

Supporting Information

Mercaptopyridine-Functionalized Au Nanoparticles for Fiber-Optic Surface Plasmon Resonance Hg²⁺ Sensing

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Contents:

Figure S-1. The molecular simulation for 4-MPY-Hg²⁺-4-MPY

Figure S-2. The electric field with the different numbers of Au NPs

Figure S-3. 4-MPY/Au NPs amplification signal stability

Figure S-4. The UV-vis absorption spectrum for different batches of Au NPs/4-MPY

Figure S-5 The sensor for Hg²⁺ detection by using different batches of 4-MPY modified Au NPs

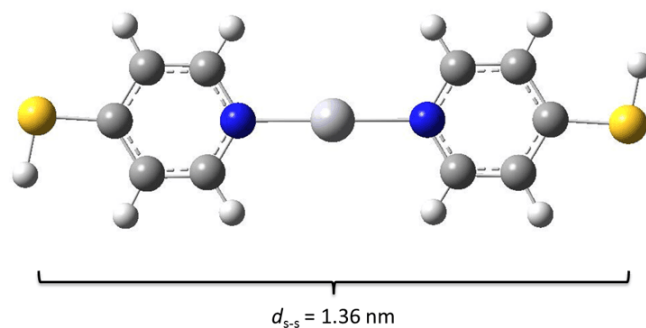
Figure S-6 The particle size distribution histogram of Au NPs

Figure S-7 SPR wavelength of Au sensor region modified with different concentration of 4-MPY

Figure S-8 Au NPs modified with different volume of 4-MPY

Figure S-9 The limit of detection (LOD) was 3.34 nM for Hg²⁺.

Table S-1 Comparison of this work with some published assays for Hg²⁺ using Au NPs.



The geometry was optimized at B3LYP/LANL2DZ level.

Figure S-1. The molecular simulation for 4-MPY- Hg^{2+} -4-MPY.

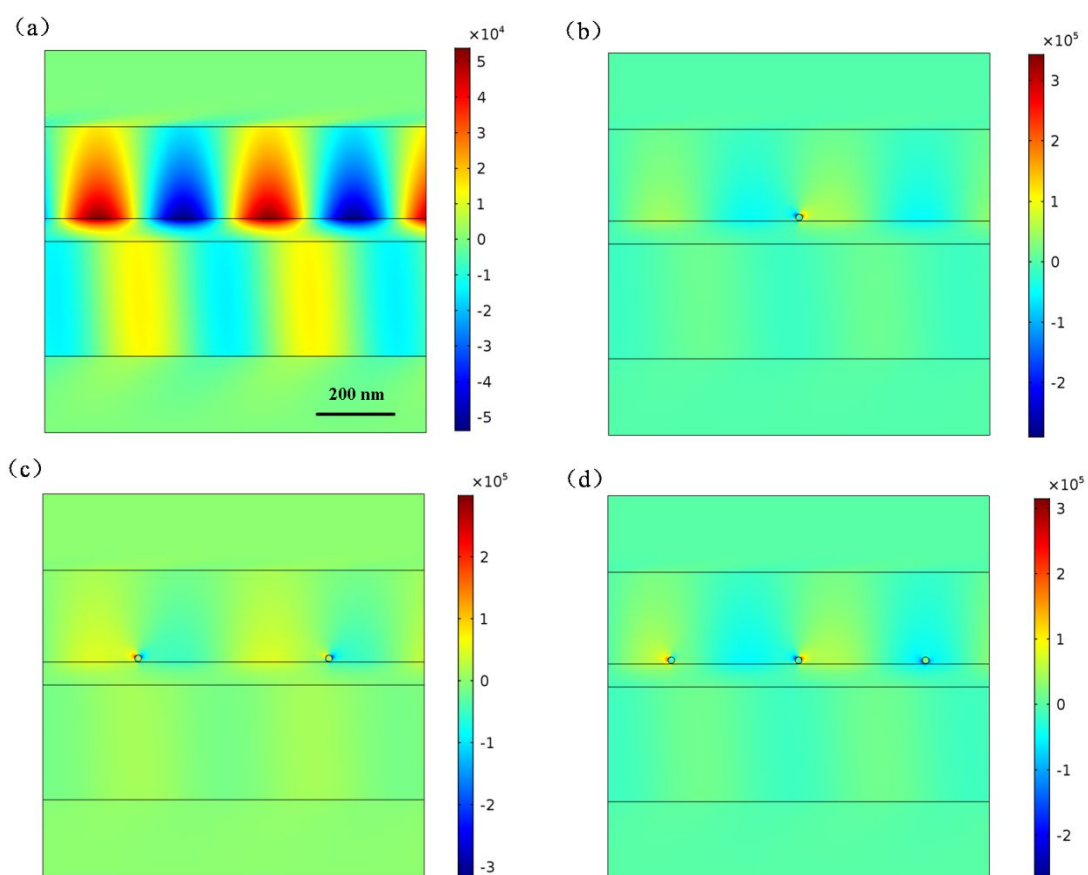


Figure S-2. The electric field with the different numbers of Au NPs (Spatial electric field ($|E_x|$))

distribution for Au NPs on SPR).

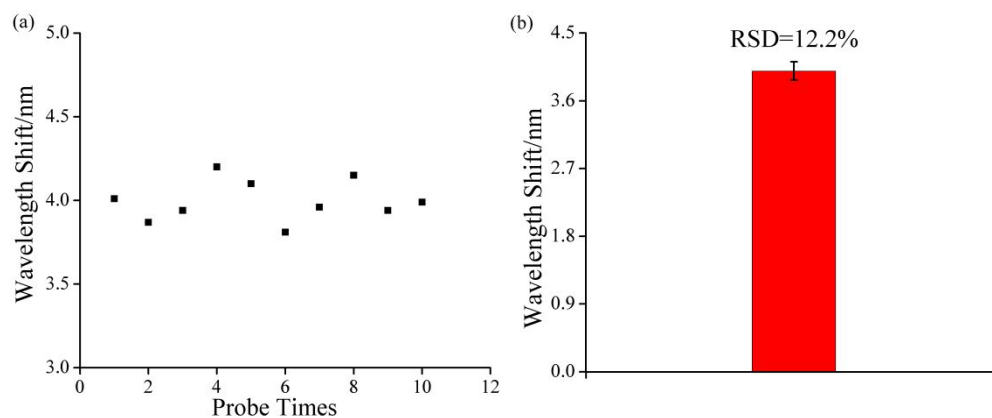


Figure S-3. (a) 4-MPY/Au NPs amplification signal stability (the concentrations of Hg^{2+} was $30\ \mu\text{M}$). (b) The relative standard deviation (RSD) of the amplification signal by Au NPs/4-MPY is about 12.2%. These results indicated that the slightly aggregation of Au NPs/4-MPY do not show obvious interference on Hg^{2+} sensing.

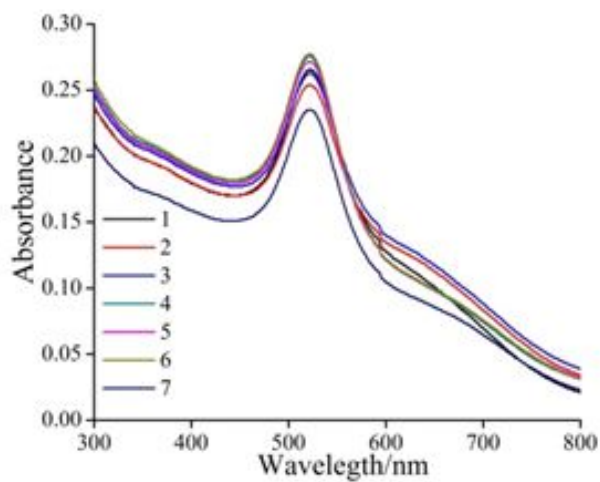


Figure S-4. The UV-vis absorption spectrum for different batches of Au NPs/4-MPY.

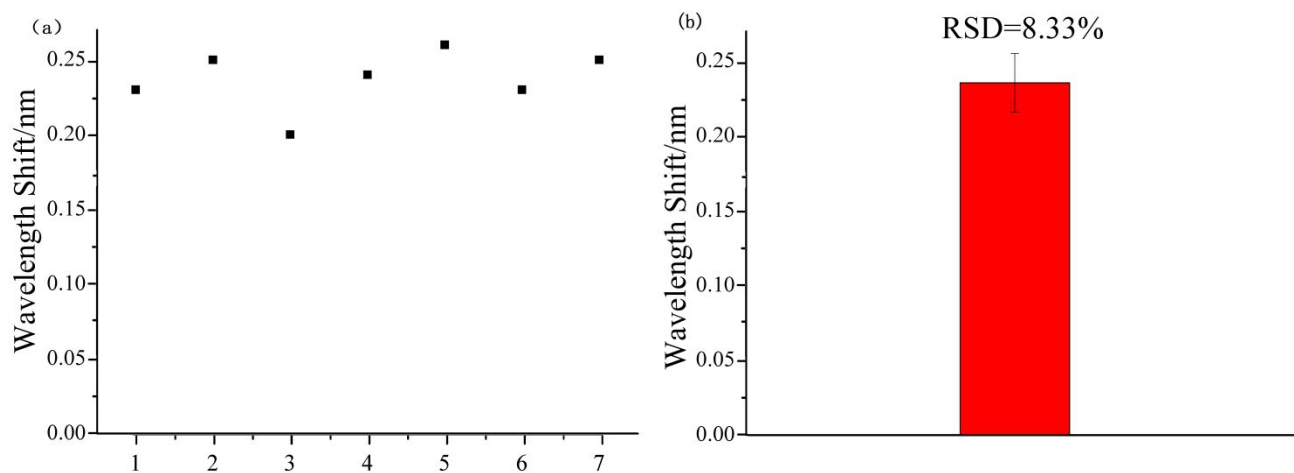


Figure S-5. Our present sensor for Hg^{2+} detection by using different batches of 4-MPY modified Au NPs. (a) 4-MPY/Au NPs amplification signal stability (the concentrations of Hg^{2+} was $1\ \mu\text{M}$). (b) The relative standard deviation (RSD) of the amplification signal by Au NPs/4-MPY is about 8.33%.

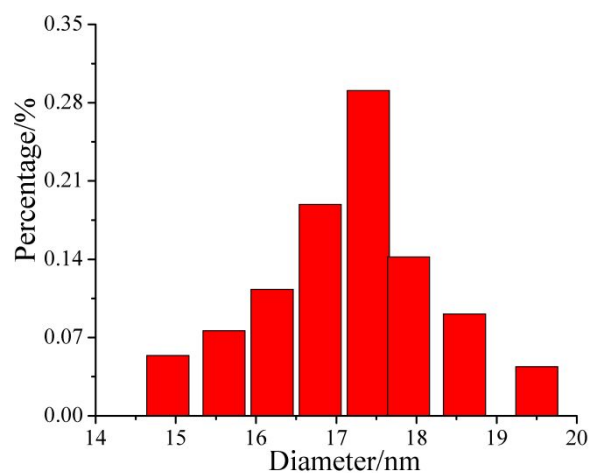


Figure S-6. The particle size distribution histogram of Au NPs.

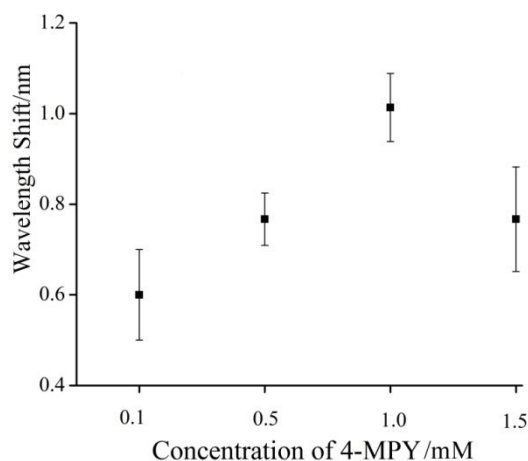


Figure S-7. SPR wavelength of Au sensor region modified with different concentration of 4-MPY (the concentration of Hg^{2+} was 500 nM). Au film modified with the 1mM 4-MPY possess the largest shift in SPR wavelength, and thus 1mM 4-MPY was selected to fabricate SPR tags for Hg^{2+} detection. Prior to apply Au NPs/4-MPY tags for Hg^{2+} detection, the optimal concentrations of 4-MPY attached on Au NPs should be considered.

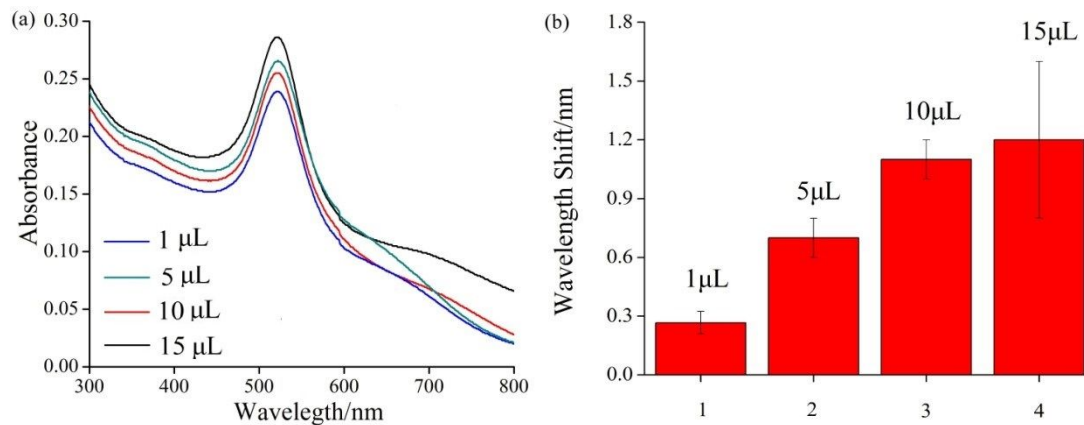


Figure S-8. Au NPs modified with different volume of 4-MPY. (a) The UV-vis of Au NPs/4-MPY (b) SPR wavelength (the concentration of Hg^{2+} was 500 nM). The Au NPs modified with 10 μL 4-MPY (1 mM) exhibits larger shift in SPR wavelength for Hg^{2+} detection. The UV-vis of Au NPs modified with 15 μL 4-MPY (1 mM) shows larger aggregation. And the SPR wavelength was not stabilizing.

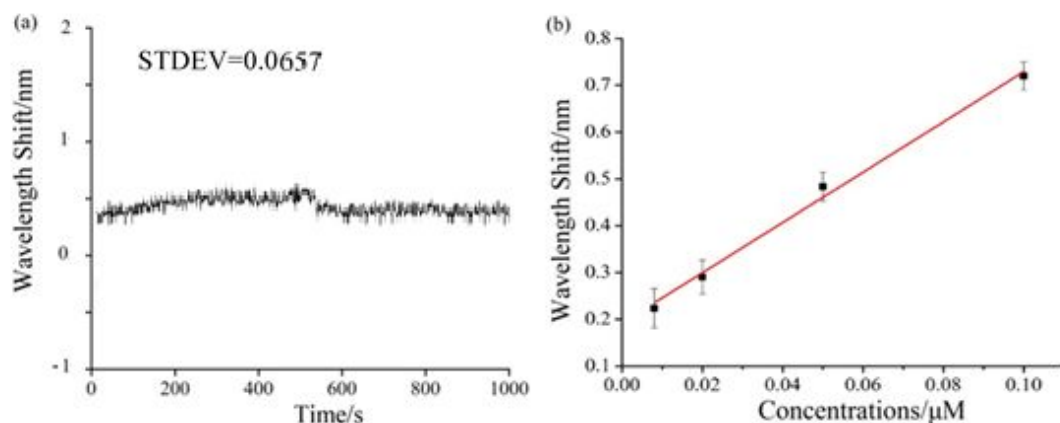


Figure S-9. (a) The STDEV of signal-to-noise was 0.0657; (b) the linear correlation with the Hg^{2+} concentration was exhibited in the concentration range from 8 to 100 nM. The limit of detection (LOD) was determined by signal-to-noise of 3 plus the background signal and obtained 3.34 nM for Hg^{2+} .

Table S-1

Comparison of this work with some published assays for Hg^{2+} using Au NPs.

Detection method	Linear range	LOD	Reference
Colorimetric sensing	0–680 nM	11.9 nM	(1)
Colorimetric	0.05–1.2 μM	20 nM	(2)
Chemiluminescent Sensor	10–600 nM,	1 nM	(3)
Colorimetric	8.76 nM–0.127mM	8.76 nM	(4)
UV–vis spectroscopy	0.05 - 1.0 μM	6.0 nM	(5)
Fluorescent	37.5 nM–12.5μM	8.6 nM	(6)
Localized Surface Plasmon Resonance	1 nM –1 mM	0.38 nM	(7)
Fluorescent	0–5.0 μM	28 nM	(8)
Electrochemical sensor	0.1 nM – 250 μM	0.01 nM	(9)
Fluorescence	0–600 nM	8 nM	(10)
Surface Plasmon Resonance	8 nM -40μM	3.34 nM	This work

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