

Human protein tyrosine phosphatase 1B inhibitors: QSAR by genetic function approximation

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Supplementary material: List of descriptors for each molecule

List of descriptors for each molecule

Compd No.	Charge	Apol	Dipole-mag	RadOfGyr	Area	MW	Vm	Density	PMI-mag	Rotl bonds	Hbond acc	Hbond don	AlogP 98
Training set													
1	0	8900	7.38	3.50	250.77	216.24	196.87	1.10	443.23	2	3	0	2.19
2	0	8850	7.36	2.91	197.21	208.60	160.11	1.30	376.32	1	4	0	1.66
3	0	7290	6.82	2.92	203.85	253.05	164.07	1.54	528.61	1	4	0	1.75
4	0	7270	3.97	2.97	227.46	331.95	182.49	1.82	713.19	1	5	0	2.50
5	0	8390	8.05	3.12	202.60	219.15	170.04	1.29	433.93	1	5	0	0.89
6	0	7420	6.68	2.88	183.74	192.15	151.08	1.27	299.45	1	4	0	1.21
7	0	9760	5.85	3.31	225.44	224.22	189.03	1.19	399.04	1	3	0	1.91
8	0	9760	7.56	7.56	229.38	224.22	189.44	1.18	447.85	1	3	0	1.91
9	0	14700	9.22	9.22	348.02	326.35	289.24	1.13	1676.79	3	3	0	4.04
10	0	15900	8.24	8.24	364.01	350.37	304.55	1.15	1150.48	2	3	0	4.34
11	0	15900	5.93	5.93	385.35	429.27	322.84	1.33	1730.00	2	4	0	5.08
12	0	15800	1.44	1.44	406.09	508.17	341.06	1.49	2085.60	2	5	0	5.83
13	0	15900	6.84	6.84	415.39	352.39	343.91	1.02	1433.34	4	3	0	4.46
14	0	16300	8.48	8.48	341.48	356.40	295.47	1.21	1432.73	2	4	0	4.49
15	0	16300	9.89	9.89	365.00	435.29	314.06	1.39	1650.41	2	5	0	5.24
16	0	13900	7.84	7.84	303.26	306.34	252.08	1.22	1020.45	2	4	0	3.15
17	0	13800	8.47	4.14	349.48	464.13	289.03	1.61	1402.24	2	6	0	4.88
18	0	16300	6.09	4.07	345.12	356.40	295.33	1.21	1117.09	2	4	0	4.49
19	0	16300	4.65	4.15	365.96	435.29	314.02	1.39	1419.32	2	5	0	5.24
20	0	17600	5.65	4.23	387.05	382.43	324.12	1.18	1204.97	3	4	0	5.10
21	0	17600	5.57	4.25	412.79	461.33	342.57	1.35	1484.01	3	5	0	5.85
22	0	14400	9.39	4.50	324.48	320.36	268.97	1.19	1230.79	3	4	0	3.62
23	0	18600	5.81	4.10	430.86	410.49	357.38	1.15	1321.54	5	4	0	5.59
24	0	11000	8.64	3.61	270.28	250.25	217.66	1.15	583.72	2	3	0	2.52
25	0	22300	7.15	5.13	525.23	486.58	429.04	1.13	2696.35	6	4	0	7.11
26	0	26000	8.88	5.51	611.42	562.68	501.62	1.12	3447.62	7	4	0	8.63
27	0	11500	7.14	3.81	289.10	264.28	234.70	1.13	692.05	3	3	0	2.97
28	0	11500	8.86	3.70	291.16	264.28	234.39	1.13	675.06	3	3	0	2.97
29	0	15700	8.63	4.20	395.36	354.40	323.04	1.10	1084.09	5	3	0	4.95
Test set													
1	0	7310	5.62	2.86	179.51	174.16	145.91	1.19	230.57	1	3	0	1.00
2	0	10400	4.89	2.95	214.95	243.05	173.65	1.40	463.56	1	5	0	2.33
3	0	9410	7.93	3.22	219.91	222.63	177.08	1.26	431.17	1	4	0	2.15
4	0	11000	7.31	7.31	261.48	250.25	217.96	1.15	687.24	2	3	0	2.52
5	0	14400	8.43	4.32	330.69	320.36	260.94	1.19	1214.08	3	4	0	3.61
6	0	14700	8.77	4.30	354.87	326.35	289.25	1.13	1016.87	3	3	0	4.04
7	0	18400	9.50	5.37	443.92	402.45	362.05	1.11	2148.66	4	3	0	5.56

Compd No.	HOMO	LUMO	Sr	DIFFV	COSV	Fo	NCOSV	ShapeRMS	SR Vol	MR	Fh2o	Foct	Hf
Training set													
1	-11.08	1.54	1.97	-257.01	153.79	0.78	43.08	0.02	453.88	42.52	-7.77	-9.65	-56.13
2	-11.47	1.22	1.27	-293.77	138.54	0.87	21.57	0.02	453.88	33.67	-8.31	-9.22	-50.26
3	0.00	0.00	1.26	-289.81	0.00	0.00	164.07	0.02	453.88	34.95	-10.19	-10.22	0.00
4	0.00	0.00	1.26	-271.39	0.00	0.00	182.49	0.02	453.88	8.39	-12.08	-12.38	0.00
5	-11.95	0.26	0.67	-283.84	138.29	0.81	31.75	0.02	453.88	33.19	2.87	3.32	-4.75
6	-11.42	1.19	0.49	-302.80	129.29	0.86	21.80	0.02	453.88	29.18	-8.25	-8.45	-87.22
7	-10.68	0.98	0.67	-264.85	139.37	0.74	49.66	1.31	453.88	8.22	-10.50	-11.45	-19.47
8	-10.53	1.34	0.67	-264.44	130.27	0.69	59.17	1.24	453.88	8.22	-10.50	-11.92	-21.87
9	-10.81	1.48	0.71	-164.64	176.59	0.61	112.65	0.72	453.88	49.02	-13.33	-13.04	-21.87
10	-9.44	0.49	1.69	-149.33	168.27	0.55	136.28	0.41	453.88	36.70	-15.13	-17.86	1685.85
11	0.00	0.00	1.69	-131.04	0.00	0.00	322.84	0.41	453.88	35.29	-16.99	-20.12	1685.85
12	0.00	0.00	1.69	-112.82	0.00	0.00	341.06	0.41	453.88	8.73	-18.88	-22.12	0.00
13	-5.14	-4.73	0.36	-109.98	206.76	0.60	137.15	0.60	453.88	58.34	-13.69	-24.28	1685.85
14	-10.59	1.48	1.74	-158.41	154.28	0.52	141.19	0.79	453.88	27.38	-16.44	-19.14	0.00
15	0.00	0.00	1.74	-139.82	0.00	0.00	314.06	0.80	453.88	0.82	-18.33	-17.67	1685.85
16	-10.46	1.43	0.39	-201.80	159.90	0.63	92.18	1.09	453.88	30.91	-14.16	-19.83	0.00
17	0.00	0.00	0.39	-164.86	0.00	0.00	289.03	1.08	453.88	12.23	-17.75	-18.13	1685.85
18	-10.73	1.46	1.66	-158.55	164.17	0.56	131.17	1.07	453.88	27.38	-16.44	-17.67	0.00
19	0.00	0.00	1.66	-139.67	0.00	0.00	314.02	0.96	453.88	0.82	-18.33	-19.83	5.03
20	-10.17	1.23	0.33	-129.76	144.56	0.45	179.56	1.14	453.88	36.70	-16.80	-18.95	5.83
21	0.00	0.00	0.33	-111.31	0.00	0.00	342.57	1.15	453.88	10.14	-18.80	-21.11	40.04
22	-10.81	1.48	0.69	184.91	144.56	0.54	124.51	0.91	453.88	46.49	-13.46	-14.43	14.46
23	-10.38	1.43	0.15	-96.50	262.09	0.73	95.29	0.70	453.88	94.68	-15.26	-19.50	40.04
24	-11.22	1.42	1.24	-236.22	190.45	0.88	27.21	0.02	453.88	42.69	-10.83	-13.04	-14.46
25	-10.33	1.51	1.71	-24.85	231.56	0.54	197.48	1.40	453.88	73.92	-18.36	-24.52	1996.84
26	-10.30	1.45	1.86	47.74	453.88	0.91	47.74	0.00	453.88	55.11	-20.88	-29.50	1996.84
27	-11.07	1.51	0.39	-219.18	132.51	0.57	102.20	1.44	453.88	57.50	-10.53	-13.49	-20.81
28	-11.25	1.47	0.39	-219.49	150.13	0.64	84.26	0.01	453.88	57.50	-10.53	-13.49	-18.58
29	-11.00	1.48	1.00	-130.84	133.71	0.41	189.33	1.44	453.88	53.50	-12.76	-18.92	5.77
Test set													
1	-11.33	1.45	1.83	-307.97	126.08	0.86	19.83	0.02	453.88	28.06	-8.33	-8.34	-44.56
2	-11.66	0.92	2.29	-280.24	151.21	0.87	22.43	0.02	453.88	5.83	-8.31	-10.38	-54.73
3	-11.36	1.24	1.26	-276.80	141.49	0.80	35.59	0.02	453.88	5.59	-8.55	-10.01	-56.23
4	-11.01	1.48	0.39	-235.92	152.13	0.70	65.83	0.72	453.88	42.69	-10.83	-11.92	-21.87
5	-10.58	1.43	0.69	-184.94	185.28	0.69	83.66	0.80	453.88	64.27	-13.46	-14.43	5.83
6	-10.85	1.48	0.69	-164.63	221.16	0.77	68.09	0.66	453.88	23.87	-13.36	-18.02	13.51
7	-10.72	1.45	0.68	-91.84	247.53	0.68	114.51	0.66	453.88	30.20	-15.86	-22.84	40.74