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Addition/Correction

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Correction to "Mutual Exclusion of Urea and Trimethylamine *N*-Oxide from Amino Acids in Mixed Solvent Environment"

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Supporting Information

In a recent publication,[1] we have made an error by incorrectly using the TMAO force-field parameters developed by Netz et al.[2] The correct σ-value for the H atoms in TMAO model by Netz is 0.2101 nm. We have rerun all the simulations involving Netz TMAO force-fields. However, we have not observed any significant changes in our data and all the conclusions drawn from our work remained unaltered. In this correction, we note the changes made in Figure 3 in the main paper as well as in Tables S1 and Table S7, Figure S3, and section 10 in the Supporting Information.

We sincerely apologize to the readers for any inconvenience caused by these errors.

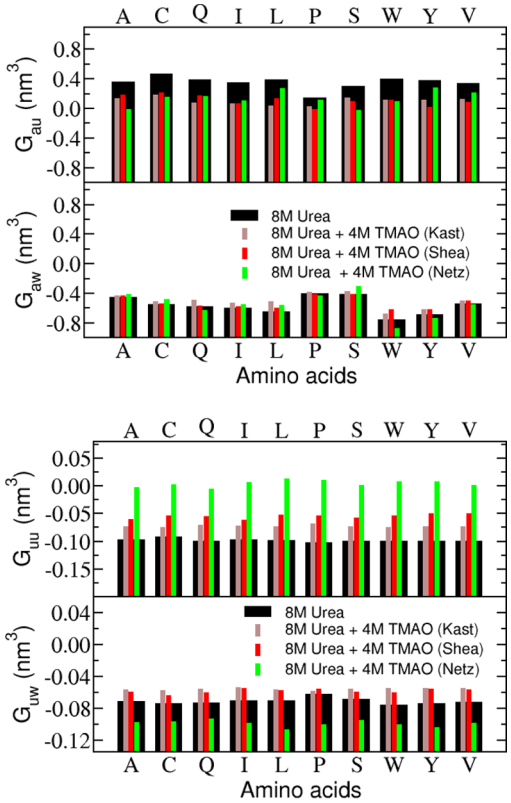

Figure 3. Comparison of KBIs with different TMAO force-fields: (a) Kast model,[3] (b) Netz model,[2] and (c) Shea model.[4] Upper panel: amino acid-urea (G_{au}) and amino acid−water (G_{aw}) Kirkwood−Buff integrals for amino acids in 8 M urea, and in the mixture of 8 M urea and 4 M TMAO solutions. Lower panel: urea−urea (G_{uu}) and urea−water (G_{uw}) Kirkwood−Buff integrals for amino acids in pure water, 8 M urea and in mixed 8 M urea and 4 M TMAO solutions. Netz model shows a very high urea−urea aggregation and eventually a lower urea−water KBI.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jpclett.5b02536.

The Supporting Information file contains simulation details including the parameters of the TMAO force fields (with the correction made to the Netz parameters), relevant KBI data and preferential binding coefficients for all systems studied, comparison of TMAO−water KBIs for different TMAO force fields (using the correct Netz parameters), comparison of KBIs obtained with GROMOS54a7 alanine + SPC/E water and with OPLS-AA alanine + TIP3P water, density maps of urea and TMAO around proline molecules and liquid phase transfer free energies of alanine and neopentane (a model hydrophobe) between water and 1 M TMAO−water solution obtained from free energy calculations (using the correct Netz parameters). (PDF)

■ ACKNOWLEDGMENTS

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■ REFERENCES

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