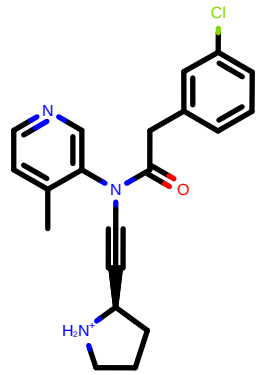
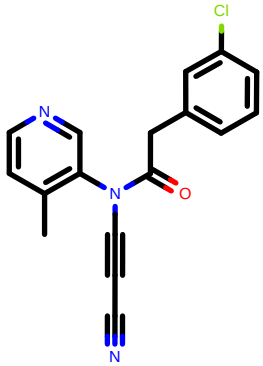
DAR-DIA-076fb6ea-10_2



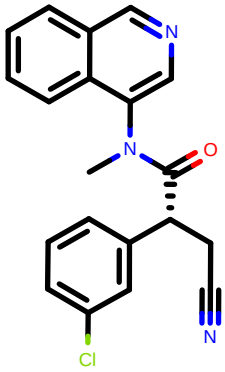
CID:	DAR-DIA-076fb6ea-10_2
SMILES:	Cc1ccncc1N(C#C[C@H]2CCC[NH2+]2)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1214
DDG (kcal/mol):	-3.87
dDDG (kcal/mol):	0.15

DAR-DIA-076fb6ea-6_1



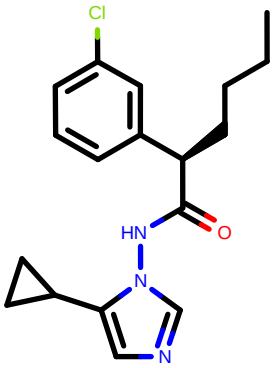
CID:	DAR-DIA-076fb6ea-6_1
SMILES:	Cc1ccncc1N(C#CC#N)C(=O)Cc2cccc(c2)Cl
RUN:	RUN1200
DDG (kcal/mol):	-3.84
dDDG (kcal/mol):	0.09

JOH-UNI-3fc3434e-7_2



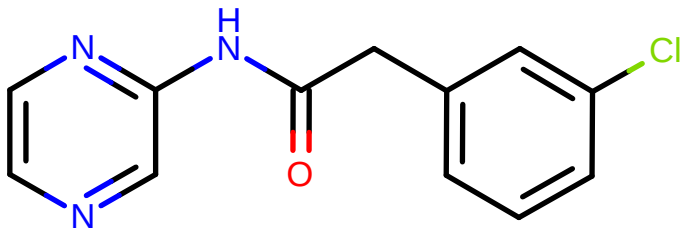
CID:	JOH-UNI-3fc3434e-7_2
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@H](CC#N)c3cccc(c3)Cl
RUN:	RUN1279
DDG (kcal/mol):	-3.54
dDDG (kcal/mol):	0.15

JAN-GHE-f4ca5a00-18_2



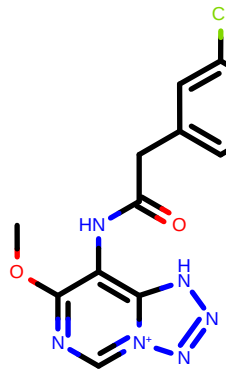
CID:	JAN-GHE-f4ca5a00-18_2
SMILES:	CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2cncc2C3CC3
RUN:	RUN931
DDG (kcal/mol):	-3.45
dDDG (kcal/mol):	0.14

JAN-GHE-5a013bed-8_1



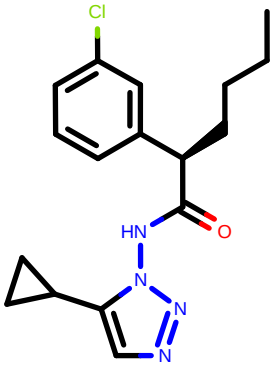
CID:	JAN-GHE-5a013bed-8_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cnccn2
RUN:	RUN785
DDG (kcal/mol):	-3.29
dDDG (kcal/mol):	0.11

EDJ-MED-97c1bf5c-2_1



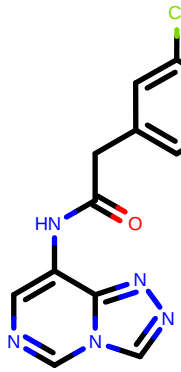
CID:	EDJ-MED-97c1bf5c-2_1
SMILES:	COc1c(c2nnnn2cn1)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1078
DDG (kcal/mol):	-3.22
dDDG (kcal/mol):	0.10

JAN-GHE-f4ca5a00-20_2



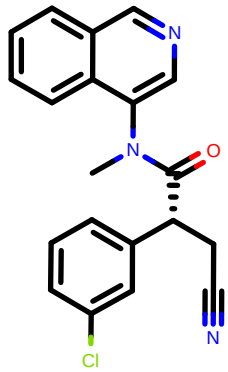
CID:	JAN-GHE-f4ca5a00-20_2
SMILES:	CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2c(cnn2)C3CC3
RUN:	RUN932
DDG (kcal/mol):	-3.21
dDDG (kcal/mol):	0.10

EDJ-MED-076d6e64-1_1



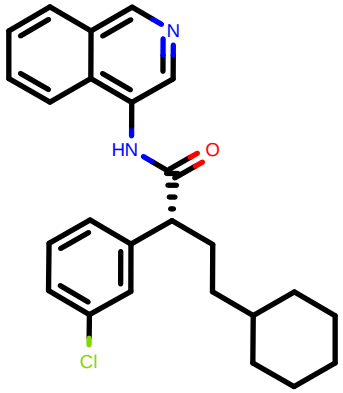
CID:	EDJ-MED-076d6e64-1_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncn3c2nnc3
RUN:	RUN1426
DDG (kcal/mol):	-3.10
dDDG (kcal/mol):	0.08

JOH-UNI-ee5ed7c8-7_2



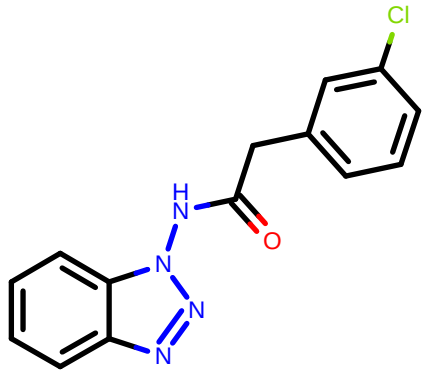
CID:	JOH-UNI-ee5ed7c8-7_2
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@H](CC#N)c3cccc(c3)Cl
RUN:	RUN1271
DDG (kcal/mol):	-3.00
dDDG (kcal/mol):	0.15

ALP-POS-3b848b35-4_2



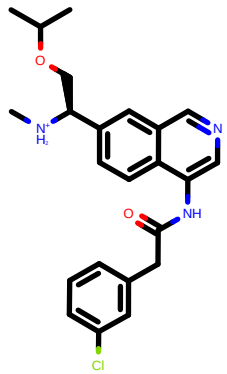
CID:	ALP-POS-3b848b35-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN934
DDG (kcal/mol):	-2.93
dDDG (kcal/mol):	0.15

MAT-POS-bfb445d4-2_1



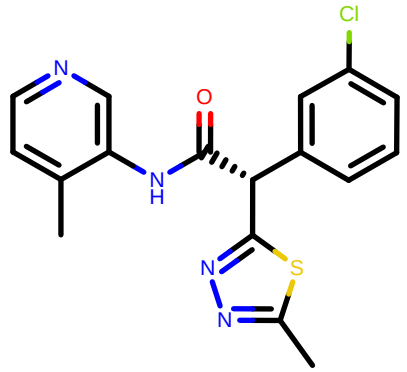
CID:	MAT-POS-bfb445d4-2_1
SMILES:	c1ccc2c(c1)nnn2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1016
DDG (kcal/mol):	-2.90
dDDG (kcal/mol):	0.08

MAK-UNK-ffc90da7-3_1



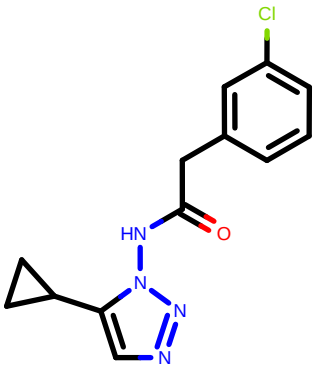
CID:	MAK-UNK-ffc90da7-3_1
SMILES:	CC(C)OC[C@@H](c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl)[NH2+]C
RUN:	RUN1082
DDG (kcal/mol):	-2.84
dDDG (kcal/mol):	0.09

SAM-UNK-2684b532-3_2



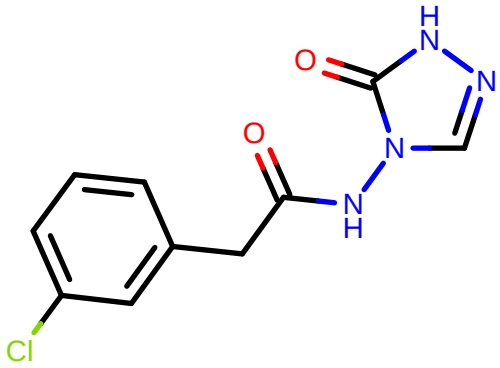
CID:	SAM-UNK-2684b532-3_2
SMILES:	Cc1ccncc1NC(=O)[C@H](c2cccc(c2)Cl)c3nnc(s3)C
RUN:	RUN876
DDG (kcal/mol):	-2.60
dDDG (kcal/mol):	0.10

JAN-GHE-f4ca5a00-17_1



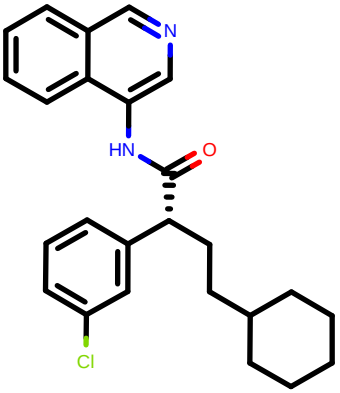
CID:	JAN-GHE-f4ca5a00-17_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nn2c(cnn2)C3CC3
RUN:	RUN894
DDG (kcal/mol):	-2.58
dDDG (kcal/mol):	0.08

JAN-GHE-5a013bed-4_1



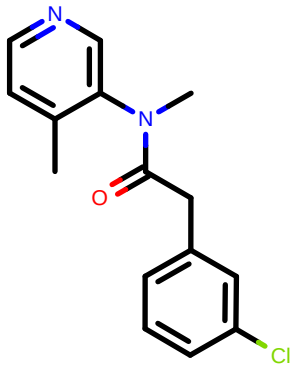
CID:	JAN-GHE-5a013bed-4_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nn2cn[nH]c2=O
RUN:	RUN803
DDG (kcal/mol):	-2.53
dDDG (kcal/mol):	0.11

MIC-UNK-c66144cb-3_2



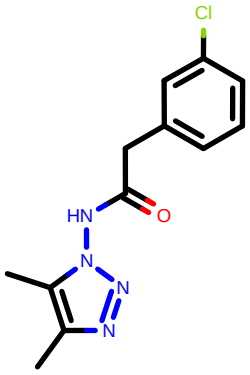
CID:	MIC-UNK-c66144cb-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN952
DDG (kcal/mol):	-2.49
dDDG (kcal/mol):	0.16

JAN-GHE-83b26c96-15_1



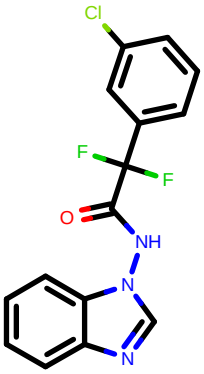
CID:	JAN-GHE-83b26c96-15_1
SMILES:	Cc1ccncc1N(C)C(=O)Cc2cccc(c2)Cl
RUN:	RUN768
DDG (kcal/mol):	-2.48
dDDG (kcal/mol):	0.09

JAN-GHE-5a013bed-1_1



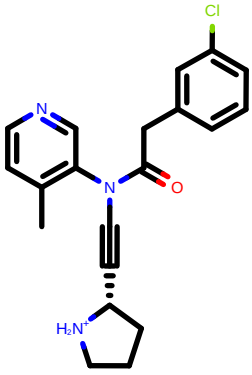
CID:	JAN-GHE-5a013bed-1_1
SMILES:	Cc1c(n(nn1)NC(=O)Cc2cccc(c2)Cl)C
RUN:	RUN791
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.08

BAR-COM-0f94fc3d-24_1



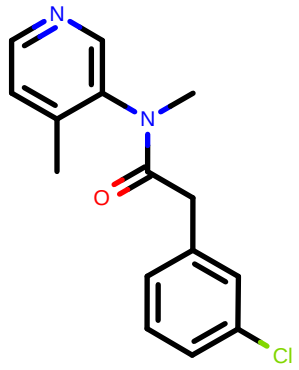
CID:	BAR-COM-0f94fc3d-24_1
SMILES:	c1ccc2c(c1)ncn2NC(=O)C(c3cccc(c3)Cl)(F)F
RUN:	RUN844
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.10

DAR-DIA-076fb6ea-10_1



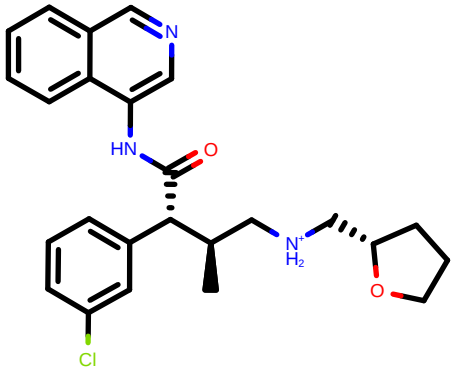
CID:	DAR-DIA-076fb6ea-10_1
SMILES:	Cc1ccncc1N(C#C[C@@H]2CCC[NH2+]2)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1208
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.12

EDG-MED-0da5ad92-1_1



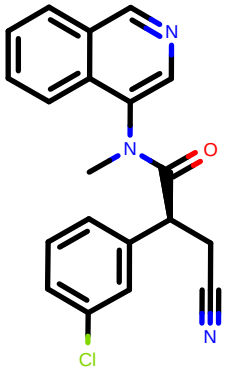
CID:	EDG-MED-0da5ad92-1_1
SMILES:	Cc1ccncc1N(C)C(=O)Cc2cccc(c2)Cl
RUN:	RUN799
DDG (kcal/mol):	-2.15
dDDG (kcal/mol):	0.09

MAK-UNK-ffc90da7-4_6



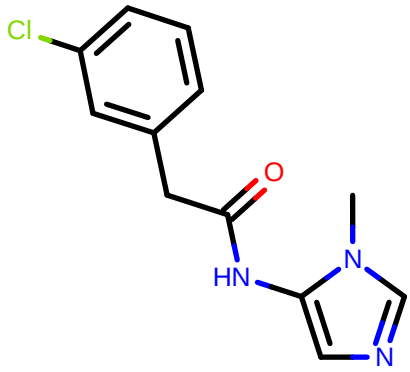
CID:	MAK-UNK-ffc90da7-4_6
SMILES:	C[C@H](C[NH2+]C[C@@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1127
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.25

JOH-UNI-3fc3434e-7_1



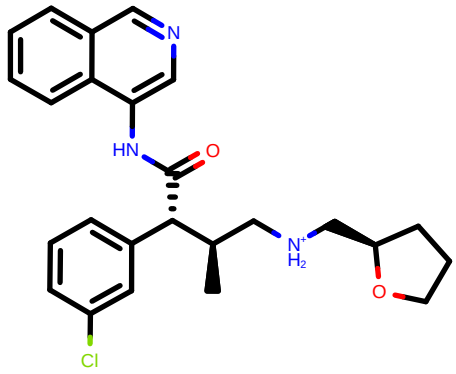
CID:	JOH-UNI-3fc3434e-7_1
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@@H](CC#N)c3cccc(c3)Cl
RUN:	RUN1276
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.13

PET-UNK-8df914d1-4_1



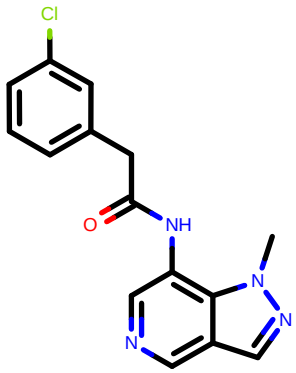
CID:	PET-UNK-8df914d1-4_1
SMILES:	Cn1cncc1NC(=O)Cc2cccc(c2)Cl
RUN:	RUN956
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.09

MAK-UNK-c749d764-22_8



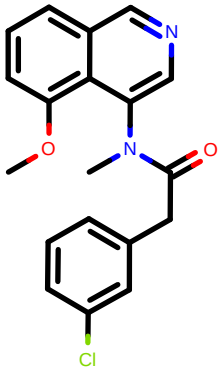
CID:	MAK-UNK-c749d764-22_8
SMILES:	C[C@H](C[NH2+]C[C@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1213
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.31

RUB-POS-1325a9ea-14_1



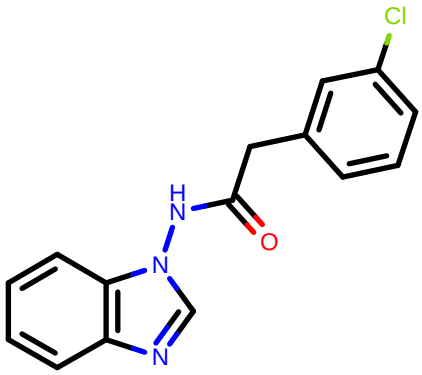
CID:	RUB-POS-1325a9ea-14_1
SMILES:	Cn1c2c(cncc2NC(=O)Cc3cccc(c3)Cl)cn1
RUN:	RUN1382
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.09

MIC-UNK-67d4a29a-4_1



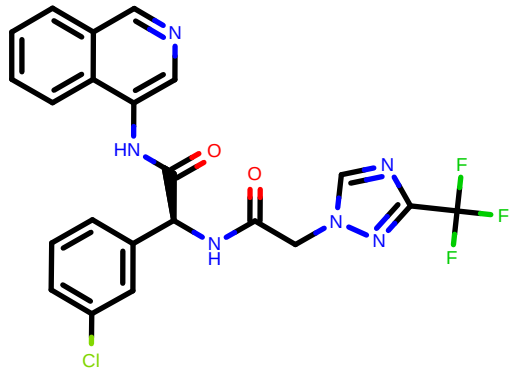
CID:	MIC-UNK-67d4a29a-4_1
SMILES:	CN(c1cncc2c1c(ccc2)OC)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1185
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.14

JAN-GHE-5a013bed-2_1



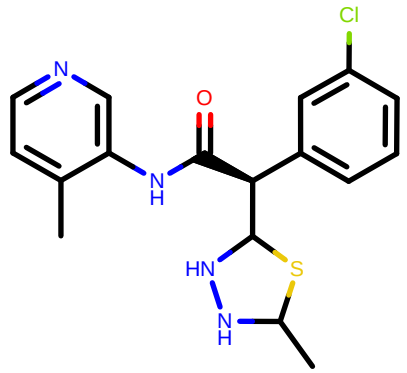
CID:	JAN-GHE-5a013bed-2_1
SMILES:	c1ccc2c(c1)ncn2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN797
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.11

EDJ-MED-ee07cf00-10_2



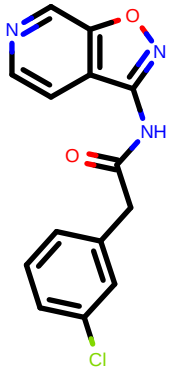
CID:	EDJ-MED-ee07cf00-10_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)Cn4cnc(n4)C(F)(F)F
RUN:	RUN1322
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.18

TRY-UNI-9f475305-3_1



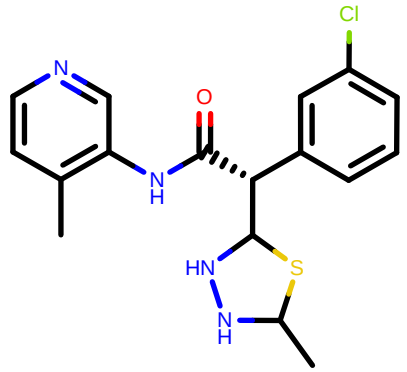
CID:	TRY-UNI-9f475305-3_1
SMILES:	Cc1ccncc1NC(=O)[C@@H](c2cccc(c2)Cl)c3nnc(s3)C
RUN:	RUN811
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.13

JIN-POS-6dc588a4-16_1



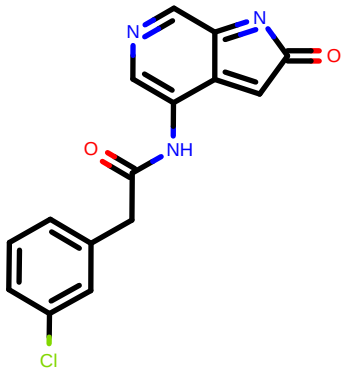
CID:	JIN-POS-6dc588a4-16_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2c3ccncc3on2
RUN:	RUN1351
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.08

TRY-UNI-9f475305-3_2



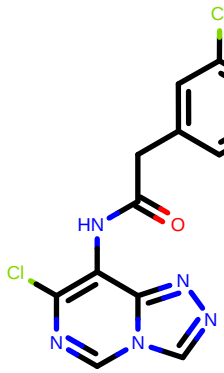
CID:	TRY-UNI-9f475305-3_2
SMILES:	Cc1ccncc1NC(=O)[C@H](c2cccc(c2)Cl)c3nnc(s3)C
RUN:	RUN804
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.11

MAT-POS-f7918075-7_1



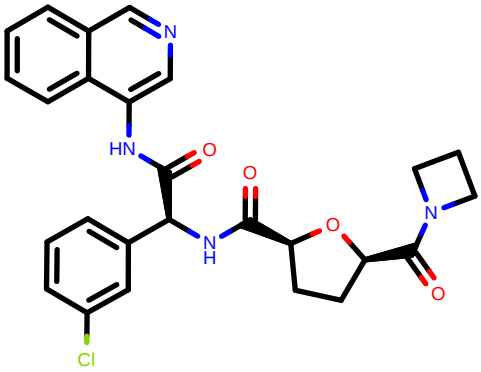
CID:	MAT-POS-f7918075-7_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2CC(=O)N3
RUN:	RUN996
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.08

EDJ-MED-c8e7a002-7_1



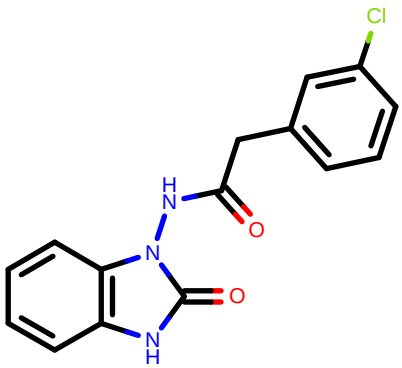
CID:	EDJ-MED-c8e7a002-7_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2c3nncn3cnc2Cl
RUN:	RUN1045
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.09

PET-UNK-1320d94d-6_1



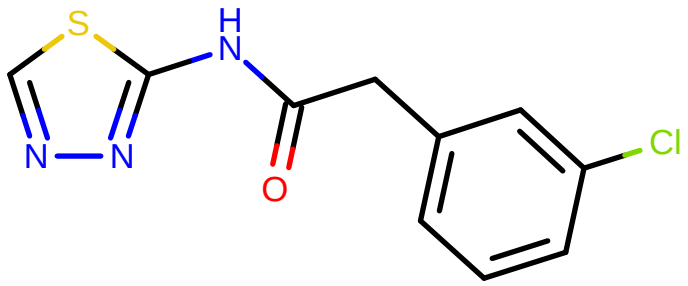
CID:	PET-UNK-1320d94d-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@@H]4CC[C@@H](O4)C(=O)N5CCC5
RUN:	RUN1436
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.20

VLA-UNK-dc1d9354-1_1



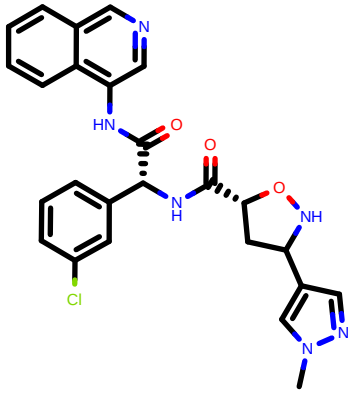
CID:	VLA-UNK-dc1d9354-1_1
SMILES:	c1ccc2c(c1)[nH]c(=O)n2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1398
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.12

JAN-GHE-5a013bed-7_1



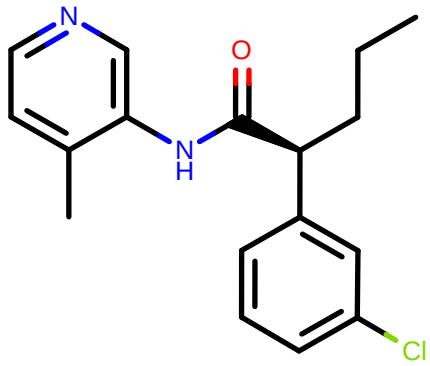
CID:	JAN-GHE-5a013bed-7_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2nncs2
RUN:	RUN808
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.09

EDJ-MED-ee07cf00-6_4



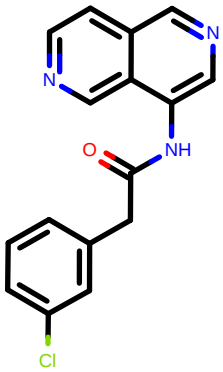
CID:	EDJ-MED-ee07cf00-6_4
SMILES:	Cn1cc(cn1)C2=NO[C@H](C2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1320
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.14

JAN-GHE-83b26c96-8_1



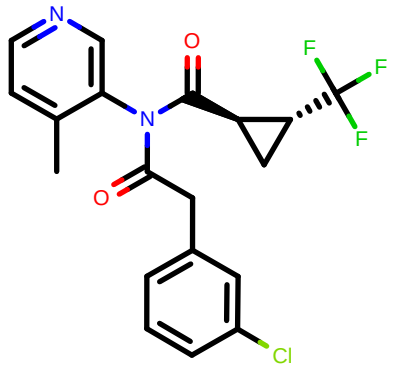
CID:	JAN-GHE-83b26c96-8_1
SMILES:	CCC[C@@H](c1cccc(c1)Cl)C(=O)Nc2cnccc2C
RUN:	RUN759
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.09

MAT-POS-f7918075-5_1



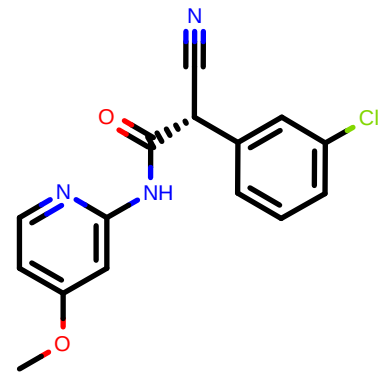
CID:	MAT-POS-f7918075-5_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cncc3
RUN:	RUN1006
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.07

JOH-UNI-a38a7bdd-7_3



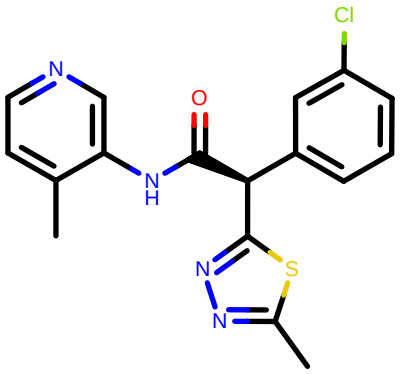
CID:	JOH-UNI-a38a7bdd-7_3
SMILES:	Cc1ccncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)[C@@H]3C[C@H]3C(F)(F)F
RUN:	RUN1232
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.13

RIT-UNK-fa3975ff-1_2



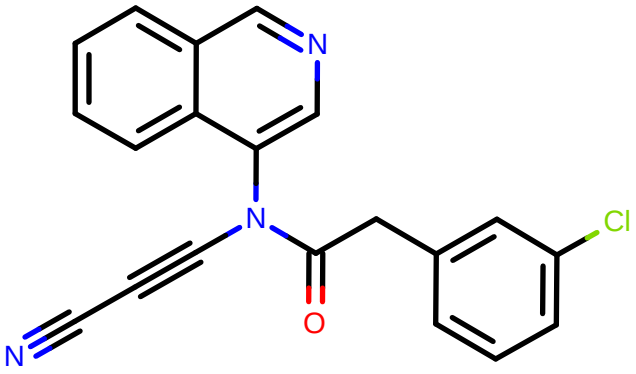
CID:	RIT-UNK-fa3975ff-1_2
SMILES:	COc1ccnc(c1)NC(=O)[C@H](C#N)c2cccc(c2)Cl
RUN:	RUN1051
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.11

SAM-UNK-2684b532-3_1



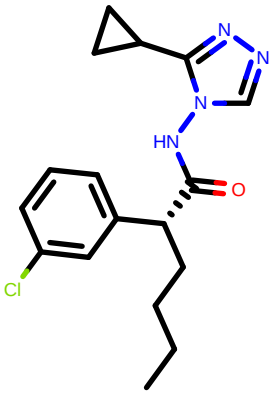
CID:	SAM-UNK-2684b532-3_1
SMILES:	Cc1ccncc1NC(=O)[C@@H](c2cccc(c2)Cl)c3nnc(s3)C
RUN:	RUN883
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.11

DAR-DIA-076fb6ea-5_1



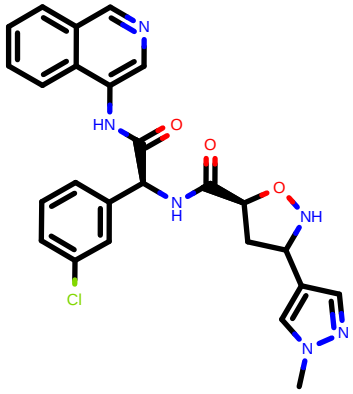
CID:	DAR-DIA-076fb6ea-5_1
SMILES:	c1ccc2c(c1)cncc2N(C#CC#N)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1201
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.13

JAN-GHE-f4ca5a00-19_2



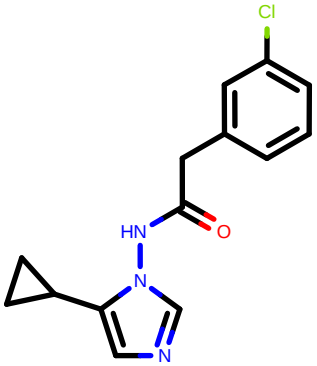
CID:	JAN-GHE-f4ca5a00-19_2
SMILES:	CCCC[C@H](c1cccc(c1)Cl)C(=O)Nn2cnnc2C3CC3
RUN:	RUN936
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.13

EDJ-MED-ee07cf00-6_1



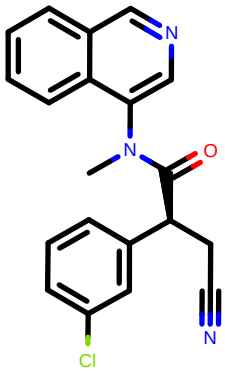
CID:	EDJ-MED-ee07cf00-6_1
SMILES:	Cn1cc(cn1)C2=NO[C@@H](C2)C(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1319
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.16

JAN-GHE-f4ca5a00-14_1



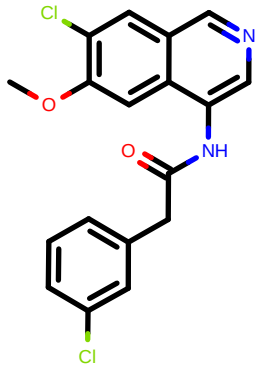
CID:	JAN-GHE-f4ca5a00-14_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nn2cncc2C3CC3
RUN:	RUN897
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.11

JOH-UNI-ee5ed7c8-7_1



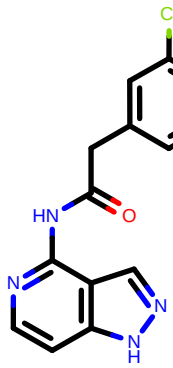
CID:	JOH-UNI-ee5ed7c8-7_1
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@@H](CC#N)c3cccc(c3)Cl
RUN:	RUN1270
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.11

PET-UNK-b38839dc-2_1



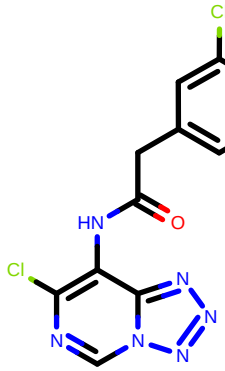
CID:	PET-UNK-b38839dc-2_1
SMILES:	COc1cc2c(cc1Cl)cncc2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1458
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.10

MAT-POS-199e2e7c-2_1



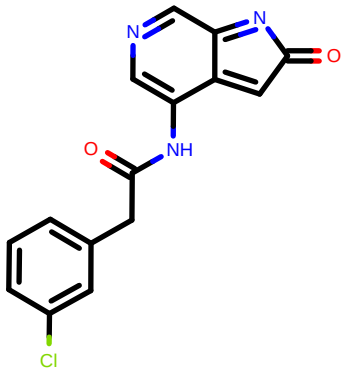
CID:	MAT-POS-199e2e7c-2_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2c3cn[nH]c3ccn2
RUN:	RUN1050
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.10

EDJ-MED-c8e7a002-8_1



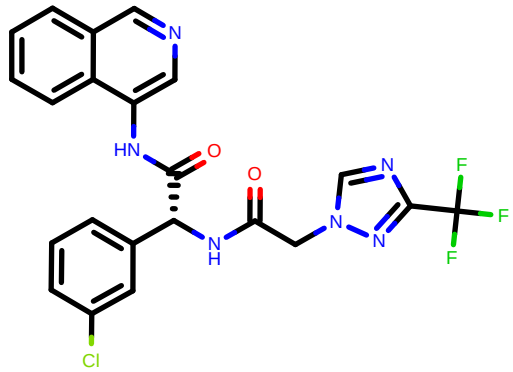
CID:	EDJ-MED-c8e7a002-8_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2c3nnnn3cnc2Cl
RUN:	RUN1042
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.10

RUB-POS-1325a9ea-1_1



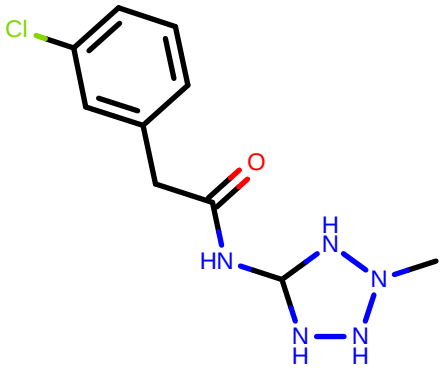
CID:	RUB-POS-1325a9ea-1_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2CC(=O)N3
RUN:	RUN1358
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.09

EDJ-MED-ee07cf00-10_1



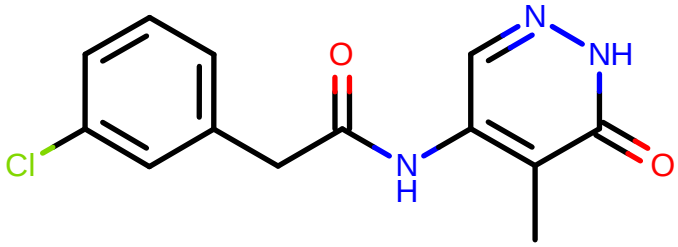
CID:	EDJ-MED-ee07cf00-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cn4cnc(n4)C(F)(F)F
RUN:	RUN1316
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.16

VLA-UNK-411a133b-1_1



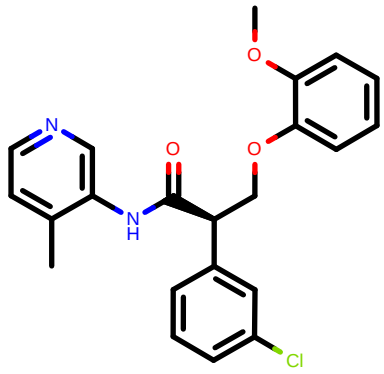
CID:	VLA-UNK-411a133b-1_1
SMILES:	Cn1nc(nn1)NC(=O)Cc2cccc(c2)Cl
RUN:	RUN1399
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.09

MIC-UNK-d935700b-1_1



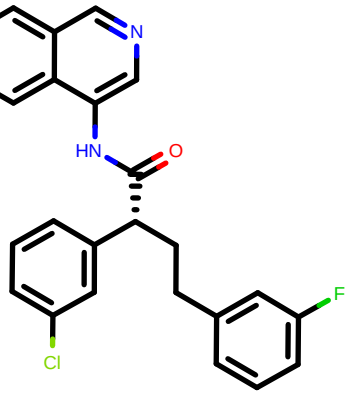
CID:	MIC-UNK-d935700b-1_1
SMILES:	Cc1c(cn[nH]c1=O)NC(=O)Cc2cccc(c2)Cl
RUN:	RUN1075
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.10

ADA-UCB-6c2cb422-9_1



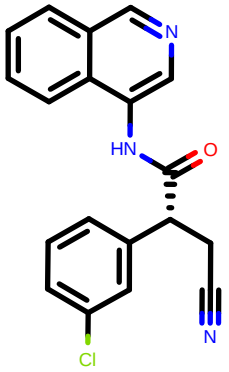
CID:	ADA-UCB-6c2cb422-9_1
SMILES:	Cc1ccncc1NC(=O)[C@@H](COc2ccccc2OC)c3cccc(c3)Cl
RUN:	RUN912
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.19

MIC-UNK-c66144cb-1_2



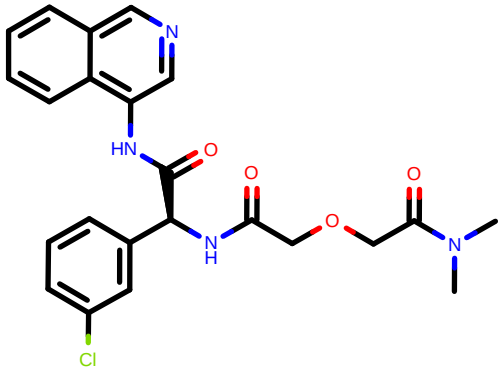
CID:	MIC-UNK-c66144cb-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CCc3cccc(c3)F)c4cccc(c4)Cl
RUN:	RUN983
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.12

JOH-UNI-3fc3434e-6_2



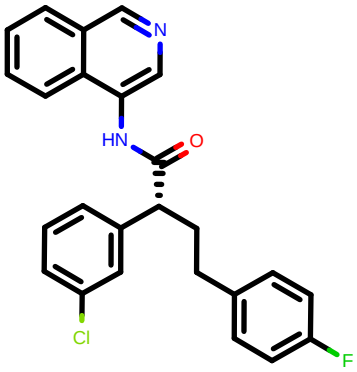
CID:	JOH-UNI-3fc3434e-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CC#N)c3cccc(c3)Cl
RUN:	RUN1284
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.09

EDJ-MED-cf4b0d25-5_1



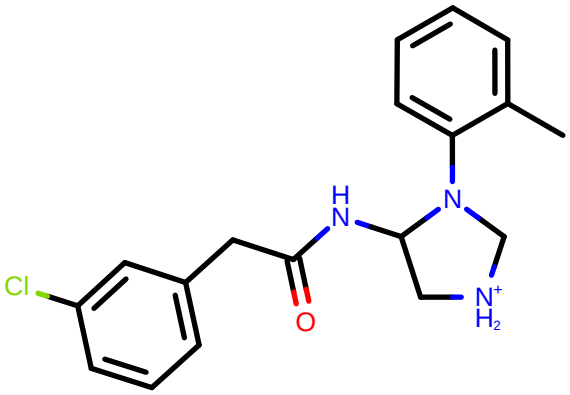
CID:	EDJ-MED-cf4b0d25-5_1
SMILES:	CN(C)C(=O)COCC(=O)N[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN1453
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.15

MIC-UNK-c66144cb-2_2



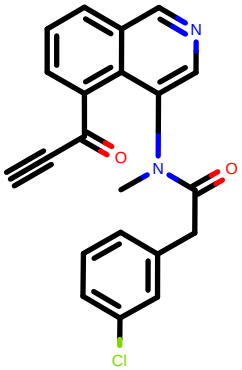
CID:	MIC-UNK-c66144cb-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CCc3ccc(cc3)F)c4cccc(c4)Cl
RUN:	RUN979
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.12

BEN-DND-1e24cf73-2_1



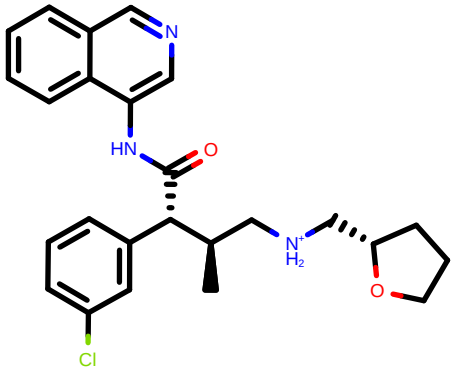
CID:	BEN-DND-1e24cf73-2_1
SMILES:	Cc1ccccc1n2cncc2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1466
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.13

JOH-UNI-3fc3434e-5_1



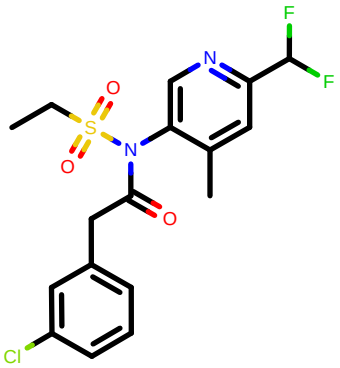
CID:	JOH-UNI-3fc3434e-5_1
SMILES:	CN(c1cncc2c1c(ccc2)C(=O)C#C)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1265
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.14

MAK-UNK-c749d764-22_6



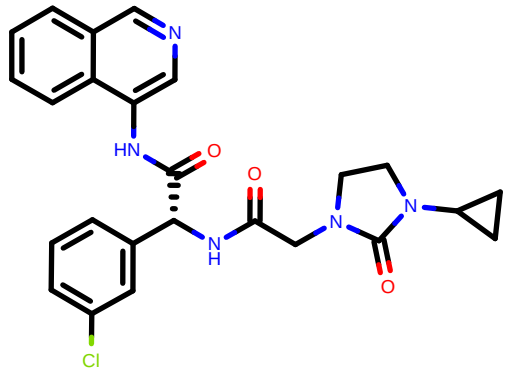
CID:	MAK-UNK-c749d764-22_6
SMILES:	C[C@H](C[NH2+]C[C@@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1187
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.26

JOH-UNI-50ce7ec3-5_1



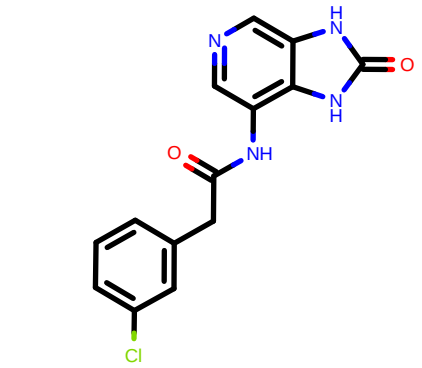
CID:	JOH-UNI-50ce7ec3-5_1
SMILES:	Cc1cc(ncc1N(C(=O)Cc2cccc(c2)Cl)S(=O)(=O)C=C)C(F)F
RUN:	RUN1309
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.16

EDJ-MED-ee07cf00-18_1



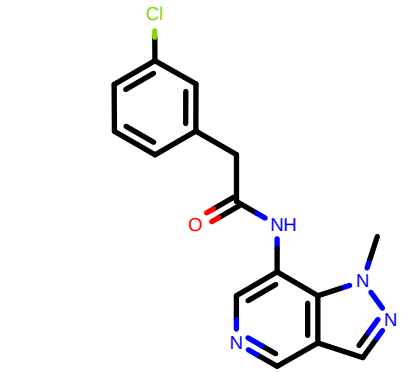
CID:	EDJ-MED-ee07cf00-18_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)CN4CCN(C4=O)C5CC5
RUN:	RUN1323
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.20

MAT-POS-f7918075-4_1



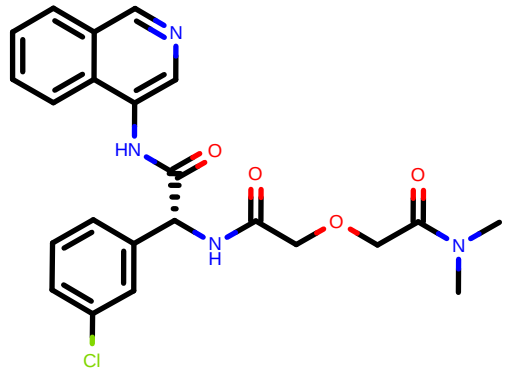
CID:	MAT-POS-f7918075-4_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2[nH]c(=O)[nH]3
RUN:	RUN998
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.08

PET-UNK-e274cad4-1_1



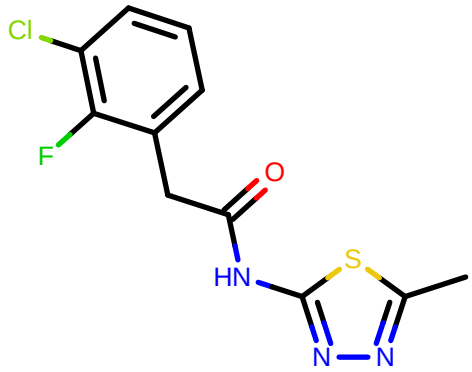
CID:	PET-UNK-e274cad4-1_1
SMILES:	Cn1c2c(cncc2NC(=O)Cc3cccc(c3)Cl)cn1
RUN:	RUN1424
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.08

EDJ-MED-cf4b0d25-5_2



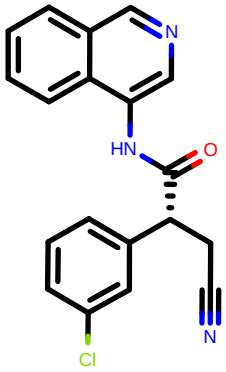
CID:	EDJ-MED-cf4b0d25-5_2
SMILES:	CN(C)C(=O)COCC(=O)N[C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN1413
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.14

JAG-UCB-a3ef7265-10_1



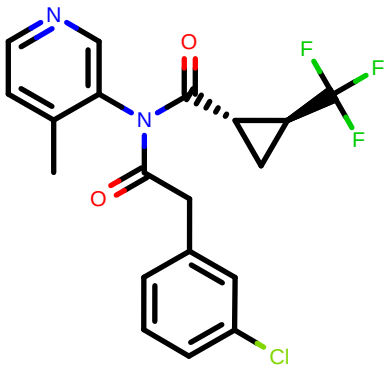
CID:	JAG-UCB-a3ef7265-10_1
SMILES:	Cc1nnc(s1)NC(=O)Cc2cccc(c2F)Cl
RUN:	RUN839
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.10

JOH-UNI-ee5ed7c8-6_2



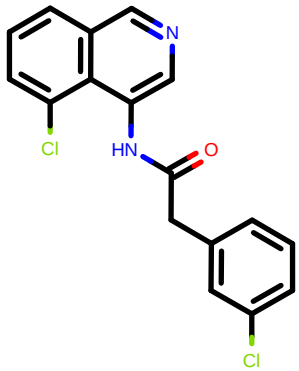
CID:	JOH-UNI-ee5ed7c8-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CC#N)c3cccc(c3)Cl
RUN:	RUN1267
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.10

JOH-UNI-a38a7bdd-7_2



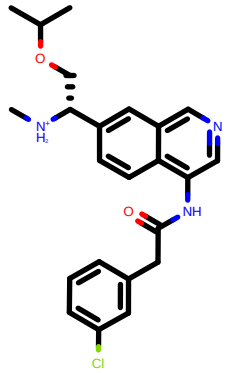
CID:	JOH-UNI-a38a7bdd-7_2
SMILES:	Cc1ccncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)[C@H]3C[C@@H]3C(F)(F)F
RUN:	RUN1244
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.14

MIC-UNK-50cce87d-2_1



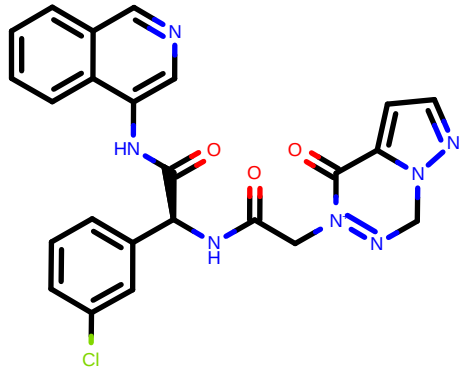
CID:	MIC-UNK-50cce87d-2_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)Cl
RUN:	RUN1077
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.08

MAK-UNK-ffc90da7-3_2



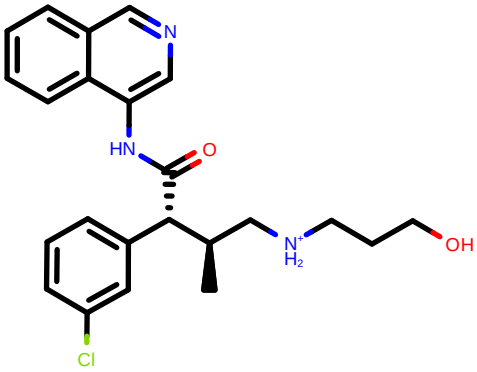
CID:	MAK-UNK-ffc90da7-3_2
SMILES:	CC(C)OC[C@H](c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl)[NH2+]C
RUN:	RUN1081
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.10

EDJ-MED-ee07cf00-17_2



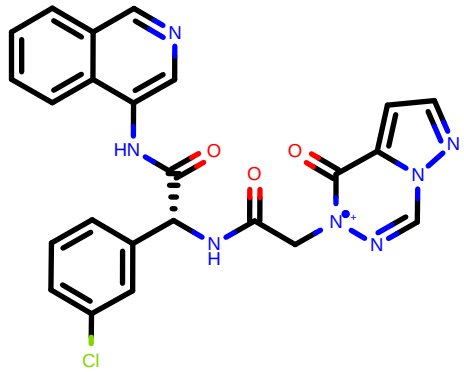
CID:	EDJ-MED-ee07cf00-17_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)Cn4c(=O)c5ccnn5cn4
RUN:	RUN1321
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.20

MAK-UNK-ffc90da7-1_4



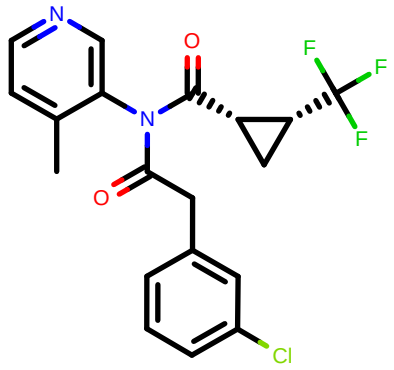
CID:	MAK-UNK-ffc90da7-1_4
SMILES:	C[C@H](C[NH2+]CCCO)[C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN1133
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.21

EDJ-MED-ee07cf00-17_1



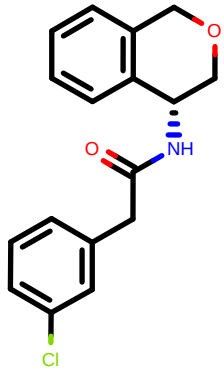
CID:	EDJ-MED-ee07cf00-17_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cn4c(=O)c5ccnn5cn4
RUN:	RUN1325
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.19

JOH-UNI-a38a7bdd-7_4



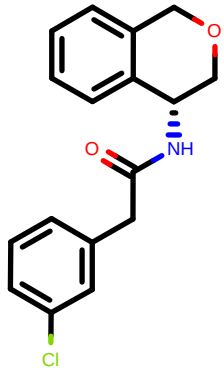
CID:	JOH-UNI-a38a7bdd-7_4
SMILES:	Cc1ccncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)[C@H]3C[C@H]3C(F)(F)F
RUN:	RUN1251
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.15

RUB-POS-1325a9ea-20_1



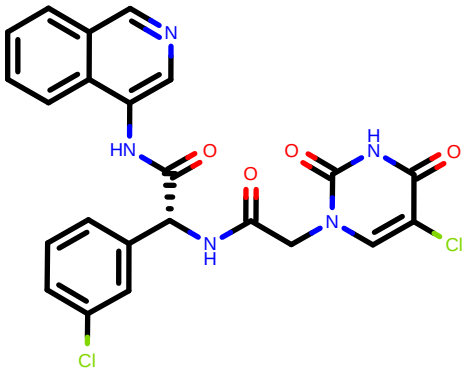
CID:	RUB-POS-1325a9ea-20_1
SMILES:	c1ccc2c(c1)COC[C@@H]2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1384
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.11

PET-UNK-f92d7c0c-2_1



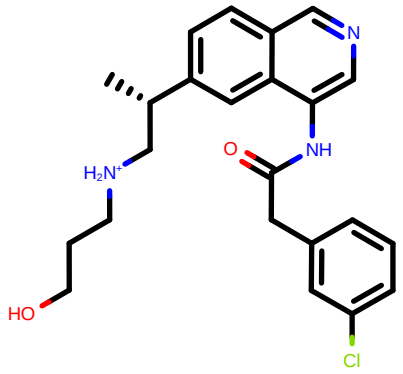
CID:	PET-UNK-f92d7c0c-2_1
SMILES:	c1ccc2c(c1)COC[C@@H]2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1403
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.10

EDJ-MED-ee07cf00-16_1



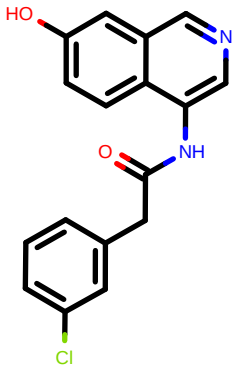
CID:	EDJ-MED-ee07cf00-16_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cn4cc(c(=O)[nH]c4=O)Cl
RUN:	RUN1302
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.17

MAK-UNK-ffc90da7-6_1



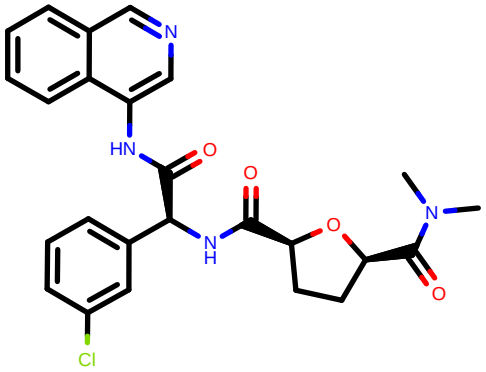
CID:	MAK-UNK-ffc90da7-6_1
SMILES:	C[C@@H](C[NH2+]CCCO)c1ccc2cncc(c2c1)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1125
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.14

MAT-POS-bb423b95-8_1



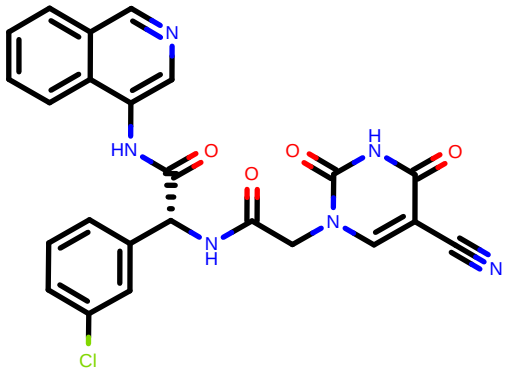
CID:	MAT-POS-bb423b95-8_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)O
RUN:	RUN1001
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.08

PET-UNK-1320d94d-2_1



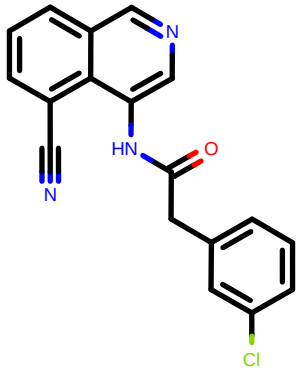
CID:	PET-UNK-1320d94d-2_1
SMILES:	CN(C)C(=O)[C@H]1CC[C@H](O1)C(=O)N[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1448
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.19

EDJ-MED-ee07cf00-8_1



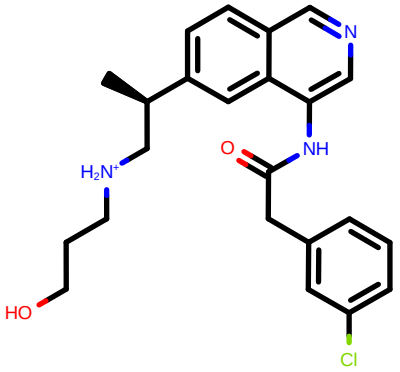
CID:	EDJ-MED-ee07cf00-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cn4cc(c(=O)[nH]c4=O)C#N
RUN:	RUN1311
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.16

PET-UNK-6314f867-3_1



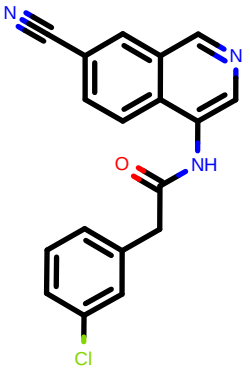
CID:	PET-UNK-6314f867-3_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)C#N
RUN:	RUN1417
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.10

MAK-UNK-ffc90da7-6_2



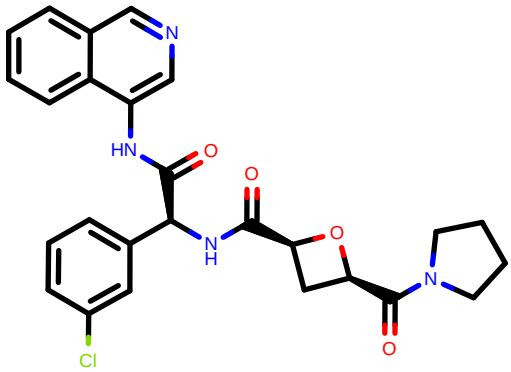
CID:	MAK-UNK-ffc90da7-6_2
SMILES:	C[C@H](C[NH2+]CCCO)c1ccc2cncc(c2c1)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1146
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.12

PET-UNK-6314f867-2_1



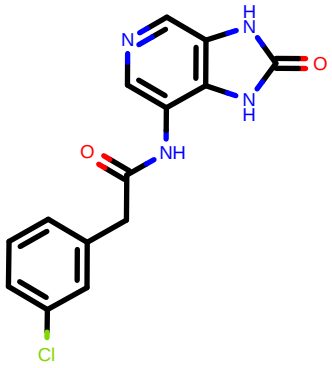
CID:	PET-UNK-6314f867-2_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccc(c3)C#N
RUN:	RUN1415
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.08

PET-UNK-1320d94d-8_1



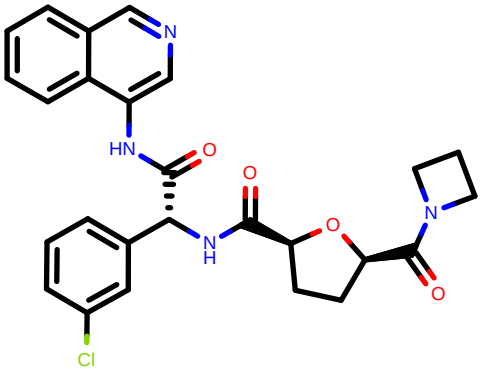
CID:	PET-UNK-1320d94d-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@@H]4C[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN1440
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.18

MIC-UNK-8971c93c-1_1



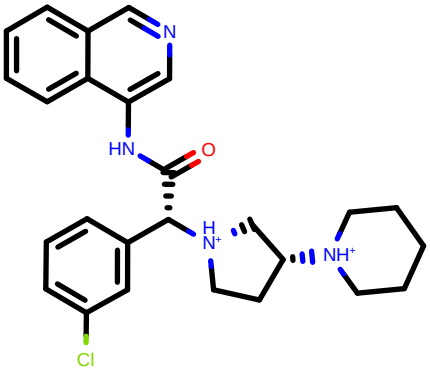
CID:	MIC-UNK-8971c93c-1_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2[nH]c(=O)[nH]3
RUN:	RUN957
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.07

PET-UNK-1320d94d-5_1



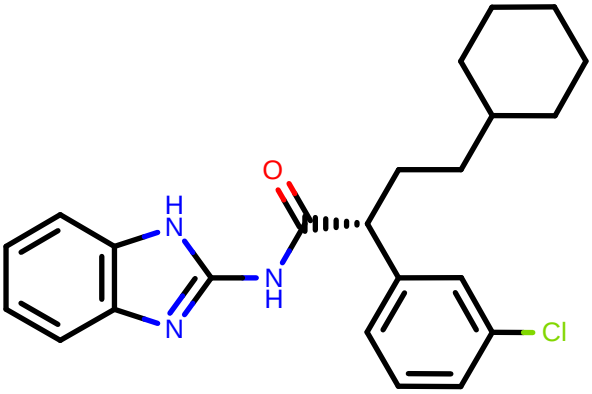
CID:	PET-UNK-1320d94d-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@@H]4CC[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN1452
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.16

MIC-UNK-5a93dd5f-12_5



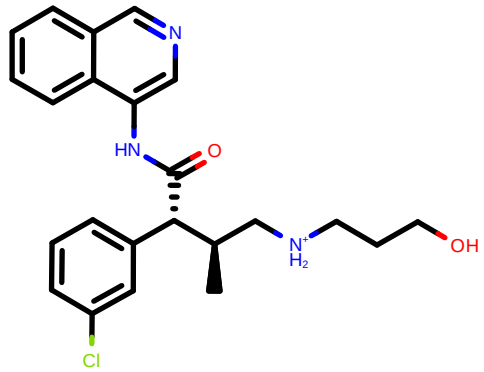
CID:	MIC-UNK-5a93dd5f-12_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@@]4CC[C@H](C4)[NH+]5CCCCC5
RUN:	RUN1179
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.16

ALP-POS-3fc1724e-8_2



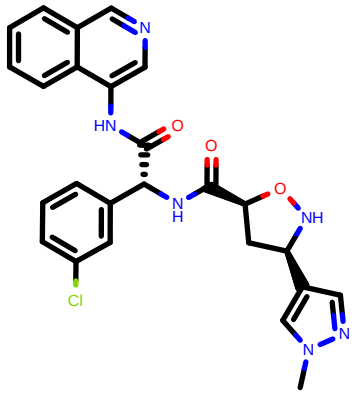
CID:	ALP-POS-3fc1724e-8_2
SMILES:	c1ccc2c(c1)[nH]c(n2)NC(=O)[C@H](CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN909
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.17

MAK-UNK-c749d764-6_4



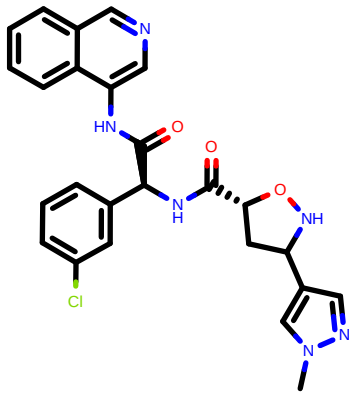
CID:	MAK-UNK-c749d764-6_4
SMILES:	C[C@H](C[NH2+]CCCO)[C@H](c1cccc(c1Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN1199
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.16

EDJ-MED-ee07cf00-6_3



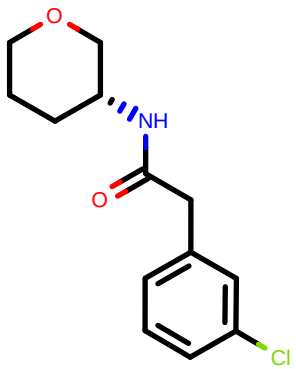
CID:	EDJ-MED-ee07cf00-6_3
SMILES:	Cn1cc(cn1)C2=NO[C@@H](C2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1313
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.15

EDJ-MED-ee07cf00-6_2



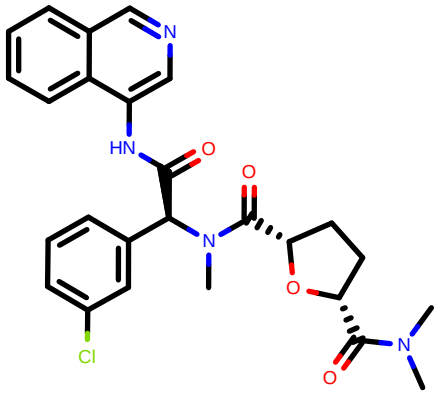
CID:	EDJ-MED-ee07cf00-6_2
SMILES:	Cn1cc(cn1)C2=NO[C@H](C2)C(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1306
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.16

PET-UNK-f92d7c0c-1_1



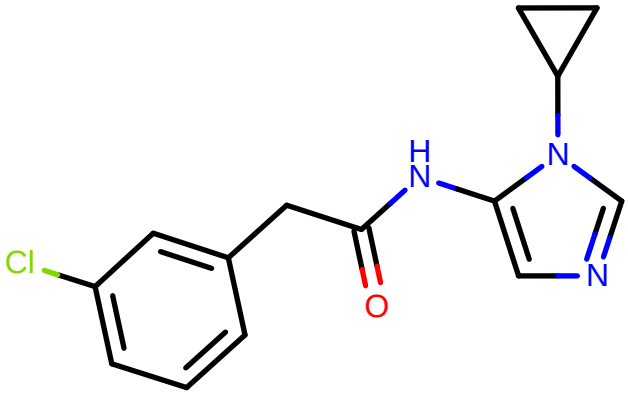
CID:	PET-UNK-f92d7c0c-1_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)N[C@@H]2CCCOC2
RUN:	RUN1412
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.10

PET-UNK-1320d94d-22_1



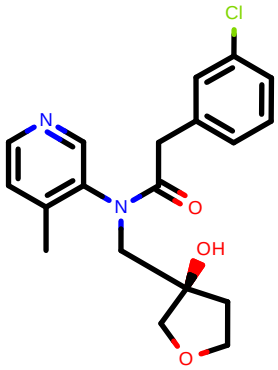
CID:	PET-UNK-1320d94d-22_1
SMILES:	CN(C)C(=O)[C@H]1CC[C@H](O1)C(=O)N(C)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1455
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.21

PET-UNK-8df914d1-5_1



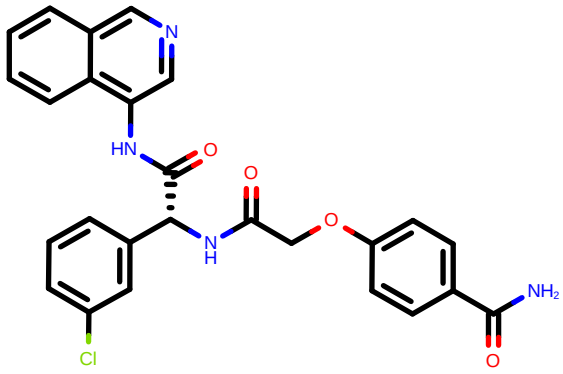
CID:	PET-UNK-8df914d1-5_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncn2C3CC3
RUN:	RUN955
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.09

BAR-COM-ebf5acce-11_1



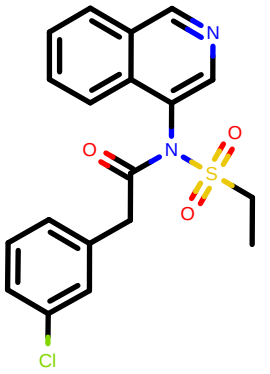
CID:	BAR-COM-ebf5acce-11_1
SMILES:	Cc1ccncc1N(C[C@@]2(CCOC2)O)C(=O)Cc3cccc(c3)Cl
RUN:	RUN801
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.19

EDJ-MED-ee07cf00-12_1



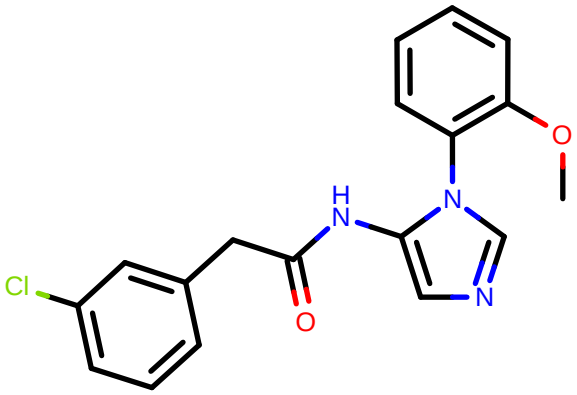
CID:	EDJ-MED-ee07cf00-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)COc4ccc(cc4)C(=O)N
RUN:	RUN1326
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.14

JOH-UNI-50ce7ec3-1_1



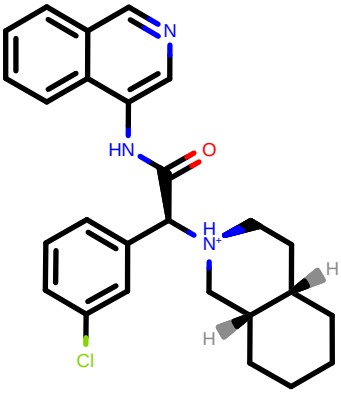
CID:	JOH-UNI-50ce7ec3-1_1
SMILES:	C=CS(=O)(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1296
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.20

BEN-DND-1e24cf73-4_1



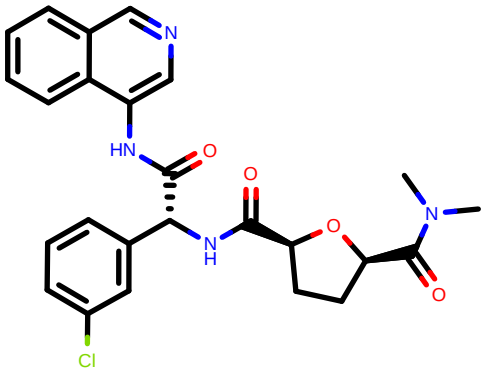
CID:	BEN-DND-1e24cf73-4_1
SMILES:	COc1ccccc1n2cncc2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1468
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.12

MIC-UNK-5a93dd5f-3_4



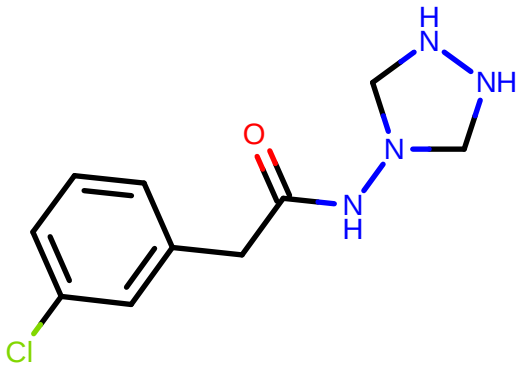
CID:	MIC-UNK-5a93dd5f-3_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@H+]4CC[C@@H]5CCCC[C@@H]5C4
RUN:	RUN1105
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.15

PET-UNK-1320d94d-1_1



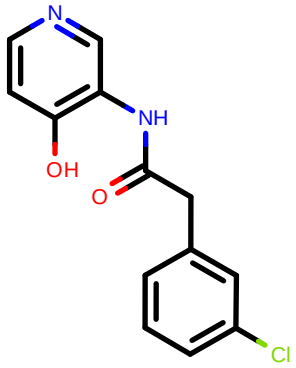
CID:	PET-UNK-1320d94d-1_1
SMILES:	CN(C)C(=O)[C@H]1CC[C@H](O1)C(=O)N[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1438
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.17

JAN-GHE-5a013bed-5_1



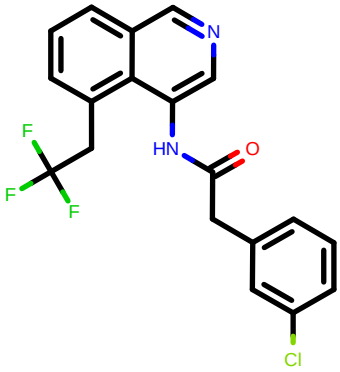
CID:	JAN-GHE-5a013bed-5_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nn2cnnc2
RUN:	RUN798
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.13

ALP-POS-95b75b4d-6_1



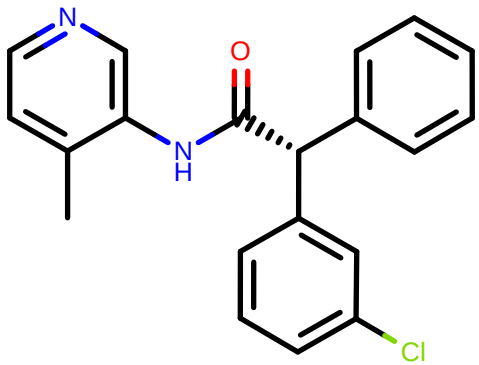
CID:	ALP-POS-95b75b4d-6_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2c[nH]ccc2=O
RUN:	RUN777
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.09

JOH-UNI-3fc3434e-3_1



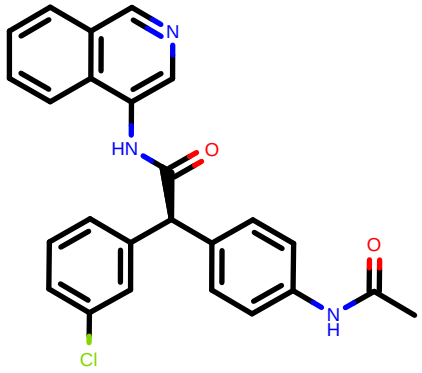
CID:	JOH-UNI-3fc3434e-3_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)CC(F)(F)F
RUN:	RUN1272
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.11

SAM-UNK-2684b532-1_2



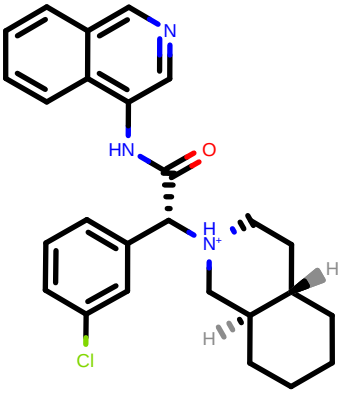
CID:	SAM-UNK-2684b532-1_2
SMILES:	Cc1ccncc1NC(=O)[C@H](c2ccccc2)c3cccc(c3)Cl
RUN:	RUN868
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.13

MIC-UNK-d36ab305-1_1



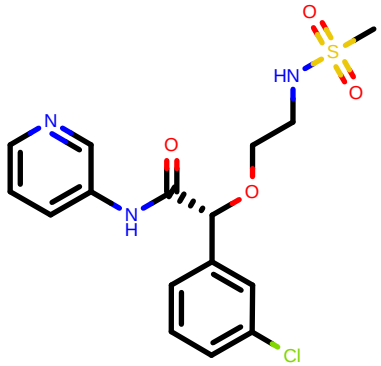
CID:	MIC-UNK-d36ab305-1_1
SMILES:	CC(=O)Nc1ccc(cc1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN975
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.14

MIC-UNK-5a93dd5f-3_9



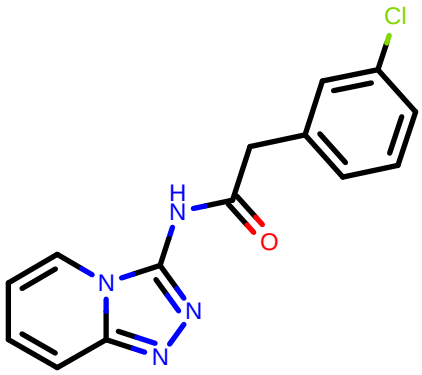
CID:	MIC-UNK-5a93dd5f-3_9
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@@H+]4CC[C@@H]5CCCC[C@H]5C4
RUN:	RUN1131
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.20

ADA-UNI-f8e79267-7_2



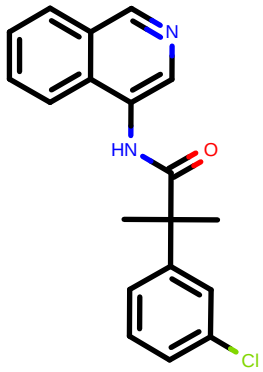
CID:	ADA-UNI-f8e79267-7_2
SMILES:	CS(=O)(=O)NCCO[C@H](c1cccc(c1)Cl)C(=O)Nc2cccnc2
RUN:	RUN743
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.17

PET-UNK-e44ffd04-1_1



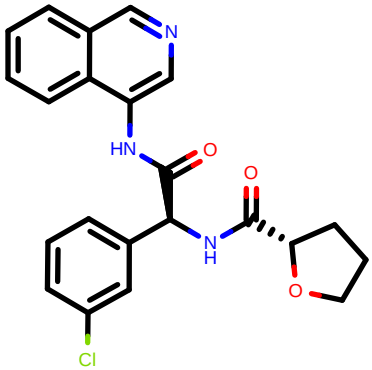
CID:	PET-UNK-e44ffd04-1_1
SMILES:	c1ccn2c(c1)nnc2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1048
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.09

NAU-LAT-2fed8305-1_1



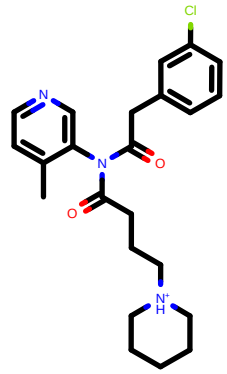
CID:	NAU-LAT-2fed8305-1_1
SMILES:	CC(C)(c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN1189
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.10

EDJ-MED-cf4b0d25-3_2



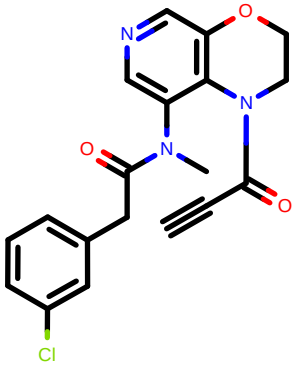
CID:	EDJ-MED-cf4b0d25-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@@H]4CCCO4
RUN:	RUN1335
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.14

DAR-DIA-076fb6ea-14_1



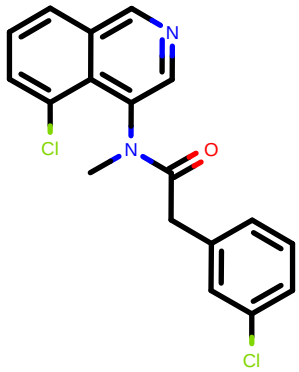
CID:	DAR-DIA-076fb6ea-14_1
SMILES:	Cc1ccncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)/C=C/C[NH+]3CCCCC3
RUN:	RUN1242
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.22

JOH-UNI-ee5ed7c8-12_1



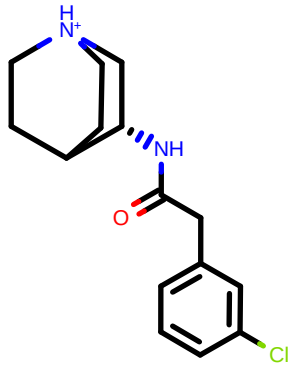
CID:	JOH-UNI-ee5ed7c8-12_1
SMILES:	CN(c1cncc2c1N(CCO2)C(=O)C#C)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1269
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.09

MIC-UNK-67d4a29a-1_1



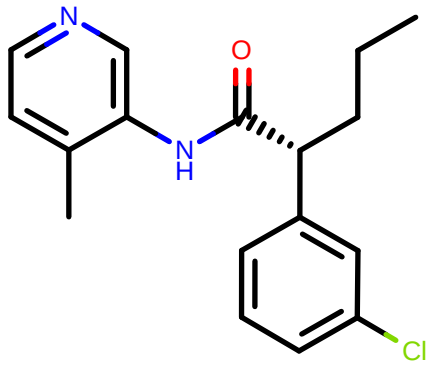
CID:	MIC-UNK-67d4a29a-1_1
SMILES:	CN(c1cncc2c1c(ccc2)Cl)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1180
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.16

MIC-UNK-13557a72-1_2



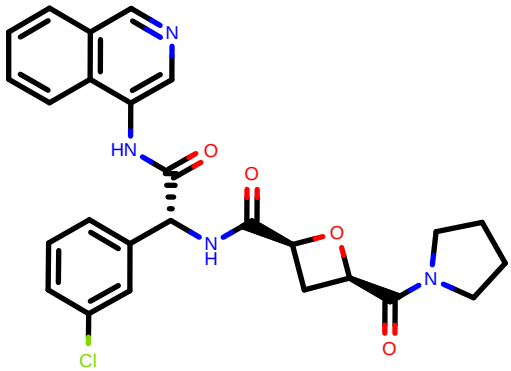
CID:	MIC-UNK-13557a72-1_2
SMILES:	c1cc(cc(c1)Cl)CC(=O)N[C@H]2C[NH+]3CCC2CC3
RUN:	RUN1009
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.11

JAN-GHE-83b26c96-8_2



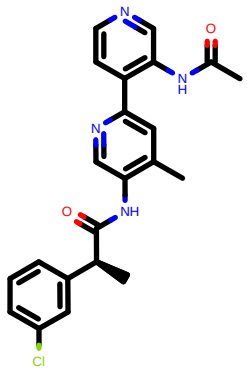
CID:	JAN-GHE-83b26c96-8_2
SMILES:	CCC[C@H](c1cccc(c1)Cl)C(=O)Nc2cnccc2C
RUN:	RUN761
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.12

PET-UNK-1320d94d-7_1



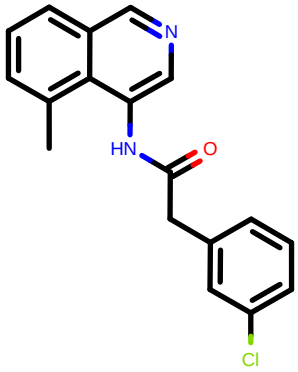
CID:	PET-UNK-1320d94d-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@@H]4C[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN1441
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.16

MAK-UNK-f203cb68-12_1



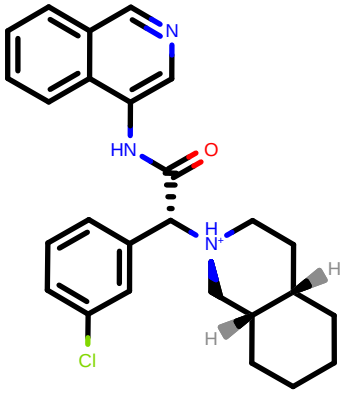
CID:	MAK-UNK-f203cb68-12_1
SMILES:	Cc1cc(ncc1NC(=O)[C@@H](C)c2cccc(c2)Cl)c3ccncc3NC(=O)C
RUN:	RUN852
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.20

RUB-POS-1325a9ea-3_1



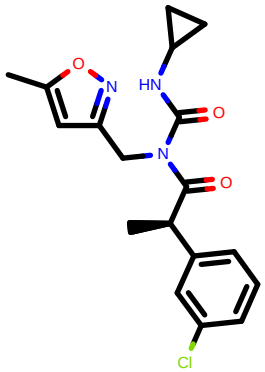
CID:	RUB-POS-1325a9ea-3_1
SMILES:	Cc1cccc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1361
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.05

MIC-UNK-5a93dd5f-3_3



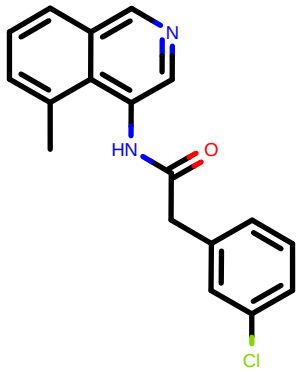
CID:	MIC-UNK-5a93dd5f-3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@H+]4CC[C@@H]5CCCC[C@@H]5C4
RUN:	RUN1115
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.21

TRY-UNI-9f475305-8_2



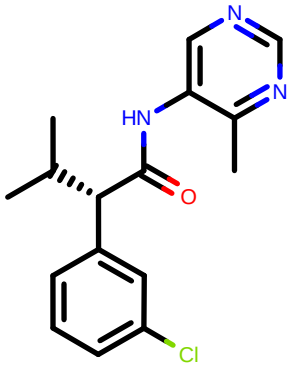
CID:	TRY-UNI-9f475305-8_2
SMILES:	Cc1cc(no1)CN(C(=O)[C@H](C)c2cccc(c2)Cl)C(=O)NC3CC3
RUN:	RUN830
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.16

MIC-UNK-50cce87d-3_1



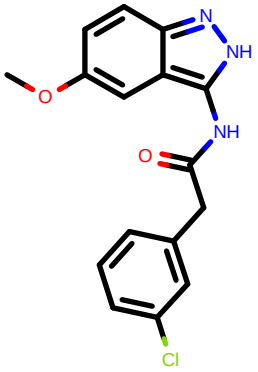
CID:	MIC-UNK-50cce87d-3_1
SMILES:	Cc1cccc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1074
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.05

JAN-GHE-83b26c96-7_2



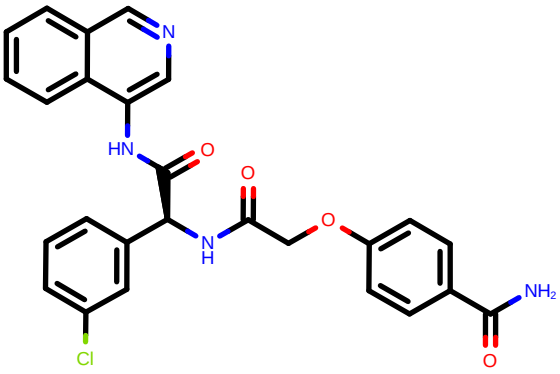
CID:	JAN-GHE-83b26c96-7_2
SMILES:	Cc1c(cncn1)NC(=O)[C@H](c2cccc(c2)Cl)C(C)C
RUN:	RUN765
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.11

EDJ-MED-c8e7a002-2_1



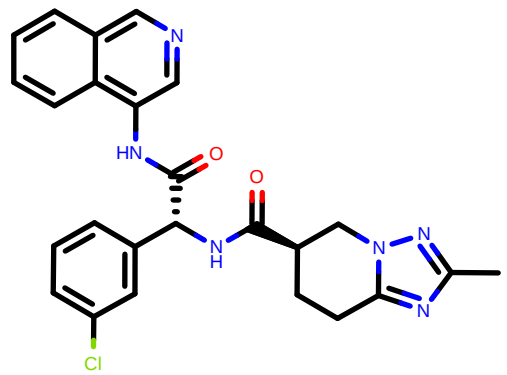
CID:	EDJ-MED-c8e7a002-2_1
SMILES:	COc1ccc2c(c1)c(n[nH]2)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1030
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.14

EDJ-MED-ee07cf00-12_2



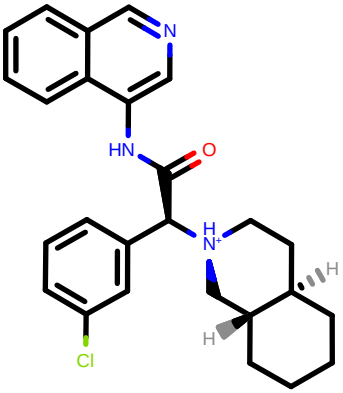
CID:	EDJ-MED-ee07cf00-12_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)COc4ccc(cc4)C(=O)N
RUN:	RUN1329
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.17

EDJ-MED-ee07cf00-13_2



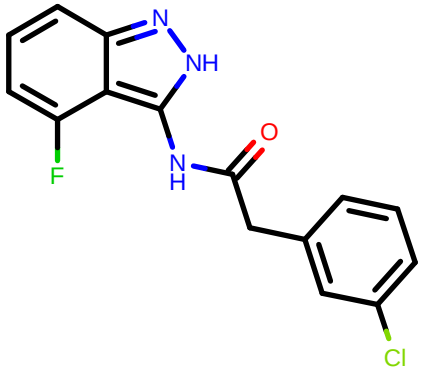
CID:	EDJ-MED-ee07cf00-13_2
SMILES:	Cc1nc2n(n1)C[C@@H](CC2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1318
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.13

MIC-UNK-5a93dd5f-3_8



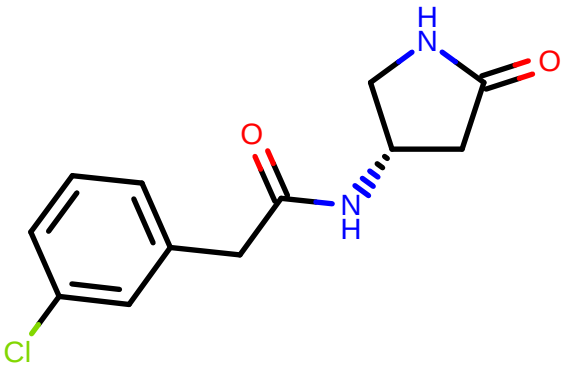
CID:	MIC-UNK-5a93dd5f-3_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@H+]4CC[C@H]5CCCC[C@@H]5C4
RUN:	RUN1126
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.16

EDJ-MED-c8e7a002-13_1



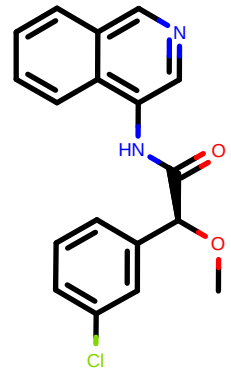
CID:	EDJ-MED-c8e7a002-13_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2c3c(cccc3F)[nH]n2
RUN:	RUN1047
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.09

ALP-POS-90e38439-3_2



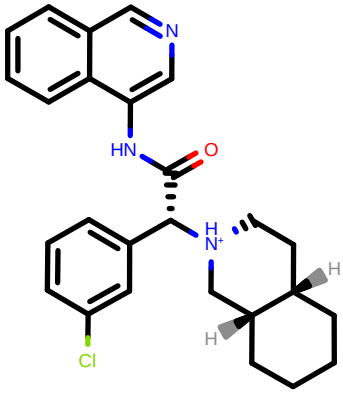
CID:	ALP-POS-90e38439-3_2
SMILES:	c1cc(cc(c1)Cl)CC(=O)N[C@H]2CC(=O)NC2
RUN:	RUN990
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.13

VLA-UNK-9a7dc93f-7_1



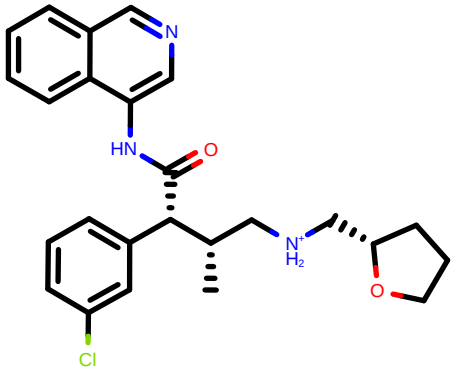
CID:	VLA-UNK-9a7dc93f-7_1
SMILES:	CO[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN1301
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.09

MIC-UNK-5a93dd5f-3_1



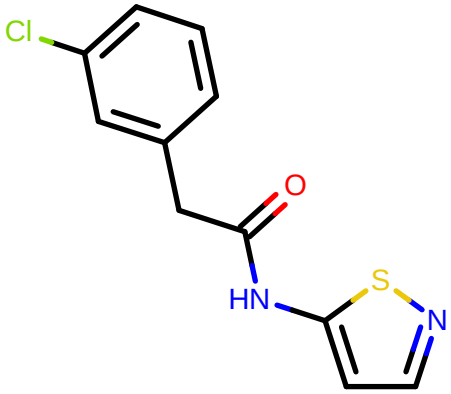
CID:	MIC-UNK-5a93dd5f-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@@H+]4CC[C@@H]5CCCC[C@@H]5C4
RUN:	RUN1123
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.20

MAK-UNK-ffc90da7-4_5



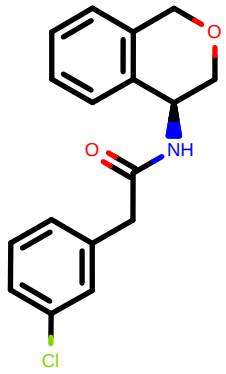
CID:	MAK-UNK-ffc90da7-4_5
SMILES:	C[C@@H](C[NH2+]C[C@@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1119
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.27

PET-UNK-158bee2a-2_1



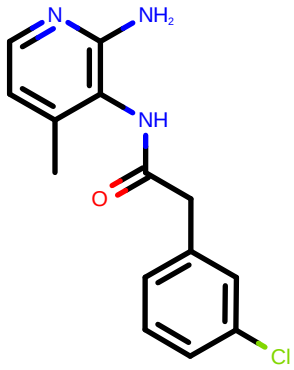
CID:	PET-UNK-158bee2a-2_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2ccns2
RUN:	RUN1430
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.08

RUB-POS-1325a9ea-20_2



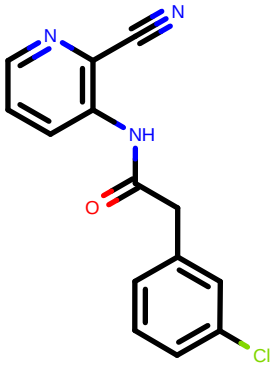
CID:	RUB-POS-1325a9ea-20_2
SMILES:	c1ccc2c(c1)COC[C@H]2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1386
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.10

EDG-MED-0da5ad92-18_1



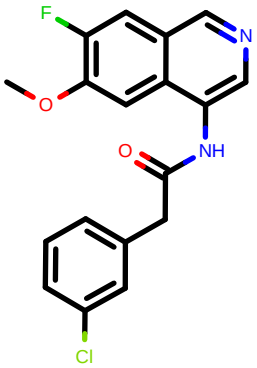
CID:	EDG-MED-0da5ad92-18_1
SMILES:	Cc1ccnc(c1NC(=O)Cc2cccc(c2)Cl)N
RUN:	RUN818
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.09

AGN-NEW-c7b24fe3-4_1



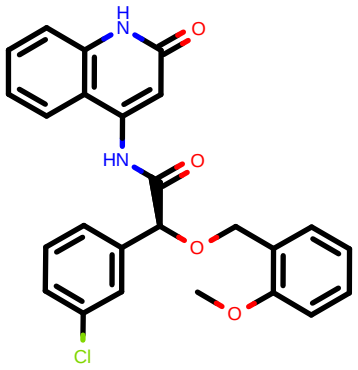
CID:	AGN-NEW-c7b24fe3-4_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cccnc2C#N
RUN:	RUN748
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.09

PET-UNK-b38839dc-1_1



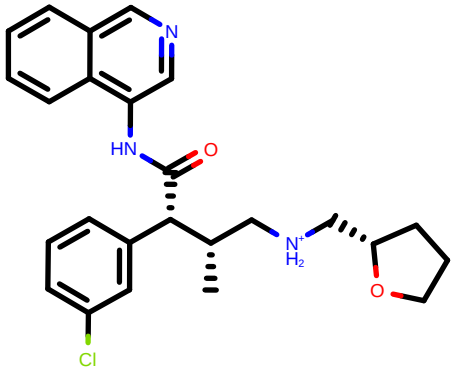
CID:	PET-UNK-b38839dc-1_1
SMILES:	COc1cc2c(cc1F)cncc2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1457
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.09

ADA-UCB-6c2cb422-11_1



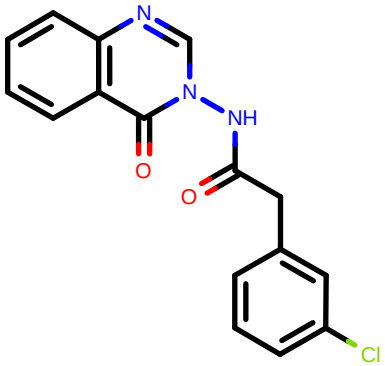
CID:	ADA-UCB-6c2cb422-11_1
SMILES:	COc1ccccc1CO[C@@H](c2cccc(c2)Cl)C(=O)Nc3cc(=O)[nH]c4c3cccc4
RUN:	RUN892
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.18

MAK-UNK-c749d764-22_5



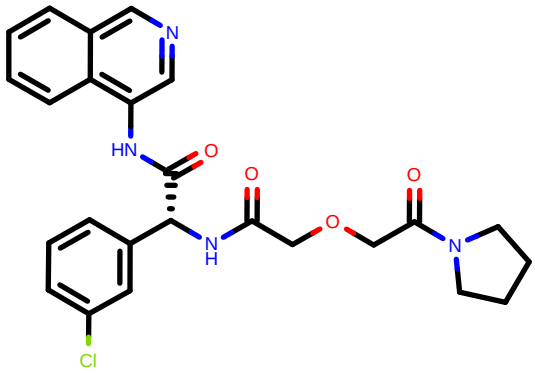
CID:	MAK-UNK-c749d764-22_5
SMILES:	C[C@@H](C[NH2+]C[C@@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1212
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.27

JAN-GHE-5a013bed-3_1



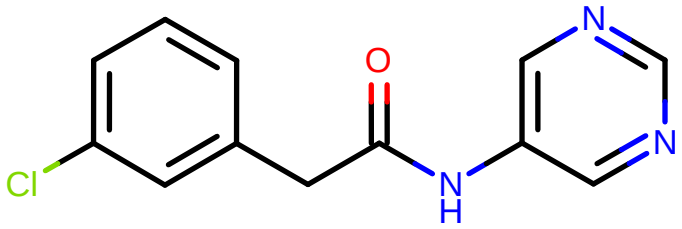
CID:	JAN-GHE-5a013bed-3_1
SMILES:	c1ccc2c(c1)c(=O)n(cn2)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN780
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.10

EDJ-MED-cf4b0d25-1_1



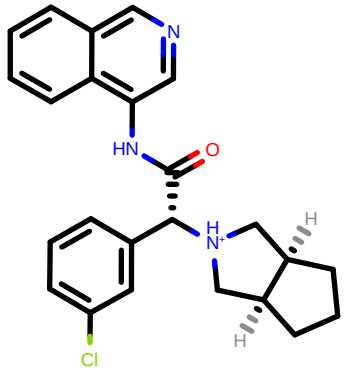
CID:	EDJ-MED-cf4b0d25-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)COCC(=O)N4CCCC4
RUN:	RUN1406
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.17

JAN-GHE-5a013bed-9_1



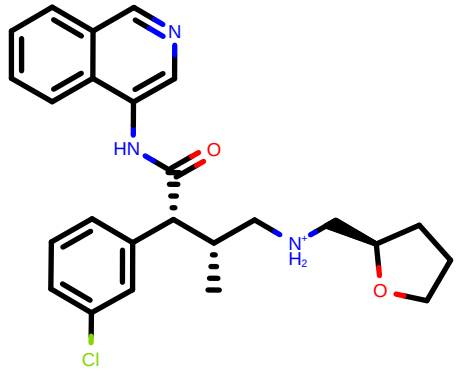
CID:	JAN-GHE-5a013bed-9_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncnc2
RUN:	RUN790
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.08

MIC-UNK-5a93dd5f-1_1



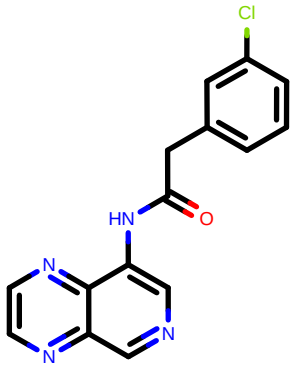
CID:	MIC-UNK-5a93dd5f-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[NH+]4C[C@H]5CCC[C@H]5C4
RUN:	RUN1096
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.18

MAK-UNK-c749d764-22_7



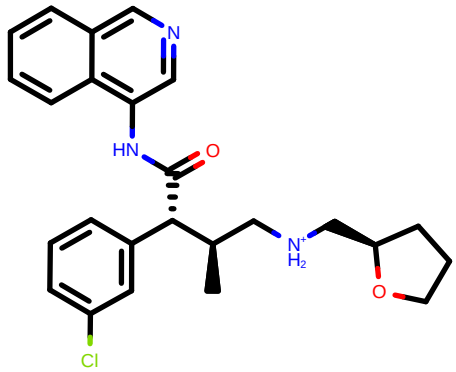
CID:	MAK-UNK-c749d764-22_7
SMILES:	C[C@@H](C[NH2+]C[C@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1216
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.28

JIN-POS-6dc588a4-10_1



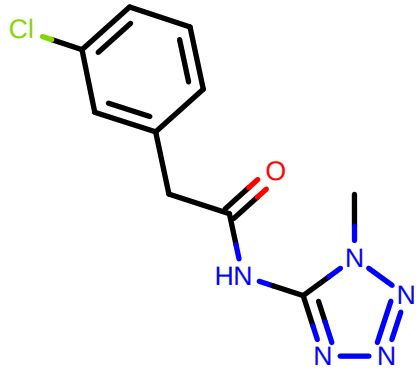
CID:	JIN-POS-6dc588a4-10_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2nccn3
RUN:	RUN1350
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.07

MAK-UNK-ffc90da7-4_8



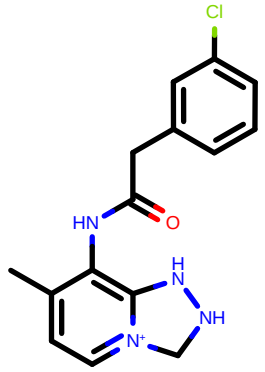
CID:	MAK-UNK-ffc90da7-4_8
SMILES:	C[C@H](C[NH2+]C[C@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1112
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.22

VLA-UNK-411a133b-2_1



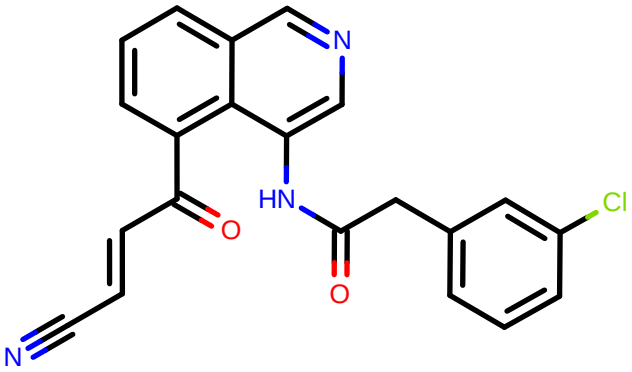
CID:	VLA-UNK-411a133b-2_1
SMILES:	Cn1c(nnn1)NC(=O)Cc2cccc(c2)Cl
RUN:	RUN1401
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.10

EDJ-MED-c8e7a002-4_1



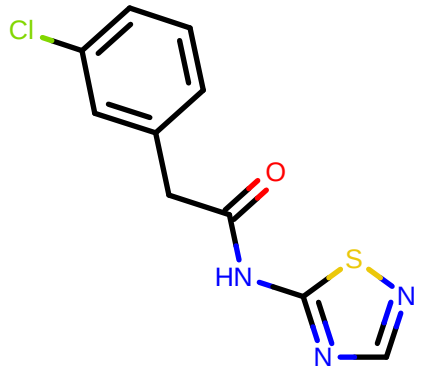
CID:	EDJ-MED-c8e7a002-4_1
SMILES:	Cc1ccn2cnnc2c1NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1040
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.10

JOH-UNI-3fc3434e-2_1



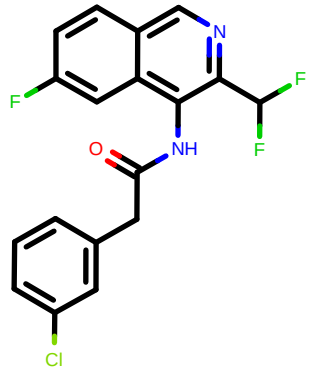
CID:	JOH-UNI-3fc3434e-2_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)C(=O)/C=C/C#N
RUN:	RUN1273
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.14

PET-UNK-158bee2a-4_1



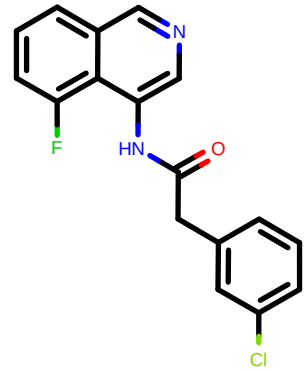
CID:	PET-UNK-158bee2a-4_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2ncns2
RUN:	RUN1434
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.09

JOH-UNI-6fede743-5_1



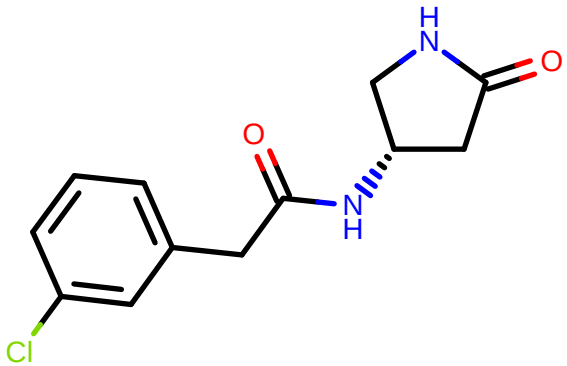
CID:	JOH-UNI-6fede743-5_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2c3cc(ccc3cnc2C(F)F)F
RUN:	RUN1194
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.13

MIC-UNK-50cce87d-1_1



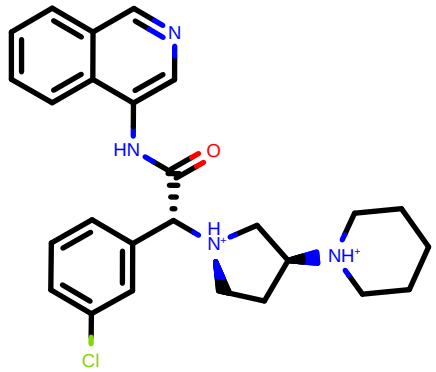
CID:	MIC-UNK-50cce87d-1_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)F
RUN:	RUN1079
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.07

MIC-UNK-42806bd5-2_2



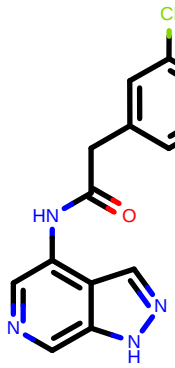
CID:	MIC-UNK-42806bd5-2_2
SMILES:	c1cc(cc(c1)Cl)CC(=O)N[C@H]2CC(=O)NC2
RUN:	RUN911
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.14

MIC-UNK-5a93dd5f-12_3



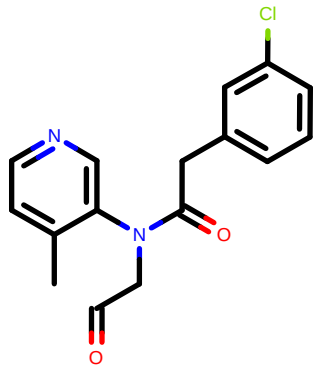
CID:	MIC-UNK-5a93dd5f-12_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@]4CC[C@@H](C4)[NH+]5CCCCC5
RUN:	RUN1178
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.16

RUB-POS-1325a9ea-13_1



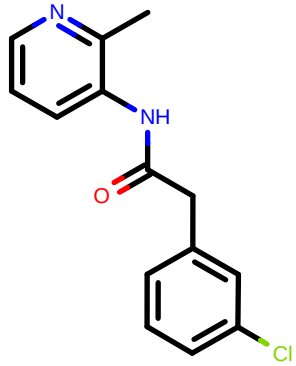
CID:	RUB-POS-1325a9ea-13_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cn[nH]3
RUN:	RUN1365
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.08

PET-UNK-bbe8d7ff-1_1



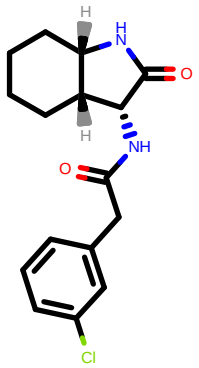
CID:	PET-UNK-bbe8d7ff-1_1
SMILES:	Cc1ccncc1N(CC=O)C(=O)Cc2cccc(c2)Cl
RUN:	RUN885
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.09

EDG-MED-0da5ad92-14_1



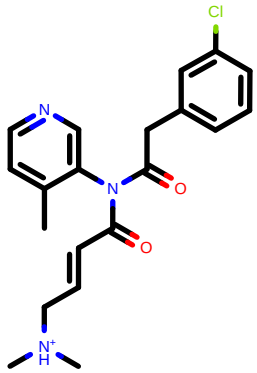
CID:	EDG-MED-0da5ad92-14_1
SMILES:	Cc1c(cccn1)NC(=O)Cc2cccc(c2)Cl
RUN:	RUN812
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.09

MIC-UNK-8373f97b-4_1



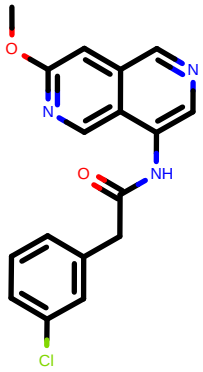
CID:	MIC-UNK-8373f97b-4_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)N[C@@H]2[C@@H]3CCCC[C@@H]3NC2=O
RUN:	RUN960
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.13

DAR-DIA-076fb6ea-13_1



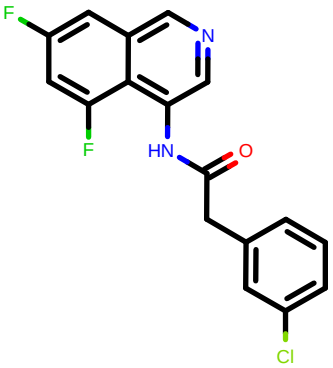
CID:	DAR-DIA-076fb6ea-13_1
SMILES:	Cc1ccncc1N(C(=O)Cc2cccc(c2)Cl)C(=O)/C=C/C[NH+](C)C
RUN:	RUN1243
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.22

PET-UNK-f4e47ebd-2_1



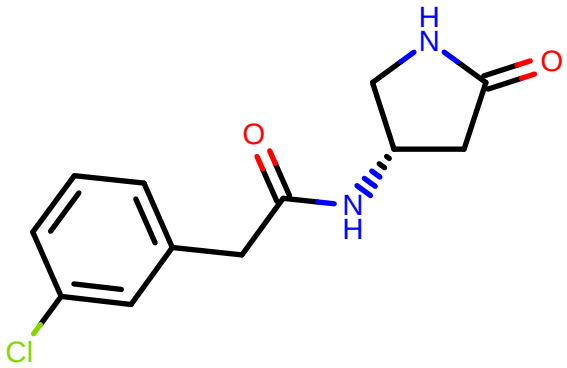
CID:	PET-UNK-f4e47ebd-2_1
SMILES:	COc1cc2cncc(c2cn1)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1422
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.09

MIC-UNK-7574fcc6-1_1



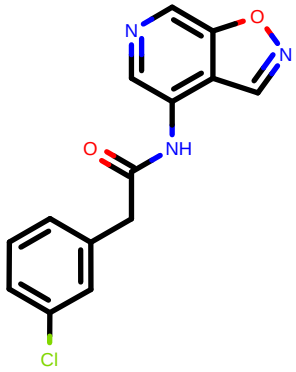
CID:	MIC-UNK-7574fcc6-1_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(cc(c3)F)F
RUN:	RUN1427
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.07

ALP-POS-8b8a49e1-5_2



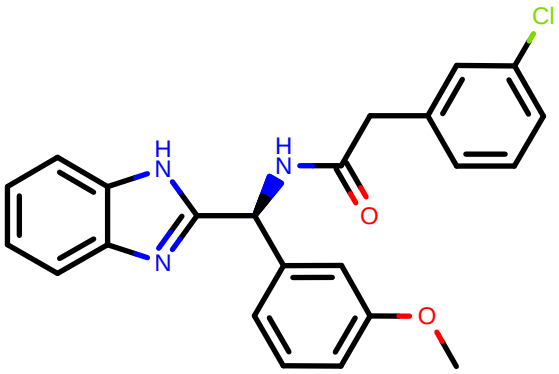
CID:	ALP-POS-8b8a49e1-5_2
SMILES:	c1cc(cc(c1)Cl)CC(=O)N[C@H]2CC(=O)NC2
RUN:	RUN1021
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.13

PET-UNK-b1ef24dc-3_1



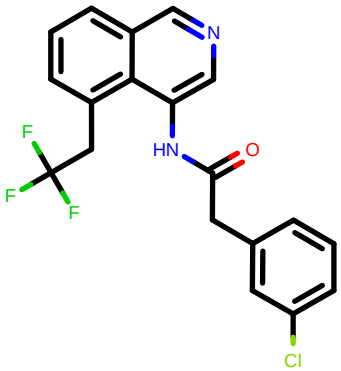
CID:	PET-UNK-b1ef24dc-3_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cno3
RUN:	RUN1425
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.08

ALP-POS-ddb41b15-9_1



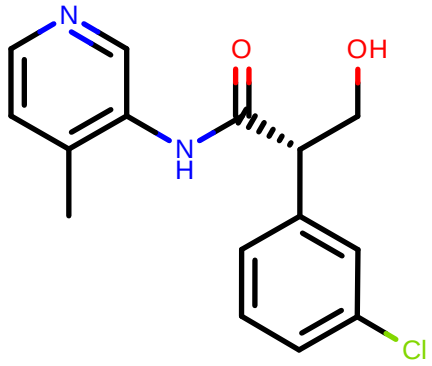
CID:	ALP-POS-ddb41b15-9_1
SMILES:	COc1cccc(c1)[C@@H](c2[nH]c3ccccc3n2)NC(=O)Cc4cccc(c4)Cl
RUN:	RUN929
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.17

JOH-UNI-ee5ed7c8-3_1



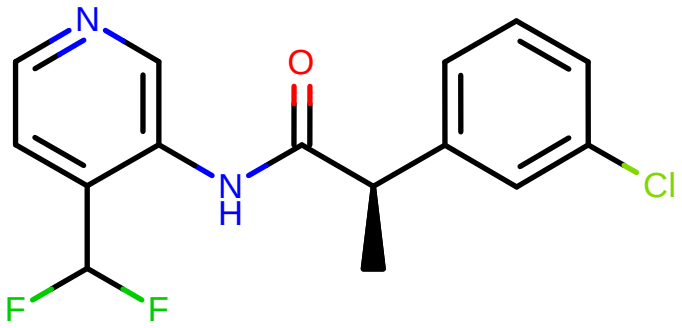
CID:	JOH-UNI-ee5ed7c8-3_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)CC(F)(F)F
RUN:	RUN1253
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.12

EDG-MED-0da5ad92-5_2



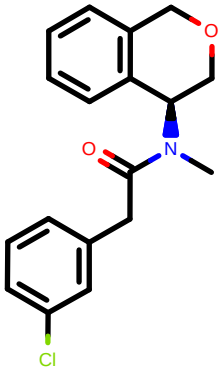
CID:	EDG-MED-0da5ad92-5_2
SMILES:	Cc1ccncc1NC(=O)[C@H](CO)c2cccc(c2)Cl
RUN:	RUN816
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.11

SAM-UNK-2684b532-5_2



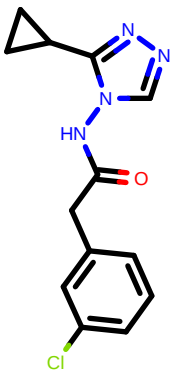
CID:	SAM-UNK-2684b532-5_2
SMILES:	C[C@H](c1cccc(c1)Cl)C(=O)Nc2cnccc2C(F)F
RUN:	RUN872
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.10

PET-UNK-f92d7c0c-9_1



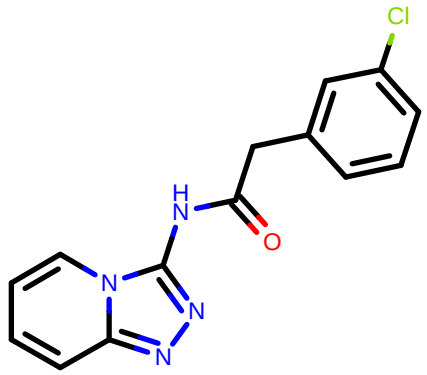
CID:	PET-UNK-f92d7c0c-9_1
SMILES:	CN([C@@H]1COCc2c1cccc2)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1416
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.13

JAN-GHE-f4ca5a00-16_1



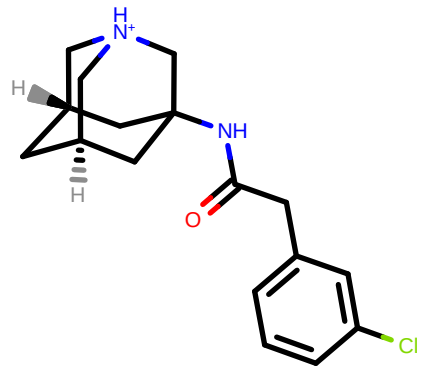
CID:	JAN-GHE-f4ca5a00-16_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nn2cnnc2C3CC3
RUN:	RUN893
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.11

NAU-LAT-a5c7d7cb-12_1



CID:	NAU-LAT-a5c7d7cb-12_1
SMILES:	c1ccn2c(c1)nnc2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1070
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.08

MIC-UNK-b12b7f76-2_1



CID:	MIC-UNK-b12b7f76-2_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)NC23C[C@H]4C[C@@H](C2)C[NH+](C4)C3
RUN:	RUN1020
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.13