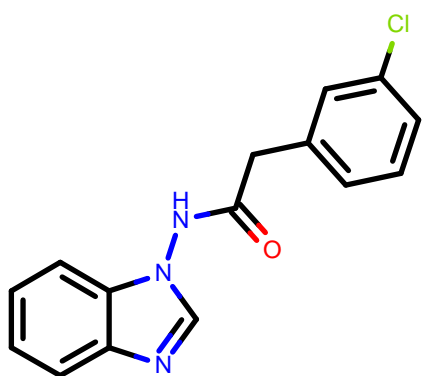
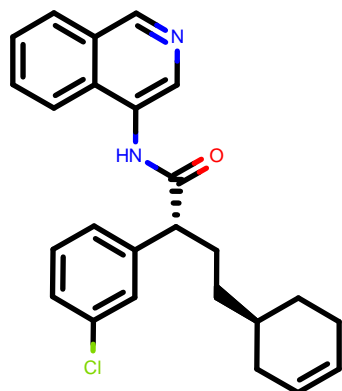


JAN-GHE-5a013bed-2_1



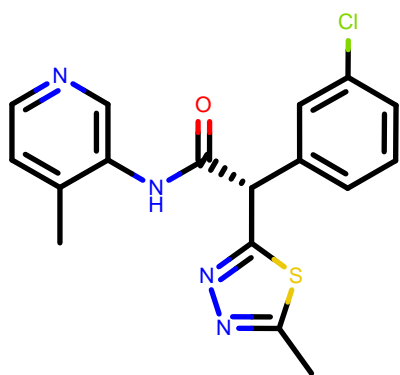
CID:	JAN-GHE-5a013bed-2_1
SMILES:	<chem>c1ccc2c(c1)ncn2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN52
DDG (kcal/mol):	-2.86
dDDG (kcal/mol):	0.10

ALP-POS-3b848b35-4_2



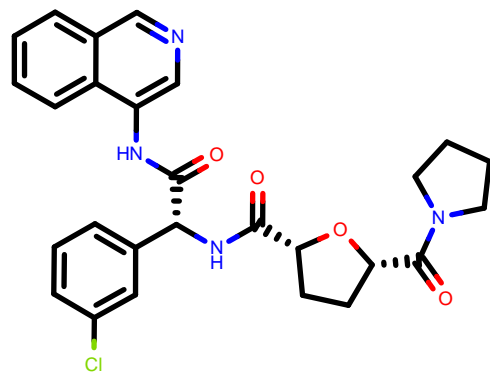
CID:	ALP-POS-3b848b35-4_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CCC3CCCCC3)c4cccc(c4)Cl</chem>
RUN:	RUN194
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.23

SAM-UNK-2684b532-3_2



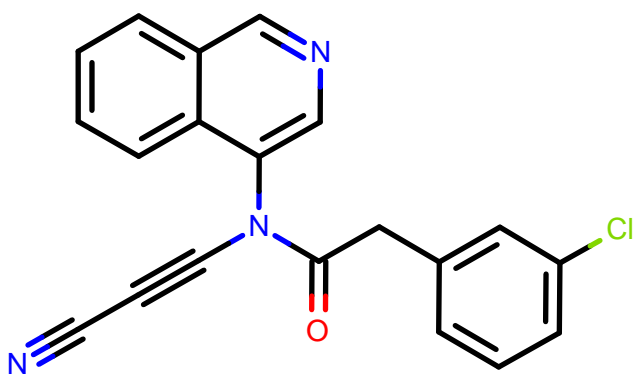
CID:	SAM-UNK-2684b532-3_2
SMILES:	<chem>Cc1ccncc1NC(=O)[C@H](c2cccc(c2)Cl)c3nnc(s3)C</chem>
RUN:	RUN145
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-11_7



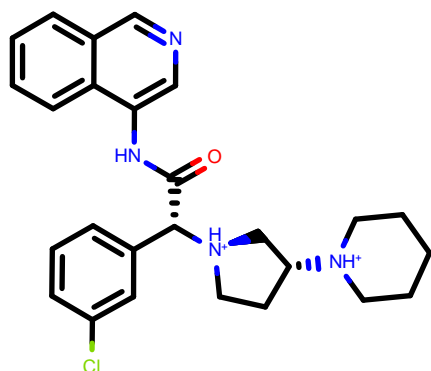
CID:	EDJ-MED-ee07cf00-11_7
SMILES:	<chem>c1ccc2c(c1)nc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@H]4CC[C@H]4O[C@H]5CCN5</chem>
RUN:	RUN595
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.20

DAR-DIA-076fb6ea-5_1



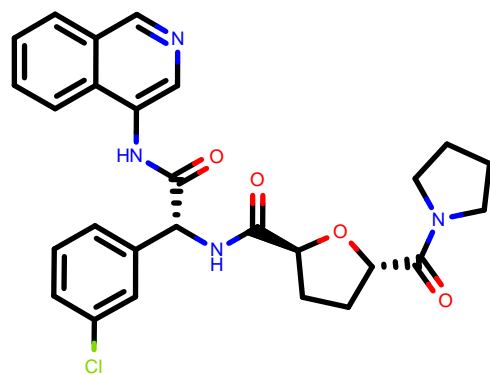
CID:	DAR-DIA-076fb6ea-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C#CC#N)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN461
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.47

MIC-UNK-5a93dd5f-12_7



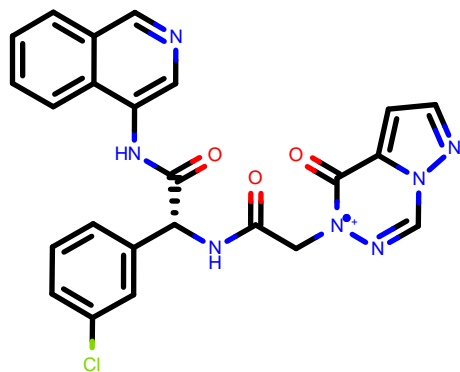
CID:	MIC-UNK-5a93dd5f-12_7
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccccc(c3)Cl)N@H4CC[C@H](C4)NH+5CCCCC5</chem>
RUN:	RUN439
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.14

PET-UNK-ac320b15-7_1



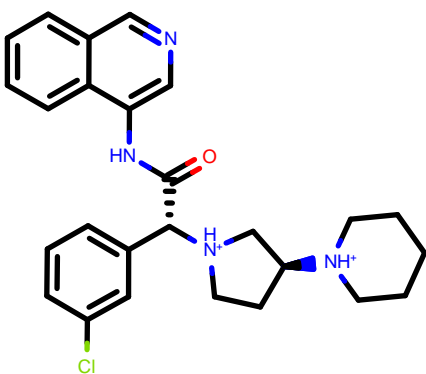
CID:	PET-UNK-ac320b15-7_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccccc(c3)Cl)N[C@@H](C4)C[C@H](O4)C5CCCCC5</chem>
RUN:	RUN757
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.17

EDJ-MED-ee07cf00-17_1



CID:	EDJ-MED-ee07cf00-17_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccccc(c3)Cl)NC(=O)Cn4c(=O)c5ccnnc5n4</chem>
RUN:	RUN602
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.26

MIC-UNK-5a93dd5f-12_1



CID: MIC-UNK-5a93dd5f-12_1

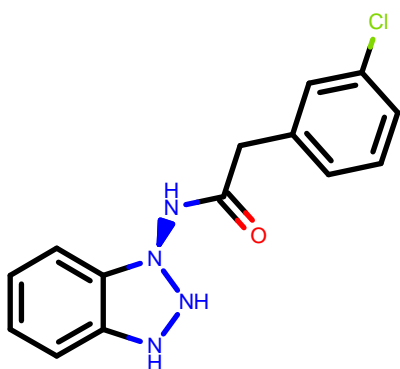
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@@]4CC[C@H](C4)[NH+]5CCCC5

RUN: RUN435

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.16

MAT-POS-bfb445d4-2_1



CID: MAT-POS-bfb445d4-2_1

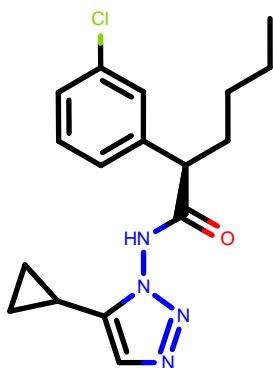
SMILES: c1ccc2c(c1)nnn2NC(=O)Cc3cccc(c3)Cl

RUN: RUN278

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.12

JAN-GHE-f4ca5a00-20_2



CID: JAN-GHE-f4ca5a00-20_2

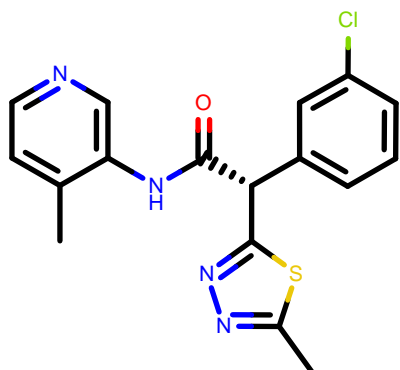
SMILES: CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2c(cnn2)C3CC3

RUN: RUN202

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.17

TRY-UNI-9f475305-3_2



CID: TRY-UNI-9f475305-3_2

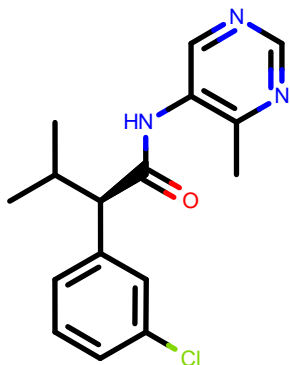
SMILES: Cc1ccncc1NC(=O)[C@@H](c2cccc(c2)Cl)c3nnc(s3)C

RUN: RUN64

DDG (kcal/mol): -1.70

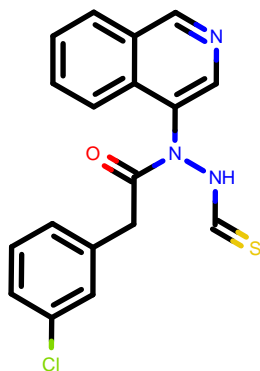
dDDG (kcal/mol): 0.14

JAN-GHE-83b26c96-7_1



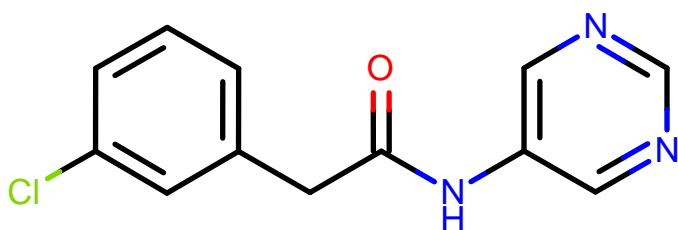
CID:	JAN-GHE-83b26c96-7_1
SMILES:	<chem>Cc1c(cncn1)NC(=O)[C@@H](c2cccc(c2)Cl)C(C)C</chem>
RUN:	RUN20
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.17

DAR-DIA-076fb6ea-15_1



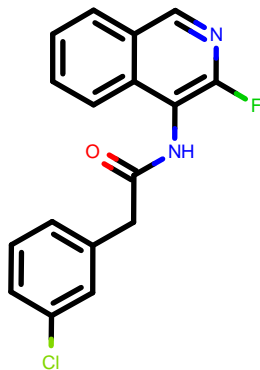
CID:	DAR-DIA-076fb6ea-15_1
SMILES:	<chem>c1ccc2c(c1)cnc2N(C(=O)Cc3cccc(c3)Cl)N=C=S</chem>
RUN:	RUN483
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.18

JAN-GHE-5a013bed-9_1



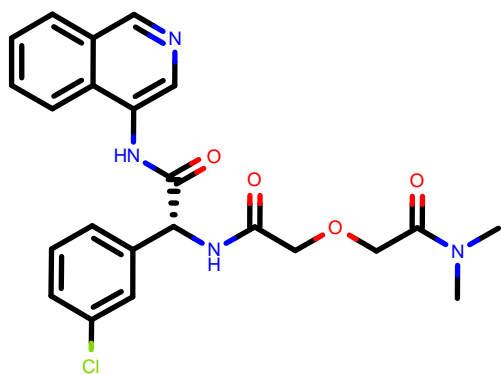
CID:	JAN-GHE-5a013bed-9_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncnc2</chem>
RUN:	RUN49
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.13

RUB-POS-1325a9ea-18_1



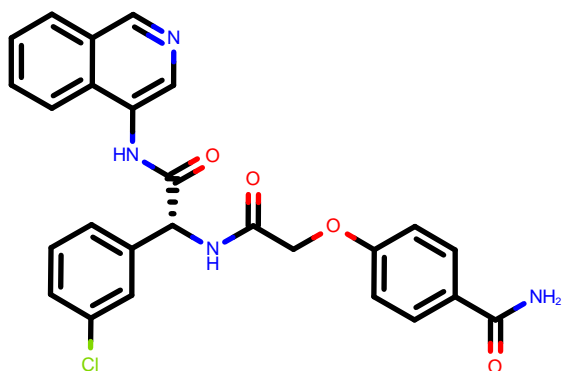
CID:	RUB-POS-1325a9ea-18_1
SMILES:	<chem>c1ccc2c(c1)cnc(c2NC(=O)Cc3cccc(c3)Cl)F</chem>
RUN:	RUN674
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.04

EDJ-MED-cf4b0d25-5_2



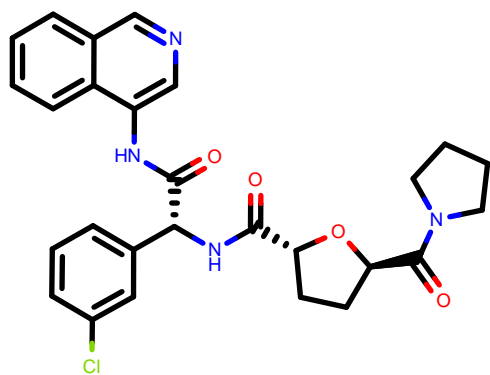
CID:	EDJ-MED-cf4b0d25-5_2
SMILES:	<chem>CN(C)C(=O)COCC(=O)N[C@@H](c1cccc(c1)Cl)C(=O)Nc2ccc3c2ccc3</chem>
RUN:	RUN716
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.18

EDJ-MED-ee07cf00-12_1



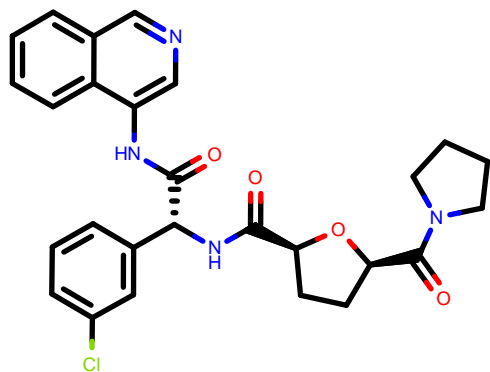
CID:	EDJ-MED-ee07cf00-12_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)Nc4ccc(cc4)C(=O)N</chem>
RUN:	RUN610
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.18

PET-UNK-ac320b15-5_1



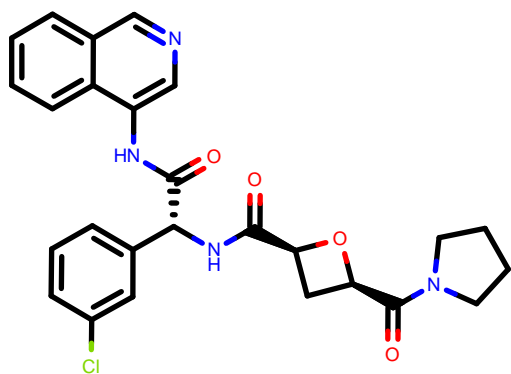
CID:	PET-UNK-ac320b15-5_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)Nc4c[nH]c4[C@@H](O4)Cl-O5NCCO5</chem>
RUN:	RUN756
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.20

EDJ-MED-ee07cf00-11_1



CID:	EDJ-MED-ee07cf00-11_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)Nc4c[nH]c4[C@@H](O4)Cl-O5NCCO5</chem>
RUN:	RUN586
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.23

PET-UNK-1320d94d-7_1



CID: PET-UNK-1320d94d-7_1

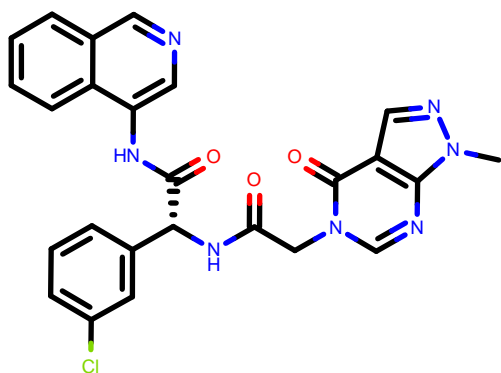
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@H(c3ccccc3)C(=O)N[C@@H](C4=CC=CC=C4)C(=O)N5CCCC5

RUN: RUN728

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.21

EDJ-MED-ee07cf00-3_2



CID: EDJ-MED-ee07cf00-3_2

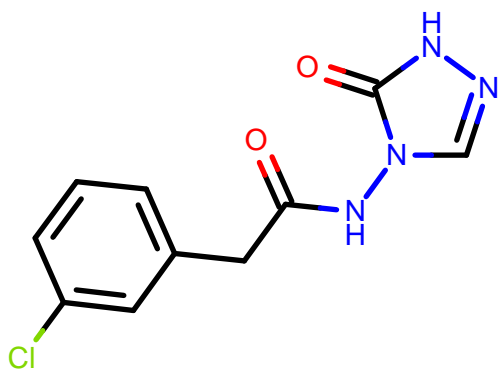
SMILES: Cn1c2c(en1)c(=O)n(cn2)CC(=O)N[C@@H](c3ccccc3)C(=O)Nc4ncnc5c4cccc5

RUN: RUN569

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.20

JAN-GHE-5a013bed-4_1



CID: JAN-GHE-5a013bed-4_1

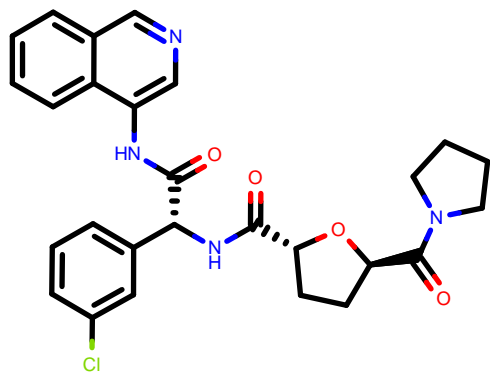
SMILES: c1cc(cc(c1)Cl)CC(=O)Nn2cn[nH]c2=O

RUN: RUN66

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.13

EDJ-MED-ee07cf00-11_3



CID: EDJ-MED-ee07cf00-11_3

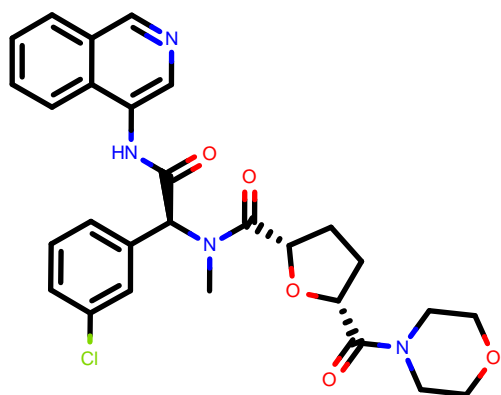
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@H(c3ccccc3)C(=O)N[C@@H](C4=CC=CC=C4)C(=O)N5CCCC5

RUN: RUN590

DDG (kcal/mol): -1.50

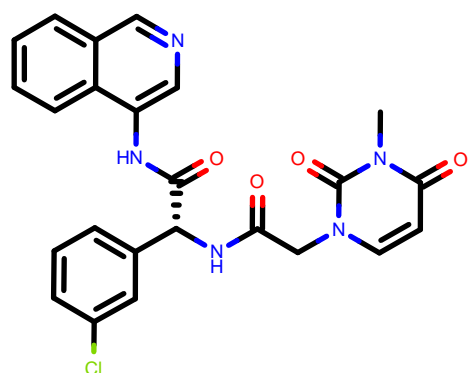
dDDG (kcal/mol): 0.20

PET-UNK-1320d94d-24_1



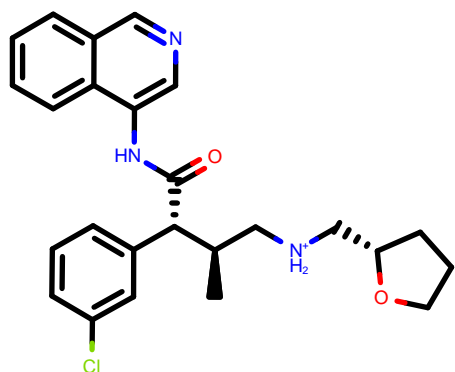
CID:	PET-UNK-1320d94d-24_1
SMILES:	<chem>CN(Cc1ccc(c1)C)C(=O)Nc2ccc3c2ccc3C(=O)C@H(Cc4cc(C)cc4)O)N5CCCC5</chem>
RUN:	RUN750
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.24

EDJ-MED-ee07cf00-1_2



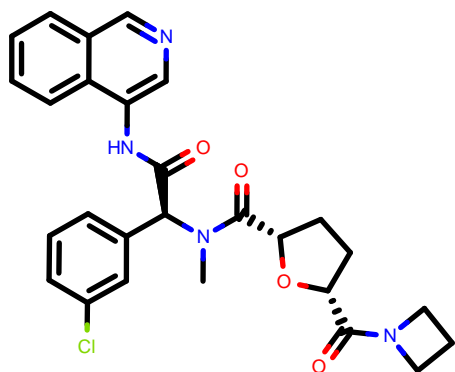
CID:	EDJ-MED-ee07cf00-1_2
SMILES:	<chem>Cn1c(=O)ccn(c1=O)CC(=O)N[C@H](c2cccc(c2)C)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN566
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.16

MAK-UNK-c749d764-22_6



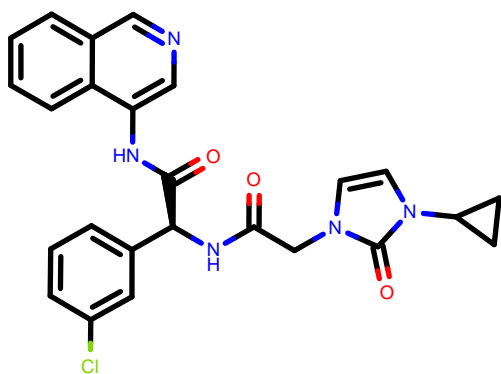
CID:	MAK-UNK-c749d764-22_6
SMILES:	<chem>C[C@H](C)[NH2+][C]C@H1CCCCO1[C@H](c2ccccc(c2)C)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN454
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.19

PET-UNK-1320d94d-26_1



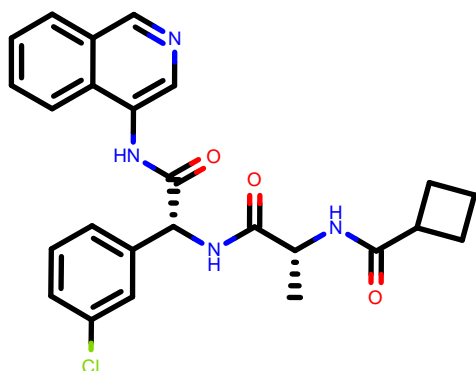
CID:	PET-UNK-1320d94d-26_1
SMILES:	<chem>CN(Cc1ccc(c1)C)C(=O)Nc2ncc3c2ccc3C(=O)C@H(Cc4c(C)cn4)O)N5CCCC5</chem>
RUN:	RUN745
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.24

EDJ-MED-ee07cf00-18_2



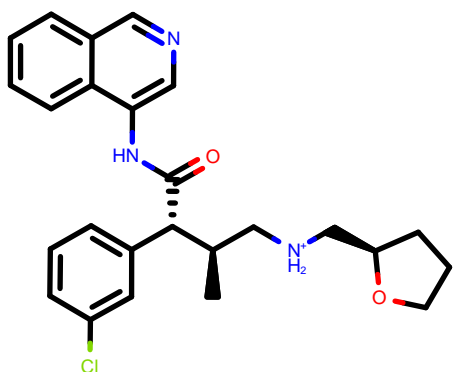
CID:	EDJ-MED-ee07cf00-18_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)C)NC(=O)CN4CCN(C4=O)C5CC5</chem>
RUN:	RUN608
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.22

EDJ-MED-ee07cf00-4_4



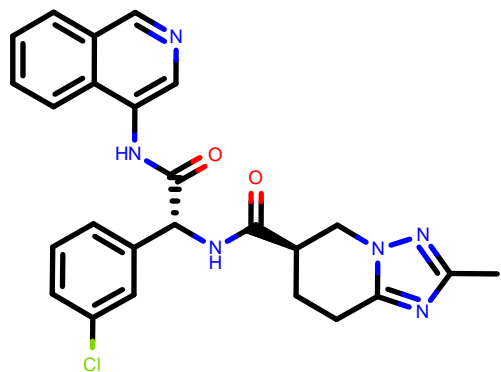
CID:	EDJ-MED-ee07cf00-4_4
SMILES:	<chem>C[C@H](C(=O)N[C@H](c1ccccc1)C)C(=O)Nc2ncc3c2ccc3)NC(=O)C4CC4</chem>
RUN:	RUN612
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.21

MAK-UNK-ffc90da7-4_8



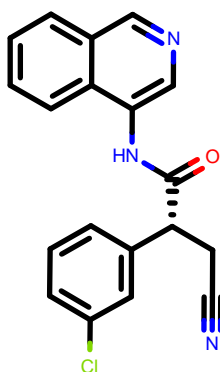
CID:	MAK-UNK-ffc90da7-4_8
SMILES:	<chem>C[C@H](C[NH2+][C@H]1CCCC1)[C@H](c2ccccc2)C)C(=O)Nc3ncc4c3ccc4</chem>
RUN:	RUN405
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.25

MAT-POS-a13804f0-1_3



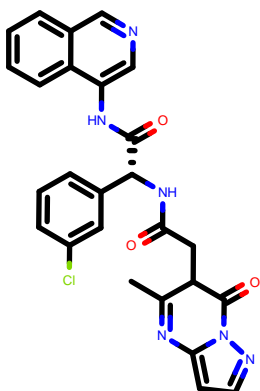
CID:	MAT-POS-a13804f0-1_3
SMILES:	<chem>Cc1nc2n(n1)C[C@H](CC2)C(=O)N[C@H](c3ccccc(c3)C)C(=O)Nc4ncc5c4ccc5</chem>
RUN:	RUN617
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.17

JOH-UNI-ee5ed7c8-6_2



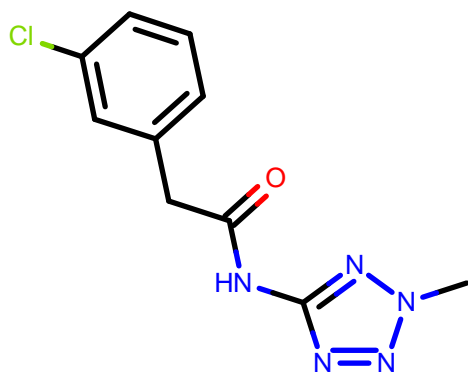
CID:	JOH-UNI-ee5ed7c8-6_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CC#N)c3cccc(c3)Cl</chem>
RUN:	RUN535
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.12

EDJ-MED-ee07cf00-2_2



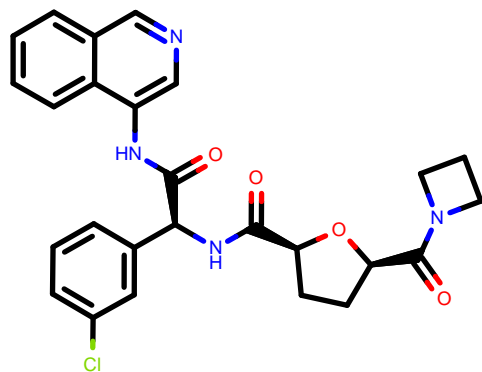
CID:	EDJ-MED-ee07cf00-2_2
SMILES:	<chem>Cc1c(c=O)n2c(n1)cd[nH]2]CC(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4ncc5o4cccc5</chem>
RUN:	RUN567
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.18

VLA-UNK-411a133b-1_1



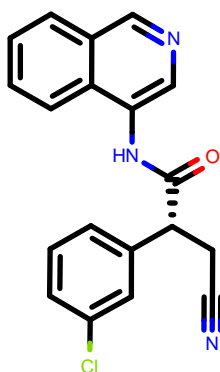
CID:	VLA-UNK-411a133b-1_1
SMILES:	<chem>Cn1nc(nn1)NC(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN685
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.12

PET-UNK-1320d94d-6_1



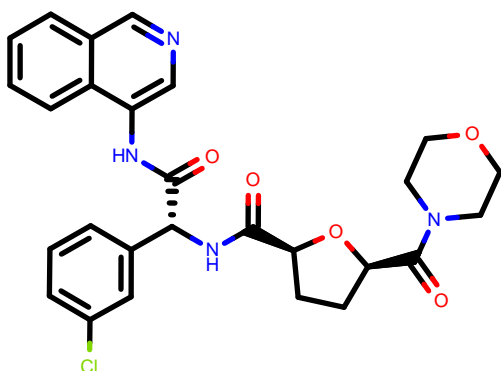
CID:	PET-UNK-1320d94d-6_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)C@H4C[C@@H](O4)C(=O)N5CCCC5</chem>
RUN:	RUN741
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.19

JOH-UNI-3fc3434e-6_2



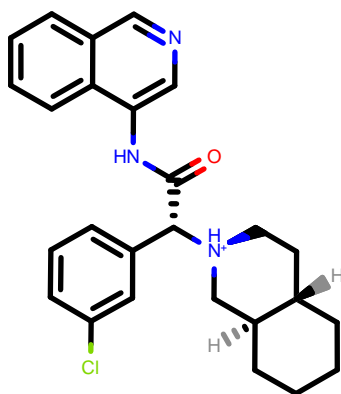
CID:	JOH-UNI-3fc3434e-6_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CC#N)c3cccc(c3)Cl</chem>
RUN:	RUN547
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.14

PET-UNK-1320d94d-3_1



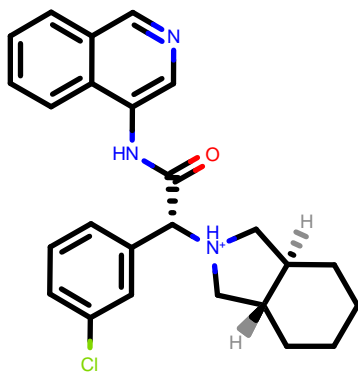
CID:	PET-UNK-1320d94d-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc3)C1NC(=O)[C@H](C@H4CC[C@H]4O)C1=O</chem>
RUN:	RUN736
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.20

MIC-UNK-5a93dd5f-3_11



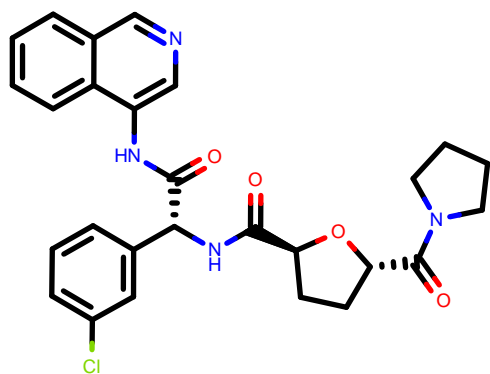
CID:	MIC-UNK-5a93dd5f-3_11
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)N@H4CC[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN396
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.22

MIC-UNK-5a93dd5f-2_3



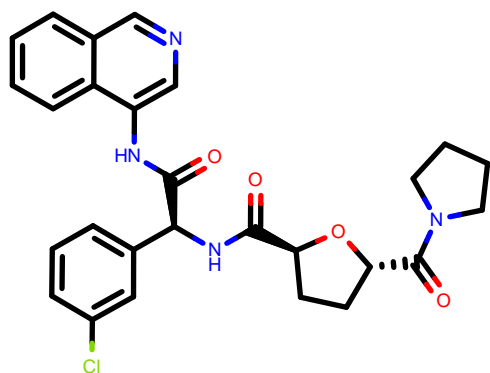
CID:	MIC-UNK-5a93dd5f-2_3
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)N+H4C[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN356
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.22

EDJ-MED-ee07cf00-11_5



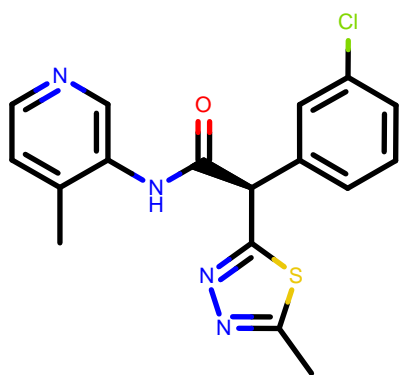
CID:	EDJ-MED-ee07cf00-11_5
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc3)C(=O)N[C@@H](O)C1=CNCC1</chem>
RUN:	RUN598
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.21

PET-UNK-ac320b15-8_1



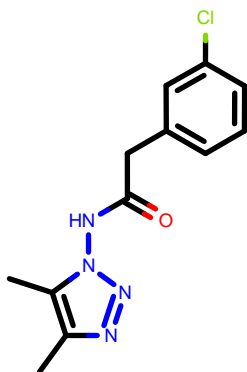
CID:	PET-UNK-ac320b15-8_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc3)C(=O)N[C@@H](O)C1=CNCC1</chem>
RUN:	RUN760
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.25

TRY-UNI-9f475305-3_1



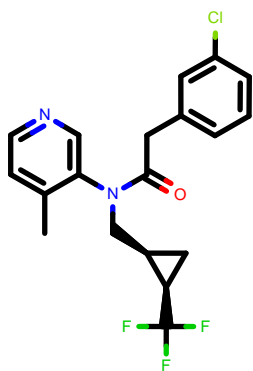
CID:	TRY-UNI-9f475305-3_1
SMILES:	<chem>Cc1ccncc1NC(=O)[C@@H](c2ccccc2)C1=CN(C)S1</chem>
RUN:	RUN69
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.14

JAN-GHE-5a013bed-1_1



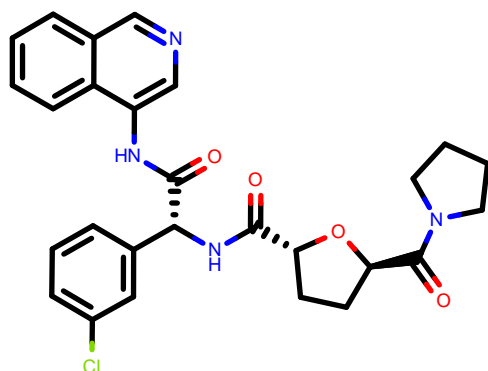
CID:	JAN-GHE-5a013bed-1_1
SMILES:	<chem>Cc1c(n(nn1)NC(=O)C)C2=CC=C(C=C2)Cl</chem>
RUN:	RUN50
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.11

JOH-UNI-a38a7bdd-8_4



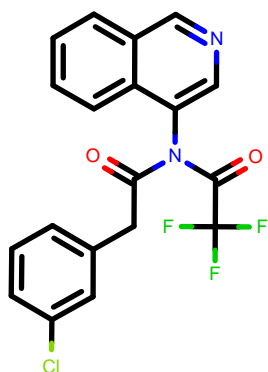
CID:	JOH-UNI-a38a7bdd-8_4
SMILES:	<chem>Cc1ccncc1N(C[C@H]2C[C@H]2C(F)(F)F)C(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN486
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.15

MAT-POS-8293a91a-2_1



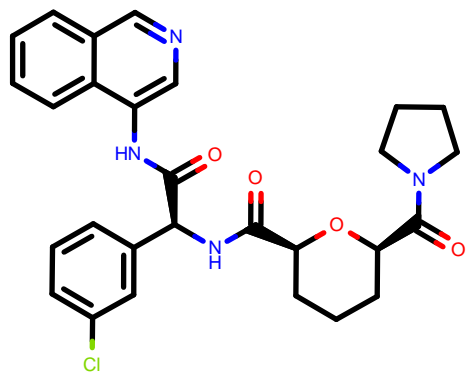
CID:	MAT-POS-8293a91a-2_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)N[C@@H](C)C(=O)N5CCCC5</chem>
RUN:	RUN774
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.20

JOH-UNI-a38a7bdd-1_1



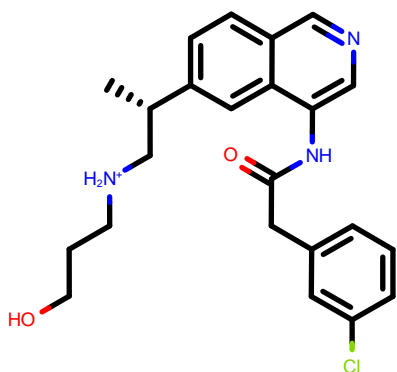
CID:	JOH-UNI-a38a7bdd-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N(C(=O)Cc3ccccc(c3)Cl)C(=O)C(F)(F)F</chem>
RUN:	RUN487
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.18

PET-UNK-1320d94d-10_1



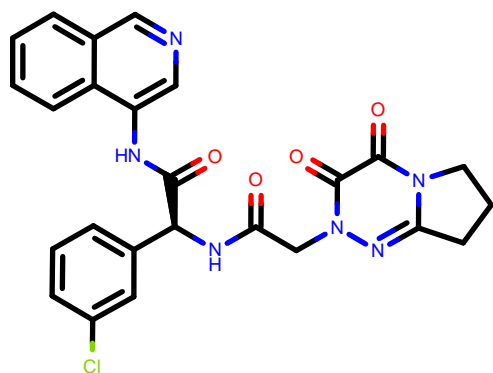
CID:	PET-UNK-1320d94d-10_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)N[C@@H](C)C(=O)N5CCCC5</chem>
RUN:	RUN738
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.26

MAK-UNK-ffc90da7-6_1



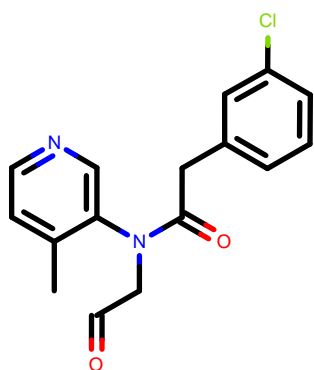
CID:	MAK-UNK-ffc90da7-6_1
SMILES:	<chem>C[C@@H](C[NH2+])CCCOc1ccc2cncc(c2c1)NC(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN415
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.18

EDJ-MED-ee07cf00-14_2



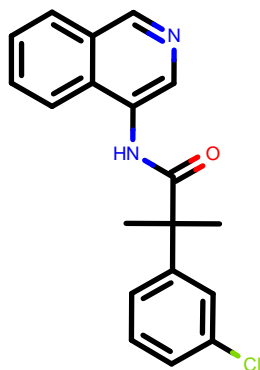
CID:	EDJ-MED-ee07cf00-14_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)NC(=O)Cn4c(=O)c(=O)n5c(n4)CCO5</chem>
RUN:	RUN601
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.23

PET-UNK-bbe8d7ff-1_1



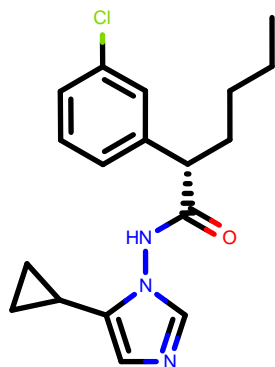
CID:	PET-UNK-bbe8d7ff-1_1
SMILES:	<chem>Cc1ccncc1N(CC=O)C(=O)Cc2ccccc(c2)Cl</chem>
RUN:	RUN147
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.17

NAU-LAT-2fed8305-1_1



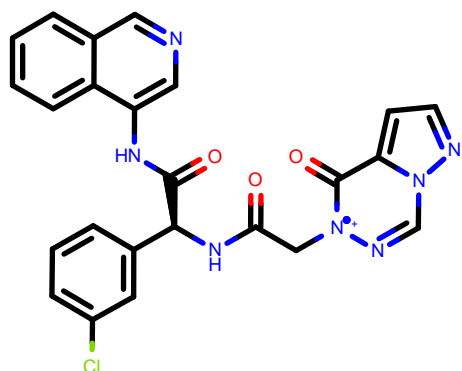
CID:	NAU-LAT-2fed8305-1_1
SMILES:	<chem>CC(C)(c1cccc(c1)Cl)C(=O)Nc2cncc3c2ccccc3</chem>
RUN:	RUN453
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.04

JAN-GHE-f4ca5a00-18_1



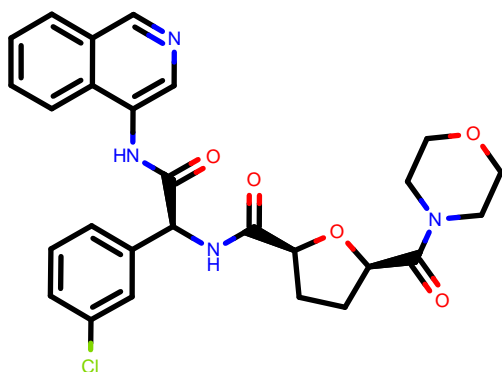
CID:	JAN-GHE-f4ca5a00-18_1
SMILES:	<chem>CCCC[C@@H](c1cccc(c1)Cl)C(=O)Nn2cncc2C3CC3</chem>
RUN:	RUN204
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.18

EDJ-MED-ee07cf00-17_2



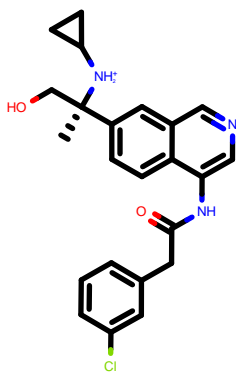
CID:	EDJ-MED-ee07cf00-17_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)Cn4c(=O)c5cnm5cn4</chem>
RUN:	RUN603
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.21

PET-UNK-1320d94d-4_1



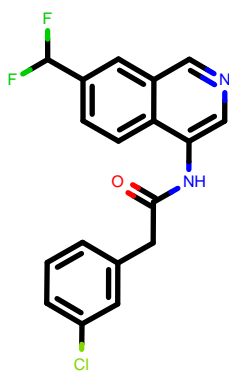
CID:	PET-UNK-1320d94d-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)C4CCOC4</chem>
RUN:	RUN730
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.26

MAK-UNK-ffc90da7-5_1



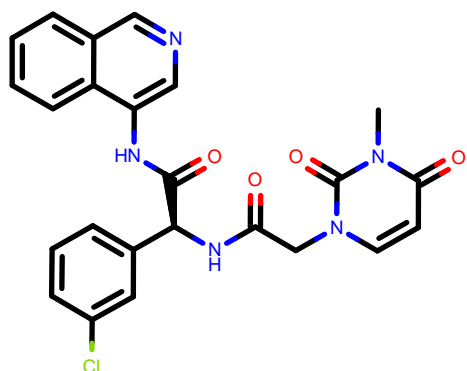
CID:	MAK-UNK-ffc90da7-5_1
SMILES:	<chem>C[C@@](O)(CO)(c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl)N2+</chem>
RUN:	RUN362
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.18

MAT-POS-c0609ef7-1_1



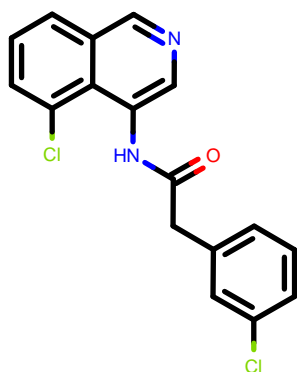
CID:	MAT-POS-c0609ef7-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)C(F)F</chem>
RUN:	RUN795
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.15

EDJ-MED-ee07cf00-1_1



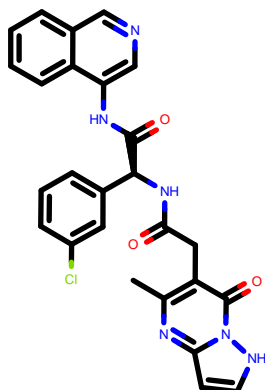
CID:	EDJ-MED-ee07cf00-1_1
SMILES:	<chem>Cn1c(=O)ccn(c1=O)CC(=O)N[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN564
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.17

MIC-UNK-50cce87d-2_1



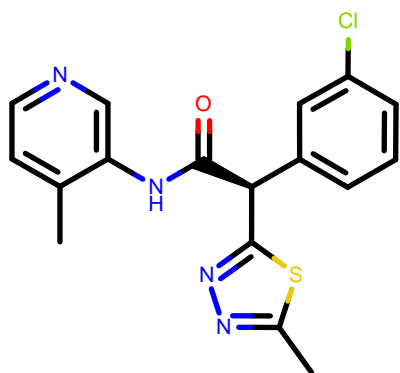
CID:	MIC-UNK-50cce87d-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)Cl</chem>
RUN:	RUN338
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-2_1



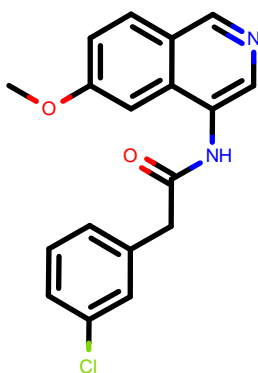
CID:	EDJ-MED-ee07cf00-2_1
SMILES:	<chem>Cc1c(c(=O)n2c(n1)cc[nH]2)CC(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN571
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.23

SAM-UNK-2684b532-3_1



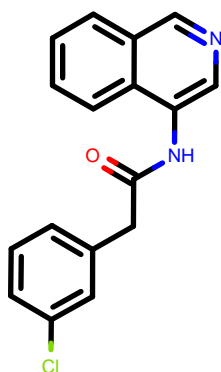
CID:	SAM-UNK-2684b532-3_1
SMILES:	<chem>Cc1ccncc1NC(=O)[C@@H](c2cccc(c2)Cl)c3nnc(s3)C</chem>
RUN:	RUN140
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.14

PET-UNK-8df914d1-1_1



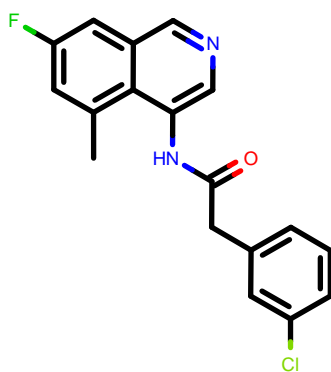
CID:	PET-UNK-8df914d1-1_1
SMILES:	<chem>COc1ccc2cnccc(c2c1)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN206
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.13

MAT-POS-f7918075-5_1



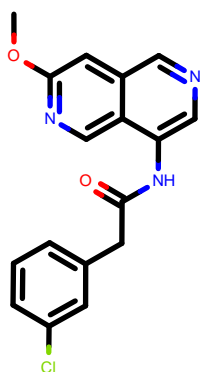
CID:	MAT-POS-f7918075-5_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cnccc3c2cnccc3</chem>
RUN:	RUN269
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.02

MAT-POS-29385cc1-4_1



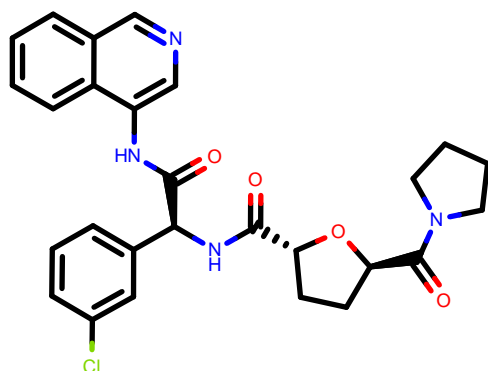
CID:	MAT-POS-29385cc1-4_1
SMILES:	<chem>Cc1cc(cc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl)F</chem>
RUN:	RUN796
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.10

PET-UNK-f4e47ebd-2_1



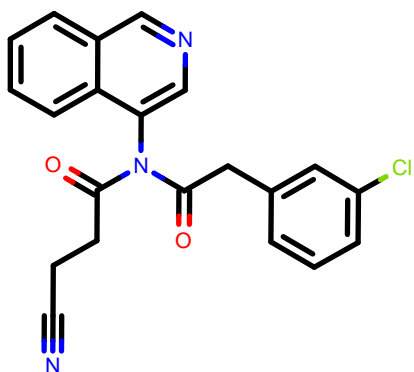
CID:	PET-UNK-f4e47ebd-2_1
SMILES:	<chem>COc1cc2cncc(c2cn1)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN708
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-11_4



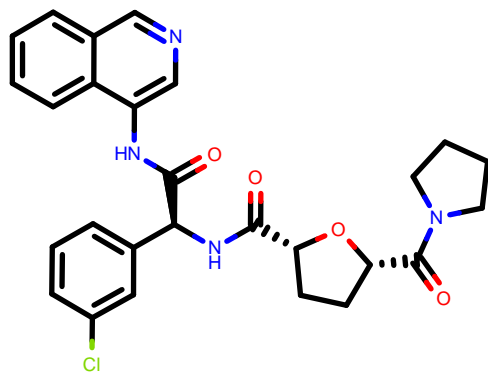
CID:	EDJ-MED-ee07cf00-11_4
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@H]4CC[C@H]4O[C@H]5CCCC5</chem>
RUN:	RUN591
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.24

DAR-DIA-56cf811e-3_1



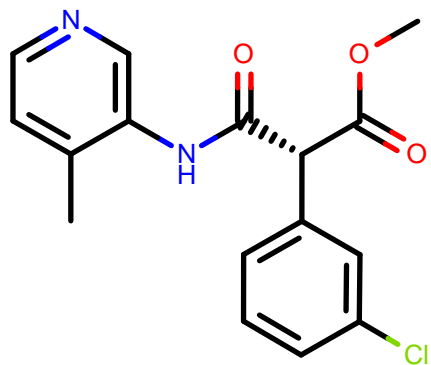
CID:	DAR-DIA-56cf811e-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)/C=C/C#N</chem>
RUN:	RUN521
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.30

EDJ-MED-ee07cf00-11_8



CID:	EDJ-MED-ee07cf00-11_8
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@H]4CC[C@H]4O[C@H]5CCCC5</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>Cc1ccncc1NC(=O)[C@@H](c2cccc(c2)Cl)C(=O)OC</chem>
RUN:	RUN272
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.13