Supplementary Material

Integrated Computational and Experimental Design of Copper–Gallic Acid Nanozymes for Selective Salbutamol Detection

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S1. FTIR and XRD characterization

In the FTIR spectrum of GA, the bands observed in the range of 4000–3000 cm^{-1} with a strong and narrow peak at 1701 cm^{-1} were attributed to the stretching vibration of the hydroxyl (OH) group and the carbonyl (C=O) group, respectively. The peaks at 1620, 1540, and 1451 cm^{-1} were characteristic of the stretching vibrations of the carbon-carbon (C-C) bonds within the aromatic ring of GA. Several other peaks observed in the range of 1300–1000 cm^{-1} corresponded to the stretching vibrations of the carbon-oxygen (C-O) bond and the bending vibration of the hydroxyl (O-H) bond of GA. The FTIR spectrum of HSs exhibited a notable increase in intensity and a shift in the position of the peaks associated with hydroxyl groups (Fig. S1). This observation further supports the formation of the metal-ligand bonds (605 cm^{-1} and 511 cm^{-1}) involving the hydroxyl groups of GA. X-ray diffraction analysis of GA showed a crystalline nature, characterized by the presence of sharp diffraction peaks at specific angles, including 20.12°, 24.9°, 28.11°, and 41.5°. The prepared HSs exhibited similar diffraction peaks to those observed for GA. However, reduced intensity and broadened peaks suggested a decrease in the crystallinity of this organic acid within the nanozymes (Fig. S2).

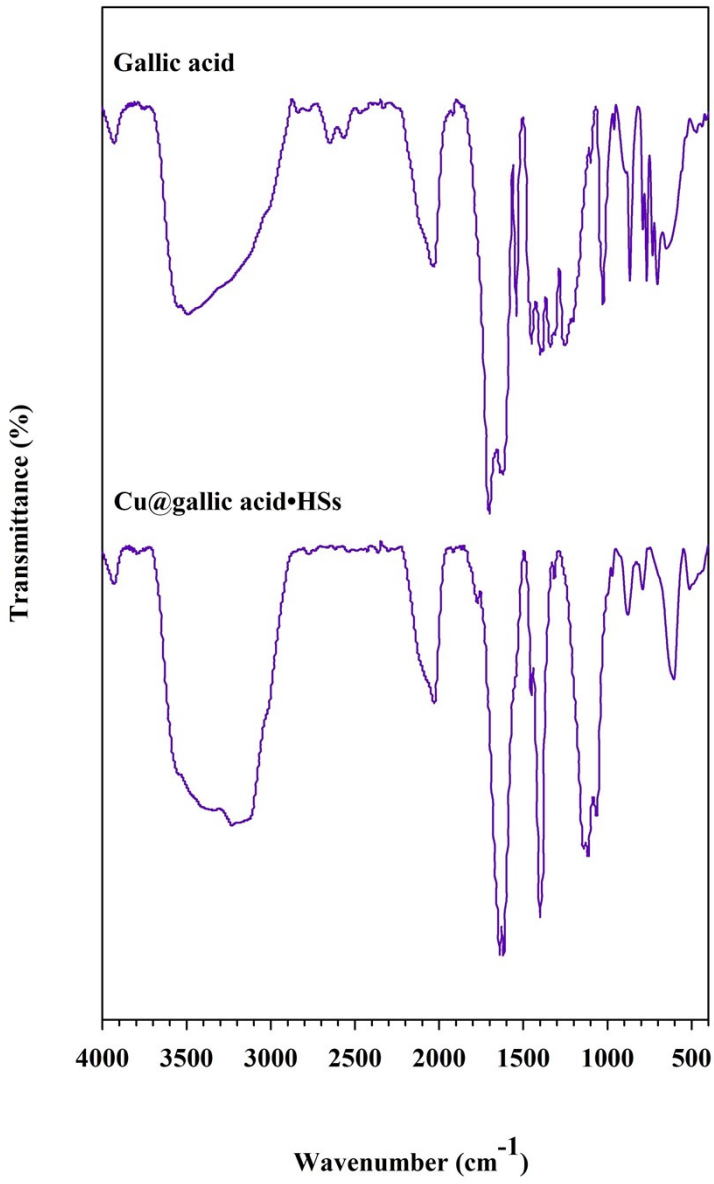

Figure S1. FTIR spectra of gallic acid and the prepared copper@gallic acid hybrid structures (Cu@GA•HSs).

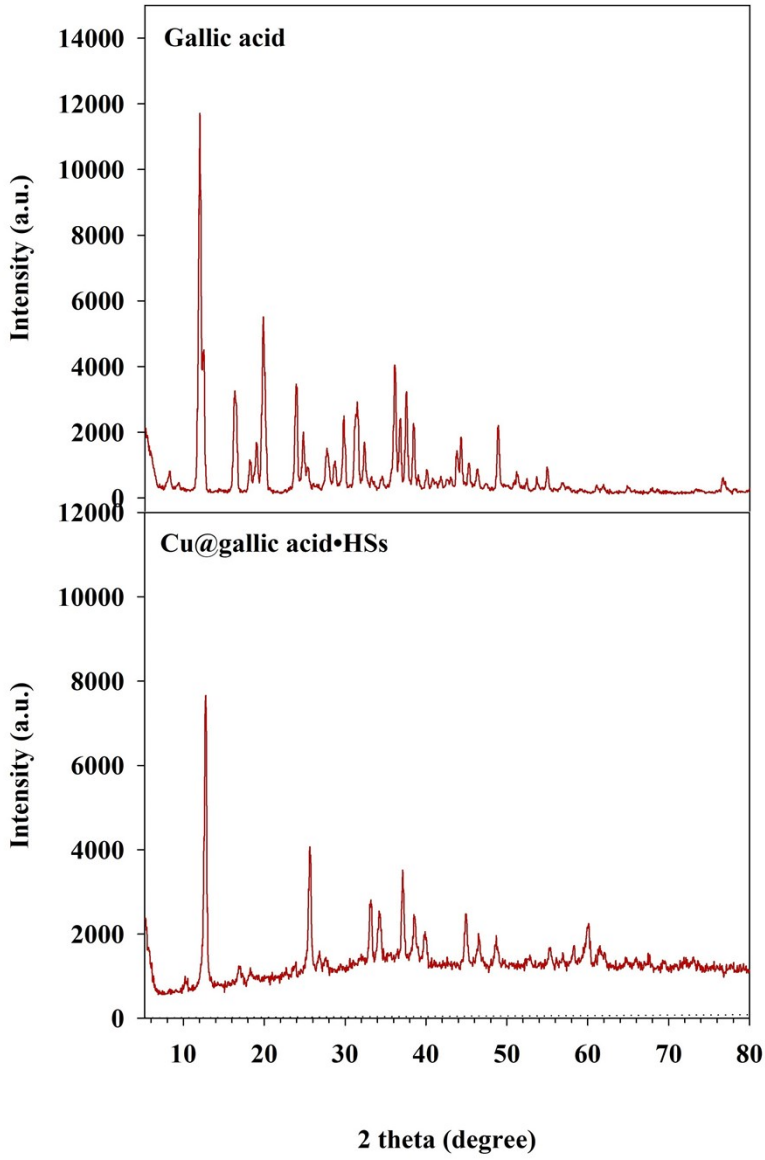

Figure S2. XRD patterns of gallic acid and copper@gallic acid hybrid structures (Cu@GA•HSs).

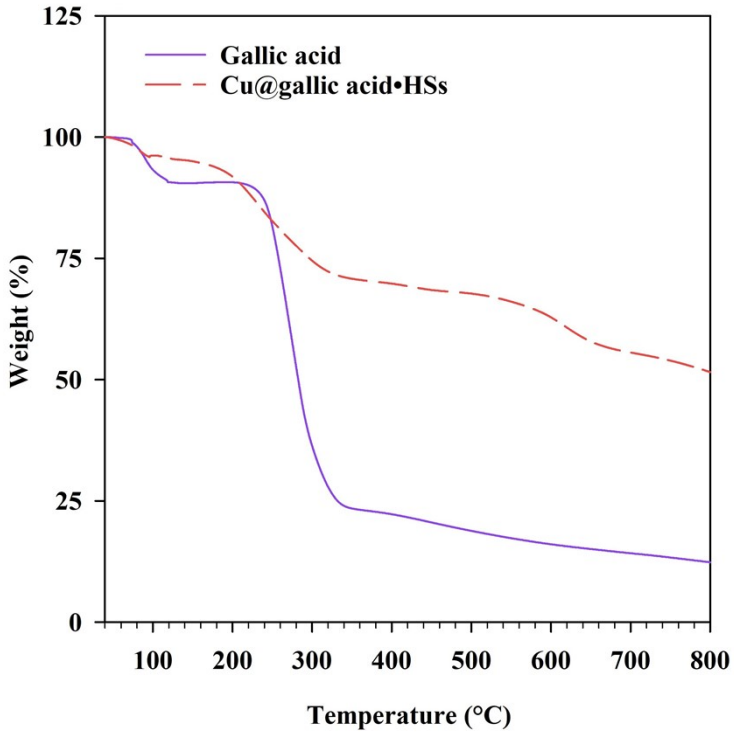

Figure S3. Thermogravimetric analysis (TGA) curves of gallic acid and Cu@gallic acid•HSs.

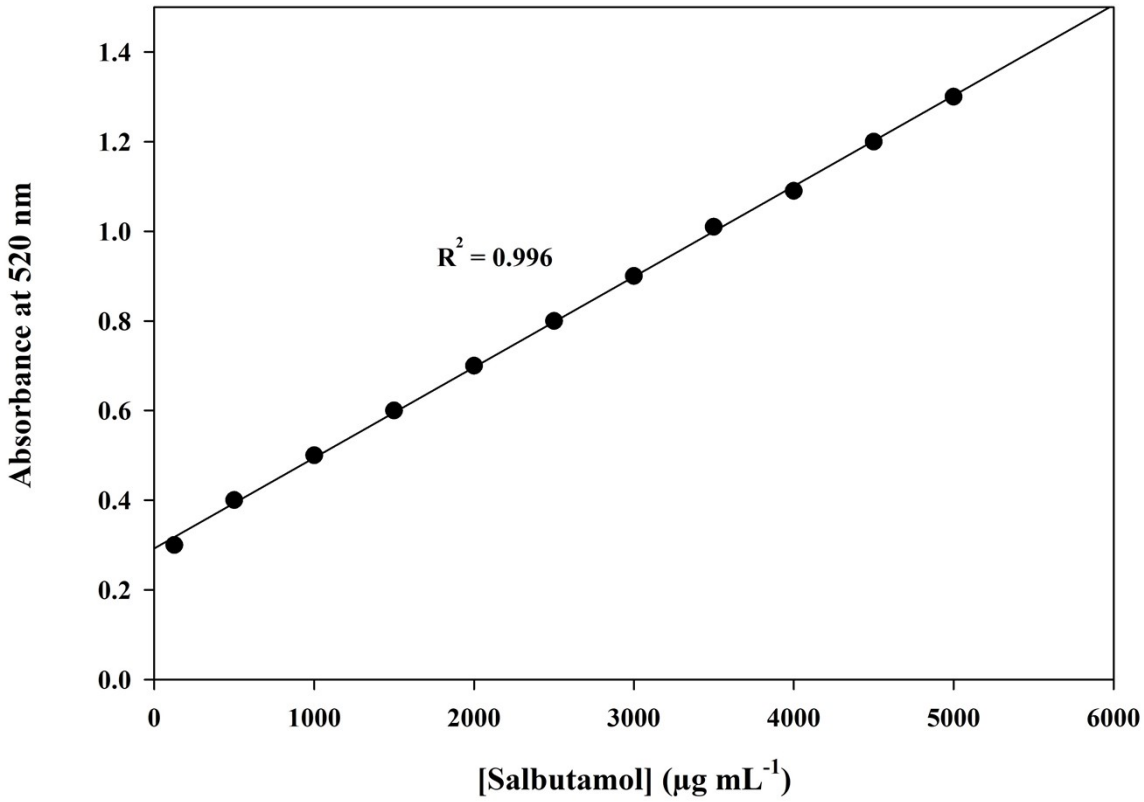

Figure S4. Calibration curve showing the relationship between salbutamol concentration and absorbance, obtained using a copper@gallic acid hybrid structure (Cu@GA•HSs)-based assay in Britton-Robinson (BR) buffer containing 4-aminoantipyrine (4-AP) at 50 °C.

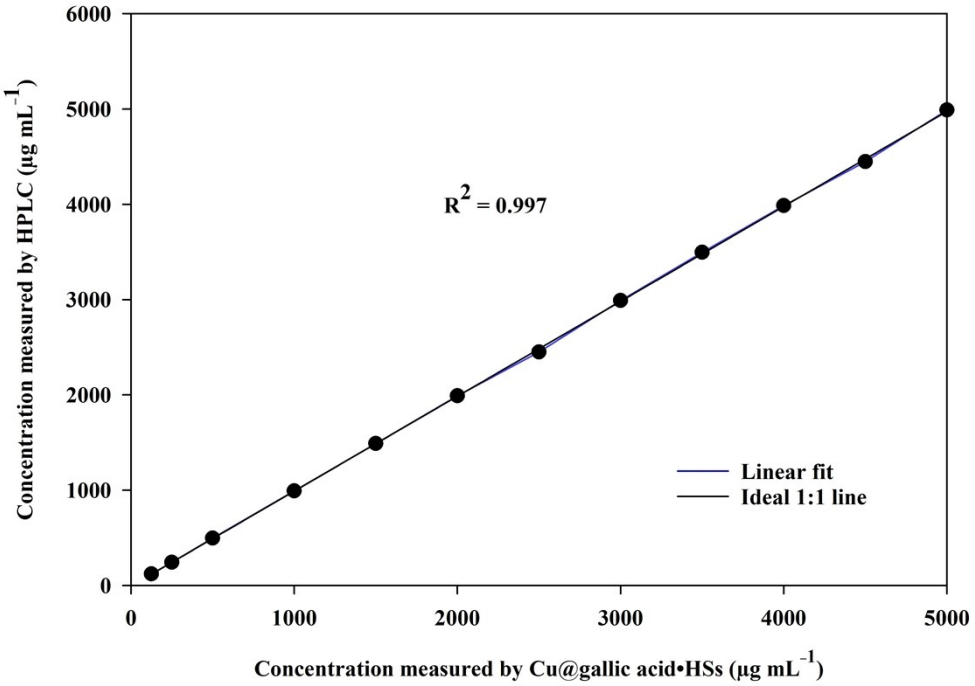

Figure S5. Correlation curve comparing the analytical response from copper@gallic acid hybrid structures (Cu@GA•HSs) with High-Performance Liquid Chromatography (HPLC) signals for the measurement of salbutamol concentration.