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Correlation Analysis of Dynamical Properties in Flexible Micellar Clusters by using Geometrical Vectors

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【INTRODUCTION】

Micellar clusters have flexible structures and various shapes such as spherical[1,2], cylindrical, disk-like, rod-like, worm-like[3], and spaghetti-like structures[4,5]. The flexible structures imply a richness of dynamic properties. In our previous work[6], we have introduced and proposed a technique to analyze dynamics of flexible structure based on the concepts of Aperture(A), Symmetry(S), Isotropy(I), and Compactness(C); namely ASIC analysis. All parameters use simple geometrical vectors and represent their physical meaning. In this talk, we discuss the technique to explain the possible shapes in biological systems such as micelle, vesicle or membrane.

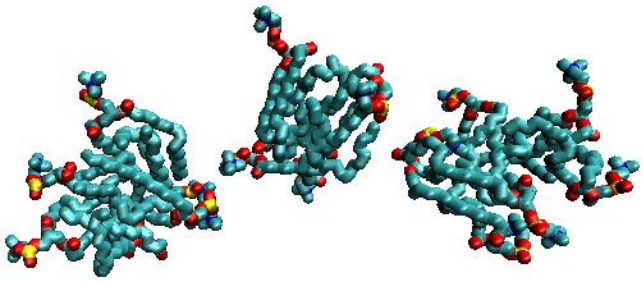

FIGURE 1. Flexible Micellar Clusters

【METHOD】

POPC (1-palmitoyl-2-oleoyl-phosphatidycholine) lipids and POPE (1-palmitoyl-2- oleoyl-phosphatidylethanolamine) lipids are interesting lipids that can be found in animals and humans. Some their technological applications are also reported. We carried out the MD simulations of 16 POPC lipids in 300 K and 340 K under a constant pressure condition (NPT) with periodic boundary using amber force field 03 and 11,326 TIP3P water molecules. In the same way, we calculate for POPE with 10,100 TIP3P water molecules. We adopted the AM1–bcc charge and use 8 Å cutoff radii for non-bond interactions. After performing 1 ns (1 MD step=2 fs, with SHAKE algorithm) for optimization and equilibration, we performed 7 ns of MD simulation. To reveal dynamic properties of flexible structure, we have proposed an analysis technique based on the concept of Aperture(A), Symmetry(S), Isotropy(I), and Compactness(C) representing tail dynamic properties, shape fluctuation, the parallelism of each lipid to one another, and cluster stability, respectively.

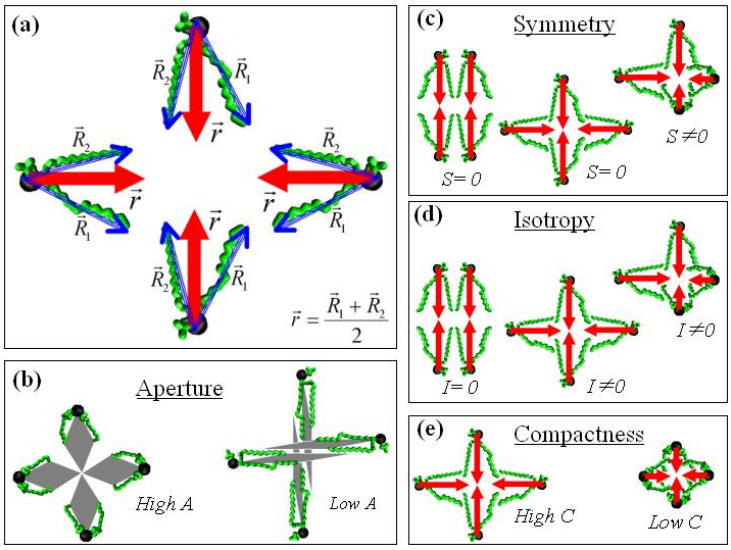

FIGURE 2. Illustration of ASIC formulation and their physical meaning.(a) Phosphate atom as center point and carbon at each edge of tail as other points.(b) Aperture is defined as summation of all the vector products. The larger the vector product is, the higher the *A*-value will become. (c) Symmetry is defined as the summation of all **r**. The more similar the length of vector **r** is, the lower the *S*-value will become. (d) Isotropy is defined as the summation of each vector product **r** with every other vector. The lower the *I*-value is, the more parallel the structure will become. (e) Compactness is defined as the summation of each length **r** . The smaller the total of each length **r** is, the more compact the structure will become. (Taken from Ref.6).

【ANALYSIS】

From the density and dynamic analyses, each parameter exhibit random processes or randomly oscillates, however, the dynamics have correlations; especially the correlation between Isotropy and Compactness. We pay attention to the correlation between Isotropy and Compactness because we find higher positive correlation between them than others and can leads consequently to the structures of micelle, vesicle, and membrane. We consider the implication that the high *I-C* correlation consistently occurs in any scale either in small or large aggregates. We interpret that the aggregates should modify their shapes to fulfill the correlations. The possible shape of *I-C* correlation for small aggregates denotes rod-like, spaghetti-like (irregular shapes), or sphere micelles with cavities, while, the possible shape of *I-C* correlation for large aggregates denotes a vesicle or membrane.

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