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Protection of HeLa Cells against ROS Stress by CuZnSOD Mimic System

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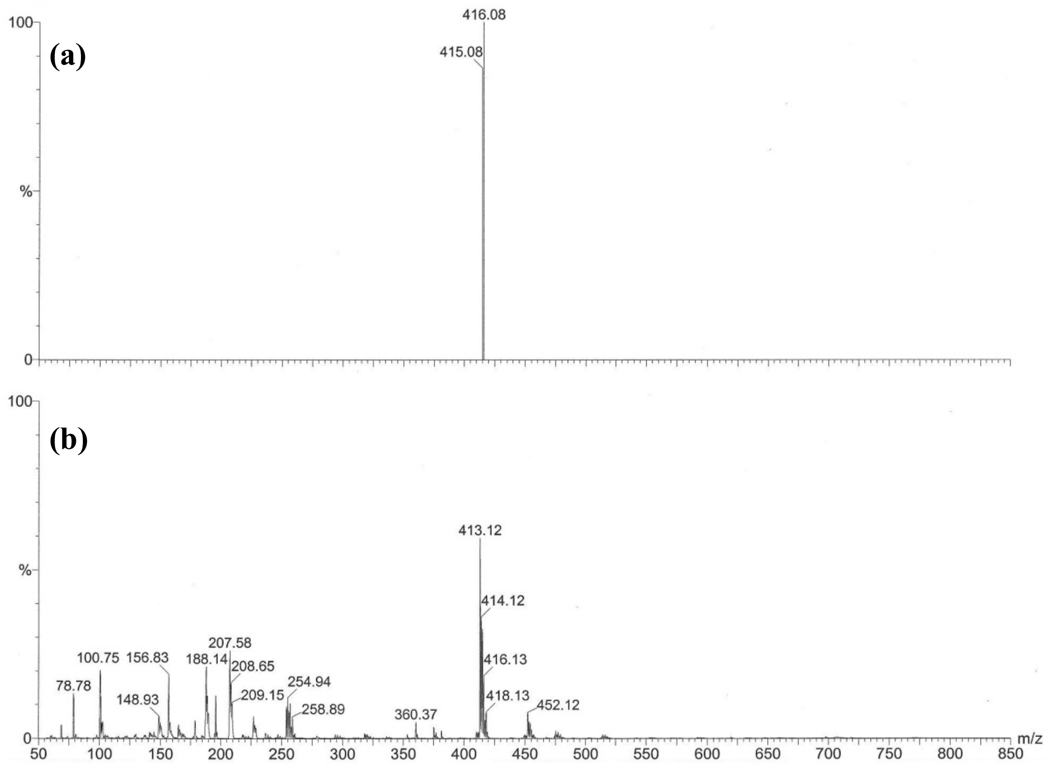
Supplementary Information for Results and Discussion:
Density Function Theory (DFT) calculations of model complex.
Figure S1. The ESI-MS spectrum of SOD–mimic CZpbi complex (as the perchlorate salt) with the focus molecular ion region: (a) simulated and (b) measured.
Figure S2. Small–angle powder XRD patterns of FITC-MSN solids and FITC-MSN-CZpbi.
Figure S3. Nitrogen adsorption–desorption isotherms plots of FITC-MSN and FITC-MSN-CZpbi.
Figure S4. TGA/DTG profiles of FITC-MSN-CZpbi and CZpbi solids. Blue line: weight loss; red line: derivative weight loss.

Density Function Theory (DFT) calculations of model complex

Since a crystallographic study of the model complex is not possible due to its unattainable single crystal form. We applied the hybrid density functional theory (DFT) (B3LYP) [30-32] in conjunction with the 6-31G* basis set to calculate the structural and conformation of copper and the rest of atoms of the model complex. The relevant structures of CZpbi complex were fully optimized in the gas phase. Open shell systems were treated using unrestricted DFT. The final theoretical structure of CZpbi is shown in Figure 1. The optimized bond distances for Cu-N's are: $Cu\text{-}N_1 = 2.017$, $Cu\text{-}N_2 = 2.000$, $Cu\text{-}N_3 = 2.121$, $Cu\text{-}N_4 = 1.998$, and $Cu\text{-}N_5 = 2.155$ Å. The bond distance for $Cu\text{-}N_1$ is indeed shorter than the average Cu-N distance of 2.112 Å in other Cu(II)Zn(II) complexes reported previously.[15]



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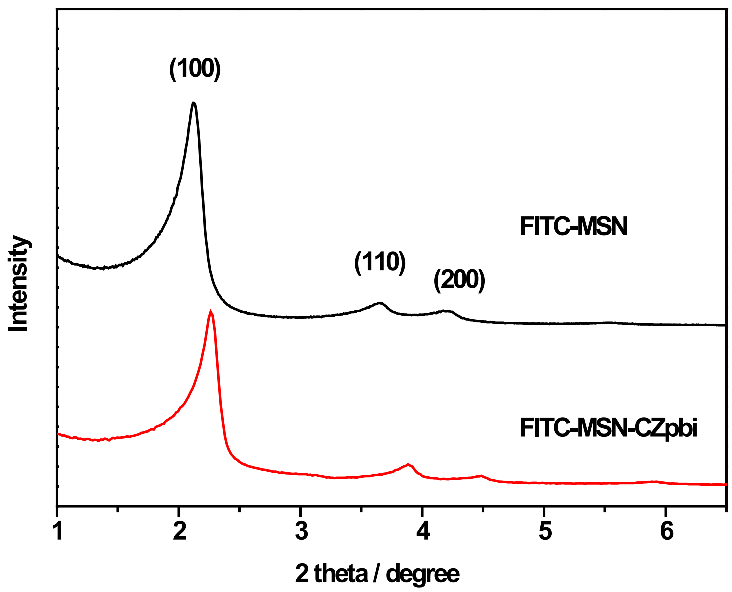

Figure S2. Small–angle powder XRD patterns for FITC-MSN solids and FITC-MSN-CZpbi.

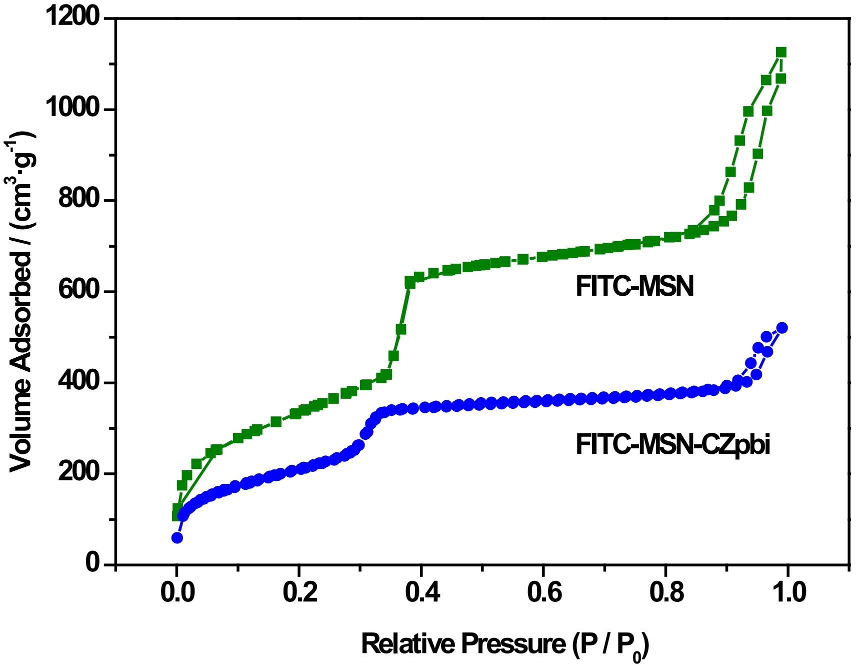

Figure S3. Nitrogen adsorption–desorption isotherms plots for FITC-MSN and FITC-MSN-CZpbi.

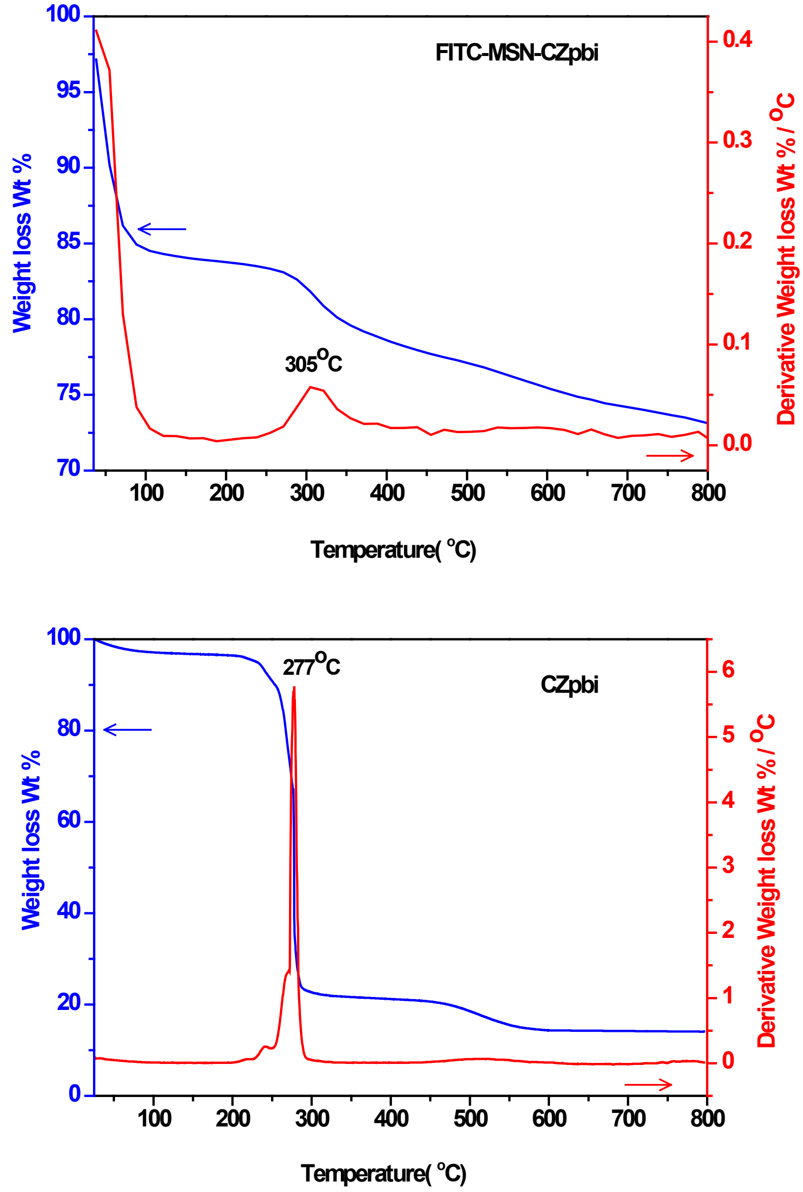

Figure S4. TGA/DTG profiles of FITC-MSN-CZpbi and CZpbi. Blue line: weight loss; red line: derivative weight loss.