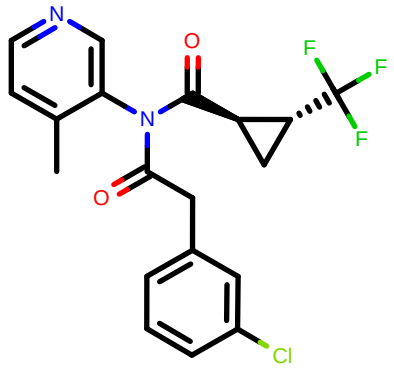
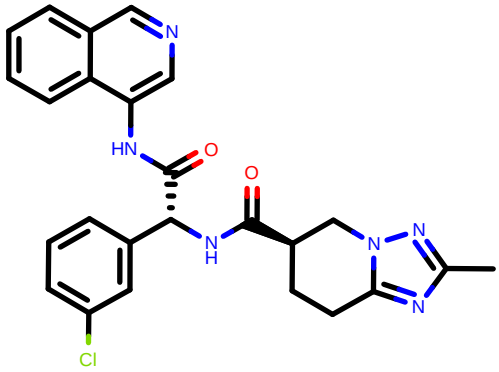
JOH-UNI-a38a7bdd-7_3



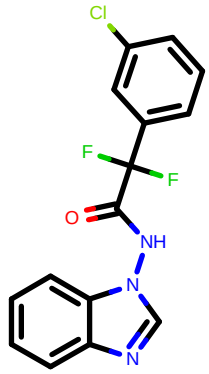
CID:	JOH-UNI-a38a7bdd-7_3
SMILES:	Cc1ccncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)[C@@H]3C[C@H]3C(F)(F)F
RUN:	RUN1312
DDG (kcal/mol):	-3.31
dDDG (kcal/mol):	0.16

EDJ-MED-ee07cf00-13_2



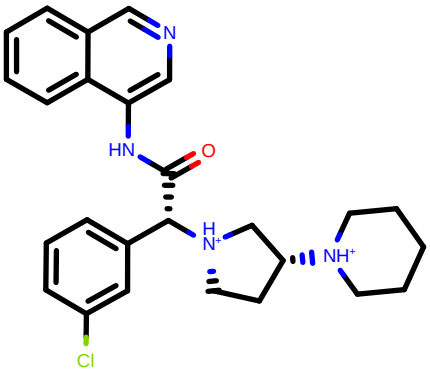
CID:	EDJ-MED-ee07cf00-13_2
SMILES:	Cc1nc2n(n1)C[C@@H](CC2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1393
DDG (kcal/mol):	-3.17
dDDG (kcal/mol):	0.20

BAR-COM-0f94fc3d-24_1



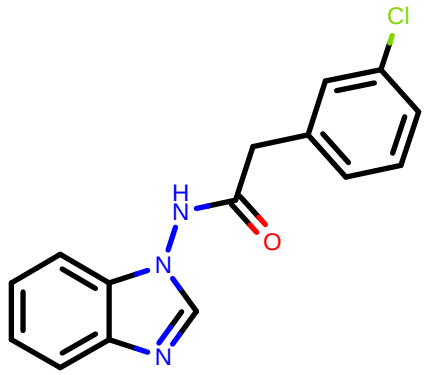
CID:	BAR-COM-0f94fc3d-24_1
SMILES:	c1ccc2c(c1)ncn2NC(=O)C(c3cccc(c3)Cl)(F)F
RUN:	RUN920
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.11

MIC-UNK-5a93dd5f-12_7



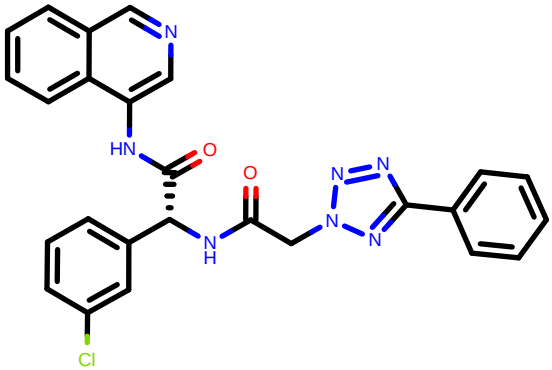
CID:	MIC-UNK-5a93dd5f-12_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@]4CC[C@H](C4)[NH+]5CCCCC5
RUN:	RUN1238
DDG (kcal/mol):	-2.59
dDDG (kcal/mol):	0.13

JAN-GHE-5a013bed-2_1



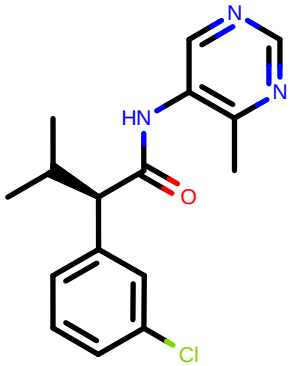
CID:	JAN-GHE-5a013bed-2_1
SMILES:	c1ccc2c(c1)ncn2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN851
DDG (kcal/mol):	-2.39
dDDG (kcal/mol):	0.10

EDJ-MED-ee07cf00-9_2



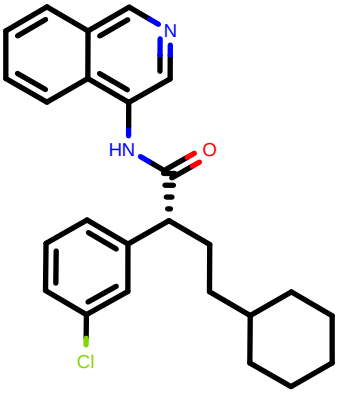
CID:	EDJ-MED-ee07cf00-9_2
SMILES:	c1ccc(cc1)c2nnn(n2)CC(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1377
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.24

JAN-GHE-83b26c96-7_1



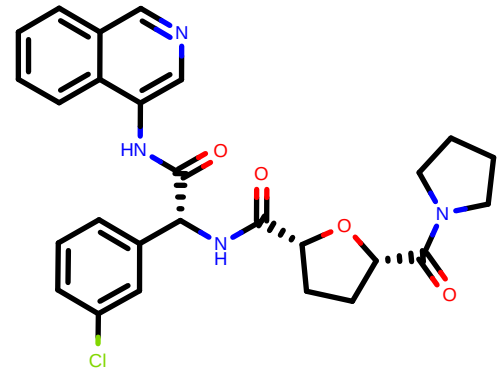
CID:	JAN-GHE-83b26c96-7_1
SMILES:	Cc1c(cncn1)NC(=O)[C@@H](c2cccc(c2)Cl)C(C)C
RUN:	RUN819
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.16

MIC-UNK-c66144cb-3_2



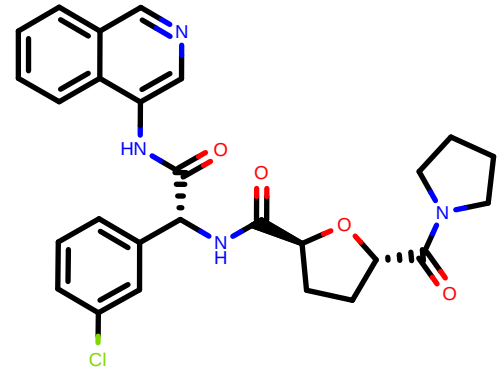
CID:	MIC-UNK-c66144cb-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN1020
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.23

MAT-POS-8293a91a-7_1



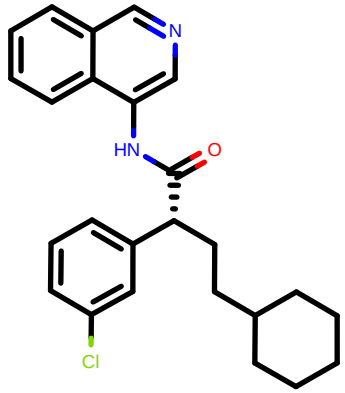
CID:	MAT-POS-8293a91a-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@H]4CC[C@H](O4)C(=O)N5CCCC5
RUN:	RUN1569
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.21

MAT-POS-8293a91a-6_1



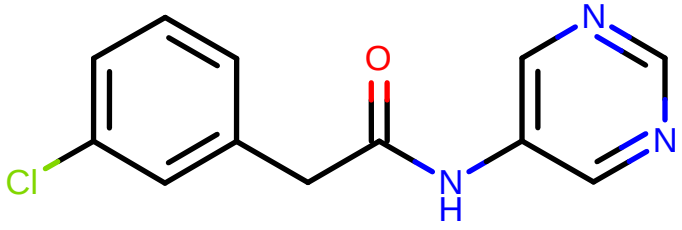
CID:	MAT-POS-8293a91a-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@@H]4CC[C@H](O4)C(=O)N5CCCC5
RUN:	RUN1578
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.19

ALP-POS-3b848b35-4_2



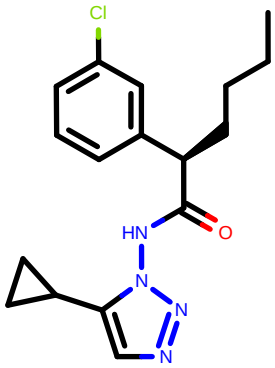
CID:	ALP-POS-3b848b35-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN993
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.20

JAN-GHE-5a013bed-9_1



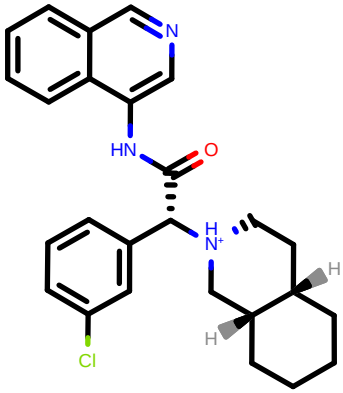
CID:	JAN-GHE-5a013bed-9_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncnc2
RUN:	RUN848
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.12

JAN-GHE-f4ca5a00-20_2



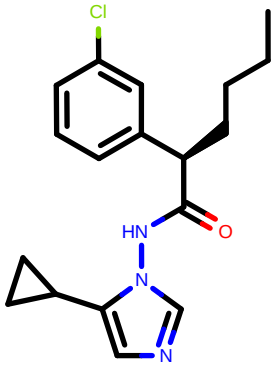
CID:	JAN-GHE-f4ca5a00-20_2
SMILES:	CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2c(cnn2)C3CC3
RUN:	RUN1001
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.15

MIC-UNK-5a93dd5f-3_1



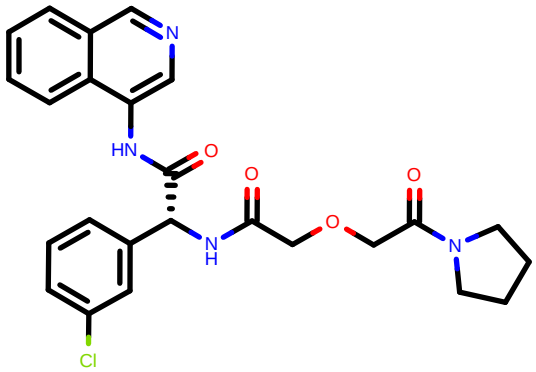
CID:	MIC-UNK-5a93dd5f-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@@H+]4CC[C@@H]5CCCC[C@@H]5C4
RUN:	RUN1189
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.14

JAN-GHE-f4ca5a00-18_2



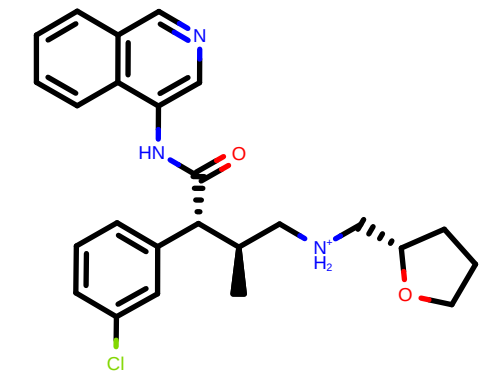
CID:	JAN-GHE-f4ca5a00-18_2
SMILES:	CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2cncc2C3CC3
RUN:	RUN1000
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.17

EDJ-MED-cf4b0d25-1_1



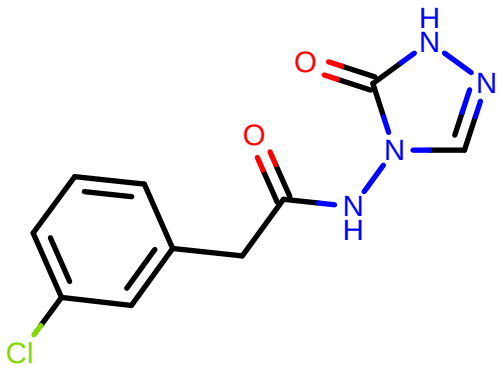
CID:	EDJ-MED-cf4b0d25-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)COCC(=O)N4CCCC4
RUN:	RUN1502
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.19

MAK-UNK-c749d764-22_6



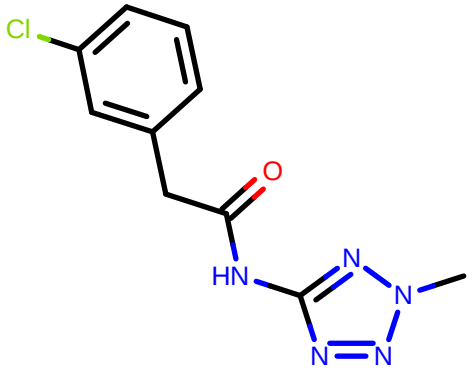
CID:	MAK-UNK-c749d764-22_6
SMILES:	C[C@H](C[NH2+]C[C@@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1253
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.20

JAN-GHE-5a013bed-4_1



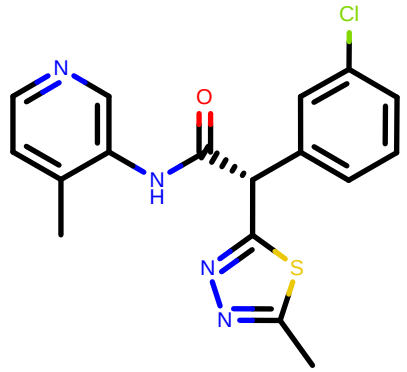
CID:	JAN-GHE-5a013bed-4_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nn2cn[nH]c2=O
RUN:	RUN865
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.12

VLA-UNK-411a133b-1_1



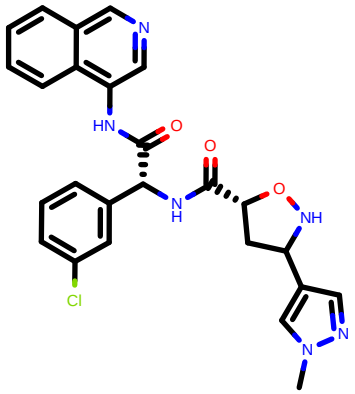
CID:	VLA-UNK-411a133b-1_1
SMILES:	Cn1nc(nn1)NC(=O)Cc2cccc(c2)Cl
RUN:	RUN1484
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.11

TRY-UNI-9f475305-3_2



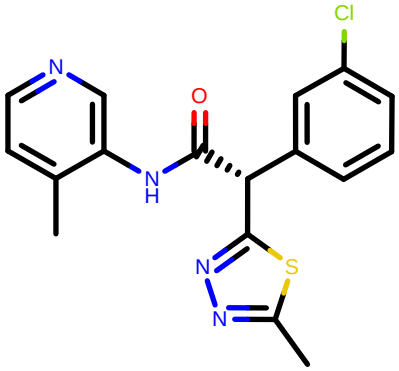
CID:	TRY-UNI-9f475305-3_2
SMILES:	Cc1ccncc1NC(=O)[C@H](c2cccc(c2)Cl)c3nnc(s3)C
RUN:	RUN863
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.12

EDJ-MED-ee07cf00-6_4



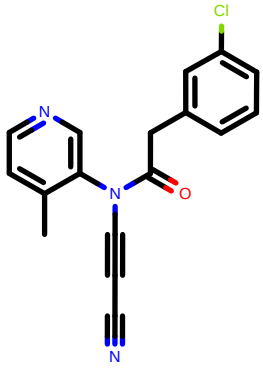
CID:	EDJ-MED-ee07cf00-6_4
SMILES:	Cn1cc(cn1)C2=NO[C@H](C2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1382
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.23

SAM-UNK-2684b532-3_2



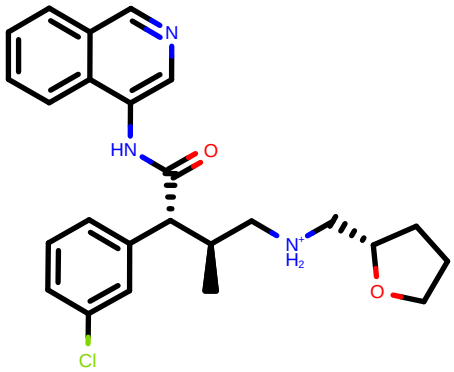
CID:	SAM-UNK-2684b532-3_2
SMILES:	Cc1ccncc1NC(=O)[C@H](c2cccc(c2)Cl)c3nnc(s3)C
RUN:	RUN944
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.12

DAR-DIA-076fb6ea-6_1



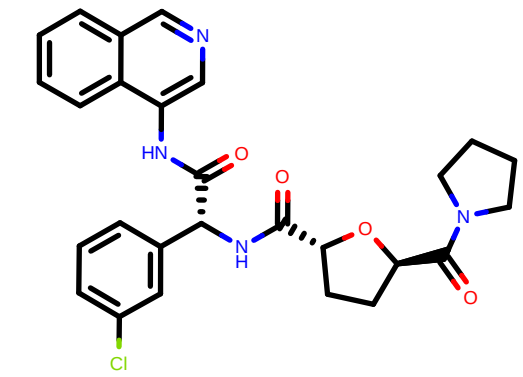
CID:	DAR-DIA-076fb6ea-6_1
SMILES:	Cc1ccncc1N(C#CC#N)C(=O)Cc2cccc(c2)Cl
RUN:	RUN1263
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.17

MAK-UNK-ffc90da7-4_6



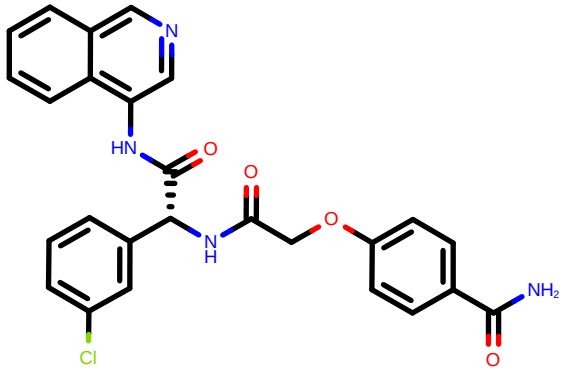
CID:	MAK-UNK-ffc90da7-4_6
SMILES:	C[C@H](C[NH2+]C[C@@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1192
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.23

PET-UNK-ac320b15-5_1



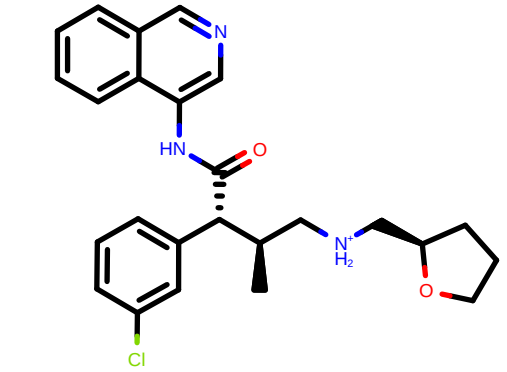
CID:	PET-UNK-ac320b15-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@H]4CC[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN1555
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.23

EDJ-MED-ee07cf00-12_1



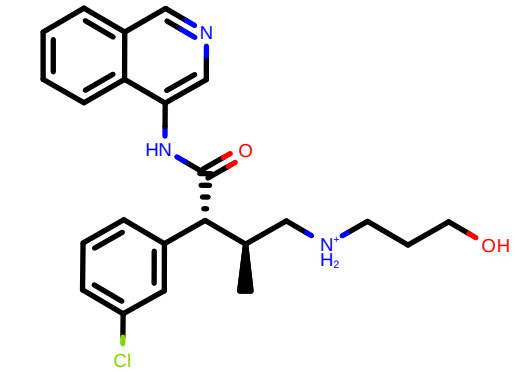
CID:	EDJ-MED-ee07cf00-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)COc4ccc(cc4)C(=O)N
RUN:	RUN1409
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.20

MAK-UNK-ffc90da7-4_8



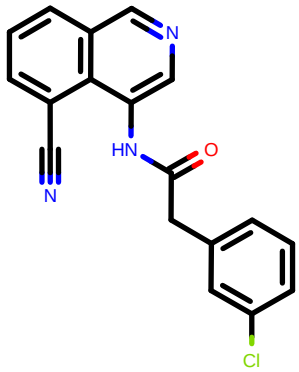
CID:	MAK-UNK-ffc90da7-4_8
SMILES:	C[C@H](C[NH2+]C[C@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1204
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.27

MAK-UNK-c749d764-6_4



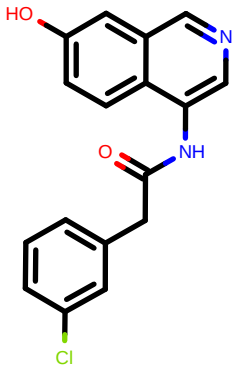
CID:	MAK-UNK-c749d764-6_4
SMILES:	C[C@H](C[NH2+]CCCO)[C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN1281
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.26

PET-UNK-6314f867-3_1



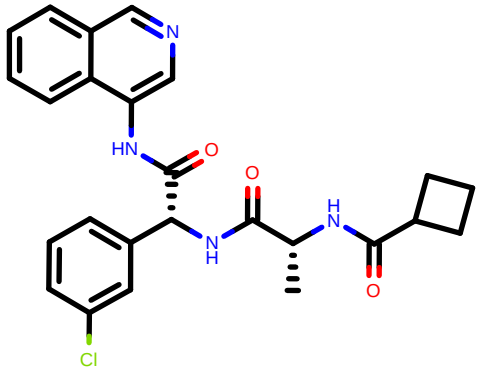
CID:	PET-UNK-6314f867-3_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)C#N
RUN:	RUN1501
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.12

MAT-POS-bb423b95-8_1



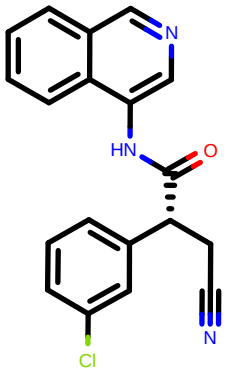
CID:	MAT-POS-bb423b95-8_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)O
RUN:	RUN1061
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.12

EDJ-MED-ee07cf00-4_4



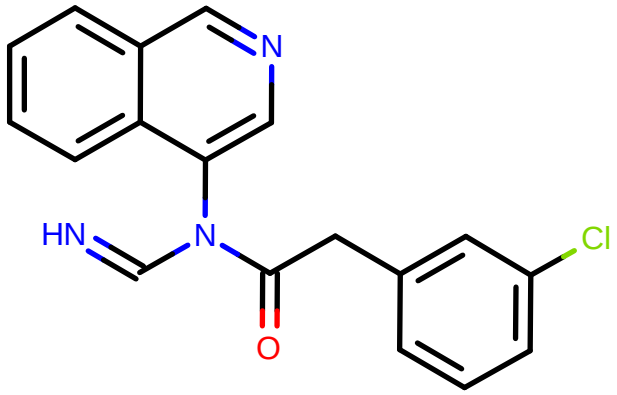
CID:	EDJ-MED-ee07cf00-4_4
SMILES:	C[C@H](C(=O)N[C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3)NC(=O)C4CCC4
RUN:	RUN1411
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.23

JOH-UNI-ee5ed7c8-6_2



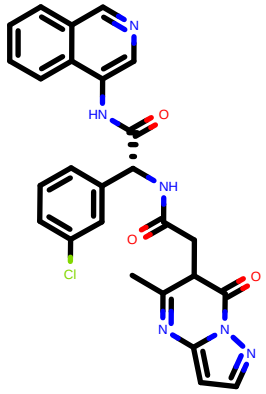
CID:	JOH-UNI-ee5ed7c8-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CC#N)c3cccc(c3)Cl
RUN:	RUN1334
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.10

PET-UNK-5ecb6237-1_1



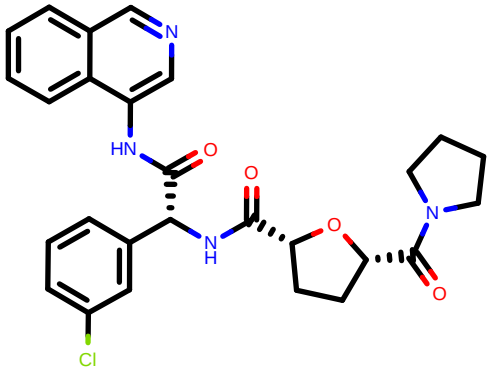
CID:	PET-UNK-5ecb6237-1_1
SMILES:	c1ccc2c(c1)cncc2N(C#N)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1121
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.15

EDJ-MED-ee07cf00-2_2



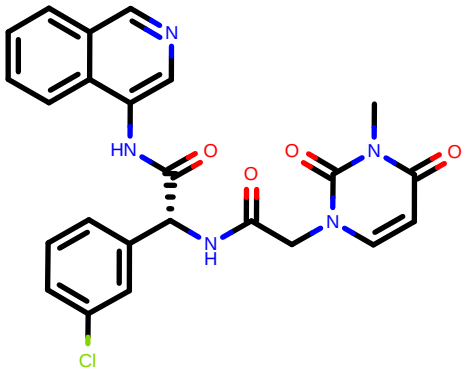
CID:	EDJ-MED-ee07cf00-2_2
SMILES:	Cc1c(c(=O)n2c(n1)cc[nH]2)CC(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1366
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.19

EDJ-MED-ee07cf00-11_7



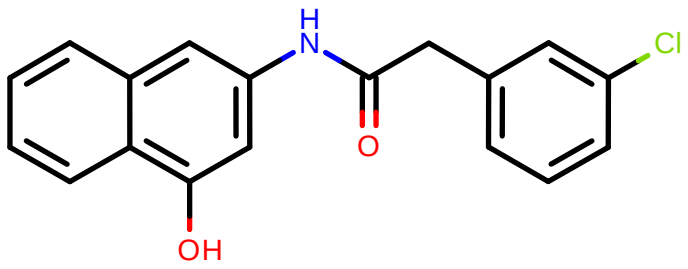
CID:	EDJ-MED-ee07cf00-11_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@H]4CC[C@H](O4)C(=O)N5CCCC5
RUN:	RUN1394
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.19

EDJ-MED-ee07cf00-1_2



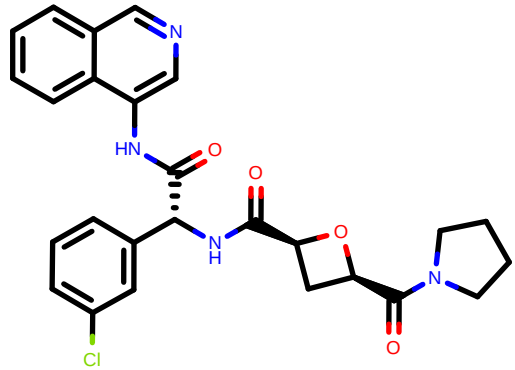
CID:	EDJ-MED-ee07cf00-1_2
SMILES:	Cn1c(=O)ccn(c1=O)CC(=O)N[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1365
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.15

ROB-UNI-daaf9793-3_1



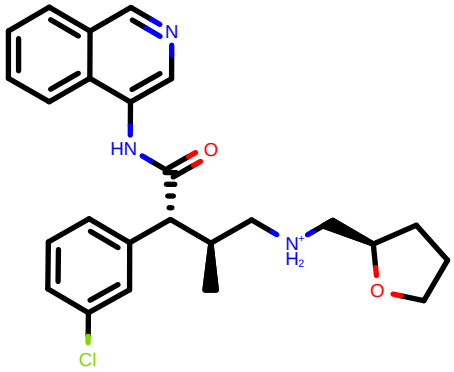
CID:	ROB-UNI-daaf9793-3_1
SMILES:	c1ccc2c(c1)cc(cc2O)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1488
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.15

PET-UNK-1320d94d-7_1



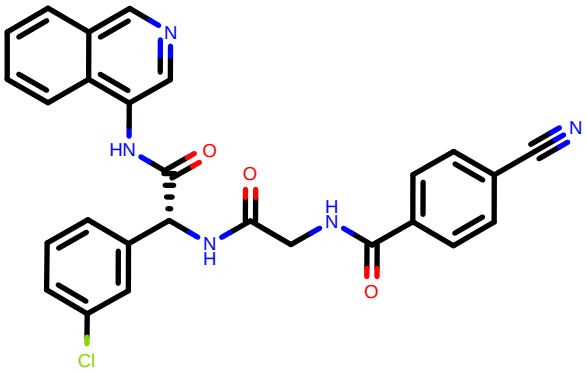
CID:	PET-UNK-1320d94d-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@@H]4C[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN1527
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.24

MAK-UNK-c749d764-22_8



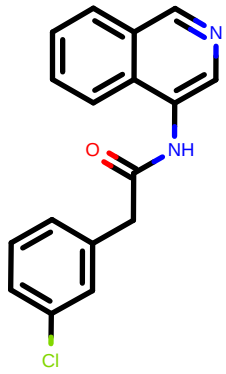
CID:	MAK-UNK-c749d764-22_8
SMILES:	C[C@H](C[NH2+]C[C@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1273
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.23

EDJ-MED-ee07cf00-5_1



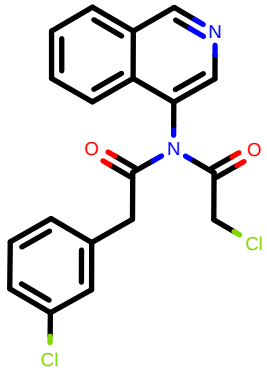
CID:	EDJ-MED-ee07cf00-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)CNC(=O)c4ccc(cc4)C#N
RUN:	RUN1406
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.22

MAT-POS-f7918075-3_1



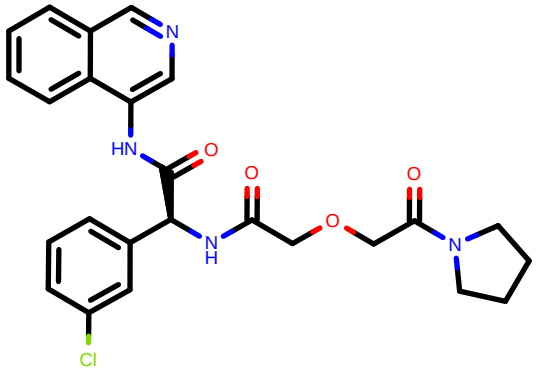
CID:	MAT-POS-f7918075-3_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccn3
RUN:	RUN1063
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.04

PET-UNK-6c2be958-1_1



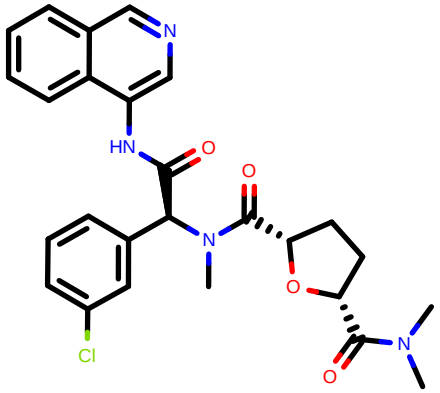
CID:	PET-UNK-6c2be958-1_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)CCl
RUN:	RUN1327
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.17

EDJ-MED-cf4b0d25-1_2



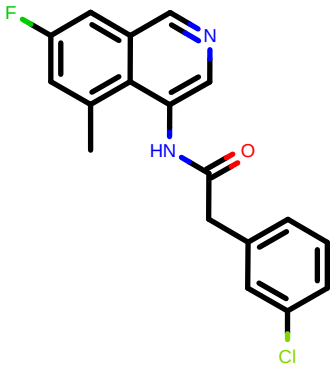
CID:	EDJ-MED-cf4b0d25-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)COCC(=O)N4CCCC4
RUN:	RUN1504
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.19

PET-UNK-1320d94d-22_1



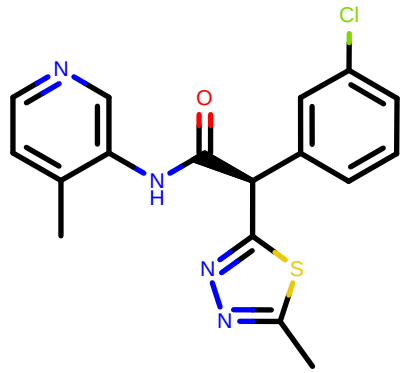
CID:	PET-UNK-1320d94d-22_1
SMILES:	CN(C)C(=O)[C@H]1CC[C@H](O1)C(=O)N(C)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1530
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.18

MAT-POS-29385cc1-4_1



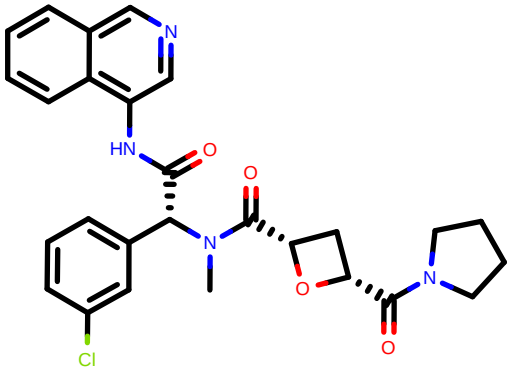
CID:	MAT-POS-29385cc1-4_1
SMILES:	Cc1cc(cc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl)F
RUN:	RUN1595
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.10

SAM-UNK-2684b532-3_1



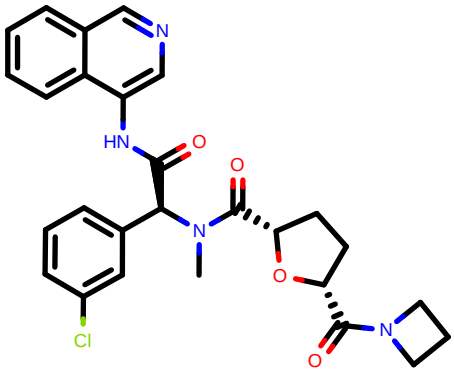
CID:	SAM-UNK-2684b532-3_1
SMILES:	Cc1ccncc1NC(=O)[C@@H](c2cccc(c2)Cl)c3nnc(s3)C
RUN:	RUN939
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.16

PET-UNK-1320d94d-27_1



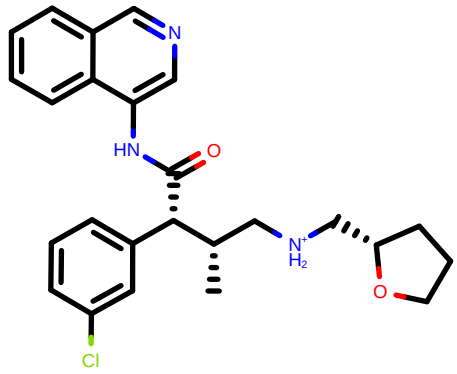
CID:	PET-UNK-1320d94d-27_1
SMILES:	CN([C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3)C(=O)[C@@H]4C[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN1539
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.21

PET-UNK-1320d94d-26_1



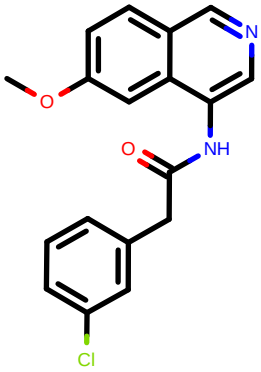
CID:	PET-UNK-1320d94d-26_1
SMILES:	CN[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3)C(=O)[C@@H]4CC[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN1544
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.19

MAK-UNK-ffc90da7-4_5



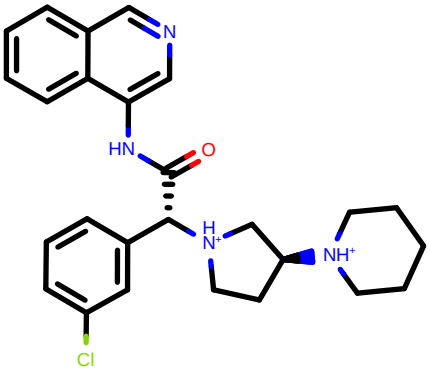
CID:	MAK-UNK-ffc90da7-4_5
SMILES:	C[C@@H](C[NH2+]C[C@@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1191
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.28

EDJ-MED-00c1612e-1_1



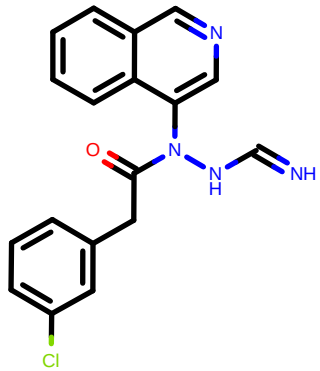
CID:	EDJ-MED-00c1612e-1_1
SMILES:	COc1ccc2cncc(c2c1)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN988
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.11

MIC-UNK-5a93dd5f-12_3



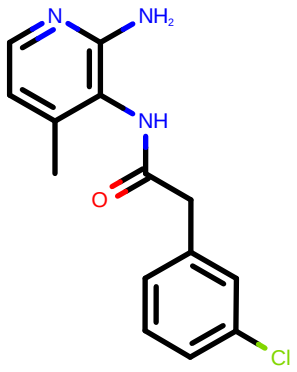
CID:	MIC-UNK-5a93dd5f-12_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@]4CC[C@@H](C4)[NH+]5CCCCC5
RUN:	RUN1242
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.18

PET-UNK-a692de38-1_1



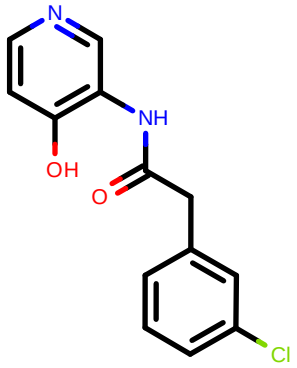
CID:	PET-UNK-a692de38-1_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)NC#N
RUN:	RUN1144
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.24

EDG-MED-0da5ad92-18_1



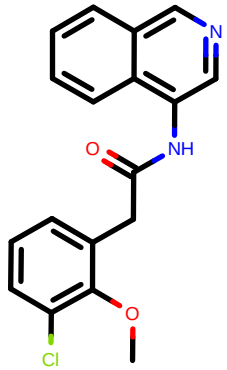
CID:	EDG-MED-0da5ad92-18_1
SMILES:	Cc1ccnc(c1NC(=O)Cc2cccc(c2)Cl)N
RUN:	RUN876
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.08

ALP-POS-95b75b4d-6_1



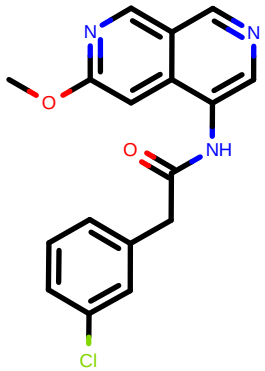
CID:	ALP-POS-95b75b4d-6_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2c[nH]ccc2=O
RUN:	RUN838
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.13

RAL-THA-2d450e86-22_1



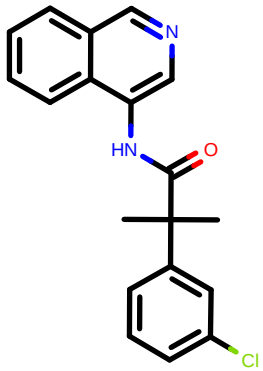
CID:	RAL-THA-2d450e86-22_1
SMILES:	COc1c(cccc1Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN1353
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.10

PET-UNK-f4e47ebd-1_1



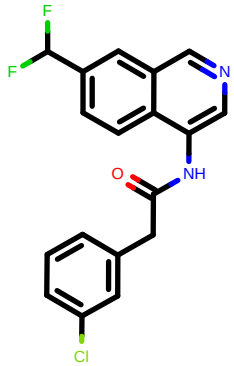
CID:	PET-UNK-f4e47ebd-1_1
SMILES:	COc1cc2c(cncc2NC(=O)Cc3cccc(c3)Cl)cn1
RUN:	RUN1506
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.13

NAU-LAT-2fed8305-1_1



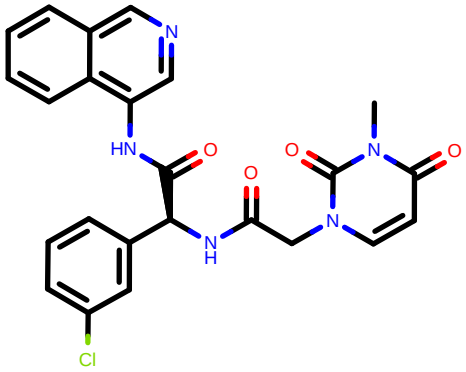
CID:	NAU-LAT-2fed8305-1_1
SMILES:	CC(C)(c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN1252
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.04

MAT-POS-c0609ef7-1_1



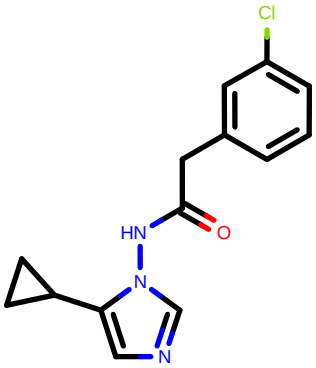
CID:	MAT-POS-c0609ef7-1_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)C(F)F
RUN:	RUN1594
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.14

EDJ-MED-ee07cf00-1_1



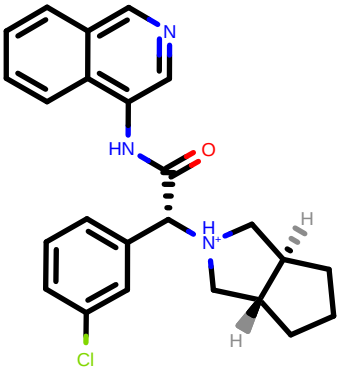
CID:	EDJ-MED-ee07cf00-1_1
SMILES:	Cn1c(=O)ccn(c1=O)CC(=O)N[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1363
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.17

JAN-GHE-f4ca5a00-14_1



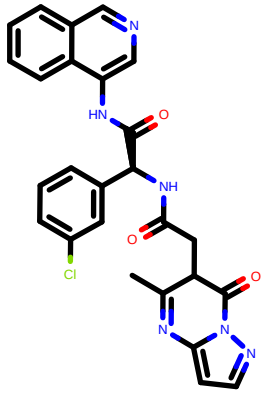
CID:	JAN-GHE-f4ca5a00-14_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nn2cncc2C3CC3
RUN:	RUN956
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.11

MIC-UNK-5a93dd5f-1_3



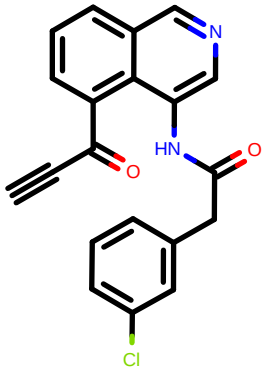
CID:	MIC-UNK-5a93dd5f-1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[NH+]4C[C@H]5CCC[C@@H]5C4
RUN:	RUN1157
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.21

EDJ-MED-ee07cf00-2_1



CID:	EDJ-MED-ee07cf00-2_1
SMILES:	Cc1c(c(=O)n2c(n1)cc[nH]2)CC(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1370
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.21

JOH-UNI-3fc3434e-1_1



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