

Internal Webinar

Impact of Macromolecular Crowding on Ligand Recognition Process

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“Macromolecular crowding” typically refers to the mutual impenetrability of various macromolecules in highly concentrated media. Biological environments usually contain various macromolecules in concentrations as high as 300-400 mg/ml occupying a total volume fraction of 30 %-40 % of the entire cellular volume. Biomolecular processes like protein-ligand binding occurring in such heterogeneous crowded media will significantly differ from dilute buffer solutions. In this seminar, I will discuss the impact of crowding on thermodynamics and kinetics of ligand recognition process of a well-studied simple prototypical cavity-ligand system using a hydrophobic cavity and Fullerene molecule as crowder and ligand. We have performed multiple biased and unbiased molecular dynamics (MD) simulations in presence and absence of crowding. Relevant thermodynamic and kinetic information was obtained by calculating free energy profiles, association & dissociation rate constants as a function of crowder concentrations. This study demonstrates that introduction of macromolecular crowders facilitates ligand binding process both kinetically and thermodynamically in relative to a dilute solution situation.

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