Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Webinar

Investigation of Protein conformations and ligand-recognition via Computer Simulation

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Proteins are not static, they are dynamic in nature. They undergo spontaneous conformational changes to participate in multiple cellular processes. These conformational changes are intrinsic in nature but can also be triggered by the processes such as biomolecular recognition. Biomolecular recognitions such as protein-ligand binding are extremely important for sustaining life in a cell and they occur at every step of life process, for example, in protein synthesis, DNA-replication, DNA-transcription, translation, cell metabolism, enzyme catalysed reactions, cell signaling pathways etc. In order to fully understand how proteins function in a cell, a deeper understanding of protein conformational change and biomolecular recognition is required.

Molecular dynamics (MD) simulations acts as computational microscope for the study of molecular biology and proven to be an efficient tool in providing the detailed atomistic insights into the dynamical process. In this seminar, I will show how MD simulations and enhanced sampling techniques can be combined with routine docking experiments to refine the outcome of the drug discovery protocol using peptidyl t-RNA hydrolase (PTH) as test case. Next, I will show how atomistic MD simulations and Markov State Model (MSM) can be effectively used to quantify conformational heterogeneity present in Cytochrome P450 (CYP450) and its role on ligand binding. Then, I will talk about a mechanism of GTP recognition by its native protein GTPase and the challenges involved in the investigation. Finally, I will talk about how coarse grained (CG) simulations can become computationally affordable and faster approach for the study of Protein-ligand recognition pathways.

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04:00 PM