

Tuesday Colloquium

“Exploring Bio-molecular Recognition using Multi-scale Computer Simulations ”

By

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Abstract:

Recognition of biomolecules is a fundamental control mechanism in eukaryotic cells. The precise targeting and versatility of these interactions such as, protein-protein, protein-ligand, and protein-membrane is the hallmark of several cellular processes that culminates into key biological functions. Therefore, an understanding of these processes on atomistic level would have significant biological and medical impacts. We use computational methods, in particular biomolecular simulations, to understand the following processes (a) mechanism of peripheral membrane proteins and followed structural changes associated with their membrane localization (b) identifying structural scaffolds existing in substrate proteins, that are targeted to chaperones, and (c) structural and dynamical information of GPCR's upon ligand binding. In this talk, I will provide a brief introduction to multi-scale computational approaches, and how they enable us to study biologically interesting problems. She will later converge to reveal our findings on the above mentioned themes.

Tuesday, February 02, 2016 at 4 p.m.

**PF AG 14, Prefabs, ABS
University of Mumbai, Kalina**