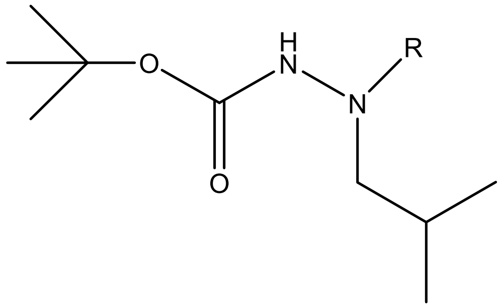
Electronic Supplementary Material (ESI) for Molecular BioSystems

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



Skeleton 1

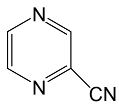
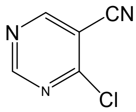
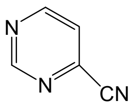
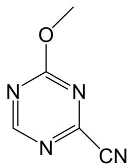
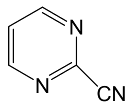
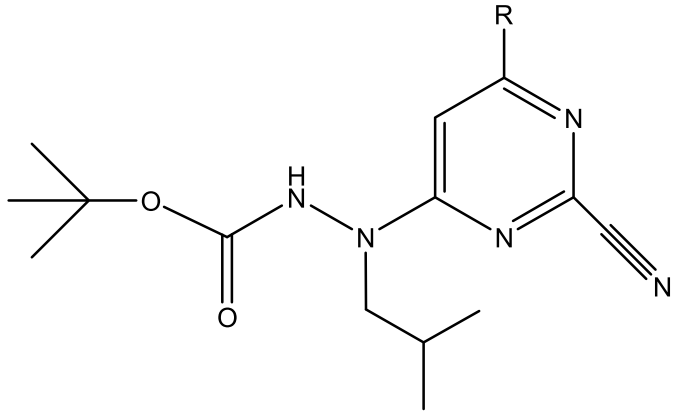
NO	R	IC_{50} (μM)
1		1.67
2		0.99
3		3.57
4		0.204
5		0.87

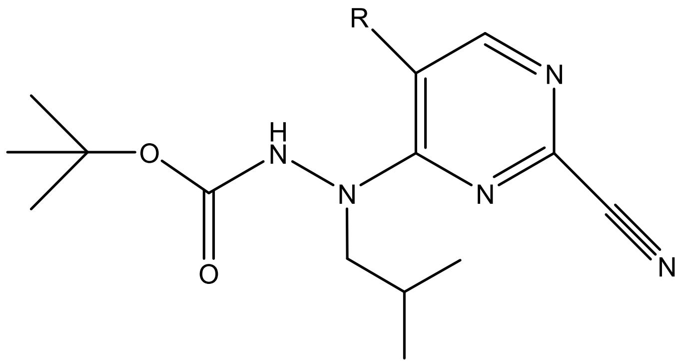
Table S2 Structure of compounds with skeleton 2 in the data set



Skeleton 2

NO	R	IC_{50} (μM)
6	H	1.86
7	CH_3	0.25
8	CO_2CH_3	1.04

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



Skeleton 3

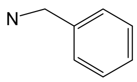
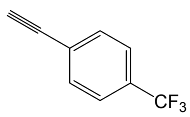
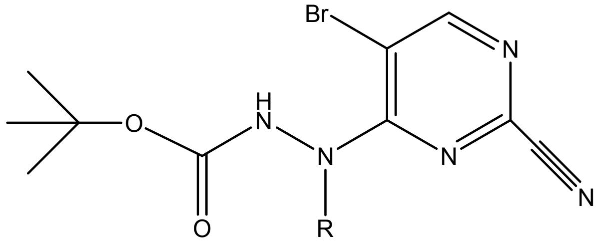
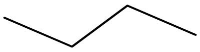
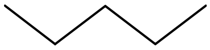
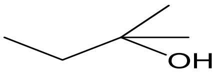
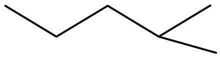
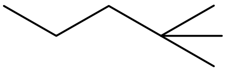
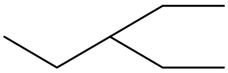
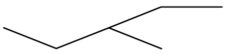
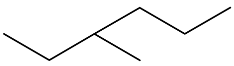
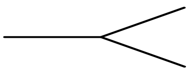
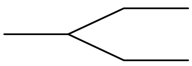
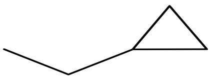
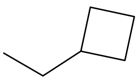
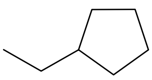
NO	R	IC_{50} (μM)
9	F	0.583
10	Br	0.092
11	Cl	0.144
12	NO_2	0.026
13	CH_3	1.15
14	CF_3	0.066
15		2.07
16		5.33
17	CH_3O	2.39

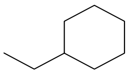
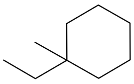
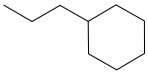
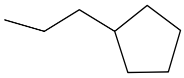
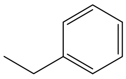
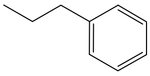
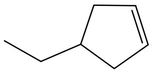
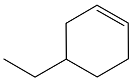
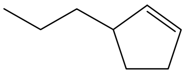
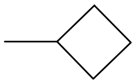
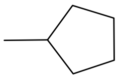
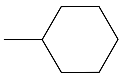
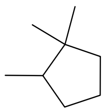
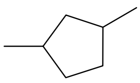
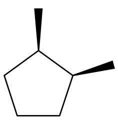
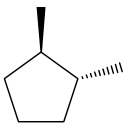
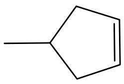
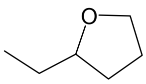
Table S4 Structure of compounds with skeleton 4 in the data set



Skeleton 4

NO	R	IC_{50} (μM)
18		0.255
19		0.125
20		0.256
21		1.05
22		0.138
23		0.283
24		0.178
25		0.187
26		0.273
27		0.054
28		0.115
29		1.33
30		3.75
31		0.413
32		0.062
33		0.01

To be continued

NO	R	IC_{50} (μM)
34		0.146
35		0.121
36		0.86
37		0.504
38		0.347
39		0.557
40		0.035
41		0.041
42		0.311
43		0.297
44		0.056
45		0.008
46		0.447
47		0.053
48		0.407
49		0.006
50		0.021
51		0.112

Electronic Supplementary Material (ESI) for Molecular BioSystems

To be continued

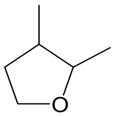
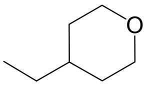
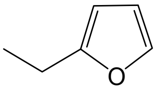
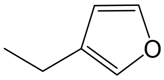
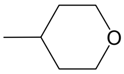
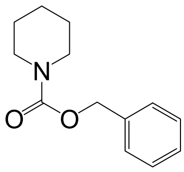
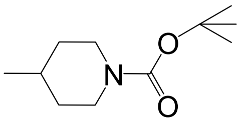
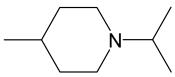
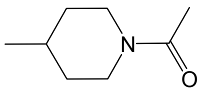
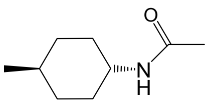
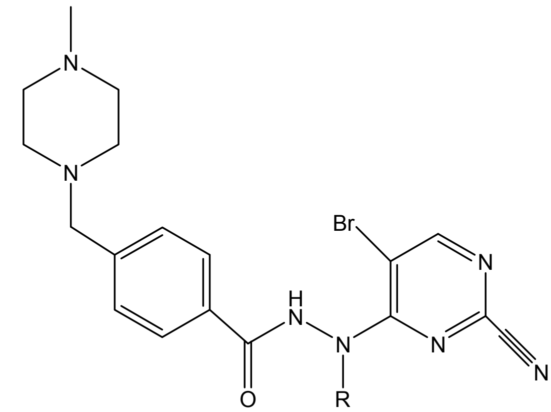
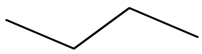
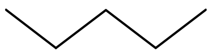
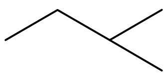
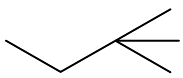
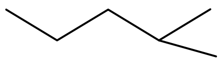
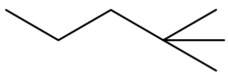
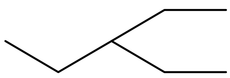
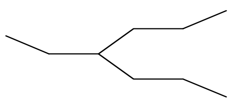
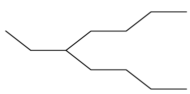
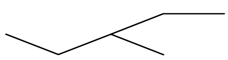
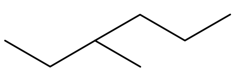
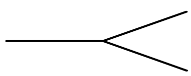
NO	R	IC_{50} (μM)
52		0.098
53		0.085
54		0.14
55		0.183
56		0.028
57		0.038
58		0.135
59		5.235
60		0.033
61		0.067

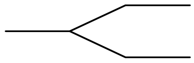
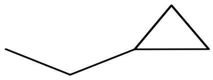
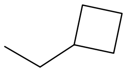
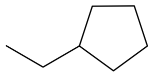
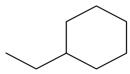
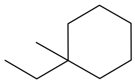
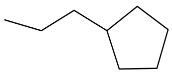
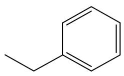
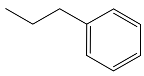
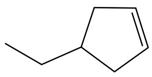
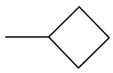
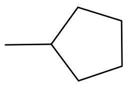
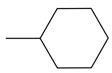
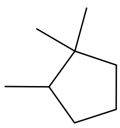
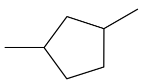
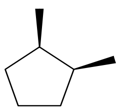
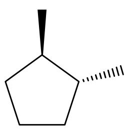
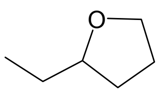
Table S5 Structure of compounds with skeleton 5 in the data set



Skeleton 5

NO	R	IC_{50} (μM)
62		0.446
63		0.105
64		0.097
65		0.126
66		0.055
67		0.158
68		0.068
69		0.039
70		0.044
71		0.802
72		0.656
73		0.035
74		0.052
75		1.37

To be continued

NO	R	IC_{50} (μM)
76		2.04
77		0.33
78		0.111
79		0.006
80		0.016
81		0.017
82		0.045
83		0.335
84		0.105
85		0.016
86		0.173
87		0.011
88		0.006
89		0.11
90		0.045
91		0.041
92		0.003
93		0.099

To be continued

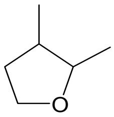
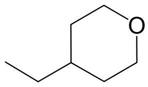
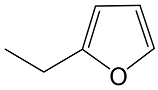
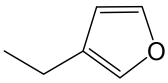
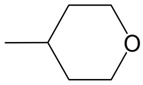
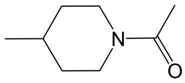
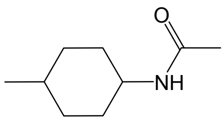
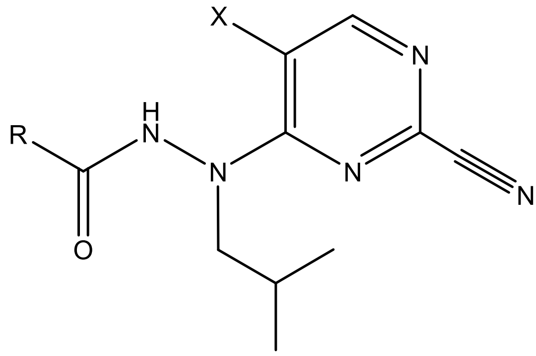
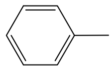
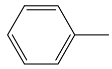
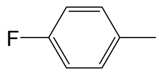
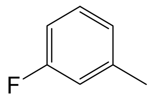
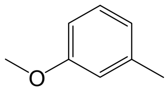
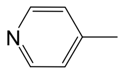
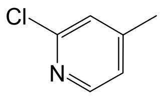
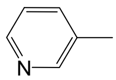
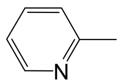
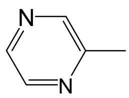
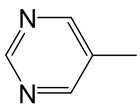
NO	R	IC_{50} (μM)
94		0.075
95		0.135
96		0.18
97		0.133
98		0.017
99		0.026
100		0.088

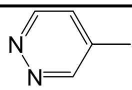
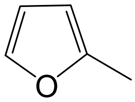
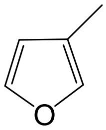
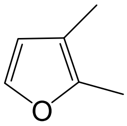
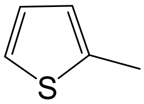
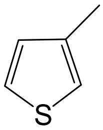
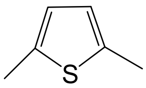
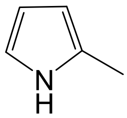
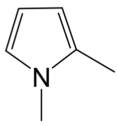
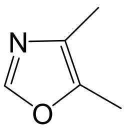
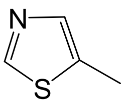
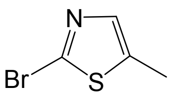
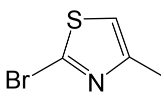
Table S6 Structure of compounds with skeleton 6 in the data set



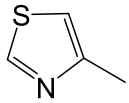
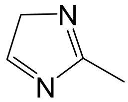
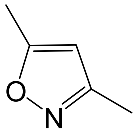
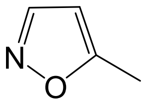
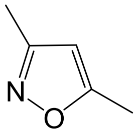
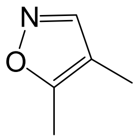
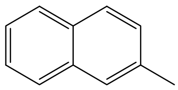
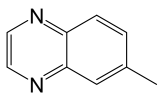
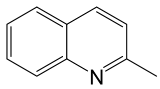
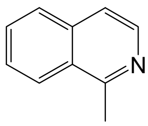
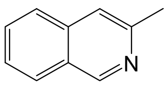
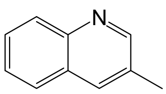
Skeleton 6

NO	X	R	IC_{50} (μM)
101	Br		0.055
102	Cl		0.08
103	Br		0.036
104	Br		0.854
105	Br		0.464
106	Br		1.05
107	Cl		0.227
108	Br		0.291
109	Br		0.093
110	Br		0.575
111	Cl		0.116

To be continued

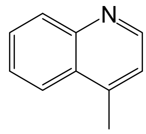
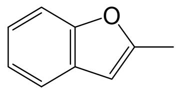
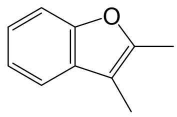
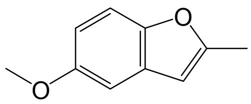
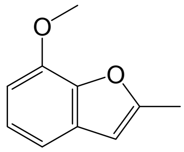
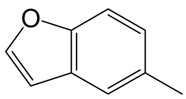
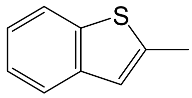
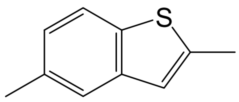
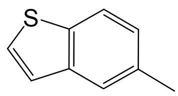
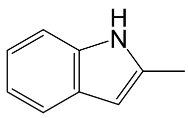
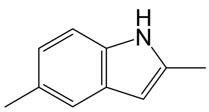
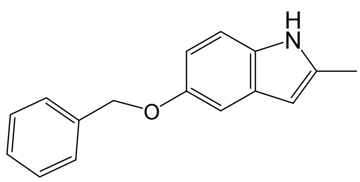
No	X	R	IC_{50} (μM)
112	Cl		0.08
113	Br		0.22
114	Cl		0.109
115	Br		0.058
116	Br		0.178
117	Br		0.229
118	Br		0.1
119	Br		0.433
120	Br		0.161
121	Br		0.161
122	Br		0.068
123	Br		0.092
124	Br		0.113

To be continued

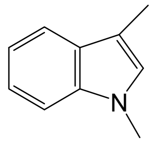
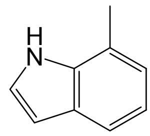
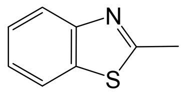
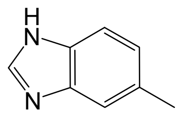
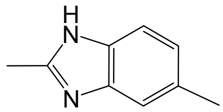
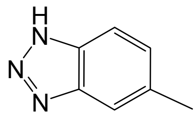
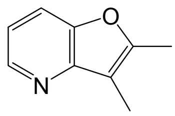
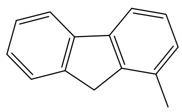
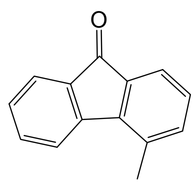
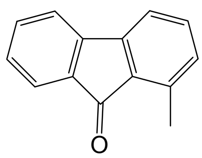
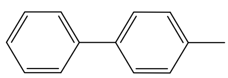
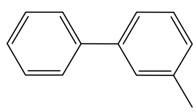
NO	X	R	IC_{50} (μM)
125	Cl		0.143
126	Br		0.119
127	Br		0.496
128	Br		0.028
129	Br		0.034
130	Br		1.22
131	Br		0.645
132	Br		1.44
133	Cl		0.254
134	Cl		0.197
135	Cl		0.333
136	Cl		0.126

Electronic Supplementary Material (ESI) for Molecular BioSystems

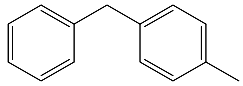
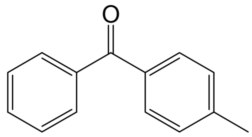
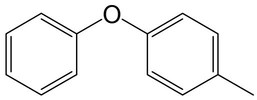
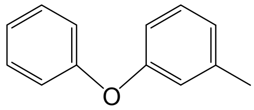
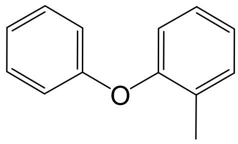
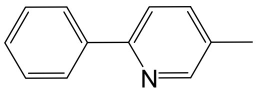
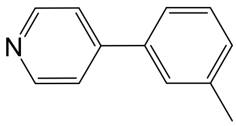
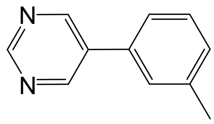
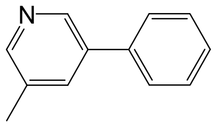
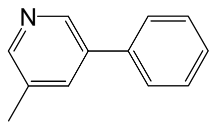
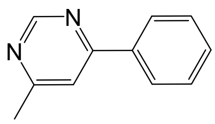
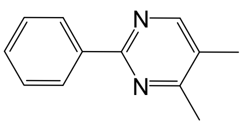
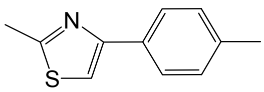
To be continued

NO	X	R	IC_{50} (μM)
137	Cl		0.044
138	Br		0.563
139	Br		1.43
140	Br		1.24
141	Br		0.399
142	Br		0.069
143	Br		0.365
144	Br		0.748
145	Br		0.154
146	Br		0.641
147	Br		1.53
148	Br		4.65

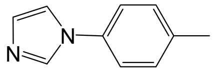
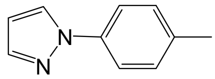
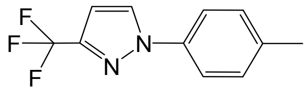
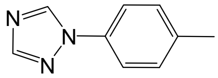
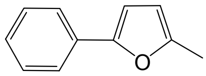
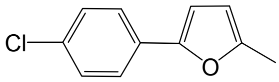
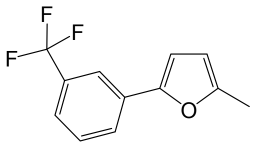
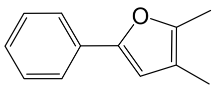
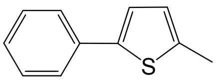
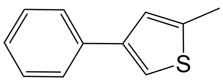
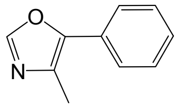
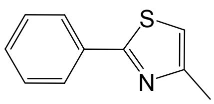
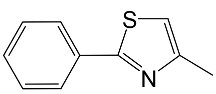
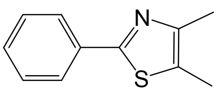
To be continued

NO	X	R	IC_{50} (μM)
149	Br		0.311
150	Br		0.342
151	Cl		0.112
152	Cl		0.093
153	Br		0.027
154	Br		0.04
155	Br		0.073
156	Br		0.329
157	Br		0.067
158	Br		0.831
159	Br		1.46
160	Cl		0.037

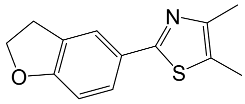
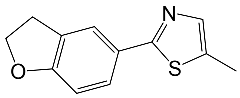
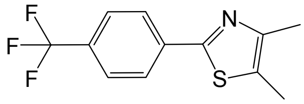
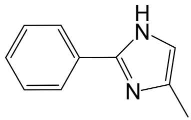
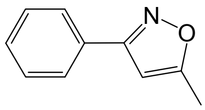
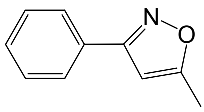
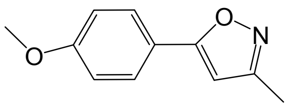
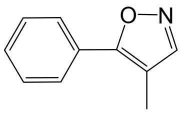
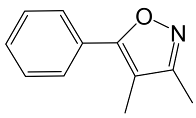
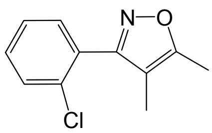
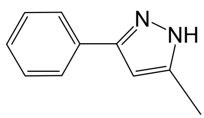
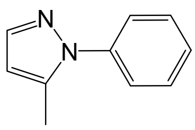
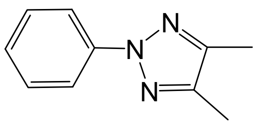
To be continued

NO	X	R	IC_{50} (μM)
161	Br		0.962
162	Br		0.115
163	Cl		0.896
164	Br		0.116
165	Br		0.066
166	Br		0.104
167	Br		0.015
168	Br		0.012
169	Br		0.004
170	Cl		0.026
171	Cl		0.03
172	Br		0.165
173	Br		0.164

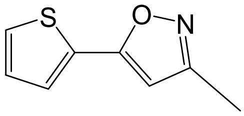
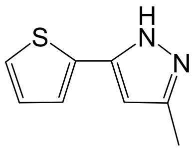
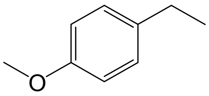
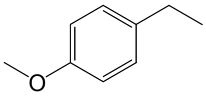
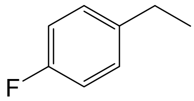
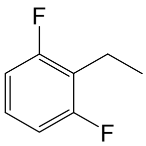
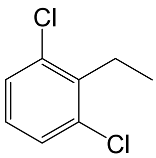
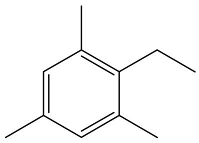
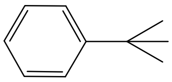
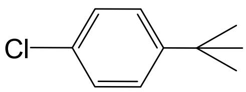
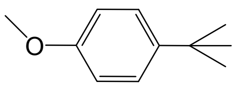
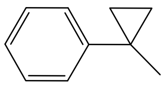
To be continued

NO	X	R	IC_{50} (μM)
174	Cl		0.239
175	Cl		0.148
176	Cl		0.144
177	Br		0.052
178	Br		0.039
179	Br		0.351
180	Br		0.097
181	Br		0.837
182	Br		0.549
183	Br		0.374
184	Br		0.374
185	Cl		0.054
186	Br		0.13
187	Cl		0.999

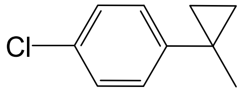
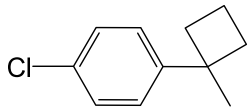
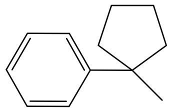
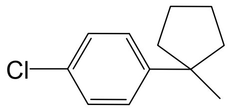
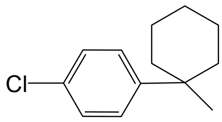
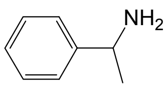
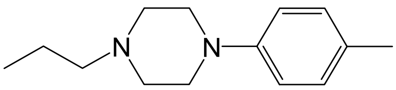
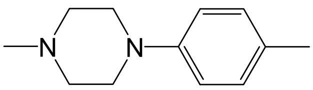
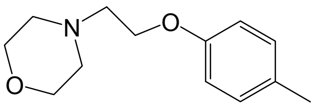
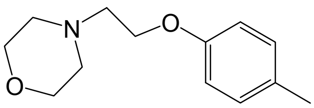
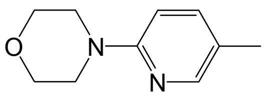
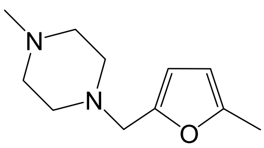
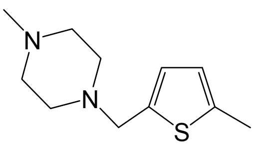
To be continued

NO	X	R	IC_{50} (μM)
188	Cl		0.95
189	Cl		0.198
190	Br		1.54
191	Br		0.146
192	Cl		0.12
193	Br		0.359
194	Cl		0.692
195	Br		0.128
196	Cl		0.071
197	Br		0.571
198	Cl		0.352
199	Br		0.063
200	Br		1.1

To be continued

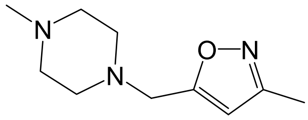
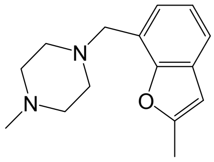
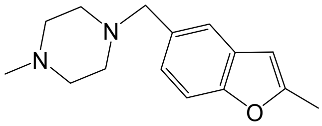
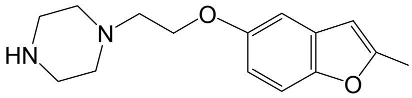
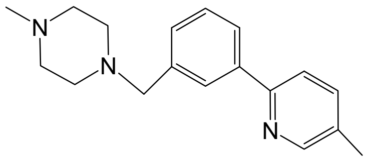
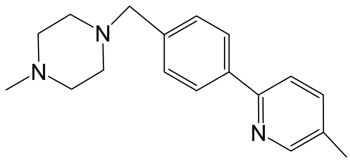
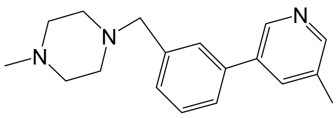
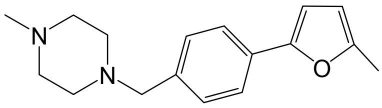
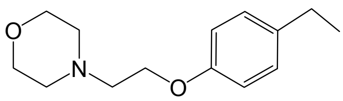
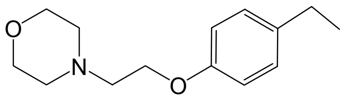
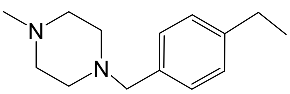
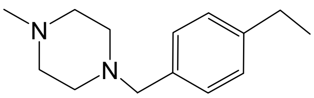
NO	X	R	IC_{50} (μM)
201	Cl		0.218
202	Br		0.451
203	Br		0.006
204	Cl		0.005
205	Br		0.004
206	Br		0.008
207	Br		0.066
208	Br		0.021
209	Br		0.06
210	Br		0.018
211	Br		0.034
212	Br		0.102

To be continued

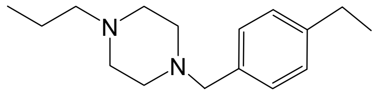
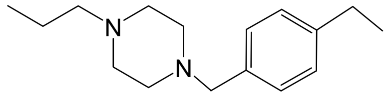
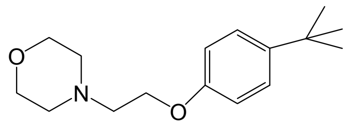
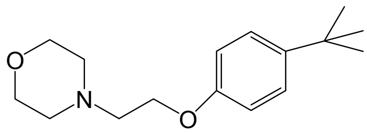
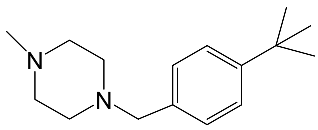
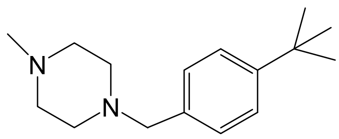
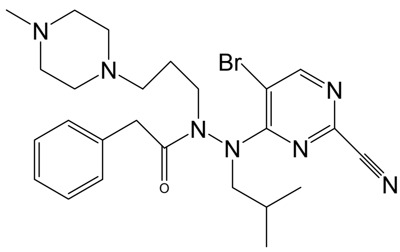
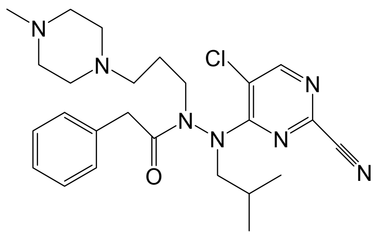
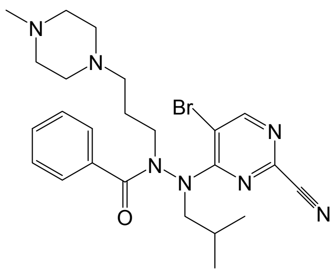
NO	X	R	IC_{50} (μM)
213	Br		0.069
214	Br		0.216
215	Br		0.137
216	Br		0.184
217	Br		1.65
218	Br		0.034
219	Br		0.032
220	Br		0.032
221	Br		0.145
222	Cl		0.09
223	Br		0.053
224	Br		0.012
225	Br		0.012

Electronic Supplementary Material (ESI) for Molecular BioSystems

To be continued

NO	X	R	IC_{50} (μM)
226	Br		0.046
227	Br		0.061
228	Br		0.029
229	Cl		0.107
230	Br		0.038
231	Br		0.026
232	Br		0.004
233	Br		0.005
234	Br		0.005
235	Cl		0.008
236	Br		0.005
237	Cl		0.005

To be continued

NO	X	R	IC_{50} (μM)
238	Br		0.003
239	Cl		0.006
240	Br		0.013
241	Cl		0.018
242	Br		0.021
243	Cl		0.046
244	Br		0.027
245	Cl		0.078
246	Br		0.078

To be continued

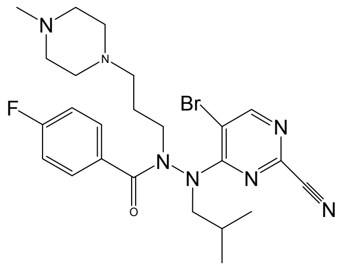
NO	X	R	IC_{50} (μM)
247	Br		0.105

Table S7 Experimental and predicted activities (pIC_{50}) for the training and test set compounds employed in CoMFA and CoMSIA analyses from the PCA division.

NO	Observed activity	Predicted
1	5.78	5.643
2*	6	6.492
3	5.45	5.67
4	6.69	6.287
5	6.06	6.179
6	5.73	6.177
7	6.6	6.475
8*	5.98	6.426
9	6.23	6.37
10	7.04	6.739
11	6.84	6.59
12	7.59	7.54
13	5.94	5.926
14	7.18	7.355
15	5.68	5.705
16	5.27	5.381
17	5.62	5.758
18	6.59	6.61
19	6.9	6.724
20	6.59	6.676
21*	5.98	6.363
22*	6.86	6.896
23	6.55	6.445
24	6.75	6.521
25	6.73	6.643
26	6.56	6.953
27	7.27	6.934
28*	6.94	6.811
29	5.88	6.693
30	5.43	5.998

To be continued

31	6.38	6.883
32	7.21	6.749
33	8	7.284
34*	6.84	6.678
35	6.92	6.822
36*	6.07	6.231
37	6.3	6.457
38	6.46	6.526
39	6.25	6.431
40	7.46	7.263
41	7.39	7.336
42	6.51	6.556
43	6.53	6.655
44	7.25	7.049
45	8.1	7.878
46	6.35	6.388
47	7.28	7.262
48	6.39	6.803
49	8.22	7.278
50	7.68	6.851
51	6.95	6.888
52	7.01	6.696
53	7.07	7.089
54*	6.85	6.717
55	6.74	6.803
56*	7.55	7.488
57	7.42	7.417
58*	6.87	7.662
59	5.28	5.096
60*	7.48	7.331
61	7.17	7.055
62	6.35	6.773

To be continued

63	6.98	6.986
64	7.01	6.863
65	6.9	6.64
66*	7.26	7.3
67	6.8	7.048
68	7.17	7.253
69	7.41	7.486
70	7.36	6.884
71	6.1	6.461
72	6.18	6.312
73	7.46	7.243
74*	7.28	7.202
75	5.86	6.193
76*	5.69	5.744
77	6.48	6.763
78	6.95	6.984
79	8.22	7.626
80	7.8	7.689
81	7.77	7.894
82	7.35	6.948
83	6.47	7.062
84	6.98	7.006
85	7.8	7.46
86	6.76	6.451
87	7.96	7.884
88*	8.22	7.814
89	6.96	7.244
90	7.35	7.515
91	7.39	7.829
92	8.52	8.619
93	7	7.211
94*	7.12	7.169

To be continued

95	6.87	7.045
96	6.74	6.931
97	6.88	6.59
98*	7.77	7.453
99	7.59	7.797
100	7.06	7.133
101	7.26	6.667
102*	7.1	6.491
103	7.44	6.935
104	6.07	6.61
105	6.33	6.636
106	5.98	6.441
107	6.64	6.826
108	6.54	6.447
109	7.03	6.855
110*	6.24	7.236
111	6.94	6.933
112	7.1	6.924
113	6.66	7.123
114	6.96	7.286
115	7.24	6.842
116	6.75	6.868
117	6.64	6.443
118	7	6.812
119	6.36	6.599
120	6.79	7.076
121	7.12	6.775
122	7.17	6.945
123	7.04	7.041
124	6.95	7.049
125	6.84	7.099
126	6.92	7.064
127*	6.3	6.303

To be continued

128	7.55	7.306
129	7.47	7.113
130	5.91	6.14
131	6.19	6.46
132*	5.84	6.433
133	6.6	6.528
134	6.71	6.786
135	6.48	6.512
136*	6.9	6.125
137	7.36	7.141
138*	6.25	6.2
139	5.84	6.301
140*	5.91	6.25
141	6.4	6.413
142	7.16	6.874
143*	6.44	6.421
144*	6.13	6.338
145	6.81	6.772
146*	6.19	6.058
147*	5.82	5.868
148*	5.33	6.383
149	6.51	6.55
150	6.47	6.265
151	6.95	6.599
152	7.03	7.258
153*	7.57	7.204
154*	7.4	7.617
155*	7.14	6.879
156*	6.48	7.23
157*	7.17	7.333
158*	6.08	6.55
159	5.84	6.141
160*	7.43	7.204

To be continued

161	6.02	5.831
162*	6.94	7.15
163	6.05	6.087
164*	6.94	6.871
165	7.18	7.22
166	6.98	6.978
167	7.82	7.782
168	7.92	7.61
169	8.4	8.169
170	7.59	7.947
171*	7.52	6.899
172*	6.78	6.848
173	6.79	6.518
174	6.62	6.616
175	6.83	6.796
176	6.84	6.65
177	7.28	7.199
178	7.41	7.023
179	6.45	6.615
180	7.01	6.979
181	6.08	6.116
182	6.26	6.676
183	6.43	6.77
184	7.03	7.252
185	7.27	7.141
186	6.89	6.935
187	6	6.1
188*	6.02	5.955
189	6.7	6.632
190*	5.81	6.04
191	6.84	6.77
192	6.92	6.648

To be continued

193	6.44	6.493
194	6.16	6.617
195	6.89	6.98
196*	7.15	7.252
197	6.24	6.322
198	6.45	6.158
199	7.2	7.668
200*	5.96	6.643
201	6.66	6.78
202*	6.35	6.253
203	8.22	8.257
204*	8.3	8.452
205	8.4	7.965
206*	8.1	7.646
207	7.18	7.537
208	7.68	7.85
209	7.22	7.167
210*	7.74	7.524
211	7.47	7.296
212	6.99	6.893
213	7.16	7.205
214*	6.67	7.151
215	6.86	6.776
216	6.74	6.721
217	5.78	5.312
218*	7.47	7.614
219	7.49	7.667
220	7.49	7.175
221	6.84	6.924
222	7.05	6.765
223	7.28	7.397
224*	7.92	8.076

To be continued

225	7.92	7.796
226*	7.34	6.968
227	7.21	7.147
228*	7.54	7.668
229	6.97	7.046
230*	7.42	7.523
231	7.59	7.633
232*	8.4	7.443
233	8.3	8.428
234*	8.3	8.414
235*	8.1	8.619
236*	8.3	8.117
237	8.3	8.323
238	8.52	8.76
239*	8.22	8.767
240*	7.89	7.397
241	7.74	7.847
242*	7.68	7.724
243*	7.34	7.753
244*	7.57	7.274
245	7.11	7.282
246	7.11	7.316
247	6.98	6.695
248$	4.74	5.237
249$	5.72	5.031
250$	5.80	6.464
251$	6.52	7.298
252$	6.96	6.891
253$	4.80	5.917

*Molecules Belonged to the Test Set.

$ Molecules Belonged to the external validation set

Table S8 Structure of compounds from the external validation set.

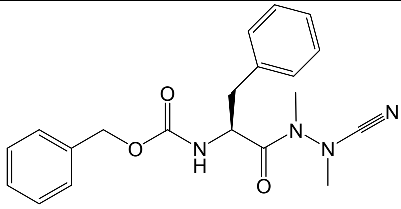
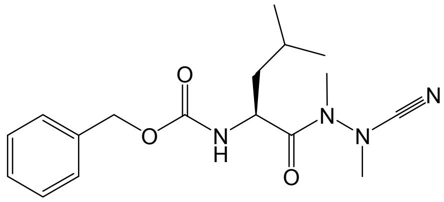
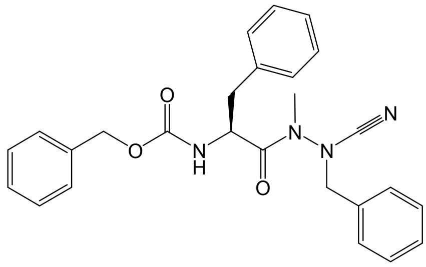
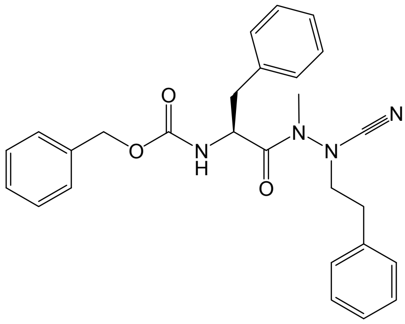
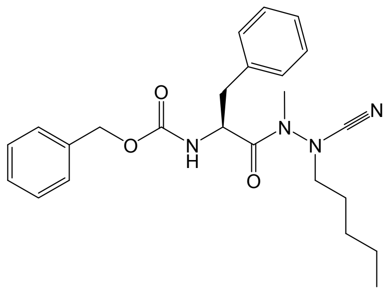
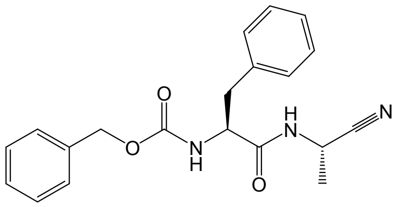
NO	R	IC_{50} (μM)
248		18.00
249		1.90
250		1.60
251		0.30
252		0.11
253		16.00

Table S9 Experimental and predicted activities (pIC_{50}) for the training and test set compounds employed in CoMFA and CoMSIA analyses from the random division.

NO	Observed activity	Predicted
1	5.78	5.524
2	6	5.965
3	5.45	5.627
4	6.69	6.053
5	6.06	6.318
6*	5.73	6.335
7*	6.6	6.342
8	5.98	6.247
9*	6.23	6.405
10	7.04	6.71
11*	6.84	6.577
12	7.59	7.573
13*	5.94	6.224
14	7.18	7.313
15	5.68	5.643
16	5.27	5.266
17	5.62	5.907
18*	6.59	6.599
19	6.9	6.682
20*	6.59	6.628
21*	5.98	6.358
22	6.86	6.83
23*	6.55	6.631
24*	6.75	6.559
25	6.73	6.675
26	6.56	6.837
27*	7.27	6.857
28	6.94	6.738
29	5.88	6.726
30	5.43	6.104

To be continued

31	6.38	6.894
32	7.21	6.799
33	8	7.242
34*	6.84	6.775
35	6.92	6.893
36	6.07	6.234
37	6.3	6.513
38	6.46	6.675
39*	6.25	6.72
40	7.46	7.142
41	7.39	7.131
42*	6.51	6.634
43*	6.53	6.707
44	7.25	7.121
45	8.1	7.789
46	6.35	6.462
47	7.28	7.197
48	6.39	6.809
49	8.22	7.247
50	7.68	6.96
51	6.95	6.872
52	7.01	6.78
53	7.07	7.199
54*	6.85	6.758
55	6.74	6.755
56	7.55	7.627
57*	7.42	6.768
58*	6.87	7.444
59	5.28	5.313
60*	7.48	7.214
61	7.17	7.106
62	6.35	6.689

To be continued

63*	6.98	6.987
64	7.01	6.852
65	6.9	6.633
66*	7.26	7.431
67	6.8	7.12
68	7.17	7.155
69	7.41	7.613
70	7.36	6.877
71	6.1	6.461
72	6.18	6.218
73	7.46	7.184
74	7.28	7.207
75	5.86	6.255
76	5.69	5.442
77	6.48	6.652
78*	6.95	6.944
79	8.22	7.513
80	7.8	7.624
81	7.77	7.987
82	7.35	7.097
83	6.47	7.249
84*	6.98	7.022
85	7.8	7.473
86	6.76	6.438
87	7.96	7.904
88	8.22	8.037
89	6.96	7.16
90*	7.35	7.469
91	7.39	7.686
92	8.52	8.709
93	7	7.06
94	7.12	7.231

To be continued

95	6.87	6.966
96	6.74	6.857
97	6.88	6.59
98	7.77	7.731
99*	7.59	7.843
100	7.06	7.14
101	7.26	6.716
102*	7.1	6.438
103	7.44	7.047
104	6.07	6.684
105*	6.33	6.9
106*	5.98	6.685
107	6.64	6.91
108*	6.54	6.574
109	7.03	6.854
110	6.24	7.1
111*	6.94	6.749
112	7.1	6.88
113	6.66	7.177
114	6.96	7.422
115	7.24	6.889
116	6.75	6.926
117	6.64	6.572
118	7	6.959
119	6.36	6.472
120*	6.79	7.214
121	7.12	6.57
122	7.17	6.916
123	7.04	6.991
124	6.95	7.126
125	6.84	7.163
126*	6.92	6.941
127	6.3	6.266

To be continued

128	7.55	7.137
129	7.47	7.063
130	5.91	6.133
131	6.19	6.559
132*	5.84	6.502
133	6.6	6.827
134	6.71	6.731
135*	6.48	6.725
136	6.9	6.383
137	7.36	7.046
138*	6.25	6.154
139	5.84	6.358
140*	5.91	6.214
141*	6.4	6.321
142*	7.16	6.937
143	6.44	6.422
144*	6.13	6.354
145	6.81	6.837
146	6.19	6.087
147*	5.82	5.834
148	5.33	5.501
149	6.51	6.669
150	6.47	6.309
151	6.95	6.537
152	7.03	7.42
153*	7.57	7.126
154	7.4	7.187
155*	7.14	6.914
156	6.48	7
157	7.17	7.425
158	6.08	6.301
159*	5.84	6.312
160	7.43	7.34

To be continued

161	6.02	5.858
162*	6.94	6.952
163	6.05	6.284
164	6.94	6.776
165*	7.18	7.364
166	6.98	6.76
167	7.82	7.811
168	7.92	7.685
169	8.4	7.956
170	7.59	7.914
171	7.52	7.093
172	6.78	6.71
173	6.79	6.729
174*	6.62	6.787
175	6.83	6.884
176	6.84	6.723
177	7.28	7.052
178	7.41	7.023
179	6.45	6.615
180*	7.01	6.901
181	6.08	6.056
182	6.26	6.599
183	6.43	6.696
184	7.03	7.15
185	7.27	7.215
186*	6.89	6.994
187	6	6.203
188	6.02	5.946
189*	6.7	6.598
190	5.81	5.806
191	6.84	6.49
192	6.92	6.496

To be continued

193	6.44	6.32
194	6.16	6.568
195*	6.89	6.843
196	7.15	7.202
197	6.24	6.64
198*	6.45	6.232
199	7.2	7.513
200	5.96	6.437
201	6.66	6.81
202	6.35	6.149
203	8.22	8.284
204	8.3	8.532
205	8.4	7.993
206	8.1	7.827
207	7.18	7.441
208	7.68	7.979
209	7.22	7.357
210*	7.74	7.553
211	7.47	7.537
212	6.99	6.976
213*	7.16	7.122
214	6.67	7.087
215	6.86	6.891
216*	6.74	6.817
217	5.78	5.512
218	7.47	7.409
219*	7.49	7.612
220	7.49	7.278
221	6.84	6.912
222	7.05	6.934
223	7.28	7.33
224	7.92	7.989

To be continued

225	7.92	7.581
226	7.34	6.991
227	7.21	7.265
228*	7.54	7.388
229*	6.97	6.901
230	7.42	7.59
231	7.59	7.516
232	8.4	8.515
233	8.3	8.308
234*	8.3	8.452
235*	8.1	8.684
236	8.3	8.09
237	8.3	8.263
238	8.52	8.431
239	8.22	8.443
240	7.89	8.012
241	7.74	7.981
242	7.68	7.602
243*	7.34	7.664
244	7.57	7.7
245	7.11	7.249
246*	7.11	6.896
247	6.98	6.854
248$	4.74	5.636
249$	5.72	6.2
250$	5.80	5.306
251$	6.52	7.272
252$	6.96	6.967
253$	4.80	6.008

*Molecules Belonged to the Test Set.

$ Molecules Belonged to the external validation set