changes of cyanobacterial transcription factor, SmtB, functioning as the sensor for zinc-ion concentration in the cell, following zinc-ion binding

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see 1TA1-02

lactalbumin

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α -Lactalbumin (α -LA) is a small globular protein and has been extensively used as a model protein for studying the mechanisms of protein folding. This protein exhibits the molten globule (MG) state under mildly denaturing conditions, which has been shown to be identical to the transient intermediate observed during the kinetic folding. The MG state of α -LA has been characterized in terms of the structure and stability. Svensson *et al.* reported that human α -LA-fatty acid complex, named HAMLET (human alpha-lactalbumin made lethal to tumor cells), induces apoptosis-like death in tumor cells. HAMLET was stable in the MG-like conformation, but the structural details are not fully understood. Peterson *et al.* reported that GAMLET (goat alpha-lactalbumin made lethal to tumor cells) also induces apoptosis in tumor cells. Previous studies have shown that the MG states were different between goat α -LA and human α -LA. In this study, we attempt to determine the oleic acid binding site of GAMLET and HAMLET by 2D-NMR. The NMR spectra of ^{15}N -labeled goat α -LA in MG state at pH 2.0 and 50 °C and GAMLET recorded at 920 MHz were studied and the backbone assignments of ^{13}C , ^{15}N -labeled goat α -LA in MG state was obtained by three-dimensional CBCACONH and HNCACB experiments. We assigned the 40 out of the 123 residues of goat α -LA in MG state. Chemical shift perturbations were used to map the binding surfaces. We found that the oleic acid binding site of GAMLET is located near the Ca^{2+} -binding site of goat α -LA. We will perform similar experiments with HAMLET and compare the results with those of GAMLET.

1P-023 異なる結合様式をもつジユビキチンの分子動力学シミュレーション
Molecular Dynamics Simulation Study of Diubiquitins with Different Linkages

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Protein ubiquitination is a post-translational modification involved in the regulation of diverse cellular processes, including protein degradation, cell signaling, DNA damage response and transport processes. Ubiquitin (Ub) can be conjugated to target proteins either as a monomer or as polyubiquitin chains, the latter can be formed though all seven lysine residues in Ub. Different Ub linkages result in various conformations of Ub chains and corresponding distinct physiological functions in cells. However, such diversity of Ub chains is not well understood. In the present study, we focused on K11-, K48-, and K63-linked diubiquitins and performed molecular dynamics simulation to reveal a variety of Ub-chain conformation and mechanisms of their specific recognition. Crystal structures of K48- and K63-linked diubiquitins (PDB ID: 1AAR and 2JF5, respectively) were used as the initial conformations for each simulation, whereas K11-linked diubiquitin structure was modeled using Ub crystal structure (PDB ID: 1UBQ) because of the absence of the crystal structure. Differences in conformations and dynamical properties among the three diubiquitins are shown. We will discuss potential mechanisms of the chain linkage specificity of polyubiquitin in the presentation.

1P-024 抗 HIV 活性を有する天然型 APOBEC3G タンパク質の構造、1 本鎖 DNA との相互作用及び酵素反応のリアルタイムモニタリング
Structure, interaction with single-stranded DNA, and real-time monitoring of the enzymatic reaction of wild-type APOBEC3G possessing anti-HIV activity

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see 1YP1-07

1P-025 翻訳後修飾を受けるタンパク質の立体構造変化データベース解析
Database analysis of protein structural changes with post-translational modifications

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Post-translational modifications, chemical modifications after the translation, occur on a wide variety of proteins. For example, phosphorylation of enzymes modulates their activities, and glycosylation of secretory proteins is necessary for their recognition processes. At the same time, proteins' structure changes are also important in controlling their functions. The aim of the study is to understand how post-translational modifications cause structural changes, and how relevant these causal relations are to the functions. For this purpose, we carried out database analysis based on the structural database. We annotated 68,928 entries in PDB in terms of the protein structure family based on the SCOP domain family to eliminate redundancy, and obtained 2,816 protein structure families. Among them, we found 186 families with multiple entries of both modified and unmodified proteins. The C_α -RMSD values between these protein pairs revealed significant structural changes between the modified and unmodified proteins; they are significantly larger than those between unmodified and unmodified protein pairs, and larger than those between modified and modified protein pairs. We will present the results of detailed analysis for these conformational changes upon modification, and discuss the relevance to their functions.

1P-026 α -ラクトアルブミンの MG 状態と生物機能
The molten globule state and the biological function of α -

1P-027 全反射赤外分光法によるマルチ銅酸化酵素のカルボン酸の機能解析
Carboxyl group functions in the multicopper oxidase CueO studied by ATR-FTIR

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Escherichia coli CueO is a multicopper oxidase, which couples the oxidation of substrate Cu(I) ion to Cu(II) with the reduction of a dioxygen molecule to two water molecules. The dioxygen activation site has one type2 and two type3 Cu ions. It has been proposed that the two key carboxylic amino acid residues, Glu506 and Asp112, could be involved in the proton transfer for the catalytic dioxygen reduction (1, 2). Redox dependent protonated state changes in carboxylic acid residues in CueO were studied by attenuated total reflection-Fourier transform infrared (ATR-FTIR) spectroscopy. Electrochemically induced reduced -minus- oxidised difference IR spectra were measured in the wild type, Glu506Gln and Asp112Asn mutants. The wild type CueO showed a positive band at 1747 cm^{-1} , which indicates the protonation of a carboxylate anion upon reduction of the trinuclear centre. The 1747(+) band was disappeared in the Glu506Gln mutant, and it was reversed in the Asp112Asn mutant. The results are discussed in relation to the reaction mechanism.

1) FEBS Lett., 580, 4069. Ueki et al.
2) J. Biol. Chem., 2009, 284, 14405. Kataoka et al.

1P-028 ビスフェノール A との相互作用はカルモジュリンのカルシウム結合能を弱める
Bisphenol A weakens Calcium Binding Affinity of Calmodulin

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see 1TA1-03

1P-029 時間領域テラヘルツ分光法でみる低振動領域におけるタンパク質の動力学転移
Low-frequency dynamical transition of proteins monitored by terahertz time-domain spectroscopy

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see 1TA1-07