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Temperature Dependences on Dynamic Structure of Spherical Micelles: A Molecular Dynamics Simulations

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[Introduction]

In order to reduce the side-effects of drugs, the drug delivery systems (DDS) such as spherical micelle and liposome has been studied intensively. For the reliable transportation of the DDS, the stability of the spherical micelle/liposome structure is known to be an important property.

Biological lipid's structures and dynamics are important. For instance, the micellar clusters is known to show some interesting phenomena. The shape and size of micelle is a function of the molecular geometry of its surfactant molecules and solution conditions such as surfactant concentration and temperature[5]. For ideal micellar size, they show definite structures. Phospholipids have important functions in biological systems. At different conditions, they show differences both structurally and dynamically.

For micellar systems, many groups have studied the temperature effects on dynamics around micelle[2),3)]. Acep Purqon's doctoral thesis[1)] give the biggest inspiration to this study. He studied seven issues on bionanocluster fluctuations. One of the issues is identifying solvent effects. He analyzed the effect of salty water and temperature on phospholipids. He newly defined four parameters, Aperture, Symmetry, Isotropy, and Compactness (ASIC), which imply the structural character of the micelle system, and found that S and A parameters increase as the temperature rises, showing irregular structure and rapid tail fluctuation. The adding salt and temperature consequently contribute to shape fluctuations as well. In contrast, the micelle system show wider fluctuation in pure water..

However, the temperature effects on the self-aggregation of micelle system and structural stability of the lipid in the micelle are still not clear. In this study,

we analyze the structure and dynamics of small spherical micelle consisting of phospholipids molecules by molecular dynamics (MD) simulations. We also study stability of spherical micelles by carried on MD simulations at several temperatures and pay attention on the dynamics of the spherical micelles.

[Method]

POPC lipid molecule was used in this study. POPC lipids are interesting lipids that can be found in animals and humans. There are several methods for lipid simulations such as Molecular Dynamics (MD), Monte Carlo, Brownian dynamics, and coarse grain. For requiring detailed information of tail dynamics of POPC (1-palmitoyl-2-oleoyl-phosphatidy-choline), we perform MD simulation using CHARMM force field and it were performed with NAMD2 program package . CHARMM force field has a more detailed description of intra molecular interactions, and richer variety of parameters for dihedral angles, many of which being developed on the basis of the quantum chemical calculations. From this point of view, CHARMM force field can have advantages in accurate description of lipid bilayers[4].

[Results]

The results of analysis of the MD simulations are reported in poster session.

(Keyword: Molecular dynamics, CHARMM, POPC, spherical micelle, temperature)

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