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Erratum

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Correction to Multiscale Reactive Molecular Dynamics for Absolute pK_a Predictions and Amino Acid Deprotonation

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With this erratum, we present a correction to the equation for the calculation of a pK_a from a PMF (eq 9 in the original publication)[1]

$$\mathrm{p}K_a = -\log\left[C^0 \int_0^{\dagger} 4\pi r^2 \exp[-\beta w(r)]\, \mathrm{d}r\right]^{-1}$$

where $w(r)$ is the free energy from the PMF, and β is the product of the simulation temperature and the Boltzmann constant. The integral is calculated from zero to the transition state, as denoted by †. C^0 is the standard state concentration whose value is 1 molecule/1660 Å^3 and results from the entropic freedom that is gained by the proton when it dissociates from the acid.[2,3] The pK_a was calculated correctly in the original publication; this correction does not influence the results presented therein.[1]

REFERENCES

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