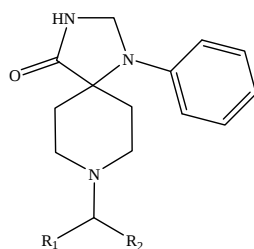
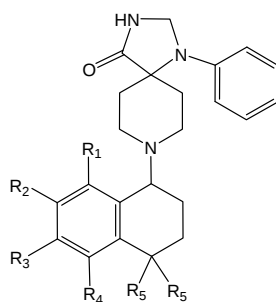


Table S1. Structures of compounds with skeleton type A in the data set.

Skeleton type A

Compound d	R ₁	R ₂	K _i (nM)
1	Ph	H	11.0
2	Cyclohexyl	H	61.2
3	2-Pyridyl	H	119.0
4	3-Pyridyl	H	133.0
5	4-Pyridyl	H	824.0
6	3-Thienyl	H	14.0
7	2-Cl-Ph	H	3.2
8	2,6-Cl ₂ -Ph	H	2.3
9	Ph	Me	3.5
10	Ph	Et	17.0
11	Ph	Propyl	2.4
12	Ph	Butyl	1.1
13	Ph	Isoamyl	1.5
14	Ph	Cyclopentyl	4.6
15	Ph	Ph	23.0
16			225.0
17			36.5
18	2-F-Ph	Ph	10.8
19	2-Cl-Ph	Ph	9.0
20	2-Me-Ph	Ph	11.5
21	4-Cl-Ph	Ph	140.0
22 [#]	2-Me-Ph	2-Me-Ph	9.0
23	2-Cl-Ph	2-Cl-Ph	6.8
24	3-Cl-Ph	3-Cl-Ph	249.0
25	2-F-Ph	2-F-Ph	6.3
26 [#]	3-F-Ph	3-F-Ph	250.0
27	4-F-Ph	4-F-Ph	49.0

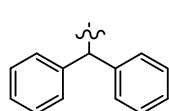
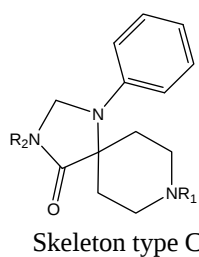
[#] Molecules belonging to the test set.

Table S2. Structures of compounds with skeleton type B in the data set.

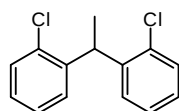
Skeleton type B

Compound	R ₁	R ₂	R ₃	R ₄	R ₅	n	K _i (nM)
28 [#]	H	H	H	H	H	0	1.2
29	H	H	H	H	H	1	1.4
30	H	H	H	H	H	2	14.5
31	H	H	H	H	CH ₃	1	1.3
32	F	H	H	H	H	1	0.3
33	H	F	H	H	H	1	0.9
34	H	H	H	F	H	1	0.8
35 [#]	Cl	H	H	H	H	1	2.6
36 [#]	H	Cl	H	H	H	1	10.8
37 [#]	H	H	H	Cl	H	1	2.0
38	H	H	Cl	H	CH ₃	1	1.4
39 [#]	H	H	F	H	CH ₃	1	8.4
40	H	Cl	Cl	H	CH ₃	1	15.1

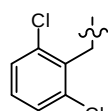
[#] Molecules belonging to the test set.

Table S3. Structures of compounds with skeleton type C in the data set.

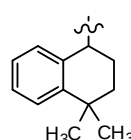
A



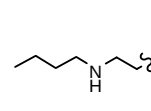
B



C



D



E

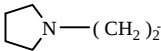
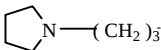
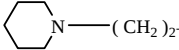
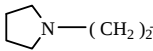
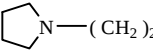
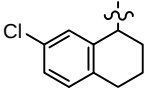
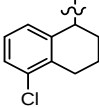
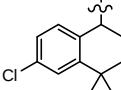
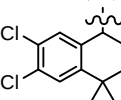
Compound	R ₁	R ₂	K _i (nM)
41	A	Me	31
42	A	Et	84
43	A	Pr	34
44 [#]	A	Bu	57
45	A	<i>i</i> -Pr	66
46	A	<i>c</i> -PrCH ₂ -	83
47	A	<i>c</i> -BuCH ₂ -	53
48 [#]	A	<i>c</i> -HexylCH ₂ -	89
49	A	Propargyl	234
50 [#]	A	Allyl	203
51	B	Bu-	48.7
52	B	<i>i</i> -Amyl	56
53	B	CH ₃ OC(O)CH ₂ -	19.5
54 [#]	B	HO(CH ₂) ₂ -	18.5
55	B	MeO(CH ₂) ₂ -	26
56 [#]	B	NH ₂ (CH ₂) ₂ -	47.8
57 [#]	B	CH ₃ NH(CH ₂) ₂ -	4.05
58	B	EtNH(CH ₂) ₂ -	2.1
59	B	<i>i</i> -PrNH(CH ₂) ₂ -	2.55
60	B	<i>c</i> -PentylNH(CH ₂) ₂ -	8.65
61	B	<i>c</i> -HexylNH(CH ₂) ₂ -	5
62 [#]	B	(CH ₃) ₂ N(CH ₂) ₂ -	3.5
63	B	<i>c</i> -PrNH(CH ₂) ₂ -	3.7
64	B	(<i>i</i> -Pr) ₂ N(CH ₂) ₂ -	12.1
65 [#]	B	BuNH(CH ₂) ₂ -	2.15
66 [#]	B	<i>i</i> -BuNH(CH ₂) ₂ -	2.75
67	B	<i>c</i> -HexylCH ₂ NH(CH ₂) ₂ -	3.8
68	B		2.25
69	B		3.2
70	B		8
71	C	CH ₃ NH(CH ₂) ₂ -	0.8
72 [#]	C	EtNH(CH ₂) ₂ -	0.7
73	C	<i>i</i> -PrNH(CH ₂) ₂ -	0.7
74	C	<i>c</i> -PrCH ₂ NH(CH ₂) ₂ -	0.5
75 [#]	C	<i>c</i> -BuNH(CH ₂) ₂ -	0.5
76	C	PrNH(CH ₂) ₂ -	0.6
77	C	<i>i</i> -BuNH(CH ₂) ₂ -	0.5
78 [#]	C	BuNH(CH ₂) ₂ -	0.4

Table S3. Cont.

Compound	R ₁	R ₂	K _i (nM)
79	C	Et ₂ N(CH ₂) ₂ -	1.0
80	C	 N—(CH ₂) ₂	2.3
81 #	D	Pr-	5.4
82	D	CH ₃ C(O)CH ₂ -	4.5
83	D	HO(CH ₂) ₂ -	1.7
84	D	CH ₃ NH(CH ₂) ₂ -	2.1
85	D	EtNH(CH ₂) ₂ -	1.6
86 #	D	<i>i</i> -PrNH(CH ₂) ₂ -	1.4
87	D	<i>c</i> -PentylNH(CH ₂) ₂ -	0.9
88	D	<i>c</i> -HexylNH(CH ₂) ₂ -	0.9
89	D	PrNH(CH ₂) ₂ -	1.0
90 #	D	CH ₂ =CHCH ₂ NH(CH ₂) ₂ -	0.9
91	D	<i>c</i> -BuNH(CH ₂) ₂ -	1.5
92 #	D	<i>c</i> -PrCH ₂ NH(CH ₂) ₂ -	0.8
93	D	<i>i</i> -BuNH(CH ₂) ₂ -	0.5
94	D	(<i>i</i> -Pr) ₂ NH(CH ₂) ₂ -	6.7
95	D	 N—(CH ₂) ₂	1.4
96	D	BuNH(CH ₂) ₂ -	0.5
97	D	<i>i</i> -AmylNH(CH ₂) ₂ -	0.4
98	D	<i>c</i> -HexylCH ₂ NH(CH ₂) ₂ -	0.7
99	D	BnNH(CH ₂) ₂ -	3.6
100		E	15.9
101		E	1.8
102		E	0.6
103		E	12.2

Molecules belonging to the test set.