

Survey No. 36/P, Gopanpally Village, Serilingampally Mandal, Ranga Reddy Dist., Hyderabad – 500 046

## Seminar

## Sculpting membranes: how proteins shape, remodel, and translocate across cellular boundaries

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Biomembrane remodelling by proteins is essential for several critical cellular functions such as intracellular cargo trafficking, transporting proteins across membranes, and autophagy. Molecular Dynamics (MD) simulations have played a pivotal role in gaining molecular insights into the mechanism of protein induced membrance remodelling. However. conventional approaches face significant challenges in capturing the relevant time and length scales. In this talk, I will first highlight how MD simulations reveal mechanistic insights into the TIM23 **complex** mediated protein insertion into the inner membrane of mitochondria. Next, I will discuss my development of a simulation framework to study COat Protein multiscale complex II (COPII) mediated membrane budding, essential for transporting protein cargoes from the ER to the Golgi apparatus. Finally, I will show how advanced machine learning-assisted MD simulations can illuminate the mechanism of lipid scrambling by **ATG9**, a key process driving phagophore expansion during autophagy.

Tuesday, Oct 14<sup>th</sup> 2025 16:00 Hrs (Tea / Coffee 15:45 Hrs) Seminar Hall, TIFRH