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Electronic Supplementary Information for

Detection of Mercury(II) Based on Hg²⁺-DNA Complexes Inducing the Aggregation
of Gold Nanoparticles

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EXPERIMENTAL SECTION

Chemicals. Trisodium citrate and all of the metal salts used in this study were purchased from Aldrich (Milwaukee, WI). Sodium phosphate dibasic anhydrous and sodium phosphate monobasic monohydrate, which were used to prepare the sodium phosphate buffer (5 mM, pH 7.4), were obtained from J. T. Baker (Phillipsburg, NJ, USA). Hydrogen tetrachloroaurate(III) trihydrate was obtained from Acros (Geel, Belgium). The OliGreen ssDNA Quantitation Reagent and Kit was obtained from Molecular Probes (Portland, OR). The probe (T₇, T₃₃, and T₈₀) and control (A₃₃ and 5'-TTTTTACCTGGGGAGTATTGCGGAGGAAGGT-3') DNA samples were purchased from Integrated DNA Technology, Inc. (Coralville, IA).

Synthesis of Au NPs. Au NPs were prepared through citrate-mediated reduction of HAuCl₄. Aqueous 1 mM HAuCl₄ (250 mL) was brought to a vigorous boil with stirring in a round-bottom flask fitted with a reflux condenser; 38.8 mM trisodium citrate (25 mL) was then added rapidly to the solution. The mixture was heated under reflux for another 15 min, during which time its color changed from pale yellow to deep red. The solution was cooled to room temperature while stirring continuously. The sizes of the nanoparticles were verified through TEM analysis (H7100, Hitachi High-Technologies Corporation, Tokyo, Japan); the Au NPs were nearly monodisperse, with an average size of 13.3 ± 0.6 nm. The particle

concentration of the Au NPs (ca. 15 nM) was determined according to Beer's law using an extinction coefficient of $10^8 \text{ M}^{-1} \text{ cm}^{-1}$ at 520 nm (double-beam UV–Vis spectrophotometer, Cintra 10e, GBC, Victoria Australia) for Au NPs of 13.3-nm diameter.

Analysis of Samples. Aliquots (30 μL) of 5 mM phosphate (pH 7.4) solutions containing Hg^{2+} (0–25 μM) and DNA (concentrations of T₇, T₃₃, T₈₀, and the control DNA: 283, 60, 25, and 60 nM, respectively) were kept at ambient temperature for 10 min. Au NP solution (2 nM) was added to the solutions, which were then incubated for 1 min. Finally, NaCl was added to each solution, which was then incubated for 10 min prior to measurement of its absorption. When conducting fluorescence measurements, aliquots (30 μL) of 5 mM sodium phosphate (pH 7.4) solutions containing Hg^{2+} (0–25 μM) and T₃₃ DNA (30 nM) were maintained at room temperature for 10 min. Au NP solution (1.0 nM) was added to each solution, which was then incubated for 1 min. Finally, OliGreen was added to each solution and incubated for 10 min prior to fluorescence measurements.

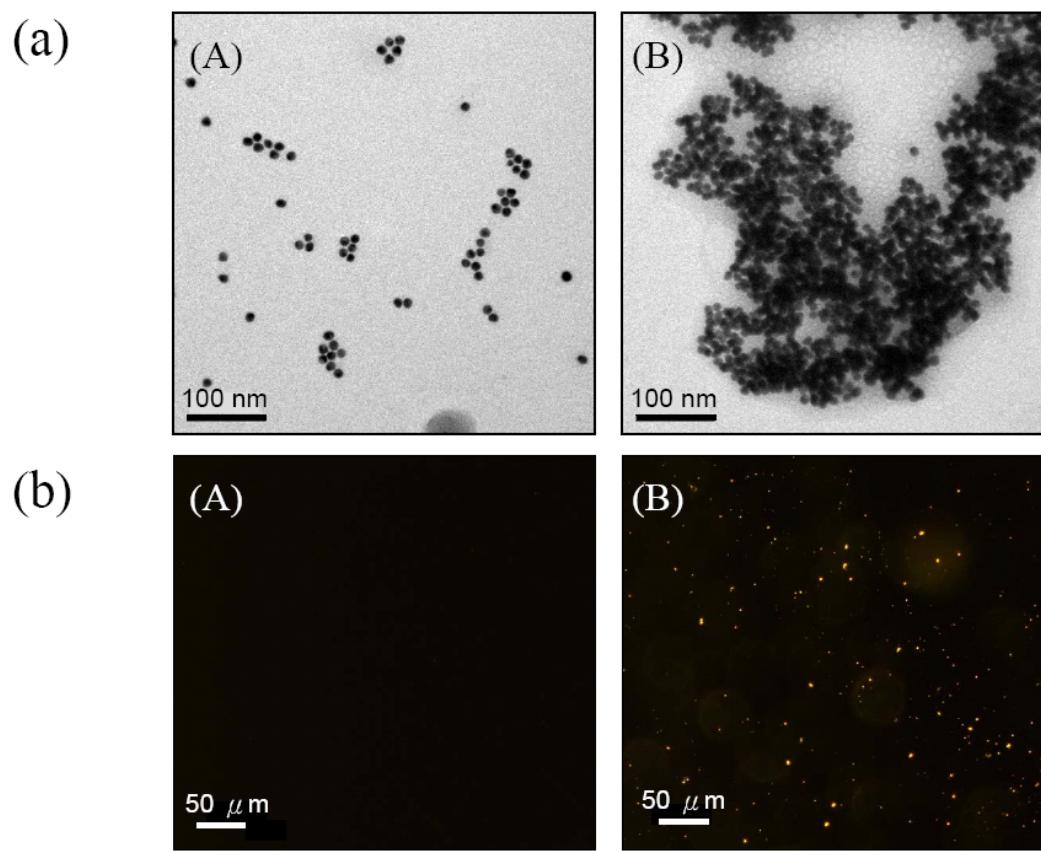


Fig. S1 (a) TEM and (b) scattering images of 5 mM phosphate solutions (pH 7.4) containing Au NPs (2 nM), T₃₃ (60 nM), and NaCl (50 mM) in the (A) absence and (B) presence of 5.0 μM Hg²⁺.

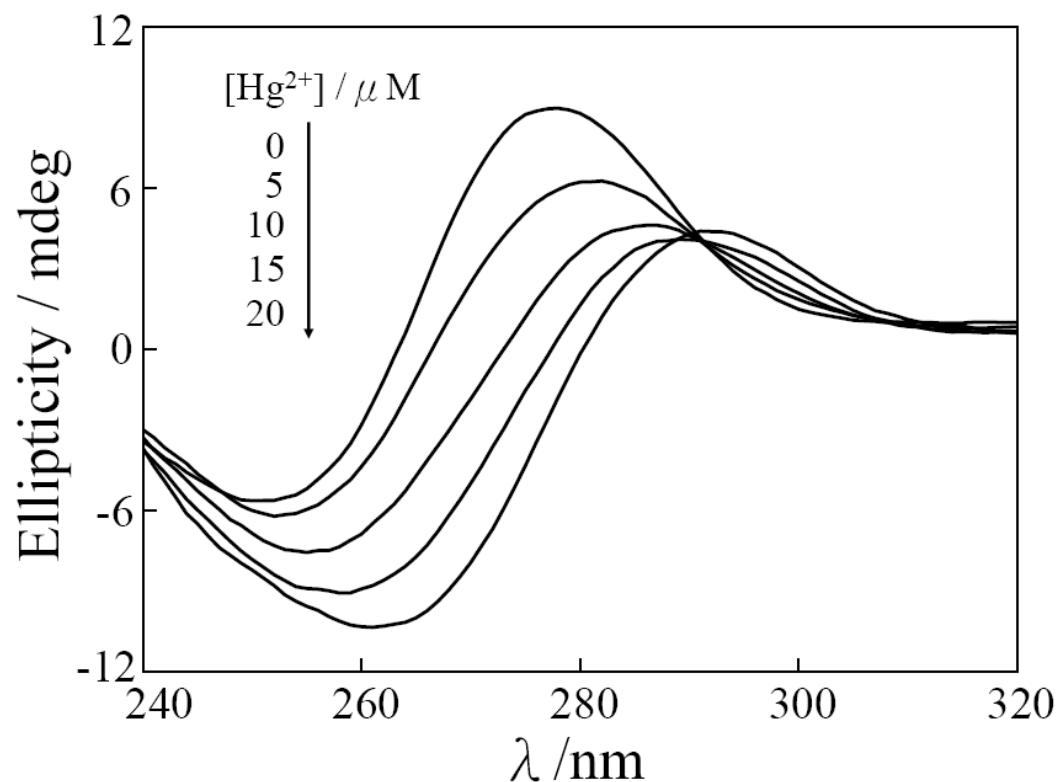


Fig. S2 Ellipticity of 500 nM T_{33} in the absence and presence of Hg^{2+} ions (5, 10, 15, and 20 μM). Buffer: 5 mM sodium phosphate (pH 7.4) was used to prepare the solutions.

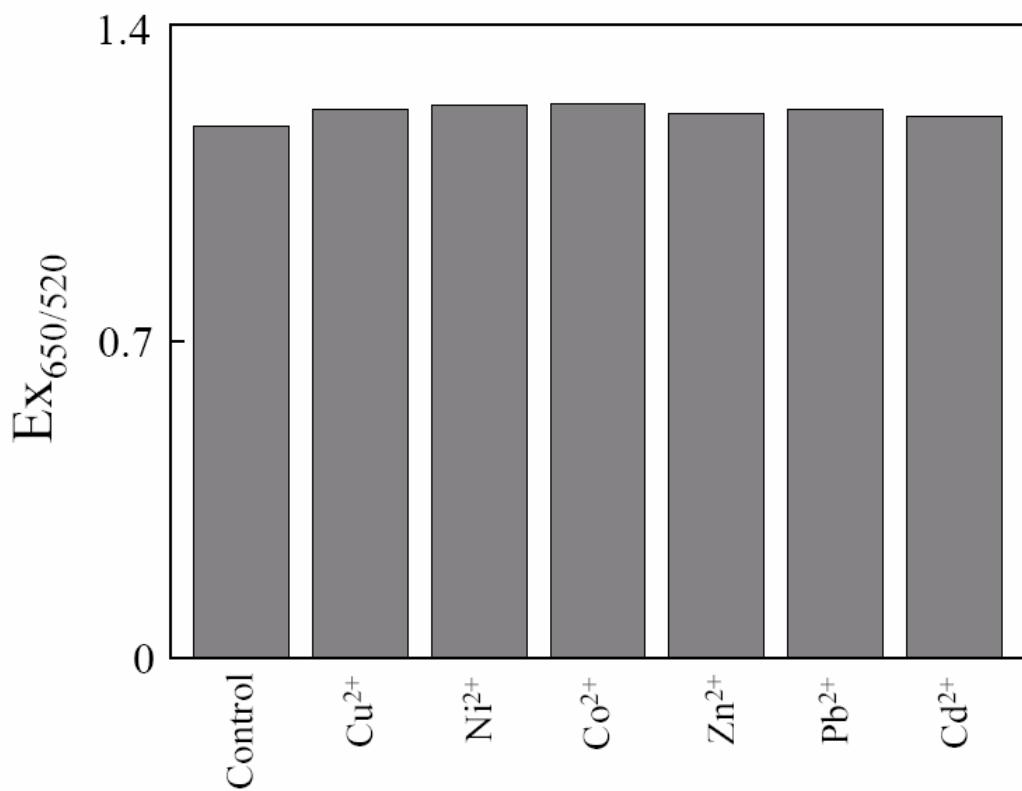


Fig. S3 Values of $Ex_{650/520}$ of solutions containing Au NPs (2 nM), T₃₃ (60 nM), 50 mM NaCl, and 5.0 μ M Hg²⁺ in the absence (control) and presence of various other metal ions (100 μ M). All other conditions were the same as those described in Fig. 2.

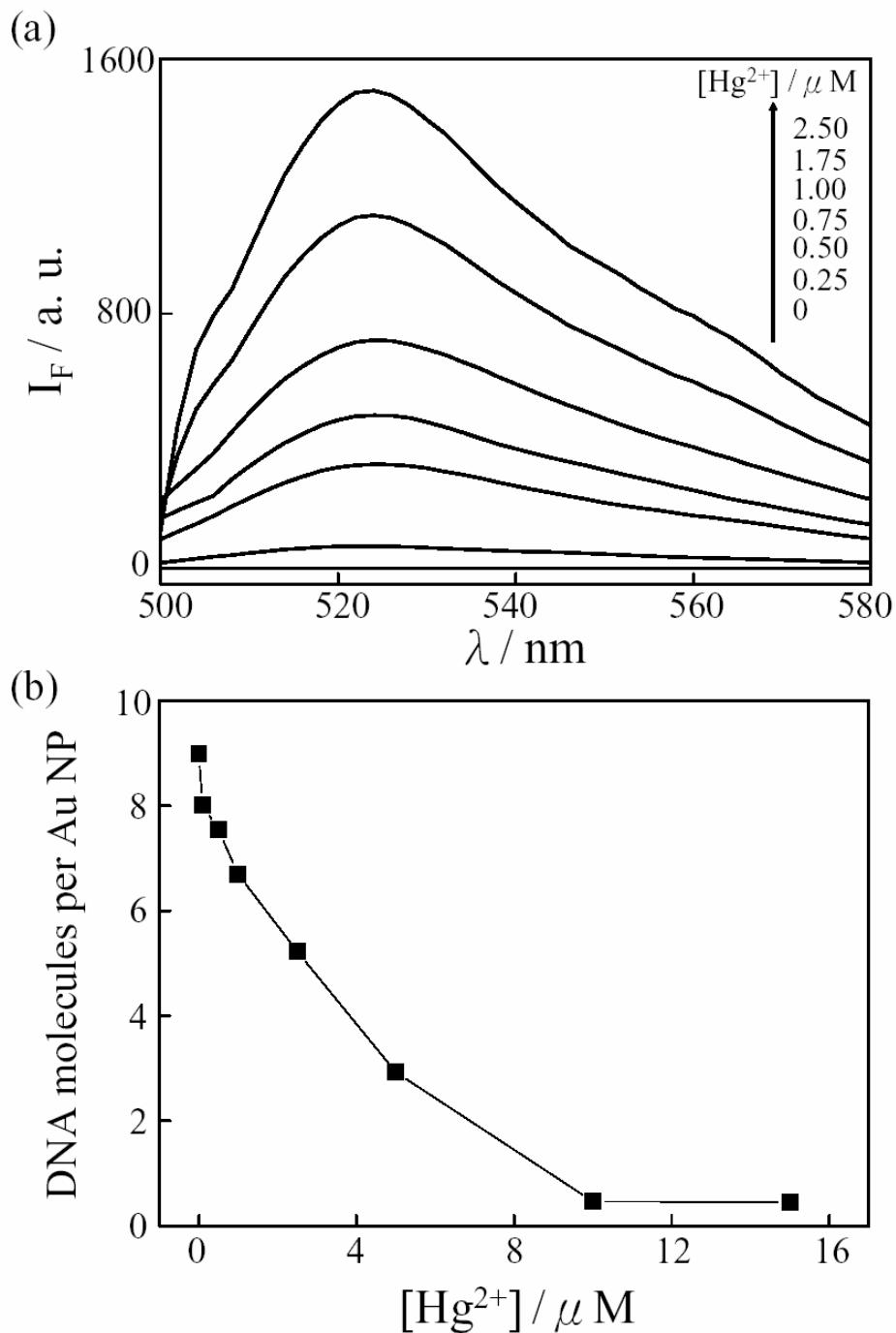


Fig. S4 (a) Fluorescence spectra of the solutions containing Au NPs (1.0 nM), T₃₃ (30 nM), and OliGreen in the presence of Hg²⁺ ions. (b) The number of DNA molecules per Au NP plotted as a function of the concentration of Hg²⁺ ions.