

## Stable Gold Nanoparticles synthesis using but-2-yne-1,4-diol – a simple approach

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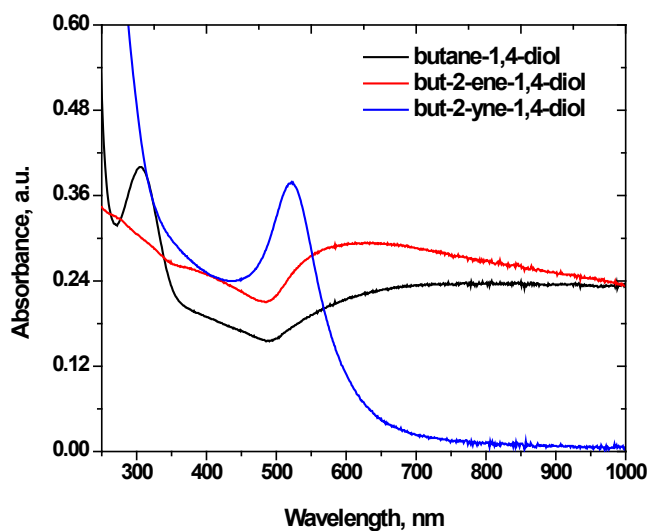
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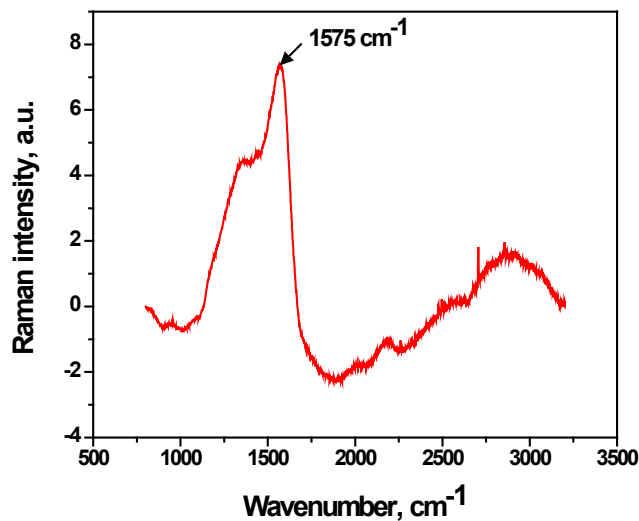
### Supporting Information

Fig.S1



UV-Vis spectra of gold nanoparticles synthesized using different diols, as labeled in the spectrum.

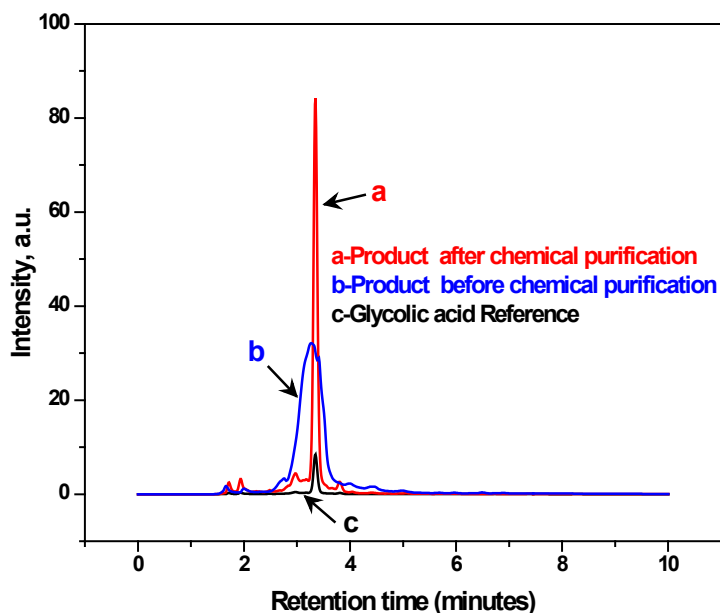
Fig.S2



Raman spectrum of gold nanoparticles derived from B≡D

Raman signals are broad in the region of 1000 to 1600  $\text{cm}^{-1}$ . It could be due to the overlap of  $-\text{CH}_2-$  and  $\text{C}=\text{O}$  bands. Though the isolated  $\text{C}=\text{O}$  stretching comes around 1700  $\text{cm}^{-1}$  (Giorgini *et al.* *J.phy.chem A* 2005, 109, 5846). Toma *et al.* reported that the citrated adsorbed on gold showed SERS (surface enhanced Raman signal) effect with an enhanced signal at 1609  $\text{cm}^{-1}$  for asymmetric and 1388  $\text{cm}^{-1}$  for symmetrical stretching, while there was no band at 1609  $\text{cm}^{-1}$  for pure sodium citrate (*J. Raman Spectrosc.* 2011, 42, 644). We observed broad peak ca. 1575  $\text{cm}^{-1}$  in Raman spectrum, which may come from the reaction product adsorbed on gold nanoparticles that contains  $\text{C}=\text{O}$  group.

Fig.S3



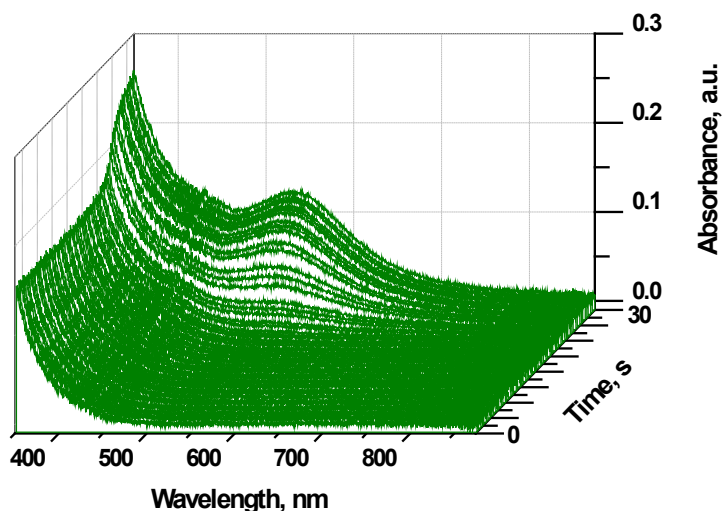
HPLC chromatograms of the extracted product of oxidation of but-2-yne-1,4-diol by  $\text{HAuCl}_4$

Mass spectrometric identification of glycolic acid is not a straightforward approach, as it does not yield significant “molecular ion peak” corresponding to its molecular weight 76.1 [SDBS database: [http://sdb.sdb.aist.go.jp/sdb/cgi-bin/direct\\_frame\\_top.cgi](http://sdb.sdb.aist.go.jp/sdb/cgi-bin/direct_frame_top.cgi)]. In such cases, chemical derivatization followed by flame ionization is used to determine glycolic acid quantitatively [C.Leboulanger, L.Serve, L.Comellas and H.Jupin, *phytochemical analysis*, vol. 9, 5–9 (1998)]. Hence, we have used a HPLC comparison of the chromatogram of the product of the reaction between  $\text{HAuCl}_4$  and butynediol with that of the reference glycolic acid sample, with good agreement. Moreover, we have also shown the presence of  $\text{C}=\text{O}$  stretching in the IR spectrum of gold nanoparticle dispersion, i.e.,  $\text{HAuCl}_4$  and But-2-yne-1,4-diol mixture.

High Performance Liquid Chromatography (HPLC) was performed using the column: C18-Phinogel column as the stationary phase with a mobile phase containing 50:50 (v/v)

water:methanol. The reaction mixture of  $\text{HAuCl}_4$  and but-2-yne-1,4-diol was purified in the following manner: the mixture was shaken with 0.1 M NaOH and washed with acetonitrile:chloroform (50:50 v/v) mixture to remove the unreacted but-2-yne-1,4-diol. The aqueous ingredients was collected into the mobile phase, i.e., 50:50 (v/v) water:methanol. The retention time ( $R_T$ ) of the product sample, thus chemically purified in the manner described above, is found to be in very good agreement with that of the reference glycolic acid sample (fig.S3). The product sample, without the abovementioned chemical treatment exhibited a broad chromatographic peak due to the presence of the reactant/other minor products (other than the major product, glycolic acid). However, the chemical treatment of the product mixture renders it amenable for identification, as an excellent agreement is found with the reference standard.

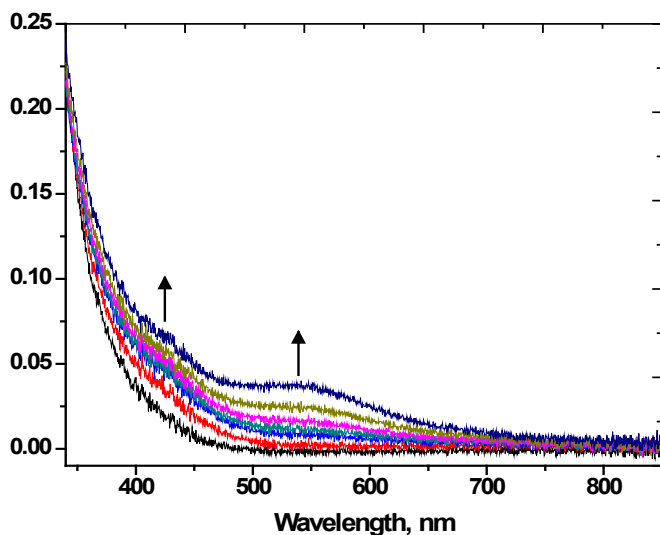
**Fig.S4**



*In situ* UV-Vis spectral monitoring of gold nanoparticle formation

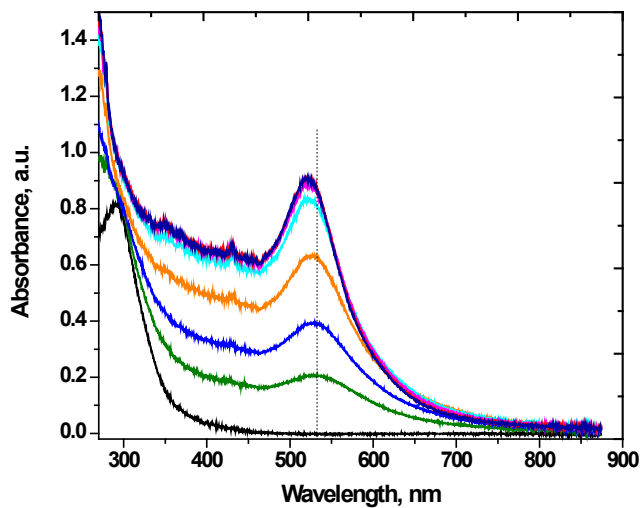
(for 30s after the addition of  $\text{B}\equiv\text{D}$ ) using Fiber-Optic UV-visible spectrometer

**Fig.S4(a)**



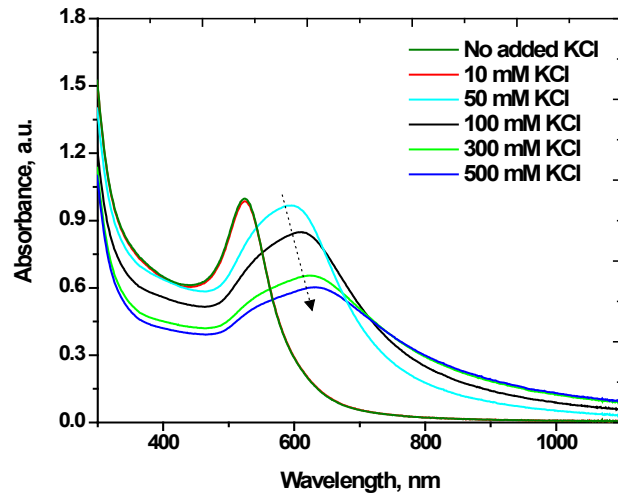
Evolution of band at  $\sim 420$  nm, before the appearance of SPR band, during the formation of gold nanoparticles (spectra are taken from fig.S3). Arrow indicates the evolution of new bands.

**Fig.S4(b)**



UV-Vis spectra recorded in every minute after the addition of B≡D. Shift in wavelength maximum is indicated by dotted vertical line.

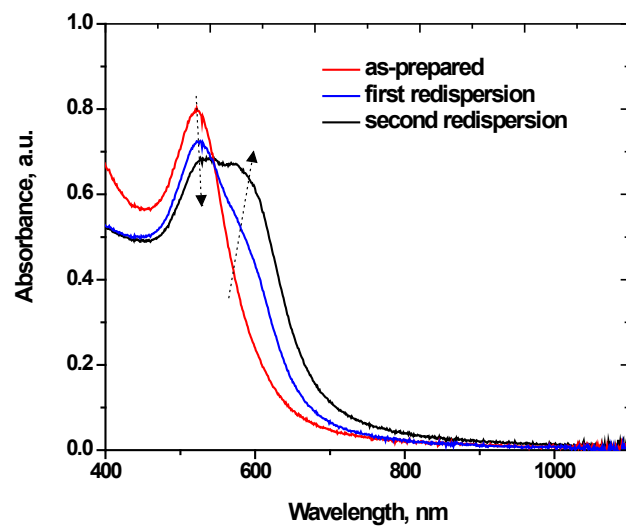
Fig.S5



UV-Vis spectra showing the effect of addition of KCl to gold nanoparticle sols.

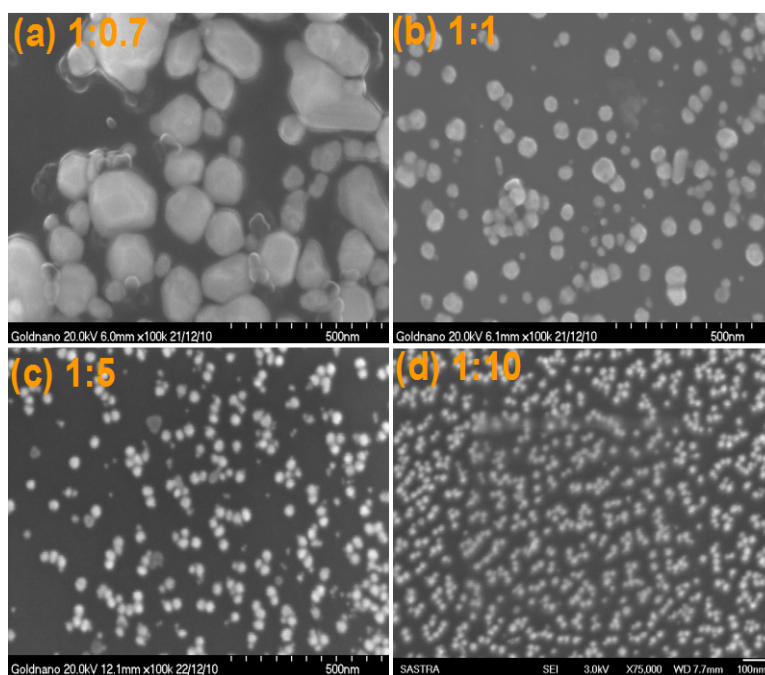
As can be seen from the spectra, addition of 10 mM KCl does not influence the SPR position and intensity. However, the wavelength maximum is red shifted as KCl concentration increases indicating particle aggregation due to increased ionic strength. This proves the electrostatic nature of the particle stabilization.

**Fig.S6**



UV-Vis spectrum of gold nanoparticles: Effect of successive centrifugation and re-dispersion of gold nanoparticles in water

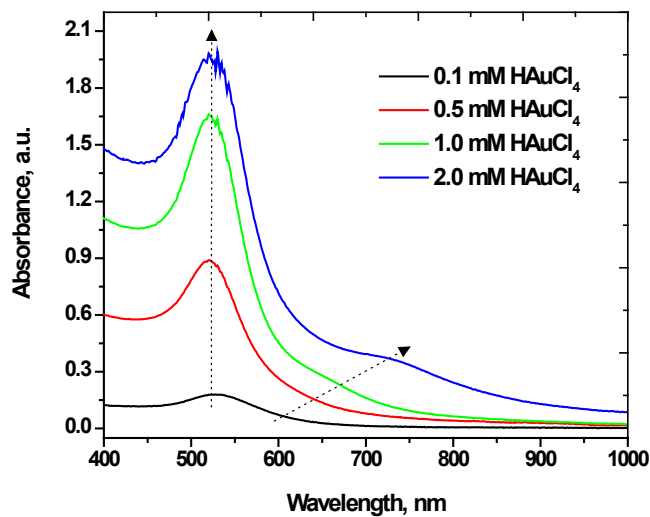
**Fig. S7**



FE-SEM images of gold nanoparticles synthesized using different molar ratios of H<sub>Au</sub>Cl<sub>4</sub> (0.25 mM) and B≡D, as labeled in each image. Scale bar: (a-c) 500 nm (x100k); (d) 100 nm (x75k).



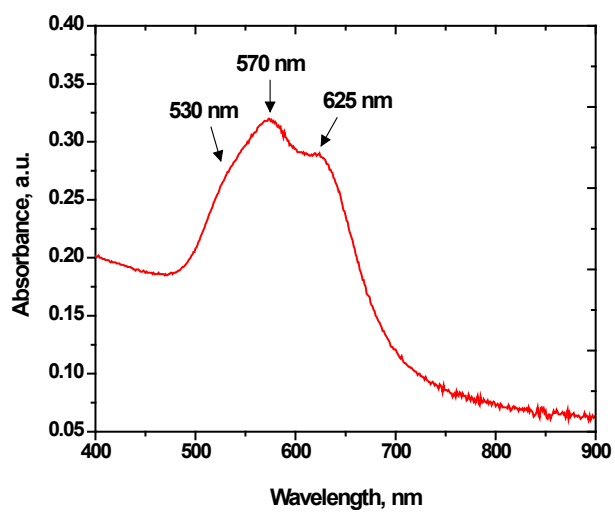
Fig.S8



UV-Vis spectrum of gold nanoparticles: Effect of concentration of HAuCl<sub>4</sub>.

As the concentration of HAuCl<sub>4</sub> increases, the wavelength maximum remains constant at 520 nm, while additional shoulders emerge in the range of 600-800 nm that increase in intensity. The latter may be associated with the formation of polyhedral particles and not due to aggregation, since the colloids continue to remain stable for several months.

**Fig.S9**



UV-visible spectrum gold nanoparticles synthesized from the mixture containing 0.1 mM

$\text{HAuCl}_4$  + 10 mM B $\equiv$ D + 1 mM CTAB