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BioSim Talk #2

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5th June 2026 (Friday)

4.00 – 5.30 pm

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

Watching Proteins Breathe: A Molecular Simulation Case Study of Hidden Hydration Pathways and Functional Dynamics in *Pseudomonas aeruginosa* PBP3 toward Next-Generation β -Lactam Design

Proteins are dynamic systems whose biological functions often depend on transient motions, fluctuating interactions, and solvent behavior that are difficult to capture using static experimental structures alone. In this seminar, I will discuss how molecular dynamics simulations can be used to uncover hidden functional dynamics in biomolecular systems using *Pseudomonas aeruginosa* Penicillin-Binding Protein 3 (PBP3) as a case study. Through analyses of loop motions, hydration networks, transient pocket formation, and active-site dynamics, we investigated how subtle chemical modifications in β -lactam scaffolds can reshape protein flexibility and alter the accessibility of catalytically important water molecules within a buried active site. The seminar will introduce practical computational workflows commonly used in biomolecular simulations, including trajectory analysis, contact dynamics, water bridge analysis, clustering approaches, pocket detection, and free energy analyses. Emphasis will be placed on how multiple complementary analyses can be integrated to construct mechanistic models from molecular simulation data. Beyond the specific biological system, the talk aims to provide a broader and intuitive perspective on how molecular simulations can serve as a discovery tool for understanding biomolecular function and guiding next-generation β -lactam design.

Link for online participation via Zoom:

Meeting ID: 813 6978 7569

Passcode: 487274

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