Supporting Information

Synthesis of water-soluble and highly fluorescent gold nanoclusters for Fe³⁺ sensing in living cells using fluorescence imaging

Jianqiao Zhang,^a Chen Cai,^b Shumaila Razzaque,^a Irshad Hussain,^{c, d} Qun-Wei Lu^{b, *} and Bien Tan^{a, *}

- a. Key Laboratory for Large-Format Battery Materials and System, Ministry of Education, Hubei Key Laboratory of Material Chemistry and Service Failure, School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, Wuhan, 430074, China. Tel/Fax: +86 27 87558172; *Email: bien.tan@mail.hust.edu.cn (Tan B)
- b. Key Laboratory of Molecular Biophysics of Ministry of Education, College of Life Science and Technology, Center for Human Genome Research, Huazhong University of Science and Technology, Wuhan, Hubei, 430074, China. Tel/Fax: +86 27 87792148; *E-mail: luqw@hust.edu.cn (Lu QW)
- c. Department of Chemistry, SBA School of Science & Engineering (SSE), Lahore University of Management Sciences (LUMS), DHA, Lahore Cantt-54792, Pakistan.
- d. US-Pakistan Center for Advanced Studies in Energy (USPCAS-E), University of Engineering and Technology (UET), Peshawar, Pakistain



Scheme S1 The schematic for synthesis of polymer ligands PTMP-PMAA.



Fig. S1 GPC elution curves of polymer ligands PTMP-PMAA with different molecular weights modified with TMSdiazomethane.

Table S1. Molecular wei	ght and pol	ydispersity c	of polymer li	gands measured b	y GPC.
-------------------------	-------------	---------------	---------------	------------------	--------

Polymer	PTMP:MAA	GPC			Yield
	(mmol:mmol)	Mn	Mw	PDI	(%)
0.5%PTMP-PMAA	0.5:100	8700	15700	1.81	98.9
1%PTMP-PMAA	1:100	5000	8400	1.70	97.3
2%PTMP-PMAA	2:100	3400	5000	1.48	90.6
3%PTMP-PMAA	3:100	1800	3000	1.71	71.2
4%PTMP-PMAA	4:100	1200	2100	1.73	68.9



Fig. S2 1H NMR of polymer ligands PTMP-PMAA dissolved in d⁶-DMSO.



Fig. S3 (A) The mixture solution of HAuCl₄ and polymer ligands PTMP-PMAA; (B) The resulting solution of Au NCs@PTMP-PMAA.



Fig. S4 (A) The 3D histogram of the influence of molecular weights and concentrations on the fluorescence intensity and (B) quantum yields of Au NCs@PTMP-PMAA; (C) DLS of the Au NCs@PTMP-PMAA prepared with polymer ligands of increasing molecular weights under 80 °C for 9 h.



Fig. S5 (A) Fluorescence emission spectra, (B) trendline, (C) UV-Vis absorption spectra and (D) DLS of the Au NCs@PTMP-PMAA prepared with increasing concentrations of 2%PTMP-PMAA (Mw=5000 g/mol) ranging from 1 to 18 mM. Insets are the photographs of the corresponding Au NCs@PTMP-PMAA solutions under visible light (upper) and 365 nm UV light (lower).



Fig. S6 (A) The 3D histogram of the influence of heating temperature and reaction time on the fluorescence intensity of Au NCs@PTMP-PMAA; (B) Fluorescence emission spectra of the Au NCs@PTMP-PMAA prepared under 80 °C with different reaction times. (C) Fluorescence emission spectra and (D) DLS of the Au NCs@PTMP-PMAA prepared under increasing heating temperature with same reaction times (9 h). The inset are photographs of the corresponding Au NCs@PTMP-PMAA solution under visible light (upper) and 365 nm UV light (lower).



Fig. S7 Normalized fluorescence emission spectra the Au NCs@PTMP-PMAA upon various excitation wavelengths ranging from 395 nm to 475 nm.



Fig. S8 DLS histogram of the Au NCs.



Fig. S9 S(2p) XPS spectra of the as-prepared Au NCs @PTMP-PMAA.



Fig. S10 Powder XRD pattern of the as-prepared Au NCs @PTMP-PMAA.The broad peaks indicated the ultrasmall particles of Au NCs.



Fig. S11 Effects of (A) ionic strength, (B) irradiation time and (C) storage time of six months on the fluorescence intensity of Au NCs.



Fig. S12 Effects of pH values on the fluorescence intensity of Au NCs@PTMP-PMAA.



Fig. S13 Effect of the incubation time for the fluorescence quenching of the Ag NCs in the presence of 20 uM, 80 μ M, 320 uM Fe³⁺.



Fig. S14 TEM images (A) and DLS (B) of Au NCs in the presence of 60 μM Fe $^{3+}$. Scale bar: 100 nm.



Fig. S15 Fluorescence intensity of Au NCs at 553 nm under different conditions. No. 1: Au NCs ; No. 2: Au NCs + Cys; No. 3: Au NCs + Fe³⁺; No. 4: Au NCs + Fe³⁺ + Cys; No. 5: Au NCs + Hg²⁺; No. 6: Au NCs + Hg²⁺ + Cys; No. 7: Au NCs + Hg²⁺ + Cys + Fe³⁺.



Fig. S16 Images of H9c2 cells incubated without Au NCs obtained (A) under bright field and (B) at the excitation wavelength of 405 nm. Scale bar: $30 \mu m$.