Supporting Information

Characterization of the Nanostructure of Complexes Formed by Single- or Double-Stranded Oligonucleotides with a Cationic Surfactant

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To be submitted to the Journal of Physical Chemistry B

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Figure S1: Size distributions of complexes formed by oligonucleotides and CTAB in H₂O with in D₂O
Figure S2: SAXS spectrum measured using a H$_2$O solution (1 mM Li$_2$SO$_4$) containing 1 mM 5’-A$_{20}$-3’ and 1 mM CTAB at 25°C.
Figure S3. The PDDF calculated from IFT analysis. (A) 1 mM 5’-A$_{20}$-3’+3 mM CTAB; (B) 1 mM ONS+1 mM CTAB; (C) 1 mM ONS+4 mM CTAB; (D) 1 mM OND+4 mM CTAB; (E) 0.5 mM 5’-A$_{20}$-3’+0.5 mM 5’-T$_{20}$-3’+5 mM CTAB
Figure S4: Comparison of form factor fits to experimental SANS data for 1 mM 5’-A\textsubscript{20}-3’ and 1 mM CTAB sample by using different parameters.

(A) $\phi=0.0002$, $r_{\text{core}}=50$ Å, average $t_{\text{shell}}=31$ Å, average $t_{\text{solvent}}=14$ Å, number of layers: 1-11 (with a mean of 6), $s=0.020664$

(B) $\phi=0.0002$, $r_{\text{core}}=55$ Å, average $t_{\text{shell}}=31$ Å, average $t_{\text{solvent}}=14$ Å, number of layers: 1-10 (with a mean of 6), $s=0.030756$

(C) $\phi=0.0002$, $r_{\text{core}}=50$ Å, average $t_{\text{shell}}=29$ Å, average $t_{\text{solvent}}=16$ Å, number of layers: 1-10 (with a mean of 6), $s=0.0372728$

(D) $\phi=0.0002$, $r_{\text{core}}=50$ Å, average $t_{\text{shell}}=31$ Å, average $t_{\text{solvent}}=14$ Å, number of layers: 1-12 (with a mean of 6), $s=0.045423$

$s$ is standard error of estimate, calculated by $s = \sqrt{\frac{\sum(y - y_{\text{ext}})^2}{n}}$

The multiple peaks/shoulders apparent in form factor fits are caused by the polydispersity in periodicity used in the calculations of the form factors (see Materials and Methods for details).
Figure S5. Distribution of hydrodynamic diameters of complexes formed in (A) an aqueous solution containing 10 mM CTAB, and (B) aqueous solution (1 mM Li$_2$SO$_4$) containing 200 μM 5’-T$_{20}$-3’ and 10 mM CTAB.
Figure S6. SANS spectrum for a D$_2$O solution (1 mM Li$_2$SO$_4$) containing 1 mM 5’-dT$_{20}$-3’ and 3 mM CTAB at 35°C and form factor fit (gray line) by using the micelle model.
Figure S7: Circular dichroism spectra of single- and double-stranded oligonucleotides in 1mM Li$_2$SO$_4$ aqueous solution, pH 5. (A) Addition of 5’-A$_{20}$-3’ to 5’-T$_{20}$-3’. The results show an increase in the magnitude of the negative CD band, which indicates an increase in the helicity of DNA,$^1$ consistent with hybridization. (B) CD spectra of OND and ONS. Relative to ONS, the CD spectrum of OND shows an increase in the magnitude of the negative CD band, as well as a blue shift of the peak position. These two differences are consistent with the presence of a duplex structure in the solution of OND. $^1$
**Figure S8.** SANS spectrum measured using a D$_2$O solution (1 mM Li$_2$SO$_4$) of 0.5 mM 5’-A$_{20}$-3’ and 0.5 mM 5’-T$_{20}$-3’ with 5 mM CTAB at 35°C.
Figure S9: SAXS spectrum measured using precipitates formed by 1 mM OND and 2 mM CTAB solution (H₂O, 1 mM Li₂SO₄, 25 °C).