

# Structure and Dynamics of Biomembranes

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**日時 (Date & Time) : 2020年3月10日 (火) 14:30 ~ 17:00**

**会場 (Venue) : 厚生棟3階大会議室 (16A棟3階)**

**主催 (Host) : 慶應義塾大学グローバルリサーチインスティテュート (KGRI)**

**講演概要 (Summary of Lecture) :**

## **Part 1: Membrane Protein Interactions with Lipids as Viewed by Molecular Simulations**

Interactions with lipids are important in the function of membrane proteins and the organization of membranes. Molecular simulations allow us to explore structural, energetic, and dynamic aspects of these interactions.

## **Part 2: Water and Ions in Membrane Nanopores and Channels: Insights from Molecular Simulations**

Molecular dynamics simulations can be used to explore the dynamic behaviour of water within nanopores and biological channels in lipid bilayer membranes. Simulation studies of the behaviour of water in idealised models of nanopores have revealed aspects of the organization and dynamics of nano-confined water, including wetting/de-wetting in narrow hydrophobic nanopores. Simulation studies of the behaviour of water in a range of biological nanopores will be discussed, including  $\beta$ -barrel protein nanopores and ion channels.

Free admission, Open to anyone,  
Pre-registration not required

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