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Comparison of Hydration Free Energy from Orthogonal Space, Random Walk, Polarizable Force Field, and Bennett Acceptance Ratio
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— The Orthogonal Space Random Walk (OSRW) method has shown enhanced sampling efficiency in free energy calculations from previous studies. In this study, the implementation of OSRW in accordance with the polarizable AMOEBA force field in TINKER molecular software package is discussed and subsequently applied to the hydration free energy calculation of 20 small organic molecules, among which 15 are positively charged and 5 are neutral. The calculated hydration free energies of these molecules are compared with the results obtained from the Bennett Acceptance Ratio method using the same force field, and excellent agreement is obtained. The convergence and the efficiency of the OSRW are also discussed and compared with BAR. OSRW reduces the computational cost for hydration free energy calculation by almost five-fold. Combining enhanced sampling techniques such as OSRW with polarizable force fields is very promising for achieving both accuracy and efficiency in general free energy calculations.

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