

## Supporting Information Available for

**Design and Synthesis of A Stable Supramolecular Trigonal Prism Formed by the Self-Assembly of A Linear Tetrakis( $\text{Zn}^{2+}$ -cyclen) Complex and Trianionic Trithiocyanuric Acid in Aqueous Solution and Its Complexation with DNA (Cyclen = 1,4,7,10-Tetraazacyclododecane).**

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**Page 3: Figure S1.** (a) UV spectral change in supramolecular trigonal prism **7** (10  $\mu\text{M}$ ) in the absence (bold curve) and upon the addition of succinimide (0~100 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  ( $\text{NaNO}_3$ ) at 25  $^\circ\text{C}$ . (b) UV spectral change of supramolecular trigonal prism **5** (10  $\mu\text{M}$ ) in the absence (bold curve) and upon the addition of succinimide (0~100 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  ( $\text{NaNO}_3$ ) at 25  $^\circ\text{C}$ . (c) Absorption change at 323 nm of **7** (open circle) and **5** (close circle) upon additional of succinimide

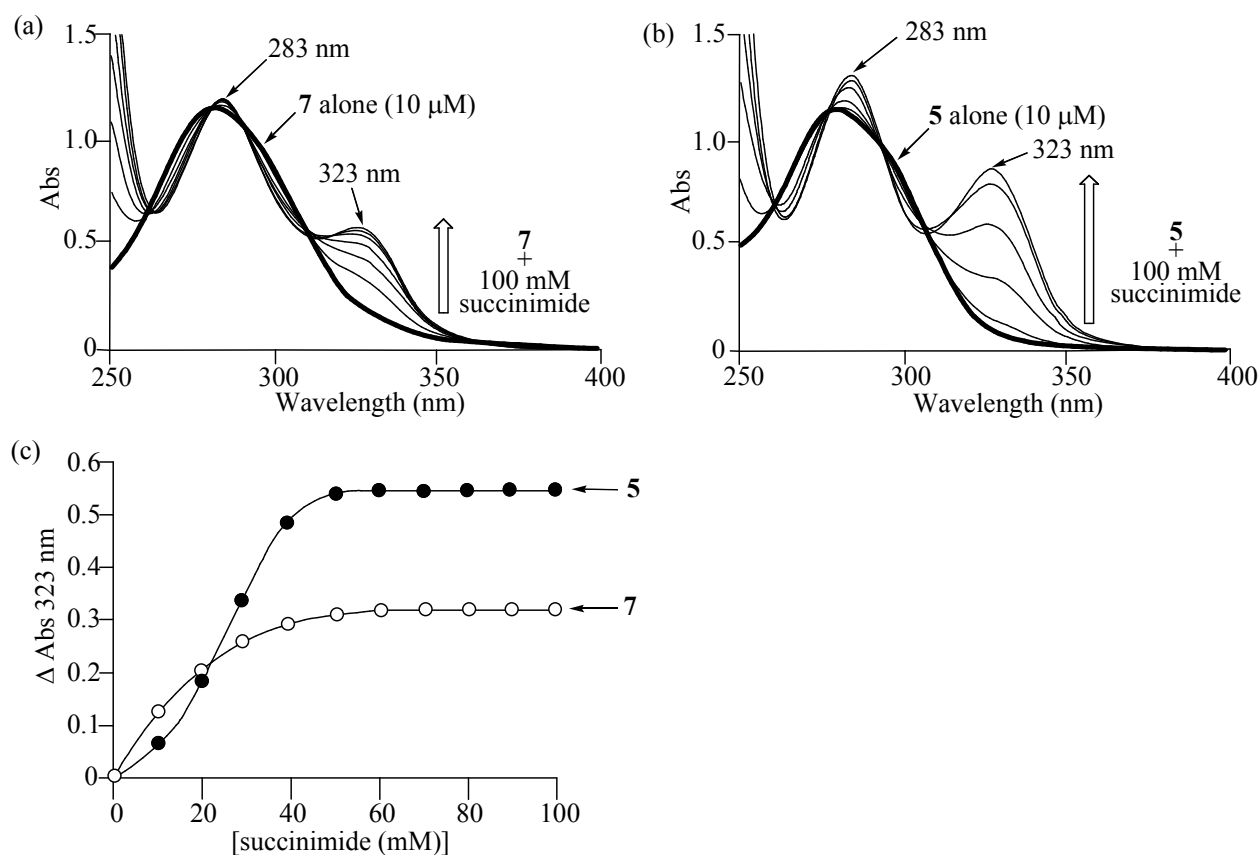
(0~100 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  ( $\text{NaNO}_3$ ) at 25 °C.

**Page 4: Figure S2.** (a) UV spectral change in supramolecular trigonal prism **7** (10  $\mu\text{M}$ ) in the absence (bold curve) and upon the addition of dithiothreitol (0~10 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  ( $\text{NaNO}_3$ ) at 25 °C. (b) UV spectral change in supramolecular trigonal prism **5** (10  $\mu\text{M}$ ) in the absence (bold curve) and upon the addition of dithiothreitol (0~10 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  ( $\text{NaNO}_3$ ) at 25 °C. (c) Absorption change at 323 nm in **7** (open circle) and **5** (close circle) upon the additional of dithiothreitol (0~10 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  ( $\text{NaNO}_3$ ) at 25 °C.

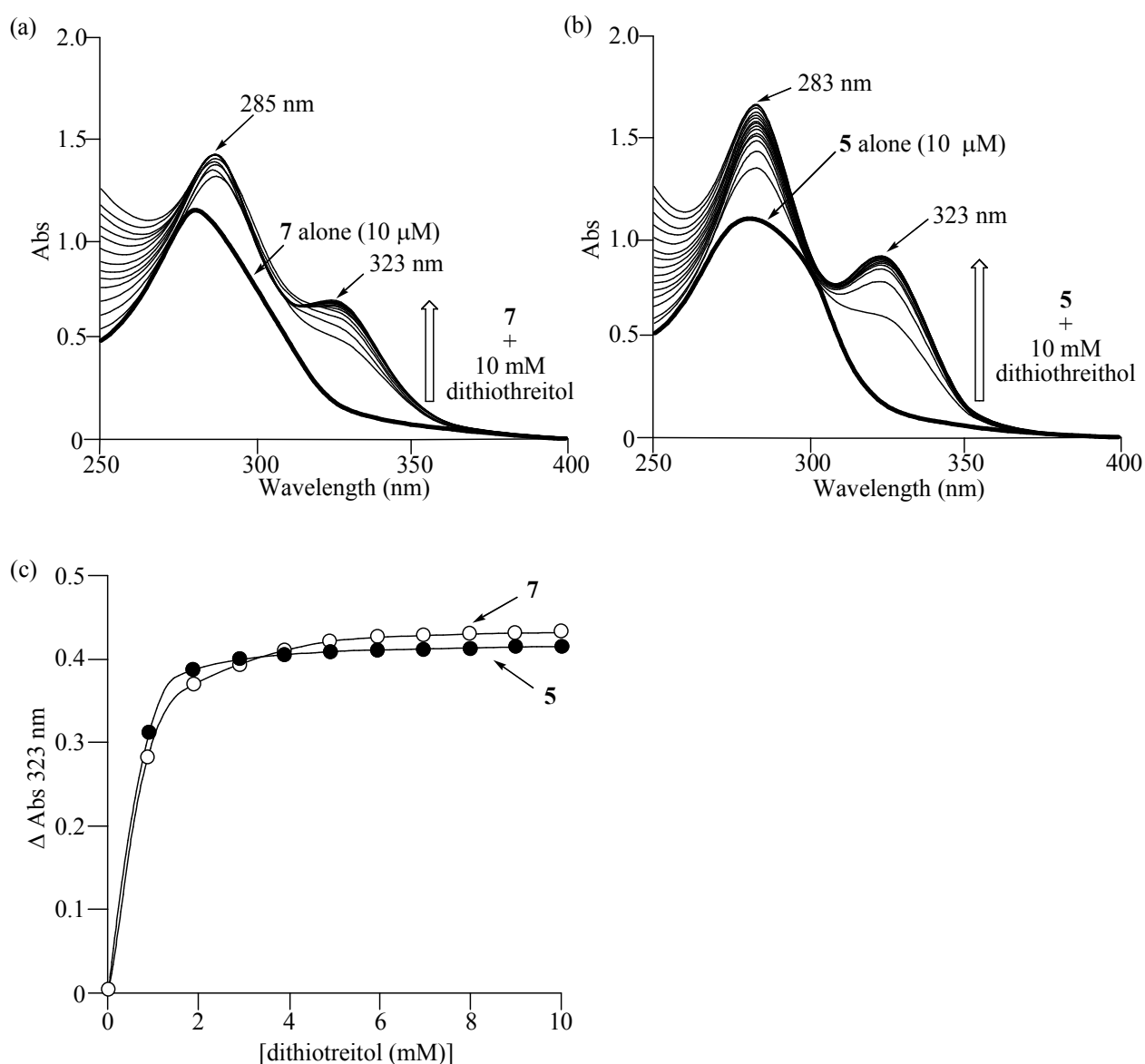
**Page 5: Figure S3.** Particle diameter distribution of ctDNA in intensity by dynamic light scattering (DSL) upon the addition of **7** and DNA-binders. (a) 100  $\mu\text{M}$  (in phosphate) ctDNA, (b) EB + ctDNA (plain curve), pentamidine + ctDNA (bold curve), and spermine + ctDNA (dashed curve), and (c) **7** + ctDNA, in 10 mM HEPES (pH 7.4) with  $I = 0.02$  ( $\text{NaNO}_3$ ) at 25 °C and  $r = 0.1$  ( $r = [\text{additive}]/[\text{ctDNA in phosphate}]$ ).

**Page 6: Figure S4.** Circular dichroism (CD) spectra of ctDNA in the absence and presence of prism **7** and DNA-binders: 100  $\mu\text{M}$  (in phosphate) ctDNA (bold curve), ctDNA + pentamidine (dashed curve), ctDNA + spermine (plain curve), and ctDNA + **7** (bold dashed curve), in 10 mM HEPES (pH 7.4) with  $I = 0.02$  ( $\text{NaNO}_3$ ) at 25 °C and  $r = 0.1$  ( $r = [\text{additive}]/[\text{ctDNA in phosphate}]$ ).

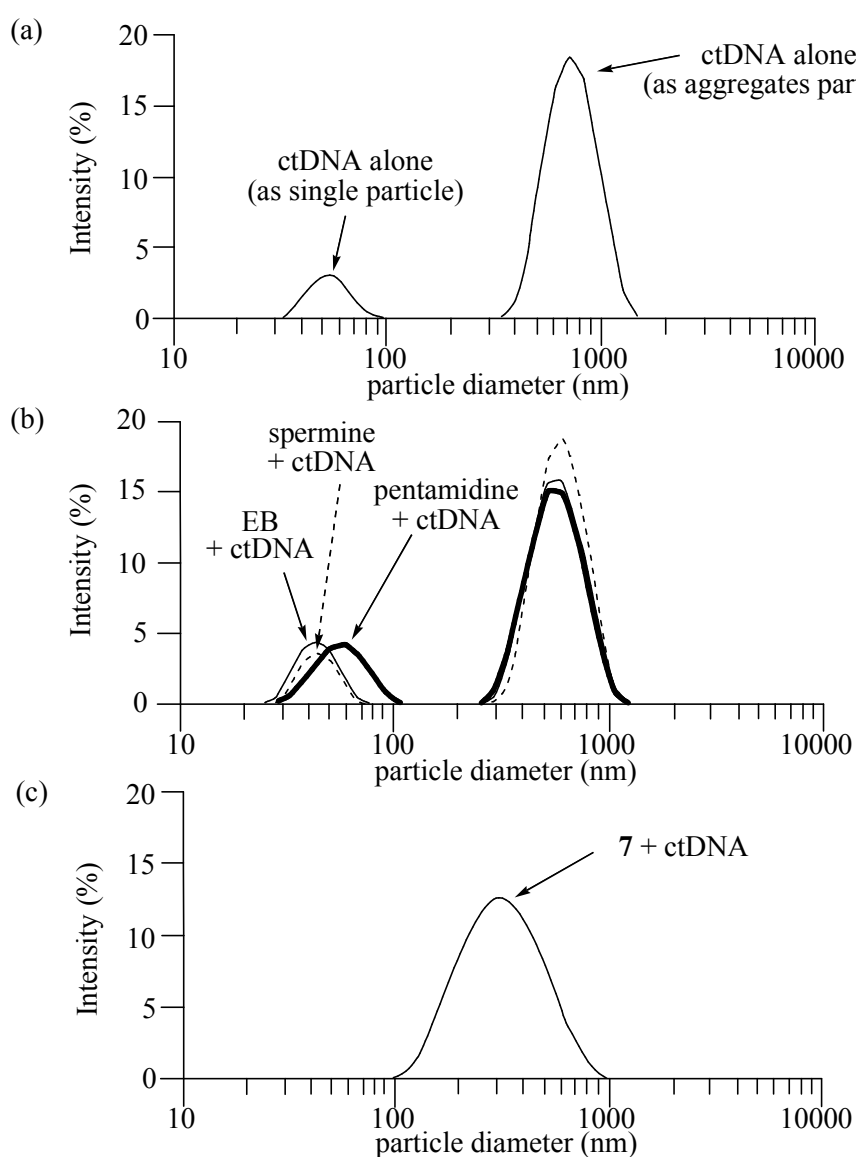
**Figure S1.** (a) UV spectral change in supramolecular trigonal prism **7** (10  $\mu\text{M}$ ) in the absence (bold curve) and upon the addition of succinimide (0~100 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  ( $\text{NaNO}_3$ ) at 25  $^\circ\text{C}$ . (b) UV spectral change in supramolecular trigonal prism **5** (10  $\mu\text{M}$ ) in the absence (bold curve) and upon the addition of succinimide (0~100 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  ( $\text{NaNO}_3$ ) at 25  $^\circ\text{C}$ . (c) Absorption change at 323 nm in **7** (open circle) and **5** (close circle) upon the additional of succinimide (0~100 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  ( $\text{NaNO}_3$ ) at 25  $^\circ\text{C}$ .



**Figure S2.** (a) UV spectral change in supramolecular trigonal prism **7** (10  $\mu$ M) in the absence (bold curve) and upon the addition of dithiothreitol (0~10 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  (NaNO<sub>3</sub>) at 25  $^{\circ}$ C. (b) UV spectral change in supramolecular trigonal prism **5** (10  $\mu$ M) in the absence (bold curve) and upon the addition of dithiothreitol (0~10 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  (NaNO<sub>3</sub>) at 25  $^{\circ}$ C. (c) Absorption change at 323 nm of **7** (open circle) and **5** (close circle) upon the additional of dithiothreitol (0~10 mM) in 10 mM HEPES (pH 7.4) with  $I = 0.1$  (NaNO<sub>3</sub>) at 25  $^{\circ}$ C.



**Figure S3.** Particle diameter distribution of ctDNA in intensity by dynamic light scattering (DSL) upon the addition of **7** and DNA-binders. (a) 100  $\mu\text{M}$  (in phosphate) ctDNA, (b) EB + ctDNA (plain curve), pentamidine + ctDNA (bold curve), and spermine + ctDNA (dashed curve), and (c) **7** + ctDNA, in 10 mM HEPES (pH 7.4) with  $I = 0.02$  ( $\text{NaNO}_3$ ) at 25  $^\circ\text{C}$  and  $r = 0.1$  ( $r = [\text{additive}]/[\text{ctDNA in phosphate}]$ ).



**Figure S4.** Circular dichroism (CD) spectra of ctDNA in the absence and presence of prism **7** and DNA-binders: 100  $\mu\text{M}$  (in phosphate) ctDNA (bold curve), ctDNA + pentamidine (dashed curve), ctDNA + spermine (plain curve), and ctDNA + **7** (bold dashed curve), in 10 mM HEPES (pH 7.4) with  $I = 0.02$  ( $\text{NaNO}_3$ ) at 25  $^\circ\text{C}$  and  $r = 0.1$  ( $r = [\text{additive}]/[\text{ctDNA in phosphate}]$ ).

