2P013 A new approach to build 3D atomic model from single electron microscope image

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We have developed a new approach to build a 3D atomic model from a single electron microscope (EM) image of a bio-molecule. In this approach, the initial structure (X-ray crystal structure or modeled structure) of the molecule is deformed by computational techniques and many atomic models with different conformations are generated. The deformation is performed in such a way that the internal energy of the molecule does not increase so much. For this purpose, the lowest frequency normal modes are used in the deformation. Then, each atomic model is projected to many different directions, and each projection is fitted to the EM image and the fitting-score is calculated. The atomic models with high fitting-scores are the candidates that reproduce the EM image.

2P014 プロリンリッチなペプチドのコンホメーション特性に関する考察

An investigation on the conformation character of proline-rich peptides

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It has been considered that proline-rich peptides would generally form the polyproline-II structure in water by the speculation on the CD spectral pattern of proline-rich peptides. In this work, theoretical investigation on the conformation character of proline-rich peptides in water was carried out by molecular dynamic simulations using gromacs algorithm. It was shown that all examined peptides dynamically fluctuate among many stable conformations. The stability of straight-rod-like conformations decreases with a decrease in proline content and the stability of compactly folded conformations increases with an increase in the content of the residue having large backbone flexibility. These results almost corresponded to the pattern of CD spectra for peptides in water.

2P015 生体電子の流れが加速する電流生成菌の細胞外電子移動機構の発見

Respiratory Electron Flow Enhances the Rate of Extracellular Electron Transport Processes in Current-Producing Bacteria

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Vectorial electron transfer (ET) sustained by positive feedbacks from structural fluctuation in photosynthesis and respiration has been predicted by theoretical studies, yet not been experimentally confirmed in molecular level. Recently we developed a 3-electrode system with electrogenic bacteria *Shewanella* to directly monitor the respiratory ET process via outer-membrane-bound deca-heme c-type cytochromes (OMDCs) in-vivo, and electrochemically identified the active state of OMDCs, which increases the ET rate 1000-fold compared with non-active state. Here we observed that respiratory electron flow itself is required to sustain OMDCs in its active state to speed up ET, suggesting OMDCs mediate the vectorial ET via its static active state under non-equilibrium condition.

2P016 再重法を用いたタンパク質力場パラメータの最適化 Optimization of force-field parameters for protein systems by an energy-based reweighting approach

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A force field is widely used in the field of molecular simulations for biomolecular systems. In this study, we propose a new method for refining force-field parameters, which modifies the force-field parameters to minimize the root-mean-square deviation of backbone dihedral angles in various protein structures. Here, we compare the experimental data obtained from NMR with the trajectory data obtained from molecular dynamics simulations. In order to decrease the simulation cost, we also apply an energy-based reweighting approach to a molecular dynamics trajectory to efficiently screen a large number of trial force fields. By using this approach, we can refine the backbone-torsion-angle parameters for each amino acid at once.

2P017 ヘモグロビンの酸素結合に伴うアロステリック転移のカメレオンモデルによる研究

A simulation study with the chameleon model: The allosteric transition of hemoglobin associated with oxygen binding

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To elucidate the mechanism of the allosteric transition of hemoglobin, we have performed molecular dynamics simulation using a newly developed potential model, 'the chameleon model'. In this model, the most stable position of locally defined potential is switched according to whether the local structure around it is similar to that in the T or R state. This gives rise to the global structural transition which is sensitively controlled by the subtle change of distance between histidine and Fe atom. Using this model system, we will discuss the molecular details of transition state in the allosteric transition process dependent on oxygen binding by characterizing the average structure of the transition state ensemble and the correlation of the movement of each residue.

2P018 天然変性タンパク質の結合と共役した折りたたみ部位の相互作用解析

Contact analysis of Protean Segments (ProSs) in intrinsically disordered proteins (IDPs)

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Intrinsically disordered proteins (IDPs) lack a stable, tertiary structure. Many regions of disordered proteins can undergo disorder to order transitions upon binding to their partners, known as coupled folding and binding mechanism. We call these regions Protean segments (ProSs). A dataset of ProSs was extracted from IDEAL database. The ProSs structures were classified into surface, interior and interface (core, rim and support). We calculated the average number of internal and external contacts of ProSs, their interaction partners and heterodimers. The results indicated that ProSs have less number of internal contacts and high number of external contacts than interaction partners and heterodimers. We will also discuss the binding efficiency of ProSs.