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Structure and Dynamics of Spherical Micelle: A Molecular Dynamics Simulation

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[Introduction]

Biological phospholipids show self-assembly processes to form certain clusters such as micelles, vesicles, and membranes. Micelles are aggregates of surfactant molecules suspended in aqueous solutions. Micelles are formed by the competition of two forces—the hydrophobic interaction between the tails provides the driving force for aggregation and the electrostatic or steric repulsion between the head groups limits the size that a micelle can attain.

For fewer lipids such as micellar clusters, they show some interesting phenomena. The micellar clusters show fluctuation shapes. The structure (shape and size) of a micelle depends both on the architecture of the constituent surfactant molecule and the solution conditions such as temperature, presence of impurities, etc [1]. In micellar size, they also can form some definite structures such as spherical, cylindrical, rod-like, disk-like, worm-like, and so on. A spherical micelle structure is formed by region double chain hydrophobic molecules and is known to exist in relatively stable in vivo.

In Acep Purqon's doctoral thesis [2], he introduced four parameters to reveal the shape fluctuations, which are Aperture, Symmetry, Isotropy, and Compactness (ASIC). ASIC analysis confirm the dynamic assumption and physical meaning: aperture concerns tail dynamics properties, symmetry concerns shape fluctuation, isotropy concerns the parallelism of each lipid to one another, and compactness concerns cluster stability. This work simulated small aggregates of lipids and examined the correlation between those parameters. From that works, we know that the correlation between Isotropy-I and Compactness-C consequently leads to the structures of micelle, vesicle, and membrane. This technique can also be modified and expanded for other cases in biological dynamics. It might be any valuable information by combining with the other parameters. The methods also can be used for larger aggregates as well.

By this previous research, it should be interesting to investigate the structure and dynamics of larger aggregates such as spherical micelle. In this study, we carry out molecular dynamics simulations for spherical 1-palmitoyl-2-oleoyl-*sn*-phosphatidylcholine (POPC) micelles in water. POPC lipids are interesting lipids can be found in animals and humans. POPC is one of synthetic phospholipids derivatives. It has two chains of hydrocarbon and a chain

of phosphatidylcholine.

[Method]

We simulate for spherical POPC micelles using CHARMM (Chemistry at HARvard Molecular Mechanics) force field. The CHARMM force field has a more detailed description of intramolecular interactions, including Urey-Bradley term for covalent angles, and a richer variety parameters for dihedral angles [3]. And the simulation will be performed by NAMD2 package.

The goal from this study is to analyze the structure and dynamics of small spherical micelle consisting of phospholipid molecules. We also examined the characteristics of the interaction between small molecules in a spherical micelles. These study of structural characteristics and dynamics are important to understand their function in biological system, such as drug delivery materials.

[Results]

The results of these simulation are reported in our poster session.

(Keyword : CHARMM, POPC, molecular dynamics, spherical micelle)

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