SUPPORT VECTOR MACHINE MODEL FOR PREDICTING ACTIVITY OF INHIBITORS AGAINST SARS-COV 3CLPRO ENZYME

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Table S1. Inhibitory activities (logIC50) of 204 compounds against SARS-CoV 3CLpro enzyme

No.	SMILES	Exp.log*IC50*	Calc. log*IC50*
	Training set		
1	ClC1=CC=C(C(N(C2=O)C(CC2)=O)=C1)OC(C3=CC=CO3)=O	1.265	1.034
2	ClCC(NC1=C(C(C2=CC=CC=C2)=O)C(C)=C(C)S1)=O	1.066	0.886
3	O=C(C4=CSN=N4)N(C2=CC=C(C(C)C)C=C2)C(C(NC3CCCC3)=O)C1=CC=CN=C1	1.449	0.764
4	O=C(C4=CC=CO4)N(C2=CC=C(C(C)CC)C=C2)C(C(NC3CCCC3)=O)C1=CC=CN=C1	0.348	0.748
5	ClC3=CC=C(C=C3)C(C1=C(C=CC=C2)C2=[N+](N1CCC(N)=O)[O-])=O	0.688	0.994
6	BrC1=CC=C(C(C(C=CC3=CC=CC=C3OC)=O)=C1)OC(C2=CC=CO2)=O	0.951	0.941
7	O=C2C1=CC=CC=C1N(CCCC3=CC=CC=C3)C2=O	1.268	0.868
8	[H]C([C@@H](NCC2N(C(C(C=C4)=CC=C4Br)=O)CC3([H])C(CCCC3)([H])C2)CC1=CNC=N1)=O	1.799	1.789
9	O=C1C2(C(C)C)CN(C(C4=CC=CC=C4[N+]([O-])=O)=O)CC(C(C)C)1CN(C(C3=CC=CC=C3[N+]([O-])=O)=O)C2	1.046	1.964
10	ClCC(N1N=C(C3=CC=CS3)CC1C2=CC=C(C)C=C2)=O	0.622	0.841
11	S=C(N/N=C/C2=CC=CC(OC)=C2)NC1=CC=CN=C1	1.410	1.400
12	O=C(CN4N=NC5=CC=CC=C45)N(C2=CC=C6C(CCC6)=C2)C(C(NCC3=CC=CO3)=O)C1=CC=CO1	1.180	1.190
13	BrC3=CC=C(C=C3)C(CN1N=NC2=CC=CC=C12)=O	0.603	1.026
14	ClC1=CC(C(C2=C(C=CC=C3)C3=[N+](N2CCC(N)=O)[O-])=O)=CC(Cl)=C1N	0.992	0.928
15	CC(C)C(O)CC/C(C)=C/CC1=C(O)C=CC(C(/C=C/C2=CC=C(O)C=C2)=O)=C1O	1.346	1.101
16	O=C(N(C4=CC=CC([N+]([O-])=O)=C4)N=C2C3=CC=CC=C3)/C2=C\C1=CC=C(C(O)=O)C=C1	0.924	1.251
17	O=C3C1=C(C(OC=C4C)=C4C3=O)C=CC2=C1C=CC=C2C	1.588	1.357
18	ClCC(N(C2=CC=CC=C2)NC(NC1=CC=CC=C1)=O)=O	0.984	1.095
19	O=C(C2=CC=CC=C2[N+]([O-])=O)NC1=CC(C3=CC=C(C)C=C3)=NN1	1.386	0.975
20	OC1=CC(O)=CC(OC2=C(O)C=C(O)C4=C2OC3=C(O)C=C(O)C=C3O4)=C1	0.944	1.145
21	O=C1C(C(CCCC(C)3CO)=C3C=C2)=C2C(OC=C4C)=C4C1=O	1.394	1.388
22	ClCC(N1N=C(C2=CC=CS2)CC1C(C=C3OC)=CC=C3OC)=O	0.362	0.352
23	O=C(C(C2=CC=NC=C2)N(C3=CC=C(C(C)(C)C)C=C3)C(C1=CC=CO1)=O)NC(C)(C)C	1.653	0.770

No.	SMILES	Exp.log*IC50*	Calc. log*IC50*
24	O=C(C3=CC=CC=C3)OC[C@H](C(NC2CCCCC2)=O)NC(/C=C/C1=CC=CC=C1)=O	1.477	1.467
25	ClC1=CC=CC=C1/C=C\C(NC2=CC=CN=C2)=O	1.383	1.393
26	O=C(C2=CC(O)=NC3=CC=CC=C23)N(CC4)CCN4C1=CC=CC(C)=C1C	0.823	0.953
27	O=C(C(C2=CC=CN=C2)N(C3=CC=C(C(C)(C)C)C=C3)C(C1=CC=CS1)=O)NC(C)(C)C	1.699	1.567
28	O=C(C)C(N(C)C2=CC=CC=C12)=C1OC(C3=CC=CO3)=O	1.656	0.958
29	O=C(C(C2=CC=CN=C2)N(C3=CC=C(C(C)(C)C)C=C3)C(C1=CC=CO1)=O)NC(C)(C)C	1.672	0.789
30	O=CC1=CN(CC3=CC=CC=C3)N=C1C2=CC=CN=C2	0.858	0.953
31	O=C2C1=CC=CC(C)=C1N(CCOC3=CC=CC=C3)C2=O	1.333	1.238
32	O=C(C2(CCCCC2)N(C(C=C5)=CC=C5OC)C(CN3N=NC4=CC=CC=C34)=O)NC1CCCC1	0.897	0.734
33	O=C(N1CCC(OC(N[C@H](C(N[C@@H](C[C@H]2C(NCC2)=O)C(O)S(=O)(O)=O)=O)CC(C)C)=O)CC1)OCC	0.944	0.954
34	O=C(C3=CC=CC=C3)O[C@@H](C(NC2CCCCC2)=O)[C@H]([C@]4=CC=CC=C4)NC(/C=C/C1=CC=CC=C1)=O	1.633	1.772
35	O=C1C(C#N)=C(C2=CC([N+]([O-])=O)=CC=C2)N=C(SCC3=CC=C([N+]([O-])=O)C=C3)N1	1.025	1.035
36	COC(C1=CNC(SSC2=CC=CC=C2C(OCC)=O)=N1)=O	0.775	0.785
37	ClC2=CC=C(C=C2)C(OC1=CC=CN=C1)=O	0.800	1.444
38	O=C(C(C2=CC=CN=C2)N(C3=CC=C(C(C)(C)C)C=C3)C(C1=CC=CO1)=O)NC(C)(C)C	0.342	0.789
39	O=C(/C=C/C3=CC(OC)=CC=C3)O[C@@H](C(NC2CCCCC2)=O)[C@H]([C@]4=CC=CC=C4)NC(/C=C/C1=CC=CC=C1)=O	1.813	1.228
40	O=C(N(C4=CC=C(C(O)=O)C=C4)N=C2C3=CC=CC=C3)/C2=C\C1=CC=C(C5=CC=CC=C5)C=C1	0.806	0.816
41	O=S(C)(N1CC(CC3=CC=CC=C3)C(OC(N[C@H](C(N[C@@H](C[C@H]2C(NCC2)=O)C=O)=O)CC(C)C)=O)CC1)=O	0.591	0.601
42	O=C1N(CC(NCC3=CC=CO3)=O)C(NC(C)1C2=CC=C4C(C=CC(OC)=C4)=C2)=O	1.493	0.866
43	OC1=CC(O)=CC(OC2=C(O)C=C(O)C4=C2OC3=C(O)C=C(OC5=C(O)C=C(OC6=C(O)C=C(O)C8=C6OC7=C(O)C=C(O)C=C7O8)C=C5O)C=C3O4)=C1	0.431	0.441
44	[H]C([C@@H](NCC3C[C@]4([H])[C@@](CCCC4)([H])[C@H](O3)CN(C)CC2=CC=CC=C2)CC1=CNC=N1)=O	2.602	2.592
45	ClC(C=C2)=CC=C2SSC1=NN=CO1	-0.287	0.261
46	O=C(CN2N=NC3=CC=CC=C23)N(C(C=C4)=CC=C4NC(C)=O)C(C(NCC1OCCC1)=O)C(C=C5)=CC=C5OC	0.971	0.981

No.	SMILES	Exp.log*IC50*	Calc. log*IC50*
47	ClC(C=C2)=CC=C2SSC1=NC=C(NC(C)=O)S1	0.354	0.344
48	OC1=CC(O)=CC(OC2=C(O)C=C(O)C4=C2OC3=C(O)C=C(OC5=C(O)C=C(O)C=C5O)C=C3O4)=C1	1.624	1.295
49	CC(C)C3=CC1=C(C(C3=O)=O)C(CCCC(C)2C)=C2C=C1	1.324	1.515
50	OC1=C2C(OC(C3=CC(C4=C5C(C(C=C(C6=CC=C(OC)C=C6)O5)=O)=C(O)C=C4O)=C(OC)C=C3)=CC2=O)=CC(OC)=C1	1.584	1.393
51	O=C(N[C@@H](CC(C)C)C(N[C@H](C(CN(NC4=O)C(C3=C4C([N+]([O-])=O)=CC=C3)=O)=O)C[C@H](CCN2)C2=O)=O)[C@@H](NC([C@H]([C@H](C)C)NC(C)=O)=O)[C@@H](C)OCC1=CC=CC=C1	-0.222	-0.212
52	FC(C=C4)=CC=C4N(N=C2C3=CC=CC=C3)C(/C2=C\C1=CC=C(C(O)=O)C=C1)=O	0.833	1.190
53	FC1=CC=CC=C1N4C(/C(C(NC4=O)=O)=C/C2=CN(CC(N5CCOCC5)=O)C3=CC=CC=C23)=O	1.535	1.341
54	O=C(C(C3=CC=CN=C3)N(C4=CC=C(C(C)CC)C=C4)C(C2=CC=CO2)=O)NC1CCCC1	0.342	0.748
55	O=C(N[C@@H](CC(C)C)C(N[C@H](C(C(F)(F)F)=O)CC1=CC=CC=C1)=O)[C@@H](NC([C@H](C)NC(OCC2=CC=CC=C2)=O)=O)[C@@H](C)C	1.000	1.314
56	CC(CC3)CCN3S(C1=CC=C(NC(C2=O)=O)C2=C1)(=O)=O	0.072	0.563
57	O=C(CN2N=NC3=CC=CC=C23)N(COC)C1=C(CC)C=CC=C1CC	1.608	1.129
58	CC(CC)(C)NC(C(C2=CN(C)C=C2)N(C1=CC=C(NC(C(C)C)=O)C=C1)C(CN(N=N4)C3=C4C=CC=C3)=O)=O	0.613	0.808
59	ClC3=CC=C(C=C3)C(NC2=CC=C1N(C)C=NC1=C2)=O	1.056	1.046
60	O=C2OC1=CC(OC(C3=CC=CO3)=O)=CC=C1C(C)=C2	0.524	0.790
61	O=C2N(CC4OC3=CC=CC=C3OC4)C(C(C2=O)=C1)=CC=C1OCC	0.633	0.922
62	ClCC(N(C(C=C3)=CC=C3[N+]([O-])=O)C1=CN(C(C)=O)C2=CC=CC=C12)=O	1.034	1.064
63	O=S(C)(N1CC(CC3=CC=CC=C3)C(OC(N[C@H](C(N[C@@H](C[C@H]2C(NCC2)=O)C(O)S(=O)(O)=O)=O)CC(C)C)=O)CC1)=O	0.633	0.623
64	BrC1=CN=CC(C(N/N=C/C(C2=CC=CC=C2C=C3)=C3O)=O)=C1	1.159	1.149
65	ClCC(N(CCC2=CC=CC=C2)CCC1=CC=CC=C1)=O	1.212	1.077
66	ClC1=CC=CC(F)=C1/C=C/C(NC2=CC=CN=C2)=O	1.566	1.438
67	[H]C([C@@H](NCC2C[C@]3([H])[C@@](CCCC3)([H])[C@H](O2)CN(C)CCCC)CC1=CNC=N1)=O	2.000	2.343
68	O=C(N(C4=CC=C(C(C)C)C=C4)N=C2C3=CC=CC=C3)/C2=C\C1=CC=C(C5=C(C(O)=O)C=CC(Cl)=C5)C=C1	0.778	1.304

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69	O=C(N1CCC(OC(N[C@H](C(N[C@@H](C[C@H]2C(NCC2)=O)C=O)=O)CC(C)C)=O)CC1)OC(C)(C)C	0.322	0.933
70	O=S(N(C)C)(C1=CC=CC(NC(CSC2=CC=CC3=CC=CN=C23)=O)=C1)=O	1.081	0.864
71	O=C(N(C4=CC=CC=C4)N=C2C3=CC=CC=C3)/C2=C\C1=CC=C(C5=C(C(O)=O)C=CC(Cl)=C5)C=C1	1.215	1.329
72	BrC(C(C)=C3)=CC=C3NC(CON(C1=C2)N=NC1=CC=C2S(=O)(C)=O)=O	1.126	0.875
73	O=C(N(C4=CC=C(C(C)(C)C)C=C4)N=C2C3=CC=CC=C3)/C2=C\C1=CC=C(C5=C(C(O)=O)C=CC(Cl)=C5)C=C1	0.763	1.310
74	O=C(N[C@@H](CC2CCCCC2)C(N[C@H](C(C(NCC4=CC=CC=C4)=O)=O)C[C@H](CCN3)C3=O)=O)/C=C/C1=CC=CC=C1	-0.149	-0.139
75	O=C(N(C4=CC=C(C#N)C=C4)N=C2C3=CC=CC=C3)/C2=C\C1=CC=C(C(O)=O)C=C1	0.740	1.254
76	FC1=CC=C(C(C2NC(C)=O)=C1)N(CCN3CCOCC3)C2=O	0.959	0.969
77	O=C([C@H](CC2CC2)N1C=CC=C(NC(OC(C)(C)C)=O)C1=O)N[C@H](C(C(NCC4=CC=CC=C4)=O)=O)C[C@H](CCN3)C3=O	-0.174	-0.047
78	OC1=CC(O)=C(C[C@@H](OC(C4=CC(O)=C(O)C(O)=C4)=O)[C@@H]([C@H]3CC(O)C(O)C(O)C3)O2)C2=C1	1.863	1.244
79	CCC(OO)CC1=C(OC)C=CC(C(/C=C/C2=CC=C(O)C=C2)=O)=C1O	1.057	1.047
80	O=C(C(C2=CC=CN=C2)N(C3=CC=C(C(C)(C)C)C=C3)C(C1=CNC=N1)=O)NC(C)(C)C	0.778	0.793
81	[H]C([C@@H](NC[C@@H]2C[C@]3([H])[C@@](CCCC3)([H])[C@H](O2)CN(C)CC(C)C)CC1=CNC=N1)=O	1.978	2.405
82	C[C@H](C)[C@@H](C(N[C@@H]([C@@H]1CCCCC1)C(N[C@@H](CC2=CNC=N2)C(C)=C)=O)=O)NC([C@H]([C@H](C)C)NC(C)=O)=O	1.991	1.426
83	CC1(C(OCC)=O)CN(C3=CC=CC=C3)CC2=C1N(CCC4=CNC5=C4C=CC=C5)N=N2	0.975	0.965
84	O=C(COC(C4=CC=CN=C4)=O)N2C1=CC=CC=C1SC3=CC=CC=C23	1.206	1.196
85	O=C(/C=C/C3=CC=CC=C3)O[C@@H](C(NC2CCCCC2)=O)[C@H]([C@]4=CC=CC=C4)NC(/C=C/C1=CC=CC=C1)=O	1.875	1.773
86	O=C2NC1=CC=C(S(N3CCN(CC4=CC(Cl)=CC=C4)CC3)(=O)=O)C=C1C2=O	1.501	0.834
87	O=C1C(C(CCCC(C)3C)=C3C=C2)=C2C(OC=C4C)=C4C1=O	1.950	1.668
88	O=C(CN3N=NC4=CC=CC=C34)N(CC5=CC=CO5)C(C(NCC2=CC=CO2)=O)C1=CC=CC(OC)=C1	0.890	0.900
89	ClCC(N1N=C(C2=CC=CS2)CC1C(C=C3OC)=CC=C3OC(F)F)=O	0.447	0.480
90	O=C(C2=CC=C1N=CSC1=C2)O	1.084	1.171

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91	OC1=C2C(OC(C3=CC(C4=C5C(C(C=C(C6=CC=C(O)C=C6)O5)=O)=C(O)C=C4O)=C(OC)C=C3)=CC2=O)=CC(OC)=C1	1.505	1.412
92	O=C(N[C@@H](CC(C)C)C(N[C@H](C(CN(NC4=O)C(C3=C4C=CC=C3)=O)=O)C[C@H](CCN2)C2=O)=O)[C@@H](NC([C@H]([C@H](C)C)NC(C)=O)=O)[C@@H](C)OCC1=CC=CC=C1	0.431	0.421
93	O=C(C(C2=CC=CN=C2)N(C3=CC=C(C(C)(C)C)C=C3)C(C1=CN=CO1)=O)NC(C)(C)C	1.591	1.324
94	O=C(CN3N=NC4=CC=CC=C34)N(C(C=C5)=CC=C5NC(C)=O)C(C(NCC2OCCC2)=O)C1=CC=CC(OC)=C1	1.049	1.039
95	O=C2N(CCN3CCOCC3)C1=CC=C(CC)C=C1C2NC(C)=O	0.817	0.903
96	O=C2NC1=CC=C(S(N3CCCCC3C)(=O)=O)C=C1C2=O	0.352	0.378
97	ClC1=CC(CC(NC2=CC=CN=C2)=O)=CC=C1Cl	1.449	1.372
98	BrC1=CC=C(C(C(/C=C\C3=CC=CC=C3F)=O)=C1)OC(C2=CC=CO2)=O	0.853	0.915
99	O=C1C(C#N)=C(C2=CC=C(OC)C=C2)N=C(SCC3=CC=C([N+]([O-])=O)C=C3)N1	1.420	1.250
100	[O-][N+]1=C3C(C=CC=C3)=C(C(C2=CC=CC([N+]([O-])=O)=C2)=O)N1CCC(N)=O	1.183	1.193
101	CC(CC)(C)NC(C(C2=CN(C)C=C2)N(C1=CC=C(NC(CC)=O)C=C1)C(CN(N=N4)C3=C4C=CC=C3)=O)=O	0.839	0.829
102	ClCC(N1N=C(C3=CC=C(C)O3)CC1C2=CC=CO2)=O	0.716	0.441
103	O=C(C(C2=CC=CN=C2)N(C3=CC=C(C(C)C)C=C3)C(C1=CC=CO1)=O)NC(C)(C)C	0.322	0.412
104	O=C([C@H](CC2CCCCC2)N1C=CC=C(NC(OC(C)(C)C)=O)C1=O)N[C@H](C(C(NC4CC4)=O)=O)C[C@H](CCN3)C3=O	0.378	0.131
105	FC4=CC=C(C5=C4)N(C(C)CC5)CC(N3CC1=C(CC3)NC2=CC=C(C)C=C12)=O	1.404	1.178
106	OC1=CC(O)=C(C(C(O)=C(C3=CC=C(O)C(O)=C3)O2)=O)C2=C1	1.863	1.086
107	O=C(C(C2=CC=CN=C2)N(C3=CC=C(C(C)(C)C)C=C3)C(C1=CN(C)C=N1)=O)NC(C)(C)C	1.875	0.755
108	CN1C=CC(CN(C2=CC=C(NC(CC)=O)C=C2)C(CN(N=N4)C3=C4C=CC=C3)=O)=C1	0.462	0.794
109	O=C(C(C2=CC=CN=C2)N(C3=CC=C(C(C)(C)C)C=C3)C(C1=CC=C(Cl)O1)=O)NC(C)(C)C	0.716	0.872
110	FC5=CC=C(C=C5)NC(C(C2=CC=CC(OC)=C2)N(C(CN3N=NC4=CC=CC=C34)=O)C1CC1)=O	1.022	1.013
111	ClC(C=C5)=CC=C5C1C(N4C=NC=C4)C(C3=CC=C(Br)C=C3)=NN1C2=CC=C(Cl)C(Cl)=C2	0.398	0.408
112	CC(CC)(C)NC(C(C2=CN(C)C=C2)N(C1=CC=C(NC(C3CCC3)=O)C=C1)C(CN(N=N5)C4=C5C=CC=C4)=O)=O	0.580	0.590
113	O=S(C)(N1CCC(OC(N[C@H](C(N[C@@H](C[C@H]2C(NCC2)=O)C(O)S(=O)(O)=O)=O)CC(C)C)=O)CC1)=O	1.624	1.366

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114	O=S(C)(N1CCC(OC(N[C@H](C(N[C@@H](C[C@H]2C(NCC2)=O)C=O)=O)CC(C)C)=O)CC1)=O	1.459	1.469
115	O=C(CN2N=NC3=CC=CC=C23)N(C(C=C4)=CC=C4NC(C)=O)C(C(NC(C)(C)CC)=O)C1=CC=CN1C	0.799	0.652
116	O=C(C2=CC(O)=NC3=CC=CC=C23)NCCOC1=CC=CC=C1OC	0.556	1.110
117	ClC(C=C2)=CC=C2SSC1=NC(C(OC)=O)=CN1	0.616	0.606
118	[H]C([C@@H](NC[C@H]2C[C@]3([H])[C@@](CCCC3)([H])[C@H](O2)CN(C)CC(C)C)CC1=CNC=N1)=O	2.415	2.405
119	O=C3C1=C(C(OC=C4C)=C4C3=O)C=CC2=C1CCCC2C(OC)=O	1.324	1.168
120	O=C3C1=C(C(OCC4C)=C4C3=O)C=CC2=C1CCCC(C)2C	2.355	1.624
121	[H]C([C@@H](NCC2C[C@]3([H])[C@@](CCCC3)([H])[C@H](O2)CN(C)CC=C)CC1=CNC=N1)=O	2.623	2.394
122	O=C(N1CCC(OC(N[C@H](C(N[C@@H](C[C@H]2C(NCC2)=O)C(O)S(=O)(O)=O)=O)CC(C)C)=O)(CC3=CC=CC=C3)CC1)OC(C)(C)C	0.799	0.819
123	O=C(OCC2=CC=CC=C2)N[C@@H](CC(C)C)C(N[C@H](C(C(F)(F)F)=O)CC1=CC=CC=C1)=O	1.176	1.186
124	O=C(CN2N=NC3=CC=CC=C23)N(C(C=C5)=CC=C5NC(C)=O)C(C(NC1CCCC1)=O)C(C=C4O)=CC=C4O	1.151	1.141
125	FC(F)(C2=CC1=[N+](N(CCC(N)=O)C(C(C3=CC=C(C)C=C3)=O)=C1C=C2)[O-])F	1.304	1.026
126	O=C3C1=C(C(OCC4C)=C4C3=O)C=CC2=C1C=CC=C2C	1.158	1.287
127	CC(CC3)CCN3S(C1=CC=C(N(C)C(C2=O)=O)C2=C1)(=O)=O	0.017	0.892
128	ClCC(N(C(C=C3)=CC=C3OC)CC1=CC(O)=NC2=CC=CC=C12)=O	1.148	1.138
129	O=C(C(O)=C3C)C=C1C3=CC=C2[C@](CC[C@@]5(C)CC=C(C)CC45)(C)[C@@]4(C)CC[C@@]12C	0.415	0.808
130	CN1C=CC(CN(C2=CC=C(NC(C3CCC3)=O)C=C2)C(CN(N=N5)C4=C5C=CC=C4)=O)=C1	0.908	0.898
131	O=C(N[C@H](C(N[C@H](C(O)S(=O)(O)=O)C[C@H]2C(NCC2)=O)=O)CC(C)C)OCC1=CC=CC=C1	-0.046	-0.056
132	C/C(C)=C/CC/C(C)=C/CC1=C(OC)C=CC(C(/C=C/C2=CC=C(O)C=C2)=O)=C1O	1.533	1.102
133	O=C(C(O)=C3C)C=C1C3=CC=C2[C@](CC[C@@]5(C)CC[C@@](C)([C@@](OC)=O)CC45)(C)[C@@]4(C)CC[C@@]12C	0.740	0.750
134	FC1=CC=CC=C1N(C(NC4=O)=O)C(/C4=C/C2=CNC3=CC=CC=C23)=O	0.976	1.300
135	FC1=CC=CC=C1N4C(/C(C(NC4=O)=O)=C/C2=CN(CC(N(CC)CC)=O)C3=CC=CC=C23)=O	1.342	1.333
136	O=C(N1CCC(OC(N[C@H](C(N[C@@H](C[C@H]2C(NCC2)=O)C(S(=O)(O)=O)O)=O)CCC)=O)CC1)OC(C)(C)C	0.708	0.718

No.	SMILES	Exp.log*IC50*	Calc. log*IC50*
137	O=C(CN1N=NC2=CC=CC=C12)N(C(C=C3)=CC=C3NC(C)=O)C(C(NC(C)(C)CC)=O)C(C=C4)=CC=C4O	1.073	1.063
138	O=C2OC1=CC(OC(C3=CC=CO3)=O)=CC=C1C(CC)=C2	0.472	0.655
139	O=C(N[C@H](C(N[C@H](C(O)S(=O)(O)=O)C[C@H]2C(NCC2)=O)=O)CC(C)C)OCC1=CC(Cl)=CC=C1	-0.301	-0.291
140	ClC1=CC=C(C(N2C(C(CC(C)CC3)C3C2=O)=O)=C1)OC(C4=CC=CO4)=O	0.732	0.898
	Validation set		
141	O=C2NC1=CC=C(S(N3CC(C)CC(C)C3)(=O)=O)C=C1C2=O	0.633	0.524
142	O=C(C3=CC=C(C)C(C)=C3)N2C1=CC=CC=C1N=C2	1.227	1.402
143	O=C(OCC1=CC=CC=C1)N[C@@H]([C@@H](C)CC)C(N[C@H](C(CF)=O)CC(N(C)C)=O)=O	0.724	1.014
144	O=C(C(C2=CC=NN=C2)N(C3=CC=C(C(C)(C)C)C=C3)C(C1=CC=CO1)=O)NC(C)(C)C	1.000	1.351
145	C[C@H](C)[C@@H](C(N[C@H](/C=C/C(OCC)=O)C[C@H](CCN1)C1=O)=O)CC([C@@H](NC([C@H](CO)NC(OC(C)(C)C)=O)=O)C(C)C)=O	1.000	1.419
146	O=C(CCC3=CC=CC=C3)O[C@@H](C(NC2CCCCC2)=O)[C@H]([C@]4=CC=CC=C4)NC(/C=C/C1=CC=CC=C1)=O	1.813	1.532
147	[O-][N+](C1=NON=C1NC(CSC2=NC=CC=C2)=O)=O	0.849	0.617
148	ClCC(N(C1C(C=C4)=CC=C4OC)N=C(C2=CNC3=CC=CC=C23)C1O)=O	0.554	1.254
149	ClCC(N4CCN(CC4)C2=C1C(CCC(C)C3)=C3SC1=NC(CC)=N2)=O	0.627	0.816
150	O=C(N1CCC(OC(N[C@H](C(N[C@@H](C[C@H]2C(NCC2)=O)C=O)=O)CC(C)C)=O)(CC3=CC=CC=C3)CC1)OC(C)(C)C	0.716	0.717
151	O=C(C(O)=C3C)C=C1C3=CC=C2[C@](CC[C@@]5(C)CC[C@@](C)([C@@](O)=O)CC45)(C)[C@@]4(C)CC[C@@]12C	1.013	0.801
152	BrC1=CC=C(C(C(C2=C3)N(C(CCl)=O)CCC2=CC(OC)=C3OC)=C1)F	0.995	1.421
153	O=C(OCC3=CC=CC=C3)N[C@@H](CC1=CC=CC=C1)C(N[C@H](C(C(F)(F)F)=O)CC2=CC=CC=C2)=O	1.301	1.352
154	[H]C([C@@H](NC[C@@H]2C[C@]3([H])[C@@](CCCC3)([H])[C@@H](O2)CN(C)CC(C)C)CC1=CNC=N1)=O	2.643	2.405
155	O=C(C(O)=C3C)C=C1C3=CC=C2[C@](CC[C@@]4(C)CC5=O)(C)[C@@](C4C[C@H]5C)(C)CC[C@@]12C	0.996	0.792
156	O=C2C1=CC=CC=C1N(C/C=C/C3=CC=CC=C3)C2=O	1.049	1.092
157	O=C(C(C2=NC=CN=C2)N(C3=CC=C(C(C)(C)C)C=C3)C(C1=CC=CO1)=O)NC(C)(C)C	0.740	0.912

No.	SMILES	Exp.log*IC50*	Calc. log*IC50*
158	O=C2N(CC4OC3=CC=CC=C3OC4)C1=CC=CC=C1C2=O	1.318	0.933
159	O=C(N(C4=CC=CC(Cl)=C4)N=C2C3=CC=CC=C3)/C2=C\C1=CC=C(C(O)=O)C=C1	1.033	1.006
160	BrC1=CC(C(N2N=C(C)C=C2C)=O)=CC=C1C	1.543	0.915
161	O=C(C3=CC=C(C)C=C3)OC2=CC=C1N(C)C=NC1=C2	1.106	1.238
162	O=C(CN2N=NC3=CC=CC=C23)N/N=C\C1=CC(OC)=C(C(OC)=C1)OC	0.714	1.026
163	CC(CC)(C)NC(C(C2=CN(C)C=C2)N(C1=CC=C(NC(C3CC3)=O)C=C1)C(CN(N=N5)C4=C5C=CC=C4)=O)=O	0.959	0.692
164	O=C(N1CCC(OC(N[C@H](C(N[C@@H](C[C@H]2C(NCC2)=O)C=O)=O)CC(C)C)=O)CC1)OCC	0.505	0.818
165	ClC3=CC=C(C=C3)C(CN1N=NC2=CC=CC=C12)=O	0.996	1.015
166	ClCC(C2=C(C)N(C(C)=C2)C1=CC=CC([N+]([O-])=O)=C1)=O	0.661	1.020
167	[H][C@](CN(C(C4=CC=C(Br)C=C4)=O)[C@@H]1CN[C@@H](CC3=CNC=N3)C([H])=O)2[C@@](CCCC2)([H])C1NC(CNC([C@H]([C@H](O)C)NC(C)=O)=O)=O	1.415	0.898
168	O=C(N3C2=CC=CC=C2SC4=CC=CC=C34)SC1=NN=C(C)S1	1.019	0.972
169	[H]C([C@@H](NC[C@H]2C[C@]3([H])[C@@](CCCC3)([H])[C@@H](O2)CN(C)CC(C)C)CC1=CNC=N1)=O	2.892	2.405
170	O=C(N[C@@H](CC(C)C)C(N[C@H](C([H])=O)CC1=CNC=C1)=O)[C@@H](NC([C@H](C)NC([C@@H](NC(C)=O)CO)=O)=O)[C@@H](C)C	1.991	1.242
171	CC1(C(OCC)=O)CN(C3=CC=CC=C3)CC2=C1N(CC4=CC=C(F)C=C4)N=N2	0.952	1.282
172	O=C(N[C@@H](CC2=CC=CC=C2)C(N[C@H](/C=C/C(OCC)=O)CC3=CC=CC=C3)=O)/C=C/C1=CC=C([N+]([O-])=O)C=C1	0.699	1.377
	Test set		
173	CC1=CC(C)=NC(SSC2=C([N+]([O-])=O)C=CC=C2)=N1	-0.036	-0.788
174	O=C(C)C1=C(N2CCCC2)NC(C3=CC=CC=C3)=C1	0.666	0.591
175	[H]C([C@@H](NCC2N(C(C(C=C5)=CC=C5C4=CC=CC=C4)=O)CC3([H])C(CCCC3)([H])C2)CC1=CNC=N1)=O	2.033	2.598
176	COC(C=C4)=CC=C4CCN(N=N2)C1=C2CN(C3=CC=CC=C3)CC1	0.949	0.632
177	OC1=CC(O)=CC(OC2=C(OC5=C(O)C=CC(O)=C5O)C=C(O)C4=C2OC3=C(O)C=C(O)C=C3O4)=C1	1.124	1.273
178	ClC(C=C5)=C(Cl)C=C5CN(N=N3)C1=C3CN(C4=CC=CC=C4)CC(C(OCC)=O)1CC2=CC=C(F)C=C2	0.975	1.810
179	C[C@H](C)[C@@H](C(N[C@H](C(CF)=O)CC(N(C)C)=O)=O)NC(OCC1=CC=CC=C1)=O	0.820	1.700

No.	SMILES	Exp.log*IC50*	Calc. log*IC50*
180	O=C(C1=C(NC(/C=C\C3=CC=CS3)=O)SC=C1C2=CC=CC=C2)O	0.718	0.495
181	BrC1=CC=C(C(C(/C=C\C3=CC=C(C)C=C3)=O)=C1)OC(C2=CC=CO2)=O	1.049	0.902
182	OC1=CC(O)=C(C[C@@H](OC(C4=CC(O)=C(O)C(O)=C4)=O)[C@H]([C@]3=CC(O)=C(O)C(O)=C3)O2)C2=C1	1.672	1.635
183	OC1=CC(O)=CC(O)=C1OC2=CC(O)=CC(O)=C2OC3=CC(C4=C(O)C=C(O)C=C4O)=C(O)C=C3O	1.352	1.317
184	OC1=CC(O)=C2C(OC(C3=CC(C4=C5C(C(C=C(C6=CC=C(O)C=C6)O5)=O)=C(O)C=C4O)=C(OC)C=C3)=CC2=O)=C1	1.859	1.453
185	BrC1=CC=C(C(C2NC(C)=O)=C1)N(CCN3CCOCC3)C2=O	0.880	0.910
186	FC1=CC=CC(CN(N=N3)C2=C3CN(C4=CC=CC=C4)CC2)=C1	1.077	1.073
187	O=C(C4=CC=CO4)N(C2=CC=C(C(C)C)C=C2)C(C(NC3CCCC3)=O)C1=CC=CN=C1	0.773	0.768
188	O=C1C(C#N)=C(C2=CC=C(Cl)C=C2)N=C(SCCC3=CC=CC=C3)N1	1.228	1.086
189	FC(F)(C1=CC(N4CCN(CC4)C(C2=CC(O)=NC3=CC=CC=C23)=O)=CC=C1)F	0.707	1.058
190	OC1=CC(O)=CC(OC2=C(O)C=C(O)C4=C2OC3=C(O)C=C6C(C5=C(O)C=C(O)C(OC7=CC(O)=CC(O)=C7)=C5O6)=C3O4)=C1	1.223	1.449
191	O=C(CN3N=NC4=CC=CC=C34)N(C2=C(C)C=C(C)C=C2C)C(C(NC(C)(C)C)=O)C1=CSC=C1	0.463	0.746
192	CN1C=CC(CN(C2=CC=C(NC(C3CC3)=O)C=C2)C(CN(N=N5)C4=C5C=CC=C4)=O)=C1	0.613	-0.153
193	CC(CC)(C)NC(C(C2=CN(C)C=C2)N(C1=CC=C(NC(C)=O)C=C1)C(CCC3=CN(C4=CC=CC=C4)N=N3)=O)=O	1.041	0.776
194	O=C(C2=CC(O)=NC3=CC=CC=C23)N1CCN(C4=CC=CC=C4)CC1	0.998	0.991
195	O=S(N(CC4)CCN4C(C2=CC(O)=NC3=CC=CC=C23)=O)(C1=C(C)C(C)=CC(C)=C1C)=O	0.684	0.888
196	O=C(C(O)=C3C)C=C1C3=CC=C2[C@](CC[C@@]5(C)CC[C@@](C)([C@@](O)=O)C[C@@]45[H])(C)[C@@]4(C)CC[C@@]12C	1.336	0.801
197	O=C2N(CC4OC3=CC=CC=C3OC4)C(C(C2=O)=C1)=CC=C1OC	0.988	0.944
198	[O-][N+]1=C2C(C=CC=C2)=C(C(C3=CC=C(C)C=C3)=O)N1CCC(N)=O	0.971	1.006
199	OC1=C(C4=C5C(C(C=C(C6=CC=C(O)C=C6)O5)=O)=C(O)C=C4O)C=C(C3=CC(C2=C(O)C=C(O)C=C2O3)=O)C=C1	0.919	1.429
200	O=C(OCC1=CC=CC=C1)N[C@@H](CC(C)C)C(N[C@H](C(CF)=O)CC(N(C)C)=O)=O	0.398	0.931
201	O=C(N[C@@H](CC1CCCCC1)C(N[C@H](C([H])=O)CC2=CNC=C2)=O)[C@@H](NC([C@H](C)NC([C@@H](NC(C)=O)CO)=O)=O)[C@@H](C)C	1.813	2.021
202	CN1C=CC(CN(C2=CC=C(NC(C(C)C)=O)C=C2)C(CN(N=N4)C3=C4C=CC=C3)=O)=C1	0.556	0.825

No.	SMILES	Exp.log*IC50*	Calc. log*IC50*
203	ClC1=CC=C(/C=C\C(NCC2=CC=CN=C2)=O)C=C1[N+]([O-])=O	1.444	1.655
204	O=C1C(C#N)=C(C2=CC=C(Cl)C=C2)N=C(SCC3=CC=C([N+]([O-])=O)C=C3)N1	0.785	1.170