Supplementary information

Interactions of Schiff-Base Ligands with Gold Nanoparticles: Structural, Optical and Electrocatalytic Studies

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Fig. S1 Crystallographic structures of the dihydroxysalophen isomers (A) 2,3-DHS; (B) 2,5-DHS obtained from the Cambridge Crystallographic Database (CDC) using MIJWUY, VEFTEG as entries, respectively. Blue and red sticks correspond to nitrogen and oxygen atoms, and dash lines indicate H-bonds. Mercury 2.3 and POV-Ray 3.6 software were used for visualization.
Fig. S2  UV-visible absorption spectra of the dihydroxysalophen isomers (A) 3,4-DHS; (B) 2,5-DHS; (C) 2,3-DHS in aqueous solution at different concentrations: $0.25 \times 10^{-5}$ M (black line); $0.5 \times 10^{-5}$ M (green line); $1 \times 10^{-5}$ M (magenta line); $2 \times 10^{-5}$ M (blue line) and $5 \times 10^{-5}$ M (red line).
**Fig. S3** Kinetic of the interaction between the 3,4-DHS (2.0x10^5 M) and citrate-AuNPs (1.8x10^-9 M) at pH 7.4 at the presence of 5 mM of tris(hydroxymethyl)aminomethane. UV-visible absorption spectra were recorded every 5 min in aqueous solution.

**Fig. S4** Absorbance FTIR spectrum of citrate-Au nanoparticles at pH 9.3. Nanoparticles were drop-cast on a BaF<sub>2</sub> window and left to dry. Vibrations at 2955, 2867, 1609, 1512 and 1456 correspond to the vibrational modes ν<sub>asy</sub>(-CH<sub>2</sub>), ν<sub>sym</sub>(-CH<sub>2</sub>), ν<sub>asy</sub>(-CO<sub>2</sub>–), ν<sub>sym</sub>(-CH<sub>2</sub>), ν<sub>sym</sub>(-CO<sub>2</sub>–), respectively. The band at approximately 3380 cm<sup>-1</sup> correspond to the ν(-OH) vibration and the bands at 1257 and 1184 cm<sup>-1</sup> are correlated with ν(-CO).
**Fig. S5** Kinetic of the interaction between the 3,4-DHS (2.0x10⁻⁵ M) and thioctic-AuNPs (1.8x10⁻⁹ M) at pH 9.3 in aqueous solution. UV-visible absorption spectra were recorded every 5 min in aqueous solution.

**Fig. S6** Emission spectra of 2,3-DHS (2.0x10⁻⁵ M) in aqueous solution containing different concentrations of AuNPs. Inset: Stern-Volmer plot of 3,4-DHS with the increasing concentrations of AuNPs. [AuNPs]: 0.0 M (black line); 7.2x10⁻¹⁰ M (green line); 1.1x10⁻⁹ M (blue line); 1.4x10⁻⁹ M (magenta line); 1.8x10⁻⁹ M (cyan line); 2.7 x 10⁻⁹ M (yellow line); 3.4 x 10⁻⁹ M (brown line).
Fig. S7 Emission spectra of 2,5-DHS (2.0x10^{-5} M) in aqueous solution containing different concentrations of AuNPs. Inset: Stern-Volmer plot of 2,5-DHS with the increasing concentrations of AuNPs. [AuNPs]: 0.0 M (black line); 7.2x10^{-10} M (green line); 1.1x10^{-9} M (blue line); 1.4x10^{-9} M (magenta line); 1.8x10^{-9} M (cyan line).
Fig. S8 Cyclic voltammograms of carbon-screen printed electrodes in 0.1 M H$_2$SO$_4$ before (red line) and after electrodeposition of citrate-AuNPs by application of a constant positive potential of +0.8 V during increasing periods of time: 15 min (green line); 30 min (blue line); 45 min (magenta line) and 60 min (cyan line). Measurements were carried out at a scan rate of 100 mV/s.
Fig. S9 Cyclic voltammograms of carbon-screen printed electrodes in phosphate buffer solution (pH 7.0) containing 10mM [Fe(CN)$_6$]$^{3-}$ before (blue line) and after electrodeposition of citrate-AuNPs (red line) by application of a constant positive potential of +0.8 V during 60 min. Measurements were carried out at a scan rate of 100 mV/s.