2P079  Intermolecular interactions and conformation of antibody dimers present in IgG1 biopharmaceuticals
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Intermolecular interactions and conformation in dimer species in Palivizumab, a monoclonal antibody (IgG1), were investigated to elucidate the physical and chemical properties of the dimerized antibody. Palivizumab solution contains approximately 1 % of dimer species with 99 % monomer. The dimer species was isolated by size exclusion chromatography (SEC) and analyzed by a number of methods. The results indicated that approximately half of the dimer species was non-covalently associated, whereas the other half was dimerized by covalent bond including disulfide and di-tyroline bonds. The dimer species were formed between Fab and Fe, or Fab and Fab. The higher-order structure and thermal stability were very similar between the dimer and monomer.

2P080 細胞膜上のガレクチン3もその細胞膜分子との複合体も、細胞膜上で極めて動的に振る舞う：超高速1分子追跡による研究
Galectin-3 and its glyco-molecule conjugates are extremely dynamic on the cell surface: detection by ultrafast single-molecule tracking
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Galectin-3 (Gal) is an N-glycan-binding lectin, whose pentamers could generate "lattices" by multiply crosslinking glyco-molecules on the plasma membrane (PM) surface, thus modulating their locations and functions. We performed ultrafast single-molecule tracking of Cy3-Gal (0.1-ms resol.), and found that each Gal molecule stays on the PM for 110 ms, and alternatingly binds and unbinds N-glycans (for 5.1 and 0.87 ms, with diffusion coefficients of 1.1 and 30 μm2/s, respectively). The latter rate is the fastest ever observed in/on the PM, suggesting Gal molecule measurement. Then extract hierarchical property of transition from the network based on transition probability between clusters of network.

2P081 分子動力学シミュレーションによる1分子FRETのデータ同化
Sequential data assimilation to single-molecule FRET photon-counting data by using molecular dynamics simulations
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Single molecule FRET (smFRET) measurement provides valuable insights into the dynamical heterogeneities of biomolecules. Here we propose a method, based on the particle filter, to sample hidden conformation states from smFRET data by using molecular dynamics simulations. In the method, a set of coarse-grained models are concurrently simulated and also filtered/resampled during the simulation like the bootstrap methods according to the likelihood of the smFRET photon-counting data in each short time bin. For emulated smFRET data of polyproline and other biomolecules, we demonstrate the performance of the method by using ten thousands of coarse-grained model simulations on K computer.

2P082 一分子数列から抽出されたマルコフ連鎖 定常ネットワークにおける連移確率が“最小小”となる分子の“状態”の同定
Identifying chemical states in Markov chain steady state network extracted from time series by finding “minimum” transition probability
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Protein dynamics is considered as having multiple time scale for execute their functions such as folding/unfolding, allosteric regulations, and signal transaction. Such property was visualized by disconnectivity graph based on potential energy profile. The approach was recently extended into disconnectivity graph based on free energy profile in equilibrium call transition disconnectivity graph. In this talk we introduce novel method to construct disconnectivity graph. Our approach is starting from Markov chain steady state network that can be extracted from time series of single molecule measurement. Then extract hierarchical property of transition from the network based on transition probability between clusters of network.

2P083 X線1分子追跡法によるII型シェパロン協同的運動評価
Cooperative Motion Analysis of group II chaperonin by X-ray Single Molecule Tracking
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Group II chaperonin, found in archaea and in the eukaryotic cytosol, is an indispensable protein that captures a nonnative protein and refolds it to the correct conformation in an ATP dependent manner. ATP-induced structural changes are essential for chaperonin activity. We had reported that the diffraeted X-ray tracking (DXT) could track ATP induced conformational change of group II chaperonin at single molecule level (Sekiguchi et al., PLoS ONE 2013). In DXT, nanocrystal immobilized on one side of chaperonin-ring is used as tracer for structural change of chaperonin. In this study, we analyzed how ATPase deficient mutant modulate dynamic motion of chaperonin and will discuss intra- and inter-ring cooperativity of group II chaperonin from motion analysis view.

2P084 X線1分子計測によるタウタンパク質分子の構造観察
Structural Fluctuations of Tau Proteins from X-ray Single Molecule Observations
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The structure of tau proteins in solution resembles that of a random coil. But, tau proteins in Alzheimer paired helical filaments-like fibers have very little secondary structure. Here, we tried to observe the structural fluctuations of tau proteins using Diffraction X-ray Tracking (DXT) as x-ray single molecule observation method. In DXT, we observed Brownian motions of recombinant tau proteins and his-tagged tau proteins, which are adsorbed on the substrate’s surface. These adsorbed tau proteins were reacted to many antibodies and were phosphorylated by several kinases. From DXT data, the tau protein combined with the antibody was confirmed that structure fluctuation had become slightly small compared with that which is not combined.