Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Dual colorimetric sensing of Ascorbic Acid and Thyroxine using Ag-EGCG-CTAB with DFT approach

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EXPERIMENTAL

Optimization and Colorimetric sensing of AA and TH

For the colorimetric sensing, 0.1 - 0.7 μM of AA and 0.1 - 0.4 μM TH were prepared from 0.1 mM stock solution.The freshly prepared Ag-EGCG-CTAB was first diluted for 5 times before using in the detection of AA. Subsequently, the prepared amount of AA was added to the Ag-EGCG-CTAB, stirred for 3 minutes and the change in absorbance maxima was analyzed using UV-Visible Spectrophotometer. On the other hand, for detection of TH, the stock solution was diluted to three times and then reaction with different concentrations of TH was analyzed by observing the change in SPR peak after 10 minutes. The reactions were performed at an ambient temperature of 30^0C. Detection limit was evaluated by calculating Standard Deviation (SD) and slope of the linear curve according to the formula LoD = 3×SD/K.

Preparation of samples for detection

For the practical analysis of AA and TH in real pharmaceutical samples, four different branding tablets were grinded and homogenized. The sample of weight equal to one tablet was dissolved in 100 ml of Milli Q water followed by sonication and centrifuged to get the clear supernatant. Further, the solutions were spiked with 5μM of AA and TH respective of their tablet solution and introduced to the colorimetric probe.

Paper based detection of AA coupled with smartphone integrated detection

Whatman 150 mm filter paper was employed in the detection of AA. With a sharp scissor, the filter papers were cut into rectangular strips of size 2 x 2 cm. The strips were then immersed in the solution of Ag-EGCG-CTAB for 24 hours at room temperature. In the next step, the strips were taken out from the solution carefully with forceps and dried naturally in room temperature. Different concentrations of AA were poured in the strips and the color change was observed. The color change was also then scanned in a Smartphone using a color

scanning application (Color Detector) and the RGB (Red, Green, Blue) intensities were noted. A graph has been plotted with the Intensity of RGB at Y axis and concentration at X axis from which we can deduce the equation of graph.

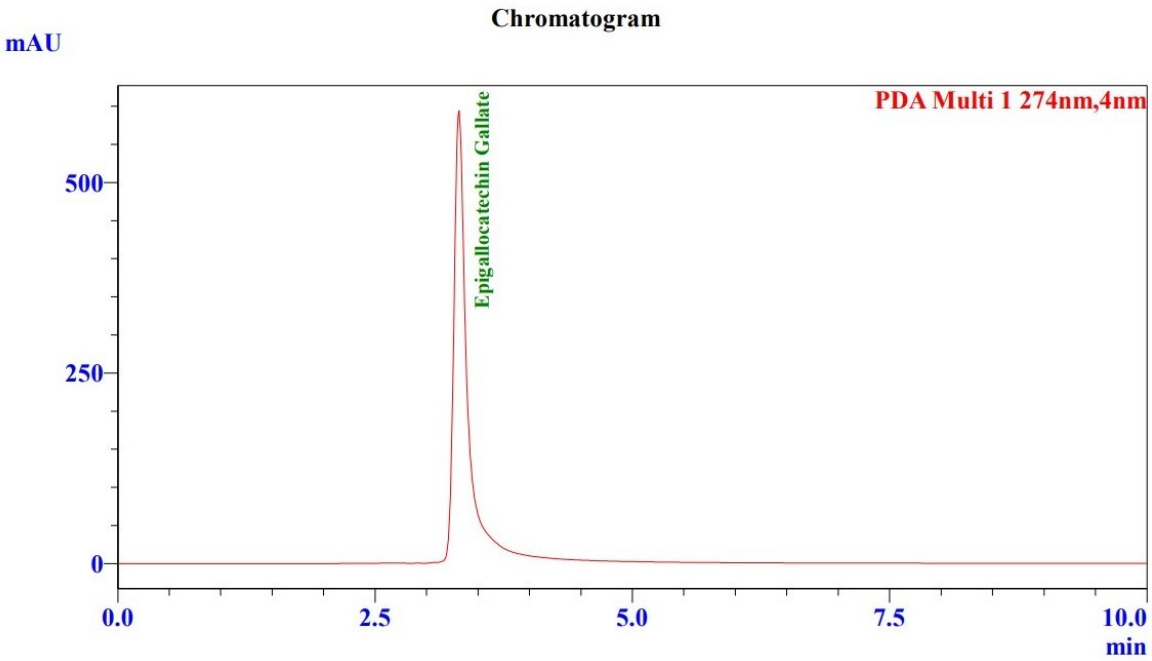


Figure S1. HPLC Chromatogram of Standard EGCG

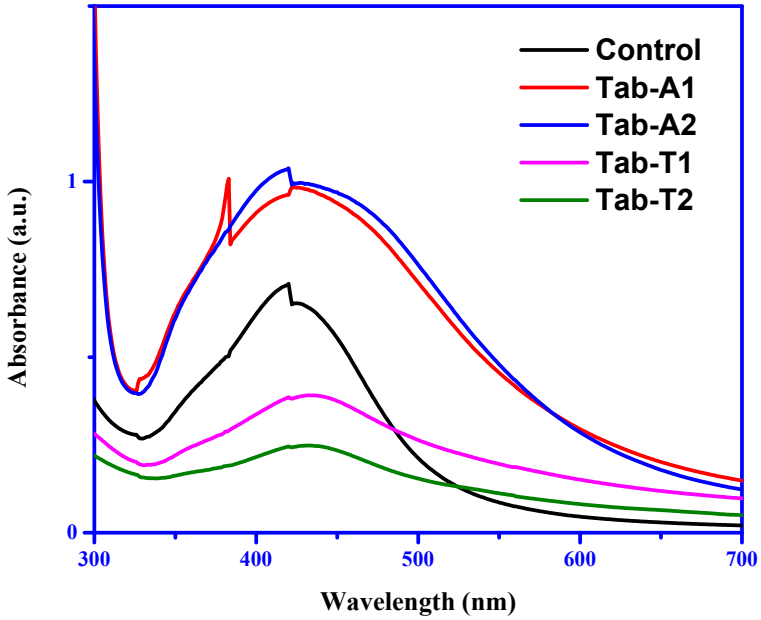


Figure S2. UV-Visible spectra of real samples.

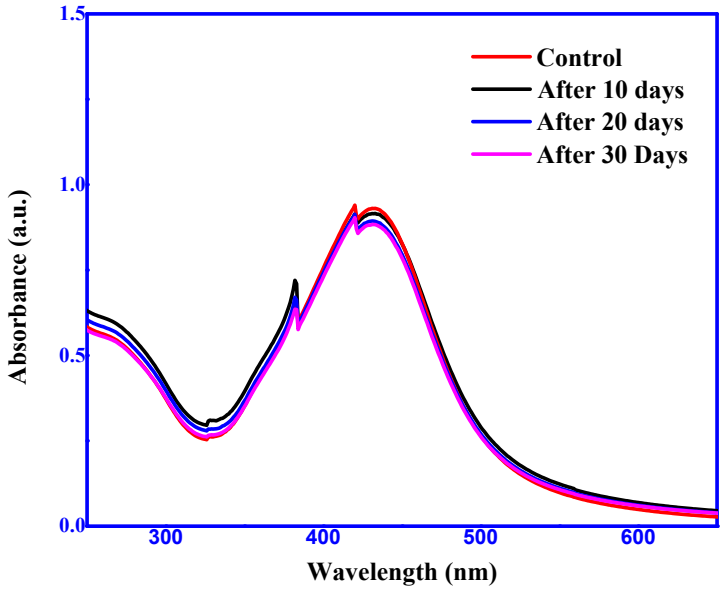


Figure. S3. Stability of the synthesized Ag-EGCG-CTAB

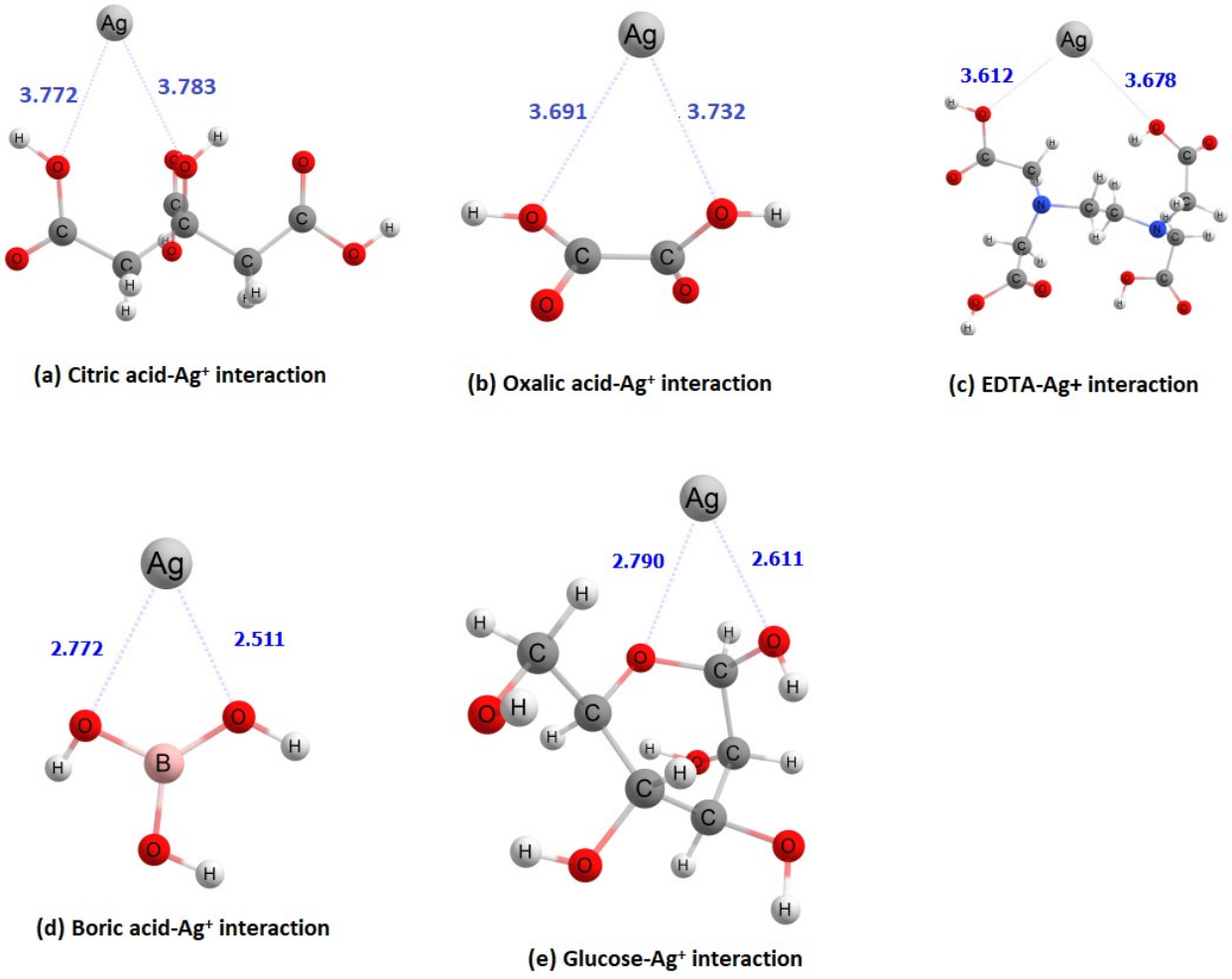
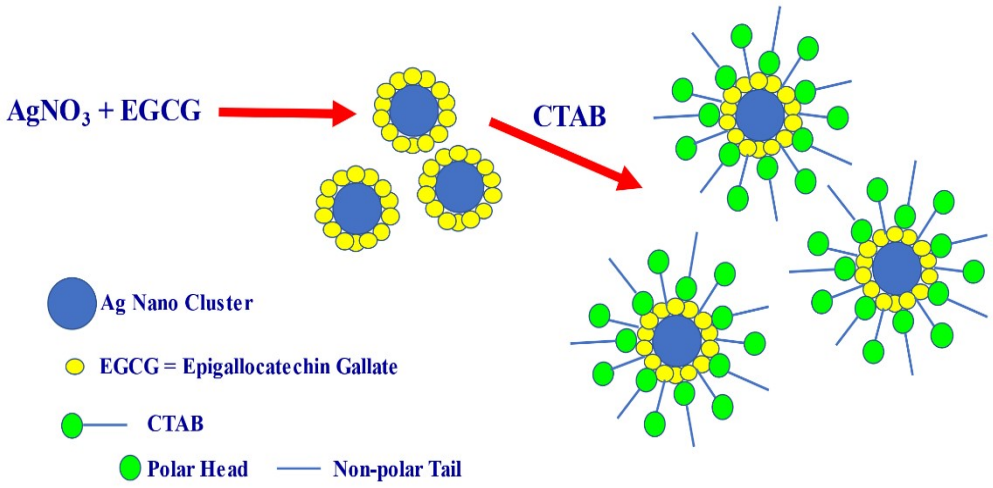


Figure S4. Interaction of Ag^+ ion with (a) Citric acid, (b) Oxalic acid (c) EDTA, (d) Boric acid and (e) Glucose.

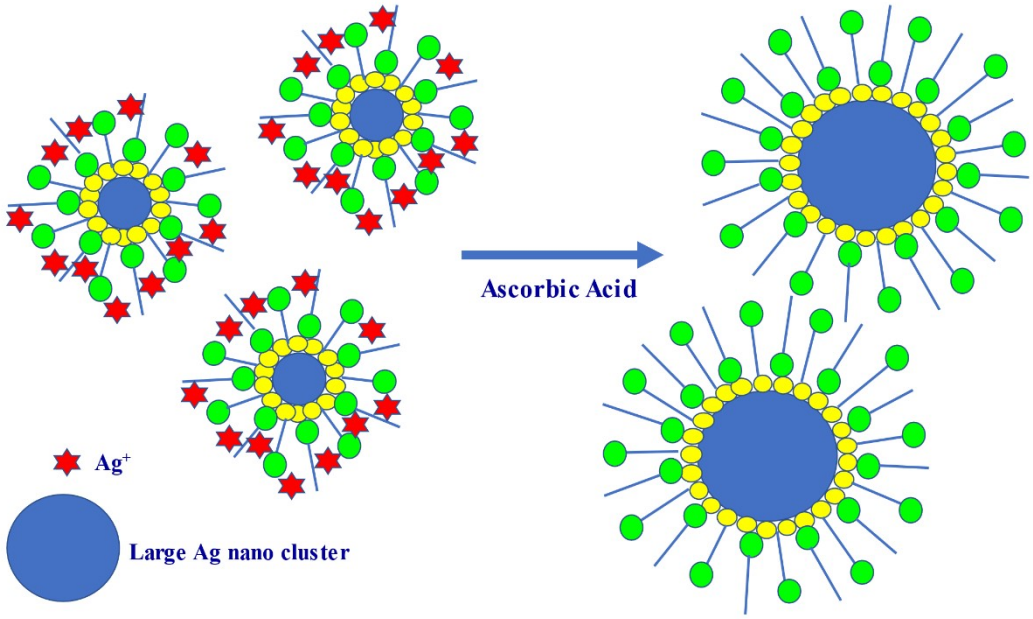
Table S1. Binding energies (kcal/mol) of Ag^+ ion with different compounds and the natural charges (in |e|) at the binding oxygen atoms of the free compounds.

Compound	Binding Energy	Natural charge at O atom
Citric acid	3.4	-0.213
Oxalic acid	4.1	-0.311
EDTA	4.7	-0.326
Boric acid	6.1	-0.388
Glucose	5.8	-0.361
AA	19.3	-0.613

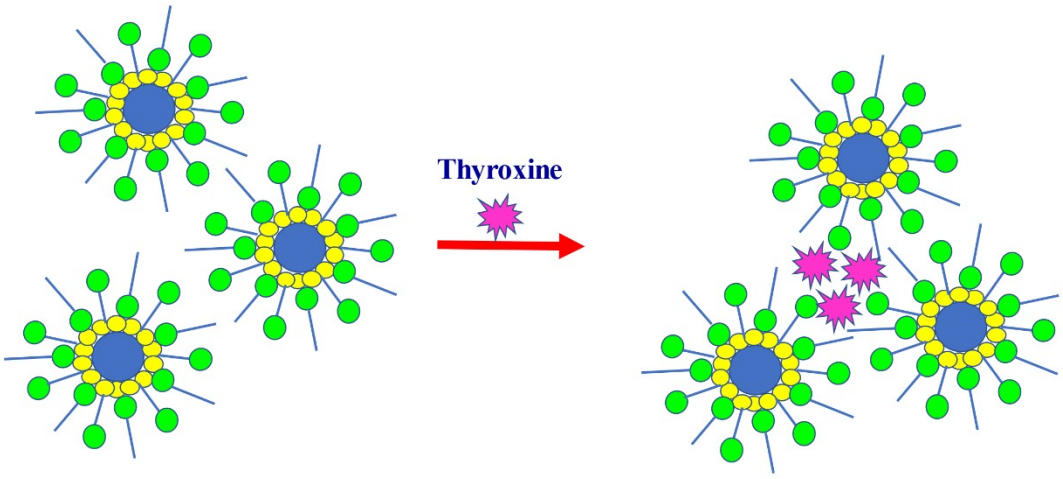
Figure S5: Interaction of CTAB with oxalic acid.



Scheme S1. Schematic illustration of Formation of Ag-EGCG-CTAB



Scheme S2. Schematic illustration of sensing mechanism of AA



Scheme S3. Schematic illustration of sensing mechanism of TH