

TATA INSTITUTE OF FUNDAMENTAL RESEARCH
DEPARTMENT OF CHEMICAL SCIENCES

DCS SEMINAR

Speaker	Prof. Shachi Gosavi National Centre for Biological Sciences, Bengaluru
Day, Date	Monday, February 20, 2023
Time	4.00 P.M.
Venue	AG-69
Title	On proteins, simple models and large conformational transitions

Abstract:

In order to function, many proteins bind ligands and change shape. This conformational change is what usually allows the protein to function, i.e., transmit a signal or perform catalysis or in some cases, stop further activity. Simple protein models which encode the two end structures of the protein can be used to understand the order of events and the molecular determinants of such conformational transitions. I will introduce such models and discuss why they work. I will then give examples of molecular dynamics simulations of different flavors of such models used in my group to understand the conformational transitions of three systems: (1) adenylate kinase (AKE; the hydrogen atom of protein conformational transitions) (2) maltose and histidine binding proteins (MBP and HisJ) and (3) cytolysin A (ClyA), a water soluble protein toxin that converts into a membrane inserted protomer. If time permits, I will talk about the folding of AKE and ClyA with such models.

S.K. Kadam