1P-097 一本鎖 DNA の両末端接触速度における長さ及び溶液の粘度依存性
The Length and Viscosity Dependence of End-to-end Collision Rates in Single-stranded DNA

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see ITP5-02

1P-098 レプリカ交換法による巨大タンパク質-核酸複合系の粗視化シミュレーション研究
Replica exchange simulations applied for coarse-grained models of giant protein-nucleic acid complex

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Transcription and translation are central processes in molecular biology and thus they have been studied extensively by various experiments. In contrast, molecular dynamics simulations are seldom applied for these processes because transcription and/or translation processes unavoidably contain huge protein-nucleic acid complex, such as chromatin, RNA polymerase, and ribosome, of which size and time-scale make simulations extremely difficult. To overcome these problems, we are currently developing a set of coarse-grained (CG) models of proteins and nucleic acids.

In this study, constructing a coarse-grained model for protein-nucleic acid complex, we apply the Hamiltonian replica exchange method (HREM) for enhanced sampling. By this approach, we can achieve efficient conformational sampling and obtain free-energy profile with arbitrary degree of freedom. Additionally, this method is considered suitable for investigation of large-scale system because of HREM's parallelization efficiency.

1P-099 タンパク質-DNA 複合体の粗視化シミュレーション: ヌクレオソームのダイナミクス
Coarse-grained simulation of protein-DNA complex: dynamics of nucleosome

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see ITP5-07

1P-100 RNA 結合タンパク質における疎水表面を用いた塩基認識機構の検証: NOVA-RNA 複合体系での研究
Study of RNA base recognition mechanism by aliphatic surface of RNA-binding protein: Case study of NOVA-RNA complex system

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see ITP5-05

1P-101 タンパク質翻訳開始複合体における 30S-mRNA 結合力の 1 分子顕微解析
Single-molecule force measurement for 30S-mRNA interaction in translation initiation

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see ITP5-06

1P-102 マウステロメア DNA の 4 本鎖 DNA 構造とマウステロメア結合蛋白質 Pot1 のテロメア DNA 結合ドメインとの相互作用

Interaction between tetraplex structure of mouse telomeric DNA and telomeric DNA binding domains of mouse telomere binding protein Pot1

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see ITP5-04

1P-103 タンパク質・DNA 間相互作用の予測のための疎視化に関する研究
Study of coarse graining for prediction of interaction between protein and DNA

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[Introduction] To predict the specific interaction between biological macromolecules such as protein and DNA, first of all, it is important to estimate which residues are involved in the interaction. Since protein and DNA are too large, it is difficult to perform accurate calculations for entire interaction between them. Therefore, we propose the partitioning of a protein into amino acid units. First, we calculate the atomic charges and the dipole moment of each model using ab initio MO method: then we express protein as a combination of the dipole moments. [Method] Concerning the main chain parts of amino acid units, we treat separately those in alpha-helix and beta-sheet. Each conformation is optimized with the side chain being fixed, and the atomic charges are calculated, which are used to calculate the unit dipole moment. The Gaussian 03 program is used for ab initio MO calculation. [Results and discussion] We use the dipole moment of each amino acid unit as a building block of proteins and several polypeptides to check the additive property. We compare the dipole moment of a whole polypeptide from combination of amino acid models with that of full electron calculation by ab initio MO method; we find the additive property in dipole moment. In addition, we modify unit building block taking account of hydrogen bonding and discuss how to deal with side-chains. We make the energy map of interaction between protein and DNA from the combination of dipole moments of amino acid units

1P-104 Rhodobacter sphaeroides 活性中心の Ab initio QM/MM による研究
Ab initio QM/MM study of photosynthesis reaction center of Rhodobacter sphaeroides

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The photosynthesis is one of the most important biological processes for the life. The first step of PS is excitation of the pigments, i.e. gathering rays of light and converting the excitation energies into the chemical energies via the electron transfer reaction in the reaction center.

In this study, we theoretically investigate the reaction center of the photosynthetic bacteria, Rhodobacter sphaeroides with including all of the protein environment. In this system, the special pair of bacteriochlorophyll is treated with QM, and other pigments are replaced by RESP charges. In order to include the surrounding environment effects, we employed the pseudo-charge and dipole closed surface (PCD-CS) method [1], for which the molecular dynamics simulation was performed. We then employed the configuration interaction single method for the QM calculations to estimate the low-lying excited states. Comparing with calculational results in vacuum, the lowest-lying spectrum is shifted to a lower value that is similar to the experimental value [2], implying that the protein environment plays an important role to determine the excited state of the special pair in this reaction center, being consistent with the previous Hartree-Fock results [3] with considering the solvent effects using Poisson-Boltzmann method.

References

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1P-105 ウシ由来シトクロム酸化酵素のヘム a およびヘム a₃ の電子構造に関する理論的研究: その酸化および還元状態の解析
Computational analysis of electronic structures of hemes a / a₃ of the bovine cytochrome c oxidase in the reduced and oxidized states

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Cytochrome c oxidase (CcO) is the terminal enzyme of the electron transport system, generating the gradient of the proton concentration between a matrix and an intermembrane space of the mitochondria. This is achieved exploiting the free energy that is released by the reduction of an oxygen molecule to two water molecules, requiring four electrons/protons. This catalytic reaction occurs in the