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

# Seminar

## Deep Learning approaches for elucidating role of small molecule and post translational modification in intrinsically disordered proteins

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Intrinsically disordered proteins (IDPs) lack a stable and well-defined secondary structure under physiological conditions. Unlike folded proteins, IDPs exhibit a rugged free energy landscape, making their characterisation challenging. Moreover, studying post translational modification (PTM) or interaction with small molecules introduce additional complexity, thereby making traditional methods insufficient. To overcome this, we have utilised deep learning methods, such as Autoencoders and Variational Autoencoders (VAEs). These techniques have enabled us to explore protein conformational landscapes, particularly in the context of phosphorylation and interaction of small molecule with α-Synuclein. We also improved the VAE model by optimising β through annealing, which enhanced its ability to characterise disordered regions and small molecule interactions in α-Synuclein and SIRT1 respectively. Additionally, combining large language models with feedforward neural networks enabled accurate prediction of phosphorylation sites, providing valuable insights into the regulation of protein function. Together, this thesis demonstrate the power of deep learning in unravelling the complexities of IDPs and their regulatory mechanisms.

***Monday, Feb 10th 2025***

***11:30 Hrs (Tea / Coffee 11:15 Hrs)***

***Auditorium, TIFRH***