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

Seminar

Lipids as modulators of protein conformations and cell fate

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Our laboratory has a long-standing interest in autophagy and, more broadly, maintains a strong focus on dynamic protein–membrane interactions. In this talk, I will present how we combine large-scale molecular dynamics simulations with experimental approaches to investigate the conformational dynamics, membrane remodeling, and how tuning protein–lipid interactions can influence cellular outcomes. Using the autophagy pathway as a model system, I will highlight how molecular-scale interactions give rise to emergent cellular behaviour across scales. First, we dissect the determinants of protein–membrane binding, identifying key interaction modes that govern LC3 recruitment to autophagosomal membranes. We show that these interactions can be tuned to modulate receptor binding and autophagy cargo recruitment. Second, we show how these interactions give rise to higher-order organization, demonstrating that LC3 proteins form spatially discrete nanoclusters under physiologically relevant, crowded membrane conditions. Third, by integrating clinically relevant variants with simulations, we demonstrate that dynamic structural ensembles capture aspects of biology that are not accessible through current state-of-the-art approaches, including AlphaFold2 and emerging ESM-based protein foundation models.

Thursday, Apr 23rd 2026

16:00 Hrs (Tea / Coffee 15:45 Hrs)

Auditorium, TIFRH