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A reconstituted active cytoskeletal networks consisting of an actin filament network coupled to myosins (motor proteins) have been shown to display rich in dynamical and mechanical behaviors that is often in contrast to passive, equilibrium system. The motor proteins, which spontaneously generate forces, kept the active cytoskeletal network out of equilibrium. The athermal fluctuations observed in the network are linked to the active force generation by motor proteins which give more relevant information including the interaction with the surrounding materials. In prior studies, only the second moment of the athermal fluctuations has been investigated. There is no reason a priori to expect Gaussian statistics in nonequilibrium systems. Indeed, the full displacement distribution of the athermal fluctuations in active cytoskeleton recently probed using video microrheology is found to be far from Gauss. In this study, we investigated the nonequilibrium statistics and dynamics of the active network by analyzing the athermal fluctuations. The model developed here is based on Levy statistics which is generally observed for the effectors whose impacts decays as $1/r^2$. It was found that the displacement distribution is obtained as a convolution of truncated Levy distribution due to the finite-size of probe particles. The truncation of Levy becomes less and power-law tail is enhanced as the probe particle gets smaller.

1PT126 Atoms in molecules 法によるタンパク質 α ヘリックス、 β シートの水素結合相互作用の理論解析

Atoms in molecules analysis of hydrogen-bond interactions in α -helix, and β -sheets of protein

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Hydrogen-bond interactions (HBIs) between biomolecular systems play an important role in physics, chemistry, and biology, and affect many biological processes, such as molecular recognition. In this study, HBIs of α -helix (AH), and parallel and antiparallel β -sheets (PBS and APBS) were investigated in terms of both energetics and topological points of view, using the electron density analyses of atoms in molecules (AIM) (Yamasaki & Nakamura, 2012) in conjunction with quantum chemical calculations. The secondary structures were built such that the numbers of peptide bonds of AH, and PBS and APBS were increased from 2 to 12 or 16, respectively, in addition to extended models, followed by refining and analyzing with DFT-M062X/6-31+G* calculations. For BS, the interaction energies (Ecp) were estimated with difference in total energy between dimer and the sum of each monomer. The basis sets superposition error was corrected by counterpoise-correction method. For AH, the correlation between total energy differences between AH and extended peptide and the sums of electron density over the bond critical points (Σ interpb) were found with r^2 of 0.99. For PBS and APBS, the correlations between Ecps and Σ interpb of HBIs were also found with r^2 of 0.99 and 0.97, respectively, implying that Ecp were well reproduced with Σ interpb. Interestingly, while Ecps were monotonically increased for PBS as the numbers of peptide bonds increased, the stepwise increase of Ecps was found for APBS, implying the cooperative HBI effect in APBS.

1PT127 Go モデルによるフォールディングシミュレーションに対する天然構造の差異の影響について

Analysis of the influence of differences in native structures of a protein on its folding simulations with a Go model

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Go model is a simple model with inter-atomic potentials between only native contacts in a given protein. The native structure of a protein is determined by X-ray crystallography or NMR spectroscopy. Although the 3D structures of a protein determined by these methods show the same structures at the level of the backbone fold, it has been reported that differences in the folding mechanisms predicted by a Go model are observed depending on whether its 3D structure has been determined by X-ray or NMR, or which structure in the NMR models has been used as a native structure. That is, we have to clarify the following points; 1) the extent of the influence of the definition of the native structure on the results of folding simulations by a Go model, 2) How can fruitful information on the folding mechanisms of a protein be extracted using NMR structural ensemble. In this study, this problem is treated by performing simulations using a coarse grained Go model which we have developed. Protein G, Protein L and α -spectrin SH3 domain are used for tests. Our results show that the differences appeared in the folding simulations in Protein L is especially large and specific. We will show the detailed results.

1PT128 光駆動性陽イオンチャネルであるチャネルロドプシンの結晶構造解析
1YS0930 Crystal Structure of a light-gated cation channel, channelrhodopsin

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Channelrhodopsin (ChR) is a light-gated cation channel derived from algae that conducts cations, including sodium ions, in a light-dependent manner. Because the inward flow of sodium ions changes the electrochemical gradient and triggers neuron firing, neurons expressing ChRs can be optically controlled with high temporal precision within systems as complex as freely moving mammals. Although ChR has been broadly applied to neuroscience research, little is known about its molecular mechanism. Here, we present the crystal structure of ChR at 2.3 angstrom resolution, showing its basic architecture and molecular mechanism, and give the long-awaited answer to the question, "Where is the cation conducting pathway?" The integration of structural and electrophysiological analyses provides insight into the molecular basis for the remarkable function of ChR, and paves the way for the precise and principled design of ChR variants with novel properties.

1PT129 DNA ポリメラーゼ η によるホスホジエステル結合形成を観察する
1YS1000 Watching DNA polymerase η make a phosphodiester bond

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A DNA polymerase catalyzes a nucleotidyl-transfer reaction with Mg^{2+} , and a new bond is formed between the 3'-OH of the primer strand and the α -phosphate of dNTP and the phosphodiester bond between α and β -phosphates of dNTP is broken. Until now, a number of structural and kinetic studies of DNA polymerases proposed the catalytic mechanism of the nucleotidyl-transfer reaction. However, the actual reaction mechanism remains unknown. In this study, we have visualized the nucleotidyl-transfer reaction process catalyzed by human DNA polymerase η (Pol η) using X-ray crystallography. Pol η , DNA and dATP were co-crystallized at pH 6.0 without Mg^{2+} . The reaction was initiated by exposing crystals to 1 mM Mg^{2+} at pH 7.0 and stopped at various time points by freezing. The substrates and two Mg^{2+} are aligned for reaction within 40 sec, but the new bond begins to form at 80 sec. Structures at reaction times from 80 to 300 sec reveal a mixture of decreasing substrate and increasing product of the nucleotidyl-transfer reaction. In sequence, the nucleophile 3'-OH is deprotonated, the deoxyribose at the primer end converts from C2'-endo to C3'-endo, and the nucleophile and the α -phosphate of dATP approach each other to form the new bond. A third Mg^{2+} ion, which arrives with the new bond and stabilizes the intermediate state, may be an appreciated feature of the two-metal-ion mechanism. Here we show a chemical bond formation at atomic resolution and in real time.

1PT130 Endo-1,3- β -glucanase・オリゴ糖複合体の MD シミュレーション
Molecular dynamics simulations of endo-1,3- β -glucanase and oligosaccharide complex

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Endo-1,3- β -glucanase from *Cellulosimicrobium cellulans* DK-1, is composed of catalytic domain and carbohydrate-binding module. The catalytic domain belongs to glycoside hydrolase family 16, and catalyzes the hydrolysis of β -1,3-glucans such as laminarin and laminarioligosaccharides. We have determined the crystal structure of catalytic domain, and analyzed its interactions with β -1,3-glucans using isothermal titration calorimetry. The catalytic domain would have six subsites for the binding of glucose units, four subsites (-4 to -1) being on the non-reducing end from the scissile glucosidic bond and two subsites (+1 and +2) on the reducing end. In this study, we carried out molecular dynamics simulations to clarify the complex structure with laminarioligosaccharides whose degrees of polymerization are 2 to 7. Each oligosaccharide was modeled