Supporting Information for

A Highly Sensitive, Colorimetric Detection of Mercury (II) in Aqueous Media by Quaternary Ammonium Groups-Capped Gold Nanoparticles at room temperature

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Materials and Instrumentation: All chemicals were purchased from major suppliers such as Alfa Aesar, Sigma-Aldrich and used as received, except for 11-mercapto-undecyl-trimethyl- ammonium, which was purchased from Prochimia. The UV-vis spectra were recorded with UV2450 spectrophotometer (Shimadzu). Mass spectrometry data were obtained with a Micromass LCT electronspray ionization time of flight (ESI TOF) with positive-ion mode. X-ray photoelectron spectroscopy (XPS) data were obtained with an ESCALab220i-XL electron spectrometer from VG Scientific using 300W radiation. Thermogravimetric analysis (TGA) of QA-AuNPs was performed using a Pyris 1 (Perkin Elmer) with a rate of 10 °C/ min from room temperature to 600 °C. Dynamic light scattering (DLS) and zeta potential (ζ) were performed on a Zeta Sizer Nano ZS (Malvern Zetasizer 3000HS and He/Ne laser at 632.8 nm at scattering angles of 90 at 25 °C). TEM images were

obtained by using a JEOL1400 TEM at an accelerating voltage of 100 kV. The solutions of AuNPs were irradiated with solar light generated by a solar light simulator (PLS-SXE300, Changtuo, Inc., China) with the intensity at ~ 396 mW/cm^2. The drinking water used in this assay is bottled water from a local supermarket.

Preparation of AuNPs: AuNPs were prepared by the citrate-mediated reduction of $HAuCl_4$.[1] A stirred aqueous solution of $HAuCl_4$ (41 mg, 1 mM) in 100 mL water was heated to reflux, and a trisodium citrate solution (114 mg, 38.8 mM) dissolved in hot water (10 mL) was added rapidly. The solution was heated under reflux with vigorous stirring for another 15 min, its color changed from pale yellow to deep red. The solution was cooled to room temperature with a slow and continuous stir. The resulting solution was filtered with a polyethersulfone membrane (filter unit is 22 μm) to remove large clusters and insoluble compounds. The sizes of the nanoparticles were about 13 nm by TEM analysis, the corresponding absorption band is at ~520 nm.

Preparation of QA-AuNPs: 11-Mercapto-undecyl-trimethyl-ammonium (MTA) modified gold nanoparticles were prepared by adding 10 mM MTA (100 μL) to the as-prepared 13-nm-diameter AuNPs solution (10 nM, 10 mL) under slow stir. 10 μL of 1 M HCl solution in water was added to the AuNPs solution. After reaction for 2 hours at room temperature, the MTA-modified AuNPs were purified by centrifugation (20 min, 14000×g) and resuspended in distilled water for five times. The concentration of the MTA-modified AuNPs was determined with the UV-vis spectra (the extinction coefficients of 13 nm of AuNPs is about $2.7\times10^8 M^{-1}cm^{-1}$).[2]

Table S1. A comparison of the QA-AuNPs and other AuNPs-based sensors for detecting Hg^{2+}

Sensor	Readout	LOD (μM)	Selectivity	Analysis time (min)	Operating temperature	References
DNA-AuNPs	Naked-eye or Absorption	0.1 [a]	Hg^{2+}	480	50 °C	(3)
DNA-AuNPs	Naked-eye or flatbed canner	0.01	Hg^{2+}	30	34 °C	(4)
DNA-AuNPs	Naked-eye or Absorption	1.0 [a]	Hg^{2+}	5	Room	(5)
DNA-AuNPs	Naked-eye or Absorption	0.01 [a]	Hg^{2+} [b]	20	Room	(6)
DNA-AuNPs	Fluorescence and naked-eye	0.04 [c]	Hg^{2+}	30	Room	(7)
Acid-AuNPs	Naked-eye or Absorption	0.1[a]	Hg^{2+} [b]	120	Room	(8)
Acid-AuNPs	Fluorescence	0.005 [c]	Hg^{2+} [b]	10	Room	(9)
Acid-AuNPs	The hyper Rayleigh scattering	0.025	Hg^{2+} [b]	<7	Room	(10)
Tween-AuNPs	Naked-eye or Absorption	0.1	Hg^{2+}, Ag^{+}	5	Room	(11)
QA-AuNPs	Naked-eye or Absorption	0.03	Hg^{2+}	<1	Room	This study

[a] Readout is UV-Vis absorption

[b] By adding masking agents

[c] Readout is fluorescence

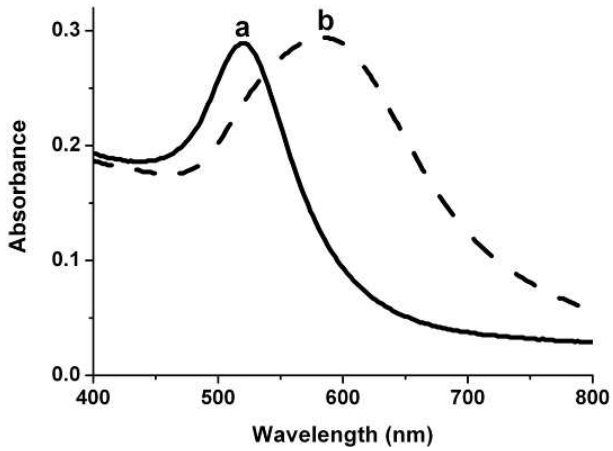

Figure S1. UV-vis absorption spectra of the QA-AuNPs in aqueous solutions with different pH values. a: pH 1.0-7.0, b: pH 9.0.

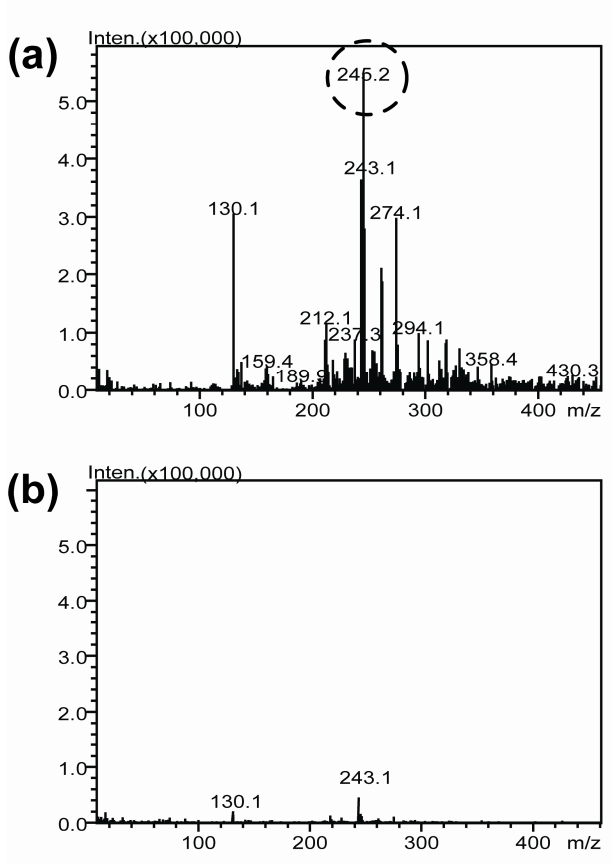

Figure S2. The ESI-MS data for the dissociated ligands from the surfaces of AuNPs (supernatant

collected after and before adding Hg^{2+}). (a) After the addition of Hg^{2+}, the value in the dashed circle is attributed to the ligands abstracted from the surfaces of AuNPs by Hg^{2+}; (b) Before the addition of Hg^{2+}.

Table S2. XPS for QA-AuNPs before (a) and after the addition of Hg^{2+} ions (b).

Elements	Au	S	C	N	Cl	O	Au/S	Au/C	Au/N
At. %(a)	36.34	2.46	50.09	3.89	2.85	4.38	14.77	0.73	9.34
At. %(b)	42.4	2.31	43.34	2.62	1.01	8.32	18.35	0.98	16.18

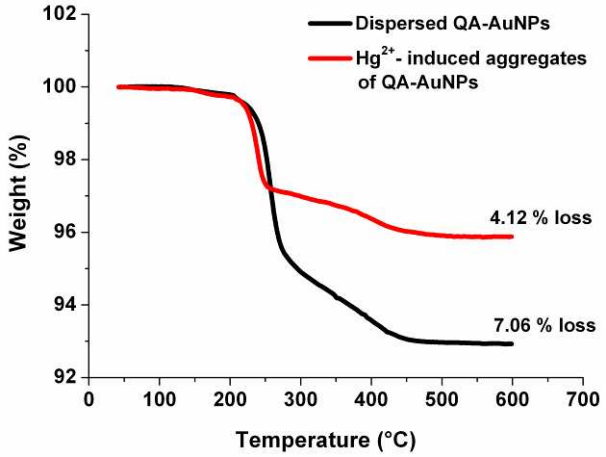

Figure S3. TGA data measuring the loss of ligands before and after adding Hg^{2+}.

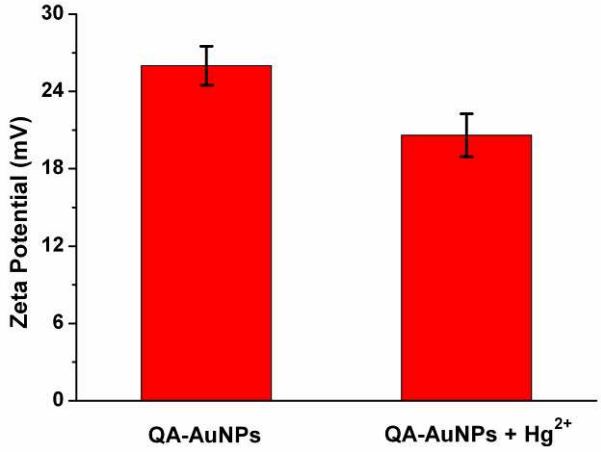

Figure S4. Zeta potential in response to QA-AuNPs before and after adding Hg^{2+}.

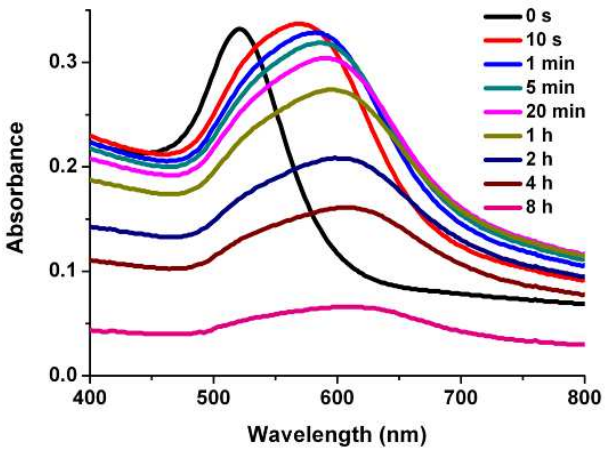

Figure S5. UV-vis absorption spectra of Hg^{2+}-caused aggregation of QA-AuNPs. The concentration of Hg^{2+} was 100 μM.

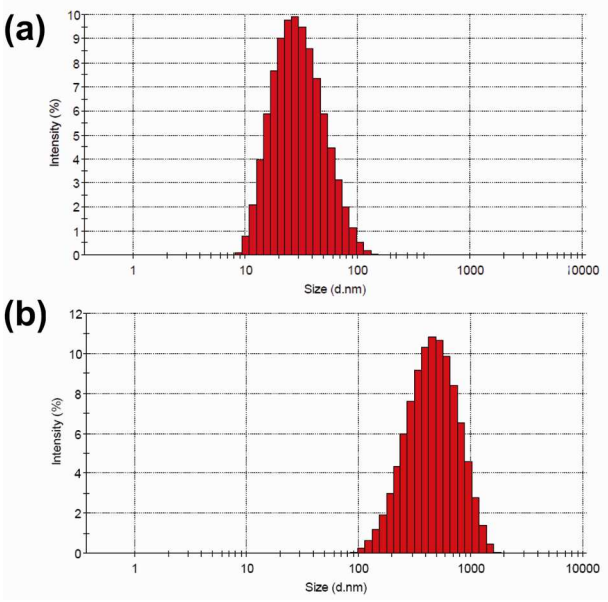

Figure S6. DLS measurements for QA-AuNPs before (a) and after (b) adding Hg^{2+}.

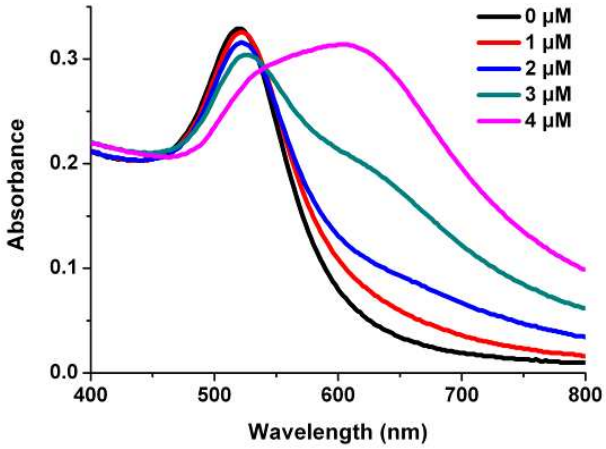

Figure S7. UV-vis absorption spectra of AuNPs in response to the low concentrations of Hg^{2+}.

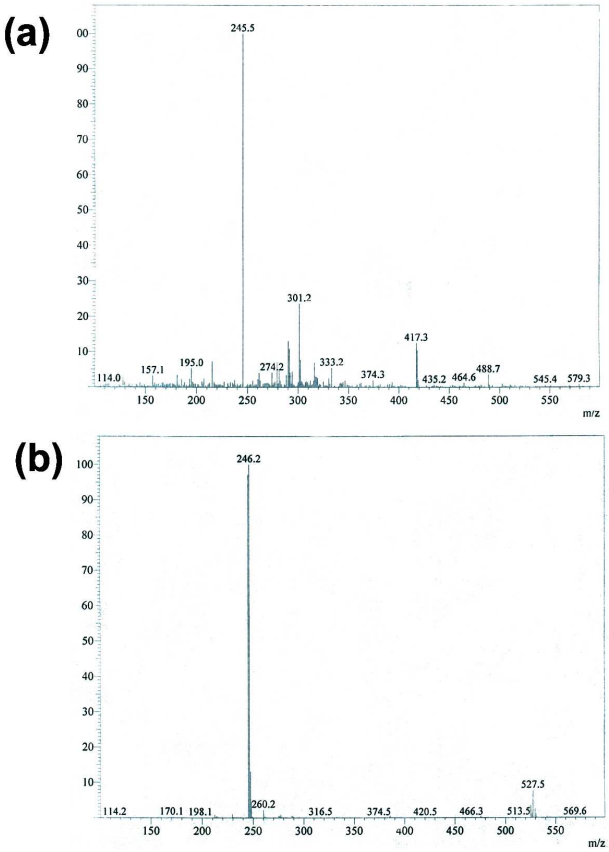

Figure S8. The ESI-MS data for (a) the dissociated ligands from the surfaces of AuNPs induced by 500 nM Hg^{2+} following by 30 s of solar light irradiation and (b) the solution of MTA that had been irradiated with 30 s of solar light.

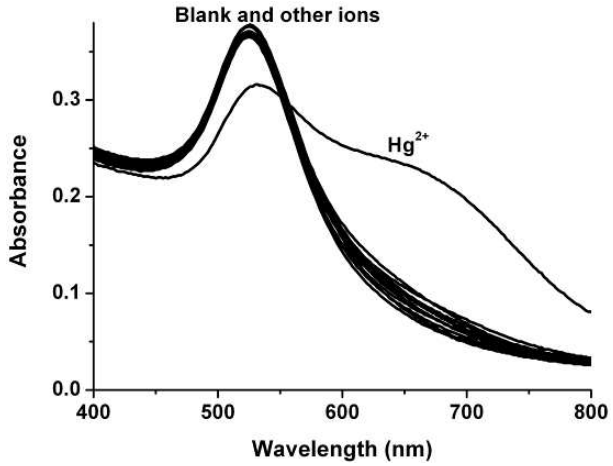

Figure S9. UV-vis absorption spectra of AuNPs that shows the selectivity of the system assisted by solar light irradiation for 30 s.

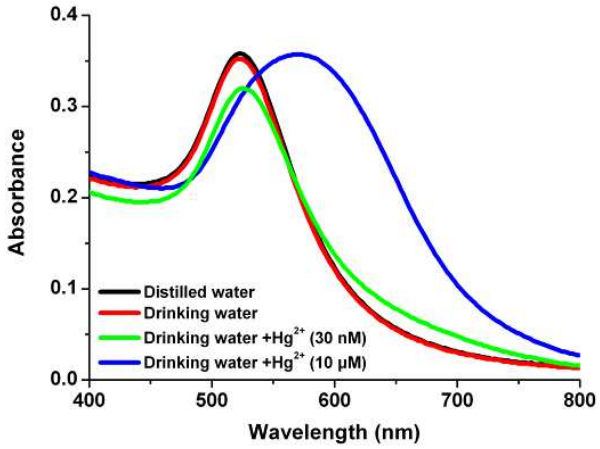

Figure S10. UV-vis spectra and colorimetric detection of Hg^{2+} in drinking water at pH 1.0: Black line, using distilled water as the solvent to disperse AuNPs; Red, using drinking water as the solvent to disperse AuNPs; Green, the drinking water solution of AuNPs added with 30 nM Hg^{2+} and irradiated with solar light for 30 s; Blue, the drinking water solution of AuNPs added with 10 μM Hg^{2+}.

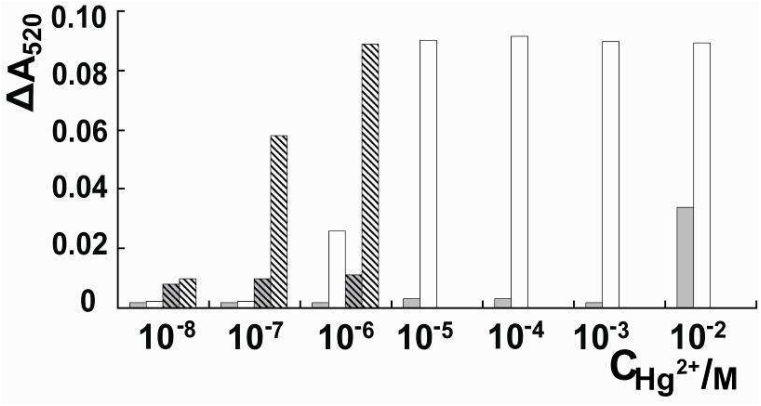

Figure S11. Selectivity of the Hg^{2+} sensor. Bars with white background represent absorbance responses after addition of various concentrations of Hg^{2+} ions together with the same concentration of other metallic ions. Bars with grey background represent absorbance responses after addition of various concentrations of other metallic ions. At lower concentrations of 3×10^{-8} ~1×10^{-6} M, the bars having biases represent absorbance response after solar light irradiation (30 s), the white and grey backgrounds represent the conditions as mentioned above.

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