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Supplementary information for:

Bio-modified Fe_3O_4 core/Au shell nanoparticles for targeting and multimodal imaging of cancer cell

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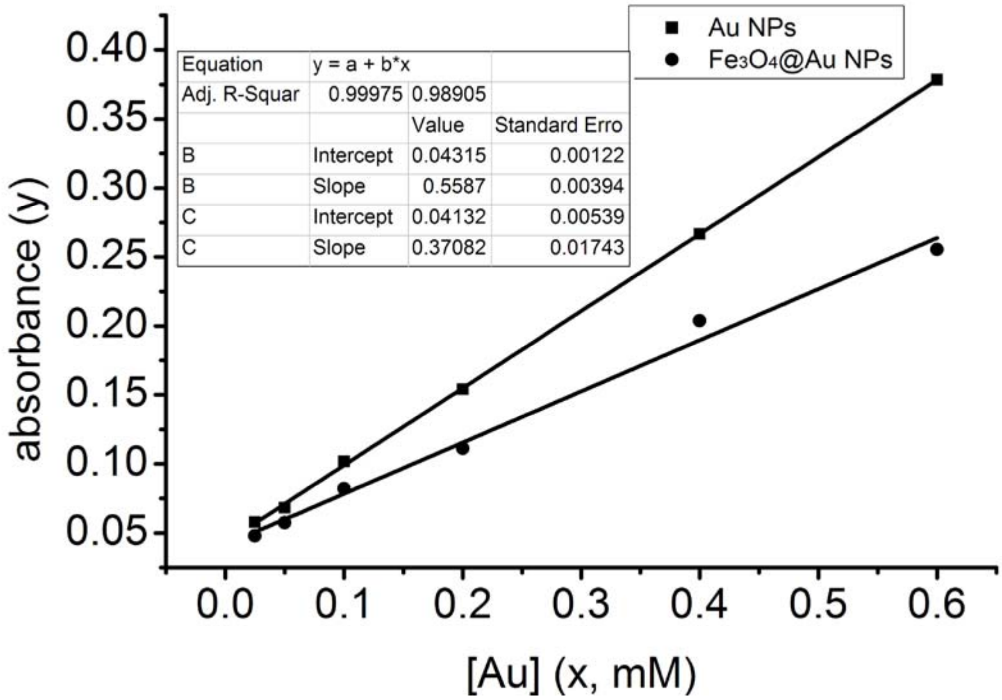

Figure S1. Standard curves of Fe_3O_4@Au nanoparticles and gold nanoparticles.

Based on the absorption peak of gold nanoparticle, a 532 nm pulse laser was used as the irradiation source in our photoacoustic imaging experiment. Therefore it is reasonable to detect the absorption cross-sections of the nanoparticles at 532 nm. We have prepared the standard solutions of Fe_3O_4@Au nanoparticles and gold nanoparticles and measured their absorbance at 532nm. Then we drew the standard curves to determine their molar absorption coefficient.

The fitted linear regression equation of gold nanoparticles and Fe_3O_4@Au nanoparticles are

$$y= 0.5587x+0.04315$$

and

$$y= 0.37082x+0.04132$$

where y is the absorbance, x is the gold concentration of nanoparticles and Fe_3O_4@Au nanoparticles (unit mM).

According to the Lambert-beer Law, the slope of the standard curve is the product of molar absorption coefficient and path length. In our experiment, we used the 96-well plate assay with a path length of 0.5cm. So the molar absorption coefficient of gold nanoparticles at 532 nm is

$$\varepsilon_1 = \frac{0.5587 mM^{-1}}{0.5 cm} \approx 1.12 \times 10^3 M^{-1} \cdot cm^{-1}$$

And the molar absorption coefficient of gold nanoparticles at 532 nm is

$$\varepsilon_2 = \frac{0.37082 mM^{-1}}{0.5 cm} \approx 0.75\times10^3 M^{-1}\cdot cm^{-1}$$

The absorption cross sections are proportional to the intensity of the absorption (or emission) between the two levels involved. The absorption of light is in general governed by the Beer-Lambert Law, for optically thin samples:

$$\ln(\frac{I_0(\lambda)}{I(\lambda)}) = \sigma(\lambda)\times l\times c'$$

where $I_0(\lambda)$ and $I(\lambda)$ are the transmitted light intensities at a wavelength λ with and without sample present, l is the path length, and c' is the molecule concentration. The constant σ is the absorption cross section. If l is in centimeters, and c' in molecules cm^{-3}, then σ has units of cm^2 $molecule^{-1}$

$$A(\lambda) = \lg(\frac{I_0(\lambda)}{I(\lambda)}) = \varepsilon(\lambda)\times l\times c$$

where the A(λ) is the absorbance at a wavelength λ, c is the molar concentration (unit M).

So the absorption cross-section at a wavelength λ

$$\sigma(\lambda) = \frac{\varepsilon(\lambda)}{N_A}\times \mathrm{In}10$$

The absorption cross-sections of gold nanoparticles (σ_1) and Fe_3O_4@Au nanoparticles (σ_2) at 532 nm are

$$\sigma_1 = 1.12\times10^3\times3.825\times10^{-24} L\cdot cm^{-1} \approx 4.28\times10^{-18} cm^2$$

$$\sigma_2 = 0.75\times10^3\times3.825\times10^{-24} L\cdot cm^{-1} \approx 2.87\times10^{-18} cm^2$$

The absorption cross-sections of Fe3O4@Au are close to that of gold nanoparticles.

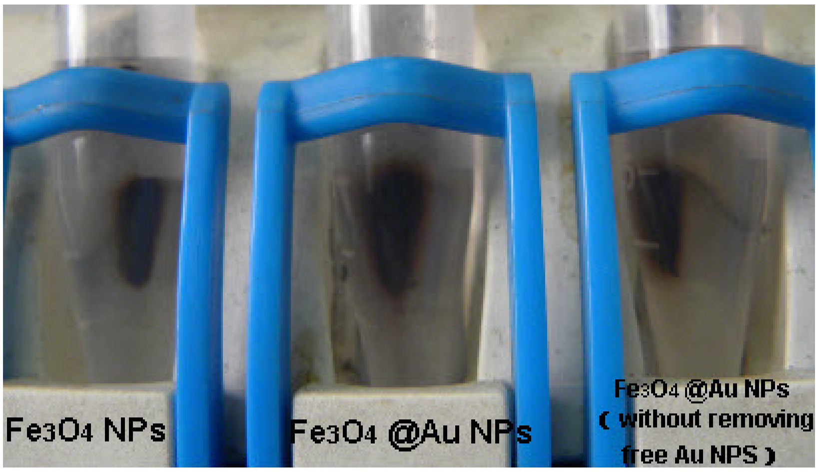

Figure S2. Magnetic separation effect of Fe_3O_4 nanoparticles, Fe_3O_4@Au nanoparticles with and without removing free gold nanoparticles.

As shown in figure S2, similar to Fe_3O_4 nanoparticles, Fe_3O_4@Au nanoparticles are attracted to the walls of the vial when a magnet is present. And there are still a few free gold nanoparticles of pink color remaining in the solution before purification. The free gold nanoparticles were separated by a magnet. Their absorbance at 532 nm was measured to be 0.0579. Basing on the standard equation of gold nanoparticles ($y= 0.5587x+0.04315$, figure S1), the Au concentration of free gold nanoparticles was calculated to be 0.026 mM, which is 2.9 % of the total Au concentration.