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

Internal Webinar

Simulations of ligand binding processes in proteins

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The presentation will discuss the application, assessment and development of high-throughput simulation protocols to investigate ligand transport processes in proteins. The challenges of rare event sampling for studying ligand binding events in haloalkane dehalogenases and the importance of knowledge-based seeding aided by Markov State Models will be discussed. In addition, the transport tools package will be introduced to address issues related to assessing large datasets of protein-ligand binding processes. Finally, the impact of hydrotropic solvents on cytochrome c dynamics will be explored, offering insights into structure-based drug design and rational protein engineering.

Thursday, Nov 2nd 2023

12:00 PM