

Supporting Information:

# Nucleic Acid-directed Self-assembly of Multifunctional Gold Nanoparticle Imaging Agents<sup>1</sup>

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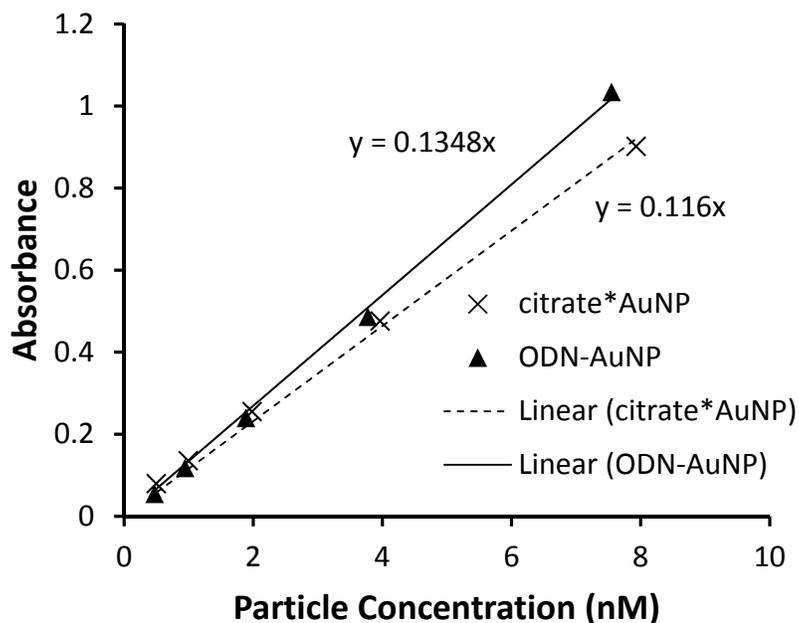
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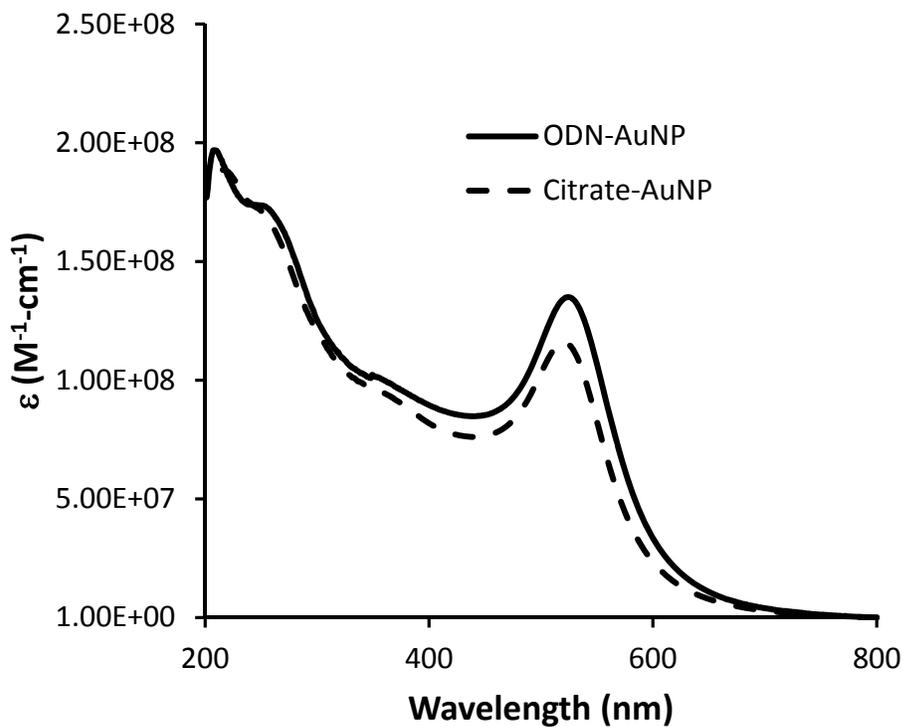
<sup>1</sup> This work is dedicated to Dr. Michael J. Welch, who passed away on May 6th, 2012.

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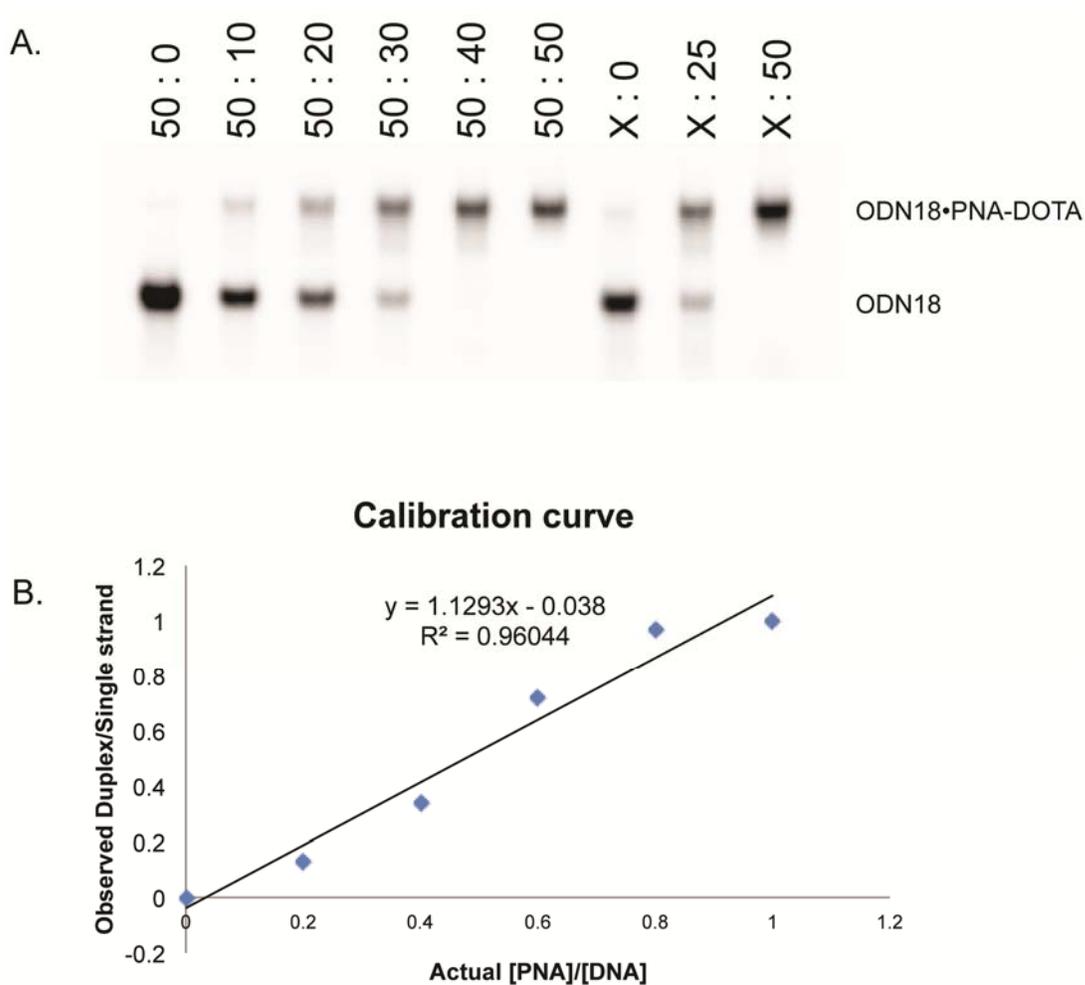
A)



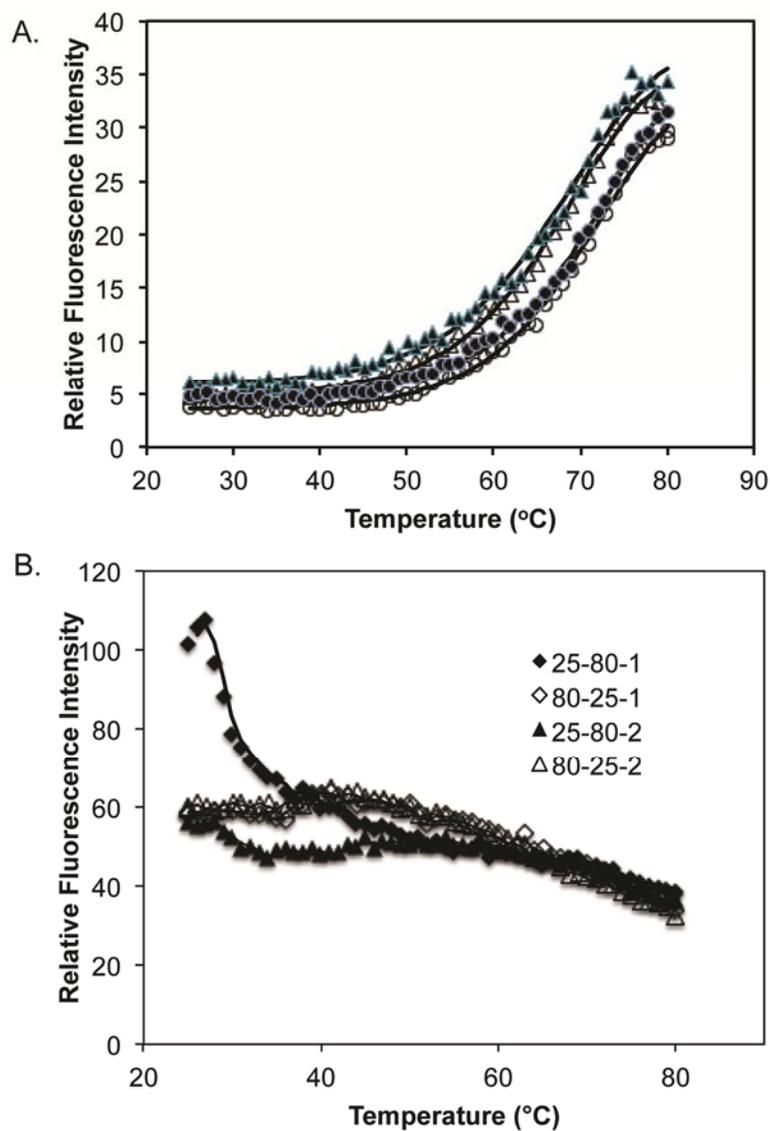
B)



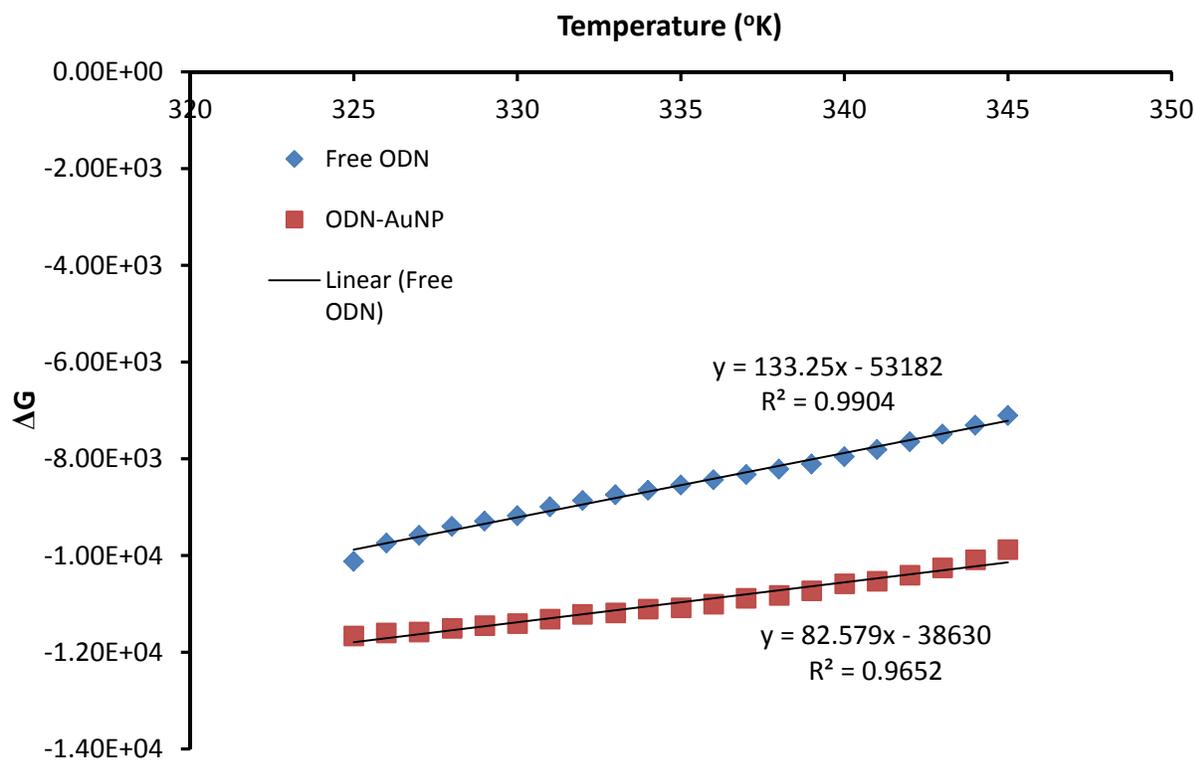
**Figure S1.** Determination of the molar absorption coefficients of the gold nanoparticles .  
A) Absorbance was measured as a function of concentration at the absorption maximum of 520 nm for the citrate•AuNP, and at 524 nm for the ODN-AuNP. The concentration of the particles was calculated as described in the experimental section. B) Molar extinction coefficient spectra for citrate-AuNP and ODN-AuNP.



**Figure S2.** Determination of the average ODN loading of ODN·AuNP. A) Gel electrophoresis of  $^{32}\text{P}$ -labeled ODN of known concentration and  $^{32}\text{P}$ -labeled ODN from cyanide treatment of ODN·AuNP that were titrated with a known concentration of PNA-DOTA. B) Calibration curve generated from lanes 1-6 of A).



**Figure S3.** A) Temperature-dependent fluorescence curves for A) Cy5-PNA·ODN-AuNP and B) Cy5-PNA. Excitation was carried out at 633 nm and emission was detected at 663 nm. The high fluorescence in the first heating curve (25-80-1) is likely an artifact.



**Figure S4.** Van't Hoff analysis of the melting temperature curve to yield  $\Delta H$  and  $\Delta S$  for PNA•ODN duplex formation with free ODN and ODN-AuNP. The fraction single strand data from Figure 6 were converted to  $K_{eq}$  values taking into account the concentration of ODN and PNA used. The  $K_{eq}$  values were then converted to  $\Delta G$  values in calories and plotted against T in degrees Kelvin. The slope from a linear fit to the data gave  $\Delta S^\circ$  in cal/deg-mol and  $\Delta H^\circ$  in calories.