Electronic Supplementary Material (ESI) for Chemical Communications

Polyelectrolyte-Assisted Transconformation of Stem-loop DNA

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Experimental Procedures

Materials: All oligonucleotides were supplied by FASMAC Co., Ltd. and purified by reverse-phase high performance liquid chromatography. Cationic comb-type copolymer PLL-*g*-Dex (Mn = 65,000) was prepared by a reductive amination reaction of PLL·HBr (Mn = 20,000, BACHEM) with dextran (Mn = 5,900, Dextran T-10, Amersham Pharmacia Biotech) as described previously.[1] The dextran content of the copolymer was 91 wt% as determined by ^{1}H NMR. DNA samples were treated by annealing (heating to 90 ^{o}C for 5 min and quick cooling on ice).

Native polyacrylamide gel electrophoresis: DNA solutions were prepared in 10 mM sodium phosphate buffer (pH 7.2) containing 0.5 mM EDTA and 150 mM NaCl with or without PLL-*g*-Dex. DNA samples were incubated at 37 ^{o}C for 1 h or 3 h. Native PAGE (13%) was performed in TBE buffer at 25 ^{o}C for 2 h at 100 V. After electrophoresis, the gel was stained with 0.01% EtBr.

Fluorescence spectroscopy: The DNA solution was dissolved in sodium phosphate buffer (10 mM sodium phosphate, 0.5 mM EDTA, 150 mM NaCl, pH 7.2). Baseline emission values were first recorded for about 5 minutes, and then PLL-*g*-Dex and PVS were successively added to the DNA solution with a syringe. The change in fluorescence intensity of the mixture (total volume 2 ml) in a 10 mm-square quartz cuvette was recorded on a JASCO FP-6500 fluorescence spectrometer (JASCO) with a Peltier thermostatically controlled cell holder at excitation and emission wavelengths of 540 nm and 570 nm, respectively.

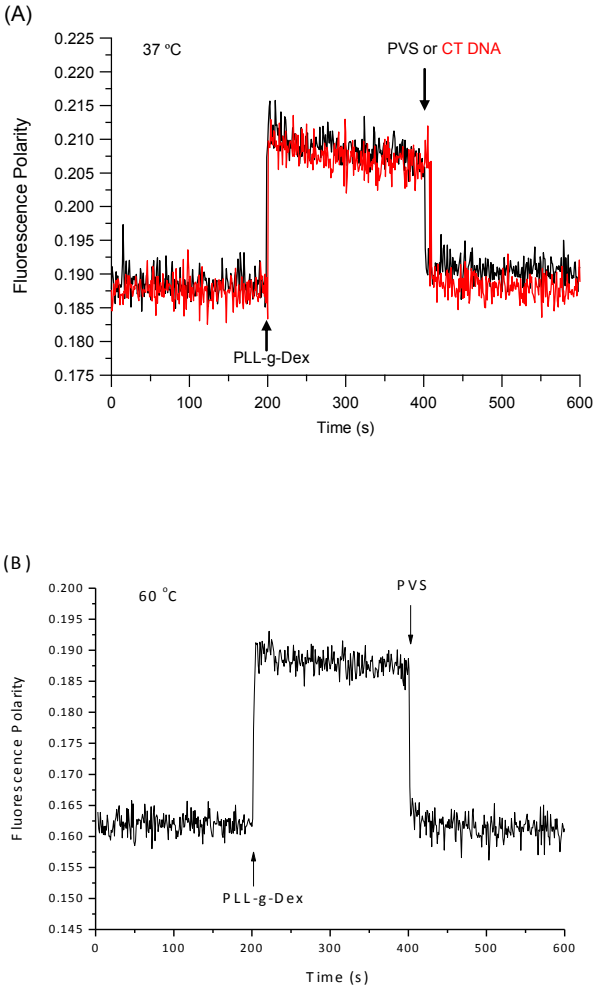
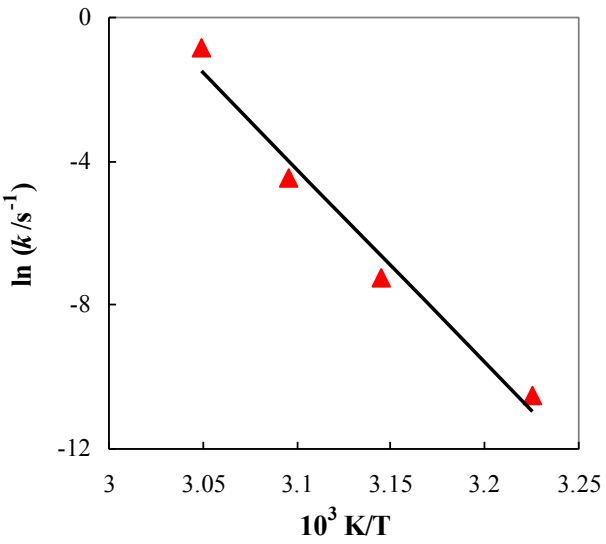


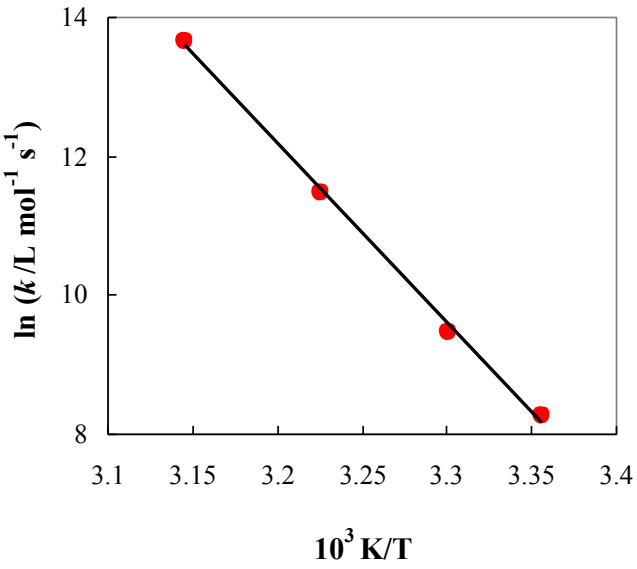
Figure S1. Effect of polyelectrolyte on the fluorescence polarity of TAMRA-labeled duplex. Experiments were performed at (A) 37 °C and (B) 60 °C in 10 mM sodium phosphate buffer (pH 7.2) containing 150 mM NaCl and 0.5 mM EDTA. Final concentration of fluorescently labeled DNA duplex (20 bp) was 50 nM. The solution was excited at 540 nm and fluorescence emission was monitored at 570 nm. PLL-*g*-Dex (*N*/*P* = 1) and PVS or calf thymus (CT) DNA (1.2 times charge concentration) were added sequentially.

A)



*E*a = 447 kJmol^{-1}

B)



*E*a = 215 kJmol^{-1}

Figure S2. Arrhenius plots for A) spontaneous dissociation of DIS25 dimer and B) PLL-g-dex-assisted dimerization of DIS25

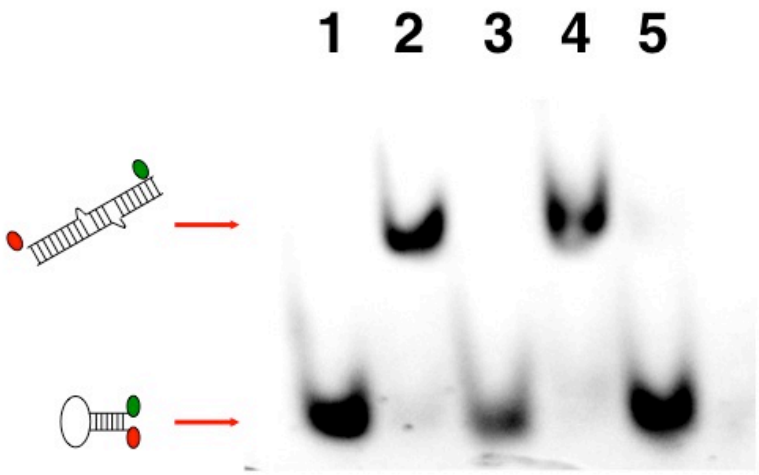


Figure S3. Gel electrophoretic analysis to confirm transconformation between dimer and monomeric stem-loop structures of DIS25 in response to successive addition of PLL-g-Dex and PVS. Gel images were acquired after EtBr staining. Lane 1: DNA alone, Lane 2: 1st PLL-*g*-Dex addition, Lane 3: 1st PVS addition, Lane 4: 2nd PLL-g-Dex addition, Lane 5: 2nd PVS addition.

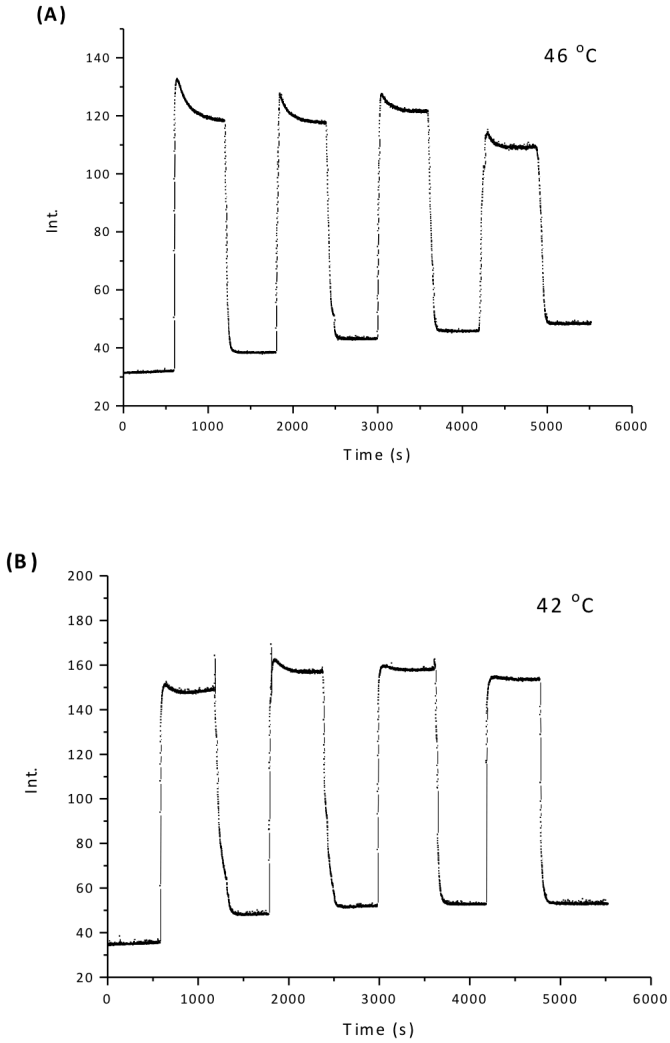


Figure S4. Polyelectrolyte-assisted transconformation of DIS derivatives. Final concentration of DNA was 50 nM. FRET assay was performed at indicated temperatures in 10 mM sodium phosphate buffer (pH 7.2, 0.5 mM EDTA, 150 mM NaCl). PLL-*g*-Dex and PVS were added successively. (A) [DIS25-2a]:[T-DIS25-2a-D] = 39:1 mixture at 46 ºC, (B) [DIS25-3a]:[T-DIS25-3a-D] = 39:1 mixture at42 ºC.