unclear. Recently, we showed that the cellular redox (reduction-oxidation) poise determines the phototactic sign: cells show positive phototaxis after treatment with reactive oxygen species (ROS), whereas they show negative phototaxis after treatment with ROS quenchers. This finding raised two questions of 1) how cellular redox poise changes in vivo and 2) what is the molecular basis for the redox-regulated switching of the phototactic sign. Regarding 1), we focused on state transitions of photosynthesis, because the ROS generation has been suggested to greatly change depending on the state of photosynthesis. Low-temperature fluorescence spectroscopy revealed that cells showing positive phototaxis are in State 1, whereas those showing negative phototaxis are in State 2. We propose a model that changes in the intracellular ROS amount, caused by state transitions, function as a signal for the phototactic sign switching. Regarding 2), we found that two previously isolated phototaxis-deficient mutants have defects in redox sensing. We also isolated a new mutant that responds to the treatment with redox reagents in an opposite manner to that of wild type. We will present the results of phenotypic analyses.

2PS051 細胞性粘菌で探る細胞運動ダイナミクスと走電性応答の関係性

Cell migration dynamics and its relevance to electrotaxis in Dictyostelium cells

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Directional cell migration is a fundamental process associated with many physiological phenomena. On the signaling process realizing directional cell migration, the dominant view is that cells respond to external signals passively and digitally. Recently, however, a complementary view in which cellular spontaneous dynamics without external signals plays an important role to produce cellular behaviors attracts considerable attention. In order to verify the latter view, a relationship between spontaneous random cell migration and directional cell migration with external guidance cues (direct current electric field) was extensively investigated in Dictyostelium discoideum. It was confirmed that a generalized Langevin model with asymmetry for cellular polarity could successfully reproduce the statistical characteristics of spontaneous cell migration. Also, it was shown that the Langevin model extended with additional velocity bias in accordance with the electric field strength could describe directional cell migration under electrotaxis quantitatively. Based on these results, the hypothesis that electrotaxis is realized by biasing spontaneous cell migration properly, and velocity memory is relevant to cellular flexible response for uncertain environment was proposed and tested through a series of electric field reversal experiments and the model simulations.

2PS052 細胞運動のための力と生化学の相互作用

Force-biochemical interaction for cell migration

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Motile cell generates traction force to show crawling migration. Although biochemical signals such as Rho family small GTPases have been well studied, it is still unclear how the migrating cell manages and integrates the traction force and biochemical signals. Our experiment using force microscopy shows that migrating Dictyostelium cell generates a small traction force at the front relative to the other directions. Keratocyte also migrates by generating relatively small traction force at the front direction. In addition, our experiment using GFP-myosin II revealed that the cell accumulates myosin II at the intracellular space where force was added from extracellular side, suggesting that the cell transduces extracellular force to a biochemical signal through myosin II accumulation. How the cell integrates intra- and extracellular interactions for migration? To examine the mechanism of the cell migration based on the experimental observations, we developed a simple computational model cell which has a hexagonal shape with a spring-dumper system and contains force-biochemical interactions. The model cell migrates on the adhesive substrate where the cell repeats adhesion and exfoliation. Using the model cell, we show that the cell can migrate to the direction at which it generates small traction force relative to the other directions. This suggests that exfoliation facilitated by myosin II accumulation not at the front side plays key role for cell migration.

2PS053 歩行中ミオシン X の高速 AFM 観察

Direct observation of walking behavior of myosin X by high-speed atomic force microscopy

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Double-headed myosin X, one of the actin-based motors, is involved in filopodia formation and intrafilopodial transport. Structurally, each head of myosin X is comprised of a motor domain, an ~11 nm long neck domain (lever-arm domain) consisting of three IQ motifs bound to calmodulins or calmodulin-like light chains, and a proximal tail of a stable alpha-helix which is hypothesized to extend the working stroke of myosin X. The head is followed by a coiled-coil domain for possible dimerization and then by two unique globular tail domains. Recently, single molecule fluorescent microscopy revealed that the artificially dimerized tail-truncated myosin X can move processively on single actin filaments with a large step size of ~34 nm [Y. Sun *et al.*, *Nat. Struct. Mol. Biol.* (2010)]. This large step size can be explained by the hypothesis of the stable alpha-helix extension to the lever arm domain [i.e., total lever arm length is estimated to be ~26 nm (~11 nm + ~15 nm)]. However, this structural evidence on the functioning molecule is still missing. Thus, here we have been performing high-speed atomic force microscopy imaging to directly observe behaviors of myosin X moving along an actin filament. We established an appropriate motility assay condition in which phospholipid bilayers were used as a substrate. Using this assay condition, we successfully visualized myosin X molecules that were moving with a large step size of ~36 nm. The details of the structural dynamics are now under investigation.

2PT001 独立してフォールドする構造ドメインデータベースの構築

I-StDom: A dataset of Independently foldable Structural Domains automatically delineated from protein structures

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Protein domains that can fold in isolation (structural domains) are significant targets in diverse areas of proteomics research as they are often readily analyzed by high-throughput methods. In this process, the ability to identify sequence regions corresponding to structural domains in novel proteins with unknown structures is an essential step. Computational methods for predicting domain regions from sequence information only are thus becoming valuable. In developing such predictors, reliable structural domain datasets are necessary as learning data.

In this study, we constructed I-StDom, a dataset of Structural Domains that can fold Independently and in isolation (ISDs). We identified ISDs from multi-domain proteins cataloged in SCOP and CATH by assuming that they form little inter-domain interactions, such as H-bonds and hydrophobic cores, and which we calculated from the protein's atomic coordinates. We parameterized interactions, and optimized them so as to select the maximal number of protein domains cataloged in PDB. 48089 ISDs were selected using the optimal parameters (less than 11 MC-MC, 9 MC-SC, and 7 SC-SC H-bonds, and 7 hydrophobic cores) with 29.7% of them having sequence similarity to a domain cataloged in PDB. This is more than 10% higher than for the unfiltered SCOP and CATH domains, which strongly suggested that domains in I-StDom can fold in isolation. I-StDom is available at <http://domserv.lab.tuat.ac.jp/i-stdom.html>.

2PT002 ADS 仮説に基づくタンパク質のデノボ立体構造予測法の開発

Development of a de novo protein structure prediction method based on the antecedent domain segment(ADS) hypothesis

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Protein structure prediction is one of the most important and fundamental problems of biology. In particular, the prediction of novel protein structures, for which we cannot use template, is a very significant from the viewpoint of biophysics. Currently, one of the most successful method for predicting novel protein structures is the fragment assembly (FA) method. The success of the method is, however, limited to low contact order (CO) proteins, probably because the FA method emphasizes local interaction too much. (R. Bonneau. *Protein Sci.* 2002;11:1937-1944). In order to predict novel protein structures with high CO, we developed a method for novel protein structures prediction. The idea of the method is based on the antecedent domain segment(ADS) hypothesis, which was originally proposed by Lupas *et al.* In this hypothesis, ancient protein structures were formed by self-assembling aggregates of short polypeptides. Our method mimick this aggregation processes for protein tertiary