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Comparison of the thermodynamic integration and free energy perturbation in the computing alchemical free energy difference

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Abstract

On an atomistic scale, free energy calculations are important for our understanding of biological processes, which provides an insight to grasp the various mechanisms. Over the years, many computational methods have been developed to calculate free energy differences such as geometrical (*e.g*. umbrella sampling) and alchemical methods. In this work, we present alchemical-free energy methods, thermodynamic integration (TI) and free energy perturbation (FEP), to investigate polarization effect of paclitaxel drug. Then, we have compared our simulation studies using TI, FEP, and Hamiltonian replica exchange FEP from the perspective of computational cost and accuracy.

Keywords: free energy perturbation, thermodynamic integration, polarization effect

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