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

Webinar

Targeting autophagy: from raw simulation trajectories to biological insights

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In cell, several biomolecules physically come together to perform a given function. The required coordination for interaction between these molecules such as proteins or lipids constitute the cornerstone of all biological processes. Not surprisingly, abrupt alterations within these complexes result in disease-state of the cell and result in damaging consequences. Atomic modelling and molecular dynamics (MD) simulations provide an opportunity to mimic physiologically-relevant molecular systems and aids in disentangling essential features for a given system under study. These simulations require high-performance supercomputing infrastructure and the present technological advances have led to an exciting phase in this field, where large supramolecular assemblies are a reality. In this talk, I will introduce key areas relevant to biomolecular dynamics and how we have utilized MD simulations to extract biological insights of protein-lipid recognition mechanisms. Lastly, I will also present our group's work on Autophagy and how we used simulations and structural bioinformatics approaches to delineate functional diversity of LC3 family members.

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4:00 PM