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BioSim Talk #7

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10th October 2025 (Friday)

4.00 – 5.30 pm

Institute for Protein Research
University of Osaka (Suita Campus)
4th floor seminar room

Simulating the Jiggling Atoms of 'Life': Is Any Extra Mile of Understanding Earned?

The atoms and molecules in nature are always jiggling and bumping into each other, which form the basis of their collective properties. Therefore, the structure-function relationships of biomolecules are sometimes non-trivial to understand from the static models of molecular structures. To go beyond, computer simulations offer scopes to witness the atoms in action, mimicking a more realistic behavior of the molecular structures and tell how exactly they are meaningfully choreographed to perform or not to perform a function. But how much can it really help to take the scientific understanding forward? Indeed, such methods provide the opportunity to distil out the molecular mechanisms with qualitative and quantitative assessments, with a statistical basis. For example, using 'standard' as well as 'enhanced' sampling methods of all-atom molecular dynamics, we have shown the thermodynamic basis of induced allosteric transitions in a kinase. This presentation will address such issues of subtle conformational changes in proteins that drive their functions, particularly in kinases, tubulin-microtubule systems, and in a few other systems. Our recent success in **applications of machine learning based methods** to analyze conformational ensembles of proteins to offer critical insights on possible molecular 'pseudo-intelligence' in kinases will also be discussed.

Link for online participation via Zoom:
Meeting ID: 817 5161 1826
Passcode: 029335

Please inform us if you will be participating online or joining our Slack channel
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