ERRATA

ADME Evaluation in Drug Discovery. 3. Modeling Blood-Brain Barrier Partitioning Using Simple Molecular Descriptors [*J. Chem. Inf. Comput. Sci. 43*, 2137−2152 (2003)] By T. J. Hou and X. J. Xu*. College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China

Pages 2140−2150. Six compounds in the training set are duplicates to six compounds in the test sets. These six compounds are 19, 21, 35, 51, 63, and 76 and should be eliminated from the training set. So the number of compounds in the training set should be 72, not 78. Moreover, the 2D structure of compound 8 in Table 1 is wrong. The QSAR models have been recalculated, yielding the following equations and associated statistical parameters. The corrected Tables 1, 4, and 5 are also listed.

$$\log BB = -0.552 + 0.236 \log P \quad (14)$$

$$(n = 72,\ r = 0.499,\ s = 0.659,\ F = 23.1)$$

$$\log BB = 0.571 - 0.0156PSA \quad (15)$$

$$(n = 72,\ r = 0.755,\ s = 0.499,\ F = 92.8)$$

$$\log BB = 0.589 - 0.0177HCPSA \quad (16)$$

$$(n = 72,\ r = 0.782,\ s = 0.474,\ F = 110.0)$$

$$\log BB = 0.219 + 0.139 \log P - 0.0158HCPSA \quad (17)$$

$$(n = 72,\ r = 0.835,\ s = 0.421,\ F = 79.4)$$

$$\log BB = 0.00845 + 0.197 \log P - 0.0135HCPSA - 0.0140 < MW - 360 > \quad (21)$$

$$(n = 72,\ r = 0.886,\ s = 0.358,\ F = 82.6)$$

10.1021/ci040020a CCC: $27.50
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Table 1. Compounds Used To Obtain the Training Set

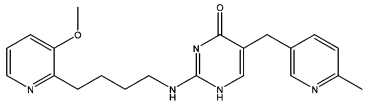
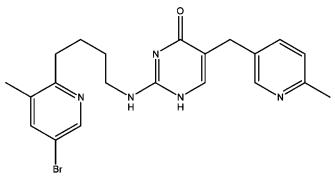
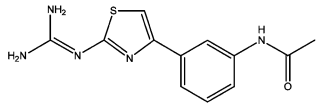
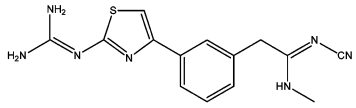
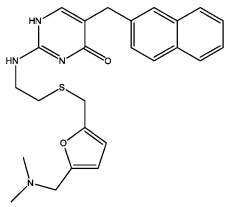
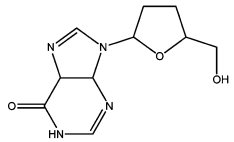
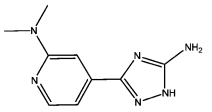
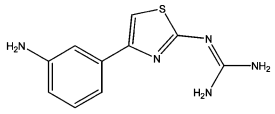
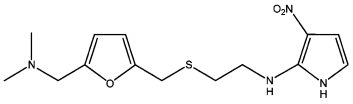
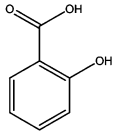
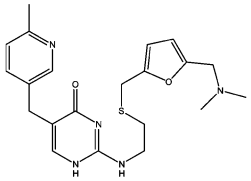
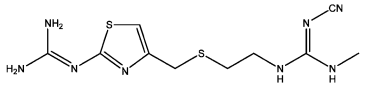
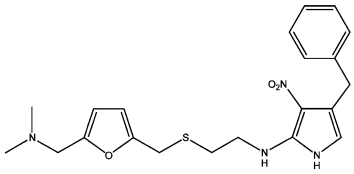
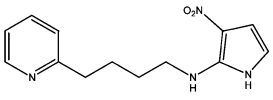
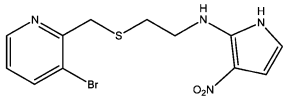
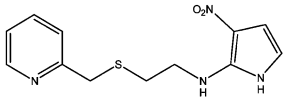
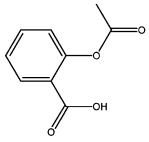
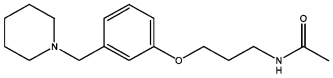
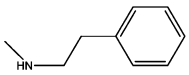
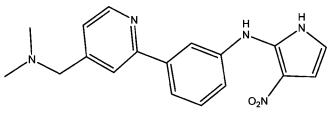
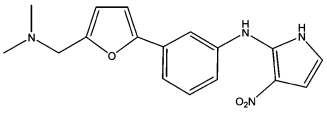
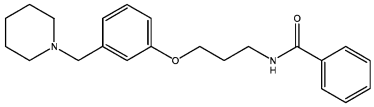
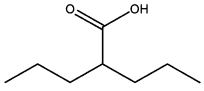
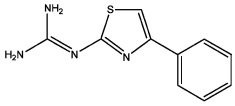
ID and name	ID and name	ID and name
1. icotidine 	2. temelastine 	3. BBcpd16 (guanidinothiazole der.) 
4. BBcpd58 (guanidinothiazole der.) 	5. SK&F 93319 	6. didanosine 
7. BBcpd10 	8. BBcpd57 (guaidinothiazole der.) 	9. BBcpd17 (ranitidine analog) 
10. salicylic acid 	11. lupitidine 	12. tiotidine 
13. BBcpd60 (ranitidine analog) 	14. zidovudine 	15. BBcpd12 (cimetidine derivative) 
16. BBcpd13 (cimetidine derivative) 	17. acetylsalicylic acid 	18. BBcpd20 (ranitidine analog) 
20. Y-G14 	22. BBcpd19 (ranitidine analog) 	23. BBcpd18 (ranitidine analog) 
24. BBcpd21 (ranitidine analog) 	25. valproic acid 	26. BBcpd15 (guanidinothiazole der.) 

Table 1 (Continued)

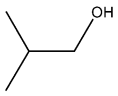
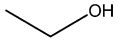
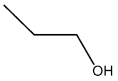
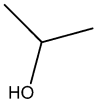
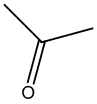
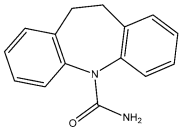
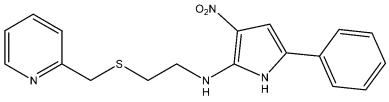
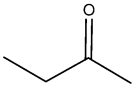
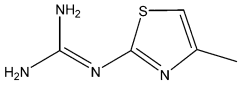
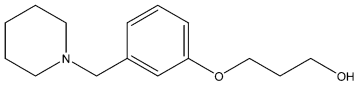
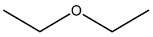
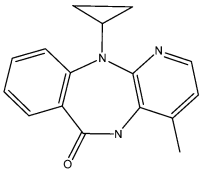
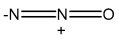
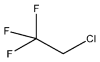
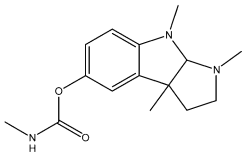
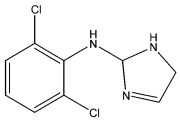
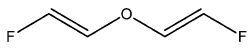
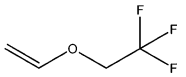
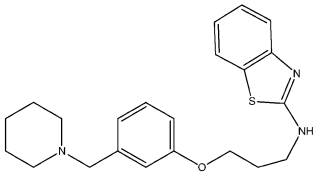
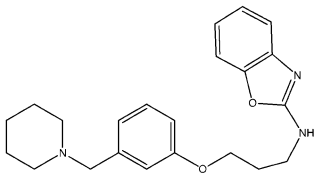
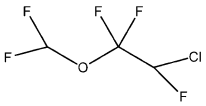
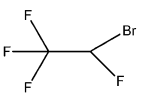
ID and name	ID and name	ID and name
27. 2-methylpropanol 	28. ethanol 	29. 1-propanol 
30. 2-propanol 	31. propanole 	32. carbamazepine 
33. BBcpd14 (cimetidine derivative) 	34. butanone 	36. ICI 17148 
37. BBcpd22 (ranitidine analog) 	38. diethyl ether 	39. nevirapine 
40. nitrogen	41. nitrous oxide 	42. methane 
43. 1,1,1-trifluoro-2-chloroethane 	44. physostigmine 	45. clonidine 
46. 	47. fluroxene 	48. zolantidine (ranitidine analog) 
49. BBcpd26 (ranitidine analog) 	50. enfluane 	52. teflurane 

Table 1 (Continued)

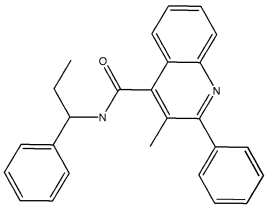
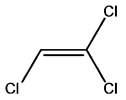
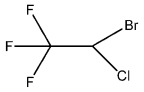
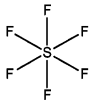
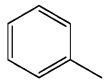
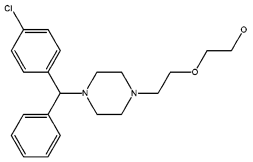
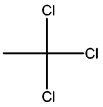
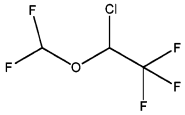
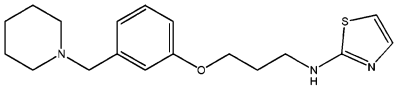
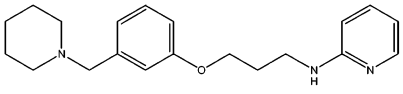
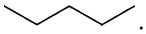
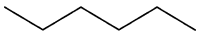
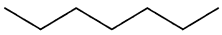
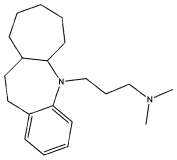
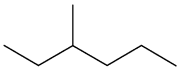
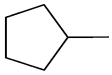
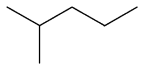
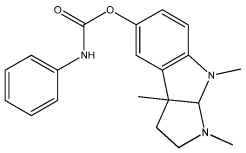
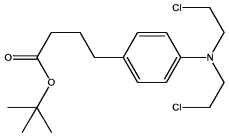
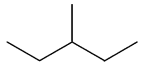
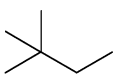
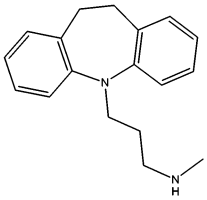
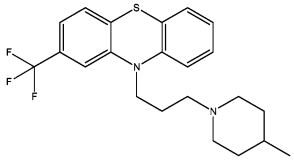
ID and name	ID and name	ID and name
53. SB-222200 	54. trichloroethene 	55. halothane 
56. sulfur hexafluoride 	57. benzene 	58. toluene 
59. hydroxyzine 	60. 1,1,1-trichloroethane 	61. isofluane 
62. BBcpd24 (ranitidine analog) 	64. BBcpd23 (ranitidine analog) 	65. pentane 
66. hexane 	67. heptane 	68. amitryptalline 
69. 3-methylhexane 	70. methylcyclopentane 	71. 2-methylpentane 
72. phenserine 	73. terbutylchlorambucil 	74. 3-methylpentane 
75. 2,2-dimethylbutane 	77. desipramine 	78. trifluoroperazine 

Table 4. Experimental and Computed log*BB* Values for Compounds in the Training Set

ID	logBB_{exp}	log*P*	PSA	HCPSA	MW_{360}	logBB_{cal}	residue	ID	logBB_{exp}	log*P*	PSA	HCPSA	MW_{360}	logBB_{cal}	residue
1	−2.00	1.72	76.79	76.79	19.46	−0.90	−1.10	40	0.03	0.00	67.06	0.00	0.00	0.05	−0.02
2	−1.88	3.01	69.36	69.36	82.36	−1.42	−0.46	41	0.03	−0.57	80.98	0.00	0.00	−0.07	0.10
3	−1.57	0.85	99.74	89.70	0.00	−0.98	−0.59	42	0.04	0.53	0.00	0.00	0.00	0.16	−0.12
4	−1.54	1.02	125.07	109.41	0.00	−1.21	−0.33	43	0.08	1.90	0.00	0.00	0.00	0.44	−0.36
5	−1.30	3.55	58.74	58.74	88.59	−1.25	−0.05	44	0.08	0.99	41.68	41.68	0.00	−0.31	0.39
6	−1.30	−1.05	92.57	92.57	0.00	−1.41	0.11	45	0.11	1.92	35.44	35.44	0.00	−0.03	0.14
7	−1.17	0.44	85.06	85.06	0.00	−1.00	−0.17	46	0.13	1.19	7.00	7.00	0.00	0.20	−0.07
8	−1.15	0.92	103.47	93.40	0.00	−1.01	−0.14	47	0.13	1.62	7.56	7.56	0.00	0.28	−0.15
9	−1.12	1.88	83.65	79.01	0.00	−0.62	−0.50	48	0.14	4.84	32.92	32.92	21.54	0.31	−0.17
10	−1.10	2.21	57.49	57.49	0.00	−0.26	−0.84	49	0.22	4.58	41.30	41.30	5.48	0.37	−0.15
11	−1.06	1.38	69.25	69.25	53.55	−1.35	0.29	50	0.24	2.78	8.15	8.15	0.00	0.51	−0.27
12	−0.82	−0.32	136.16	118.01	0.00	−1.60	0.78	52	0.27	2.13	0.00	0.00	0.00	0.49	−0.22
13	−0.73	3.66	80.50	77.09	54.53	−0.99	0.26	53	0.30	5.61	34.22	34.22	20.49	0.46	−0.16
14	−0.72	−0.97	133.67	99.88	0.00	−1.49	0.77	54	0.34	2.26	0.00	0.00	0.00	0.52	−0.18
15	−0.67	3.10	69.05	69.05	0.00	−0.23	−0.44	55	0.35	2.75	0.00	0.00	0.00	0.62	−0.27
16	−0.66	2.16	83.75	79.52	0.00	−0.57	−0.09	56	0.36	3.03	0.00	0.00	0.00	0.68	−0.32
17	−0.50	1.22	64.61	64.61	0.00	−0.56	0.06	57	0.37	2.06	0.00	0.00	0.00	0.47	−0.10
18	−0.46	1.52	39.37	39.37	0.00	−0.16	−0.30	58	0.37	2.50	0.00	0.00	0.00	0.57	−0.20
20	−0.42	0.49	25.21	25.21	0.00	−0.19	−0.23	59	0.39	2.72	33.23	33.23	14.91	−0.04	0.43
22	−0.28	2.96	82.81	79.44	0.00	−0.40	0.12	60	0.40	2.39	0.00	0.00	0.00	0.54	−0.14
23	−0.27	3.00	81.86	77.82	0.00	−0.37	0.10	61	0.42	2.62	7.64	7.64	0.00	0.49	−0.07
24	−0.24	3.29	36.47	36.47	0.00	0.24	−0.48	62	0.44	3.28	33.4	33.4	0.00	0.28	0.16
25	−0.22	2.09	44.28	44.28	0.00	−0.11	−0.11	64	0.69	3.24	33.22	33.22	0.00	0.27	0.42
26	−0.18	1.73	72.57	62.45	0.00	−0.43	0.25	65	0.76	2.96	0.00	0.00	0.00	0.66	0.10
27	−0.17	0.57	23.98	23.98	0.00	−0.16	−0.01	66	0.80	3.47	0.00	0.00	0.00	0.77	0.03
28	−0.16	−0.10	24.93	24.93	0.00	−0.31	0.15	67	0.81	3.97	0.00	0.00	0.00	0.87	−0.06
29	−0.16	0.24	24.94	24.94	0.00	−0.24	0.08	68	0.83	4.43	4.54	4.54	0.00	0.91	−0.08
30	−0.15	0.30	23.81	23.81	0.00	−0.21	0.06	69	0.90	3.98	0.00	0.00	0.00	0.87	0.03
31	−0.15	−0.09	20.56	20.56	0.00	−0.25	0.10	70	0.93	3.16	0.00	0.00	0.00	0.70	0.23
32	−0.14	2.77	43.34	43.34	0.00	0.04	−0.18	71	0.97	3.46	0.00	0.00	0.00	0.77	0.20
33	−0.12	3.93	81.53	79.23	8.46	−0.32	0.20	72	1.00	3.30	36.56	36.56	0.00	0.24	0.76
34	−0.08	0.44	18.73	18.73	0.00	−0.11	0.03	73	1.00	4.03	19.64	19.64	0.32	0.62	0.38
36	−0.04	−0.06	74.17	64.04	0.00	−0.82	0.78	74	1.01	3.47	0.00	0.00	0.00	0.77	0.24
37	−0.02	1.78	34.58	34.58	0.00	−0.05	0.03	75	1.04	3.45	0.00	0.00	0.00	0.76	0.28
38	0.00	1.12	7.18	7.18	0.00	0.18	−0.18	77	1.20	3.88	14.58	14.58	0.00	0.66	0.54
39	0.00	2.50	40.83	40.83	0.00	0.02	−0.02	78	1.44	6.63	4.46	4.46	46.52	0.71	0.73

Table 5. Experimental and Predicted log*BB* Values for Compounds Comprising Test Sets Using Equation 21

ID	logBB_{exp}	HCPSA	log*P*	MW_{360}	logBB_{cah}	residue	ID	logBB_{exp}	HCPSA	log*P*	MW_{360}	logBB_{cah}	residue
B1[c]	**−1.30**	**40.85**	**2.37**	**0.00**	**−0.01**	**−1.29**	C6	−0.18	43.69	3.68	0.00	0.23	−0.41
B2	−1.40	44.10	−0.12	0.00	−0.57	−0.83	C7	0.11	42.68	2.27	0.00	−0.05	0.16
B3	−0.43	59.67	2.13	0.00	−0.31	−0.12	C8	0.55	43.79	1.50	0.00	−0.23	0.78
B4	0.25	36.28	2.77	0.00	0.14	0.11	C9	0.12	79.95	2.05	0.00	−0.60	0.72
B5	−0.30	24.56	0.65	0.00	−0.15	−0.15	C10	−1.42	78.16	0.46	0.00	−0.90	−0.52
B6	−0.06	14.05	0.82	0.00	0.03	−0.09	C11	0.04	40.54	3.1	0.00	0.15	−0.11
B7	−0.42	43.62	0.26	0.00	−0.48	0.06	C12	0.49	19.35	2.62	0.00	0.33	0.16
B8	−0.16	35.12	2.18	0.00	0.03	−0.19	**C13**[c]	**−1.26**	**67.29**	**3.37**	**0.00**	**−0.15**	**−1.11**
B9	0.00	47.70	2.91	0.00	0.01	−0.01	C14	0.61	64.09	2.23	0.00	−0.35	0.96
B10	−0.34	62.95	1.95	0.00	−0.39	0.05	C15	0.39	37.72	2.73	0.00	0.11	0.28
B11	−0.30	50.02	1.21	0.00	−0.37	0.07	C16	0.83	3.94	4.11	0.00	0.85	−0.02
B12	−1.34	71.21	0.03	13.80	−1.09	−0.25	C17	1.20	9.72	5.32	0.00	1.02	0.18
B13	−1.82	92.94	−0.96	29.80	−1.82	0.00	C18	0.36	21.71	3.36	0.00	0.45	−0.09
B14	0.89	3.76	4.32	0.00	0.89	0.00	C19	−0.70	51.08	5.13	94.61	−0.90	0.20
r						0.94	C20	1.23	4.01	3.99	0.00	0.82	0.41
MUE[a]						0.15	C21	1.06	3.98	4.62	0.00	0.95	0.11
SSE[b]						0.86	C22	0.24	3.71	5.37	10.59	0.96	−0.72
rmse						0.26	C23	−0.52	49.26	1.16	0.00	−0.37	−0.15
C1	−0.29	62.68	−0.89	0.00	−0.98	0.69	*r*						0.78
C2	−0.06	45.53	−0.53	0.00	−0.67	0.61	*MUE*[a]						0.38
C3	−0.10	20.56	1.51	0.00	0.09	−0.19	*SSE*[b]						4.75
C4	−1.23	70.08	1.33	0.00	−0.62	−0.61	rmse						0.46
C5	−0.31	54.76	0.61	0.00	−0.56	0.25							

[a] *MUE* represents mean unsigned error. [b] *SSE* represents sum of square error. [c] **B1** and **C13** are not included in the calculations of *r*, *MUE*, *SSE*, and rmse.

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