一般社団法人日本生物物理学会　第 9 回 Biophysics and Physicobiology 論文賞受賞講演会

The 9th Award Seminar for outstanding Biophysics and Physicobiology paper

オーガナイザー：日本生物物理学会 Biophysics and Physicobiology 論文賞選考委員会
Organizers: Award committee for outstanding Biophysics and Physicobiology paper
日　時：9 月 16 日（水）12:20 ～ 13:00 ／ Sep.16 Wed.
会　場：オンライン開催／ Online
形　式：講演会／ Lecture

第 9 回 Biophysics and Physicobiology 論文賞受賞者

坂野貴子，Md. Iqbal Mahmood，山下雄史，藤谷秀章
Takako Sakano, Md. Iqbal Mahmood, Takefumi Yamashita, Hideaki Fujitani
東京大学先端科学技術研究センター
Research Center for Advanced Science and Technology, The University of Tokyo

MD シミュレーションによるタンパク質－リガンド相互作用の研究
Molecular dynamics study on protein-ligand interaction

Understanding of the protein-ligand interaction is a key issue for the drug development [1]. Thus, many drug design software suites have been developed to predict the binding affinity based on the docking method. In the standard docking method, the binding affinity is predicted as an empirical binding score, following the protein-ligand complex structure prediction. Accordingly, the accurate prediction of the protein-ligand complex structure is quite important. Here, we utilized the molecular dynamics (MD) simulation to check the stability of the predicted complex structure. Although in the docking we used protein structures obtained by the high-resolution X-ray crystallography experiments, we often observed the complex structures were largely changed in the MD simulations, which indicated that the predicted complex structures were not the most stable. When the complex structure was unstable, we further observed that the ligand was dissociated from the protein. In this sense, we consider that the MD simulation can provide the information about the protein-ligand complex structure and modify the complex structure predicted by the docking [2]. Today, due to the advancement of computer power, as symbolized by the supercomputers, K and Fugaku, the MD simulation becomes a popular method and is applied to more challenging problems. This seminar will review and discuss the recent MD studies on the ligand-protein simulation.

[1] Yamashita, T. et al. (2015). *Chem. Pharm. Bull.,* 63: 147-155.
[2] Sakano, T., Mahmood, M. I., Yamashita, T., & Fujitani, H. (2016). *Biophys. Physicobiol.*, 13: 181-194.