

Supporting Information of

2,3,4-Trihydroxy benzophenone as a novel reducing agent for one-step synthesis of size-optimized gold nanoparticles and their application in colorimetric sensing of adenine at nanomolar concentration

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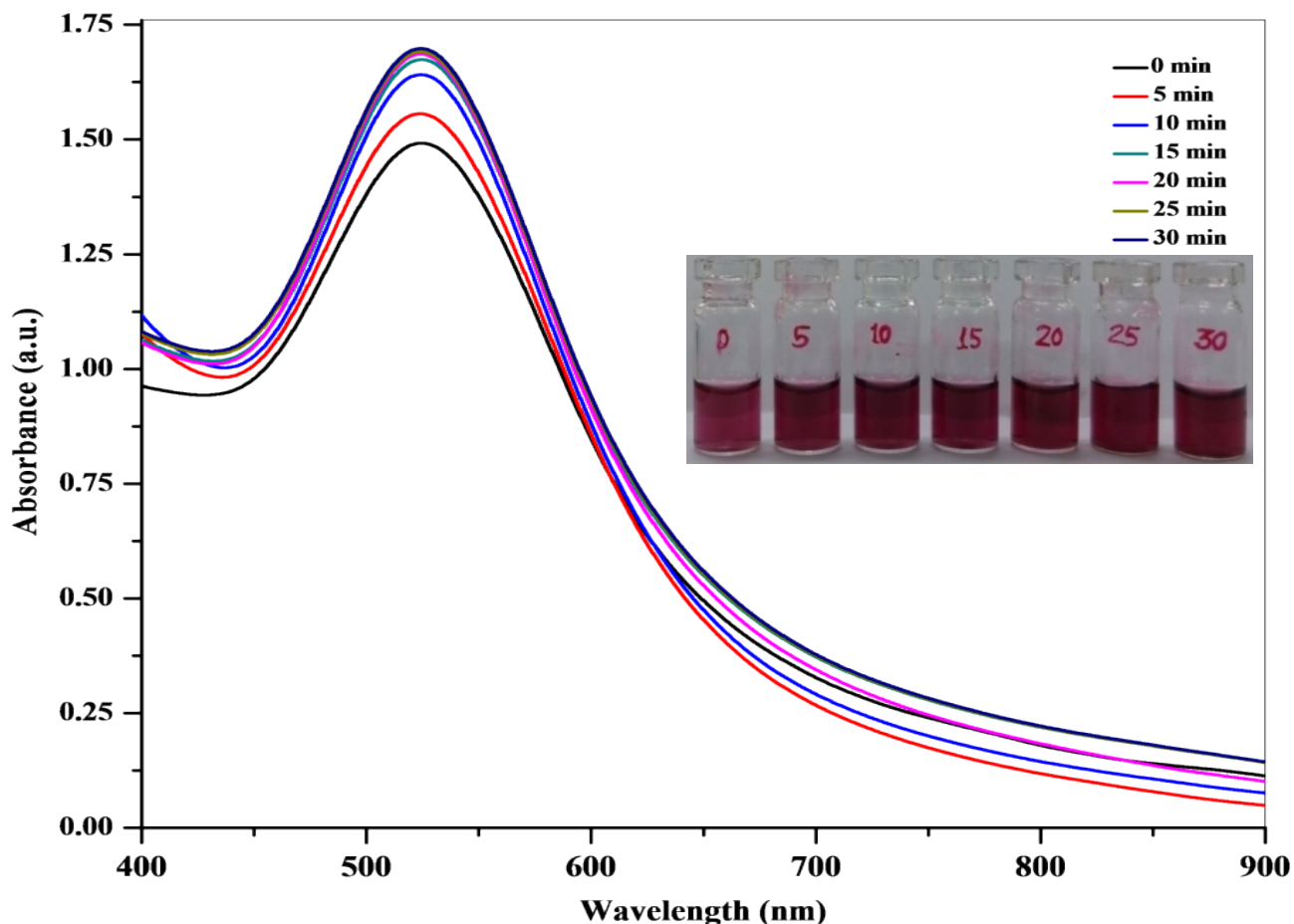


Figure S1. UV-visible absorption spectra of Au NPs by using THB (2.5 mM) as a reducing and capping agent at different reaction time from 0 to 30 min.

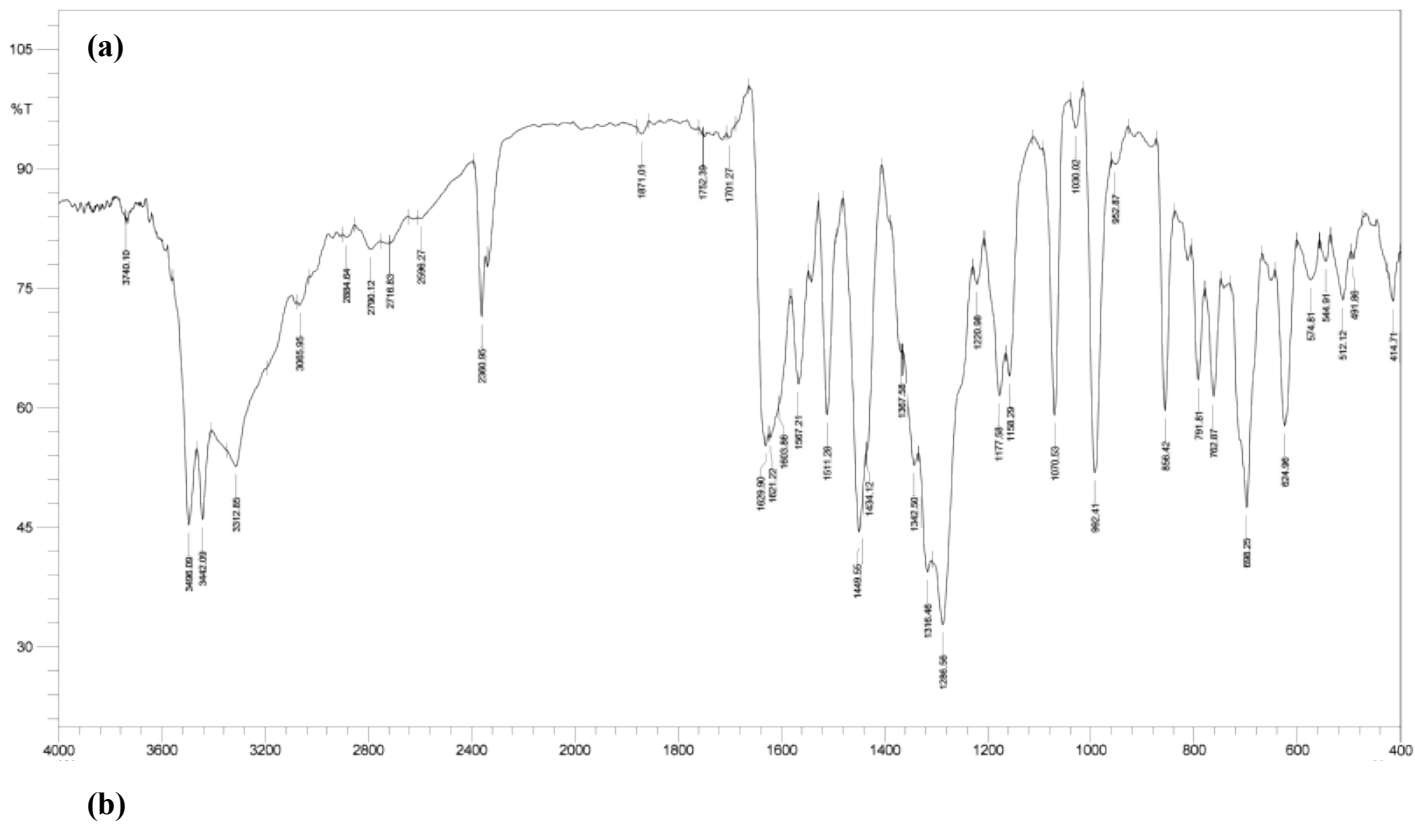


Figure S2. FT-IR of (a) pure THB and (b) THB reduced Au NPs.

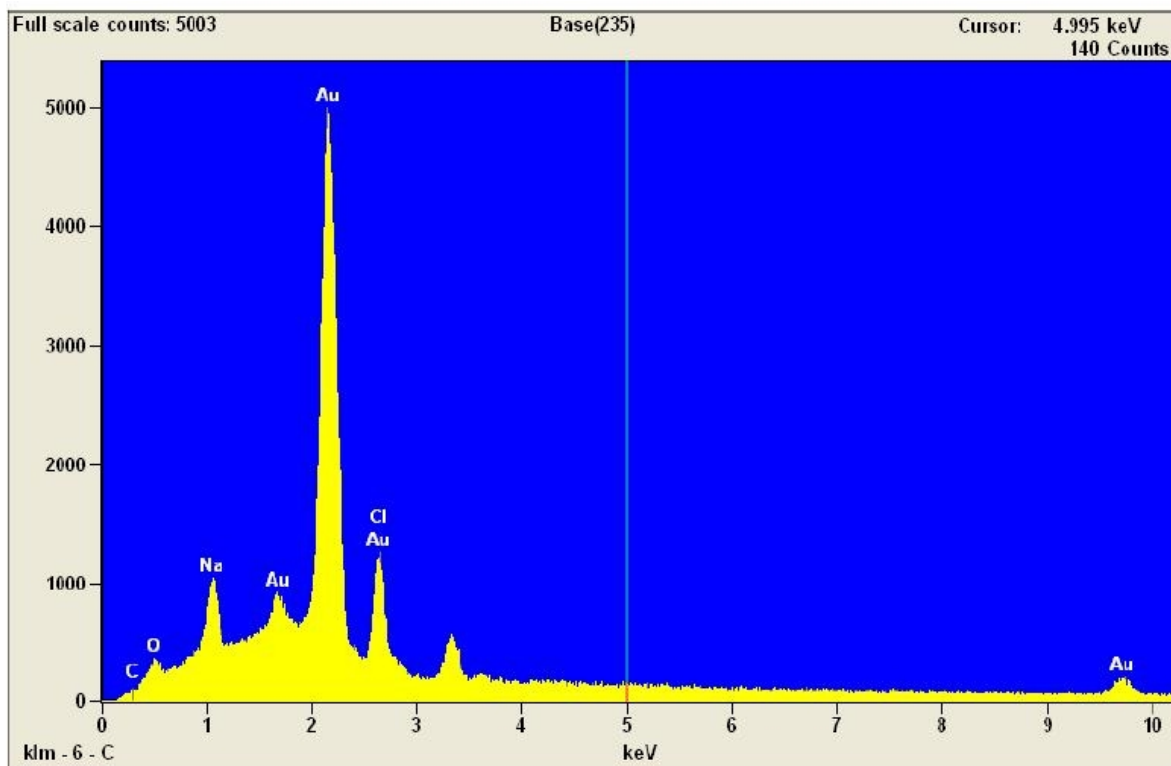


Figure S3. SEM/EDX spectrum of THB-Au NPs

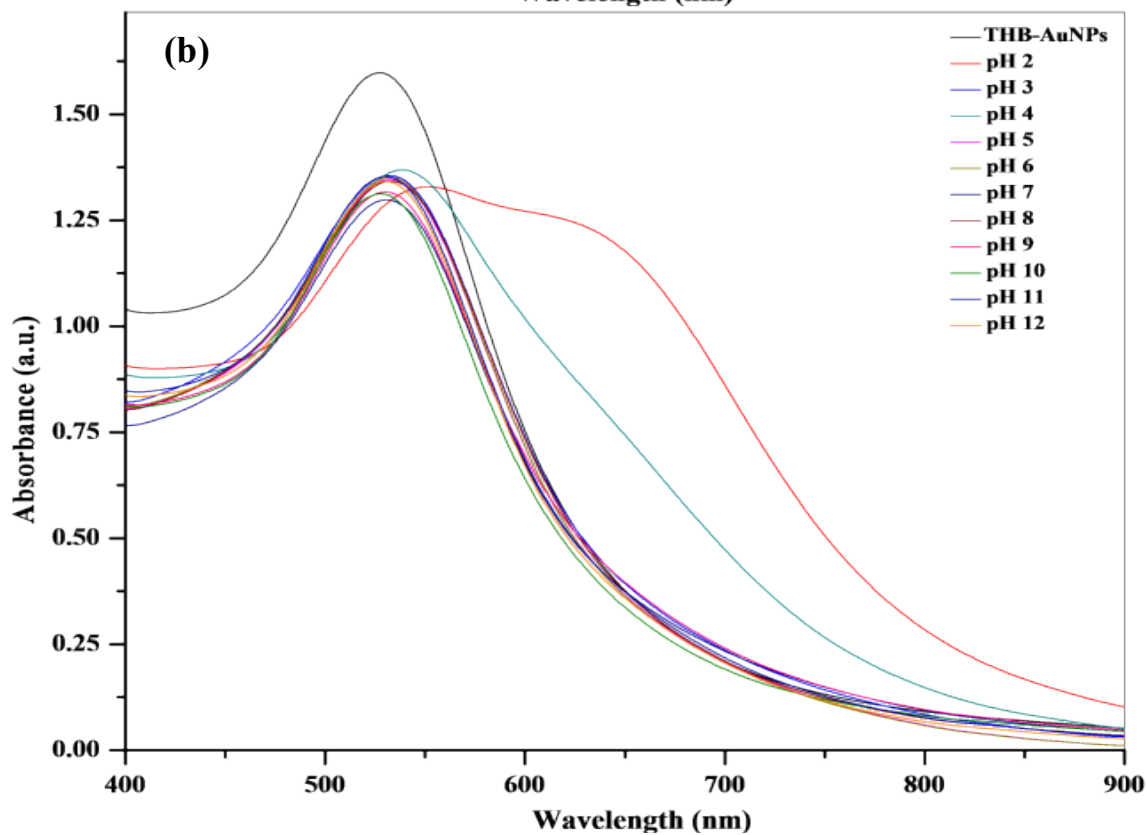
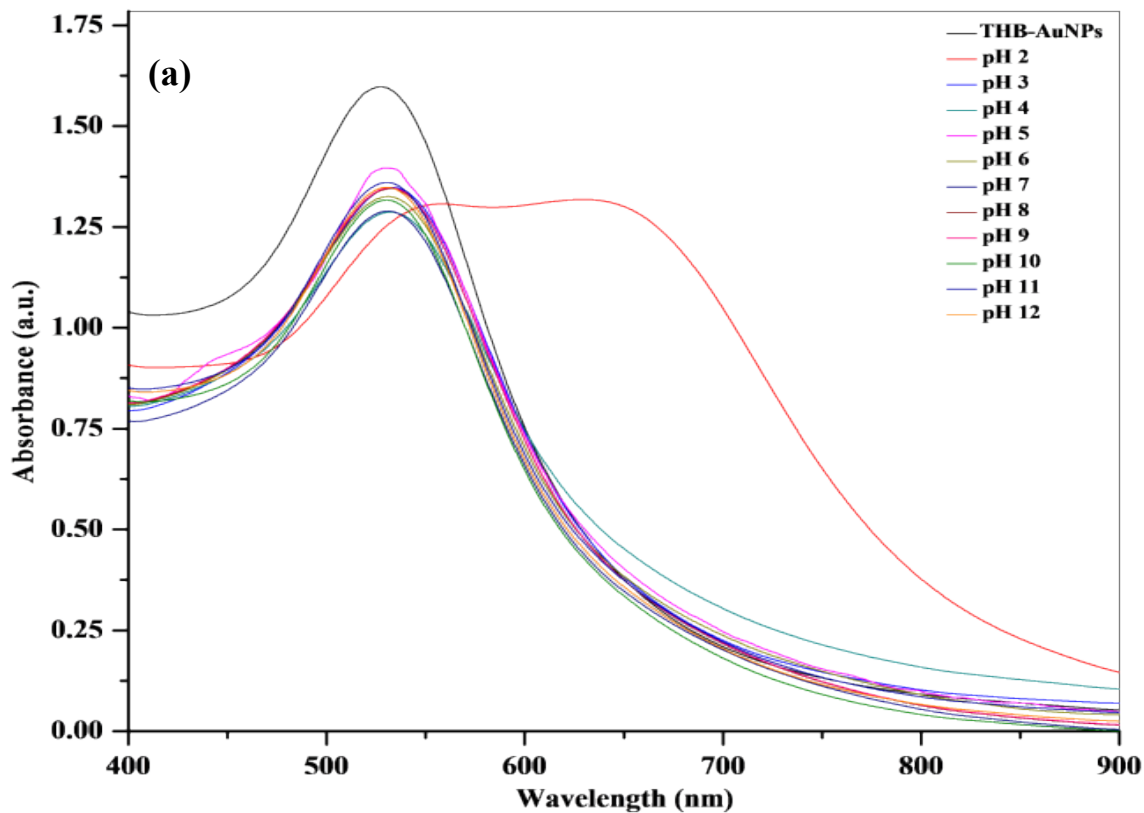


Figure S4. UV-visible absorption spectra of THB-Au NPs in the presence of adenine (0.1 mM) at (a) ammonium acetate and (b) sodium acetate buffers pH in the range of 2.0 to 12.0.

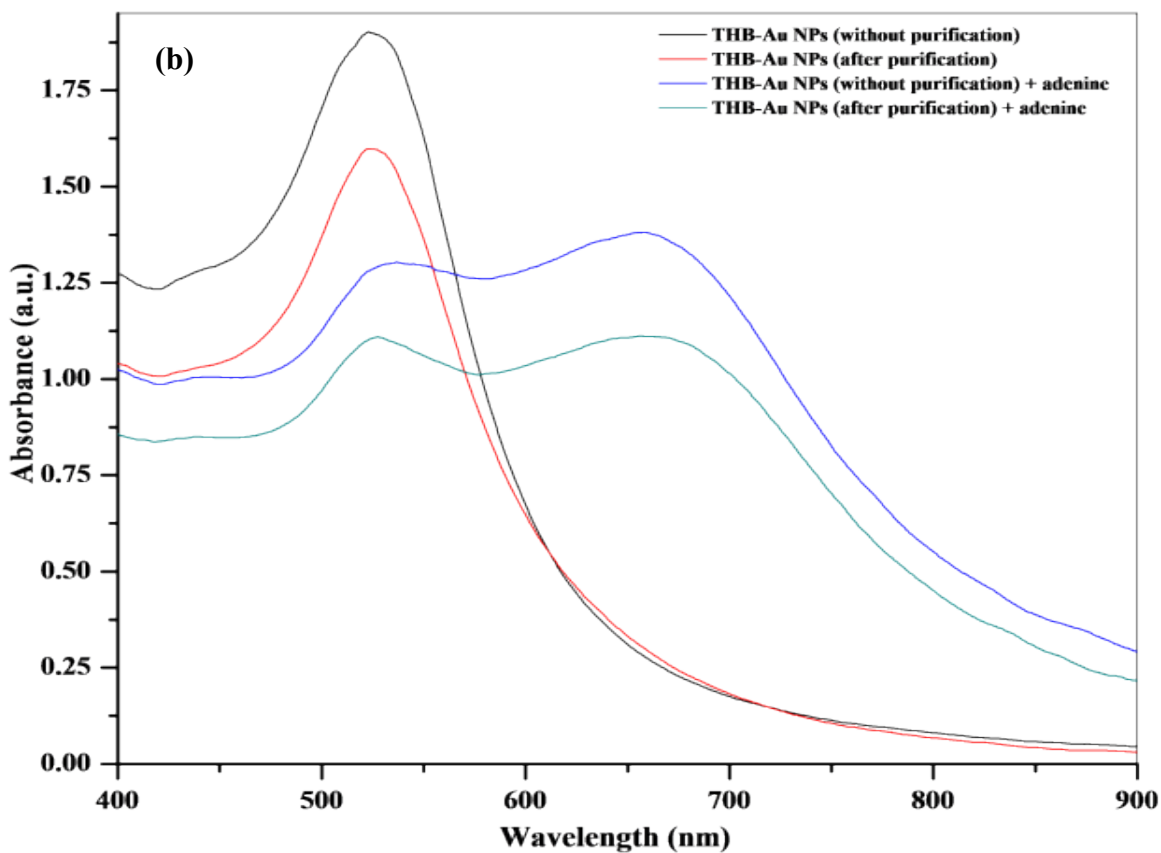
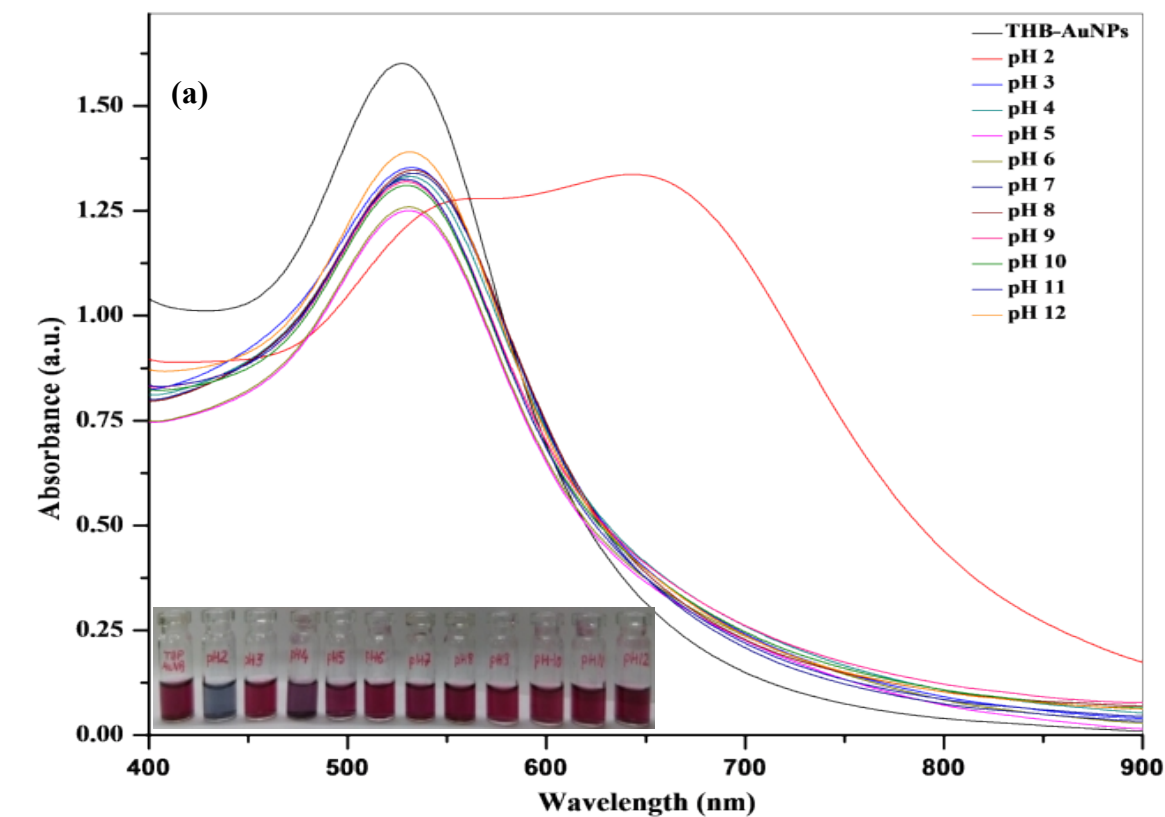


Figure S5. (a) UV-visible absorption spectra of THB-Au NPs in the presence of adenine (0.1 mM) at Tris-HCl pH in the range of 2.0 to 12.0. UV-visible absorption spectra of purified and unpurified THB-Au NPs in the presence of adenine (0.1 mM) at PBS pH 4.0.

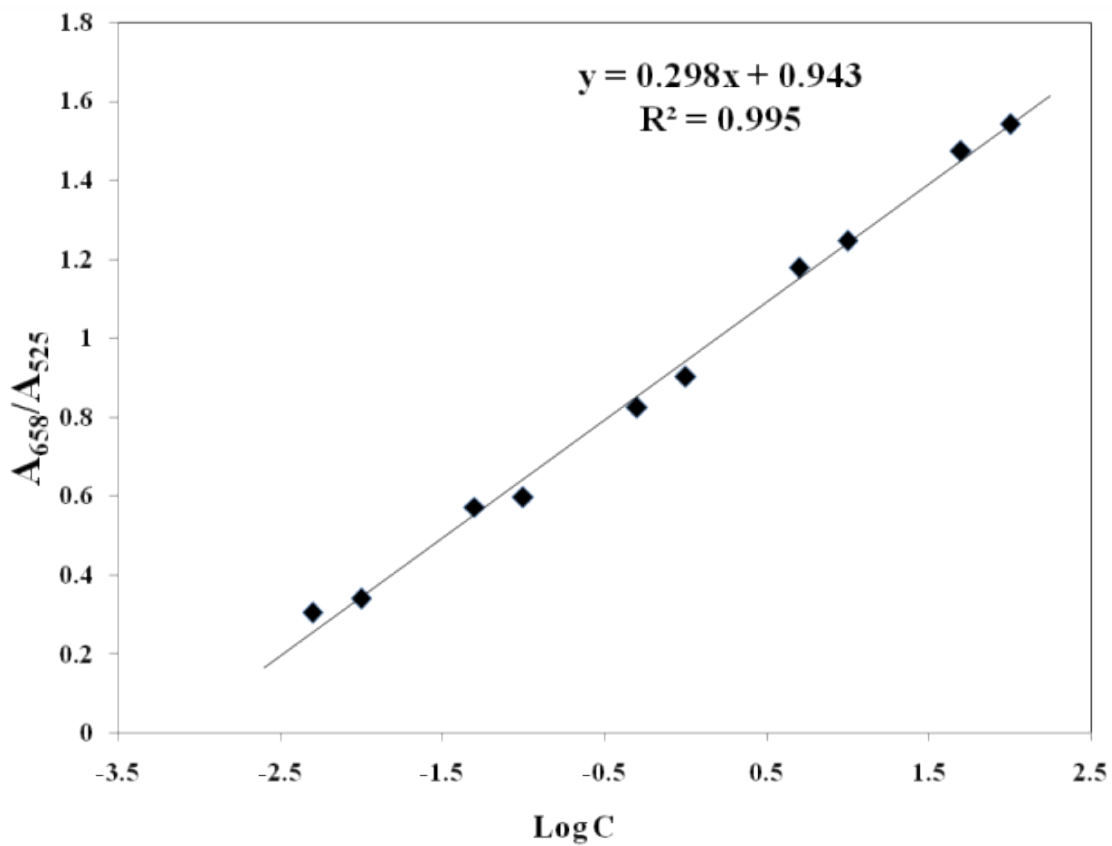


Figure S6. Calibration graph plotted between the absorption ratio (A_{658}/A_{525}) and log of adenine concentration (0.005 – 100 μM) at PBS pH 4.0.

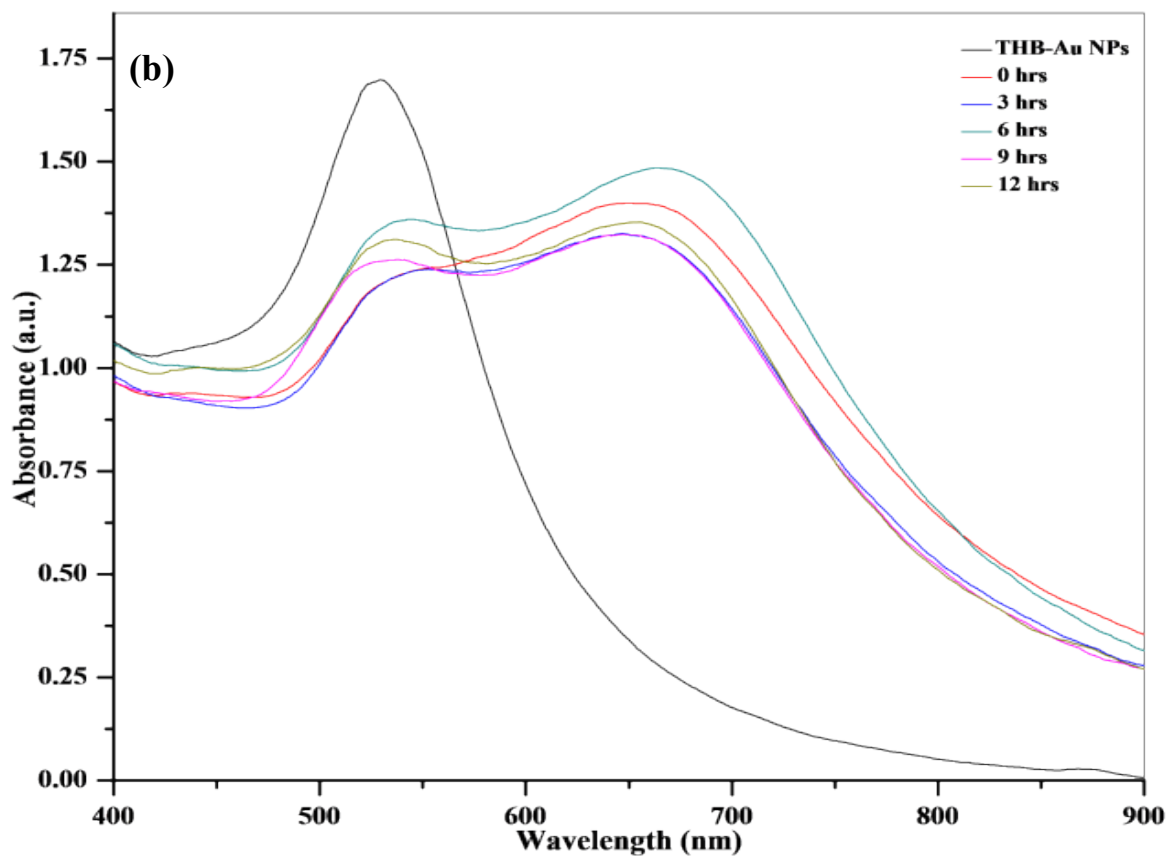
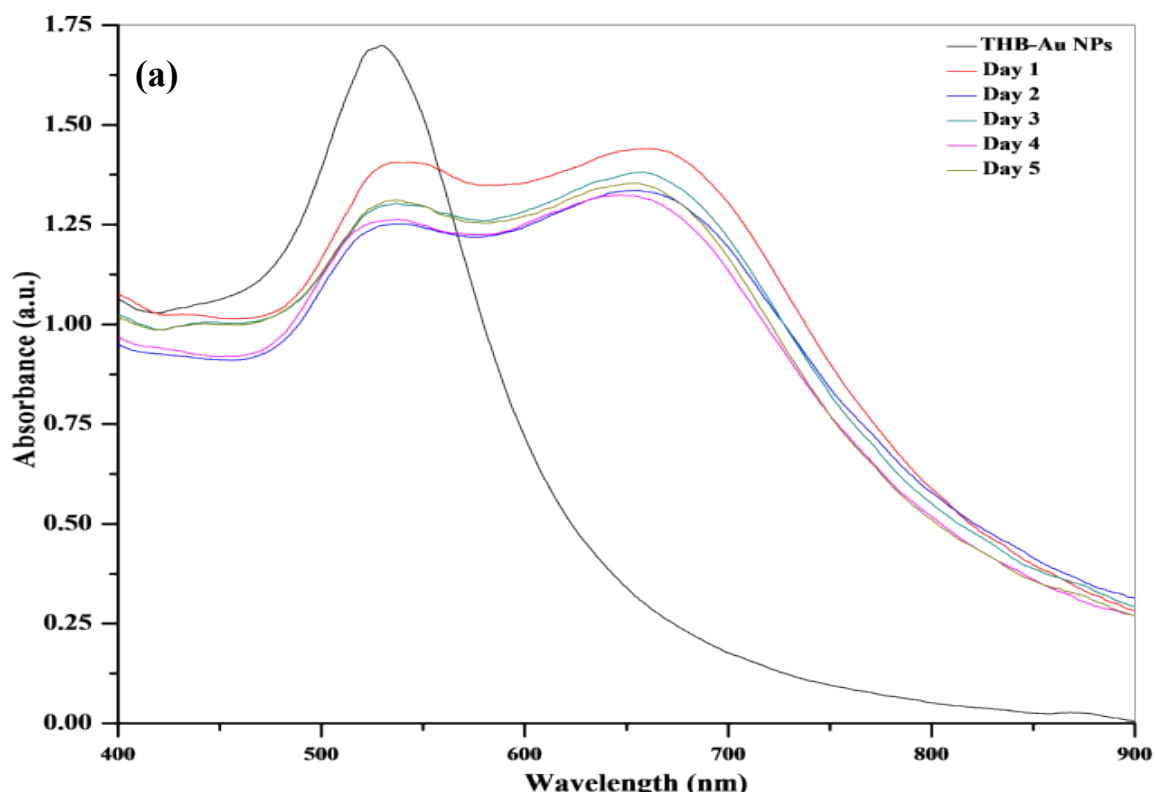


Figure S7. UV-visible absorption spectra of THB-Au NPs with spiked adenine ($100 \mu\text{M}$) in urine and serum samples at (a) inter- and (b) intra- day.

The calculation for the number of THB molecules per Au particle are as follows:

The average number of THB molecules on the surfaces of single Au NPs can be calculated from UV-visible absorption spectra and TEM analysis, using following formula.

$$N = N_m / N_p \text{ ----- (1)}$$

where N is the number of THB molecules per nanoparticle, N_m is the number of THB molecules (N_m) = $C_a \times 6.023 \times 10^{23}$ ----- (2)

The concentration (C_a) of THB was calculated from the intensity of THB in water using the absorption spectroscopy (C_a) = 0.178 mM

Therefore, the number of THB molecules (N_m) = 1.07×10^{20} ----- (3)

Similarly, the number of nanoparticles may be estimated by the following formula

$$N_p = W / W_{np} \text{ ----- (4)}$$

where N_p is the number of nanoparticles, W is the weight of Au formed theoretically, 398 g of $\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$ on reduction will give 198 g of Au.

The concentration of $\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$ = 1 mM, from that 1000 mL solution contains (W) = 198×10^{-3} g of Au.

From the TEM data, we can estimate the radius of the nanoparticle as well as can calculate the weight of each nanoparticle using following formula

The weight of 12.5 nm (d) nanoparticles (W_{np}) = 15.29×10^{-18} g ----- (5)

Thus the number of 12.5 nm present in 1000 mL of gold colloids (N_p) = 5.2×10^{17}

From the above, the number of THB molecules per nanoparticle (N) = $N_m / N_p \sim 206$

Hence, the number of THB molecules per nanoparticle ~ 206