An IPR seminar series supported by
WPI-PRIMe and ASPiRE

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

Dr. Hisham M. Dokainish

Laboratory of Vaccine Design, Research Center for Vaccine Development, National Institute of Infectious Diseases, Japan

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