Contribution ID: **263** Type: **Invited Speaker**

Molecular Dynamics Simulations and Gaussian Network Model in Improving Protein–Protein Binding Affinity: HIV and Dengue Cases

Tuesday 29 November 2016 10:55 (20 minutes)

Conformational dynamics of proteins have been suggested to play crucial roles in protein-protein binding and dissociation which are the two fundamental steps of protein–protein interactions, and determine the binding affinity. Intrinsic disorder in specific protein regions plays its role in recognition and such disordered protein regions may control the degree of motion between domains and in fact confer advantages over folded proteins in binding. Not surprisingly, a major endeavor in recent years has been to develop models and methods for simulating the dynamics of proteins, and relating the observed behavior to experimental data. Here, we demonstrate how protein dynamics dictate the binding affinity through the atomistic molecular dynamics simulations (MDs) and Gaussian Network Model (GNM), an elastic network model introduced at the amino acid residue level. A study cases for HIV and Dengue will be discussed. Comparison of both methods will be discussed. Binding free energy from longtime-scale molecular dynamics simulation under graphic processing units (GPUs) computing and mode shape analysis from GNM can be used to distinguish the higher/lower affinity protein towards the protein target.

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Session Classification: Heron 1

Track Classification: Theory and simulation related to nanosystem