

Table S1. Predicted pIC₅₀ of MLR and SVM models

Compound	pIC ₅₀	SVM		MLR	
		Predicted pIC ₅₀	Residual	Predicted pIC ₅₀	Residual
1	4.09	4.66	0.57	5.58	1.49
2	4.72	4.56	-0.17	4.59	-0.13
3	6.57	4.99	-1.57	6.03	-0.54
4	4.72	5.18	0.45	4.97	0.25
5	4.30	5.42	1.12	4.71	0.41
6	4.01	3.63	-0.38	4.30	0.29
7	5.34	4.71	-0.63	4.19	-1.15
8	4.85	5.90	1.05	5.16	0.31
9	5.70	5.37	-0.33	5.84	0.14
10	6.00	6.55	0.55	6.30	0.30
11	6.80	5.11	-1.68	5.48	-1.32
12	7.72	5.38	-2.34	6.23	-1.49
13	7.68	7.65	-0.03	7.06	-0.62
14	7.92	9.05	1.13	8.36	0.44
15	7.60	7.66	0.06	7.21	-0.39
16	9.40	8.97	-0.43	9.11	-0.29
17	8.30	8.66	0.36	8.23	-0.07
18	7.92	8.50	0.59	7.98	0.06
19	7.31	7.83	0.52	7.82	0.51
20	7.77	8.42	0.65	8.06	0.29
21	7.98	8.61	0.63	8.62	0.64
22	7.74	9.11	1.37	8.91	1.17
23	9.05	9.54	0.50	9.66	0.62
24	9.10	10.26	1.16	11.14	2.04
25	9.70	9.10	-0.60	9.66	-0.04
26	9.22	9.77	0.55	9.44	0.22
27	8.03	8.15	0.11	7.68	-0.35
28	5.72	5.86	0.14	5.93	0.21
29	5.47	5.36	-0.11	5.71	0.24
30	5.12	5.19	0.07	5.05	-0.07
31	5.82	5.34	-0.48	5.98	0.15
32	5.82	5.01	-0.81	5.26	-0.57
33	5.10	5.45	0.36	5.91	0.81
34	7.09	5.75	-1.34	5.89	-1.20

35	5.62	7.05	1.43	6.49	0.87
36	5.89	5.23	-0.65	5.47	-0.41
37	6.00	5.18	-0.82	5.25	-0.75
38	4.92	4.82	-0.11	4.80	-0.12
39	4.82	5.26	0.44	5.32	0.50
40	5.82	5.34	-0.48	5.52	-0.30
41	5.70	5.85	0.15	6.55	0.85
42	5.89	5.07	-0.82	5.23	-0.65
43	4.96	5.53	0.58	5.10	0.14
44	5.00	5.77	0.76	4.98	-0.02
45	5.32	5.55	0.24	5.93	0.61
46	5.28	5.28	0.00	5.46	0.18
47	5.82	5.74	-0.08	5.30	-0.52
48	5.80	5.31	-0.49	5.11	-0.69
49	5.77	5.23	-0.54	5.01	-0.76
50	5.54	5.46	-0.08	4.75	-0.79
51	5.51	5.18	-0.33	5.21	-0.29
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52*	6.06	6.82	0.76	7.14	1.08
53*	4.68	4.08	-0.59	4.85	0.18
54*	5.04	6.62	1.57	6.62	1.58
55*	8.70	9.63	0.93	9.68	0.98
56*	7.65	8.18	0.53	8.64	0.98
57*	8.35	9.61	1.26	8.98	0.63
58*	5.68	5.26	-0.41	5.30	-0.38
59*	5.52	4.53	-0.99	4.49	-1.03
60*	5.55	5.29	-0.27	5.44	-0.11
61*	6.12	5.81	-0.31	6.37	0.25
62*	5.06	5.28	0.22	4.64	-0.41

*Compound for test set