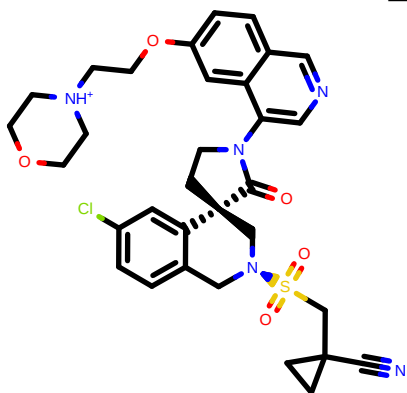
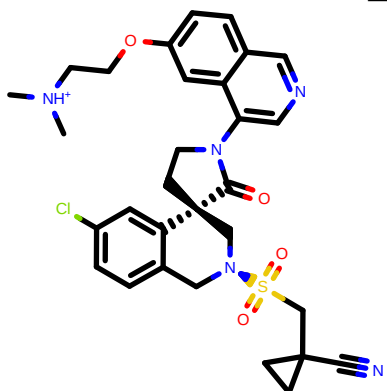


EDJ-MED-468565e0-2_1



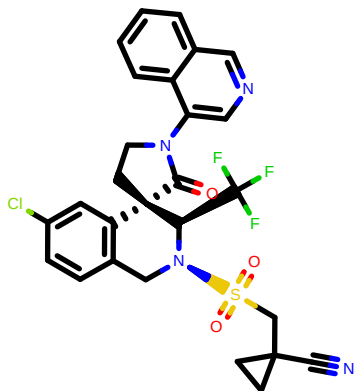
CID:	EDJ-MED-468565e0-2_1
SMILES:	<chem>c1cc2nccc(c2cc1OCC[NH+]3CCOCC3)N4C[C@]5(C4=O)C[N@]6Cc6c6cc(c65)C5(S(=O)(=O)CC7(C)C7)C#N</chem>
RUN:	RUN999
DDG (kcal/mol):	-4.78
dDDG (kcal/mol):	0.66

LUO-POS-8484f2d3-1_1



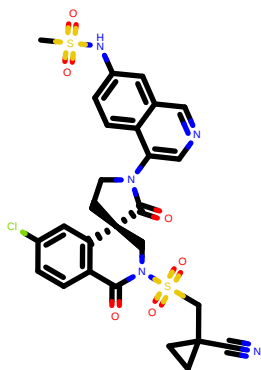
CID:	LUO-POS-8484f2d3-1_1
SMILES:	<chem>C[NH+]1CjCCOc1ccc2nccc(c2c1)N3CC[C@]4(C3=O)C[N@]5Cc5c4cc(c5)C5(S(=O)(=O)CC6(C)C6)C#N</chem>
RUN:	RUN995
DDG (kcal/mol):	-4.23
dDDG (kcal/mol):	0.62

VLA-UNK-61877630-9_1



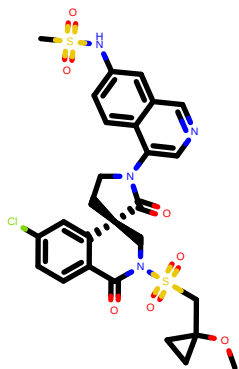
CID:	VLA-UNK-61877630-9_1
SMILES:	<chem>c1ccc2c(c1)nccc2N3CC[C@]4(C3=O)C5cc(c5c5C[N@]6[C@]4C@H4C(F)(F)F)S(=O)(=O)CC6(C)C6)C#N</chem>
RUN:	RUN968
DDG (kcal/mol):	-3.55
dDDG (kcal/mol):	0.35

EDJ-MED-9f4ac58c-3_1



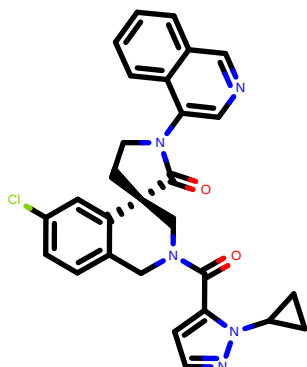
CID:	EDJ-MED-9f4ac58c-3_1
SMILES:	<chem>C5(S(=O)(=O)Nc1ccc2c(c1)nccc2N3CC[C@]4(C3=O)C[N@]5Cc5c4cc(c5)C5(S(=O)(=O)CC6(C)C6)C#N</chem>
RUN:	RUN997
DDG (kcal/mol):	-3.52
dDDG (kcal/mol):	0.48

EDJ-MED-9f4ac58c-7_1



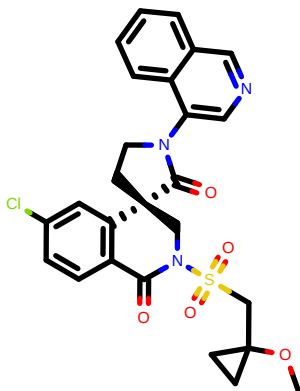
CID:	EDJ-MED-9f4ac58c-7_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4ncc5c4ccc(c5)N[S](=O)(=O)C6CC(=O)C6)Cl</chem>
RUN:	RUN985
DDG (kcal/mol):	-3.50
dDDG (kcal/mol):	0.43

MAT-POS-be048f2c-7_1



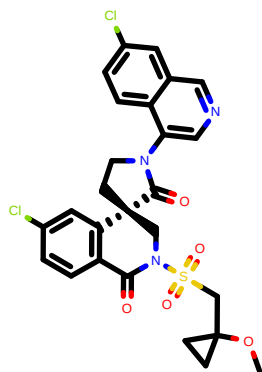
CID:	MAT-POS-be048f2c-7_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@]4(C3=O)CN(Cc5c4cc(cc5)Cl)C(=O)c6ccnn6C7CC7</chem>
RUN:	RUN918
DDG (kcal/mol):	-3.26
dDDG (kcal/mol):	0.14

EDJ-MED-9f4ac58c-6_1



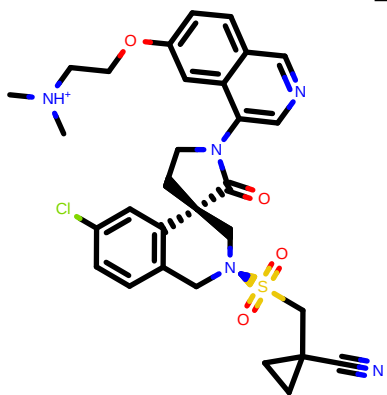
CID:	EDJ-MED-9f4ac58c-6_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cnc5c4ccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN885
DDG (kcal/mol):	-3.20
dDDG (kcal/mol):	0.38

EDJ-MED-9f4ac58c-5_1



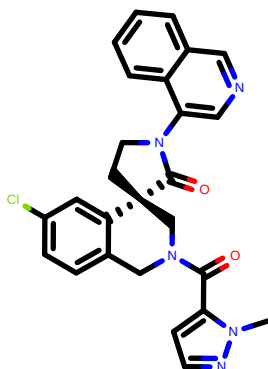
CID:	EDJ-MED-9f4ac58c-5_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cnc5c4ccc(c5)Cl)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN934
DDG (kcal/mol):	-3.12
dDDG (kcal/mol):	0.34

MAT-POS-38eb6498-1_1



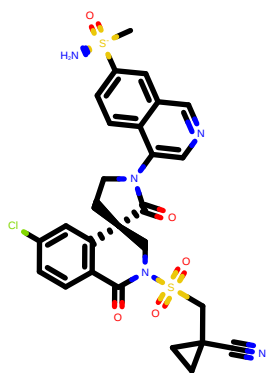
CID:	MAT-POS-38eb6498-1_1
SMILES:	<chem>C[NH+](C)CCOC1ccc2ncnc(c2c1)NCC[C@]4(C3=O)C[N@]5Cc5c4cc(c5)C(S(=O)(=O)CC6CC6)C#N</chem>
RUN:	RUN990
DDG (kcal/mol):	-2.94
dDDG (kcal/mol):	0.63

EDJ-MED-cc48ee33-3_1



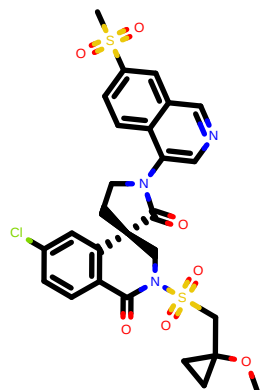
CID:	EDJ-MED-cc48ee33-3_1
SMILES:	<chem>Cn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5cccc6)Cl</chem>
RUN:	RUN836
DDG (kcal/mol):	-2.87
dDDG (kcal/mol):	0.10

EDJ-MED-7d88f880-3_2



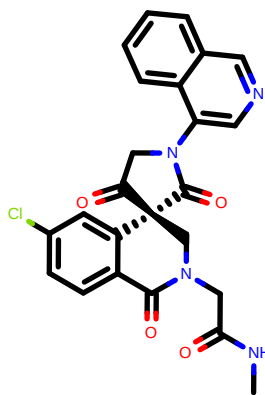
CID:	EDJ-MED-7d88f880-3_2
SMILES:	<chem>C[S@](=N)(=O)c1ccc2c(c1)ncnc2N3CC[C@]4(C3=O)C[N@]5Cc5c4cc(c5)C(S(=O)(=O)CC6CC6)C#N</chem>
RUN:	RUN983
DDG (kcal/mol):	-2.87
dDDG (kcal/mol):	0.59

EDJ-MED-9f4ac58c-8_1



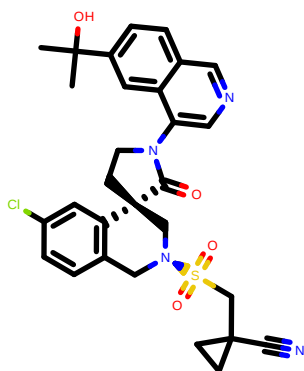
CID:	EDJ-MED-9f4ac58c-8_1
SMILES:	<chem>COC1(CC1)C(S(=O)(=O)N2C[C@]3(CCN(C3=O)c4cnc5c4ccc(c5)S(=O)(=O)C)C6cc(ccc6C2=O)Cl</chem>
RUN:	RUN977
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.46

EDJ-MED-a12e3a20-2_1



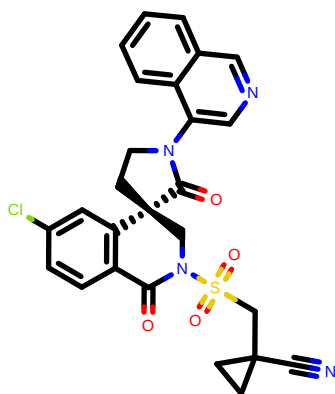
CID:	EDJ-MED-a12e3a20-2_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(c3cc(ccc3C1=O)C)C(=O)CN(C2=O)c4cncc5c4cccc5</chem>
RUN:	RUN802
DDG (kcal/mol):	-2.76
dDDG (kcal/mol):	0.12

MAT-POS-853c0ffa-11_1



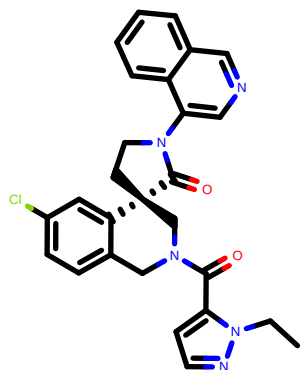
CID:	MAT-POS-853c0ffa-11_1
SMILES:	<chem>CC(C)(c1ccc2nccc(c2c1)N3CC[C@@]4(C3=O)C[N@H](C5c4cc(cc5)C)S(=O)(=O)CC6(C)C6)C#N</chem>
RUN:	RUN973
DDG (kcal/mol):	-2.67
dDDG (kcal/mol):	0.38

EDJ-MED-9f4ac58c-2_1



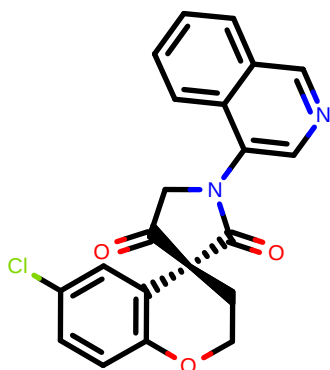
CID:	EDJ-MED-9f4ac58c-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)C)S(=O)(=O)CC6(C)C6)C#N</chem>
RUN:	RUN888
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.44

MAT-POS-be048f2c-5_1



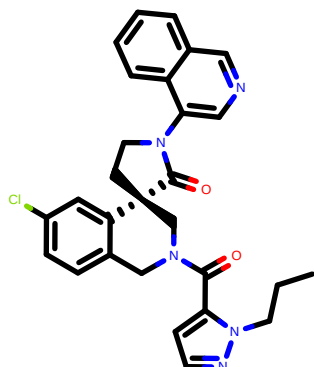
CID:	MAT-POS-be048f2c-5_1
SMILES:	<chem>CCn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl</chem>
RUN:	RUN887
DDG (kcal/mol):	-2.54
dDDG (kcal/mol):	0.17

DAR-DIA-0f7b7cd9-9_1



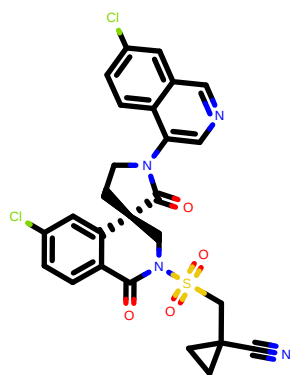
CID:	DAR-DIA-0f7b7cd9-9_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN707
DDG (kcal/mol):	-2.50
dDDG (kcal/mol):	0.07

MAT-POS-be048f2c-8_1



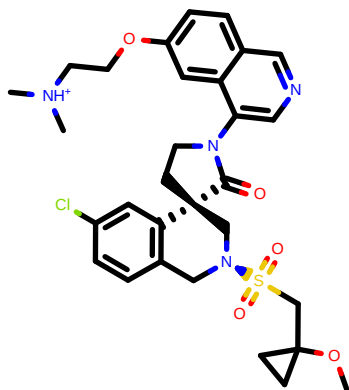
CID:	MAT-POS-be048f2c-8_1
SMILES:	<chem>CCc1c(ccn1)C(=O)N2Cc3ccc(cc3[C@@]4(C2)CCN(C4=O)c5cnccc6c5cccc6)Cl</chem>
RUN:	RUN910
DDG (kcal/mol):	-2.47
dDDG (kcal/mol):	0.17

EDJ-MED-9f4ac58c-1_1



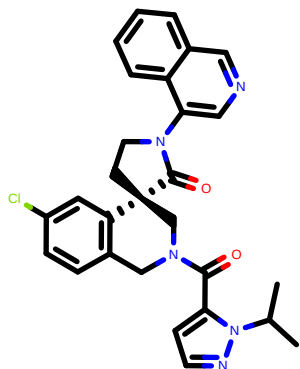
CID:	EDJ-MED-9f4ac58c-1_1
SMILES:	<chem>c1cc2c(cc1Cl)cncc2N3CC[C@]4(C3=O)CN(C(=O)c5c4cc(cc5Cl)S(=O)(=O)CC6(Cc6)C#N</chem>
RUN:	RUN929
DDG (kcal/mol):	-2.44
dDDG (kcal/mol):	0.34

MAT-POS-853c0ffa-10_1



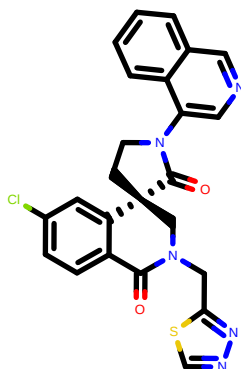
CID:	MAT-POS-853c0ffa-10_1
SMILES:	<chem>C[NH+](C)CCOC1ccc2ccc(cc2c1)N3CC[C@]4(C3=O)C[N+]([C@@]5C4cc(cc5Cl)S(=O)(=O)CC6(Cc6)OC</chem>
RUN:	RUN992
DDG (kcal/mol):	-2.43
dDDG (kcal/mol):	0.46

MAT-POS-be048f2c-6_1



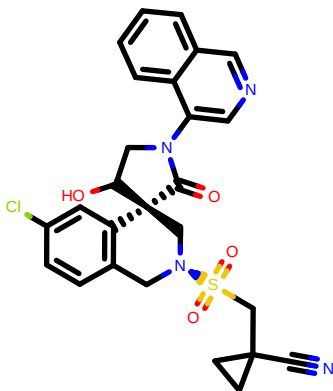
CID:	MAT-POS-be048f2c-6_1
SMILES:	<chem>CC(C)n1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5ccccc6)Cl</chem>
RUN:	RUN935
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.26

PET-UNK-6af7266d-3_1



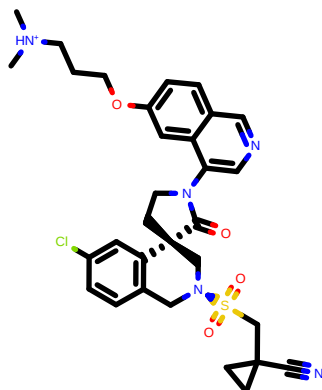
CID:	PET-UNK-6af7266d-3_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nncc6</chem>
RUN:	RUN806
DDG (kcal/mol):	-2.22
dDDG (kcal/mol):	0.11

EDJ-MED-a12e3a20-1_1



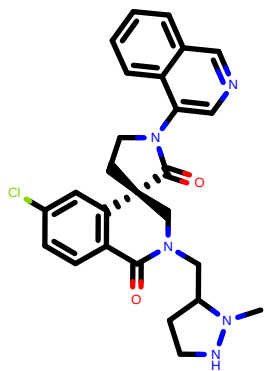
CID:	EDJ-MED-a12e3a20-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC(=O)[C@@]4(C3=O)C[N@](C5c4cc(cc5)Cl)S(=O)(=O)CC6(Cc6)C#N</chem>
RUN:	RUN913
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.39

MAT-POS-40ad851a-4_1



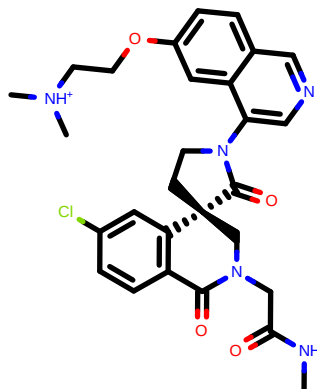
CID:	MAT-POS-40ad851a-4_1
SMILES:	<chem>C[NH+]([C]CCCC1ccc2cnc(c2c1)N3CC[C@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(Cc6)C#N</chem>
RUN:	RUN994
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.69

EDJ-MED-cc48ee33-7_1



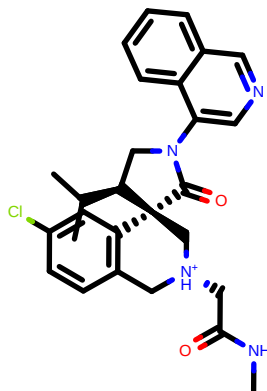
CID:	EDJ-MED-cc48ee33-7_1
SMILES:	<chem>Cn1c(ccn1)CN2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN820
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.19

EDJ-MED-b6c6ee2b-5_1



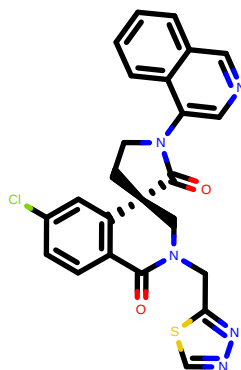
CID:	EDJ-MED-b6c6ee2b-5_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)OCC[NH+](C)C)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN984
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.28

MAT-POS-50a80394-6_2



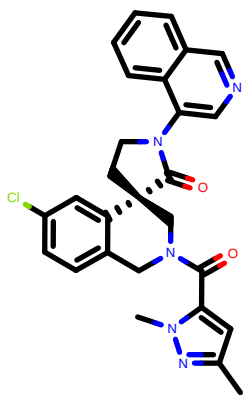
CID:	MAT-POS-50a80394-6_2
SMILES:	<chem>CC(C)[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)C)CC(=O)NC)c4cncc5c4cccc5</chem>
RUN:	RUN853
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.22

PET-UNK-6af7266d-1_1



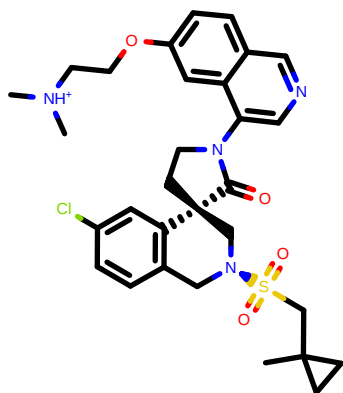
CID:	PET-UNK-6af7266d-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nncc6</chem>
RUN:	RUN805
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.10

EDJ-MED-cc48ee33-5_1



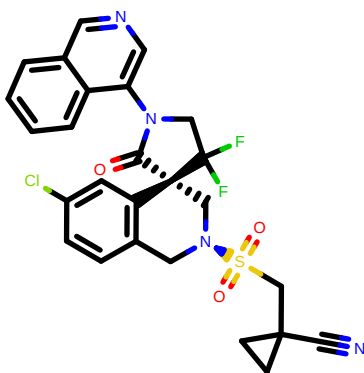
CID:	EDJ-MED-cc48ee33-5_1
SMILES:	<chem>Cc1cc(n(n1)C)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccccc6)Cl</chem>
RUN:	RUN884
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.17

MAT-POS-853c0ffa-19_1



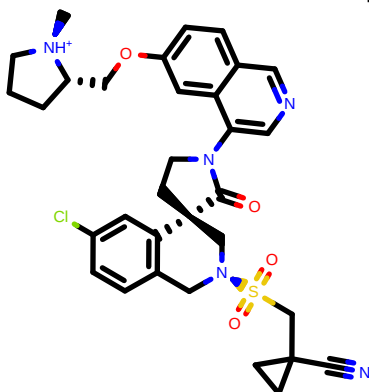
CID:	MAT-POS-853c0ffa-19_1
SMILES:	<chem>CC1(C)CS(=O)(=O)N[C@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccccc6)OCC(NH+)[C@]7(C)C</chem>
RUN:	RUN987
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.44

EDJ-MED-7e491f08-1_1



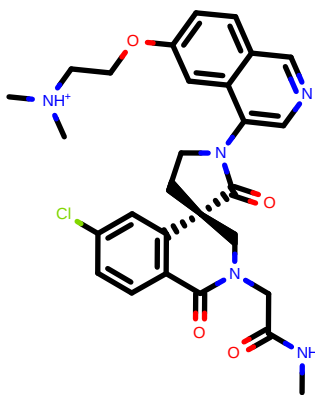
CID:	EDJ-MED-7e491f08-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC([C@]4(C3=O)C[N+]56)C6c5ccc(cc5O)S(=O)(=O)C6(C)N(F)F</chem>
RUN:	RUN947
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.48

MAT-POS-40ad851a-1_2



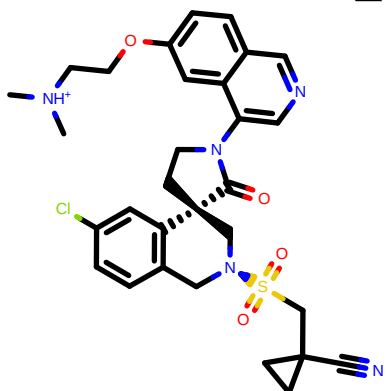
CID:	MAT-POS-40ad851a-1_2
SMILES:	<chem>C[N+]([H])1CCC[C@H]1CCc2ccc3ncc(c3c2)N4CC([C@]5(C4=O)C[N+]6)C6c5ccc(cc5O)S(=O)(=O)C6(C)N(F)F</chem>
RUN:	RUN1000
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.70

MAT-POS-38eb6498-4_1



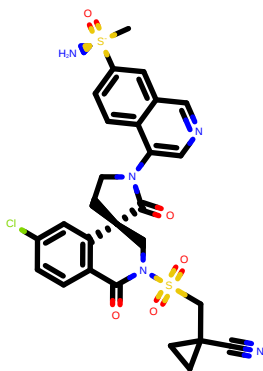
CID:	MAT-POS-38eb6498-4_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)OCC[NH+](C)C)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN978
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.28

MAT-POS-853c0ffa-9_1



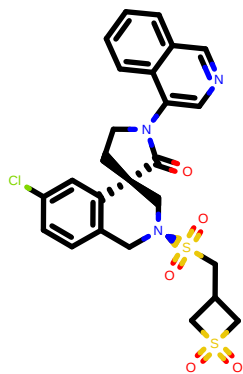
CID:	MAT-POS-853c0ffa-9_1
SMILES:	<chem>C[NH+](C)CCOc1ccc2nccc(c2c1)N3CC[C@]4(C3=O)C[N@](C5c4cc(cc5)S(=O)(=O)CC6(C)C#N</chem>
RUN:	RUN986
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.75

EDJ-MED-7d88f880-3_1



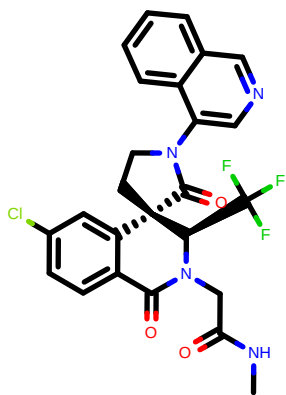
CID:	EDJ-MED-7d88f880-3_1
SMILES:	<chem>C[S@]([N])(=O)c1ccc2c(c1)ncc2N3CC[C@]4(C3=O)C[N@](C5c4cc(cc5)S(=O)(=O)CC6(C)C#N</chem>
RUN:	RUN979
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.57

ALP-POS-ecbed2ba-5_1



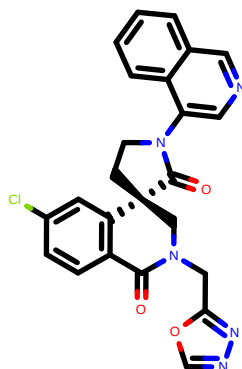
CID:	ALP-POS-ecbed2ba-5_1
SMILES:	<chem>c1ccc2c(c1)ncc2N3CC[C@]4(C3=O)C[N@](C5c4cc(cc5)S(=O)(=O)CC6CS(=O)(=O)C6</chem>
RUN:	RUN905
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.97

VLA-UNK-61877630-3_1



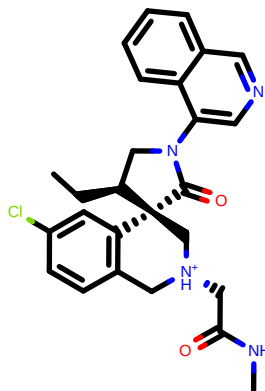
CID:	VLA-UNK-61877630-3_1
SMILES:	<chem>CNC(=O)CN1[C@@H]([C@H]2(CCN(C2=O)c3cncc4c3ccoc4)c5cc(ccc5C1=O)Cl)C(F)(F)F</chem>
RUN:	RUN927
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.16

PET-UNK-aa57768f-7_1



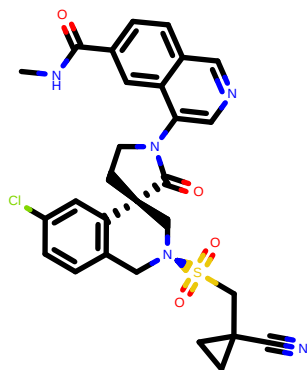
CID:	PET-UNK-aa57768f-7_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)C6nncoc6</chem>
RUN:	RUN790
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.10

MAT-POS-50a80394-5_2



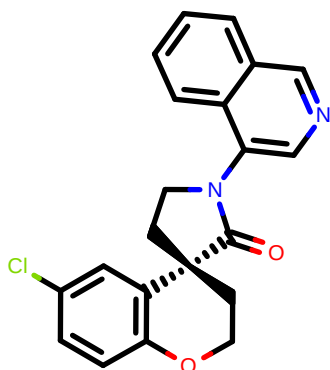
CID:	MAT-POS-50a80394-5_2
SMILES:	<chem>CC[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4ccoc5</chem>
RUN:	RUN828
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.20

MAT-POS-38eb6498-2_1



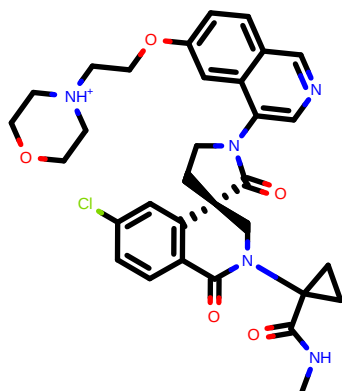
CID:	MAT-POS-38eb6498-2_1
SMILES:	<chem>CNC(=O)c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@H](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6C#NCC6</chem>
RUN:	RUN966
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.41

EDJ-MED-159244ea-1_1



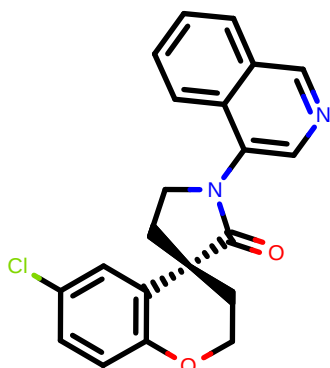
CID:	EDJ-MED-159244ea-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN682
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.05

EDJ-MED-dfa1d800-2_1



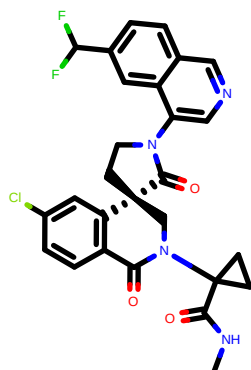
CID:	EDJ-MED-dfa1d800-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCCC6)c7cc(ccc7C2=O)Cl</chem>
RUN:	RUN1012
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.30

MAT-POS-983b399a-1_1



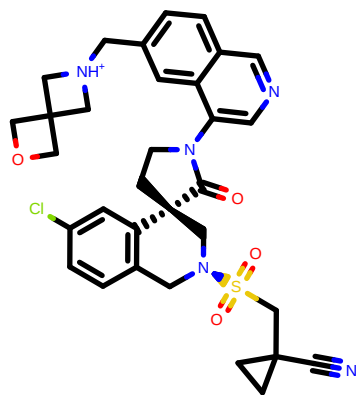
CID:	MAT-POS-983b399a-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN691
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.05

EDJ-MED-5cd3920d-4_1



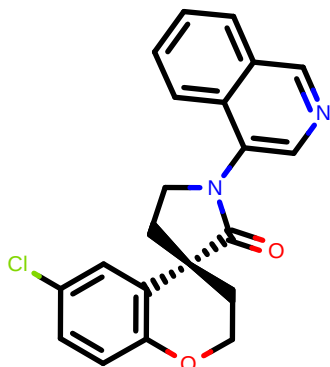
CID:	EDJ-MED-5cd3920d-4_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)C(F)F)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN930
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.15

EDJ-MED-ee81482e-5_1



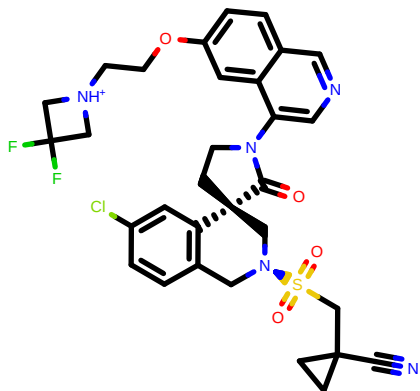
CID:	EDJ-MED-ee81482e-5_1
SMILES:	<chem>c1cc2nccc(c2cc1)[NH+]3CC4(C3)COC4N5CC[C@H](C5=O)C[NH@]1C2C6cc(cc7C2)S(=O)(=O)CC8(C7)CC8C1N</chem>
RUN:	RUN1014
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.53

ALP-POS-477dc5b7-4_1



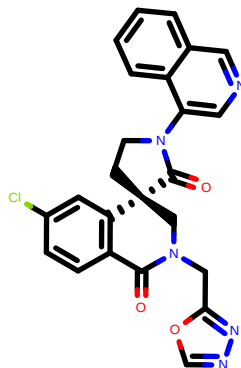
CID:	ALP-POS-477dc5b7-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOC5c4cc(cc5)Cl</chem>
RUN:	RUN695
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.05

EDJ-MED-468565e0-5_1



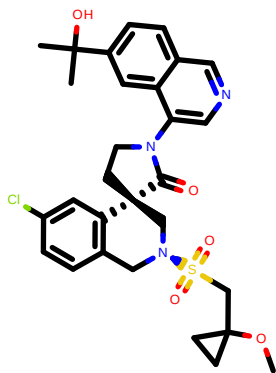
CID:	EDJ-MED-468565e0-5_1
SMILES:	<chem>c1cc2nccc(c2cc1OCCN3CC(C3)(F)F)N4CC[C@H](C4=O)C[NH@]1C2C6cc(ccc6)C2)S(=O)(=O)CC7(C7)C1N</chem>
RUN:	RUN1009
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.52

PET-UNK-aa57768f-1_1



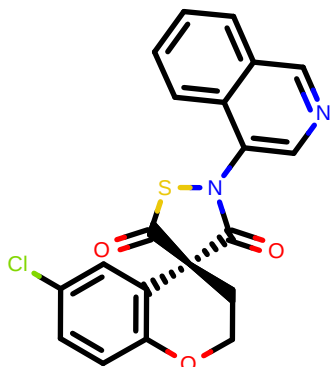
CID:	PET-UNK-aa57768f-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6</chem>
RUN:	RUN781
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.09

MAT-POS-853c0ffa-12_1



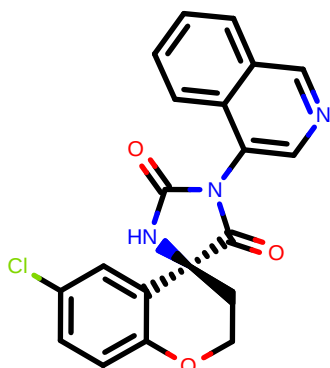
CID:	MAT-POS-853c0ffa-12_1
SMILES:	<chem>CC(C)(c1ccc2ncc(c2c1)n3cc[C@@H]4[C@H](C3=O)C[nH]4)[C@H](C5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC7O</chem>
RUN:	RUN976
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.39

DAR-DIA-0f7b7cd9-8_1



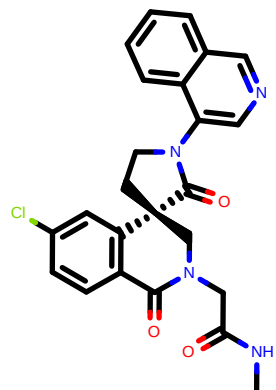
CID:	DAR-DIA-0f7b7cd9-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H]4(CCOc5c4cc(cc5)Cl)C(=O)S3</chem>
RUN:	RUN716
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.08

VLA-UCB-29506327-1_1



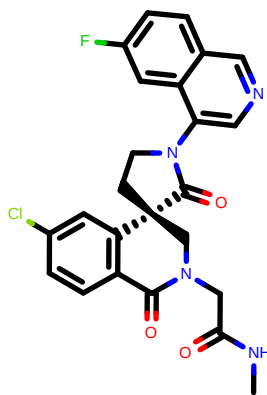
CID:	VLA-UCB-29506327-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H]4(CCOc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN697
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.05

PET-UNK-14142a25-10_1



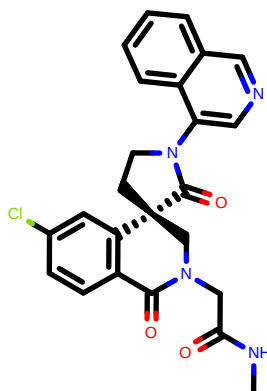
CID:	PET-UNK-14142a25-10_1
SMILES:	<chem>CNC(=O)CN1C[C@H]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN734
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.11

EDG-MED-b1ef7fe3-2_1



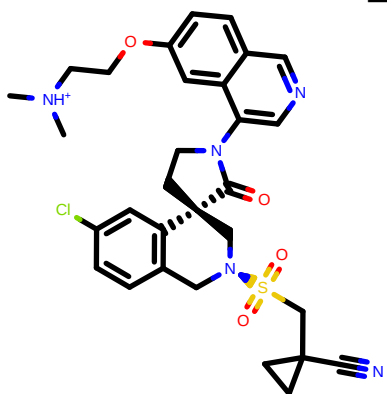
CID:	EDG-MED-b1ef7fe3-2_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN768
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.10

LUO-POS-9931618f-1_1



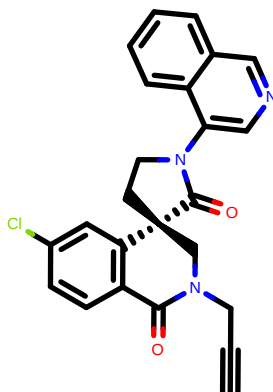
CID:	LUO-POS-9931618f-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN748
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.11

LUO-POS-8484f2d3-2_1



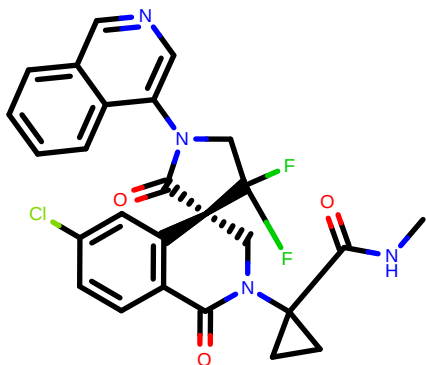
CID:	LUO-POS-8484f2d3-2_1
SMILES:	<chem>C[NH+]([C-])COC1ccc2cncc(c2c1)N3C[C@]4(CCN(C3=O)C[N+]([C-])C5c4cc(cc5)O)S(=O)(=O)CC6(CCC6)C#N</chem>
RUN:	RUN991
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.60

PET-UNK-aa57768f-9_1



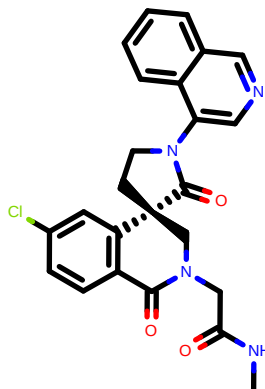
CID:	PET-UNK-aa57768f-9_1
SMILES:	<chem>C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN712
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.09

EDJ-MED-7e491f08-2_1



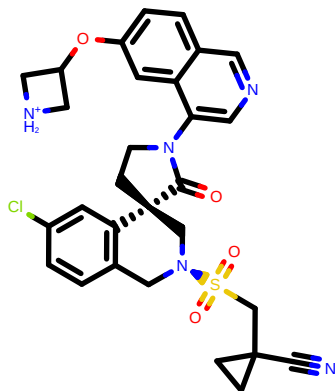
CID:	EDJ-MED-7e491f08-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(c4cc(ccc4C2=O)C)C(=O)N(CC3(F)F)c5cncc6c5cccc6</chem>
RUN:	RUN907
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.15

EDJ-MED-8bb691af-8_1



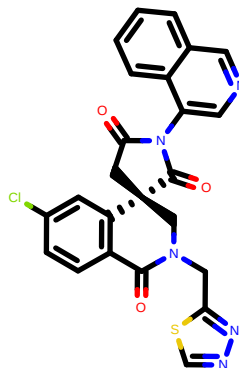
CID:	EDJ-MED-8bb691af-8_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN730
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.10

EDJ-MED-ee81482e-1_1



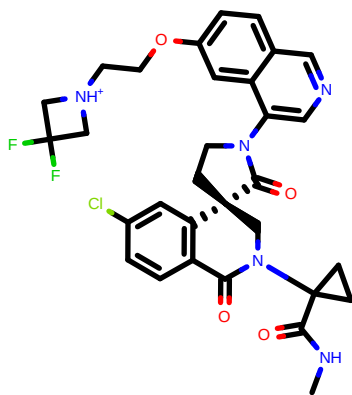
CID:	EDJ-MED-ee81482e-1_1
SMILES:	<chem>c1cc2ncc(c2cc1OC3C[NH2+])C3[N4CC]C[C@]5([C4=O]C[N6])C6c5cc(cc6)C)S(=O)(=O)CC7(C7)C#N</chem>
RUN:	RUN1015
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.42

PET-UNK-6af7266d-2_1



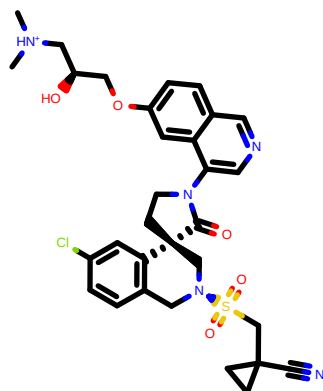
CID:	PET-UNK-6af7266d-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@]4(C3=O)CN(C(=O)c5c4cc(cc5)C)Cc6nncc6</chem>
RUN:	RUN840
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.12

EDJ-MED-dfa1d800-5_1



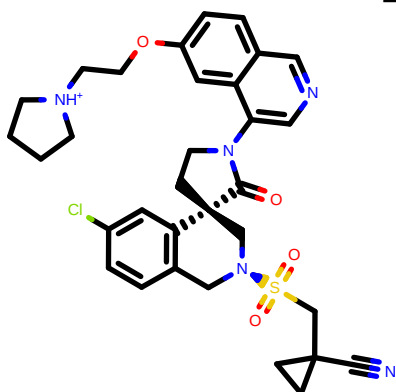
CID:	EDJ-MED-dfa1d800-5_1
SMILES:	<chem>CNC(=O)C1(C(C1)N2C[C@H]3(CCN(C(C3=O)C4cccc5c4ccc(cc5)OCCN6CC(C6)(F)F)C7cc(ccc7C2=O)Cl</chem>
RUN:	RUN993
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.23

EDJ-MED-ee81482e-3_1



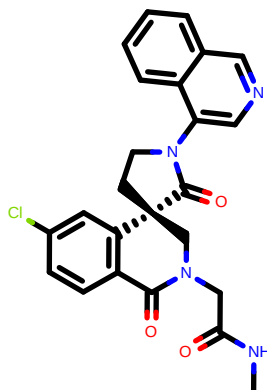
CID:	EDJ-MED-ee81482e-3_1
SMILES:	<chem>C[NH+](C)[C@H](C)[C@@H](CO)C1ccc2ccc(cc21)N3CC[C@H]4(C3=O)C[N@H]5C6c4ccc(cc6)S(=O)(=O)CC7(C)C7C8=NO</chem>
RUN:	RUN1002
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.62

EDJ-MED-468565e0-1_1



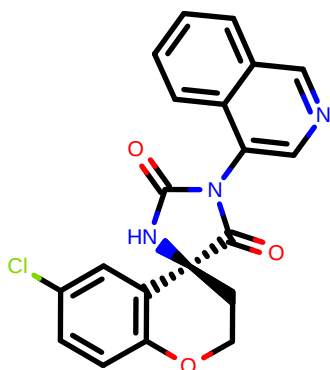
CID:	EDJ-MED-468565e0-1_1
SMILES:	<chem>c1cc2ccc(cc2c1OCC[NH+])C3CCCC3N4CC[C@H]5(C4=O)C[N@H]6C7c6ccc(cc7)S(=O)(=O)CC7(C)C7C8=NO</chem>
RUN:	RUN1006
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.61

EDJ-MED-fd8ed875-3_1



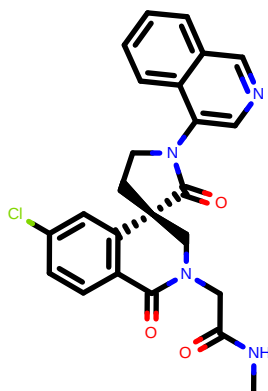
CID:	EDJ-MED-fd8ed875-3_1
SMILES:	<chem>CNC(=O)CN1C[C@H]2(C=CN(C2=O)C3cnc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN753
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.09

VLA-UNK-cf7facf1-1_1



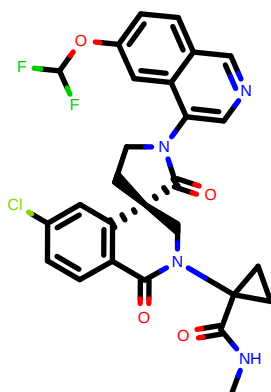
CID:	VLA-UNK-cf7facf1-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN699
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.05

PET-UNK-14142a25-1_1



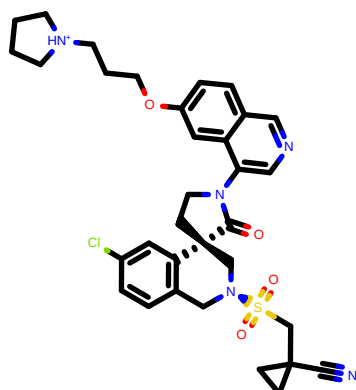
CID:	PET-UNK-14142a25-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN732
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.11

EDJ-MED-5cd3920d-3_1



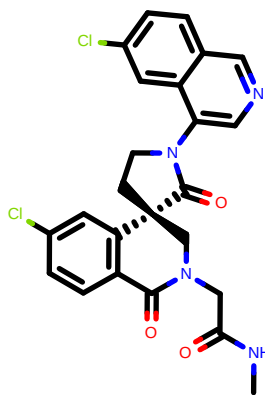
CID:	EDJ-MED-5cd3920d-3_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OC(F)F)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN967
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.15

MAT-POS-40ad851a-5_1



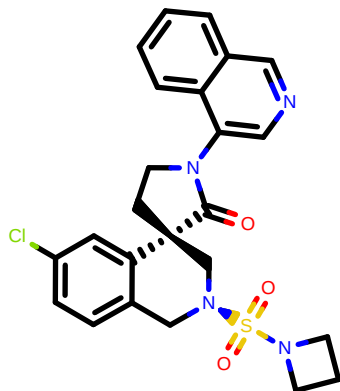
CID:	MAT-POS-40ad851a-5_1
SMILES:	<chem>c1cc2nccc(c2cc1OCCC[NH+])3CCCC3N4CC[C@]5([C@H](C4=O)[C@H]5)Cc6c5ccc(c6)C7S(=O)(=O)CC7(C)C#N</chem>
RUN:	RUN1013
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.49

LUO-POS-8c3e556a-1_1



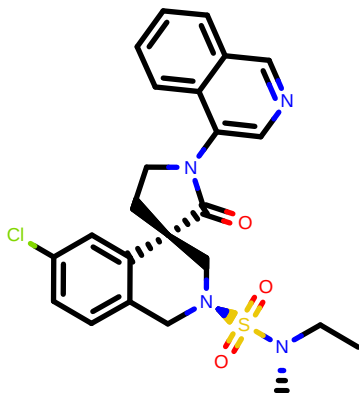
CID:	LUO-POS-8c3e556a-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN795
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.12

ALP-POS-ecbed2ba-20_1



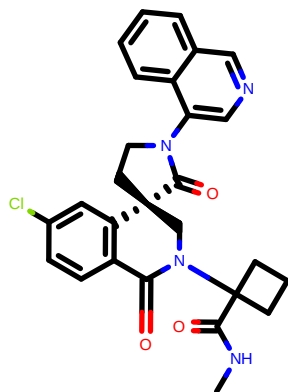
CID:	ALP-POS-ecbed2ba-20_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CCC6</chem>
RUN:	RUN788
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.65

ALP-POS-ecbed2ba-18_1



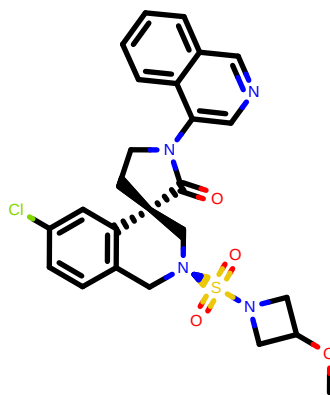
CID:	ALP-POS-ecbed2ba-18_1
SMILES:	<chem>CC[N@@](C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccc5)Cl</chem>
RUN:	RUN786
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.21

EDJ-MED-98c0a822-3_1



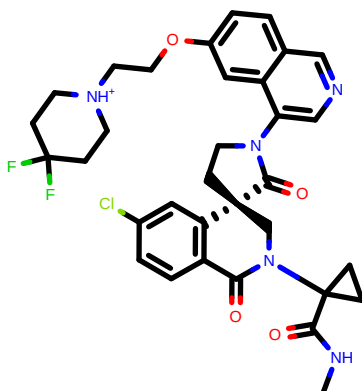
CID:	EDJ-MED-98c0a822-3_1
SMILES:	<chem>CNC(=O)C1(CCC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN866
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.19

ALP-POS-ecbed2ba-10_1



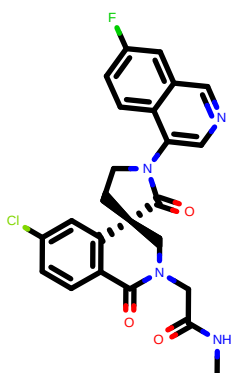
CID:	ALP-POS-ecbed2ba-10_1
SMILES:	<chem>COC1CN(C1)S(=O)(=O)N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5ccc6)Cl</chem>
RUN:	RUN862
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.36

EDJ-MED-dfa1d800-4_1



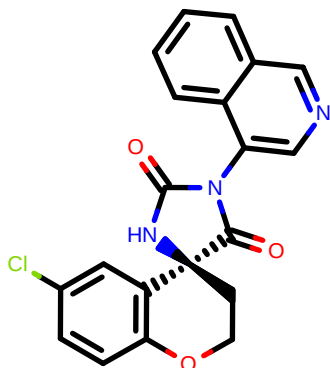
CID:	EDJ-MED-dfa1d800-4_1
SMILES:	<chem>CNC(=O)C1(C1)N2C[C@]3(C)CCN(C3=O)c4cnc5c4cc(cc5)OC(NH)6CCC(C6)F(F)F7cc(ccc7C2=O)Cl</chem>
RUN:	RUN1005
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.32

EDG-MED-b1ef7fe3-3_1



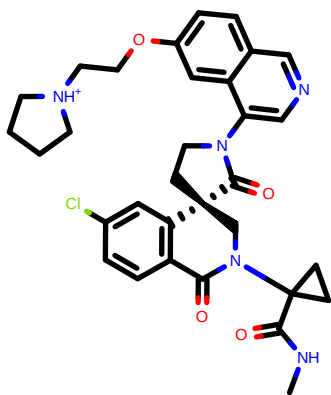
CID:	EDG-MED-b1ef7fe3-3_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cnc4c3ccc(c4)F)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN773
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.11

VLA-UCB-34f3ed0c-11_1



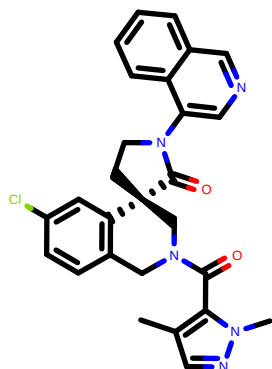
CID:	VLA-UCB-34f3ed0c-11_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN689
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.05

EDJ-MED-dfa1d800-1_1



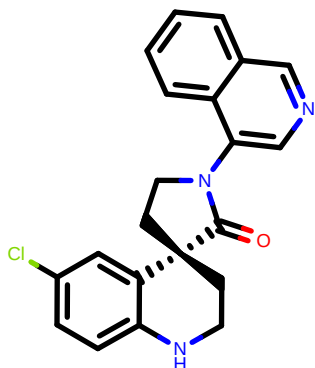
CID:	EDJ-MED-dfa1d800-1_1
SMILES:	<chem>CNC(=O)C1CC1N2C[C@]3(CCN(C3=O)c4cccc5c4cc(cc5)OC[C@H]1)CCCC6c7cc(ccc7C2=O)Cl</chem>
RUN:	RUN988
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.33

EDJ-MED-cc48ee33-4_1



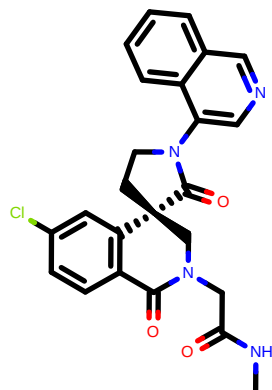
CID:	EDJ-MED-cc48ee33-4_1
SMILES:	<chem>Cc1cnnc(c1C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl)C</chem>
RUN:	RUN881
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.22

DAR-DIA-6be260fc-5_1



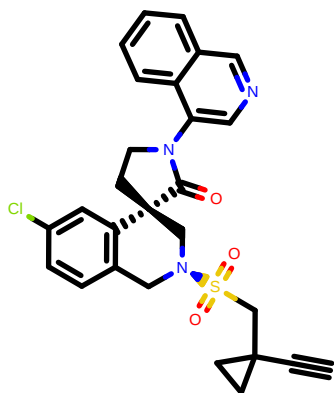
CID:	DAR-DIA-6be260fc-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCNc5c4cc(cc5)Cl</chem>
RUN:	RUN692
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.09

LUO-POS-9931618f-2_1



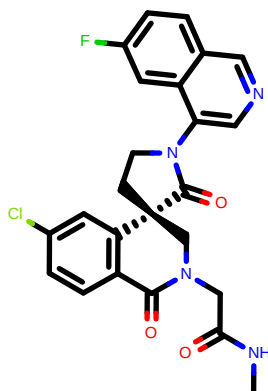
CID:	LUO-POS-9931618f-2_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN752
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.11

PET-UNK-94036022-2_1



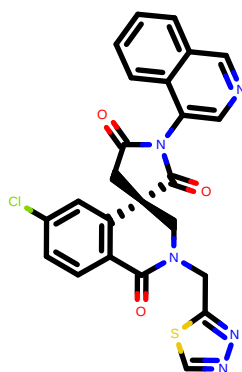
CID:	PET-UNK-94036022-2_1
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)N@@J2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cccc65cccc6)Cl</chem>
RUN:	RUN890
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.30

EDJ-MED-b6c6ee2b-6_1



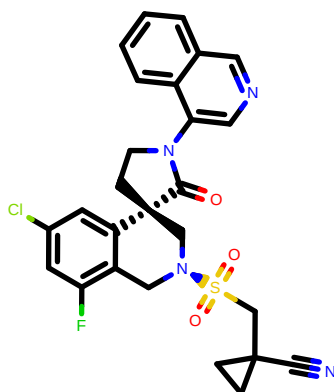
CID:	EDJ-MED-b6c6ee2b-6_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4F)c5ccc(ccc5C1=O)Cl</chem>
RUN:	RUN785
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.11

PET-UNK-6af7266d-4_1



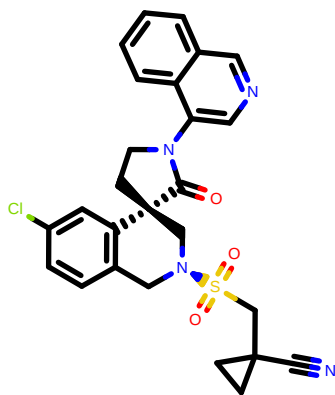
CID:	PET-UNK-6af7266d-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nncc6</chem>
RUN:	RUN845
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.11

VLA-UNK-61877630-7_1



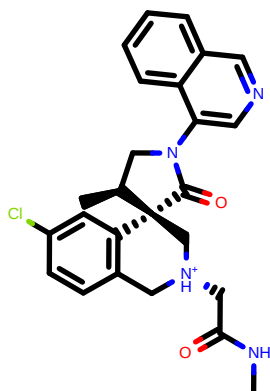
CID:	VLA-UNK-61877630-7_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)C[N@](C5c4cc(cc5F)Cl)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN917
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.42

EDJ-MED-8bb691af-6_1



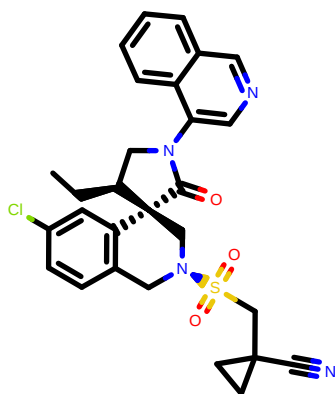
CID:	EDJ-MED-8bb691af-6_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](C5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN847
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.42

MAT-POS-50a80394-4_2



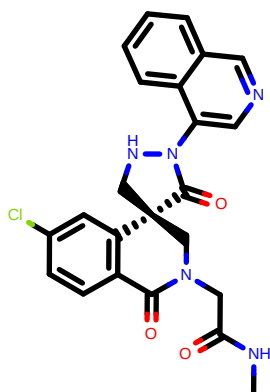
CID:	MAT-POS-50a80394-4_2
SMILES:	<chem>C[C@H]1CN(C(=O)[C@@]12C[N@](H+)(C3c2cc(cc3)Cl)CC(=O)NC)C4cccc5C4cccc5</chem>
RUN:	RUN784
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.24

MAT-POS-50a80394-2_2



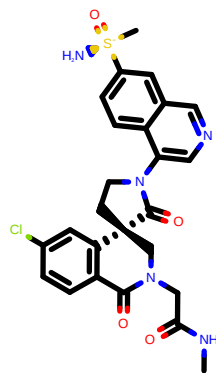
CID:	MAT-POS-50a80394-2_2
SMILES:	<chem>CC[C@H]1CN(C(=O)[C@@]12C[N@](H+)(C3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C5cccc5C5cccc5</chem>
RUN:	RUN950
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.55

EDJ-MED-fed7ac0b-1_1



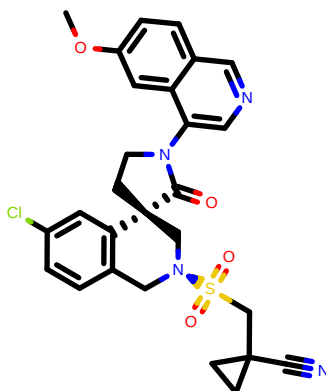
CID:	EDJ-MED-fed7ac0b-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CNN(C2=O)C3cnc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN744
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.11

EDJ-MED-7d88f880-1_2



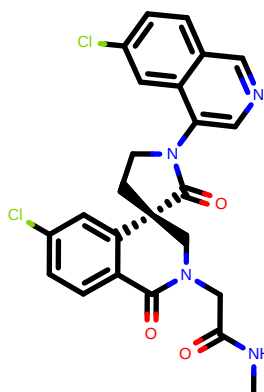
CID:	EDJ-MED-7d88f880-1_2
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)[S@]1(=N)(=O)C)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN904
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.18

EDJ-MED-b6c6ee2b-3_1



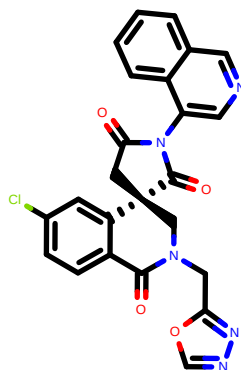
CID:	EDJ-MED-b6c6ee2b-3_1
SMILES:	<chem>COc1ccc2nccc(c2c1)N3CC[C@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN953
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.34

LUO-POS-8c3e556a-2_1



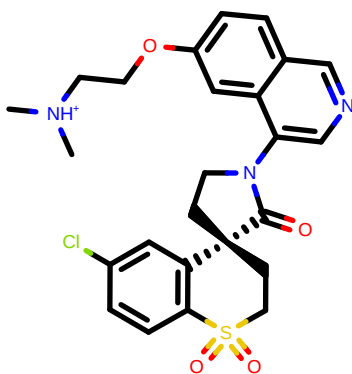
CID:	LUO-POS-8c3e556a-2_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN793
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.13

12_-111-3e02a1cd-1_1



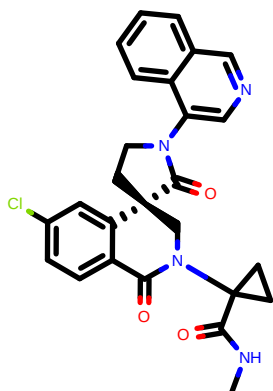
CID:	12_-111-3e02a1cd-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)C6c6nnc6</chem>
RUN:	RUN842
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.10

EDJ-MED-d4864bdc-4_1



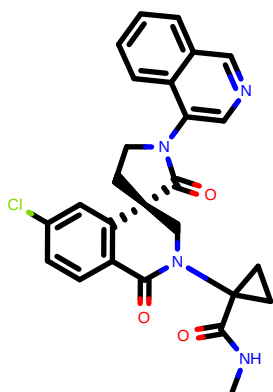
CID:	EDJ-MED-d4864bdc-4_1
SMILES:	<chem>C[NH+](C)CCOc1ccc2ncoc(c2c1)N3CC[C@@]4(C3=O)CCS(=O)(=O)c5cc(cc5)Cl</chem>
RUN:	RUN839
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.28

MAT-POS-e48723dc-1_1



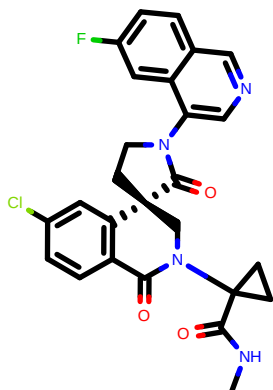
CID:	MAT-POS-e48723dc-1_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN833
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.13

EDJ-MED-976a33d5-1_1



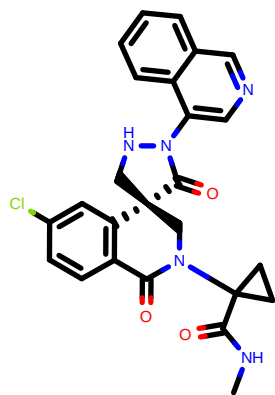
CID:	EDJ-MED-976a33d5-1_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN816
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.14

EDJ-MED-b6c6ee2b-7_1



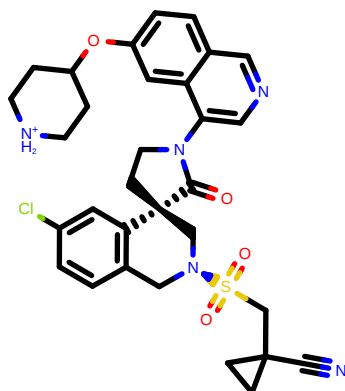
CID:	EDJ-MED-b6c6ee2b-7_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@@]3(CCN(C3=O)c4cncc5c4cc(cc5)F)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN871
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.14

EDJ-MED-fed7ac0b-2_1



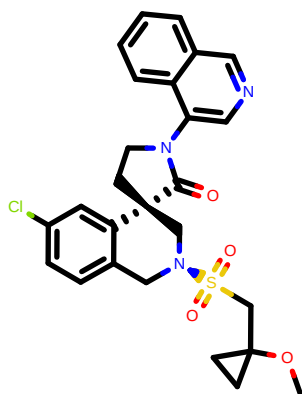
CID:	EDJ-MED-fed7ac0b-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cnc5c4cccc5)c6cc(c6c6C2=O)Cl</chem>
RUN:	RUN824
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.13

EDJ-MED-ee81482e-4_1



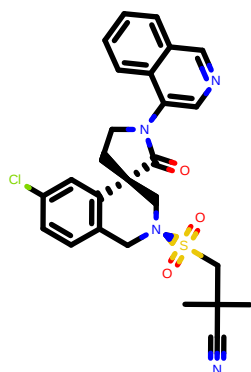
CID:	EDJ-MED-ee81482e-4_1
SMILES:	<chem>c1cc2nccc(2cc1OC3CC[NH2+](CC3)N4CC[C@]5(C(=O)C[N@]6(Cc6c5cc(6)C)S(=O)(=O)CC7(C)C7)C#N</chem>
RUN:	RUN1008
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.52

ALP-POS-ecbed2ba-6_1



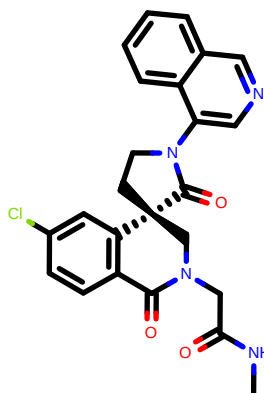
CID:	ALP-POS-ecbed2ba-6_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5cccc6)Cl</chem>
RUN:	RUN876
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.27

ALP-POS-ecbed2ba-13_1



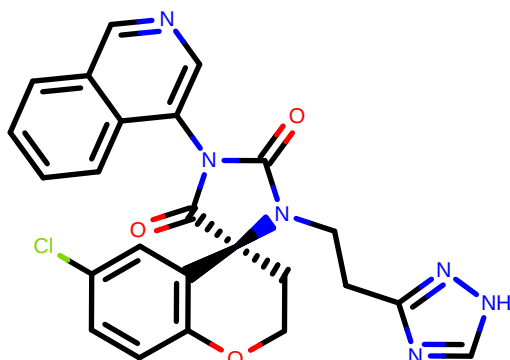
CID:	ALP-POS-ecbed2ba-13_1
SMILES:	<chem>CC(C)(CS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl)C#N</chem>
RUN:	RUN855
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.34

MIK-ENA-794411b8-1_1



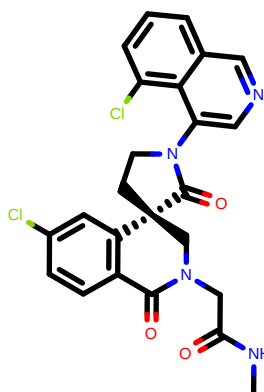
CID:	MIK-ENA-794411b8-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN761
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.13

VLA-UNK-f702bf1c-8_1



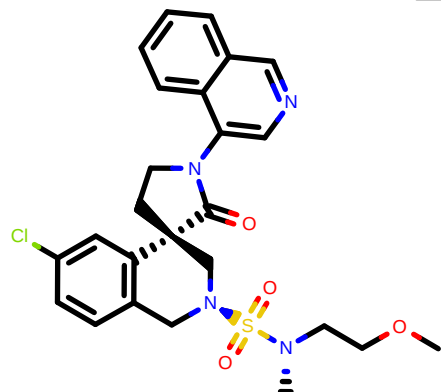
CID:	VLA-UNK-f702bf1c-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCc6[nH]ncc6</chem>
RUN:	RUN830
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.17

MAT-POS-853c0ffa-1_1



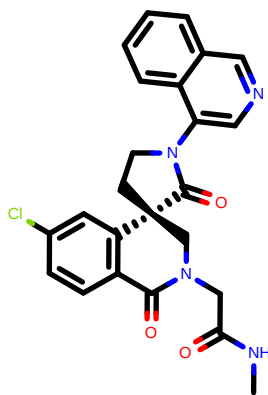
CID:	MAT-POS-853c0ffa-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(cc4)Cl)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN772
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.15

ALP-POS-ecbed2ba-21_1



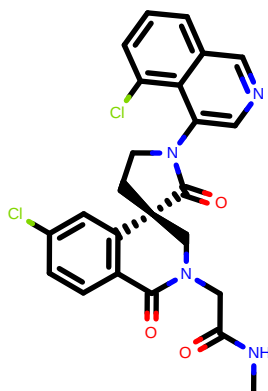
CID:	ALP-POS-ecbed2ba-21_1
SMILES:	<chem>C[N@](CCOC)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccc5)Cl</chem>
RUN:	RUN870
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.22

MIK-ENA-37e0b697-1_1



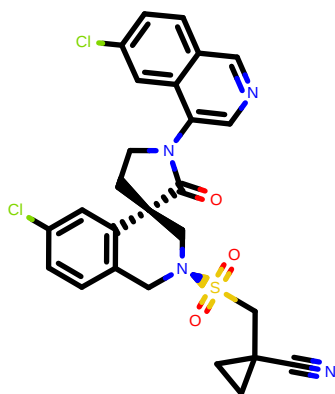
CID:	MIK-ENA-37e0b697-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN758
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.13

MAT-POS-1d5ab790-3_1



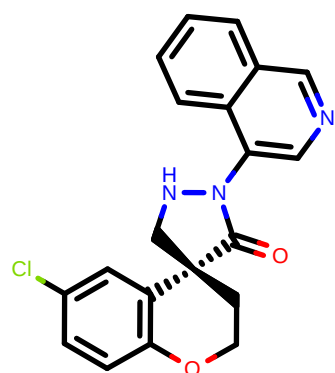
CID:	MAT-POS-1d5ab790-3_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(cc4)Cl)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN799
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.15

EDJ-MED-b6c6ee2b-4_1



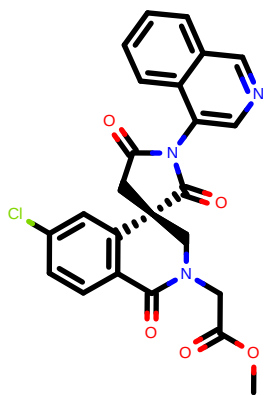
CID:	EDJ-MED-b6c6ee2b-4_1
SMILES:	<chem>c1cc2cncc(c2cc1C)N3CC[C@@]4(C3=O)C[N@](C5c4cc(cc5)Cl)S(=O)(=O)CC6(C6)C#N</chem>
RUN:	RUN919
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.37

BEN-BAS-c2bc0d80-3_1



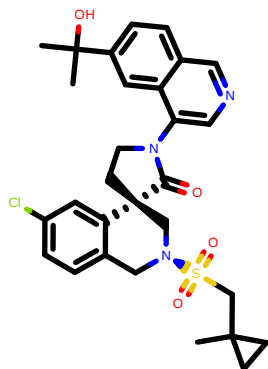
CID:	BEN-BAS-c2bc0d80-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)CN3</chem>
RUN:	RUN694
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.05

PET-UNK-77d5678a-6_1



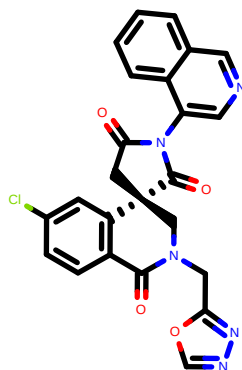
CID:	PET-UNK-77d5678a-6_1
SMILES:	<chem>COC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN797
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.08

MAT-POS-853c0ffa-20_1



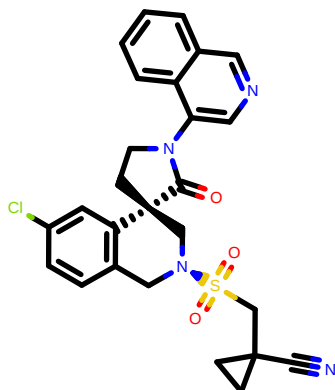
CID:	MAT-POS-853c0ffa-20_1
SMILES:	<chem>CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)C(C)O)Cl</chem>
RUN:	RUN970
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.34

PET-UNK-77d5678a-5_1



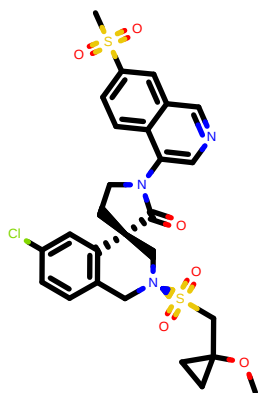
CID:	PET-UNK-77d5678a-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6</chem>
RUN:	RUN834
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.11

ALP-POS-ecbed2ba-4_1



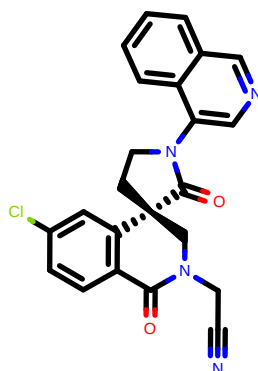
CID:	ALP-POS-ecbed2ba-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)C[N@](C5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN869
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.38

MAT-POS-853c0ffa-16_1



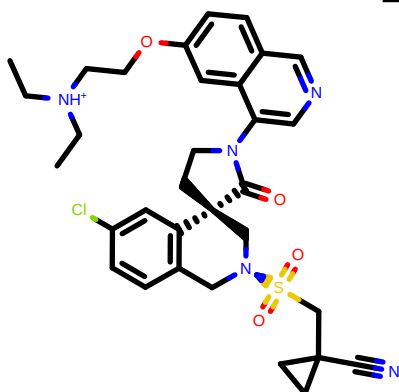
CID:	MAT-POS-853c0ffa-16_1
SMILES:	<chem>COC1(CC1)C5(=O)(=O)N@]2C3ccc(cc3[C@@]4(C2)CN(C4=O)c5ccc6c(ccc6)S(=O)(=O)C7Cl</chem>
RUN:	RUN972
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.30

PET-UNK-aa57768f-2_1



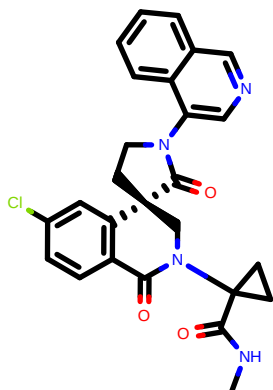
CID:	PET-UNK-aa57768f-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N</chem>
RUN:	RUN720
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.07

MAT-POS-40ad851a-3_1



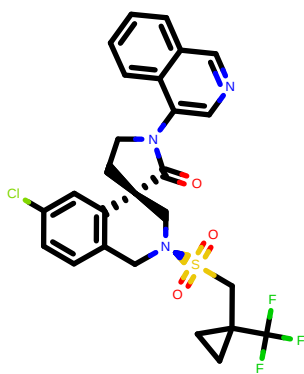
CID:	MAT-POS-40ad851a-3_1
SMILES:	<chem>CC[NH+](C)CC(CO)c1ccc2nc(cc2c1)N3CC[C@@]4(C3=O)CN(C4=O)c5c4cc(cc5)Cl)S(=O)(=O)C6C7C8C9C#N</chem>
RUN:	RUN1011
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.60

MAT-POS-e48723dc-2_1



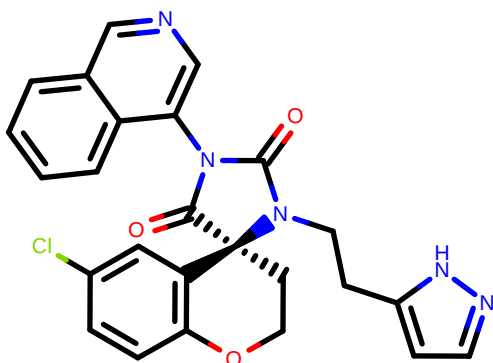
CID:	MAT-POS-e48723dc-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN835
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.15

VLA-UNK-61877630-10_1



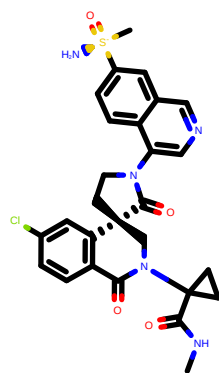
CID:	VLA-UNK-61877630-10_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(C)C(F)(F)F</chem>
RUN:	RUN941
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.35

VLA-UNK-f702bf1c-1_1



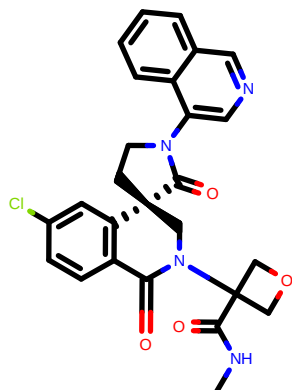
CID:	VLA-UNK-f702bf1c-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6ccn[nH]6</chem>
RUN:	RUN809
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.15

EDJ-MED-7d88f880-2_2



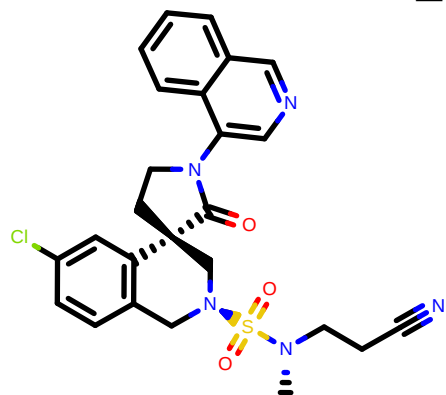
CID:	EDJ-MED-7d88f880-2_2
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)[S@]([N])(=O)C)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN951
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.23

EDJ-MED-98c0a822-4_1



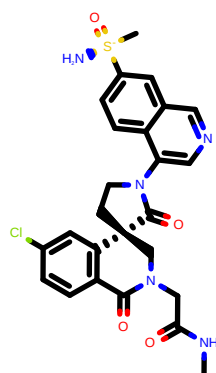
CID:	EDJ-MED-98c0a822-4_1
SMILES:	<chem>CNC(=O)C1(COC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN868
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.15

ALP-POS-ecbed2ba-16_1



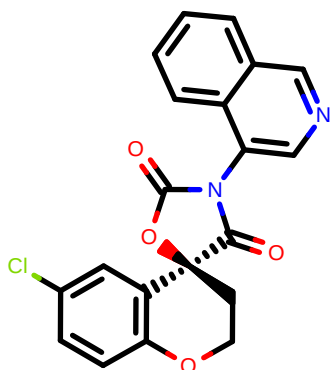
CID:	ALP-POS-ecbed2ba-16_1
SMILES:	<chem>C#N@([CCC#N]S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN860
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.72

EDJ-MED-7d88f880-1_1



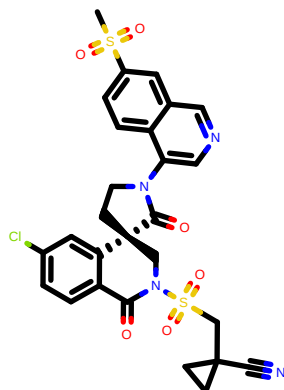
CID:	EDJ-MED-7d88f880-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)[S@]([N])(=O)C)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN903
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.17

MAT-POS-ec6d90b7-1_1



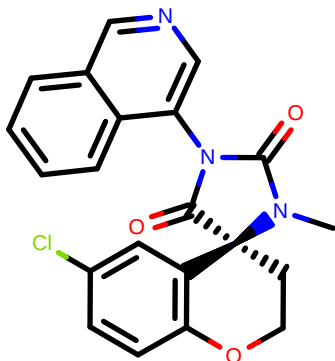
CID:	MAT-POS-ec6d90b7-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O</chem>
RUN:	RUN698
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.03

EDJ-MED-9f4ac58c-4_1



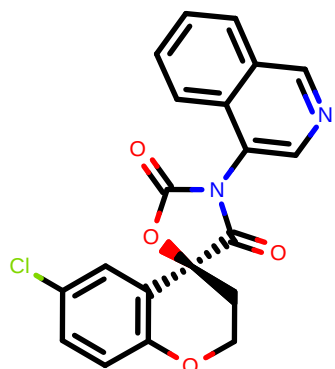
CID:	EDJ-MED-9f4ac58c-4_1
SMILES:	<chem>CS(=O)(=O)c1ccc2c(c1)cncc2N3C[C@]([N])(C3=O)CN(C(=O)c4c5cc(cc5)O)c5cc(ccc5)C#N</chem>
RUN:	RUN963
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.71

BEN-BAS-c2bc0d80-7_1



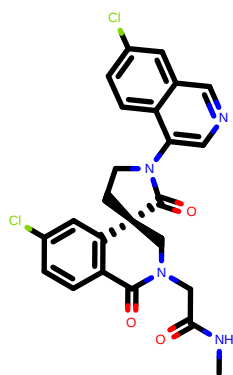
CID:	BEN-BAS-c2bc0d80-7_1
SMILES:	<chem>CN1C(=O)N(C(=O))[C@@]12CCOC3c2cc(cc3)Cl)c4cncc5c4cccc5</chem>
RUN:	RUN709
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.07

MAT-POS-90505e2b-1_1



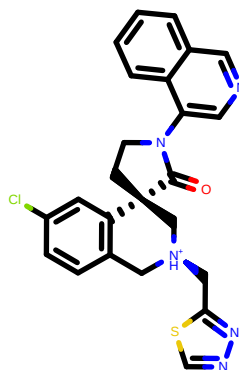
CID:	MAT-POS-90505e2b-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O</chem>
RUN:	RUN690
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.03

EDG-MED-b1ef7fe3-4_1



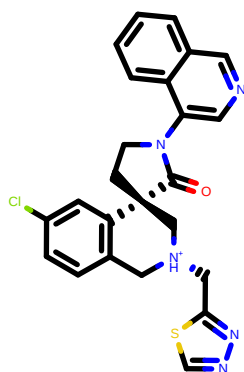
CID:	EDG-MED-b1ef7fe3-4_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)Cl)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN771
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.15

MAT-POS-96396902-1_1



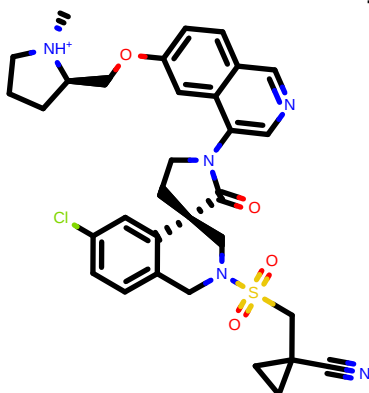
CID:	MAT-POS-96396902-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H]5(Cc5c4cc(cc5)Cl)Cc6nncc6</chem>
RUN:	RUN782
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.14

PET-UNK-7e9559de-1_1



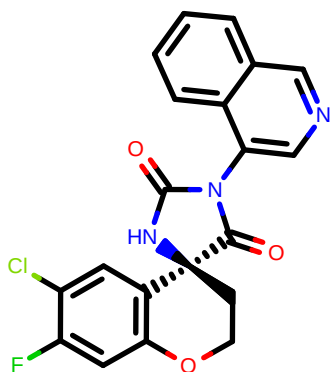
CID:	PET-UNK-7e9559de-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@H](C3=O)C[N@H+](Cc5c4cc(cc5)Cl)C6nncs6</chem>
RUN:	RUN755
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.18

MAT-POS-40ad851a-1_1



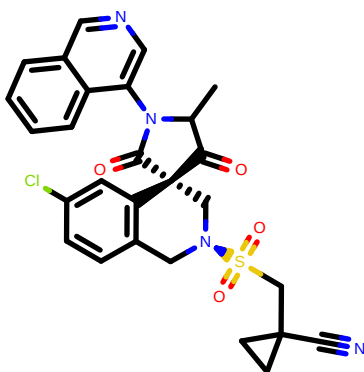
CID:	MAT-POS-40ad851a-1_1
SMILES:	<chem>C[N@H+](CCCC[C@H](H)COC2cc3ncc(c3c2)N4CC[C@H](C4=O)C[N@H](Cc5c5cc(cc5)O)S(=O)(=O)CC7(C7)C#N</chem>
RUN:	RUN1003
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.67

VLA-UNK-3a43cd95-1_1



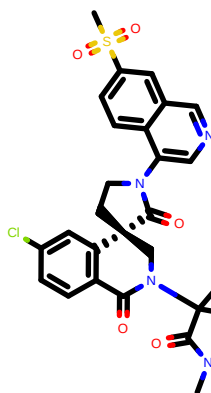
CID:	VLA-UNK-3a43cd95-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H](C3=O)(CCOC5c4cc(c(c5)F)Cl)NC3=O</chem>
RUN:	RUN706
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.05

PET-UNK-94036022-13_1



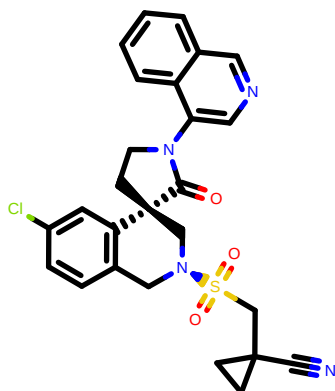
CID:	PET-UNK-94036022-13_1
SMILES:	<chem>C=C1C(=O)C@H2(C1N@H)C3c3cc(cc3)C]S(=O)(=O)CC4(C4)C[NH]C(=O)N1c5ccc6cc5ccc6</chem>
RUN:	RUN954
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.43

EDJ-MED-976a33d5-2_1



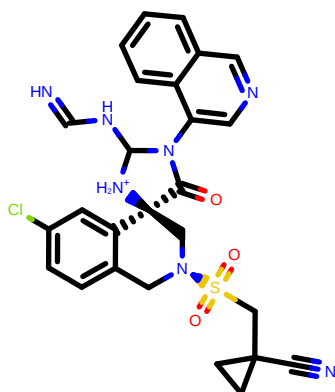
CID:	EDJ-MED-976a33d5-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C(C@)3(CCN(C3=O)c4cncc5c4ccc(c5)S(=O)(=O)C)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN946
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.20

MIK-ENA-5d9157e9-2_1



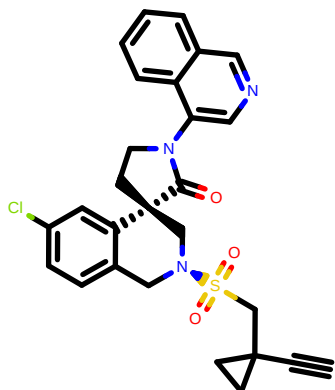
CID:	MIK-ENA-5d9157e9-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC(C@@)4(C3=O)C(N@)(C5c4cc(c5)Cl)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN874
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.41

LUO-POS-b5068a05-2_1



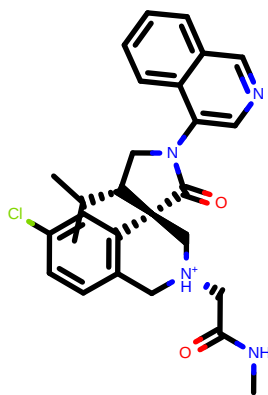
CID:	LUO-POS-b5068a05-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C(C@@)4(C3=O)C(N@)(C5c4cc(c5)Cl)S(=O)(=O)CC6(CC6)C#N=C3N=C#N</chem>
RUN:	RUN962
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.27

PET-UNK-94036022-9_1



CID:	PET-UNK-94036022-9_1
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)N@2C3ccc(cc3C@)4(C2)CCN(C4=O)c5cncc6c5ccc6)Cl</chem>
RUN:	RUN891
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.29

MAT-POS-50a80394-6_1



CID: MAT-POS-50a80394-6_1

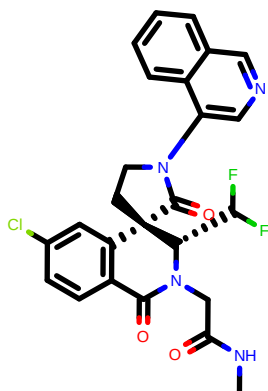
SMILES: CC(C)[C@@H]1CN(C(=O)[C@@H]12C[N@@H+](Cc3c2cc(cc3)C)CC(=O)NC)c4cccc5

RUN: RUN843

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.22

VLA-UNK-61877630-6_2



CID: VLA-UNK-61877630-6_2

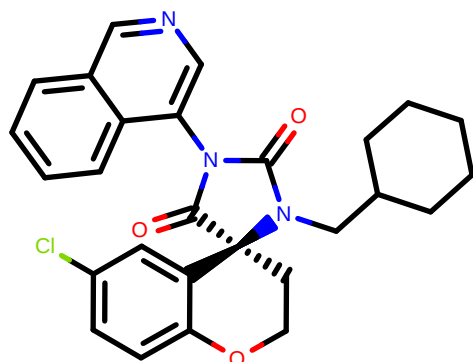
SMILES: CNC(=O)CN1[C@H]([C@H]12(CCN(C2=O)c3cccc4c3cccc4)c5cc(ccc5C1=O)Cl)C(F)F

RUN: RUN880

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.19

VLA-UCB-34f3ed0c-14_1



CID: VLA-UCB-34f3ed0c-14_1

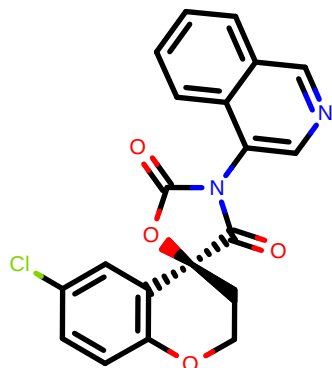
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@H]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCCC6

RUN: RUN800

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.15

MAT-POS-ec6d90b7-2_1



CID: MAT-POS-ec6d90b7-2_1

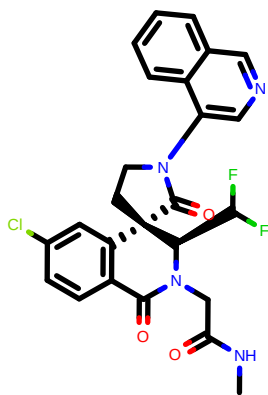
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@H]4(CCOc5c4cc(cc5)Cl)OC3=O

RUN: RUN710

DDG (kcal/mol): -0.32

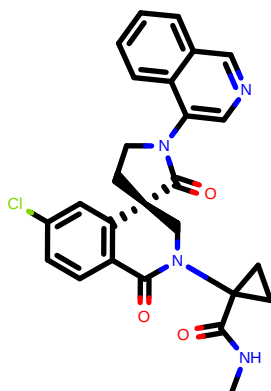
dDDG (kcal/mol): 0.03

VLA-UNK-61877630-6_1



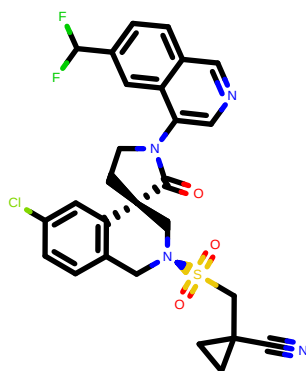
CID:	VLA-UNK-61877630-6_1
SMILES:	<chem>CNC(=O)CN1[C@@H]([C@H]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl)C(F)F</chem>
RUN:	RUN878
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.23

MAT-POS-576f7758-2_1



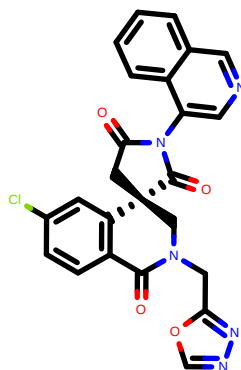
CID:	MAT-POS-576f7758-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@H]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN822
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.14

EDJ-MED-5cd3920d-2_1



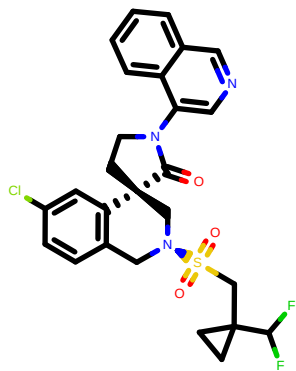
CID:	EDJ-MED-5cd3920d-2_1
SMILES:	<chem>c1cc2ncc(c2c1C(F)F)N(C)C[C@H]4(C3=O)CN([C@H]4Cc5cc(cc5)S(=O)(=O)CC6C(C)C#N</chem>
RUN:	RUN971
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.42

PET-UNK-77d5678a-2_1



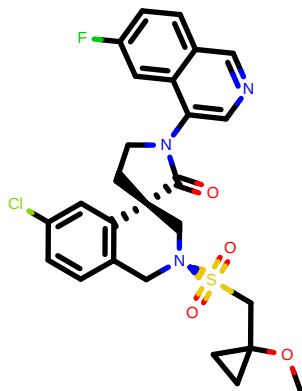
CID:	PET-UNK-77d5678a-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@H]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6</chem>
RUN:	RUN837
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.10

EDJ-MED-5cd3920d-5_1



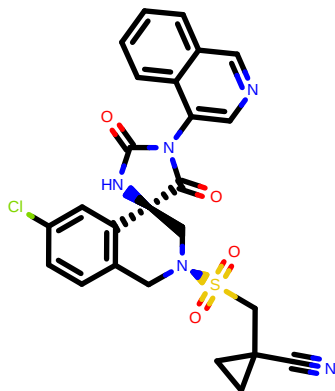
CID:	EDJ-MED-5cd3920d-5_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@]4(C3=O)C[N@](C5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)F</chem>
RUN:	RUN932
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.42

MAT-POS-853c0ffa-14_1



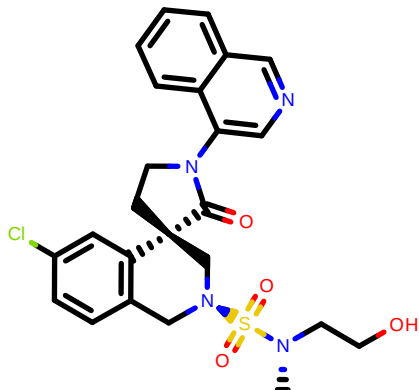
CID:	MAT-POS-853c0ffa-14_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5cc(cc6)F)Cl</chem>
RUN:	RUN926
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.41

MAT-POS-c2d406ed-1_1



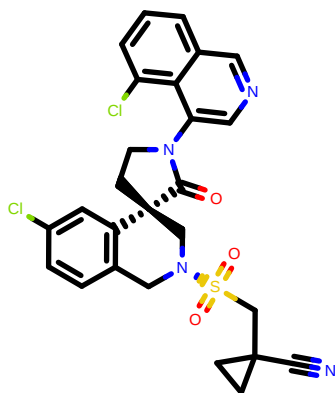
CID:	MAT-POS-c2d406ed-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)[C@]4(C3)C[N@](C5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN892
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.28

ALP-POS-ecbed2ba-19_1



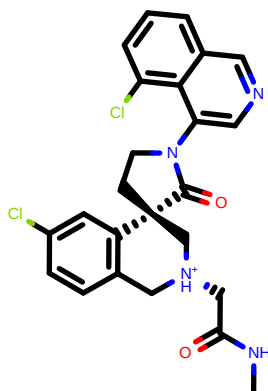
CID:	ALP-POS-ecbed2ba-19_1
SMILES:	<chem>C[N@](CCO)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4ccc5)Cl</chem>
RUN:	RUN814
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.32

MAT-POS-1d5ab790-1_1



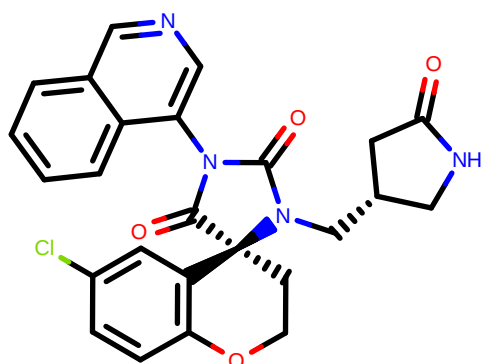
CID:	MAT-POS-1d5ab790-1_1
SMILES:	<chem>c1cc2cncc(c2c(c1)C)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN909
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.43

MAT-POS-1d5ab790-2_1



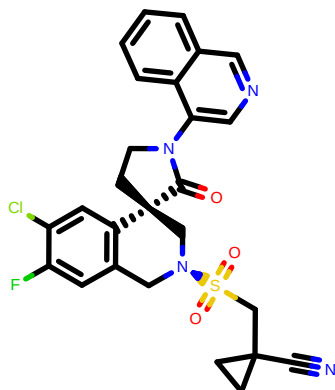
CID:	MAT-POS-1d5ab790-2_1
SMILES:	<chem>CNC(=O)C[N@](H)[+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl</chem>
RUN:	RUN766
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.23

VLA-UNK-f702bf1c-4_1



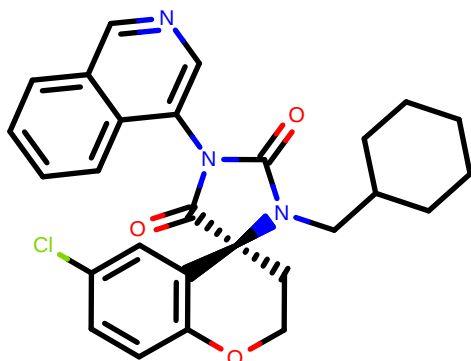
CID:	VLA-UNK-f702bf1c-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@](H)6CC(=O)NC6</chem>
RUN:	RUN811
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.17

VLA-UNK-61877630-8_1



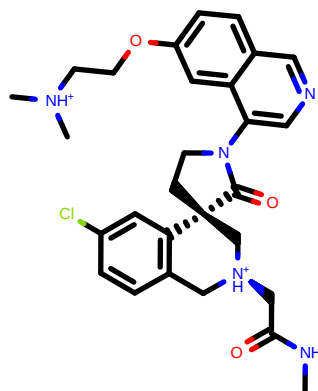
CID:	VLA-UNK-61877630-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(c(c5)F)Cl)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN945
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.41

VLA-UNK-f702bf1c-6_1



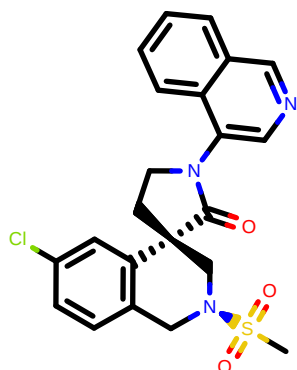
CID:	VLA-UNK-f702bf1c-6_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCC6</chem>
RUN:	RUN817
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.14

MAT-POS-38eb6498-3_1



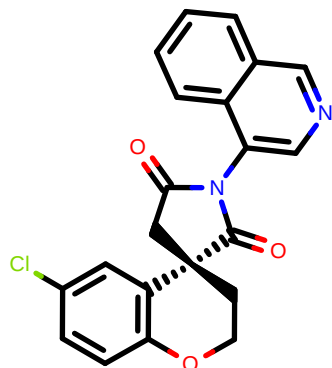
CID:	MAT-POS-38eb6498-3_1
SMILES:	<chem>CNC(=O)C[N@H]1Cc2ccc(cc2[C@@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+])([C]C)Cl</chem>
RUN:	RUN949
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.42

EDJ-MED-7587a9ee-3_1



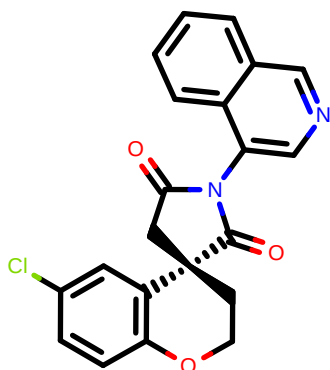
CID:	EDJ-MED-7587a9ee-3_1
SMILES:	<chem>CS(=O)(=O)[N@]1Cc2ccc(cc2[C@@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN725
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.16

MAT-POS-94643566-1_1



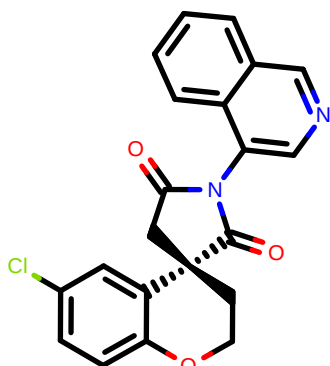
CID:	MAT-POS-94643566-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN701
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.01

BEN-BAS-c2bc0d80-6_1



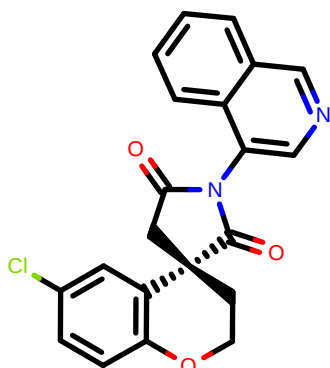
CID:	BEN-BAS-c2bc0d80-6_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN696
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.00

VLA-UCB-05e51b3f-5_1



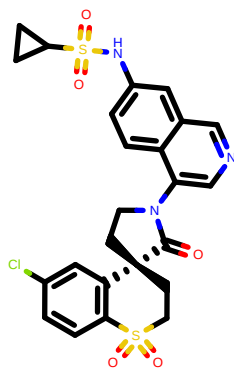
CID:	VLA-UCB-05e51b3f-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN703
DDG (kcal/mol):	-0.00
dDDG (kcal/mol):	0.00

VLA-UCB-50c39ae8-2_1



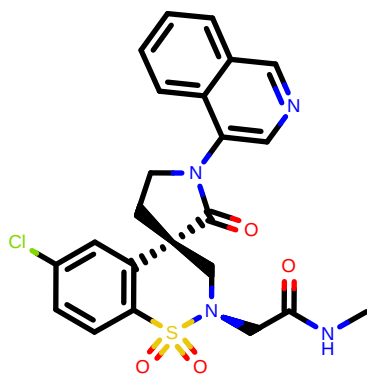
CID:	VLA-UCB-50c39ae8-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN693
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.00

EDJ-MED-edc5c6cb-2_1



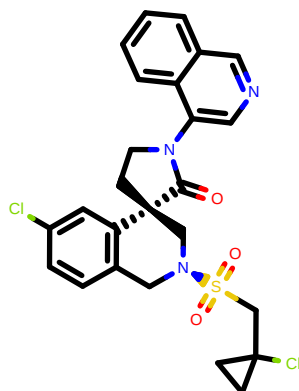
CID:	EDJ-MED-edc5c6cb-2_1
SMILES:	<chem>c1cc2c(cc1NS(=O)(=O)C3CC3)cncc2N4CC[C@@]5(C4=O)CCS(=O)(=O)c6c5cc(cc6)Cl</chem>
RUN:	RUN883
DDG (kcal/mol):	0.01
dDDG (kcal/mol):	0.17

ALP-POS-4483ae88-2_1



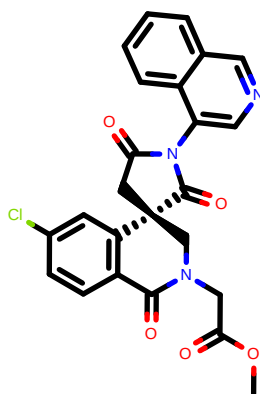
CID:	ALP-POS-4483ae88-2_1
SMILES:	<chem>CNC(=O)C[N+]([O-])C1C[C@H]2(CCN(C2=O)c3cncc4c3ccoc4)c5cc(ccc5S1(=O)=O)Cl</chem>
RUN:	RUN774
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.21

PET-UNK-94036022-10_1



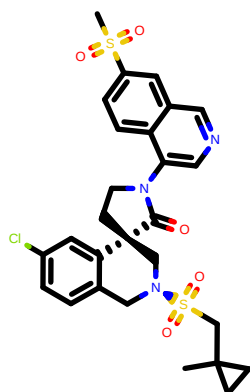
CID:	PET-UNK-94036022-10_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@H]4(C3=O)C[N+]([O-])C5c4cc(cc5Cl)S(=O)(=O)CC6(Cc6)Cl</chem>
RUN:	RUN846
DDG (kcal/mol):	0.04
dDDG (kcal/mol):	0.29

12_-111-3e02a1cd-2_1



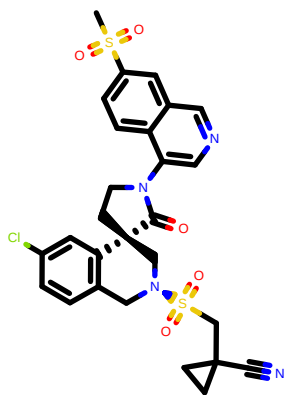
CID:	12_-111-3e02a1cd-2_1
SMILES:	<chem>COC(=O)CN1C[C@H]2(CC(=O)N(C2=O)c3cncc4c3ccoc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN794
DDG (kcal/mol):	0.05
dDDG (kcal/mol):	0.11

MAT-POS-853c0ffa-22_1



CID:	MAT-POS-853c0ffa-22_1
SMILES:	<chem>CC1(CC1)C5(=O)(=O)[N+]([O-])C2C3ccccc3[C@H]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)Cl</chem>
RUN:	RUN957
DDG (kcal/mol):	0.08
dDDG (kcal/mol):	0.34

MAT-POS-853c0ffa-15_1



CID:

MAT-POS-853c0ffa-15_1

SMILES:

CS(=O)(=O)c1ccc2c(c1)nccc2N3CC[C@H](C3=O)C[N@H](C5c4ccc(C)S(=O)(=O)CC6CC6)C#N

RUN:

RUN958

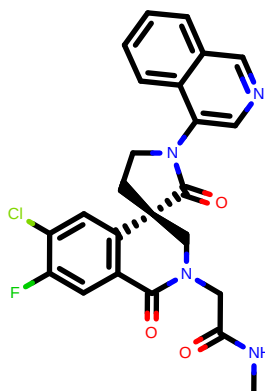
DDG (kcal/mol):

0.10

dDDG (kcal/mol):

0.48

VLA-UNK-61877630-5_1



CID:

VLA-UNK-61877630-5_1

SMILES:

CNC(=O)CN1C[C@H]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(c(c5C1=O)F)Cl

RUN:

RUN801

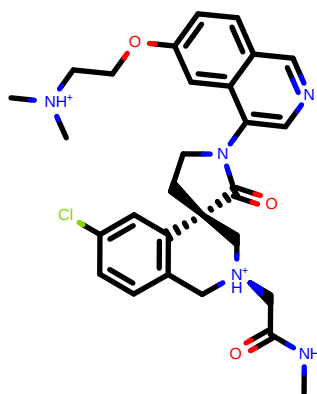
DDG (kcal/mol):

0.10

dDDG (kcal/mol):

0.12

EDJ-MED-b6c6ee2b-1_1



CID:

EDJ-MED-b6c6ee2b-1_1

SMILES:

CNC(=O)C[N@H]1Cc2ccc(cc2[C@H]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl

RUN:

RUN965

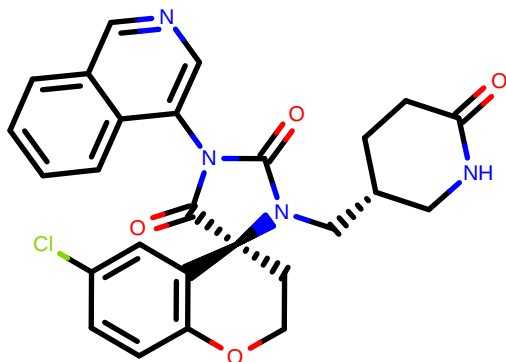
DDG (kcal/mol):

0.12

dDDG (kcal/mol):

0.41

VLA-UNK-f702bf1c-5_1



CID:

VLA-UNK-f702bf1c-5_1

SMILES:

c1ccc2c(c1)nccc2N3C(=O)[C@H](C@H4(CCOc5c4cc(cc5)C)N(C3=O)C[C@H]6CCCC(=O)NC6

RUN:

RUN844

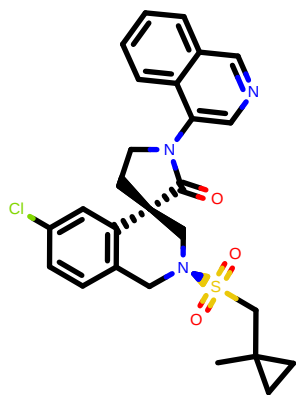
DDG (kcal/mol):

0.12

dDDG (kcal/mol):

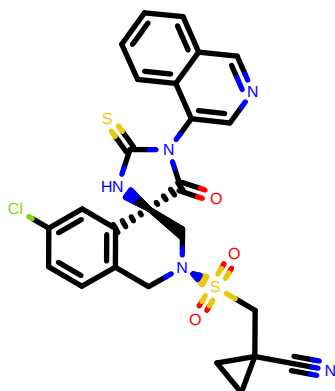
0.22

ALP-POS-ecbed2ba-3_1



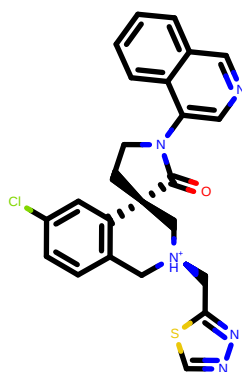
CID:	ALP-POS-ecbed2ba-3_1
SMILES:	<chem>CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5ccccc6)Cl</chem>
RUN:	RUN813
DDG (kcal/mol):	0.13
dDDG (kcal/mol):	0.25

MAT-POS-c2d406ed-3_1



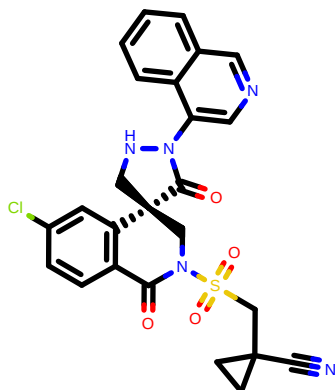
CID:	MAT-POS-c2d406ed-3_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@]4(C3=O)C[N@]5(Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N3=S</chem>
RUN:	RUN902
DDG (kcal/mol):	0.13
dDDG (kcal/mol):	0.26

PET-UNK-7e9559de-4_1



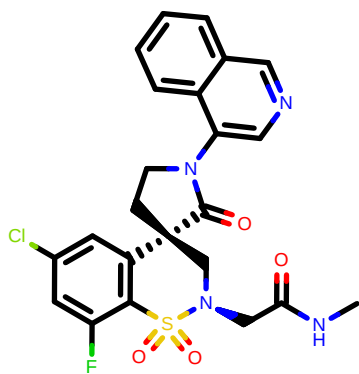
CID:	PET-UNK-7e9559de-4_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@]4(C3=O)C[N@H]5(Cc5c4cc(cc5)Cl)Cc6nncs6</chem>
RUN:	RUN789
DDG (kcal/mol):	0.14
dDDG (kcal/mol):	0.17

EDJ-MED-fed7ac0b-3_1



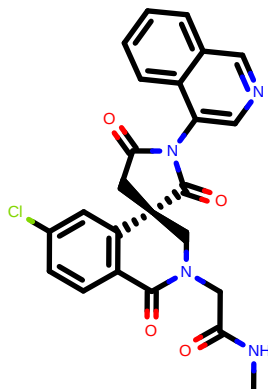
CID:	EDJ-MED-fed7ac0b-3_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@]4(CN3)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN900
DDG (kcal/mol):	0.15
dDDG (kcal/mol):	0.66

VLA-UNK-f2612802-3_1



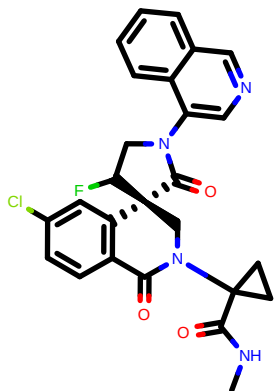
CID:	VLA-UNK-f2612802-3_1
SMILES:	<chem>CNC(=O)C[N@@]1C[C@]2(CC(N(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)F)Cl</chem>
RUN:	RUN841
DDG (kcal/mol):	0.18
dDDG (kcal/mol):	0.24

LUO-POS-868e8996-7_1



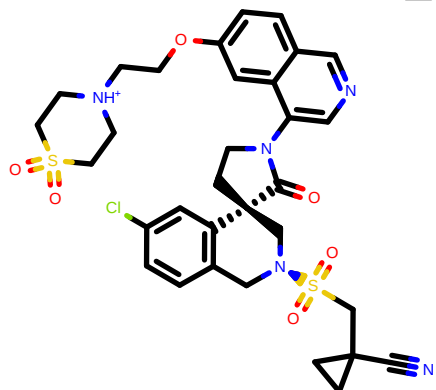
CID:	LUO-POS-868e8996-7_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN770
DDG (kcal/mol):	0.19
dDDG (kcal/mol):	0.11

EDJ-MED-fd8ed875-6_1



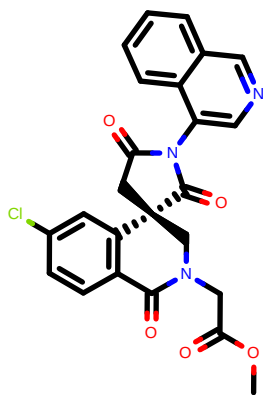
CID:	EDJ-MED-fd8ed875-6_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@@]3(c4cc(ccc4C2=O)Cl)C(=CN(C3=O)c5cncc6c5cccc6)F</chem>
RUN:	RUN872
DDG (kcal/mol):	0.22
dDDG (kcal/mol):	0.21

EDJ-MED-468565e0-3_1



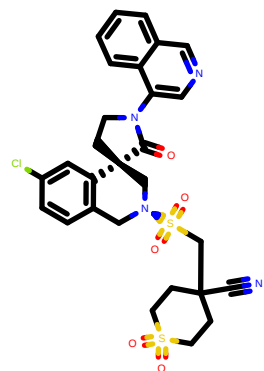
CID:	EDJ-MED-468565e0-3_1
SMILES:	<chem>c1cc2ncc(c2cc1OCCN3CCS(=O)(=O)CC3)N4C[C@@]5(c4cc(ccc4C2=O)Cl)N(C5=O)c6cncc7c6cccc7)C(=O)C7(C7)C#N</chem>
RUN:	RUN1019
DDG (kcal/mol):	0.23
dDDG (kcal/mol):	0.59

PET-UNK-77d5678a-3_1



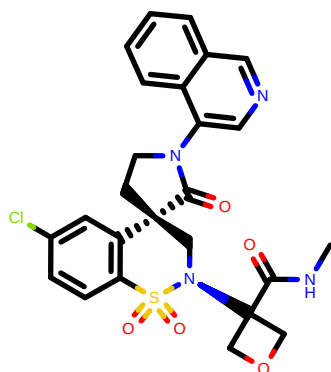
CID:	PET-UNK-77d5678a-3_1
SMILES:	<chem>COC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN804
DDG (kcal/mol):	0.26
dDDG (kcal/mol):	0.10

ALP-POS-ecbed2ba-2_1



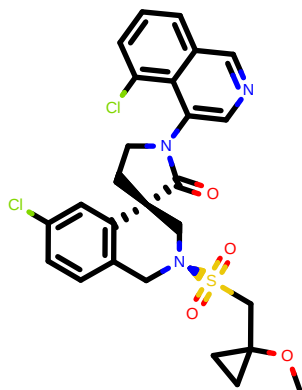
CID:	ALP-POS-ecbed2ba-2_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@]4(C3=O)C[N@@](C5c4cc(c5)C1S(=O)(=O)CC6(CCS(=O)(=O)CC6)C#N</chem>
RUN:	RUN982
DDG (kcal/mol):	0.28
dDDG (kcal/mol):	0.30

EDJ-MED-98c0a822-2_1



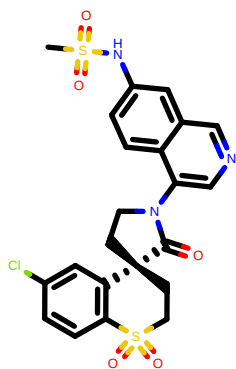
CID:	EDJ-MED-98c0a822-2_1
SMILES:	<chem>CNC(=O)C1(COC1)[N@@]2C[C@]3(CC(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl</chem>
RUN:	RUN924
DDG (kcal/mol):	0.29
dDDG (kcal/mol):	0.34

MAT-POS-853c0ffa-7_1



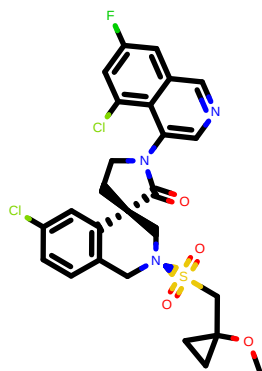
CID:	MAT-POS-853c0ffa-7_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc6)Cl)Cl</chem>
RUN:	RUN911
DDG (kcal/mol):	0.30
dDDG (kcal/mol):	0.38

EDJ-MED-edc5c6cb-1_1



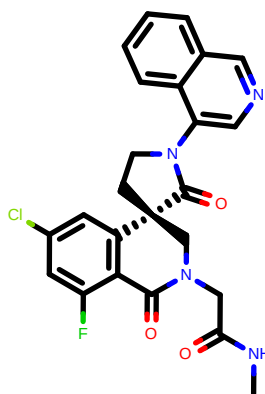
CID:	EDJ-MED-edc5c6cb-1_1
SMILES:	<chem>CS(=O)(=O)Nc1ccc2c(c1)ncnc2N3CC[C@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN792
DDG (kcal/mol):	0.32
dDDG (kcal/mol):	0.15

MAT-POS-853c0ffa-8_1



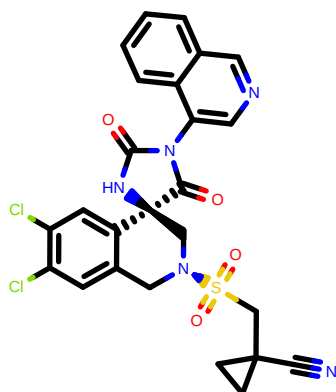
CID:	MAT-POS-853c0ffa-8_1
SMILES:	<chem>COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5ncnc6c5c(cc6)F)Cl</chem>
RUN:	RUN938
DDG (kcal/mol):	0.33
dDDG (kcal/mol):	0.32

VLA-UNK-61877630-4_1



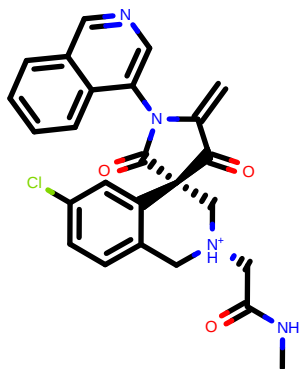
CID:	VLA-UNK-61877630-4_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cnc4c3cccc4)c5cc(cc(c5C1=O)F)Cl</chem>
RUN:	RUN787
DDG (kcal/mol):	0.34
dDDG (kcal/mol):	0.11

JOH-MSK-ccc6e4c0-1_1



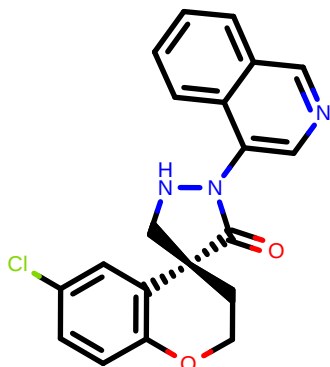
CID:	JOH-MSK-ccc6e4c0-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)[C@]4(C)[C@H](N3)Cc5c4cc(c(c5)Cl)C7S(=O)(=O)CC8(CO8)CN(NC3=O</chem>
RUN:	RUN956
DDG (kcal/mol):	0.34
dDDG (kcal/mol):	0.25

PET-UNK-94036022-14_1



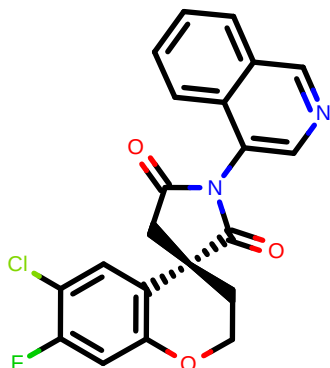
CID:	PET-UNK-94036022-14_1
SMILES:	<chem>CNC(=O)C[NH+]1C2ccc(cc2[C@]3(C1)C(=O)C(=O)N(C3=O)c4cncc5c4ccc5)Cl</chem>
RUN:	RUN829
DDG (kcal/mol):	0.35
dDDG (kcal/mol):	0.18

BRU-THA-73c97d88-1_1



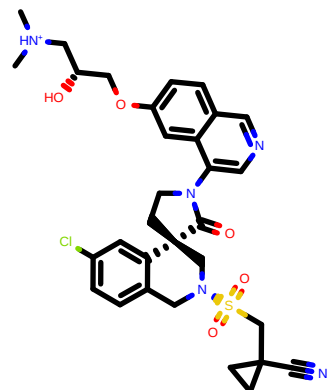
CID:	BRU-THA-73c97d88-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C=N3</chem>
RUN:	RUN684
DDG (kcal/mol):	0.36
dDDG (kcal/mol):	0.05

VLA-UNK-3a43cd95-3_1



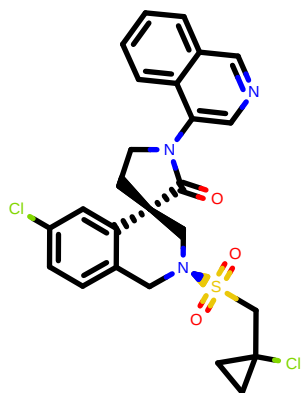
CID:	VLA-UNK-3a43cd95-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(c(c5)F)Cl</chem>
RUN:	RUN702
DDG (kcal/mol):	0.38
dDDG (kcal/mol):	0.08

EDJ-MED-ee81482e-3_2



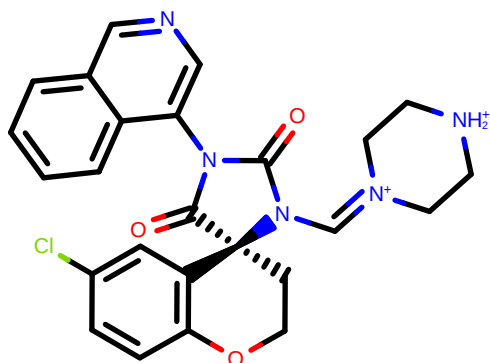
CID:	EDJ-MED-ee81482e-3_2
SMILES:	<chem>C[NH+](C)C[C@H](COc1ccc2ncc(c2c1)N3CC[C@H]4(C3=O)C[N@]5(Cc5c4cc(c5)C)S(=O)(=O)C6(C)C6)C#N</chem>
RUN:	RUN1017
DDG (kcal/mol):	0.38
dDDG (kcal/mol):	0.59

PET-UNK-94036022-3_1



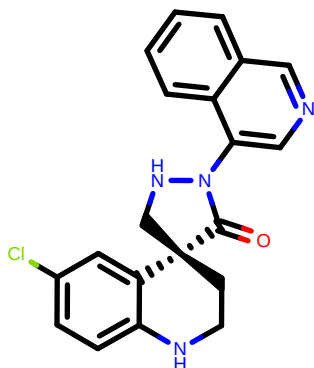
CID:	PET-UNK-94036022-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C[C@@]4(C3=O)C[N@@](C5c4cc(cc5)Cl)S(=O)(=O)CC6(Cc6)Cl</chem>
RUN:	RUN852
DDG (kcal/mol):	0.38
dDDG (kcal/mol):	0.25

VLA-UCB-34f3ed0c-15_1



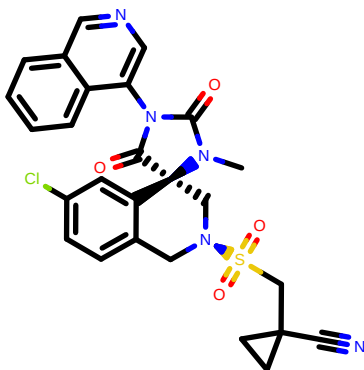
CID:	VLA-UCB-34f3ed0c-15_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CN6CC[NH2+][C6]</chem>
RUN:	RUN807
DDG (kcal/mol):	0.39
dDDG (kcal/mol):	0.35

BRU-THA-55eab31a-1_1



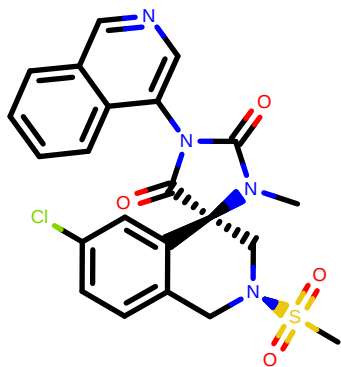
CID:	BRU-THA-55eab31a-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCNc5c4cc(cc5)Cl)C=N3</chem>
RUN:	RUN688
DDG (kcal/mol):	0.40
dDDG (kcal/mol):	0.08

MAT-POS-c2d406ed-2_1



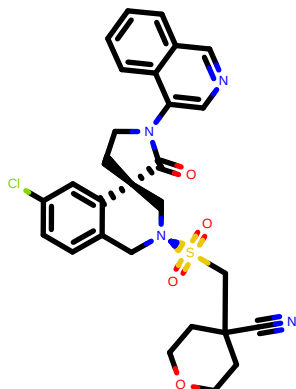
CID:	MAT-POS-c2d406ed-2_1
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@]12C[N@@](C3c2cc(cc3)Cl)S(=O)(=O)CC4(Cc4)N5cncdc5ccccc6</chem>
RUN:	RUN922
DDG (kcal/mol):	0.40
dDDG (kcal/mol):	0.28

MAT-POS-2e8b2191-8_1



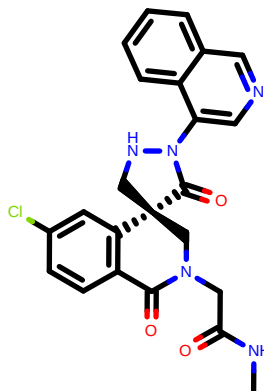
CID:	MAT-POS-2e8b2191-8_1
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@H]12C[N@@](C3c2cc(cc3C)S(=O)(=O)C4Cncc5c4cccc5</chem>
RUN:	RUN740
DDG (kcal/mol):	0.44
dDDG (kcal/mol):	0.12

ALP-POS-ecbed2ba-11_1



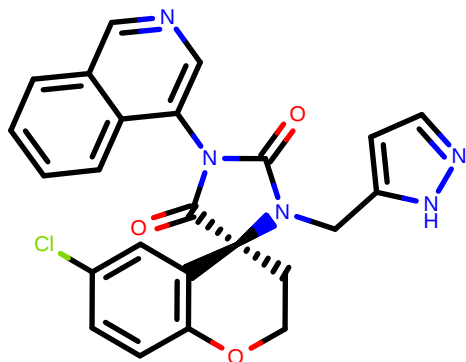
CID:	ALP-POS-ecbed2ba-11_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3CC[C@@H]4(C3=O)C[N@@](C5c4cc(cc5)C)S(=O)(=O)C6(CCCOC6)C#N</chem>
RUN:	RUN969
DDG (kcal/mol):	0.48
dDDG (kcal/mol):	0.68

EDJ-MED-fed7ac0b-4_1



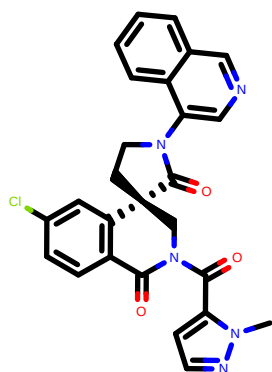
CID:	EDJ-MED-fed7ac0b-4_1
SMILES:	<chem>CNC(=O)CN1C[C@H]2(C=NN(C2=O)c3cnc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN741
DDG (kcal/mol):	0.49
dDDG (kcal/mol):	0.10

VLA-UNK-f702bf1c-2_1



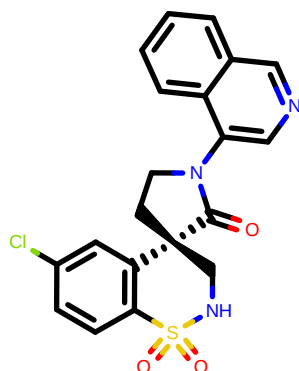
CID:	VLA-UNK-f702bf1c-2_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)[C@@H]4(CCOc5c4cc(cc5)C)N(C3=O)C6ccn[nH]6</chem>
RUN:	RUN762
DDG (kcal/mol):	0.49
dDDG (kcal/mol):	0.17

EDJ-MED-cc48ee33-2_1



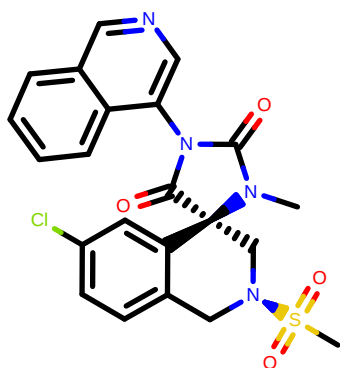
CID:	EDJ-MED-cc48ee33-2_1
SMILES:	<chem>Cn1c(cn1)C(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN894
DDG (kcal/mol):	0.54
dDDG (kcal/mol):	0.17

EDJ-MED-f9b78f78-4_1



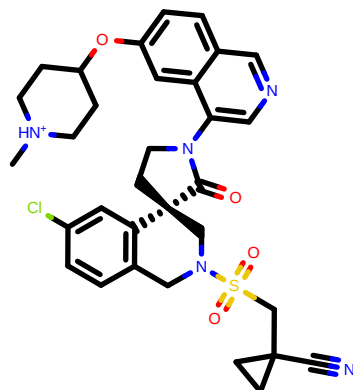
CID:	EDJ-MED-f9b78f78-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN722
DDG (kcal/mol):	0.54
dDDG (kcal/mol):	0.11

EDJ-MED-7587a9ee-1_1



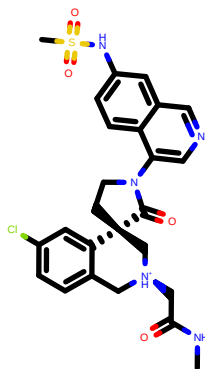
CID:	EDJ-MED-7587a9ee-1_1
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5</chem>
RUN:	RUN736
DDG (kcal/mol):	0.55
dDDG (kcal/mol):	0.10

LUO-POS-d1147590-1_1



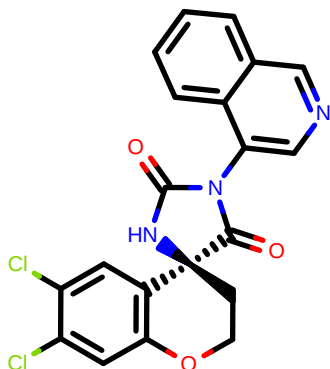
CID:	LUO-POS-d1147590-1_1
SMILES:	<chem>C[NH+]1CCCC(C1)Oc2cc3ncc(c3c2)N4CC[C@]5([C@@]4=O)C[N@@](Cc6c5cc(cc6)C)S(=O)(=O)C7C7C7C7N</chem>
RUN:	RUN1007
DDG (kcal/mol):	0.57
dDDG (kcal/mol):	0.80

MAT-POS-b4d6b7fc-7_1



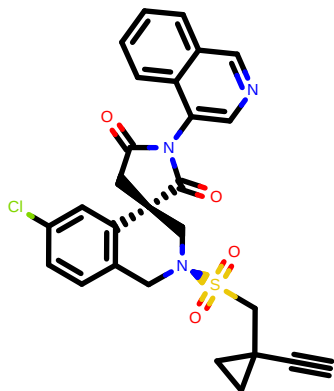
CID:	MAT-POS-b4d6b7fc-7_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cccc5c4ccc(cc5)NS(=O)(=O)C)Cl</chem>
RUN:	RUN908
DDG (kcal/mol):	0.61
dDDG (kcal/mol):	0.28

VLA-UNK-56836b69-2_1



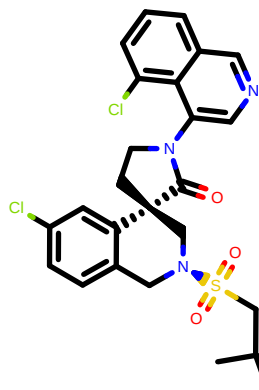
CID:	VLA-UNK-56836b69-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4ccc(c(c5)Cl)Cl)NC3=O</chem>
RUN:	RUN708
DDG (kcal/mol):	0.63
dDDG (kcal/mol):	0.08

PET-UNK-94036022-4_1



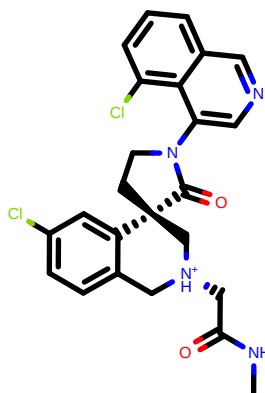
CID:	PET-UNK-94036022-4_1
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cccc6c5ccc6)Cl</chem>
RUN:	RUN916
DDG (kcal/mol):	0.67
dDDG (kcal/mol):	0.32

MAT-POS-853c0ffa-17_1



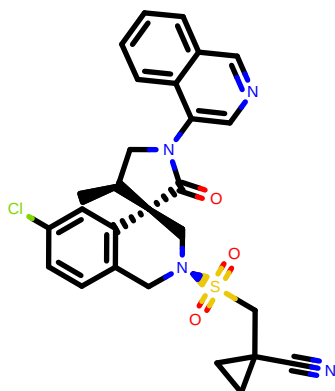
CID:	MAT-POS-853c0ffa-17_1
SMILES:	<chem>CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cccc6c5ccc6)Cl</chem>
RUN:	RUN856
DDG (kcal/mol):	0.67
dDDG (kcal/mol):	0.29

MAT-POS-b4d6b7fc-6_1



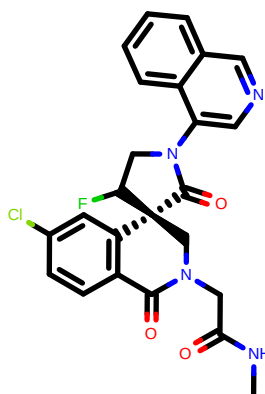
CID:	MAT-POS-b4d6b7fc-6_1
SMILES:	<chem>CNC(=O)C[N+]([H])1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4c(ccc5)C]Cl</chem>
RUN:	RUN756
DDG (kcal/mol):	0.70
dDDG (kcal/mol):	0.22

MAT-POS-50a80394-1_2



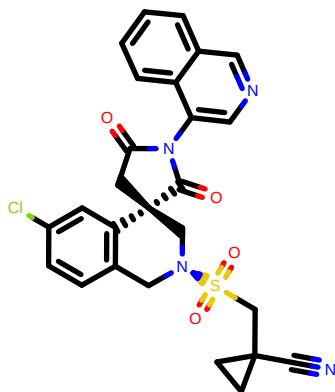
CID:	MAT-POS-50a80394-1_2
SMILES:	<chem>C[C@H]1CN(C(=O)[C@@]12C[N+]([H])C3Cc2cc(cc3)C)S(=O)(=O)CC4(Cc5[nH]c5nc6c5ccccc6</chem>
RUN:	RUN906
DDG (kcal/mol):	0.71
dDDG (kcal/mol):	0.50

EDJ-MED-fd8ed875-5_1



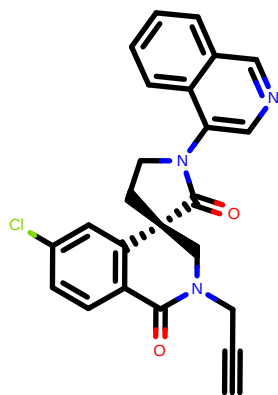
CID:	EDJ-MED-fd8ed875-5_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(c3cc(ccc3C1=O)Cl)C(=CN(C2=O)c4cnc5c4cccc5)F</chem>
RUN:	RUN810
DDG (kcal/mol):	0.75
dDDG (kcal/mol):	0.28

LUO-POS-868e8996-9_1



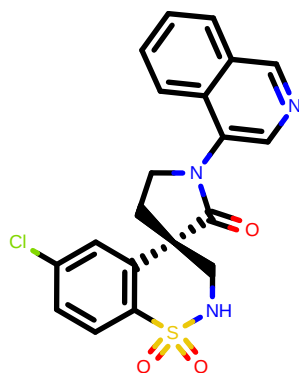
CID:	LUO-POS-868e8996-9_1
SMILES:	<chem>c1ccc2c(c1)nccc2N3C(=O)C[C@]4(C3=O)C[N+]([H])C5Cc4ccc5C)S(=O)(=O)CC6(Cc7[nH]c7nc8c7ccccc8</chem>
RUN:	RUN895
DDG (kcal/mol):	0.76
dDDG (kcal/mol):	0.42

PET-UNK-aa57768f-3_1



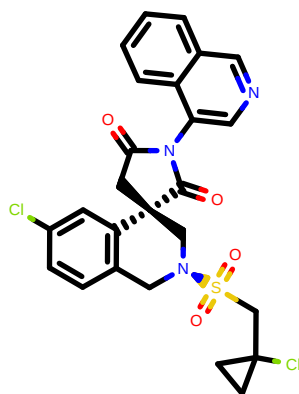
CID:	PET-UNK-aa57768f-3_1
SMILES:	<chem>C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN717
DDG (kcal/mol):	0.78
dDDG (kcal/mol):	0.14

ALP-POS-4483ae88-1_1



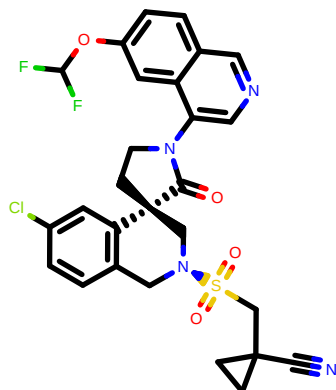
CID:	ALP-POS-4483ae88-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN713
DDG (kcal/mol):	0.81
dDDG (kcal/mol):	0.11

PET-UNK-94036022-5_1



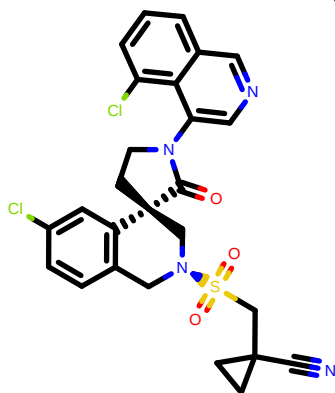
CID:	PET-UNK-94036022-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@]4(C3=O)C[N@@]5(Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(Cc6)Cl</chem>
RUN:	RUN897
DDG (kcal/mol):	0.83
dDDG (kcal/mol):	0.30

EDJ-MED-5cd3920d-1_1



CID:	EDJ-MED-5cd3920d-1_1
SMILES:	<chem>c1cc2ncc(c2cc1OC(F)F)N3CC[C@]4(C3=O)C[N@@]5(Cc5c4cc(cc5)C(F)(F)F)S(=O)(=O)CC6(Cc6)C#N</chem>
RUN:	RUN989
DDG (kcal/mol):	0.85
dDDG (kcal/mol):	0.40

MAT-POS-853c0ffa-5_1



CID:

MAT-POS-853c0ffa-5_1

SMILES:

c1cc2nccc(c2c(c1)C)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N

RUN:

RUN896

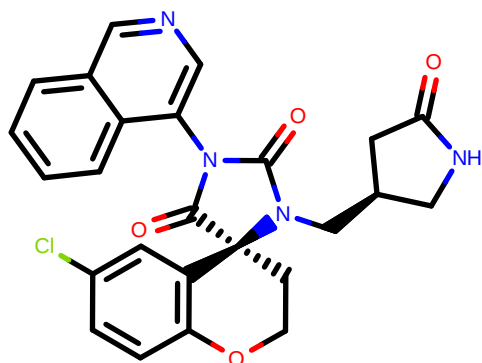
DDG (kcal/mol):

0.86

dDDG (kcal/mol):

0.46

VLA-UNK-f702bf1c-4_2



CID:

VLA-UNK-f702bf1c-4_2

SMILES:

c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C3=O)C(Cc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CC(=O)NCC6

RUN:

RUN823

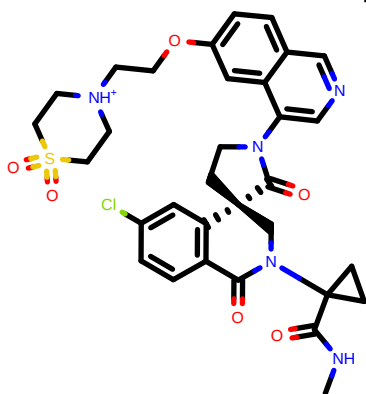
DDG (kcal/mol):

0.86

dDDG (kcal/mol):

0.25

EDJ-MED-dfa1d800-3_1



CID:

EDJ-MED-dfa1d800-3_1

SMILES:

ONC(=O)C1(CC1)N2C[C@]3(B(CCN(C3=O)c4cncc5c4cc(cc5)OCCN6CCS(=O)(=O)CC6)c7cc(c7)C2=O)Cl

RUN:

RUN1001

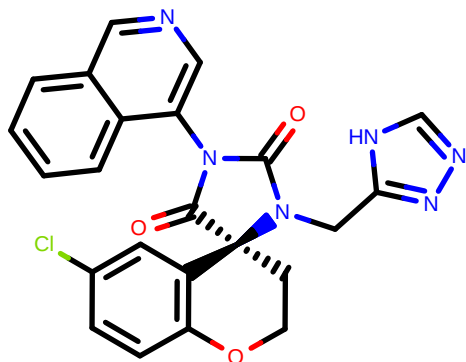
DDG (kcal/mol):

0.90

dDDG (kcal/mol):

0.33

VLA-UNK-f702bf1c-3_1



CID:

VLA-UNK-f702bf1c-3_1

SMILES:

c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C3=O)C(Cc5c4cc(cc5)Cl)N(C3=O)C6[nH]ncn6

RUN:

RUN767

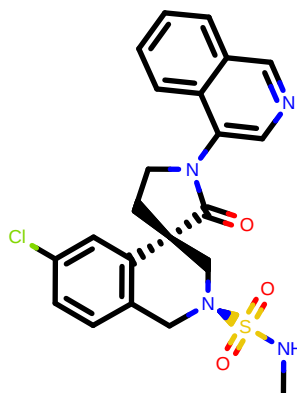
DDG (kcal/mol):

0.92

dDDG (kcal/mol):

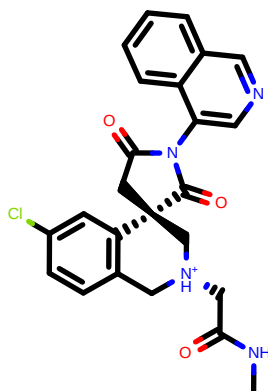
0.15

LUO-POS-ed2cfb03-2_1



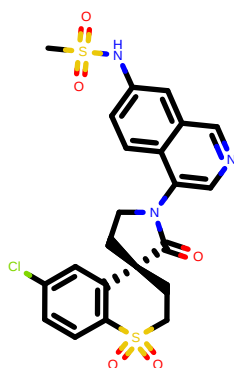
CID:	LUO-POS-ed2cfb03-2_1
SMILES:	<chem>CNS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN746
DDG (kcal/mol):	0.93
dDDG (kcal/mol):	0.37

JOH-MSK-1f2dff76-2_1



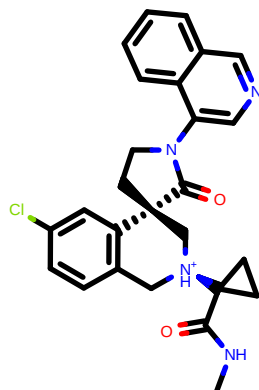
CID:	JOH-MSK-1f2dff76-2_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN759
DDG (kcal/mol):	0.94
dDDG (kcal/mol):	0.26

EDJ-MED-94fddcec-7_1



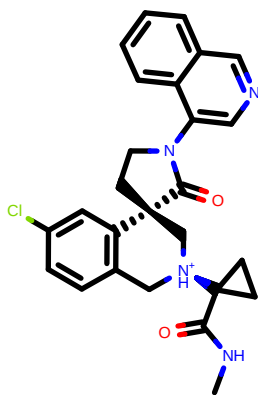
CID:	EDJ-MED-94fddcec-7_1
SMILES:	<chem>CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@]4(C3=O)CCS(=O)(=O)c5ccc(cc5)Cl</chem>
RUN:	RUN778
DDG (kcal/mol):	0.96
dDDG (kcal/mol):	0.18

MAT-POS-69786b79-1_1



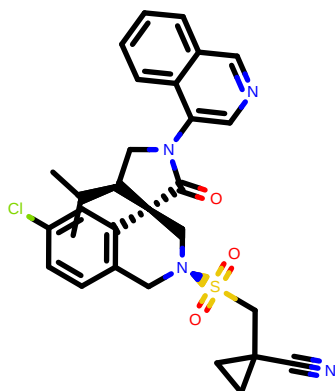
CID:	MAT-POS-69786b79-1_1
SMILES:	<chem>CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl</chem>
RUN:	RUN827
DDG (kcal/mol):	0.97
dDDG (kcal/mol):	0.17

MAT-POS-576f7758-1_1



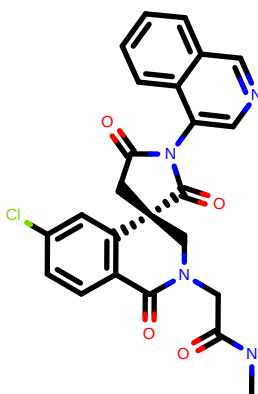
CID:	MAT-POS-576f7758-1_1
SMILES:	<chem>CNC(=O)C1(CC1)[N@H+]2C3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5ccccc6)Cl</chem>
RUN:	RUN831
DDG (kcal/mol):	0.97
dDDG (kcal/mol):	0.17

MAT-POS-50a80394-3_2



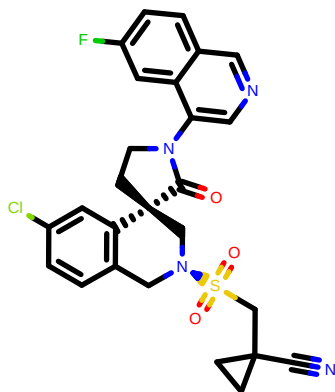
CID:	MAT-POS-50a80394-3_2
SMILES:	<chem>Cc1c(C)[C@H]1CN(C(=O)[C@]12C[N+]4(C)[C@H]5Cnc6c5ccccc6)S(=O)(=O)CC4(C4)C1N4c5cnc6c5ccccc6</chem>
RUN:	RUN959
DDG (kcal/mol):	0.98
dDDG (kcal/mol):	0.46

LUO-POS-868e8996-8_1



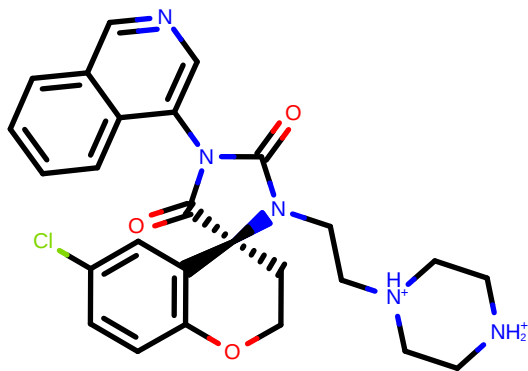
CID:	LUO-POS-868e8996-8_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cnc4c3ccccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN775
DDG (kcal/mol):	0.99
dDDG (kcal/mol):	0.11

MAT-POS-853c0ffa-13_1



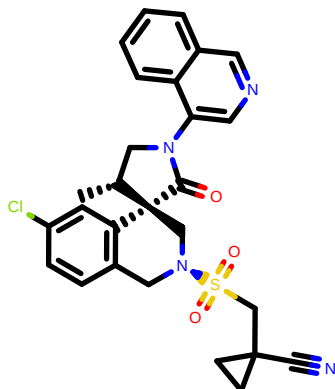
CID:	MAT-POS-853c0ffa-13_1
SMILES:	<chem>c1cc2cnc3c(c2cc1F)N3CC[C@@]4(C3=O)C[N+]5(Cc6c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C1N</chem>
RUN:	RUN901
DDG (kcal/mol):	1.00
dDDG (kcal/mol):	0.37

VLA-UNK-f702bf1c-7_1



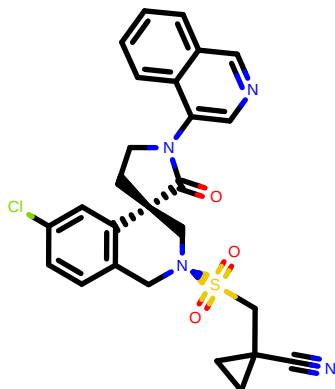
CID:	VLA-UNK-f702bf1c-7_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H]4(CCOc5c4cc(cc5)C)N(C3=O)CCN6CC[NH2+][CC6]</chem>
RUN:	RUN849
DDG (kcal/mol):	1.01
dDDG (kcal/mol):	0.24

MAT-POS-50a80394-1_1



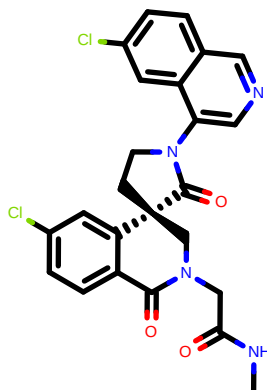
CID:	MAT-POS-50a80394-1_1
SMILES:	<chem>C[C@@H]1CN(C(=O)[C@@H]2C[C@H]3[C@@H](C2c2cc(cc3)C)S(=O)(=O)CC4(C#N)C5CNC6S5ccccc6</chem>
RUN:	RUN915
DDG (kcal/mol):	1.02
dDDG (kcal/mol):	0.45

MIK-ENA-5d9157e9-1_1



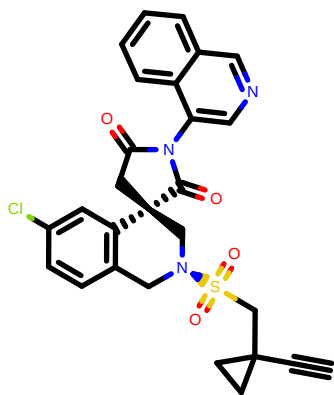
CID:	MIK-ENA-5d9157e9-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@H]4(C3=O)C[N@@H]5(Cc5c4cc(cc5)C)S(=O)(=O)CC6(C#N)C#N</chem>
RUN:	RUN875
DDG (kcal/mol):	1.02
dDDG (kcal/mol):	0.44

EDG-MED-b1ef7fe3-1_1



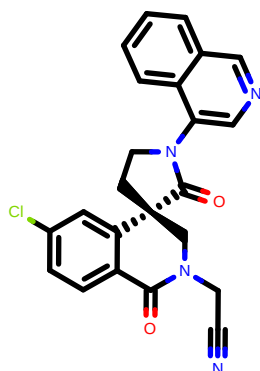
CID:	EDG-MED-b1ef7fe3-1_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5ccc(ccc5C1=O)Cl</chem>
RUN:	RUN765
DDG (kcal/mol):	1.07
dDDG (kcal/mol):	0.23

PET-UNK-94036022-11_1



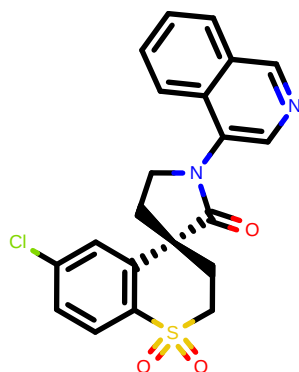
CID:	PET-UNK-94036022-11_1
SMILES:	<chem>C#CC1(CC1)CS(=O)(=O)N@@]2Cc3ccc(cc3[C@@]4(C2)CC(=O)N(C4=O)c5cccc6c5cccc6)Cl</chem>
RUN:	RUN899
DDG (kcal/mol):	1.08
dDDG (kcal/mol):	0.32

PET-UNK-aa57768f-8_1



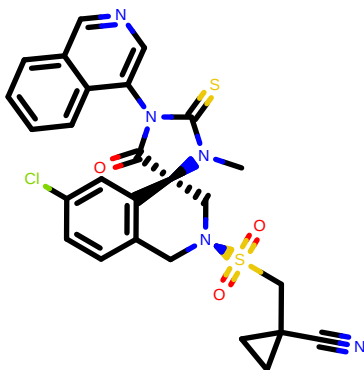
CID:	PET-UNK-aa57768f-8_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N</chem>
RUN:	RUN721
DDG (kcal/mol):	1.09
dDDG (kcal/mol):	0.15

EDJ-MED-94fddcec-4_1



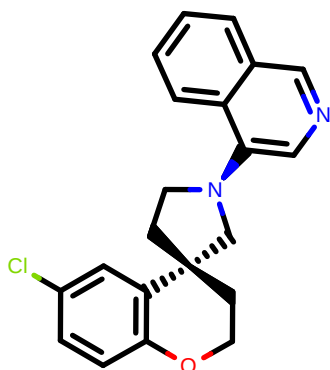
CID:	EDJ-MED-94fddcec-4_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN723
DDG (kcal/mol):	1.12
dDDG (kcal/mol):	0.12

MAT-POS-c2d406ed-4_1



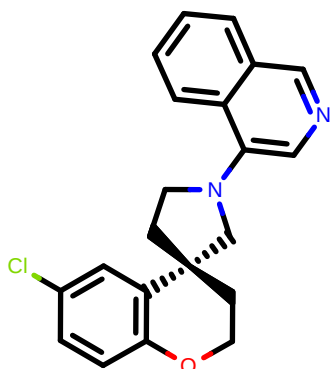
CID:	MAT-POS-c2d406ed-4_1
SMILES:	<chem>CN1C(=S)N(C(=O)[C@@]1)2C#N@@]3Cc4ccc(cc4)C(=O)N(C(=O)CC4(C#N)c5cccc6c5cccc6)Cl</chem>
RUN:	RUN933
DDG (kcal/mol):	1.16
dDDG (kcal/mol):	0.29

MAT-POS-983b399a-2_1



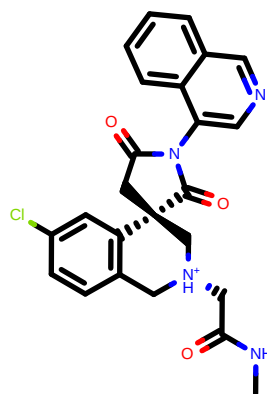
CID:	MAT-POS-983b399a-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN680
DDG (kcal/mol):	1.18
dDDG (kcal/mol):	0.08

EDJ-MED-159244ea-2_1



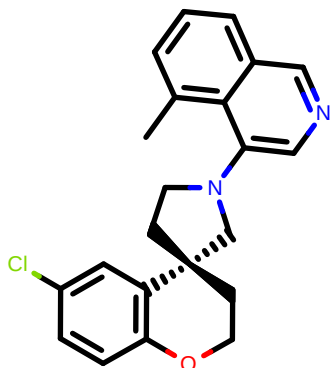
CID:	EDJ-MED-159244ea-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN683
DDG (kcal/mol):	1.21
dDDG (kcal/mol):	0.08

MAT-POS-1bed62cf-3_1



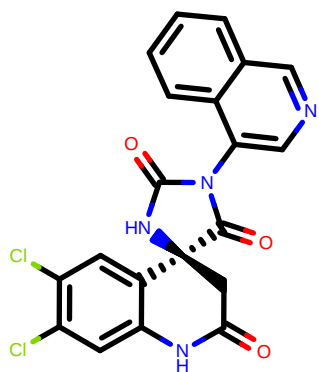
CID:	MAT-POS-1bed62cf-3_1
SMILES:	<chem>CNC(=O)C[N+]([H])1Cc2ccc(cc2[C@@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN749
DDG (kcal/mol):	1.22
dDDG (kcal/mol):	0.25

EDJ-MED-a6bab6fb-1_1



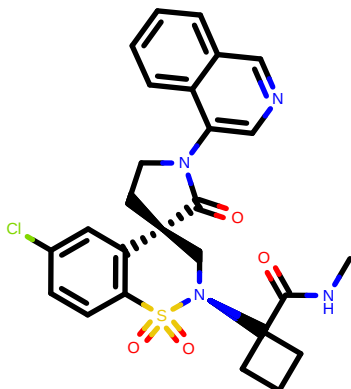
CID:	EDJ-MED-a6bab6fb-1_1
SMILES:	<chem>Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN685
DDG (kcal/mol):	1.28
dDDG (kcal/mol):	0.08

VLA-UNK-56836b69-5_1



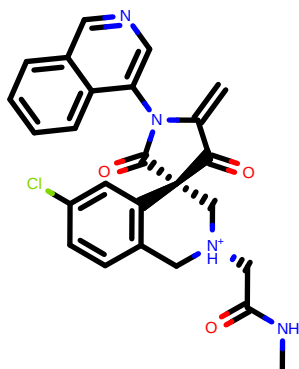
CID:	VLA-UNK-56836b69-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CC(=O)Nc5c4cc(c(c5)Cl)Cl)NC3=O</chem>
RUN:	RUN727
DDG (kcal/mol):	1.30
dDDG (kcal/mol):	0.11

EDJ-MED-98c0a822-1_1



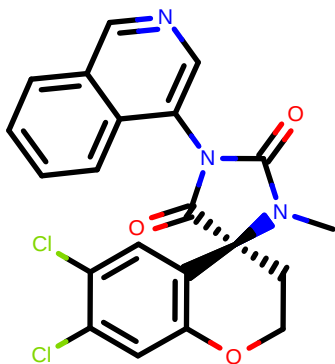
CID:	EDJ-MED-98c0a822-1_1
SMILES:	<chem>CNC(=O)C1(CCC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl</chem>
RUN:	RUN928
DDG (kcal/mol):	1.31
dDDG (kcal/mol):	0.56

PET-UNK-94036022-7_1



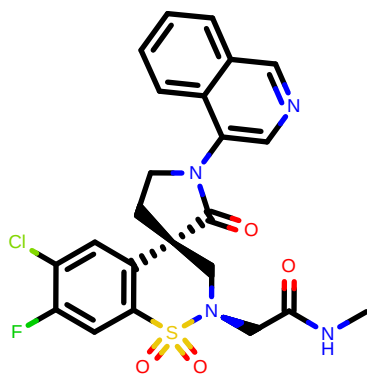
CID:	PET-UNK-94036022-7_1
SMILES:	<chem>CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=O)N(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN803
DDG (kcal/mol):	1.33
dDDG (kcal/mol):	0.27

VLA-UNK-56836b69-3_1



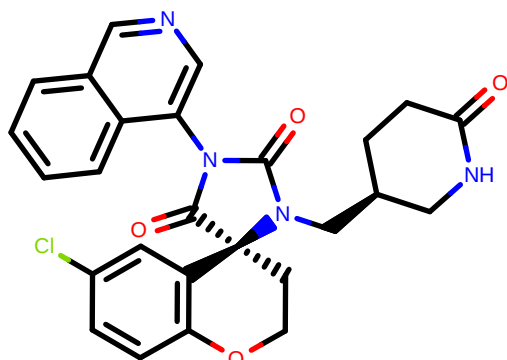
CID:	VLA-UNK-56836b69-3_1
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@]12CCOCc3c2cc(c(c3)Cl)Cl)c4cncc5c4cccc5</chem>
RUN:	RUN704
DDG (kcal/mol):	1.33
dDDG (kcal/mol):	0.07

VLA-UNK-f2612802-2_1



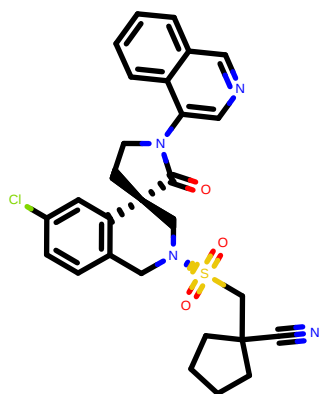
CID:	VLA-UNK-f2612802-2_1
SMILES:	<chem>CNC(=O)C[N+]([O-])C1C[C@H]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(c(cc5S1(=O)=O)F)Cl</chem>
RUN:	RUN854
DDG (kcal/mol):	1.34
dDDG (kcal/mol):	0.23

VLA-UNK-f702bf1c-5_2



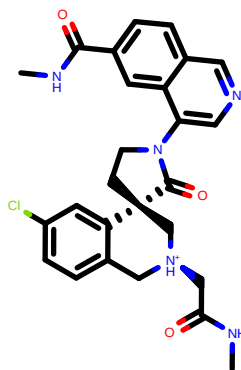
CID:	VLA-UNK-f702bf1c-5_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CCC(=O)NC6</chem>
RUN:	RUN848
DDG (kcal/mol):	1.41
dDDG (kcal/mol):	0.19

ALP-POS-ecbed2ba-15_1



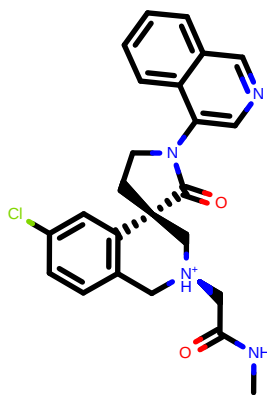
CID:	ALP-POS-ecbed2ba-15_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@H]4(C3=O)C[N+]([O-])C5c4cc(cc5)Cl)S(=O)(=O)CC6(CCCC6)C#N</chem>
RUN:	RUN939
DDG (kcal/mol):	1.42
dDDG (kcal/mol):	0.40

MAT-POS-38eb6498-5_1



CID:	MAT-POS-38eb6498-5_1
SMILES:	<chem>CNC(=O)C[N+]([O-])C1C2ccc(cc2[C@@H]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)C(=O)NC)Cl</chem>
RUN:	RUN867
DDG (kcal/mol):	1.42
dDDG (kcal/mol):	0.20

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:

RUN769

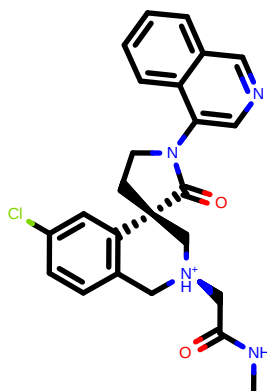
DDG (kcal/mol):

1.45

dDDG (kcal/mol):

0.19

LUO-POS-868e8996-12_1



CID:

LUO-POS-868e8996-12_1

SMILES:

CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl

RUN:

RUN757

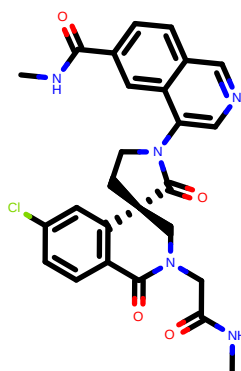
DDG (kcal/mol):

1.46

dDDG (kcal/mol):

0.19

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:

RUN893

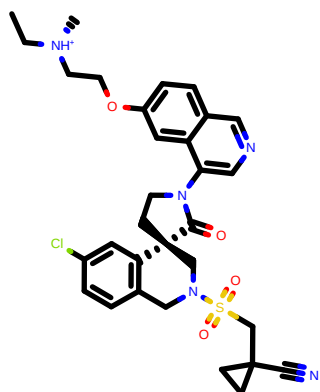
DDG (kcal/mol):

1.46

dDDG (kcal/mol):

0.21

MAT-POS-40ad851a-2_1



CID:

MAT-POS-40ad851a-2_1

SMILES:

CC[N@H+]([C]C)CCOc1ccc2nccc(c2c1)N3CC[C@]4([C]3=O)C[N@H]5C6Cc4cc(c5)C(S(=O)(=O)CC6)CC6c7n

RUN:

RUN998

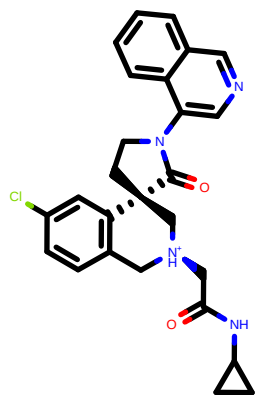
DDG (kcal/mol):

1.46

dDDG (kcal/mol):

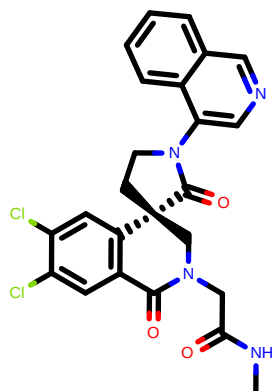
0.77

MAT-POS-69786b79-2_1



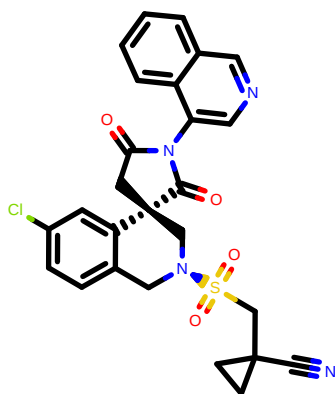
CID:	MAT-POS-69786b79-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H]1(Cc5c4cc(cc5)Cl)CC(=O)NC6CC6</chem>
RUN:	RUN808
DDG (kcal/mol):	1.48
dDDG (kcal/mol):	0.23

ALP-POS-afe0272e-2_1



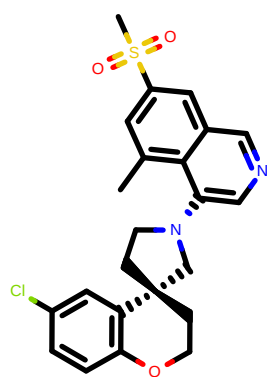
CID:	ALP-POS-afe0272e-2_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccccc4)c5cc(c(cc5C1=O)Cl)Cl</chem>
RUN:	RUN798
DDG (kcal/mol):	1.48
dDDG (kcal/mol):	0.16

MAT-POS-1bed62cf-1_1



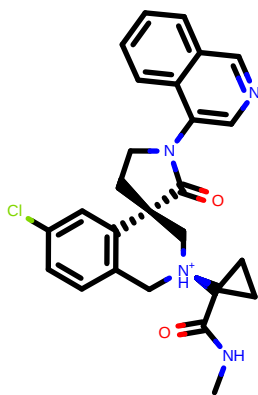
CID:	MAT-POS-1bed62cf-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@]4(C3=O)C[N@]5(Cc6c4cc(cc6)S(=O)(=O)CC7C#N)CC7</chem>
RUN:	RUN877
DDG (kcal/mol):	1.49
dDDG (kcal/mol):	0.41

EDJ-MED-d7486dd1-1_1



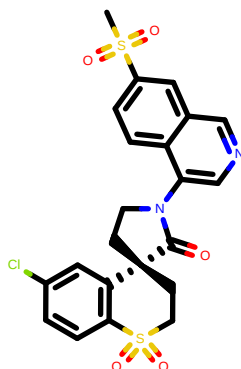
CID:	EDJ-MED-d7486dd1-1_1
SMILES:	<chem>Cc1cc(cc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl)S(=O)(=O)C</chem>
RUN:	RUN718
DDG (kcal/mol):	1.49
dDDG (kcal/mol):	0.14

ALP-POS-ecbed2ba-7_1



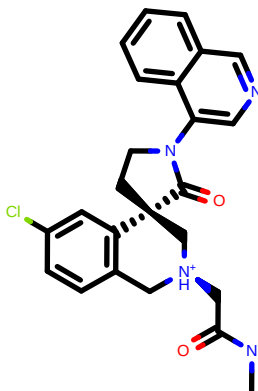
CID:	ALP-POS-ecbed2ba-7_1
SMILES:	<chem>CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5ccccc6)Cl</chem>
RUN:	RUN796
DDG (kcal/mol):	1.49
dDDG (kcal/mol):	0.23

EDJ-MED-94fddcec-5_1



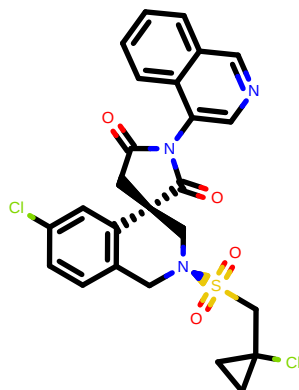
CID:	EDJ-MED-94fddcec-5_1
SMILES:	<chem>CS(=O)(=O)c1ccc2c(c1)cnc2N3CC[C@]4(C3=O)CCS(=O)(=O)c5c4cc(c5)Cl</chem>
RUN:	RUN742
DDG (kcal/mol):	1.53
dDDG (kcal/mol):	0.16

MAT-POS-c7726e07-5_1



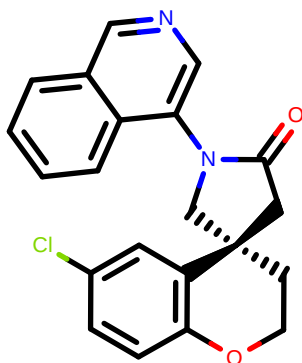
CID:	MAT-POS-c7726e07-5_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4ccccc5)Cl</chem>
RUN:	RUN747
DDG (kcal/mol):	1.54
dDDG (kcal/mol):	0.20

PET-UNK-94036022-12_1



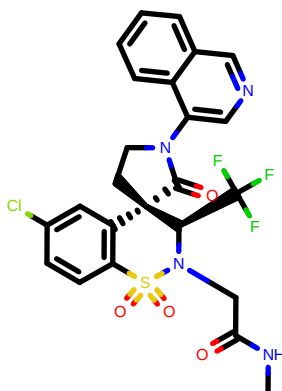
CID:	PET-UNK-94036022-12_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)C[C@]4(C3=O)C[N@]5(Cc6c4cc(c5)Cl)S(=O)(=O)CC6(Cc6)Cl</chem>
RUN:	RUN882
DDG (kcal/mol):	1.60
dDDG (kcal/mol):	0.31

MAT-POS-983b399a-3_1



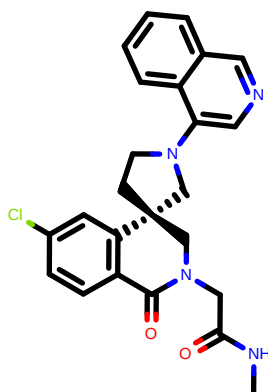
CID:	MAT-POS-983b399a-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O</chem>
RUN:	RUN686
DDG (kcal/mol):	1.60
dDDG (kcal/mol):	0.04

VLA-UNK-f2612802-1_1



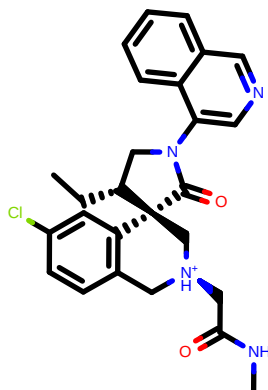
CID:	VLA-UNK-f2612802-1_1
SMILES:	<chem>CNC(=O)C[N@@]1[C@@H]([C@@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1=O)=O)C(F)F)F</chem>
RUN:	RUN948
DDG (kcal/mol):	1.61
dDDG (kcal/mol):	0.42

EDJ-MED-8bb691af-7_1



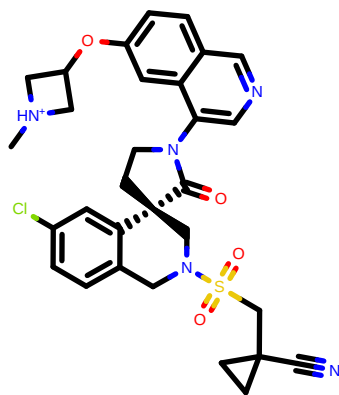
CID:	EDJ-MED-8bb691af-7_1
SMILES:	<chem>CNC(=O)CN1C[C@@]2(CCN(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN731
DDG (kcal/mol):	1.63
dDDG (kcal/mol):	0.13

MAT-POS-50a80394-5_1



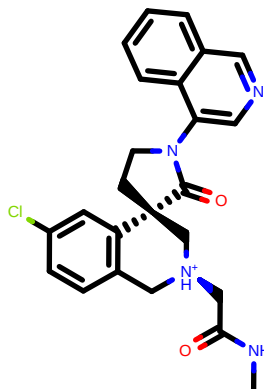
CID:	MAT-POS-50a80394-5_1
SMILES:	<chem>CC[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5</chem>
RUN:	RUN815
DDG (kcal/mol):	1.69
dDDG (kcal/mol):	0.21

EDJ-MED-ee81482e-2_1



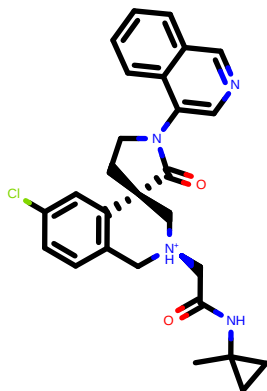
CID:	EDJ-MED-ee81482e-2_1
SMILES:	<chem>C[NH+]1CC(C1)Oc2ccc3nccc(c3c2)N4CC[C@]5(C4=O)C[N@](Cc6c5ccc(c6)C)S(=O)(=O)CC7(Cc7)C#N</chem>
RUN:	RUN996
DDG (kcal/mol):	1.69
dDDG (kcal/mol):	0.50

EDJ-MED-8bb691af-4_1



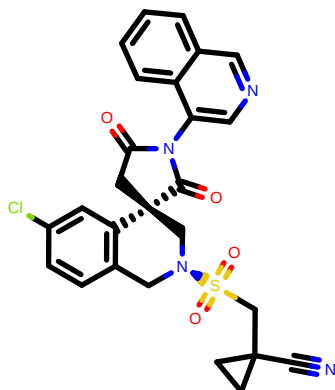
CID:	EDJ-MED-8bb691af-4_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN745
DDG (kcal/mol):	1.69
dDDG (kcal/mol):	0.17

MAT-POS-69786b79-3_1



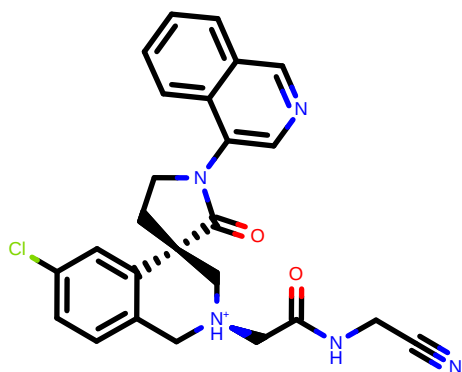
CID:	MAT-POS-69786b79-3_1
SMILES:	<chem>CC1(CC1)NC(=O)C[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cnc6c5cccc6)Cl</chem>
RUN:	RUN863
DDG (kcal/mol):	1.70
dDDG (kcal/mol):	0.25

LUO-POS-868e8996-10_1



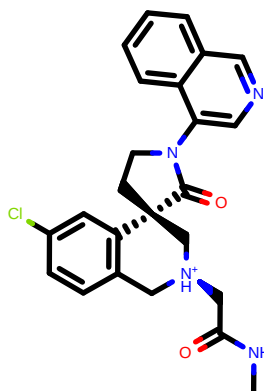
CID:	LUO-POS-868e8996-10_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)C[C@]4(C3=O)C[N@](Cc5c4cc(c5)Cl)S(=O)(=O)CC6(Cc6)C#N</chem>
RUN:	RUN886
DDG (kcal/mol):	1.82
dDDG (kcal/mol):	0.39

ALP-POS-ecbed2ba-14_1



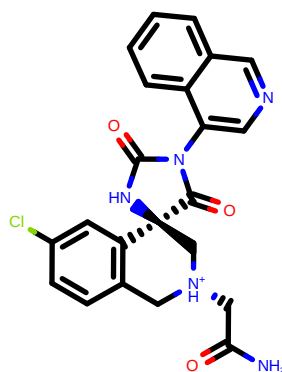
CID:	ALP-POS-ecbed2ba-14_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC#N</chem>
RUN:	RUN776
DDG (kcal/mol):	1.84
dDDG (kcal/mol):	0.19

LUO-POS-868e8996-11_1



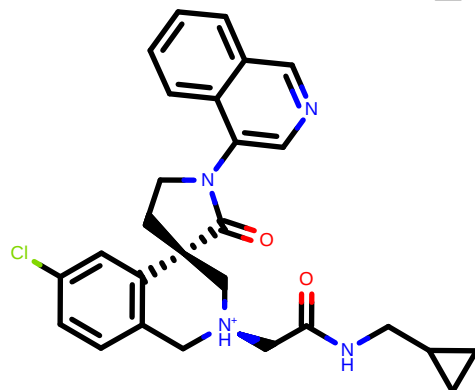
CID:	LUO-POS-868e8996-11_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN751
DDG (kcal/mol):	1.85
dDDG (kcal/mol):	0.20

VLA-MRT-a639d434-2_1



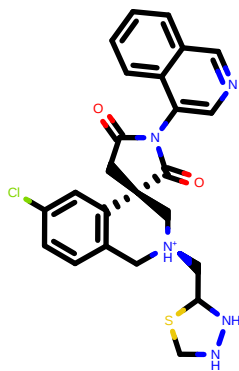
CID:	VLA-MRT-a639d434-2_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@@]4(C)[C]N@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O</chem>
RUN:	RUN760
DDG (kcal/mol):	1.85
dDDG (kcal/mol):	0.23

ALP-POS-ecbed2ba-12_1



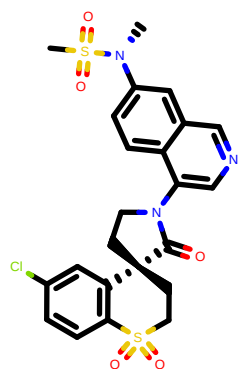
CID:	ALP-POS-ecbed2ba-12_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC6CC6</chem>
RUN:	RUN857
DDG (kcal/mol):	1.90
dDDG (kcal/mol):	0.21

PET-UNK-77d5678a-4_1



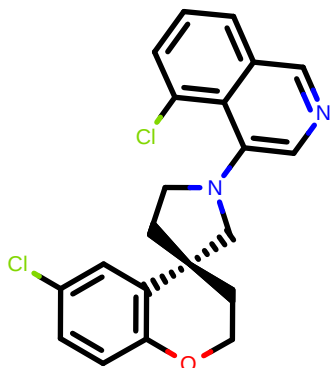
CID:	PET-UNK-77d5678a-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@H+]([C@H]4Cc5cc(cc5)Cl)Cc6nncs6</chem>
RUN:	RUN819
DDG (kcal/mol):	1.91
dDDG (kcal/mol):	0.18

EDJ-MED-94fddcec-6_1



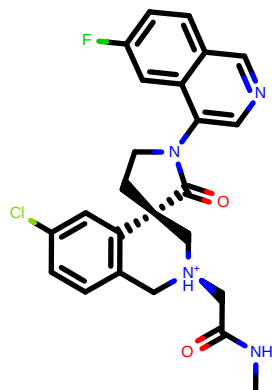
CID:	EDJ-MED-94fddcec-6_1
SMILES:	<chem>C[N@]([c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5cc(cc5)Cl)S(=O)(=O)C</chem>
RUN:	RUN821
DDG (kcal/mol):	1.93
dDDG (kcal/mol):	0.20

EDJ-MED-e78d5f1a-1_1



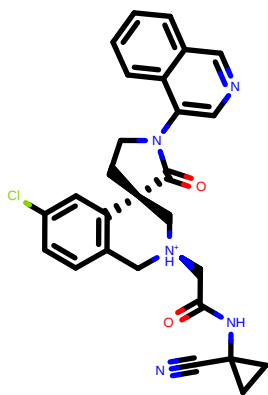
CID:	EDJ-MED-e78d5f1a-1_1
SMILES:	<chem>c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN687
DDG (kcal/mol):	1.95
dDDG (kcal/mol):	0.12

LUO-POS-b4dec3be-1_1



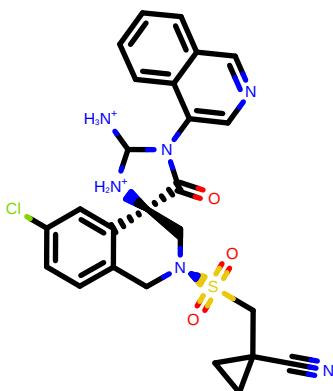
CID:	LUO-POS-b4dec3be-1_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl</chem>
RUN:	RUN777
DDG (kcal/mol):	1.97
dDDG (kcal/mol):	0.19

MAT-POS-69786b79-4_1



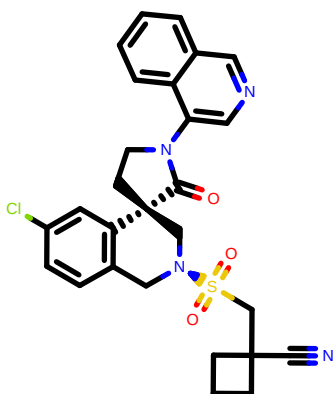
CID:	MAT-POS-69786b79-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C(=O)C[NH+](Cc5c4cc(cc5)Cl)CC(=O)NC6(CC6)C#N</chem>
RUN:	RUN861
DDG (kcal/mol):	1.99
dDDG (kcal/mol):	0.28

LUO-POS-eaf50f21-1_1



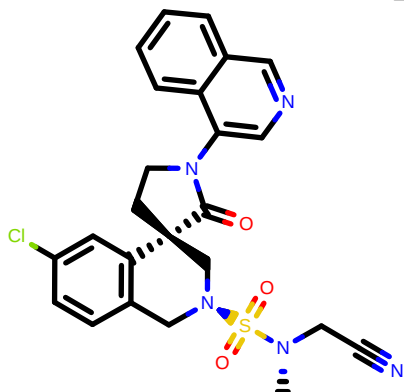
CID:	LUO-POS-eaf50f21-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@H](C[NH+])Cc4c4cc(cc4)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN937
DDG (kcal/mol):	2.03
dDDG (kcal/mol):	0.40

ALP-POS-ecbed2ba-8_1



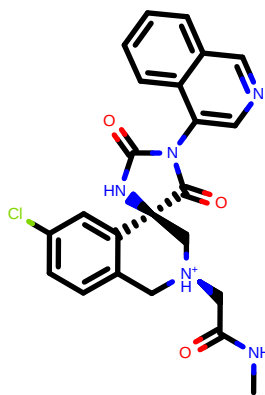
CID:	ALP-POS-ecbed2ba-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C(=O)C[NH+](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCC6)C#N</chem>
RUN:	RUN898
DDG (kcal/mol):	2.03
dDDG (kcal/mol):	0.58

ALP-POS-ecbed2ba-17_1



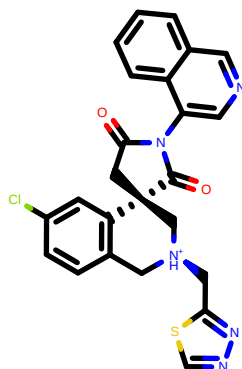
CID:	ALP-POS-ecbed2ba-17_1
SMILES:	<chem>C[NH+](CC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4ccc5c4ccc5)Cl</chem>
RUN:	RUN818
DDG (kcal/mol):	2.07
dDDG (kcal/mol):	0.69

VLA-MRT-a639d434-1_1



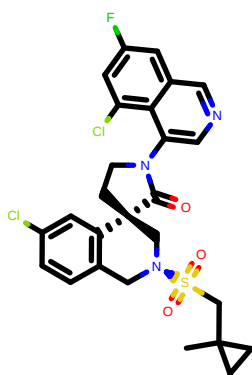
CID:	VLA-MRT-a639d434-1_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@@]3(C1)C(=O)N(C(=O)N3)c4cnc5c4cccc5)Cl</chem>
RUN:	RUN733
DDG (kcal/mol):	2.07
dDDG (kcal/mol):	0.18

PET-UNK-77d5678a-1_1



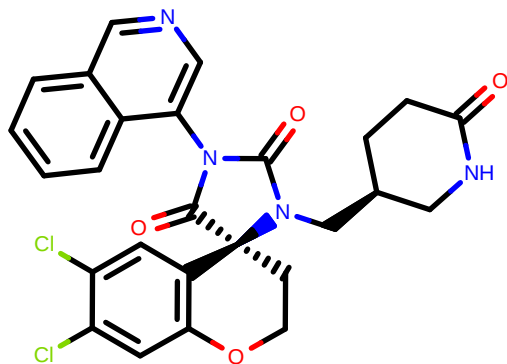
CID:	PET-UNK-77d5678a-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)C[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6</chem>
RUN:	RUN825
DDG (kcal/mol):	2.11
dDDG (kcal/mol):	0.18

MAT-POS-853c0ffa-18_1



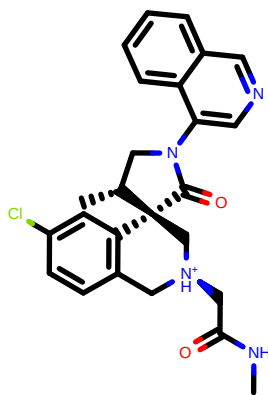
CID:	MAT-POS-853c0ffa-18_1
SMILES:	<chem>CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@@]4(C2)CCN(C4=O)c5cnc6c5c(cc(c6)F)Cl</chem>
RUN:	RUN889
DDG (kcal/mol):	2.19
dDDG (kcal/mol):	0.31

JOH-MSK-b735e33c-1_2



CID:	JOH-MSK-b735e33c-1_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)Cl)N(C3=O)C[C@H]6CCC(=O)NC6</chem>
RUN:	RUN920
DDG (kcal/mol):	2.19
dDDG (kcal/mol):	0.21

MAT-POS-50a80394-4_1



CID: MAT-POS-50a80394-4_1

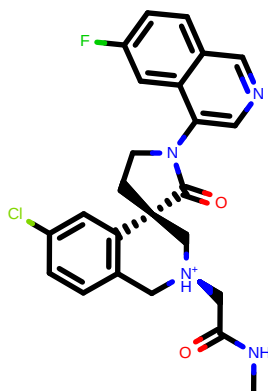
SMILES: C[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)Nc4cnc5c4cccc5

RUN: RUN780

DDG (kcal/mol): 2.23

dDDG (kcal/mol): 0.23

MAT-POS-b4d6b7fc-5_1



CID: MAT-POS-b4d6b7fc-5_1

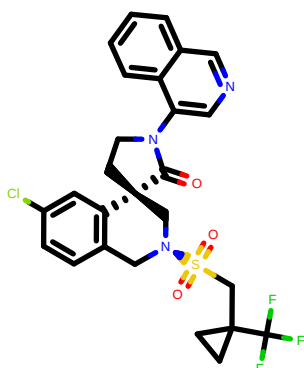
SMILES: CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)CCN(C3=O)c4cnc5c4cc(cc5)F)Cl

RUN: RUN754

DDG (kcal/mol): 2.29

dDDG (kcal/mol): 0.19

EDJ-MED-5cd3920d-6_1



CID: EDJ-MED-5cd3920d-6_1

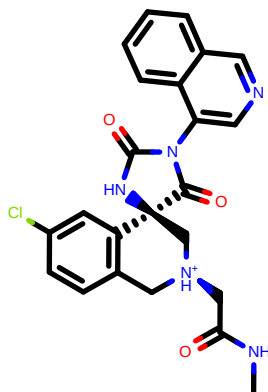
SMILES: c1ccc2c(c1)cnc2N3CC[C@]4(C3=O)C[N@](C5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)(F)F

RUN: RUN944

DDG (kcal/mol): 2.31

dDDG (kcal/mol): 0.46

VLA-MRT-8c78ee15-3_1



CID: VLA-MRT-8c78ee15-3_1

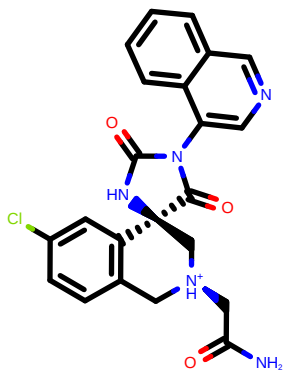
SMILES: CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cnc5c4cccc5)Cl

RUN: RUN750

DDG (kcal/mol): 2.32

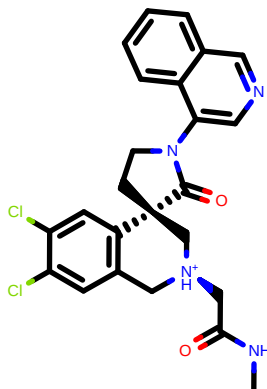
dDDG (kcal/mol): 0.21

VLA-MRT-8c78ee15-4_1



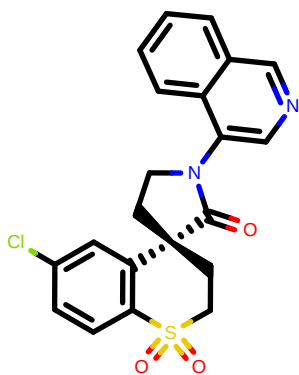
CID:	VLA-MRT-8c78ee15-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H](C[N@H+](Cc5c4cc(cc5)C)CC(=O)N)NC3=O</chem>
RUN:	RUN737
DDG (kcal/mol):	2.32
dDDG (kcal/mol):	0.16

ALP-POS-afe0272e-1_1



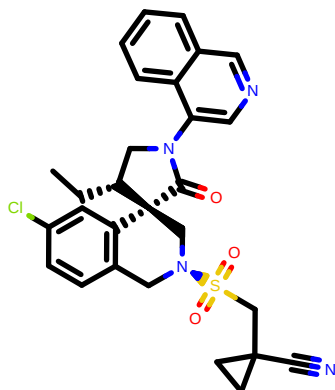
CID:	ALP-POS-afe0272e-1_1
SMILES:	<chem>CNC(=O)C[N@H+][C@@H](Cc2cc(c(cc2[C@@H]3(C1)CCN(C3=O)c4cncc5c4cccc5)C)C)Cl</chem>
RUN:	RUN779
DDG (kcal/mol):	2.47
dDDG (kcal/mol):	0.24

EDJ-MED-d4864bdc-3_1



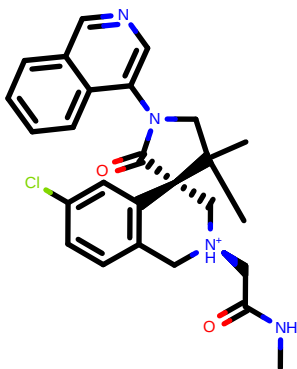
CID:	EDJ-MED-d4864bdc-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@H](C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN711
DDG (kcal/mol):	2.48
dDDG (kcal/mol):	0.21

MAT-POS-50a80394-2_1



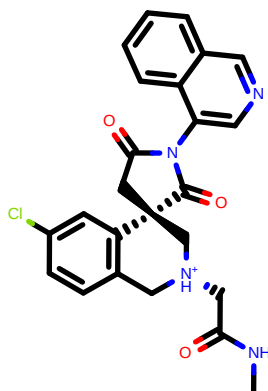
CID:	MAT-POS-50a80394-2_1
SMILES:	<chem>CC[C@@H]1CN(C(=O)[C@@H]1C2CN@H)(Cc3c2cc(c3)C)S(=O)(=O)CC4(C4)C#N)c5cncc6c5cccc6</chem>
RUN:	RUN936
DDG (kcal/mol):	2.49
dDDG (kcal/mol):	0.53

MAT-POS-50a80394-7_1



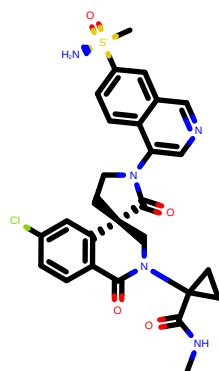
CID:	MAT-POS-50a80394-7_1
SMILES:	<chem>CC1(CN(C(=O)[C@@H]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5)C</chem>
RUN:	RUN851
DDG (kcal/mol):	2.50
dDDG (kcal/mol):	0.28

JOH-MSK-1f2dff76-1_1



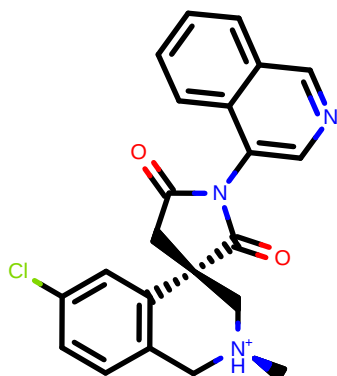
CID:	JOH-MSK-1f2dff76-1_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2cccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN783
DDG (kcal/mol):	2.57
dDDG (kcal/mol):	0.32

EDJ-MED-7d88f880-2_1



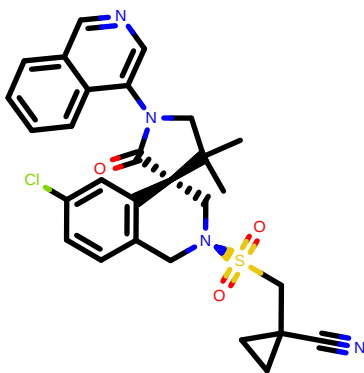
CID:	EDJ-MED-7d88f880-2_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)[S@H](=N)(=O)C16cc(ccc6C2=O)Cl</chem>
RUN:	RUN952
DDG (kcal/mol):	2.67
dDDG (kcal/mol):	0.30

JOH-MSK-51c67e7d-1_1



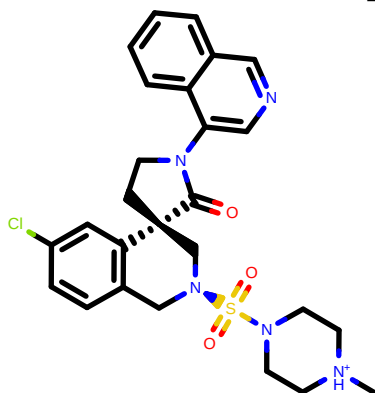
CID:	JOH-MSK-51c67e7d-1_1
SMILES:	<chem>C[N@H+]1Cc2cccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN726
DDG (kcal/mol):	2.72
dDDG (kcal/mol):	0.10

MAT-POS-50a80394-8_1



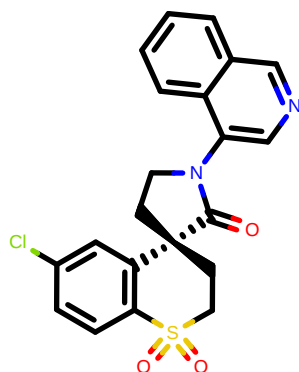
CID:	MAT-POS-50a80394-8_1
SMILES:	<chem>CC1(CN(C(=O)C)C@H)2C[N+]([O-])C3C2CC(C3)S(=O)(=O)CC4(CCNc5ccc6c5ccc6)C</chem>
RUN:	RUN943
DDG (kcal/mol):	2.73
dDDG (kcal/mol):	0.63

LUO-POS-ed2cfb03-1_1



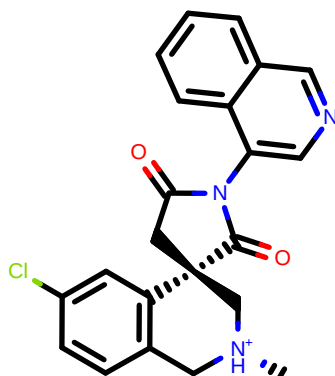
CID:	LUO-POS-ed2cfb03-1_1
SMILES:	<chem>C[NH+]1CCN(CC1)S(=O)(=O)[N+]([O-])2Cc3ccc(cc3)[C@H]4(C2)CCN(C4=O)c5ccc6c5ccc6)Cl</chem>
RUN:	RUN912
DDG (kcal/mol):	2.73
dDDG (kcal/mol):	0.92

ALP-POS-41e2080f-1_1



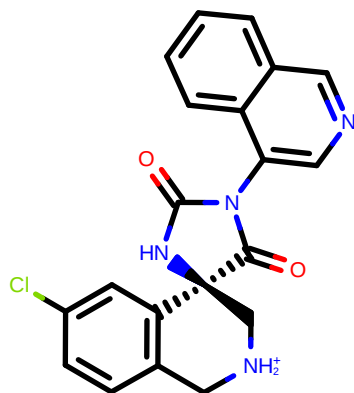
CID:	ALP-POS-41e2080f-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@H]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl</chem>
RUN:	RUN705
DDG (kcal/mol):	2.78
dDDG (kcal/mol):	0.21

JOH-MSK-51c67e7d-2_1



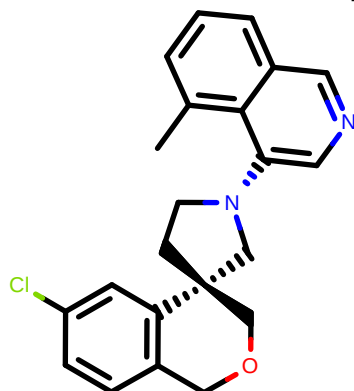
CID:	JOH-MSK-51c67e7d-2_1
SMILES:	<chem>C[N+]([O-])1Cc2ccc(cc2[C@H]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN729
DDG (kcal/mol):	2.79
dDDG (kcal/mol):	0.17

VLA-MRT-8c78ee15-1_1



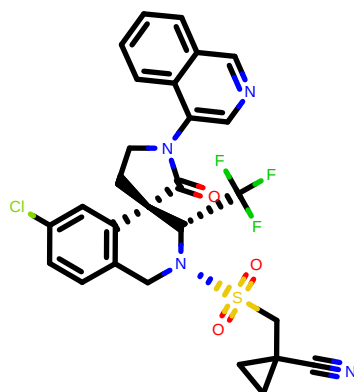
CID:	VLA-MRT-8c78ee15-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@@]4(C)[C](NH2+)[C]c5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN728
DDG (kcal/mol):	2.80
dDDG (kcal/mol):	0.17

EDJ-MED-f3cfbbb5-1_1



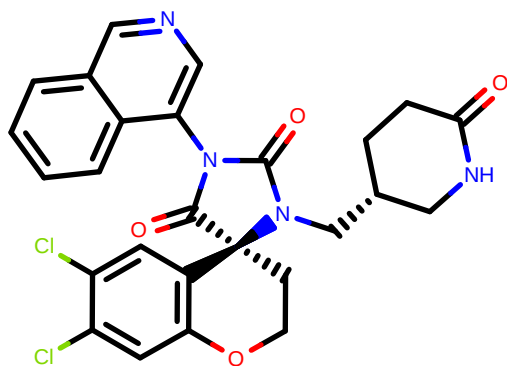
CID:	EDJ-MED-f3cfbbb5-1_1
SMILES:	<chem>Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl</chem>
RUN:	RUN700
DDG (kcal/mol):	2.84
dDDG (kcal/mol):	0.07

VLA-UNK-61877630-9_2



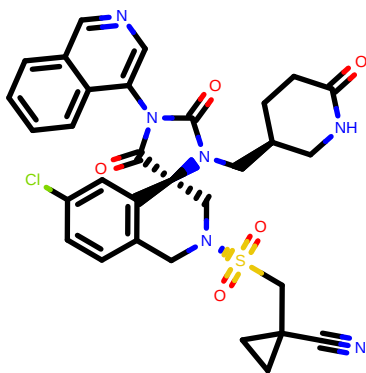
CID:	VLA-UNK-61877630-9_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3CC[C@@]4(C3=O)c5cc(cc5C)N[C@@]4(C)C(F)(F)F)S(=O)(=O)CC(C#N)C1</chem>
RUN:	RUN960
DDG (kcal/mol):	2.85
dDDG (kcal/mol):	0.36

JOH-MSK-b735e33c-1_1



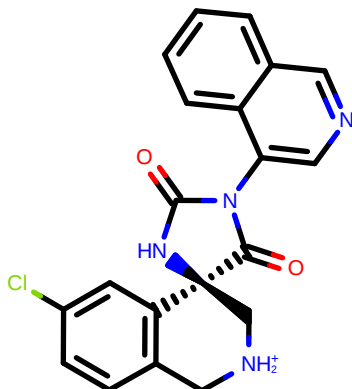
CID:	JOH-MSK-b735e33c-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@@]4(C)C(COCc5c4cc(c(c5)Cl)C)N(C3=O)C[C@@]4(C)C(=O)NC6</chem>
RUN:	RUN921
DDG (kcal/mol):	2.94
dDDG (kcal/mol):	0.26

JOH-MSK-949975c8-1_2



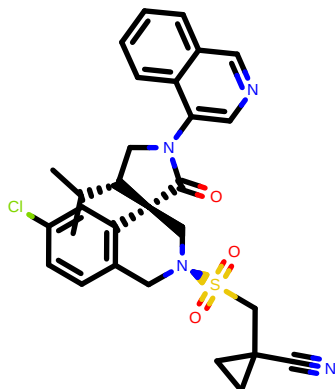
CID:	JOH-MSK-949975c8-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H]4C(N@H)(C5c4cc(cc5)C)S(=O)(=O)CC6(Cc7H)N(C3=O)C@H7CCCC(=O)NC7</chem>
RUN:	RUN1010
DDG (kcal/mol):	2.95
dDDG (kcal/mol):	0.40

VLA-MRT-a639d434-3_1



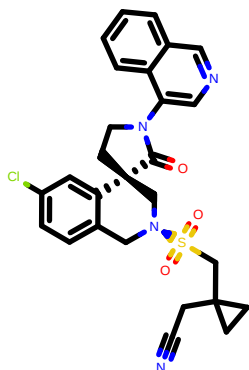
CID:	VLA-MRT-a639d434-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H]4C(NH2+)Cc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN724
DDG (kcal/mol):	2.97
dDDG (kcal/mol):	0.20

MAT-POS-50a80394-3_1



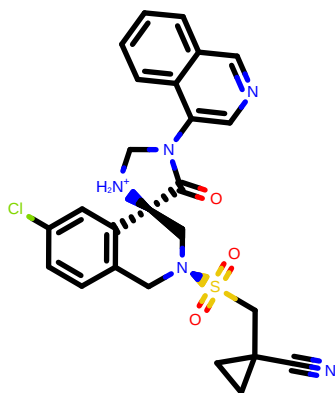
CID:	MAT-POS-50a80394-3_1
SMILES:	<chem>CC(C)[C@@H]1CN(C(=O)[C@@H]2C[N@H]1)(C3c2cc(cc3)C)S(=O)(=O)CC4(Cc5H)N(C3=O)C@H5CCCC65CCCC6</chem>
RUN:	RUN964
DDG (kcal/mol):	3.01
dDDG (kcal/mol):	0.41

ALP-POS-ecbed2ba-22_1



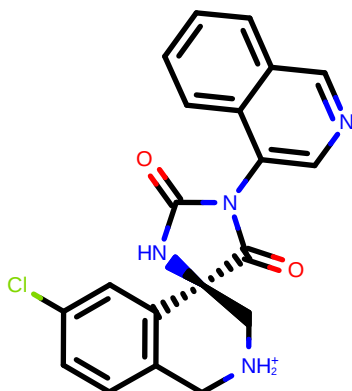
CID:	ALP-POS-ecbed2ba-22_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@@H]4(C3=O)C[N@H](C5c4cc(cc5)C)S(=O)(=O)CC6(Cc7H)N(C3=O)C@H7CCCC65CCCC6</chem>
RUN:	RUN931
DDG (kcal/mol):	3.12
dDDG (kcal/mol):	0.45

EDG-MED-00af8776-1_1



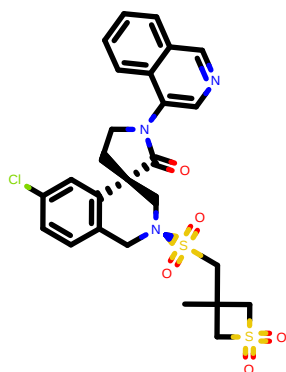
CID:	EDG-MED-00af8776-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=N)N(C@H)4(C3=O)C(N@H)C5c4cc(cc5C)S(=O)(=O)CC6(CO)C#N</chem>
RUN:	RUN873
DDG (kcal/mol):	3.19
dDDG (kcal/mol):	0.38

VLA-MRT-8c78ee15-2_1



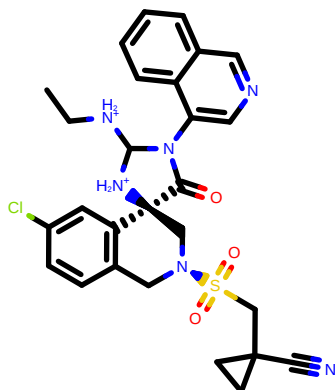
CID:	VLA-MRT-8c78ee15-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@H]4(C[NH2+])Cc5c4cc(cc5Cl)NC3=O</chem>
RUN:	RUN719
DDG (kcal/mol):	3.27
dDDG (kcal/mol):	0.20

ALP-POS-ecbed2ba-1_1



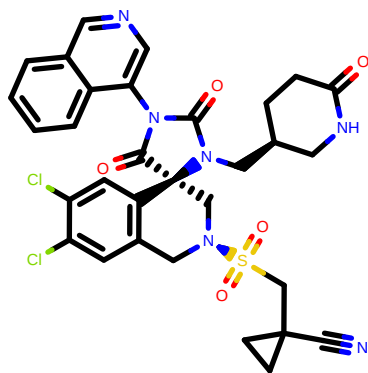
CID:	ALP-POS-ecbed2ba-1_1
SMILES:	<chem>CC1(CS(=O)(=O)C1)CS(=O)(=O)N@2Cc3ccc(cc3[C@@H]4(C2)CCN(C4=O)c5ncc6c5ccccc6)Cl</chem>
RUN:	RUN925
DDG (kcal/mol):	3.29
dDDG (kcal/mol):	0.54

LUO-POS-eaf50f21-5_1



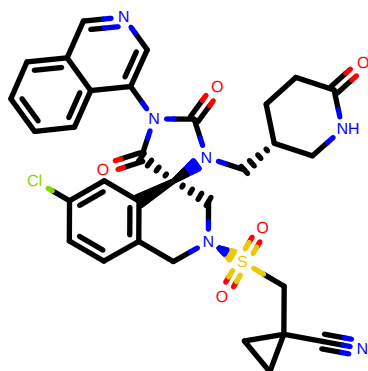
CID:	LUO-POS-eaf50f21-5_1
SMILES:	<chem>CC(NH+)-C1N[C@@H]2(C1N@H)C3Cc2ccc(cc3C)S(=O)(=O)CC4(Cc5c4cc(cc5O)N1c5ncc6c5ccccc6</chem>
RUN:	RUN975
DDG (kcal/mol):	3.39
dDDG (kcal/mol):	0.36

JOH-MSK-cef8a2bc-1_2



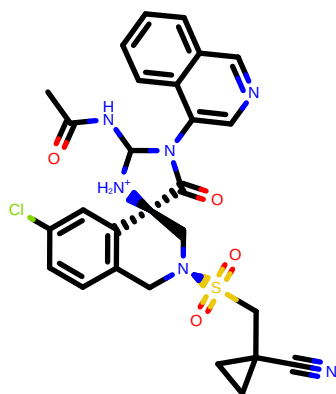
CID:	JOH-MSK-cef8a2bc-1_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)[C@H](C[N@H]C5c4ccc(cc5)C(=O)S(=O)(=O)CC6(Cc7cncnc7)N(C3=O)C[C@H]7CCCC(=O)NC7</chem>
RUN:	RUN1018
DDG (kcal/mol):	3.42
dDDG (kcal/mol):	0.38

JOH-MSK-949975c8-1_1



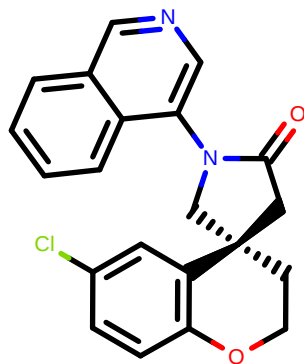
CID:	JOH-MSK-949975c8-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N3C(=O)[C@H](C[N@H]C5c4ccc(cc5)C(=O)S(=O)(=O)CC6(Cc7cncnc7)N(C3=O)C[C@H]7CCCC(=O)NC7</chem>
RUN:	RUN1016
DDG (kcal/mol):	3.50
dDDG (kcal/mol):	0.46

LUO-POS-eaf50f21-3_1



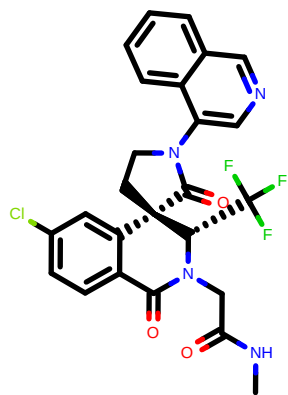
CID:	LUO-POS-eaf50f21-3_1
SMILES:	<chem>CC(=O)NC1=[NH+][C@H]2[C@H](C[N@H]C3c4ccc(cc3)C(=O)S(=O)(=O)CC4(Cc5cncnc5)N(C1=O)N1c5cccnc5c5ccc6</chem>
RUN:	RUN981
DDG (kcal/mol):	3.63
dDDG (kcal/mol):	0.51

EDJ-MED-159244ea-3_1



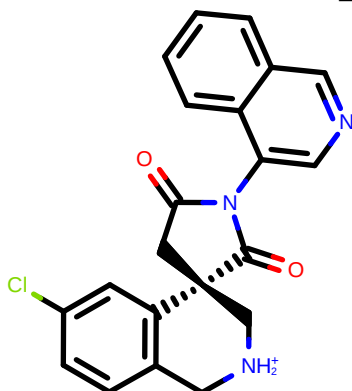
CID:	EDJ-MED-159244ea-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O</chem>
RUN:	RUN681
DDG (kcal/mol):	3.63
dDDG (kcal/mol):	0.08

VLA-UNK-61877630-3_2



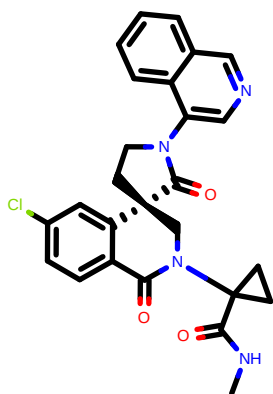
CID:	VLA-UNK-61877630-3_2
SMILES:	<chem>CNC(=O)CN1[C@H]([C@H]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)C)C(F)(F)F</chem>
RUN:	RUN914
DDG (kcal/mol):	3.65
dDDG (kcal/mol):	0.33

JOH-MSK-1f2dff76-4_1



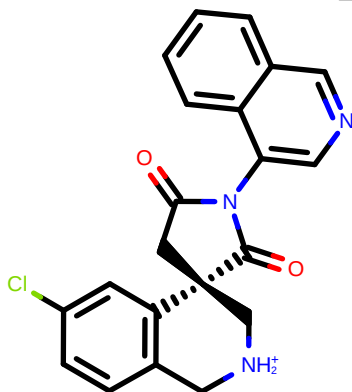
CID:	JOH-MSK-1f2dff76-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[NH2+][C]5c4cc(cc5)Cl</chem>
RUN:	RUN715
DDG (kcal/mol):	3.73
dDDG (kcal/mol):	0.14

EDJ-MED-fd8ed875-4_1



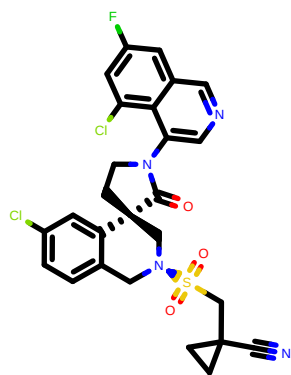
CID:	EDJ-MED-fd8ed875-4_1
SMILES:	<chem>CNC(=O)C1(CC1)N2C[C@]3(C=CN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl</chem>
RUN:	RUN832
DDG (kcal/mol):	3.87
dDDG (kcal/mol):	0.25

JOH-MSK-1f2dff76-3_1



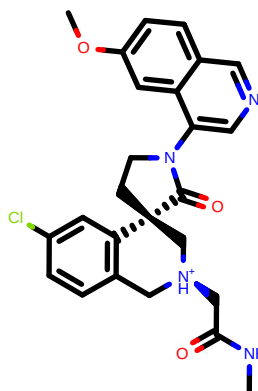
CID:	JOH-MSK-1f2dff76-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[NH2+][C]5c4cc(cc5)Cl</chem>
RUN:	RUN714
DDG (kcal/mol):	3.95
dDDG (kcal/mol):	0.14

MAT-POS-853c0ffa-6_1



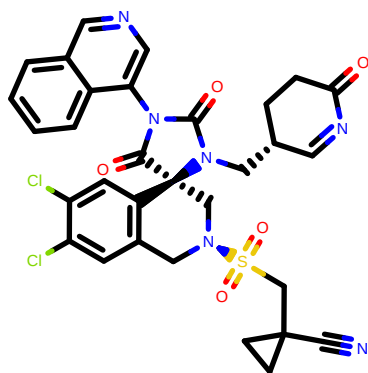
CID:	MAT-POS-853c0ffa-6_1
SMILES:	<chem>c1cc2(cc1C)C@H]3[C@@H](CN(C3=O)c4ncc5c4(cc(c5)F)C1C[N@H](C2)S(=O)(=O)CC6(CO6)CN</chem>
RUN:	RUN940
DDG (kcal/mol):	4.04
dDDG (kcal/mol):	0.37

EDJ-MED-b6c6ee2b-2_1



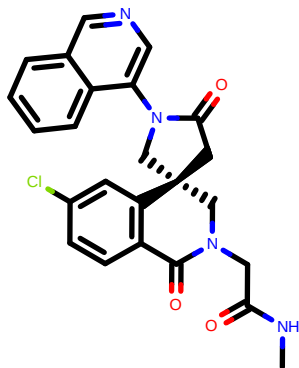
CID:	EDJ-MED-b6c6ee2b-2_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@H]3(C1)CCN(C3=O)c4ncc5c4cc(cc5)OC)Cl</chem>
RUN:	RUN812
DDG (kcal/mol):	4.09
dDDG (kcal/mol):	0.26

JOH-MSK-cef8a2bc-1_1



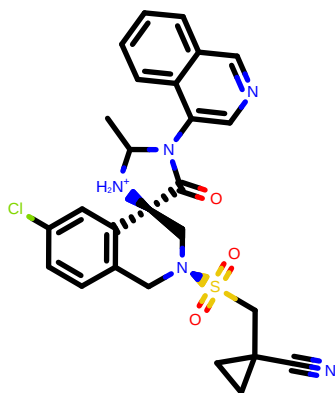
CID:	JOH-MSK-cef8a2bc-1_1
SMILES:	<chem>c1ccc2(c(c1)nc3c2N3C(=O)C@H]4[C@@H](CN(C4=O)C5c4cc(cc5)C)S(=O)(=O)CC6(CO6)CN(NC3=O)C[C@H]7CCC(=O)N7</chem>
RUN:	RUN1004
DDG (kcal/mol):	4.12
dDDG (kcal/mol):	0.46

EDJ-MED-8bb691af-9_1



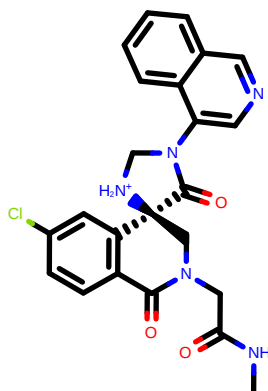
CID:	EDJ-MED-8bb691af-9_1
SMILES:	<chem>CNC(=O)CN1C[C@H]2(CC(=O)N(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem>
RUN:	RUN739
DDG (kcal/mol):	4.20
dDDG (kcal/mol):	0.13

EDG-MED-b6bce001-2_1



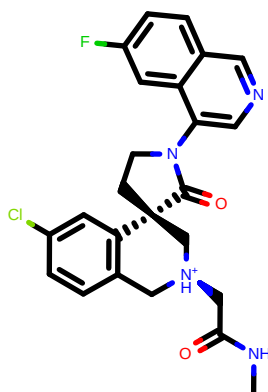
CID:	EDG-MED-b6bce001-2_1
SMILES:	<chem>CC1=[NH+][C@]2[C@]3[C@]4(Cc3c2cc(cc3Cl)S(=O)(=O)CC4(C)C#N)C(=O)N1c5ncc6c5ccccc6</chem>
RUN:	RUN923
DDG (kcal/mol):	4.21
dDDG (kcal/mol):	0.32

EDJ-MED-fd8ed875-1_1



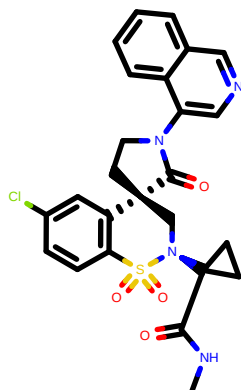
CID:	EDJ-MED-fd8ed875-1_1
SMILES:	<chem>CNC(=O)CN1C[C@]2(c3cc(ccc3C1=O)C)C(=O)N(C=[NH+])c4cnc5c4cccc5</chem>
RUN:	RUN763
DDG (kcal/mol):	4.23
dDDG (kcal/mol):	0.11

LUO-POS-b4dec3be-2_1



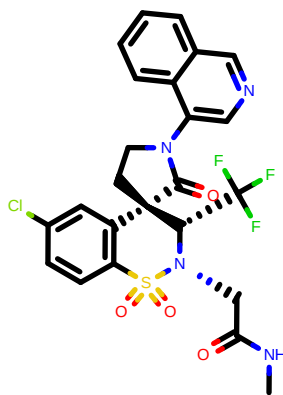
CID:	LUO-POS-b4dec3be-2_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2cc(ccc2[C@]3(C1)CCN(C3=O)c4cnc5c4ccc(cc5)F)Cl</chem>
RUN:	RUN791
DDG (kcal/mol):	4.43
dDDG (kcal/mol):	0.26

EDJ-MED-976a33d5-3_1



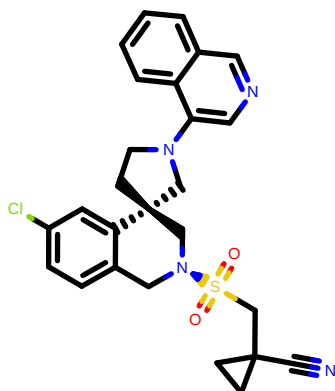
CID:	EDJ-MED-976a33d5-3_1
SMILES:	<chem>CNC(=O)C1(CC1)[N@]2C[C@]3(CCN(C3=O)c4cnc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl</chem>
RUN:	RUN864
DDG (kcal/mol):	4.51
dDDG (kcal/mol):	0.49

VLA-UNK-f2612802-1_2



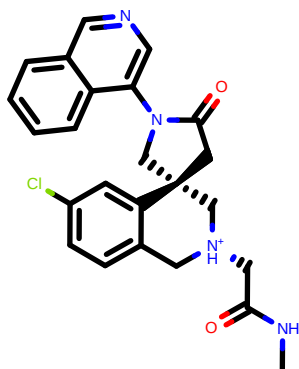
CID:	VLA-UNK-f2612802-1_2
SMILES:	<chem>CNC(=O)C[N+]([C@H]1[C@@H]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)C)C(F)(F)F</chem>
RUN:	RUN942
DDG (kcal/mol):	4.73
dDDG (kcal/mol):	0.39

EDJ-MED-8bb691af-2_1



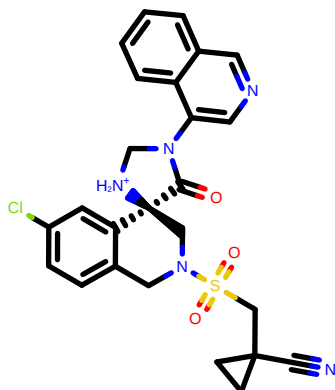
CID:	EDJ-MED-8bb691af-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3)C[N+]([C@@H]5Cc6cc(cc5C)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN826
DDG (kcal/mol):	4.90
dDDG (kcal/mol):	0.39

EDJ-MED-8bb691af-3_1



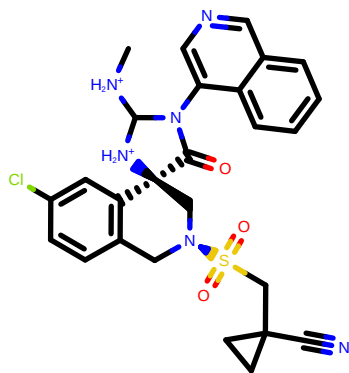
CID:	EDJ-MED-8bb691af-3_1
SMILES:	<chem>CNC(=O)C[N+]([H+])1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3)c4cncc5c4cccc5)Cl</chem>
RUN:	RUN735
DDG (kcal/mol):	5.08
dDDG (kcal/mol):	0.30

EDG-MED-b6bce001-1_1



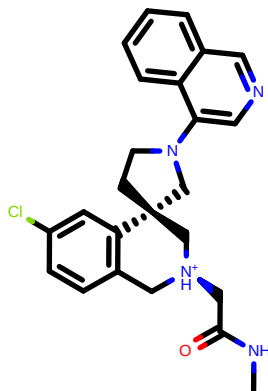
CID:	EDG-MED-b6bce001-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=N[+]([C@]4(C3=O)C[N+]([C@@H]5Cc6cc(cc5C)S(=O)(=O)CC6(CC6)C#N</chem>
RUN:	RUN879
DDG (kcal/mol):	5.13
dDDG (kcal/mol):	0.65

LUO-POS-eaf50f21-2_1



CID:	LUO-POS-eaf50f21-2_1
SMILES:	<chem>C[NH+]C1C1N(C@2[C@H]N(C)C2)C3C2C(C3)S(=O)(=O)CC4(C)C4N(C)C1=O</chem>
RUN:	RUN961
DDG (kcal/mol):	5.93
dDDG (kcal/mol):	0.73

EDJ-MED-8bb691af-1_1



CID:	EDJ-MED-8bb691af-1_1
SMILES:	<chem>CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3)c4ncc5c4ccc5)Cl</chem>
RUN:	RUN743
DDG (kcal/mol):	5.95
dDDG (kcal/mol):	0.21