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

Webinar

Navigating biomolecular energy landscapes using different flavours of coarse-Graining

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During the last few decades, the energy landscape framework has emerged both as a conceptual and a computational tool to understand the intimate connections between biomolecular structure, dynamics and ultimately function. In practice, determining the global topography of the landscape using standard computer simulation techniques have proved challenging because of large free energy barriers that lead to rare event dynamics. In this context, a coarse-graining of the landscape in terms of stationary points can prove effective. In the first part of my talk, I will highlight how this approach can be exploited to obtain key insights into RNA folding, as well as conformational switching between different secondary structure elements of a designed peptide. In the second part, I will illustrate how coarse-graining the degrees of freedom can also be a viable route in the computer simulation of biomolecules. I will discuss how sequence-dependent aggregation propensities of Aβ peptides may be understood in terms of the cryptic signatures of fibril- like configurations encoded within the monomer free energy landscapes.

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04:00 PM