

Supplementary Materials

A new pH dependent macrocyclic Rhodamine B-based fluorescent probe for copper detection in white wine

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Table of contents

NMR measurements	2
¹ H and ¹³ C NMR spectra were recorded on a Bruker 300 and 500 NMR spectrometer.....	2
Figure 1: ¹ H NMR spectrum Probe 3 (300 MHz, D ₂ O, 300 K).....	2
Figure 2: ¹³ C NMR of probe 3 (75 MHz, D ₂ O, 300 K)	2
HR-mass measurements	3
Figure 3: Figure 3: ESI-TOF spectrum of Probe 3.....	3
FT-IR measurements	4
Figure 4: FTIR spectrum of Probe 3.....	4
UV-vis spectra of Probe 3	5
Figure 5: UV-visible absorption spectra of Probe 3 (1 μM) in buffer solution 4.7 with addition of [Cu ²⁺].....	5
Figure 6: Regression curve of the absorbance of Probe 3 alone at different concentrations in distilled water..	5

NMR measurements

^1H and ^{13}C NMR spectra were recorded on a Bruker 300 and 500 NMR spectrometer. Chemical shifts were reported in parts per million using tetramethylsilane (TMS) as the internal standard.

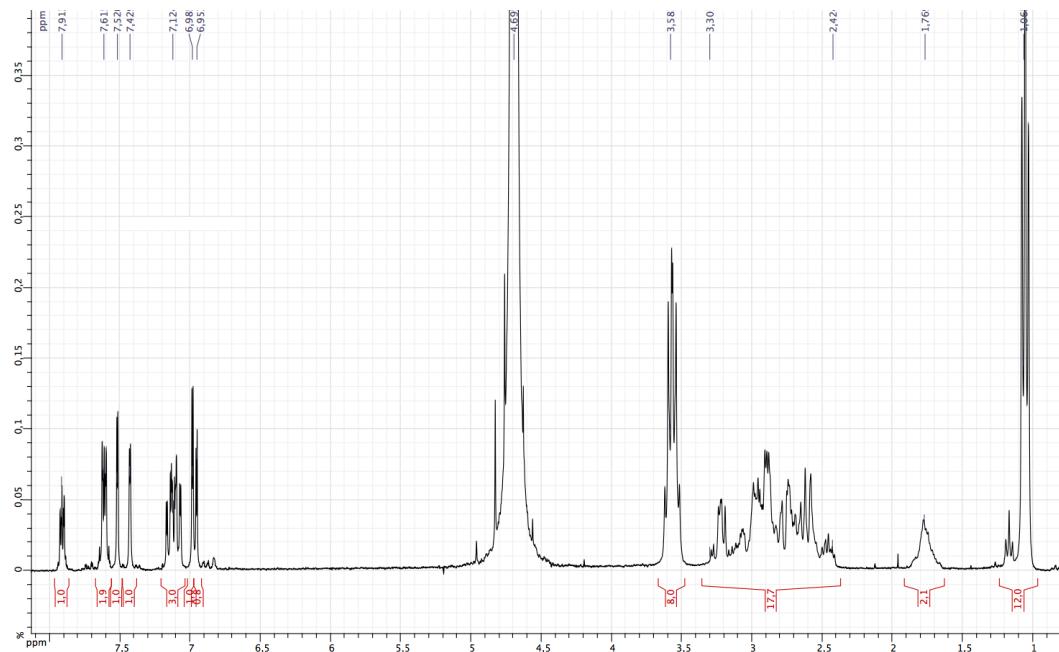


Figure 1. ^1H NMR spectrum Probe 3 (300 MHz, D_2O , 300 K).

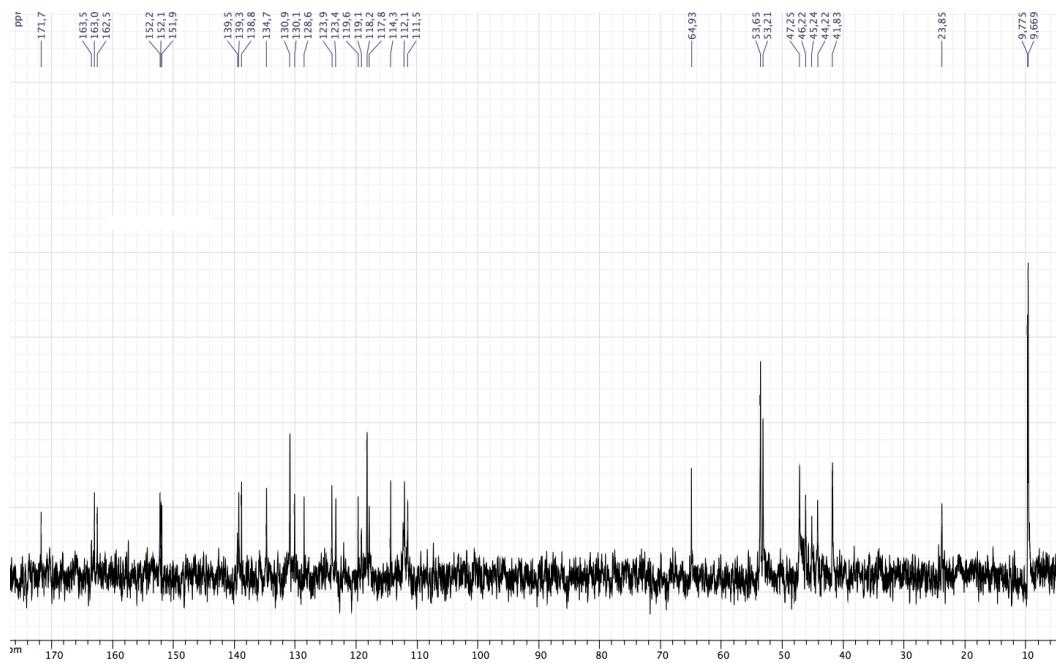


Figure 2. ^{13}C NMR of Probe 3 (75 MHz, D_2O , 300 K).

HR-mass measurements

The high resolution and accurate mass measurements were carried out using a Bruker microTOF-Q™ ESI-TOF (Electro Spray Ionization – Time of Flight) and a Thermo Scientific® LTQ Orbitrap mass spectrometer.

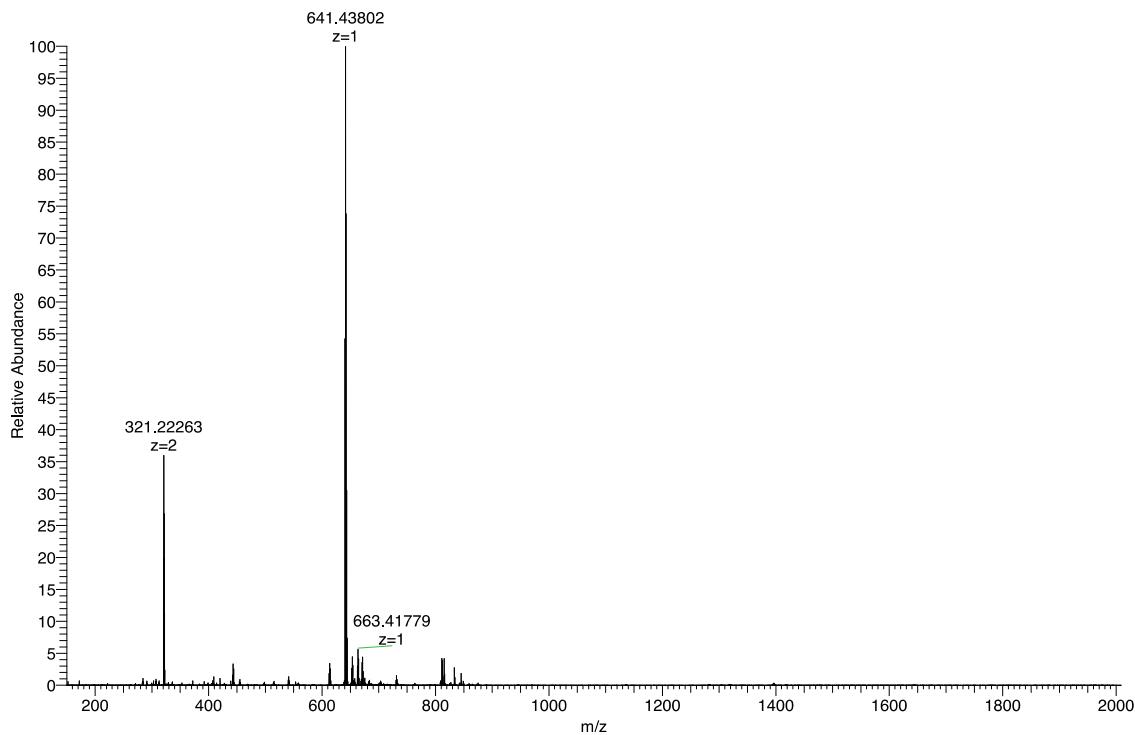


Figure 3. ESI-TOF spectrum of Probe 3.

FT-IR measurements

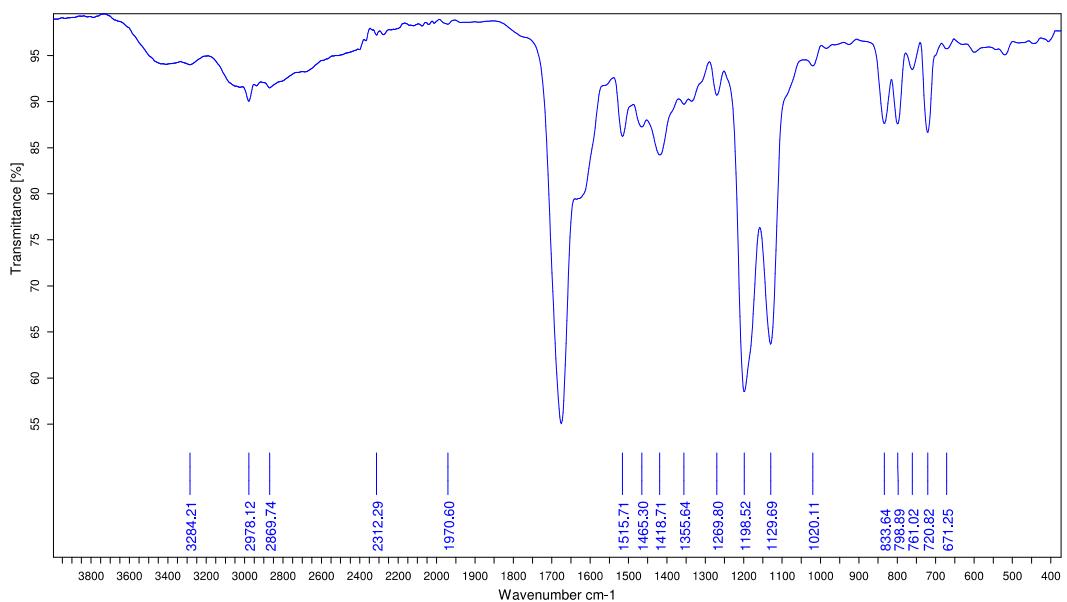


Figure 4. FTIR spectrum of Probe 3.

UV-vis spectra of Probe 3 in presence of copper (II) ions at different concentrations

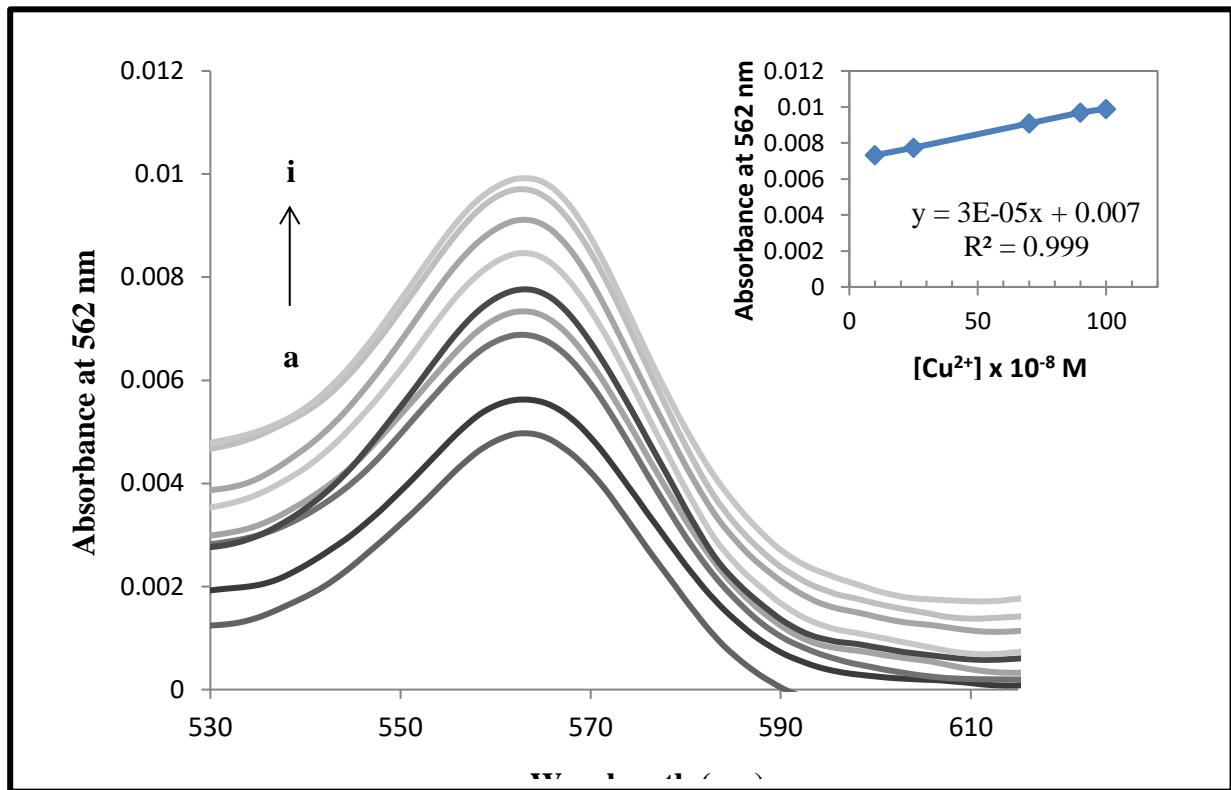


Figure 5. UV-visible absorption spectra of Probe 3 (1 μ M) in buffer solution 4.7 (0.1 M potassium dihydrogen phthalate buffer solution 10/2.72, v/v) with addition of $[Cu^{2+}]$ a: 0 M, b: 5×10^{-8} M, c: 10×10^{-8} M, d: 25×10^{-8} M, e: 35×10^{-8} M, f: 45×10^{-8} M, g: 70×10^{-8} M, h: 90×10^{-8} M, i: 1 μ M.

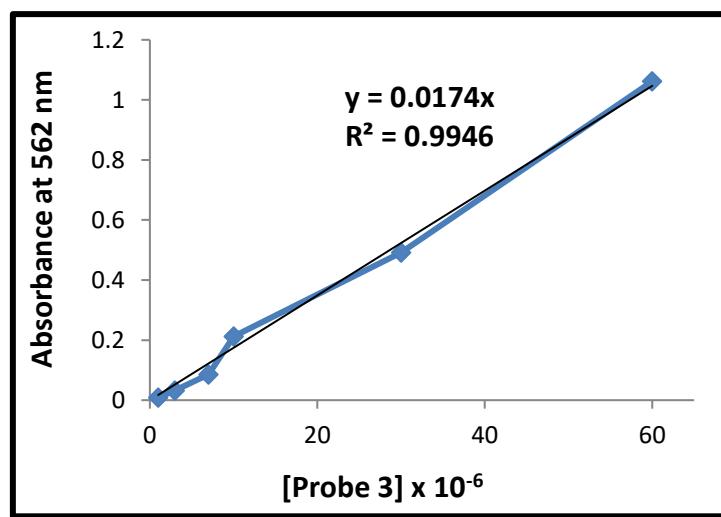


Figure 6. Regression curve of the absorbance of Probe 3 alone at different concentrations (from 0 to 60×10^{-6} M) in distilled water.

$$\epsilon = 0.0174 \text{ L/mol} \times \text{cm}$$

$$\epsilon = \frac{A}{Cl}; A: \text{absorbance} = y; C: \text{concentration} = x \text{ (mol/L)}; l: \text{width of cuvette} = 1 \text{ (cm)}.$$