1P019 タンパク質の構造コンプライアンス特性の計算
Computation of the Structural Compliance Characteristics of Proteins

Keisuke Arikawa (*Fcl. Eng., Kanagawa Inst. of Tech.*)

We developed a method for calculating the structural compliance of proteins using PDB data. The protein model used in this method consists of main chains, springs between the alpha carbons, and constraints of distances between the specific alpha carbons. The method is formulated not just for a single protein molecule model but for a system containing multiple molecule models, with the prospect of efficient computation including parallel and incremental computation. We confirmed that it was possible to calculate the structural compliance of a system containing more than eight thousand amino acid residues. The calculated results provide information regarding the motion of molecules in the system as well as the structural compliance characteristics.

1P022 アラニンペプチドモデルにおける溶媒和自由エネルギーの加算性
Analysis of additivity in the alanine peptide model of protein solvation by molecular simulations

Hironori Kokubo, B. M. Pettitt (*UTMB*)

The protein solvation model implying additivity of the alanine peptide free energy of solvation is computationally tested by solvation free energy simulations. We found that both the fixed extended conformations and the flexible ones showed the ideally additive solvation free energy as the chain length increased. The slope of the total solvation free energy of the extended conformations was negatively larger than that of the flexible ones as expected. However, we found that the vdW solvation free energy decreased as the chain length increased for the extended peptides, on the other hand, it increased as the chain length increased for the flexible peptides. We discuss these trends and their implications in protein solvation.

1P020 NRSF/REST の競合誘起天然変性に起因する動的特性
Dynamical Property due to Frustration Induced Intrinsic Disorder of NRSF/REST

Katsuyoshi Matsushita^{1,3}, Hidetoshi Sugihara^{1,3}, Macoto Kikuchi^{1,3,4}, Tomoaki Nogawa⁵, Munetaka Sasaki⁶ (¹*Cybermedia Centery, Osaka University*, ²*Institute for Protein Research, Osaka University*, ³*Graduate School of Science, Osaka University*, ⁴*Graduate School of Frontier Biosciences, Osaka University*, ⁵*Faculty of Medicine, Toho University*, ⁶*Department of Applied Physics, Tohoku University*)

An intrinsically disordered region in NRSF/REST exhibits a coupled binding and folding [1]. Recently, we theoretically investigated this coupled folding and binding, and proposed the hypothesis that the cooperativity between the folding and binding is induced by the frustrating interaction in this region [2]. The frustrating interaction is expected to exert effects on the kinetics of the coupled folding and binding. The effects on the kinetics are still unclear.

In the present work, we develop an analytical method of folding kinetics. We apply this method to a model of NRSF/REST and describe the frustration effects on the coupled folding and binding.

[1] M. Nomura et al., *J. Mol. Bio.* 354 (2005) 903.

[2] K. Matsushita and M. Kikuchi, *J. Chem. Phys.* 138 (2013) 105101.

1P023 MD シミュレーションによる設計したタンパク質間相互作用面の評価
Evaluation of the designed protein binding interfaces as studied by MD simulation

Masaki Fukuda, Hironao Yamada, Takeshi Miyakawa, Ryota Morikawa, Masako Takasu, Satoshi Akanuma, Akihiko Yamagishi (*Sch. of Life Sci., Tokyo Univ. of Pharm. and Life Sci.*)

The purpose of our study is to design protein surfaces which induce a protein-protein interaction. We mimicked naturally occurring 4-helix bundle that are found at interfaces between two proteins. To strengthen the protein-protein interaction, we introduced hydrophobic residues on the surface and charged residues on the side of interface *in silico*. We evaluated the binding of two protein molecules with the designed interface by molecular dynamics simulation. Then, we analyzed the distance between the interfaces, solvent-accessible surface area, root mean square fluctuation, and short-range (1nm) part of Coulomb potential energy in the system. We eventually found an interface that seemed to be suitable for inducing the protein-protein interaction.

1P021 Adaptive lambda square dynamics シミュレーション：生体分子の効率的な構造探索法
Adaptive lambda square dynamics simulation: an efficient conformational sampling method for biomolecules

Jinzen Ikebe, Shun Sakuraba, Hidetoshi Kono (*MMS, JAEA*)

A novel, efficient sampling method for biomolecules is proposed. The partial multicanonical molecular dynamics (partial McMD) was recently developed as a generalized ensemble (GE) method to focus sampling only on a part of a system (GEPS); however, it was not tested well. We found that partial McMD did not work well for poly-lysine decapeptide and gave significantly worse sampling efficiency than a conventional GE. Herein, we elucidate the fundamental reason for this and propose a novel GEPS, adaptive lambda square dynamics (ALSD), which can resolve the problem faced when using partial McMD. We demonstrate that ALSD greatly increases the sampling efficiency over a conventional GE.

1P024 赤外分光法によるカルシウム結合タンパク質並びにカルシウム結合ペプチドアナログの配位構造解析
Coordination to divalent cations by calcium-binding proteins and calcium-binding peptide analogues studied by FTIR spectroscopy

Masayuki Nara¹, Hisayuki Morii², Masaru Tanokura³ (¹*College of Liberal Arts and Sciences, Tokyo Medical and Dental University*, ²*National Institute of Advanced Industrial Science and Technology (AIST)*, ³*Graduate School of Agricultural and Life Sciences, University of Tokyo*)

EF-hand motif is a Ca²⁺ binding domain in common between many intracellular Ca²⁺-binding proteins such as calmodulin and troponin C. FTIR spectroscopy has been applied to study Ca²⁺-binding proteins and the synthetic peptide analogues corresponding to the EF-hand motif. The COO⁻ stretching vibration modes can be used to identify the coordination modes of COO⁻ groups of Ca²⁺-binding proteins to metal ions: bidentate, unidentate, and pseudo-bridging. As a result, the downshift of the COO⁻ antisymmetric stretching mode from 1565 cm⁻¹ to 1555 - 1540 cm⁻¹ upon Ca²⁺ binding was a commonly observed feature of FTIR spectra for EF-hand proteins. The implication of COO⁻ stretches was discussed on the basis of the FTIR spectra of calcium-binding peptide analogues.