3P049 糖鎖の構造多形予測に向けた CHARMM 力場の改良
Revised CHARMM carbohydrate force field for improved description of conformational diversity of N-glycans

Suyong Re¹, Shigehisa Watabe², Wataru Nishima¹, Yuji Sugita¹ (¹*Wako Inst., Riken*, ²*Grad. Sch. Sci. Eng., Chuo Univ.*)

Glycans-protein interaction is essential for a variety of biological functions and diseases. However, the inherent flexibility of the glycan molecules makes conventional X-ray or NMR structural analysis quite difficult. Here, we employ molecular dynamics (MD) simulations to reveal the glycan-protein complex structures in atomic details. To this end, we revised the current CHARMM force field for carbohydrates by refitting the parameters so as to increase the accuracy in the potential for the α 1-6 glycosidic bond. Replica-exchange MD simulations, with extensive sampling of N-glycan structures in solution, show that our revised force field parameters better reproduce the experimental NMR data and more accurately represent glycan rotameric conformations.

3P050 Structural insights into enzyme-bound flavin adenine dinucleotides (FAD)

Gopi Kuppuraj¹, Fumiko Suzuki¹, Masahiko Ikeuchi², Kei Yura¹ (¹*Centre for Informational Biology, Ochanomizu University, Bunkyo, Tokyo*, ²*Department of Life Sciences (Biology), University of Tokyo, Komaba, Meguro, Tokyo*)

The coenzyme FAD is an absolute requirement for certain enzymes to carry out metabolic reactions and to repair DNA damaged by UV radiation. Hence, understanding the conformations adopted by FAD bound to different enzymes is essential. Here, we sampled 927 enzyme-bound FAD conformations in the Protein data Bank (PDB). The results show that FAD exists in a variety of conformations from compact to “open” structures. FAD dihedral angle distributions indicate that structures are locally conserved to recognize different chemical groups within the coenzyme. The conclusions provided herein may prove valuable in the development of rotamer libraries and fragment-based approaches for docking/drug targets in the aforementioned FAD-bound enzymes.

3P051 金属結合によるヒトプリオンペプチドの配位モード
Coordination mode in human prion peptide caused by metal binding

Kazuya Iwama, Masahiro Yagi, Haruto Onda, Wakako Hiraoka (*Graduate School and Technology, Meiji University*)

In this report we investigated the conformational change in human prion protein (huPrP) which have flexible regions caused by metal binding, such as Cu²⁺, Ni²⁺ and Co²⁺.

Metal binding to peptide fragments containing His96 and/or His 111 was examined using visible absorption spectra and Circular Dichroism (CD). Secondary structure of peptide fragments was observed using Far-UV CD. Vis absorption and Vis CD indicated the characteristic spectra from metal binding, which were derived from d-d transition of metal ion. Far-UV CD spectra showed coordination modes depended on pH value, metal and chain length of huPrP.

We will also investigate metal binding mode of other huPrP peptide fragments to more understand mechanism of prion diseases.

3P052 二次元蛍光寿命相関分光法による BdpA 変性状態における構造ダイナミクスの解析
Two-dimensional fluorescence lifetime correlation spectroscopy on the conformational dynamics of the unfolded state of BdpA

Takuhiko Otsu¹, Kunihiro Ishii¹, Hiroyuki Oikawa², Munehito Arai³, Satoshi Takahashi², Tahei Tahara¹ (¹*Mol. Spectrosc. lab., RIKEN*, ²*IMRAM, Tohoku Univ.*, ³*Grad. Sch. Arts. Sci., Univ. Tokyo*)

Characterization of the unfolded state of protein is highly required to understand the initial stage of protein folding. This state does not possess a well-defined structure but is described as an ensemble of conformers. However, the sensitivity, time resolution and quantitativity provided by conventional analytical methods are not sufficient to fully explore it. We have recently developed two-dimensional fluorescence lifetime correlation spectroscopy and applied it to examine the unfolded ensemble of B domain of protein A (BdpA). The results showed the presence of two distinct unfolded ensembles (extended and compact). It was also revealed that the compact unfolded ensemble is highly heterogeneous and the dynamics in the ensemble occur within 10 microseconds.

3P053 タンパク質中のトリプトファン残基の近紫外円二色性と紫外共鳴ラマンスペクトルの特性
Some basic properties of near-UV circular dichroism and UV resonance Raman spectra of tryptophan residues in proteins

Shigenori Nagatomo¹, Masako Nagai², Takashi Ogura³, Teizo Kitagawa³ (¹*Dept. Chem., Univ. Tsukuba*, ²*Res. Center Micro-Nano Tech., Hosei Univ.*, ³*Grad. Sch. Life. Sci., Univ. Hyogo*)

Near-UV circular dichroism (CD) and UV resonance Raman (UVRR) spectra of L-Trp residues and model compounds were investigated to utilize Trp signals of proteins as a structural marker. All the indole-C₃ derivatives except for L-Trp gave no CD bands (L_a and L_b), indicating that the asymmetric carbon (C _{α}) is essential to appearance of CD. The 229-nm excited UVRR spectra were almost the same between L-Trp and indole-C₃ derivatives, suggesting that Raman intensity comes from resonance with B_b but not with L_a or L_b . Both UVRR and CD spectra of L-Trp were influenced by protonation of amino- and/or carboxyl-groups, suggesting that these protonations are communicated to indole through σ -bonds containing C _{α} and influence both chirality and the electronic state.

3P054 テラヘルツ時間領域分光法によるトレハロースにコートされたタンパク質の低振動ダイナミクス
Low-frequency dynamics of Trehalose-coated Lysozyme studied by terahertz time-domain spectroscopy

Risa Okada¹, Naoki Yamamoto², Atsuo Tamura¹, Keisuke Tominaga^{1,2} (¹*Grad. Sch. Sci., Univ. Kobe*, ²*Molecular Photoscience Research Center, Univ. Kobe*)

It is known that trehalose preserves proteins from damage such as denaturation due to dehydration or extreme change in temperature. This function of trehalose is related to inhibition of protein collective motions, which correspond to low-frequency motions in several wavenumber regions. In this study, we measured low-frequency dynamics of trehalose-coated lysozyme by terahertz time-domain spectroscopy to understand effect of coating by trehalose from 83 K to 293 K. Terahertz absorption coefficients increase linearly as the temperature increasing. In contrast to the case of hydrated lysozyme, “dynamical transition”, in which increasing rate of absorption coefficients become more intense, is never observed in this temperature region.