Theoretical study of a coarse-grained model for folding and association of a protein complex

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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. Protein association is related to protein folding. Folding and association of a small homotetrameric protein BBAT1 has been investigated by using all-atom Go model [1]. In our previous studies, we have constructed a simple coarse-grained potential to represent the effective interaction between amino acid residues in a water solvent by using all-atom molecular dynamics (MD) simulation. We also have reproduced the complex structure of GCN4-pLI tetramer and investigated the free energy landscape for protein association by using our coarse-grained model for monomers constrained to native structure [2, 3].

In this study, we develop our coarse-grained model for folding and association of protein complex and investigate association pathway related to folding of small protein complex, such as GCN4-pLI. We perform the Langevin dynamics simulation with our coarse-grained model for unfolded monomers of GCN4-pLI. To check the validity of our coarse-grained model, root mean square deviation, radius of gyration, and so on are calculated and compared with the results for BBAT1.

References

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