

SUPPORTING INFORMATION

Copper-phthalocyanine coordination polymer as a reusable catechol oxidase biomimetic catalyst

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NMR characterization:

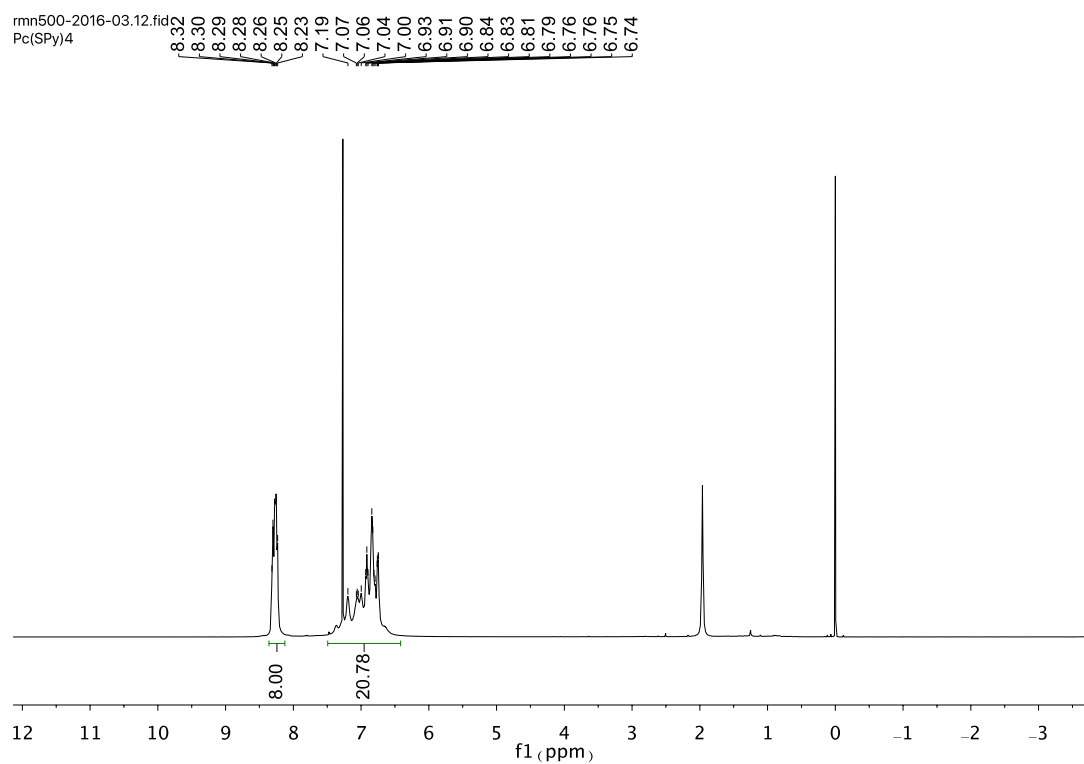


Figure S1. ^1H -NMR spectrum of H_2PcSPy .

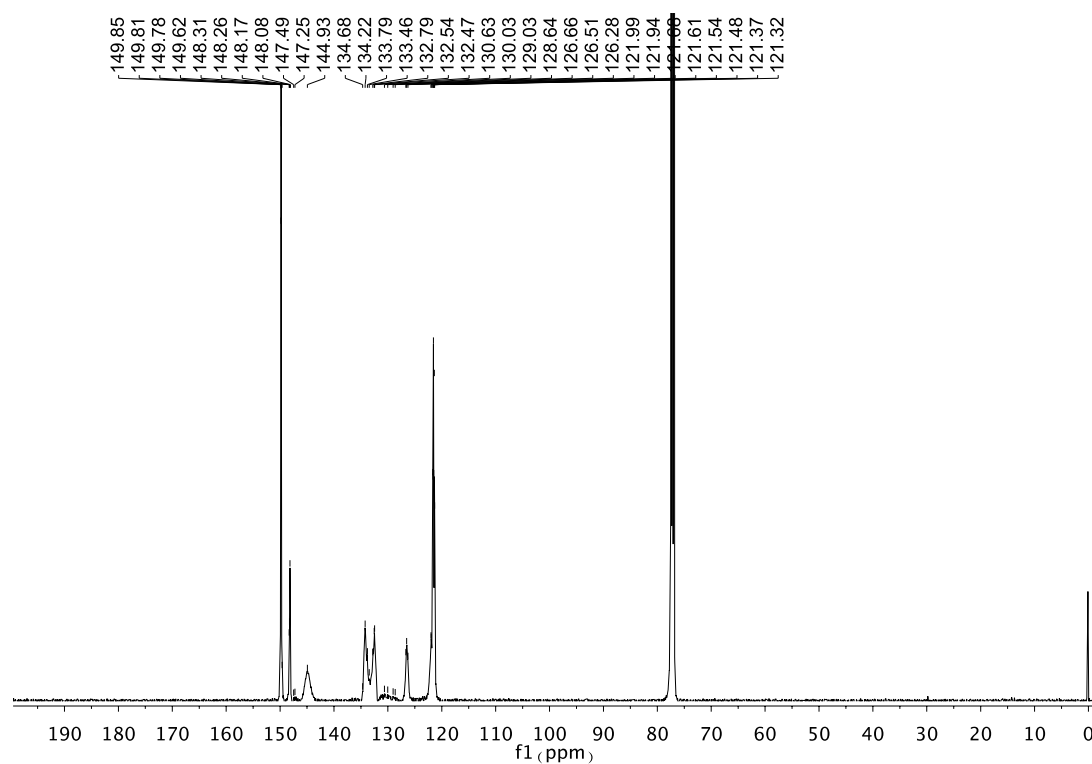


Figure S2. ^{13}C -NMR spectrum of H_2PcSPy .

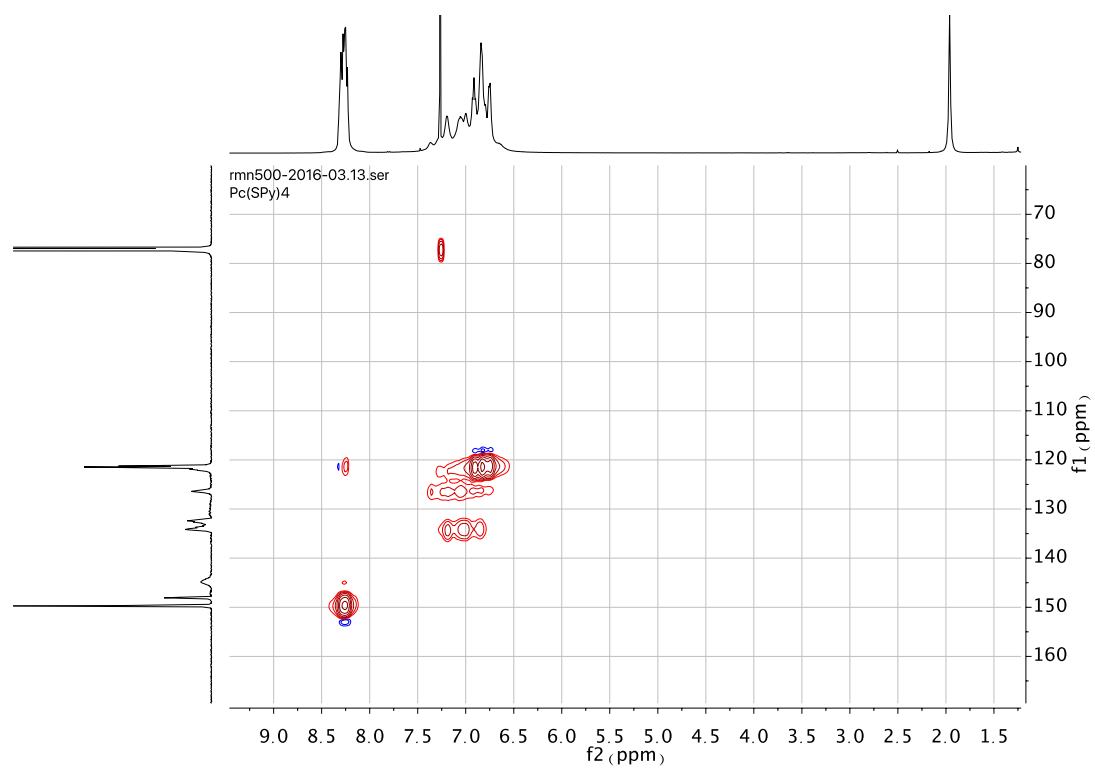


Figure S3. HSQC spectrum of H_2PcSPy .

Mass spectrometry:

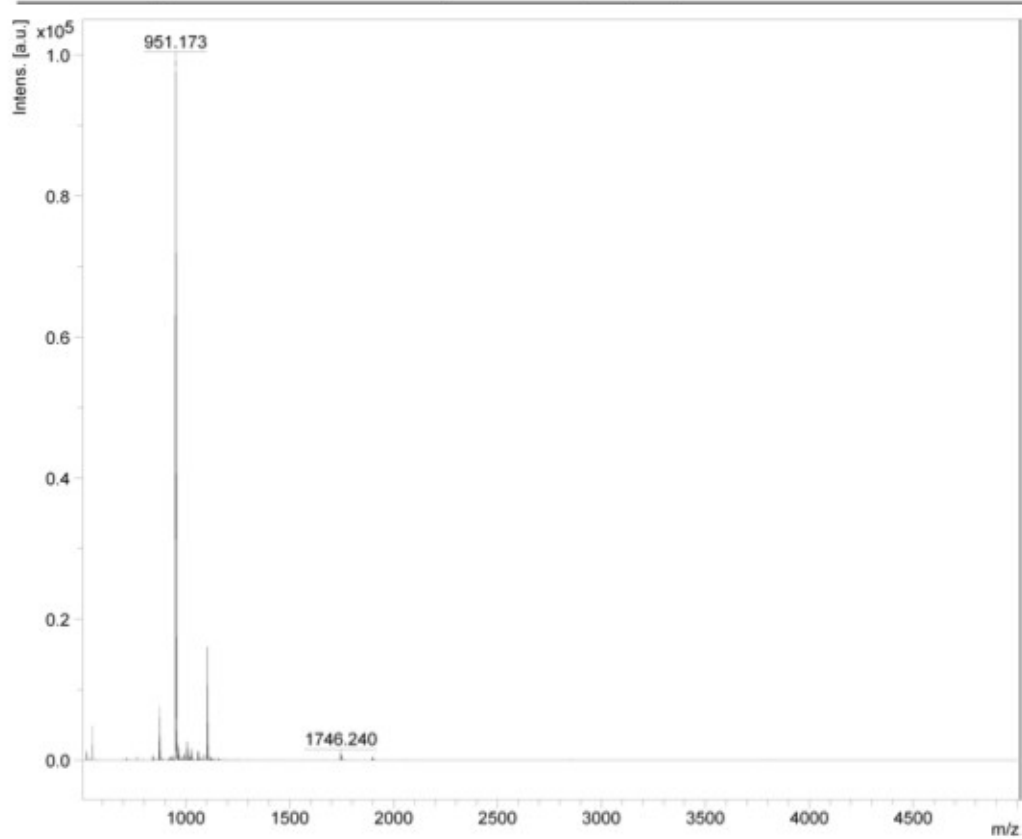


Figure S4. MALDI-TOF mass spectrum of H_2PcSPy .

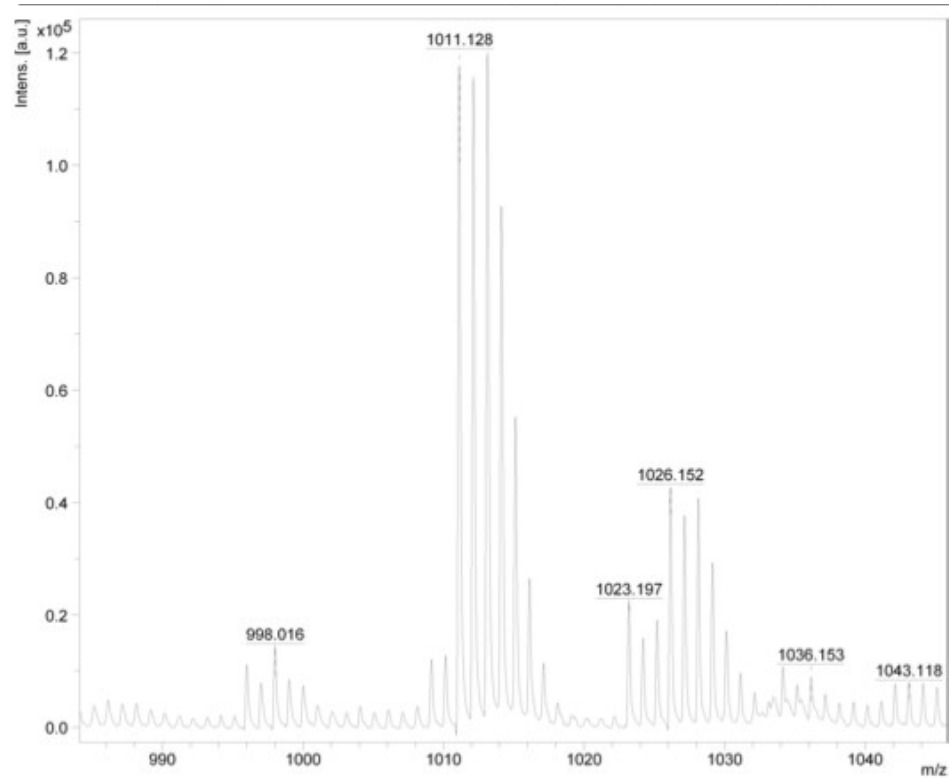


Figure S5. MALDI-TOF mass spectrum of $CuPcSPy$

Fluorescence:

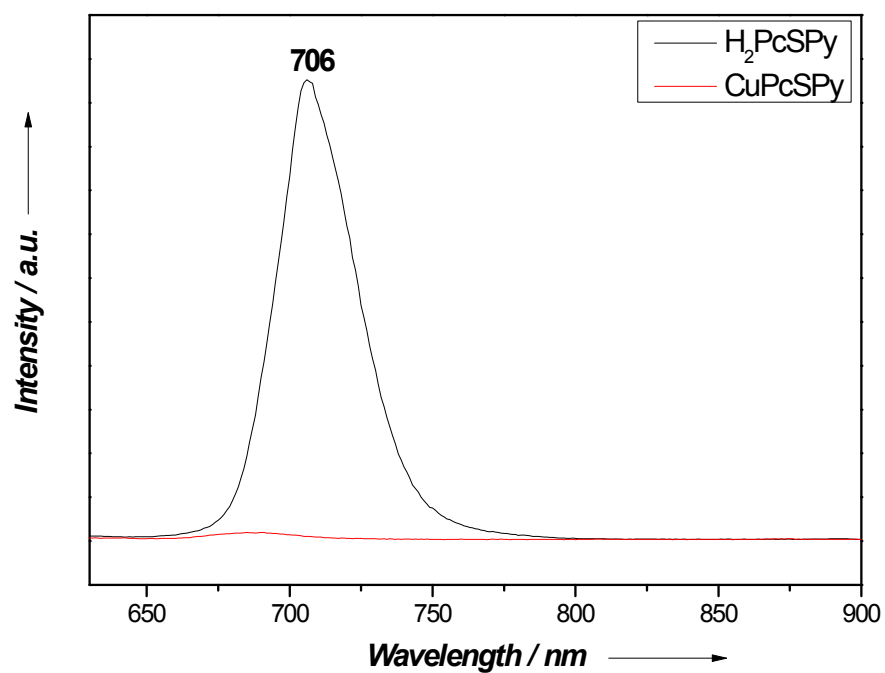


Figure S6. Normalized fluorescence spectra of compounds **H₂PcSPy** and **CuPcSPy** by excitation at $\lambda = 610$ nm (OD for samples at 610 nm = 0.05).

ATR-FTIR Spectroscopy:

Table S1. Band assignments for phthalocyanine and copper-phthalocyanines.

H ₂ PcSPy	CuPcSPy	Cu ₄ CuPcSPy	Band assignment
3282			NH stretching
3039	3054		Ar-H stretching
	1706		C=O stretching from DMF molecules
1603			N–H deformation
1569	1573	1571	C=C stretching
1536	1542		C=N stretching
1500	1506	1505	C- N stretching
1477	1479	1482	C–H in-plane bending
1442	1439	1442	C–C stretching in isoindole
1299			N–H deformation
1256	1253	1256	C–N stretching in isoindole
	1143	1139	C–H in-plane deformation
1128			C–H in-plane deformation
1102	1100	1098	C–H in-plane deformation
1061	1064	1062	C–H in-plane deformation
1006			N–H in-plane bending vibration
	918	919	Metal ligand vibration
741	744	743	C–H out-of-plane deformation
		724	C–H out-of-plane deformation
700	704	706	C–H out-of-plane deformation
669	671	673	C-S-C stretching
636	638	637	C–C out-of-plane ring deformation

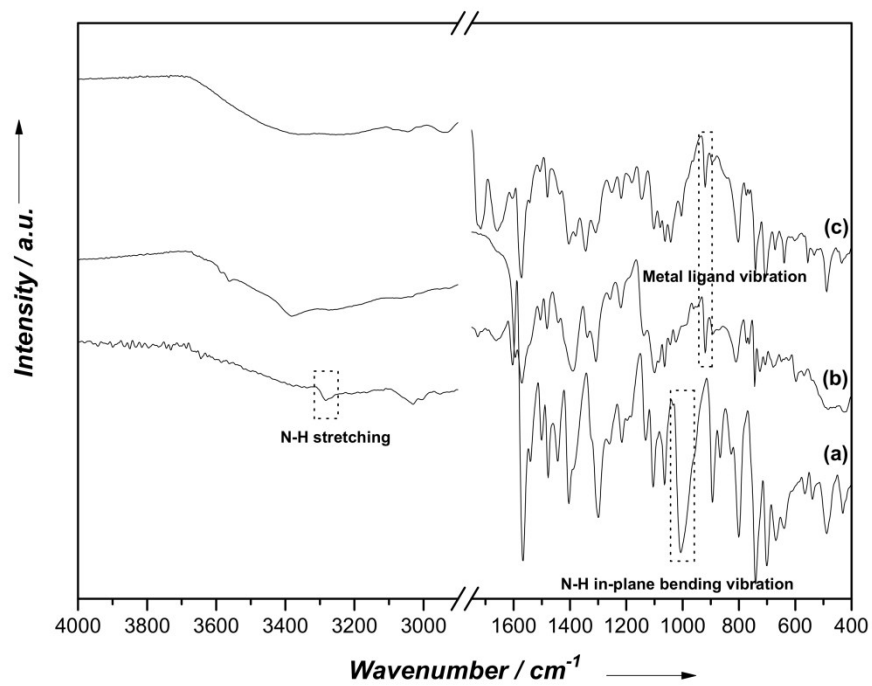


Figure S7. ATR-FTIR spectra of the metal-free phthalocyanine and copper phthalocyanines: (a) **H₂PcSPy**, (b) **Cu₄CuPcSPy** and (c) **CuPcSPy**.

Electrochemical studies:

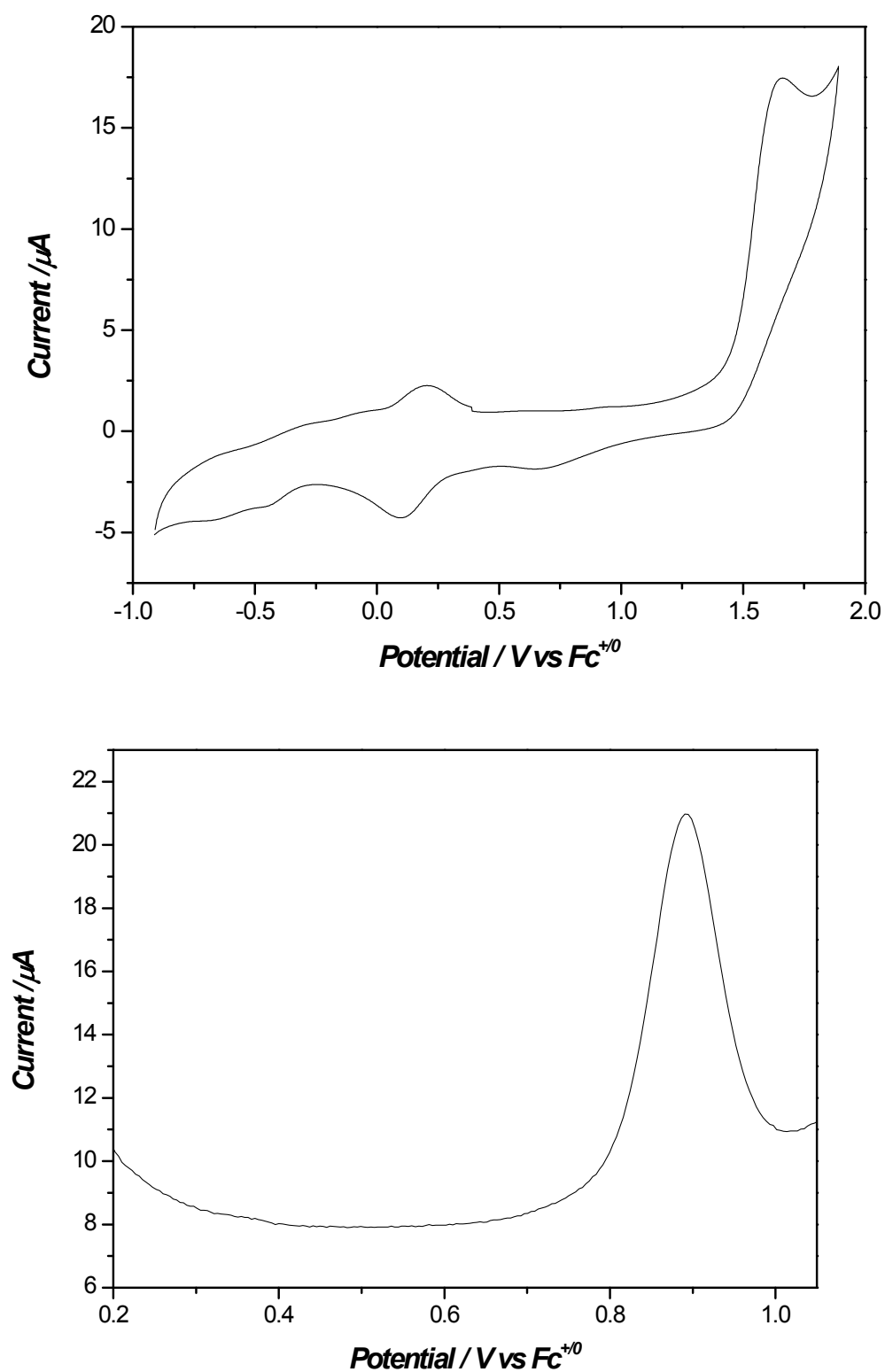


Figure S8. Cyclic voltammetry of 0.1 mM of H_2PcSPy in 0.1 M TBAPF_6 in dimethylformamide as support electrolyte. Ferrocene (Fc) in DMF (+0.39 V versus Ag/AgCl) was employed as internal standard.

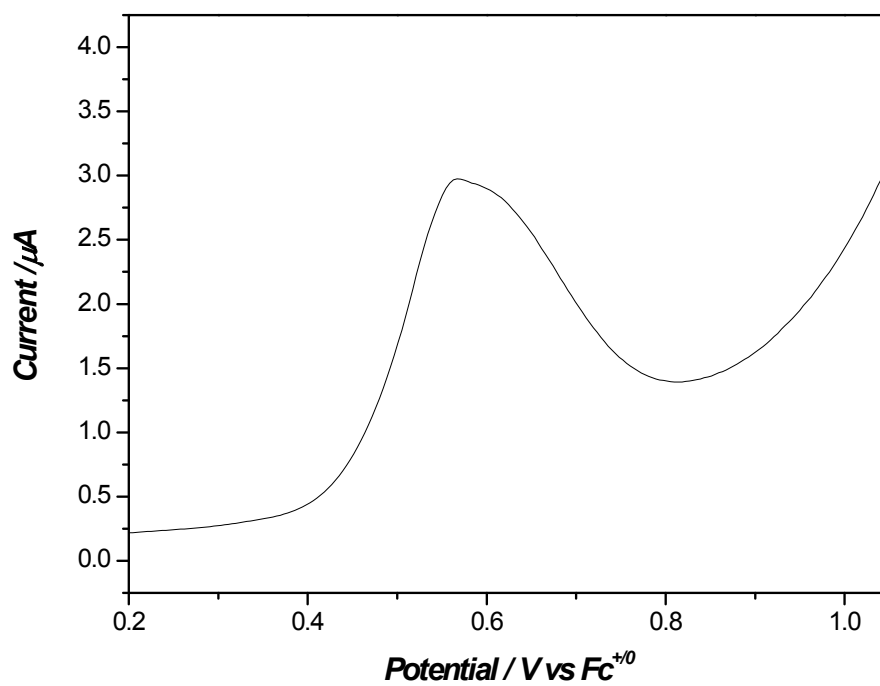
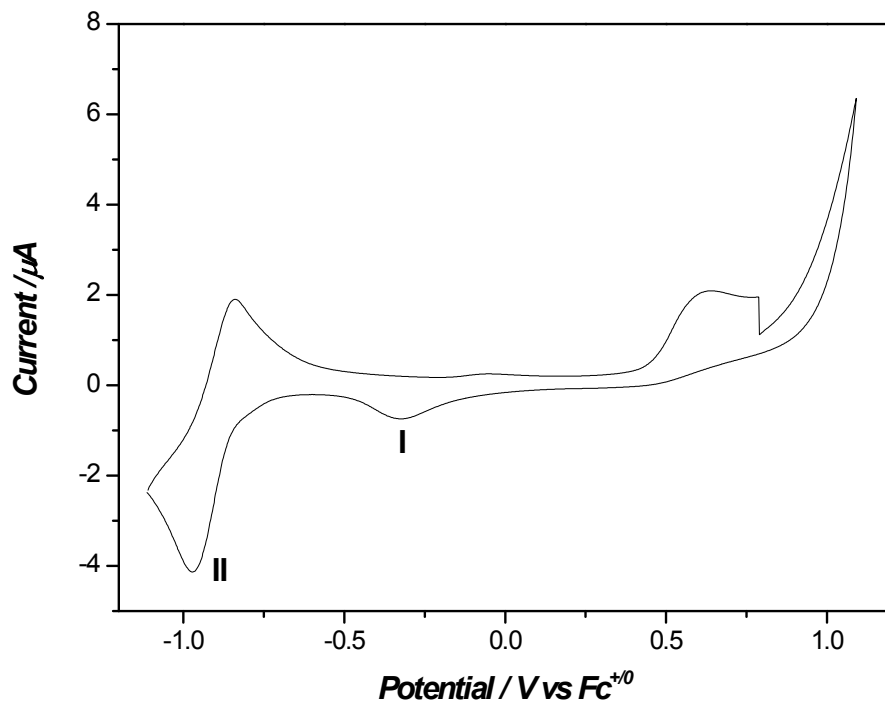


Figure S9. Cyclic voltammetry of 0.1 mM of **CuPcSPy** in 0.1 M TBAPF₆ in dimethylformamide as support electrolyte. Ferrocene in DMF (+0.39 V versus Ag/AgCl) was employed as internal standard.

PXRD:

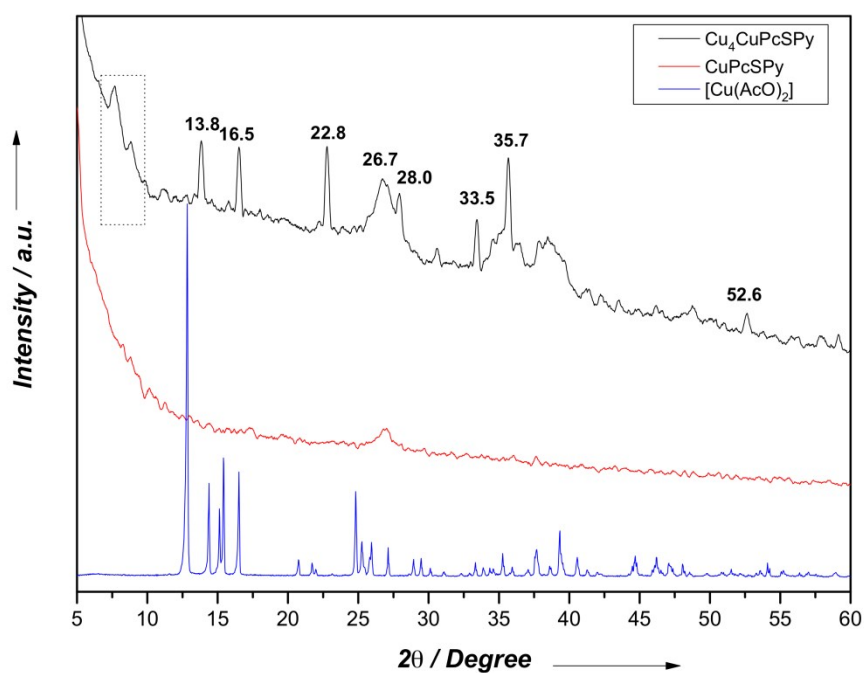


Figure S10. PXRD patterns of **Cu₄CuPcSPy** (black line), **CuPcSPy** (red line) and **[Cu(AcO)₂]** (blue line).

EPR:

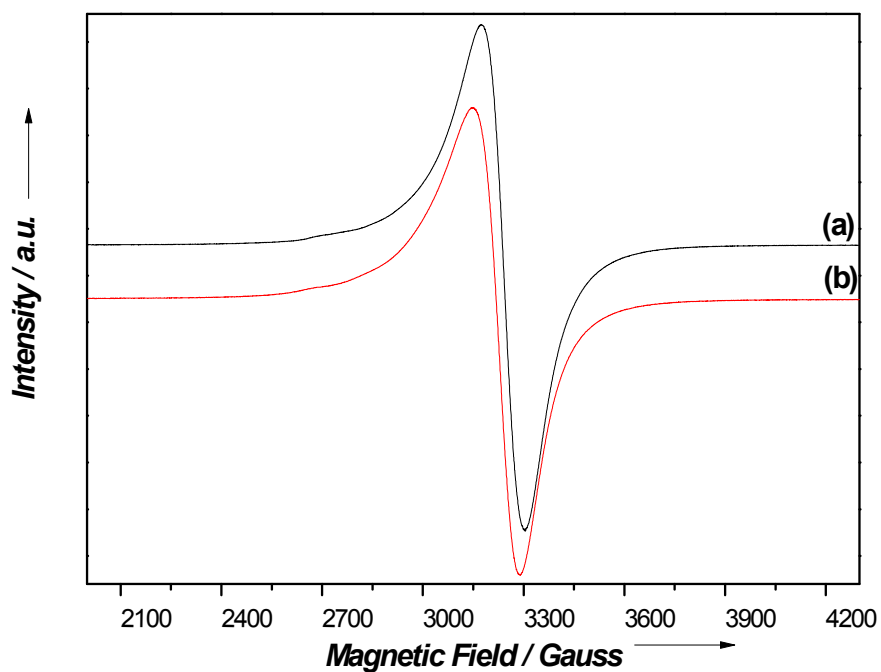


Figure S11. EPR spectra of powder samples at 77 K for (a) **CuPcSPy** and (b) **Cu₄CuPcSPy**.

UV-Vis spectrophotometry:

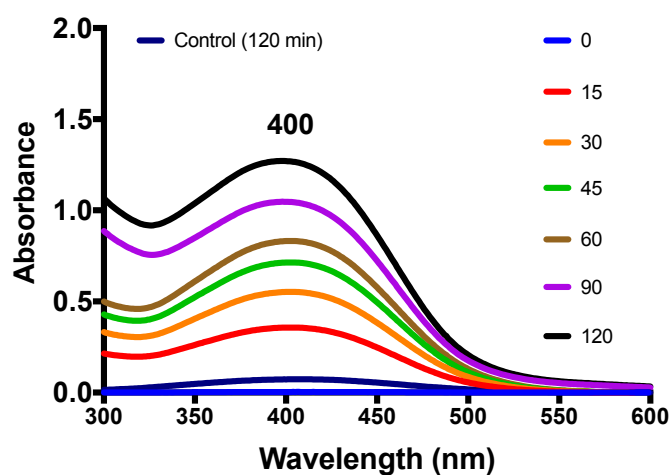


Figure S12. UV-Vis scans for the formation of the 3,5-DTBQ from 3,5-DTBC as a function of time.

Stability of the $\text{Cu}_4\text{CuPcSPy}$ catalyst

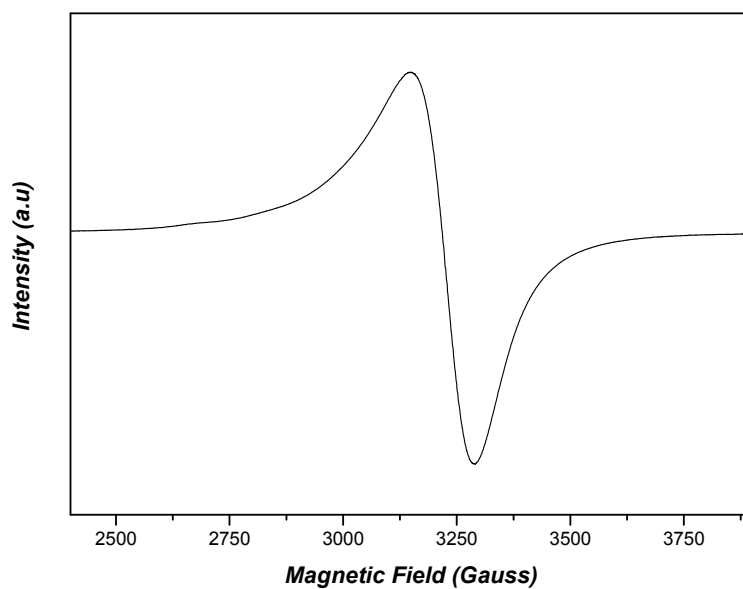


Figure S13. EPR spectrum for $\text{Cu}_4\text{CuPcSPy}$ recovered after the first reuse as catalyst in 3,5-DTBC oxidation.

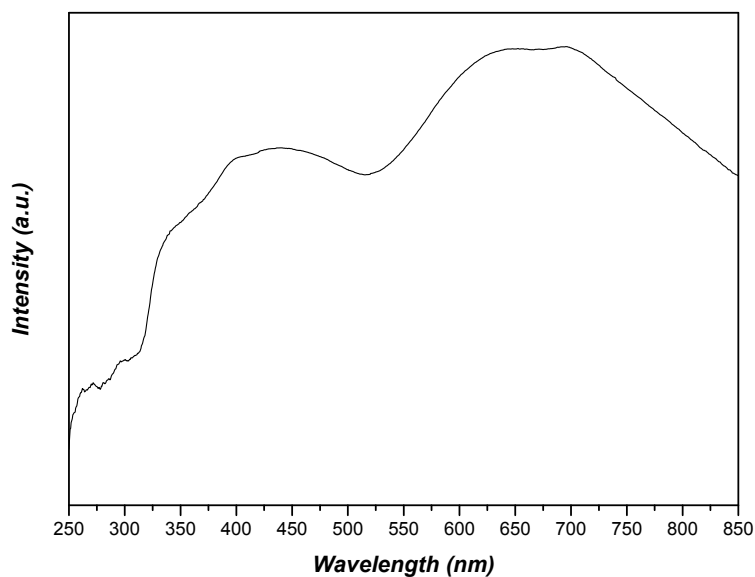


Figure S14. UV-Vis spectrum for **Cu₄CuPcSPy** recovered after the first reuse as catalyst in 3,5-DTBC oxidation.

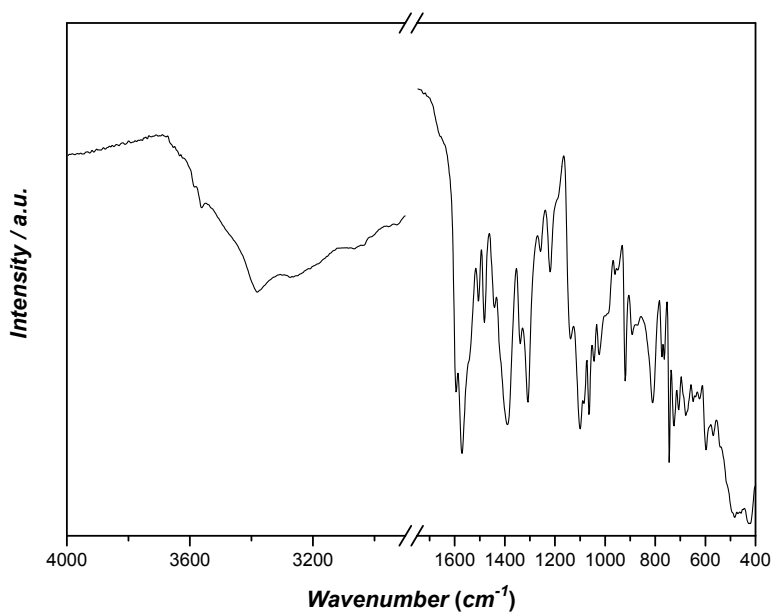


Figure S15. ATR-FTIR spectrum for **Cu₄CuPcSPy** recovered after the first reuse as catalyst in 3,5-DTBC oxidation.