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Facile One-Pot Synthesis of Gold Nanoclusters and their Sensing protocol

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Electronic Supplementary Material
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Au-NPs Synthesis details:

For the preparation of Au-NPs following conditions were used; an amount of 160 µL (varied for various reactions) of tetrachloroauric (III) acid (from 50 mM stock solution of $HAuCl_4.3H_2O$) and the desired amount of amoxicillin (from 50 mM stock suspension of amoxicillin), as amoxicillin has low solubility in water therefore suspension was used which was stirred and sonicated well before use. Reaction mixture was kept on stirring for 1h then we added 80 µL (varied for various reactions, Table 1) of sodium borohydride (freshly prepared 880 mM solution of $NaBH_4$) at once along with vigorous stirring. The resulting mixture was stirred for 3 h at room temperature and UV-vis spectra were recorded. Photoluminescence spectra of the nanoparticles produced using the method in which the solution is reduced with $NaBH_4$, excited at 360 nm, exhibit a maximum emission around 435–440 nm. Solid Au-NPs were collected by freeze drying the clear reaction mixtures for FT-IR and TEM studies.

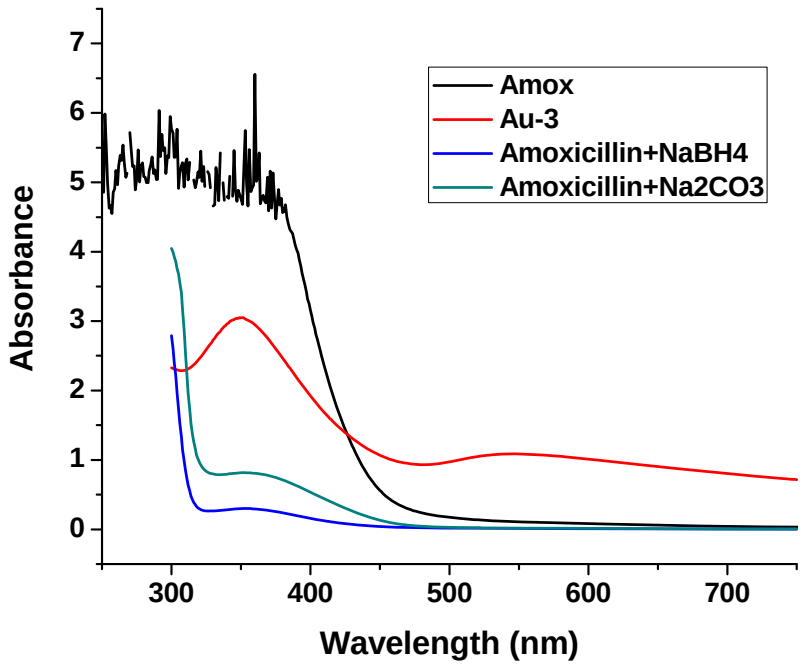

Figure ES1: Absorption spectra confirming the formation of salt of amoxicillin

Na^+ of the $NaBH_4$ and of Na_2CO_3 combines with amoxicillin and gives its salt which is indicated by its absorbance peak at 350 nm in the UV spectra (Fig. ES1)

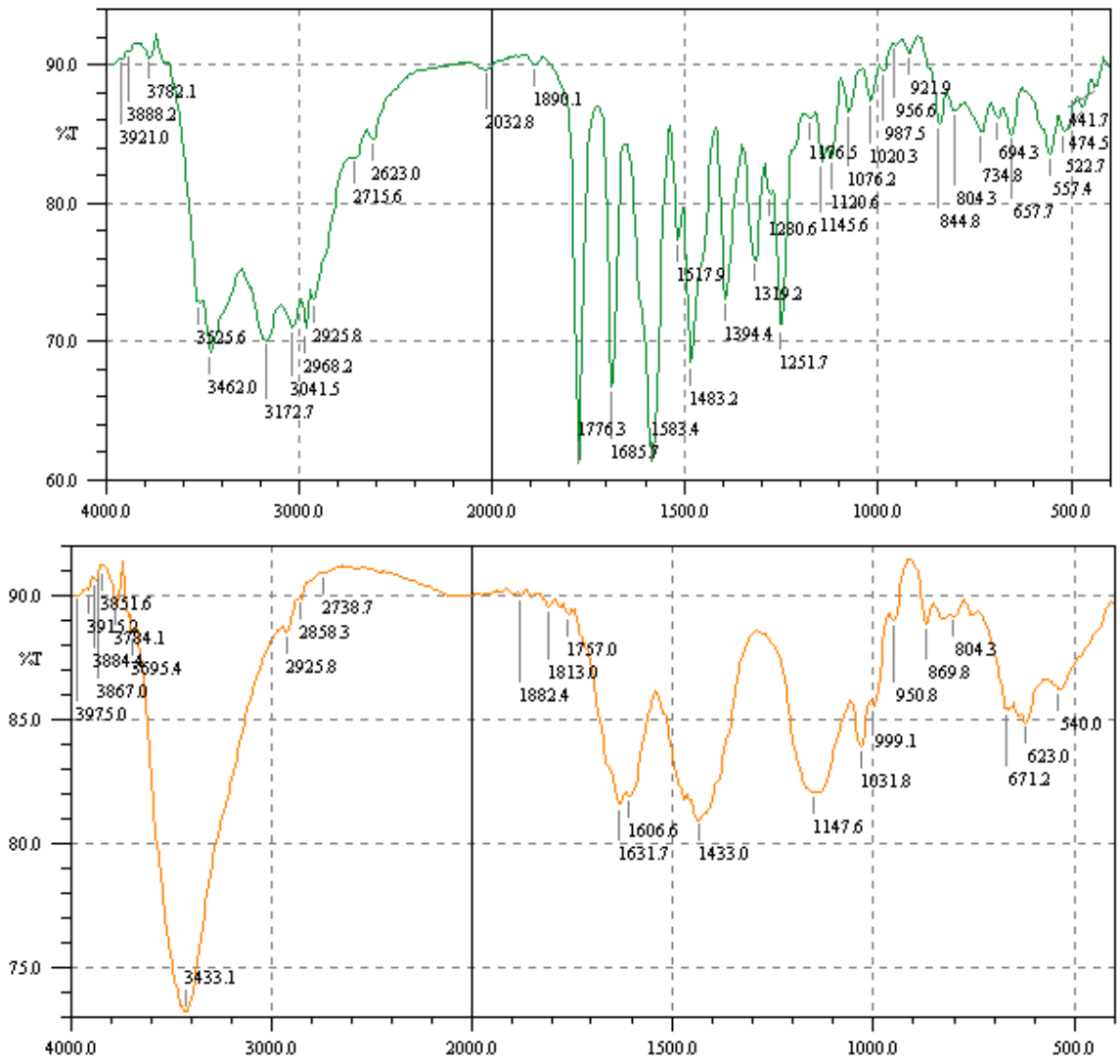

Figure ES2: FTIR spectra of amoxicillin (upper) and Au-3NPs (lower)

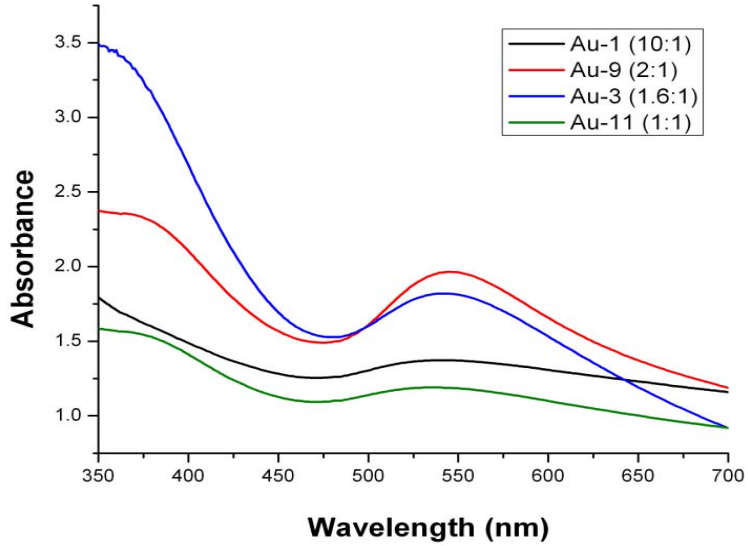

Figure ES3: UV-vis spectra of Au- NPs with different ligand ratios in 5mL deionized water

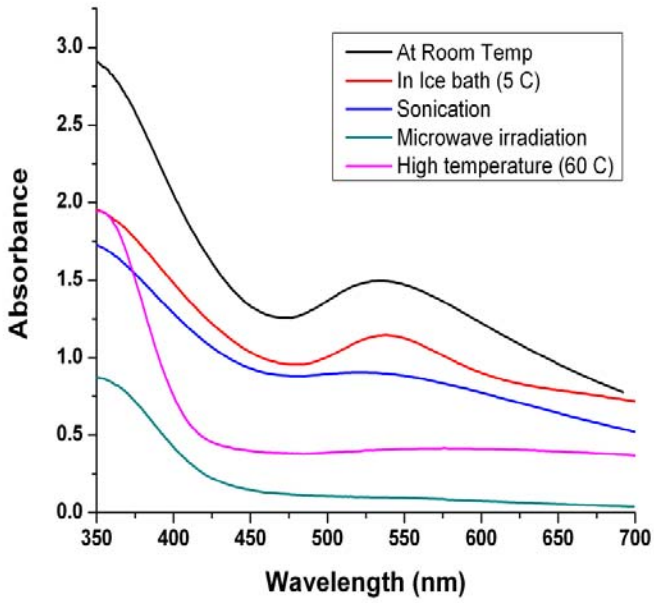

Figure ES4: UV-vis spectra of Au-NPs prepared with different synthetic routes

As shown in figure (ES4), results of gold nanoclusters formation at higher temperature (60°C) were not noteworthy. Same was the case under microwave irradiation followed by appearance of black precipitates. Sonication gave slight better results but it's rather time compromising technique. Ice cold conditions, was the 2nd best route for synthesis of Au-NPs using amoxicillin which improved the efficiency as more nanopartciles were formed under cold conditions.

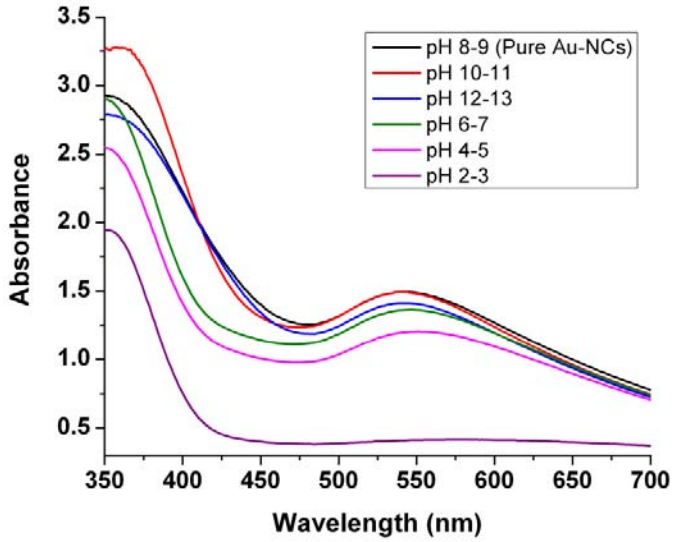

Figure ES5a: Effect of pH on stability of Au-3NPs: same day (5a)

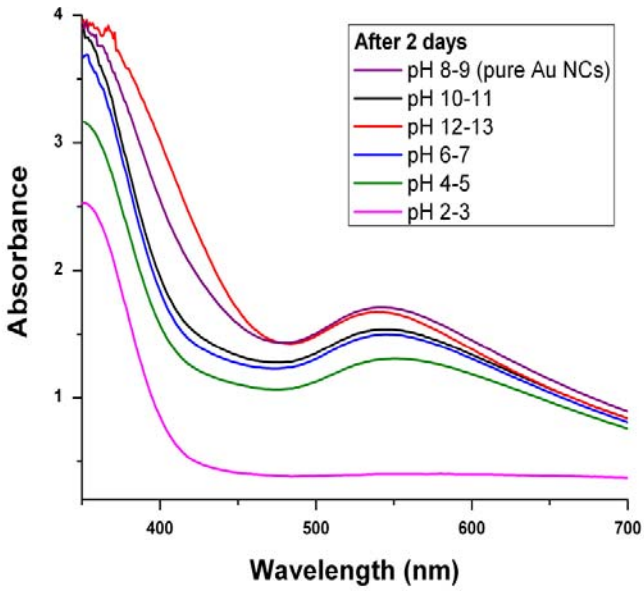

Figure ES5b: Effect of pH on stability of Au-3NPs: after 2 days (5b)

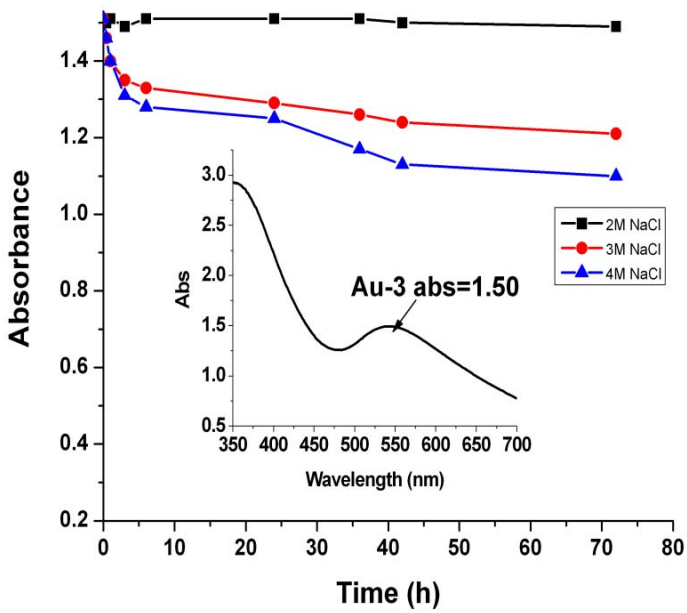

Figure ES6: Effect of NaCl on stability of Au-3NPs (■= 2M NaCl, ●= 3 M NaCl, ▲= 4M NaCl) inset shows absorbance spectra of Au-3NPs

With 2M NaCl, after a week's time, microscopic precipitates were noticed at the bottom of vials which shows that they are stable to salt solutions for quite a long time.

Temperature effect on stability of Au-NPs:

Temperature effects on stability of Au-NPs were also studied under a wide temperature range and NPs were found to be stable up to 80°C. For this purpose Au-NPs were heated for 30 minutes at different temperature between 20-80°C and the stability was checked by observing absorbance and through formation of precipitates as seen from naked eye. Above 80°C the gold nanoparticles start coagulation and form precipitates which shows instability of gold nanoparticles at higher temperature.

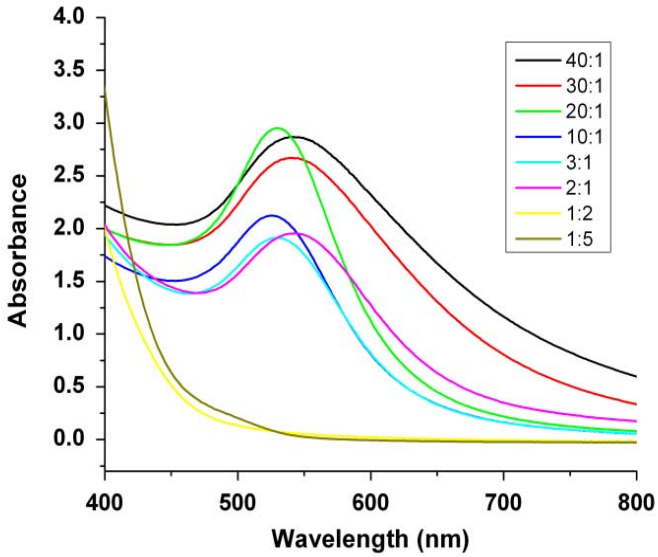

Figure ES7: UV-vis spectra showing different gold to ligand ratios using triethylamine as reducing agent

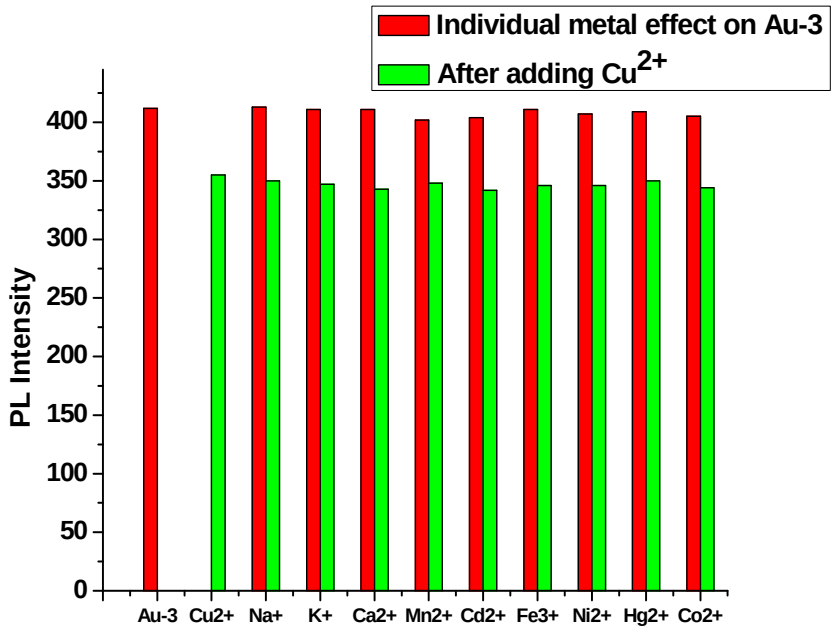

Figure ES8: Study of interfering species on Au-3NPs for detection of Cu^{2+}

Conditions: 1×10^{-6}M Cu^{2+}; 1×10^{-4}M metal species

Red bars and green bars represent the individual metal ion′s responses, and the mixture of Cu^{2+} and corresponding metal ions on Au-3NPs, respectively. Excellent selectivity for Cu^{2+} detection was achieved over alkali, alkaline earth, and heavy transition-metal ions, and this technique shows great promise for point-of-use and in-field detection of environmentally toxic copper.

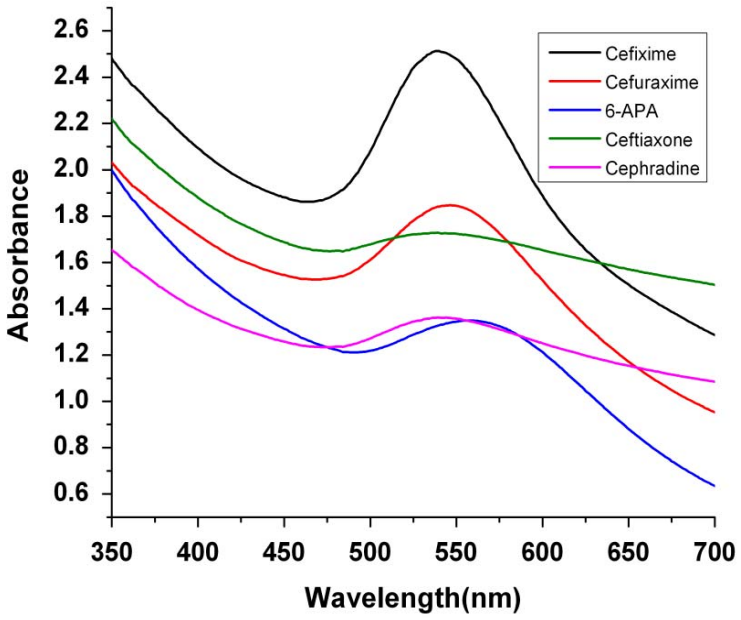

Figure ES9: UV-vis spectra of Au-NPs with different β-lactam antibiotics

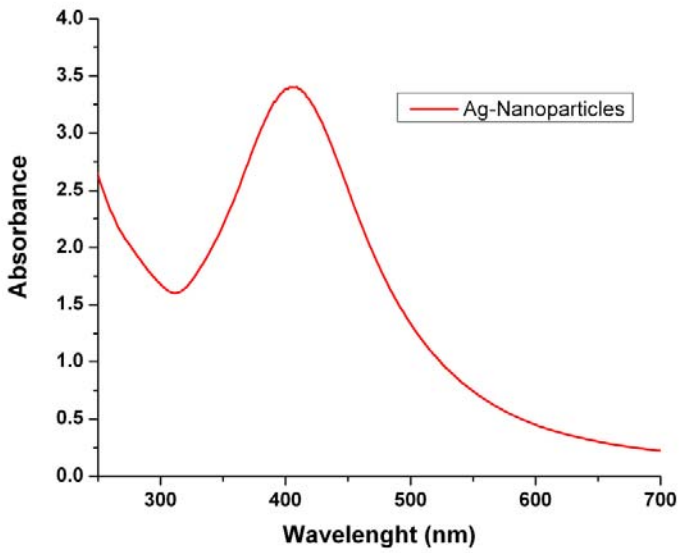

Figure ES10: UV-vis spectra of Ag-nanoparticles stabilized with amoxicillin

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Table ES1: Optimized/optical parameters for Synthesis and Stabilization of Au-NPs with few other β-lactam antibiotics

S. No.	Beta lactam antibiotic	Au:ligand	λ^{abs}/ abs ^{max} (nm)
1	**6-APA**	5:1	560/1.349
2	**Ceftriaxone**	10:1	544/1.361
3	**Cefuraxime**	30:1	547/1.847
4	**Cefradine**	10:1	544/1.361
5	**Cefixime**	10:1	539/2.513

Conditions: $HAuCl_4$; 50mM, Ligand; 50mM, $NaBH_4$; 880mM