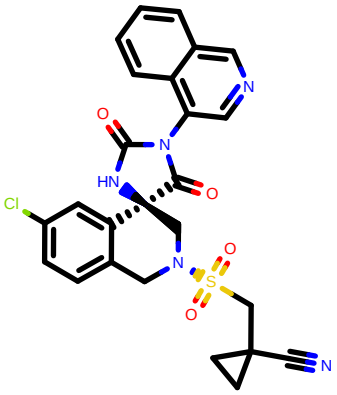
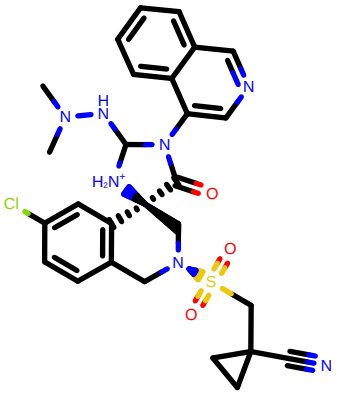
MAT-POS-c2d406ed-1_2



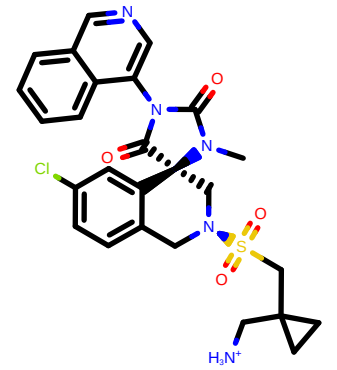
CID:	MAT-POS-c2d406ed-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=O
RUN:	RUN310
DDG (kcal/mol):	-4.01
dDDG (kcal/mol):	0.29

LUO-POS-b5068a05-1_2



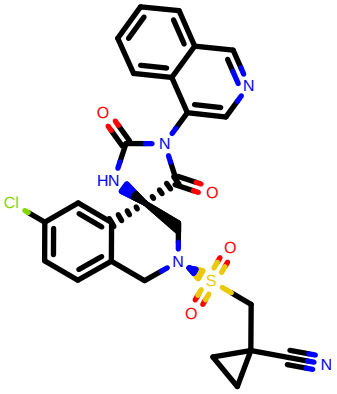
CID:	LUO-POS-b5068a05-1_2
SMILES:	C[NH+](C)NC1=N[C@]2(C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN424
DDG (kcal/mol):	-3.44
dDDG (kcal/mol):	0.51

MAT-POS-c2d406ed-2_2



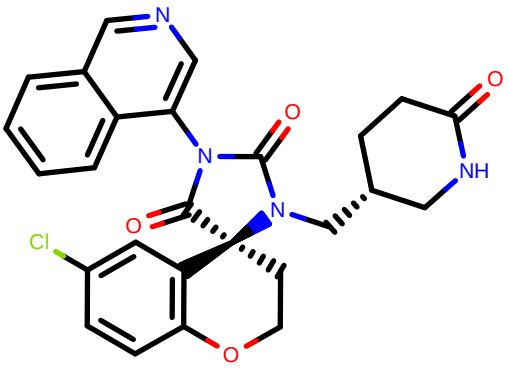
CID:	MAT-POS-c2d406ed-2_2
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN364
DDG (kcal/mol):	-2.49
dDDG (kcal/mol):	0.30

MAT-POS-c2d406ed-1_1



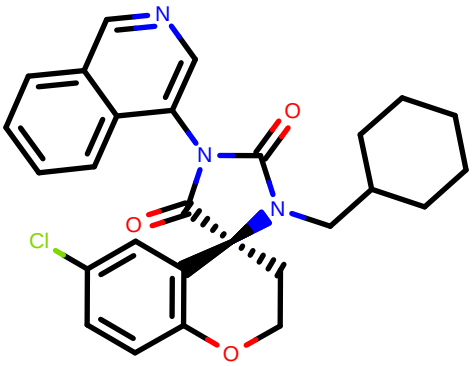
CID:	MAT-POS-c2d406ed-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=O
RUN:	RUN320
DDG (kcal/mol):	-2.48
dDDG (kcal/mol):	0.19

VLA-UNK-f702bf1c-5_1



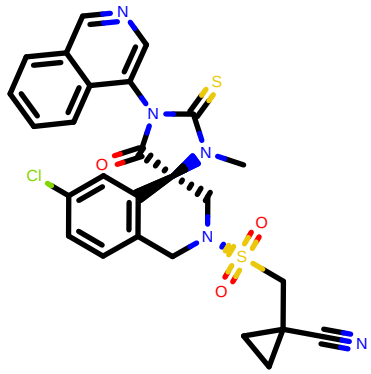
CID:	VLA-UNK-f702bf1c-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@@H]6CCC(=O)NC6
RUN:	RUN227
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.16

VLA-UNK-f702bf1c-6_1



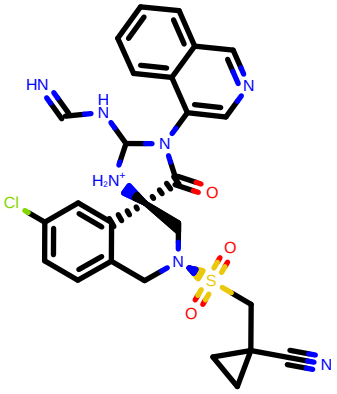
CID:	VLA-UNK-f702bf1c-6_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCCC6
RUN:	RUN181
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.11

MAT-POS-c2d406ed-4_2



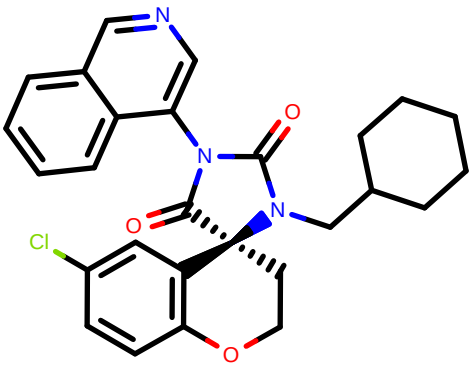
CID:	MAT-POS-c2d406ed-4_2
SMILES:	CN1C(=S)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN368
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.39

LUO-POS-b5068a05-2_2



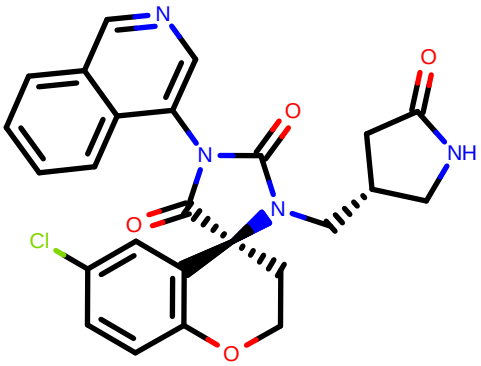
CID:	LUO-POS-b5068a05-2_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)N=C3NC#N
RUN:	RUN412
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.34

VLA-UCB-34f3ed0c-14_1



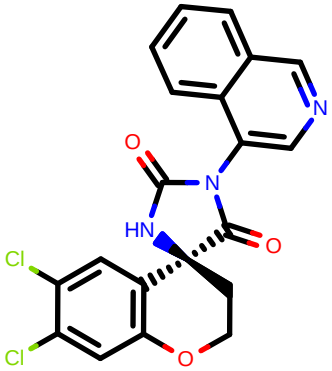
CID:	VLA-UCB-34f3ed0c-14_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCCC6
RUN:	RUN174
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.12

VLA-UNK-f702bf1c-4_1



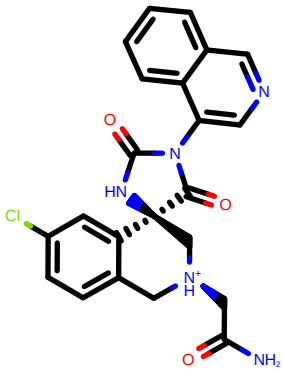
CID:	VLA-UNK-f702bf1c-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@@H]6CC(=O)NC6
RUN:	RUN189
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.12

VLA-UNK-56836b69-2_1



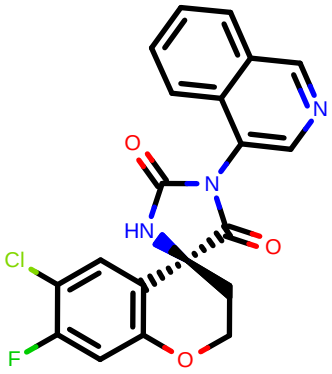
CID:	VLA-UNK-56836b69-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)Cl)NC3=O
RUN:	RUN33
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.07

VLA-MRT-8c78ee15-4_2



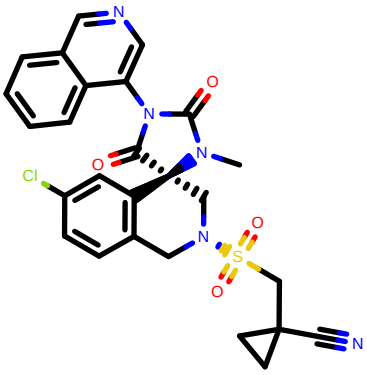
CID:	VLA-MRT-8c78ee15-4_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN64
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.14

VLA-UNK-3a43cd95-1_1



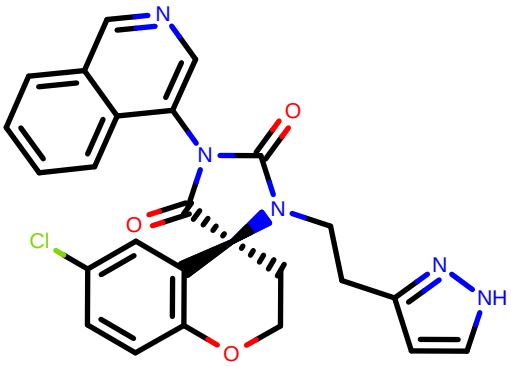
CID:	VLA-UNK-3a43cd95-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)F)Cl)NC3=O
RUN:	RUN42
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.06

MAT-POS-c2d406ed-2_1



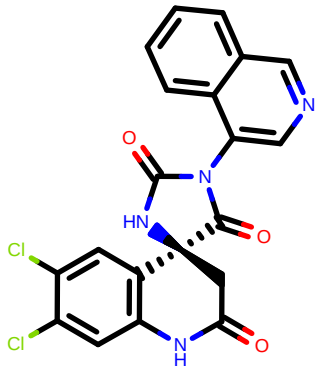
CID:	MAT-POS-c2d406ed-2_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN362
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.16

VLA-UNK-f702bf1c-1_1



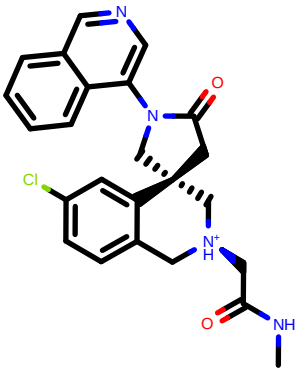
CID:	VLA-UNK-f702bf1c-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCc6ccn[nH]6
RUN:	RUN190
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.12

VLA-UNK-56836b69-5_1



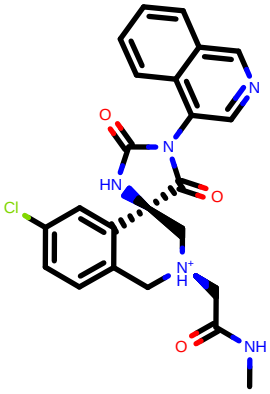
CID:	VLA-UNK-56836b69-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CC(=O)Nc5c4cc(c(c5)Cl)Cl)NC3=O
RUN:	RUN43
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.09

EDJ-MED-8bb691af-3_2



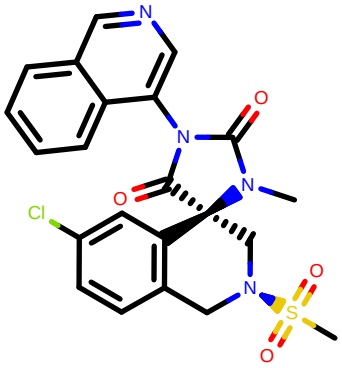
CID:	EDJ-MED-8bb691af-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3)c4cncc5c4cccc5)Cl
RUN:	RUN68
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.17

VLA-MRT-a639d434-1_2



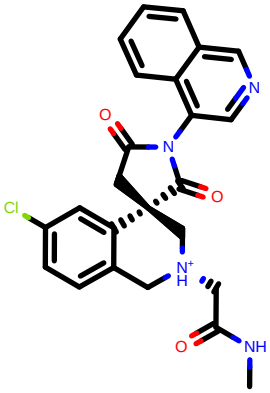
CID:	VLA-MRT-a639d434-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN97
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.19

MAT-POS-2e8b2191-8_1



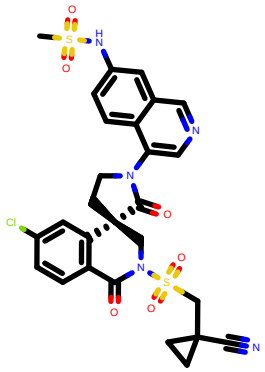
CID:	MAT-POS-2e8b2191-8_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN87
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.11

JOH-MSK-1f2dff76-1_1



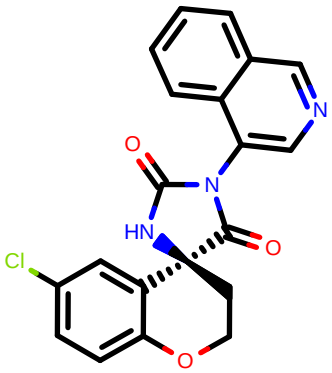
CID:	JOH-MSK-1f2dff76-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN127
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.26

EDJ-MED-9f4ac58c-3_1



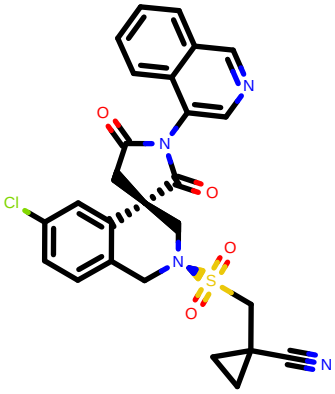
CID:	EDJ-MED-9f4ac58c-3_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN431
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.60

VLA-UCB-34f3ed0c-11_1



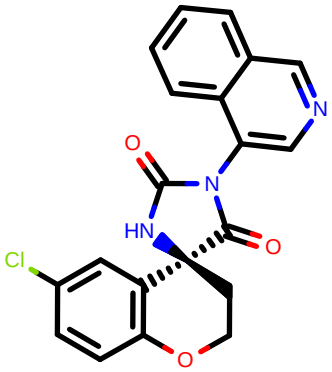
CID:	VLA-UCB-34f3ed0c-11_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN27
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.04

LUO-POS-868e8996-9_1



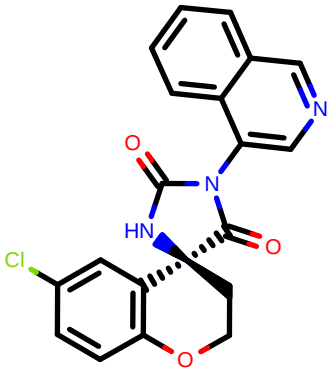
CID:	LUO-POS-868e8996-9_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN295
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.26

VLA-UCB-29506327-1_1



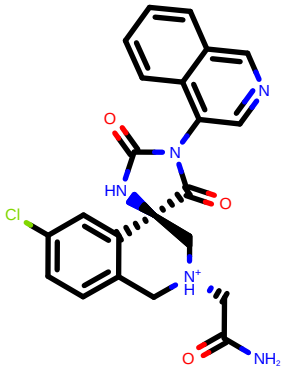
CID:	VLA-UCB-29506327-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN29
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.05

VLA-UNK-cf7facf1-1_1



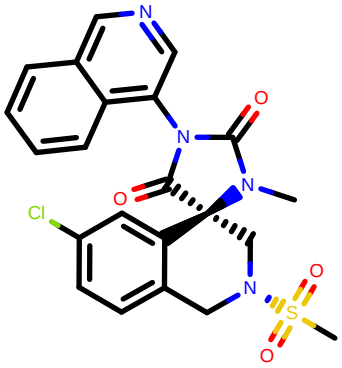
CID:	VLA-UNK-cf7facf1-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN22
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.05

VLA-MRT-a639d434-2_1



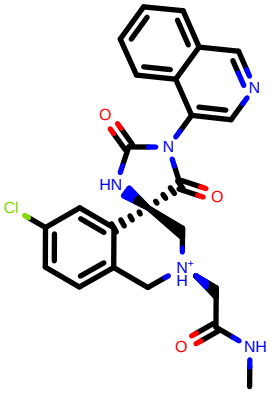
CID:	VLA-MRT-a639d434-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN65
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.18

EDJ-MED-7587a9ee-1_2



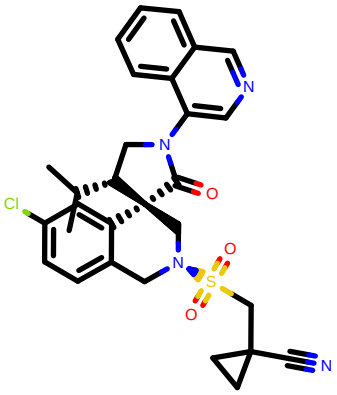
CID:	EDJ-MED-7587a9ee-1_2
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN86
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.09

VLA-MRT-8c78ee15-3_2



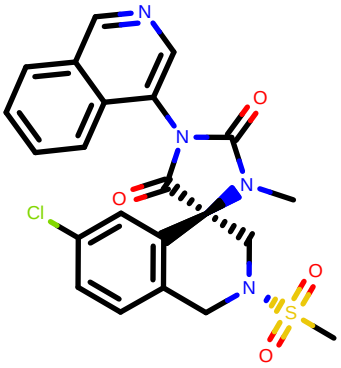
CID:	VLA-MRT-8c78ee15-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN93
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.19

MAT-POS-50a80394-3_3



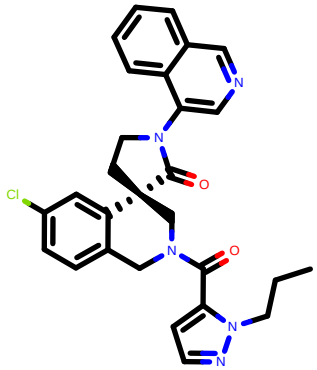
CID:	MAT-POS-50a80394-3_3
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN397
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.44

MAT-POS-2e8b2191-8_2



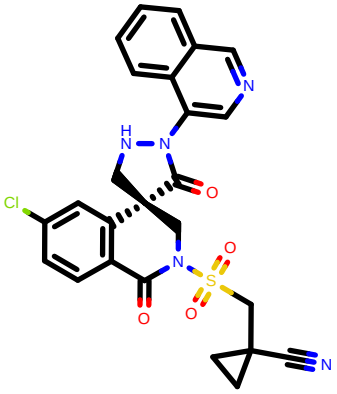
CID:	MAT-POS-2e8b2191-8_2
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN95
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.10

MAT-POS-be048f2c-8_1



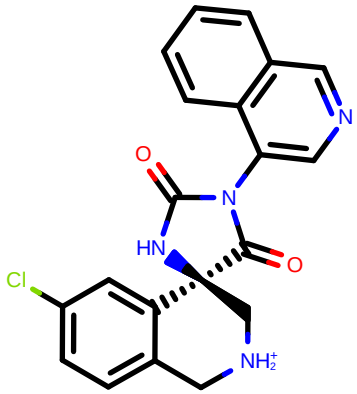
CID:	MAT-POS-be048f2c-8_1
SMILES:	CCCn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN340
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.14

EDJ-MED-fed7ac0b-3_1



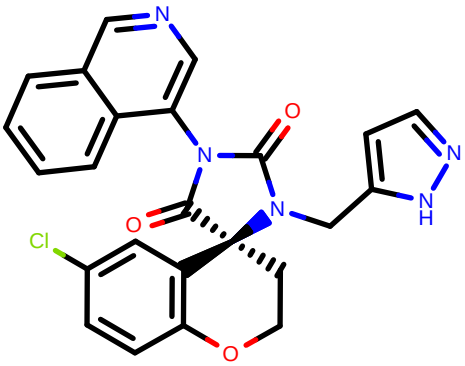
CID:	EDJ-MED-fed7ac0b-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@]4(CN3)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN323
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.40

VLA-MRT-8c78ee15-1_1



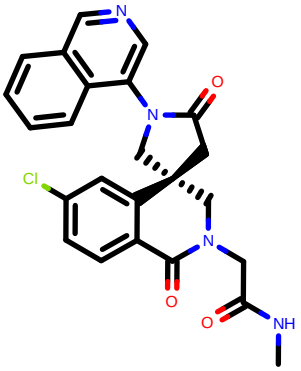
CID:	VLA-MRT-8c78ee15-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN31
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.16

VLA-UNK-f702bf1c-2_1



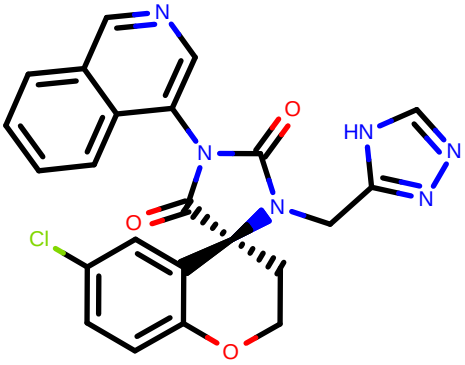
CID:	VLA-UNK-f702bf1c-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)Cc6ccn[nH]6
RUN:	RUN136
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.11

EDJ-MED-8bb691af-9_1



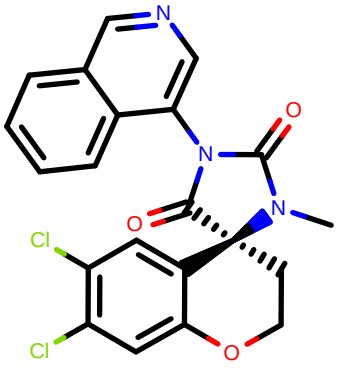
CID:	EDJ-MED-8bb691af-9_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN92
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.10

VLA-UNK-f702bf1c-3_1



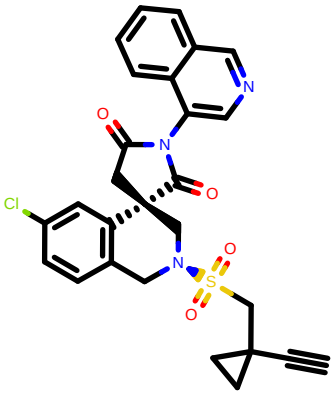
CID:	VLA-UNK-f702bf1c-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)Cc6[nH]ncn6
RUN:	RUN137
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.13

VLA-UNK-56836b69-3_1



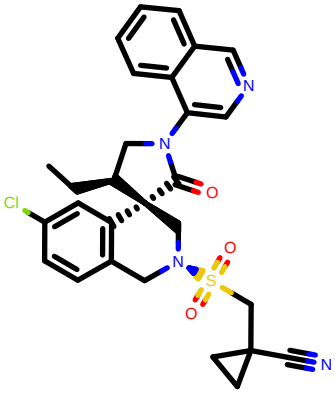
CID:	VLA-UNK-56836b69-3_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(c(c3)Cl)Cl)c4cncc5c4cccc5
RUN:	RUN37
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.08

PET-UNK-94036022-4_1



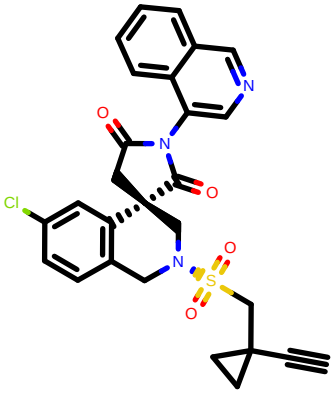
CID:	PET-UNK-94036022-4_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN336
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.24

MAT-POS-50a80394-2_2



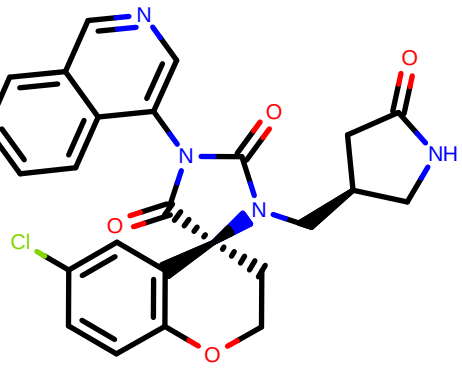
CID:	MAT-POS-50a80394-2_2
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN369
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.44

PET-UNK-94036022-11_2



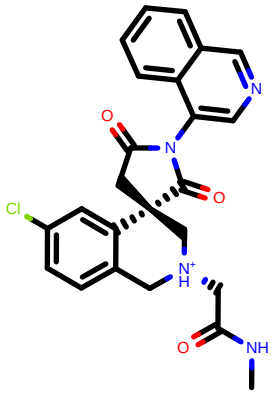
CID:	PET-UNK-94036022-11_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN341
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.31

VLA-UNK-f702bf1c-4_2



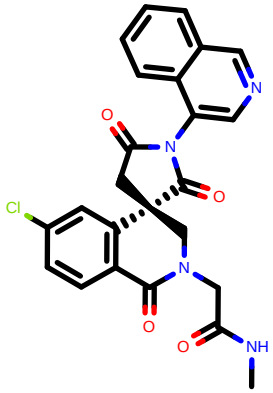
CID:	VLA-UNK-f702bf1c-4_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CC(=O)NC6
RUN:	RUN187
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.12

JOH-MSK-1f2dff76-2_1



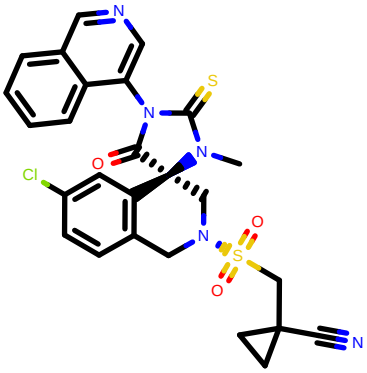
CID:	JOH-MSK-1f2dff76-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN131
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.23

MAT-POS-1bed62cf-2_1



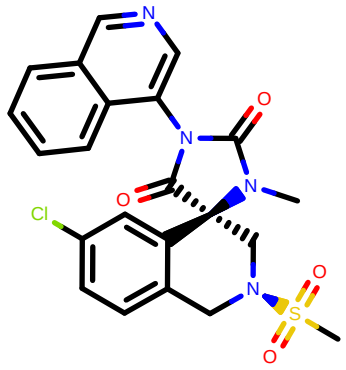
CID:	MAT-POS-1bed62cf-2_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN135
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.09

MAT-POS-c2d406ed-4_1



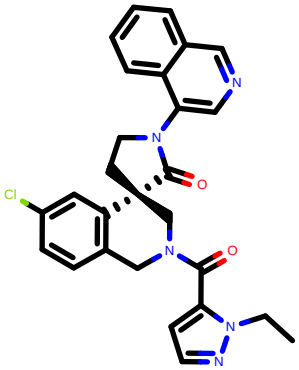
CID:	MAT-POS-c2d406ed-4_1
SMILES:	CN1C(=S)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN365
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.28

EDJ-MED-7587a9ee-1_1



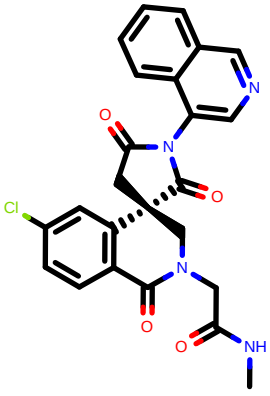
CID:	EDJ-MED-7587a9ee-1_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN85
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.10

MAT-POS-be048f2c-5_1



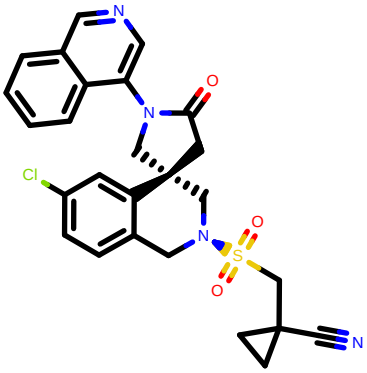
CID:	MAT-POS-be048f2c-5_1
SMILES:	CCn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN278
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.11

LUO-POS-868e8996-8_1



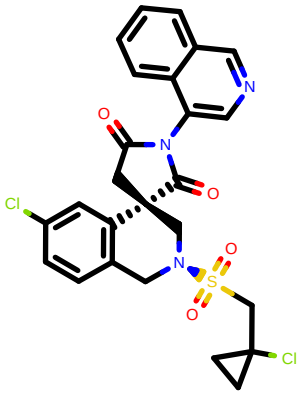
CID:	LUO-POS-868e8996-8_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN145
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.10

EDJ-MED-8bb691af-5_2



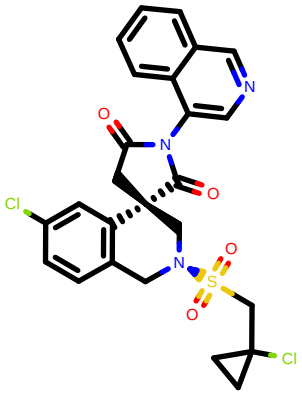
CID:	EDJ-MED-8bb691af-5_2
SMILES:	c1ccc2c(c1)cncc2N3C[C@]4(CC3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN234
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.38

PET-UNK-94036022-5_1



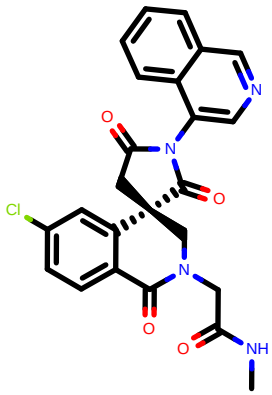
CID:	PET-UNK-94036022-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN280
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.21

PET-UNK-94036022-5_2



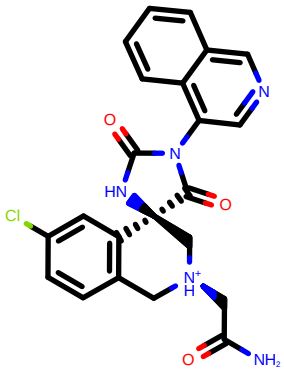
CID:	PET-UNK-94036022-5_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN282
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.30

LUO-POS-868e8996-7_1



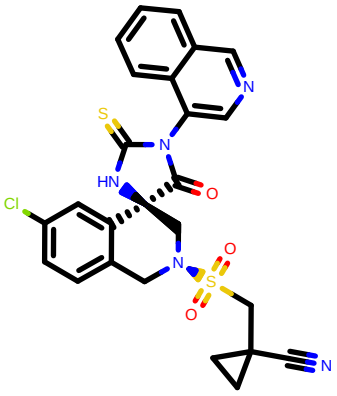
CID:	LUO-POS-868e8996-7_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN143
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.10

VLA-MRT-a639d434-2_2



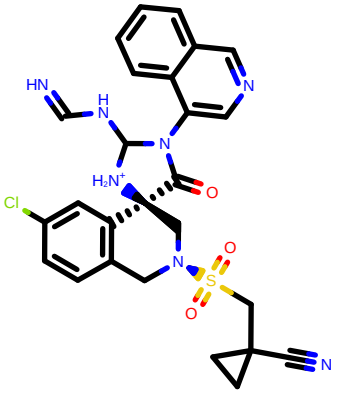
CID:	VLA-MRT-a639d434-2_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN67
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.18

MAT-POS-c2d406ed-3_1



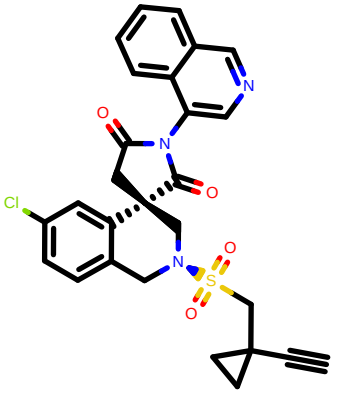
CID:	MAT-POS-c2d406ed-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=S
RUN:	RUN324
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.27

LUO-POS-b5068a05-2_1



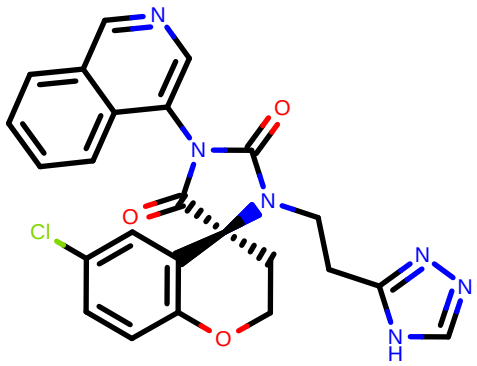
CID:	LUO-POS-b5068a05-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)N=C3NC#N
RUN:	RUN405
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.28

PET-UNK-94036022-11_1



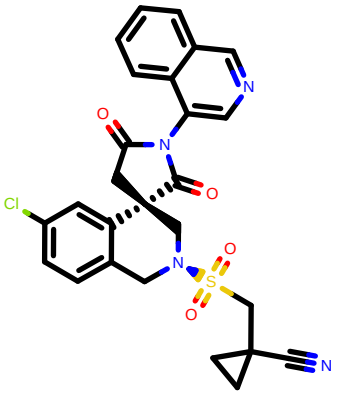
CID:	PET-UNK-94036022-11_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN351
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.23

VLA-UNK-f702bf1c-8_1



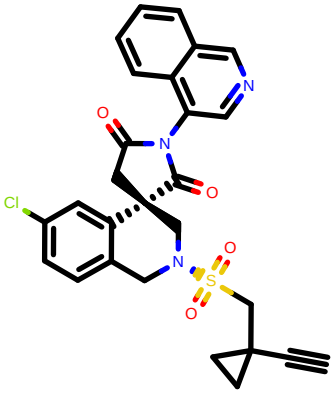
CID:	VLA-UNK-f702bf1c-8_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCc6[nH]ncn6
RUN:	RUN192
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.19

MAT-POS-1bed62cf-1_1



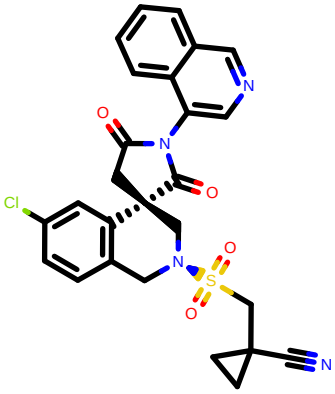
CID:	MAT-POS-1bed62cf-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN291
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.29

PET-UNK-94036022-4_2



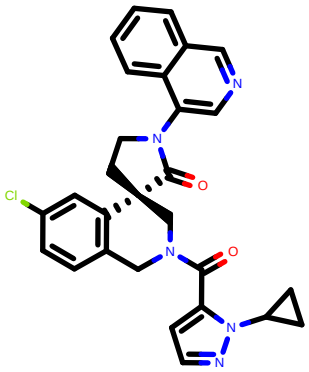
CID:	PET-UNK-94036022-4_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN349
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.34

MAT-POS-1bed62cf-1_2



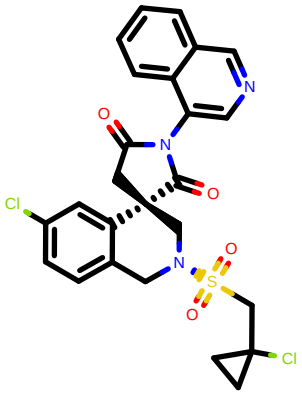
CID:	MAT-POS-1bed62cf-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN287
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.39

MAT-POS-be048f2c-7_1



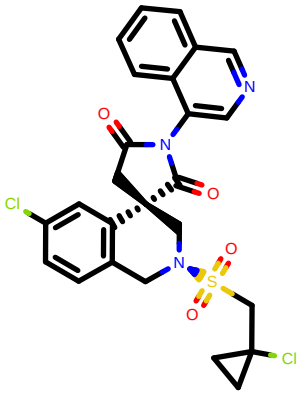
CID:	MAT-POS-be048f2c-7_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(Cc5c4cc(cc5)Cl)C(=O)c6ccnn6C7CC7
RUN:	RUN326
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.14

PET-UNK-94036022-12_2



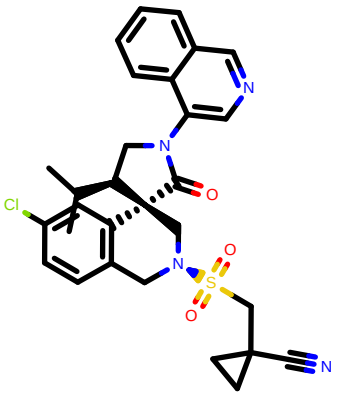
CID:	PET-UNK-94036022-12_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN290
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.30

PET-UNK-94036022-12_1



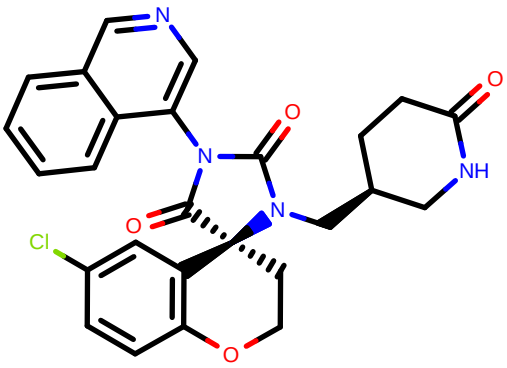
CID:	PET-UNK-94036022-12_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN288
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.25

MAT-POS-50a80394-3_2



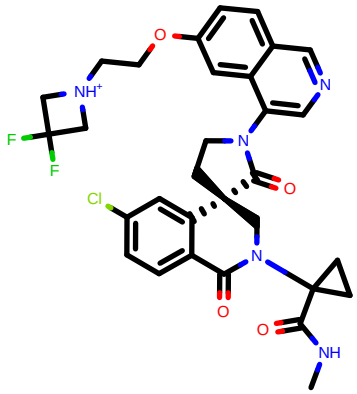
CID:	MAT-POS-50a80394-3_2
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN393
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.43

VLA-UNK-f702bf1c-5_2



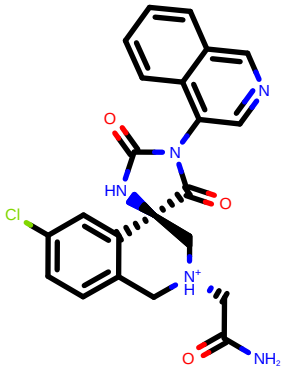
CID:	VLA-UNK-f702bf1c-5_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CCC(=O)NC6
RUN:	RUN228
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.14

EDJ-MED-dfa1d800-5_1



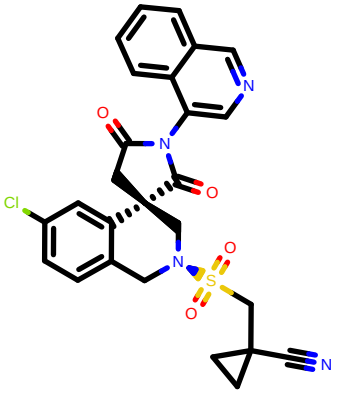
CID:	EDJ-MED-dfa1d800-5_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCCN6CC(C6)(F)F)c7cc(ccc7C2=O)Cl
RUN:	RUN459
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.19

VLA-MRT-8c78ee15-4_1



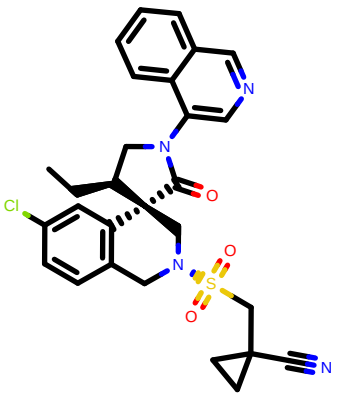
CID:	VLA-MRT-8c78ee15-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN63
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.20

LUO-POS-868e8996-10_1



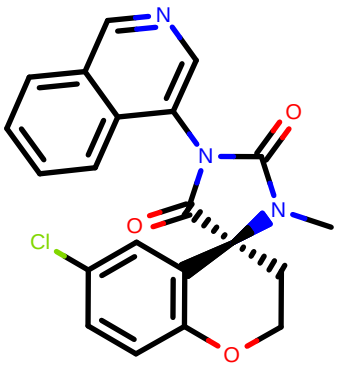
CID:	LUO-POS-868e8996-10_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN296
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.29

MAT-POS-50a80394-2_4



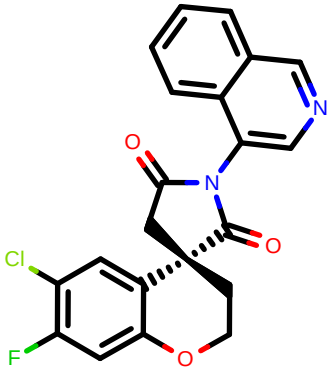
CID:	MAT-POS-50a80394-2_4
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5ncc6c5cccc6
RUN:	RUN374
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.36

BEN-BAS-c2bc0d80-7_1



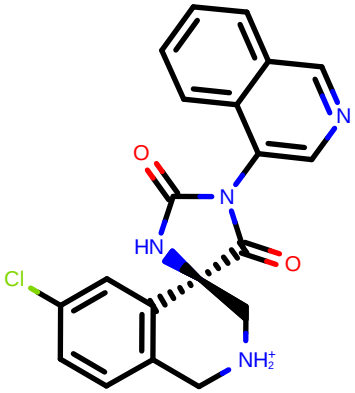
CID:	BEN-BAS-c2bc0d80-7_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(cc3)Cl)c4cncc5c4cccc5
RUN:	RUN34
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.06

VLA-UNK-3a43cd95-3_1



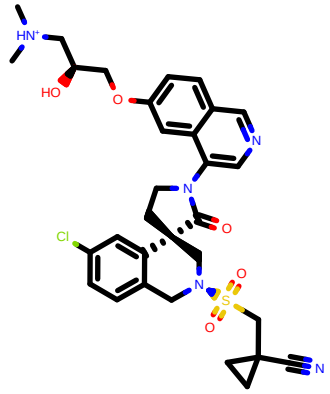
CID:	VLA-UNK-3a43cd95-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(c(c5)F)Cl
RUN:	RUN38
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.04

VLA-MRT-8c78ee15-2_1



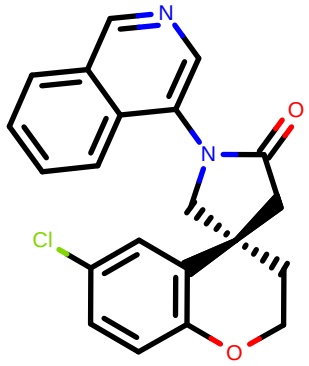
CID:	VLA-MRT-8c78ee15-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN36
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.16

EDJ-MED-ee81482e-3_3



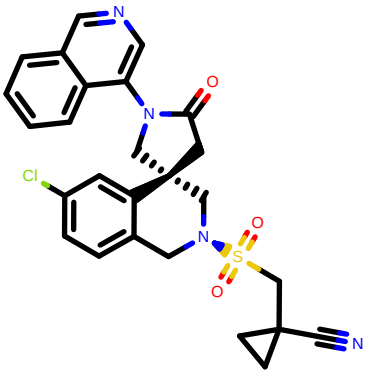
CID:	EDJ-MED-ee81482e-3_3
SMILES:	C[NH+](C)C[C@@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN456
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.88

MAT-POS-983b399a-3_1



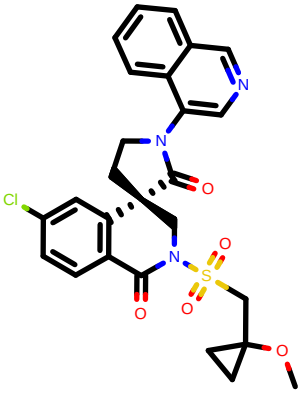
CID:	MAT-POS-983b399a-3_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O
RUN:	RUN25
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.06

EDJ-MED-8bb691af-5_1



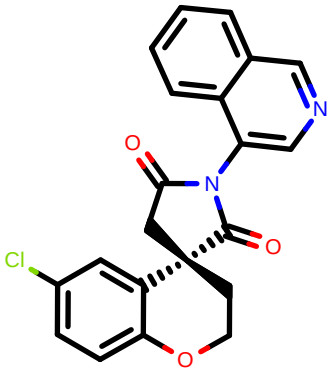
CID:	EDJ-MED-8bb691af-5_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@]4(CC3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN231
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.37

EDJ-MED-9f4ac58c-6_1



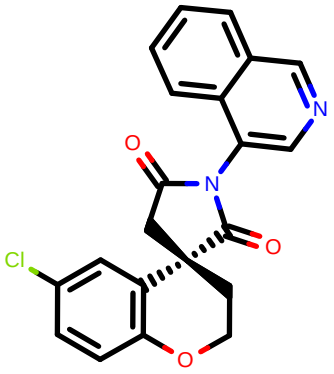
CID:	EDJ-MED-9f4ac58c-6_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN298
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.36

VLA-UCB-05e51b3f-5_1



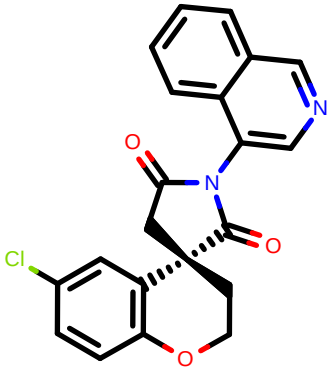
CID:	VLA-UCB-05e51b3f-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN17
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.00

BEN-BAS-c2bc0d80-6_1



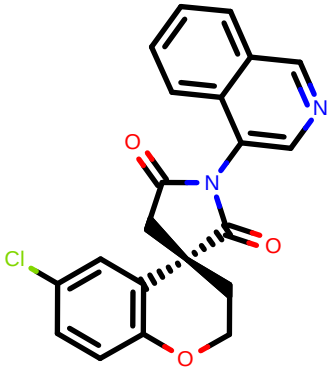
CID:	BEN-BAS-c2bc0d80-6_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN20
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.00

MAT-POS-94643566-1_1



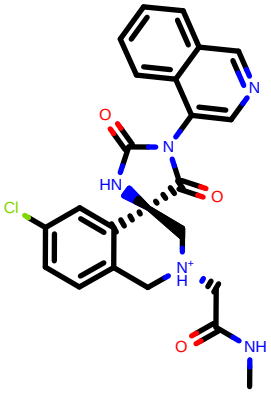
CID:	MAT-POS-94643566-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN21
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.00

VLA-UCB-50c39ae8-2_1



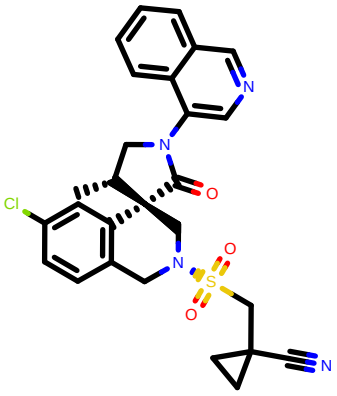
CID:	VLA-UCB-50c39ae8-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN18
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.00

VLA-MRT-a639d434-1_1



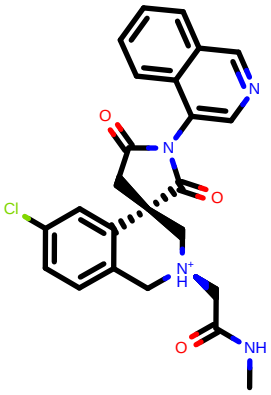
CID:	VLA-MRT-a639d434-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN88
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.23

MAT-POS-50a80394-1_3



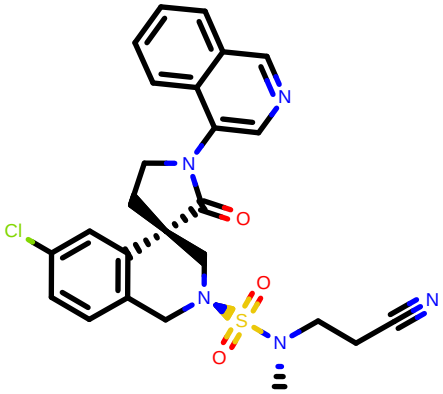
CID:	MAT-POS-50a80394-1_3
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5ncc6c5cccc6
RUN:	RUN338
DDG (kcal/mol):	0.03
dDDG (kcal/mol):	0.43

JOH-MSK-1f2dff76-1_2



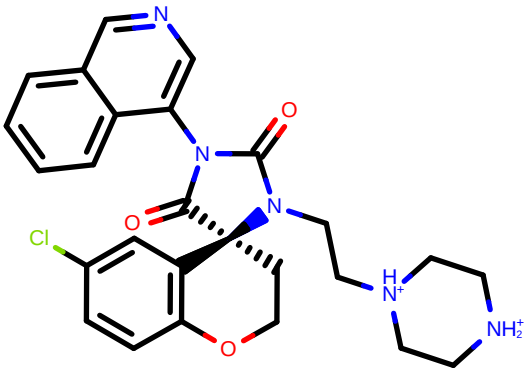
CID:	JOH-MSK-1f2dff76-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN132
DDG (kcal/mol):	0.03
dDDG (kcal/mol):	0.15

ALP-POS-ecbed2ba-16_3



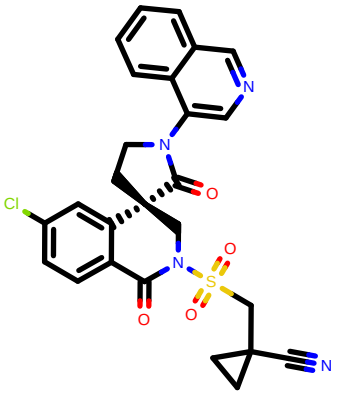
CID:	ALP-POS-ecbed2ba-16_3
SMILES:	C[N@@](CCC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN257
DDG (kcal/mol):	0.08
dDDG (kcal/mol):	0.67

VLA-UNK-f702bf1c-7_1



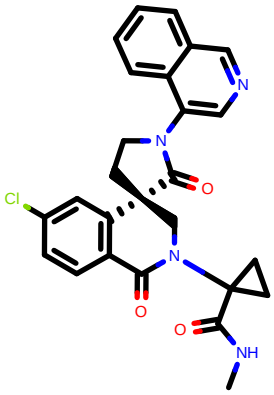
CID:	VLA-UNK-f702bf1c-7_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCN6CC[NH2+]CC6
RUN:	RUN230
DDG (kcal/mol):	0.08
dDDG (kcal/mol):	0.19

EDJ-MED-9f4ac58c-2_1



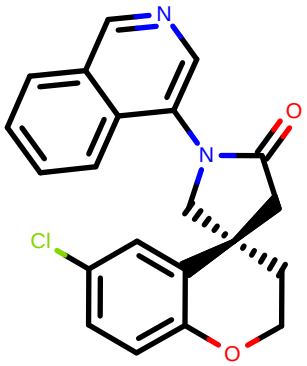
CID:	EDJ-MED-9f4ac58c-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN294
DDG (kcal/mol):	0.12
dDDG (kcal/mol):	0.39

MAT-POS-576f7758-2_1



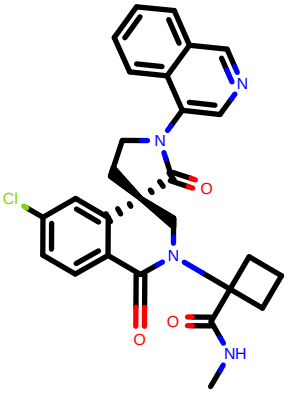
CID:	MAT-POS-576f7758-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN205
DDG (kcal/mol):	0.14
dDDG (kcal/mol):	0.11

EDJ-MED-159244ea-3_1



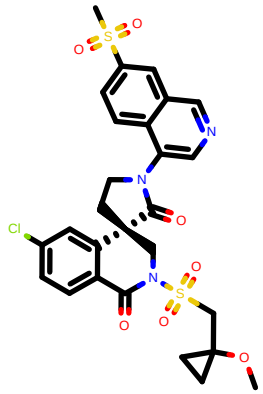
CID:	EDJ-MED-159244ea-3_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O
RUN:	RUN7
DDG (kcal/mol):	0.18
dDDG (kcal/mol):	0.07

EDJ-MED-98c0a822-3_1



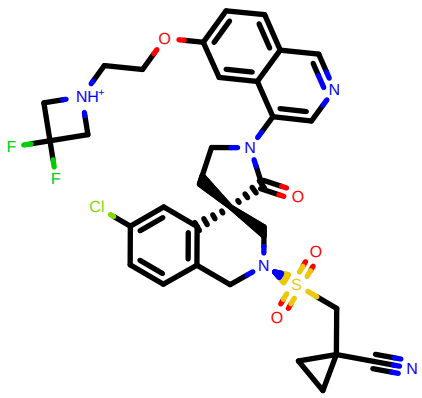
CID:	EDJ-MED-98c0a822-3_1
SMILES:	CNC(=O)C1(CCC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN272
DDG (kcal/mol):	0.21
dDDG (kcal/mol):	0.20

EDJ-MED-9f4ac58c-8_1



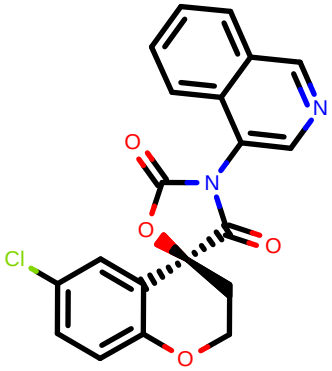
CID:	EDJ-MED-9f4ac58c-8_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)S(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN422
DDG (kcal/mol):	0.23
dDDG (kcal/mol):	0.47

EDJ-MED-468565e0-5_1



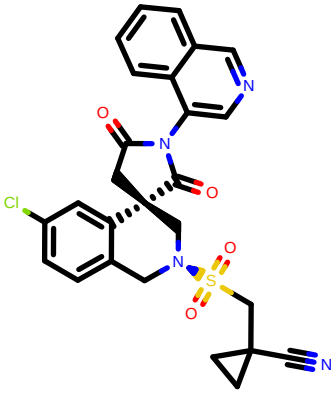
CID:	EDJ-MED-468565e0-5_1
SMILES:	c1cc2cncc(c2cc1OCCN3CC(C3)(F)F)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN475
DDG (kcal/mol):	0.26
dDDG (kcal/mol):	0.44

MAT-POS-90505e2b-1_1



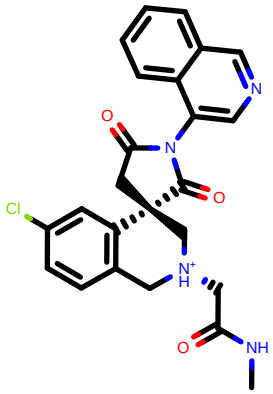
CID:	MAT-POS-90505e2b-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN23
DDG (kcal/mol):	0.26
dDDG (kcal/mol):	0.03

LUO-POS-868e8996-10_2



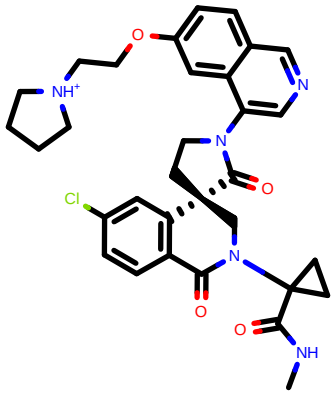
CID:	LUO-POS-868e8996-10_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN297
DDG (kcal/mol):	0.34
dDDG (kcal/mol):	0.41

MAT-POS-1bed62cf-3_1



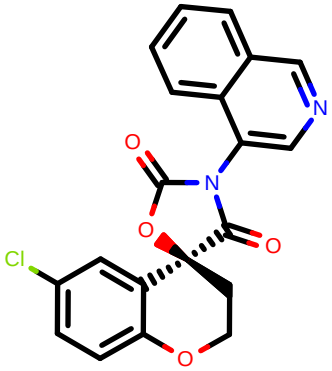
CID:	MAT-POS-1bed62cf-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN98
DDG (kcal/mol):	0.34
dDDG (kcal/mol):	0.24

EDJ-MED-dfa1d800-1_1



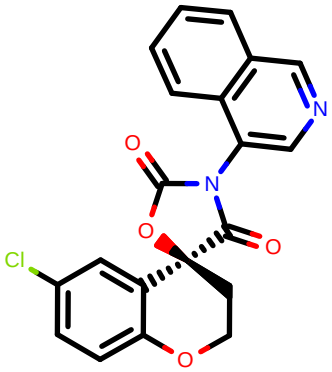
CID:	EDJ-MED-dfa1d800-1_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCCC6)c7cc(ccc7C2=O)Cl
RUN:	RUN439
DDG (kcal/mol):	0.40
dDDG (kcal/mol):	0.28

MAT-POS-ec6d90b7-1_1



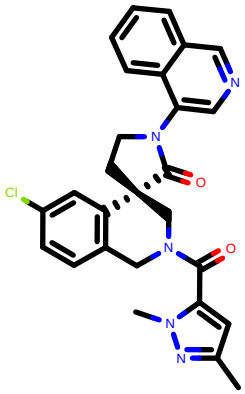
CID:	MAT-POS-ec6d90b7-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN24
DDG (kcal/mol):	0.40
dDDG (kcal/mol):	0.03

MAT-POS-ec6d90b7-2_1



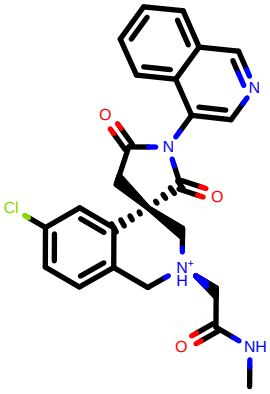
CID:	MAT-POS-ec6d90b7-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN26
DDG (kcal/mol):	0.41
dDDG (kcal/mol):	0.03

EDJ-MED-cc48ee33-5_1



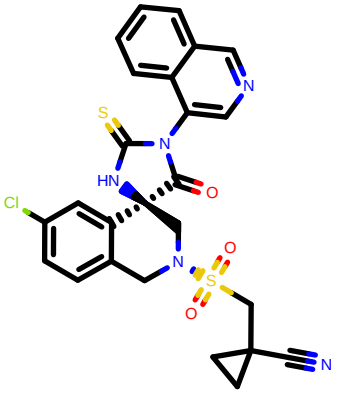
CID:	EDJ-MED-cc48ee33-5_1
SMILES:	Cc1cc(n(n1)C)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN276
DDG (kcal/mol):	0.41
dDDG (kcal/mol):	0.13

MAT-POS-1bed62cf-3_2



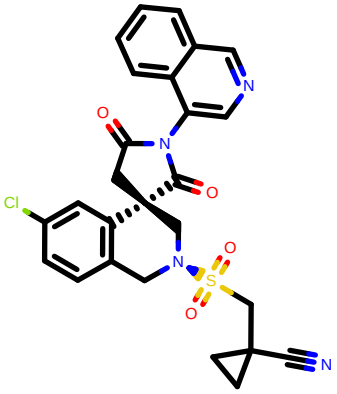
CID:	MAT-POS-1bed62cf-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN94
DDG (kcal/mol):	0.47
dDDG (kcal/mol):	0.17

MAT-POS-c2d406ed-3_2



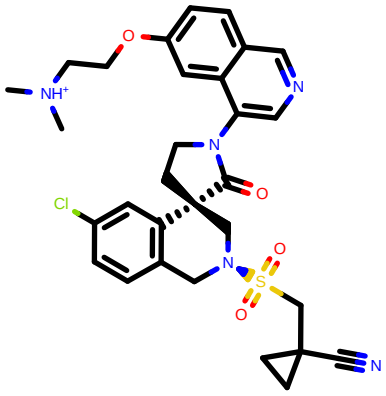
CID:	MAT-POS-c2d406ed-3_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=S
RUN:	RUN325
DDG (kcal/mol):	0.48
dDDG (kcal/mol):	0.29

LUO-POS-868e8996-9_2



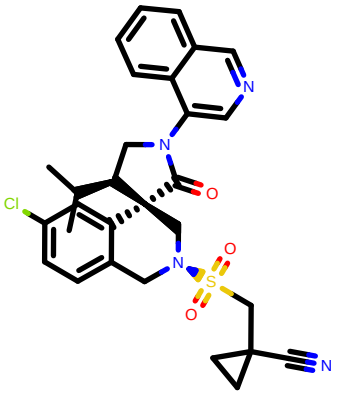
CID:	LUO-POS-868e8996-9_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN293
DDG (kcal/mol):	0.48
dDDG (kcal/mol):	0.40

MAT-POS-853c0ffa-9_1



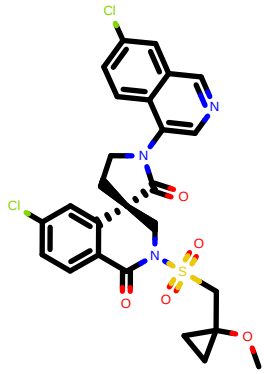
CID:	MAT-POS-853c0ffa-9_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN435
DDG (kcal/mol):	0.52
dDDG (kcal/mol):	0.49

MAT-POS-50a80394-3_4



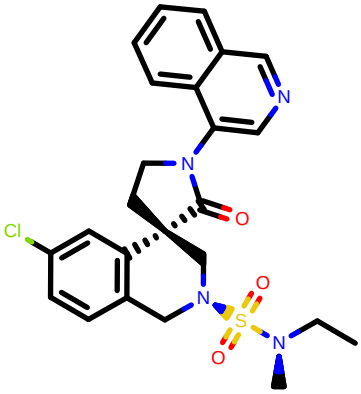
CID:	MAT-POS-50a80394-3_4
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN398
DDG (kcal/mol):	0.53
dDDG (kcal/mol):	0.45

EDJ-MED-9f4ac58c-5_1



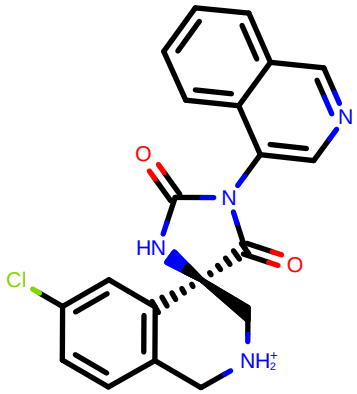
CID:	EDJ-MED-9f4ac58c-5_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)Cl)c6cc(ccc6C2=O)Cl
RUN:	RUN356
DDG (kcal/mol):	0.59
dDDG (kcal/mol):	0.36

ALP-POS-ecbed2ba-18_3



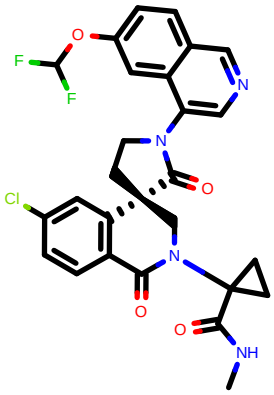
CID:	ALP-POS-ecbed2ba-18_3
SMILES:	CC[N@@](C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN154
DDG (kcal/mol):	0.65
dDDG (kcal/mol):	0.55

VLA-MRT-a639d434-3_1



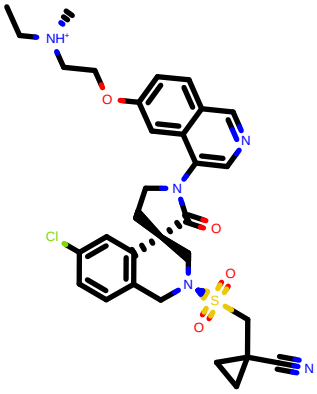
CID:	VLA-MRT-a639d434-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN39
DDG (kcal/mol):	0.66
dDDG (kcal/mol):	0.19

EDJ-MED-5cd3920d-3_1



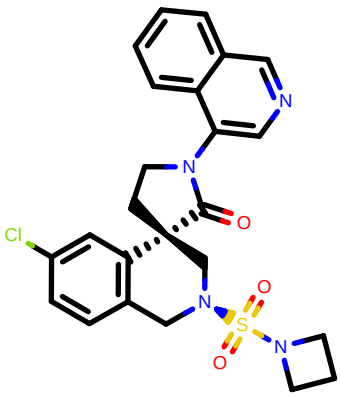
CID:	EDJ-MED-5cd3920d-3_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OC(F)F)c6cc(ccc6C2=O)Cl
RUN:	RUN421
DDG (kcal/mol):	0.67
dDDG (kcal/mol):	0.14

MAT-POS-40ad851a-2_2



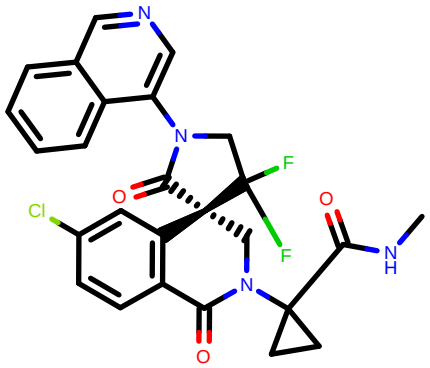
CID:	MAT-POS-40ad851a-2_2
SMILES:	CC[N@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN451
DDG (kcal/mol):	0.72
dDDG (kcal/mol):	0.59

ALP-POS-ecbed2ba-20_2



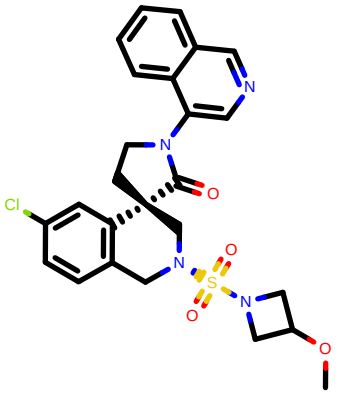
CID:	ALP-POS-ecbed2ba-20_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CCC6
RUN:	RUN155
DDG (kcal/mol):	0.72
dDDG (kcal/mol):	0.71

EDJ-MED-7e491f08-2_1



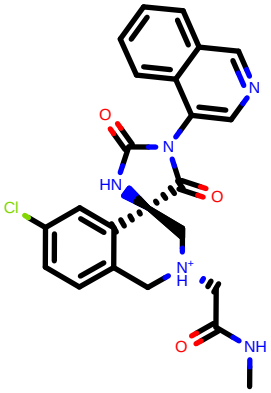
CID:	EDJ-MED-7e491f08-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(c4cc(ccc4C2=O)Cl)C(=O)N(CC3(F)F)c5cncc6c5cccc6
RUN:	RUN344
DDG (kcal/mol):	0.73
dDDG (kcal/mol):	0.15

ALP-POS-ecbed2ba-10_2



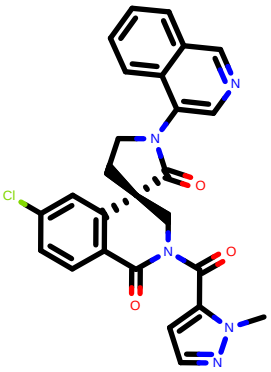
CID:	ALP-POS-ecbed2ba-10_2
SMILES:	COC1CN(C1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN253
DDG (kcal/mol):	0.79
dDDG (kcal/mol):	0.71

VLA-MRT-8c78ee15-3_1



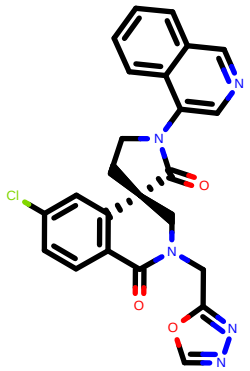
CID:	VLA-MRT-8c78ee15-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN90
DDG (kcal/mol):	0.80
dDDG (kcal/mol):	0.23

EDJ-MED-cc48ee33-2_1



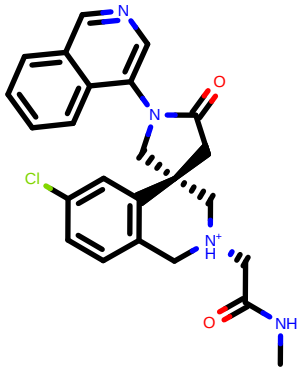
CID:	EDJ-MED-cc48ee33-2_1
SMILES:	Cn1c(ccn1)C(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN269
DDG (kcal/mol):	0.82
dDDG (kcal/mol):	0.14

PET-UNK-aa57768f-7_1



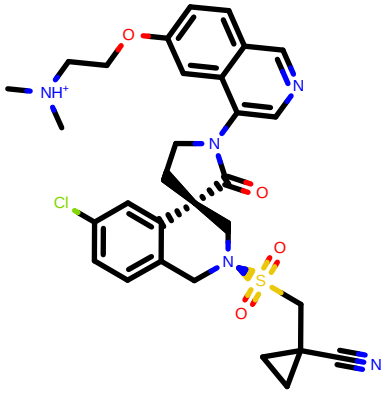
CID:	PET-UNK-aa57768f-7_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN159
DDG (kcal/mol):	0.85
dDDG (kcal/mol):	0.10

EDJ-MED-8bb691af-3_1



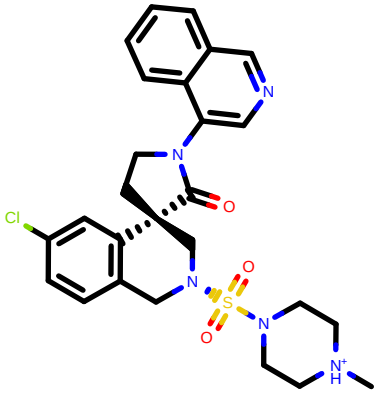
CID:	EDJ-MED-8bb691af-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3)c4cncc5c4cccc5)Cl
RUN:	RUN66
DDG (kcal/mol):	0.86
dDDG (kcal/mol):	0.18

MAT-POS-853c0ffa-9_2



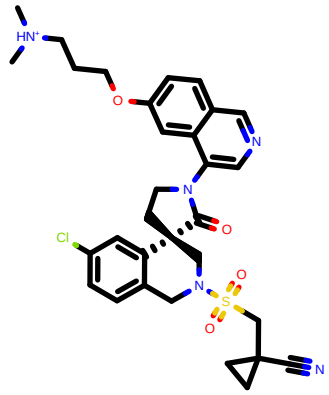
CID:	MAT-POS-853c0ffa-9_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN436
DDG (kcal/mol):	0.87
dDDG (kcal/mol):	0.75

LUO-POS-ed2cfb03-1_2



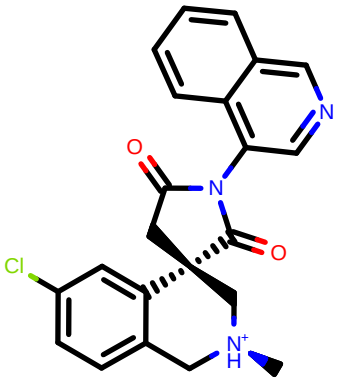
CID:	LUO-POS-ed2cfb03-1_2
SMILES:	C[NH+]1CCN(CC1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN347
DDG (kcal/mol):	0.91
dDDG (kcal/mol):	0.49

MAT-POS-40ad851a-4_2



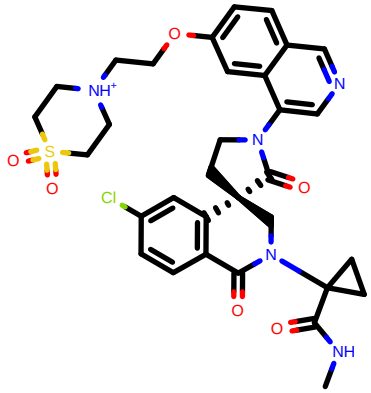
CID:	MAT-POS-40ad851a-4_2
SMILES:	C[NH+](C)CCCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN453
DDG (kcal/mol):	0.95
dDDG (kcal/mol):	0.55

JOH-MSK-51c67e7d-2_2



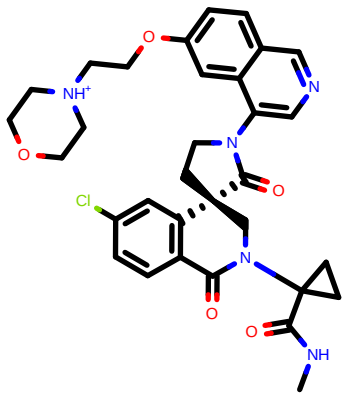
CID:	JOH-MSK-51c67e7d-2_2
SMILES:	C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN48
DDG (kcal/mol):	0.96
dDDG (kcal/mol):	0.08

EDJ-MED-dfa1d800-3_1



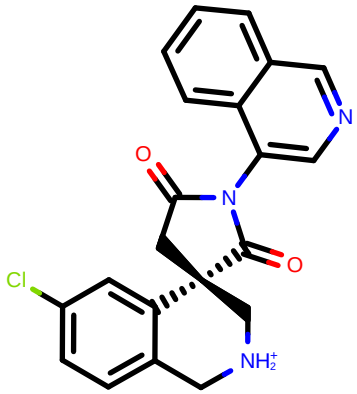
CID:	EDJ-MED-dfa1d800-3_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCCN6CCS(=O)(=O)CC6)c7cc(ccc7C2=O)Cl
RUN:	RUN485
DDG (kcal/mol):	0.97
dDDG (kcal/mol):	0.27

EDJ-MED-dfa1d800-2_1



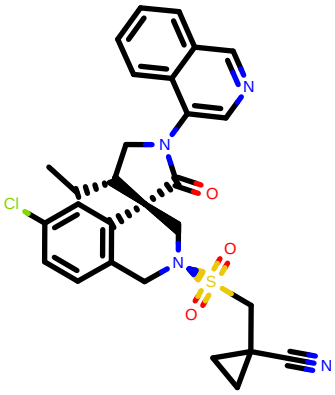
CID:	EDJ-MED-dfa1d800-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCOCC6)c7cc(ccc7C2=O)Cl
RUN:	RUN461
DDG (kcal/mol):	0.99
dDDG (kcal/mol):	0.29

JOH-MSK-1f2dff76-4_1



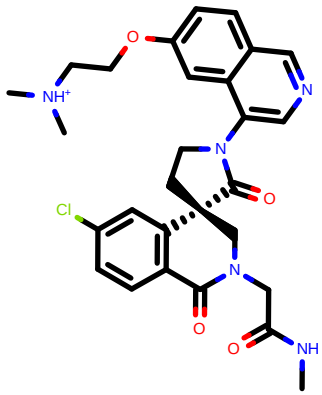
CID:	JOH-MSK-1f2dff76-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[NH2+]Cc5c4cc(cc5)Cl
RUN:	RUN32
DDG (kcal/mol):	1.00
dDDG (kcal/mol):	0.15

MAT-POS-50a80394-2_3



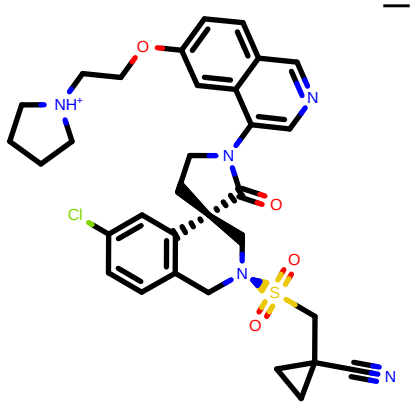
CID:	MAT-POS-50a80394-2_3
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN366
DDG (kcal/mol):	1.01
dDDG (kcal/mol):	0.37

EDJ-MED-b6c6ee2b-5_1



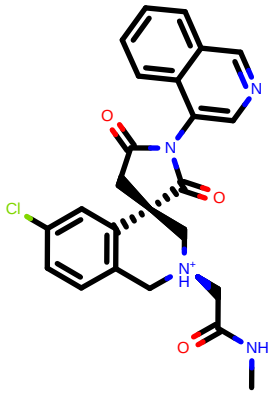
CID:	EDJ-MED-b6c6ee2b-5_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)OCC[NH+](C)C)c5cc(ccc5C1=O)Cl
RUN:	RUN425
DDG (kcal/mol):	1.03
dDDG (kcal/mol):	0.24

EDJ-MED-468565e0-1_1



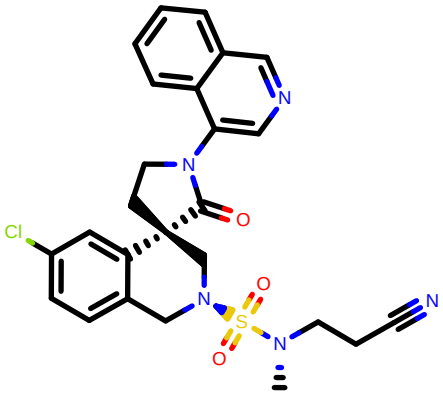
CID:	EDJ-MED-468565e0-1_1
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN472
DDG (kcal/mol):	1.03
dDDG (kcal/mol):	0.73

JOH-MSK-1f2dff76-2_2



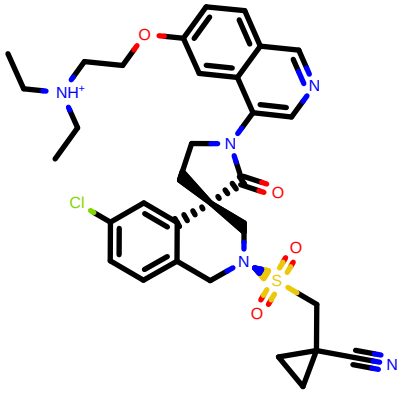
CID:	JOH-MSK-1f2dff76-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN134
DDG (kcal/mol):	1.03
dDDG (kcal/mol):	0.18

ALP-POS-ecbed2ba-16_1



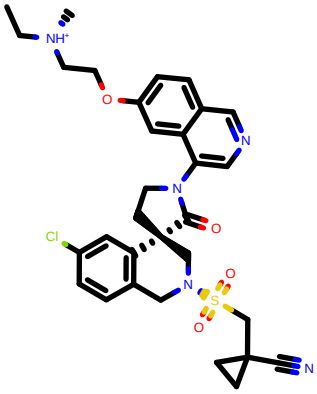
CID:	ALP-POS-ecbed2ba-16_1
SMILES:	C[N@@](CCC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN256
DDG (kcal/mol):	1.06
dDDG (kcal/mol):	0.34

MAT-POS-40ad851a-3_1



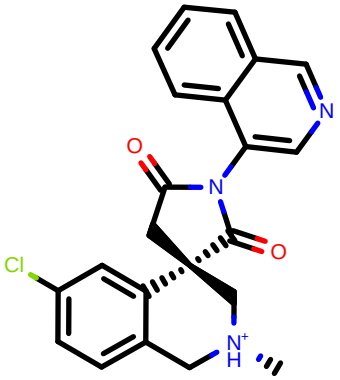
CID:	MAT-POS-40ad851a-3_1
SMILES:	CC[NH+](CC)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN468
DDG (kcal/mol):	1.06
dDDG (kcal/mol):	0.68

MAT-POS-40ad851a-2_4



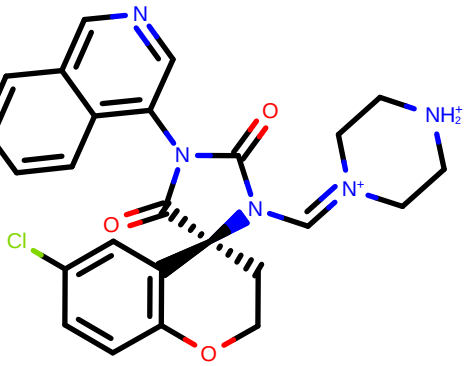
CID:	MAT-POS-40ad851a-2_4
SMILES:	CC[N@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN449
DDG (kcal/mol):	1.08
dDDG (kcal/mol):	0.57

JOH-MSK-51c67e7d-2_1



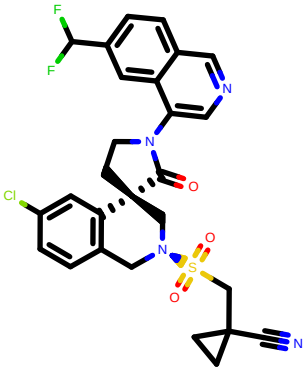
CID:	JOH-MSK-51c67e7d-2_1
SMILES:	C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN45
DDG (kcal/mol):	1.10
dDDG (kcal/mol):	0.13

VLA-UCB-34f3ed0c-15_1



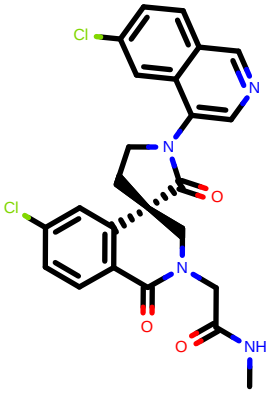
CID:	VLA-UCB-34f3ed0c-15_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CN6CC[NH2+]CC6
RUN:	RUN188
DDG (kcal/mol):	1.12
dDDG (kcal/mol):	0.29

EDJ-MED-5cd3920d-2_1



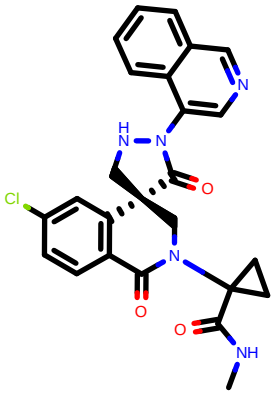
CID:	EDJ-MED-5cd3920d-2_1
SMILES:	c1cc2cncc(c2cc1C(F)F)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN396
DDG (kcal/mol):	1.12
dDDG (kcal/mol):	0.30

EDG-MED-b1ef7fe3-1_1



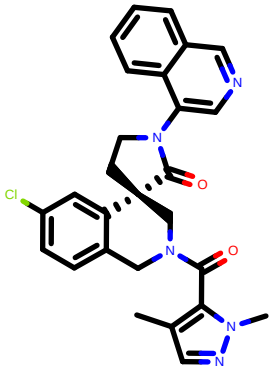
CID:	EDG-MED-b1ef7fe3-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN133
DDG (kcal/mol):	1.17
dDDG (kcal/mol):	0.13

EDJ-MED-fed7ac0b-2_1



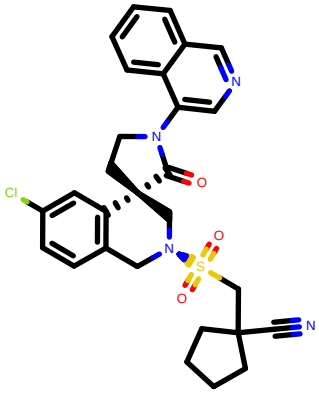
CID:	EDJ-MED-fed7ac0b-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CNN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN213
DDG (kcal/mol):	1.18
dDDG (kcal/mol):	0.14

EDJ-MED-cc48ee33-4_1



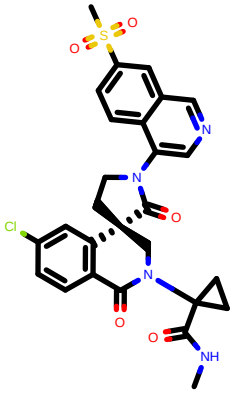
CID:	EDJ-MED-cc48ee33-4_1
SMILES:	Cc1cnn(c1C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl)C
RUN:	RUN270
DDG (kcal/mol):	1.20
dDDG (kcal/mol):	0.16

ALP-POS-ecbed2ba-15_1



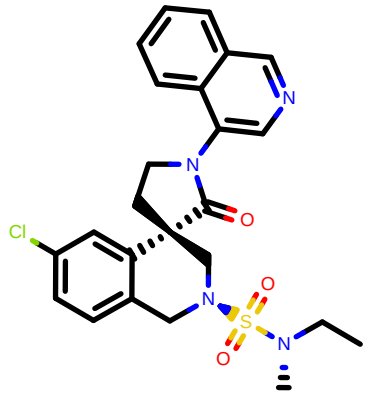
CID:	ALP-POS-ecbed2ba-15_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCCC6)C#N
RUN:	RUN358
DDG (kcal/mol):	1.24
dDDG (kcal/mol):	0.42

EDJ-MED-976a33d5-2_1



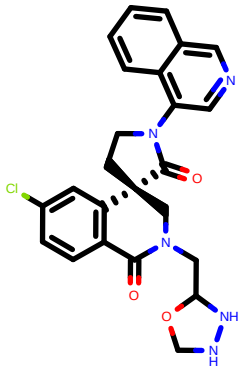
CID:	EDJ-MED-976a33d5-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)S(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN394
DDG (kcal/mol):	1.26
dDDG (kcal/mol):	0.16

ALP-POS-ecbed2ba-18_4



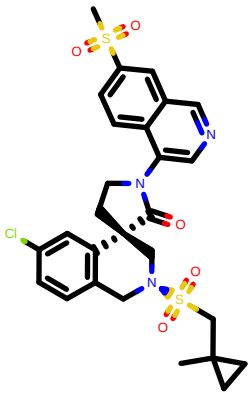
CID:	ALP-POS-ecbed2ba-18_4
SMILES:	CC[N@](C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN156
DDG (kcal/mol):	1.27
dDDG (kcal/mol):	0.53

PET-UNK-aa57768f-1_1



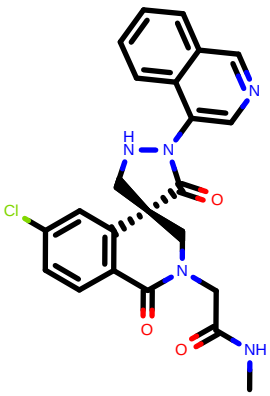
CID:	PET-UNK-aa57768f-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN144
DDG (kcal/mol):	1.30
dDDG (kcal/mol):	0.14

MAT-POS-853c0ffa-22_2



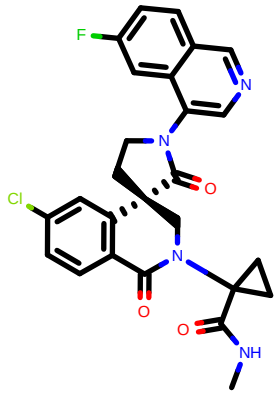
CID:	MAT-POS-853c0ffa-22_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN389
DDG (kcal/mol):	1.34
dDDG (kcal/mol):	0.38

EDJ-MED-fed7ac0b-1_1



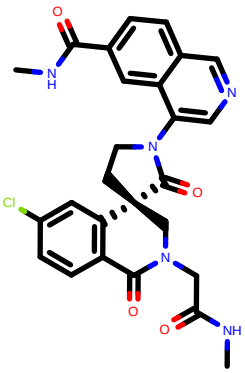
CID:	EDJ-MED-fed7ac0b-1_1
SMILES:	CNC(=O)CN1C[C@]2(CNN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN110
DDG (kcal/mol):	1.36
dDDG (kcal/mol):	0.15

EDJ-MED-b6c6ee2b-7_1



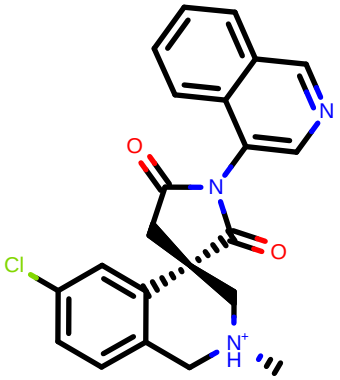
CID:	EDJ-MED-b6c6ee2b-7_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)F)c6cc(ccc6C2=O)Cl
RUN:	RUN279
DDG (kcal/mol):	1.36
dDDG (kcal/mol):	0.15

MAT-POS-38eb6498-6_1



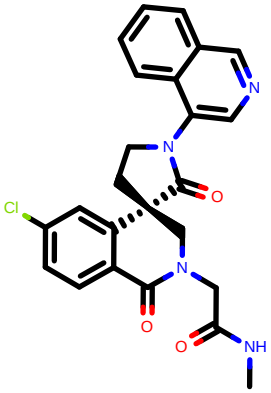
CID:	MAT-POS-38eb6498-6_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)C(=O)NC)c5cc(ccc5C1=O)Cl
RUN:	RUN319
DDG (kcal/mol):	1.37
dDDG (kcal/mol):	0.16

JOH-MSK-51c67e7d-1_1



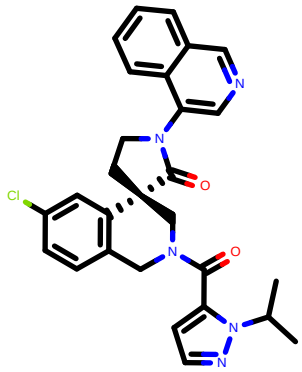
CID:	JOH-MSK-51c67e7d-1_1
SMILES:	C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN44
DDG (kcal/mol):	1.37
dDDG (kcal/mol):	0.14

PET-UNK-14142a25-10_1



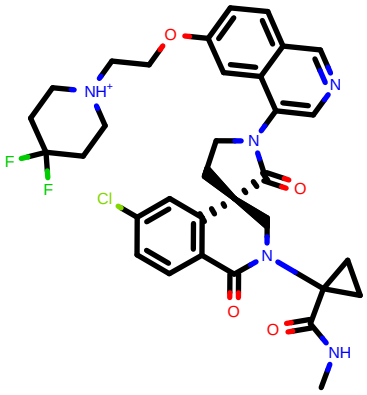
CID:	PET-UNK-14142a25-10_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN105
DDG (kcal/mol):	1.38
dDDG (kcal/mol):	0.13

MAT-POS-be048f2c-6_1



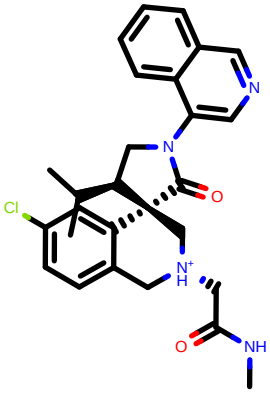
CID:	MAT-POS-be048f2c-6_1
SMILES:	CC(C)n1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN331
DDG (kcal/mol):	1.40
dDDG (kcal/mol):	0.19

EDJ-MED-dfa1d800-4_1



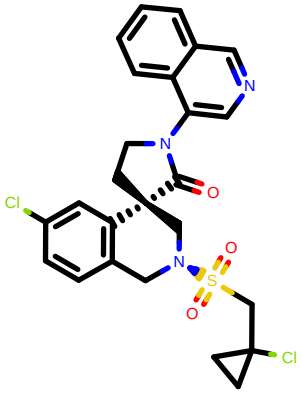
CID:	EDJ-MED-dfa1d800-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCC(CC6)(F)F)c7cc(ccc7C2=O)Cl
RUN:	RUN483
DDG (kcal/mol):	1.40
dDDG (kcal/mol):	0.30

MAT-POS-50a80394-6_2



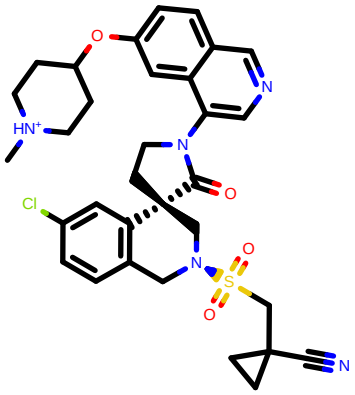
CID:	MAT-POS-50a80394-6_2
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN222
DDG (kcal/mol):	1.41
dDDG (kcal/mol):	0.20

PET-UNK-94036022-3_2



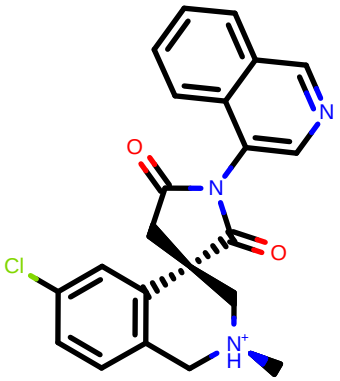
CID:	PET-UNK-94036022-3_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN224
DDG (kcal/mol):	1.43
dDDG (kcal/mol):	0.31

LUO-POS-d1147590-1_2



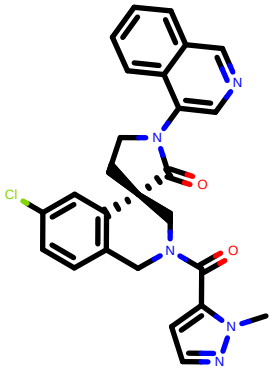
CID:	LUO-POS-d1147590-1_2
SMILES:	C[NH+]1CCC(CC1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN476
DDG (kcal/mol):	1.48
dDDG (kcal/mol):	0.67

JOH-MSK-51c67e7d-1_2



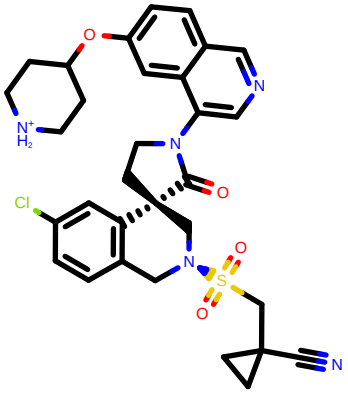
CID:	JOH-MSK-51c67e7d-1_2
SMILES:	C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN47
DDG (kcal/mol):	1.50
dDDG (kcal/mol):	0.08

EDJ-MED-cc48ee33-3_1



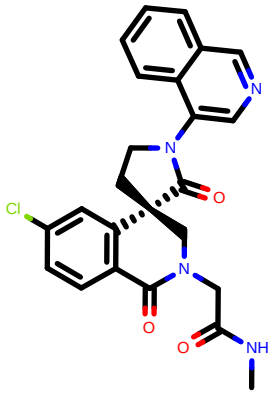
CID:	EDJ-MED-cc48ee33-3_1
SMILES:	Cn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN211
DDG (kcal/mol):	1.52
dDDG (kcal/mol):	0.16

EDJ-MED-ee81482e-4_1



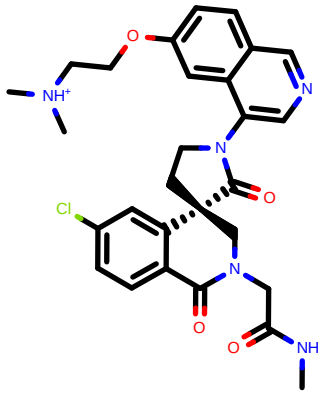
CID:	EDJ-MED-ee81482e-4_1
SMILES:	c1cc2cncc(c2cc1OC3CC[NH2+]CC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN447
DDG (kcal/mol):	1.54
dDDG (kcal/mol):	0.40

PET-UNK-14142a25-1_1



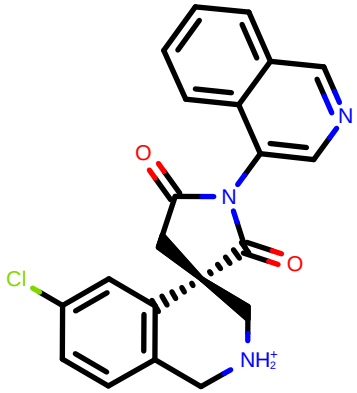
CID:	PET-UNK-14142a25-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN102
DDG (kcal/mol):	1.56
dDDG (kcal/mol):	0.13

MAT-POS-38eb6498-4_1



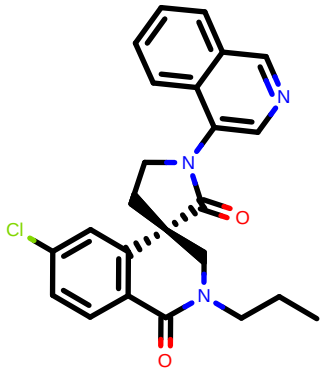
CID:	MAT-POS-38eb6498-4_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)OCC[NH+](C)C)c5cc(ccc5C1=O)Cl
RUN:	RUN415
DDG (kcal/mol):	1.57
dDDG (kcal/mol):	0.28

JOH-MSK-1f2dff76-3_1



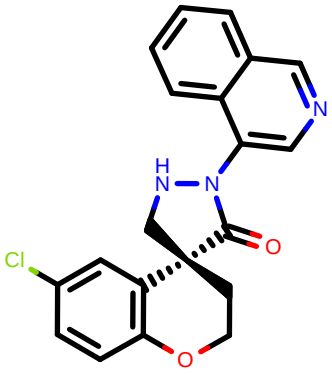
CID:	JOH-MSK-1f2dff76-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[NH2+]Cc5c4cc(cc5)Cl
RUN:	RUN40
DDG (kcal/mol):	1.58
dDDG (kcal/mol):	0.15

PET-UNK-aa57768f-3_1



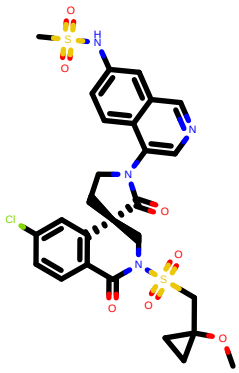
CID:	PET-UNK-aa57768f-3_1
SMILES:	C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN54
DDG (kcal/mol):	1.60
dDDG (kcal/mol):	0.14

BEN-BAS-c2bc0d80-3_1



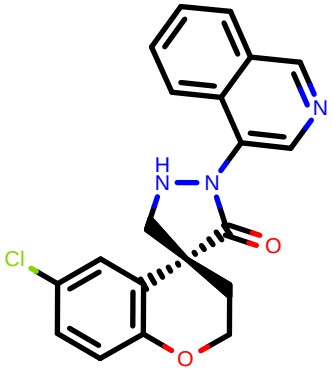
CID:	BEN-BAS-c2bc0d80-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)CN3
RUN:	RUN10
DDG (kcal/mol):	1.61
dDDG (kcal/mol):	0.09

EDJ-MED-9f4ac58c-7_1



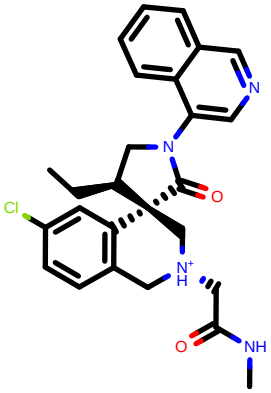
CID:	EDJ-MED-9f4ac58c-7_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN429
DDG (kcal/mol):	1.64
dDDG (kcal/mol):	0.55

BRU-THA-73c97d88-1_1



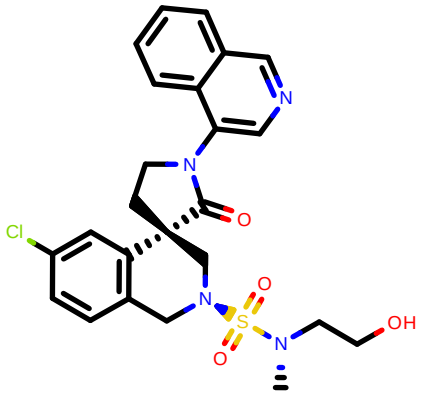
CID:	BRU-THA-73c97d88-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C=N3
RUN:	RUN13
DDG (kcal/mol):	1.66
dDDG (kcal/mol):	0.08

MAT-POS-50a80394-5_2



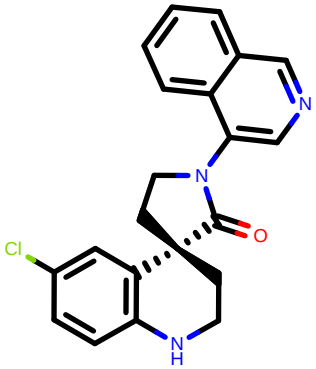
CID:	MAT-POS-50a80394-5_2
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN165
DDG (kcal/mol):	1.66
dDDG (kcal/mol):	0.25

ALP-POS-ecbed2ba-19_4



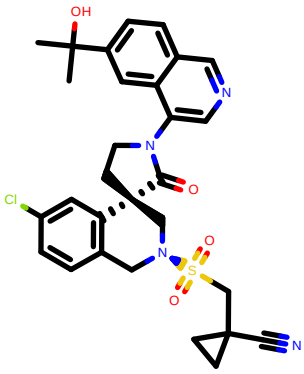
CID:	ALP-POS-ecbed2ba-19_4
SMILES:	C[N@](CCO)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN219
DDG (kcal/mol):	1.70
dDDG (kcal/mol):	0.70

DAR-DIA-6be260fc-5_1



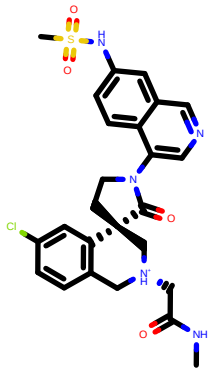
CID:	DAR-DIA-6be260fc-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCNc5c4cc(cc5)Cl
RUN:	RUN4
DDG (kcal/mol):	1.70
dDDG (kcal/mol):	0.09

MAT-POS-853c0ffa-11_1



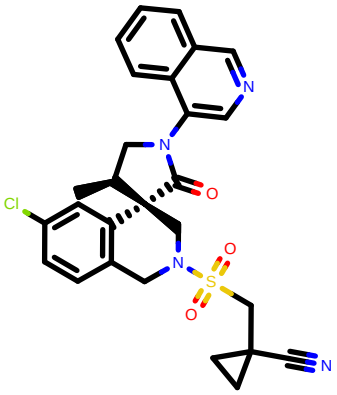
CID:	MAT-POS-853c0ffa-11_1
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN408
DDG (kcal/mol):	1.74
dDDG (kcal/mol):	0.39

MAT-POS-b4d6b7fc-7_1



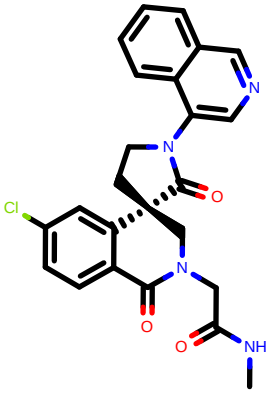
CID:	MAT-POS-b4d6b7fc-7_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)Cl
RUN:	RUN292
DDG (kcal/mol):	1.74
dDDG (kcal/mol):	0.23

MAT-POS-50a80394-1_2



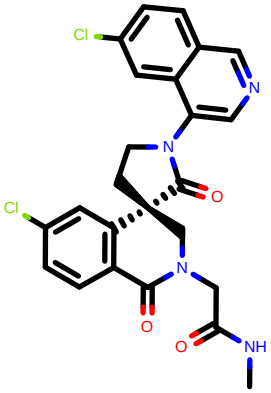
CID:	MAT-POS-50a80394-1_2
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5ncc6c5cccc6
RUN:	RUN339
DDG (kcal/mol):	1.75
dDDG (kcal/mol):	0.48

LUO-POS-9931618f-1_1



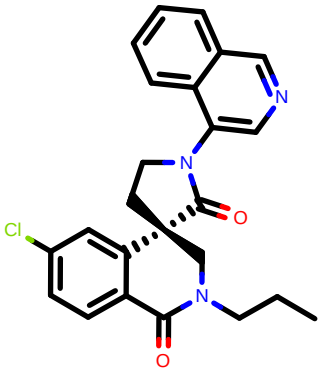
CID:	LUO-POS-9931618f-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN120
DDG (kcal/mol):	1.76
dDDG (kcal/mol):	0.15

LUO-POS-8c3e556a-1_1



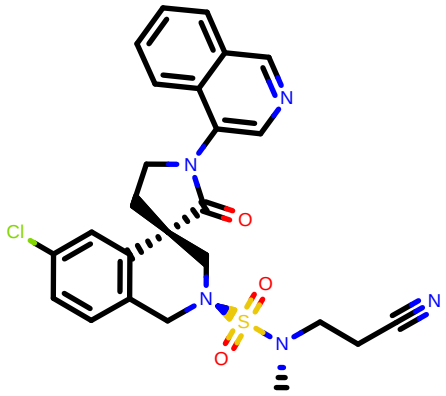
CID:	LUO-POS-8c3e556a-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN177
DDG (kcal/mol):	1.76
dDDG (kcal/mol):	0.15

PET-UNK-aa57768f-9_1



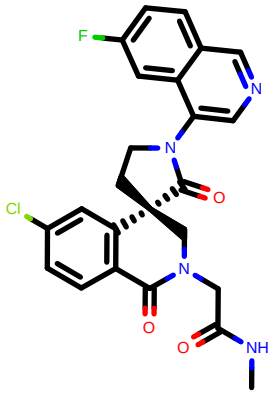
CID:	PET-UNK-aa57768f-9_1
SMILES:	C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN58
DDG (kcal/mol):	1.76
dDDG (kcal/mol):	0.15

ALP-POS-ecbed2ba-16_4



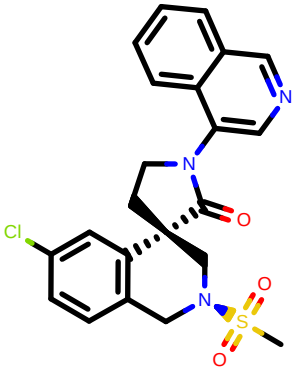
CID:	ALP-POS-ecbed2ba-16_4
SMILES:	C[N@](CCC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN258
DDG (kcal/mol):	1.77
dDDG (kcal/mol):	0.59

EDG-MED-b1ef7fe3-2_1



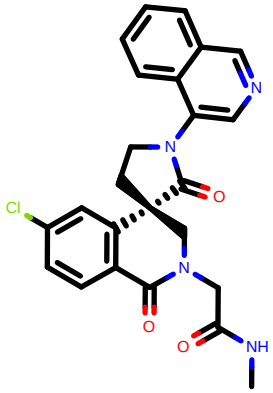
CID:	EDG-MED-b1ef7fe3-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN142
DDG (kcal/mol):	1.77
dDDG (kcal/mol):	0.12

EDJ-MED-7587a9ee-3_1



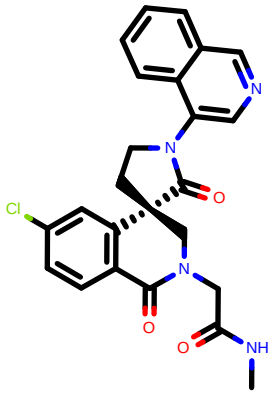
CID:	EDJ-MED-7587a9ee-3_1
SMILES:	CS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN50
DDG (kcal/mol):	1.79
dDDG (kcal/mol):	0.17

LUO-POS-9931618f-2_1



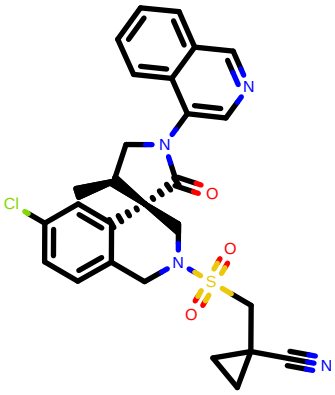
CID:	LUO-POS-9931618f-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN118
DDG (kcal/mol):	1.80
dDDG (kcal/mol):	0.14

EDJ-MED-fd8ed875-3_1



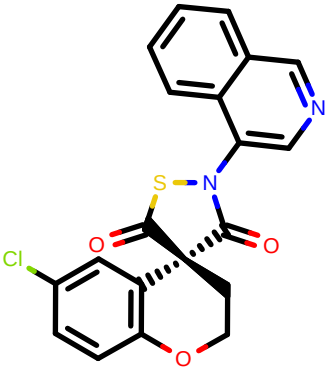
CID:	EDJ-MED-fd8ed875-3_1
SMILES:	CNC(=O)CN1C[C@]2(C=CN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN115
DDG (kcal/mol):	1.81
dDDG (kcal/mol):	0.11

MAT-POS-50a80394-1_4



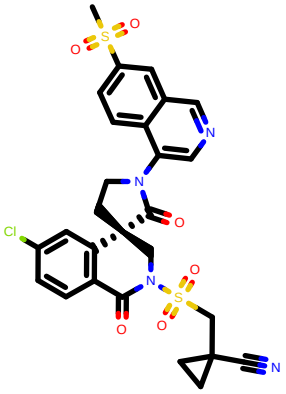
CID:	MAT-POS-50a80394-1_4
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN343
DDG (kcal/mol):	1.83
dDDG (kcal/mol):	0.43

DAR-DIA-0f7b7cd9-8_1



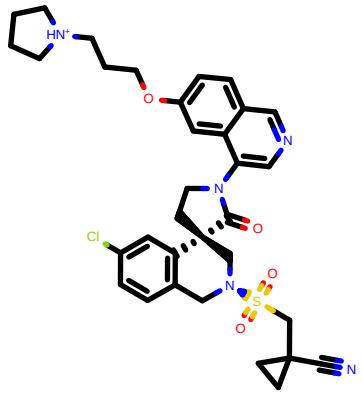
CID:	DAR-DIA-0f7b7cd9-8_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C(=O)S3
RUN:	RUN28
DDG (kcal/mol):	1.85
dDDG (kcal/mol):	0.07

EDJ-MED-9f4ac58c-4_1



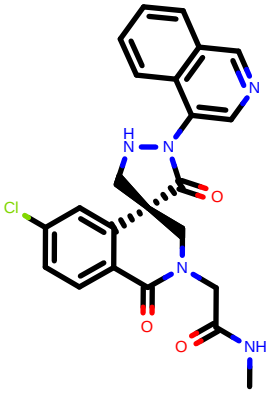
CID:	EDJ-MED-9f4ac58c-4_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN416
DDG (kcal/mol):	1.89
dDDG (kcal/mol):	0.54

MAT-POS-40ad851a-5_2



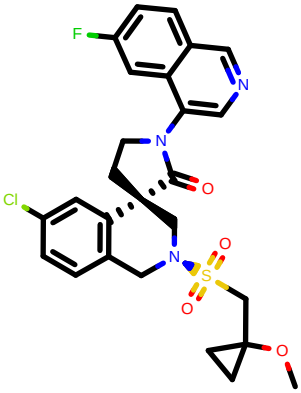
CID:	MAT-POS-40ad851a-5_2
SMILES:	c1cc2cncc(c2cc1OCCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN473
DDG (kcal/mol):	1.90
dDDG (kcal/mol):	0.63

EDJ-MED-fed7ac0b-4_1



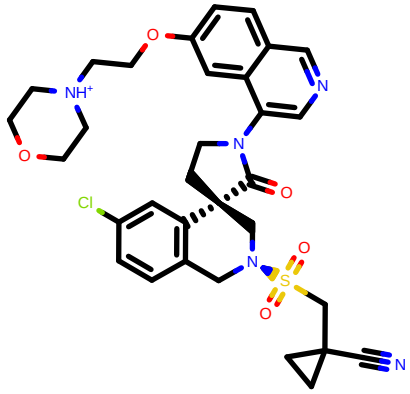
CID:	EDJ-MED-fed7ac0b-4_1
SMILES:	CNC(=O)CN1C[C@]2(C=NN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN106
DDG (kcal/mol):	1.91
dDDG (kcal/mol):	0.13

MAT-POS-853c0ffa-14_1



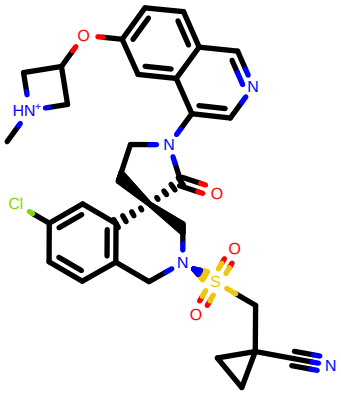
CID:	MAT-POS-853c0ffa-14_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN307
DDG (kcal/mol):	1.91
dDDG (kcal/mol):	0.26

EDJ-MED-468565e0-2_1



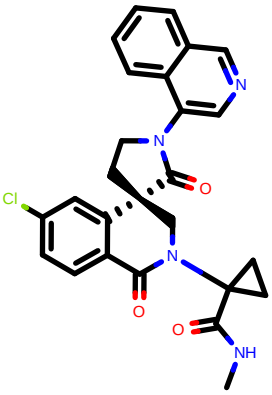
CID:	EDJ-MED-468565e0-2_1
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCOCC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN470
DDG (kcal/mol):	1.92
dDDG (kcal/mol):	0.63

EDJ-MED-ee81482e-2_1



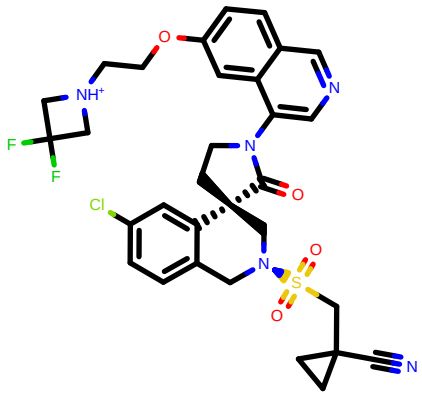
CID:	EDJ-MED-ee81482e-2_1
SMILES:	C[NH+]1CC(C1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN442
DDG (kcal/mol):	1.93
dDDG (kcal/mol):	0.42

EDJ-MED-fd8ed875-4_1



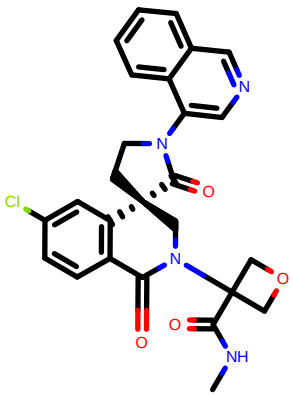
CID:	EDJ-MED-fd8ed875-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(C=CN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN212
DDG (kcal/mol):	1.93
dDDG (kcal/mol):	0.14

EDJ-MED-468565e0-5_2



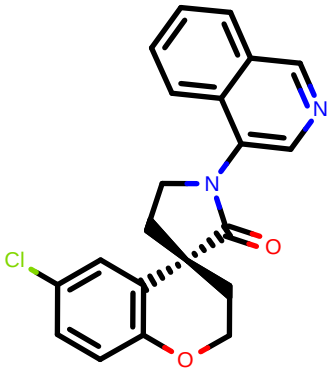
CID:	EDJ-MED-468565e0-5_2
SMILES:	c1cc2cncc(c2cc1OCCN3CC(C3)(F)F)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN467
DDG (kcal/mol):	1.95
dDDG (kcal/mol):	0.54

EDJ-MED-98c0a822-4_1



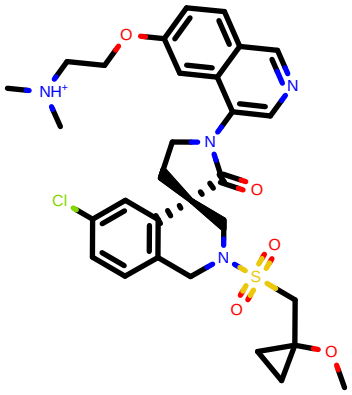
CID:	EDJ-MED-98c0a822-4_1
SMILES:	CNC(=O)C1(COC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN273
DDG (kcal/mol):	1.96
dDDG (kcal/mol):	0.15

MAT-POS-983b399a-1_1



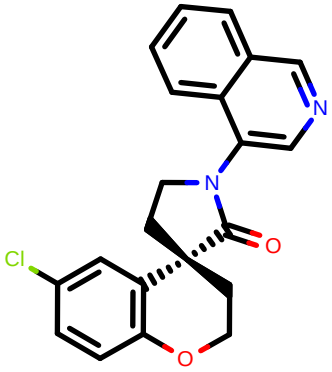
CID:	MAT-POS-983b399a-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN9
DDG (kcal/mol):	2.00
dDDG (kcal/mol):	0.09

MAT-POS-853c0ffa-10_2



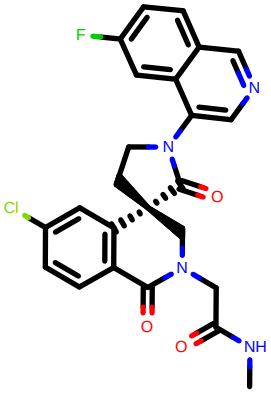
CID:	MAT-POS-853c0ffa-10_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC
RUN:	RUN438
DDG (kcal/mol):	2.00
dDDG (kcal/mol):	0.49

EDJ-MED-159244ea-1_1



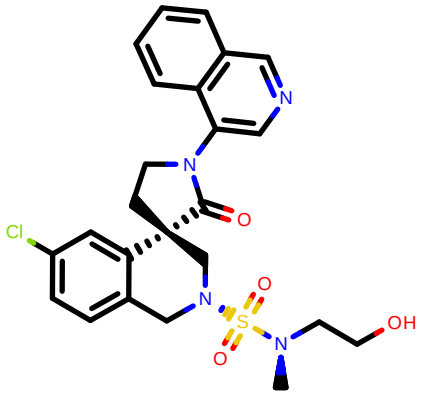
CID:	EDJ-MED-159244ea-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN8
DDG (kcal/mol):	2.01
dDDG (kcal/mol):	0.09

EDJ-MED-b6c6ee2b-6_1



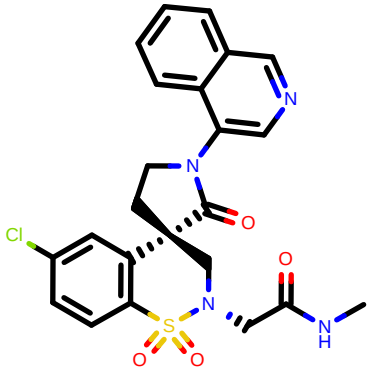
CID:	EDJ-MED-b6c6ee2b-6_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN183
DDG (kcal/mol):	2.02
dDDG (kcal/mol):	0.14

ALP-POS-ecbed2ba-19_2



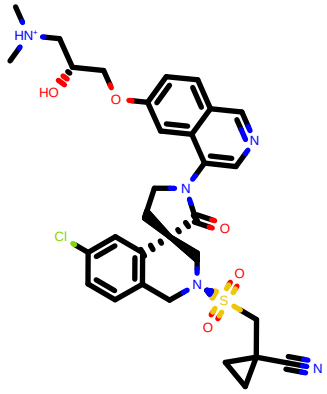
CID:	ALP-POS-ecbed2ba-19_2
SMILES:	C[N@](CCO)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN215
DDG (kcal/mol):	2.06
dDDG (kcal/mol):	0.28

ALP-POS-4483ae88-2_2



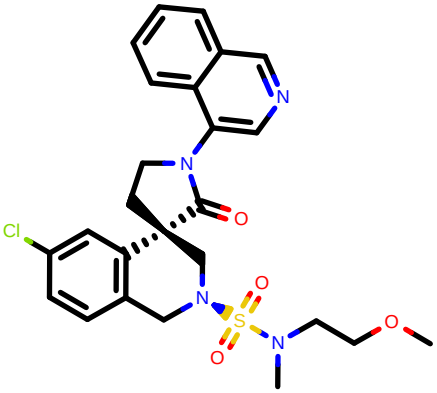
CID:	ALP-POS-4483ae88-2_2
SMILES:	CNC(=O)C[N@]1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)Cl
RUN:	RUN146
DDG (kcal/mol):	2.07
dDDG (kcal/mol):	0.19

EDJ-MED-ee81482e-3_4



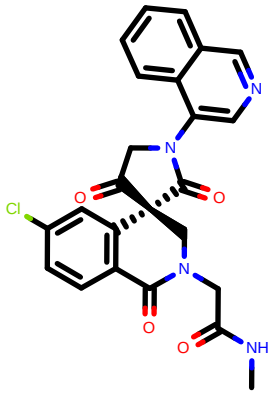
CID:	EDJ-MED-ee81482e-3_4
SMILES:	C[NH+](C)C[C@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN457
DDG (kcal/mol):	2.08
dDDG (kcal/mol):	0.89

ALP-POS-ecbed2ba-21_1



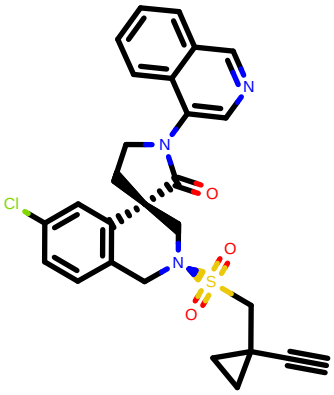
CID:	ALP-POS-ecbed2ba-21_1
SMILES:	C[N@@](CCOC)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN261
DDG (kcal/mol):	2.09
dDDG (kcal/mol):	0.28

EDJ-MED-a12e3a20-2_1



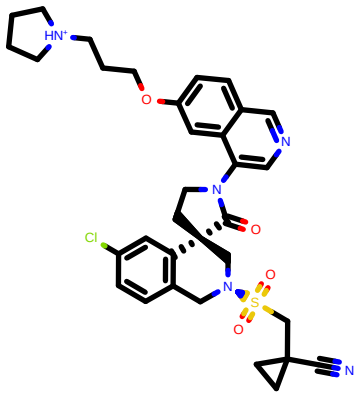
CID:	EDJ-MED-a12e3a20-2_1
SMILES:	CNC(=O)CN1C[C@@]2(c3cc(ccc3C1=O)Cl)C(=O)CN(C2=O)c4cncc5c4cccc5
RUN:	RUN166
DDG (kcal/mol):	2.09
dDDG (kcal/mol):	0.14

PET-UNK-94036022-2_1



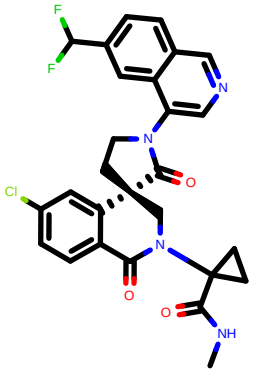
CID:	PET-UNK-94036022-2_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN284
DDG (kcal/mol):	2.10
dDDG (kcal/mol):	0.30

MAT-POS-40ad851a-5_1



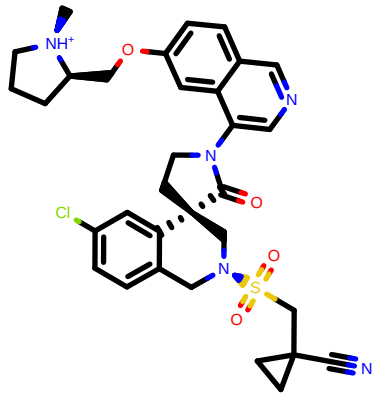
CID:	MAT-POS-40ad851a-5_1
SMILES:	c1cc2cncc(c2cc1OCCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN482
DDG (kcal/mol):	2.11
dDDG (kcal/mol):	0.65

EDJ-MED-5cd3920d-4_1



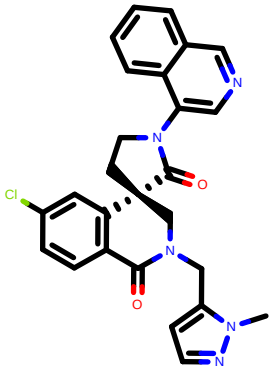
CID:	EDJ-MED-5cd3920d-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)C(F)F)c6cc(ccc6C2=O)Cl
RUN:	RUN378
DDG (kcal/mol):	2.13
dDDG (kcal/mol):	0.21

MAT-POS-40ad851a-1_1



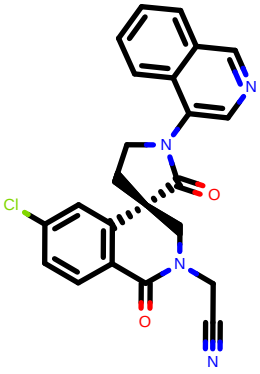
CID:	MAT-POS-40ad851a-1_1
SMILES:	C[N@@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN464
DDG (kcal/mol):	2.13
dDDG (kcal/mol):	0.50

EDJ-MED-cc48ee33-7_1



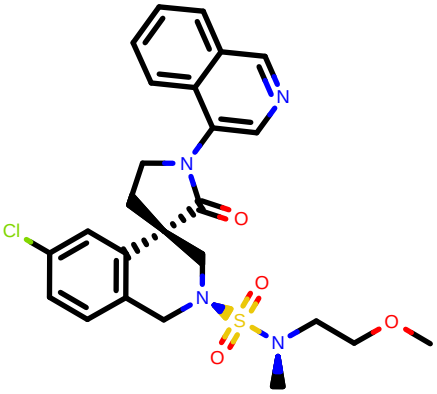
CID:	EDJ-MED-cc48ee33-7_1
SMILES:	Cn1c(ccn1)CN2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN208
DDG (kcal/mol):	2.14
dDDG (kcal/mol):	0.21

PET-UNK-aa57768f-8_1



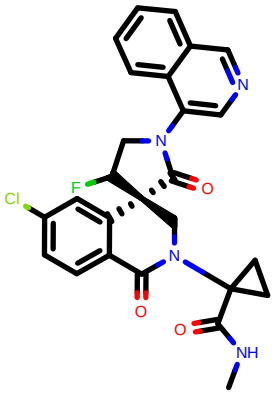
CID:	PET-UNK-aa57768f-8_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N
RUN:	RUN62
DDG (kcal/mol):	2.19
dDDG (kcal/mol):	0.11

ALP-POS-ecbed2ba-21_2



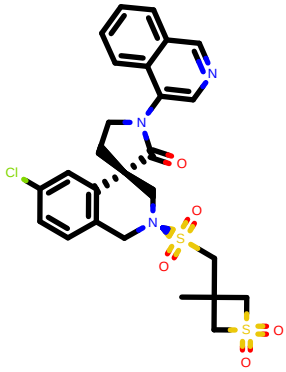
CID:	ALP-POS-ecbed2ba-21_2
SMILES:	C[N@](CCOC)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN263
DDG (kcal/mol):	2.26
dDDG (kcal/mol):	0.30

EDJ-MED-fd8ed875-6_1



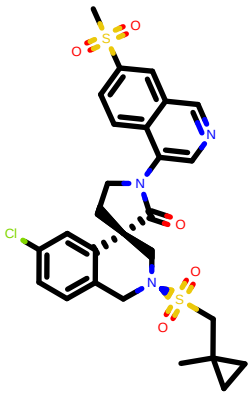
CID:	EDJ-MED-fd8ed875-6_1
SMILES:	CNC(=O)C1(CC1)N2C[C@@]3(c4cc(ccc4C2=O)Cl)C(=CN(C3=O)c5cncc6c5cccc6)F
RUN:	RUN286
DDG (kcal/mol):	2.26
dDDG (kcal/mol):	0.16

ALP-POS-ecbed2ba-1_2



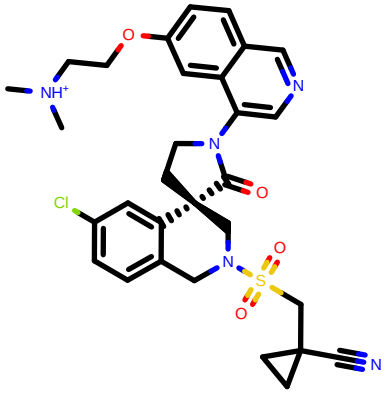
CID:	ALP-POS-ecbed2ba-1_2
SMILES:	CC1(CS(=O)(=O)C1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN360
DDG (kcal/mol):	2.26
dDDG (kcal/mol):	0.64

MAT-POS-853c0ffa-22_1



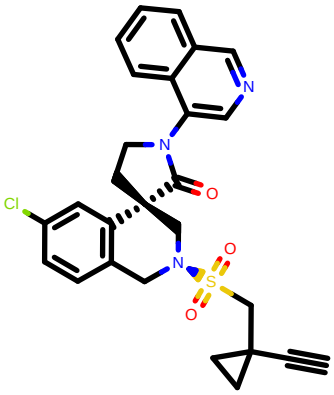
CID:	MAT-POS-853c0ffa-22_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN387
DDG (kcal/mol):	2.28
dDDG (kcal/mol):	0.30

LUO-POS-8484f2d3-1_1



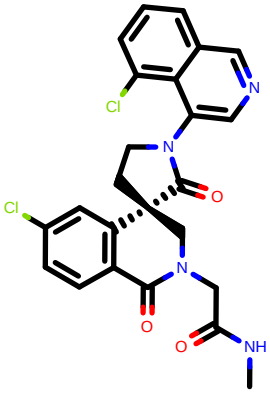
CID:	LUO-POS-8484f2d3-1_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN445
DDG (kcal/mol):	2.29
dDDG (kcal/mol):	0.63

PET-UNK-94036022-9_1



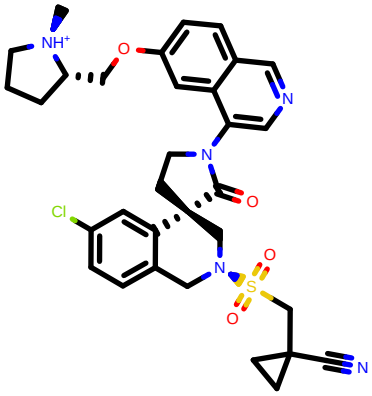
CID:	PET-UNK-94036022-9_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN274
DDG (kcal/mol):	2.30
dDDG (kcal/mol):	0.28

MAT-POS-1d5ab790-3_1



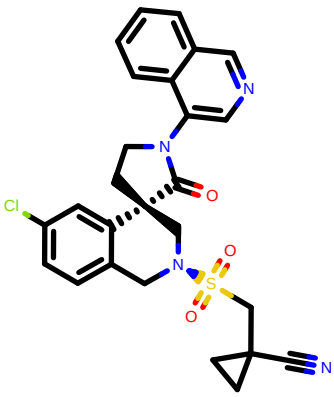
CID:	MAT-POS-1d5ab790-3_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(ccc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN168
DDG (kcal/mol):	2.30
dDDG (kcal/mol):	0.12

MAT-POS-40ad851a-1_3



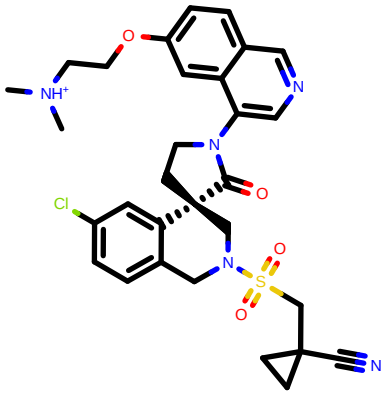
CID:	MAT-POS-40ad851a-1_3
SMILES:	C[N@@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN462
DDG (kcal/mol):	2.31
dDDG (kcal/mol):	0.53

EDJ-MED-8bb691af-6_1



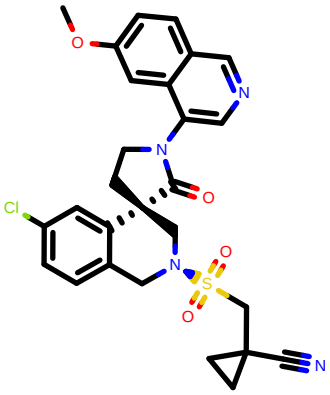
CID:	EDJ-MED-8bb691af-6_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN233
DDG (kcal/mol):	2.32
dDDG (kcal/mol):	0.34

LUO-POS-8484f2d3-1_2



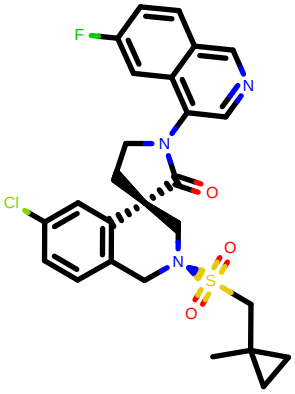
CID:	LUO-POS-8484f2d3-1_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN441
DDG (kcal/mol):	2.33
dDDG (kcal/mol):	0.65

EDJ-MED-b6c6ee2b-3_1



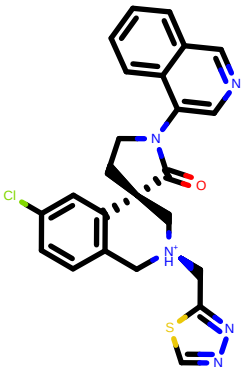
CID:	EDJ-MED-b6c6ee2b-3_1
SMILES:	COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN372
DDG (kcal/mol):	2.33
dDDG (kcal/mol):	0.49

MAT-POS-853c0ffa-21_1



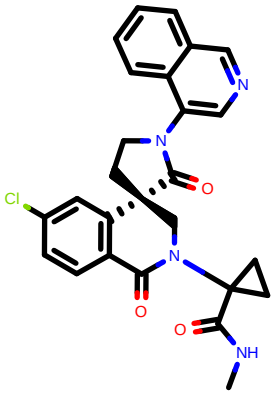
CID:	MAT-POS-853c0ffa-21_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN238
DDG (kcal/mol):	2.33
dDDG (kcal/mol):	0.26

PET-UNK-7e9559de-4_2



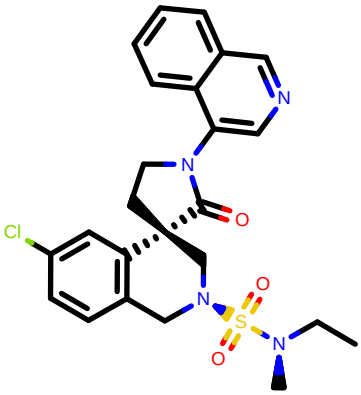
CID:	PET-UNK-7e9559de-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN116
DDG (kcal/mol):	2.36
dDDG (kcal/mol):	0.16

EDJ-MED-976a33d5-1_1



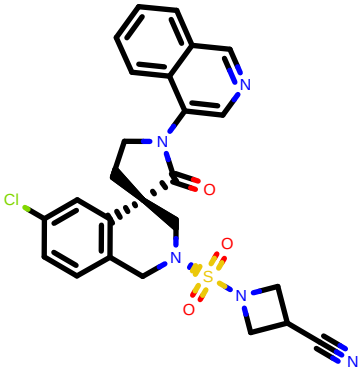
CID:	EDJ-MED-976a33d5-1_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN210
DDG (kcal/mol):	2.37
dDDG (kcal/mol):	0.19

ALP-POS-ecbed2ba-18_1



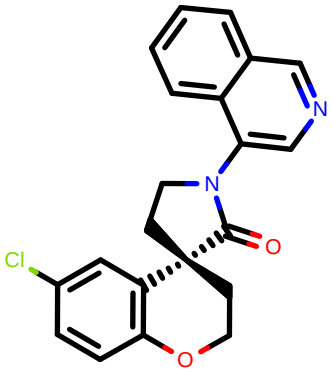
CID:	ALP-POS-ecbed2ba-18_1
SMILES:	CC[N@@](C)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN151
DDG (kcal/mol):	2.37
dDDG (kcal/mol):	0.29

ALP-POS-ecbed2ba-9_2



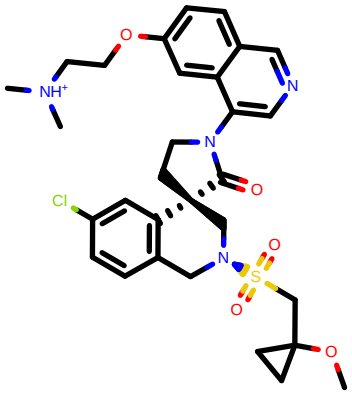
CID:	ALP-POS-ecbed2ba-9_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CC(C6)C#N
RUN:	RUN239
DDG (kcal/mol):	2.37
dDDG (kcal/mol):	0.62

ALP-POS-477dc5b7-4_1



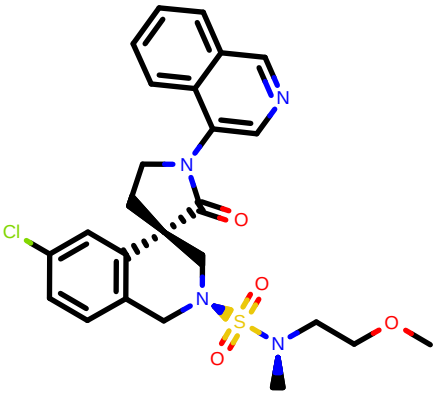
CID:	ALP-POS-477dc5b7-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN6
DDG (kcal/mol):	2.38
dDDG (kcal/mol):	0.13

MAT-POS-853c0ffa-10_1



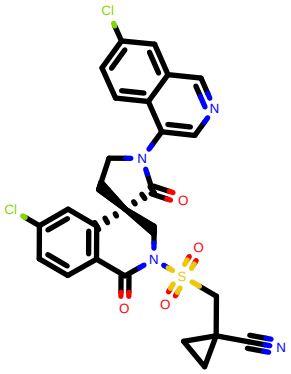
CID:	MAT-POS-853c0ffa-10_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5Cl)S(=O)(=O)CC6(CC6)OC
RUN:	RUN434
DDG (kcal/mol):	2.39
dDDG (kcal/mol):	0.54

ALP-POS-ecbed2ba-21_3



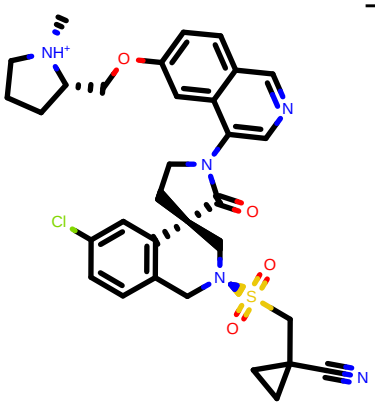
CID:	ALP-POS-ecbed2ba-21_3
SMILES:	C[N@@](CCOC)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN260
DDG (kcal/mol):	2.41
dDDG (kcal/mol):	0.68

EDJ-MED-9f4ac58c-1_1



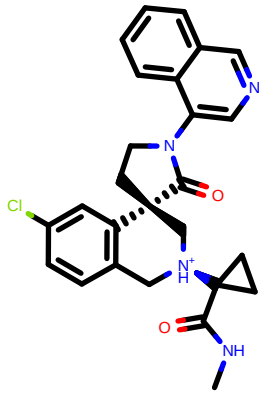
CID:	EDJ-MED-9f4ac58c-1_1
SMILES:	c1cc2c(cc1Cl)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN353
DDG (kcal/mol):	2.41
dDDG (kcal/mol):	0.38

MAT-POS-40ad851a-1_4



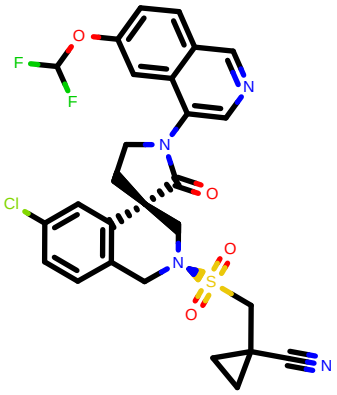
CID:	MAT-POS-40ad851a-1_4
SMILES:	C[N@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN465
DDG (kcal/mol):	2.41
dDDG (kcal/mol):	0.54

MAT-POS-69786b79-1_2



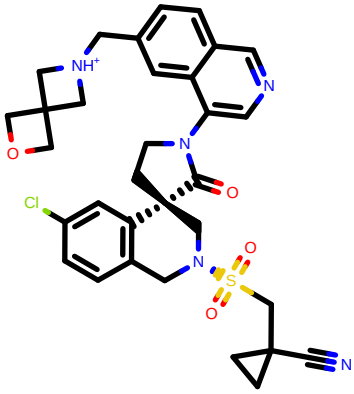
CID:	MAT-POS-69786b79-1_2
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN160
DDG (kcal/mol):	2.42
dDDG (kcal/mol):	0.17

EDJ-MED-5cd3920d-1_2



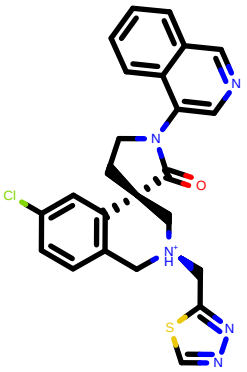
CID:	EDJ-MED-5cd3920d-1_2
SMILES:	c1cc2cncc(c2cc1OC(F)F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN428
DDG (kcal/mol):	2.42
dDDG (kcal/mol):	0.45

EDJ-MED-ee81482e-5_2



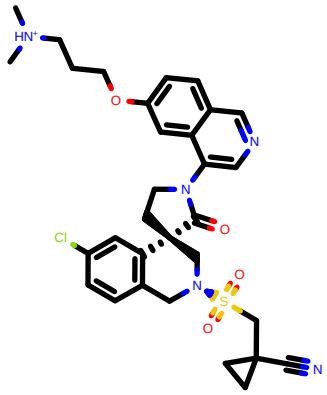
CID:	EDJ-MED-ee81482e-5_2
SMILES:	c1cc2cncc(c2cc1C[NH+]3CC4(C3)COC4)N5CC[C@@]6(C5=O)C[N@](Cc7c6ccc(cc7)Cl)S(=O)(=O)CC8(CC8)C#N
RUN:	RUN460
DDG (kcal/mol):	2.44
dDDG (kcal/mol):	0.45

MAT-POS-96396902-1_2



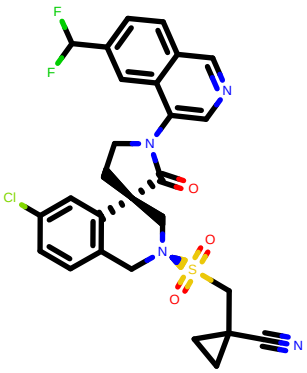
CID:	MAT-POS-96396902-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN125
DDG (kcal/mol):	2.45
dDDG (kcal/mol):	0.17

MAT-POS-40ad851a-4_1



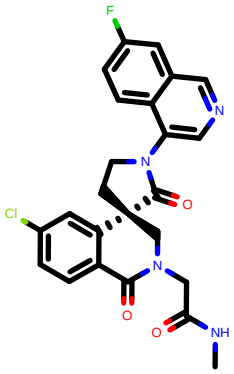
CID:	MAT-POS-40ad851a-4_1
SMILES:	C[NH+](C)CCCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN454
DDG (kcal/mol):	2.46
dDDG (kcal/mol):	0.41

EDJ-MED-5cd3920d-2_2



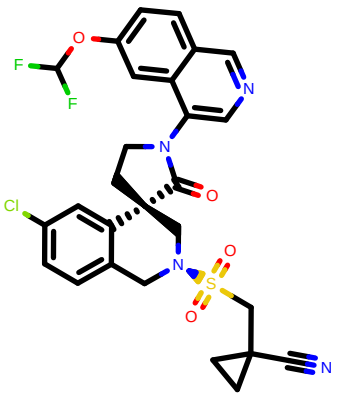
CID:	EDJ-MED-5cd3920d-2_2
SMILES:	c1cc2cncc(c2cc1C(F)F)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN399
DDG (kcal/mol):	2.47
dDDG (kcal/mol):	0.33

EDG-MED-b1ef7fe3-3_1



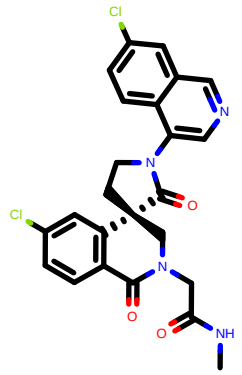
CID:	EDG-MED-b1ef7fe3-3_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN147
DDG (kcal/mol):	2.47
dDDG (kcal/mol):	0.16

EDJ-MED-5cd3920d-1_1



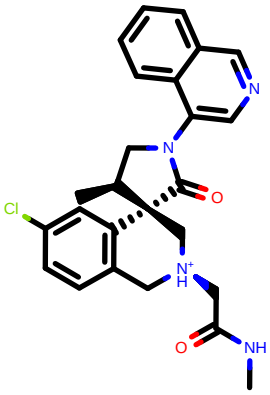
CID:	EDJ-MED-5cd3920d-1_1
SMILES:	c1cc2cncc(c2cc1OC(F)F)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN423
DDG (kcal/mol):	2.48
dDDG (kcal/mol):	0.35

EDG-MED-b1ef7fe3-4_1



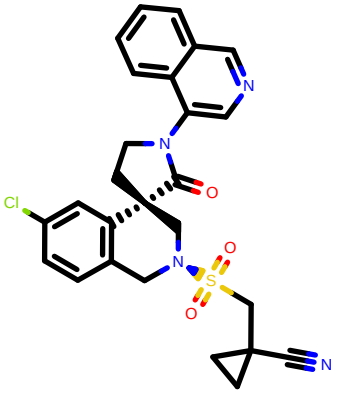
CID:	EDG-MED-b1ef7fe3-4_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN140
DDG (kcal/mol):	2.48
dDDG (kcal/mol):	0.21

MAT-POS-50a80394-4_4



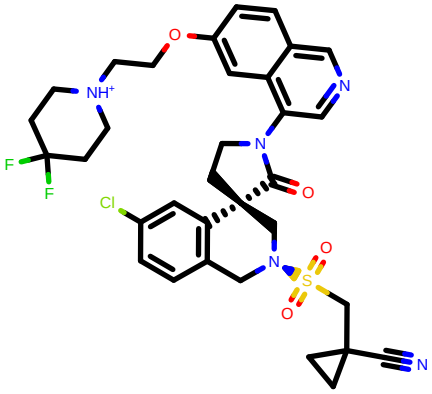
CID:	MAT-POS-50a80394-4_4
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN124
DDG (kcal/mol):	2.49
dDDG (kcal/mol):	0.24

EDJ-MED-8bb691af-6_2



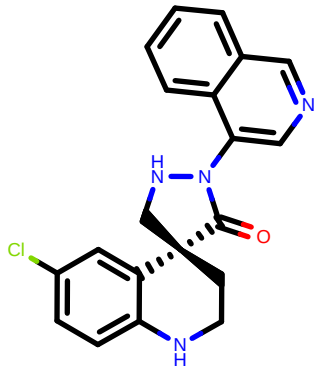
CID:	EDJ-MED-8bb691af-6_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN235
DDG (kcal/mol):	2.51
dDDG (kcal/mol):	0.53

EDJ-MED-468565e0-4_1



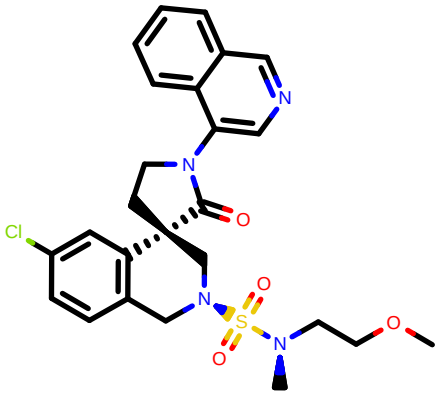
CID:	EDJ-MED-468565e0-4_1
SMILES:	c1cc2ncc(c2cc1OCC[NH+]3CCC(CC3)(F)F)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN486
DDG (kcal/mol):	2.53
dDDG (kcal/mol):	0.74

BRU-THA-55eab31a-1_1



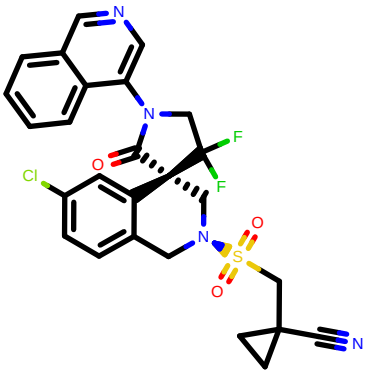
CID:	BRU-THA-55eab31a-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCNc5c4cc(cc5)Cl)C=N3
RUN:	RUN19
DDG (kcal/mol):	2.57
dDDG (kcal/mol):	0.11

ALP-POS-ecbed2ba-21_4



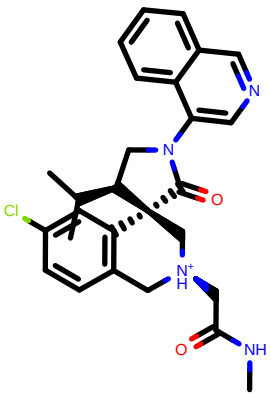
CID:	ALP-POS-ecbed2ba-21_4
SMILES:	C[N@](CCOC)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN267
DDG (kcal/mol):	2.57
dDDG (kcal/mol):	0.70

EDJ-MED-7e491f08-1_1



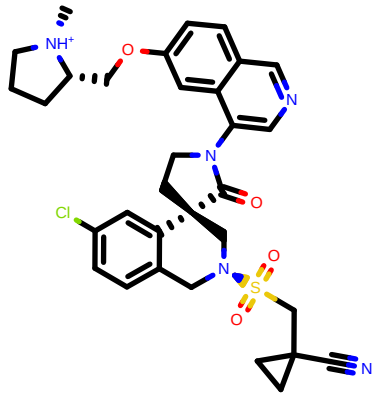
CID:	EDJ-MED-7e491f08-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)(F)F
RUN:	RUN373
DDG (kcal/mol):	2.58
dDDG (kcal/mol):	0.41

MAT-POS-50a80394-6_4



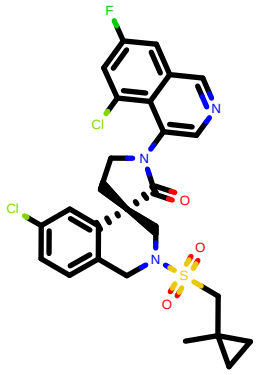
CID:	MAT-POS-50a80394-6_4
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN214
DDG (kcal/mol):	2.59
dDDG (kcal/mol):	0.42

MAT-POS-40ad851a-1_8



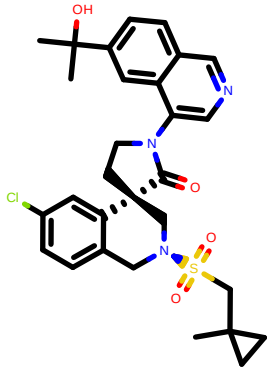
CID:	MAT-POS-40ad851a-1_8
SMILES:	C[N@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN469
DDG (kcal/mol):	2.59
dDDG (kcal/mol):	0.58

MAT-POS-853c0ffa-18_2



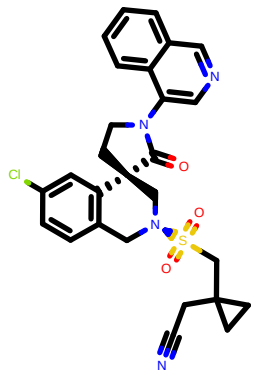
CID:	MAT-POS-853c0ffa-18_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN306
DDG (kcal/mol):	2.59
dDDG (kcal/mol):	0.30

MAT-POS-853c0ffa-20_1



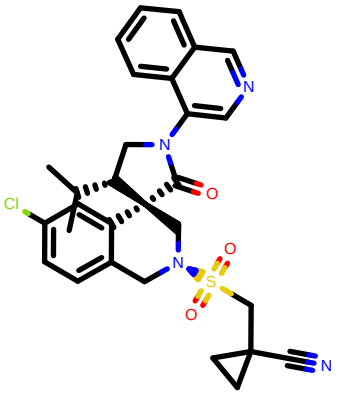
CID:	MAT-POS-853c0ffa-20_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)C(C)(C)O)Cl
RUN:	RUN391
DDG (kcal/mol):	2.60
dDDG (kcal/mol):	0.32

ALP-POS-ecbed2ba-22_1



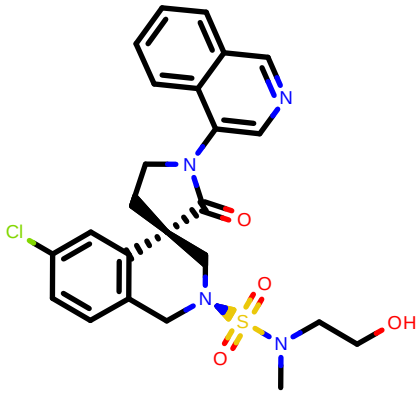
CID:	ALP-POS-ecbed2ba-22_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)CC#N
RUN:	RUN318
DDG (kcal/mol):	2.60
dDDG (kcal/mol):	0.42

MAT-POS-50a80394-3_1



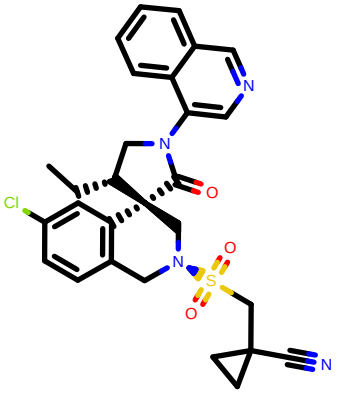
CID:	MAT-POS-50a80394-3_1
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN385
DDG (kcal/mol):	2.61
dDDG (kcal/mol):	0.62

ALP-POS-ecbed2ba-19_1



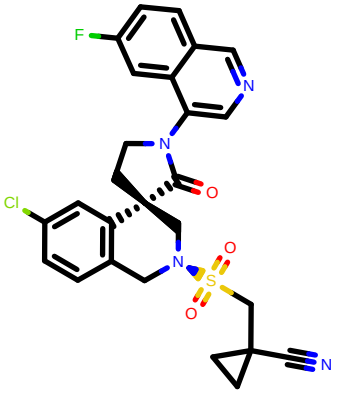
CID:	ALP-POS-ecbed2ba-19_1
SMILES:	C[N@@](CCO)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN209
DDG (kcal/mol):	2.61
dDDG (kcal/mol):	0.30

MAT-POS-50a80394-2_1



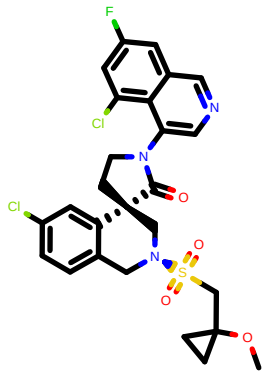
CID:	MAT-POS-50a80394-2_1
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN363
DDG (kcal/mol):	2.63
dDDG (kcal/mol):	0.42

MAT-POS-853c0ffa-13_1



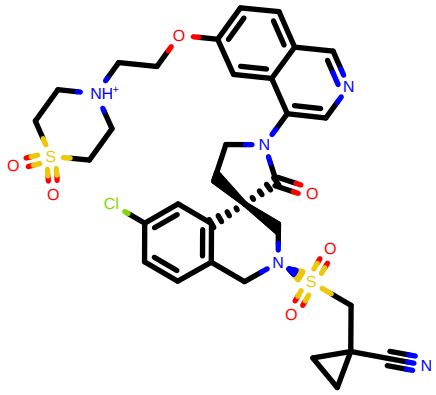
CID:	MAT-POS-853c0ffa-13_1
SMILES:	c1cc2cncc(c2cc1F)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN304
DDG (kcal/mol):	2.67
dDDG (kcal/mol):	0.34

MAT-POS-853c0ffa-8_1



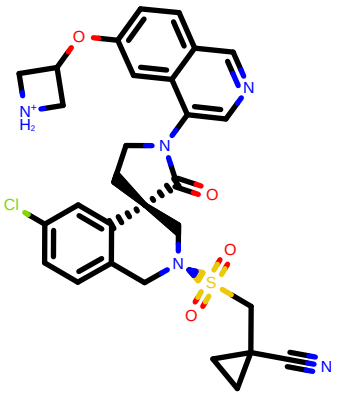
CID:	MAT-POS-853c0ffa-8_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN357
DDG (kcal/mol):	2.67
dDDG (kcal/mol):	0.31

EDJ-MED-468565e0-3_1



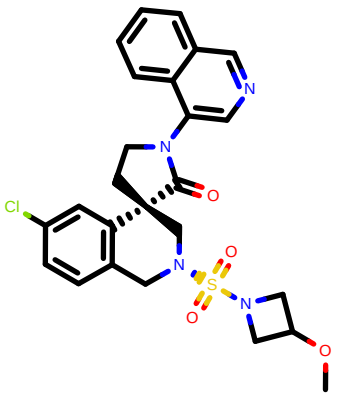
CID:	EDJ-MED-468565e0-3_1
SMILES:	c1cc2cncc(c2cc1OCCN3CCS(=O)(=O)CC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN474
DDG (kcal/mol):	2.69
dDDG (kcal/mol):	0.49

EDJ-MED-ee81482e-1_1



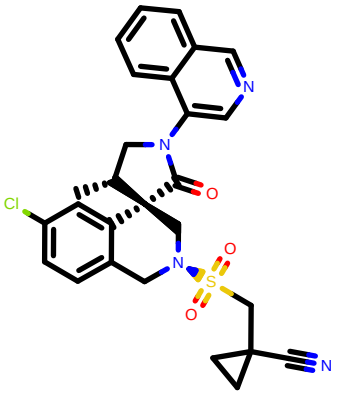
CID:	EDJ-MED-ee81482e-1_1
SMILES:	c1cc2cncc(c2cc1OC3C[NH2+]C3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN433
DDG (kcal/mol):	2.70
dDDG (kcal/mol):	0.57

ALP-POS-ecbed2ba-10_1



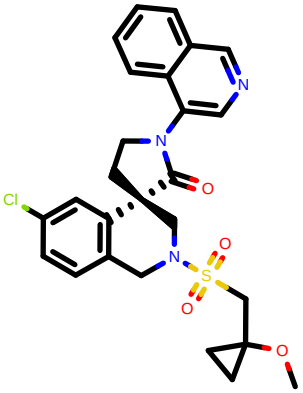
CID:	ALP-POS-ecbed2ba-10_1
SMILES:	COC1CN(C1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN251
DDG (kcal/mol):	2.71
dDDG (kcal/mol):	0.45

MAT-POS-50a80394-1_1



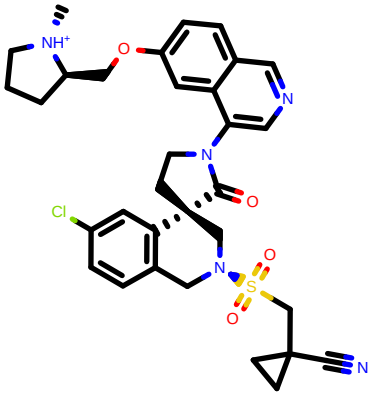
CID:	MAT-POS-50a80394-1_1
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN337
DDG (kcal/mol):	2.72
dDDG (kcal/mol):	0.42

ALP-POS-ecbed2ba-6_2



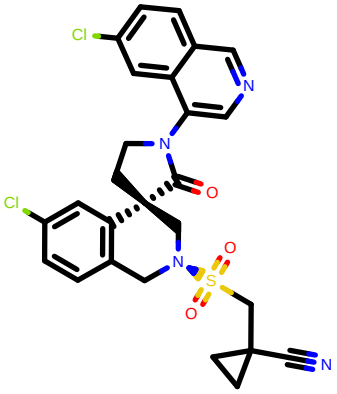
CID:	ALP-POS-ecbed2ba-6_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN236
DDG (kcal/mol):	2.74
dDDG (kcal/mol):	0.43

MAT-POS-40ad851a-1_6



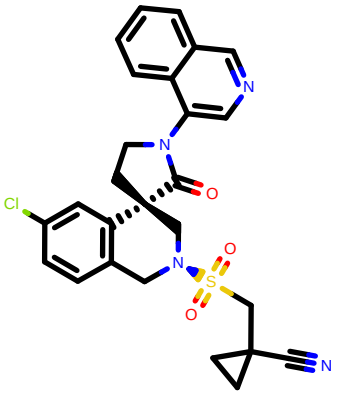
CID:	MAT-POS-40ad851a-1_6
SMILES:	C[N@H+]1CCC[C@@H]1COc2ccc3ncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN471
DDG (kcal/mol):	2.75
dDDG (kcal/mol):	0.76

EDJ-MED-b6c6ee2b-4_1



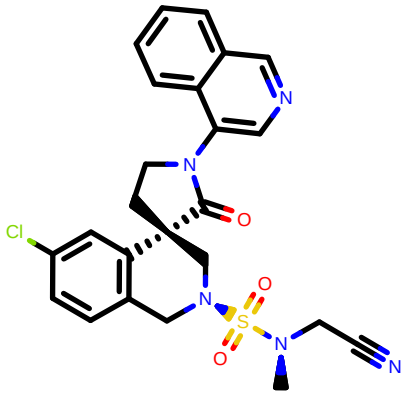
CID:	EDJ-MED-b6c6ee2b-4_1
SMILES:	c1cc2cncc(c2cc1Cl)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN329
DDG (kcal/mol):	2.75
dDDG (kcal/mol):	0.33

MIK-ENA-5d9157e9-2_1



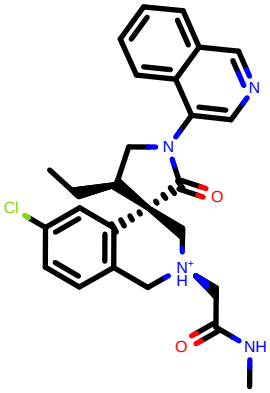
CID:	MIK-ENA-5d9157e9-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN264
DDG (kcal/mol):	2.77
dDDG (kcal/mol):	0.33

ALP-POS-ecbed2ba-17_2



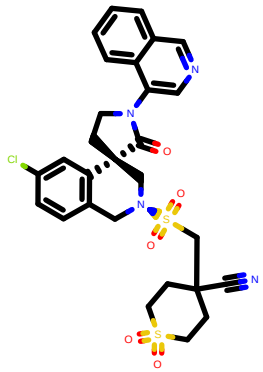
CID:	ALP-POS-ecbed2ba-17_2
SMILES:	C[N@](CC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN198
DDG (kcal/mol):	2.78
dDDG (kcal/mol):	0.26

MAT-POS-50a80394-5_4



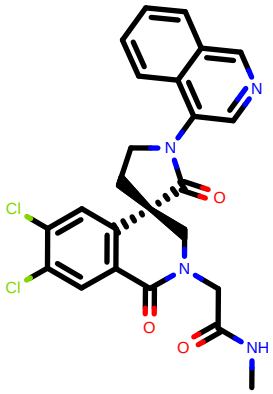
CID:	MAT-POS-50a80394-5_4
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN175
DDG (kcal/mol):	2.79
dDDG (kcal/mol):	0.23

ALP-POS-ecbed2ba-2_2



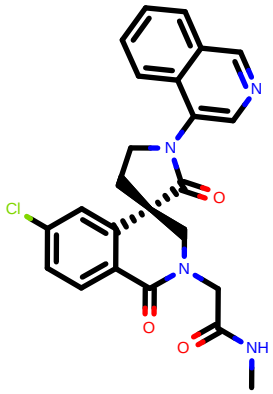
CID:	ALP-POS-ecbed2ba-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCS(=O)(=O)CC6)C#N
RUN:	RUN414
DDG (kcal/mol):	2.82
dDDG (kcal/mol):	0.36

ALP-POS-afe0272e-2_1



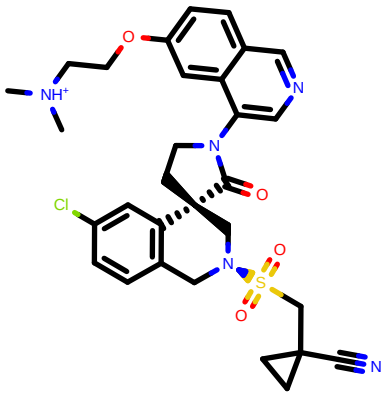
CID:	ALP-POS-afe0272e-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(c(cc5C1=O)Cl)Cl
RUN:	RUN164
DDG (kcal/mol):	2.82
dDDG (kcal/mol):	0.13

EDJ-MED-8bb691af-8_1



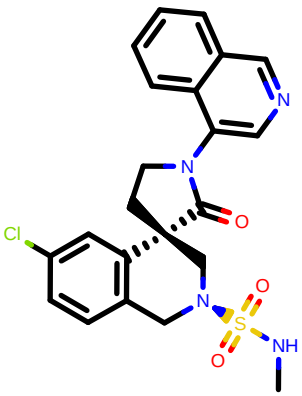
CID:	EDJ-MED-8bb691af-8_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN91
DDG (kcal/mol):	2.84
dDDG (kcal/mol):	0.18

LUO-POS-8484f2d3-2_1



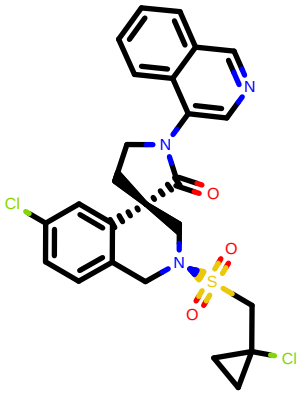
CID:	LUO-POS-8484f2d3-2_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN437
DDG (kcal/mol):	2.84
dDDG (kcal/mol):	0.64

LUO-POS-ed2cfb03-2_2



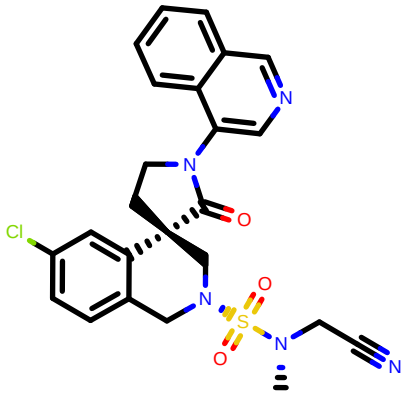
CID:	LUO-POS-ed2cfb03-2_2
SMILES:	CNS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN89
DDG (kcal/mol):	2.85
dDDG (kcal/mol):	0.43

PET-UNK-94036022-3_1



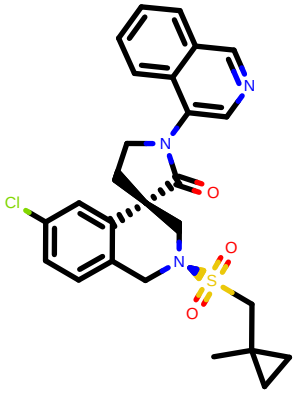
CID:	PET-UNK-94036022-3_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN226
DDG (kcal/mol):	2.85
dDDG (kcal/mol):	0.31

ALP-POS-ecbed2ba-17_1



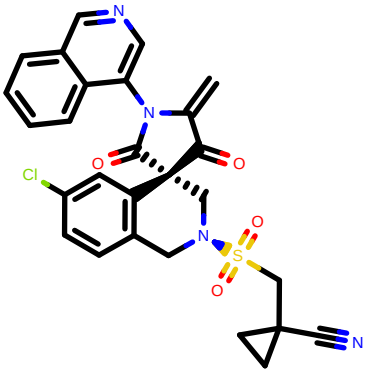
CID:	ALP-POS-ecbed2ba-17_1
SMILES:	C[N@@](CC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN201
DDG (kcal/mol):	2.85
dDDG (kcal/mol):	0.27

ALP-POS-ecbed2ba-3_2



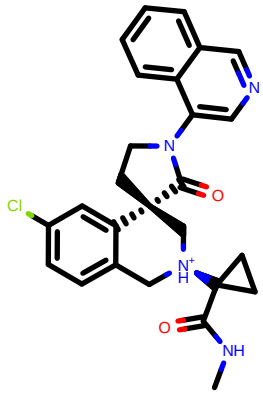
CID:	ALP-POS-ecbed2ba-3_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN200
DDG (kcal/mol):	2.86
dDDG (kcal/mol):	0.32

PET-UNK-94036022-13_1



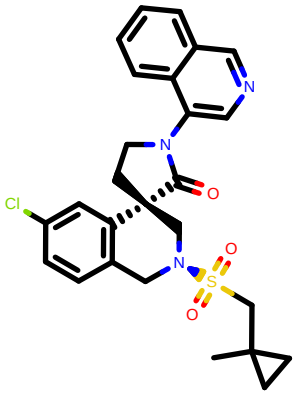
CID:	PET-UNK-94036022-13_1
SMILES:	C=C1C(=O)[C@]2(C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN384
DDG (kcal/mol):	2.87
dDDG (kcal/mol):	0.36

MAT-POS-576f7758-1_2



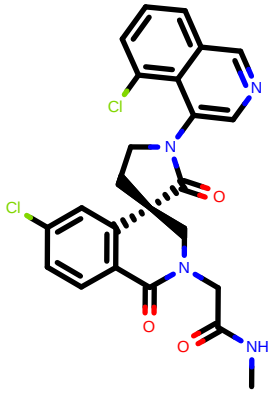
CID:	MAT-POS-576f7758-1_2
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN167
DDG (kcal/mol):	2.88
dDDG (kcal/mol):	0.16

ALP-POS-ecbed2ba-3_1



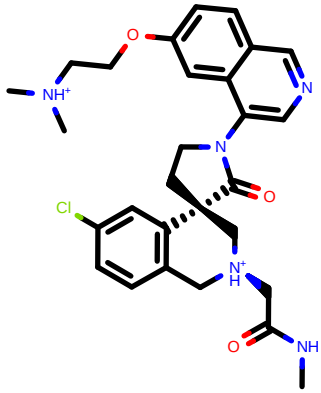
CID:	ALP-POS-ecbed2ba-3_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN199
DDG (kcal/mol):	2.89
dDDG (kcal/mol):	0.36

MAT-POS-853c0ffa-1_1



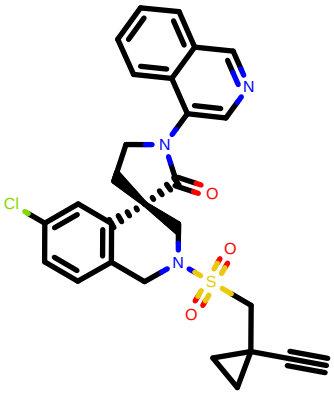
CID:	MAT-POS-853c0ffa-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(ccc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN149
DDG (kcal/mol):	2.90
dDDG (kcal/mol):	0.18

MAT-POS-38eb6498-3_2



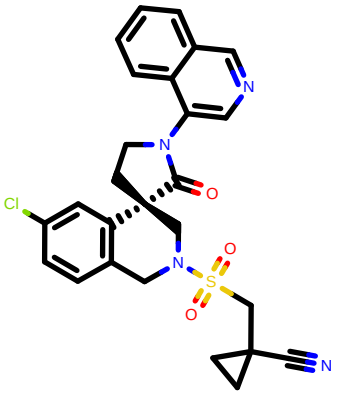
CID:	MAT-POS-38eb6498-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN390
DDG (kcal/mol):	2.91
dDDG (kcal/mol):	0.40

PET-UNK-94036022-2_2



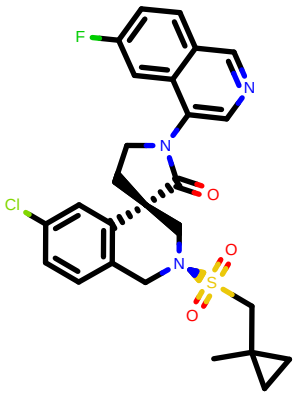
CID:	PET-UNK-94036022-2_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN283
DDG (kcal/mol):	2.92
dDDG (kcal/mol):	0.40

ALP-POS-ecbed2ba-4_2



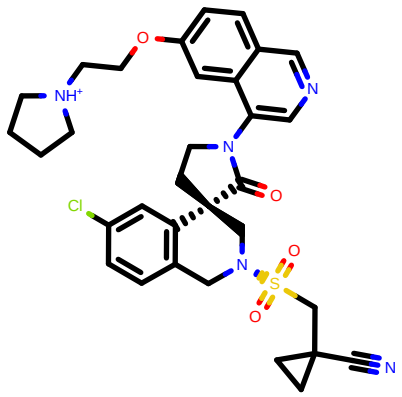
CID:	ALP-POS-ecbed2ba-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN240
DDG (kcal/mol):	2.94
dDDG (kcal/mol):	0.40

MAT-POS-853c0ffa-21_2



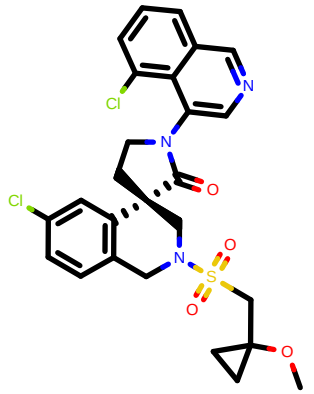
CID:	MAT-POS-853c0ffa-21_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN242
DDG (kcal/mol):	2.94
dDDG (kcal/mol):	0.48

EDJ-MED-468565e0-1_2



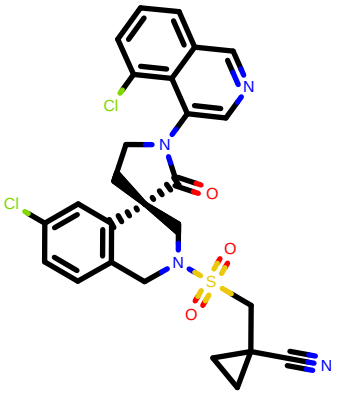
CID:	EDJ-MED-468565e0-1_2
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN479
DDG (kcal/mol):	2.95
dDDG (kcal/mol):	0.66

MAT-POS-853c0ffa-7_1



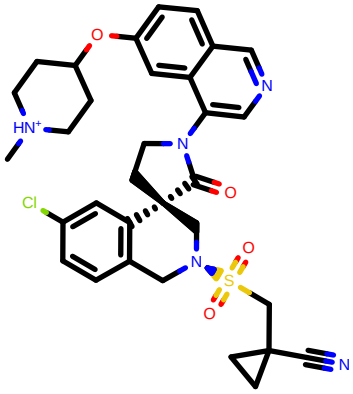
CID:	MAT-POS-853c0ffa-7_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN301
DDG (kcal/mol):	2.96
dDDG (kcal/mol):	0.32

MAT-POS-1d5ab790-1_2



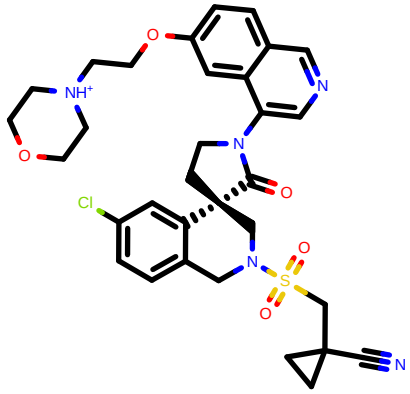
CID:	MAT-POS-1d5ab790-1_2
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN321
DDG (kcal/mol):	2.96
dDDG (kcal/mol):	0.47

LUO-POS-d1147590-1_1



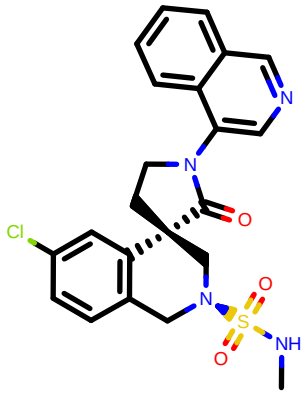
CID:	LUO-POS-d1147590-1_1
SMILES:	C[NH+]1CCC(CC1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN478
DDG (kcal/mol):	2.97
dDDG (kcal/mol):	0.56

EDJ-MED-468565e0-2_2



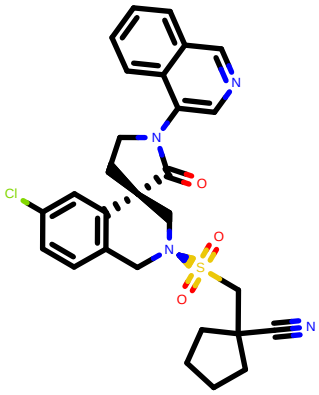
CID:	EDJ-MED-468565e0-2_2
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCOCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN481
DDG (kcal/mol):	2.97
dDDG (kcal/mol):	0.69

LUO-POS-ed2cfb03-2_1



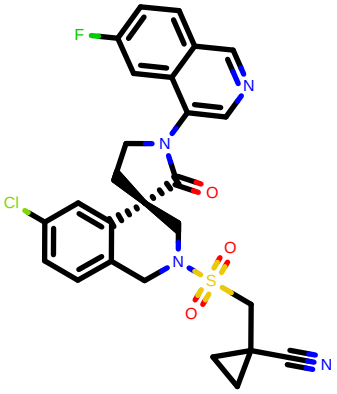
CID:	LUO-POS-ed2cfb03-2_1
SMILES:	CNS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN96
DDG (kcal/mol):	2.98
dDDG (kcal/mol):	0.22

ALP-POS-ecbed2ba-15_2



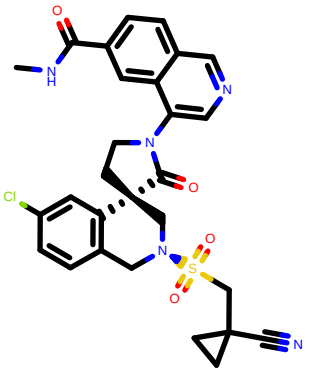
CID:	ALP-POS-ecbed2ba-15_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCCC6)C#N
RUN:	RUN359
DDG (kcal/mol):	2.99
dDDG (kcal/mol):	0.51

MAT-POS-853c0ffa-13_2



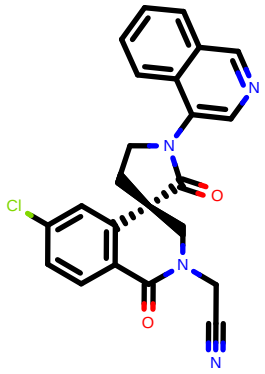
CID:	MAT-POS-853c0ffa-13_2
SMILES:	c1cc2cncc(c2cc1F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN303
DDG (kcal/mol):	3.01
dDDG (kcal/mol):	0.36

MAT-POS-38eb6498-2_1



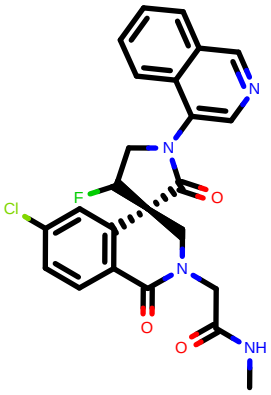
CID:	MAT-POS-38eb6498-2_1
SMILES:	CNC(=O)c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN410
DDG (kcal/mol):	3.01
dDDG (kcal/mol):	0.42

PET-UNK-aa57768f-2_1



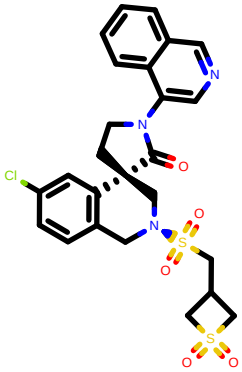
CID:	PET-UNK-aa57768f-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N
RUN:	RUN60
DDG (kcal/mol):	3.01
dDDG (kcal/mol):	0.17

EDJ-MED-fd8ed875-5_1



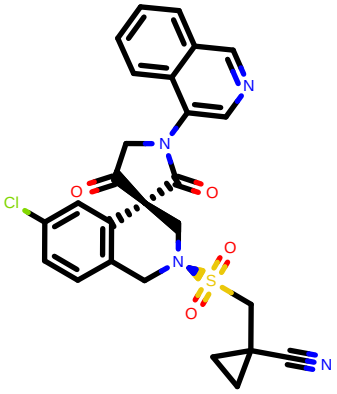
CID:	EDJ-MED-fd8ed875-5_1
SMILES:	CNC(=O)CN1C[C@@]2(c3cc(ccc3C1=O)Cl)C(=CN(C2=O)c4cncc5c4cccc5)F
RUN:	RUN170
DDG (kcal/mol):	3.03
dDDG (kcal/mol):	0.17

ALP-POS-ecbed2ba-5_2



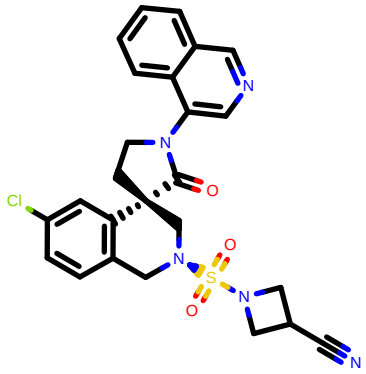
CID:	ALP-POS-ecbed2ba-5_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6CS(=O)(=O)C6
RUN:	RUN314
DDG (kcal/mol):	3.03
dDDG (kcal/mol):	0.69

EDJ-MED-a12e3a20-1_1



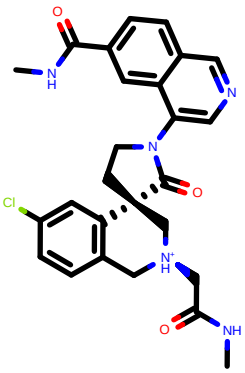
CID:	EDJ-MED-a12e3a20-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN327
DDG (kcal/mol):	3.07
dDDG (kcal/mol):	0.50

ALP-POS-ecbed2ba-9_1



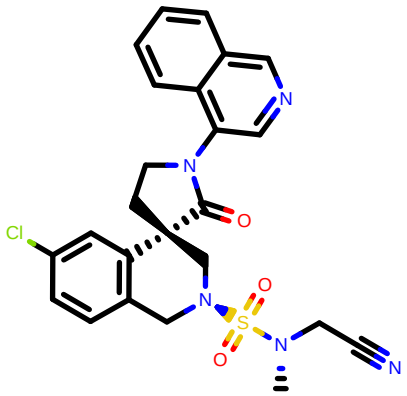
CID:	ALP-POS-ecbed2ba-9_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CC(C6)C#N
RUN:	RUN248
DDG (kcal/mol):	3.08
dDDG (kcal/mol):	0.50

MAT-POS-38eb6498-5_2



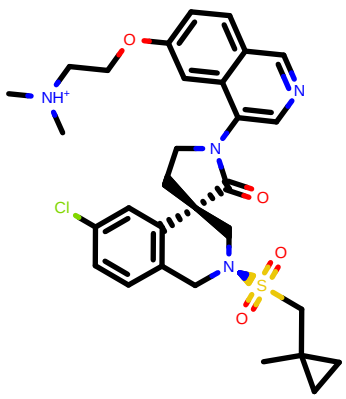
CID:	MAT-POS-38eb6498-5_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)C(=O)NC)Cl
RUN:	RUN277
DDG (kcal/mol):	3.11
dDDG (kcal/mol):	0.19

ALP-POS-ecbed2ba-17_3



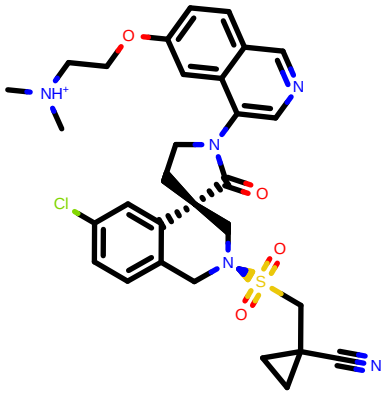
CID:	ALP-POS-ecbed2ba-17_3
SMILES:	C[N@@](CC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN207
DDG (kcal/mol):	3.12
dDDG (kcal/mol):	0.65

MAT-POS-853c0ffa-19_1



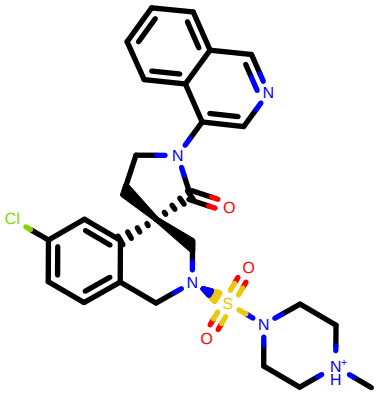
CID:	MAT-POS-853c0ffa-19_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(cc6)OCC[NH+](C)C)Cl
RUN:	RUN427
DDG (kcal/mol):	3.14
dDDG (kcal/mol):	0.43

MAT-POS-38eb6498-1_1



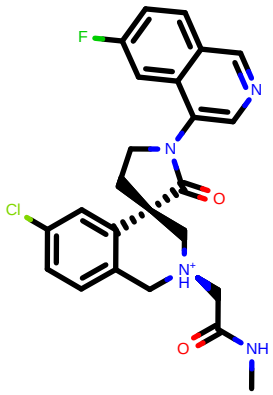
CID:	MAT-POS-38eb6498-1_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN440
DDG (kcal/mol):	3.14
dDDG (kcal/mol):	0.78

LUO-POS-ed2cfb03-1_1



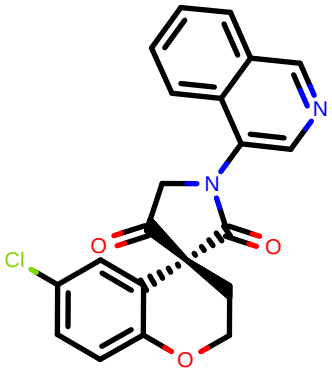
CID:	LUO-POS-ed2cfb03-1_1
SMILES:	C[NH+]1CCN(CC1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN345
DDG (kcal/mol):	3.15
dDDG (kcal/mol):	0.28

MAT-POS-b4d6b7fc-5_2



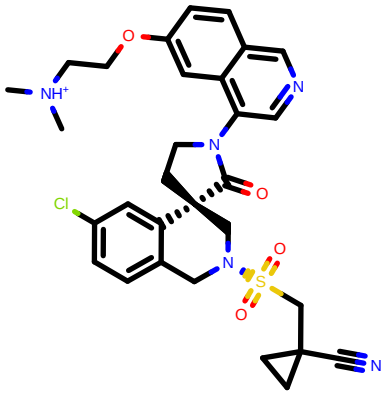
CID:	MAT-POS-b4d6b7fc-5_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN103
DDG (kcal/mol):	3.16
dDDG (kcal/mol):	0.22

DAR-DIA-0f7b7cd9-9_1



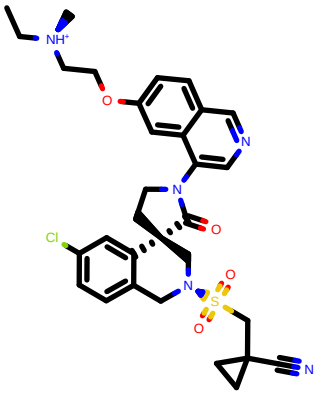
CID:	DAR-DIA-0f7b7cd9-9_1
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN30
DDG (kcal/mol):	3.17
dDDG (kcal/mol):	0.15

LUO-POS-8484f2d3-2_2



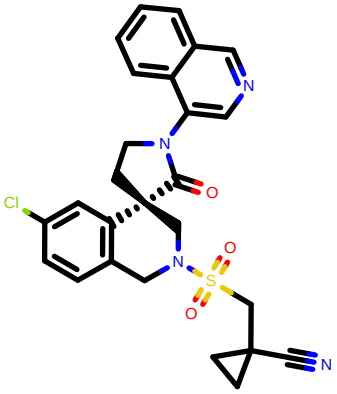
CID:	LUO-POS-8484f2d3-2_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN446
DDG (kcal/mol):	3.17
dDDG (kcal/mol):	0.71

MAT-POS-40ad851a-2_1



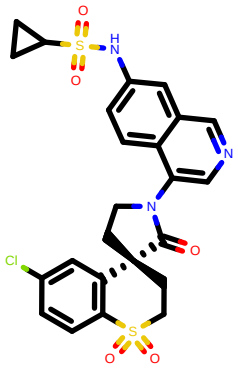
CID:	MAT-POS-40ad851a-2_1
SMILES:	CC[N@@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN448
DDG (kcal/mol):	3.19
dDDG (kcal/mol):	0.58

MIK-ENA-5d9157e9-2_2



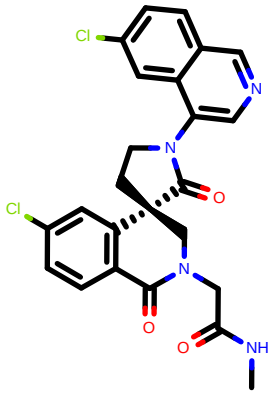
CID:	MIK-ENA-5d9157e9-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN266
DDG (kcal/mol):	3.19
dDDG (kcal/mol):	0.45

EDJ-MED-ede5c6cb-2_1



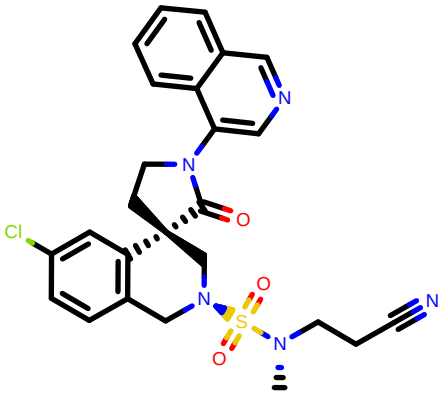
CID:	EDJ-MED-ede5c6cb-2_1
SMILES:	c1cc2c(cc1NS(=O)(=O)C3CC3)cncc2N4CC[C@@]5(C4=O)CCS(=O)(=O)c6c5cc(cc6)Cl
RUN:	RUN289
DDG (kcal/mol):	3.20
dDDG (kcal/mol):	0.20

LUO-POS-8c3e556a-2_1



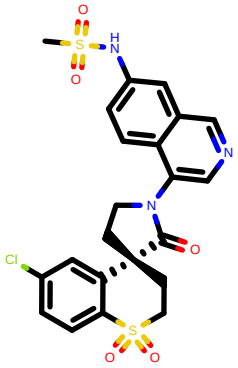
CID:	LUO-POS-8c3e556a-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN180
DDG (kcal/mol):	3.21
dDDG (kcal/mol):	0.19

ALP-POS-ecbed2ba-16_2



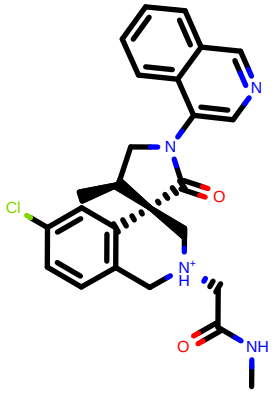
CID:	ALP-POS-ecbed2ba-16_2
SMILES:	C[N@](CCC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN249
DDG (kcal/mol):	3.21
dDDG (kcal/mol):	0.32

EDJ-MED-94fddcec-7_1



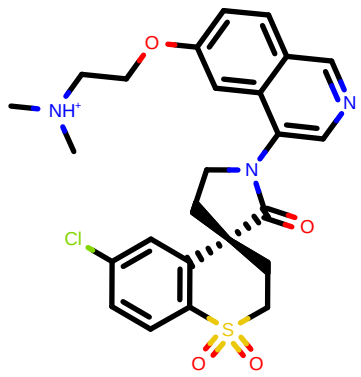
CID:	EDJ-MED-94fddcec-7_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN150
DDG (kcal/mol):	3.23
dDDG (kcal/mol):	0.17

MAT-POS-50a80394-4_2



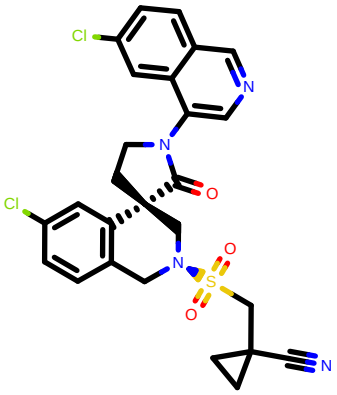
CID:	MAT-POS-50a80394-4_2
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN122
DDG (kcal/mol):	3.24
dDDG (kcal/mol):	0.31

EDJ-MED-d4864bdc-4_1



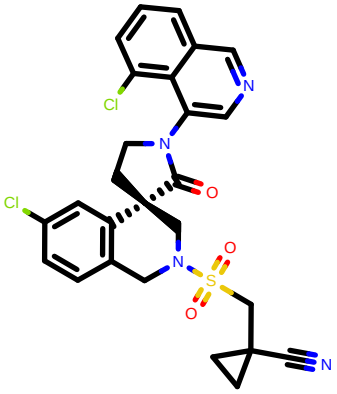
CID:	EDJ-MED-d4864bdc-4_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN229
DDG (kcal/mol):	3.24
dDDG (kcal/mol):	0.23

EDJ-MED-b6c6ee2b-4_2



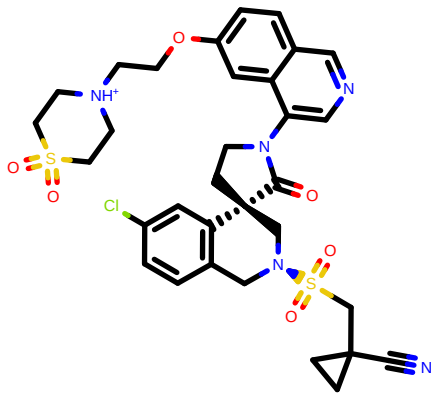
CID:	EDJ-MED-b6c6ee2b-4_2
SMILES:	c1cc2cncc(c2cc1Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN335
DDG (kcal/mol):	3.25
dDDG (kcal/mol):	0.48

MAT-POS-853c0ffa-5_2



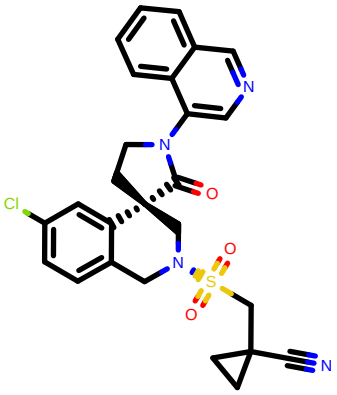
CID:	MAT-POS-853c0ffa-5_2
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN300
DDG (kcal/mol):	3.27
dDDG (kcal/mol):	0.44

EDJ-MED-468565e0-3_2



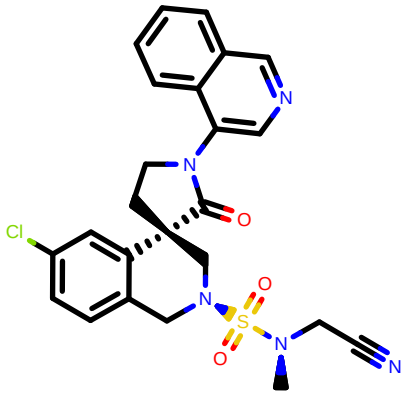
CID:	EDJ-MED-468565e0-3_2
SMILES:	c1cc2cncc(c2cc1OCCN3CCS(=O)(=O)CC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN484
DDG (kcal/mol):	3.30
dDDG (kcal/mol):	0.67

ALP-POS-ecbed2ba-4_1



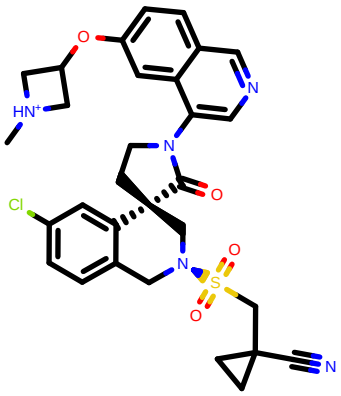
CID:	ALP-POS-ecbed2ba-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN241
DDG (kcal/mol):	3.32
dDDG (kcal/mol):	0.40

ALP-POS-ecbed2ba-17_4



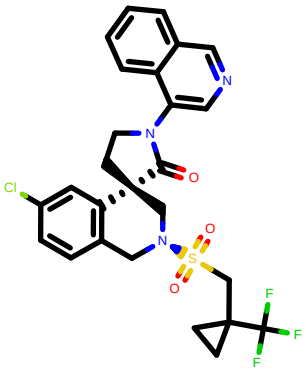
CID:	ALP-POS-ecbed2ba-17_4
SMILES:	C[N@](CC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN202
DDG (kcal/mol):	3.34
dDDG (kcal/mol):	0.67

EDJ-MED-ee81482e-2_2



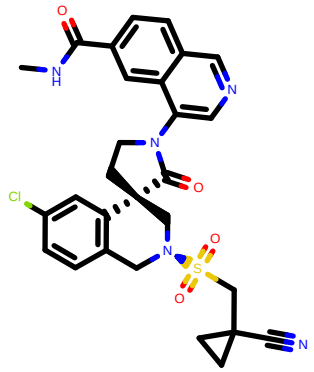
CID:	EDJ-MED-ee81482e-2_2
SMILES:	C[NH+]1CC(C1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN443
DDG (kcal/mol):	3.36
dDDG (kcal/mol):	0.77

EDJ-MED-5cd3920d-6_1



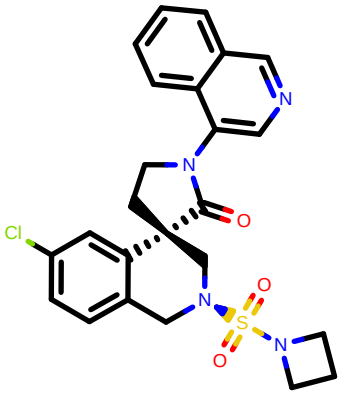
CID:	EDJ-MED-5cd3920d-6_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)(F)F
RUN:	RUN375
DDG (kcal/mol):	3.39
dDDG (kcal/mol):	0.35

MAT-POS-38eb6498-2_2



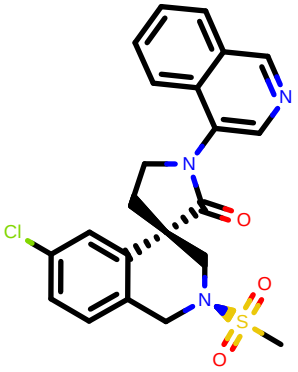
CID:	MAT-POS-38eb6498-2_2
SMILES:	CNC(=O)c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN411
DDG (kcal/mol):	3.41
dDDG (kcal/mol):	0.47

ALP-POS-ecbed2ba-20_1



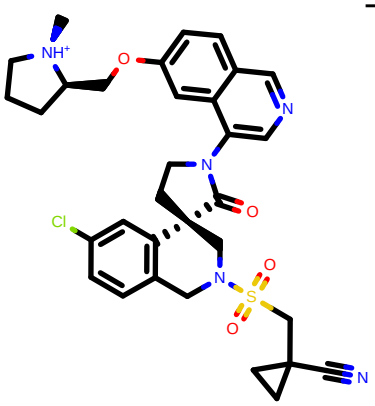
CID:	ALP-POS-ecbed2ba-20_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CCC6
RUN:	RUN158
DDG (kcal/mol):	3.42
dDDG (kcal/mol):	0.47

EDJ-MED-7587a9ee-3_2



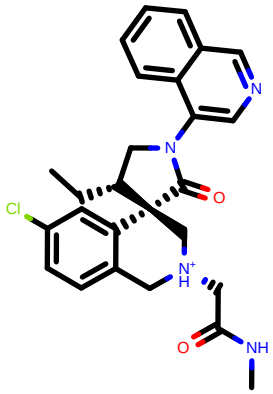
CID:	EDJ-MED-7587a9ee-3_2
SMILES:	CS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN49
DDG (kcal/mol):	3.42
dDDG (kcal/mol):	0.17

MAT-POS-40ad851a-1_5



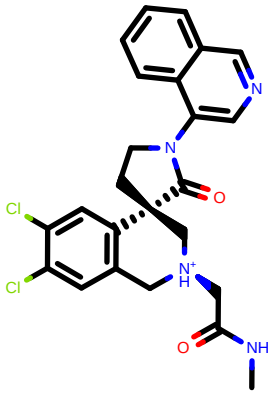
CID:	MAT-POS-40ad851a-1_5
SMILES:	C[N@@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN463
DDG (kcal/mol):	3.46
dDDG (kcal/mol):	0.81

MAT-POS-50a80394-5_1



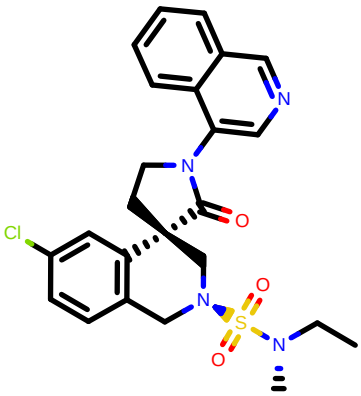
CID:	MAT-POS-50a80394-5_1
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN172
DDG (kcal/mol):	3.50
dDDG (kcal/mol):	0.27

ALP-POS-afe0272e-1_2



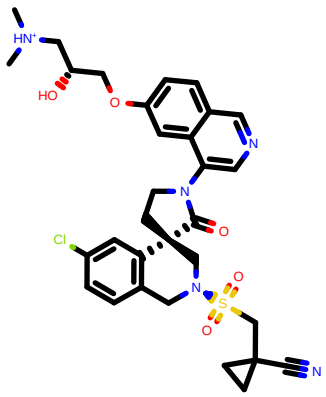
CID:	ALP-POS-afe0272e-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2cc(c(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)Cl
RUN:	RUN111
DDG (kcal/mol):	3.50
dDDG (kcal/mol):	0.24

ALP-POS-ecbed2ba-18_2



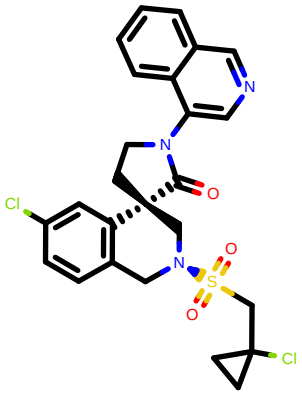
CID:	ALP-POS-ecbed2ba-18_2
SMILES:	CC[N@](C)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN152
DDG (kcal/mol):	3.51
dDDG (kcal/mol):	0.32

EDJ-MED-ee81482e-3_2



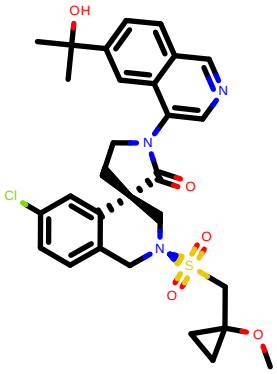
CID:	EDJ-MED-ee81482e-3_2
SMILES:	C[NH+](C)C[C@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4ccc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN455
DDG (kcal/mol):	3.53
dDDG (kcal/mol):	0.54

PET-UNK-94036022-10_1



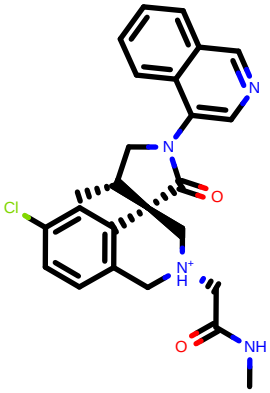
CID:	PET-UNK-94036022-10_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN225
DDG (kcal/mol):	3.54
dDDG (kcal/mol):	0.38

MAT-POS-853c0ffa-12_1



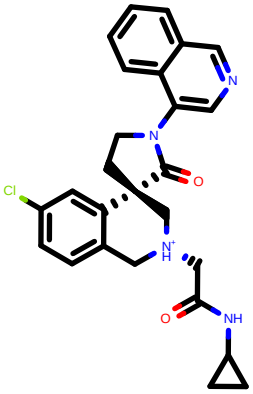
CID:	MAT-POS-853c0ffa-12_1
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC)O
RUN:	RUN409
DDG (kcal/mol):	3.54
dDDG (kcal/mol):	0.42

MAT-POS-50a80394-4_1



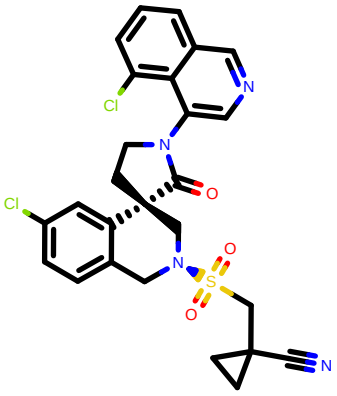
CID:	MAT-POS-50a80394-4_1
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN121
DDG (kcal/mol):	3.56
dDDG (kcal/mol):	0.25

MAT-POS-69786b79-2_1



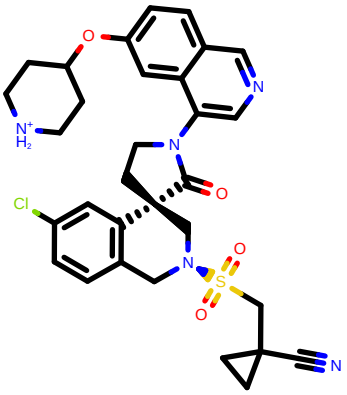
CID:	MAT-POS-69786b79-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6CC6
RUN:	RUN161
DDG (kcal/mol):	3.56
dDDG (kcal/mol):	0.30

MAT-POS-1d5ab790-1_1



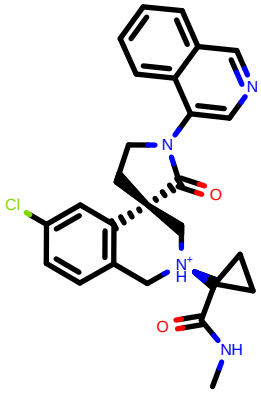
CID:	MAT-POS-1d5ab790-1_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN316
DDG (kcal/mol):	3.57
dDDG (kcal/mol):	0.34

EDJ-MED-ee81482e-4_2



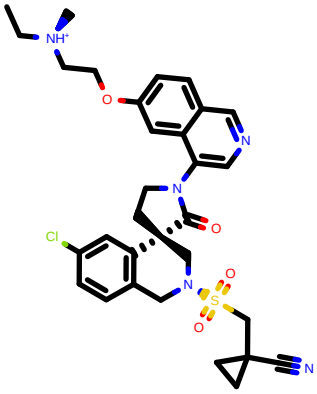
CID:	EDJ-MED-ee81482e-4_2
SMILES:	c1cc2cncc(c2cc1OC3CC[NH2+]CC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN432
DDG (kcal/mol):	3.58
dDDG (kcal/mol):	0.83

ALP-POS-ecbed2ba-7_2



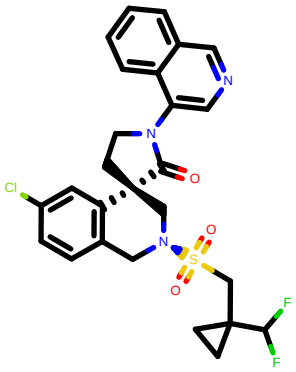
CID:	ALP-POS-ecbed2ba-7_2
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN139
DDG (kcal/mol):	3.58
dDDG (kcal/mol):	0.18

MAT-POS-40ad851a-2_3



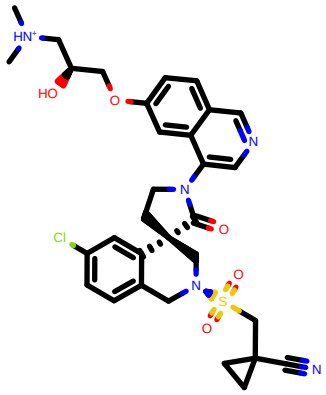
CID:	MAT-POS-40ad851a-2_3
SMILES:	CC[N@@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN450
DDG (kcal/mol):	3.58
dDDG (kcal/mol):	0.63

EDJ-MED-5cd3920d-5_1



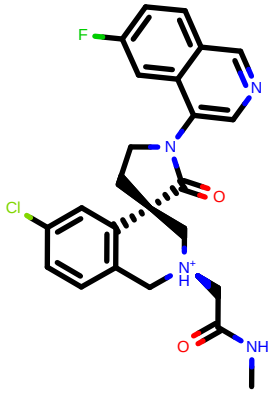
CID:	EDJ-MED-5cd3920d-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)F
RUN:	RUN342
DDG (kcal/mol):	3.59
dDDG (kcal/mol):	0.46

EDJ-MED-ee81482e-3_1



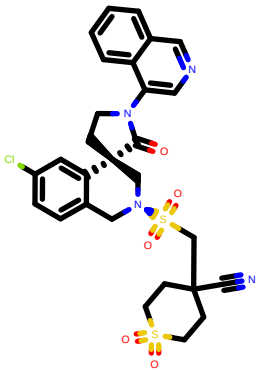
CID:	EDJ-MED-ee81482e-3_1
SMILES:	C[NH+](C)C[C@@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN452
DDG (kcal/mol):	3.59
dDDG (kcal/mol):	0.55

LUO-POS-b4dec3be-2_2



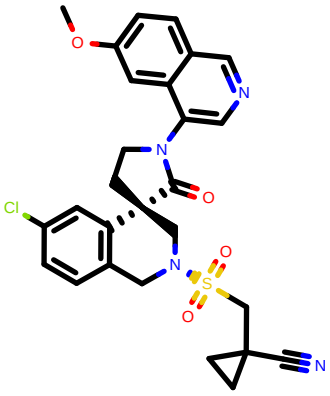
CID:	LUO-POS-b4dec3be-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN128
DDG (kcal/mol):	3.59
dDDG (kcal/mol):	0.20

ALP-POS-ecbed2ba-2_1



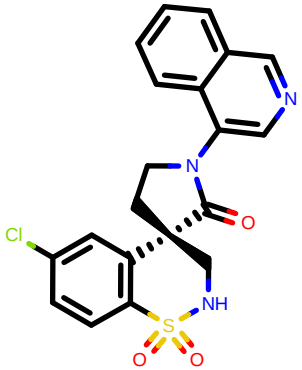
CID:	ALP-POS-ecbed2ba-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCS(=O)(=O)CC6)C#N
RUN:	RUN419
DDG (kcal/mol):	3.59
dDDG (kcal/mol):	0.44

EDJ-MED-b6c6ee2b-3_2



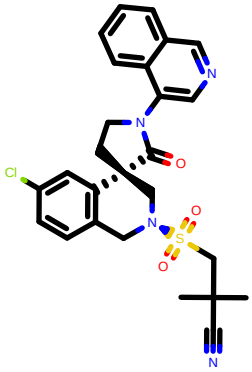
CID:	EDJ-MED-b6c6ee2b-3_2
SMILES:	COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN377
DDG (kcal/mol):	3.60
dDDG (kcal/mol):	0.45

ALP-POS-4483ae88-1_1



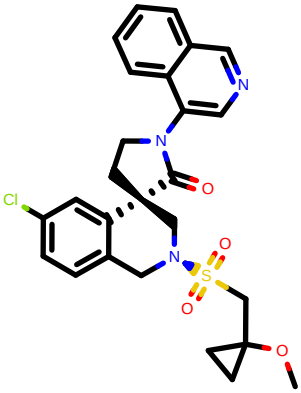
CID:	ALP-POS-4483ae88-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN51
DDG (kcal/mol):	3.61
dDDG (kcal/mol):	0.14

ALP-POS-ecbed2ba-13_1



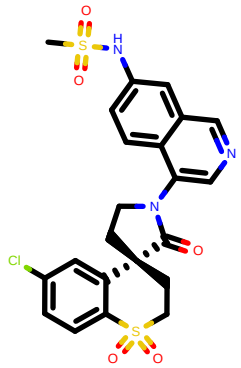
CID:	ALP-POS-ecbed2ba-13_1
SMILES:	CC(C)(CS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)C#N
RUN:	RUN254
DDG (kcal/mol):	3.64
dDDG (kcal/mol):	0.36

ALP-POS-ecbed2ba-6_1



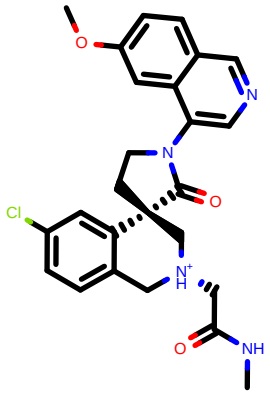
CID:	ALP-POS-ecbed2ba-6_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN243
DDG (kcal/mol):	3.65
dDDG (kcal/mol):	0.34

EDJ-MED-ede5c6cb-1_1



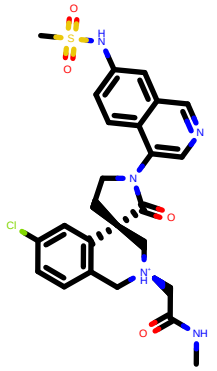
CID:	EDJ-MED-ede5c6cb-1_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN176
DDG (kcal/mol):	3.67
dDDG (kcal/mol):	0.19

EDJ-MED-b6c6ee2b-2_1



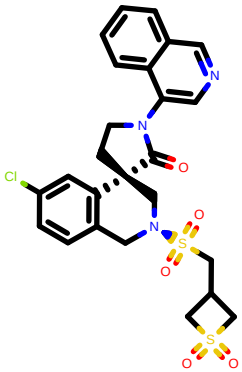
CID:	EDJ-MED-b6c6ee2b-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OC)Cl
RUN:	RUN178
DDG (kcal/mol):	3.67
dDDG (kcal/mol):	0.29

MAT-POS-b4d6b7fc-7_2



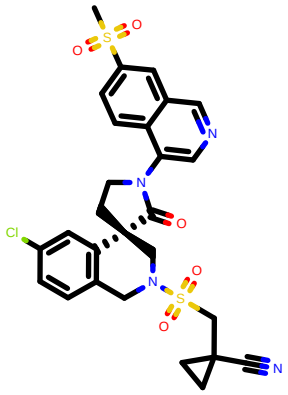
CID:	MAT-POS-b4d6b7fc-7_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)Cl
RUN:	RUN322
DDG (kcal/mol):	3.69
dDDG (kcal/mol):	0.26

ALP-POS-ecbed2ba-5_1



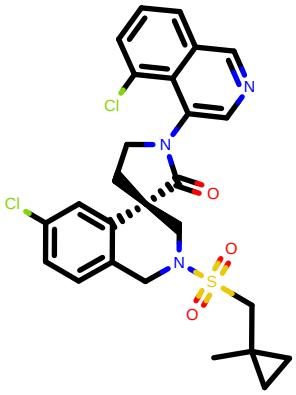
CID:	ALP-POS-ecbed2ba-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6CS(=O)(=O)C6
RUN:	RUN308
DDG (kcal/mol):	3.70
dDDG (kcal/mol):	0.82

MAT-POS-853c0ffa-15_2



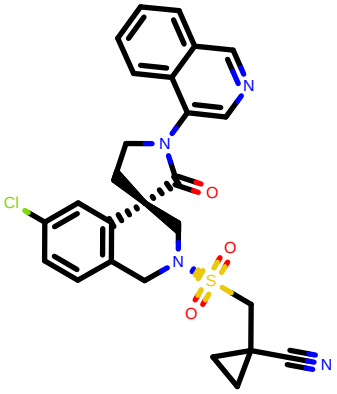
CID:	MAT-POS-853c0ffa-15_2
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN403
DDG (kcal/mol):	3.73
dDDG (kcal/mol):	0.59

MAT-POS-853c0ffa-17_2



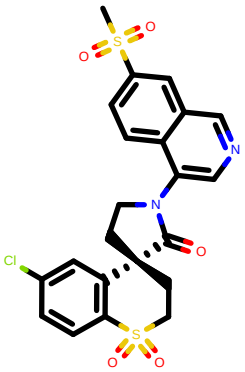
CID:	MAT-POS-853c0ffa-17_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN237
DDG (kcal/mol):	3.76
dDDG (kcal/mol):	0.28

MIK-ENA-5d9157e9-1_2



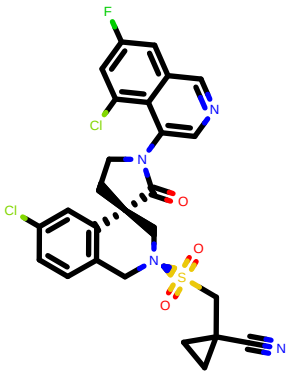
CID:	MIK-ENA-5d9157e9-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN259
DDG (kcal/mol):	3.82
dDDG (kcal/mol):	0.45

EDJ-MED-94fddcec-5_1



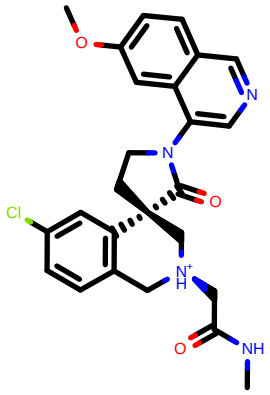
CID:	EDJ-MED-94fddcec-5_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN101
DDG (kcal/mol):	3.82
dDDG (kcal/mol):	0.15

MAT-POS-853c0ffa-6_1



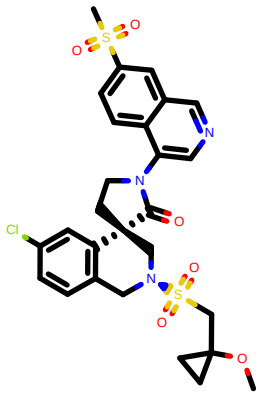
CID:	MAT-POS-853c0ffa-6_1
SMILES:	c1cc2c(cc1Cl)[C@@]3(CCN(C3=O)c4cncc5c4c(cc(c5)F)Cl)C[N@@](C2)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN350
DDG (kcal/mol):	3.85
dDDG (kcal/mol):	0.54

EDJ-MED-b6c6ee2b-2_2



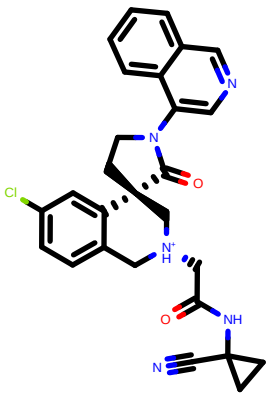
CID:	EDJ-MED-b6c6ee2b-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OC)Cl
RUN:	RUN171
DDG (kcal/mol):	3.86
dDDG (kcal/mol):	0.23

MAT-POS-853c0ffa-16_2



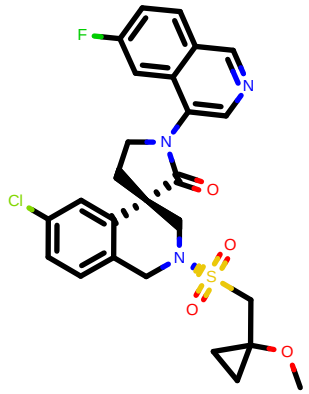
CID:	MAT-POS-853c0ffa-16_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN407
DDG (kcal/mol):	3.87
dDDG (kcal/mol):	0.43

MAT-POS-69786b79-4_1



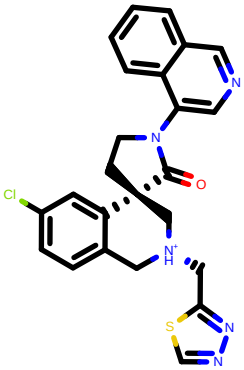
CID:	MAT-POS-69786b79-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6(CC6)C#N
RUN:	RUN268
DDG (kcal/mol):	3.88
dDDG (kcal/mol):	0.30

MAT-POS-853c0ffa-14_2



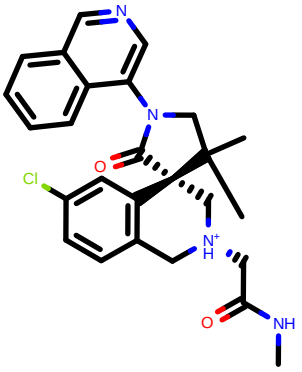
CID:	MAT-POS-853c0ffa-14_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN309
DDG (kcal/mol):	3.88
dDDG (kcal/mol):	0.48

PET-UNK-7e9559de-4_1



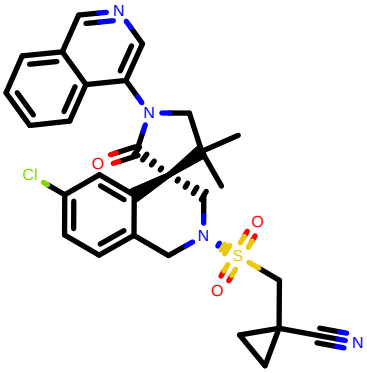
CID:	PET-UNK-7e9559de-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN114
DDG (kcal/mol):	3.91
dDDG (kcal/mol):	0.17

MAT-POS-50a80394-7_1



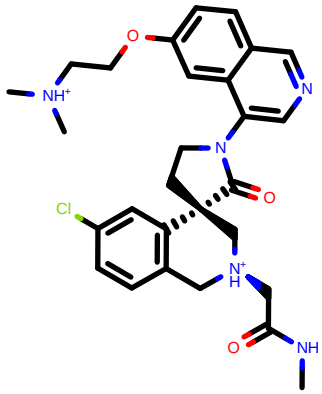
CID:	MAT-POS-50a80394-7_1
SMILES:	CC1(CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5)C
RUN:	RUN169
DDG (kcal/mol):	3.91
dDDG (kcal/mol):	0.29

MAT-POS-50a80394-8_2



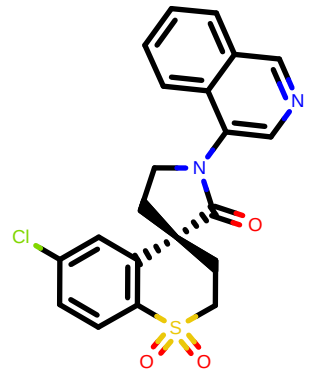
CID:	MAT-POS-50a80394-8_2
SMILES:	CC1(CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6)C
RUN:	RUN367
DDG (kcal/mol):	3.91
dDDG (kcal/mol):	0.52

EDJ-MED-b6c6ee2b-1_2



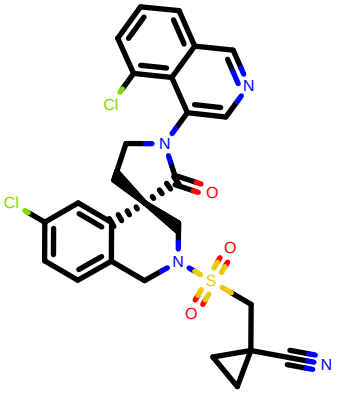
CID:	EDJ-MED-b6c6ee2b-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN395
DDG (kcal/mol):	3.93
dDDG (kcal/mol):	0.40

EDJ-MED-d4864bdc-3_1



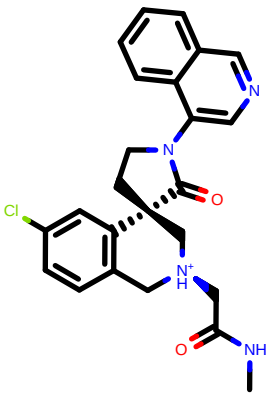
CID:	EDJ-MED-d4864bdc-3_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN35
DDG (kcal/mol):	3.94
dDDG (kcal/mol):	0.13

MAT-POS-853c0ffa-5_1



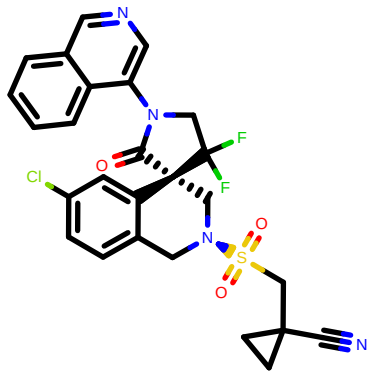
CID:	MAT-POS-853c0ffa-5_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN299
DDG (kcal/mol):	3.94
dDDG (kcal/mol):	0.42

EDJ-MED-8bb691af-4_2



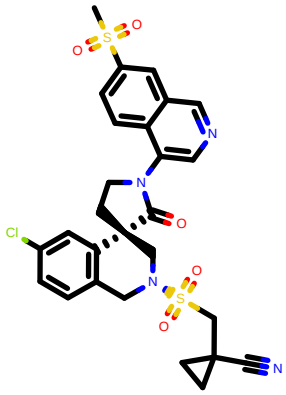
CID:	EDJ-MED-8bb691af-4_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN69
DDG (kcal/mol):	3.95
dDDG (kcal/mol):	0.21

EDJ-MED-7e491f08-1_2



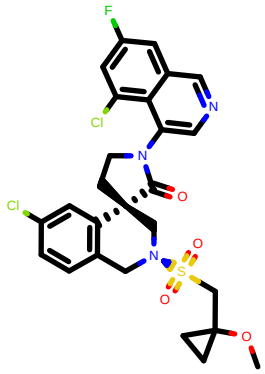
CID:	EDJ-MED-7e491f08-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)(F)F
RUN:	RUN376
DDG (kcal/mol):	3.98
dDDG (kcal/mol):	0.61

MAT-POS-853c0ffa-15_1



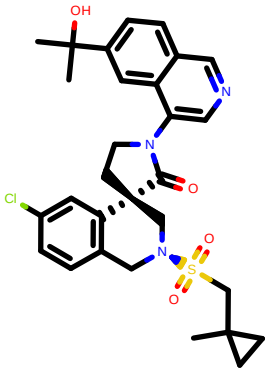
CID:	MAT-POS-853c0ffa-15_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN401
DDG (kcal/mol):	3.99
dDDG (kcal/mol):	0.55

MAT-POS-853c0ffa-8_2



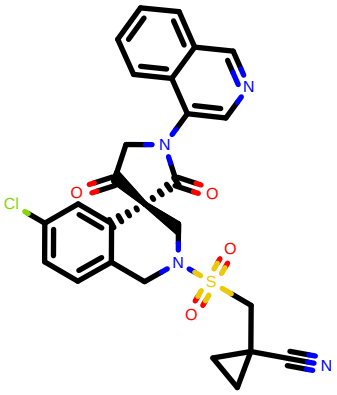
CID:	MAT-POS-853c0ffa-8_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN361
DDG (kcal/mol):	4.03
dDDG (kcal/mol):	0.37

MAT-POS-853c0ffa-20_2



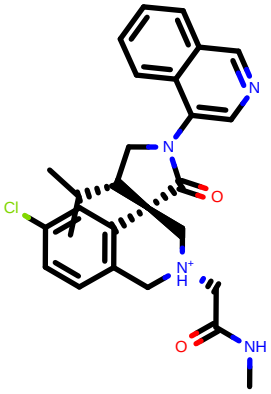
CID:	MAT-POS-853c0ffa-20_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)C(C)(C)O)Cl
RUN:	RUN392
DDG (kcal/mol):	4.04
dDDG (kcal/mol):	0.53

EDJ-MED-a12e3a20-1_2



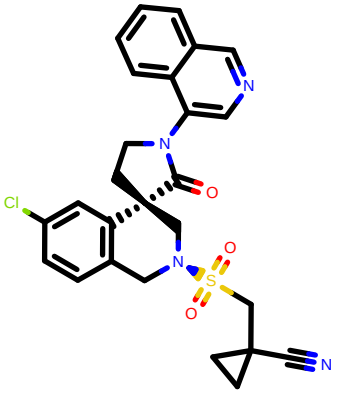
CID:	EDJ-MED-a12e3a20-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN332
DDG (kcal/mol):	4.04
dDDG (kcal/mol):	0.51

MAT-POS-50a80394-6_1



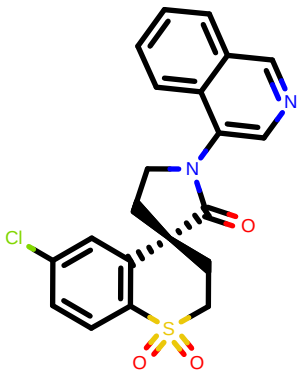
CID:	MAT-POS-50a80394-6_1
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN220
DDG (kcal/mol):	4.04
dDDG (kcal/mol):	0.29

MIK-ENA-5d9157e9-1_1



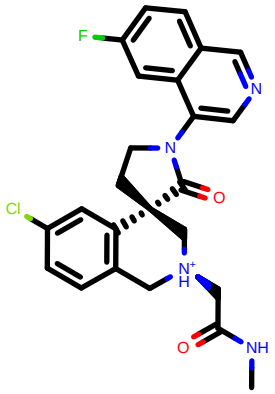
CID:	MIK-ENA-5d9157e9-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN262
DDG (kcal/mol):	4.07
dDDG (kcal/mol):	0.46

EDJ-MED-94fddcec-4_1



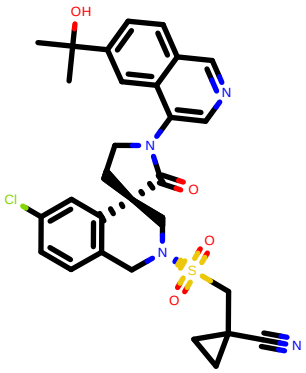
CID:	EDJ-MED-94fddcec-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN41
DDG (kcal/mol):	4.13
dDDG (kcal/mol):	0.16

LUO-POS-b4dec3be-1_2



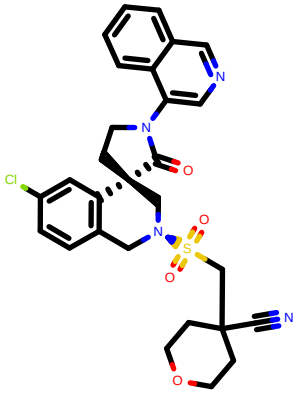
CID:	LUO-POS-b4dec3be-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN129
DDG (kcal/mol):	4.15
dDDG (kcal/mol):	0.19

MAT-POS-853c0ffa-11_2



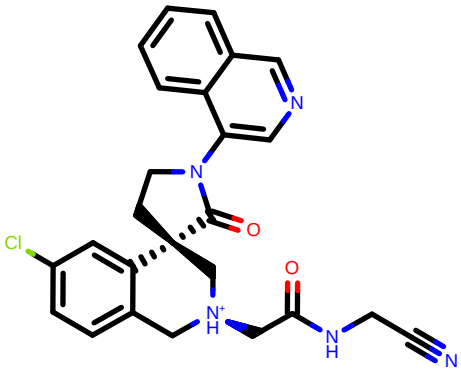
CID:	MAT-POS-853c0ffa-11_2
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN413
DDG (kcal/mol):	4.16
dDDG (kcal/mol):	0.45

ALP-POS-ecbed2ba-11_1



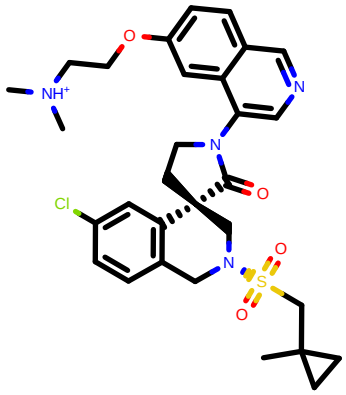
CID:	ALP-POS-ecbed2ba-11_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCOCC6)C#N
RUN:	RUN381
DDG (kcal/mol):	4.16
dDDG (kcal/mol):	0.67

ALP-POS-ecbed2ba-14_2



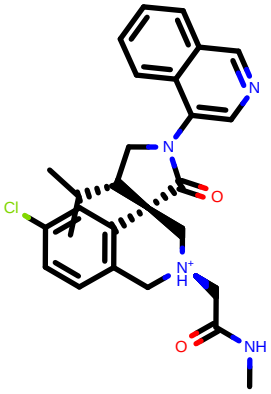
CID:	ALP-POS-ecbed2ba-14_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC#N
RUN:	RUN141
DDG (kcal/mol):	4.20
dDDG (kcal/mol):	0.26

MAT-POS-853c0ffa-19_2



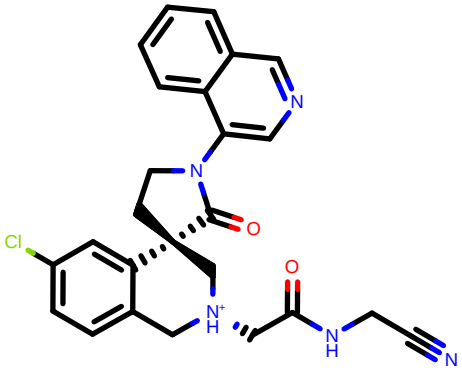
CID:	MAT-POS-853c0ffa-19_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)OCC[NH+](C)C)Cl
RUN:	RUN426
DDG (kcal/mol):	4.23
dDDG (kcal/mol):	0.56

MAT-POS-50a80394-6_3



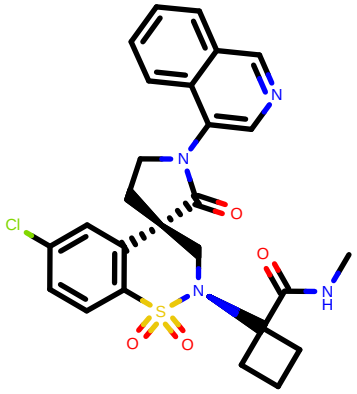
CID:	MAT-POS-50a80394-6_3
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN223
DDG (kcal/mol):	4.23
dDDG (kcal/mol):	0.41

ALP-POS-ecbed2ba-14_1



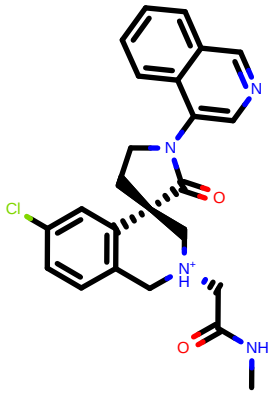
CID:	ALP-POS-ecbed2ba-14_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC#N
RUN:	RUN153
DDG (kcal/mol):	4.27
dDDG (kcal/mol):	0.28

EDJ-MED-98c0a822-1_2



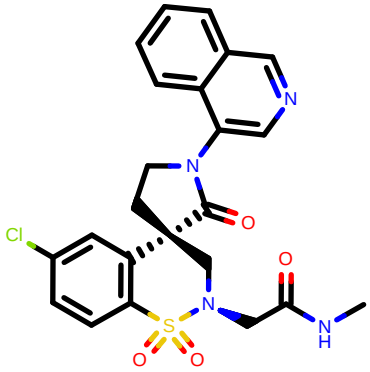
CID:	EDJ-MED-98c0a822-1_2
SMILES:	CNC(=O)C1(CCC1)[N@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN330
DDG (kcal/mol):	4.27
dDDG (kcal/mol):	0.39

LUO-POS-868e8996-12_1



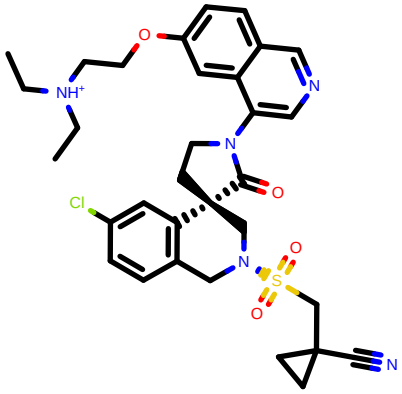
CID:	LUO-POS-868e8996-12_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN79
DDG (kcal/mol):	4.27
dDDG (kcal/mol):	0.26

ALP-POS-4483ae88-2_1



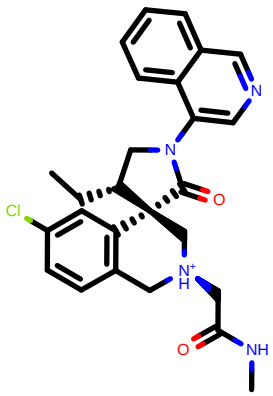
CID:	ALP-POS-4483ae88-2_1
SMILES:	CNC(=O)C[N@@]1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)Cl
RUN:	RUN138
DDG (kcal/mol):	4.28
dDDG (kcal/mol):	0.22

MAT-POS-40ad851a-3_2



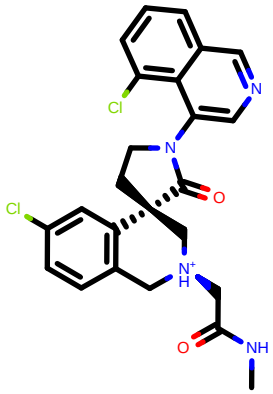
CID:	MAT-POS-40ad851a-3_2
SMILES:	CC[NH+](CC)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN466
DDG (kcal/mol):	4.29
dDDG (kcal/mol):	0.64

MAT-POS-50a80394-5_3



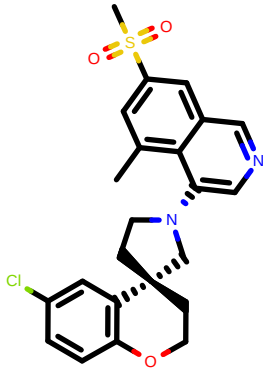
CID:	MAT-POS-50a80394-5_3
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN173
DDG (kcal/mol):	4.29
dDDG (kcal/mol):	0.22

MAT-POS-b4d6b7fc-6_2



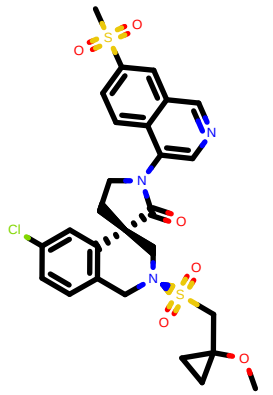
CID:	MAT-POS-b4d6b7fc-6_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN104
DDG (kcal/mol):	4.29
dDDG (kcal/mol):	0.22

EDJ-MED-d7486dd1-1_2



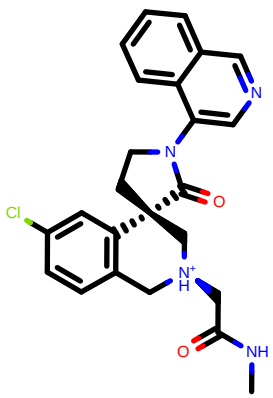
CID:	EDJ-MED-d7486dd1-1_2
SMILES:	Cc1cc(cc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN56
DDG (kcal/mol):	4.30
dDDG (kcal/mol):	0.12

MAT-POS-853c0ffa-16_1



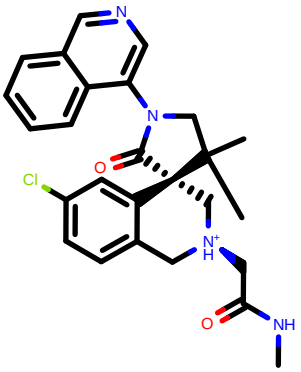
CID:	MAT-POS-853c0ffa-16_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN400
DDG (kcal/mol):	4.30
dDDG (kcal/mol):	0.38

LUO-POS-868e8996-11_2



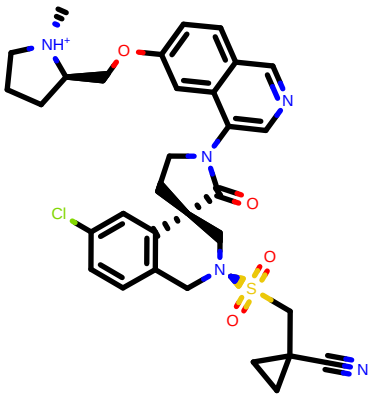
CID:	LUO-POS-868e8996-11_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN84
DDG (kcal/mol):	4.32
dDDG (kcal/mol):	0.26

MAT-POS-50a80394-7_2



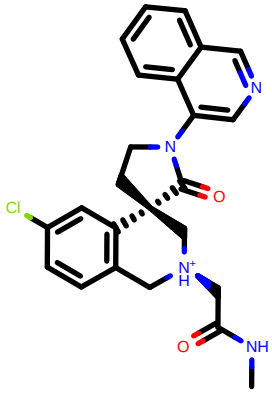
CID:	MAT-POS-50a80394-7_2
SMILES:	CC1(CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5)C
RUN:	RUN179
DDG (kcal/mol):	4.34
dDDG (kcal/mol):	0.24

MAT-POS-40ad851a-1_2



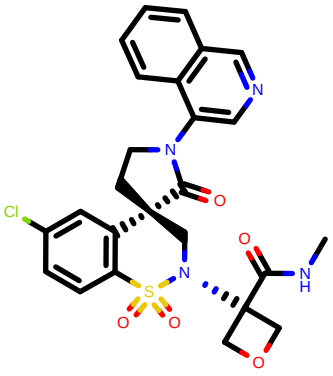
CID:	MAT-POS-40ad851a-1_2
SMILES:	C[N@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN480
DDG (kcal/mol):	4.35
dDDG (kcal/mol):	0.76

MAT-POS-c7726e07-5_2



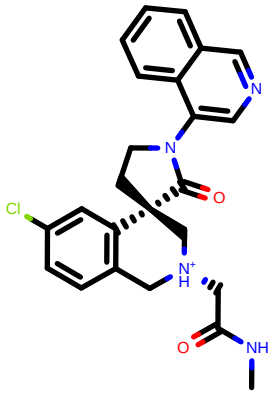
CID:	MAT-POS-c7726e07-5_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN74
DDG (kcal/mol):	4.36
dDDG (kcal/mol):	0.20

EDJ-MED-98c0a822-2_2



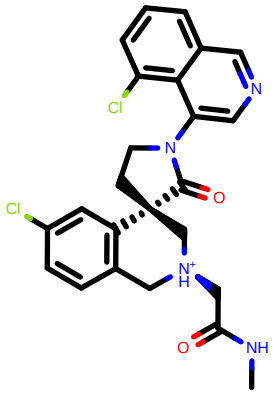
CID:	EDJ-MED-98c0a822-2_2
SMILES:	CNC(=O)C1(COC1)[N@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN334
DDG (kcal/mol):	4.36
dDDG (kcal/mol):	0.27

MAT-POS-c7726e07-6_1



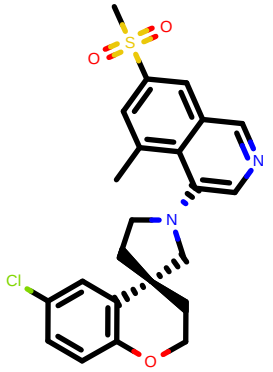
CID:	MAT-POS-c7726e07-6_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN78
DDG (kcal/mol):	4.38
dDDG (kcal/mol):	0.24

MAT-POS-1d5ab790-2_2



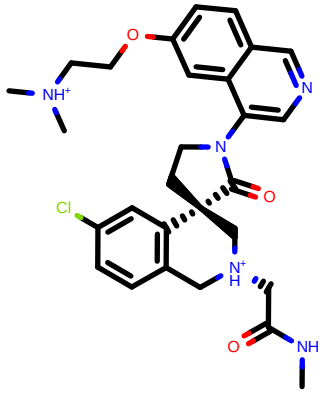
CID:	MAT-POS-1d5ab790-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN112
DDG (kcal/mol):	4.42
dDDG (kcal/mol):	0.23

EDJ-MED-d7486dd1-1_1



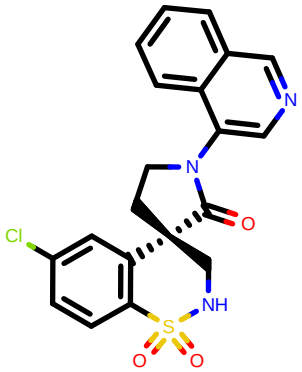
CID:	EDJ-MED-d7486dd1-1_1
SMILES:	Cc1cc(cc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN53
DDG (kcal/mol):	4.48
dDDG (kcal/mol):	0.11

EDJ-MED-b6c6ee2b-1_1



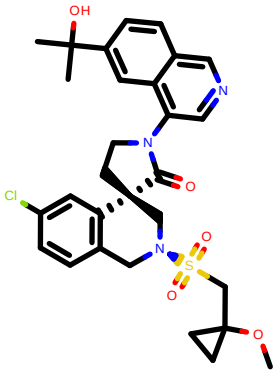
CID:	EDJ-MED-b6c6ee2b-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN383
DDG (kcal/mol):	4.48
dDDG (kcal/mol):	0.38

EDJ-MED-f9b78f78-4_1



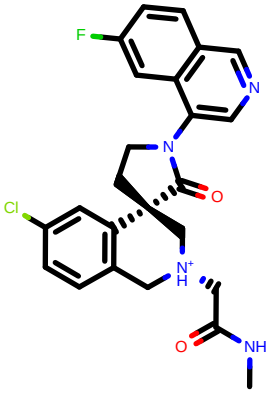
CID:	EDJ-MED-f9b78f78-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN52
DDG (kcal/mol):	4.49
dDDG (kcal/mol):	0.16

MAT-POS-853c0ffa-12_2



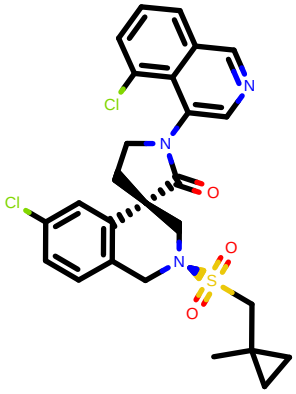
CID:	MAT-POS-853c0ffa-12_2
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC)O
RUN:	RUN404
DDG (kcal/mol):	4.49
dDDG (kcal/mol):	0.50

LUO-POS-b4dec3be-2_1



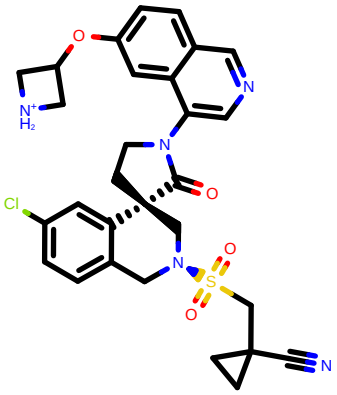
CID:	LUO-POS-b4dec3be-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN130
DDG (kcal/mol):	4.50
dDDG (kcal/mol):	0.28

MAT-POS-853c0ffa-17_1



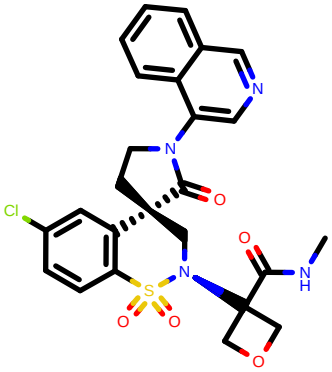
CID:	MAT-POS-853c0ffa-17_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN232
DDG (kcal/mol):	4.51
dDDG (kcal/mol):	0.33

EDJ-MED-ee81482e-1_2



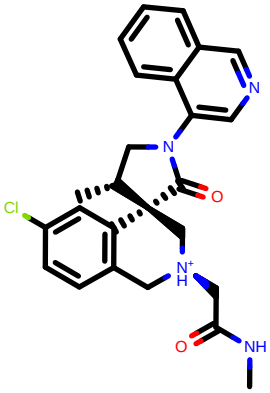
CID:	EDJ-MED-ee81482e-1_2
SMILES:	c1cc2cncc(c2cc1OC3C[NH2+]C3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN430
DDG (kcal/mol):	4.53
dDDG (kcal/mol):	0.49

EDJ-MED-98c0a822-2_1



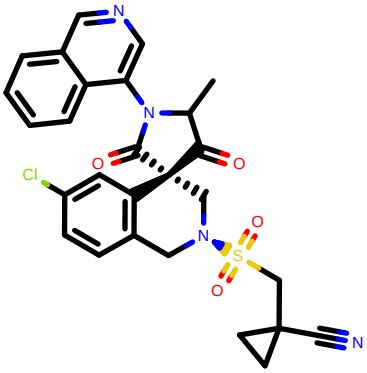
CID:	EDJ-MED-98c0a822-2_1
SMILES:	CNC(=O)C1(COC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN333
DDG (kcal/mol):	4.54
dDDG (kcal/mol):	0.25

MAT-POS-50a80394-4_3



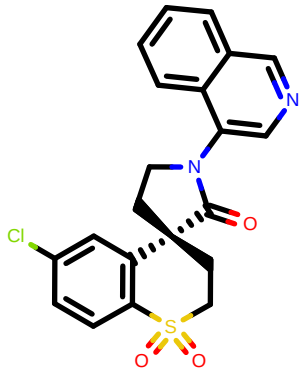
CID:	MAT-POS-50a80394-4_3
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN119
DDG (kcal/mol):	4.62
dDDG (kcal/mol):	0.23

PET-UNK-94036022-6_1



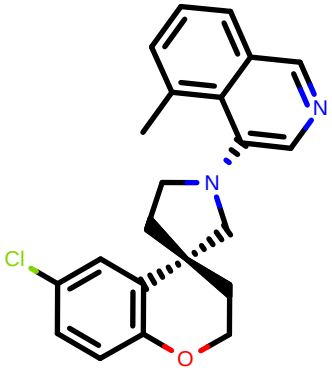
CID:	PET-UNK-94036022-6_1
SMILES:	C=C1C(=O)[C@]2(C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN380
DDG (kcal/mol):	4.64
dDDG (kcal/mol):	0.33

ALP-POS-41e2080f-1_1



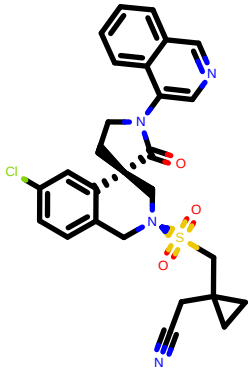
CID:	ALP-POS-41e2080f-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN46
DDG (kcal/mol):	4.66
dDDG (kcal/mol):	0.17

EDJ-MED-a6bab6fb-1_1



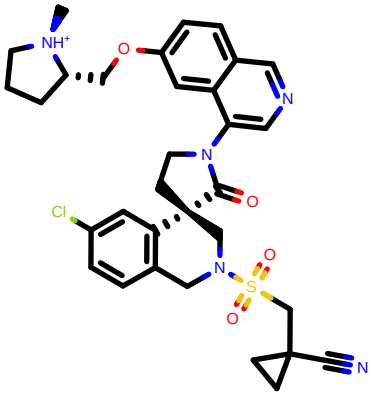
CID:	EDJ-MED-a6bab6fb-1_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN16
DDG (kcal/mol):	4.67
dDDG (kcal/mol):	0.08

ALP-POS-ecbed2ba-22_2



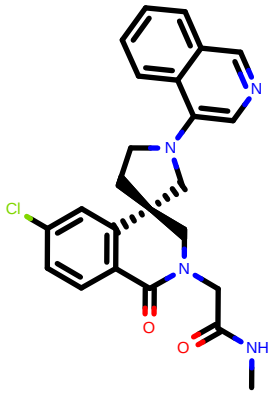
CID:	ALP-POS-ecbed2ba-22_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN311
DDG (kcal/mol):	4.70
dDDG (kcal/mol):	0.41

MAT-POS-40ad851a-1_7



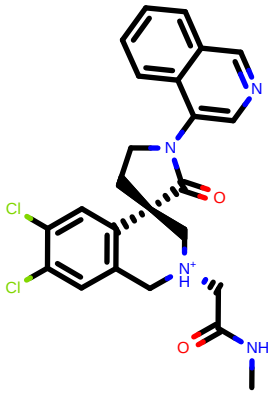
CID:	MAT-POS-40ad851a-1_7
SMILES:	C[N@@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN477
DDG (kcal/mol):	4.73
dDDG (kcal/mol):	0.66

EDJ-MED-8bb691af-7_2



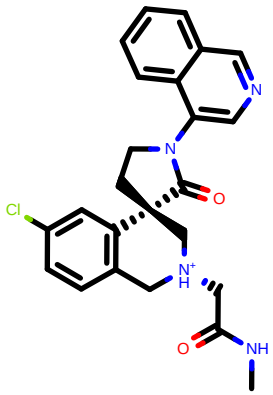
CID:	EDJ-MED-8bb691af-7_2
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN70
DDG (kcal/mol):	4.77
dDDG (kcal/mol):	0.12

ALP-POS-afe0272e-1_1



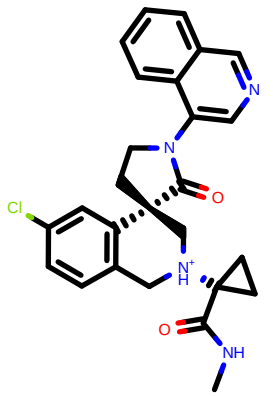
CID:	ALP-POS-afe0272e-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2cc(c(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)Cl
RUN:	RUN107
DDG (kcal/mol):	4.81
dDDG (kcal/mol):	0.28

MAT-POS-c7726e07-5_1



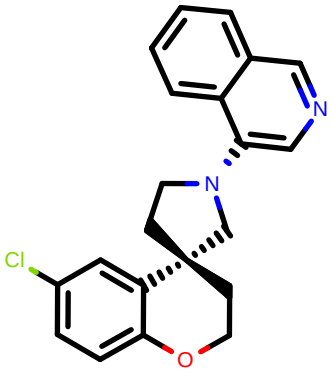
CID:	MAT-POS-c7726e07-5_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN77
DDG (kcal/mol):	4.84
dDDG (kcal/mol):	0.27

ALP-POS-ecbed2ba-7_1



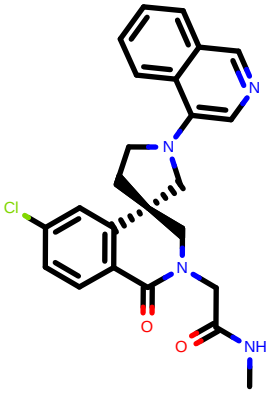
CID:	ALP-POS-ecbed2ba-7_1
SMILES:	CNC(=O)C1(CC1)[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN148
DDG (kcal/mol):	4.84
dDDG (kcal/mol):	0.16

MAT-POS-983b399a-2_1



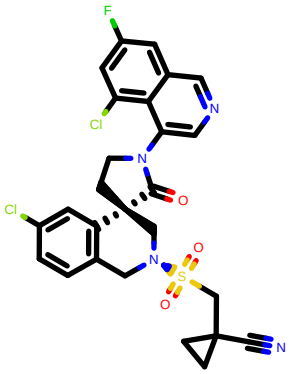
CID:	MAT-POS-983b399a-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN1
DDG (kcal/mol):	4.87
dDDG (kcal/mol):	0.08

EDJ-MED-8bb691af-7_1



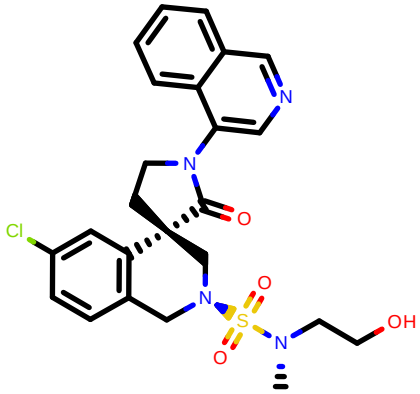
CID:	EDJ-MED-8bb691af-7_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN73
DDG (kcal/mol):	4.87
dDDG (kcal/mol):	0.11

MAT-POS-853c0ffa-6_2



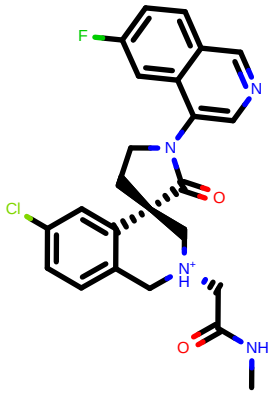
CID:	MAT-POS-853c0ffa-6_2
SMILES:	c1cc2c(cc1Cl)[C@@]3(CCN(C3=O)c4cncc5c4c(cc(c5)F)Cl)C[N@](C2)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN354
DDG (kcal/mol):	4.88
dDDG (kcal/mol):	0.55

ALP-POS-ecbed2ba-19_3



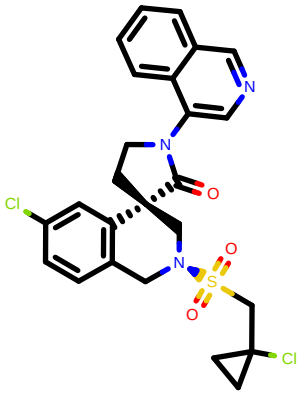
CID:	ALP-POS-ecbed2ba-19_3
SMILES:	C[N@@](CCO)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN221
DDG (kcal/mol):	4.89
dDDG (kcal/mol):	0.73

MAT-POS-b4d6b7fc-5_1



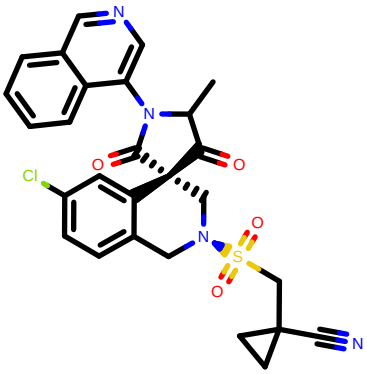
CID:	MAT-POS-b4d6b7fc-5_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN99
DDG (kcal/mol):	4.92
dDDG (kcal/mol):	0.26

PET-UNK-94036022-10_2



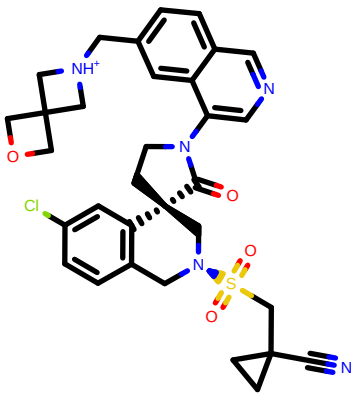
CID:	PET-UNK-94036022-10_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN216
DDG (kcal/mol):	4.93
dDDG (kcal/mol):	0.49

PET-UNK-94036022-6_2



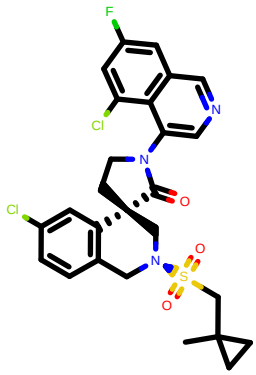
CID:	PET-UNK-94036022-6_2
SMILES:	C=C1C(=O)[C@]2(C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN382
DDG (kcal/mol):	4.94
dDDG (kcal/mol):	0.49

EDJ-MED-ee81482e-5_1



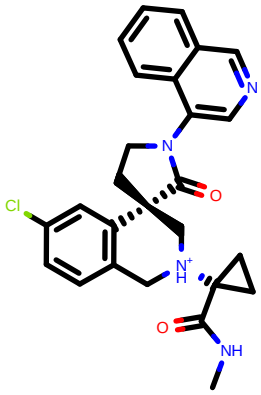
CID:	EDJ-MED-ee81482e-5_1
SMILES:	c1cc2cncc(c2cc1C[NH+]3CC4(C3)COC4)N5CC[C@@]6(C5=O)C[N@@](Cc7c6cc(cc7Cl)S(=O)(=O)CC8(CC8)C#N
RUN:	RUN458
DDG (kcal/mol):	4.96
dDDG (kcal/mol):	0.42

MAT-POS-853c0ffa-18_1



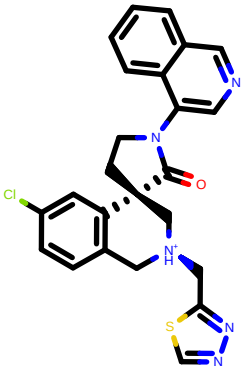
CID:	MAT-POS-853c0ffa-18_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN313
DDG (kcal/mol):	4.97
dDDG (kcal/mol):	0.41

MAT-POS-69786b79-1_1



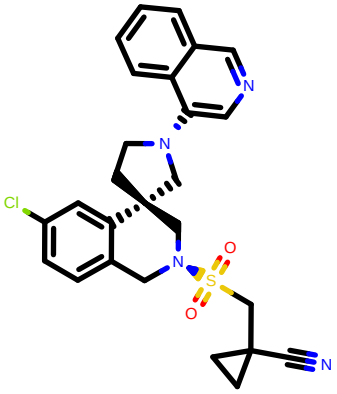
CID:	MAT-POS-69786b79-1_1
SMILES:	CNC(=O)C1(CC1)[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN157
DDG (kcal/mol):	4.97
dDDG (kcal/mol):	0.18

PET-UNK-7e9559de-1_2



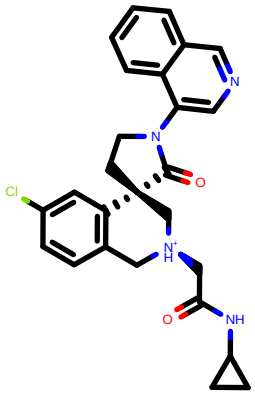
CID:	PET-UNK-7e9559de-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN117
DDG (kcal/mol):	4.99
dDDG (kcal/mol):	0.17

EDJ-MED-8bb691af-2_3



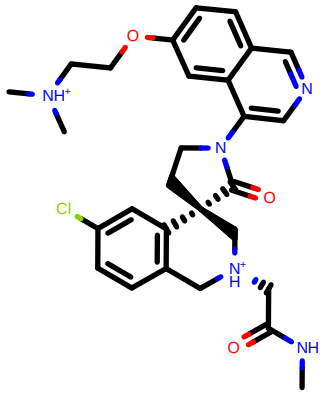
CID:	EDJ-MED-8bb691af-2_3
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN193
DDG (kcal/mol):	4.99
dDDG (kcal/mol):	0.33

MAT-POS-69786b79-2_2



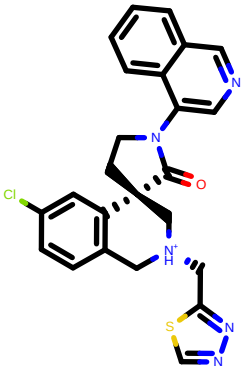
CID:	MAT-POS-69786b79-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6CC6
RUN:	RUN162
DDG (kcal/mol):	5.01
dDDG (kcal/mol):	0.23

MAT-POS-38eb6498-3_1



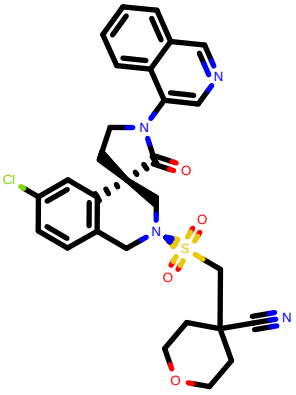
CID:	MAT-POS-38eb6498-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN379
DDG (kcal/mol):	5.01
dDDG (kcal/mol):	0.32

MAT-POS-96396902-1_1



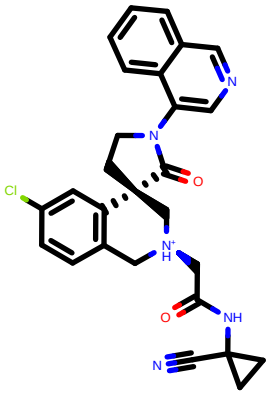
CID:	MAT-POS-96396902-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN126
DDG (kcal/mol):	5.03
dDDG (kcal/mol):	0.18

ALP-POS-ecbed2ba-11_2



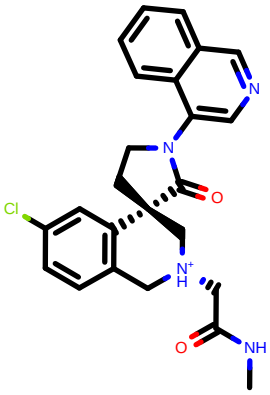
CID:	ALP-POS-ecbed2ba-11_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCOCC6)C#N
RUN:	RUN388
DDG (kcal/mol):	5.07
dDDG (kcal/mol):	0.57

MAT-POS-69786b79-4_2



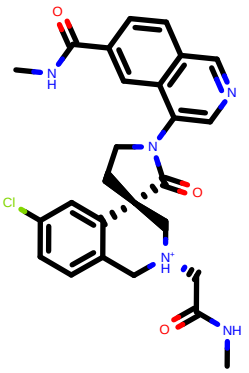
CID:	MAT-POS-69786b79-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6(CC6)C#N
RUN:	RUN275
DDG (kcal/mol):	5.07
dDDG (kcal/mol):	0.27

LUO-POS-868e8996-11_1



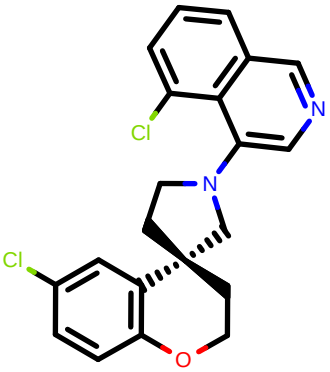
CID:	LUO-POS-868e8996-11_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN81
DDG (kcal/mol):	5.10
dDDG (kcal/mol):	0.26

MAT-POS-38eb6498-5_1



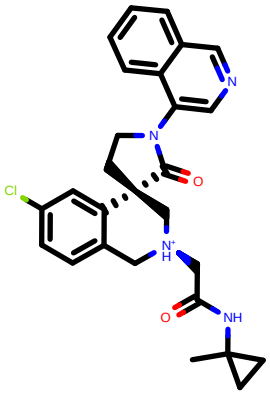
CID:	MAT-POS-38eb6498-5_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)C(=O)NC)Cl
RUN:	RUN265
DDG (kcal/mol):	5.13
dDDG (kcal/mol):	0.22

EDJ-MED-e78d5f1a-1_2



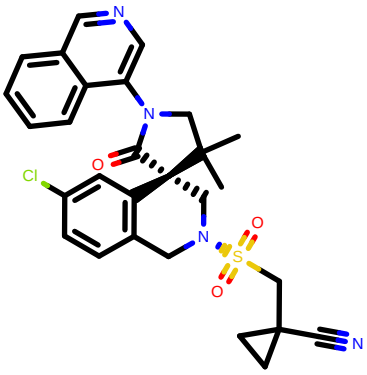
CID:	EDJ-MED-e78d5f1a-1_2
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN14
DDG (kcal/mol):	5.15
dDDG (kcal/mol):	0.08

MAT-POS-69786b79-3_2



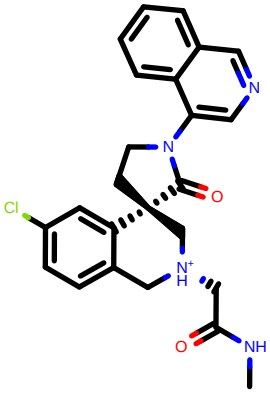
CID:	MAT-POS-69786b79-3_2
SMILES:	CC1(CC1)NC(=O)C[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN217
DDG (kcal/mol):	5.16
dDDG (kcal/mol):	0.26

MAT-POS-50a80394-8_1



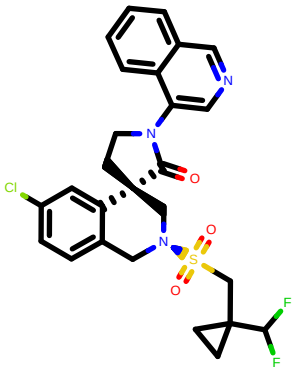
CID:	MAT-POS-50a80394-8_1
SMILES:	CC1(CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6)C
RUN:	RUN371
DDG (kcal/mol):	5.17
dDDG (kcal/mol):	0.54

EDJ-MED-8bb691af-4_1



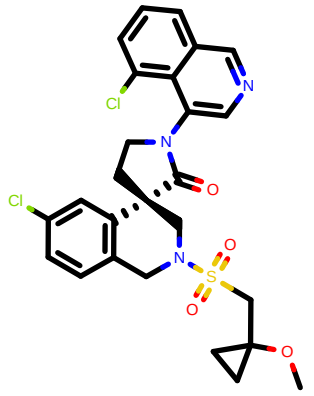
CID:	EDJ-MED-8bb691af-4_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN71
DDG (kcal/mol):	5.20
dDDG (kcal/mol):	0.27

EDJ-MED-5cd3920d-5_2



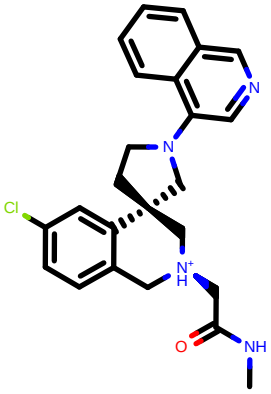
CID:	EDJ-MED-5cd3920d-5_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)F
RUN:	RUN346
DDG (kcal/mol):	5.20
dDDG (kcal/mol):	0.41

MAT-POS-853c0ffa-7_2



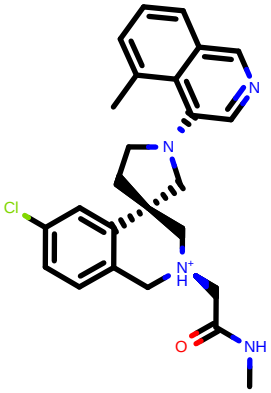
CID:	MAT-POS-853c0ffa-7_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN302
DDG (kcal/mol):	5.23
dDDG (kcal/mol):	0.40

EDJ-MED-8bb691af-1_4



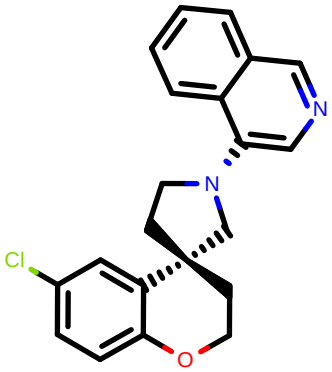
CID:	EDJ-MED-8bb691af-1_4
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3)c4cncc5c4cccc5)Cl
RUN:	RUN61
DDG (kcal/mol):	5.25
dDDG (kcal/mol):	0.15

EDJ-MED-3656d29d-1_4



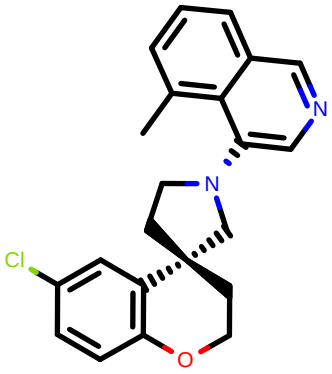
CID:	EDJ-MED-3656d29d-1_4
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC
RUN:	RUN76
DDG (kcal/mol):	5.26
dDDG (kcal/mol):	0.16

EDJ-MED-159244ea-2_2



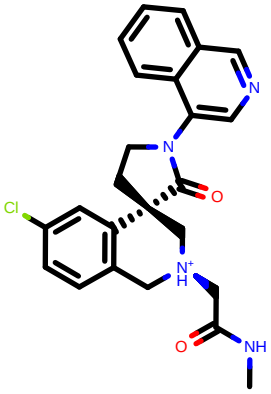
CID:	EDJ-MED-159244ea-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN2
DDG (kcal/mol):	5.27
dDDG (kcal/mol):	0.08

EDJ-MED-a6bab6fb-1_2



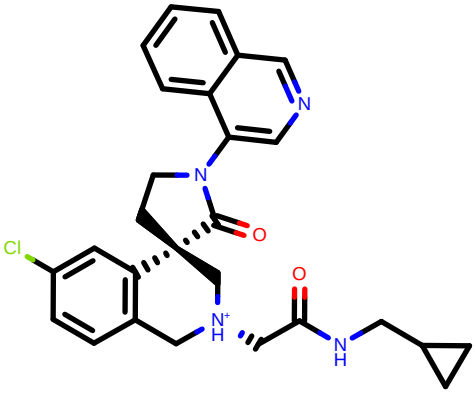
CID:	EDJ-MED-a6bab6fb-1_2
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN5
DDG (kcal/mol):	5.29
dDDG (kcal/mol):	0.08

MAT-POS-c7726e07-6_2



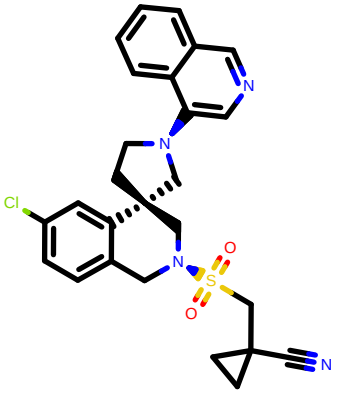
CID:	MAT-POS-c7726e07-6_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN82
DDG (kcal/mol):	5.29
dDDG (kcal/mol):	0.25

ALP-POS-ecbed2ba-12_1



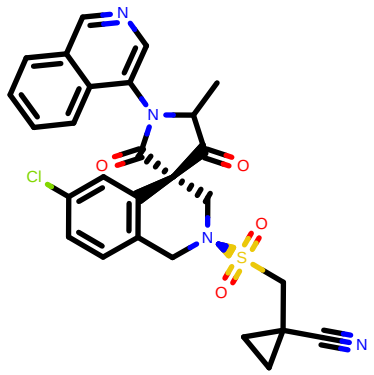
CID:	ALP-POS-ecbed2ba-12_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC6CC6
RUN:	RUN204
DDG (kcal/mol):	5.29
dDDG (kcal/mol):	0.29

EDJ-MED-8bb691af-2_1



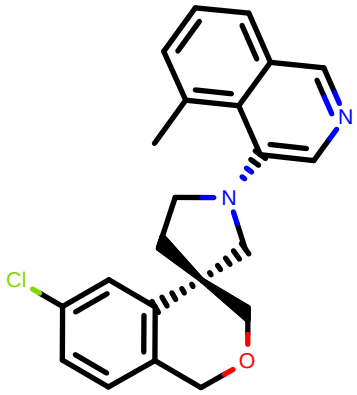
CID:	EDJ-MED-8bb691af-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN191
DDG (kcal/mol):	5.29
dDDG (kcal/mol):	0.31

PET-UNK-94036022-13_2



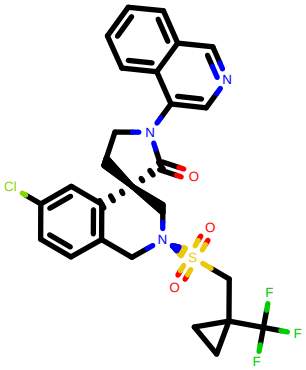
CID:	PET-UNK-94036022-13_2
SMILES:	C=C1C(=O)[C@]2(C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN386
DDG (kcal/mol):	5.30
dDDG (kcal/mol):	0.44

EDJ-MED-f3cfbbb5-1_2



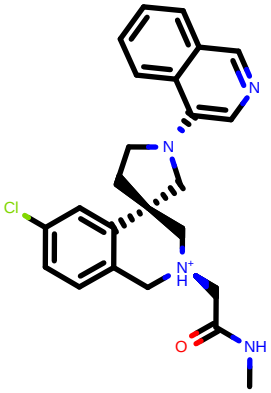
CID:	EDJ-MED-f3cfbbb5-1_2
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl
RUN:	RUN12
DDG (kcal/mol):	5.33
dDDG (kcal/mol):	0.07

EDJ-MED-5cd3920d-6_2



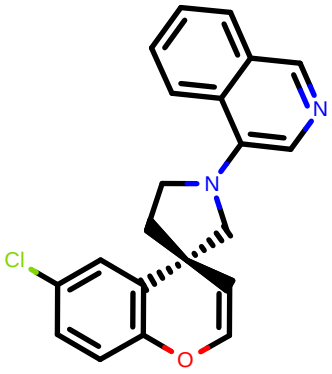
CID:	EDJ-MED-5cd3920d-6_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)(F)F
RUN:	RUN370
DDG (kcal/mol):	5.35
dDDG (kcal/mol):	0.36

EDJ-MED-8bb691af-1_2



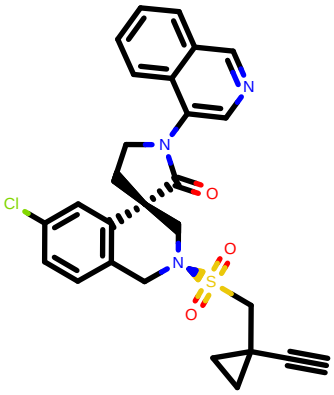
CID:	EDJ-MED-8bb691af-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3)c4cncc5c4cccc5)Cl
RUN:	RUN57
DDG (kcal/mol):	5.39
dDDG (kcal/mol):	0.16

EDJ-MED-159244ea-2_1



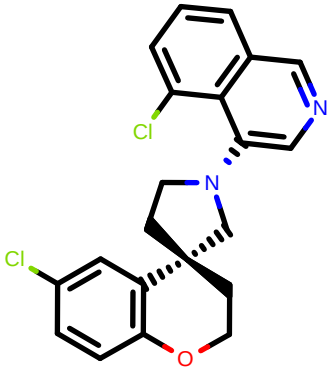
CID:	EDJ-MED-159244ea-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN3
DDG (kcal/mol):	5.41
dDDG (kcal/mol):	0.08

PET-UNK-94036022-9_2



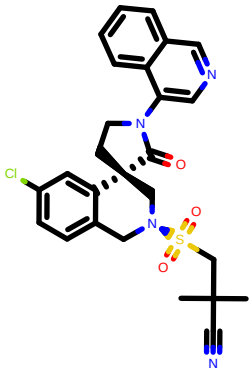
CID:	PET-UNK-94036022-9_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN285
DDG (kcal/mol):	5.41
dDDG (kcal/mol):	0.50

EDJ-MED-e78d5f1a-1_1



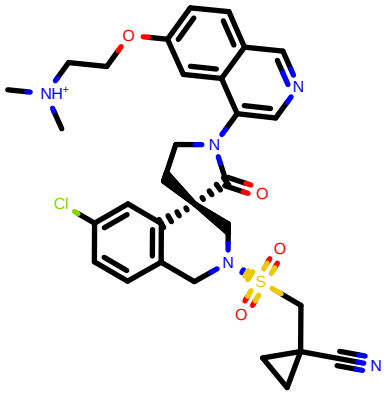
CID:	EDJ-MED-e78d5f1a-1_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN15
DDG (kcal/mol):	5.43
dDDG (kcal/mol):	0.07

ALP-POS-ecbed2ba-13_2



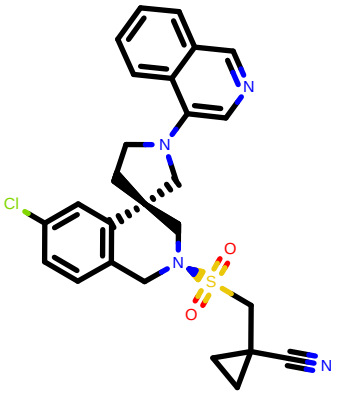
CID:	ALP-POS-ecbed2ba-13_2
SMILES:	CC(C)(CS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)C#N
RUN:	RUN246
DDG (kcal/mol):	5.46
dDDG (kcal/mol):	0.42

MAT-POS-38eb6498-1_2



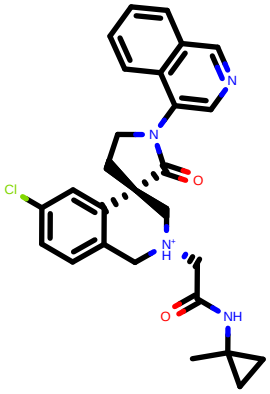
CID:	MAT-POS-38eb6498-1_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN444
DDG (kcal/mol):	5.52
dDDG (kcal/mol):	0.61

EDJ-MED-8bb691af-2_4



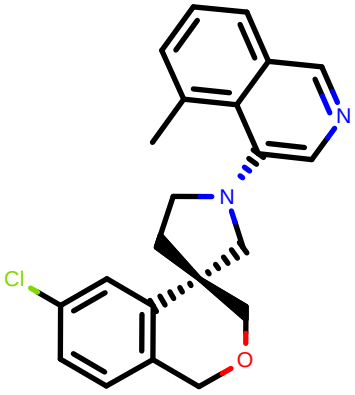
CID:	EDJ-MED-8bb691af-2_4
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN196
DDG (kcal/mol):	5.52
dDDG (kcal/mol):	0.41

MAT-POS-69786b79-3_1



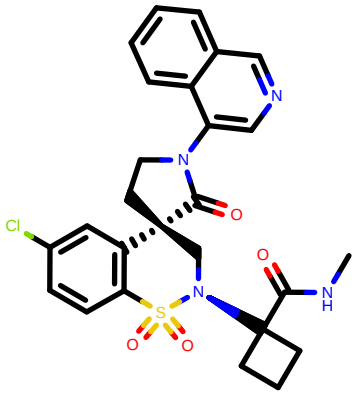
CID:	MAT-POS-69786b79-3_1
SMILES:	CC1(CC1)NC(=O)C[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN206
DDG (kcal/mol):	5.52
dDDG (kcal/mol):	0.30

EDJ-MED-f3cfbbb5-1_1



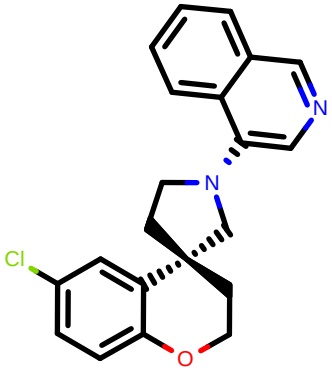
CID:	EDJ-MED-f3cfbbb5-1_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl
RUN:	RUN11
DDG (kcal/mol):	5.53
dDDG (kcal/mol):	0.07

EDJ-MED-98c0a822-1_1



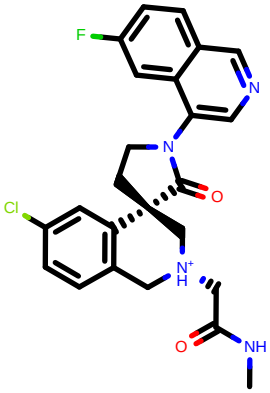
CID:	EDJ-MED-98c0a822-1_1
SMILES:	CNC(=O)C1(CCC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN328
DDG (kcal/mol):	5.53
dDDG (kcal/mol):	0.39

MAT-POS-983b399a-2_2



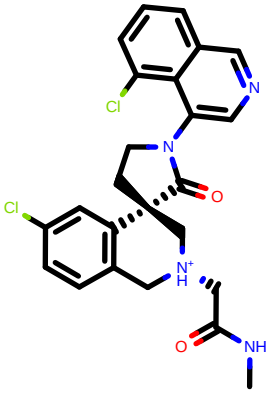
CID:	MAT-POS-983b399a-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN0
DDG (kcal/mol):	5.60
dDDG (kcal/mol):	0.07

LUO-POS-b4dec3be-1_1



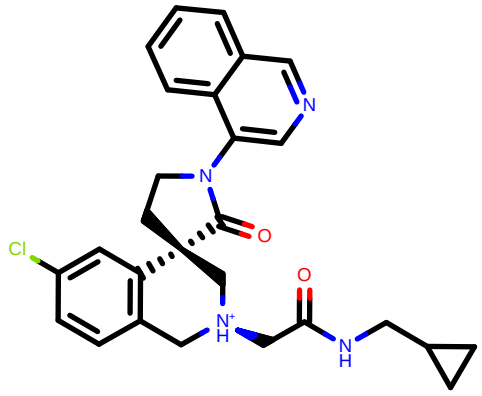
CID:	LUO-POS-b4dec3be-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN123
DDG (kcal/mol):	5.61
dDDG (kcal/mol):	0.19

MAT-POS-b4d6b7fc-6_1



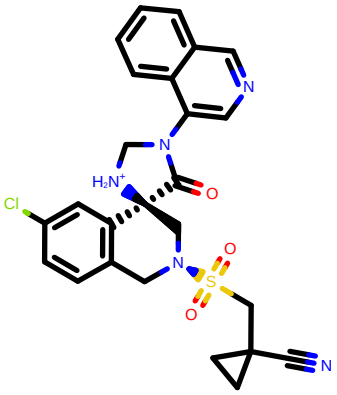
CID:	MAT-POS-b4d6b7fc-6_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN100
DDG (kcal/mol):	5.64
dDDG (kcal/mol):	0.24

ALP-POS-ecbed2ba-12_2



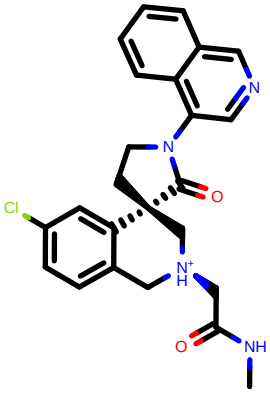
CID:	ALP-POS-ecbed2ba-12_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC6CC6
RUN:	RUN203
DDG (kcal/mol):	5.68
dDDG (kcal/mol):	0.21

EDG-MED-b6bce001-1_2



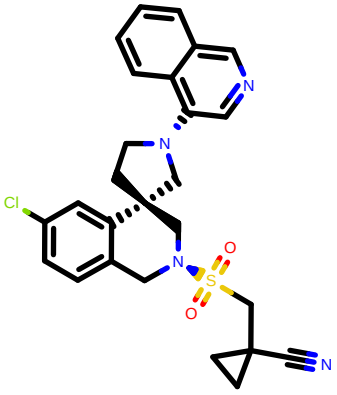
CID:	EDG-MED-b6bce001-1_2
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@]([Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN252
DDG (kcal/mol):	5.72
dDDG (kcal/mol):	0.44

LUO-POS-868e8996-12_2



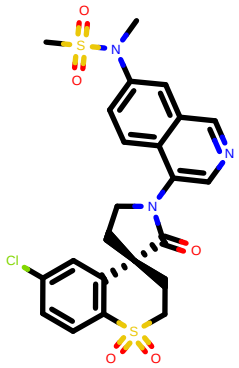
CID:	LUO-POS-868e8996-12_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN83
DDG (kcal/mol):	5.73
dDDG (kcal/mol):	0.22

EDJ-MED-8bb691af-2_2



CID:	EDJ-MED-8bb691af-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN194
DDG (kcal/mol):	5.74
dDDG (kcal/mol):	0.33

EDJ-MED-94fddcec-6_2



CID:	EDJ-MED-94fddcec-6_2
SMILES:	C[N@](c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN195
DDG (kcal/mol):	5.88
dDDG (kcal/mol):	0.22