Supporting Information

Accelerated Color Change of Gold Nanoparticles Assembled by DNAsymes for Simple and Fast Colorimetric Pb^{2+} Detection

Juewen Liu and Yi Lu

Department of Chemistry

University of Illinois at Urbana-Champaign

Urbana, Illinois 61801, USA
Figure S1. Stability of DNA-functionalized 42 nm diameter gold nanoparticles in the presence of 500 mM NaCl. Nanoparticles functionalized with 3′- and 5′-thiol modified DNA were mixed with equal concentration. The UV-vis spectroscopy of the sample was monitored for 30 minutes. The change of extinction ratio is presented in (A). Spectra of the sample at several time points were presented in (B). The buffer conditions were 25 mM Tris acetate, pH 8.2. No DNAzyme was added. The results show that the nanoparticles are stable in high NaCl concentration.
Figure S2. (A) to (C): Secondary structures of the substrate strand (35SubAu) predicted by the Mfold

A. 35 ºC, dG=-1.3
B. 25 ºC, dG=-3.2
C. 5 ºC, dG=-7.8
program (available at http://www.bioinfo.rpi.edu/applications/mfold)\textsuperscript{1} at different temperatures. The NaCl concentration was input to be 0.3 M. The ribonucleoside adenosine (rA) was replaced with a deoxyribonucleoside adenosine for calculating the structure by the mfold program. With the decrease of temperature, more and more local secondary structures have been stabilized. The dG (free energy change) decreases with decreasing of temperature, indicating that more energy is needed to melt the local structures of the DNA at lower temperature. (D): Melting curve of the substrate (35SubAu) alone in 300 mM NaCl, 25 mM tris acetate buffer, pH 8.2 (blue). The melting temperature was determined to be 44 °C (inset). As a control experiment, the temperature-dependent absorption change of a polyT (5´-TTTTT-3´) was also measured (black curve). No significant changes were observed from 10 to 61 °C for the polyT.
Figure S3. The effect of temperature on the rate of nanoparticle aggregation assembled by a 24-mer complementary strand DNA to the two 12-mer DNA on nanoparticles (3′DNA$_{Au}$ and 5′DNA$_{Au}$). The sequence of the 24-mer DNA is 5′-ACTCATCTGTGATGTCAACTCGTG-3′. Comparing this figure and Figure 5, it can be concluded that the temperature-dependent rate of aggregation is also general to simple complementary DNA assembled systems.
Figure S4. Melting temperature of 35SubAu and 17E assembled 42 nm gold nanoparticle aggregates. The aggregates were prepared by allowing nanoparticles (0.11 nM) and the enzyme (2 µM) and substrate (3 nM) to assemble at room temperature for half an hour (300 mM NaCl, 25 mM Tris acetate buffer, pH 8.2). The aggregates were diluted by adding the same volume of the same buffer with 300 mM NaCl. Temperature was then increased and the extinction at 260 nm was monitored. Then melting temperature was determined to be 53 ºC. The significant increase of extinction at 260 upon melting and the very sharp melting transition suggests that the nanoparticles were reversibly assembly by the DNAzyme were experienced a cooperative melting behavior.\textsuperscript{2} The melting temperature is higher than that obtained for nanoparticle aggregates aligned in a “head-to-tail” manner (T\textsubscript{m} = 46 ºC for aggregates formed by 13 nm particles aligned in a “head-to-tail” manner in 300 mM NaCl).

References: