2020-08-14-nucleophilic-displacement
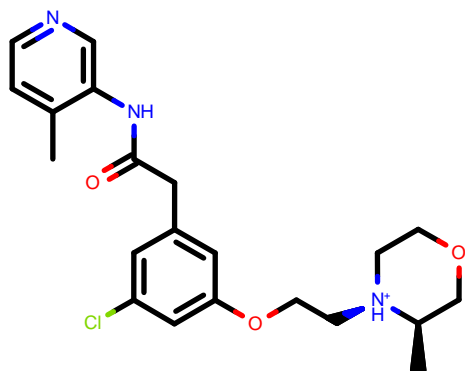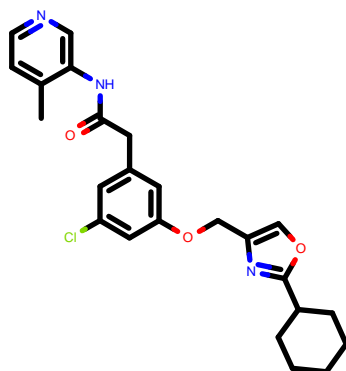
EN300-170738

CID:	EN300-170738
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC[N@H+]3CCOC[C@@H]3C
RUN:	RUN3598
DDG (kcal/mol):	-4.21
dDDG (kcal/mol):	0.19

EN300-382173

CID:	EN300-382173
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3coc(n3)C4CCCCC4
RUN:	RUN176
DDG (kcal/mol):	-2.94
dDDG (kcal/mol):	0.11

EN300-1920731
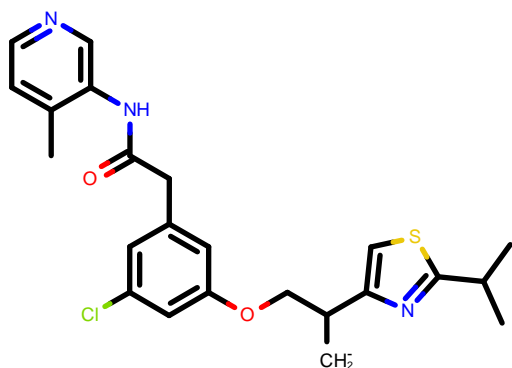
|	
CID:	EN300-1920731
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=C)c3csc(n3)C(C)C
RUN:	RUN4616
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.30

EN300-718949
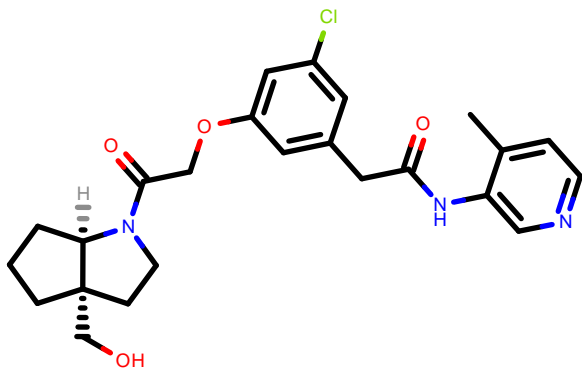
|	
CID:	EN300-718949
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)N3CC[C@]4([C@H]3CCC4)CO
RUN:	RUN3613
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.17

EN300-185424
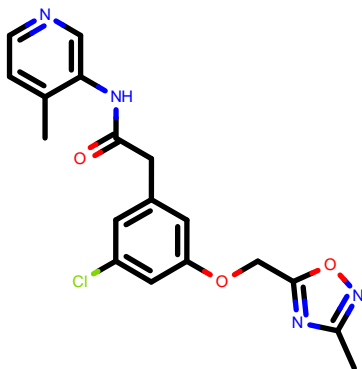
CID:	EN300-185424
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3nc(no3)C
RUN:	RUN1591
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.09

EN300-1863798
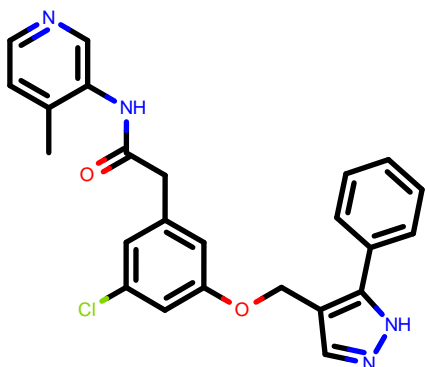
CID:	EN300-1863798
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn[nH]c3c4ccccc4
RUN:	RUN1112
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.13
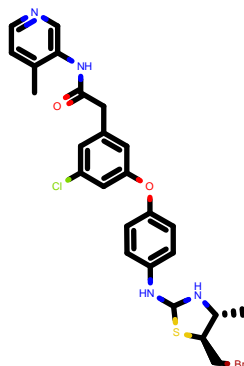
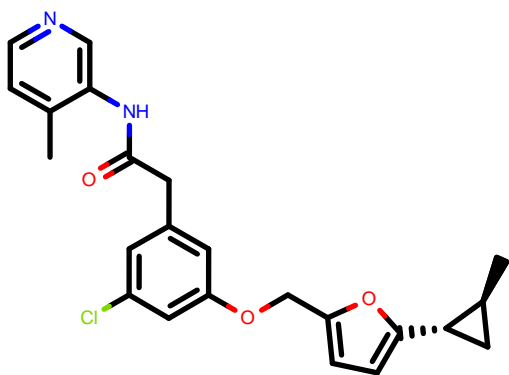# EN300-1274653

CID:	EN300-1274653
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+][C@@H]([C@H](S4)CBr)C
RUN:	RUN3789
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.14

EN300-1266528
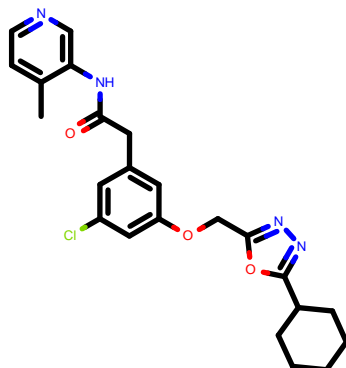
CID:	EN300-1266528
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3nnc(o3)C4CCCCC4
RUN:	RUN88
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.13

EN300-1940535

CID:	EN300-1940535
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(o3)[C@H]4C[C@H]4C
RUN:	RUN106
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.12

EN300-330332
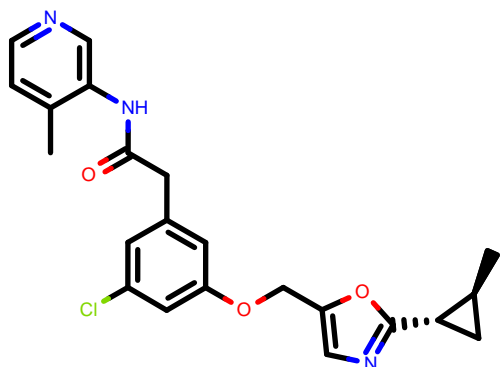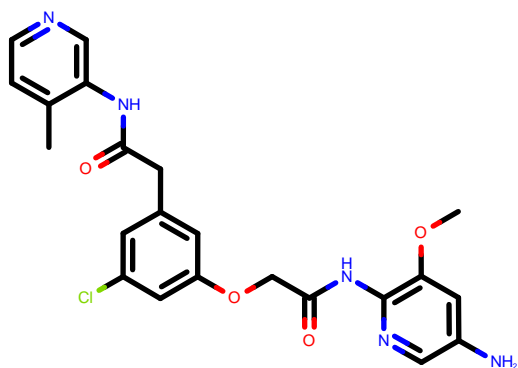

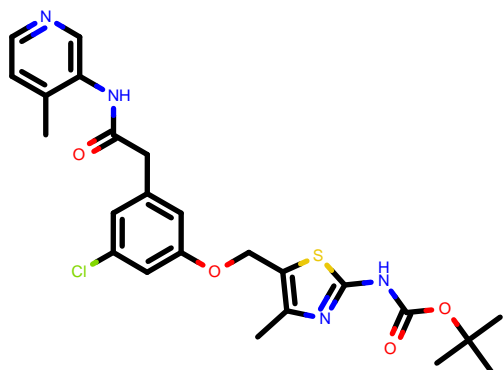|	
CID:	EN300-330332
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnc(o3)[C@H]4C[C@H]4C
RUN:	RUN324
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.12

EN300-377745

CID:	EN300-377745
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)Nc3c(cc(cn3)N)OC
RUN:	RUN3338
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.16

EN300-1886131

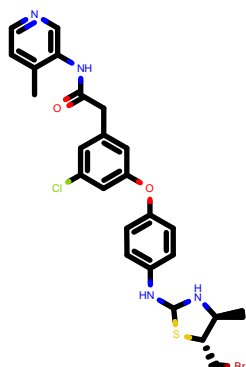|	
CID:	EN300-1886131
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(nc(s3)NC(=O)OC(C)(C)C)C
RUN:	RUN4609
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.37

EN300-1084907
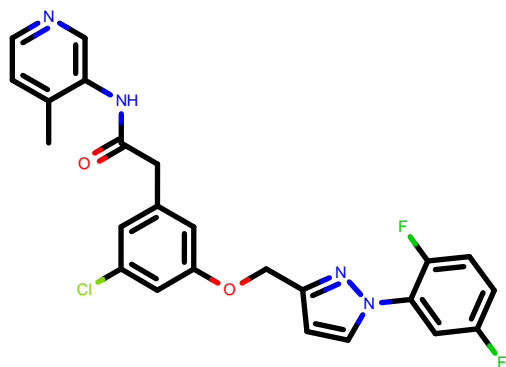
CID:	EN300-1084907
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccn(n3)c4cc(ccc4F)F
RUN:	RUN180
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.13

EN300-1274653

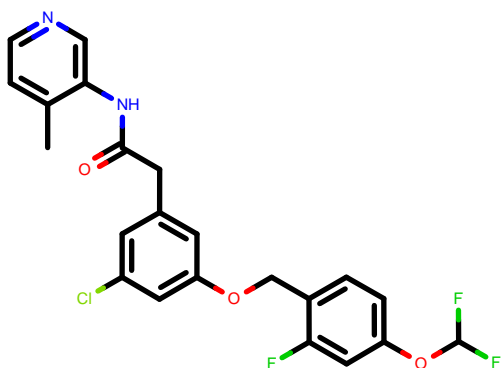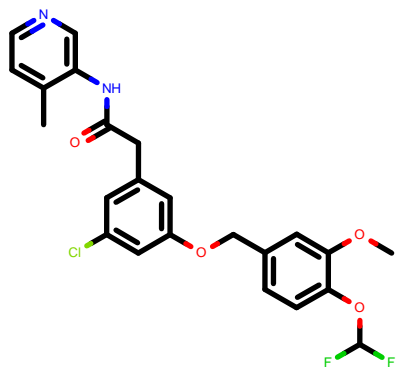|	
CID:	EN300-1274653
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+][C@H]([C@@H](S4)CBr)C
RUN:	RUN3262
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.13

EN300-1929484

CID:	EN300-1929484
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(cc3F)OC(F)F
RUN:	RUN1708
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.13

EN300-155655

CID:	EN300-155655
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3)OC)OC(F)F
RUN:	RUN2011
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.16

2020-08-14-nucleophilic-displacement
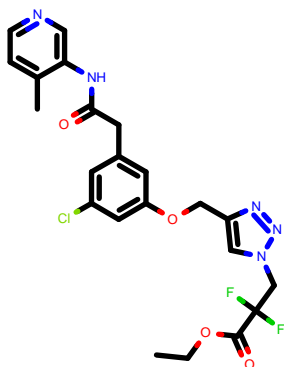
EN300-843777
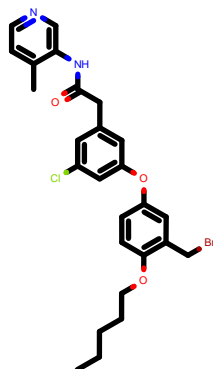
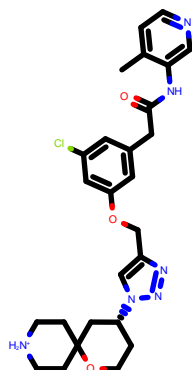|	
CID:	EN300-843777
SMILES:	CCOC(=O)C(Cn1cc(nn1)COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)(F)F
RUN:	RUN997
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.16

EN300-70105

CID:	EN300-70105
SMILES:	CCCCCOc1ccc(cc1CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
RUN:	RUN2809
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.16

EN300-843582

CID:	EN300-843582
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nn3)[C@@H]4CCOC5(C4)CC[NH2+]CC5
RUN:	RUN907
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.17

EN300-1915724
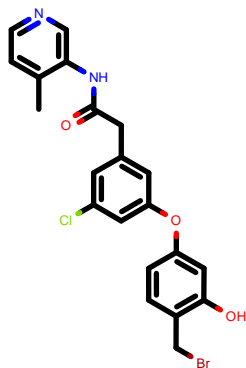
CID:	EN300-1915724
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)O)CBr
RUN:	RUN566
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.10

EN300-1909681
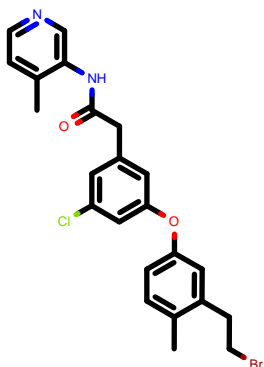
CID:	EN300-1909681
SMILES:	Cc1ccc(cc1CCBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
RUN:	RUN2206
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.12

EN300-844309
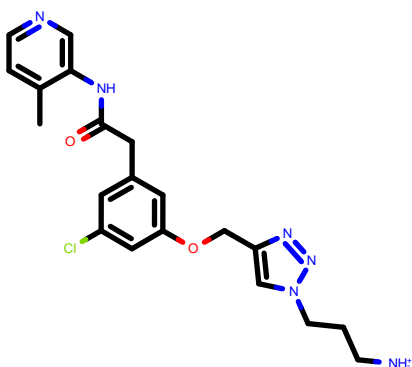
CID:	EN300-844309
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nn3)CCC[NH3+]
RUN:	RUN645
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.13

EN300-1274638
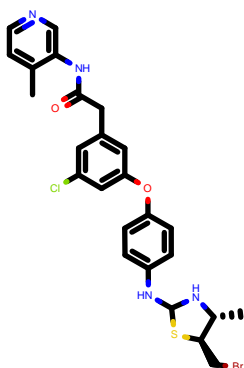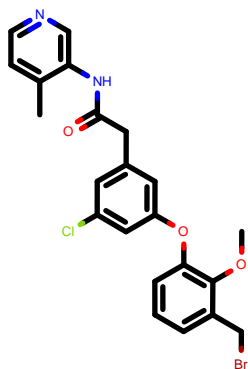

CID:	EN300-1274638
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+][C@@H]([C@H](S4)CBr)C
RUN:	RUN3788
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.14

EN300-60436
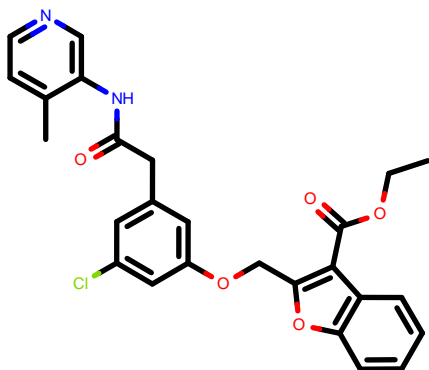
CID:	EN300-60436
SMILES:	CCOC(=O)c1c2ccccc2oc1COc3cc(cc(c3)Cl)CC(=O)Nc4cnccc4C
RUN:	RUN4577
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.30

EN300-1910987

CID:	EN300-1910987
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3OC)CBr
RUN:	RUN1168
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.13

EN300-1938856
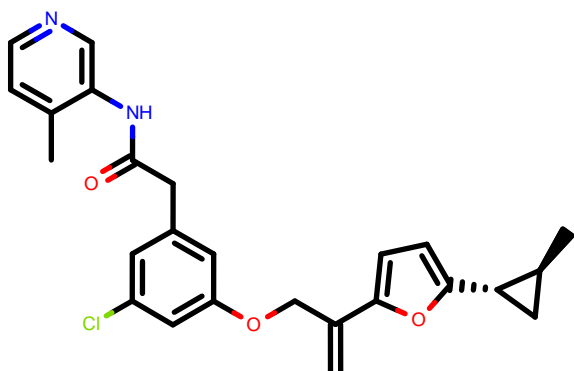
CID:	EN300-1938856
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=C)c3ccc(o3)[C@H]4C[C@@H]4C
RUN:	RUN4615
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.37

EN300-701252
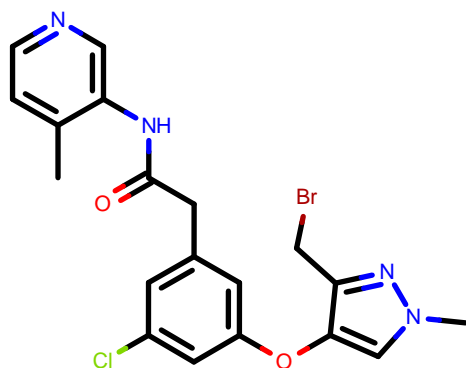
CID:	EN300-701252
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cn(nc3CBr)C
RUN:	RUN1206
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.11

EN300-24531
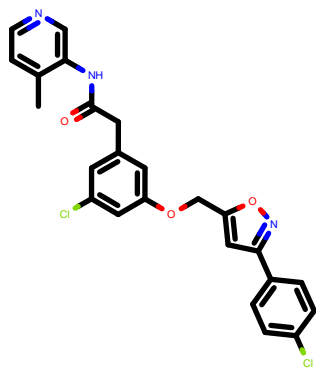
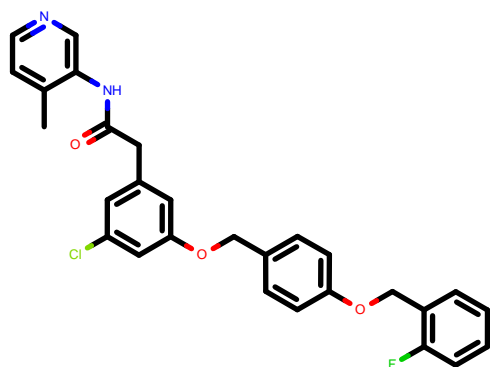|	
CID:	EN300-24531
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4ccc(cc4)Cl
RUN:	RUN3389
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.14

EN300-1897350
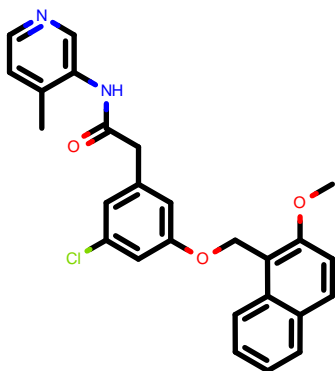
CID:	EN300-1897350
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c4ccccc4ccc3OC
RUN:	RUN3624
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.16

EN300-378667

CID:	EN300-378667
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(cc3)OCc4ccccc4F
RUN:	RUN2751
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.15

EN300-24227
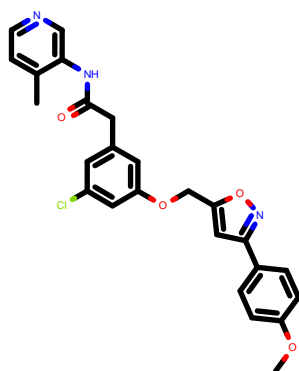
CID:	EN300-24227
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4ccc(cc4)OC
RUN:	RUN3755
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.15

EN300-2009659
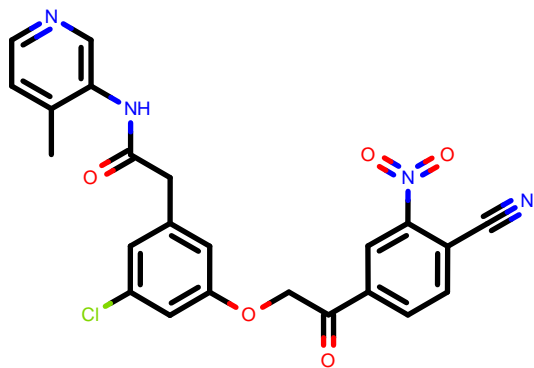
CID:	EN300-2009659
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)c3ccc(c(c3)N(=O)=O)C#N
RUN:	RUN4481
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.20

EN300-301686
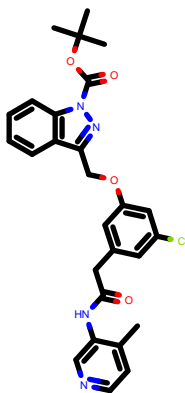
CID:	EN300-301686
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c4ccccc4n(n3)C(=O)OC(C)(C)C
RUN:	RUN4523
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.27

EN300-1274639
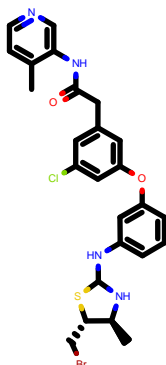
CID:	EN300-1274639
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3)NC4=[NH+][C@H]([C@@H](S4)CBr)C
RUN:	RUN1452
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.16

EN300-1914939
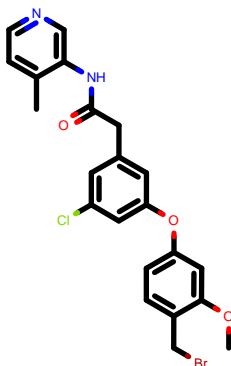
CID:	EN300-1914939
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)OC)CBr
RUN:	RUN2542
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.12

EN300-372060
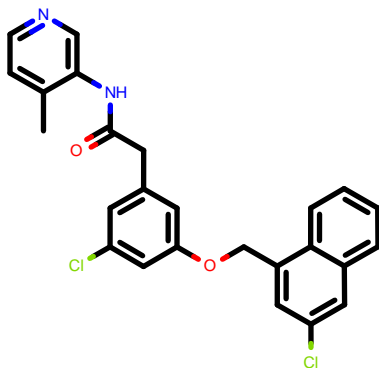
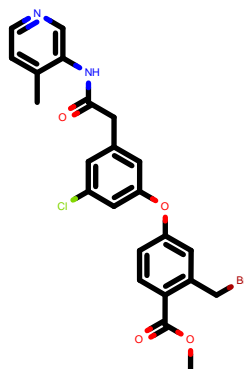|	
CID:	EN300-372060
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(cc4c3cccc4)Cl
RUN:	RUN2293
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.12

EN300-1926474
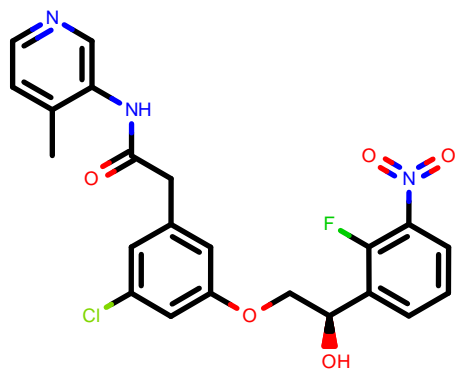
|	
CID:	EN300-1926474
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3cccc(c3F)N(=O)=O)O
RUN:	RUN1782
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.17

EN300-117814

|	
CID:	EN300-117814
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)CBr)C(=O)OC
RUN:	RUN1589
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.12

EN300-1918362
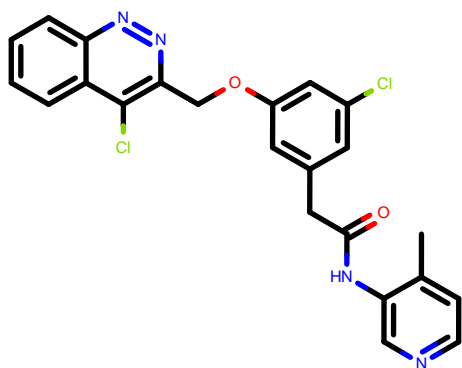
CID:	EN300-1918362
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(c4ccccc4nn3)Cl
RUN:	RUN3740
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.14

EN300-87636
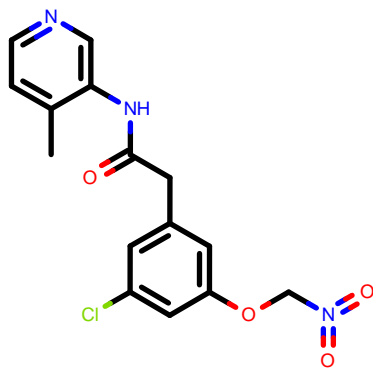
|	
CID:	EN300-87636
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCN(=O)=O
RUN:	RUN786
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.08

EN300-1296572
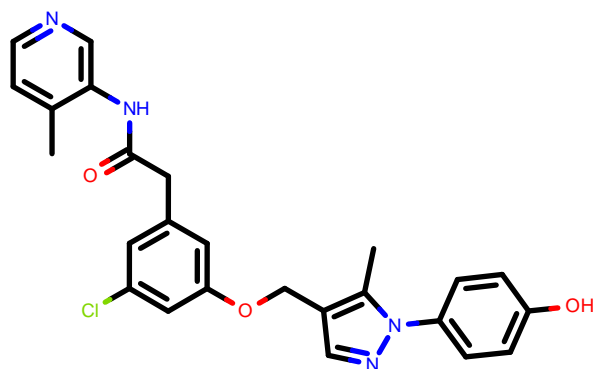
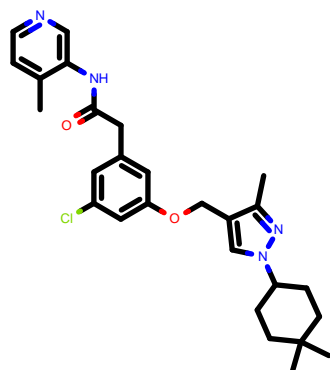|	
CID:	EN300-1296572
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnn(c3C)c4ccc(cc4)O
RUN:	RUN1383
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.15

EN300-1910562
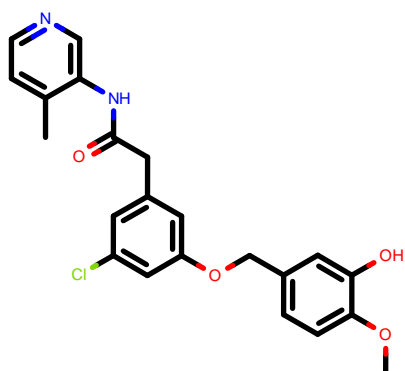
CID:	EN300-1910562
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3)O)OC
RUN:	RUN2172
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.14

EN300-1912582
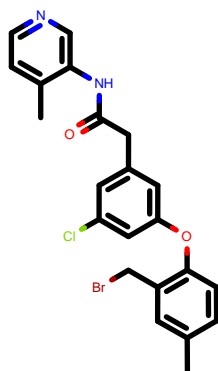
CID:	EN300-1912582
SMILES:	Cc1ccc(c(c1)CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
RUN:	RUN1011
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.14

EN300-1461330

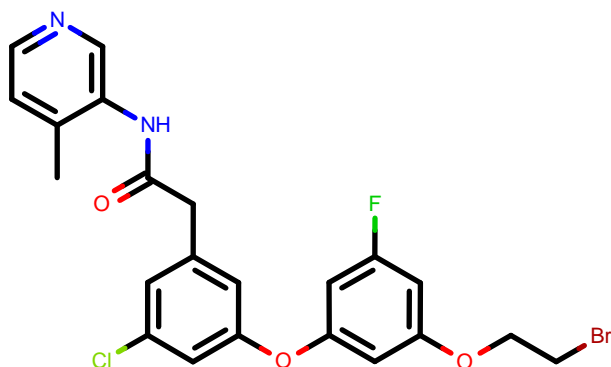|	
CID:	EN300-1461330
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nc3C)C4CCC(CC4)(C)C
RUN:	RUN735
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.16

EN300-1912943
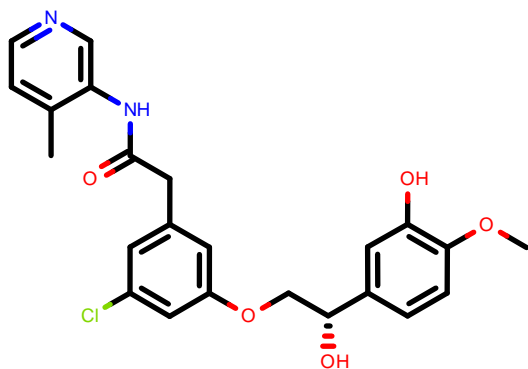
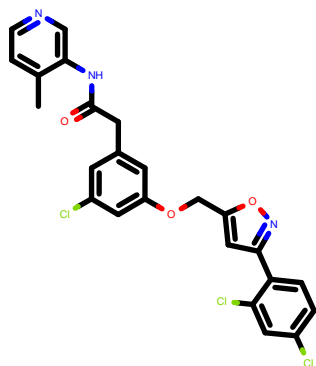|	
CID:	EN300-1912943
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3ccc(c(c3)O)OC)O
RUN:	RUN3195
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.20

EN300-160173

CID:	EN300-160173
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(cc(c3)F)OCCBr
RUN:	RUN2023
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.16

EN300-24230

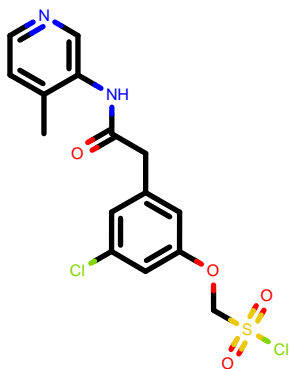|	
CID:	EN300-24230
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4ccc(cc4Cl)Cl
RUN:	RUN3009
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.16

EN300-1591418
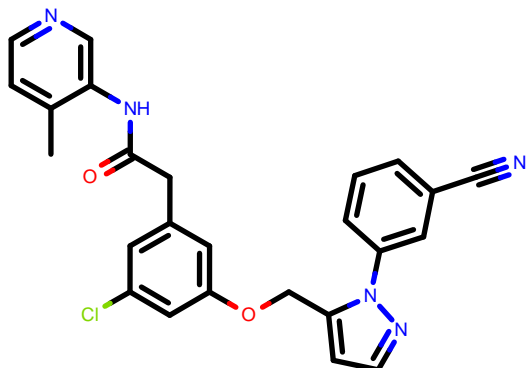
CID:	EN300-1591418
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccnn3c4cccc(c4)C#N
RUN:	RUN1247
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.16

EN300-4257713

CID:	EN300-4257713
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCS(=O)(=O)Cl
RUN:	RUN548
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.08

EN300-1918008
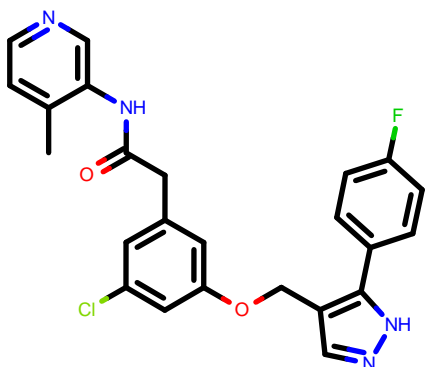
CID:	EN300-1918008
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn[nH]c3c4ccc(cc4)F
RUN:	RUN1345
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.14

EN300-1917400
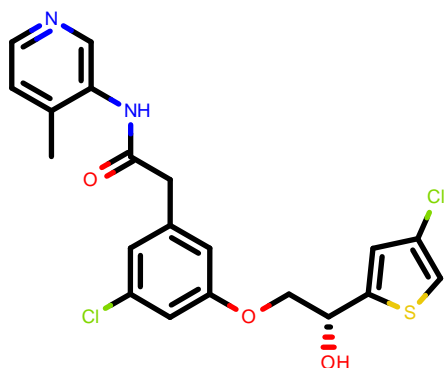
CID:	EN300-1917400
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3cc(cs3)Cl)O
RUN:	RUN2584
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.18

EN300-156205
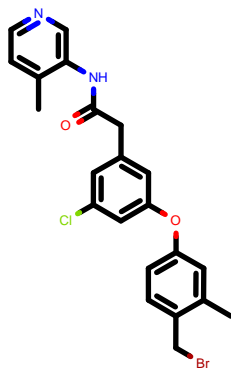
CID:	EN300-156205
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C)CBr
RUN:	RUN1704
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.10

EN300-1894071
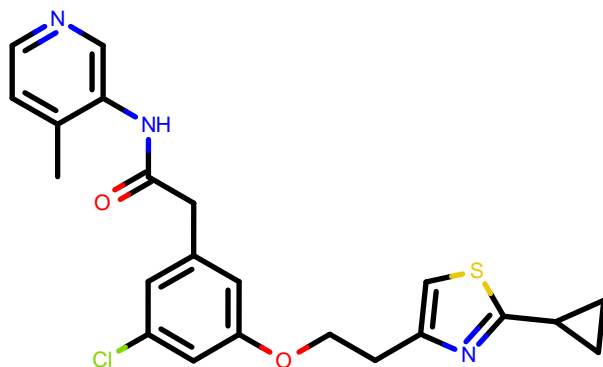
CID:	EN300-1894071
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3csc(n3)C4CC4
RUN:	RUN2324
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.16

EN300-7437130
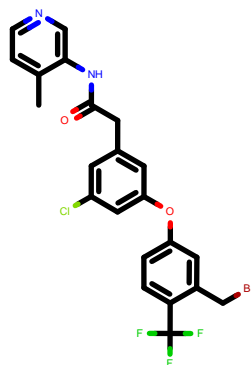
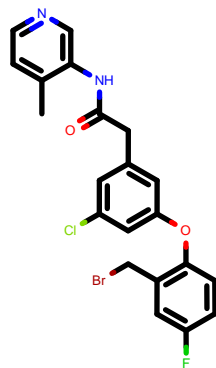|	
CID:	EN300-7437130
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)CBr)C(F)(F)F
RUN:	RUN3604
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.12

EN300-1724721
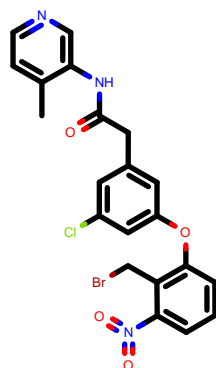
CID:	EN300-1724721
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3CBr)N(=O)=O
RUN:	RUN2085
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.13

EN300-29546

CID:	EN300-29546
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)F
RUN:	RUN1118
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.13

EN300-7494548
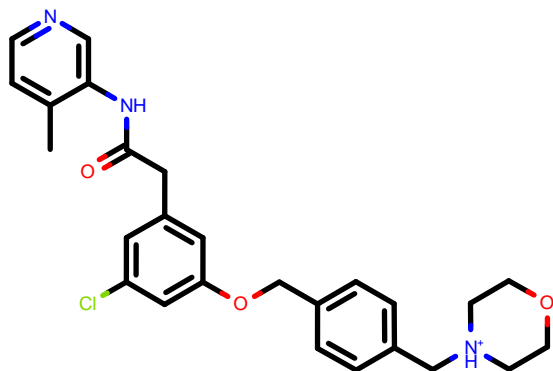
CID:	EN300-7494548
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(cc3)C[NH+]4CCOCC4
RUN:	RUN3552
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.15

EN300-643001
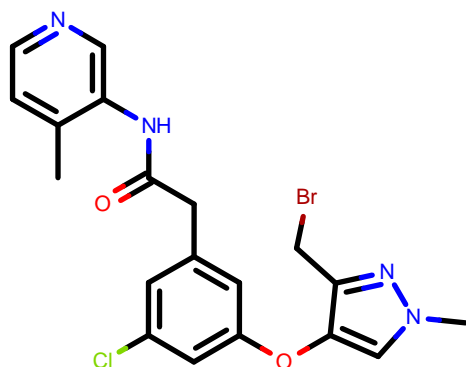
CID:	EN300-643001
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cn(nc3CBr)C
RUN:	RUN1207
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.13

EN300-7377816
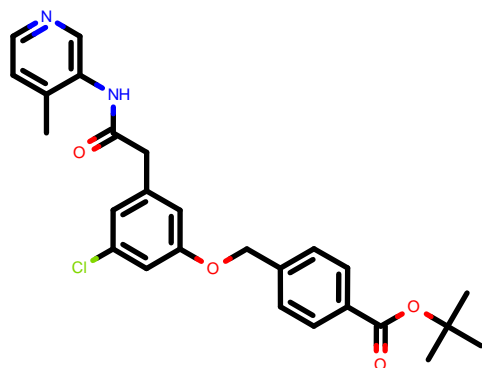
CID:	EN300-7377816
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(cc3)C(=O)OC(C)(C)C
RUN:	RUN4473
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.17

EN300-1277860
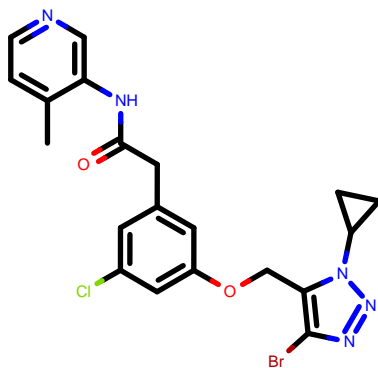
CID:	EN300-1277860
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(nnn3C4CC4)Br
RUN:	RUN1144
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.13

EN300-740743
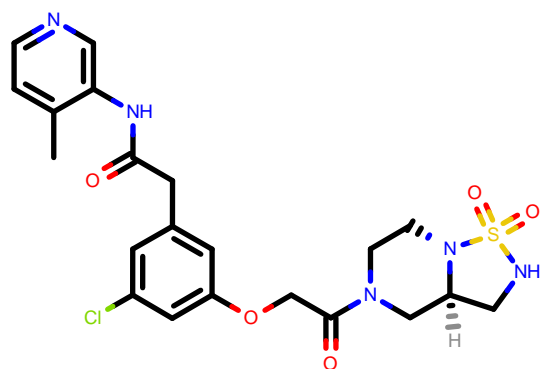
CID:	EN300-740743
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc2)Cl)OCC(=O)N3CC[N@@]4[C@H](C3)CNS4(=O)=O
RUN:	RUN3691
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.17

EN300-154526
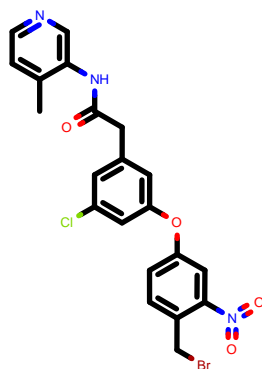
CID:	EN300-154526
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc2)Cl)Oc3ccc(c(c3)N(=O)=O)CBr
RUN:	RUN2558
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.13

EN300-43523
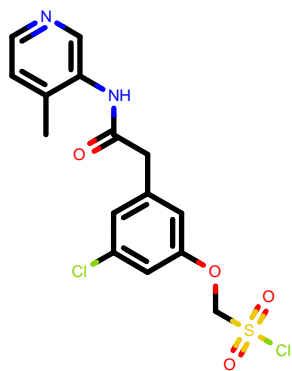
CID:	EN300-43523
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc2)Cl)OCS(=O)(=O)Cl
RUN:	RUN547
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.09

EN300-1296574
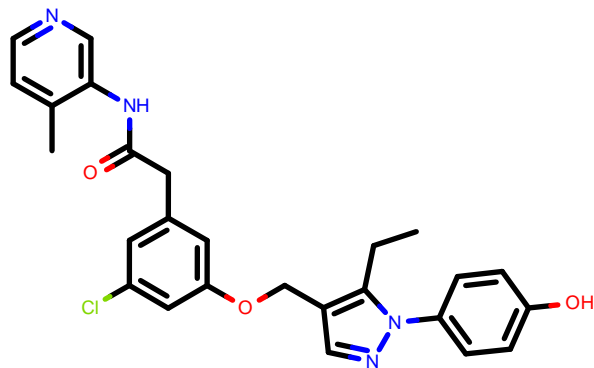
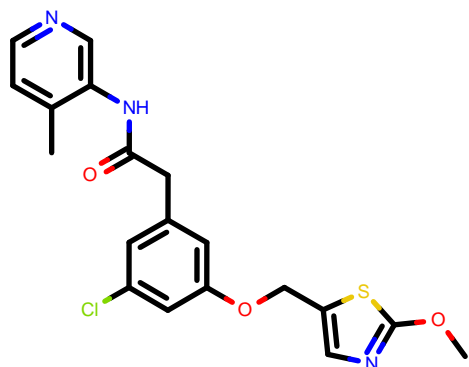|	
CID:	EN300-1296574
SMILES:	CCc1c(cnn1c2ccc(cc2)O)COc3cc(cc(c3)Cl)CC(=O)Nc4cnccc4C
RUN:	RUN1221
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.14

EN300-6776042
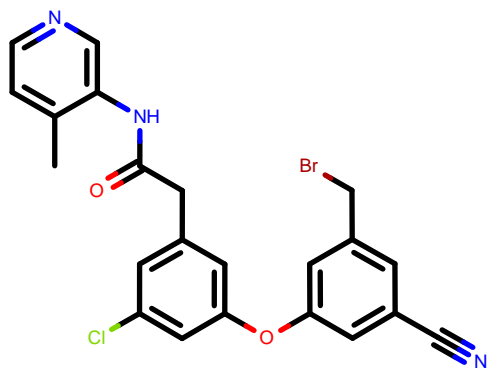
CID:	EN300-6776042
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(cc(c3)C#N)CBr
RUN:	RUN3182
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.12

EN300-1918616

CID:	EN300-1918616
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnc(s3)OC
RUN:	RUN838
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.13

EN300-843597
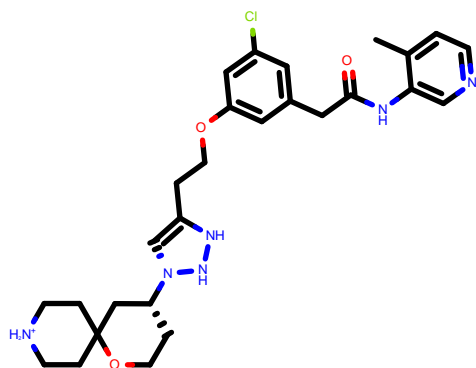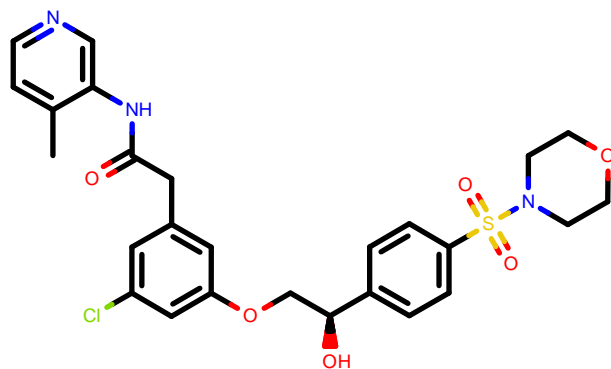

|	
CID:	EN300-843597
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cn(nn3)[C@@H]4CCOC5(C4)CC[NH2+]CC5
RUN:	RUN4546
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.37

EN300-13933
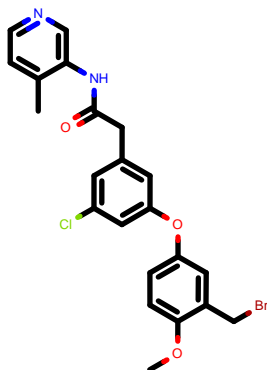
|	
CID:	EN300-13933
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)CBr)OC
RUN:	RUN2655
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.13

EN300-87708

| CID:	EN300-87708
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3ccc(cc3)S(=O)(=O)N4CCOCC4)O
RUN:	RUN4605
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.58

EN300-1461309
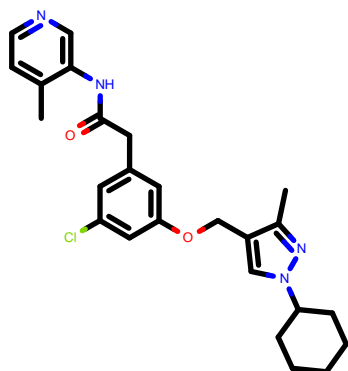
CID:	EN300-1461309
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nc3C)C4CCCCC4
RUN:	RUN678
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.13

EN300-195084
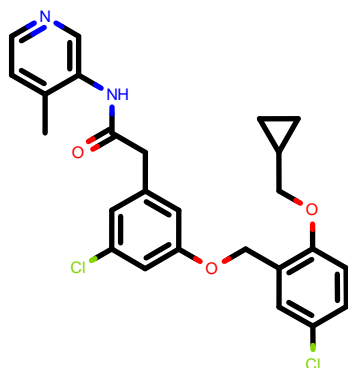
CID:	EN300-195084
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(ccc3OCC4CC4)Cl
RUN:	RUN1831
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.16

EN300-1897461
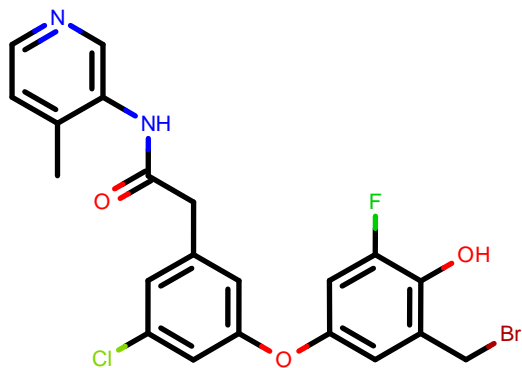
CID:	EN300-1897461
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(c(c(c3)F)O)CBr
RUN:	RUN2052
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.12

EN300-1274654
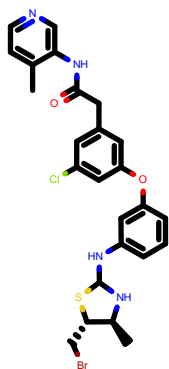
CID:	EN300-1274654
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3)NC4=[NH+][C@H]([C@@H](S4)CBr)C
RUN:	RUN1453
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.17

EN300-674719
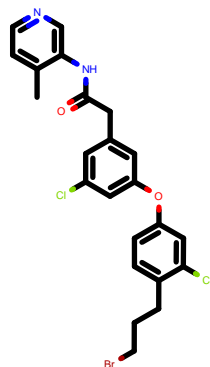
CID:	EN300-674719
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)Cl)CCCBr
RUN:	RUN1823
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.13

EN300-1132718
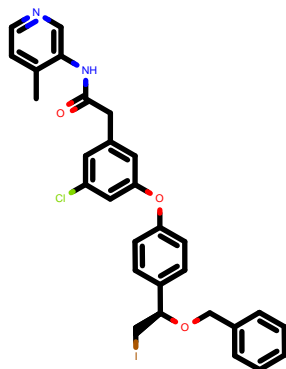
CID:	EN300-1132718
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@H](Cl)OCc4ccccc4
RUN:	RUN3652
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.19

EN300-1916362
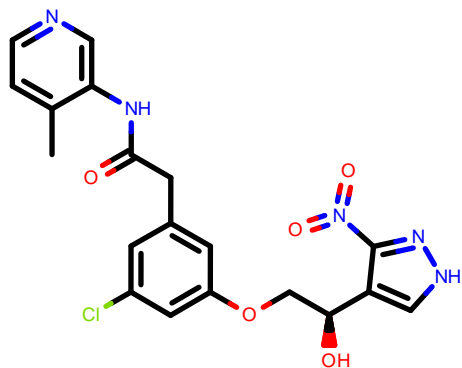
CID:	EN300-1916362
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3c[nH]nc3N(=O)=O)O
RUN:	RUN4562
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.54

EN300-127722
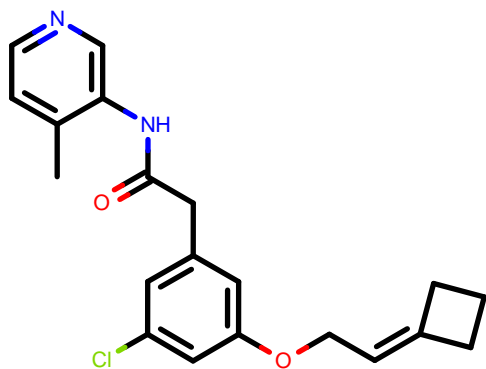
CID:	EN300-127722
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC=C3CCC3
RUN:	RUN4513
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.14

EN300-1927181
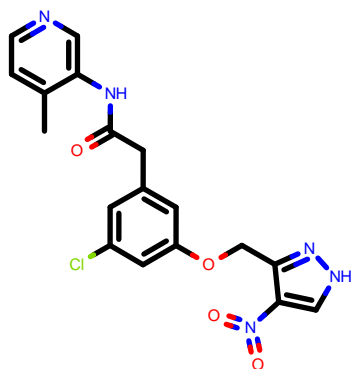
CID:	EN300-1927181
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(c[nH]n3)N(=O)=O
RUN:	RUN933
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.11

EN300-6245905
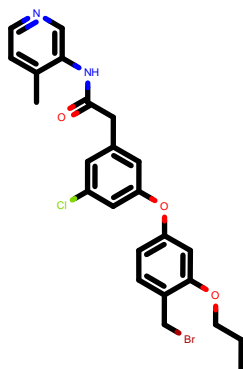
CID:	EN300-6245905
SMILES:	CCCOc1cc(ccc1CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
RUN:	RUN2010
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.14

EN300-366127
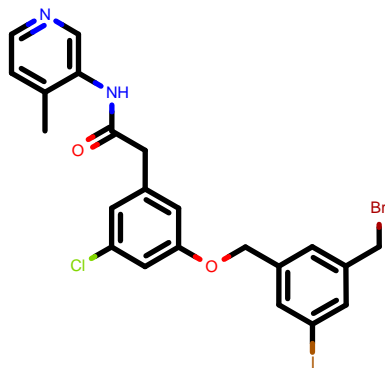
CID:	EN300-366127
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(cc(c3)I)CBr
RUN:	RUN1570
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.13

EN300-1132707
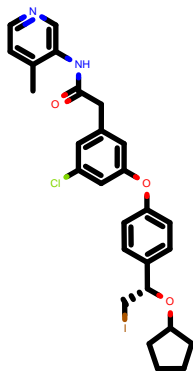
CID:	EN300-1132707
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](CI)OC4CCCC4
RUN:	RUN1347
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.17

EN300-3051713
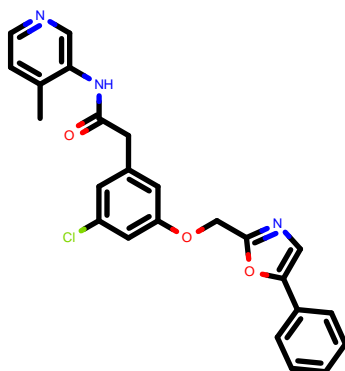
CID:	EN300-3051713
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ncc(o3)c4ccccc4
RUN:	RUN348
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.14

EN300-64239
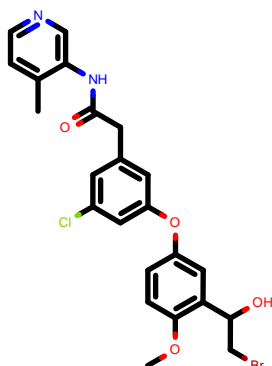
CID:	EN300-64239
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C(=O)CBr)OC
RUN:	RUN2827
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.16

EN300-1910335
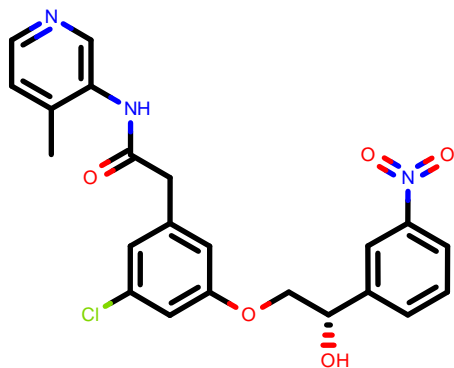
CID:	EN300-1910335
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3cccc(c3)N(=O)=O)O
RUN:	RUN3297
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.17

EN300-1274638
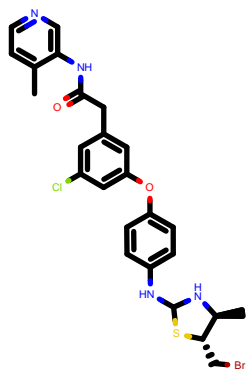
CID:	EN300-1274638
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+]([C@H]([C@@H](S4)CBr)C
RUN:	RUN3261
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.15

EN300-378599
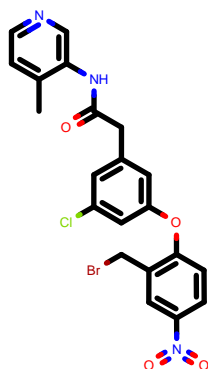
CID:	EN300-378599
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)N(=O)=O
RUN:	RUN2138
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.14

EN300-219510
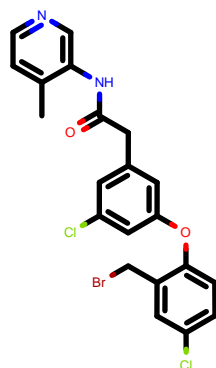
CID:	EN300-219510
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)Cl
RUN:	RUN1021
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.13

EN300-16612
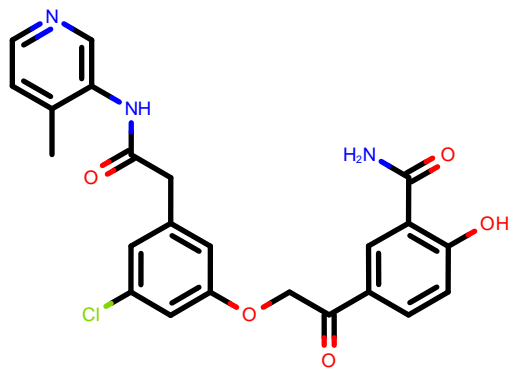
CID:	EN300-16612
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)c3ccc(c(c3)C(=O)N)O
RUN:	RUN4581
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.44

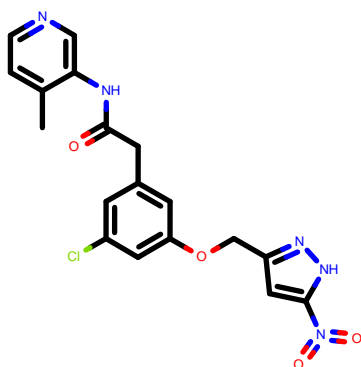# EN300-695739
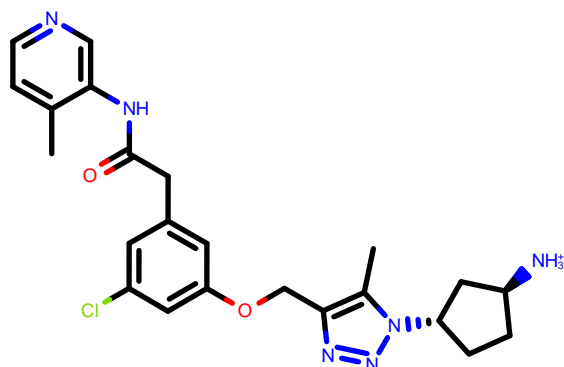
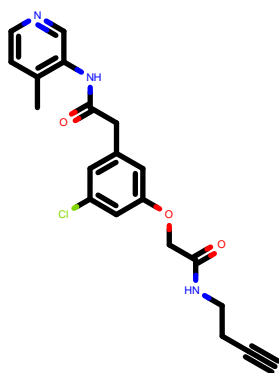|	
CID:	EN300-695739
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(nn3)[C@@H]4CC[C@@H](C4)[NH3+])C
RUN:	RUN1003
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.17

EN300-1923485

CID:	EN300-1923485
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc([nH]n3)N(=O)=O
RUN:	RUN2661
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.13

EN300-135871

CID:	EN300-135871
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)NCCC#C
RUN:	RUN2631
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.14

EN300-1864036
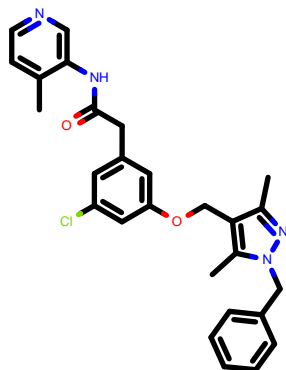
CID:	EN300-1864036
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(nn(c3C)Cc4ccccc4)C
RUN:	RUN301
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.13

EN300-76253
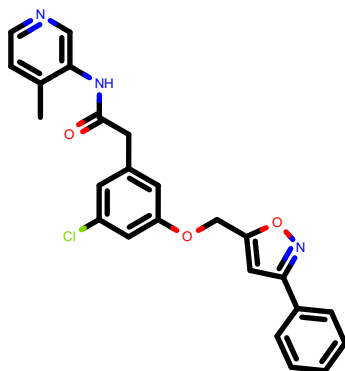
CID:	EN300-76253
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4ccccc4
RUN:	RUN3107
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.14

EN300-1936709
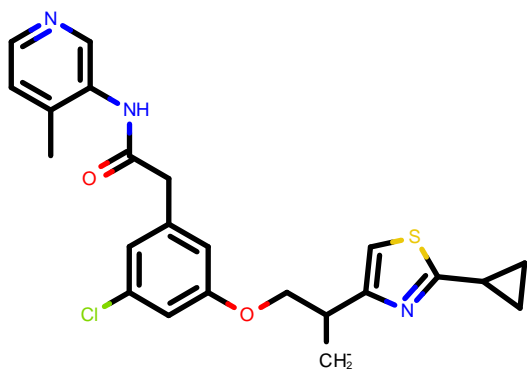
CID:	EN300-1936709
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=C)c3csc(n3)C4CC4
RUN:	RUN4484
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.23

EN300-844238
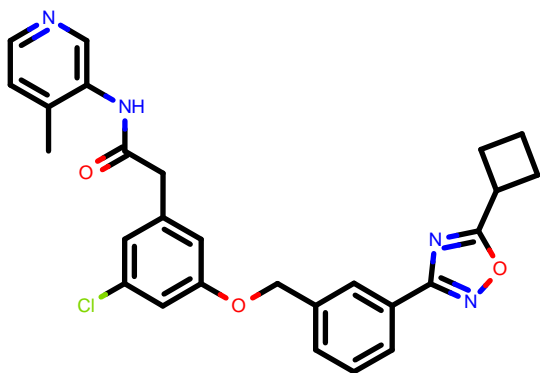
CID:	EN300-844238
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccc(c3)c4nc(on4)C5CCC5
RUN:	RUN2993
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.18

EN300-300079
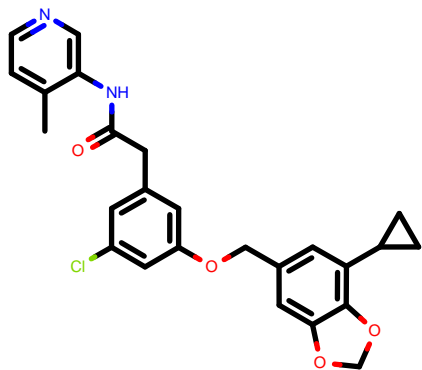
CID:	EN300-300079
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(c4c(c3)OCO4)C5CC5
RUN:	RUN3418
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.16

EN300-75651
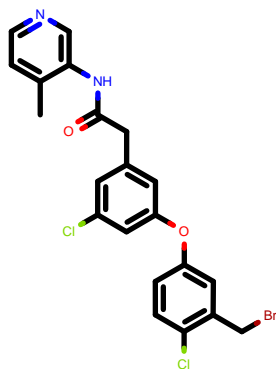
CID:	EN300-75651
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)CBr)Cl
RUN:	RUN2571
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.11

EN300-738987
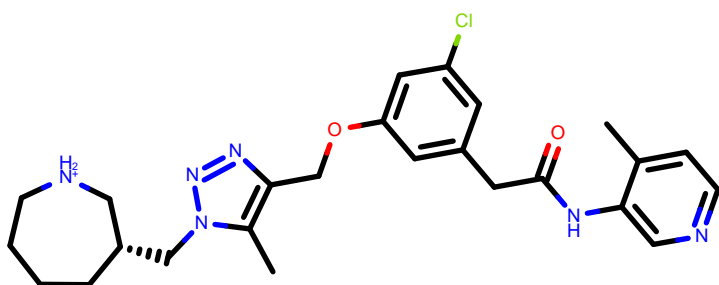
CID:	EN300-738987
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(nn3C[C@@H]4CCCC[NH2+]C4)C
RUN:	RUN392
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.14

EN300-1916571
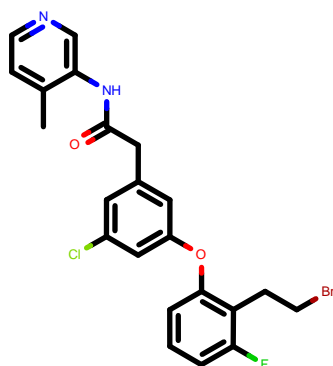
CID:	EN300-1916571
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3CCBr)F
RUN:	RUN1098
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.14

EN300-177132
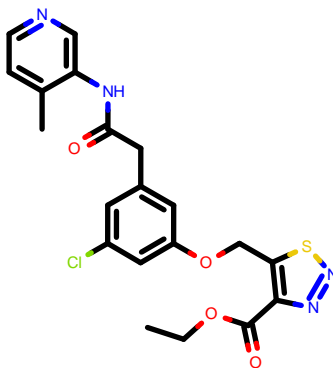
CID:	EN300-177132
SMILES:	CCOC(=O)c1c(snn1)COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
RUN:	RUN361
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.12

EN300-1563127

CID:	EN300-1563127
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3)C)C(=O)OC
RUN:	RUN4415
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.19

EN300-767696

CID:	EN300-767696
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccc(c3)c4ccc(cc4)[C@@H]5CCO5
RUN:	RUN2490
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.17

EN300-1613392

CID:	EN300-1613392
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(oc(=O)o3)c4cccc(c4)N(=O)=O
RUN:	RUN2799
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.22

EN300-658821

CID:	EN300-658821
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3CBr)OC)C(=O)OC
RUN:	RUN2540
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.20

EN300-1910378

CID:	EN300-1910378
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)CCBr)C
RUN:	RUN434
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.10

EN300-38958
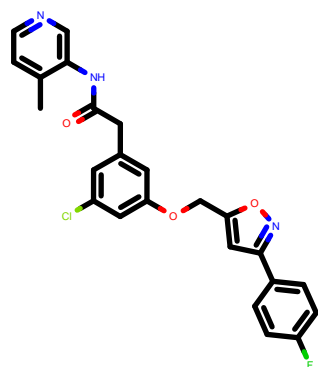
CID:	EN300-38958
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4ccc(cc4)F
RUN:	RUN3479
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.14

EN300-14247
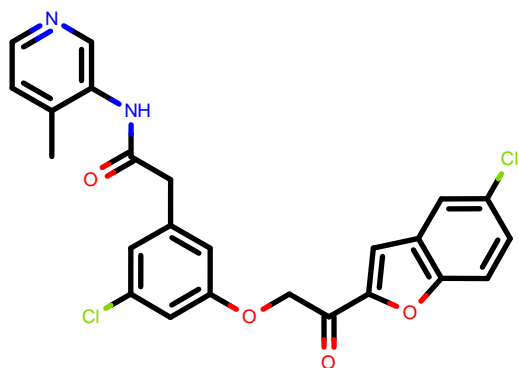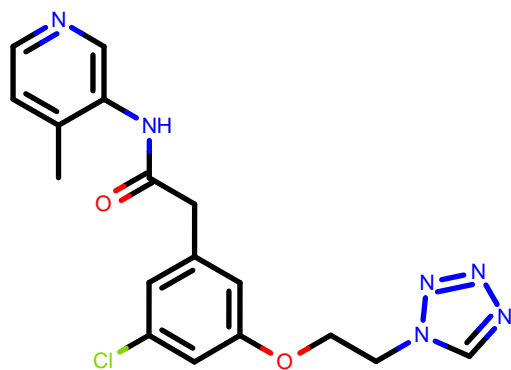

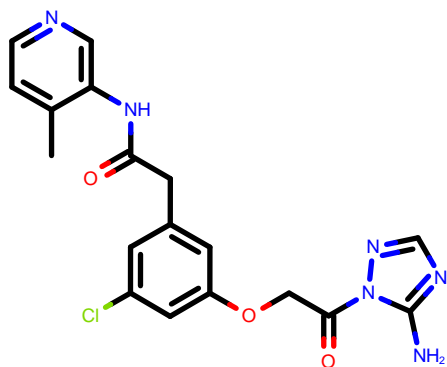|	
CID:	EN300-14247
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)c3cc4cc(ccc4o3)Cl
RUN:	RUN4540
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.29

EN300-379812

CID:	EN300-379812
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCn3cnnn3
RUN:	RUN4327
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.17

EN300-7464827

CID:	EN300-7464827
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)n3c(ncn3)N
RUN:	RUN4391
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.18

EN300-66387
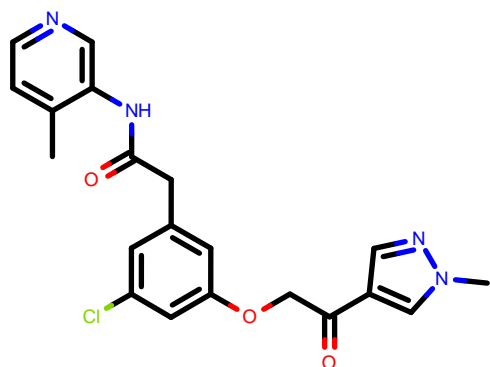
CID:	EN300-66387
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)c3cnn(c3)C
RUN:	RUN4599
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.48

EN300-380073
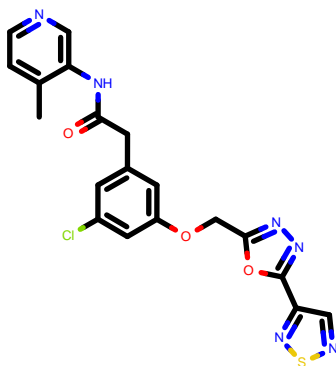
CID:	EN300-380073
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3nnc(o3)c4cnsn4
RUN:	RUN1159
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.15

EN300-738987
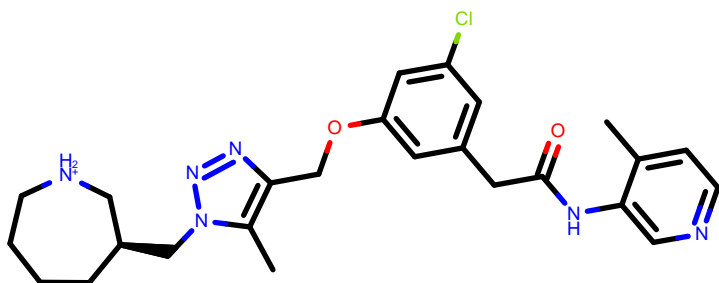
CID:	EN300-738987
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(nn3)C[C@H]4CCCC[NH2+]C4)C
RUN:	RUN640
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.16

EN300-1132699
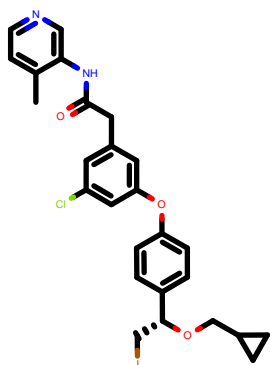
CID:	EN300-1132699
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)OCC4CC4
RUN:	RUN1728
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.15

EN300-6764228
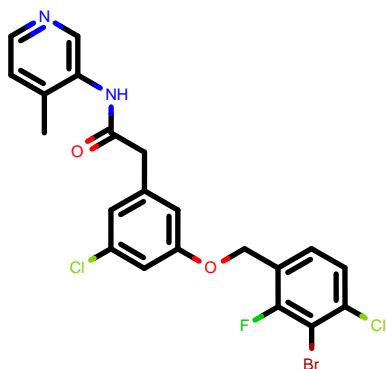
CID:	EN300-6764228
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3F)Br)Cl
RUN:	RUN1389
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.13

EN300-77512
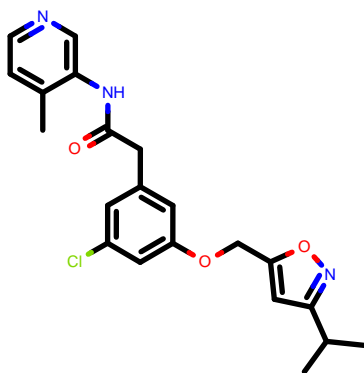
CID:	EN300-77512
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)C(C)C
RUN:	RUN1518
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.12

EN300-99500
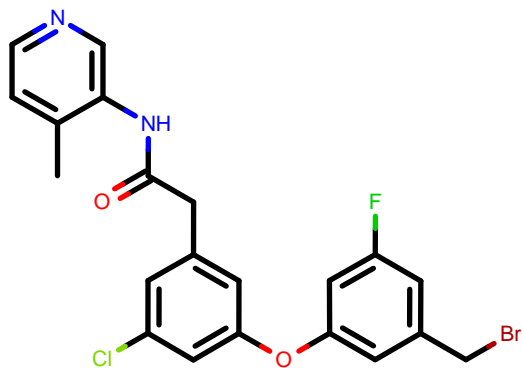
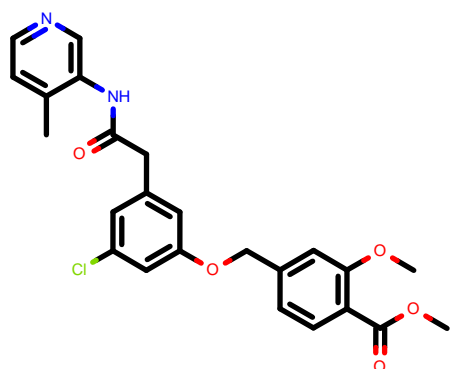| CID:	EN300-99500
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(cc(c3)F)CBr
RUN:	RUN1809
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.11

EN300-1919504
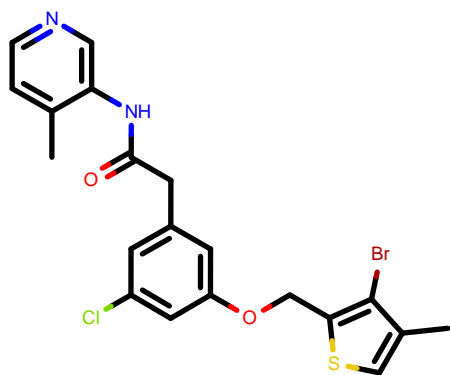
CID:	EN300-1919504
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(c(cs3)C)Br
RUN:	RUN183
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.09

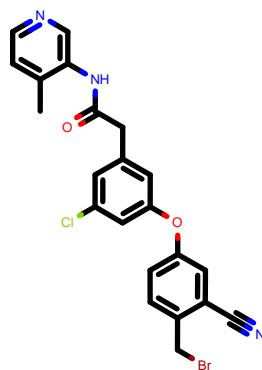## EN300-123146

|	
CID:	EN300-123146
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3)OC)C(=O)OC
RUN:	RUN4346
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.17

EN300-1697674
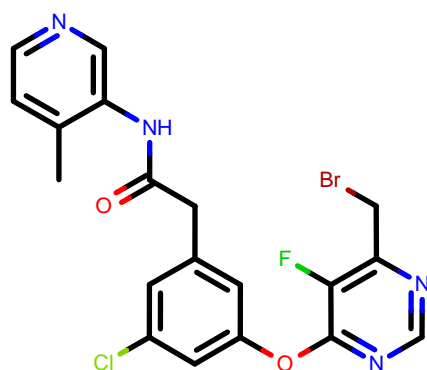
CID:	EN300-1697674
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3c(c(ncn3)CBr)F
RUN:	RUN3759
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.12

EN300-107185

CID:	EN300-107185
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C#N)CBr
RUN:	RUN3171
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.14

EN300-269986
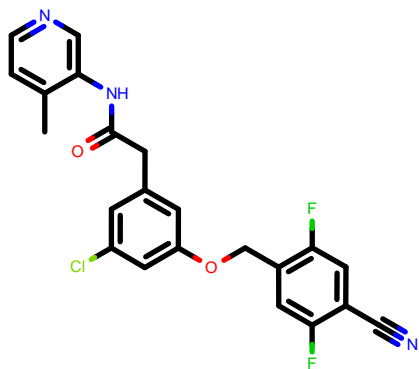
CID:	EN300-269986
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(c(cc3F)C#N)F
RUN:	RUN4230
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.13

EN300-1927497
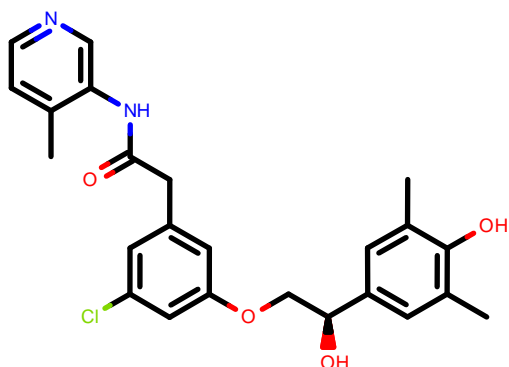
CID:	EN300-1927497
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3cc(c(c(c3)C)O)C)O
RUN:	RUN3223
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.18

EN300-87674
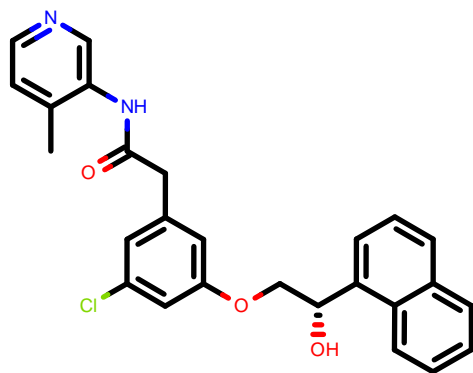
CID:	EN300-87674
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3cccc4c3cccc4)O
RUN:	RUN3047
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.15

EN300-7425216
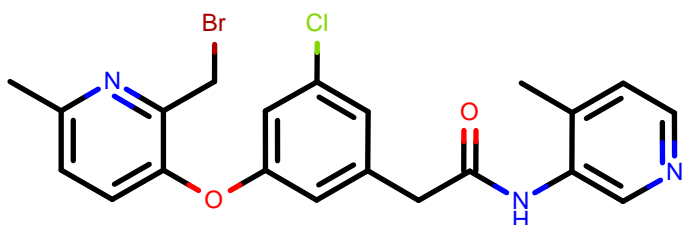
CID:	EN300-7425216
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(nc3CBr)C
RUN:	RUN2873
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.12

EN300-1274638
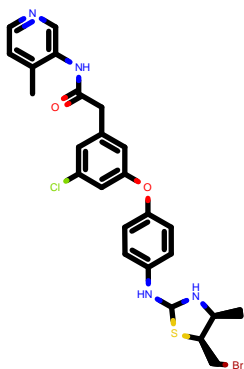
CID:	EN300-1274638
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+][C@H]([C@H](S4)CBr)C
RUN:	RUN3760
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.16

EN300-1896632
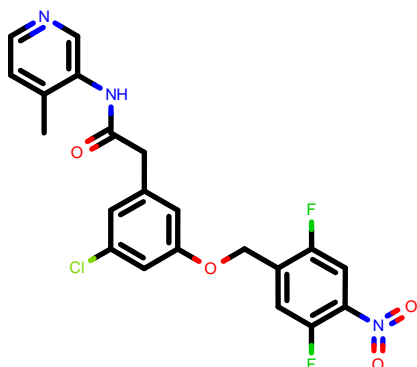
CID:	EN300-1896632
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(c(cc3F)N(=O)=O)F
RUN:	RUN3666
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.14

EN300-764780
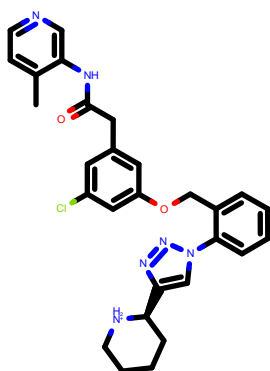
CID:	EN300-764780
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccccc3n4cc(nn4)[C@H]5CCCC[NH2+]5
RUN:	RUN4329
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.23

EN300-1921394
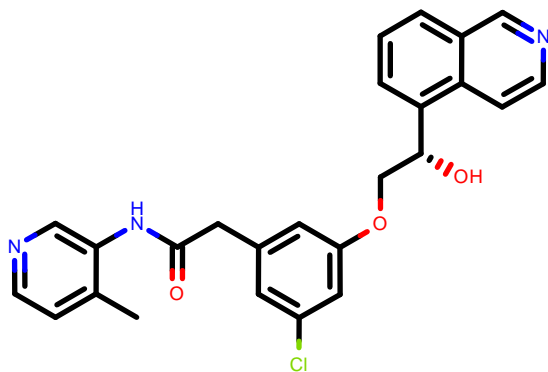
CID:	EN300-1921394
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3cccc4c3ccnc4)O
RUN:	RUN3296
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.16

EN300-1915625
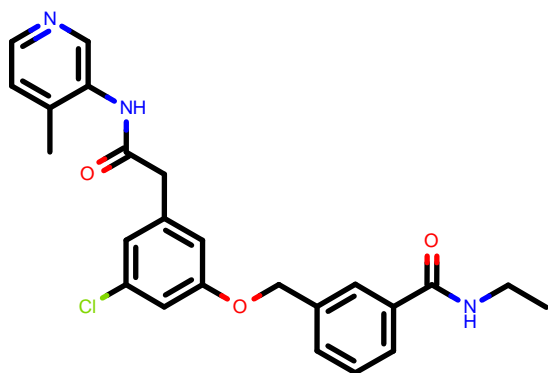
CID:	EN300-1915625
SMILES:	CCNC(=O)c1cccc(c1)COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
RUN:	RUN571
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.15

EN300-7434416
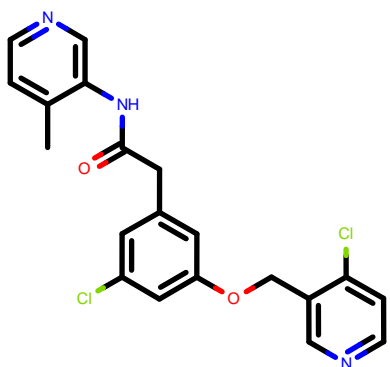
CID:	EN300-7434416
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnccc3Cl
RUN:	RUN1026
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.11

EN300-1137140
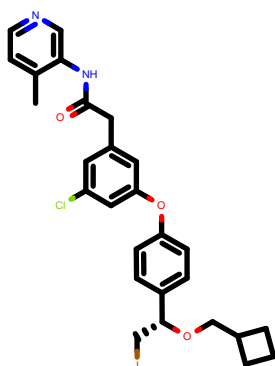
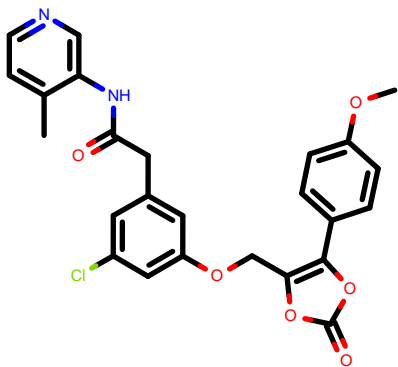| CID:	EN300-1137140
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)OCC4CCC4
RUN:	RUN1359
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.16

EN300-35204
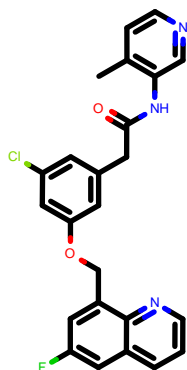
CID:	EN300-35204
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(cc4c3nccc4)F
RUN:	RUN1226
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.14

EN300-1613389

CID:	EN300-1613389
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(oc(=O)o3)c4ccc(cc4)OC
RUN:	RUN2575
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.19

EN300-224566
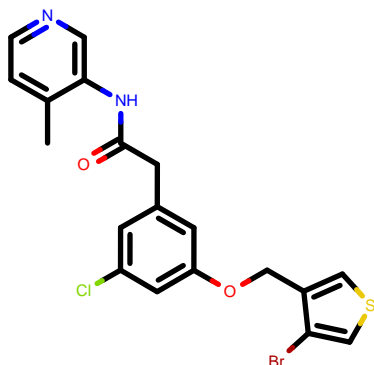
CID:	EN300-224566
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cscc3Br
RUN:	RUN333
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.09

EN300-7427269
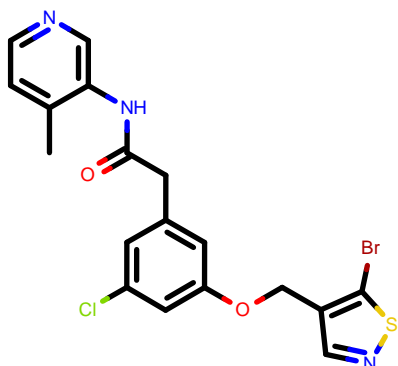
CID:	EN300-7427269
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnsc3Br
RUN:	RUN834
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.11

EN300-180043
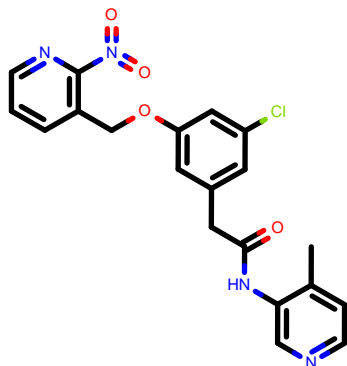
CID:	EN300-180043
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccnc3N(=O)=O
RUN:	RUN1551
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.12

EN300-1916585
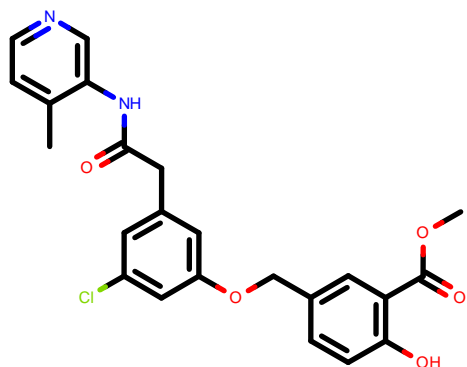
CID:	EN300-1916585
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3)C(=O)OC)O
RUN:	RUN1342
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.17

EN300-841086
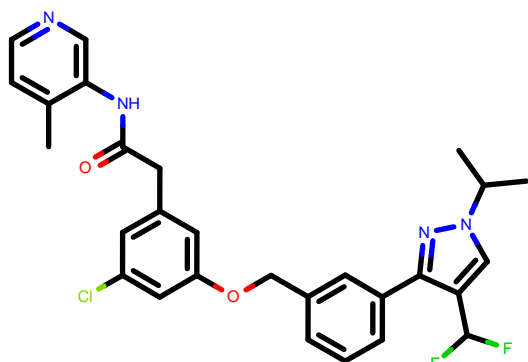
CID:	EN300-841086
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccc(c3)c4c(cn(n4)C(C)C)C(F)F
RUN:	RUN798
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.20

EN300-766689
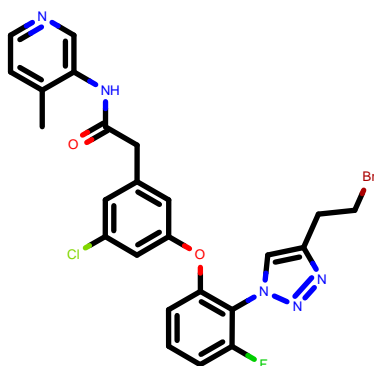
CID:	EN300-766689
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3n4cc(nn4)CCBr)F
RUN:	RUN3550
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.21

EN300-202844
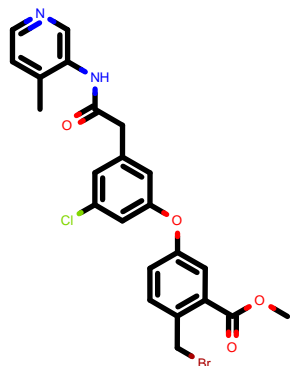
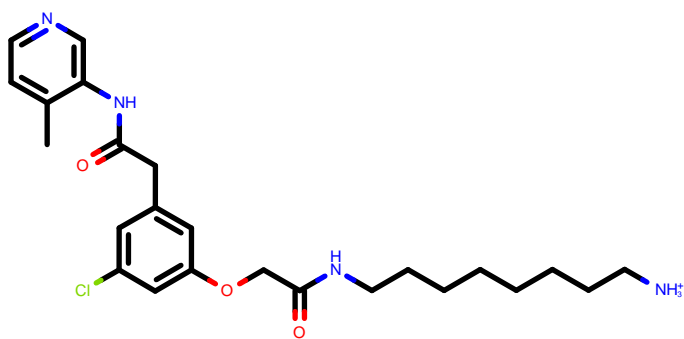| CID:	EN300-202844
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C(=O)OC)CBr
RUN:	RUN2367
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.14

EN300-1906910
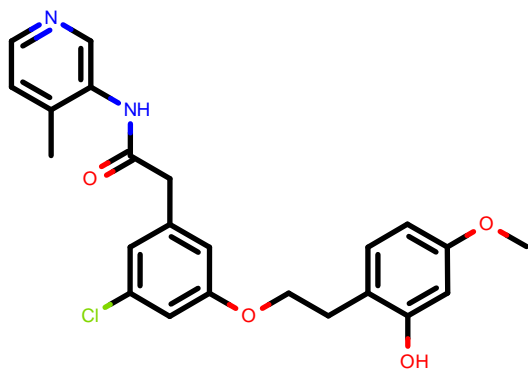
CID:	EN300-1906910
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3ccc(cc3O)OC
RUN:	RUN2912
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.14

EN300-7456768

CID:	EN300-7456768
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)NCCCCCCCC[NH3+]
RUN:	RUN1899
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.24

EN300-706185
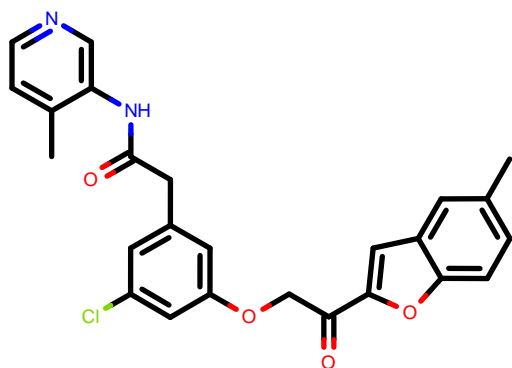
CID:	EN300-706185
SMILES:	Cc1ccc2c(c1)cc(o2)C(=O)COc3cc(cc(c3)Cl)CC(=O)Nc4cnccc4C
RUN:	RUN4521
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.25

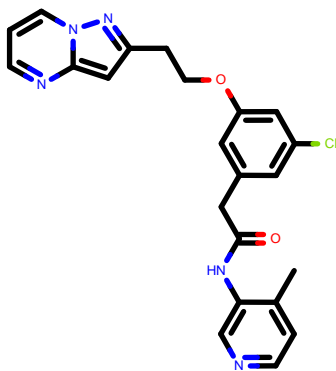## EN300-1132709
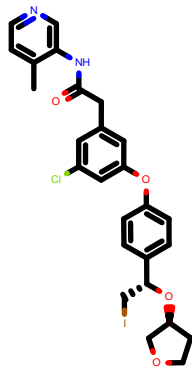
| CID:	EN300-1132709
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)O[C@H]4CCOC4
RUN:	RUN2020
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.15

EN300-1921187

CID:	EN300-1921187
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cc4ncccn4n3
RUN:	RUN4291
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.20

EN300-1132829
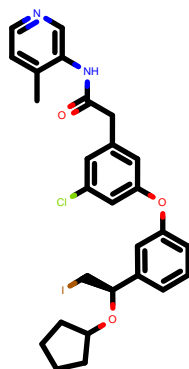
CID:	EN300-1132829
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3)[C@H](Cl)OC4CCCC4
RUN:	RUN1260
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.18

EN300-127870
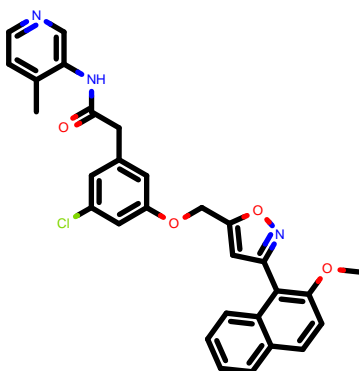
CID:	EN300-127870
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4c5ccccc5ccc4OC
RUN:	RUN3778
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.22

EN300-1613387
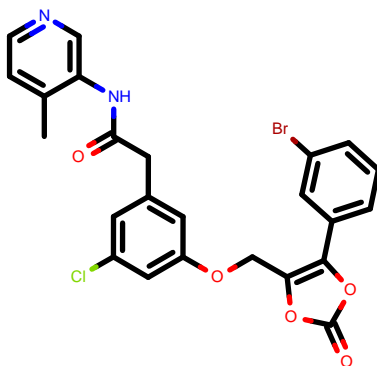
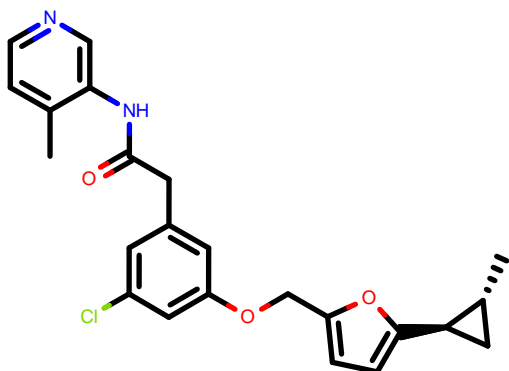|	
CID:	EN300-1613387
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(oc(=O)o3)c4cccc(c4)Br
RUN:	RUN1307
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.19

EN300-728709
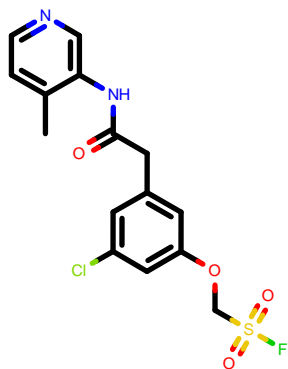
CID:	EN300-728709
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCS(=O)(=O)F
RUN:	RUN302
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.09

EN300-1940535

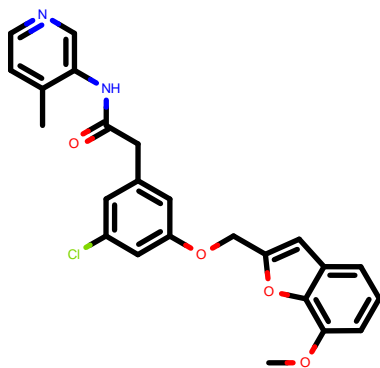| CID:	EN300-1940535
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(o3)[C@@H]4C[C@H]4C
RUN:	RUN161
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.11

EN300-219845
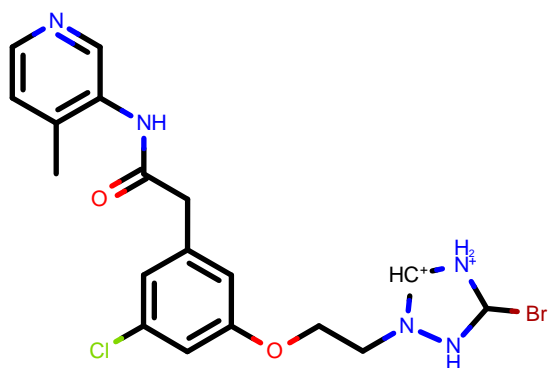
CID:	EN300-219845
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCn3cnc(n3)Br
RUN:	RUN2721
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.15

EN300-236658

CID:	EN300-236658
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc4cccc(c4o3)OC
RUN:	RUN2648
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.16

EN300-254027
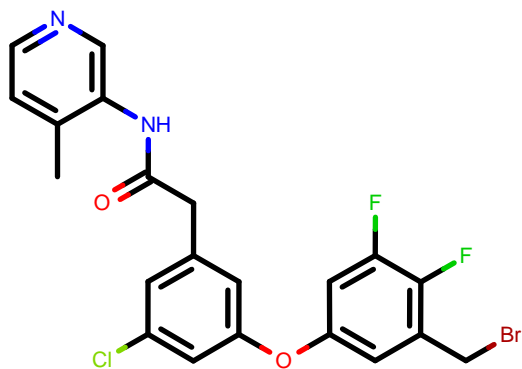
CID:	EN300-254027
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(c(c(c3)F)F)CBr
RUN:	RUN2633
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.12

EN300-118287
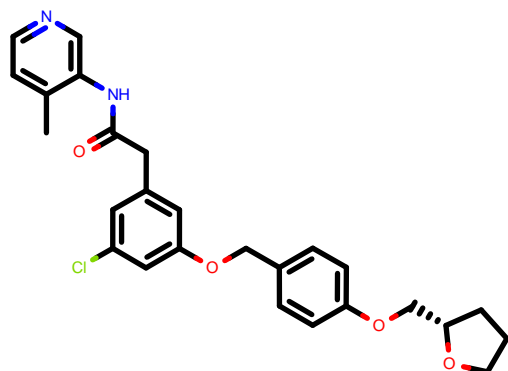
CID:	EN300-118287
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(cc3)OC[C@@H]4CCCO4
RUN:	RUN3490
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.15

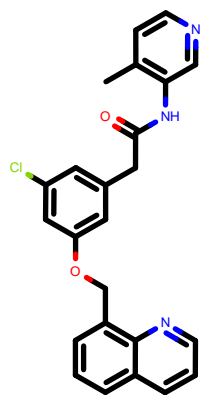## EN300-43569
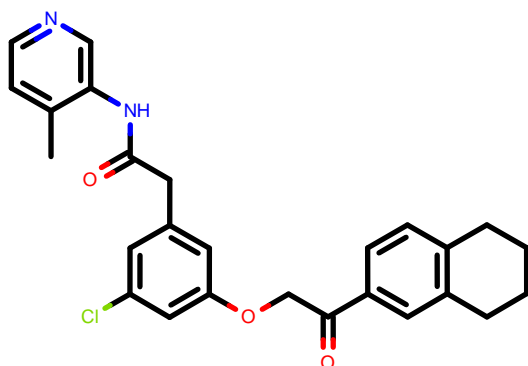
CID:	EN300-43569
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)c3ccc4c(c3)CCCC4
RUN:	RUN4494
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.21

EN300-1456498
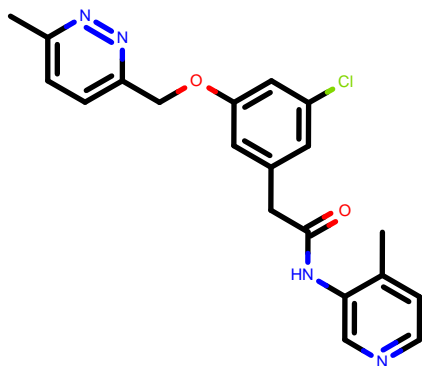
CID:	EN300-1456498
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(nn3)C
RUN:	RUN1684
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.12

EN300-125523

CID:	EN300-125523
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccc4c3nccc4
RUN:	RUN274
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.14

EN300-1897611
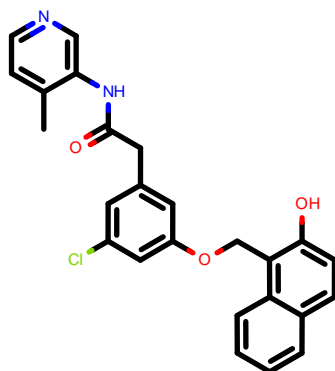
CID:	EN300-1897611
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c4ccccc4ccc3O
RUN:	RUN2647
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.14

EN300-1937083
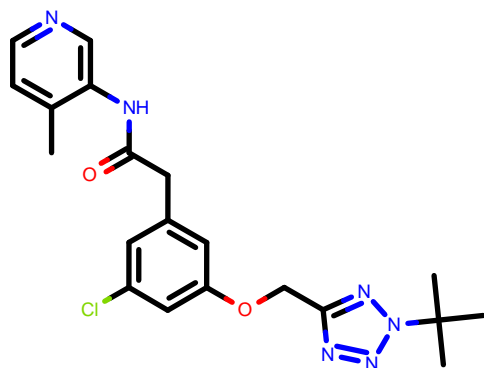
CID:	EN300-1937083
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3nnn(n3)C(C)(C)C
RUN:	RUN1770
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.12

EN300-1934022
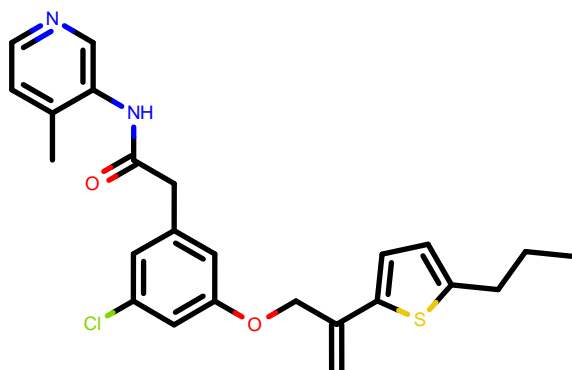
CID:	EN300-1934022
SMILES:	CCCc1ccc(s1)C(=C)COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
RUN:	RUN4524
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.22

EN300-1256145
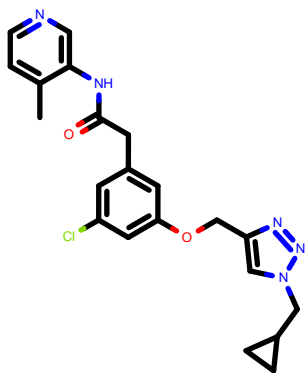
CID:	EN300-1256145
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nn3)CC4CC4
RUN:	RUN398
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.11

EN300-24109
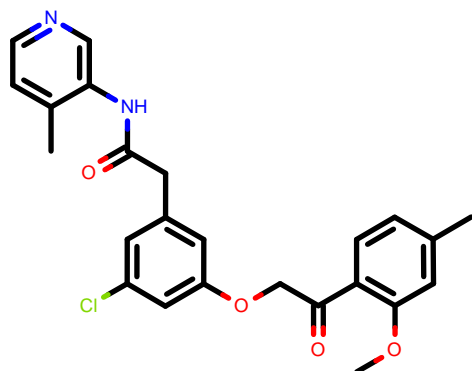
CID:	EN300-24109
SMILES:	Cc1ccc(c(c1)OC)C(=O)COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
RUN:	RUN4349
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.23

EN300-374640
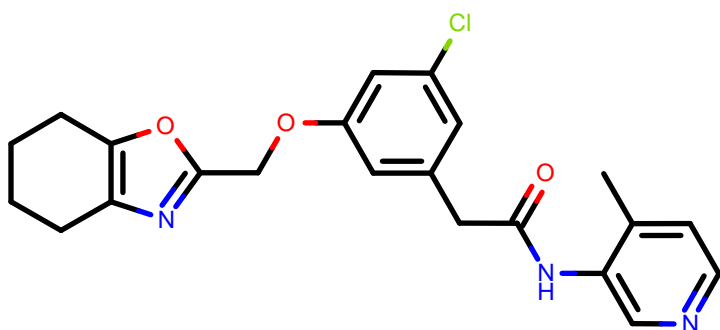
|	
CID:	EN300-374640
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3nc4c(o3)CCCC4
RUN:	RUN3442
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.11

EN300-1864735
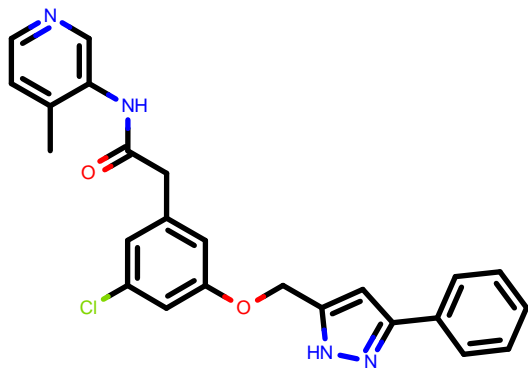
|	
CID:	EN300-1864735
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(n[nH]3)c4ccccc4
RUN:	RUN2573
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.15

EN300-764389
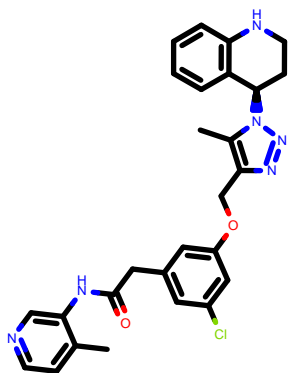
CID:	EN300-764389
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(n(nn3)[C@@H]4CCNc5c4cccc5)C
RUN:	RUN830
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.16

EN300-257065
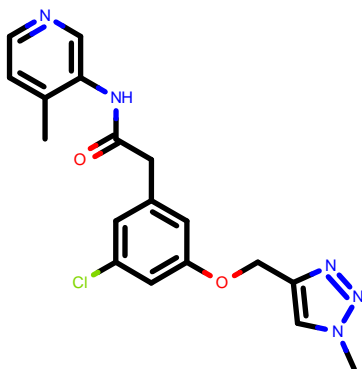
CID:	EN300-257065
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nn3)C
RUN:	RUN1272
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.09

EN300-379204
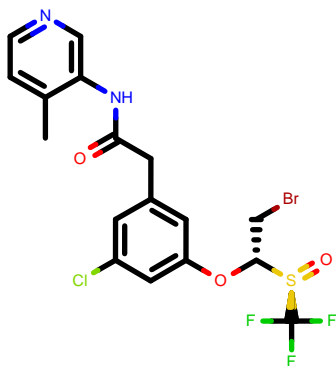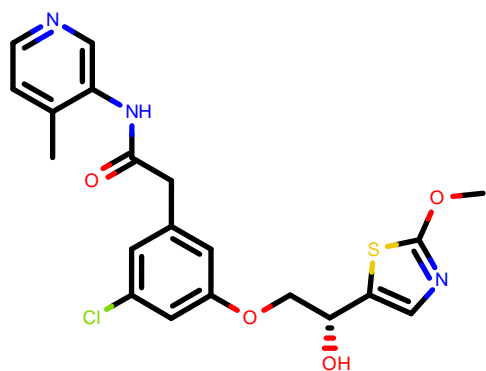
|	
CID:	EN300-379204
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)O[C@H](CBr)[S@@](=O)C(F)(F)F
RUN:	RUN3252
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.14

EN300-1280988
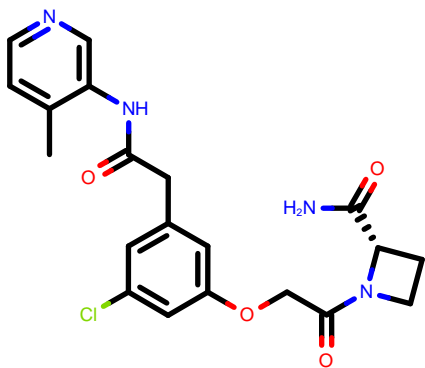
|	
CID:	EN300-1280988
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)N3CC[C@H]3C(=O)N
RUN:	RUN4578
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.27

EN300-1918941

CID:	EN300-1918941
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3cnc(s3)OC)O
RUN:	RUN3118
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.19

EN300-1277859
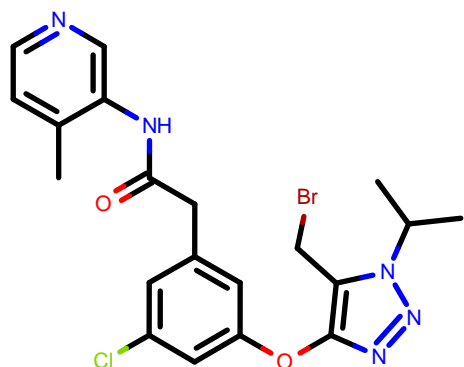
CID:	EN300-1277859
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3c(n(nn3)C(C)C)CBr
RUN:	RUN184
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.11

EN300-843012
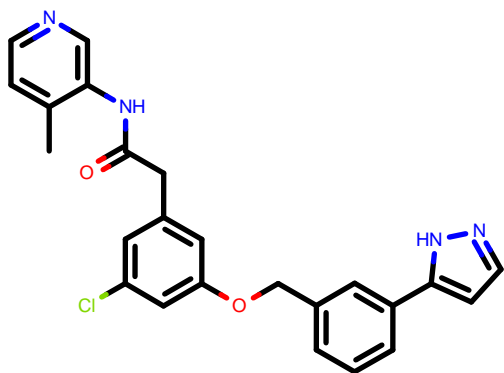
CID:	EN300-843012
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccc(c3)c4ccn[nH]4
RUN:	RUN876
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.12

EN300-1274631
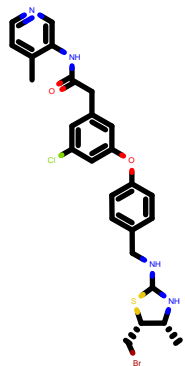
CID:	EN300-1274631
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)C/[NH+]=C\4/N[C@@H]([C@@H](S4)CBr)C
RUN:	RUN1822
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.16

EN300-139605
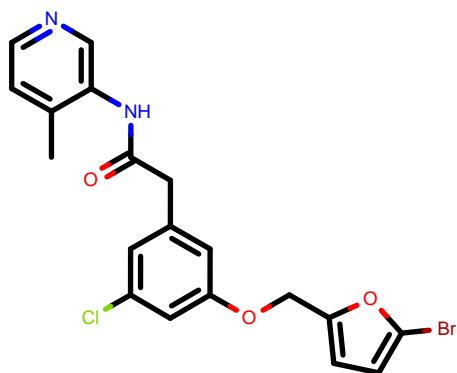
CID:	EN300-139605
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(o3)Br
RUN:	RUN316
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.11

EN300-121881
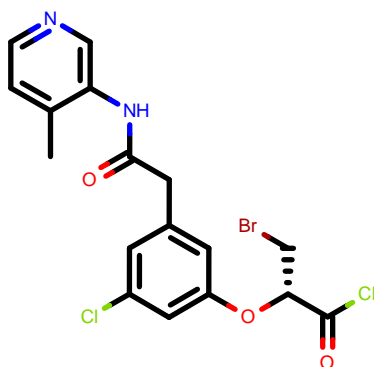
CID:	EN300-121881
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)O[C@H](CBr)C(=O)Cl
RUN:	RUN3472
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.14

EN300-1893407
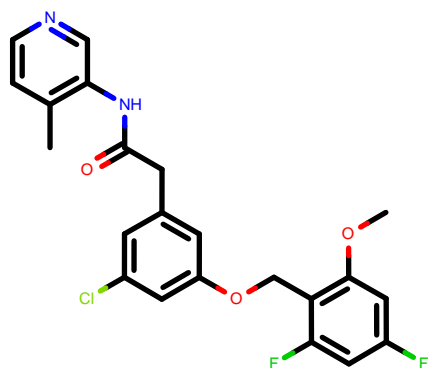
|	
CID:	EN300-1893407
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(cc(cc3F)F)OC
RUN:	RUN1620
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.12

EN300-1934449
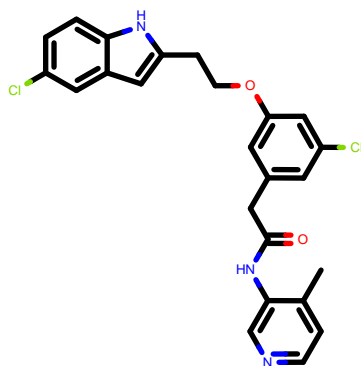
|	
CID:	EN300-1934449
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cc4cc(ccc4[nH]3)Cl
RUN:	RUN3668
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.15

EN300-1117588
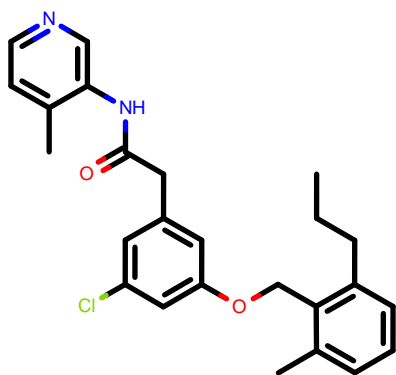
CID:	EN300-1117588
SMILES:	CCCc1cccc(c1COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)C
RUN:	RUN4303
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.13

EN300-99101
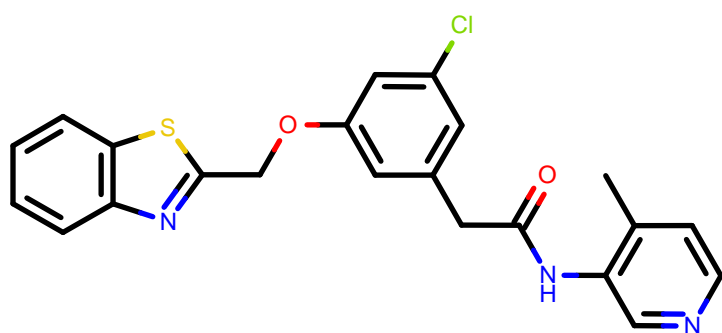
CID:	EN300-99101
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3nc4ccccc4s3
RUN:	RUN3682
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.13

EN300-1894400
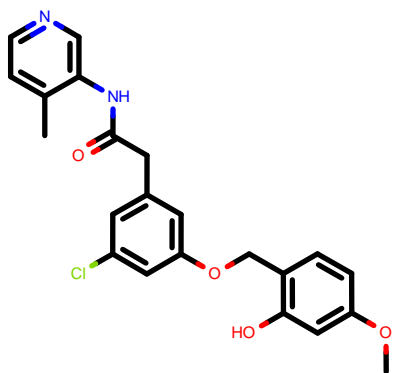
CID:	EN300-1894400
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(cc3O)OC
RUN:	RUN2847
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.13

EN300-1918983
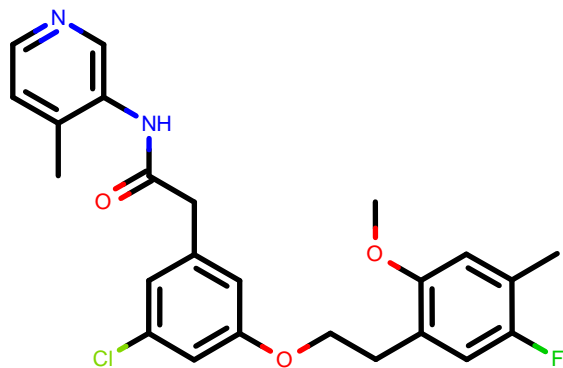
CID:	EN300-1918983
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cc(c(cc3OC)C)F
RUN:	RUN3513
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.15

EN300-313279
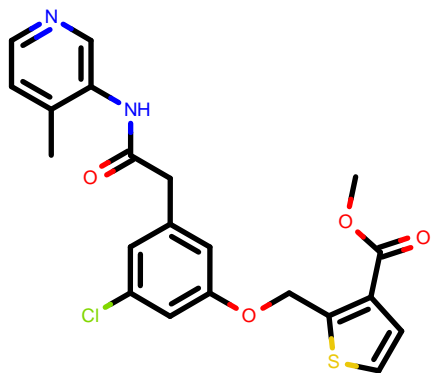
CID:	EN300-313279
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(ccs3)C(=O)OC
RUN:	RUN970
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.12

EN300-2003699
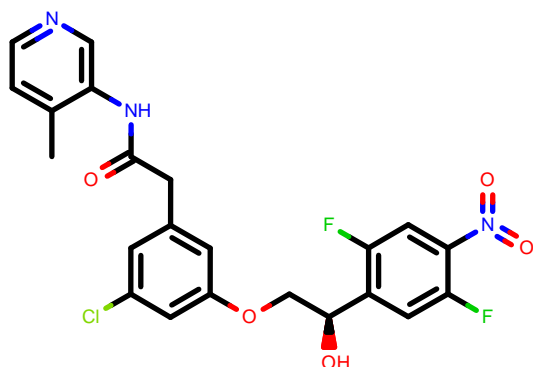
CID:	EN300-2003699
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3cc(c(cc3F)N(=O)=O)F)O
RUN:	RUN2754
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.20

EN300-1706848
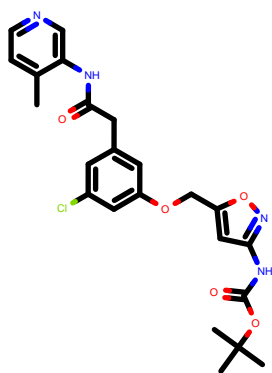
CID:	EN300-1706848
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)NC(=O)OC(C)(C)C
RUN:	RUN2157
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.15

EN300-703228
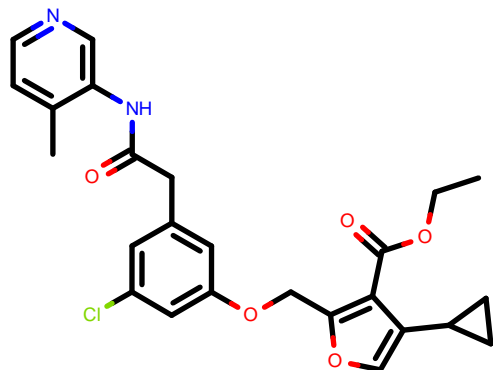
CID:	EN300-703228
SMILES:	CCOC(=O)c1c(coc1COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)C4CC4
RUN:	RUN1126
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.15

EN300-1939155
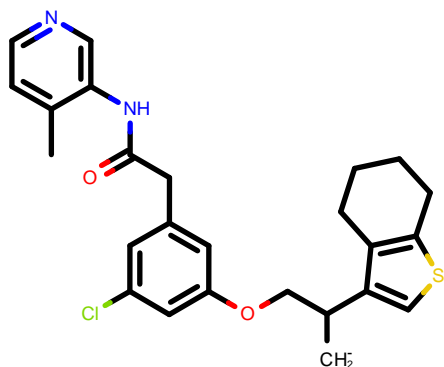
CID:	EN300-1939155
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=C)c3csc4c3CCCC4
RUN:	RUN4498
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.20

EN300-76695
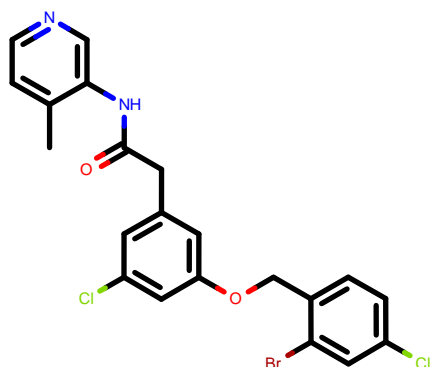
CID:	EN300-76695
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(cc3Br)Cl
RUN:	RUN3337
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.14

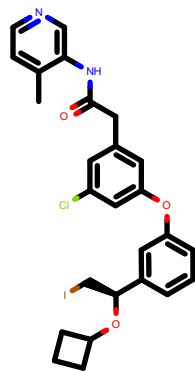# EN300-1921759
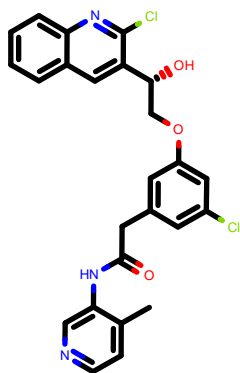
CID:	EN300-1921759
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3cc4ccccc4nc3Cl)O
RUN:	RUN4336
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.22

EN300-740100
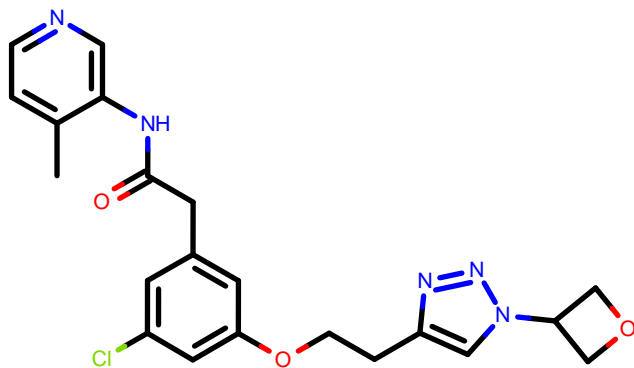
CID:	EN300-740100
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cn(nn3)C4COC4
RUN:	RUN3372
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.17

EN300-1132820

CID:	EN300-1132820
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3)[C@H](Cl)OC4CCC4
RUN:	RUN546
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.14

EN300-189792
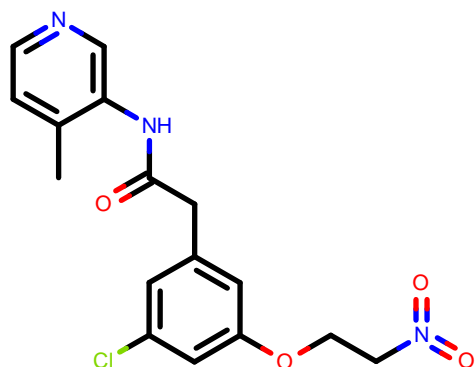
CID:	EN300-189792
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCN(=O)=O
RUN:	RUN1898
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.10

EN300-1910456
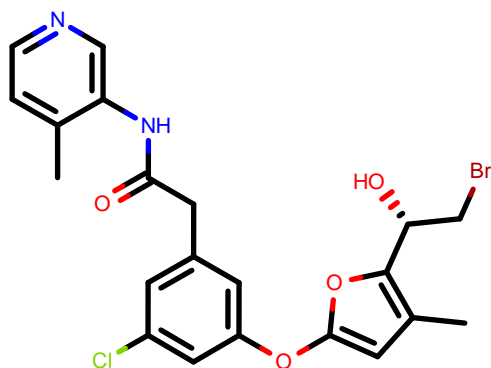
CID:	EN300-1910456
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)[C@@H](CBr)O)C
RUN:	RUN77
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.16

EN300-840854
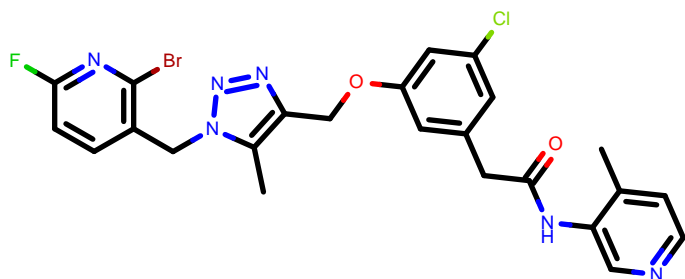
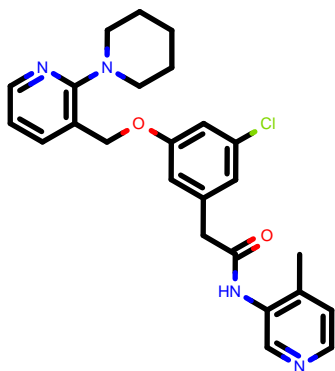|	
CID:	EN300-840854
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(n(nn3)Cc4ccc(nc4Br)F)C
RUN:	RUN1094
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.16

EN300-1145382
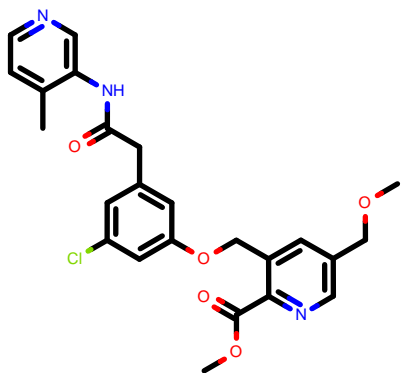
|	
CID:	EN300-1145382
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(cnc3C(=O)OC)COC
RUN:	RUN4276
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.17

EN300-1913480

CID:	EN300-1913480
SMILES:	Cc1ccnccc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccnc3N4CCCCC4
RUN:	RUN3408
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.17

EN300-1895232
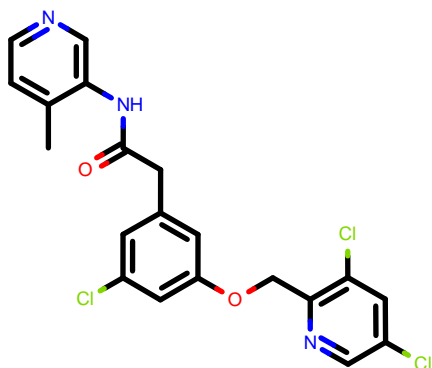
CID:	EN300-1895232
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(cc(cn3)Cl)Cl
RUN:	RUN2929
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.12

EN300-10621
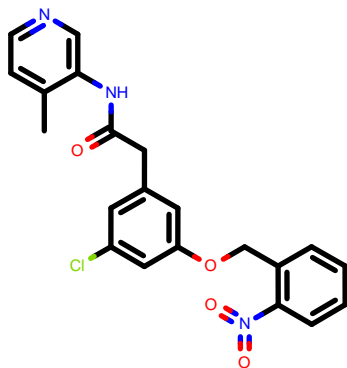
CID:	EN300-10621
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccccc3N(=O)=O
RUN:	RUN1965
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.13

EN300-1613388
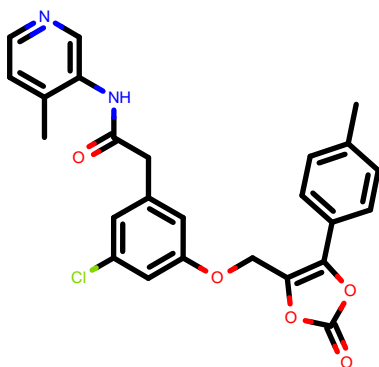
CID:	EN300-1613388
SMILES:	Cc1ccc(cc1)c2c(oc(=O)o2)COc3cc(cc(c3)Cl)CC(=O)Nc4cnccc4C
RUN:	RUN2168
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.18

EN300-13565
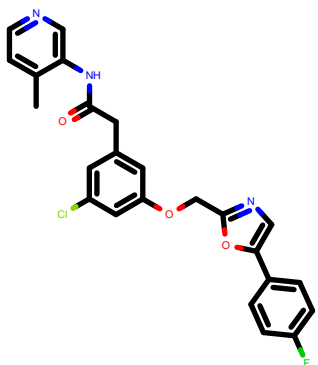
CID:	EN300-13565
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ncc(o3)c4ccc(cc4)F
RUN:	RUN591
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.14

EN300-1910385
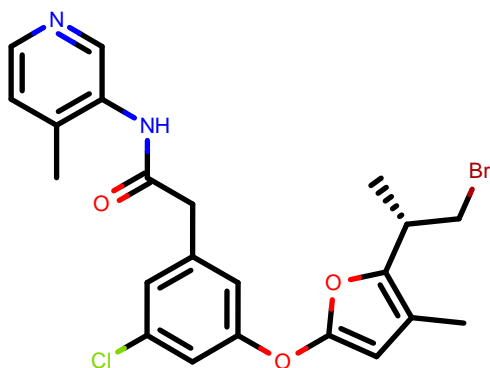
CID:	EN300-1910385
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)[C@H](C)CBr)C
RUN:	RUN602
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.11

EN300-1117578
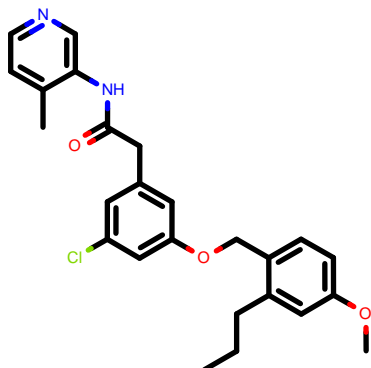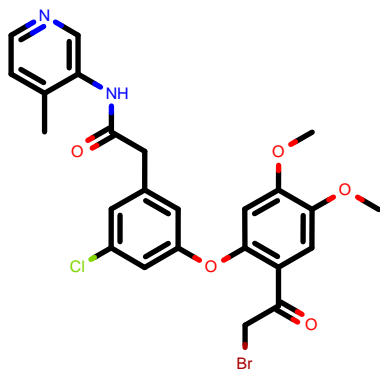

CID:	EN300-1117578
SMILES:	CCCc1cc(ccc1COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)OC
RUN:	RUN4356
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.15

EN300-170062

CID:	EN300-170062
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3C(=O)CBr)OC)OC
RUN:	RUN1973
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.20

EN300-1910226
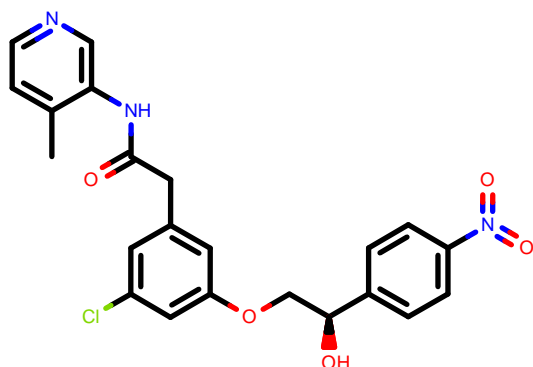
CID:	EN300-1910226
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3ccc(cc3)N(=O)=O)O
RUN:	RUN2028
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.18

EN300-20767
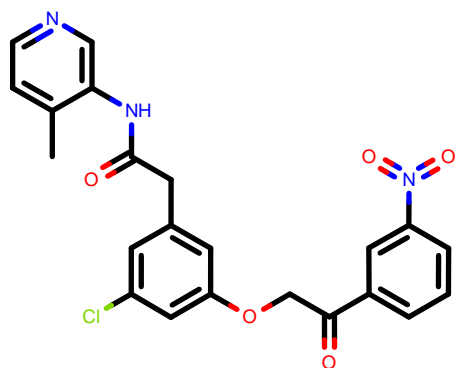
CID:	EN300-20767
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)c3cccc(c3)N(=O)=O
RUN:	RUN4590
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.34

EN300-703231
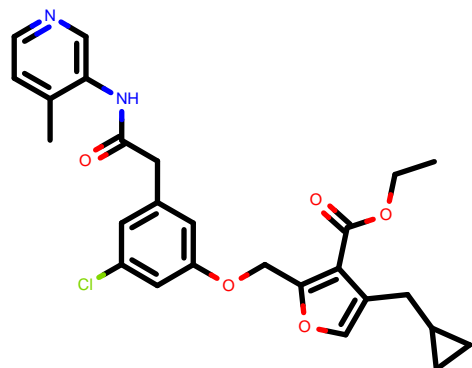
CID:	EN300-703231
SMILES:	CCOC(=O)c1c(coc1COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)CC4CC4
RUN:	RUN1063
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.17

EN300-367729
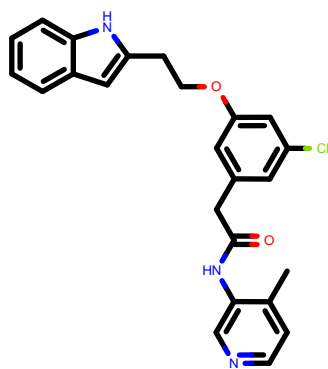
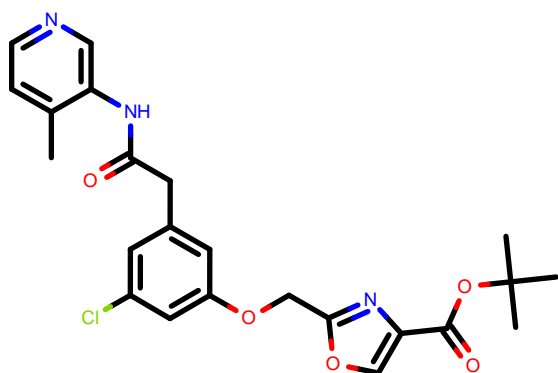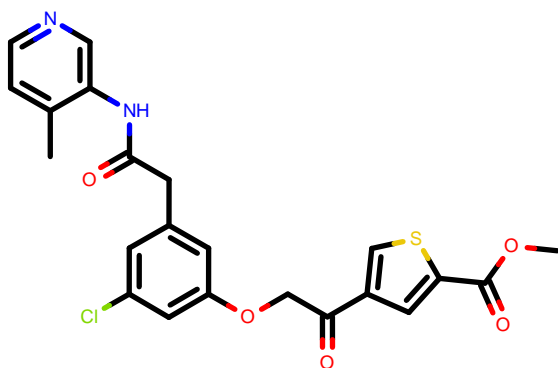|	
CID:	EN300-367729
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cc4ccccc4[nH]3
RUN:	RUN3481
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.15

EN300-1609143

CID:	EN300-1609143
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3nc(co3)C(=O)OC(C)(C)C
RUN:	RUN364
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.14

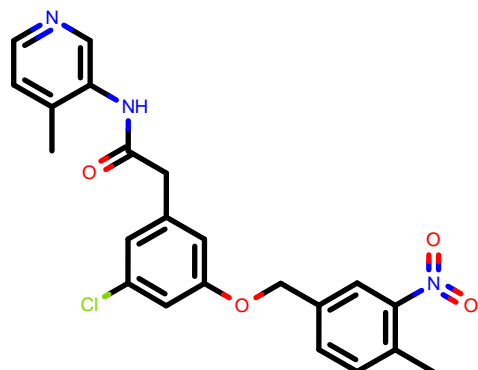# EN300-1700433

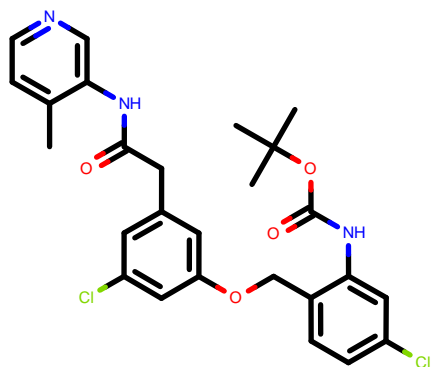|	
CID:	EN300-1700433
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)c3cc(sc3)C(=O)OC
RUN:	RUN4283
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.17

EN300-210903

CID:	EN300-210903
SMILES:	Cc1ccc(cc1N(=O)=O)COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
RUN:	RUN2470
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.14

EN300-1889287

| CID:	EN300-1889287
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(cc3NC(=O)OC(C)(C)C)Cl
RUN:	RUN2123
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.18

EN300-764382
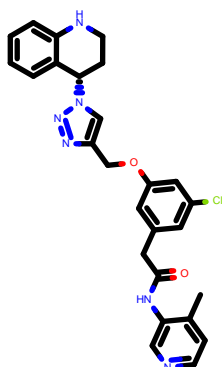
CID:	EN300-764382
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nn3)[C@H]4CCNc5c4cccc5
RUN:	RUN1176
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.17

EN300-1912469
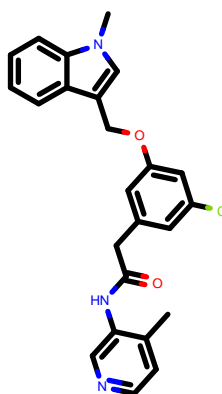
CID:	EN300-1912469
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(c4c3cccc4)C
RUN:	RUN435
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.10

EN300-1921861
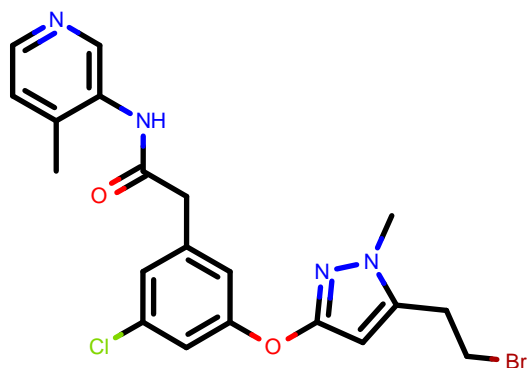
CID:	EN300-1921861
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(n(n3)C)CCBr
RUN:	RUN226
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.12

EN300-364189
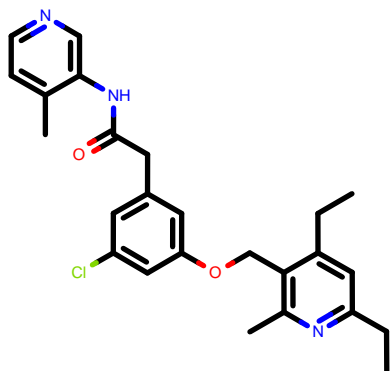
CID:	EN300-364189
SMILES:	CCc1cc(nc(c1COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)C)CC
RUN:	RUN4567
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.29

EN300-695729
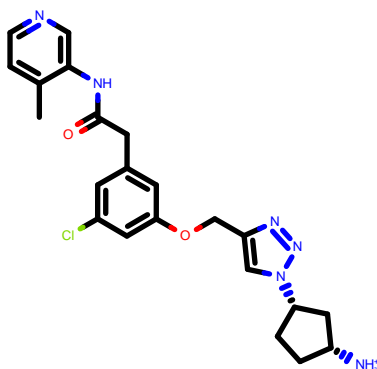
CID:	EN300-695729
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nn3)[C@H]4CC[C@H](C4)[NH3+]
RUN:	RUN1073
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.16

EN300-14150
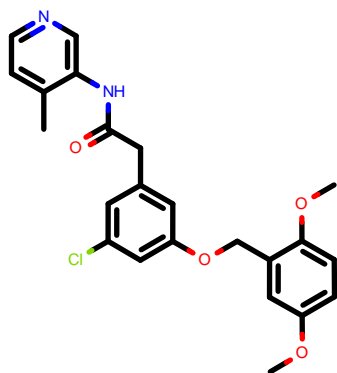
CID:	EN300-14150
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(ccc3OC)OC
RUN:	RUN2092
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.14

EN300-2966841
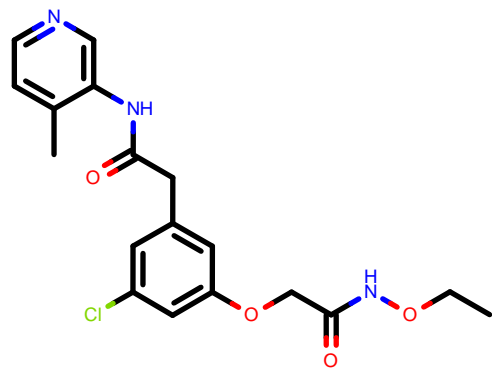
CID:	EN300-2966841
SMILES:	CCONC(=O)COc1cc(cc(c1)Cl)CC(=O)Nc2cnccc2C
RUN:	RUN43
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.10

EN300-1136771
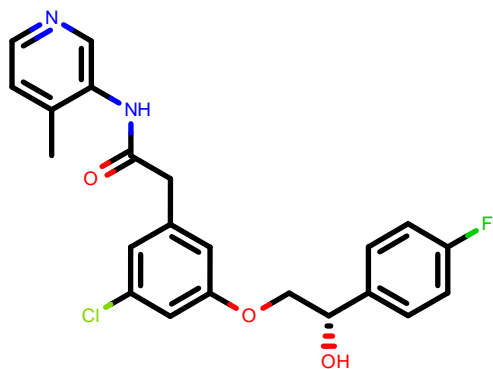
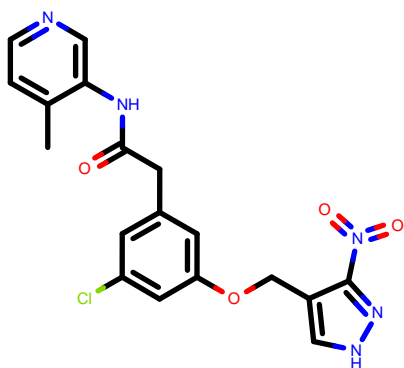|	
CID:	EN300-1136771
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3ccc(cc3)F)O
RUN:	RUN2852
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.17

EN300-1613383
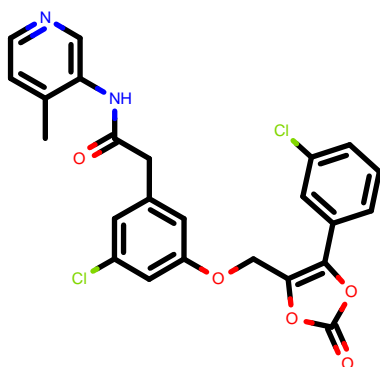
CID:	EN300-1613383
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(oc(=O)o3)c4cccc(c4)Cl
RUN:	RUN1379
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.18

EN300-1915974

CID:	EN300-1915974
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c[nH]nc3N(=O)=O
RUN:	RUN2156
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.12

EN300-1896524
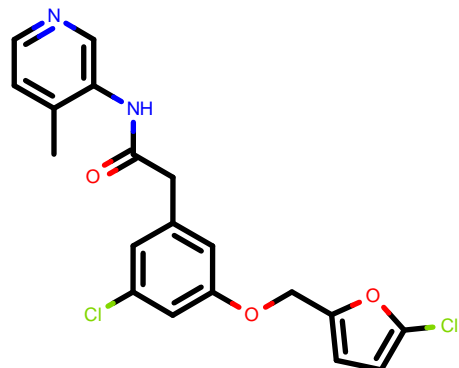
CID:	EN300-1896524
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(o3)Cl
RUN:	RUN384
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.11

EN300-4263497
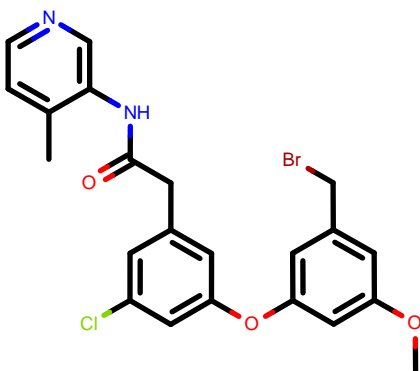
CID:	EN300-4263497
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(cc(c3)OC)CBr
RUN:	RUN2446
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.12

EN300-7433156
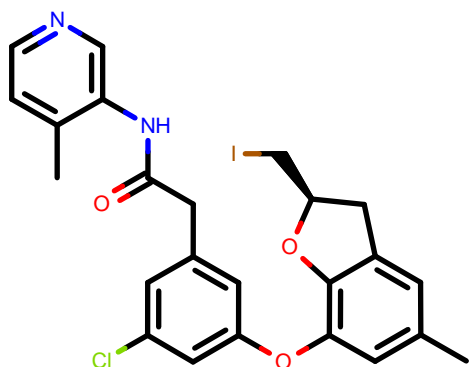
CID:	EN300-7433156
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(cc4c3O[C@@H](C4)Cl)C
RUN:	RUN2999
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.16

EN300-382760
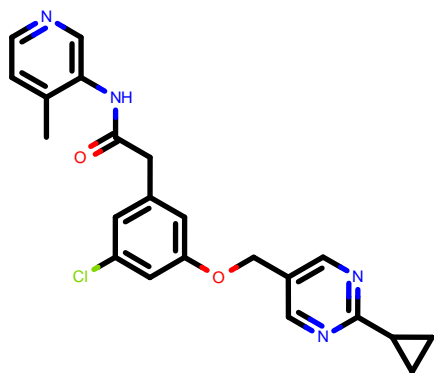
CID:	EN300-382760
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnc(nc3)C4CC4
RUN:	RUN2654
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.13

EN300-1897863
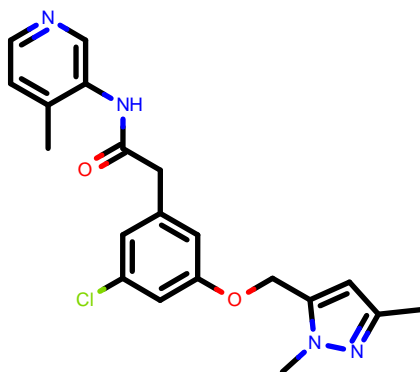
CID:	EN300-1897863
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(nn3C)C
RUN:	RUN956
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.12

EN300-1908580
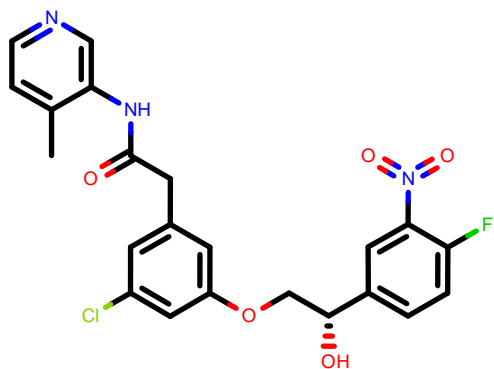
CID:	EN300-1908580
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3ccc(c(c3)N(=O)=O)F)O
RUN:	RUN3152
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.19

EN300-1921979
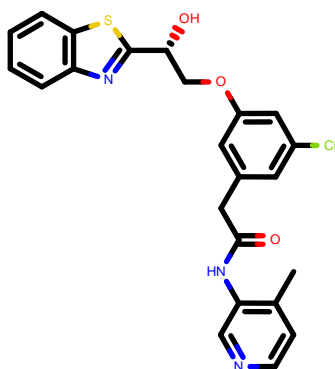
CID:	EN300-1921979
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3nc4ccccc4s3)O
RUN:	RUN3104
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.22

EN300-1904938
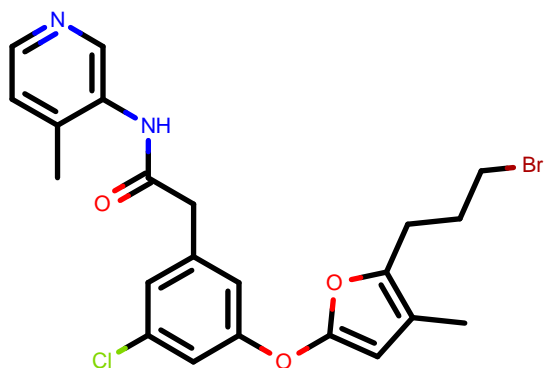
CID:	EN300-1904938
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)CCCBr)C
RUN:	RUN373
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.12

EN300-7493972
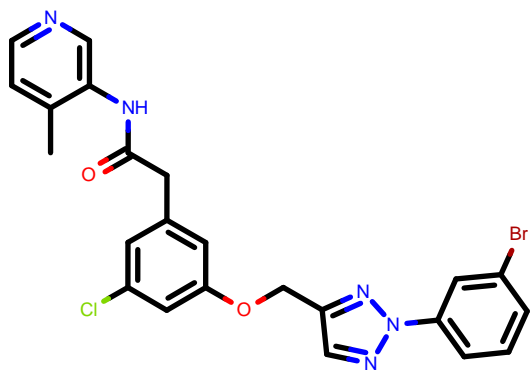
CID:	EN300-7493972
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnn(n3)c4cccc(c4)Br
RUN:	RUN1316
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.14

EN300-138681
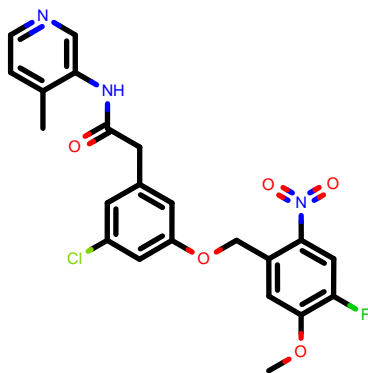
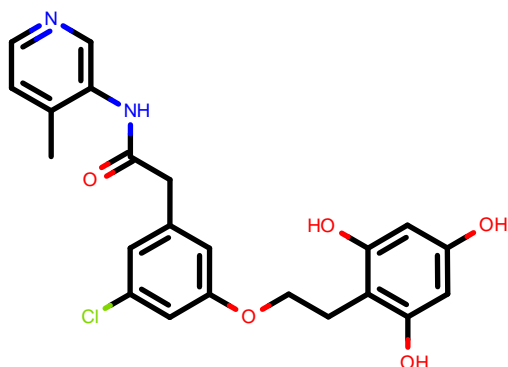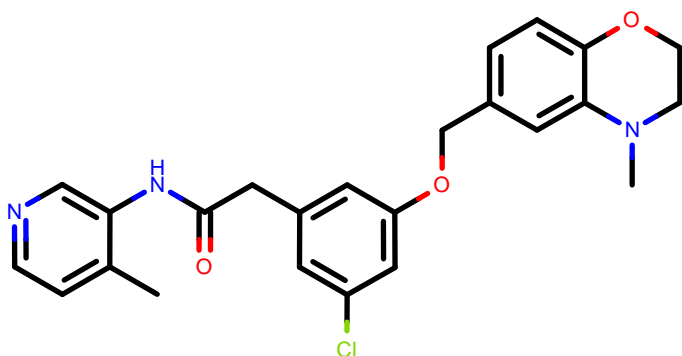|	
CID:	EN300-138681
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(c(cc3N(=O)=O)F)OC
RUN:	RUN4536
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.28

EN300-1934062

CID:	EN300-1934062
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3c(cc(cc3O)O)O
RUN:	RUN2850
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.13

EN300-1917568

CID:	EN300-1917568
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc4c(c3)[N@@](CCO4)C
RUN:	RUN1675
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.12

EN300-2002092
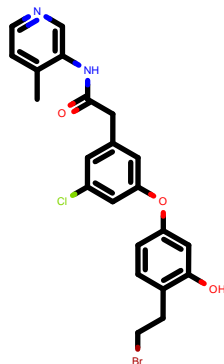
CID:	EN300-2002092
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)O)CCBr
RUN:	RUN700
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.12

EN300-1165403

CID:	EN300-1165403
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c4cc(ccc4sn3)O
RUN:	RUN405
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.12

EN300-134559

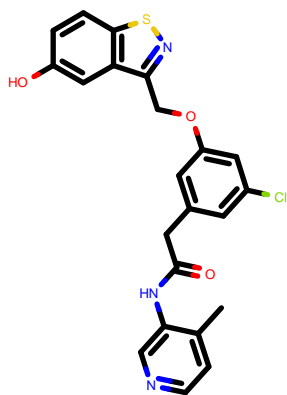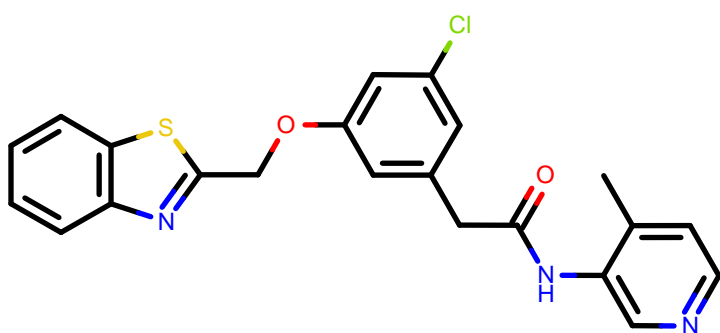| CID:	EN300-134559
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3nc4ccccc4s3
RUN:	RUN3684
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.12

EN300-1908666
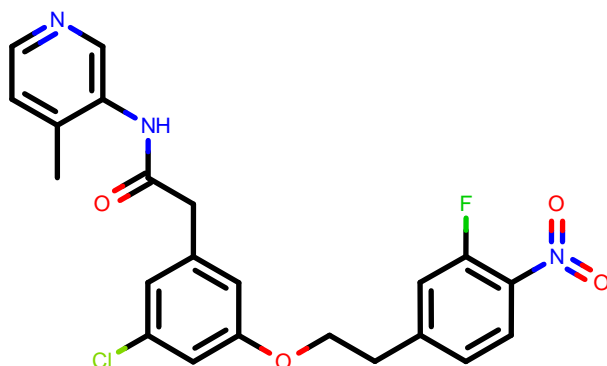
CID:	EN300-1908666
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3ccc(c(c3)F)N(=O)=O
RUN:	RUN3114
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.14

EN300-1915476
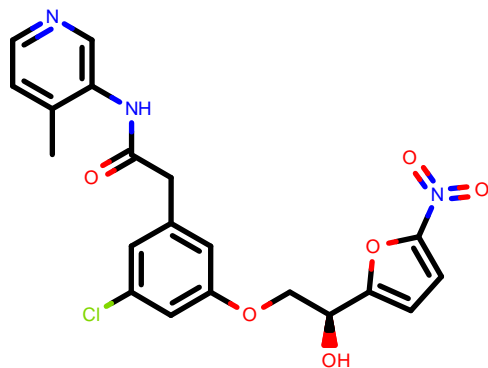
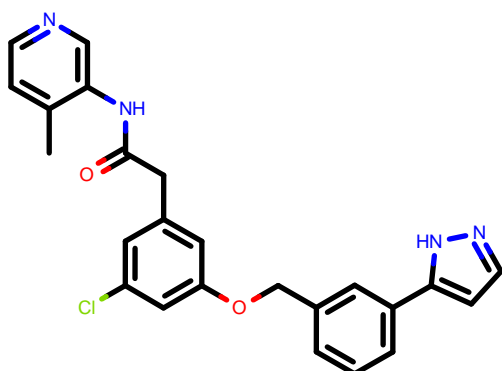| CID:	EN300-1915476
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3ccc(o3)N(=O)=O)O
RUN:	RUN1400
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.19

EN300-1136777
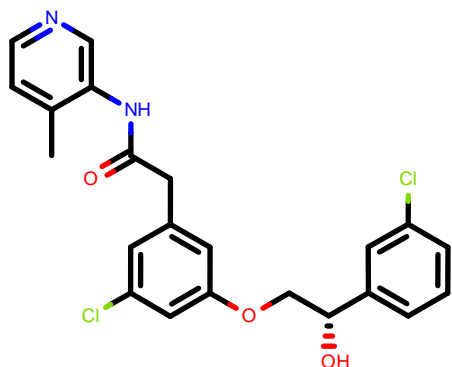
CID:	EN300-1136777
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3cccc(c3)Cl)O
RUN:	RUN2701
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.17

EN300-26674128

CID:	EN300-26674128
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccc(c3)c4ccn[nH]4
RUN:	RUN877
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.13

EN300-396514
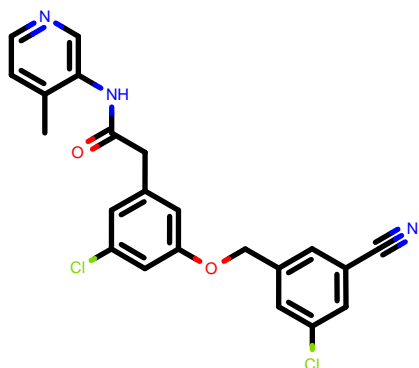
CID:	EN300-396514
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(cc(c3)Cl)C#N
RUN:	RUN2105
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.13

EN300-1997073
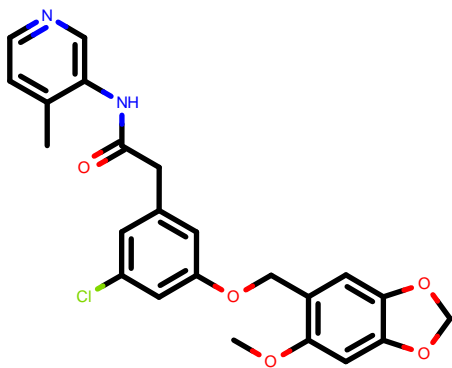
CID:	EN300-1997073
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc4c(cc3OC)OCO4
RUN:	RUN3647
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.15

EN300-216088
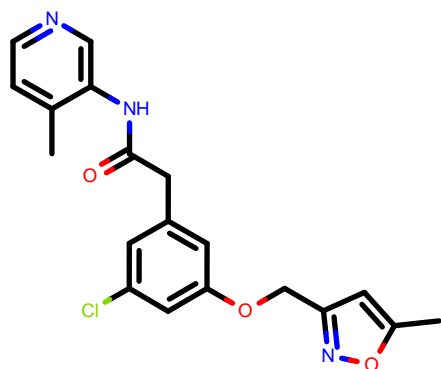
CID:	EN300-216088
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(on3)C
RUN:	RUN989
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.11

EN300-1246893
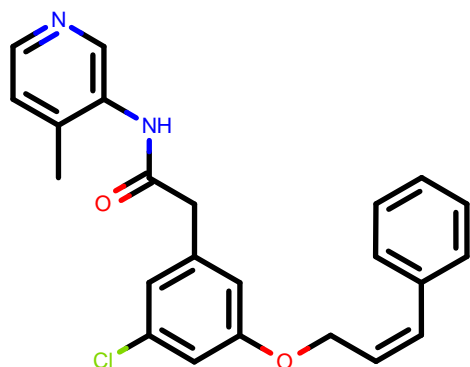
CID:	EN300-1246893
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC/C=C\c3ccccc3
RUN:	RUN1067
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.11

EN300-674675
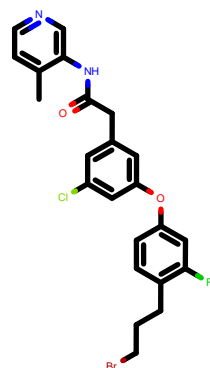
CID:	EN300-674675
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)F)CCCBr
RUN:	RUN1103
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.12

EN300-1653517
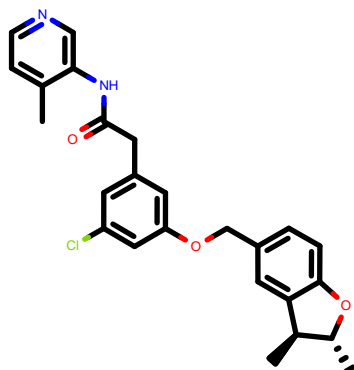
CID:	EN300-1653517
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc4c(c3)[C@@H]([C@@H](O4)C)C
RUN:	RUN1588
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.14

EN300-28768
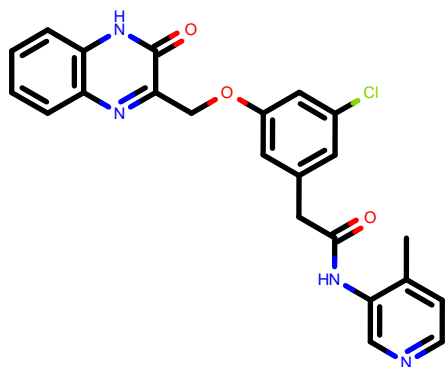
CID:	EN300-28768
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(=O)[nH]c4ccccc4n3
RUN:	RUN3274
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.15

EN300-6245933

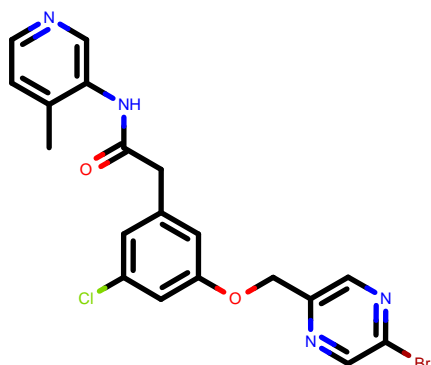|	
CID:	EN300-6245933
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnc(cn3)Br
RUN:	RUN3059
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.12

EN300-260177
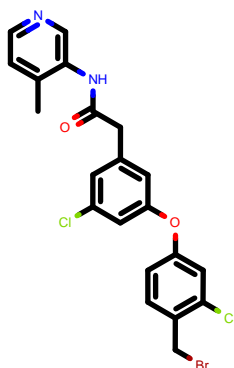
CID:	EN300-260177
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)Cl)CBr
RUN:	RUN1848
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.12

EN300-1296576
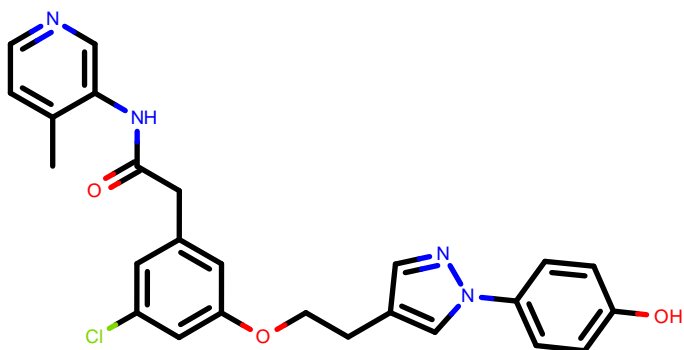
CID:	EN300-1296576
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cnn(c3)c4ccc(cc4)O
RUN:	RUN4341
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.16

EN300-26952

CID:	EN300-26952
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)c3ccc(c(c3)N(=O)=O)Cl
RUN:	RUN4419
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.20

EN300-1132820

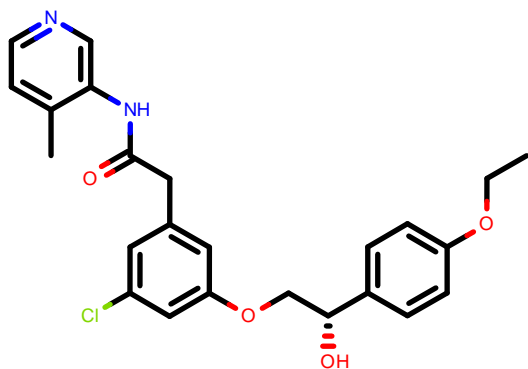|	
CID:	EN300-1132820
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3)[C@@H](CI)OC4CCC4
RUN:	RUN692
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.16

EN300-310116

CID:	EN300-310116
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccc(c3C)OC
RUN:	RUN2457
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.13

EN300-1274639

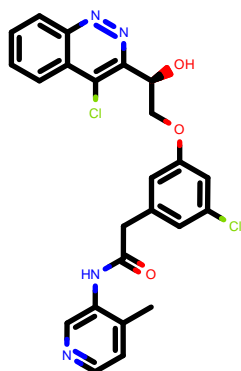|	
CID:	EN300-1274639
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3)NC4=[NH+][C@@H]([C@@H](S4)CBr)C
RUN:	RUN1646
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.17

EN300-87706

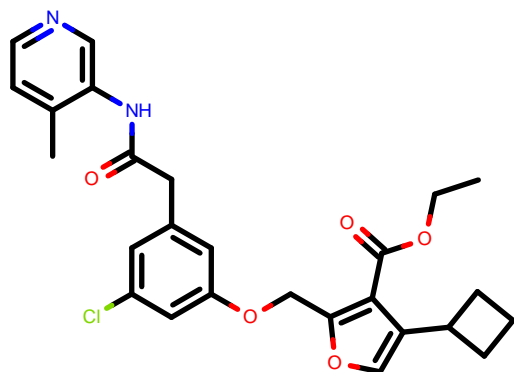|	
CID:	EN300-87706
SMILES:	CCOc1ccc(cc1)[C@@H](COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)O
RUN:	RUN2940
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.20

EN300-1918363

CID:	EN300-1918363
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3c(c4ccccc4nn3)Cl)O
RUN:	RUN4539
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.33

EN300-1918995
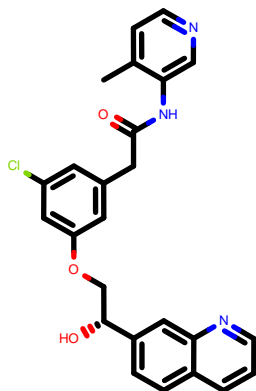
CID:	EN300-1918995
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3ccc4cccnc4c3)O
RUN:	RUN2919
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.18

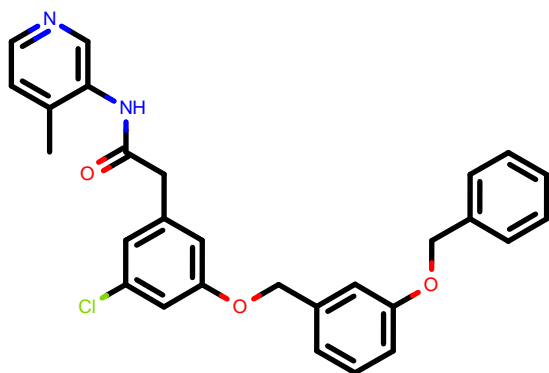# EN300-703234

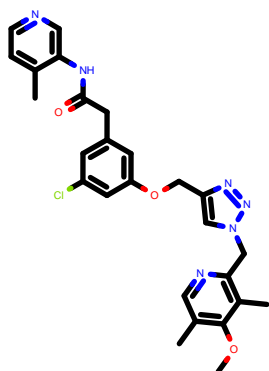|	
CID:	EN300-703234
SMILES:	CCOC(=O)c1c(coc1COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)C4CCC4
RUN:	RUN1813
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.17

EN300-59530

CID:	EN300-59530
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccc(c3)OCc4ccccc4
RUN:	RUN1147
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.15

EN300-766154

CID:	EN300-766154
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nn3)Cc4c(c(c(cn4)C)OC)C
RUN:	RUN2176
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.18

EN300-1898328
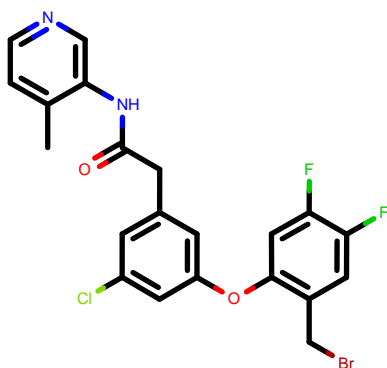
CID:	EN300-1898328
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3CBr)F)F
RUN:	RUN1288
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.13

EN300-1912781
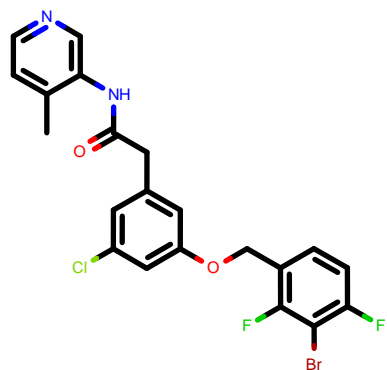
CID:	EN300-1912781
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3F)Br)F
RUN:	RUN1244
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.15

EN300-2010197
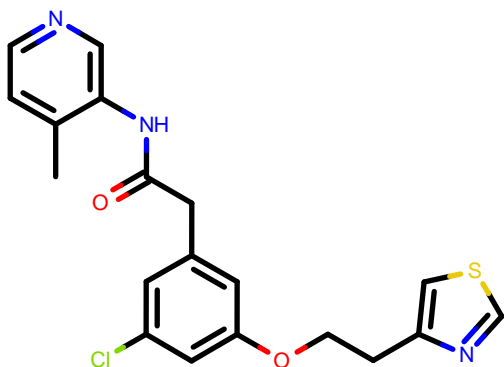
CID:	EN300-2010197
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cscn3
RUN:	RUN3276
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.13

EN300-1897247
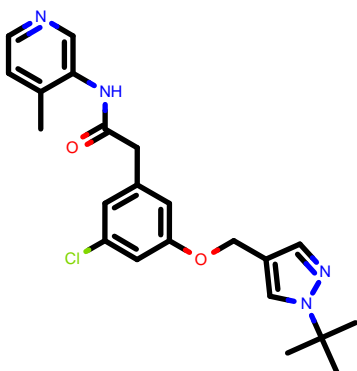
CID:	EN300-1897247
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnn(c3)C(C)(C)C
RUN:	RUN889
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.13

EN300-695755
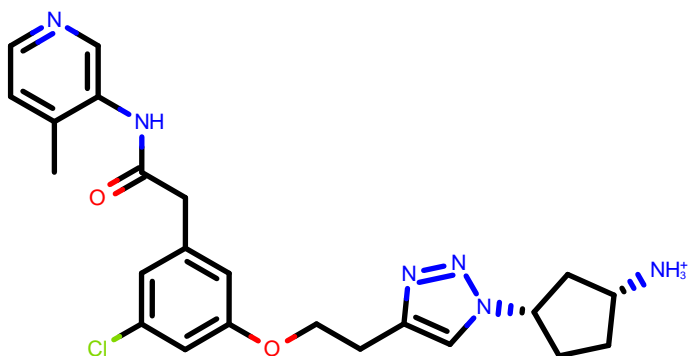
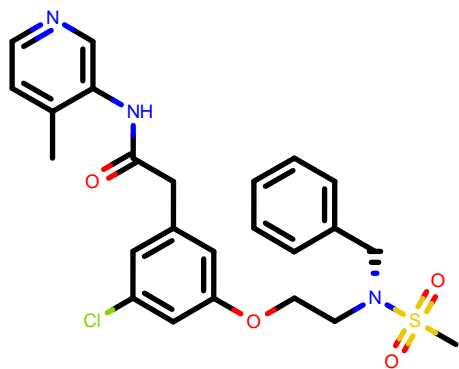|	
CID:	EN300-695755
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cn(nn3)[C@H]4CC[C@H](C4)[NH3+]
RUN:	RUN4348
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.27

EN300-1938792
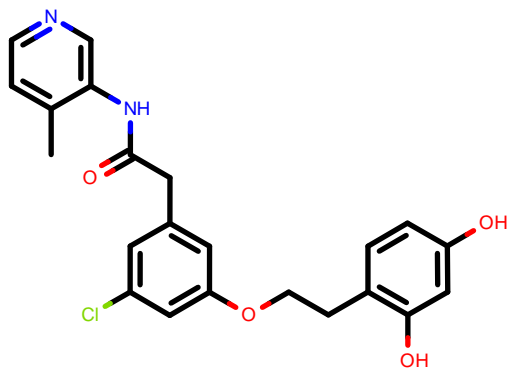
CID:	EN300-1938792
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3ccc(cc3O)O
RUN:	RUN3037
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.14

EN300-175288

CID:	EN300-175288
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC[N@](Cc3ccccc3)S(=O)(=O)C
RUN:	RUN4600
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.64

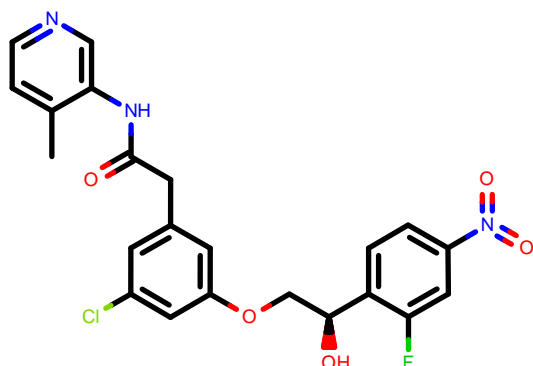# EN300-7464360
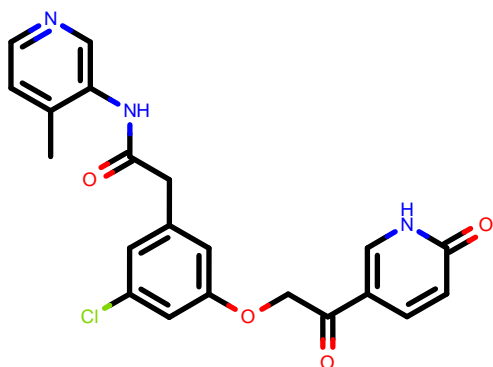
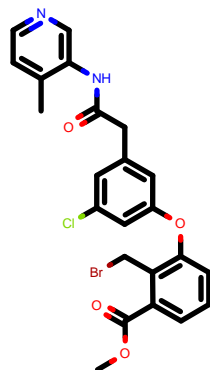| CID:	EN300-7464360
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)c3ccc(=O)[nH]c3
RUN:	RUN4552
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.29

EN300-1917759

CID:	EN300-1917759
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3ccc(cc3F)N(=O)=O)O
RUN:	RUN1698
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.19

EN300-222255

CID:	EN300-222255
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3CBr)C(=O)OC
RUN:	RUN3088
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.16

EN300-1865390
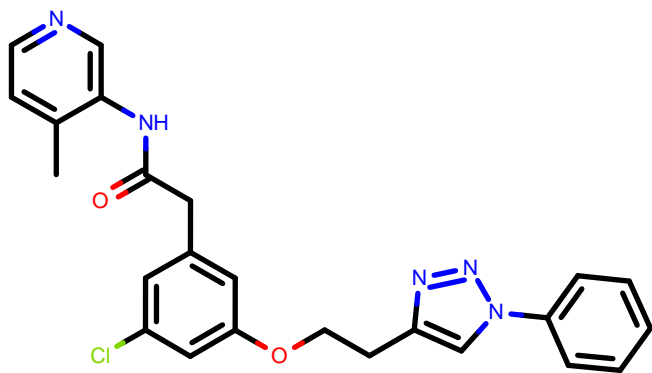
CID:	EN300-1865390
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cn(nn3)c4ccccc4
RUN:	RUN4613
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.40

EN300-1926794
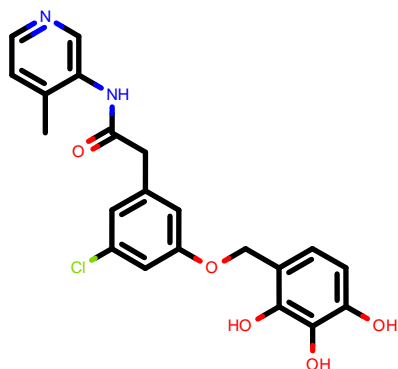
CID:	EN300-1926794
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3O)O)O
RUN:	RUN2116
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.17

EN300-45396
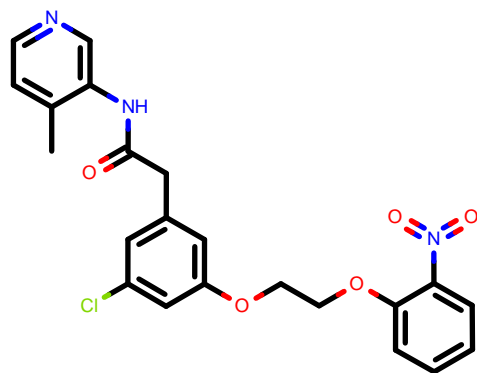
CID:	EN300-45396
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCOc3ccccc3N(=O)=O
RUN:	RUN3014
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.20

EN300-1926690
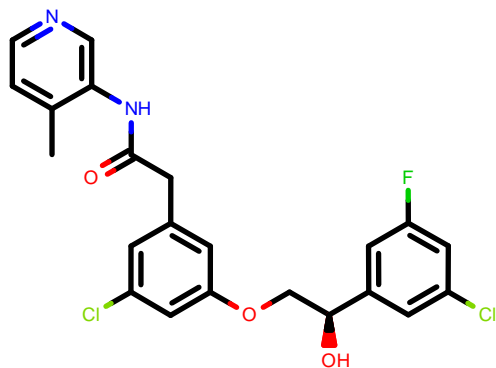
CID:	EN300-1926690
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3cc(cc(c3)Cl)F)O
RUN:	RUN2350
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.21

EN300-50577
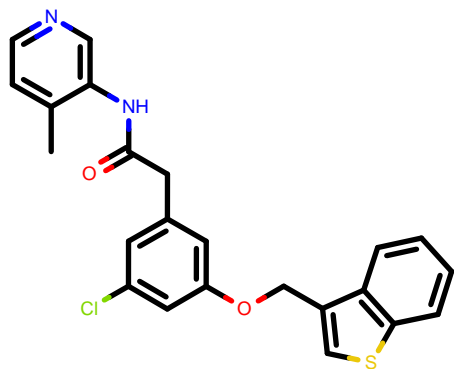
CID:	EN300-50577
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3csc4c3cccc4
RUN:	RUN55
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.11

EN300-1613316
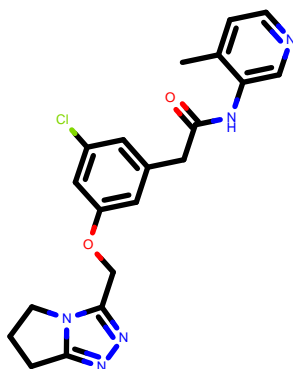
CID:	EN300-1613316
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3nnc4n3CCC4
RUN:	RUN357
DDG (kcal/mol):	-0.00
dDDG (kcal/mol):	0.13