2P067 タバコモザイクウイルス外被蛋白質会合体の安定性
Stability of the Tobacco Mosaic Virus Coat Protein Assemblage

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Tobacco mosaic virus coat protein (TMVCP) is known to form self-assemblies such as single-helical rods or disks. We have produced TMVCP in E.coli by using an auto-inducing expression system with a yield of more than a hundred mg of pure protein per three liter of culture. In 20 mM TrisCl, pH 7.4, the dissociation of a disk-like assemblage of the produced TMVCP occurred in the urea-concentration range of 0 to 2 M, and the unfolding of the secondary structure in the range of 2 to 4 M. Thermodynamic analyses based on a simple all-at-once association scheme showed that a decrease in the dissociation free energy change by only several kJ per mol of monomeric protein unit caused the assembly to be dissociated.

2P068 計算化学的手法によるアデニル酸キナーゼの反応機構の研究
Computational Study on the reaction mechanism of adenylate kinase

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Adenylate kinase catalyzes the reaction: ATP + AMP + Mg²⁺ → ADP + ADP + Mg²⁺. We have been studying the theoretical model of the reaction using MM/QM method. We constructed the model of complex structure of enzyme and substrates, ATP and AMP with Mg ion with some water molecules surrounding the active center using MM or MD calculation with AMBER99 force field. The truncated models were used for the calculations with ONIOM method, and the reactant, product, transition structures were optimized. The highest level of the theory (B3LYP/6-31+G(d):Amber(embed)) with 853 atoms (89 atoms in QM) gives the reaction barrier of about 19 kcal/mol. The details about the model size, the conformational differences, or the free energy profiles, will be discussed.

2P069 局所パッキングパターンによる GroEL 基質蛋白質の構造的特徴の記述
Discrimination of GroEL substrate proteins using a small set of packing-patterns

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Chaperonin GroEL plays an essential role in preventing protein misfolding by assisting the folding reaction. Recent proteome-wide experiments indicate a strong correlation between GroEL substrate proteins and their structure, e.g. α/β class folds are enriched in substrates. This suggests that folded structure can be related to the specific substrate recognition by GroEL. Here, we analyzed GroEL substrates by focusing on the local packing-patterns of secondary structures shared among them, applying a non-sequential structure comparison method MICAN. As a result, a decision tree was derived to discriminate the substrates from others with more than 95% sensitivity. The packing-patterns used in the decision tree will be discussed in terms of the GroEL-substrate recognition.

2P070 天然変性タンパク質としてのグループ3 LEA モデルペプチドの役割-乾燥に伴うリボソームの融合を防止する効果-
A role of group-3 LEA model peptides as IDPs. Protective effects on desiccation-induced liposome fusion

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The following four peptides were tested as candidates of anti-fusion reagents for dried liposomes prepared with POPC: 1) PvLEA-22, which consists of two tandem repeats of the 11-mer motif characteristic to LEA proteins from an African sleeping chironomide, 2) its control, i.e. the peptide with the amino acid composition identical with that of PvLEA-22, although its sequence is scrambled. 3) Poly-L-glutamic acid, and 4) Poly-L-lysine. Based upon the results of the size distribution measurements and the leakage tests of a fluorescent marker inside liposomes, we argue that the protective efficiency of the peptides depends not only on the amino acid composition but also on their sequence.

2P071 An activation mechanism of human Cu,Zn-superoxide dismutase by its copper chaperone, CCS

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A catalytic copper ion in human Cu,Zn-superoxide dismutase (SOD1) is supplied by the copper chaperone for SOD1 (CCS). CCS is composed of three domains, among which domain I and III have Cu(I)-binding Cys-x-x-Cys (CxxC) and Cys-x-Cys (Cx'C) motifs, respectively. While both motifs have been known to tightly bind to cuprous ion, it remains controversial as to which motif is important for donating a copper ion to SOD1. Here, we show that the CxC motif in domain III is essential for human SOD1 activation; and in contrast, the CxxC motif in domain I was not necessary. Investigation on the roles of CCS domain I in SOD1 activation are currently in progress using our yeast model expressing human SOD1 and human CCS proteins.

2P072 変異体を用いた分子動力学シミュレーションによる電位依存性カリウムチャネルのイオン透過機構の解析
Analysis of the ion permeation mechanism of Kv1.2 using the molecular dynamics simulations of a single point mutant

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Voltage-gated potassium channels play a crucial role in recovering membrane potentials from its depolarized state. Potassium ions permeate outward through the selectivity filter (SF) in single-file, which requires the entering ions to be dehydrated in the central cavity. Here we analyzed the mechanism of ion permeation by performing the molecular dynamics simulations of recently reported single point mutant of Kv-channel with high conductance under several conditions. In the ion permeation process through this mutant channel entering of ions into the cavity is not a rate-limiting step. These results suggested that the water molecules in the central cavity having orientation tend to push ions toward SF though the external field is required for the permeation through SF.