Protein–protein interactions of Azurin complex in the liquid system

M. Rusmerryani, M. Takasu*, K. Kawaguchi, H. Saito, H. Nagao

Institute of Science and Engineering, Kanazawa University, Kakuma, Kanazawa 920-1192 Japan
*aSchool of Life Sciences, Tokyo University of Pharmacy and Life Sciences, Hachioji, Tokyo 192-0392, Japan

micke@wriron1.s.kanazawa-u.ac.jp

Proteins perform their biological functions in a crowded environment where other macromolecules, such as lipid, nucleic acids, and other proteins exist. Recent studies focus mainly on the dynamics of single protein. Nevertheless, the existence of other proteins may affect the protein dynamics in the real system. Using computational studies, we investigate the protein–protein interactions for gaining insights into the effects from the presence of other proteins on protein conformational changes. In this work, we apply a coarse-grained model where several atoms are represented by one large particle. We carry out molecular dynamics simulation with a topology-based potential interactions to simulate dynamical properties of Pseudomonas Aeruginosa azurin complex systems[1]. It is important to characterize the protein interactions in azurin since azurin plays an essential role as an electron carrier in bacterial respiration.

We treat the intramolecular interactions at the residue level with the implementation of the off lattice Gō-like model to represent the bonded and non-bonded interactions among the residues inside the chain[2,3]. Meanwhile, the intermolecular interactions among the chains are represented by 12-6 Lennard-Jones potential to describe the strongly repulsive and weakly attractive interactions in the liquid system[4]. Moreover, different values of initial distance and various configuration systems are used to gain deep understanding into the long range interaction based on their distance separation by using the autocorrelation function and statistical analysis. These studies will provide valuable insights for further investigation on protein–protein interaction in more realistic system.

Keywords: azurin, protein–protein interaction, coarse-grained, Gō model, long range interaction