Development and Use of Hydrophobic Surface Area (HSA) Descriptors for Computer-Assisted Quantitative Structure-Activity and Structure-Property Relationship Studies

Stanton, D.T.; Mattioni, B.E.; Knittel, J.J.; Jurs, P.C.

SUPPORTING INFORMATION

The following table contains the observed and computed activity values for the 47 biaryl amides used in the development of the MIC model. The compounds are identified in the text using the numbers shown.

The structures and data were taken from previous work by Stanton, et al., *J. Chem. Inf. Comput. Sci.*, **2003**. (in press). The structures are identified using the same numbers used in the previous work.

Observed and computed (Fitted) activity values for the 47 biarylamides.

Compound Number	Observed Activity (Log 1/MIC, μM)	Fitted Activity (Log 1/MIC, μM)
1	-0.544	-0.344
2	-1.668	-1.328
3	-1.279	-0.952
4	-1.750	-1.637
5	-0.716	-0.993
6	-0.813	-0.844
7	-1.398	-1.504
8	-2.000	-1.992
9	-1.636	-1.354
10	-1.248	-1.454
11	-1.549	-1.471
12	-0.544	-1.004
13	-1.045	-1.171
14	-1.297	-1.378
15	-1.900	-1.895
16	-0.544	-0.368
17	-0.301	-0.464
18	-0.602	-0.416
19	-1.549	-1.622
20	-0.944	-1.257
21	-0.716	-0.672
22	-0.643	-0.777
23	-0.919	-0.988
24	-0.544	-0.547
25	-0.892	-0.859
26	-0.447	-0.387
27	-1.449	-1.833
28	-1.449	-1.273
29	-1.449	-1.397
30	-0.845	-1.009
31	-1.498	-1.659
32	-1.248	-1.344
33	-1.097	-1.100
34	-1.941	-1.561
35	-1.498	-1.338
36	-1.519	-1.301
37	-1.849	-1.681
38	-0.279	-0.409
39	-0.806	-0.650
40	-0.613	-0.802
41	-1.818	-1.651
42	-1.076	-1.188
43	-0.041	-0.110
44	-0.519	-0.657
45	-1.149	-1.110
46	-1.196	-1.035
47	-1.667	-1.711

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SUPPORTING INFORMATION

The following structures are those used in the development of the MIC model for the biaryl amides. The compounds are identified in the text using the numbers shown.

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SUPPORTING INFORMATION

The following table contains the observed and computed activity values for the 97 structures used in the development of the two blood-brain barrier penetration models (both with and without including the HSAs). The compounds are identified in the text using the numbers with the “**BB-**” prefix, as shown.

Observed and computed activity values for the 97 structures used in the development of the two blood-brain barrier penetration models (both with and without including the HSAs).

Compound ID	Observed Log BB	Fitted Log BB (5-var. Model excluding the HSAs)	Fitted Log BB (4-var. Model including the HSA)
BB-001	-0.745	-0.827	-0.755
BB-002	-0.700	-0.744	-0.675
BB-003	-1.300	-1.565	-1.281
BB-004	-1.060	-1.739	-1.660
BB-005	-0.730	-0.954	-0.538
BB-006	0.300	0.090	0.581
BB-007	-2.000	-1.395	-1.329
BB-008	-1.820	-1.234	-1.748
BB-009	1.440	0.743	0.608
BB-010	-1.880	-1.204	-1.158
BB-011	0.140	0.240	0.618
BB-012	0.220	-0.132	0.281
BB-013	-0.120	-0.763	-0.368
BB-014	-0.240	-0.286	0.231
BB-015	-1.340	-0.752	-1.251
BB-016	0.390	-0.133	-0.005
BB-017	-0.280	-0.406	-0.344
BB-018	-0.300	-0.446	-0.767
BB-019	-1.260	-0.844	-1.007
BB-021	1.000	0.333	0.582
BB-022	-0.270	-0.528	-0.447
BB-023	0.690	0.255	0.694
BB-024	0.440	0.128	0.436
BB-025	0.360	0.135	0.032
BB-026	-0.071	-0.151	0.020
BB-027	-1.120	-0.804	-0.614
BB-028	-1.540	-1.530	-1.623
BB-029	0.550	1.424	0.647
BB-030	0.044	0.004	-0.403
BB-031	0.490	0.273	0.206
BB-032	0.830	0.911	0.930
BB-033	-1.230	-0.705	-0.758
BB-034	-0.460	-0.324	-0.234
BB-035	0.886	0.762	0.833
BB-036	1.060	1.259	1.017
BB-037	-0.820	-1.632	-1.793
BB-038	-0.670	-0.399	-0.212
BB-039	-0.430	-0.452	-0.648
BB-041	1.200	0.806	0.790
BB-042	1.230	1.210	1.088
BB-043	0.079	0.425	0.343
BB-044	0.000	0.293	0.337
BB-045	-0.160	-0.128	0.195
BB-047	-0.660	-0.594	-0.534
BB-048	-1.570	-0.865	-1.157
BB-049	-0.340	0.043	0.050
BB-050	0.250	-0.074	0.042
BB-051	-0.720	-1.215	-1.370
BB-052	-1.700	-0.759	-0.728
BB-053	-0.020	-0.001	-0.038

Observed and computed activity values for the 97 structures used in the development of the two blood-brain barrier penetration models (both with and without including the HSAs).

Compound ID	Observed Log BB	Fitted Log BB (5-var. Model excluding the HSAs)	Fitted Log BB (4-var. Model including the HSA)
BB-054	0.000	-0.105	-0.047
BB-055	-1.420	-1.125	-0.842
BB-056	-1.300	-1.152	-1.283
BB-057	-1.150	-0.906	-1.347
BB-058	0.120	-0.548	-0.405
BB-059	-1.170	-0.577	-0.825
BB-060	-0.180	-0.381	-0.674
BB-061	-0.180	-0.134	-0.092
BB-062	0.110	0.077	0.333
BB-064	-0.055	-0.615	-0.590
BB-065	-0.097	-0.132	-0.006
BB-066	-0.290	-0.844	-0.712
BB-067	-0.500	-0.595	-0.718
BB-068	-1.400	-0.778	-0.492
BB-069	-0.520	-0.565	-0.522
BB-070	-0.060	0.244	0.302
BB-071	-0.310	-0.391	-0.593
BB-072	-0.040	-0.479	-0.773
BB-073	0.240	0.161	-0.011
BB-074	0.420	0.141	-0.032
BB-075	-0.300	0.145	0.192
BB-076	-0.220	-0.130	-0.023
BB-077	-1.100	-0.388	-0.506
BB-078	0.130	0.103	0.060
BB-079	-0.420	-0.115	-0.256
BB-080	0.810	0.861	0.680
BB-081	0.900	0.767	0.683
BB-082	0.270	0.426	0.159
BB-083	0.370	0.660	0.592
BB-084	0.350	0.502	0.171
BB-086	0.370	0.633	0.559
BB-087	1.040	0.784	0.515
BB-088	0.800	0.756	0.638
BB-089	0.930	0.768	0.797
BB-090	0.970	0.769	0.656
BB-091	1.010	0.776	0.586
BB-092	0.080	0.487	0.203
BB-093	-0.080	-0.334	0.005
BB-094	0.000	-0.040	0.492
BB-095	-0.170	-0.156	-0.057
BB-096	0.760	0.755	0.605
BB-097	0.400	0.637	0.353
BB-098	0.340	0.330	0.252
BB-099	-0.160	-0.212	-0.048
BB-100	-0.150	-0.188	-0.037
BB-101	-0.150	-0.457	-0.058
BB-102	-0.160	-0.304	-0.116

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SUPPORTING INFORMATION

The following structures are those used in the development of the blood-brain barrier (BBB) penetration models. The compounds are identified in the text using the numbers with the “**BB-**” prefix, as shown.

These structures were originally taken from the work described by Rose et al., *J. Chem. Inf. Comput. Sci.* **2002**, 42, 651-666. Corrections were made to several of the structures from the original report. Those corrections are reflected in this compilation.