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Direct comparison of the theory of molecular solvation with molecular dynamics and experiment TYLER LUCHKO, IN SUK JOUNG, GEORGE GIAMBASU, BioMaPS Institute, Rutgers University, DARRIN YORK, DAVID A. CASE, BioMaPS Institute and Chemistry & Chemical Biology, Rutgers University — The reference interaction site model (RISM) provides complete equilibrium sampling of bulk solvent and solvent around a solute of arbitrary shape and size at a fraction of the computational cost of explicit solvent molecular dynamics (MD). Though based on first principles, approximations must be made to achieve numerical solutions. In this study, we first compare RISM to MD and experimental results for bulk solutions of aqueous monovalent ions using the Joung-Cheatham parameters with SPC/E and TIP3P water subject to several approximate closures. Then, using the same parameters and approximations, we evaluate the distribution of water and ions around a 24 base pair strand of DNA, once again, comparing to MD results and experimental observables. In both cases RISM gives the correct qualitative behavior and, often, the correct quantitative behavior. However, this strongly depends on the closure relation used, with higher order, HNC-like closures usually giving better results.

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