

Impact of pyridine-2-carboxaldehyde-derived aroylhydrazones on the copper-catalyzed oxidation of the M112A PrP₁₀₃₋₁₁₂ mutant fragment

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Supplementary Material

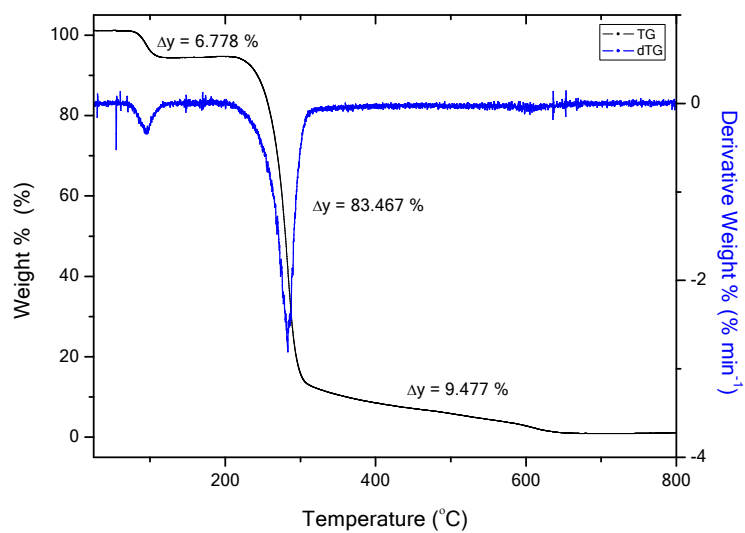


Figure S1. Thermal decomposition of HPCFur between 25 and 800 °C, as shown by its TG (black) and dTG (blue) curves.

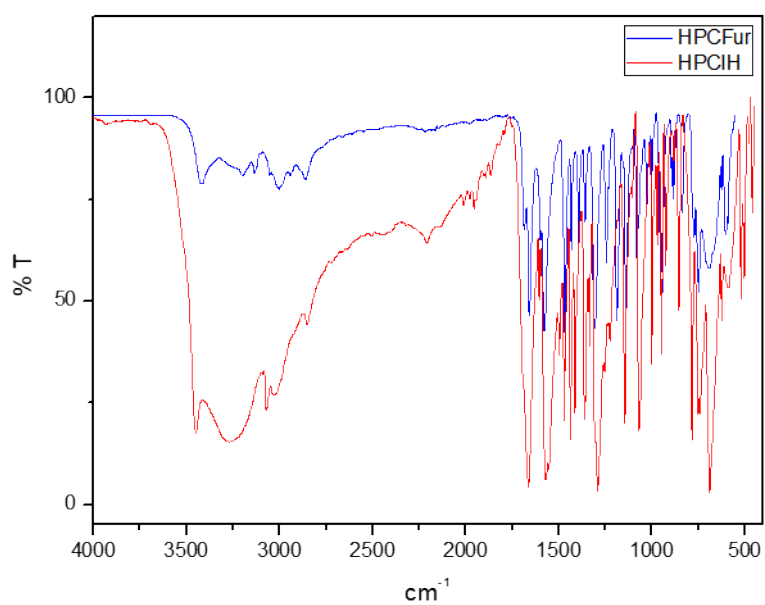


Figure S2. Mid-infrared spectra of the aroylhydrazones: HPCFur (blue) and HPCIH (red), from 4000 to 400 cm⁻¹, at room temperature, in KBr pellets.

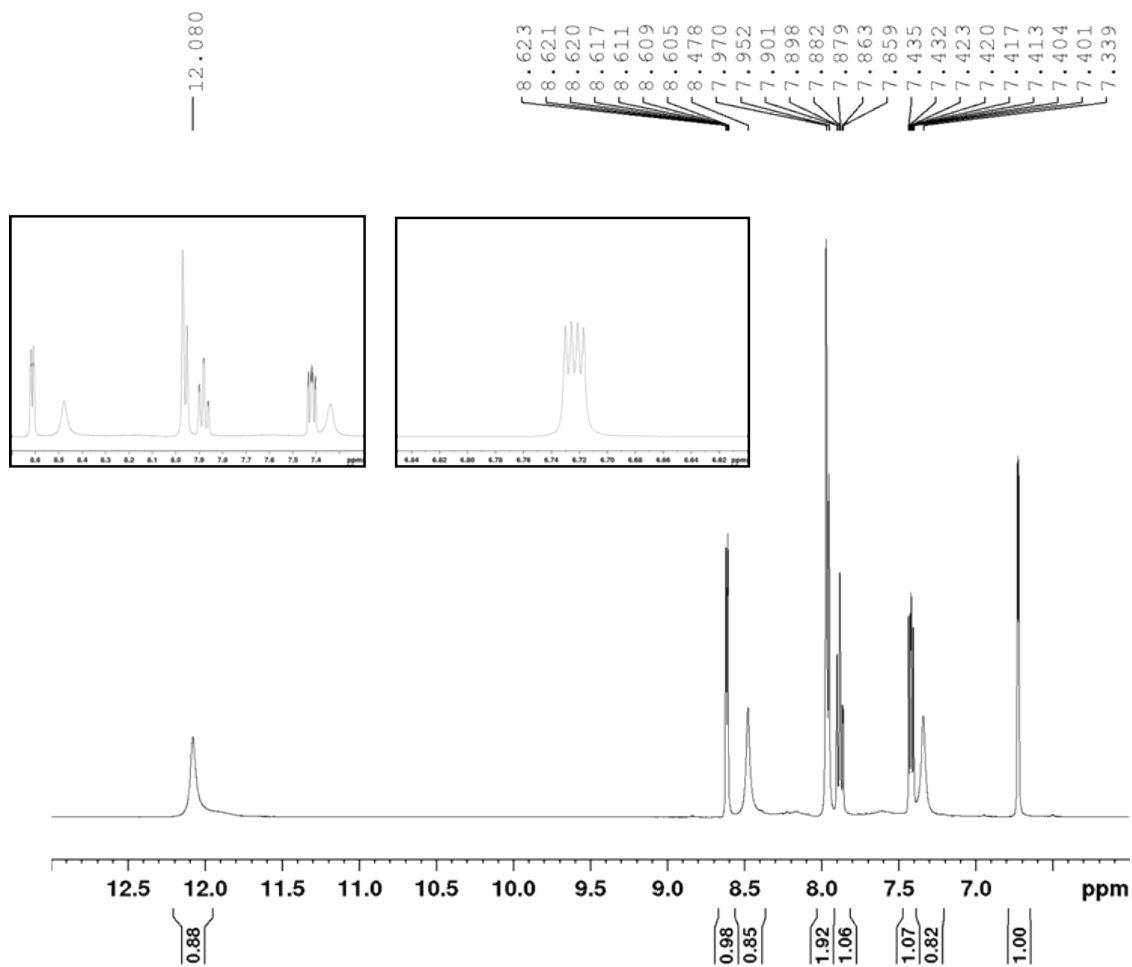


Figure S3. ^1H (400 MHz) NMR spectrum of HPCFur in DMSO- d_6 , at room temperature.

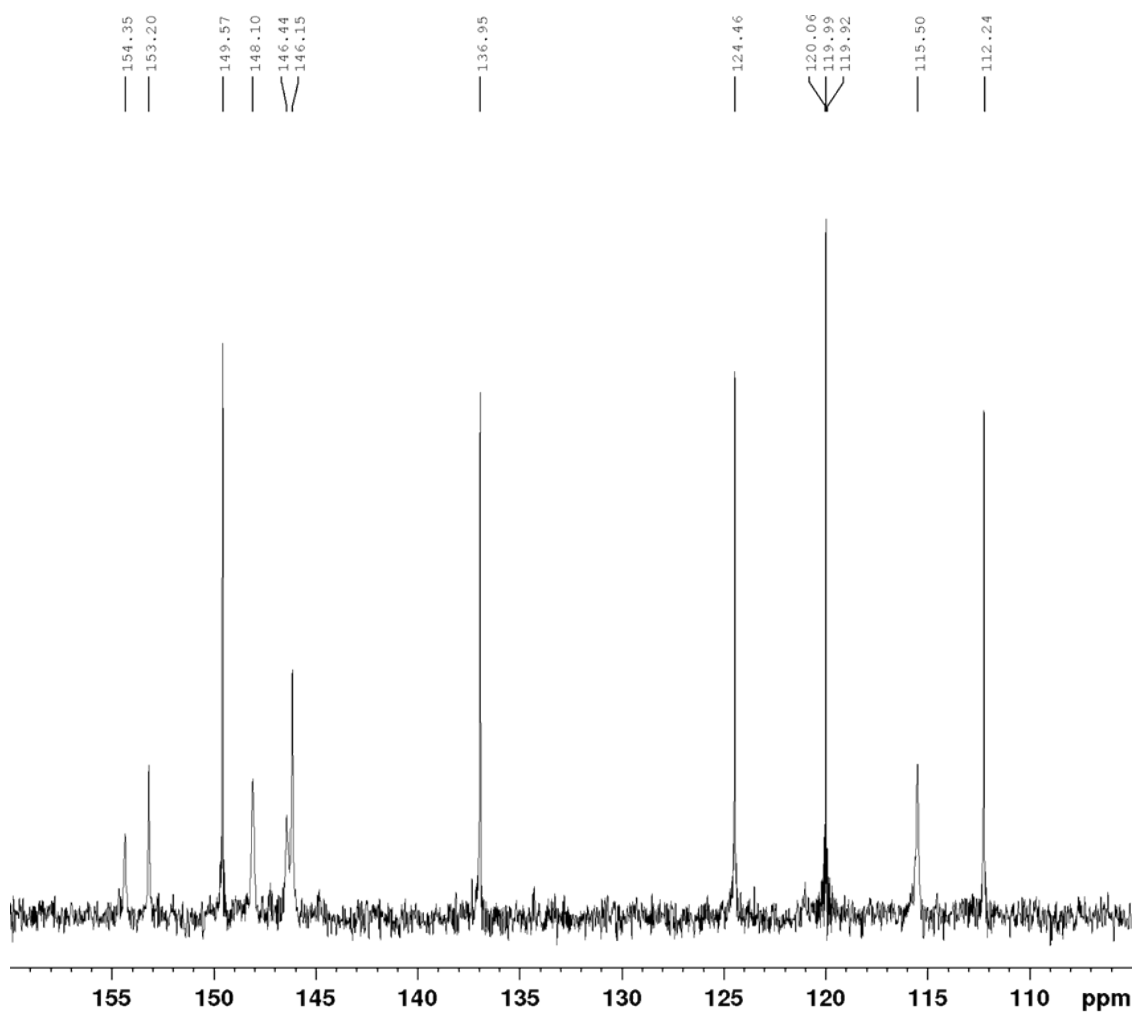


Figure S4. ^{13}C (100 MHz) NMR spectrum of HPCFur in DMSO- d_6 , at room temperature.

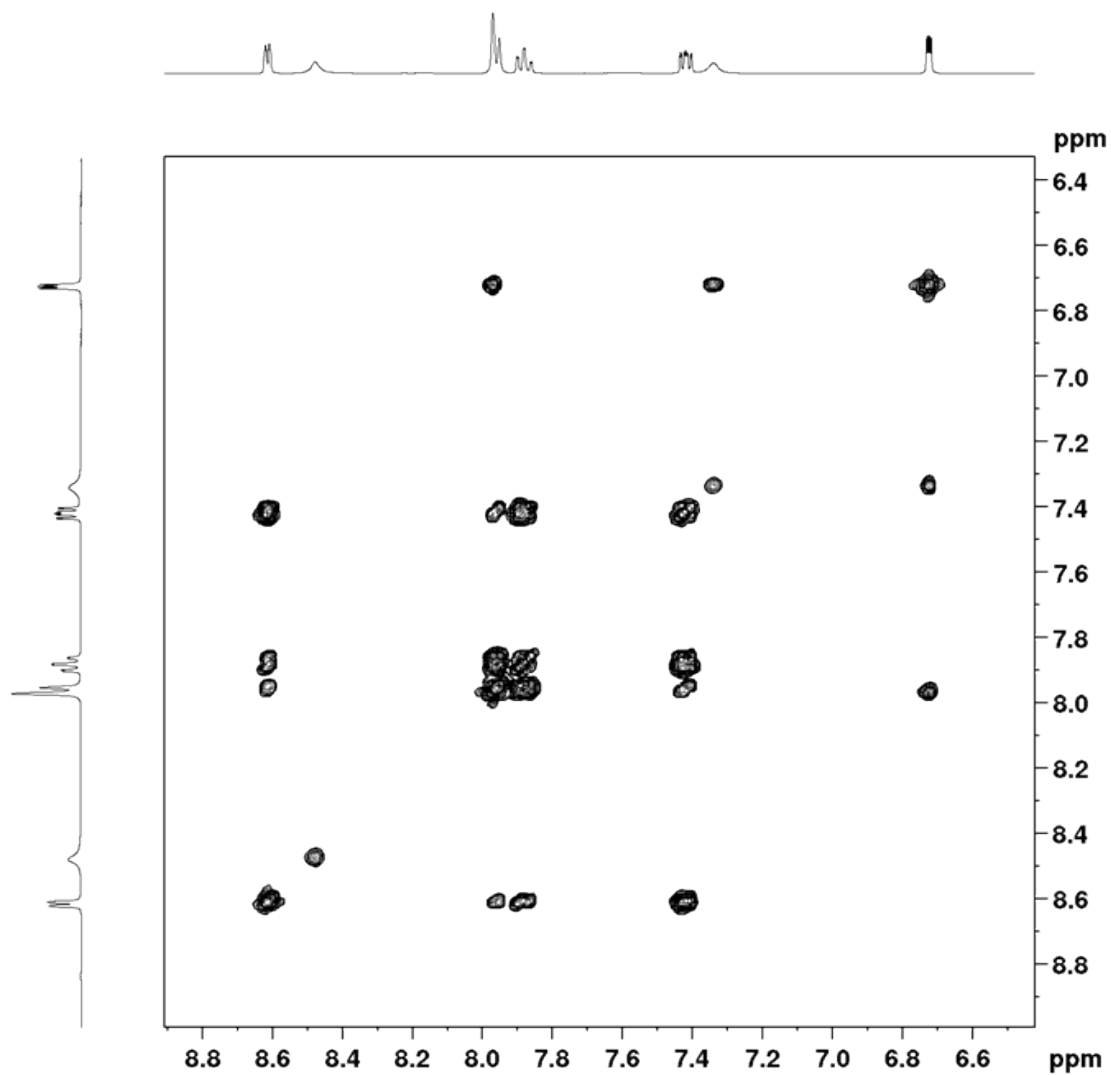


Figure S5. COSY contour map (400 MHz) of HPCFur in DMSO-d₆, at room temperature.

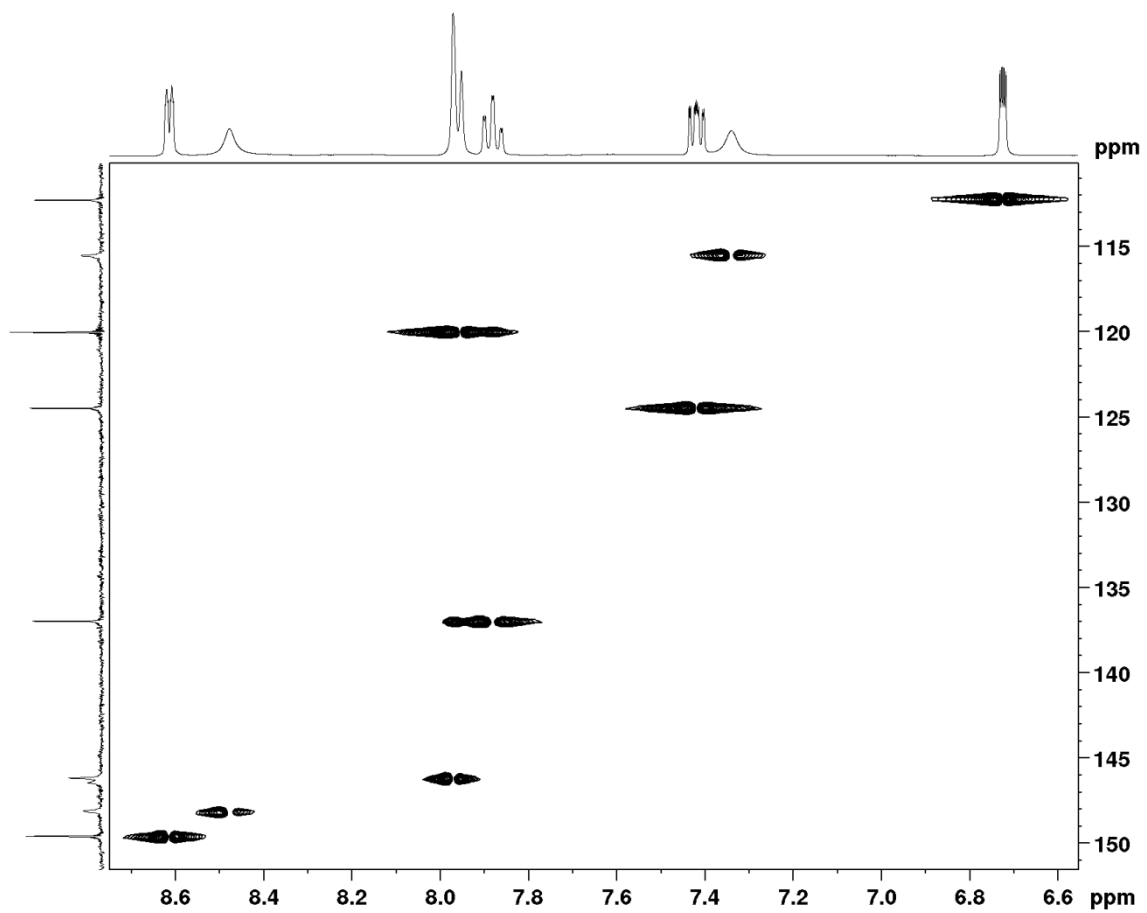


Figure S6. ^1H - ^{13}C HSQC contour map (400 MHz) of HPCFur in DMSO- d_6 , at room temperature.

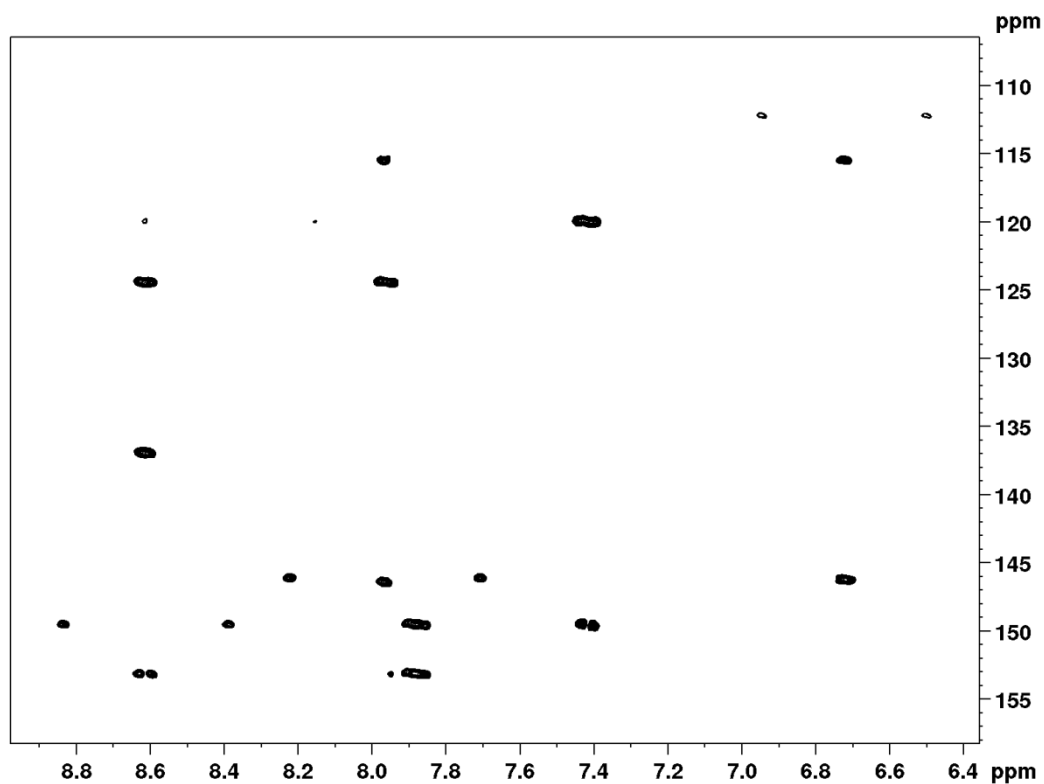


Figure S7. ^1H - ^{13}C HMBC contour map (400 MHz) of HPCFur in DMSO- d_6 , at room temperature.

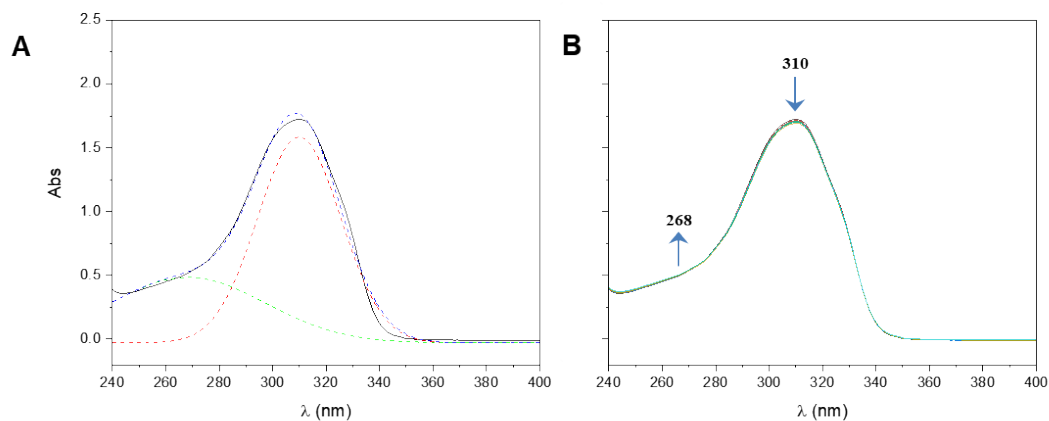


Figure S8. Electronic spectra of HPCFur (50 μM) in a 1% DMSO/water solution. (A) Fit Peak showing the two main spectral components in green and red dotted lines, as well as the cumulative fit in blue. Performed in Origin 2018. (B) Stability evaluation along 12 hours.

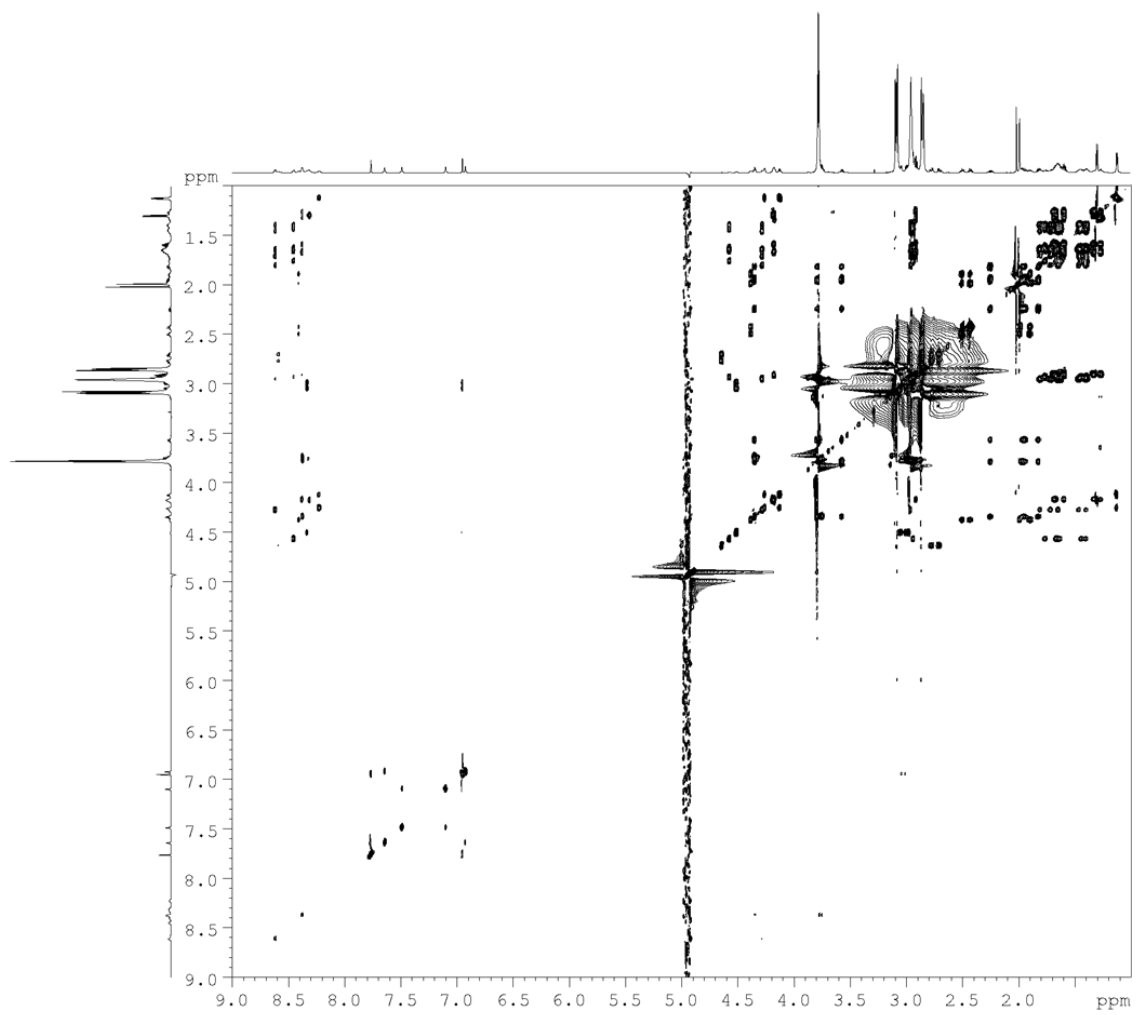


Figure S9. ^1H - ^1H TOCSY contour map (800 MHz) of dMKHA in HEPES buffer pH 7.4, at 5 °C.

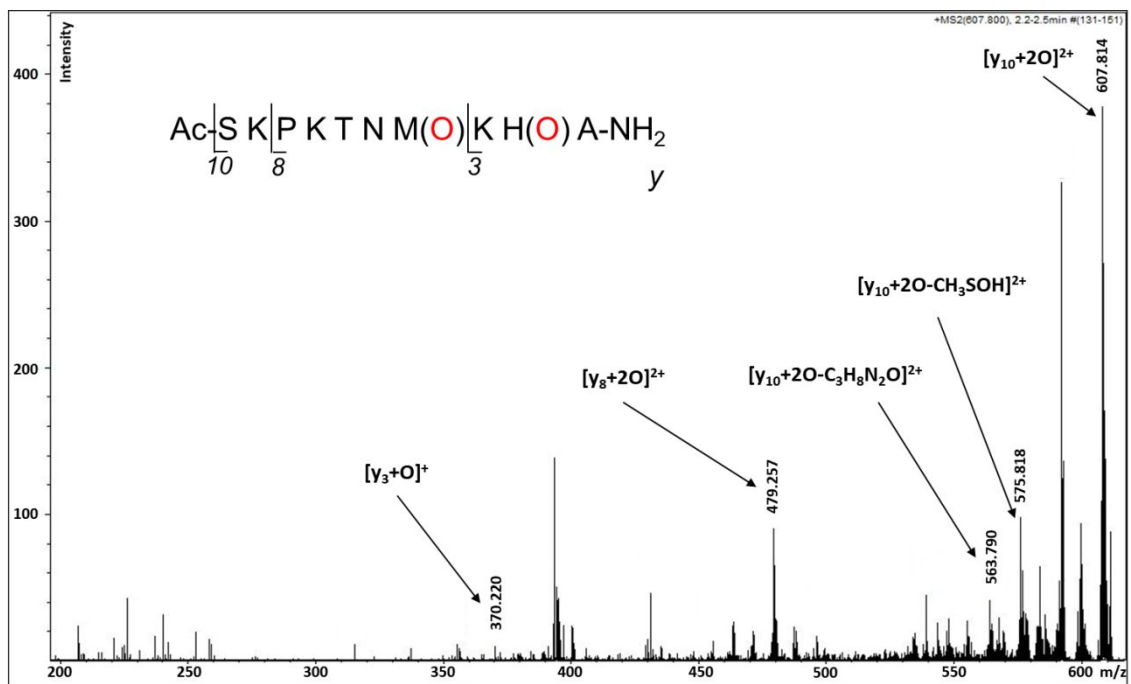


Figure S10. MS/MS spectrum of the doubly oxidized dM(O)KH(O)A product.

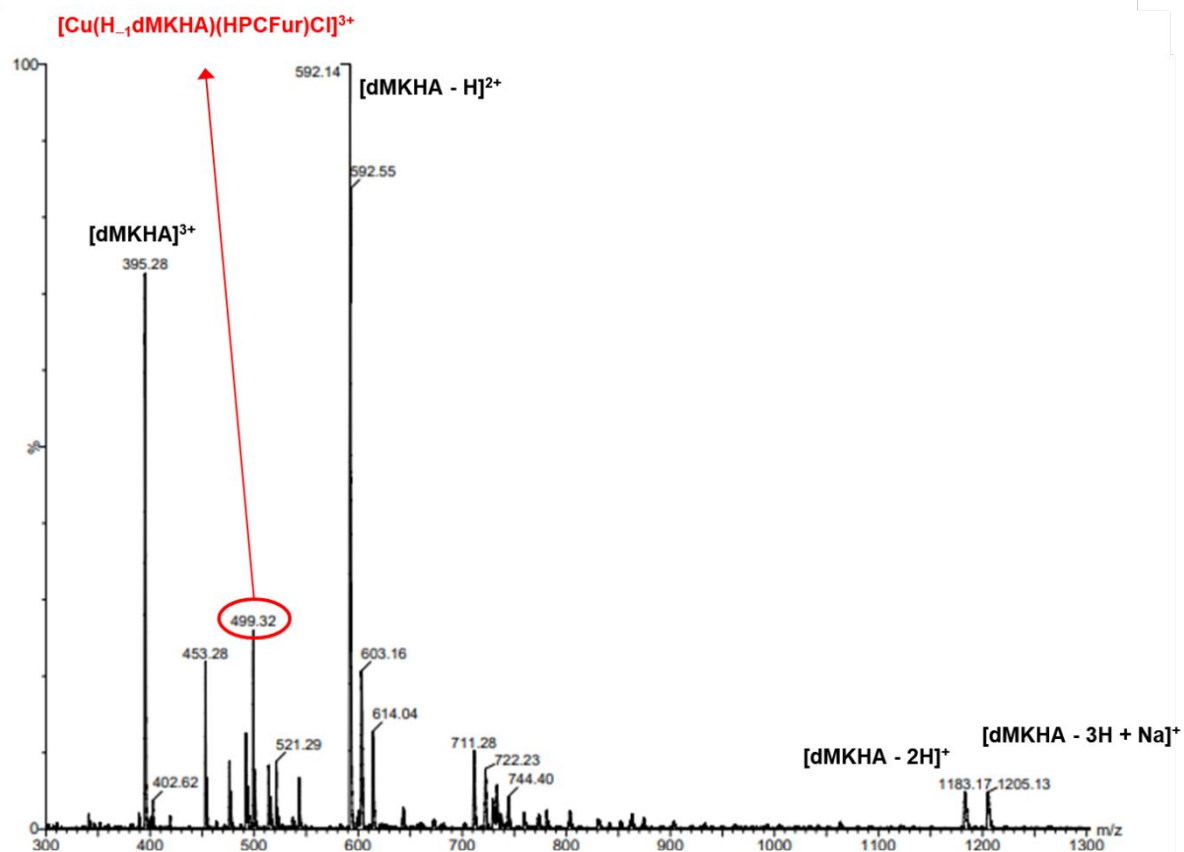


Figure S11. ESI-MS(+) spectrum of a mixture containing dMKHA (5 mM), Cu²⁺ (0.5 mM) and HPCFur (2.5 mM), at pH 7.4. The ternary species $[Cu(H_{-1}dMKHA)(HPCFur)Cl]^{3+}$ is observed at m/z 499.32.