Pyridoxal conjugated gold nanoparticles for distinct colorimetric detection of chromium(III) and iodide ions in biological and environmental fluids

Shilpa Bothra, Rajender Kumar and Suban K Sahoo*

Department of Applied Chemistry, SV National Institute of Technology (SVNIT), Surat-395007, India.

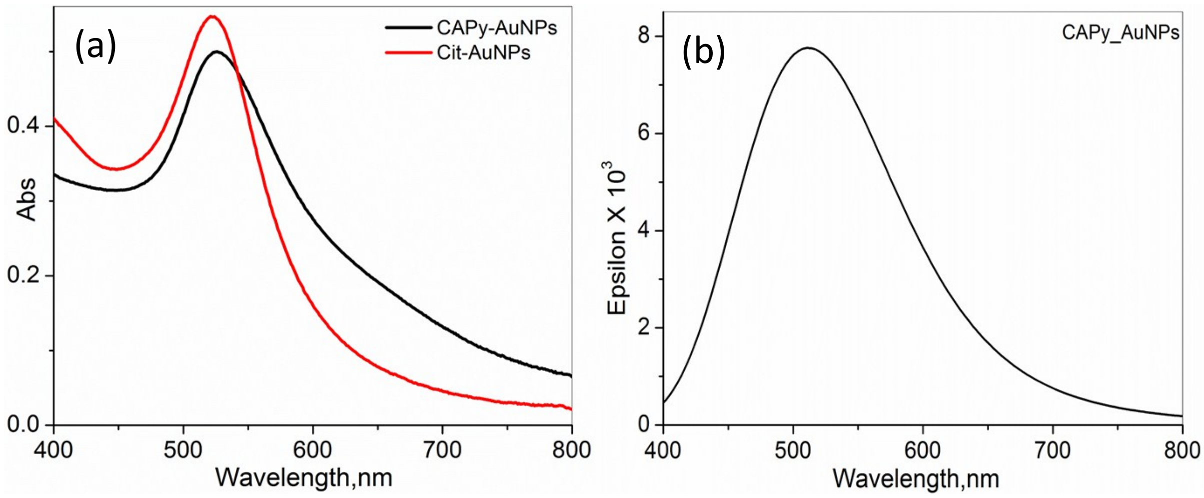

Fig. S1. (a) UV-Vis spectra of the citrate capped AuNPs and CAPy-AuNPs and (b) TD-DFT calculated UV-Vis spectra of CAPy-Au_6.

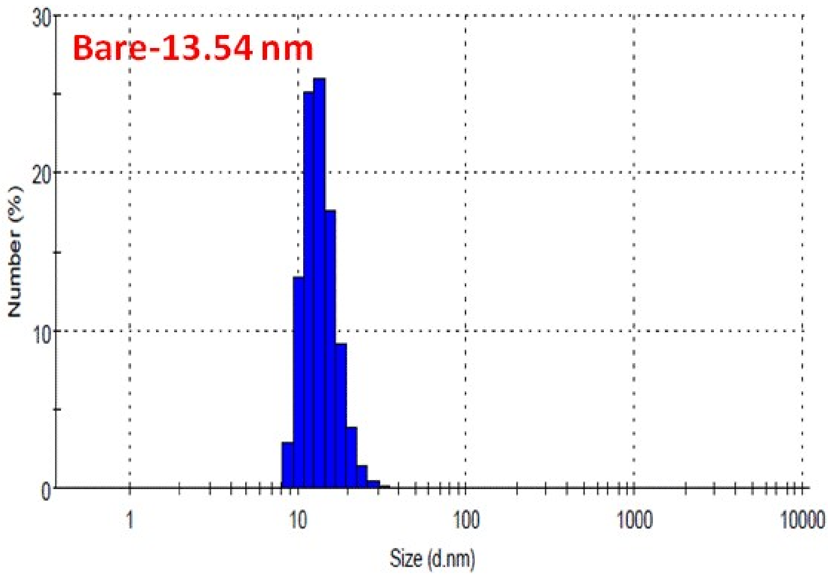

Fig. S2. DLS data of citrate capped AuNPs.

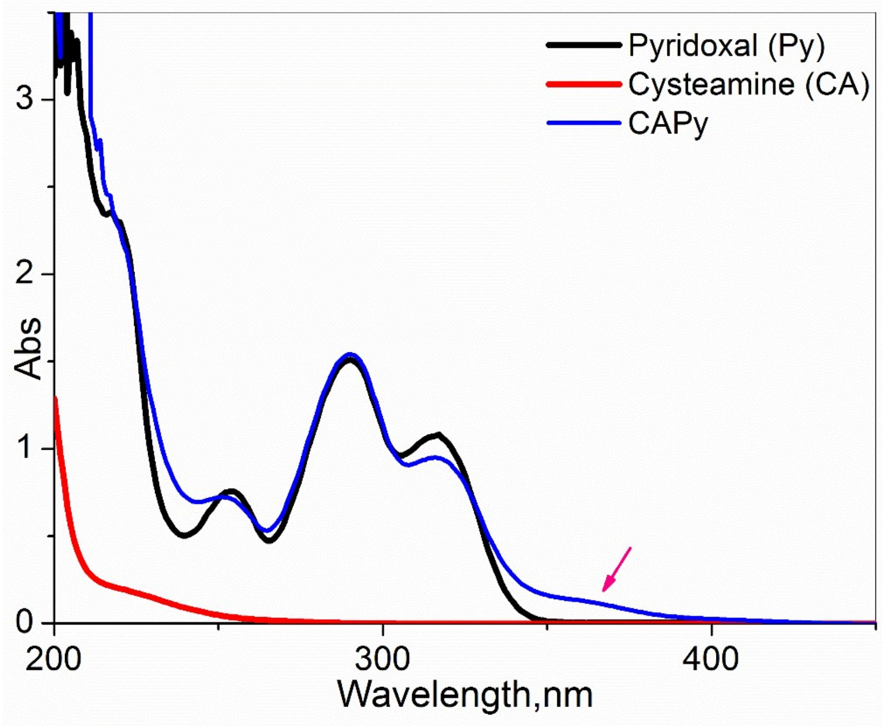

Fig. S3. UV-Visible analysis for the interaction between CA and Py.

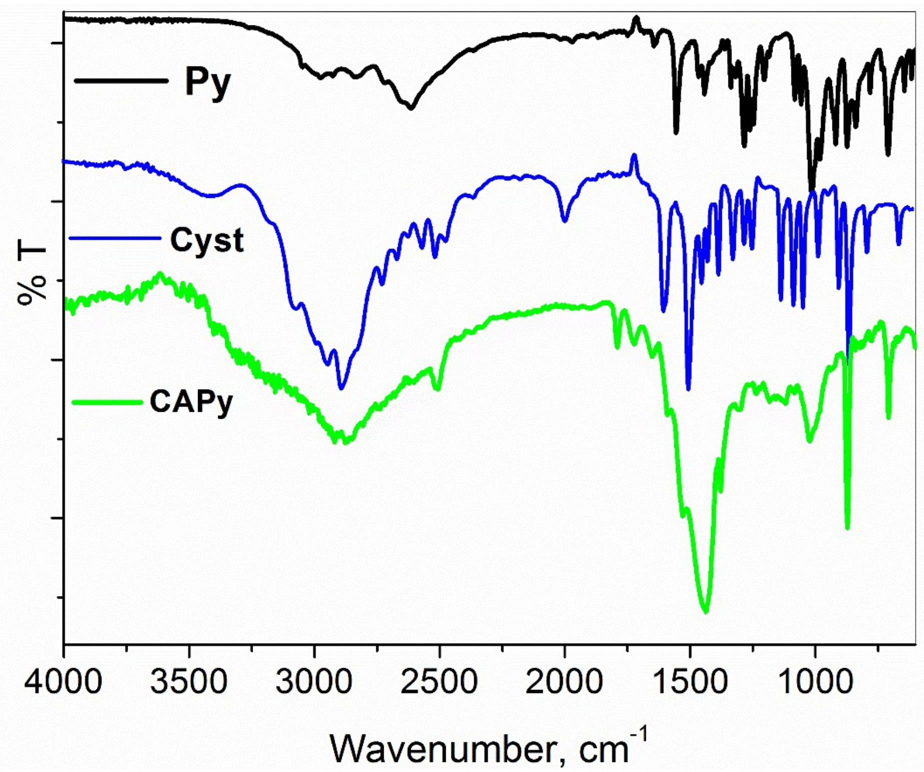

Fig. S4. FTIR analysis for the interaction between CA and Py.

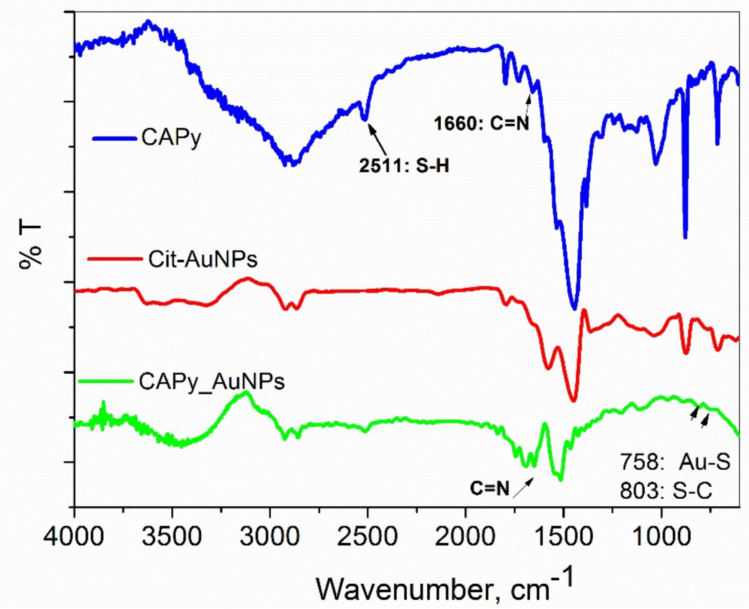

Fig. S5. FTIR spectra of bare AuNPs, capping agent CAPy and CAPy-AuNPs.

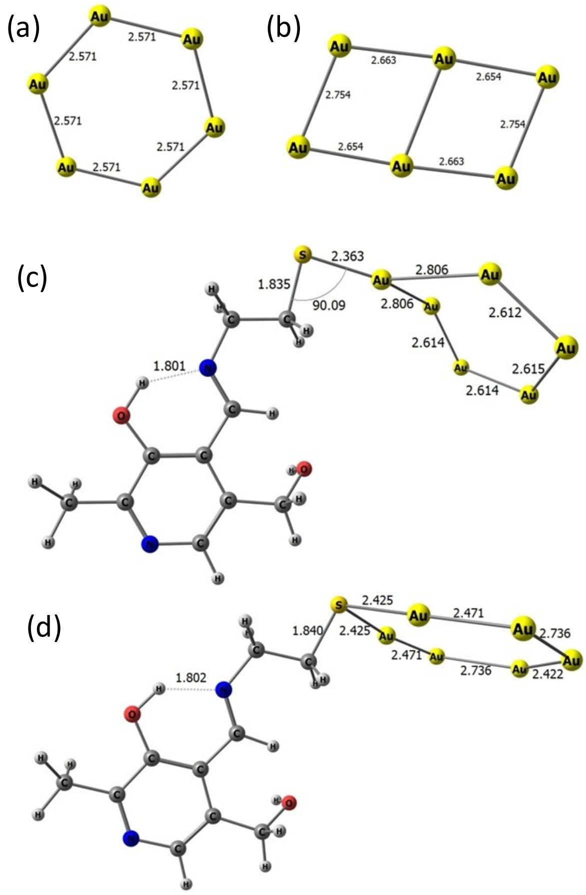

Fig. S6. Optimized structure of Au_6 (**a**) and CAPy-Au_6 (**c, d**) by semi-empirical PM6 method and Au_6 (**b**) by B3LYP/LANL2DZ method in the gas phase. The structure '**d**' is energetically more stable (-22.16 kcal/mol) then the '**c**', where the thiol group of CAPy interacting with the two Au atoms.

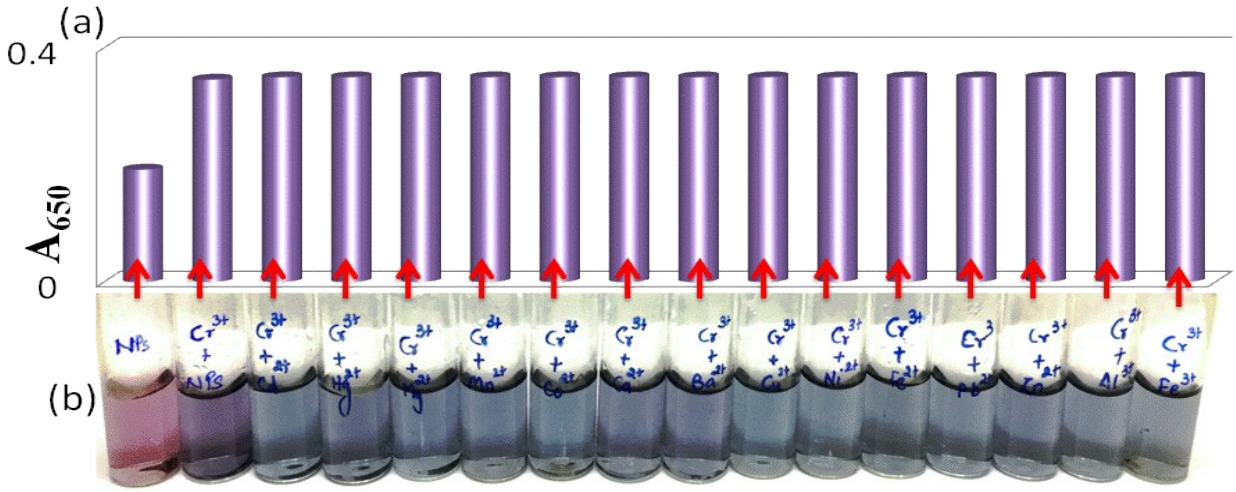

Fig. S7. (a) Bar graph at wavelength 650 nm and (b) naked-eye responses depicting the selectivity of CAPy-AuNPs in presence of equivalent molar concentration of Cr^{3+} ($2.5x10^{-4}$M) and other metal ions ($2.5x10^{-4}$M).

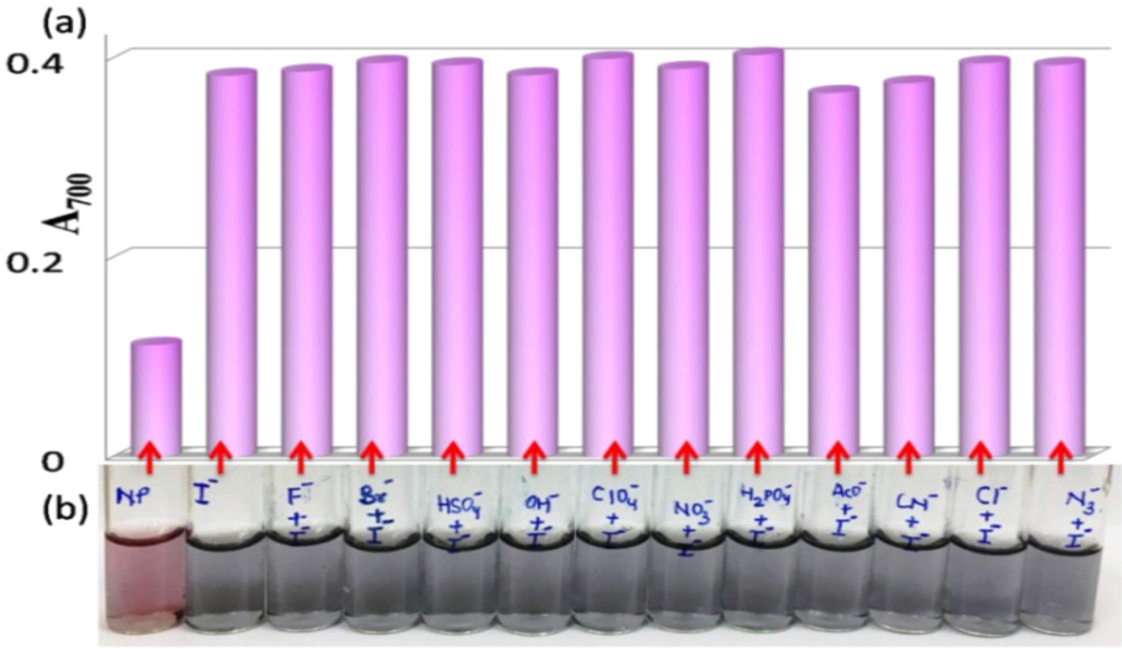

Fig. S8. (a) Bar graph at wavelength 700 nm and (b) naked-eye responses depicting the selectivity of CAPy-AuNPs in presence of equivalent molar concentration of I^- ($1x10^{-4}$M) and other anions ($1x10^{-4}$M).

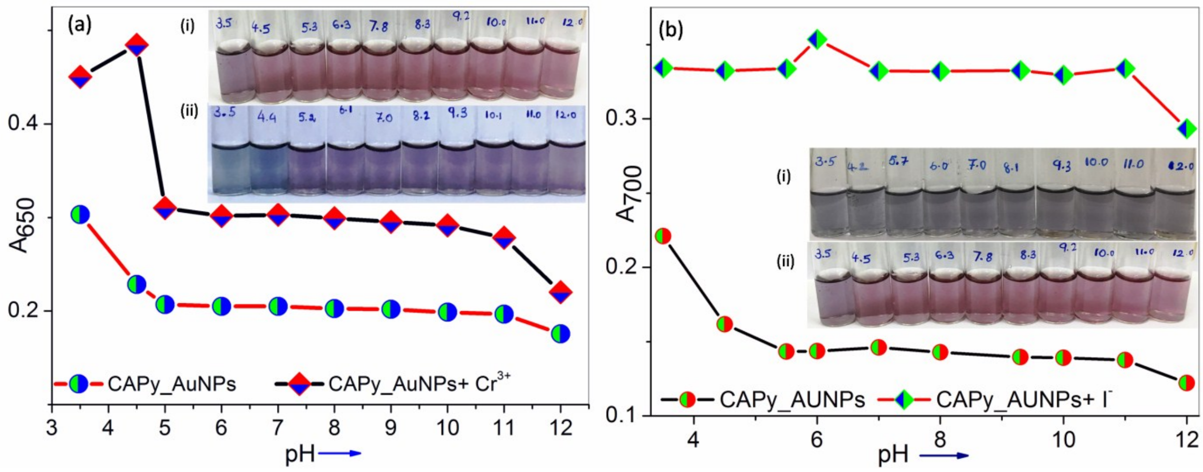

Fig. S9. Effects of change of pH on (a) CAPy-AuNPs solution in the absence and presence of Cr^{3+} and (b) CAPy-AuNPs in the absence and presence of I^-.

Table S1. Brief account of various colorimetric NPs systems reported for Cr^{3+} and I^- detection.

Developed system	Detecting Ions	LOD (M)	Real samples	References
AgNP-I	Cr^{3+}	0.441×10^{-6}	-	1
PAH-AuNPs		1.17×10^{-6}	Milk powder, milk, lake water	2
PDCA- AuNPs		2.27×10^{-6}	-	3
GA-AuNPs		0.05×10^{-6}	Lake and tap water	4
CAPy-AuNPs		$\mathbf{11.5 \times 10^{-6}}$	**Tap and river water, liquid milk, milk powder**	**This study**
Virgin AgNPs	I^-	0.32×10^{-6} Fe^{3+} 1.32×10^{-6} Cr^{3+}	-	5
Cit-Core/Shell Cu@AuNPs		5×10^{-6}	-	6
Au@Ag core–shell NPs with Cu^{2+}		0.5×10^{-6}	Drinking water , Dried kelps,Agarose gels	7
ATTP-AuNPs		15×10^{-9}	Lake water	8
CAPy-AuNPs		$\mathbf{5.89 \times 10^{-7}}$	**Tap and river water, urine**	**This Study**

Table S2. Brief account of various reported official methods for Cr^{3+} and I^- detection.

Detected Ion	Method	LOD	Reference
Cr^{3+}	ICP-MS	0.03 μg/L	9
	AAS	5.0 ng	10
	GFAAS	0.03–0.04 μg/L	11
	HRS	25 ppt	12
	DPSV	0.4 μM	13
	AAS	0.19 ng mL^{-1}	14
	Chemiluminescence	5×10^{-10} M	15
I^-	Total reflection X-ray fluorescence	180 μg L^{-1}	16
	Molecular absorption spectrometry	60 μg L^{-1}	17
	Flow-injection cold-vapor AAS	3.6 μg L^{-1}	18
	ISE	1.47 μg L^{-1}	19
	ICP-OES	4.5 μg L^{-1}	20
	Capillary Electrophoresis	0.06 μM	21
	ICP-MS	0.19 ng g^{-1}	22

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