

## **Students' Annual Seminar**

### **Elucidating PTM and interaction of small molecule with IDPs using deep learning and language models**

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Phosphorylation of IDPs results in subtle conformational changes undetectable by traditional methods. Employing deep learning and molecular dynamics, our study finds modifications in both intra-molecular interactions and the local environment and helps elucidate the impacts of phosphorylation on IDPs. We have also investigated the interaction between a small molecule, fasudil and alpha-synuclein ( $\alpha$ S) using Markov State Modelling and VAE. Our study identifies diverse conformational states influenced by fasudil, expanding the ensemble of  $\alpha$ S. Thermodynamic analysis highlights how fasudil modulates  $\alpha$ S's structural repertoire by affecting backbone entropy, presenting a mechanism for conformational changes in IDPs. Additionally, large language models predict PTM sites, providing insights into their functional consequences across biological contexts.

***Tuesday, Mar 5<sup>th</sup> 2024***

***14:00 Hrs (Tea / Coffee 13:45 Hrs)***

***Seminar Hall, TIFR-H***