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BioSim Talk #4
10h July 2026 (Friday)
1.30 – 3.00 pm

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

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Integrating AI and Molecular Simulation for Antibody and Protein Design

Proteins perform a wide range of biological functions through complex relationships between sequence, structure, dynamics, and molecular interactions. Understanding these relationships is essential for developing next-generation vaccines and therapeutics. However, protein function often depends not only on static structures but also on conformational flexibility and dynamic behavior, making rational protein engineering a challenging task. Recent advances in artificial intelligence and molecular simulation have expanded our ability to analyze and design proteins, yet understanding which molecular features determine stability and function remains a major challenge.

One of the most effective approaches to address these problems is the integration of AI-based design with molecular simulation and structural analysis. In this presentation, I will describe how these computational methods can be applied to both antibody engineering and de novo protein design. First, I will present our efforts to understand antibody breadth through the analysis of CDRH3 conformational dynamics and structural features associated with broad antigen recognition. I will then introduce an AI-guided protein design framework that combines sequence generation, structure prediction, and molecular simulation to identify and prioritize novel protein candidates. Together, these studies illustrate how integrating AI with physics-based modeling can both reveal fundamental principles of protein function and accelerate the design of next-generation biomolecules.

Link for online participation via Zoom:

Meeting ID: 814 1451 0156

Passcode: 891973

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

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