1P019 Expression and Structural Analysis of Two Kinds of Perireceptor Proteins (PRPs)

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Around olfactory dendrites there are soluble proteins in the high concentration, suggesting an important role in the odour or pheromone perception. In insects two classes of soluble proteins have been so far identified, odorant-binding proteins (OBPs) and chemosensory proteins (CSPs). However, we found only OBPs from common Japanese newt. We call them perireceptor protein (PRP) and study to elucidate the role in chemosensation. We have cloned, expressed and analyzed two kinds of OBPs (Cp-Lip1, -Lip2) of *Cynops pyrrhogaster*, and CSP7 found in the aunt chemosensory organ. In the present study, the expression and purification of Cp-Lip1 and CSP7 and the fluorescent assay and CD measurements are reported.

1P020 SepCysE の機能・構造解析による Cys-tRNA^{Cys} 生合成機構の解明

The study on the structure and function of SepCysE related to Cys-tRNA^{Cys} synthesis

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In the synthesis process of aa-tRNA, amino acid is normally attached to tRNA directly by aminoacyl-tRNA synthetase (aaRS). However, methanogenic archaea require two enzymes to form Cys-tRNA^{Cys} synthesis in indirectly pathway, which tRNA^{Cys} is acylated with phosphoserine (Sep) to form Sep-tRNA^{Cys} by phosphoseryl-tRNA synthetase (SepRS), and then Sep is converted to Cys by Sep-tRNA:Cys-tRNA synthetase (SepCysS). Here we revealed a crystal structure of SepCysS in complex with SepCysE that is recently discovered as an essential factor for Cys-tRNA^{Cys} synthesis. Moreover, we carried out binding assay with SepRS, SepCysS and SepCysE. The results indicated that these three proteins form a stable complex as a functional unit.

1P021 タンパク質レアイベントを抽出する効率的構造サンプリング法

Enhanced conformational sampling methods for extracting biological rare events of proteins

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Biological rare events are related to functions of proteins. In the most of biological processes, the rare events are observed as structural transitions related to the biological functions. In this study, we propose two enhanced conformational sampling methods by repeating (i) Selections of seeds and (ii) Conformational re-sampling for the seeds. One is Fluctuation Flooding Method (FFM), where largely fluctuating structures projected onto low frequency modes are selected as the seeds. Another is Outlier FLOODing Method (OFLOOD), where sparse distributions of states of proteins (outliers) in conformational spaces are selected as the seeds. We show these simple protocols might drastically promote structural transitions like a conformational flooding from the seeds.

1P022 遷移温度付近のシニョリンの緩和モード解析 Relaxation Mode Analysis of Chignolin at Transition Temperature

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Relaxation mode analysis (RMA) developed to investigate "dynamic" properties of polymer, homo-polymer, systems. In the method, slow relaxation modes are extracted from a molecular dynamics simulation. In RMA, the time correlation matrices of structural fluctuations for two different times are calculated. Then, by solving a generalized eigenvalue problem for these matrices, the relaxation rates and modes are estimated from the eigenvalues and eigenvectors, respectively. RMA has been applied to protein systems to investigate dynamic properties of structural fluctuations. Here, we present the results of RMA for a simulation of chignolin at a transition temperature in which many transitions between the global energy minimum state and metastable states are observed.

1P023 真空紫外円二色性分光による α_1 酸性糖蛋白質と生体膜の相互作用機構の解明

Interaction Mechanism of α_1 -Acid Glycoprotein with Biomembrane Characterized by Vacuum-Ultraviolet Circular Dichroism Spectroscopy

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α_1 -Acid glycoprotein (AGP) interacts with biomembrane to change the conformation ($\alpha \rightarrow \beta$ transition) and decrease the drug (hormone)-binding capacity. To clarify the interaction mechanism, the vacuum-ultraviolet circular dichroism spectra of AGP were measured in the presence or absence of phosphatidylcholine (PC), phosphatidic acid (PA), and phosphatidylglycerol (PG) liposomes. It was found that the helical regions of AGP increased upon interacting with the PA and PG liposomes, the latter more strongly inducing the helices. However, there was no secondary-structure change of AGP in the PC liposome. These results suggest that the polar head groups of phospholipids play an important role and their negative net charge is essential for the AGP biomembrane interaction.

1P024 レチノール結合タンパク質とカルパインの立体構造上に形成されたイントロンの平面

Planes formed with 4 introns in tertiary structures of RBP & calpain D-VI

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We report a novel relationship between introns and the tertiary structures of retinol binding protein and calpain domain VI. We identified "intron-positions" on the residues on which or just after which introns are found in their corresponding nucleotide sequences, and then found that 4 intron-positions form a plane. We also found some relationships between the planes and the ligands. To evaluate the statistical significance of the planarity, we calculated the mean distance of each intron-position from the plane defined by the other three intron-positions, and simulated to confirm that their probabilities are significantly smaller than those calculated from randomly generated locations.