1P073 様々なアルカン産生シアノバクテリアに由来するアシルACP還元酵素の活性比較
Comparison of the activities of acyl-ACP reductases from various alkane producing cyanobacteria
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Some kinds of cyanobacteria generates alkanes and alkox-ones with acyl-ACP reductase (AAR) and aldehyde decarboxylase (AD). AAR reduces fatty acyl-ACP into aldehyde, which is then transformed into alkane by AD. It is experimentally shown that activities of AD vary between species of cyanobacteria. However, differences in activities of AAR from various alkane producing cyanobacteria has not been investigated. To reveal them, we have synthesized AAR genes of various cyanobacteria including Synechococcus elongatus PCC 7942, Nostoc punctiforme PCC 73102, and Synechocystis sp. PCC 6803. Each AAR protein is overexpressed in E. coli, and the amount of aldehydes produced in E. coli is measured by GC-MS. Detailed results will be presented in the poster.

1P074 ニトリルヒドラターゼの触媒機構に関する理論的研究
Theoretical Study on Catalytic Mechanism of Nitrile Hydratase
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Nitrile hydratase (NHase) catalyses hydration of nitrile to the corresponding amide and has been used as a biocatalyst in chemical industry. However, the detailed catalytic mechanism of this enzyme has not yet elucidated. In the present study, we analyze several proposed reaction pathways of NHases comprising Fe(III) at the active site by using Quantum Mechanics / Molecular Mechanics (QM/MM) method. First we analyze three reaction mechanisms which have been suggested in previous theoretical studies using active-site models (Hopmann et al., 2007&2008) to reveal the effects of surrounding protein environment on the reaction process.

1P075 アデニル酸キナーゼ反応機構に関する ONIOM 法による研究
Study on the reaction mechanism of adenylate kinase with ONIOM method
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In order to elucidate the nature of the reaction of adenylate kinase, which catalyzes the reaction: ATP + AMP + Mg2+ -> ADP + ADP + Mg2+, we have been studying the theoretical model using molecular mechanics and quantum chemistry.

We constructed the model of complex structure of enzyme and substrates, ATP and AMP with Mg ion with some water molecules surrounding the active center using MM or MD calculation with AMBER99 force field. The truncated models were used for the calculations with ONIOM method, and the reactant, product, transition structures were optimized.

In these calculations, small barrier shown in the low level model vanishes with the higher level, and the present highest model gives the reaction barrier of about 19 kcal/mol, and 10 kcal/mol exothermicity.

1P076 トレオニン合成酵素における反応制御機構の理論的解明
Theoretical elucidation on the reaction control mechanism in Threonine Synthase

Threonine synthase (TS) catalyzes the last step of L-Thr biosynthesis and its reaction is the most complex among the PLP enzymes. To elucidate the detailed mechanism, we performed comparative Quantum Mechanics/Molecular Mechanics calculations with an exhaustive search for the reaction pathways in the reaction-specificity-determining-process. Satisfactory agreements with the experimental data were obtained. Contrary to the earlier proposal, the base that abstracts a proton from the attacking water was the Lys61 amino group rather than the phosphate ion. We also determined that phosphate ion forms a stable H-bond with the L-Thr moiety, which is critical for the reaction specificity. Additionally, a new mechanism was proposed for the transaldolization process.

1P077 生体分子の分子動力学に対する時系列解析ー運動変化と構造変化の関係を探究ー
Time-series analysis of molecular dynamics: Conformational change and dynamics of collective behavior
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Dynamics of proteins have harmonic and unharmonic motion. In recent years, the wavelet transformation as a method to analyze unharmonic motion has been proposed.

We aim to develop analysis for MD simulations, focusing in particular on the relationship between conformational change and motion of proteins. In this study, we analyze a trajectory data of chignolin (consisting of 10 amino acid residues) from all atom MD simulation. Our method is "Wavelet PCA", which combines the wavelet transformation and the principal component analysis (PCA). Wavelet PCA can be applied to characterize frequency of each of degrees of freedom of proteins.

We find that conformational change from folded to misfolded states results in shift to a lower frequency side.

1P078 それぞれが複数の立体構造からなる複数の蛋白質構造の比較解析
Superposition of protein structures each of which is a set of multiple conformations
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The mathematics for superposition of two protein conformations are well known. Methods for superimposing more than two conformations have been reported in recent years. Stepping further, we propose a method for superimposing multiple protein structures simultaneously each having multiple conformations. The method is based on mixed-effects models and uses maximum a posteriori estimation, i.e., the deviations of individual proteins are estimated by borrowing information from overall conformations. The portions that have deviations are narrowed by means of L1-regularization to clarify the characteristic deviation of each protein molecule. We will illustrate the applications of the method for analyzing molecular dynamics trajectories.