1P070 Designing T cell epitope peptides that bind promiscuously to several HLA class I molecules
 ○宇高 恵子¹, 平地 泰子¹, 片岡 佐登¹
¹高知大・医・免疫
 Designing T cell epitope peptides that bind promiscuously to several HLA class I molecules
 Keiko Udaka, Yasuko Hirachi, Sayo Kataoka (Department of Immunology, Kochi Medical School)

A major obstacle to design a peptide vaccine to induce cytotoxic T lymphocytes (CTLs) for viruses and malignant tumors is a polymorphic nature of HLA class I genes. Since HLA genes are believed to be under an evolutionary pressure to diversify their ligand repertoire finding a peptide that binds to several HLA molecules is rather a rare event. However, in order to develop a vaccine for the public it is pivotal to find promiscuous peptides that bind to several HLA class I molecules which are frequently found in a target population. We have previously developed a computational method to identify HLA class I binding peptides in collaboration with NEC corporation. By exploiting the programs to predict HLA-A*2402, A*0201 and A*0206 peptides we identified several rare peptides from WT1 tumor antigen that promiscuously bind to all three HLA allomorphs. Computational predictions were verified by peptide binding experiments that also revealed the size of repertoire overlap between different HLA allomorphs. Interestingly, recently diversified HLA molecules largely share the repertoire while evolutionary distant HLA molecules exhibited more distinct peptide repertoires. This observation supports a long standing hypothesis that polymorphism of the MHC genes is driven by a selective pressure for diversification.

1P072 アミノ酸配列における電荷周期性の解析によるゲノム比較
 ○柯 関聡¹, 美宅 成樹¹
¹名大院・工・応用物理
 Genome comparison by analysis of charge periodicity in amino acid sequences
 Runcong Ke and Shigeki Mitaku. (Dept Appl Phys, Graduate School of Engineering, Nagoya Univ)

Protein structure and stability are related to the physical and chemical properties of a protein. Recently, we analyzed all amino acid sequences coded in human and yeast genomes by the autocorrelation function of charge sequences, showing a significant charge periodicity of 28 residues for human and no peak for yeast. The proteins with charge periodicity of 28 residues were selected and the ratio of this type of proteins was approximately 3% of the total human proteome. A question arises at which point of evolution from yeast to human the ratio of the proteins with charge periodicity of 28 residues in the total ORFs significantly increased.

In this work, we analyzed all amino acid sequences from 268 biological genomes, including 248 prokaryotes, 10 invertebrates and 10 vertebrates, by the autocorrelation function of the charge distribution. The result indicated very sharp positive correlation of the multiple of 28 residues for vertebrates, positive correlation for invertebrates and non-correlation for prokaryotes. The proteins with charge periodicity of 28 residues existed in all organisms and the dependence of the number of this type of protein on the total ORFs had two branches: the branch of vertebrates and that of other organisms. When we studied the intracellular localization of these proteins by analyzing the database SWISS-PROT, this type of protein from vertebrates contains many nuclear proteins such as transcriptional factor. The role of charge periodicity of 28 residues in amino acid sequence will be discussed.

1P071 データベース解析によるタンパク質の極性原子周辺の水和構造予測
 ○松岳 大輔¹, 中迫 雅由¹
¹慶應大院・基礎理工・物理
 Prediction of hydration structures around polar protein atoms through a data-base analysis
 Daisuke Matsuoka (1) and Masayoshi Nakasako (1). (1: Graduate School of Science and Technology, Keio University)

Polar atoms on the surface of proteins work as sites to anchor networks of hydrogen bond organized by hydration water molecules. The networks are thought to have great influences on the dynamics, function and folding of proteins. About 20 years ago, an analysis of 16 high-resolution crystal structures by Thanki *et al.* demonstrated that water molecules bind to polar atoms so as to satisfy the stereochemistry of hydrogen bond [1].

Now, more than 40,000 protein structures have been registered in the Protein Data Bank. Among them, about 17,000 structures with many hydration water molecules were determined by X-ray diffraction at resolutions of better than 2.2 Å. Thus we examined systematically spatial distributions of water molecules around polar atoms of proteins and arrangements of water molecules with the new version of the FESTKOP program suite developed for hydration structure analyses [2]. Through the analyses, we determined the 3D-distribution profile of the first hydration sites around polar atoms. In addition, we also verified the tetrahedral arrangement of water molecules in the water-water hydrogen bonds formed around the polar atoms. With these results, we are trying to predict hydration structures around polar atoms of proteins.

[1] N. Thanki, J. M. Thornton & J. M. Goodfellow (1988) *J. Mol. Biol.*, **202**, 637-657
 [2] M. Nakasako (1999) *J. Mol. Biol.*, **289**, 547-564

1P073 生体系時系列データから動力学諸量を抽出する方法論
 ○寺本 央¹, 小松崎 民樹¹
¹神戸大・理・地惑
 From time series of biological systems to their dynamical
 Hiroshi Teramoto (1) and Tamiki Komatsuzaki (1). (1: Department of Earth and Planetary Sciences, Faculty of Science, Kobe University)

Thanks to the development of experimental technology, a lot of interesting time series data at the single molecular level is available nowadays. One of the outstanding experiments is the experiment of structural dynamics of the hairpin ribozyme done by X. Zhuang et. al. [1] which reveals the long term memory effects of that molecule.

However, the understanding of their underlying dynamics is still in its infancy since there are tremendous number of degree of freedom that are involved in those phenomena and their time evolutionary equations are too complicated to be analyzed.

On the contrary, from experimental 1-dimensional time series data, there are several approaches aiming at extracting several dynamical variables such as embedded dimension, Lyapunov exponent, etc. Yet, there are roughly two problems for most of these methods, too. One is that a lot of data points are required to calculate these variables. The other is that it is very difficult to extract local, transient and intermittent behavior by these methods. The main purpose of this study is to overcome these difficulties. To achieve this goal, in this talk, we propose a new method to extract the dynamical variables, based on ε-machine [2] which is shown to be the unique, simplest machine among the machines which have the maximum predictability [3].

[1] X. Zhuang et. al. Science 296, 1473 (2002).
 [2] J. P. Crutchfield and Karl Young, Phys. Rev. Lett. 63, 105 (1989).
 [3] C. R. Shalizi and J. P. Crutchfield, J. Stat. Phys. 63, 817 (2001).