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BioSim Talk #10
23th January 2026 (Friday)
4.30 – 6.00 pm
Institute for Protein Research
University of Osaka (Suita Campus)
2nd Conference room (large)

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Toward FAIR (Findable, Accessible, Interoperable, Reusable) Data in Molecular Dynamics

As molecular dynamics (MD) simulations become central to fields like molecular biology, systems biology, and drug design, they are increasingly integrated into a broader scientific ecosystem driven by machine learning, supercomputing, and large-scale data. But this integration exposes a critical weakness: the lack of data standardization. MD simulations produce complex datasets across varied software and file formats, often lacking consistent metadata or documentation. This makes the data difficult to share, reproduce, or reuse, unlike in areas like genomics or structural biology, where standardization is more established. In this talk, I introduce the FAIR principles as a way to address the challenges of standardizing MD data. I discuss how they have been applied in molecular dynamics, including efforts that gained momentum during the COVID-19 pandemic. I also examine the current state of data handling in the field and some of the difficulties that persist.

Link for online participation via Zoom:
Meeting ID: 832 6502 9407
Passcode: 965258
Please inform us if you will be participating online or joining our Slack channel
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