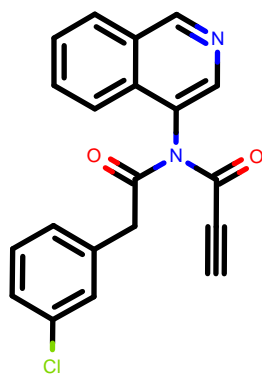
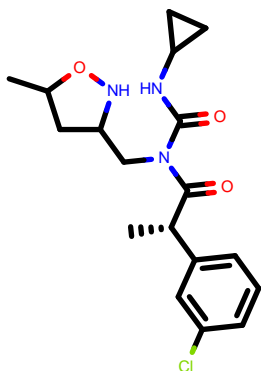


DAR-DIA-56cf811e-1_1



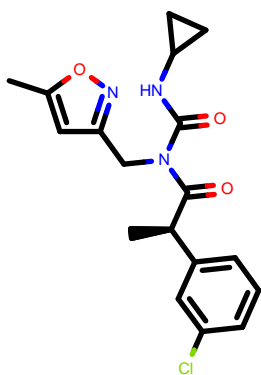
CID:	DAR-DIA-56cf811e-1_1
SMILES:	<chem>C#CC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1308
DDG (kcal/mol):	-6.36
dDDG (kcal/mol):	0.14

TRY-UNI-9f475305-8_1



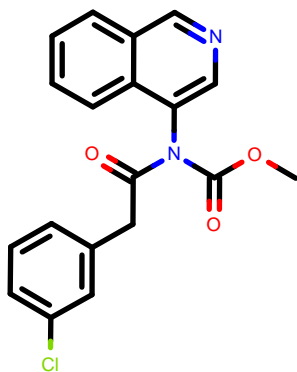
CID:	TRY-UNI-9f475305-8_1
SMILES:	<chem>Cc1cc(no1)CN(C(=O)[C@@H](C)c2cccc(c2)Cl)C(=O)NC3CC3</chem>
RUN:	RUN886
DDG (kcal/mol):	-6.06
dDDG (kcal/mol):	0.25

TRY-UNI-9f475305-8_2



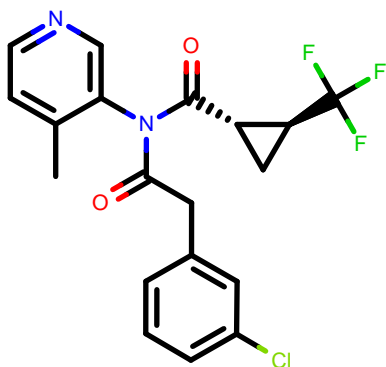
CID:	TRY-UNI-9f475305-8_2
SMILES:	<chem>Cc1cc(no1)CN(C(=O)[C@H](C)c2cccc(c2)Cl)C(=O)NC3CC3</chem>
RUN:	RUN891
DDG (kcal/mol):	-5.84
dDDG (kcal/mol):	0.25

PET-UNK-12d8d43f-2_1



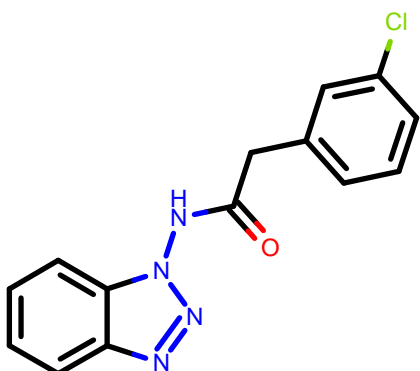
CID:	PET-UNK-12d8d43f-2_1
SMILES:	<chem>COC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1317
DDG (kcal/mol):	-5.13
dDDG (kcal/mol):	0.16

JOH-UNI-a38a7bdd-7_2



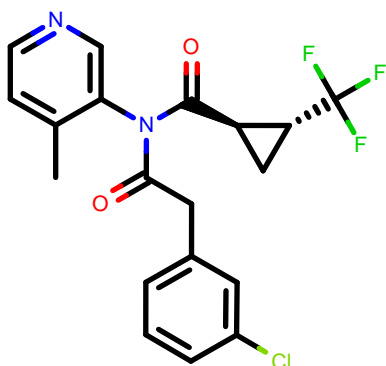
CID:	JOH-UNI-a38a7bdd-7_2
SMILES:	<chem>Cc1ccnc1N(C(=O)Cc2cccc(c2)Cl)C(=O)[C@H]3C[C@@H]3C(F)(F)F</chem>
RUN:	RUN1300
DDG (kcal/mol):	-3.91
dDDG (kcal/mol):	0.19

MAT-POS-bfb445d4-2_1



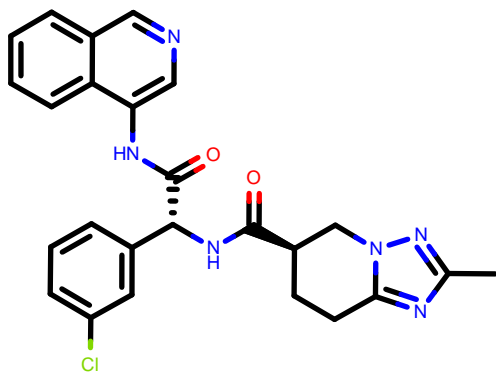
CID:	MAT-POS-bfb445d4-2_1
SMILES:	<chem>c1ccc2c(c1)nnn2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1077
DDG (kcal/mol):	-3.87
dDDG (kcal/mol):	0.11

JOH-UNI-a38a7bdd-7_3



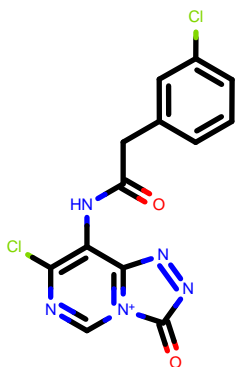
CID:	JOH-UNI-a38a7bdd-7_3
SMILES:	<chem>Cc1ccnc1N(C(=O)Cc2cccc(c2)Cl)C(=O)[C@@H]3C[C@H]3C(F)(F)F</chem>
RUN:	RUN1312
DDG (kcal/mol):	-3.31
dDDG (kcal/mol):	0.16

EDJ-MED-ee07cf00-13_2



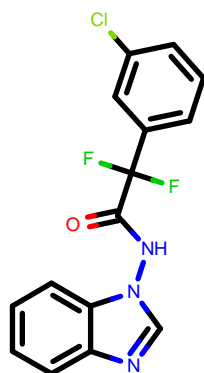
CID:	EDJ-MED-ee07cf00-13_2
SMILES:	<chem>Cc1nc2n(n1)C[C@@H](CC2)C(=O)N[C@@H](c3ccccc(c3)Cl)C(=O)Nc4cnccc5c4ccccc5</chem>
RUN:	RUN1393
DDG (kcal/mol):	-3.17
dDDG (kcal/mol):	0.20

EDJ-MED-c8e7a002-17_1



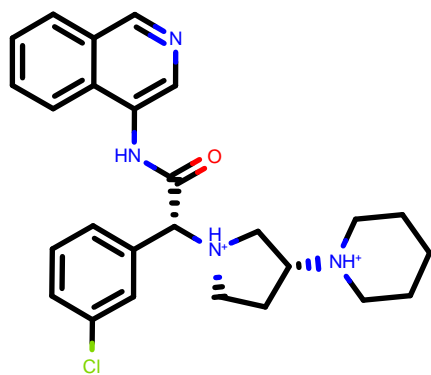
CID:	EDJ-MED-c8e7a002-17_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3n[nH]c(=O)n3cnc2Cl</chem>
RUN:	RUN1110
DDG (kcal/mol):	-2.96
dDDG (kcal/mol):	0.10

BAR-COM-0f94fc3d-24_1



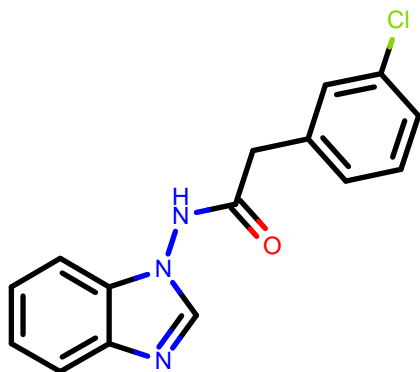
CID:	BAR-COM-0f94fc3d-24_1
SMILES:	<chem>c1ccc2c(c1)ncn2NC(=O)C(c3ccccc(c3)Cl)(F)F</chem>
RUN:	RUN920
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.11

MIC-UNK-5a93dd5f-12_7



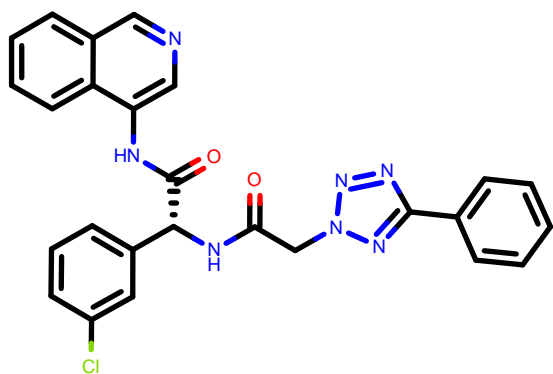
CID:	MIC-UNK-5a93dd5f-12_7
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc(c3)Cl)N@J4CC[C@H](C4)[NH+]5CCCC5</chem>
RUN:	RUN1238
DDG (kcal/mol):	-2.59
dDDG (kcal/mol):	0.13

JAN-GHE-5a013bed-2_1



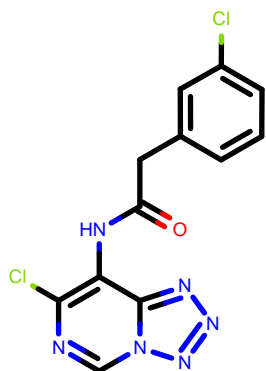
CID:	JAN-GHE-5a013bed-2_1
SMILES:	<chem>c1ccc2c(c1)ncn2NC(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN851
DDG (kcal/mol):	-2.39
dDDG (kcal/mol):	0.10

EDJ-MED-ee07cf00-9_2



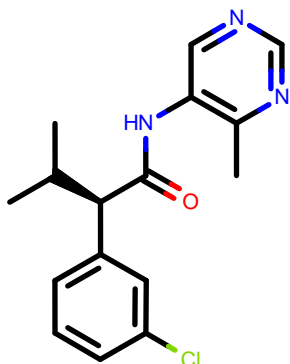
CID:	EDJ-MED-ee07cf00-9_2
SMILES:	<chem>c1ccc(cc1)c2nnn(n2)CC(=O)N[C@H](c3ccccc(c3)Cl)C(=O)Nc4ncnc5c4ccccc5</chem>
RUN:	RUN1377
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.24

EDJ-MED-c8e7a002-8_1



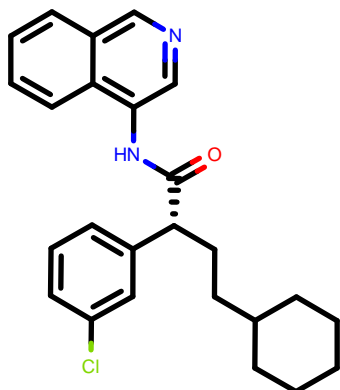
CID:	EDJ-MED-c8e7a002-8_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3nnnn3cnc2Cl</chem>
RUN:	RUN1100
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.13

JAN-GHE-83b26c96-7_1



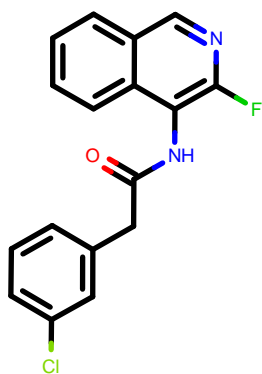
CID:	JAN-GHE-83b26c96-7_1
SMILES:	<chem>Cc1c(cncn1)NC(=O)[C@H](c2cccc(c2)Cl)C(C)C</chem>
RUN:	RUN819
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.16

MIC-UNK-c66144cb-3_2



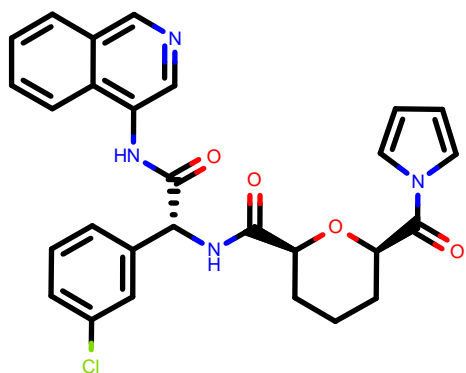
CID:	MIC-UNK-c66144cb-3_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@H](CCC3CCCCC3)c4ccccc4Cl</chem>
RUN:	RUN1020
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.23

RUB-POS-1325a9ea-18_1



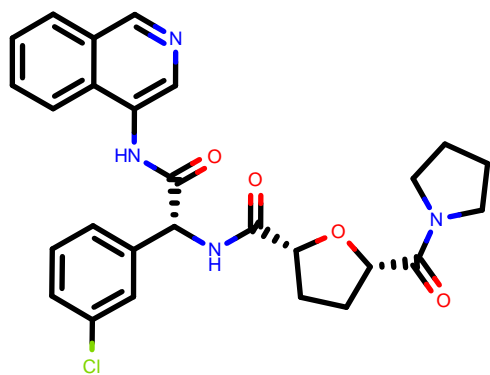
CID:	RUB-POS-1325a9ea-18_1
SMILES:	<chem>c1ccc2c(c1)cnc(c2NC(=O)Cc3ccccc(c3)Cl)F</chem>
RUN:	RUN1473
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.03

PET-UNK-1320d94d-9_1



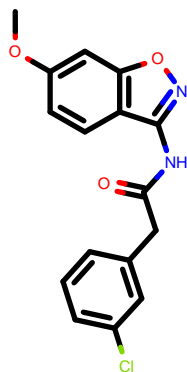
CID:	PET-UNK-1320d94d-9_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)C[C@@H](c3ccccc3)C(NC(=O)C[C@@H](c4ccccc4)[C@@H](O4)Cl)O4N5CCCC5</chem>
RUN:	RUN1536
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.24

MAT-POS-8293a91a-7_1



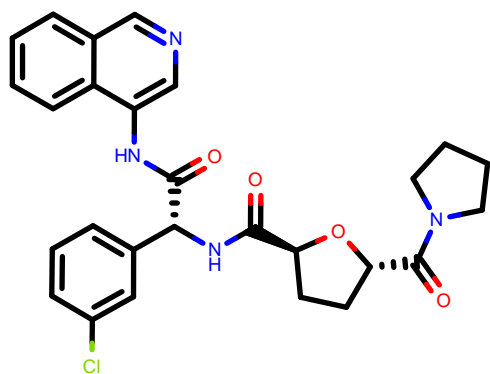
CID:	MAT-POS-8293a91a-7_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)C[C@@H](c3ccccc3)C(NC(=O)C[C@@H](c4ccccc4)[C@@H](O4)Cl)O4N5CCCC5</chem>
RUN:	RUN1569
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.21

EDJ-MED-c8e7a002-1_1



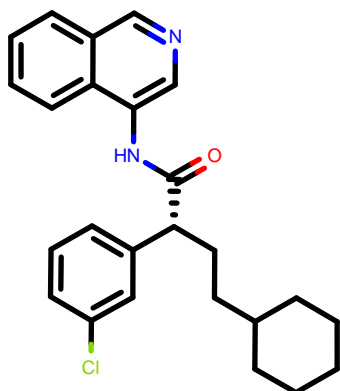
CID:	EDJ-MED-c8e7a002-1_1
SMILES:	<chem>COc1ccc2c(c1)onc2NC(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN1095
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.13

MAT-POS-8293a91a-6_1



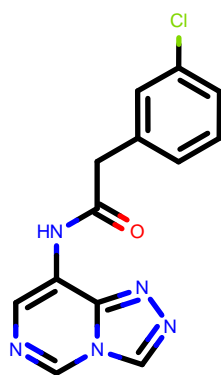
CID:	MAT-POS-8293a91a-6_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc3)C(=O)N[C@@H](C4=CC=C(C=C4)Cl)C(=O)N5CCCC5</chem>
RUN:	RUN1578
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.19

ALP-POS-3b848b35-4_2



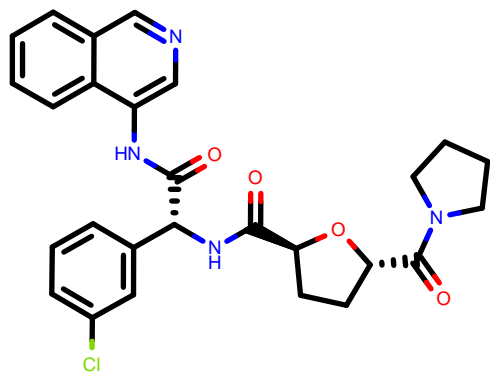
CID:	ALP-POS-3b848b35-4_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](CCCC3CCCCC3)c4ccccc4Cl</chem>
RUN:	RUN993
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.20

EDJ-MED-076d6e64-1_1



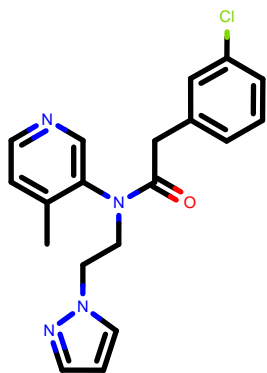
CID:	EDJ-MED-076d6e64-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncn3c2nnc3</chem>
RUN:	RUN1512
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.10

PET-UNK-ac320b15-7_1



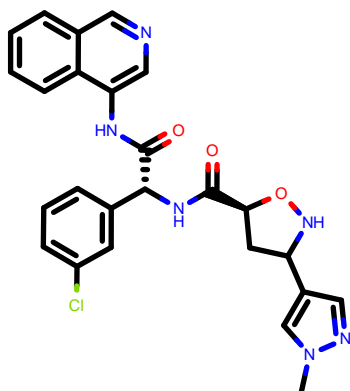
CID:	PET-UNK-ac320b15-7_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc3)C(=O)N[C@@H](C4=CC=C(C=C4)Cl)C(=O)N5CCCC5</chem>
RUN:	RUN1556
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.20

BAR-COM-ebf5acce-14_1



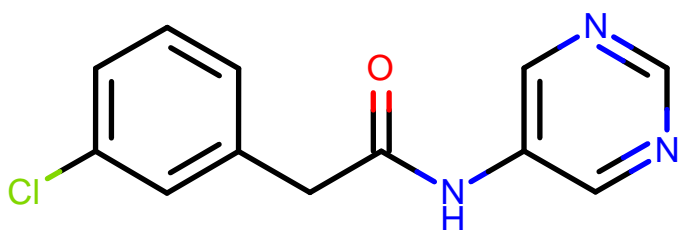
CID:	BAR-COM-ebf5acce-14_1
SMILES:	<chem>Cc1ccncc1N(CCn2ccccn2)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN861
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.20

EDJ-MED-ee07cf00-6_3



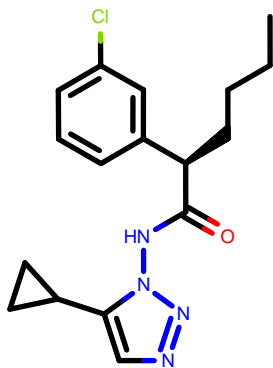
CID:	EDJ-MED-ee07cf00-6_3
SMILES:	<chem>Cn1cc(en1)C2=NO[C@@H](C2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN1383
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.18

JAN-GHE-5a013bed-9_1



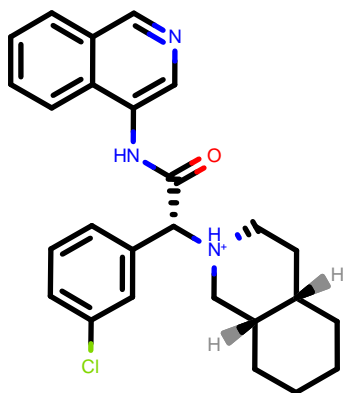
CID:	JAN-GHE-5a013bed-9_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncnc2</chem>
RUN:	RUN848
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.12

JAN-GHE-f4ca5a00-20_2



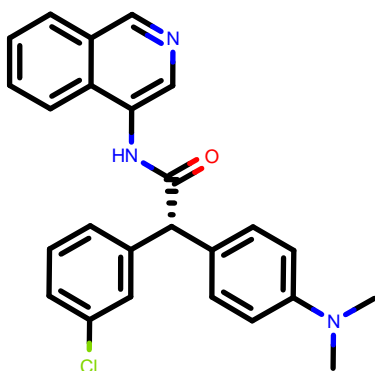
CID:	JAN-GHE-f4ca5a00-20_2
SMILES:	<chem>CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2c(cnn2)C3CC3</chem>
RUN:	RUN1001
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.15

MIC-UNK-5a93dd5f-3_1



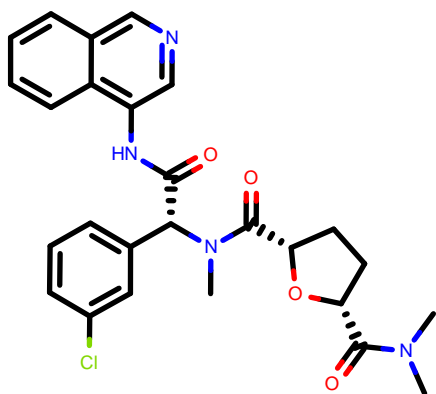
CID:	MIC-UNK-5a93dd5f-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)N[+]@H+J4CC[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN1189
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.14

MIC-UNK-d36ab305-4_2



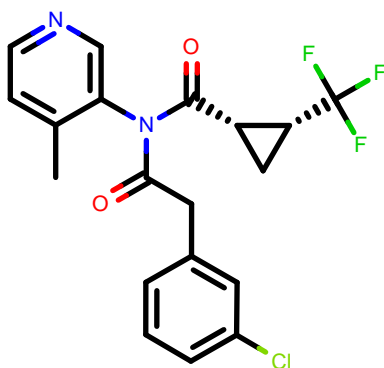
CID:	MIC-UNK-d36ab305-4_2
SMILES:	<chem>CN(C)c1ccc(cc1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1043
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.15

PET-UNK-1320d94d-21_1



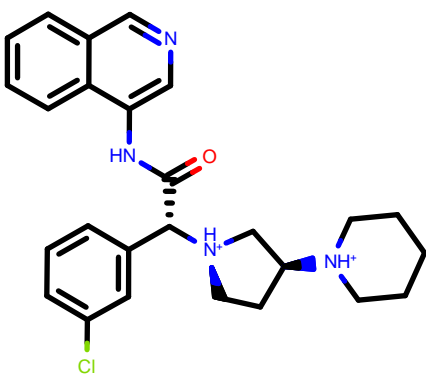
CID:	PET-UNK-1320d94d-21_1
SMILES:	<chem>CN(C)C(=O)[C@H]1CC[C@H](O1)C(=O)N(C)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1531
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.21

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:	RUN1314
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.18

MIC-UNK-5a93dd5f-12_1



CID: MIC-UNK-5a93dd5f-12_1

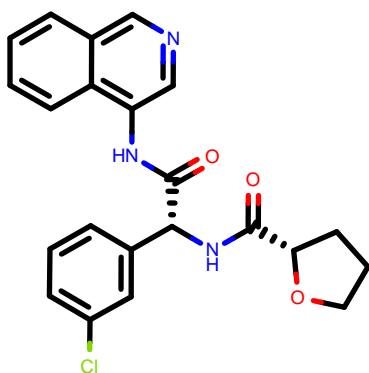
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](c3cccc(c3)Cl)N@[4]CC[C@@H](C4)[NH+]5CCCCC5

RUN: RUN1234

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.15

EDJ-MED-cf4b0d25-3_1



CID: EDJ-MED-cf4b0d25-3_1

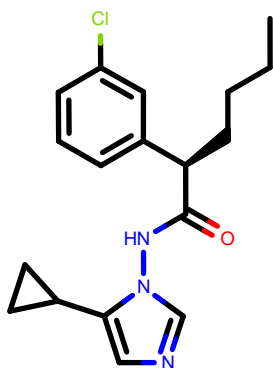
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@@H]4CCCC4

RUN: RUN1426

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.17

JAN-GHE-f4ca5a00-18_2



CID: JAN-GHE-f4ca5a00-18_2

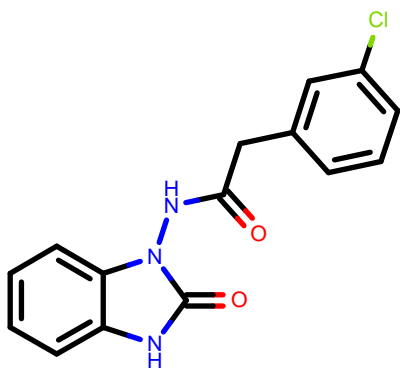
SMILES: CCCC[C@@H](c1cccc(c1)Cl)C(=O)Nn2cnc2C3CC3

RUN: RUN1000

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.17

VLA-UNK-dc1d9354-1_1



CID: VLA-UNK-dc1d9354-1_1

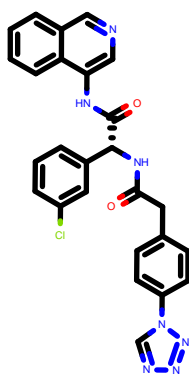
SMILES: c1ccc2c(c1)[nH]c(=O)n2NC(=O)Cc3cccc(c3)Cl

RUN: RUN1483

DDG (kcal/mol): -1.83

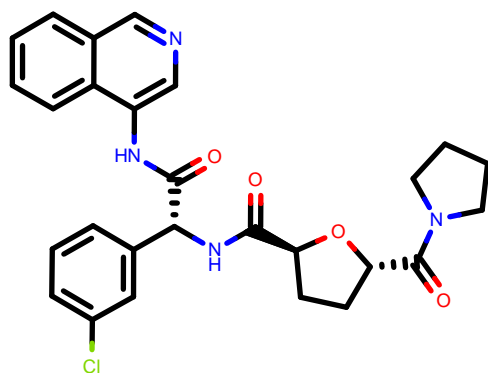
dDDG (kcal/mol): 0.14

EDJ-MED-ee07cf00-15_1



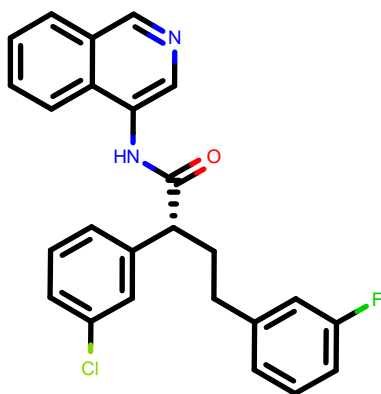
CID:	EDJ-MED-ee07cf00-15_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccccc(c3)C)NC(=O)Cc4ccc(cc4)n5cnnn5</chem>
RUN:	RUN1398
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.22

EDJ-MED-ee07cf00-11_5



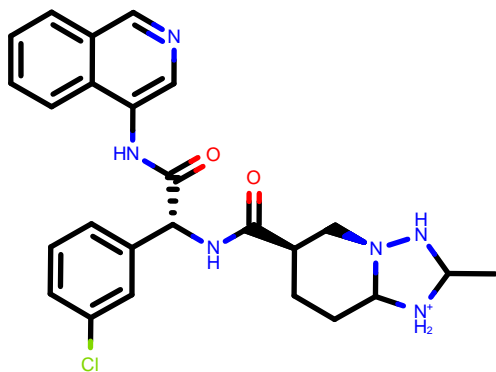
CID:	EDJ-MED-ee07cf00-11_5
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccccc(c3)C)NC(=O)C@H(Cc4ccoc4)N5CCCC5</chem>
RUN:	RUN1397
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.19

MIC-UNK-c66144cb-1_2



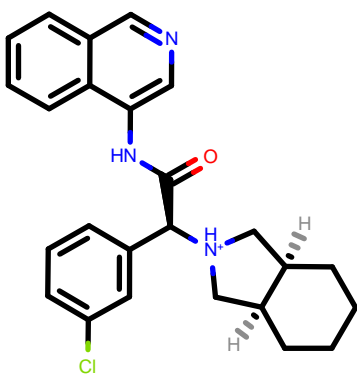
CID:	MIC-UNK-c66144cb-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](CCc3ccccc(c3)F)c4ccccc(c4)Cl</chem>
RUN:	RUN1047
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.23

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)Nc4cnc(C)c4</chem>
RUN:	RUN1416
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.19

MIC-UNK-5a93dd5f-2_2



CID: MIC-UNK-5a93dd5f-2_2

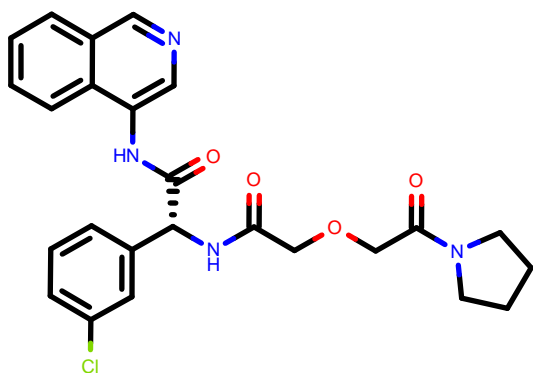
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)[NH+]4C[C@H]5CCCC[C@H]5C4

RUN: RUN1150

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.23

EDJ-MED-cf4b0d25-1_1



CID: EDJ-MED-cf4b0d25-1_1

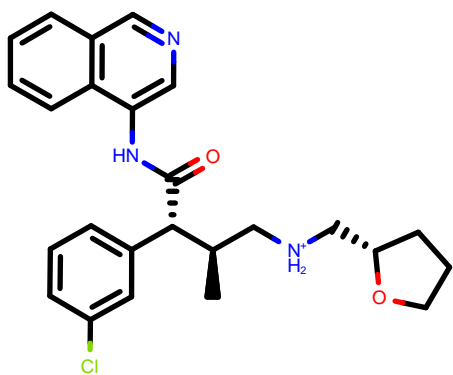
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)NC(=O)COCC(=O)N4CCCC4

RUN: RUN1502

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.19

MAK-UNK-c749d764-22_6



CID: MAK-UNK-c749d764-22_6

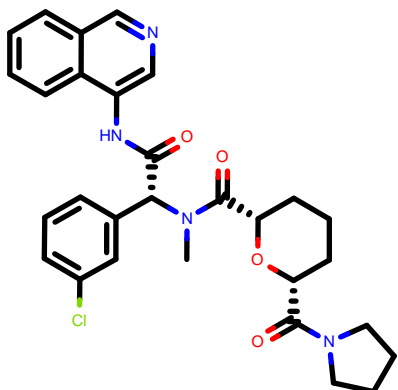
SMILES: C[C@H](C)[C][NH2+][C]C@H1CCCCO1[C@H](c2ccccc(c2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN1253

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.20

PET-UNK-1320d94d-29_1



CID: PET-UNK-1320d94d-29_1

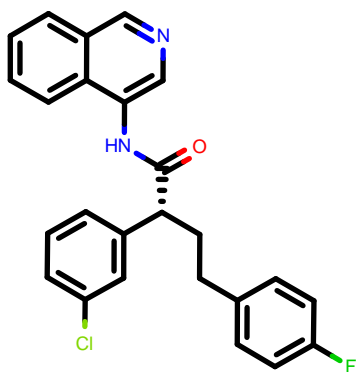
SMILES: CN[C@H](c1ccc(c1)Cl)C(=O)Nc2nccc3c2ccc3Cl(=O)C@H4CCCC[C@H]4[C@@H]5C1CCCC15

RUN: RUN1542

DDG (kcal/mol): -1.67

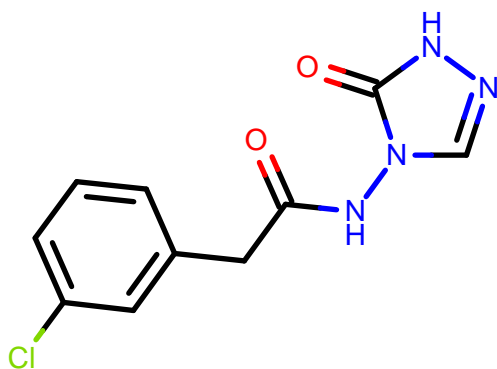
dDDG (kcal/mol): 0.21

MIC-UNK-c66144cb-2_2



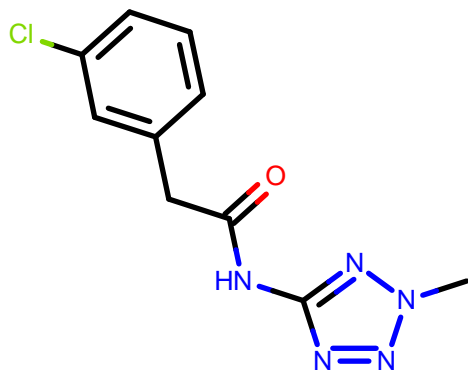
CID:	MIC-UNK-c66144cb-2_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CCc3cccc(cc3)F)c4cccc(c4)Cl</chem>
RUN:	RUN1044
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.19

JAN-GHE-5a013bed-4_1



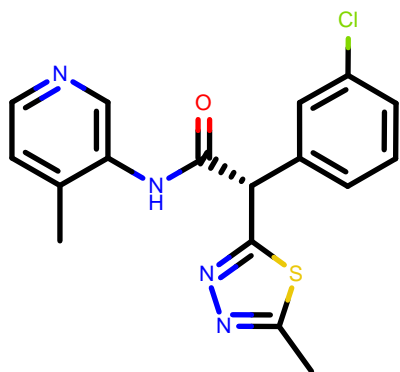
CID:	JAN-GHE-5a013bed-4_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2cn[nH]c2=O</chem>
RUN:	RUN865
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.12

VLA-UNK-411a133b-1_1



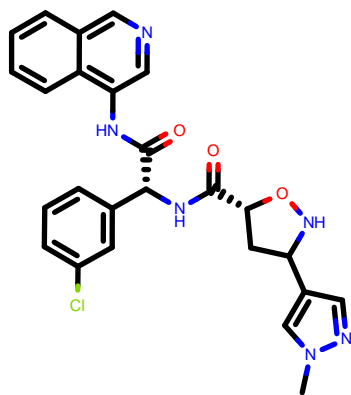
CID:	VLA-UNK-411a133b-1_1
SMILES:	<chem>Cn1nc(nn1)NC(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN1484
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.11

TRY-UNI-9f475305-3_2



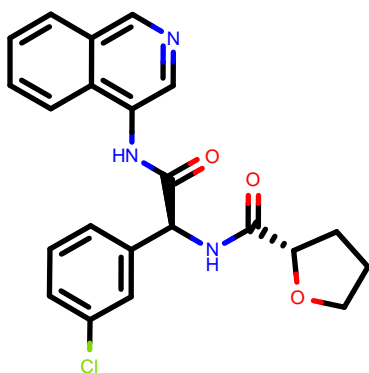
CID:	TRY-UNI-9f475305-3_2
SMILES:	<chem>Cc1ccncc1NC(=O)[C@H](c2cccc(c2)Cl)c3nnc(s3)C</chem>
RUN:	RUN863
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.12

EDJ-MED-ee07cf00-6_4



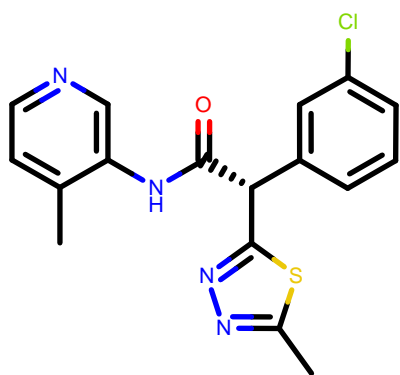
CID:	EDJ-MED-ee07cf00-6_4
SMILES:	<chem>Cn1cc(en1)C2=NO[C@H](C2)C(=O)N[C@H](c3ccccc(c3)Cl)C(=O)Nc4nccc5c4ccccc5</chem>
RUN:	RUN1382
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.23

EDJ-MED-cf4b0d25-3_2



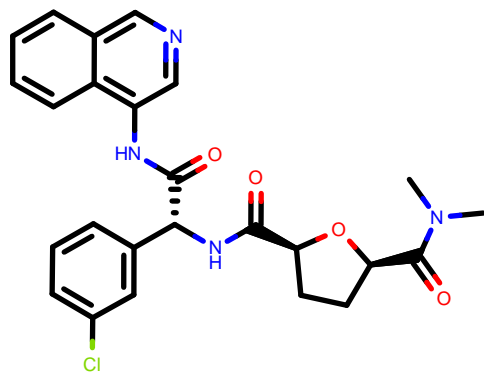
CID:	EDJ-MED-cf4b0d25-3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)NC(=O)[C@@H]4CCCCO4</chem>
RUN:	RUN1424
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.17

SAM-UNK-2684b532-3_2



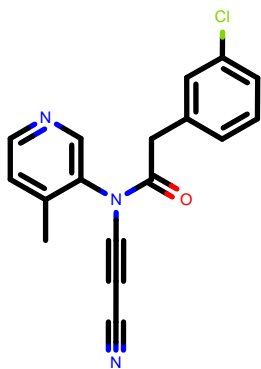
CID:	SAM-UNK-2684b532-3_2
SMILES:	<chem>Cc1ccncc1NC(=O)[C@H](c2ccccc(c2)Cl)c3nnc(s3)C</chem>
RUN:	RUN944
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.12

PET-UNK-1320d94d-1_1



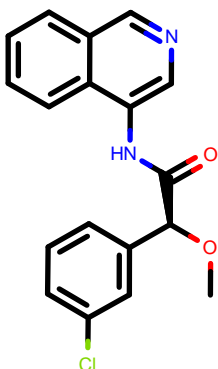
CID:	PET-UNK-1320d94d-1_1
SMILES:	<chem>CN(C)C(=O)[C@H]1CC[C@H](O1)C(=O)N[C@H](c2ccccc(c2)Cl)C(=O)Nc3nccc4c3ccccc4</chem>
RUN:	RUN1526
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.20

DAR-DIA-076fb6ea-6_1



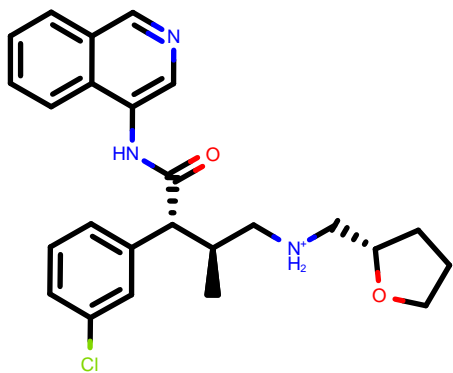
CID:	DAR-DIA-076fb6ea-6_1
SMILES:	<chem>Cc1ccncc1N(C#CC#N)C(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN1263
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.17

VLA-UNK-9a7dc93f-7_1



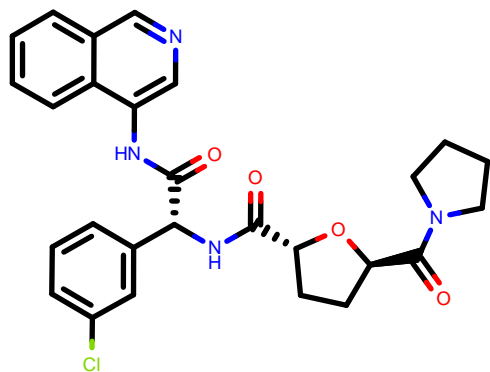
CID:	VLA-UNK-9a7dc93f-7_1
SMILES:	<chem>CO[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN1380
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.05

MAK-UNK-ffc90da7-4_6



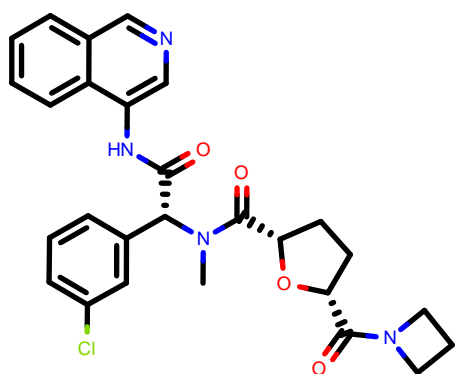
CID:	MAK-UNK-ffc90da7-4_6
SMILES:	<chem>C[C@H](C[NH2+][C@@@H]1CCCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1192
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.23

PET-UNK-ac320b15-5_1



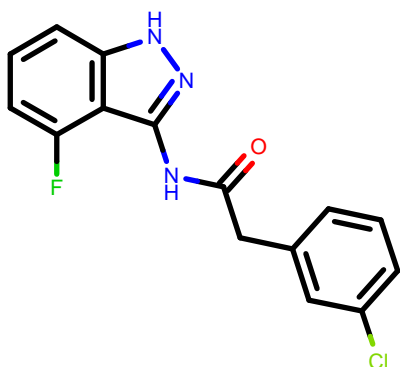
CID:	PET-UNK-ac320b15-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)N(C)C(=O)[C@H](O)C1CCN1</chem>
RUN:	RUN1555
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.23

PET-UNK-1320d94d-25_1



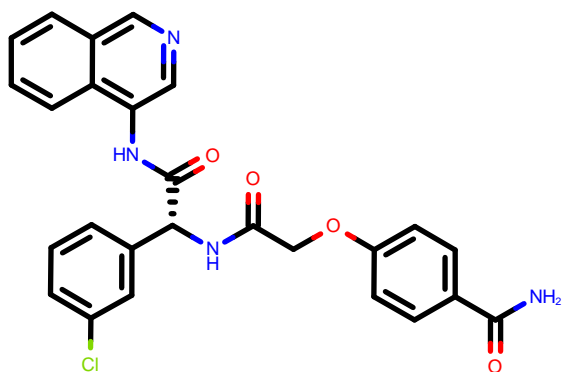
CID:	PET-UNK-1320d94d-25_1
SMILES:	<chem>CN1[C@@H](c1ccc(c1)C)C(=O)Nc2oc3c2ccc3C1=O[C@@H](C)C[C@@H](O4C1=O)N5CCCC5</chem>
RUN:	RUN1546
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.19

EDJ-MED-c8e7a002-13_1



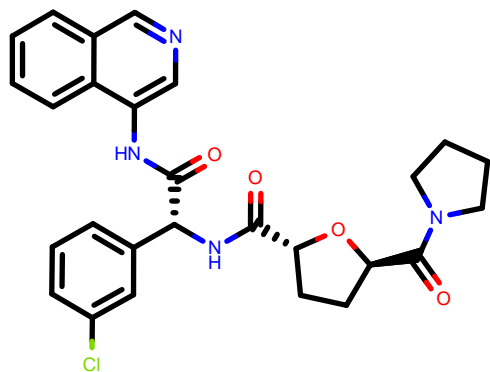
CID:	EDJ-MED-c8e7a002-13_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3c(cccc3F)[nH]n2</chem>
RUN:	RUN1109
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-12_1



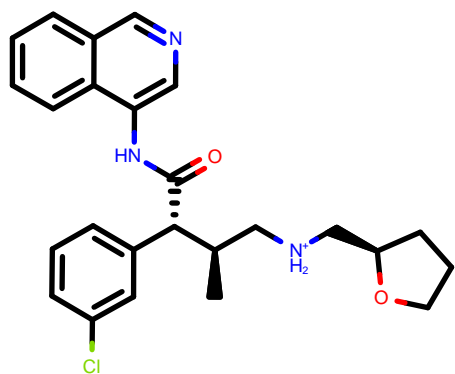
CID:	EDJ-MED-ee07cf00-12_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccc(c3)C)N(C(=O)COc4ccc(cc4)C)C(=O)N</chem>
RUN:	RUN1409
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.20

MAT-POS-8293a91a-2_1



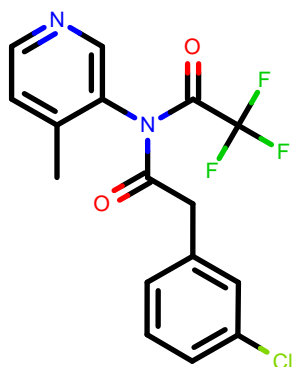
CID:	MAT-POS-8293a91a-2_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccc(c3)C)N(C(=O)C1=O)[C@@H](O4C1=O)N5CCCC5</chem>
RUN:	RUN1573
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.19

MAK-UNK-ffc90da7-4_8



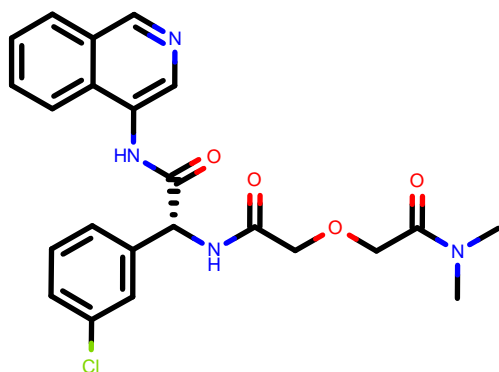
CID:	MAK-UNK-ffc90da7-4_8
SMILES:	<chem>C[C@H](C[NH2+][C][C@H]1CCCCO1)[C@H](c2ccccc2)C(=O)Nc3nccc4c3cccc4</chem>
RUN:	RUN1204
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.27

JOH-UNI-a38a7bdd-3_1



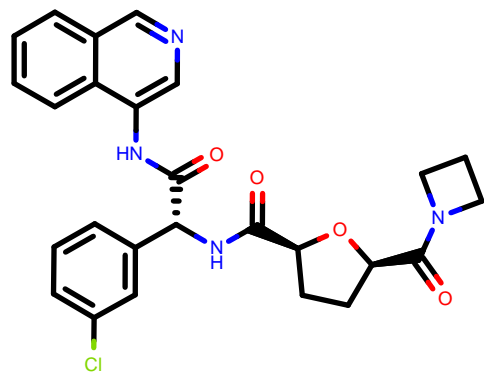
CID:	JOH-UNI-a38a7bdd-3_1
SMILES:	<chem>Cc1ccncc1N(C(=O)Cc2ccccc2)C(=O)C(F)(F)F</chem>
RUN:	RUN1291
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.16

EDJ-MED-cf4b0d25-5_2



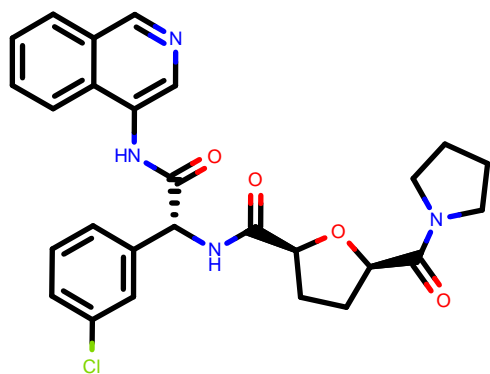
CID:	EDJ-MED-cf4b0d25-5_2
SMILES:	<chem>CN(C)C(=O)COCC(=O)N[C@H](c1ccccc1)C(=O)Nc2nccc3c2cccc3</chem>
RUN:	RUN1515
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.17

PET-UNK-1320d94d-5_1



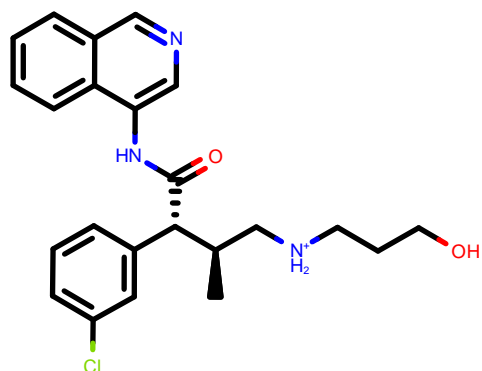
CID:	PET-UNK-1320d94d-5_1
SMILES:	<chem>c1ccc2c(c1)nccc2N[C@H](c3ccccc3)C(=O)N[C@H](O4CCOC4)C(=O)N5CCCC5</chem>
RUN:	RUN1532
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.20

EDJ-MED-ee07cf00-11_1



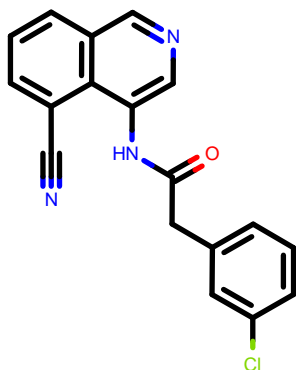
CID:	EDJ-MED-ee07cf00-11_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](C)[C@@H](c3ccc(c3)NC(=O)[C@H](C)[C@@H](O4C[C@H]5CNCC5)O4)C(=O)N5CCCC5</chem>
RUN:	RUN1385
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.19

MAK-UNK-c749d764-6_4



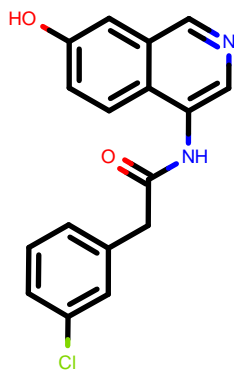
CID:	MAK-UNK-c749d764-6_4
SMILES:	<chem>C[C@H](C)[C@H](C)CC(=O)[C@H](c1ccc(c1)Cl)C(=O)Nc2cnc3c2ccc3O</chem>
RUN:	RUN1281
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.26

PET-UNK-6314f867-3_1



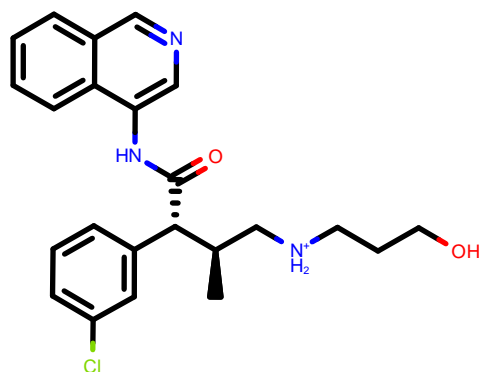
CID:	PET-UNK-6314f867-3_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cnc3c2c(c3)C#N</chem>
RUN:	RUN1501
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.12

MAT-POS-bb423b95-8_1



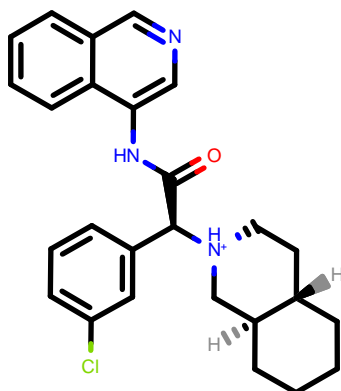
CID:	MAT-POS-bb423b95-8_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cnc3c2ccc(c3)O</chem>
RUN:	RUN1061
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.12

MAK-UNK-ffc90da7-1_4



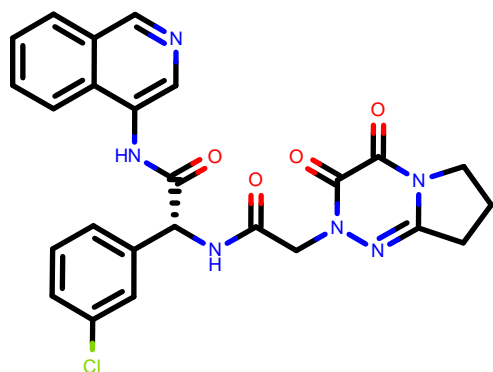
CID:	MAK-UNK-ffc90da7-1_4
SMILES:	<chem>C[C@H](C[NH2+]CCCO)[C@H](c1cccc(c1)Cl)C(=O)Nc2cccc3c2cccc3</chem>
RUN:	RUN1207
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.23

MIC-UNK-5a93dd5f-3_10



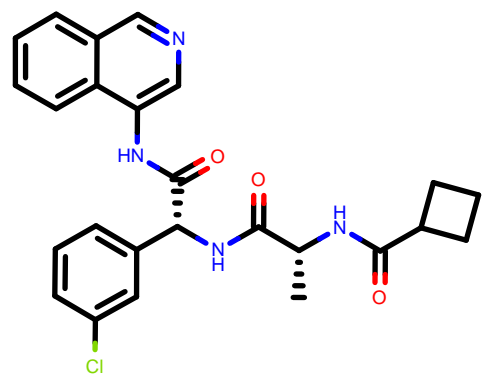
CID:	MIC-UNK-5a93dd5f-3_10
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)N@@H4CC[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN1187
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.25

EDJ-MED-ee07cf00-14_1



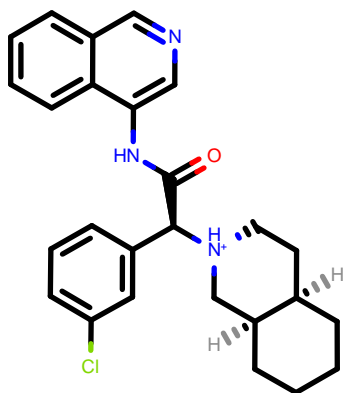
CID:	EDJ-MED-ee07cf00-14_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)Cn4c(=O)c(=O)n5c(n4)CCO5</chem>
RUN:	RUN1395
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.28

EDJ-MED-ee07cf00-4_4



CID:	EDJ-MED-ee07cf00-4_4
SMILES:	<chem>C[C@H](C(=O)N[C@H](c1cccc(c1)Cl)C(=O)Nc2cccc3c2cccc3)NC(=O)C4CCC4</chem>
RUN:	RUN1411
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.23

MIC-UNK-5a93dd5f-3_14



CID: MIC-UNK-5a93dd5f-3_14

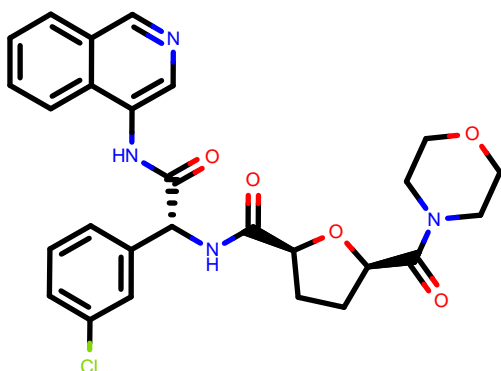
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](c3cccc(c3)Cl)N@@H+4CC[C@H]5CCCC[C@H]5C4

RUN: RUN1190

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.24

PET-UNK-1320d94d-3_1



CID: PET-UNK-1320d94d-3_1

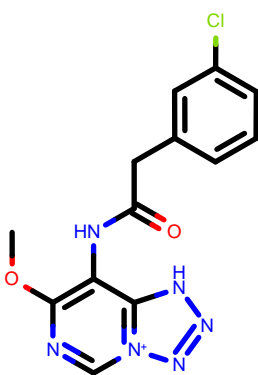
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](c3cccc(c3)Cl)N[C@@H]4C[C@H](O4)C1=NC=CC=C1

RUN: RUN1535

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.23

EDJ-MED-97c1bf5c-2_1



CID: EDJ-MED-97c1bf5c-2_1

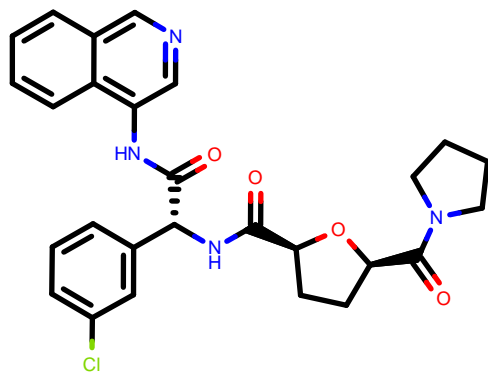
SMILES: COc1c(c2nnnn2cn1)NC(=O)Cc3cccc(c3)Cl

RUN: RUN1134

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.13

MAT-POS-a13804f0-4_1



CID: MAT-POS-a13804f0-4_1

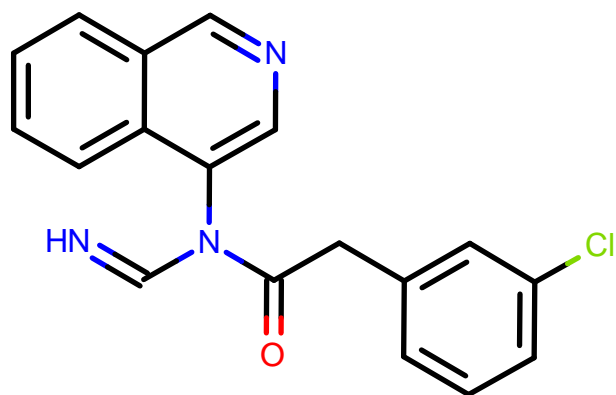
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](c3cccc(c3)Cl)N[C@@H]4C[C@H](O4)C1=CC=CC=C1

RUN: RUN1419

DDG (kcal/mol): -1.20

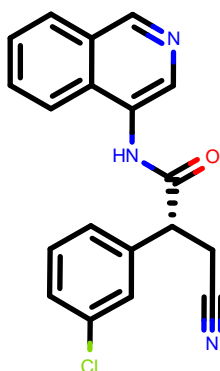
dDDG (kcal/mol): 0.22

PET-UNK-5ecb6237-1_1



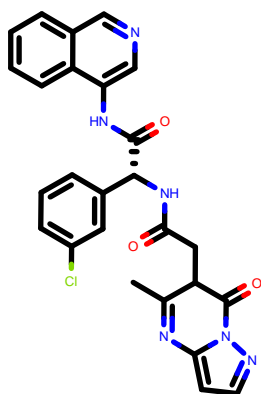
CID:	PET-UNK-5ecb6237-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C#N)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1121
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.15

JOH-UNI-ee5ed7c8-6_2



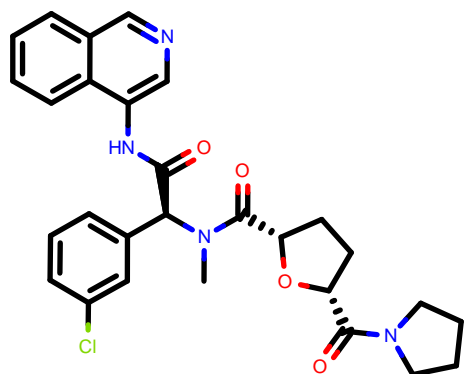
CID:	JOH-UNI-ee5ed7c8-6_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CC#N)c3cccc(c3)Cl</chem>
RUN:	RUN1334
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.10

EDJ-MED-ee07cf00-2_2



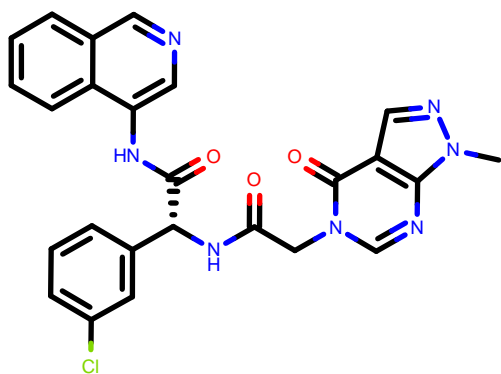
CID:	EDJ-MED-ee07cf00-2_2
SMILES:	<chem>Cc1c(c(=O)n2c(n1)cd[nH]2)CC(=O)N[C@H](c3cccc(c3)C)C(=O)Nc4ncnc5o4cccc5</chem>
RUN:	RUN1366
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.19

PET-UNK-10339a1d-1_1



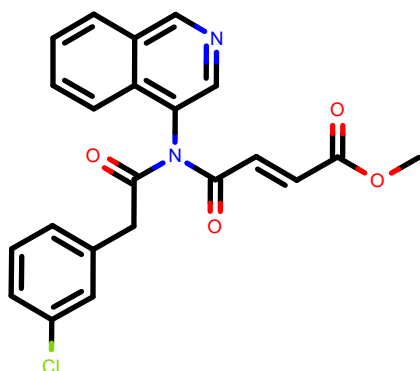
CID:	PET-UNK-10339a1d-1_1
SMILES:	<chem>CN[C@H](c1cccc(c1)C)C(=O)Nc2ncnc3c2cccc3C(=O)C[C@H](c4cccc(c4)O)N5CCCC5</chem>
RUN:	RUN1523
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.21

EDJ-MED-ee07cf00-3_2



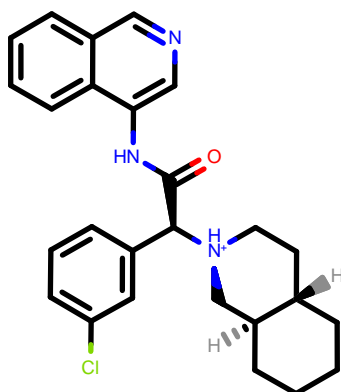
CID:	EDJ-MED-ee07cf00-3_2
SMILES:	<chem>Cn1c2c(en1)c(=O)n(en2)CC(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN1368
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.18

DAR-DIA-076fb6ea-3_1



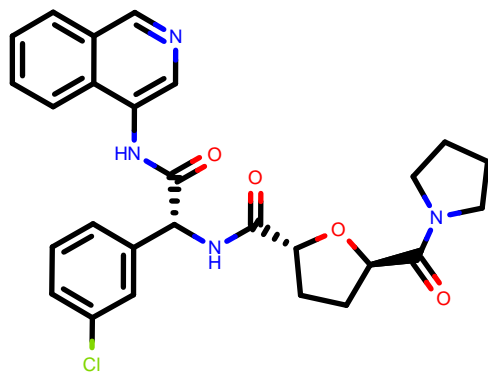
CID:	DAR-DIA-076fb6ea-3_1
SMILES:	<chem>COC(=O)/C=C/C(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1318
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.24

MIC-UNK-5a93dd5f-3_12



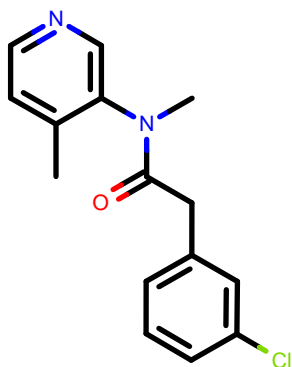
CID:	MIC-UNK-5a93dd5f-3_12
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@H]4CC[C@@H]5CCCC[C@H]5C4</chem>
RUN:	RUN1194
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.23

EDJ-MED-ee07cf00-11_3



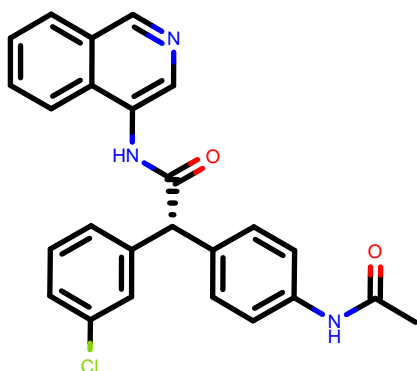
CID:	EDJ-MED-ee07cf00-11_3
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)N[C@H]4CC[C@@H]5CCCC[C@H]5C4</chem>
RUN:	RUN1389
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.19

JAN-GHE-83b26c96-15_1



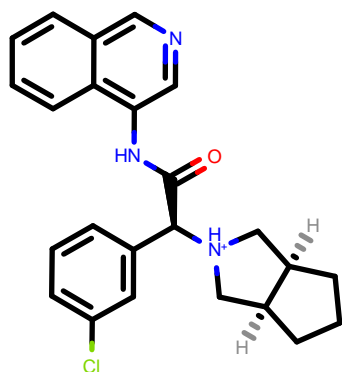
CID:	JAN-GHE-83b26c96-15_1
SMILES:	<chem>Cc1ccncc1N(C)C(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN835
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.16

MIC-UNK-d36ab305-1_2



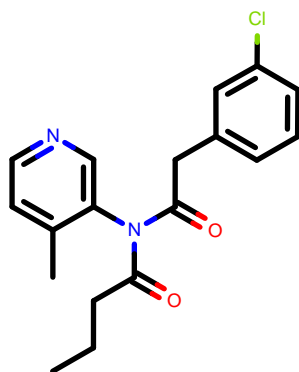
CID:	MIC-UNK-d36ab305-1_2
SMILES:	<chem>CC(=O)Nc1ccc(cc1)[C@H](c2cccc(c2)Cl)C(=O)Nc3ccc4c3cccc4</chem>
RUN:	RUN1041
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.14

MIC-UNK-5a93dd5f-1_2



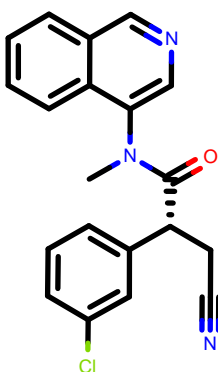
CID:	MIC-UNK-5a93dd5f-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)N[H+]4C[C@H]5CC[C@H]5C4</chem>
RUN:	RUN1152
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.22

DAR-DIA-076fb6ea-7_1



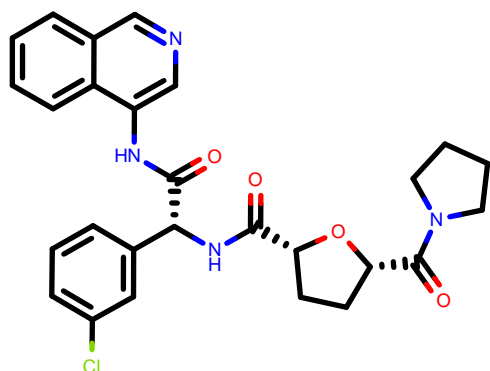
CID:	DAR-DIA-076fb6ea-7_1
SMILES:	<chem>Cc1ccncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)C=C</chem>
RUN:	RUN1279
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.16

JOH-UNI-3fc3434e-7_2



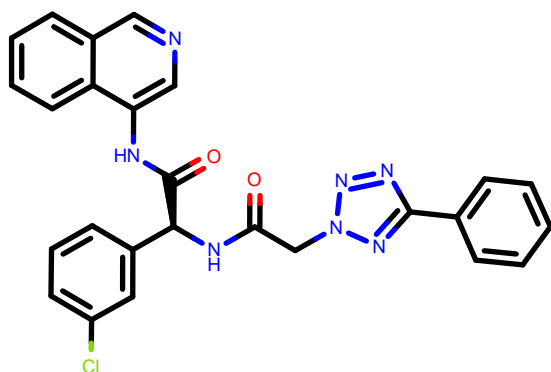
CID:	JOH-UNI-3fc3434e-7_2
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)[C@H](CC#N)c3cccc(c3)Cl</chem>
RUN:	RUN1355
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.25

EDJ-MED-ee07cf00-11_7



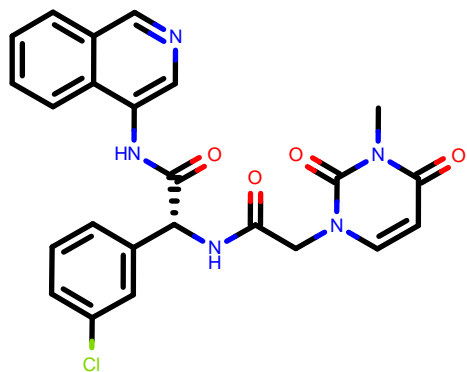
CID:	EDJ-MED-ee07cf00-11_7
SMILES:	<chem>c1ccc2c(c1)cncc2N[C@@H](C#O)c3cccc(c3)C(=O)[C@@H](C4CCN4)O5NCCCC5</chem>
RUN:	RUN1394
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.19

EDJ-MED-ee07cf00-9_1



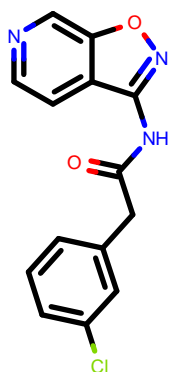
CID:	EDJ-MED-ee07cf00-9_1
SMILES:	<chem>c1ccc(cc1)c2nnn(n2)CC(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN1376
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.19

EDJ-MED-ee07cf00-1_2



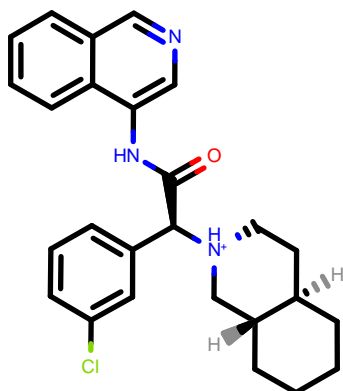
CID:	EDJ-MED-ee07cf00-1_2
SMILES:	<chem>Cn1c(=O)ccn(c1=O)CC(=O)N[C@H](c2cccc(c2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN1365
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.15

JIN-POS-6dc588a4-16_1



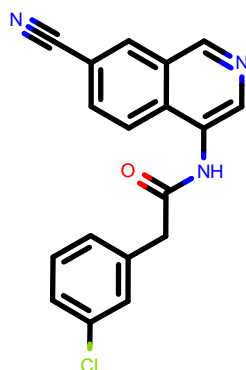
CID:	JIN-POS-6dc588a4-16_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3ccncc3on2</chem>
RUN:	RUN1440
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.11

MIC-UNK-5a93dd5f-3_6



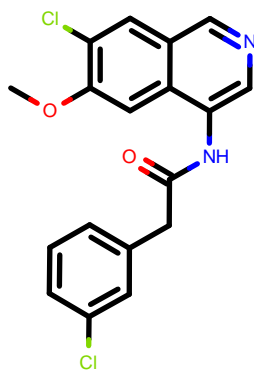
CID:	MIC-UNK-5a93dd5f-3_6
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)[C@H](c3cccc(c3)Cl)N@@H4CC[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN1169
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.23

PET-UNK-6314f867-2_1



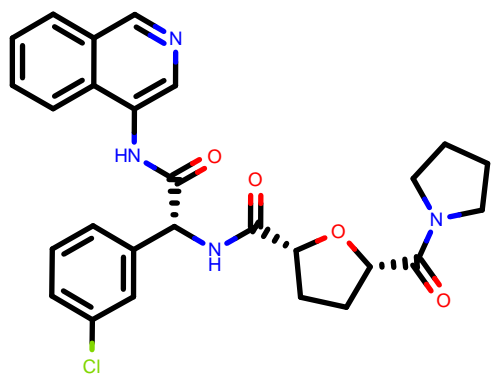
CID:	PET-UNK-6314f867-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cnccc3c2ccc(c3)C#N</chem>
RUN:	RUN1499
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.16

PET-UNK-b38839dc-2_1



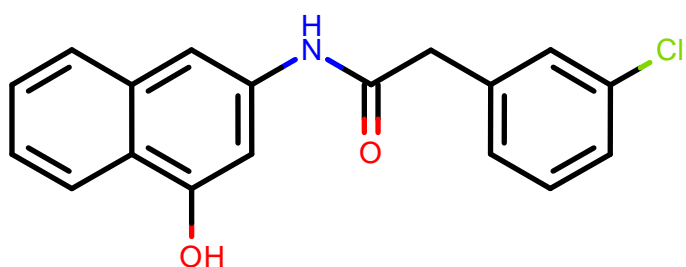
CID:	PET-UNK-b38839dc-2_1
SMILES:	<chem>COc1cc2c(cc1Cl)ncc2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1580
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.15

PET-UNK-ac320b15-9_1



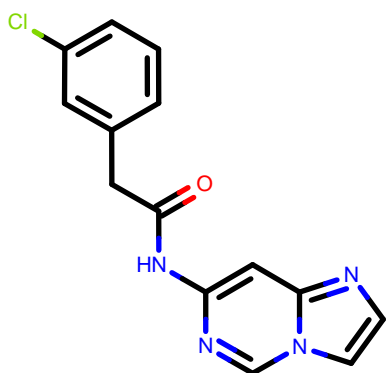
CID:	PET-UNK-ac320b15-9_1
SMILES:	<chem>c1ccc2c(c1)nc2N(C(=O)[C@@H](c3cccc(c3)N(C(=O)[C@@H](C4CC[C@H]4)O4)Cl)O)N6CCCC6</chem>
RUN:	RUN1567
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.20

ROB-UNI-daaf9793-3_1



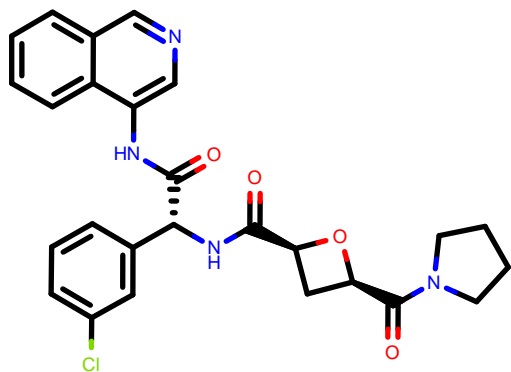
CID:	ROB-UNI-daaf9793-3_1
SMILES:	<chem>c1ccc2c(c1)cc(cc2O)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1488
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.15

JIN-POS-6dc588a4-17_1



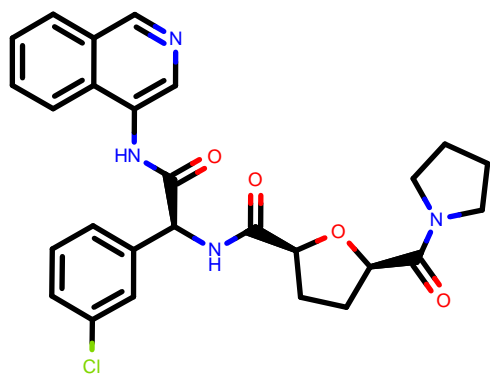
CID:	JIN-POS-6dc588a4-17_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cc3nccn3cn2</chem>
RUN:	RUN1449
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.17

PET-UNK-1320d94d-7_1



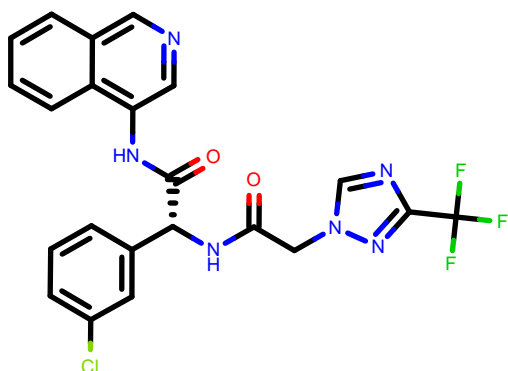
CID:	PET-UNK-1320d94d-7_1
SMILES:	<chem>c1ccc2c(c1)nc2N(C(=O)[C@@H](c3cccc(c3)N(C(=O)[C@@H](C4CC[C@H]4)O4)Cl)O)N6CCCC6</chem>
RUN:	RUN1527
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.24

MAT-POS-a13804f0-4_2



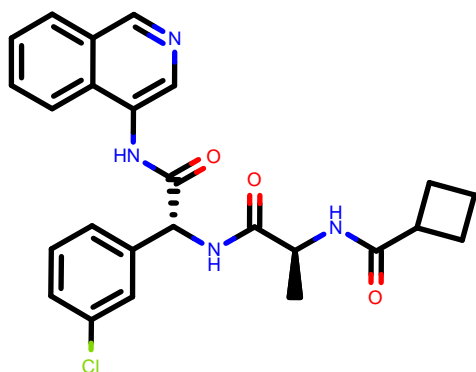
CID:	MAT-POS-a13804f0-4_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccc(c3)C)NC(=O)[C@@H](C)C(=O)N6CCCC6</chem>
RUN:	RUN1423
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.22

EDJ-MED-ee07cf00-10_1



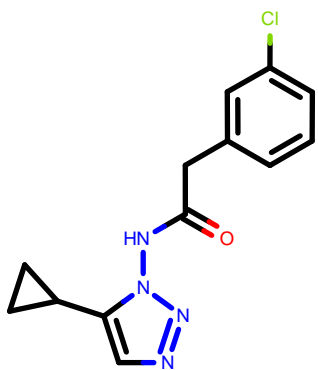
CID:	EDJ-MED-ee07cf00-10_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)N3C(=O)Cn4nc(n4)C(F)(F)F</chem>
RUN:	RUN1381
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.27

EDJ-MED-ee07cf00-4_3



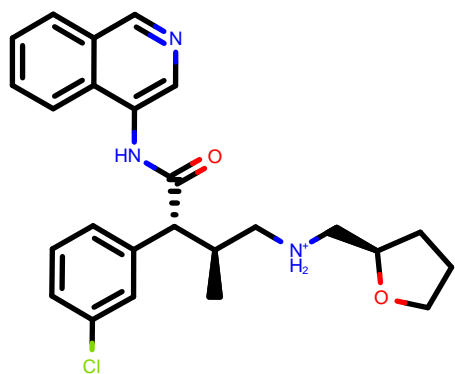
CID:	EDJ-MED-ee07cf00-4_3
SMILES:	<chem>C[C@@H](C(=O)N[C@@H](c1cccc(c1)C)C(=O)Nc2ccc3c2ccc3)NC(=O)C4CCCC4</chem>
RUN:	RUN1408
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.21

JAN-GHE-f4ca5a00-17_1



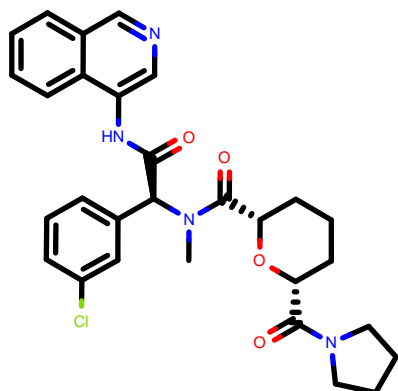
CID:	JAN-GHE-f4ca5a00-17_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2c(cnn2)C3CC3</chem>
RUN:	RUN958
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.12

MAK-UNK-c749d764-22_8



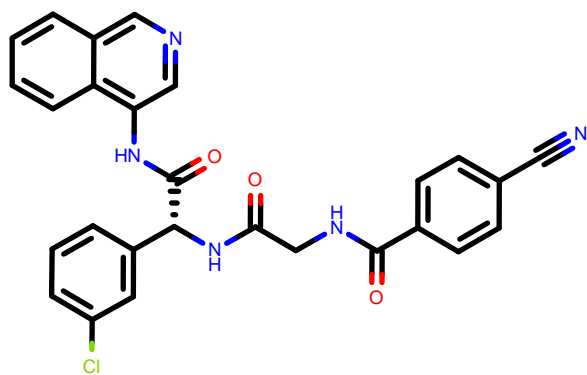
CID:	MAK-UNK-c749d764-22_8
SMILES:	<chem>C[C@H](C[NH2+][C][C@H]1CCCC1)[C@H](C2CCCC2)C(=O)Nc3nccc4c3cccc4</chem>
RUN:	RUN1273
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.23

PET-UNK-1320d94d-30_1



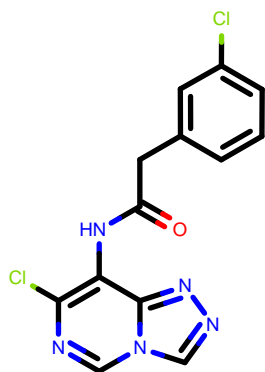
CID:	PET-UNK-1320d94d-30_1
SMILES:	<chem>CN(C@@H)(c1cccc1)C(C)(=O)Nc2ncc3c2cccc3C(=O)C@H(C4CC[C@H](O4)C=O)N5CCCC5</chem>
RUN:	RUN1562
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.19

EDJ-MED-ee07cf00-5_1



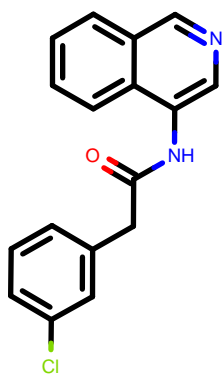
CID:	EDJ-MED-ee07cf00-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C][C@H](c3cccc(c3)C)NC(=O)CNC(=O)c4ccc(cc4)C#N</chem>
RUN:	RUN1406
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.22

EDJ-MED-c8e7a002-7_1



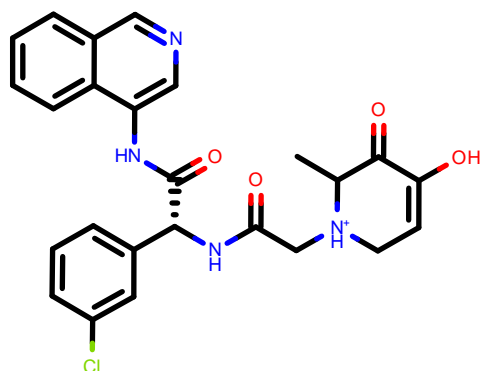
CID:	EDJ-MED-c8e7a002-7_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3nncn3cnc2Cl</chem>
RUN:	RUN1103
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.14

MAT-POS-f7918075-3_1



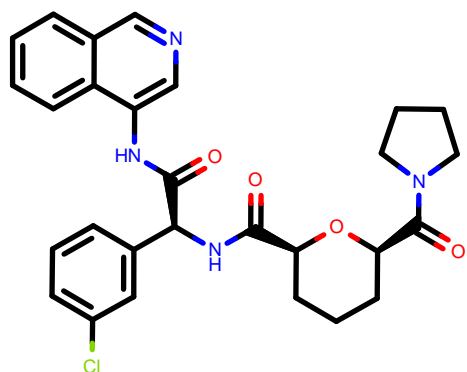
CID:	MAT-POS-f7918075-3_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccn3</chem>
RUN:	RUN1063
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.04

EDJ-MED-ee07cf00-7_2



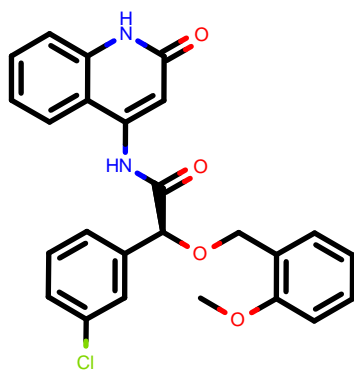
CID:	EDJ-MED-ee07cf00-7_2
SMILES:	<chem>Cc1c(c(=O)ccn1CC(=O)N[C@H](c2ccccc2)Cl)C(=O)Nc3cncc4c3cccc4[O]</chem>
RUN:	RUN1374
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.26

PET-UNK-1320d94d-10_1



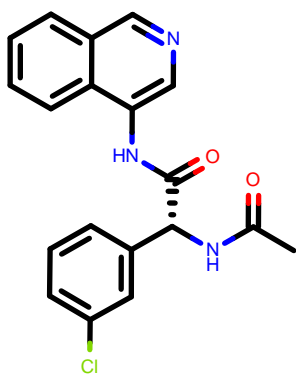
CID:	PET-UNK-1320d94d-10_1
SMILES:	<chem>c1ccc2c(c1)ccc2NCl(=O)[C@H](c3ccccc3)C(=O)N[C@@H](C4CC[C@H]4)C(=O)N5CCCC5</chem>
RUN:	RUN1537
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.21

ADA-UCB-6c2cb422-11_1



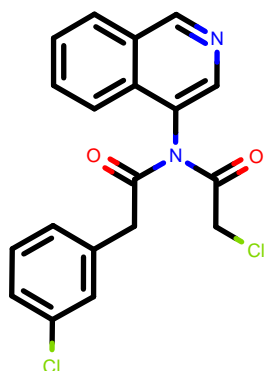
CID:	ADA-UCB-6c2cb422-11_1
SMILES:	<chem>COc1ccccc1CO[C@H](c2ccccc2)Cl)C(=O)Nc3cc(=O)[nH]c4c3ccccc4</chem>
RUN:	RUN957
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.24

EDJ-MED-cf4b0d25-4_2



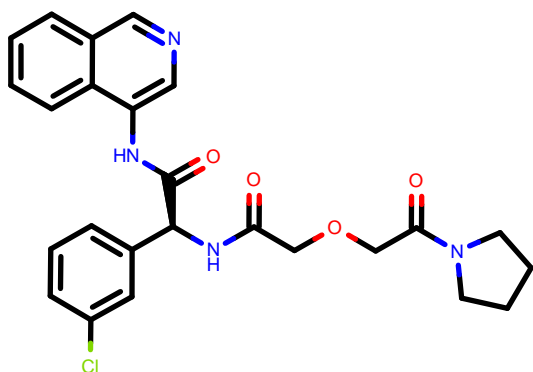
CID:	EDJ-MED-cf4b0d25-4_2
SMILES:	<chem>CC(=O)N[C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN1421
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.15

PET-UNK-6c2be958-1_1



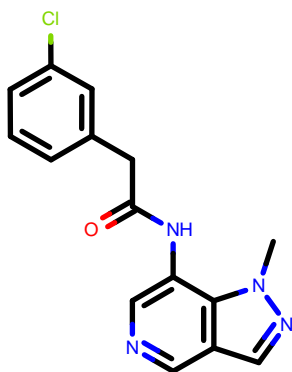
CID:	PET-UNK-6c2be958-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)CCl</chem>
RUN:	RUN1327
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.17

EDJ-MED-cf4b0d25-1_2



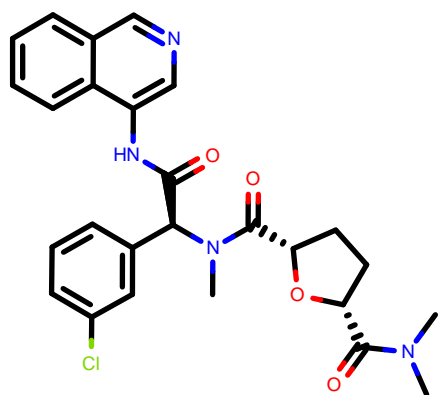
CID:	EDJ-MED-cf4b0d25-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)COCC(=O)N4CCCC4</chem>
RUN:	RUN1504
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.19

PET-UNK-e274cad4-1_1



CID:	PET-UNK-e274cad4-1_1
SMILES:	<chem>Cn1c2c(cncc2NC(=O)Cc3cccc(c3)Cl)cn1</chem>
RUN:	RUN1509
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.12

PET-UNK-1320d94d-22_1



CID: PET-UNK-1320d94d-22_1

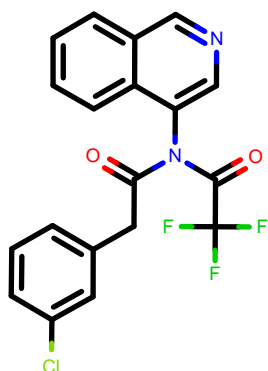
SMILES: CN(C)C(=O)[C@H]1CC[C@H](O1)C(=O)N(C)[C@@H](c2ccccc2Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN1530

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.18

JOH-UNI-a38a7bdd-1_1



CID: JOH-UNI-a38a7bdd-1_1

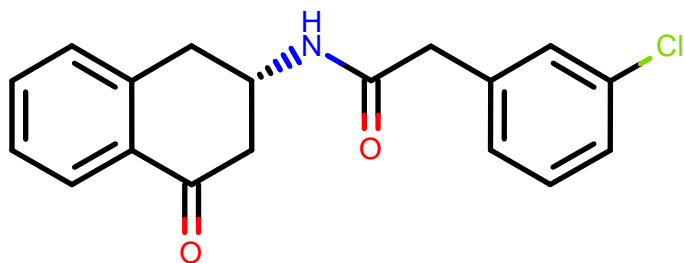
SMILES: c1ccc2c(c1)cncc2N(C(=O)Cc3ccccc(c3)Cl)C(=O)C(F)(F)F

RUN: RUN1286

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.17

ROB-UNI-daaf9793-4_1



CID: ROB-UNI-daaf9793-4_1

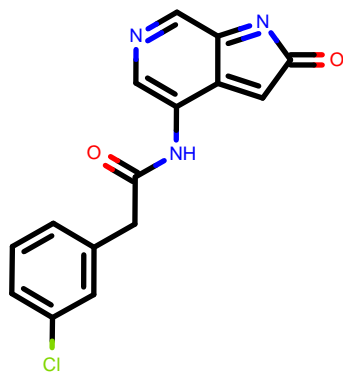
SMILES: c1ccc2c(c1)C[C@@H](CC2=O)NC(=O)Cc3ccccc(c3)Cl

RUN: RUN1489

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.14

MAT-POS-f7918075-7_1



CID: MAT-POS-f7918075-7_1

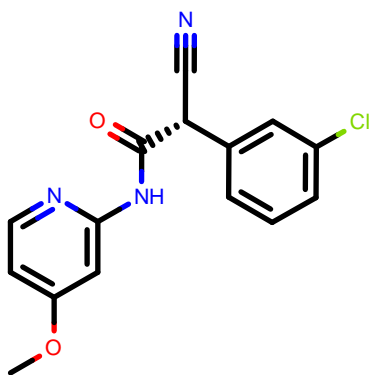
SMILES: c1cc(cc(c1)Cl)CC(=O)Nc2cnccc3c2CC(=O)N3

RUN: RUN1069

DDG (kcal/mol): -0.56

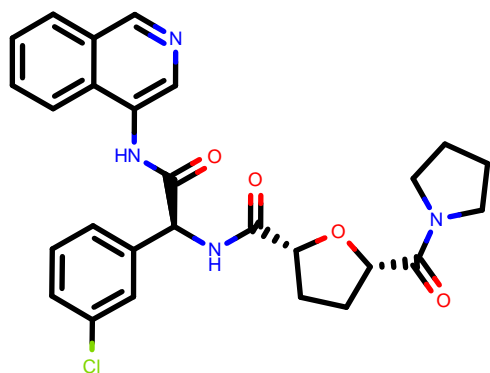
dDDG (kcal/mol): 0.14

RIT-UNK-fa3975ff-1_2



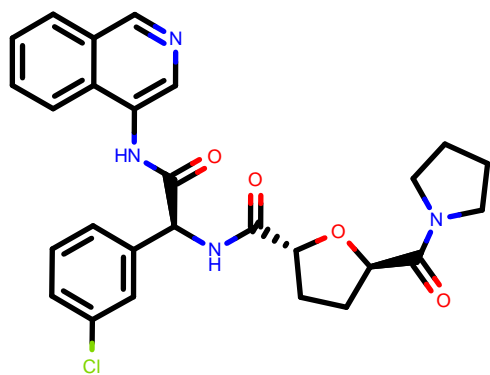
CID:	RIT-UNK-fa3975ff-1_2
SMILES:	<chem>COc1ccnc(c1)NC(=O)[C@H](C#N)c2cccc(c2)Cl</chem>
RUN:	RUN1119
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.25

MAT-POS-8293a91a-7_2



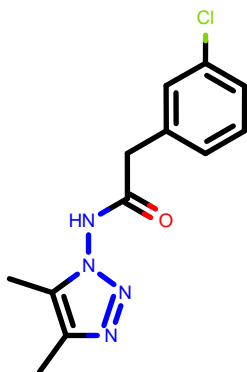
CID:	MAT-POS-8293a91a-7_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)NC(=O)[C@H](C#N)C(=O)N5CCCC5</chem>
RUN:	RUN1584
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.24

PET-UNK-ac320b15-6_1



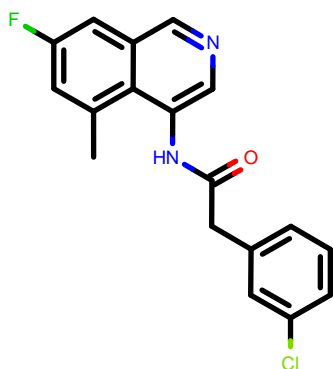
CID:	PET-UNK-ac320b15-6_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)NC(=O)[C@H](C#N)C(=O)N5CCCC5</chem>
RUN:	RUN1564
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.28

JAN-GHE-5a013bed-1_1



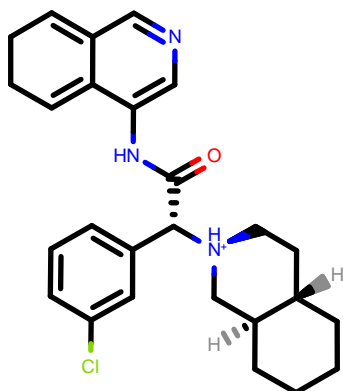
CID:	JAN-GHE-5a013bed-1_1
SMILES:	<chem>Cc1c(n(nn1)NC(=O)Cc2cccc(c2)Cl)C</chem>
RUN:	RUN849
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.12

MAT-POS-29385cc1-4_1



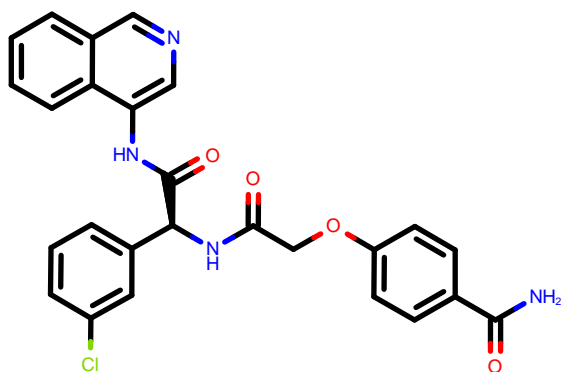
CID:	MAT-POS-29385cc1-4_1
SMILES:	<chem>Cc1cc(cc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl)F</chem>
RUN:	RUN1595
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.10

MIC-UNK-5a93dd5f-3_11



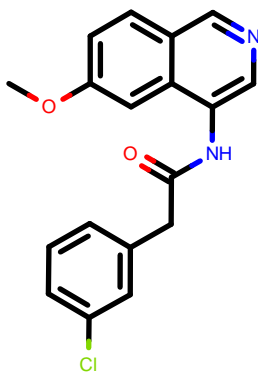
CID:	MIC-UNK-5a93dd5f-3_11
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)Cl)N@H4CC[C@@H]5CCCC[C@H]5C4</chem>
RUN:	RUN1195
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.23

EDJ-MED-ee07cf00-12_2



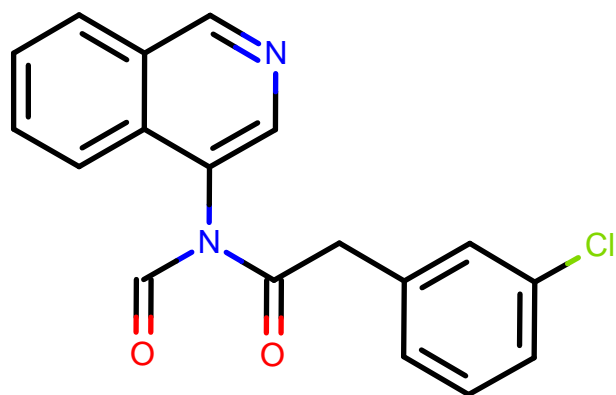
CID:	EDJ-MED-ee07cf00-12_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)COc4ccc(cc4)N</chem>
RUN:	RUN1414
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.17

PET-UNK-8df914d1-1_1



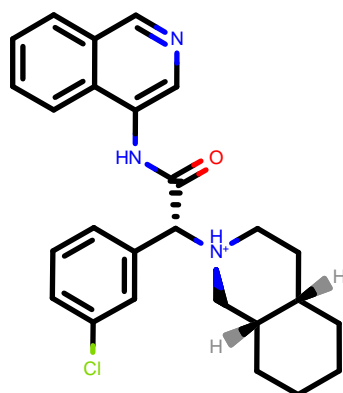
CID:	PET-UNK-8df914d1-1_1
SMILES:	<chem>COc1ccc2cnccc(c2c1)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1005
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.12

PET-UNK-12d8d43f-1_1



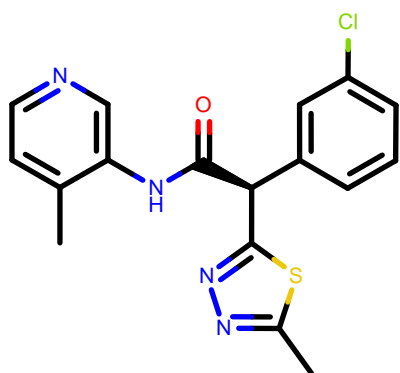
CID:	PET-UNK-12d8d43f-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C=O)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1309
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.13

MIC-UNK-5a93dd5f-3_3



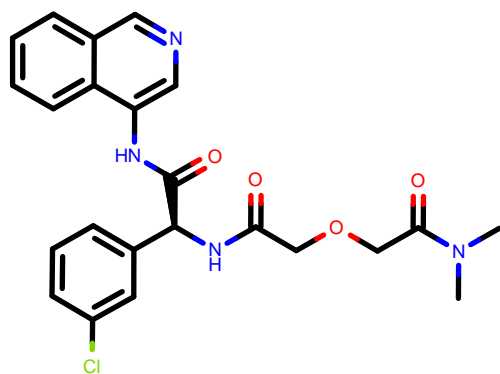
CID:	MIC-UNK-5a93dd5f-3_3
SMILES:	<chem>c1ccc2c(c1)nc2N(C(=O)[C@@H](c3cccc(c3)Cl)N@H)4CC[C@@H]5CCCC[C@H]5C4</chem>
RUN:	RUN1188
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.24

SAM-UNK-2684b532-3_1



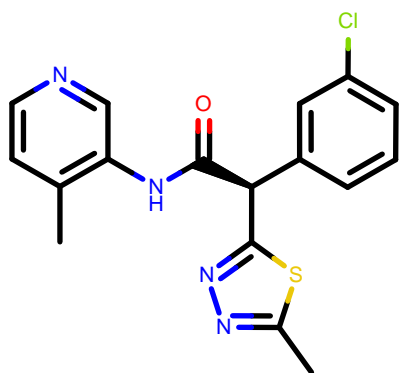
CID:	SAM-UNK-2684b532-3_1
SMILES:	<chem>Cc1ccncc1NC(=O)[C@@H](c2cccc(c2)Cl)c3nnc(s3)C</chem>
RUN:	RUN939
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.16

EDJ-MED-cf4b0d25-5_1



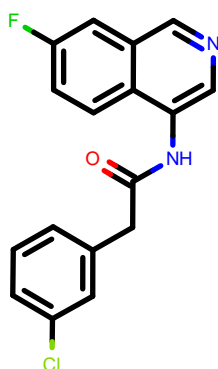
CID:	EDJ-MED-cf4b0d25-5_1
SMILES:	<chem>CN(C)C(=O)COCC(=O)N[C@@H](c1cccc(c1)Cl)C(=O)Nc2ncc3c2cccc3</chem>
RUN:	RUN1525
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.18

TRY-UNI-9f475305-3_1



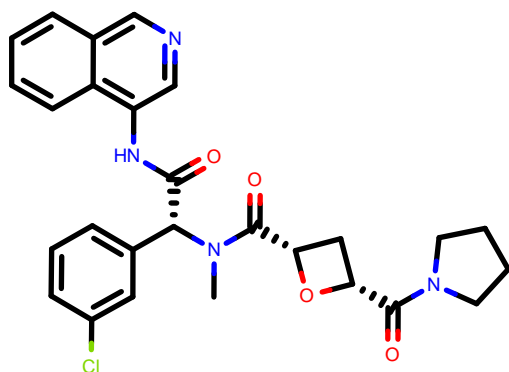
CID:	TRY-UNI-9f475305-3_1
SMILES:	<chem>Cc1ccccc1NC(=O)[C@@H](c2cccc(c2)Cl)c3nnc(s3)C</chem>
RUN:	RUN868
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.14

JIN-POS-6dc588a4-11_1



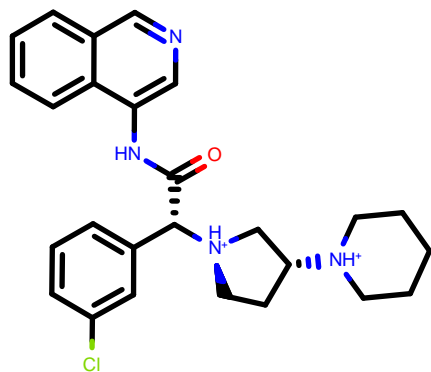
CID:	JIN-POS-6dc588a4-11_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)F</chem>
RUN:	RUN1438
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.10

PET-UNK-1320d94d-27_1



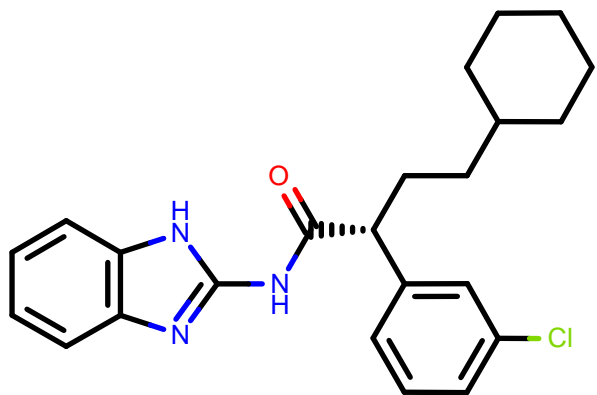
CID:	PET-UNK-1320d94d-27_1
SMILES:	<chem>CN(C@H)(c1ccc(c1)Cl)C(=O)Nc2cncc3c2ccc3Cl=O[C@@H](C)C@H)(O4)Cl=O5CCCC5</chem>
RUN:	RUN1539
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.21

MIC-UNK-5a93dd5f-12_5



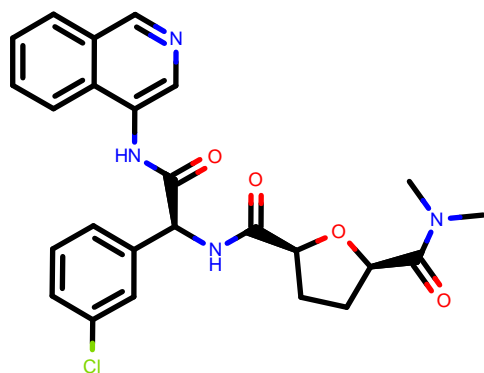
CID:	MIC-UNK-5a93dd5f-12_5
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc(c3)Cl)N@@4CC[C@H](C4)N5CCCC5</chem>
RUN:	RUN1244
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.16

ALP-POS-3fc1724e-8_2



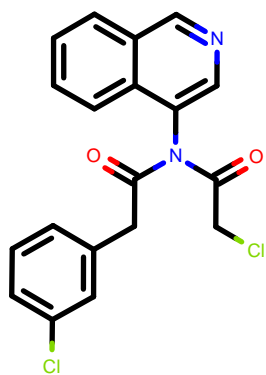
CID:	ALP-POS-3fc1724e-8_2
SMILES:	<chem>c1ccc2c(c1)[nH]c(n2)NC(=O)[C@H](CCCC3CCCCC3)c4ccccc4Cl</chem>
RUN:	RUN970
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.27

PET-UNK-1320d94d-2_1



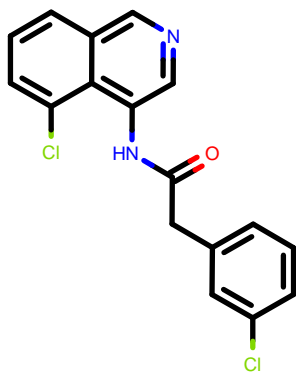
CID:	PET-UNK-1320d94d-2_1
SMILES:	<chem>CN(C)C(=O)C@H1CC[C@H](O1)C(=O)N[C@@H](C2CCCC2)C(=O)Nc3nccc4c3ccc4</chem>
RUN:	RUN1528
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.20

VLA-UCB-05e51b3f-15_1



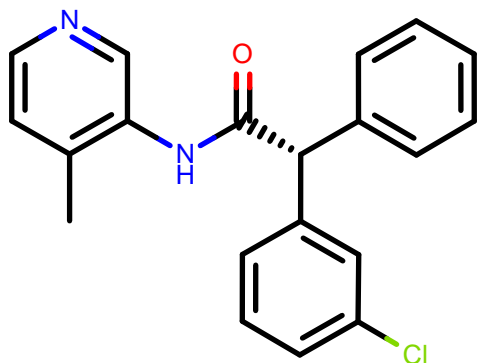
CID:	VLA-UCB-05e51b3f-15_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)Cc3ccccc(c3)Cl)C(=O)CCl</chem>
RUN:	RUN1098
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.16

MIC-UNK-50cce87d-2_1



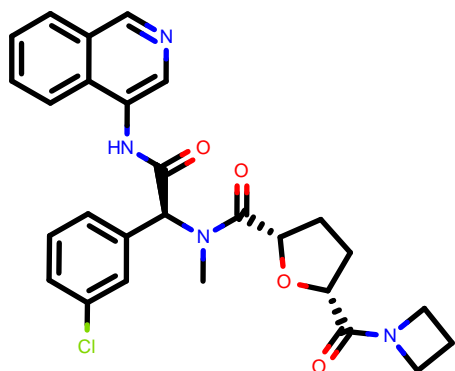
CID:	MIC-UNK-50cce87d-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)Cl</chem>
RUN:	RUN1137
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.10

SAM-UNK-2684b532-1_2



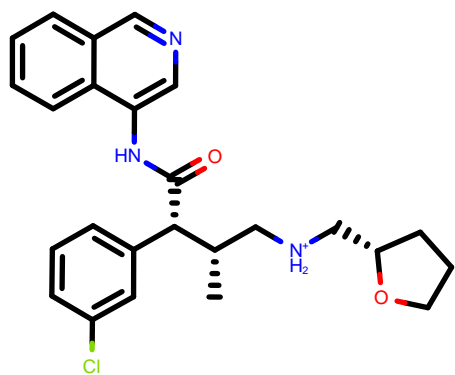
CID:	SAM-UNK-2684b532-1_2
SMILES:	<chem>Cc1ccncc1NC(=O)[C@H](c2ccccc2)c3cccc(c3)Cl</chem>
RUN:	RUN932
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.15

PET-UNK-1320d94d-26_1



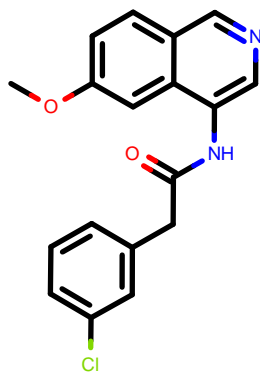
CID:	PET-UNK-1320d94d-26_1
SMILES:	<chem>CN[C@@H](c1cccc(c1)C(=O)N2cnc3c2ccccc3)C(=O)[C@@H](C)C(=O)N[C@@H](O4)C(=O)N5CCCC5</chem>
RUN:	RUN1544
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.19

MAK-UNK-ffc90da7-4_5



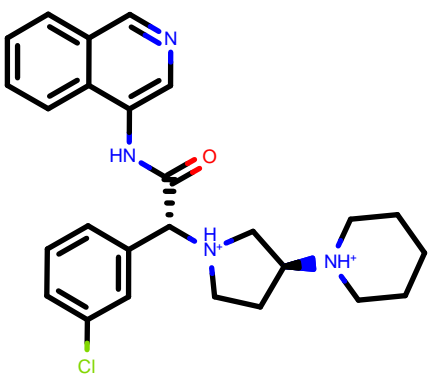
CID:	MAK-UNK-ffc90da7-4_5
SMILES:	<chem>C[C@@H](C)[NH2+][C]C@@H1CCCCO1[C@H](c2ccccc2)C(=O)Nc3cnc4c3ccccc4</chem>
RUN:	RUN1191
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.28

EDJ-MED-00c1612e-1_1



CID:	EDJ-MED-00c1612e-1_1
SMILES:	<chem>COc1ccc2cnc(c2c1)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN988
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.11

MIC-UNK-5a93dd5f-12_3



CID: MIC-UNK-5a93dd5f-12_3

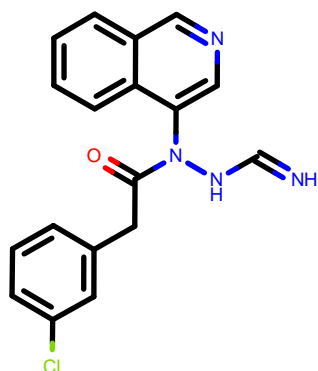
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc(c3)Cl)N@H4C[C@@H](C4)[NH+]5CCCCC5

RUN: RUN1242

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.18

PET-UNK-a692de38-1_1



CID: PET-UNK-a692de38-1_1

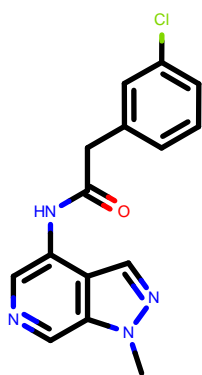
SMILES: c1ccc2c(c1)ncnc2N(C(=O)Cc3ccccc(c3)Cl)NC#N

RUN: RUN1144

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.24

RUB-POS-1325a9ea-15_1



CID: RUB-POS-1325a9ea-15_1

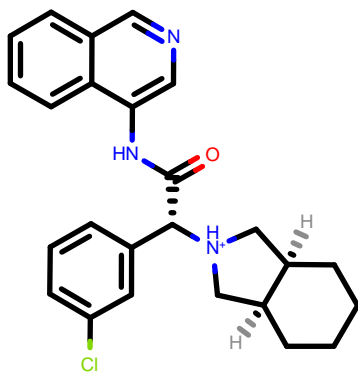
SMILES: Cn1c2cncc(c2cn1)NC(=O)Cc3ccccc(c3)Cl

RUN: RUN1476

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.13

MIC-UNK-5a93dd5f-2_1



CID: MIC-UNK-5a93dd5f-2_1

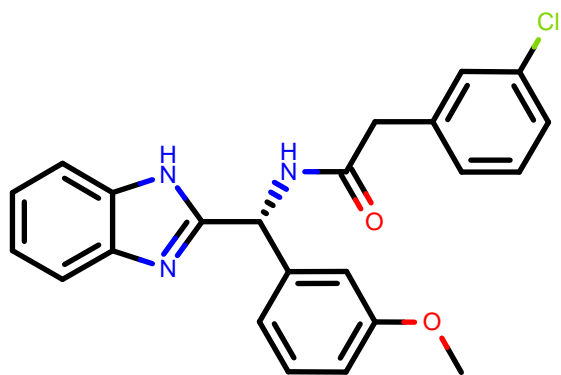
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc(c3)Cl)N+4C[C@@H]5CCCC[C@@H]5C4

RUN: RUN1151

DDG (kcal/mol): -0.27

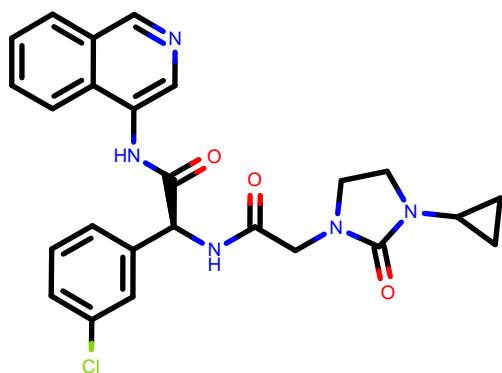
dDDG (kcal/mol): 0.22

ALP-POS-ddb41b15-9_2



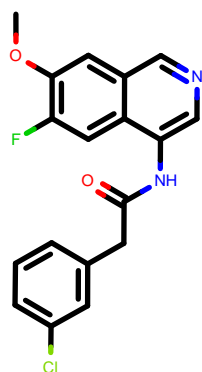
CID:	ALP-POS-ddb41b15-9_2
SMILES:	<chem>COc1cccc(c1)[C@H](c2[nH]c3ccccc3n2)NC(=O)Cc4cccc(c4)Cl</chem>
RUN:	RUN981
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.26

EDJ-MED-ee07cf00-18_2



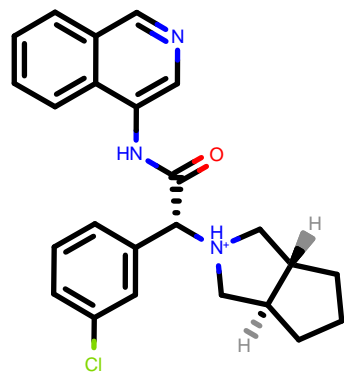
CID:	EDJ-MED-ee07cf00-18_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc(c3)Cl)NC(=O)CN4CCN(C4=O)C5CC5</chem>
RUN:	RUN1407
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.22

MAT-POS-29385cc1-2_1



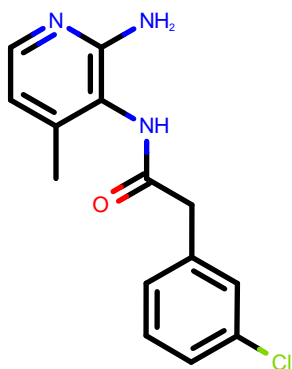
CID:	MAT-POS-29385cc1-2_1
SMILES:	<chem>COc1cc2cncnc(c2cc1F)NC(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN1593
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.12

MIC-UNK-5a93dd5f-1_5



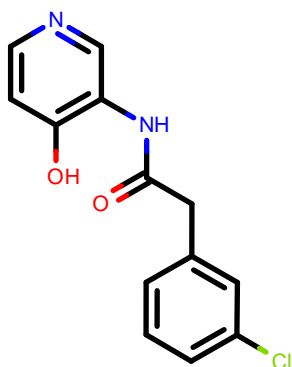
CID:	MIC-UNK-5a93dd5f-1_5
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc(c3)Cl)[NH+]4C[C@@H]5CC[C@H]5C4</chem>
RUN:	RUN1159
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.24

EDG-MED-0da5ad92-18_1



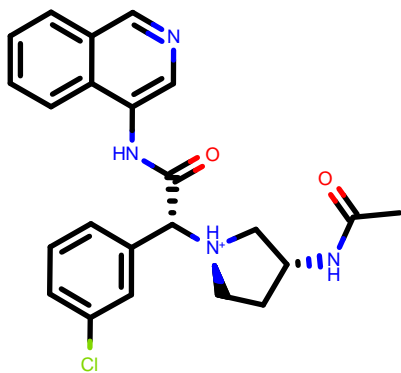
CID:	EDG-MED-0da5ad92-18_1
SMILES:	<chem>Cc1ccnc(c1NC(=O)Cc2cccc(c2)Cl)N</chem>
RUN:	RUN876
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.08

ALP-POS-95b75b4d-6_1



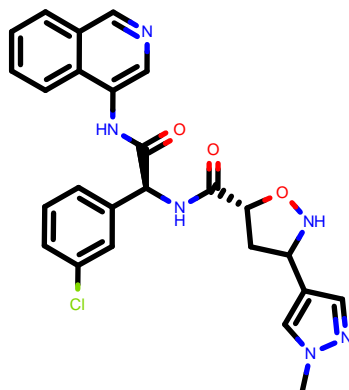
CID:	ALP-POS-95b75b4d-6_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c[nH]ccc2=O</chem>
RUN:	RUN838
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.13

MIC-UNK-5a93dd5f-5_7



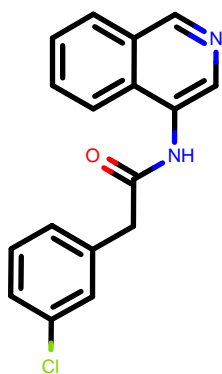
CID:	MIC-UNK-5a93dd5f-5_7
SMILES:	<chem>CC(=O)N[C@@H]1CC[N@H+]1C1[C@H](c2cccc(c2)Cl)C(=O)Nc3nccc4c3ccc4</chem>
RUN:	RUN1210
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.22

EDJ-MED-ee07cf00-6_2



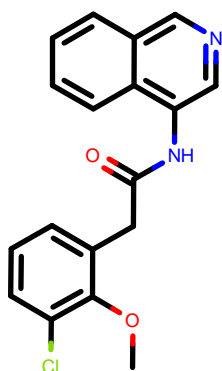
CID:	EDJ-MED-ee07cf00-6_2
SMILES:	<chem>Cn1cc(en1)C2=NO[C@H](C2)C(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN1379
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.21

MAT-POS-f7918075-5_1



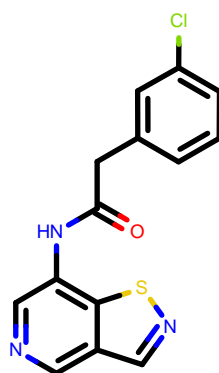
CID:	MAT-POS-f7918075-5_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cncc3</chem>
RUN:	RUN1068
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.02

RAL-THA-2d450e86-22_1



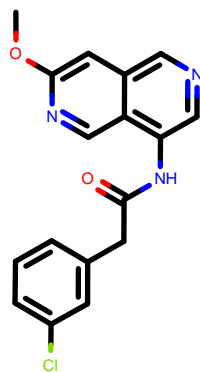
CID:	RAL-THA-2d450e86-22_1
SMILES:	<chem>COc1c(cccc1Cl)CC(=O)Nc2cncc3c2ccccc3</chem>
RUN:	RUN1353
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.10

PET-UNK-b1ef24dc-2_1



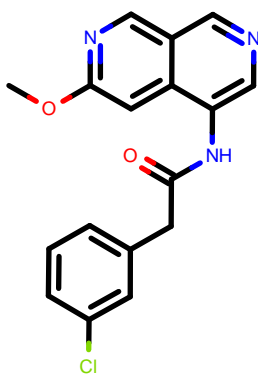
CID:	PET-UNK-b1ef24dc-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2snc3</chem>
RUN:	RUN1514
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.11

PET-UNK-f4e47ebd-2_1



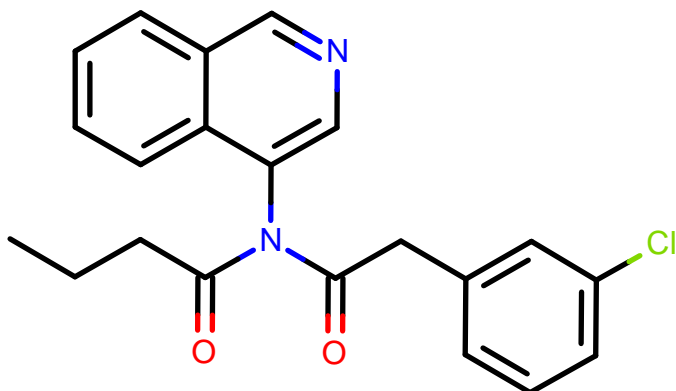
CID:	PET-UNK-f4e47ebd-2_1
SMILES:	<chem>COc1cc2cncc(c2cn1)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1507
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.16

PET-UNK-f4e47ebd-1_1



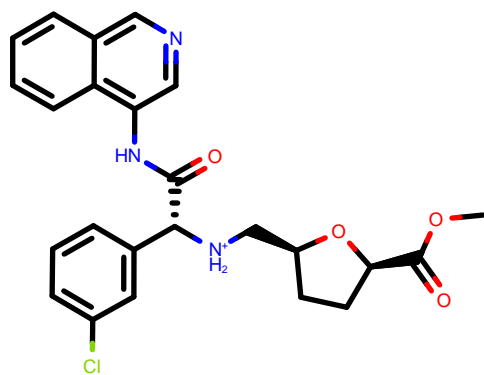
CID:	PET-UNK-f4e47ebd-1_1
SMILES:	<chem>COc1cc2c(cnc2NC(=O)Cc3cccc(c3)Cl)cn1</chem>
RUN:	RUN1506
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.13

DAR-DIA-076fb6ea-8_1



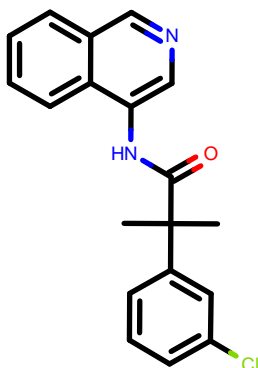
CID:	DAR-DIA-076fb6ea-8_1
SMILES:	<chem>C=CC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1276
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.20

MAT-POS-d8472c4f-2_2



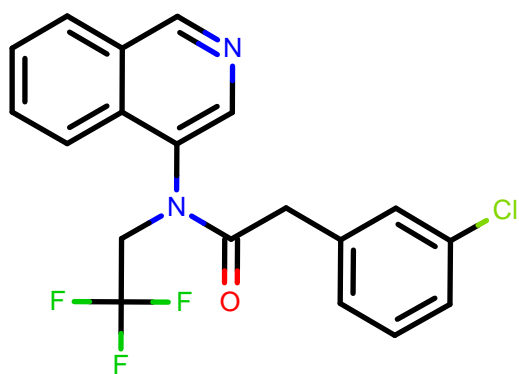
CID:	MAT-POS-d8472c4f-2_2
SMILES:	<chem>COC(=O)[C@H]1CC[C@H](O1)C[NH2+][C@H](c2cccc(c2)Cl)C(=O)Nc3ncc4c3ccc4</chem>
RUN:	RUN1561
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.25

NAU-LAT-2fed8305-1_1



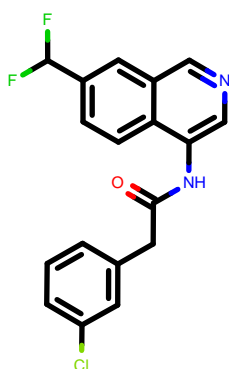
CID:	NAU-LAT-2fed8305-1_1
SMILES:	<chem>CC(C)(c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN1252
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.04

JOH-UNI-a38a7bdd-2_1



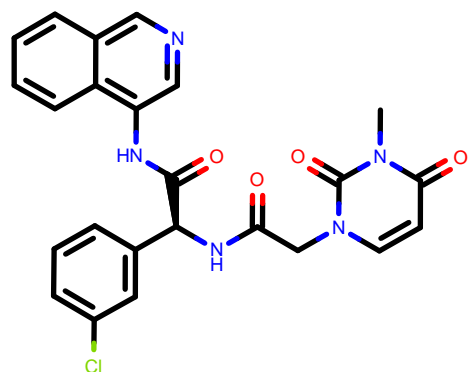
CID:	JOH-UNI-a38a7bdd-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(CC(F)(F)F)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1268
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.29

MAT-POS-c0609ef7-1_1



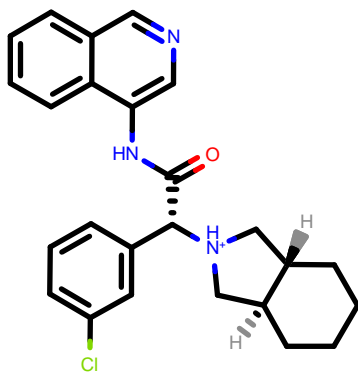
CID:	MAT-POS-c0609ef7-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)C(F)F</chem>
RUN:	RUN1594
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.14

EDJ-MED-ee07cf00-1_1



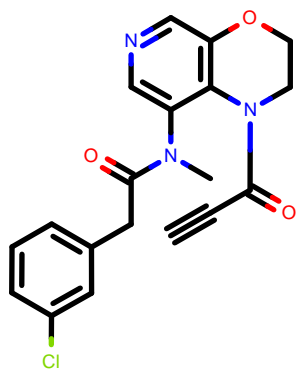
CID:	EDJ-MED-ee07cf00-1_1
SMILES:	<chem>Cn1c(=O)ccn(c1=O)CC(=O)N[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1363
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.17

MIC-UNK-5a93dd5f-2_5



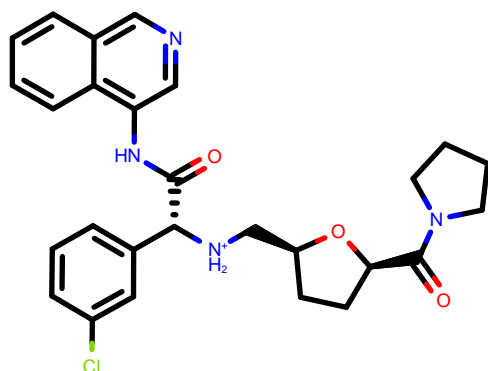
CID:	MIC-UNK-5a93dd5f-2_5
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)N[C@@H]4C[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN1148
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.22

JOH-UNI-3fc3434e-12_1



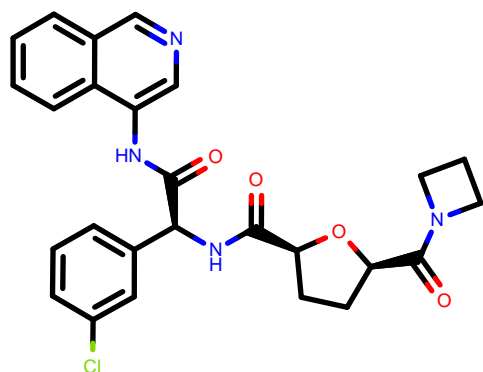
CID:	JOH-UNI-3fc3434e-12_1
SMILES:	<chem>CN(c1cncc2c1N(CCO2)C(=O)C#C)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1343
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.14

EDJ-MED-cf4b0d25-2_1



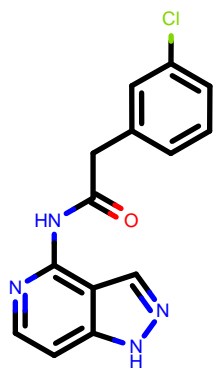
CID:	EDJ-MED-cf4b0d25-2_1
SMILES:	<chem>c1ccc2(c1)ncnc2NC(=O)C@H(c3cccc(c3)C)N12+1C(C@H)4CC(C@H)O4(C)=O#N5CCCC5</chem>
RUN:	RUN1447
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.32

PET-UNK-1320d94d-6_1



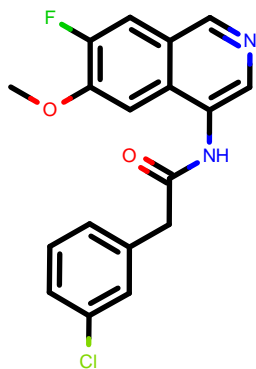
CID:	PET-UNK-1320d94d-6_1
SMILES:	<chem>c1ccc2(c1)ncnc2NC(=O)C@H(c3cccc(c3)C)N(C)=O(C@H)4CC(C@H)O4(C)=O#N5CCCC5</chem>
RUN:	RUN1540
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.22

MAT-POS-199e2e7c-2_1



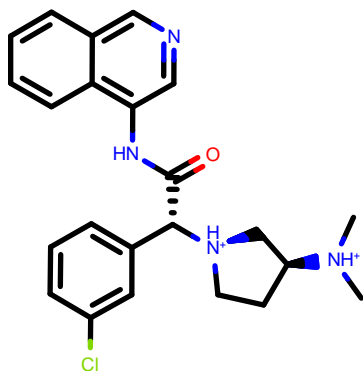
CID:	MAT-POS-199e2e7c-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3cn[nH]c3ccn2</chem>
RUN:	RUN1114
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.14

MAT-POS-29385cc1-1_1



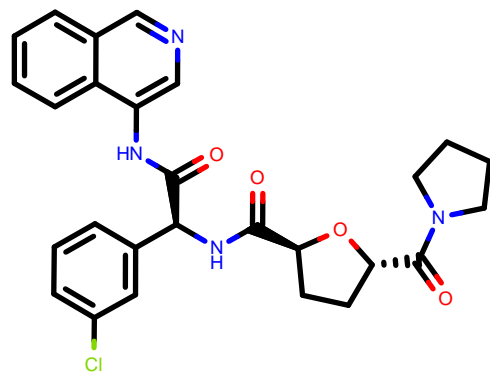
CID:	MAT-POS-29385cc1-1_1
SMILES:	<chem>COc1cc2c(cc1F)cncc2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1596
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.13

MIC-UNK-5a93dd5f-9_8



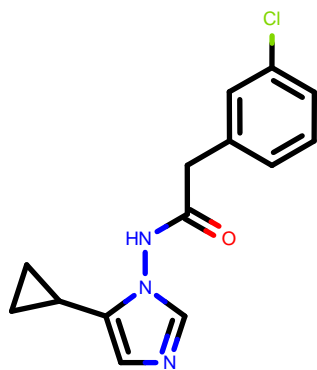
CID:	MIC-UNK-5a93dd5f-9_8
SMILES:	<chem>CN(C)[C@H]1CC[N@H+](C1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1228
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.19

PET-UNK-ac320b15-8_1



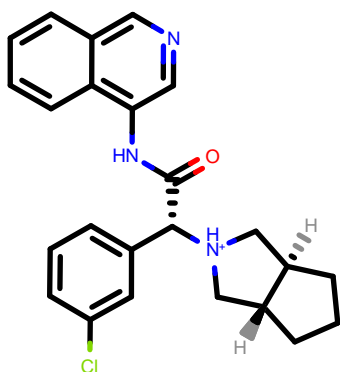
CID:	PET-UNK-ac320b15-8_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3cccc(c3)Cl)N(C(=O)O)C@H(C)C@H(O)Cl=O</chem>
RUN:	RUN1559
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.19

JAN-GHE-f4ca5a00-14_1



CID:	JAN-GHE-f4ca5a00-14_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2cncc2C3CC3</chem>
RUN:	RUN956
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.11

MIC-UNK-5a93dd5f-1_3



CID: MIC-UNK-5a93dd5f-1_3

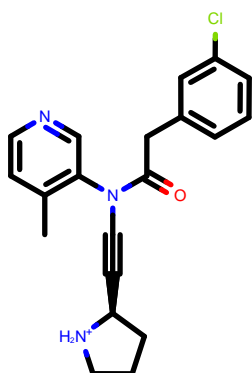
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[NH+]4C[C@H]5CC[C@@H]5C4

RUN: RUN1157

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.21

DAR-DIA-076fb6ea-10_2



CID: DAR-DIA-076fb6ea-10_2

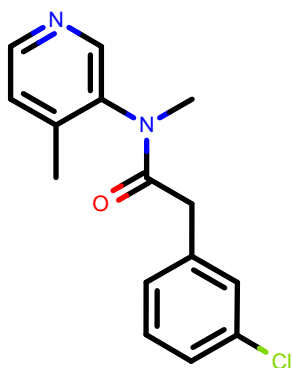
SMILES: Cc1ccncc1N(C#C[C@H]2CCCC[NH2+]2)C(=O)Cc3cccc(c3)Cl

RUN: RUN1277

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.22

EDG-MED-0da5ad92-1_1



CID: EDG-MED-0da5ad92-1_1

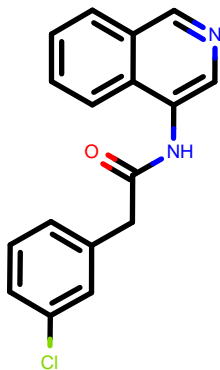
SMILES: Cc1ccncc1N(C)C(=O)Cc2cccc(c2)Cl

RUN: RUN847

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.14

MAT-POS-bb423b95-1_1



CID: MAT-POS-bb423b95-1_1

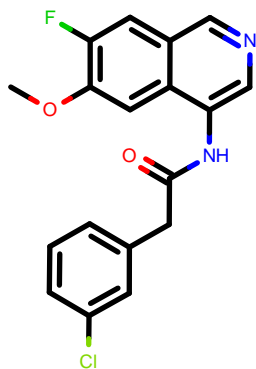
SMILES: c1cc(cc(c1)Cl)CC(=O)Nc2cnc3c2ccnc3

RUN: RUN1054

DDG (kcal/mol): -0.07

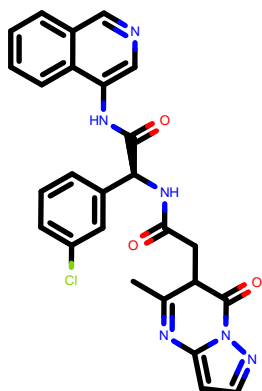
dDDG (kcal/mol): 0.02

PET-UNK-b38839dc-1_1



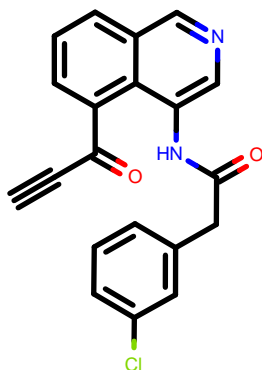
CID:	PET-UNK-b38839dc-1_1
SMILES:	<chem>COc1cc2c(cc1F)cncc2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1568
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-2_1



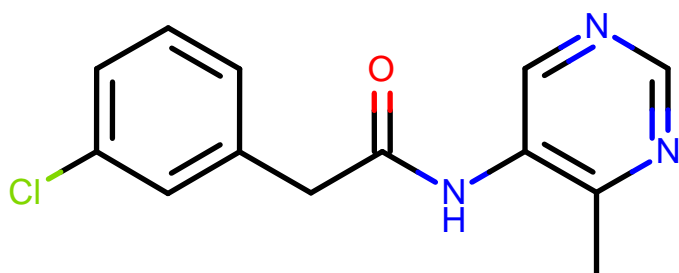
CID:	EDJ-MED-ee07cf00-2_1
SMILES:	<chem>Cc1c(c(=O)n2c(n1)cc[nH]2)CC(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN1370
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.21

JOH-UNI-3fc3434e-1_1



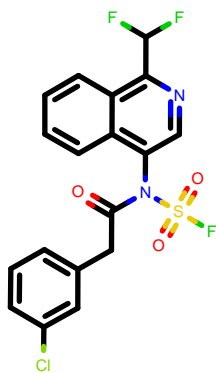
CID:	JOH-UNI-3fc3434e-1_1
SMILES:	<chem>C#CC(=O)c1cccc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN1322
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.16

ABI-SAT-4d06482b-2_1



CID:	ABI-SAT-4d06482b-2_1
SMILES:	<chem>Cc1c(cncn1)NC(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN943
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.11

JOH-UNI-50ce7ec3-4_1



CID:	JOH-UNI-50ce7ec3-4_1
SMILES:	<chem>c1ccc2c(c1)c(nc2C(F)F)N(C(=O)Cc3cccc(c3)Cl)S(=O)(=O)F</chem>
RUN:	RUN1364
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.45