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: 0.25×10^{-5} M (black line); 0.5×10^{-5} M (green line); 1×10^{-5} M (magenta line); 2×10^{-5} M (blue line) and 5×10^{-5} M (red line).



Fig. S3 Kinetic of the interaction between the 3,4-DHS $(2.0 \times 10^{-5} \text{ M})$ and citrate-AuNPs $(1.8 \times 10^{-9} \text{ M})$ 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 BaF₂ window and left to dry. Vibrations at 2955, 2867, 1609, 1512 and 1456 correspond to the vibrational modes $v_{asy}(-CH_2)$, $v_{sym}(-CH_2)$, $v_{asy}(-CO_2^-)$, $v_{sym}(-CH_2)$, $v_{sym}(-CO_2^-)$

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Fig. S5 Kinetic of the interaction between the 3,4-DHS $(2.0 \times 10^{-5} \text{ M})$ and thioctic-AuNPs $(1.8 \times 10^{-9} \text{ M})$ 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); 2.7×10^{-9} M (yellow line); 3.4×10^{-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 $0.1 \text{ M H}_2\text{SO}_4$ 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.