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

# Internal Webinar

## Atomistic Insights into Protein Regulation and RNA–Protein Interactions from Molecular Dynamics Simulations

## T S Sreevidya

### IMSc, Chennai

My research uses atomistic molecular dynamics simulations and molecular modelling to understand how molecular-scale interactions govern biomolecular structure, dynamics, and function. During my PhD, I investigated mutation-induced changes in global dynamics and allosteric signalling in proteins, combining long-timescale MD simulations with interaction network analysis. These approaches were applied to study substitution mutations in 14–3–3 proteins and phosphorylation-regulated catalytic loop dynamics in the phosphatase PTP–PEST, providing mechanistic insight into experimentally observed functional changes. I also modelled the PTP–PEST–AMPKα complex to support experimental identification of AMPKα as a novel substrate. My current work extends these approaches to RNA–protein systems, examining polycation–siRNA complex formation and the role of sequence, charge distribution, and chemical specificity in determining complex stability and organisation.

***Friday, Jan 30th 2026***

***12:00 Hrs***