JCTC Journal of Chemical Theory and Computation

Erratum

pubs.acs.org/JCTC

Correction to Balanced Protein–Water Interactions Improve Properties of Disordered Proteins and Non-Specific Protein Association

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J. Chem. Theory Comput. **2014**, *10* (11), 5113−5124. DOI:10.1021/ct500569b

In our paper[1] we did not properly acknowledge the contribution by Head-Gordon and co-workers[2] (ref 41 of our manuscript). These authors used a similar modification of the mixing rules for protein−water interactions, although the correction was applied on a per-atom basis to both the characteristic distance (sigma) and energy (epsilon) parameters rather than using a single scaling factor for epsilon as we did. Head-Gordon and co-workers used extensive solvation free energy data on model organic compounds to fit their parameters, whereas we used FRET efficiencies for a single unfolded protein (cold shock protein) to estimate our scaling parameter. Overall, we reached qualitatively similar conclusions regarding the solvation free energies of force fields with Amber 94[3] Lennard-Jones parameters being too unfavorable, as reported previously by these authors.[2] The more systematic approach of Nerenberg et al. showed a mean signed error of solvation free energies close to zero for their optimized force field.[2]

We would also like to make a specific correction to the sentence on page 5115, which is inaccurate: "Recently, a full parametrization of protein Lennard-Jones parameters to reproduce solvation free energies showed some promising results, but unfortunately resulted in very unstable folded proteins". Instead, it should read as follows: "Recently, a rescaling of protein−water Lennard-Jones parameters to reproduce solvation free energies showed some promising results for correcting protein−protein interactions using concentrated solutions of glycine and leucine dipeptides. In conjunction with a 12-10 van der Waals (vdW) term to replace the standard 12-6 vdW potential to model the nonelectrostatic part of the hydrogen bonding between the backbone carbonyl oxygens and amide protons, this modification resulted in stable folded proteins."

REFERENCES

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Published: March 18, 2015

DOI: 10.1021/acs.jctc.5b00219
J. Chem. Theory Comput. 2015, 11, 1978−1978