Supporting Information

Computational screening of potential inhibitors of *Desulfobacter postgatei* for pyrite scale prevention in oil and gas wells

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Table S1. Sequence alignments and RMSD of model and template protein

PROTEIN	TYPE	SEQUENCE
D. postgatei	MODEL	MSKLVAPHGGKGLVCCKLEGAALEAERKKAAGLKKIEISSQVKGDLIMLGIGGFSPLNGFMTKADWKSVC EDFLLANGTFWPVPVMLDASAADAAAIKVGDEITLERNGEIYATMKIEEKFEMTEAEKKWECEKVYKGHG EESDDKVFWEIALKDHPGVQMVMARKEFCLAGPVKVLSEGEFPEKFKGVYLTPAETRAIMDEKGWANVAS MQLRNPMHRSHEHLCKIALDVCDGVLIHSLIGNLKPGDIPADVRIKCIDTLIKGYFVPEHVINAGYPLDM RYAGPREALLHATFRQNYGVNKMIIGRDHAGVGDFYTLFEAQEIFDTIPTPEDPGKRLLCEPLKIDWTFY CHKCDGMASMRTCPHGKDDRVILSGTKLRHALSNNQPVVDHFGREEVLVILREYYASLTEKVEVKLQSHA EGTKM
A. vinosum (PDBID:4DNX)	TEMPLATE	---MIKPVGSDELRPRFVYDPEQHHRLSSEAESLPSVIVSSQAAGNAVMLGAGYFSPLDG FMNLADALSSAQSMTLTDGRFFPVPLLCLLES--ADAIAGATRIALRDPNVEGNPVLAVM DVTAVEQVSDAQMALMTEQVYGTSD----------PKHPGVETFNSQGRTAISGPIQ VLNFSYFQTDFPDTFRTAVEIRHEIQERGWQKIVAFQTRNPMHRAHEELCKMAMEAVEAD GVVIHMLLGQLKPGDIPAPVRDAAIRTMAELYFPPNTVMVTGYGFDMLYAGPREAVLHAY FRQNMGATHFIIGRDHAGVGDYYGPFDAQTIFDDA----VPTDVLAIEIFRADNTAYSKK LGRVVMMRDAPDHTPDDFIQLSGTRVREMLGQGEAPPPEFSRPEVAQILMDYYRSLPQ-- ----------
ALIGNMENT RMSD		---711010122122223-777111111111121111111110011000000000000000 000000110000000000000000000112345--874445532111235----5211000 000111111111111111110002256----------6210001112222211000000 001111112212222221111111110000000000000000000000000000023--320 000000000000000000000011222222200122111100000000000000000000 000000110000000000000000000000000233----777765321111100000122 22211112223677-761110000000000111111010000111111111101245----

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Table S2. AutoDock Vina molecular docking results from first virtual screening

#	SMILES	DOCKING SCORE
1	N12CN(C3C=CC=CC=3C)CSC1=C([C@H](C1=C(OC)C=CC3C=CC=CC1=3)CC2=O)C#N	-9.5
2	S(=O)(=O)(N1CCC2(CC1)NC1C=C(F)C=CC=1N1C=CC=C12)C1=CC=CC=C1Cl	-9.3
3	[C@]12(C)C(=O)/C(=C(\C)/NC3=CC=C4C(C(=O)C=CO4)=C3)/C(C=C1OC1=C(C(O)=C(C)C(O)=C21)C(C)=O)=O	-9.1
4	N12N=C(C3C=CC(=CC=3)F)CSC1=NC1=C(C(C)=C(S1)C(=O)NC1C=C(C)C=C(C)C=1)C2=O	-9.1
5	**[C@@]12(/C=N/C3C=CC=C(C)C=3)C3C=CC=CC=3[C@@H]([C@H]3[C@@H]1C(=O)N(C3=O)C1C=CC(=CC=1)OC)C1C=CC=CC2=1**	**-8.7**
6	C1(NC2=CC=CC(Cl)=C2)O[C@@H](C2=CC3OCCOC=3C=C2N=1)C1=CC=CC=C1	-8.7
7	N1(N(C)C(=C(/C=N/N=C(/NC2=NC=CC=C2)\C2=NC=CC=C2)C1=O)C)C1=CC=CC=C1	-8.6
8	C1(C(=O)N2CCC(CC2)C(=O)NC2=CC=CC(F)=C2)N=NN2C=C(C)NC(=O)C=12	-8.5
9	N1C(=O)C(CCC(=O)N2CCN(CC2)C2=CC=C(F)C=C2)=NNC=1C1=CC(OC)=C(C=C1)OCC1C=CC=CC=1F	-8.5
10	C12C(CCCC=1NC(C1C=CC(C3C=CC=CC=3)=NC=1[C@@H]2O)=O)=O	-8.4
11	**C1(C#N)=C(SCC(OC)=O)NC([C@H](C21CCCCC2)C1SC=C(C2=CC=CC=C2)N=1)=N[H]**	**-8.4**
12	C12N=C(NCC3=CC=C(C=C3)OC)C3=C(C=CS3)N1N=NC=2S(=O)(=O)C1C=CC(=CC=1)C	-8.3
13	S1(=O)(=O)C2C=CC=CC=2OC2C=CC3=C(C(/C=N/NC(N)=O)=CN3)C1=2	-8.3
14	FC1=CC(NC(NN/C=C2\C3=C(C=CC=C3)C(=O)NC\2=O)=O)=CC(F)=C1	-8.3
15	NC1=C(C2NC(=O)[C@@]3(NN=C(C4=CC=CC=C4)C3)NN=2)C=CC=C1	-8.2
16	C[C@@H]1C2N(C=NN=2)CCN1S(C1CN(C(C2=CC(Cl)=CC=C2)=O)C1)(=O)=O	-8.2
17	**C12N=C(O)C[C@@H](C3C=CC(=C(Cl)C=3)O)C=1C(=NN2C1C=CC(=NN=1)O)C**	**-8.2**
18	N1C(N[C@H](C2C=CC(OC)=CC=2)C(=C1)C1OC2=CC(=C(C=C2C=1C(C1C=CC(C)=CC=1)=O)C#N)C#N)=O	-8.2
19	[C@]12(C[C@H](ON1[C@H](N(C1C=CC=CC=1)C2)C1=CC=C(OC)C(OC)=C1)C1C=CC=CC=1)C1=CC=CC=C1	-8.2
20	N1=C(C2=CC=C(C=C2)CS(=O)(=O)C2=CC=C(C=C2)C)ON=C1C1=CC=C2C(=C1)N=C(O2)C	-8.1
21	C12NC3=C(C=CC=C3)N1/C(/C=C(C)C=2C#N)=N/C1C=CC(=CC=1)Cl	-8.1
22	N12C(=O)/C(/SC1=NC(C1C=CC=CC=1)=C2C1=CC=CC=C1)=N/NC1=CC=C(C=C1)N(=O)=O	-8.1
23	C1(C(=O)NN2C=C(C(OCC)=O)C(C3C=C(F)C(F)=C(F)C2=3)=O)=CN(CC)C2=C(C=C(C(N3CCCC3)=C2)F)C1=O	-8.1

24	C1(=NC(CSC2=NC=CC=N2)=CC(=O)N1)N/C(/NC1C=CC(=CC=1)CC)=N/C(C1C=CC=CC=1)=O	-8.1
25	S(=O)(=O)(C1C=CC2=C(CCCC2)C=1)NC1C=CC=CC=1SCC1=CC(=O)N2C(C=CC(C)=C2)=N1	-8
26	C1(C(=O)NC[P+](C2C=CC=CC=2)(C2=CC=CC=C2)C2C=CC=CC=2)=CC2=C(C=CC=C2)O1	-8
27	COC(/C(/CC(C1=CC=CC=C1)=O)=N\N=C1\C2=C(C=CC=C2)NC(=O)N\1)=O	-8
28	C1(=C(C)C=CC2=CC=CC=C12)[C@H](O)C1C=CC(=CC=1)C1C=CC=CC=1	-8
29	C1(C2C[C@H](C3=CC=C(C=C3)OC)SC3C=CC=CC=3N=2)C(=O)N(C)C(N(C)C=1O)=S	-8
30	CN1C2=C(CC[C@@H](C3ON=C(C4(C5=C(F)C=C(F)C=C5)CCCCC4)N=3)C2)N=N1	-8
31	FC1=CC=C(C#CCN2C(=O)[C@]3(C4=C(C=CC=C4)OCC3)NC2=O)C=C1	-8
32	CC1=C(C)C2=C(N=C(N=C2N)CN2CCC(C3SC4=C(C=CC=C4)N=3)CC2)O1	-7.9
33	N12ON=C(C3C(C)=C(C)C=C(C)C=3C)N1C1C(=CC=CC=1)N2C(=O)C1=CC=C(C=C1)S(=O)(=O)N1CCOCC1	-7.9
34	C1(C(N)=O)C2N=C(O)C=C(O)C=2SC=1SCC(C1=CC=CC=C1)=O	-7.9
35	O=N(C1=CC=C(/C=N/N2C(=S)NN=C2N2C(C3=CC=CC=C3)=CC(C3=CC=CC=C3)=N2)C=C1)=O	-7.9
36	CN1C2=C(C=C(C=C2)Cl)N=C1NS(/C=C/C1=CC=CC=C1)(=O)=O	-7.9
37	C1(=C(C)SC2N=CN(CC(=O)N3CCN(CC3)C3C=CC=CC=3)C(=O)C1=2)S(=O)(=O)N1C[C@@H](C)C[C@@H](C)C1	-7.9
38	C1(/NC2=C(C)C=C(C=C2C(C)=N/1)C)=N\C1NCN(CN=1)CC1=CC=CC=N1	-7.9
39	CC(NC1=CC=C(C2C[C@@H](C3SC=CC=3)N(S(C3=CC=C(C)C=C3)(=O)=O)N=2)C=C1)=O	-7.9
40	N12N=C(N=C1S/C(/C2=O)=C1/C2C=C(Br)C=CC=2N(CC2=CC=CC=C2)C/1=O)C1C=CC(=CC=1)OC	-7.9
41	C12(CCN(CC1)C(C)C)N[C@@H](CC(C1C=CC(=CC=1)C)=N2)C1C=C(Cl)C=CC=1O	-7.8
42	C1(=O)C2C=CC=CC=2SC2=CC(=CC=C2N1C1CC1)NC(=O)C1C=CC(=CC=1)C(F)(F)F	-7.8
43	C1(OS(=O)(=O)C2=CC=C3C(C=CC=C3)=C2)=CC(=O)N(N=C1C(OCC)=O)C1C=CC(=CC=1)C	-7.8
44	C1(/C=C/[C@@H]2C[C@@H](O)CC(=O)O2)C(C2C=CC(=CC=2)F)=C2C=CC=CC2=NC=1C1CC1	-7.8
45	CC[C@@H]1N(C(C2C=C3S(NC4N(C3=CC=2)N=CN=4)(=O)=O)=O)CCCC1	-7.8
46	C1(C2=CC=NC(C)=N2)=C(C)N=C(C2CCN(CC2)C(=O)C2=CC=NO2)S1	-7.8
47	CC1=C(C)OC(CNC(C2=CC(N(=O)=O)=C(NC3=CC=CC=C3)C=C2)=O)=N1	-7.8
48	C12[C@@H](C3C=CC(=CC=3)C)N=C(NC=1C1C(=CC=CC=1)NC2=O)NC1SC2=C(C=CC=C2)N=1	-7.8
49	C1(=CC=NN1C(=O)NC1=CC=CC=C1)C1ON=C(C2=CC=CC=C2)C=1	-7.8
50	C1(NC(=O)NC2=CC=CC=C2OCC)C2=CC(F)=CC=C2NC=1C1=CC=NC=C1	-7.7
51	C12C(=O)CC(CC=1NC1=C(C=CC=C1)S[C@@H]2C1C=CC(=C(Cl)C=1)Cl)(C)C	-7.7
52	N1(C2C=CC=CC=2C=CC2C=CC=CC1=2)C(=O)N1CCCCC1	-7.7
53	C12C=C(SC=1N=C(C)N=C2OC1C=CC2=C(OCO2)C=1)C1=CC=CC=C1	-7.7

54	C1(CN2CCN(CC2)C2CCOCC2)=C(O)OC=C(CN2CCN(CC2)C2C=CC(=CC=2)F)C1=O	-7.7
55	S1(=O)(=O)C2=CC=C(C=C2N=C(CCC(=O)N[C@@H](C)C2C=CC3=C(OCCO3)C=2)N1)C	-7.7
56	C1(/S/C(/N(CC=C)C/1=O)=C1\C(C)=NN(C2=CC=C(C=C2)Cl)C\1=O)=C1/SC2=C(C=CC=C2)N/1CC	-7.7
57	N1(CC2=CC=C(C=C2)Cl)C2C=CC=CC=2C(/C=N/N=C2\SC3C(=CC=CC=3)N\2)=C1	-7.7
58	C1(=C/C2=CC(=CC=C2N2CCN(CC2)CC)N(=O)=O)\C(O)=NC(=NC\1=O)O	-7.7
59	CC1=C(C(NNC(NC2C(=O)N(CC3=CC=C(C)C=C3)C=CC=2)=O)=O)SC=N1	-7.7
60	N1(CCC(=O)NC2C=CC(=CC=2)S(=O)(=O)NC2ON=C(C)C=2C)C(=O)C2=C(C=CC=C2)C1=O	-7.6
61	FC1=C(NNC(C#CC2=CC3=C(OCO3)C=C2)=O)C=C(C(F)(F)F)C=C1	-7.6
62	CC1=C(Cl)C=C2C(OC(C=C2CN2CCN(C(N3CCCC3)=O)CC2)=O)=C1	-7.6
63	C1(C(=O)NNC(=O)C2=CC=CC=C2Br)OC2=C(/C(/CCC2)=N/NC2C=CC=CC=2)C=1C	-7.6
64	S(=O)(=O)(C1C=CC(=CC=1)C)NC(=O)NC1C=CC(=CC=1)C1OCCN=1	-7.6
65	C[C@@H](C1=C(C)C2=C(C=CC=C2)S1)OC(C1=NC=C2C(C(NC=N2)=O)=C1)=O	-7.6
66	N12NC(C(/N=N/C3C=CC=CC=3)=C1N=NC(C#N)=C2N)=O	-7.6
67	N1(CC(O)=NC2=CC=CC=C12)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](CC1C=CC=CC=1)C(O)=O	-7.5
68	FC1=CC=C(CONC(C2C(C3=C(Cl)C=CC=C3)=NNC=2)=O)C=C1	-7.5
69	C1(OCCSC=1C1C=CC=CC=1)C(=O)/N=C1/NN=C(SCC2C=CC(=CC=2)Cl)S/1	-7.5
70	C12[C@H](C3C=NN(C)C=3)C3=C(C)NN=C3OC=1N=CN1N=C(C3=CC=CC=C3N(=O)=O)N=C21	-7.5
71	CN1N=C(C(F)(F)F)C(CNC(/C=C/C2OC3=C(C=CC=C3)N=2)=O)=C1	-7.4
72	N12N=NN=C1NC(C1C=CC(=CC=1)C(C)C)=C[C@@H]2C1C=CC=C(OC)C=1OC	-7.4
73	C1(=C/C(=O)C2=CC=CS2)\NC2C=CC(=CC=2OC\1=O)N(=O)=O	-7.4
74	N12C(C3C=CC(=CC=3)Cl)=CN=C1C(=C(N)O2)/N=N/C1=CC=CC=C1	-7.4
75	C1(C2=CC=C(C=C2)/N=C/C2=CC=C(C(Cl)=C2)Cl)=CC2C=CC=CC=2OC1=O	-7.4
76	N12C(=O)C(=CN=C1OC(C1C=CC(=CC=1)OC)=N2)NC(=O)C1=CC=CC=C1Cl	-7.4
77	C12C3C=COC=3CCC=1C(=NN2C1C=CC(=CC=1)C(=O)NC(C)C)C(F)(F)F	-7.4
78	C12=C(C=CC3C(=CC(=O)OC1=3)C)O/C(=N\NC1=CC=C(C=C1)Cl)/C2=O	-7.4
79	CC1=C(CC(NC2SC(CC3=C(Cl)C=CC(Cl)=C3)=CN=2)=O)C(=O)NC(C2=CN=CC=C2)=N1	-7.4
80	C12N=C(N)C3=C(C=CC=C3)N1C1=C(C(CCC1)=O)[C@@H](C1=CC=C(C=C1)OC)C=2C#N	-7.4
81	O1C(C2C=CC=CC=2)=C2C=CC(C3C=CC=C1C=32)=O	-7.4
82	FC1=C(NC2=C3C(C=CC=C3)=NC(C(F)(F)F)=N2)C=C(Cl)C=C1	-7.4
83	N1=C(C2CC2)ON=C1C1=CC=CN=C1SCC(=O)N1CCN(CC1)C1CCN(CC1)C	-7.4
84	FC1=CC(C2OC(CN3C(=O)C4=C(CCC4)N=C3)=NC=2)=CC=C1	-7.4
85	COCC(N(CC(NC1OC(C2=CC=CC=C2)=C(C2=CC=CC=C2)N=1)=O)C)=O	-7.4
86	C12SSC(=S)C=1C1=C(C=CC(OC)=C1)N(C(=O)CC1=CC=C(C=C1)F)C2(C)C	-7.3
87	C1(OC[C@H](CSCC2C=CC(=CC=2)F)N=1)C1=CC=CN1CC1=CC=C(C=C1)C	-7.3
88	N1C(NC2C=CC(=CC=2)CC)=NC(=NC=1C1=CC2=C(C=CC=C2)O1)N	-7.3

89	N12C(=O)[C@@H](C3C=CC=CC=3Cl)SC(C(N)=O)=C1/C(/C(N)=C2C(OCC)=O)=C/C1=CC=CC=C1Cl	-7.3
90	C(C1=NOC(C2SC=CC=2)=C1)N1[C@H](C2=CC=CC=C2)C2N(C=CC=2)CC1	-7.3
91	C1(C=C(C=NC=1SC1=CC=CC(Cl)=C1)C1=CC=CC(=C1)C(F)(F)F)C#N	-7.3
92	C12[C@H](CC(NC=1C(=C(C(O)=O)S2)C1=CC=C(C=C1)F)=O)C1C=CC=CC=1OCCC	-7.3
93	C1C=C2C=C(C(=O)/C(=C/NC(=S)NC3C=CC(S(=O)(=O)N)=CC=3)/C#N)C=CC2=CC=1	-7.3
94	CN(CC1C2=C(C=CC=C2)OC=1C(NC1SC(/C=C/C2OC=CC=2)=NN=1)=O)C	-7.3
95	FC1=C(F)C=C2C(N=C(NC2=O)CC2NN=C(C3=CC=CC=C3)N=2)=C1	-7.3
96	CC1=C(C)C=C(C(NC2C(=O)OC(C(F)(F)F)=CC=2)=O)C=C1	-7.3
97	[C@@H]12N=NN(CC3C(=CC=CC=3F)Cl)[C@@H]1C(N(C1C=CC(=CC=1)Cl)C2=O)=O	-7.3
98	O1C(=C([C@H](C2=CC=C(CC)S2)C2C(N(C3C=CC=CC=3C=21)C)=O)C#N)N	-7.3
99	[C@@]1(C(F)(F)F)(NC(=O)C2C=CC(=CC=2)C(C)(C)C)C(=O)N(C2CC(C)(C)CC(=O)C1=2)CCCC	-7.3
100	N1=C(C2=C(N)N(C3=CC(C)=CC=C3)N=C2N=C1NCC1=CN=CC=C1)C1=CSC=C1	-7.3
101	C12C(N)=C(C(=O)OCC)OC=1N=C(C1C=CC(Cl)=CC=1)C=C2C(F)(F)F	-7.2
102	C1C[C@]2(CC=CCC2)CN(C2=NC(C3=NC=CN=C3)=CC=N2)C1	-7.2
103	C12C3(CCCCC3)CC3C(=CC=CC=3)C=1N=C(CC1=CC=CC=C1)N=C2SCC	-7.2
104	C1(C(OC)=O)=C(C)N(C(=O)/C/1=C\C1C=C(N(C2C=CC(=CC=2)OC)C=1C)C)C1C=CC(=C(Cl)C=1)C	-7.2
105	O=C(NN1C(=O)C2=C(C=CC=C2)N=C1)CN1N=NC(C2=CC=CC=C2)=C1	-7.2
106	NC1=CC=C(C2=CC(C)(C)[C@H](N)C(C)=C2)C=C1C	-7.2
107	C1([C@H](C([C@H]([C@@H](C(=O)OC)C=1O)C1C=CC=CC=1F)(C#N)C#N)C1=CC=C(C=C1)C)C(=O)OC	-7.2
108	C1(OC(=O)C2=CC=C(C=C2)N(=O)=O)OC(=NC=1/C=N/C1C=CC(=CC=1)OC)C1=CC=CC=C1	-7.2
109	ClC1=C(Cl)C=C(CN(C(C2OCCOC=2)=O)CC2=NC=CC=C2)C=C1	-7.2
110	[C@@]12(C[C@H]3CC[C@@H]1C[C@@H]3C(NCCCN1CCCC1=O)=O)OC1C=CC=CC=1C(=O)N2	-7.2
111	C1([C@H](CCC)N2CCN(CC2)C2C=CC=CC=2OC)=NN=NN1CC1=CC=CS1	-7.2
112	N12N=C(SC1=NN=C2C1C=C(Cl)C=CC=1F)C1CCC1	-7.2
113	CCC(NC1=CC=C(C2CSC(NCC3=CC4=C(OCO4)C=C3)=NN=2)C=C1)=O	-7.2
114	C1(SCCOC=1C)C(=O)NC1C=CC=C(C=1)C(=O)NCC1C=CC(=CC=1)OC(C)C	-7.2

115	FC1=C(F)C=C(N2CCCCC2)C(NC(N2C[C@H](N3N=NC=C3)CCC2)=O)=C1	-7.2
116	CC(C1N(CC(NC2=C(C3=CC(F)=C(F)C(F)=C3)C=CC=C2)=O)N=NN=1)C	-7.2
117	O[C@]1(C(F)(F)F)CN(C(C2=C(NC3=CC=CC=C3)C=CC=C2)=O)CC1	-7.2
118	[C@@]1(C)(C2=CC=CC=C2)OC(=O)C=C(C2C=CC=CC=2)O1	-7.1
119	C1(/NN=C(CSCC2C=CC(=CC=2)Cl)S/1)=N\C(=O)NC1C=CC(=C(Cl)C=1)Cl	-7.1
120	N1(C[C@@H](CO)C[C@H](CN2CCOCC2)C1)C(=O)C1C=COC2=CC=CC=C2C=1	-7.1
121	S1(=O)(=O)C(C2=CC=C(C=C2)C(C)C)=C(C(NC2C=CC(=C(C)C=2)C)=N1)C	-7.1
122	CC(OCCCN1/C(=N\[H])/C(=C2\N(C)C3=C(C=CC=C3)N\2C)/C(=O)C1)C	-7.1
123	O=C([C@@]12C[C@@H]3C[C@@H](C[C@@H](C3)C1)C2)CN=P(C1=CC=CC=C1)(C1=CC=CC=C1)C1=CC=CC=C1	-7.1
124	O=C1C2=C(C=CC=C2)C(C2=CC=CC=C2)=NN1CN1CC=C(C2SC=CC=2)CC1	-7.1
125	S1(=O)(=O)C2C=CC=CC=2C(OC2C=CC(=CC=2Br)F)=N1	-7.1
126	N12C(=O)C=C(N=C1NC(NC[C@@H]1CCCO1)=N[C@H]2[C@@H]1CCC=CC1)C	-7.1
127	C12=C(C3=CC=CO3)C(C#N)=C(N=C1SC1C(=CC=CC=1)N=C2N)N	-7.1
128	C12N=C(N(C(C)=O)C=1SC(C1C=CC=CC=1)=NN2C(C)=O)C1C=CC=CC=1	-7.1
129	N12N=CN=C1N=C(C(CC)=C2SC1=CC=C(C=C1)NC(=O)NC1=CC=C(C(Cl)=C1)F)C	-7.1
130	C[C@@H]1N(CC2=C(C(NNC3=NC(C)=NC(C)=C3)=O)OC=C2)C2=C(C=CC=C2)C1	-7.1
131	NC1=C(S(N2C3=C(C=CC=C3)C=CCC2)(=O)=O)C=C(Br)C=N1	-7.1
132	CCC1N=C(NC(/C(/C#N)=C/C2=C(C)N(C[C@@H]3OCCC3)C(C)=C2)=O)NN=1	-7.1
133	C12NC3=C(C=CC=C3)C=1N=C(C)N(/N=C/C1C=CC=C(C=1)N(=O)=O)C2=O	-7.1
134	FC1=C(Br)C=C2C(OC(N2CC2N=C(C3CCCCC3)ON=2)=O)=C1	-7.1
135	C[C@H]1CN(CN2C(=S)N3C(SC4=C3C=CC=C4)=N2)CCC1	-7.1
136	C12=C(NC)C(N)=CN=C1C(=C(F)C=C2F)F	-7.1
137	C1(C(=O)N/N=C/C2C=C(C=C(Br)C=2O)N(=O)=O)=NN(C(C2C=CC=CC=2)=N1)C1C=CC=CC=1	-7.1
138	CC1=C2C(C=CC=C2)=NC(SCC(C2OC3=C(C=CC=C3)C=2)=O)=C1	-7.1

139	C[C@H](C(/C(/C#N)=C1\NC2=C(C=CC=C2)N\1)=O)SC1N(C)C=NN=1	-7.1
140	CN1N=CC(C2=NC(/C=C/C3=CC4=C(OCC(N4)=O)C=C3)=NC=C2)=C1	-7.1
141	CC1C(/C=C2/C(=O)C3=C(C=CC(N(=O)=O)=C3)CC/2)=C(OC2=CN=CC=C2)N(C)N=1	-7.1
142	N1(/N=C/C2=CC(OC)=C(C(Br)=C2)OCC=C)C(=O)C2=CC=C3C4C(=CC=C(C2=4)C1=O)CC3	-7.1
143	C[C@@H](C(N([C@@H]1CS(=O)(=O)CC1)C)=O)N1CCC(C2OC(C)=C(C3=CC=CC=C3)N=2)CC1	-7
144	N1(CCN=C1SCC1C=CC=CC=1F)C(=O)C1=CC(Cl)=CC=C1OC	-7
145	C1(COC(=O)C2C3C=CC=CC=3OC3C=CC=CC2=3)C(=CC=CC=1F)Cl	-7
146	FC(C1=NC=C(S(NC2SN=C(C3=CC=NC=C3)N=2)(=O)=O)C=C1)(F)F	-7
147	C1(/S[C@@H](C(=O)N/1CC)CC(=O)NC1=CC=C(C=C1)Cl)=N\S(=O)(=O)C1=CC=C(C=C1)Cl	-7
148	C1(C(=O)C2C=CC=CC=2C(=O)C=1[N+]1C=CC(=CC=1)CC)[N-]S(C1=CC=CC=C1)(=O)=O	-7
149	C1(=NN=NN1C1C=CC=CC=1)S/C=C\C(C1C=CC(C)=CC=1C)=O	-7
150	C1(C2CCN(CC=2SC=1N)C(C)C)S(C1C=CC=CC=1)(=O)=O	-7
151	C1(=O)/C(=C\C2C=CC3OCOC=3C=2)/SC(NC2=CC(N(=O)=O)=CC=C2)=C1C(=O)OC	-7
152	N1(C2=CC=CC(=C2)C(F)(F)F)C(CNC(CC2C=CC3=C(OCO3)C=2)=O)=NN=C1SC[C@@H]1CCCO1	-7
153	C1(=S)N(NC(=O)C2C=CC=C(OC)C=2)[C@@H](C(=O)N1C1=CC=C(C=C1)OC)CC(=O)NC1=CC=C(C=C1)F	-7
154	ClC1=CC(NS(C2=CC=C(NC(C3CCC(=O)NN=3)=O)C=C2)(=O)=O)=CC=C1	-7
155	FC1=C(N2CCN(S(C3=CN=C(C4=CC=CC=C4)N=C3)(=O)=O)CC2)C=CC=C1	-7
156	C1(OC(/C(=C/C2C=CC=CC=2Cl)/N=1)=O)C1=C(C)ON=C1C1=CC=CC=C1	-7
157	NC(C1C=CC(N2C[C@H](C(=O)O)S(=O)(=O)CC2)=C(N(=O)=O)C=1)=O	-7
158	C12C3CCN(CC=3SC=1N[C@H](C1=CC=C(C=C1)CC)N=C2O)C(OCC)=O	-7
159	CC(C1C2=C(N=CC(C(OCCCC3=NN4C(N=C(C=C4C)C)=N3)=O)=C2)ON=1)C	-7
160	CC1=C(Cl)C=C(NP2(C=C(C3=CC=CC=C3)OC(C3=CC=CC=C3)=C2)=O)C=C1	-7
161	N1(C=CN=C(SCC2C=CC(=CC=2)Cl)C1=O)C1C=CC(=C(C)C=1)C	-7
162	C1(/NN=C(CCC)S/1)=N\C(CCC(=O)N1CCN(CC1)[C@@H](C1=CC=CC=C1)C1C=CC(=CC=1)Cl)=O	-7

163	CN1N=CC(N2C(=O)[C@H](NC(/C=C/C3=C(C#N)C=CC=C3)=O)CC2)=C1	-6.9
164	CC(C1OC2=C(C=C(C=C2)NS(/C=C/C2=CC=CC=C2)(=O)=O)N=1)(C)C	-6.9
165	[C@@]12(SC(=C(C)N1C1C=CC=CC=1)C(OC)=O)N(C1=CC=C(C=C1)Cl)N=C(C(OC)=O)S2	-6.9
166	C1(N(=O)=O)C=C(N(CC2=NN=C(NC3C=CN(CC4=CC=CC=C4Cl)N=3)S2)N=1)C	-6.9
167	O=C1C(C)=CN=C(NC2C=C(N3CCN(C)CC3)C=CC=2)N1	-6.9
168	N1(CC(=O)NC2SC=C(C3=CC=C(C=C3)Br)N=2)N=C(OC1=S)C1=CC=CC=C1	-6.9
169	O=S1(N(CC2N=C(C3SC=CC=3)ON=2)C2=C(C=CC=C2)N1CC1N=C(C2SC=CC=2)ON=1)=O	-6.9
170	C1C[C@H](C2SC(C3ON=C(C4=C(OC5=CC=CC=C5)N=CC=C4)N=3)=CN=2)OC1	-6.9
171	OC1=C(CNC(NNC(CC2=NC=CC=C2)=O)=O)C2=C(CCCC2)C=C1	-6.9
172	N12C(C)=CC=C1S[C@H](C(=O)NC1=CC=CC(C)=C1)[C@H](C1C=CC(=CC=1)OC)N2	-6.9
173	C(C)(C)(C)CCN[C@@H]1C[C@H]([C@@H]([C@H]1CC1=CC=NC(C2=CC=CN=C2)=N1)CO)O	-6.9
174	O=N(C1=NC=C(S(N[C@@H]2C3=C(C=CC(=C3)F)SCC2)(=O)=O)C=C1)=O	-6.9
175	O=C(C1=C(CSC2SCCN=2)C=CC=C1)N[C@@H]1[C@H](C2=CC=CC=C2)OCC1	-6.9
176	C1(C(=O)N(C)CC2SC=CN=2)C(OC)=CC(N2CCN(CC[C@H](C)C3=CC=C(C)O3)CCC=12)=O	-6.9
177	CC1SC=C(C2=CC(NC(C3=C(Cl)C=C(N4N=NN=C4)C=C3)=O)=CC=C2)N=1	-6.9
178	FC1=CC(COC2=CC3=C(C=CC(O3)=O)C=C2)=CN=C1	-6.9
179	[C@]12(C#N)[C@@H]3CCCC[C@@]3(O/C/1=N/[H])O[C@H](C1=CC=C(C(OC)=C1)OCC)C2(C#N)C#N	-6.9
180	O=C(N1CC2=C(C=CC=C2)S(=O)(=O)CC1)[C@@H]1N2C(=CC=C2)C(=O)CC1	-6.9
181	O=C(N1CC(=O)N(C2SC=CC=2)CC1)NCCC1NC2=C(C=CC=C2)N=1	-6.9
182	FC1=NC=CC(NNC(COC2=CC(N3C(=O)CCC3)=CC=C2)=O)=C1	-6.8
183	[C@]12(CC[C@](/C(=N/O)/C1=O)(C)C2(C)C)C(=O)N1CCOCC1	-6.8
184	ClC1=C([C@@H]2OCCN([C@@H]3C=CCCC3)C2)C=CC=C1	-6.8
185	COC(C1=CC(C2SC=C(CN3C(C#N)=C(C#N)N=C3N)N=2)=CC=C1)=O	-6.8
186	CO[C@@H](C1=CC=C(F)C=C1)CS(NC1C(C(N)=O)=NN(C)C=1)(=O)=O	-6.8

187	C12=CC(Cl)=CC=C1N=C(N=C2C1C=CC=CC=1)Cl	-6.8
188	N1(C2C=CC(=C(Cl)C=2)Cl)C(=O)/C(=C/N2CCN(CC2)C(=O)C2=CC=CO2)/C(NC1=S)=O	-6.8
189	C12C(=CC=NC1=CC(Cl)=CC=2)NNC1=CC=C(C=C1)C(O)=O	-6.8
190	C1(=C/NC2C(C)=CC=C(Cl)C=2)/[C@H]2CC[C@@](C2(C)C)(C)C/1=O	-6.8
191	C1(C(=O)N2CCN(CC2)S(=O)(=O)C2CC2)N=NN(C2=CC=C(C=C2)OC)N=1	-6.8
192	CCN1C(N2CCOCC2)=NN=C1SCN1C2=C(C=CC=C2)N=N1	-6.8
193	CN(CN1N=C(C2=CC=NC=C2)C(N(=O)=O)=C1)CC1SC=C(C(F)(F)F)N=1	-6.8
194	N1=NC2C(=CC=CC=2)N1C/C(/C)=N/NC(=O)C1=CC=C(C=C1)Br	-6.8
195	N1(C2CC2)C(=O)N(N=C1C1=CC=CS1)CCNS(=O)(=O)C1=CC=C(C(Cl)=C1)F	-6.8
196	N1(C(=O)CSC2=NN=C(N/N=C/C3=CC=C(OCC4C=CC(=CC=4)F)O3)N2)C(C)=CC(C)=N1	-6.8
197	C1(/C=N/NC(C2C=CC=CC=2)=O)C=C(SC=1Cl)C1C=CC=CC=1	-6.8
198	ClC1=C(NNC(NC2=NN3C(C=CC=C3)=N2)=O)C(Cl)=CC=C1	-6.8
199	C1(=NC=CN1[C@H]1CCC2=C(C=NN2)C1)C1=CC=C(C2C=CNN=2)S1	-6.8
200	CC1=NC(C)=C(C#N)C(OCC2N=NN(C3=CC=C(Cl)C=C3)C=2)=C1	-6.8
201	C1(SC2C(=CC=C(C)C=2)N=1)NC1OC2=C(C=CC(C)=C2C)N=1	-6.8
202	O=C1/C(=C/NNC2=CC3=C(C=CC=C3)C=C2)/N=C(C2SC=CC=2)O1	-6.8
203	CC(C1N=C(NC(N2CC3C(=C(C=C(C=3)F)F)CC2)=O)SN=1)(C)C	-6.8
204	C1(NC(N)=N[H])NC2C(=CC=CC=2)N=1	-6.8
205	C1(C2=CC=CS2)=NC2(N=C1SCC(=O)NC1C=CC(=CC=1)F)CCCCCC2	-6.8
206	N1(OC2C=CC(=CC=2N(=O)=O)N(=O)=O)C(=O)C2=CC=CC3C=C(O)C=C(C2=3)C1=O	-6.8
207	C1(NC(=O)CN2C=CC3=C(C=C(C(OC)=C3)OC)CC2=O)=NN=C(CC(C)C)S1	-6.8
208	ClC1=CC=C(S(C2=C(N3CCCCC3)OC(/C=C/C3=CC=CC=C3)=N2)(=O)=O)C=C1	-6.7
209	C1(SC2C=CC(=CC=2)Cl)OC(=CC=1Br)/C=N/C1=CC=C(C=C1)Cl	-6.7
210	CCOC(C1=CC=C(NC(CN2C(CC3=C(C)C=C(C(C)(C)C)C=C3C)=NCC2)=O)C=C1)=O	-6.7

211	CC1=C(F)C=C(CS(NC2OC(C3CC3)=NN=2)(=O)=O)C=C1	-6.7
212	N1(C2C(C)=CC=CC=2C)N=NN=C1C(C)(C)/N=C/C1C=CC=C(C=1)N(=O)=O	-6.7
213	C1(SCC(=O)N2CCC[C@@H](C2)C2C(C)=CN=C(SC[C@H]3CCCO3)N=2)SC=C(C)N=1	-6.7
214	CC1=C(Cl)C(C(N2C=C/C(=N\CC(F)(F)F)/C=C2)=O)=CC=C1	-6.7
215	C1(C=COC=1)C1=NC=CN=C1CNC(=O)C1C=CC(=CC=1)N1C=CC=C1	-6.7
216	C1(C(=O)NC(=S)NC2=CC=CC(=C2)CCC(=O)N(C)C)=C(Cl)C2=C(C=C(C=C2)OC)S1	-6.7
217	C(/NC(=O)C1C=C(OC)C(=C(OC)C=1)OC)(\C(=O)NC1=CC=CC=C1)=C\C1=CC=C(C)O1	-6.7
218	C1(C(O)=NC=C(C(OC)=O)C=1O)[C@H](C1C=CC(=CC=1)Br)CC(N)=O	-6.7
219	C1(/N=C/C2=CC=C(C3=CC=C(C(Cl)=C3)F)O2)=NN=CN1	-6.7
220	CS(C1SC=C(C(OC2=C(OCC(F)(F)F)C=CC=C2)=O)C=1)(=O)=O	-6.7
221	[C@H]12C[C@H]1C(=NN=C2C1C=CC(=CC=1)C)O	-6.7
222	CC1=C(F)C=C(CNC(C2=C(N3N=CN=C3)C=C(Br)C=C2)=O)C=C1	-6.7
223	C12C=CC=CC=1NC=C2C[C@H](C(=O)O)NC[C@](O)(C)C#CCCC	-6.7
224	CC1C(CCC(NN2C(=O)C3(CCCCC3)NC2=O)=O)=C(C)ON=1	-6.7
225	N1(C2C=CC(=CC=2)Cl)[C@H](C2=CC=CS2)N(N=C1C(C)=O)C1C=CC(=CC=1)Cl	-6.7
226	C1(NC(CC)=O)=NN=C(SCC2OC=C(C(=O)C=2)OC(=O)C2=CC=CC(=C2)C(F)(F)F)S1	-6.7
227	CN1N=CC(C2=C(C(N3CCC([C@H](C4=CC=C(F)C=C4)O)CC3)=O)C=NO2)=C1	-6.7
228	N1=C(O)[C@@H](S/C/1=N\N=C1\CCCCCC\1)CC(=O)NC1=CC=C(C=C1)OCC	-6.7
229	N12[C@@](O)(CSC1=NC(NCC)=N/C/2=N\CC)NC1C(Cl)=CC=C(Cl)C=1	-6.7
230	C1(C#N)SC2=C(C=CC=C2)C=1OCC1=CC=C(C(Cl)=C1)Cl	-6.7
231	CC(N1N=NC(C2CCN(C(N[C@@H]3C(C)(C)CCC3)=O)CCC=2)=C1)C	-6.7
232	N1(N=C(/C(=C(\C)/OCC)/C1=O)C(F)(F)F)C1SC2=C(C=CC=C2)N=1	-6.7
233	COC1=NC=C(N2/C(=C(\C#N)/C#N)/S/C(=C\C3N(C)N=CC=3)/C2=O)C=C1	-6.7
234	C12C(=O)CC(CC1=N[C@H]1[C@H](CCCC1)NC=2)(C)C	-6.7

235	CNC1SC=C(CNC(NC2=C(Cl)C=C3C(OCCCO3)=C2)=O)N=1	-6.7
236	C[C@@H]1S(=O)(=O)CCN(CC2=NN(C3=CC=CC=C3)C=N2)C1	-6.7
237	N1(C)C(SCN2N=CC(N(=O)=O)=C2)=NN=C1C1=CC=CC(Cl)=C1	-6.7
238	N12C(=O)N(C3C=CC=CC=3)C(=O)N1[C@@H]1CC=C[C@H]2CC1	-6.6
239	C1(C(O)=O)N=C(OC=1SC1=CC=C(C=C1)Cl)C1=CC=CC=C1	-6.6
240	S1C(C2=CC=CN=C2)=NN=C1/N=N/C1C=CC(=CC=1)O	-6.6
241	CC1=C(C2OC(SCC(NC3N(CC4OC=CC=4)C(C)=C(C)C=3C#N)=O)=NN=2)C=CO1	-6.6
242	C1(=CC=C(C)C=C1)S(=O)(=O)OC[C@H](O)CCOS(=O)(=O)C1=CC=C(C)C=C1	-6.6
243	CC(C1SC(CNC(NC2=CC3=C(CCCC3)N=C2)=O)=NN=1)(C)C	-6.6
244	CCN1N=CC(OC(C[C@@H]2C(=O)NC3=C(C=CC(=C3)Cl)S2)=O)=C1	-6.6
245	C12C=C(O)C=CC=1OC=C(/C=C/C(O)=O)C2=O	-6.6
246	N12C(C)=NN=C1C=C(N1CCN(CC1)CC1=CSC3CCCCC1=3)C=N2	-6.6
247	CCC1N=C(N2CCN(CN3C(=O)N(C4=CC=CC=C4)N=N3)CC2)SN=1	-6.6
248	C(=O)(C1=CC=CC(C)=C1)NNC(=O)/C=C/C(O)=O	-6.6
249	CC(NC1=CC(NC(NCCCSC2SC=CN=2)=O)=C(Cl)C=C1)=O	-6.6
250	C1(NC(=O)CN2C(C)=C(C(C(F)F)=N2)Cl)C(C)=NN(C)C=1C	-6.6
251	FC1=CC(F)=C(N2C(=O)C[C@H](C(N3C[C@H](C4=NOC=N4)OCC3)=O)C2)C=C1	-6.6
252	N12C(=O)C3=C(C=CC=C3)[C@@H]1C[C@@]([H])(C1=CC=CN21)O	-6.6
253	CC1OC([C@](C(F)(F)F)(CC(NNC2=NC3=C(C=CC=C3)C=C2)=O)O)=CC=1	-6.6
254	C1(=NNC(SCC)=C1C(OCC)=O)N1C=CC2=C(C=NC3=NC(COC)=NN23)C1=O	-6.6
255	FC1=CC=C(/C=C(/C(NNC(CC2=CN=CC=C2)=O)=O)\C#N)C=C1	-6.6
256	C[S@@](C1N(C2OC3=C(C=C(C=C3)F)N=2)C=NN=1)=O	-6.6
257	N1C(C)=NC(=CC=1N/N=C/C1C=CC(=CC=1OC)OC)C1C=CC=CC=1	-6.6
258	C12N=C(C)S[C@H](C3CCCCC3)C=1C(NN2C(C)C)=O	-6.6

259	S(=O)(=O)(C1=CC=CC2=CC=CN=C12)NC1C2C=CC=CC=2OC=1C#N	-6.6
260	C[C@@H]1CN(S(NC2C(C(F)F)=NNC=2C)(=O)=O)CCC1	-6.6
261	C1(C=C(Br)C=CC=1F)C(=O)C1C=CC(=CC=1)F	-6.6
262	CN1C2=C(C=C(C=C2)F)N=C(COC2=C(F)C(F)=CC(Br)=C2)C1=O	-6.6
263	C1(N/N=C(/C2=CC=CC=C2)\C(C2C=CC=CC=2)=O)=NN=C(C)N1N	-6.6
264	C1(C(CC)=NNC=1N)C1C=CC=CC=1C	-6.5
265	N1(C=COC=C1/N=C/C1=CC=CC=C1)CC1=CC=CC=C1	-6.5
266	[C@]12(CC[C@](C1(C)C)(C)[C@H]2Br)C(=O)O/N=C1\C[C@H]2C(C)(C)[C@]\1(C)CC2	-6.5
267	C(=O)(C(C1=CC=CC=C1)C1C=CC=CC=1)N/N=C(/C)\CCCC	-6.5
268	NC1=NC([C@H](C(C2C=C(Cl)SC=2)=O)C#N)=NC(N)=N1	-6.5
269	C1(=C/C(N)=O)/[C@H]2CC[C@@](C2(C)C)(C)C/1=O	-6.5
270	C1(=CSC(=S)N1NC1C=CC=CC=1)C1=CC=C(Cl)C(C)=C1	-6.5
271	S1(=O)(=O)N(CC2C=CC=CC=2)C2=CC=CC=C2C(=O)/C/1=C\NC1C=CC=CC=1	-6.5
272	FC(C1=NN(COC(OC2CCCCC2)=O)C(=O)C=C1)(F)F	-6.5
273	COC1=C(OCC2=CC=NC=C2)C=C(NC(C2OCCCC=2)=O)C=C1	-6.5
274	S1(=O)(=O)C2=CC=CC=C2N(N=C1C(=O)N1CCCCC1)CC(OCC)=O	-6.5
275	C1(=NC=CN=C1OC1=CC=CC(C(F)(F)F)=C1)/C(/N)=N/OC(=O)C1SC=CC=1	-6.5
276	C1(CC2=CC=C(C(=O)NC3=C(F)C=CC(F)=C3)O2)C(C)=NOC=1C	-6.5
277	O=S(C1C2C(=NSN=2)C=CC=1)(NCC1=NC=C(C2=CC=CC=C2)C=N1)=O	-6.5
278	[C@]12(C(C)C)CC[C@@]([C@@H](OC(=O)NC3C=CC=CC=3)C1)(C)O2	-6.5
279	FC1=C(C2OC=C(CN3C(=O)C4=C(C=CS4)N=C3)N=2)C(F)=CC=C1	-6.5
280	C1(C(OCC)=O)SC(=NC=1CSC1N=C(C(F)F)C=C(C)C=1C#N)NC1CC1	-6.5
281	FC(C1N=C(CN2C[C@H](S(NC3CCCC3)(=O)=O)CCC2)ON=1)F	-6.5
282	N1(CC[C@@H](OC2C=CC(C)=NN=2)C1)C(=O)C1C=COC=1	-6.5

283	C1(NC2C=CC(=CC=2)F)C(=O)C(C=1C1=CC=C(C=C1)C(C)C)=O	-6.5
284	CSCCNC(NNC(C1C(C2SC(C)=CC=2)=CNC=1)=O)=S	-6.5
285	CC1C(/C=C2/C(=O)N=C(NC3=C(C)C=CC(C)=C3)S/2)=C(C)NN=1	-6.5
286	N1(C2=CC=C(C=N2)F)C2C=CN=C(C)C=2N=C1	-6.5
287	FC1=C(Cl)C=C(CS(NCC2OC3=C(C=CC=C3)C=2)(=O)=O)C=C1	-6.5
288	CN1C2=C(C=CC=C2)C(/C=C/C(NCCCS(CC2=CC=CC=C2)(=O)=O)=O)=C1	-6.5
289	FC(C(NC1(C2N3C(=NCC3)SC=2)CCCCC1)=O)(F)F	-6.5
290	C[C@@H](CS(C)(=O)=O)CSC1=C2C(C=CC=C2)=NC(C(F)(F)F)=N1	-6.5
291	CN1[C@H](CCN2C(=O)OC(C3=CC=C(F)C=C3)=N2)CCCC1	-6.5
292	COC1=C(C2SC=C(CSC3OC(C4OC=CC=4)=NN=3)N=2)C=C(Br)C=C1	-6.5
293	CC1=C(C)N=NC(OCC2OC(C3=CC=CC=C3)=CN=2)=C1	-6.5
294	CCCC1N=C(/C(/CC)=C/C2=CN(CCCl)N=C2)NC(=O)C=1	-6.5
295	N1=C(NC2=CC=C(C(OC)=C2)OC)ON=C1C1=CC=C(C=C1)OC	-6.5
296	CCN1N=CC(C2CCN(CN3C(=S)NN=C3CC3SC=CC=3)CC2)=C1	-6.5
297	CCN1C2=C(C=C(C=C2)C#N)N=C1NC(CC1=C(Cl)C=CC=C1F)=O	-6.5
298	CCCOC1=CC(CCNC(N2CCN(C3=NN=CC=C3)CCC2)=O)=CC=C1	-6.5
299	C12C=C(C=CC=1C(=O)C1=C(C=CC=C1)C2=O)OC(C)=O	-6.5
300	C(C1O[C@@H]2C(=O)C3=C(C(=O)[C@H]2C=1)C=CC=C3)(=O)C	-6.5
301	O=C(C1C(=O)OC2=C(C=CC=C2)C=1)NNC(NCCC1SC=CC=1)=S	-6.4
302	C1S[C@H](C2=CC=C3OCOC3=C2)C2C=NNC=2NC1=O	-6.4
303	C1(C#N)=C(C=CC2C=CC=CC=2O)C(O/C/1=C(/C#N)\C#N)(C)C	-6.4
304	FC(COCCNC(NNC1=C(Br)C=C(F)C=C1)=O)F	-6.4
305	N1(C(CC)=O)/C(=N/C2C=CC=CC=2C)/SC(C)=C1OC(CC)=O	-6.4
306	N12C(=O)[C@@H](N=C1C1=C(C=C(C(OC)=C1)OC)NC2=S)CCC(OC)=O	-6.4

307	N1=C(N)N[C@@](C2=CC=C(C)C=C2)(CC2=CC=CO2)C1=O	-6.4
308	C12=CC=C(Br)C=C1C(=N[C@H](OC(=O)C)C(=O)N2CC(=O)OC)C1C=CC=CC=1	-6.4
309	C1(=CSC=C1C1=CC(C)=NC(F)=C1)C(F)F	-6.4
310	C1(CN)C(C)=NOC=1C1C=CC2=C(C=1)OC(N2)=O	-6.4
311	CCC([C@@H]1OCC[C@H](NC(/C=C/C2OC(C(C)C)=NN=2)=O)C1)CC	-6.4
312	C1(C=C(C(O)=C(C(C)(C)C)C=1)C(C)(C)C)[C@@H]1NN=C(C2C=CC=CC=2)S1	-6.4
313	C1(C)C=CC(S(=O)(=O)NN2CCS(=O)(=O)CC2)=CC=1	-6.4
314	C12N(C3C=CC(=CC=3)C)CCN1C(C(=O)N(CC(NCCC1C=CC=CC=1)=O)N=2)=O	-6.4
315	FC1=C(F)C=C(NNC(C(NC2=CN=C(C3CC3)N=C2)=O)=O)C(F)=C1	-6.4
316	O=N(C1=C2C(C=CC=C2)=C(OC2=C(F)C(F)=NC(F)=C2F)C=C1)=O	-6.4
317	C1(=O)N(N(C)C)C=CC2N=C3C=CN(CCC4CCCCC=4)C(=O)C3=CC1=2	-6.4
318	S(C1C=CC=CC=1)(=O)(=O)/C(/C#N)=C(/SCC1=CC=CC(C)=C1)\NC1C(C)=CC(=CC=1C)C	-6.4
319	C1(=CC=C(Br)S1)[C@](CN)(O)C1=CC=CC(F)=C1	-6.4
320	C1(=C(/NCC2C=CC=CC=2)\NCC2C=CC=CC=2)/C(=O)C2C(=CC=CC=2)C/1=O	-6.4
321	CCN(C1=C(C)C=CC=C1)CCNC1=C(N(=O)=O)C=C(S(C)(=O)=O)S1	-6.4
322	O=C(C1=CC=CC=C1)N/N=C1/NN2C(=NN=C2)C=C/1	-6.4
323	ClC1=NC=C(NS(C2CCOC3=C(C=CC=C3)C=2)(=O)=O)C=C1	-6.4
324	COC(C1=C(C)C(C(O)=O)=C(S(NC2=CC3=C(N4C(=N3)CCCCC4)C=C2)(=O)=O)S1)=O	-6.4
325	C12N=NC(=C(C)N1N=C(C(F)(F)F)N=2)C(OCC)=O	-6.4
326	CC1=C(COC(C2CCN(C(N3CCCC3)=O)CC2)=O)C=CO1	-6.4
327	CC[C@H](N1N=C(C2=CC=C(Cl)C=C2)N=N1)C(OCC1=NC(C)=NC(C)=C1)=O	-6.4
328	N(C1C=C(C(=CC=1C)[C@H](C1C=CC(=CC=1)Cl)C#N)Cl)(=O)=O	-6.3
329	CCN(CC(F)(F)F)C[C@@H]1CN(CC2N(C(F)F)C=CN=2)CC1	-6.3
330	C1(=CC=C(C(C)(C)CN)N1)C1C=C(Br)C=CC=1F	-6.3

331	O=S(/C=C/C1=CC=CC=C1)(OC1=C2C(OCCO2)=CC=C1)=O	-6.3
332	N1=C(N=C(CC(=O)OCC)N=C1N1CCOCC1)OC1C=CC(OCC)=NN=1	-6.3
333	CCOC(/C=C1/N(CCOC(CCC2C(=O)NC(=O)NC=2C)=O)C(=O)CS/1)=O	-6.3
334	CN1[C@H](C2ON=C(C)N=2)CN(C2C(=O)N(C(F)F)C=CN=2)CC1	-6.3
335	C1(=NON=C1N)N(CC1C=CC=CC=1Br)/N=N/C1=NON=C1N	-6.3
336	COC1=CC(N(=O)=O)=C(NNC(C2=C(C(C)(C)C)N=NS2)=O)C=C1	-6.3
337	N(/C1C=CC(=CC=1)C(C)(C)C)=N\C1C=CC(=CC=1)C(C)(C)C	-6.3
338	CC1=CC=C(SC2=NN=C(SC3=CC=C(C)C=C3)C=C2)C=C1	-6.3
339	O=N(C1=CC(S(NC2=NC=C(Br)N=C2)(=O)=O)=CC(F)=C1)=O	-6.3
340	CC1CN(C(NC2=NC=C(Br)C(N3CCOCC3)=C2)=O)CCC=1	-6.3
341	CCN(CC1=C(OC(F)(F)F)C=C(F)C=C1)CC(NC(C)C)=O	-6.3
342	ClC1=C(N2CCSCC2)C=CC(NC(NOCC2=CN=CC=C2)=O)=C1	-6.3
343	N[C@H]1[C@@H]2C[C@@H](CC2)[C@H]1C(NC1=CC(I)=CC=C1)=O	-6.3
344	O=S(C1=CC=CC=C1)(N(C1SC=CN=1)CC1ON=C(C2=COC=C2)N=1)=O	-6.3
345	[N+]12CC(=CSC=1N(C1C=CC=CC2=1)CC1=CC=CC=C1)C	-6.3
346	C(=O)(N/N=C/C1C=C(CC=C)C(=C(OCC)C=1)O)NC1C=CC=C(Cl)C=1	-6.3
347	N1C(/C=C/C=C2\C(C)=CC(C)=[NH+]\2)=C(C)C=C1C	-6.3
348	C1(C(=O)/N=C2\SC=C(C(OCC)=O)N\2)=CC(=NN1C)C1=CC=CC=C1	-6.3
349	OC(C1SC(/C=C/C2C=CC(F)=C(N(=O)=O)C=2)=NC=1)=O	-6.3
350	FC(OC1=CC2=C(C=C(S(OC3=C(F)N=CC=C3)(=O)=O)CC2)C=C1)F	-6.3
351	S(=O)(=O)(C1C(C)=CC(=C(C)C=1)C)N1CCN=C1N1CCCCC1	-6.3
352	C1(C(Cl)=CC=CC=1Cl)C(=O)/N=C1\NCCN\1	-6.3
353	NC1(C2N=C(C3ON=C(C4C=CC=CN=4)C=3)ON=2)CCC1	-6.3
354	O=C(OC1=C2C(C=CC=C2)=CC=C1)CC1C2=C(C=CC=C2)ON=1	-6.3

355	CC(CCC1=CC=C(OC2=NC(N)=NC(Cl)=C2)C=C1)=O	-6.3
356	CCOCCN(CN1C(=S)N(C2=C(Cl)C=CC=C2)C(N2CCCC2)=N1)C	-6.3
357	C1(/C=C/C2=CC=CO2)N(CCOC2C=C(C)C=C(C)C=2)C2C(=CC=CC=2)N=1	-6.3
358	N1(C(S)=NN=C1[C@H](CC)N1C=C(C=N1)Cl)C1C=NN(CC2=CC=C(C=C2)C)C=1	-6.3
359	N1(C2=NC=CC=N2)C(Cl)=NC(C2=CC=CC(OC)=C2)=N1	-6.3
360	O=C(C1N(C2=CC=CC=C2)N=C(C2CC2)C=1)N=S1(CCCC1)=O	-6.3
361	FC([C@@H](C1=NC=CC=C1)OC([C@@H]1ON=C(C2=CC=CC=C2)C1)=O)(F)F	-6.3
362	O=S(OC1=CC=C(N2N=NN=C2)C=C1)(CC1C2=C(C=CC=C2)ON=1)=O	-6.3
363	COC(C1=CC(NS(CC2=CC(F)=C(C)C=C2)(=O)=O)=C(Cl)C=C1)=O	-6.3
364	O=S(C1=CN=C(C#N)C=C1)(NC1OC(C2=CN(C3=CC=CC=C3)N=C2)=NN=1)=O	-6.3
365	N1=C(C)C[C@H](CNC(=O)NC2=CC=C(C=C2F)F)O1	-6.3
366	FC1=C(NNC(CCCCC2N=NNC=2)=O)C(F)=CC=C1	-6.3
367	C1(SCCNC(=O)C2C=C(C)NC(=O)C=2)=NN=NN1C	-6.3
368	O=S(CC1C2=C(CCC2)N(C2=CC=CC=C2)N=1)(CC1SC=CN=1)=O	-6.3
369	CC1C(C(N2C[C@H](CN(S(=O)(=O)C)CC(=O)O)OCC2)=O)=CSC=1	-6.3
370	[C@H]12[C@@H](C3=CC=CS3)N(O[C@H]1C(N(CC)C2=O)=O)C1C=CC=CC=1	-6.2
371	P(CO)(=O)(C1C=CC(=CC=1)Cl)C1C=CC(=CC=1)Cl	-6.2
372	O=C(C1C=CC2N(CCS(N=2)(=O)=O)C=1)NC1C(C2=CC=CC=C2)=NNC=1	-6.2
373	C1(=C(N/N=C/C2CCCCC=2C#C)C=CC(N(=O)=O)=C1)N(=O)=O	-6.2
374	N1(C)C(F)=C(/C=N/NC(=O)COC2C=CC(=CC=2F)F)C(C)=N1	-6.2
375	N1(C(=O)/C=C/C2=CC=CO2)C=NC(C2C=CC=CC=2)=N1	-6.2
376	COC1=CC=C(N(C(COC2=CC=C(C3OC=NN=3)C=C2)=O)CC2SC=CC=2)C=C1	-6.2
377	C1(C(=O)NC2=CC=C(C=C2)OC)=NOC2C3=C(SC=C3)CCC1=2	-6.2
378	C1(N/N=C/C2C=CC(=CC=2Cl)Cl)C(Cl)=C(Cl)C(=C(Cl)N=1)C#N	-6.2

379	ClC1=NC=C(C(NC2CCN(S(CC3=CC=CC=C3)(=O)=O)CC2)=O)N=C1	-6.2
380	N1(CNC2C(=NC=NC1=2)N)[C@@H]1O[C@H]([C@H](OC(C)=O)[C@@H]1OC(C)=O)COC(C)=O	-6.2
381	CN1C(=S)N[C@@H](C2N=C(C3=CC=C(Cl)C=C3)SC=2)C(C(NC2=NOC(C)=C2)=O)=C1C	-6.2
382	O=S(C1NC=CN=1)(CC1=C2C(OCCO2)=CC=C1)=O	-6.2
383	S(=O)(=O)(NC1=CC=C(C=C1)N(=O)=O)[C@@H]1CCS(=O)(=O)C1	-6.2
384	O=C(N1CCN(C2NN=C(C3CC3)C=2)CC1)CSC1N2C(C=CC=C2)=NN=1	-6.2
385	CC1=CC(S(NC2=C(N3N=CC=C3)N=CC(Br)=C2)(=O)=O)=CC=C1	-6.2
386	C1C(CO)=CC=C2[C@H]3C[C@H](C=C3)C2=1	-6.2
387	C1(Cl)C(=O)NN=CC=1N/N=C\[C@@H]1CCC=CC1	-6.2
388	CC1SC(C(NNS(C2=C(C(F)(F)F)C=CC=C2)(=O)=O)=O)=CC=1	-6.2
389	O=C(O[C@H](C1=CC=CC=C1)C1SC=CN=1)CCC1OC(C2=CC=CC=C2)=NN=1	-6.2
390	ClC1=CC=C(SC2=C(NC(COC(CC3=CSC=C3)=O)=O)C=CC=C2)C=C1	-6.2
391	CC1([C@H](OCC2=CC=CC=C2)C[C@@H]1NS(NCC(F)(F)F)(=O)=O)C	-6.2
392	S(=O)(=O)(CCOC1=CC=C(C=C1)F)NC1=NC=CC=N1	-6.2
393	COC(C1=CC(C2N=C(C3OCCOC=3)ON=2)=CC=C1)=O	-6.2
394	CC(OC(N[C@@H]1CN(CCOC2=CC(N(=O)=O)=CC=C2)CC1)=O)(C)C	-6.2
395	C1(SC2=CC=C(/C=N/NC(=O)C3=CC=CC=C3N(=O)=O)O2)SC2=C(C=CC(OCC)=C2)N=1	-6.2
396	C1(N)N(CCO)N=C(CCC2CCCCC2)C=1N	-6.2
397	C=CCN1C2=C(C=CC=C2)N=C1SCC1N=C2N(C=CS2)C=1	-6.2
398	O1C=CN=C1C(=O)C1C=C(F)C(F)=C(F)C=1	-6.2
399	C12NCCCN1C=C(C1=CC=C(C=C1)CCC)N=2	-6.2
400	CC1=C2C(CCCC2)=NC(NS(C2=CN(C3=C(F)C=CC=C3)N=C2)(=O)=O)=N1	-6.2
401	C(F)(F)(F)C1C=CC=C(C=1)C(=O)N/N=C/C=C/C1=CC=CO1	-6.2
402	C[C@H](C(NNC1=NC2=C(C=CC=C2)N=C1)=O)SC1SC2=C(C=CC=C2)N=1	-6.2

403	CCC1=C(CC)C=C(NC(CCN/C(/O)=C2\C(=O)C=CC=N\2)=O)C=C1	-6.2
404	CC1=CC(C)=C(C[S@](CC(NCCOC2=CC(F)=CC=C2)=O)=O)C(C)=C1	-6.2
405	ClC1=C(NC(CN2CCN(CC3=NOC=C3)CC2)=O)C=C2C(OCCO2)=C1	-6.2
406	C12SC(=CC=1C(OC(C1=CC=C(C=C1)C(C)(C)C)=N2)=O)C	-6.2
407	C1(C(OC)=O)SN=C(C2=CC=C(C=C2)F)C=1N	-6.2
408	CC1N(C)C=C(C(/C=C/C2=CC(C)=C(OC(F)F)C(C)=C2)=O)N=1	-6.2
409	CC1N(C)C(CNC2=C(Cl)C=C(F)C(Br)=C2)=NN=1	-6.2
410	CN1C([C@@H]2[C@@H](NC(NC[C@@H]3SCCCC3)=O)CCCO2)=NC=C1	-6.2
411	O1[C@@H]2CO[C@H]1C(C[C@@H]2SC1C(C)=CC=C(C(C)(C)C)C=1)=O	-6.2
412	CNC(C1=CC=C(CN(CN2C(=O)C3=C(N(N=C3)C)N=N2)C)C=C1)=O	-6.2
413	CS(CC1(CC1)CC(OC1=C(C2=CC=CC=C2)C=CC=C1)=O)(=O)=O	-6.2
414	ClC1C=CC2N(CC3=C(/C(/N=2)=N\C(C2SC=CC=2)=O)C=CC=C3)C=1	-6.2
415	CC(C1=CC=C(C2SC(CSCC3N(C)C=NN=3)=CN=2)C=C1)C	-6.2
416	FC(C1=CN=C(NNC(C2SC=C(Br)N=2)=O)C=C1)(F)F	-6.2
417	N1(C2=CC=CC=C2Cl)C(C)=CC(C)(C)N=C1S	-6.1
418	C1(NC2C=CC(=C(N)C=2)OC)NCCN=1	-6.1
419	CC1N(CCN2C3=C(C=CC=N3)OC2=O)C(Br)=C(N(=O)=O)N=1	-6.1
420	CN1N=CC(C(NC2=CC(OS(C3OC=CC=3)(=O)=O)=CC=C2)=O)=C1	-6.1
421	O=C(C1C(C#CC2C=CC=CC=2)=CC=CC=1)OCC	-6.1
422	CC1=C2C(CCCN2S(C2=C3N(CCCO3)N=C2)(=O)=O)=CC(Cl)=C1	-6.1
423	O=C(NNC(NCC1=CC=CC=C1)=S)CSCC1=CC=C(C#N)C=C1	-6.1
424	S(C1C=CC=CC=1)(=O)(=O)/C(/C#N)=C(/[H])\C1=CC=C(C2C=CC(=CC=2)C(OCC)=O)O1	-6.1
425	C12N=CC=CC=1N=NN2OCC(=O)NC1=CC=C(Cl)C=C1	-6.1
426	C[C@@H](N1N=CN=C1)C(NNC(C1=CC(N(=O)=O)=CC=C1)=O)=O	-6.1

427	N1(CC(C)C)C(=O)/C(/N=C1SCC(=O)NC1SC2=C(CCCC2)C=1C(OC)=O)=C\C1=CC=C(C)S1	-6.1
428	CC1=C(OS(C2=C(Cl)N(C)C=N2)(=O)=O)C=CC(N(=O)=O)=C1	-6.1
429	CN(C1=NC(COC(C2=C(S(N3CCSCC3)(=O)=O)C=CS2)=O)=NC(N)=N1)C	-6.1
430	S(C1C=CC=CC=1)(=O)(=O)/N=C1\SC(=C(C(=O)N[C@@H](CCSC)C(OC)=O)N\1)C	-6.1
431	BrC1=CC=C(C2=NC(CS(C3SC=CC=3)(=O)=O)=CC=N2)C=C1	-6.1
432	N1(N(/C(=N/C(=O)C2C=CC(C(C)(C)C)=CC=2)/N=N1)C(C1C=CC(C(C)(C)C)=CC=1)=O)CCCC	-6.1
433	C1C=CC([C@@H]2C(C(OC)=O)=C(C)NC(C)=C2N(=O)=O)=C(C(F)(F)F)C=1	-6.1
434	C1(S(CCC)(=O)=O)=C(C(=O)C2C=CC(=CC=2)OC)N2C(C(C)=CC(C)=C2)=C1S(CCC)(=O)=O	-6.1
435	C1(N(=O)=O)=C(C=CC2=NSN=C12)SC1N=NN(C2CCCCC2)N=1	-6.1
436	C(=S)(N1CCOCC1)N[C@H](C(Cl)(Cl)Cl)NC(=O)C1=CC=CC2C=CC=CC1=2	-6.1
437	C1(N(C)C)=NC(OCCNC(=O)NC2C=CC=CC=2)=NC(OC)=N1	-6.1
438	CC1=CC(OCC2ON=C(C3=NC=CN=C3)N=2)=C(F)C=C1	-6.1
439	S(N)(=O)(=O)[C@H]1CCOC2C(=CC(Cl)=CC1=2)Cl	-6.1
440	N1C(=CSC=1NC1C=CC(OC)=CC=1OC)C1C=COC=1	-6.1
441	N1(/N=C/C2=CC=C(C(COC3C=CC=C(Cl)C=3Cl)=C2)OC)C(S)=NN=C1C(F)F	-6.1
442	CC(N1C=C(S(NC2SC(CC3=CC=CC=C3)=CN=2)(=O)=O)N=C1)C	-6.1
443	CCCC(N1[C@@H](C(NCCN2CC=C(C)CC2)=O)CCC1)=O	-6.1
444	C1(C(=O)C2C=CC3=C(OCCO3)C=2)=CC2=C(C(C)=NC=C2CNCCOC)O1	-6.1
445	NC1=NC(N2N=CC=C2)=CC(NCC2CCOCC2)=N1	-6.1
446	CN(S(/C(/C#N)=C\C1=CC2=C(CCC2)C=C1)(=O)=O)C	-6.1
447	COC1=C(OC2SC(N(=O)=O)=CN=2)C=CC(/C=C/C)=C1	-6.1
448	CCCCN1N=C(C)C(C(OC[C@@H]2ON=C(C3=CC=CC=C3)NC2)=O)=C1	-6.1
449	CN(S(C1=CC2=C(N=NN2OCC2N(C(F)F)C=CN=2)C=C1)(=O)=O)C	-6.1
450	CSCC[C@@H](C1NC2=C(C=CC=C2)N=1)NC(/C(/F)=C(\C)/C)=O	-6.1

451	CN1C(=O)C(Br)=CC(NC(NCC2N3C(C=CC=C3)=NN=2)=O)=C1	-6.1
452	CC1=CC(C)=C(OC[C@@H](CN2CCN(C/C=C/C3=CC=CC=C3)CC2)O)C=C1	-6.1
453	O=N(C1=CC(/C=C/C(O[C@@H](C(F)(F)F)[C@@H]2OCCC2)=O)=CC=C1)=O	-6.1
454	ClC1=NC(=C2C(=N1)N(C=N2)[C@H]1[C@@H]([C@@H]([C@@H](CO)O1)F)O)N	-6.1
455	C[C@@H](C1=CSC=C1)NCC1=C(OC2=CC(F)=CC=C2)N=CC=C1	-6.1
456	IC1=C(C(N2C[C@H]3N(CCOC3)CC2)=O)C=NN1	-6.1
457	CCN1C(=O)NN=C1SCC(C1SC(N2CCCCC2)=NC=1)=O	-6.1
458	C1(SCCCN=1)NC1=C(CC)C=CC=C1C	-6.1
459	C1(CN(CC2=CC=CC=C2)CN(C2C=CC(=CC=2)C(O)=O)N=1)N(=O)=O	-6.1
460	S(=O)(=O)(C1C=CC(=CC=1)C)/N=C(/C1=CC=C(C=C1)Cl)\NC(OCC)=S	-6.1
461	S1(=O)(=O)N=C(C2=CC=CO2)C=C(C(=O)NC2=CC=CC=C2C(OC)=O)N1C	-6.1
462	FC(C1=CC=C(C#CCNCC2=NNC=C2)C=C1)(F)F	-6.1
463	CN(C1=CC=C([S@](C)(=NC(C2=NC=C(C)N=C2)=O)=O)C=C1)C	-6.1
464	N1(C(C)=C(N=N1)/C(/C)=N/N=C(\C)/C1=CC=C(C=C1)N(=O)=O)C1=NON=C1N	-6.1
465	N1(CC)C(=O)/C(/NC1=O)=C\C1=CC(Cl)=CC(I)=C1O	-6.1
466	C(/C#N)(\C(N)=O)=C(\O)/C(/O)=C\C(=O)C1=CC=C(C=C1)Cl	-6.1
467	CN1C(=O)N(C)C(=O)C(C#N)=C1NCCC1N2C(CCCC2)=NN=1	-6.1
468	CC[C@H](OC1=C(/C=C/C(OCCC2=NC=CN=C2)=O)C=CC=C1)C	-6.1
469	C1(/C=N/NC2SC3=C(C=CC=C3)N=2)C(C)=NN(CCO)C=1C	-6.1
470	C(F)(F)(F)C1=CC=CC=C1NC(=S)NN1C=NN=C1	-6.1
471	C1(=NSC(O)=C1N)NC1C=CC(Cl)=CC=1Cl	-6
472	C/C(/C)=C(/C(NNC1ON=C(C2=CC=NC=C2)N=1)=O)\F	-6
473	N1(NC(=O)NS(=O)(=O)C2C=CC(=CC=2N(=O)=O)Cl)C(C(C)(C)C)=NN=C(SC)C1=O	-6
474	FC1(CCC(C(OCCOC2=NC(Cl)=CN=C2)=O)CC1)F	-6

475	COC1=C(C2OC(C[S@@](CC3=C(Cl)C=CC(Cl)=C3)=O)=NN=2)C=CC=C1	-6
476	CCS(CCCCCN1N=C(C2=CC(C)=C(F)C=C2)N=N1)(=O)=O	-6
477	CCOC(C1=NNC(NC(C2SC3=C(COCC3)C=2)=O)=C1)=O	-6
478	C12C3=CC=CC=C3SCC=1C=C(C(NCCCN(C(C)C)CC1=CC=CC=C1)=O)S2	-6
479	N1C2=CC=CC=C2CC[C@@H](SCCC(=O)NC2=CC=CC3=C2C=CC=N3)C=1O	-6
480	S1(=O)(=O)C[C@@H]2[C@H](C1)N(C(=O)S2)C1=CC=C(C=C1)C	-6
481	CC1=CC=C(C)N1C1SC=CC=1C(=O)O	-6
482	C[C@@H](C1=CC(F)=CC=C1)C(N1OCCC1)=O	-6
483	CC1=NOC([C@@H]2N(S(C3N(C)N=C(C)C=3C(F)F)(=O)=O)CCC2)=C1	-6
484	C1(=C(CCC)C=NC(C)=N1)N1CCN(CC1)C/C(/C)=C/C1=CC=CO1	-6
485	S(F)(=O)(=O)C1C=CC=CC=1NC(=O)C(F)(F)F	-6
486	CC1=C(O)C(NC(/C=C/SC2=CC=CC=C2)=O)=CC=C1	-6
487	S(C1=CC=CC=C1)(=O)(=O)[C@H]1CCCCCC/C/1=N\O	-6
488	O=C(C1=C(CO/C(=N/O)/N)CS[C@@]2([C@H](NC(=O)/C(=N\OC)/C3OC=CC=3)C(=O)N12)[H])O	-6
489	C1(ON=C(C2C=CC=CC=2Br)C=1)S(F)(=O)=O	-6
490	C1(=O)N(CC2C=CC=CC=2)C=CN(CC(O)=O)C1=O	-6
491	C12C(C)=CC(=NC=1SC(C#N)=C2/N=C/C1C=CC(=CC=1)Br)C	-6
492	CC1OC(COC(/C=C/C2=CC(F)=CC=C2)=O)=NC=1	-6
493	C1(C(C)=NON=1)NC(=O)C1N=CN=C(N2CCCC2)C=1	-6
494	OC[C@H]1C=C[C@@H](NC(NCC2(C3=CC=C(F)C=C3)CC2)=O)C1	-6
495	NC(NC(OCCCSCC1=C(Cl)C=CC=C1)=O)=O	-6
496	CSC1=CC(NC(CN2C(=O)C3=C(C=CC=C3)S2)=O)=CC=C1	-6
497	CC(C1=CC(C(C)C)=C(S(N2C(C)=C(SC3=CC=CC=C3)C(C)=N2)(=O)=O)C(C(C)C)=C1)C	-6
498	O=C(C1SC(S(C2=CC=CC=C2)(=O)=O)=CC=1)NCC1=COC=C1	-6

499	COCCNC(CN1CCN(CN2C(=S)SC(NC3=C(C)C=CC=C3)=N2)CC1)=O	-6
500	N1(C2C=CC(=CC=2)C)C(=O)/C(=C(\C)/NCCO)/C(=NC1=O)O	-6

Table S3. K_{DEEP} machine learning results from second virtual screening

#	SMILES	pK$_d$
1	N1(C(S)=NN=C1[C@H](CC)N1C=C(C=N1)Cl)C1C=NN(CC2=CC=C(C=C2)C)C=1	7.14
2	CCOC(/C=C1/N(CCOC(CCC2C(=O)NC(=O)NC=2C)=O)C(=O)CS/1)=O	7.12
3	**C1(C#N)=C(SCC(OC)=O)NC([C@H](C21CCCCC2)C1SC=C(C2=CC=CC=C2)N=1)=N[H]**	**7.03**
4	C1(C(OCC)=O)SC(=NC=1CSC1N=C(C(F)F)C=C(C)C=1C#N)NC1CC1	6.97
5	N1=C(C2CC2)ON=C1C1=CC=CN=C1SCC(=O)N1CCN(CC1)C1CCN(CC1)C	6.86
6	CC(C1C2=C(N=CC(C(OCCCC3=NN4C(N=C(C=C4C)C)=N3)=O)=C2)ON=1)C	6.84
7	C1(=NNC(SCC)=C1C(OCC)=O)N1C=CC2=C(C=NC3=NC(COC)=NN23)C1=O	6.74
8	C1(C(=O)N(C)CC2SC=CN=2)C(OC)=CC(N2CCN(CC[C@H](C)C3=CC=C(C)O3)CCC=12)=O	6.74
9	C(/NC(=O)C1C=C(OC)C(=C(OC)C=1)OC)(\C(=O)NC1=CC=CC=C1)=C\C1=CC=C(C)O1	6.72
10	N12N=NN=C1NC(C1C=CC(=CC=1)C(C)C)=C[C@@H]2C1C=CC=C(OC)C=1OC	6.71
11	C1(SCC(=O)N2CCC[C@@H](C2)C2C(C)=CN=C(SC[C@H]3CCCO3)N=2)SC=C(C)N=1	6.70
12	C1(/NC2=C(C)C=C(C=C2C(C)=N/1)C)=N\C1NCN(CN=1)CC1=CC=CC=N1	6.69
13	N12[C@@](O)(CSC1=NC(NCC)=N/C/2=N\CC)NC1C(Cl)=CC=C(Cl)C=1	6.69
14	N1(CCC(=O)NC2C=CC(=CC=2)S(=O)(=O)NC2ON=C(C)C=2C)C(=O)C2=C(C=CC=C2)C1=O	6.69
15	C1(C(O)=NC=C(C(OC)=O)C=1O)[C@H](C1C=CC(=CC=1)Br)CC(N)=O	6.65
16	C=CCN1C2=C(C=CC=C2)N=C1SCC1N=C2N(C=CS2)C=1	6.64
17	C(C1=NOC(C2SC=CC=2)=C1)N1[C@H](C2=CC=CC=C2)C2N(C=CC=2)CC1	6.63
18	CC1C(/C=C2/C(=O)C3=C(C=CC(N(=O)=O)=C3)CC/2)=C(OC2=CN=CC=C2)N(C)N=1	6.60
19	CNC1SC=C(CNC(NC2=C(Cl)C=C3C(OCCCO3)=C2)=O)N=1	6.59
20	**C12N=C(O)C[C@@H](C3C=CC(=C(Cl)C=3)O)C=1C(=NN2C1C=CC(=NN=1)O)C**	**6.58**
21	**[C@@]12(/C=N/C3C=CC=C(C)C=3)C3C=CC=CC=3[C@@H]([C@H]3[C@@H]1C(=O)N(C3=O)C1C=CC(=CC=1)OC)C1C=CC=CC2=1**	**6.56**
22	CN1C2=C(C=C(C=C2)Cl)N=C1NS(/C=C/C1=CC=CC=C1)(=O)=O	6.54

23	C12C(N)=C(C(=O)OCC)OC=1N=C(C1C=CC(Cl)=CC=1)C=C2C(F)(F)F	6.51
24	CCN1C2=C(C=C(C=C2)C#N)N=C1NC(CC1=C(Cl)C=CC=C1F)=O	6.51
25	C1(C(=O)NC(=S)NC2=CC=CC(=C2)CCC(=O)N(C)C)=C(Cl)C2=C(C=C(C=C2)OC)S1	6.50
26	C1([C@H](C([C@H]([C@@H](C(=O)OC)C=1O)C1C=CC=CC=1F)(C#N)C#N)C1=CC=C(C=C1)C)C(=O)OC	6.50
27	CC1N(CCN2C3=C(C=CC=N3)OC2=O)C(Br)=C(N(=O)=O)N=1	6.49
28	C12N(C3C=CC(=CC=3)C)CCN1C(C(=O)N(CC(NCCC1C=CC=CC=1)=O)N=2)=O	6.49
29	C1(=NC=CN1[C@H]1CCC2=C(C=NN2)C1)C1=CC=C(C2C=CNN=2)S1	6.49
30	C1(C2=CC=NC(C)=N2)=C(C)N=C(C2CCN(CC2)C(=O)C2=CC=NO2)S1	6.48
31	N12C(=O)[C@@H](C3C=CC=CC=3Cl)SC(C(N)=O)=C1/C(/C(N)=C2C(OCC)=O)=C/C1=CC=CC=C1Cl	6.46
32	S(=O)(=O)(C1C=CC2=C(CCCC2)C=1)NC1C=CC=CC=1SCC1=CC(=O)N2C(C=CC(C)=C2)=N1	6.46
33	N12C(=O)C=C(N=C1NC(NC[C@@H]1CCCO1)=N[C@H]2[C@@H]1CCC=CC1)C	6.45
34	C1(NC(=O)CN2C=CC3=C(C=C(C(OC)=C3)OC)CC2=O)=NN=C(CC(C)C)S1	6.44
35	CCOCCN(CN1C(=S)N(C2=C(Cl)C=CC=C2)C(N2CCCC2)=N1)C	6.43
36	N1(N(C)C(=C(/C=N/N=C(/NC2=NC=CC=C2)\C2=NC=CC=C2)C1=O)C)C1=CC=CC=C1	6.35
37	C[C@@H]1CN(S(NC2C(C(F)F)=NNC=2C)(=O)=O)CCC1	6.35
38	ClC1=C(Cl)C=C(CN(C(C2OCCOC=2)=O)CC2=NC=CC=C2)C=C1	6.34
39	N12N=C(C3C=CC(=CC=3)F)CSC1=NC1=C(C(C)=C(S1)C(=O)NC1C=C(C)C=C(C)C=1)C2=O	6.34
40	CN1C2=C(CC[C@@H](C3ON=C(C4(C5=C(F)C=C(F)C=C5)CCCCC4)N=3)C2)N=N1	6.34
41	CCS(CCCCCN1N=C(C2=CC(C)=C(F)C=C2)N=N1)(=O)=O	6.34
42	C1(C(=O)N2CCC(CC2)C(=O)NC2=CC=CC(F)=C2)N=NN2C=C(C)NC(=O)C=12	6.33
43	CC[C@@H]1N(C(C2C=C3S(NC4N(C3=CC=2)N=CN=4)(=O)=O)=O)CCCC1	6.32
44	C1(C2C[C@H](C3=CC=C(C=C3)OC)SC3C=CC=CC=3N=2)C(=O)N(C)C(N(C)C=1O)=S	6.31
45	C12C(=O)CC(CC=1NC1=C(C=CC=C1)S[C@@H]2C1C=CC(=C(Cl)C=1)Cl)(C)C	6.30
46	CCCC1N=C(/C(/CC)=C/C2=CN(CCCl)N=C2)NC(=O)C=1	6.29

47	C1(/S[C@@H](C(=O)N/1CC)CC(=O)NC1=CC=C(C=C1)Cl)=N\S(=O)(=O)C1=CC=C(C=C1)Cl	6.28
48	N12C(=O)/C(/SC1=NC(C1C=CC=CC=1)=C2C1=CC=CC=C1)=N/NC1=CC=C(C=C1)N(=O)=O	6.28
49	FC1=C(NC2=C3C(C=CC=C3)=NC(C(F)(F)F)=N2)C=C(Cl)C=C1	6.27
50	FC(C1=NC=C(S(NC2SN=C(C3=CC=NC=C3)N=2)(=O)=O)C=C1)(F)F	6.26
51	C1([C@H](CCC)N2CCN(CC2)C2C=CC=CC=2OC)=NN=NN1CC1=CC=CS1	6.26
52	C1(/C=C/[C@@H]2C[C@@H](O)CC(=O)O2)C(C2C=CC(=CC=2)F)=C2C=CC=CC2=NC=1C1CC1	6.26
53	O1C(=C([C@H](C2=CC=C(CC)S2)C2C(N(C3C=CC=CC=3C=21)C)=O)C#N)N	6.25
54	CC(C1OC2=C(C=C(C=C2)NS(/C=C/C2=CC=CC=C2)(=O)=O)N=1)(C)C	6.19
55	FC1=CC=C(CONC(C2C(C3=C(Cl)C=CC=C3)=NNC=2)=O)C=C1	6.18
56	N12C(C3C=CC(=CC=3)Cl)=CN=C1C(=C(N)O2)/N=N/C1=CC=CC=C1	6.15
57	S(=O)(=O)(C1C=CC(=CC=1)C)/N=C(/C1=CC=C(C=C1)Cl)\NC(OCC)=S	6.14
58	C1(C(=O)N2CCN(CC2)S(=O)(=O)C2CC2)N=NN(C2=CC=C(C=C2)OC)N=1	6.13
59	C1(/S/C(/N(CC=C)C/1=O)=C1\C(C)=NN(C2=CC=C(C=C2)Cl)C\1=O)=C1/SC2=C(C=CC=C2)N/1CC	6.13
60	CCN1C(=O)NN=C1SCC(C1SC(N2CCCCC2)=NC=1)=O	6.12
61	CC1=C(F)C=C(CNC(C2=C(N3N=CN=C3)C=C(Br)C=C2)=O)C=C1	6.11
62	N1=C(N=C(CC(=O)OCC)N=C1N1CCOCC1)OC1C=CC(OCC)=NN=1	6.11
63	N12CN(C3C=CC=CC=3C)CSC1=C([C@H](C1=C(OC)C=CC3C=CC=CC1=3)CC2=O)C#N	6.11
64	C12C3(CCCCC3)CC3C(=CC=CC=3)C=1N=C(CC1=CC=CC=C1)N=C2SCC	6.10
65	CC1=C(COC(C2CCN(C(N3CCCC3)=O)CC2)=O)C=CO1	6.10
66	C1(/C=C/C2=CC=CO2)N(CCOC2C=C(C)C=C(C)C=2)C2C(=CC=CC=2)N=1	6.09
67	C(=O)(C(C1=CC=CC=C1)C1C=CC=CC=1)N/N=C(/C)\CCCC	6.09
68	CCN1N=CC(C2CCN(CN3C(=S)NN=C3CC3SC=CC=3)CC2)=C1	6.09
69	CC1=C(C2OC(SCC(NC3N(CC4OC=CC=4)C(C)=C(C)C=3C#N)=O)=NN=2)C=CO1	6.08
70	C1(SCCOC=1C)C(=O)NC1C=CC=C(C=1)C(=O)NCC1C=CC(=CC=1)OC(C)C	6.08

71	CN(S(C1=CC2=C(N=NN2OCC2N(C(F)F)C=CN=2)C=C1)(=O)=O)C	6.07
72	O=C([C@@]12C[C@@H]3C[C@@H](C[C@@H](C3)C1)C2)CN=P(C1=CC=CC=C1)(C1=CC=CC=C1)C1=CC=CC=C1	6.07
73	CCC1N=C(N2CCN(CN3C(=O)N(C4=CC=CC=C4)N=N3)CC2)SN=1	6.07
74	C1(C(=O)NNC(=O)C2=CC=CC=C2Br)OC2=C(/C(/CCC2)=N/NC2C=CC=CC=2)C=1C	6.06
75	C12N=C(C)S[C@H](C3CCCCC3)C=1C(NN2C(C)C)=O	6.05
76	CC1=C(C)OC(CNC(C2=CC(N(=O)=O)=C(NC3=CC=CC=C3)C=C2)=O)=N1	6.05
77	C1(N(=O)=O)C=C(N(CC2=NN=C(NC3C=CN(CC4=CC=CC=C4Cl)N=3)S2)N=1)C	6.03
78	FC1=C(Br)C=C2C(OC(N2CC2N=C(C3CCCCC3)ON=2)=O)=C1	6.01
79	C1(NC2=CC=CC(Cl)=C2)O[C@@H](C2=CC3OCCOC=3C=C2N=1)C1=CC=CC=C1	6.01
80	[C@@]12(SC(=C(C)N1C1C=CC=CC=1)C(OC)=O)N(C1=CC=C(C=C1)Cl)N=C(C(OC)=O)S2	6.01
81	C1(OC[C@H](CSCC2C=CC(=CC=2)F)N=1)C1=CC=CN1CC1=CC=C(C=C1)C	6.01
82	C1(C2=CC=CS2)=NC2(N=C1SCC(=O)NC1C=CC(=CC=1)F)CCCCCC2	5.98
83	NC1=NC([C@H](C(C2C=C(Cl)SC=2)=O)C#N)=NC(N)=N1	5.97
84	O=C(C1=C(CSC2SCCN=2)C=CC=C1)N[C@@H]1[C@H](C2=CC=CC=C2)OCC1	5.97
85	COC1=CC(N(=O)=O)=C(NNC(C2=C(C(C)(C)C)N=NS2)=O)C=C1	5.96
86	C[C@@H]1C2N(C=NN=2)CCN1S(C1CN(C(C2=CC(Cl)=CC=C2)=O)C1)(=O)=O	5.95
87	C1(C2=CC=C(C=C2)/N=C/C2=CC=C(C(Cl)=C2)Cl)=CC2C=CC=CC=2OC1=O	5.94
88	N1(C2C=CC(=CC=2)Cl)[C@H](C2=CC=CS2)N(N=C1C(C)=O)C1C=CC(=CC=1)Cl	5.93
89	COC1=C(OCC2=CC=NC=C2)C=C(NC(C2OCCCC=2)=O)C=C1	5.92
90	CSCC[C@@H](C1NC2=C(C=CC=C2)N=1)NC(/C(/F)=C(\C)/C)=O	5.91
91	FC(C(NC1(C2N3C(=NCC3)SC=2)CCCCC1)=O)(F)F	5.91
92	C1(=C/NC2C(C)=CC=C(Cl)C=2)/[C@H]2CC[C@@](C2(C)C)(C)C/1=O	5.91
93	CC(NC1=CC=C(C2C[C@@H](C3SC=CC=3)N(S(C3=CC=C(C)C=C3)(=O)=O)N=2)C=C1)=O	5.89
94	CCCCN1N=C(C)C(C(OC[C@@H]2ON=C(C3=CC=CC=C3)NC2)=O)=C1	5.88

95	C1C[C@]2(CC=CCC2)CN(C2=NC(C3=NC=CN=C3)=CC=N2)C1	5.88
96	C12N=C(NCC3=CC=C(C=C3)OC)C3=C(C=CS3)N1N=NC=2S(=O)(=O)C1C=CC(=CC=1)C	5.86
97	CN(CC1C2=C(C=CC=C2)OC=1C(NC1SC(/C=C/C2OC=CC=2)=NN=1)=O)C	5.85
98	C12(CCN(CC1)C(C)C)N[C@@H](CC(C1C=CC(=CC=1)C)=N2)C1C=C(Cl)C=CC=1O	5.84
99	C12[C@H](CC(NC=1C(=C(C(O)=O)S2)C1=CC=C(C=C1)F)=O)C1C=CC=CC=1OCCC	5.84
100	C1C=C2C=C(C(=O)/C(=C/NC(=S)NC3C=CC(S(=O)(=O)N)=CC=3)/C#N)C=CC2=CC=1	5.83
101	O=C(C1C(=O)OC2=C(C=CC=C2)C=1)NNC(NCCC1SC=CC=1)=S	5.82
102	FC1=CC=C(C#CCN2C(=O)[C@]3(C4=C(C=CC=C4)OCC3)NC2=O)C=C1	5.80
103	C12=CC=C(Br)C=C1C(=N[C@H](OC(=O)C)C(=O)N2CC(=O)OC)C1C=CC=CC=1	5.80
104	C1(SCCNC(=O)C2C=C(C)NC(=O)C=2)=NN=NN1C	5.79
105	C1C=CC([C@@H]2C(C(OC)=O)=C(C)NC(C)=C2N(=O)=O)=C(C(F)(F)F)C=1	5.77
106	N1(CCN=C1SCC1C=CC=CC=1F)C(=O)C1=CC(Cl)=CC=C1OC	5.75
107	CC1C(C(N2C[C@H](CN(S(=O)(=O)C)CC(=O)O)OCC2)=O)=CSC=1	5.74
108	N1(/N=C/C2=CC(OC)=C(C(Br)=C2)OCC=C)C(=O)C2=CC=C3C4C(=CC=C(C2=4)C1=O)CC3	5.74
109	CCN(CC1=C(OC(F)(F)F)C=C(F)C=C1)CC(NC(C)C)=O	5.73
110	O=C1C2=C(C=CC=C2)C(C2=CC=CC=C2)=NN1CN1CC=C(C2SC=CC=2)CC1	5.73
111	N1C(N[C@H](C2C=CC(OC)=CC=2)C(=C1)C1OC2=CC(=C(C=C2C=1C(C1C=CC(C)=CC=1)=O)C#N)C#N)=O	5.71
112	N12C(C)=NN=C1C=C(N1CCN(CC1)CC1=CSC3CCCCC1=3)C=N2	5.70
113	C1(OS(=O)(=O)C2=CC=C3C(C=CC=C3)=C2)=CC(=O)N(N=C1C(OCC)=O)C1C=CC(=CC=1)C	5.70
114	N12N=C(SC1=NN=C2C1C=C(Cl)C=CC=1F)C1CCC1	5.69
115	C[C@@H](C1=CSC=C1)NCC1=C(OC2=CC(F)=CC=C2)N=CC=C1	5.69
116	S(=O)(=O)(N1CCC2(CC1)NC1C=C(F)C=CC=1N1C=CC=C12)C1=CC=CC=C1Cl	5.69
117	[C@]12(C[C@H](ON1[C@H](N(C1C=CC=CC=1)C2)C1=CC=C(OC)C(OC)=C1)C1C=CC=CC=1)C1=CC=CC=C1	5.69
118	C1(NC2C=CC(=CC=2)F)C(=O)C(C=1C1=CC=C(C=C1)C(C)C)=O	5.69

119	N1(C2C=CC=CC=2C=CC2C=CC=CC1=2)C(=O)N1CCCCC1	5.69
120	C12SSC(=S)C=1C1=C(C=CC(OC)=C1)N(C(=O)CC1=CC=C(C=C1)F)C2(C)C	5.69
121	S1(=O)(=O)C2C=CC=CC=2OC2C=CC3=C(C(/C=N/NC(N)=O)=CN3)C1=2	5.67
122	O=C(NNC(NCC1=CC=CC=C1)=S)CSCC1=CC=C(C#N)C=C1	5.66
123	C1(=C(C)SC2N=CN(CC(=O)N3CCN(CC3)C3C=CC=CC=3)C(=O)C1=2)S(=O)(=O)N1C[C@@H](C)C[C@@H](C)C1	5.65
124	C1(C=C(C=NC=1SC1=CC=CC(Cl)=C1)C1=CC=CC(=C1)C(F)(F)F)C#N	5.65
125	N1=C(NC2=CC=C(C(OC)=C2)OC)ON=C1C1=CC=C(C=C1)OC	5.64
126	C12C=CC=CC=1NC=C2C[C@H](C(=O)O)NC[C@](O)(C)C#CCCC	5.64
127	[C@]12(C)C(=O)/C(=C(\C)/NC3=CC=C4C(C(=O)C=CO4)=C3)/C(C=C1OC1=C(C(O)=C(C)C(O)=C21)C(C)=O)=O	5.63
128	C(=O)(N/N=C/C1C=C(CC=C)C(=C(OCC)C=1)O)NC1C=CC=C(Cl)C=1	5.62
129	C1(C(=O)NC[P+](C2C=CC=CC=2)(C2=CC=CC=C2)C2C=CC=CC=2)=CC2=C(C=CC=C2)O1	5.62
130	N12C(=O)[C@@H](N=C1C1=C(C=C(C(OC)=C1)OC)NC2=S)CCC(OC)=O	5.61
131	O[C@]1(C(F)(F)F)CN(C(C2=C(NC3=CC=CC=C3)C=CC=C2)=O)CC1	5.61
132	[C@]12(C(C)C)CC[C@@]([C@@H](OC(=O)NC3C=CC=CC=3)C1)(C)O2	5.60
133	C[C@@H](CS(C)(=O)=O)CSC1=C2C(C=CC=C2)=NC(C(F)(F)F)=N1	5.60
134	COC(/C(/CC(C1=CC=CC=C1)=O)=N\N=C1\C2=C(C=CC=C2)NC(=O)N\1)=O	5.59
135	O=C(NN1C(=O)C2=C(C=CC=C2)N=C1)CN1N=NC(C2=CC=CC=C2)=C1	5.59
136	CC1=C(F)C=C(CS(NC2OC(C3CC3)=NN=2)(=O)=O)C=C1	5.58
137	CC[C@H](OC1=C(/C=C/C(OCCC2=NC=CN=C2)=O)C=CC=C1)C	5.57
138	N1(C2C(C)=CC=CC=2C)N=NN=C1C(C)(C)/N=C/C1C=CC=C(C=1)N(=O)=O	5.56
139	C1(N(=O)=O)=C(C=CC2=NSN=C12)SC1N=NN(C2CCCCC2)N=1	5.56
140	C[C@H](C(/C(/C#N)=C1\NC2=C(C=CC=C2)N\1)=O)SC1N(C)C=NN=1	5.55
141	COC1=NC=C(N2/C(=C(\C#N)/C#N)/S/C(=C\C3N(C)N=CC=3)/C2=O)C=C1	5.54
142	CC(N1N=NC(C2CCN(C(N[C@@H]3C(C)(C)CCC3)=O)CCC=2)=C1)C	5.54

143	S1(=O)(=O)C2=CC=C(C=C2N=C(CCC(=O)N[C@@H](C)C2C=CC3=C(OCCO3)C=2)N1)C	5.54
144	FC(C1N=C(CN2C[C@H](S(NC3CCCC3)(=O)=O)CCC2)ON=1)F	5.54
145	C1(C(=O)C2C=CC=CC=2C(=O)C=1[N+]1C=CC(=CC=1)CC)[N-]S(C1=CC=CC=C1)(=O)=O	5.53
146	C12=C(C3=CC=CO3)C(C#N)=C(N=C1SC1C(=CC=CC=1)N=C2N)N	5.51
147	C[C@H]1CN(CN2C(=S)N3C(SC4=C3C=CC=C4)=N2)CCC1	5.50
148	N1(C(CC)=O)/C(=N/C2C=CC=CC=2C)/SC(C)=C1OC(CC)=O	5.50
149	CN1N=CC(C2=NC(/C=C/C3=CC4=C(OCC(N4)=O)C=C3)=NC=C2)=C1	5.49
150	C1(=O)/C(=C\C2C=CC3OCOC=3C=2)/SC(NC2=CC(N(=O)=O)=CC=C2)=C1C(=O)OC	5.49
151	C1(=C(C)C=CC2=CC=CC=C12)[C@H](O)C1C=CC(=CC=1)C1C=CC=CC=1	5.49
152	C1(C2CCN(CC=2SC=1N)C(C)C)S(C1C=CC=CC=1)(=O)=O	5.48
153	CCCOC1=CC(CCNC(N2CCN(C3=NN=CC=C3)CCC2)=O)=CC=C1	5.47
154	C1(=O)C2C=CC=CC=2SC2=CC(=CC=C2N1C1CC1)NC(=O)C1C=CC(=CC=1)C(F)(F)F	5.47
155	CC1=C(C)C2=C(N=C(N=C2N)CN2CCC(C3SC4=C(C=CC=C4)N=3)CC2)O1	5.46
156	C1(CN(CC2=CC=CC=C2)CN(C2C=CC(=CC=2)C(O)=O)N=1)N(=O)=O	5.45
157	CCCC(N1[C@@H](C(NCCN2CC=C(C)CC2)=O)CCC1)=O	5.45
158	C12C(CCCC=1NC(C1C=CC(C3C=CC=CC=3)=NC=1[C@@H]2O)=O)=O	5.45
159	CN1C([C@@H]2[C@@H](NC(NC[C@@H]3SCCCC3)=O)CCCO2)=NC=C1	5.44
160	P(CO)(=O)(C1C=CC(=CC=1)Cl)C1C=CC(=CC=1)Cl	5.43
161	FC1=C(N2CCN(S(C3=CN=C(C4=CC=CC=C4)N=C3)(=O)=O)CC2)C=CC=C1	5.42
162	C1(C(=O)NC2=CC=C(C=C2)OC)=NOC2C3=C(SC=C3)CCC1=2	5.42
163	C1(=C(N/N=C/C2CCCCC=2C#C)C=CC(N(=O)=O)=C1)N(=O)=O	5.42
164	S(=O)(=O)(C1C=CC(=CC=1)C)NC(=O)NC1C=CC(=CC=1)C1OCCN=1	5.42
165	C[C@@H](C(N([C@@H]1CS(=O)(=O)CC1)C)=O)N1CCC(C2OC(C)=C(C3=CC=CC=C3)N=2)CC1	5.42
166	C12C3CCN(CC=3SC=1N[C@H](C1=CC=C(C=C1)CC)N=C2O)C(OCC)=O	5.41

167	CCC1=C(CC)C=C(NC(CCN/C(/O)=C2\C(=O)C=CC=N\2)=O)C=C1	5.41
168	C1(/C=N/NC2SC3=C(C=CC=C3)N=2)C(C)=NN(CCO)C=1C	5.40
169	C1(=C/C(=O)C2=CC=CS2)\NC2C=CC(=CC=2OC\1=O)N(=O)=O	5.40
170	CC(OC(N[C@@H]1CN(CCOC2=CC(N(=O)=O)=CC=C2)CC1)=O)(C)C	5.39
171	FC(OC1=CC2=C(C=C(S(OC3=C(F)N=CC=C3)(=O)=O)CC2)C=C1)F	5.39
172	CC[C@H](N1N=C(C2=CC=C(Cl)C=C2)N=N1)C(OCC1=NC(C)=NC(C)=C1)=O	5.37
173	FC1=C(F)C=C(N2CCCCC2)C(NC(N2C[C@H](N3N=NC=C3)CCC2)=O)=C1	5.36
174	C1(=NON=C1N)N(CC1C=CC=CC=1Br)/N=N/C1=NON=C1N	5.36
175	C1(C)C=CC(S(=O)(=O)NN2CCS(=O)(=O)CC2)=CC=1	5.36
176	CC(OCCCN1/C(=N\[H])/C(=C2\N(C)C3=C(C=CC=C3)N\2C)/C(=O)C1)C	5.35
177	C1(=NSC(O)=C1N)NC1C=CC(Cl)=CC=1Cl	5.35
178	CN(CN1N=C(C2=CC=NC=C2)C(N(=O)=O)=C1)CC1SC=C(C(F)(F)F)N=1	5.35
179	[C@]12(CC[C@](/C(=N/O)/C1=O)(C)C2(C)C)C(=O)N1CCOCC1	5.35
180	C1(C=COC=1)C1=NC=CN=C1CNC(=O)C1C=CC(=CC=1)N1C=CC=C1	5.34
181	CC(NC1=CC(NC(NCCCSC2SC=CN=2)=O)=C(Cl)C=C1)=O	5.32
182	C12SC(=CC=1C(OC(C1=CC=C(C=C1)C(C)(C)C)=N2)=O)C	5.32
183	S1(=O)(=O)C2=CC=CC=C2N(N=C1C(=O)N1CCCCC1)CC(OCC)=O	5.32
184	FC1=C(NNC(C#CC2=CC3=C(OCO3)C=C2)=O)C=C(C(F)(F)F)C=C1	5.31
185	O=N(C1=CC(S(NC2=NC=C(Br)N=C2)(=O)=O)=CC(F)=C1)=O	5.30
186	CN(C1=CC=C([S@](C)(=NC(C2=NC=C(C)N=C2)=O)=O)C=C1)C	5.29
187	S(N)(=O)(=O)[C@H]1CCOC2C(=CC(Cl)=CC1=2)Cl	5.27
188	CN1N=C(C(F)(F)F)C(CNC(/C=C/C2OC3=C(C=CC=C3)N=2)=O)=C1	5.27
189	NC(C1C=CC(N2C[C@H](C(=O)O)S(=O)(=O)CC2)=C(N(=O)=O)C=1)=O	5.27
190	N1(C[C@@H](CO)C[C@H](CN2CCOCC2)C1)C(=O)C1C=COC2=CC=CC=C2C=1	5.26

191	CCN1N=CC(OC(C[C@@H]2C(=O)NC3=C(C=CC(=C3)Cl)S2)=O)=C1	5.26
192	CC1OC([C@](C(F)(F)F)(CC(NNC2=NC3=C(C=CC=C3)C=C2)=O)O)=CC=1	5.26
193	CCN(CC(F)(F)F)C[C@@H]1CN(CC2N(C(F)F)C=CN=2)CC1	5.25
194	N1(/N=C/C2=CC=C(C(COC3C=CC=C(Cl)C=3Cl)=C2)OC)C(S)=NN=C1C(F)F	5.24
195	C12NC3=C(C=CC=C3)C=1N=C(C)N(/N=C/C1C=CC=C(C=1)N(=O)=O)C2=O	5.22
196	C(C)(C)(C)CCN[C@@H]1C[C@H]([C@@H]([C@H]1CC1=CC=NC(C2=CC=CN=C2)=N1)CO)O	5.20
197	S(F)(=O)(=O)C1C=CC=CC=1NC(=O)C(F)(F)F	5.18
198	CCC([C@@H]1OCC[C@H](NC(/C=C/C2OC(C(C)C)=NN=2)=O)C1)CC	5.18
199	N1(C=COC=C1/N=C/C1=CC=CC=C1)CC1=CC=CC=C1	5.16
200	N1(N=C(/C(=C(\C)/OCC)/C1=O)C(F)(F)F)C1SC2=C(C=CC=C2)N=1	5.15
201	CS(C1SC=C(C(OC2=C(OCC(F)(F)F)C=CC=C2)=O)C=1)(=O)=O	5.15
202	FC(C1=CC=C(C#CCNCC2=NNC=C2)C=C1)(F)F	5.15
203	CC1=CC=C(SC2=NN=C(SC3=CC=C(C)C=C3)C=C2)C=C1	5.14
204	[C@@H]12N=NN(CC3C(=CC=CC=3F)Cl)[C@@H]1C(N(C1C=CC(=CC=1)Cl)C2=O)=O	5.13
205	NC1=C(C2NC(=O)[C@@]3(NN=C(C4=CC=CC=C4)C3)NN=2)C=CC=C1	5.12
206	C(F)(F)(F)C1C=CC=C(C=1)C(=O)N/N=C/C=C/C1=CC=CO1	5.12
207	N1(C)C(SCN2N=CC(N(=O)=O)=C2)=NN=C1C1=CC=CC(Cl)=C1	5.11
208	C1(=NN=NN1C1C=CC=CC=1)S/C=C\C(C1C=CC(C)=CC=1C)=O	5.11
209	CN1[C@H](CCN2C(=O)OC(C3=CC=C(F)C=C3)=N2)CCCC1	5.11
210	N1(CC(O)=NC2=CC=CC=C12)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](CC1C=CC=CC=1)C(O)=O	5.11
211	N1=C(C)C[C@H](CNC(=O)NC2=CC=C(C=C2F)F)O1	5.09
212	CN1C(=O)N(C)C(=O)C(C#N)=C1NCCC1N2C(CCCC2)=NN=1	5.08
213	FC1(CCC(C(OCCOC2=NC(Cl)=CN=C2)=O)CC1)F	5.07
214	CC1([C@H](OCC2=CC=CC=C2)C[C@@H]1NS(NCC(F)(F)F)(=O)=O)C	5.07

215	C12C(=O)CC(CC1=N[C@H]1[C@H](CCCC1)NC=2)(C)C	5.06
216	C(/C#N)(\C(N)=O)=C(\O)/C(/O)=C\C(=O)C1=CC=C(C=C1)Cl	5.05
217	C1(SC2C=CC(=CC=2)Cl)OC(=CC=1Br)/C=N/C1=CC=C(C=C1)Cl	5.03
218	NC1=C(S(N2C3=C(C=CC=C3)C=CCC2)(=O)=O)C=C(Br)C=N1	5.03
219	N1(C2=CC=C(C=N2)F)C2C=CN=C(C)C=2N=C1	4.99
220	S(=O)(=O)(NC1=CC=C(C=C1)N(=O)=O)[C@@H]1CCS(=O)(=O)C1	4.99
221	N1C(=CSC=1NC1C=CC(OC)=CC=1OC)C1C=COC=1	4.99
222	C1(NC(=O)CN2C(C)=C(C(C(F)F)=N2)Cl)C(C)=NN(C)C=1C	4.98
223	ClC1=C(NC(CN2CCN(CC3=NOC=C3)CC2)=O)C=C2C(OCCO2)=C1	4.96
224	CC1OC(COC(/C=C/C2=CC(F)=CC=C2)=O)=NC=1	4.95
225	C[C@@H]1S(=O)(=O)CCN(CC2=NN(C3=CC=CC=C3)C=N2)C1	4.95
226	CC(CCC1=CC=C(OC2=NC(N)=NC(Cl)=C2)C=C1)=O	4.93
227	ClC1=C([C@@H]2OCCN([C@@H]3C=CCCC3)C2)C=CC=C1	4.93
228	[C@@]1(C)(C2=CC=CC=C2)OC(=O)C=C(C2C=CC=CC=2)O1	4.91
229	N1(C2=CC=CC=C2Cl)C(C)=CC(C)(C)N=C1S	4.91
230	C1(SC2C(=CC=C(C)C=2)N=1)NC1OC2=C(C=CC(C)=C2C)N=1	4.89
231	O=C(C1=CC=CC=C1)N/N=C1/NN2C(=NN=C2)C=C/1	4.89
232	COC1=C(OC2SC(N(=O)=O)=CN=2)C=CC(/C=C/C)=C1	4.87
233	CCN1C(N2CCOCC2)=NN=C1SCN1C2=C(C=CC=C2)N=N1	4.86
234	NC1(C2N=C(C3ON=C(C4C=CC=CN=4)C=3)ON=2)CCC1	4.86
235	O=S(C1NC=CN=1)(CC1=C2C(OCCO2)=CC=C1)=O	4.85
236	C12N=CC=CC=1N=NN2OCC(=O)NC1=CC=C(Cl)C=C1	4.84
237	ClC1C=CC2N(CC3=C(/C(/N=2)=N\C(C2SC=CC=2)=O)C=CC=C3)C=1	4.84
238	CC1=C(Cl)C=C2C(OC(C=C2CN2CCN(C(N3CCCC3)=O)CC2)=O)=C1	4.79

239	O=C(C1N(C2=CC=CC=C2)N=C(C2CC2)C=1)N=S1(CCCC1)=O	4.76
240	C12N=NC(=C(C)N1N=C(C(F)(F)F)N=2)C(OCC)=O	4.75
241	C1C(CO)=CC=C2[C@H]3C[C@H](C=C3)C2=1	4.71
242	COC(C1=CC(C2N=C(C3OCCOC=3)ON=2)=CC=C1)=O	4.70
243	CN(S(/C(/C#N)=C\C1=CC2=C(CCC2)C=C1)(=O)=O)C	4.68
244	C[S@@](C1N(C2OC3=C(C=C(C=C3)F)N=2)C=NN=1)=O	4.66
245	C(C1O[C@@H]2C(=O)C3=C(C(=O)[C@H]2C=1)C=CC=C3)(=O)C	4.65
246	S(=O)(=O)(CCOC1=CC=C(C=C1)F)NC1=NC=CC=N1	4.58
247	C1(C(C)=NON=1)NC(=O)C1N=CN=C(N2CCCC2)C=1	4.51
248	N12NC(C(/N=N/C3C=CC=CC=3)=C1N=NC(C#N)=C2N)=O	4.48
249	CC1=C(C)N=NC(OCC2OC(C3=CC=CC=C3)=CN=2)=C1	4.46
250	N1(CC(=O)NC2SC=C(C3=CC=C(C=C3)Br)N=2)N=C(OC1=S)C1=CC=CC=C1	4.27
251	C1(/N=C/C2=CC=C(C3=CC=C(C(Cl)=C3)F)O2)=NN=CN1	4.26
252	N12C(=O)C(=CN=C1OC(C1C=CC(=CC=1)OC)=N2)NC(=O)C1=CC=CC=C1Cl	4.18
253	CN1N=CC(C(NC2=CC(OS(C3OC=CC=3)(=O)=O)=CC=C2)=O)=C1	4.18
254	C1(NC(CC)=O)=NN=C(SCC2OC=C(C(=O)C=2)OC(=O)C2=CC=CC(=C2)C(F)(F)F)S1	4.18
255	CN1C2=C(C=CC=C2)C(/C=C/C(NCCCS(CC2=CC=CC=C2)(=O)=O)=O)=C1	4.18
256	N1C(=O)C(CCC(=O)N2CCN(CC2)C2=CC=C(F)C=C2)=NNC=1C1=CC(OC)=C(C=C1)OCC1C=CC=CC=1F	4.18
257	FC1=CC(NC(NN/C=C2\C3=C(C=CC=C3)C(=O)NC\2=O)=O)=CC(F)=C1	4.18
258	N1=C(C2=CC=C(C=C2)CS(=O)(=O)C2=CC=C(C=C2)C)ON=C1C1=CC=C2C(=C1)N=C(O2)C	4.18
259	C12NC3=C(C=CC=C3)N1/C(/C=C(C)C=2C#N)=N/C1C=CC(=CC=1)Cl	4.18
260	C1(C(=O)NN2C=C(C(OCC)=O)C(C3C=C(F)C(F)=C(F)C2=3)=O)=CN(CC)C2=C(C=C(C(N3CCCC3)=C2)F)C1=O	4.18
261	N12ON=C(C3C(C)=C(C)C=C(C)C=3C)N1C1C(=CC=CC=1)N2C(=O)C1=CC=C(C=C1)S(=O)(=O)N1CCOCC1	4.18
262	C1(C(N)=O)C2N=C(O)C=C(O)C=2SC=1SCC(C1=CC=CC=C1)=O	4.18

263	O=N(C1=CC=C(/C=N/N2C(=S)NN=C2N2C(C3=CC=CC=C3)=CC(C3=CC=CC=C3)=N2)C=C1)=O	4.18
264	N12N=C(N=C1S/C(/C2=O)=C1/C2C=C(Br)C=CC=2N(CC2=CC=CC=C2)C/1=O)C1C=CC(=CC=1)OC	4.18
265	C12[C@@H](C3C=CC(=CC=3)C)N=C(NC=1C1C(=CC=CC=1)NC2=O)NC1SC2=C(C=CC=C2)N=1	4.18
266	C1(=CC=NN1C(=O)NC1=CC=CC=C1)C1ON=C(C2=CC=CC=C2)C=1	4.18
267	N1(CC2=CC=C(C=C2)Cl)C2C=CC=CC=2C(/C=N/N=C2\SC3C(=CC=CC=3)N\2)=C1	4.18
268	C1(=C/C2=CC(=CC=C2N2CCN(CC2)CC)N(=O)=O)\C(O)=NC(=NC\1=O)O	4.18
269	CC1=C(C(NNC(NC2C(=O)N(CC3=CC=C(C)C=C3)C=CC=2)=O)=O)SC=N1	4.18
270	C[C@@H](C1=C(C)C2=C(C=CC=C2)S1)OC(C1=NC=C2C(C(NC=N2)=O)=C1)=O	4.18
271	C1(OCCSC=1C1C=CC=CC=1)C(=O)/N=C1/NN=C(SCC2C=CC(=CC=2)Cl)S/1	4.18
272	C12[C@H](C3C=NN(C)C=3)C3=C(C)NN=C3OC=1N=CN1N=C(C3=CC=CC=C3N(=O)=O)N=C21	4.18
273	C12C3C=COC=3CCC=1C(=NN2C1C=CC(=CC=1)C(=O)NC(C)C)C(F)(F)F	4.18
274	CC1=C(CC(NC2SC(CC3=C(Cl)C=CC(Cl)=C3)=CN=2)=O)C(=O)NC(C2=CN=CC=C2)=N1	4.18
275	C12N=C(N)C3=C(C=CC=C3)N1C1=C(C(CCC1)=O)[C@@H](C1=CC=C(C=C1)OC)C=2C#N	4.18
276	O1C(C2C=CC=CC=2)=C2C=CC(C3C=CC=C1C=32)=O	4.18
277	N1C(NC2C=CC(=CC=2)CC)=NC(=NC=1C1=CC2=C(C=CC=C2)O1)N	4.18
278	FC1=C(F)C=C2C(N=C(NC2=O)CC2NN=C(C3=CC=CC=C3)N=2)=C1	4.18
279	CC1=C(C)C=C(C(NC2C(=O)OC(C(F)(F)F)=CC=2)=O)C=C1	4.18
280	[C@@]1(C(F)(F)F)(NC(=O)C2C=CC(=CC=2)C(C)(C)C)C(=O)N(C2CC(C)(C)CC(=O)C1=2)CCCC	4.18
281	N1=C(C2=C(N)N(C3=CC(C)=CC=C3)N=C2N=C1NCC1=CN=CC=C1)C1=CSC=C1	4.18
282	C1(C(OC)=O)=C(C)N(C(=O)/C/1=C\C1C=C(N(C2C=CC(=CC=2)OC)C=1C)C)C1C=CC(=C(Cl)C=1)C	4.18
283	NC1=CC=C(C2=CC(C)(C)[C@H](N)C(C)=C2)C=C1C	4.18
284	[C@@]12(C[C@H]3CC[C@@H]1C[C@@H]3C(NCCCN1CCCC1=O)=O)OC1C=CC=CC=1C(=O)N2	4.18
285	CCC(NC1=CC=C(C2CSC(NCC3=CC4=C(OCO4)C=C3)=NN=2)C=C1)=O	4.18
286	C1(/NN=C(CSCC2C=CC(=CC=2)Cl)S/1)=N\C(=O)NC1C=CC(=C(Cl)C=1)Cl	4.18

287	S1(=O)(=O)C2C=CC=CC=2C(OC2C=CC(=CC=2Br)F)=N1	4.18
288	C12N=C(N(C(C)=O)C=1SC(C1C=CC=CC=1)=NN2C(C)=O)C1C=CC=CC=1	4.18
289	C[C@@H]1N(CC2=C(C(NNC3=NC(C)=NC(C)=C3)=O)OC=C2)C2=C(C=CC=C2)C1	4.18
290	CCC1N=C(NC(/C(/C#N)=C/C2=C(C)N(C[C@@H]3OCCC3)C(C)=C2)=O)NN=1	4.18
291	C12=C(NC)C(N)=CN=C1C(=C(F)C=C2F)F	4.18
292	C1(C(=O)N/N=C/C2C=C(C=C(Br)C=2O)N(=O)=O)=NN(C(C2C=CC=CC=2)=N1)C1C=CC=CC=1	4.18
293	CC1=C2C(C=CC=C2)=NC(SCC(C2OC3=C(C=CC=C3)C=2)=O)=C1	4.18
294	N1(C2=CC=CC(=C2)C(F)(F)F)C(CNC(CC2C=CC3=C(OCO3)C=2)=O)=NN=C1SC[C@@H]1CCCO1	4.18
295	C1(=S)N(NC(=O)C2C=CC=C(OC)C=2)[C@@H](C(=O)N1C1=CC=C(C=C1)OC)CC(=O)NC1=CC=C(C=C1)F	4.18
296	ClC1=CC(NS(C2=CC=C(NC(C3CCC(=O)NN=3)=O)C=C2)(=O)=O)=CC=C1	4.18
297	C1(OC(/C(=C/C2C=CC=CC=2Cl)/N=1)=O)C1=C(C)ON=C1C1=CC=CC=C1	4.18
298	CC1=C(Cl)C=C(NP2(C=C(C3=CC=CC=C3)OC(C3=CC=CC=C3)=C2)=O)C=C1	4.18
299	C1(/NN=C(CCC)S/1)=N\C(CCC(=O)N1CCN(CC1)[C@@H](C1=CC=CC=C1)C1C=CC(=CC=1)Cl)=O	4.18
300	O=C1C(C)=CN=C(NC2C=C(N3CCN(C)CC3)C=CC=2)N1	4.18
301	O=S1(N(CC2N=C(C3SC=CC=3)ON=2)C2=C(C=CC=C2)N1CC1N=C(C2SC=CC=2)ON=1)=O	4.18
302	OC1=C(CNC(NNC(CC2=NC=CC=C2)=O)=O)C2=C(CCCC2)C=C1	4.18
303	N12C(C)=CC=C1S[C@H](C(=O)NC1=CC=CC(C)=C1)[C@H](C1C=CC(=CC=1)OC)N2	4.18
304	CC1SC=C(C2=CC(NC(C3=C(Cl)C=C(N4N=NN=C4)C=C3)=O)=CC=C2)N=1	4.18
305	[C@]12(C#N)[C@@H]3CCCC[C@@]3(O/C/1=N/[H])O[C@H](C1=CC=C(C(OC)=C1)OCC)C2(C#N)C#N	4.18
306	O=C(N1CC2=C(C=CC=C2)S(=O)(=O)CC1)[C@@H]1N2C(=CC=C2)C(=O)CC1	4.18
307	O=C(N1CC(=O)N(C2SC=CC=2)CC1)NCCC1NC2=C(C=CC=C2)N=1	4.18
308	FC1=NC=CC(NNC(COC2=CC(N3C(=O)CCC3)=CC=C2)=O)=C1	4.18
309	COC(C1=CC(C2SC=C(CN3C(C#N)=C(C#N)N=C3N)N=2)=CC=C1)=O	4.18
310	CO[C@@H](C1=CC=C(F)C=C1)CS(NC1C(C(N)=O)=NN(C)C=1)(=O)=O	4.18

311	C12=CC(Cl)=CC=C1N=C(N=C2C1C=CC=CC=1)Cl	4.18
312	C12C(=CC=NC1=CC(Cl)=CC=2)NNC1=CC=C(C=C1)C(O)=O	4.18
313	N1=NC2C(=CC=CC=2)N1C/C(/C)=N/NC(=O)C1=CC=C(C=C1)Br	4.18
314	N1(C2CC2)C(=O)N(N=C1C1=CC=CS1)CCNS(=O)(=O)C1=CC=C(C(Cl)=C1)F	4.18
315	N1(C(=O)CSC2=NN=C(N/N=C/C3=CC=C(OCC4C=CC(=CC=4)F)O3)N2)C(C)=CC(C)=N1	4.18
316	C1(/C=N/NC(C2C=CC=CC=2)=O)C=C(SC=1Cl)C1C=CC=CC=1	4.18
317	ClC1=C(NNC(NC2=NN3C(C=CC=C3)=N2)=O)C(Cl)=CC=C1	4.18
318	O=C1/C(=C/NNC2=CC3=C(C=CC=C3)C=C2)/N=C(C2SC=CC=2)O1	4.18
319	CC(C1N=C(NC(N2CC3C(=C(C=C(C=3)F)F)CC2)=O)SN=1)(C)C	4.18
320	C1(NC(N)=N[H])NC2C(=CC=CC=2)N=1	4.18
321	N1(OC2C=CC(=CC=2N(=O)=O)N(=O)=O)C(=O)C2=CC=CC3C=C(O)C=C(C2=3)C1=O	4.18
322	ClC1=CC=C(S(C2=C(N3CCCCC3)OC(/C=C/C3=CC=CC=C3)=N2)(=O)=O)C=C1	4.18
323	CCOC(C1=CC=C(NC(CN2C(CC3=C(C)C=C(C(C)(C)C)C=C3C)=NCC2)=O)C=C1)=O	4.18
324	[C@H]12C[C@H]1C(=NN=C2C1C=CC(=CC=1)C)O	4.18
325	CC1C(CCC(NN2C(=O)C3(CCCCC3)NC2=O)=O)=C(C)ON=1	4.18
326	CN1N=CC(C2=C(C(N3CCC([C@H](C4=CC=C(F)C=C4)O)CC3)=O)C=NO2)=C1	4.18
327	N1=C(O)[C@@H](S/C/1=N\N=C1\CCCCCC\1)CC(=O)NC1=CC=C(C=C1)OCC	4.18
328	N12C(=O)N(C3C=CC=CC=3)C(=O)N1[C@@H]1CC=C[C@H]2CC1	4.18
329	C1(C(O)=O)N=C(OC=1SC1=CC=C(C=C1)Cl)C1=CC=CC=C1	4.18
330	S1C(C2=CC=CN=C2)=NN=C1/N=N/C1C=CC(=CC=1)O	4.18
331	C1(=CC=C(C)C=C1)S(=O)(=O)OC[C@H](O)CCOS(=O)(=O)C1=CC=C(C)C=C1	4.18
332	CC(C1SC(CNC(NC2=CC3=C(CCCC3)N=C2)=O)=NN=1)(C)C	4.18
333	C12C=C(O)C=CC=1OC=C(/C=C/C(O)=O)C2=O	4.18
334	FC1=CC(F)=C(N2C(=O)C[C@H](C(N3C[C@H](C4=NOC=N4)OCC3)=O)C2)C=C1	4.18

335	N12C(=O)C3=C(C=CC=C3)[C@@H]1C[C@@]([H])(C1=CC=CN21)O	4.18
336	FC1=CC=C(/C=C(/C(NNC(CC2=CN=CC=C2)=O)=O)\C#N)C=C1	4.18
337	N1C(C)=NC(=CC=1N/N=C/C1C=CC(=CC=1OC)OC)C1C=CC=CC=1	4.18
338	S(=O)(=O)(C1=CC=CC2=CC=CN=C12)NC1C2C=CC=CC=2OC=1C#N	4.18
339	C1(C=C(Br)C=CC=1F)C(=O)C1C=CC(=CC=1)F	4.18
340	CN1C2=C(C=C(C=C2)F)N=C(COC2=C(F)C(F)=CC(Br)=C2)C1=O	4.18
341	C1(N/N=C(/C2=CC=CC=C2)\C(C2C=CC=CC=2)=O)=NN=C(C)N1N	4.18
342	[C@]12(CC[C@](C1(C)C)(C)[C@H]2Br)C(=O)O/N=C1\C[C@H]2C(C)(C)[C@]\1(C)CC2	4.18
343	C1(=C/C(N)=O)/[C@H]2CC[C@@](C2(C)C)(C)C/1=O	4.18
344	C1(=CSC(=S)N1NC1C=CC=CC=1)C1=CC=C(Cl)C(C)=C1	4.18
345	C1(=NC=CN=C1OC1=CC=CC(C(F)(F)F)=C1)/C(/N)=N/OC(=O)C1SC=CC=1	4.18
346	C1(CC2=CC=C(C(=O)NC3=C(F)C=CC(F)=C3)O2)C(C)=NOC=1C	4.18
347	O=S(C1C2C(=NSN=2)C=CC=1)(NCC1=NC=C(C2=CC=CC=C2)C=N1)=O	4.18
348	FC1=C(C2OC=C(CN3C(=O)C4=C(C=CS4)N=C3)N=2)C(F)=CC=C1	4.18
349	CSCCNC(NNC(C1C(C2SC(C)=CC=2)=CNC=1)=O)=S	4.18
350	CC1C(/C=C2/C(=O)N=C(NC3=C(C)C=CC(C)=C3)S/2)=C(C)NN=1	4.18
351	FC1=C(Cl)C=C(CS(NCC2OC3=C(C=CC=C3)C=2)(=O)=O)C=C1	4.18
352	COC1=C(C2SC=C(CSC3OC(C4OC=CC=4)=NN=3)N=2)C=C(Br)C=C1	4.18
353	C12C=C(C=CC=1C(=O)C1=C(C=CC=C1)C2=O)OC(C)=O	4.18
354	C1S[C@H](C2=CC=C3OCOC3=C2)C2C=NNC=2NC1=O	4.18
355	C1(C#N)=C(C=CC2C=CC=CC=2O)C(O/C/1=C(/C#N)\C#N)(C)C	4.18
356	FC(COCCNC(NNC1=C(Br)C=C(F)C=C1)=O)F	4.18
357	N1=C(N)N[C@@](C2=CC=C(C)C=C2)(CC2=CC=CO2)C1=O	4.18
358	C1(=CSC=C1C1=CC(C)=NC(F)=C1)C(F)F	4.18

359	C1(CN)C(C)=NOC=1C1C=CC2=C(C=1)OC(N2)=O	4.18
360	C1(C=C(C(O)=C(C(C)(C)C)C=1)C(C)(C)C)[C@@H]1NN=C(C2C=CC=CC=2)S1	4.18
361	FC1=C(F)C=C(NNC(C(NC2=CN=C(C3CC3)N=C2)=O)=O)C(F)=C1	4.18
362	O=N(C1=C2C(C=CC=C2)=C(OC2=C(F)C(F)=NC(F)=C2F)C=C1)=O	4.18
363	C1(=O)N(N(C)C)C=CC2N=C3C=CN(CCC4CCCCC=4)C(=O)C3=CC1=2	4.18
364	S(C1C=CC=CC=1)(=O)(=O)/C(/C#N)=C(/SCC1=CC=CC(C)=C1)\NC1C(C)=CC(=CC=1C)C	4.18
365	C1(=CC=C(Br)S1)[C@](CN)(O)C1=CC=CC(F)=C1	4.18
366	C1(=C(/NCC2C=CC=CC=2)\NCC2C=CC=CC=2)/C(=O)C2C(=CC=CC=2)C/1=O	4.18
367	ClC1=NC=C(NS(C2CCOC3=C(C=CC=C3)C=2)(=O)=O)C=C1	4.18
368	COC(C1=C(C)C(C(O)=O)=O)=C(S(NC2=CC3=C(N4C(=N3)CCCCC4)C=C2)(=O)=O)S1)=O	4.18
369	N(C1C=C(C(=CC=1C)[C@H](C1C=CC(=CC=1)Cl)C#N)Cl)(=O)=O	4.18
370	C1(=CC=C(C(C)(C)CN)N1)C1C=C(Br)C=CC=1F	4.18
371	CN1[C@H](C2ON=C(C)N=2)CN(C2C(=O)N(C(F)F)C=CN=2)CC1	4.18
372	N(/C1C=CC(=CC=1)C(C)(C)C)=N\C1C=CC(=CC=1)C(C)(C)C	4.18
373	CC1CN(C(NC2=NC=C(Br)C(N3CCOCC3)=C2)=O)CCC=1	4.18
374	ClC1=C(N2CCSCC2)C=CC(NC(NOCC2=CN=CC=C2)=O)=C1	4.18
375	N[C@H]1[C@@H]2C[C@@H](CC2)[C@H]1C(NC1=CC(I)=CC=C1)=O	4.18
376	O=S(C1=CC=CC=C1)(N(C1SC=CN=1)CC1ON=C(C2=COC=C2)N=1)=O	4.18
377	[N+]12CC(=CSC=1N(C1C=CC=CC2=1)CC1=CC=CC=C1)C	4.18
378	N1C(/C=C/C=C2\C(C)=CC(C)=[NH+]\2)=C(C)C=C1C	4.18
379	C1(C(=O)/N=C2\SC=C(C(OCC)=O)N\2)=CC(=NN1C)C1=CC=CC=C1	4.18
380	OC(C1SC(/C=C/C2C=CC(F)=C(N(=O)=O)C=2)=NC=1)=O	4.18
381	S(=O)(=O)(C1C(C)=CC(=C(C)C=1)C)N1CCN=C1N1CCCCC1	4.18
382	C1(C(Cl)=CC=CC=1Cl)C(=O)/N=C1\NCCN\1	4.18

383	O=C(OC1=C2C(C=CC=C2)=CC=C1)CC1C2=C(C=CC=C2)ON=1	4.18
384	FC([C@@H](C1=NC=CC=C1)OC([C@@H]1ON=C(C2=CC=CC=C2)C1)=O)(F)F	4.18
385	O=S(OC1=CC=C(N2N=NN=C2)C=C1)(CC1C2=C(C=CC=C2)ON=1)=O	4.18
386	COC(C1=CC(NS(CC2=CC(F)=C(C)C=C2)(=O)=O)=C(Cl)C=C1)=O	4.18
387	O=S(C1=CN=C(C#N)C=C1)(NC1OC(C2=CN(C3=CC=CC=C3)N=C2)=NN=1)=O	4.18
388	O=S(CC1C2=C(CCC2)N(C2=CC=CC=C2)N=1)(CC1SC=CN=1)=O	4.18
389	[C@H]12[C@@H](C3=CC=CS3)N(O[C@H]1C(N(CC)C2=O)=O)C1C=CC=CC=1	4.18
390	O=C(C1C=CC2N(CCS(N=2)(=O)=O)C=1)NC1C(C2=CC=CC=C2)=NNC=1	4.18
391	N1(C)C(F)=C(/C=N/NC(=O)COC2C=CC(=CC=2F)F)C(C)=N1	4.18
392	N1(C(=O)/C=C/C2=CC=CO2)C=NC(C2C=CC=CC=2)=N1	4.18
393	COC1=CC=C(N(C(COC2=CC=C(C3OC=NN=3)C=C2)=O)CC2SC=CC=2)C=C1	4.18
394	C1(N/N=C/C2C=CC(=CC=2Cl)Cl)C(Cl)=C(Cl)C(=C(Cl)N=1)C#N	4.18
395	ClC1=NC=C(C(NC2CCN(S(CC3=CC=CC=C3)(=O)=O)CC2)=O)N=C1	4.18
396	N1(CNC2C(=NC=NC1=2)N)[C@@H]1O[C@H]([C@H](OC(C)=O)[C@@H]1OC(C)=O)COC(C)=O	4.18
397	CN1C(=S)N[C@@H](C2N=C(C3=CC=C(Cl)C=C3)SC=2)C(C(NC2=NOC(C)=C2)=O)=C1C	4.18
398	O=C(N1CCN(C2NN=C(C3CC3)C=2)CC1)CSC1N2C(C=CC=C2)=NN=1	4.18
399	CC1=CC(S(NC2=C(N3N=CC=C3)N=CC(Br)=C2)(=O)=O)=CC=C1	4.18
400	C1(Cl)C(=O)NN=CC=1N/N=C\[C@@H]1CCC=CC1	4.18
401	CC1SC(C(NNS(C2=C(C(F)(F)F)C=CC=C2)(=O)=O)=O)=CC=1	4.18
402	O=C(O[C@H](C1=CC=CC=C1)C1SC=CN=1)CCC1OC(C2=CC=CC=C2)=NN=1	4.18
403	ClC1=CC=C(SC2=C(NC(COC(CC3=CSC=C3)=O)=O)C=CC=C2)C=C1	4.18
404	C1(SC2=CC=C(/C=N/NC(=O)C3=CC=CC=C3N(=O)=O)O2)SC2=C(C=CC(OCC)=C2)N=1	4.18
405	C1(N)N(CCO)N=C(CCC2CCCCC2)C=1N	4.18
406	O1C=CN=C1C(=O)C1C=C(F)C(F)=C(F)C=1	4.18

407	C12NCCCN1C=C(C1=CC=C(C=C1)CCC)N=2	4.18
408	CC1=C2C(CCCC2)=NC(NS(C2=CN(C3=C(F)C=CC=C3)N=C2)(=O)=O)=N1	4.18
409	C[C@H](C(NNC1=NC2=C(C=CC=C2)N=C1)=O)SC1SC2=C(C=CC=C2)N=1	4.18
410	CC1=CC(C)=C(C[S@](CC(NCCOC2=CC(F)=CC=C2)=O)=O)C(C)=C1	4.18
411	C1(C(OC)=O)SN=C(C2=CC=C(C=C2)F)C=1N	4.18
412	CC1N(C)C=C(C(/C=C/C2=CC(C)=C(OC(F)F)C(C)=C2)=O)N=1	4.18
413	O1[C@@H]2CO[C@H]1C(C[C@@H]2SC1C(C)=CC=C(C(C)(C)C)C=1)=O	4.18
414	CNC(C1=CC=C(CN(CN2C(=O)C3=C(N(N=C3)C)N=N2)C)C=C1)=O	4.18
415	CC(C1=CC=C(C2SC(CSCC3N(C)C=NN=3)=CN=2)C=C1)C	4.18
416	FC(C1=CN=C(NNC(C2SC=C(Br)N=2)=O)C=C1)(F)F	4.18
417	C1(NC2C=CC(=C(N)C=2)OC)NCCN=1	4.18
418	O=C(C1C(C#CC2C=CC=CC=2)=CC=CC=1)OCC	4.18
419	CC1=C2C(CCCN2S(C2=C3N(CCCO3)N=C2)(=O)=O)=CC(Cl)=C1	4.18
420	S(C1C=CC=CC=1)(=O)(=O)/C(/C#N)=C(/[H])\C1=CC=C(C2C=CC(=CC=2)C(OCC)=O)O1	4.18
421	C[C@@H](N1N=CN=C1)C(NNC(C1=CC(N(=O)=O)=CC=C1)=O)=O	4.18
422	N1(CC(C)C)C(=O)/C(/N=C1SCC(=O)NC1SC2=C(CCCC2)C=1C(OC)=O)=C\C1=CC=C(C)S1	4.18
423	CN(C1=NC(COC(C2=C(S(N3CCSCC3)(=O)=O)C=CS2)=O)=NC(N)=N1)C	4.18
424	S(C1C=CC=CC=1)(=O)(=O)/N=C1\SC(=C(C(=O)N[C@@H](CCSC)C(OC)=O)N\1)C	4.18
425	N1(N(/C(=N/C(=O)C2C=CC(C(C)(C)C)=CC=2)/N=N1)C(C1C=CC(C(C)(C)C)=CC=1)=O)CCCC	4.18
426	C1(S(CCC)(=O)=O)=C(C(=O)C2C=CC(=CC=2)OC)N2C(C(C)=CC(C)=C2)=C1S(CCC)(=O)=O	4.18
427	C(=S)(N1CCOCC1)N[C@H](C(Cl)(Cl)Cl)NC(=O)C1=CC=CC2C=CC=CC1=2	4.18
428	C1(N(C)C)=NC(OCCNC(=O)NC2C=CC=CC=2)=NC(OC)=N1	4.18
429	CC1=CC(OCC2ON=C(C3=NC=CN=C3)N=2)=C(F)C=C1	4.18
430	C1(C(=O)C2C=CC3=C(OCCO3)C=2)=CC2=C(C(C)=NC=C2CNCCOC)O1	4.18

431	CN1C(=O)C(Br)=CC(NC(NCC2N3C(C=CC=C3)=NN=2)=O)=C1	4.18
432	CC1=CC(C)=C(OC[C@@H](CN2CCN(C/C=C/C3=CC=CC=C3)CC2)O)C=C1	4.18
433	O=N(C1=CC(/C=C/C(O[C@@H](C(F)(F)F)[C@@H]2OCCC2)=O)=CC=C1)=O	4.18
434	ClC1=NC(=C2C(=N1)N(C=N2)[C@H]1[C@@H]([C@@H]([C@@H](CO)O1)F)O)N	4.18
435	IC1=C(C(N2C[C@H]3N(CCOC3)CC2)=O)C=NN1	4.18
436	C1(SCCCN=1)NC1=C(CC)C=CC=C1C	4.18
437	S1(=O)(=O)N=C(C2=CC=CO2)C=C(C(=O)NC2=CC=CC=C2C(OC)=O)N1C	4.18
438	N1(C(C)=C(N=N1)/C(/C)=N/N=C(\C)/C1=CC=C(C=C1)N(=O)=O)C1=NON=C1N	4.18
439	N1(CC)C(=O)/C(/NC1=O)=C\C1=CC(Cl)=CC(I)=C1O	4.18
440	C/C(/C)=C(/C(NNC1ON=C(C2=CC=NC=C2)N=1)=O)\F	4.18
441	N1(NC(=O)NS(=O)(=O)C2C=CC(=CC=2N(=O)=O)Cl)C(C(C)(C)C)=NN=C(SC)C1=O	4.18
442	CCOC(C1=NNC(NC(C2SC3=C(COCC3)C=2)=O)=C1)=O	4.18
443	C12C3=CC=CC=C3SCC=1C=C(C(NCCCN(C(C)C)CC1=CC=CC=C1)=O)S2	4.18
444	N1C2=CC=CC=C2CC[C@@H](SCCC(=O)NC2=CC=CC3=C2C=CC=N3)C=1O	4.18
445	S1(=O)(=O)C[C@@H]2[C@H](C1)N(C(=O)S2)C1=CC=C(C=C1)C	4.18
446	CC1=CC=C(C)N1C1SC=CC=1C(=O)O	4.18
447	C[C@@H](C1=CC(F)=CC=C1)C(N1OCCC1)=O	4.18
448	CC1=NOC([C@@H]2N(S(C3N(C)N=C(C)C=3C(F)F)(=O)=O)CCC2)=C1	4.18
449	C1(=C(CCC)C=NC(C)=N1)N1CCN(CC1)C/C(/C)=C/C1=CC=CO1	4.18
450	CC1=C(O)C(NC(/C=C/SC2=CC=CC=C2)=O)=CC=C1	4.18
451	S(C1=CC=CC=C1)(=O)(=O)[C@H]1CCCCCC/C/1=N\O	4.18
452	O=C(C1=C(CO/C(=N/O)/N)CS[C@@]2([C@H](NC(=O)/C(=N\OC)/C3OC=CC=3)C(=O)N12)[H])O	4.18
453	C12C(C)=CC(=NC=1SC(C#N)=C2/N=C/C1C=CC(=CC=1)Br)C	4.18
454	OC[C@H]1C=C[C@@H](NC(NCC2(C3=CC=C(F)C=C3)CC2)=O)C1	4.18

455	NC(NC(OCCCSCC1=C(Cl)C=CC=C1)=O)=O	4.18
456	CSC1=CC(NC(CN2C(=O)C3=C(C=CC=C3)S2)=O)=CC=C1	4.18
457	CC(C1=CC(C(C)C)=C(S(N2C(C)=C(SC3=CC=CC=C3)C(C)=N2)(=O)=O)C(C(C)C)=C1)C	4.18
458	O=C(C1SC(S(C2=CC=CC=C2)(=O)=O)=CC=1)NCC1=COC=C1	4.18
459	COCCNC(CN1CCN(CN2C(=S)SC(NC3=C(C)C=CC=C3)=N2)CC1)=O	4.18
460	N1(C2C=CC(=CC=2)C)C(=O)/C(=C(\C)/NCCO)/C(=NC1=O)O	4.18
461	C1(CN2CCN(CC2)C2CCOCC2)=C(O)OC=C(CN2CCN(CC2)C2C=CC(=CC=2)F)C1=O	4.18
462	C1C[C@H](C2SC(C3ON=C(C4=C(OC5=CC=CC=C5)N=CC=C4)N=3)=CN=2)OC1	4.18
463	N1(C=CN=C(SCC2C=CC(=CC=2)Cl)C1=O)C1C=CC(=C(C)C=1)C	4.18
464	S1(=O)(=O)N(CC2C=CC=CC=2)C2=CC=CC=C2C(=O)/C/1=C\NC1C=CC=CC=1	4.18
465	BrC1=CC=C(C2=NC(CS(C3SC=CC=3)(=O)=O)=CC=N2)C=C1	4.18
466	S1(=O)(=O)C(C2=CC=C(C=C2)C(C)C)=C(C(NC2C=CC(=C(C)C=2)C)=N1)C	4.18
467	C1(OC(=O)C2=CC=C(C=C2)N(=O)=O)OC(=NC=1/C=N/C1C=CC(=CC=1)OC)C1=CC=CC=C1	4.18
468	N1(C2C=CC(=C(Cl)C=2)Cl)C(=O)/C(=C/N2CCN(CC2)C(=O)C2=CC=CO2)/C(NC1=S)=O	4.18
469	CS(CC1(CC1)CC(OC1=C(C2=CC=CC=C2)C=CC=C1)=O)(=O)=O	4.18
470	CC1=NC(C)=C(C#N)C(OCC2N=NN(C3=CC=C(Cl)C=C3)C=2)=C1	4.18
471	CC(C1N(CC(NC2=C(C3=CC(F)=C(F)C(F)=C3)C=CC=C2)=O)N=NN=1)C	4.17
472	C12C=C(SC=1N=C(C)N=C2OC1C=CC2=C(OCO2)C=1)C1=CC=CC=C1	4.17
473	CC1=C(Cl)C(C(N2C=C/C(=N\CC(F)(F)F)/C=C2)=O)=CC=C1	4.17
474	C1(ON=C(C2C=CC=CC=2Br)C=1)S(F)(=O)=O	4.17
475	C12=C(C=CC3C(=CC(=O)OC1=3)C)O/C(=N\NC1=CC=C(C=C1)Cl)/C2=O	4.17
476	O=N(C1=NC=C(S(N[C@@H]2C3=C(C=CC(=C3)F)SCC2)(=O)=O)C=C1)=O	4.17
477	FC(C1=NN(COC(OC2CCCCC2)=O)C(=O)C=C1)(F)F	4.17
478	C1(=NC(CSC2=NC=CC=N2)=CC(=O)N1)N/C(/NC1C=CC(=CC=1)CC)=N/C(C1C=CC=CC=1)=O	4.17

479	NC1=NC(N2N=CC=C2)=CC(NCC2CCOCC2)=N1	4.17
480	N12N=CN=C1N=C(C(CC)=C2SC1=CC=C(C=C1)NC(=O)NC1=CC=C(C(Cl)=C1)F)C	4.17
481	COCC(N(CC(NC1OC(C2=CC=CC=C2)=C(C2=CC=CC=C2)N=1)=O)C)=O	4.17
482	O=S(/C=C/C1=CC=CC=C1)(OC1=C2C(OCCO2)=CC=C1)=O	4.17
483	CC1N(C)C(CNC2=C(Cl)C=C(F)C(Br)=C2)=NN=1	4.17
484	N1(C2=NC=CC=N2)C(Cl)=NC(C2=CC=CC(OC)=C2)=N1	4.17
485	FC1=CC(C2OC(CN3C(=O)C4=C(CCC4)N=C3)=NC=2)=CC=C1	4.17
486	CC(N1C=C(S(NC2SC(CC3=CC=CC=C3)=CN=2)(=O)=O)N=C1)C	4.17
487	CN1N=CC(N2C(=O)[C@H](NC(/C=C/C3=C(C#N)C=CC=C3)=O)CC2)=C1	4.17
488	CCN(C1=C(C)C=CC=C1)CCNC1=C(N(=O)=O)C=C(S(C)(=O)=O)S1	4.17
489	COC1=C(C2OC(C[S@@](CC3=C(Cl)C=CC(Cl)=C3)=O)=NN=2)C=CC=C1	4.17
490	C1(C#N)SC2=C(C=CC=C2)C=1OCC1=CC=C(C(Cl)=C1)Cl	4.17
491	CC1=C(OS(C2=C(Cl)N(C)C=N2)(=O)=O)C=CC(N(=O)=O)=C1	4.17
492	FC1=CC(COC2=CC3=C(C=CC(O3)=O)C=C2)=CN=C1	4.17
493	C(F)(F)(F)C1=CC=CC=C1NC(=S)NN1C=NN=C1	4.17
494	C1(COC(=O)C2C3C=CC=CC=3OC3C=CC=CC2=3)C(=CC=CC=1F)Cl	4.17
495	FC1=C(NNC(CCCCC2N=NNC=2)=O)C(F)=CC=C1	4.17
496	C1(C(CC)=NNC=1N)C1C=CC=CC=1C	4.17
497	C(=O)(C1=CC=CC(C)=C1)NNC(=O)/C=C/C(O)=O	4.16
498	N1(CC[C@@H](OC2C=CC(C)=NN=2)C1)C(=O)C1C=COC=1	4.16
499	C1(NC(=O)NC2=CC=CC=C2OCC)C2=CC(F)=CC=C2NC=1C1=CC=NC=C1	4.16
500	C1(=O)N(CC2C=CC=CC=2)C=CN(CC(O)=O)C1=O	3.35

Table S4. The amino residues in the active site of *D. postgatei (Homology model)* and *A. vinsoum* (Template protein).

The amino residues in the binding modes are highlighted in green while the amino residues that appear in both template protein and model are highlighted in yellow.

D. postgatei (Homology model)						*A. vinsoum* (Template protein)				
POSITION	**RESIDUE**	**X-coordinate**	**Y-coordinate**	**Z-coordinate**		**POSITION**	**RESIDUE**	**X-coordinate**	**Y-coordinate**	**Z-coordinate**
1	ASP155	15.274	-9.108	14.765		1	PRO144	22.312	29.337	19.782
2	ASP155	16.386	-9.166	12.115		2	PRO144	24.355	29.315	21.018
3	HIS156	12.673	-9.342	14.533		3	PHE198	3.742	15.969	19.644
4	PRO157	12.504	-5.861	17.041		4	PHE198	3.492	23.086	17.731
5	PRO157	13.102	-7.509	15.438		5	PHE198	3.035	22.612	21.962
6	PRO157	14.563	-6.654	18.032		6	PHE198	3.396	24.021	19.98
7	GLY158	11.14	-9.681	21.135		7	PHE198	4.425	18.343	17.956
8	LYS160	16.327	-7.453	22.852		8	GLN199	6.299	19.248	18.692
9	LYS160	16.817	-8.236	20.643		9	GLN199	6.64	21.552	20.605
10	TYR182	12.275	-1.041	31.825		10	GLN199	9.671	20.765	21.063
11	TYR186	12.673	7.164	31.866		11	GLN199	11.826	21.257	20.985
12	TYR186	13.076	6.294	31.913		12	GLN199	12.994	20.39	20.007
13	ALA210	-6.144	5.049	23.073		13	THR200	4.926	24.079	24.339
14	ALA210	-5.408	4.012	26.291		14	THR200	7.598	22.758	22.569
15	LEU211	-2.966	5.896	20.707		15	ARG201	10.701	24.808	24.489
16	LEU211	-3.33	9.728	20.644		16	ARG201	10.742	25.584	26.09
17	GLN212	0.128	3.211	22.495		17	ARG201	11.176	22.655	25.559
18	GLN212	0.776	5.85	21.697		18	ARG201	11.111	23.457	27.146
19	GLN212	2.342	3.701	23.546		19	ARG201	12.849	25.068	21.542
20	LEU213	4.898	8.32	19.727		20	ARG201	13.062	23.963	24.925

21	ARG214	6.511	6.835	24.950		21	ARG201	13.083	24.949	26.407
22	ARG214	7.055	4.018	20.876		22	ARG201	13.537	27.225	21.666
23	ARG214	8.187	0.883	19.658		23	ARG201	13.317	26.855	25.142
24	ARG214	8.042	8.773	24.588		24	ARG201	13.744	28.004	23.223
25	ARG214	10.342	1.672	20.176		25	ASN202	4.752	24.518	26.777
26	ARG214	9.591	4.646	22.138		26	ASN202	7.356	24.934	25.688
27	ARG214	9.544	5.367	20.511		27	ASN202	9.168	28.177	26.464
28	ARG214	10.551	3.274	20.854		28	PRO203	2.844	26.948	26.322
29	ASN215	6.138	8.858	22.058		29	MET204	1.83	23.829	23.587
30	ASN215	9.187	8.312	20.086		30	MET204	1.269	26.038	24.813
31	ASN215	10.709	8.105	20.932		31	HIS205	-0.657	29.988	24.396
32	MET217	-1.736	13.64	23.577		32	HIS205	0.177	27.96	24.673
33	MET217	0.752	14.023	20.340		33	HIS205	1.375	30.257	26.311
34	MET217	2.083	12.95	22.837		34	HIS205	1.235	30.666	28.774
35	HIS218	3.037	14.836	17.988		35	ALA207	-2.882	29.645	21.487
36	HIS218	2.753	17.734	18.420		36	ALA207	-2.172	30.906	19.389
37	HIS218	5.443	18.578	17.683		37	HIS208	-1.173	27.547	21.081
38	HIS218	6.103	15.401	17.416		38	HIS208	1.57	26.728	18.384
39	SER220	-2.723	13.554	14.940		39	HIS208	4.483	27.98	21.214
40	SER220	0.454	14.663	12.406		40	GLU210	-7.593	27.36	18.783
41	SER220	1.586	12.948	13.476		41	LEU211	1.856	24.156	14.737
42	HIS221	-3.223	12.742	18.386		42	LEU211	1.451	24.003	16.463
43	HIS221	2.016	8.498	16.589		43	LEU211	1.049	25.497	15.584
44	HIS221	2.385	12.691	16.294		44	LYS213	-8.013	22.258	19.997

45	LEU224	-3.3	8.778	14.980		45	MET214	-7.147	23.584	12.463
46	CYS225	-7.004	10.675	19.888		46	MET214	-6.529	23.797	14.118
47	ILE237	0.303	9.569	26.879		47	MET214	-6.198	26.291	14.415
48	HIS238	-1.571	6.873	26.641		48	MET214	-5.096	22.399	11.837
49	SER239	4.899	7.696	28.059		49	MET214	-5.658	21.838	15.375
50	LEU240	6.23	3.393	25.679		50	MET214	-4.449	22.636	13.478
51	LEU240	7.467	4.767	27.727		51	ALA215	-4.159	16.495	11.87
52	LEU240	7.638	1.571	24.803		52	ALA218	-5.606	19.002	9.004
53	LEU240	7.613	1.915	27.143		53	ILE226	3.916	18.013	25.283
54	ILE241	9.76	3.681	32.372		54	LEU229	12.115	20.157	27.759
55	GLY242	11.258	1.741	29.277		55	LEU229	12.116	20.727	24.953
56	GLY242	10.636	4.381	30.130		56	LEU230	11.473	16.243	28.86
57	GLY242	12.792	4.353	29.940		57	LEU230	12.651	18.872	29.873
58	ASN243	14.446	3.268	27.274		58	LEU230	15.575	18.17	28.603
59	ASN243	16.006	1.035	28.862		59	GLY231	16.842	20.261	29.549
60	ASN243	16.554	-0.57	30.271		60	GLN232	17.128	24.073	31.222
61	LEU244	14.371	7.68	25.842		61	LEU233	12.981	25.644	32.696
62	LEU244	14.843	5.883	26.741		62	LYS234	16.948	26.912	28.765
63	LEU244	14.69	8.953	27.044		63	LYS234	16.192	26.517	28.086
64	LEU244	16.422	5.04	28.972		64	LYS234	20.59	26.13	27.066
65	LEU244	17.328	9.948	25.647		65	PRO235	14.572	32.404	30.01
66	LEU244	17.251	9.672	27.404		66	PRO235	18.27	30.637	29.906
67	LEU244	17.569	4.305	26.035		67	GLY236	10.334	31.929	31.057
68	LEU244	17.663	6.806	27.516		68	GLY236	11.951	33.579	32.489
69	LYS245	11.312	0.694	24.105		69	GLY236	12.465	33.635	30.786

70	LYS245	10.868	2.513	22.615		70	ASP237	10.618	29.492	30.422
71	LYS245	12.226	0.547	22.740		71	ASP237	12.146	28.724	28.662
72	LYS245	11.616	3.068	24.131		72	ASP237	13.08	30.48	31.602
73	LYS245	12.92	1.061	24.146		73	ILE238	9	28.157	31.375
74	LYS245	14.049	3.609	24.196		74	ARG243	6.341	22.596	32.716
75	LYS245	14.66	2.177	23.333		75	ARG243	6.014	24.516	30.508
76	LYS245	17.024	3.594	23.727		76	ARG243	10.385	21.775	30.029
77	LYS245	17.037	6.728	23.035		77	ILE247	-0.705	21.861	29.147
78	PRO246	16.982	6.599	19.576		78	MET250	-5.311	23.175	26.439
79	PRO246	20.68	6.083	20.090		79	MET250	-4.126	23.514	28.427
80	GLY247	16.965	8.998	18.742		80	MET250	-3.181	22.513	25.589
81	GLY247	17.77	10.322	19.618		81	PHE267	17.722	16.593	20.931
82	GLY247	18.661	8.787	21.119		82	PHE267	18.064	17.929	24.219
83	ASP248	12.972	6.09	23.082		83	ASP268	20.613	18.728	21.698
84	ASP248	13.145	8.695	23.933		84	MET269	15.68	24.378	20.673
85	ASP248	15.664	11.083	23.274		85	MET269	17.155	21.611	23.07
86	ILE249	12.517	10.908	23.146		86	MET269	17.376	24.896	20.821
87	ILE249	12.19	12.953	21.772		87	MET269	18.58	20.444	20.775
88	ILE249	14.402	14.009	22.143		88	MET269	18.396	22.912	20.626
89	ILE249	13.6	15.532	22.593		89	MET269	19.215	20.917	23.489
90	PRO250	14.678	11.387	27.906		90	MET269	19.131	23.03	22.242
91	PRO250	15.884	12.836	25.058		91	MET269	21.493	21.895	21.046
92	ALA251	11.731	10.043	31.165		92	TYR271	18.789	24.874	17.066
93	ALA251	13.515	11.411	29.969		93	TYR271	18.627	27.341	18.813
94	ARG254	7.257	9.842	30.256		94	TYR271	19.409	22.976	18.214

95	ARG254	6.82	10.424	25.768		95	TYR271	19.932	26.52	21.856
96	ARG254	9.424	9.338	26.801		96	TYR271	19.758	26.707	23.211
97	ARG254	9.889	8.483	28.259		97	TYR271	19.006	27.266	23.419
98	ILE258	2.363	16.485	25.473		98	TYR271	21.664	25.294	22.163
99	ILE258	4.396	12.118	25.762		99	TYR271	22.064	24.962	19.737
100	LEU278	7.225	-2.466	28.244		100	PRO274	15.755	22.074	6.807
101	LEU278	7.063	-1.326	30.319		101	PRO274	16.374	25.013	9.427
102	ASP279	7.299	-5.594	26.504		102	PRO274	17.453	24.266	6.963
103	ASP279	8.127	-5.197	29.546		103	ARG275	18.251	20.544	9.371
104	ASP279	10.58	-5.72	26.907		104	ARG275	18.86	21.329	9.192
105	ASP279	11.056	-4.044	29.367		105	ARG275	20.713	19.743	8.814
106	ASP279	11.835	-6.126	29.364		106	GLU276	17.888	20.385	16.879
107	MET280	6.428	-1.925	23.937		107	GLU276	18.12	21.57	16.559
108	MET280	7.345	-0.534	22.201		108	HIS280	15.06	18.675	18.312
109	MET280	8.072	-1.372	24.336		109	ARG284	10.841	17.004	17.941
110	MET280	9.334	-5.901	23.473		110	ARG284	10.567	16.995	20.183
111	MET280	9.062	-3.026	22.949		111	PHE292	4.147	14.509	11.299
112	MET280	9.683	-0.285	22.718		112	PHE292	7.766	17.435	16.739
113	ARG281	2.866	-8.317	25.529		113	ILE293	2.459	21.586	14.892
114	ARG281	5.236	-7.516	24.306		114	ILE293	4.068	21.625	14.133
115	ARG281	6.094	-9.073	24.379		115	ILE293	6.184	19.797	14.118
116	ARG281	8.177	-8.274	20.328		116	GLY295	8.084	25.411	10.684
117	ARG281	7.96	-8.16	22.837		117	ARG296	5.208	33.129	6.487
118	TYR282	6.864	-5.142	18.563		118	ARG296	7.33	33.797	6.908
119	TYR282	6.603	-5.587	20.769		119	ARG296	8.114	33.352	8.412
120	TYR282	8.535	-3.809	17.102		120	ASP297	12.554	29.738	13.066

121	TYR282	10.363	-5.613	20.496		121	ASP297	12.812	30.74	10.511
122	TYR282	9.539	-1.635	17.701		122	HIS298	9.949	21.14	15.164
123	TYR282	11.37	-3.445	21.101		123	HIS298	9.229	20.757	15.887
124	TYR282	10.866	-0.469	19.166		124	HIS298	10.953	25.136	14.277
125	HIS291	-2.791	-3.106	22.577		125	HIS298	13.729	24.542	12.782
126	HIS291	2.263	-2.978	23.918		126	ALA299	12.43	24.749	15.632
127	HIS291	1.673	-1.722	21.612		127	ALA299	14.22	22.116	15.477
128	PHE294	-1.459	-0.168	28.331		128	GLY300	15.478	28.152	13.579
129	PHE294	-0.384	-3.922	26.607		129	GLY300	16.415	28.234	16.51
130	PHE294	-0.202	-1.464	26.654		130	VAL301	17.939	29.077	13.902
131	MET303	-3.546	0.413	21.642		131	VAL301	17.667	30.747	16.378
132	ILE304	-6.567	3.711	21.274		132	VAL301	19.007	31.033	13.542
133	ILE304	-4.605	2.652	19.265		133	VAL301	20.88	30.1	18.062
134	ILE304	-4.493	4.492	17.862		134	VAL301	20.393	31.478	17.047
135	ILE305	-4.036	-1.8	18.205		135	VAL301	21.42	28.683	16.177
136	ILE305	-3.994	1.279	17.274		136	GLY302	17.468	33.611	12.964
137	GLY306	-2.672	0.628	13.076		137	GLY302	18.484	32.735	16.149
138	GLY306	-2.772	2.228	15.620		138	GLY302	20.428	33.513	14.288
139	GLY306	-2.707	3.741	13.737		139	ASP303	16.922	36.207	10.491
140	ARG307	-2.462	3.355	9.215		140	ASP303	17.882	34.071	10.689
141	ARG307	-1.856	3.307	11.625		141	ASP303	18.053	37.205	8.865
142	ARG307	-0.098	1.468	9.019		142	ASP303	19.462	33.487	8.484
143	ARG307	0.694	1.648	12.290		143	ASP303	19.712	36.212	11.08
144	ASP308	1.479	-2.075	11.486		144	ASP303	20.479	34.154	12.192

145	ASP308	1.987	-1.5	9.181		145	TYR304	19.883	31.845	11.118
146	ASP308	2.778	-0.772	13.766		146	TYR304	20.799	29.468	10.62
147	ASP308	2.891	0.631	11.330		147	TYR304	20.231	29.973	7.242
148	ASP308	3.701	-0.928	11.611		148	TYR304	21.329	31.689	8.605
149	ASP308	3.713	-0.114	8.962		149	TYR304	22.717	31.586	14.308
150	HIS309	-1.445	-0.209	15.637		150	TYR304	23.873	31.27	9.487
151	HIS309	-1.022	-0.15	20.517		151	TYR305	16.363	28.361	9.394
152	HIS309	-0.628	0.916	18.279		152	TYR305	18.114	28.954	6.988
153	HIS309	-0.333	-1.197	13.519		153	GLY306	14.515	29.867	4.629
154	HIS309	1.298	-3.205	15.650		154	PRO307	10.206	31.355	4.985
155	ALA310	1.957	-2.89	19.257		155	PRO307	10.143	31.922	7.914
156	ALA310	2.483	-0.642	17.004		156	PRO307	10.382	32.895	5.859
157	ALA310	4.651	-4.388	17.079		157	PRO307	12.531	31.596	4.788
158	GLY311	4.689	-3.475	13.474		158	PRO307	12.669	32.517	6.305
159	GLY311	7.075	-2.644	15.223		159	PHE308	6.497	30.999	4.746
160	VAL312	8.206	-5.789	11.730		160	PHE308	8.442	25.991	4.654
161	VAL312	9.218	-4.645	15.469		161	PHE308	8.293	29.492	3.918
162	VAL312	9.035	-3.188	13.426		162	ASP309	13.617	22.798	5.238
163	VAL312	11.28	-4.951	13.272		163	ASP309	13.328	24.906	3.997
164	VAL312	11.13	-3.588	14.407		164	ASP309	14.341	27.239	3.306
165	VAL312	11.556	-5.207	15.011		165	ASP309	15.572	25.028	5.164
166	GLY313	8.16	-4.294	9.315		166	ASP309	16.257	27.529	4.315
167	GLY313	10.454	-3.579	11.686		167	ALA310	12.727	24.785	7.524
168	GLY313	10.71	-5.981	10.283		168	ALA310	13.501	23.536	9.633

169	GLY313	11.056	-4.367	9.617		169	THR312	9.209	22.91	0.974
170	ASP314	7.68	-5.547	6.962		170	THR312	9.716	23.893	2.368
171	ASP314	9.26	-4.857	5.282		171	THR312	12.38	23.547	1.975
172	ASP314	9.548	-7.901	6.394		172	THR312	12.507	24.302	1.396
173	ASP314	10.039	-6.567	8.358		173	ILE313	15.335	20.684	4.898
174	ASP314	10.895	-6.335	4.981		174	ILE313	17.59	20.298	5.707
175	PHE315	7.932	-7.667	9.558		175	PHE314	10.782	18.327	5.987
176	PHE315	11.162	-8.689	11.702		176	ILE327	3.163	16.72	6.904
177	TYR316	4.87	-6.908	9.565		177	PHE328	-2.852	21.775	9.827
178	GLY317	0.021	-4.965	9.150		178	ARG329	1.925	20	7.181
179	MET318	-0.259	-3.879	6.206		179	ARG329	3.785	22.879	6.068
180	MET318	0.516	-0.06	5.675		180	ARG329	4.895	22.162	3.863
181	MET318	1.464	-2.195	5.099		181	ARG329	6.13	19.574	4.247
182	MET318	3.513	-1.357	6.053		182	ARG329	6.486	21.489	0.709
183	MET318	2.992	-0.383	4.657		183	ALA330	3.338	24.198	11.894
184	MET318	3.76	-1.968	4.400		184	ASP331	0.907	28.435	11.793
185	GLU320	0.662	-5.671	12.323		185	ASP331	0.726	28.737	8.47
186	ALA321	-1.579	-4.392	14.682		186	ASP331	2.445	29.947	6.624
187	PHE325	-6.405	-5.254	18.141		187	ASP331	3.359	28.266	9.868
188	ILE345	-5.608	5.083	14.478		188	ASP331	3.132	30.519	8.619
189	ILE345	-6.237	6.274	16.658		189	ASN332	1.767	31.014	12.87
190	ILE345	-4.454	6.339	12.669		190	ASN332	1.165	33.362	12.206
191	ASP346	-4.296	4.79	9.646		191	ASN332	2.932	34.22	9.94
192	ASP346	-4.163	7.798	10.375		192	ASN332	3.922	32.488	12.367
193	TRP347	-1.007	8.959	6.736		193	ASN332	4.572	34.061	10.538
194	TRP347	0.075	5.966	2.360		194	THR333	-2.443	28.133	15.166

195	TRP347	-0.194	6.262	5.663		195	THR333	-2.117	29.994	16.584
196	TRP347	-0.444	6.518	8.906		196	THR333	-1.807	33.444	14.383
197	TRP347	1.495	4.069	3.048		197	ALA334	-3.571	35.404	13.235
198	TRP347	1.118	4.492	8.006		198	TYR335	-9.599	32.604	18.441
199	TRP347	1.84	3.569	5.498		199	TYR335	-7.82	34.342	18.047
200	THR348	-2.268	13.029	11.530		200	VAL342	-5.441	30.519	16.265
201	THR348	-1.199	12.614	7.659		201	MET344	-3.322	24.492	10.746
202	PHE349	-1.361	15.147	7.161		202	MET345	-4.756	32.418	6.168
203	PHE349	0.434	14.731	5.610		203	MET345	-3.343	34.428	8.122
204	PHE349	1.013	10.55	4.925		204	MET345	-2.348	35.665	10.482
205	ILE372	2.774	14.184	4.367		205	MET345	-2.003	33.32	8.498
206	LEU373	3.167	15.796	7.037		206	MET345	-0.59	34.539	11.615
207	LEU373	4.499	17.845	8.649		207	ARG346	-2.058	23.992	6.462
208	LEU373	4.558	15.183	9.004		208	ARG346	-2.167	31.015	7.275
209	SER374	7.106	11.995	7.136		209	ARG346	-2.593	31.647	4.533
210	SER374	9.378	12.169	7.555		210	ARG346	-1.195	27.588	3.964
211	GLY375	6.532	11.91	10.778		211	ARG346	-0.461	23.36	6.811
212	GLY375	7.219	12.067	12.979		212	ARG346	-0.678	28.777	6.709
213	GLY375	6.989	13.826	12.841		213	ARG346	-0.546	30.623	5.478
214	GLY375	9.497	13.882	13.096		214	ARG346	0.267	27.477	4.973
215	THR376	9.046	11.834	10.735		215	ASP347	-5.736	27.614	7.1
216	THR376	11.447	9.639	9.764		216	ASP347	-4.294	25.496	6.611
217	THR376	11.471	12.231	12.159		217	PHE356	-5.976	37.446	12.664
218	THR376	13.405	11.005	9.301		218	PHE356	-5.892	38.366	9.3

219	THR376	13.463	11.406	11.034		219	PHE356	-5.967	38.801	11.511
220	THR376	13.303	12.703	9.826		220	GLN358	-2.325	38.795	12.933
221	LYS377	10.337	15.497	6.935		221	GLN358	-2.946	39.998	18.663
222	LYS377	9.639	15.875	6.188		222	GLN358	-1.469	39.207	16.304
223	LYS377	11.811	15.214	5.426		223	GLN358	0.116	36.941	13.581
224	LYS377	12.422	15.099	7.093		224	LEU359	-2.137	36.945	18.582
225	LEU378	5.643	16.669	13.802		225	LEU359	-1.217	40.408	22.011
226	LEU378	8.483	15.974	13.506		226	SER360	1.845	36.076	19.747
227	ARG379	13.333	13.794	16.717		227	SER360	0.966	38.71	20.546
228	ARG379	14.311	12.032	15.307		228	SER360	3.073	38.187	19.263
229	ARG379	13.801	15.499	16.514		229	GLY361	3.945	33.45	22.725
230	ARG379	15.442	11.035	12.092		230	GLY361	3.297	34.735	20.901
231	ARG379	16.303	13.209	11.922		231	THR362	4.827	36.271	22.456
232	ARG379	15.785	14.031	16.171		232	THR362	5.882	38.415	22.66
233	ARG379	16.094	14.346	13.239		233	THR362	6.114	39.777	24.719
234	LYS380	14.646	15.819	8.339		234	THR362	8.114	37.672	22.614
235	LYS380	15.23	15.754	10.766		235	ARG363	1.446	41.362	22.311
236	LYS380	15.794	16.963	12.836		236	ARG363	3.06	40.759	22.756
237	SER383	17.104	17.803	15.987		237	VAL364	0.523	33.877	27.842
238	PHE392	1.115	17.101	8.595		238	ARG365	6.326	34.095	29.229
239	VAL397	6.47	20.15	20.943		239	ARG365	7.794	35.902	28.093
240	LEU401	11.658	17.421	22.086		240	ARG365	7.5	35.602	30.722
241	TYR405	14.812	15.171	18.954		241	ARG365	7.384	38.391	30.575
242	TYR405	16.949	15.932	19.321		242	ARG365	9.141	39.119	27.653

						243	GLU366	6.493	41.965	26.481
						244	PHE378	-5.526	32.61	22.483
						245	PHE378	-4.189	34.085	20.671
						246	PHE378	-4.746	35.464	18.667
						247	ARG380	-5.956	29.157	27.714
						248	LEU387	1.474	30.68	31.356
						249	LEU387	2.763	28.412	33.01
						250	MET46	16.645	12.605	20.887