2P007 β -sheet 中でのヘア傾向は edge strand と central strand では全く異なる
Pairing propensity in β -sheets is quite different between edge and central strands

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We analyzed residue pairing patterns in β -sheets to understand the mechanism of β -sheet formation which is one of the key steps for forming the tertiary structure of proteins. Only 12 pairs showed different pairing propensity between hydrogen-bonding (HB) and non-bonding (nHB) pairs in anti-parallel sheets when pairs including Pro were neglected. When edge and central strand pairs were distinguished, however, 37 and 39 pairs showed different pairing propensity for edge and central strand pairs, respectively, and only 7 of these pairs showed similar propensity between edge and central strand pairs. These results indicated that edge and central pairs possessed quite different propensity each other and this difference might be one of criteria to select edge strand pairs.

2P008 最適化した力場のアミノ酸ごとのパラメータ依存性について
Parameter dependency of an optimized force field for each amino acid

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A force field is widely used in the field of molecular simulations for biomolecular systems. Recently, we proposed a new method for refining force-field parameters, which modifies the force-field parameters for each amino acid to minimize the root-mean-square deviation of backbone dihedral angles in various protein structures. Here, we compared the experimental data obtained from NMR with the trajectory data obtained from molecular dynamics simulations. In addition, we also applied an energy-based reweighting approach to a molecular dynamics trajectory to efficiently screen a large number of trial force fields in order to decrease the simulation cost. In this study, we examined the parameter dependency of optimized force field for each amino acid.

2P009 固体 NMR および MD シミュレーションによるヒトカルシトニン線維形成機構と構造の解析
Fibrillation mechanism and fibril structure of human calcitonin as studied by solid-state NMR and MD simulation

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Human calcitonin (hCT) is known to form amyloid fibrils by taking two step autocatalytic reaction mechanisms. In the initial stage of fibrillation of hCT in HEPES solution, spherical stage of intermediates were observed by TEM experiment. This result gain insight into the fibrillation mechanism of hCT. To determine the fibril structure of hCT in phosphate buffer at pH7.5, ¹³C-¹⁵N internuclear distance were evaluated using [1-¹³C]Phe16, [¹⁵N]Phe19-hCT by means of REDOR experiment in solid-state NMR. REDOR results indicated that Phe19 and Phe16 located one residue away registry in the antiparallel β -sheet structure. MD simulation results indicate that the fibril structure is stabilized by interactions between inter-strand aromatic interchain.

2P010 4量体型サルコシン酸化酵素の分子動力学シミュレーション: 水分子の透過経路解析
Molecular dynamics simulation of heterotetrameric sarcosine oxidase: pathways of water molecules

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Heterotetrameric sarcosine oxidase (SO) containing FAD and FMN catalyzes the oxidative demethylation of sarcosine. The structural and biochemical analyses have shown that the SO-dimethylglycine (DMG) complex contains a large cavity near the catalytic site and have suggested channeling of reactants and products through several tunnels. Toward realistic simulations of channeling, we have carried out molecular dynamics simulations for the SO-DMG complex using the GROMACS program with the Amber force field. As a result, the structure simulated was in good agreement with the X-ray data. In our present study, the trajectories of water molecules were analyzed accurately to understand their pathways and obtain new insights into the channeling related to the catalysis of SO.

2P011 生体高分子中性子結晶構造解析におけるフーリエマップ改善のための実践的考察
A practical study for the improvement on the Fourier map in neutron protein crystallography(NPC)

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Neutron scattering length (b [cm]) is independent of $\sin\theta/\lambda$ unlike X-ray atomic form factor (f [cm]). However, the resolution or a set of reflections of NPC has been determined as observed minimum d-spacing by considering R-merge etc, like in case of X-ray's. In order to find new criteria in NPC, we drew several Fourier maps by including a set of calculated Fc(hkl) from neutron PDB data, which consists of only larger |Fc|s than the mean value at the higher resolution range, and found that the quality of the map became better than one at the conventional resolution. This suggests that the practical improvement on the map will be possible if we use reflections ignored by the conventional method.

2P012 分子動力学シミュレーションによる GLP-1 と Exendin-4 の構造解析
Structure Analysis of GLP-1 and Exendin-4 by Molecular Dynamics Simulation

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We analyzed the structure of glucagon-like peptide-1 (GLP-1) and exendin-4 by molecular dynamics (MD) simulation. GLP-1, a peptide of 30 amino acids, enhances insulin secretion when it binds to GLP-1 receptor (GLP-1R) in pancreas. This function is beneficial for treatment of type II diabetes. However, GLP-1 is decomposed by dipeptidyl peptidase-4 (DPP-4), and the activity is turned off. On the other hand, exendin-4 is a GLP-1R agonist and it has the resistance to DPP-4. We have performed MD simulation and compared the conformation of GLP-1 and exendin-4. In our simulations, we studied the effects on the conformations of several conditions of environment, for example, with 0.9 % NaCl in water solvent system.