سمینار هفتگی ماده چگال نرم

Computing Absolute Binding Affinities by Streamlined Alchemical Free Energy Perturbation (SAFEP) Method

Abstract

Many biological processes are controlled by the interaction between two or more biomolecules which is measured by binding free energy. Nonetheless, accurate computing binding affinity remains a challenge and costly for speeding up the discovery of small molecules and studying the function of protein membranes. The streamlined alchemical free energy perturbation method termed SAFEP [1], introduces a simplified framework for computing absolute binding affinity, significantly reducing computation time. This approach implements a single roto-translational restraint that takes in all ligand binding modes while nullifying the relative motion of the ligand with respect to the receptor. Additionally, SAFEP provides a user-friendly interface using the Colvar module [2] that makes the scheme adaptable to a variety of systems even interacting with symmetric ligands [3]. SAFEP allows the user to integrate other features based on their interests, due to the subtleties of each system [4].

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