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

Students' Annual Seminar

Understanding the role of phosphorylation and small molecule interaction with IDPs using deep learning

Subinoy Adhikari

IDPs exist in a multitude of dynamically flexible distinct conformational states. The high dimensional input features which describe the heterogeneous conformational space of IDPs have nonlinear relationships, and dimension reduction using a deep learning algorithm "autoencoder" (AE) is suited, to project the atomistically simulated conformation ensemble of Ash1 and Sic1 proteins along their respective latent space, which is further refined by developing individual Markov State Models thereby capturing similarities and differences up on phosphorylation of IDPs. AE was also used to project αSyn data in its apo state and in presence of fasudil, into states which identified residues which predominantly interact with fasudil and is consistent with the experimental results. Finally I would like to introduce to generative modelling using variational AE (VAE) which is used to create conformational ensemble of IDPs and predicting time series data using long short term memory (LSTM) neural network.

Monday, Apr 3rd 2023

4:00 PM (Tea / Coffee 3.45 PM)

Seminar Hall, TIFR-H