Theoretical study of a coarse grained model of electrostatic 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. In our previous studies, we have 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 [1]. We have also constructed the coarse grained potential to represent the effective interaction between hydrophobic amino acid residues in a water solvent by using aaMD simulations and reproduced the complex structure of GCN4-pLI tetramer by the coarse grained simulation [2].

The purpose of this study is to construct the coarse grained potential for the effective interaction between charged amino acid residues and polar amino acid residues in a water solvent. In the first step, the effective interaction between two amino acid side chains analogues in a water solvent is calculated as a function of the distance between them by using aaMD simulations. The coarse grained potential function is constructed to represent the effective interaction obtained by the aaMD simulations. In the second step, the Langevin dynamics simulation with the coarse grained potential is performed to reproduce the complex structure of small protein.

References

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

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