

Supporting Information

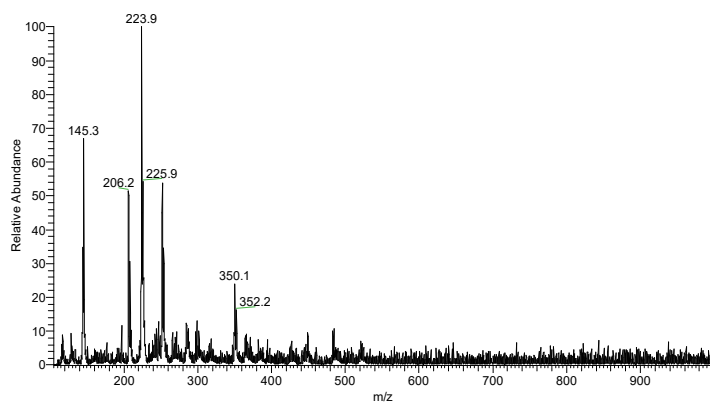


Figure S1. ESI-MS spectrum of 8AQ and Cu²⁺ at 2:1 ratio (pH 7.0)

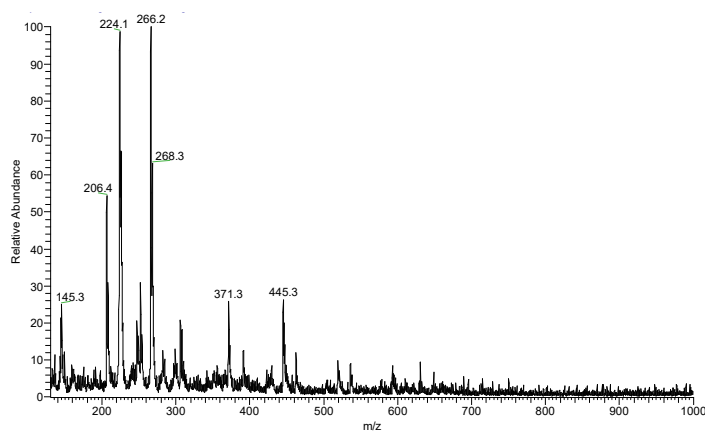


Figure S2. ESI-MS spectrum of 8AQ and Cu²⁺ at 1:1 ratio (pH 7.0)

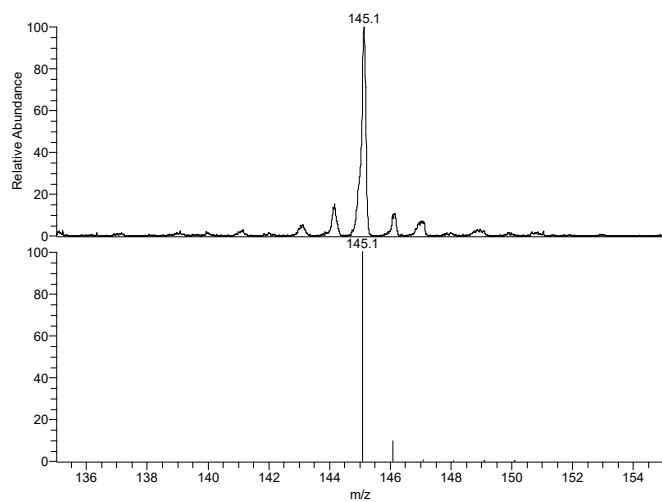


Figure S3. Zoom scan spectrum and isotopic pattern simulation of the protonated adduct [L+H]⁺ of 8AQ (C₉H₉N₂)

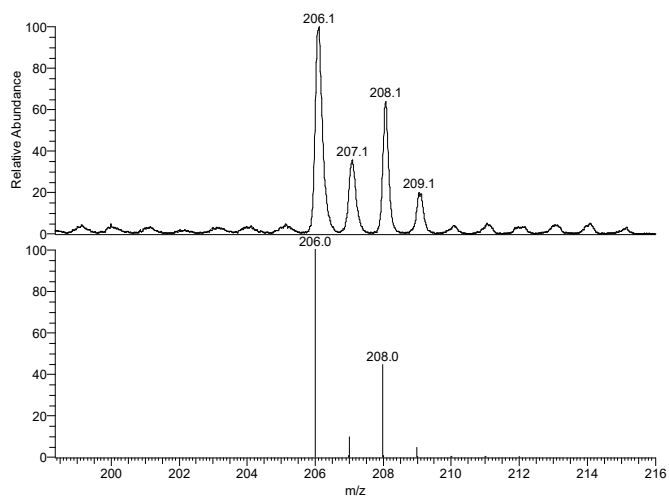


Figure S4. Zoom scan spectrum and isotopic pattern simulation of $[\text{Cu}^{\text{II}}\text{-L-H}]^+$ species of 8AQ ($\text{CuC}_9\text{H}_7\text{N}_2$)

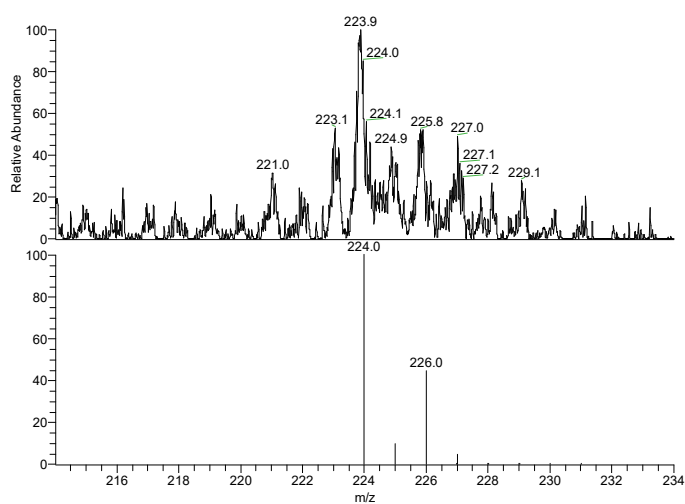


Figure S5. Zoom scan spectrum and isotopic pattern simulation of $[\text{Cu}^{\text{II}}\text{-L+H}_2\text{O-H}]^+$ species of 8AQ ($\text{CuC}_9\text{H}_9\text{N}_2\text{O}$)

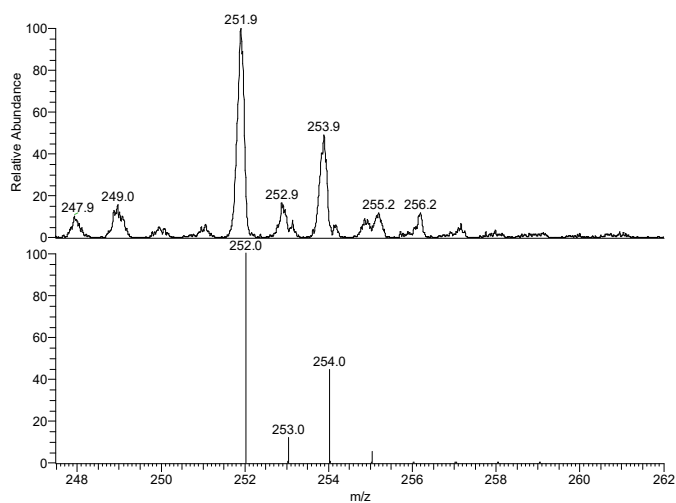


Figure S6. Zoom scan spectrum and isotopic pattern simulation of $[\text{Cu}^{\text{II}}\text{-L+C}_2\text{H}_6\text{O-H}]^+$ species of 8AQ ($\text{CuC}_{11}\text{H}_{13}\text{N}_2\text{O}$)

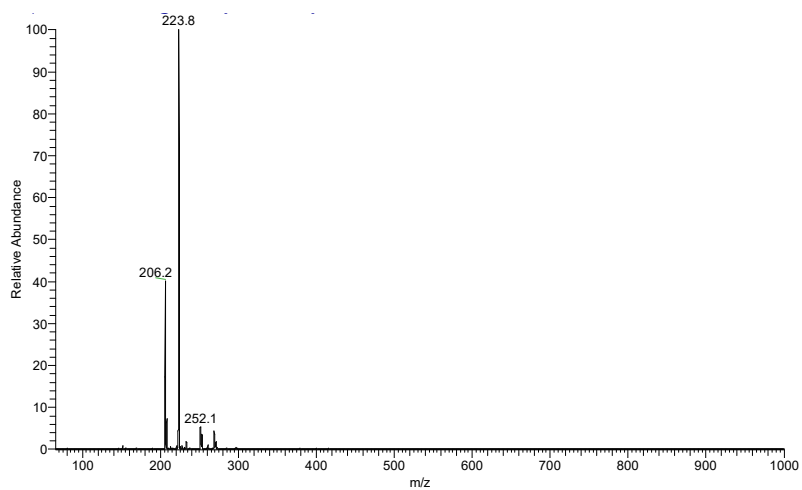


Figure S7. MS/MS spectrum of m/z 252.1 found in the mixture 8AQ-Cu²⁺

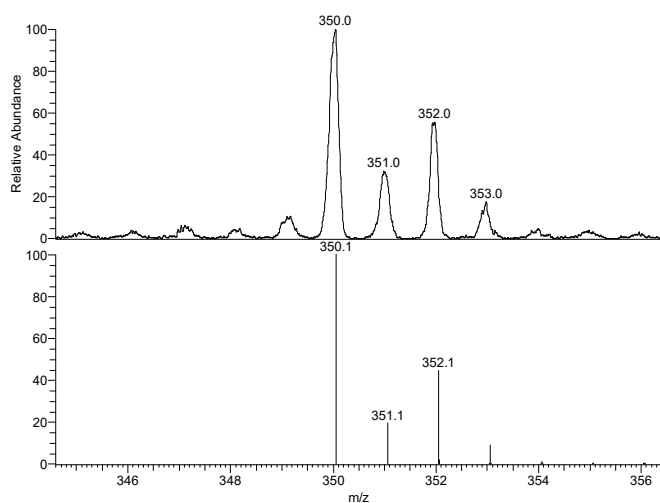


Figure S8. Zoom Scan spectrum and isotopic pattern simulation of the main copper(II) species of 8AQ [Cu^{II}L₂-H]⁺ (Cu₁₈H₁₅N₄) detected at M/L 1:2 ratio and pH 7.0

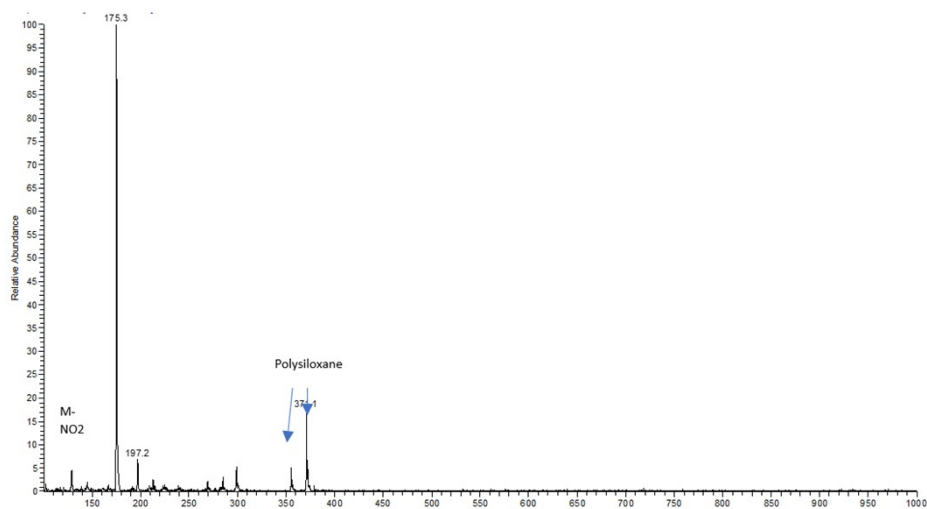


Figure S9. ESI-MS spectrum of 8NQ and Cu²⁺ at 1:1 ratio (pH 7.0)

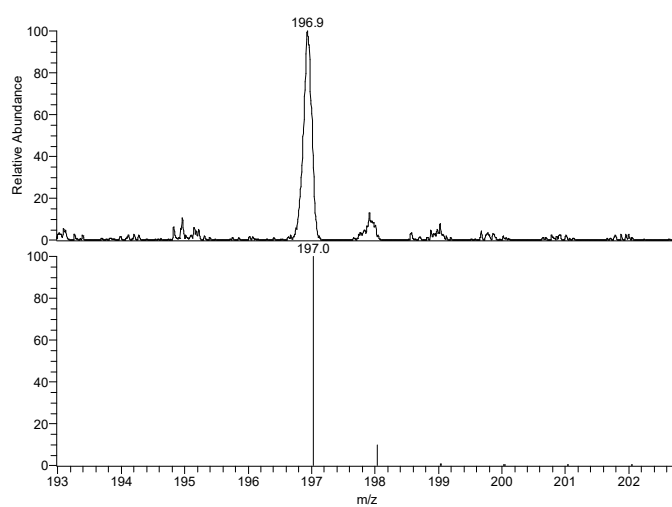
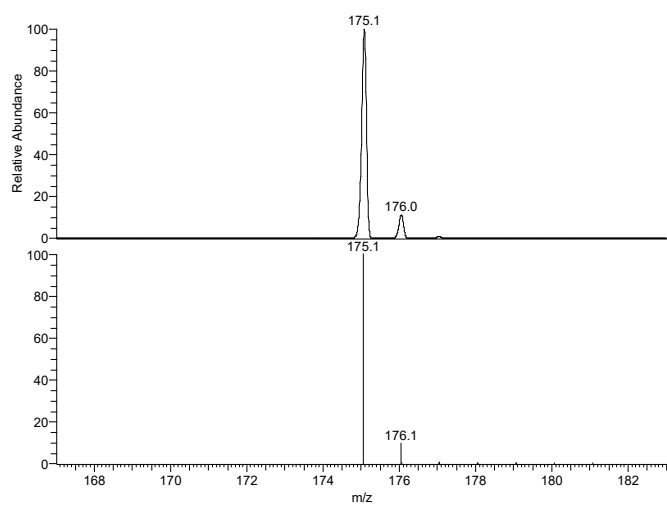
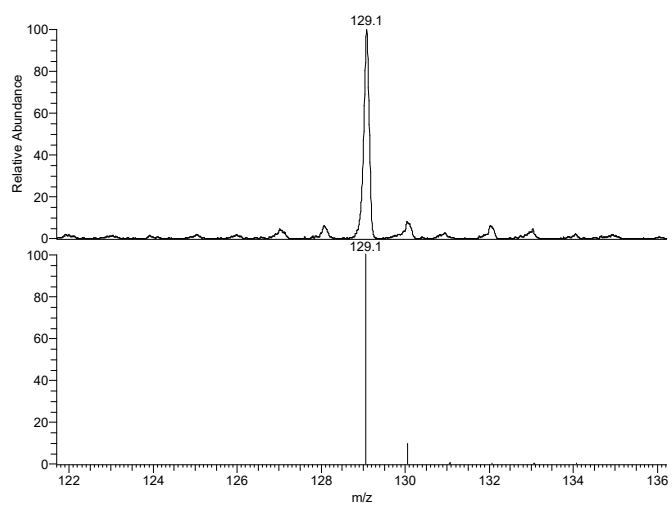


Figure S10. Zoom Scan spectra and isotopic pattern simulations of the main species of 8NQ detected at M/L 1:1 ratio and pH 7.0

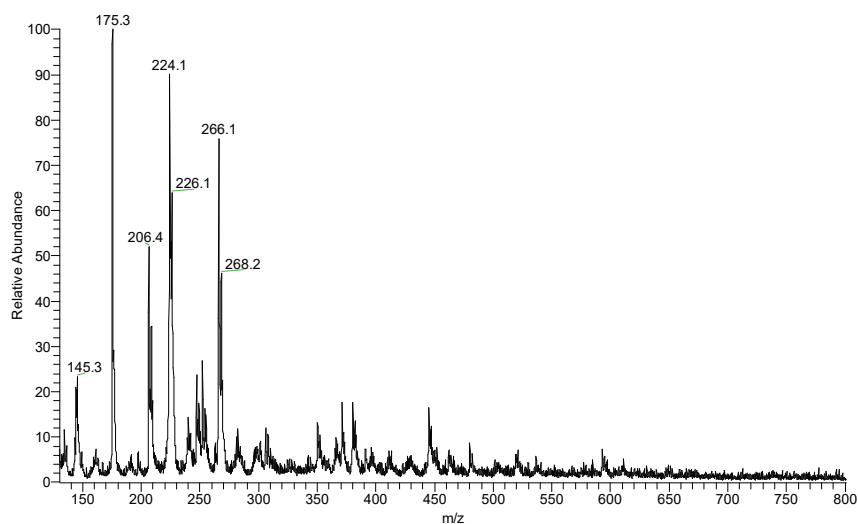


Figure S11. ESI-MS spectrum of the mixture 8NQ-8AQ-Cu²⁺ at ratio 1:1:1 (pH 7.0)

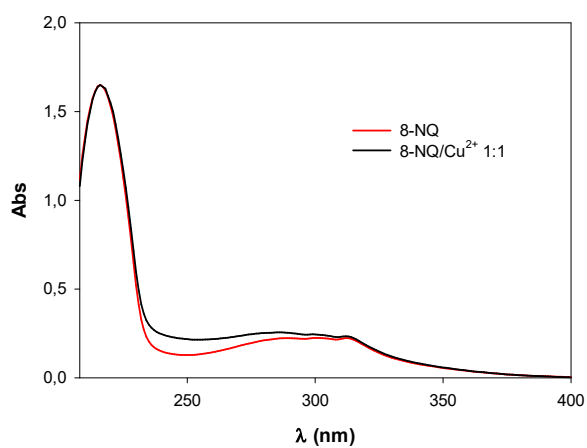


Figure S12. UV-vis spectra of 8NQ (50 μM) in the presence and in the absence of Cu²⁺ (1 equiv) in MOPS 10 mM /EtOH 80:20 at pH 7.4 and 25°C

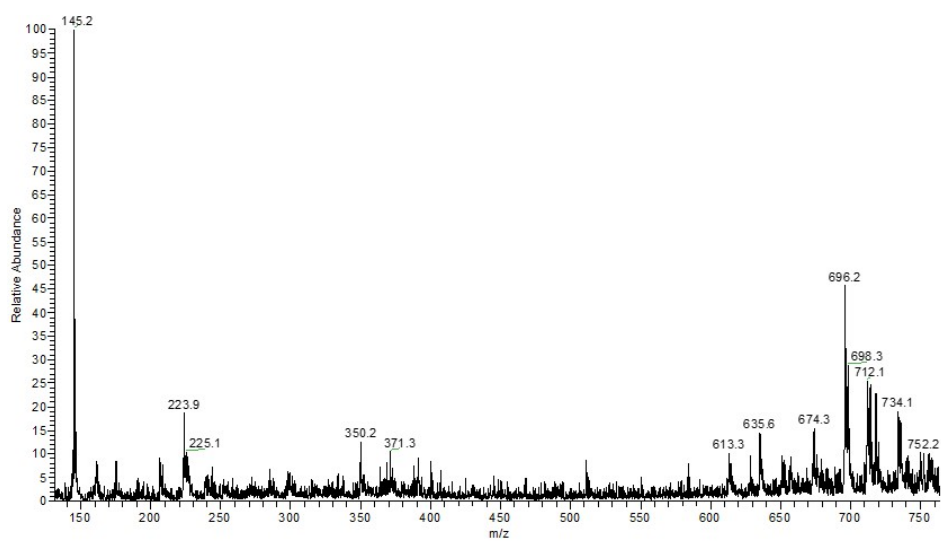


Figure S13. ESI-MS spectrum of 8AQ-Cu²⁺-GSH at 1:1:2 ratio (pH 7.0)

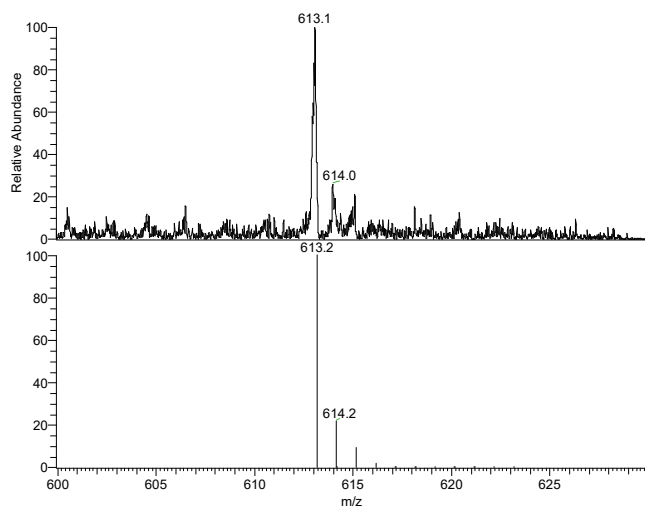


Figure S14. Zoom Scan spectrum and isotopic pattern simulation of the peak at m/z 613.1 attributable at $[GSSG+H]^+$ in the mixture 8AQ-Cu²⁺-GSH 1:1:2

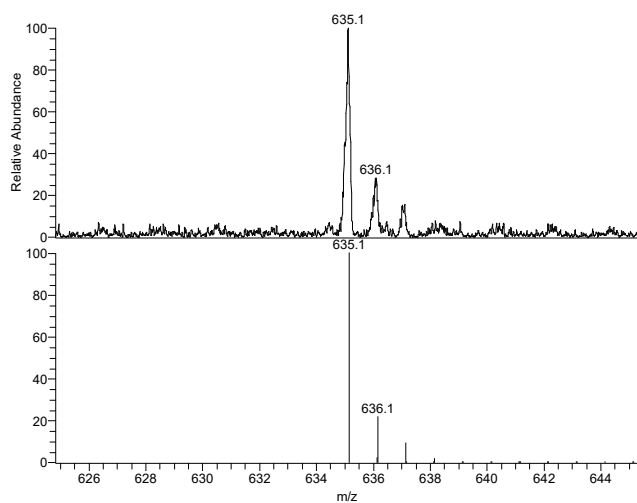


Figure S15. Zoom Scan spectrum and isotopic pattern simulation of the peak at m/z 635.1 attributable at $[GSSG+Na]^+$ ($C_{20}H_{32}N_6O_{12}S_2Na$) in the mixture 8AQ-Cu²⁺-GSH 1:1:2

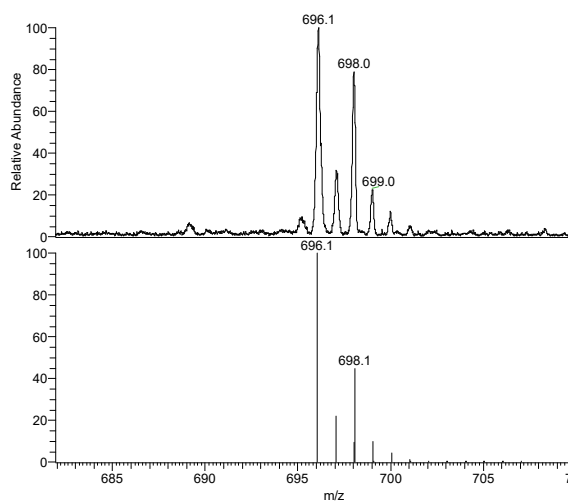


Figure S16. Zoom Scan spectrum and isotopic pattern simulation of the peak at m/z 696.1 attributable at $[CuGSSG+Na-2H]^+$ ($CuC_{20}H_{30}N_6O_{12}S_2Na$) in the mixture 8AQ-Cu²⁺-GSH 1:1:2

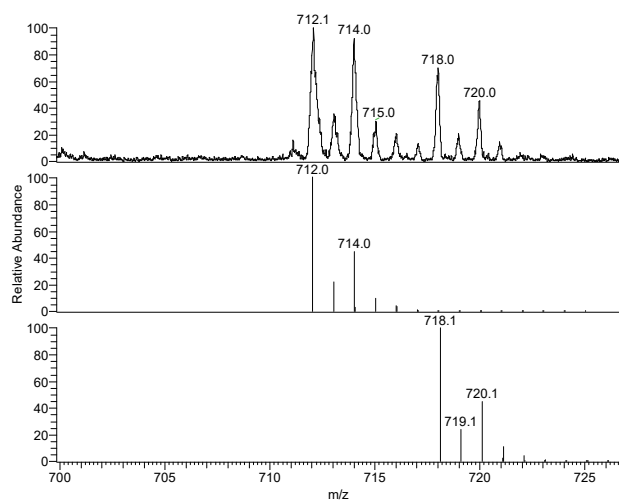


Figure S17. Zoom Scan spectra and isotopic pattern simulations of the peaks at m/z 712.1 and 718.0 attributable, respectively, at $[\text{CuGSSG}+\text{K}-2\text{H}]^+$ and $[\text{CuGSSG}+\text{C}_2\text{H}_6\text{O}-\text{H}]^+$ ($\text{CuC}_{20}\text{H}_{30}\text{N}_6\text{O}_{12}\text{S}_2\text{K}$ and $\text{CuC}_{22}\text{H}_{35}\text{N}_6\text{O}_{13}\text{S}_2$) in the mixture 8AQ- Cu^{2+} -GSH 1:1:2

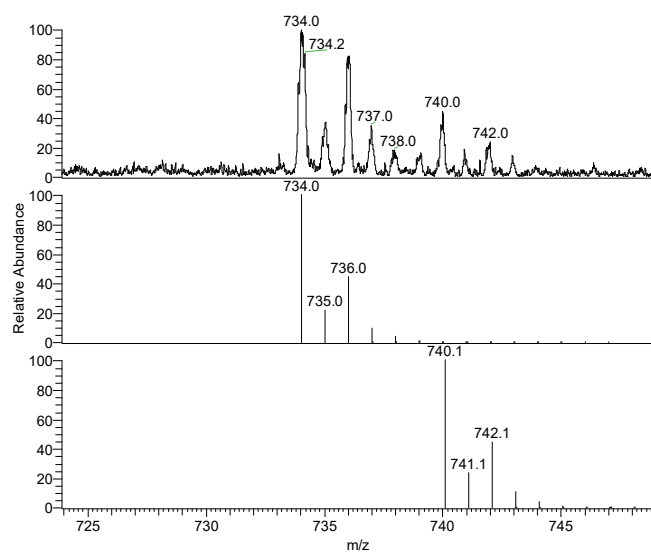


Figure S18. Zoom Scan spectra and isotopic pattern simulations of the peaks at m/z 734.0 and 740.1 attributable, respectively, at $[\text{CuGSSG}+\text{Na}+\text{K}-3\text{H}]^+$ and $[\text{CuGSSG}+\text{Na}+\text{C}_2\text{H}_6\text{O}-2\text{H}]^+$ ($\text{CuC}_{20}\text{H}_{29}\text{N}_6\text{O}_{12}\text{S}_2\text{KNa}$ and $\text{CuC}_{22}\text{H}_{34}\text{N}_6\text{O}_{13}\text{S}_2\text{Na}$) in the mixture 8AQ- Cu^{2+} -GSH 1:1:2

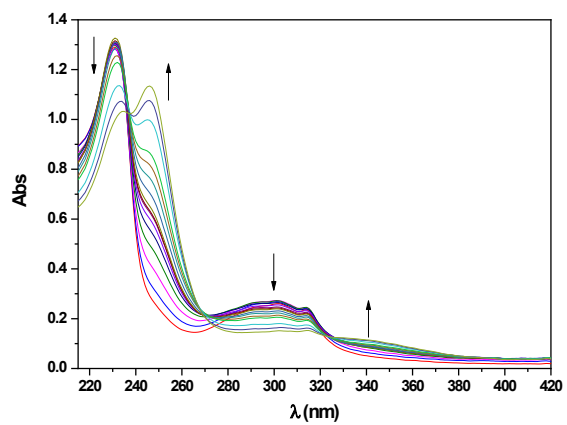


Figure S19. Titration of 8AQ-Cu²⁺ at a 1:1 ratio (red line) with DMEM. For better clarity, the spectra underwent subtraction of the contribution of DMEM alone at the same concentration).