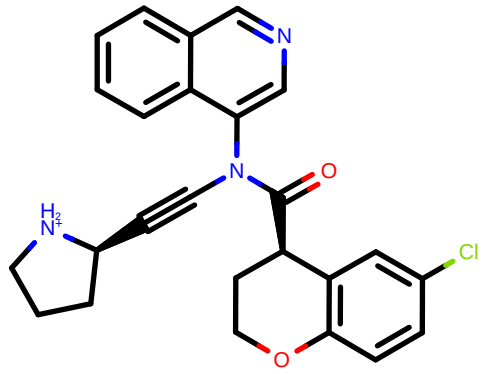
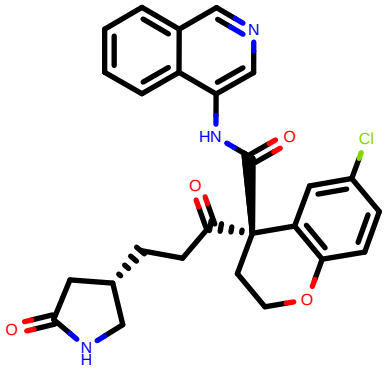
DAR-DIA-5ff57136-12_2



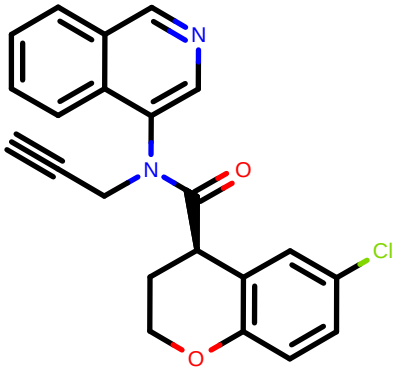
CID:	DAR-DIA-5ff57136-12_2
SMILES:	c1ccc2c(c1)cncc2N(C#C[C@H]3CCCN3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN95
DDG (kcal/mol):	-2.87
dDDG (kcal/mol):	0.22

VLA-UCB-34f3ed0c-21_2



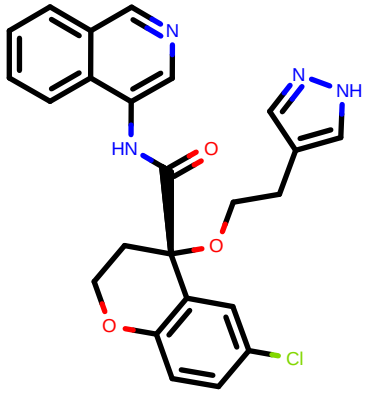
CID:	VLA-UCB-34f3ed0c-21_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@H]5CC(=O)NC5
RUN:	RUN0
DDG (kcal/mol):	-2.78
dDDG (kcal/mol):	0.37

DAR-DIA-5ff57136-13_1



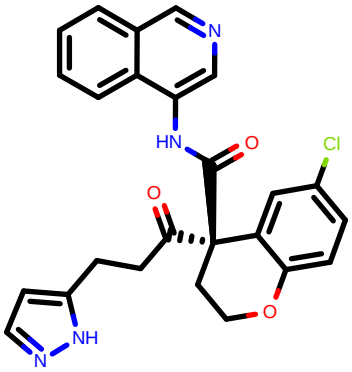
CID:	DAR-DIA-5ff57136-13_1
SMILES:	C#CCN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN92
DDG (kcal/mol):	-2.73
dDDG (kcal/mol):	0.13

EDJ-MED-28ec730d-5_1



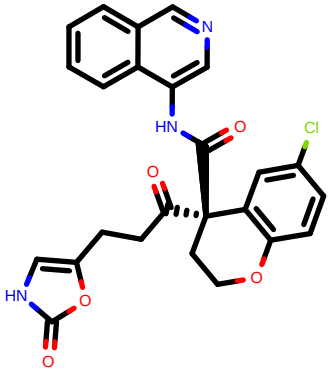
CID:	EDJ-MED-28ec730d-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5c[nH]nc5
RUN:	RUN31
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.23

VLA-UCB-34f3ed0c-8_1



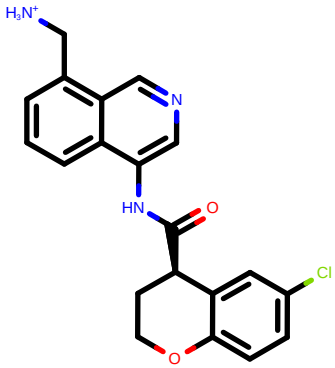
CID:	VLA-UCB-34f3ed0c-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5cc[nH]n5
RUN:	RUN76
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.22

VLA-UCB-34f3ed0c-9_1



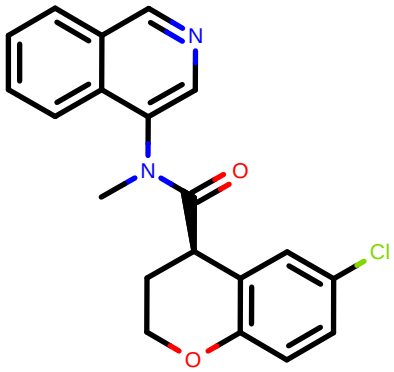
CID:	VLA-UCB-34f3ed0c-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5c[nH]c(=O)o5
RUN:	RUN72
DDG (kcal/mol):	-2.59
dDDG (kcal/mol):	0.27

MAK-UNK-8be7dca9-6_1



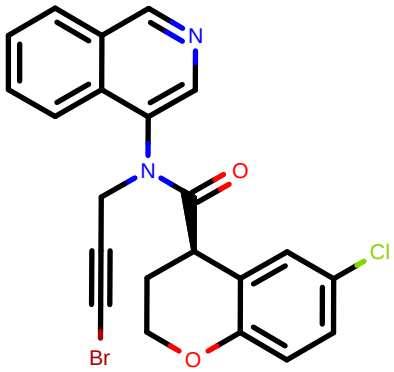
CID:	MAK-UNK-8be7dca9-6_1
SMILES:	c1cc(c2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)CN
RUN:	RUN42
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.09

MAK-UNK-3875bbc8-2_1



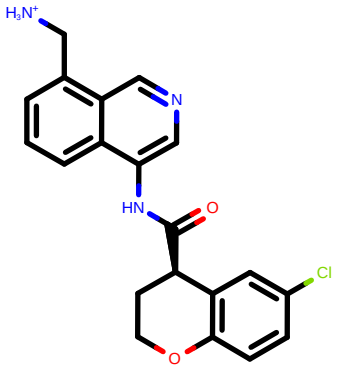
CID:	MAK-UNK-3875bbc8-2_1
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN49
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.07

DAR-DIA-5ff57136-17_1



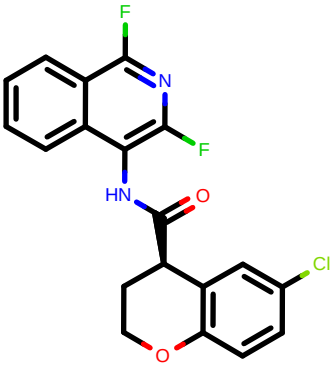
CID:	DAR-DIA-5ff57136-17_1
SMILES:	c1ccc2c(c1)cncc2N(CC#CBr)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN69
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.17

NAU-LAT-b7d8c353-8_1



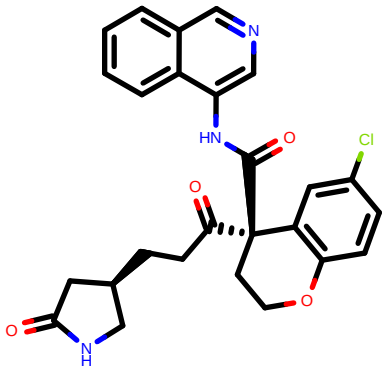
CID:	NAU-LAT-b7d8c353-8_1
SMILES:	c1cc(c2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)CN
RUN:	RUN41
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.09

JOH-SUS-a69c159d-6_1



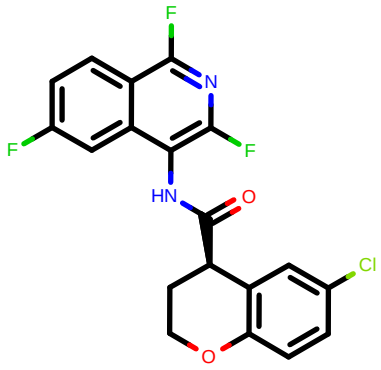
CID:	JOH-SUS-a69c159d-6_1
SMILES:	c1ccc2c(c1)c(c(nc2F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN70
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.05

VLA-UCB-34f3ed0c-21_1



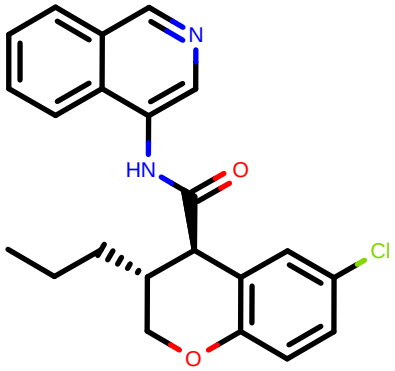
CID:	VLA-UCB-34f3ed0c-21_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@@H]5CC(=O)NC5
RUN:	RUN27
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.31

JOH-SUS-a69c159d-7_1



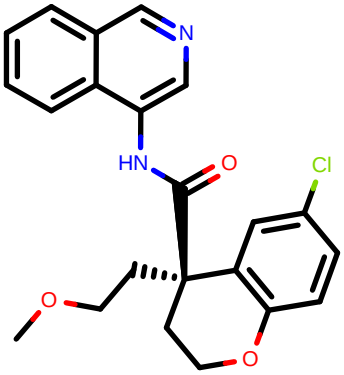
CID:	JOH-SUS-a69c159d-7_1
SMILES:	c1cc2c(cc1F)c(c(nc2F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN71
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.05

EDJ-MED-e4b030d8-6_1



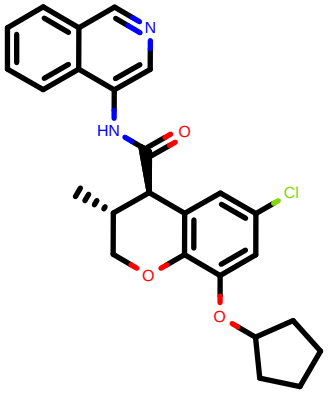
CID:	EDJ-MED-e4b030d8-6_1
SMILES:	CCC[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN7
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.10

EDJ-MED-28ec730d-2_1



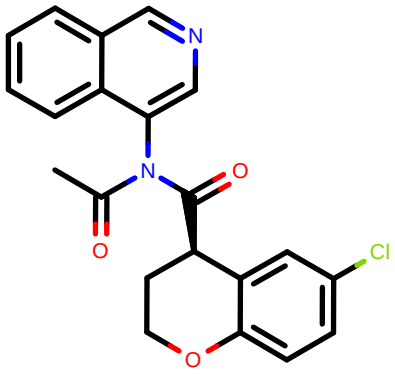
CID:	EDJ-MED-28ec730d-2_1
SMILES:	COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN77
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.17

DAR-DIA-0d514e7d-4_1



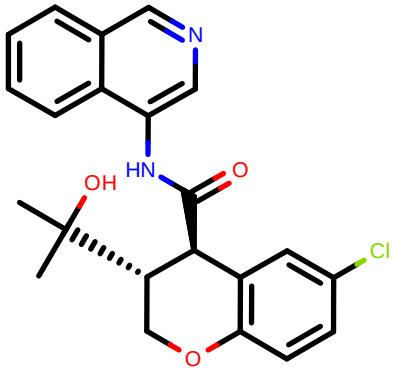
CID:	DAR-DIA-0d514e7d-4_1
SMILES:	C[C@H]1COc2c(cc(cc2OC3CCCC3)Cl)[C@@H]1C(=O)Nc4cncc5c4cccc5
RUN:	RUN93
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.21

VLA-UCB-50c39ae8-1_1



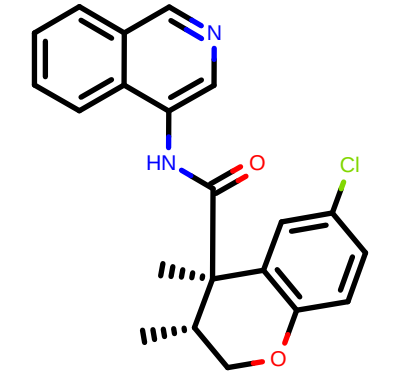
CID:	VLA-UCB-50c39ae8-1_1
SMILES:	CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN94
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.16

BEN-BAS-5c03e89e-1_2



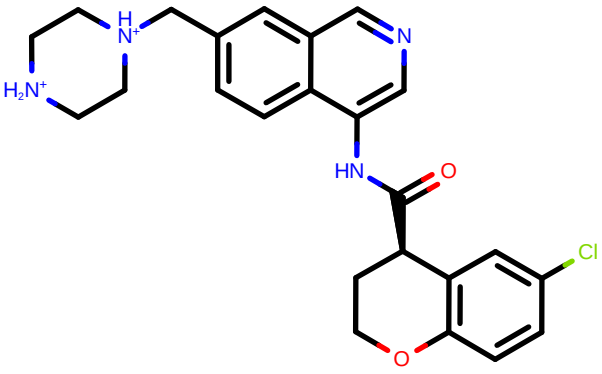
CID:	BEN-BAS-5c03e89e-1_2
SMILES:	CC(C)([C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)O
RUN:	RUN14
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.11

DAR-DIA-0d514e7d-28_1



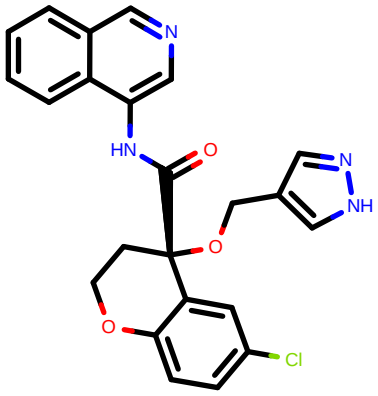
CID:	DAR-DIA-0d514e7d-28_1
SMILES:	C[C@H]1COc2ccc(cc2[C@]1(C)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN6
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.09

MAK-UNK-8be7dca9-1_1



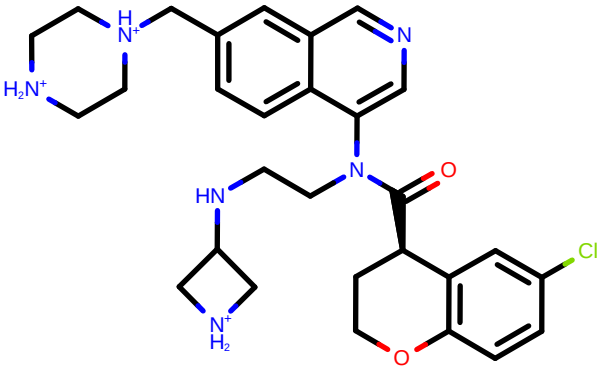
CID:	MAK-UNK-8be7dca9-1_1
SMILES:	c1cc2c(cc1CN3CCNCC3)cncc2NC(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN2
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.12

EDJ-MED-28ec730d-4_1



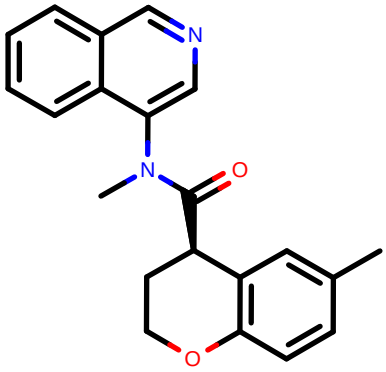
CID:	EDJ-MED-28ec730d-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5c[nH]nc5
RUN:	RUN65
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.21

MAK-UNK-83e0a0b4-2_1



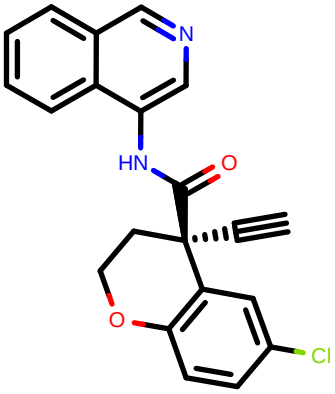
CID:	MAK-UNK-83e0a0b4-2_1
SMILES:	c1cc2c(cc1CN3CCNCC3)cncc2N(CCNC4CNC4)C(=O)[C@@H]5CCOc6c5cc(cc6)Cl
RUN:	RUN34
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.33

MAK-UNK-3875bbc8-1_1



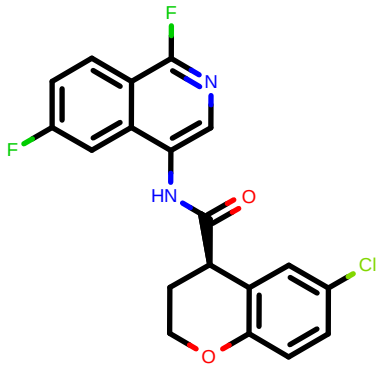
CID:	MAK-UNK-3875bbc8-1_1
SMILES:	Cc1ccc2c(c1)[C@@H](CCO2)C(=O)N(C)c3cncc4c3cccc4
RUN:	RUN32
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.09

PET-UNK-29afea89-1_1



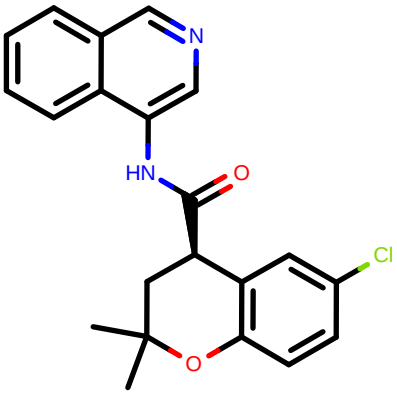
CID:	PET-UNK-29afea89-1_1
SMILES:	C#C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN40
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.10

JOH-SUS-a69c159d-5_1



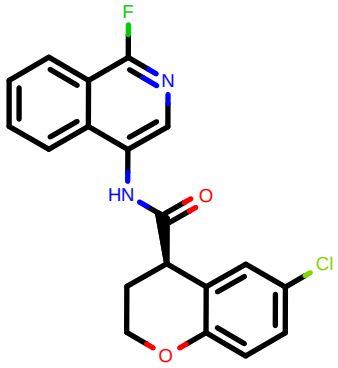
CID:	JOH-SUS-a69c159d-5_1
SMILES:	c1cc2c(cc1F)c(cnc2F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN52
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.03

ADA-UCB-dc2b944c-16_1



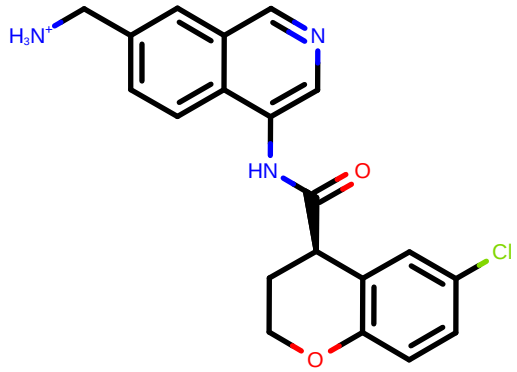
CID:	ADA-UCB-dc2b944c-16_1
SMILES:	CC1(C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4)C
RUN:	RUN43
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.10

JOH-SUS-a69c159d-2_1



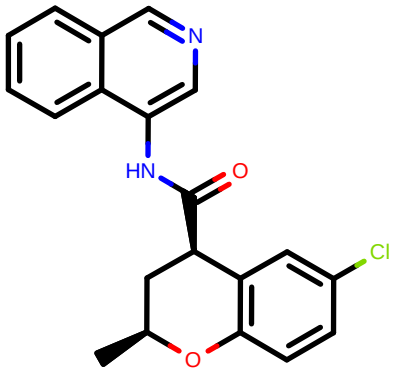
CID:	JOH-SUS-a69c159d-2_1
SMILES:	c1ccc2c(c1)c(cnc2F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN50
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.03

MAK-UNK-8be7dca9-5_1



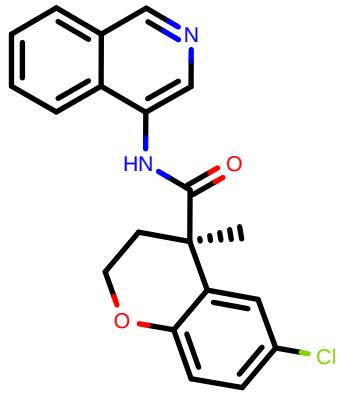
CID:	MAK-UNK-8be7dca9-5_1
SMILES:	c1cc2c(cc1CN)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN19
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.08

ALP-POS-d3acb8cc-1_1



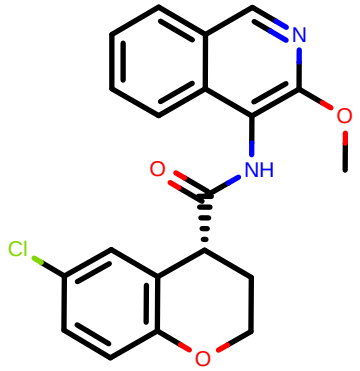
CID:	ALP-POS-d3acb8cc-1_1
SMILES:	C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN23
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.08

DAR-DIA-6a508060-10_2



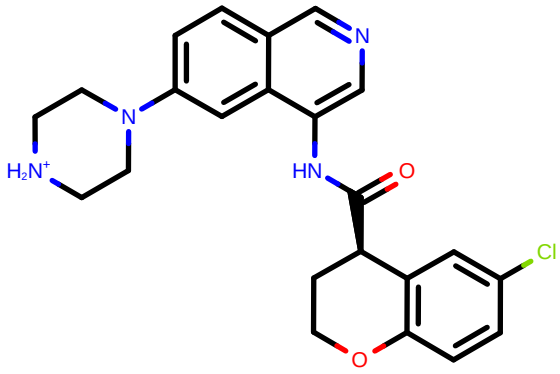
CID:	DAR-DIA-6a508060-10_2
SMILES:	C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.10

JOH-UNI-f51e3bbc-4_1



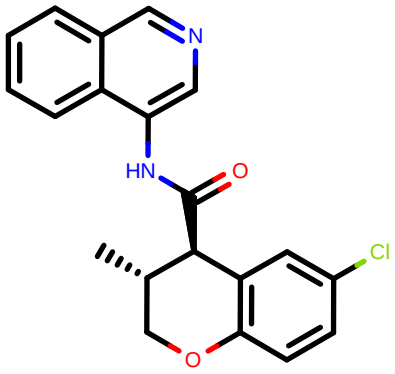
CID:	JOH-UNI-f51e3bbc-4_1
SMILES:	COc1c(c2ccccc2cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN75
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.13

MAK-UNK-8be7dca9-4_1



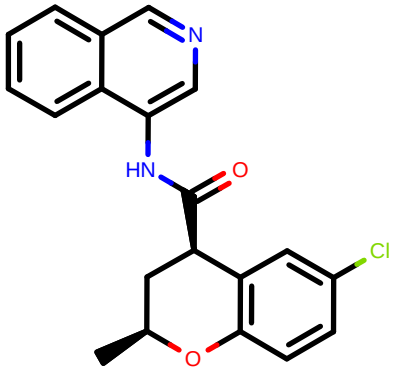
CID:	MAK-UNK-8be7dca9-4_1
SMILES:	c1cc2cncc(c2cc1N3CCNCC3)NC(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN56
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.08

MAT-POS-8a69d52e-4_2



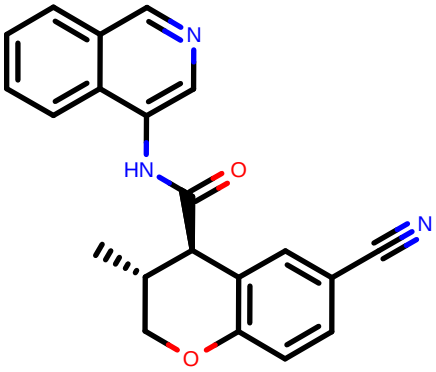
CID:	MAT-POS-8a69d52e-4_2
SMILES:	C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN13
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.05

EDJ-MED-e4b030d8-3_1



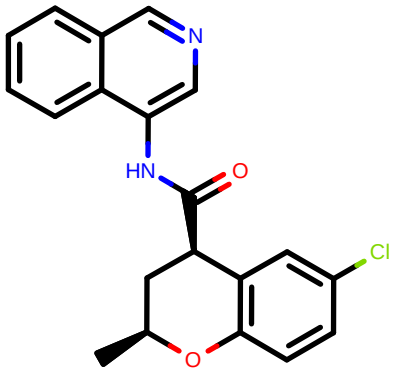
CID:	EDJ-MED-e4b030d8-3_1
SMILES:	C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN22
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.09

DAR-DIA-0d514e7d-8_1



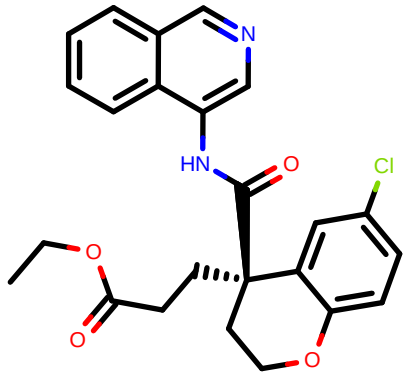
CID:	DAR-DIA-0d514e7d-8_1
SMILES:	C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)C#N
RUN:	RUN18
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.07

MAT-POS-8a69d52e-1_4



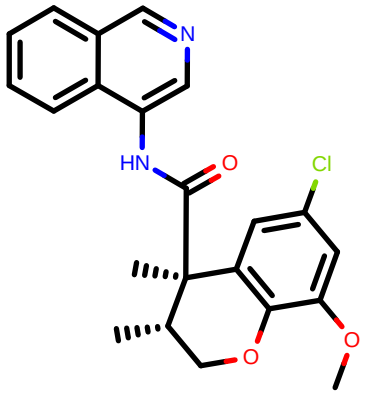
CID:	MAT-POS-8a69d52e-1_4
SMILES:	C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN21
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.09

JAG-UCB-706446eb-4_1



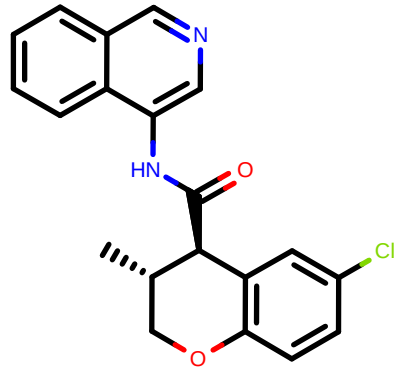
CID:	JAG-UCB-706446eb-4_1
SMILES:	CCOC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.21

DAR-DIA-0d514e7d-25_1



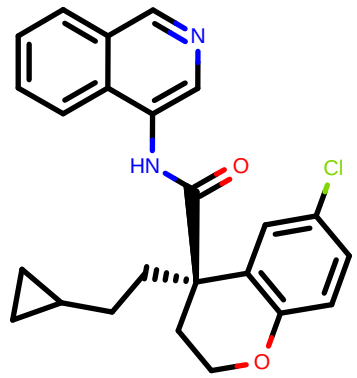
CID:	DAR-DIA-0d514e7d-25_1
SMILES:	C[C@H]1COc2c(cc(cc2OC)Cl)[C@]1(C)C(=O)Nc3cncc4c3cccc4
RUN:	RUN73
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.13

EDJ-MED-e4b030d8-11_1



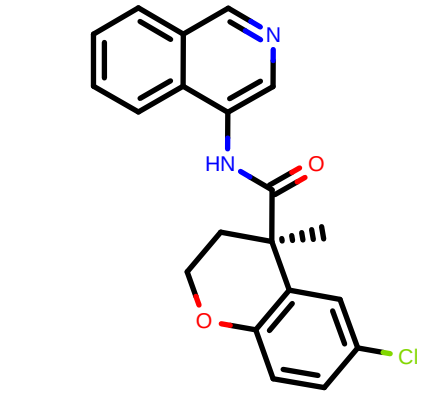
CID:	EDJ-MED-e4b030d8-11_1
SMILES:	C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN12
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.06

ALP-POS-477dc5b7-3_1



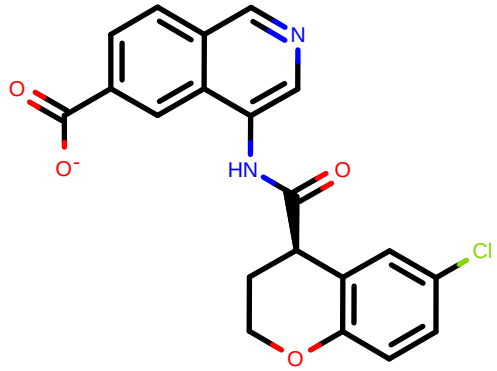
CID:	ALP-POS-477dc5b7-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CC5
RUN:	RUN96
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.21

EDJ-MED-e4b030d8-13_1



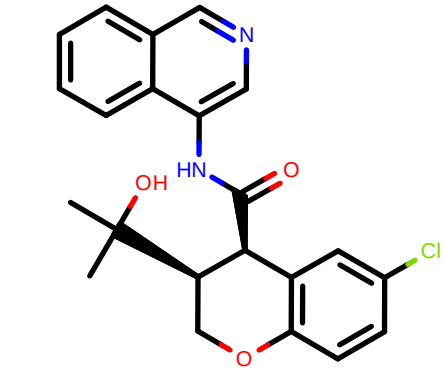
CID:	EDJ-MED-e4b030d8-13_1
SMILES:	C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN8
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.09

MAK-UNK-8be7dca9-7_1



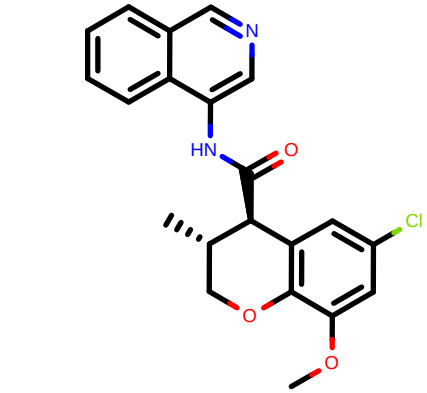
CID:	MAK-UNK-8be7dca9-7_1
SMILES:	c1cc2cncc(c2cc1C(=O)O)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN29
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.08

BEN-BAS-5c03e89e-1_1



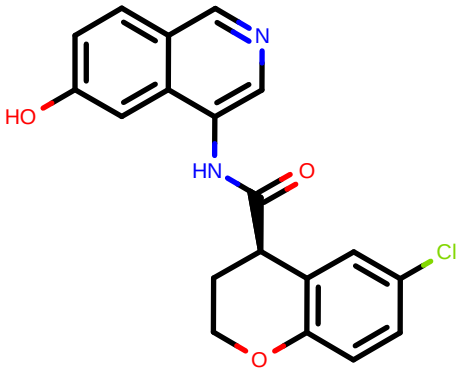
CID:	BEN-BAS-5c03e89e-1_1
SMILES:	CC(C)([C@@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)O
RUN:	RUN97
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.18

DAR-DIA-0d514e7d-1_1



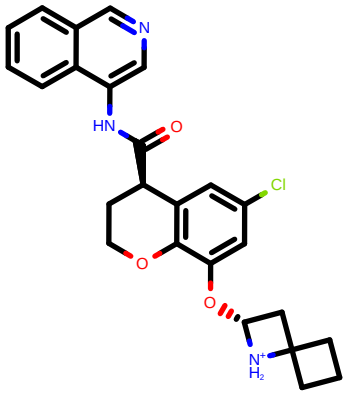
CID:	DAR-DIA-0d514e7d-1_1
SMILES:	C[C@H]1COc2c(cc(cc2OC)Cl)[C@@H]1C(=O)Nc3cncc4c3cccc4
RUN:	RUN79
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.11

BEN-DND-c852c98b-4_1



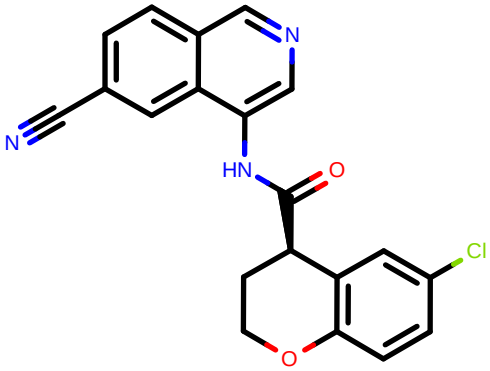
CID:	BEN-DND-c852c98b-4_1
SMILES:	c1cc2cncc(c2cc1O)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN33
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.04

DAR-DIA-23e5a6a0-2_1



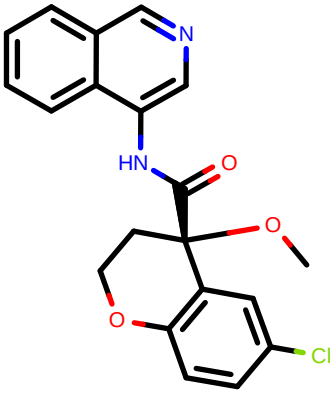
CID:	DAR-DIA-23e5a6a0-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@@H]5CC6(N5)CCC6)Cl
RUN:	RUN81
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.36

BEN-DND-c852c98b-1_1



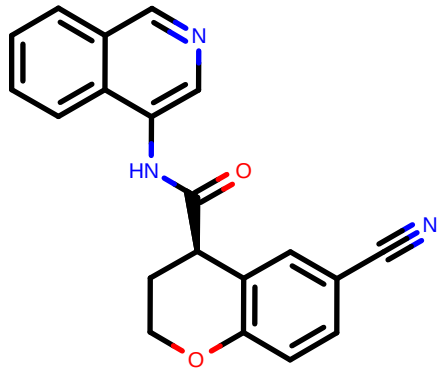
CID:	BEN-DND-c852c98b-1_1
SMILES:	c1cc2cncc(c2cc1C#N)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN25
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.04

PET-UNK-29afea89-2_1



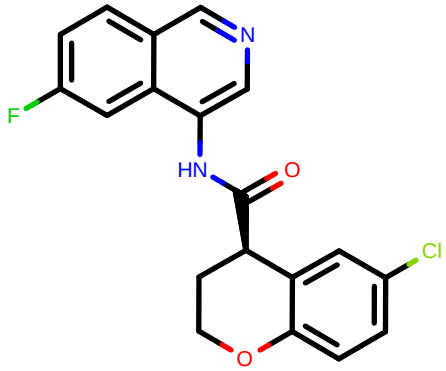
CID:	PET-UNK-29afea89-2_1
SMILES:	CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN55
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.13

DAR-DIA-6a508060-3_1



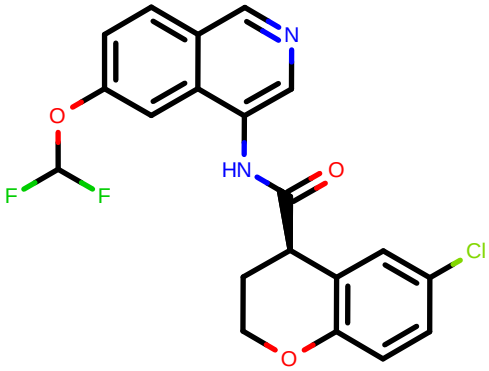
CID:	DAR-DIA-6a508060-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)C#N
RUN:	RUN26
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.06

ALP-POS-696356e4-1_1



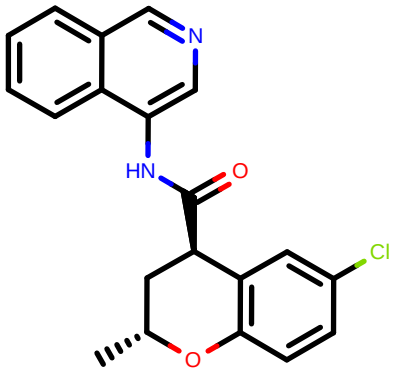
CID:	ALP-POS-696356e4-1_1
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN20
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.03

BEN-DND-c852c98b-6_1



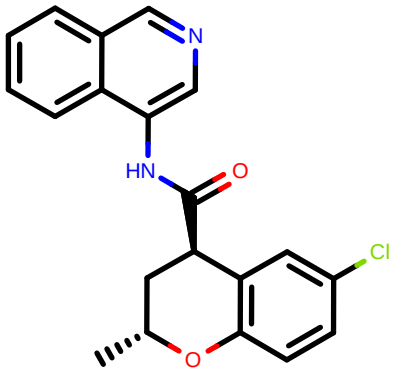
CID:	BEN-DND-c852c98b-6_1
SMILES:	c1cc2cncc(c2cc1OC(F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN53
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.06

MAT-POS-8a69d52e-1_3



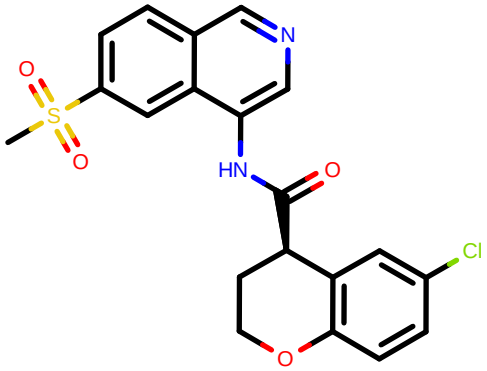
CID:	MAT-POS-8a69d52e-1_3
SMILES:	C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN37
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.04

EDJ-MED-e4b030d8-2_1



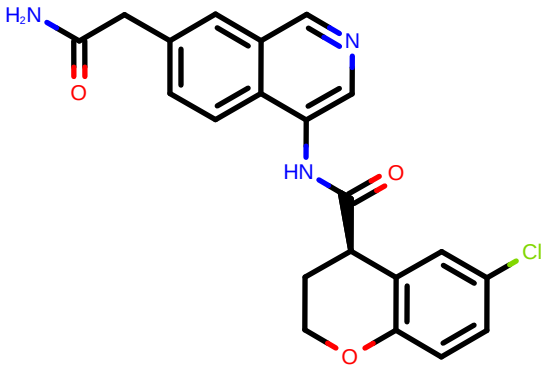
CID:	EDJ-MED-e4b030d8-2_1
SMILES:	C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN36
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.04

BEN-DND-c852c98b-5_1



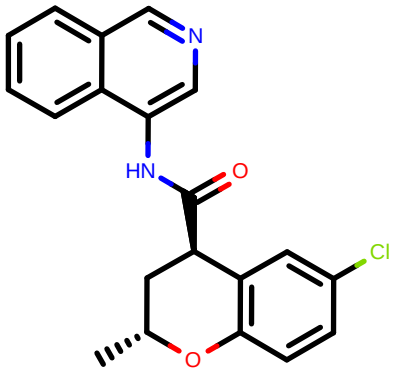
CID:	BEN-DND-c852c98b-5_1
SMILES:	CS(=O)(=O)c1ccc2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN54
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.08

MAK-UNK-8be7dca9-2_1



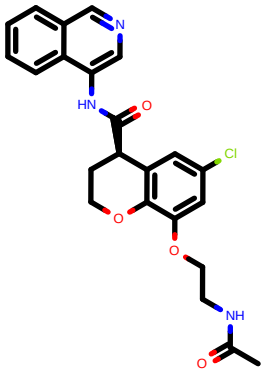
CID:	MAK-UNK-8be7dca9-2_1
SMILES:	c1cc2c(cc1CC(=O)N)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN59
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.09

ALP-POS-d3acb8cc-4_1



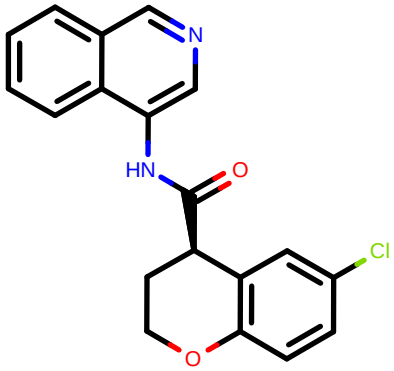
CID:	ALP-POS-d3acb8cc-4_1
SMILES:	C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN38
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.05

NAU-LAT-0543f7f2-10_2



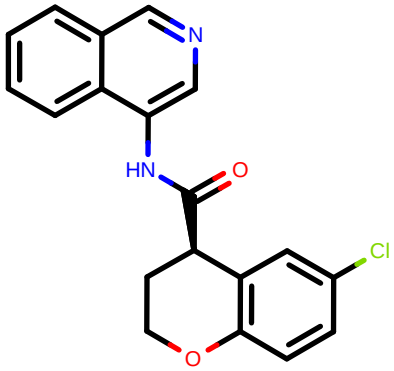
CID:	NAU-LAT-0543f7f2-10_2
SMILES:	CC(=O)NCCOc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN60
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.33

MAT-POS-f7918075-1_1



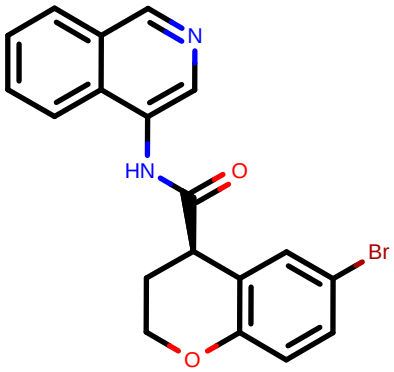
CID:	MAT-POS-f7918075-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN17
DDG (kcal/mol):	0.01
dDDG (kcal/mol):	0.03

VLA-UCB-1dbca3b4-15_1



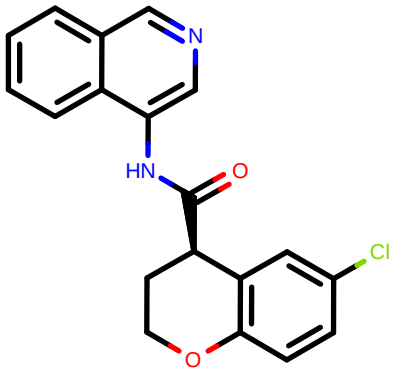
CID:	VLA-UCB-1dbca3b4-15_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN15
DDG (kcal/mol):	0.01
dDDG (kcal/mol):	0.02

MAT-POS-11b63608-1_1



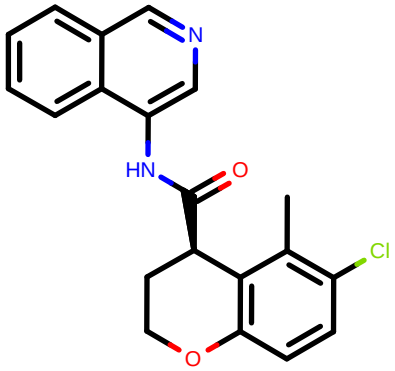
CID:	MAT-POS-11b63608-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Br
RUN:	RUN39
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.05

MAT-POS-b3e365b9-1_1



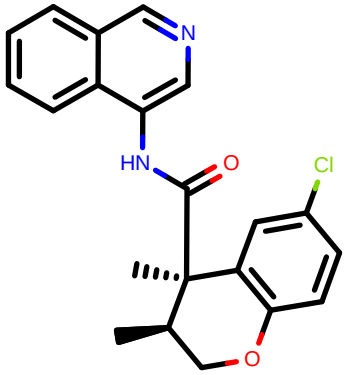
CID:	MAT-POS-b3e365b9-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN16
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.02

EDJ-MED-e4b030d8-8_1



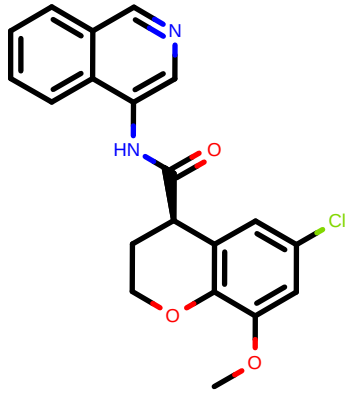
CID:	EDJ-MED-e4b030d8-8_1
SMILES:	Cc1c(ccc2c1[C@@H](CCO2)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN44
DDG (kcal/mol):	0.03
dDDG (kcal/mol):	0.08

DAR-DIA-0d514e7d-29_1



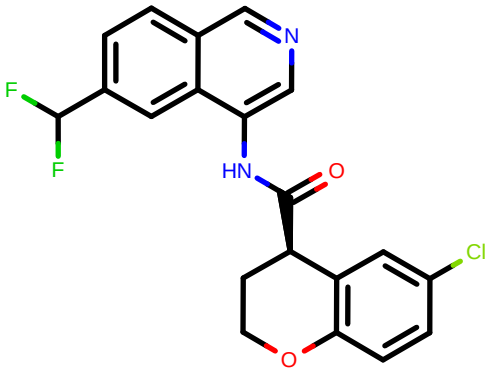
CID:	DAR-DIA-0d514e7d-29_1
SMILES:	C[C@@H]1COc2ccc(cc2[C@]1(C)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN85
DDG (kcal/mol):	0.06
dDDG (kcal/mol):	0.17

EDJ-MED-e4b030d8-7_1



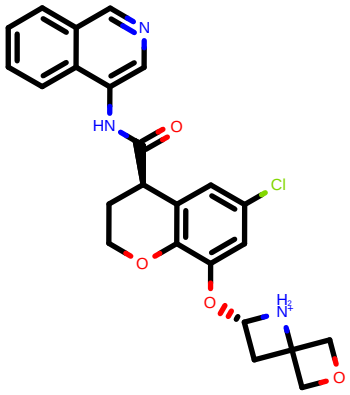
CID:	EDJ-MED-e4b030d8-7_1
SMILES:	COc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN83
DDG (kcal/mol):	0.09
dDDG (kcal/mol):	0.14

BEN-DND-c852c98b-7_1



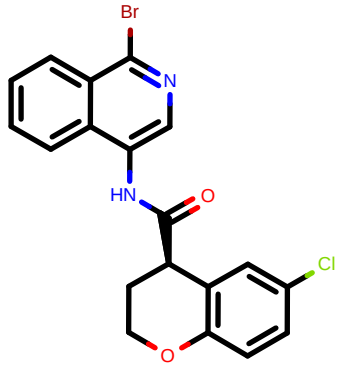
CID:	BEN-DND-c852c98b-7_1
SMILES:	c1cc2cncc(c2cc1C(F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN35
DDG (kcal/mol):	0.18
dDDG (kcal/mol):	0.05

DAR-DIA-23e5a6a0-3_2



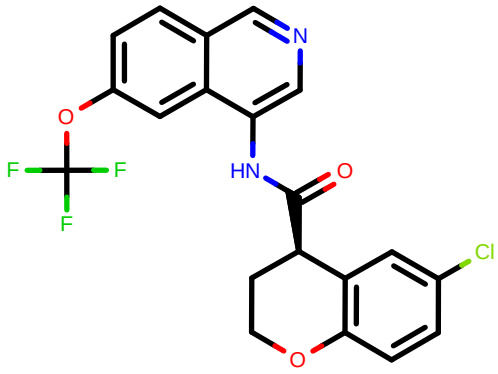
CID:	DAR-DIA-23e5a6a0-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@H]5CC6(N5)COC6)Cl
RUN:	RUN91
DDG (kcal/mol):	0.19
dDDG (kcal/mol):	0.49

ADA-UCB-dc2b944c-11_1



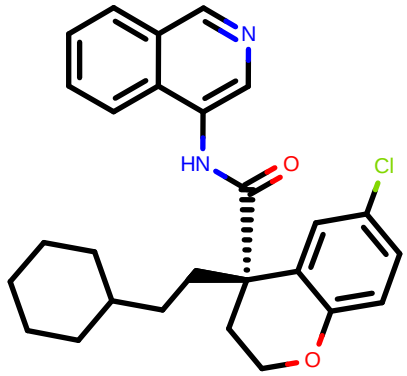
CID:	ADA-UCB-dc2b944c-11_1
SMILES:	c1ccc2c(c1)c(cnc2Br)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN67
DDG (kcal/mol):	0.20
dDDG (kcal/mol):	0.07

BEN-DND-c852c98b-2_1



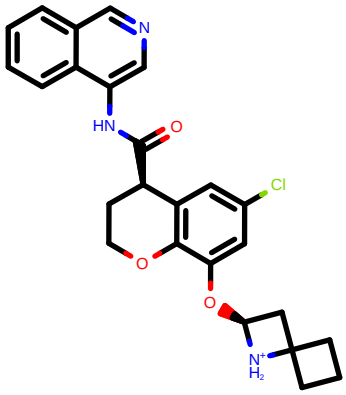
CID:	BEN-DND-c852c98b-2_1
SMILES:	c1cc2cncc(c2cc1OC(F)(F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN61
DDG (kcal/mol):	0.23
dDDG (kcal/mol):	0.06

VLA-UCB-05e51b3f-13_1



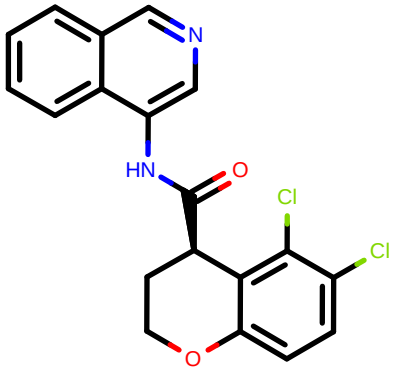
CID:	VLA-UCB-05e51b3f-13_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CCC5CCCCC5
RUN:	RUN89
DDG (kcal/mol):	0.24
dDDG (kcal/mol):	0.28

DAR-DIA-23e5a6a0-2_2



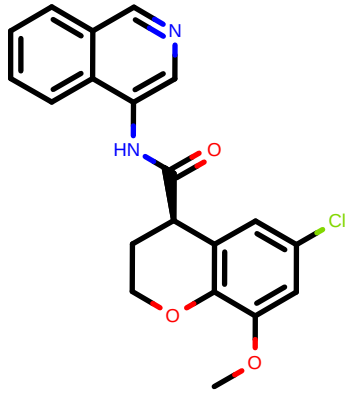
CID:	DAR-DIA-23e5a6a0-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@H]5CC6(N5)CCC6)Cl
RUN:	RUN88
DDG (kcal/mol):	0.33
dDDG (kcal/mol):	0.31

EDJ-MED-e4b030d8-10_1



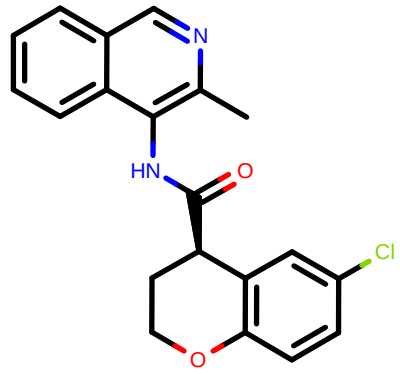
CID:	EDJ-MED-e4b030d8-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3c(c(cc4)Cl)Cl
RUN:	RUN46
DDG (kcal/mol):	0.33
dDDG (kcal/mol):	0.10

DAR-DIA-6a508060-4_2



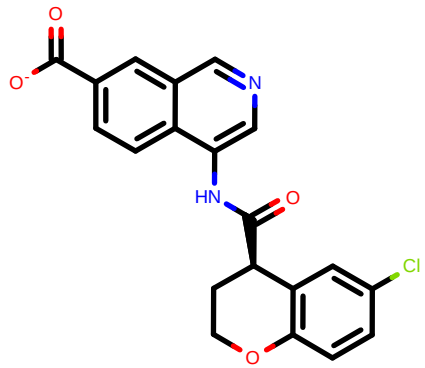
CID:	DAR-DIA-6a508060-4_2
SMILES:	COc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN82
DDG (kcal/mol):	0.35
dDDG (kcal/mol):	0.10

ADA-UCB-dc2b944c-10_1



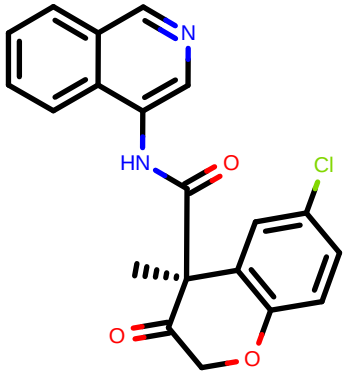
CID:	ADA-UCB-dc2b944c-10_1
SMILES:	Cc1c(c2ccccc2cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN51
DDG (kcal/mol):	0.39
dDDG (kcal/mol):	0.09

MAK-UNK-8be7dca9-9_1



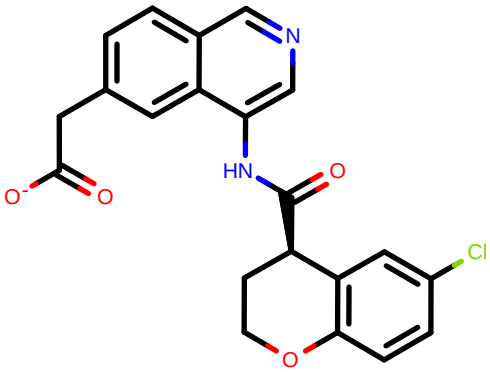
CID:	MAK-UNK-8be7dca9-9_1
SMILES:	c1cc2c(cc1C(=O)O)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN47
DDG (kcal/mol):	0.60
dDDG (kcal/mol):	0.06

EDJ-MED-e4b030d8-1_1



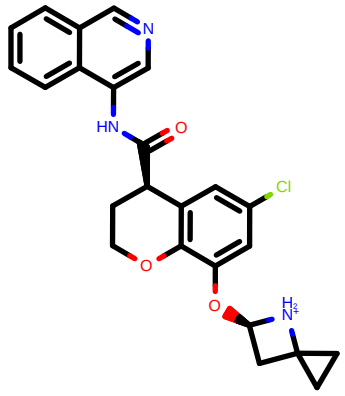
CID:	EDJ-MED-e4b030d8-1_1
SMILES:	C[C@@]1(c2cc(ccc2OCC1=O)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN11
DDG (kcal/mol):	0.64
dDDG (kcal/mol):	0.10

MAK-UNK-8be7dca9-8_1



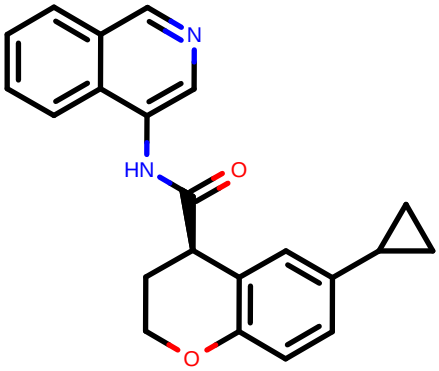
CID:	MAK-UNK-8be7dca9-8_1
SMILES:	c1cc2cncc(c2cc1CC(=O)O)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN57
DDG (kcal/mol):	0.65
dDDG (kcal/mol):	0.07

DAR-DIA-23e5a6a0-5_1



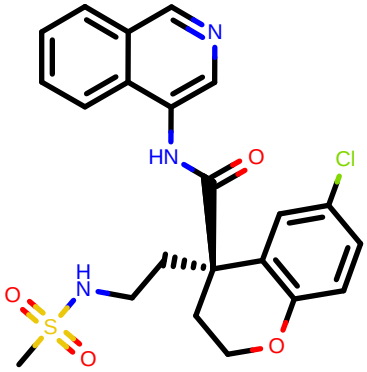
CID:	DAR-DIA-23e5a6a0-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@@H]5CC6(N5)CC6)Cl
RUN:	RUN84
DDG (kcal/mol):	0.68
dDDG (kcal/mol):	0.37

DAR-DIA-6a508060-8_1



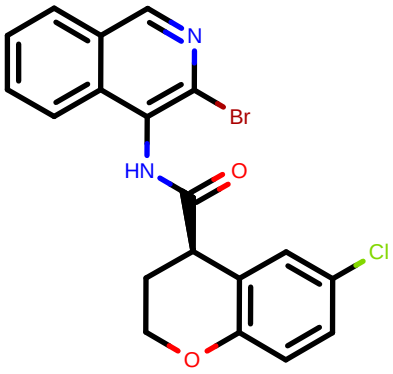
CID:	DAR-DIA-6a508060-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)C5CC5
RUN:	RUN68
DDG (kcal/mol):	0.71
dDDG (kcal/mol):	0.11

DAR-DIA-6a508060-13_2



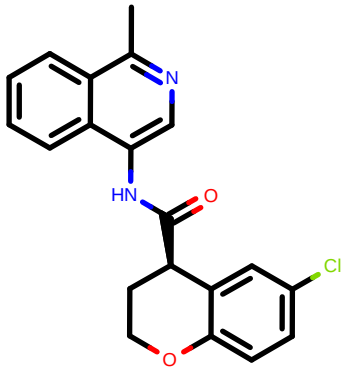
CID:	DAR-DIA-6a508060-13_2
SMILES:	CS(=O)(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN28
DDG (kcal/mol):	0.72
dDDG (kcal/mol):	0.27

ADA-UCB-dc2b944c-9_1



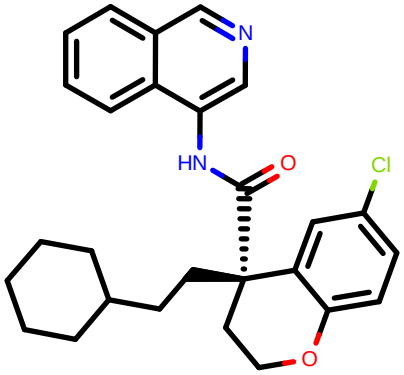
CID:	ADA-UCB-dc2b944c-9_1
SMILES:	c1ccc2c(c1)cnc(c2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)Br
RUN:	RUN58
DDG (kcal/mol):	0.75
dDDG (kcal/mol):	0.12

ADA-UCB-dc2b944c-12_1



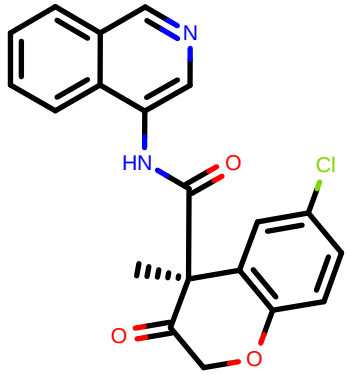
CID:	ADA-UCB-dc2b944c-12_1
SMILES:	Cc1c2ccccc2c(cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN64
DDG (kcal/mol):	0.81
dDDG (kcal/mol):	0.05

DAR-DIA-6a508060-9_2



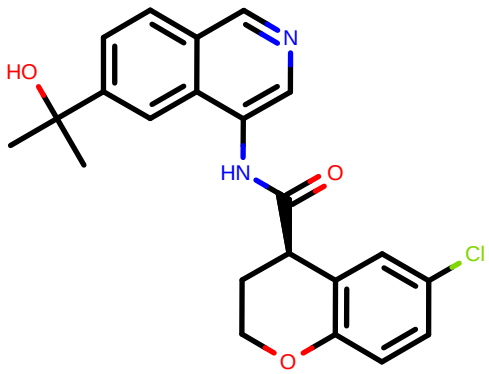
CID:	DAR-DIA-6a508060-9_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CCC5CCCCC5
RUN:	RUN90
DDG (kcal/mol):	0.82
dDDG (kcal/mol):	0.27

VLA-UCB-1dbca3b4-14_1



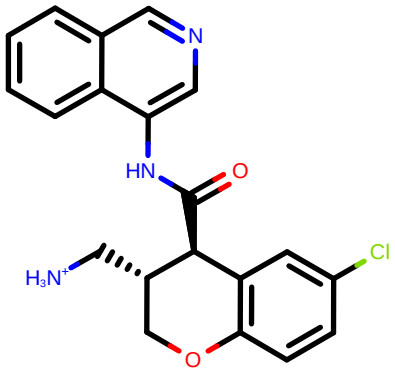
CID:	VLA-UCB-1dbca3b4-14_1
SMILES:	C[C@@]1(c2cc(ccc2OCC1=O)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10
DDG (kcal/mol):	0.85
dDDG (kcal/mol):	0.10

BEN-DND-c852c98b-3_1



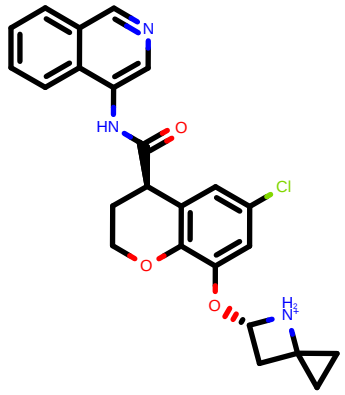
CID:	BEN-DND-c852c98b-3_1
SMILES:	CC(C)(c1ccc2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)O
RUN:	RUN45
DDG (kcal/mol):	0.86
dDDG (kcal/mol):	0.08

MAK-UNK-8be7dca9-3_2



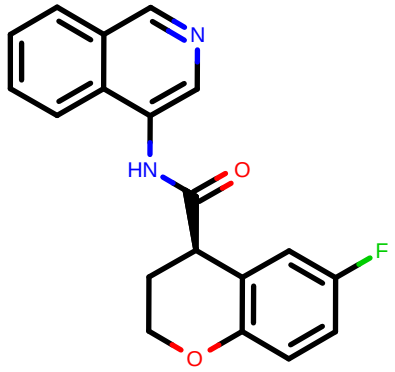
CID:	MAK-UNK-8be7dca9-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4OC[C@@H]3CN)Cl
RUN:	RUN48
DDG (kcal/mol):	0.90
dDDG (kcal/mol):	0.13

DAR-DIA-23e5a6a0-5_2



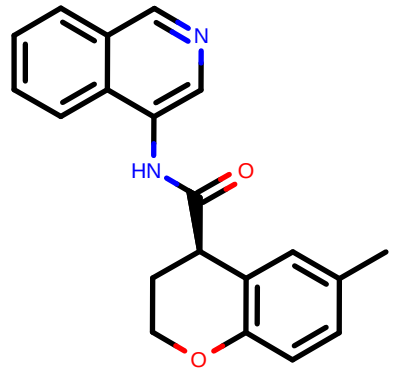
CID:	DAR-DIA-23e5a6a0-5_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@H]5CC6(N5)CC6)Cl
RUN:	RUN80
DDG (kcal/mol):	0.96
dDDG (kcal/mol):	0.30

ADA-UCB-dc2b944c-7_1



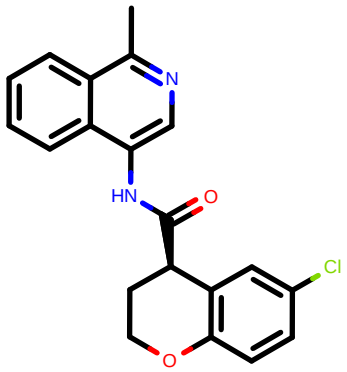
CID:	ADA-UCB-dc2b944c-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)F
RUN:	RUN4
DDG (kcal/mol):	0.98
dDDG (kcal/mol):	0.06

ADA-UCB-dc2b944c-5_1



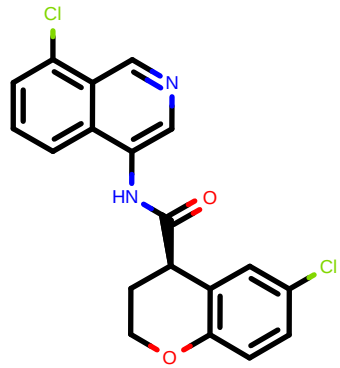
CID:	ADA-UCB-dc2b944c-5_1
SMILES:	Cc1ccc2c(c1)[C@@H](CCO2)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5
DDG (kcal/mol):	1.01
dDDG (kcal/mol):	0.05

JOH-SUS-a69c159d-1_1



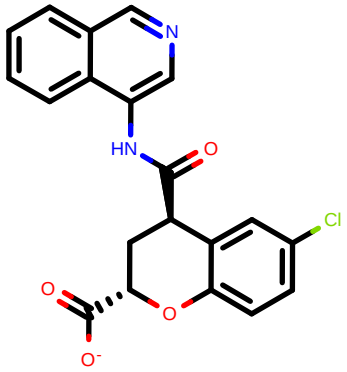
CID:	JOH-SUS-a69c159d-1_1
SMILES:	Cc1c2ccccc2c(cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN63
DDG (kcal/mol):	1.06
dDDG (kcal/mol):	0.05

ADA-UCB-dc2b944c-8_1



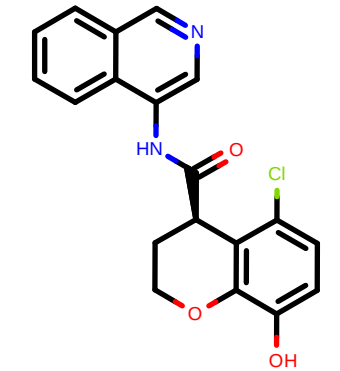
CID:	ADA-UCB-dc2b944c-8_1
SMILES:	c1cc2c(cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)c(c1)Cl
RUN:	RUN30
DDG (kcal/mol):	1.27
dDDG (kcal/mol):	0.05

MAK-UNK-8be7dca9-10_3



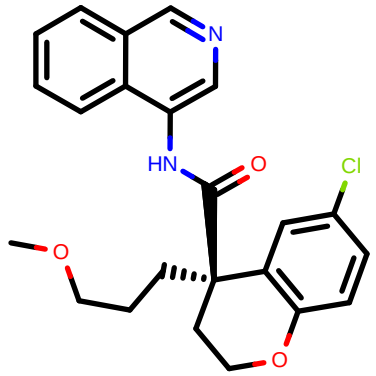
CID:	MAK-UNK-8be7dca9-10_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[C@H](Oc4c3cc(cc4)Cl)C(=O)O
RUN:	RUN86
DDG (kcal/mol):	1.50
dDDG (kcal/mol):	0.08

ALP-UNI-4b8a177c-1_1



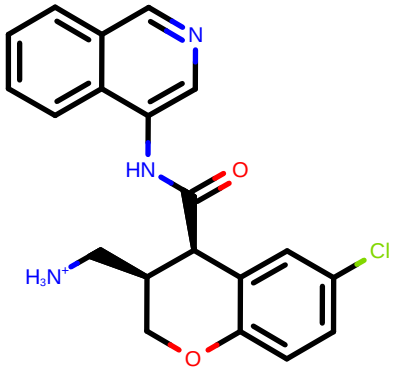
CID:	ALP-UNI-4b8a177c-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3c(ccc4O)Cl
RUN:	RUN74
DDG (kcal/mol):	2.03
dDDG (kcal/mol):	0.18

EDJ-MED-28ec730d-1_1



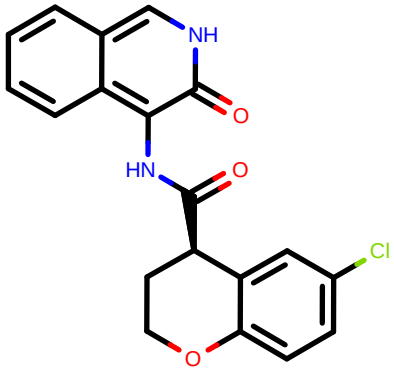
CID:	EDJ-MED-28ec730d-1_1
SMILES:	COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN62
DDG (kcal/mol):	2.22
dDDG (kcal/mol):	0.22

MAK-UNK-8be7dca9-3_4



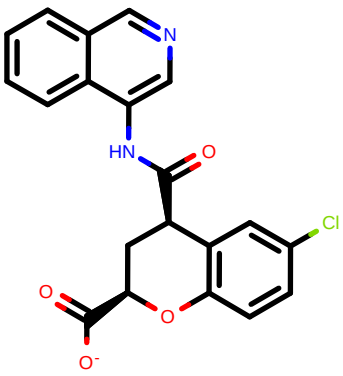
CID:	MAK-UNK-8be7dca9-3_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4OC[C@H]3CN)Cl
RUN:	RUN24
DDG (kcal/mol):	2.31
dDDG (kcal/mol):	0.14

JOH-UNI-f51e3bbc-3_1



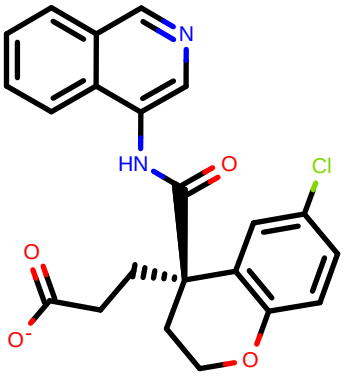
CID:	JOH-UNI-f51e3bbc-3_1
SMILES:	c1ccc2c(c1)cnc(c2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)O
RUN:	RUN87
DDG (kcal/mol):	2.39
dDDG (kcal/mol):	0.16

MAK-UNK-8be7dca9-10_1



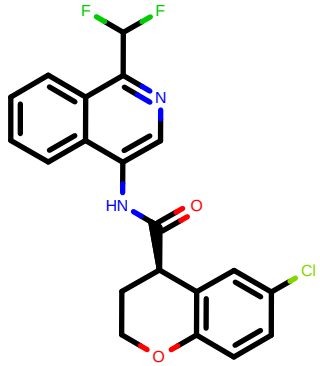
CID:	MAK-UNK-8be7dca9-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[C@@H](Oc4c3cc(cc4)Cl)C(=O)O
RUN:	RUN66
DDG (kcal/mol):	3.09
dDDG (kcal/mol):	0.12

JAG-UCB-706446eb-3_1



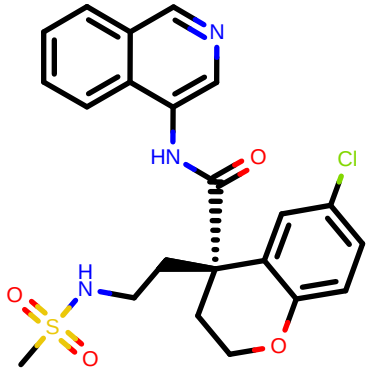
CID:	JAG-UCB-706446eb-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)O
RUN:	RUN3
DDG (kcal/mol):	3.23
dDDG (kcal/mol):	0.24

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)Nc3cncc4c3cccc4
RUN:	RUN99
DDG (kcal/mol):	4.51
dDDG (kcal/mol):	0.27