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[2] J. Grumelard et al., *Chem. Commun.* (2004).

2A1636 細胞動態シミュレーションのための粗視化膜モデルの構築

Simplified coarse-grained model of cellular membranes to simulate dynamic features of cells

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Living cells have dynamic and characteristic shapes relating to their functions. To understand cells as molecular systems, it is dispensable to develop numerical modeling and to simulate cellular membranes. However, it takes a huge amount of time to simulate the membrane dynamics in an entire cell. To eliminate this very high cost of computation time, we constructed a simple coarse-grained model of cell membrane instead of dealing with individual lipid molecules. The coarse-grained modeling has proved appropriate for protein folding studies, explaining some features of folding rate and mechanism. A simplifying feature of these coarse-grained protein models has treated implicitly the aqueous solvent environment, solvent frictional forces, and random collisions, which were described by Langevin dynamics. Here we further simplified the coarse-grained model. In our model, a membrane element was substituted for some lipid molecules. Simulation of a spherically arranged liposome were used as a simplest membrane model to examine the potential energy functions. Directional asymmetry of the potential function between the elements was the key to stabilize the spherical shape of the liposome. The present simplified coarse-grained modeling of membranes will provide a facile means to simulate a dynamic shape and functions of complex cellular membranes at the cellular level.

2A1648 メリチンのリン脂質膜内での非アレニウス揺らぎ

Melittin-fluctuation within a phospholipid membrane according to non-Arrhenius law

Masayuki Higashi, Kazumi Saikusa, Akinori Awazu, Syunsuke Izumi (Department of mathematical and life sciences, Graduate school of science, Hiroshima university)

Membrane proteins play important roles of signaling processes in cells. In general, not only the protein structures but also the dynamics and fluctuations induced by the lipid-protein interactions contribute dominantly to their functional performances. Melittin is the peptide toxin composed of 26 amino acid residues (GIGAVLKVLTTGLPALISWIKRKRQQ-NH₂). This molecule is often considered as a model of transmembrane subunit of membrane proteins since it takes membrane penetration structure by interacting with a phospholipids membrane. In this study, we focus on the fluctuation of melittin within a phospholipid membrane experimentally and theoretically.

First, we analyzed the fluctuation of melittin within Egg-York-phospholipid liposome by sequential acetylation and mass spectrometry. The reaction rate of acetylated melittin decreased exponentially at low temperature. However, the reaction rate became almost constant for more than 30°C. This non-Arrhenius behavior was not observed in the case of other phospholipids. It was suggested that non-Arrhenius behavior depends on the phase transition of phospholipid liposome.

Next, we simulated a coarse-grained model of melittin within a membrane. We obtained qualitatively the similar phenomena to that obtained in experiments. We found the amplification of the lipid fluctuation by temperature increase causes the hindering of intra-membrane migration of melittin and acetylation. Thus, non-Arrhenius behavior is realized by the excluded volume effect among melittin and fluctuating lipid.

2A1700 脂質膜上において誘起される PH ドメインの構造変化および機能の解析

Conformational alteration of SWAP-70 PH domain induced at the membrane surface

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We investigated conformational alteration of the pleckstrin homology (PH) domain of switch-associated protein-70 (SWAP-70) induced at the membrane surface. The SWAP-70 PH domain has a typical PH domain tertiary structure

that consists of a β -sandwich and a C-terminal α -helix located at one of the splayed corner of the β -sandwich in solution. The SWAP-70 PH domain contains a phosphatidylinositol 3,4,5-trisphosphate (PtdIns(3,4,5)P₃)-specific binding site and a nuclear localization signal (NLS) sequence which localize SWAP-70 to the plasma membrane and the nucleus, respectively. Far-UV CD and solid-state NMR spectroscopies indicated that the C-terminal α -helix undergoes conformational transition to form a disordered structure when the PH domain binds to PtdIns(3,4,5)P₃ embedded in lipid bilayer vesicles. This conformational alteration is not detected for the PH domain bound to Ins(1,3,4,5)P₄, head-group analog of PtdIns(3,4,5)P₃, in solution. Exposure of the NLS sequence located in the C-terminal α -helix would be modulated by the conformational alteration induced at the membrane surface. This suggests that the functional relocalization of SWAP-70 is regulated by interaction between plasma membrane and the PH domain. The conformation of the SWAP-70 PH domain at the membrane surface was also found to be regulated by condition of the membrane interface, such as ion concentration and lipid composition.

14:00~17:00 B 会場 / Room B

水・水和／電解質

Water & Hydration & Electrolyte

2B1412 イオンと生体分子周囲の水の動的性質の評価：MD および QM 計算

Assessment of dynamic properties of water around ions and biomolecules: MD and QM calculations

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Ions and water around biomolecules play important roles and are supposed to change the physico-chemical properties during enzymatic reaction such as ATP hydrolysis. Mobility change of water molecules in ionic solutions has been a long standing issue in the field of spectroscopy; however, the molecular mechanism is still controversial. To elucidate the properties, classical MD simulations of water molecules around several types of solutes (polyphosphates, AMP, 20 amino acids, and monovalent ions) were done with several conventional water models. The decreased mobility of water molecules was reproduced in our simulations while the increased mobility could not. Therefore, we examined ion/water interactions through QM calculations based on TIP5P water model and improved the interaction potential. This newly developed model could reproduce the increased mobility around several ions.

2B1424 分子サイズの溶質分子による水の分極の分子動力学シミュレーション

Molecular Dynamics Study of the Static Water-Polarizability Caused by a Molecular-Sized Ion

Yoji Kubota, Ryo Akiyama (Department of Chemistry, Kyushu University)

The dielectric response of water governed by solute molecules has been studied using various methods because it is an important topic in the study of electron transfer reactions and in calculations on the hydration energy of a solute. The linear response approximation, for example the Born model, is frequently adopted to estimate the solvation energy of a solute molecule immersed in a solvent. In the approximation the dielectric constant is not dependent on the charge of solute molecules. Hence, the response of a solvent's polarization has been examined based on a molecular picture using integral equation theories and molecular simulation methods. Here, we examined water polarization phenomena caused by a charge of a solute, because there is a qualitative discrepancy in the calculated results between various methods. In the present study, the polarization was calculated using MD simulations. The finite size effect was examined and we set a basic cell large enough. In case of a positive solute, the dependence of the polarizability on the value of solute charge showed a maximum. However, the response to the solute charge was not saturated, and it approached a linear response behavior. The feature for a negative solute was almost the same, but much more remarkable. Therefore the water's state is drastically changed from -e to +e. These results also indicate a fine structure in the polarizability curve. We will discuss the relation between the electrostatic fluctuation of water and the hyper mobile water.