Compound No.	SMILES	pIC50 (IC50 in microM)	
1	ClC1=CC(NC(=O)CSC2=NC=CC(=N2)C2=CSC(=N2)C2=CC=CC=C2)=CC(Cl)=C1	-0.477121255	
2	CN1N=C(C=C1C(F)(F)F)C1=CC=C(S1)C1=CC=NC(SCC(=O)NC2=CC=C(Cl)C=C2)=N1	-1	
3	CSC1=C(C(C)=C(S1)C1=NC(C)=CS1)C1=CC=NC(SCC(=O)NC2=CC=C(Cl)C=C2)=N1	-1.041392685	
4	CSC1=C(C(C)=C(S1)C1=NC(C)=CS1)C1=CC=NC(SCC(=O)NC2=CC=CC=C2Cl)=N1	BLINDED	*
5	CC1=NC(=CS1)C1=NC(=CS1)C1=NC(SCC(=O)NC2=CC=C(Cl)C=C2)=NC=C1	-1.146128036	
6	ClC1=CC=C(NC(=O)CSC2=NC=CC(=N2)C2=CC(=NO2)C2=CC=CC=C2)C=C1	-1.176091259	
7	FC(F)(F)C1=CC=C(NC(=O)CSC2=NC(=CC=N2)C2=CC(=NO2)C2=CC=C(Cl)C=C2Cl)C=C1	-1.176091259	
8	ClC1=CC=C(NC(=O)CSC2=NC=CC(=N2)C2=CC(=NO2)C2=C(Cl)C=CC=C2)C=C1	-1.176091259	
9	CCCC1=CC(Cl)=NC(SCC(=O)NC2=CC=C(Cl)C=C2)=N1	-1.477121255	
10	COC1=CC(=CC=C1)C1=C(C#N)C(=O)NC(SCC(=O)NC2=CC=C(C=C2)S(N)(=O)=O)=N1	-1.602059991	
11	CC(C)C1=CC=C(NC(=O)CSC2=NC(=CC=N2)C2=CC=CS2)C=C1	-1.602059991	
12	COC1=C(OC)C=C(NC(=O)CSC2=NC(O)=CC(=N2)C2=CC=CC=C2)C=C1	-1.653212514	
13	COC1=CC=CC(=C1)C1=C(C#N)C(=O)NC(SCC(=O)NC2=CC=C(C=C2)C(C)=O)=N1	-1.77815125	
14	CCC(SC1=NC(C2=CC=CC(OC)=C2)=C(C#N)C(=O)N1)C(=O)NC1=CC=CC(=C1)C(C)=O	-1.77815125	
15	CC1=CC(=O)NC(SCC(=O)NC2=C(OC3=CC=CC=C3)C=CC(Cl)=C2)=N1	-2	
16	CC1=CC(O)=NC(SCC(=O)NC2=CC=C(OC3=CC=C(Cl)C=C3)C=C2)=N1	-2.301029996	
17	CC(C)C1=CC=C(NC(=O)CSC2=NC=CC(=N2)C2=CSC(COC3=C(Cl)C=CC=C3)=N2)C=C1	-2.301029996	
18	COC(OC)C1=CC(O)=NC(SCC(=O)NC2=CC=C(C=C2)C(F)(F)F)=N1	-2.301029996	
19	CCCCC1=CC=C(NC(=O)CSC2=NC(C3CCCCC3)=C(C#N)C(=O)N2)C(C)=C1	-2.301029996	
20	FC(F)(F)C1=CC=CC(NC(=O)CSC2=NC(C3=CC=CC=C3)=C(C#N)C(=O)N2)=C1	-2.301029996	
21	CCOC(=O)C1=CN=C(SCC(=O)NC2=CC=C(C=C2)[N+]([O-])=O)N=C1N	-2.397940009	
22	CCOC1=CC=C(C=C1)N1C(=O)CC(SC2=NC(C)=CC(C)=N2)C1=O	-2.477121255	
23	COC1=CC=CC(=C1)C1=C(C#N)C(=O)NC(SCC(=O)NC2=CC=C(C=C2)[N+]([O-])=O)=N1	BLINDED	*
24	CC(SC1=NC(C2=CC=CC=C2)=C(C#N)C(=O)N1)C(=O)NC1=CC=C(Cl)C=C1	-2.477121255	
25	CC(C)(C)C1=CC=C(NC(=O)CSC2=NC(C3CCCCC3)=C(C#N)C(=O)N2)C=C1	-2.544068044	
26	COC1=CC=C(C=C1)C1=NC(SCC(=O)NC2=CC=C(C=C2)C(C)C)=NC=C1	-2.602059991	
27	CC1=NC(SCC(=O)NC2=CC=C(Cl)C=C2F)=NC(=C1)C(F)(F)F	-2.698970004	
28	CC1=COC2=C1C(=O)C(=O)C1=C3CCCC(C)(C)C3=CC=C21	BLINDED	*
29	CC1=COC2=C1C(=O)C(=O)C1=C3CCCC(C)(CO)C3=CC=C21	-1.394451681	
30	COC(=O)C1(C)CCCC2=C3C(=O)C(=O)C4=C(OC=C4C)C3=CC=C12	-1.324282455	
31	CC1COC2=C1C(=O)C(=O)C1=C3CCCC(C)(C)C3=CC=C21	-2.35545152	
32	CC1=COC2=C1C(=O)C(=O)C1=C2C=CC2=C(C)C=CC=C12	-1.587710965	
33	CC1COC2=C1C(=O)C(=O)C1=C2C=CC2=C(C)C=CC=C12	-1.158362492	

34	CC(C)C1=CC2=CC=C3C(CCCC3(C)C)=C2C(=O)C1=O	-1.324282455	
35	CC1=C(Cl)C=C(Cl)C(=C1)S(=O)(=O)C1=C(C=C(C=C1[N+]([O-])=O)C(F)(F)F)[N+]([O-])=O	0.522878745	
36	ClC(Cl)=C(Cl)C(=O)OC1=CC=C(C=C1)S(=O)(=O)C1=CC=C(OC(=O)C(Cl)=C(Cl)Cl)C=C1	0.045757491	
37	NC1=NC=C(C(N)=N1)S(=O)(=O)C1=CC=C(Cl)C=C1	-0.77815125	
38	[O-][N+](=O)C1=CC(=CC=C1S(=O)(=O)C1=CC=C(Cl)C=C1)C(F)(F)F	-1.079181246	
39	CC1=C(C(C)=C(C#N)C(=N1)S(=O)(=O)C1=CC=CC=C1)[N+]([O-])=O	-1.113943352	
40	CC1=CC=C(C=C1)S(=O)(=O)C1=NC(C)=C(C(C)=C1C#N)[N+]([O-])=O	-1.113943352	
41	[O-][N+](=O)C1=C[N+]([O-])=C(C=C1)S(=O)(=O)C1=CC=C(Cl)C=C1	-1.176091259	
42	CCOC(=O)C(=C\NC1=CC=C(C=C1)S(=O)(=O)C1=CC=C(N\C=C(/C#N)C(=O)OCC)C=C1)\C#N	BLINDED	*
43	OC(=O)C1=CC=C(C=C1)S(=O)(=O)C1=CC(Br)=C(O)C(Br)=C1	-1.204119983	
44	CC(=O)C1=CC=CC=C1S(=O)(=O)C1=CC=CC=C1C(O)=O	-1.204119983	
45	[O-][N+](=O)C1=CC=C(C=C1)S(=O)(=O)C1=CC=C(C=C1)[N+]([O-])=O	-1.397940009	
46	CCOC(=O)C(=CNC1=CC=C(C=C1)S(=O)(=O)C1=CC=C(NC=C(C(=O)OCC)C(=O)OCC)C=C1)C(=O)OCC	BLINDED	*
47	FC(F)(F)C1=NN=C(N1)SC(=O)C1=CC=C(O1)C#CC1=CC=CC=C1	-0.477121255	
48	CN1N=C(C=C1C1=CC=C(S1)C(=O)NC1=C(C(C)=NO1)[N+]([O-])=O)C(F)(F)F	-0.698970004	
49	CC1=C(C=C(O1)C(C)(C)C)C1=NNC(NS(=O)(=O)C2=CC=CS2)=C1	-1	
50	CSC1=NNC(NC(=O)C2=CC=CS2)=C1S(=O)(=O)C1=CC=C(Cl)C=C1	-1.176091259	
51	CC1(C)CC2=C(SC(NCC3=CC=CO3)=C2C(=O)C1)C#N	-1.204119983	
52	CSC1=NN(C2=C(C(C)=NN2C)[N+]([O-])=O)C(C2=CC=CS2)=C1C#N	-1.255272505	
53	ClC1=CC=C(S1)C1=CSC(CS(=O)(=O)C2=CC=CS2)=N1	-1.255272505	
54	CN1N=C(C)C(=C1NCC1=CC=C(S1)C1=CC=CS1)[N+]([O-])=O	-1.301029996	
55	O=C(CC1=NCCS1)C1=NC=CS1	-1.602059991	
56	ClC1=CC=C(C=C1)C1=CC=C(O1)C(=O)OC1=CN=CC(Cl)=C1	1.200659451	
57	[O-][N+](=O)C1=CC=C(C=C1)C1=CC=C(O1)C(=O)OC1=CN=CC(Cl)=C1	1.22184875	
58	[O-][N+](=O)C1=C(C=CC(Cl)=C1)C1=CC=C(O1)C(=O)OC1=CN=CC(Cl)=C1	BLINDED	*
59	[O-][N+](=O)C1=C(C=CC=C1)C1=CC=C(O1)C(=O)OC1=CN=CC(Cl)=C1	0.681936665	
60	[O-][N+](=O)C1=CC=CC(=C1)C1=CC=C(O1)C(=O)OC1=CN=CC(Cl)=C1	0.301029996	
61	ClC1=CC(OC(=O)C2=CC=NC=C2)=CN=C1	0.785156152	
62	ClC1=CC(OC(=O)C2=CN=CC=C2)=CN=C1	0.156767222	
63	ClC1=CC=C(C=C1)C(=O)OC1=CN=CC(Cl)=C1	BLINDED	*
64	[O-][N+](=O)C1=C(C=CC=C1)C(=O)OC1=CN=CC(Cl)=C1	0.477555766	
65	[O-][N+](=O)C1=CC=CC(=C1)C(=O)OC1=CN=CC(Cl)=C1	0.164943898	
66	ClC1=CC(OC(=O)C2=C3C=CC=CC3=CC=C2)=CN=C1	0.906578315	
67	ClC1=CC(OC(=O)C2=CC3=C(OC2=O)C=CC=C3)=CN=C1	0.966576245	

68	CN1CCN(CC1)S(=O)(=O)C1=CC2=C(NC(=O)C2=O)C=C1	BLINDED	*
69	ClC1=CC(CN2CCN(CC2)S(=O)(=O)C2=CC3=C(NC(=O)C3=O)C=C2)=CC=C1	-1.501196242	
70	COC1=CC(CN2CCN(CC2)S(=O)(=O)C2=CC3=C(NC(=O)C3=O)C=C2)=CC(OC)=C1OC	-1.50623436	
71	O=C1NC2=C(C=C(C=C2)S(=O)(=O)N2CCN(CCC3=CC=CC=C3)CC2)C1=O	-1.542949849	
72	O=C(N1CCN(CC1)S(=O)(=O)C1=CC2=C(NC(=O)C2=O)C=C1)C1=CC=CO1	-1.003029471	
73	O=C1NC2=C(C=C(C=C2)S(=O)(=O)N2CCN(CC2)C2=CC=CC=N2)C1=O	-1.710371264	
74	O=C1NC2=C(C=C(C=C2)S(=O)(=O)N2CCCCC2)C1=O	BLINDED	*
75	O=C1NC2=C(C=C(C=C2)S(=O)(=O)N2CCOCC2)C1=O	-1.102433706	
76	CC1CCN(CC1)S(=O)(=O)C1=CC2=C(NC(=O)C2=O)C=C1	-0.071882007	
77	CC1CCCCN1S(=O)(=O)C1=CC2=C(NC(=O)C2=O)C=C1	-0.352182518	
78	CC1CC(C)CN(C1)S(=O)(=O)C1=CC2=C(NC(=O)C2=O)C=C1	-0.633468456	
79	CN1C(=O)C(=O)C2=C1C=CC(=C2)S(=O)(=O)N1CCN(C)CC1	-1.072984745	
80	CN1CCN(CC1)S(=O)(=O)C1=CC2=C(C=C1)N(CC1=CC=CC=C1)C(=O)C2=O	-1.827369273	
81	CN1C(=O)C(=O)C2=C1C=CC(=C2)S(=O)(=O)N1CCOCC1	-0.996073654	
82	O=C1N(CC2=CC=CC=C2)C2=C(C=C(C=C2)S(=O)(=O)N2CCOCC2)C1=O	-1.14176323	
83	CC1CCN(CC1)S(=O)(=O)C1=CC2=C(C=C1)N(CC1=CC=CC=C1)C(=O)C2=O	-0.017033339	
84	CC1CCN(CC1)S(=O)(=O)C1=CC2=C(C=C1)N(C)C(=O)C2=O	-1.2509077	
85	CC1CC(C)CN(C1)S(=O)(=O)C1=CC2=C(C=C1)N(CC1=CC=CC=C1)C(=O)C2=O	-0.450249108	
86	CN1CCN(CC1)S(=O)(=O)C1=CC=C2N(CC3=CC=C4C=CC=CC4=C3)C(=O)C(=O)C2=C1	-1.918606915	
87	O=C1N(CC2=CC=C3C=CC=CC3=C2)C2=CC=C(C=C2C1=O)S(=O)(=O)N1CCN(CCC2=CC=CC=C2)CC1	-1.14176323	
88	O=C1N(CC2=CC=C3C=CC=CC3=C2)C2=CC=C(C=C2C1=O)S(=O)(=O)N1CCN(CC1)C1=CC=CC=N1	-0.741939078	
89	O=C1N(CC2=CC=C3C=CC=CC3=C2)C2=CC=C(C=C2C1=O)S(=O)(=O)N1CCCCC1	-1.146128036	
90	O=C1N(CC2=CC=C3C=CC=CC3=C2)C2=CC=C(C=C2C1=O)S(=O)(=O)N1CCOCC1	-1.600646236	
91	CC1CCN(CC1)S(=O)(=O)C1=CC=C2N(CC3=CC=C4C=CC=CC4=C3)C(=O)C(=O)C2=C1	-0.227886705	
92	CC1CC(C)CN(C1)S(=O)(=O)C1=CC=C2N(CC3=CC=C4C=CC=CC4=C3)C(=O)C(=O)C2=C1	-0.672097858	
93	CC1=C(CN2C(=O)C(=O)C3=CC(=CC=C23)C#N)C(C)=NO1	-0.857332496	
94	FC1=CC(Cl)=C(CN2C(=O)C(=O)C3=CC(I)=CC=C23)C=C1	-0.973127854	
95	IC1=CC=C2N(CC3COC4=C(O3)C=CC=C4)C(=O)C(=O)C2=C1	BLINDED	*
96	O=C1N(CC2=CC3=CC=CC=C3S2)C2=CC=CC=C2C1=O	-1.117602692	
97	[O-][N+](=O)C1=C2N(CC3=CC4=CC=CC=C4S3)C(=O)C(=O)C2=CC=C1	-0.301029996	
98	BrC1=C2N(CC3=CC4=CC=CC=C4S3)C(=O)C(=O)C2=CC=C1	0.008773924	
99	FC1=CC=C2N(CC3=CC4=CC=CC=C4S3)C(=O)C(=O)C2=C1	-0.683047038	
100	IC1=CC=C2N(CC3=CC4=CC=CC=C4S3)C(=O)C(=O)C2=C1	0.022276395	
101	ClC1=C2C(=O)C(=O)N(CC3=CC4=CC=CC=C4S3)C2=CC=C1	-1.049218023	

102	IC1=CC=C2N(C\C=C\C3=CC4=CC=CC=C4S3)C(=O)C(=O)C2=C1	-1.371067862
103	ClC1=CC=C(NC(=O)C2=CC=C(CN3C(=O)C(=O)C4=CC(I)=CC=C34)S2)C=C1	-1.099335278
104	IC1=CC=C2N(CC3=CC=C(S3)C(=O)N3CCCCC3)C(=O)C(=O)C2=C1	-1.243038049