Supporting Information

DNA tetraplex structure formation from human telomeric repeat motif (TTAGGG):(CCCTAA) in nanocavity water pools of reverse micelles

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Materials and Methods

Oligonucleotides and buffer. High performance liquid chromatography (HPLC) purification grade oligonuleotides d[AGGG(TTAGGG)$_3$] and d[(CCCTAA)$_3$C CCT] were purchased from Hokkido System Science (Sapporo, Japan). Single strand concentrations of oligonucleotides were determined by measuring the absorbance at 260 nm at a high temperature using a Simadzu 1700 spectrophotometer (Shimadzu, Kyoto, Japan) connected to a thermoprogrammer. Single strand extinction coefficients were calculated from mononucleotide and dinucleotide data using the nearest-neighbour approximation. [#E. G. Richards, Use of tables in calculation of absorption, optical rotator dispersion and circular dichroism of polyribonucleotides. #G. D. Fasman, Ed. Handbook of Biochemistry and Molecular Biology, 3rd ed., CRC Press: Cleveland, OH, 1975; Vol. 1, pp 596-603.]. The surfactant, bis(2-ethylhexyl)sulfosuccinate (AOT) was Sigma product and used without further purification. Isooctane was purchased from Wako Chemicals.

Preparation of reverse micelle encapsulated DNA samples. AOT reverse micelle (AOT RM) encapsulated DNA samples were prepared as follows. Required amount of surfactant, AOT was dissolved in isooctane to prepare fresh 0.1 M solution. 250 μM DNA stock solutions were prepared in a buffer containing 10 mM sodium phosphate (pH 7.0), 10 mM NaCl, and 1 mM Na_2EDTA. 32 μl of stock DNA solutions were then injected to 2 ml 0.1 M AOT solution followed by the addition of required amount of the buffer, which was used to prepare stock DNA solution to achieve desired ω (10, 20, and 30). The solutions were then stirred for several minutes and resulting transparent solutions were used for further studies. The interior water pools of AOT RM used in this study with ω values of 10, 20, and 30 have diameters of 38, 68, and 98 Å, respectively. [J. Zhou, C. Wei, G. Jia, X. Wang, Z. Feng and C. Li, *Chem. Comm*., 2010, **46**, 1700–1702] It is important to note that the water pool of AOT RM throughout this work were a buffer containing 10 mM sodium phosphate (pH 7.0), 10 mM NaCl, and 1 mM Na_2EDTA except otherwise stated. In 2 ml solution the resulting concentrations of DNAs were 4μM. Reference DNA samples in bulk dilute conditions were prepared by dissolving the stock DNA solutions in the same buffer, which was used to prepare stock solution.

Circular dichroism (CD) measurements. CD experiments utilized a JASCO J-820 spectropolarimeter (JASCO, Japan) and were performed at different temperatures in a 1.0-

mm path length cuvette at 4 μM total strand concentration of nucleic acid. The CD spectra shown are the average of at least three scans measured from 240 to 350 nm at a scan rate of 50 nm min^{-1}. The temperature of the cell holder was regulated by a JASCO PTC-348 temperature controller, and the cuvette-holding chamber was flushed with a constant stream of dry N_2 gas to avoid condensation of water on the cuvette exterior. Before measurement, samples were heated to 95 °C, cooled at a rate of 1 °C min^{-1}, and incubated at 5 °C for 1 hour. Thermal denaturation of all the structures were measured both in the dilute and reverse micellar conditions at indicated wavelengths. The heating rates were 0.5 °C min^{-1}.

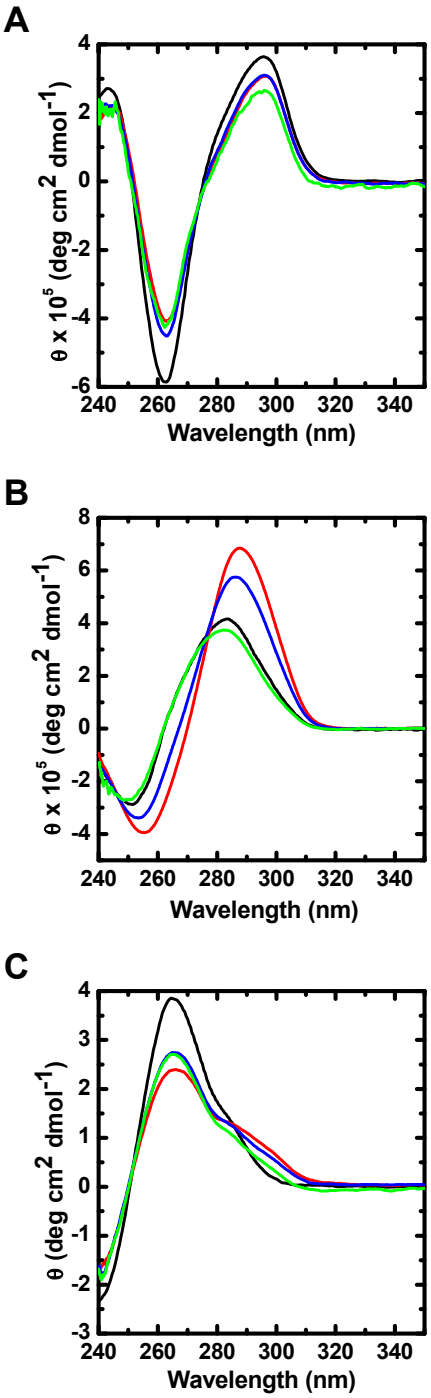

Fig. S1 CD spectra at 5 °C of **(A)** 4 μM 22AG, **(B)** 4 μM 22CT, and **(C)** 2 μM 22AG + 2 μM 22CT in dilute solution (black) and in AOT RMs with ω = 10 (red), ω = 20 (blue), and ω = 30 (green).

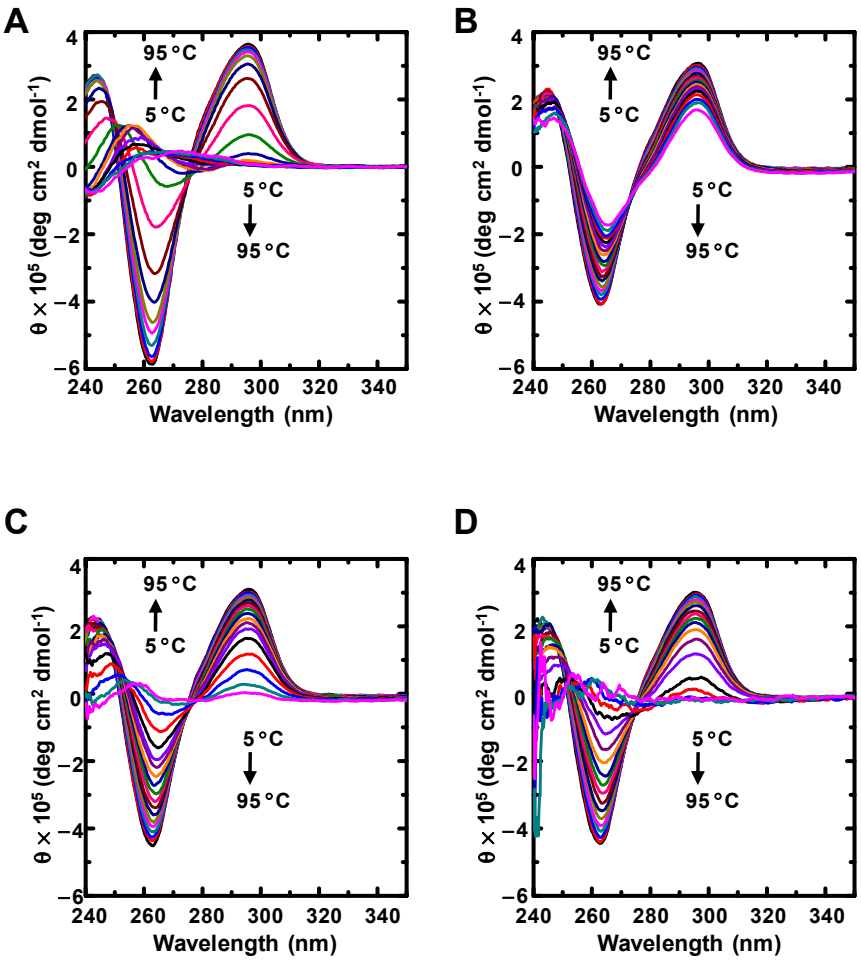

Fig. S2 CD spectra of 4 μM 22AG in **(A)** dilute solution and in AOT RMs at **(B)** ω = 10, **(C)** ω = 20, and **(D)** ω = 30 at temperatures from 5 °C to 95 °C.

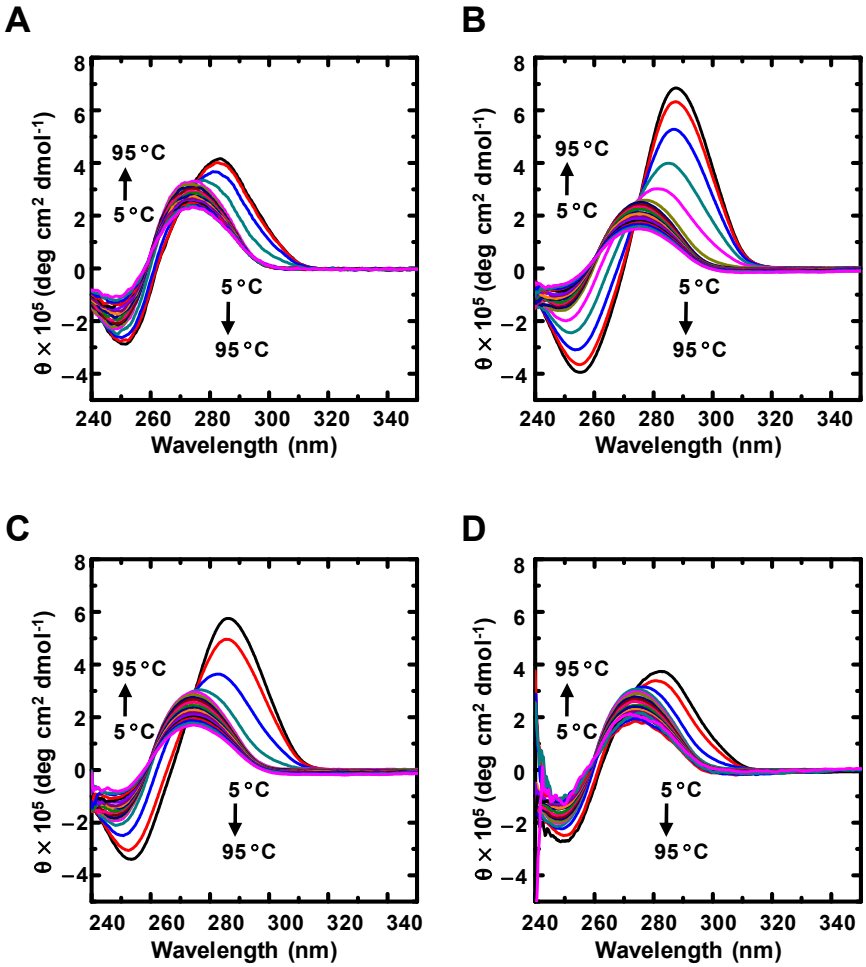

Fig. S3 CD spectra of 4 μM 22CT in **(A)** dilute solution and in AOT RMs at **(B)** ω = 10, **(C)** ω = 20, and **(D)** ω = 30 at temperatures from 5 °C to 95 °C.

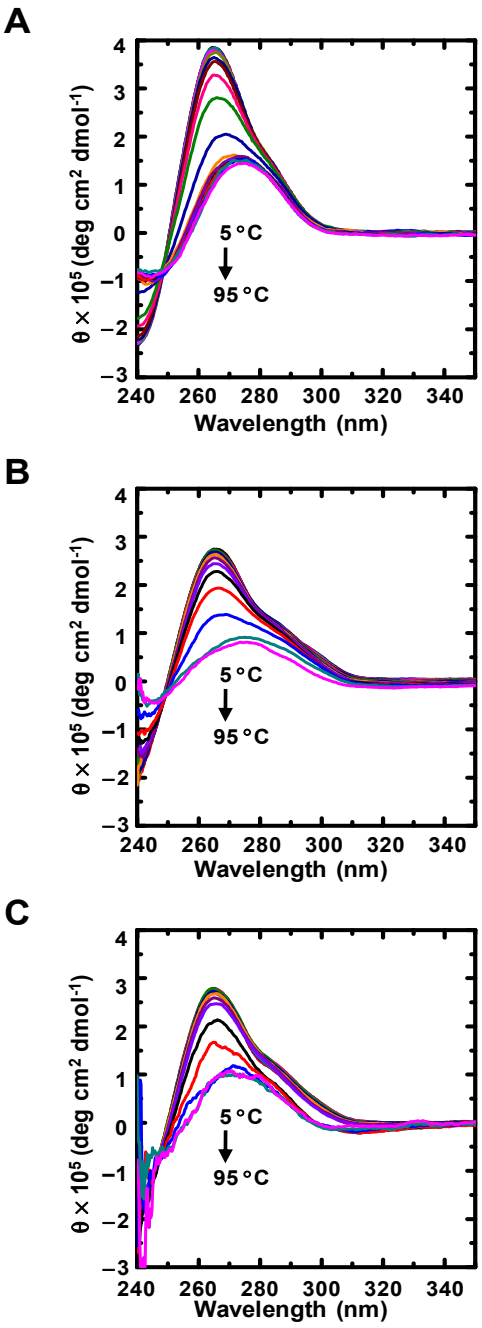

Fig. S4 CD spectra of 4 μM total strand concentration of the equimolar mixture of 22AG and 22CT in **(A)** dilute solution and in AOT RMs at **(B)** ω = 20 and **(C)** ω = 30 at temperatures from 5 °C to 95 °C.

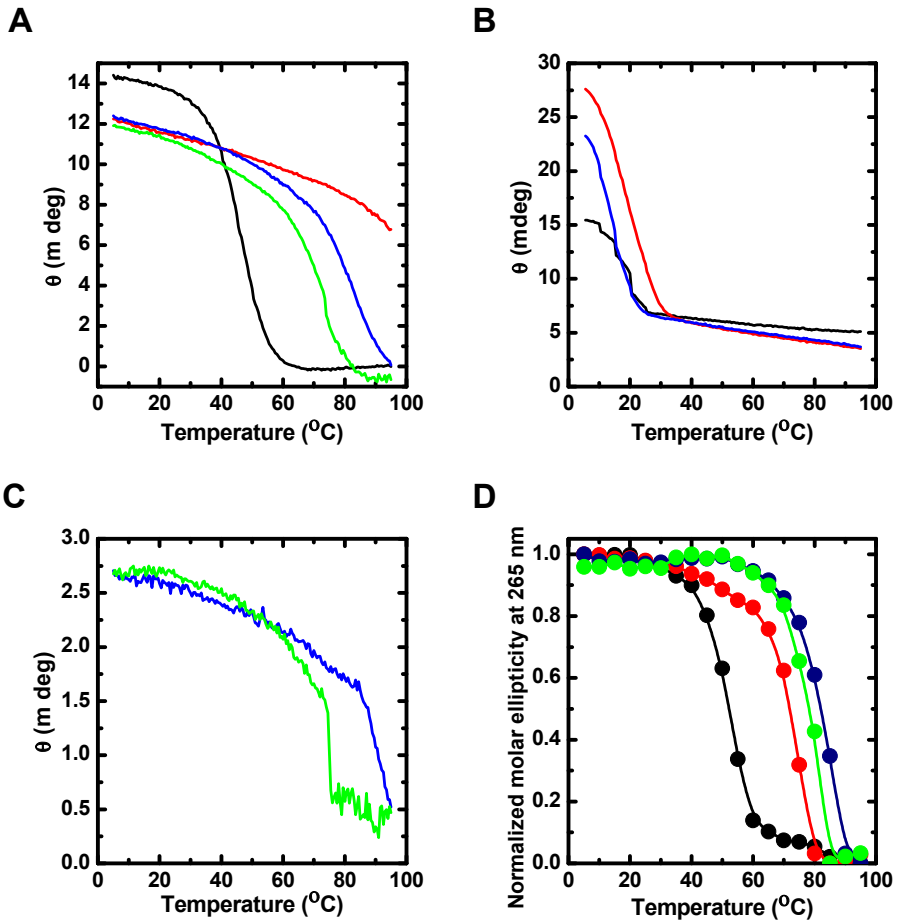

Fig. S5 CD melting curves of **(A)** 4 μM 22AG at 295 nm, **(B)** 4 μM 22CT at 287 nm, **(C)** 2 μM 22AG + 2 μM 22CT at 295 nm, and **(D)** 2 μM 22AG + 2 μM 22CT at 265 nm in dilute solution (black) and in AOT RMs at ω = 10 (red), ω = 20 (blue), and ω = 30 (green).