

## **Seminar**

### **Understanding large conformational transitions in proteins using simplified models**

**Sachi Gosavi**

**NCBS, Bangalore**

In order to function, many proteins bind ligands and change shape. This final shape is what usually allows the protein to transmit a signal or perform catalysis or in some cases stop further activity. The energy landscapes of proteins which perform conformational conversion need to not only (1) enable protein folding to the correct (ligand-binding capable) active structure but to also (2) then enable the change of shape to the correct final structure. We have simulated the conformational transitions of several model proteins using simplified models. I will describe our studies on three very different proteins adenylate kinase (AKE), cytolysin A (clyA) and alpha1-antitrypsin (A1AT) which allow us to understand some general constraints that sculpt the landscapes of proteins that perform conformational transitions.

***Monday, Dec 12<sup>th</sup> 2022***

***4:00 PM (Tea/Coffee at 3:45 PM)***

***Auditorium, TIFR-H***