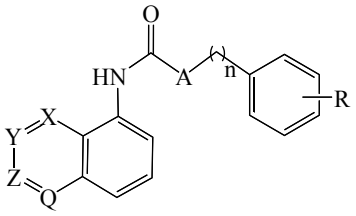
Table S1 Structures of compounds with skeleton 1 in the data set

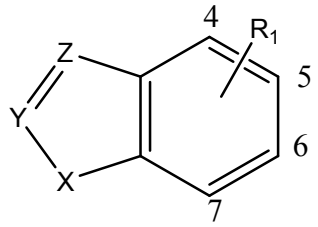


Skeleton 1

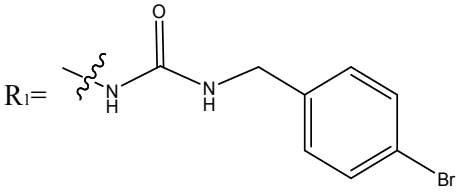
Compound	X	Y	Z	Q	A	n	R	IC_{50}(nM)
1	CH	CH	CH	N	NH	0	$3-SCF_3$	1500
2	N	CH	CH	CH	NH	0	$3-SCF_3$	420
3	CH	CH	N	CH	NH	0	$3-SCF_3$	44
4	CH	N	CH	CH	NH	0	$3-SCF_3$	1100
5	CH	CH	N	CH	NH	1	$4-CF_3$	4
6	CH	CH	N	CH	NH	1	$2-CF_3$	87
7	CH	CH	N	CH	NH	2	$3-CF_3$	51
8	CH	CH	N	CH	NH	2	$4-CF_3$	19
9	CH	CH	N	CH	NH	1	$3-CF_3$	20
10	N	CH	N	CH	NH	1	$4-CF_3$	42
11	N	CH	N	CH	NH	1	$4-Br$	170
12	CH	N	N	CH	NH	0	$4-CF_3$	175
13	N	CH	CH	N	NH	1	$3-SCF_3$	1700
14[b]	CH	CH	N	N	NH	1	3,4-di-Cl	189
15	CH	CH	N	CH	O	1	$4-CF_3$	37
16	CH	CH	N	CH	O	1	4-Me	313
17	CH	CH	N	CH	O	1	4-Cl	110
18	CH	CH	N	CH	O	1	4-Br	318
19	CH	CH	N	CH	O	1	4-t-Bu	223

[b] Compound contains methyl group at 3-position.

Table S2 Structures of compounds with skeleton 2 in the data set

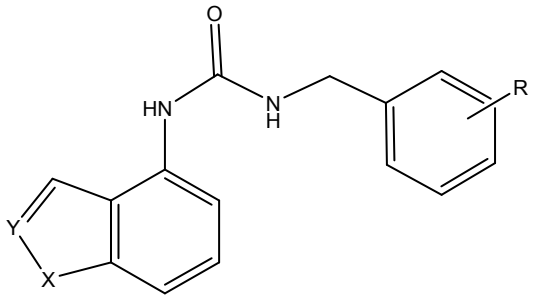


Skeleton 2



Compound	R_1	X	Y	Z	IC_{50}(nM)
20	4	NH	CH	CH	110
21	5	NH	CH	CH	5850
22	6	NH	CH	CH	3010
23	7	NH	CH	CH	180
24	4	NH	N	CH	13
25	5	NH	N	CH	3540
26	4	NH	C-CH_3	C-CH_3	1470
27	4	N-CH_3	N	CH	76
28	4	NH	CH	N	2470

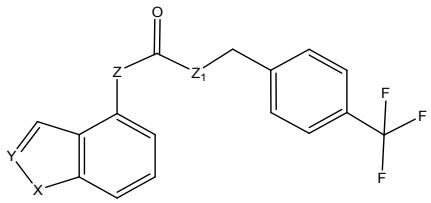
Table S3 Structures of compounds with skeleton 3 in the data set



Skeleton 3

Compound	X	Y	R	IC_{50}(nM)
29	NH	CH	3,4-DiCl	220
30	NH	CH	4-CF_3	60
31	NH	CH	4-OCF_3	80
32	NH	CH	3-F, 4-CF_3	40
33	NH	CH	4-Cl, 3-CF_3	70
34	NH	CH	4-Cl	150
35	NH	CH	3-F	2700
36	NH	CH	4-F	2710
37	NH	N	3,4-DiCl	21
38	NH	N	4-CF_3	9
39	NH	N	4-OCF_3	11
40	NH	N	3-CF_3	44
41	N-CH_3	N	4-OCF_3	35
42	N-CH_3	N	4-Cl	60
43	N-CH_3	N	4-F	720
44	N-CH_3	N	3,4-DiCl	120

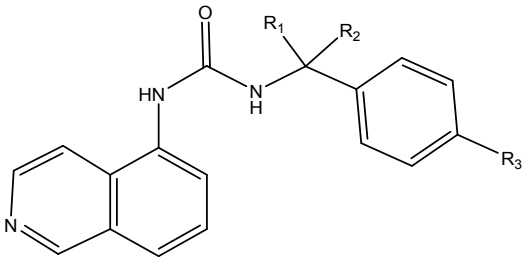
Table S4 Structures of compounds with skeleton 4 in the data set



Skeleton 4

Compound	X	Y	Z	Z_1	IC_{50}(nM)
45	NH	N	CH_2	NH	10200
46	NH	CH	CH_2	NH	520
47	NH	CH	NH	O	940

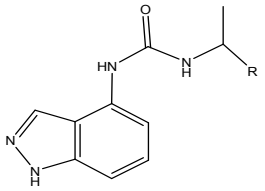
Table S5 Structures of compounds with skeleton 5 in the data set



Skeleton 5

Compound	R_1	R_2	R_3	IC_{50}(nM)
48	Me	H	4-CF_3	22
49	Me	H	4-Br	26
50	Me	H	4-t-Bu	24
51	Me	H	3-F, 4-CF_3	19
52	Ph	H	4-CF_3	147
53	Ph	H	4-t-Bu	125
54	Ph	H	4-Piperidino	171
55	Ph	H	H	600
56	Me	H	2-Me, 4-t-Bu	46
57	Me	H	2-Et, 4-t-Bu	20
58	Me	H	2,4-di-t-Bu	17
59	Et	H	3-F, 4-CF_3	109
60	Et	H	H	2580
61	Me_2NCH_2	H	H	31000
62	$NCCH_2$	H	H	15900
63	Cyclopropyl	H	4-CF_3	149
64	Cyclopentyl	H	4-CF_3	476
65	Cyclohexyl	H	4-CF_3	287
66	Me	Me	4-Cl	143
67	Me	Me	4-CF_3	94

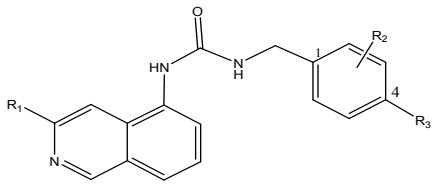
Table S6 Structures of compounds with skeleton 6 in the data set



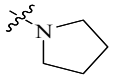
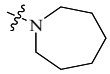
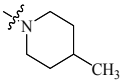
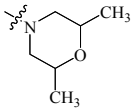
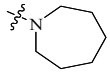
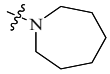
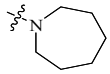
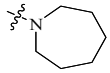
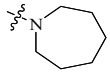
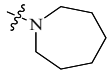
Skeleton 6

Compound	R_2	IC_{50}(nM)
68	(S)4-CF_3-pheyl	248
69	(R)4-CF_3-pheyl	41
70	(S)4-Me-pheyl	749
71	(R)4-Me-pheyl	73
72	naphthyl	3750
73	naphthyl	123

Table S7 Structures of compounds with skeleton 7 in the data set



Skeleton 7

Compound	R_1	R_2	R_3	IC_{50}(nM)
74	H	H	NMe_2	157
75	H	H		5.3
76	H	H		7.3
77	H	H		3.3
78	H	H		4.7
79	H	H		9.3
80	H	H		91
81	H	H		258
82	H	H		23.8
83	H	H		3.3
84	CH_3	H		3.8
85	NH_2	H		9.8
86	Cl	H		156
87	H	2-Cl		5.2
88	H	2-CF_3		5.7
89	H	3-CF_3		4.6
90	H	3-F		2.8
91	H	3,5-diF		9.3

To be continued

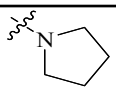
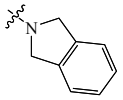
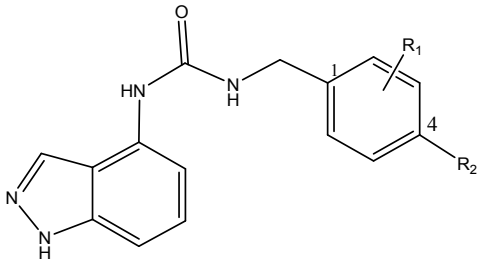
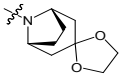
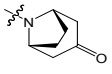
92	CH_3	3-F		15.5
93	CH_3	3-F		7360
94	NH_2	3-CF_3		14.0

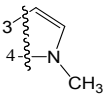
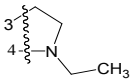
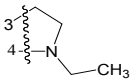
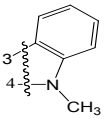
Table S8 Structures of compounds with skeleton 8 in the data set



Skeleton 8

Compound	R^3	R^4	IC_{50}(nM)
95	2-Cl		190
96	2-CF_3		133
97	2-CF_3		29.5
98	3-F		14.2
99	3,5-diF		39.3
100	H		18.0
101	2-Cl		58.8
102	2-CF_3		54.5
103	3-CF_3		26.9
104	2-Cl		20.4
105	2-Br		43.2
106	3-F		14.8
107	3,5-diF		12.6
108	2,3-diF		25.5
109	2,5-diF		21.3
110	2,5-diF		82.0
111	2,5-diF		157

To be continued

112[b]			1850
113			285
114[b]			305
115			902
116	3-CH_3		19.8
117	2-CH_3		29.0
118			35.3
119			10.3

[b] Compound contains a methyl group at the N-1 indazole.

Table S9 Structures of compounds with skeleton 9 in the data set

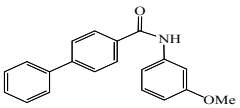
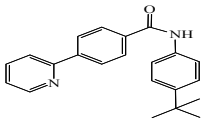
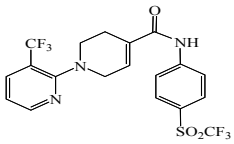
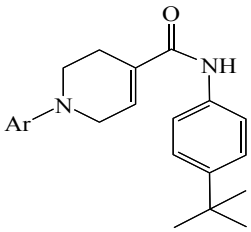
Compound	Structure	IC_{50}(nM)
120		147
121		42
122		24

Table S10 Structures of compounds with skeleton 10 in the data set



Skeleton 10

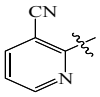
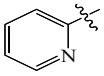
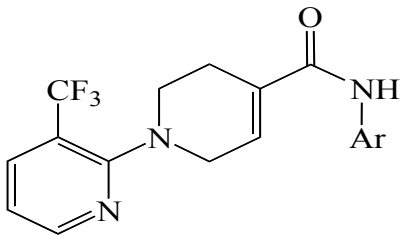
Compound	Ar	IC_{50}(nM)	Compound	Ar	IC_{50}(nM)
123		6	127		19
124		10	128		14
125		78	129		10
126		27	130		265

Table S11 Structures of compounds with skeleton 11 in the data set



Skeleton 11

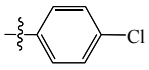
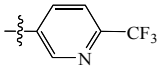
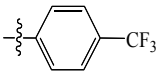
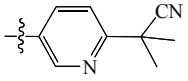
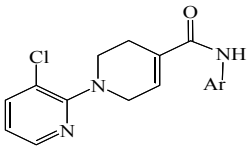
Compound	Ar	IC_{50}(nM)	Compound	Ar	IC_{50}(nM)
131		19	133		42
132		8	134		41

Table S12 Structures of compounds with skeleton 12 in the data set



Skeleton 12

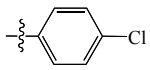
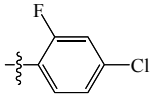
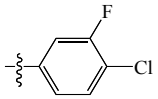
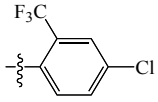
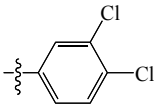
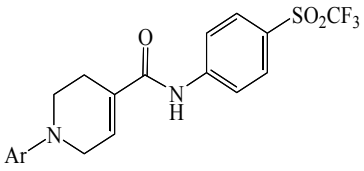
Compound	Ar	IC_{50}(nM)	Compound	Ar	IC_{50}(nM)
135		33	138		618
136		78	139		2746
137		124			

Table S13 Structures of compounds with skeleton 13 in the data set



Skeleton 13

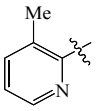
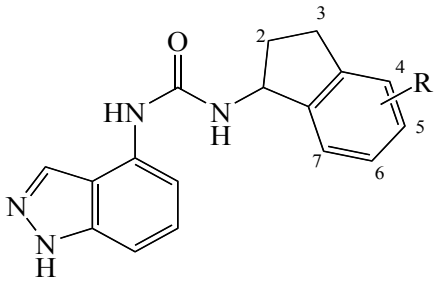
Compound	Ar	IC_{50}(nM)	Compound	Ar	IC_{50}(nM)
140		41	143		95
141		67	144		44
142		35			

Table S14 Structures of compounds with skeleton 14 in the data set



Skeleton 14

Compound	R	IC_{50}(nM)
145	5-CF_3	3
146	5- *tert*-Bu	6
147	5-Br	9
148	5-Cl	10
149	5-F	52
150	5-piperidino	14
151	4-piperidino	10
152	4-(4-CF_3-piperidino)	7
153	4-cyclopropyl	5
154	5-cyclopropyl	4
155	4-CF_3	10
156	4-*tert*-Bu	4
157	5-OMe	40
158	4-pyrrolidino	21
159	4-C(CN)Me_2	19
160	4-morpholino	65
161	5-F, 4-morpholino	5
162	4-Me	46
163	5-Me	11
164	6-Me	7200
165	7-Me	595
166	H	151

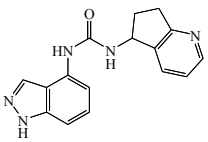
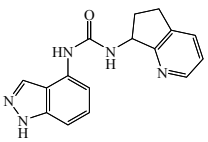
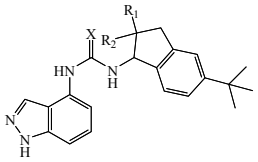
Compound	R	IC_{50}(nM)
167		5820
168		1350

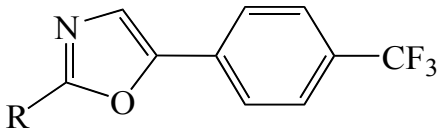
Table S15 Structures of compounds with skeleton 15 in the data set



Skeleton 15

Compound	R_1	R_2	X	IC_{50}(nM)
169	H	H	S	97
170	F	H	O	35
171	F	F	O	216

Table S16 Structures of compounds with skeleton 16 in the data set



Skeleton 16

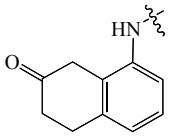
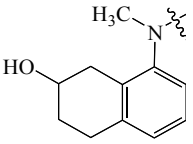
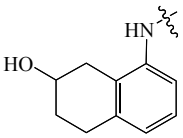
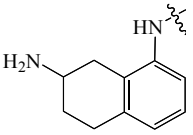
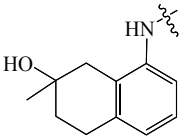
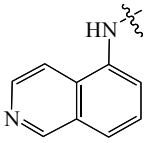
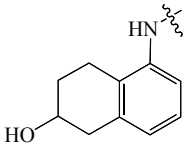
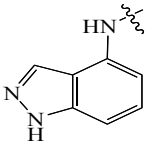
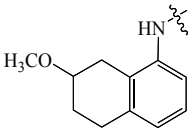
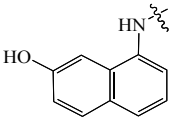
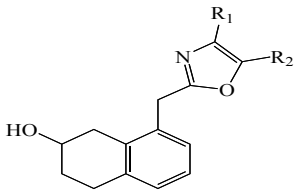
Compound	R	IC_{50}(nM)	Compound	R	IC_{50}(nM)
172		374	177		277
173		8.3	178		327
174		840	179		229
175		120	180		101
176		150	181		10

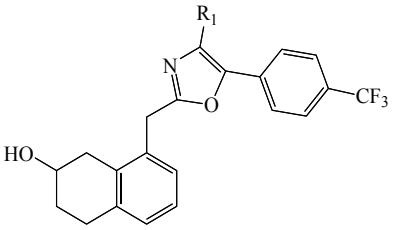
Table S17 Structures of compounds with skeleton 17 in the data set



Skeleton 17

Compound	R_4	R_5	IC_{50}(nM)
182	H	Ph	187
183	H	2-CH_3-Ph	416
184	H	3-CH_3-Ph	157
185	H	4-CH_3-Ph	62
186	H	4-t-Bu-Ph	26
187	H	4-Cl-Ph	15
188	H	4-OCH_3-Ph	81
189	H	4-Pyrrolidinyl-Ph	101
190	H	Benzyl	1820
191	Ph	H	864

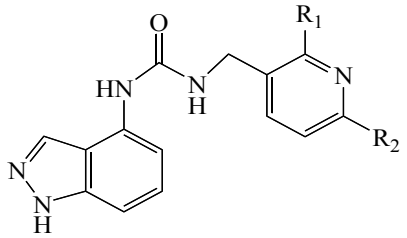
Table S18 Structures of compounds with skeleton 18 in the data set



Skeleton 18

Compound	R_4	IC_{50}(nM)	Compound	R_4	IC_{50}(nM)
192	Me	3.2	195	Br	9
193	Et	2.1	196	4-CN-Ph	2.0
194	i-Pr	114	197	4-F-Ph	1.3

Table S19 Structures of compounds with skeleton 19 in the data set



Skeleton 19

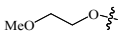
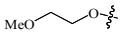
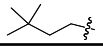
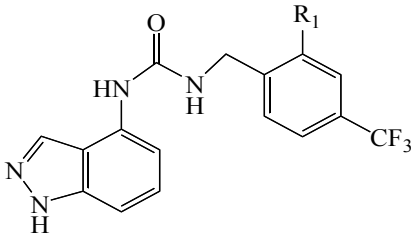
Compound	R_1	R_2	IC_{50}(nM)
198	H	CF_3	184
199		CF_3	3.5
200		Me	16
201		ph	14
202		CF_3	12
203		Me	125
204	Pho-	CF_3	9
205		CF_3	18
206		CF_3	12
207		CF_3	6
208		CF_3	5

Table S20 Structures of compounds with skeleton 20 in the data set



Skeleton 20

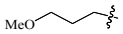
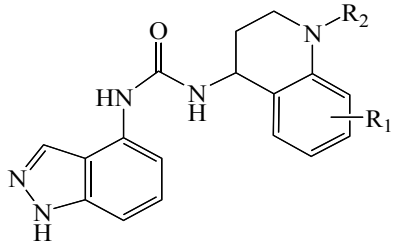
Compound	R_1	IC_{50}(nM)
209		8
210		8
211	PhO-	9
212	*i*Pr	9
213		6
214		4.3

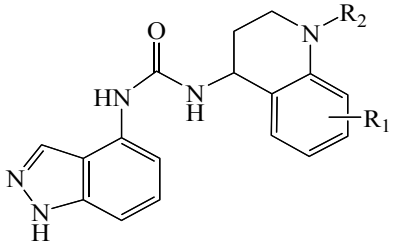
Table S21 Structures of compounds with skeleton 21 in the data set



Skeleton 21

Compound	R^1	IC_{50}(nM)
215	7-CF_3	11
216	7-OCF_3	8
217	7-tBu	43
218	8-CF_3	5
219	8-OCF_3	5
220	8-tBu	5
221	8-Cyclohexyl	15
222	8-Piperidino	16
223	8-Morpholino	110
224	6-Me	933
225	6-F	718
226	H	234

Table S22 Structures of compounds with skeleton 22 in the data set



Skeleton 22

Compound	R^1	R^2	IC_{50}(nM)
227	H	Methyl	215
228	7-F	Methyl	34
229	7-CF_3	Methyl	7
230	8-tBu	Methyl	6
231	7-tBu	Methyl	115
232	6-tBu	Methyl	853
233	6-OMe	Methyl	1380
234	H	Benzyl	70
235	6-F	Benzyl	66
236	6-tBu	Benzyl	121
45	6-OMe	Benzyl	160
46	6-OMe	Cydohexylmethyl	196
133	8-Cl	3-Methylbutyl	11