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Supporting Information

Cationic and Anionic Reverse Micelles as the Molecular Crowding Container for G-quadruplex Structure

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Materials and Methods

Materials

The high performance liquid chromatography purified human teleomere sequence (5′-$AG_3(T_2AG_3)_3$, the Hum 22) was purchased from Sigma Aldrich and was used without further purification. The CTAB (BioXtra, >99%), AOT (BirXtra, >97%), TMPyP4 (>97%), NaCl (BioXtra, >99.5%) and KCl (For molecular biology, >99%) were also purchased from Sigma Aldrich and were used as received. The CTAC was purchased from Alfa Aser (96%). The isooctane (>99%) and 1-hexanol (>99%) were purchased from Macron™ and Alfa Aser, respectively. The deionized water (resistivity>18.2 MΩ-cm at 25°C) was obtained from Barnstead™ EasyPure™ II water purification system (Thermo Scientific™) and was used in all experiments.

Sample preparation

DNA preparation

The Hum 22 was dissolved in deionized water. The single strand concentration of oligonucleotide was estimated by measuring the absorbance at 260 nm (ε=228500 M^{-1} cm^{-1}). After determining the concentration of oligonucleotide, the proper volume of high concentration oligonucleotide was added to the Tris buffer solution (10 mM tris, pH=7.4) or the buffers that containing Na^+ or K^+ ions. The samples were heated to 95°C for 10 minutes and slowly cooled down to the room temperature. After cooling down to the room temperature, the samples were stored in the 4˚C refrigerator for at least 8 hours to ensure the formation of G-quadruplex structure.

Preparation of DNA encapsulated reverse micelles.

The cationic or anionic surfactants were dissolved in organic solvents (0.1M AOT in isooctane, 0.2 M CTAB and CTAC in isooctane: 1-hexanol=7:1 solution). The proper amounts of buffer or highly concentrate nucleic acid stock solution were directly injected into the solution (ω=20 in AOT, ω=25 in CTAB and ω=20 in CTAC RMs) and sonicated for 1 hr. In RMs, the finial concentration of DNA was control at 2 μM.

CD spectroscopy

The CD spectra were obtained using Jasco J-810 spectropolarimeter (JASCO, Japan). The spectra were obtained in a 1 cm path length quartz cuvette. The temperature was controlled at 25°C using temperature accessory (JASCO, PTC-423S). The spectra were recorded from 220 to 350 nm at a scanning rate of 100 nm/min. Each spectrum was scanned three times and the background CD spectrum was subtracted.

UV-Vis steady state spectra, melting curve and Job plot analysis

The UV-Vis absorption spectra were obtained using a Cary 100 spectrophotometer (Cary-100, Agilent) with 1 cm quartz cuvette. The temperature of the samples was

controled with a peltier thermostatted multicell holder accessory. The melting curves of the samples were monitored at 295 nm and increasing with the temperature gradient of 0.4˚C/nm. For the Job plot measurements, the temperature of the samples were controlled at 25˚C, and the total concentration of the Hum 22+TMPyP4 was 2μM in buffer or 20% PEG 400 and 1μM in CTAB RMs.

Estimation of the concentration of free Na^+ ions in AOT RMs

For the AOT RMs (ω=20), the hydrodynamics radius is 6 nm, considering the thickness of the surfactant monolayer is ~1 nm, the radius of the central water pool is ~5 nm, which corresponds to the volume of 5.24×10^{-22} liter. Because each droplet is composed of ~300 surfactants, the concentration of the total available Na^+

$$= \frac{300}{6.02 \times 10^{23}} \times \frac{1}{5.24 \times 10^{-22}} = 0.95\,\mathrm{M}$$

According to the MD simulation result, about 16 % of Na^+ ions (~150 mM) is free dissociated in ω=10 AOT RMs. Since the percentage of the dissociated Na^+ will also increase with the ω, we expected that the concentration of the dissociated Na^+ in ω=20 AOT RMs should be in the range between 200~300 mM, which is comparable to the 300 mM Na^+ ions we used.

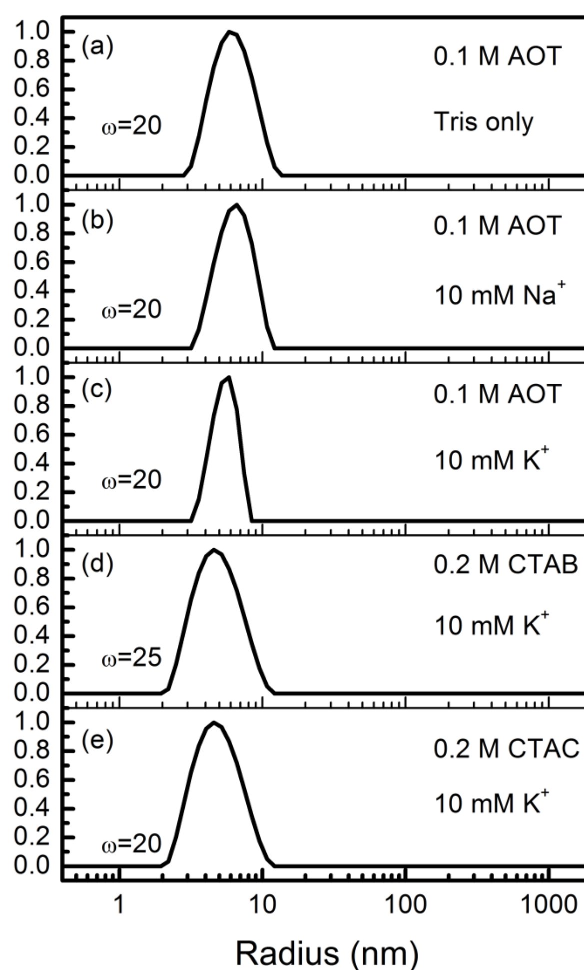

Figure S_1: The size distribution of (a-c) AOT, (d) CTAB and (e)CTAC reverse micelles. As depicted, the hydrodynamic radius of the reverse micelle was ~6 nm in all cases.

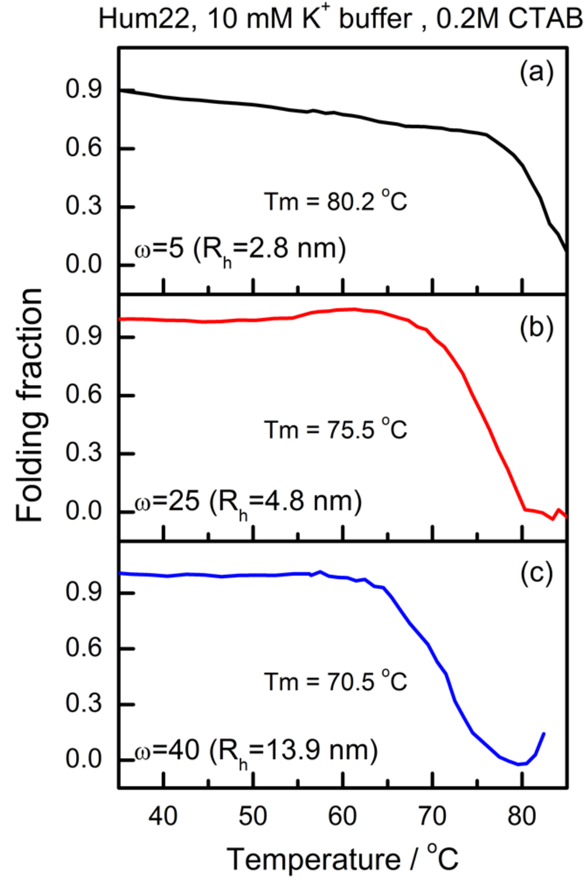

Figure S_2: The melting curve of Hum 22 in (a) ω=5 (b) ω=25 (c) ω=40 CTAB RMs. The hydrodynamics radius (R_h) was estimated by the DLS method.

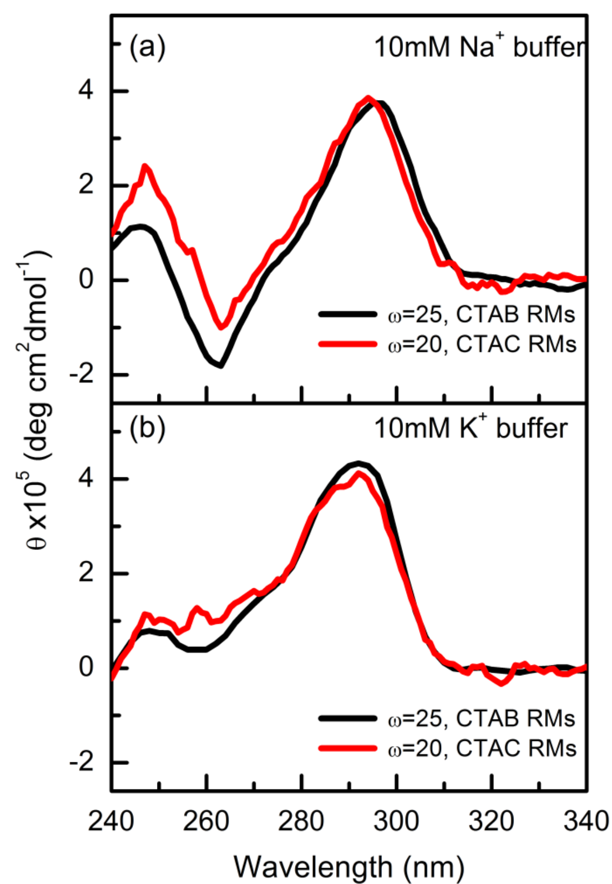

Figure S_3: The CD spectra of Hum 22 in CTAB (black) and CTAC (red) RMs containing 10 mM (a) NaCl and (b) KCl Tris buffer solutions.

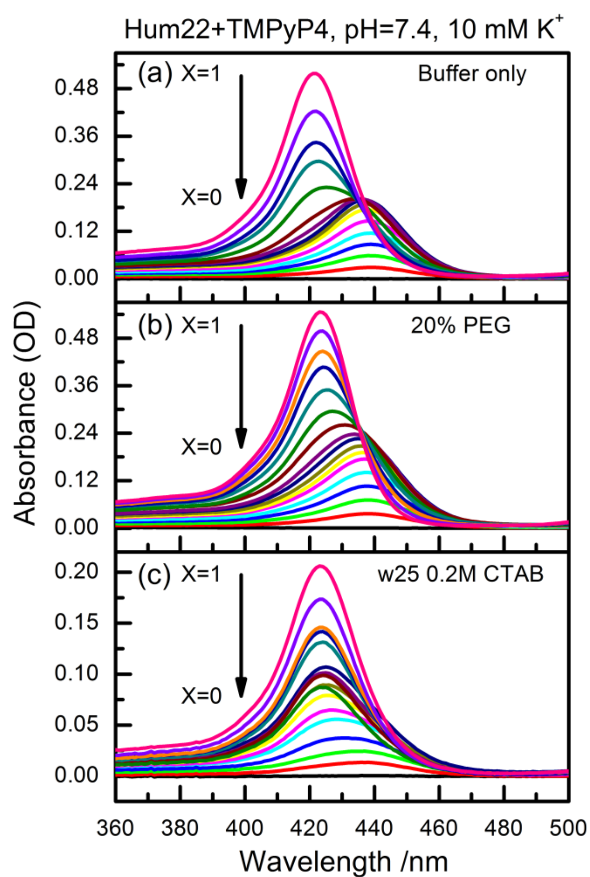

Figure S_4: The absorption spectra of TMPyP4 binding with different mole fraction of Hum 22 in (a) Buffer (b) 20% PEG 400 and (c) CTAB RMs.

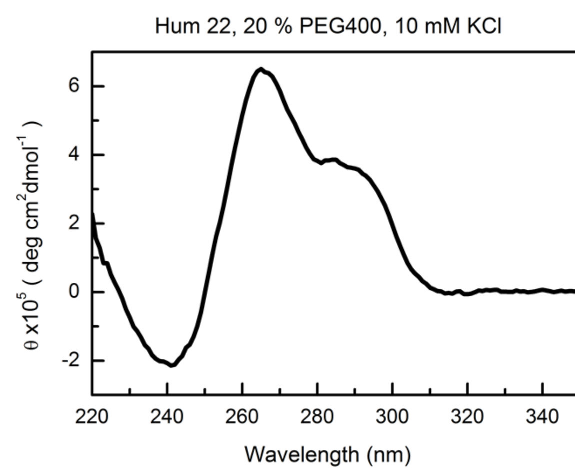

Figure S_5: The CD spectrum of Hum 22 in 20 % PEG400 solution.