Supporting Information

SVM Model for Virtual Screening of Lck Inhibitors

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Table 1. Database of collected compounds used for building SVM model and validation.

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
1	1	59	Train	C1(=C(C(=C2C(=C1[H])N=C(C(=C2N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])O[H])[H])[H])[H])[H])[H])C4=C(SC(=N4)C([H])=O)[H]	17600705
2	2	13	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])O[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
3	3	130	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3[H])[H])[H])O[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
4	4	73	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3[H])C([H])([H])[H])[H])O[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
5	5	190	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3[H])[H])C([H])([H])[H])O[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
6	6	41	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3Br)[H])[H])O[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
7	7	880	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C(C([H])([H])[H])(C([H])([H])[H])[H])[H])O[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
8	8	89	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
9	9	40	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])O[H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
10	10	100	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])O[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
11	11	270	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])F)[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
12	12	380	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])Cl)[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
13	13	86	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])OC([H])([H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
14	14	97	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])N([H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
15	15	1300	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(=O)N([H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
16	16	9300	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(=O)N(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
17	17	7700	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])N(S(=O)(=O)C([H])([H])[H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
18	18	3400	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N([H])[H])([H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
19	19	2700	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3[H])[H])[H])OC([H])([H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
20	20	3300	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3[H])[H])[H])F)[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
21	21	1800	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3[H])[H])[H])N(C([H])([H])[H])C(=O)C([H])([H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
22	22	1100	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3[H])[H])F)[H])F)[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
23	23	8.5	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])O[H])[H])[H])[H])=C(C(=C(C(=C1[H])S(=O)(=O)N([H])[H])[H])[H])[H]	17600705
24	24	54	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])OC([H])([H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])S(=O)(=O)N([H])[H])[H])[H])[H]	17600705
25	25	350	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C(=C(C(=C3[H])[H])F)[H])F)[H])[H])=C(C(=C(C(=C1[H])S(=O)(=O)N([H])[H])[H])[H])[H]	17600705
26	26	3000	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C4=C(C(=C3[H])[H])N=C(S4)[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
27	27	16000	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C4=C(C(=C3[H])[H])N=C(N4C([H])([H])[H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
28	28	3000	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C4=C(C(=C3[H])[H])N(N=C4[H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
29	29	1800	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C4=C(C(=C3[H])[H])N(C(=N4)[H])C([H])([H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
30	30	4400	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C4=C(C(=C3[H])[H])N=NN4[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
31	31	8200	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C(C4=C(C(=C3[H])[H])C(=NN4C([H])([H])[H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
32	32	560	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3[H])[H])[H])N=C(C(=C4[H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
33	33	490	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3[H])[H])[H])N=NN4[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
34	34	1400	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3[H])[H])[H])C(=NN4[H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
35	35	5600	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3[H])[H])[H])N(C(=N4)C([H])([H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
36	36	100	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3[H])[H])[H])N(N=C4[H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
37	37	12	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3C([H])([H])[H])[H])[H])N(N=C4[H])[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
38	38	520	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3[H])C([H])([H])[H])[H])N(N=C4[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
39	39	55	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3[H])[H])C([H])([H])[H])N(N=C4[H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
40	40	1600	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3[H])[H])[H])N(N=C4[H])C([H])([H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
41	41	2800	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3C([H])([H])[H])[H])[H])N(N=C4[H])C([H])([H])[H])[H])[H])=C(C(=C(C(=C1[H])C(=O)N([H])[H])[H])[H])[H]	17600705
42	42	33	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3[H])[H])[H])N(N=C4[H])[H])[H])[H])=C(C(=C(C(=C1[H])S(=O)(=O)N([H])[H])[H])[H])[H]	17600705
43	43	19	Train	C1(N(C2=NC(=C(C(=N2)[H])[H])N(C3=C4C(=C(C(=C3C([H])([H])[H])[H])[H])N(N=C4[H])[H])[H])[H])=C(C(=C(C(=C1[H])S(=O)(=O)N([H])[H])[H])[H])[H]	17600705
44	2	1	Train	N1=C(C(=C(N=C1C([H])([H])[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])C([H])([H])[H]	15546730
45	9	0.6	Train	C1(=C(C(=C(C(=C1[H])[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])[H])[H]	15546730
46	10	1.2	Train	C1(=C(C(=C(N=C1[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])[H])[H]	15546730
47	11	6	Train	C1(=C(C(=C(C(=N1)[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])[H])[H]	15546730
48	12	10	Train	N1=C(C(=C(C(=C1[H])[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])[H]	15546730
49	13	4	Train	N1=C(C(=C(C(=N1)[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])[H]	15546730
50	14	374	Train	C1(C(C(C(C(C1([H])[H])([H])[H])(N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	15546730
51	15	1	Train	C1(=C(C(=C(N=C1C([H])([H])[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])[H])[H]	15546730
52	16	1.1	Train	C1(=C(C(=C(N=C1[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])[H])C([H])([H])[H]	15546730
53	17	0.5	Train	C1(=C(C(=C(N=C1[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])C([H])([H])[H]	15546730
54	18	7.3	Train	C1(=C(C(=C(N=C1[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])C([H])([H])[H])[H])[H]	15546730
55	19	4	Train	C1(=C(C(=C(N=C1C([H])([H])[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])Cl)[H])[H])[H])C([H])([H])[H])[H]	15546730
56	20	50	Train	C1(=C(N=C(N=C1C([H])([H])[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])Cl)[H])[H])C([H])([H])[H])[H]	15546730
57	21	2	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])C([H])([H])[H])[H]	15546730
58	22	0.4	Train	N1=C(C(=C(N=C1[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])N(C(C(N4C(C(C(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	15546730
59	23	4	Train	N1=C(C(=C(N=C1[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])N(C(C(N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	15546730
60	24	1	Train	N1=C(C(=C(N=C1[H])N(C2SC(=C(N=2)[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H]	15546730
61	25	1	Train	C1(=C(C(=C(N=C1N2C([C@@](N(C(C2([H])[H])([H])[H])[H])[H])(C([H])([H])[H])[H])([H])[H])[H])N(C3SC(=C(N=3)[H])C(=O)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])[H])[H]	15546730
62	26	1	Train	C1(=C(C(=C(N=C1N(C(C(N2C(C(OC(C2([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])N(C3SC(=C(N=3)[H])C(=O)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])[H])[H])[H])[H]	15546730
63	43	0.7	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])/C(=C(/C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])[H])[H])[H])[H])=O	12672234
64	44	2	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])/C(=C(/C(N5C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])=O	12672234
65	45	10	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])/C(=C(/C(N(C([H])([H])[H])[H])C(C5C(=C(C(=C(C=5[H])[H])[H])[H])[H])([H])[H])([H])[H])[H])[H])=O	12672234
66	46	3	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])/C(=C(/C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])[H])[H])[H])=O	12672234
67	1	>10000	Train	N1=C(C(=C(N=C1N([C@](C([H])([H])[H])(C(O[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])N(C2C(=C(C(=C(C=2[H])[H])F)[H])[H])C(=O)N(C3=C(Cl)C(=C(C(=C3[H])[H])[H])[H])[H])[H])[H]	16682201
68	2	3860	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])F)[H])[H])[H]	16682201
69	7a	1820	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2[H])[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])F)[H])[H])[H]	16682201
70	7b	3130	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2[H])[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])[H])[H])[H]	16682201
71	7c	301	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	16682201
72	7d	190	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2C([H])([H])[H])[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	16682201

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
73	7e	4290	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2[H])[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
74	7f	6	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H]	16682201
75	7g	9	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2C([H])([H])[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H]	16682201
76	7h	708	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2[H])[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])[H])[H])[H]	16682201
77	7i	87	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	16682201
78	7j	28	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2C([H])([H])[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])[H])([H])[H])([H])[H])[H])[H]	16682201
79	7k	96	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2C(F)(F)F)[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
80	7l	418	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(F)C(=C(C(=C2F)[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
81	7m	>10000	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(OC([H])([H])[H])C(=C(C(=C2[H])[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	16682201
82	8a	1450	Train	N1=C(C(=C(N=C1[H])N(C(C2=C(C(=C(C(=C2[H])[H])[H])[H])[H])[H])([H])[H])C(=O)N(C3=C(Cl)C(=C(C(=C3C([H])([H])[H])[H])[H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])F)[H])[H])[H]	16682201
83	8b	>10000	Train	N1=C(C(=C(N=C1[H])N(C(C2=C(C(=C(C(=C2[H])[H])[H])[H])[H])[H])([H])[H])C(=O)N(C3=C(Cl)C(=C(C(=C3[H])[H])[H])[H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])[H])[H]	16682201
84	8c	>10000	Train	N1=C(C(=C(N=C1[H])N(C(C2=C(C(=C(C(=C2[H])[H])N(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])C(=O)N(C3=C(Cl)C(=C(C(=C3[H])[H])[H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])[H]	16682201
85	8d	4490	Train	N1=C(C(=C(N=C1[H])N(C(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2[H])[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N(C(C([H])([H])[H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])[H]	16682201
86	8e	971	Train	N1=C(C(=C(N=C1[H])N(C(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2C([H])([H])[H])[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])[H]	16682201
87	8f	229	Train	N1=C(C(=C(N=C1[H])N(C(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
88	8g	155	Train	N1=C(C(=C(N=C1[H])N(C(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
89	8h	230	Train	N1=C(C(=C(N=C1[H])N(N2C(C(N(C(C2([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])C(=O)N(C3=C(Cl)C(=C(C(=C3Cl)[H])[H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	16682201
90	8i	>10000	Train	N1=C(C(=C(N=C1[H])N(C2C(=C(N=C(C=2[H])[H])[H])[H])C(=O)N(C3=C(Cl)C(=C(C(=C3Cl)[H])[H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N5C(C(OC(C5([H])[H])([H])[H])([H])[H])[H])[H])[H])[H]	16682201
91	9a	>10000	Train	N1=C(C(=C(N=C1[H])N(C2=C(C(=C(C(=C2[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C(=O)N(C3=C(Cl)C(=C(C(=C3Cl)[H])[H])[H])[H])[H])N(C([H])([H])[H])[H]	16682201
92	9b	2350	Train	N1=C(C(=C(N=C1[H])N(C(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C([H])([H])[H])[H]	16682201
93	9c	>10000	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
94	9d	5990	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
95	9e	>10000	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C3(C(C(OC(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	16682201
96	9f	>10000	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(Cl)C(=C(C(=C2Cl)[H])[H])[H])[H])[H])N(C(C(N3C(C(OC(C3([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
97	10a	2580	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])([H])[H])[H])OC([H])([H])[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
98	10b	3	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])O[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	16682201
99	10c	4	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])O[H])[H])[H])[H])N(C3=C(C(=C(C(=C3[H])[H])N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	16682201
100	16a	4	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(=O)N(C3=NOC(=C3[H])C(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	16682201

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101	16b	32	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(=O)N(C3=C(C(=C(C(=C3[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H]	16682201
102	18a	149	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])N(C(C3N(C4=C(C=3[H])C(=C(C(=C4[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])[H])N(C5=C(C(=C(C(=C5[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
103	18b	52	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])N(C(C3SC4=C(C=3[H])C(=C(C(=C4[H])[H])[H])[H])=O)[H])[H])[H])[H])N(C5=C(C(=C(C(=C5[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
104	18c	3	Train	N1=C(C(=C(N=C1[H])N(C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])N(C(C3=C(C(=C(C(=C3[H])C(F)(F)(F)F)[H])[H])[H])=O)[H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16682201
105	2	110	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])[H])[H])[H])C([H])([H])[H])C([H])([H])[H])[H])=O	12672234
106	12	23	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])[H])[H])[H])C([H])([H])[H])C([H])([H])[H])[H])=O	12672234
107	40	>2500	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C(C([H])([H])[H])([H])[H])[H])[H])[H])C([H])([H])[H])C([H])([H])[H])[H])=O	12672234
108	41	>2000	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N=C(N3C([H])([H])[H])N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])[H])[H])C([H])([H])[H])C([H])([H])[H])[H])=O	12672234
109	14	87	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4[H])[H])[H])[H])Cl)Cl)C([H])([H])[H])[H])[H])C(=O)OC([H])([H])[H]C([H])([H])[H])[H])=O	12672234
110	16	700	Train	C(C(C1=C(N(C(C2=C1C(=C(C3=C2N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])=O)[H])C([H])([H])[H])([H])[H])(=O)O[H]	12672234
111	18	120	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C(C(=O)N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C([H])([H])[H])[H])=O	12672234
112	19	30	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C([H])([H])[H])[H])=O	12672234
113	49	120	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C(C(C(=O)N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C([H])([H])[H])[H])=O	12672234
114	50	460	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C(C(=O)N(C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])C([H])([H])[H])[H])=O	12672234
115	51	740	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C(C(=O)N5C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C([H])([H])[H])[H])=O	12672234
116	52	440	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C(C(=O)N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])C([H])([H])[H])[H])=O	12672234
117	53	110	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C(C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C([H])([H])[H])[H])=O	12672234
118	54	27	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C(C(O[H])([H])[H])([H])[H])C([H])([H])[H])[H])=O	12672234
119	23	50	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])C5=C(C(=C(N=C5F)F)[H])[H])[H])C([H])([H])[H])C([H])([H])[H])[H])=O	12672234
120	26	26	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])C(N(C(C(O[H])([H])[H])([H])[H])[H])([H])[H])[H])C([H])([H])[H])C([H])([H])[H])[H])=O	12672234
121	27	180	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])C(N(C(C5C(=C(C(=C(C=5[H])[H])OC([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C([H])([H])[H])[H])=O	12672234
122	28	170	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])C(=O)[H])[H])=O	12672234
123	29	770	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])C(O[H])([H])[H])[H])=O	12672234
124	30	2000	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])C(N(C(C5=C(C(=C(C(=C5[H])[H])[H])[H])([H])[H])([H])[H])([H])[H])[H])=O	12672234
125	31	570	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])[C@@](O[H])(C(=C([H])[H])[H])[H])[H])=O	12672234
126	32	45	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])C(=C([H])[H])[H])[H])=O	12672234
127	36	86	Train	C(/C(=C(/C1N(C(C2=C(C=1C([H])([H])[H])C(=C(C3=C2N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])=O)[H])[H])[H])(=O)OC([H])([H])[H]	12672234
128	37	360	Train	C(C(C(C1N(C(C2=C(C=1C([H])([H])[H])C(=C(C3=C2N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])=O)[H])([H])[H])([H])[H])(=O)OC([H])([H])[H]	12672234
129	38	9	Train	C(/C(=C(/C1N(C(C2=C(C=1C([H])([H])[H])C(=C(C3=C2N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])=O)[H])[H])[H])(O[H])([H])[H]	12672234
130	34	4	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])/C(=C(/C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])=O	12672234
131	35	2	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])/C(=C(/C(N([H])[H])([H])[H])[H])[H])[H])=O	12672234
132	39	2	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])[H])C([H])([H])[H])/C(=C(/C(N(C(C([H])([H])[H])([H])[H])([H])([H])[H])([H])[H])[H])[H])=O	12672234

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
133	42	780	Train	C1(N(C(=C(C2C(=C(C3=C(C1=2)N(C(=N3)N(C4C(=C(C(=C(C=4Cl)[H])[H])[H])Cl)[H])C([H])([H])[H])[H])[H])C([H])([H])[H])C([H])([H])[H])C(C([H])([H])[H])([H])[H])[H])=O	12672234
134	2	31	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C([H])([H])[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])[H]	17234410
135	3	5200	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])[H])[H]	17234410
136	4	9650	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])N([H])[H])[H]	17234410
137	5	20800	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])N(C(=O)C(C(N6C(C(C(C6([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	17234410
138	6	6850	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])N(C(=O)N(C(C(N6C(C(C(C6([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	17234410
139	7	>50000	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])C(=O)O[H])[H]	17234410
140	8	380	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])C(=O)N([H])[H])[H]	17234410
141	9	140	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])C(=O)N(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	17234410
142	10	17600	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])C(N6C(C(N(C(C6([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])=O)[H]	17234410
143	11	240	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])C(=O)N(C(C(N6C(C(C(C6([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	17234410
144	12	541	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C([H])=C(\[H])C(=O)N([H])[H])[H]	17234410
145	13	130	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N(C6(C(C(N(C(C6([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])=O)[H])[H])[H]	17234410
146	14	770	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C([H])=C(\[H])C(O[H])([H])[H])[H]	17234410
147	15	4810	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])C(C(C(O[H])([H])[H])([H])[H])([H])[H])[H]	17234410
148	16	230	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C([H])=C(\[H])C(N([H])[H])([H])[H])[H])[H]	17234410
149	17	4470	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(\C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])[H])[H]	17234410
150	18	290	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])[H])[H]	17234410
151	19	1370	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N(S(=O)(=O)C([H])([H])[H])[H])([H])[H])([H])[H])[H]	17234410
152	20	6700	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N(C(=O)NC6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H])([H])[H])[H])[H])[H]	17234410
153	21	720	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N(C(=O)C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	17234410
154	22	290	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N6C(C(N(C(C6([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	17234410
155	25	190	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N(C6(C(C(N(C(C6([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	17234410
156	26	110	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N([C@@]6(C(C([C@](C(C6([H])[H])([H])[H])(N([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	17234410
157	27	480	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N([C@@]6(C(C([C@@](C(C6([H])[H])([H])[H])[H])(N([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	17234410
158	28	210	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N6C(C(C(C(C6([H])[H])([H])[H])O[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	17234410
159	23	2950	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N6C(C(N(C(C6([H])[H])([H])[H])[H])C7=C(C(=C(C(=C7[H])[H])[H])[H])[H])([H])[H])([H])[H])[H])[H]	17234410
160	24	1520	Train	N1=C(C(=C2C(=C1N([H])[H])C(=C(S2)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])N(C(C4N(C5=C(C=4[H])C(=C(C(=C5[H])[H])[H])[H])C([H])([H])[H])=O)[H])[H])[H])/C(=C(/C(N6C(C(N(C(C6([H])[H])([H])[H])C([H])([H])[H])=C([H])[H])([H])[H])([H])[H])([H])[H])[H]	17234410

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161	1	0.2	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N([H])[H]	16970394
162	9	0.3	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
163	27	0.01	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
164	28	0.3	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C5C(=C(C(=C4[H])[H])[H])C(C(C5([H])[H])([H])[H])([H])[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
165	29	1	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])OC5(C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
166	30	0.5	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])Cl)C(F)(F)F)[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
167	31	3	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])Cl)C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
168	32	0.5	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4OC5(C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
169	33	48	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
170	34	2	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4N5C(C(N(C5=O)C([H])([H])[H])([H])[H])([H])[H])([H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
171	35	0.4	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4N(C(=O)N(C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
172	36	0.5	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4N(C(=O)C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
173	37	2	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4N5C(C(C5=O)(C([H])([H])[H])C([H])([H])[H])([H])[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
174	38	10	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
175	39	35	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N([H])[H]	16970394
176	40	150	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3[H])[H])F)C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N([H])[H]	16970394
177	41	4	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3Cl)[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N([H])[H]	16970394
178	42	0.5	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])F)C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N(C([H])([H])[H])[H]	16970394
179	43	0.9	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])F)C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N([H])[H]	16970394
180	44	200	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)C([H])([H])[H])[H])N([H])[H]	16970394
181	13	0.3	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])N(C(=O)C4=C(C(=C(C(=C4[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])N(C([H])([H])[H])[H]	16970394
182	14	8	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])N(C(=O)N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])N(C([H])([H])[H])[H]	16970394
183	15	297	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])N(C4N(C5=C(N=4)C(=C(C(=C5[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])N(C([H])([H])[H])[H]	16970394
184	45	94	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])[H])[H])[H])N([H])[H]	16970394
185	24	5550	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])C#N)[H])[H])[H])[H])[H]	11012022
186	25	529	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])C(O[H])([H])[H])[H])[H])[H]	11012022
187	26	751	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])C(O[H])([H])[H])[H])[H])[H])[H]	11012022
188	27	15800	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])C(=O)O[H])[H])[H])[H]	11012022
189	28	1310	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])C(=O)O[H])[H])[H])[H])[H]	11012022
190	1	3200	Train	N1=C(N=C2C(=C1[H])C(=C(N(N2C([H])([H])[H])C([H])([H])[H])C3=C(C(=C(C(=C3Cl)[H])[H])[H])[H])Cl)[H])N(C4=C(C(=C(C(=C4[H])[H])F)[H])[H])[H]	16757169
191	12a	124	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])F)[H])[H])[H]	16757169
192	12b	182	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H]	16757169
193	12c	2814	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C([H])([H])[H])[H]	16757169
194	12d	71	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])OC([H])([H])[H])[H])[H])[H]	16757169
195	12e	179	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])[H])OC([H])([H])[H])[H])[H]	16757169
196	12f	7269	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])[H])[H])OC([H])([H])[H])[H]	16757169
197	12g	285	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])OC(C([H])([H])[H])([H])[H])[H])[H])[H]	16757169

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198	12h	143	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])C(=O)OC([H])([H])[H])[H])[H])[H]	16757169
199	12i	26	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])N(C([H])([H])[H])C([H])([H])[H])[H])[H])[H]	16757169
200	12j	43	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])[H])[H])[H]	16757169
201	12k	21	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	16757169
202	12l	3	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])N6C(C(OC(C6([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	16757169
203	12m	2	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])N(C5=C(C(=C(C(=C5[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])[H])([H])[H])([H])[H])[H])[H])[H]	16757169
204	12n	4802	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])OC([H])([H])[H])[H])[H])N(C5=C(C(=C(C(=C5[H])[H])F)[H])[H])[H]	16757169
205	12o	2837	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])OC([H])([H])[H])[H])[H])[H])N(C5=C(C(=C(C(=C5[H])[H])N(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H]	16757169
206	12p	10	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])O[H])[H])[H])N(C5=C(C(=C(C(=C5[H])[H])N(C([H])([H])[H])C([H])([H])[H])[H])[H])[H]	16757169
207	12q	47	Train	N1=C(N=C2C(=C1[H])C(=C(N3N2C(C(C3=O)([H])[H])([H])[H])C4=C(C(=C(C(=C4Cl)[H])[H])[H])O[H])[H])[H])N(C5=C(C(=C(C(=C5[H])[H])N6C(C(N(C(C6([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H]	16757169
208	2	100	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	12039590
209	3	42	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@]3(C(C(OC3([H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	12039590
210	4	120	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(OC(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	12039590
211	5	130	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C(O[H])([H])[H])([H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H]	12039590
212	6	890	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C(N([H])[H])([H])[H])([H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H]	12039590
213	7	46	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@]3(C(N(OC3([H])[H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	12039590
214	8	240	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@]3(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	12039590
215	9	170	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	12039590
216	10	520	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(C(C(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])OC6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H])[H]	12039590
217	11	82	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(C(C(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])OC6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H])[H]	12039590
218	12	240	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])OC6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H]	12039590
219	13	15	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])OC6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H]	12039590
220	1	15	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])OC6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H]	12039591
221	2	40	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])OC6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H]	12039591
222	3	40	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])N(C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H])[H])[H]	12039591
223	4	110	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])C(C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H])[H])[H])[H]	12039591
224	5	93	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])N(C(=O)C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H])[H])[H]	12039591
225	6	4	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])N(C(=O)OC(C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])([H])[H])[H])OC([H])([H])[H])[H])[H]	12039591
226	7	209	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])N(C(=O)N(C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H])[H])[H]	12039591
227	8	3120	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])N(S(=O)(=O)C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])OC([H])([H])[H])[H])[H]	12039591

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
228	9	167	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])[H])N(S(=O)(=O)N(C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H])[H])[H]	12039591
229	10	55	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])[H])N(C(C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])([H])[H])[H])[H])OC([H])([H])[H])[H])[H]	12039591
230	11	28	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])[H])N(C(=O)C(C(C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])([H])[H])[H])[H])OC([H])([H])[H])[H])[H]	12039591
231	12	92	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])[H])N(C(=O)C(C([H])([H])[H])(C([H])([H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H])[H])[H]	12039591
232	13	31	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])[H])N(C(=O)C(C(C([H])([H])[H])(C([H])([H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H])[H])[H]	12039591
233	14	19	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])[H])N(C(=O)[C@]6([C@@](C6([H])[H])(C7=C(C(=C(C(=C7[H])[H])[H])[H])[H])[H])[H])O)C([H])([H])[H])[H])[H]	12039591
234	15	10	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])[H])N(C(=O)C6=C(C7=C(O6)C(=C(C(=C7[H])[H])[H])[H])[H])[H])OC([H])([H])[H])[H])[H]	12039591
235	16	50	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])[H])N(C(C(C6=C(C7=C(N6[H])C(=C(C(=C7[H])[H])[H])[H])[H])([H])[H])([H])[H])[H])[H])[H])[H]	12039591
236	46	0.6	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C)C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N([H])[H]	16970394
237	47	0.2	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C)C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])N(C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16970394
238	48	3	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C)C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N(C(C(N5C(C(OC(C5([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16970394
239	49	0.4	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C)C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N(C(C(C(N5C(C(OC(C5([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16970394
240	50	14	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C)C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N(C(C(C(N5C(C(OC(C5([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C([H])([H])[H]	16970394
241	51	6	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C)C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N(C(C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16970394
242	52	6	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C)C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N(C(C(N5C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16970394
243	53	0.6	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C)C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N(C5(C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16970394
244	54	1	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C)C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N(C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	16970394
245	55	0.07	Train	N1=C(N=C2C(=C1[H])C(=C(C(=C2[H])[H])C)C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)C([H])([H])[H])[H])=O)[H])[H])N(C5(C(C5([H])[H])([H])[H])[H])[H])[H]	16970394
246	1	14	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16884310
247	25	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16884310
248	26	12	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16884310
249	27	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC(C([H])([H])[H])(C([H])([H])[H])[H])[H])F)[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16884310
250	28	2	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16884310
251	29	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C(C3=C(C(=C(C(=C3[H])OC([H])([H])[H])[H])[H])OC([H])([H])[H])([H])[H])N(C4=C(C(=C(C(=C4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16884310

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
252	30	10	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C4C(=C3[H])C(=C(C(=C4[H])[H])[H])[H])[H])N(C5=C(C(=C(C(=C5[H])[H])N6C(C(N(C(C6([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	16884310
253	31	13	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3[H])[H])C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])N(C5=C(C(=C(C(=C5[H])[H])N6C(C(N(C(C6([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H]	16884310
254	32	49	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3[H])C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])N(C5=C(C(=C(C(=C5[H])[H])N6C(C(N(C(C6([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H]	16884310
255	33	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H])[H])[H]	16884310
256	34	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])O C([H])([H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H])[H])[H]	16884310
257	35	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])F)[H])[H]	16884310
258	36	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	16884310
259	37	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(C(N([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	16884310
260	38	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])F)[H])[H]	16884310
261	39	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])O C([H])([H])[H])OC(C(N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H])[H])[H]	16884310
262	40	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])O C([H])([H])[H])OC(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H])[H])[H]	16884310
263	41	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	16884310
264	42	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(C(N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H])[H])[H]	16884310
265	43	0.6	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])O C([H])([H])[H])OC(C(C(N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H])[H])[H]	16884310
266	44	1	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(C(N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])F)[H])[H]	16884310
267	45	2	Train	N1=C(N=C(C(=C1[H])[H])N(C(OC2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)C3=C(C(=C(C(=C3OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])F)[H])[H]	16884310
268	A420983	37	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(C6=C(C7=C(N6C([H])([H])[H])C(=C(C(=C7[H])[H])[H])[H])[H])[H])[H])[H])[H]	16216497
269	1	141	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(C6=C(C(=C(C(=C6F)[H])C(F)(F)F)[H])[H])=O)[H])[H])[H])[H]	16216497
270	2	196	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	16216497
271	3	80	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])[H])C4=C(C(=C(C(=C4[H])OC([H])([H])[H])N(C(C5=C(C(=C(C(=C5F)[H])C(F)(F)F)[H])[H])=O)[H])[H])[H])[H]	16216497
272	4	106	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])C4=C(C(=C(C(=C4[H])OC([H])([H])[H])N(C(C5=C(C(=C(C(=C5F)[H])C(F)(F)F)[H])[H])=O)[H])[H])[H])[H]	16216497
273	5	341	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])([H])[H])([H])[H])([H])[H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(C6=C(C(=C(C(=C6F)[H])C(F)(F)F)[H])[H])=O)[H])[H])[H])[H]	16216497
274	6	102	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(C6=C(C(=C(C(=C6F)[H])C(F)(F)F)[H])[H])=O)[H])[H])[H])[H]	16216497

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275	7	23	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(C6=C(C(=C(C(=C6F)[H])C(F)(F)F)[H])[H])=O)[H])[H])[H])[H]	16216497
276	8	93	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(N(C(C4([H])[H])([H])[H])C(=O)C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(C6=C(C(=C(C(=C6F)[H])C(F)(F)F)[H])[H])=O)[H])[H])[H])[H]	16216497
277	9	106	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=C(C(=C(C(=C6[H])[H])N(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])[H]	16216497
278	10	8960	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=C(C(=C(C(=C6[H])[H])C([H])([H])[H])[H])[H])[H])[H])[H]	16216497
279	11	2350	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=C(C(=C(C(=C6[H])[H])OC(F)(F)F)[H])[H])[H])[H])[H]	16216497
280	12	23200	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=C(C(=C(C(=C6[H])O[H])[H])[H])[H])[H])[H])[H]	16216497
281	13	318	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=NC7=C(N6C([H])([H])[H])C(=C(C(=C7[H])[H])[H])[H])[H])[H])[H]	16216497
282	14	107	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=C(C7=C(N6C([H])([H])[H])C(=C(C(=C7[H])[H])[H])[H])[H])[H])[H])[H]	16216497
283	15	54	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=C(C7=C(N6C([H])([H])[H])C(=C(C(=C7[H])Cl)[H])[H])[H])[H])[H])[H]	16216497
284	16	3480	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=C(C7=C(N6C([H])([H])[H])C(=C(C(=C7[H])C#N)[H])[H])[H])[H])[H])[H]	16216497
285	17	>50000	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=C(C7=C(N6C([H])([H])[H])C(=C(C(=C7[H])C(=O)N([H])[H])[H])[H])[H])[H])[H]	16216497
286	18	9180	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=NC7=C(C(=C6[H])O[H])C(=C(C(=C7[H])[H])[H])[H])[H])[H]	16216497
287	19	7.4	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C3(C(C(N(C(C3([H])[H])([H])[H])C4(C(C(N(C(C4([H])[H])([H])[H])C(=O)C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=C(C7=C(N6C([H])([H])[H])C(=C(C(=C7[H])[H])[H])[H])[H])[H])[H])[H]	16216497
288	1	170	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4[H])[H])[H])[H])Br)[H])=C(N=C3[H])[H])[H])[H])[H]	12372522
289	2	2	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	12372522
290	2a	2.4	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])C([H])([H])[H])[H])[H])=C(N=C3[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	12372522
291	11a	4	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])O[H])O[H]	12372522
292	11b	4	Train	C12=C(C(=C3C(=C1[H])N4C(C(=N3)N(C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C4[H])[H])[H])OC(O2)([H])[H]	12372522
293	11c	10	Train	C12=C(C(=C3C(=C1[H])N4C(C(=N3)N(C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C4[H])[H])[H])OC(C(O2)([H])[H])([H])[H]	12372522
294	11d	3	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])OC([H])([H])[H]	12372522
295	11f	8.7	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])OC([H])([H])[H])[H]	12372522
296	11g	280	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])OC([H])([H])[H])[H])[H]	12372522
297	11h	9.4	Train	C1(=C(C(=C2C(=C1OC([H])([H])[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])[H]	12372522
298	11i	240	Train	C1(=C(C(=C2C(=C1OC(C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])([H])[H])[H])N4C(C(=N2)N(C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C4[H])[H])[H])[H])[H]	12372522
299	11j	100	Train	C1(=C(C(=C2C(=C1[N+](=O)[O-])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])C([H])([H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	12372522
300	11k	70	Train	C1(=C(C(=C2C(=C1N([H])[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])C([H])([H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	12372522
301	11l	26	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])F	12372522
302	11m	15	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])Br	12372522
303	11n	26	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])C(=O)OC([H])([H])[H]	12372522
304	11o	24	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])[N+](=O)[O-]	12372522
305	11p	100	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])C#N	12372522
306	11q	7	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N([H])[H]	12372522
307	11r	3	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N(C(=O)C([H])([H])[H])[H]	12372522

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
308	11s	14	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])Br)[H]	12372522
309	11t	21	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N([H])[H])[H]	12372522
310	11u	11	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N(C(=O)C([H])([H])[H])[H])[H]	12372522
311	11v	30	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])C(=O)N([H])[H])[H]	12372522
312	12a	5	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N(C([H])([H])[H])C([H])([H])[H]	12372522
313	12b	2	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H]	12372522
314	12c	10	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N(C(C([H])([H])[H])([H])[H])[H]	12372522
315	12d	6	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H]	12372522
316	12e	7	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N(C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	12372522
317	12f	3	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N(C(C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	12372522
318	12g	4	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H]	12372522
319	12h	3	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])[H])([H])[H])([H])[H]	12372522
320	12i	1	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H]	12372522
321	12j	2	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H]	12372522
322	12k	9	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C(=O)[H])([H])[H])([H])[H]	12372522
323	12l	3	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N5C([C@@](N([C@@](C5([H])[H])(C([H])([H])[H])[H])[H])(C([H])([H])[H])[H])([H])[H]	12372522
324	12m	9	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])N5C(C(N(C(C(C5([H])[H])([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H]	12372522
325	12n	9	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H]	12372522
326	12o	10	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	12372522
327	12p	9	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N(C(C(C(N(C([H])([H])[H])C([H])([H])H])([H])[H])([H])[H])[H])[H]	12372522
328	12q	6	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])[H]	12372522
329	12r	11	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])[H])([H])[H])([H])[H])[H])[H]	12372522
330	12s	8	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H]	12372522
331	12t	13	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N5C([C@@](N([C@@](C5([H])[H])(C([H])([H])[H])[H])[H])(C([H])([H])[H])[H])([H])[H])[H]	12372522
332	12u	36	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])OC([H])([H])[H])OC(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	12372522
333	12v	18	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])OC([H])([H])[H])N5C([C@@](N([C@@](C5([H])[H])(C([H])([H])[H])[H])[H])(C([H])([H])[H])[H])([H])[H])[H]	12372522
334	12w	2.4	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])OC(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H]	12372522
335	12x	5.4	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N(C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])OC([H])([H])[H]	12372522
336	12y	1.7	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])OC([H])([H])[H]	12372522
337	12z	5	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4F)[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])N(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H]	12372522
338	13	3	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=C(N=C3C([H])([H])[H])[H])[H])[H])N(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])OC([H])([H])[H]	12372522
339	13	9	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=C2[H])[H])[H])[H]	15317463
340	10	30	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)[H])[H])[H]	15317463
341	14	1400	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(N=C2[H])[H])[H]	15317463
342	15	77	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=NC(=C2[H])[H])[H]	15317463

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
343	16	90	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])N=C(C(=C2[H])[H])[H]	15317463
344	17	150	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])C([H])([H])[H])[H])N=C(C(=C2[H])[H])[H]	15317463
345	18	>780	Train	[C@@]12([C@@](N=C(C3N1C(=NC=3[H])C([H])([H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])[H])Cl)[H])(N=C(N2C([H])([H])[H])[H])[H]	15317463
346	19	>780	Train	[C@@]12([C@@](N=C(C3N1C(=NC=3[H])C([H])([H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])[H])Cl)[H])(N(=C(N2C([H])([H])[H])[H])(C([H])([H])[H])[H])[H])[H]	15317463
347	20	>780	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])N=C(N=C2[H])OC([H])([H])[H]	15317463
348	21	9	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=C2[H])[H])OC([H])([H])[H])[H]	15317463
349	12	25	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)Cl)[H])[H]	15317463
350	22a	19	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)OC([H])([H])[H])[H])[H]	15317463
351	22b	1	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N(C([H])([H])[H])C([H])([H])[H])[H])[H]	15317463
352	22c	2	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])[H])[H]	15317463
353	22d	71	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N(C([H])([H])[H])C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H]	15317463
354	22e	5	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C(=NC(=C5[H])[H])[H])[H])[H]	15317463
355	22f	1	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	15317463
356	22g	7	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	15317463
357	22h	1	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C(C(N(C(C5([H])[H])([H])[H])[H])([H])[H])([H])[H])[H])[H]	15317463
358	22i	1	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H]	15317463
359	22j	6	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C(C(N(C(C(C5([H])[H])([H])[H])([H])[H])[H])([H])[H])([H])[H])[H])[H]	15317463
360	22k	2	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@@](N([C@@](C5([H])[H])C([H])([H])[H])[H])[H])(C([H])([H])[H])[H])([H])[H])[H]	15317463
361	23	29	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=NC(=C2[H])N5C([C@@](N([C@@](C5([H])[H])C([H])([H])[H])[H])[H])(C([H])([H])[H])[H])([H])[H]	15317463
362	24a	163	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(N=C2[H])N5C(C(N(C(C5([H])[H])([H])[H])[H])([H])[H])([H])[H])[H]	15317463
363	24b	240	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(N=C2[H])N(C([H])([H])[H])C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H]	15317463
364	24c	103	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(N=C2[H])N(C([H])([H])[H])C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	15317463
365	25	4	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@](C(C5([H])[H])([H])[H])(O[H])[H])([H])[H])[H])[H])[H]	15317463
366	26	8	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@@](C(C5([H])[H])([H])[H])O[H])[H])([H])[H])[H])[H]	15317463
367	27	5	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@]([C@@](C5([H])[H])O[H])[H])O[H])[H])([H])[H])[H])[H]	15317463
368	28	13	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@@]([C@](C5([H])[H])(O[H])[H])(O[H])[H])([H])[H])[H])[H])[H]	15317463
369	29	6	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@](C(C5([H])[H])([H])[H])(N([H])[H])[H])([H])[H])[H])[H]	15317463
370	30	7	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@@](C(C5([H])[H])([H])[H])(N([H])[H])[H])([H])[H])[H])[H]	15317463
371	4	4	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@@](N(C(C5([H])[H])([H])[H])[H])(C([H])([H])[H])[H])([H])[H])[H])[H]	15317463
372	31	2	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@](N(C(C5([H])[H])([H])[H])[H])(C([H])([H])[H])[H])([H])[H])[H])[H]	15317463
373	32	5	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@@](N(C(C5([H])[H])([H])[H])[H])(C(O[H])([H])[H])[H])([H])[H])[H])[H]	15317463
374	33	3	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C([C@](N(C(C5([H])[H])([H])[H])[H])(C(O[H])([H])[H])[H])([H])[H])[H])[H]	15317463
375	34	9	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C(C(N(C(C5([H])[H])([H])[H])C(C(O[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	15317463
376	35	2	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N5C(C(N(C(C5([H])[H])([H])[H])C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	15317463
377	36	4	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N(C(C(O[H])([H])[H])([H])[H])C(C(O[H])([H])[H])([H])[H])([H])[H])[H]	15317463
378	37	7	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N(C([H])([H])[H])C([C@](C(O[H])([H])[H])O[H])[H])([H])[H])[H])[H]	15317463
379	38	13	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N(C([H])([H])[H])C([C@@](C(O[H])([H])[H])(O[H])[H])([H])[H])[H])[H]	15317463
380	39	3	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N(C([H])([H])[H])C(C(O[H])([H])[H])([H])[H])([H])[H])[H]	15317463

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
381	40	3	Train	C12=C(N=C(C3N1C(=NC=3[H])[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])C(=C(C(=N2)N(C([H])([H])[H])C(C(O[H])([H])[H])([H])[H])[H])[H]	15317463
382	1	0.2	Train	C1(=NC(=C2C(=N1)C(=C(C(=C2[H])[H])C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])C(N(C4=C(C(=C(C(=C4[H])C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])[H])N([H])[H]	18083554
383	2	53	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3[H])C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)OC([H])([H])[H])N(C([H])([H])[H])[H]	18083554
384	3	7	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3F)C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)OC([H])([H])[H])N(C([H])([H])[H])[H]	18083554
385	4	44	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3C([H])([H])[H])C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)OC([H])([H])[H])N(C([H])([H])[H])[H]	18083554
386	5	25	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3[H])C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])N(C([H])([H])[H])[H]	18083554
387	6	41	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3[H])C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])N(C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18083554
388	7	101	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3[H])C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)OC([H])([H])[H])N(C4(C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])[H])[H])[H]	18083554
389	8	22	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3[H])C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)OC([H])([H])[H])N(C(C(N4C(C(OC(C4([H])[H])([H])[H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H]	18083554
390	9	19	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3C([H])([H])[H])C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)OC([H])([H])[H])N(C(C(C(N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])[H])([H])[H])([H])[H])[H])[H]	18083554
391	10	45	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3C([H])([H])[H])C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)OC([H])([H])[H])N(C(C(C(C(N(C([H])([H])[H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18083554
392	11	0.6	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3F)C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)OC([H])([H])[H])N(C4=C(C(=C(C(=C4[H])[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18083554
393	20	147	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2[C@]3(C(C([C@](C(C3([H])[H])([H])[H])(N4C(C(N(C(C4([H])[H])([H])[H])C(=O)C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C5=C(C(=C(C(=C5[H])OC([H])([H])[H])N(C(=O)C6=C(C7=C(N6C([H])([H])[H])C(=C(C(=C7[H])[H])[H])[H])[H])[H])[H])[H])[H]	16216497
394	1	5000	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N([H])[H])C([H])([H])[H])=O)[H]	14592495
395	7a	1500	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	14592495
396	7b	28000	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2Cl)[H])[H])[H])C([H])([H])[H])[H])[H]	14592495
397	7c	4400	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H]	14592495
398	7d	1400	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])Br)[H])C([H])([H])[H])[H]	14592495
399	7e	12500	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2Cl)[H])[H])[H])Cl)[H]	14592495
400	7g	>50000	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])C([H])([H])[H])C(=O)N([C@@](C([H])([H])[H])(C(C([H])([H])[H])C([H])([H])[H])([H])[H])[H])[H]	14592495
401	7t	700	Train	C1(=C(N=C(S1)N(C(OC([H])([H])[H])=O)[H])C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	14592495
402	7u	360	Train	C1(=C(N=C(S1)N(C(=O)C2OC(=C(C=2[H])[H])[H])[H])C([H])([H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	14592495
403	7v	800	Train	C1(=C(N=C(S1)N(C(=O)C2=C(C(=C(C(=C2[H])[H])[H])[H])[H])[H])C([H])([H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	14592495
404	7w	240	Train	C1(=C(N=C(S1)N(C(=O)N(C([H])([H])[H])[H])[H])C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	14592495
405	7x	30	Train	C1(=C(N=C(S1)N(C(=O)N(C(C(C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C([H])([H])[H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	14592495
406	7y	710	Train	C1(=C(N=C(S1)N(C(=O)C2OC(=C(C=2[H])[H])[H])[H])C([H])([H])[H])C(=O)N(C3=C(C(=C(C(=C3Cl)[H])[H])[H])C([H])([H])[H])[H]	14592495
407	7z	4500	Train	C1(=C(N=C(S1)N(C(=O)C2=C(C(=C(C(=C2[H])[H])[H])[H])[H])[H])C([H])([H])[H])C(=O)N(C3=C(C(=C(C(=C3Cl)[H])[H])[H])C([H])([H])[H])[H]	14592495
408	7aa	620	Train	C1(=C(N=C(S1)N(C(=O)N(C(C(C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C([H])([H])[H])[H])C(=O)N(C2=C(C(=C(C(=C2Cl)[H])[H])[H])C([H])([H])[H])[H]	14592495
409	7bb	>50000	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])C([H])([H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])C([H])([H])[H]	14592495
410	7cc	>50000	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)C([H])([H])[H])C([H])([H])[H]C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	14592495
411	8	>30000	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])C(C([H])([H])[H])([H])[H]C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	14592495
412	9	>30000	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])C2=C(C(=C(C(=C2[H])[H])[H])[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	14592495
413	10	>30000	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])C(F)(F)F)C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])[H]	14592495
414	11a	>30000	Train	C1(=C(N=C(S1)N(C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])=O)[H])[H])C(=O)N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	14592495

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
415	11b	3100	Train	C1(=C(N=C(S1)N(C(C2=C(C(=C(O2)[H])[H])[H])=O)[H])[H])C(=O)N(C3=C(C(=C(C(=C3Cl)[H])[H])[H])C([H])([H])[H])[H]	14592495
416	11c	890	Train	C1(=C(N=C(S1)N(C(C2=C(C(=C(C(=C2[H])[H])[H])[H])[H])=O)[H])[H])C(=O)N(C3=C(C(=C(C(=C3Cl)[H])[H])[H])C([H])([H])[H])[H]	14592495
417	11d	35	Train	C1(=C(N=C(S1)N(C(C2(C(C2([H])[H])([H])[H])[H])=O)[H])[H])C(=O)N(C3=C(C(=C(C(=C3Cl)[H])[H])[H])C([H])([H])[H])[H]	14592495
418	11e	18	Train	C1(=C(N=C(S1)N(C(C2(C(C2([H])[H])([H])[H])[H])=O)[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])C([H])([H])[H])[H]	14592495
419	7dd	1400	Train	C1(=C(N=C(S1)N(C(C2(C(C2([H])[H])([H])[H])[H])=O)[H])C([H])([H])[H])C(=O)N(C3=C(C(=C(C(=C3Cl)[H])[H])[H])C([H])([H])[H])[H]	14592495
420	1	170	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Br)[H])[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
421	2	>50000	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Br)[H])[H])[H])[H])[H])=NC(=C3[H])[H])[H])[H])[H]	11992777
422	6a	3170	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4(C(C(C(C(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
423	6b	3170	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4(C(C4([H])[H])([H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
424	6c	2680	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C(C(C([H])([H])[H])([H])[H])([H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
425	6d	>12500	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C(C(C(C(C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
426	6f	4390	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C(C(C4=C(C(=C(C(=C4[H])Cl)[H])[H])[H])([H])[H])([H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
427	6g	820	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(N=C4[H])[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
428	6h	>12500	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=NC(=C4[H])[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
429	7a	3700	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)OC4=C(C(=C(C(=C4Br)[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
430	7b	>12500	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)SC4=C(C(=C(C(=C4Br)[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
431	7c	>12500	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)C(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])C([H])([H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
432	7d	>12500	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])[H])C([H])([H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
433	7e	60	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C(C4=C(C(=C(C(=C4Br)[H])[H])[H])[H])=O)[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
434	7f	>12500	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])[H])[H])=O)[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
435	7g	810	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C(C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)=O)[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
436	7h	890	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
437	7i	390	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4F)[H])[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
438	7j	1330	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4[H])F)[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
439	7k	60	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
440	7l	5520	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4OC([H])([H])[H])[H])[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
441	7m	12500	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4[N+](=O)[O-])[H])[H])[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
442	PP1	5	Train	C12=C(C(=NN1C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])C([H])([H])[H])[H])[H])C(=NC(=N2)[H])N([H])[H]	8557675
443	PP2	4	Train	C12=C(C(=NN1C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])Cl)[H])[H])C(=NC(=N2)[H])N([H])[H]	8557675
444	5a	1500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[H])C([H])([H])[H])=O)[H]	17154512
445	5b	28000	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])C([H])([H])[H])=O)[H]	17154512
446	5c	4400	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[H])C([H])([H])[H])=O)[H]	17154512
447	5d	1400	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])Br)[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])=O)[H]	17154512
448	5e	12500	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])=O)[H]	17154512
449	7a	700	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)OC([H])([H])[H])[H])C([H])([H])[H])=O)[H]	17154512
450	7c	480	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)C([H])([H])[H])[H])C([H])([H])[H])=O)[H]	17154512
451	7d	800	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
452	7e	12080	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[H])C([H])([H])[H])=O)[H]	17154512
453	7f	360	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)C3=C(C(=C(O3)[H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
454	7g	1200	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)C3C(=C(OC=3[H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
455	7h	180	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)C3C(=C(SC=3[H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
456	7i	390	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3C(=C(SC=3[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
457	7k	710	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3=C(C(=C(O3)[H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
458	7j	130	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3=C(C(=C(S3)[H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
459	7l	4470	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
460	7m	1400	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3(C(C3([H])[H])([H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
461	8a	240	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)N(C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
462	8b	160	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)N(C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
463	8c	30	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)N(C(C(C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
464	8d	1300	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)N(C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
465	8e	130	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)N(C(C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])([H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
466	8f	620	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)N(C(C(C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C([H])([H])[H])=O)[H]	17154512
467	7n	35	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3(C(C3([H])[H])([H])[H])[H])[H])[H])=O)[H]	17154512
468	7o	22000	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C(C([H])([H])[H])([H])[H])[H])[H])[H])=O)[H]	17154512
469	7p	15000	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)[C@]3([C@@](C3([H])[H])(C([H])([H])[H])[H])[H])[H])[H])=O)[H]	17154512
470	7q	15000	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)[C@]3(C([C@]3(C([H])([H])[H])[H])([H])[H])[H])[H])[H])=O)[H]	17154512
471	7r	890	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])[H])[H])=O)[H]	17154512
472	7s	2230	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3=C(C(=C(S3)[H])[H])[H])[H])[H])=O)[H]	17154512
473	7t	17	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3C(=C(SC=3[H])[H])[H])[H])[H])=O)[H]	17154512
474	7u	29000	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3=C(C(=C(O3)[H])[H])[H])[H])[H])=O)[H]	17154512
475	7v	17000	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3(C(C(C3([H])[H])([H])[H])([H])[H])[H])[H])[H])=O)[H]	17154512
476	7w	1340	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C(=O)C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])=O)[H]	17154512
477	11	9	Train	C12=C(N=C(S1)N(C(=O)C3(C(C3([H])[H])([H])[H])[H])[H])C(=C(C(=C2[H])C(N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=O)[H])[H]	17154512
478	12a	1.2	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=C(C(=N3)[H])[H])[H])[H])[H])[H])=O)[H]	17154512
479	12b	6.7	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=C(N=C3[H])[H])[H])[H])[H])[H])=O)[H]	17154512
480	12c	9.4	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=NC(=C3[H])[H])[H])[H])[H])[H])=O)[H]	17154512
481	12d	1.2	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C3=C(C(=C(C(=N3)[H])[H])[H])[H])[H])[H])=O)[H]	17154512
482	12e	5	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C3=C(C(=C(C(=N3)[H])[H])[H])[H])[H])[H])=O)[H]	17154512
483	12f	4	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=C(N=N3)[H])[H])[H])[H])[H])=O)[H]	17154512
484	12g	0.3	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C3=C(C(=C(N=N3)[H])[H])[H])[H])[H])=O)[H]	17154512
485	12h	6.3	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(N=C(C(=N3)[H])C([H])([H])[H])C([H])([H])[H])[H])[H])=O)[H]	17154512
486	12i	4.9	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C3=C(N=C(C(=N3)[H])[H])[H])[H])[H])=O)[H]	17154512
487	12j	0.6	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=C(C(=N3)C([H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	17154512
488	12k	0.5	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=C(C(=N3)[H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	17154512
489	12l	4	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=C(C(=N3)C([H])([H])[H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	17154512
490	12m	1	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=NC(=N3)C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	17154512
491	12n	50	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=NC(=C(C(=N3)C([H])([H])[H])[H])C([H])([H])[H])[H])[H])=O)[H]	17154512
492	12o	3	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C3=C(C(=NC(=N3)C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	17154512
493	7n	>12500	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4[H])[H])Br)[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
494	7o	240	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])C([H])([H])[H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
495	7p	30	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])C([H])([H])[H])[H])C([H])([H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
496	7q	40	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
497	7r	16	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])C([H])([H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
498	7s	50	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Br)[H])[H])[H])Br)[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
499	7t	9	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])Cl)[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
500	7u	360	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4F)[H])[H])[H])F)[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
501	7v	9	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])C([H])([H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
502	7w	1690	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C(C([H])([H])[H])([H])[H])[H])[H])[H])C(C([H])([H])[H])([H])[H])[H])[H])=C(N=C3[H])[H])[H])[H])[H]	11992777
503	12a	>12500	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Br)[H])[H])[H])[H])[H])=C(N=C3[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	11992777
504	12b	30	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])[H])[H])=C(N=C3[H])C([H])([H])[H])[H])[H])[H]	11992777
505	12c	180	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Br)[H])[H])[H])[H])[H])=C(N=C3C([H])([H])[H])[H])[H])[H])[H]	11992777
506	12d	7.4	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])C([H])([H])[H])[H])=C(N=C3C([H])([H])[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	11992777
507	12e	6.2	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])C([H])([H])[H])[H])=C(N=C3C(O[H])([H])[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	11992777
508	12f	10	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])C([H])([H])[H])[H])=C(N=C3C(=O)[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	11992777
509	12g	4.3	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])C([H])([H])[H])[H])=C(N=C3/C(=N/O[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	11992777
510	12h	53	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])C([H])([H])[H])[H])=C(N=C3[C@@](O[H])(C([H])([H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	11992777
511	12j	69	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])C([H])([H])[H])[H])=C(N=C3C(C(C(O[H])([H])[H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	11992777
512	12k	665	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])C([H])([H])[H])[H])=C(N=C3C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H]	11992777
513	12l	2.4	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])C([H])([H])[H])[H])=C(N=C3[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	11992777
514	12m	2	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])C([H])([H])[H])[H])=C(N=C3[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	11992777
515	4	75	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H])[H]	11012021
516	5	11	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H]	11012021
517	6	16	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	11012021
518	7	240	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@]3(C(C(C([C@]3(O[H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	11012021
519	8	5	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@]3(C(C([C@@](C3([H])[H])(O[H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	11012021
520	9	23	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2[C@]3(C([C@@]([C@@](C3([H])[H])(O[H])[H])(O[H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	11012021
521	10	1180	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	11012021
522	2	380	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])Cl)C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	11012022
523	3	75	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])Br)C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	11012022
524	5	69	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])C#N)C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	11012022
525	6	290	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C(O[H])([H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	11012022
526	9	3090	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C(N([H])[H])([H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	11012022
527	10	1060	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C(=O)O[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	11012022
528	11	26200	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C(=O)N([H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	11012022
529	13	11	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H]	11012022
530	14	75	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H]	11012022
531	16	30	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])O[H])[H])[H])[H])[H])[H]	11012022
532	17	3	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])N([H])[H])[H])[H])[H])[H])[H]	11012022
533	19	1010	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])N([H])[H])[H])[H])[H]	11012022
534	20	2110	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])OC([H])([H])[H])[H])[H])[H]	11012022

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
535	21	633	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])O[H])[H])[H])[H]	11012022
536	22	790	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])[N+](=O)[O-])[H])[H])[H]	11012022
537	23	459	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])C#N)[H])[H])[H]	11012022
538	13	20	Train	C12=C(N=C(S1)N(C3=NC(=NC(=C3[H])C([H])([H])[H])C([H])([H])[H])[H])C(=C(C(=C2[H])C(N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=O)[H])[H]	17154512
539	13a	0.5	Train	C12=C(N=C(S1)N(C3=NC(=C(C(=C3[H])[H])[H])N(C(C(O[H])([H])[H])([H])[H])[H])[H])C(=C(C(=C2[H])C(N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])Cl)[H])=O)[H])[H]	17154512
540	12p	<0.2	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=C(C(=N3)N(C(C(O[H])([H])[H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	17154512
541	12q	0.5	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=C(C(=N3)N(C(C(C(N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])=O)[H]	17154512
542	12r	<0.5	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=C(C(=N3)N(C(C(C(N4C(=NC(=C4[H])[H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	17154512
543	12s	0.5	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=NC(=N3)[H])N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])=O)[H]	17154512
544	12t	1.3	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=NC(=N3)C([H])([H])[H])N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])=O)[H]	17154512
545	12u	0.7	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=NC(=N3)C([H])([H])[H])N(C(C(C(N4C(C(OC(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])=O)[H]	17154512
546	12v	0.2	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=NC(=N3)C([H])([H])[H])N(C(C(O[H])([H])[H])([H])[H])([H])[H])([H])[H])=O)[H]	17154512
547	12w	0.7	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=NC(=N3)C([H])([H])[H])N4C(C(C(C(C4([H])[H])([H])[H])(C(O[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])[H])=O)[H]	17154512
548	2	0.4	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])Cl)N(C(C2=C(N=C(S2)N(C3=C(C(=NC(=N3)C([H])([H])[H])N4C(C(N(C(C4([H])[H])([H])[H])C(C(O[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])=O)[H]	17154512
549	1	81	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H]	17276681
550	6	2100	Train	N1=C(N=C2C(=C1N(C([C@]3(OC(C(C3([H])[H])([H])[H])([H])[H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H]	17276681
551	8	210	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H]	17276681
552	13	22	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H])[H]	17276681
553	14	54	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17276681
554	15	30	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(=C(N=C5[H])[H])[H])([H])[H])([H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17276681
555	16	19	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])[H])([H])[H])(C([H])([H])[H])[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H]	17276681
556	17	29	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17276681
557	18	1600	Train	N1=C(N=C2C(=C1N(C(C(C3=C(C(=NC(=C3[H])[H])[H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17276681
558	19	170	Train	N1=C(N=C2C(=C1N(C(C(C3=C(N=C(C(=C3[H])[H])[H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17276681
559	20	380	Train	N1=C(N=C2C(=C1N(C(C(C(N3C(=NC(=C3[H])[H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17276681
560	2	122	Train	N1=C(N=C2C(=C1N(C([C@]3(C(C(C(O3)([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H]	17280833
561	3	81	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H]	17280833
562	17	6	Train	N1=C(N=C2C(=C1N(C([C@]3(C(C(C(O3)([H])[H])([H])[H])([H])[H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H]	17280833
563	18	11	Train	N1=C(N=C2C(=C1N(C([C@]3(C(C(C(O3)([H])[H])([H])[H])([H])[H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
564	19	8	Train	N1=C(N=C2C(=C1N(C([C@]3(C(C(C(O3)([H])[H])([H])[H])([H])[H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])OC([H])([H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
565	20	6	Train	N1=C(N=C2C(=C1N(C([C@]3(C(C(C(O3)([H])[H])([H])[H])([H])[H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])C(N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
566	21	11	Train	N1=C(N=C2C(=C1N(C([C@]3(C(C(C(O3)([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])C(N5C(C(N(C(C5([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])=O)[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
567	22	11	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
568	23	42	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C5=C(C(=C4[H])[H])N(C(C(O5)([H])[H])([H])[H])C([H])([H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
569	24	27	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
570	25	22	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])=O)[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
571	26	14	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H]	17280833
572	27	9	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
573	28	22	Train	N1=C(N=C2C(=C1N(C(C(N3C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])([H])[H])OC([H])([H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
574	29	14	Train	N1=C(N=C2C(=C1N(C(C(C3(C(C(N(C(C3([H])[H])([H])[H])[H])([H])[H])([H])[H])[H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
575	30	5	Train	N1=C(N=C2C(=C1N(C(C(C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])([H])[H])([H])[H])[H])C(=C(O2)C4=C(C(=C(C(=C4[H])[H])OC(C(N5C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])C6=C(C(=C(C(=C6[H])[H])[H])[H])[H])[H]	17280833
576	31	83	Train	N1=C(N=C2C(=C1N(C(C([H])([H])[H])(C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C(=C(O2)C3=C(C(=C(C(=C3[H])[H])OC(C(N4C(C(C(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	17280833
577	32	36	Train	N1=C(N=C2C(=C1N(C(C([H])([H])[H])(C([H])([H])[H])[H])[H])[H])C(=C(O2)C3=C(C(=C(C(=C3[H])[H])OC(C(N4C(C(C(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H]	17280833
578	1	4	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H]	12852972
579	2	0.5	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)N(C(C(O[H])([H])[H])([H])[H])[H])[H])[H])[H])[H]	12852972
580	3	1	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)N(C([C@]5(C(C(C(O5)([H])[H])([H])[H])([H])[H])[H])[H])[H])C([H])([H])[H])[H])[H]	12852972
581	6a	15070	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N([H])[H]	12852972
582	6b	1740	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H]	12852972
583	6c	>3100	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C(C4(C(C4([H])[H])([H])[H])[H])([H])[H])[H]	12852972
584	6d	>3100	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=NC(=C(S4)[H])[H])[H]	12852972
585	6e	>3100	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=NC(=C(N4[H])[H])[H])[H]	12852972
586	6f	>3100	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(N(C(=N4)[H])[H])[H])[H]	12852972
587	6g	>3100	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=NC(=NN4[H])[H])[H]	12852972
588	6h	138	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])[H])[H])[H])[H]	12852972
589	6i	>3100	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=C(N=C4[H])[H])[H])[H])[H])[H]	12852972
590	6j	>3100	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=NC(=C4[H])[H])[H])[H])[H])[H]	12852972
591	6k	>3100	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=NC(=C(C(=N4)[H])[H])[H])[H])[H]	12852972
592	6l	403	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])[H])[H])[H])[H]	12852972
593	6m	1890	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=NC(=C(N=N4)[H])[H])[H]	12852972
594	6n	235	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(N=C(C(=N4)[H])[H])[H])[H]	12852972
595	6o	327	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H]	12852972
596	6p	>3100	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=NC(=C(N4[H])[H])[H])[H])[H]	12852972
597	6q	1590	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4C(=C(N(N=4)[H])[H])[H])[H]	12852972
598	6r	84	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])[H])[H])[H])[H]	12852972
599	6s	27	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])[H])[H])[H]	12852972

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600	6t	41	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(N4C(C(=C(C(=N4)[H])[H])[H])([H])[H])[H]	12852972
601	6u	15	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=NC(=C(N=C4[H])[H])[H])[H]	12852972
602	6v	>3100	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])[H])C([H])([H])[H])[H]	12852972
603	6w	32	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])C([H])([H])[H])[H])[H]	12852972
604	6x	72	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])C([H])([H])[H])[H])[H])[H]	12852972
605	6y	180	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)C([H])([H])[H])[H])[H])[H])[H]	12852972
606	6z	17	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])C([H])([H])[H])[H])C([H])([H])[H])[H]	12852972
607	6aa	84	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])[H])[H])[H]	12852972
608	6ab	20	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])C([H])([H])[H])[H])[H]	12852972
609	6ac	35	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])C([H])([H])[H])[H])[H])[H]	12852972
610	6ad	9	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)C([H])([H])[H])[H])[H])[H])[H]	12852972
611	6ae	8	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)C([H])([H])[H])[H])C([H])([H])[H])[H])[H]	12852972
612	6af	5	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])C(C([H])([H])[H])([H])[H])[H])[H]	12852972
613	6ag	403	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])N([H])[H])[H])[H]	12852972
614	6ah	9	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])[H])[H]	12852972
615	6ai	1	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])C(N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	12852972
616	6aj	1	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)[H])[H])C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	12852972
617	6ak	2	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)N([H])[H])[H])[H])[H])[H]	12852972
618	6al	10	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])[H])[H])[H])[H]	12852972
619	6am	13	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	12852972
620	6an	2	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)N(C(C(N(C(=O)C([H])([H])[H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H]	12852972
621	6ao	6	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=C(C(=N4)N(C(C(C([H])([H])[H])(C([H])([H])[H])N([H])[H])([H])[H])[H])[H])[H])[H]	12852972
622	6ap	53	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)C([H])([H])[H])C([H])([H])[H])[H])[H]	12852972
623	6aq	77	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])C(C([H])([H])[H])([H])[H])[H])[H]	12852972
624	6ar	31	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)Cl)[H])[H])[H]	12852972
625	6as	20	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)N(C([H])([H])[H])[H])[H])[H])[H]	12852972
626	6at	3	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)N(C(C(O[H])([H])[H])([H])[H])[H])[H])[H])[H]	12852972
627	6au	21	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])C([H])([H])[H])[H])[H]	12852972
628	6av	5	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])C(C([H])([H])[H])([H])[H])[H])[H]	12852972
629	6aw	20	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])Cl)[H])[H]	12852972
630	6ax	13	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])OC([H])([H])[H])[H])[H]	12852972
631	6ay	8	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])N([H])[H])[H])[H]	12852972
632	6az	2	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])N(C([H])([H])[H])[H])[H])[H]	12852972
633	6ba	8	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])N(C(C(O[H])([H])[H])([H])[H])[H])[H])[H]	12852972
634	6bb	6	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)[H])N(C(C(N(C(=O)C([H])([H])[H])[H])([H])[H])([H])[H])[H])[H])[H]	12852972
635	6bc	20	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)C([H])([H])[H])C([H])([H])[H])[H])[H]	12852972

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
636	6bd	7	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)C([H])([H])[H])C(N(C([H])([H])[H])[H])([H])[H])[H])[H]	12852972
637	6be	6	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)C([H])([H])[H])C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	12852972
638	6bg	2	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)N(C(C(O[H])([H])[H])([H])[H])[H])C([H])([H])[H])[H])[H]	12852972
639	6bh	6	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)N(C(C(C([H])([H])[H])C([H])([H])[H])O[H])([H])[H])[H])C([H])([H])[H])[H])[H]	12852972
640	6bi	10	Train	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])Cl)[H])[H])SC(=N2)N(C4=C(C(=NC(=N4)C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])C([H])([H])[H])[H])[H])[H]	12852972
641	8	19600	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])O[H])[H])O[H]	14980632
642	9	26000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[H])OC([H])([H])[H])[H])[H])[H])[H]	14980632
643	10	34900	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])O[H])O[H])[H])[H])O[H])[H])O[H]	14980632
644	11	39000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])O[H])[H])[H])[H])[H])[H])O[H]	14980632
645	12	46000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])N([H])[H])[H])[H])[H])N([H])[H])O[H])N([H])[H]	14980632
646	13	56000	Train	C1(=C(C(=C2C(=C1N([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])N([H])[H])[H])[H])[H])[H])OC([H])([H])[H])[H]	14980632
647	14	60000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])O[H])[H]	14980632
648	15	69000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)O[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[H])OC([H])([H])[H])[H])O[H])[H])O[H]	14980632
649	16	99000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)O[H])C3=C(C(=C(C(=C3[H])O[H])[H])O[H])[H])O[H])[H])O[H]	14980632
650	17	103000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])N([H])[H])[H]	14980632
651	18	106000	Train	C1(=C(C(=C2C(=C1N([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])N([H])[H])[H]	14980632
652	19	117000	Train	C1(=C(C(=C2C(=C1N([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])O[H])[H]	14980632
653	20	118000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])[H])O[H])[H]	14980632
654	21	120000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[H])OC([H])([H])[H])[H])[H])[H])O[H]	14980632
655	22	119400	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])O[Si](C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])O[H])[H]	14980632
656	23	123000	Train	C1(=C(C(=C2C(=C1N([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])[H])[H]	14980632
657	24	130450	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[H])OC([H])([H])[H])[H])[H])O[H])[H]	14980632
658	25	138000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])[H])O[H]	14980632
659	26	141000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])N([H])[H])O[H]	14980632
660	27	169000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])[H])[H])O[H]	14980632
661	28	177600	Train	C1(=C(C(=C2C(=C1O[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])O[H])[H])[H])[H])[H])[H])O[H]	14980632
662	29	200000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])N([H])[H])[H])[H])[H])[H])N([H])[H])[H]	14980632
663	30	210000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])[H])[H]	14980632
664	31	223000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])O[H])N([H])[H])[H]	14980632
665	32	296000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)O[H])C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])O[H])[H])O[H]	14980632
666	33	281000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])O[H])[H])OC([H])([H])[H]	14980632
667	34	315000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])O[H])[H])[H])[H])O[H])[H])[H]	14980632
668	35	315000	Train	C1(=C(C(=C2C(=C1O[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])[H])[H])O[H]	14980632
669	36	326000	Train	C1(=C(C(=C2C(=C1N([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])O[H])[H])[H]	14980632
670	37	331000	Train	C1(=C(C(=C2C(=C1N([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])[H])O[H]	14980632
671	38	335800	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])[H])[H])O[H]	14980632
672	39	373000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[Si](C([H])([H])[H])(C([H])([H])[H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])OC([H])([H])[H])[H])[H])O[H])[H]	14980632
673	40	382000	Train	C1(=C(C(=C2C(=C1N([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])OC([H])([H])[H])[H]	14980632
674	41	395000	Train	C1(=C(C(=C2C(=C1O[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])O[H]	14980632

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675	42	439000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])[H])[H])[H]	14980632
676	43	504000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])[H])[H])[H]	14980632
677	44	502000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])N([H])[H])[H])[H])[H])[H])N([H])[H])O[H]	14980632
678	45	754000	Train	C1(=C(C(=C2C(=C1N([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])N([H])[H])O[H]	14980632
679	46	810000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])[H]	14980632
680	47	976000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])O[Si](C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])O[H]	14980632
681	48	1032000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])[H])[H])OC([H])([H])[H]	14980632
682	49	1272000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[H])OC([H])([H])[H])[H])[H])[H])O[H]	14980632
683	50	1530000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[Si](C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])OC([H])([H])[H])[H])[H])[H])O[H]	14980632
684	51	1565000	Train	C1(=C(C(=C2C(=C1[N+](=O)[O-])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[N+](=O)[O-])O[H]	14980632
685	52	1596000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])[H])[H]	14980632
686	53	1621000	Train	C1(=C(C(=C2C(=C1N([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])OC([H])([H])[H])[H])[H]	14980632
687	54	1876000	Train	C1(=C(C(=C2C(=C1[N+](=O)[O-])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[H])O[H]	14980632
688	55	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H]	14980632
689	12	84	Train	N1=C(N=C(C(=C1[H])C(N(C2=C(C(=C(C(=C2C([H])([H])[H])[H])[H])C(N(C3=C(C(=C(C(=C3F)C(F)(F)F)[H])[H])[H])[H])=O)[H])[H])=O)N(C([H])([H])[H])[H])N(C([H])([H])[H])[H]	18083554
690	1	4200	Train	O1C2=C(C(=N1)C3=C(C(=NC(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
691	1	6800	Train	O1C2=C(C(=N1)C3=C(C(=NC(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])N([H])[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
692	6	193	Train	N1C2=C(N(C=1[H])C3=C(C(=NC(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
693	7	24	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
694	6	>10000	Train	N1C2=C(N(C=1[H])C3=C(C(=NC(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])OC([H])([H])[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
695	7	7700	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])OC([H])([H])[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
696	6	5664	Train	N1C2=C(N(C=1[H])C3=C(C(=NC(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])C(=O)N([H])[H])[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
697	6	8640	Train	N1C2=C(N(C=1[H])C3=C(C(=NC(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])N(C(=O)C([H])([H])[H])[H])[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
698	6	>10000	Train	N1C2=C(N(C=1[H])C3=C(C(=NC(=N3)N(C4=C(C(=C(C(=C4[H])[H])[H])O[H])[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
699	7	>10000	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])F)[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
700	8	>10000	Train	N1C2=C(N(C=1[H])C3=NC(=NC(=C3[H])N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
701	4	1286	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])[H])Cl)C(=C(C(=C2[H])[H])[H])[H]	16997556
702	12a	294	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])N([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
703	12b	79	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])N(C([H])([H])[H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
704	12c	384	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])N(C([H])([H])[H])C([H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
705	12d	71	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])OC([H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
706	12e	137	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])[H])N5C(C(OC(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
707	12f	3	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H])[H]	16997556
708	12g	3	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])[H])OC(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
709	12h	867	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])OC([H])([H])[H])[H])[H])[H])OC(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
710	12i	17	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])[H])N(C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H])[H]	16997556
711	12j	65	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])[H])OC(C(N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H])[H]	16997556

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712	12k	3	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])N(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
713	12l	44	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])N(C(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
714	12m	130	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])N(C(C(C(N5C(C(N(C(C5([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
715	12n	45	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])N(C(C(N5C(C(N(C(C5([H])[H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
716	12o	165	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])N(N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
717	12p	519	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])N(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
718	12q	43	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])C(C5(C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
719	12r	333	Train	N1C2=C(N(C=1[H])C3=NC(=C(C(=N3)N(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])O[H])[H])[H])C(C(C(C5(C(C(N(C(C5([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])C(=C(C(=C2[H])[H])[H])[H]	16997556
720	4	1600	Train	C1(=C(C(=C(C(=C1[H])[H])C([C@@](C(N([C@](C(N([C@](C(N([C@](C(=O)N(C([H])([H])[H])[H])([C@@](C([H])([H])[H])(C(C([H])([H])[H])([H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])=O)(C(C(C(=O)O[H])([H])[H])([H])[H])[H])[H])=O)(C(C(C(=O)O[H])([H])[H])([H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H]	11992778
721	7	1600	Train	C1(=C(C(=C(C(=C1[H])[H])C([C@](N(C(C([H])([H])[H])=O)[H])(C(=O)N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N([C@@](C(=O)N(C([H])([H])[H])[H])([C@](C(C([H])([H])[H])([H])[H])(C([H])([H])[H])[H])([H])[H])[H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])[H])[H])OP(=O)(O[H])O[H]	11992778
722	20	1500	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])([H])[H])[H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
723	21	400	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C4=C(C(=C(C(=C4[H])[H])Cl)[H])[H])([H])[H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
724	22	10000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C4=C(C(=C(C(=C4[H])[H])O[H])[H])[H])([H])[H])[H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
725	23	8500	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])([H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
726	24	6000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C(C([H])([H])[H])([H])[H])([H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
727	25	1900	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C(C(C([H])([H])[H])([H])[H])([H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
728	26	1800	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C(C(C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
729	27	1200	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C([C@](C(C([H])([H])[H])([H])[H])(C([H])([H])[H])[H])([H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
730	29	1600	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C4(C(C(C(C(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
731	30	1100	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C45C([C@@]6(C([C@@](C([C@](C4([H])[H])(C6([H])[H])[H])([H])[H])(C5([H])[H])[H])([H])[H])([H])[H])([H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
732	31	1900	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C4C(=C(C(=C5C(=C(C(=C(C=45)[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
733	28	1800	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C(C(C(C([H])([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
734	32	1100	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N(C4C(=C(C(=C5C(=C(C(=C(C=45)[H])[H])[H])[H])[H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
735	33	1200	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N([C@]4(C(C(C5C(=C(C(=C(C4=5)[H])[H])[H])[H])([H])[H])([H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
736	34	7700	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N([C@@]4(C([C@](C5C(=C(C(=C(C4=5)[H])[H])[H])[H])(C(=O)O[H])[H])([H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
737	35	7300	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N([C@]4(C([C@@](C5C(=C(C(=C(C4=5)[H])[H])[H])[H])(C(=O)O[H])[H])([H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
738	36	100	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N([C@@]4(C([C@@](C5C(=C(C(=C(C4=5)[H])[H])[H])[H])(C(=O)O[H])[H])([H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
739	56	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H]	14980632
740	57	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H]	14980632
741	58	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])OC(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H])[H])[H]	14980632
742	59	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])OC(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H]	14980632
743	60	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])OC(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H])[H]	14980632
744	61	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])[H])Br)[H])[H])[H])[H]	14980632
745	62	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[H])[H]	14980632
746	63	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])OC([H])([H])[H]	14980632
747	64	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])OC([H])([H])[H])[H]	14980632
748	65	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])O[H])[H])O[H]	14980632
749	66	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[H])[H]	14980632
750	67	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[N+](=O)[O-])[H]	14980632
751	68	>2000000	Train	C1(=C(C(=C2C(=C1[N+](=O)[O-])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[H])[H]	14980632
752	69	>2000000	Train	C1(=C(C(=C2C(=C1[N+](=O)[O-])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])OC([H])([H])[H])[H]	14980632
753	70	>2000000	Train	C1(=C(C(=C2C(=C1[N+](=O)[O-])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])OC([H])([H])[H])[H])[H]	14980632
754	71	1928000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])OC(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])([H])[H])[H])[H])[H])[H])O[H]	14980632
755	72	>2000000	Train	C1(=C(C(=C2C(=C1OC([H])([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])OC([H])([H])[H]	14980632
756	73	>2000000	Train	C1(=C(C(=C2C(=C1O[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[Si](C([H])([H])[H])(C([H])([H])[H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])OC([H])([H])[H])[H])[H])O[H]	14980632
757	74	>2000000	Train	C1(=C(C(=C2C(=C1OC(=O)C([H])([H])[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[Si](C([H])([H])[H])(C([H])([H])[H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])OC([H])([H])[H])[H])[H])OC(=O)C([H])([H])[H]	14980632
758	75	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])OC([H])([H])[H])[H]	14980632
759	76	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])O[H]	14980632
760	77	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[H])OC([H])([H])[H])[H])[H])[H])OC(=O)C([H])([H])[H]	14980632
761	78	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O[Si](C([H])([H])[H])(C([H])([H])[H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])OC([H])([H])[H])[H])[H])OC(=O)C([H])([H])[H]	14980632
762	79	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])OC([H])([H])[H]	14980632
763	80	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])[H])[H]	14980632
764	81	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])OC(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])([H])[H])[H])[H])O[H])[H])[H]	14980632
765	82	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])OC([H])([H])[H])[H])[H])[H])[H])[H]	14980632
766	83	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])Br)[H])[H])[H])[H])[H]	14980632
767	84	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[H])[H])[H]	14980632
768	85	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])OC([H])([H])[H]	14980632
769	86	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])OC([H])([H])[H])[H]	14980632

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
770	87	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])OC(C4=C(C(=C(C(=C4[H])[H])[H])[H])([H])[H])OC(C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	14980632
771	88	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O C([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H]	14980632
772	89	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])[H])[H]	14980632
773	90	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])O C([H])([H])[H])[H])[H])[H])[H])[H]	14980632
774	91	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)O[H])C3=C(C(=C(C(=C3[H])[H])OC([H])([H])[H])[H])[H])[H])[H])[H]	14980632
775	92	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])[H])[H])OC([H])([H])[H]	14980632
776	93	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])[H])OC([H])([H])[H])[H]	14980632
777	94	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])N(C(=O)C([H])([H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H]	14980632
778	95	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])N(C(=O)C([H])([H])[H])[H])[H])[H])[H])OC([H])([H])[H])[H]	14980632
779	96	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[H])OC([H])([H])[H]	14980632
780	97	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])OC([H])([H])[H])[H]	14980632
781	98	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])O[H])[H])O[H]	14980632
782	99	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[H])[N+](=O)[O-])O[H]	14980632
783	100	>2000000	Train	C1(=C(C(=C2C(=C1[N+](=O)[O-])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])O[H])[H])[H]	14980632
784	37	2000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N([C@]4(C([C@](C5C(=C(C(=C(C4=5)[H])[H])[H])[H])(C(=O)O[H])[H])([H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
785	38	30	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N([C@@]4(C([C@](C5C(=C(C(=C(C4=5)[H])[H])[H])[H])(C(=O)O[H])[H]) ([H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
786	39	2800	Train	C1(=C(C(=C(C(=C1[H])C([C@@](C(N([C@]2(C(C(C(N3N(C2=O)[C@@](C(C(C3([H])[H])([H])[H])([H])[H])(C(=O)N([C@]4(C([C@@](C5C(=C(C(=C(C4=5)[H])[H])[H])[H])(C(=O)O[H])[H]) ([H])[H])[H])[H])[H])=O)([H])[H])([H])[H])[H])[H])=O)(N(C(=O)C([H])([H])[H])[H])([H])[H])[H])[H])OP(=O)(O[H])O[H])[H]	11992778
787	1	1710	Train	C1(=NC(=NC(=C1[H])[H])N(C2=C(C(=C(C(=C2[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])[H])[H])[H]	15032728
788	3	504	Train	C1(=C(C(=C(C(=C1[H])N(C2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H])[H])[H])[H]	15032728
789	5	602	Train	C1(=C(C(=C(C(=C1[H])C(C2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H])[H])[H])[H]	15032728
790	7	125	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H])[H])[H]	15032728
791	7	2695	Train	C1(=C(C(=C(C(=C1[H])S(C2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])(=O)=O)[H])[H])[H])[H]	15032728
792	15	1300	Train	O=C(C1=NC(=NC(=C1[H])[H])N(C2=C(C(=C(C(=C2[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])C3=C(C(=C(C(=C3[H])[H])[H])[H])[H]	15032728
793	17	523	Train	C1(=C(C(=C(C(=C1[H])OC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H])[H])[H])[H]	15032728
794	18	1300	Train	C1(=C(C(=C(C(=C1[H])SC2=C(C(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H])[H])[H])[H]	15032728
795	19	91	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])OC([H])([H])[H])[H])[H])[H]	15032728
796	20	43	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])OC([H])([H])[H])[H])[H]	15032728
797	21	70	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])OC([H])([H])[H])[H]	15032728
798	22	32	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])Br)[H])[H]	15032728
799	23	85	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H])Br)[H]	15032728
800	24	135	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])C#N)[H])[H]	15032728
801	25	13	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])C(=O)O[H])[H])[H]	15032728
802	26	56	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])C(=O)OC(C([H])([H])[H])([H])[H])[H])[H]	15032728
803	27	84	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])C(=O)ON([H])[H])[H])[H]	15032728
804	28	4	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC(C(N4C(C(C(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])OC([H])([H])[H])[H])[H]	15032728
805	29	3	Train	C1(=C(C(=C(C(=C1[H])SC2=NC(=NC(=C2[H])[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H]) OC([H])([H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])OC([H])([H])[H])[H])[H]	15032728

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
806	6	24000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](OC(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)(C(O[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
807	7	20000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N(C(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)[H])(C(O[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
808	8	21000	Train	C1(=C(C(=C(C(=C1[H])C([C@](N(C(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)[H])(C(O[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
809	9	15000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](OC(C(C(C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])([H])[H])([H])[H])=O)(C(O[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
810	4	13000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N(C(C(C(C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])([H])[H])([H])[H])=O)[H])(C(O[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
811	10	71000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N(C(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)[H])(C(OC([H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
812	11	32000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N(C(C(C(C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])([H])[H])([H])[H])=O)[H])(C(OC([H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
813	12	21000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N(C(C(C2=C(C(=C(C(=C2[H])O[H])O[H])[H])[H])([H])[H])=O)[H])(C(OC([H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
814	13	19000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N(C(C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])=O)[H])(C(OC([H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
815	14	80000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](OC(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)(C(OC([H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
816	15	91000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](OC(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)(C(OC(C([H])([H])[H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
817	16	145000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](OC(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)(C(OC(C(C([H])([H])[H])([H])[H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
818	17	110000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](OC(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)(C(OC(C([H])([H])[H])(C([H])([H])[H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
819	5	127000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](OC(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)(C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
820	18	>500000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](OC(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)(C(N(C(C(C(C(C(C(=O)OC([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
821	19	>500000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N(C(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])OC([H])([H])[H])[H])[H])[H])[H])=O)[H])(C(OC([H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
822	20	>500000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N(C(/C(=C(/C2=C(C(=C(C(=C2[H])[H])OC([H])([H])[H])O[H])[H])[H])[H])=O)[H])(C(OC([H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
823	21	>500000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N(C(/C(=C(/C2=C(C(=C(C(=C2[H])[H])OC([H])([H])[H])OC([H])([H])[H])([H])[H])[H])=O)[H])(C(OC([H])([H])[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
824	22	>500000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N(C(/C(=C(/C2=C(C(=C(C(=C2[H])[H])O[H])O[H])[H])[H])[H])[H])=O)[H])(C(OC([H])([H])[H])=O)[H])([H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	17418581
825	23	>500000	Train	O(C(/C(=C(/C1=C(C(=C(C(=C1[H])[H])O[H])O[H])[H])[H])[H])[H])=O)[H]	17418581
826	24	>500000	Train	C1(=C(C(=C(C(=C1[H])C([C@@](N([H])[H])(C(O[H])=O)[H])([H])[H])[H])[H])O[H])O[H]	17418581
827	1	7400	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])O[H])[H])O[H]	14980632
828	2	13000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)O[H])C3=C(C(=C(C(=C3[H])O[H])O[H])[H])[H])O[H])[H])O[H]	14980632
829	3	14000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)O[H])C3=C(C(=C(C(=C3[H])O[H])O[H])[H])[H])[H])[H])O[H]	14980632
830	4	14800	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])O[H])[H])O[H]	14980632
831	5	15730	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])O[H])[H])[H]	14980632
832	6	15730	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])O[H])[H])[H])[H])[H])O[H])[H]	14980632
833	7	18000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])N([H])[H])O[H])N([H])[H]	14980632
834	101	>2000000	Train	C1(=C(C(=C2C(=C1[N+](=O)[O-])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[H])[N+](=O)[O-])[H]	14980632
835	102	>2000000	Train	C1(=C(C(=C2C(=C1[N+](=O)[O-])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])[H])[H])O[H])[H]	14980632
836	103	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])[N+](=O)[O-])[H])[H])O[H])[N+](=O)[O-])[H]	14980632
837	104	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N+](=O)[O-])[H])[H])[H])[N+](=O)[O-])O[H])[N+](=O)[O-]	14980632
838	17	1200	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])[H])N([H])[H])[H])[H])[H])O[H])[H]	1995903
839	13	>2000000	Train	C1(=C(C(=C2C(=C1[H])OC(=C(C2=O)C(=O)OC([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])N(C(C4=C(C(=C(C(=C4[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])=O)[H])[H])[H])[H])[H])[H]	1995903
840	1	3200	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N([H])[H])C([H])([H])[H])=O)[H]	12798323
841	9	3000	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(N=C(S2)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])C([H])([H])[H])=O)[H]	12798323
842	10	15000	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N([H])[H])[H])[H])=O)[H]	12798323
843	5a	290	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
844	11	3230	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])N(C(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
845	12	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])N(C(=N3)N([H])[H])[H])[H])[H])=O)[H]	12798323

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
846	13	7250	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])OC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
847	14	23000	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])OC(=N3)N([H])[H])[H])[H])=O)[H]	12798323
848	15	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=N2)SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
849	16	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=N2)SC(=N3)N([H])[H])[H])[H])=O)[H]	12798323
850	17	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(=O)C2C(=C(C(=C3C=2SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])[H]	12798323
851	18	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(=O)C2=C(C(=C3C(=C2[H])N=C(S3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H]	12798323
852	19	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(=O)C2C(=C(C(=C3C=2N=C(S3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])[H]	12798323
853	20	4400	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2Cl)SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
854	21	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])Cl)=O)[H]	12798323
855	22	5600	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])C([H])([H])[H])[H])=O)[H]	12798323
856	23	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])OC([H])([H])[H])[H])=O)[H]	12798323
857	5b	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])Br)[H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
858	5c	70	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
859	5d	90	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
860	5e	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C(C(O[H])([H])[H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
861	5f	>12500	Train	C1(=C(C(=C(C(=C1O[H])[H])[H])[H])C(=O)C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
862	5g	>12500	Train	C1(=C(C(=C(C(=C1Br)C([H])([H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
863	5h	110	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])Br)[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
864	5i	4270	Train	C1(=C(C(=C(C(=C1Br)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
865	5j	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])Br)C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
866	5k	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])C(C([H])([H])[H])(C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
867	5l	>12500	Train	C1(=C(C(=C(C(=C1OC([H])([H])[H])[H])[H])[H])[H])OC([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
868	5m	3120	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C(=O)OC([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
869	5n	200	Train	C1(=C(C(=C(C(=C1Br)[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
870	5o	310	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C(O[H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
871	5p	9650	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C2=C(C(=C(C(=C2[H])[H])[H])[H])[H])[H])C([H])([H])[H])N(C(C3=C(C(=C4C(=C3[H])SC(=N4)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
872	7a	120	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)C([H])([H])[H])[H])[H])[H])=O)[H]	12798323
873	7b	>12500	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
874	7c	700	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)C(C([H])([H])[H])(C([H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
875	7d	20	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)C4(C(C4([H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
876	7e	15	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)C4(C(C4([H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
877	7f	1800	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)C(C([H])([H])[H])(C([H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
878	7g	11	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)[C@]4(C([C@]4(C([H])([H])[H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
879	7h	9	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)C4(C(C4([H])[H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
880	7i	666	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)C4(C(C(C4([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
881	7j	272	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)[C@]4(OC(C(C4([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
882	7k	565	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)C(C4=C(C(=C(C(=C4C([H])([H])[H])[H])[H])[H])[H])([H])[H])[H])[H])[H])=O)[H]	12798323
883	7l	7	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)[C@]4(C([C@]4(C([H])([H])[H])[H])([H])[H])[H])[H])[H])=O)[H]	12798323
884	7m	27	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)[C@]4(C([C@]4(C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
885	7n	337	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)[C@]4([C@@](C4([H])[H])(C([H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
886	7o	85	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)C(C4(C(C4([H])[H])([H])[H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
887	7p	7	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)[C@]4(C([C@]4(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
888	7q	3	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)[C@]4(C([C@]4(C(O[H])([H])[H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
889	7r	11	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)[C@]4(C([C@]4(C([C@]5(N(C(C(C5([H])[H])([H])[H])[H])([H])[H])[H])([H])[H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
890	8a	130	Train	C1(=C(C(=C(C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C([H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
891	8b	380	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
892	8c	1730	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
893	8d	300	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C4(C(C4([H])[H])([H])[H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
894	8e	330	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C(C(C(C([H])([H])[H])([H])[H])[H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
895	8f	70	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
896	8j	90	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C4(C(C4([H])[H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
897	8h	100	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
898	8i	80	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N([C@]4(C(C4([H])[H])(C([H])([H])[H])[H])C([H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
899	8k	45	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C4(C(C(C(C4([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
900	8l	39	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C(C4=C(C(=C(O4)[H])[H])[H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
901	8m	19	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C(C(C(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
902	8n	2010	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C4=C(C(=C(C(=N4)[H])[H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
903	8o	>3125	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C4=NC(=C(C(=N4)[H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
904	8p	123	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C4=C(C(=C(C(=C4[H])[H])F)[H])[H])[H])[H])[H])[H])=O)[H]	12798323
905	8q	87	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C(C4=C(C(=C(C(=C4[H])[H])F)[H])[H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
906	2	4	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
907	8s	55	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N([C@]4(C(C4([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
908	8t	30	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
909	8u	7	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C(C([C@]4(C(C(C(N4C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])([H])[H])[H])[H])[H])[H])[H])[H])=O)[H]	12798323
910	8v	4	Train	C1(=C(C(=C(C(=C1Cl)[H])[H])[H])C([H])([H])[H])N(C(C2=C(C(=C3C(=C2[H])SC(=N3)N(C(=O)N(C4(C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])[H])(C([H])([H])[H])C([H])([H])[H])([H])[H])[H])[H])[H])[H])=O)[H]	12798323
911	3	50000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])[H])Cl)[H])[H])[H])[H])[H]	10.1016/S0960-894X(97)00034-6
912	4	5000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])[H])Cl)[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-7
913	5	1000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])OC3=C(C(=C(C(=C3[H])[H])[H])Cl)[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-8
914	6	2500	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])SC3=C(C(=C(C(=C3[H])[H])[H])Cl)[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-9

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
915	7	10000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-10
916	8	>100000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])C([H])([H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-11
917	9	10000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-12
918	10	500	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-13
919	11	20000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C(C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])([H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-14
920	12	10000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])[H])F)[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-15
921	13	50000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C4C(=C3[H])C(C(C4([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-16
922	14	3000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-17
923	15	>100000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-18
924	16	10000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])OC([H])([H])[H])[H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-19
925	17	10000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-20
926	18	>50000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])SC3=C(C(=C(C(=C3[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-21
927	19	>100000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])C([H])([H])[H])[H])C([H])([H])[H]	10.1016/S0960-894X(97)00034-22
928	20	>100000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-23
929	21	>100000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)Cl)N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-24
930	22	10000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-25
931	23	>50000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])[H])Cl	10.1016/S0960-894X(97)00034-26
932	24	5000	Train	C1(=C(C(=C2C(=C1[H])C(=NC(=N2)[H])OC3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H]	10.1016/S0960-894X(97)00034-27
933	25	10000	Train	C12=C(C(=NC(=N1)[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])C(=NN2[H])[H]	10.1016/S0960-894X(97)00034-28
934	26	50000	Train	C12=C(C(=NC(=N1)[H])N(C3=C(C(=C(C(=C3[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H])[H])N=C(N2[H])[H]	10.1016/S0960-894X(97)00034-29
935	12i	238	Train	C1(=C(C(=C2C(=C1[H])N3C(C(=N2)N(C4=C(C(=C(C(=C4Cl)[H])[H])[H])C([H])([H])[H])[H])=C(N=C3[C@@](O[H])(C(C([H])([H])[H])(C([H])([H])[H])[H])[H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	11992777
936	12	328000	Train	C1(=C(C(=C2C(=C1O[H])OC(=C(C2=O)[H])C3=C(C(=C(C(=C3[H])OC([H])([H])[H])C([H])([H])[H])OC([H])([H])[H])[H])[H])[H])O[H]	1800636
937	2	<8	Train	N1=C(N=C2C(=C1N(C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H])C(=C(C(=C2[H])[H])[H])[H])[H]	11012021
938	3	220	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])C3=C(C(=C(C(=C3[H])[H])Cl)[H])[H])[H]	11012021
939	Staurosporine	3	Train	N12[C@]3([C@]([C@](C([C@@](N4C5C1=C(C6=C(C=5C7C(=C(C(=C(C4=7)[H])[H])[H])[H])C(N(C6([H])[H])[H])=O)C8C(=C(C(=C(C2=8)[H])[H])[H])[H])(O3)[H])([H])[H])(N(C([H])([H])[H])[H])[H])(OC([H])([H])[H])[H])C([H])([H])[H]	8557675
940	Genistein	4500	Train	C1(=C(C(=O)C2C(O[H])=C(C(O[H])=C(C=2O1)[H])[H])C3C(=C(C(O[H])=C(C=3[H])[H])[H])[H])[H]	8557675
941	166326	<5	Train	C(O[C@@]1([C@](OC([H])([H])[H])(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])([H])([H])[H]	10974196
942	173952	<5	Train	C(O[C@@]1([C@](OC([H])([H])[H])(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])O[H])[H])[H])[H])[H])[H])[H])([H])([H])[H]	10974196
943	173955	<5	Train	N(C(=O)N(C1C(=C(C(=C(C=1[H])C(F)(F)F)[H])[H])F)[H])(C2C(=C(C(=C(C=2[H])[H])C3C4=C(N=C(N=C4N([H])[H])[H])SC=3C([H])([H])[H])[H])[H])[H]	10974196
944	173956	<5	Train	N(C(=O)N(C1C(=C(C(=C(C=1[H])[H])[H])C([H])([H])[H])[H])[H])(C2C(=C(C(=C(C=2[H])[H])C3C4=C(N=C(N=C4N([H])[H])[H])SC=3[H])[H])[H])[H]	10974196
945	173958	<5	Train	C1(C2C(=C(C(=C(C=2[H])C(N(C3C(=C(C(=C(C=3[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])C([H])([H])[H])=C(C4=C(C(=C1[H])[H])N=C(N=C4[H])N([H])[H])[H]	10974196
946	179483	<5	Train	C(C1C(=C(C(=C(C=1[H])C(N(C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N([H])[H])[H])[H]	10974196
947	180970	<5	Train	N1=C(N=C2C(=C1[H])C([C@@](C(N2C([H])([H])[H])=O)(C3=C(C(=C(C(=C3Cl)[H])[H])[H])Cl)[H])([H])[H])N(C4=C(C(=C(C(=C4[H])[H])F)C([H])([H])[H])[H])[H]	10974196
948	6l	7	Train	C1(=C(C(=C(C(=C1N(C2=NN3C(=C2C(=O)N([H])[H])N=C(C(=C3N([C@@](C(C4=C(C(=C(C(=C4[H])[H])[H])[H])[H])([H])[H])(C(O[H])([H])[H])[H])[H])[H])C5(C(C5([H])[H])([H])[H])[H])[H])[H])OC([H])([H])[H])[H])OC([H])([H])[H])[H]	17997320
949	13	0.4	Train	C1(=C(C(=C(C(=C1C([H])([H])[H])N(C(=O)C2SC(=NC=2[H])N(C3=C(C(=NC(=N3)C([H])([H])[H])N4C(C(N(C(C4([H])[H])([H])[H])C(C(O[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])Cl)[H])[H])[H]	15615512
950	83	60	Train	C1(=C(C(=C(C(=C1[H])OC([H])([H])[H])[H])C2=C(C3C(N(C2=O)C(C([H])([H])[H])([H])[H])=NC(=NC=3[H])N(C4=C(C(=C(C(=C4[H])[H])OC(C(N(C(C([H])([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H]	12171566
951	84	1800	Train	C1(=C(C(=C(C(=C1[H])OC([H])([H])[H])[H])C2=C(C3C(N(C2=O)C(C([H])([H])[H])([H])[H])=NC(=NC=3[H])N(C4=C(C(=NC(=C4[H])[H])[H])[H])[H])[H])[H])OC([H])([H])[H]	12171566
952	42	13	Train	C1(=C(C(=C(C(=C1[H])C([H])([H])[H])C2C(=C3C(=C(C=2[H])C([H])([H])[H])N=C(N=N3)N(C4=C(C(=C(C(=C4[H])[H])O[C@@](C([H])([H])[H])(N5C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H])C([H])([H])[H])[H])[H]	16931012

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
953	24	>5000	Train	N1=C(N=C(C2N1C(=C(C=2C(OC([C@]3(OC(C(N(C3([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])N(C4=C(C5=C(C(=C4[H])[H])N(N=C5[H])C(C6=C(C(=C(C(=C6[H])[H])[H])F)[H])([H])[H])[H])[H])[H]	17270437
954	1a	>5000	Train	C12N(N=C(N=C1N(C3=C(C4=C(C(=C3[H])[H])N(N=C4[H])C(C5=C(C(=C(C(=C5[H])[H])[H])F)[H])([H])[H])[H])[H])[H])C(=C(C=2C(OC([C@]6(OC(C(N(C6([H])[H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	17606372
955	1c	710	Train	C12N(N=C(N=C1N(C3=C(C4=C(C(=C3[H])[H])N(N=C4[H])C(C5=C(C(=C(C(=C5[H])[H])[H])F)[H])([H])[H])[H])[H])[H])C(=C(C=2C(N6C(C(C(C(C6([H])[H])([H])[H])(N([H])[H])[H])([H])[H])([H])[H])([H])[H])[H])[H]	17606372
956	3	341	Train	C1(=C(C(=C2C(=C1[H])N(C(=N2)C3=C(C(=C(N(C3=O)[H])[H])[H])N(C([C@](C4=C(C(=C(C(=C4[H])Cl)[H])[H])[H])(O[H])[H])([H])[H])[H])[H])[H])C([H])([H])[H])[H])N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])[H]	16134929
957	1	151	Train	N1=C(N=C2C(=C1N([H])[H])C(=NN2C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C3=C(C(=C(C(=C3[H])[H])C([H])([H])[H])[H])[H])[H])[H]	11012021
958	1	16	Train	N1=C(N=C2C(=C1N([H])[H])C(=C(N2C3(C(C(C(C3([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])C4=C(C(=C(C(=C4[H])[H])OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H])[H]	11012022
959	4	88	Train	C(O[C@@]1([C@](OC([H])([H])[H])(C(=C2C(=C1[H])C(=NC(=N2)[H])N(C3=C(C(=C(C(=C3[H])[H])OC4=C(C(=C(C(=C4[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H]	11401553
960	15	7	Train	C(C1C(=C(C(=C(C=1[H])C(N(C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N([H])[H])[H])[H]	17064066
961	33	<4	Train	C(C1C(=C(C(=C(C=1[H])C(N(C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H]	17064066
962	1	59	Train	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H]	18006306
963	3	170	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N([H])[H]	18353642
964	4a	21	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C([H])([H])[H])[H])[H]	18353642
965	4b	16	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H])[H]	18353642
966	4c	16	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C5(C(C(C(C5([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18353642
967	4d	94	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H])[H]	18353642
968	4e	125	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N([C@]5(C(=C(C(=C(N5[H])[H])[H])[H])[H])[H])[H])[H])[H])[H]	18353642
969	4f	30	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)C([H])([H])[H])[H]	18353642
970	4g	30	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])[H])[H])[H]	18353642
971	4h	8	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)OC(C(OC([H])([H])[H])([H])[H])([H])[H])[H])[H]	18353642
972	4i	112	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)OC5=C(C(=C(C(=C5[H])[H])[H])[H])[H])[H])[H]	18353642
973	4j	131	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)OC5=C(C(=C(C(=C5[H])[H])OC([H])([H])[H])[H])[H])[H])[H]	18353642
974	9a	81	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18353642
975	9b	58	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(C(N5C(C(N(C(C5([H])[H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18353642
976	9c	78	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(C(C(N5C(C(OC(C5([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18353642
977	9d	16	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N([C@]5(C(=C(C(=C(N5[H])[H])[H])[H])C([H])([H])[H])[H])[H])[H]	18353642
978	9e	53	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N([C@]5(N(C(=C(C(=N5)C([H])([H])[H])[H])[H])C([H])([H])[H])[H])[H])[H]	18353642
979	9f	0.6	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C5=NC(=NC(=C5[H])C([H])([H])[H])C([H])([H])[H])[H]	18353642
980	9g	4	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N([C@]5(N(C(=C(N=C5[H])[H])[H])[H])[H])[H])[H]	18353642
981	9h	8	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C5=NOC(=C5[H])C([H])([H])[H])[H]	18353642

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982	15a	7	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])F)[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H]	18353642
983	15b	15	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])N5C(=NC(=C5[H])C([H])([H])[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H]	18353642
984	15c	19	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])C(F)(F)F)[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H]	18353642
985	15d	50	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])Cl)C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H]	18353642
986	15e	158	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])OC([H])([H])[H])[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H]	18353642
987	15f	112	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C([H])([H])[H])[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H])[H]	18353642
988	15g	104	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])Cl)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H]	18353642
989	15h	9	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)[C@]4(N(C(=C(C(=C4[H])[H])[H])C(C([H])([H])[H])([H])C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H]	18353642
990	15i	12	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(S4)C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H])[H])[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H]	18353642
991	2	36	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[H]	18353642
992	16	955	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[H]	18353642
993	18	>10000	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])C([H])([H])[H]	18353642
994	20	2099	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])N(C(=O)C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])Br)[H])[H])[H])SC(=N2)N(N5C([C@@](OC(C5([H])[H])([H])[H])C(C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H]	18353642
995	21	118	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])[H])[H])SC(=N2)N(C(=O)N(C(C([H])([H])[H])([H])[H])[H])[H])[H]	18353642
996	22	139	Validation	C12=C(C(=C(C(=C1[H])[H])C(=O)N(C3=C(C([H])([H])[H])C(=C(C(=C3[H])C(N(C4=C(C(=C(C(=C4[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])[H])[H])SC(=N2)N(C(=O)N(C5(C(C(C(C5([H])[H])([H])[H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18353642
997	34	0.2	Validation	C1(C2C(=C(C(=C(C=2[H])C(N(C3C(=C(C(=C(C=3[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])C([H])([H])[H])=C(C4=C(C(=C1[H])[H])N=C(N=C4[H])N([H])[H])[H]	18321037
998	10a	15	Validation	C(C1C(=C(C(=C(C=1[H])C(N(C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N([H])[H])[H])[H]	18321037
999	10b	0.5	Validation	C(C1C(=C(C(=C(C=1[H])C(N(C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])=O)[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18321037
1000	1	6	Validation	N1=C(N=C(N=C1[H])N2C(N(C3=C(C(=C(C(=C3[H])[H])[H])[H])[H])[H])=NC4=C2C(=C(C(=C4[H])[H])[H])[H])N(C5=C(C(=C(C(=C5[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H]	18278858
1001	2	1	Validation	N1=C(N=C(N=C1[H])N2C(N(C3=C(C(=C(C(=C3C([H])([H])[H])[H])[H])[H])C([H])([H])[H])[H])=NC4=C2C(=C(C(=C4[H])[H])[H])[H])N(C5=C(C(=C(C(=C5[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H]	18278858
1002	24	27	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])OC([H])([H])[H])OC([H])([H])[H])OC([H])([H])[H])[H])[H]	18278858
1003	25	7	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])[H])N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18278858
1004	26	5	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])OC([H])([H])[H])N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18278858
1005	27	28	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])[H])OC(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18278858
1006	28	20	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])[H])OC(C(C(N(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18278858
1007	29	19	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])OC([H])([H])[H])[H])OC(C(N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18278858
1008	30	6	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])OC([H])([H])[H])[H])OC(C(N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H]	18278858

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
1009	31	23	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])F)OC(C(N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18278858
1010	32	10	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])OC([H])([H])[H])OC(C(N7C(C(OC(C7([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H])[H])[H]	18278858
1011	33	12	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])[H])OC(C(C(N7C(C(C(C(C7([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18278858
1012	34	12	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])OC([H])([H])[H])OC(C(C(N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18278858
1013	35	6	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5C([H])([H])[H])[H])[H])[H])C([H])([H])[H])=O)N(C6=C(C(=C(C(=C6[H])OC([H])([H])[H])OC(C(C(N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])OC([H])([H])[H])[H])[H]	18278858
1014	36	10	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5Cl)[H])[H])[H])Cl)=O)N(C6=C(C(=C(C(=C6[H])[H])N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18278858
1015	37	8	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5Cl)[H])Cl)[H])Cl)=O)N(C6=C(C(=C(C(=C6[H])[H])N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18278858
1016	38	350	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])C([H])([H])[H])[H])[H])=O)N(C6=C(C(=C(C(=C6[H])[H])N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18278858
1017	39	96	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])C([H])([H])[H])[H])=O)N(C6=C(C(=C(C(=C6[H])[H])N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18278858
1018	40	190	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])[H])OC([H])([H])[H])[H])=O)N(C6=C(C(=C(C(=C6[H])[H])N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18278858
1019	41	23	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5OC([H])([H])[H])[H])[H])Cl)[H])=O)N(C6=C(C(=C(C(=C6[H])[H])N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18278858
1020	42	4600	Validation	N1=C(N=C2C(=C1[H])C(N(C3N2C4=C(N=3)C(=C(C(=C4[H])[H])[H])[H])C5=C(C(=C(C(=C5[H])[H])OC(C(C([H])([H])[H])([H])[H])([H])[H])[H])[H])=O)N(C6=C(C(=C(C(=C6[H])[H])N7C(C(N(C(C7([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18278858
1021	35	0.4	Validation	C1(C2C(=C(C(=C(C=2[H])N(C(=O)C3C(=C(C(=C(C=3[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])C([H])([H])[H])=C(C4=C(C(=C1[H])[H])N=C(N=C4[H])N([H])[H])[H]	18321037
1022	13a	14	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N([H])[H])[H])[H]	18321037
1023	13b	0.6	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H]	18321037
1024	36	7	Validation	C1(C2C(=C(C(=C(C=2[H])N(C(=O)N(C3C(=C(C(=C(C=3[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])C([H])([H])[H])=C(C4=C(C(=C1[H])[H])N=C(N=C4[H])N([H])[H])[H]	18321037
1025	23a	63	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)N(C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N([H])[H])[H])[H]	18321037
1026	23b	0.6	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)N(C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H]	18321037
1027	37	239	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])[H])[H])[H]	18321037
1028	13c	24	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C(C(C(N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18321037
1029	13e	72	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C(C(N4C(C(OC(C4([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])[H])[H])[H]	18321037
1030	13d	1310	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4(C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H]	18321037
1031	14	48	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C([H])([H])[H])[H])[H])[H])C([H])([H])[H])(=O)N(C2C(=NC(=NC=2[H])N(C3C(=C(C(=C(C=3[H])[H])N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H]	18321037
1032	15	14	Validation	O1N=C(C(=C1C([H])([H])[H])C(=O)N(C2C(=C(C(=C(C=2[H])[H])C([H])([H])[H])C(N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H])=O)[H])[H])[H]	18321037
1033	16	5	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])[H])[H])[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H]	18321037
1034	17	5	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])[H])[H])OC([H])([H])[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H]	18321037
1035	18	0.3	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])C(F)(F)F)[H])F)[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H]	18321037
1036	19	0.8	Validation	C(C1C(=C(C(=C(C=1[H])[H])[H])C(F)(F)F)C([H])([H])[H])(=O)N(C2C(=C(C(=C(C=2[H])[H])C([H])([H])[H])C(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])[H])[H])[H])[H])[H])[H])[H])[H]	18321037

No.	Compound ID	IC50 (nM)	Dataset	SMILES	Reference: DOI / PubMed Unique Identifier
1037	20	1.3	Validation	O1C(OC2C1=C(C(=C(C=2[H])C(=O)N(C3C(=C(C(=C(C=3[H])[H])C([H])([H])[H])C(=O)N(C4C(=NC(=NC=4[H])N(C5C(=C(C(=C(C=5[H])[H])N6C(C(N(C(C6([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])(F)F	18321037
1038	21	1.5	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H]	18321037
1039	22	1.4	Validation	C(C1C(=C(C(=C(C=1[H])N(C(=O)C2C(=C(C(=C(C=2[H])OC([H])([H])[H])[H])OC([H])([H])[H])[H])[H])[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H]	18321037
1040	32	1.8	Validation	C(C1C(=C(C(=C(C=1[H])[H])[H])N(C(=O)C2C(=C(C3=C(C=2[H])OC(O3)(F)F)[H])[H])[H])Cl)(=O)N(C4C(=NC(=NC=4[H])N(C5C(=C(C(=C(C=5[H])[H])N6C(C(N(C(C6([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H]	18321037
1041	33	6	Validation	C(C1C(=C(C(=C(C=1[H])[H])[H])N(C(=O)C2C(=C(C3=C(C=2[H])OC(O3)(F)F)[H])[H])[H])C(C([H])([H])[H])([H])[H])(=O)N(C4C(=NC(=NC=4[H])N(C5C(=C(C(=C(C=5[H])[H])N6C(C(N(C(C6([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H]	18321037
1042	29	6	Validation	C(C1C(=C(C(=C(C=1C([H])([H])[H])[H])[H])[H])N(C(=O)C2C(=C(C(=C(C=2[H])[H])[H])C(F)(F)F)[H])[H])C([H])([H])[H])(=O)N(C3C(=NC(=NC=3[H])N(C4C(=C(C(=C(C=4[H])[H])N5C(C(N(C(C5([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H]	18321037
1043	27	10	Validation	C(C1C(=C(C(=C(C=1Cl)[H])[H])[H])Cl)(=O)N(C2C(=NC(=NC=2[H])N(C3C(=C(C(=C(C=3[H])[H])N4C(C(N(C(C4([H])[H])([H])[H])C([H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H])([H])[H]	18321037