4s Cirse: a Novel Solvation Energy Potential for Simulation and Design of Biomolecules

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Abstract: Accurate solvation models are essential in order to perform accurate simulations of biomolecules. For problems such as flexible protein-protein docking, solvation effects often contribute significantly to the pathway of approach and the final free-energy of interaction. Explicit water significantly adds to the degrees of freedom of the system, hence it cannot be used for an exhaustive protein docking, interface prediction or design calculations. In this poster, I will present results from a novel pairwise solvation model, CIRSE, that has been optimized against the Poisson-Boltzmann solvent approximation. The pairwise nature of our model augmented by a all-atom force-field enables to perform rapid searches in conformation space to predict side-chain conformations at protein interfaces. Further, our folding simulations of small peptides also indicate the suitability of CIRSE for molecular dynamics and Monte-Carlo studies of biomolecules.