**3P031** Gliding and binding of mycoplasma on uniform sialylated oligosaccharide

Taishi Kasai, Tasuku Hamaguchi, Makoto Miyata (Osaka City University, Graduate School of Science)

Mycoplasmas glide in the direction of the membrane protrusion at a pole. Generally, mycoplasmas glide on mixed sialylated oligosaccharides (SOs), and the gliding motility on uniform SO has never been observed. In the present study, we analyzed binding and gliding of M. mobile on a plastic plate covered by 53 uniform oligosaccharides on isolated spots. The gliding speed related inversely to the affinity of mycoplasma to the SO, suggesting that the mycoplasma legs generate drag force in gliding. Mycoplasma cells glided faster, more constantly, with accelerated pivoting on uniform SO than on mixed SO, suggesting that they can glide efficiently on uniform SO and processively on mixed SO.

**3P032** Ant HIV factor APOBEC3Gの基質認識及びスライディング機構の実時間NMR解析

Substrate Recognition and Sliding Properties of an Anti-HIV Factor APOBEC3G analyzed by Real-Time NMR Monitoring Strategy

Keisuke Kamba1,2, Takashi Nagata1,2, Masato Katahira1,2 (1Inst. of Advanced Energy, Kyoto Univ., 2Grad. Sch. of Energy Science, Kyoto Univ.)

Human APOBEC3G protein (A3G) destroys the HIV genomic information by converting cytidines into uridines in the minus DNA strand synthesized from RNA genome of HIV. This deamination activity of A3G is only targeted towards DNA. A3G effectively deaminates cytidines that are located close to the 5' end. The mechanism of the DNA recognition by A3G has not been clarified so far. In this study, we have applied the real-time NMR monitoring strategy to the systematically designed oligonucleotides: DNAs that are partially substituted with RNA or abasic nucleotides. We will discuss the identified DNA determinants for the recognition by A3G and A3G's DNA sliding property.

**3P033** セルラーゼTrCel7Aの基質取り込み機構に関する分子シミュレーション研究

Molecular simulation study on the mechanism of substrate uptake in cellulase TrCel7A

Takashi Kanazawa, Minoru Sakurai, Tadaomi Furuta (Center for Biod. Res. Info., Tokyo Tech)

Cellulohydrolases is an enzyme that hydrolyzes glycosidic linkages in cellulose, and its catalytic domain has a tunnel for substrate to pass through. Here, we conducted MD simulations of the catalytic domain and free energy calculations to examine the contribution of four tryptophan residues (W38, W40, W367, W376), which are lined up along the tunnel, for initial threading of a cellulose chain into the catalytic tunnel of the Family 7 cellulohydrolase from Trichoderma reesei (TrCel7A). Simulations for W40A and W38A mutants revealed the role of these tryptophan residues in initial uptake. Moreover, we would discuss the dynamics of entire TrCel7A bound to crystalline cellulose toward further understanding of cellulose decrystallization.

**3P034** レプリカ交換MD及びフラグメントMO計算によるアミロイドβダイマーの水中での安定構造の探索

Replica exchange MD and ab initio fragment MO calculations for searching stable conformations of amyloid-b dimer in water

Hiromi Ishimura, Akisumi Okamoto, Atsushi Yano, Noriyuki Kurita (Toyohashi University of Technology)

The aggregation of amyloid-B peptides (ABs) is involved in the pathogenesis of Alzheimer’s disease, and the conformations of AB aggregates have been investigated widely. In the present study, we performed replica exchange molecular dynamics simulations to obtain various conformations of AB(1-42) dimer in explicit water molecules and determined the most stable conformation of the solvated AB dimer by ab initio fragment molecular orbital calculations. In addition, the specific interactions between AB monomers were investigated to elucidate which residues of AB contribute to the AB dimerization in water.

**3P035** Elastic Network Modelを用いたABCトランスポーターのglobal motionの解析

Global motion of ABC transporters using nonlinear relaxation dynamics in elastic network model

Naoki Arai, Tadaomi Furuta, Minoru Sakurai (Center for Biol. Res. & inform., Tokyo Tech)

ABC transporters have two TMDs and two NBDs. TMD and NBD are connected with ICL. Although several X-ray structures have been reported, their dynamic properties are not well understood. This study investigated the structural transition and communication between TMDs and NBDs by applying nonlinear relaxation dynamics in elastic network model (ENM) (Togashi et al. PNAS 2007) to MsbA. At first, ENM was constructed from its X-ray structure. Then, we added a force of bringing the two NBDs approaching each other as a simulation of ATP binding, but the TMDs never opened outward. Next, a force of rotating the NBDs was added. Then, the TMD opening was observed. The detailed analysis suggested that the motion of TMDs opening results from power transmission through ICL.

**3P036** 一酸化炭素型ヘモグロビンの光解離中間体のX線結晶構造

X-ray crystal structures of carbonmonoxy hemoglobin photolysis intermediates


Hemoglobin (Hb) is an αβ4 tetrameric oxygen transport protein that binds gaseous ligands such as O2 and CO cooperatively at the four heme irons. Although Hb was one of the first protein structures ever to be solved by X-ray crystallography, its static structures do not tell us much about the gas migration pathway from the outside of the protein to the deeply buried heme. We report a series of X-ray crystal structures of the photolysis intermediates of HbCO at 140 K, visualizing the irradiation time-dependent position of CO in the α and β subunits. Photo-dissociated CO moves toward the protein internal cavities with shift of amino acid residues around the cavities. We assign the individual ligand migration pathways in both subunits of Hb.