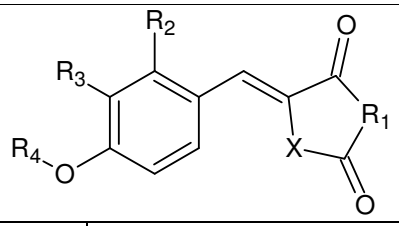
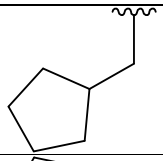
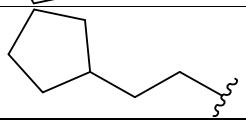
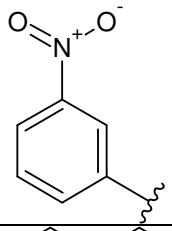
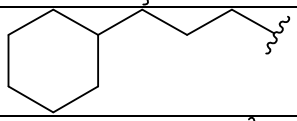
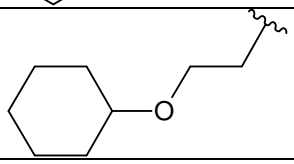
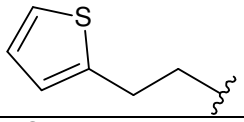
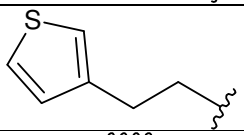
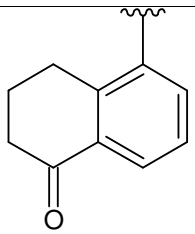
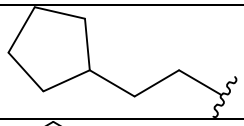
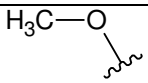
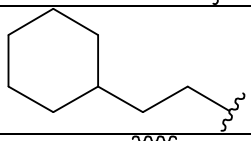
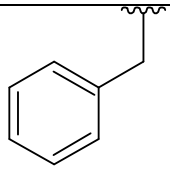
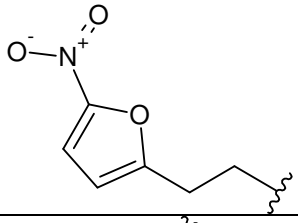
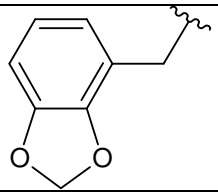
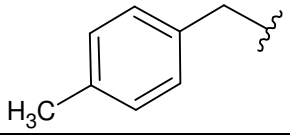
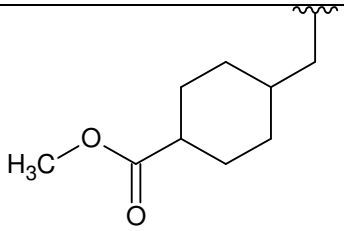
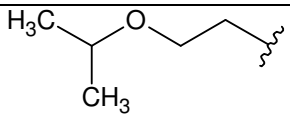
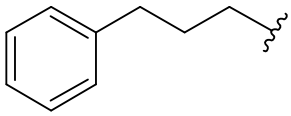
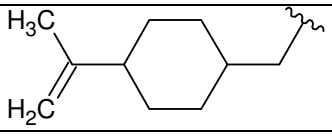
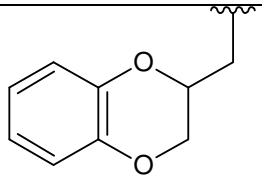
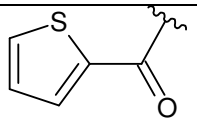
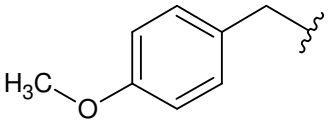
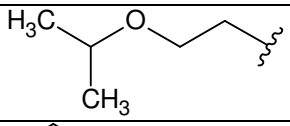
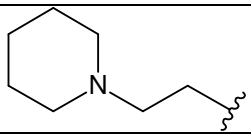
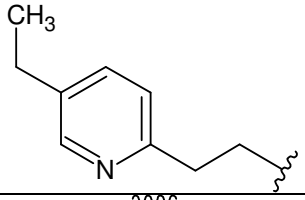
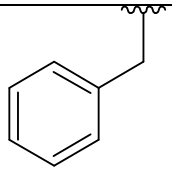
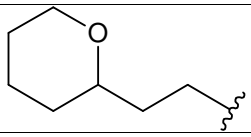
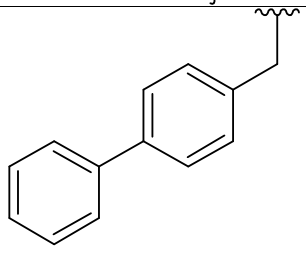
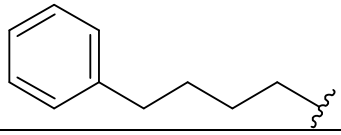
Supplementary Material

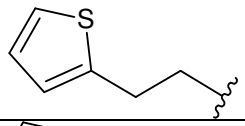
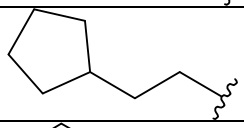
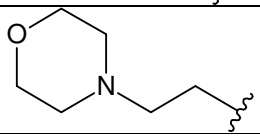
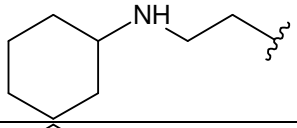
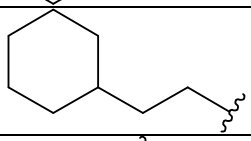
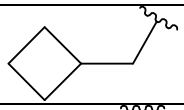
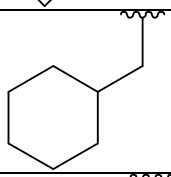
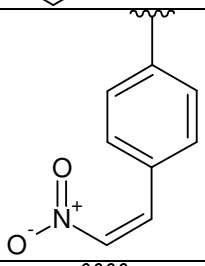
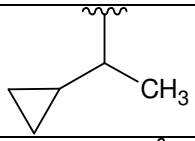
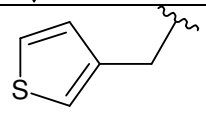
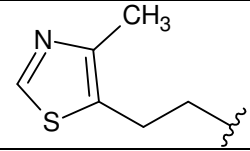
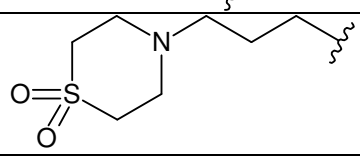
Table A: The 2D chemical structures of training compounds with their IC_{50}.

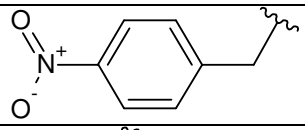
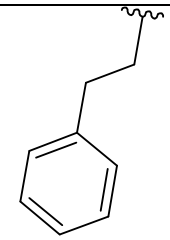
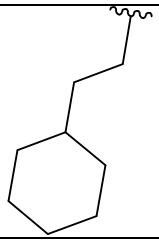
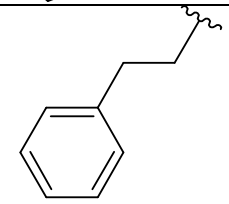
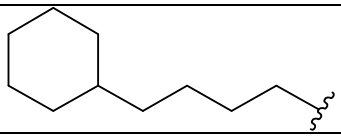
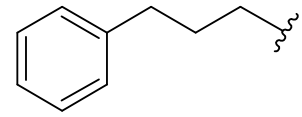
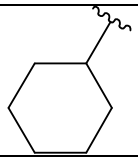
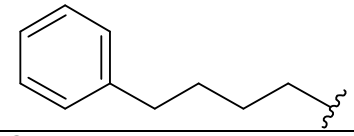
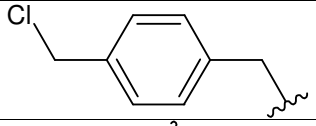
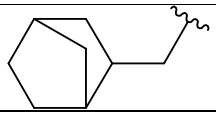


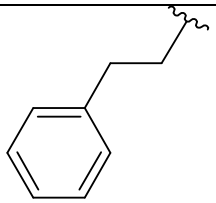
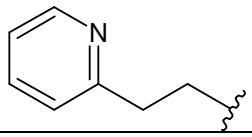
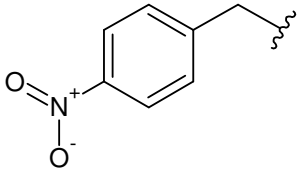
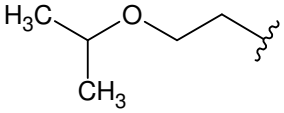
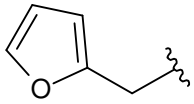
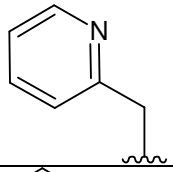
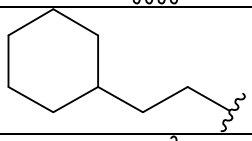
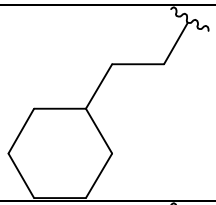
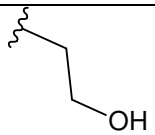
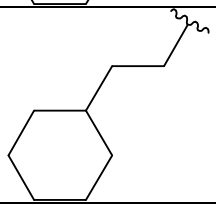
#	R_1	R_2	R_3	R_4	X	Activity (nM)	Reference
1	H	H	Cl		S	11	[16]
3	H	Cl	H		S	42	[16]
4	H	H	Cl		S	100	[16]
8	H	H	Cl		S	10	[13]
9	H	H	Cl		S	20	[16]
10	H	H	H		S	31	[12]
12	H	H	H		S	60	[12]
13	H	H	Cl		S	71	[16]

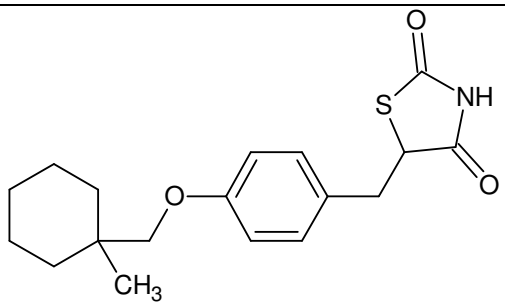
14	H	H	Cl		S	99	[16]
16	H	H			S	25	[13]
18	H	H	Cl		S	48	[16]
20	H	H	Cl		S	123	[16]
21	H	H	Cl		S	193	[16]
22	H	H	H		S	232	[12]
23	H	H	H		S	620	[12]
25	H	H	H		S	1248	[12]
26	H	Cl	H		S	52	[16]
27	H	H	Cl		S	75	[16]

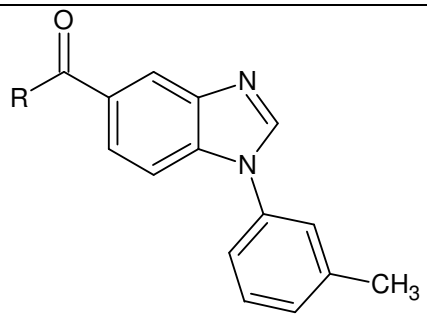
28	H	H	H		S	172	[12]
29	H	H	Cl		S	264	[16]
31	H	H	H		S	529	[12]
32	H	Cl	H		S	1050	[16]
33	H	H	H		S	1442	[12]
35	H	H	Cl		S	2077	[16]
40	H	Cl	H		S	487	[16]
42	H	H	H		S	750	[12]
43	H	H	H		S	814	[12]
49	H	Cl	H		S	81	[16]

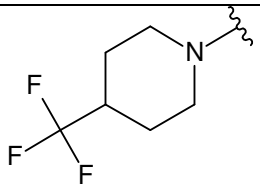
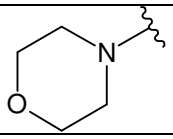
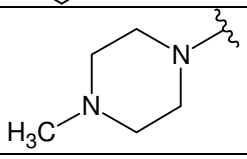
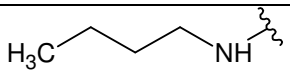
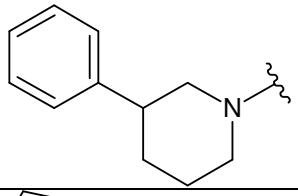
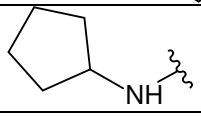
50	H	H	Cl		S	84	[16]
52	H	H	H		S	116	[12]
56	H	H	H		S	713	[12]
59	H	H	H		S	3719	[12]
60	H	H	ClI		S	8	[13]
61	H	H	Cl		S	9	[16]
62	H	H	Cl		S	28	[13]
63	H	H	Cl		S	59	[16]
65	H	H	Cl		S	132	[16]
66	H	H	H		S	429	[12]
67	H	H	H		S	636	[12]
68	H	H	H		S	1960	[12]

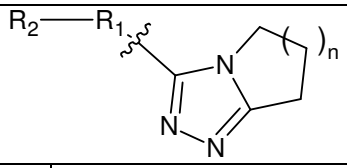
69	H	Cl	H		S	4540	[16]
70	H	H	Br		S	4	[14]
71	H	H	Br		S	19	[13]
72	H	H	Cl		S	20	[16]
73	H	H	Cl		S	24	[13]
74	H	H	Cl		S	38	[16]
75	H	H	Cl		S	47	[13]
76	H	H	Cl		S	48	[16]
78	H	H	H		S	124	[12]
79	H	H	Cl		S	165	[16]

80	H	Cl	H		S	178	[16]
82	H	H	H		S	660	[12]
83	H	H	Cl		S	930	[16]
85	H	H	Cl		S	2738	[16]
5	H	H	H		S	893	[12]
6	H	H	H		S	2585	[12]
15	H	H	H		CH_2	3789	[12]
24	H	H	H		NH	865	[12]
54		H	H		S	526	[12]

#	2D Structure	Activity (nM)	Reference
44		2700	[15]



#	R	Activity (nM)	Reference
34		1524	[15]
36		3040	[15]
45		2710	[15]
58		1358	[15]
81		429	[15]
84		961	[15]



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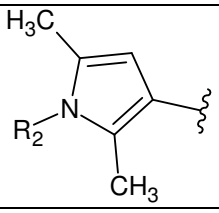
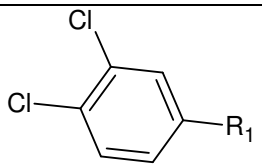
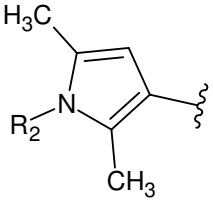
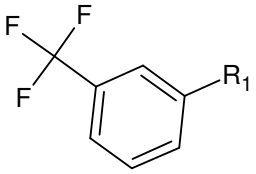
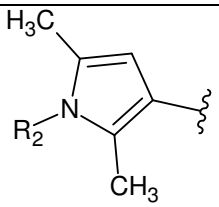
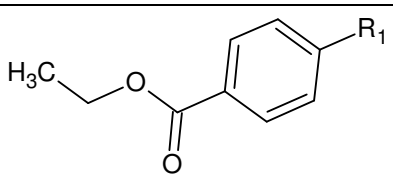
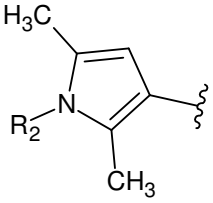
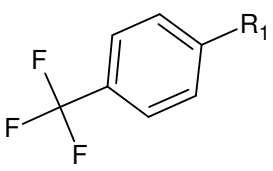
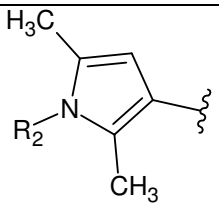
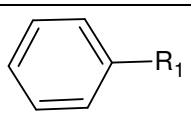
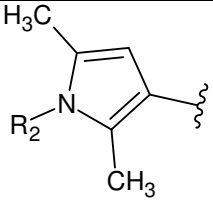
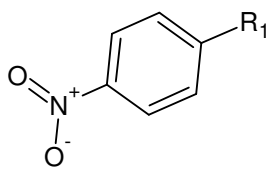
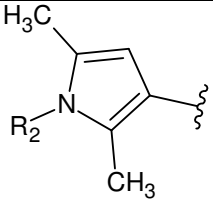
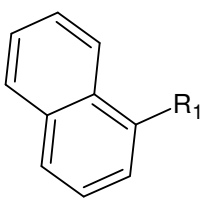
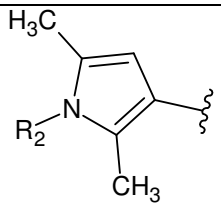
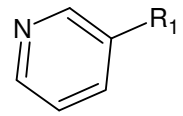
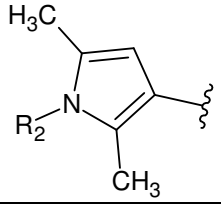
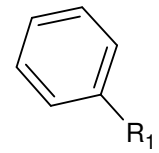
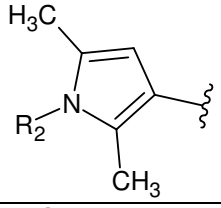
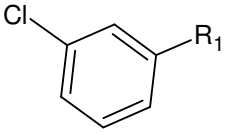
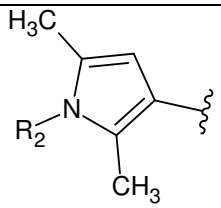
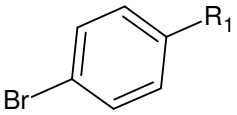
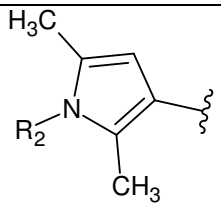
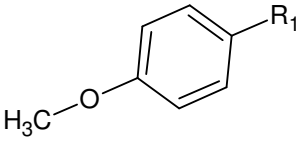
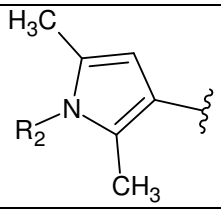
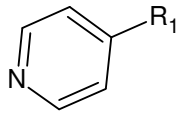
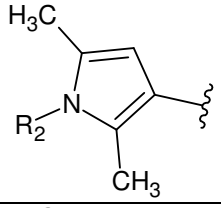
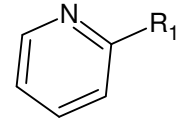
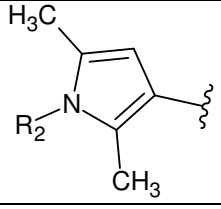
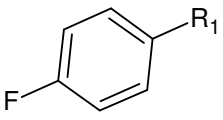
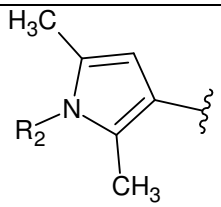
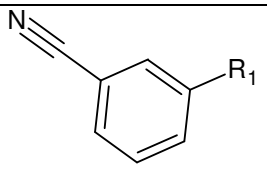
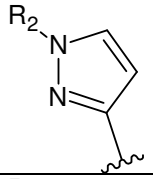
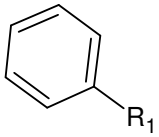
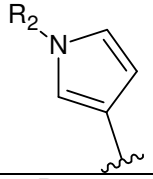
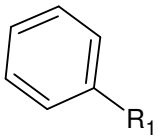
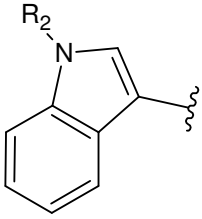
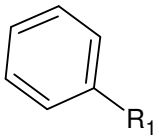
2	3			22	[15]
11	3			48	[15]
17	3			38	[15]
19	3			68	[15]
30	5			383	[15]
37	3			108	[15]
38	3			108	[15]

39	3			271	[15]
46	3			3040	[15]
47	3			34	[15]
48	3			48	[15]
51	3			86	[15]
53	3			383	[15]
57	3			1078	[15]
64	3			121	[15]

77	3			76	[15]
7	3			3827	[15]
41	3			607	[15]
55	3			681	[15]