

Supporting Informations

3-D QSAR Studies on Histone Deacetylase Inhibitors. A GOLPE/GRID Approach on Different Series of Compounds

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Model 12 calculated pIC₅₀ for the training set and predicted pIC₅₀ for TestSet-1 and TestSet-2 are given.

Table A. Model 12 calculated pIC₅₀ values for the training set					
entry	Actual pIC₅₀	Calculated pIC₅₀	entry	Actual pIC₅₀	Calculated pIC₅₀
1	7.00	7.08	50	5.62	5.60
5	5.70	5.66	51	7.00	6.56
7	7.00	6.65	52	6.00	6.60
9	6.52	6.90	53	5.30	5.84
13	6.74	6.75	54	4.28	4.22
15	6.85	6.96	55	3.96	3.90
17	6.05	5.97	68	4.25	3.74
19	6.82	6.77	69	4.14	3.89
21	6.74	6.22	70	4.16	4.60
23	7.00	6.92	72	4.13	4.10
25	5.96	6.25	73	4.46	4.49
26	7.10	7.00	74	4.69	4.55
27	6.85	6.97	75	4.43	5.08
28	6.48	6.85	76	5.57	5.33
29	6.47	6.86	78	6.11	6.09
30	6.42	6.75	80	4.18	4.96
31	6.28	6.79	81	4.97	4.85
32	6.12	6.13	82	4.77	4.98
33	6.12	6.08	83	5.92	6.24
34	6.60	6.82	84	5.85	5.87
35	6.07	6.14	86	5.83	5.80
36	6.68	6.79	88	6.70	5.83
37	6.05	5.96	89	5.89	6.03
38	6.44	6.68	91	5.00	4.97
39	7.40	7.28	92	7.37	6.85
40	6.15	6.03	93	6.89	6.62
41	6.92	6.75	94	6.96	7.03
42	7.46	7.49	95	7.15	6.91
43	6.30	6.54	96	6.58	6.51
44	5.42	5.52	97	6.68	6.72
45	5.62	5.45	98	7.00	6.71
46	5.42	4.76	99	6.84	6.76
47	5.41	5.53	100	6.51	6.45
48	5.72	5.41	101	6.94	6.44
49	5.54	5.43	SAHA	7.30	7.22
			TSA	8.14	7.70

Table B. Model 12 predicted pIC₅₀ values for the test sets					
TestSet-1			TestSet-2		
entry	Actual pIC₅₀	Predicted pIC₅₀	entry	Actual pIC₅₀	Predicted pIC₅₀
102	6.55	6.25	109	7.42	5.86
103	5.28	5.88	110	6.64	6.18
104	4.62	5.91	111	6.90	5.19
105	4.60	5.95	112	7.74	6.64
106	6.57	6.56	113	7.43	7.18
107	5.10	6.28	114	7.21	5.74
108	4.99	6.07	115	6.67	6.32
			116	6.96	6.07
			117	6.87	6.21
			118	7.92	7.04
			119	7.46	7.02
			120	7.46	6.75