BioSim Talk #15

Gert-Jan Bekker, PhD.

Specially appointed Assist. Prof. (Lecturer),
PDBj & Lab for Protein Crystallography

17th March 2025 (Monday)
4.30 – 6.00 pm

Institute for Protein Research
Osaka U. (Suita Campus)
2nd floor conference room (medium)

Practical tools for preparing and running MD simulations using GROMACS

Over the past decade, I have developed several tools for the preparation, execution and analysis of MD simulations using GROMACS. In this talk I will introduce those tools, how they can be obtained and executed for your own simulations. Example tools include “autoBuild” to prepare protein-ligand complexes, “gmxrunner” for running automatic execution of long MD simulations on supercomputers, a standard protocol for running and analyzing enhanced sampling McMD simulations and Molmil for visualization of structures & trajectories. For each of the tools I will prepare some examples for attendees to try. Finally, I'll reserve about 30 minutes for general questions (including ones beyond the scope of this talk).

Link for online participation via Zoom:
Meeting ID: 867 7426 7402
Passcode: 468127
Please inform us if you will be participating online or joining our slack
sandhyatiwari@protein.osaka-u.ac.jp, shinobu.ai.prime@osaka-u.ac.jp