encountered in this ECT is alignment accuracy of tilted projection images. Here, three ET software packages (IMOD, Inspect3D and TEMography) are well known and applied to tilt series alignment in different ways. In our previous work, we have acquired tilt series from axonemes by cryo-transmission electron microscopy (cryo-TEM), and reconstructed the 3D structure using IMOD, Inspect3D and Eos we have developed, mainly. IMOD can automatically determine tilt axis by using fiducial marker, while Inspect3D needs to manually determine tilt axis but gave us more precise alignment than that of IMOD, judging from obtained 3D. Thus we decided to compare them systematically, i. e., our present purpose is to evaluate the quality of 3D reconstruction and the usability of these software packages, show the pros and cons of them systematically and then make our developed Eos more convenient with higher analysis ability. We acquired tilt series of model structure (phantom data) and axonemes by cryo-TEM, and computed the 3D structure using IMOD, Inspect3D, TEMography and Eos from each of them, respectively. Comparison between them will here be reported and discussed.

1PT187 Gibbs energies of secondary structures for α -Chymotrypsinogen A investigated by FT-IR spectroscopy

Koichi Murayama (Grad. Sch. Med., Gifu Univ.)

FT-IR spectra were measured over a temperature range of 25-90 degree, to investigate difference in Gibbs energies of secondary structures for α -Chymotrypsinogen A (a-ctg). The curve fitting method combined with Fourier self-deconvolution technique allowed us to explore details of the secondary structure. The spectra of a-ctg in the amide I' region reveal eight bands for anti-parallel β -sheet, turn, α -helix, β -sheet, intermolecular β -sheet and side chain vibration below 70 degree. Additional band for disordered appears over 70 degree in the spectra. Then, Gibbs energies for secondary structures and their transition temperatures (T_m) were calculated. The T_m for the four bands due to the α -helix, turn and disordered structures are found to be around 60 degree. Corresponding values for anti-parallel β -sheet and side chain are higher by about 67 degree, and those for β -sheet, inter-molecular β -sheet structures were around 63-64 degree. The Gibbs energies were obtained about 11-16 kJmol⁻¹ for α -helix, β -sheet and turn. The value for intermolecular β -sheets was much higher than others, suggesting that intermolecular β -sheets formation need more energy than other secondary structures. In this study, I will discuss Gibbs energy and T_m values for secondary structures of a-ctg obtained from FT-IR spectroscopy in details.

1PT188 TIP3P モデルおよび Generalized Born モデルを併用した分子動力学計算によるタンパク質の構造サンプリング

Improvement of sampling efficiency through combined use of molecular dynamics simulations with implicit and explicit solvent models

Hiroko Kondo^{1,2}, Noriaki Okimoto², Makoto Taiji^{1,2} (¹Department of Computational Biology, the University of Tokyo, ²Laboratory for Computational Molecular Design, Quantitative Biology Center (QBiC), RIKEN)

Various experimental and computational studies have indicated that the protein conformation and its function are closely linked. Investigating their dynamical properties is consequently important to understand their functional properties. The molecular dynamics (MD) simulation is powerful tool for these analyses because we can observe the kinetics of protein at the atomic level. It is however that the time scale of the simulation is not enough for examining the significant event including protein folding, domain movement, and so on. Therefore the enhanced sampling methods to overcome this computational limitation are so important.

In this study we aim at the improvement of sampling efficiency, reduction in actual simulation time by combining the results from implicit solvent simulations and those of explicit one; the former is used for reducing the sampling space and the latter for correcting the conformational distribution sampled by the former simulation. The replica exchange method was adopted for rough conformational sampling with implicit solvent followed by the explicit solvent simulation. Here, we performed conformational sampling of a mini protein, chignolin to examine the efficiency of our method. The results show that our new method covered a wider region of conformational space as compared with the conventional MD simulation with the explicit solvation model.

1PT189 生体分子の分子動力学に対する時系列解析—集団運動の揺らぎと構造変化の関係を調べる—

Time-series analysis of molecular dynamics: Conformational change and dynamics of collective behavior

Kana Fuji¹, Masakazu Sekijima², Hiroshi Fujisaki³, Mikito Toda⁴ (¹Graduate of school Humanities and Sciences, Nara Women's Univ., ²GSIC, Tokyo Tech, ³Phys., Nippon Medical School, ⁴Sci., Nara Women's Univ.)

Our study aims to analyze time series data of molecular dynamics simulation for proteins to extract collective behavior involving side chains and water molecules. Our methodology consists of the following two steps: (1) conformational analysis (dihedral principal component analysis) (2) dynamical analysis (the wavelet transformation and singular value decomposition(SVD)). The wavelet transformation enables us to investigate time-varying features of oscillatory motions, and SVD extracts collective variables involving multiple amino residues[1].

Our system is chignolin. In our previous work, we analyzed time series data using implicit solvent method for dynamics simulation. Here, we study data using explicit solvent method and will compare these two cases.

In particular, we aim to extract collective behavior involving not only the main chain but also the side chain. By analyzing relationship of collective behavior between the main chain and the side chains, we can understand to what extent collective behavior involving the main chain provides us with information concerning collective behavior with the side chains. Furthermore, we expect that the study of collective behavior involving the side chain will give us an important clue to understand molecular functions for other proteins.

[1]M.Kamada,et. al,Chem.Phys.Lett.502(2011)241-7.

1PT190 イオンモビリティ質量分析と分子動力学シミュレーションを用いた気相中におけるヒストン多量体の構造解析

Characterization of histone multimers in the gas phase by ion mobility mass spectrometry and molecular dynamics simulation

Kazumi Saikusa¹, Sotaro Fuchigami¹, Kyohei Takahashi¹, Yuuki Asano¹, Aritaka Nagadoi¹, Hiroaki Tachiwana², Hitoshi Kurumizaka², Mitsunori Ikeguchi¹, Yoshifumi Nishimura¹, Satoko Akashi¹ (¹Yokohama City Univ., ²Waseda Univ.)

Nucleosome core particle (NCP) is the basic structural unit of eukaryotic chromatin. In order to understand the mechanism of the NCP assembly and disassembly, structural characterization of the histone multimers, H2A/H2B dimer and H3/H4 tetramer, should be of great help. However, these atomic-level structures have not been determined. In the present study, human histone multimers were prepared and characterized by electrospray ionization ion mobility mass spectrometry (ESI-IM-MS) and molecular dynamics (MD) simulation. Experimentally obtained arrival times of these histone multimer ions showed rather wide distributions, which suggested that histone multimers had various conformations. To probe the conformers' structures, several MD simulations of the histone multimers were carried out in solution and in vacuo, and it was identified that the histone multimers had a variety of structure. In addition, the simulation showed that the conformers with smaller CCS values had more compact tail regions than those with larger CCS values. On the other hand, the CCS values of the folded core structure were almost kept identical in the analyzed conformers. This implies that the disordered regions brought about the structural variety of histone multimers. This paper presents that the combination of IM-MS and MD simulation enables comprehensive characterization of the gas-phase structures of biomolecular complexes containing disordered regions.

1PT191 カーネル正準相関分析と離散ウェーブレット変換を用いたタンパク質立体構造の時系列解析

Time-series analysis for protein dynamics using discrete wavelet transform with kernel canonical correlation analysis

Mayumi Kamada¹, Mikito Toda², Tatsuya Akutsu¹ (¹Inst. Chem. Res., Kyoto University, ²Phys. Dept., Nara Womens Univ.)

Structural dynamics of proteins play an important role in expression of protein functions. In particular, slow collective motions of proteins make a large contribution to performing its functions. To understand a correlation between protein functions and structural dynamics, we need a method to extract slow collective motions from structural dynamics without losing important information, and correctly characterize them. For this purpose, we use the discrete wavelet transformation (DWT) for the time-series data of protein structures obtained from molecular dynamics (MD) simulation. DWT is one of time-frequency analysis methods used for denoising and data composition, and