

Simultaneously Fluctuations on Mutual Bionanoclusters

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[INTRODUCTION]

Phospholipids in aqueous solutions have important functions in biological systems. At different conditions, they show certain fluctuations concerning with their cluster shapes. For fewer numbers of lipids, Marrink et al. have discussed in scaling of cluster properties and divided them into six different cluster sizes [1]. We have discussed the dynamical properties since the shape may act as diagnostics of anomalous behavior [2]. In this talk, we evaluate the shape fluctuations by using a concept of symmetry as a physical meaning [3]. We pay attention on mutual clusters and their simultaneously fluctuations [4].

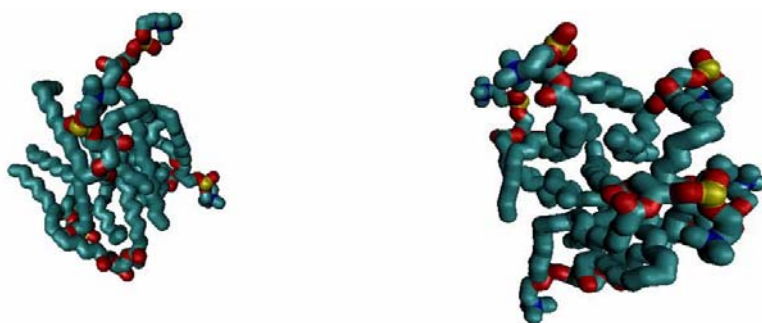


Figure 1. Mutual bionanoclusters analysis. Each cluster consists of several lipids. The shape fluctuations are calculated by Symmetry- S parameter and analyzed by direction correlation.

[METHOD]

We carried out the MD simulations of 16 POPC (1-palmitoyl-2-oleoyl- phosphatidyl choline) 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 ways, we simulated POPE (1-palmitoyl- 2-oleoyl- phosphatidylethanolamine) lipids in 10,100 TIP3P water molecules. We defined a parameter for analyzing shape fluctuations in mutual bionanoclusters by evaluating disordered shapes in connection with a concept of symmetry shapes. Symmetry- S represents whether a cluster has structurally symmetric or has asymmetric (irregular) shape. It evaluated a degree of symmetry or orderness from 3D actual position. Furthermore, we introduced direction correlation by calculating Symmetry- S to analyze the fluctuation patterns simultaneously. We also evaluated them in delayed time.

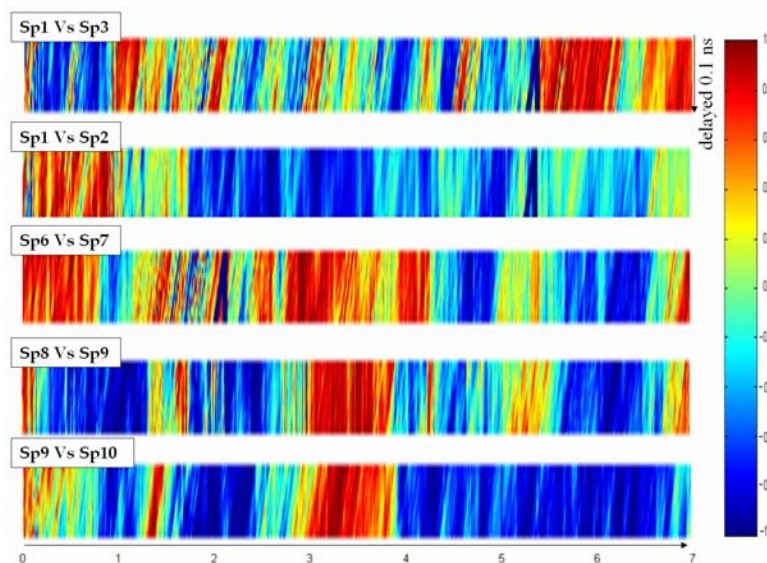


Figure.2. Simultaneously fluctuations in mutual bionanoclusters show certain pattern particularly for same number of lipids. (Taken from Ref.4).

【ANALYSIS】

We analyze the fluctuations both individual and mutual clusters. For individual clusters, they fluctuate randomly. In contrast, for mutual clusters, they apparently show certain patterns [4-6]. They also show certain patterns in delayed time analysis and seem periodically occurring for same number of lipids. We also analyze several aspects such as effects of number of lipids, odd-even number, temperature, distribution, jump motions and so on.

References

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