Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Seminar

How, when and why do drugs unbind: predictive all-atom simulations

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Using molecular dynamics (MD) simulations to study the kinetics of drug unbinding is a desirable but difficult task primarily due to the extremely long timescales involved. Recent progress in enhanced sampling methods, including the development of new sampling approaches, makes it possible to address this and a range of related problems with full atomistic resolution, reaching timescales previously unattainable in MD simulations. In this talk, I will summarize the key principles behind these approaches. I will then highlight some applications calculating pathways, timescales and rate-determining steps of ligand unbinding in various systems including an FDA-approved anti-cancer drug as it unbinds from host kinase and biotin-streptavidin.

Thursday, Nov 9th 2017

04:00 PM (Tea/Coffee at 03:30 PM)

Auditorium, TIFR-H