molecules in the groove on each structure. The variability of the conformation was different depending on the solvation condition. The DNA conformation seemed to be influenced by the localization of the water molecules in the groove.

3PT109 Model for self-assembly of flexible DNA motifs using stacking interactions

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Molecular Clusters (MCs) with variable number of constituents seem to be possible if building units are properly designed. Recently, concentration-dependent self-assembly of MCs was demonstrated by utilizing both flexibility of DNA motifs and inter-molecular binding by sticky-ends (He, Y. et al., *Nature* 2008). Here we propose a cluster of DNA motifs by using DNA blunt-end stacking and flexibility introduced into the motif. First, we study an abstract model of flexible planar monomers (triangle with sticky sides A and B, and shrinkable side C. Angle between A and B is about 60 deg.) that move randomly on a surface colliding against each other. Sides A and B of different monomers can stack, thus forming a flexible dimer. Over time we expect to obtain clusters from dimers up to hexamers. We simulated the dynamics of the cluster formation based on chemical kinetics successfully applied to rigid monomers (Hosokawa, K. et al. *Artificial life* 1995). Our simulation shows that the amount of trimers overcomes the tetramers. However, contrary to the work of Hosokawa et al., dimers and pentamers seem to be equally formed. Second, to realize the concept, we have designed a DNA motif with blunt-end stacking interactions, which were proved to be a potential tool for self-assembling larger DNA structures (Woo, S. et al., *Nature Chemistry* 2011).

3PT110 A Growth mechanism of DNA tile array

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We report a growing mechanism of DXAB (DNA double-crossover AB-staggered) tile array known to form planar structures and grow to micro-scale. DXAB tile array is a kind of DNA tile arrays and can work as a scaffold to control positions of nano-particles. Growth mechanisms of the array are important information to set its properties, such as size, accuracy of position control, yield, or the required time of annealing. Here, we report that the growth of array is a co-operative phenomenon in narrow temperature range. This transition width is shorter than a prediction by model based on lengths of the sticky-ends. This has been visualized by fluorescence optical microscope, because, unlike the tiles' assembly, growth of the tile arrays cannot be observed in melting curve. From this knowledge we show two applications, making big isolated sheets and shortening the annealing time in protocol, as examples. These experimental results demonstrate that such knowledge about growth mechanisms is useful to control properties of DNA nanostructures.

3PT111 DNA ナノ構造を用いた DNA-RNA ポリメラーゼ・ハイブリッド ナノマシンの構築と機能評価

Construction and functional analysis of DNA origami base DNA-RNAP hybrid nanomachine

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DNA nanotechnology has recently developed a new nanoscale device called as DNA origami tile (DNA origami). DNA origami is a method for folding long single strand DNA into arbitrary two or three dimensional structures and can be used as a molecular platform which allows proteins and other molecules to place with precisely controlled patterns at nanometer order. Here, we applied DNA origami technology into transcription system. Transcription system is thought to couple to other system in *E. coli* (e.g. translation and replication). And reconstitution of such sequential reactions *in vitro* is important for science and engineering, for which the DNA origami technology may provide platform. As a first step, we assembled T7 RNA polymerase (T7-RNAP) on DNA origami. Rectangle DNA origami (90 x 60 nm) are prepared as reported (Rothenmund *Nature* 2006), and SNAP-tag protein fused T7-RNAP (T7-RNAP-SNAP) were site-specifically anchored on DNA origami through its specific ligand (benzylguanine (BG)-ligand) included on the DNA origami. With the optimized assembly condition, we succeeded in measuring the activity of T7 assembled DNA origami (T7-Tile). We will check the effect of the number and the layout

of T7-RNAP on the activity of T7-Tile.

3PT112 リボソームへの DNA リングの吸着

Adsorption of DNA ring onto Liposome

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The various molecular devices made of biomolecules such as nucleic acid, protein and lipid are reported. We are now able to design each devices with certain complexity, although it is still difficult to combine multiple devices into one functional system. Embedding various molecular devices within a given-size compartment is one of the potential solutions to solve this problem and enable us to achieve programmed behavior of the system. A key component to realize this concept is a channel device integrated into the compartment, which allows materials pass through the compartment.

Here, we adopt a phospholipid as material for micron-sized compartment, and DNA nanostructure for the channel device embedded on the compartment surface. In the design of the DNA channel, we have been inspired by the macrocyclic resorcin channel, which is an artificial mimic of a natural ion channel. We have adopted the T-motif DNA ring that has a similar structure to this. The surface of the DNA ring is hydrophilic, therefore, has affinity to the lipid membrane surface. In order to integrate the ring into the membrane, hydrophobic groups are attached to the DNA rings. We adopt Cholesteryl-TEG as the hydrophobic groups and confirmed the formation of those DNA rings. We also found that DNA structures tend to rest on the lipid membrane surface by giving positive charge to the lipid. Currently, we are working on the optimization of the lipid composition to give an appropriate charge condition.

3PT113 脂質二重膜上での DNA ナノ構造の基板上成長

Substrate-Assisted Self-Assembly of DNA Nanostructure on lipid bilayer

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Substrate-Assisted Self-Assembly (SASA) by Hamada *et al.* enables us to make large 2-D DNA nanostructures that are difficult for conventional self-assembly in free solution. So far, limited materials, e.g., cleaved mica, are known for suitable substrate for the method. It is necessary to extend the method to utilize various materials for the substrate. However, the process of SASA is very complex and not yet thoroughly understood.

To model SASA, we divide it into adsorption and self-assembly processes. The adsorption process is described by DLVO theory. Following Sushko, we can calculate energy of DNA adsorption by DLVO. We also measured minimal length of DNA, or equivalently energy per base pair, to be absorbed on mica substrate. In order to extend SASA to other materials, measured absorption energy between DNA and mica surface roughly indicates the feasible condition for SASA. Based on this consideration, we chose lipid bilayer (DOPG) for the substrate, because the calculated energy between 100 base pairs of DNA and the bilayer is enough to absorb when magnesium ion concentration is 12.5 mM. However, we haven't confirmed DNA adsorption under this condition. Currently, we are working on experiments to search appropriate conditions for SASA.

3PT114 中性膜に結合した LFampinB の膜結合構造と膜親和性の固体 NMR と QCM による解析

Structure and affinity of bovine lactoferrampin bind to neutral model membrane as studied by by solid state NMR and QCM

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Recently antimicrobial peptide is focus attention on a potential alternative for antibiotics. Analysis of membrane bound structure of peptide provides important information on efficiency and side effect of medicine.

Bovine lactoferrampin (LFampinB) is an antimicrobial peptide found in the N1-domain of bovine lactoferrin (268-284) and consists of 17 amino acid residues. Bovine lactoferrin (bLF) is an iron binding glyco protein with innate immunity factor in mammalian secretory fluid for example, tear saliva and milk.

In this study, the structure of LFampinB bound to the neutral membrane was determined using chemical shift oscillation analysis by observing the chemical