

## Supporting Information

### Differentiation of biothiols from other sulfur-containing biomolecules using iodide-capped gold nanoparticles

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#### Calculation of the concentration of the GNPs (*c*):

The total mass of GNPs in the colloidal solution = The total mass of Au in added HAuCl<sub>4</sub>.

$$(4/3\pi r^3) \times \rho \times (6.02 \times 10^{23}) \times c \times V = m_{\text{HAuCl}_4} \times (M_{\text{Au}}/M_{\text{HAuCl}_4})$$

$$[(4/3 \times 3.14 \times (20 \times 10^{-7} \text{ cm})^3)] \times 19.30 \text{ g/cm}^3 \times (6.02 \times 10^{23}) \times c \text{ mol/cm}^3 \times 60 \text{ cm}^3 \\ = (60 \text{ g} \times 0.01\%) \times (197/340)$$

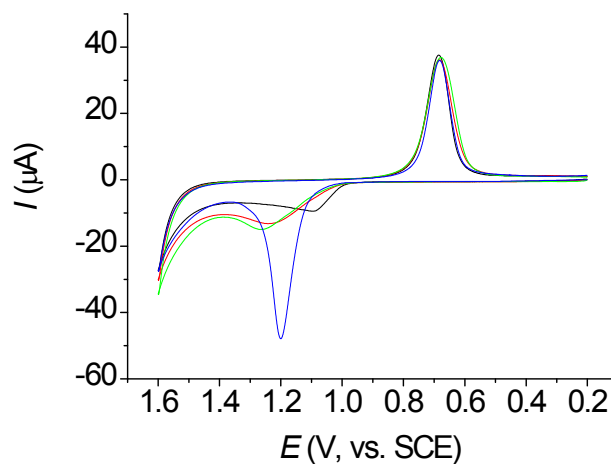
$$c = 1.48 \times 10^{-13} \text{ mol/cm}^3 = 1.48 \times 10^{-4} \text{ nmol/cm}^3 = 0.148 \text{ nmol/l}$$

Where *r* (= 20 nm) is the radius of GNPs, *ρ* (= 19.30 g/cm<sup>3</sup>) is the density of bulk gold, *V* (= 60 cm<sup>3</sup>) is the volume of the colloidal solution, *m*<sub>HAuCl<sub>4</sub></sub> (=60 g × 0.01%) is the mass of added HAuCl<sub>4</sub>, *M*<sub>Au</sub> is the atomic weight of Au, and *M*<sub>HAuCl<sub>4</sub></sub> is the molecular weight of HAuCl<sub>4</sub>.

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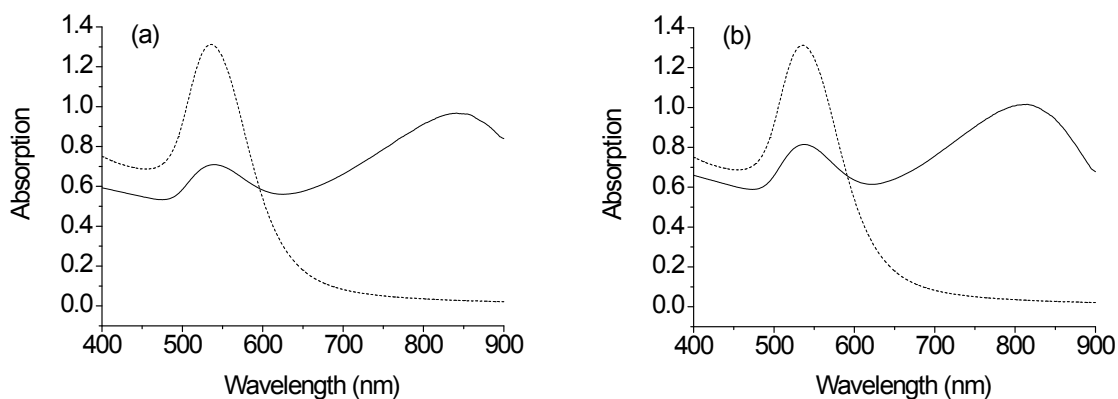
\* Corresponding author.

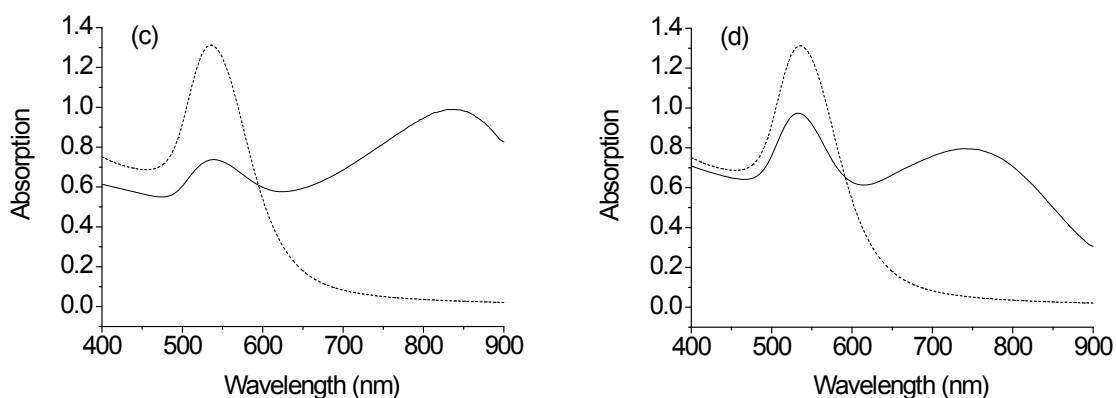
E-mail address: lntukj@163.com (J.-F. Kong), zfchen@tongji.edu.cn (Z.-F. Chen).



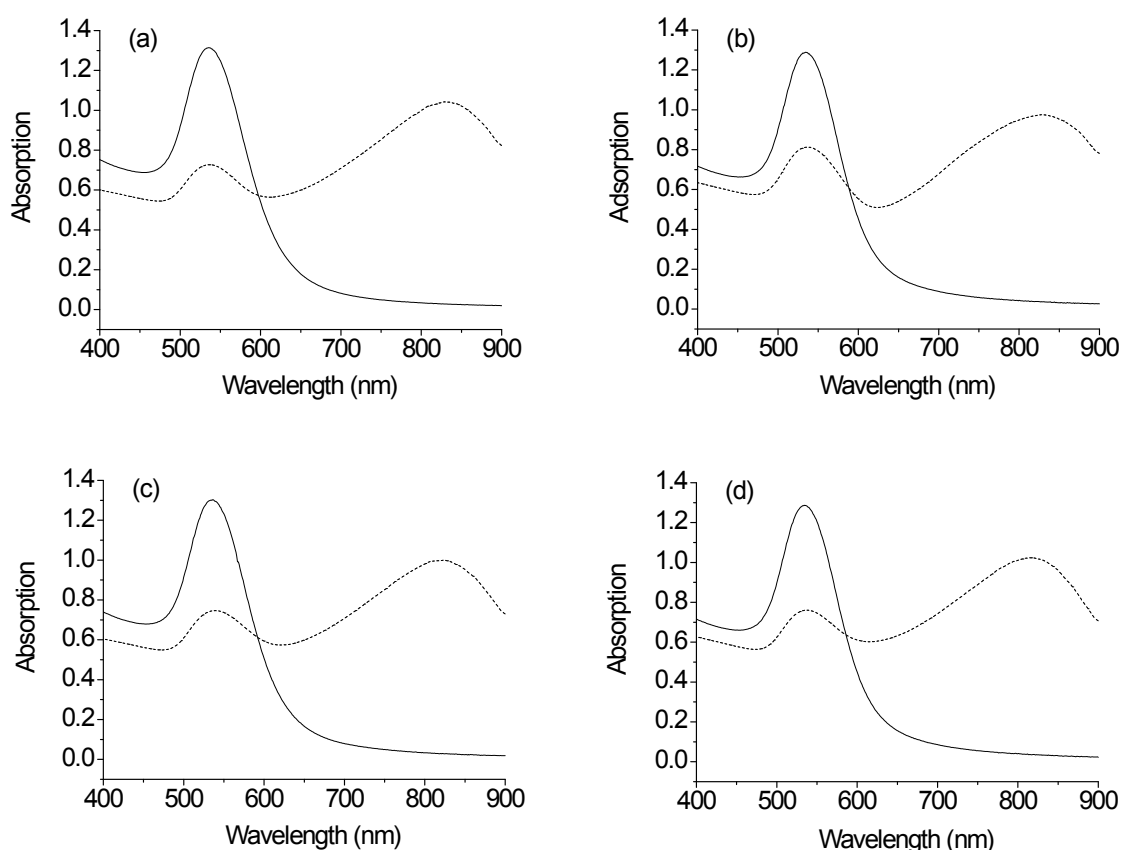
**Figure S1.** Cyclic voltammograms of bare Au (black line), Cl<sup>-</sup>-Au (red line), Br<sup>-</sup>-Au (green line) and I<sup>-</sup>-Au (blue line) electrodes in 0.15 M PBS (pH 3.0). Scan rate, 100 mV/s.

Prior to the experiments, a bare polycrystalline gold electrode of 2 mm diameter was wet polished with 0.05  $\mu\text{m}$  Al<sub>2</sub>O<sub>3</sub> powders to obtain a mirror surface followed by sonication in distilled water for 10 s, and was subjected to repeated scanning in a wide potential range in 0.1 M H<sub>2</sub>SO<sub>4</sub> solution until reproducible voltammograms were obtained. The halide-modified Au electrodes (Cl<sup>-</sup>-Au, Br<sup>-</sup>-Au or I<sup>-</sup>-Au) were prepared by dipping the pretreated Au electrode into 0.1 M aqueous solutions of different halide salts for 20 min followed by a thoroughly rinsing with distilled water.

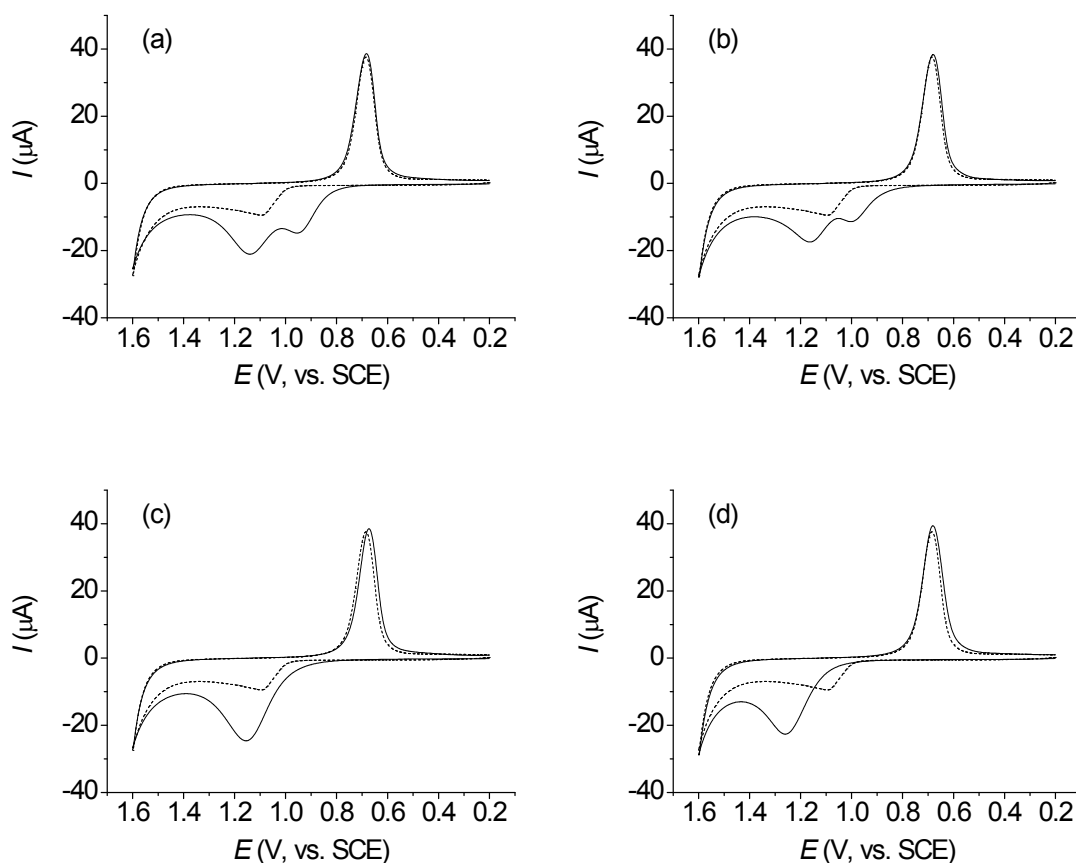




**Figure S2.** UV-vis spectra of 40 nm iodide-capped GNPs in the presence of 5  $\mu\text{M}$  cysteamine (a), 2-mercaptoethanol (b), 2-mercaptoethylamine (c), and 6-mercapto-1-hexanol (d). The corresponding dashed lines represent the UV-vis spectra of GNPs before adding analytes. All the spectra were acquired at 10 min after the addition of analytes.

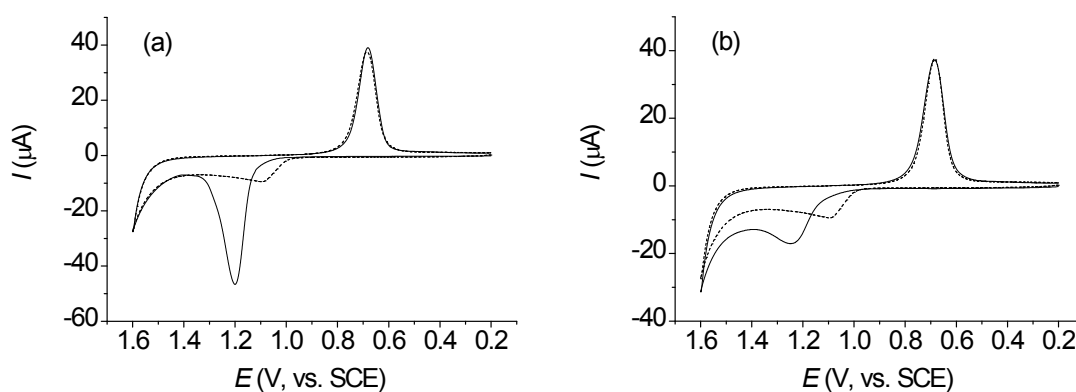


**Figure S3.** UV-vis spectra of 40 nm iodide-capped GNPs in the presence of 100  $\mu\text{M}$  cystamine (a), 2,2'-thiodiethanol (b), thiourea (c), and thiocarbohydrazide (d). The corresponding dashed lines represent the UV-vis spectra of GNPs without any capping in the presence of 2  $\mu\text{M}$  cystamine, 40  $\mu\text{M}$  2,2'-thiodiethanol, 2  $\mu\text{M}$  thiourea and 2  $\mu\text{M}$  thiocarbohydrazide. The spectra of solid line and dashed line were acquired at 60 min and 2 min, respectively, after the addition of the analytes.



**Figure S4.** Cyclic voltammograms of Cys-Au (a), Hcy-Au (b), CysGly-Au (c), and Glu-Au (d) electrodes in 0.15 M PBS (pH 3.0). Scan rate, 100 mV/s. The dashed line represents the cyclic voltammogram of bare Au electrode under the same experimental condition.

The biothiols-modified Au electrodes (Cys-Au, Hcy-Au, CysGly-Au or Glu-Au) were prepared by dipping the pretreated Au electrodes into 10 mM aqueous solutions of the corresponding biothiols for 10 min followed by a thoroughly rinsing with distilled water.



**Figure S5.** Cyclic voltammograms of FSN-Au (a) and Brij 35-Au (b) electrodes in 0.15 M PBS (pH 3.0). Scan rate, 100 mV/s. The dashed line represents the cyclic voltammogram of bare Au electrode under the same experimental condition.

The FSN-modified Au electrode (FSN-Au) and Brij 35-modified Au electrode (Brij 35-Au) were obtained by dipping the pretreated Au electrode into 5 wt % FSN and Brij 35 aqueous solutions for 10 min, respectively, followed by a thoroughly rinsing with distilled water.