3P013 金属結合に伴う 3 ヘリックスバンドル形成の動的構造解析
Dynamic structural analysis of three-helix bundle formation induced by metal-ion binding

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We designed a 72-residue protein based on a *de novo* designed three-helix bundle protein, α_3 D, reported previously. In order to evaluate the conformational change from random to three-helix bundle structure only in the presence of metal-ion, three residues in the hydrophobic core of α_3 D were replaced to His, and additional several residues were replaced to Ala. We analyzed the metal-ion dependent helix formation of overexpressed and purified α_3 D-His using circular dichroism spectrometry. We further analyzed the Laue diffraction spots from gold nanocrystal attached to the introduced Met of α_3 D-His in the presence or absence of metal-ion using the single-molecule detection system called diffracted X-ray tracking. The dynamic property of α_3 D-His was evaluated.

3P014 Membrane-Induced Conformations of Proteins Characterized by Vacuum-Ultraviolet Circular-Dichroism and Flow Linear-Dichroism

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Vacuum-ultraviolet (VUV) circular-dichroism (CD) and flow linear-dichroism (FLD) spectra of α -lactalbumin, β -lactoglobulin, and thioredoxin were measured down to 170 nm in the presence (pH 4.5) and absence (pH 7.5) of phosphoglyceride liposome in order to clarify the conformations of these proteins interacting with membrane. The VUVCD analysis showed that the α -helix regions on the secondary-structure sequence largely increase due to liposome binding in all proteins. The FLD spectra indicated that the membrane-induced helix regions interact with the surface of liposome. These results suggest that a VUVCD coupled with a FLD spectroscopy can give new insight into the conformations of proteins interacting with membrane.

3P015 創薬等支援技術基盤プラットフォーム事業におけるタンパク質 X 線溶液散乱
Bio-SAXS in the Platform for Drug Discovery, Informatics, and Structural Life Science (PDIS)

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PDIS is a national platform project started from FY2012 to promote the structural life science. KEK is one of groups to support the structural analysis studied by protein crystallography and protein solution scattering, supplying the beamtime of Photon Factory. Biomolecule small-angle X-ray scattering (Bio-SAXS) is a powerful technique for analyzing not only the protein structure in the solution but the molecular arrangement of complexes by ab-initio method. The hybrid analysis using PX and SAXS would lead to the further understanding about a structure state of biomolecules. We now support measurement and analysis of beginners of Bio-SAXS and improve the core technologies in the Bio-SAXS experiment.

3P016 分子動力学法によるラミニン由来ペプチドの研究
Study of peptides derived from laminin by molecular dynamics simulations

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We are analyzing the EF1 (DYATLQLQEGRLHFMFDLG, mouse $\alpha 1$ chain 2762-2780 residues) and the EF2 (DFATVQLRNGFPYFSYDLG, mouse $\alpha 2$ chain residues 2808-2826) peptides derived from the laminin. Laminin, a glycoprotein which is a component of basement membrane, has diverse biological activities. In previous research (EF1 and EF2), relation of structure to biological activity was indicated. Thus, we study the differences of dynamical properties in EF1 and EF2. In our previous research, we showed that hairpin-structure is found in EF1 (but not in EF2) by simulated annealing. In this study, we investigate the behavior of EF1 and EF2 peptides at 300K and 1bar. We calculate RMSD and RMSF. Furthermore, we will analyze our results by using PCA.

3P017 分子動力学法を用いたラミニン $\alpha 2$ 由来ペプチド A2G80 の構造決定因子の同定
Identification of structure determinant amino acid residues in the A2G80 peptide derived from laminin $\alpha 2$ by molecular dynamics simulation

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Laminins are glycoproteins composed of α , β , and γ chains. Laminins have diverse biological functions, such as cell adhesion, migration and angiogenesis. Laminin $\alpha 2$ chain is expressed in muscle and nerve tissues, and the interaction between laminin $\alpha 2$ chain and α -dystroglycan (α DG) is essential for proper muscle function.

The A2G80 peptide derived from laminin $\alpha 2$ chain binds to α DG specifically. We performed molecular dynamics simulation of A2G80 to compare with crystal structure obtained by X-rays. Furthermore, to identify structure determinants, alanine-substituted peptides were also simulated, and compared with their circular dichroic spectra.

3P018 分子動力学計算による 4 量体型サルコシン酸化酵素の酵素—基質アナログ複合体の動的挙動解析
Behavior of enzyme-substrate analogue complex of heterotetrameric sarcosine oxidase studied by molecular dynamics simulation

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Heterotetrameric sarcosine oxidase (SO) catalyzes oxidative demethylation of sarcosine to generate glycine and hydrogen peroxide. SO is composed of four non-identical subunits, and FAD, FMN, NAD⁺, and Zn²⁺. The structural and biochemical analyses have shown that the SO-dimethylglycine (DMG) complex contains a large cavity and suggested channeling of oxygen, sarcosine, and products through the cavity. Toward realistic simulations of channeling, we have carried out molecular dynamics simulations for the SO-DMG complex using the GROMACS program with the GROMOS force field. In the present study, we are performing more accurate simulations by using the AMBER force field than the previous one. As a result, the structure simulated was in good agreement with X-ray data.