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Telomeric DNA at the ends of eukaryotic chromosomes consists of tandemly repeated G-rich sequences with a single-stranded 3' overhang. Pot1 is a protein to bind with the single-stranded telomeric DNA. Here, we examined the thermodynamic properties of the interaction between a single-stranded telomeric DNA-binding domain (ssDBD) of Pot1 and the single-stranded telomeric DNA (ssDNA) by isothermal titration calorimetry. The signs of the observed ΔH and ΔS were negative. Because the observed negative ΔS is unfavorable for the interaction, the interaction is driven by the negative ΔH . On the other hand, the negative ΔH and the positive ΔS were previously reported for the interaction between a double-stranded DNA (dsDNA) and a double-stranded DNA-binding protein (dsDBD). Thus, the observed negative ΔS for the ssDNA-ssDBD interaction mainly due to the conformational restraint of ssDNA is in sharp contrast with the positive ΔS previously reported for the dsDNA-dsDBD interaction probably resulting from the release of water molecules upon binding with dsDNA. We have also investigated the temperature dependence of the thermodynamic parameters for the ssDNA-ssDBD interaction. The negative ΔH decreased and the positive $-T\Delta S$ increased with increasing temperature. Because the temperature dependencies of ΔH and $-T\Delta S$ had the opposite signs, their contributions to the temperature dependence of ΔG was almost canceled out. The enthalpy-entropy compensation has been also observed for the dsDNA-dsDBD interaction.

1P134 核様体タンパク質 Fis と Dps による DNA 折り畳み様式の差異
Difference in the action of *Escherichia Coli* nucleoid proteins, Fis and Dps, on DNA conformation

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In *Escherichia Coli* K12, 4.6 M bp of genomic DNA is folded inside a cell with 2 μm long and 1 μm in diameter. In the cell cycle, the genomic DNA is tightly packed in the stationary phase rather than that in the exponential phase. However, the manner of the conformational change of DNA has not been clarified yet.

In present study, we study conformational transition of giant DNA under the intracellular model solution of *E. Coli* containing spermidine and nucleoid proteins, by using fluorescent microscopy. We find that Fis, the most abundant nucleoid protein in exponential-phase, induces ON/OFF switching of DNA under the presence of spermidine. On the other hand, Dps, the most abundant in stationary-phase, exhibits continuous transition of DNA folding under the same condition of spermidine. These results suggest that genome DNA with Fis can be adapted to the abrupt change of structural change and protein expression of DNA accompanied by the cell division. On the contrary, mild transition of DNA with Dps concerns with the function to maintain expression level of genomic DNA in the stationary phase.

1P135 不完全な繰り返し単位を有する出芽酵母テロメア DNA 配列の 4 本鎖 DNA 構造の解析
Analyses of the quadruplex structures of irregularly repetitive telomeric DNA sequences from budding yeast

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Telomeric DNA at the ends of linear eukaryotic chromosomes consists of tandemly repeated G-rich sequences. The G-rich sequences have the ability to form quadruplex structures with Na^+ or K^+ , where four guanines align with each other through non-Watson-Crick G:C base pair hydrogen bonds to form a square planar configuration. Although the quadruplex structures of perfectly repetitive telomeric DNA sequences from *Tetrahymena*, *Oxytricha*, and vertebrates have been well-characterized, few studies have been reported on the quadruplex structures of irregularly repetitive telomeric DNA sequences from budding yeast. Here, we examined the quadruplex structures of the telomeric DNA sequences from budding yeast, TELG4: 5'-(TGGGTGTG)₄-3', TELGG4: 5'-(TGGGTGTGG)₄-3', TGTGTELG4: 5'-(TGTGTGGGTGTG)₄-3', TGTGTELGG4: 5'-(TGTGTGGGTGTGG)₄-3' with 150 mM Na^+ or K^+ . Native gel electrophoresis, UV melting and CD spectroscopy revealed that the main component for all of the sequences was compact intramolecular quadruplex with either Na^+ or K^+ . With K^+ , the strand orientation of the quadruplex was parallel for all of the sequences, but with Na^+ , it was antiparallel for TELG4 and a mixture of parallel and antiparallel for the other three sequences. The thermal stability of the quadruplex with K^+ was significantly higher than that with Na^+ . These results indicate that the observed variety of the quadruplex structures depends on the base

sequence and the type of the coexisting cations.

1P136 タンパク質-DNA 複合体の粗視化シミュレーション: ヌクレオソームの力学的なアンジッピング
Coarse-grained simulation of protein-DNA complex: mechanical unzipping of nucleosome

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Eucaryotic chromosome is composed of repeating nucleosomes, that are the most basic structural units. Structure and dynamics of nucleosomes are of central importance in genome packaging and gene regulation. The nucleosome is a protein-DNA complex where 147 DNA base-pairs are wrapped around histone proteins, which is very large system for standard molecular dynamics simulations at the moment. Thus, molecular simulation by a coarse-grained (CG) model can be very powerful. Recently, large-amplitude protein dynamics has been investigated by CG models, such as Go-like model, and some CG DNA models that can treat both single- and double-stranded DNAs have been proposed. Here putting them together and modeling interaction between them, we develop a CG model for protein-DNA complex and implement it in the general software of CG biomolecular simulations, which we call CafeMol. This model describes not only the large conformational change of protein-DNA complex, but also melting process of DNA duplex. Using this new model, we investigate large-scale conformational dynamics of nucleosomes. Here we simulated mechanical unzipping process of nucleosome, which recently has been investigated by single molecule experiment[1]. We observed various kind of unzipping behavior depending on environmental condition, such as friction and ion concentration. [1] M.A. Hall, A. Shundrovsky, L. Bai, R.M. Fulbright, J.T. Lis, and M.D. Wang, Nature Struct. Mol. Biol. 16, 124-129 (2009)

1P137 RNA-タンパク質複合体の粗視化シミュレーションモデル: 全原子モデルに基づく導出
Coarse-grained model of RNA-protein complexes based on all-atom simulations

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Recently various functional RNA molecules and RNA-protein complexes have been focused and studied experimentally due to their essential functions, especially related to genetic mechanisms such as transcription and translation. Although molecular dynamics simulation is a good tool to investigate such biological phenomena at atomic resolution, it is seldom applied to these processes because of its large system size and relatively long time scale.

To overcome these limitations, here we constructed a coarse-grained (CG) model of nucleic acids and complexes with protein. In the model, each nucleotide is represented as three CG beads; phosphate, sugar and base, and interactions are modeled with Go-like potential which makes the native structure the most stable. For high accuracy, we used a multiscale modeling method, called the fluctuation matching method. In this procedure, firstly all-atom MD simulations are performed, and then that information is used to decide CG parameters by matching mean-square fluctuations through iterative CG-model simulations. To confirm the accuracy and availability, we try to reproduce dynamic behavior of functional RNA and its complex. Using several reference structures corresponding to distinct functional states, this model should have potential to reproduce conformational change and be useful to study RNA-related biomolecular functions.

1P138 Electronic structures of the novel [4Fe-4S] cluster in dark-1YA0945 operative protochlorophyllide oxidoreductase

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The [4Fe-4S] clusters are ubiquitous in nature and play important roles in electron transfer and catalysis such as in ferredoxins and nitrogenases. The accessible oxidation states and the redox potentials of these [4Fe-4S] sites are enormously diverse.

Recently, a X-ray structure of the dark-operative protochlorophyllide (Pchl) oxidoreductase (DPOR) catalyzing the stereo-specific reduction of Pchl to form chlorophyllide *a* has been determined at 2.3 angstrom resolution. The [4Fe-4S] cluster in DPOR (NB cluster) has a unique feature that one of iron is chelated by a carboxylate group of Asp36 unlike conventional [4Fe-4S] clusters coordinated by four Cys residues. The enzyme activities of the mutant of the NB cluster, which was altered to Cys (D36C), were examined, and the D36C mutant almost abolished the activity. The crystal structure of the D36C mutant had the conventional [4Fe-4S] cluster chelated by four Cys residues, suggesting that the Asp ligation is essential for the catalysis.

We have investigated the electronic structures of the NB cluster to elucidate the role of the Asp ligation to the [4Fe-4S] cluster in the catalysis of DPOR