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BioSim Talk #8

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November 22nd 2024 (Fri)

4.30 – 6.00 pm

Institute for Protein Research
Osaka U. (Suita Campus)

2nd floor conference room (#202)

What can we learn from SAXS data? An example of complementary analysis with MD simulation

Molecular dynamics simulation enables us to sample dynamic structures of biomolecules with high spatio-temporal resolution. However, due to the difficulties of reproducing the real ensemble from MD simulation, it is important to compare with experimental data. Among various experimental methods, Small-angle X-ray scattering (SAXS) can provide information on structural ensemble in solution at ambient temperature without any observational bias, even though structural information encoded in the profile is limited to low-resolution. In fact, SAXS data can also reveal a variety of molecular properties. In this talk, the principle of the measurement and analysis will be briefly explained, and then the study of molecular dynamics using SAXS and MD calculations will be presented.

Link for online participation via Zoom:

Meeting ID: 849 9164 5171

Passcode: 098186

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

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