

Supplementary Material

Effect of Metal Environment and Immobilization on the Catalytic Activity of a Cu Superoxide Dismutase Mimic

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Table S1. Crystal data and structure refinement for [Cu(pypapn)(ClO₄)₂]

Empirical formula	C ₂₁ H ₂₄ Cl ₂ CuN ₄ O ₈
Formula weight	594.88
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, F d d 2
Unit cell dimensions	a = 16.2282(3) Å α = 90° b = 30.3060(6) Å β = 90° c = 9.6575(2) Å γ = 90°
Volume	4749.67(16) Å ³
Z, Calculated density	8, 1.664 g/cm ³
Absorption coefficient	1.201 mm ⁻¹
F(000)	2440
Crystal size	0.093 x 0.105 x 0.112 mm
Theta range for data collection	2.848 to 28.289 deg
Limiting indices	-21<=h<=21, -40<=k<=40, -12<=l<=12
Reflections collected / unique	33929 / 2941 [R(int) = 0.0745]
Completeness to theta = 25.24	99.5 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2941 / 1 / 165
Goodness-of-fit on F ²	1.057
Final R indices [I>2sigma(I)]	R1 = 0.0334, wR2 = 0.0604
R indices (all data)	R1 = 0.0538, wR2 = 0.0666
Largest diff. peak and hole	0.231 and -0.248 e.Å ⁻³

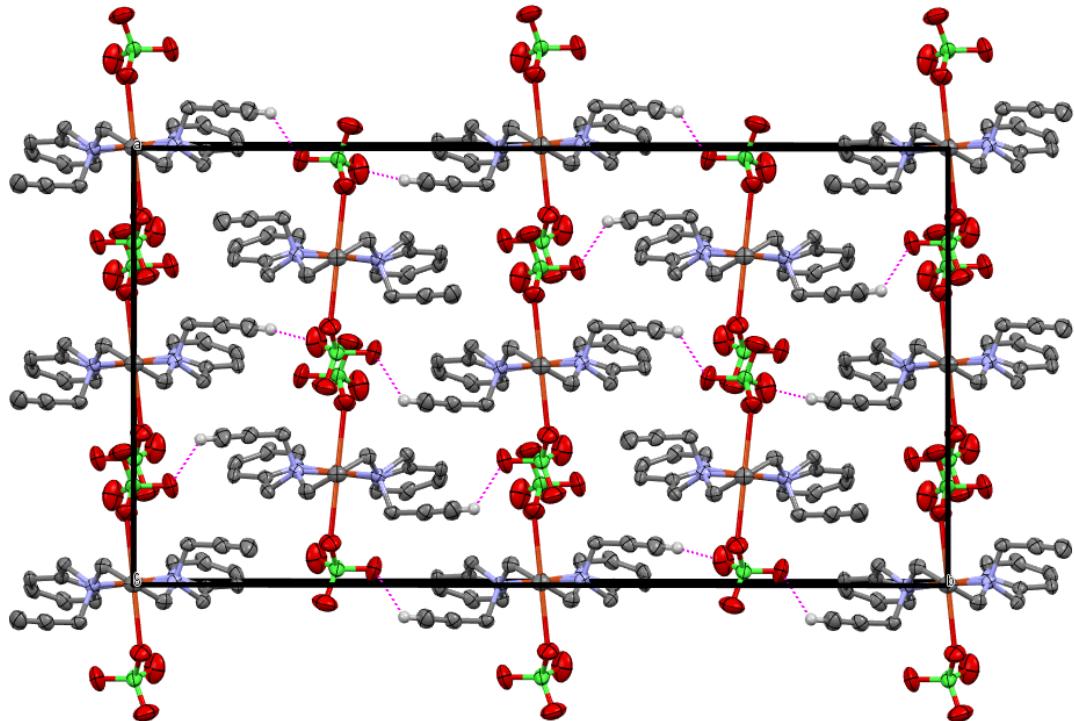


Figure S1. Crystal packing diagram for $[\text{Cu}(\text{pypapn})(\text{ClO}_4)_2]$ viewed along the crystallographic c -axis, showing the intermolecular hydrogen-bonding interactions between perchlorate and the alkyne H as dashed lines. H atoms not involved in these interactions are omitted for clarity.

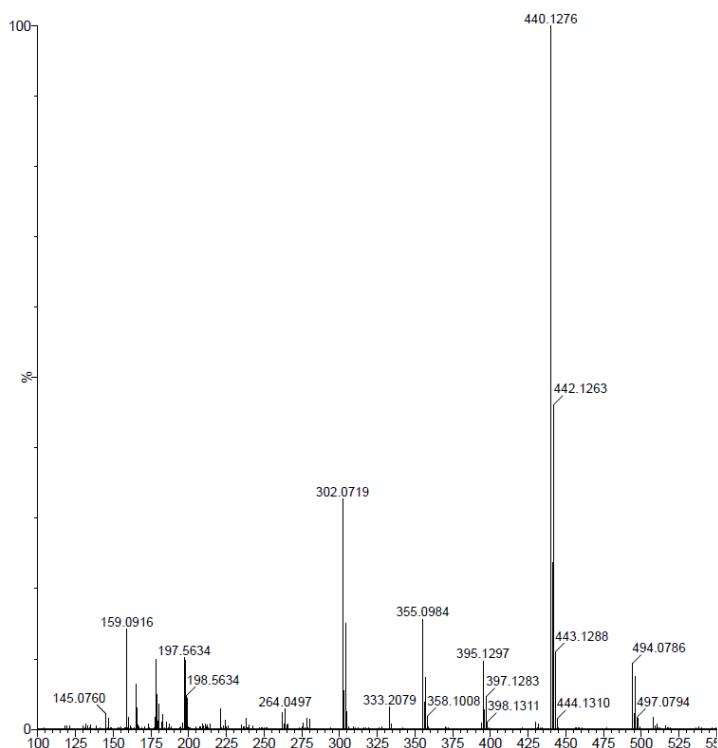


Figure S2. HRMS of $[\text{Cy}(\text{pypapn})(\text{ClO}_4)_2]$ in acetonitrile

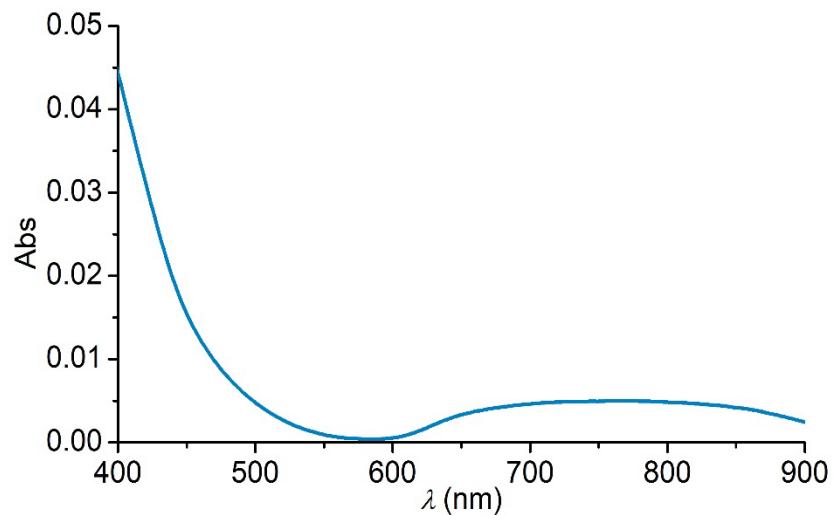


Figure S3. Electronic spectrum of 5×10^{-4} M $[\text{Cu}(\text{pypapn})(\text{ClO}_4)_2]$ in DMF

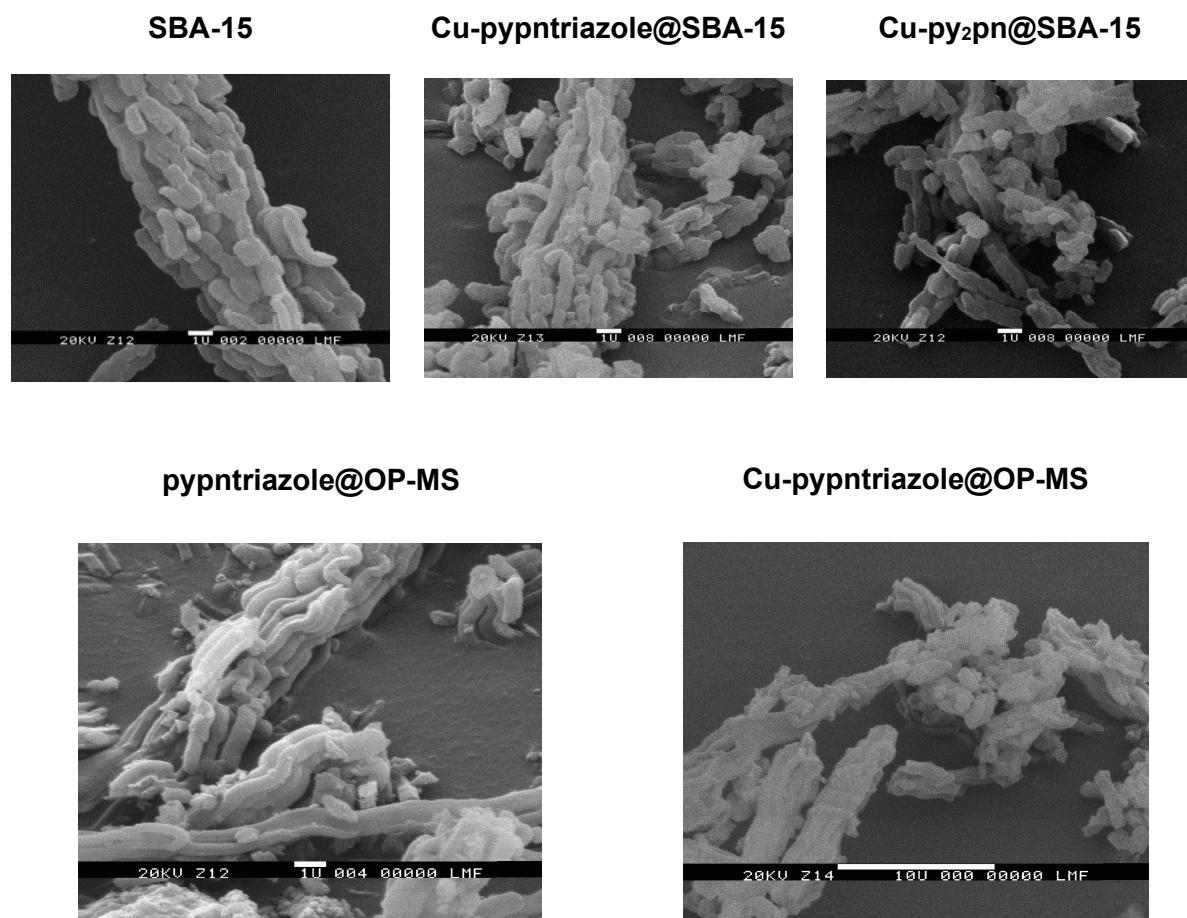


Figure S4. SEM images of the mesoporous silica and the hybrid materials

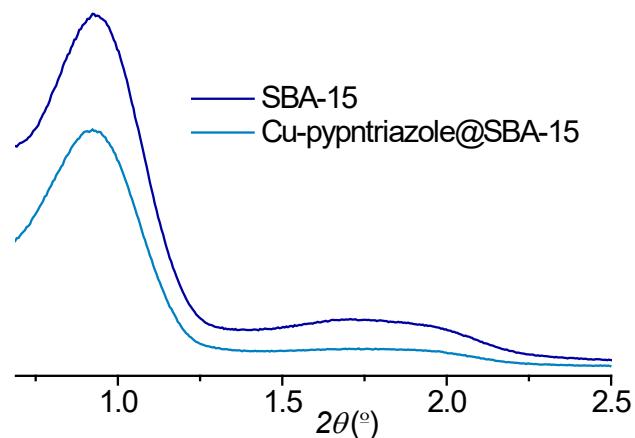
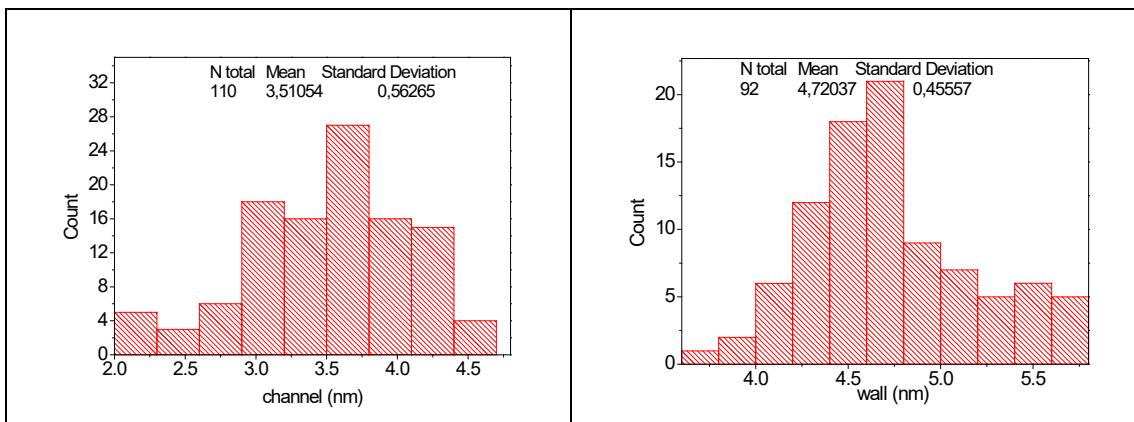


Chart S1. Structures of complexes listed in Table 2

