Electronic Supplementary Information

Single cytidine units-templated syntheses of multicolored water-soluble Au nanoclusters

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Table S1 Feed amount for preparation of multicolored Au NCs

	$HAuCl_4$ (20 mM)	CMP or Cyt (20 mM)	H_2O	Citrate (500 mM)
b-Au-CMP b-Au-Cyt	0.1 mL	0.2 mL	1.5 mL	0.2 mL, pH 5
g-Au-Cyt	0.1 mL	0.1 mL	1.6 mL	0.2 mL, pH 7
y-Au-CMP	0.1 mL	0.2 mL	1.5 mL	0.2 mL, pH 4

Table S2 Photophysical properties of Au NCs

	UV peak (nm)	Excitation peaks (nm)	Emission peak (nm)	Quantum Yield (%)*	Lifetime (ratio) (ns)
b-AuCMP	280, 330	360	470	3.3	6.28(0.62), 15.55 (0.23), 0.82 (0.15)
g-AuCyt	283, 380	350, 440	505	0.6	5.53 (0.52), 0.22 (0.48)
y-AuCMP	280	380, 520	550	0.4	4.15 (0.14), 0.02 (0.86)

* take quinine sulfate in 0.1 N sulfuric acid as a standard (55%).

Fig. S1. Photos taken at 1 min after addition of $AgNO_3$ (final concentration: 1 mM) to mixture containing only 1 mM $AuCl_4^-$ (left) or 1 mM $AuCl_4^-$ and 2 mM cytidine (right). The right sample was cloudy while the left one kept clear.

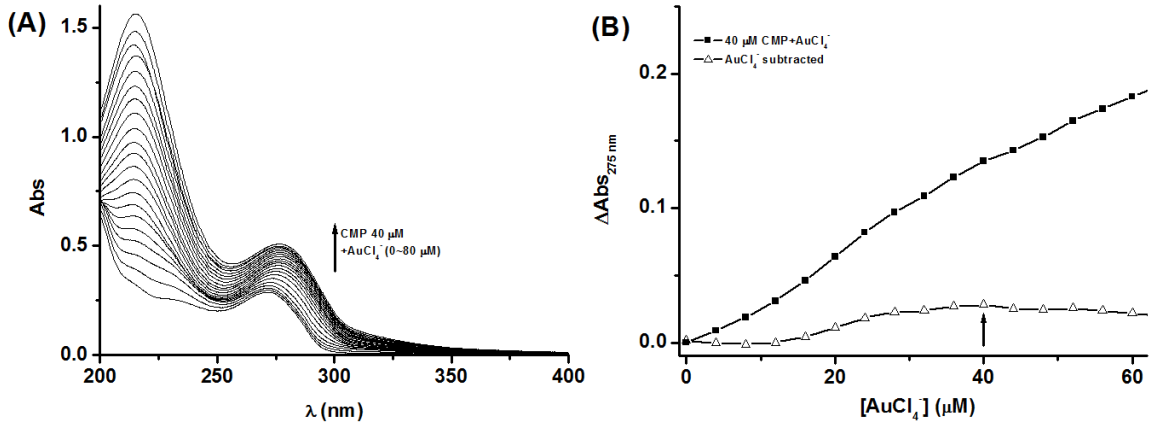

Fig. S2. (A) Titration of $AuCl_4^-$ to 40 μM CMP monitored by UV spectra. (B) The relationship of apparent increment (solid cube) and subtracted increment (hollow triangle) in peak absorbance at 275 nm and concentration of $AuCl_4^-$. The maximum $\Delta Abs_{275\ nm}$ appears at addition of 40 μM $AuCl_4^-$, indicating a "saturated" complexation ratio of 1:1.

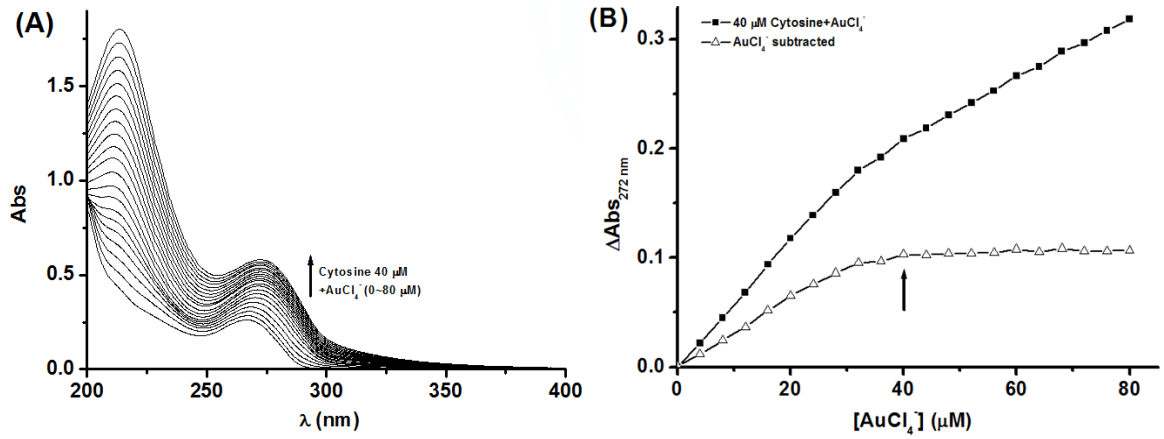

Fig. S3. (A) Titration of $AuCl_4^-$ to 40 μM cytosine monitored by UV spectra. (B) The relationship of apparent increment (solid cube) and subtracted increment (hollow triangle) in peak absorbance at 272 nm and concentration of $AuCl_4^-$. The maximum $\Delta Abs_{272\ nm}$ appears at addition of 40 μM $AuCl_4^-$, indicating a "saturated" complexation ratio of 1:1.

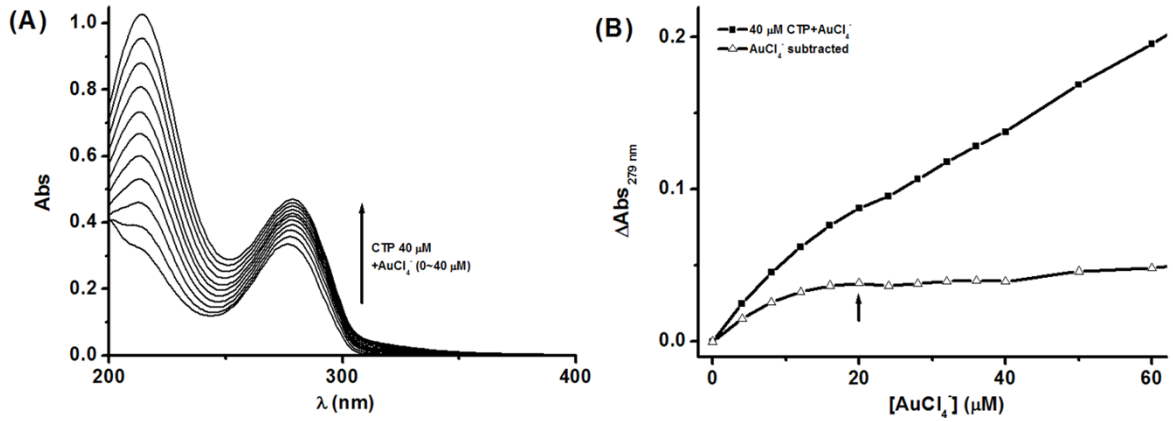

Fig. S4. (A) Titration of $AuCl_4^-$ to 40 μM CTP monitored by UV spectra. (B) The relationship of apparent increment (solid cube) and subtracted increment (hollow triangle) in peak absorbance at 279 nm and concentration of $AuCl_4^-$. The maximum $\Delta Abs_{279\ nm}$ appears at addition of 20 μM $AuCl_4^-$, indicating a "saturated" complexation ratio of 1:2.

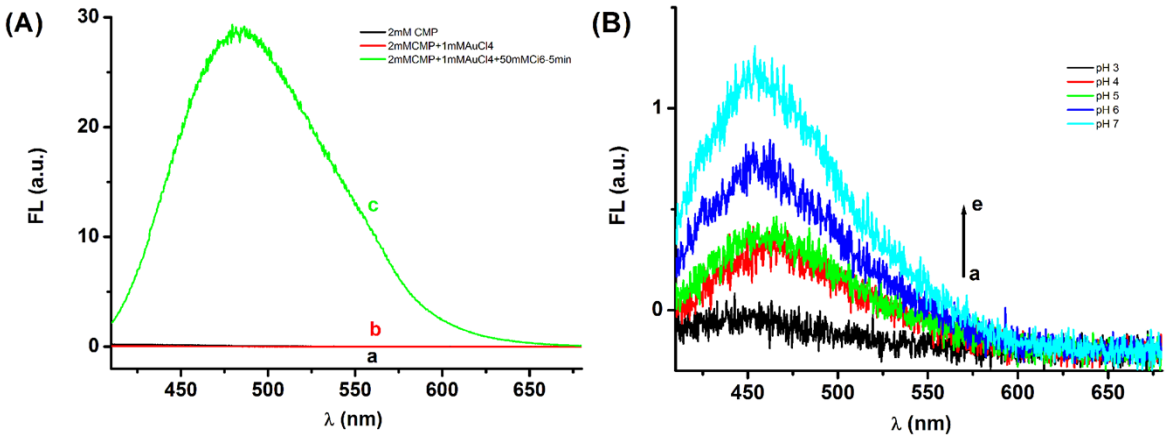

Fig. S5. (A) FL emission spectra for CMP (a), Au-CMP precursors before (b) and after (c) reduction by citrate at pH 6 for 5 min (excitation at 360 nm); (B) FL emission spectra of Au-CTP (molar ratio of 1:2) after reduction by citrate of pH 3~7 (a~e) for 60 min (excitation at 350 nm). Excitation/emission slit width: 3/3 nm.

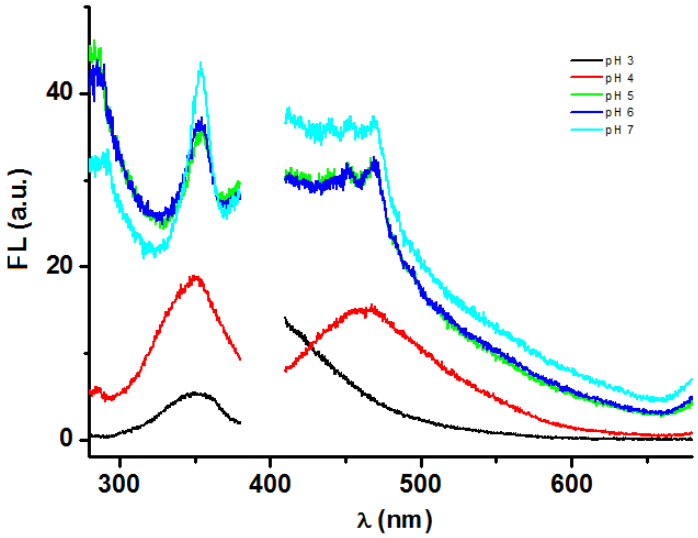

Fig. S6. FL emission spectra of Au-cytosine (molar ratio of Au:cytosine =1:1) at pH 3~7 after reduction for 1 h. Excitation wavelength: 360 nm. Excitation/emission slit width: 5/5 nm.

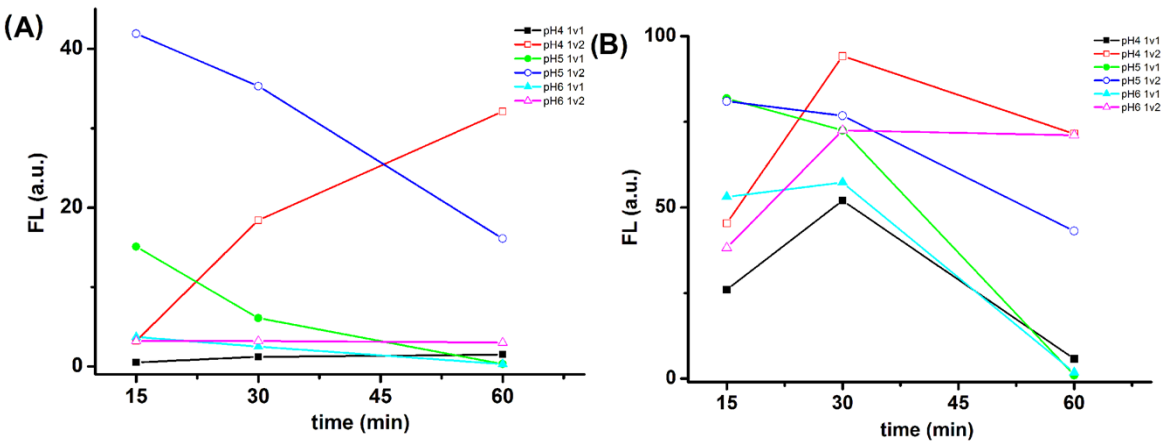

Fig. S7. Dependence of FL peak intensity on reduction time using Au-Cyt (A) or Au-CMP (B) precursors at a molar ratio of 1:1 (solid symbols) or 1:2 (hollow symbols) at pH 4 (square), 5 (round) and 6 (triangle), respectively. Excitation wavelength: 360 nm. Excitation/emission slit width: 3/3 nm.

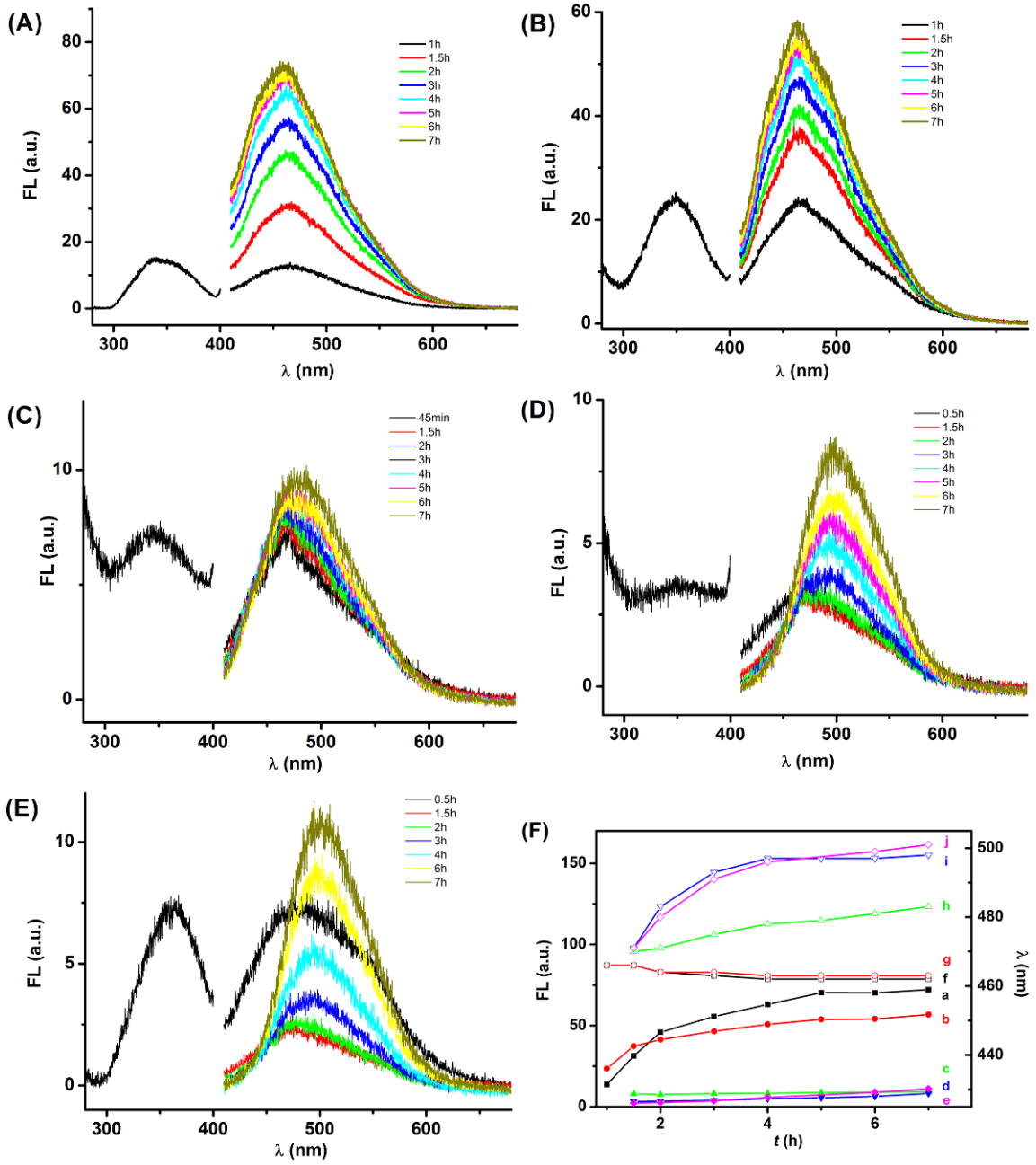

Fig. S8. FL emission spectra for Au-Cyt (molar ratio of Au:Cyt =1:1) by reduction of citrate at pH 3~7 (A~E) for 1~7 h. Excitation wavelength: 350 nm. Excitation/emission slit width: 5/5 nm. (F) The changes in FL peak intensity (solid, a~e) or wavelength (hollow, f~j) depend upon reduction time at pH 3 (a, f), 4 (b, g), 5 (c, h), 6 (d, i) and 7 (e, j).

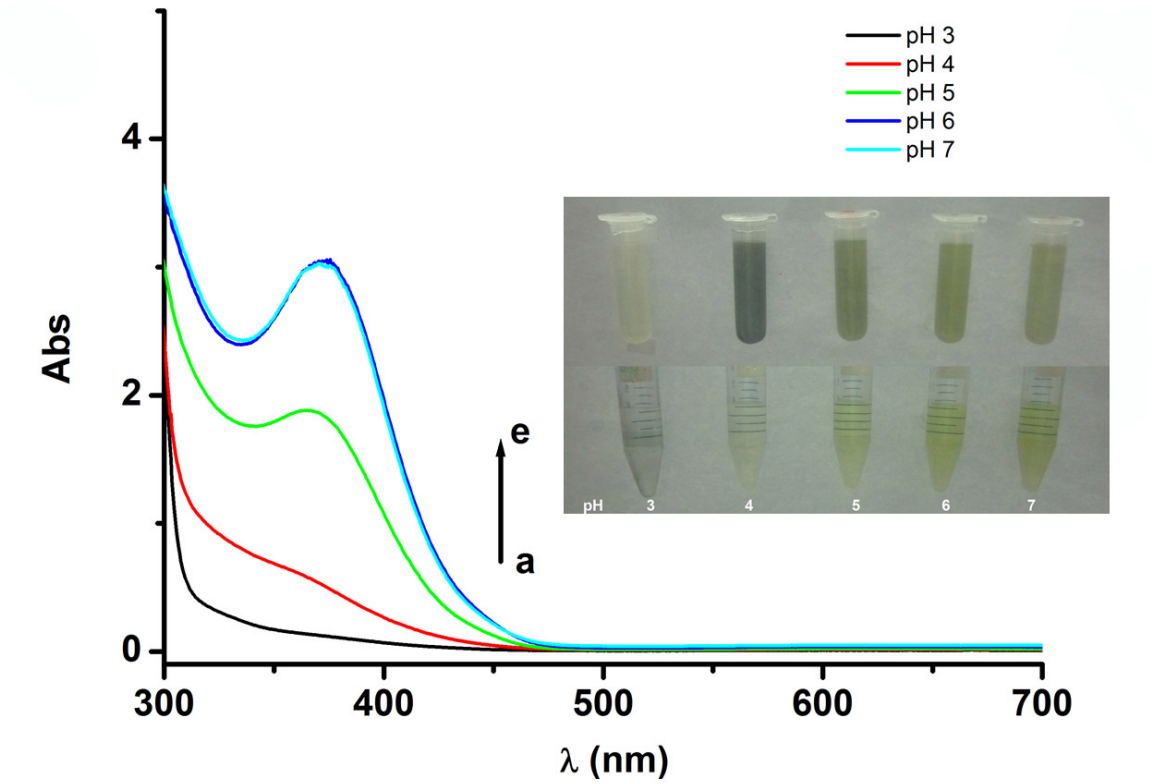

Fig. S9. UV-Vis absorption spectra of the mixture filtrate after reduction by citrate at pH 3~7 (a~e) for 7 h. Inset: Photos of the mixtures containing $AuCl_4^-$ (1.0 mM), Cyt (1.0 mM) and citrate (50.0 mM) at different pH for 7-h reduction before (top) and after (down) treatment with 0.22 μm filter. Note that the blue mixture at pH 4 before filtration is caused by the aggregated Au NPs.

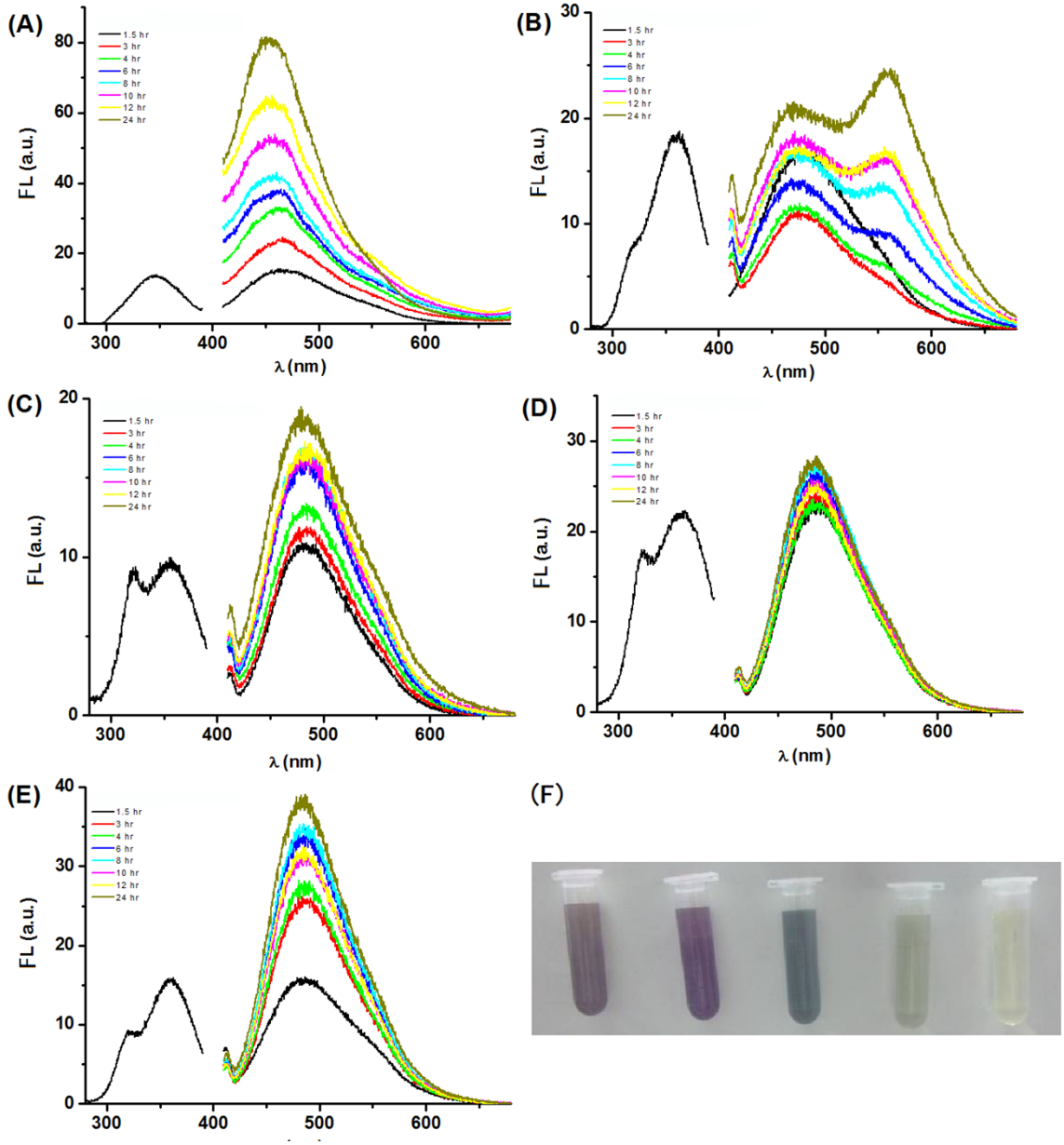

Fig. S10. Study on the FL dependence of Au-CMP (molar ratio of Au:CMP =1:1) on incubation time at pH 3~7 (A~E), with an excitation wavelength at 350 nm for pH 3 and 360 nm for pH 4~7. Excitation/emission slit width: 5/5 nm. (F) Photos of the mixtures containing $AuCl_4^-$ (1.0 mM), CMP (1.0 mM) and citrate (50.0 mM) at pH 3~7 (from left to right) after 3-h incubation.

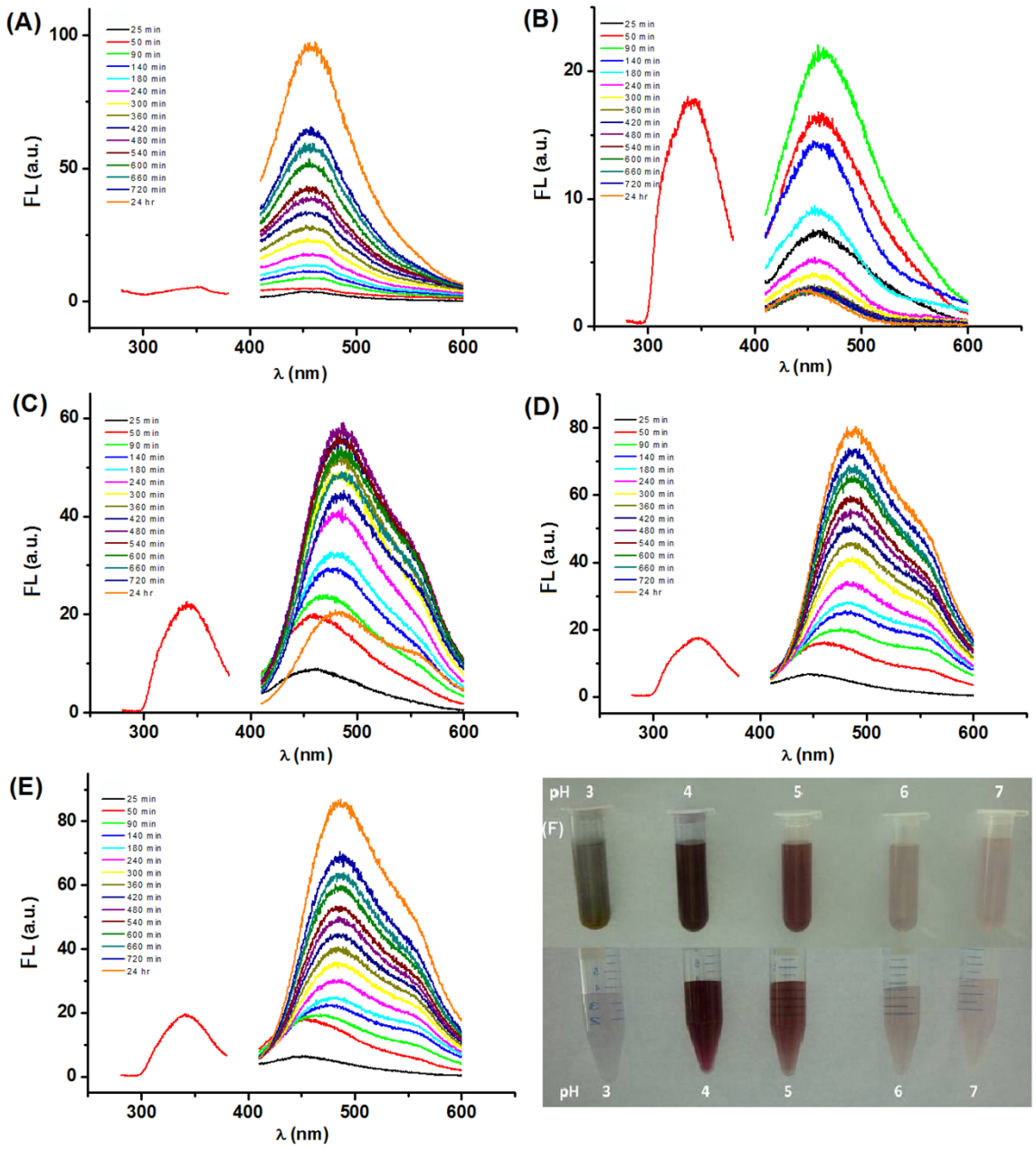

Fig. S11. Study on the FL dependence of Au-CTP (molar ratio of Au:CTP =1:2) on incubation time at pH 3~7 (A~E). Excitation wavelength: 350 nm. Excitation/emission slit width: 5/5 nm. (F) Photos of the mixtures containing $AuCl_4^-$ (1.0 mM), CTP (2.0 mM) and citrate (50.0 mM) incubated at different pH for 24-h before (top) and after (down) treatment with 0.22 μm filter.

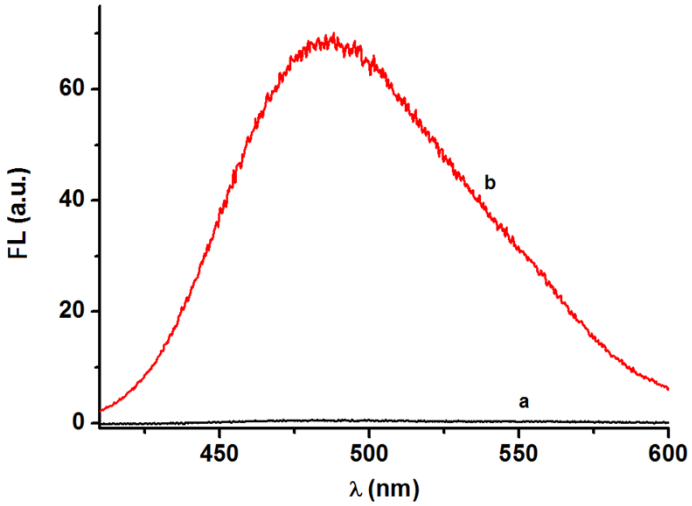

Fig. S12. FL emission spectra for solution in the ultrafilter (i.e., MW≥10 KDa) (a) and filtrate (i.e., MW<10 KDa) (b) after ultrafiltration of the mixture containing $AuCl_4^-$ (1.0 mM), CTP (2.0 mM) and citrate (50.0 mM, pH 7) incubated for 8-h. Excitation wavelength: 350 nm. Excitation/emission slit width: 5/5 nm. The fluorescent components are only found in the filtrate, suggesting that their MW is lower than 10 KDa.

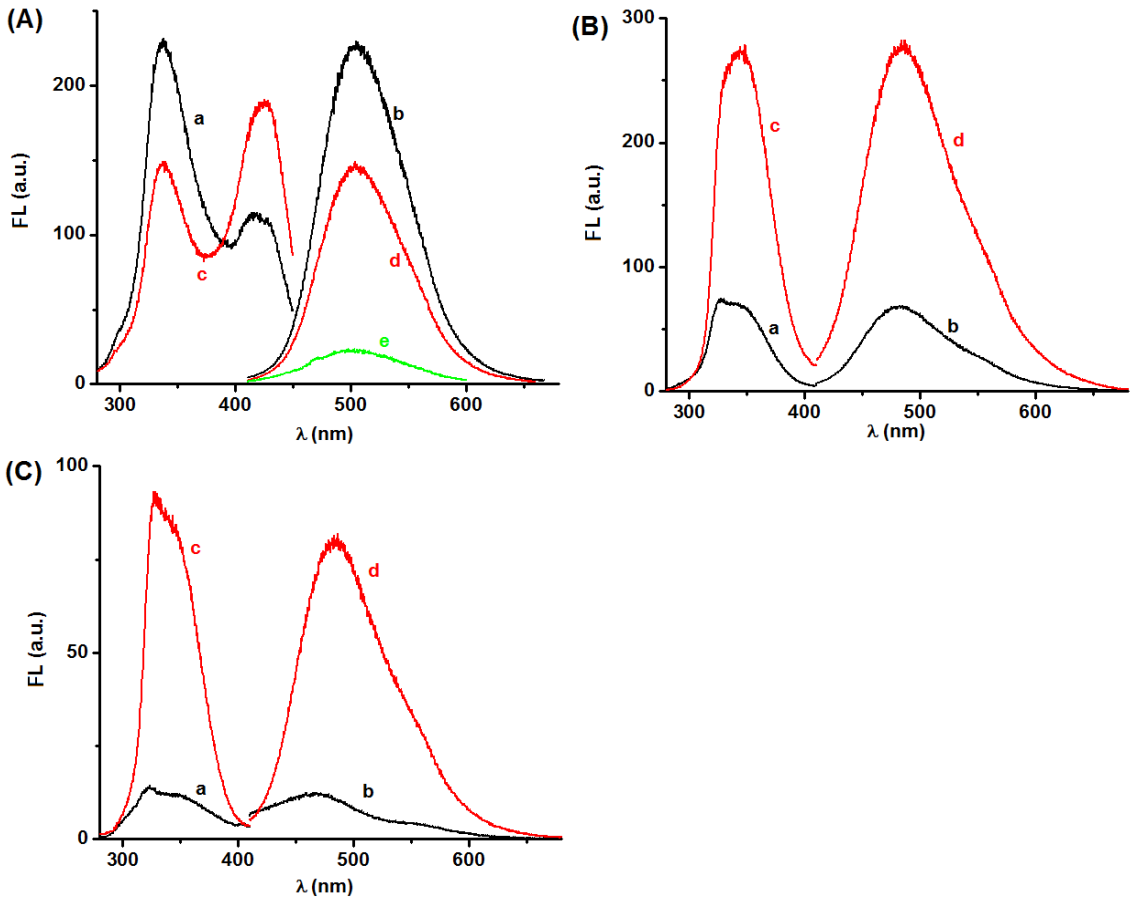

Fig. S13. FL excitation (a, c) and emission (b, d) spectra for Au-Cyt (A), Au-CMP (B) and Au-CTP (C) complexes at a molar ratio of 1:1 (a, b) or 1:2 (c, d) by reduction of citrate (pH 6.0) at 80 °C for 1 h. Excitation wavelength: 350 nm. Excitation/emission slit width: 5/5 nm. Curve e in part (A) shows the emission spectrum for Au-Cyt (1:1) excited at 680 nm.

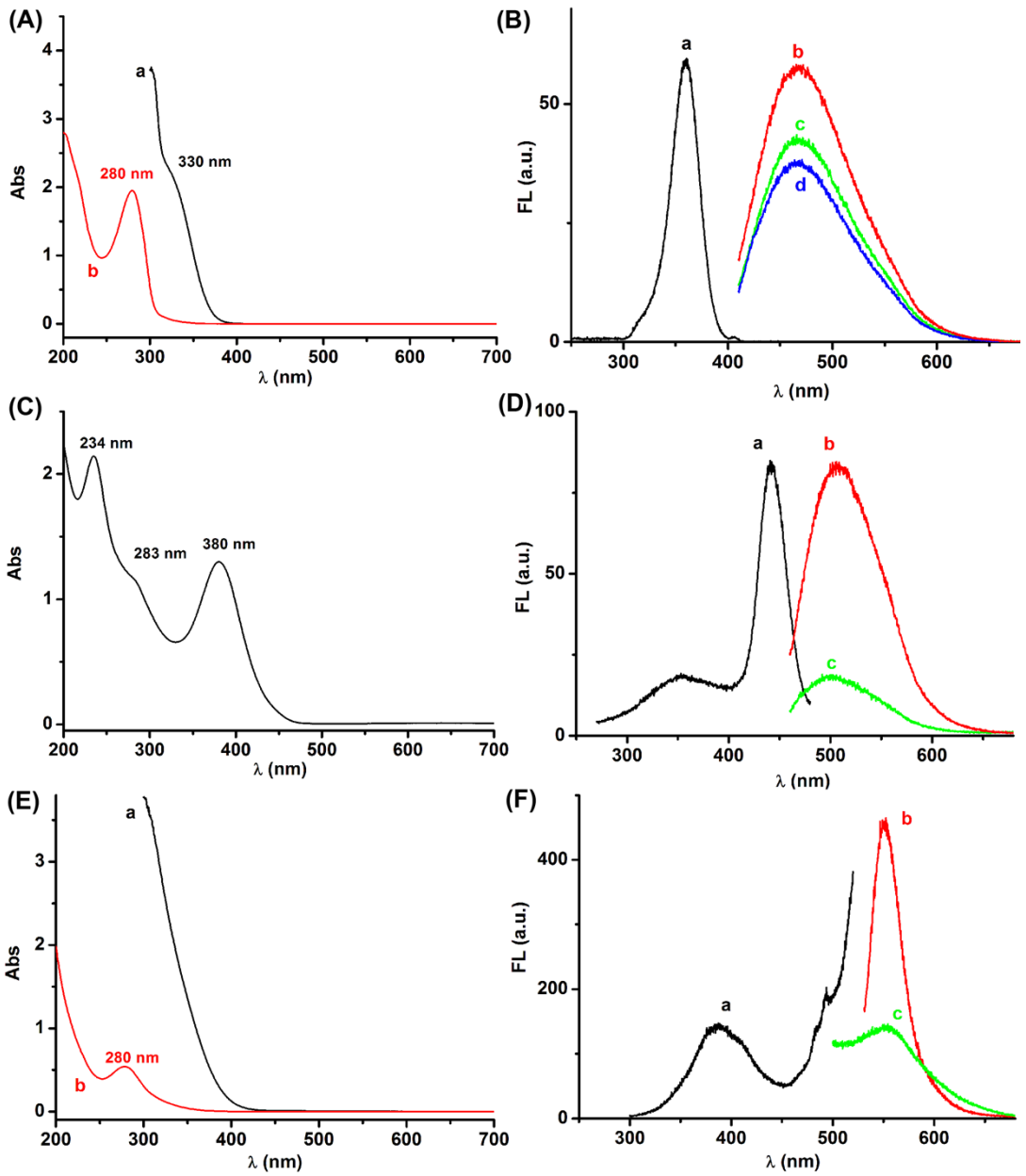

Fig. S14. The UV-vis spectra (A, C, E) and fluorescent spectra (B, D, F) for b-Au-CMP (A, B), g-Au-Cyt (C, D) and y-Au-CMP (E, F) in deionized water: (A, E) The UV-vis spectra for samples of ~1 mg/mL (a) or ~0.1 mg/mL (b); (C) UV-vis spectra for sample of ~1 mg/mL; (B) The excitation spectra with λ_{em} at 470 nm (a) and emission spectra with λ_{ex} at 360 nm (b), 350 nm (c), 370 nm (d); (D) The excitation spectra with λ_{em} at 505 nm (a) and emission spectra with λ_{ex} at 440 nm (b), 350 nm (c); (F) The excitation spectra with λ_{em} at 550 nm (a) and emission spectra with λ_{ex} at 520 nm (b), 380 nm (c). The Excitation/emission slit width is 3/3 nm in (B) and 5/5 nm in (D) and (F),

respectively.

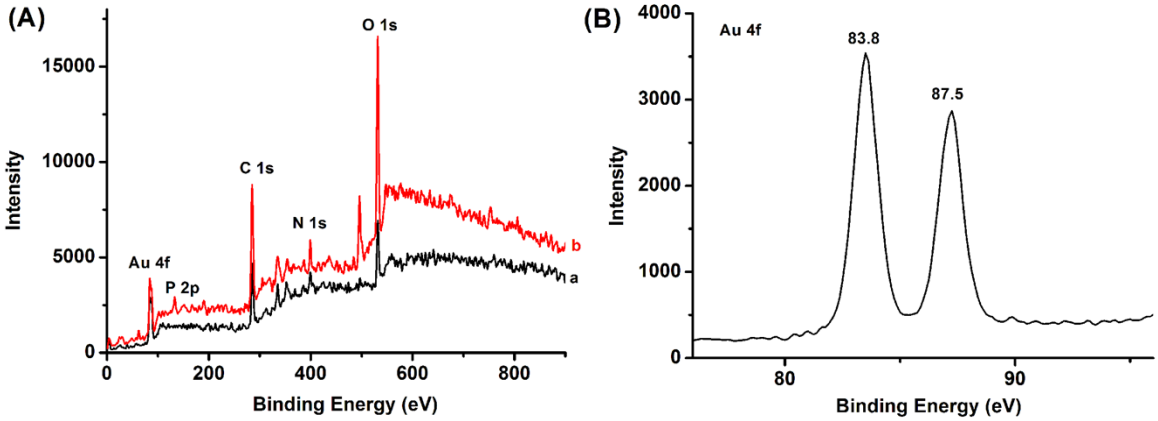

Fig. S15. (A) The XPS spectra for g-Au-Cyt (molar ratio of 1:1) (a) and b-Au-CMP (molar ratio of 1:2) (b). (B) The magnified Au 4f zone in (A).