Additions and Corrections

2001, Volume 44

Jay T. Goodwin, Robert A. Conradi, Norman F. H. Ho, and Philip S. Burton*: Physicochemical Determinants of Passive Membrane Permeability: Role of Solute Hydrogen-Bonding Potential and Volume.

Page 3722. In line 25, "... from log $P_{\text{hydrocarbon/water}}$ − log $P_{\text{octanol/water}}$..." should be "... from log $P_{\text{octanol/water}}$ − log $P_{\text{hydrocarbon/water}}$...". In Table 1, the values for log p_{trans} should be *negative* in sign.

Page 3733. In Table 2, the values for log $P_{\text{octanol/water}}$ for compounds **1** and **2**, all values of log $P_{\text{hydrocarbon/water}}$, and all values of log $P_{\text{heptane/glycol}}$ should be negative in sign.

Table 1. Permeability Data for Compounds **1**−**12**

	p_{eff}			$p_{\text{eff,verapamil}}$						log
compound	AP → BL[a]	BL → AP[a]	ratio[b]	AP → BL[a]	BL → AP[a]	ratio[b]	p_{mono}[c]	p_{para}[c]	p_{trans}[c]	p_{trans}
1	0.17	0.24	1.4	0.14	0.12	0.9	0.14	0.60	0.00	
2	0.24	0.38	1.6	0.25	0.25	1.0	0.25	0.56	0.00	
3a	0.91	1.84	2.0	0.89	0.78	0.9	0.9	0.48	0.42	−6.38
4	1.41	2.24	1.6	1.52	1.42	0.9	1.56	0.44	1.12	−5.95
5a	2.75	5.19	1.9	2.80	2.64	0.9	2.95	0.37	2.58	−5.59
6	7.20	14.5	2.0	8.93	9.02	1.0	10.7	0.36	10.3	−4.99
7	21.9	20.6	0.9	22.6	20.8	0.9	38.4	0.77	37.6	−4.42
8	24.6	22.9	0.9	25.2	23.5	0.9	46.5	0.71	45.8	−4.34
9a	34.5	32.4	0.9	35.1	33.0	0.9	97.0	0.60	96.4	−4.02
10	42.6	47.2	1.1	47.4	47.7	1.0	343	0.56	342	−3.47
11a	52.0	56.8	1.1	55.1	59.5	1.1				
12	58.3	58.4	1.0	55.5	55.6	1.0				

[a] AP → BL = apical-to-basolateral permeability; BL → AP = basolateral-to-apical permeability. [b] Ratio of BL → AP to AP → BL permeabilities. [c] p_{mono} = monolayer permeability, p_{para} = paracellular permeability, p_{trans} = transcellular permeability; permeabilities are given in units of 10^{-6} centimeters per second. Standard errors in permeabilities are ≤10%, $n \geq 4$, except for compounds **7**, **8**, **9a**, and **10**, where the standard error is ≤30%. The mass balances for all permeabilities determined are 100% (±10%).

Table 2. Physicochemical Data for Compounds **1**−**12**

compound	MW	tHB[a]	dHB[a]	aHB[a]	log $P_{\text{octanol/water}}$[b]	log $P_{\text{heptane/water}}$[b]	Δ log P[b]	log $P_{\text{heptane/glycol}}$[b]
1	277	6	3	3	−0.30	−6.30	6.00	−6.17
2	291	6	3	3	−0.06	−6.26	6.20	−5.83
3a	319	6	3	3	0.66	−5.33	5.99	−5.79
4	333	6	3	3	1.24	−4.61	5.85	−5.43
5a	367	6	3	3	1.44	−4.15	5.59	−5.34
6	373	6	3	3	2.40	−3.41	5.81	−5.03
7	220	4	2	2	0.48	−3.73	4.21	−5.00
8	234	4	2	2	0.76	−3.53	4.29	−4.40
9a	262	4	2	2	1.59	−2.64	4.23	−3.77
10	276	4	2	2	2.03	−2.14	4.17	−3.69
11a	310	4	2	2	2.32	−2.00	4.32	−3.70
12	316	4	2	2	3.13	−0.90	4.03	−3.41

[a] tHB = total number of solute hydrogen bonds possible, dHB = number of donor hydrogen bonds, aHB = number of acceptor hydrogen bonds. [b] Standard error for log $P_{\text{octanol/water}} \leq 15\%$, for log $P_{\text{heptane/water}} \leq 10\%$, for $\Delta \log P \leq 15\%$, and for log $P_{\text{heptane/ethylene glycol}} \leq 5\%$; $n \geq 2$ for all solvent partition experiments.

JM0200963

10.1021/jm0200963
Published on Web 04/10/2002