3P007 Systematic structural study of single amino acid insertion mutants of YFP

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YFP is a mutant derivative of green fluorescent protein, and is widely used as a fluorescent indicator in molecular biology. Recently we found that YFP mutant variants with single amino acid insertion in $\beta 7$ showed various fluorescence responses to environmental change. The fluorescence responses depend on the nature of the inserted amino acid residue. To elucidate the molecular mechanism how the insertion affects the fluorescent property, we prepared twenty single amino acid insertion variants of YFP and solved the structures. Here we show the structures of eighteen mutant YFPs. They show unexpected conformational variation in $\beta 7$ dependent on the inserted residue. We will discuss the relationship between the mutant structure and the fluorescent property.

3P008 分子動力学シミュレーションを用いた Hras-GTP 複合体の溶媒水と複合体の水素結合の解析

Analysis of hydrogen bonds between solvent water and atoms in the Hras-GTP complex by molecular dynamics simulations

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In order to understand the mechanism of hydrolysis of GTP in the Hras-GTP complex, we study the structures of the Hras-GTP and GDP complexes in water solvent by molecular dynamics (MD) simulations. We evaluated the potential parameters around Mg²⁺ in Hras-GTP and GDP complexes by quantum chemical calculations. We performed MD simulations of the Hras-GTP and GDP complexes in water solvent using parameters of AMBER03 and our parameters around Mg²⁺. We found that the site dipole fields around GTP are different from those around GDP. We proposed that this difference causes the difference of hydrolyzability between GTP and GDP.

In this study, we analyze the individual hydrogen bonds between solvent water and atoms in the Hras-GTP complex.

3P009 固体 NMR を用いたヌクレオソームにおけるヒストン H2A、H4 の構造解析

Structural analysis of histone H2A, H4 in nucleosome using by solid-state NMR

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In eukaryotic cells the fundamental structural unit of chromatin is a nucleosome core, consisting of two copies of four histones and DNA, whose crystalline structures have been determined. However in the crystals the N- and C-terminal histone tails, which are responsible for gene regulations by their chemical modifications could not be well identified. Here, we have examined the structures of N- and C-terminal histone tails of H2A and H4 in a model of chromatin by solid-state NMR and MD simulations. These suggested that both histone tails in chromatin hold flexible random coil structures, which might play significant roles in gene regulations.

3P010 細胞接着ペプチドと $\alpha 2\beta 1$ インテグリン I ドメインとの結合シミュレーション

Docking simulation of cell adhesion peptide and $\alpha 2\beta 1$ integrin I domain

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Laminins, which are glycoprotein in basement membrane, have diverse biological activities. EF1 peptide (DYATLQLQEGRLHFMFDLG) derived from $\alpha 1$ chain of laminin has cell adhesion mediated by $\alpha 2\beta 1$ integrin. Suzuki et al. analyzed active core sequences to investigate minimal sequences of EF1 and found that cell adhesion of EF1 is conformation-dependent by cyclization of minimal sequences of EF1. Previously, we showed that EF1 has hairpin structure by simulated annealing, and we studied dynamical behavior of EF1 in water solution (300K, 1bar). We are also interested in relationship of structure between EF1 and receptor. In this study, we perform docking simulation of EF1 and $\alpha 2\beta 1$ integrin. We use structure of $\alpha 2\beta 1$ integrin I domain determined by X-ray diffraction.

3P011 DFTB+ソフトウェアへの REUS 法の導入

Implementation of Replica-Exchange Umbrella Sampling to the DFTB+ Simulation Package

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We have investigated the computational methods which combined the self-consistent-charge Density Functional based Tight Binding (DFTB) method[1] for fast calculations of quantum effects and the Replica-Exchange Umbrella Sampling (REUS)[2] for enhanced conformational sampling. One of the excellent QM-MD simulation package named DFTB+ does not have REUS method incorporated. We thus modified DFTB+ to include the REUS method. We will compare the results of DFTB+ calculations with those by another simulation package and present the results in small molecules.

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[2] Y. Sugita, A. Kitao, and Y. Okamoto, J. Chem. Phys. 113, 6042 (2000).

3P012 Preliminary study of voltage-gated proton channel in activated state for X-ray crystallography

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Voltage-gated proton channel (VSOP) has a voltage sensor domain that is similar to the voltage sensors of canonical voltage-gated ion channels, but it lack of ion pore domain. VSOP is related to superoxide production in phagocytes and human sperm motility. We recently determined the crystal structure of VSOP, which showed first resting-state structure as voltage sensor, and it showed that the proton pathway was closed. We are trying to determine the crystal structure in activated-state, which is expected to understand the gating mechanism of VSOP. In our poster, we will discuss the procedure to prepare the activated-state of VSOP using gel filtration chromatography with anti-VSOP Fab fragment labeled fluorescence.