

Copper-induced Fluorescence Quenching in a *Bis*[2-(2'hydroxyphenyl)benzoxazole]pyridinium Derivative for Quantification of Cu²⁺ in Solution

Supporting Information

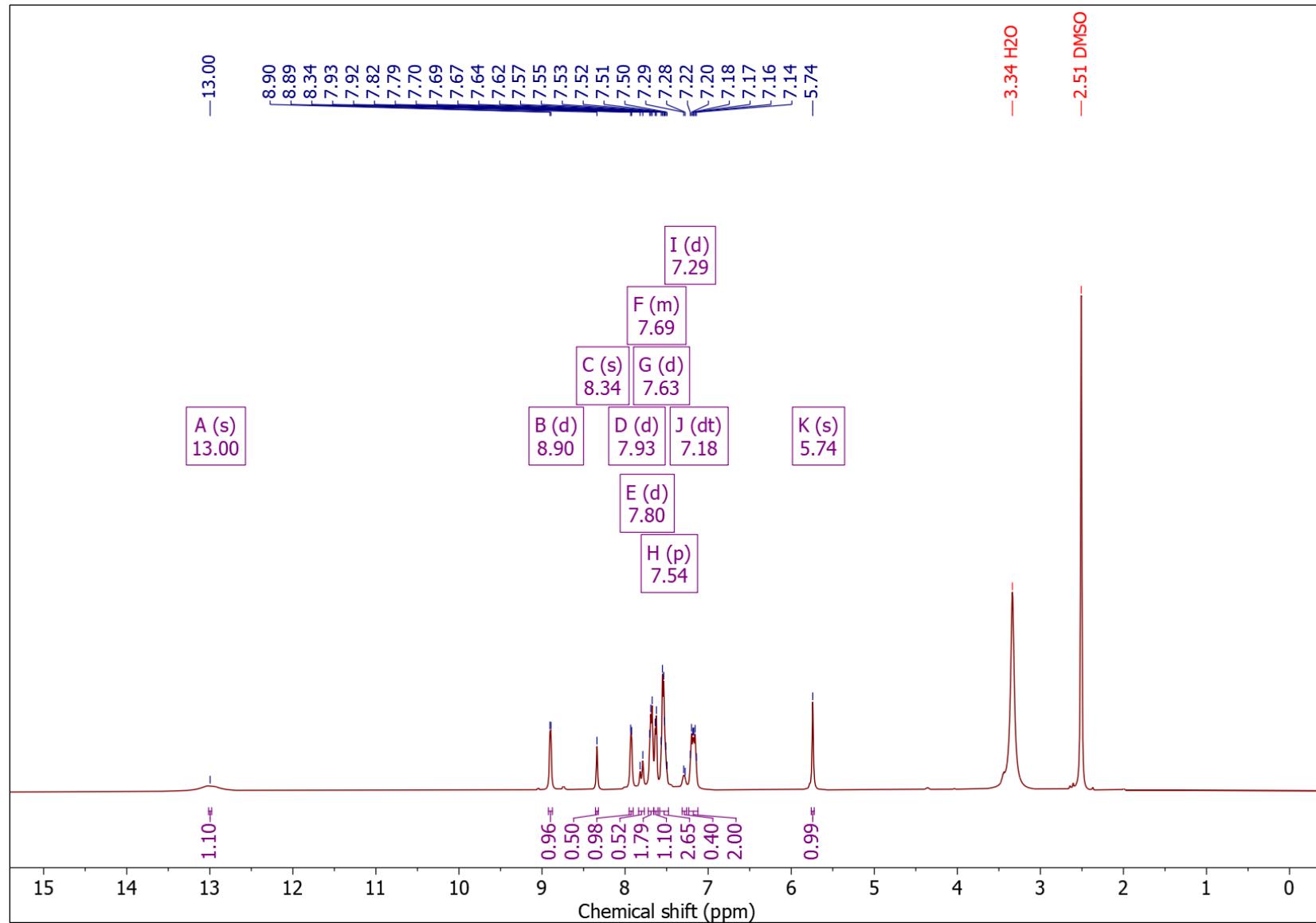


Figure S1.1 ^1H NMR spectra of **2** (500 MHz in $\text{DMSO}-d_6$).

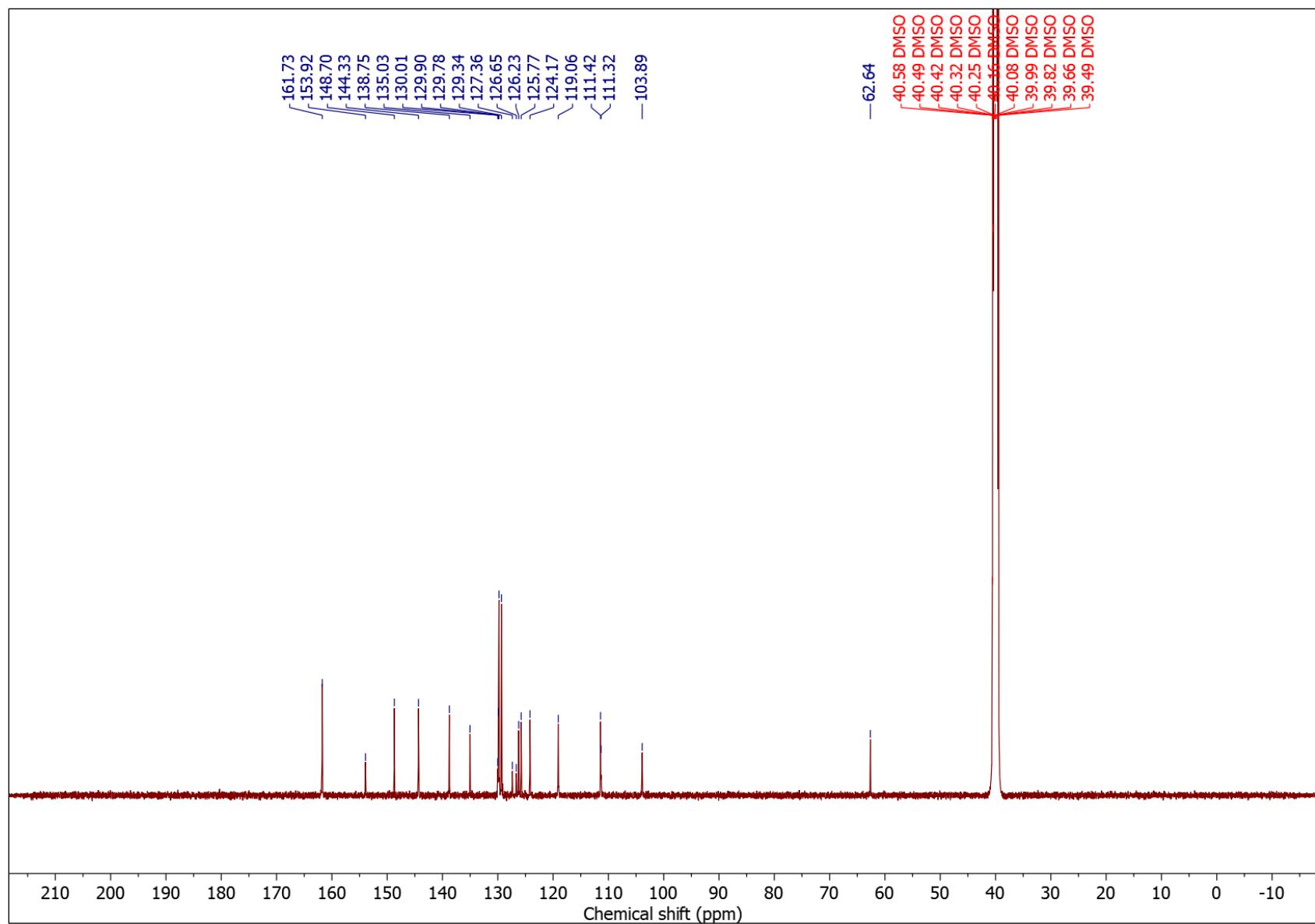


Figure S1.2 ^{13}C NMR spectra of **2** (126 MHz in $\text{DMSO}-d_6$).

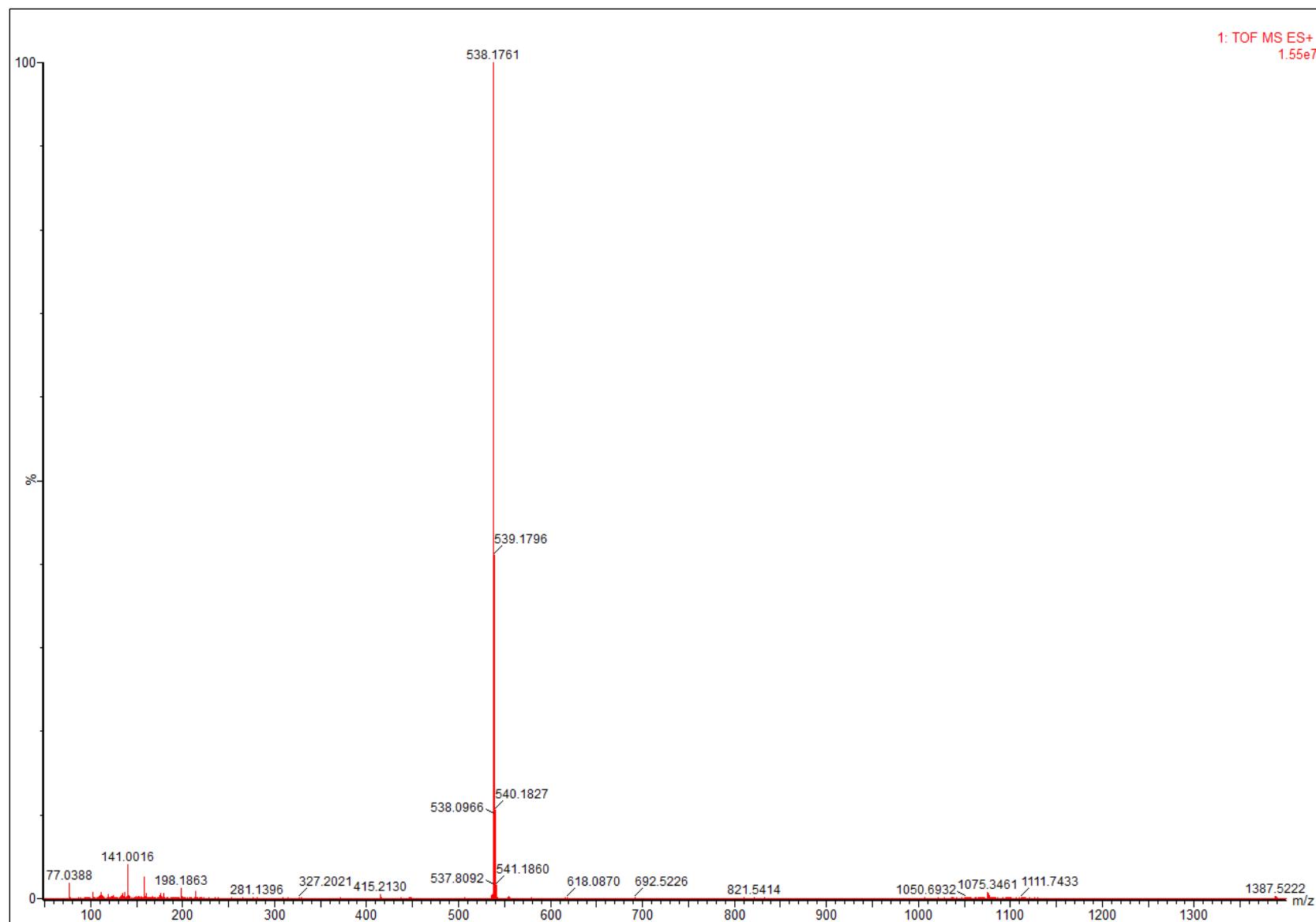


Figure S1.3 High-resolution mass spectra (TOF MS ES+) of **2**.

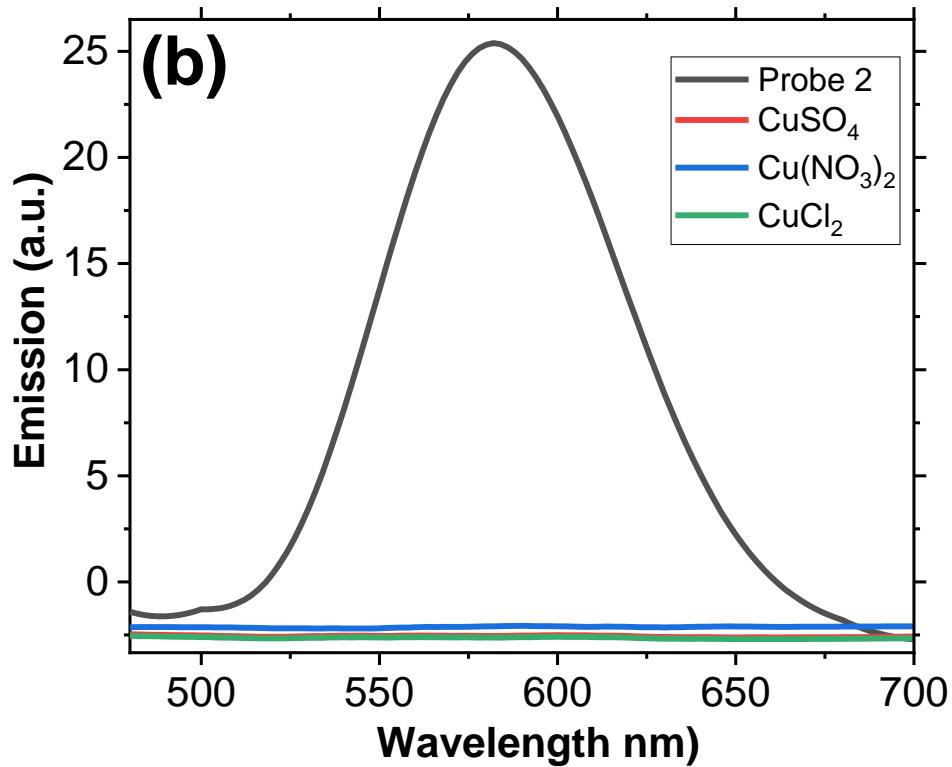
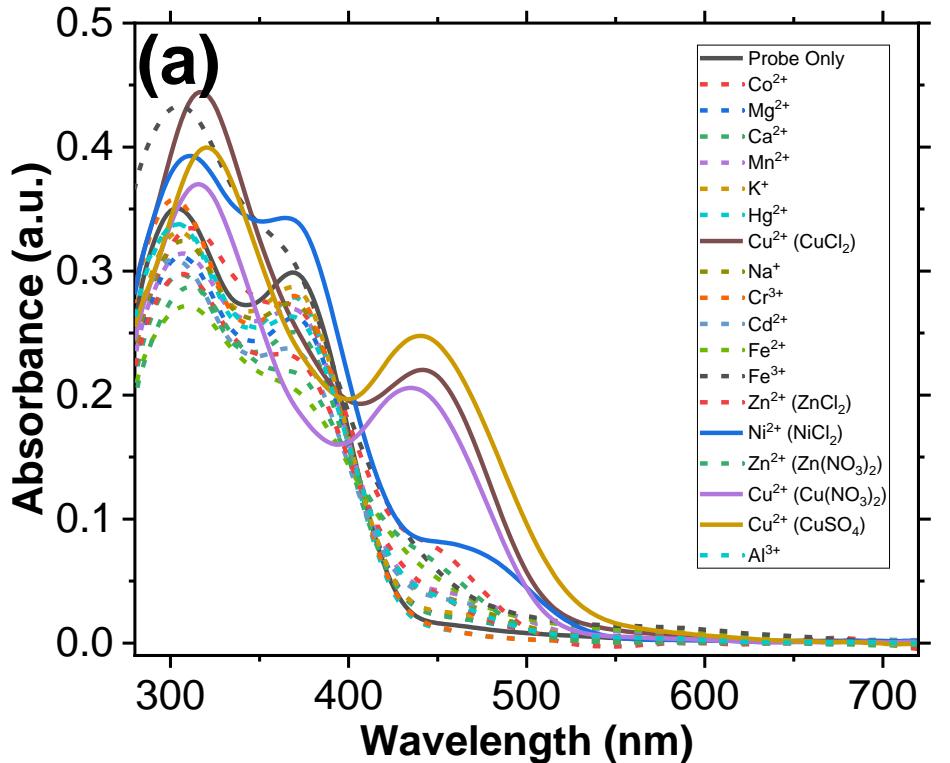


Figure S2. Absorbance (a) and emission (b) spectra recorded for probe **2** (1×10^{-5} M) in acetonitrile upon addition of 10 equivalence of different Cu^{2+} species at room temperature.

Table S1.1 LOD and LOQ calculation based on ratiometric absorbance (A_{440}/A_{370}) Data

SUMMARY OUTPUT

<i>Regression Statistics</i>	
Multiple R	0.997065
R Square	0.994139
Adjusted R Square	0.993488
Standard Error	0.02914
Observations	11

ANOVA

	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>
Regression	1	1.296204	1.296204	1526.511	2.34E-11
Residual	9	0.007642	0.000849		
Total	10	1.303846			

	<i>Coefficients</i>	<i>Standard</i>		<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>	<i>Lower 95.0%</i>	<i>Upper 95.0%</i>
		<i>Error</i>	<i>t Stat</i>					
Intercept	0.047079	0.016437	2.864174	0.018653	0.009895	0.084262	0.009895	0.084262
X Variable 1	1.085526	0.027784	39.07058	2.34E-11	1.022675	1.148378	1.022675	1.148378

SE Intercept **0.016437**
SD Intercept **0.004956**
Slope **0.10855**

LOD **0.150665**
LOQ **0.45656**

Table S1.2 LOD and LOQ calculation based on ratiometric fluorescence data (I_{6585}/I_{585})

SUMMARY OUTPUT

<i>Regression Statistics</i>	
Multiple R	0.995593
R Square	0.991206
Adjusted R Square	0.989007
Standard Error	0.032597
Observations	6

ANOVA

	df	SS	MS	Significance	
				F	F
Regression	1	0.47903	0.47903	450.8357	2.91E-05
Residual	4	0.00425	0.001063		
Total	5	0.48328			

	Coefficients	Standard		P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
		Coefficients	Error					
Intercept	0.958402	0.023592	40.62459	2.19E-06	0.892901	1.023903	0.892901	1.023903
X Variable 1	-0.08272	0.003896	-21.2329	2.91E-05	-0.09354	-0.07191	-0.09354	-0.07191

SE Intercept **0.023592**

SD Intercept **0.009631**

Slope **0.0827**

LOD **0.384319**

LOQ **1.164602**

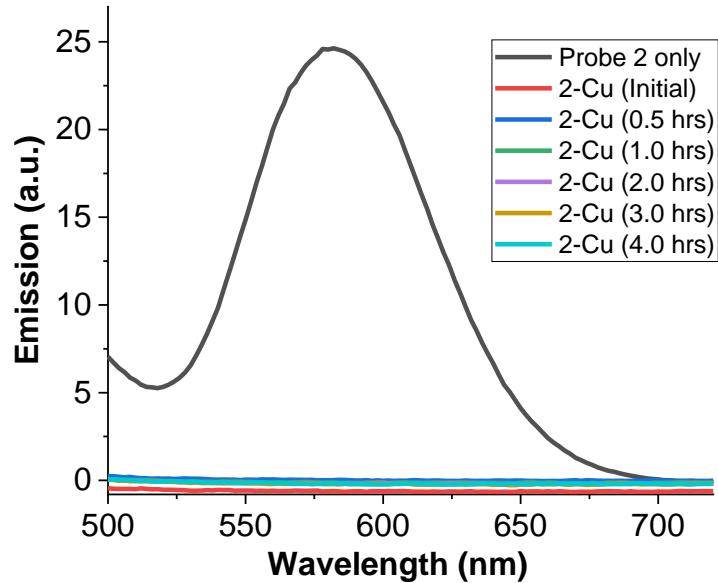


Figure S3 The evaluation of the stability of the **2-Cu** complex (10 μM in acetonitrile) by fluorescence analysis at room temperature.

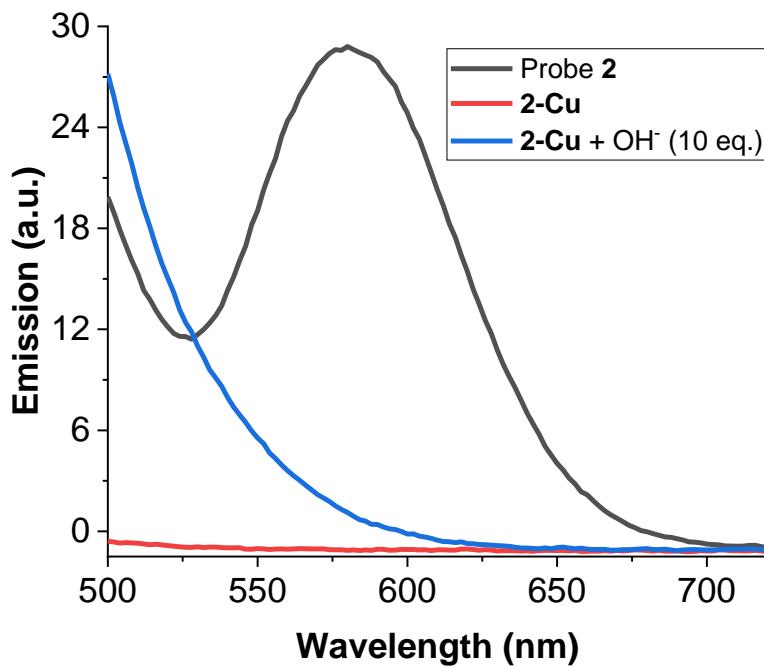


Figure S4 The evaluation of the stability of the **2-Cu** complex (10 μM in acetonitrile) by fluorescence in the presence of strong base (NaOH) at room temperature.

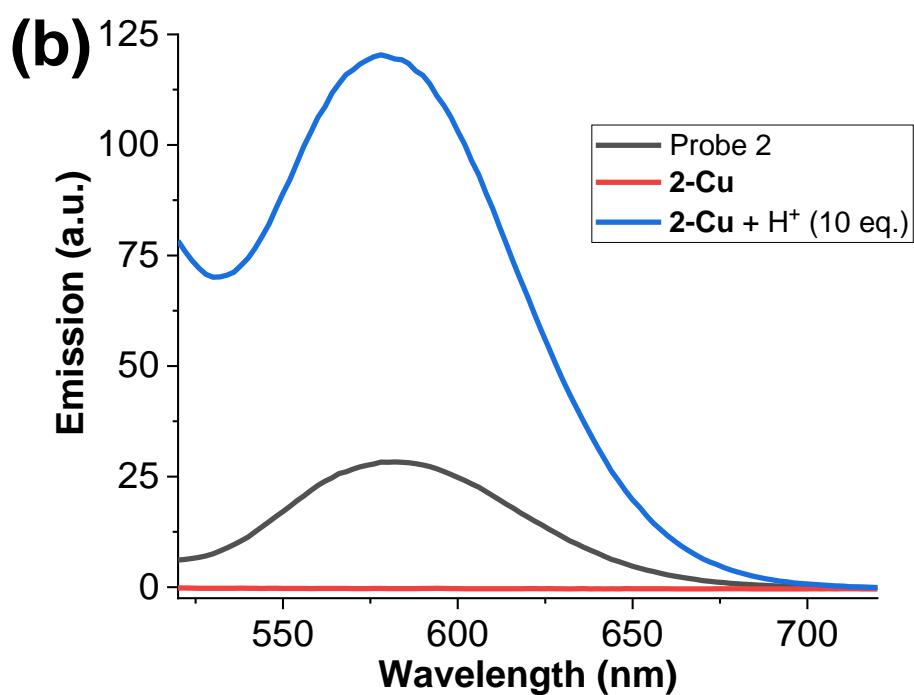
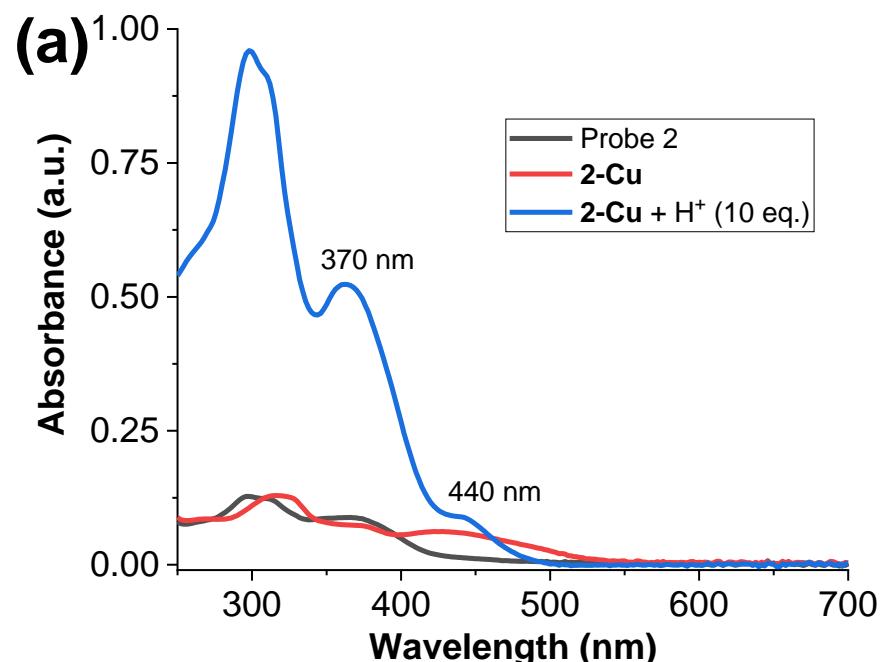


Figure S5 The evaluation of the stability of the **2-Cu** complex (10 μM in acetonitrile) by absorbance (a) and emission (b) in the presence of strong acid (HCl) at room temperature.

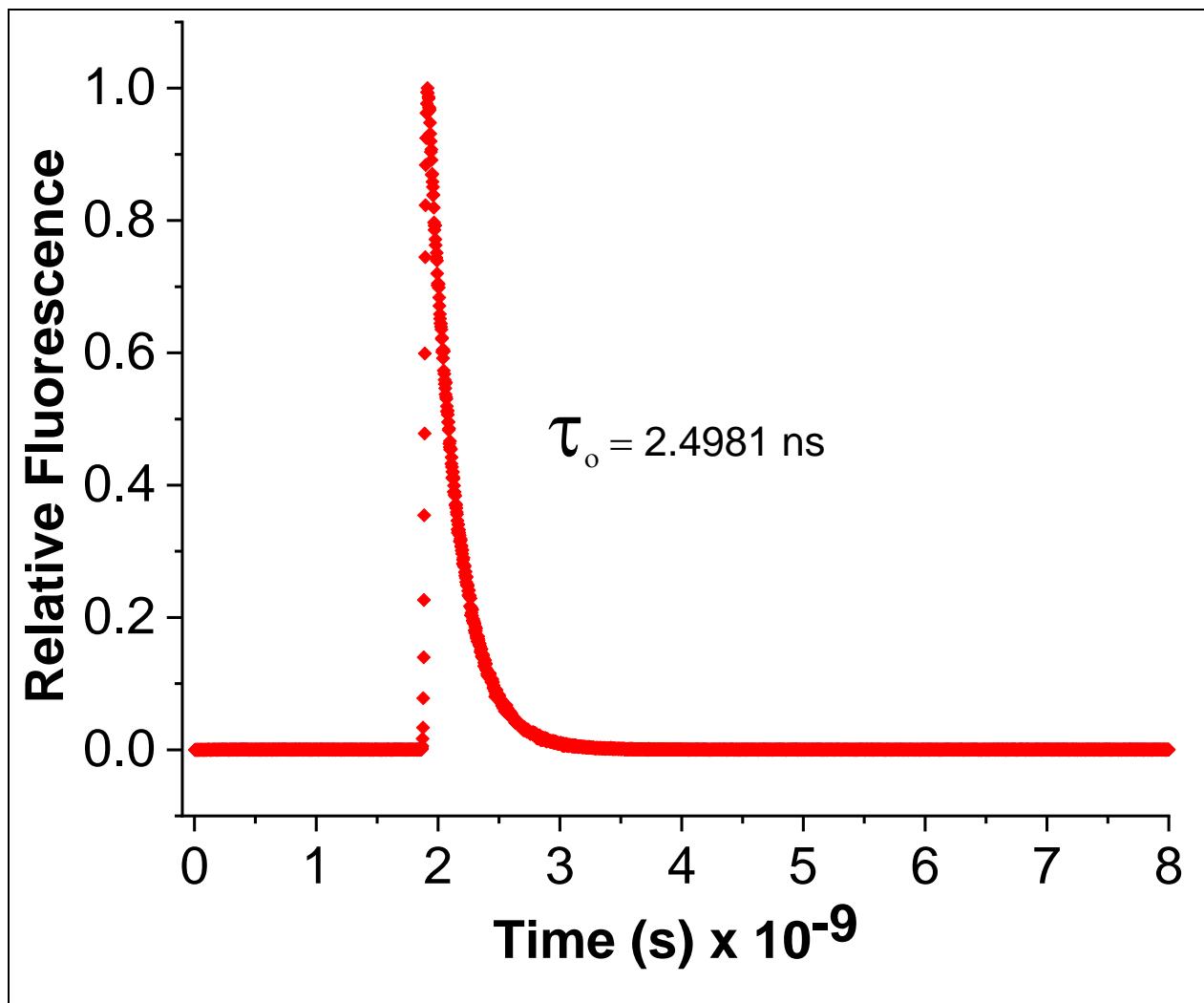


Figure S6 The fluorescence life-time measurement for probe **2** (10 μM) in acetonitrile at 25 °C.