

Supporting Information

Nanofiber formation from sequence-selective DNA-templated self-assembly of a thymidylic acid-appended bolaamphiphile

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Sample Preparation

Thymidylic acid-appended bolaamphiphile **1** was synthesized by the phosphoramidite technique described with its stereochemistry in reference 10. Synthetic oligonucleotides **2**, **3**, **4**, and **5** were purchased from Fasmac Co (Kanagawa, Japan). Bolaamphiphile **1** was dissolved in a 0.1× TE buffer solution (1.0 mM tris-HCl and 0.1 mM EDTA, pH = 8.0) by sonication and heating at 90 °C for 30 min. Templates **2** and **3** were added to the solution and the solution was divided into three portions and gradually cooled to room temperature to form whitish viscous solutions. Solutions of either the target oligonucleotide (**4**) or a non-target oligonucleotide (**5**) in 0.1× TE buffer were added to each of two portions, and no oligonucleotide was added to the third portion. These three portions were kept at 20 °C for one day prior to analysis. The final concentrations of bolaamphiphile **1** and oligonucleotides **2**, **3**, **4**, and **5** were 1.8×10^{-2} M, 9.0×10^{-4} M, 9.0×10^{-4} M, 1×10^{-4} M, and 1×10^{-4} M, respectively.

AFM Observation

One microliter of each aqueous solution was placed on highly oriented pyrolytic graphite and dried in air for a few minutes. The specimen was then washed with 10 μ l of cold Millipore water 2 times and blotted with filter paper. Tapping-mode AFM was

carried out with a Nanonavi station and an S-image system (SII NanoTechnology Inc., Tokyo, Japan) using a silicon micro-cantilever (spring constant 40 N m^{-1} , frequency $\approx 120 \text{ kHz}$, Olympus).

UV melting curve measurements

Solutions of **1** alone, **1/2/3/4**, **1/2/3**, and **2/3/4** were prepared in $0.1\times$ TE buffer using the similar procedure described in sample preparation and subjected to UV melting experiments in a quartz cell ($l = 1.0 \text{ cm}$). The concentrations of **1**, **2**, **3**, and **4** were $3.6 \times 10^{-5} \text{ M}$, $1.8 \times 10^{-6} \text{ M}$, $1.8 \times 10^{-6} \text{ M}$, and $2 \times 10^{-7} \text{ M}$, respectively. The UV absorbance at 260 nm was measured with a UV-1800 spectrometer (Shimadzu Co., Kyoto, Japan) at a heating rate of $0.5 \text{ degC min}^{-1}$ after annealing at $10 \text{ }^\circ\text{C}$ for 30 minutes, and T_m analyses were conducted using a TMSPC-8 system (Shimadzu Co., Kyoto, Japan). T_m values were calculated from the first-derivative curves of the UV melting curve measurements as shown in Figure S1. The UV melting curve of the **1/2/3/5** system was obtained by the similar procedure described above and T_m was appeared at $57 \text{ }^\circ\text{C}$ as shown in Figure S2.

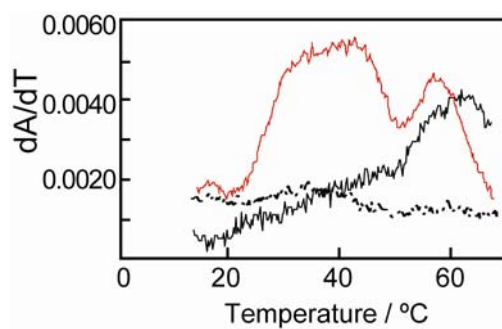


Figure S1 The first-derivative curves of the UV melting curves shown in Figure 3 for the **1/2/3/4** (red), **1/2/3** (black), and **2/3/4** (dotted) systems.

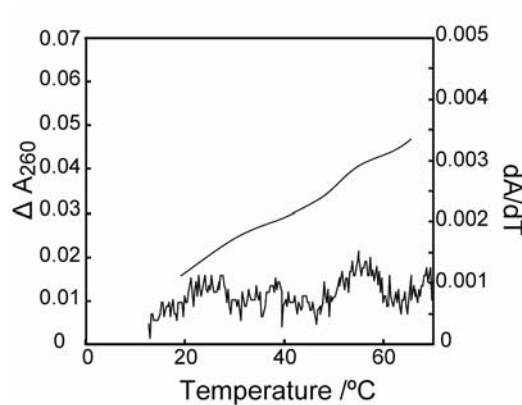


Figure S2 The melting and first-derivative curves of the **1/2/3/5** system in $0.1\times$ TE buffer solution.