Theoretical study on intermolecular interaction and structural stability of plastocyanin and cytochrome f complex by using the Gō-like model

Satoshi Nakagawa, Shogo Kinoshita, Kazutomo Kawaguchi, Hidemi Nagao

Graduate School of Natural Science and Technology, Kanazawa University

In photosynthesis, plastocyanin(Pc) is a blue copper protein and transfers one electron from cytochrome f(Cyt$f$) in cytochrome b_6f complex to P700 in Photosystem I by diffusing in the lumen side of the thylakoid membrane. When Pc receives and donates an electron, Pc is associated with Cyt$f$ and P700, respectively. Although the complex structure of Pc-Cyt$f$ has already analyzed by NMR, the complex structure of Pc-P700 has not been analyzed yet. In order to investigate both association process and diffusion process of Pc, coarse-grained simulation is efficient to simulate large system sizes on long time scale. In our pervious study, we have developed coarse-grained intermolecular interaction including only hydrophobic interaction and succeeded in obtaining the complex structure of GCN4-pLI[1].

In this study, we apply this intermolecular interaction to Pc-Cyt$f$ complex to explore native complex structure. Before performing coarse-grained simulation, some parameters involved in our coarse-grained model are estimated by all-atom simulation of amino acid side chains. We introduce the effects of multibody interaction to our coarse-grained model. Performing coarse-grained simulation, we evaluate stability of complex structure and discuss the effects of multibody interaction.

References

[1] K. Kawaguchi, et al., *Mol. Phys.,* (2016) DOI:10.1080/00268976.2016.1234652, in press