

SUPPORTING INFORMATION

QSAR Modeling on Benzo[*c*]phenanthridine Analogues as Topoisomerase I Inhibitors and Anti-cancer Agents

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Figure S1. Process of 2D-QSAR in Rapidminer software

Table S1. Dataset of 133 BCPs compounds with their cytotoxicity on RPMI8402 cell line: experimental pIC₅₀ value and predictive results

Table S2. Dataset of 101 BCPs compounds with their cytotoxicity on CPTK5 cell line: experimental pIC₅₀ value and predictive results

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Model 1. 2D QSAR model on RPMI8402 cytotoxicity

Model 2. 2D QSAR model on CPTK5 cytotoxicity

Model 3. 2D QSAR model on P388 cytotoxicity

Model 4. 2D QSAR model on CPT45 cytotoxicity

Model 5. 2D QSAR model on KB3-1 cytotoxicity

Model 6. 2D QSAR model on KBV-1 cytotoxicity

Model 7. 2D QSAR model on KBH5.0 cytotoxicity

Model 8. 2D QSAR model on topoisomerase-1 inhibitory activity

Model 9. Hologram QSAR model on RPMI8402 cytotoxicity

Model 10. Hologram QSAR model on CPTK5 cytotoxicity

Model 11. Hologram QSAR model on P388 cytotoxicity

Model 12. Hologram QSAR model on CPT45 cytotoxicity

Model 13. Hologram QSAR model on KB3-1 cytotoxicity

Model 14. QSAR model on KBV-1 cytotoxicity

Model 15. Hologram QSAR model on KBH5.0 cytotoxicity

Model 16. Hologram QSAR model on topoisomerase-1 inhibitory activity

Model 17-18. 3D QSAR model on RPMI8402 cytotoxicity

Model 19. 3D QSAR model on CPTK5 cytotoxicity

Model 20. 3D QSAR model on P388 cytotoxicity

Model 21. 3D QSAR model on CPT45 cytotoxicity

Model 22-25. 3D QSAR model on KB3-1 cytotoxicity

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Model 27. 3D QSAR model on KBH5.0 cytotoxicity

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Table S9. Several new designed BCPs compound with predictive activity from QSAR models

Part S. Calculation of r_m^2 metrics and references.

Figure S1. Process of 2D-QSAR in Rapidminer software

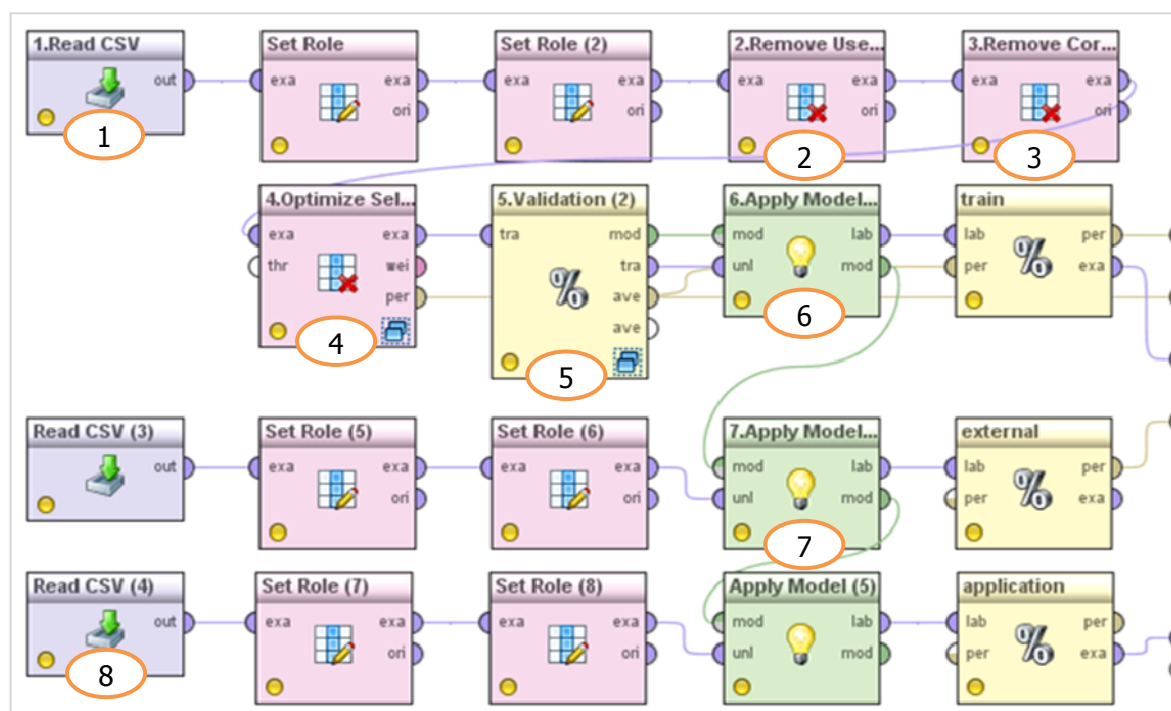


Table S1. Dataset of 133 BCPs compounds with their cytotoxicity on RPMI8402 cell line: experimental pIC₅₀ value and predictive results

No	Name	pIC50/RPMI	pIC50/RPMI-S43	pIC50/RPMI-S45	pIC50/RPMI-151	pIC50/RPMI-2D
1	BMCL_02_3333_4C	2.00	2.10	2.07	1.74	1.41
2	BMC_03_1475_12	0.35	-0.11	-0.06	-0.22	0.43
3	BMC_03_1475_14	-1.00	-0.21	-0.61	-0.16	0.17
4	BMC_03_1475_15	0.49	0.26	0.38	0.00	0.52
5	BMC_03_1475_2B	-0.88	-1.66	-0.85	-1.07	-0.13
6	BMC_03_1475_5	-0.74	-0.40	-0.68	-0.74	-0.50
7	BMC_03_1475_8	-0.60	0.21	-0.06	-0.92	-0.45
8	BMC_03_1475_9	-1.59	-1.25	-0.89	-1.23	-0.86
9	BMC_03_1809_5A	-1.15	-1.20	-0.80	-0.81	-0.54
10	BMC_03_1809_5B	-1.34	-1.26	-0.74	-1.80	-0.61
11	BMC_03_1809_6	-0.70	-1.54	-1.01	-0.39	-0.88
12	BMC_03_2061_3C	2.52	1.53	1.56	1.91	1.96
13	BMC_03_2061_3D	0.47	1.39	1.14	1.39	1.54
14	BMC_03_2061_3F	1.10	1.45	1.51	1.71	1.16
15	BMC_03_2061_3G	0.82	1.53	1.44	1.54	1.04
16	BMC_03_2061_3H	1.70	1.25	1.25	1.52	1.22
17	BMC_03_2061_3I	1.59	1.39	1.73	1.65	1.49
18	BMC_03_2061_3J	-0.20	0.30	-0.27	-0.18	1.53
19	BMC_03_2061_3K	1.36	1.29	1.20	1.30	1.28
20	BMC_03_2061_4A	1.77	1.44	1.58	1.65	1.38
21	BMC_03_2061_4B	0.80	0.97	0.94	0.16	1.27
22	BMC_03_2061_9K	1.41	1.75	1.64	1.26	1.49
23	BMC_03_3795_10A	0.40	0.13	-0.30	0.16	0.37
24	BMC_03_3795_10C	-1.52	-0.47	-1.01	-0.56	0.40
25	BMC_03_3795_10D	0.80	0.38	0.27	0.40	0.01
26	BMC_03_3795_10E	-0.88	0.10	-0.47	0.05	0.74
27	BMC_03_3795_12B	0.70	-0.01	-0.06	0.63	-0.70
28	BMC_03_3795_12D	0.52	0.77	0.99	0.23	-0.47
29	BMC_03_3795_3	-0.65	-1.67	-0.97	-0.11	-0.14
30	BMC_03_3795_5	1.15	0.37	0.19	-0.21	0.48
31	BMC_03_521_7B	-0.36	-0.26	-0.45	-0.72	-0.93
32	BMC_03_521_7C	-0.90	-0.56	-0.70	-0.93	-0.72
33	BMC_03_521_7D	-1.11	-0.44	-0.58	-0.78	-0.85
34	BMC_03_521_7E	-0.93	-0.96	-0.94	-0.66	-1.59
35	BMC_03_521_7G	-0.20	-0.40	-0.60	-0.60	-1.08
36	BMC_03_521_7H	-0.60	-0.62	-0.68	-0.43	-0.21
37	BMC_04_3731_2	3.00	2.41	2.53	2.08	1.64
38	BMC_04_3731_3A	0.66	0.59	0.59	0.96	0.75
39	BMC_04_3731_3B	1.12	0.82	0.93	0.90	1.13
40	BMC_04_3731_4A	0.19	0.42	0.44	0.73	0.59
41	BMC_04_3731_4B	1.00	0.82	0.96	0.88	0.24
42	BMC_04_3731_5	1.00	0.64	0.66	0.69	0.39
43	BMC_04_5585_15B	3.30	1.76	2.32	2.44	2.15
44	BMC_04_5585_15D	3.00	2.58	2.82	2.61	1.88

No	Name	pIC50/RPMI	pIC50/RPMI-S43	pIC50/RPMI-S45	pIC50/RPMI-151	pIC50/RPMI-2D
45	BMC_04_795_1B	2.40	2.38	2.60	2.25	2.27
46	BMC_04_795_1C	0.59	0.54	0.08	0.90	1.55
47	BMC_04_795_1D	2.40	2.13	2.12	2.06	1.54
48	BMC_04_795_1E	2.00	1.09	1.31	2.02	1.38
49	BMC_04_795_1F	2.52	2.34	2.33	2.43	2.17
50	BMC_04_795_1G	2.52	2.38	2.33	2.40	2.11
51	BMC_04_795_1H	1.10	2.20	1.94	1.91	1.70
52	BMC_04_795_2	0.62	1.31	1.06	1.10	1.22
53	BMC_05_6782_7A	1.07	1.22	1.17	1.31	0.80
54	BMC_05_6782_7B	1.52	1.35	1.68	1.38	1.32
55	BMC_05_6782_7C	1.52	1.57	1.74	1.39	1.34
56	BMC_05_6782_7D	1.40	1.15	1.31	1.26	1.38
57	BMC_05_6782_7E	0.66	0.62	0.42	1.42	1.00
58	BMC_05_6782_9C	2.70	1.95	2.27	1.40	2.12
59	BMC_05_6782_9D	0.30	0.56	0.17	1.36	1.41
60	BMC_05_6782_9E	2.22	1.61	1.66	1.39	1.68
61	BMC_05_6782_9F	1.47	0.78	1.07	0.97	0.84
62	BMC_05_6782_9G	0.35	0.83	0.04	0.50	0.94
63	BMC_05_6782_9H	2.52	1.62	1.79	1.52	1.36
64	BMC_05_6782_9I	1.26	1.56	1.57	1.47	2.05
65	BMC_05_6782_9J	1.19	1.25	1.05	0.99	1.94
66	BMC_05_6782_9K	1.30	1.58	1.57	1.21	1.63
67	BMC_05_6782_9L	0.77	0.49	0.28	1.62	1.21
68	BMC_06_3131_10B	2.52	2.19	2.63	2.31	2.27
69	BMC_06_3131_10C	2.52	2.61	2.94	2.50	2.14
70	BMC_06_3131_10F	2.40	2.43	2.46	2.72	1.44
71	BMC_06_3131_10G	1.46	2.46	2.61	2.45	1.96
72	BMC_06_3131_10I	1.52	1.77	1.95	2.23	1.94
73	BMC_06_3131_10J	1.30	0.95	2.02	1.26	0.71
74	BMC_06_3131_10K	1.64	2.14	1.72	1.99	1.29
75	BMC_06_3131_10L	2.70	1.85	2.04	2.39	1.52
76	BMC_06_3131_10M	2.70	2.31	2.72	2.40	2.26
77	BMC_08_8598_10	0.92	1.03	0.93	0.81	0.07
78	BMC_08_8598_12	0.92	1.04	0.98	0.87	0.60
79	BMC_08_8598_13	1.00	0.59	0.57	1.30	1.06
80	BMC_08_8598_14	0.26	1.13	0.86	0.01	0.42
81	BMC_08_8598_15	1.22	1.24	1.35	1.77	0.51
82	BMC_08_8598_17	1.70	1.70	1.78	1.65	1.06
83	BMC_08_8598_19	1.22	0.67	1.05	1.53	1.34
84	BMC_08_8598_21	0.55	0.67	0.51	0.26	1.04
85	BMC_08_8598_23	1.46	0.87	1.26	0.58	2.12
86	BMC_08_8598_9	-1.00	0.53	0.19	-0.66	0.14
87	BMC_09_2877_10	0.42	1.29	1.26	1.05	1.23
88	BMC_09_2877_11	1.60	1.33	1.39	0.90	0.73
89	BMC_09_2877_12	1.52	1.72	1.99	1.00	1.45
90	BMC_09_2877_14	-0.60	0.96	0.67	1.10	1.30

No	Name	pIC50/RPMI	pIC50/RPMI-S43	pIC50/RPMI-S45	pIC50/RPMI-151	pIC50/RPMI-2D
91	BMC_09_2877_16	0.22	0.77	0.58	1.01	0.71
92	BMC_09_2877_17	1.35	1.50	0.99	1.54	1.39
93	BMC_09_2877_18	0.74	1.38	1.69	0.83	1.43
94	BMC_09_2877_19	0.52	1.19	0.28	1.40	0.88
95	BMC_09_2877_20	0.00	1.17	1.05	0.90	1.00
96	BMC_09_2877_21	0.52	1.16	0.37	0.86	1.16
97	BMC_09_2877_22	1.62	1.18	1.14	1.49	1.32
98	BMC_09_2877_3	3.15	2.48	2.88	2.45	2.24
99	BMC_09_2877_7	2.52	0.91	0.95	1.13	0.64
100	BMC_09_2877_8	1.48	1.42	1.31	1.04	0.80
101	BMC_09_2877_9	1.48	1.25	1.09	1.17	1.07
102	JMC_03_2254_16A	0.62	0.84	0.91	0.63	1.45
103	JMC_03_2254_3	1.22	0.80	0.65	0.62	0.91
104	JMC_03_2254_4B	0.47	0.71	0.47	0.62	1.15
105	JMC_03_2254_6B	1.10	0.89	1.06	0.83	1.55
106*	BMCL_02_3333_3C	0.82	1.64	3.34	1.45	1.06
107*	BMC_03_1475_11	-1.61	0.02	1.53	-0.03	0.04
108*	BMC_03_1475_7	-0.30	0.27	1.62	-0.83	-0.17
109*	BMC_03_1809_7	-0.70	-1.68	1.03	-0.70	-1.22
110*	BMC_03_2061_3B	0.24	0.31	2.14	0.16	1.27
111*	BMC_03_2061_3E	1.52	1.56	3.05	1.68	2.03
112*	BMC_03_3795_10B	0.22	-0.23	1.05	-0.01	0.00
113*	BMC_03_3795_10F	-0.15	-0.28	0.74	0.11	0.34
114*	BMC_03_3795_12C	-1.26	-0.15	1.62	0.31	-0.30
115*	BMC_03_3795_4	0.40	0.34	1.65	0.20	-0.19
116*	BMC_03_521_7F	-0.59	-0.88	0.92	-0.51	-0.86
117*	BMC_04_3731_3C	1.74	0.84	2.88	1.01	0.78
118*	BMC_04_3731_3D	-0.74	-0.76	0.65	0.78	1.16
119*	BMC_04_3731_4C	1.40	0.75	2.85	0.84	0.61
120*	BMC_04_3731_4D	-0.60	0.27	2.24	0.95	0.60
121*	BMC_05_6782_1	2.70	1.44	3.32	1.65	1.38
122*	BMC_05_6782_9A	2.52	1.83	3.86	1.40	2.06
123*	BMC_05_6782_9B	3.40	1.80	3.65	1.56	1.80
124*	BMC_06_3131_10D	2.52	2.48	4.17	2.63	1.91
125*	BMC_08_8598_11	1.00	0.90	2.39	0.00	0.67
126*	BMC_08_8598_16	1.49	1.25	3.10	1.08	0.78
127*	BMC_08_8598_18	1.46	1.07	2.69	0.11	1.39
128*	BMC_08_8598_20	0.85	0.72	2.50	0.17	1.32
129*	BMC_08_8598_22	-0.20	0.61	2.53	0.35	0.74
130*	BMC_09_2877_15	1.40	1.36	3.37	1.03	1.03
131*	BMC_09_2877_6	1.52	1.11	2.97	0.92	0.05
132*	JMC_03_2254_5B	1.60	1.04	3.12	0.78	1.18
133*	LDDD_04_198_1	2.40	1.23	2.86	1.54	1.52

*: external test set

Table S2. Dataset of 101 BCPs compounds with their cytotoxicity on CPTK5 cell line: experimental pIC₅₀ value and predictive results

No	Name	pIC50/CPTk5	pIC50/CPTk5-SH44	pIC50/CPTk5-53	pIC50/CPTk5-2D
1	BMC_03_1475_12	-2.00	-1.48	-0.83	-0.47
2	BMC_03_1475_15	0.42	-0.54	-0.41	-0.60
3	BMC_03_1475_2B	-0.99	-1.60	-0.56	0.08
4	BMC_03_1475_5	-1.00	-0.88	-1.54	-1.39
5	BMC_03_1475_8	-1.45	-0.52	-1.36	-1.18
6	BMC_03_1475_9	-1.79	-1.95	-1.59	-1.02
7	BMC_03_1809_5A	-1.20	-1.04	-0.55	-0.64
8	BMC_03_1809_5B	-1.04	-0.98	-0.99	-0.64
9	BMC_03_1809_6	-0.88	-0.99	-0.38	-0.99
10	BMC_03_2061_3C	0.41	-0.09	-0.11	-0.05
11	BMC_03_2061_3D	-1.00	-0.36	-0.36	-0.46
12	BMC_03_2061_3J	-1.10	-0.76	-0.68	-0.36
13	BMC_03_2061_4A	-0.60	0.03	-0.17	0.11
14	BMC_03_2061_4B	0.40	0.09	-0.36	0.18
15	BMC_03_3795_10A	0.70	-0.21	-0.21	-0.22
16	BMC_03_3795_10C	-1.85	-1.26	-0.86	-0.57
17	BMC_03_3795_10D	0.85	0.84	-0.09	-0.41
18	BMC_03_3795_10E	-1.40	-1.01	-0.76	-0.90
19	BMC_03_3795_12B	0.70	-0.05	0.29	-0.27
20	BMC_03_3795_12D	0.52	0.86	0.14	-0.11
21	BMC_03_3795_3	-1.04	-1.71	-0.14	0.08
22	BMC_03_3795_5	-0.74	-0.47	-0.92	-0.12
23	BMC_03_521_7B	-0.75	-0.97	-1.67	-0.56
24	BMC_03_521_7D	-1.60	-0.90	-1.36	-1.39
25	BMC_03_521_7E	-1.36	-1.34	-0.83	-1.18
26	BMC_03_521_7G	-1.15	-0.66	-1.19	-1.67
27	BMC_03_521_7H	-1.48	-1.42	-1.54	-0.72
28	BMC_04_3731_2	0.22	0.07	-0.35	-0.02
29	BMC_04_3731_3A	-0.48	-0.42	-0.12	-0.76
30	BMC_04_3731_3B	-0.53	-0.49	0.17	-0.81
31	BMC_04_3731_4B	-0.32	-0.82	0.09	-0.62
32	BMC_04_3731_5	-0.23	-0.37	0.05	-1.25
33	BMC_04_5585_15B	0.70	0.54	0.51	0.09
34	BMC_04_5585_15D	-0.18	-0.02	0.20	0.22
35	BMC_04_795_1B	0.29	0.01	-0.40	0.14
36	BMC_04_795_1C	-0.56	-1.03	-0.61	0.04
37	BMC_04_795_1D	-1.00	-0.36	-0.54	0.24
38	BMC_04_795_1F	0.22	-0.04	-0.29	-0.18
39	BMC_04_795_1G	-0.04	-0.11	-0.29	0.02
40	BMC_04_795_1H	-0.90	-0.25	-0.56	-0.59
41	BMC_04_795_2	-0.40	-0.52	-1.30	-0.65
42	BMC_05_6782_7B	0.14	0.23	0.14	-0.15
43	BMC_05_6782_7C	0.00	0.13	0.03	-0.39

No	Name	pIC50/CPTk5	pIC50/CPTk5-SH44	pIC50/CPTk5-53	pIC50/CPTk5-2D
44	BMC_05_6782_7D	-0.35	-0.04	-0.19	-0.43
45	BMC_05_6782_7E	-0.18	0.17	0.14	0.01
46	BMC_05_6782_9C	0.12	-0.07	-0.13	0.23
47	BMC_05_6782_9D	-0.70	-0.47	-0.55	-0.23
48	BMC_05_6782_9E	-0.24	-0.25	-0.37	-0.01
49	BMC_05_6782_9F	-1.00	-0.88	-0.77	-0.73
50	BMC_05_6782_9H	-0.34	-0.15	-0.28	-0.33
51	BMC_05_6782_9I	-0.81	-0.33	-0.30	-0.13
52	BMC_05_6782_9J	-0.70	-0.27	-0.49	-0.74
53	BMC_05_6782_9K	-0.32	-0.11	-0.47	-0.02
54	BMC_05_6782_9L	-0.30	-0.49	-0.76	-0.11
55	BMC_06_3131_10B	0.74	0.51	0.79	0.33
56	BMC_06_3131_10C	0.05	0.24	0.14	0.34
57	BMC_06_3131_10F	0.40	-0.25	0.09	0.27
58	BMC_06_3131_10I	0.52	0.55	0.68	0.09
59	BMC_06_3131_10J	-0.32	-0.93	-0.01	-0.23
60	BMC_06_3131_10K	-0.28	-0.42	0.11	-0.32
61	BMC_06_3131_10L	0.52	0.47	0.35	0.27
62	BMC_06_3131_10M	0.40	0.33	0.45	0.20
63	BMC_08_8598_12	-0.32	0.42	-0.38	0.38
64	BMC_08_8598_13	-0.43	0.26	-0.28	0.99
65	BMC_08_8598_17	0.48	0.79	0.61	0.55
66	BMC_08_8598_19	0.54	0.23	0.20	0.80
67	BMC_08_8598_23	0.20	0.52	0.52	-0.18
68	BMC_09_2877_10	0.52	0.65	1.06	-0.03
69	BMC_09_2877_11	0.60	0.70	0.62	-0.14
70	BMC_09_2877_12	0.35	0.73	0.47	-0.22
71	BMC_09_2877_17	1.08	0.54	0.72	1.27
72	BMC_09_2877_18	0.85	0.71	0.58	-0.06
73	BMC_09_2877_19	0.66	0.68	0.89	0.63
74	BMC_09_2877_20	-0.36	0.54	0.51	0.10
75	BMC_09_2877_21	-0.32	0.41	0.48	-0.32
76	BMC_09_2877_22	1.52	0.65	0.97	0.10
77	BMC_09_2877_3	0.68	0.46	0.45	0.17
78	BMC_09_2877_7	2.52	0.16	-0.07	0.89
79	BMC_09_2877_8	1.48	1.23	0.90	1.16
80	BMC_09_2877_9	1.46	0.80	0.81	0.86
81	BMC_03_1475_11*	-1.61	-0.43	-0.92	-0.47
82	BMC_03_1475_7*	-0.70	-0.95	-1.40	-1.18
83	BMC_03_1809_7*	-0.93	-2.04	-0.49	-0.99
84	BMC_03_2061_3B*	-0.53	-0.86	-0.36	0.18
85	BMC_03_2061_3E*	0.05	-0.06	-0.08	0.02
86	BMC_03_3795_10B*	0.10	-0.75	-0.41	-0.57
87	BMC_03_3795_10F*	-0.04	-0.26	-0.37	-0.90
88	BMC_03_3795_4*	0.40	-0.10	0.11	0.08
89	BMC_03_521_7F*	-1.40	-1.03	-0.97	-0.99

No	Name	pIC50/CPTk5	pIC50/CPTk5-SH44	pIC50/CPTk5-53	pIC50/CPTk5-2D
90	BMC_04_3731_3C*	0.10	-0.39	-0.19	-0.81
91	BMC_04_3731_3D*	-1.08	-1.29	0.20	-0.73
92	BMC_04_3731_4A*	-0.30	-0.63	-0.14	-0.62
93	BMC_04_3731_4C*	-0.15	-0.29	-0.09	-0.62
94	BMC_04_3731_4D*	-0.90	-0.41	0.23	-0.62
95	BMC_05_6782_1*	0.05	0.03	-0.17	0.11
96	BMC_05_6782_9A*	0.00	0.13	-0.36	-0.18
97	BMC_05_6782_9B*	-0.48	-0.15	-0.48	0.13
98	BMC_06_3131_10D*	0.07	0.16	0.19	0.02
99	BMC_08_8598_16*	0.70	0.81	0.21	-0.14
100	BMC_08_8598_18*	0.46	0.37	-0.53	1.27
101	BMC_09_2877_6*	1.52	0.21	0.31	-0.05

*: external test set

Table S3. Dataset of 82 BCPs compounds with their cytotoxicity on P388 cell line: experimental pIC₅₀ value and predictive results

STT	Tên	pIC50/P388	pIC50/P388-S15	pIC50/P388-353	pIC50/P388-2D
1	BMC_03_3795_10A	0.72	0.31	0.30	0.70
2	BMC_03_3795_10C	-0.65	-0.36	-0.04	-0.20
3	BMC_03_3795_10E	-0.38	0.05	0.16	-0.23
4	BMC_03_3795_12B	0.54	0.25	0.58	0.16
5	BMC_03_3795_12D	1.00	0.96	0.92	0.53
6	BMC_03_3795_3	0.35	-0.17	0.93	1.08
7	BMC_03_3795_5	0.48	0.73	0.73	1.17
8	BMC_04_3731_2	2.70	2.29	1.84	1.87
9	BMC_04_3731_3A	0.72	0.94	0.75	0.38
10	BMC_04_3731_3B	1.52	1.25	0.77	1.44
11	BMC_04_3731_3C	1.40	1.25	0.74	0.60
12	BMC_04_3731_3D	-0.78	-0.61	0.63	0.40
13	BMC_04_3731_4A	0.46	0.88	0.58	0.60
14	BMC_04_3731_4B	1.22	1.29	0.64	1.38
15	BMC_04_3731_5	1.15	1.08	0.57	0.82
16	BMC_04_5585_15B	2.52	1.95	2.89	2.83
17	BMC_04_5585_15D	2.52	2.95	3.09	2.57
18	BMC_04_795_1B	2.70	2.53	1.91	2.46
19	BMC_04_795_1C	0.96	0.75	1.91	1.80
20	BMC_04_795_1D	2.40	2.11	1.83	1.69
21	BMC_04_795_1E	1.70	1.93	1.92	2.12
22	BMC_04_795_1F	2.52	2.28	2.03	2.45
23	BMC_04_795_1G	2.52	2.30	2.05	2.20
24	BMC_04_795_1H	1.10	2.03	1.94	1.43
25	BMC_04_795_2	1.05	1.15	1.33	1.05
26	BMC_05_6782_7A	1.40	1.21	1.28	1.03
27	BMC_05_6782_7B	1.85	1.67	1.30	1.02
28	BMC_05_6782_7C	1.70	2.08	1.37	1.14

STT	Tên	pIC50/P388	pIC50/P388-S15	pIC50/P388-353	pIC50/P388-2D
29	BMC_05_6782_7D	1.40	1.54	1.46	1.56
30	BMC_05_6782_7E	0.57	0.49	1.30	1.11
31	BMC_05_6782_9C	2.70	2.28	1.42	1.66
32	BMC_05_6782_9D	0.82	0.94	1.39	1.04
33	BMC_05_6782_9E	2.40	1.90	1.45	2.04
34	BMC_05_6782_9F	1.46	1.11	1.23	1.54
35	BMC_05_6782_9G	0.46	0.23	1.10	0.86
36	BMC_05_6782_9H	2.52	1.85	1.56	1.93
37	BMC_05_6782_9I	2.00	1.83	1.58	2.32
38	BMC_05_6782_9J	1.35	1.51	1.47	1.53
39	BMC_05_6782_9K	1.52	2.12	1.37	2.05
40	BMC_05_6782_9L	0.89	0.70	1.47	1.17
41	BMC_06_3131_10C	2.52	2.71	2.95	2.78
42	BMC_08_8598_10	1.22	1.19	1.26	0.52
43	BMC_08_8598_12	1.59	1.31	1.32	1.75
44	BMC_08_8598_13	1.00	1.10	1.55	1.55
45	BMC_08_8598_14	0.74	1.45	1.11	0.62
46	BMC_08_8598_15	1.15	1.57	1.24	0.84
47	BMC_08_8598_17	1.82	1.83	1.51	1.54
48	BMC_08_8598_19	1.40	1.06	1.30	1.31
49	BMC_08_8598_21	1.60	1.08	1.27	1.15
50	BMC_08_8598_23	1.82	1.38	1.36	1.52
51	BMC_08_8598_9	-0.60	0.87	1.08	0.42
52	BMC_09_2877_10	0.55	1.20	1.06	1.44
53	BMC_09_2877_11	1.80	1.22	1.10	1.86
54	BMC_09_2877_12	1.52	1.78	1.18	0.82
55	BMC_09_2877_14	-0.20	0.98	1.29	0.34
56	BMC_09_2877_16	0.32	0.90	1.32	0.62
57	BMC_09_2877_17	1.52	1.94	1.28	2.25
58	BMC_09_2877_18	1.42	1.62	1.09	0.91
59	BMC_09_2877_19	1.52	1.17	1.33	0.85
60	BMC_09_2877_20	-0.15	1.44	1.11	1.05
61	BMC_09_2877_21	0.39	0.13	1.16	0.64
62	BMC_09_2877_22	1.70	1.52	1.20	1.33
63	BMC_09_2877_3	2.70	2.30	2.86	2.83
64	BMC_09_2877_7	2.70	0.99	1.20	2.48
65	BMC_09_2877_8	2.30	1.82	1.26	1.50
66	BMC_09_2877_9	1.60	1.39	1.30	1.23
67	BMC_03_3795_10B*	0.80	-0.05	0.05	0.04
68	BMC_03_3795_10F*	0.44	0.01	0.18	0.01
69	BMC_03_3795_12C*	-0.42	-0.15	0.62	-0.08
70	BMC_03_3795_4*	0.64	0.68	0.91	1.08
71	BMC_04_3731_4C*	1.70	1.22	0.63	1.14
72	BMC_04_3731_4D*	-0.48	0.91	0.74	0.87
73	BMC_05_6782_1*	3.00	1.44	1.25	2.24
74	BMC_05_6782_9A*	2.52	2.00	1.39	1.58

STT	Tên	pIC50/P388	pIC50/P388-S15	pIC50/P388-353	pIC50/P388-2D
75	BMC_05_6782_9B*	3.15	2.38	1.45	1.66
76	BMC_08_8598_11*	0.92	0.97	1.08	2.50
77	BMC_08_8598_16*	1.85	1.53	1.28	1.60
78	BMC_08_8598_18*	1.40	1.87	1.10	2.19
79	BMC_08_8598_20*	1.46	0.99	1.24	0.35
80	BMC_08_8598_22*	0.01	1.04	1.30	0.59
81	BMC_09_2877_15*	1.52	1.17	1.31	1.16
82	BMC_09_2877_6*	1.52	1.13	1.07	0.52

*: external test set

Table S4. Dataset of 73 BCPs compounds with their cytotoxicity on CPT45 cell line: experimental pIC₅₀ value and predictive results

No	Name	pIC50/CPT45	pIC50/CPT45-S53	pIC50/CPT45-199	pIC50/CPT45-2D
1	BMC_03_3795_10A	0.74	-0.03	-0.90	0.20
2	BMC_03_3795_10C	-1.34	-0.31	-0.94	-0.47
3	BMC_03_3795_10E	-1.28	-0.23	-1.02	-0.70
4	BMC_03_3795_12B	0.28	0.19	0.63	0.49
5	BMC_03_3795_12D	0.74	0.61	0.52	0.40
6	BMC_03_3795_3	0.34	-0.05	0.81	0.80
7	BMC_04_3731_2	0.44	0.49	0.58	0.91
8	BMC_04_3731_3A	-0.32	0.30	-0.11	0.12
9	BMC_04_3731_3B	0.47	0.32	0.38	0.08
10	BMC_04_3731_3D	-0.85	-0.97	-0.03	-0.24
11	BMC_04_3731_4A	0.68	0.19	0.32	0.10
12	BMC_04_3731_4B	0.64	0.34	0.23	0.13
13	BMC_04_3731_5	0.52	0.31	0.26	0.41
14	BMC_04_5585_15B	1.70	1.03	1.56	1.37
15	BMC_04_5585_15D	0.64	0.94	1.24	0.15
16	BMC_04_795_1B	0.55	0.40	0.45	0.40
17	BMC_04_795_1C	0.25	-0.39	0.58	0.74
18	BMC_04_795_1D	-0.08	0.42	0.62	0.17
19	BMC_04_795_1E	-0.26	-0.22	0.50	-0.10
20	BMC_04_795_1F	0.59	0.40	0.41	0.30
21	BMC_04_795_1G	0.57	0.35	0.30	-0.01
22	BMC_04_795_1H	-0.04	0.18	-0.09	0.34
23	BMC_04_795_2	0.96	0.16	0.53	0.85
24	BMC_05_6782_7A	-0.51	0.94	0.92	0.28
25	BMC_05_6782_7B	1.48	1.23	1.02	0.74
26	BMC_05_6782_7C	1.70	1.31	1.04	0.40
27	BMC_05_6782_7D	0.89	0.88	1.07	-0.16
28	BMC_05_6782_7E	0.60	0.62	0.96	0.39
29	BMC_05_6782_9C	0.27	0.57	0.52	0.85
30	BMC_05_6782_9D	0.52	0.01	0.38	0.53
31	BMC_05_6782_9E	0.43	0.12	0.41	0.58
32	BMC_05_6782_9F	-0.44	-0.05	-0.39	0.51

No	Name	pIC50/CPT45	pIC50/CPT45-S53	pIC50/CPT45-199	pIC50/CPT45-2D
33	BMC_05_6782_9G	-0.81	-0.66	-1.00	-0.18
34	BMC_05_6782_9H	0.48	0.25	0.37	-0.11
35	BMC_05_6782_9I	0.00	0.02	0.26	-0.47
36	BMC_05_6782_9J	-0.13	-0.02	-0.13	0.37
37	BMC_05_6782_9K	0.47	0.50	0.67	1.06
38	BMC_05_6782_9L	-0.42	-0.84	0.09	0.30
39	BMC_06_3131_10C	1.52	1.32	1.38	0.99
40	BMC_08_8598_12	0.52	0.59	0.73	1.07
41	BMC_08_8598_13	-0.30	0.47	0.12	0.92
42	BMC_08_8598_14	-1.00	0.28	0.49	0.33
43	BMC_08_8598_17	0.74	0.88	0.16	0.28
44	BMC_08_8598_19	0.70	0.74	0.71	0.23
45	BMC_08_8598_23	0.59	0.56	0.26	0.98
46	BMC_09_2877_10	0.54	0.91	0.73	0.35
47	BMC_09_2877_11	0.52	0.98	0.75	0.40
48	BMC_09_2877_12	0.52	1.15	0.71	0.46
49	BMC_09_2877_17	1.43	1.17	1.03	1.19
50	BMC_09_2877_18	1.00	0.91	0.70	0.16
51	BMC_09_2877_19	1.22	1.09	0.94	1.48
52	BMC_09_2877_20	-0.32	0.64	0.63	-0.17
53	BMC_09_2877_21	0.29	1.22	0.58	0.48
54	BMC_09_2877_22	1.62	0.73	0.76	1.84
55	BMC_09_2877_3	1.82	1.42	1.51	1.51
56	BMC_09_2877_7	2.70	0.74	0.90	1.67
57	BMC_09_2877_8	1.82	1.68	1.10	1.76
58	BMC_09_2877_9	1.60	1.27	0.82	0.57
59	BMC_03_3795_10B*	0.60	-0.28	-0.92	-0.48
60	BMC_03_3795_10F*	0.05	-0.11	-1.04	-0.49
61	BMC_03_3795_12C*	-0.42	0.04	0.67	0.54
62	BMC_03_3795_4*	0.59	0.42	0.81	1.03
63	BMC_04_3731_3C*	0.70	0.30	0.36	-0.07
64	BMC_04_3731_4C*	0.48	0.26	0.21	0.00
65	BMC_04_3731_4D*	-0.54	-0.19	0.26	-0.29
66	BMC_05_6782_1*	0.64	0.34	0.50	1.15
67	BMC_05_6782_9A*	0.49	0.65	0.53	1.09
68	BMC_05_6782_9B*	0.11	0.65	0.53	0.72
69	BMC_08_8598_11*	-1.00	0.46	0.68	1.69
70	BMC_08_8598_16*	0.74	0.72	0.72	0.33
71	BMC_08_8598_18*	0.46	0.67	0.72	1.15
72	BMC_09_2877_15*	0.52	0.88	0.70	0.34
73	BMC_09_2877_6*	1.52	0.94	0.90	0.20

*: external test set

Table S5. Dataset of 83 BCPs compounds with their cytotoxicity on KB3-1 cell line: experimental pIC₅₀ value and predictive results

No	Name	pIC ₅₀ /KB3	pIC ₅₀ /KB3-S34	pIC ₅₀ /KB3-E12	pIC ₅₀ /KB3-H34	pIC ₅₀ /KB3-EH32	pIC ₅₀ /KB3-61	pIC ₅₀ /KB3-2D
1	BMC_03_1475_11	-1.76	-0.25	-0.27	-0.73	-0.36	-0.43	-0.39
2	BMC_03_1475_12	0.41	-0.24	-0.83	-0.80	-0.79	-0.49	-0.02
3	BMC_03_1475_14	-1.00	-0.48	-0.20	-1.17	-0.44	-0.62	-0.35
4	BMC_03_1475_15	0.68	0.16	-0.29	0.23	-0.18	-0.15	-0.08
5	BMC_03_1475_2B	-1.08	-1.25	-1.57	-1.20	-1.42	0.34	0.29
6	BMC_03_1475_5	-0.81	-0.05	-0.39	-0.21	-0.38	-0.68	-1.17
7	BMC_03_1475_6	-1.43	-0.79	-1.27	-0.79	-1.15	-0.55	-0.34
8	BMC_03_1475_7	-0.51	0.18	-0.07	-0.34	-0.19	-0.57	-1.11
9	BMC_03_1475_8	-0.52	0.13	-0.09	-0.22	-0.16	-0.60	-1.39
10	BMC_03_1475_9	-1.45	-1.64	-1.49	-1.63	-1.43	-0.63	-0.87
11	BMC_03_3795_10A	0.80	0.07	0.83	0.58	0.60	0.34	0.32
12	BMC_03_3795_10C	-0.85	-0.35	0.06	-0.29	-0.17	-0.02	-0.09
13	BMC_03_3795_10D	0.74	0.79	0.78	0.77	0.61	0.31	0.38
14	BMC_03_3795_10E	-0.48	-0.19	0.22	0.15	0.07	0.13	0.71
15	BMC_03_3795_12B	0.64	-0.22	0.49	-0.06	0.33	0.32	-0.65
16	BMC_03_3795_12D	0.72	1.00	0.90	0.90	0.80	0.31	0.19
17	BMC_03_3795_3	-0.74	-1.35	-1.59	-0.88	-1.36	0.38	0.13
18	BMC_03_3795_5	1.30	0.24	0.17	-0.07	0.05	-0.34	0.39
19	BMC_04_5585_15B	2.52	1.84	1.71	2.13	2.06	2.12	1.76
20	BMC_04_5585_15D	2.22	2.22	2.03	2.32	2.07	2.47	1.96
21	BMC_05_6782_7A	1.22	0.93	1.13	0.81	0.88	1.02	1.48
22	BMC_05_6782_7B	1.47	1.40	1.13	1.16	1.05	1.10	1.13
23	BMC_05_6782_7C	1.26	1.87	1.05	1.20	0.96	1.21	1.25
24	BMC_05_6782_7D	1.35	1.12	1.20	1.43	1.18	1.33	1.35
25	BMC_05_6782_7E	0.33	0.53	0.95	0.74	0.87	1.14	0.93
26	BMC_05_6782_9C	2.22	1.69	1.55	1.71	1.61	1.04	1.57
27	BMC_05_6782_9D	0.35	0.55	0.92	0.84	0.91	0.98	1.08
28	BMC_05_6782_9E	1.52	1.46	1.47	1.41	1.50	1.08	1.70
29	BMC_05_6782_9F	1.22	0.95	1.04	1.22	1.01	0.61	0.59
30	BMC_05_6782_9G	0.30	0.40	1.15	0.42	1.04	0.18	0.55
31	BMC_05_6782_9H	2.52	1.61	1.49	1.55	1.58	1.21	1.70
32	BMC_05_6782_9I	1.74	1.57	1.50	1.50	1.57	1.25	2.05
33	BMC_05_6782_9J	1.00	1.45	1.49	1.19	1.56	1.42	1.72
34	BMC_05_6782_9K	1.35	1.90	1.25	1.32	1.33	1.05	1.26
35	BMC_05_6782_9L	0.60	0.23	0.88	0.61	0.89	1.23	1.33
36	BMC_06_3131_10B	2.22	2.13	1.98	2.03	1.92	2.28	1.77
37	BMC_06_3131_10C	2.52	2.22	2.05	2.18	1.99	2.31	2.20
38	BMC_06_3131_10F	2.40	2.23	2.03	2.28	2.08	2.58	1.76
39	BMC_06_3131_10G	1.35	2.10	1.93	2.18	2.08	2.25	1.96
40	BMC_06_3131_10I	1.52	1.97	2.02	2.00	1.97	2.45	2.04
41	BMC_06_3131_10J	1.40	1.55	1.15	1.73	1.42	1.53	1.50
42	BMC_06_3131_10K	1.42	1.36	2.00	1.70	1.90	1.86	0.90
43	BMC_06_3131_10L	2.40	1.45	1.99	1.97	2.11	2.10	1.75

No	Name	pIC50/KB3	pIC50 /KB3-S34	pIC50 /KB3-E12	pIC50 /KB3-H34	pIC50 /KB3-EH32	pIC50 /KB3-61	pIC50 /KB3-2D
44	BMC_06_3131_10M	2.22	1.84	2.00	1.92	2.02	2.17	2.02
45	BMC_08_8598_10	0.82	0.81	1.04	0.90	1.07	0.95	0.44
46	BMC_08_8598_12	1.52	1.02	1.28	1.52	1.47	1.02	1.10
47	BMC_08_8598_13	1.22	1.25	1.54	1.26	1.93	1.34	1.19
48	BMC_08_8598_14	0.74	0.90	0.98	0.79	0.85	0.90	0.99
49	BMC_08_8598_15	0.82	1.28	0.72	1.04	0.94	1.13	1.06
50	BMC_08_8598_17	1.68	1.69	1.47	1.59	1.92	1.28	1.21
51	BMC_08_8598_19	1.46	1.60	0.85	1.08	0.71	1.09	1.16
52	BMC_08_8598_21	0.64	1.04	1.34	0.99	1.14	0.94	0.88
53	BMC_08_8598_23	1.57	1.34	1.53	1.45	1.36	1.06	1.47
54	BMC_09_2877_10	0.52	1.23	1.02	1.04	1.03	1.04	1.70
55	BMC_09_2877_11	1.30	1.26	1.29	1.47	1.31	1.08	1.14
56	BMC_09_2877_12	1.60	1.83	1.16	1.57	1.21	1.08	1.05
57	BMC_09_2877_14	-0.18	0.79	1.14	1.06	1.17	0.85	1.24
58	BMC_09_2877_16	0.22	0.96	1.10	0.95	0.89	0.87	0.50
59	BMC_09_2877_17	0.80	0.92	0.89	1.21	0.85	0.82	1.25
60	BMC_09_2877_18	1.40	1.56	0.94	1.52	1.18	1.00	1.16
61	BMC_09_2877_19	0.49	0.37	0.89	0.42	0.50	0.80	1.01
62	BMC_09_2877_20	0.40	1.53	1.35	1.30	1.11	1.13	0.92
63	BMC_09_2877_21	0.77	0.52	0.96	0.90	1.15	1.34	1.13
64	BMC_09_2877_22	1.60	1.55	1.26	1.78	1.67	1.08	1.34
65	BMC_09_2877_3	2.52	2.00	2.03	2.08	2.00	2.25	1.65
66	BMC_09_2877_7	2.40	0.66	1.27	0.74	1.02	0.80	1.31
67	BMC_09_2877_8	1.52	1.29	1.04	1.12	1.21	0.99	0.88
68	BMC_09_2877_9*	1.52	0.97	1.15	1.17	1.05	0.81	1.64
69	BMC_03_3795_10B*	0.52	-0.36	-0.04	-0.29	-0.19	-0.06	-0.46
70	BMC_03_3795_10F*	0.12	-0.19	0.36	0.21	0.13	0.11	0.35
71	BMC_03_3795_12C*	-1.11	-0.22	-0.03	-0.15	-0.07	0.25	-0.28
72	BMC_03_3795_4*	0.52	0.28	0.94	0.63	0.76	0.40	0.13
73	BMC_05_6782_1*	2.30	0.99	0.97	0.92	1.06	2.23	1.01
74	BMC_05_6782_9A*	2.30	1.71	1.50	1.59	1.55	1.00	1.46
75	BMC_05_6782_9B*	2.52	1.82	1.38	1.60	1.51	1.02	1.58
76	BMC_06_3131_10D*	2.70	2.12	2.02	2.21	2.05	2.43	2.20
77	BMC_08_8598_11*	0.89	0.63	1.12	0.83	0.89	0.75	1.31
78	BMC_08_8598_16*	1.70	1.29	0.87	1.47	1.08	1.11	1.14
79	BMC_08_8598_18*	1.52	1.38	0.87	1.36	0.72	0.90	1.26
80	BMC_08_8598_20*	1.26	0.77	1.33	1.10	1.20	0.96	1.24
81	BMC_08_8598_22*	-0.08	1.16	1.35	1.10	1.13	0.94	0.51
82	BMC_09_2877_15*	1.51	0.98	1.15	1.02	1.05	0.87	0.88
83	BMC_09_2877_6*	1.35	0.87	1.05	0.77	0.95	0.99	0.44

*: external test set

Table S6. Dataset of 81 BCPs compounds with their cytotoxicity on KBV-1 cell line: experimental pIC₅₀ value and predictive results

No	Name	pIC50/KBV	pIC50/KBV-S34	pIC50/KBV-71	pIC50/KBV-2D
1	BMC_03_1475_12	0.19	0.16	-0.20	0.53
2	BMC_03_1475_15	0.77	0.27	-0.04	1.48
3	BMC_03_1475_2B	-1.28	-1.01	0.18	-0.37
4	BMC_03_1475_5	-0.54	0.04	-0.32	-0.75
5	BMC_03_1475_6	-1.46	-0.91	-0.39	-1.21
6	BMC_03_1475_8	-0.40	0.11	-0.37	-0.85
7	BMC_03_1475_9	-1.88	-2.06	-1.02	-1.11
8	BMC_03_3795_10A	0.62	0.30	0.68	0.13
9	BMC_03_3795_10C	-0.34	0.21	0.49	0.20
10	BMC_03_3795_10D	0.62	0.66	0.05	-0.20
11	BMC_03_3795_10E	0.52	0.24	0.63	0.84
12	BMC_03_3795_12B	0.57	0.20	0.27	0.33
13	BMC_03_3795_12D	0.60	0.62	-0.43	-0.18
14	BMC_03_3795_3	-0.26	-1.03	0.20	0.45
15	BMC_03_3795_5	0.92	0.27	-0.22	0.52
16	BMC_04_5585_15B	2.15	1.09	1.52	0.93
17	BMC_05_6782_7A	0.51	0.48	0.58	0.81
18	BMC_05_6782_7B	0.66	0.49	0.55	0.55
19	BMC_05_6782_7C	1.00	0.87	0.58	0.37
20	BMC_05_6782_7D	0.64	0.54	0.66	0.32
21	BMC_05_6782_7E	-0.36	-0.17	0.58	-0.18
22	BMC_05_6782_9C	0.96	0.93	0.20	0.21
23	BMC_05_6782_9D	-0.26	0.07	0.15	-0.33
24	BMC_05_6782_9E	0.33	0.22	0.27	0.81
25	BMC_05_6782_9F	0.17	0.01	-0.42	0.20
26	BMC_05_6782_9G	-0.90	-0.92	-0.88	-0.24
27	BMC_05_6782_9H	0.82	0.21	0.21	0.41
28	BMC_05_6782_9I	0.74	0.01	0.33	0.42
29	BMC_05_6782_9J	-0.88	-0.22	-0.10	0.24
30	BMC_05_6782_9K	-0.65	0.58	0.26	-0.25
31	BMC_05_6782_9L	-0.30	-0.36	0.03	0.10
32	BMC_06_3131_10B	1.82	1.46	1.51	1.44
33	BMC_06_3131_10C	1.92	1.52	1.60	2.06
34	BMC_06_3131_10F	1.64	1.19	1.70	1.46
35	BMC_06_3131_10G	0.92	1.25	1.40	0.97
36	BMC_06_3131_10I	1.05	1.38	1.48	1.49
37	BMC_06_3131_10J	0.60	0.57	0.56	0.00
38	BMC_06_3131_10K	0.92	0.96	0.97	0.57
39	BMC_06_3131_10L	1.80	1.02	1.60	0.96
40	BMC_06_3131_10M	1.19	1.28	1.56	1.41
41	BMC_08_8598_10	0.40	0.49	0.40	0.68
42	BMC_08_8598_13	0.60	0.63	0.54	1.17
43	BMC_08_8598_14	0.35	0.46	0.05	-0.09

No	Name	pIC50/KBV	pIC50/KBV-S34	pIC50/KBV-71	pIC50/KBV-2D
44	BMC_08_8598_15	0.44	0.62	0.51	0.24
45	BMC_08_8598_19	0.40	0.68	0.51	0.39
46	BMC_08_8598_21	0.38	0.59	0.08	0.19
47	BMC_08_8598_23	-0.15	0.33	0.02	0.22
48	BMC_09_2877_10	0.36	0.86	0.52	0.60
49	BMC_09_2877_11	0.30	0.91	0.47	0.36
50	BMC_09_2877_12	1.10	1.29	0.48	0.48
51	BMC_09_2877_16	0.15	0.64	0.24	0.05
52	BMC_09_2877_17	0.43	0.33	0.28	0.90
53	BMC_09_2877_18	0.30	0.87	0.45	-0.24
54	BMC_09_2877_19	0.40	0.00	0.34	0.30
55	BMC_09_2877_20	-0.60	0.56	0.47	-0.23
56	BMC_09_2877_21	-0.28	-0.22	0.44	0.39
57	BMC_09_2877_22	1.57	0.57	0.39	1.54
58	BMC_09_2877_7	1.80	0.47	0.33	1.06
59	BMC_09_2877_8	0.77	0.49	0.54	1.04
60	BMC_09_2877_9	-0.25	0.49	0.18	0.04
61	BMC_03_1475_11*	-2.30	0.21	-0.15	0.46
62	BMC_03_1475_7*	-0.40	0.23	-0.32	-1.20
63	BMC_03_3795_10B*	0.40	0.21	0.53	0.21
64	BMC_03_3795_10F*	0.44	0.24	0.63	0.93
65	BMC_03_3795_12C*	-0.36	0.15	0.22	0.36
66	BMC_03_3795_4*	0.70	0.27	0.20	0.46
67	BMC_04_5585_15D*	2.22	1.28	1.65	0.76
68	BMC_05_6782_1*	2.30	0.31	1.18	0.90
69	BMC_05_6782_9A*	0.66	0.64	0.21	0.36
70	BMC_05_6782_9B*	0.49	0.81	0.21	0.64
71	BMC_06_3131_10D*	2.40	1.30	1.54	1.49
72	BMC_08_8598_11*	0.52	0.37	0.20	0.67
73	BMC_08_8598_12*	0.80	0.55	0.44	0.22
74	BMC_08_8598_16*	0.30	0.64	0.43	-0.07
75	BMC_08_8598_17*	1.22	0.73	0.57	0.90
76	BMC_08_8598_18*	0.48	0.47	0.13	0.78
77	BMC_08_8598_20*	0.40	0.50	0.06	0.14
78	BMC_08_8598_22*	-0.60	0.64	0.04	-0.30
79	BMC_09_2877_15*	1.00	0.61	0.27	0.23
80	BMC_09_2877_3*	2.40	1.35	1.54	0.85
81	BMC_09_2877_6*	1.12	0.56	0.39	0.93

*: external test set

Table S7. Dataset of 60 BCPs compounds with their cytotoxicity on KBH5.0 cell line: experimental pIC₅₀ value and predictive results

No	Name	pIC ₅₀ /KBH	pIC ₅₀ /KBH-CoMFAS43	pIC ₅₀ /KBH-S43	pIC ₅₀ /KBH-59	pIC ₅₀ /KBH-2D
1	BMC_04_5585_15B	2.40	1.60	1.45	1.91	1.65
2	BMC_04_5585_15D	2.15	1.79	1.68	1.86	1.69
3	BMC_05_6782_7A	0.92	0.94	0.82	0.98	1.03
4	BMC_05_6782_7B	1.14	1.09	0.95	0.97	0.78
5	BMC_05_6782_7C	1.19	1.13	1.26	0.93	0.75
6	BMC_05_6782_7D	0.96	0.94	0.97	0.83	0.72
7	BMC_05_6782_7E	0.28	0.40	0.26	0.93	0.83
8	BMC_05_6782_9C	1.30	1.39	1.32	0.78	1.44
9	BMC_05_6782_9D	0.05	0.12	0.43	0.60	0.69
10	BMC_05_6782_9E	1.15	0.76	0.68	0.80	1.13
11	BMC_05_6782_9F	0.46	0.46	0.51	-0.11	-0.10
12	BMC_05_6782_9G	-0.81	-0.98	-0.61	-0.74	-0.55
13	BMC_05_6782_9H	1.30	0.93	0.68	0.86	1.16
14	BMC_05_6782_9I	1.40	0.82	0.51	0.88	1.21
15	BMC_05_6782_9J	-0.18	0.29	0.32	0.29	0.10
16	BMC_05_6782_9K	0.30	0.92	1.17	0.82	1.34
17	BMC_05_6782_9L	0.19	-0.01	0.11	0.38	0.85
18	BMC_06_3131_10B	2.05	1.87	1.73	1.70	1.76
19	BMC_06_3131_10C	2.30	2.13	1.87	1.79	1.61
20	BMC_06_3131_10F	1.66	1.66	1.60	1.84	1.66
21	BMC_06_3131_10G	0.82	1.59	1.62	1.63	0.93
22	BMC_06_3131_10I	1.30	1.44	1.63	1.67	1.84
23	BMC_06_3131_10J	0.77	1.00	0.84	0.70	0.58
24	BMC_06_3131_10K	1.15	1.23	1.22	1.07	0.72
25	BMC_06_3131_10L	1.70	1.19	1.26	1.96	1.68
26	BMC_06_3131_10M	1.07	1.70	1.56	1.88	1.57
27	BMC_08_8598_10	0.40	0.53	0.54	0.55	0.45
28	BMC_08_8598_12	0.68	0.62	0.57	0.62	0.96
29	BMC_08_8598_13	0.54	0.57	0.57	0.53	0.24
30	BMC_08_8598_14	0.38	0.48	0.49	0.84	0.83
31	BMC_08_8598_15	0.49	0.58	0.58	0.59	0.46
32	BMC_08_8598_19	0.89	0.95	0.90	0.60	0.53
33	BMC_08_8598_21	0.32	0.64	0.63	0.69	1.00
34	BMC_08_8598_23	0.70	0.68	0.58	0.58	0.99
35	BMC_09_2877_10	0.31	0.91	1.14	0.69	0.46
36	BMC_09_2877_11	0.70	0.99	1.19	0.72	0.93
37	BMC_09_2877_12	1.15	1.63	1.64	0.77	0.51
38	BMC_09_2877_16	0.42	0.58	0.92	0.80	0.53
39	BMC_09_2877_17	0.54	0.67	0.77	1.01	1.07
40	BMC_09_2877_18	0.74	1.31	1.25	0.63	0.81
41	BMC_09_2877_19	0.49	0.30	0.26	1.02	0.98
42	BMC_09_2877_20	0.02	0.80	0.95	0.67	0.86
43	BMC_09_2877_21	0.26	0.05	0.30	0.46	0.52

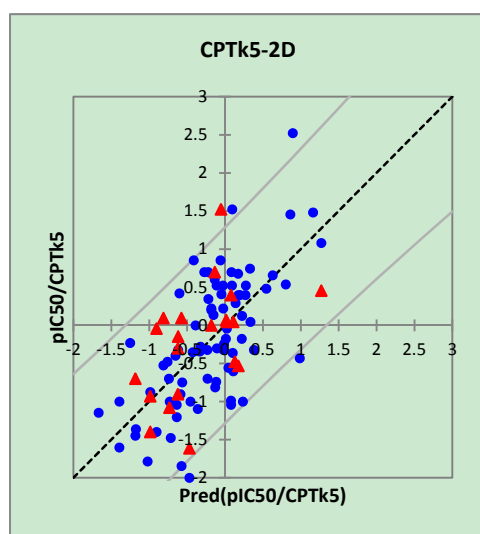
No	Name	pIC50/KBH	pIC50 /KBH-CoMFAS43	pIC50 /KBH-S43	pIC50 /KBH-59	pIC50 /KBH-2D
44	BMC_09_2877_22	1.42	1.06	0.99	0.65	0.40
45	BMC_09_2877_3	2.40	1.88	1.68	1.79	1.52
46	BMC_09_2877_7	1.72	0.88	0.73	1.12	1.32
47	BMC_09_2877_8	1.22	0.88	0.87	0.66	0.89
48	BMC_09_2877_9	1.40	0.88	0.89	1.04	0.87
49	BMC_05_6782_1*	2.22	0.50	0.44	1.43	1.47
50	BMC_05_6782_9A*	1.22	1.22	1.10	0.78	1.03
51	BMC_05_6782_9B*	1.70	1.28	1.27	0.77	1.36
52	BMC_06_3131_10D*	2.40	1.76	1.66	1.85	1.64
53	BMC_08_8598_11*	0.54	0.78	0.58	0.94	1.27
54	BMC_08_8598_16*	0.96	0.66	0.61	0.64	0.93
55	BMC_08_8598_17*	1.40	0.67	0.63	0.66	-0.05
56	BMC_08_8598_18*	1.15	0.52	0.64	0.82	1.02
57	BMC_08_8598_20*	-0.43	0.55	0.55	0.77	1.55
58	BMC_08_8598_22*	-0.56	0.56	0.59	0.60	0.49
59	BMC_09_2877_15*	1.10	0.82	0.90	0.89	1.04
60	BMC_09_2877_6*	1.10	0.88	0.82	0.81	0.45

*: External test set

Table S8. Dataset of 94 BCPs compounds with experimental topoisomerase-1 inhibitory value and predictive results

No	Name	pIC50/TOP1	pIC50/TOP1-E34	pIC50/TOP1-H64	pIC50/TOP1-307	pIC50/TOP1-2D
1	BMC_03_1475_12	-1.78	-2.11	-2.31	-1.68	-1.38
2	BMC_03_1475_14	-2.30	-2.32	-2.61	-1.71	-2.09
3	BMC_03_1475_15	-1.30	-1.26	-1.12	-1.71	-0.74
4	BMC_03_1475_2B	-1.30	-2.15	-1.92	-0.62	-1.63
5	BMC_03_1475_5	-1.30	-1.30	-1.64	-2.01	-2.14
6	BMC_03_1475_8	-2.00	-1.03	-1.43	-1.76	-0.94
7	BMC_03_1809_6	-2.20	-1.99	-1.75	-1.48	-1.91
8	BMC_03_3795_10A	-0.90	-1.45	-1.25	-1.58	-1.25
9	BMC_03_3795_10C	-2.30	-2.30	-2.36	-2.08	-1.82
10	BMC_03_3795_10E	-2.70	-1.98	-1.88	-1.78	-1.68
11	BMC_03_3795_3	-2.00	-2.36	-1.98	-0.79	-1.42
12	BMC_03_3795_5	-0.90	-0.99	-1.35	-1.20	-0.82
13	BMC_03_521_7C	-2.20	-1.17	-1.11	-1.66	-1.66
14	BMC_03_521_7G	-0.60	-1.22	-1.04	-1.39	-1.82
15	BMC_04_3731_2	0.52	0.05	0.20	-0.58	-0.57
16	BMC_04_3731_3A	-0.95	-0.89	-1.03	-0.79	-1.59
17	BMC_04_3731_3B	-0.78	-0.71	-1.00	-1.02	-0.83
18	BMC_04_3731_4A	-2.00	-1.11	-1.42	-1.19	-1.47
19	BMC_04_3731_4B	-1.08	-0.60	-0.82	-1.15	-0.71
20	BMC_04_3731_5	-1.00	-0.82	-1.09	-1.26	-1.23
21	BMC_04_5585_15B	0.22	0.31	0.36	0.36	0.38
22	BMC_04_5585_15D	1.70	0.29	-0.11	0.55	-0.21
23	BMC_04_795_1B	0.52	0.05	0.21	-0.44	0.12
24	BMC_04_795_1C	-2.00	-1.92	-1.07	-0.65	-0.48
25	BMC_04_795_1D	0.30	-0.02	-0.29	-0.37	0.24
26	BMC_04_795_1F	0.70	-0.12	-0.03	-0.34	-0.20
27	BMC_04_795_1G	-0.30	-0.18	-0.08	-0.29	-0.38
28	BMC_04_795_1H	-1.30	-0.44	-0.73	-0.71	-0.94
29	BMC_04_795_2	-1.00	-1.27	-1.15	-1.39	-0.80
30	BMC_05_6782_7A	-1.00	-0.52	-0.81	-0.63	-0.72
31	BMC_05_6782_7B	-0.70	-0.12	-0.47	-0.70	-0.37
32	BMC_05_6782_7C	0.00	0.21	-0.46	-0.77	-0.67
33	BMC_05_6782_7D	-0.90	-1.18	-0.45	-0.94	-0.54
34	BMC_05_6782_7E	-0.81	-0.98	-0.80	-0.66	-0.58
35	BMC_05_6782_9C	0.40	-0.18	-0.06	-0.09	0.15
36	BMC_05_6782_9D	-1.00	-0.94	-0.44	-0.18	-0.50
37	BMC_05_6782_9E	0.15	-0.43	-0.48	-0.06	0.66
38	BMC_05_6782_9F	-1.08	-1.06	-0.17	-1.30	-1.48
39	BMC_05_6782_9G	-1.78	-1.85	-1.54	-2.36	-1.79
40	BMC_05_6782_9H	0.22	-0.05	-0.11	0.04	0.58
41	BMC_05_6782_9I	-0.18	-0.15	-0.23	0.09	0.28
42	BMC_05_6782_9J	0.52	-0.09	0.37	-0.33	-0.21

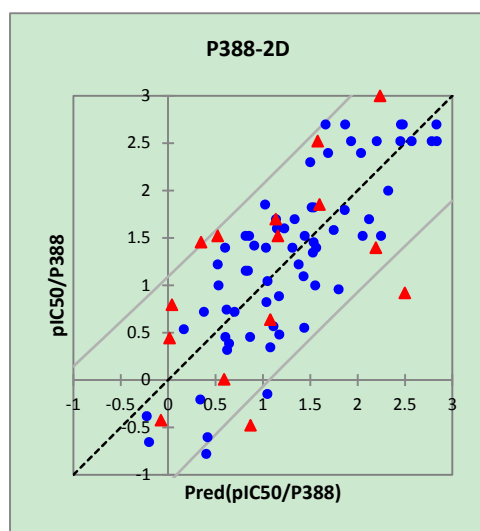
No	Name	pIC50/TOP1	pIC50/TOP1-E34	pIC50/TOP1-H64	pIC50/TOP1-307	pIC50/TOP1-2D
43	BMC_05_6782_9K	-0.70	0.05	-0.44	-0.15	0.34
44	BMC_05_6782_9L	-0.48	-0.86	-0.50	-0.29	-0.61
45	BMC_06_3131_10B	-0.08	0.49	0.33	0.38	0.21
46	BMC_06_3131_10C	0.70	0.39	0.17	0.40	0.73
47	BMC_06_3131_10F	-0.48	0.14	-0.19	0.60	-0.37
48	BMC_06_3131_10G	-0.95	0.28	0.28	0.23	-0.38
49	BMC_06_3131_10I	0.35	0.32	0.33	0.60	0.00
50	BMC_06_3131_10K	-1.11	-0.60	-0.63	-0.86	-1.01
51	BMC_06_3131_10L	0.46	0.18	0.53	0.32	0.36
52	BMC_06_3131_10M	0.82	0.37	0.40	0.30	0.50
53	BMC_08_8598_10	0.70	-0.18	-0.01	0.08	-0.67
54	BMC_08_8598_12	0.70	0.09	1.06	0.10	0.33
55	BMC_08_8598_13	0.70	0.40	0.60	0.67	0.30
56	BMC_08_8598_17	0.40	0.69	0.85	0.77	-0.15
57	BMC_08_8598_19	0.10	0.45	-0.22	0.19	-0.30
58	BMC_08_8598_21	0.10	0.12	0.44	0.40	-0.03
59	BMC_08_8598_23	0.70	0.10	0.98	0.35	0.63
60	BMC_09_2877_10	-0.89	-0.05	-0.54	-0.21	-0.48
61	BMC_09_2877_11	0.52	0.02	-0.03	-0.27	0.24
62	BMC_09_2877_12	0.30	0.25	-0.16	-0.24	-0.24
63	BMC_09_2877_14	0.10	-0.38	-0.31	-0.24	0.13
64	BMC_09_2877_16	-0.04	-0.34	-0.45	-0.09	-0.55
65	BMC_09_2877_17	-0.89	-0.73	-0.97	-0.79	-0.52
66	BMC_09_2877_18	-1.00	0.01	-0.31	-0.32	-0.50
67	BMC_09_2877_19	-1.18	-1.13	-1.09	-0.79	-0.64
68	BMC_09_2877_20	0.70	0.14	-0.40	-0.21	-0.29
69	BMC_09_2877_21	-0.96	-0.89	-0.42	-0.18	-0.13
70	BMC_09_2877_22	-0.28	0.08	0.06	-0.40	0.65
71	BMC_09_2877_3	0.22	0.39	0.41	0.26	0.07
72	BMC_09_2877_7	-0.67	-0.52	-0.55	-0.58	-0.60
73	BMC_09_2877_8	-0.04	-0.08	-0.73	-0.21	-0.35
74	BMC_09_2877_9	-0.96	-0.38	-0.62	-0.78	-1.07
75	BMC_03_1475_11*	-3.00	-1.81	-2.12	-1.74	-1.15
76	BMC_03_1475_7*	-1.30	-0.99	-1.44	-1.80	-0.75
77	BMC_03_1809_7*	-2.30	-2.31	-1.99	-1.36	-1.91
78	BMC_03_3795_10B*	-2.30	-2.07	-2.35	-2.04	-1.83
79	BMC_03_3795_10F*	-1.00	-1.73	-1.80	-1.73	-1.66
80	BMC_03_3795_12C*	-2.00	-2.07	-1.85	-1.25	-2.00
81	BMC_03_3795_4*	-1.00	-0.95	-0.82	-0.78	-1.44
82	BMC_03_521_7F*	-1.30	-1.20	-0.94	-1.36	-1.60
83	BMC_04_3731_3C*	-0.30	-0.88	-1.10	-1.06	-0.98
84	BMC_04_3731_4C*	-0.78	-0.87	-1.12	-1.11	-0.86
85	BMC_04_795_1E*	-0.70	-0.98	-1.22	-0.18	-0.93
86	BMC_05_6782_1*	0.52	-0.51	-0.79	-0.60	0.01
87	BMC_05_6782_9A*	0.30	-0.03	-0.15	-0.18	0.49
88	BMC_05_6782_9B*	0.22	-0.15	-0.31	-0.22	0.15



The relationship between observed and predicted data from QSAR model and its 95% confidence interval of CPTk5 cell line

Model 3. 2D QSAR on P388

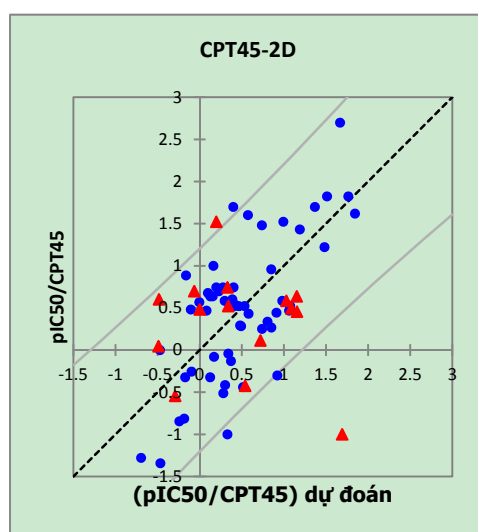
No	Descriptor	1	2	3	4	5	6	7	8	9	10	Y=	p
1	diameter	1,00										0,566	0,808 0,000
2	petitjean	0,10	1,00									-7,136	-0,251 0,014
3	GCUT_SLOGP_0	0,05	0,04	1,00								1,051	0,338 0,001
4	a_nO	0,28	-0,05	0,30	1,00							-2,683	-26,447 0,000
5	PEOE_VSA+3	0,30	0,14	-0,11	0,19	1,00						-0,147	-14,915 0,000
6	PEOE_VSA-0	0,23	-0,22	0,13	0,11	0,08	1,00					0,022	6,890 0,000
7	PEOE_VSA_NEG	0,51	-0,21	0,29	0,17	-0,12	0,64	1,00				0,112	37,212 0,000
5	vsa_acc	0,15	0,07	0,25	0,39	0,02	0,03	0,28	1,00			0,419	45,254 0,000
9	vsa_other	0,15	-0,02	0,33	0,84	0,17	-0,07	0,12	0,32	1,00		0,147	18,039 0,000
10	SlogP	0,58	-0,11	0,21	0,16	0,26	0,18	0,44	-0,34	0,06	1,00	-1,681	-15,893 0,000
coff												-15,908	



The relationship between observed and predicted data from QSAR model and its 95% confidence interval of P388 cell line

Model 4. 2D QSAR on CPT45-2D

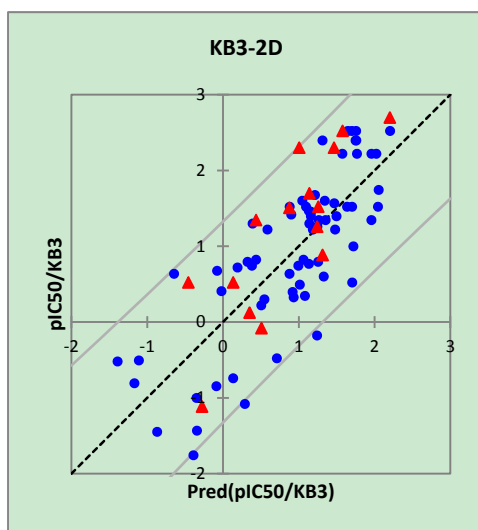
No	descriptor	1	2	3	4	5	6	7	8	9	Y=	p	
1	BCUT_PEOE_1	1,00									-19,423	-0,973	0,000
2	GCUT_PEOE_1	0,75	1,00								20,756	0,514	0,000
3	chi1v_C	-0,22	0,03	1,00							-1,699	-1,988	0,000
4	PEOE_VSA_FHYD	0,03	0,16	0,25	1,00						19,864	0,957	0,000
5	PEOE_VSA_FNEG	-0,03	0,05	0,13	0,00	1,00					-24,092	-1,376	0,000
6	PEOE_VSA_NEG	0,28	0,33	0,56	-0,03	0,64	1,00				0,065	2,310	0,000
7	vsa_other	-0,04	-0,28	0,11	-0,66	-0,01	0,15	1,00			0,056	0,735	0,000
8	SlogP_VSA1	0,07	-0,15	-0,05	-0,33	0,14	0,33	0,41	1,00		-0,060	-0,673	0,000
9	SlogP_VSA5	0,71	0,68	-0,17	0,08	-0,08	0,29	-0,20	-0,09	1,00	-0,013	-0,629	0,000
Coff											-8,798		



The relationship between observed and predicted data from QSAR model and its 95% confidence interval of CPT45 cell line

Model 5. 2D QSAR on KB3-2D

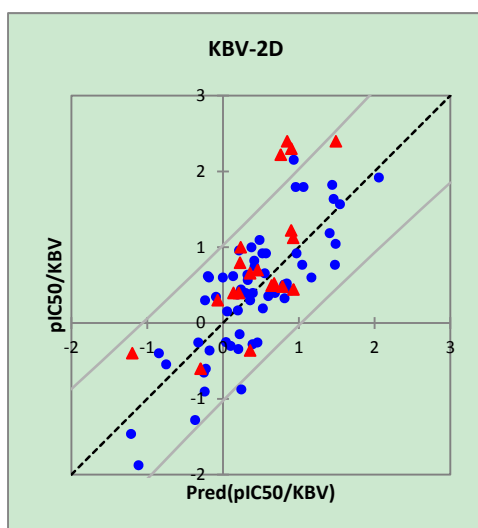
[illegible]



The relationship between observed and predicted data from QSAR model and its 95% confidence interval of KB3 cell line

Model 6. 2D QSAR on KBV cell line

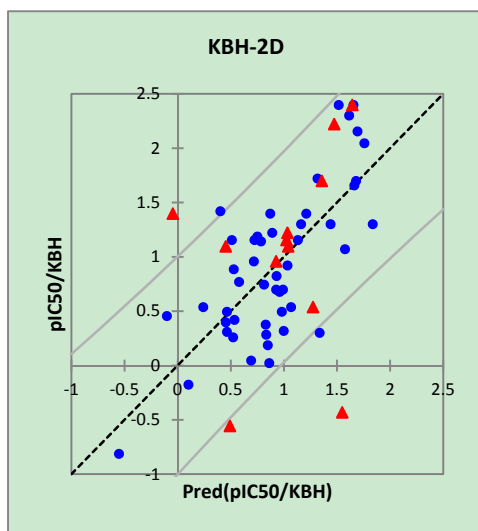
No	Descriptor	1	2	3	4	5	6	7	8	Y=	P
1	BCUT_PEOE_2	1,00								9,713	0,761 0,000
2	GCUT_PEOE_1	-0,38	1,00							12,877	0,308 0,002
3	a_aro	0,42	0,25	1,00						-0,193	-0,621 0,000
4	PEOE_VSA+3	-0,23	0,17	-0,03	1,00					0,035	0,308 0,002
5	opr_leadlike	0,12	-0,28	-0,41	-0,12	1,00				0,728	0,441 0,000
6	a_acc	-0,50	0,18	-0,01	0,28	-0,39	1,00			0,597	0,741 0,000
7	vsa_pol	-0,08	-0,24	0,02	0,14	-0,09	0,72	1,00		-0,033	-0,328 0,001
8	SlogP_VSA9	-0,14	0,12	0,27	0,13	-0,28	0,28	0,19	1,00	0,017	0,392 0,000
Coff										0,092	



The relationship between observed and predicted data from QSAR model and its 95% confidence interval of KBV cell line

Model 7. 2D QSAR model on KBH

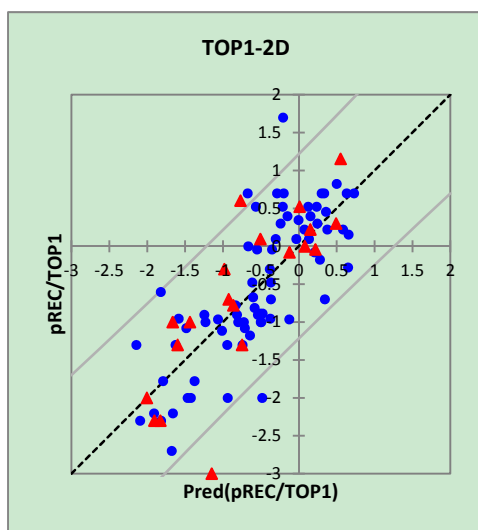
No	Descriptor	1	2	3	4	5	6	Y=	Chuẩn	p
1	a_aro	1,00						-0,271	-1,040	0,000
2	a_nN	0,07	1,00					0,665	0,656	0,000
3	a_nO	-0,02	-0,02	1,00				-0,278	-0,268	0,026
4	PEOE_VSA+0	0,02	0,77	0,03	1,00			-0,019	-0,935	0,000
5	vsa_acc	0,06	0,52	0,46	0,52	1,00		0,065	0,635	0,000
6	SlogP	0,76	-0,12	0,03	0,11	-0,07	1,00	0,546	0,632	0,000
Coff								4,195		



The relationship between observed and predicted data from QSAR model and its 95% confidence interval of KBH cell line

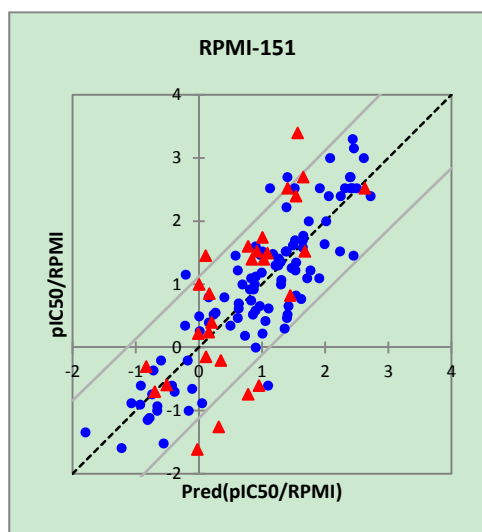
Model 8. 2D QSAR on Topoisomerase 1 inhibitory activity

No	Descriptor	1	2	3	4	5	6	7	8	9	10	Y=	p	
1	GCUT_SLOGP_1	1,00										-13,772	-0,306	0,001
2	a_ICM	-0,44	1,00									27,553	1,597	0,000
3	b_1rotR	0,50	0,06	1,00								7,250	0,351	0,000
4	a_nN	0,04	0,65	0,51	1,00							-0,567	-0,577	0,000
5	PEOE_VSA+3	-0,33	0,04	0,06	-0,08	1,00						0,038	0,368	0,000
6	PEOE_VSA-1	0,32	-0,26	-0,01	0,02	-0,22	1,00					-0,021	-0,477	0,000
7	opr_leadlike	-0,16	-0,04	-0,45	-0,35	-0,26	-0,04	1,00				0,459	0,237	0,008
8	SlogP	0,52	-0,62	0,25	-0,40	0,11	0,47	-0,32	1,00			0,393	0,320	0,000
9	SlogP_VSA5	0,54	-0,14	0,66	0,21	-0,06	-0,33	-0,13	0,04	1,00		-0,013	-0,501	0,000
10	density	-0,67	0,74	-0,45	0,03	0,19	-0,25	0,15	-0,42	-0,54	1,00	-71,331	-1,546	0,000
Coff												5,063		

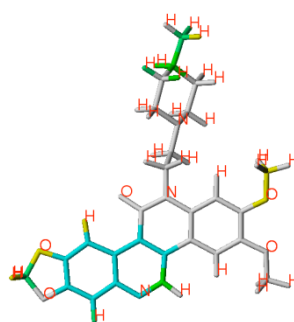


The relationship between observed and predicted data from QSAR model and its 95% confidence interval of topoisomerase -1 inhibitory activity

Model 9. Hologram QSAR on RPMI-151



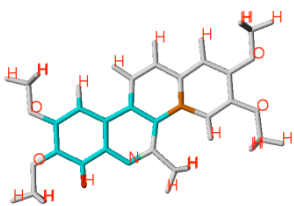
The relationship between observed and predicted data from QSAR model and its 95% confidence interval of RPMI cell line



BMC_06_3131_10F

Exp: 2,39790

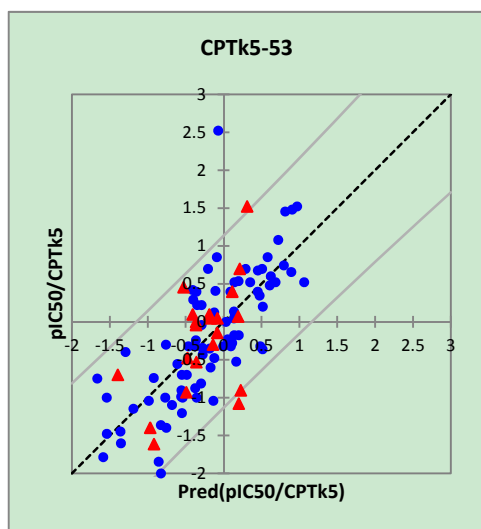
Pred: 2,71781



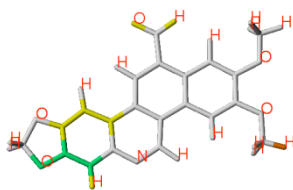
BMC_03_1809_5B

Exp: -1,34240

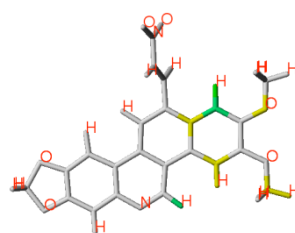
Pred: -1,79618

Model 10. Hologram QSAR on CPTk5-53

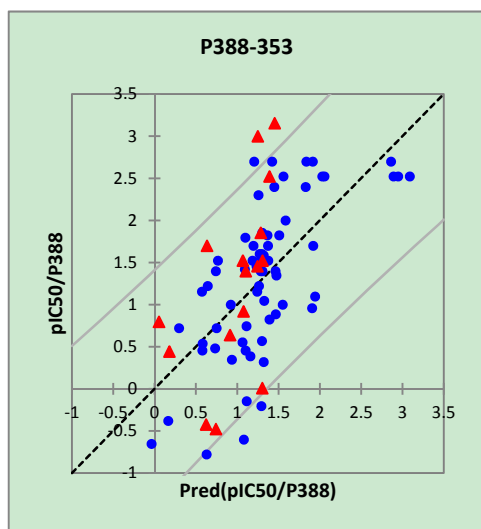
The relationship between observed and predicted data from QSAR model and its 95% confidence interval of CPTk5 cell line



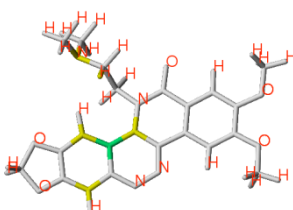
BMC_09_2877_7
Exp 2,52290
Pred: -0,07129



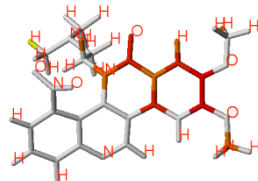
BMC_03_1475_12
Exp: -2,00
Pred: -0,82801

Model 11. Hologram QSAR on P388-353

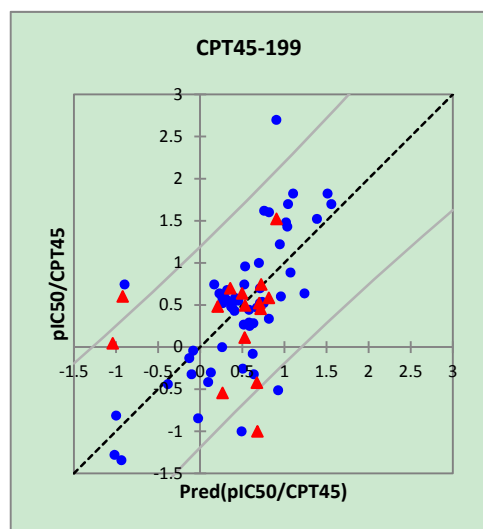
The relationship between observed and predicted data from QSAR model and its 95% confidence interval of P388 cell line



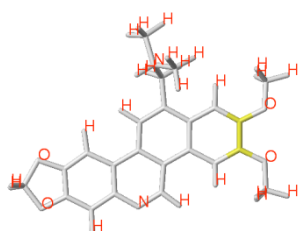
BMC_04_3731_2
Exp: 2,69900
Pred: 2,16123



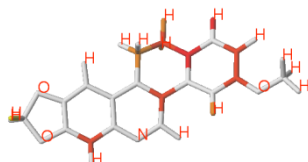
BMC_04_3731_3D
Exp: -0,77820
Pred: -1,04515

Model 12. Hologram QSAR on CPT45-199

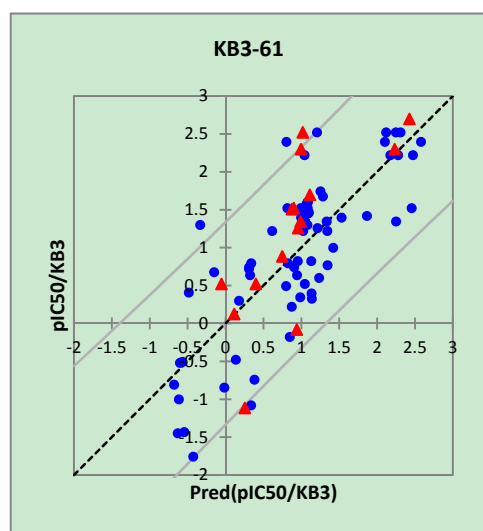
The relationship between observed and predicted data from QSAR model and its 95% confidence interval of CPT45 cell line



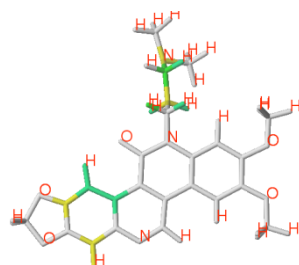
BMC_09_2877_8
Exp: 1,82390
Pred: 1,10111



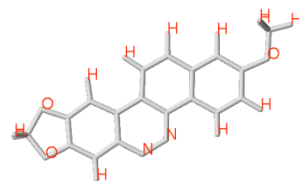
BMC_03_3795_10C
Exp: -1,34240
Pred: -0,93813

Model 13. Hologram QSAR on KB3-61

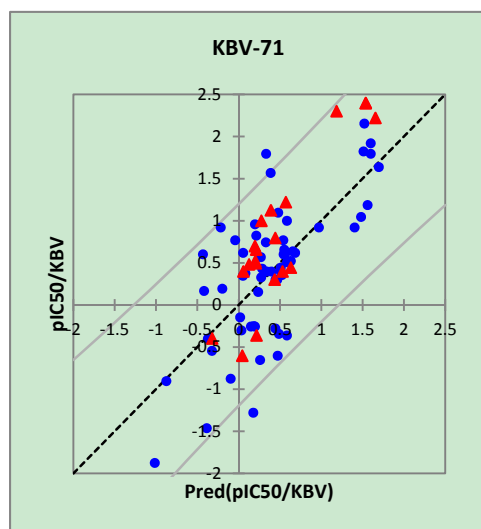
The relationship between observed and predicted data from QSAR model and its 95% confidence interval of KB3 cell line



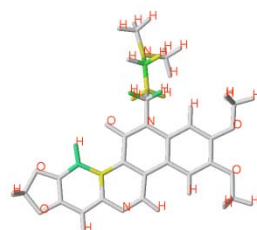
BMC_04_5585_15B
Exp: 2,52290
Pred: 2,11754



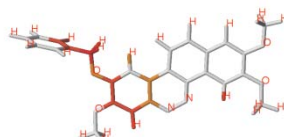
BMC_03_1475_11
Exp: -1,75590
Pred: -0,42833

Model 14. Hologram QSAR on KBV-71

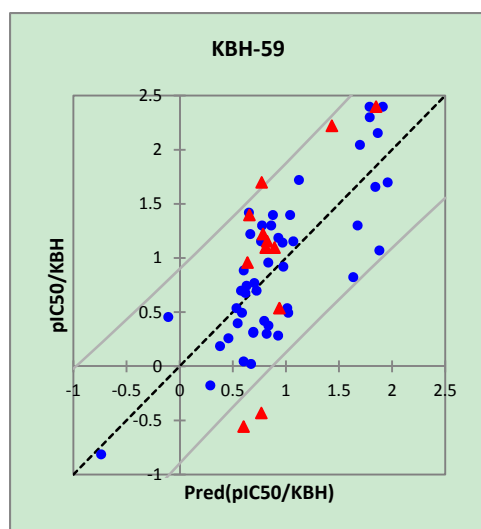
The relationship between observed and predicted data from QSAR model and its 95% confidence interval of KBV cell line



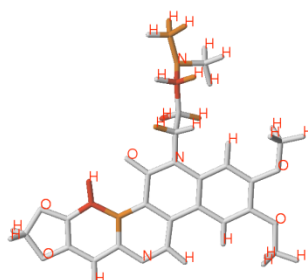
BMC_04_5585_15B
Exp: 2,15490
Pred: 1,52010



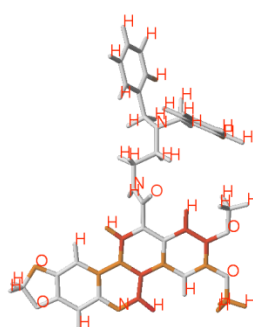
BMC_03_1475_11
Exp: -1,87510
Pred: -1,01580

Model 15. Hologram QSAR on KBH-59

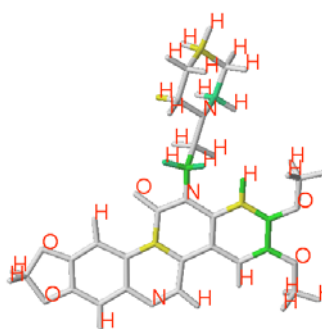
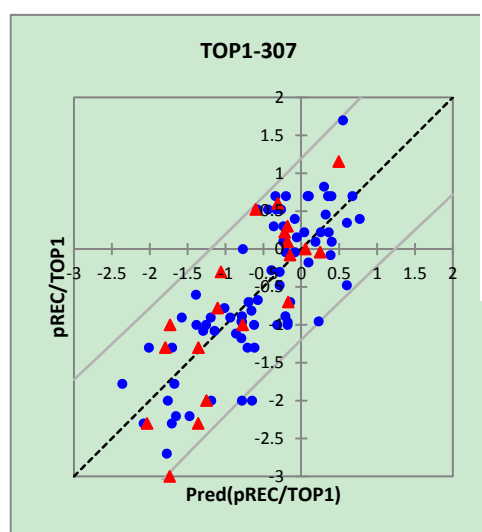
The relationship between observed and predicted data from QSAR model and its 95% confidence interval of KBH cell line



BMC_04_5585_15B
Exp: 2,39790
Pred: 1,91122

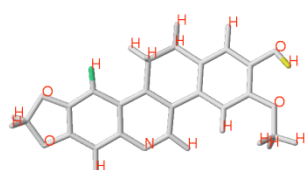


BMC_05_6782_9G
Exp: -0,81290
Pred: -0,73965

Model 16. Hologram QSAR on TOP1 inhibitory activity

BMC_04_5585_15D

Exp: 1,69900
Pred: 0,5483835



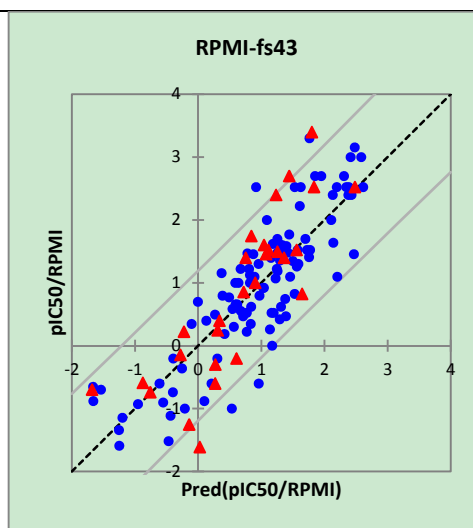
BMC_03_3795_10E

Exp: -2,69900
Pred: -1,77674

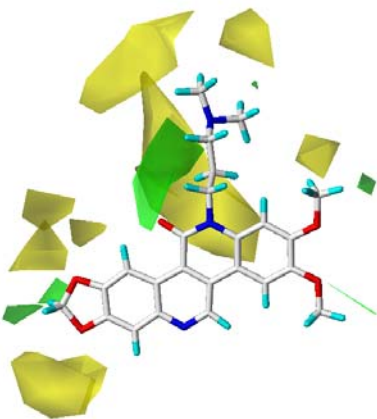
The relationship between observed and predicted data from QSAR model and its 95% confidence interval of Top1 inhibitory activity

Model 17-18. 3D-QSAR on RPMI cytotoxicity

RPMI	q ² for each column filter values				
Descriptor fields	1	2	3	4	5
S	0,573	0,572	0,568	0,57	0,562
E	0,491	0,491	0,49	0,474	0,469
H	0,494	0,493	0,488	0,477	0,461
D	0	0	0	0	0
A	0,279	0,279	0,278	0,279	0,275
s,e	0,555	0,557	0,559	0,551	0,55
s,h	0,546	0,55	0,549	0,545	0,542
s,d	0,554	0,552	0,524	0,536	0,56
s,a	0,496	0,499	0,502	0,493	0,487
e,h	0,526	0,526	0,525	0,517	0,508
e,d	0,458	0,456	0,447	0,443	0,457
e,a	0,478	0,477	0,468	0,456	0,452
h,d	0,454	0,444	0,436	0,446	0,456
h,a	0,425	0,423	0,404	0,4	0,392
d,a	0,242	0,246	0,258	0,253	0,267
s,e,h	0,543	0,545	0,546	0,539	0,539
s,e,d	0,531	0,534	0,528	0,522	0,534
s,e,a	0,524	0,525	0,515	0,507	0,511
s,h,d	0,529	0,532	0,52	0,524	0,545
s,h,a	0,473	0,477	0,473	0,47	0,471
s,d,a	0,451	0,455	0,44	0,447	0,498
e,h,d	0,493	0,492	0,484	0,47	0,484



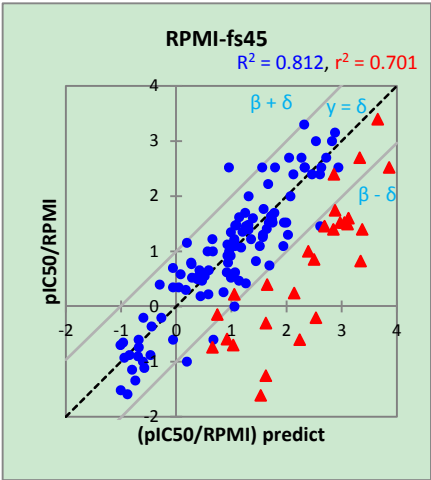
e,h,a	0,495	0,494	0,489	0,481	0,477
e,d,a	0,444	0,448	0,435	0,416	0,467
h,d,a	0,375	0,375	0,373	0,363	0,385
s,e,h,d	0,526	0,526	0,52	0,511	0,522
s,e,h,a	0,519	0,519	0,51	0,507	0,507
s,e,d,a	0,494	0,496	0,485	0,474	0,501
s,h,d,a	0,469	0,469	0,451	0,445	0,466
e,h,d,a	0,467	0,466	0,452	0,434	0,464
s,e,h,d,a	0,495	0,498	0,491	0,484	0,495
CoMFA	0,579	0,581	0,585	0,581	0,574



BMC_04_5585_15B

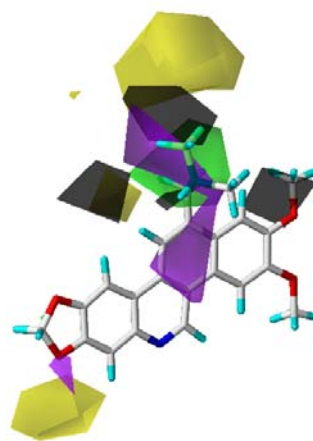
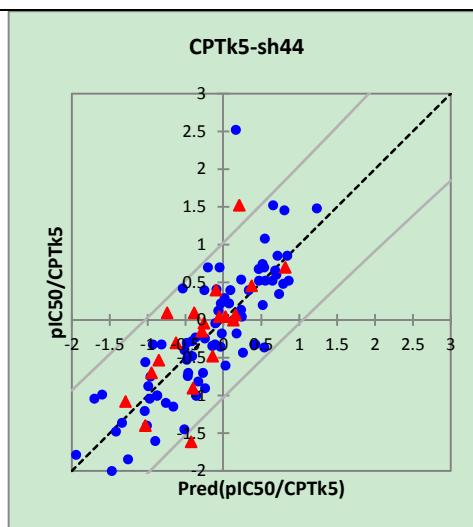
pIC₅₀ pred (exp): 1,709 (3,301)

CoMFA(s) 0,609 0,609 0,608 0,607 0,597



Model 19. 3D-QSAR on CPTk5 cytotoxicity

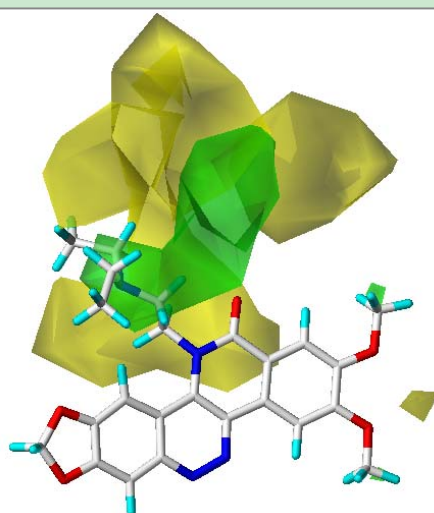
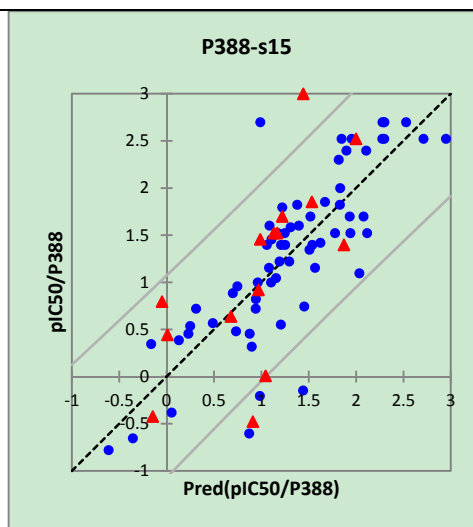
CPTk5	q ² for each column filter values				
Descriptor field	1	2	3	4	5
S	0,308	0,308	0,304	0,301	0,302
E	0,222	0,221	0,218	0,207	0,204
H	0,283	0,287	0,288	0,269	0,262
D	0,000	0,000	0,000	0,000	0,006
A	0,068	0,071	0,077	0,067	0,064
s,e	0,226	0,230	0,229	0,219	0,219
s,h	0,326	0,333	0,336	0,338	0,335
s,d	-	-	-	-	-
s,a	-	-	-	-	-
e,h	0,219	0,219	0,217	0,195	0,193
e,d	-	-	-	-	-
e,a	-	-	-	-	-
h,d	-	-	-	-	-
h,a	-	-	-	-	-
d,a	-	-	-	-	-
s,e,h	0,250	0,254	0,253	0,241	0,238
s,e,d	-	-	-	-	-
s,e,a	-	-	-	-	-
s,h,d	-	-	-	-	-
s,h,a	-	-	-	-	-
s,d,a	-	-	-	-	-
e,h,d	-	-	-	-	-
e,h,a	-	-	-	-	-
e,d,a	-	-	-	-	-
h,d,a	-	-	-	-	-
s,e,h,d	-	-	-	-	-
s,e,h,a	-	-	-	-	-
s,e,d,a	-	-	-	-	-
s,h,d,a	-	-	-	-	-
e,h,d,a	-	-	-	-	-
s,e,h,d,a	-	-	-	-	-
CoMFA	0,216	0,221	0,226	0,242	0,204
CoMFA(s)	0,305	0,306	0,304	0,294	0,232



BMC_09_2877_8
pIC₅₀ pred (exp): 1,230 (1,481)

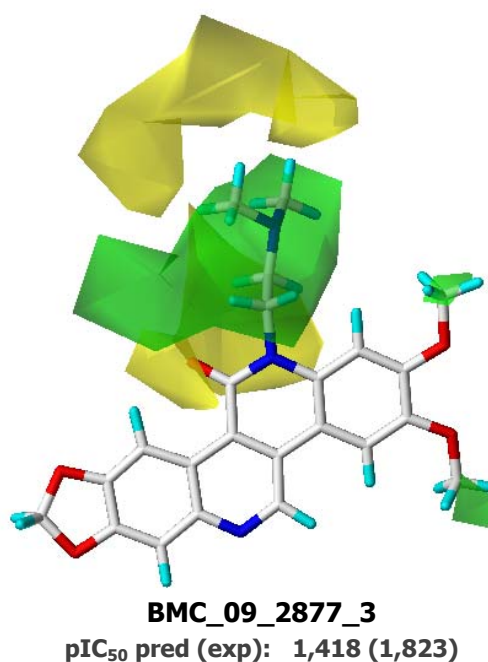
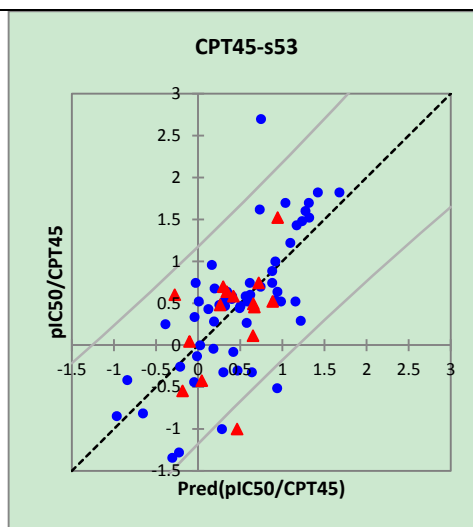
Model 20. 3D-QSAR on P388 cytotoxicity

P388	q ² for each column filter values				
Descriptor field	1	2	3	4	5
S	0,309	0,304	0,295	0,280	0,264
E	0,098	0,098	0,063	0,050	0,002
H	0,151	0,139	0,140	0,138	0,138
D	0,000	0,000	0,000	0,000	0,000
a	0,000	0,000	0,000	0,000	0,000
s,e	0,300	0,295	0,280	0,268	0,250
s,h	0,265	0,266	0,270	0,275	0,277
s,d	-	-	-	-	-
s,a	-	-	-	-	-
e,h	0,168	0,167	0,152	0,147	0,107
e,d	-	-	-	-	-
e,a	-	-	-	-	-
h,d	-	-	-	-	-
h,a	-	-	-	-	-
d,a	-	-	-	-	-
s,e,h	0,229	0,235	0,222	0,226	0,204
s,e,d	-	-	-	-	-
s,e,a	-	-	-	-	-
s,h,d	-	-	-	-	-
s,h,a	-	-	-	-	-
s,d,a	-	-	-	-	-
e,h,d	-	-	-	-	-
e,h,a	-	-	-	-	-
e,d,a	-	-	-	-	-
h,d,a	-	-	-	-	-
s,e,h,d	-	-	-	-	-
s,e,h,a	-	-	-	-	-
s,e,d,a	-	-	-	-	-
s,h,d,a	-	-	-	-	-
e,h,d,a	-	-	-	-	-
s,e,h,d,a	-	-	-	-	-
CoMFA	0,188	0,168	0,180	0,176	0,136
CoMFA(s)	0,293	0,293	0,293	0,289	0,283

**BMC_04_795_1B**pIC₅₀ pred (exp): 2,699 (2,526)

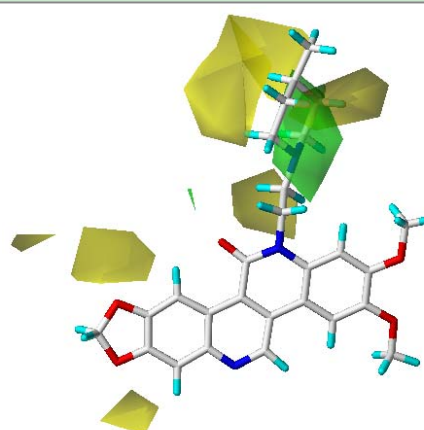
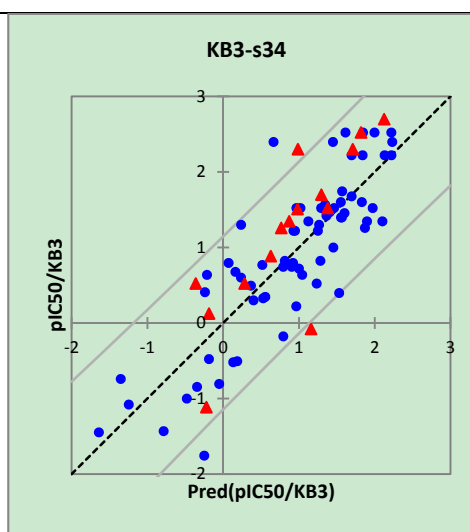
Model 21. 3D-QSAR on CPT45 cytotoxicity

CPT45	q ² for each column filter values				
Descriptor field	1	2	3	4	5
s	0,196	0,197	0,200	0,201	0,201
e	0,007	0,008	0,010	0,009	0,005
h	0,000	0,000	0,000	0,000	0,000
d	0,000	0,000	0,000	0,000	0,000
a	0,000	0,000	0,000	0,000	0,000
s,e	0,018	0,019	0,020	0,019	0,018
s,h	-	-	-	-	-
s,d	-	-	-	-	-
s,a	-	-	-	-	-
e,h	-	-	-	-	-
e,d	-	-	-	-	-
e,a	-	-	-	-	-
h,d	-	-	-	-	-
h,a	-	-	-	-	-
d,a	-	-	-	-	-
s,e,h	-	-	-	-	-
s,e,d	-	-	-	-	-
s,e,a	-	-	-	-	-
s,h,d	-	-	-	-	-
s,h,a	-	-	-	-	-
s,d,a	-	-	-	-	-
e,h,d	-	-	-	-	-
e,h,a	-	-	-	-	-
e,d,a	-	-	-	-	-
h,d,a	-	-	-	-	-
s,e,h,d	-	-	-	-	-
s,e,h,a	-	-	-	-	-
s,e,d,a	-	-	-	-	-
s,h,d,a	-	-	-	-	-
e,h,d,a	-	-	-	-	-
s,e,h,d,a	-	-	-	-	-
CoMFA	0,000	0,000	0,000	0,000	0,000
CoMFA(s)	0,092	0,092	0,092	0,084	0,085

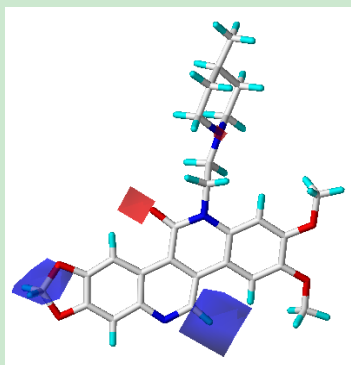
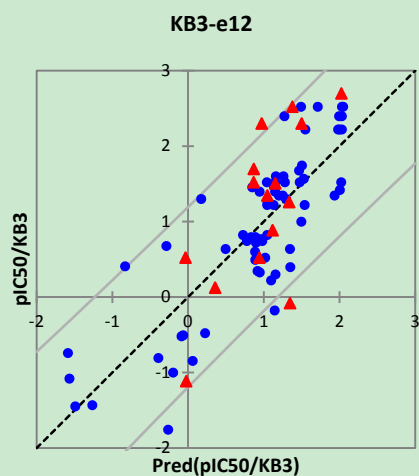


Model 22-25. 3D-QSAR on KB3 cytotoxicity

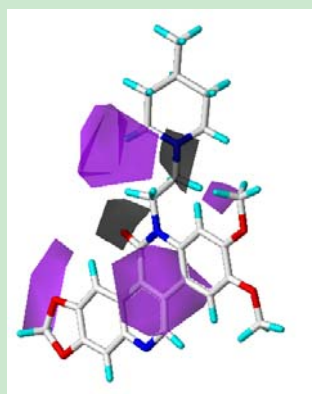
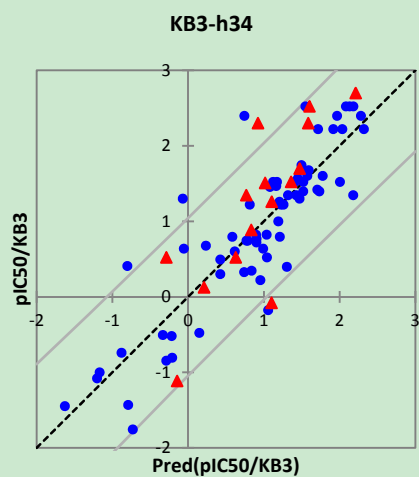
KB3	q ² for each column filter values				
Descriptor field	1	2	3	4	5
s	0,583	0,583	0,584	0,579	0,575
e	0,552	0,551	0,553	0,540	0,542
h	0,542	0,541	0,539	0,509	0,485
d	0,014	0,013	0,004	0,000	0,000
a	0,414	0,415	0,417	0,423	0,429
s,e	0,580	0,580	0,580	0,576	0,576
s,h	0,551	0,555	0,555	0,545	0,536
s,d	0,448	0,446	0,473	0,485	0,502
s,a	0,498	0,507	0,501	0,503	0,505
e,h	0,582	0,581	0,582	0,571	0,560
e,d	0,560	0,562	0,568	0,545	0,534
e,a	0,561	0,558	0,552	0,550	0,547
h,d	0,437	0,438	0,438	0,411	0,406
h,a	0,466	0,465	0,465	0,463	0,467
d,a	0,409	0,412	0,417	0,423	0,427
s,e,h	0,585	0,581	0,584	0,579	0,570
s,e,d	0,578	0,578	0,586	0,584	0,575
s,e,a	0,563	0,564	0,562	0,561	0,558
s,h,d	0,514	0,527	0,533	0,528	0,516
s,h,a	0,511	0,515	0,511	0,510	0,511
s,d,a	0,499	0,507	0,514	0,530	0,509
e,h,d	0,563	0,565	0,573	0,560	0,552
e,h,a	0,560	0,557	0,551	0,546	0,540
e,d,a	0,526	0,528	0,533	0,531	0,520
h,d,a	0,444	0,446	0,445	0,443	0,449
s,e,h,d	0,572	0,574	0,579	0,571	0,562
s,e,h,a	0,569	0,569	0,565	0,561	0,555
s,e,d,a	0,548	0,551	0,555	0,558	0,544
s,h,d,a	0,493	0,507	0,515	0,518	0,501
e,h,d,a	0,528	0,529	0,530	0,523	0,513
s,e,h,d,a	0,545	0,547	0,543	0,540	0,537
CoMFA	0,549	0,549	0,546	0,547	0,551
CoMFA(s)	0,573	0,574	0,573	0,571	0,565



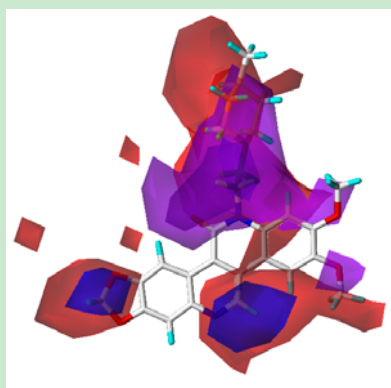
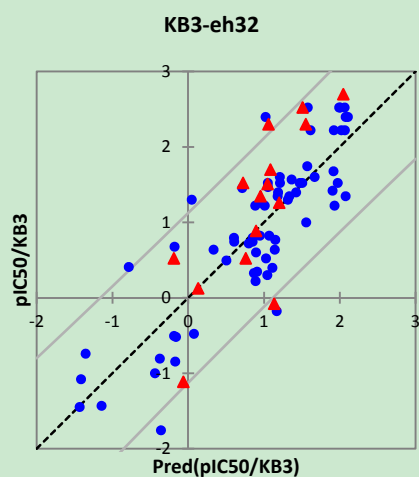
BMC_06_3131_10F
pIC₅₀ pred (exp): 2,229 (2,398)



BMC_06_3131_10F
pIC50 pred (exp): 2,229
(2,398)



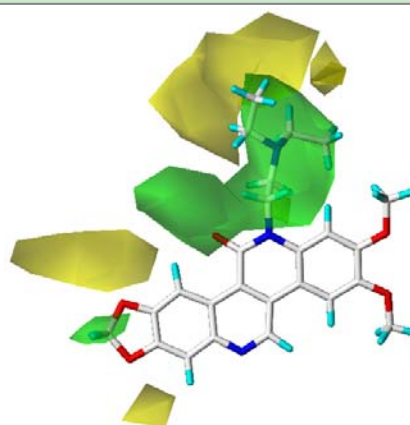
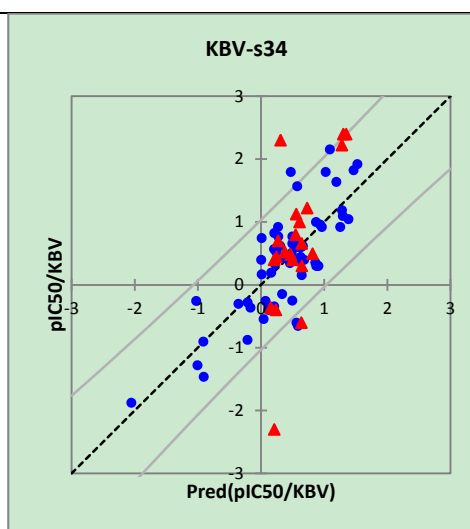
BMC_06_3131_10F
pIC50 pred (exp): 2,280 (2,398)



BMC_06_3131_10F
pIC50 pred (exp):
2,280 (2,398)

Model 26. 3D-QSAR on KBV cytotoxicity

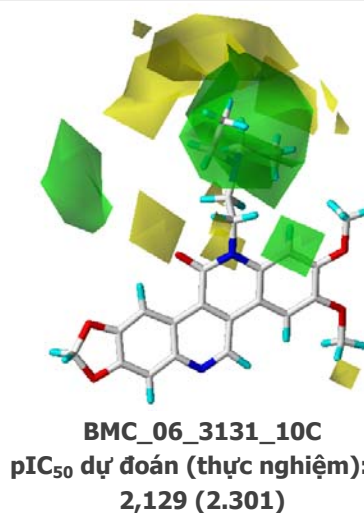
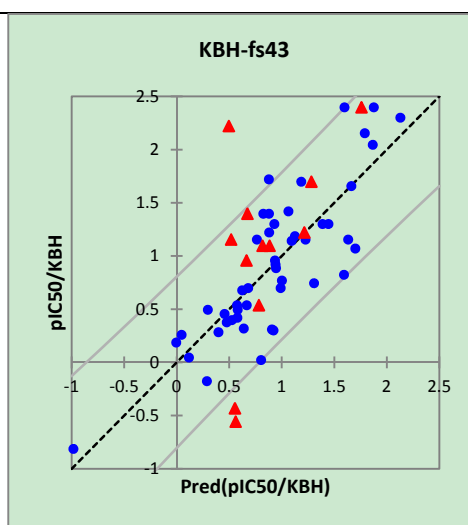
KBV	q ² for each column filter values				
Descriptor field	1	2	3	4	5
S	0,370	0,369	0,372	0,367	0,357
E	0,347	0,347	0,341	0,340	0,314
H	0,225	0,224	0,224	0,219	0,219
D	0,000	0,000	0,000	0,000	0,006
a	0,199	0,198	0,200	0,209	0,225
s,e	0,342	0,342	0,341	0,334	0,302
s,h	0,270	0,274	0,275	0,267	0,255
s,d	-	-	-	-	-
s,a	0,351	0,362	0,364	0,360	0,375
e,h	0,324	0,322	0,319	0,302	0,284
e,d	-	-	-	-	-
e,a	0,315	0,316	0,306	0,303	0,277
h,d	-	-	-	-	-
h,a	0,249	0,249	0,246	0,242	0,242
d,a	-	-	-	-	-
s,e,h	0,327	0,327	0,325	0,313	0,286
s,e,d	-	-	-	-	-
s,e,a	0,306	0,299	0,296	0,285	0,266
s,h,d	-	-	-	-	-
s,h,a	0,259	0,263	0,253	0,250	0,247
s,d,a	-	-	-	-	-
e,h,d	-	-	-	-	-
e,h,a	0,294	0,292	0,280	0,274	0,268
e,d,a	-	-	-	-	-
h,d,a	-	-	-	-	-
s,e,h,d	-	-	-	-	-
s,e,h,a	0,310	0,308	0,296	0,278	0,270
s,e,d,a	-	-	-	-	-
s,h,d,a	-	-	-	-	-
e,h,d,a	-	-	-	-	-
s,e,h,d,a	-	-	-	-	-
CoMFA	0,356	0,350	0,323	0,321	0,307
CoMFA(s)	0,370	0,369	0,372	0,367	0,357



BMC_06_3131_10C
pIC₅₀ pred (exp):
1,523 (1,920)

Model 27. 3D-QSAR on KBH cytotoxicity

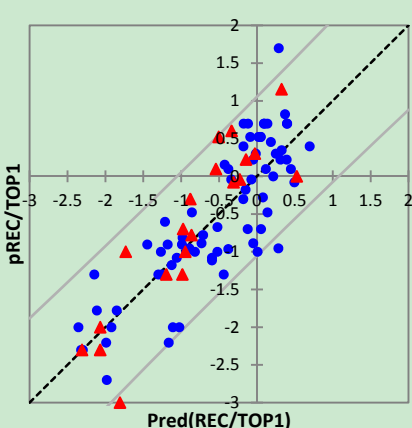
KBH	q ² for each column filter values				
Descriptor field	1	2	3	4	5
s	0,277	0,273	0,267	0,257	0,249
e	0,247	0,243	0,312	0,281	0,239
h	0,219	0,219	0,219	0,218	0,220
d	0,000	0,000	0,000	0,000	0,000
a	0,217	0,217	0,219	0,221	0,217
s,e	0,243	0,238	0,240	0,239	0,231
s,h	0,208	0,203	0,200	0,199	0,197
s,d	-	-	-	-	-
s,a	0,215	0,212	0,211	0,226	0,203
e,h	0,264	0,265	0,268	0,268	0,266
e,d	-	-	-	-	-
e,a	0,221	0,216	0,224	0,230	0,219
h,d	-	-	-	-	-
h,a	0,219	0,217	0,218	0,220	0,219
d,a	-	-	-	-	-
s,e,h	0,255	0,254	0,256	0,255	0,251
s,e,d	-	-	-	-	-
s,e,a	0,217	0,212	0,218	0,223	0,213
s,h,d	-	-	-	-	-
s,h,a	0,221	0,219	0,220	0,221	0,219
s,d,a	-	-	-	-	-
e,h,d	-	-	-	-	-
e,h,a	0,232	0,231	0,234	0,235	0,233
e,d,a	-	-	-	-	-
h,d,a	-	-	-	-	-
s,e,h,d	-	-	-	-	-
s,e,h,a	0,234	0,233	0,235	0,237	0,234
s,e,d,a	-	-	-	-	-
s,h,d,a	-	-	-	-	-
e,h,d,a	-	-	-	-	-
s,e,h,d,a	-	-	-	-	-
CoMFA	0,138	0,129	0,141	0,154	0,169
CoMFA(s)	0,328	0,329	0,328	0,330	0,332



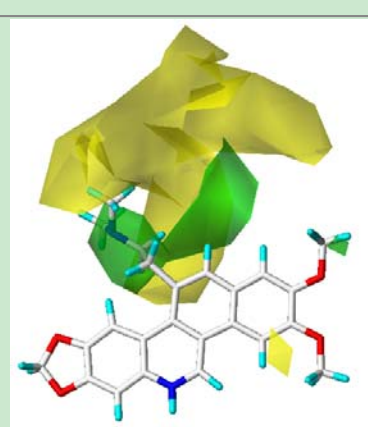
Model 28-29. 3D-QSAR on Topoisomerase -1 inhibitory activity

TOP1	q ² for each column filter values				
Descriptor field	1	2	3	4	5
s	0,425	0,423	0,423	0,379	0,379
e	0,287	0,289	0,289	0,280	0,267
h	0,340	0,340	0,341	0,346	0,341
d	0,126	0,108	0,077	0,038	0,019
a	0,113	0,112	0,096	0,078	0,082
s,e	0,310	0,315	0,320	0,315	0,306
s,h	0,364	0,365	0,368	0,367	0,351
s,d	0,403	0,390	0,397	0,377	0,331
s,a	0,293	0,279	0,281	0,277	0,268
e,h	0,329	0,331	0,324	0,307	0,300
e,d	0,367	0,361	0,343	0,287	0,255
e,a	0,330	0,332	0,323	0,306	0,293
h,d	0,360	0,334	0,323	0,301	0,280
h,a	0,315	0,284	0,261	0,256	0,237
d,a	0,137	0,137	0,136	0,123	0,130
s,e,h	0,336	0,340	0,344	0,335	0,329
s,e,d	0,405	0,402	0,393	0,366	0,350
s,e,a	0,333	0,336	0,325	0,322	0,308
s,h,d	0,403	0,390	0,386	0,377	0,367
s,h,a	0,326	0,318	0,313	0,312	0,302
s,d,a	0,293	0,262	0,267	0,245	0,245
e,h,d	0,369	0,359	0,345	0,310	0,300
e,h,a	0,335	0,334	0,326	0,313	0,306
e,d,a	0,327	0,306	0,288	0,257	0,256
h,d,a	0,193	0,180	0,175	0,164	0,166
s,e,h,d	0,393	0,387	0,380	0,359	0,347
s,e,h,a	0,348	0,349	0,345	0,338	0,327
s,e,d,a	0,370	0,353	0,343	0,322	0,315
s,h,d,a	0,296	0,273	0,279	0,267	0,272
e,h,d,a	0,319	0,305	0,294	0,267	0,275
s,e,h,d,a	0,351	0,341	0,339	0,319	0,322
CoMFA	0,292	0,298	0,303	0,324	0,307
CoMFA(s)	0,366	0,366	0,360	0,348	0,343

TOP1-s34



BMC_08_8598_17
pIC50 pred (exp)
0,694 (0,398)



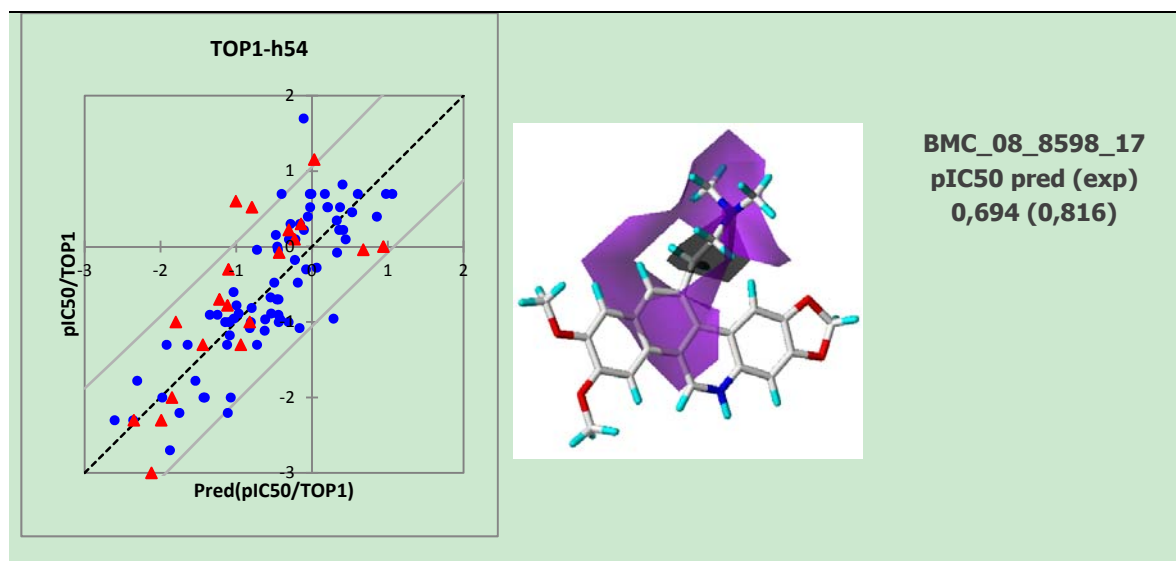
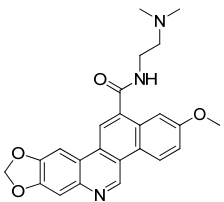
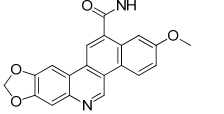
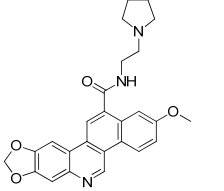
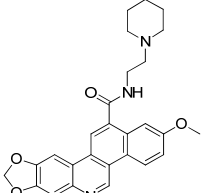
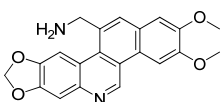
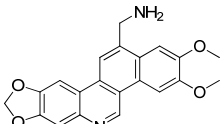
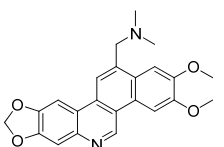


Table S10. Several new designed BCPs compound with predictive activity from QSAR models

Chemical structure	Predicted pIC50 RPMI cytotoxicity			Predicted pIC50 KB3 cytotoxicity			Predicted pREC (TopI)		
	2D-QSAR	H-QSAR	3D-QSAR	2D-QSAR	H-QSAR	3D-QSAR	2D-QSAR	H-QSAR	3D-QSAR
	1.988	1.524	1.674	0.762	0.890	1.237	0.233	-0.689	-0.557
	1.749	1.533	1.870	0.882	0.963	0.657	0.230	-0.623	-1.208
	1.208	1.654	1.669	1.010	0.863	1.298	0.298	-0.533	-0.539
	1.822	1.754	1.747	1.370	0.865	1.364	-0.046	-0.505	-0.169
	0.613	0.679	0.705	0.941	0.881	0.856	0.095	0.080	-0.052
	0.542	0.391	1.060	0.940	0.663	0.925	-0.151	-0.300	-0.196
	0.814	0.492	1.254	0.880	0.761	1.403	-0.432	-0.278	0.083

Part S. Calculation of r_m^2 metrics

Determination coefficient r_m^2 for the least squares regression line (without intercept) correlating observed (y-axis) and predicted (x-axis) values proposed by Roy *et al.* [1-3] was also applied to validate our QSAR models. This metric is calculated based on the correlations between the observed and predicted values with (r^2) and without (r_0^2) intercept for the least squares regression lines as shown in the following equation:

$$r_m^2 = r^2 \times (1 - \sqrt{r^2 + r_0^2}) \quad (1)$$

Average of r_m^2 and $r_m^{/2}$ are performed by $\overline{r_m^2} = \frac{r_m^2 + r_m^{/2}}{2}$ with r_m^2 is validation metric calculated according to Eq. (1) using observed (y-axis) and predicted (x-axis) values; and $r_m^{/2}$ is validation metric calculated according to Eq. (1) using observed (x-axis) and predicted (y-axis) values. Absolute difference between r_m^2 and $r_m^{/2}$ was also calculated by $r_m^2 = r_m^2 - r_m^{/2}$ [1-3].

References

1. Roy, K.; Mitra, I.; Kar, S.; Ojha, P.K.; Das, R.N.; Kabir, H. Comparative Studies on Some Metrics for External Validation of QSPR Models. *J. Chem. Inf. Model.* **2012**, *52*, 396–408
2. Ojha, P.K.; Mitra, I.; Das, R.N.; Roy, K. Further exploring r_m^2 metrics for validation of QSPR models. *Chemometr. Intell. Lab.* **2011**, *107*, 194–205.
3. Pratim Roy, P.; Paul, S.; Mitra, I.; Roy, K. On Two Novel Parameters for Validation of Predictive QSAR Models. *Molecules* **2009**, *14*, 1660–1701.