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

Webinar

Exploring Protein Dynamics: Conformational heterogeneity and Collective Variables

Dube Dheeraj Prakashchand

TCIS, Hyderabad

Proteins are bio-macromolecules, which are basically polymer chains of amino acids, and are one of the most essential nutrients required in the sustenance of a living organism. The various functionalities of proteins can be closely linked with their dynamical properties, which are intrinsically encoded in their amino acids sequence. Thus, decoding various protein functions demands a detailed knowledge about the ensemble of diverse conformational meta-stable states adopted by the protein. Employing ideas which were earlier successful in addressing important phenomena in crystalline solids, we have defined a new collective variable, NAP, which quantifies non-affine thermally excited displacements of proteins. We have shown that all the key dynamical phenomena like allostery, ligand-binding and folding can be investigated by tracking down the various regional predominant non-affine modes of fluctuations. Identification of non-affine fluctuations in protein offers a distinct advantage for understanding the bio-macromolecular dynamics and its quantifier GNAP holds the promise of acting as an optimal CV for projecting the free energy landscape. The availability of an analytical expression for GNAP makes it possible to patch it with any standard MD analysis tool for post-simulation analysis. This holds future promises of driving a biophysical process along its collective non-affine displacement using enhanced sampling techniques.

Thursday, Nov 19th 2020

4:00 PM