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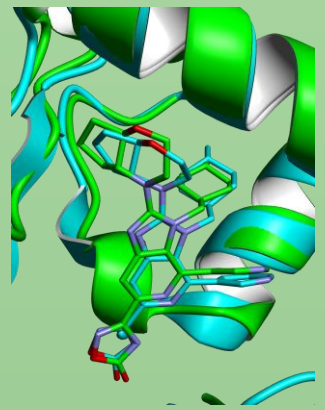

# BioSim Talk #7


## Gert-Jan Bekker, PhD.

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


**November 1st 2024 (Fri)**
**4.00 – 5.30 pm**

Institute for Protein Research
Osaka U. (Suita Campus)
2nd floor conference room (#202)

***Dynamic docking using Multicanonical MD***

Multicanonical Molecular Dynamics (McMD) based dynamic docking is a powerful tool to not only predict the native binding configuration between two flexible molecules, but it can also be used to accurately simulate the binding/unbinding pathway. Furthermore, it can also predict alternative binding sites, including allosteric ones, by employing an exhaustive sampling approach. Since McMD-based dynamic docking accurately samples binding/unbinding events, it can thus be used to determine the molecular mechanism of binding between molecules. In this talk I will showcase various applications of McMD-based dynamic docking, applied to small ligands, medium-sized ligands, peptides to their receptors, as well as protein-protein docking. Finally, I will demonstrate how anyone*** can perform McMD-based dynamic docking simulations, by showcasing the dynamic docking between MDM2 and a medium-sized compound, including all the steps involved in preparing the system, executing the simulations and analyzing the results.

*** NB: you do need to have a desktop/workstation/server/cluster (don't do this on a laptop/phone)

Link for online participation via Zoom:
Meeting ID: 821 3683 8780
Passcode: 762776
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