Invited Talk

Macromolecular Simulations Using Continuum Solvent Models

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It is often useful in computer simulations to use a simple description of solvation effects, instead of explicitly representing the individual solvent molecules. Continuum dielectric models often work well in describing the thermodynamic aspects of aqueous solvation, and approximations to such models that avoid the need to solve the Poisson equation are attractive because of their computational efficiency. I will discuss one approach, the generalized Born model, which is simple and fast enough to be used for molecular dynamics simulations of proteins and nucleic acids. Strengths and weaknesses will be discussed, both for fidelity to the underlying continuum model, and for the ability to replace explicit consideration of solvent molecules in macromolecular simulations. The focus will be on versions of the generalized Born model that have a pairwise analytical form, and therefore fit most naturally into conventional molecular mechanics calculations. I will discuss both static energetic analysis and molecular dynamics simulations using the new methods, looking at pKa calculations and discussing also new ideas that may lead to signficantly different theories over the next few years.