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Locating structural energy minimum of biological molecules in explicit solvent ERIC DYKEMAN, OTTO SANKEY, Arizona State University — Biological molecules in waters often adopt several structural conformers. These structures correspond to the various local energy minima on the solute-solvent potential energy hyper-surface. Methods capable of predicting the various conformations that a molecule can adopt in solution have involved, (naming a few), annealing and replica exchange molecular dynamics simulations. However, implementation of these methods with systems containing explicit solvent still requires large amounts of computation time due to the requirement of a small time step. The recent development of the activation relaxation technique (ART) of Mousseau et al. provides an alternative that may reduce computational costs. Instead of following a Newtonian trajectory, ART locates local energy minima through a series of activations to energy saddles followed by relaxation to a local energy minimum. Here we discuss extensions of the method to explicit solvent models. This development and extension of the technique offers insight into how water affects the potential energy surface of molecules in solution.

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