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Corrigendum

Corrigendum for Biophysical Chemistry 124 (2006) 279–291

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An error was discovered in the computer script used to calculate the relative free energies in the reduced models that were reported in Table 2. In some of the calculations, the ion position was not fixed at the origin and the rigid geometry of the TIP3 water molecules was not constrained. This resulted in free energies that were too favorable for Na^+ over K^+ in some of the free energy perturbation molecular dynamics (FEP/MD) calculations. The corrected values are given in the amended version of Table 2. Furthermore, the text (p. 287, left column, line 8) should be revised as: "For example, as shown in Table 2, a binding site with four carbonyl groups and four water molecules is considerably less selective for K^+ over Na^+". This correction explains and resolves the apparent discrepancy between different computations carried out on identical reduced models noted elsewhere [1,2]. The corrected values display the same trend as reported previously, albeit the variations in free energies are smaller. The general conclusions about the importance of the chemical type of ligands on the ion selectivity remain unchanged.

Table 2
The variation of ΔΔG as a function of a toy model ligand composition[1].

Number of carbonyls	Number of water molecules	ΔΔG (kcal/mol)
8	0	6.2
7	1	4.9
6	2	4.0
5	3	3.2
4	4	2.5
6	0	3.6
5	1	3.2
4	2	2.5

[1] The difference in hydration free energy between Na^+ and K^+ is 18.4 kcal/mol. The cation Lennard–Jones parameters Emin and Rmin/2 were −0.0469, 1.40375 and −0.087, 1.76375, for Na^+ and K^+, respectively; pair-specific Lennard–Jones parameters for the ion–carbonyl interactions used for Na^+ and K^+ were −0.1021763, 3.64275 and −0.07502, 3.2975, respectively. For these parameters, the difference in hydration free energy between Na^+ and K^+ is 18.4 kcal/mol.

References

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[2] S. Varma, D.M. Rogers, L.R. Pratt, S.B. Rempe, Perspectives on: ion selectivity: design principles for K^+ selectivity in membrane transport, J. Gen. Physiol. 137 (2011) 479–488.

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