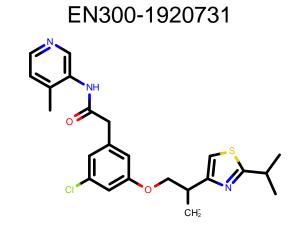
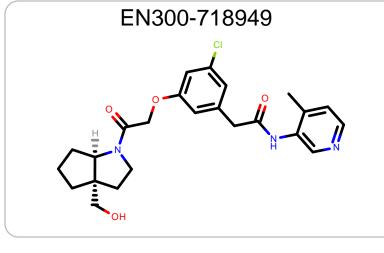
RUN:

DDG (kcal/mol):

EN300-170738	
NH	
CI O H	
EN300-382173	

NH N
EN300-382173

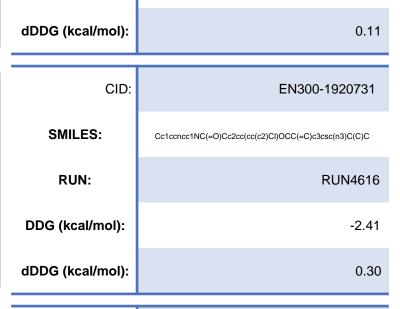




CID:	EN300-170738
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC[N@H+]3CCOC[C@@H]3C
RUN:	RUN3598
DDG (kcal/mol):	-4.21
dDDG (kcal/mol):	0.19
CID:	EN300-382173
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3coc(n3)C4CCCCC4

RUN176

-2.94

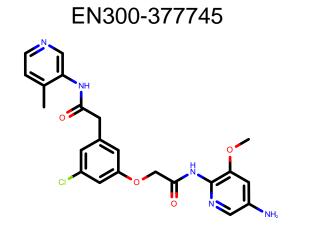


CID:	EN300-718949
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)N3CC[C@]4([C@H]3CCC4)C0
RUN:	RUN3613
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.17

EN300-185424	CID:	EN300-185424
NH	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
CI	dDDG (kcal/mol):	0.13
EN300-1274653	CID:	EN300-1274653
	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+]]C@@HJ((C@H](S4)CBr)C
	RUN:	RUN3789
	DDG (kcal/mol):	-1.44
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~		
S Br	dDDG (kcal/mol):	0.14
EN300-1266528	dDDG (kcal/mol):  CID:	0.14 EN300-1266528
EN300-1266528		
EN300-1266528	CID:	EN300-1266528
EN300-1266528	CID:	EN300-1266528  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3nnc(o3)C4CCCCC4

EN300-1940535
NH NH
EN300-330332

<b>L</b> 11000 00000 <b>L</b>
NH O



EN300-1886131
NH

CID:	EN300-1940535
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(o3)[C@H]4C[C@H]4C
RUN:	RUN106
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.12
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

dDDG (kcal/mol):	0.12
CID:	EN300-377745
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)Nc3c(cc(cn3)N)OC
RUN:	RUN3338
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.16

CID:	EN300-1886131
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(nc(s3)NC(=0)OC(C)(C)C)C
RUN:	RUN4609
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.37

<b>'</b>	hilic-displacement	
EN300-1084907	CID:	EN300-1084907
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccn(n3)c4cc(ccc4F)F
	RUN:	RUN180
	DDG (kcal/mol):	-1.27
₩ ¥ F	dDDG (kcal/mol):	0.13
EN300-1274653	CID:	EN300-1274653
	SMILES:	Cc1cancc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+][C@H]([C@@H](S4)CBr)C
	RUN:	RUN3262
	DDG (kcal/mol):	-1.27
S Br	dDDG (kcal/mol):	0.13
EN300-1929484	CID:	EN300-1929484
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(cc3F)OC(F)F
	RUN:	RUN1708
	DDG (kcal/mol):	-1.27
F C	dDDG (kcal/mol):	0.13
EN300-155655	CID:	EN300-155655

EN300-155655	CID:	EN300-155655
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3)OC)OC(F)F
	RUN:	RUN2011
	DDG (kcal/mol):	-1.25
F F	dDDG (kcal/mol):	0.16

EN300-843777	CID:	EN300-843777
NH NH	SMILES:	CCOC(=0)C(Cn1cc(nn1)COc2cc(cc(c2)Cl)CC(=0)Nc3cnccc3C)(F)F
	RUN:	RUN997
CI O N	DDG (kcal/mol):	-1.19
<b>→°</b> ★F	dDDG (kcal/mol):	0.16
EN300-70105	CID:	EN300-70105
<b>V</b> o	SMILES:	CCCCCOc1ccc(cc1CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
	RUN:	RUN2809
Br Br	DDG (kcal/mol):	-1.18
	dDDG (kcal/mol):	0.16
EN300-843582	CID:	EN300-843582
	SMILES:	$\label{eq:concetNC} CctccncctNC(=0)Cc2cc(cc(c2)Cl)OCc3cn(nn3)[C@@H]4CCOC5(C4)CC[NH2+]CC5$
	RUN:	RUN907
o <u></u>		
	DDG (kcal/mol):	-1.16
	DDG (kcal/mol):	-1.16 0.17
EN300-1915724		
	dDDG (kcal/mol):	0.17
	dDDG (kcal/mol):	0.17 EN300-1915724
	dDDG (kcal/mol):  CID:  SMILES:	0.17  EN300-1915724  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)O)CBr

EN300-1909681	CID:	EN300-1909681
NH NH	SMILES:	Cc1ccc(cc1CCBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
	RUN:	RUN2206
	DDG (kcal/mol):	-1.14
Br	dDDG (kcal/mol):	0.12
EN300-844309	CID:	EN300-844309
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cn(nn3)CCC[NH3+]
	RUN:	RUN645
	DDG (kcal/mol):	-1.13
	dDDG (kcal/mol):	0.13
NH;		0.13
EN300-1274638	CID:	EN300-1274638
EN300-1274638		
EN300-1274638	CID:	EN300-1274638
EN300-1274638	CID:	EN300-1274638  Cc1concc1NC(=0)Cc2cc(cc(c2)Ci)Oc3ccc(cc3)NC4=[NH+][C@@H]((C@H](S4)CBr)C
EN300-1274638	CID: SMILES: RUN:	EN300-1274638  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+][C@@H]([C@H](S4)CBr)C  RUN3788
EN300-1274638  EN300-60436	CID: SMILES: RUN: DDG (kcal/mol):	EN300-1274638  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+][C@@H]([C@H](S4)CBr)C  RUN3788  -1.13
NH N	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1274638  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Ci)Oc3ccc(cc3)NC4=[NH+][C@@H]([C@H](S4)CBr)C  RUN3788  -1.13  0.14
NH N	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1274638  CctccncctNC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+][C@@H]([C@H](S4)CBt)C  RUN3788  -1.13  0.14  EN300-60436
NH N	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-1274638  Ce1cence1NC(=0)Ce2cc(cc(e2)Cl)Oc3ccc(cc3)NC4=[NH+][C@@H]([C@H](S4)CBr)C  RUN3788  -1.13  0.14  EN300-60436  CCOC(=0)c1c2cccc2oc1COc3cc(cc(c3)Cl)CC(=0)Nc4cnccc4C

·	milic-displacement	
EN300-1910987	CID:	EN300-1910987
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3OC)CBr
	RUN:	RUN1168
	DDG (kcal/mol):	-1.12
Br	dDDG (kcal/mol):	0.13
EN300-1938856	CID:	EN300-1938856
	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=C)c3ccc(c3)[C@H]4C[C@@H]4C
NH NH	RUN:	RUN4615
	DDG (kcal/mol):	-1.12
CI ON	dDDG (kcal/mol):	0.37
EN300-701252	CID:	EN300-701252
	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cn(nc3CBr)C
Br	RUN:	RUN1206
	DDG (kcal/mol):	-1.11
CI ON	dDDG (kcal/mol):	0.11
EN300-24531	CID:	EN300-24531
	CID.	EN300-2453 I
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4ccc(cc4)Cl
	RUN:	RUN3389
	DDG (kcal/mol):	-1.09
	dDDG (kcal/mol):	0.14

	milic-displacement	
EN300-1897350	CID:	EN300-1897350
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c4ccccc4ccc3OC
	RUN:	RUN3624
CI CONTRACTOR OF THE PROPERTY	DDG (kcal/mol):	-1.05
	dDDG (kcal/mol):	0.16
EN300-378667	CID:	EN300-378667
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(cc3)OCc4ccccc4F
	RUN:	RUN2751
	DDG (kcal/mol):	-1.05
F	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
NH NH	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):

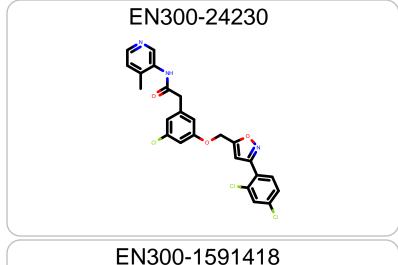
EN300-301686 ✓	CID:	EN300-301686
	SMILES:	$\label{eq:concc1NC} Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c4ccccc4n(n3)C(=O)OC(C)(C)C$
	RUN:	RUN4523
cl o	DDG (kcal/mol):	-1.02
	dDDG (kcal/mol):	0.27
EN300-1274639	CID:	EN300-1274639
NH O	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3)NC4=[NH+][C@H]([C@@H](S4)CBr)C
ه ا	RUN:	RUN1452
HN S	DDG (kcal/mol):	-1.02
Br	dDDG (kcal/mol):	0.16
EN300-1914939	CID:	EN300-1914939
EN300-1914939	CID:	EN300-1914939  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)OC)CBr
EN300-1914939		
EN300-1914939	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)OC)CBr
EN300-1914939	SMILES: RUN:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)OC)CBr
EN300-1914939  EN300-372060	SMILES: RUN: DDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)OC)CBr  RUN2542 -1.00
NH NH NH	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)OC)CBr  RUN2542  -1.00  0.12
NH NH NH	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)OC)CBr  RUN2542  -1.00  0.12
NH NH NH	SMILES: RUN: DDG (kcal/mol): dDDG (kcal/mol): CID: SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)OC)CBr  RUN2542  -1.00  0.12  EN300-372060  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(cc4c3cccc4)Cl

2020-00-14-Hucleop	•	
EN300-1926474	CID:	EN300-1926474
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@@H](c3cccc(c3F)N(=0)=0)O
	RUN:	RUN1782
	DDG (kcal/mol):	-0.98
CI OH	dDDG (kcal/mol):	0.17
EN300-117814	CID:	EN300-117814
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)CBr)C(=O)OC
	RUN:	RUN1589
Br Br	DDG (kcal/mol):	-0.96
. <b>∠</b> .	alDDC (Iso al/m al).	
l	dDDG (kcal/mol):	0.12
EN300-1918362	CID:	0.12 EN300-1918362
EN300-1918362		
EN300-1918362	CID:	EN300-1918362
N CI	CID:	EN300-1918362  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(c4ccccc4nn3)Cl
N CI	CID: SMILES: RUN:	EN300-1918362  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(c4ccccc4nn3)Cl  RUN3740
N CI	CID: SMILES: RUN: DDG (kcal/mol):	EN300-1918362  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(c4ccccc4nn3)Cl  RUN3740  -0.95
CI CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1918362  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(c4ccccc4nn3)Cl  RUN3740  -0.95
CI CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1918362  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(c4ccccc4nn3)Cl  RUN3740  -0.95  0.14  EN300-87636
CI CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-1918362  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(c4ccccc4nn3)Cl  RUN3740  -0.95  0.14  EN300-87636  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCN(=0)=0

EN300-1296572	CID:	EN300-1296572
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnn(c3C)c4ccc(cc4)O
	RUN:	RUN1383
	DDG (kcal/mol):	-0.94
CI	dDDG (kcal/mol):	0.15
EN300-1910562	CID:	EN300-1910562
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3)O)OC
	RUN:	RUN2172
CI OH	DDG (kcal/mol):	-0.93
	dDDG (kcal/mol):	0.14
EN300-1912582	CID:	EN300-1912582
EN300-1912582	CID:	EN300-1912582  Cc1ccc(c(c1)CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
EN300-1912582		
NH NH	SMILES:	Cc1ccc(c(c1)CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
NH NH	SMILES: RUN:	Cc1ccc(c(c1)CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
NH NH	SMILES:  RUN:  DDG (kcal/mol):	Cc1ccc(c(c1)CBr)Oc2cc(cc(c2)Cl)CC(=0)Nc3cnccc3C  RUN1011  -0.92
NH O O O O O O O O O O O O O O O O O O O	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccc(c(c1)CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C  RUN1011  -0.92  0.14
NH O O O O O O O O O O O O O O O O O O O	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccc(c(c1)CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C  RUN1011  -0.92  0.14  EN300-1461330
NH O O O O O O O O O O O O O O O O O O O	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	Cc1ccc(c(c1)CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C  RUN1011  -0.92  0.14  EN300-1461330  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nc3C)C4CCC(CC4)(C)C

EN300-1912943	
NH NH	
OH OH	
CI OH	

EN300-160173	
-N.	
NH	
Br	



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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

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

dDDG (kcal/mol):	0.16
CID:	EN300-24230
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4ccc(cc4Cl)Cl
RUN:	RUN3009
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.16
CID:	EN200 1501419

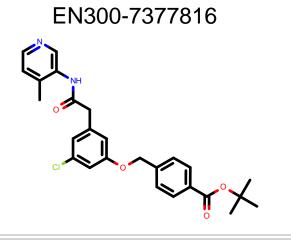
CID:	EN300-1591418
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccnn3c4cccc(c4)C#N
RUN:	RUN1247
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.16

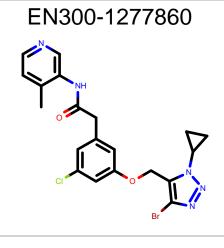
ENIOCO 4057740		
EN300-4257713	CID:	EN300-4257713
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCS(=O)(=O)Cl
	RUN:	RUN548
CI	DDG (kcal/mol):	-0.89
S CI	dDDG (kcal/mol):	0.08
EN300-1918008	CID:	EN300-1918008
NH E	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cn[nH]c3c4ccc(cc4)F
	RUN:	RUN1345
	DDG (kcal/mol):	-0.87
CI NH	dDDG (kcal/mol):	0.14
EN300-1917400	CID:	EN300-1917400
EN300-1917400	CID:	EN300-1917400  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3cc(cs3)Cl)O
EN300-1917400		
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3cc(cs3)Cl)O
NH NH	SMILES: RUN:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3cc(cs3)Cl)O
NH O CI CI	SMILES:  RUN:  DDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3cc(cs3)Cl)O  RUN2584  -0.87
NH OH CI	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3cc(cs3)Cl)O  RUN2584  -0.87
NH OH CI	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3cc(cs3)Cl)O  RUN2584  -0.87  0.18
NH OH CI	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3cc(cs3)Cl)O  RUN2584  -0.87  0.18  EN300-156205  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C)CBr

2020 00 11 1100100		
EN300-1894071	CID:	EN300-1894071
	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3csc(n3)C4CC4
NH ONH	RUN:	RUN2324
	DDG (kcal/mol):	-0.86
CI	dDDG (kcal/mol):	0.16
EN300-7437130	CID:	EN300-7437130
	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)CBr)C(F)(F)F
	RUN:	RUN3604
CI Br	DDG (kcal/mol):	-0.86
F F	dDDG (kcal/mol):	0.12
	azzo (neaginoi)i	0.12
EN300-1724721	CID:	EN300-1724721
EN300-1724721		
EN300-1724721	CID:	EN300-1724721
NH NH	CID:	EN300-1724721  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3CBr)N(=0)=0
NH NH	CID: SMILES: RUN:	EN300-1724721  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3CBr)N(=0)=0  RUN2085
NH NH	CID: SMILES: RUN: DDG (kcal/mol):	EN300-1724721  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3CBr)N(=0)=0  RUN2085  -0.85
NH ONH ON NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1724721  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3CBr)N(=0)=0  RUN2085  -0.85
NH ONH ON NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1724721  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3CBr)N(=0)=0  RUN2085  -0.85  0.13
NH ONH ON NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-1724721  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3CBr)N(=O)=O  RUN2085  -0.85  0.13  EN300-29546  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)F

EN300-7494548
NH NH
CI NO N
EN300-643001

N
NH O Br





ilic-displacement	
CID:	EN300-7494548
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(cc3)C[NH+]4CCOCC4
RUN:	RUN3552
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.15
CID:	EN300-643001
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cn(nc3CBr)C
RUN:	RUN1207

dDDG (kcal/mol):	0.13
CID:	EN300-7377816
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(cc3)C(=0)OC(C)(C)C
RUN:	RUN4473
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.17
CID:	EN300-1277860

-0.84

DDG (kcal/mol):

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

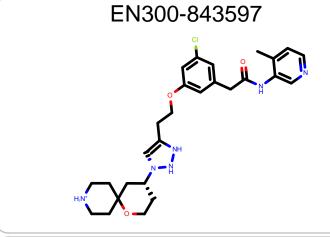
2020 00 11 110000		
EN300-740743	CID:	EN300-740743
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)N3CC[N@ @]4[C@H](C3)CNS4(=0)=0
	RUN:	RUN3691
N. N	DDG (kcal/mol):	-0.83
CI	dDDG (kcal/mol):	0.17
EN300-154526	CID:	EN300-154526
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)N(=0)=0)CBr
	RUN:	RUN2558
	DDG (kcal/mol):	-0.82
N Rr	dDDG (kcal/mol):	0.13
J.	)	0.13
EN300-43523	CID:	EN300-43523
EN300-43523		
EN300-43523	CID:	EN300-43523
NH NH	CID:	EN300-43523  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCS(=0)(=0)Cl
NH O	CID:  SMILES:  RUN:	EN300-43523  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCS(=0)(=0)Cl  RUN547
NH O	CID: SMILES: RUN: DDG (kcal/mol):	EN300-43523  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCS(=0)(=0)Cl  RUN547  -0.81
NH O O O O O O O O O O O O O O O O O O O	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-43523  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCS(=0)(=0)Cl  RUN547  -0.81  0.09
NH O O O O O O O O O O O O O O O O O O O	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-43523  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCS(=O)(=O)Cl  RUN547  -0.81  0.09
NH O O O O O O O O O O O O O O O O O O O	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-43523  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCS(=0)(=0)Cl  RUN547  -0.81  0.09  EN300-1296574  CCc1c(cnn1c2ccc(cc2)0)COc3cc(cc(c3)Cl)CC(=0)Nc4cnccc4C

RUN:

SMILES:

EN300-6776042
NH NH
Br
CI O N
EN300-1918616

EN300-1918616	
NH NH	



EN300-13933
V _o NH
Br

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
OID	EN000 4040040
CID:	EN300-1918616
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnc(s3)OC

**RUN838** 

DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.13
CID:	EN300-843597
SMILES:	$\label{eq:Concorn} Cctccncc1NC(=0)Cc2cc(cc(c2)Cl)OCCc3cn(nn3)[C@@H]4CCOC5(C4)CC[NH2+]CC5$
RUN:	RUN4546
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.37
CID:	EN300-13933

Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)CBr)OC

2020-08-14-nucleopnilic-displacement			
EN300-87708	CID:	EN300-87708	
NH	SMILES:	$\label{eq:concentration} Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC(C@@H](c3ccc(cc3)S(=0)(=0)N4CCOCC4)O$	
	RUN:	RUN4605	
	DDG (kcal/mol):	-0.75	
CI OH	dDDG (kcal/mol):	0.58	
EN300-1461309	CID:	EN300-1461309	
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nc3C)C4CCCCC4	
	RUN:	RUN678	
CI N	DDG (kcal/mol):	-0.74	
	dDDG (kcal/mol):	0.13	
EN300-195084	CID:	EN300-195084	
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(ccc3OCC4CC4)Cl	
	RUN:	RUN1831	
CI CI	DDG (kcal/mol):	-0.74	
CI	dDDG (kcal/mol):	0.16	
EN300-1897461	CID:	EN300-1897461	
	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(c(c3)F)O)CBr	
F F	RUN:	RUN2052	
ОН	DDG (kcal/mol):	-0.72	

dDDG (kcal/mol):

EN300-1274654	CID:	EN300-1274654
NH O	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3)NC4=[NH+][C@H]([C@@H](S4)CBr)C
a Company of the comp	RUN:	RUN1453
HN CO	DDG (kcal/mol):	-0.72
S NH Br	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
Br Br	dDDG (kcal/mol):	0.13
	)	
EN300-1132718	CID:	EN300-1132718
EN300-1132718	CID:	EN300-1132718  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@H](Cl)OCc4ccccc4
EN300-1132718		
EN300-1132718	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@H](Cl)OCc4ccccc4
EN300-1132718	SMILES: RUN:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@H](Cl)OCc4ccccc4  RUN3652
EN300-1132718  EN300-1916362	SMILES: RUN: DDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@H](Cl)OCc4ccccc4  RUN3652  -0.71
EN300-1916362	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@H](Cl)OCc4ccccc4  RUN3652  -0.71  0.19
EN300-1916362	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@H](Cl)OCc4ccccc4  RUN3652  -0.71  0.19  EN300-1916362
EN300-1916362	SMILES: RUN: DDG (kcal/mol): dDDG (kcal/mol): CID: SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@H](Cl)OCc4ccccc4  RUN3652  -0.71  0.19  EN300-1916362  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@@H](c3c[nH]nc3N(=0)=0)0

EN300-127722	CID:	EN300-127722
	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC=C3CCC3
T NH	RUN:	RUN4513
	DDG (kcal/mol):	-0.70
CI	dDDG (kcal/mol):	0.14
EN300-1927181	CID:	EN300-1927181
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(c[nH]n3)N(=0)=0
	RUN:	RUN933
CI NH	DDG (kcal/mol):	-0.70
° ≥ _N	-IDDO (Iso al/m al)	
Ö	dDDG (kcal/mol):	0.11
EN300-6245905	CID:	0.11 EN300-6245905
EN300-6245905		
EN300-6245905	CID:	EN300-6245905
EN300-6245905	CID:	EN300-6245905  CCCOc1cc(ccc1CBr)Oc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C
EN300-6245905	CID: SMILES: RUN:	EN300-6245905  CCCOc1cc(ccc1CBr)Oc2cc(cc(c2)Cl)CC(=0)Nc3cnccc3C  RUN2010
EN300-6245905  EN300-366127	CID: SMILES: RUN: DDG (kcal/mol):	EN300-6245905  CCCOc1cc(ccc1CBr)Oc2cc(cc(c2)Cl)CC(=0)Nc3cnccc3C  RUN2010  -0.70
	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-6245905  CCCOc1cc(ccc1CBr)Oc2cc(cc(c2)Cl)CC(=0)Nc3cnccc3C  RUN2010  -0.70  0.14
	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-6245905  CCCOc1cc(ccc1CBr)Oc2cc(cc(c2)Cl)CC(=0)Nc3cnccc3C  RUN2010  -0.70  0.14  EN300-366127
	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-6245905  CCCOc1cc(ccc1CBr)Oc2cc(cc(c2)Cl)CC(=0)Nc3cnccc3C  RUN2010  -0.70  0.14  EN300-366127  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(cc(c3)l)CBr

EN300-1132707	CID:	EN300-1132707
NH O	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)OC4CCCC4
	RUN:	RUN1347
	DDG (kcal/mol):	-0.68
	dDDG (kcal/mol):	0.17
EN300-3051713	CID:	EN300-3051713
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ncc(o3)c4ccccc4
	RUN:	RUN348
CI N	DDG (kcal/mol):	-0.68
	dDDG (kcal/mol):	0.14
		0.14
EN300-64239	CID:	EN300-64239
EN300-64239		
EN300-64239	CID:	EN300-64239
EN300-64239	CID:	EN300-64239  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C(=0)CBr)OC
EN300-64239	CID: SMILES: RUN:	EN300-64239  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C(=0)CBr)OC  RUN2827
EN300-64239  September 2015  EN300-1910335	CID: SMILES: RUN: DDG (kcal/mol):	EN300-64239  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C(=0)CBr)OC  RUN2827  -0.68
EN300-1910335	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-64239  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C(=0)CBr)OC  RUN2827  -0.68  0.16
NH OH OH Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-64239  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C(=0)CBr)OC  RUN2827  -0.68  0.16
EN300-1910335	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-64239  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C(=0)CBr)OC  RUN2827  -0.68  0.16  EN300-1910335  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3cccc(c3)N(=0)=0)O

EN300-1274638	CID:	EN300-1274638
NH O	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+][C@H]([C@@H](S4)CBr)C
a Co	RUN:	RUN3261
	DDG (kcal/mol):	-0.66
S Br	dDDG (kcal/mol):	0.15
EN300-378599	CID:	EN300-378599
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)N(=O)=O
	RUN:	RUN2138
CI Br	DDG (kcal/mol):	-0.65
o s ^ň so	dDDG (kcal/mol):	0.14
EN300-219510	dDDG (kcal/mol):  CID:	0.14 EN300-219510
EN300-219510		
EN300-219510	CID:	EN300-219510
EN300-219510	CID:	EN300-219510  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)Cl
EN300-219510	CID: SMILES: RUN:	EN300-219510  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)Cl  RUN1021
EN300-219510  EN300-16612	CID: SMILES: RUN: DDG (kcal/mol):	EN300-219510  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)Cl  RUN1021  -0.62
NH O CI Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-219510  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)Cl  RUN1021  -0.62  0.13
NH O CI Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-219510  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)Cl  RUN1021  -0.62  0.13
EN300-16612	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-219510  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(cc3CBr)Cl  RUN1021  -0.62  0.13  EN300-16612  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCC(=O)c3ccc(c(c3)C(=O)N)O

EN300-695739	CID:	EN300-695739
NH NH	SMILES:	Cc1cencc1NC(=0)Cc2cc(cc(c2)Ci)OCc3c(n(nn3)[C@@H]4CC[C@@H](C4)[NH3+])C
	RUN:	RUN1003
NH ₃	DDG (kcal/mol):	-0.61
N=N NIII	dDDG (kcal/mol):	0.17
EN300-1923485	CID:	EN300-1923485
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc([nH]n3)N(=O)=O
	RUN:	RUN2661
CI NH	DDG (kcal/mol):	-0.61
N=°	dDDG (kcal/mol):	0.13
O O		51.15
EN300-135871	CID:	EN300-135871
EN300-135871		
EN300-135871	CID:	EN300-135871
EN300-135871	CID:	EN300-135871  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)NCCC#C
EN300-135871	CID:  SMILES:  RUN:	EN300-135871  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)NCCC#C  RUN2631
EN300-135871  EN300-1864036	CID: SMILES: RUN: DDG (kcal/mol):	EN300-135871  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)NCCC#C  RUN2631  -0.60
N N N N N N N N N N N N N N N N N N N	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-135871  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)NCCC#C  RUN2631  -0.60  0.14
N N N N N N N N N N N N N N N N N N N	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-135871  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)NCCC#C  RUN2631  -0.60  0.14  EN300-1864036
N N N N N N N N N N N N N N N N N N N	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-135871  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)NCCC#C  RUN2631  -0.60  0.14  EN300-1864036  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(nn(c3C)Cc4ccccc4)C

2020 00 11 1100.00	orillic-displacement	
EN300-76253	CID:	EN300-76253
NH NH	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(=0)Cc2cc(cc(c2)Cl)OCC(=C)c3csc(n3)C4CC4
	RUN:	RUN4484
	DDG (kcal/mol):	-0.57
CI O N CH ₂	dDDG (kcal/mol):	0.23
EN300-844238	CID:	EN300-844238
NH NH	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
NH NH	SMILES:	Cc1ccncc1NC(=0)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
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)CBr)Cl
	RUN:	RUN2571
	DDG (kcal/mol):	-0.56
CI Br	dDDG (kcal/mol):	0.11
EN300-738987	CID:	EN300-738987
CI	SMILES:	Cet cence 1NC (= O) Ce2 ce(ce(c2)CI) OCc3e(n(m3)C[C@@H]4CCCC[NH2+]C4) Cencer Center
the New York	RUN:	RUN392
	DDG (kcal/mol):	-0.55
· ·	dDDG (kcal/mol):	0.14
EN300-1916571	CID:	EN300-1916571
EN300-1916571	CID:	EN300-1916571  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3CCBr)F
EN300-1916571		
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3CCBr)F
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3CCBr)F
NH NH	SMILES: RUN: DDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3CCBr)F  RUN1098  -0.54
NH O D D D D D D D D D D D D D D D D D D	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3CCBr)F  RUN1098  -0.54  0.14
NH O D D D D D D D D D D D D D D D D D D	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3CCBr)F  RUN1098  -0.54  0.14  EN300-177132
NH O D D D D D D D D D D D D D D D D D D	SMILES: RUN: DDG (kcal/mol): dDDG (kcal/mol): CID: SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3CCBr)F  RUN1098  -0.54  0.14  EN300-177132  CCOC(=O)c1c(snn1)COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C

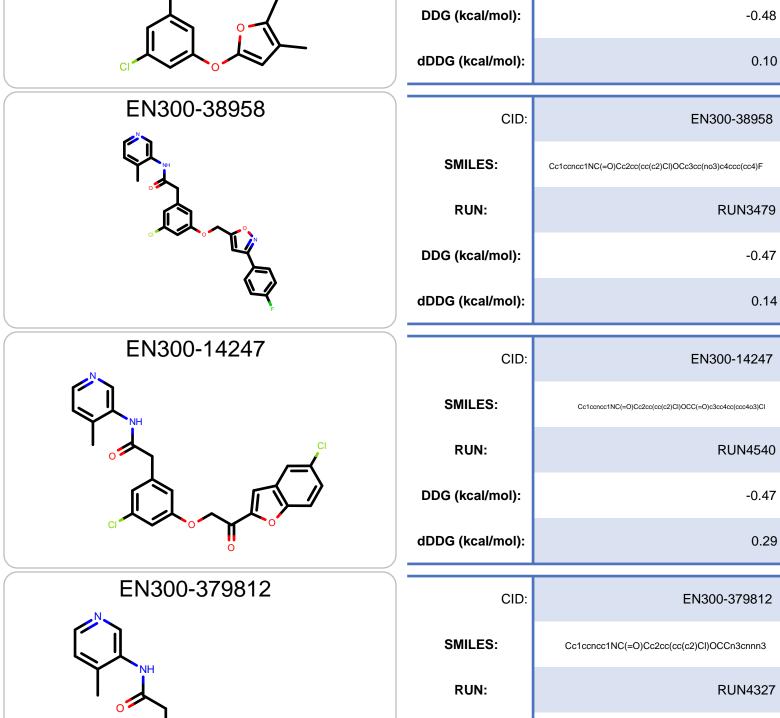
	nilic-displacement	
EN300-1563127	CID:	EN300-1563127
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3)C)C(=0)OC
	RUN:	RUN4415
CI C	DDG (kcal/mol):	-0.51
	dDDG (kcal/mol):	0.19
EN300-767696	CID:	EN300-767696
NH	SMILES:	$\label{eq:conc} Cc1ccncc1NC(=0)Cc2cc(cc(c2)CI)OCc3cccc(c3)c4ccc(cc4)[C@@H]SCCO5$
	RUN:	RUN2490
	DDG (kcal/mol):	-0.51
	dDDG (kcal/mol):	0.17
EN300-1613392	CID:	EN300-1613392
NH O	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(ac(=0)o3)c4cccc(c4)N(=0)=0
	RUN:	RUN2799
CI CO	DDG (kcal/mol):	-0.51
, A	dDDG (kcal/mol):	0.22
EN300-658821	CID:	EN300-658821
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3CBr)OC)C(=0)OC
	RUN:	RUN2540

DDG (kcal/mol):

dDDG (kcal/mol):

-0.49

2020-08-14-nucleop	hilic-displacement	
EN300-1910378	CID:	EN300-1910378
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)CCBr)C
Br	RUN:	RUN434
	DDG (kcal/mol):	-0.48
CI	dDDG (kcal/mol):	0.10
EN300-38958	CID:	EN300-38958
NH.	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4ccc(cc4)F
	RUN:	RUN3479
	DDG (kcal/mol):	-0.47
	dDDG (kcal/mol):	0.14

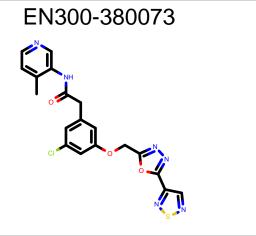


RUN434

EN300-38958	CID:	EN300-38958
	SMILES:	Cc1ccncc1NC(=0)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
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)c3cc4cc(ccc4o3)Cl
CI	RUN:	RUN4540
	DDG (kcal/mol):	-0.47
CI O O O	dDDG (kcal/mol):	0.29
EN300-379812	CID:	EN300-379812
	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCn3cnnn3
NH ONH	RUN:	RUN4327
N=N	DDG (kcal/mol):	-0.47
	dDDG (kcal/mol):	0.17
- 2	27 -	

EN300-7464827	
NH	
CI N N	
Ö NH ₂	=:
EN300-66387	

EN300-00307
NH NH CI



El	N300-738987	
	CI	

CID:	EN300-7464827
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)n3c(ncn3)N
RUN:	RUN4391
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.18
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

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

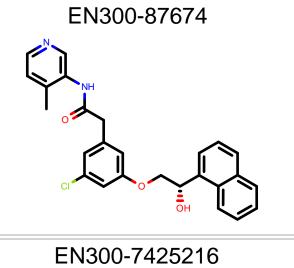
CID:	EN300-738987
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(n(nn3)C[C@H]4CCCC[NH2+]C4)C
RUN:	RUN640
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.16

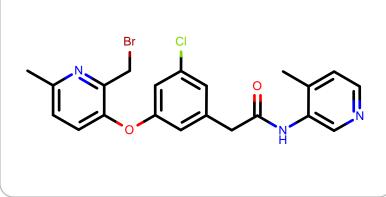
EN300-1132699	CID:	EN300-1132699
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)OCC4CC4
	RUN:	RUN1728
	DDG (kcal/mol):	-0.44
j, ✓	dDDG (kcal/mol):	0.15
EN300-6764228	CID:	EN300-6764228
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3F)Br)Cl
	RUN:	RUN1389
	DDG (kcal/mol):	-0.44
F CI	dDDC (kaal/mal).	0.40
Br	dDDG (kcal/mol):	0.13
EN300-77512	CID:	EN300-77512
EN300-77512		
EN300-77512	CID:	EN300-77512
NH NH	CID:	EN300-77512  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)C(C)C
NH NH	CID: SMILES: RUN:	EN300-77512  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)C(C)C  RUN1518
NH NH	CID: SMILES: RUN: DDG (kcal/mol):	EN300-77512  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)C(C)C  RUN1518  -0.44
NH CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-77512  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)C(C)C  RUN1518  -0.44  0.12
EN300-99500	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-77512  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)C(C)C  RUN1518  -0.44  0.12  EN300-99500
EN300-99500	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-77512  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)C(C)C  RUN1518  -0.44  0.12  EN300-99500  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(cc(c3)F)CBr

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EN300-1919504	CID:	EN300-1919504
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(c(cs3)C)Br
	RUN:	RUN183
Br A	DDG (kcal/mol):	-0.43
CI	dDDG (kcal/mol):	0.09
EN300-123146	CID:	EN300-123146
NH NH	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
		0.11
EN300-1697674	CID:	EN300-1697674
EN300-1697674		
NH Br	CID:	EN300-1697674
NH NH	CID:	EN300-1697674  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3c(c(ncn3)CBr)F
NH Br	CID:  SMILES:  RUN:	EN300-1697674  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3c(c(ncn3)CBr)F  RUN3759
NH Br	SMILES: RUN: DDG (kcal/mol):	EN300-1697674  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3c(c(ncn3)CBr)F  RUN3759  -0.42
NH Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1697674  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3c(c(ncn3)CBr)F  RUN3759  -0.42  0.12
NH Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1697674  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3c(c(ncn3)CBr)F  RUN3759  -0.42  0.12
NH Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-1697674  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3c(c(ncn3)CBr)F  RUN3759  -0.42  0.12  EN300-107185  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C#N)CBr

EN300-269986	,
NH	
¥ NNN NNNNNNNNNNNNNNNNNNNNNNNNNNNNNNNN	

EN300-1927497	
NH	
OH OH	
ОН	





CID:	EN300-269986
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(c(cc3F)C#N)F
RUN:	RUN4230
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.13
CID:	EN300-1927497

RUN:	RUN3223
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.18

Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C @ @ H](c3cc(c(c3)C)O)C)O

SMILES:

dDDG (kcal/mol):	0.18
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
	_

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
NH NH	SMILES:	$\label{eq:concentration} Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)NC4=[NH+][C@H][C@H][C4]CBr]C$
	RUN:	RUN3760
	DDG (kcal/mol):	-0.38
S Br	dDDG (kcal/mol):	0.16
EN300-1896632	CID:	EN300-1896632
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(c(cc3F)N(=O)=O)F
	RUN:	RUN3666
cı Co	DDG (kcal/mol):	-0.37
N°°		
F Ö	dDDG (kcal/mol):	0.14
EN300-764780	dDDG (kcal/mol):	0.14 EN300-764780
EN300-764780		
EN300-764780	CID:	EN300-764780
EN300-764780	CID:	EN300-764780  Cc1ccncctNC(=0)Cc2cc(cc(c2)Cl)OCc3ccccc3n4cc(nn4) C@H]SCCCC[NH2+]5
EN300-764780	CID: SMILES: RUN:	EN300-764780  CetecneetNC(=0)Ge2cc(cc(c2)Cl)OCc3ccccc3n4cc(nn4)(C@HIJ5CCCC(NH2+)5  RUN4329
EN300-764780  EN300-1921394	CID:  SMILES:  RUN:  DDG (kcal/mol):	EN300-764780  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccccc3n4cc(nn4)[C@H]5CCCC[NH2+j5]  RUN4329  -0.37
	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-764780  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccccc3n4cc(nn4)(C@H]5CCCC(NH2+j5)  RUN4329  -0.37
	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-764780  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccccc3n4cc(nn4)(C@HIJSCCCC(NH2+)5  RUN4329  -0.37  0.23
EN300-1921394	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-764780  Ce1cence1NC(=0)Ce2cc(cc(e2)Cl)OCc3ccccc3n4cc(nn4)(C@HIJ5CCCC(NH2+)5  RUN4329  -0.37  0.23  EN300-1921394  Ce1cence1NC(=0)Ce2cc(cc(e2)Cl)OC[C@H](c3cccc4c3ccnc4)0

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EN300-1915625	CID:	EN300-1915625
NH	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
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnccc3Cl
	RUN:	RUN1026
CI	DDG (kcal/mol):	-0.36
	dDDG (kcal/mol):	0.11
		0.11
EN300-1137140	CID:	EN300-1137140
EN300-1137140		
EN300-1137140	CID:	EN300-1137140
EN300-1137140	CID:	EN300-1137140  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)OCC4CCC4
EN300-1137140	CID: SMILES: RUN:	EN300-1137140  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)OCC4CCC4  RUN1359
EN300-1137140  EN300-35204	CID: SMILES: RUN: DDG (kcal/mol):	EN300-1137140  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)OCC4CCC4  RUN1359  -0.36
NH NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1137140  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)OCC4CCC4  RUN1359  -0.36  0.16
NH NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1137140  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)OCC4CCC4  RUN1359  -0.36  0.16
NH NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-1137140  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(cc3)[C@@H](Cl)OCC4CCC4  RUN1359  -0.36  0.16  EN300-35204  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(cc4c3nccc4)F

EN300-1613389	CID:	EN300-1613389
NH O	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(oc(=0)o3)c4ccc(cc4)OC
	RUN:	RUN2575
	DDG (kcal/mol):	-0.34
	dDDG (kcal/mol):	0.19
EN300-224566	CID:	EN300-224566
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cscc3Br
	RUN:	RUN333
CI CO	DDG (kcal/mol):	-0.34
	dDDG (kcal/mol):	0.09
Br	da a community	0.00
EN300-7427269	CID:	EN300-7427269
EN300-7427269	CID:	EN300-7427269
NH NH	CID: SMILES:	EN300-7427269  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cnsc3Br
NH O	CID: SMILES: RUN:	EN300-7427269  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cnsc3Br  RUN834
NH O	CID: SMILES: RUN: DDG (kcal/mol):	EN300-7427269  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cnsc3Br  RUN834  -0.34
NH O CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-7427269  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cnsc3Br  RUN834  -0.34  0.11
NH O CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-7427269  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cnsc3Br  RUN834  -0.34  0.11
NH O CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-7427269  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cnsc3Br  RUN834  -0.34  0.11  EN300-180043  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccnc3N(=O)=O

2020 00 14 Hudicop	hilic-displacement	
EN300-1916585	CID:	EN300-1916585
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3)C(=O)OC)O
	RUN:	RUN1342
	DDG (kcal/mol):	-0.33
ОН	dDDG (kcal/mol):	0.17
EN300-841086	CID:	EN300-841086
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccc(c3)c4c(cn(n4)C(C)C)C(F)F
<b>&gt;</b>	RUN:	RUN798
	DDG (kcal/mol):	-0.33
F F	dDDG (kcal/mol):	0.20
EN300-766689	CID:	EN300-766689
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3n4cc(nn4)CCBr)F
Br	RUN:	RUN3550
	DDG (kcal/mol):	-0.33
F TN	dDDG (kcal/mol):	0.21
EN300-202844	CID:	EN300-202844
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)C(=O)OC)CBr
	RUN:	RUN2367

DDG (kcal/mol):

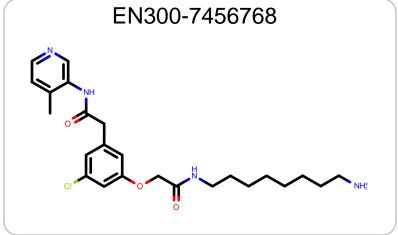
dDDG (kcal/mol):

-0.33

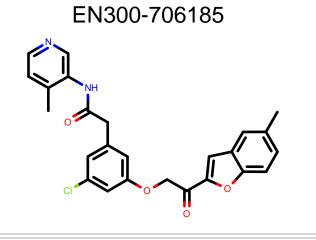
EN300-1906910	
NH	
CI OH	
	$\leq$

910	
OH OH	
700	

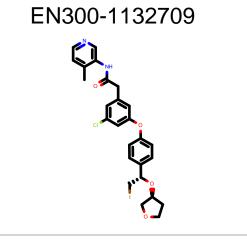
CID:	EN300-1906910
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3ccc(cc3O)OC
RUN:	RUN2912
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.14



CID:	EN300-7456768
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)NCCCCCCC[NH3+]
RUN:	RUN1899
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.24



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



CID:	EN300-1132709
SMILES:	Cc1ccncc1NC(=0)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
CI	RUN:	RUN4291
O HN	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
EN300-127870	CID:	EN300-127870  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4c5cccc5ccc4OC
EN300-127870		
EN300-127870	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4c5cccc5ccc4OC
EN300-127870	SMILES: RUN:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4c5ccccc5ccc4OC
EN300-127870  EN300-1613387	SMILES: RUN: DDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4c5ccccc5ccc4OC  RUN3778  -0.31
NH CI	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4c5ccccc5ccc4OC  RUN3778  -0.31
NH CI	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4c5ccccc5ccc40C  RUN3778  -0.31  0.22
NH CI	SMILES: RUN: DDG (kcal/mol): dDDG (kcal/mol): CID: SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(no3)c4c5ccccc5ccc4OC  RUN3778  -0.31  0.22  EN300-1613387  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c(oc(=O)o3)c4cccc(c4)Br

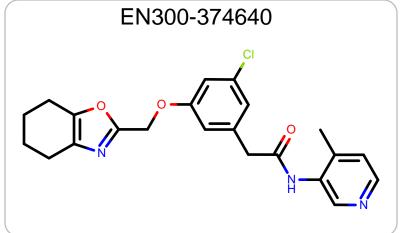
	primo diopidoornorit	
EN300-728709	CID:	EN300-728709
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCS(=O)(=O)F
	RUN:	RUN302
CI	DDG (kcal/mol):	-0.31
S F	dDDG (kcal/mol):	0.09
EN300-1940535	CID:	EN300-1940535
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(c3)[C@@H]4C[C@H]4C
	RUN:	RUN161
	DDG (kcal/mol):	-0.31
CI	dDDG (kcal/mol):	0.11
EN300-219845	CID:	EN300-219845
	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCn3cnc(n3)Br
NH O	RUN:	RUN2721
HC+- N	DDG (kcal/mol):	-0.30
CI N N N Br	dDDG (kcal/mol):	0.15
EN300-236658	CID:	EN300-236658
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc4cccc(c4o3)OC
	RUN:	RUN2648
	DDG (kcal/mol):	-0.30
	dDDG (kcal/mol):	0.16

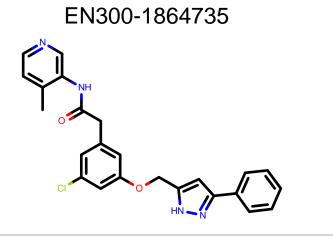
2020-00-14-Hucieo		
EN300-254027	CID:	EN300-254027
	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(c(c3)F)F)CBr
NH F	RUN:	RUN2633
	DDG (kcal/mol):	-0.29
CI	dDDG (kcal/mol):	0.12
EN300-118287	CID:	EN300-118287
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(cc3)OC[C@@H]4CCCO4
	RUN:	RUN3490
	DDG (kcal/mol):	-0.28
	dDDG (kcal/mol):	0.15
		0.13
EN300-43569	CID:	EN300-43569
EN300-43569	CID:	EN300-43569
NH NH	CID:	EN300-43569  Ce1cance1NC(=0)Ce2cc(cc(c2)Cl)OCC(=0)c3ccc4c(c3)CCCC4
NH NH	CID: SMILES: RUN:	EN300-43569  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)c3ccc4c(c3)CCCC4  RUN4494
	CID: SMILES: RUN: DDG (kcal/mol):	EN300-43569  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)c3ccc4c(c3)CCCC4  RUN4494  -0.28
NH O CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-43569  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)c3ccc4c(c3)CCCC4  RUN4494  -0.28
NH O CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-43569  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)c3ccc4c(c3)CCCC4  RUN4494  -0.28  0.21
NH O CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-43569  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)c3ccc4c(c3)CCCC4  RUN4494  -0.28  0.21  EN300-1456498  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(nn3)C

EN300-125523	CID:	EN300-125523
○ NH	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
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c4ccccc4ccc3O
ОН	RUN:	RUN2647
CI	DDG (kcal/mol):	-0.27
	dDDC (lead/mal).	0.44
	dDDG (kcal/mol):	0.14
EN300-1937083	CID:	EN300-1937083
EN300-1937083	CID:	EN300-1937083
NH NH	CID:	EN300-1937083  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3nnn(n3)C(C)(C)C
NH NH	CID: SMILES: RUN:	EN300-1937083  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3nnn(n3)C(C)(C)C  RUN1770
NH NH	CID: SMILES: RUN: DDG (kcal/mol):	EN300-1937083  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3nnn(n3)C(C)(C)C  RUN1770  -0.27
NH ON NH ON NH	CID: SMILES: RUN: DDG (kcal/mol): dDDG (kcal/mol):	EN300-1937083  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3nnn(n3)C(C)(C)C  RUN1770  -0.27  0.12
NH ON NH ON NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1937083  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3nnn(n3)C(C)(C)C  RUN1770  -0.27  0.12
NH ON NH ON NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-1937083  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3nnn(n3)C(C)(C)C  RUN1770  -0.27  0.12  EN300-1934022  CCCc1ccc(s1)C(=C)COc2cc(cc(c2)Cl)CC(=0)Nc3cnccc3C

EN300-1256145
NH O
$\triangleleft$
FN300-24109

## NH CI





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

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

dDDG (kcal/mol):	0.23
CID:	EN300-374640
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3nc4c(o3)CCCC4
RUN:	RUN3442
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.11

CID:	EN300-1864735
SMILES:	Cc1ccncc1NC(=0)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(=0)(Cc2cc(cc(c2)Cl)OCc3c(n(nn3)[C@@HJ4CCNc5c4cccc5)C
	RUN:	RUN830
N.	DDG (kcal/mol):	-0.26
	dDDG (kcal/mol):	0.16
EN300-257065	CID:	EN300-257065
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(nn3)C
	RUN:	RUN1272
CI NN	DDG (kcal/mol):	-0.26
	dDDG (kcal/mol):	0.09
	)	
EN300-379204	CID:	EN300-379204
EN300-379204	CID:	EN300-379204  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)O[C@H](CBr)[S@@](=0)C(F)(F)F
EN300-379204		
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)O[C@H](CBr)[S@@](=0)C(F)(F)F
NH NH	SMILES: RUN:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Q[C@H](CBr)[S@@](=0)C(F)(F)F  RUN3252
NH NH	SMILES: RUN: DDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)O[C@H](CBr)[S@@](=0)C(F)(F)F  RUN3252  -0.25
NH Br	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)O[C@H](CBr)[S@@](=0)C(F)(F)F  RUN3252  -0.25
EN300-1280988	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)O[C@H](CBr)[S@@](=0)C(F)(F)F  RUN3252  -0.25  0.14  EN300-1280988
NH Br	SMILES: RUN: DDG (kcal/mol): dDDG (kcal/mol): CID: SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Q[C@H](CBr)[S@@](=Q)C(F)(F)F  RUN3252  -0.25  0.14  EN300-1280988  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)QCC(=0)N3CC[C@H]3C(=Q)N

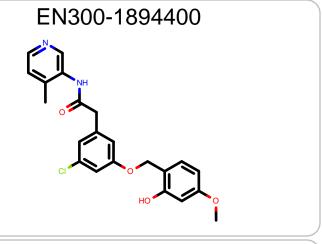
	hilic-displacement	
EN300-1918941	CID:	EN300-1918941
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@H](c3cnc(s3)OC)O
	RUN:	RUN3118
	DDG (kcal/mol):	-0.24
CI OH	dDDG (kcal/mol):	0.19
EN300-1277859	CID:	EN300-1277859
	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3c(n(nn3)C(C)C)CBr
Br NH	RUN:	RUN184
	DDG (kcal/mol):	-0.24
CI N N	dDDG (kcal/mol):	0.11
EN300-843012	CID:	EN300-843012
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cccc(c3)c4ccn[nH]4
	RUN:	RUN876
HNNN	DDG (kcal/mol):	-0.24
	dDDG (kcal/mol):	0.12
EN300-1274631	CID:	EN300-1274631
No.	SMILES:	$\label{eq:concentration} Cc + 1 + Cc + Cc + Cc + Cc + Cc + Cc + $

211000 121 1001	CID:	EN300-1274631
	SMILES:	eq:conconconconconconconconconconconconconc
	RUN:	RUN1822
	DDG (kcal/mol):	-0.24
Br	dDDG (kcal/mol):	0.16
- 4	3 -	

2020 00 11 110000	•	
EN300-139605	CID:	EN300-139605
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(o3)Br
	RUN:	RUN316
	DDG (kcal/mol):	-0.23
CI	dDDG (kcal/mol):	0.11
EN300-121881	CID:	EN300-121881
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)O[C@H](CBr)C(=O)Cl
	RUN:	RUN3472
Br	DDG (kcal/mol):	-0.23
CI O O O	dDDG (kcal/mol):	0.14
EN300-1893407	CID:	EN300-1893407
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(cc(cc3F)F)OC
	RUN:	RUN1620
	DDG (kcal/mol):	-0.23
F F	dDDG (kcal/mol):	0.12
EN300-1934449	CID:	EN300-1934449
	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cc4cc(ccc4[nH]3)Cl
CI	RUN:	RUN3668
HN	DDG (kcal/mol):	-0.23
	dDDG (kcal/mol):	0.15

EN300-1117588
NH NH
CI
EN200 00101

EN300-99101	
S CI	



EN300-1918983
N S
\text{\text{NH}}
CI

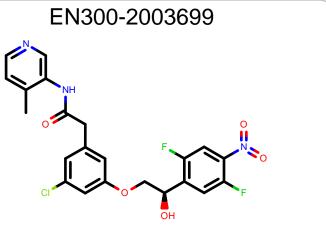
CID:	EN300-1117588
SMILES:	CCCc1cccc(c1COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)C
RUN:	RUN4303
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.13
OID	EN000 00404

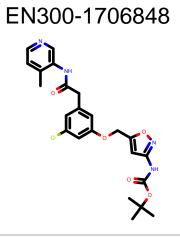
CID:	EN300-99101
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3nc4ccccc4s3
RUN:	RUN3682
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.13

DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.13
CID:	EN300-1894400
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(cc3O)OC
RUN:	RUN2847
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.13
CID:	EN300-1918983

CID.	EN300-1910903
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
NH ONH CI
EN300 3003600





EN300-70	3228
NH NH	
CI	

CID:	EN300-313279
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(ccs3)C(=0)OC
RUN:	RUN970
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.12
CID:	EN300-2003699

SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@@H](c3cc(c(cc3F)N(=0)=0)F)O
RUN:	RUN2754
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.20

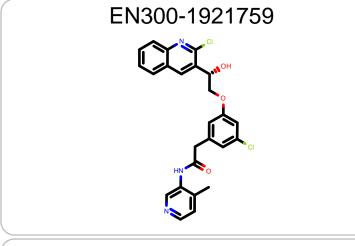
dDDG (kcal/mol):	0.20
CID:	EN300-1706848
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(no3)NC(=0)OC(C)(C)C
RUN:	RUN2157
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.15
CID.	FN300-703228

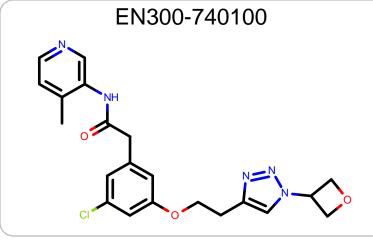
CID:	EN300-703228
SMILES:	CCOC(=0)c1c(coc1C0c2cc(cc(c2)Cl)CC(=0)Nc3enccc3C)C4CC4
RUN:	RUN1126
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.15

NH OCH ₂
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EN300-1939155
NH CH ₂
EN300-76695

EN300-70093	
NH ON THE STATE OF	
Br	





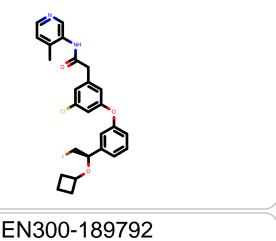
•	
CID:	EN300-1939155
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=C)c3csc4c3CCCC4
RUN:	RUN4498
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.20
CID:	EN300-76695

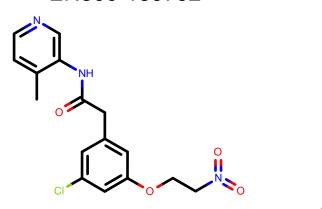
CID:	EN300-76695
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3ccc(cc3Br)Cl
RUN:	RUN3337
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.14

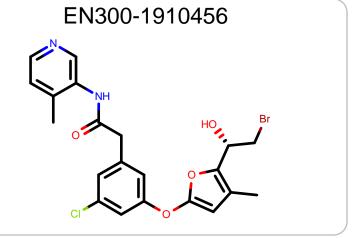
CID:	EN300-1921759
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3cc4ccccc4nc3Cl)O
RUN:	RUN4336
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.23

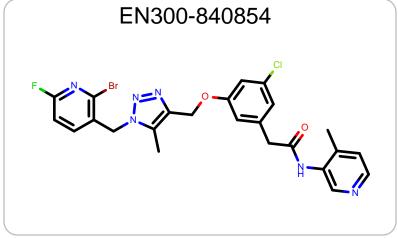
CID:	EN300-740100
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cn(nn3)C4COC4
RUN:	RUN3372
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.17

EN300-1132820	
NH NH	
	)
FN300-189792	









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
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

dDDG (kcal/mol):	0.10
CID:	EN300-1910456
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)[C@@H](CBr)O)C
RUN:	RUN77
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.16

CID:	EN300-840854
SMILES:	Cc1ccncc1NC(=0)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
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(cnc3C(=0)OC)COC
	RUN:	RUN4276
	DDG (kcal/mol):	-0.18
	dDDG (kcal/mol):	0.17
EN300-1913480	CID:	EN300-1913480
	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccnc3N4CCCCC4
CI	RUN:	RUN3408
	DDG (kcal/mol):	-0.18
	dDDG (kcal/mol):	0.17
	)	
EN300-1895232	CID:	EN300-1895232
	CID:	EN300-1895232  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(cc(cn3)Cl)Cl
EN300-1895232		
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(cc(cn3)Cl)Cl
NH NH	SMILES: RUN:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(cc(cn3)Cl)Cl
NH NH	SMILES:  RUN:  DDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(cc(cn3)Cl)Cl  RUN2929  -0.18
NH CI	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(cc(cn3)Cl)Cl  RUN2929  -0.18  0.12
NH CI	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(cc(cn3)Cl)Cl  RUN2929  -0.18  0.12
NH CI	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(cc(cn3)Cl)Cl  RUN2929  -0.18  0.12  EN300-10621  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccccc3N(=0)=0

EN300-1613388	CID:	EN300-1613388
NH NH	SMILES:	Cc1ccc(cc1)c2c(cc(=O)o2)COc3cc(cc(c3)Cl)CC(=O)Nc4cnccc4C
	RUN:	RUN2168
CI	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
		0.14
EN300-1910385	CID:	EN300-1910385
EN300-1910385		
NH Br	CID:	EN300-1910385
NH NH	CID:	EN300-1910385  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)[C@H](C)CBt)C
NH Br	CID: SMILES: RUN:	EN300-1910385  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)[C@H](C)CBr)C  RUN602
NH O MH	CID: SMILES: RUN: DDG (kcal/mol):	EN300-1910385  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)[C@H](C)CBt)C  RUN602  -0.17
NH Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1910385  Cc1ccncc1NC(=0)Cc2cc(cc(c2)CI)Oc3cc(c(o3)[C@H](C)CBt)C  RUN602  -0.17  0.11
NH Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1910385  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(a3)[C@H](C)CBr)C  RUN602  -0.17  0.11  EN300-1117578
NH Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-1910385  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)[C@H](C)CBr)C  RUN602  -0.17  0.11  EN300-1117578  CCCc1cc(ccc1COc2cc(cc(c2)Cl)CC(=0)Nc3cnccc3C)OC

dDDG (kcal/mol):

SMILES:

CID:

CID:

EN300-170062
EN200 1010226

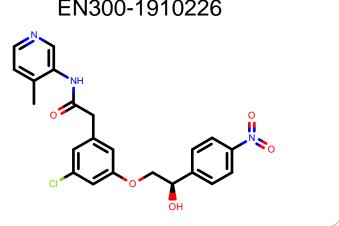
CID:	EN300-170062
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3C(=0)CBr)OC)OC
RUN:	RUN1973
DDG (kcal/mol):	-0.17

0.20

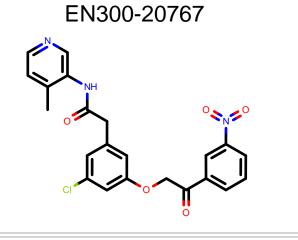
EN300-1910226

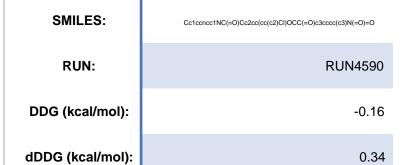
EN300-20767

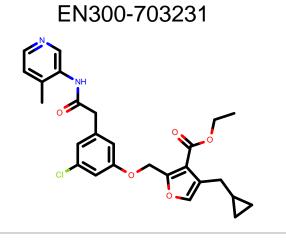
Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC[C@@H](c3ccc(cc3)N(=O)=O)O



RUN:	RUN2028
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.18

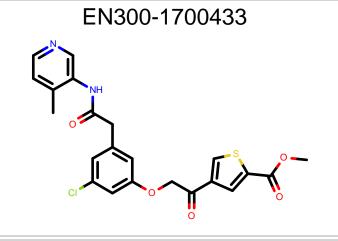


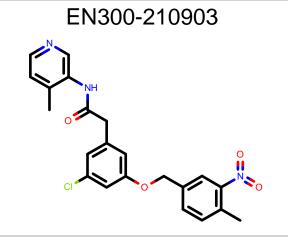




CID:	EN300-703231
SMILES:	CCOC(=O)c1c(coc1COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)CC4CC4
RUN:	RUN1063
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.17

	EN300-367729
	EN300-1609143
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CID:	EN300-367729
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCCc3cc4ccccc4[nH]3
RUN:	RUN3481
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.15
CID:	EN300-1609143

SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3nc(co3)C(=0)OC(C)(C)C
RUN:	RUN364
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.14

dDDG (kcal/mol):	0.14
CID:	EN300-1700433
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)c3cc(sc3)C(=0)OC
RUN:	RUN4283
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.17

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

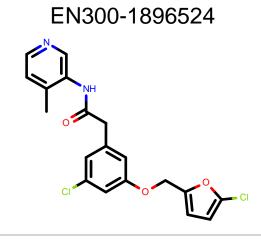
EN300-1889287	CID:	EN300-1889287
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(cc3NC(=0)OC(C)(C)C)Cl
	RUN:	RUN2123
NH NH	DDG (kcal/mol):	-0.15
CI	dDDG (kcal/mol):	0.18
EN300-764382	CID:	EN300-764382
	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cn(nn3)[C@H]4CCNc5c4cccc5
	RUN:	RUN1176
	DDG (kcal/mol):	-0.15
	dDDG (kcal/mol):	0.17
EN300-1912469	CID:	EN300-1912469
EN300-1912469	CID:	EN300-1912469  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cn(c4c3cccc4)C
EN300-1912469		
EN300-1912469	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cn(c4c3cccc4)C
EN300-1912469	SMILES: RUN:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(c4c3cccc4)C
EN300-1912469  EN300-1921861	SMILES: RUN: DDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cn(c4c3cccc4)C  RUN435  -0.15
HN CI	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cn(c4c3cccc4)C  RUN435  -0.15
HN CI	SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(c4c3cccc4)C  RUN435  -0.15  0.10
HN CI	SMILES: RUN: DDG (kcal/mol): dDDG (kcal/mol): CID: SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cn(c4c3cccc4)C  RUN435  -0.15  0.10  EN300-1921861  Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(n(n3)C)CCBr

2020 00 11 11401000		
EN300-364189	CID:	EN300-364189
NH	SMILES:	CCc1cc(nc(c1COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)C)CC
	RUN:	RUN4567
o Control of the cont	DDG (kcal/mol):	-0.14
	dDDG (kcal/mol):	0.29
EN300-695729	CID:	EN300-695729
NH NH	SMILES:	Cc1canca1NC(=0)Cc2cc(cc(c2)Cl)OCc3cn(nn3)(C@H]4CC[C@H](C4)(NH3+]
	RUN:	RUN1073
	DDG (kcal/mol):	-0.14
O _{**} , _{NH;}	dDDG (kcal/mol):	0.16
· · · ·		0.10
EN300-14150	CID:	EN300-14150
	CID:	EN300-14150
EN300-14150	CID:	EN300-14150  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(ccc3OC)OC
EN300-14150	CID: SMILES: RUN:	EN300-14150  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(ccc3OC)OC  RUN2092
EN300-14150	CID: SMILES: RUN: DDG (kcal/mol):	EN300-14150  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(ccc3OC)OC  RUN2092  -0.14
EN300-14150	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-14150  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(ccc3OC)OC  RUN2092  -0.14  0.14
EN300-14150	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-14150  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(ccc3OC)OC  RUN2092  -0.14  0.14  EN300-2966841
EN300-14150  EN300-2966841	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-14150  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(ccc3OC)OC  RUN2092  -0.14  0.14  EN300-2966841  CCONC(=0)COc1cc(cc(c1)Cl)CC(=0)Nc2cnccc2C

EN300-1136771
NH NH
CI OH
EN300-1613383

NH CI	L14300-1013303
	NH CI

EN300-1915974
NH
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CI
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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
CID:	EN300-1613383

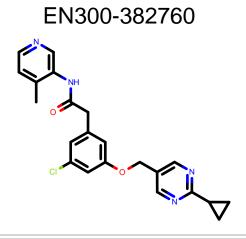
CID:	EN300-1613383
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3c(oc(=0)o3)c4cccc(c4)Cl
RUN:	RUN1379
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.18

CID:	EN300-1915974
SMILES: Cc1ccncc1NC(=0)Cc2c	c(cc(c2)Cl)OCc3c[nH]nc3N(=O)=O
RUN:	RUN2156
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.12

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
NH NH
S Br
FN300-7433156

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EN300-7433156	
NH NH	



EN300-1897863
NH
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N N

EN300-4263497
Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cc(cc(c3)OC)CBr
RUN2446
-0.13
0.12
EN300-7433156

CID:	EN300-7433156
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(cc4c3O[C@@H](C4)Cl)C
RUN:	RUN2999
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.16
	·

dDDG (kcal/mol):	0.16
CID:	EN300-382760
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cnc(nc3)C4CC4
RUN:	RUN2654
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.13

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

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EN300-1908580	CID:	EN300-1908580
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3ccc(c(c3)N(=0)=0)F)O
	RUN:	RUN3152
	DDG (kcal/mol):	-0.12
CI OH	dDDG (kcal/mol):	0.19
EN300-1921979	CID:	EN300-1921979
	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC(C@H](c3nc4ccccc4s3)O
CI	RUN:	RUN3104
HN	DDG (kcal/mol):	-0.12
	IDD 0 (1 1/ 1)	
N -	dDDG (kcal/mol):	0.22
EN300-1904938	CID:	0.22 EN300-1904938
EN300-1904938		
NH Br	CID:	EN300-1904938
NH NH	CID:	EN300-1904938  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)CCCBr)C
NH Br	CID: SMILES: RUN:	EN300-1904938  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)CCCBr)C  RUN373
NH O Br	CID: SMILES: RUN: DDG (kcal/mol):	EN300-1904938  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)CCCBr)C  RUN373  -0.12
NH O Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1904938  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)CCCBr)C  RUN373  -0.12
NH O Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1904938  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)CCCBr)C  RUN373  -0.12  0.12  EN300-7493972
NH O Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-1904938  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(o3)CCCBr)C  RUN373  -0.12  0.12  EN300-7493972  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cnn(n3)c4cccc(c4)Br

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EN300-138681	CID:	EN300-138681
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(c(cc3N(=0)=0)F)OC
	RUN:	RUN4536
	DDG (kcal/mol):	-0.11
F	dDDG (kcal/mol):	0.28
EN300-1934062	CID:	EN300-1934062
NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3c(cc(cc3O)O)O
	RUN:	RUN2850
HO OH	DDG (kcal/mol):	-0.11
CI	dDDG (kcal/mol):	0.13
EN300-1917568	CID:	EN300-1917568
	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc4c(c3)[N@@](CCO4)C
	RUN:	RUN1675
	DDG (kcal/mol):	-0.11
CI	dDDG (kcal/mol):	0.12
EN300-2002092	CID:	EN300-2002092
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)O)CCBr
	RUN:	RUN700
	DDG (kcal/mol):	-0.11

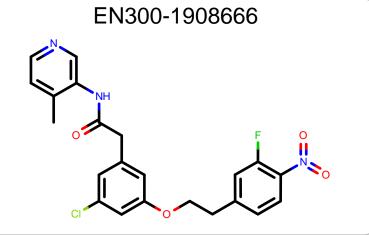
dDDG (kcal/mol):

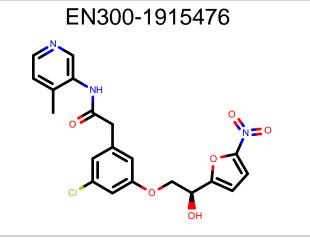
0.12

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FN300-134559

EN300-11	65403	
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HN	<b>\</b> 0	
	1	
N	<b>-/</b>	

EN300-134559	
S O O O O O O O O O O O O O O O O O O O	





EN300-1165403
cncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3c4cc(ccc4sn3)O
RUN405
-0.11
0.12

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

dDDG (kcal/mol):	0.12
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

CID:	EN300-1915476
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@@H](c3ccc(o3)N(=0)=0)0
RUN:	RUN1400
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.19

EN300-1136777	
NH	
CI OH	
EN300-26674128	

EN300-1136777	
NH CI	
CI OH	

SMILI	
RUN	
DDG (kca	
dDDG (kc	

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

EN300-26674128

**RUN877** 

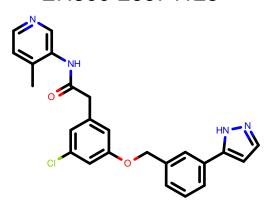
-0.10

0.13

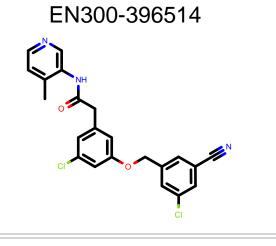
**RUN2105** 

-0.10

0.13

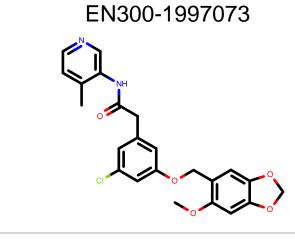


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NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cccc(c3)c4ccn[nH]4
	RUN:	RUN87
HNNN	DDG (kcal/mol):	-0.10
	dDDG (kcal/mol):	0.1;
		·



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	CID:	EN300-396514
	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc(cc(c3)Cl)C#N
	RUN:	RUN210
	DDG (kcal/mol):	-0.1
	dDDG (kcal/mol):	0.1

CID:

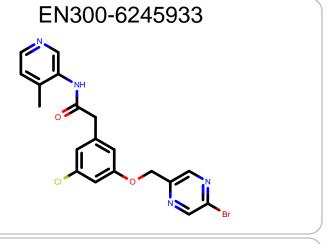


CID:	EN300-1997073
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cc4c(cc3OC)OCO4
RUN:	RUN3647
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.15

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EN300-216088	CID:	EN300-216088
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCc3cc(on3)C
	RUN:	RUN989
	DDG (kcal/mol):	-0.09
CI	dDDG (kcal/mol):	0.11
EN300-1246893	CID:	EN300-1246893
	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OC/C=C\c3ccccc3
NH NH	RUN:	RUN1067
	DDG (kcal/mol):	-0.09
	dDDG (kcal/mol):	0.11
	and a continuous	0.11
EN300-674675	CID:	EN300-674675
EN300-674675		
EN300-674675	CID:	EN300-674675
EN300-674675	CID:	EN300-674675  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)F)CCCBr
EN300-674675	CID: SMILES: RUN:	EN300-674675  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)F)CCCBr  RUN1103
EN300-674675  EN300-1653517	CID: SMILES: RUN: DDG (kcal/mol):	EN300-674675  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)F)CCCBr  RUN1103  -0.09
NH CI SHE F	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-674675  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)F)CCCBr  RUN1103  -0.09  0.12
NH CI SHE F	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-674675  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3ccc(c(c3)F)CCCBr  RUN1103  -0.09  0.12
NH CI SHE F	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-674675  Cc1ccncc1NC(=0)Cc2cc(cc(c2)CI)Oc3ccc(c(c3)F)CCCBr  RUN1103  -0.09  0.12  EN300-1653517  Cc1ccncc1NC(=0)Cc2cc(cc(c2)CI)OCc3ccc4c(c3)[C@@H](C@@H](O4)C)C

EN300-28768	
CI CI	
HN	

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



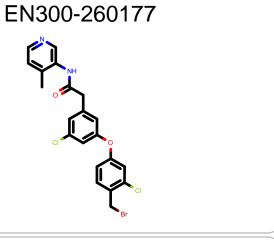
RUN:	RUN3059
DDG (kcal/mol):	-0.09
IDDO (1 1/ 1)	0.40

EN300-6245933

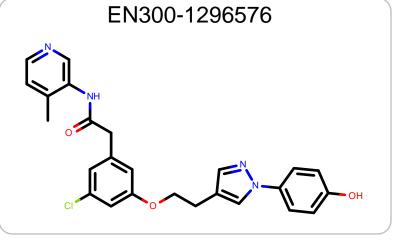
Cc1ccncc1NC(=O)Cc2cc(cc(c2)CI)OCc3cnc(cn3)Br

CID:

SMILES:



dDDG (kcal/mol):	0.12
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



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
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC(=0)c3ccc(c(c3)N(=0)=0)Cl
	RUN:	RUN4419
	DDG (kcal/mol):	-0.08
CI	dDDG (kcal/mol):	0.20
EN300-1132820	CID:	EN300-1132820
NH NH	SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)Oc3cccc(c3)[C@@H](Cl)OC4CCC4
	RUN:	RUN692
	DDG (kcal/mol):	-0.08
	-IDDO (Isaal/masi)s	0.40
	dDDG (kcal/mol):	0.16
EN300-310116	CID:	0.16 EN300-310116
EN300-310116		
EN300-310116	CID:	EN300-310116
NH NH	CID:	EN300-310116  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cccc(c3C)OC
NH NH	CID: SMILES: RUN:	EN300-310116  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cccc(c3C)OC  RUN2457
NH NH	CID: SMILES: RUN: DDG (kcal/mol):	EN300-310116  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cccc(c3C)OC  RUN2457  -0.08
NH CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-310116  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cccc(c3C)OC  RUN2457  -0.08  0.13
NH CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-310116  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cccc(c3C)OC  RUN2457  -0.08  0.13
NH CI	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-310116  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cccc(c3C)OC  RUN2457  -0.08  0.13  EN300-1274639  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3)NC4=[NH+][C8@H]([C8@H](C4)CBr)C

2020 00 11 11401000		
EN300-87706	CID:	EN300-87706
NH NH	SMILES:	CCOc1ccc(cc1)[C@@H](COc2cc(cc(c2)Cl)CC(=O)Nc3cnccc3C)O
	RUN:	RUN2940
	DDG (kcal/mol):	-0.07
CI OH	dDDG (kcal/mol):	0.20
EN300-1918363	CID:	EN300-1918363
ОН	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@@H](c3c(c4ccccc4nn3)Cl)O
	RUN:	RUN4539
HN	DDG (kcal/mol):	-0.07
	dDDG (kcal/mol):	0.33
	,	0.55
EN300-1918995	CID:	EN300-1918995
EN300-1918995		
EN300-1918995	CID:	EN300-1918995
EN300-1918995	CID:	EN300-1918995  Cc1cancc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3ccc4ccanc4c3)O
EN300-1918995	CID: SMILES: RUN:	EN300-1918995  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3ccc4cccnc4c3)O  RUN2919
O NH	CID: SMILES: RUN: DDG (kcal/mol):	EN300-1918995  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3ccc4cccnc4c3)O  RUN2919  -0.07
CI NH NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1918995  Cc1cancc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3ccc4cccnc4c3)O  RUN2919  -0.07  0.18
CI NH NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1918995  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Ci)OC(C@H)(c3ccc4cccnc4c3)O  RUN2919  -0.07  0.18
CI NH NH	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-1918995  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@H](c3ccc4cccnc4c3)O  RUN2919  -0.07  0.18  EN300-703234  CCOC(=0)c1c(coc1COc2cc(cc(c2)Cl)CC(=0)Nc3cnccc3C)C4CCC4

2020 00 11 11401000		
EN300-59530	CID:	EN300-59530
NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cccc(c3)OCc4ccccc4
	RUN:	RUN1147
	DDG (kcal/mol):	-0.07
	dDDG (kcal/mol):	0.15
EN300-766154	CID:	EN300-766154
NH NH	SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cn(nn3)Cc4c(c(c(cn4)C)OC)C
	RUN:	RUN2176
	DDG (kcal/mol):	-0.07
<b>&gt;=</b>	dDDC (kool/mol)	0.40
<b>,</b>	dDDG (kcal/mol):	0.18
EN300-1898328	CID:	EN300-1898328
EN300-1898328		
EN300-1898328	CID:	EN300-1898328
NH NH	CID:	EN300-1898328  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3CBr)F)F
NH NH	CID: SMILES: RUN:	EN300-1898328  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3CBr)F)F  RUN1288
NH NH	CID: SMILES: RUN: DDG (kcal/mol):	EN300-1898328  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3CBr)F)F  RUN1288  -0.06
NH O CI Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1898328  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3CBr)F)F  RUN1288  -0.06
NH O CI Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):	EN300-1898328  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3CBr)F)F  RUN1288  -0.06  0.13
NH O CI Br	CID:  SMILES:  RUN:  DDG (kcal/mol):  dDDG (kcal/mol):  CID:  SMILES:	EN300-1898328  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cc(c(cc3CBr)F)F  RUN1288  -0.06  0.13  EN300-1912781  Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(c(c3F)Br)F

EN300-2010197
NH NH
CI
FN300-1897247

EN300-1897247	
NH NH	
CI N	

EN300-695755
NH NH
N=N NH\$
CI

EN300-1938792
NH OH CI

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

SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3cnn(c3)C(C)(C)C	
RUN:	RUN889	
DDG (kcal/mol):	-0.05	
dDDG (kcal/mol):	0.13	

EN300-1897247

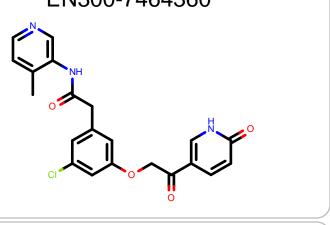
CID:

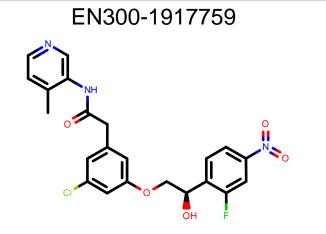
dDDG (kcai/moi):	0.13
CID:	EN300-695755
SMILES:	Cc1ccncc1NC(=0)/Cc2cc(cc(c2)Cl)/OCCc3cn(nn3) C@HJ4CC[C@HJ(C4)[NH3+]
RUN:	RUN4348
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.27

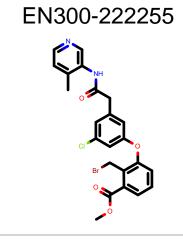
CID:	EN300-1938792
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCCc3ccc(cc3O)O
RUN:	RUN3037
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.14

EN300-175288
CI No.
EN200 7464260

EN300-173200
NH N
FN300-7464360







CID:	EN300-175288
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCC[N@](Cc3ccccc3)S(=0)(=0)C
RUN:	RUN4600
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.64
CID:	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

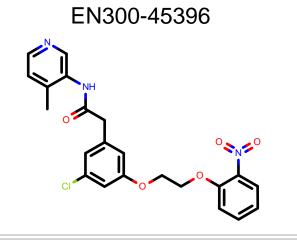
CID:	EN300-1917759
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OC[C@@H](c3ccc(cc3F)N(=0)=0)O
RUN:	RUN1698
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.19

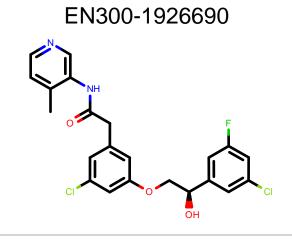
CID:	EN300-222255
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)Oc3cccc(c3CBr)C(=0)OC
RUN:	RUN3088
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.16
<u> </u>	

EN300-1865390
NH NH
EN300-1926794

EN300-1865390	
NH	
N=N	
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L11000 1020101	
NH NH	
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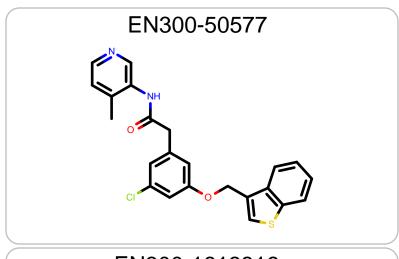


CID:	EN300-1865390
SMILES:	Cc1ccncc1NC(=O)Cc2cc(cc(c2)Cl)OCCc3cn(nn3)c4ccccc4
RUN:	RUN4613
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.40
CID:	EN300-1926794

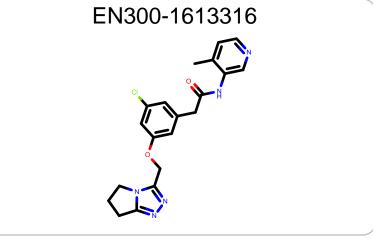
SMILES:	Cc1ccncc1NC(=0)Cc2cc(cc(c2)Cl)OCc3ccc(c(c30)O)O
RUN:	RUN2116
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.17

dbbg (kcai/illoi).	0.17
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

CID:	EN300-1926690
SMILES:	Cc1ccncc1NC(=0)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



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



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