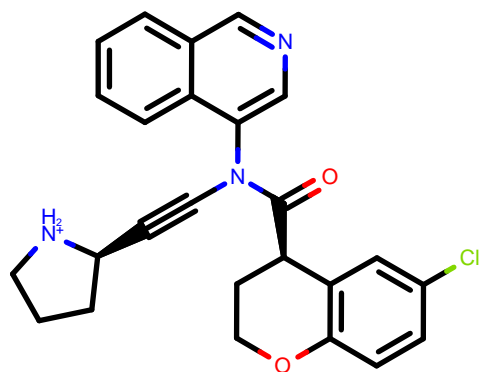
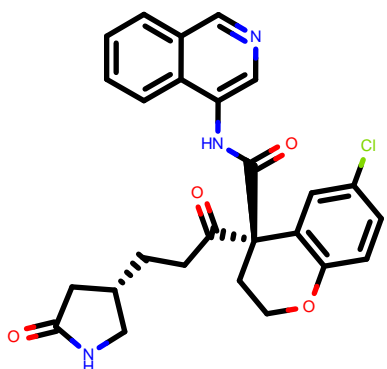


DAR-DIA-5ff57136-12_2



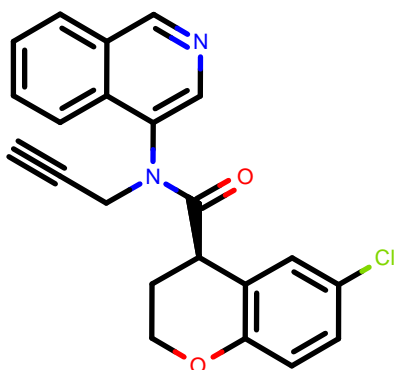
CID:	DAR-DIA-5ff57136-12_2
SMILES:	<chem>c1ccc2c(c1)cncc2N(C#C[C@H]3CCCN3)C(=O)[C@@H]4CCOCc5ccc(cc5)Cl</chem>
RUN:	RUN95
DDG (kcal/mol):	-2.87
dDDG (kcal/mol):	0.22

VLA-UCB-34f3ed0c-21_2



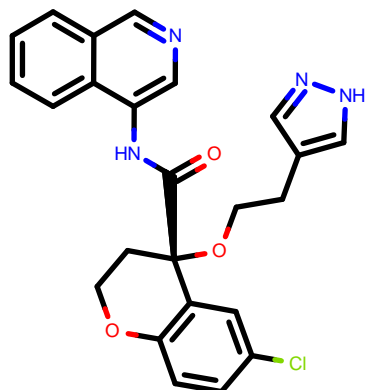
CID:	VLA-UCB-34f3ed0c-21_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@H]5CC(=O)NC5</chem>
RUN:	RUN0
DDG (kcal/mol):	-2.78
dDDG (kcal/mol):	0.37

DAR-DIA-5ff57136-13_1



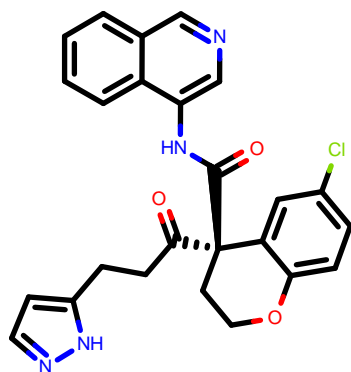
CID:	DAR-DIA-5ff57136-13_1
SMILES:	<chem>C#CCN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN92
DDG (kcal/mol):	-2.73
dDDG (kcal/mol):	0.13

EDJ-MED-28ec730d-5_1



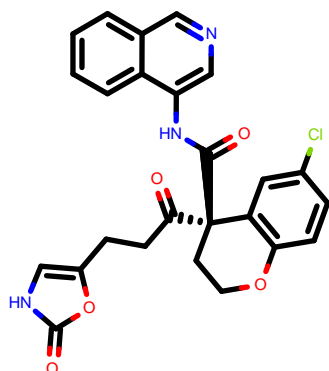
CID:	EDJ-MED-28ec730d-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)OCCc5c[nH]nc5</chem>
RUN:	RUN31
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.23

VLA-UCB-34f3ed0c-8_1



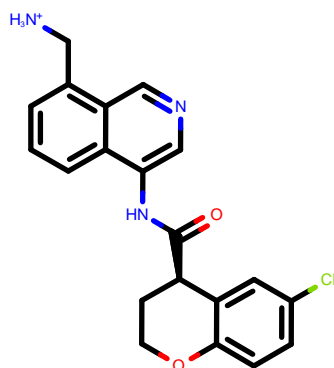
CID:	VLA-UCB-34f3ed0c-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5c[nH]5</chem>
RUN:	RUN76
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.22

VLA-UCB-34f3ed0c-9_1



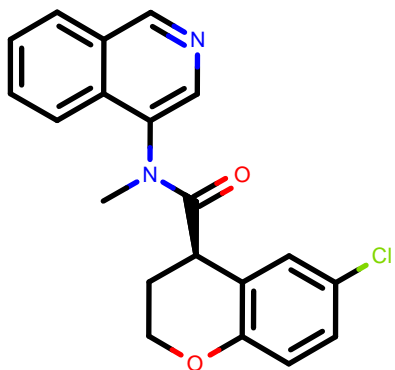
CID:	VLA-UCB-34f3ed0c-9_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5c[nH]c(=O)o5</chem>
RUN:	RUN72
DDG (kcal/mol):	-2.59
dDDG (kcal/mol):	0.27

MAK-UNK-8be7dca9-6_1



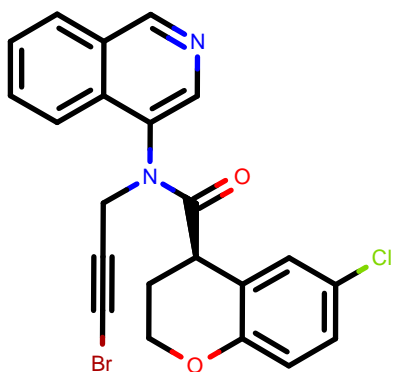
CID:	MAK-UNK-8be7dca9-6_1
SMILES:	<chem>c1cc(c2cncc(c2c1)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CN</chem>
RUN:	RUN42
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.09

MAK-UNK-3875bbc8-2_1



CID:	MAK-UNK-3875bbc8-2_1
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN49
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.07

DAR-DIA-5ff57136-17_1



CID: DAR-DIA-5ff57136-17_1

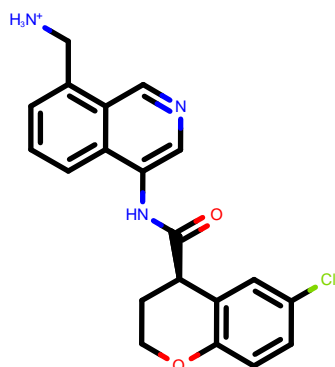
SMILES: c1ccc2c(c1)cncc2N(CC#CCBr)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN69

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.17

NAU-LAT-b7d8c353-8_1



CID: NAU-LAT-b7d8c353-8_1

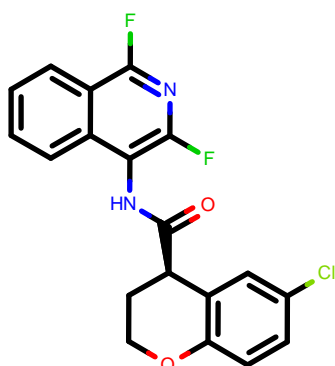
SMILES: c1cc(c2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)CN

RUN: RUN41

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.09

JOH-SUS-a69c159d-6_1



CID: JOH-SUS-a69c159d-6_1

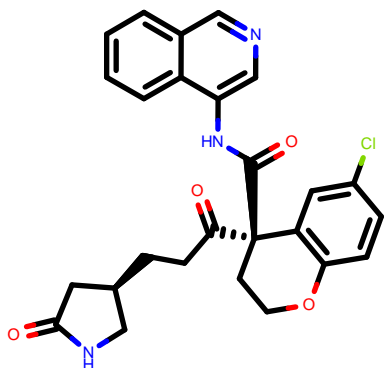
SMILES: c1ccc2c(c1)c(c(nc2F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN70

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.05

VLA-UCB-34f3ed0c-21_1



CID: VLA-UCB-34f3ed0c-21_1

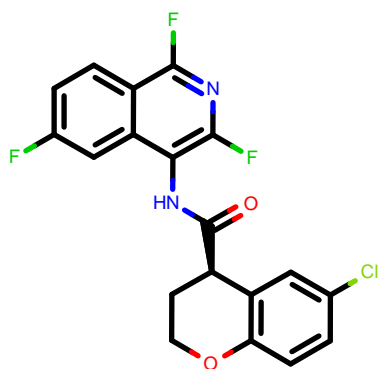
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)C(=O)CC[C@@H]5CC(=O)NC5

RUN: RUN27

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.31

JOH-SUS-a69c159d-7_1



CID: JOH-SUS-a69c159d-7_1

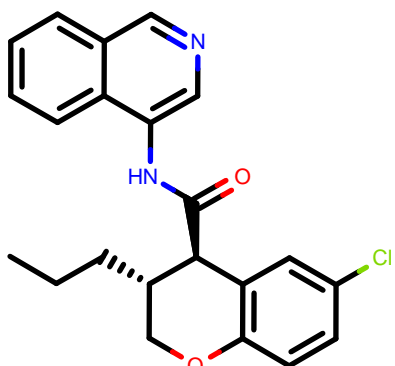
SMILES: c1cc2c(cc1F)c(nc2F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN71

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.05

EDJ-MED-e4b030d8-6_1



CID: EDJ-MED-e4b030d8-6_1

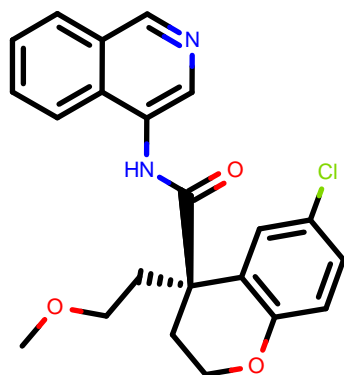
SMILES: CCC[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3ncc4c3ccc4)Cl

RUN: RUN7

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.10

EDJ-MED-28ec730d-2_1



CID: EDJ-MED-28ec730d-2_1

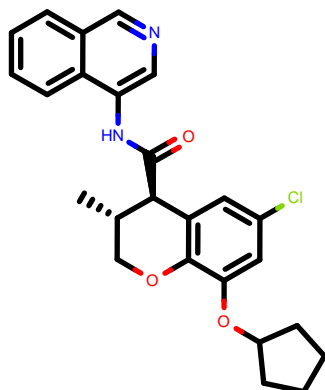
SMILES: COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN77

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.17

DAR-DIA-0d514e7d-4_1



CID: DAR-DIA-0d514e7d-4_1

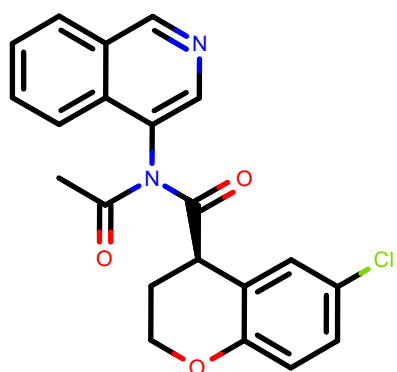
SMILES: C[C@H]1COc2c(cc(cc2OC3CCCC3)Cl)[C@@H]1C(=O)Nc4cncc5c4ccc5

RUN: RUN93

DDG (kcal/mol): -1.60

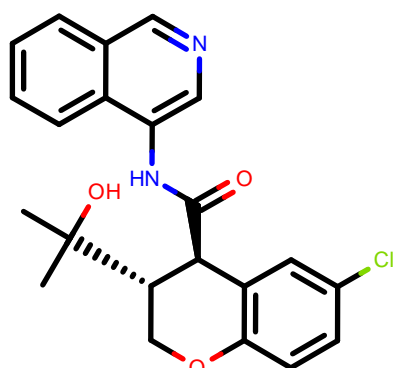
dDDG (kcal/mol): 0.21

VLA-UCB-50c39ae8-1_1



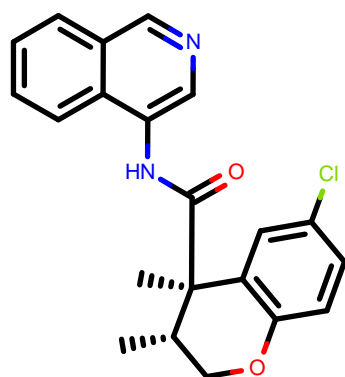
CID:	VLA-UCB-50c39ae8-1_1
SMILES:	<chem>CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN94
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.16

BEN-BAS-5c03e89e-1_2



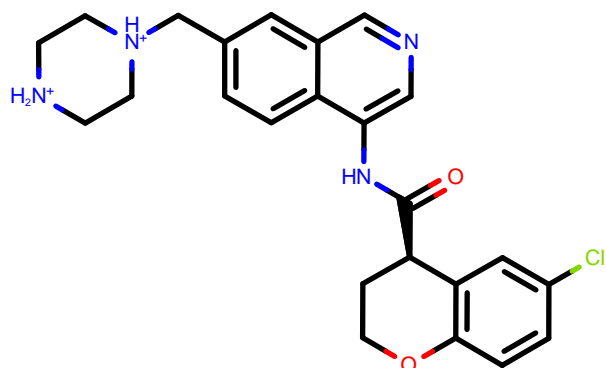
CID:	BEN-BAS-5c03e89e-1_2
SMILES:	<chem>CC(C)(C)[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)O</chem>
RUN:	RUN14
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.11

DAR-DIA-0d514e7d-28_1



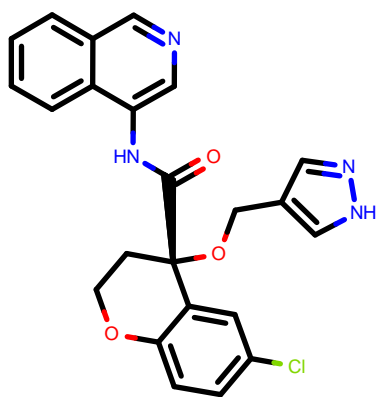
CID:	DAR-DIA-0d514e7d-28_1
SMILES:	<chem>C[C@H]1COc2ccc(cc2[C@]1(C)C(=O)Nc3cncc4c3cccc4)Cl</chem>
RUN:	RUN6
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.09

MAK-UNK-8be7dca9-1_1



CID:	MAK-UNK-8be7dca9-1_1
SMILES:	<chem>c1cc2c(cc1CN3CCNCC3)cncc2NC(=O)[C@@H]4CCOC5c4cc(cc5)Cl</chem>
RUN:	RUN2
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.12

EDJ-MED-28ec730d-4_1



CID: EDJ-MED-28ec730d-4_1

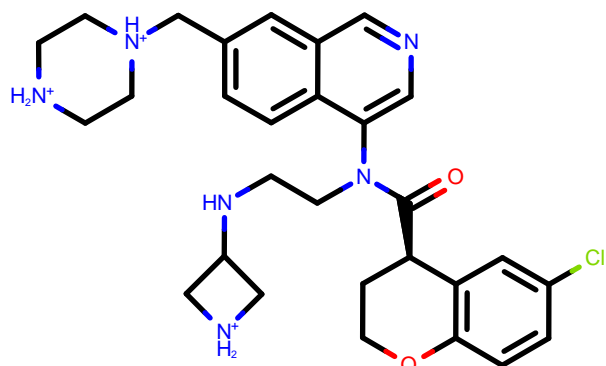
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5c[nH]nc5

RUN: RUN65

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.21

MAK-UNK-83e0a0b4-2_1



CID: MAK-UNK-83e0a0b4-2_1

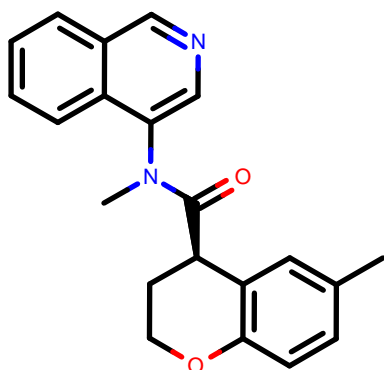
SMILES: c1cc2c(cc1CN3CCNCC3)cnc2N(CCN4CNCC4)C(=O)[C@@]5C@H]5CCOC6c5cc(cc6)Cl

RUN: RUN34

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.33

MAK-UNK-3875bbc8-1_1



CID: MAK-UNK-3875bbc8-1_1

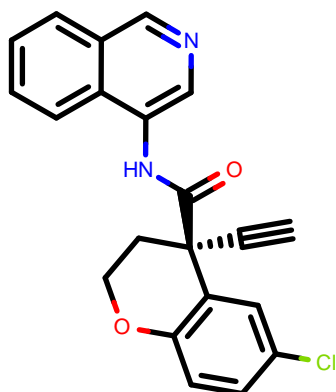
SMILES: Cc1ccc2c(c1)[C@@]3[C@@]4(CCO2)C(=O)N(C)C3cnc4c3cccc4

RUN: RUN32

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.09

PET-UNK-29afea89-1_1



CID: PET-UNK-29afea89-1_1

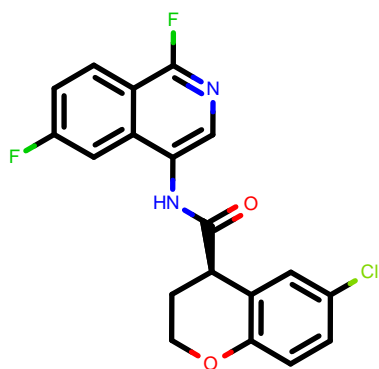
SMILES: C#[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN40

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.10

JOH-SUS-a69c159d-5_1



CID: JOH-SUS-a69c159d-5_1

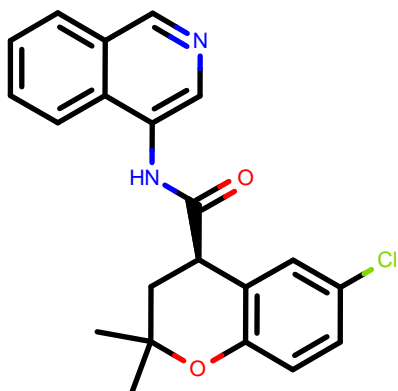
SMILES: c1cc2c(cc1F)c(cnc2F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN52

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.03

ADA-UCB-dc2b944c-16_1



CID: ADA-UCB-dc2b944c-16_1

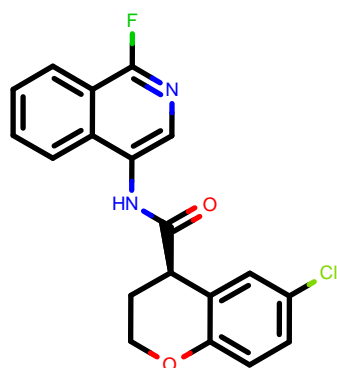
SMILES: CC1(C)[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4)C

RUN: RUN43

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.10

JOH-SUS-a69c159d-2_1



CID: JOH-SUS-a69c159d-2_1

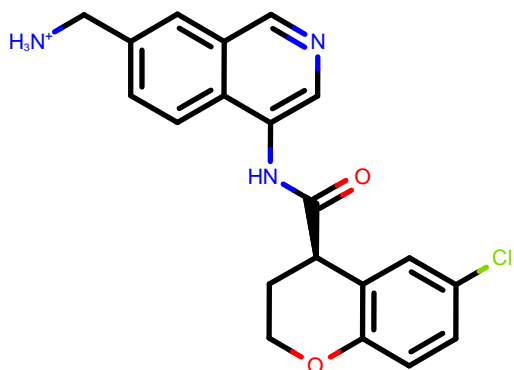
SMILES: c1ccc2c(c1)c(cnc2F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN50

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.03

MAK-UNK-8be7dca9-5_1



CID: MAK-UNK-8be7dca9-5_1

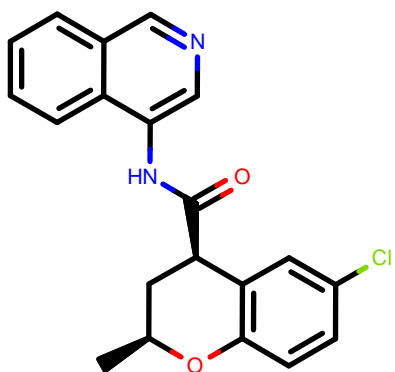
SMILES: c1cc2c(cc1CN)cnc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN19

DDG (kcal/mol): -0.96

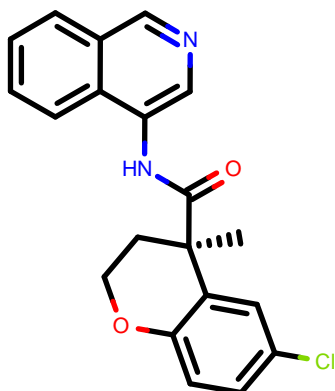
dDDG (kcal/mol): 0.08

ALP-POS-d3acb8cc-1_1



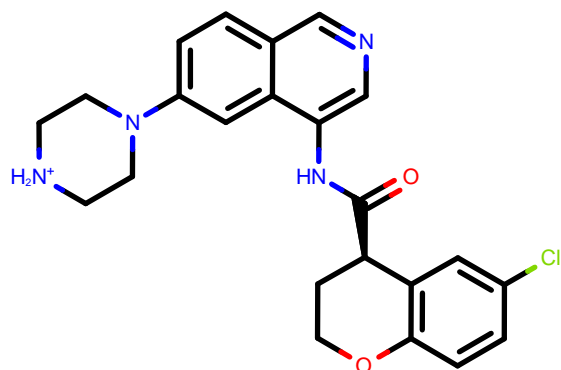
CID:	ALP-POS-d3acb8cc-1_1
SMILES:	<chem>C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN23
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.08

DAR-DIA-6a508060-10_2



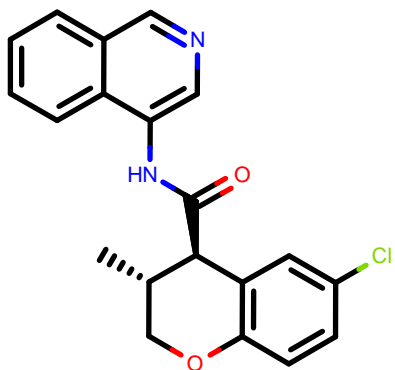
CID:	DAR-DIA-6a508060-10_2
SMILES:	<chem>C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN9
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.10

MAK-UNK-8be7dca9-4_1



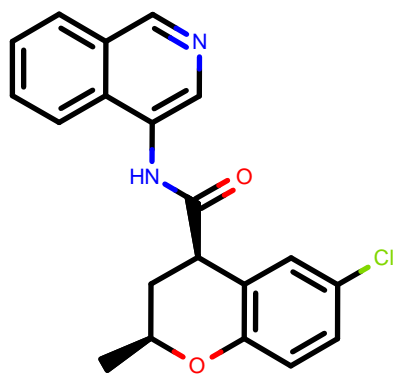
CID:	MAK-UNK-8be7dca9-4_1
SMILES:	<chem>c1cc2nccc(c2cc1N3CCNCC3)NC(=O)[C@@H]4CCOCc5c4cc(cc5)Cl</chem>
RUN:	RUN56
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.08

MAT-POS-8a69d52e-4_2



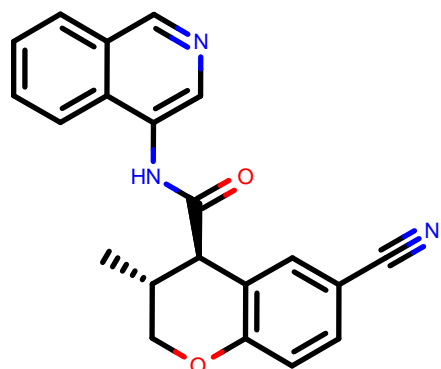
CID:	MAT-POS-8a69d52e-4_2
SMILES:	<chem>C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl</chem>
RUN:	RUN13
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.05

EDJ-MED-e4b030d8-3_1



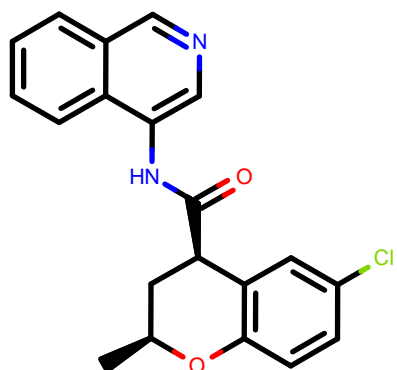
CID:	EDJ-MED-e4b030d8-3_1
SMILES:	<chem>C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN22
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.09

DAR-DIA-0d514e7d-8_1



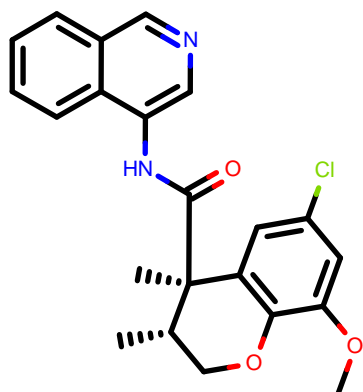
CID:	DAR-DIA-0d514e7d-8_1
SMILES:	<chem>C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)C#N</chem>
RUN:	RUN18
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.07

MAT-POS-8a69d52e-1_4



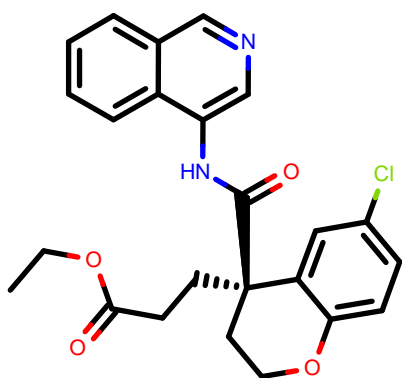
CID:	MAT-POS-8a69d52e-1_4
SMILES:	<chem>C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN21
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.09

DAR-DIA-0d514e7d-25_1



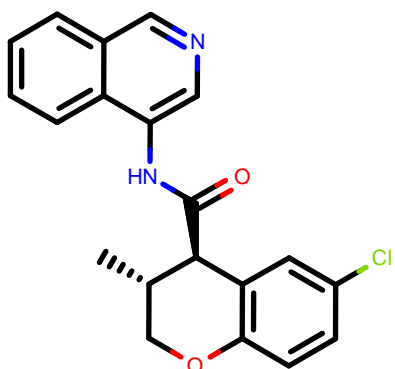
CID:	DAR-DIA-0d514e7d-25_1
SMILES:	<chem>C[C@H]1COc2c(cc(cc2OC)Cl)[C@]1(C)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN73
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.13

JAG-UCB-706446eb-4_1



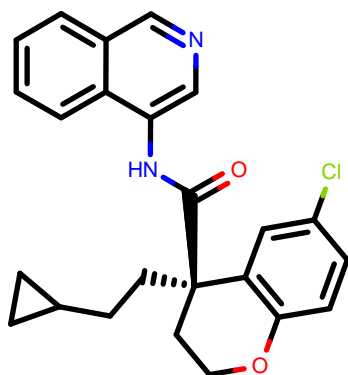
CID:	JAG-UCB-706446eb-4_1
SMILES:	<chem>CCOC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.21

EDJ-MED-e4b030d8-11_1



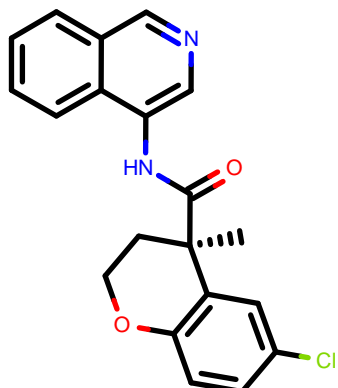
CID:	EDJ-MED-e4b030d8-11_1
SMILES:	<chem>C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl</chem>
RUN:	RUN12
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.06

ALP-POS-477dc5b7-3_1



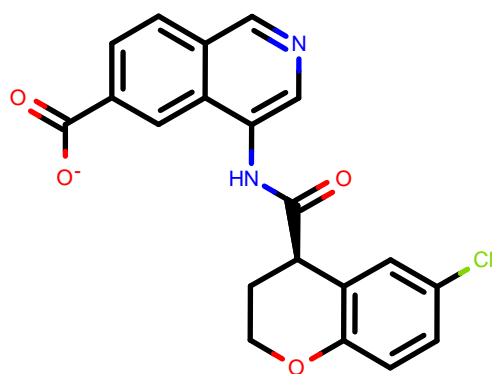
CID:	ALP-POS-477dc5b7-3_1
SMILES:	<chem>c1ccc2c(e1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CC5</chem>
RUN:	RUN96
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.21

EDJ-MED-e4b030d8-13_1



CID:	EDJ-MED-e4b030d8-13_1
SMILES:	<chem>C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN8
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.09

MAK-UNK-8be7dca9-7_1



CID: MAK-UNK-8be7dca9-7_1

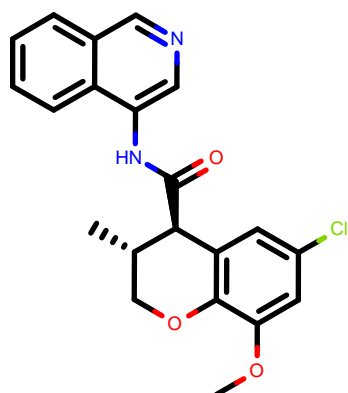
SMILES: c1cc2cnc(c2cc1C(=O)O)NC(=O)[C@@H]3CCOCc4cc(cc4)Cl

RUN: RUN29

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.08

DAR-DIA-0d514e7d-1_1



CID: DAR-DIA-0d514e7d-1_1

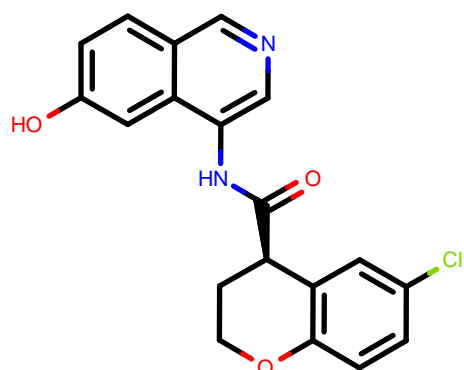
SMILES: C[C@H]1COc2c(cc2OC)Cl][C@@H]1C(=O)Nc3cnc4c3ccccc4

RUN: RUN79

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.11

BEN-DND-c852c98b-4_1



CID: BEN-DND-c852c98b-4_1

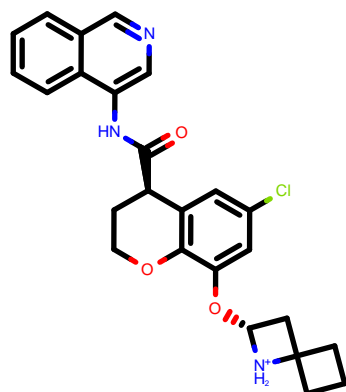
SMILES: c1cc2cnc(c2cc1O)NC(=O)[C@@H]3CCOCc4cc(cc4)Cl

RUN: RUN33

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.04

DAR-DIA-23e5a6a0-2_1



CID: DAR-DIA-23e5a6a0-2_1

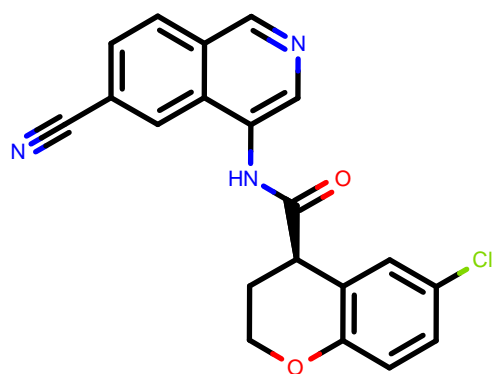
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4ccc(cc4O)[C@@H]5CC6(N5)C(C6)Cl

RUN: RUN81

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.36

BEN-DND-c852c98b-1_1



CID: BEN-DND-c852c98b-1_1

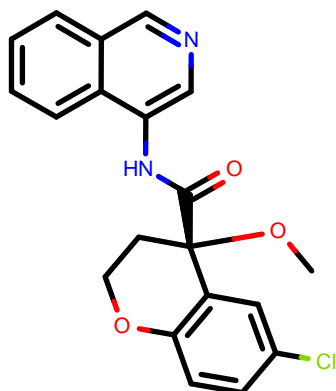
SMILES: c1cc2cncc(c2cc1C#N)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN25

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.04

PET-UNK-29afea89-2_1



CID: PET-UNK-29afea89-2_1

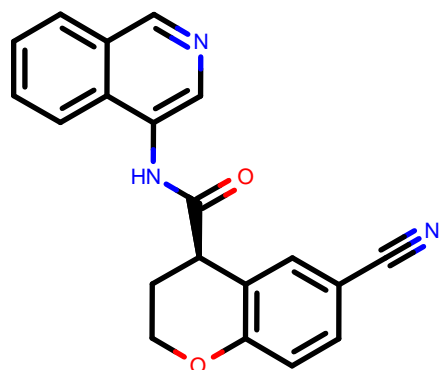
SMILES: CO[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN55

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.13

DAR-DIA-6a508060-3_1



CID: DAR-DIA-6a508060-3_1

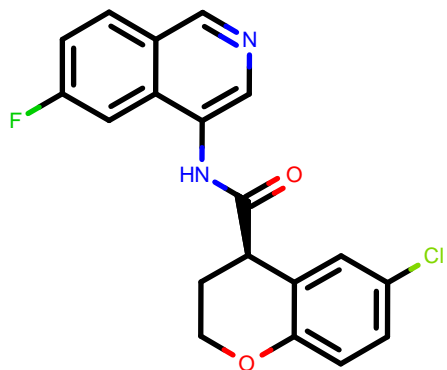
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)C#N

RUN: RUN26

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.06

ALP-POS-696356e4-1_1



CID: ALP-POS-696356e4-1_1

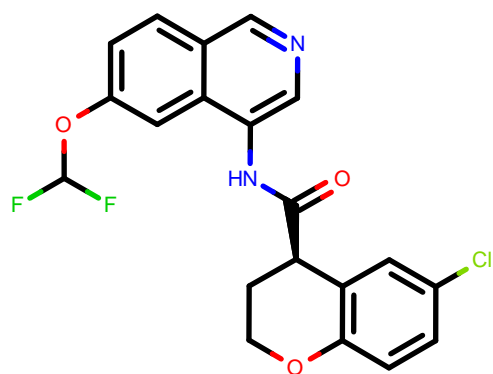
SMILES: c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN20

DDG (kcal/mol): -0.16

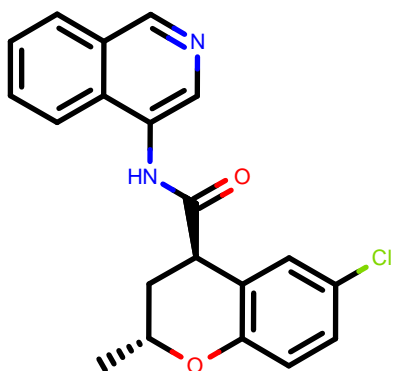
dDDG (kcal/mol): 0.03

BEN-DND-c852c98b-6_1



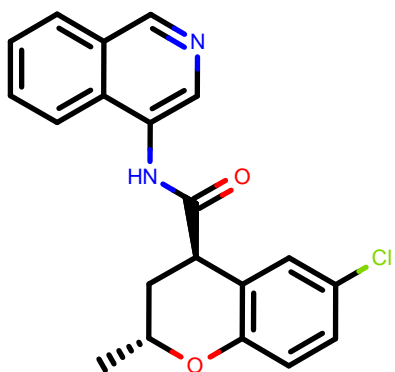
CID:	BEN-DND-c852c98b-6_1
SMILES:	<chem>c1cc2cncc(c2cc1OC(F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN53
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.06

MAT-POS-8a69d52e-1_3



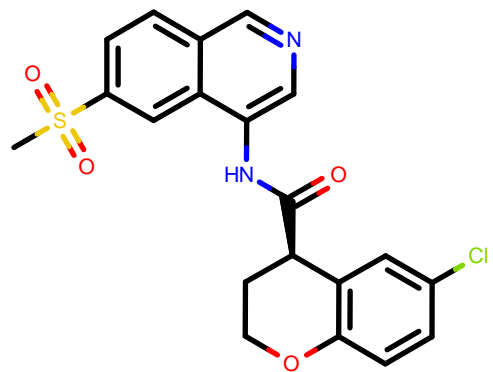
CID:	MAT-POS-8a69d52e-1_3
SMILES:	<chem>C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN37
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.04

EDJ-MED-e4b030d8-2_1



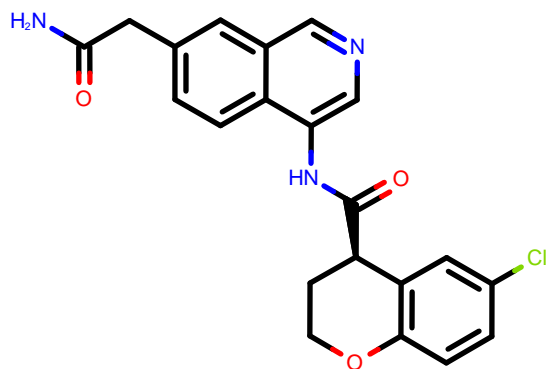
CID:	EDJ-MED-e4b030d8-2_1
SMILES:	<chem>C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN36
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.04

BEN-DND-c852c98b-5_1



CID:	BEN-DND-c852c98b-5_1
SMILES:	<chem>CS(=O)(=O)c1ccc2cncc(c2c1)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN54
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.08

MAK-UNK-8be7dca9-2_1



CID: MAK-UNK-8be7dca9-2_1

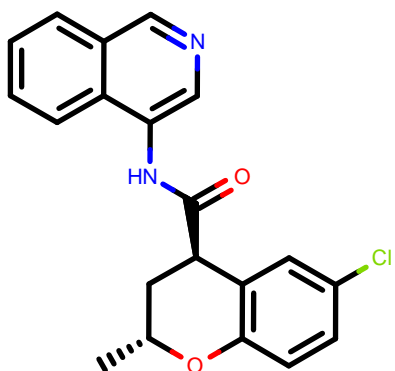
SMILES: c1cc2c(cc1CC(=O)N)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN59

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.09

ALP-POS-d3acb8cc-4_1



CID: ALP-POS-d3acb8cc-4_1

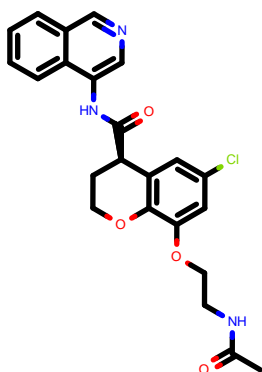
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN38

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.05

NAU-LAT-0543f7f2-10_2



CID: NAU-LAT-0543f7f2-10_2

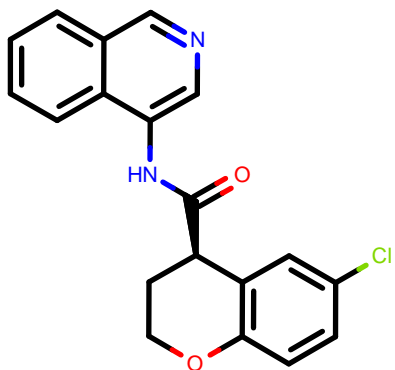
SMILES: CC(=O)NCCOc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN60

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.33

MAT-POS-f7918075-1_1



CID: MAT-POS-f7918075-1_1

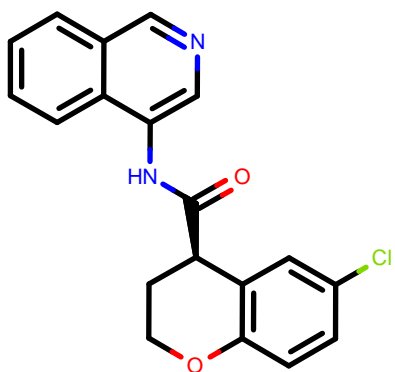
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN17

DDG (kcal/mol): 0.01

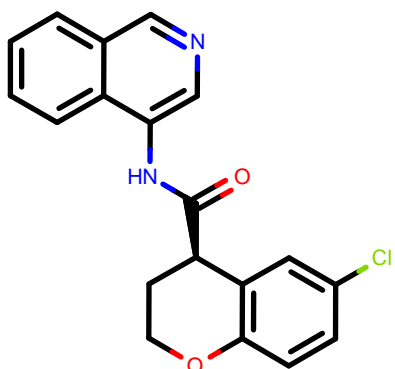
dDDG (kcal/mol): 0.03

VLA-UCB-1dbca3b4-15_1



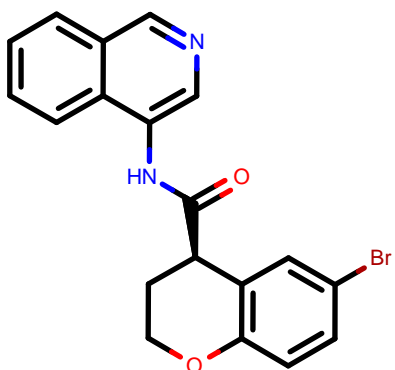
CID:	VLA-UCB-1dbca3b4-15_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN15
DDG (kcal/mol):	0.01
dDDG (kcal/mol):	0.02

MAT-POS-b3e365b9-1_1



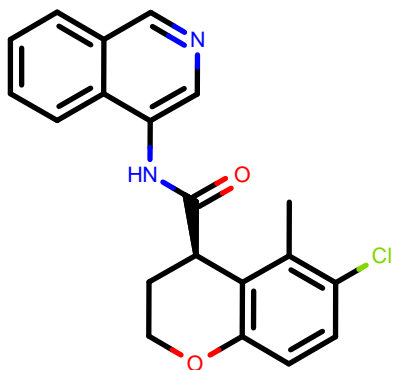
CID:	MAT-POS-b3e365b9-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN16
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.02

MAT-POS-11b63608-1_1



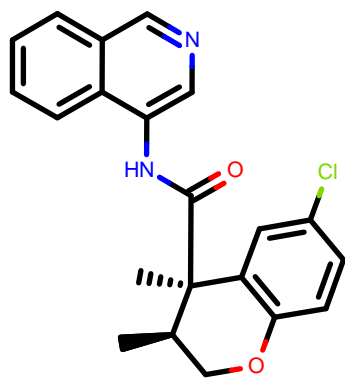
CID:	MAT-POS-11b63608-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)Br</chem>
RUN:	RUN39
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.05

EDJ-MED-e4b030d8-8_1



CID:	EDJ-MED-e4b030d8-8_1
SMILES:	<chem>Cc1c(ccc2c1[C@@H](CCO2)C(=O)Nc3cncc4c3ccc4)Cl</chem>
RUN:	RUN44
DDG (kcal/mol):	0.03
dDDG (kcal/mol):	0.08

DAR-DIA-0d514e7d-29_1



CID: DAR-DIA-0d514e7d-29_1

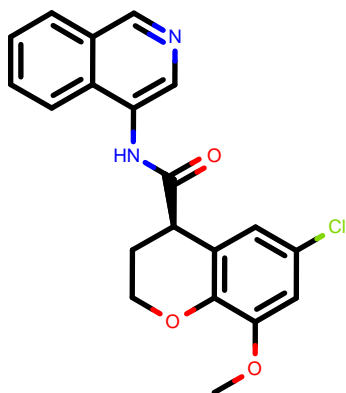
SMILES: C[C@@H]1COc2ccc(cc2[C@]1(C)C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN85

DDG (kcal/mol): 0.06

dDDG (kcal/mol): 0.17

EDJ-MED-e4b030d8-7_1



CID: EDJ-MED-e4b030d8-7_1

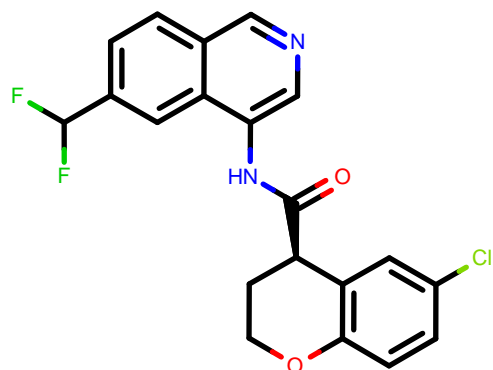
SMILES: COc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN83

DDG (kcal/mol): 0.09

dDDG (kcal/mol): 0.14

BEN-DND-c852c98b-7_1



CID: BEN-DND-c852c98b-7_1

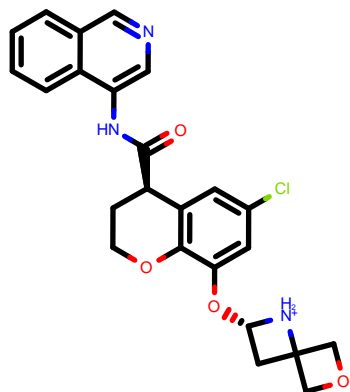
SMILES: c1cc2cncc(c2cc1C(F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN35

DDG (kcal/mol): 0.18

dDDG (kcal/mol): 0.05

DAR-DIA-23e5a6a0-3_2



CID: DAR-DIA-23e5a6a0-3_2

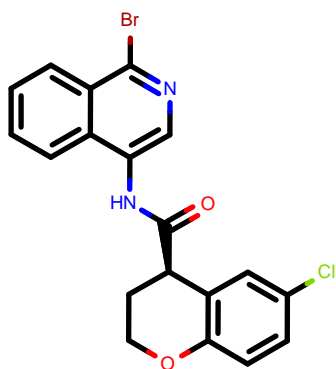
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O)[C@H]5CC6(N5)COC6)Cl

RUN: RUN91

DDG (kcal/mol): 0.19

dDDG (kcal/mol): 0.49

ADA-UCB-dc2b944c-11_1



CID: ADA-UCB-dc2b944c-11_1

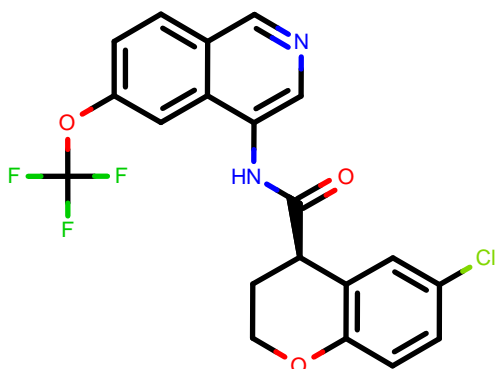
SMILES: c1ccc2c(c1)c(cnc2Br)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN67

DDG (kcal/mol): 0.20

dDDG (kcal/mol): 0.07

BEN-DND-c852c98b-2_1



CID: BEN-DND-c852c98b-2_1

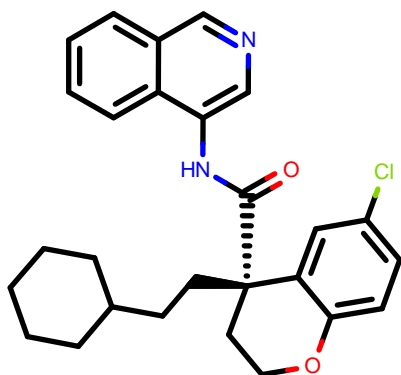
SMILES: c1cc2nc(c2cc1OC(F)(F)F)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN61

DDG (kcal/mol): 0.23

dDDG (kcal/mol): 0.06

VLA-UCB-05e51b3f-13_1



CID: VLA-UCB-05e51b3f-13_1

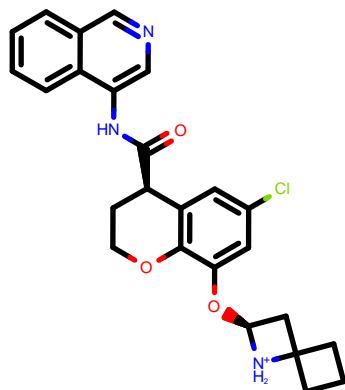
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCCCC5

RUN: RUN89

DDG (kcal/mol): 0.24

dDDG (kcal/mol): 0.28

DAR-DIA-23e5a6a0-2_2



CID: DAR-DIA-23e5a6a0-2_2

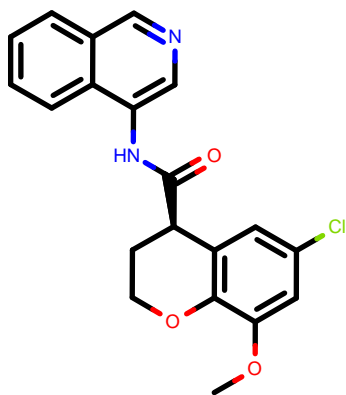
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOCc4c3cc(cc4O)[C@H]5CC6(N5)CCC6)Cl

RUN: RUN88

DDG (kcal/mol): 0.33

dDDG (kcal/mol): 0.31

DAR-DIA-6a508060-4_2



CID: DAR-DIA-6a508060-4_2

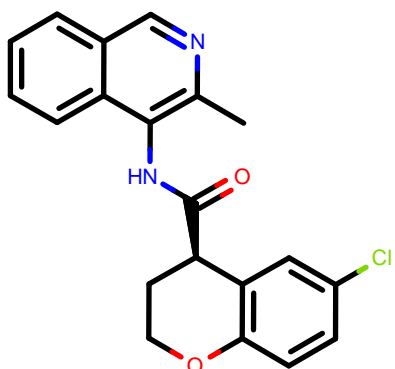
SMILES: COc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN82

DDG (kcal/mol): 0.35

dDDG (kcal/mol): 0.10

ADA-UCB-dc2b944c-10_1



CID: ADA-UCB-dc2b944c-10_1

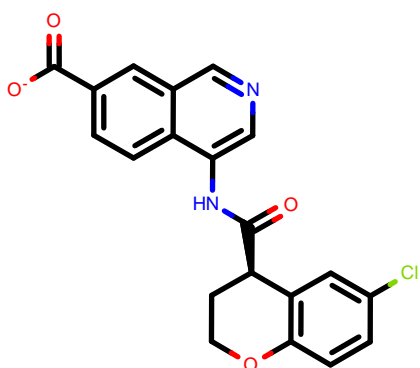
SMILES: Cc1c(c2cccc2cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN51

DDG (kcal/mol): 0.39

dDDG (kcal/mol): 0.09

MAK-UNK-8be7dca9-9_1



CID: MAK-UNK-8be7dca9-9_1

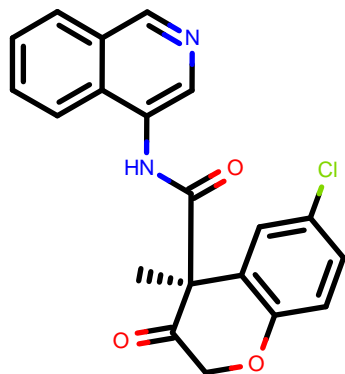
SMILES: c1cc2c(cc1C(=O)O)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN47

DDG (kcal/mol): 0.60

dDDG (kcal/mol): 0.06

EDJ-MED-e4b030d8-1_1



CID: EDJ-MED-e4b030d8-1_1

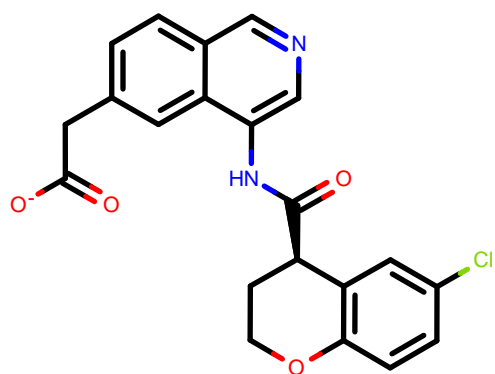
SMILES: C[C@@]1(c2cc(ccc2OCC1=O)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN11

DDG (kcal/mol): 0.64

dDDG (kcal/mol): 0.10

MAK-UNK-8be7dca9-8_1



CID: MAK-UNK-8be7dca9-8_1

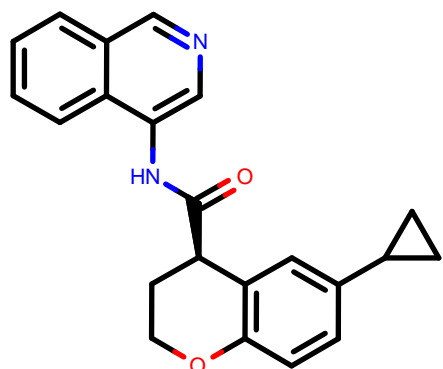
SMILES: c1cc2cncc(c2cc1CC(=O)O)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN57

DDG (kcal/mol): 0.65

dDDG (kcal/mol): 0.07

DAR-DIA-6a508060-8_1



CID: DAR-DIA-6a508060-8_1

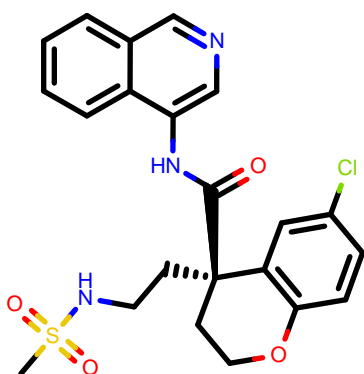
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)C5CC5

RUN: RUN68

DDG (kcal/mol): 0.71

dDDG (kcal/mol): 0.11

DAR-DIA-6a508060-13_2



CID: DAR-DIA-6a508060-13_2

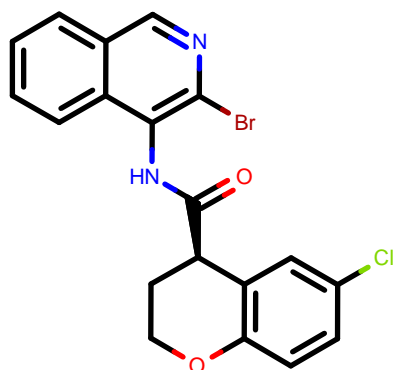
SMILES: CS(=O)(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN28

DDG (kcal/mol): 0.72

dDDG (kcal/mol): 0.27

ADA-UCB-dc2b944c-9_1



CID: ADA-UCB-dc2b944c-9_1

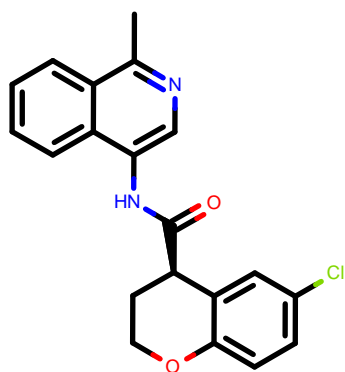
SMILES: c1ccc2c(c1)nc(c2NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl)Br

RUN: RUN58

DDG (kcal/mol): 0.75

dDDG (kcal/mol): 0.12

ADA-UCB-dc2b944c-12_1



CID: ADA-UCB-dc2b944c-12_1

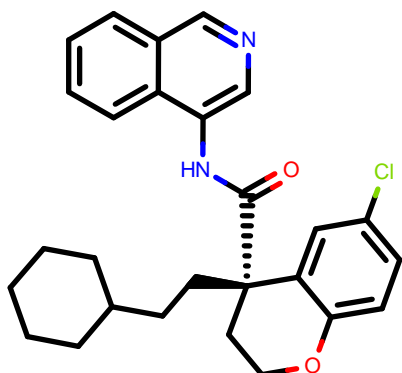
SMILES: Cc1c2ccccc2c(cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN64

DDG (kcal/mol): 0.81

dDDG (kcal/mol): 0.05

DAR-DIA-6a508060-9_2



CID: DAR-DIA-6a508060-9_2

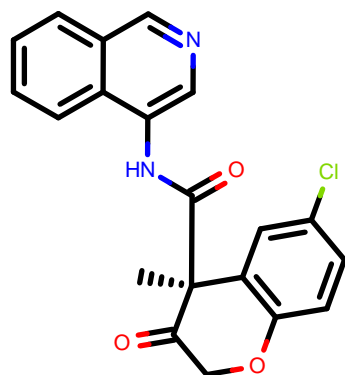
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CCCC5

RUN: RUN90

DDG (kcal/mol): 0.82

dDDG (kcal/mol): 0.27

VLA-UCB-1dbca3b4-14_1



CID: VLA-UCB-1dbca3b4-14_1

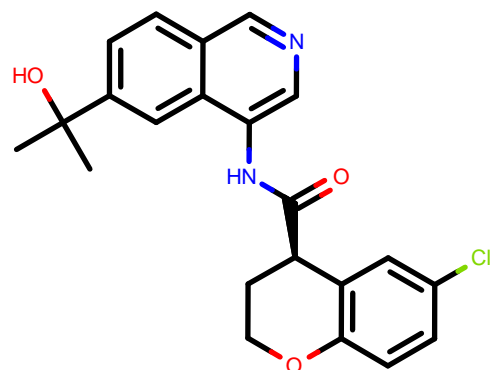
SMILES: C[C@@]1(c2cc(ccc2OCC1=O)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN10

DDG (kcal/mol): 0.85

dDDG (kcal/mol): 0.10

BEN-DND-c852c98b-3_1



CID: BEN-DND-c852c98b-3_1

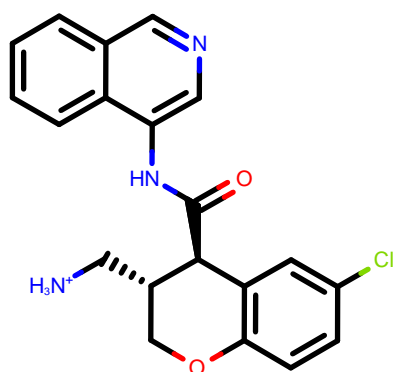
SMILES: CC(C)(c1ccc2nccc(c2c1)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O

RUN: RUN45

DDG (kcal/mol): 0.86

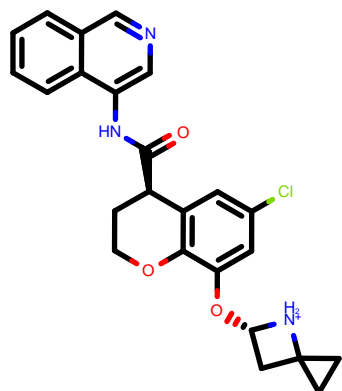
dDDG (kcal/mol): 0.08

MAK-UNK-8be7dca9-3_2



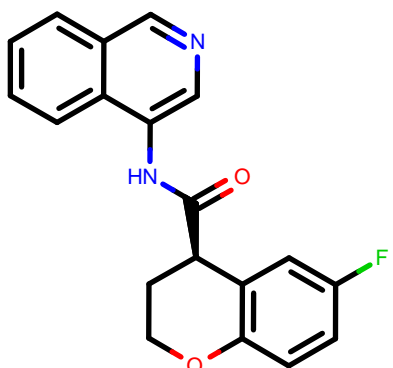
CID:	MAK-UNK-8be7dca9-3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3c4cc(ccc4OC[C@@H]3CN)Cl</chem>
RUN:	RUN48
DDG (kcal/mol):	0.90
dDDG (kcal/mol):	0.13

DAR-DIA-23e5a6a0-5_2



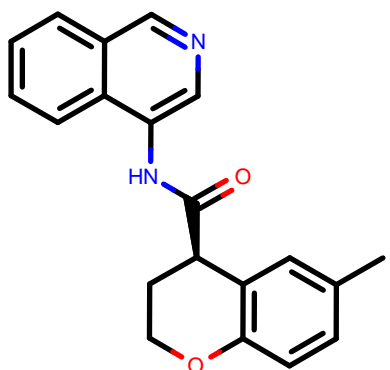
CID:	DAR-DIA-23e5a6a0-5_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4O[C@@H]5CC6(N5)CC6)Cl</chem>
RUN:	RUN80
DDG (kcal/mol):	0.96
dDDG (kcal/mol):	0.30

ADA-UCB-dc2b944c-7_1



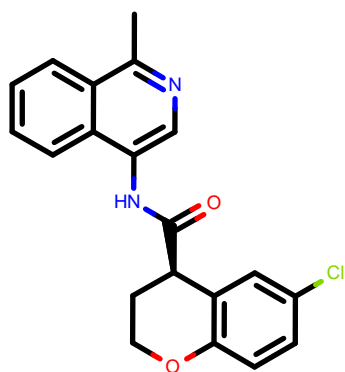
CID:	ADA-UCB-dc2b944c-7_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4)F</chem>
RUN:	RUN4
DDG (kcal/mol):	0.98
dDDG (kcal/mol):	0.06

ADA-UCB-dc2b944c-5_1



CID:	ADA-UCB-dc2b944c-5_1
SMILES:	<chem>Cc1ccc2c(c1)[C@@H]3(CCO2)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN5
DDG (kcal/mol):	1.01
dDDG (kcal/mol):	0.05

JOH-SUS-a69c159d-1_1



CID: JOH-SUS-a69c159d-1_1

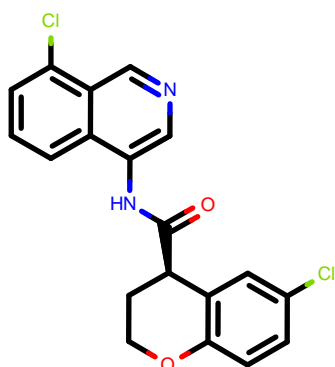
SMILES: Cc1c2cccc2c(cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN63

DDG (kcal/mol): 1.06

dDDG (kcal/mol): 0.05

ADA-UCB-dc2b944c-8_1



CID: ADA-UCB-dc2b944c-8_1

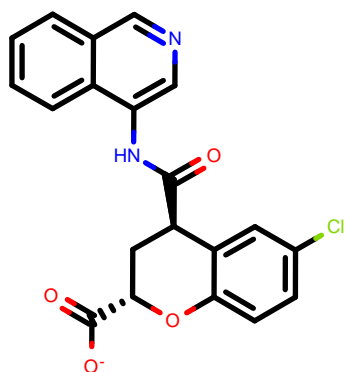
SMILES: c1cc2c(cnc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)c(c1)Cl

RUN: RUN30

DDG (kcal/mol): 1.27

dDDG (kcal/mol): 0.05

MAK-UNK-8be7dca9-10_3



CID: MAK-UNK-8be7dca9-10_3

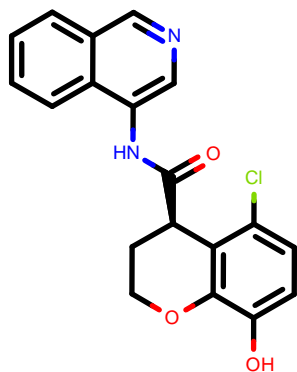
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3C[C@H](Oc4c3cc(cc4)Cl)C(=O)O

RUN: RUN86

DDG (kcal/mol): 1.50

dDDG (kcal/mol): 0.08

ALP-UNI-4b8a177c-1_1



CID: ALP-UNI-4b8a177c-1_1

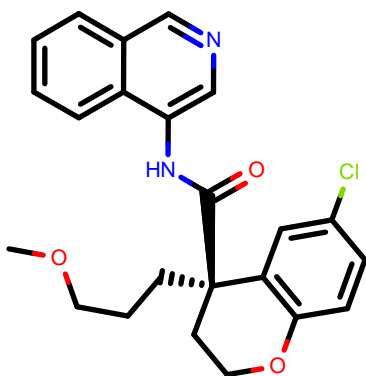
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOc4c3c(ccc4O)Cl

RUN: RUN74

DDG (kcal/mol): 2.03

dDDG (kcal/mol): 0.18

EDJ-MED-28ec730d-1_1



CID: EDJ-MED-28ec730d-1_1

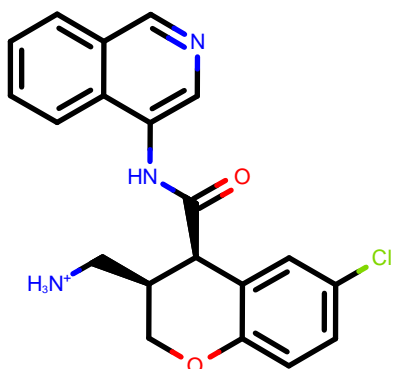
SMILES: COCCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN62

DDG (kcal/mol): 2.22

dDDG (kcal/mol): 0.22

MAK-UNK-8be7dca9-3_4



CID: MAK-UNK-8be7dca9-3_4

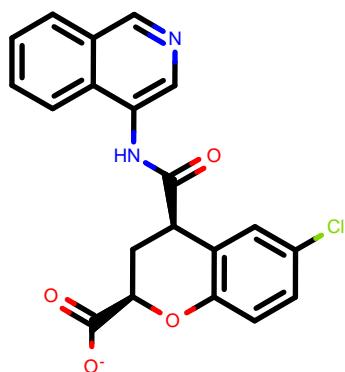
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4OC[C@H]3CN)Cl

RUN: RUN24

DDG (kcal/mol): 2.31

dDDG (kcal/mol): 0.14

MAK-UNK-8be7dca9-10_1



CID: MAK-UNK-8be7dca9-10_1

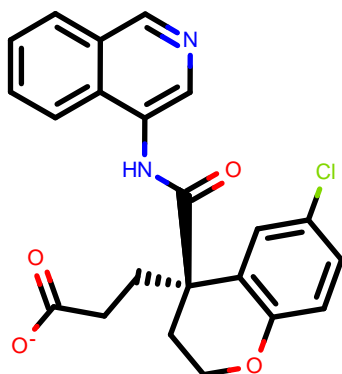
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[C@@H](O4c3cc(cc4)Cl)C(=O)O

RUN: RUN66

DDG (kcal/mol): 3.09

dDDG (kcal/mol): 0.12

JAG-UCB-706446eb-3_1



CID: JAG-UCB-706446eb-3_1

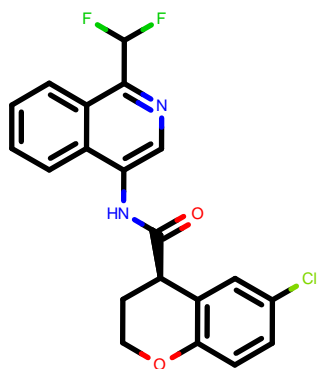
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCC(=O)O

RUN: RUN3

DDG (kcal/mol): 3.23

dDDG (kcal/mol): 0.24

JOH-SUS-a69c159d-3_1



CID: JOH-SUS-a69c159d-3_1

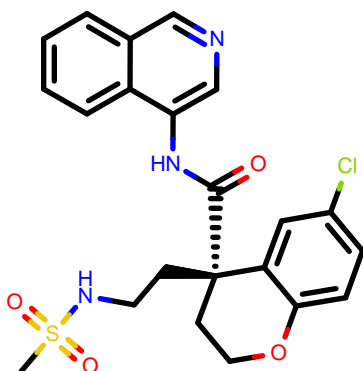
SMILES: c1ccc2c(c1)c(cnc2C(F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN98

DDG (kcal/mol): 3.81

dDDG (kcal/mol): 0.15

DAR-DIA-6a508060-13_1



CID: DAR-DIA-6a508060-13_1

SMILES: CS(=O)(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN99

DDG (kcal/mol): 4.51

dDDG (kcal/mol): 0.27