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

Internal Seminar

Mechanistic insights into multi-drug cooperativity, nanopore transport and toxin-mediated membrane remodelling from multiscale simulations

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The molecular principles governing drug cooperativity, substrate translocation, and toxin-induced membrane remodelling remain a central challenge in chemical biology and biophysics. In this talk, I will present three complementary computational studies that investigate these processes across atomistic to mesoscopic scales. Together, these studies provide an integrated mechanistic insight into multi-drug interactions in human cytochrome P450, selective molecular transport mediated by porins, and pneumolysin-induced membrane perturbation, advancing our molecular understanding of cooperativity, biosensing, and host-pathogen interactions.

Friday, Dec 5th 2025

11:30 Hrs

Seminar Hall, TIFRH