



BioSim Talk #3

An IPR seminar series supported by WPI PRIME and ASPIRE

Date: August 1st 2024 (Thu)

Time: 4.30 – 6.00 pm

Venue: 2F Conference Room (#202), Institute for Protein Research, Osaka U. (Suita Campus), +Zoom

Speaker: Sandhya Tiwari, PhD.

Institute for Protein Research (IPR), Osaka University

Title: How to use elastic network models to study protein flexibility

Understanding protein flexibility is crucial for comprehending biological functions. Elastic network models (ENMs) have emerged as powerful tools for studying the dynamic aspects of protein structures with computational efficiency and minimalistic assumptions. This talk will delve into the foundational principles of ENMs, highlighting their reliance on simplified physical models to predict the motions of proteins around their equilibrium positions. Moreover, the focus will shift to the application of ENMs in normal mode analysis and coarse-grained simulations. The results from ENM-based analyses have been used to interpret the intrinsic flexibility of protein structures, assess the impact of mutations on stability, understand allosteric signaling pathways, and characterize the conservation of dynamics across protein homologues and proteins with similar topologies.

Link for online participation:

Meeting ID: 883 7289 5325

Passcode: 747062

Please kindly let us know if you will be participating online.

