Reversible Condensation of DNA using a Redox-Active Surfactant

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Supplemental Materials

Comparison of Size Distributions Obtained by using CONTIN and NNLS Algorithms

We compared the size distributions obtained from light scattering measurements by using the CONTIN and NNLS algorithms. Analysis of three samples containing DNA and 5μM reduced FTMA at 90° (5 measurements per sample) using NNLS revealed a bimodal distribution of hydrodynamic sizes (Figure S1). This size distribution was in good agreement with the size distribution obtained using CONTIN (also shown in Figure S1).

Concentration of FTMA Required to Compact all DNA in Solution

Using the data in Figure 5, we calculated the fraction of DNA in solution that was compacted as a function of FTMA concentration (Figure S2). Inspection of Figure S2 reveals that the DNA in solution was completely compacted by the FTMA when the concentration of FTMA in solution was 10μM.

Electrochemical and Chemical Transformations DNA/FTMA Complexes

The current measured during the electrochemical oxidation of complexes of DNA and 30μM reduced FTMA is shown in Figure S3. We measured the current passed between the working and counter electrodes to decrease with time. This observation is consistent with oxidation of FTMA.[1] We also measured the optical absorbance spectra of the solutions before and after oxidation at wavelengths between 190nm and 800nm (Figure S4). For reference, Figure S4 shows the absorption spectra of samples prepared by mixing DNA with either reduced or oxidized FTMA at a final concentration of 30μM FTMA. The sample containing the oxidized FTMA was characterized by a peak in absorbance at 625nm, which was absent for reduced FTMA. When the reduced FTMA + DNA solution was oxidized electrochemically as described in the Methods section, the final solution also exhibited a peak at 625nm at a magnitude very similar to a sample prepared by mixing oxidized FTMA and DNA. When combining the data in Figure S3 and Figure S4, we concluded that the solution of DNA and 30μM reduced FTMA was fully oxidized after application of a potential of 400mV for 50 minutes.

We added ascorbic acid to a solution of oxidized FTMA and DNA (prepared by electrochemical oxidation of reduced FTMA when mixed with DNA). Inspection of the optical absorbance spectrum of this sample in Figure S4 reveals no peak at 625nm (as observed with oxidized FTMA) providing evidence that FTMA was reduced by ascorbic acid. When ascorbic acid was added to a solution of DNA mixed with oxidized FTMA, the peak at 625nm was also eliminated. As a control, we added ascorbic acid to a

solution of DNA and to a solution of DNA in the presence of 30μM reduced FTMA (Figure S4 and Table S1). No change was observed in the absorbance spectra in the range of 500 – 800nm. We concluded that the oxidized FTMA was fully reduced by the ascorbic acid in the presence of DNA.

Influence of Oxidizing Potential on DNA

To assess the potential influence that an oxidizing potential may cause to the conformation of DNA in solution, we applied a potential of 400mV for 1-1.5 hours to a solution of DNA in the absence of FTMA. Subsequent DLS measurements revealed no change in the ACF of the solution after the applied potential as compared to the ACF of the DNA without an applied potential. We then added reduced FTMA to the solution of DNA that was pre-exposed to an oxidizing potential to a final concentration of 30μM reduced FTMA and performed measurements of DLS. The addition of reduced FTMA led to shorter relaxation times, similar to the relaxation times present for a solution prepared by mixing DNA with reduced FTMA. We concluded that the applied potential did not interfere with the ability of FTMA to interact with DNA and cause a change in conformation. We also note that several past studies have reported that potentials of greater than 1200mV are required to oxidize the base pairs of DNA.[2-4] The low potentials used in our experiment are unlikely to cause damage to DNA.

References

(1) Rosslee, C. A.; Khripin, C.; Foley, T. M. D.; Abbott, N. L. *AIChE Journal* **2004**, *50*, 708-714.

(2) Ye, Y.; Ju, H. *Sensors* **2003**, *3*, 128-145.

(3) Teijeiro, C.; Nejedly, K.; Palecek, E. *Journal of Biomolecular Structure & Dynamics* **1993**, *11*, 313-331.

(4) Palecek, E.; Jelen, F.; Trnkova, L. *General Physiology and Biophysics* **1986**, *5*, 315-329.

Tables

Table S1. Absorbance measurements of 5μM DNA and 30μM FTMA complexes prepared by *in situ* electrochemical oxidation and subsequent chemical reduction by ascorbic acid. All absorbance measurements are reported relative to a sample containing 5μM DNA in 1mM Li_2SO_4.

Sample	**Absorbance at 625nm (x1000)**
DNA + reduced FTMA	0.53 ± 0.06
DNA + oxidized FTMA	8.36 ± 0.09
DNA + FTMA oxidized *in situ*	8.29 ± 0.12
DNA + ascorbic acid	-0.11 ± 0.07
DNA + oxidized FTMA + 30μM ascorbic acid	0.30 ± 0.07
DNA + reduced FTMA + 30μM ascorbic acid	0.12 ± 0.08
DNA + FTMA oxidized *in situ* + 30μM ascorbic acid	0.52 ± 0.08

Figures

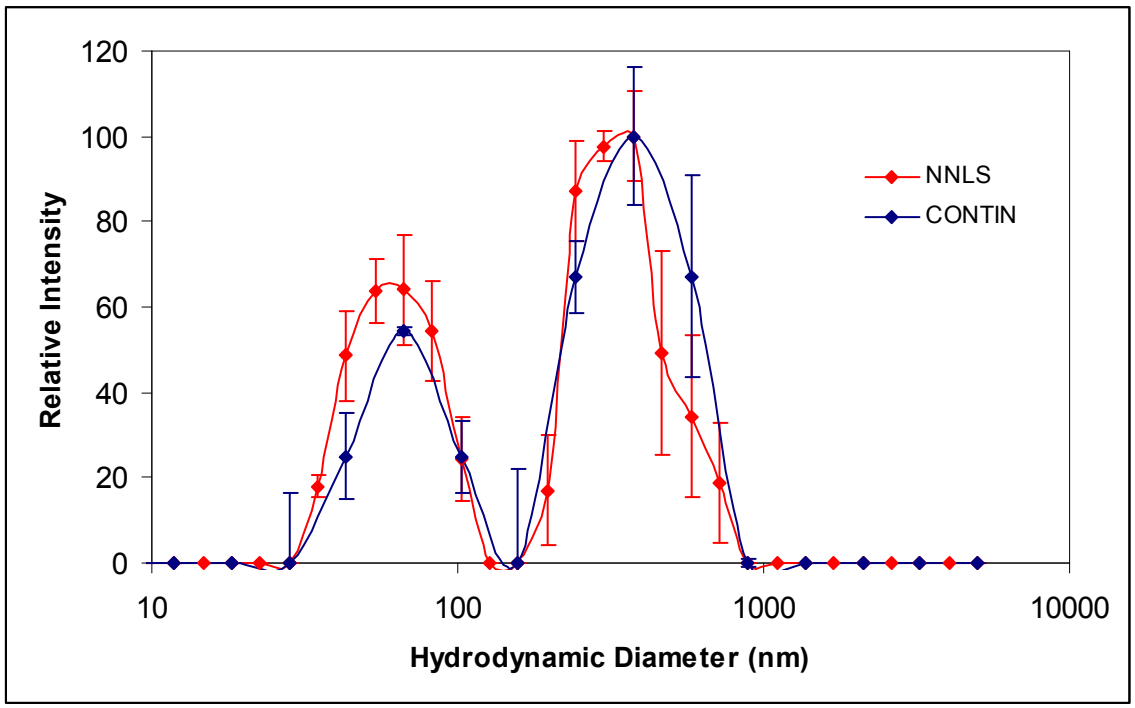

Figure S1. Comparison of size distributions obtained using CONTIN and NNLS algorithms.

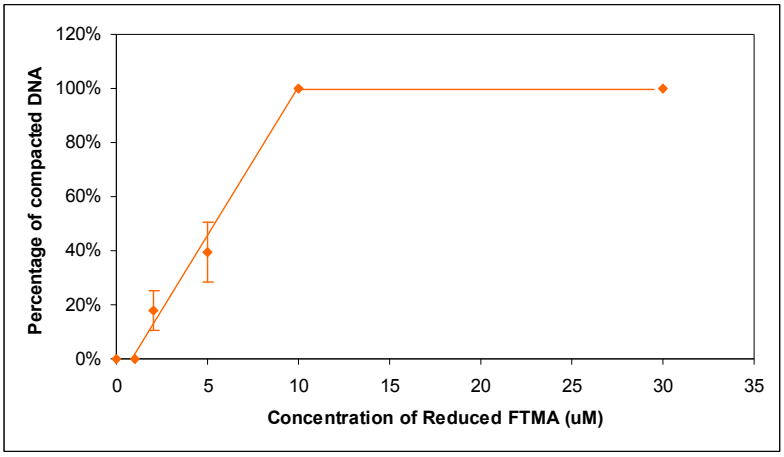

Figure S2: Fraction of DNA compacted as a function of concentration of FTMA in solution.

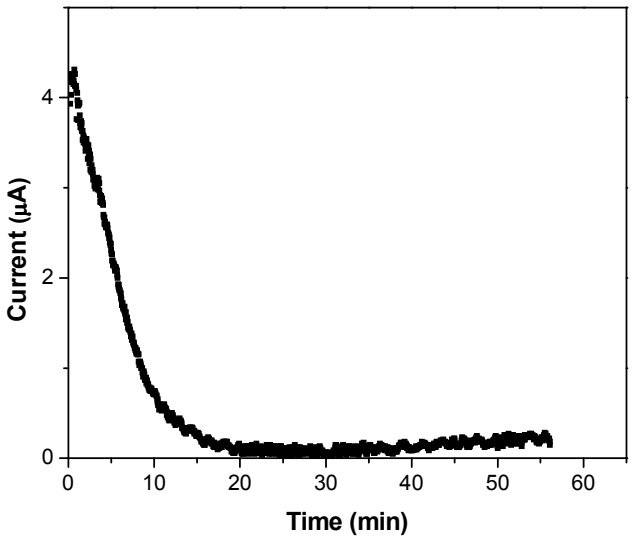

Figure S3. Oxidation of 5μM DNA and 30μM reduced FTMA using 400mV at room temperature.

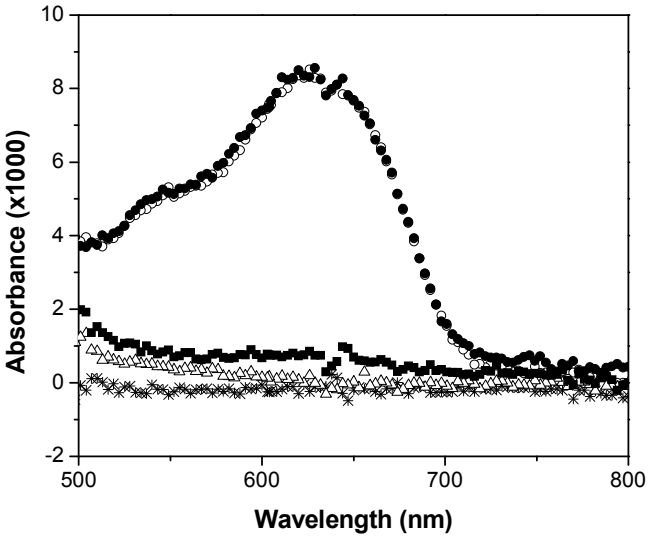

Figure S4. UV-visible spectrophotometry of 5μM DNA and 30μM FTMA. The symbols correspond to solutions of DNA mixed with oxidized FTMA (●), DNA mixed with reduced FTMA (■), complexes prepared by *in situ* oxidation of reduced FTMA DNA (○), complexes prepared by *in situ* oxidation of reduced FTMA and DNA followed by addition of L-ascorbic acid to a final concentration of 30μM (Δ), DNA without FTMA in the presence of 30μM ascorbic acid (*).