3P266 保存された連続反応を用いた代謝系のモジュール構造の同定とその進化に関する考察**Identification of metabolic pathway modules by conserved reaction sequences and its application to evolutionary analysis**

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Enzymatic reactions are key components in the metabolic pathway and have been classified in several ways. We have also developed a classification system for the enzymatic reactions based on chemical transformation mechanisms. Using this classification system, we extracted and annotated conserved sequences of reactions from the KEGG PATHWAY database, successfully defined 33 functionally well explained sequences, and termed them as reaction modules. These modules often correspond to gene clusters on bacterial genomes even though they are defined only based on chemical reactions. We also found that some modules are repeatedly used and/or combined with specific partner modules, indicating an evolutionary aspect of the metabolic pathway.

**3P269 間期染色体の3Dモデル：ゲノム構造と機能の理解に向けて
3D model of interphase chromosomes: toward understanding of genome structure and function**

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Recent progress of the chromosome conformation capture technology such as 3C and Hi-C enabled studies of the spatial organization of genome-wide chromosome structures. Yet, how the 3D structure of the genome affects gene function (ex. transcription, replication, etc.) remains elusive. Using published data and computational approaches, we examined the gene positioning and other properties for several organisms, compared them with the chromatin organization, and then revealed some functional role of the spatial organization of the genome.

**3P267 Lysozyme スーパーファミリーを用いた遠縁タンパク質間のフォールディング部位の頑健性についての解析
The analysis of the robust folding units among highly diverse proteins in the lysozyme superfamily**

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The relationships between the evolution of protein and the protein folding mechanisms are not completely elucidated. In the lysozyme superfamily the structural similarity of each type of lysozyme suggests they have a common ancestor despite their low sequence similarity. In this study, we examine the robustness of folding nuclei of the lysozyme superfamily. That is, location of the possible folding nuclei of these proteins is predicted only from their amino acid sequences based on the inter-residue average distance statistics. The phylogenetic trees are built using the multiple sequence alignment to investigate the evolutionary change of the possible folding nuclei. The results suggest the robustness of folding nuclei during the evolution of the lysozyme superfamily.

**3P270 Krylov 部分空間法による相関したブラウンノイズの計算
Krylov subspace methods for computing correlated Brownian noise vectors in Brownian dynamics simulations with hydrodynamic interactions**

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Brownian dynamics is a molecular simulation algorithm that can incorporate hydrodynamic interactions between particles. In the simulations, a Cholesky factorization is commonly used to compute correlated Brownian noise vectors. However, this factorization is an $O(N^3)$ operation for an N -particle system, which is generally the bottleneck in the Brownian dynamics. Here, we study methods based on Krylov subspace approximations for computing Brownian noise vectors to overcome this difficulty. We show that the computational time of Krylov subspace methods scales very nearly as $O(N^2)$ without any loss of simulation accuracy. Thus, Krylov subspace methods are recommended for performing large-scale Brownian dynamics simulations with hydrodynamic interactions.

**3P268 天然変性タンパク質における自然淘汰のdN/dS比に関する解析
Estimating the strength of natural selection on intrinsically disordered proteins in terms of dN/dS ratio**

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A significant fraction of eukaryotic proteins includes intrinsically disordered regions (IDR) that do not exhibit compact rigid structure under physiological conditions. Typically, functional fragments in IDRs switch to more ordered states upon binding to target molecules, a phenomenon known as coupled folding and binding (CFB). We conducted an analysis to compare the degree of selective pressure observed between ordered regions, IDRs, and functional IDRs. dN/dS, that represents the vulnerability of amino acid substitutions relative to the neutral nucleotide mutation rate, of the functional IDRs suggests that the regions have been subjected to stronger negative selection than IDRs. Higher dN/dS of IDRs may be accounted for by the abundance of neutrally evolved codons.

3P271 3P271 は 2P183 に移動しました。