1P145   フォトクロミック化合物フルギミドを結合したミオシン頭部ドメインのX線小角散乱**Small-angle X-ray Scattering Study of Photochromic Fulgimide-bound Myosin**

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To clarify the structure of myosin head domain that bounds the photochromic fulgimide ATP analog, we have carried out the small-angle X-ray scattering experiments.

Fulgimide compound synthesized de novo by Maruta et al is a photochromic molecule that changes color and ring structure by light irradiation. It is possible to have an ATP similar structure to triphosphorylates fulgimide which binds to the ATP binding site of S1. We have examined the global structural changes of S1 by binding fulgimide ATP analog and light irradiation, using small-angle X-ray scattering. The S1 bound fulgimide ATP analog showed the shape change such as the radius of gyration increased when UV light was irradiated.

**1P146   ATP 結合で誘起されるミオシンの誘電応答
Dielectric response of myosin induced by ATP binding**

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Binding of a ligand induces allosteric response in a protein. The allosteric response is often understood by a sort of the principle of leverage. However, the ligand, with specific distribution of electric charge, should induce a large-scale response of protein through the rearrangements of charges and dipoles in the protein. Myosin, a well-studied molecular motor, is a typical allosteric protein, the ligands of which are a nucleotide and a divalent cation. When Mg-ATP binds to myosin, myosin dissociates from actin, the mechanism of which is still unclear. By conducting extensive all-atom model molecular dynamics simulation, we investigated the dielectric response of myosin upon ATP binding, and discuss the role of this dielectric response in the motor function.

1P147   Multiscale analysis of functional motions in F1-ATPase: From Pi release to elasticity and friction of γ -subunit rotation

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F1-ATPase, the catalytic domain of ATP synthase, synthesizes most of the ATP in living organisms. Running in reverse powered by ATP hydrolysis, it creates torque on its central γ -subunit. First, we use molecular dynamics (MD) simulations to study the timing of Pi release coupled to the rotation. On the basis of metadynamics simulations and rate calculations, we clarify the timing and pathway of Pi release. Second, from the MD trajectories we construct a simple model to deduce elasticity and friction of γ -rotation. The deduced elastic properties are consistent with experiments. According to our analysis, the work performed in the torque-driven rotation is mostly stored as elastic energy with remarkably little dissipation, which explains high efficiency of the motor.

1P148   Molecular mechanism of the epsilon subunit from F-type ATP synthases studied by Molecular Dynamics simulations

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ATP synthases are the main producer of ATP, the universal energy source in all living cells. For ATP synthesis, they use a transmembrane electrochemical gradient. Vice versa they can generate an electrochemical gradient, hydrolysing ATP. While in mammals a pH dependent inhibitory protein IF1 regulates the ATP hydrolysis activity, bacteria avoid ATP hydrolysis by the [ATP] dependent subunit epsilon, which carries out a conformational change from the contracted to the inhibitory extended state if [ATP] gets too low. Understanding the ATP hydrolysis prevention mechanisms in bacteria, might help to develop new antibiotics. Using MD simulations and taking previous experiments into account, we propose novel features for the bacterial epsilon subunit of F-type ATP synthases.

**1P149   ダイナクチンのアンテナ構造
Antenna structure of Dynactin Complex**

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Dynactin is a multi-molecular protein complex which regulates dynein activity. Previously we have shown that the coiled coil 1 domain (CC1) of p150 extrudes from the dynactin head and forms an antenna structure. Since CC1 directly binds dynein and regulates dynein activity, we purified CC1 fragments with different lengths and restricted the dynein binding region. By estimating molecular weight, each of the CC1 fragments appeared as a mixture of dimer and tetramer. We further purified the first half and the second half fragments of the CC1 and found that they did not bind each other. These results suggest the folding model that CC1 makes a parallel dimer first and then folds back at some middle points.

1P150   Structure of dimeric axonemal dynein in cilia suggests an alternative mechanism of force generation

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The ciliary outer arm dynein produces force during ciliary beating. However, it is still unknown how the ciliary dynein translocate the microtubule using the two different types of heads. Here, we analyzed the conformational change and its distribution in each dynein head of mouse respiratory cilia by cryo-electron tomography and image processing. Most of two heads were in the same form and tightly packed in the non-nucleotide condition, whereas they were dissociated and alternatively moves in the presence of nucleotide. In a significant number of dyneins in the presence of ADP/Vi, two heads overlap each other in the proximal shifting form, indicating that ciliary heterodimeric dynein translocates a microtubule by moving with short steps.