Supplementary Material (ESI) for Chemical Communications

Supporting Information

Formation and stabilization of G-quadruplex in nanosized water pool

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1. Materials and methods

1.1. Materials

The high performance liquid chromatography (HPLC) purification grade DNA oligonucleotides and fluorophore-labeled DNA oligonucleotides, 5′-GGG(TTAGGG)$_3$-3′ and 5′-FAM-GGG(TTAGGG)$_3$-TAMRA-3′ (Donor fluorophore FAM: 6-carboxyfluorescein; acceptor fluorophore TAMRA: 6-carboxy-tetramethylrhodamine), were purchased from Sangon (Shanghai, China) and TaKaRa Biotech (Dalian, China), respectively. The strand concentrations were determined by measuring the absorbance at 260 nm at a high temperature, using the extinction coefficient values obtained in the web (http://scitools.idtdna.com/analyzer/Applications/oligoanalyzer/). AOT was purchased from Sigma Aldrich (>99% purity) and used without any further purification. HPLC quality of isooctane (2,2,4-trimethyl pentane, Kermel, Tianjin) was used as received. Water used in all the experiments was distilled and deionized using a Milli-Q A10 water purification system.

1.2. Sample preparation

To make nucleic acids micellar solutions at a concentration of 100 mM AOT and a w_0 20 ([H_2O]/[AOT]), AOT solution (100 mM) was prepared first by dissolving the appropriate mass of AOT in isooctane, then added the proper amounts of water and shaken vigorously for several minutes. Afterwards, aliquots of the stock nucleic acid solution were directly injected into AOT/isooctane/water reverse micelles (the final w_0 20 was achieved by adjusting the amounts of water) and shook until a clear

solution resulted. Control samples of nucleic acids in bulk buffer containing 150 mM Na^+ or K^+ were prepared by heating to 90 ^oC for 5 min, then cooling slowly to room temperature before use except otherwise stated.

1.3. CD spectroscopy

CD spectra were obtained on a Jasco J-810 spectropolarimeter (JASCO, Japan). Samples were prepared as described above before collecting CD spectra. The CD spectra were obtained in a 0.1 cm path length cuvette by taking the average of three scans recorded from 220 to 320 nm at a scanning rate of 50 nm/min at room temperature. A background CD spectrum was subtracted from the average scan for each sample.

1.4. Fluorescence spectroscopy

Fluorescence spectra were taken on a spectrofluorometer model FLS 920 (Edinburgh Analytical Instruments, U.K.) at room temperature. Spectra were collected from 500 to 700 nm while exciting at 480 nm, with the excitation and emission slits being 2 and 2 nm, respectively. In these measurements, the path lengths of the quartz cell used were 0.2 cm in the excitation direction and 1 cm in the emission direction. The contribution from direct excitation of TAMRA was neglected. All emission spectra were corrected with background fluorescence and instrument response.

1.5. UV spectroscopy

UV absorption was carried out on a Shimadzu 2450 spectrophotometer (Shimadzu, Japan) and UV melting experiments were on the same machine equipped with a

Peltier temperature control accessory. All UV/Vis spectra were measured in a sealed quartz cell with a path length of 1.0 cm. The samples were treated as described above before collecting UV spectra. Melting curves of samples were measured at 295 nm with the temperature gradient of 1 ^{o}C /min.

Fig. S1

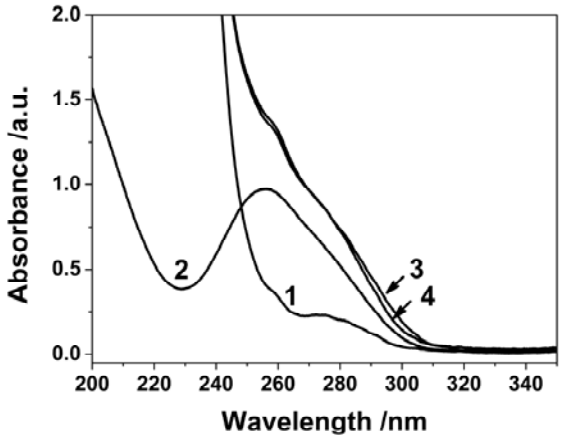

Fig. S1 Absorption spectra of the DNA-free reverse micelles (1), DNA in bulk water (2) and solubilized in the reverse micelles (w_o = 20) (3). The sum of the absorbance value of DNA in bulk water and that of DNA-free reverse micelles (4).

Fig. S2

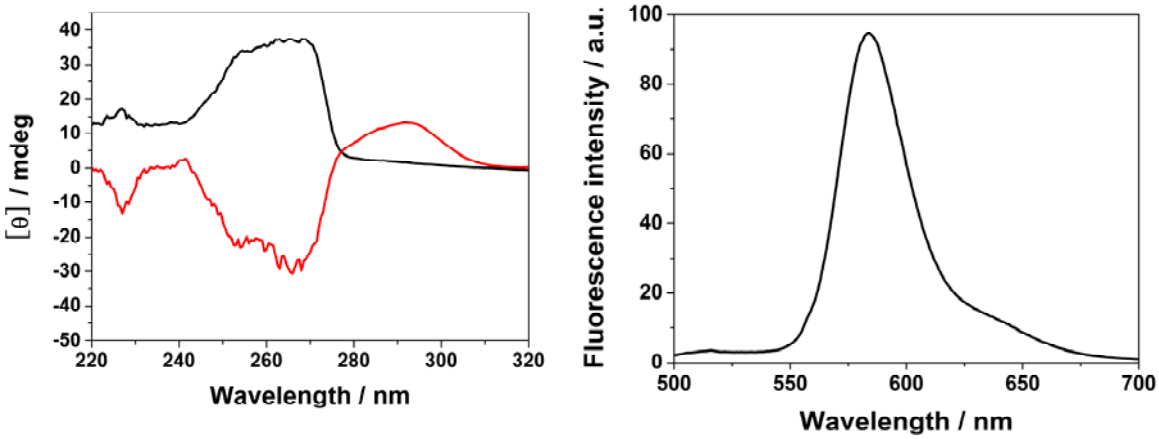

Fig. S2 (left) CD spectra of DNA-free reverse micelles (baseline, black) and 4 μM HTS in the water pool of reverse micelles formed by CTAB (cyltrimethylammonium bromide, w_o = 20, decane:hexanol, 6:1, v/v red). The spectrum of HTS is strange because the reverse micelles has strong absorption below 280 nm (maybe results from the contamination), therefore, the baseline cannot be deducted well. The experiments were performed in OLIS CD instrument and using 1 cm path length cuvette. **(right)** The fluorescence spectra of 100 nM HTS in the water pool of reverse micelles formed by CTAB (cyltrimethylammonium bromide, w_o = 20, decane:hexanol, 6:1, v/v).

Fig. S3

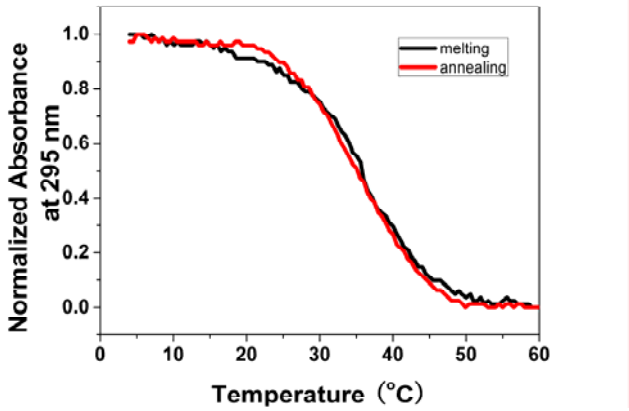

Fig. S3 The melting and annealing curves of HTS at 295 nm in bulk water.

Fig. S4

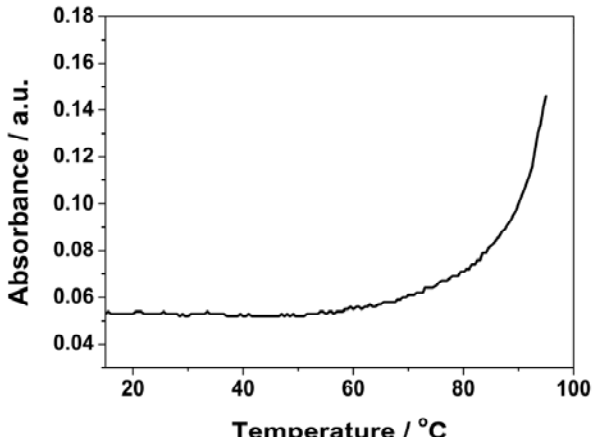

Fig. S4 The absorption spectrum of AOT reverse micelles (w_o = 20) at 295 nm in the absence of DNA as the increasing temperature.

Fig.S5

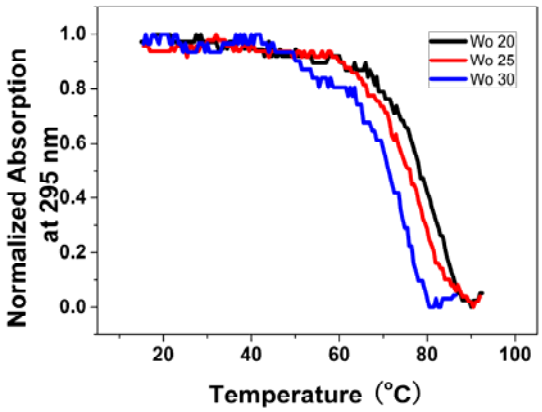

Fig. S5 The melting curves of HTS at 295 nm in the reverse micelles (w_o = 20, 25 and 30).