An IPR seminar series supported by
WPI-PRIMe and ASPiRE

BioSim Talk #2

Sandhya Tiwari

Independent Associate Professor (PI)
Lab. for Biomolecular Modeling and Dynamics,
Institute for Protein Research,
The University of Osaka

20th June 2025 (Friday)
3.30 – 5.00 pm
Institute for Protein Research
Osaka U. (Suita Campus)
4th floor seminar room

Analyzing protein-protein coupled motions from whole-complex dynamics

Understanding how proteins behave within complexes is vital for unraveling their functional roles. In this talk, I will present recent insights into the intrinsic dynamics of protein–protein complexes, focusing on how the inclusion or exclusion of binding partners affects protein flexibility. Using elastic network models (ENMs) and normal mode analysis, we distinguish between self-coupled and directly coupled motions, showing that partner proteins can induce long-range dynamical effects that may not be evident when treated implicitly. I will include recent work involving the analysis of PAS domain interactions in bHLH PAS domain transcription factors, revealing different patterns of dynamics related to the binding interface according to protein class. Furthermore, I will show how this method can be adapted to analyze coupled motions as captured in MD simulations.

Link for online participation via Zoom:
Meeting ID: 857 7049 5531
Passcode: 102874
Please inform us if you will be participating online or joining our Slack channel

sandhyatiwari@protein.osaka-u.ac.jp, shinobu.ai.prime@osaka-u.ac.jp