

Supplementary Information

Synthesis of highly fluorescent gold nanoclusters and its use in sensitive analysis of metal ions

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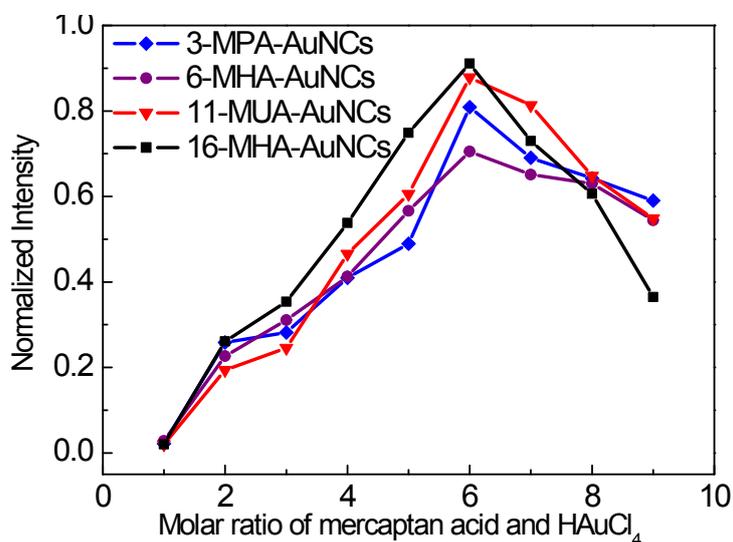


Fig. S1 Emission wavelength of four kinds of clusters operated from different molar ratio of mercaptan acid and HAuCl₄.

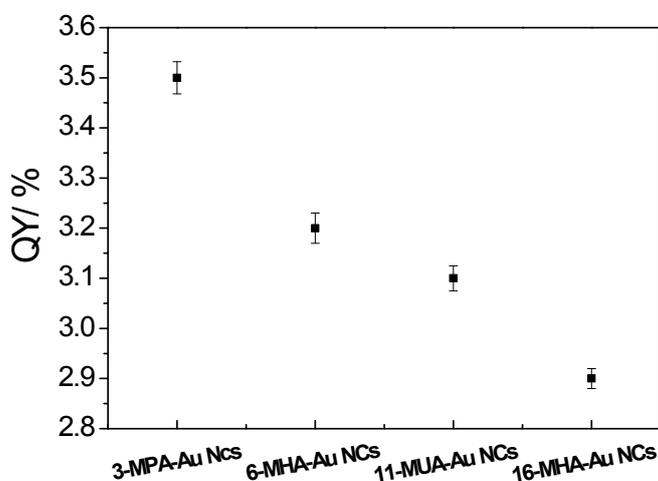


Fig.S2 The QY (%) of Au NCs (3-MPA-Au NCs, 6-MHA-Au NCs, 11-MUA-Au NCs and 16-MHA-Au NCs).

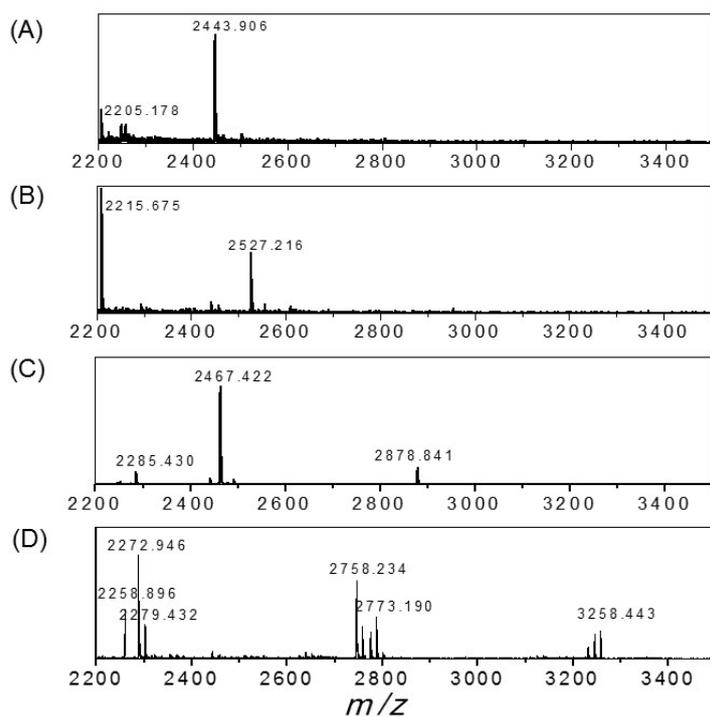


Fig. S3 MALDI-TOF mass spectrometry of four kinds of clusters operated in the positive ion mode. DCTB (1000ppm, dissolved in chloroform) was used as matrix. (A) 3-MPA-Au NCs (B) 6-MHA-Au NCs (C) 11-MUA-Au NCs (D) 16-MHA-Au NCs.

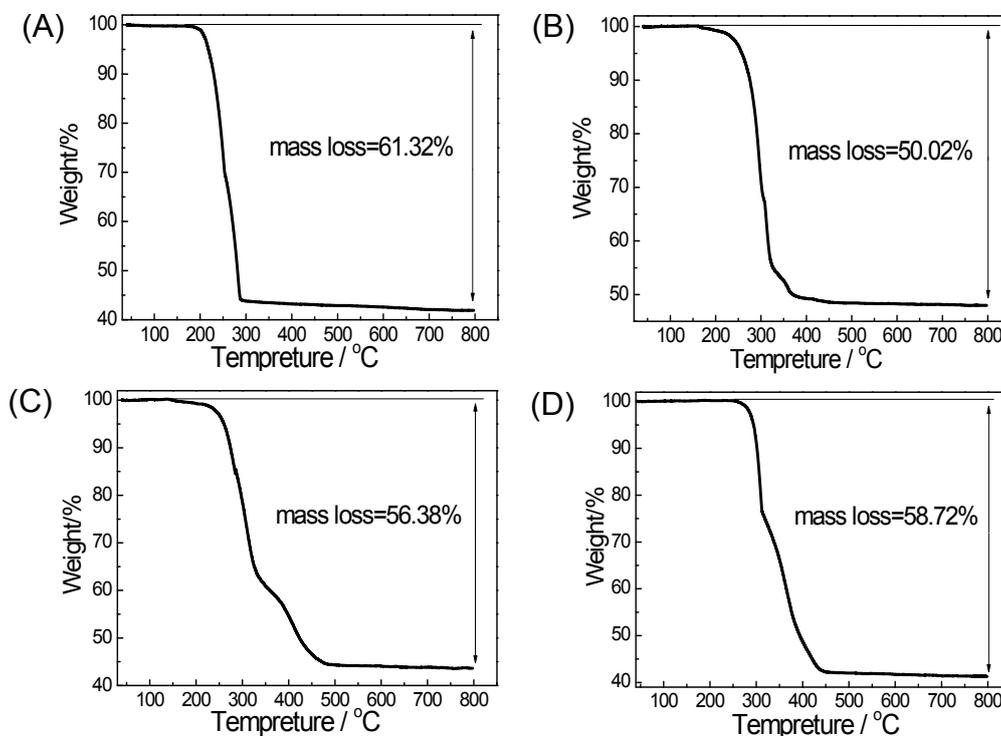


Fig. S4 TGA thermogram of four kinds of Au NCs with a heating rate of 10°C/min. (A) 3-MPA-Au NCs, (B) 6-MHA-Au NCs, (C) 11-MUA-Au NCs, (D) 16-MHA-Au NCs.

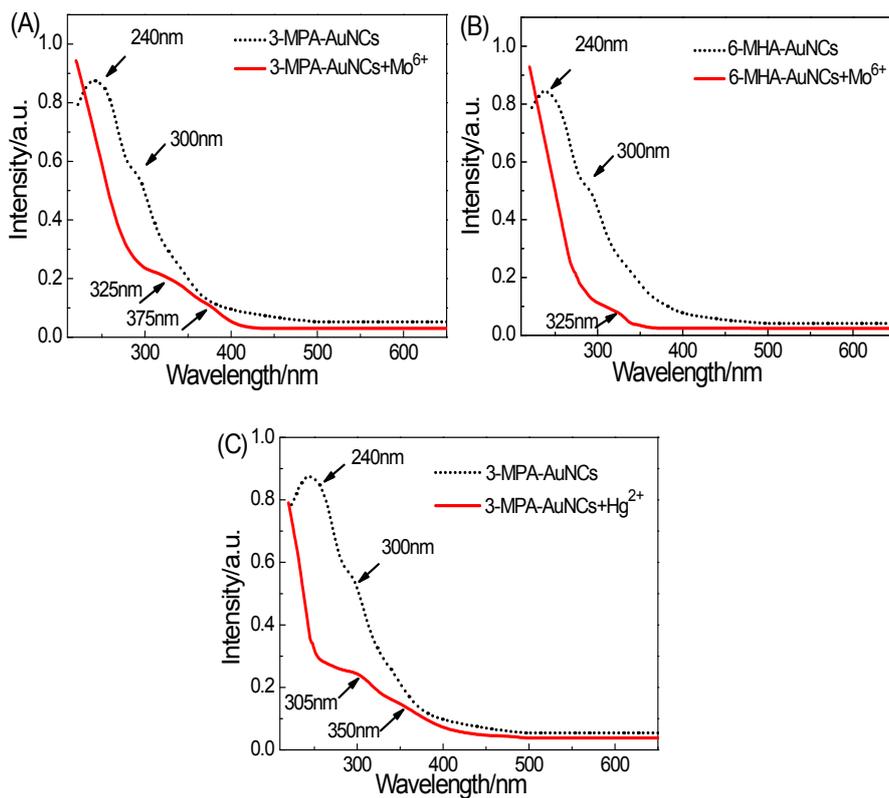


Fig. S5 The absorption spectrum of two kinds of Au NCs in the presence (solid line) and absence (dash line) of metal ions.

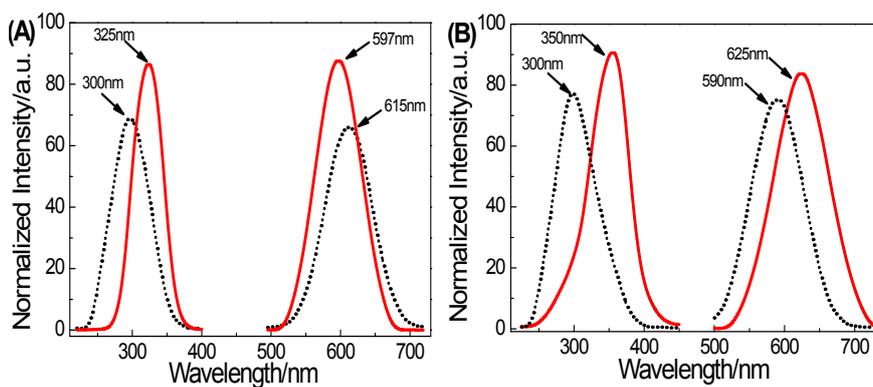


Fig. S6 Emission and excitation wavelength of two kinds of Au NCs in the presence (solid line) and absence (dash line) of metal ions. **(A)** 6-MHA-Au NCs added Mo(VI), **(B)** 3-MPA-Au NCs added Hg(II).

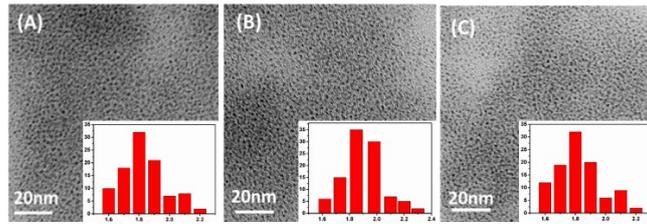


Fig. S7 TEM images of the Au NCs in the presence of metal ions. **(A)** 3-MPA-Au NCs added Mo(VI), **(B)** 6-MHA-Au NCs added Mo(VI), **(C)** 3-MPA-Au NCs added Hg(II).

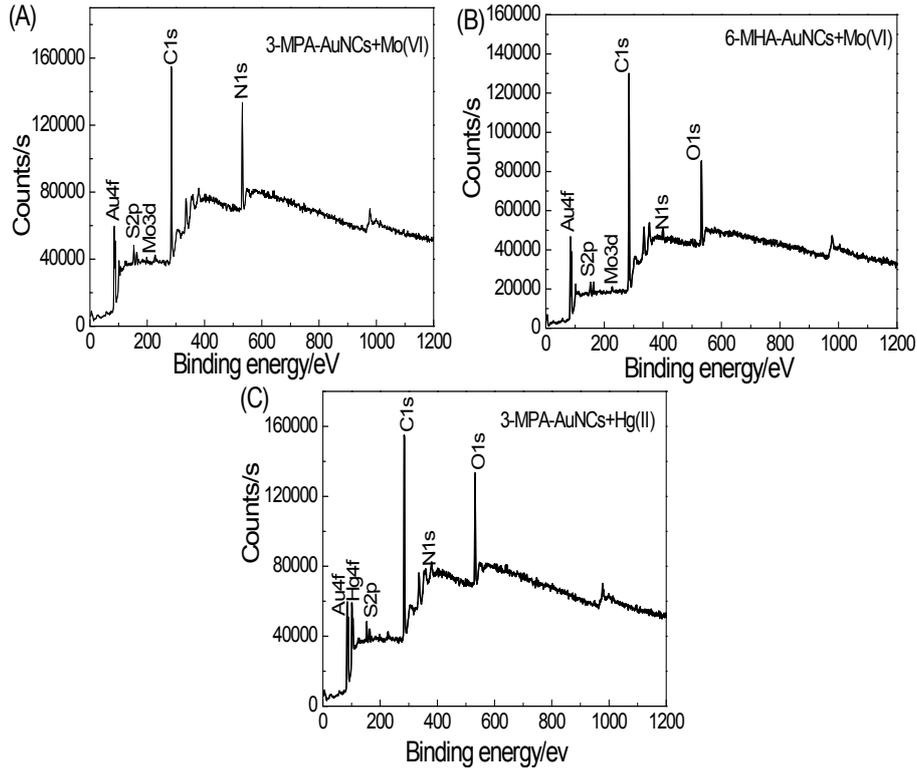


Fig. S8 The XPS spectrum of 3-MPA-Au NCs added Mo(VI), 6-MHA-Au NCs added Mo(VI), 3-MPA-Au NCs added Hg(II).

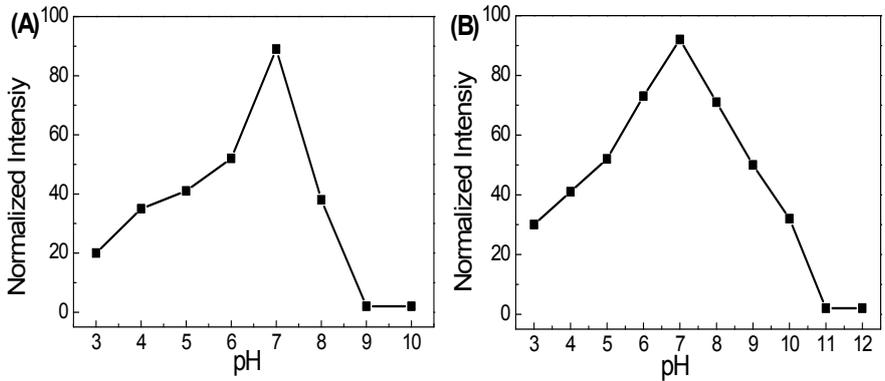


Fig. S9 Fluorescence intensity of 3-MPA-Au NCs, **(A)** and 6-MHA-Au NCs, **(B)** in the HEPES buffer (25mM) at different pH.

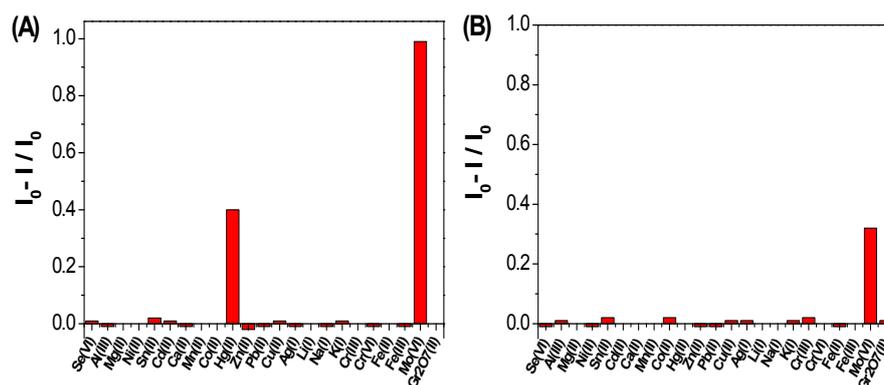


Fig. S10 The Fluorescence intensity ratios $I_0 - I / I_0$ (where I and I_0 are the corresponding fluorescence intensities in the presence and absence of metal ions, respectively) for the (A) 3-MPA-Au NCs and (B) 6-MHA-Au NCs measured various individual metal ions in 25 mM HEPES buffer at pH 7.0.

Table S1. The Fluorescent wavelength of Au NCs added metal ions

Metal ion	3-MPA-Au NCs	6-MHA-Au NCs
Se(VI)	590nm	615nm
Al(III)	590nm	615nm
Mg(II)	590nm	615nm
Ni(II)	590nm	615nm
Sn(II)	590nm	615nm
Cd(II)	590nm	615nm
Ca(II)	590nm	615nm
Mn(II)	590nm	615nm
Co(II)	590nm	615nm
Hg(II)	625nm	615nm
Zn(II)	590nm	615nm
Pb(II)	590nm	615nm
Cu(II)	590nm	615nm
Ag(I)	590nm	615nm
Li(I)	590nm	615nm
Na(I)	590nm	615nm
K(I)	590nm	615nm
Cr(III)	590nm	615nm
Cr(VI)	590nm	615nm
Fe(II)	590nm	615nm
Fe(III)	590nm	615nm
Mo(VI)	590nm	597nm
Gr ₂ O ₇ (II)	590nm	615nm

Table S2. Detection results of Mo(VI) in real samples

Real sample	Concentration of metal ion standard solution	ICP-MS (mean±RSD, n=3)	Colorimetric card 3-MPA-Au NCs (+Mo(VI))	Colorimetric card 6-MHA-Au NCs (+Mo(VI))
tap water	0	1.241±0.023μM	 (1-4 μM)	 (0-2.0μM)
	4.5μM	5.713±0.024μM	 (4.0-15.0 μM)	 (6.0-15.0μM)
	20.00 μM	21.224±0.021μM	 (15.0-30.0 μM)	 (15.0-25.0μM)
	35.00 μM	36.238±0.023μM	 (30.0-40.0 μM)	 (25.0-40.0μM)
bottled water	0 μM	0 μM	 (0μM)	 (0μM)
	4.5 μM	4.513±0.023 μM	 (4.0-15.0 μM)	 (2.0-6.0μM)
	20.00 μM	20.016±0.022 μM	 (15.0-30.0 μM)	 (15.0-25.0μM)
	35.00 μM	34.981±0.031 μM	 (30.0-40.0 μM)	 (25.0-40.0μM)

Table S3. Detection results of Hg(II) in real samples

Real sample	Concentration of metal ion standard solution	ICP-MS (mean±RSD, n=3)	Colorimetric card 3-MPA-Au NCs (+Hg(II))
tap water	0μM	0μM	 (0μM)
	0.07μM	0.071±0.001μM	 (0.05-0.2μM)
	6.00μM	5.982±0.022μM	 (5.0-7.5μM)
	13.00μM	13.021±0.025μM	 (7.5-15μM)
bottled water	0μM	0μM	 (0μM)
	0.07μM	0.069±0.001μM	 (0.05-0.2μM)
	6.00μM	5.993±0.024μM	 (5.0-7.5μM)
	13.00μM	13.011±0.023μM	 (7.5-15μM)