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

Seminar

Investigation of Protein Conformation and ligand-recognition using Computer Simulations

Bhupendra Ramesh Dandekar

TCIS, Hyderabad

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 recognition (such as protein-ligand binding) is extremely important for sustaining life in a cell. They occur at every step of the life process, for example, in protein synthesis, DNA-replication, DNA transcription-translation, enzyme-catalysed reactions, multiple cell signalling pathways etc. In order to fully understand how proteins function in a cell, a deeper understanding of protein conformational changes and biomolecular recognitions is required.

Molecular dynamics (MD) simulations act as a computational microscope for the study of molecular biology and have proven to be an efficient tool for providing detailed atomistic insights into the dynamical process. In this seminar, I will talk about how MD simulations and enhanced sampling techniques can be combined with routine docking virtual screening (VS) experiments to refine the outcome of the drug discovery protocols using peptidyl t-RNA hydrolase (PTH) as a test case. Next, I will talk about how atomistic MD simulations and Markov State Model (MSM) can be effectively used to quantify the conformational heterogeneity present in Cytochrome P450 (CYP450) protein and the conformational plasticity present in GTPase protein along with their role in ligand binding processes. Finally, I will talk about how coarse-grained (CG) simulations can become a computationally affordable and faster approach for the study of Protein-ligand bindings and their multiple recognition pathways.

Tuesday, April 5th 2022

11:30 AM

Auditorium