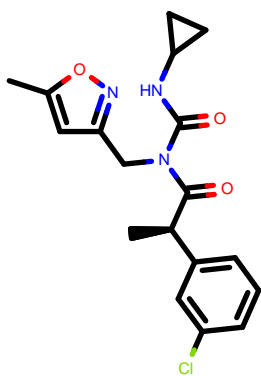
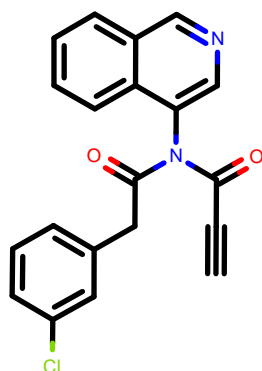


TRY-UNI-9f475305-8_2



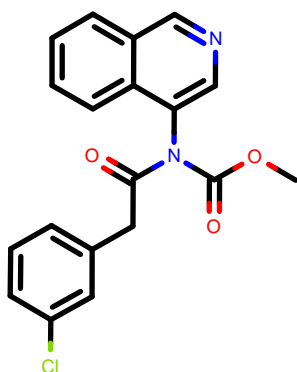
CID:	TRY-UNI-9f475305-8_2
SMILES:	<chem>Cc1cc(no1)CN(C(=O))[C@H](C)c2cccc(c2)ClC(=O)NC3CC3</chem>
RUN:	RUN92
DDG (kcal/mol):	-6.62
dDDG (kcal/mol):	0.26

DAR-DIA-56cf811e-1_1



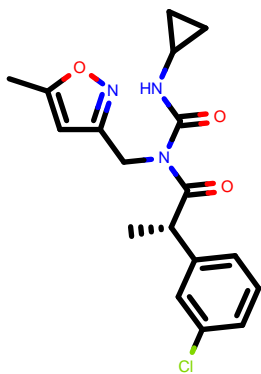
CID:	DAR-DIA-56cf811e-1_1
SMILES:	<chem>C#CC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN509
DDG (kcal/mol):	-6.32
dDDG (kcal/mol):	0.15

PET-UNK-12d8d43f-2_1



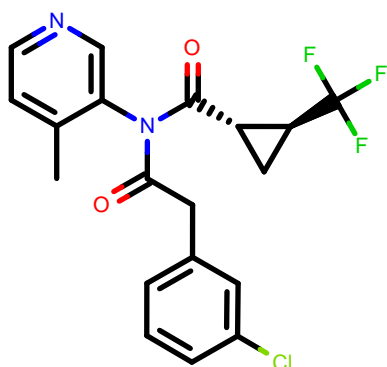
CID:	PET-UNK-12d8d43f-2_1
SMILES:	<chem>COC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN518
DDG (kcal/mol):	-5.44
dDDG (kcal/mol):	0.17

TRY-UNI-9f475305-8_1



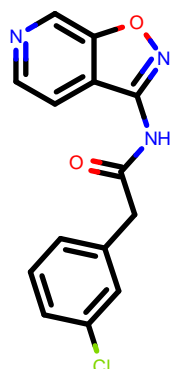
CID:	TRY-UNI-9f475305-8_1
SMILES:	<chem>Cc1cc(no1)CN(C(=O))[C@@H](C)c2cccc(c2)ClC(=O)NC3CC3</chem>
RUN:	RUN87
DDG (kcal/mol):	-5.13
dDDG (kcal/mol):	0.21

JOH-UNI-a38a7bdd-7_2



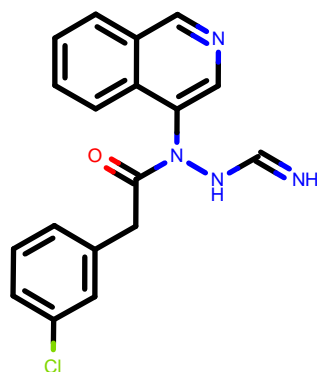
CID:	JOH-UNI-a38a7bdd-7_2
SMILES:	<chem>Cc1cncc1N(C(=O)Cc2ccccc2Cl)C(=O)C@H]3C[C@@H]3C(F)(F)F</chem>
RUN:	RUN501
DDG (kcal/mol):	-4.52
dDDG (kcal/mol):	0.17

JIN-POS-6dc588a4-16_1



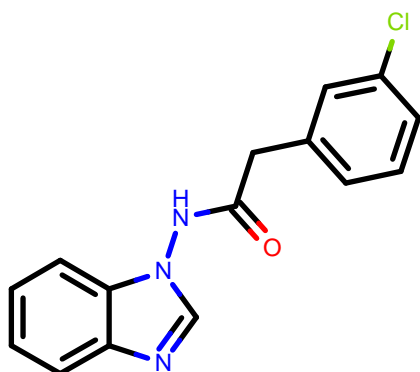
CID:	JIN-POS-6dc588a4-16_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3ccncc3on2</chem>
RUN:	RUN641
DDG (kcal/mol):	-3.44
dDDG (kcal/mol):	0.10

PET-UNK-a692de38-1_1



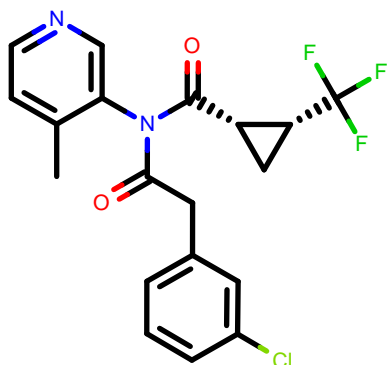
CID:	PET-UNK-a692de38-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)Cc3ccccc(c3)Cl)NC#N</chem>
RUN:	RUN345
DDG (kcal/mol):	-3.09
dDDG (kcal/mol):	0.23

JAN-GHE-5a013bed-2_1



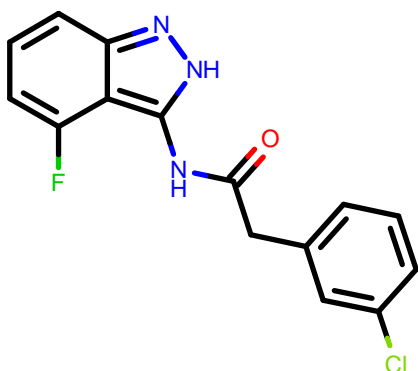
CID:	JAN-GHE-5a013bed-2_1
SMILES:	<chem>c1ccc2c(c1)ncn2NC(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN52
DDG (kcal/mol):	-2.86
dDDG (kcal/mol):	0.10

JOH-UNI-a38a7bdd-7_4



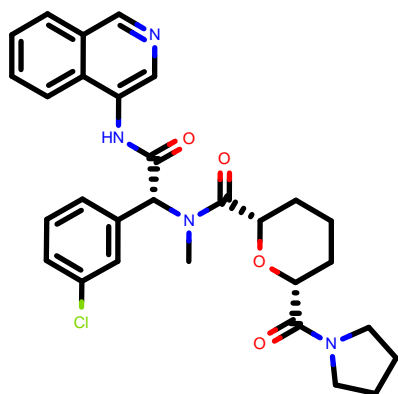
CID:	JOH-UNI-a38a7bdd-7_4
SMILES:	<chem>Cc1cncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)[C@H]3C[C@H]3C(F)(F)F</chem>
RUN:	RUN515
DDG (kcal/mol):	-2.83
dDDG (kcal/mol):	0.18

EDJ-MED-c8e7a002-13_1



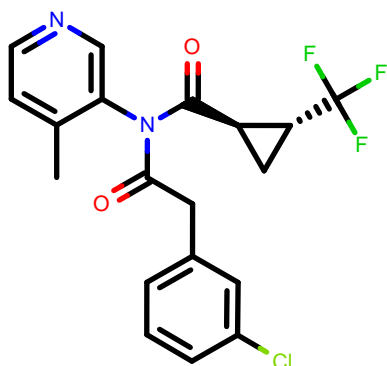
CID:	EDJ-MED-c8e7a002-13_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3c(cccc3F)[nH]n2</chem>
RUN:	RUN310
DDG (kcal/mol):	-2.69
dDDG (kcal/mol):	0.14

PET-UNK-1320d94d-29_1



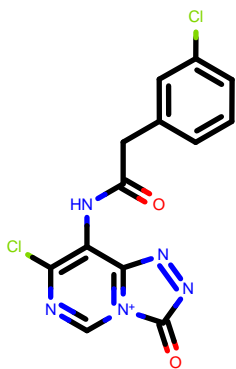
CID:	PET-UNK-1320d94d-29_1
SMILES:	<chem>CN[C@H](c1cccc(c1)Cl)C(=O)Nc2nc3c2cccc3Cl=O[C@@H]4CC[C@]([H])O4C(=O)N5CCCC5</chem>
RUN:	RUN743
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.26

JOH-UNI-a38a7bdd-7_3



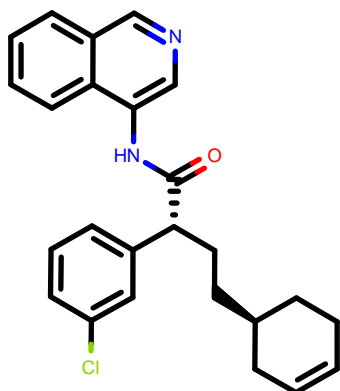
CID:	JOH-UNI-a38a7bdd-7_3
SMILES:	<chem>Cc1cncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)[C@@H]3C[C@H]3C(F)(F)F</chem>
RUN:	RUN513
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.16

EDJ-MED-c8e7a002-17_1



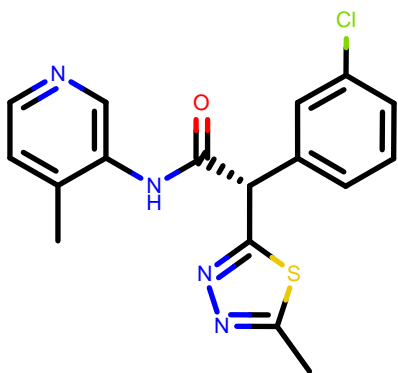
CID:	EDJ-MED-c8e7a002-17_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3n[nH]c(=O)n3cnc2Cl</chem>
RUN:	RUN311
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.10

ALP-POS-3b848b35-4_2



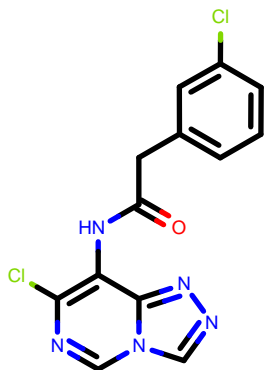
CID:	ALP-POS-3b848b35-4_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@H](CCCCCCCC3)c4cccc(c4)Cl</chem>
RUN:	RUN194
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.23

SAM-UNK-2684b532-3_2



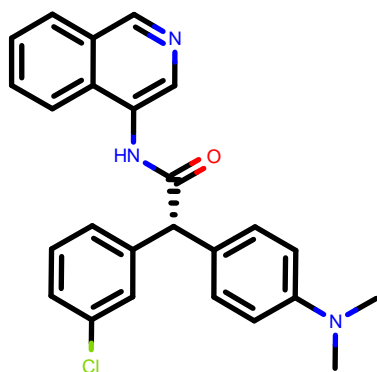
CID:	SAM-UNK-2684b532-3_2
SMILES:	<chem>Cc1ccncc1NC(=O)[C@H](c2cccc(c2)Cl)c3nnc(s3)C</chem>
RUN:	RUN145
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.13

EDJ-MED-c8e7a002-7_1



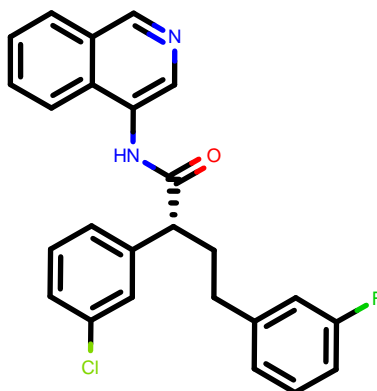
CID:	EDJ-MED-c8e7a002-7_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3nncn3cnc2Cl</chem>
RUN:	RUN304
DDG (kcal/mol):	-2.35
dDDG (kcal/mol):	0.14

MIC-UNK-d36ab305-4_2



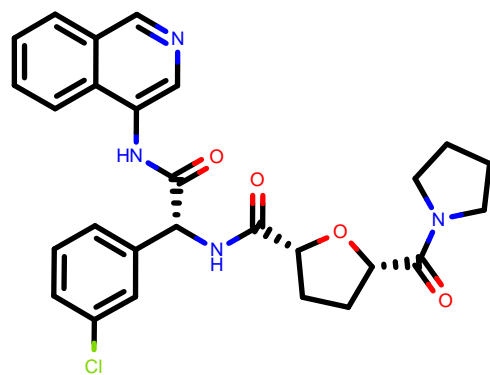
CID:	MIC-UNK-d36ab305-4_2
SMILES:	<chem>CN(C)c1ccc(cc1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN244
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.17

MIC-UNK-c66144cb-1_2



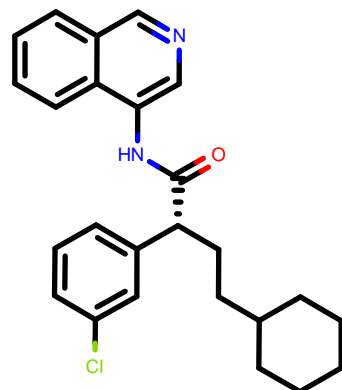
CID:	MIC-UNK-c66144cb-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CCc3cccc(c3)F)c4cccc(c4)Cl</chem>
RUN:	RUN248
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.21

EDJ-MED-ee07cf00-11_7



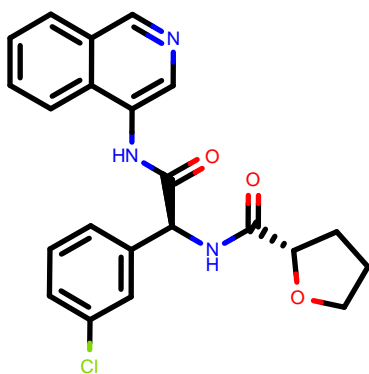
CID:	EDJ-MED-ee07cf00-11_7
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@H](C4CCN4)O5CCCCO5</chem>
RUN:	RUN595
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.20

MIC-UNK-c66144cb-3_2



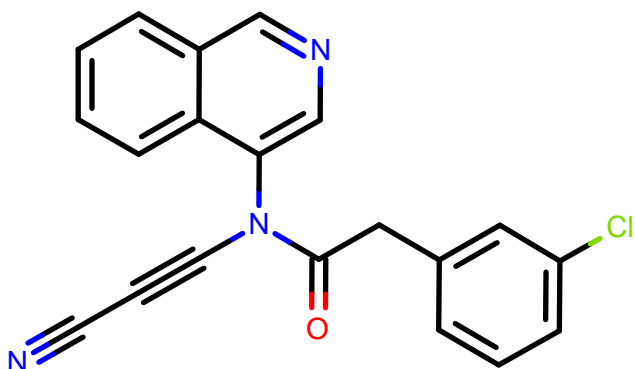
CID:	MIC-UNK-c66144cb-3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CCCC3CCCCC3)c4cccc(c4)Cl</chem>
RUN:	RUN221
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.22

EDJ-MED-cf4b0d25-3_2



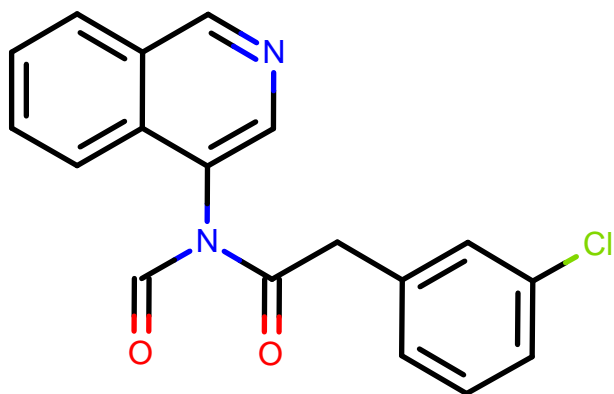
CID:	EDJ-MED-cf4b0d25-3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@@H]4CCCCO4</chem>
RUN:	RUN625
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.19

DAR-DIA-076fb6ea-5_1



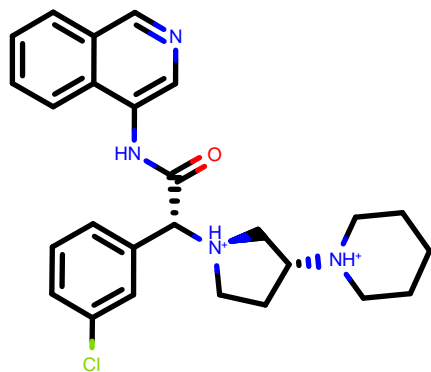
CID:	DAR-DIA-076fb6ea-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C#CC#N)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN461
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.47

PET-UNK-12d8d43f-1_1



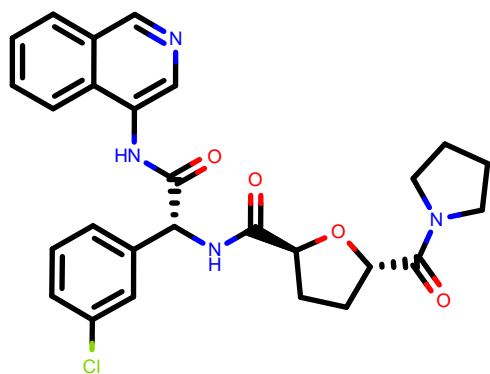
CID:	PET-UNK-12d8d43f-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C=O)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN510
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.13

MIC-UNK-5a93dd5f-12_7



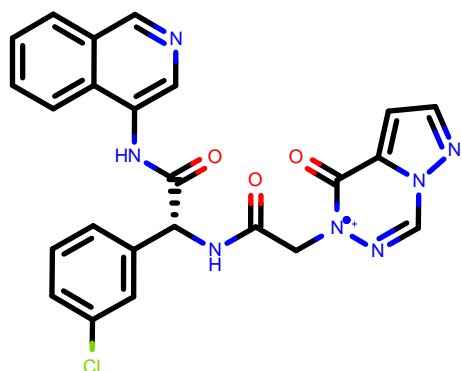
CID:	MIC-UNK-5a93dd5f-12_7
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@]4CC[C@H](C4)[NH+]5CCCCC5</chem>
RUN:	RUN439
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.14

PET-UNK-ac320b15-7_1



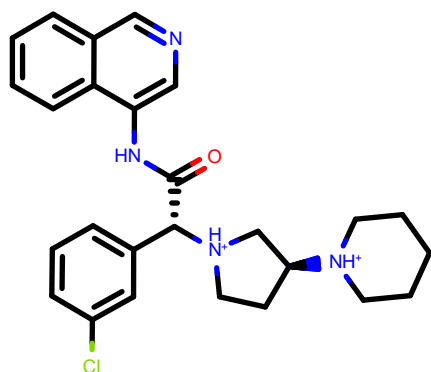
CID:	PET-UNK-ac320b15-7_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)N[C@@H](C4CCN4)C(=O)N5CCCC5</chem>
RUN:	RUN757
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.17

EDJ-MED-ee07cf00-17_1



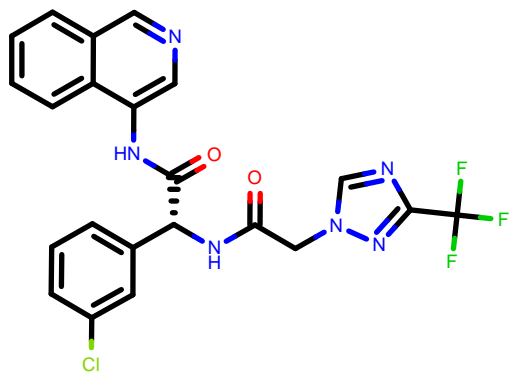
CID:	EDJ-MED-ee07cf00-17_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)N[C@@H](C4=CN=CN4)C(=O)N5C=NN=C5</chem>
RUN:	RUN602
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.26

MIC-UNK-5a93dd5f-12_1



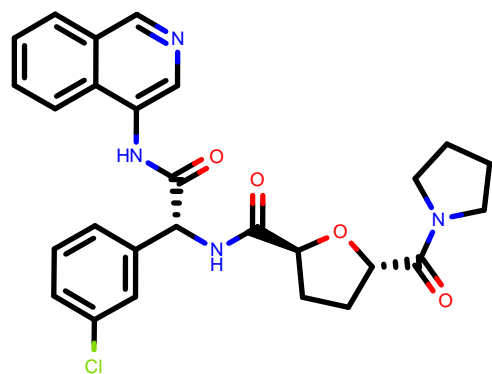
CID:	MIC-UNK-5a93dd5f-12_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)N[C@@H](C4CCN4)C(=O)N5CCCC5</chem>
RUN:	RUN435
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.16

EDJ-MED-ee07cf00-10_1



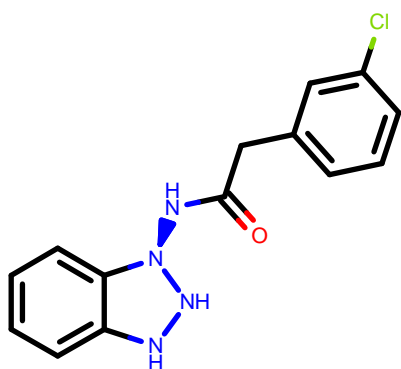
CID:	EDJ-MED-ee07cf00-10_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)N[C@@H](C4=CN=CN4)C(F)(F)F</chem>
RUN:	RUN582
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.20

MAT-POS-8293a91a-6_1



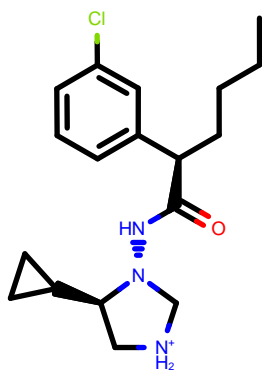
CID:	MAT-POS-8293a91a-6_1
SMILES:	<chem>c1ccc2c(c1)nncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@@H](O4C[C@H]4)C5=CNCC5</chem>
RUN:	RUN779
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.21

MAT-POS-bfb445d4-2_1



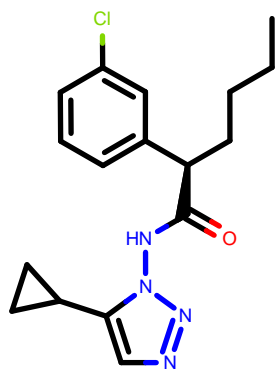
CID:	MAT-POS-bfb445d4-2_1
SMILES:	<chem>c1ccc2c(c1)nnn2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN278
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.12

JAN-GHE-f4ca5a00-18_2



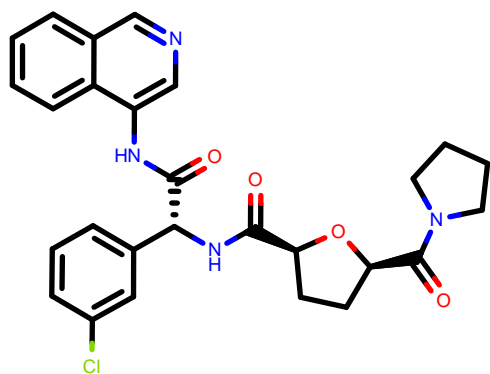
CID:	JAN-GHE-f4ca5a00-18_2
SMILES:	<chem>CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2cncc2C3CC3</chem>
RUN:	RUN201
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.16

JAN-GHE-f4ca5a00-20_2



CID:	JAN-GHE-f4ca5a00-20_2
SMILES:	<chem>CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2c(cnn2)C3CC3</chem>
RUN:	RUN202
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.17

MAT-POS-a13804f0-4_1



CID: MAT-POS-a13804f0-4_1

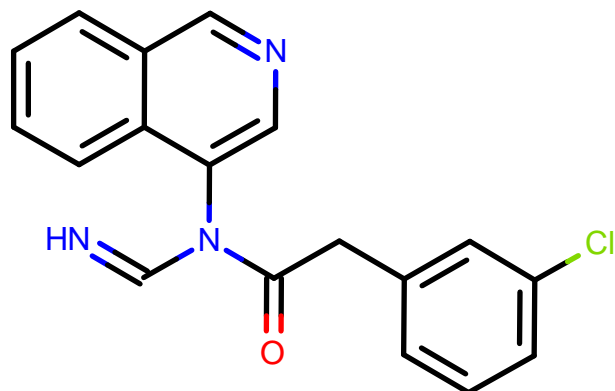
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@H](c3ccc(c3)C)NC(=O)[C@@H](c4cc(C)cc4)C(=O)N5CCCC5

RUN: RUN620

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.23

PET-UNK-5ecb6237-1_1



CID: PET-UNK-5ecb6237-1_1

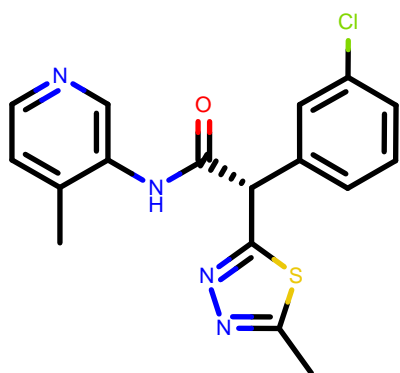
SMILES: c1ccc2c(c1)cncc2N(C#N)C(=O)Cc3cccc(c3)Cl

RUN: RUN322

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.14

TRY-UNI-9f475305-3_2



CID: TRY-UNI-9f475305-3_2

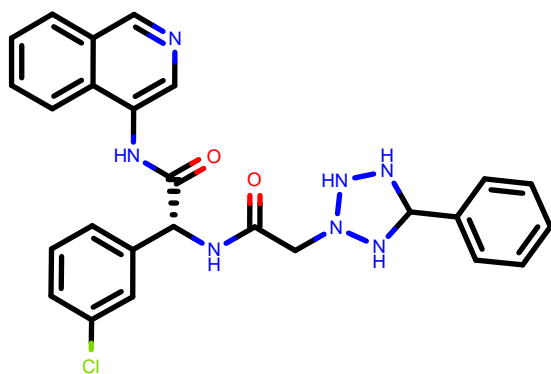
SMILES: Cc1ccncc1NC(=O)[C@H](c2cccc(c2)Cl)c3nnc(s3)C

RUN: RUN64

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.14

EDJ-MED-ee07cf00-9_2



CID: EDJ-MED-ee07cf00-9_2

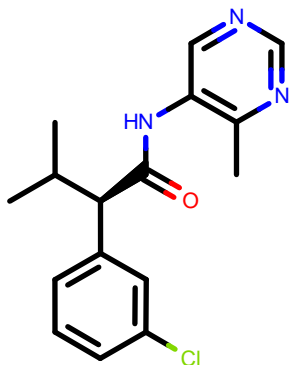
SMILES: c1ccc(cc1)c2nnn(n2)CC(=O)N[C@@H](c3cccc(c3)Cl)C(=O)N4cncnc5c4ccccc5

RUN: RUN578

DDG (kcal/mol): -1.69

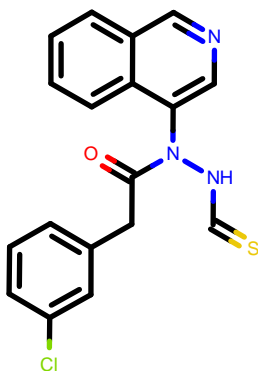
dDDG (kcal/mol): 0.23

JAN-GHE-83b26c96-7_1



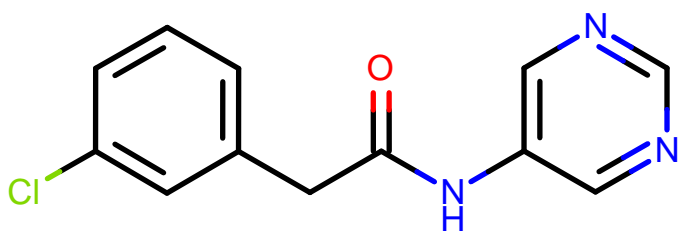
CID:	JAN-GHE-83b26c96-7_1
SMILES:	<chem>Cc1c(cncn1)NC(=O)[C@@H](c2cccc(c2)Cl)C(C)C</chem>
RUN:	RUN20
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.17

DAR-DIA-076fb6ea-15_1



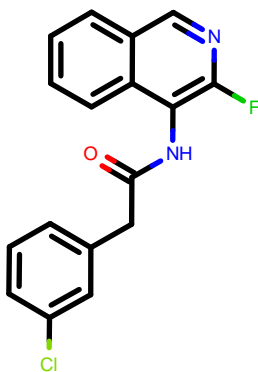
CID:	DAR-DIA-076fb6ea-15_1
SMILES:	<chem>c1ccc2c(c1)cnc2N(C(=O)Cc3cccc(c3)Cl)N=C=S</chem>
RUN:	RUN483
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.18

JAN-GHE-5a013bed-9_1



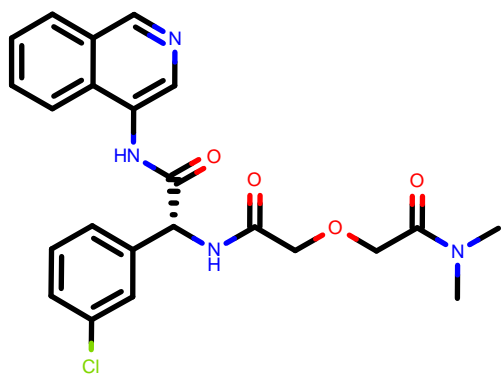
CID:	JAN-GHE-5a013bed-9_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncnc2</chem>
RUN:	RUN49
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.13

RUB-POS-1325a9ea-18_1



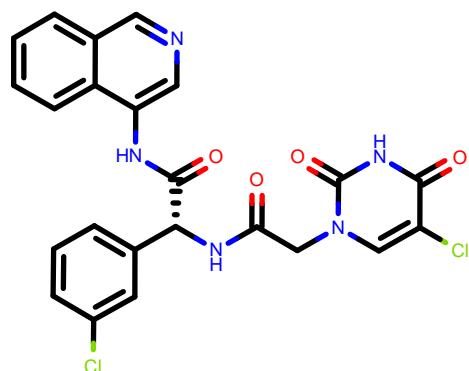
CID:	RUB-POS-1325a9ea-18_1
SMILES:	<chem>c1ccc2c(c1)cnc(c2NC(=O)Cc3cccc(c3)Cl)F</chem>
RUN:	RUN674
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.04

EDJ-MED-cf4b0d25-5_2



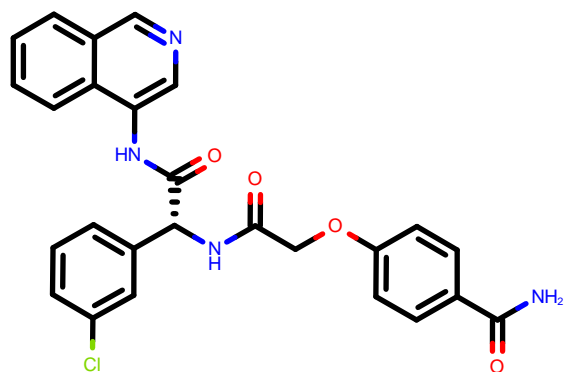
CID:	EDJ-MED-cf4b0d25-5_2
SMILES:	<chem>CN(C)C(=O)COCC(=O)N[C@@H](c1cccc(e1)Cl)C(=O)Nc2ccc3c2ccc3</chem>
RUN:	RUN716
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.18

EDJ-MED-ee07cf00-16_1



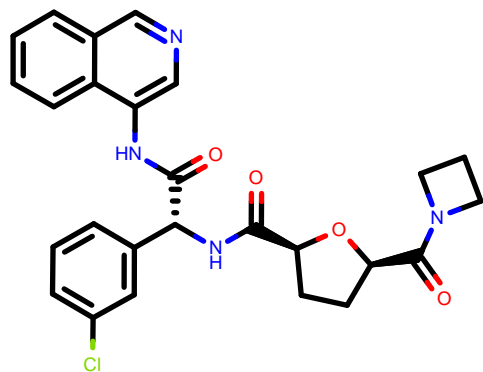
CID:	EDJ-MED-ee07cf00-16_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cn4cc(c(=O)[nH]4=O)Cl</chem>
RUN:	RUN593
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.17

EDJ-MED-ee07cf00-12_1



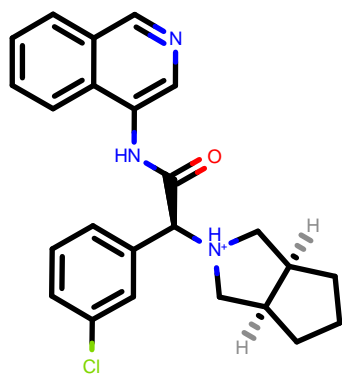
CID:	EDJ-MED-ee07cf00-12_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)COc4ccc(cc4)C(=O)N</chem>
RUN:	RUN610
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.18

PET-UNK-1320d94d-5_1



CID:	PET-UNK-1320d94d-5_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)C@H4OC@H4C(=O)N5CCO5</chem>
RUN:	RUN733
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.20

MIC-UNK-5a93dd5f-1_2



CID: MIC-UNK-5a93dd5f-1_2

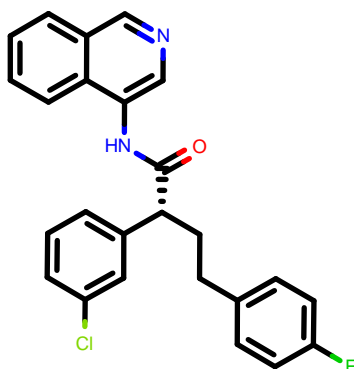
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)N+H4C[C@H]5CC[C@H]5C4

RUN: RUN353

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.18

MIC-UNK-c66144cb-2_2



CID: MIC-UNK-c66144cb-2_2

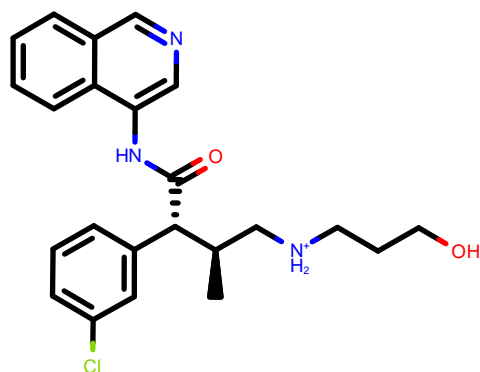
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](CCc3cccc(c3)F)c4cccc(c4)Cl

RUN: RUN245

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.20

MAK-UNK-c749d764-6_4



CID: MAK-UNK-c749d764-6_4

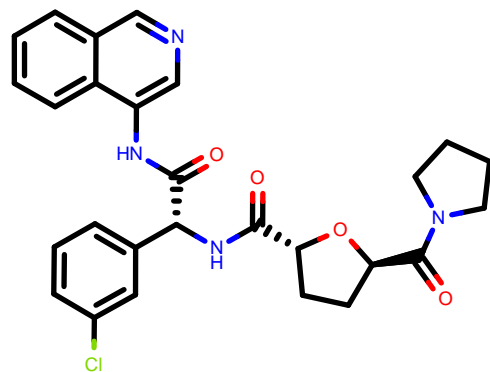
SMILES: C[C@H](C[NH2+])CCCO[C@H](c1cccc(c1)Cl)C(=O)Nc2cccc3c2cccc3

RUN: RUN482

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.24

PET-UNK-ac320b15-5_1



CID: PET-UNK-ac320b15-5_1

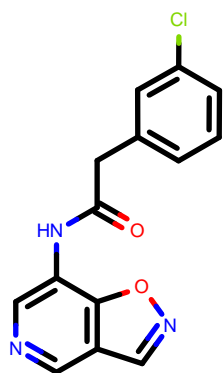
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)N(C=O)[C@H]4[C@@H](O)C[C@H]4O5CCCC5

RUN: RUN756

DDG (kcal/mol): -1.57

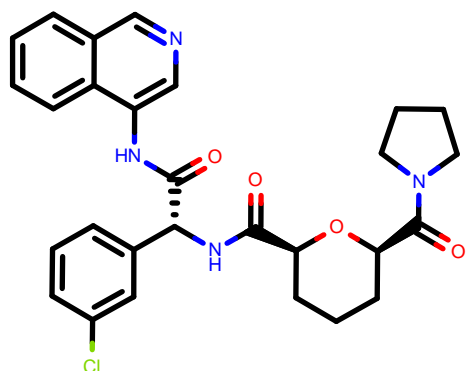
dDDG (kcal/mol): 0.20

PET-UNK-b1ef24dc-1_1



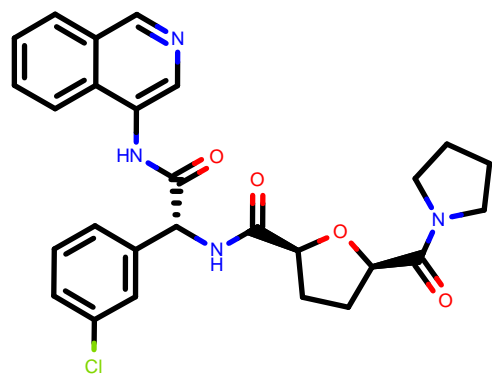
CID:	PET-UNK-b1ef24dc-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2onc3</chem>
RUN:	RUN711
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.13

PET-UNK-1320d94d-9_1



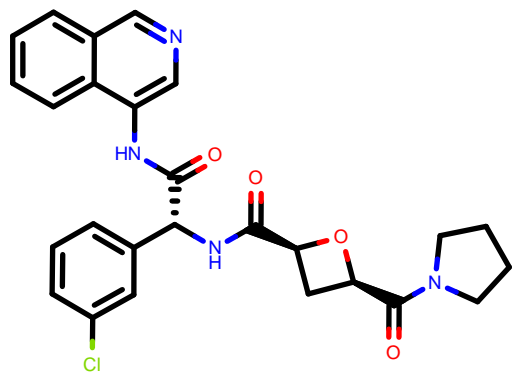
CID:	PET-UNK-1320d94d-9_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)C@H](c3ccccc3)C1NC(=O)C@H](C4CC[C@H]4)O1NSCCCC5</chem>
RUN:	RUN737
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.25

EDJ-MED-ee07cf00-11_1



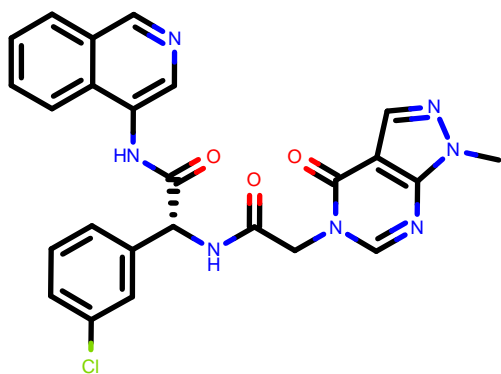
CID:	EDJ-MED-ee07cf00-11_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)C@H](c3ccccc3)C1NC(=O)C@H](C4CC[C@H]4)O1NSCCCC5</chem>
RUN:	RUN586
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.23

PET-UNK-1320d94d-7_1



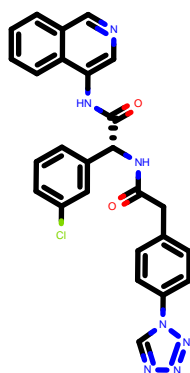
CID:	PET-UNK-1320d94d-7_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)C@H](c3ccccc3)C1NC(=O)C@H](C4CC[C@H]4)O1NSCCCC5</chem>
RUN:	RUN728
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.21

EDJ-MED-ee07cf00-3_2



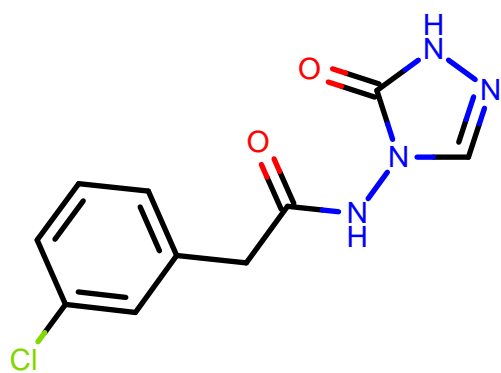
CID:	EDJ-MED-ee07cf00-3_2
SMILES:	<chem>Cn1c2c(en1)c(=O)n(en2)CC(=O)N[C@@H](c3ccccc(c3)Cl)C(=O)Nc4nc5c5c4ccc5</chem>
RUN:	RUN569
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.20

EDJ-MED-ee07cf00-15_1



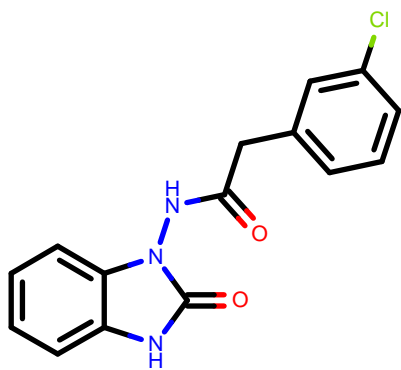
CID:	EDJ-MED-ee07cf00-15_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccccc(c3)Cl)NC(=O)Cc4ccc(cc4)n5cn[nH]5</chem>
RUN:	RUN599
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.25

JAN-GHE-5a013bed-4_1



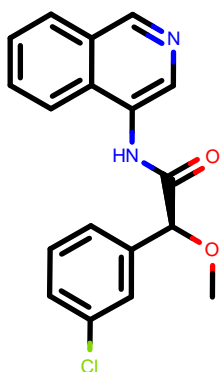
CID:	JAN-GHE-5a013bed-4_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2cn[nH]c2=O</chem>
RUN:	RUN66
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.13

VLA-UNK-dc1d9354-1_1



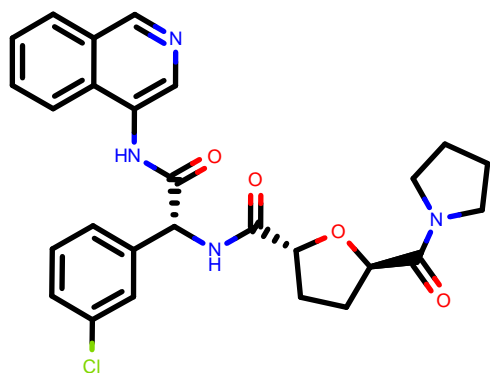
CID:	VLA-UNK-dc1d9354-1_1
SMILES:	<chem>c1ccc2c(c1)[nH]c(=O)n2NC(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN684
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.15

VLA-UNK-9a7dc93f-7_1



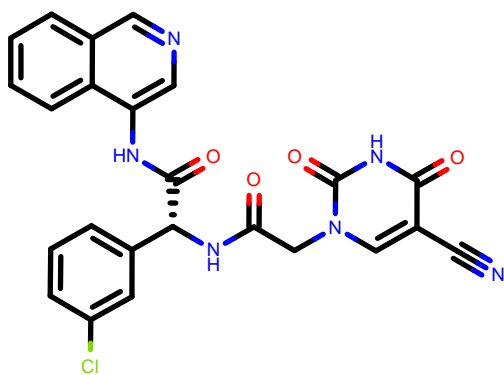
CID:	VLA-UNK-9a7dc93f-7_1
SMILES:	<chem>CO[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN581
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.04

EDJ-MED-ee07cf00-11_3



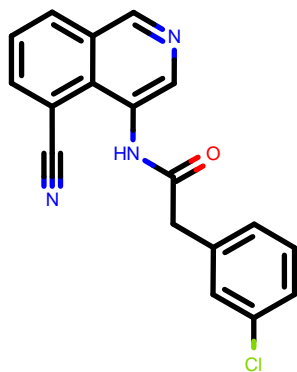
CID:	EDJ-MED-ee07cf00-11_3
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)C[C@@H](c4ccccc4)N5CCCC5</chem>
RUN:	RUN590
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.20

EDJ-MED-ee07cf00-8_1



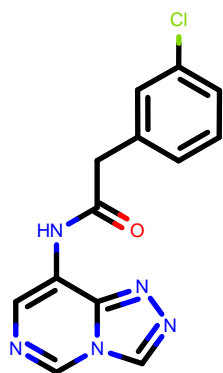
CID:	EDJ-MED-ee07cf00-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cn4cc(c(=O)[nH]c4=O)C#N</chem>
RUN:	RUN574
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.17

PET-UNK-6314f867-3_1



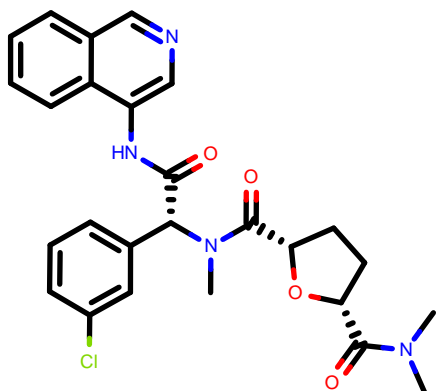
CID:	PET-UNK-6314f867-3_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)C#N</chem>
RUN:	RUN702
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.13

EDJ-MED-076d6e64-1_1



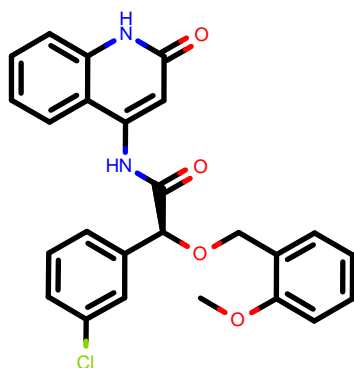
CID:	EDJ-MED-076d6e64-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncn3c2nnc3</chem>
RUN:	RUN713
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.12

PET-UNK-1320d94d-21_1



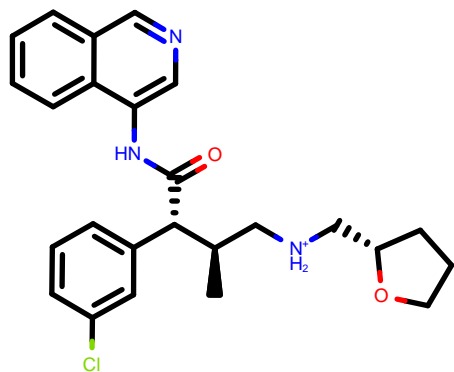
CID:	PET-UNK-1320d94d-21_1
SMILES:	<chem>CN(C)C(=O)[C@H]1CC[C@H](O1)C(=O)N(C)[C@H](c2ccccc2)C(=O)Nc3ncoc4c3ccoc4</chem>
RUN:	RUN732
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.22

ADA-UCB-6c2cb422-11_1



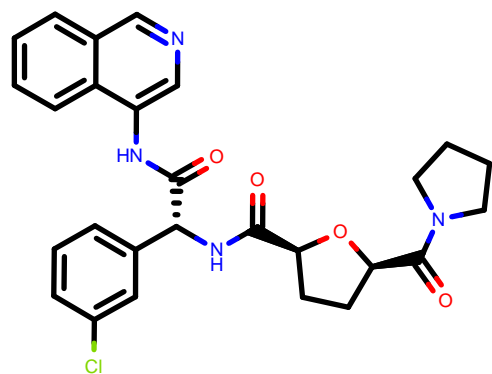
CID:	ADA-UCB-6c2cb422-11_1
SMILES:	<chem>COc1ccccc1CO[C@@H](c2ccccc2)C(=O)Nc3cc(=O)[nH]c4c3ccccc4</chem>
RUN:	RUN158
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.23

MAK-UNK-ffc90da7-4_6



CID:	MAK-UNK-ffc90da7-4_6
SMILES:	<chem>C[C@H](C)[C@H](N)C[C@H](c1ccccc1)C(=O)Nc2cncoc2</chem>
RUN:	RUN393
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.20

MAT-POS-7174c657-6_1



CID: MAT-POS-7174c657-6_1

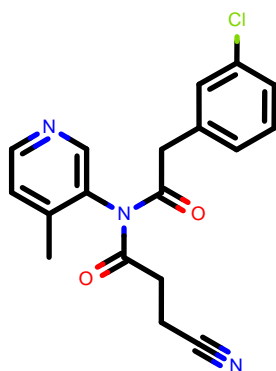
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](C)[c3cccc(c3)C]NC(=O)[C@@H](C)C[C@@H](O4)C1=O9NSCCCC5

RUN: RUN798

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.23

DAR-DIA-56cf811e-4_1



CID: DAR-DIA-56cf811e-4_1

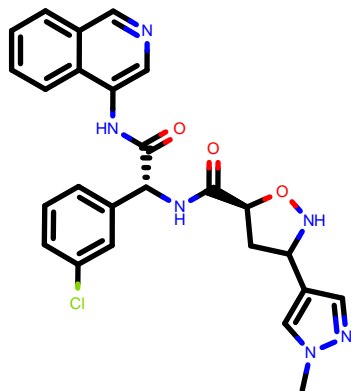
SMILES: Cc1ccncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)C=C/C#N

RUN: RUN524

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.20

EDJ-MED-ee07cf00-6_3



CID: EDJ-MED-ee07cf00-6_3

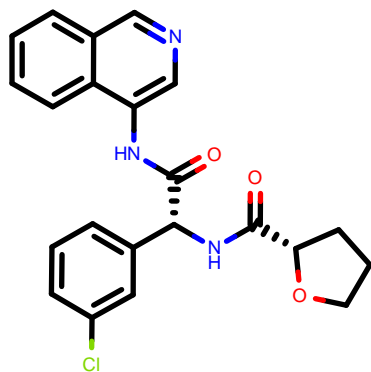
SMILES: Cn1cc(en1)C2=NO[C@@H](C2)C(=O)N[C@@H](c3cccc(c3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN584

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.19

EDJ-MED-cf4b0d25-3_1



CID: EDJ-MED-cf4b0d25-3_1

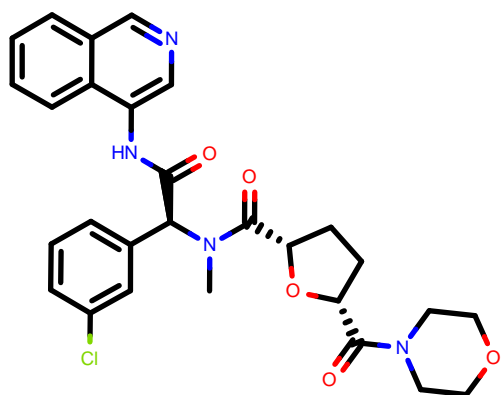
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](C)[c3cccc(c3)C]NC(=O)[C@@H](C)C4CCCO4

RUN: RUN627

DDG (kcal/mol): -1.26

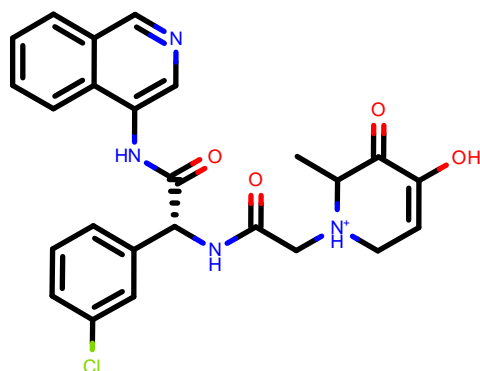
dDDG (kcal/mol): 0.16

PET-UNK-1320d94d-24_1



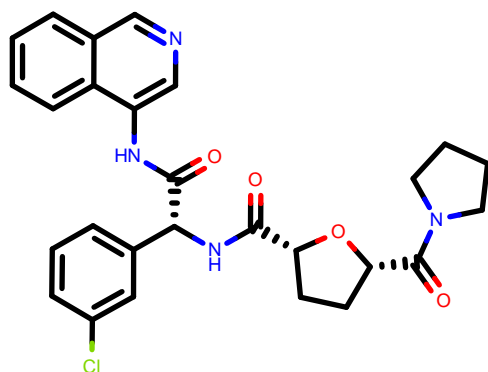
CID:	PET-UNK-1320d94d-24_1
SMILES:	<chem>CN(C@H)(c1ccc(c1)C)C(=O)Nc2ccc3c2ccc3C(-O)(C@H)C4C@H)(O4)C(-O)N5CCCC5</chem>
RUN:	RUN750
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.24

EDJ-MED-ee07cf00-7_2



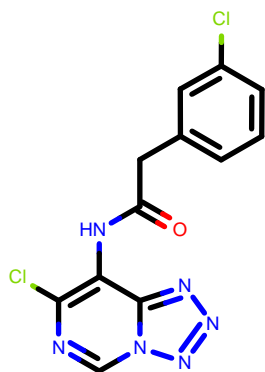
CID:	EDJ-MED-ee07cf00-7_2
SMILES:	<chem>Cc1c(c(=O)ccn1CC(=O)N)C@H)(c2ccc(c2)C)C(=O)Nc3ccc4c3ccc4[O-]</chem>
RUN:	RUN575
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.24

MAT-POS-8293a91a-7_1



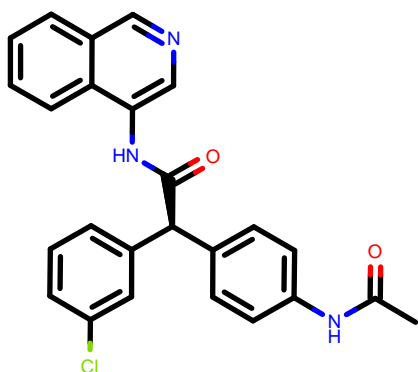
CID:	MAT-POS-8293a91a-7_1
SMILES:	<chem>c1ccc2c(c1)ccc2N(C(=O)N)C@H)(c3ccc(c3)C)N(C(=O)N)C4C@H)(O4)C(-O)N5CCCC5</chem>
RUN:	RUN770
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.22

EDJ-MED-c8e7a002-8_1



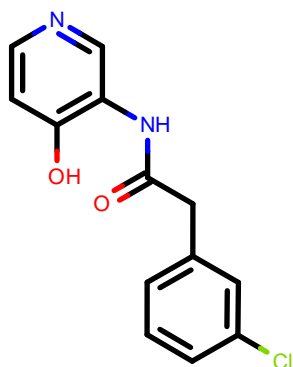
CID:	EDJ-MED-c8e7a002-8_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3nnnn3cnc2Cl</chem>
RUN:	RUN301
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.15

MIC-UNK-d36ab305-1_1



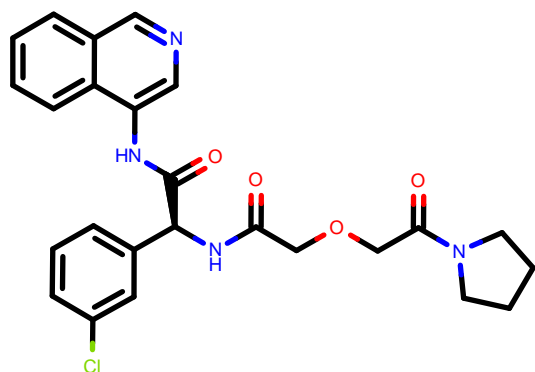
CID:	MIC-UNK-d36ab305-1_1
SMILES:	<chem>CC(=O)Nc1ccc(cc1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3ccc4c3cccc4</chem>
RUN:	RUN240
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.18

ALP-POS-95b75b4d-6_1



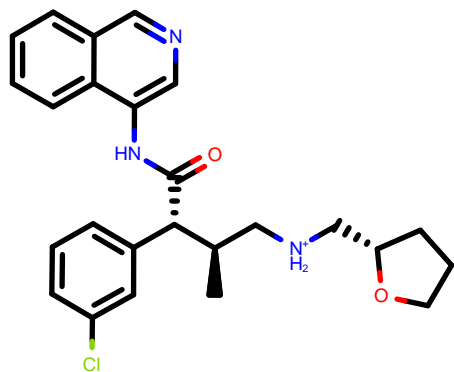
CID:	ALP-POS-95b75b4d-6_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c[nH]ccc2=O</chem>
RUN:	RUN39
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.12

EDJ-MED-cf4b0d25-1_2



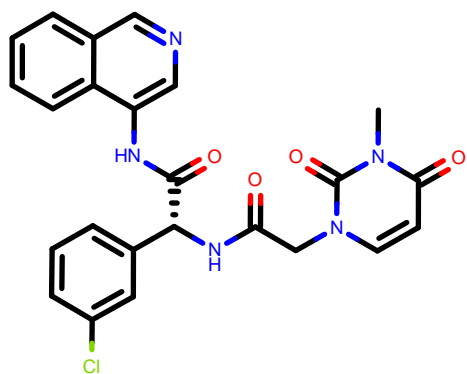
CID:	EDJ-MED-cf4b0d25-1_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)COCC(=O)N4CCCC4</chem>
RUN:	RUN705
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.22

MAK-UNK-c749d764-22_6



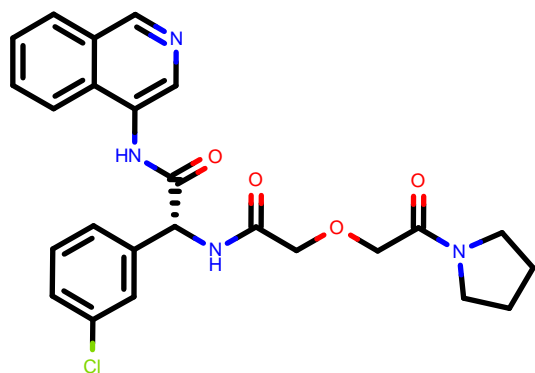
CID:	MAK-UNK-c749d764-22_6
SMILES:	<chem>C[C@H](C)[C](NH2+)[C]C@H1CCCCO1[C@H](c2cccc(c2)Cl)C(=O)Nc3ccc4c3cccc4</chem>
RUN:	RUN454
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.19

EDJ-MED-ee07cf00-1_2



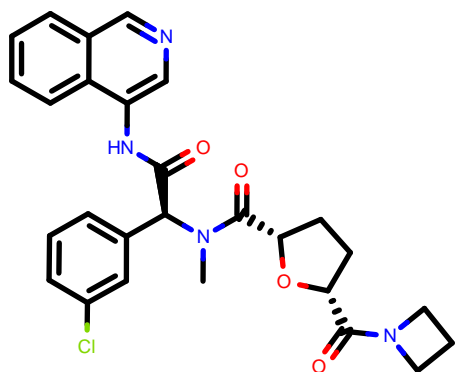
CID:	EDJ-MED-ee07cf00-1_2
SMILES:	<chem>Cn1c(=O)ccn(c1=O)CC(=O)N[C@H](c2cccc(c2)C)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN566
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.16

EDJ-MED-cf4b0d25-1_1



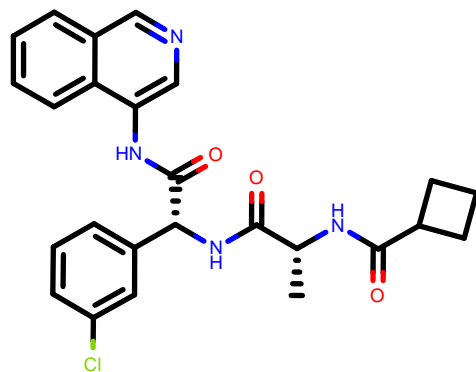
CID:	EDJ-MED-cf4b0d25-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)C)NC(=O)COCC(=O)N4CCCC4</chem>
RUN:	RUN703
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.19

PET-UNK-1320d94d-26_1



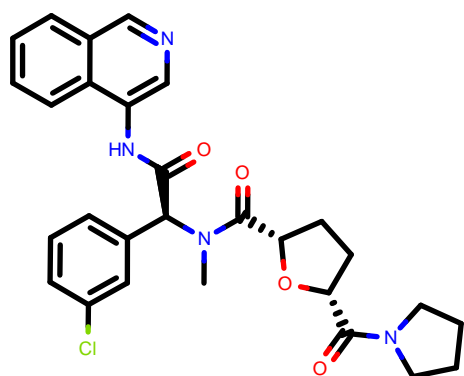
CID:	PET-UNK-1320d94d-26_1
SMILES:	<chem>CN[C@@H](c1cccc(c1)C)C(=O)Nc2cncc3c2cccc3C(=O)C@@H4C[C@@H](O4)C(=O)N5CCCC5</chem>
RUN:	RUN745
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.24

EDJ-MED-ee07cf00-4_4



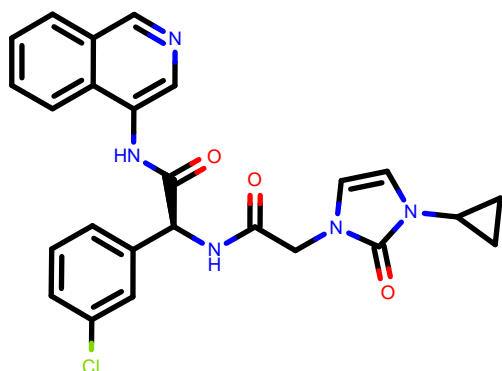
CID:	EDJ-MED-ee07cf00-4_4
SMILES:	<chem>C[C@@H](C(=O)N[C@H](c1cccc(c1)C)C(=O)Nc2cncc3c2cccc3)NC(=O)C4CC4</chem>
RUN:	RUN612
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.21

ALP-POS-a9ad2217-2_1



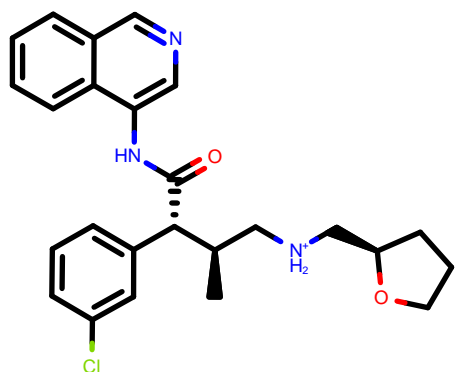
CID:	ALP-POS-a9ad2217-2_1
SMILES:	<chem>CN[C@@H](c1cccc(c1)C(=O)Nc2ccc3c2ccc3C(=O)C[C@@H]4CC[C@H]4)C(=O)N5CCCC5</chem>
RUN:	RUN723
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.21

EDJ-MED-ee07cf00-18_2



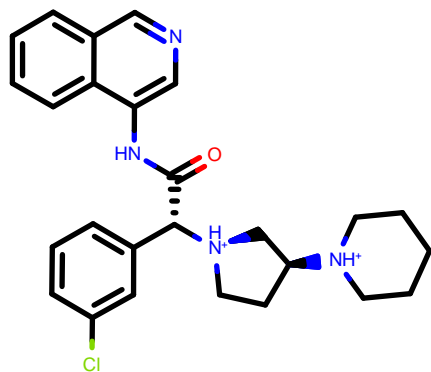
CID:	EDJ-MED-ee07cf00-18_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)C)N(C=O)CN4CCN(C4=O)C5CC5</chem>
RUN:	RUN608
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.22

MAK-UNK-ffc90da7-4_8



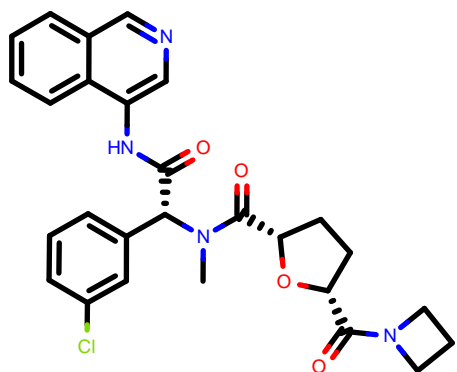
CID:	MAK-UNK-ffc90da7-4_8
SMILES:	<chem>C[C@@H](C[NH2+][C@@H]1CCCCO1)[C@@H](c2ccccc2)C(=O)Nc3cccc4c3ccc4</chem>
RUN:	RUN405
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.25

MIC-UNK-5a93dd5f-12_3



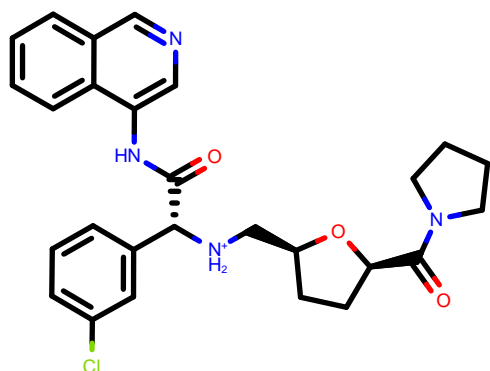
CID:	MIC-UNK-5a93dd5f-12_3
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C)N@HCC[C@@H](C4)N[H+]5CCCC5</chem>
RUN:	RUN443
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.19

PET-UNK-1320d94d-25_1



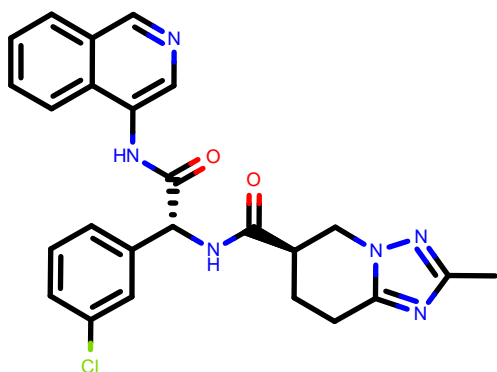
CID:	PET-UNK-1320d94d-25_1
SMILES:	<chem>CN1C=CNc2ccccc2C(=O)C(C)C(=O)N5CCCC5</chem>
RUN:	RUN747
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.20

EDJ-MED-cf4b0d25-2_1



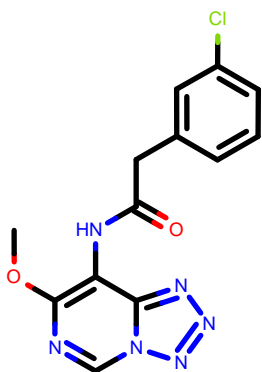
CID:	EDJ-MED-cf4b0d25-2_1
SMILES:	<chem>C1CC2C1)NCC(=O)C(C)C(=O)N3CCCC3C(=O)N4CCCC4</chem>
RUN:	RUN648
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.36

MAT-POS-a13804f0-1_3



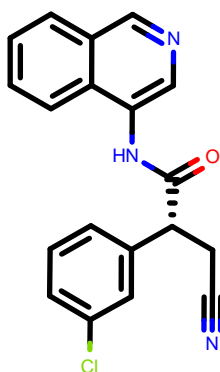
CID:	MAT-POS-a13804f0-1_3
SMILES:	<chem>Cc1nc2n(n1)C(C)C(=O)N(C)C(=O)N3CCCC3C(=O)N4CCCC4</chem>
RUN:	RUN617
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.17

EDJ-MED-97c1bf5c-2_1



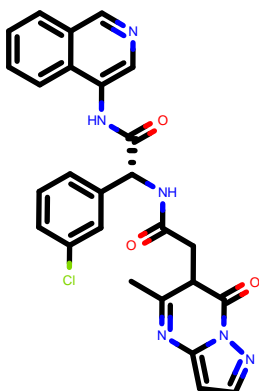
CID:	EDJ-MED-97c1bf5c-2_1
SMILES:	<chem>COc1c(c2nnnn2cn1)NC(=O)Cc3ccccc3Cl</chem>
RUN:	RUN335
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.11

JOH-UNI-ee5ed7c8-6_2



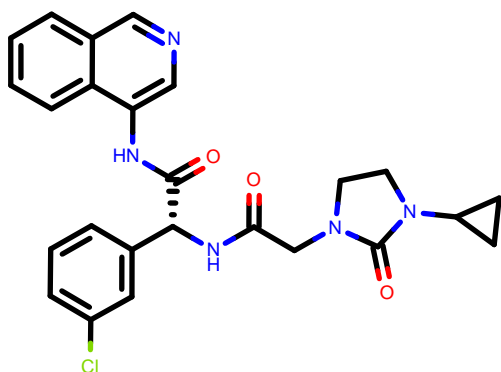
CID:	JOH-UNI-ee5ed7c8-6_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CC#N)c3cccc(c3)Cl</chem>
RUN:	RUN535
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.12

EDJ-MED-ee07cf00-2_2



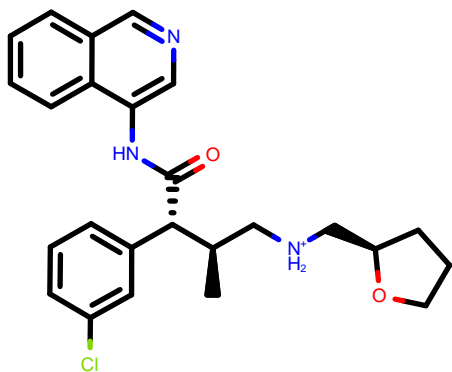
CID:	EDJ-MED-ee07cf00-2_2
SMILES:	<chem>Cc1c(c(O)n2c(n1)cd[nH]2)CC(=O)N[C@H](c3cccc(c3)C)C(=O)Nc4ncc5o4cccc5</chem>
RUN:	RUN567
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.18

EDJ-MED-ee07cf00-18_1



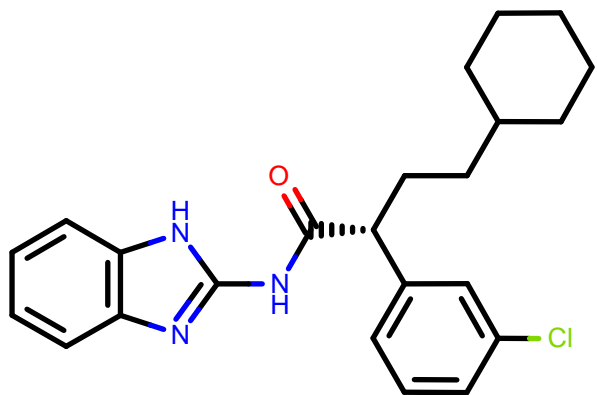
CID:	EDJ-MED-ee07cf00-18_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)C)NC(=O)CN4CCN(C4=O)C5CC5</chem>
RUN:	RUN606
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.23

MAK-UNK-c749d764-22_8



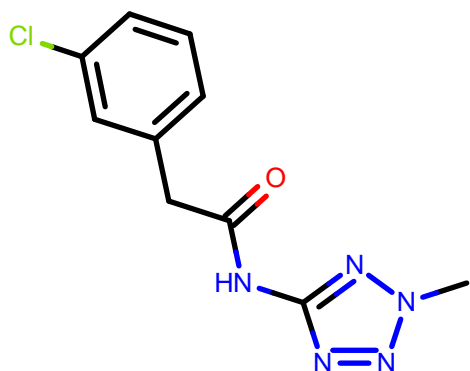
CID:	MAK-UNK-c749d764-22_8
SMILES:	<chem>C[C@H](C)[NH2+][C][C@H]1CCCCO1[C@H](c2ccccc2)C)C(=O)Nc3nccc4c3cccc4</chem>
RUN:	RUN474
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.25

ALP-POS-3fc1724e-8_2



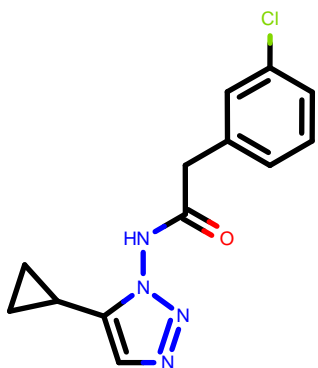
CID:	ALP-POS-3fc1724e-8_2
SMILES:	<chem>c1ccc2c(c1)[nH]c(n2)NC(=O)[C@H](CCC3CCCCC3)c4ccc(c4)Cl</chem>
RUN:	RUN171
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.29

VLA-UNK-411a133b-1_1



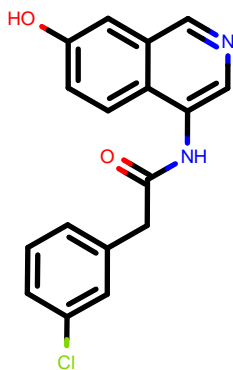
CID:	VLA-UNK-411a133b-1_1
SMILES:	<chem>Cn1nc(nn1)NC(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN685
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.12

JAN-GHE-f4ca5a00-17_1



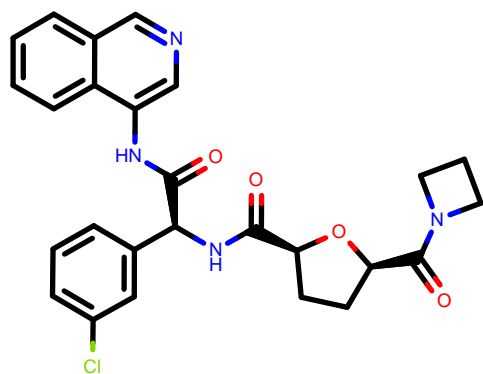
CID:	JAN-GHE-f4ca5a00-17_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2c(cnn2)C3CC3</chem>
RUN:	RUN159
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.13

MAT-POS-bb423b95-8_1



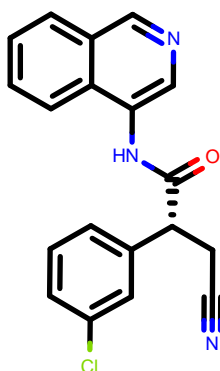
CID:	MAT-POS-bb423b95-8_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cnc3c2ccc(c3)O</chem>
RUN:	RUN262
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.10

PET-UNK-1320d94d-6_1



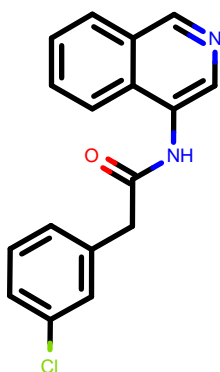
CID:	PET-UNK-1320d94d-6_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3cccc(c3)C)NC(=O)C@@H4C[C@@H](O4)C(=O)N5CCCC5</chem>
RUN:	RUN741
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.19

JOH-UNI-3fc3434e-6_2



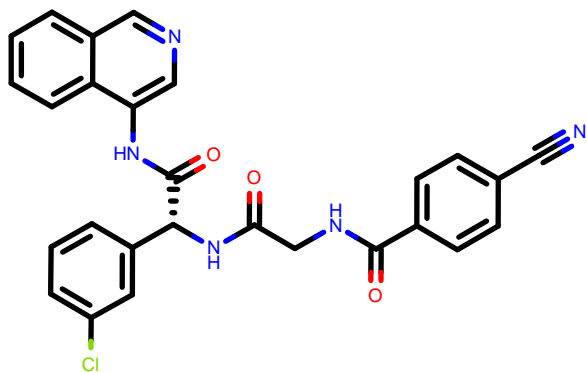
CID:	JOH-UNI-3fc3434e-6_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CC#N)c3cccc(c3)Cl</chem>
RUN:	RUN547
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.14

RUB-POS-1325a9ea-17_1



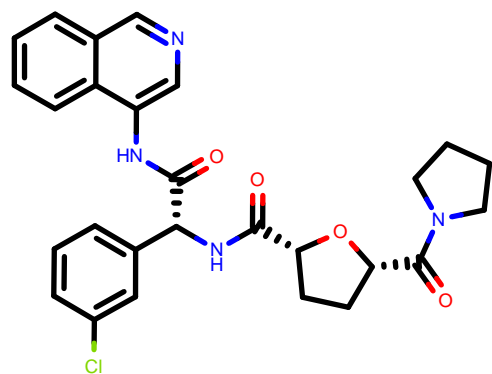
CID:	RUB-POS-1325a9ea-17_1
SMILES:	<chem>c1ccc2c(c1)c(cnc2F)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN672
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.03

EDJ-MED-ee07cf00-5_1



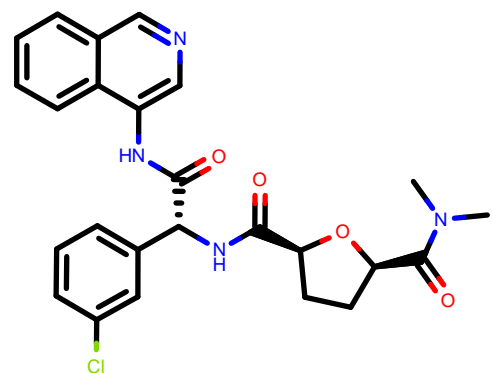
CID:	EDJ-MED-ee07cf00-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)C)NC(=O)CNC(=O)c4ccc(cc4)C#N</chem>
RUN:	RUN607
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.21

PET-UNK-ac320b15-9_1



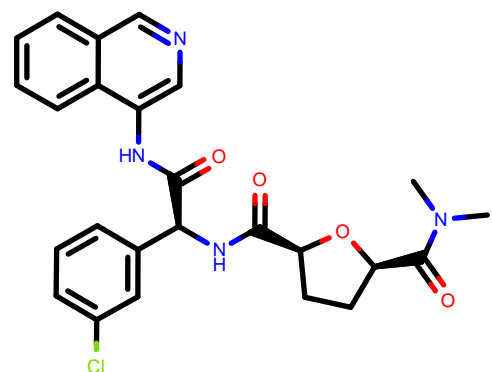
CID:	PET-UNK-ac320b15-9_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N[C@@H](C(=O)N[C@@H](C3CCCC3)N[C@@H](C(=O)N[C@@H](C4CCCC4)O)N6CCCC6</chem>
RUN:	RUN768
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.20

PET-UNK-1320d94d-1_1



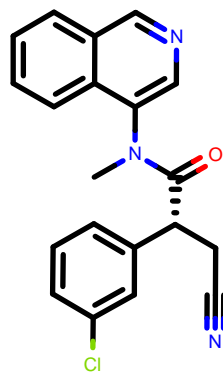
CID:	PET-UNK-1320d94d-1_1
SMILES:	<chem>CN(C)C(=O)[C@@H](C(=O)N[C@@H](O1)C(=O)N[C@@H](C2CCCC2)C)C(=O)Nc3nccc4c3cccc4</chem>
RUN:	RUN727
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.19

PET-UNK-1320d94d-2_1



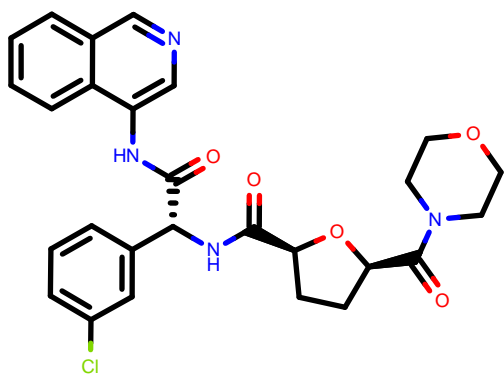
CID:	PET-UNK-1320d94d-2_1
SMILES:	<chem>CN(C)C(=O)[C@@H](C(=O)N[C@@H](O1)C(=O)N[C@@H](C2CCCC2)C)C(=O)Nc3nccc4c3cccc4</chem>
RUN:	RUN729
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.21

JOH-UNI-ee5ed7c8-7_2



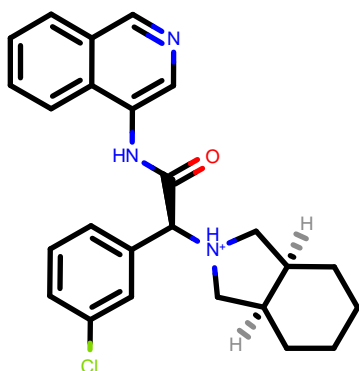
CID:	JOH-UNI-ee5ed7c8-7_2
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)[C@@H](C(=O)N[C@@H](C#N)c3cccc(c3)Cl</chem>
RUN:	RUN542
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.27

PET-UNK-1320d94d-3_1



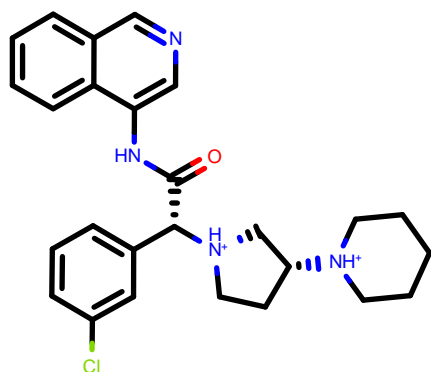
CID:	PET-UNK-1320d94d-3_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)N[C@@H](C4=CC=C4)N5CCOCC5</chem>
RUN:	RUN736
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.20

MIC-UNK-5a93dd5f-2_2



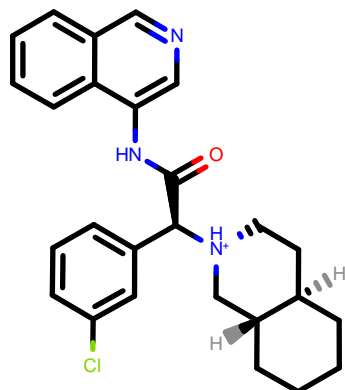
CID:	MIC-UNK-5a93dd5f-2_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc3)C(=O)N[C@@H](C4=CC=C4)N5C6CCCCC5C6</chem>
RUN:	RUN351
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.23

MIC-UNK-5a93dd5f-12_5



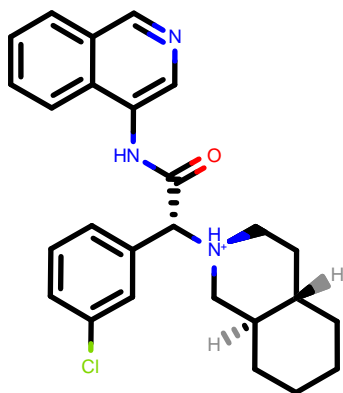
CID:	MIC-UNK-5a93dd5f-12_5
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)N[C@@H](C4=CC=C4)N5C6CCCCC56</chem>
RUN:	RUN445
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.18

MIC-UNK-5a93dd5f-3_6



CID:	MIC-UNK-5a93dd5f-3_6
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc3)C(=O)N[C@@H](C4=CC=C4)N5C6CCCCC56</chem>
RUN:	RUN370
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.20

MIC-UNK-5a93dd5f-3_11



CID: MIC-UNK-5a93dd5f-3_11

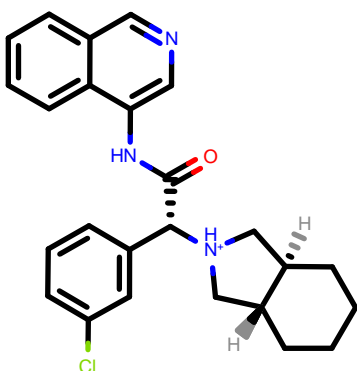
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc(c3)Cl)N@H4CC[C@@H]5CCCC[C@H]5C4

RUN: RUN396

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.22

MIC-UNK-5a93dd5f-2_3



CID: MIC-UNK-5a93dd5f-2_3

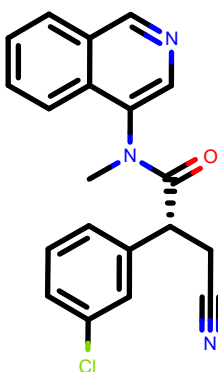
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc(c3)Cl)N+4C[C@H]5CCCC[C@H]5C4

RUN: RUN356

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.22

JOH-UNI-3fc3434e-7_2



CID: JOH-UNI-3fc3434e-7_2

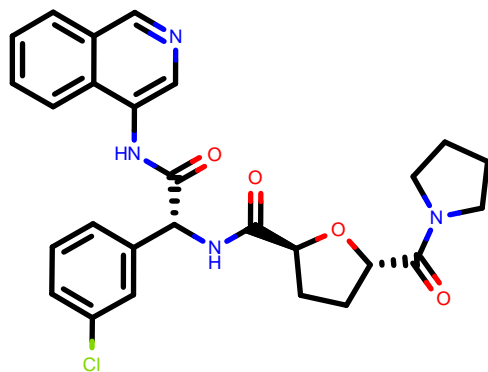
SMILES: CN(c1cnc2c1cccc2)C(=O)[C@H](CC#N)c3ccccc(c3)Cl

RUN: RUN556

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.24

EDJ-MED-ee07cf00-11_5



CID: EDJ-MED-ee07cf00-11_5

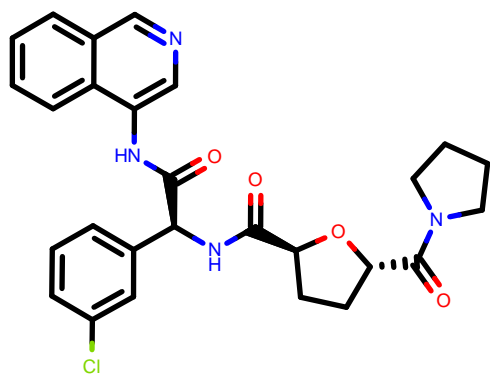
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc(c3)Cl)N[C@@H]4C[C@H](O4)C5=CNCC5

RUN: RUN598

DDG (kcal/mol): -0.70

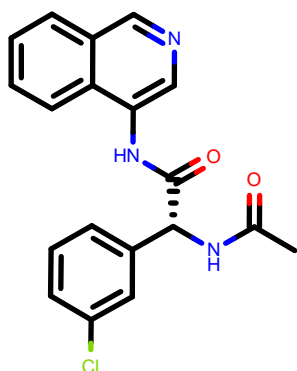
dDDG (kcal/mol): 0.21

PET-UNK-ac320b15-8_1



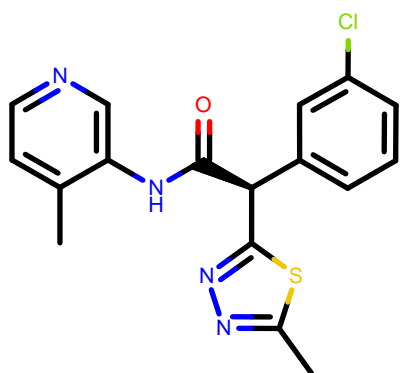
CID:	PET-UNK-ac320b15-8_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N[C@@H](C(=O)N[C@@H](c3ccccc3)C)N[C@@H](C(=O)Nc4cncnc4)O[C@@H](C5=CNCC5)C6=CC=CC=C6</chem>
RUN:	RUN760
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.25

EDJ-MED-cf4b0d25-4_2



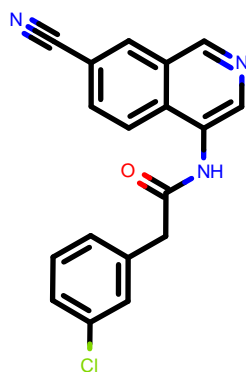
CID:	EDJ-MED-cf4b0d25-4_2
SMILES:	<chem>CC(=O)N[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncnc2c3ccccc3</chem>
RUN:	RUN622
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.14

TRY-UNI-9f475305-3_1



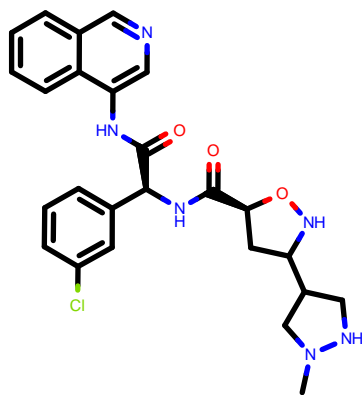
CID:	TRY-UNI-9f475305-3_1
SMILES:	<chem>Cc1ccncc1NC(=O)[C@@H](c2ccccc2)C)N[C@@H](c3nnc(s3)C</chem>
RUN:	RUN69
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.14

PET-UNK-6314f867-2_1



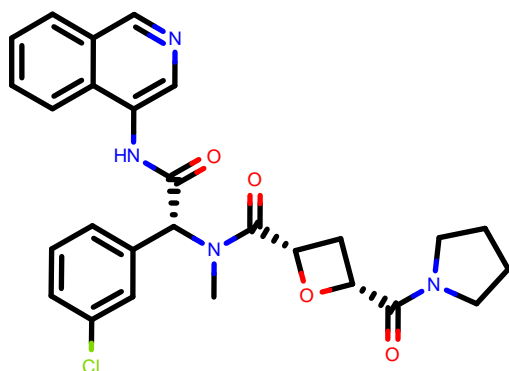
CID:	PET-UNK-6314f867-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncnc2c3ccccc3)C#N</chem>
RUN:	RUN700
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-6_1



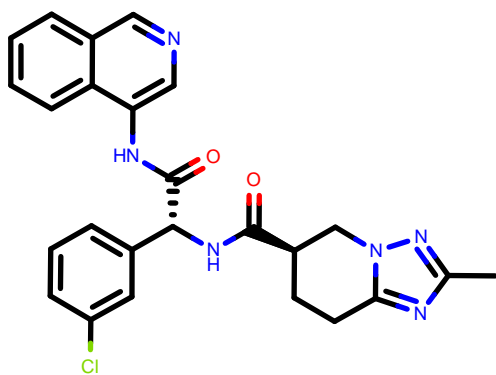
CID:	EDJ-MED-ee07cf00-6_1
SMILES:	<chem>Cn1cc(n1)C2=NO[C@@H](C2)C(=O)N[C@@H](c3ccccc3)C(=O)Nc4nccc5c4ccccc5</chem>
RUN:	RUN579
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.21

PET-UNK-1320d94d-27_1



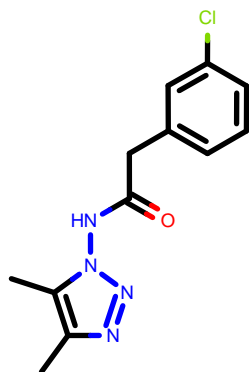
CID:	PET-UNK-1320d94d-27_1
SMILES:	<chem>CN[C@@H](c1ccccc1)C(=O)N[C@@H](C2=O)C(=O)N[C@@H](C2)C(=O)Nc3nccc4c3ccccc4</chem>
RUN:	RUN740
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.21

EDJ-MED-ee07cf00-13_2



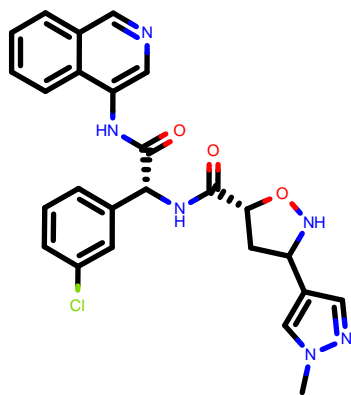
CID:	EDJ-MED-ee07cf00-13_2
SMILES:	<chem>Cc1nc2n(n1)C[C@@H](CC2)C(=O)N[C@@H](c3ccccc3)C(=O)Nc4nccc5c4ccccc5</chem>
RUN:	RUN594
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.19

JAN-GHE-5a013bed-1_1



CID:	JAN-GHE-5a013bed-1_1
SMILES:	<chem>Cc1c(n(nn1)NC(=O)Cc2cccc(c2)Cl)C</chem>
RUN:	RUN50
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.11

EDJ-MED-ee07cf00-6_4



CID: EDJ-MED-ee07cf00-6_4

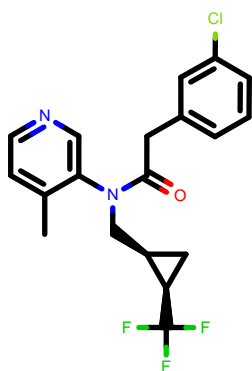
SMILES: Cn1cc(en1)C2=NO[C@H](C2)C(=O)N[C@H](c3ccccc(c3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN583

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.21

JOH-UNI-a38a7bdd-8_4



CID: JOH-UNI-a38a7bdd-8_4

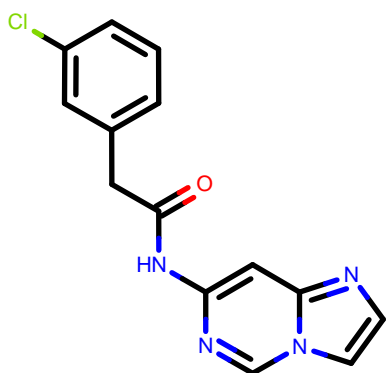
SMILES: Cc1ccncc1N(C[C@H]2C[C@H]2C(F)(F)F)C(=O)Cc3ccccc(c3)Cl

RUN: RUN486

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.15

JIN-POS-6dc588a4-17_1



CID: JIN-POS-6dc588a4-17_1

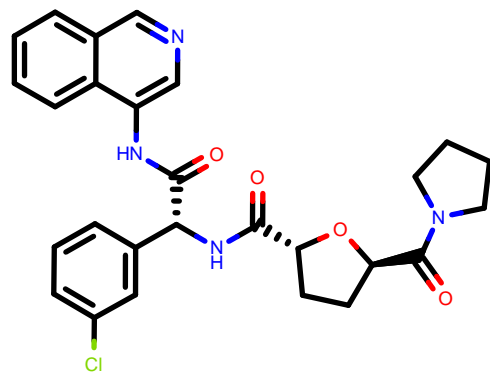
SMILES: c1cc(cc(c1)Cl)CC(=O)Nc2cc3nccn3cn2

RUN: RUN650

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.16

MAT-POS-8293a91a-2_1



CID: MAT-POS-8293a91a-2_1

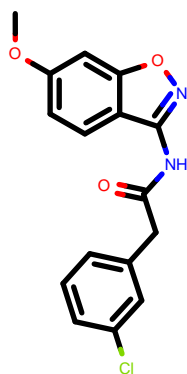
SMILES: c1ccc2c(c1)cncc2N[C@H](C[C@H](c3ccccc3)C)N[C@H](c4ccccc4)C(=O)N5CCCC5

RUN: RUN774

DDG (kcal/mol): -0.54

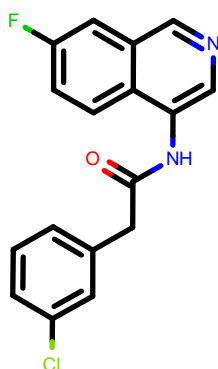
dDDG (kcal/mol): 0.20

EDJ-MED-c8e7a002-1_1



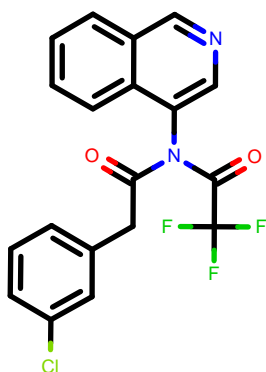
CID:	EDJ-MED-c8e7a002-1_1
SMILES:	<chem>COc1ccc2c(c1)onc2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN296
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.16

JIN-POS-6dc588a4-11_1



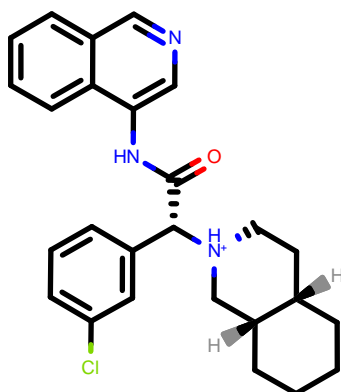
CID:	JIN-POS-6dc588a4-11_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)F</chem>
RUN:	RUN639
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.10

JOH-UNI-a38a7bdd-1_1



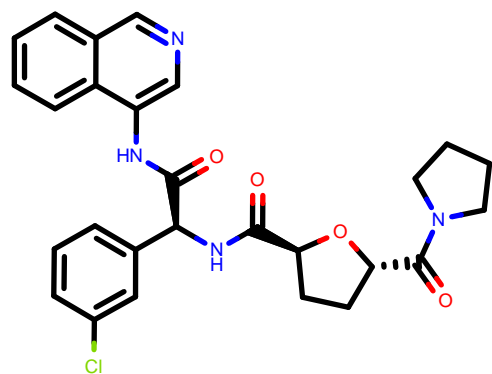
CID:	JOH-UNI-a38a7bdd-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)C(F)(F)F</chem>
RUN:	RUN487
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.18

MIC-UNK-5a93dd5f-3_1



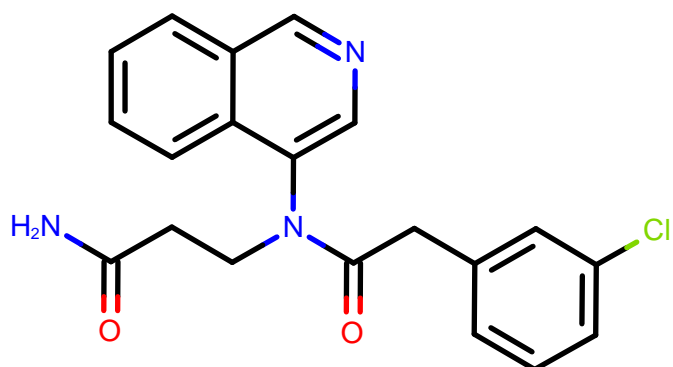
CID:	MIC-UNK-5a93dd5f-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@@H+]4CC[C@@H]5CCCC[C@@H]5C4</chem>
RUN:	RUN390
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.19

MAT-POS-8293a91a-6_2



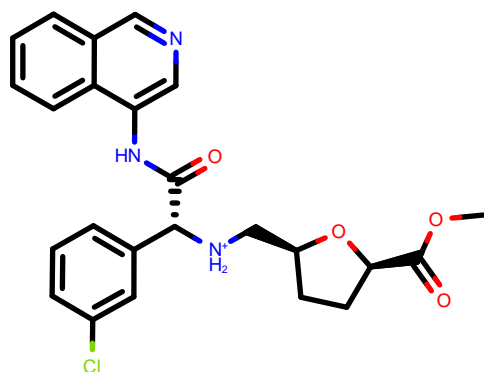
CID:	MAT-POS-8293a91a-6_2
SMILES:	<chem>c1ccc2c(c1)ncnc2N(C(=O)[C@@H](c3ccccc3)C)N(C(=O)C@H(C)O4C1=O)N6CCCC5</chem>
RUN:	RUN776
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.22

NAU-LAT-4ce8bf23-2_1



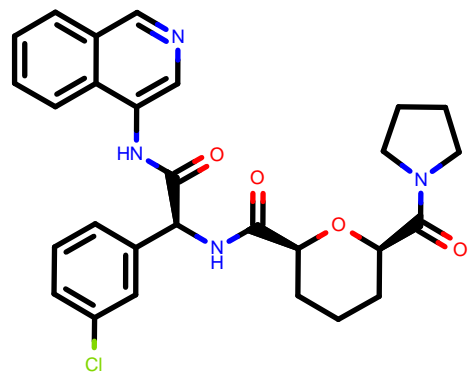
CID:	NAU-LAT-4ce8bf23-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(CCC(=O)N)C(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN462
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.25

MAT-POS-d8472c4f-2_2



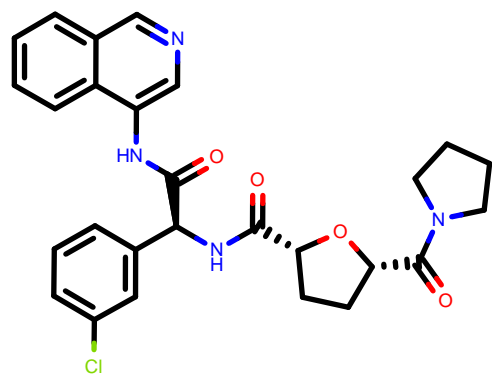
CID:	MAT-POS-d8472c4f-2_2
SMILES:	<chem>COC(=O)[C@H](C)C[C@@H](O)C1N[C@@H](C)C(=O)Nc3ccccc3</chem>
RUN:	RUN762
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.28

PET-UNK-1320d94d-10_1



CID:	PET-UNK-1320d94d-10_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N(C(=O)[C@@H](c3ccccc3)C)N(C(=O)C@H(C)O4C1=O)N6CCCC5</chem>
RUN:	RUN738
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.26

PET-UNK-ac320b15-10_1



CID: PET-UNK-ac320b15-10_1

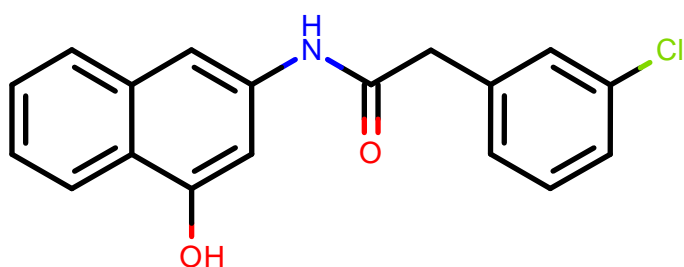
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)NC(=O)[C@H](O)C[C@H](O)N5CCCC5

RUN: RUN755

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.20

ROB-UNI-daaf9793-3_1



CID: ROB-UNI-daaf9793-3_1

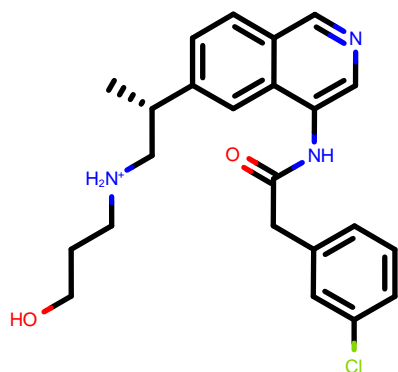
SMILES: c1ccc2c(c1)cc(cc2O)NC(=O)Cc3ccccc(c3)Cl

RUN: RUN689

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.13

MAK-UNK-ffc90da7-6_1



CID: MAK-UNK-ffc90da7-6_1

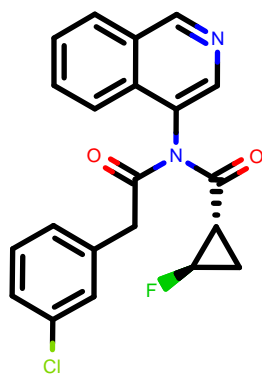
SMILES: C[C@@H](C[NH2+])CCCOc1ccc2cncc(c2c1)NC(=O)Cc3ccccc(c3)Cl

RUN: RUN415

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.18

JOH-UNI-a38a7bdd-5_3



CID: JOH-UNI-a38a7bdd-5_3

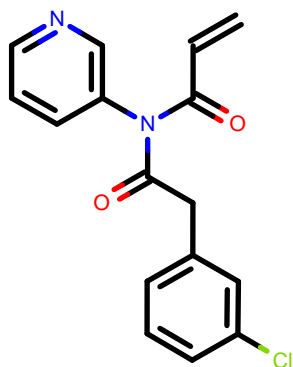
SMILES: c1ccc2c(c1)cncc2N(C(=O)Cc3ccccc(c3)Cl)C(=O)[C@@H](O)C[C@H](O)N4F

RUN: RUN497

DDG (kcal/mol): -0.43

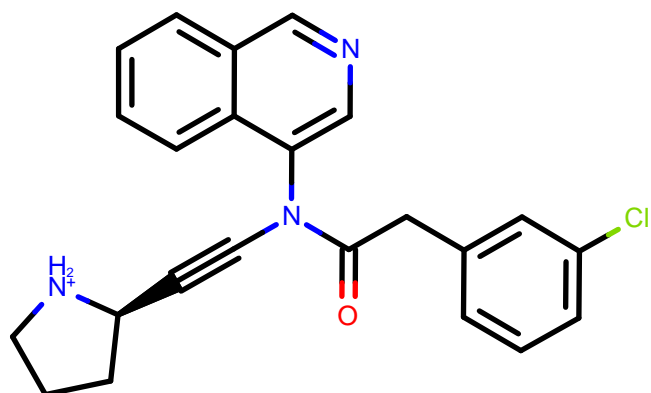
dDDG (kcal/mol): 0.21

PET-UNK-e8c7a26f-2_1



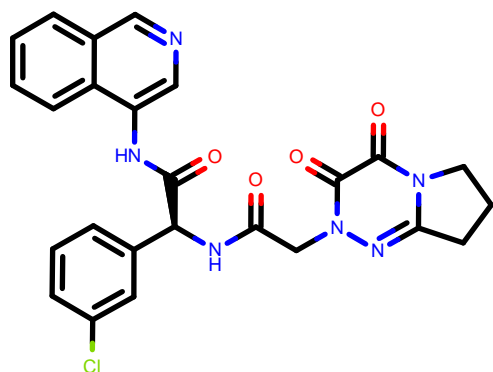
CID:	PET-UNK-e8c7a26f-2_1
SMILES:	<chem>C=CC(=O)N(c1ccnc1)C(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN611
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.17

DAR-DIA-076fb6ea-9_2



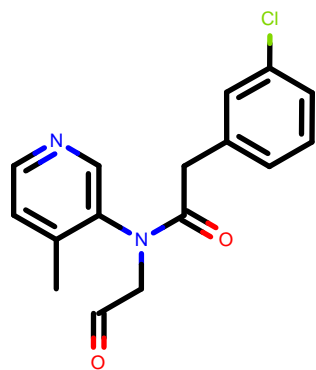
CID:	DAR-DIA-076fb6ea-9_2
SMILES:	<chem>c1ccc2c(c1)cncc2N(C#C[C@H]3CCCC[NH2+])C(=O)Cc4cccc(c4)Cl</chem>
RUN:	RUN473
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.36

EDJ-MED-ee07cf00-14_2



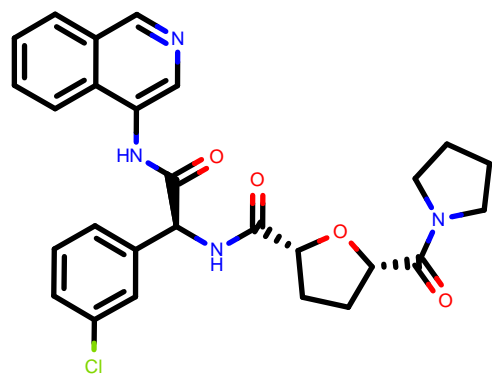
CID:	EDJ-MED-ee07cf00-14_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)Cn4c(c=O)c(=O)n5c(n4)CC5</chem>
RUN:	RUN601
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.23

PET-UNK-bbe8d7ff-1_1



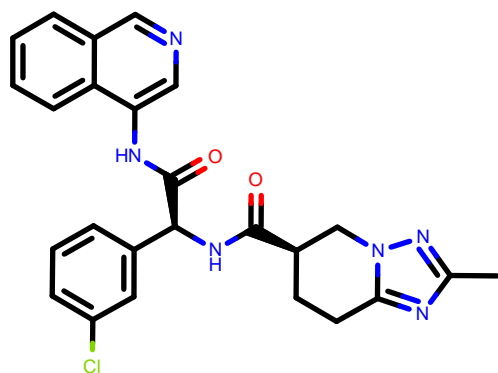
CID:	PET-UNK-bbe8d7ff-1_1
SMILES:	<chem>Cc1ccncc1N(CC=O)C(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN147
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.17

MAT-POS-8293a91a-7_2



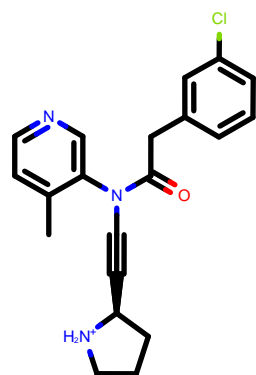
CID:	MAT-POS-8293a91a-7_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)C)NC(=O)[C@H]4CC[C@H](O4)C(=O)N5CCCC5</chem>
RUN:	RUN785
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.21

MAT-POS-a13804f0-1_1



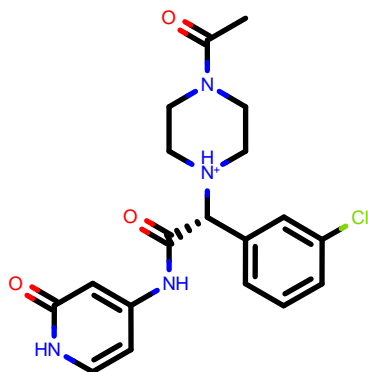
CID:	MAT-POS-a13804f0-1_1
SMILES:	<chem>Cc1nc2n(n1)C[C@@H](CC2)C(=O)N[C@@H](c3ccccc(c3)C)C(=O)Nc4cncc5c4ccccc5</chem>
RUN:	RUN616
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.22

DAR-DIA-076fb6ea-10_2



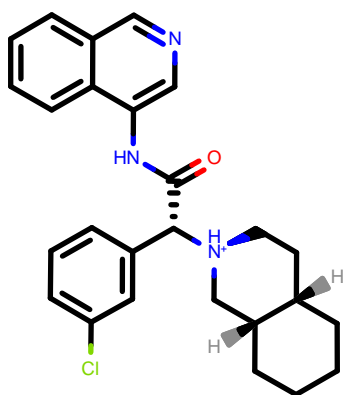
CID:	DAR-DIA-076fb6ea-10_2
SMILES:	<chem>Cc1ccncc1N(C#C[C@H]2CCC[NH2+]2)C(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN478
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.22

NAU-LAT-a5c7d7cb-6_2



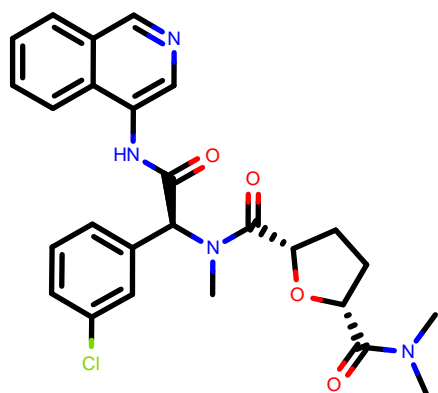
CID:	NAU-LAT-a5c7d7cb-6_2
SMILES:	<chem>CC(=O)N1CC[NH+](CC1)[C@H](c2ccccc(c2)Cl)C(=O)Nc3cc[nH]c(=O)c3</chem>
RUN:	RUN334
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.25

MIC-UNK-5a93dd5f-3_3



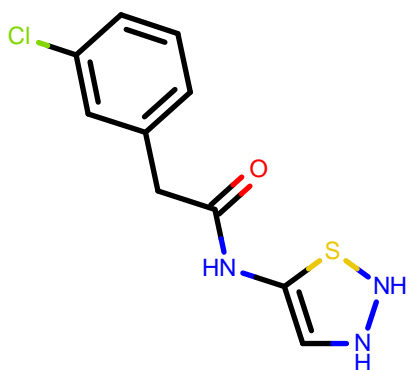
CID:	MIC-UNK-5a93dd5f-3_3
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)Cl)N@H+4CC[C@@H]5CCCC[C@@H]5C4</chem>
RUN:	RUN389
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.23

PET-UNK-1320d94d-22_1



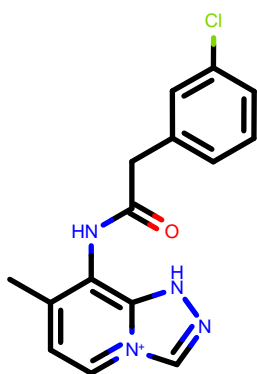
CID:	PET-UNK-1320d94d-22_1
SMILES:	<chem>CN(C)C(=O)[C@@H]1CC[C@H](O1)C(=O)N(C)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cccc4c3cccc4</chem>
RUN:	RUN731
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.17

JAN-GHE-5a013bed-6_1



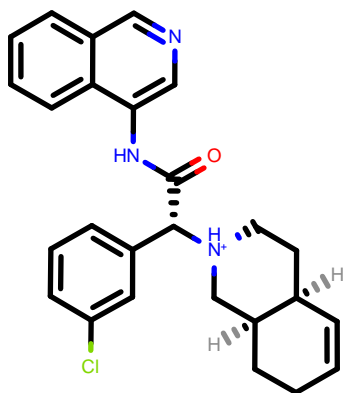
CID:	JAN-GHE-5a013bed-6_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cnns2</chem>
RUN:	RUN60
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.13

EDJ-MED-c8e7a002-4_1



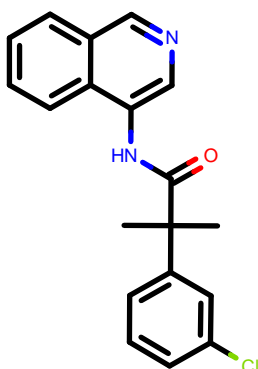
CID:	EDJ-MED-c8e7a002-4_1
SMILES:	<chem>Cc1ccn2cnnc2c1NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN300
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.15

MIC-UNK-5a93dd5f-3_13



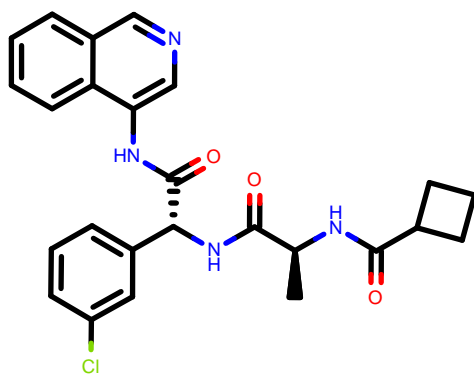
CID:	MIC-UNK-5a93dd5f-3_13
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)Cl)N@H4CC[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN402
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.20

NAU-LAT-2fed8305-1_1



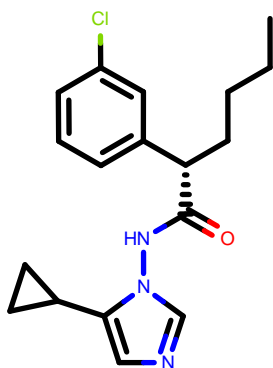
CID:	NAU-LAT-2fed8305-1_1
SMILES:	<chem>CC(C)(c1cccc(c1)Cl)C(=O)Nc2cncc3c2ccccc3</chem>
RUN:	RUN453
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.04

EDJ-MED-ee07cf00-4_3



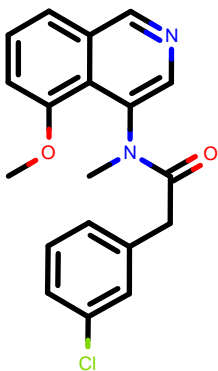
CID:	EDJ-MED-ee07cf00-4_3
SMILES:	<chem>C[C@@H](C(=O)N[C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2ccccc3)NC(=O)C4CCC4</chem>
RUN:	RUN609
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.20

JAN-GHE-f4ca5a00-18_1



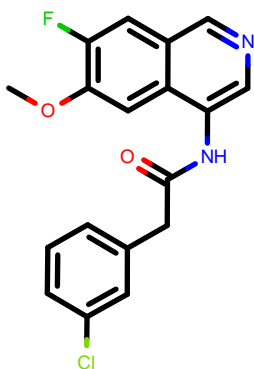
CID:	JAN-GHE-f4ca5a00-18_1
SMILES:	<chem>CCCC[C@@H](c1cccc(c1)Cl)C(=O)Nn2cncc2C3CC3</chem>
RUN:	RUN204
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.18

MIC-UNK-67d4a29a-4_1



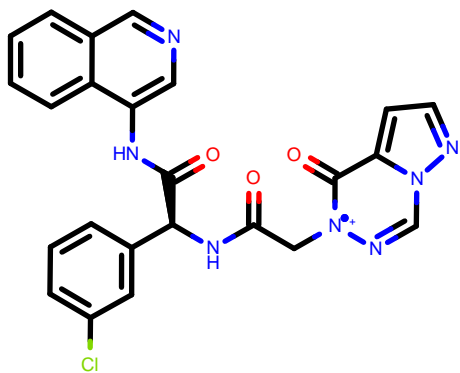
CID:	MIC-UNK-67d4a29a-4_1
SMILES:	<chem>CN(c1ccc2c1c(ccc2)OC)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN450
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.27

MAT-POS-29385cc1-1_1



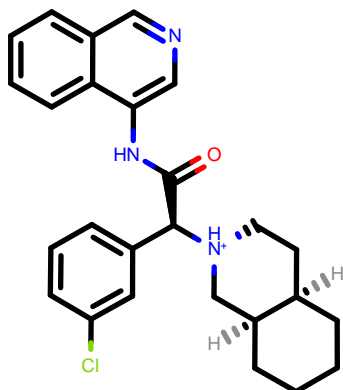
CID:	MAT-POS-29385cc1-1_1
SMILES:	<chem>COc1cc2c(cc1F)cncc2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN797
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-17_2



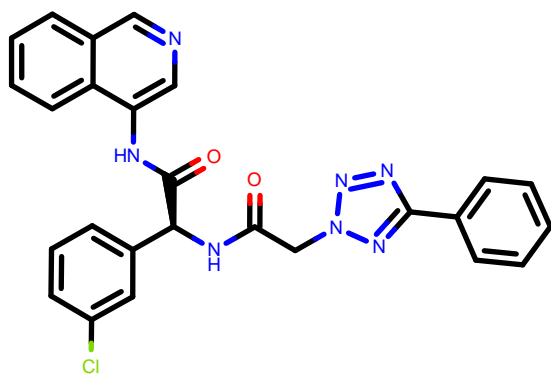
CID:	EDJ-MED-ee07cf00-17_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)O)NC(=O)Cn4c(=O)c5cn[nH]5c4</chem>
RUN:	RUN603
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.21

MIC-UNK-5a93dd5f-3_14



CID:	MIC-UNK-5a93dd5f-3_14
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@@H]4CC[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN391
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.27

EDJ-MED-ee07cf00-9_1



CID: EDJ-MED-ee07cf00-9_1

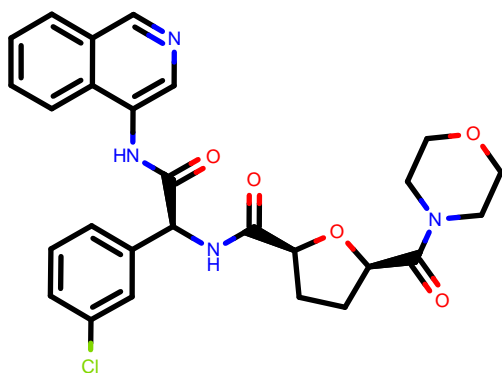
SMILES: c1ccc(cc1)c2nnc(n2)CC(=O)N[C@@H](c3ccccc(c3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN577

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.23

PET-UNK-1320d94d-4_1



CID: PET-UNK-1320d94d-4_1

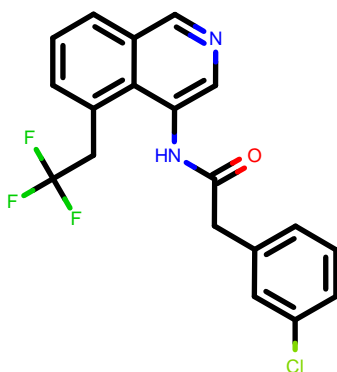
SMILES: c1ccc2c(c1)cnc2N[C@@H](C)[C@@H](c3ccccc3)C(=O)N[C@@H](C4CCOC4)C(=O)N5CCOCC5

RUN: RUN730

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.26

JOH-UNI-3fc3434e-3_1



CID: JOH-UNI-3fc3434e-3_1

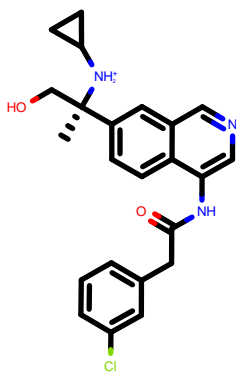
SMILES: c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)CC(F)(F)F

RUN: RUN537

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.14

MAK-UNK-ffc90da7-5_1



CID: MAK-UNK-ffc90da7-5_1

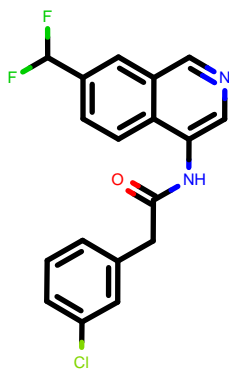
SMILES: C[C@@H](CO)(c1ccc2c(c1)cnc2N[C@@H](C)N)N[C@@H](C)C(=O)Nc3ccccc(c3)Cl

RUN: RUN362

DDG (kcal/mol): -0.22

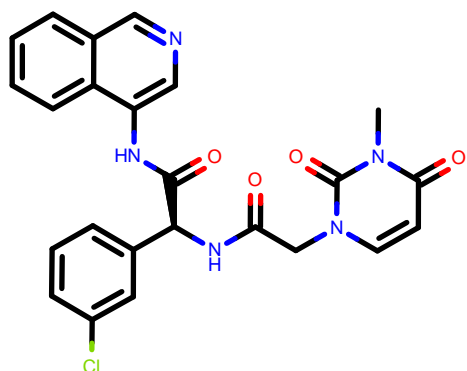
dDDG (kcal/mol): 0.18

MAT-POS-c0609ef7-1_1



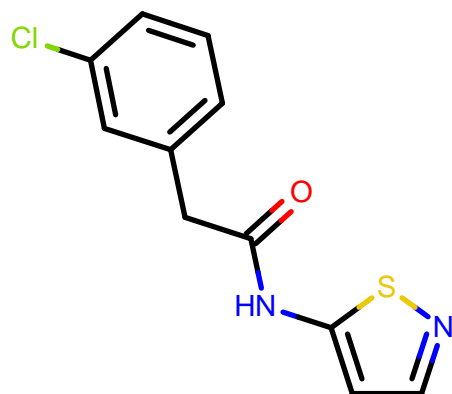
CID:	MAT-POS-c0609ef7-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)C(F)F</chem>
RUN:	RUN795
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.15

EDJ-MED-ee07cf00-1_1



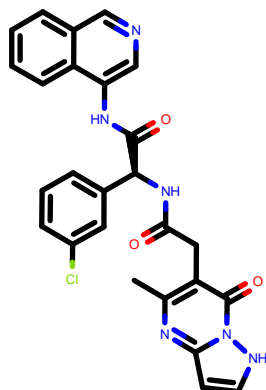
CID:	EDJ-MED-ee07cf00-1_1
SMILES:	<chem>Cn1c(=O)ccn(c1=O)CC(=O)N[C@@H](c2cccc(c2)Cl)C(=O)Nc3nccc4c3cccc4</chem>
RUN:	RUN564
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.17

PET-UNK-158bee2a-2_1



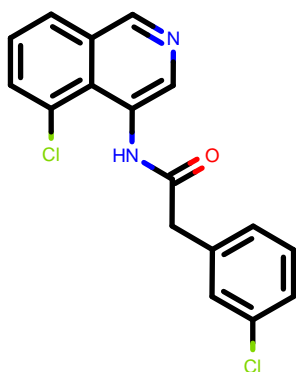
CID:	PET-UNK-158bee2a-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2ccns2</chem>
RUN:	RUN719
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-2_1



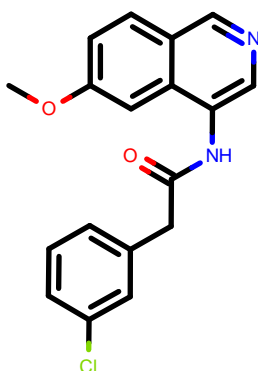
CID:	EDJ-MED-ee07cf00-2_1
SMILES:	<chem>Cc1c(c(=O)n2c(n1)cc[nH]2)CC(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4nccc5c4cccc5</chem>
RUN:	RUN571
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.23

MIC-UNK-50cce87d-2_1



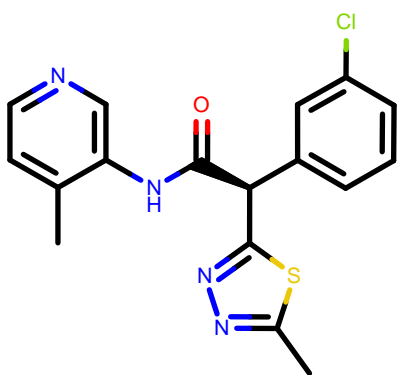
CID:	MIC-UNK-50cce87d-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)Cl</chem>
RUN:	RUN338
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.13

PET-UNK-8df914d1-1_1



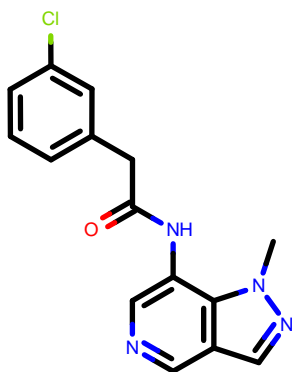
CID:	PET-UNK-8df914d1-1_1
SMILES:	<chem>COc1ccc2cncc(c2c1)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN206
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.13

SAM-UNK-2684b532-3_1



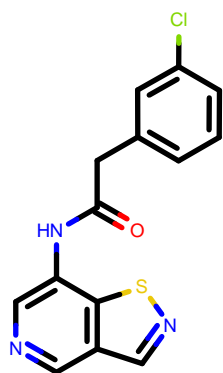
CID:	SAM-UNK-2684b532-3_1
SMILES:	<chem>Cc1cncc1NC(=O)[C@@H](c2cccc(c2)Cl)c3nnc(s3)C</chem>
RUN:	RUN140
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.14

PET-UNK-e274cad4-1_1



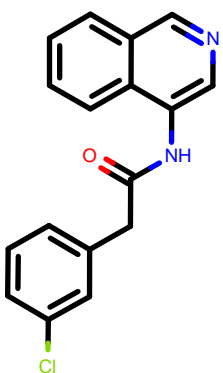
CID:	PET-UNK-e274cad4-1_1
SMILES:	<chem>Cn1c2c(cncc2NC(=O)Cc3cccc(c3)Cl)cn1</chem>
RUN:	RUN710
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.14

PET-UNK-b1ef24dc-2_1



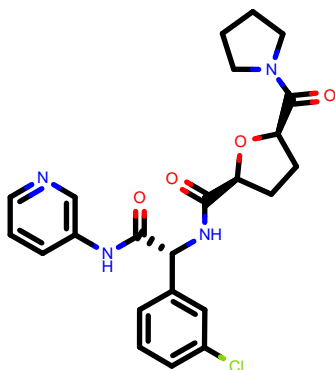
CID:	PET-UNK-b1ef24dc-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2snc3</chem>
RUN:	RUN715
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.11

MAT-POS-f7918075-5_1



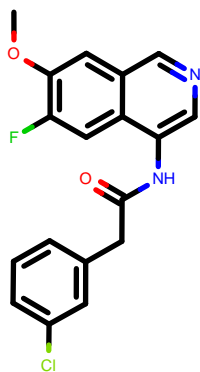
CID:	MAT-POS-f7918075-5_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cncc3</chem>
RUN:	RUN269
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.02

PET-UNK-ac320b15-3_1



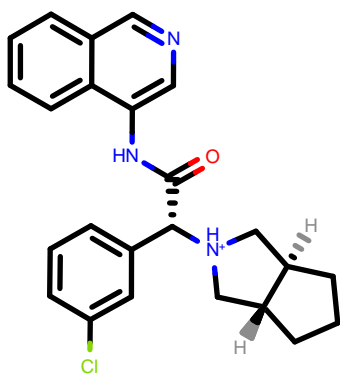
CID:	PET-UNK-ac320b15-3_1
SMILES:	<chem>c1cc(cc1)Cl[C@@H](C(=O)Nc2ccnc2)NC(=O)[C@@H]3CC[C@H](O3)C(=O)N4CCCC4</chem>
RUN:	RUN754
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.26

MAT-POS-29385cc1-2_1



CID:	MAT-POS-29385cc1-2_1
SMILES:	<chem>COc1cc2cncc(c2cc1F)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN794
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.14

MIC-UNK-5a93dd5f-1_3



CID: MIC-UNK-5a93dd5f-1_3

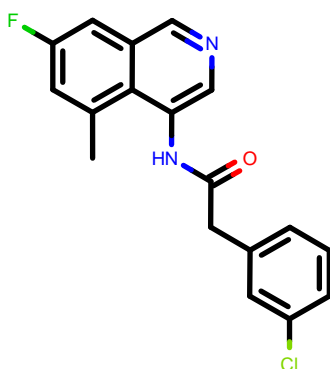
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](c3cccc(c3)Cl)[NH+]4C[C@H]5CCC[C@@H]5C4

RUN: RUN358

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.21

MAT-POS-29385cc1-4_1



CID: MAT-POS-29385cc1-4_1

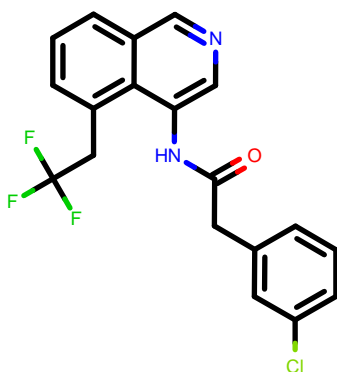
SMILES: Cc1cc(cc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl)F

RUN: RUN796

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.10

JOH-UNI-ee5ed7c8-3_1



CID: JOH-UNI-ee5ed7c8-3_1

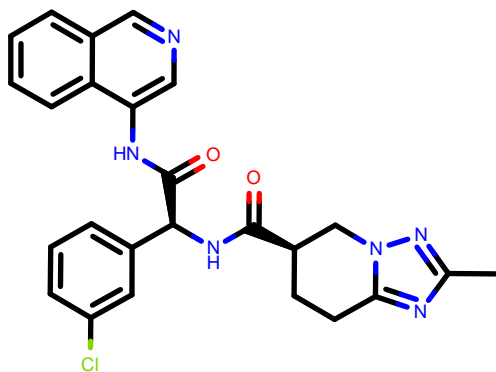
SMILES: c1cc(cc(c1)Cl)CC(=O)Nc2cnc3c2c(ccc3)CC(F)(F)F

RUN: RUN506

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.17

EDJ-MED-ee07cf00-13_1



CID: EDJ-MED-ee07cf00-13_1

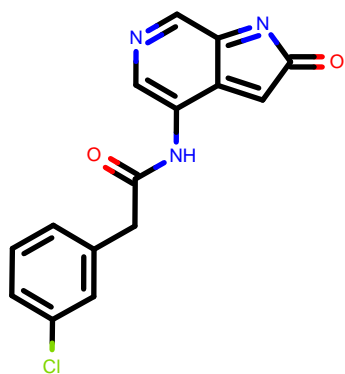
SMILES: Cc1nc2n(n1)C[C@@H](CC2)C(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN587

DDG (kcal/mol): -0.15

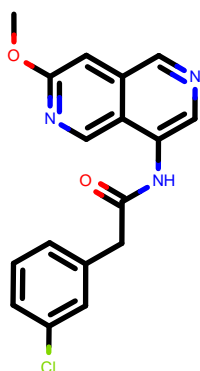
dDDG (kcal/mol): 0.22

MAT-POS-f7918075-7_1



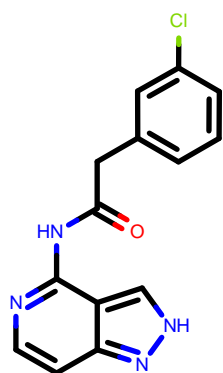
CID:	MAT-POS-f7918075-7_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2CC(=O)N3</chem>
RUN:	RUN270
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.14

PET-UNK-f4e47ebd-2_1



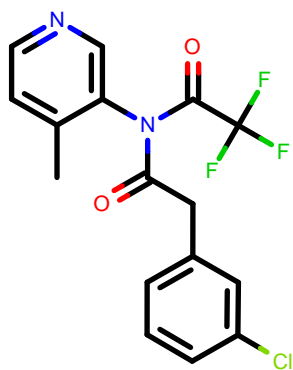
CID:	PET-UNK-f4e47ebd-2_1
SMILES:	<chem>COC1CC2CNCC(C2CN1)NC(=O)CC3CCCC(C3)Cl</chem>
RUN:	RUN708
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.13

MAT-POS-199e2e7c-2_1



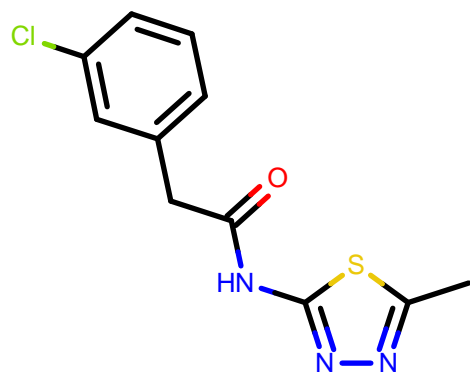
CID:	MAT-POS-199e2e7c-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3cn[nH]c3ccn2</chem>
RUN:	RUN315
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.15

JOH-UNI-a38a7bdd-3_1



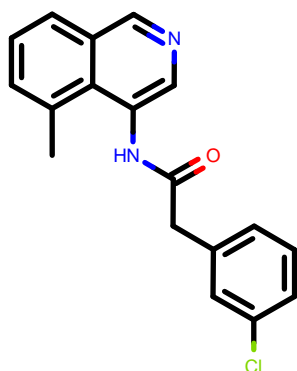
CID:	JOH-UNI-a38a7bdd-3_1
SMILES:	<chem>Cc1ccncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)C(F)(F)F</chem>
RUN:	RUN492
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.15

JAG-UCB-a3ef7265-10_1



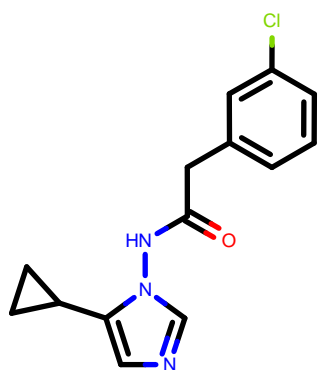
CID:	JAG-UCB-a3ef7265-10_1
SMILES:	<chem>Cc1nnc(s1)NC(=O)Cc2cccc(c2F)Cl</chem>
RUN:	RUN107
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.13

MIC-UNK-50cce87d-3_1



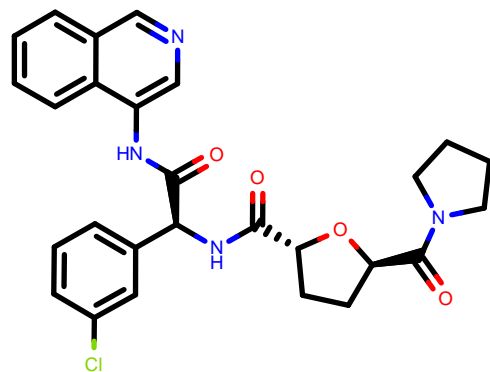
CID:	MIC-UNK-50cce87d-3_1
SMILES:	<chem>Cc1cccc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN340
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.10

JAN-GHE-f4ca5a00-14_1



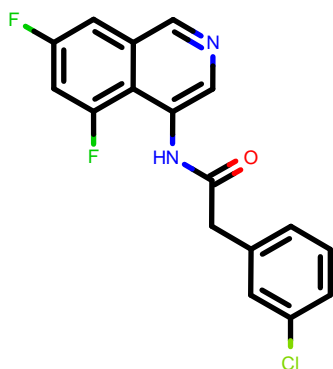
CID:	JAN-GHE-f4ca5a00-14_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2cncc2C3CC3</chem>
RUN:	RUN157
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-11_4



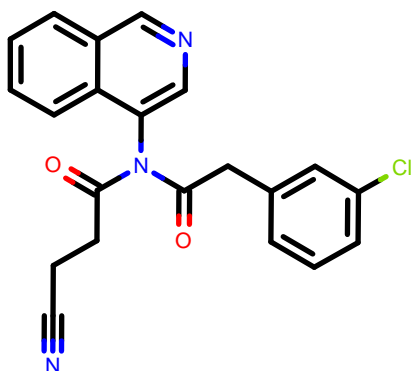
CID:	EDJ-MED-ee07cf00-11_4
SMILES:	<chem>c1ccc2c1)cnc2N(C(=O)C1=CC=C(C=C1)Cl)C(=O)O[C@H](C1=CC=CC=C1)C(=O)N2CCCC2</chem>
RUN:	RUN591
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.24

MIC-UNK-7574fcc6-1_1



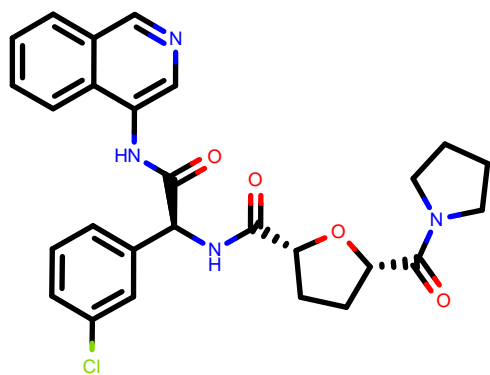
CID:	MIC-UNK-7574fcc6-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(cc(c3)F)F</chem>
RUN:	RUN721
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.13

DAR-DIA-56cf811e-3_1



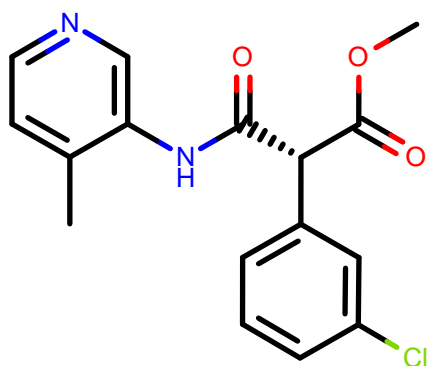
CID:	DAR-DIA-56cf811e-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)CC3CCCC(c3)Cl)C(=O)/C=C/C#N</chem>
RUN:	RUN521
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.30

EDJ-MED-ee07cf00-11_8



CID:	EDJ-MED-ee07cf00-11_8
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)NC(=O)[C@H](O)C[C@H](O4)C(=O)N5CCCC5</chem>
RUN:	RUN597
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.24

MAT-POS-1e5f28a7-1_1



CID:	MAT-POS-1e5f28a7-1_1
SMILES:	<chem>Cc1cncc1NC(=O)[C@@H](c2ccccc(c2)Cl)C(=O)OC</chem>
RUN:	RUN272
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.13