

Riron Seminar

Date: July 27, 2018 (Fri.) 4 P.M.–5 P.M

Place: ISSP Main building Fl. 6 A615

Lecturer: **Prof. Yasuteru SHIGETA**

(Affiliation) (*Center for Computational Sciences, University of Tsukuba*)

Title: **Computational analyses on structure and function relationship of proteins**

(The talk is given in Japanese but the slides are prepared in English.)

Abstract:

Proteins are macromolecular compounds with extremely complex structures and drive various biological functions *in vivo* such as molecular recognition, signal transduction, enzymatic reaction, and etc. Since it is expected that there is a correlation between the structure and the function (structure-function relationship), the three-dimensional structures of many proteins have been clarified by experimental methods such as X-ray diffraction experiment and nuclear magnetic resonance method (NMR). Especially, dynamic information of a protein is recently obtained by state-of-the-art experimental techniques such as X-ray free electron laser, cryo-electron microscopy, AFM and STM, and etc., which enable ones to elucidate protein functions in detail. Under such circumstances, theoretical calculations become more important to confirm experimental facts at the microscopic level and predict its vital role.

With recent progress in both supercomputer architectures and computational methodologies to analyze biomolecules, the field of chemical reaction analysis occurring *in vivo* has made remarkable progress. In this seminar, molecular dynamics simulations and first-principles methods for analyzing biological phenomena are reviewed. We will also provide the latest research topics that our laboratory is conducting especially on free energy analyses of folding and domain motion of proteins, how to evaluate physical properties of proteins, enzymatic reactions are introduced.

1. R. Harada, Y. Takano, T. Baba, Y. Shigeta, “Simple, Yet Powerful Methodologies for Conformational Sampling of Proteins”, *Phys. Chem. Chem. Phys.* (**invited feature article**) **17**, 6155-6173 (2015).

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2. J. Fujita, R. Harada, Y. Maeda, Y. Saito, E. Mizohata, T. Inoue, Y. Shigeta, H. Matsumura, " Identification of the key interactions in structural transition pathway of FtsZ from *Staphylococcus aureus*", *J. Struct. Biol.* **198**, 65-73 (2017).
3. R. Harada, Y. Shigeta, "How low-resolution data can predict conformational changes of a protein: a molecular dynamics study", *Phys. Chem. Chem. Phys.* **20**, 17790-17798 (2018).
4. M. Shoji, H. Isobe, Y. Shigeta, T. Nakajima, K. Yamaguchi, "Concerted Mechanism of Water Insertion and O₂ Release during the S₄ to S₀ Transition of the Oxygen-Evolving Complex in Photosystem II", *J. Phys Chem. B* **122** (25), 6491-6502 (2018).
5. K. Kamiya, T. Baba, M. Boero, T. Matsui, S. Negoro, Y. Shigeta, "A Nylon-oligomer Hydrolase Promoting Cleavage Reactions in Unnatural Amide Compounds", *J. Phys Chem. Lett.* **5**, 1210-1216 (2014).
6. K. Kamiya, Y. Shigeta, "First-principles Molecular Dynamics Studies on the Atomistic Behavior of His503 in Bovine Cytochrome *c* Oxidase", *Biochim. Biophys. Acta*, **1807**, 1328-1335 (2011).