1P055 タンパク質の構造・安定性に及ぼす環状オリゴ糖およびポリオール
の添加効果
Effects of polyol and cyclic oligosaccharide on structure and stability of protein

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Polyol and cyclic oligosaccharide (cyclodextrin, CD) influence structure and stability of protein through hydrophobic interaction. We have determined thermodynamic properties of molten globule (MG) state of cytochrome c induced by polyol and unfolded state by temperature with CD. In this study, to reveal the thermodynamic properties of MG state of myoglobin, thermal denaturation of myoglobin in aqueous sorbitol solution were measured by circular dichroism and DSC. Sorbitol induced the MG state from acid unfolded state at pH2, 290 K, and over 3 M of sorbitol, and the MG state was unfolded by increasing temperature with low cooperativity. The kinetic properties of MG state was determined by stopped flow measurement.

1P056 タンパク質の熱安定性に及ぼすシクロデキストリンの包接効果
Inclusion effects of cyclodextrin on thermal stability of proteins

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The protein structure is maintained by a significant small stability as a compensated result of hydrophobic interaction, hydrogen bond, electrostatic interaction, structural entropy, and other enthalpic and entropic factors. Cyclodextrins (CDs) can influence the conformation and stability of protein via their inclusion ability. In this study, thermal denaturations of several globular proteins in aqueous CD solutions were measured by DSC. CD concentration dependence of midpoint temperature and change in enthalpy for thermal denaturation of proteins indicate the CD destabilized the folded state of proteins by stabilizing the unfolded state due to inclusion. The effect was dependent on the property of proteins.

1P057 粗視化シミュレーションを用いたSTMVの自己組織化についての理論的研究
Theoretical study on the self-assembly of satellite tobacco mosaic virus using coarse grained simulation

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Satellite tobacco mosaic virus (STMV) is composed of 60 identical copies of a single protein with an icosahedral structure. In this work, we investigate the assembly mechanism of the STMV particle by simulations with Go like model, which is a kind of coarse grained model. For the purpose of understanding the assembly mechanism of a virus particle, it is significant to study interactions both intra- and inter-subunits of capsid proteins because the interactions highly contribute to the structural stability of a whole virus particle. Electrostatic, Van der Waals, hydrophobic and hydrogen bonding interactions are applied to protein-protein interactions. We then discuss the stability and which interaction is dominant for completing the assembly of the STMV particle.

1P058 バクテリア細胞質の全原子分子動力学シミュレーション
All-Atom Molecular Dynamics Simulation of Bacterial Cytoplasm

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Computer simulation of the realistic cellular environment is one of the major challenges for biophysical scientists. It is indispensable in obtaining the molecular-level dynamic picture of the biochemical reaction networks. For this purpose, we constructed all-atom model of cytoplasm in the Mycoplasma genitalium, the smallest bacteria. The size of the system is 50x50x50 nm, which is greatly exceeds that of typical MD simulations, covering about 1% of the volume of an entire cell. Using the trajectories generated by highly parallelized MD program GENESIS on K computer, the dynamics of the macromolecules/metabolites are analyzed. The correlation between MD-derived spatiotemporal data with experimentally known biochemical reaction networks is also discussed.

1P059 分子動力学シミュレーションによる構造エントロピー計算法の比較
Comparison of calculation methods of configurational entropy from molecular dynamics simulation trajectories

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Configurational entropy (S^c) is one of important properties in many biomolecular processes such as molecular binding. So far, many methods to calculate S^c from trajectories of the molecular dynamics simulations have been proposed. Recently, Harpole and Sharp proposed the Clausius method which enables us to exactly calculate the temperature difference in S^c without any approximations such as quasi-harmonic distributions.^[1]

In this study, we compared results of the Clausius method with those of several methods for entropy calculation, including quasi-harmonic methods based on principal component analysis using Cartesian coordinates.

[1] K. W. Harpole and K. A. Sharp, *J. Phys. Chem. B*, **115**, 9461(2011).

1P060 分子モデリング法を用いた酸変性アポミオグロビンの構造解析
A Conformational Analysis of Acid Unfolded Apomyoglobin using a Novel Molecular Modeling Method

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The unfolded protein in solution consists of an ensemble with a great number of conformations. It is necessary to integrate diverse experimental data for elucidating its structural properties. We developed a new computational method for generating conformations of unfolded protein (Seki, Y. et al., *JCTC*, **2011**). Using our method, we have tried to find an ensemble which best reproduces experimental data obtained from both residual dipolar couplings of NMR and solution X-ray scattering. As a result, it was clarified that structural properties of the acid-unfolded (AU) apomyoglobin. In the annual meeting, we will discuss differences in structural properties between urea unfolded state and AU state.