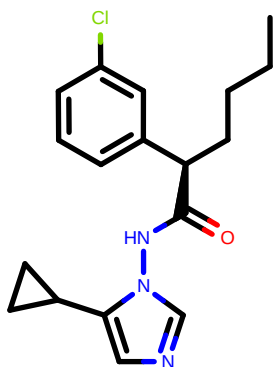
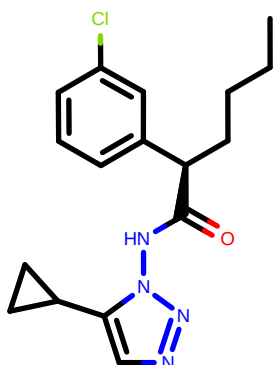


JAN-GHE-f4ca5a00-18_2



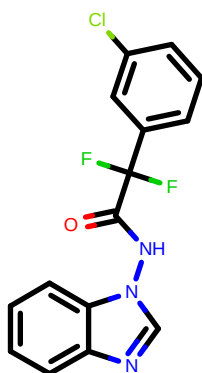
CID:	JAN-GHE-f4ca5a00-18_2
SMILES:	<chem>CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2cncc2C3CC3</chem>
RUN:	RUN196
DDG (kcal/mol):	-4.84
dDDG (kcal/mol):	0.16

JAN-GHE-f4ca5a00-20_2



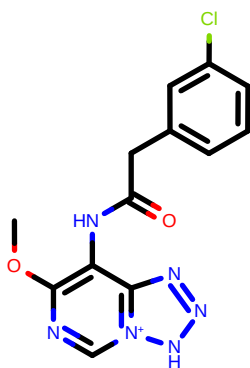
CID:	JAN-GHE-f4ca5a00-20_2
SMILES:	<chem>CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2c(cnn2)C3CC3</chem>
RUN:	RUN197
DDG (kcal/mol):	-4.56
dDDG (kcal/mol):	0.11

BAR-COM-0f94fc3d-24_1



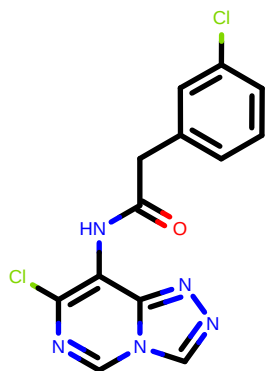
CID:	BAR-COM-0f94fc3d-24_1
SMILES:	<chem>c1ccc2c(c1)ncn2NC(=O)C(c3cccc(c3)Cl)(F)F</chem>
RUN:	RUN109
DDG (kcal/mol):	-3.08
dDDG (kcal/mol):	0.09

EDJ-MED-97c1bf5c-2_1



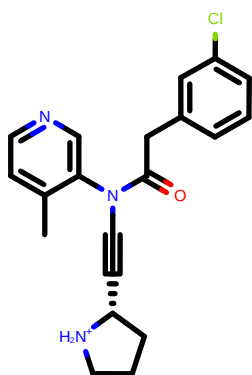
CID:	EDJ-MED-97c1bf5c-2_1
SMILES:	<chem>COc1c(c2nnnn2cn1)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN343
DDG (kcal/mol):	-2.94
dDDG (kcal/mol):	0.11

EDJ-MED-c8e7a002-7_1



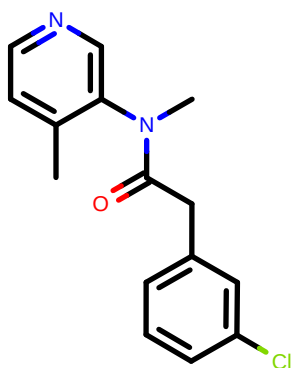
CID:	EDJ-MED-c8e7a002-7_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3nnnc3cnc2Cl</chem>
RUN:	RUN310
DDG (kcal/mol):	-2.90
dDDG (kcal/mol):	0.11

DAR-DIA-076fb6ea-10_1



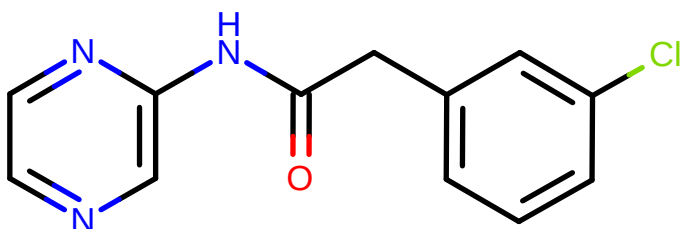
CID:	DAR-DIA-076fb6ea-10_1
SMILES:	<chem>Cc1ccncc1N(C#C[C@H]2CCCC[NH2+](2)C(=O)Cc3ccccc3)Cl</chem>
RUN:	RUN473
DDG (kcal/mol):	-2.82
dDDG (kcal/mol):	0.12

JAN-GHE-83b26c96-15_1



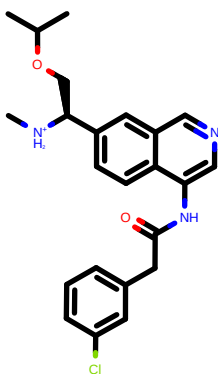
CID:	JAN-GHE-83b26c96-15_1
SMILES:	<chem>Cc1ccncc1N(C)C(=O)Cc2ccccc2)Cl</chem>
RUN:	RUN33
DDG (kcal/mol):	-2.82
dDDG (kcal/mol):	0.09

JAN-GHE-5a013bed-8_1



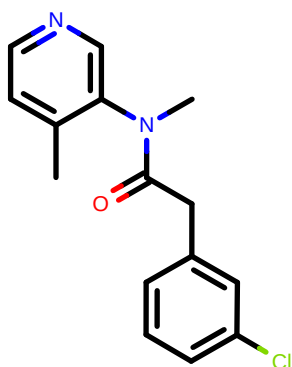
CID:	JAN-GHE-5a013bed-8_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cnccn2</chem>
RUN:	RUN50
DDG (kcal/mol):	-2.81
dDDG (kcal/mol):	0.11

MAK-UNK-ffc90da7-3_1



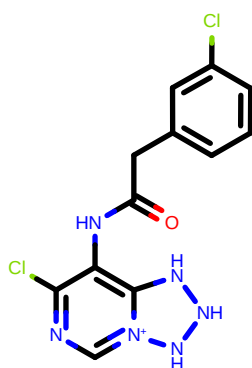
CID:	MAK-UNK-ffc90da7-3_1
SMILES:	<chem>CC(C)OC[C@H](c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl)[NH2+]</chem>
RUN:	RUN347
DDG (kcal/mol):	-2.76
dDDG (kcal/mol):	0.09

EDG-MED-0da5ad92-1_1



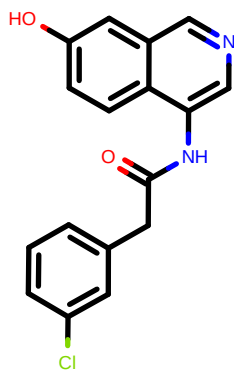
CID:	EDG-MED-0da5ad92-1_1
SMILES:	<chem>Cc1ccncc1N(C)C(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN64
DDG (kcal/mol):	-2.65
dDDG (kcal/mol):	0.09

EDJ-MED-c8e7a002-8_1



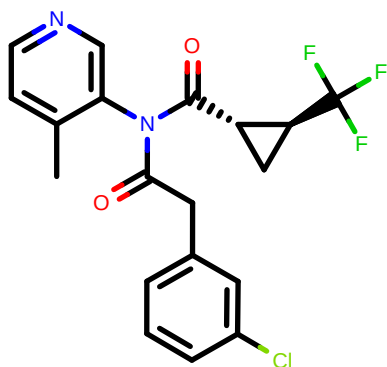
CID:	EDJ-MED-c8e7a002-8_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3nnnn3cnc2Cl</chem>
RUN:	RUN307
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.10

MAT-POS-bb423b95-8_1



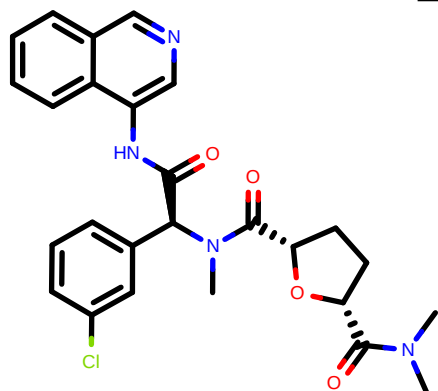
CID:	MAT-POS-bb423b95-8_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)O</chem>
RUN:	RUN266
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.07

JOH-UNI-a38a7bdd-7_2



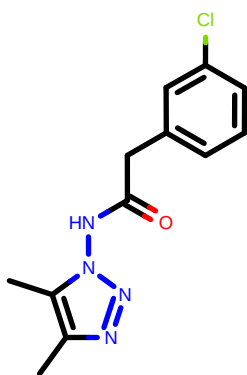
CID:	JOH-UNI-a38a7bdd-7_2
SMILES:	<chem>Cc1cncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)[C@H]3C[C@H]3C(F)(F)F</chem>
RUN:	RUN509
DDG (kcal/mol):	-2.51
dDDG (kcal/mol):	0.13

PET-UNK-1320d94d-22_1



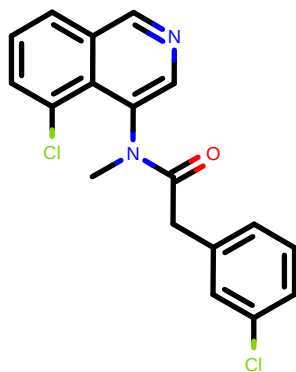
CID:	PET-UNK-1320d94d-22_1
SMILES:	<chem>CN(C)C(=O)[C@H]1CC[C@H](O1)C(=O)N(C)[C@H]2c2ccc(c2)Cl)C(=O)Nc3nccc4c3ccc4</chem>
RUN:	RUN720
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.19

JAN-GHE-5a013bed-1_1



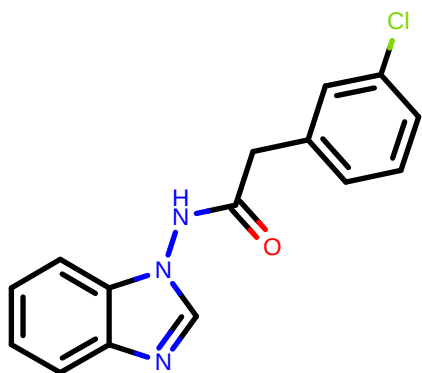
CID:	JAN-GHE-5a013bed-1_1
SMILES:	<chem>Cc1c(n(nn1)NC(=O)Cc2cccc(c2)Cl)C</chem>
RUN:	RUN56
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.08

MIC-UNK-67d4a29a-1_1



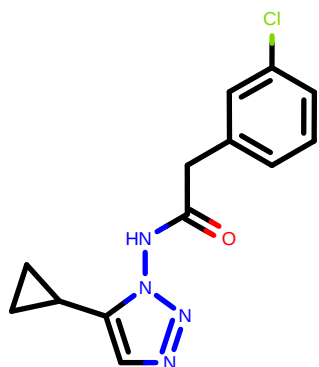
CID:	MIC-UNK-67d4a29a-1_1
SMILES:	<chem>CN(c1cncc2c1c(ccc2)Cl)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN445
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.14

JAN-GHE-5a013bed-2_1



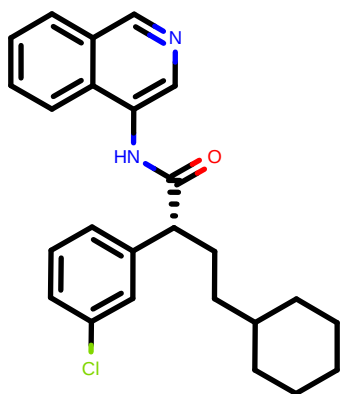
CID:	JAN-GHE-5a013bed-2_1
SMILES:	<chem>c1ccc2c(c1)ncn2NC(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN62
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.11

JAN-GHE-f4ca5a00-17_1



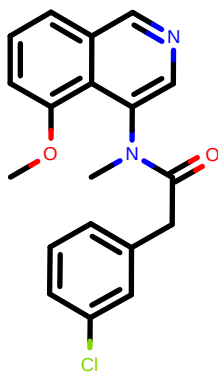
CID:	JAN-GHE-f4ca5a00-17_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2c(cnn2)C3CC3</chem>
RUN:	RUN159
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.09

MIC-UNK-c66144cb-3_2



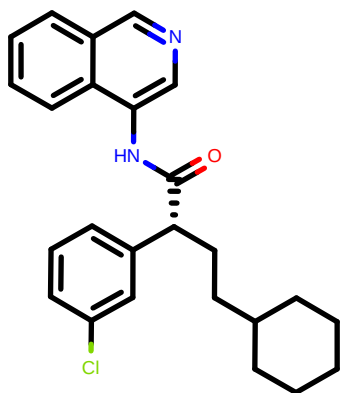
CID:	MIC-UNK-c66144cb-3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CCCCCCCC3)c4ccccc(c4)Cl</chem>
RUN:	RUN217
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.17

MIC-UNK-67d4a29a-4_1



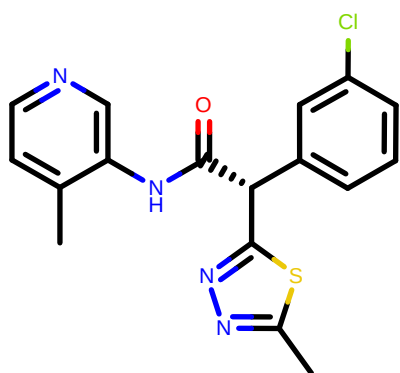
CID:	MIC-UNK-67d4a29a-4_1
SMILES:	<chem>CN(c1cncc2c1c(ccc2)OC)C(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN450
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.14

ALP-POS-3b848b35-4_2



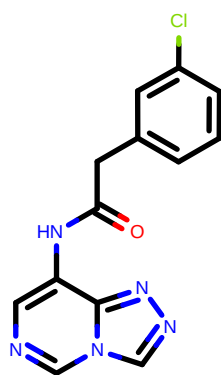
CID:	ALP-POS-3b848b35-4_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CCCCCCCC3)c4cccc(c4)Cl</chem>
RUN:	RUN199
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.17

TRY-UNI-9f475305-3_2



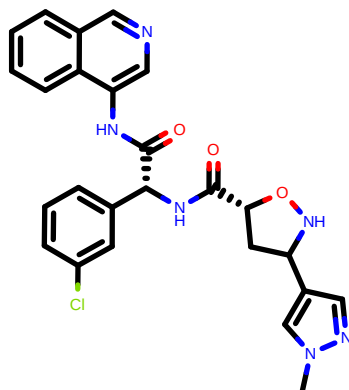
CID:	TRY-UNI-9f475305-3_2
SMILES:	<chem>Cc1ccncc1NC(=O)[C@H](c2cccc(c2)Cl)c3nnc(s3)C</chem>
RUN:	RUN69
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.11

EDJ-MED-076d6e64-1_1



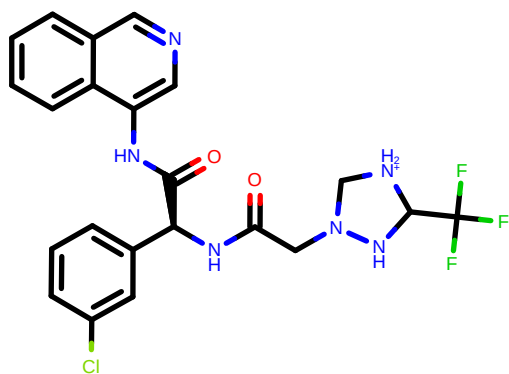
CID:	EDJ-MED-076d6e64-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncn3c2nnc3</chem>
RUN:	RUN691
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.08

EDJ-MED-ee07cf00-6_4



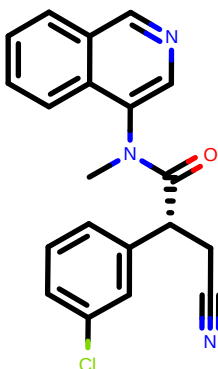
CID:	EDJ-MED-ee07cf00-6_4
SMILES:	<chem>Cn1cc(en1)C2=NO[C@H](C2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN585
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-10_2



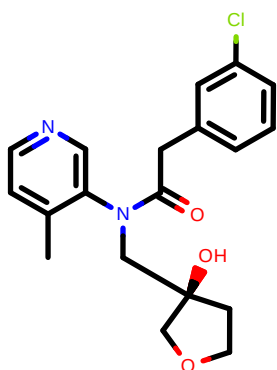
CID:	EDJ-MED-ee07cf00-10_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)Cn4cnc(n4)C(F)(F)F</chem>
RUN:	RUN587
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.18

JOH-UNI-ee5ed7c8-7_2



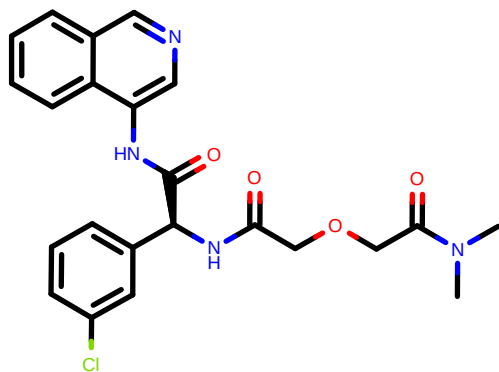
CID:	JOH-UNI-ee5ed7c8-7_2
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)[C@H](CC#N)c3cccc(c3)Cl</chem>
RUN:	RUN536
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.15

BAR-COM-ebf5acce-11_1



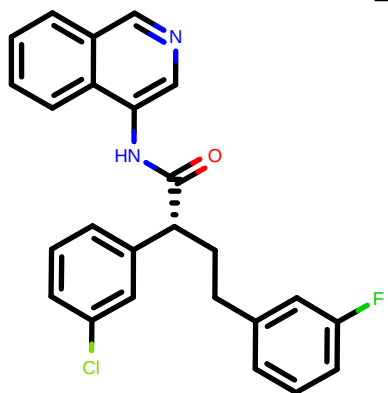
CID:	BAR-COM-ebf5acce-11_1
SMILES:	<chem>Cc1cncc1N(C[C@@H]2(CCOC2)O)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN66
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.18

EDJ-MED-cf4b0d25-5_1



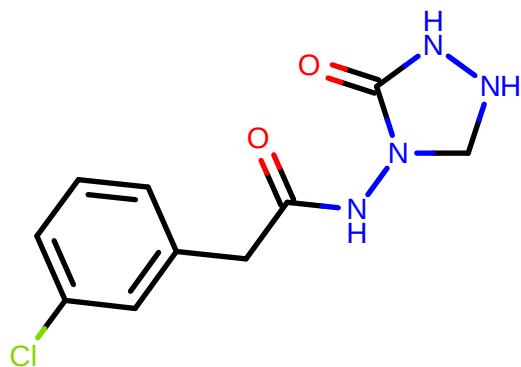
CID:	EDJ-MED-cf4b0d25-5_1
SMILES:	<chem>CN(C)C(=O)COCC(=O)N[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN718
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.16

MIC-UNK-c66144cb-1_2



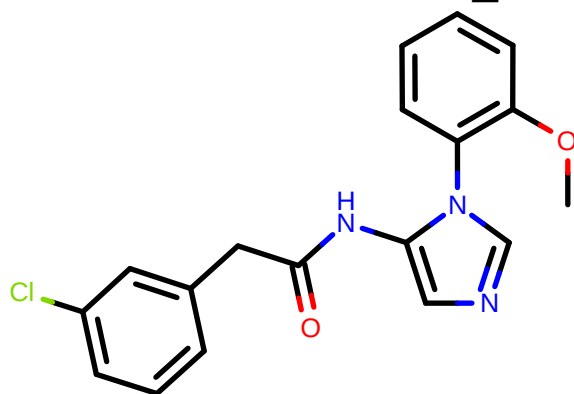
CID:	MIC-UNK-c66144cb-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CCc3ccccc(c3)F)c4ccccc(c4)Cl</chem>
RUN:	RUN248
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.12

JAN-GHE-5a013bed-4_1



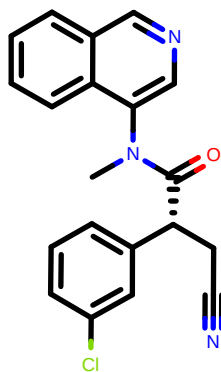
CID:	JAN-GHE-5a013bed-4_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2cn[nH]c2=O</chem>
RUN:	RUN68
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.12

BEN-DND-1e24cf73-4_1



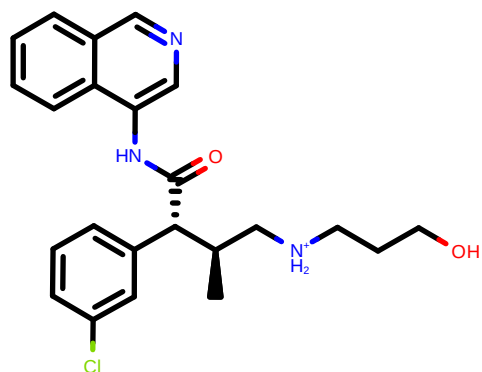
CID:	BEN-DND-1e24cf73-4_1
SMILES:	<chem>COc1cccc1n2cncc2NC(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN733
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.12

JOH-UNI-3fc3434e-7_2



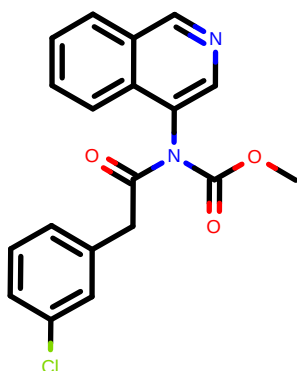
CID:	JOH-UNI-3fc3434e-7_2
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)[C@H](CC#N)c3ccccc(c3)Cl</chem>
RUN:	RUN544
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.16

MAK-UNK-c749d764-6_4



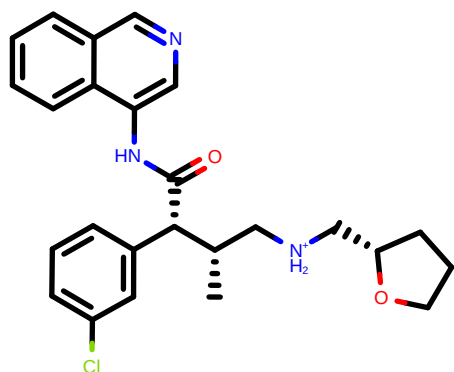
CID:	MAK-UNK-c749d764-6_4
SMILES:	<chem>C[C@H](C[NH2+])CCCO)[C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN464
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.21

PET-UNK-12d8d43f-2_1



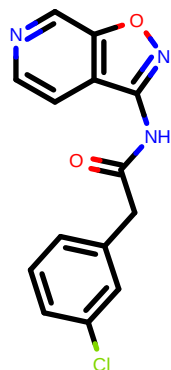
CID:	PET-UNK-12d8d43f-2_1
SMILES:	<chem>COC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN527
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.11

MAK-UNK-ffc90da7-4_5



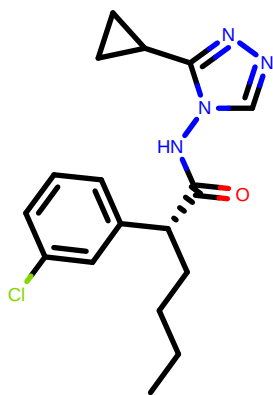
CID:	MAK-UNK-ffc90da7-4_5
SMILES:	<chem>C[C@@H](C[NH2+])C[C@@H]1CCCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN384
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.29

JIN-POS-6dc588a4-16_1



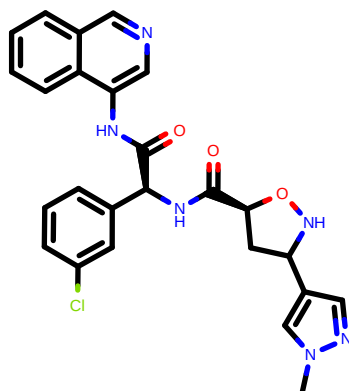
CID:	JIN-POS-6dc588a4-16_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3ccncc3on2</chem>
RUN:	RUN616
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.08

JAN-GHE-f4ca5a00-19_2



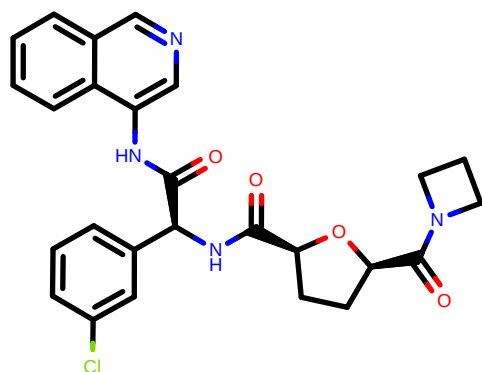
CID:	JAN-GHE-f4ca5a00-19_2
SMILES:	<chem>CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2cnnc2C3CC3</chem>
RUN:	RUN201
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.16

EDJ-MED-ee07cf00-6_1



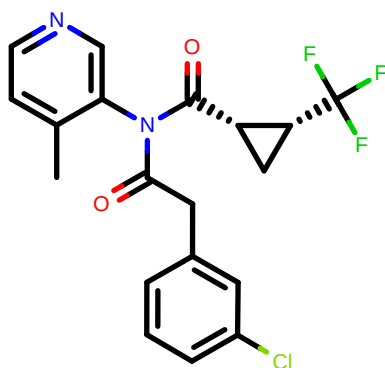
CID:	EDJ-MED-ee07cf00-6_1
SMILES:	<chem>Cn1cc(en1)C2=NO[C@H](C2)C(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN584
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.17

PET-UNK-1320d94d-6_1



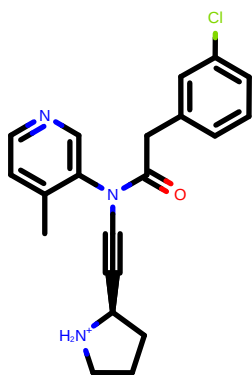
CID:	PET-UNK-1320d94d-6_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@@H](O)C[C@H](O4)C(=O)N5CCCC5</chem>
RUN:	RUN701
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.20

JOH-UNI-a38a7bdd-7_4



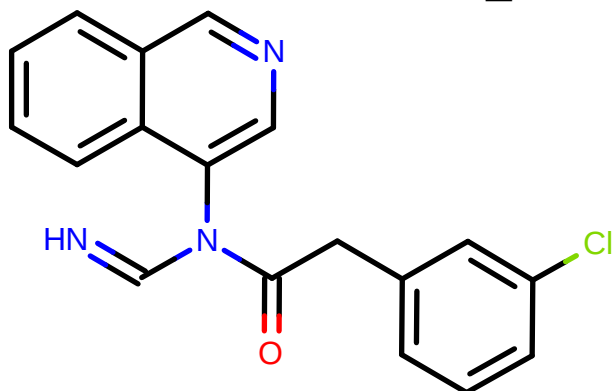
CID:	JOH-UNI-a38a7bdd-7_4
SMILES:	<chem>Cc1cncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)[C@H]3C[C@H]3C(F)(F)F</chem>
RUN:	RUN516
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.14

DAR-DIA-076fb6ea-10_2



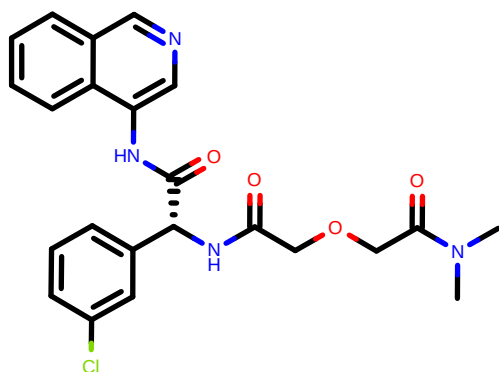
CID:	DAR-DIA-076fb6ea-10_2
SMILES:	<chem>Cc1ccncc1N(C#C[C@H]2CCC[NH2+])C(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN479
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.10

PET-UNK-5ecb6237-1_1



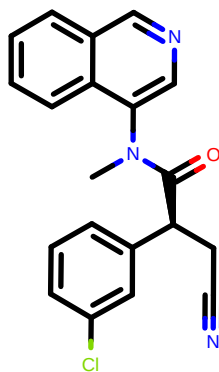
CID:	PET-UNK-5ecb6237-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C#N)C(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN327
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.09

EDJ-MED-cf4b0d25-5_2



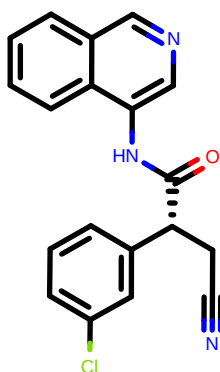
CID:	EDJ-MED-cf4b0d25-5_2
SMILES:	<chem>CN(C)C(=O)COCC(=O)N[C@H](c1ccccc1)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN678
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.14

JOH-UNI-ee5ed7c8-7_1



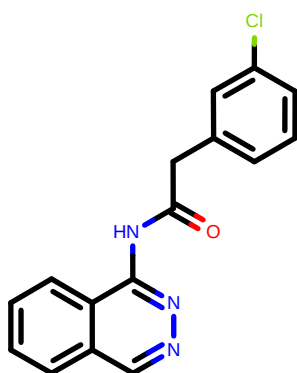
CID:	JOH-UNI-ee5ed7c8-7_1
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)[C@@H](CC#N)c3ccccc(c3)Cl</chem>
RUN:	RUN535
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.12

JOH-UNI-3fc3434e-6_2



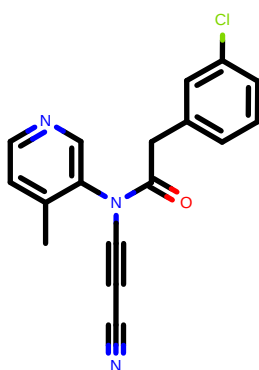
CID:	JOH-UNI-3fc3434e-6_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CC#N)c3cccc(c3)Cl</chem>
RUN:	RUN549
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.10

EDJ-MED-50fe53e8-1_1



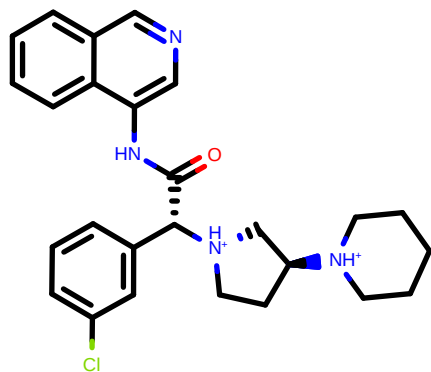
CID:	EDJ-MED-50fe53e8-1_1
SMILES:	<chem>c1ccc2c(c1)cnnc2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN195
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.08

DAR-DIA-076fb6ea-6_1



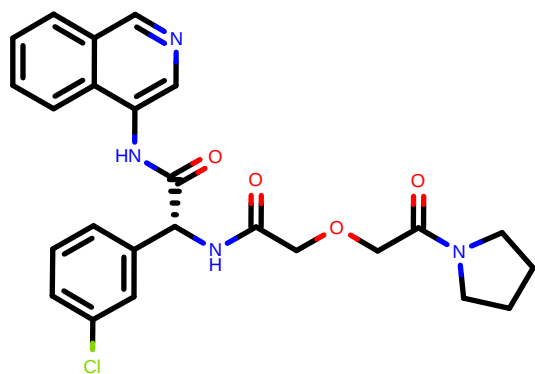
CID:	DAR-DIA-076fb6ea-6_1
SMILES:	<chem>Cc1ccncc1N(C#CC#N)C(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN465
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.09

MIC-UNK-5a93dd5f-12_3



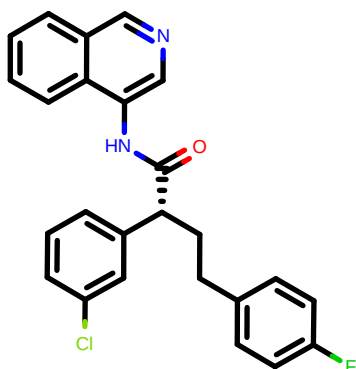
CID:	MIC-UNK-5a93dd5f-12_3
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@](C#N)C[C@H](C4)N[H+]5CCCCC5</chem>
RUN:	RUN443
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.17

EDJ-MED-cf4b0d25-1_1



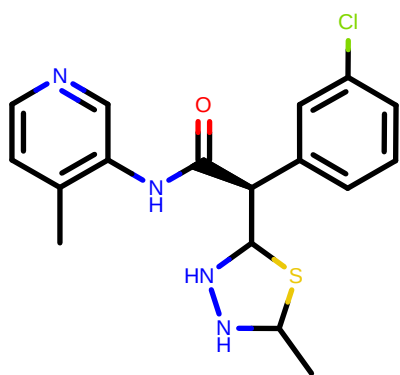
CID:	EDJ-MED-cf4b0d25-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)COC(=O)N4CCCC4</chem>
RUN:	RUN671
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.18

MIC-UNK-c66144cb-2_2



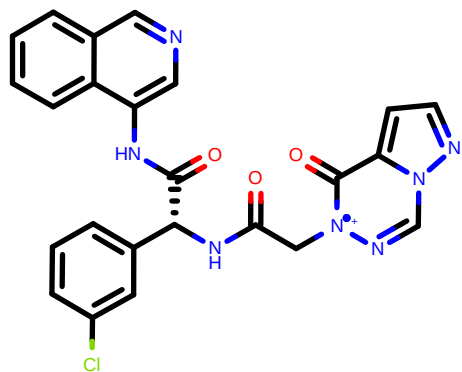
CID:	MIC-UNK-c66144cb-2_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](CCc3cccc(c3)F)c4cccc(c4)Cl</chem>
RUN:	RUN244
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.12

TRY-UNI-9f475305-3_1



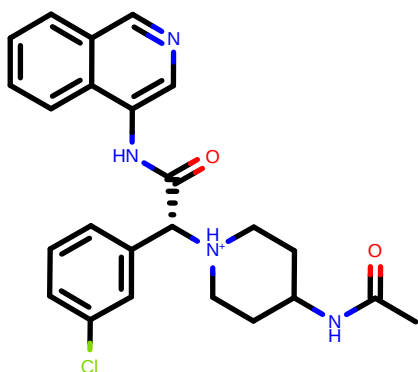
CID:	TRY-UNI-9f475305-3_1
SMILES:	<chem>Cc1ccncc1NC(=O)[C@@H](c2cccc(c2)Cl)c3nncc(s3)C</chem>
RUN:	RUN76
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-17_1



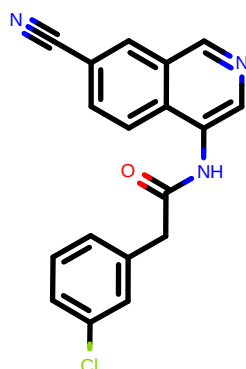
CID:	EDJ-MED-ee07cf00-17_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cn4c(=O)c5ccnn5cn4</chem>
RUN:	RUN590
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.19

MIC-UNK-5a93dd5f-4_2



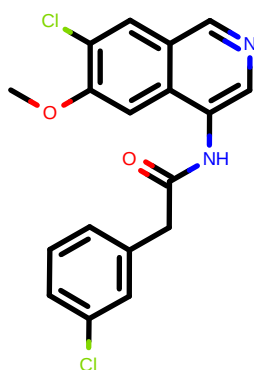
CID:	MIC-UNK-5a93dd5f-4_2
SMILES:	<chem>CC(=O)NC1CC[NH+](CC1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN400
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.38

PET-UNK-6314f867-2_1



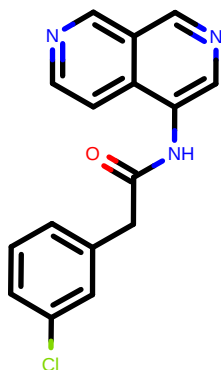
CID:	PET-UNK-6314f867-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)C#N</chem>
RUN:	RUN680
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.08

PET-UNK-b38839dc-2_1



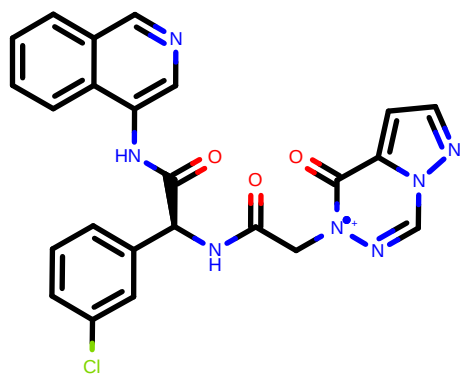
CID:	PET-UNK-b38839dc-2_1
SMILES:	<chem>COc1cc2c(cc1Cl)cncc2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN723
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.10

MAT-POS-bb423b95-1_1



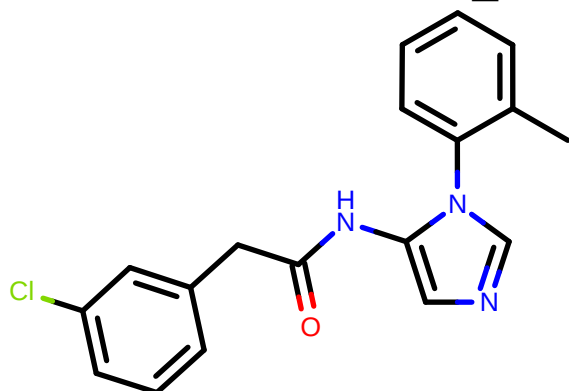
CID:	MAT-POS-bb423b95-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccnc3</chem>
RUN:	RUN257
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.08

EDJ-MED-ee07cf00-17_2



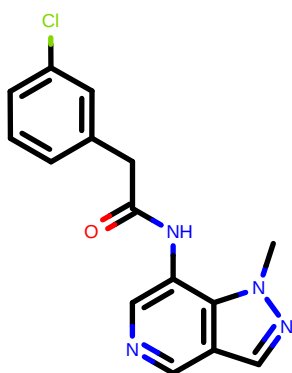
CID:	EDJ-MED-ee07cf00-17_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)C)NC(=O)Cn4c(=O)c5cnrn5cn4</chem>
RUN:	RUN586
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.23

BEN-DND-1e24cf73-2_1



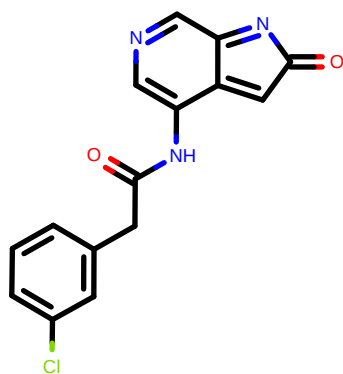
CID:	BEN-DND-1e24cf73-2_1
SMILES:	<chem>Cc1ccccc1n2cncc2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN731
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.11

RUB-POS-1325a9ea-14_1



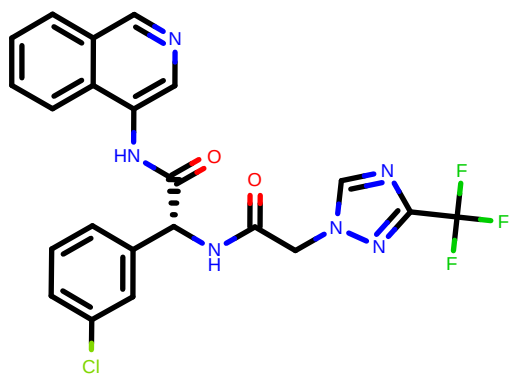
CID:	RUB-POS-1325a9ea-14_1
SMILES:	<chem>Cn1c2c(cncc2NC(=O)Cc3cccc(c3)Cl)cn1</chem>
RUN:	RUN647
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.08

MAT-POS-f7918075-7_1



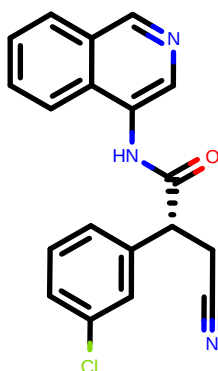
CID:	MAT-POS-f7918075-7_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2CC(=O)N3</chem>
RUN:	RUN261
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.09

EDJ-MED-ee07cf00-10_1



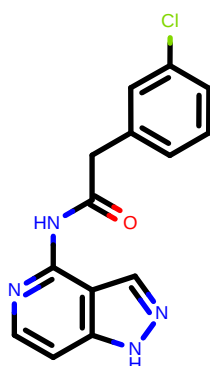
CID:	EDJ-MED-ee07cf00-10_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cn4nc(n4)C(F)(F)F</chem>
RUN:	RUN581
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.16

JOH-UNI-ee5ed7c8-6_2



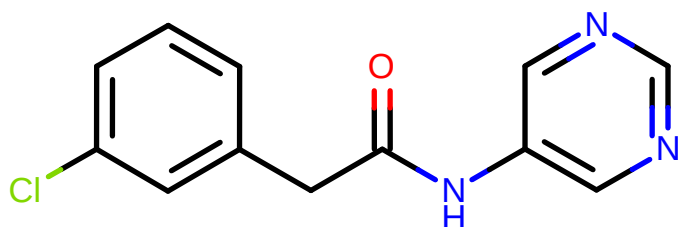
CID:	JOH-UNI-ee5ed7c8-6_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](CC#N)(CC#N)c3cccc(c3)Cl</chem>
RUN:	RUN532
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.10

MAT-POS-199e2e7c-2_1



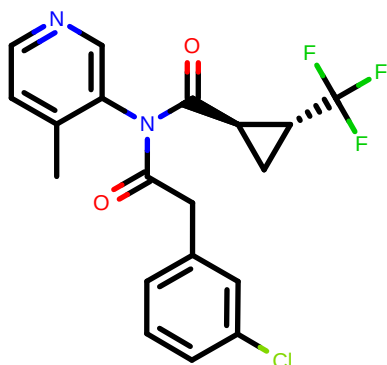
CID:	MAT-POS-199e2e7c-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3cn[nH]c3ccn2</chem>
RUN:	RUN315
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.11

JAN-GHE-5a013bed-9_1



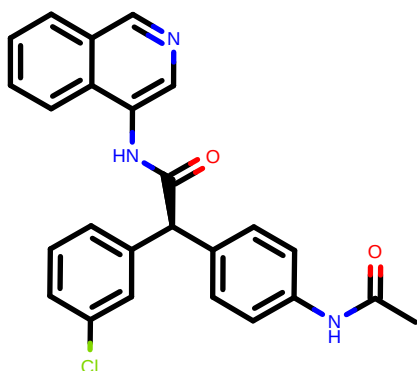
CID:	JAN-GHE-5a013bed-9_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncnc2</chem>
RUN:	RUN55
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.09

JOH-UNI-a38a7bdd-7_3



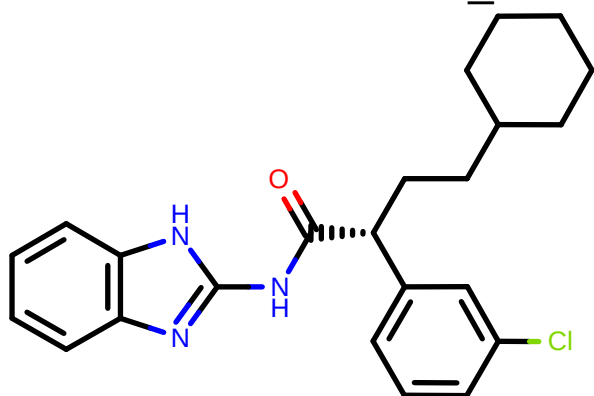
CID:	JOH-UNI-a38a7bdd-7_3
SMILES:	<chem>Cc1cncc1N(C(=O)Cc2ccccc2Cl)C(=O)[C@H]3C[C@H]3C(F)(F)F</chem>
RUN:	RUN497
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.13

MIC-UNK-d36ab305-1_1



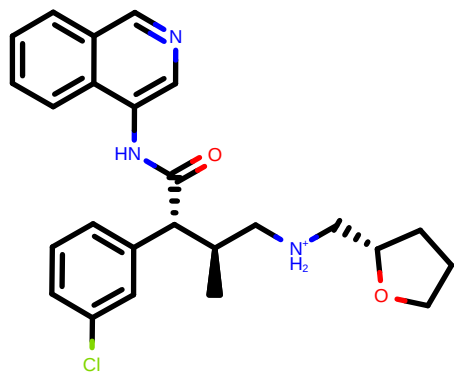
CID:	MIC-UNK-d36ab305-1_1
SMILES:	<chem>CC(=O)Nc1ccc(cc1)[C@@H](c2ccccc2Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN240
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.14

ALP-POS-3fc1724e-8_2



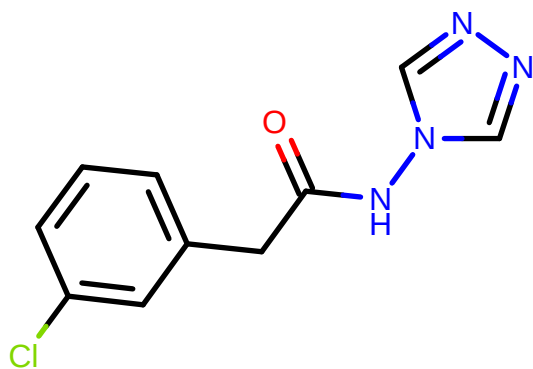
CID:	ALP-POS-3fc1724e-8_2
SMILES:	<chem>c1ccc2c(c1)[nH]c(n2)NC(=O)[C@H](CCCC3CCCCC3)c4ccccc4Cl</chem>
RUN:	RUN174
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.17

MAK-UNK-c749d764-22_6



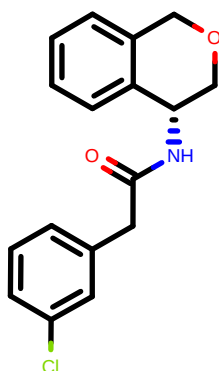
CID:	MAK-UNK-c749d764-22_6
SMILES:	<chem>C[C@H](C[NH2+][C]([NH2+])C(=O)[C@H]1CCCCO1)[C@H](c2ccccc2Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN452
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.25

JAN-GHE-5a013bed-5_1



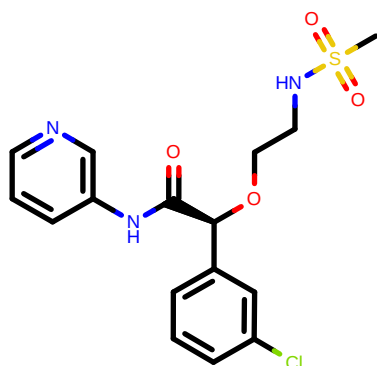
CID:	JAN-GHE-5a013bed-5_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2cnnc2</chem>
RUN:	RUN63
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.12

RUB-POS-1325a9ea-20_1



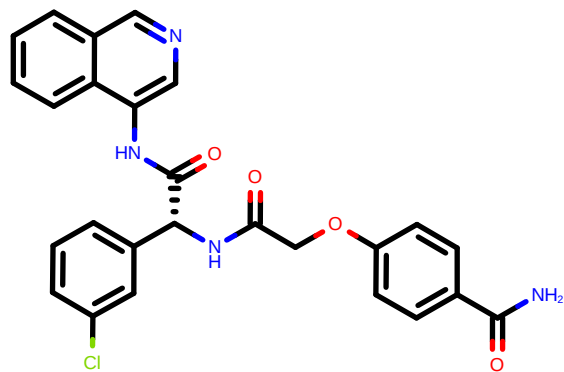
CID:	RUB-POS-1325a9ea-20_1
SMILES:	<chem>c1ccc2c(c1)COC[C@@H]2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN649
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.10

ADA-UNI-f8e79267-7_1



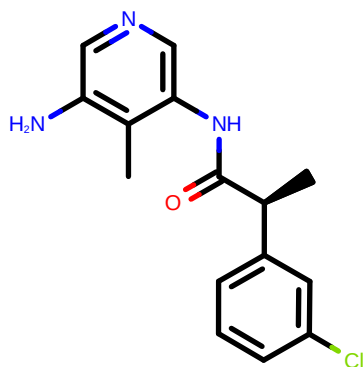
CID:	ADA-UNI-f8e79267-7_1
SMILES:	<chem>CS(=O)(=O)NCCO[C@@H](c1cccc(c1)Cl)C(=O)Nc2ccncc2</chem>
RUN:	RUN19
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.15

EDJ-MED-ee07cf00-12_1



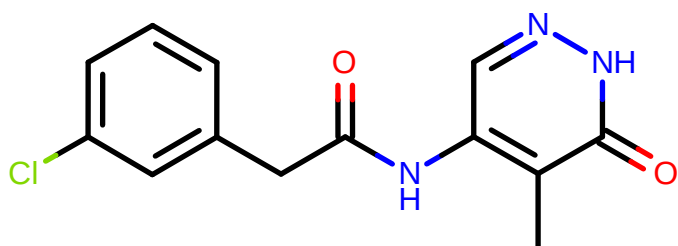
CID:	EDJ-MED-ee07cf00-12_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)COc4ccc(cc4)C(=O)N</chem>
RUN:	RUN591
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.16

TRY-UNI-714a760b-15_1



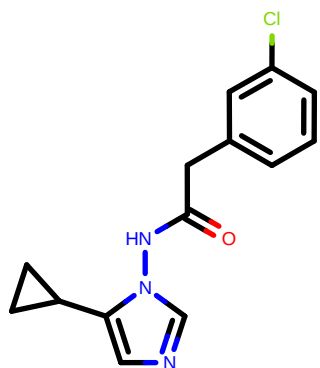
CID:	TRY-UNI-714a760b-15_1
SMILES:	<chem>Cc1c(cnc1NC(=O)[C@@H](C)c2ccccc2)Cl)N</chem>
RUN:	RUN4
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.08

MIC-UNK-d935700b-1_1



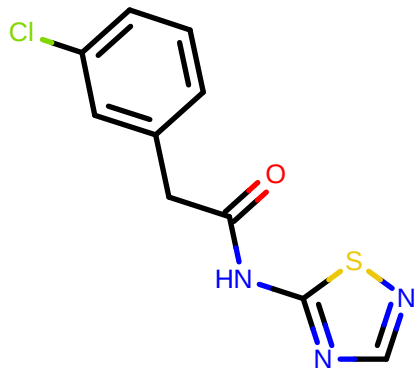
CID:	MIC-UNK-d935700b-1_1
SMILES:	<chem>Cc1c(c[nH]c1=O)NC(=O)Cc2ccccc2)Cl</chem>
RUN:	RUN340
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.11

JAN-GHE-f4ca5a00-14_1



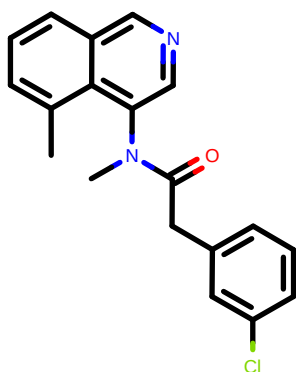
CID:	JAN-GHE-f4ca5a00-14_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2cncc2C3CC3</chem>
RUN:	RUN162
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.12

PET-UNK-158bee2a-4_1



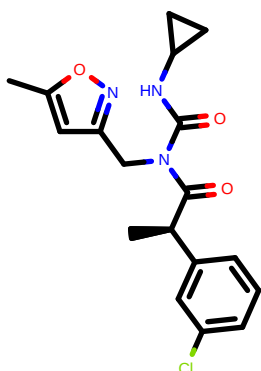
CID:	PET-UNK-158bee2a-4_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2ncns2</chem>
RUN:	RUN699
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.10

MIC-UNK-67d4a29a-3_1



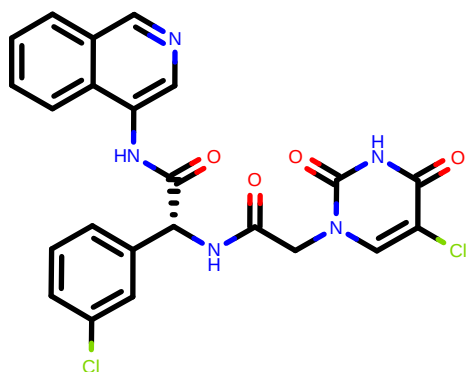
CID:	MIC-UNK-67d4a29a-3_1
SMILES:	<chem>Cc1cccc2c1c(cnc2)N(C)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN448
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.16

TRY-UNI-9f475305-8_2



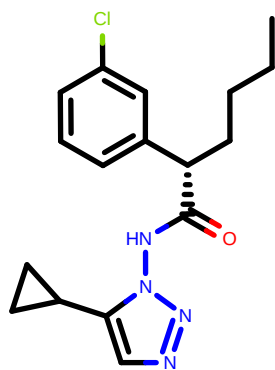
CID:	TRY-UNI-9f475305-8_2
SMILES:	<chem>Cc1cc(no1)CN(C(=O)[C@H](C)c2cccc(c2)Cl)C(=O)NC3CCC3</chem>
RUN:	RUN95
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.16

EDJ-MED-ee07cf00-16_1



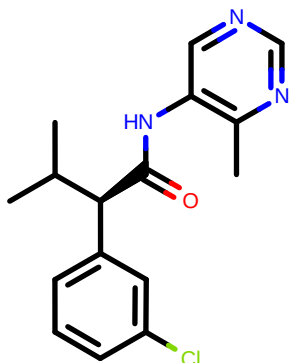
CID:	EDJ-MED-ee07cf00-16_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](C)c3cccc(c3)Cl)NC(=O)Cn4cc(c(c=O)[nH])c4=O)Cl</chem>
RUN:	RUN567
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.19

JAN-GHE-f4ca5a00-20_1



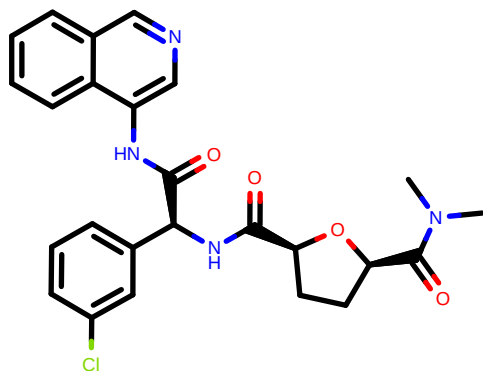
CID:	JAN-GHE-f4ca5a00-20_1
SMILES:	<chem>CCCC[C@H](C1CCCC(C1)Cl)C(=O)Nn2c(cnn2)C3CCC3</chem>
RUN:	RUN207
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.12

JAN-GHE-83b26c96-7_1



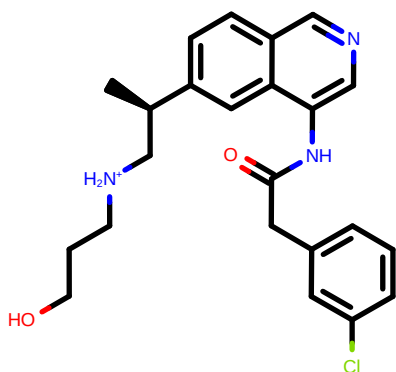
CID:	JAN-GHE-83b26c96-7_1
SMILES:	<chem>Cc1c(cncn1)NC(=O)[C@@H](c2cccc(c2)Cl)C(C)C</chem>
RUN:	RUN22
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.11

PET-UNK-1320d94d-2_1



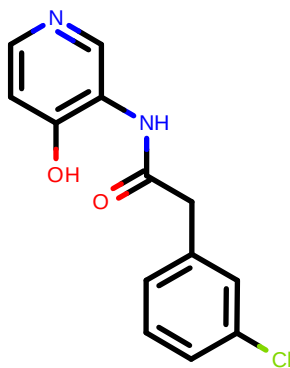
CID:	PET-UNK-1320d94d-2_1
SMILES:	<chem>CN(C)C(=O)[C@@H](C)CC[C@H](O1)C(=O)N[C@@H](c2cccc(c2)Cl)C(=O)Nc3nccc4c3ccc4</chem>
RUN:	RUN713
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.18

MAK-UNK-ffc90da7-6_2



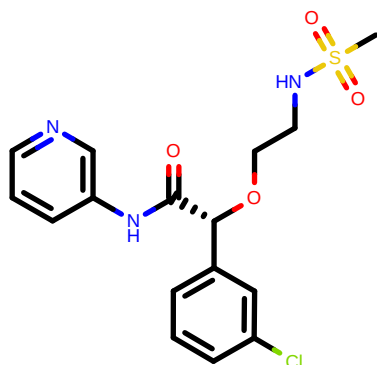
CID:	MAK-UNK-ffc90da7-6_2
SMILES:	<chem>C[C@H](C[NH2+])CCCO)c1ccc2nccc(c2c1)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN411
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.13

ALP-POS-95b75b4d-6_1



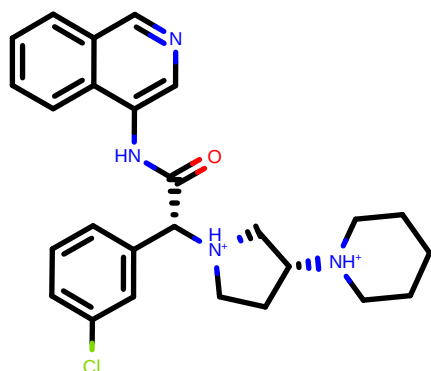
CID:	ALP-POS-95b75b4d-6_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c[nH]ccc2=O</chem>
RUN:	RUN42
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.09

ADA-UNI-f8e79267-7_2



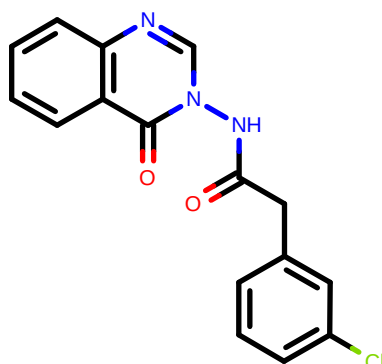
CID:	ADA-UNI-f8e79267-7_2
SMILES:	<chem>CS(=O)(=O)NCCO[C@H](c1cccc(c1)Cl)C(=O)Nc2ccnc2</chem>
RUN:	RUN8
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.15

MIC-UNK-5a93dd5f-12_5



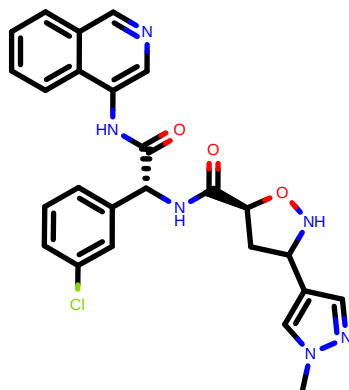
CID:	MIC-UNK-5a93dd5f-12_5
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc3Cl)[N+]([O-])C4CC[C@H](C4)[NH+]5CCCCC5</chem>
RUN:	RUN444
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.18

JAN-GHE-5a013bed-3_1



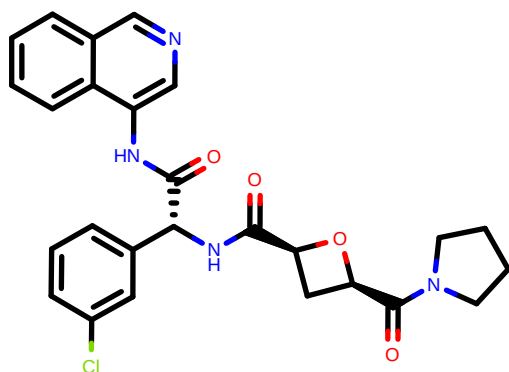
CID:	JAN-GHE-5a013bed-3_1
SMILES:	<chem>c1ccc2c(c1)c(=O)n(cn2)NC(=O)Cc3ccccc3Cl</chem>
RUN:	RUN45
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.10

EDJ-MED-ee07cf00-6_3



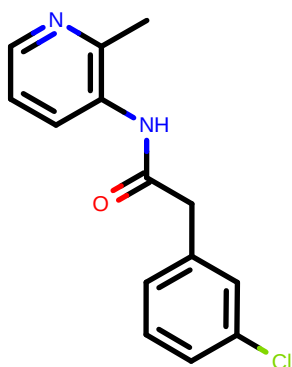
CID:	EDJ-MED-ee07cf00-6_3
SMILES:	<chem>Cn1cc(cn1)C2=NO[C@H](C2)C(=O)N[C@H](c3ccccc3Cl)C(=O)Nc4cccc5c4cccc5</chem>
RUN:	RUN578
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.15

PET-UNK-1320d94d-7_1



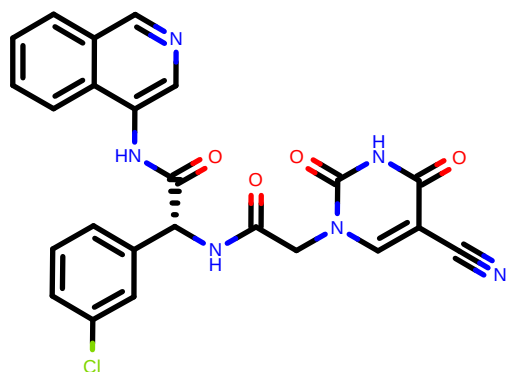
CID:	PET-UNK-1320d94d-7_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)C)NC(=O)[C@@H](C4C[C@H](O4)C)=O</chem>
RUN:	RUN706
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.17

EDG-MED-0da5ad92-14_1



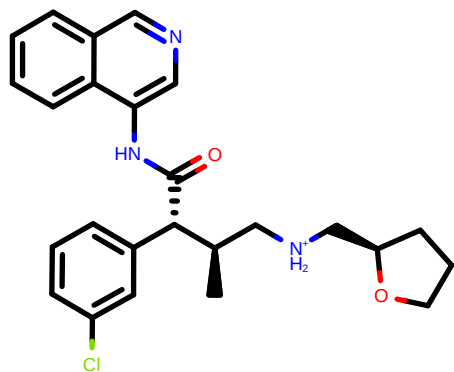
CID:	EDG-MED-0da5ad92-14_1
SMILES:	<chem>Cc1c(cccn1)NC(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN77
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.12

EDJ-MED-ee07cf00-8_1



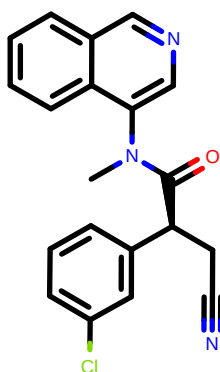
CID:	EDJ-MED-ee07cf00-8_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)C)NC(=O)Cn4cc(c(=O)[nH]c4=O)C#N</chem>
RUN:	RUN576
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.18

MAK-UNK-c749d764-22_8



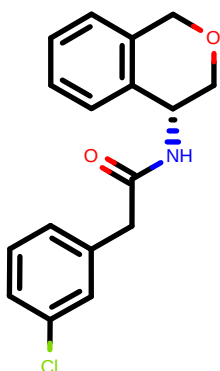
CID:	MAK-UNK-c749d764-22_8
SMILES:	<chem>C[C@H](C[NH2+][C@H]1CCCCO1)[C@H](c2cccc(c2)C)C(=O)Nc3nccc4c3cccc4</chem>
RUN:	RUN478
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.24

JOH-UNI-3fc3434e-7_1



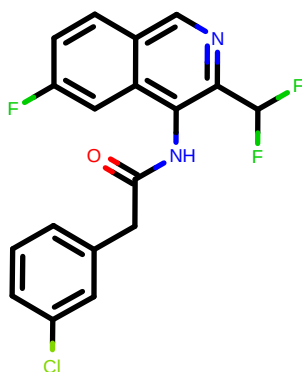
CID:	JOH-UNI-3fc3434e-7_1
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)[C@@H](CC#N)c3cccc(c3)Cl</chem>
RUN:	RUN541
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.13

PET-UNK-f92d7c0c-2_1



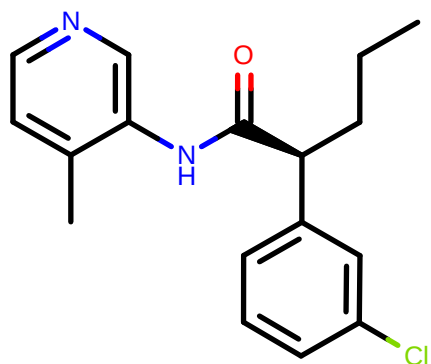
CID:	PET-UNK-f92d7c0c-2_1
SMILES:	<chem>c1ccc2c(c1)COC[C@@H]2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN668
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.11

JOH-UNI-6fede743-5_1



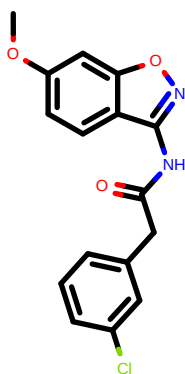
CID:	JOH-UNI-6fede743-5_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3cc(ccc3cnc2C(F)F)F</chem>
RUN:	RUN459
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.13

JAN-GHE-83b26c96-8_1



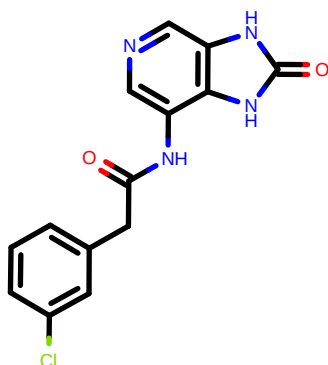
CID:	JAN-GHE-83b26c96-8_1
SMILES:	<chem>CCC[C@@H](c1cccc(c1)Cl)C(=O)Nc2cnccc2C</chem>
RUN:	RUN24
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.10

EDJ-MED-c8e7a002-1_1



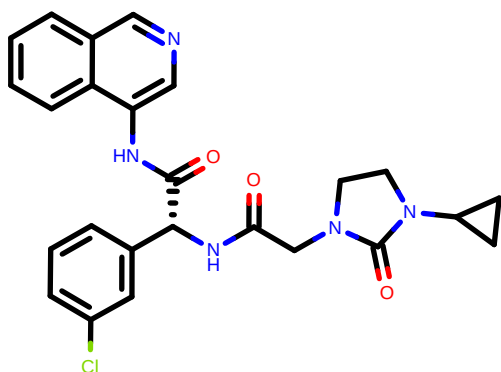
CID:	EDJ-MED-c8e7a002-1_1
SMILES:	<chem>COc1ccc2c(c1)onc2NC(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN296
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.13

MAT-POS-f7918075-4_1



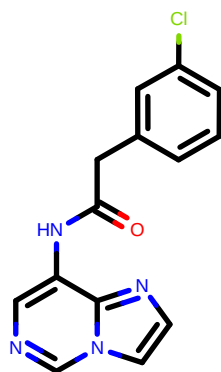
CID:	MAT-POS-f7918075-4_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2[nH]c(=O)[nH]3</chem>
RUN:	RUN263
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.08

EDJ-MED-ee07cf00-18_1



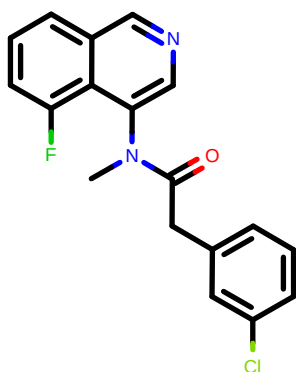
CID:	EDJ-MED-ee07cf00-18_1
SMILES:	<chem>c1ccc2c(c1)onc2NC(=O)[C@@H](c3ccccc(c3)Cl)NC(=O)CN4CCN(C4=O)C5CC5</chem>
RUN:	RUN588
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.18

RUB-POS-1325a9ea-8_1



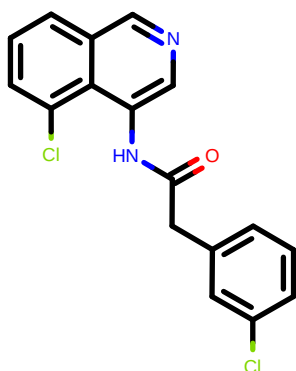
CID:	RUB-POS-1325a9ea-8_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncn3c2ncc3</chem>
RUN:	RUN643
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.09

MIC-UNK-67d4a29a-2_1



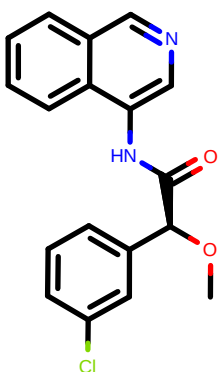
CID:	MIC-UNK-67d4a29a-2_1
SMILES:	<chem>CN(c1cncc2c1c(ccc2)F)C(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN451
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.12

MIC-UNK-50cce87d-2_1



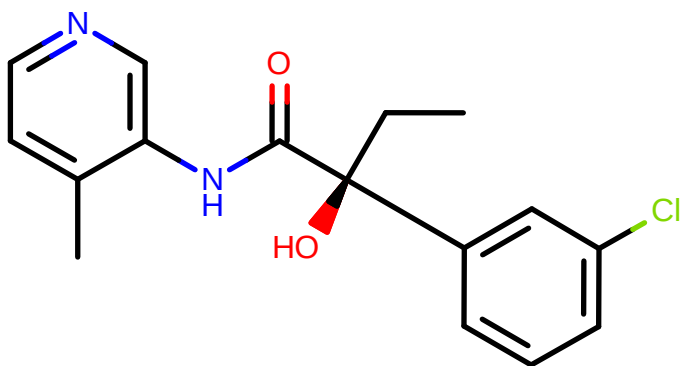
CID:	MIC-UNK-50cce87d-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)Cl</chem>
RUN:	RUN342
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.08

VLA-UNK-9a7dc93f-7_1



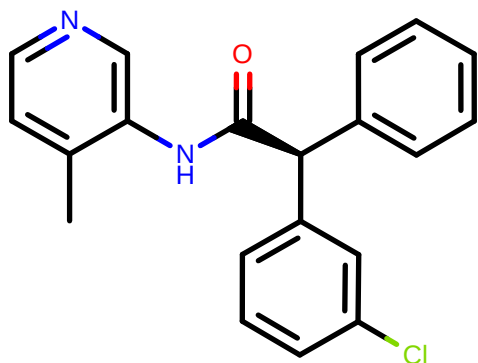
CID:	VLA-UNK-9a7dc93f-7_1
SMILES:	<chem>CO[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN566
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.09

BAR-COM-0f94fc3d-38_2



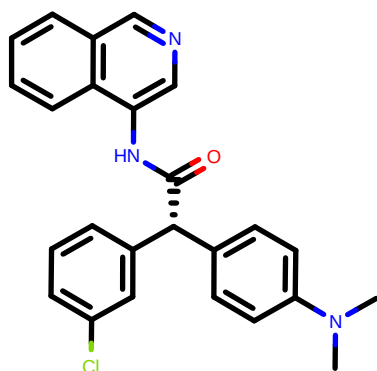
CID:	BAR-COM-0f94fc3d-38_2
SMILES:	<chem>CC[C@](c1cccc(c1)Cl)(C(=O)Nc2cnccc2C)O</chem>
RUN:	RUN123
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.11

SAM-UNK-2684b532-1_1



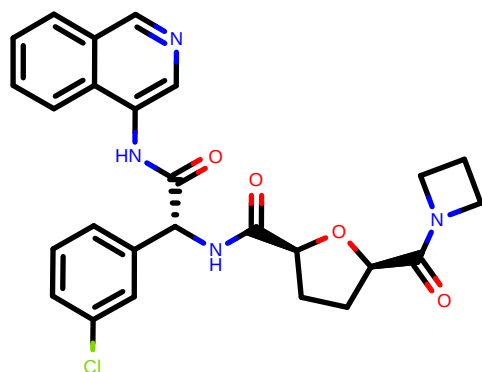
CID:	SAM-UNK-2684b532-1_1
SMILES:	<chem>Cc1ccncc1NC(=O)[C@@H](c2ccccc2)c3cccc(c3)Cl</chem>
RUN:	RUN124
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.10

MIC-UNK-d36ab305-4_2



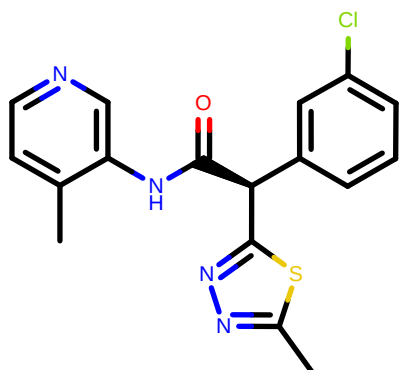
CID:	MIC-UNK-d36ab305-4_2
SMILES:	<chem>CN(C)c1ccc(cc1)[C@H](c2ccccc2)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN247
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.13

PET-UNK-1320d94d-5_1



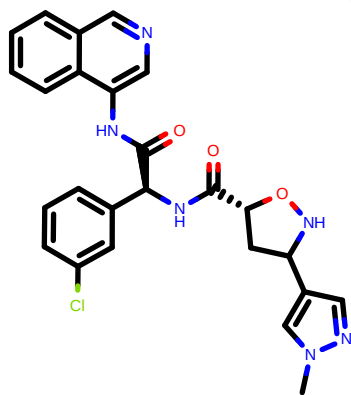
CID:	PET-UNK-1320d94d-5_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc3)C(=O)Nc4cnc(c4)C(=O)Nc5ccccc5</chem>
RUN:	RUN717
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.17

SAM-UNK-2684b532-3_1



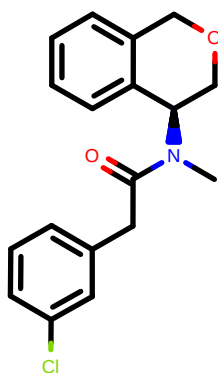
CID:	SAM-UNK-2684b532-3_1
SMILES:	<chem>Cc1ccncc1NC(=O)[C@@H](c2ccccc2)Cl)c3nncc(s3)C</chem>
RUN:	RUN148
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-6_2



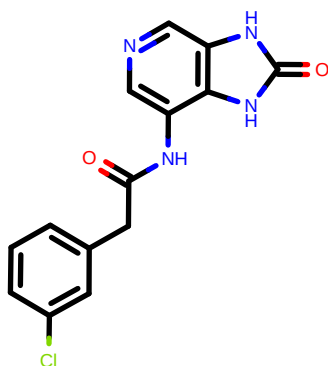
CID:	EDJ-MED-ee07cf00-6_2
SMILES:	<chem>Cn1cc(cn1)C2=NO[C@H](C2)C(=O)N[C@@H](c3ccccc3)C(=O)Nc4cncc5c4ccccc5</chem>
RUN:	RUN571
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.17

PET-UNK-f92d7c0c-9_1



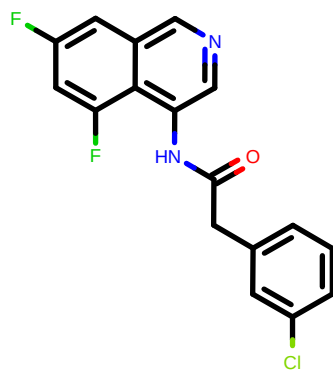
CID:	PET-UNK-f92d7c0c-9_1
SMILES:	<chem>CN([C@@H]1COCc2c1cccc2)C(=O)Cc3ccccc3)Cl</chem>
RUN:	RUN681
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.13

MIC-UNK-8971c93c-1_1



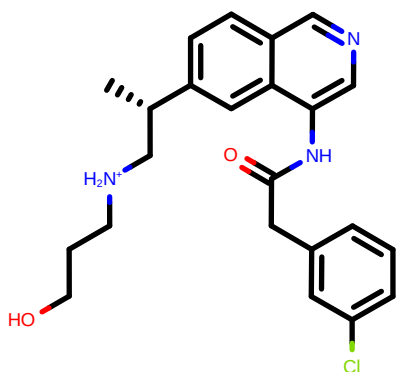
CID:	MIC-UNK-8971c93c-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2[nH]c(=O)[nH]3</chem>
RUN:	RUN222
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.07

MIC-UNK-7574fcc6-1_1



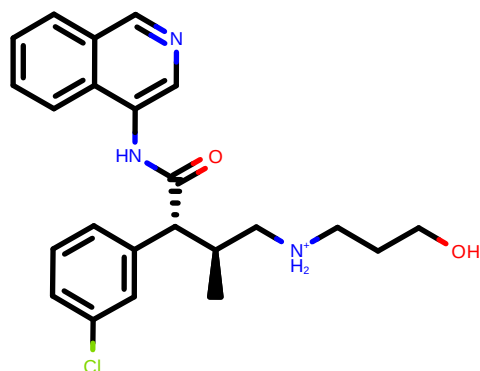
CID:	MIC-UNK-7574fcc6-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(cc(c3)F)F</chem>
RUN:	RUN692
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.06

MAK-UNK-ffc90da7-6_1



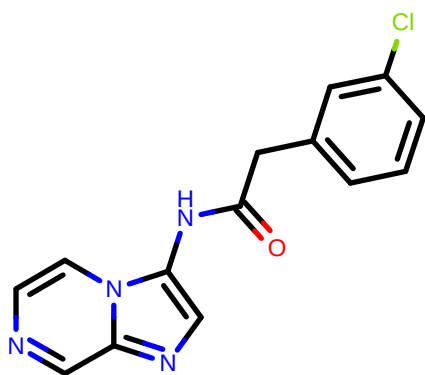
CID:	MAK-UNK-ffc90da7-6_1
SMILES:	<chem>C[C@@H](C[NH2+])CCCO)c1ccc2cnc(c2c1)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN390
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.14

MAK-UNK-ffc90da7-1_4



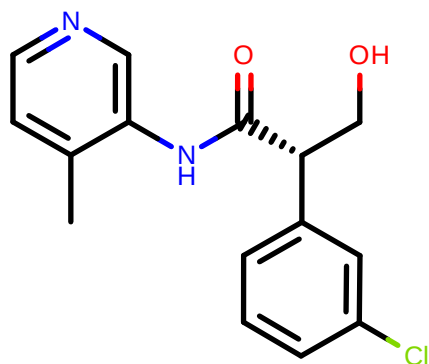
CID:	MAK-UNK-ffc90da7-1_4
SMILES:	<chem>C[C@H](C[NH2+])CCCO)[C@H](c1cccc(c1)Cl)C(=O)Nc2cnc3c2cccc3</chem>
RUN:	RUN398
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.18

EDJ-MED-6e43a462-5_1



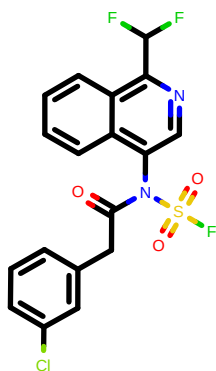
CID:	EDJ-MED-6e43a462-5_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c[nH+]c3n2ccnc3</chem>
RUN:	RUN714
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.12

EDG-MED-0da5ad92-5_2



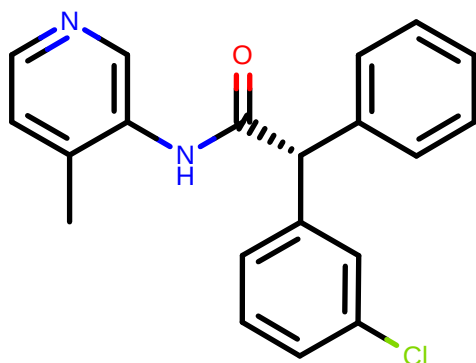
CID:	EDG-MED-0da5ad92-5_2
SMILES:	<chem>Cc1ccncc1NC(=O)[C@H](CO)c2cccc(c2)Cl</chem>
RUN:	RUN81
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.12

JOH-UNI-50ce7ec3-4_1



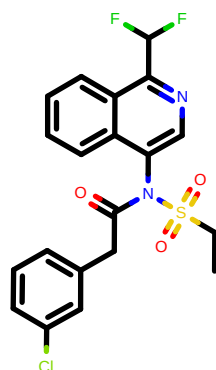
CID:	JOH-UNI-50ce7ec3-4_1
SMILES:	<chem>c1ccc2c(c1)c(cnc2C(F)F)N(C(=O)Cc3cccc(c3)Cl)S(=O)(=O)F</chem>
RUN:	RUN568
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.30

SAM-UNK-2684b532-1_2



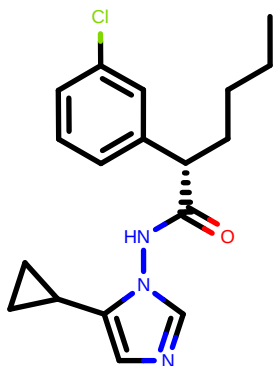
CID:	SAM-UNK-2684b532-1_2
SMILES:	<chem>Cc1ccncc1NC(=O)[C@H](c2ccccc2)c3cccc(c3)Cl</chem>
RUN:	RUN133
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.15

JOH-UNI-50ce7ec3-3_1



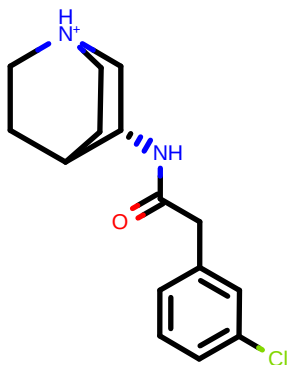
CID:	JOH-UNI-50ce7ec3-3_1
SMILES:	<chem>C=CS(=O)(=O)N(c1cnc(c2c1cccc2)C(F)F)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN570
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.24

JAN-GHE-f4ca5a00-18_1



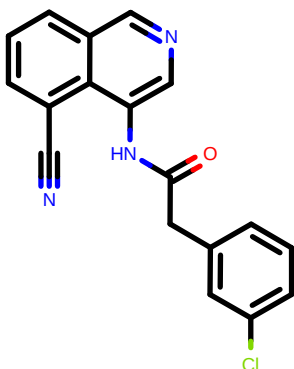
CID:	JAN-GHE-f4ca5a00-18_1
SMILES:	<chem>CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2cncc2C3CC3</chem>
RUN:	RUN185
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.15

MIC-UNK-13557a72-1_2



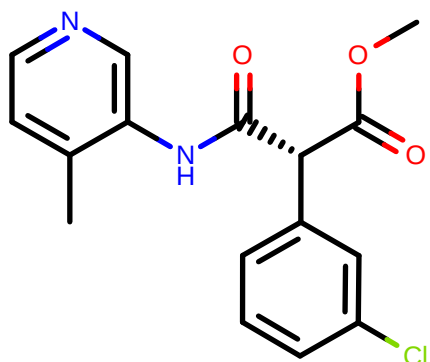
CID:	MIC-UNK-13557a72-1_2
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)N[C@H]2C[NH+]3CCCC2CC3</chem>
RUN:	RUN274
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.13

PET-UNK-6314f867-3_1



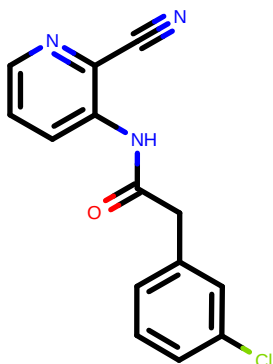
CID:	PET-UNK-6314f867-3_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)C#N</chem>
RUN:	RUN682
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.11

MAT-POS-1e5f28a7-1_1



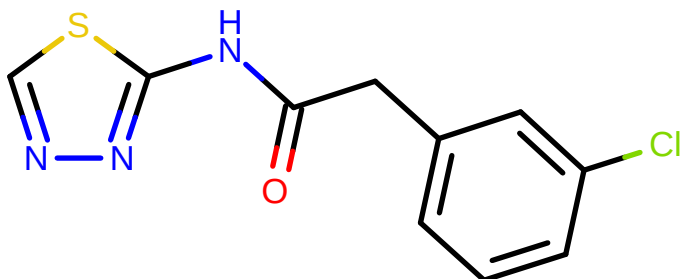
CID:	MAT-POS-1e5f28a7-1_1
SMILES:	<chem>Cc1ccncc1NC(=O)[C@@H](c2cccc(c2)Cl)C(=O)OC</chem>
RUN:	RUN276
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.12

AGN-NEW-c7b24fe3-4_1



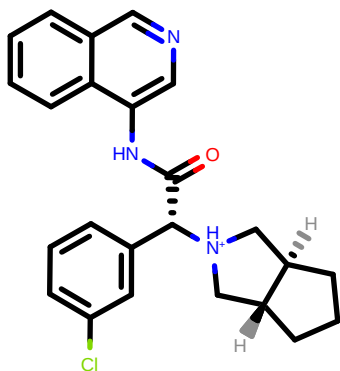
CID:	AGN-NEW-c7b24fe3-4_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cccnc2C#N</chem>
RUN:	RUN13
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.09

JAN-GHE-5a013bed-7_1



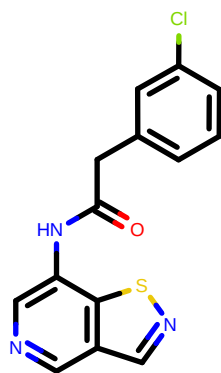
CID:	JAN-GHE-5a013bed-7_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2nncs2</chem>
RUN:	RUN73
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.09

MIC-UNK-5a93dd5f-1_3



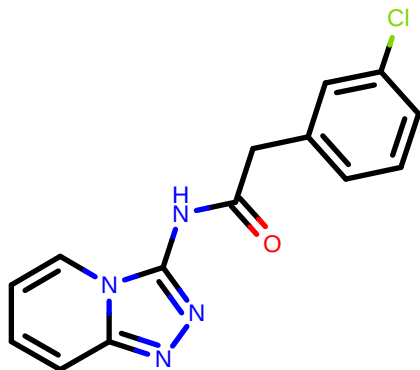
CID:	MIC-UNK-5a93dd5f-1_3
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)[C@@H](c3cccc(c3)Cl)[NH+]4C[C@H](5CCC[C@H]5C4</chem>
RUN:	RUN362
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.21

PET-UNK-b1ef24dc-2_1



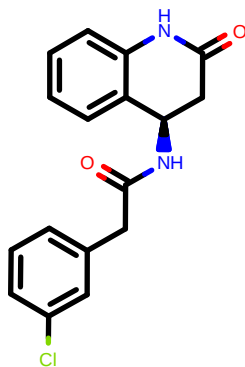
CID:	PET-UNK-b1ef24dc-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2snc3</chem>
RUN:	RUN696
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.07

BEN-DND-02317c5c-8_1



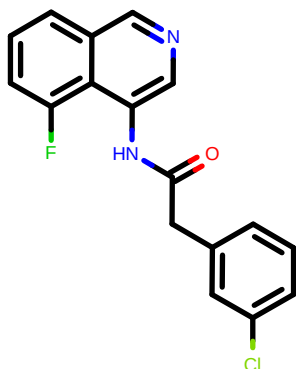
CID:	BEN-DND-02317c5c-8_1
SMILES:	<chem>c1ccn2c(c1)nnc2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN672
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.09

NAU-LAT-a5c7d7cb-14_1



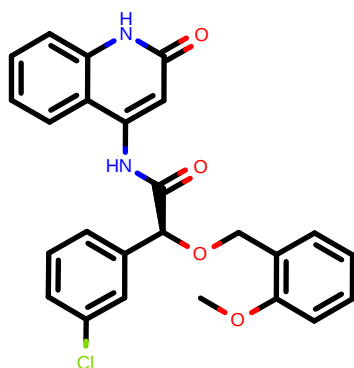
CID:	NAU-LAT-a5c7d7cb-14_1
SMILES:	<chem>c1ccc2c(c1)[C@@H](CC(=O)N2)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN321
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.13

MIC-UNK-50cce87d-1_1



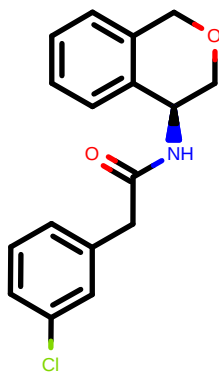
CID:	MIC-UNK-50cce87d-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)F</chem>
RUN:	RUN344
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.07

ADA-UCB-6c2cb422-11_1



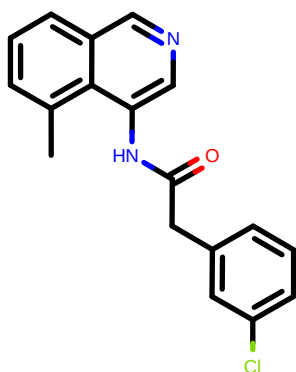
CID:	ADA-UCB-6c2cb422-11_1
SMILES:	<chem>COc1ccccc1CO[C@@H](c2cccc(c2)Cl)C(=O)Nc3cc(=O)[nH]c4c3cccc4</chem>
RUN:	RUN157
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.18

RUB-POS-1325a9ea-20_2



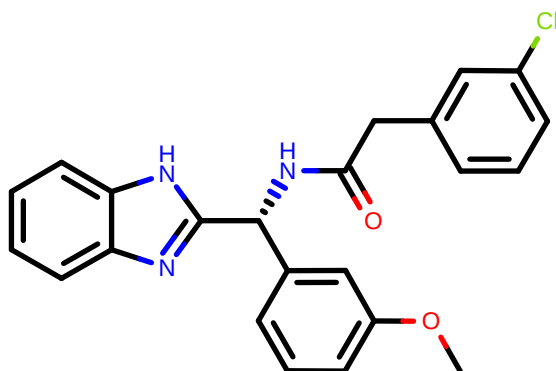
CID:	RUB-POS-1325a9ea-20_2
SMILES:	<chem>c1ccc2c(c1)COC[C@H]2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN651
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.10

MIC-UNK-50cce87d-3_1



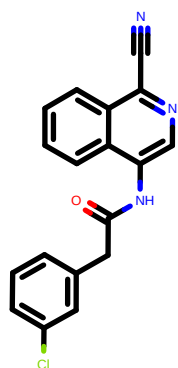
CID:	MIC-UNK-50cce87d-3_1
SMILES:	<chem>Cc1cccc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN339
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.06

ALP-POS-ddb41b15-9_2



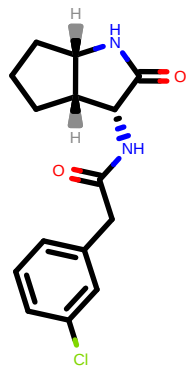
CID:	ALP-POS-ddb41b15-9_2
SMILES:	<chem>COc1cccc(c1)[C@H](c2[nH]c3ccccc3n2)NC(=O)Cc4cccc(c4)Cl</chem>
RUN:	RUN188
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.21

JIN-POS-6dc588a4-24_1



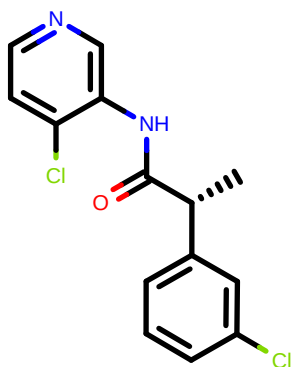
CID:	JIN-POS-6dc588a4-24_1
SMILES:	<chem>c1ccc2c(c1)c(cnc2C#N)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN632
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.08

MIC-UNK-8373f97b-5_1



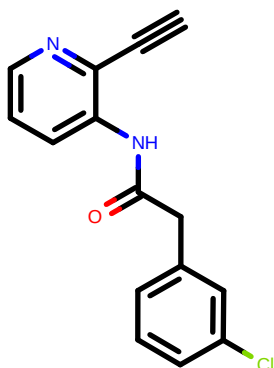
CID:	MIC-UNK-8373f97b-5_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)N[C@@H]2[C@@H]3CCC[C@@H]3NC2=O</chem>
RUN:	RUN239
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.13

SAM-UNK-2684b532-7_2



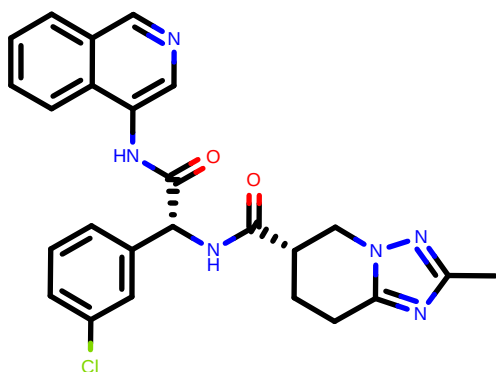
CID:	SAM-UNK-2684b532-7_2
SMILES:	<chem>C[C@H](c1cccc(c1)Cl)C(=O)Nc2cnccc2Cl</chem>
RUN:	RUN134
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.08

AGN-NEW-c7b24fe3-5_1



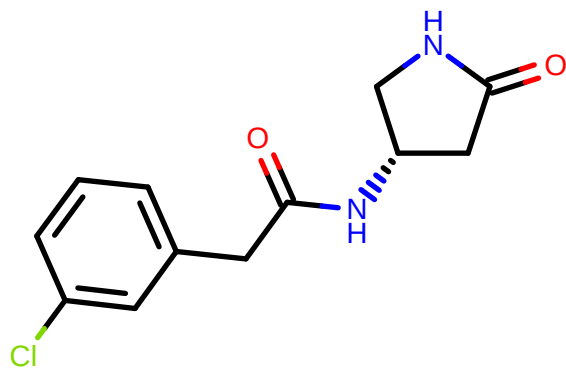
CID:	AGN-NEW-c7b24fe3-5_1
SMILES:	<chem>C#Cc1c(cccn1)NC(=O)Cc2cccc(c2)Cl</chem>
RUN:	RUN10
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.10

MAT-POS-a13804f0-1_4



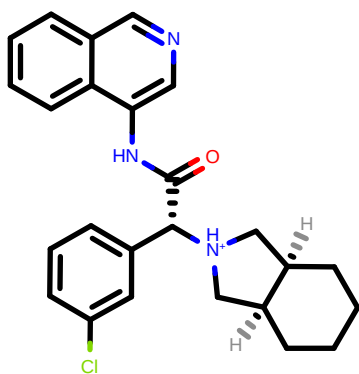
CID:	MAT-POS-a13804f0-1_4
SMILES:	<chem>Cc1nc2n(n1)C[C@H](CC2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4cnccc5c4cccc5</chem>
RUN:	RUN596
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.14

ALP-POS-90e38439-3_2



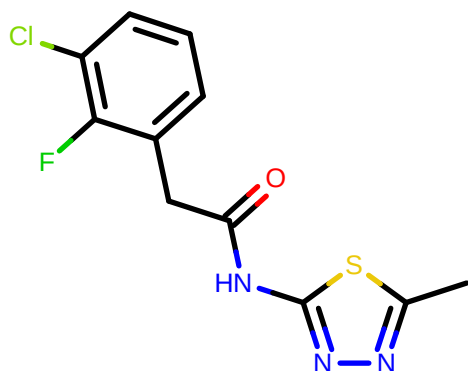
CID:	ALP-POS-90e38439-3_2
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)N[C@H]2CC(=O)NC2</chem>
RUN:	RUN255
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.14

MIC-UNK-5a93dd5f-2_1



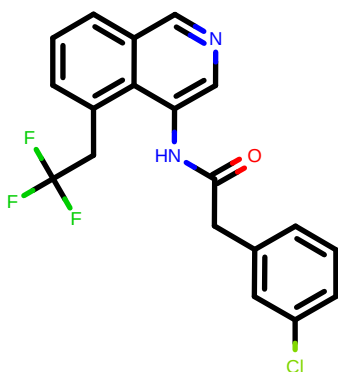
CID:	MIC-UNK-5a93dd5f-2_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3ccccc(c3)Cl)N+4C[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN354
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.20

JAG-UCB-a3ef7265-10_1



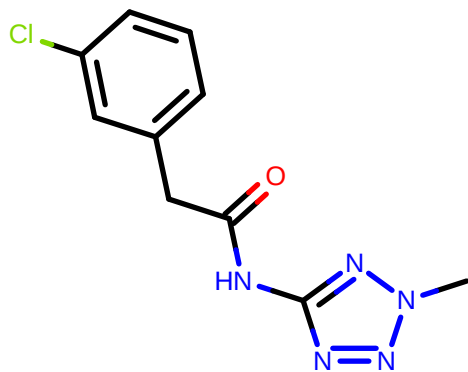
CID:	JAG-UCB-a3ef7265-10_1
SMILES:	<chem>Cc1nnc(s1)NC(=O)Cc2ccccc(c2F)Cl</chem>
RUN:	RUN104
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.10

JOH-UNI-3fc3434e-3_1



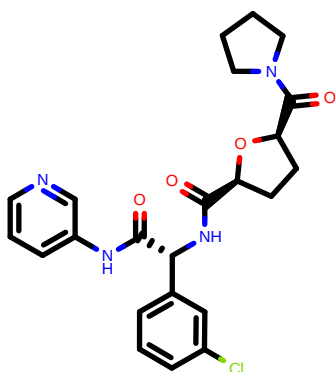
CID:	JOH-UNI-3fc3434e-3_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)CC(F)(F)F</chem>
RUN:	RUN537
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.13

VLA-UNK-411a133b-1_1



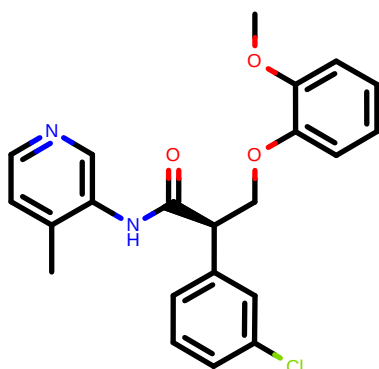
CID:	VLA-UNK-411a133b-1_1
SMILES:	<chem>Cn1nc(nn1)NC(=O)Cc2ccccc(c2)Cl</chem>
RUN:	RUN664
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.09

PET-UNK-ac320b15-3_1



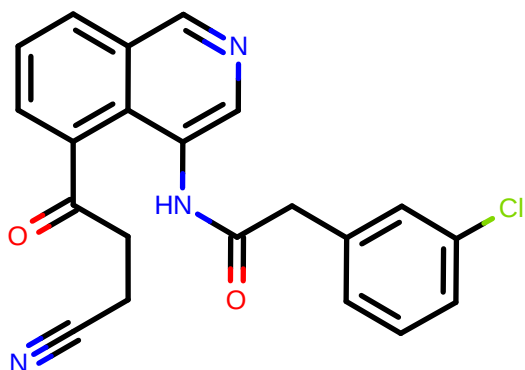
CID:	PET-UNK-ac320b15-3_1
SMILES:	<chem>c1cc(cc(c1)Cl)[C@H](C(=O)Nc2ccnc2)NC(=O)[C@@H](C3CC[C@H](O3)C(=O)N4CCCC4</chem>
RUN:	RUN709
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.17

ADA-UCB-6c2cb422-9_1



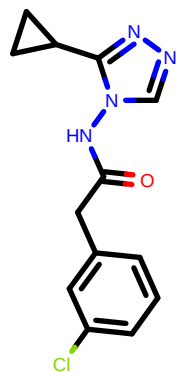
CID:	ADA-UCB-6c2cb422-9_1
SMILES:	<chem>Cc1ccncc1NC(=O)[C@@H](C(=O)c2ccccc2OC)c3ccccc3Cl</chem>
RUN:	RUN177
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.21

JOH-UNI-3fc3434e-2_1



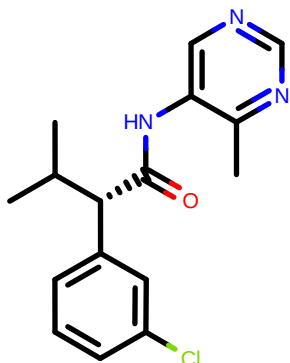
CID:	JOH-UNI-3fc3434e-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)C(=O)/C=C/C#N</chem>
RUN:	RUN538
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.14

JAN-GHE-f4ca5a00-16_1



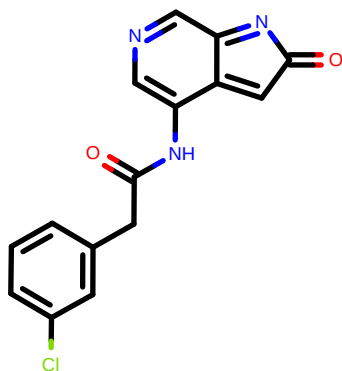
CID:	JAN-GHE-f4ca5a00-16_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nn2cnnc2C3CC3</chem>
RUN:	RUN158
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.11

JAN-GHE-83b26c96-7_2



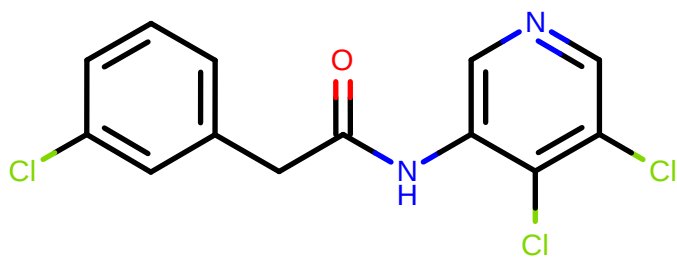
CID:	JAN-GHE-83b26c96-7_2
SMILES:	<chem>Cc1c(cncn1)NC(=O)[C@H](c2cccc(c2)Cl)C(C)C</chem>
RUN:	RUN30
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.11

RUB-POS-1325a9ea-1_1



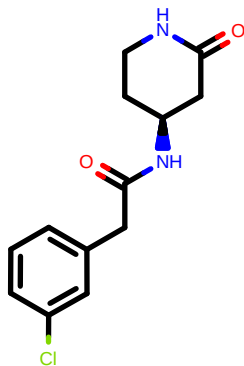
CID:	RUB-POS-1325a9ea-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2CC(=O)N3</chem>
RUN:	RUN623
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.08

JAN-GHE-5a013bed-10_1



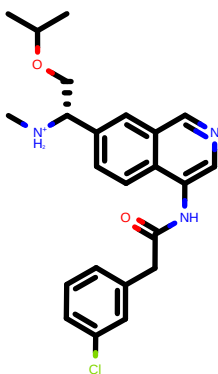
CID:	JAN-GHE-5a013bed-10_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc(c2Cl)Cl</chem>
RUN:	RUN46
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.08

ALP-POS-8b8a49e1-8_2



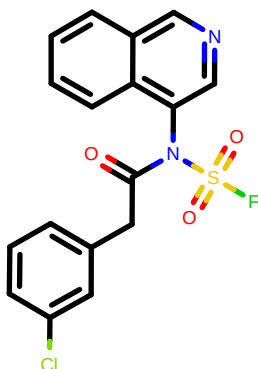
CID:	ALP-POS-8b8a49e1-8_2
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)N[C@H]2CCNC(=O)C2</chem>
RUN:	RUN294
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.16

MAK-UNK-ffc90da7-3_2



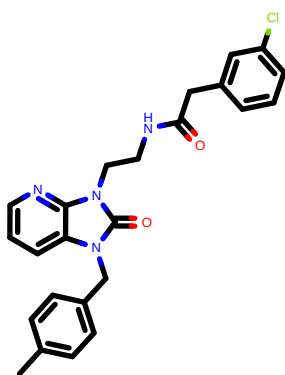
CID:	MAK-UNK-ffc90da7-3_2
SMILES:	<chem>CC(C)OC[C@H](c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl)[NH2+][C]</chem>
RUN:	RUN346
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.11

JOH-UNI-50ce7ec3-2_1



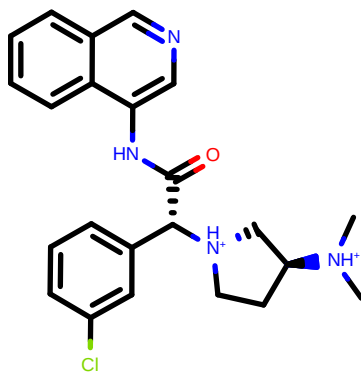
CID:	JOH-UNI-50ce7ec3-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)S(=O)(=O)F</chem>
RUN:	RUN564
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.25

MAR-TRE-f6f5f473-93_1



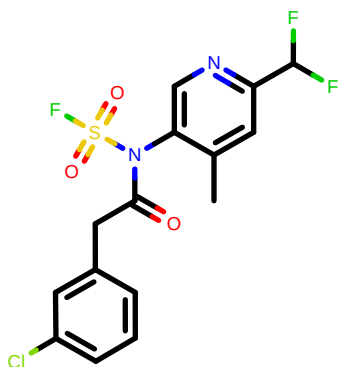
CID:	MAR-TRE-f6f5f473-93_1
SMILES:	<chem>Cc1ccc(cc1)Cn2c3ccncc3n(c2=O)CCNC(=O)Cc4cccc(c4)Cl</chem>
RUN:	RUN175
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.18

MIC-UNK-5a93dd5f-9_6



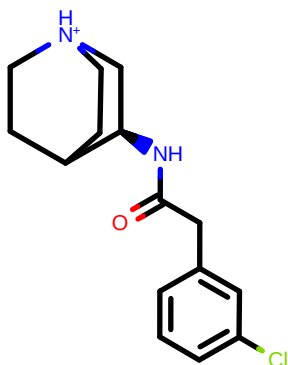
CID:	MIC-UNK-5a93dd5f-9_6
SMILES:	<chem>CN(C)[C@H](H)1CC[N@@H+](C1)[C@H](c2cccc(c2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN427
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.25

JOH-UNI-50ce7ec3-6_1



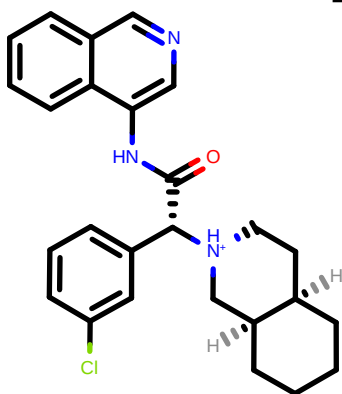
CID:	JOH-UNI-50ce7ec3-6_1
SMILES:	<chem>Cc1cc(ncc1N(C(=O)Cc2cccc(c2)Cl)S(=O)(=O)F)C(F)F</chem>
RUN:	RUN563
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.24

MIC-UNK-13557a72-1_1



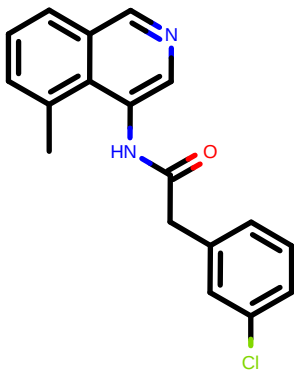
CID:	MIC-UNK-13557a72-1_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)N[C@@H]2C[NH+]3CCCC2CC3</chem>
RUN:	RUN282
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.12

MIC-UNK-5a93dd5f-3_13



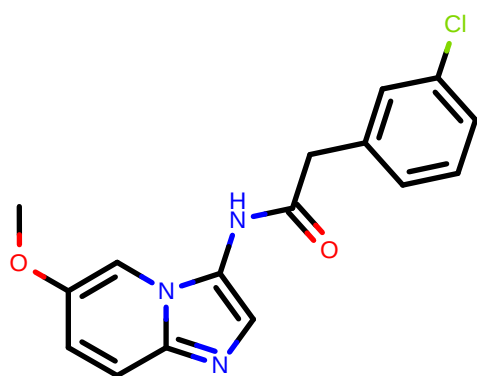
CID:	MIC-UNK-5a93dd5f-3_13
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H](c3cccc(c3)Cl)[N+]([H])4CC[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN397
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.21

RUB-POS-1325a9ea-3_1



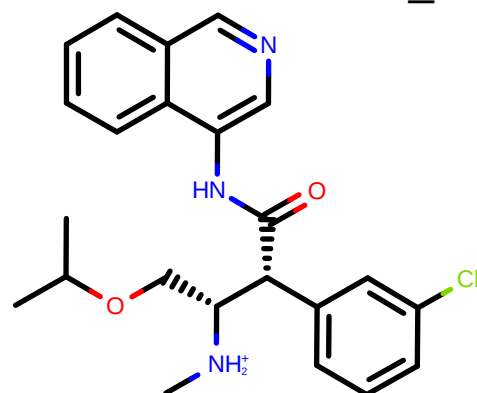
CID:	RUB-POS-1325a9ea-3_1
SMILES:	<chem>Cc1cccc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN626
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.06

EDJ-MED-6e43a462-2_1



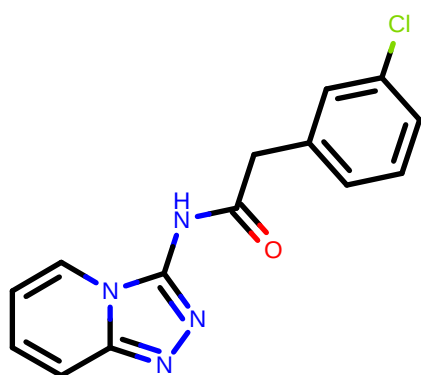
CID:	EDJ-MED-6e43a462-2_1
SMILES:	<chem>COc1ccc2[nH+]cc(n2c1)NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN708
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.16

MAK-UNK-ffc90da7-7_2



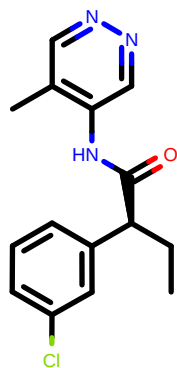
CID:	MAK-UNK-ffc90da7-7_2
SMILES:	<chem>CC(C)OC[C@H]([C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3)[NH2+]C</chem>
RUN:	RUN364
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.44

PET-UNK-e44ffd04-1_1



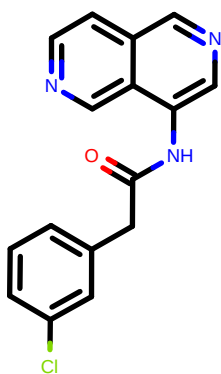
CID:	PET-UNK-e44ffd04-1_1
SMILES:	<chem>c1ccn2c(c1)nnc2NC(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN313
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.09

JAN-GHE-83b26c96-1_1



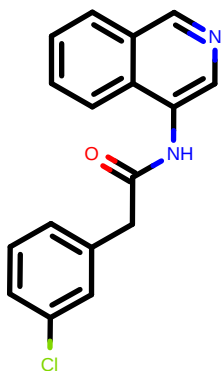
CID:	JAN-GHE-83b26c96-1_1
SMILES:	<chem>CC[C@@H]([C@H](c1cccc(c1)Cl)C(=O)Nc2cnnc2C</chem>
RUN:	RUN18
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.09

MAT-POS-f7918075-5_1



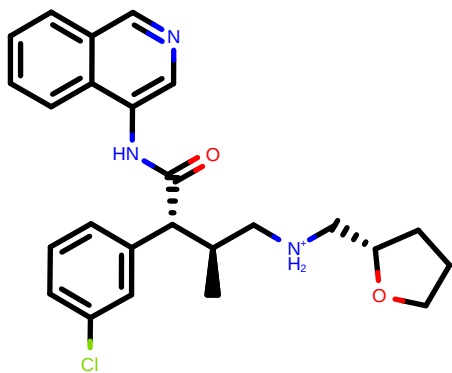
CID:	MAT-POS-f7918075-5_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cncc3</chem>
RUN:	RUN271
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.08

ADA-UCB-6c2cb422-1_1



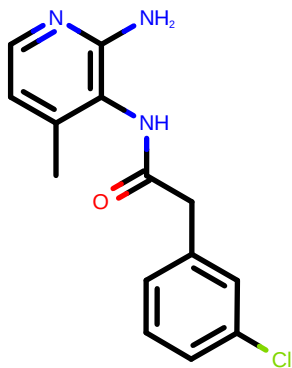
CID:	ADA-UCB-6c2cb422-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN154
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.02

MAK-UNK-ffc90da7-4_6



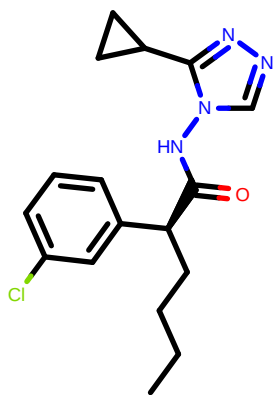
CID:	MAK-UNK-ffc90da7-4_6
SMILES:	<chem>C[C@H](C)[NH2+][C]([C@@H]1CCCCO1)[C@H](c2ccccc2)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN392
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.24

EDG-MED-0da5ad92-18_1



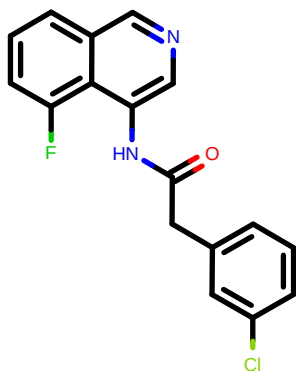
CID:	EDG-MED-0da5ad92-18_1
SMILES:	<chem>Cc1ccnc(c1NC(=O)Cc2ccccc(c2)Cl)N</chem>
RUN:	RUN83
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.09

JAN-GHE-f4ca5a00-19_1



CID:	JAN-GHE-f4ca5a00-19_1
SMILES:	<chem>CCCC[C@@H](c1cccc(c1)Cl)C(=O)Nn2cnnc2C3CC3</chem>
RUN:	RUN205
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.16

RUB-POS-1325a9ea-2_1



CID:	RUB-POS-1325a9ea-2_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)F</chem>
RUN:	RUN636
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.07