Supporting Information

Quantitative Measurements of Thermodynamics and Kinetics of Polythiophene-DNA Complex Formation in DNA Detection

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<table>
<thead>
<tr>
<th>Name</th>
<th>Sequence</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_1$</td>
<td>5’TAA CAA TAA TCC CTC</td>
<td>DNA probe</td>
</tr>
<tr>
<td>$X_1'$</td>
<td>5’-TAA CAA TAA TCC CTC A$_{20}$-C$_3$-S-S-C$_3$-OH</td>
<td>DNA probe to bind on silica nanoparticles</td>
</tr>
<tr>
<td>$Y_1$</td>
<td>5’-GAG GGA TTA TTG TTA</td>
<td>DNA Complementary to $X_1$, $X_1'$</td>
</tr>
</tbody>
</table>

Zheng and He “Quantitative Measurements of Thermodynamics and Kinetics…” SI Table
Calculation of surface density of immobilized polymer-ssDNA duplex on silica nanoparticles:
Volume of 100-nm silica nanoparticle, \( V = (\pi/6)D^3 = (3.14/6)(10^{-5}\text{ cm})^3 = 5.2*10^{-16}\text{ cm}^3; \)
Surface area of 100-nm silica nanoparticle, \( S = \pi D^2 = 3.14*(10^{-5}\text{ cm})^2 = 3.14*10^{-10}\text{ cm}^2; \)
Weight of silica nanoparticle, \( W = \rho V = (1.96\text{ g/mL})*(5.2*10^{-16}\text{ cm}^3) = 1.02*10^{-15}\text{ g}; \)
For 100 \( \mu\text{L} \) of 15mg/mL particle solution, total weight of particle, \( W_t; \)
\[ W_t = (100*10^{-6}\text{ L})* (15\text{ mg/mL}) = 1.5*10^{-3}\text{ g}; \]
Number of particles in solution, \( N = W_t/W = (1.5*10^{-3}\text{ g})/(1.02*10^{-15}\text{ g}) = 1.5*10^{12}; \)
Total surface area of particles, \( S_t = N*S = (1.5*10^{12})* (3.14*10^{-10}\text{ cm}^2) =471 \text{ cm}^2; \)
Surface density of immobilized polymer-ssDNA duplex on particles, \( \Gamma; \)
\[ \Gamma = \frac{\text{mole of duplex}}{S_t} = \frac{(100*10^{-6}\text{ L})*(16*10^{-6}\text{ mol/L})}{(471\text{ cm}^2)} \approx 3*10^{-12}\text{ mol/cm}^2 = 3\text{ pmol/cm}^2. \]
Supporting Figure 1. (A) Absorbance and (B) fluorescence emission profiles of conjugated polymer-DNA complexes: (a) free polymer, (b) polymer/ssDNA duplexes, and (c) polymer/dsDNA triplexes.

Zheng and He “Quantitative Measurements of Thermodynamics and Kinetics...” SI Fig 1.
Supporting Figure 2. Melting curves of the polymer-ssDNA duplexes in 10 mM PB buffer monitored at 260 nm (black squares) and 500 nm (red circles). The corresponding solid lines are the best fit of experimental data.

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Supporting Figure 3. The melting curves of dsDNA in solution without (red triangles) or with (blue circles) the extra A\textsubscript{20} spacer. The presence of A\textsubscript{20} as the spacer only slightly changed the melting temperature of dsDNA at the absence polymer with the calculated K value increased from 2.2 x 10\textsuperscript{-8} to 4.3 x 10\textsuperscript{-8}. No stability change was observed for the polymer-dsDNA system, primarily due to the much higher temperature needed to dissociate polymer-dsDNA triplexes that no polymer-ssA\textsubscript{20}, if any, would be able to survive.

Zheng and He “Quantitative Measurements of Thermodynamics and Kinetics...” SI Fig 3.
Supporting Figure 4. Arrhenius plots for conjugated polymer-bound DNA hybridization in solution phase and on particle phase. Association rate constants were determined from the fitting curves recorded at different temperatures.