3P206 並列化された粗視化シミュレーションを用いたベシクルの構造安定性に関する理論的研究**Theoretical study on the structural stability of the vesicle by parallelized coarse-grained simulation**

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Biomembrane has lipid bilayer structure and the function as protein transporting. Lipid bilayer has a property to bend. Lipid bilayer on large scale is transformed from plane membrane to spherical membrane which is called vesicle. In this study, we perform molecular dynamics (MD) simulation of the vesicle to study structural stability by using different parameters of the interaction between two lipid molecules. We use coarse-grained model in which the lipid molecules are represented as 3 elastic chains of beads and develop MD program to perform parallel calculation for large scale and long time simulation. We observe membrane properties such as curvature. We will report the stability of the vesicle and the acceleration of MD simulation by parallel calculation.

3P207 Effect of cholesterol and 7-ketocholesterol on localization of Alzheimer's amyloid beta (A β -42) in membrane domains

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Lipid raft domains are considered as sites for amyloid beta (A β) binding in cell membranes. Cholesterol (Chol) and its oxidized derivative, 7-ketocholesterol (7keto), have been reported to affect A β /membranes interaction. However, very little is known about their effects on A β localization in membrane domains.

We have shown that Chol controlled the association of A β with Lo domains of model membranes. 7keto did not significantly increase A β localization in Lo domains but facilitated the peptide to insert into Ld phase. The effect of Chol and 7keto on the interaction of A β with membrane domains has been discussed by means of their ability to change membrane fluidity. These results are useful for understanding the role of Chol and its oxidation in A β -induced cytotoxicity.

**3P208 脂質酸化物による生体模倣膜のドメイン形成
Effects of lipid oxidation products on domain formation of biomimetic membrane**

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Lipid rafts, physiologically important domains in plasma membranes, may be formed by mainly saturated lipids and cholesterol. Lipid oxidation has been reported to change dynamics of membranes¹. However, the influence of lipid oxidation on domain structure and stability of membranes has not been well understood.

We made phase diagrams of membranes containing oxidized cholesterols, such as 7-ketocholesterol and 7 β -hydroxycholesterol. We found that nonanal, an oxidized product of dioleoylphosphatidylcholine, significantly affects domain structure. Further, we characterized miscibility temperatures of oxidized membranes. Finally, the mechanism behind domain formation and stability of oxidized lipid-containing membranes was discussed.

[1] T. Yoda, et al., Chem. Lett. (2010)

3P209 遠心式マイクロ流体デバイスによる細胞サイズリボソームの作製**The synthesis of cell-sized liposomes by centrifuge-based microfluidic device**

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Cell-sized liposomes are widely used to mimic the bio-membrane in biophysics and biochemistry. To efficiently use liposome for biological application, the production methods are required to control unilamellarity, encapsulation efficiency, and size. In recently, microfluidics method for producing a cell-sized liposomes have been proposed. However, the utility of this technology is low because to make microchannel requires for a microfabrication process. Here, we constructed simple production method of cell-sized liposomes as control unilamellarity, encapsulation efficiency, and size by centrifuge-based droplet shooting device (Maeda et al., Adv. Mater. 2012). We hope that this method will allow to make cell-sized liposomes for a given biological application.

3P210 脂質側方拡散を増幅させる新規拡張アンサンブル法の開発と応用**Acceleration of lipid lateral diffusion by generalized-ensemble molecular dynamics simulation**

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Conformational sampling is important for simulating complex biomolecular systems. In this study, we propose a new generalized-ensemble simulation algorithm for membrane systems, which we call the surface-tension replica-exchange molecular dynamics method. In the method, each replica is simulated in the NPyT ensemble, where surface tensions in a pair of replicas are exchanged at certain intervals during the simulation. We tested the method on a fully hydrated DPPC lipid bilayer system. We observe that large-scale lateral deformation of DPPC membranes takes place in all of the replicas. There is accelerated lateral diffusion of lipid molecules compared with conventional MD simulation. Our method could be applicable to a wide variety of biological membrane systems.

3P211 Time-resolved 3D Quantification and Analysis of Membrane-Lipid Signaling in Dictyostelium

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On the basis of 3D time-resolved observations on actin-polymerization-inhibited Dictyostelium cells using ultra-fast spin confocal microscopy, we systematically analyze and map the dynamics and patterns of membrane-bounded PIP3 molecules. We show that a whole zoo of pattern formation is possible, even exotic ones such as periodic target waves, bouncing waves and standing waves. Quantitative analysis of a large ensemble of cells lead to unique dependencies that are found to be bounded by the geometrical constrain of the cell membrane. We additionally performed realistic 3D stochastic simulations and compare the results with our experimental findings.

This study is a unique (may be first) attempt to analyze and understand pattern formation in chemotactic cells in 3D.