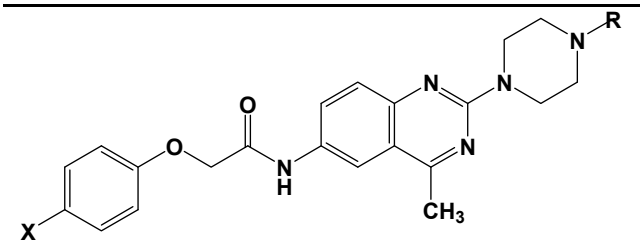
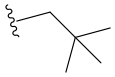
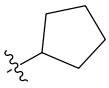
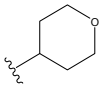
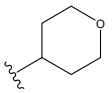
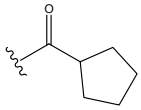
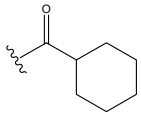
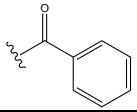
Supplementary Information

Table S1. Structures and pIC_{50} values of compounds with skeleton type A in the data set.

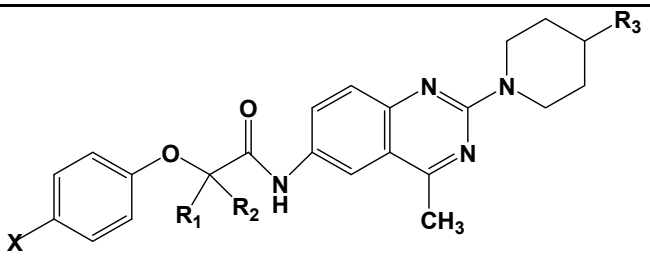


Skeleton type A

Compound	X	R	pIC_{50}(M)
1[#]	Cl	Me	6.66
2	Cl	Et	6.16
3	Cl		6.11
4	Cl	^{c}Pr	6.57
5	Cl		7.02
6	Cl		7.35
7	OCF_3		8.15
8	Cl	CO^{i}Pr	6.65
9	OCF_3	CO^{i}Pr	7.44
10	Cl	$COCH_2{}^{i}Pr$	6.85
11	Cl	$COCH_2OMe$	6.67
12	Cl	CO^{c}Pr	6.60
13[#]	OCF_3	CO^{c}Pr	7.31
14	Cl	CO^{c}Bu	6.49
15	OCF_3	CO^{c}Bu	7.08
16[#]	Cl		6.52
17[#]	Cl		6.94
18	Cl		5.14

[#] Molecules belonging to the test set. [i] means iso-. [c] means cycloalkane.

Table S2. Structures and pIC_{50} values of compounds with skeleton type B in the data set.

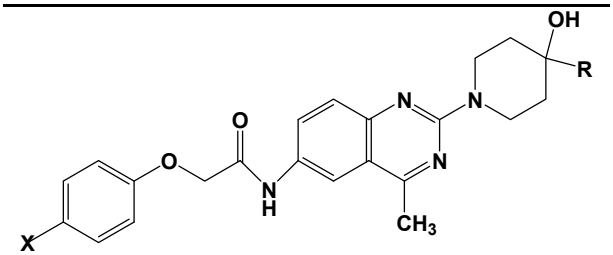


Skeleton type B

Compound	X	R_1	R_2	R_3	pIC_{50}(M)
19[#]	Cl	H	H	H	6.74
20[#]	Cl	H	H	OH	6.82
21	Cl	H	H	OMe	6.67
22	Cl	H	H	$CONH^iPr$	7.82
23[#]	OCF_3	H	H	$CONH^iPr$	7.77
24	OCF_3	H	H	$CONMe_2$	7.33
25	OCF_3	H	H	$CONH^cPr$	8.05
26[#]	OCF_3	H	H	$CONH_2$	7.64
27[#]	OCF_3	H	H	CO^cPr	8.00
28	Cl	H	H	NH_2	6.82
29	OCF_3	H	H	NH_2	7.66
30[#]	Cl	H	H	$NHCO^iPr$	7.82
31	Cl	H	H	$NHCONH^iPr$	8.15
32[#]	Cl	H	H	Pyrrolidine	7.70
33[#]	Cl	Me	H	Pyrrolidine	6.59
34	OCF_3	H	H	Pyrrolidine	7.51
35	OCF_3	H	H	Morpholine	8.22
36	OCF_3	H	H	2−Pyrrolidinone	7.72

[#] Molecules belonging to the test set.

Table S3. Structures and pIC_{50} values of compounds with skeleton type C in the data set.



Skeleton type C

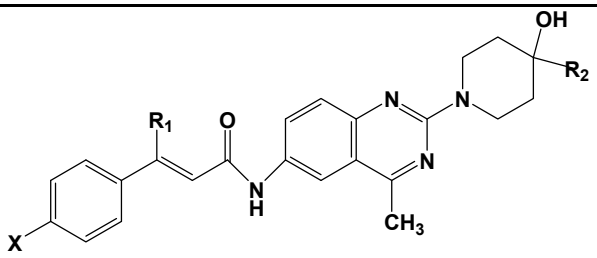
Compound	X	R	pIC_{50}(M)
37	Cl	Me	6.63
38	Cl	Et	6.68
39	OCF_3	Et	6.94
40	OCF_3	*c*−Pr	7.00
41	OCF_3	*c*−Bu	7.10

Table S3. *Cont.*

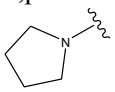
Compound	X	R	pIC_{50}(M)
42	OCF_3	*c*−Hexyl	6.49
43	OCF_3	$CONH_2$	6.20
44[#]	OCF_3	Ph	6.45
45	OCF_3	*p*−F−phenyl	6.82
46[#]	OCF_3	*m*−F−phenyl	6.20
47	OCF_3	5−F−2−pyridyl	6.67

[#] Molecules belonging to the test set.

Table S4. Structures and pIC_{50} values of compounds with skeleton type D in the data set.

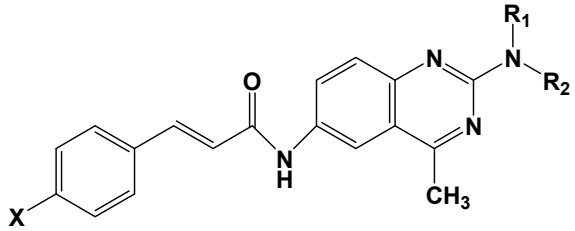


Skeleton type D

Compound	X	R_1	R_2	pIC_{50}(M)
48	OCF_3	H	H	7.21
49[#]	Cl	H	H	6.97
50[#]	Cl	Me	H	6.17
51[#]	OCF_3	H	^{c}Pr	6.68
52	OCF_3	Me	^{c}Pr	6.45
53	Cl	H	^{c}Pr	6.83
54	Cl	Me	^{c}Pr	6.27
55[#]	Me	H	^{c}Pr	6.46
56[#]	CF_3	H	^{c}Pr	6.63
57[#]	OMe	H	^{c}Pr	6.94
58	CHF_2	H	^{c}Pr	6.91
59[#]	$OCHF_2$	H	^{c}Pr	6.70
60	o,p−DiCl	H	^{c}Pr	6.21
61		H	^{c}Pr	5.74
62	Cl	H	Ph	5.96
63	Cl	H	^{c}Bu	6.69
64[#]	Cl	H	^{i}Pr	6.77
65[#]	Cl	H	^{n}Pr	6.61
66[#]	Cl	H	Et	6.57
67[#]	Cl	H	CH_2Ac	6.82
68	Cl	H	$(CH_2)_2OH$	6.66
69[#]	Cl	H	(CH2)2OMe	6.61

[#] Molecules belonging to the test set. [n] means neo-.

Table S5. Structures and pIC_{50} values of compounds with skeleton type E in the data set.

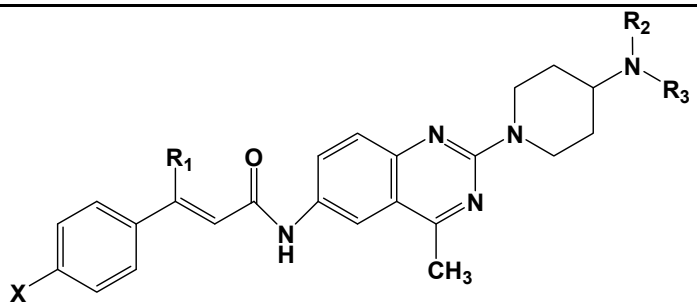


Skeleton type E

Compound	X	R_1	R_2	pIC_{50}(M)
70[#]	Cl	*c*−Pentyl	Me	6.40
71	Cl	*c*−Pentyl	$(CH_2)_2OH$	6.07
72[#]	Cl	H	$(CH_2)_2OH$	6.26
73	OCF_3	H	$(CH_2)_3OH$	7.44
74[#]	OCF_3	^{i}Pr	$(CH_2)_3OH$	6.54
75[#]	OCF_3	H	$(CH_2)_2NHMs$	6.77
76	OCF_3	H	$(CH_2)_3NHMs$	7.27
77	OCF_3	H	$(CH_2)_2NHCO^{c}Pr$	7.21
78	OCF_3	H	$(CH_2)_3NHCO^{c}Pr$	7.20
79	OCF_3	H	$(CH_2)_3CONH^{c}Pr$	7.70

[#] Molecules belonging to the test set.

Table S6. Structures and pIC_{50} values of compounds with skeleton type F in the data set.



Skeleton type F

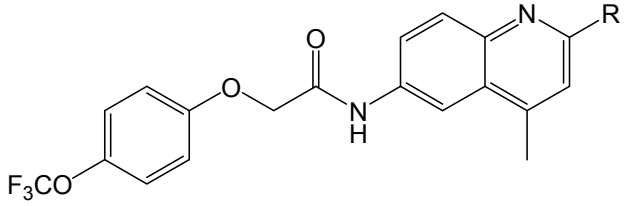
Compound	X	R_1	R_2 R_3	pIC_{50}(M)
80	Cl	H	$-(CH_2)_2O(CH_2)_2-$	7.80
81	OCF_3	H	$-(CH_2)_2O(CH_2)_2-$	8.00
82	OCF_3	H	$-COCH_2O(CH_2)_2-$	7.52
83	OCF_3	H	$-CO(CH_2)_4-$	7.29
84	OCF_3	H	$-CO(CH_2)_3-$	7.96
85	OCF_3	Me	$-CO(CH_2)_3-$	7.16
86	Cl	H	$-CO(CH_2)_3-$	7.13
87	Cl	Me	$-CO(CH_2)_3-$	7.09
88	OCF_3	H	$-SO_2(CH_2)_3-$	8.40
89[#]	OCF_3	H	$-CO(CH_2)_2CO-$	7.03
90	OCF_3	H	$-COO(CH_2)_2-$	7.39

Table S6. *Cont.*

Compound	X	R_1	R_2	R_3	pIC_{50}(M)
91[#]	OCF_3	H	$-COOCMe_2CH_2-$		7.17
92	OCF_3	H	$-CONH(CH_2)_2-$		7.18
93	OCF_3	H	$-CONMe(CH_2)_2-$		7.68
94[#]	OCF_3	H	$-SO_2NH(CH_2)_2-$		6.84
95	OCF_3	H	$-SO_2NMe(CH_2)_2-$		6.55
96	Cl	H	H	CO^cPr	6.65
97	Cl	H	H	SO_2Me	7.51
98	Cl	Me	H	SO_2Me	6.95
99	Cl	H	H	$COCH_2OH$	7.39
100[#]	Cl	H	H	$COCH_2OMe$	7.35
101	OCF_3	H	H	$COCH_2OH$	7.59
102[#]	OCF_3	H	H	$COCH_2OMe$	7.49
103	OCF_3	H	Me	$COCH_2OH$	7.35
104	OCF_3	H	Me	$COCH_2OH$	7.04
105	OCF_3	H	H	SO_2NMe_2	6.98

[#] Molecules belonging to the test set.

Table S7. Structures and pIC_{50} values of compounds with skeleton type H in the data set.



Skeleton type G

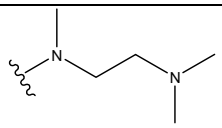
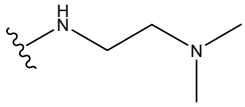
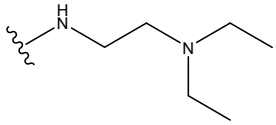
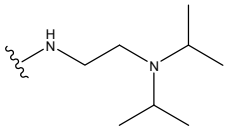
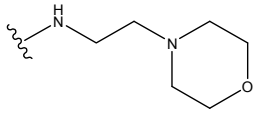
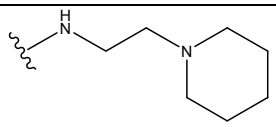
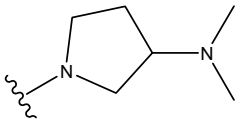
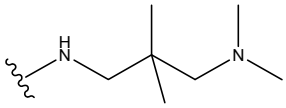
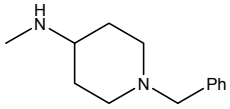
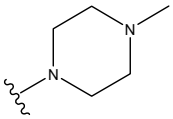
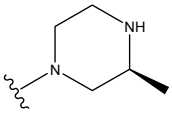
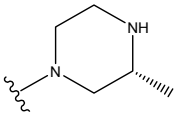
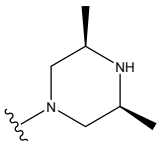
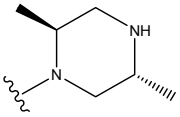
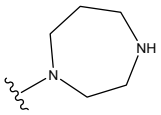
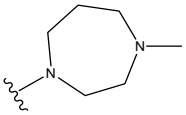
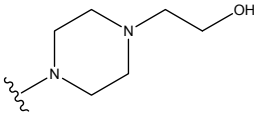
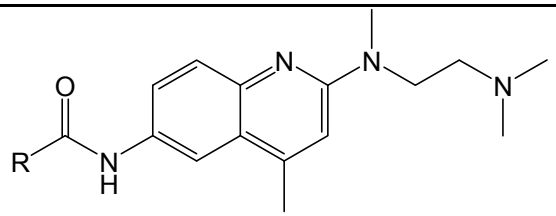
Compound	R	pIC_{50}(M)
106		7.74
107		7.74
108		7.82
109		7.66
110		8.02

Table S7. *Cont.*

Compound	R	pIC_{50}(M)
111[#]		8.28
112		8.21
113[#]		7.80
114		7.40
115		7.54
116[#]		7.89
117		7.74
118		7.06
119		7.70
120		7.92
121		7.70
122		8.30

[#] Molecules belonging to the test set.

Table S8. Structures and pIC_{50} values of compounds with skeleton type I in the data set.



Skeleton type H

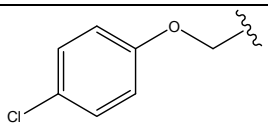
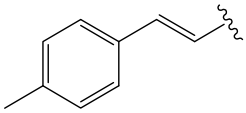
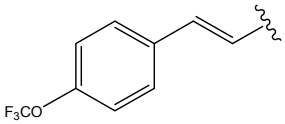
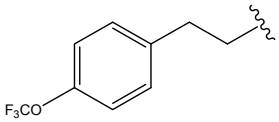
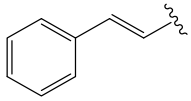
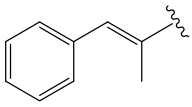
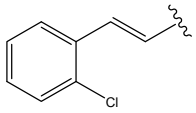
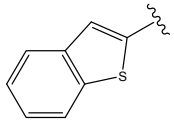
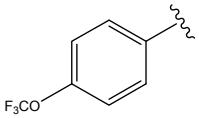
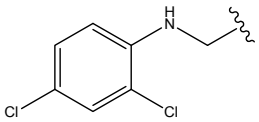
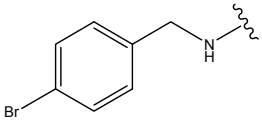
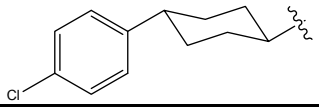
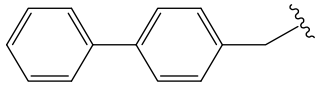
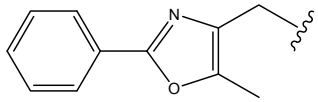
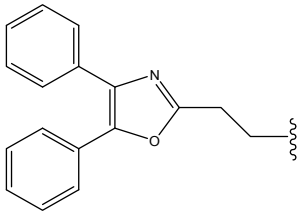
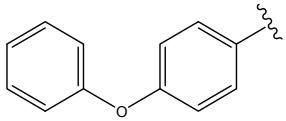
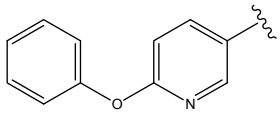
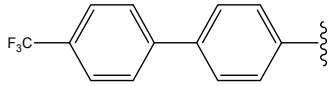
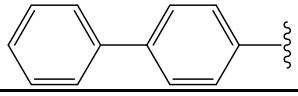
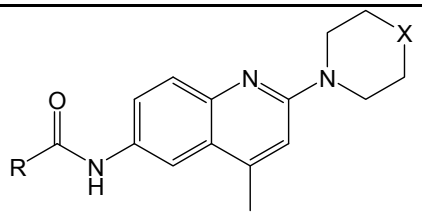
Compound	R	pIC_{50}(M)
123		7.08
124		7.32
125#		7.72
126#		7.40
127#		5.16
128		5.02
129		5.60
130		5.68
131		5.56
132#		6.90
133		6.57
134		6.37

Table S8. *Cont.*

Compound	R	pIC_{50}(M)
135		5.48
136		6.25
137		6.79
138		6.68
139		6.98
140		7.20
141		7.38

[#] Molecules belonging to the test set.

Table S9. Structures and pIC_{50} values of compounds with skeleton type J in the data set.



Skeleton type I

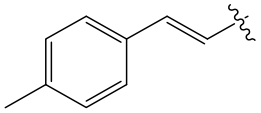
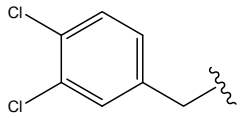
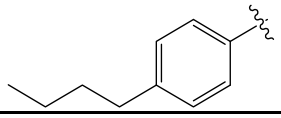
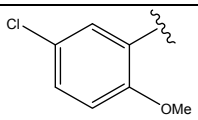
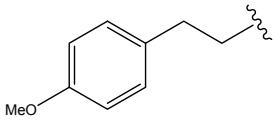
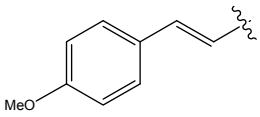
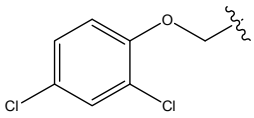
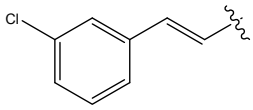
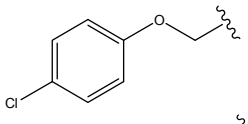
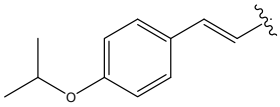
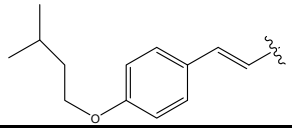
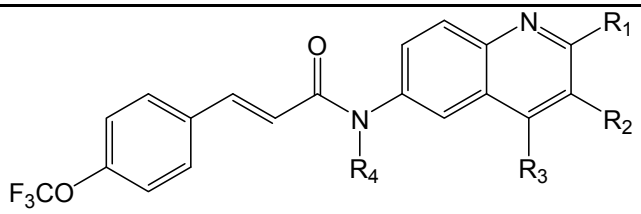
Compound	R	X	pIC_{50}(M)
142		NMe	7.35
143[#]		NEt	6.14
144		NEt	6.94

Table S9. *Cont.*

Compound	R	X	pIC50(M)
145[#]		NEt	5.58
146		NEt	6.60
147[#]		NEt	7.80
148[#]		Net	7.62
149[#]		NMe	5.74
150[#]		Net	7.66
151		NEt	7.02
152[#]		NMe	6.36

[#] Molecules belonging to the test set.

Table S10. Structures and pIC_{50} values of compounds with skeleton type K in the data set.



Skeleton type J

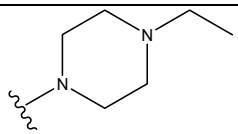
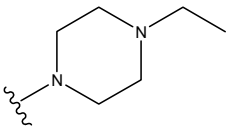
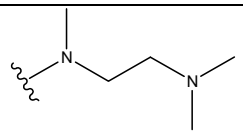
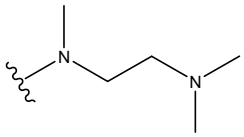
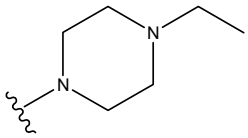
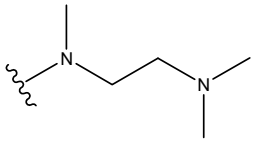
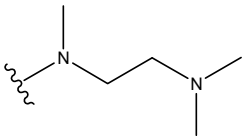
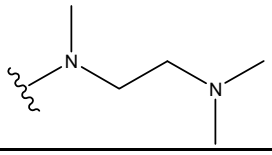
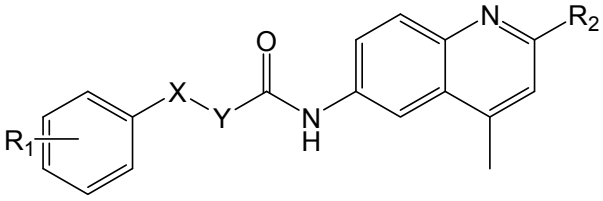
Compound	R1	R2	R3	R4	pIC_{50}(M)
153		H	Me	H	7.80
154		H	Me	H	6.46

Table S10. *Cont.*

Compound	R1	R2	R3	R4	pIC50(M)
155		H	H	H	6.76
156[#]		H	H	H	6.09
157		Me	H	H	6.32
158[#]		Me	H	H	5.98
159		H	Et	H	6.62
160[#]		H	Me	Me	5.96

[#] Molecules belonging to the test set.

Table S11. Structures and pIC_{50} values of compounds with skeleton type L in the data set.



Skeleton type K

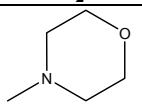
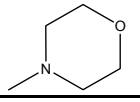
Compound	R_1	X−Y	R_2	pIC_{50}(M)
161	2,4−Cl_2	O−CH_2		7.23
162	4−CF_3O	O−CH_2		7.09

Table S11. *Cont.*

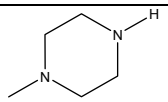
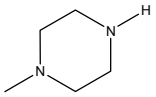
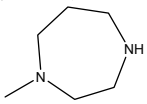
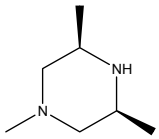
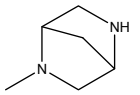
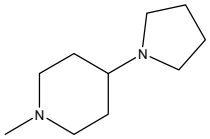
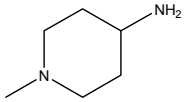
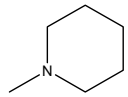
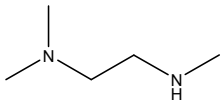
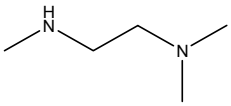
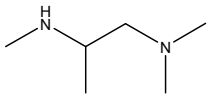
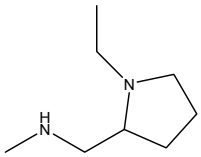
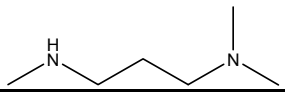
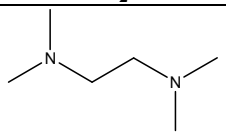
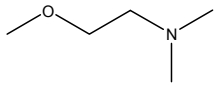
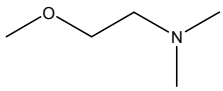
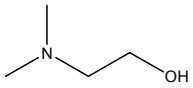
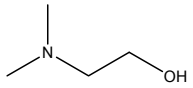
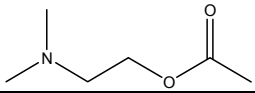
Compound	R1	X−Y	R2	pIC50(M)
163[#]	2,4−Cl_2	O−CH_2		7.80
164	4−CF_3O	CH=CH		7.19
165[#]	4−CF_3O	CH=CH		7.64
166	4−CF_3O	CH=CH		6.39
167	4−CF_3O	O−CH_2		8.01
168[#]	4−CF_3O	O−CH_2		8.15
169	4−CF_3O	O−CH_2		8.46
170[#]	4−CF_3O	O−CH_2		7.01
171[#]	2,4−Cl_2	O−CH_2		8.16
172	4−CF_3O	CH=CH		7.89
173	4−CF_3O	CH=CH		7.66
174	4−CF_3O	O−CH_2		7.68
175	4−CF_3O	O−CH_2		8.42

Table S11. *Cont*.

Compound	R_1	X−Y	R_2	pIC_{50}(M)
176[#]	2,4−Cl_2	O−CH_2		8.03
177[#]	2,4−Cl_2	O−CH_2		6.74
178	4−CF_3O	CH=CH		6.38
179	2,4−Cl_2	O−CH_2		7.37
180[#]	4−CF_3O	CH=CH		7.39
181	2,4−Cl_2	O−CH_2		7.54

[#] Molecules belonging to the test set.

Table S12. Q^2, R^2_{ncv} and R^2_{pred} of all 34 possible combinations of different descriptor fields.

No.	PLS Statistics	Q^2	R^2_{ncv}	R^2_{pred}
	CoMFA			
1	*S*	0.280	0.784	0.265
2	*E*	0.296	0.644	0.262
3	*SE*	0.372	0.896	0.544
	CoMSIA			
4	S	0.206	0.405	−0.211
5	*E*	0.321	0.628	0.225
6	*H*	0.368	0.662	0.514
7	*D*	0.234	0.499	0.074
8	*A*	0.169	0.368	−0.363
9	*SE*	0.319	0.658	−0.044
10	*SH*	0.376	0.677	0.459
11	*SD*	0.093	0.498	0.381
12	*SA*	0.254	0.772	0.501
13	*EH*	0.368	0.736	0.498
14	*ED*	0.302	0.687	0.425
15	*EA*	0.412	0.713	0.460
16	*HD*	0.397	0.757	0.639
17	*HA*	0.463	0.874	0.643

Table S12. *Cont.*

No.	PLS Statistics	Q^2	R^2_{ncv}	R^2_{pred}
18	*DA*	0.204	0.648	0.264
19	*SEH*	0.389	0.689	0.536
20	*SED*	0.288	0.655	0.448
21	*SEA*	0.386	0.831	0.488
22	*SHD*	0.398	0.771	0.662
23	*SHA*	0.453	0.868	0.665
24	*SDA*	0.413	0.837	0.609
25	*EHD*	0.405	0.801	0.616
26	*EHA*	0.434	0.886	0.635
27	*EDA*	0.446	0.834	0.514
28	*HDA*	0.477	0.889	0.576
29	*SEHD*	0.404	0.805	0.658
30	*SEHA*	0.428	0.875	0.666
31	*SEDA*	0.454	0.861	0.582
32	*SHDA*	0.509	0.841	0.745
33	*EHDA*	0.476	0.838	0.687
34	*SEHDA*	0.469	0.890	0.657

Table S13. Observed and predicted MCHR1 antagonist activities (pIC_{50}, M).

Compound	Observed Activities	CoMFA		CoMSIA	
		Predicted	Residue	Predicted	Residue
1	6.66	6.511	−0.149	6.583	−0.077
2	6.16	6.477	0.317	6.496	0.336
3	6.11	6.169	0.059	6.054	−0.056
4	6.57	6.464	−0.106	6.471	−0.099
5	7.02	7.096	0.076	6.66	−0.36
6	7.35	7.309	−0.041	7.15	−0.2
7	8.15	8.075	−0.075	7.959	−0.191
8	6.65	7.01	0.36	6.652	0.002
9	7.44	7.227	−0.213	6.855	−0.585
10	6.85	6.729	−0.121	6.491	−0.359
11	6.67	6.789	0.119	6.556	−0.114
12	6.6	6.648	0.048	6.615	0.015
13	7.31	7.016	−0.294	6.821	−0.489
14	6.49	6.557	0.067	6.673	0.183
15	7.08	7.336	0.256	7.398	0.318
16	6.52	6.255	−0.265	6.596	0.076
17	6.94	7.027	0.087	6.623	−0.317
18	5.14	4.603	−0.537	5.063	−0.077
19	6.74	6.956	0.216	7.016	0.276
20	6.82	7.12	0.3	6.928	0.108
21	6.67	6.902	0.232	6.951	0.281
22	7.82	7.926	0.106	7.684	−0.136
23	7.77	8.059	0.289	7.803	0.033

Table S13. *Cont.*

Compound	Observed Activities	CoMFA		CoMSIA	
		Predicted	Residue	Predicted	Residue
24	7.33	7.227	−0.103	7.182	−0.148
25	8.05	8.116	0.066	7.897	−0.153
26	7.64	7.529	−0.111	7.966	0.326
27	8	7.633	−0.367	7.153	−0.847
28	6.82	6.932	0.112	7.31	0.49
29	7.66	7.152	−0.508	7.499	−0.161
30	7.82	7.547	−0.273	7.365	−0.455
31	8.15	8.278	0.128	8.002	−0.148
32	7.7	7.024	−0.676	7.196	−0.504
33	6.59	6.079	−0.511	6.565	−0.025
34	7.51	7.054	−0.456	7.323	−0.187
35	8.22	8.123	−0.097	7.948	−0.272
36	7.72	7.799	0.079	7.848	0.128
37	6.63	6.784	0.154	6.916	0.286
38	6.68	6.615	−0.065	6.823	0.143
39	6.94	6.755	−0.185	7.024	0.084
40	7	6.9	−0.1	7.003	0.003
41	7.1	6.96	−0.14	6.813	−0.287
42	6.49	6.873	0.383	6.631	0.141
43	6.2	6.36	0.16	6.031	−0.169
44	6.45	6.994	0.544	6.898	0.448
45	6.82	6.916	0.096	7.116	0.296
46	6.2	6.523	0.323	6.086	−0.114
47	6.67	6.651	−0.019	6.82	0.15
48	7.21	7.131	−0.079	7.099	−0.111
49	6.97	6.643	−0.327	6.802	−0.168
50	6.17	6.331	0.161	6.585	0.415
51	6.68	7.152	0.472	6.957	0.277
52	6.45	6.629	0.179	6.875	0.425
53	6.83	6.584	−0.246	6.627	−0.203
54	6.27	6.057	−0.213	6.452	0.182
55	6.46	7.027	0.567	6.633	0.173
56	6.63	6.545	−0.085	6.796	0.166
57	6.94	6.872	−0.068	6.62	−0.32
58	6.91	6.805	−0.105	6.448	−0.462
59	6.7	6.218	−0.482	6.58	−0.12
60	6.21	6.153	−0.057	5.904	−0.306
61	5.74	5.902	0.162	5.668	−0.072
62	5.96	6.058	0.098	6.265	0.305
63	6.69	6.499	−0.191	6.635	−0.055
64	6.77	6.336	−0.434	6.449	−0.321
65	6.61	6.749	0.139	6.481	−0.129
66	6.57	6.34	−0.23	6.602	0.032

Table S13. *Cont.*

Compound	Observed Activities	CoMFA		CoMSIA	
		Predicted	Residue	Predicted	Residue
67	6.82	6.031	−0.789	6.825	0.005
68	6.66	6.476	−0.184	6.716	0.056
69	6.61	6.59	−0.02	6.937	0.327
70	6.4	6.213	−0.187	6.507	0.107
71	6.07	6.257	0.187	6.154	0.084
72	6.26	6.8	0.54	6.742	0.482
73	7.44	7.421	−0.019	7.19	−0.25
74	6.54	6.677	0.137	6.739	0.199
75	6.77	7.204	0.434	6.978	0.208
76	7.27	7.185	−0.085	7.119	−0.151
77	7.21	7.279	0.069	7.047	−0.163
78	7.2	7.213	0.013	6.976	−0.224
79	7.7	7.536	−0.164	7.672	−0.028
80	7.8	7.708	−0.092	7.796	−0.004
81	8	8.14	0.14	8.058	0.058
82	7.52	7.181	−0.339	7.298	−0.222
83	7.29	7.49	0.2	7.333	0.043
84	7.96	7.896	−0.064	7.451	−0.509
85	7.16	7.431	0.271	7.336	0.176
86	7.13	7.055	−0.075	7.231	0.101
87	7.09	6.903	−0.187	6.964	−0.126
88	8.4	7.995	−0.405	7.978	−0.422
89	7.03	6.942	−0.088	7.19	0.16
90	7.39	7.307	−0.083	7.643	0.253
91	7.17	7.536	0.366	7.69	0.52
92	7.18	7.696	0.516	6.973	−0.207
93	7.68	7.844	0.164	7.74	0.06
94	6.84	7.933	1.093	7.025	0.185
95	6.55	6.92	0.37	7	0.45
96	6.65	6.659	0.009	6.785	0.135
97	7.51	7.342	−0.168	7.501	−0.009
98	6.95	6.9	−0.05	7.295	0.345
99	7.39	7.465	0.075	7.442	0.052
100	7.35	6.61	−0.74	7.102	−0.248
101	7.59	7.736	0.146	7.584	−0.006
102	7.49	7.491	0.001	7.427	−0.063
103	7.35	7.052	−0.298	7.394	0.044
104	7.04	7.014	−0.026	7.257	0.217
105	6.98	7.047	0.067	7.208	0.228
106	7.74	7.618	−0.122	7.381	−0.359
107	7.74	7.955	0.215	8.103	0.363
108	7.82	7.497	−0.323	7.417	−0.403
109	7.66	7.623	−0.037	7.9	0.24

Table S13. *Cont.*

Compound	Observed Activities	CoMFA		CoMSIA	
		Predicted	Residue	Predicted	Residue
110	8.02	8.283	0.263	8.494	0.474
111	8.28	8.346	0.066	8.292	0.012
112	8.21	7.872	−0.338	7.679	−0.531
113	7.8	7.635	−0.165	8.138	0.338
114	7.4	7.444	0.044	7.391	−0.009
115	7.54	7.697	0.157	7.69	0.15
116	7.89	7.709	−0.181	7.686	−0.204
117	7.74	7.768	0.028	7.648	−0.092
118	7.06	7.097	0.037	7.003	−0.057
119	7.7	7.681	−0.019	7.63	−0.07
120	7.92	7.843	−0.077	8.091	0.171
121	7.7	7.564	−0.136	7.546	−0.154
122	8.3	8.307	0.007	8.425	0.125
123	7.08	6.793	−0.287	7.071	−0.009
124	7.32	6.997	−0.323	6.723	−0.597
125	7.72	7.807	0.087	7.173	−0.547
126	7.4	7.017	−0.383	6.874	−0.526
127	5.16	6.374	1.214	5.862	0.702
128	5.02	5.427	0.407	5.949	0.929
129	5.6	5.737	0.137	5.653	0.053
130	5.68	5.937	0.257	6.262	0.582
131	5.56	5.749	0.189	5.606	0.046
132	6.9	5.842	−1.058	6.509	−0.391
133	6.57	6.318	−0.252	6.868	0.298
134	6.37	6.136	−0.234	6.367	−0.003
135	5.48	5.431	−0.049	5.4	−0.08
136	6.25	6.387	0.137	6.275	0.025
137	6.79	6.896	0.106	7.37	0.58
138	6.68	6.74	0.06	6.543	−0.137
139	6.98	6.916	−0.064	6.788	−0.192
140	7.2	7.299	0.099	7.193	−0.007
141	7.38	7.093	−0.287	6.823	−0.557
142	7.35	7.009	−0.341	6.825	−0.525
143	6.14	6.546	0.406	6.373	0.233
144	6.94	7.104	0.164	7.003	0.063
145	5.58	5.924	0.344	5.836	0.256
146	6.6	6.721	0.121	6.761	0.161
147	7.8	8.482	0.682	7.255	−0.545
148	7.62	7.438	−0.182	7.686	0.066
149	5.74	6.483	0.743	6.4	0.66
150	7.66	7.257	−0.403	7.54	−0.12
151	7.02	7.121	0.101	6.979	−0.041
152	6.36	7.246	0.886	6.971	0.611

Table S13. *Cont.*

Compound	Observed Activities	CoMFA		CoMSIA	
		Predicted	Residue	Predicted	Residue
153	7.8	7.066	−0.734	7.049	−0.751
154	6.46	6.895	0.435	6.951	0.491
155	6.76	6.574	−0.186	6.557	−0.203
156	6.09	6.799	0.709	6.323	0.233
157	6.32	6.628	0.308	6.866	0.546
158	5.98	6.363	0.383	6.254	0.274
159	6.62	6.877	0.257	6.709	0.089
160	5.96	6.875	0.915	6.459	0.499
161	7.23	7.207	−0.023	7.17	−0.06
162	7.09	7.497	0.407	7.527	0.437
163	7.8	7.389	−0.411	7.35	−0.45
164	7.19	7.137	−0.053	7.05	−0.14
165	7.64	7.185	−0.455	7.232	−0.408
166	6.39	6.866	0.476	6.733	0.343
167	8.01	7.911	−0.099	7.946	−0.064
168	8.15	7.997	−0.153	7.765	−0.385
169	8.46	8.032	−0.428	8.511	0.051
170	7.01	6.898	−0.112	7.277	0.267
171	8.16	7.339	−0.821	7.802	−0.358
172	7.89	7.515	−0.375	7.481	−0.409
173	7.66	7.526	−0.134	7.442	−0.218
174	7.68	7.534	−0.146	7.891	0.211
175	8.42	8.51	0.09	8.201	−0.219
176	8.03	7.875	−0.155	7.5	−0.53
177	6.74	6.365	−0.375	6.335	−0.405
178	6.38	6.77	0.39	6.564	0.184
179	7.37	7.575	0.205	7.635	0.265
180	7.39	7.224	−0.166	6.908	−0.482
181	7.54	7.864	0.324	7.657	0.117