

SUPPLEMENTARY INFORMATION

Gold nanoparticles as colorimetric sensors for the detection of DNA bases and related compounds

Emilia Iglesias

Departamento de Química. Facultad de Ciencias. Campus A Zapateira. Universidad de La Coruña. 15008-La Coruña. SPAIN. emilia.iglesias@udc.es

Figure S1: The spectra of the compounds studied in both neutral and mild acid aqueous solution.

Figure S2: Experiments to compare the effect of small amounts of acetic acid in the gold nanoparticles aggregation mediated by thiourea.

Figure S3: Optimized structures of thiourea and 4-thiouracil.

Figure S4: Experiments to demonstrate the effect of order addition of 2-thiouracil, 4-thiouracil, and AuNPs solution in the mixture.

Figure S5: First-order plot of absorbance *versus* time corresponding to AuNPs aggregation process mediated by adenine and guanine

Figure S6: Histogram of size distribution of synthesized nanoparticles.

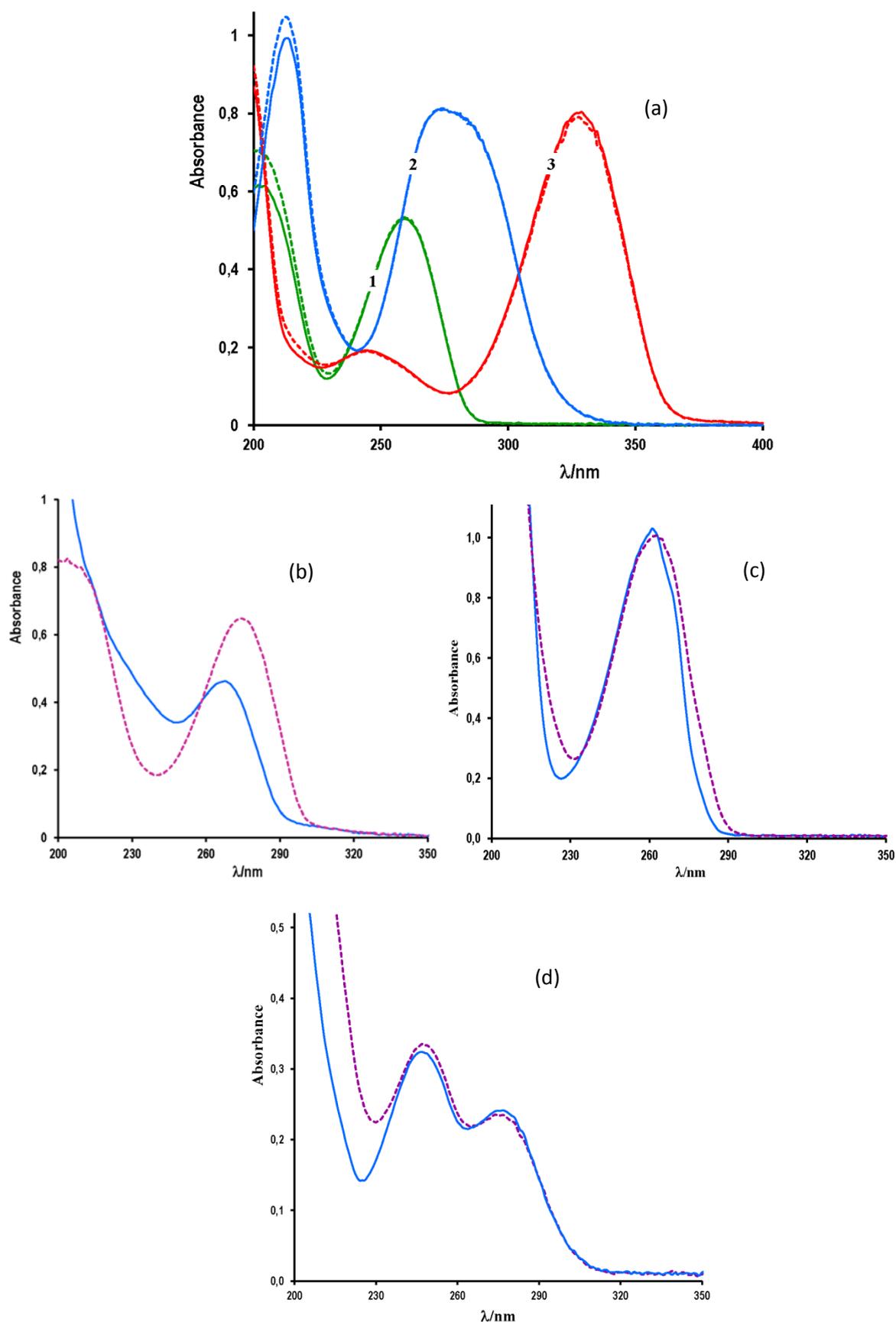


Figure S1. UV-Vis absorption spectrum **(a)** of (1)Uracil 65 μM ; (2)2-thiouracil 58 μM , and (3)4-thiouracil 42 μM , in water and in 1.74 mM acetic acid (*dashed line*); **(b)**cytosine 65 μM in water and in 1.74 mM acetic acid (*dashed line*), and **(c)**adenine 77.6 μM , in water and in 10.4 mM acetic acid (*dashed line*); **(d)**guanine 50 μM in water and in 10.4 mM acetic acid (*dashed line*).

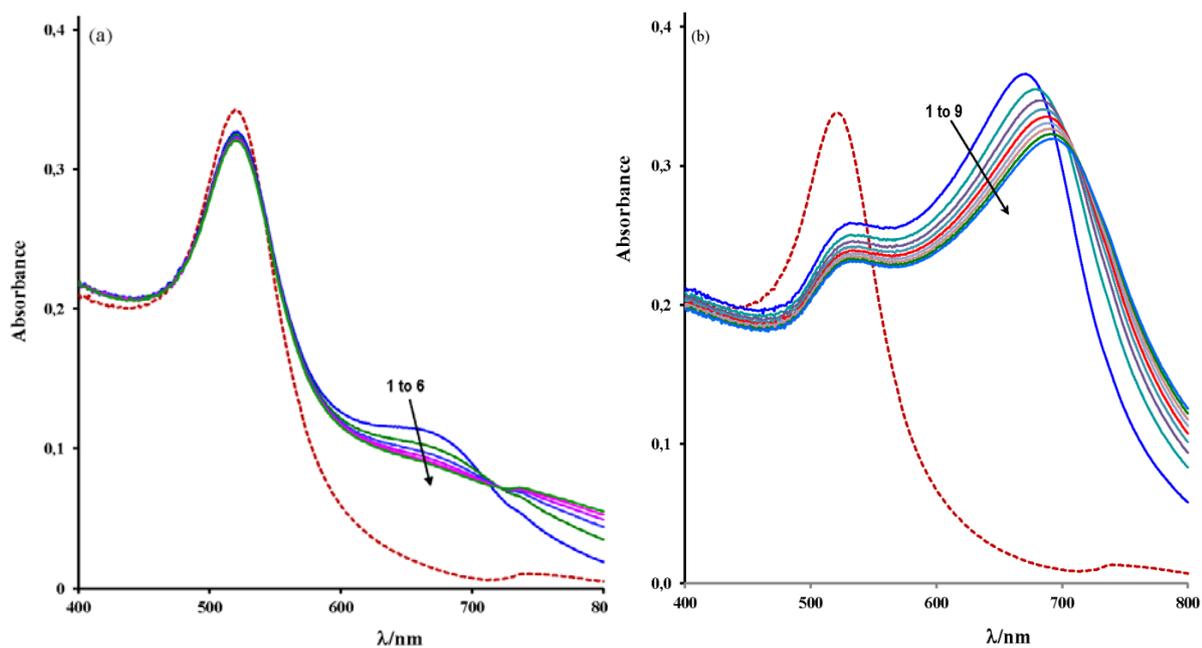


Figure S2. The absorption spectra evolution of AuNPs solution in the presence of 1.12 μM of thiourea (a) in the absence of acetic acid, and (b) at 1.6 mM of acetic acid; (- - -) only AuNPs; (scans 1 to 6 or 1 to 9) at 3 min interval.

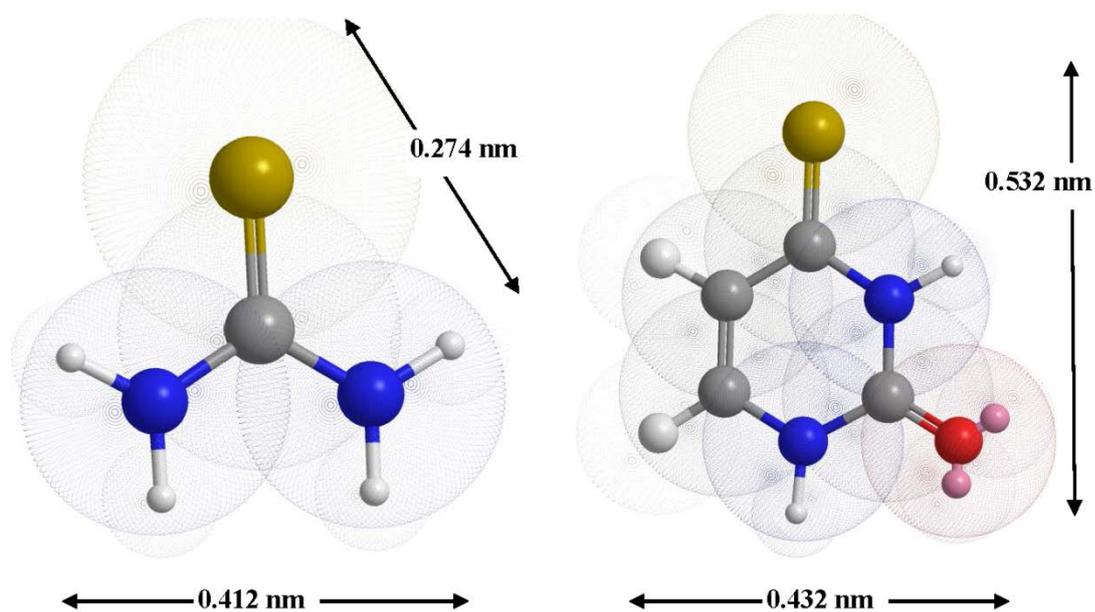


Figure S3. Cross-section dimensions of the optimized structures of thiourea and 4-thiouracil

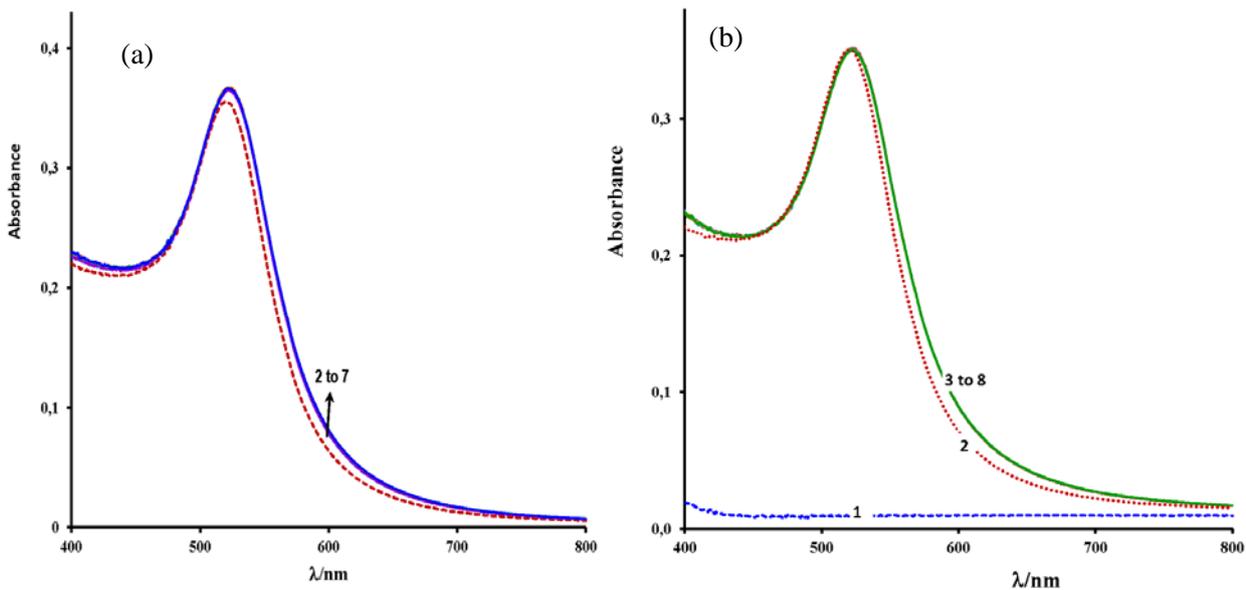


Figure S4. UV-Vis spectrum of gold nanoparticles solution (- - -) and in the presence of (a) 93,9 μM of 2TU recorded at 3 min interval (curves 2 to 6), and after the addition of 25.3 μM of 4-thiouracil (curve 7); no changes have been observed, and (b) 93,9 μM of both 2TU and 4TU but in the absence of AuNPs (dashed line 1); only AuNPs in the absence of 2TU and 4TU (dotted line 2), and with the three additives: 2TU, 4TU and AuNPs added in this order (curves 3 to 8 recorded at 3 min interval). The different additives were added into the same sample successively, the effect of volume increase has been corrected.

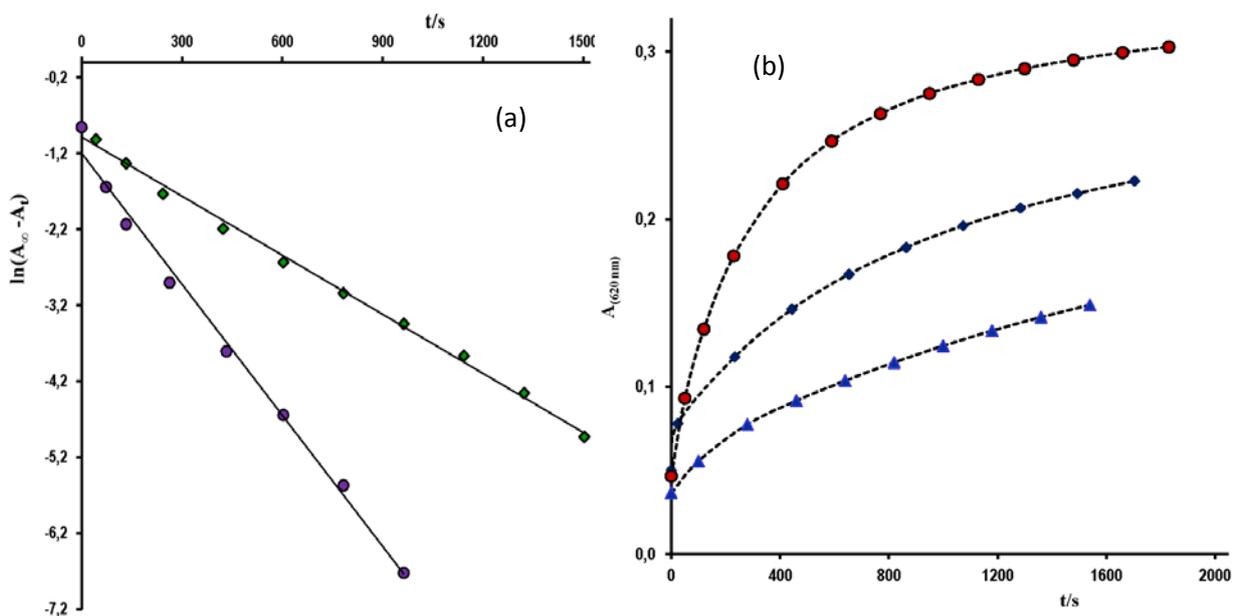


Figure S5. (a) Linear form of the first-order rate equation $\{A_t = A_\infty - (A_\infty - A_0) \exp(-k \cdot t)\}$ for the absorbance increase at 670 nm as a function of time corresponding to the SPR band of gold nanoparticles solution in the presence of adenine at (\blacklozenge) $[\text{A}] = 1.55 \mu\text{M}$, and (\bullet) $[\text{A}] = 38.8 \mu\text{M}$. (b) Increase absorbance at 620 nm due to the evolution of the SPR band of gold NPs in the presence of guanine at (\blacktriangle) $[\text{G}] = 5.6 \mu\text{M}$; (\blacklozenge) $[\text{G}] = 8.4 \mu\text{M}$, and (\bullet) $[\text{G}] = 8.4 \mu\text{M}$, $[\text{Mn}^{2+}] = 0.046 \text{ mM}$.

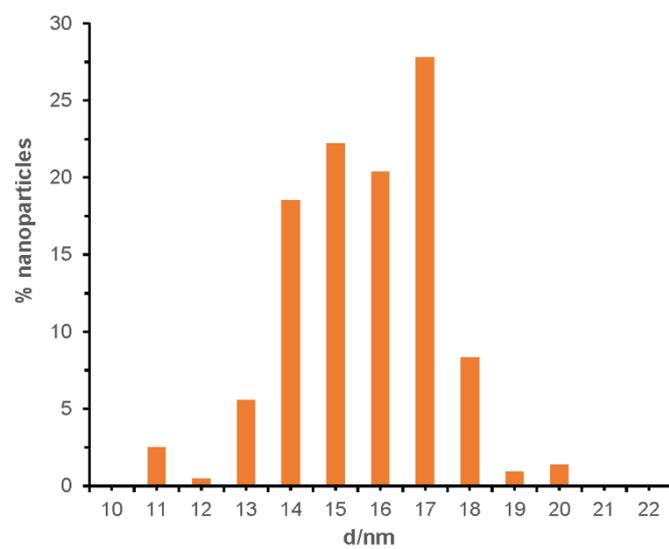


Figure S6. Size distributions of synthesized gold nanoparticles