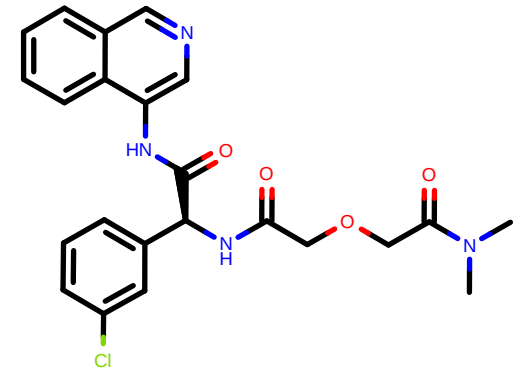
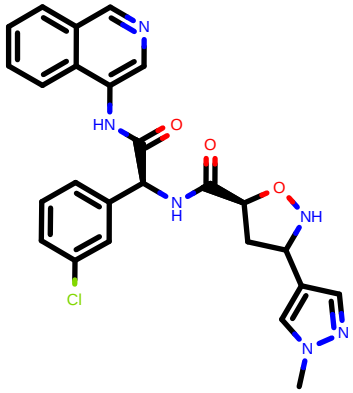
EDJ-MED-cf4b0d25-5_1



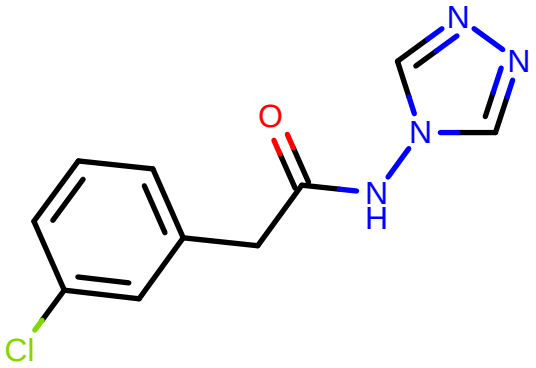
CID:	EDJ-MED-cf4b0d25-5_1
SMILES:	CN(C)C(=O)COCC(=O)N[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN718
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.16

EDJ-MED-ee07cf00-6_1



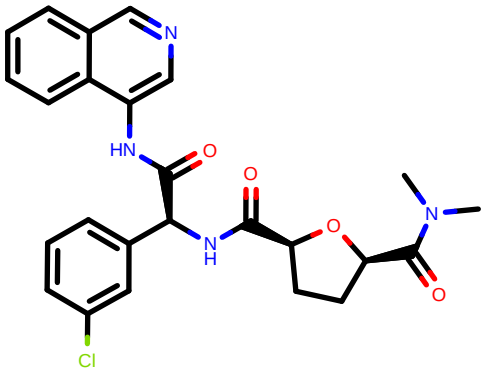
CID:	EDJ-MED-ee07cf00-6_1
SMILES:	Cn1cc(cn1)C2=NO[C@@H](C2)C(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN584
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.17

JAN-GHE-5a013bed-5_1



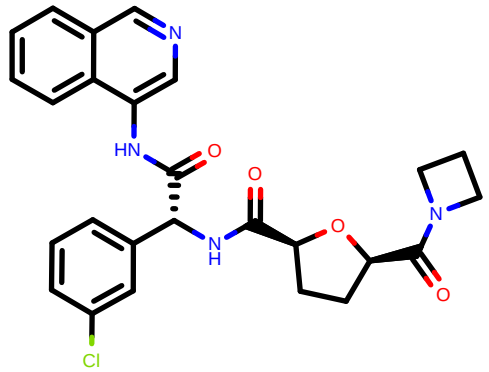
CID:	JAN-GHE-5a013bed-5_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nn2cnnc2
RUN:	RUN63
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.12

PET-UNK-1320d94d-2_1



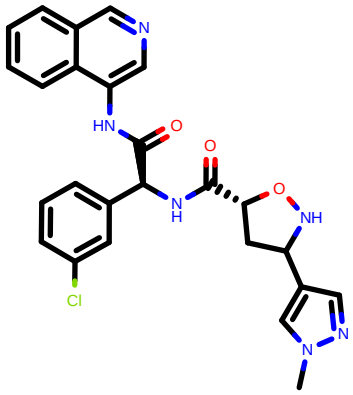
CID:	PET-UNK-1320d94d-2_1
SMILES:	CN(C)C(=O)[C@H]1CC[C@H](O1)C(=O)N[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN713
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.18

PET-UNK-1320d94d-5_1



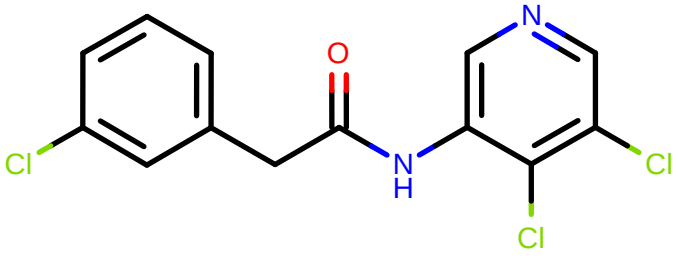
CID:	PET-UNK-1320d94d-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@@H]4CC[C@@H](O4)C(=O)N5CCC5
RUN:	RUN717
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.17

EDJ-MED-ee07cf00-6_2



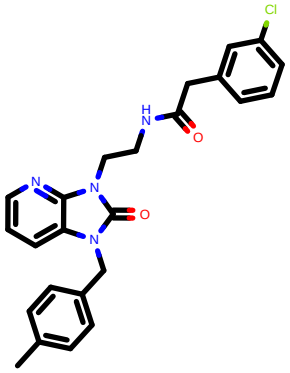
CID:	EDJ-MED-ee07cf00-6_2
SMILES:	Cn1cc(cn1)C2=NO[C@H](C2)C(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN571
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.17

JAN-GHE-5a013bed-10_1



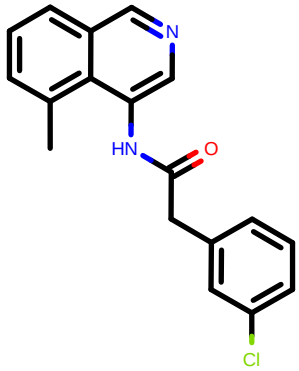
CID:	JAN-GHE-5a013bed-10_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc(c2Cl)Cl
RUN:	RUN46
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.08

MAR-TRE-f6f5f473-93_1



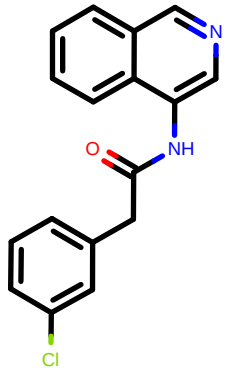
CID:	MAR-TRE-f6f5f473-93_1
SMILES:	Cc1ccc(cc1)Cn2c3cccnc3n(c2=O)CCNC(=O)Cc4cccc(c4)Cl
RUN:	RUN175
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.18

RUB-POS-1325a9ea-3_1



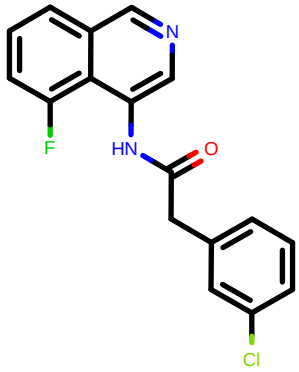
CID:	RUB-POS-1325a9ea-3_1
SMILES:	Cc1cccc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN626
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.06

ADA-UCB-6c2cb422-1_1



CID:	ADA-UCB-6c2cb422-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN154
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.02

RUB-POS-1325a9ea-2_1



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