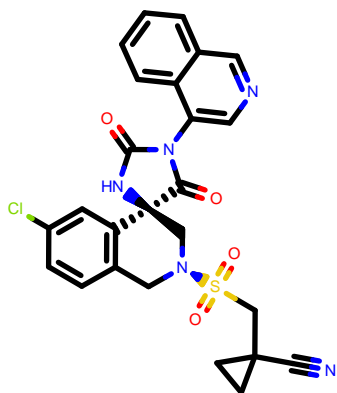
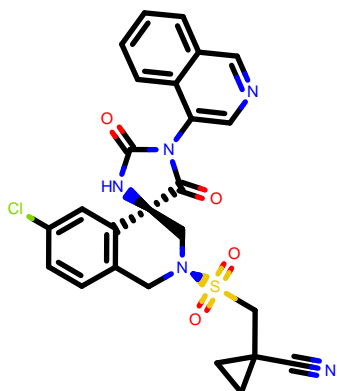


MAT-POS-c2d406ed-1_2



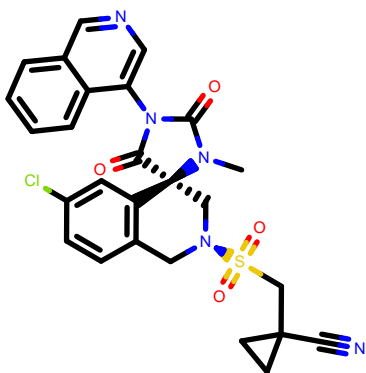
CID:	MAT-POS-c2d406ed-1_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@@]4[C@N@](C5c4cc(cc5)C)S(=O)(=O)CC6(CC6)C#N)NC3=O</chem>
RUN:	RUN797
DDG (kcal/mol):	-2.98
dDDG (kcal/mol):	0.28

MAT-POS-c2d406ed-1_1



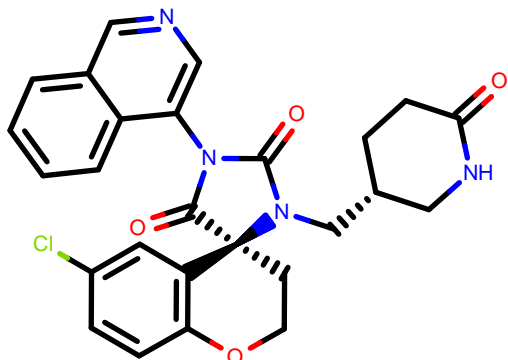
CID:	MAT-POS-c2d406ed-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@@]4[C@N@](C5c4cc(cc5)C)S(=O)(=O)CC6(CC6)C#N)NC3=O</chem>
RUN:	RUN807
DDG (kcal/mol):	-2.95
dDDG (kcal/mol):	0.20

MAT-POS-c2d406ed-2_2



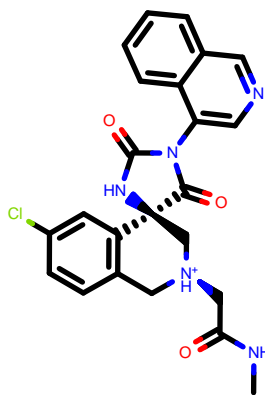
CID:	MAT-POS-c2d406ed-2_2
SMILES:	<chem>CN1C(=O)N(C1=O)[C@@]12[C@N@](C3c2cc(cc3)C)S(=O)(=O)CC4(CC4)C#N)5cnc6c5ccccc6</chem>
RUN:	RUN851
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.27

VLA-UNK-f702bf1c-5_1



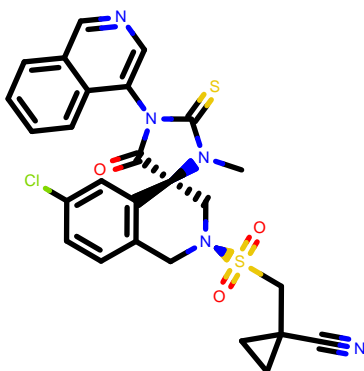
CID:	VLA-UNK-f702bf1c-5_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@@]4(CC)C5c4cc(cc5)C)N(C3=O)C[C@@]H6CCCC(=O)NC6</chem>
RUN:	RUN714
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.19

VLA-MRT-8c78ee15-3_2



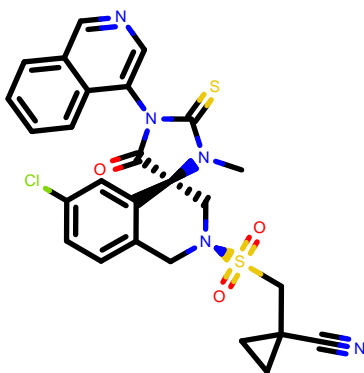
CID:	VLA-MRT-8c78ee15-3_2
SMILES:	<chem>CNC(=O)C[N@H]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4ccc5)Cl</chem>
RUN:	RUN580
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.19

MAT-POS-c2d406ed-4_2



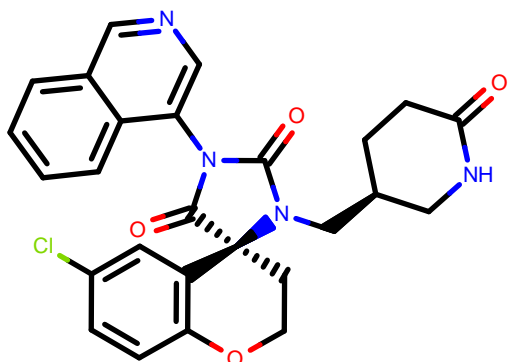
CID:	MAT-POS-c2d406ed-4_2
SMILES:	<chem>CN1C(=S)N(C1=O)[C@@]12CN(C@)C3c2ccc(cc3C)S(=O)(=O)CC4(C4)C#N5cnc6c5ccc6</chem>
RUN:	RUN855
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.31

MAT-POS-c2d406ed-4_1



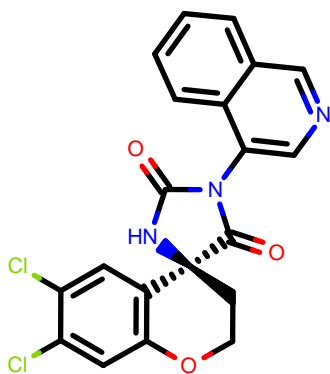
CID:	MAT-POS-c2d406ed-4_1
SMILES:	<chem>CN1C(=S)N(C1=O)[C@@]12CN(C@)C3c2ccc(cc3C)S(=O)(=O)CC4(C4)C#N5cnc6c5ccc6</chem>
RUN:	RUN852
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.25

VLA-UNK-f702bf1c-5_2



CID:	VLA-UNK-f702bf1c-5_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(ccc5)Cl)N(C3=O)C[C@@H]6CCC(=O)NC6</chem>
RUN:	RUN715
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.15

VLA-UNK-56836b69-2_1



CID: VLA-UNK-56836b69-2_1

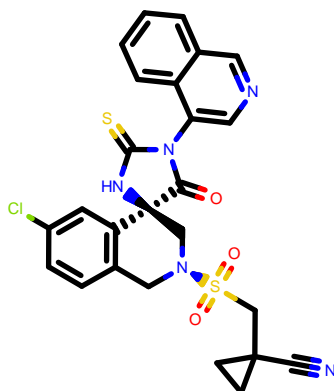
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)Cl)NC3=O

RUN: RUN520

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.08

MAT-POS-c2d406ed-3_2



CID: MAT-POS-c2d406ed-3_2

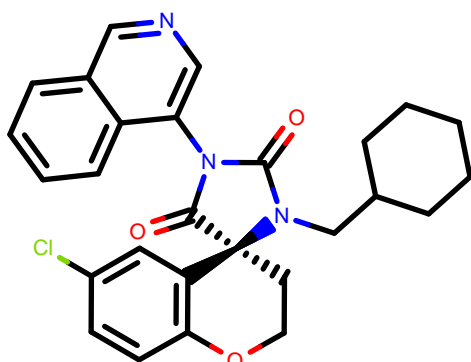
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](C5c54cc(c(c5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=S

RUN: RUN812

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.34

VLA-UNK-f702bf1c-6_1



CID: VLA-UNK-f702bf1c-6_1

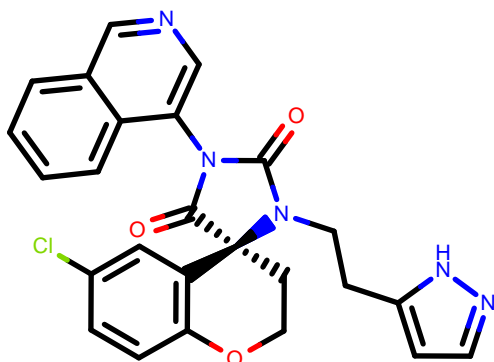
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)N(C3=O)CC6CCCC6

RUN: RUN668

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.15

VLA-UNK-f702bf1c-1_1



CID: VLA-UNK-f702bf1c-1_1

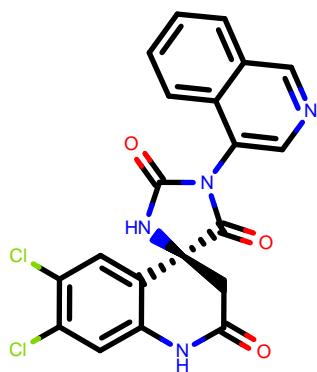
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)N(C3=O)CC6CC[nH]6

RUN: RUN677

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.13

VLA-UNK-56836b69-5_1



CID: VLA-UNK-56836b69-5_1

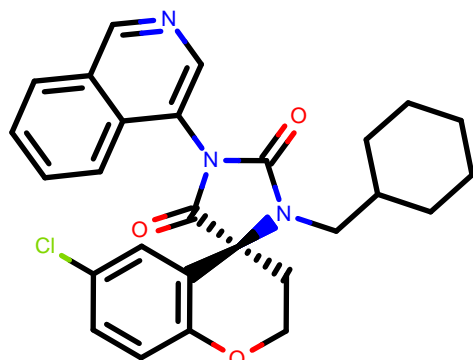
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CC(=O)Nc5c4cc(c(c5)Cl)Cl)NC3=O

RUN: RUN530

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.10

VLA-UCB-34f3ed0c-14_1



CID: VLA-UCB-34f3ed0c-14_1

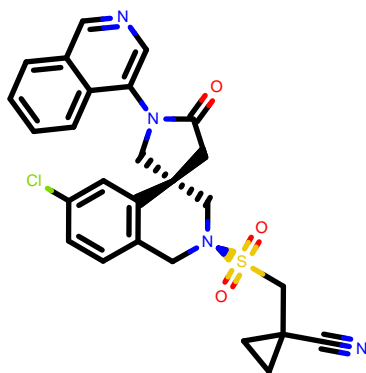
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)N(C3=O)CC6CCCC6

RUN: RUN661

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.15

EDJ-MED-8bb691af-5_1



CID: EDJ-MED-8bb691af-5_1

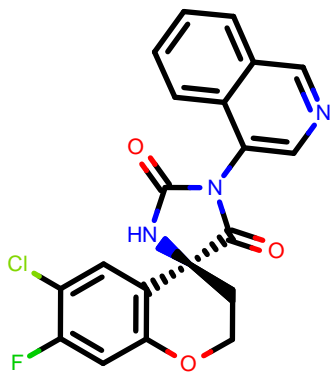
SMILES: c1ccc2c(c1)cncc2N3C[C@@]4(CC3=O)C[N@@]5(Cc5c4cc(c(c5)Cl)S(=O)(=O)CC6(Cc6)C#N

RUN: RUN718

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.35

VLA-UNK-3a43cd95-1_1



CID: VLA-UNK-3a43cd95-1_1

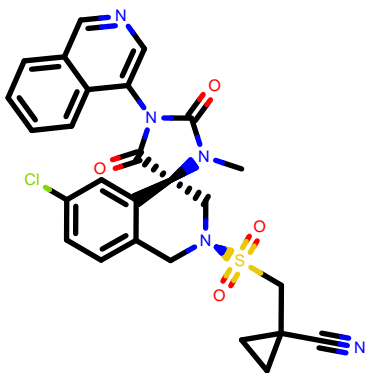
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOCc5c4cc(c(c5)F)Cl)NC3=O

RUN: RUN529

DDG (kcal/mol): -1.69

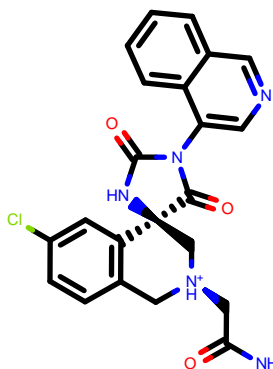
dDDG (kcal/mol): 0.07

MAT-POS-c2d406ed-2_1



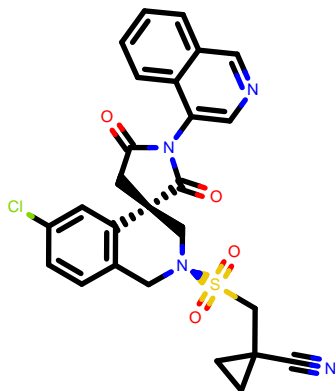
CID:	MAT-POS-c2d406ed-2_1
SMILES:	<chem>CN1C(=O)N(C1=O)C(C@@H)2CN(C@@H)2C3C2C(=O)C3C(S(=O)(=O)CC4C#N)C5=O=C6C=C6</chem>
RUN:	RUN849
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.19

VLA-MRT-a639d434-2_2



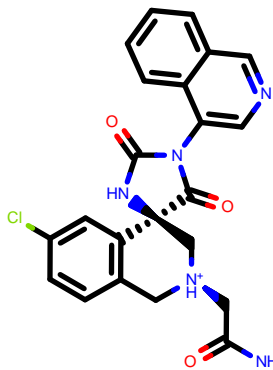
CID:	VLA-MRT-a639d434-2_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H](C[N@H+](C5=C4C=C(C=C5)C)C(=O)N)NC3=O</chem>
RUN:	RUN554
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.17

LUO-POS-868e8996-9_1



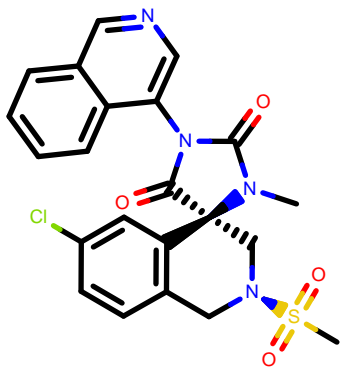
CID:	LUO-POS-868e8996-9_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H](C3=O)C[N@H+](C5=C4C=C(C=C5)C)S(=O)(=O)CC6C=C6C#N</chem>
RUN:	RUN782
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.28

VLA-MRT-8c78ee15-4_2



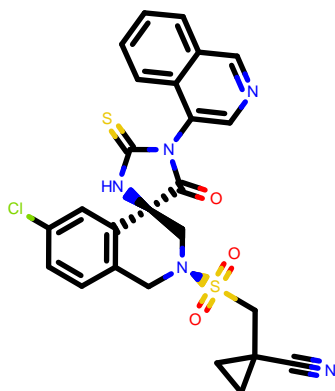
CID:	VLA-MRT-8c78ee15-4_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H](C[N@H+](C5=C4C=C(C=C5)C)C(=O)N)NC3=O</chem>
RUN:	RUN551
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.16

MAT-POS-2e8b2191-8_2



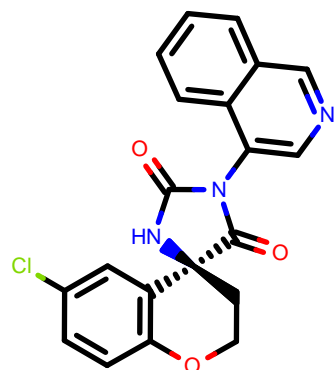
CID:	MAT-POS-2e8b2191-8_2
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@H]2C[N@@H]3C[C@@H](C)S(=O)(=O)C4=CC=CC=C4)C2=O</chem>
RUN:	RUN582
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.12

MAT-POS-c2d406ed-3_1



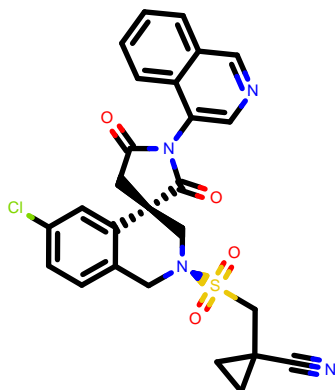
CID:	MAT-POS-c2d406ed-3_1
SMILES:	<chem>C1CC2C(C1)NCC2N3C(=O)[C@@H](C3)N[C@@H]4C(C)S(=O)(=O)C5=CC=CC=C5</chem>
RUN:	RUN811
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.23

VLA-UCB-34f3ed0c-11_1



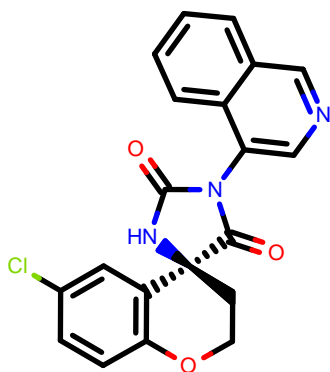
CID:	VLA-UCB-34f3ed0c-11_1
SMILES:	<chem>C1CC2C(C1)NCC2N3C(=O)[C@@H](C3)N[C@@H]4C(C)S(=O)(=O)C5=CC=CC=C5</chem>
RUN:	RUN514
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.05

LUO-POS-868e8996-10_1



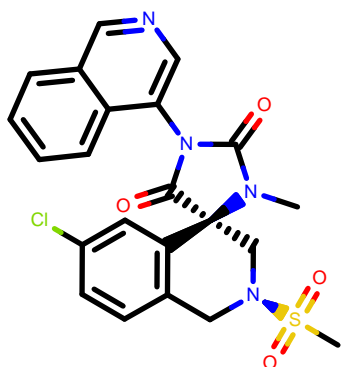
CID:	LUO-POS-868e8996-10_1
SMILES:	<chem>C1CC2C(C1)NCC2N3C(=O)[C@@H](C3)N[C@@H]4C(C)S(=O)(=O)C5=CC=CC=C5</chem>
RUN:	RUN783
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.26

VLA-UNK-cf7facf1-1_1



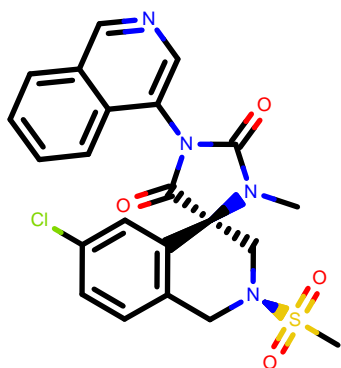
CID:	VLA-UNK-cf7facf1-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN509
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.05

EDJ-MED-7587a9ee-1_2



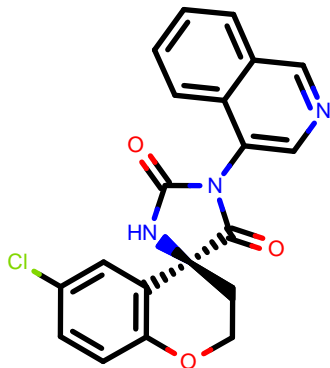
CID:	EDJ-MED-7587a9ee-1_2
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@]12C[N@@]3(Cc3c2cc(cc3)Cl)S(=O)(=O)C)4cncoc5c4cccc5</chem>
RUN:	RUN573
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.11

EDJ-MED-7587a9ee-1_1



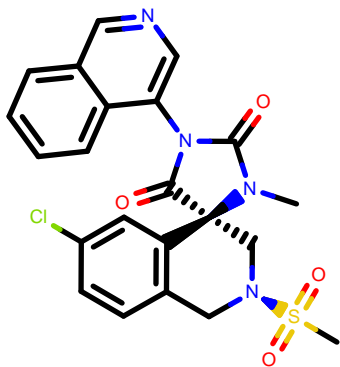
CID:	EDJ-MED-7587a9ee-1_1
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@]12C[N@@]3(Cc3c2cc(cc3)Cl)S(=O)(=O)C)4cncoc5c4cccc5</chem>
RUN:	RUN572
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.12

VLA-UCB-29506327-1_1



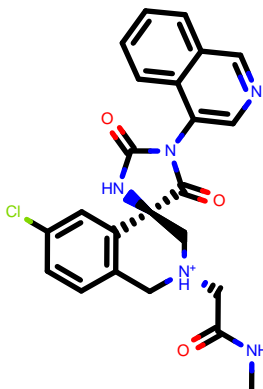
CID:	VLA-UCB-29506327-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN516
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.06

MAT-POS-2e8b2191-8_1



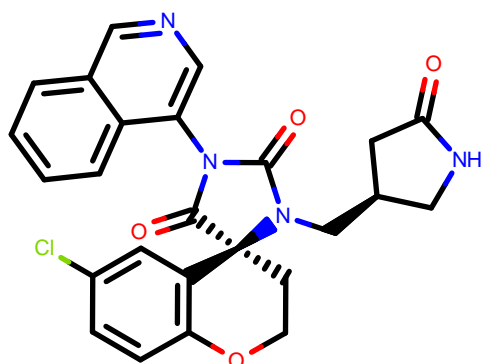
CID:	MAT-POS-2e8b2191-8_1
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@]1)2C[N@@]3C3c2cc(cc3)C(S(=O)(=O)C)4cnc5c4cccc5</chem>
RUN:	RUN574
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.12

VLA-MRT-a639d434-1_1



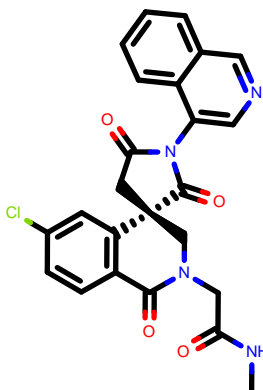
CID:	VLA-MRT-a639d434-1_1
SMILES:	<chem>CNC(=O)C[N@@H+]1Cc2ccc(cc2)[C@@]3(C1)C(=O)N(C(=O)N3)c4cnc5c4cccc5Cl</chem>
RUN:	RUN575
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.23

VLA-UNK-f702bf1c-4_2



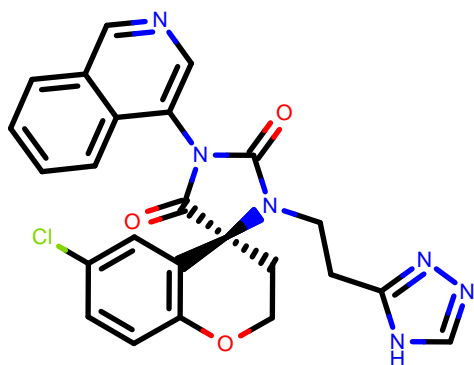
CID:	VLA-UNK-f702bf1c-4_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)C)N(C3=O)C[C@H]6CC(=O)N6</chem>
RUN:	RUN674
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.14

MAT-POS-1bed62cf-2_1



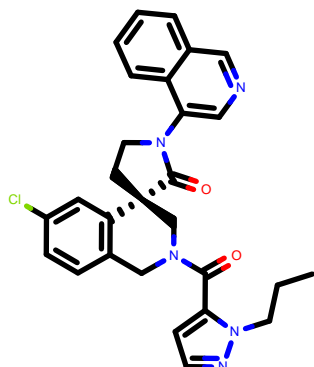
CID:	MAT-POS-1bed62cf-2_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(CC(=O)N(C2=O)c3cnc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN622
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.10

VLA-UNK-f702bf1c-8_1



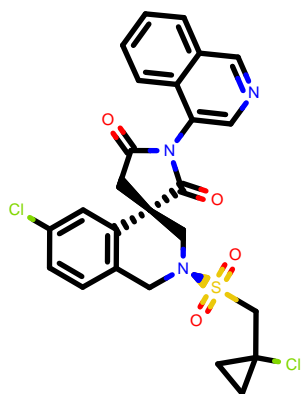
CID:	VLA-UNK-f702bf1c-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)C)N(C3=O)CCc6[nH]nc6</chem>
RUN:	RUN679
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.20

MAT-POS-be048f2c-8_1



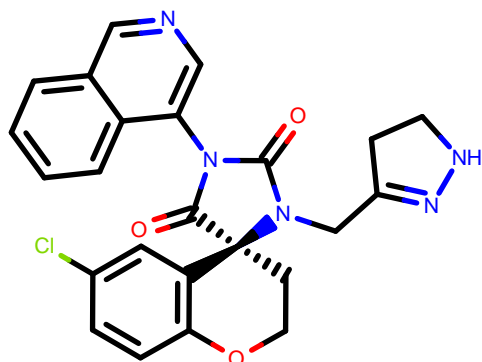
CID:	MAT-POS-be048f2c-8_1
SMILES:	<chem>CCCN1c(ccn1)C(=O)N2C3ccc(cc3[C@@]4(C2)CCN(C4=O)c5nccc6c5ccc6)Cl</chem>
RUN:	RUN827
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.17

PET-UNK-94036022-5_1



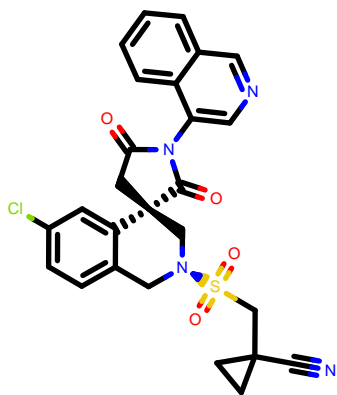
CID:	PET-UNK-94036022-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C3=O)[N@@]5(Cc5c4cc(cc5)C)S(=O)(=O)CC6(Cc6)Cl</chem>
RUN:	RUN767
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.24

VLA-UNK-f702bf1c-2_1



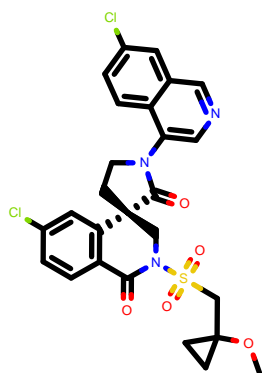
CID:	VLA-UNK-f702bf1c-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)C)N(C3=O)CC6c[nH]6</chem>
RUN:	RUN623
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.12

LUO-POS-868e8996-9_2



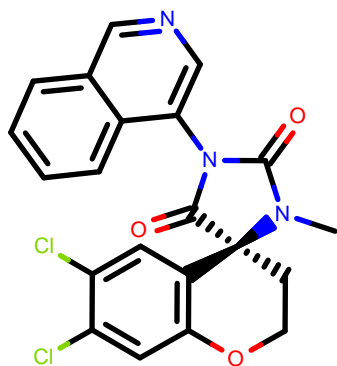
CID:	LUO-POS-868e8996-9_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)C[C@@]4(C3=O)C[N@@]5Cc5c4cc(c5)ClS(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN780
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.35

EDJ-MED-9f4ac58c-5_1



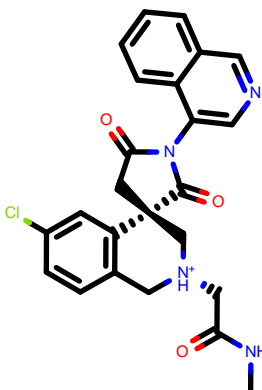
CID:	EDJ-MED-9f4ac58c-5_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)N2C[C@@]3(CCN(C3=O)c4ncc5c4ccc(c5)Cl)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN843
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.33

VLA-UNK-56836b69-3_1



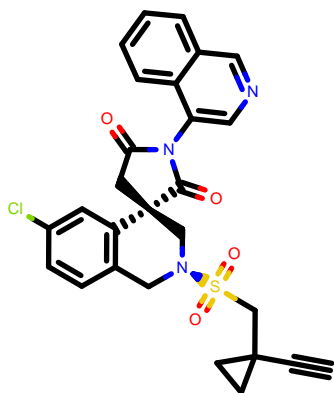
CID:	VLA-UNK-56836b69-3_1
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(c(c3)Cl)Cl)c4cnc5c4cccc5</chem>
RUN:	RUN524
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.10

JOH-MSK-1f2dff76-1_1



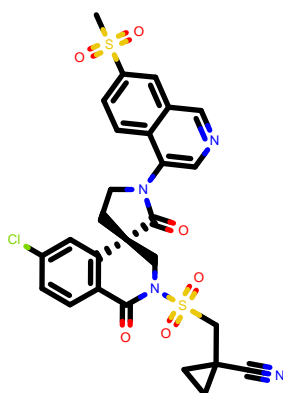
CID:	JOH-MSK-1f2dff76-1_1
SMILES:	<chem>CNC(=O)C[N@@H+]1Cc2ccc(cc2)[C@@]3(C1)CC(=O)N(C3=O)c4cnc5c4cccc5Cl</chem>
RUN:	RUN614
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.27

PET-UNK-94036022-11_1



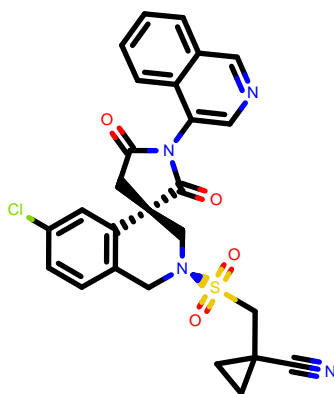
CID:	PET-UNK-94036022-11_1
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)N@@2C=C3ccc(cc3)C@4(C2)CC(=O)N(C4=O)c5ccc6c5ccc6)Cl</chem>
RUN:	RUN838
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.25

EDJ-MED-9f4ac58c-4_1



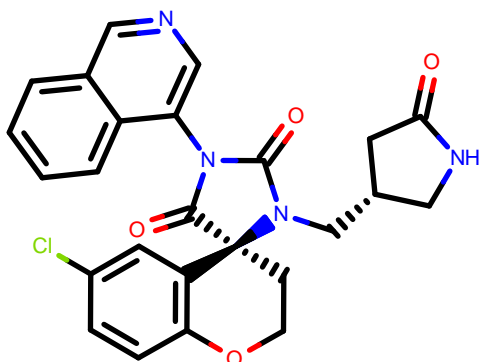
CID:	EDJ-MED-9f4ac58c-4_1
SMILES:	<chem>CS(=O)(=O)c1ccc2c(c1)ncnc2N3C[C@@H](C3=O)CN(C1=O)c5c4ccc(cc5)C(Si(=O)(=O)C6=CC=CC=C6)C#N</chem>
RUN:	RUN903
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.36

MAT-POS-1bed62cf-1_1



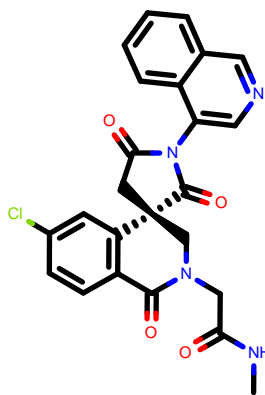
CID:	MAT-POS-1bed62cf-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)C[C@@H](C3=O)C[N@@H](C5=C4ccc(cc5)C(Si(=O)(=O)C6=CC=CC=C6)C#N</chem>
RUN:	RUN778
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.30

VLA-UNK-f702bf1c-4_1



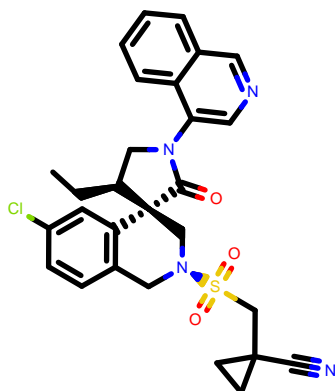
CID:	VLA-UNK-f702bf1c-4_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)C[C@@H](C3=O)C[C@@H](C4=O)C[C@@H](C4=O)C5=CC=CC=C5</chem>
RUN:	RUN676
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.16

LUO-POS-868e8996-7_1



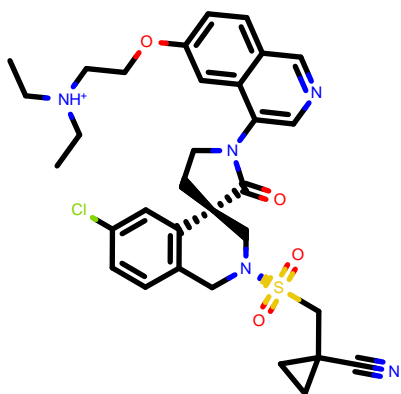
CID:	LUO-POS-868e8996-7_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN630
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.12

MAT-POS-50a80394-2_2



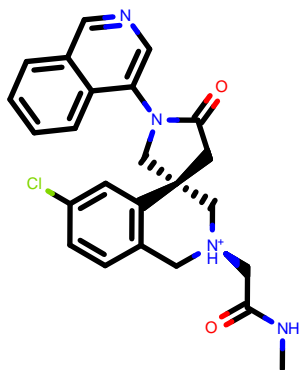
CID:	MAT-POS-50a80394-2_2
SMILES:	<chem>CC[C@H]1CN(C1=O)[C@@]2(CN[C@@]3(Cc3cc2cc3)C)S(=O)(=O)CC4(C4)CN(C5C=CC6C5=CC=CC6)C#N</chem>
RUN:	RUN856
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.54

MAT-POS-40ad851a-3_1



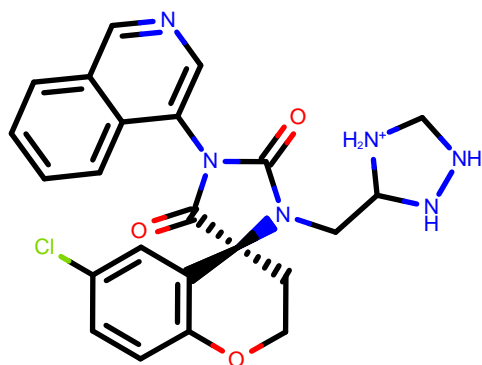
CID:	MAT-POS-40ad851a-3_1
SMILES:	<chem>CC[NH+](CC)CCOC1=CC=C2C=CC(=C2)N3C(C)C[C@@]4(C3=O)CN[C@@]5(Cc5cc4cc5)C)S(=O)(=O)CC6(C6)C#N</chem>
RUN:	RUN955
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.52

EDJ-MED-8bb691af-3_2



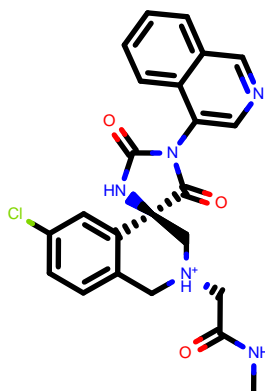
CID:	EDJ-MED-8bb691af-3_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2cccc(c2)[C@]3(C1)CC(=O)N(C3)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN555
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.18

VLA-UNK-f702bf1c-3_1



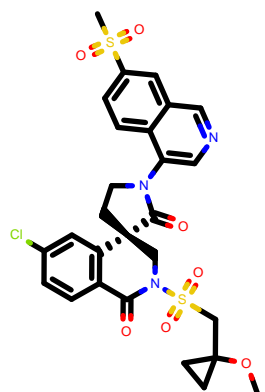
CID:	VLA-UNK-f702bf1c-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCCOc5c4cc(cc5)C)N(C3=O)C6([nH])nc6</chem>
RUN:	RUN624
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.13

VLA-MRT-8c78ee15-3_1



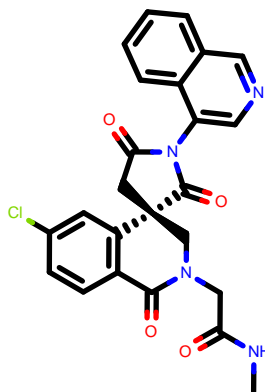
CID:	VLA-MRT-8c78ee15-3_1
SMILES:	<chem>CNC(=O)CN[CH+]1Cc2ccc(cc2)[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5Cl</chem>
RUN:	RUN577
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.23

EDJ-MED-9f4ac58c-8_1



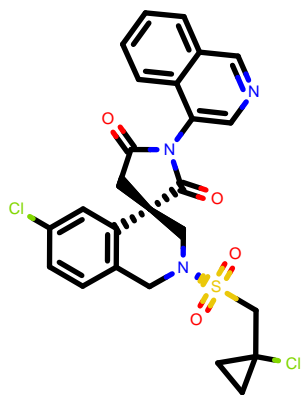
CID:	EDJ-MED-9f4ac58c-8_1
SMILES:	<chem>COC1(C(C1)CS(=O)(=O)N2C[C@@]3(CCN(C3=O)c4cncc4c3cccc4)c5[Si](=O)(=O)C)C6[cc]c6C2=O)Cl</chem>
RUN:	RUN909
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.40

LUO-POS-868e8996-8_1



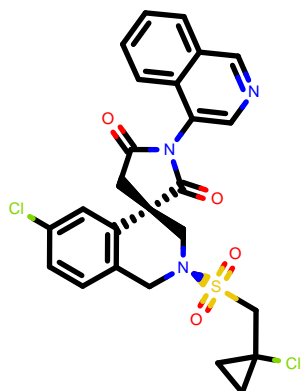
CID:	LUO-POS-868e8996-8_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN632
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.11

PET-UNK-94036022-5_2



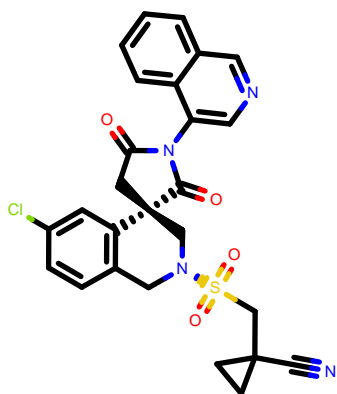
CID:	PET-UNK-94036022-5_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)C[C@@H](C3=O)C[N@@]1Cc5c4cc(cc5)ClS(=O)(=O)CC6(Cc6)Cl</chem>
RUN:	RUN769
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.31

PET-UNK-94036022-12_1



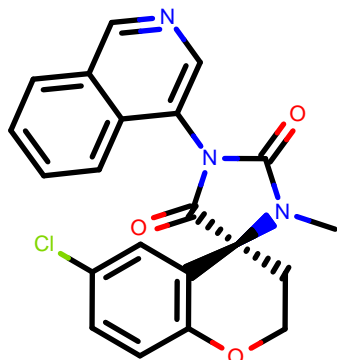
CID:	PET-UNK-94036022-12_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)C[C@@H](C3=O)C[N@@]1Cc5c4cc(cc5)ClS(=O)(=O)CC6(Cc6)Cl</chem>
RUN:	RUN775
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.24

MAT-POS-1bed62cf-1_2



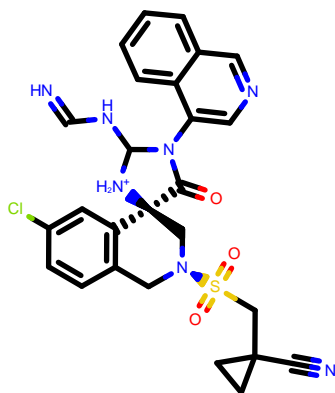
CID:	MAT-POS-1bed62cf-1_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)C[C@@H](C3=O)C[N@@]1Cc5c4cc(cc5)ClS(=O)(=O)CC6(Cc6)C#N</chem>
RUN:	RUN774
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.47

BEN-BAS-c2bc0d80-7_1



CID:	BEN-BAS-c2bc0d80-7_1
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@H]12CCOCc3c2cc(cc3)Cl)c4ncc5c4cccc5</chem>
RUN:	RUN521
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.07

LUO-POS-b5068a05-2_1



CID: LUO-POS-b5068a05-2_1

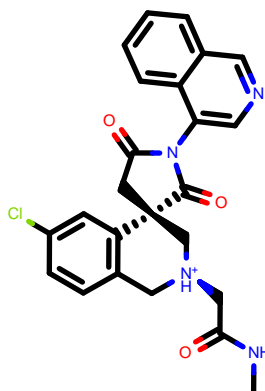
SMILES: c1ccc2c(c1)ncnc2N3C(=O)C[C@@H](C[N+]#N)C(C#N)S(=O)(=O)CC4(C)CN(C)C4

RUN: RUN892

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.29

MAT-POS-1bed62cf-3_2



CID: MAT-POS-1bed62cf-3_2

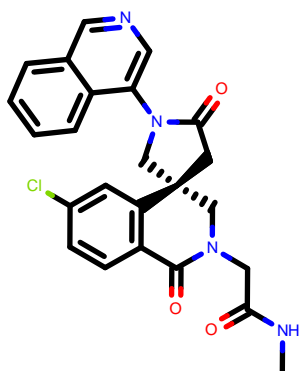
SMILES: CNC(=O)C[N+](H)1Cc2ccc(cc2)[C@]3(C1)CC(=O)N(C3=O)c4cncnc5c4ccc5Cl

RUN: RUN581

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.15

EDJ-MED-8bb691af-9_1



CID: EDJ-MED-8bb691af-9_1

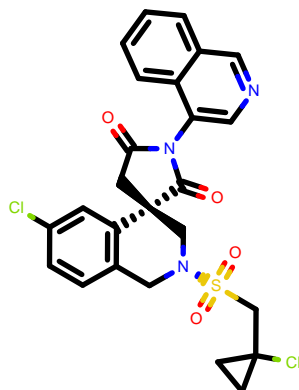
SMILES: CNC(=O)CN1C[C@]2(CC(=O)N(C2)c3cnc4c3ccc4)c5cc(ccc5C1=O)Cl

RUN: RUN579

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.14

PET-UNK-94036022-12_2



CID: PET-UNK-94036022-12_2

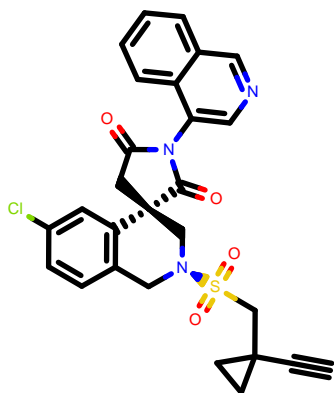
SMILES: c1ccc2c(c1)ncnc2N3C(=O)C[C@@H](C3=O)C[N+]#N)C(C#N)S(=O)(=O)CC4(C)CN(C)C4

RUN: RUN777

DDG (kcal/mol): -0.36

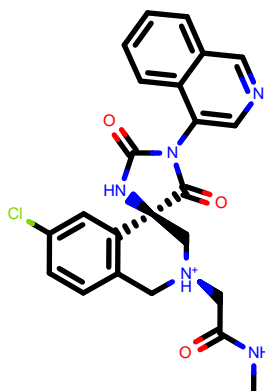
dDDG (kcal/mol): 0.36

PET-UNK-94036022-4_2



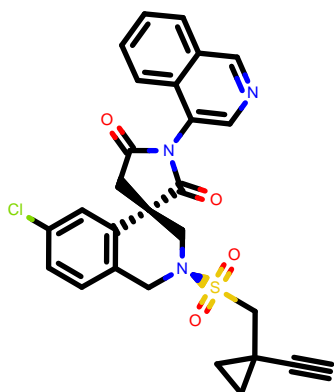
CID:	PET-UNK-94036022-4_2
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)N@[2]C2C3ccc(cc3)C@[4](C2)CC(=O)N(C4=O)c5nc6c65ccc6)Cl</chem>
RUN:	RUN836
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.32

VLA-MRT-a639d434-1_2



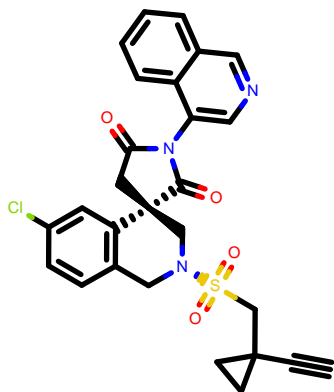
CID:	VLA-MRT-a639d434-1_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2)C@[3](C1)C(=O)N(C(=O)N3)c4nc5c4ccc5)Cl</chem>
RUN:	RUN584
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.23

PET-UNK-94036022-4_1



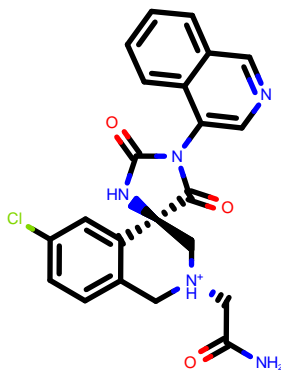
CID:	PET-UNK-94036022-4_1
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)N@[2]C2C3ccc(cc3)C@[4](C2)CC(=O)N(C4=O)c5nc6c65ccc6)Cl</chem>
RUN:	RUN823
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.25

PET-UNK-94036022-11_2



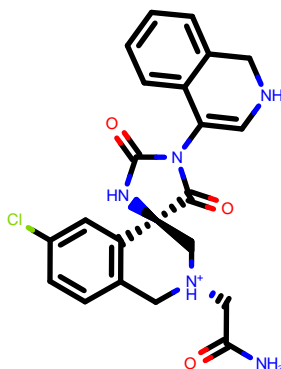
CID:	PET-UNK-94036022-11_2
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)N@[2]C2C3ccc(cc3)C@[4](C2)CC(=O)N(C4=O)c5nc6c65ccc6)Cl</chem>
RUN:	RUN828
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.34

VLA-MRT-8c78ee15-4_1



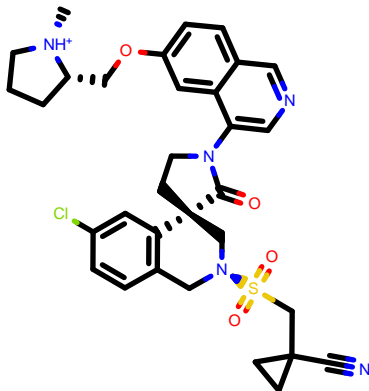
CID:	VLA-MRT-8c78ee15-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H](C[N+]([H+])C5c4cc(cc5)C)CC(=O)N)NC3=O</chem>
RUN:	RUN550
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.19

VLA-MRT-a639d434-2_1



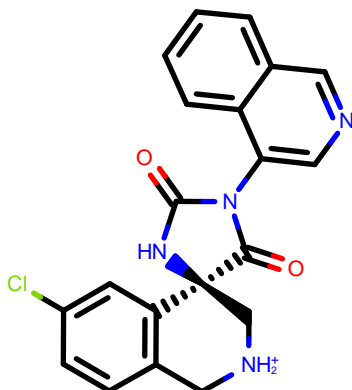
CID:	VLA-MRT-a639d434-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H](C[N+]([H+])C5c4cc(cc5)C)CC(=O)N)NC3=O</chem>
RUN:	RUN552
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.20

MAT-POS-40ad851a-1_4



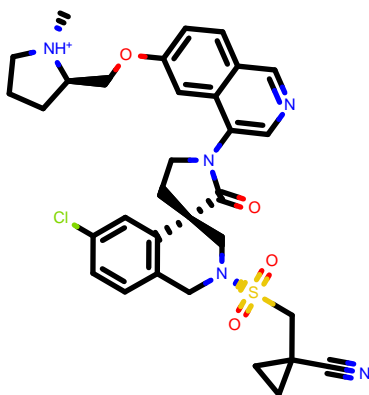
CID:	MAT-POS-40ad851a-1_4
SMILES:	<chem>C[N+]([H+])1CC[C@H]1COc2ccc3ncnc(c3c2)N4CC[C@@H]5(C4=O)C[N+]([H+])C6c5cc(cc6)C(S(=O)(=O)CC7C(C7)C#N)</chem>
RUN:	RUN952
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.45

VLA-MRT-8c78ee15-1_1



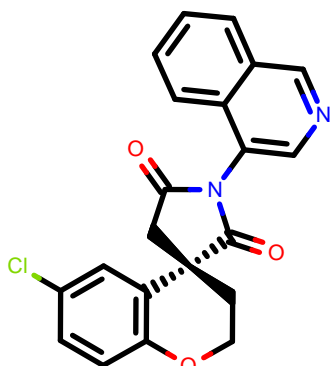
CID:	VLA-MRT-8c78ee15-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H](C[NH2+])Cc5c4cc(cc5)C)NC3=O</chem>
RUN:	RUN518
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.20

MAT-POS-40ad851a-1_6



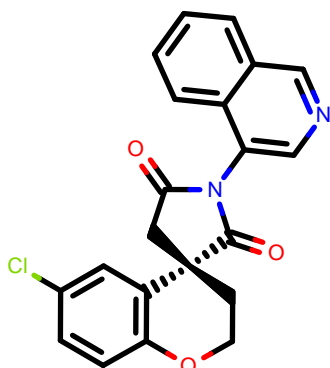
CID:	MAT-POS-40ad851a-1_6
SMILES:	<chem>C1N([H])CCC1C2C3C4C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100</chem>
RUN:	RUN958
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.61

VLA-UCB-50c39ae8-2_1



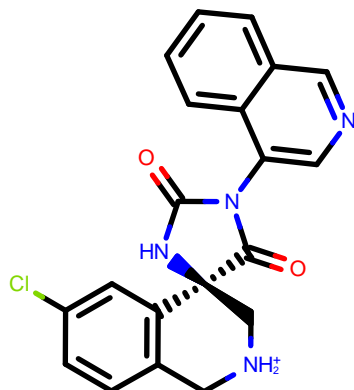
CID:	VLA-UCB-50c39ae8-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN505
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.03

VLA-UCB-05e51b3f-5_1



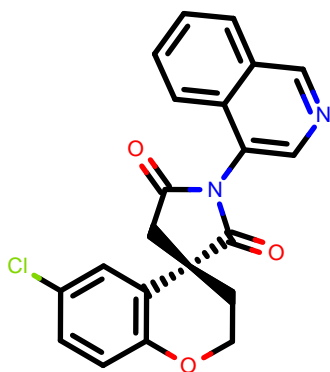
CID:	VLA-UCB-05e51b3f-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN504
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.02

VLA-MRT-a639d434-3_1



CID:	VLA-MRT-a639d434-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C3=O)[C@H](N)Cc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN526
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.21

MAT-POS-94643566-1_1



CID: MAT-POS-94643566-1_1

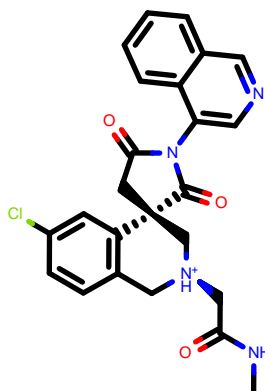
SMILES: c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(c5)Cl

RUN: RUN508

DDG (kcal/mol): 0.03

dDDG (kcal/mol): 0.02

JOH-MSK-1f2dff76-1_2



CID: JOH-MSK-1f2dff76-1_2

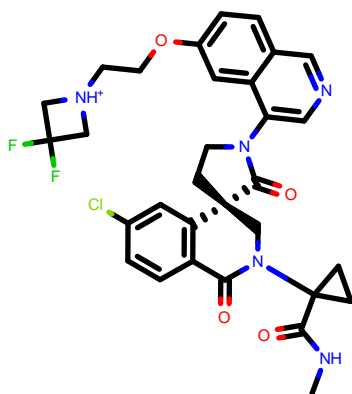
SMILES: CNC(=O)C[NH+]1Cc2cccc(cc2)[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5Cl

RUN: RUN619

DDG (kcal/mol): 0.09

dDDG (kcal/mol): 0.16

EDJ-MED-dfa1d800-5_1



CID: EDJ-MED-dfa1d800-5_1

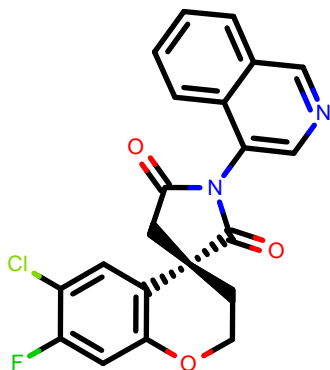
SMILES: CNC(=O)C1(C(C1)N2C[C@]3(C)CCN(C3=O)c4cncc5c4cccc5)OCCN6CC(C6)(F)F)c7ccc7C2=OCl

RUN: RUN946

DDG (kcal/mol): 0.14

dDDG (kcal/mol): 0.21

VLA-UNK-3a43cd95-3_1



CID: VLA-UNK-3a43cd95-3_1

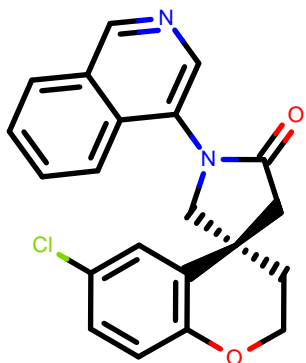
SMILES: c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(c(c5)F)Cl

RUN: RUN525

DDG (kcal/mol): 0.15

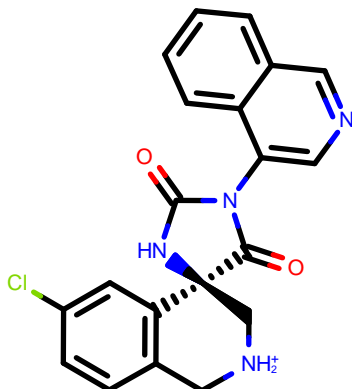
dDDG (kcal/mol): 0.05

MAT-POS-983b399a-3_1



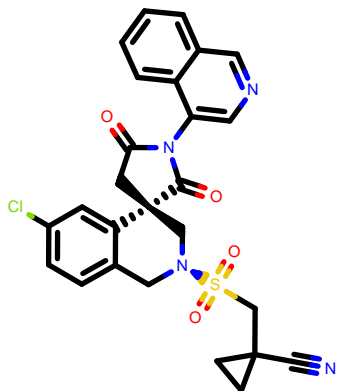
CID:	MAT-POS-983b399a-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O</chem>
RUN:	RUN512
DDG (kcal/mol):	0.15
dDDG (kcal/mol):	0.08

VLA-MRT-8c78ee15-2_1



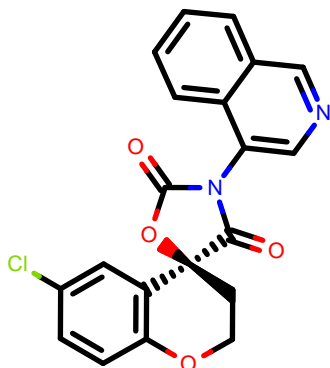
CID:	VLA-MRT-8c78ee15-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+])Cc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN523
DDG (kcal/mol):	0.17
dDDG (kcal/mol):	0.19

LUO-POS-868e8996-10_2



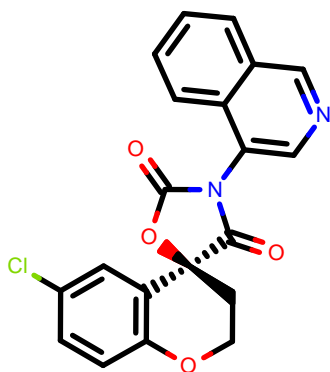
CID:	LUO-POS-868e8996-10_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@]5(Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CO6)C#N</chem>
RUN:	RUN784
DDG (kcal/mol):	0.19
dDDG (kcal/mol):	0.40

MAT-POS-90505e2b-1_1



CID:	MAT-POS-90505e2b-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O</chem>
RUN:	RUN510
DDG (kcal/mol):	0.19
dDDG (kcal/mol):	0.04

MAT-POS-ec6d90b7-2_1



CID: MAT-POS-ec6d90b7-2_1

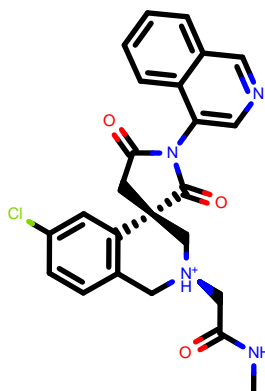
SMILES: c1ccc2c(c1)cnc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O

RUN: RUN513

DDG (kcal/mol): 0.19

dDDG (kcal/mol): 0.04

JOH-MSK-1f2dff76-2_2



CID: JOH-MSK-1f2dff76-2_2

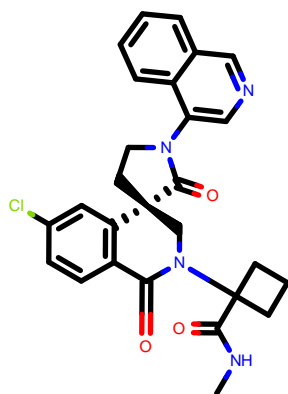
SMILES: CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cnc5c4cccc5)Cl

RUN: RUN621

DDG (kcal/mol): 0.23

dDDG (kcal/mol): 0.17

EDJ-MED-98c0a822-3_1



CID: EDJ-MED-98c0a822-3_1

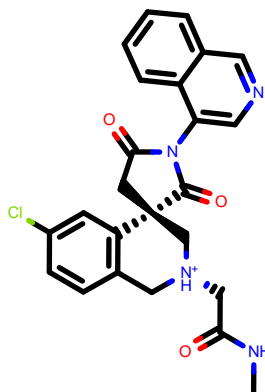
SMILES: CNC(=O)C1(CCC1)N2C[C@]3(CCN(C3=O)c4cnc5c4cccc5)c6ccc(cc6C2=O)Cl

RUN: RUN759

DDG (kcal/mol): 0.24

dDDG (kcal/mol): 0.22

MAT-POS-1bed62cf-3_1



CID: MAT-POS-1bed62cf-3_1

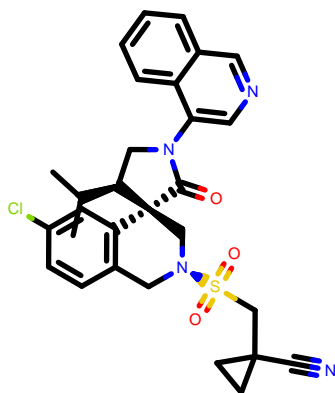
SMILES: CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cnc5c4cccc5)Cl

RUN: RUN585

DDG (kcal/mol): 0.25

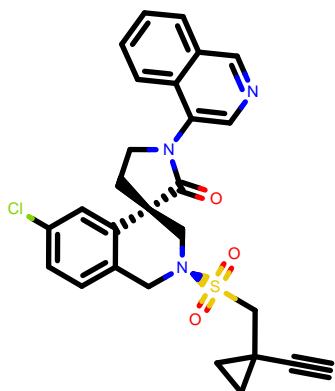
dDDG (kcal/mol): 0.26

MAT-POS-50a80394-3_2



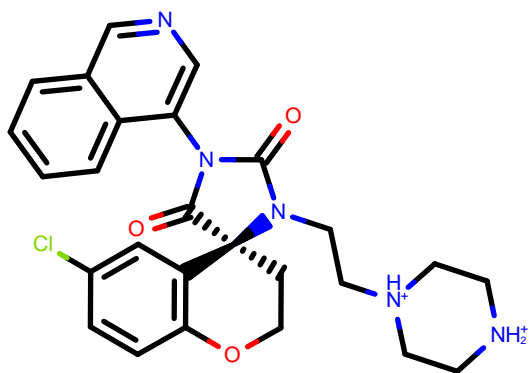
CID:	MAT-POS-50a80394-3_2
SMILES:	<chem>CCC[C@H]1CN(C(=O)[C@@H]2CN[C@@H]3C2cc3C1)S(=O)(=O)CC4(C4)C#N5C6cc65C6cc6</chem>
RUN:	RUN880
DDG (kcal/mol):	0.25
dDDG (kcal/mol):	0.36

PET-UNK-94036022-2_1



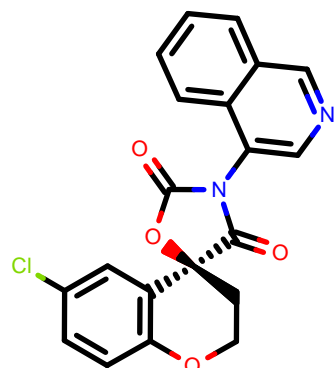
CID:	PET-UNK-94036022-2_1
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)[N@@H]2C3ccccc3[C@H]4(C2)CCN(C4=O)c5ccc6c5C6cc6Cl</chem>
RUN:	RUN771
DDG (kcal/mol):	0.27
dDDG (kcal/mol):	0.35

VLA-UNK-f702bf1c-7_1



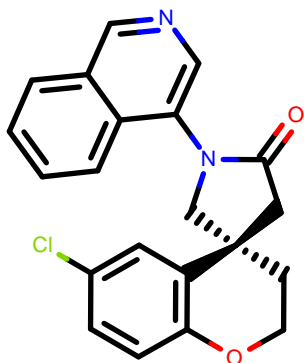
CID:	VLA-UNK-f702bf1c-7_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)[C@@H]4(CCOc5c4cc(cc5)C1)N(C3=O)CCN6CC[NH2+][C6]</chem>
RUN:	RUN717
DDG (kcal/mol):	0.38
dDDG (kcal/mol):	0.25

MAT-POS-ec6d90b7-1_1



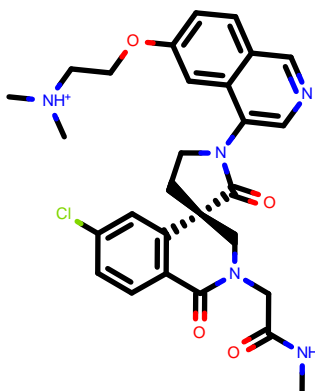
CID:	MAT-POS-ec6d90b7-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)[C@@H]4(CCOc5c4cc(cc5)C1)OC3=O</chem>
RUN:	RUN511
DDG (kcal/mol):	0.40
dDDG (kcal/mol):	0.04

EDJ-MED-159244ea-3_1



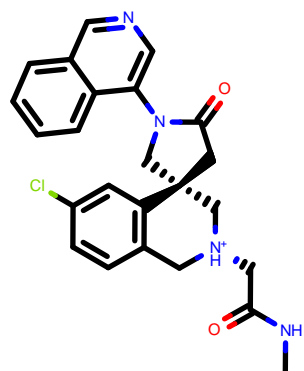
CID:	EDJ-MED-159244ea-3_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O</chem>
RUN:	RUN494
DDG (kcal/mol):	0.48
dDDG (kcal/mol):	0.12

EDJ-MED-b6c6ee2b-5_1



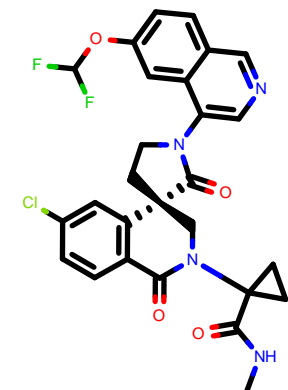
CID:	EDJ-MED-b6c6ee2b-5_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(CCN(C2=O)c3cnc4c3cc(cc4)OC[NH+](C)C)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN912
DDG (kcal/mol):	0.51
dDDG (kcal/mol):	0.30

EDJ-MED-8bb691af-3_1



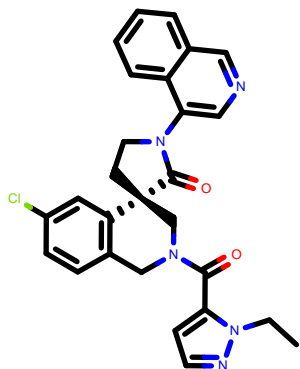
CID:	EDJ-MED-8bb691af-3_1
SMILES:	<chem>CNC(=O)CN[C@@H]1Cc2ccc(cc2[C@@]3(C1)CC(=O)N(C3)c4cnc5c4ccc5)Cl</chem>
RUN:	RUN553
DDG (kcal/mol):	0.52
dDDG (kcal/mol):	0.19

EDJ-MED-5cd3920d-3_1



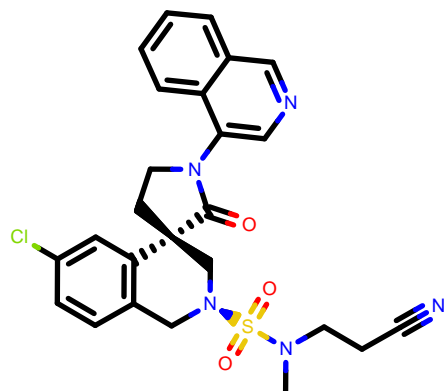
CID:	EDJ-MED-5cd3920d-3_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@@]3(CCN(C3=O)c4cnc5c4cc(cc5)OC(F)F)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN908
DDG (kcal/mol):	0.52
dDDG (kcal/mol):	0.15

MAT-POS-be048f2c-5_1



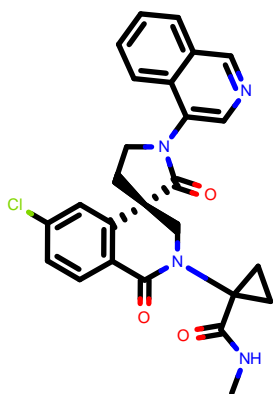
CID:	MAT-POS-be048f2c-5_1
SMILES:	<chem>CCn1c(ccn1)C(=O)N2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5cccc6)Cl</chem>
RUN:	RUN765
DDG (kcal/mol):	0.53
dDDG (kcal/mol):	0.19

ALP-POS-ecbed2ba-16_4



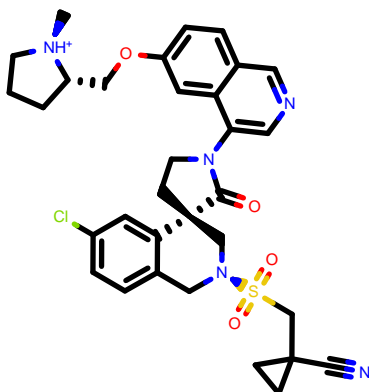
CID:	ALP-POS-ecbed2ba-16_4
SMILES:	<chem>C[N@]([CC#N])S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN745
DDG (kcal/mol):	0.54
dDDG (kcal/mol):	0.51

EDJ-MED-976a33d5-1_1



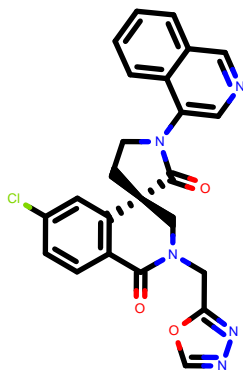
CID:	EDJ-MED-976a33d5-1_1
SMILES:	<chem>CNC(=O)C1(CC1)N2[C@]3([CCN(C3=O)c4cnc5c4cccc5)c6ccc(cc6C2=O)Cl</chem>
RUN:	RUN697
DDG (kcal/mol):	0.60
dDDG (kcal/mol):	0.13

MAT-POS-40ad851a-1_3



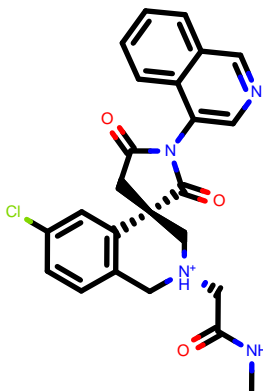
CID:	MAT-POS-40ad851a-1_3
SMILES:	<chem>C[NH+]1CCCC1[H]1CCc2ccc3ccc(cc2N4CC[C@]5(C4=O)C[N@]6[C@]c7c5cc(c7)Cl)S(=O)(=O)CC7(C)CN</chem>
RUN:	RUN949
DDG (kcal/mol):	0.69
dDDG (kcal/mol):	0.50

PET-UNK-aa57768f-7_1



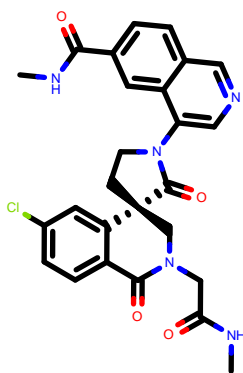
CID:	PET-UNK-aa57768f-7_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)C6nnc6</chem>
RUN:	RUN646
DDG (kcal/mol):	0.76
dDDG (kcal/mol):	0.13

JOH-MSK-1f2dff76-2_1



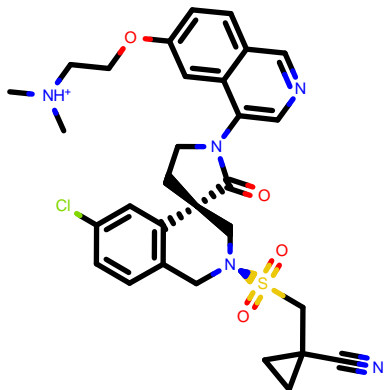
CID:	JOH-MSK-1f2dff76-2_1
SMILES:	<chem>CNC(=O)CN[C@@H]1Cc2ccc(cc2[C@@]3(C1)CC(=O)N(C3=O)c4cnc5c4ccc5)Cl</chem>
RUN:	RUN618
DDG (kcal/mol):	0.80
dDDG (kcal/mol):	0.25

MAT-POS-38eb6498-6_1



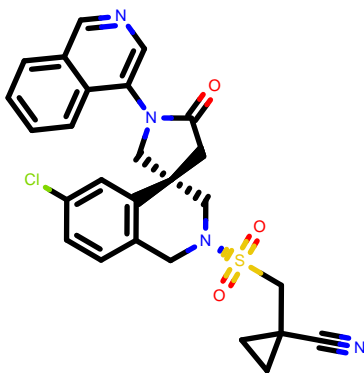
CID:	MAT-POS-38eb6498-6_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(CCN(C2=O)c3ccc4c3cc(cc4)C(=O)NC)c5ccc(cc5C1=O)Cl</chem>
RUN:	RUN806
DDG (kcal/mol):	0.80
dDDG (kcal/mol):	0.14

LUO-POS-8484f2d3-2_1



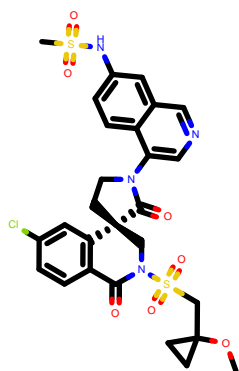
CID:	LUO-POS-8484f2d3-2_1
SMILES:	<chem>C[NH+]C)CCO1ccc2nccc2c1)N3CC[C@@]4(C3=O)CN(B@)C5c4ccc(cc5)O[S(=O)(=O)C6C6]c#N</chem>
RUN:	RUN924
DDG (kcal/mol):	0.81
dDDG (kcal/mol):	0.60

EDJ-MED-8bb691af-5_2



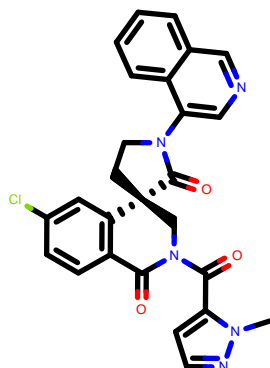
CID:	EDJ-MED-8bb691af-5_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3C[C@@H](C(=O)N[C@@H](Cc5c4ccc(cc5)Cl)S(=O)(=O)CC6(C(=O)C)C#N</chem>
RUN:	RUN721
DDG (kcal/mol):	0.81
dDDG (kcal/mol):	0.32

EDJ-MED-9f4ac58c-7_1



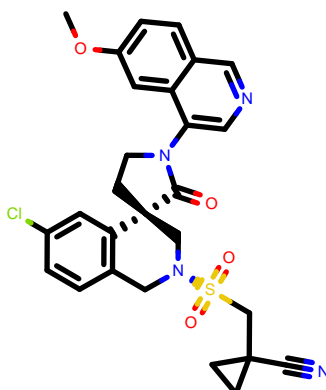
CID:	EDJ-MED-9f4ac58c-7_1
SMILES:	<chem>COc1cc2cnc(c2c1)N3CC[C@@H](C(=O)N[C@@H](Cc4ccc5c4ccc(c5)NS(=O)(=O)C)C6(C)C</chem>
RUN:	RUN916
DDG (kcal/mol):	0.82
dDDG (kcal/mol):	0.44

EDJ-MED-cc48ee33-2_1



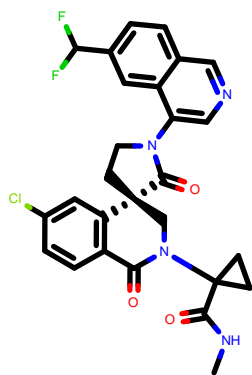
CID:	EDJ-MED-cc48ee33-2_1
SMILES:	<chem>Cn1c(cn1)C(=O)N2C[C@@H](C(=O)N[C@@H](Cc3ccc4c3ccc(c4)C)S(=O)(=O)CC6(C(=O)C)C</chem>
RUN:	RUN756
DDG (kcal/mol):	0.84
dDDG (kcal/mol):	0.17

EDJ-MED-b6c6ee2b-3_2



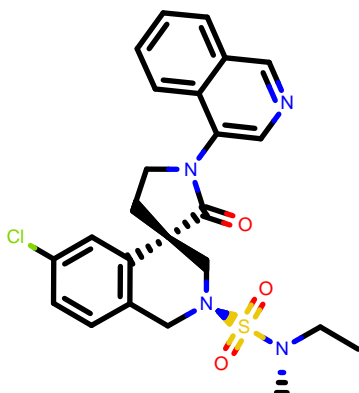
CID:	EDJ-MED-b6c6ee2b-3_2
SMILES:	<chem>COc1ccc2nc(c2c1)N3CC[C@@H](C(=O)N[C@@H](Cc5c4ccc(cc5)Cl)S(=O)(=O)CC6(C(=O)C)C#N</chem>
RUN:	RUN864
DDG (kcal/mol):	0.85
dDDG (kcal/mol):	0.55

EDJ-MED-5cd3920d-4_1



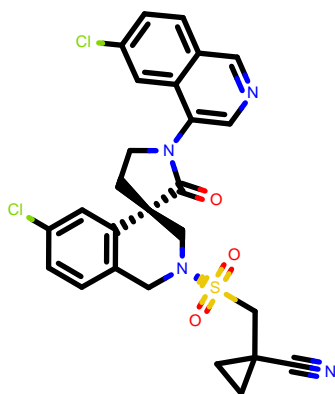
CID:	EDJ-MED-5cd3920d-4_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)4cnc5c4cc(c5)C(F)F)c6cc(c6C2=O)Cl</chem>
RUN:	RUN865
DDG (kcal/mol):	0.86
dDDG (kcal/mol):	0.15

ALP-POS-ecbed2ba-18_4



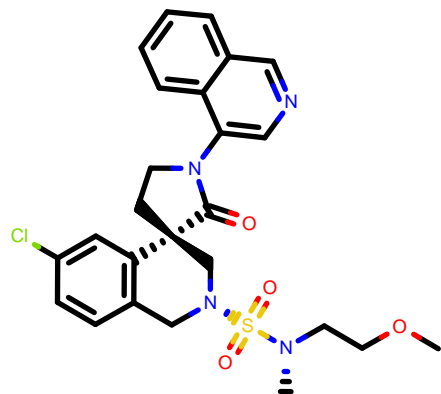
CID:	ALP-POS-ecbed2ba-18_4
SMILES:	<chem>CC[N@](C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)4cnc5c4cc5)Cl</chem>
RUN:	RUN643
DDG (kcal/mol):	0.88
dDDG (kcal/mol):	0.50

EDJ-MED-b6c6ee2b-4_2



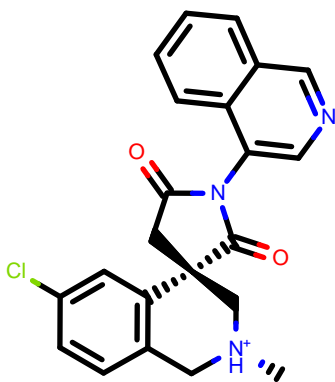
CID:	EDJ-MED-b6c6ee2b-4_2
SMILES:	<chem>c1cc2nccc(c2cc1Cl)N3CC[C@]4(C3=O)C[N@](C5c4cc(c5)Cl)S(=O)(=O)CC6(C6)C#N</chem>
RUN:	RUN822
DDG (kcal/mol):	0.88
dDDG (kcal/mol):	0.34

ALP-POS-ecbed2ba-21_3



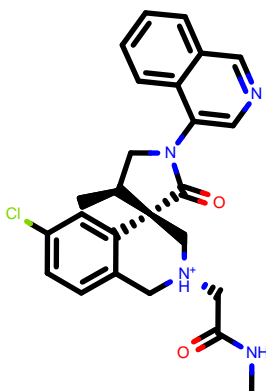
CID:	ALP-POS-ecbed2ba-21_3
SMILES:	<chem>C[N@](C)CCOC)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)4cnc5c4cc5)Cl</chem>
RUN:	RUN747
DDG (kcal/mol):	0.90
dDDG (kcal/mol):	0.63

JOH-MSK-51c67e7d-1_1



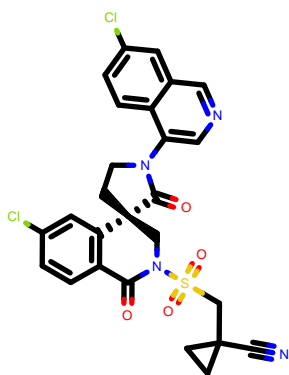
CID:	JOH-MSK-51c67e7d-1_1
SMILES:	<chem>C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN531
DDG (kcal/mol):	0.91
dDDG (kcal/mol):	0.13

MAT-POS-50a80394-4_2



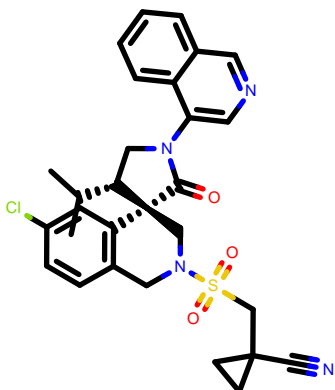
CID:	MAT-POS-50a80394-4_2
SMILES:	<chem>C[C@H]1CN(C(=O)[C@@]12C[N@@H+]Cc3c2cc(cc3)C)CC(=O)NC)c4cncc5c4cccc5</chem>
RUN:	RUN609
DDG (kcal/mol):	0.93
dDDG (kcal/mol):	0.25

EDJ-MED-9f4ac58c-1_1



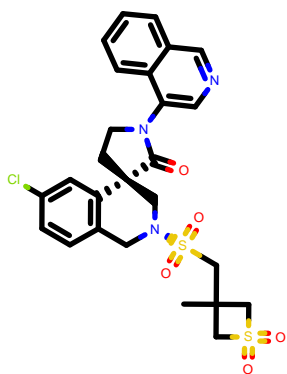
CID:	EDJ-MED-9f4ac58c-1_1
SMILES:	<chem>c1cc2c(cc1Cl)cncc2N3CC[C@@]14(C3=O)CN(C(=O)c5c4cc(cc5)O)S(=O)(=O)CC6(C)C#N</chem>
RUN:	RUN840
DDG (kcal/mol):	0.93
dDDG (kcal/mol):	0.37

MAT-POS-50a80394-3_3



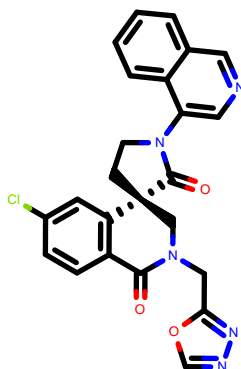
CID:	MAT-POS-50a80394-3_3
SMILES:	<chem>CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@@H+]Cc3c2cc(cc3)C)S(=O)(=O)CC4(C)C#N)c5cncc6c5cccc6</chem>
RUN:	RUN884
DDG (kcal/mol):	0.95
dDDG (kcal/mol):	0.50

ALP-POS-ecbed2ba-1_2



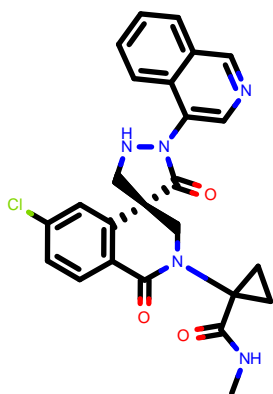
CID:	ALP-POS-ecbed2ba-1_2
SMILES:	<chem>CC1(CS(=O)(=O)C1)CS(=O)(=O)N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5ccc6c5ccc6)Cl</chem>
RUN:	RUN847
DDG (kcal/mol):	0.97
dDDG (kcal/mol):	0.49

PET-UNK-aa57768f-1_1



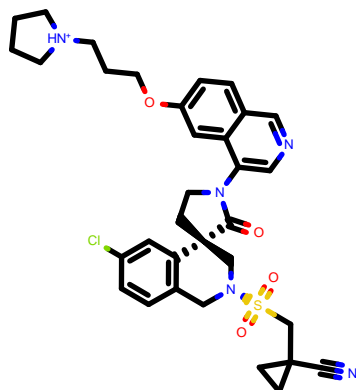
CID:	PET-UNK-aa57768f-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)C6Nnco6</chem>
RUN:	RUN631
DDG (kcal/mol):	0.97
dDDG (kcal/mol):	0.15

EDJ-MED-fed7ac0b-2_1



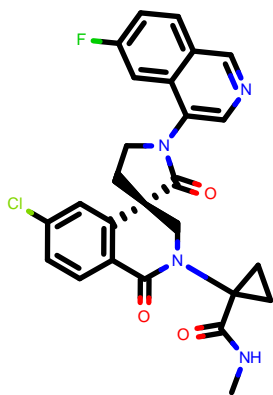
CID:	EDJ-MED-fed7ac0b-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CNN(C3=O)c4cnc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN700
DDG (kcal/mol):	0.97
dDDG (kcal/mol):	0.14

MAT-POS-40ad851a-5_2



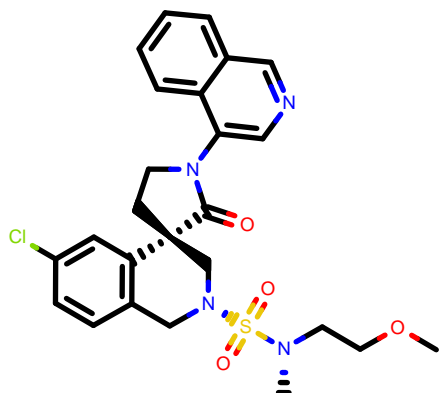
CID:	MAT-POS-40ad851a-5_2
SMILES:	<chem>c1cc2nccc2cc1OCC[NH+]3CCDC3N4CC[C@]5(C4=O)C(N@]6Cc6c5cc6)C1S(=O)(=O)CC7C7c#N</chem>
RUN:	RUN960
DDG (kcal/mol):	0.98
dDDG (kcal/mol):	0.50

EDJ-MED-b6c6ee2b-7_1



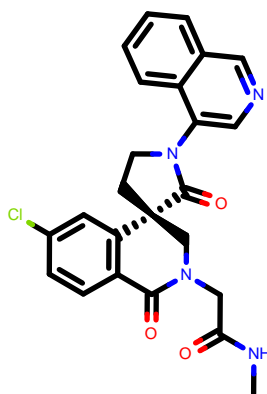
CID:	EDJ-MED-b6c6ee2b-7_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cnc5c4cc(cc5)F)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN766
DDG (kcal/mol):	0.99
dDDG (kcal/mol):	0.15

ALP-POS-ecbed2ba-21_4



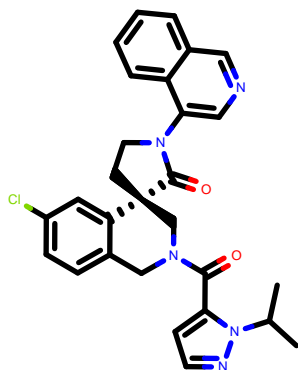
CID:	ALP-POS-ecbed2ba-21_4
SMILES:	<chem>C[N@](COC)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN754
DDG (kcal/mol):	1.00
dDDG (kcal/mol):	0.47

PET-UNK-14142a25-1_1



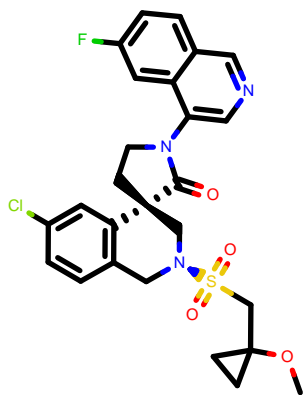
CID:	PET-UNK-14142a25-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cnc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN589
DDG (kcal/mol):	1.02
dDDG (kcal/mol):	0.13

MAT-POS-be048f2c-6_1



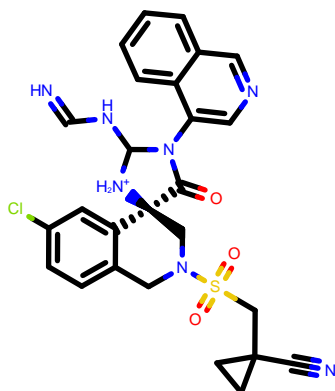
CID:	MAT-POS-be048f2c-6_1
SMILES:	<chem>CC(C)n1c(ccn1)C(=O)N2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5cccc6)Cl</chem>
RUN:	RUN818
DDG (kcal/mol):	1.03
dDDG (kcal/mol):	0.25

MAT-POS-853c0ffa-14_2



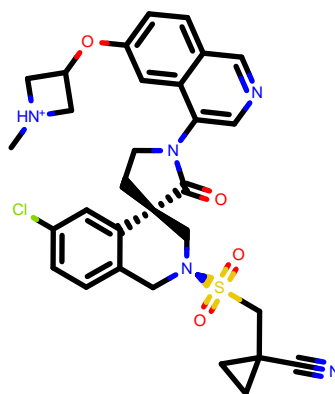
CID:	MAT-POS-853c0ffa-14_2
SMILES:	<chem>COC1(CC1)CS(=O)=[O]N@]2C=C3ccc(cc3[C@]4(C2)CCN(C4=O)c5ccc6c5cc(cc6)F)Cl</chem>
RUN:	RUN796
DDG (kcal/mol):	1.04
dDDG (kcal/mol):	0.28

LUO-POS-b5068a05-2_2



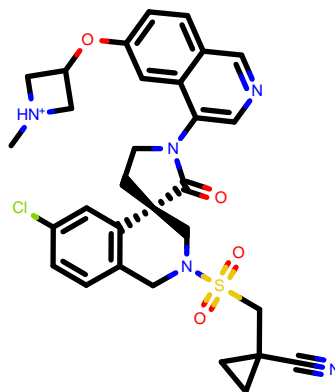
CID:	LUO-POS-b5068a05-2_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)N[C@@H](C3)N@]4C=CN=C5C=C(C=C5)S(=O)(=O)C6=CC=CC=C6N=C3NC#N</chem>
RUN:	RUN899
DDG (kcal/mol):	1.07
dDDG (kcal/mol):	0.33

EDJ-MED-ee81482e-2_2



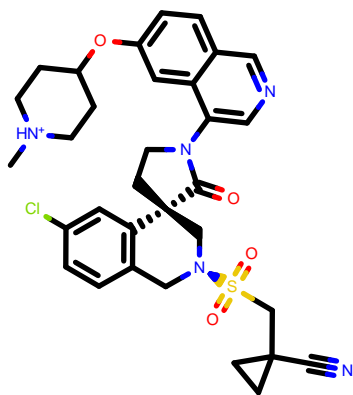
CID:	EDJ-MED-ee81482e-2_2
SMILES:	<chem>C[NH+]1CC(C1)Oc2ccc3ncnc3c2N4CC[C@]5(C4=O)C[N@]6C=C6C=CC=C6C(S(=O)(=O)C7=CC=CC=C7)C#N</chem>
RUN:	RUN930
DDG (kcal/mol):	1.08
dDDG (kcal/mol):	0.41

EDJ-MED-ee81482e-2_1



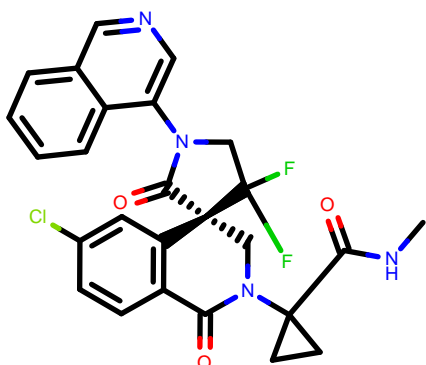
CID:	EDJ-MED-ee81482e-2_1
SMILES:	<chem>C[NH+]1CC(C1)Oc2ccc3ncnc3c2N4CC[C@]5(C4=O)C[N@]6C=C6C=CC=C6C(S(=O)(=O)C7=CC=CC=C7)C#N</chem>
RUN:	RUN929
DDG (kcal/mol):	1.09
dDDG (kcal/mol):	0.36

LUO-POS-d1147590-1_1



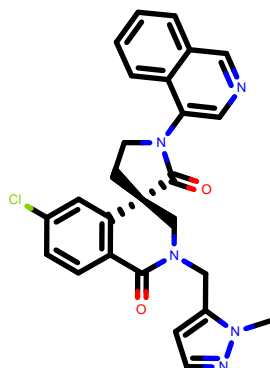
CID:	LUO-POS-d1147590-1_1
SMILES:	<chem>C[NH+]CCCC(C1)O2ccc3ccc(c3c2)N4C[C@@]5(C4=O)CN(C)C66c6c6c6)C1S(+O)-O)CC7(C)CN</chem>
RUN:	RUN965
DDG (kcal/mol):	1.10
dDDG (kcal/mol):	0.48

EDJ-MED-7e491f08-2_1



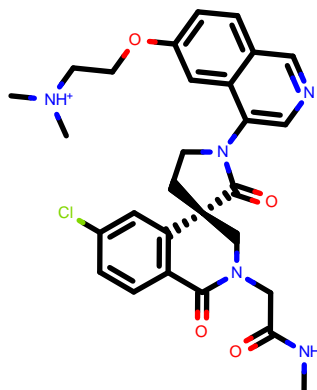
CID:	EDJ-MED-7e491f08-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(c4cc(ccc4C2=O)C)C(=O)N(CC3(F)F)c5ccc6c5ccc6</chem>
RUN:	RUN831
DDG (kcal/mol):	1.10
dDDG (kcal/mol):	0.16

EDJ-MED-cc48ee33-7_1



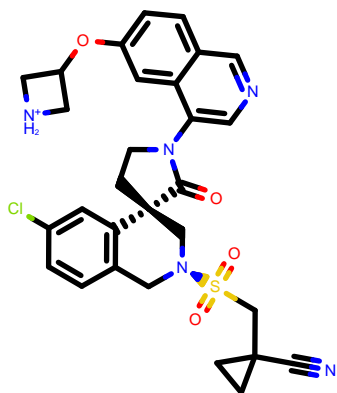
CID:	EDJ-MED-cc48ee33-7_1
SMILES:	<chem>Cn1c(ccn1)CN2C[C@]3(CCN(C3=O)c4cnc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN695
DDG (kcal/mol):	1.13
dDDG (kcal/mol):	0.21

MAT-POS-38eb6498-4_1



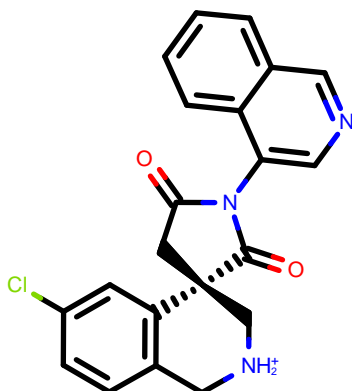
CID:	MAT-POS-38eb6498-4_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3ccc4c3cc(cc4)OC[NH+](C)C)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN902
DDG (kcal/mol):	1.15
dDDG (kcal/mol):	0.25

EDJ-MED-ee81482e-1_1



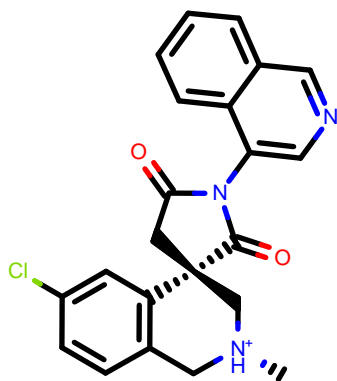
CID:	EDJ-MED-ee81482e-1_1
SMILES:	<chem>c1cc2ncc(c2cc1OC3CNH2+)(C3)N4CC(C@@H)(C4=O)CN(C)C5c6ccccc6(C)S(=O)(=O)CC7(C)C#N</chem>
RUN:	RUN920
DDG (kcal/mol):	1.15
dDDG (kcal/mol):	0.36

JOH-MSK-1f2dff76-3_1



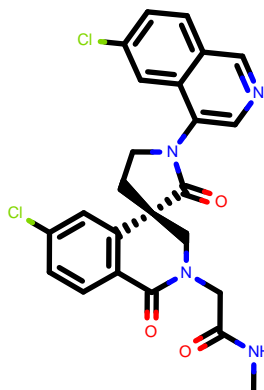
CID:	JOH-MSK-1f2dff76-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@H](C3=O)CNH2+)(C5c6ccccc5)Cl</chem>
RUN:	RUN527
DDG (kcal/mol):	1.17
dDDG (kcal/mol):	0.17

JOH-MSK-51c67e7d-2_1



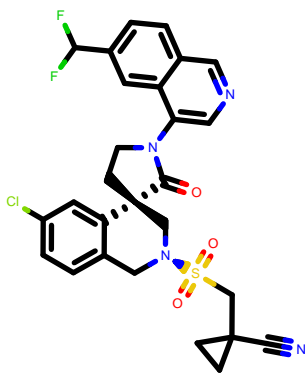
CID:	JOH-MSK-51c67e7d-2_1
SMILES:	<chem>C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN532
DDG (kcal/mol):	1.19
dDDG (kcal/mol):	0.14

LUO-POS-8c3e556a-1_1



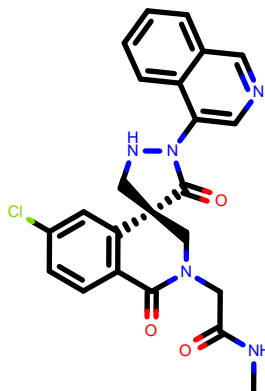
CID:	LUO-POS-8c3e556a-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5ccc(cc5C1=O)Cl</chem>
RUN:	RUN664
DDG (kcal/mol):	1.19
dDDG (kcal/mol):	0.13

EDJ-MED-5cd3920d-2_2



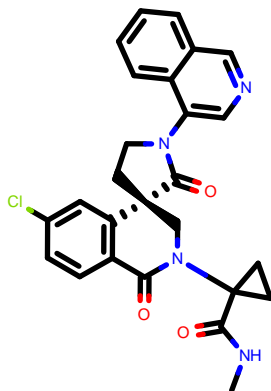
CID:	EDJ-MED-5cd3920d-2_2
SMILES:	<chem>c1cc2ncc(c2c1C(F)F)N3CC(C@H)4(C3=O)C(N#)C5c4ccc(c5)C(S(=O)(=O)C6=CC6)CN</chem>
RUN:	RUN886
DDG (kcal/mol):	1.27
dDDG (kcal/mol):	0.41

EDJ-MED-fed7ac0b-1_1



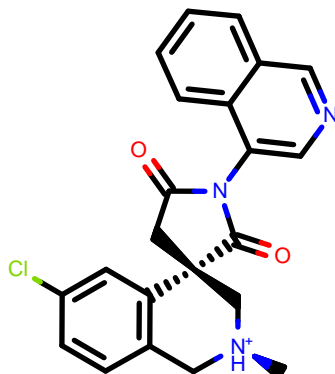
CID:	EDJ-MED-fed7ac0b-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CNN(C2=O)c3cnc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN597
DDG (kcal/mol):	1.27
dDDG (kcal/mol):	0.16

MAT-POS-576f7758-2_1



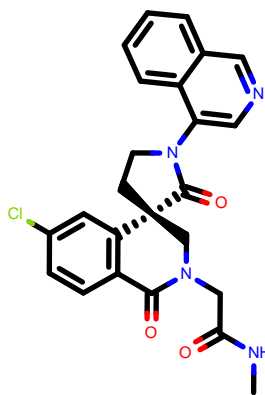
CID:	MAT-POS-576f7758-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cnc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN692
DDG (kcal/mol):	1.29
dDDG (kcal/mol):	0.16

JOH-MSK-51c67e7d-2_2



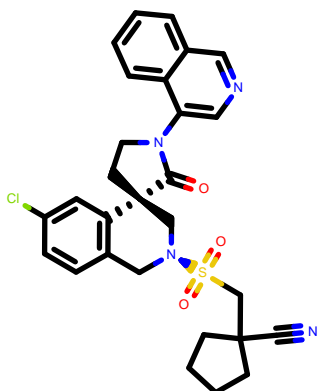
CID:	JOH-MSK-51c67e7d-2_2
SMILES:	<chem>C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN535
DDG (kcal/mol):	1.29
dDDG (kcal/mol):	0.10

LUO-POS-9931618f-1_1



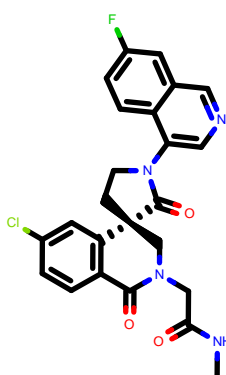
CID:	LUO-POS-9931618f-1_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN607
DDG (kcal/mol):	1.46
dDDG (kcal/mol):	0.13

ALP-POS-ecbed2ba-15_1



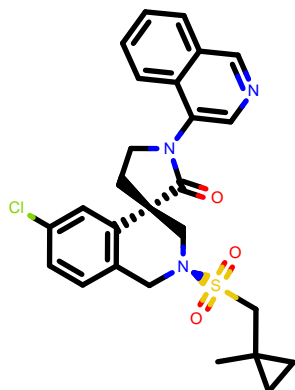
CID:	ALP-POS-ecbed2ba-15_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@@]4(C3=O)CN[C@@]5(Cc6ccccc6)S(=O)(=O)C5=O</chem>
RUN:	RUN845
DDG (kcal/mol):	1.47
dDDG (kcal/mol):	0.37

EDG-MED-b1ef7fe3-3_1



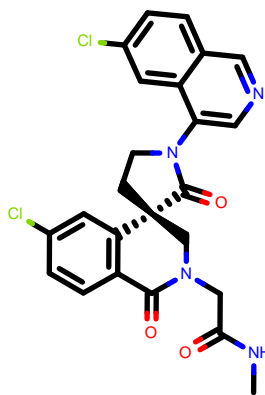
CID:	EDG-MED-b1ef7fe3-3_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(CCN(C2=O)c3cncc4c3ccc(c4)F)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN634
DDG (kcal/mol):	1.49
dDDG (kcal/mol):	0.14

ALP-POS-ecbed2ba-3_1



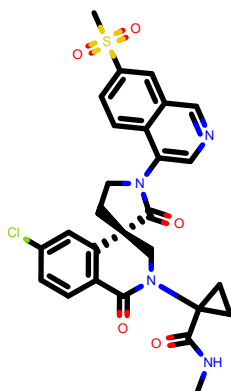
CID:	ALP-POS-ecbed2ba-3_1
SMILES:	<chem>CC1(CC1)CS(=O)(=O)N[C@@]2(Cc3ccccc3)[C@@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl</chem>
RUN:	RUN686
DDG (kcal/mol):	1.51
dDDG (kcal/mol):	0.24

LUO-POS-8c3e556a-2_1



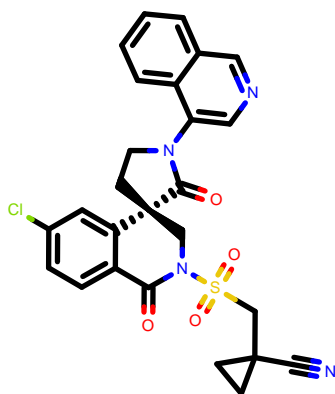
CID:	LUO-POS-8c3e556a-2_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4Cl)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN667
DDG (kcal/mol):	1.52
dDDG (kcal/mol):	0.14

EDJ-MED-976a33d5-2_1



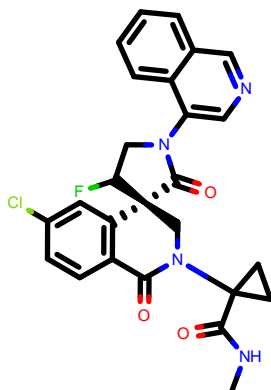
CID:	EDJ-MED-976a33d5-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)S(=O)(=O)C)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN881
DDG (kcal/mol):	1.54
dDDG (kcal/mol):	0.16

EDJ-MED-9f4ac58c-2_1



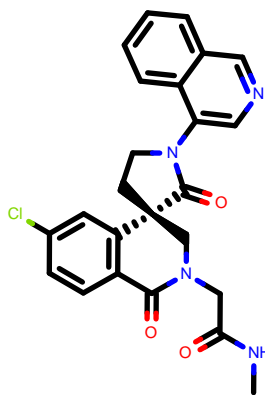
CID:	EDJ-MED-9f4ac58c-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C[C@]4(C3=O)CN(C(=O)c5c4cc(c5)O)S(=O)(=O)CC6(C6)C#N</chem>
RUN:	RUN781
DDG (kcal/mol):	1.55
dDDG (kcal/mol):	0.43

EDJ-MED-fd8ed875-6_1



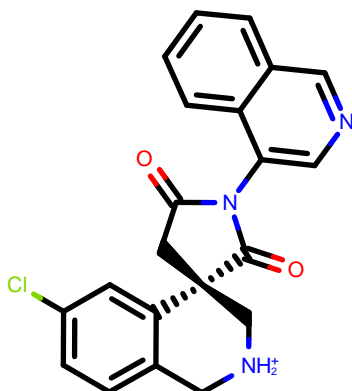
CID:	EDJ-MED-fd8ed875-6_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(c4cc(ccc4C2=O)Cl)C(=CN(C3=O)c5cncc6c5ccc6)F</chem>
RUN:	RUN773
DDG (kcal/mol):	1.56
dDDG (kcal/mol):	0.17

LUO-POS-9931618f-2_1



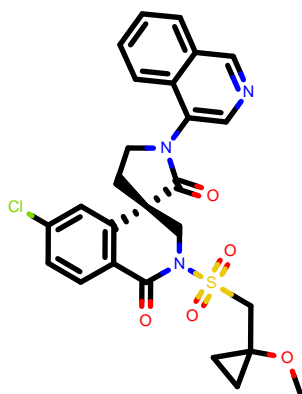
CID:	LUO-POS-9931618f-2_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncoc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN605
DDG (kcal/mol):	1.59
dDDG (kcal/mol):	0.15

JOH-MSK-1f2dff76-4_1



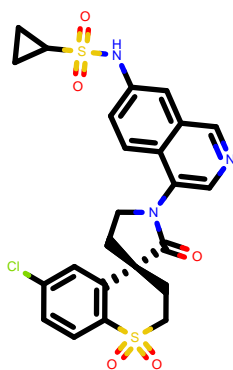
CID:	JOH-MSK-1f2dff76-4_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)C[C@@]4(C3=O)C[NH2+]Cc5c4cc(cc5)Cl</chem>
RUN:	RUN519
DDG (kcal/mol):	1.59
dDDG (kcal/mol):	0.17

EDJ-MED-9f4ac58c-6_1



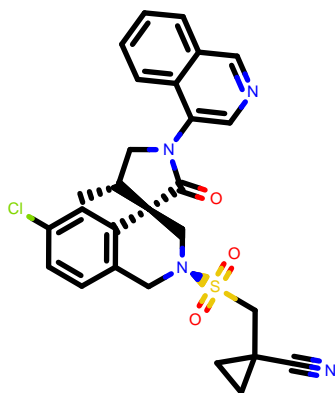
CID:	EDJ-MED-9f4ac58c-6_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cnc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN785
DDG (kcal/mol):	1.60
dDDG (kcal/mol):	0.38

EDJ-MED-edc5c6cb-2_1



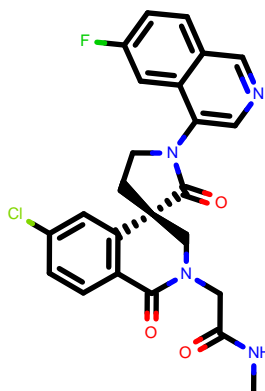
CID:	EDJ-MED-edc5c6cb-2_1
SMILES:	<chem>c1cc2c(cc1NS(=O)(=O)C3CC3)cnc2N4CC[C@@]5(C4=O)CCS(=O)(=O)c6c5cc(cc6)Cl</chem>
RUN:	RUN776
DDG (kcal/mol):	1.61
dDDG (kcal/mol):	0.20

MAT-POS-50a80394-1_3



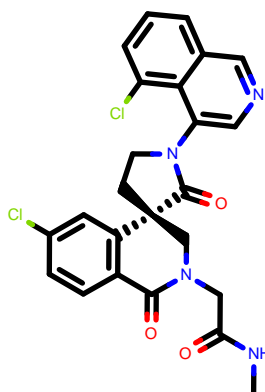
CID:	MAT-POS-50a80394-1_3
SMILES:	<chem>C[C@H]1CN(C1=O)C[C@]2(CN2)C3=CC=CC=C3S(=O)(=O)CC4(CCN4)C5=CC=CC=C5</chem>
RUN:	RUN825
DDG (kcal/mol):	1.64
dDDG (kcal/mol):	0.31

EDJ-MED-b6c6ee2b-6_1



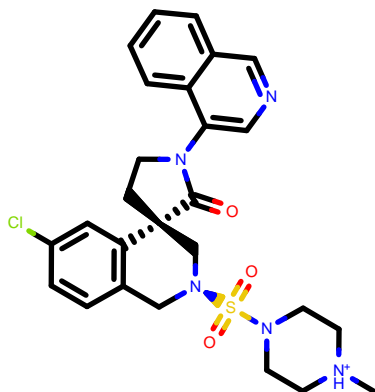
CID:	EDJ-MED-b6c6ee2b-6_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3nccc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN670
DDG (kcal/mol):	1.67
dDDG (kcal/mol):	0.15

MAT-POS-1d5ab790-3_1



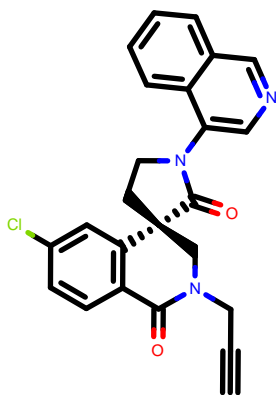
CID:	MAT-POS-1d5ab790-3_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3nccc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN655
DDG (kcal/mol):	1.67
dDDG (kcal/mol):	0.14

LUO-POS-ed2cfb03-1_1



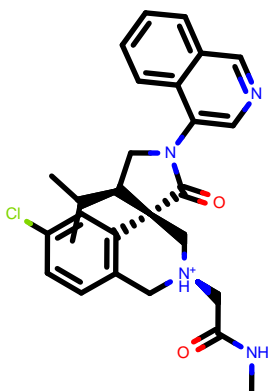
CID:	LUO-POS-ed2cfb03-1_1
SMILES:	<chem>C[NH+]1CCN(CC1)S(=O)(=O)N@@2C=C3CC(=O)C@H(C2)CCN(C4=O)C5=CC=CC=C5C6=CC=C6Cl</chem>
RUN:	RUN832
DDG (kcal/mol):	1.68
dDDG (kcal/mol):	0.26

PET-UNK-aa57768f-9_1



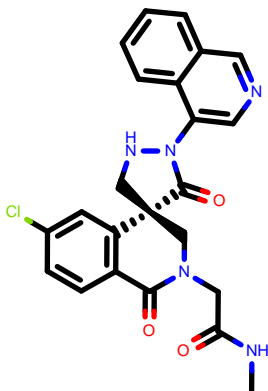
CID:	PET-UNK-aa57768f-9_1
SMILES:	<chem>C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN545
DDG (kcal/mol):	1.69
dDDG (kcal/mol):	0.13

MAT-POS-50a80394-6_4



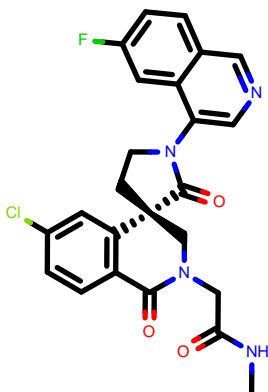
CID:	MAT-POS-50a80394-6_4
SMILES:	<chem>CC(C)[C@H]1CN(C(=O)[C@@]12C[N@H+]C3c2cc(cc3)C)CC(=O)N(C)C4cncc5c4cccc5</chem>
RUN:	RUN701
DDG (kcal/mol):	1.70
dDDG (kcal/mol):	0.32

EDJ-MED-fed7ac0b-4_1



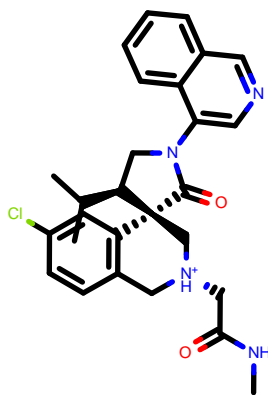
CID:	EDJ-MED-fed7ac0b-4_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(C=NN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN593
DDG (kcal/mol):	1.70
dDDG (kcal/mol):	0.13

EDG-MED-b1ef7fe3-2_1



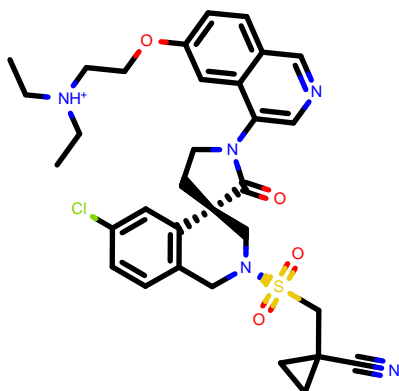
CID:	EDG-MED-b1ef7fe3-2_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN629
DDG (kcal/mol):	1.72
dDDG (kcal/mol):	0.13

MAT-POS-50a80394-6_2



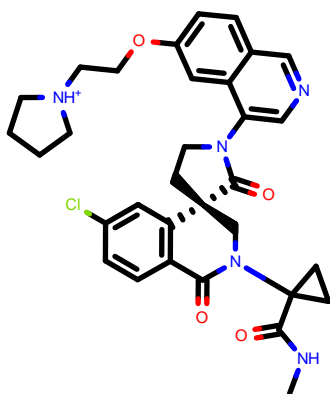
CID:	MAT-POS-50a80394-6_2
SMILES:	<chem>CC(C)[C@H]1CN(C(=O)[C@@]12C[N@@H+][C@]3c2cc(cc3)C)CC(=O)NC)c4cnc5c4ccc5</chem>
RUN:	RUN709
DDG (kcal/mol):	1.73
dDDG (kcal/mol):	0.24

MAT-POS-40ad851a-3_2



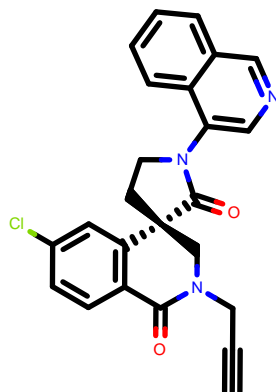
CID:	MAT-POS-40ad851a-3_2
SMILES:	<chem>CC[NH+](C)CCOC1c2c2nc2c2e1N3CC[C@]4[C@@]3O[C@N5]C654cc(cc5)C(S(=O)(=O)C6)C6#N</chem>
RUN:	RUN953
DDG (kcal/mol):	1.74
dDDG (kcal/mol):	0.70

EDJ-MED-dfa1d800-1_1



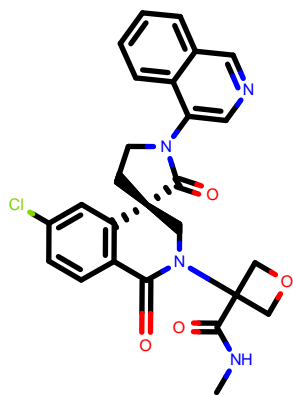
CID:	EDJ-MED-dfa1d800-1_1
SMILES:	<chem>CNC1=O[C@@]1(C2)N2C[C@]3[C@@]1CN(C3=O)c4cnc5c4ccc5)OCC[NH+]6CCCC6c7cc(cc7)C2=O)Cl</chem>
RUN:	RUN926
DDG (kcal/mol):	1.74
dDDG (kcal/mol):	0.32

PET-UNK-aa57768f-3_1



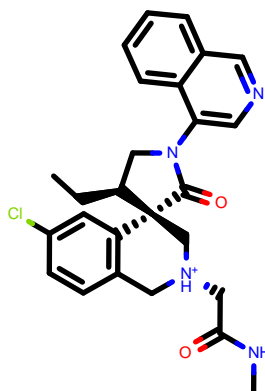
CID:	PET-UNK-aa57768f-3_1
SMILES:	<chem>C#CCN1C[C@@]2(CCN(C2=O)c3cnc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN541
DDG (kcal/mol):	1.75
dDDG (kcal/mol):	0.15

EDJ-MED-98c0a822-4_1



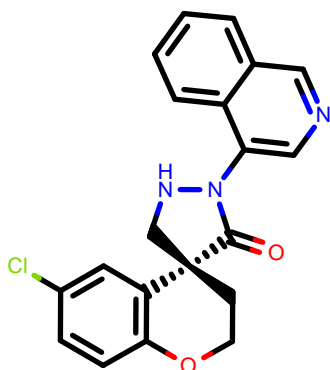
CID:	EDJ-MED-98c0a822-4_1
SMILES:	<chem>CNC(=O)C1(COC1)N2C[C@]3(CCN(C3=O)c4cnc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN760
DDG (kcal/mol):	1.76
dDDG (kcal/mol):	0.16

MAT-POS-50a80394-5_2



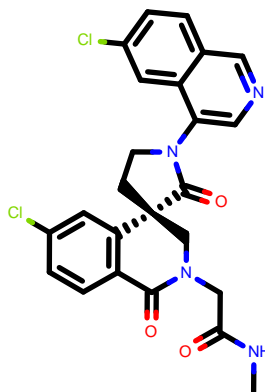
CID:	MAT-POS-50a80394-5_2
SMILES:	<chem>CC[C@H]1CN(C(=O)[C@@]12C[N@@H+]Cc3c2cc(cc3)C)CC(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN652
DDG (kcal/mol):	1.76
dDDG (kcal/mol):	0.23

BRU-THA-73c97d88-1_1



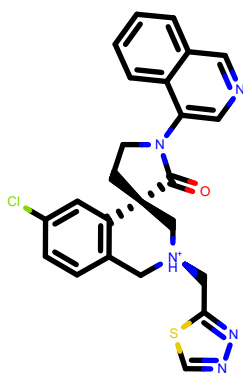
CID:	BRU-THA-73c97d88-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C=N3</chem>
RUN:	RUN500
DDG (kcal/mol):	1.78
dDDG (kcal/mol):	0.09

EDG-MED-b1ef7fe3-1_1



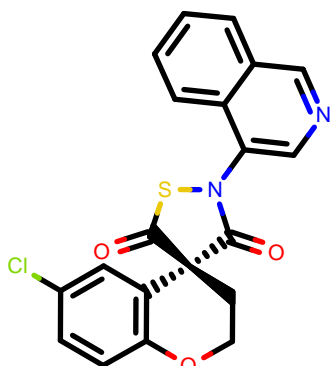
CID:	EDG-MED-b1ef7fe3-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN620
DDG (kcal/mol):	1.79
dDDG (kcal/mol):	0.16

PET-UNK-7e9559de-4_2



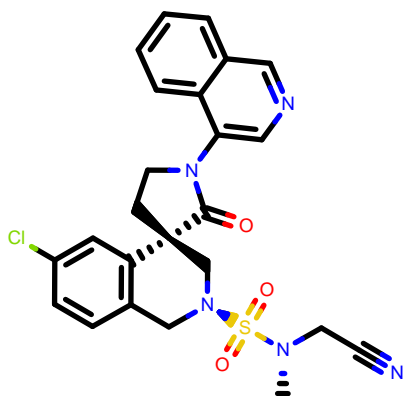
CID:	PET-UNK-7e9559de-4_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+]1Cc5c4cc(cc5)C1Cc6nncs6</chem>
RUN:	RUN603
DDG (kcal/mol):	1.83
dDDG (kcal/mol):	0.16

DAR-DIA-0f7b7cd9-8_1



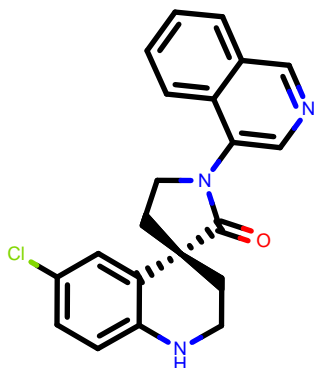
CID:	DAR-DIA-0f7b7cd9-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C3=O)C[N@H+]1Cc5c4cc(cc5)C1C(=O)S3</chem>
RUN:	RUN515
DDG (kcal/mol):	1.83
dDDG (kcal/mol):	0.10

ALP-POS-ecbed2ba-17_1



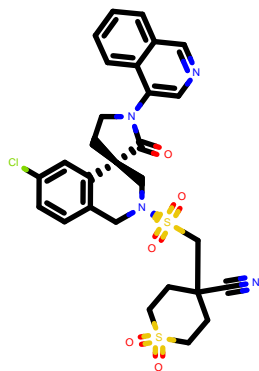
CID:	ALP-POS-ecbed2ba-17_1
SMILES:	<chem>C[N@@]1(CC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@@]3(C1)CCN(C3=O)c4ncc5c4cccs5)Cl</chem>
RUN:	RUN688
DDG (kcal/mol):	1.84
dDDG (kcal/mol):	0.23

DAR-DIA-6be260fc-5_1



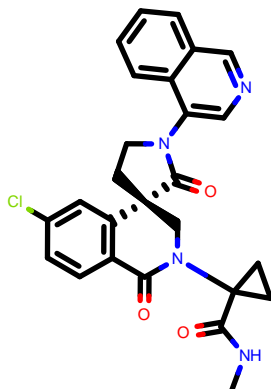
CID:	DAR-DIA-6be260fc-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCNc5c4cc(cc5)Cl</chem>
RUN:	RUN491
DDG (kcal/mol):	1.87
dDDG (kcal/mol):	0.10

ALP-POS-ecbed2ba-2_2



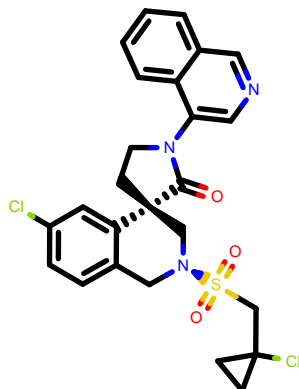
CID:	ALP-POS-ecbed2ba-2_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@H](C3=O)C[N@]1Cc5c4c(cc5)C(S(=O)(=O)CC6(CCS(=O)(=O)CC6)CN</chem>
RUN:	RUN901
DDG (kcal/mol):	1.90
dDDG (kcal/mol):	0.37

EDJ-MED-fd8ed875-4_1



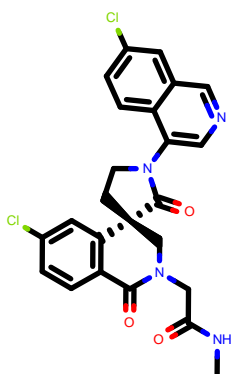
CID:	EDJ-MED-fd8ed875-4_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3[C=C=CN(C3=O)c4cnc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN699
DDG (kcal/mol):	1.92
dDDG (kcal/mol):	0.17

PET-UNK-94036022-10_2



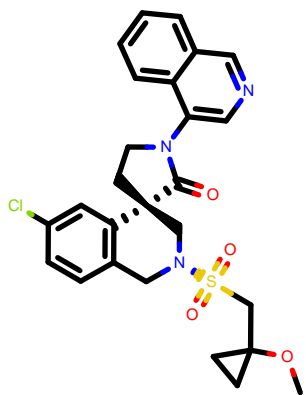
CID:	PET-UNK-94036022-10_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@H](C3=O)C[N@]1Cc5c4c(cc5)C(S(=O)(=O)CC6(COC6)(CC6)Cl</chem>
RUN:	RUN703
DDG (kcal/mol):	1.93
dDDG (kcal/mol):	0.37

EDG-MED-b1ef7fe3-4_1



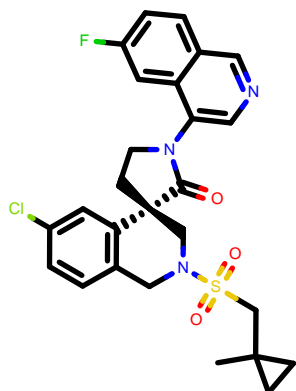
CID:	EDG-MED-b1ef7fe3-4_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cnc4c3ccc(c4)C)C5CC(CCC5C1=O)Cl</chem>
RUN:	RUN627
DDG (kcal/mol):	1.93
dDDG (kcal/mol):	0.17

ALP-POS-ecbed2ba-6_1



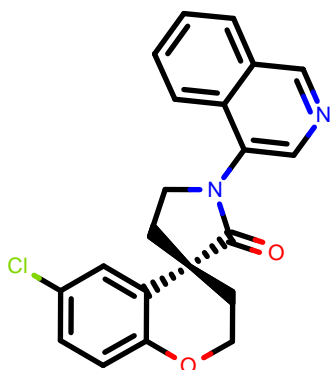
CID:	ALP-POS-ecbed2ba-6_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@H](C2)CCN(C4=O)c5cnc6c5ccc6)Cl</chem>
RUN:	RUN730
DDG (kcal/mol):	1.94
dDDG (kcal/mol):	0.33

MAT-POS-853c0ffa-21_1



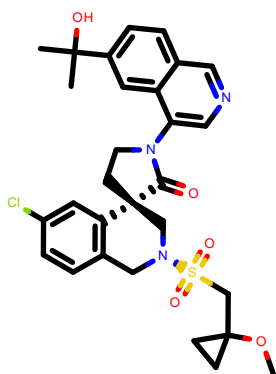
CID:	MAT-POS-853c0ffa-21_1
SMILES:	<chem>CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@H](C2)CCN(C4=O)c5cnc6c5cc(c6)F)Cl</chem>
RUN:	RUN725
DDG (kcal/mol):	1.94
dDDG (kcal/mol):	0.30

MAT-POS-983b399a-1_1



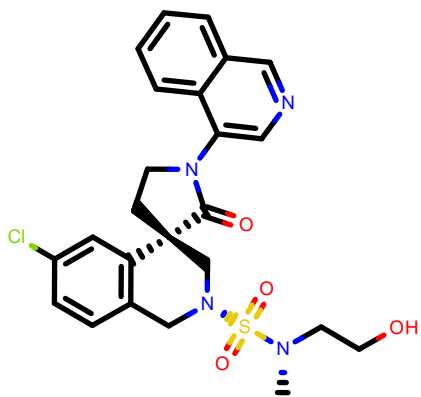
CID:	MAT-POS-983b399a-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN496
DDG (kcal/mol):	1.95
dDDG (kcal/mol):	0.10

MAT-POS-853c0ffa-12_1



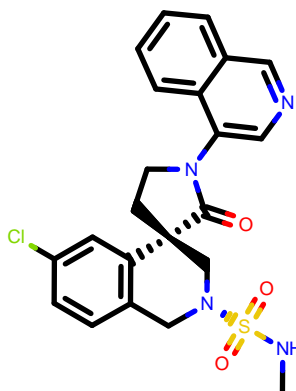
CID:	MAT-POS-853c0ffa-12_1
SMILES:	<chem>CC(C)(c1ccc2nc(c2c1)N3CC[C@@]4(C3=O)CN@@]5Cc6ccc(cc6)Cl)S(=O)(=O)CO</chem>
RUN:	RUN896
DDG (kcal/mol):	1.96
dDDG (kcal/mol):	0.41

ALP-POS-ecbed2ba-19_4



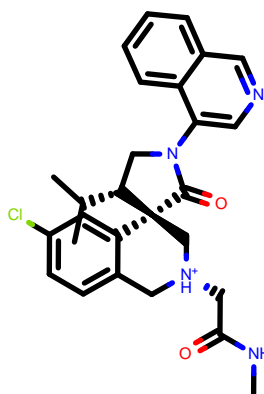
CID:	ALP-POS-ecbed2ba-19_4
SMILES:	<chem>C[N@]([CCO]S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN706
DDG (kcal/mol):	2.03
dDDG (kcal/mol):	0.81

LUO-POS-ed2cfb03-2_2



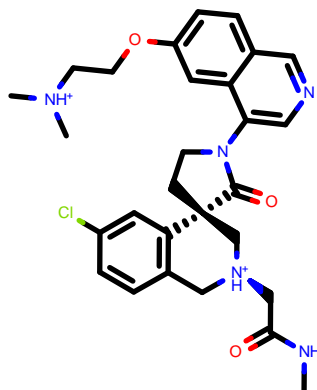
CID:	LUO-POS-ed2cfb03-2_2
SMILES:	<chem>CNS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN576
DDG (kcal/mol):	2.05
dDDG (kcal/mol):	0.42

MAT-POS-50a80394-6_1



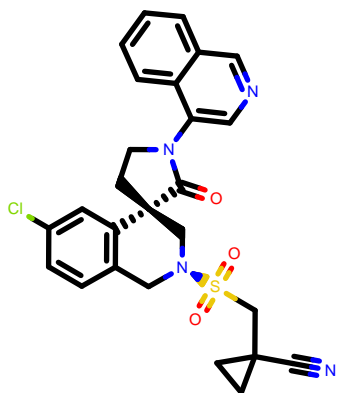
CID:	MAT-POS-50a80394-6_1
SMILES:	<chem>CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@@H+]Cc3c2cc(cc3)C)CC(=O)NC)c4cncc5c4cccc5</chem>
RUN:	RUN707
DDG (kcal/mol):	2.06
dDDG (kcal/mol):	0.26

MAT-POS-38eb6498-3_2



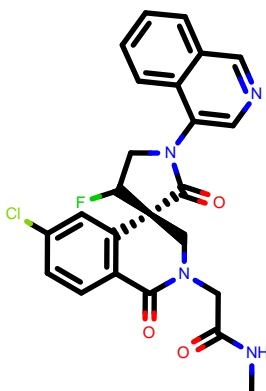
CID:	MAT-POS-38eb6498-3_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(cc5)OCC[NH+](C)C)Cl</chem>
RUN:	RUN877
DDG (kcal/mol):	2.06
dDDG (kcal/mol):	0.35

MIK-ENA-5d9157e9-2_2



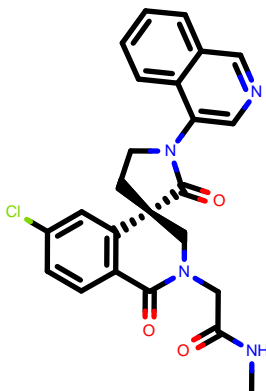
CID:	MIK-ENA-5d9157e9-2_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@]5Cc5c4cc(cc5)ClS(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN753
DDG (kcal/mol):	2.07
dDDG (kcal/mol):	0.50

EDJ-MED-fd8ed875-5_1



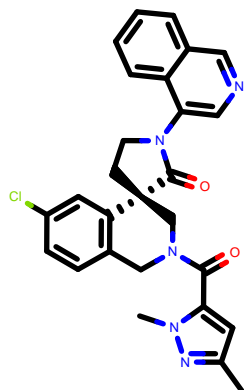
CID:	EDJ-MED-fd8ed875-5_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(c3cc(ccc3C1=O)Cl)C(=CN(C2=O)c4cncc5c4cccc5)F</chem>
RUN:	RUN657
DDG (kcal/mol):	2.10
dDDG (kcal/mol):	0.12

EDJ-MED-8bb691af-8_1



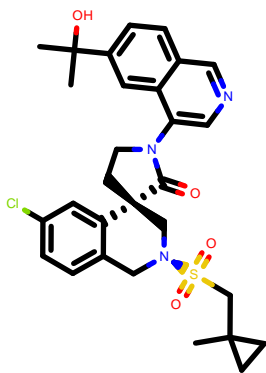
CID:	EDJ-MED-8bb691af-8_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN578
DDG (kcal/mol):	2.10
dDDG (kcal/mol):	0.18

EDJ-MED-cc48ee33-5_1



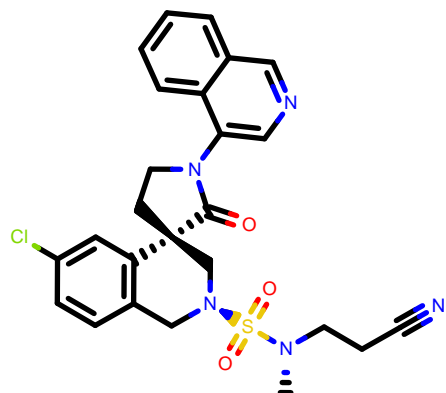
CID:	EDJ-MED-cc48ee33-5_1
SMILES:	<chem>Cc1cc(n(n1)C)C(=O)N2C3ccc(cc3[C@@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl</chem>
RUN:	RUN763
DDG (kcal/mol):	2.12
dDDG (kcal/mol):	0.20

MAT-POS-853c0ffa-20_1



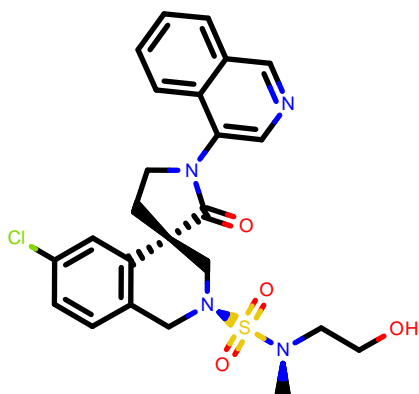
CID:	MAT-POS-853c0ffa-20_1
SMILES:	<chem>CC1(C)C(S(=O)(=O)N@2[C@@H](C)CCN(C4=O)C5=CC=CC=C5C1)C(O)Cl</chem>
RUN:	RUN878
DDG (kcal/mol):	2.13
dDDG (kcal/mol):	0.26

ALP-POS-ecbed2ba-16_1



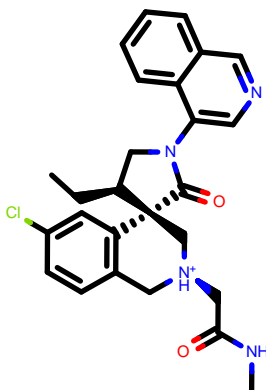
CID:	ALP-POS-ecbed2ba-16_1
SMILES:	<chem>C[N@@]1CCC#N)S(=O)(=O)N@@1C2CCCC2[C@@]3(C1)CCN(C3=O)C4=CC=CC=C4</chem>
RUN:	RUN743
DDG (kcal/mol):	2.14
dDDG (kcal/mol):	0.32

ALP-POS-ecbed2ba-19_2



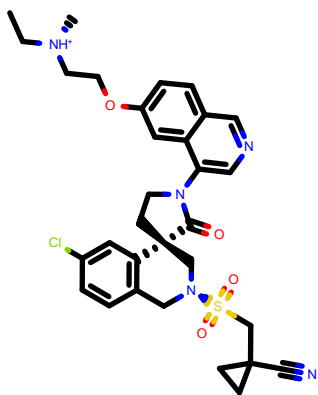
CID:	ALP-POS-ecbed2ba-19_2
SMILES:	<chem>C[N@@]1(CCO)S(=O)(=O)N@@1C2CCCC2[C@@]3(C1)CCN(C3=O)C4=CC=CC=C4</chem>
RUN:	RUN702
DDG (kcal/mol):	2.15
dDDG (kcal/mol):	0.34

MAT-POS-50a80394-5_4



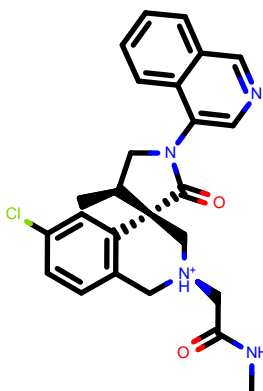
CID:	MAT-POS-50a80394-5_4
SMILES:	<chem>CC[C@H]1CN(C(=O)[C@@]12C[N@H+]1C2)C(=O)N(C)C(=O)C4=CC=CC=C4</chem>
RUN:	RUN662
DDG (kcal/mol):	2.16
dDDG (kcal/mol):	0.25

MAT-POS-40ad851a-2_4



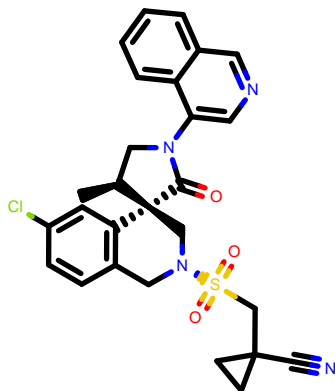
CID:	MAT-POS-40ad851a-2_4
SMILES:	<chem>CC[NH+](C)CCOC1=CC=C2C(=N1)N(C)C(C)C(=O)N(C)C3=CC=C(C=C3)S(=O)(=O)CC6=CC=CN</chem>
RUN:	RUN936
DDG (kcal/mol):	2.19
dDDG (kcal/mol):	0.66

MAT-POS-50a80394-4_4



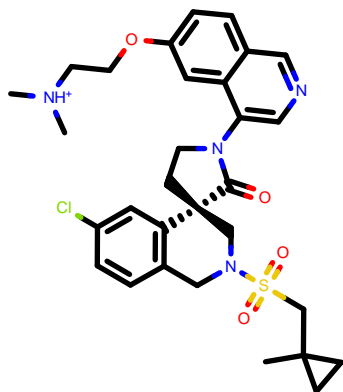
CID:	MAT-POS-50a80394-4_4
SMILES:	<chem>C[C@H]1CN(C(=O)[C@@]12C[NH+]([C@H]2)C3=CC=C(C=C3)C)C(=O)NC(=O)C4=CC=CC=C4</chem>
RUN:	RUN611
DDG (kcal/mol):	2.19
dDDG (kcal/mol):	0.22

MAT-POS-50a80394-1_4



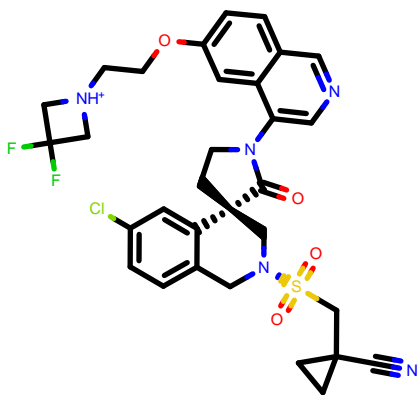
CID:	MAT-POS-50a80394-1_4
SMILES:	<chem>C[C@H]1CN(C(=O)[C@@]12C[NH+]([C@H]2)C3=CC=C(C=C3)S(=O)(=O)CC4=CC=C(C=C4)C#N)C5=CC=CC=C5</chem>
RUN:	RUN830
DDG (kcal/mol):	2.20
dDDG (kcal/mol):	0.50

MAT-POS-853c0ffa-19_2



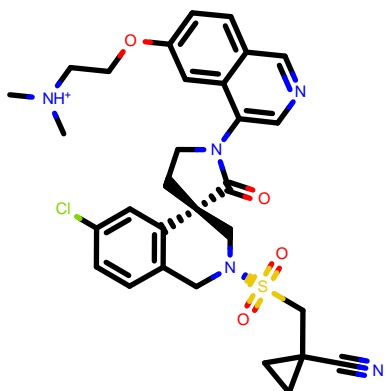
CID:	MAT-POS-853c0ffa-19_2
SMILES:	<chem>CC1(C)CS(=O)(=O)[N+](C)C2=CC=C(C=C2)C3=CC=C(C=C3)S(=O)(=O)CC4=CC=CC(=O)N(C)C(C)C1</chem>
RUN:	RUN913
DDG (kcal/mol):	2.22
dDDG (kcal/mol):	0.44

EDJ-MED-468565e0-5_1



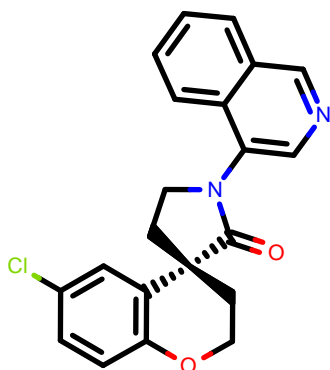
CID:	EDJ-MED-468565e0-5_1
SMILES:	<chem>c1cc2ncc(c2cc1OCCN3CC(C3)F)F)N4CC[C@@]5(C4=O)C(N@B)C6c5cc(c6)C(S(=O)(=O)CC7(C)C7)C#N</chem>
RUN:	RUN962
DDG (kcal/mol):	2.23
dDDG (kcal/mol):	0.57

MAT-POS-38eb6498-1_1



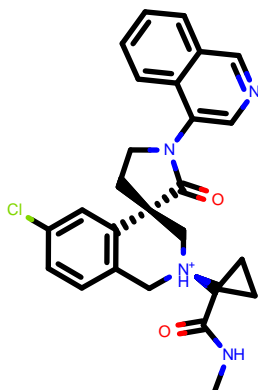
CID:	MAT-POS-38eb6498-1_1
SMILES:	<chem>C[NH+]C)CCO1ccc2ncc(c2c1)N3CC[C@@]4(C3=O)C(N@B)C5c4cc(c5)C(S(=O)(=O)CC6(C)C6)C#N</chem>
RUN:	RUN927
DDG (kcal/mol):	2.24
dDDG (kcal/mol):	0.71

ALP-POS-477dc5b7-4_1



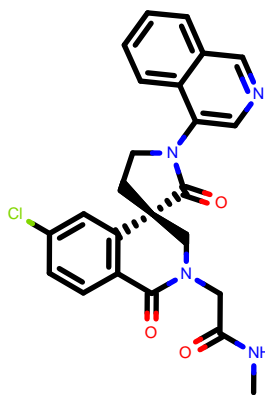
CID:	ALP-POS-477dc5b7-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN493
DDG (kcal/mol):	2.28
dDDG (kcal/mol):	0.11

MAT-POS-576f7758-1_2



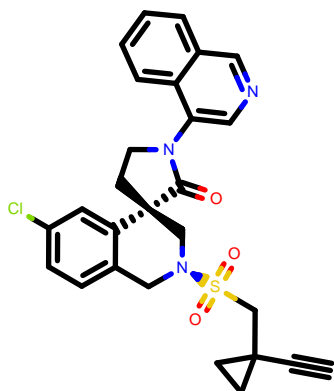
CID:	MAT-POS-576f7758-1_2
SMILES:	<chem>CNC(=O)C1(CC1)[N@H+]2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5ccccc6)Cl</chem>
RUN:	RUN654
DDG (kcal/mol):	2.33
dDDG (kcal/mol):	0.17

EDJ-MED-fd8ed875-3_1



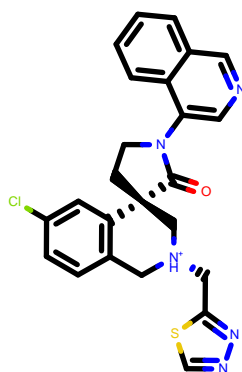
CID:	EDJ-MED-fd8ed875-3_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(C=CN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN602
DDG (kcal/mol):	2.34
dDDG (kcal/mol):	0.15

PET-UNK-94036022-9_1



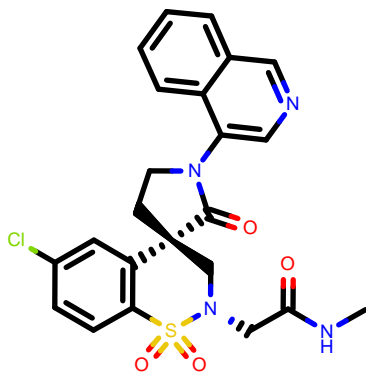
CID:	PET-UNK-94036022-9_1
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)N@@]2C=C3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl</chem>
RUN:	RUN761
DDG (kcal/mol):	2.35
dDDG (kcal/mol):	0.27

PET-UNK-7e9559de-1_1



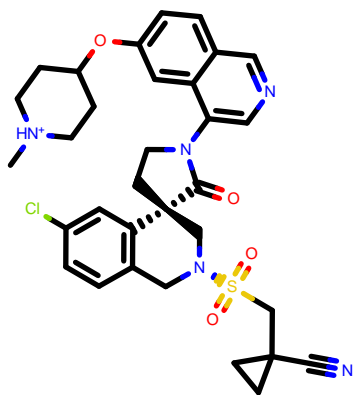
CID:	PET-UNK-7e9559de-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)C[N@@H]5C=C4c(c5)ClC6=NC=CS6</chem>
RUN:	RUN600
DDG (kcal/mol):	2.36
dDDG (kcal/mol):	0.21

ALP-POS-4483ae88-2_2



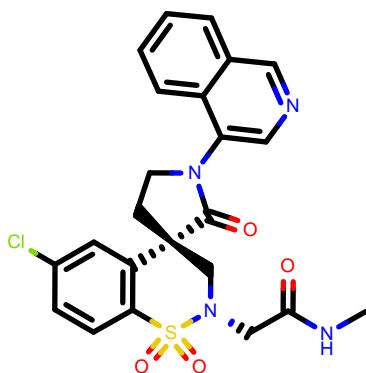
CID:	ALP-POS-4483ae88-2_2
SMILES:	<chem>CNC(=O)C[N@]1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)Cl</chem>
RUN:	RUN633
DDG (kcal/mol):	2.37
dDDG (kcal/mol):	0.21

LUO-POS-d1147590-1_2



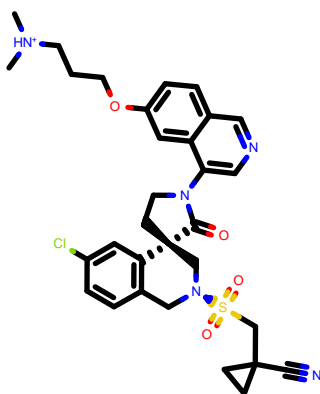
CID:	LUO-POS-d1147590-1_2
SMILES:	<chem>C[NH+](CCC(CC1)Oc2cc3nccc3c2)N4CC[C@H]5(C4=O)C[N@H]6c6c6cc6)C1S(=O)(=O)CC7(C)C7c#N</chem>
RUN:	RUN963
DDG (kcal/mol):	2.37
dDDG (kcal/mol):	0.73

ALP-POS-4483ae88-2_1



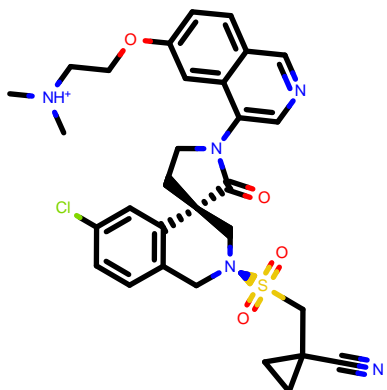
CID:	ALP-POS-4483ae88-2_1
SMILES:	<chem>CNC(=O)C[N@H]1C[C@H]2(CCN(C2=O)c3nccc4c3ccc4)c5cc(ccc5S1(=O)=O)Cl</chem>
RUN:	RUN625
DDG (kcal/mol):	2.38
dDDG (kcal/mol):	0.20

MAT-POS-40ad851a-4_1



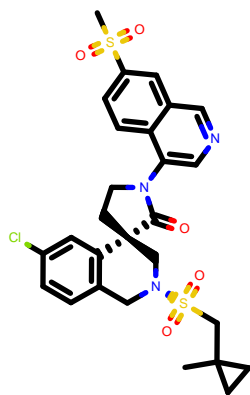
CID:	MAT-POS-40ad851a-4_1
SMILES:	<chem>C[NH+](C)CCOC1ccc2nccc2c1)N3CC[C@H]4(C3=O)C[N@H]5(Cc54cc5)C1S(=O)(=O)CC6(C)C6c#N</chem>
RUN:	RUN941
DDG (kcal/mol):	2.40
dDDG (kcal/mol):	0.35

LUO-POS-8484f2d3-1_1



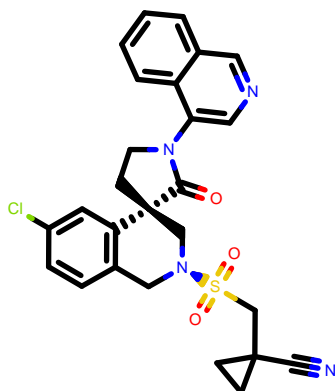
CID:	LUO-POS-8484f2d3-1_1
SMILES:	<chem>C[NH+](C)CCOC1ccc2nccc2c1)N3CC[C@H]4(C3=O)C[N@H]5(Cc54cc5)C1S(=O)(=O)CC6(C)C6c#N</chem>
RUN:	RUN932
DDG (kcal/mol):	2.41
dDDG (kcal/mol):	0.65

MAT-POS-853c0ffa-22_1



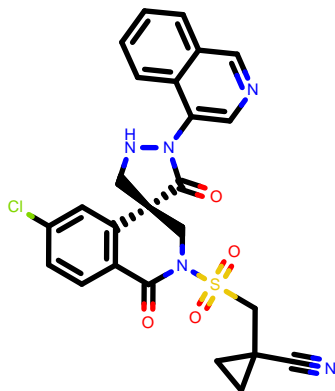
CID:	MAT-POS-853c0ffa-22_1
SMILES:	<chem>CC1(CC1)CS(=O)=O[N@@]2[C@@]3C=CC(=O)N[C@@]4(C2)CCN(C4=O)c5ccc6c5ccc6(S(=O)(=O)C1)C1</chem>
RUN:	RUN874
DDG (kcal/mol):	2.46
dDDG (kcal/mol):	0.29

MIK-ENA-5d9157e9-2_1



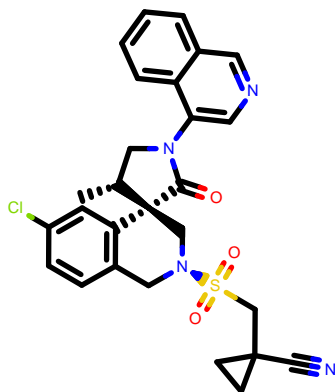
CID:	MIK-ENA-5d9157e9-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC(C@@H)(C3=O)C(N@@)C(C5=O)C(=O)C(C6)(CC6)C#N</chem>
RUN:	RUN751
DDG (kcal/mol):	2.47
dDDG (kcal/mol):	0.35

EDJ-MED-fed7ac0b-3_1



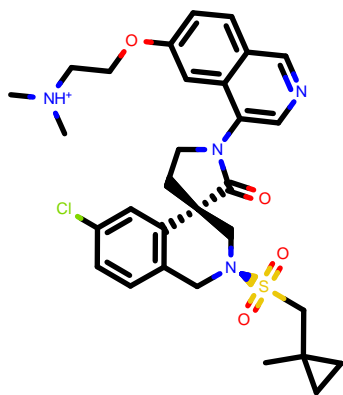
CID:	EDJ-MED-fed7ac0b-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C(C@@H)(CN3)CN(C(=O)c5c4cc(cc5)O)S(=O)(=O)C(C6)(CC6)C#N</chem>
RUN:	RUN810
DDG (kcal/mol):	2.48
dDDG (kcal/mol):	0.41

MAT-POS-50a80394-1_1



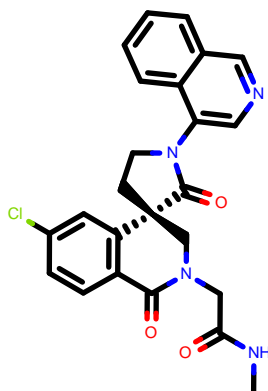
CID:	MAT-POS-50a80394-1_1
SMILES:	<chem>C[C@@H]1CN(C1=O)[C@@]2[C@@]3C=CC(=O)N[C@@]4(C2)CCN(C4=O)c5ccc6c5ccc6(S(=O)(=O)C1)C1</chem>
RUN:	RUN824
DDG (kcal/mol):	2.48
dDDG (kcal/mol):	0.38

MAT-POS-853c0ffa-19_1



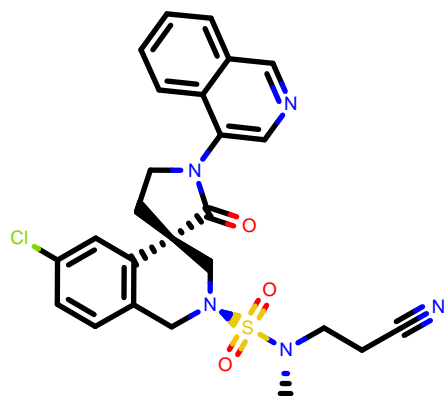
CID:	MAT-POS-853c0ffa-19_1
SMILES:	<chem>CC1(CC1)CS(=O)(=O)N@]2C3ccc(cc3)C@]4(C2)CCN(C4=O)c5ccc6c5cc(c6)OCCN(H)C]C]Cl</chem>
RUN:	RUN914
DDG (kcal/mol):	2.50
dDDG (kcal/mol):	0.47

PET-UNK-14142a25-10_1



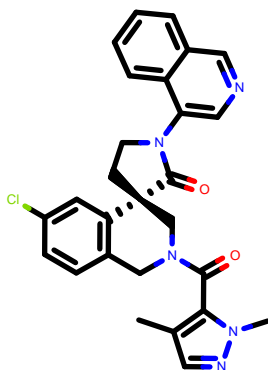
CID:	PET-UNK-14142a25-10_1
SMILES:	<chem>CNC(=O)CN1C]C@]2(CCN(C2=O)c3cnc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN592
DDG (kcal/mol):	2.52
dDDG (kcal/mol):	0.17

ALP-POS-ecbed2ba-16_3



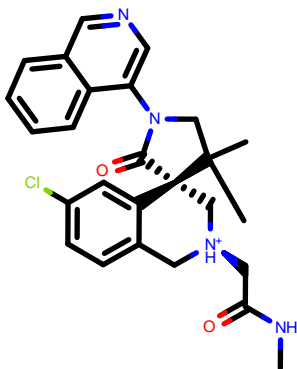
CID:	ALP-POS-ecbed2ba-16_3
SMILES:	<chem>C]N@]([CC#N)S(=O)(=O)[N@]1Cc2ccc(cc2)C@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN744
DDG (kcal/mol):	2.52
dDDG (kcal/mol):	0.59

EDJ-MED-cc48ee33-4_1



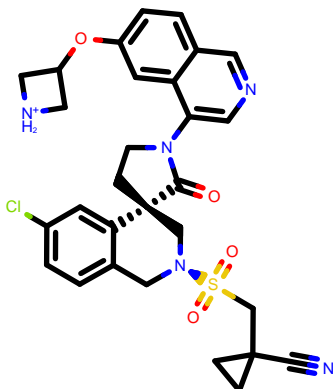
CID:	EDJ-MED-cc48ee33-4_1
SMILES:	<chem>Cc1ann(c1C(=O)N2Cc3ccc(cc3)C@]4(C2)CCN(C4=O)c5cnc6c5cccc6)Cl]C</chem>
RUN:	RUN757
DDG (kcal/mol):	2.59
dDDG (kcal/mol):	0.19

MAT-POS-50a80394-7_2



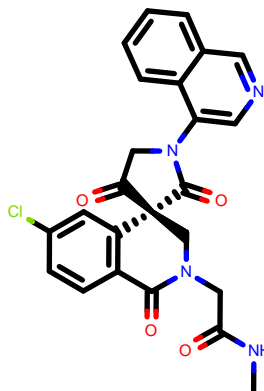
CID:	MAT-POS-50a80394-7_2
SMILES:	<chem>CC1(CN(C(=O)[C@@]1)2C[N@H+](C3c2cc(cc3)C)CC(=O)NC)c4cccc5c4cccc5C</chem>
RUN:	RUN666
DDG (kcal/mol):	2.60
dDDG (kcal/mol):	0.22

EDJ-MED-ee81482e-1_2



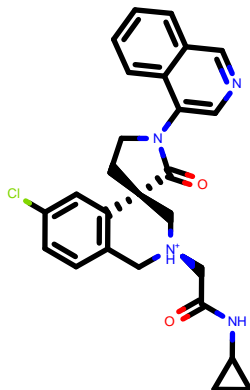
CID:	EDJ-MED-ee81482e-1_2
SMILES:	<chem>c1cc2ccc(c2c1OC3C[NH2+](C3)N4CC[C@@]5(C4=O)C(N8)C6c5ccc(c6)C(S(=O)(=O)C7)C(C7)C#N</chem>
RUN:	RUN917
DDG (kcal/mol):	2.60
dDDG (kcal/mol):	0.56

EDJ-MED-a12e3a20-2_1



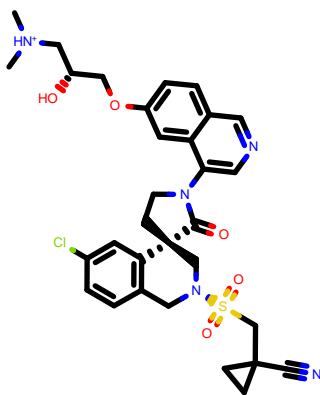
CID:	EDJ-MED-a12e3a20-2_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(c3ccc(ccc3C1=O)C)C(=O)CN(C2=O)c4cccc5c4cccc5</chem>
RUN:	RUN653
DDG (kcal/mol):	2.60
dDDG (kcal/mol):	0.15

MAT-POS-69786b79-2_2



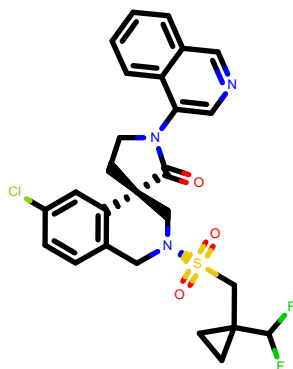
CID:	MAT-POS-69786b79-2_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)C)CC(=O)NC6CC6</chem>
RUN:	RUN649
DDG (kcal/mol):	2.61
dDDG (kcal/mol):	0.25

EDJ-MED-ee81482e-3_2



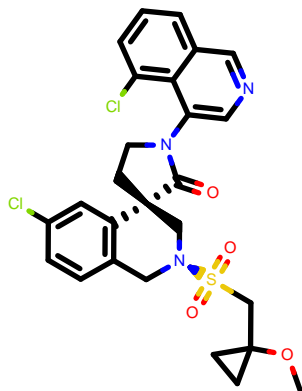
CID:	EDJ-MED-ee81482e-3_2
SMILES:	<chem>C[NH+]C[C]C[C@H](COc1ccc2mcc(c2c1)N3CC[C@]4(C3=O)CN[C@@]5C5c4cc(cc5C)S(=O)(=O)CC6(C)C#N</chem>
RUN:	RUN942
DDG (kcal/mol):	2.63
dDDG (kcal/mol):	0.49

EDJ-MED-5cd3920d-5_1



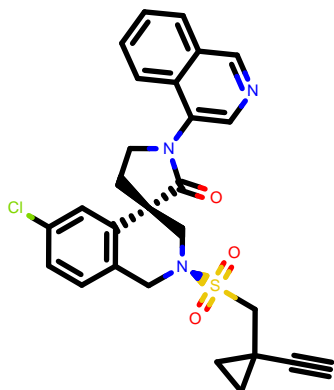
CID:	EDJ-MED-5cd3920d-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)C[N@@]5(C5c4cc(cc5C)S(=O)(=O)CC6(C)C(F)F</chem>
RUN:	RUN829
DDG (kcal/mol):	2.63
dDDG (kcal/mol):	0.42

MAT-POS-853c0ffa-7_2



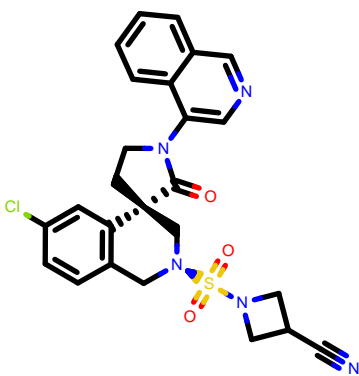
CID:	MAT-POS-853c0ffa-7_2
SMILES:	<chem>COc1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5ncc6c5c(ccc6)C)Cl</chem>
RUN:	RUN789
DDG (kcal/mol):	2.65
dDDG (kcal/mol):	0.33

PET-UNK-94036022-9_2



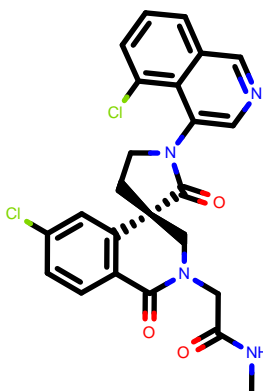
CID:	PET-UNK-94036022-9_2
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5ncc6c5c(ccc6)C)Cl</chem>
RUN:	RUN772
DDG (kcal/mol):	2.66
dDDG (kcal/mol):	0.35

ALP-POS-ecbed2ba-9_1



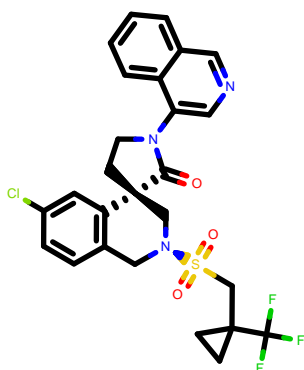
CID:	ALP-POS-ecbed2ba-9_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@H](C3=O)C[N@@]([C@H]4CC(=O)S(=O)(=O)N6CC(C6)C#N</chem>
RUN:	RUN735
DDG (kcal/mol):	2.68
dDDG (kcal/mol):	0.49

MAT-POS-853c0ffa-1_1



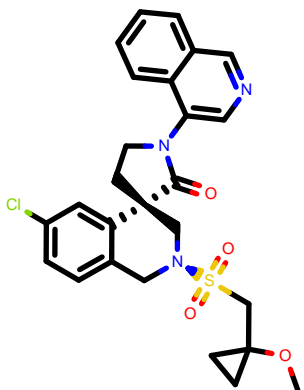
CID:	MAT-POS-853c0ffa-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(ccc4)Cl)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN636
DDG (kcal/mol):	2.71
dDDG (kcal/mol):	0.17

EDJ-MED-5cd3920d-6_1



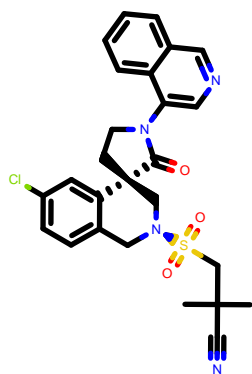
CID:	EDJ-MED-5cd3920d-6_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@H](C3=O)C[N@@]([C@H]4CC(=O)S(=O)(=O)C(F)(F)F</chem>
RUN:	RUN862
DDG (kcal/mol):	2.72
dDDG (kcal/mol):	0.39

ALP-POS-ecbed2ba-6_2



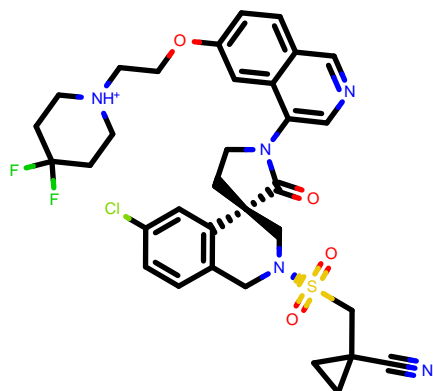
CID:	ALP-POS-ecbed2ba-6_2
SMILES:	<chem>COC1(CC1)CS(=O)(=O)[N@]2C3CC(=O)C[C@H](C2)CCN(C4=O)c5ccccc5C4C1</chem>
RUN:	RUN723
DDG (kcal/mol):	2.72
dDDG (kcal/mol):	0.42

ALP-POS-ecbed2ba-13_1



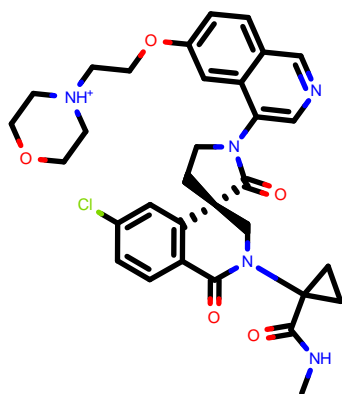
CID:	ALP-POS-ecbed2ba-13_1
SMILES:	<chem>CC(C)(CS(=O)(=O)[N@@]1[C@@]2CCCC2[C@@]3(C1)CCN(C3=O)c4cnc5c4ccc5)C1C#N</chem>
RUN:	RUN741
DDG (kcal/mol):	2.73
dDDG (kcal/mol):	0.34

EDJ-MED-468565e0-4_1



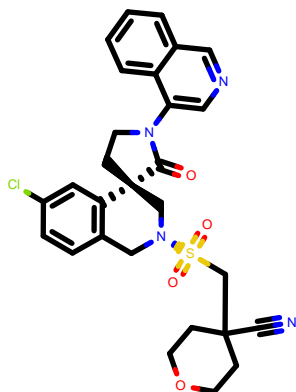
CID:	EDJ-MED-468565e0-4_1
SMILES:	<chem>c1cc2ccc2cc1OCC[NH+]3CCCC(C3)F(F)N4CC[C@@]5(C4+O)[N@@]6C8c6cc(cc8)C1S(=O)(=O)CC7C7C#N</chem>
RUN:	RUN973
DDG (kcal/mol):	2.75
dDDG (kcal/mol):	0.64

EDJ-MED-dfa1d800-2_1



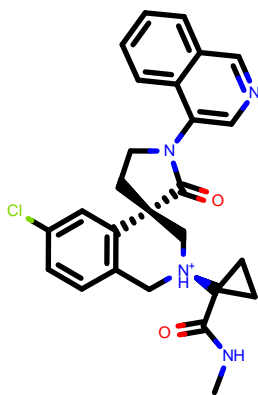
CID:	EDJ-MED-dfa1d800-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@@]3(CCN(C3=O)c4cnc5c4ccc5)OCC[NH+]6CCCCO6c7ccc(cc7C2=O)C1</chem>
RUN:	RUN948
DDG (kcal/mol):	2.78
dDDG (kcal/mol):	0.26

ALP-POS-ecbed2ba-11_1



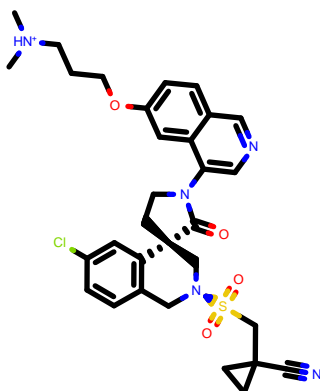
CID:	ALP-POS-ecbed2ba-11_1
SMILES:	<chem>c1ccc2(c1)ncnc2N3CC[C@@]4(C)[C@@]5(CN3)C6c5c4ccc5)C1S(=O)(=O)CC6(COCCO6)C#N</chem>
RUN:	RUN868
DDG (kcal/mol):	2.80
dDDG (kcal/mol):	0.53

ALP-POS-ecbed2ba-7_2



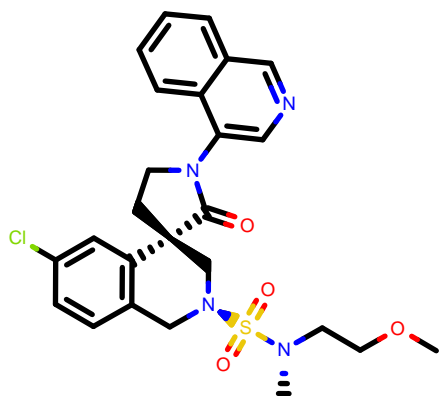
CID:	ALP-POS-ecbed2ba-7_2
SMILES:	<chem>CNC(=O)C1(CC1)[N@H+]2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5ccc6)Cl</chem>
RUN:	RUN626
DDG (kcal/mol):	2.80
dDDG (kcal/mol):	0.15

MAT-POS-40ad851a-4_2



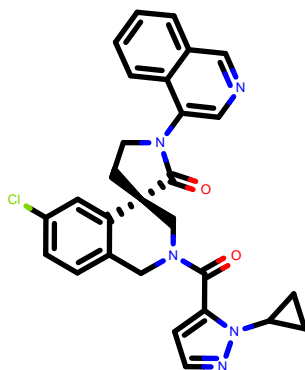
CID:	MAT-POS-40ad851a-4_2
SMILES:	<chem>C[NH+](C)CCCC1ccc2ncoc2c1N3CC[C@]4(C3=O)C[N@](C5=C4C(=O)C1S(=O)(=O)CC6(C)C6)C#N</chem>
RUN:	RUN940
DDG (kcal/mol):	2.82
dDDG (kcal/mol):	0.59

ALP-POS-ecbed2ba-21_1



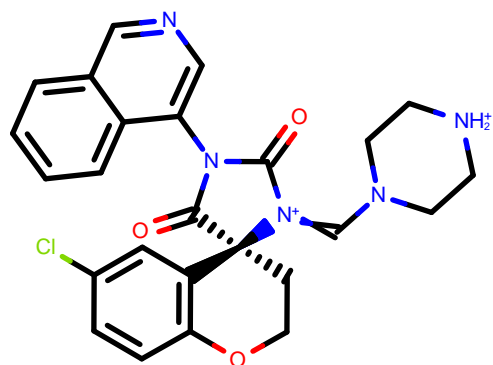
CID:	ALP-POS-ecbed2ba-21_1
SMILES:	<chem>C[N@](C)(CCOC)S(=O)(=O)[N@]1C2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4ccc5)Cl</chem>
RUN:	RUN748
DDG (kcal/mol):	2.82
dDDG (kcal/mol):	0.43

MAT-POS-be048f2c-7_1



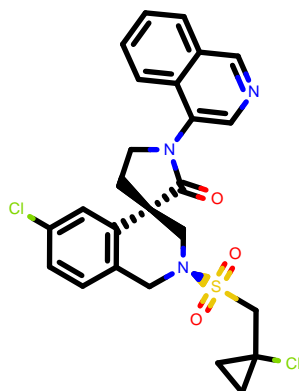
CID:	MAT-POS-be048f2c-7_1
SMILES:	<chem>c1ccc2c(c1)nc2N3CC[C@]4(C3=O)C[N](C5=C4C(=O)C1C(=O)c6cnn67CC7</chem>
RUN:	RUN813
DDG (kcal/mol):	2.82
dDDG (kcal/mol):	0.23

VLA-UCB-34f3ed0c-15_1



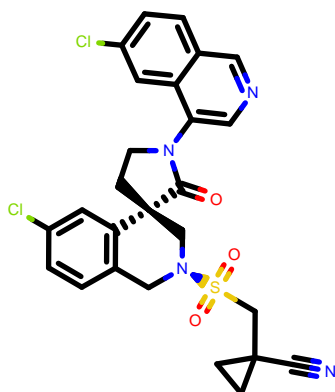
CID:	VLA-UCB-34f3ed0c-15_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@@H](C(=O)c5c4cc(cc5)C)N(C3=O)CN6CC[NH2+]CC6</chem>
RUN:	RUN675
DDG (kcal/mol):	2.83
dDDG (kcal/mol):	0.28

PET-UNK-94036022-10_1



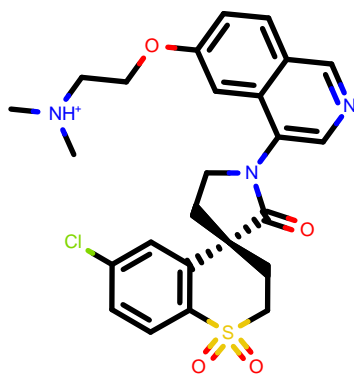
CID:	PET-UNK-94036022-10_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C[C@@H](C(=O)C)N[C@@H](C5c4cc(cc5)C)S(=O)(=O)CC6(CO6)Cl</chem>
RUN:	RUN712
DDG (kcal/mol):	2.83
dDDG (kcal/mol):	0.23

EDJ-MED-b6c6ee2b-4_1



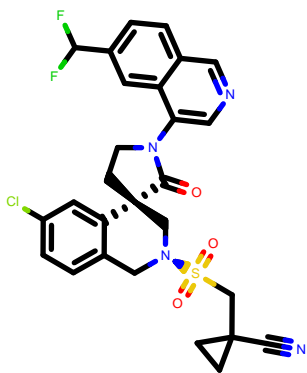
CID:	EDJ-MED-b6c6ee2b-4_1
SMILES:	<chem>c1cc2nccc(c2cc1C)N3CC[C@@H](C(=O)C)N[C@@H](C5c4cc(cc5)C)S(=O)(=O)CC6(CO6)N</chem>
RUN:	RUN816
DDG (kcal/mol):	2.83
dDDG (kcal/mol):	0.44

EDJ-MED-d4864bdc-4_1



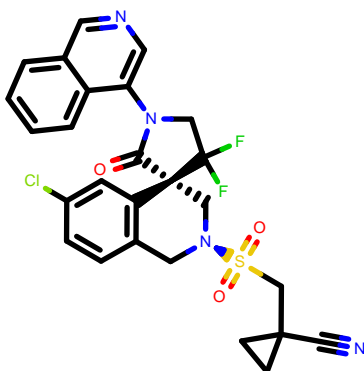
CID:	EDJ-MED-d4864bdc-4_1
SMILES:	<chem>C[NH+]C)CCOC1ccc2nccc(c2c1)N3CC[C@@H](C(=O)C)S(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN716
DDG (kcal/mol):	2.84
dDDG (kcal/mol):	0.28

EDJ-MED-5cd3920d-2_1



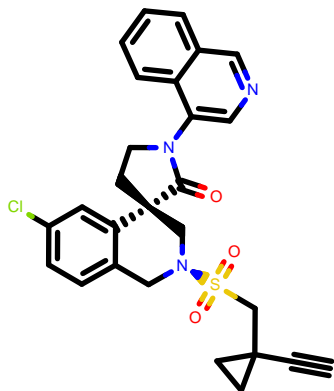
CID:	EDJ-MED-5cd3920d-2_1
SMILES:	<chem>c1cc2ccc2cc1C(F)F)N3CC[C@@H](C3=O)C(N8@)C6c4ccc5C(S(=O)(=O)CC6)C#N</chem>
RUN:	RUN883
DDG (kcal/mol):	2.90
dDDG (kcal/mol):	0.42

EDJ-MED-7e491f08-1_1



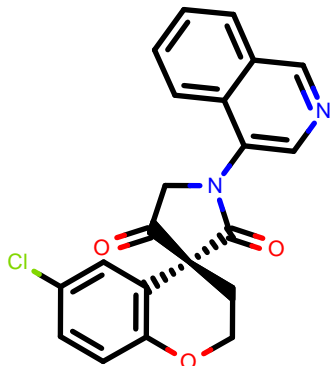
CID:	EDJ-MED-7e491f08-1_1
SMILES:	<chem>c1ccc2c(c1)ccc2N3CC[C@@H](C3=O)C(N8@)C6c4ccc5C(S(=O)(=O)CC6)C#N)F</chem>
RUN:	RUN860
DDG (kcal/mol):	2.94
dDDG (kcal/mol):	0.32

PET-UNK-94036022-2_2



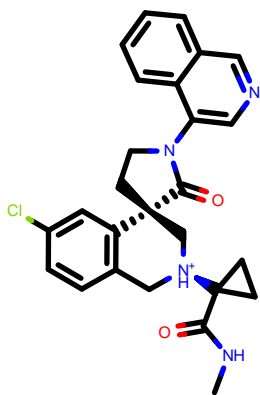
CID:	PET-UNK-94036022-2_2
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3)[C@@H](C2)CCN(C4=O)c5ccc6c5ccc6)Cl</chem>
RUN:	RUN770
DDG (kcal/mol):	2.97
dDDG (kcal/mol):	0.32

DAR-DIA-0f7b7cd9-9_1



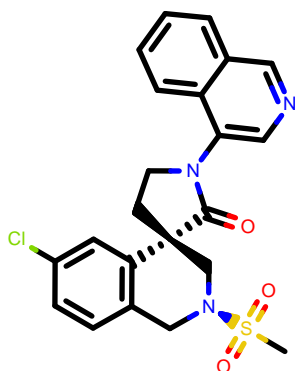
CID:	DAR-DIA-0f7b7cd9-9_1
SMILES:	<chem>c1ccc2c(c1)ccc2N3CC(=O)[C@@H](C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN517
DDG (kcal/mol):	2.98
dDDG (kcal/mol):	0.12

MAT-POS-69786b79-1_2



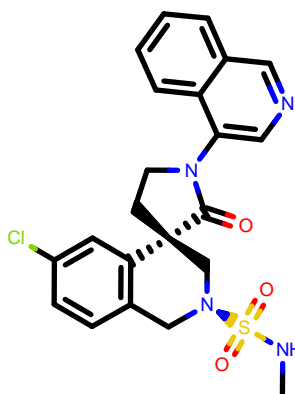
CID:	MAT-POS-69786b79-1_2
SMILES:	<chem>CNC(=O)C1(CC1)[N@H+]2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5ccc6c5ccc6)Cl</chem>
RUN:	RUN647
DDG (kcal/mol):	3.03
dDDG (kcal/mol):	0.21

EDJ-MED-7587a9ee-3_1



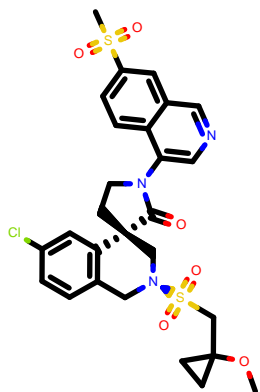
CID:	EDJ-MED-7587a9ee-3_1
SMILES:	<chem>CS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4ccc5c4ccc5)Cl</chem>
RUN:	RUN537
DDG (kcal/mol):	3.05
dDDG (kcal/mol):	0.21

LUO-POS-ed2cfb03-2_1



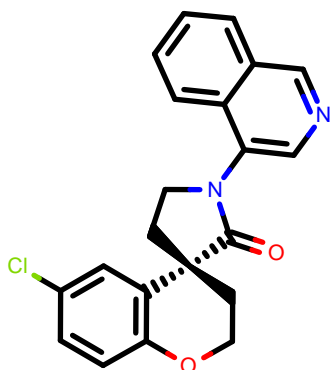
CID:	LUO-POS-ed2cfb03-2_1
SMILES:	<chem>CNS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4ccc5c4ccc5)Cl</chem>
RUN:	RUN583
DDG (kcal/mol):	3.07
dDDG (kcal/mol):	0.28

MAT-POS-853c0ffa-16_1



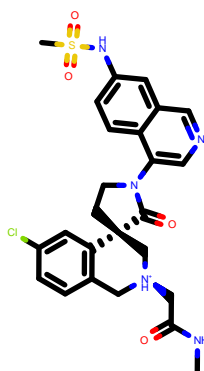
CID:	MAT-POS-853c0ffa-16_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)[N@@]2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5ccc6c5ccc6)S(=O)(=O)Cl</chem>
RUN:	RUN887
DDG (kcal/mol):	3.08
dDDG (kcal/mol):	0.33

EDJ-MED-159244ea-1_1



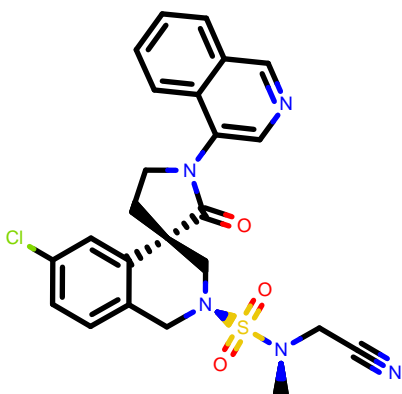
CID:	EDJ-MED-159244ea-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN495
DDG (kcal/mol):	3.08
dDDG (kcal/mol):	0.14

MAT-POS-b4d6b7fc-7_2



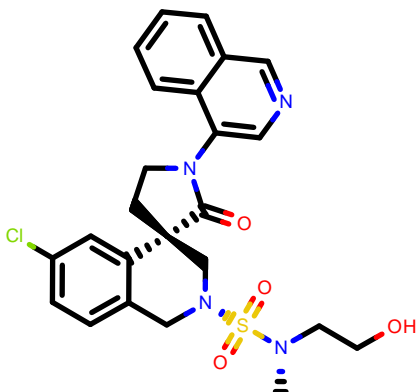
CID:	MAT-POS-b4d6b7fc-7_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2)[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)Cl</chem>
RUN:	RUN809
DDG (kcal/mol):	3.09
dDDG (kcal/mol):	0.26

ALP-POS-ecbed2ba-17_3



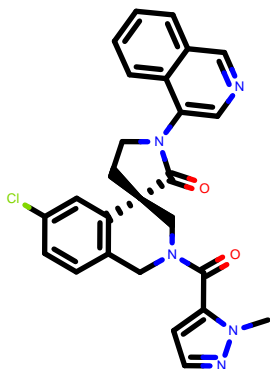
CID:	ALP-POS-ecbed2ba-17_3
SMILES:	<chem>C[N@@]([C]C#N)S(=O)(=O)[N@]1Cc2ccc(cc2)[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(c5)Cl</chem>
RUN:	RUN694
DDG (kcal/mol):	3.09
dDDG (kcal/mol):	0.49

ALP-POS-ecbed2ba-19_3



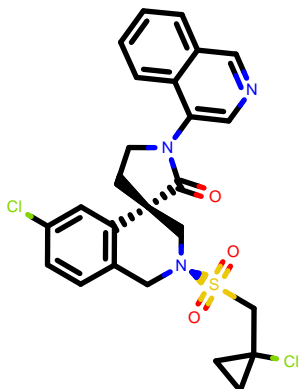
CID:	ALP-POS-ecbed2ba-19_3
SMILES:	<chem>C[N@@]([C]CO)S(=O)(=O)[N@]1Cc2ccc(cc2)[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(c5)Cl</chem>
RUN:	RUN708
DDG (kcal/mol):	3.10
dDDG (kcal/mol):	0.41

EDJ-MED-cc48ee33-3_1



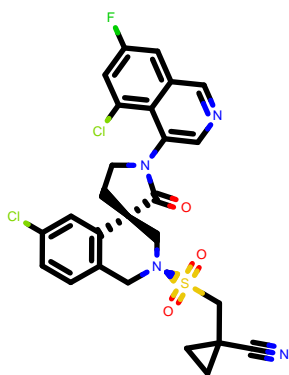
CID:	EDJ-MED-cc48ee33-3_1
SMILES:	<chem>Cn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl</chem>
RUN:	RUN698
DDG (kcal/mol):	3.14
dDDG (kcal/mol):	0.24

PET-UNK-94036022-3_1



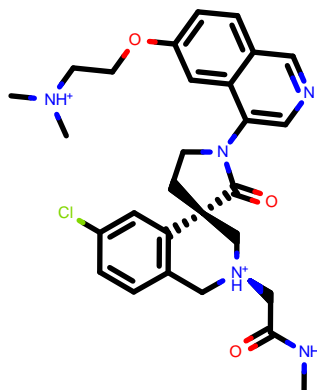
CID:	PET-UNK-94036022-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@]5(Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CO6)Cl</chem>
RUN:	RUN713
DDG (kcal/mol):	3.15
dDDG (kcal/mol):	0.36

MAT-POS-853c0ffa-6_2



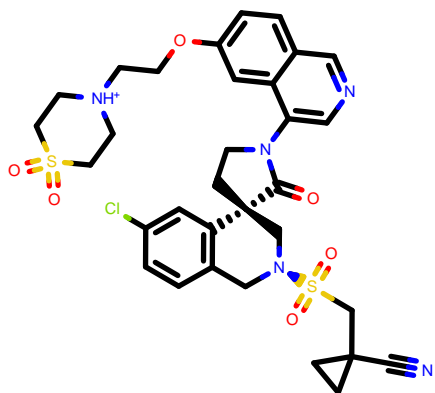
CID:	MAT-POS-853c0ffa-6_2
SMILES:	<chem>c1cc2c(c1)C[C@@]3(C)CCN(C3=O)c4ncc5c4(cc(c5)F)C1[N@@]2(C)Si(O)=O)CC6(CO6)C#N</chem>
RUN:	RUN841
DDG (kcal/mol):	3.18
dDDG (kcal/mol):	0.41

EDJ-MED-b6c6ee2b-1_2



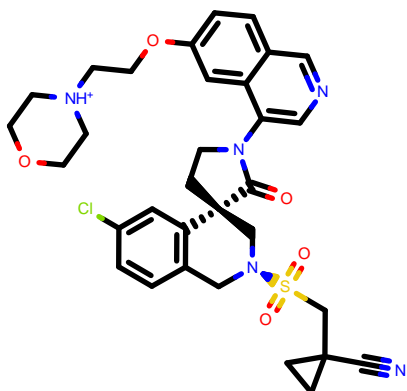
CID:	EDJ-MED-b6c6ee2b-1_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)CCN(C3=O)c4ncc5c4cc(cc5)OCC[NH+](C)C)Cl</chem>
RUN:	RUN882
DDG (kcal/mol):	3.20
dDDG (kcal/mol):	0.35

EDJ-MED-468565e0-3_1



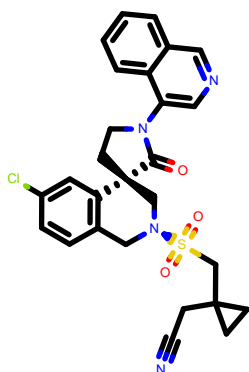
CID:	EDJ-MED-468565e0-3_1
SMILES:	<chem>c1cc2ccc(cc1OCN3CCS(=O)(=O)CC3)N4CC[C@@]5(C4=O)C(N@@)C6c6cc(cc6)C1S(=O)(=O)CC7(C)C#N</chem>
RUN:	RUN961
DDG (kcal/mol):	3.21
dDDG (kcal/mol):	0.64

EDJ-MED-468565e0-2_1



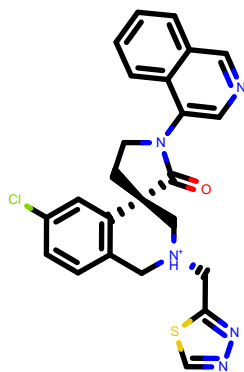
CID:	EDJ-MED-468565e0-2_1
SMILES:	<chem>c1cc2ccc(cc1OC(NH)3CCOCC3)N4CC[C@@]5(C4=O)C(N@@)C6c6cc(cc6)C1S(=O)(=O)CC7(C)C#N</chem>
RUN:	RUN957
DDG (kcal/mol):	3.22
dDDG (kcal/mol):	0.46

ALP-POS-ecbed2ba-22_1



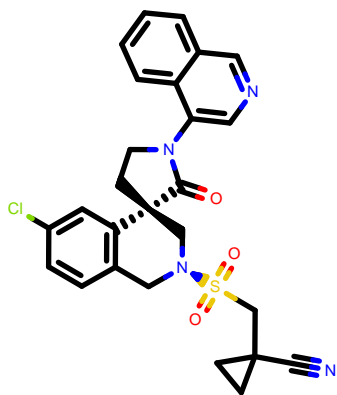
CID:	ALP-POS-ecbed2ba-22_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C(N@@)C5c4cc(cc5)C1S(=O)(=O)CC6(C)C#N</chem>
RUN:	RUN805
DDG (kcal/mol):	3.23
dDDG (kcal/mol):	0.39

PET-UNK-7e9559de-4_1



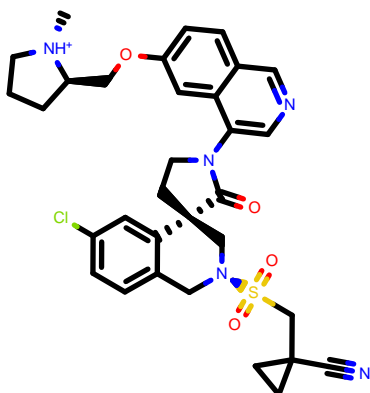
CID:	PET-UNK-7e9559de-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C(N@@)C5c4cc(cc5)C1C6nncs6</chem>
RUN:	RUN601
DDG (kcal/mol):	3.24
dDDG (kcal/mol):	0.20

MIK-ENA-5d9157e9-1_2



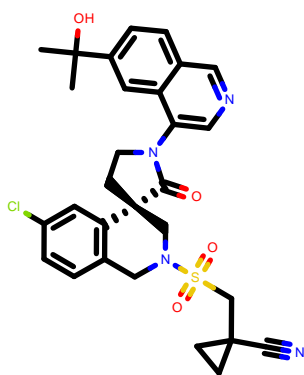
CID:	MIK-ENA-5d9157e9-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@]5Cc5c4cc(c5)ClS(=O)(=O)CC6(Cc6)C#N</chem>
RUN:	RUN746
DDG (kcal/mol):	3.25
dDDG (kcal/mol):	0.40

MAT-POS-40ad851a-1_2



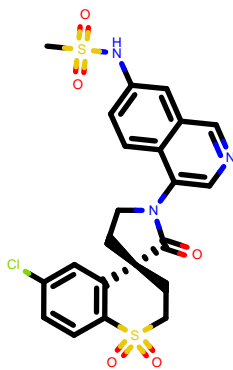
CID:	MAT-POS-40ad851a-1_2
SMILES:	<chem>C[N@@H]1CCC[C@H]1COc2ccc3ncc(c3c2)N4CC[C@@]5(C4=O)C[N@@]6Cc6c5cc(c6)ClS(=O)(=O)CC7(Cc7)C#N</chem>
RUN:	RUN967
DDG (kcal/mol):	3.26
dDDG (kcal/mol):	0.54

MAT-POS-853c0ffa-11_2



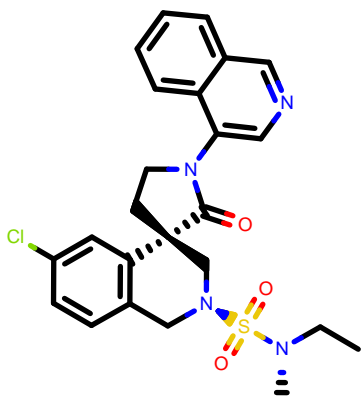
CID:	MAT-POS-853c0ffa-11_2
SMILES:	<chem>CC(C)(c1ccc2ncc(c2c1)N3CC[C@@]4(C3=O)C[N@@]5Cc5c4cc(c5)ClS(=O)(=O)CC6(Cc6)C#N)O</chem>
RUN:	RUN900
DDG (kcal/mol):	3.27
dDDG (kcal/mol):	0.54

EDJ-MED-94fddcec-7_1



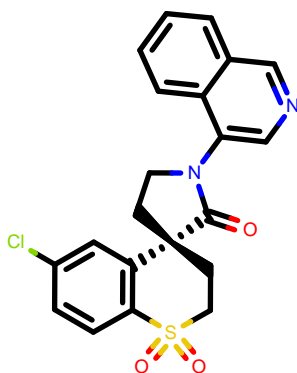
CID:	EDJ-MED-94fddcec-7_1
SMILES:	<chem>CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(c5)Cl</chem>
RUN:	RUN637
DDG (kcal/mol):	3.27
dDDG (kcal/mol):	0.21

ALP-POS-ecbed2ba-18_2



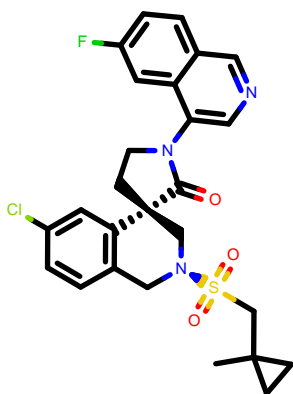
CID:	ALP-POS-ecbed2ba-18_2
SMILES:	<chem>CC(N@)C(S(=O)(=O)N@@)1Cc2ccc(cc2[C@@]3(C1)CCN(C3=O)c4ncc5c4ccc5)Cl</chem>
RUN:	RUN639
DDG (kcal/mol):	3.36
dDDG (kcal/mol):	0.36

EDJ-MED-94fddcec-4_1



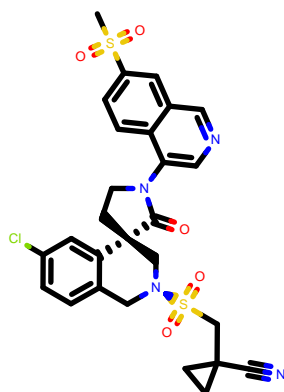
CID:	EDJ-MED-94fddcec-4_1
SMILES:	<chem>c1ccc2c(c1)ncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(c5)Cl</chem>
RUN:	RUN528
DDG (kcal/mol):	3.37
dDDG (kcal/mol):	0.12

MAT-POS-853c0ffa-21_2



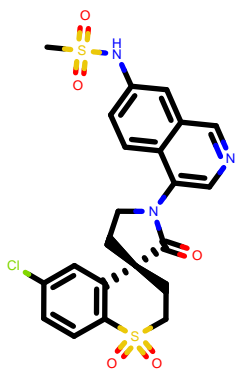
CID:	MAT-POS-853c0ffa-21_2
SMILES:	<chem>CC1(CC1)CS(=O)(=O)N@]2Cc3ccc(cc3[C@@]4(C2)CCN(C4=O)c5ncc6c5cc(cc6)F)Cl</chem>
RUN:	RUN729
DDG (kcal/mol):	3.37
dDDG (kcal/mol):	0.42

MAT-POS-853c0ffa-15_1



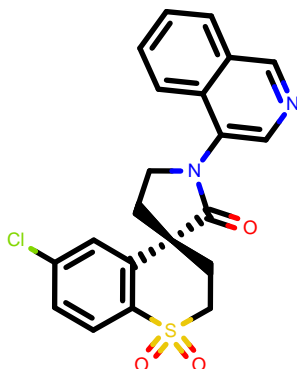
CID:	MAT-POS-853c0ffa-15_1
SMILES:	<chem>CS(=O)(=O)c1ccc2c(c1)ncc2N3CC[C@@]4(C3=O)C[N@@]5C6c4ccc5)O(S(=O)(=O)CC6)C#N</chem>
RUN:	RUN888
DDG (kcal/mol):	3.37
dDDG (kcal/mol):	0.51

EDJ-MED-edc5c6cb-1_1



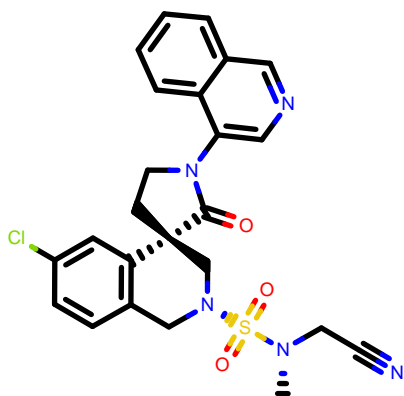
CID:	EDJ-MED-edc5c6cb-1_1
SMILES:	<chem>CS(=O)(=O)Nc1ccc2c(c1)ncnc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN663
DDG (kcal/mol):	3.39
dDDG (kcal/mol):	0.19

ALP-POS-41e2080f-1_1



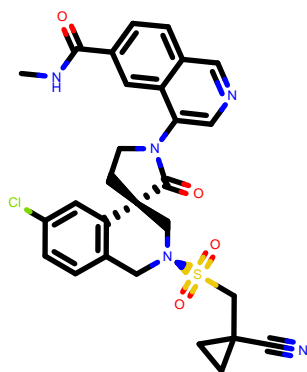
CID:	ALP-POS-41e2080f-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN533
DDG (kcal/mol):	3.39
dDDG (kcal/mol):	0.18

ALP-POS-ecbed2ba-17_4



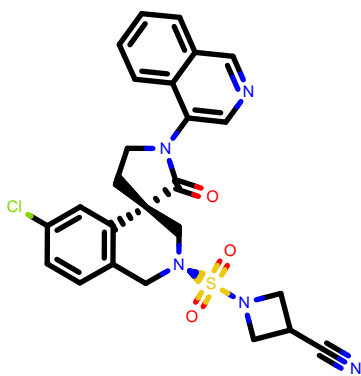
CID:	ALP-POS-ecbed2ba-17_4
SMILES:	<chem>C[N@](CC#N)S(=O)(=O)[N@]1C2ccccc2[C@@]3(C1)CCN(C3=O)c4ncnc5c4cccc5)Cl</chem>
RUN:	RUN689
DDG (kcal/mol):	3.41
dDDG (kcal/mol):	0.53

MAT-POS-38eb6498-2_1



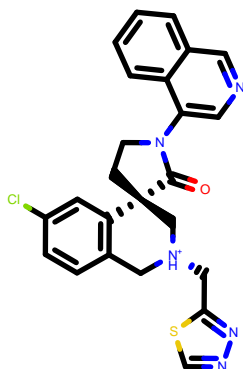
CID:	MAT-POS-38eb6498-2_1
SMILES:	<chem>CNC(=O)c1ccc2ncnc(c2c1)N3CC[C@@]4(C3=O)C[N@]5(Cc6c4ccc(cc6)S(=O)(=O)OC6CCCC6)C#N</chem>
RUN:	RUN897
DDG (kcal/mol):	3.41
dDDG (kcal/mol):	0.37

ALP-POS-ecbed2ba-9_2



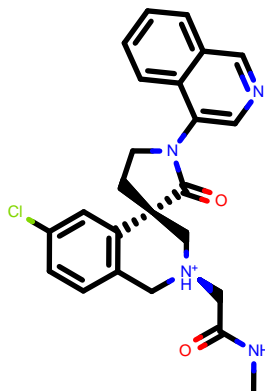
CID:	ALP-POS-ecbed2ba-9_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@@H](C3=O)C[N@@](Cc5c4cc(cc5)C)S(=O)(=O)N6CC(C6)C#N</chem>
RUN:	RUN726
DDG (kcal/mol):	3.45
dDDG (kcal/mol):	0.52

MAT-POS-96396902-1_1



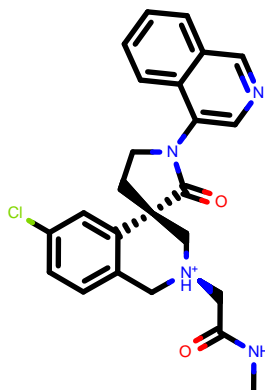
CID:	MAT-POS-96396902-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@@H](C3=O)C[N@@H](Cc5c4cc(cc5)C)C6nncs6</chem>
RUN:	RUN613
DDG (kcal/mol):	3.50
dDDG (kcal/mol):	0.19

EDJ-MED-8bb691af-4_2



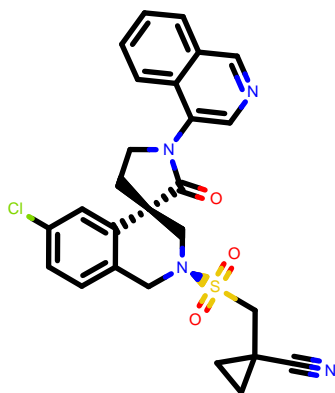
CID:	EDJ-MED-8bb691af-4_2
SMILES:	<chem>CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN556
DDG (kcal/mol):	3.51
dDDG (kcal/mol):	0.23

LUO-POS-868e8996-11_2



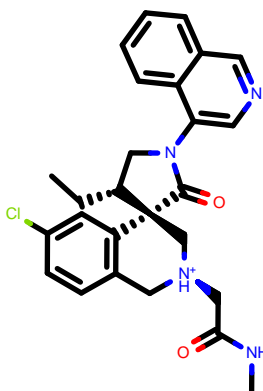
CID:	LUO-POS-868e8996-11_2
SMILES:	<chem>CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN571
DDG (kcal/mol):	3.52
dDDG (kcal/mol):	0.20

MIK-ENA-5d9157e9-1_1



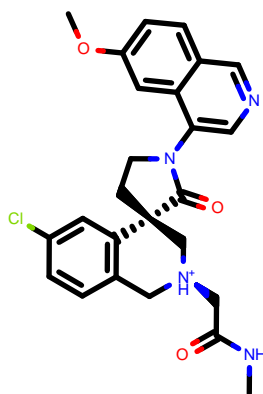
CID:	MIK-ENA-5d9157e9-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@H](C3=O)C[N@@]([C@H](C5=O)C5)S(=O)(=O)CC6(C6)C#N</chem>
RUN:	RUN749
DDG (kcal/mol):	3.52
dDDG (kcal/mol):	0.52

MAT-POS-50a80394-5_3



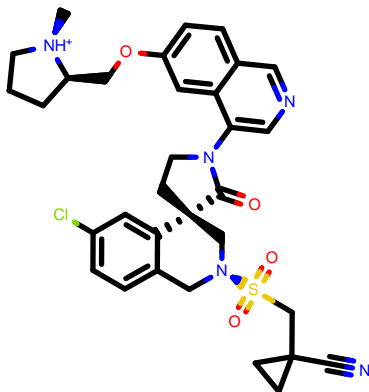
CID:	MAT-POS-50a80394-5_3
SMILES:	<chem>CC[C@@H]1CN(C(=O)[C@@]12C[N@H+]([C@H]2C3=O)C3)CC(=O)NC)c4ccc5c4ccc5</chem>
RUN:	RUN660
DDG (kcal/mol):	3.54
dDDG (kcal/mol):	0.29

EDJ-MED-b6c6ee2b-2_2



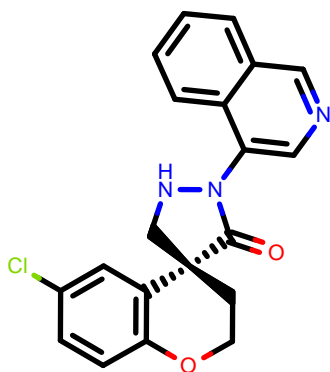
CID:	EDJ-MED-b6c6ee2b-2_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2)[C@@]2[C@H]3(C1)CCN(C3=O)c4ccc5c4cc(OC)c1</chem>
RUN:	RUN658
DDG (kcal/mol):	3.56
dDDG (kcal/mol):	0.25

MAT-POS-40ad851a-1_1



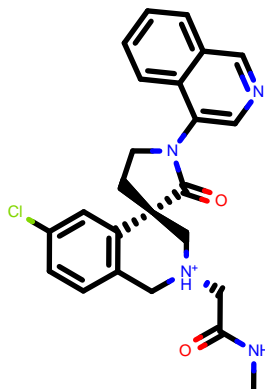
CID:	MAT-POS-40ad851a-1_1
SMILES:	<chem>C#N[C@@H]1CC[C@H]([C@@H]1)COc2ccc3nccc(c32)N4CC[C@H]5(C4=O)C[N@@]([C@H]5C6=O)C6)S(=O)(=O)CC7(C7)C#N</chem>
RUN:	RUN951
DDG (kcal/mol):	3.56
dDDG (kcal/mol):	0.52

BEN-BAS-c2bc0d80-3_1



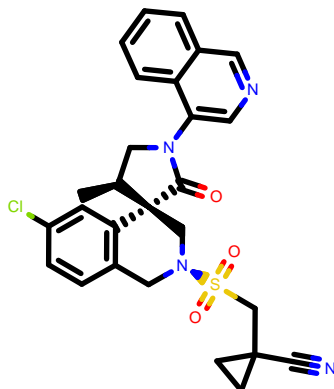
CID:	BEN-BAS-c2bc0d80-3_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)CN3</chem>
RUN:	RUN497
DDG (kcal/mol):	3.56
dDDG (kcal/mol):	0.15

MAT-POS-c7726e07-6_1



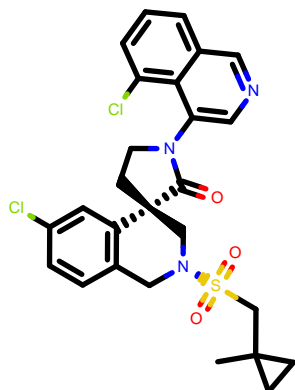
CID:	MAT-POS-c7726e07-6_1
SMILES:	<chem>CNC(=O)[N+]([H])1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4ccc5)Cl</chem>
RUN:	RUN565
DDG (kcal/mol):	3.57
dDDG (kcal/mol):	0.25

MAT-POS-50a80394-1_2



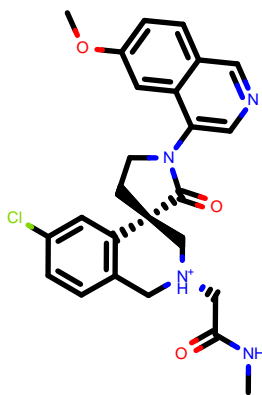
CID:	MAT-POS-50a80394-1_2
SMILES:	<chem>C[C@H]1CN(C1=O)[C@@]2(CN1)C(=O)N3C(=O)[C@@]4(C2)CCN(C4=O)c5cnc6c5ccc6</chem>
RUN:	RUN826
DDG (kcal/mol):	3.58
dDDG (kcal/mol):	0.48

MAT-POS-853c0ffa-17_2



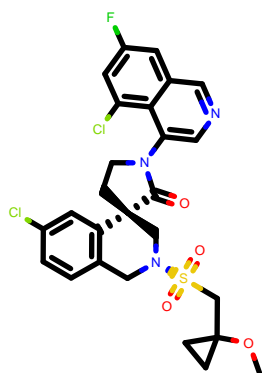
CID:	MAT-POS-853c0ffa-17_2
SMILES:	<chem>CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5c(ccc6)Cl)Cl</chem>
RUN:	RUN724
DDG (kcal/mol):	3.59
dDDG (kcal/mol):	0.30

EDJ-MED-b6c6ee2b-2_1



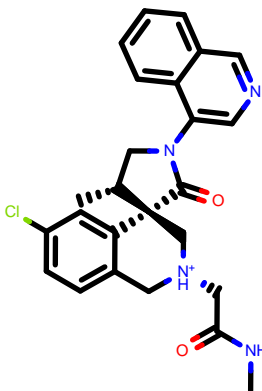
CID:	EDJ-MED-b6c6ee2b-2_1
SMILES:	<chem>CNC(=O)C[N+]([O-])C1Cc2ccc(cc2)C[C@]3(C1)CCN(C3=O)c4ccc5c4cc(=O)c5)OC1</chem>
RUN:	RUN665
DDG (kcal/mol):	3.59
dDDG (kcal/mol):	0.27

MAT-POS-853c0ffa-8_1



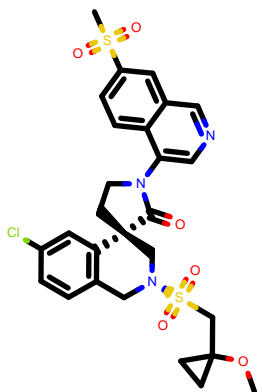
CID:	MAT-POS-853c0ffa-8_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)[N+]([O-])C2Cc3ccc(cc3)C[C@]4(C2)CCN(C4=O)c5ccc6c5cc(=O)c6)F)Cl</chem>
RUN:	RUN844
DDG (kcal/mol):	3.61
dDDG (kcal/mol):	0.32

MAT-POS-50a80394-4_1



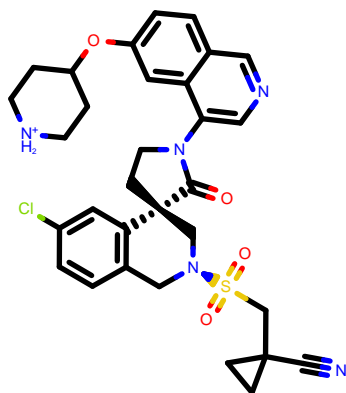
CID:	MAT-POS-50a80394-4_1
SMILES:	<chem>C[C@@H]1CN(C(=O)[C@@]12C[N+]([O-])C3Cc2ccc(cc3)C)CC(=O)NC)c4ccc5c4ccc5</chem>
RUN:	RUN608
DDG (kcal/mol):	3.62
dDDG (kcal/mol):	0.24

MAT-POS-853c0ffa-16_2



CID:	MAT-POS-853c0ffa-16_2
SMILES:	<chem>COC1(CC1)CS(=O)(=O)[N+]([O-])C2Cc3ccc(cc3)C[C@]4(C2)CCN(C4=O)c5ccc6c5ccc(=O)c6)S(=O)(=O)Cl</chem>
RUN:	RUN894
DDG (kcal/mol):	3.63
dDDG (kcal/mol):	0.48

EDJ-MED-ee81482e-4_1



CID: EDJ-MED-ee81482e-4_1

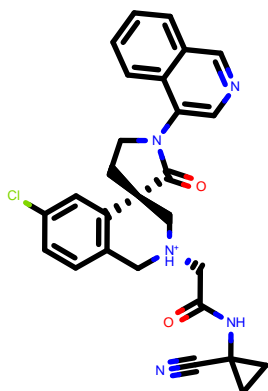
SMILES: c1cc2mcc(c2cc1OC3CQ[NH2+])C3)N4CC[C@@]5(C4=O)C[N@@]6C665cc(c6)C1S(=O)=O)CC7(C)C7#N

RUN: RUN934

DDG (kcal/mol): 3.67

dDDG (kcal/mol): 0.41

MAT-POS-69786b79-4_1



CID: MAT-POS-69786b79-4_1

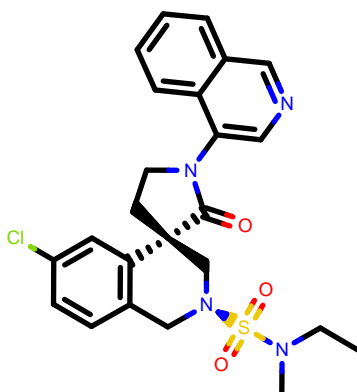
SMILES: c1ccc2c(c1)ncnc2N3CC[C@@]4(C3=O)C[N@@]5H+][C5c4cc(cc5)Cl)CC(=O)NC6(C)C6#N

RUN: RUN755

DDG (kcal/mol): 3.68

dDDG (kcal/mol): 0.33

ALP-POS-ecbed2ba-18_1



CID: ALP-POS-ecbed2ba-18_1

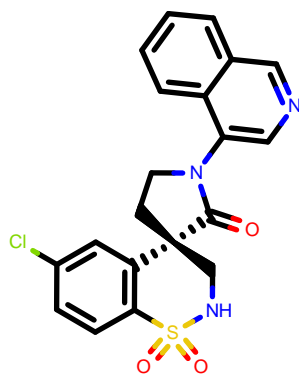
SMILES: CC[N@@]5(C)S(=O)(=O)[N@@]6[C@@]1C2ccc(cc2[C@@]3(C1)CCN(C3=O)c4ncc5c4ccc5)Cl

RUN: RUN638

DDG (kcal/mol): 3.68

dDDG (kcal/mol): 0.37

EDJ-MED-f9b78f78-4_1



CID: EDJ-MED-f9b78f78-4_1

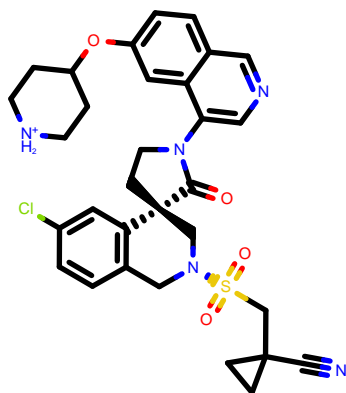
SMILES: c1ccc2c(c1)ncnc2N3CC[C@@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl

RUN: RUN539

DDG (kcal/mol): 3.69

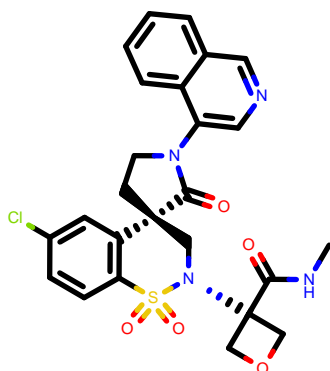
dDDG (kcal/mol): 0.15

EDJ-MED-ee81482e-4_2



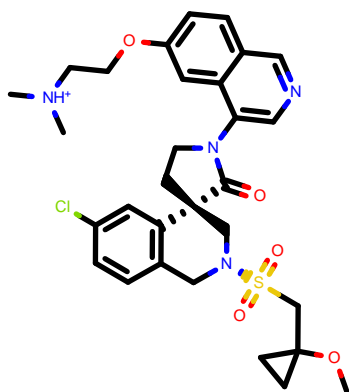
CID:	EDJ-MED-ee81482e-4_2
SMILES:	<chem>c1c2nccc2cc1OC3CC[NH2+]CC3N4CC[C@]5[C@@H](C4=O)C[N@]6Cc6fcoc6)C[S+](=O)(=O)CC7(C)C#N</chem>
RUN:	RUN919
DDG (kcal/mol):	3.70
dDDG (kcal/mol):	0.60

EDJ-MED-98c0a822-2_2



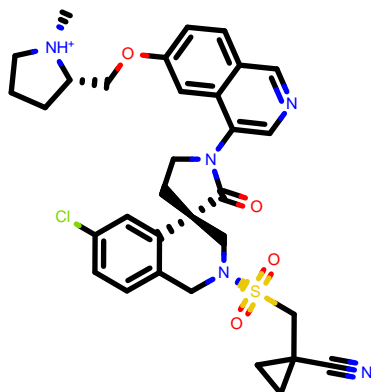
CID:	EDJ-MED-98c0a822-2_2
SMILES:	<chem>CNC(=O)C1(COC1)[N@]2C[C@]3(CCN(C3=O)c4nccc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl</chem>
RUN:	RUN821
DDG (kcal/mol):	3.72
dDDG (kcal/mol):	0.24

MAT-POS-853c0ffa-10_2



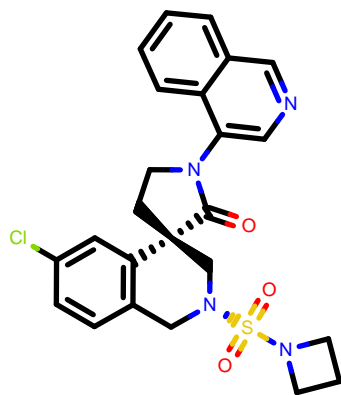
CID:	MAT-POS-853c0ffa-10_2
SMILES:	<chem>C[NH+]1CCOC1ccc2nccc2c21N3CC[C@]4(C3=O)C[N@]5Cc5fcoc5)C[S+](=O)(=O)CC6(C)C#N</chem>
RUN:	RUN925
DDG (kcal/mol):	3.72
dDDG (kcal/mol):	0.53

MAT-POS-40ad851a-1_8



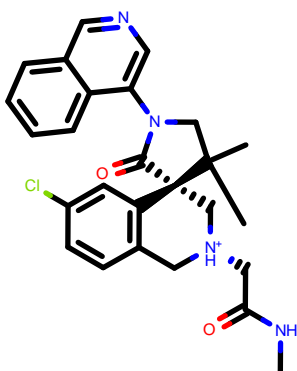
CID:	MAT-POS-40ad851a-1_8
SMILES:	<chem>C[NH+]1CCC[C@H]1COC2ccc3nccc3c21N4CC[C@]5[C@@H](C4=O)C[N@]6Cc6fcoc6)C[S+](=O)(=O)CC7(C)C#N</chem>
RUN:	RUN956
DDG (kcal/mol):	3.73
dDDG (kcal/mol):	0.59

ALP-POS-ecbed2ba-20_1



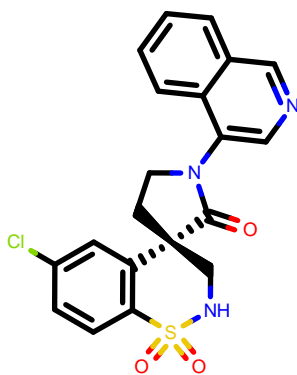
CID:	ALP-POS-ecbed2ba-20_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@@H](C3=O)C[N@@]1[Cc5c4cc(cc5)Cl]S(=O)(=O)N6CC6</chem>
RUN:	RUN645
DDG (kcal/mol):	3.74
dDDG (kcal/mol):	0.47

MAT-POS-50a80394-7_1



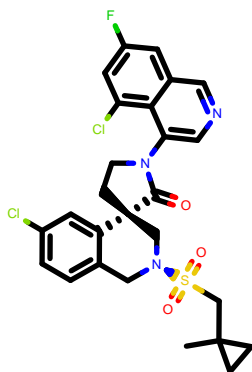
CID:	MAT-POS-50a80394-7_1
SMILES:	<chem>CC1(CN(C(=O)[C@@]12C[N@@H+]1[Cc3c2cc(cc3)Cl)CC(=O)NC)C4cnc5c4cccc5)C</chem>
RUN:	RUN656
DDG (kcal/mol):	3.74
dDDG (kcal/mol):	0.25

ALP-POS-4483ae88-1_1



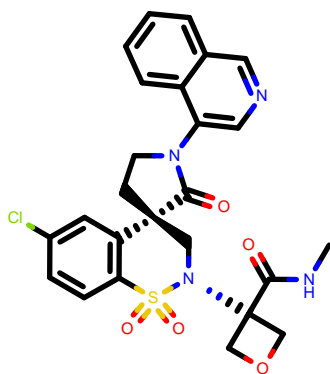
CID:	ALP-POS-4483ae88-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN538
DDG (kcal/mol):	3.75
dDDG (kcal/mol):	0.15

MAT-POS-853c0ffa-18_2



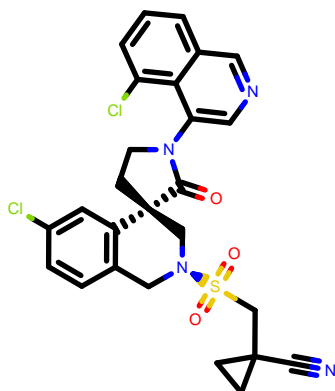
CID:	MAT-POS-853c0ffa-18_2
SMILES:	<chem>CC1(CC1)CS(=O)(=O)[N@]2C3ccc(cc3[C@@]4(C2)CCN(C4=O)c5cnc6c5c(cc6)F)Cl</chem>
RUN:	RUN793
DDG (kcal/mol):	3.76
dDDG (kcal/mol):	0.31

EDJ-MED-98c0a822-2_1



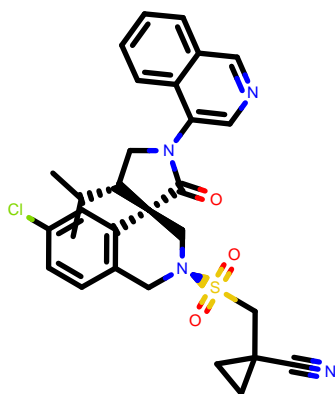
CID:	EDJ-MED-98c0a822-2_1
SMILES:	<chem>CNC(=O)C1(COC1)N@@@2C[C@@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl</chem>
RUN:	RUN820
DDG (kcal/mol):	3.77
dDDG (kcal/mol):	0.22

MAT-POS-1d5ab790-1_2



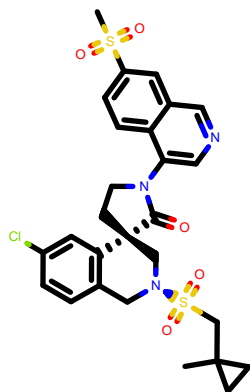
CID:	MAT-POS-1d5ab790-1_2
SMILES:	<chem>c1cc2nccc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@@]5(Cc5c4cc(c5)Cl)S(=O)(=O)CC6(Cc6)C#N</chem>
RUN:	RUN808
DDG (kcal/mol):	3.77
dDDG (kcal/mol):	0.38

MAT-POS-50a80394-3_1



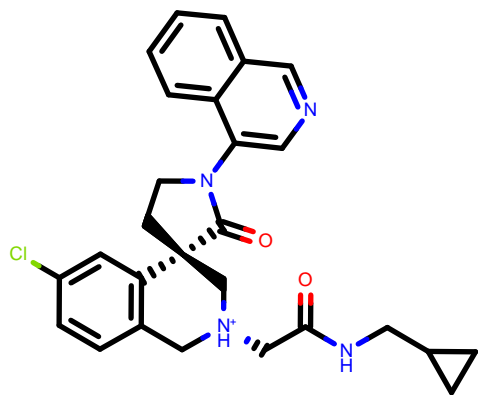
CID:	MAT-POS-50a80394-3_1
SMILES:	<chem>CC(C)[C@@H]1CN(C1=O)[C@@]2(CN@@@3)C3=O)C[N@@]4(Cc4c3cc(c4)S(=O)(=O)CC5(Cc5)C#N)C5=O</chem>
RUN:	RUN872
DDG (kcal/mol):	3.77
dDDG (kcal/mol):	0.41

MAT-POS-853c0ffa-22_2



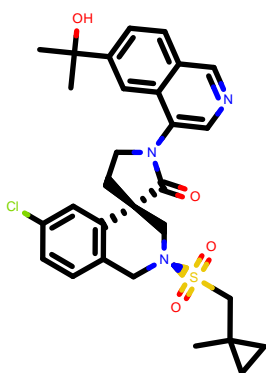
CID:	MAT-POS-853c0ffa-22_2
SMILES:	<chem>CC1(Cc1(CS1=O)=O)N@@2C3c4cc(c3)C[C@@]4(C2)CCN(C4=O)c5cncc6c5ccc6(S1=O)=O)Cl</chem>
RUN:	RUN876
DDG (kcal/mol):	3.80
dDDG (kcal/mol):	0.34

ALP-POS-ecbed2ba-12_1



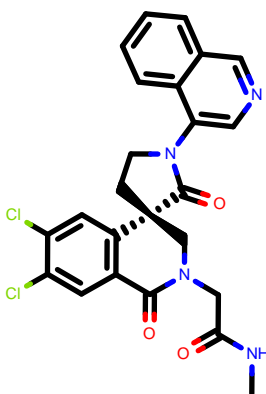
CID:	ALP-POS-ecbed2ba-12_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@]4(C3=O)CN@@H](C=C4c5cc(cc5)Cl)CC(=O)NCC6CC6</chem>
RUN:	RUN691
DDG (kcal/mol):	3.81
dDDG (kcal/mol):	0.30

MAT-POS-853c0ffa-20_2



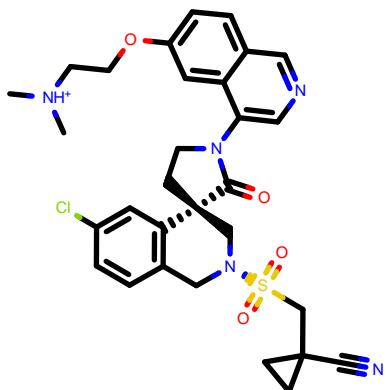
CID:	MAT-POS-853c0ffa-20_2
SMILES:	<chem>CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)OCN(C4=O)c5cnc6c5cc(cc6)C)(C)O)Cl</chem>
RUN:	RUN879
DDG (kcal/mol):	3.82
dDDG (kcal/mol):	0.46

ALP-POS-afe0272e-2_1



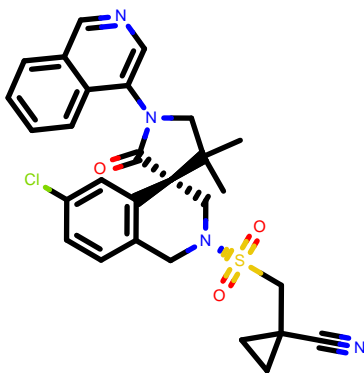
CID:	ALP-POS-afe0272e-2_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cnc4c3cccc4)c5cc(c(cc5C1=O)Cl)Cl</chem>
RUN:	RUN651
DDG (kcal/mol):	3.83
dDDG (kcal/mol):	0.17

LUO-POS-8484f2d3-1_2



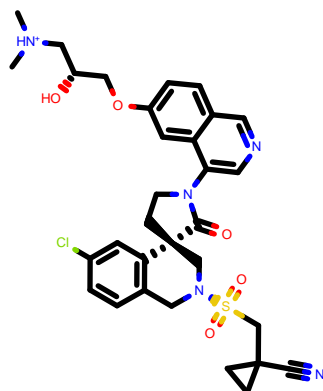
CID:	LUO-POS-8484f2d3-1_2
SMILES:	<chem>C[NH+](C)CCOC1cc2nnc2c1N3CC[C@]4(C3=O)CN@@H](C=C4c5cc(cc5)O)S(=O)(=O)CC6CC6#N</chem>
RUN:	RUN928
DDG (kcal/mol):	3.84
dDDG (kcal/mol):	0.88

MAT-POS-50a80394-8_2



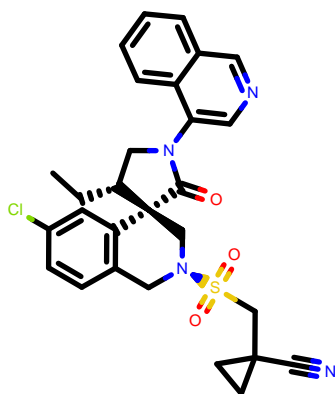
CID:	MAT-POS-50a80394-8_2
SMILES:	<chem>CC1(CN(C(=O)[C@@]12CN@]C(Cc2cc(cc3C)S(=O)(=O)CC4(CC4)C#N)c5nccc6c5cccc6)C</chem>
RUN:	RUN854
DDG (kcal/mol):	3.86
dDDG (kcal/mol):	0.47

EDJ-MED-ee81482e-3_4



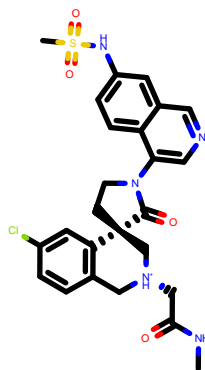
CID:	EDJ-MED-ee81482e-3_4
SMILES:	<chem>C[NH+](C)[C@H](COc1ccc2ncc(c2c1)N(C)C[C@@]3(C)C#N@]C(Cc3cc(cc4C)S(=O)(=O)CC5(CC5)C#N)O</chem>
RUN:	RUN944
DDG (kcal/mol):	3.86
dDDG (kcal/mol):	0.70

MAT-POS-50a80394-2_1



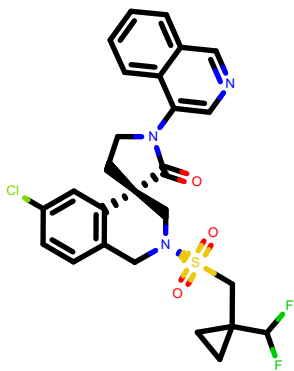
CID:	MAT-POS-50a80394-2_1
SMILES:	<chem>CC[C@@]1(C)CN(C(=O)[C@@]12CN@]C(Cc2cc(cc3C)S(=O)(=O)CC4(CC4)C#N)c5nccc6c5cccc6</chem>
RUN:	RUN850
DDG (kcal/mol):	3.86
dDDG (kcal/mol):	0.44

MAT-POS-b4d6b7fc-7_1



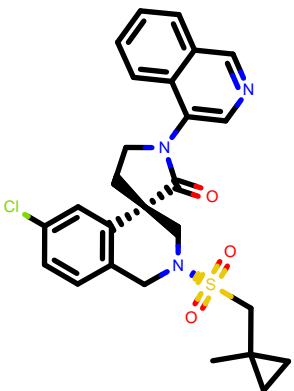
CID:	MAT-POS-b4d6b7fc-7_1
SMILES:	<chem>CNC(=O)[C][N@@]([H+])1Cc2ccc(cc2)[C@@]3(C)C[N](C3=O)c4cnc5c4ccc(c5)NS(=O)(=O)C)Cl</chem>
RUN:	RUN779
DDG (kcal/mol):	3.87
dDDG (kcal/mol):	0.28

EDJ-MED-5cd3920d-5_2



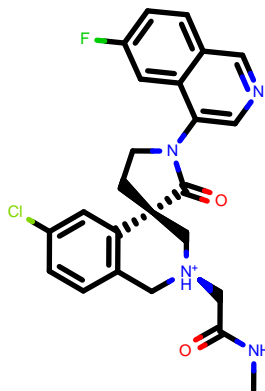
CID:	EDJ-MED-5cd3920d-5_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@@]4(C3=O)C[N@]5C5c4cc(cc5)C(S(=O)(=O)CC6(CC6)C(F)F</chem>
RUN:	RUN833
DDG (kcal/mol):	3.89
dDDG (kcal/mol):	0.41

ALP-POS-ecbed2ba-3_2



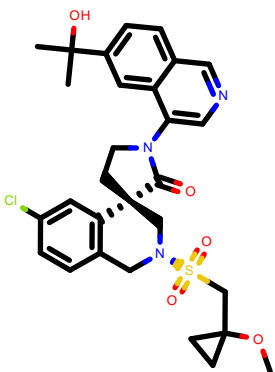
CID:	ALP-POS-ecbed2ba-3_2
SMILES:	<chem>CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5ccc6c5ccc6)Cl</chem>
RUN:	RUN687
DDG (kcal/mol):	3.91
dDDG (kcal/mol):	0.40

LUO-POS-b4dec3be-1_2



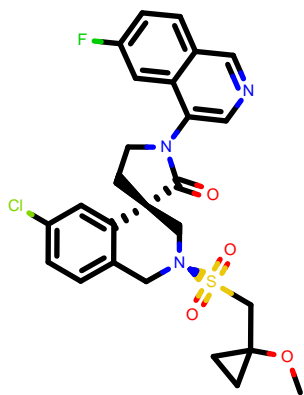
CID:	LUO-POS-b4dec3be-1_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4ccc5c4cc(cc5)F)Cl</chem>
RUN:	RUN616
DDG (kcal/mol):	3.94
dDDG (kcal/mol):	0.23

MAT-POS-853c0ffa-12_2



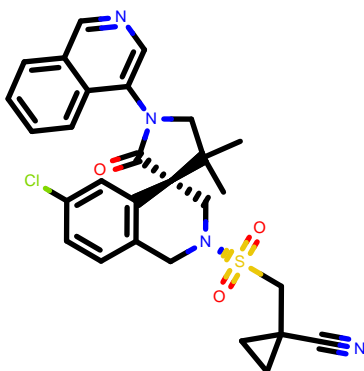
CID:	MAT-POS-853c0ffa-12_2
SMILES:	<chem>CC(C)(c1ccc2mcc(c2c1)N3CC[C@@]4(C3=O)C[N@]5C5c4cc(cc5)C(S(=O)(=O)CC6(CC6)OC)O</chem>
RUN:	RUN891
DDG (kcal/mol):	3.95
dDDG (kcal/mol):	0.41

MAT-POS-853c0ffa-14_1



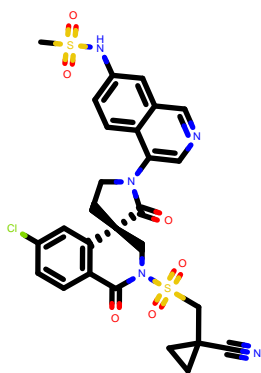
CID:	MAT-POS-853c0ffa-14_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)N@@]2C3ccc(cc3C@]4(C2)CCN(C4=O)c5ccc6c5cc(cc6)F)C1</chem>
RUN:	RUN794
DDG (kcal/mol):	3.98
dDDG (kcal/mol):	0.41

MAT-POS-50a80394-8_1



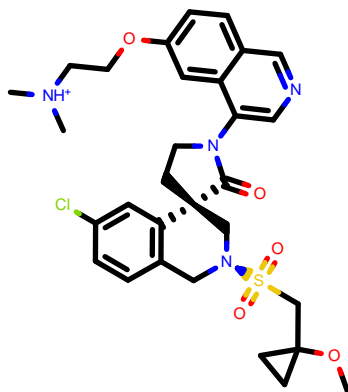
CID:	MAT-POS-50a80394-8_1
SMILES:	<chem>CC1(CN(C1=O)C@@]12CN@@]3)C3c2cc(cc3C)S(=O)(=O)CC4(CC4)CNc5ccc6c5ccccc6)C</chem>
RUN:	RUN858
DDG (kcal/mol):	3.98
dDDG (kcal/mol):	0.64

EDJ-MED-9f4ac58c-3_1



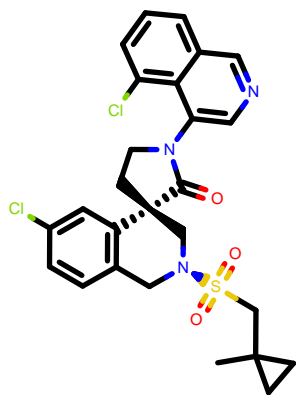
CID:	EDJ-MED-9f4ac58c-3_1
SMILES:	<chem>CS(=O)(=O)Nc1ccc2c(c1)ncnc2N3CC(C@@]4(C3=O)CN(C1=O)c5ccc6c5ccccc6)C4N</chem>
RUN:	RUN918
DDG (kcal/mol):	3.99
dDDG (kcal/mol):	0.47

MAT-POS-853c0ffa-10_1



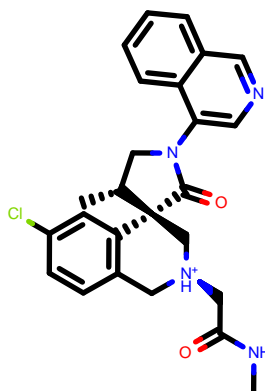
CID:	MAT-POS-853c0ffa-10_1
SMILES:	<chem>C[NH+]([C]COCc1ccc2nc(c12)c1n3cc(C@@]4(C3=O)CN@@]5)C5c4ccc6c5ccccc6)S(=O)(=O)COC</chem>
RUN:	RUN921
DDG (kcal/mol):	4.01
dDDG (kcal/mol):	0.42

MAT-POS-853c0ffa-17_1



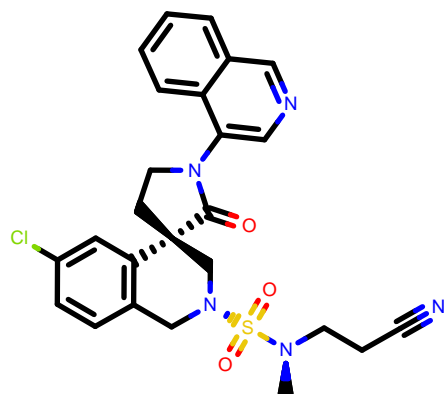
CID:	MAT-POS-853c0ffa-17_1
SMILES:	<chem>CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3)[C@H](C2)CCN(C4=O)c5ncc6c5c(ccc6)Cl</chem>
RUN:	RUN719
DDG (kcal/mol):	4.01
dDDG (kcal/mol):	0.34

MAT-POS-50a80394-4_3



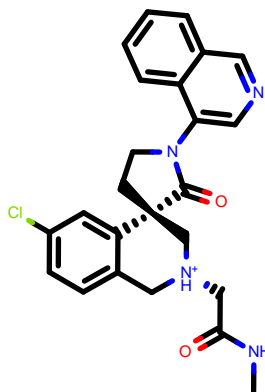
CID:	MAT-POS-50a80394-4_3
SMILES:	<chem>C[C@@H]1CN(C(=O)[C@@]12C[N@H+]Cc3c2cc(cc3)Cl)CC(=O)NC)c4ncc5c4cccc5</chem>
RUN:	RUN606
DDG (kcal/mol):	4.02
dDDG (kcal/mol):	0.21

ALP-POS-ecbed2ba-16_2



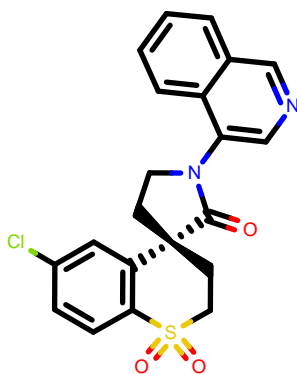
CID:	ALP-POS-ecbed2ba-16_2
SMILES:	<chem>C[N@](CCC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2)[C@]3(C1)CCN(C3=O)c4ncc5c4cccc5)Cl</chem>
RUN:	RUN736
DDG (kcal/mol):	4.08
dDDG (kcal/mol):	0.38

LUO-POS-868e8996-11_1



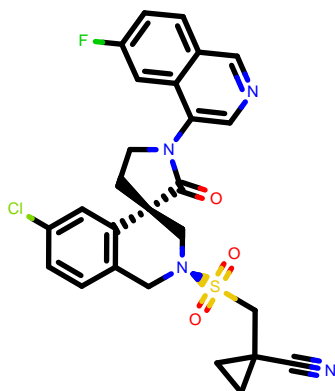
CID:	LUO-POS-868e8996-11_1
SMILES:	<chem>CNC(=O)C[N@@H+]1Cc2ccc(cc2)[C@]3(C1)CCN(C3=O)c4ncc5c4cccc5)Cl</chem>
RUN:	RUN568
DDG (kcal/mol):	4.11
dDDG (kcal/mol):	0.27

EDJ-MED-d4864bdc-3_1



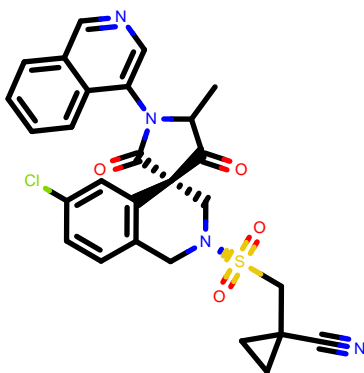
CID:	EDJ-MED-d4864bdc-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN522
DDG (kcal/mol):	4.12
dDDG (kcal/mol):	0.17

MAT-POS-853c0ffa-13_1



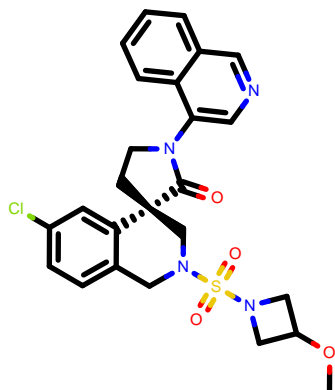
CID:	MAT-POS-853c0ffa-13_1
SMILES:	<chem>c1cc2nccc(c2cc1F)N3CC[C@@]4(C3=O)C[N@@]5(Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(Cc6)C#N</chem>
RUN:	RUN791
DDG (kcal/mol):	4.15
dDDG (kcal/mol):	0.30

PET-UNK-94036022-13_1



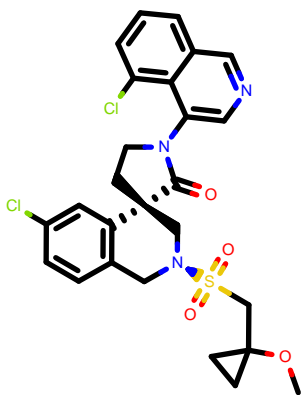
CID:	PET-UNK-94036022-13_1
SMILES:	<chem>C=C1C=O[C@@]2(CN@@3)C3C2cc(c3)C)S(=O)(=O)CC4(Cc4)C#N[C@@]1(O)N1c5ccc6c5ccc6</chem>
RUN:	RUN871
DDG (kcal/mol):	4.19
dDDG (kcal/mol):	0.44

ALP-POS-ecbed2ba-10_1



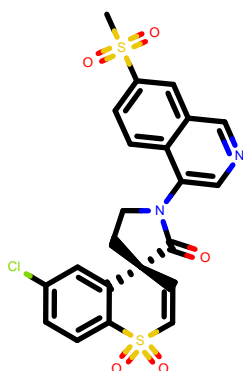
CID:	ALP-POS-ecbed2ba-10_1
SMILES:	<chem>COC1CN(C1)S(=O)(=O)[N@@]2C3ccc(cc3)C@4(C2)CCN(C4=O)c5ccc6c5ccc6)Cl</chem>
RUN:	RUN738
DDG (kcal/mol):	4.19
dDDG (kcal/mol):	0.51

MAT-POS-853c0ffa-7_1



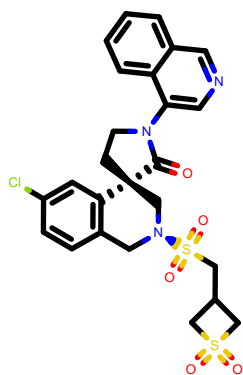
CID:	MAT-POS-853c0ffa-7_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)N@@2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5ccc6c5c(ccc6)Cl)Cl</chem>
RUN:	RUN788
DDG (kcal/mol):	4.22
dDDG (kcal/mol):	0.58

EDJ-MED-94fddcec-5_1



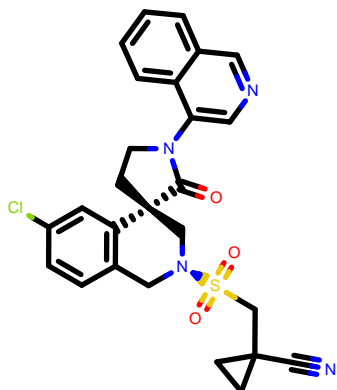
CID:	EDJ-MED-94fddcec-5_1
SMILES:	<chem>CS(=O)(=O)c1ccc2c(c1)ncnc2N3CC[C@]4(C3=O)CCS(=O)(=O)c5c4cc(c5)Cl</chem>
RUN:	RUN588
DDG (kcal/mol):	4.22
dDDG (kcal/mol):	0.20

ALP-POS-ecbed2ba-5_2



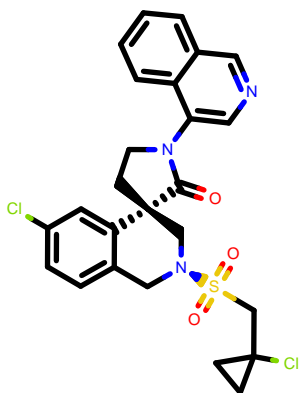
CID:	ALP-POS-ecbed2ba-5_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@]4(C3=O)C[N@@]5(Cc5c4cc(c5)Cl)S(=O)(=O)CC6CS(=O)(=O)C6</chem>
RUN:	RUN801
DDG (kcal/mol):	4.22
dDDG (kcal/mol):	0.81

EDJ-MED-8bb691af-6_1



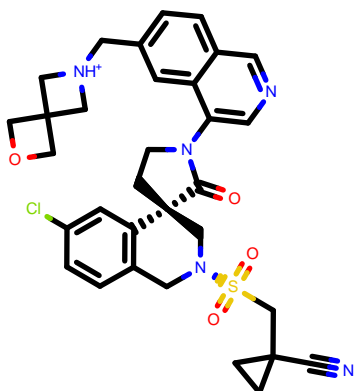
CID:	EDJ-MED-8bb691af-6_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@]4(C3=O)C[N@@]5(Cc5c4cc(c5)Cl)S(=O)(=O)CC6(Cc6)C#N</chem>
RUN:	RUN720
DDG (kcal/mol):	4.22
dDDG (kcal/mol):	0.31

PET-UNK-94036022-3_2



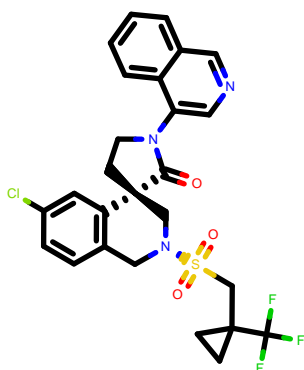
CID:	PET-UNK-94036022-3_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@]5C5c4cc(cc5)ClS(=O)(=O)CC6(C)CC6Cl</chem>
RUN:	RUN711
DDG (kcal/mol):	4.23
dDDG (kcal/mol):	0.38

EDJ-MED-ee81482e-5_2



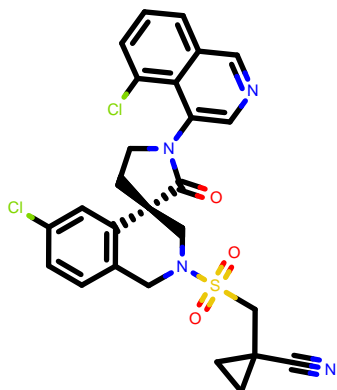
CID:	EDJ-MED-ee81482e-5_2
SMILES:	<chem>c1cc2ncc(c2cc1C[NH+]3CC4(C3)COC4N5CC[C@@]6(C5=O)C[N@@]7C7c6cc(cc7)ClS(=O)(=O)CC8(C)CC8#N</chem>
RUN:	RUN947
DDG (kcal/mol):	4.25
dDDG (kcal/mol):	0.54

EDJ-MED-5cd3920d-6_2



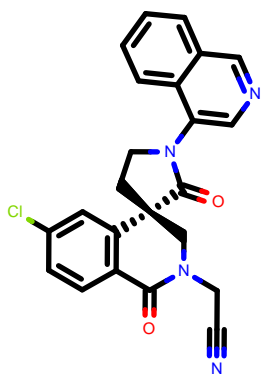
CID:	EDJ-MED-5cd3920d-6_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@]5C5c4cc(cc5)ClS(=O)(=O)CC6(C)C(F)C(F)F6</chem>
RUN:	RUN857
DDG (kcal/mol):	4.25
dDDG (kcal/mol):	0.37

MAT-POS-853c0ffa-5_2



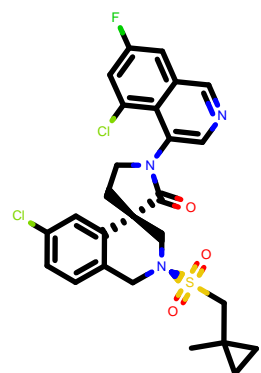
CID:	MAT-POS-853c0ffa-5_2
SMILES:	<chem>c1cc2ncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@@]5C5c4cc(cc5)ClS(=O)(=O)CC6(C)C#N6</chem>
RUN:	RUN787
DDG (kcal/mol):	4.30
dDDG (kcal/mol):	0.74

PET-UNK-aa57768f-2_1



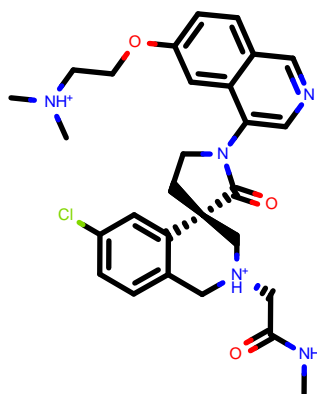
CID:	PET-UNK-aa57768f-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N</chem>
RUN:	RUN547
DDG (kcal/mol):	4.31
dDDG (kcal/mol):	0.11

MAT-POS-853c0ffa-18_1



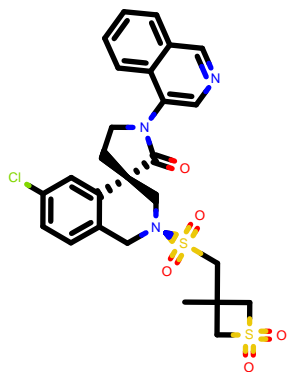
CID:	MAT-POS-853c0ffa-18_1
SMILES:	<chem>CC1(CC1)CS(=O)(=O)N@@]2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5ccc6c5c(cc6)F)Cl</chem>
RUN:	RUN800
DDG (kcal/mol):	4.31
dDDG (kcal/mol):	0.30

EDJ-MED-b6c6ee2b-1_1



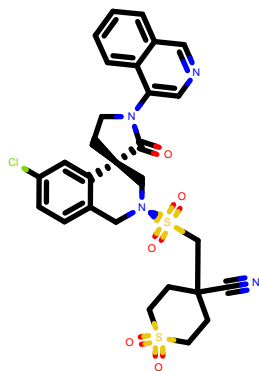
CID:	EDJ-MED-b6c6ee2b-1_1
SMILES:	<chem>CNC(=O)C[N@@]([H+])1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4ccc5c4cc(cc5)OCC([NH+](C)C)Cl</chem>
RUN:	RUN870
DDG (kcal/mol):	4.35
dDDG (kcal/mol):	0.37

ALP-POS-ecbed2ba-1_1



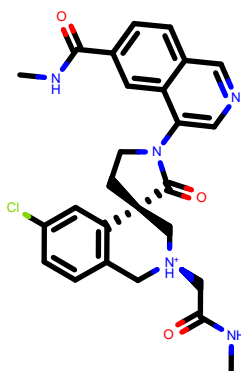
CID:	ALP-POS-ecbed2ba-1_1
SMILES:	<chem>CC1(CS(=O)(=O)C1)CS(=O)(=O)N@@]2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5ccc6c5c(cc6)Cl</chem>
RUN:	RUN842
DDG (kcal/mol):	4.35
dDDG (kcal/mol):	0.47

ALP-POS-ecbed2ba-2_1



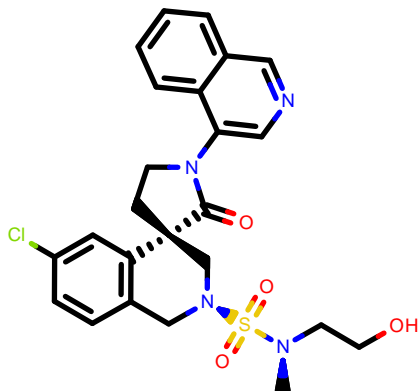
CID:	ALP-POS-ecbed2ba-2_1
SMILES:	<chem>C1CC2(C1)NCC(C)C(C)N(C)C2C3=CC=CC=C3C4=CC=C(C=C4)S(=O)(=O)CC5=CC=C(C=C5)C#N</chem>
RUN:	RUN906
DDG (kcal/mol):	4.35
dDDG (kcal/mol):	0.42

MAT-POS-38eb6498-5_2



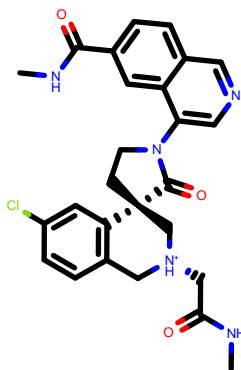
CID:	MAT-POS-38eb6498-5_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2)C@3(C1)CCN(C3=O)c4ccc5c4cc(c5)C(=O)NC)Cl</chem>
RUN:	RUN764
DDG (kcal/mol):	4.38
dDDG (kcal/mol):	0.34

ALP-POS-ecbed2ba-19_1



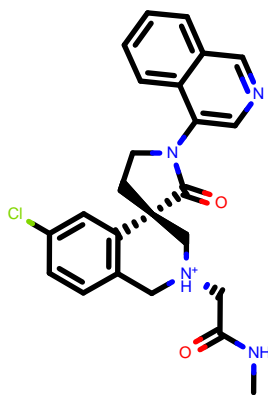
CID:	ALP-POS-ecbed2ba-19_1
SMILES:	<chem>C[N@]([C]CO)S(=O)(=O)[N@]1Cc2ccc(cc2)C@3(C1)CCN(C3=O)c4ccc5c4cc(c5)Cl</chem>
RUN:	RUN696
DDG (kcal/mol):	4.39
dDDG (kcal/mol):	0.41

MAT-POS-38eb6498-5_1



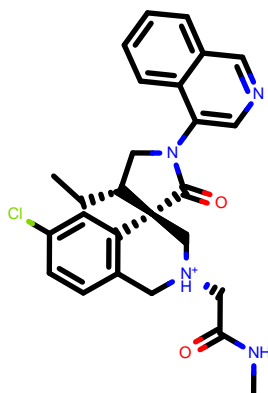
CID:	MAT-POS-38eb6498-5_1
SMILES:	<chem>CNC(=O)C[N@]([H+]1Cc2ccc(cc2)C@3(C1)CCN(C3=O)c4ccc5c4cc(c5)C(=O)NC)Cl</chem>
RUN:	RUN752
DDG (kcal/mol):	4.40
dDDG (kcal/mol):	0.27

EDJ-MED-8bb691af-4_1



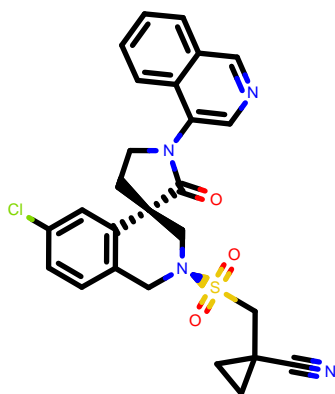
CID:	EDJ-MED-8bb691af-4_1
SMILES:	<chem>CNC(=O)C[NH+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN558
DDG (kcal/mol):	4.41
dDDG (kcal/mol):	0.30

MAT-POS-50a80394-5_1



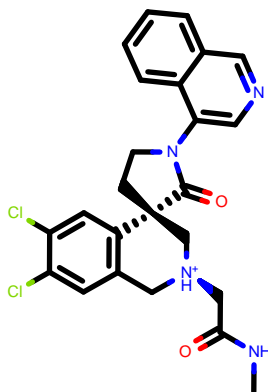
CID:	MAT-POS-50a80394-5_1
SMILES:	<chem>CC[C@]1CN(C(=O)[C@]2[C@H]12C[NH+]1Cc3ccc(cc3)C)CC(=O)NC)c4cnc5c4cccc5</chem>
RUN:	RUN659
DDG (kcal/mol):	4.42
dDDG (kcal/mol):	0.32

ALP-POS-ecbed2ba-4_2



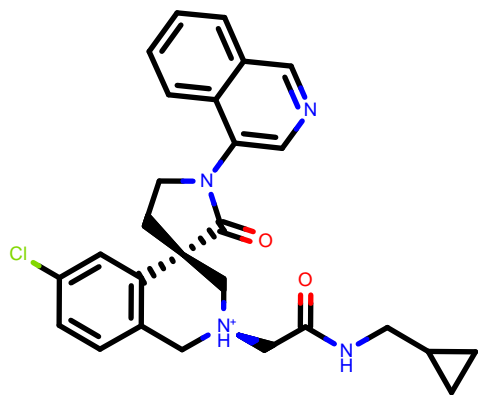
CID:	ALP-POS-ecbed2ba-4_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@]4(C3=O)C[NH+]1Cc5ccc(cc5)C1S(=O)(=O)CC6(C)C6#N</chem>
RUN:	RUN727
DDG (kcal/mol):	4.43
dDDG (kcal/mol):	0.60

ALP-POS-afe0272e-1_2



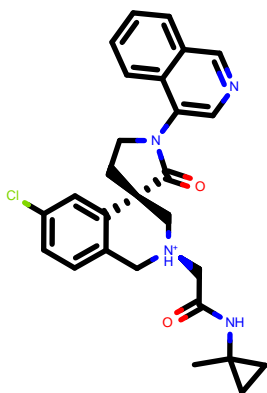
CID:	ALP-POS-afe0272e-1_2
SMILES:	<chem>CNC(=O)C[NH+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN598
DDG (kcal/mol):	4.46
dDDG (kcal/mol):	0.26

ALP-POS-ecbed2ba-12_2



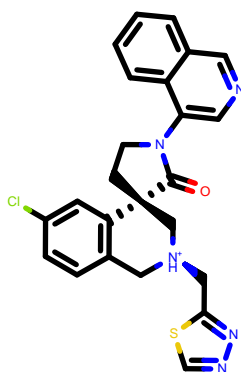
CID:	ALP-POS-ecbed2ba-12_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@H](C3=O)C[N@H](Cc5c4cc(cc5)Cl)CC(=O)NCC6CC6</chem>
RUN:	RUN690
DDG (kcal/mol):	4.47
dDDG (kcal/mol):	0.22

MAT-POS-69786b79-3_2



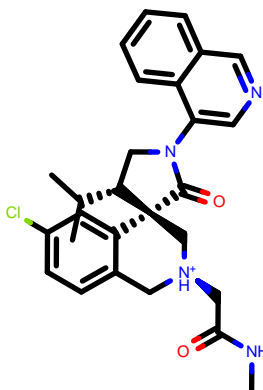
CID:	MAT-POS-69786b79-3_2
SMILES:	<chem>CC1(CC1)NC(=O)C[N@H]2Cc3ccc(cc3[C@H](C2)CCN(C4=O)c5nccc6c5ccc6)Cl</chem>
RUN:	RUN704
DDG (kcal/mol):	4.47
dDDG (kcal/mol):	0.35

MAT-POS-96396902-1_2



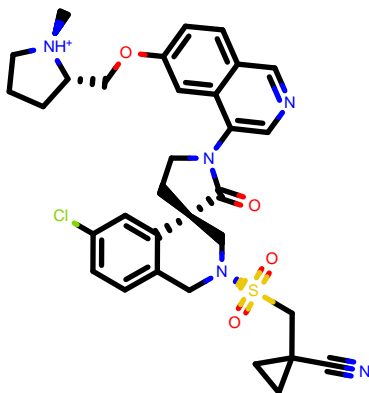
CID:	MAT-POS-96396902-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@H](C3=O)C[N@H](Cc5c4cc(cc5)Cl)C6nncs6</chem>
RUN:	RUN612
DDG (kcal/mol):	4.48
dDDG (kcal/mol):	0.17

MAT-POS-50a80394-6_3



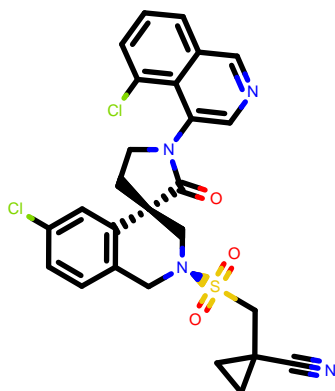
CID:	MAT-POS-50a80394-6_3
SMILES:	<chem>CC[C@H](C1CN(C(=O)[C@H]12C[N@H](Cc3c2cc(cc3)Cl)CC(=O)NC)c4ncc5c4ccc5</chem>
RUN:	RUN710
DDG (kcal/mol):	4.51
dDDG (kcal/mol):	0.30

MAT-POS-40ad851a-1_7



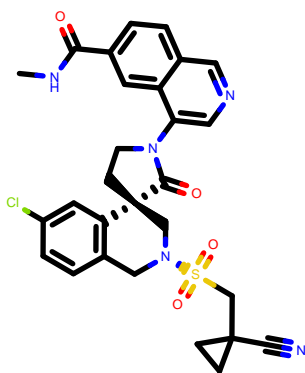
CID:	MAT-POS-40ad851a-1_7
SMILES:	<chem>C[N+]1CCCC[C@H]1CCc2cc3nnc(c3c2)N4CC[C@@]5(C4=O)C[N@@]6Cc6cc(cc6)C(S(=O)(=O)CC7C#N)C#N</chem>
RUN:	RUN964
DDG (kcal/mol):	4.51
dDDG (kcal/mol):	0.79

MAT-POS-1d5ab790-1_1



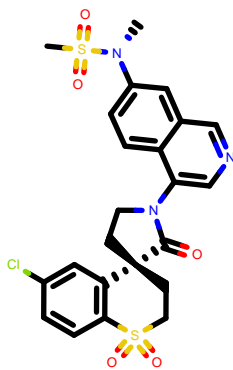
CID:	MAT-POS-1d5ab790-1_1
SMILES:	<chem>c1cc2ncc(c2c1)C1N3CC[C@@]4(C3=O)C[N@@]5]C6c6cc(cc6)C(S(=O)(=O)CC7C#N)C#N</chem>
RUN:	RUN803
DDG (kcal/mol):	4.52
dDDG (kcal/mol):	0.55

MAT-POS-38eb6498-2_2



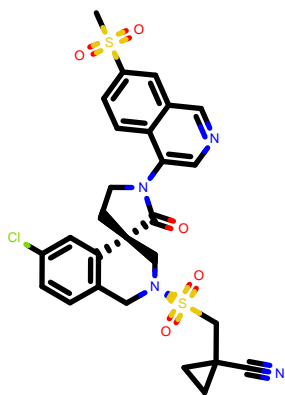
CID:	MAT-POS-38eb6498-2_2
SMILES:	<chem>CNC(=O)c1cc2ncc(c2c1)N3CC[C@@]4(C3=O)C[N@@]5]C6c6cc(cc6)C(S(=O)(=O)CC7C#N)C#N</chem>
RUN:	RUN898
DDG (kcal/mol):	4.53
dDDG (kcal/mol):	0.53

EDJ-MED-94fddcec-6_2



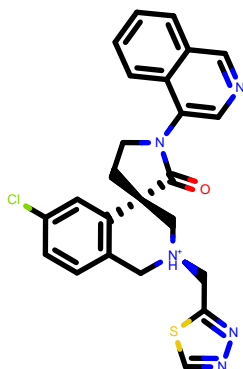
CID:	EDJ-MED-94fddcec-6_2
SMILES:	<chem>C[N@@]1c1ccc2c(c1)ncnc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)C(S(=O)(=O)C</chem>
RUN:	RUN682
DDG (kcal/mol):	4.53
dDDG (kcal/mol):	0.23

MAT-POS-853c0ffa-15_2



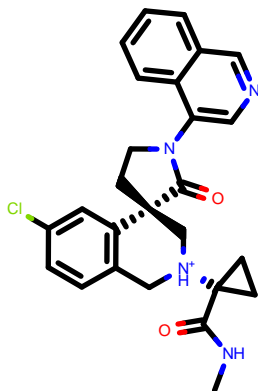
CID:	MAT-POS-853c0ffa-15_2
SMILES:	<chem>CS(=O)(=O)C1CC2C(C1)NCC2C(C)C@H(C3=O)C[N@H]C(C5=CC(=O)C(S(=O)(=O)CC6)C6)C#N</chem>
RUN:	RUN890
DDG (kcal/mol):	4.54
dDDG (kcal/mol):	0.63

PET-UNK-7e9559de-1_2



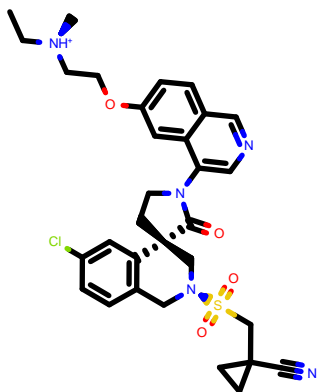
CID:	PET-UNK-7e9559de-1_2
SMILES:	<chem>C1CC2C(C1)CNC2N3CC(C)@H(C3=O)C[N@H]C(C5=CC(=O)C(S(=O)(=O)C)C6)NCS6</chem>
RUN:	RUN604
DDG (kcal/mol):	4.55
dDDG (kcal/mol):	0.21

MAT-POS-69786b79-1_1



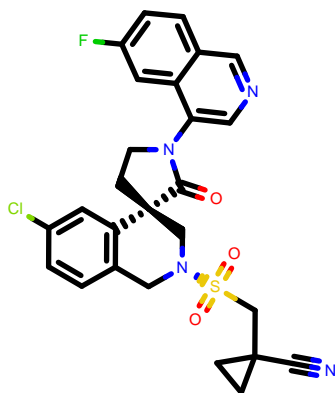
CID:	MAT-POS-69786b79-1_1
SMILES:	<chem>CNC(=O)C1(CC1)N@H+2C3CC(C)C@H(C3)4(C2)CCN(C4=O)S5CC6(C5)C6)Cl</chem>
RUN:	RUN644
DDG (kcal/mol):	4.57
dDDG (kcal/mol):	0.22

MAT-POS-40ad851a-2_1



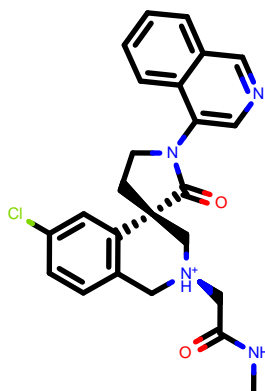
CID:	MAT-POS-40ad851a-2_1
SMILES:	<chem>CC[NH+]C(C)COC1CC2C(C1)NCC2C(C)C@H(C3=O)C[N@H]C(C5=CC(=O)C(S(=O)(=O)CC6)C6)C#N</chem>
RUN:	RUN935
DDG (kcal/mol):	4.58
dDDG (kcal/mol):	0.49

MAT-POS-853c0ffa-13_2



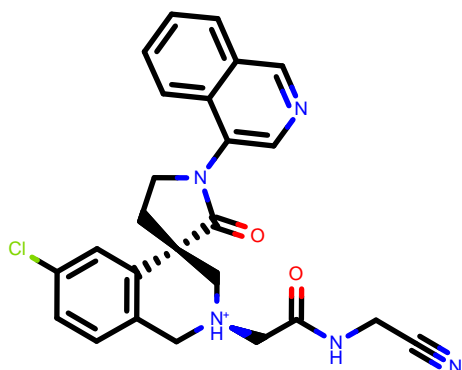
CID:	MAT-POS-853c0ffa-13_2
SMILES:	<chem>c1cc2cncoc(c2cc1F)N3CC[C@@H](C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN790
DDG (kcal/mol):	4.60
dDDG (kcal/mol):	0.49

MAT-POS-c7726e07-5_2



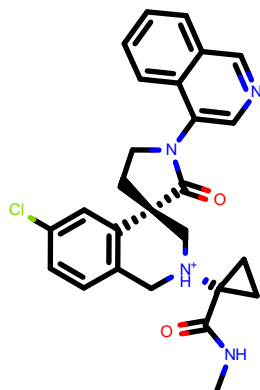
CID:	MAT-POS-c7726e07-5_2
SMILES:	<chem>CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN561
DDG (kcal/mol):	4.61
dDDG (kcal/mol):	0.31

ALP-POS-ecbed2ba-14_2



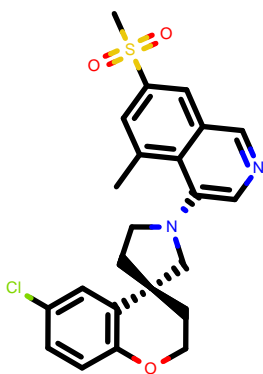
CID:	ALP-POS-ecbed2ba-14_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@H](C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC#N</chem>
RUN:	RUN628
DDG (kcal/mol):	4.62
dDDG (kcal/mol):	0.25

MAT-POS-576f7758-1_1



CID:	MAT-POS-576f7758-1_1
SMILES:	<chem>CNC(=O)C1(CC1)N@@H+]2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5cccc6)Cl</chem>
RUN:	RUN650
DDG (kcal/mol):	4.63
dDDG (kcal/mol):	0.20

EDJ-MED-d7486dd1-1_1



CID: EDJ-MED-d7486dd1-1_1

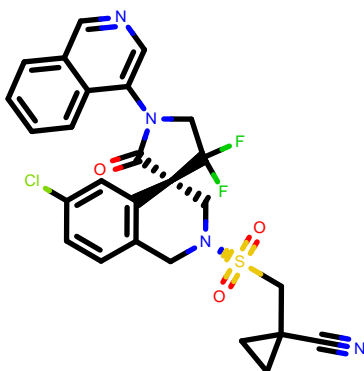
SMILES: Cc1cc(cc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl)S(=O)(=O)C

RUN: RUN540

DDG (kcal/mol): 4.63

dDDG (kcal/mol): 0.11

EDJ-MED-7e491f08-1_2



CID: EDJ-MED-7e491f08-1_2

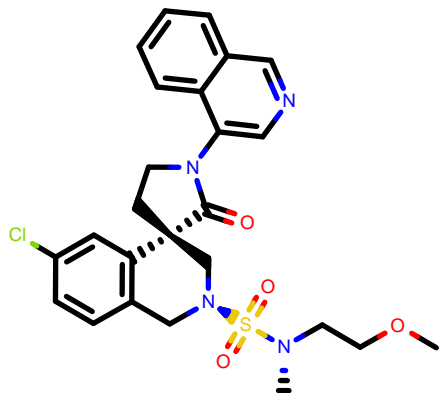
SMILES: c1ccc2c(c1)ncnc2N3CC[C@@]4(C3)C(=O)N(C)C5c4cc(cc5)Cl)S(=O)(=O)CC6(C)C#N)F)F

RUN: RUN863

DDG (kcal/mol): 4.64

dDDG (kcal/mol): 0.61

ALP-POS-ecbed2ba-21_2



CID: ALP-POS-ecbed2ba-21_2

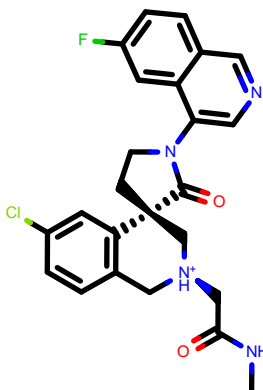
SMILES: C[N@](C)C(=O)S(=O)(=O)N[C@@]1(Cc2ccc(cc2)C@]3(C1)CCN(C3=O)c4ccc5c4cc5)Cl

RUN: RUN750

DDG (kcal/mol): 4.65

dDDG (kcal/mol): 0.33

LUO-POS-b4dec3be-2_2



CID: LUO-POS-b4dec3be-2_2

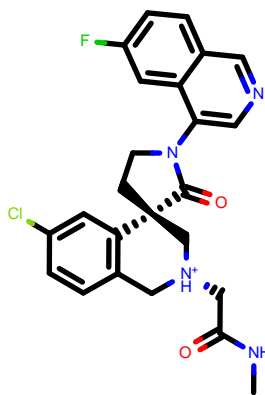
SMILES: CNC(=O)C[N@H+]1Cc2ccc(cc2)C@]3(C1)CCN(C3=O)c4ccc5c4cc5)F)Cl

RUN: RUN615

DDG (kcal/mol): 4.66

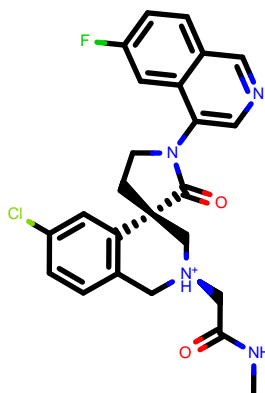
dDDG (kcal/mol): 0.25

MAT-POS-b4d6b7fc-5_1



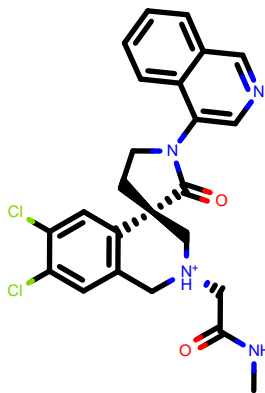
CID:	MAT-POS-b4d6b7fc-5_1
SMILES:	<chem>CNC(=O)C[N+]([H])1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl</chem>
RUN:	RUN586
DDG (kcal/mol):	4.66
dDDG (kcal/mol):	0.27

MAT-POS-b4d6b7fc-5_2



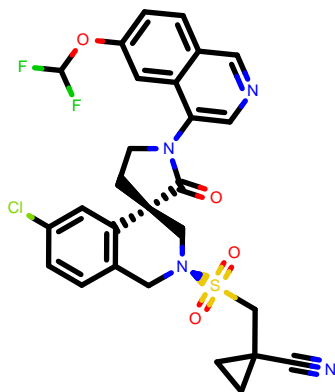
CID:	MAT-POS-b4d6b7fc-5_2
SMILES:	<chem>CNC(=O)C[N+]([H])1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl</chem>
RUN:	RUN590
DDG (kcal/mol):	4.67
dDDG (kcal/mol):	0.22

ALP-POS-afe0272e-1_1



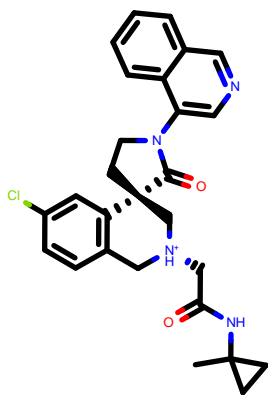
CID:	ALP-POS-afe0272e-1_1
SMILES:	<chem>CNC(=O)C[N+]([H])1Cc2cc(c(c2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)Cl</chem>
RUN:	RUN594
DDG (kcal/mol):	4.67
dDDG (kcal/mol):	0.32

EDJ-MED-5cd3920d-1_1



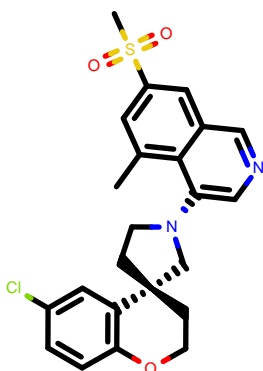
CID:	EDJ-MED-5cd3920d-1_1
SMILES:	<chem>c1cc2ncc(c2c1OC(F)F)N3CC[C@]4(C3=O)C[N+]([H])C5c4ccc(c5)S(=O)(=O)C6CC6)C#N</chem>
RUN:	RUN910
DDG (kcal/mol):	4.69
dDDG (kcal/mol):	0.35

MAT-POS-69786b79-3_1



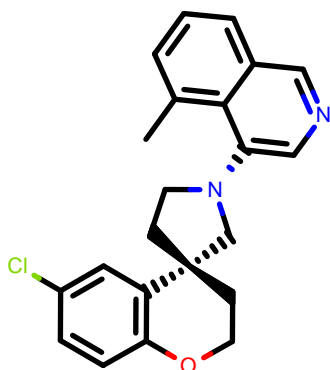
CID:	MAT-POS-69786b79-3_1
SMILES:	<chem>CC1(CC1)NC(=O)C[N+]([H])2Cc3ccc(cc3[C@@]4(C2)CCN(C4=O)c5ccc6c5ccc6)Cl</chem>
RUN:	RUN693
DDG (kcal/mol):	4.70
dDDG (kcal/mol):	0.33

EDJ-MED-d7486dd1-1_2



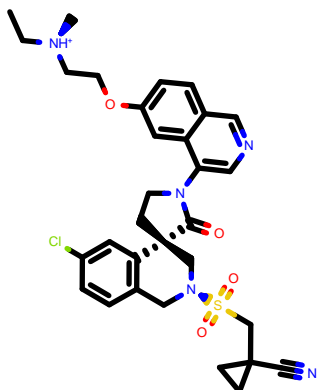
CID:	EDJ-MED-d7486dd1-1_2
SMILES:	<chem>Cc1cc(cc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl)S(=O)(=O)C</chem>
RUN:	RUN543
DDG (kcal/mol):	4.71
dDDG (kcal/mol):	0.11

EDJ-MED-a6bab6fb-1_1



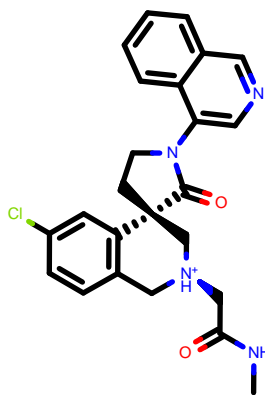
CID:	EDJ-MED-a6bab6fb-1_1
SMILES:	<chem>Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN503
DDG (kcal/mol):	4.81
dDDG (kcal/mol):	0.09

MAT-POS-40ad851a-2_3



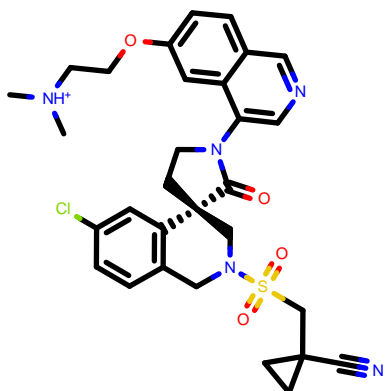
CID:	MAT-POS-40ad851a-2_3
SMILES:	<chem>CC[NH+]([H])C(CCCOc1ccc2nc(c2c1)N3CC[C@@]4(C3)O[C]N8)Cc5c4cc(cc5)Cl)S(=O)(=O)CC6C6c#N</chem>
RUN:	RUN937
DDG (kcal/mol):	4.84
dDDG (kcal/mol):	0.65

MAT-POS-c7726e07-6_2



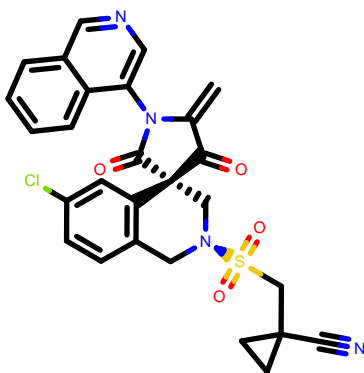
CID:	MAT-POS-c7726e07-6_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4ccc5)Cl</chem>
RUN:	RUN569
DDG (kcal/mol):	4.84
dDDG (kcal/mol):	0.26

LUO-POS-8484f2d3-2_2



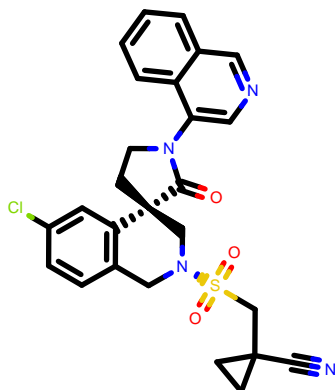
CID:	LUO-POS-8484f2d3-2_2
SMILES:	<chem>C[NH+]1C(CCOc1ccc2ncnc2c1)N(C)C@ @]4(C3=O)C[N@]5Cc6c4ccc5)ClS(=O)(=O)CC6(C)C#N</chem>
RUN:	RUN933
DDG (kcal/mol):	4.92
dDDG (kcal/mol):	0.65

PET-UNK-94036022-13_2



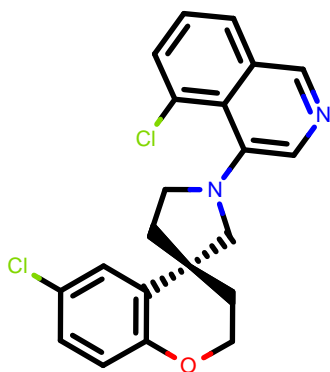
CID:	PET-UNK-94036022-13_2
SMILES:	<chem>C=C1C(=O)C@]2(C1N@]3C3c2ccc(c3)ClS(=O)(=O)CC4(C)C#N)Cl(=O)N1c5ccc6c5cccc6</chem>
RUN:	RUN873
DDG (kcal/mol):	4.92
dDDG (kcal/mol):	0.47

EDJ-MED-8bb691af-6_2



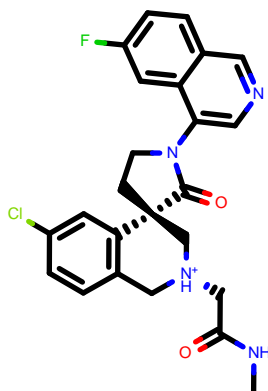
CID:	EDJ-MED-8bb691af-6_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@ @]4(C3=O)C[N@]5Cc5c4ccc(c5)ClS(=O)(=O)CC6(C)C#N</chem>
RUN:	RUN722
DDG (kcal/mol):	4.92
dDDG (kcal/mol):	0.49

EDJ-MED-e78d5f1a-1_1



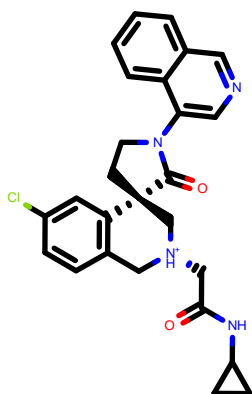
CID:	EDJ-MED-e78d5f1a-1_1
SMILES:	<chem>c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN502
DDG (kcal/mol):	4.96
dDDG (kcal/mol):	0.10

LUO-POS-b4dec3be-1_1



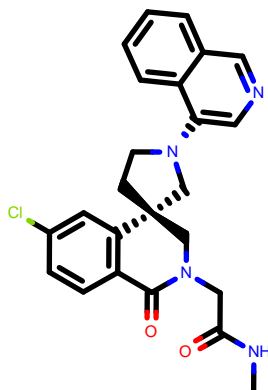
CID:	LUO-POS-b4dec3be-1_1
SMILES:	<chem>CNC(=O)C[NH+]1C2ccc(cc2[C@@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl</chem>
RUN:	RUN610
DDG (kcal/mol):	4.98
dDDG (kcal/mol):	0.26

MAT-POS-69786b79-2_1



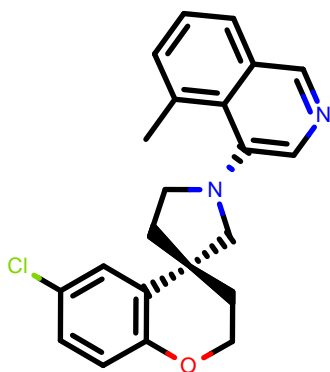
CID:	MAT-POS-69786b79-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[NH+]1C5c4cc(cc5)Cl)CC(=O)N6CC6</chem>
RUN:	RUN648
DDG (kcal/mol):	4.98
dDDG (kcal/mol):	0.24

EDJ-MED-8bb691af-7_2



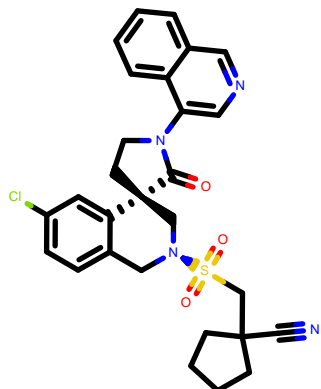
CID:	EDJ-MED-8bb691af-7_2
SMILES:	<chem>CNC(=O)CN1C[C@@]2(CCN(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN557
DDG (kcal/mol):	5.00
dDDG (kcal/mol):	0.14

EDJ-MED-a6bab6fb-1_2



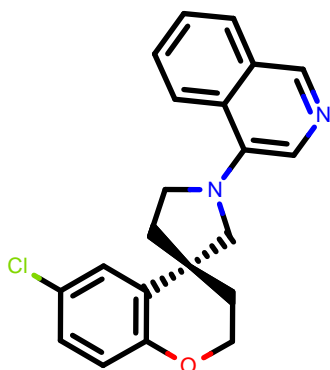
CID:	EDJ-MED-a6bab6fb-1_2
SMILES:	<chem>Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN492
DDG (kcal/mol):	5.01
dDDG (kcal/mol):	0.09

ALP-POS-ecbed2ba-15_2



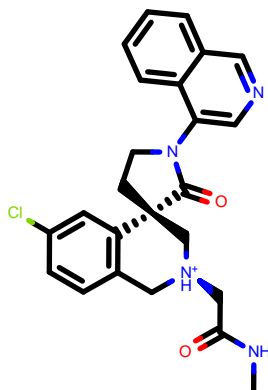
CID:	ALP-POS-ecbed2ba-15_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3=O)C[N@@]5C5c4cc(cc5)ClS(=O)(=O)CC6(CCCC6)C#N</chem>
RUN:	RUN846
DDG (kcal/mol):	5.04
dDDG (kcal/mol):	0.47

EDJ-MED-159244ea-2_1



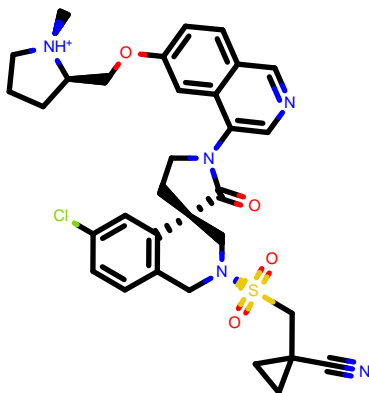
CID:	EDJ-MED-159244ea-2_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN490
DDG (kcal/mol):	5.10
dDDG (kcal/mol):	0.09

LUO-POS-868e8996-12_2



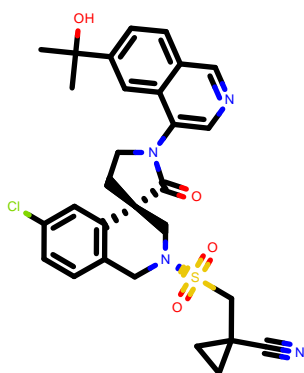
CID:	LUO-POS-868e8996-12_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN570
DDG (kcal/mol):	5.14
dDDG (kcal/mol):	0.22

MAT-POS-40ad851a-1_5



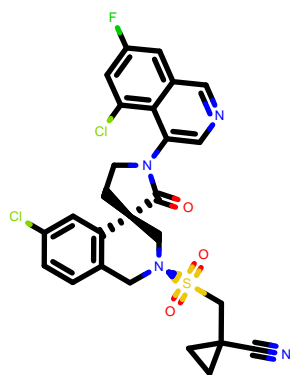
CID:	MAT-POS-40ad851a-1_5
SMILES:	<chem>CN=[C+]1CCC[C@H]1CC[C@@H]2C=CC(=O)N2C3=CC=C(C=C3)N4C[C@@H]5[C@@H](C=C4)O[C@H]6C=C(C=C6)C7=CN</chem>
RUN:	RUN950
DDG (kcal/mol):	5.17
dDDG (kcal/mol):	0.68

MAT-POS-853c0ffa-11_1



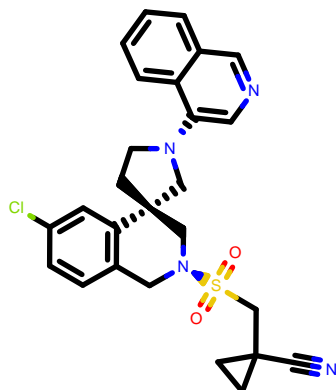
CID:	MAT-POS-853c0ffa-11_1
SMILES:	<chem>CC(C)(C1=CC=C(C=C1)N(C)C)O[C@H]2C=CC(=O)N2C3=CC=C(C=C3)N4C[C@@H]5[C@@H](C=C4)O[C@H]6C=C(C=C6)C7=CN</chem>
RUN:	RUN895
DDG (kcal/mol):	5.18
dDDG (kcal/mol):	0.46

MAT-POS-853c0ffa-6_1



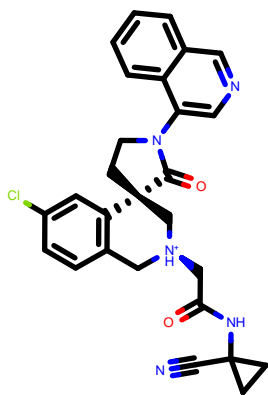
CID:	MAT-POS-853c0ffa-6_1
SMILES:	<chem>C1=CC=C(C=C1)N(C)C[C@@H]2C=CC(=O)N2C3=CC=C(C=C3)N4C[C@@H]5[C@@H](C=C4)O[C@H]6C=C(C=C6)C7=CN</chem>
RUN:	RUN837
DDG (kcal/mol):	5.19
dDDG (kcal/mol):	0.45

EDJ-MED-8bb691af-2_3



CID:	EDJ-MED-8bb691af-2_3
SMILES:	<chem>C1=CC=C(C=C1)N(C)C[C@@H]2C=CC(=O)N2C3=CC=C(C=C3)N4C[C@@H]5[C@@H](C=C4)O[C@H]6C=C(C=C6)C7=CN</chem>
RUN:	RUN680
DDG (kcal/mol):	5.19
dDDG (kcal/mol):	0.40

MAT-POS-69786b79-4_2



CID: MAT-POS-69786b79-4_2

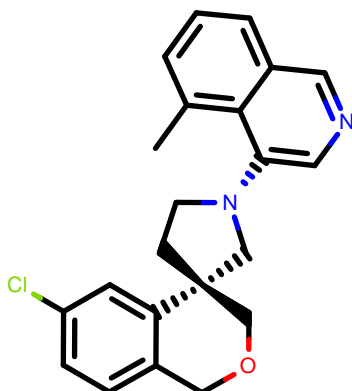
SMILES: c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+]([C@H]4)C(=O)NC6(C(C6)C#N

RUN: RUN762

DDG (kcal/mol): 5.34

dDDG (kcal/mol): 0.25

EDJ-MED-f3cfbbb5-1_2



CID: EDJ-MED-f3cfbbb5-1_2

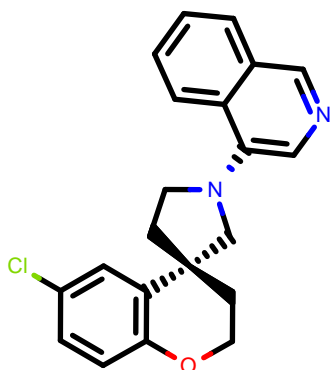
SMILES: Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl

RUN: RUN499

DDG (kcal/mol): 5.36

dDDG (kcal/mol): 0.09

MAT-POS-983b399a-2_1



CID: MAT-POS-983b399a-2_1

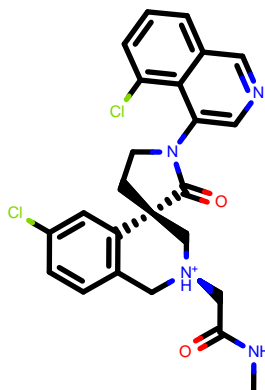
SMILES: c1ccc2c(c1)cncc2N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl

RUN: RUN488

DDG (kcal/mol): 5.36

dDDG (kcal/mol): 0.09

MAT-POS-b4d6b7fc-6_2



CID: MAT-POS-b4d6b7fc-6_2

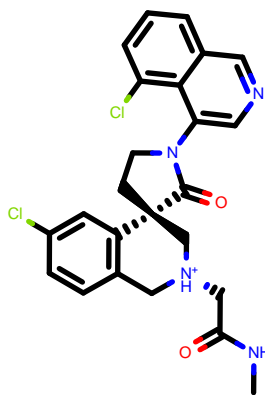
SMILES: CNC(=O)C[N@H+]1C2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4(ccc5)Cl)Cl

RUN: RUN591

DDG (kcal/mol): 5.38

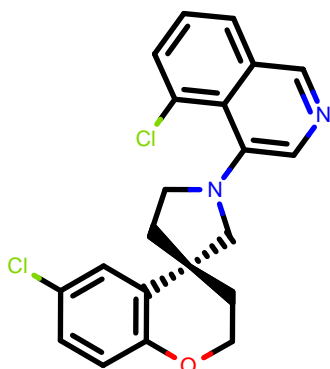
dDDG (kcal/mol): 0.27

MAT-POS-1d5ab790-2_1



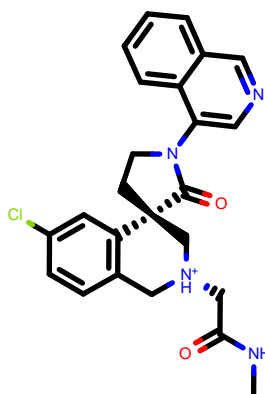
CID:	MAT-POS-1d5ab790-2_1
SMILES:	<chem>CNC(=O)C[N+]([H])1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl</chem>
RUN:	RUN595
DDG (kcal/mol):	5.40
dDDG (kcal/mol):	0.27

EDJ-MED-e78d5f1a-1_2



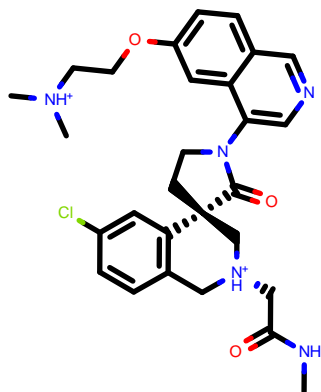
CID:	EDJ-MED-e78d5f1a-1_2
SMILES:	<chem>c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN501
DDG (kcal/mol):	5.40
dDDG (kcal/mol):	0.08

LUO-POS-868e8996-12_1



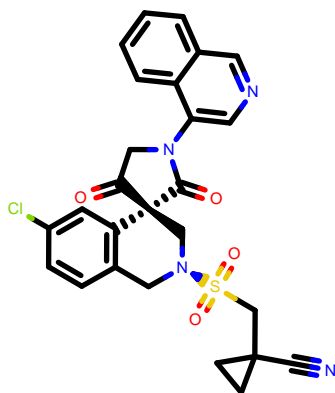
CID:	LUO-POS-868e8996-12_1
SMILES:	<chem>CNC(=O)C[N+]([H])1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccccc5)Cl</chem>
RUN:	RUN566
DDG (kcal/mol):	5.40
dDDG (kcal/mol):	0.29

MAT-POS-38eb6498-3_1



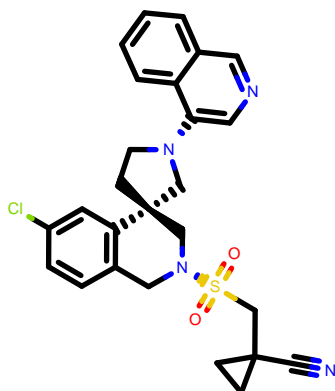
CID:	MAT-POS-38eb6498-3_1
SMILES:	<chem>CNC(=O)C[N+]([H])1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(ccc5)OCC[NH+](C)Cl)Cl</chem>
RUN:	RUN866
DDG (kcal/mol):	5.42
dDDG (kcal/mol):	0.34

EDJ-MED-a12e3a20-1_1



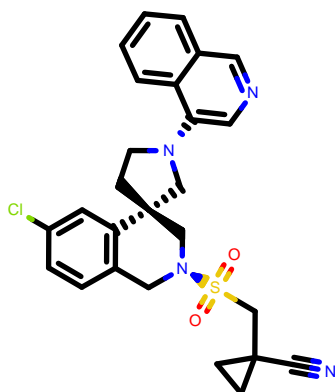
CID:	EDJ-MED-a12e3a20-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC(=O)[C@@H](C3=O)C[N@@]1Cc5c4ccc(c5)C(S(=O)(=O)CC6(C)C6)C#N</chem>
RUN:	RUN814
DDG (kcal/mol):	5.42
dDDG (kcal/mol):	0.31

EDJ-MED-8bb691af-2_4



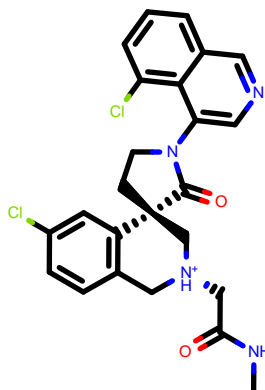
CID:	EDJ-MED-8bb691af-2_4
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3)C[N@@]1Cc5c4ccc(c5)C(S(=O)(=O)CC6(C)C6)C#N</chem>
RUN:	RUN683
DDG (kcal/mol):	5.43
dDDG (kcal/mol):	0.34

EDJ-MED-8bb691af-2_2



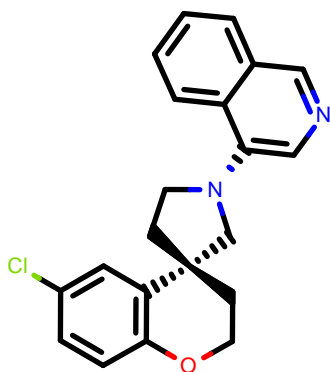
CID:	EDJ-MED-8bb691af-2_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3)C[N@@]1Cc5c4ccc(c5)C(S(=O)(=O)CC6(C)C6)C#N</chem>
RUN:	RUN681
DDG (kcal/mol):	5.43
dDDG (kcal/mol):	0.37

MAT-POS-b4d6b7fc-6_1



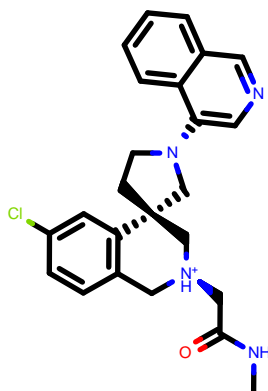
CID:	MAT-POS-b4d6b7fc-6_1
SMILES:	<chem>CNC(=O)C[N@@H+]1C2ccc(cc2C@]3(C1)CCN(C3=O)c4cnc5c4c(ccc5)C)Cl</chem>
RUN:	RUN587
DDG (kcal/mol):	5.50
dDDG (kcal/mol):	0.26

MAT-POS-983b399a-2_2



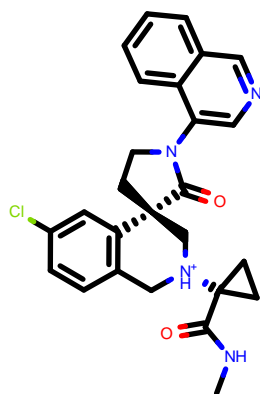
CID:	MAT-POS-983b399a-2_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN487
DDG (kcal/mol):	5.52
dDDG (kcal/mol):	0.09

EDJ-MED-8bb691af-1_4



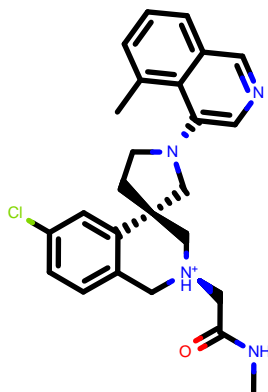
CID:	EDJ-MED-8bb691af-1_4
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)CCN(C3)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN548
DDG (kcal/mol):	5.55
dDDG (kcal/mol):	0.16

ALP-POS-ecbed2ba-7_1



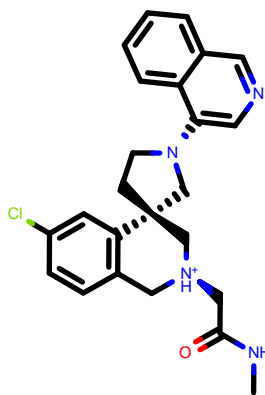
CID:	ALP-POS-ecbed2ba-7_1
SMILES:	<chem>CNC(=O)C1(CC1)N@H+]2Cc3ccc(cc3[C@@]4(C2)CCN(C4=O)c5cnc6c5cccc6)Cl</chem>
RUN:	RUN635
DDG (kcal/mol):	5.57
dDDG (kcal/mol):	0.20

EDJ-MED-3656d29d-1_3



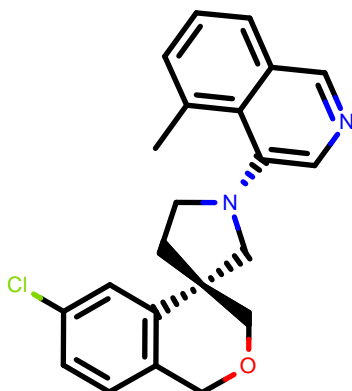
CID:	EDJ-MED-3656d29d-1_3
SMILES:	<chem>Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)C[N@H+](C5c4cc(cc5)C)C(=O)NC</chem>
RUN:	RUN567
DDG (kcal/mol):	5.58
dDDG (kcal/mol):	0.16

EDJ-MED-8bb691af-1_2



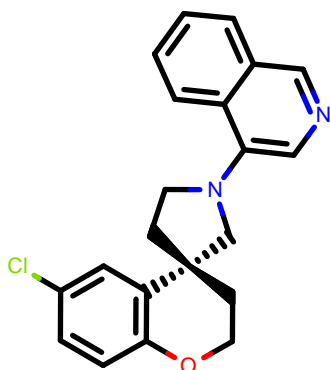
CID:	EDJ-MED-8bb691af-1_2
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)CCN(C3)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN544
DDG (kcal/mol):	5.59
dDDG (kcal/mol):	0.19

EDJ-MED-f3cfbbb5-1_1



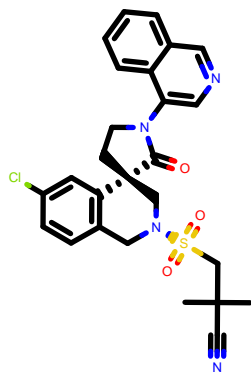
CID:	EDJ-MED-f3cfbbb5-1_1
SMILES:	<chem>Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl</chem>
RUN:	RUN498
DDG (kcal/mol):	5.63
dDDG (kcal/mol):	0.08

EDJ-MED-159244ea-2_2



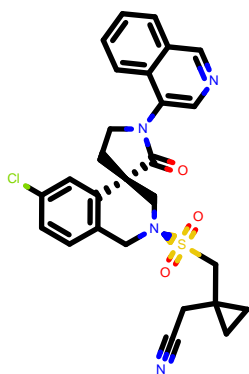
CID:	EDJ-MED-159244ea-2_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl</chem>
RUN:	RUN489
DDG (kcal/mol):	5.65
dDDG (kcal/mol):	0.10

ALP-POS-ecbed2ba-13_2



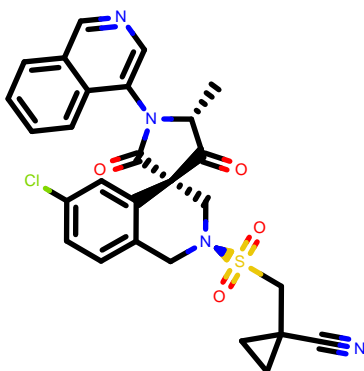
CID:	ALP-POS-ecbed2ba-13_2
SMILES:	<chem>CC(C)(CS(=O)(=O)[N@]1Cc2ccc(cc2[C@@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)C#N</chem>
RUN:	RUN733
DDG (kcal/mol):	5.65
dDDG (kcal/mol):	0.40

ALP-POS-ecbed2ba-22_2



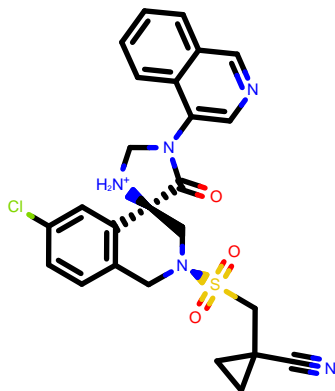
CID:	ALP-POS-ecbed2ba-22_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@@]4(C3=O)C[N@]([C@5c4cc(cc5)Cl])S(=O)(=O)CC6(CC6)CC#N</chem>
RUN:	RUN798
DDG (kcal/mol):	5.72
dDDG (kcal/mol):	0.44

PET-UNK-94036022-6_1



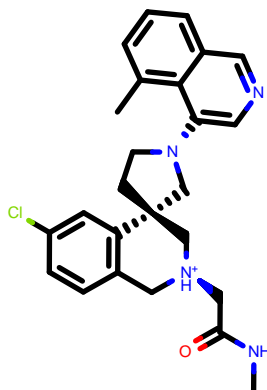
CID:	PET-UNK-94036022-6_1
SMILES:	<chem>C=C1C=O[C@]2(CN@]3C)S(=O)(=O)CC4(CN)C1=O[N15cnc6c5ccc6</chem>
RUN:	RUN867
DDG (kcal/mol):	5.74
dDDG (kcal/mol):	0.43

EDG-MED-00af8776-1_2



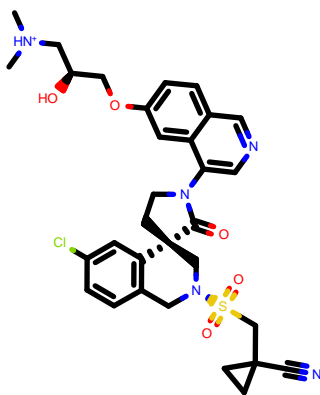
CID:	EDG-MED-00af8776-1_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C=[NH+]4C@]([C3=O)C[N@]([C@5c4cc(cc5)Cl])S(=O)(=O)CC6(CO6)C#N</chem>
RUN:	RUN737
DDG (kcal/mol):	5.75
dDDG (kcal/mol):	0.38

EDJ-MED-3656d29d-1_4



CID:	EDJ-MED-3656d29d-1_4
SMILES:	<chem>Cc1cccc2c1c(nc2)N3CC[C@@]4(C3)C[N@]([C@5c4cc(cc5)Cl])C1CC1=O)NC</chem>
RUN:	RUN563
DDG (kcal/mol):	5.91
dDDG (kcal/mol):	0.21

EDJ-MED-ee81482e-3_3



CID:	EDJ-MED-ee81482e-3_3
SMILES:	<chem>C[NH+](C)C(C @ H)(COc1ccc2ncnc2c1)N3CC(C @ H)(C3-O)C(N @)C5c4ccc(cc5C)S(-O)(-O)CC6(C)C#N6</chem>
RUN:	RUN943
DDG (kcal/mol):	5.94
dDDG (kcal/mol):	0.79