Theoretical study on effective interaction between protein molecules

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Association of protein molecules plays a key role in many protein functions, such as signal transduction, transcription, and electron transport in photosynthesis. We have discussed the association of protein molecules by using coarse grained model in which protein-protein interaction is represented by only van der Waals interaction [1]. We have also investigated that the effective attraction interacts between a protein molecule and its ligand molecule in a water solvent by using all-atom molecular dynamics (aaMD) simulations [2].

In this study, we construct the coarse grained model to represent the effective interaction between protein molecules in a water solvent. First, the effective interaction between two amino acid side chains in a water solvent is calculated as a function of the distance between them by using aaMD simulations. The coarse grained potential function for each amino acid side chain is constructed to represent the effective interaction obtained by the aaMD simulations. Then, the effective interaction between two α-helices in a water solvent is calculated by using the coarse grained potential function, and is compared with that calculated by using aaMD simulations.

References

[1] M. Rusmerryani, et al., *JPS Conf. Proc.*, **1** (2014) 012054.

[2] K. Kawaguchi, et al., *Chem. Phys. Lett.*, **588** (2013) 226.