

Supplementary Information

4D-QSAR Study of 17 β -Hydroxysteroid Dehydrogenase Type 3 Inhibitors

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Table S1. Results of internal and external prediction for model 1, and values of the selected descriptors

Compound	Molecular descriptor								Real pIC ₅₀	Pred. pIC ₅₀	Residual
	20_17_17_LJ	11_10_12_C	18_24_22_LJ	17_15_15_LJ	19_10_19_LJ	10_18_23_C	20_17_16_LJ	12_21_17_C			
1	153.93	-1.21	-0.31	164.21	1.09	-8.59	160.93	1.31	7.85	7.26	0.59
2	178.50	0.73	-0.39	157.43	13.57	-7.34	150.86	-18.33	6.05	6.76	-0.71
3	187.63	-0.21	-0.43	164.25	-5.55	-4.10	157.43	-1.39	6.92	6.93	-0.01
4	183.65	0.53	-0.44	164.61	54.42	-4.55	156.46	-1.07	6.52	7.14	-0.62
5	175.92	5.13	-0.33	167.88	-1.84	-21.48	163.12	4.09	6.72	6.36	0.36
7	157.96	0.79	-0.62	166.34	-5.58	-16.04	153.37	-4.98	7.12	6.97	0.15
8	163.47	-2.98	-0.98	159.93	133.31	-1.42	178.21	-3.01	7.05	7.59	-0.54
9	156.57	-9.26	-0.84	178.15	21.55	2.21	153.11	0.10	7.89	8.40	-0.51
10	148.47	-5.83	-1.23	181.30	-10.82	-1.77	153.23	0.51	8.22	8.22	0.00
11	138.85	-1.72	-1.25	167.44	-11.76	-3.52	135.44	4.07	8.15	8.15	0.00
12	152.00	-3.97	-0.83	170.79	-9.57	-1.32	169.57	-12.62	7.22	7.50	-0.28
13	156.86	-6.17	-1.38	193.74	142.20	-3.96	160.32	-3.63	8.10	8.46	-0.36
15	144.92	-4.21	-1.80	181.15	-9.36	-0.31	164.82	7.40	8.22	8.35	-0.13
16	142.16	-6.22	-0.30	190.50	145.98	-0.38	140.71	4.27	8.70	8.79	-0.09
17	152.15	-0.70	-1.02	171.69	167.02	-4.67	149.98	-5.51	8.52	7.79	0.73
18	142.85	-2.09	-1.09	165.54	152.77	-7.36	153.27	-2.17	7.72	7.98	-0.26
19	168.26	1.96	-0.47	178.10	182.40	-6.47	161.12	-5.29	7.64	7.34	0.30
20	181.52	-14.75	-0.95	159.80	-9.03	4.35	175.24	-15.44	7.62	7.50	0.12
21	151.47	0.58	-0.30	146.16	21.21	-3.63	150.48	-11.22	7.25	6.96	0.29
23	156.06	0.03	-0.21	167.46	-7.16	-11.19	155.00	-9.73	7.38	6.95	0.43
25	155.31	1.33	-0.22	170.46	141.27	-9.26	165.97	-8.70	7.60	7.11	0.49

Table S1. Results of internal and external prediction for model 1, and values of the selected descriptors (cont.)

Compound	Molecular descriptor								Real pIC ₅₀	Pred. pIC ₅₀	Residual
	20_17_17_LJ	11_10_12_C	18_24_22_LJ	17_15_15_LJ	19_10_19_LJ	10_18_23_C	20_17_16_LJ	12_21_17_C			
27	135.66	1.40	-0.41	190.89	140.36	-4.97	140.28	-8.25	7.68	8.28	-0.60
29	165.84	2.08	1.40	160.83	-3.35	-4.49	159.84	-12.81	6.05	6.51	-0.46
30	165.90	-1.11	-0.29	167.04	34.04	-1.57	169.47	3.83	7.13	7.39	-0.26
31	147.23	-3.83	-0.94	155.65	134.37	-3.83	167.97	-1.48	7.67	7.75	-0.08
32	165.41	-5.65	-0.38	169.26	135.24	-2.82	154.92	3.99	8.40	7.90	0.50
34	159.42	-0.70	-0.48	172.68	57.33	-2.22	156.26	9.31	7.68	7.81	-0.13
35	158.76	-1.21	-0.58	179.32	-4.35	-0.64	168.79	9.48	7.70	7.75	-0.05
36	152.84	-2.96	-0.72	172.64	131.43	-3.53	151.93	-0.43	8.40	7.97	0.43
37	153.45	1.65	-0.66	163.66	-6.16	-20.01	160.15	18.73	6.91	7.36	-0.45
39	157.79	0.94	4.55	181.45	-7.90	-10.74	154.90	5.16	6.60	6.21	0.39
40	161.77	2.94	-0.53	163.19	-5.38	25.18	155.70	17.33	8.70	7.52	1.18
42	158.68	-7.32	-0.84	173.37	54.23	-18.66	157.80	5.80	8.30	7.66	0.64
43	157.41	4.22	-1.31	173.30	-2.98	-15.74	150.12	33.23	7.92	7.83	0.09
44	146.71	-12.24	-0.31	158.88	134.37	-8.39	140.64	6.62	8.30	8.48	-0.18
45	169.73	-24.97	-0.50	178.73	-7.26	-7.27	157.85	0.34	9.00	8.38	0.62
46	148.96	2.17	-1.07	162.78	-8.71	-4.75	150.15	4.57	7.05	7.62	-0.57
47	169.23	-4.47	-0.83	181.89	131.60	-10.10	170.78	5.53	7.40	7.85	-0.45
49	156.88	13.50	-0.61	187.00	15.99	-14.53	160.38	13.15	7.05	6.90	0.15
External validation											
6		5.35	-0.42	188.82	134.59	-0.29	160.48	10.27	8.52	7.85	0.67
14	137.17	-4.54	-0.34	177.15	150.03	-0.74	145.80	1.21	8.70	8.46	0.24

Table S1. Results of internal and external prediction for model 1, and values of the selected descriptors (cont.)

Compound	Molecular descriptor								Real pIC ₅₀	Pred. pIC ₅₀	Residual
	20_17_17_LJ	11_10_12_C	18_24_22_LJ	17_15_15_LJ	19_10_19_LJ	10_18_23_C	20_17_16_LJ	12_21_17_C			
22	155.40	-3.43	-0.45	164.60	134.50	-9.40	166.55	-14.39	7.60	7.26	0.34
24	160.20	0.11	-0.24	167.53	-7.41	-9.52	168.26	-9.28	6.52	6.85	-0.33
26	159.89	-5.46	-0.34	155.76	-7.26	-2.07	169.71	7.47	7.24	7.53	-0.29
28	160.38	-4.52	-0.42	158.90	-5.66	-2.30	192.60	6.71	7.05	7.28	-0.23
33	160.58	-4.21	-0.80	160.85	130.68	-6.93	170.18	-1.24	7.17	7.54	-0.37
38	162.18	-3.74	-0.50	171.29	-1.58	-9.28	159.64	0.09	7.70	7.43	0.27
41	145.73	-1.93	-0.98	157.25	132.07	0.48	152.26	39.52	8.40	8.77	-0.37
48	161.30	4.87	-0.58	168.30	51.32	-5.38	156.46	-0.31	7.05	7.15	-0.10

pIC₅₀: $-\log IC_{50}$ (IC₅₀: half-maximal inhibitory concentration); Pred. pIC₅₀: predicted pIC₅₀.

