- 3P076 蛋白質分子内における不對稱性基の統計解析
○西上 慎哉¹、松本 博希¹、関 安孝¹、曾田 邦嗣¹
¹長岡技科大・生物系
- 3aF13 Statistical Analysis of Unpaired Polar Groups in Protein Interior
Shin-ya Nishiue (1), Hiroki Matsumoto (1), Yasutaka Seki(1) and Kunitsugu Soda(1). (1:Department of Bioengineering, Nagaoka University of Technology)

It has been known that several unpaired polar groups are found in the interior of native protein structure. The typical structural stability of protein is 60 kJ/mol, which correspond to the energy of a few H-bonds. Hence, an unpaired polar group in the interior of a protein should significantly decrease its structural stability. The purpose of this study is to reveal (1) how many unpaired polar groups exist in protein interior; and (2) how these unpaired polar groups cancel the disadvantage. To achieve the aim, using Thornton's method, we examined unpaired polar groups in protein interior of 914 species of proteins, whose structures are determined with high accuracy. Moderate criteria of $d(H...A) \leq 0.3$ nm and $\angle DH A \geq 60^\circ$ were taken for the H-bond formation of D(donor)-H...A (accepter) type. The result of analysis shows that the total polar groups contain 2.9 % unpaired polar groups or 2.2 % donor and 3.9 % acceptor groups. Especially, the polar groups found in the unpaired state with high percentage are the imino groups of His (14.7 %), the amino groups of Asn and Gln (17.1 %) among the possible donors, and the imino N atom of His (19.8 %) and the hydroxyl O atom of Thr, Ser, Tyr (24.9 %) among the possible accepters. As much as 77.8 % the H atoms in the unpaired polar groups neighbor at least one N atom or S atom or C atom in an aromatic ring within 0.3 nm. In the poster presentation, we will report what role is played by the atoms that are found around unpaired polar groups with high probability.

- 3P078 蛋白質 2 分子複合体の基準振動の包括的解析
○猿渡 茂¹、輪湖 博²
¹北里大学・理・物理、²早大・社会科学
- Comprehensive Analyses of Normal Modes of Dimeric Protein Complexes
Shigeru Endo (1) and Hiroshi Wako (2) (1: Dept Physics, School of Science, Kitasato Univ.; 2: School of Social Sciences, Waseda Univ.)

We carried out normal mode analyses (NMA) of more than 2,500 typical proteins registered in PDB, and we have built *ProMode* (a database of normal mode analysis of proteins)⁽¹⁾, in which monomeric proteins and each subunit in complexes were registered. At present the comprehensive normal mode analysis of protein complexes is in progress. About the selection of homodimers we referred to the classification of homo protein-protein interfaces⁽²⁾. As typical hetero-protein systems protease-inhibitor and proteinous antigen-Fv fragment complexes were selected.

Low-frequency normal modes which appear newly with the complex formation are important motions in the dynamics of the complex, because a basic function of proteins is achieved by binding to other molecules. In the normal mode analysis of the protein complex, the normal mode which changes a distance between the centers of mass of the molecules is considered to cause the dissociation of the complex and relate to the pathway of the complex formation. In a preliminary survey, such external translational mode was hardly observed. Other normal modes that change the intermolecular orientation were generally observed. Such modes show the relative rotation of each molecule as a rigid body. The details of the statistics will be discussed in the meeting.

1. <http://promode.socs.waseda.ac.jp>
2. <http://pre-s.protein.osaka-u.ac.jp/~classppi/>

- 3P077 ProMode データを利用したタンパク質の基準振動解析プログラムの開発
○輪湖 博¹、富澤 裕樹²、猿渡 茂³
¹早大・社会科学、²(株)サイエンスハウス、³北里大学・理・物理
- Development of a program with user-friendly GUI to perform normal mode analysis of proteins by ProMode users themselves
Hiroshi Wako (1), Yuhki Tomizawa (2) and Shigeru Endo (3) (1: Sch Social Sciences, Waseda Univ.; 2: Sciencehouse Inc.; 3: Dept Physics, Sch Science, Kitasato Univ.)

Normal mode analysis (NMA) is one of popular methods to reveal dynamic aspects of proteins. Although the NMA is much faster than molecular dynamics simulation, it is still too time consuming for non-expert researchers on computational studies to perform. In such situation we have developed the database ProMode to present the NMA results on the web, and now the data for more than 2,500 proteins are given in it. However, we have a problem in ProMode that the NMA can potentially generate enormous amount of data. For example, correlations between atomic displacements can be calculated for any atom pairs and furthermore, it can be calculated for any normal modes. However, the number of modes is as many as 1,000 to 2,000 for the proteins with 100 to 300 residues, when dihedral angles are used as independent variable to represent their three-dimensional structures. In fact we present the data only for the twenty lowest-frequency modes in ProMode. We guess that many researchers want to obtain more data for a specific protein they are interested in. So, we developed the program with user-friendly GUI to perform the NMA of proteins by users themselves. By providing the intermediate data generated in the NMA calculation including the most time-consuming parts (energy minimization and diagonalization of the matrix) through ProMode, the calculation can be perform in very short time (a few to a dozen of minutes on a regular PC). The details of the functions implemented in the program will be discussed in the meeting.

- 3P079 分子動力学シミュレーションによる PhoB DNA 結合タンパクのダイナミクス解析
○山根 努¹、岡村 英保¹、池口 満徳¹、西村 善文¹、木寺 詔紀¹
¹横浜市立大学大学院
- Dynamics of PhoB protein as revealed in the comparison between molecular dynamics simulation and NMR relaxation experiments
Tsutomu Yamane, Hideyasu Okamura, Mitsunori Ikeguchi, Yoshifumi Nishimura & Akinori Kidera(International Graduate School of Arts and Sciences, Yokohama City Univ.)

PhoB is a transcription activator protein which is involved in the regulation of the pho regulon of 39 genes. Recently, Okamura et al. carried out an NMR relaxation study for both DNA bound and unbound forms of the PhoB DNA-binding/transactivation domain. Their model-free analyses clarified that the hydrophobic core of the DNA-binding domain were clearly divided into a soft-core and a hard-core, and that the flexibility of the soft-core decreased upon DNA binding. In the present study, we performed molecular dynamics (MD) simulation for the DNA bound and unbound forms of the PhoB DNA-binding domain to calculate the order parameters for the backbone NH (S_{NH}^2) and for methyl-averaging axis (S_{axis}^2). The results of our calculations successfully reproduced the experimentally determined parameters of the NMR experiments. To establish the structural basis for the difference in dynamics, we applied the Voronoi analysis to the MD trajectories, and compared the volume of the core regions. It was found that the soft-core reduced the average volume as well as the volume fluctuation upon DNA binding. This result suggests that the interactions between the soft-core and DNA reducing volume could be ascribed to the change in the order parameters upon DNA binding. Further analyses are underway to elucidate the relation between the order parameters and protein dynamics.