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

Seminar

Reframing biomolecular recognition: multi-site binding, allostery and machine learned insights

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TIFR, Hyderabad

We investigated the complexities of biomolecular recognition through atomistic simulations of protein-ligand systems. Using unbiased molecular dynamics, machine learning, and experimental validation, we uncover novel mechanisms such as pre-binding selectivity filters in biosensors, multi-substrate occupancy in cytochrome P450, and mixed binding modes in Hsp90. We also introduce a machine learning tool, unsupervised-random-forest, for structural insight from simulations and benchmark existing simulation techniques. These studies offer fresh mechanistic and computational frameworks for understanding and engineering biomolecular recognition.

Monday, Dec 22nd 2025

14:30 Hrs (Tea / Coffee 14:15 Hrs)

Auditorium, TIFRH