

## Supplementary Information

### Near-infrared aza-BODIPY fluorescent probe for selective Cu<sup>2+</sup> detection and its potential in living cell imaging

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1. ESI-MS, <sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of <b>2</b>	S2
2. ESI-MS, <sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of <b>1</b>	S4
3. The effect of pH value on the fluorescence intensity of <b>1</b> in the absence and present of Cu <sup>2+</sup>	S6
4. The effect of coexisting anion in fluorescence emissions of <b>1</b>	S6
5. HOMOs, LUMOs and energy gaps of the <b>1</b> and <b>1</b> :Cu <sup>2+</sup> complexation.	S7

## Mass Spectrum List Report

### Analysis Info

Analysis Name OSSSUS600131003.d  
Method Tune\_wide\_POS\_pin\_600.m  
Sample Name aza-BDP-aceBr  
aza-BDP-aceBr

Acquisition Date 1/31/2017 12:03:31 PM  
Operator Administrator  
Instrument micrOTOF 72

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	50 V
Scan Range	n/a	Capillary Exit	250.0 V	Set Pulsar Pull	337 V
Scan Begin	50 m/z	Hexapole RF	600.0 V	Set Pulsar Push	337 V
Scan End	3000 m/z	Skimmer 1	75.0 V	Set Reflector	1300 V
		Hexapole 1	25.0 V	Set Flight Tube	9000 V
				Set Detector TOF	2295 V

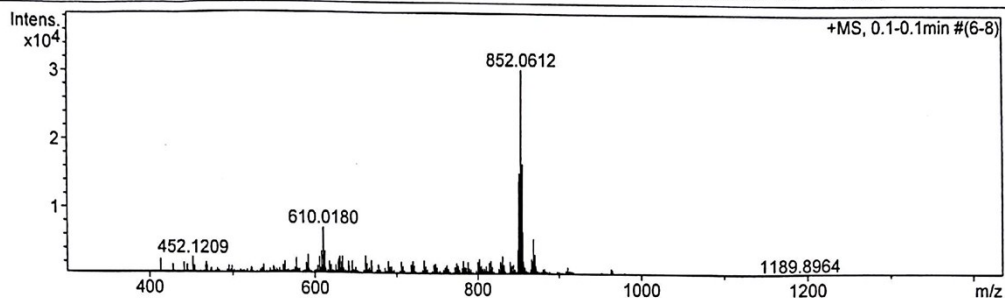


Fig. S1 HR-ESI MS of compound **2**: C<sub>38</sub>H<sub>30</sub>BBr<sub>2</sub>F<sub>2</sub>N<sub>5</sub>O<sub>4</sub>Na<sup>+</sup> calcd. 852.0603; m/z [M+Na]<sup>+</sup> found 852.0612.

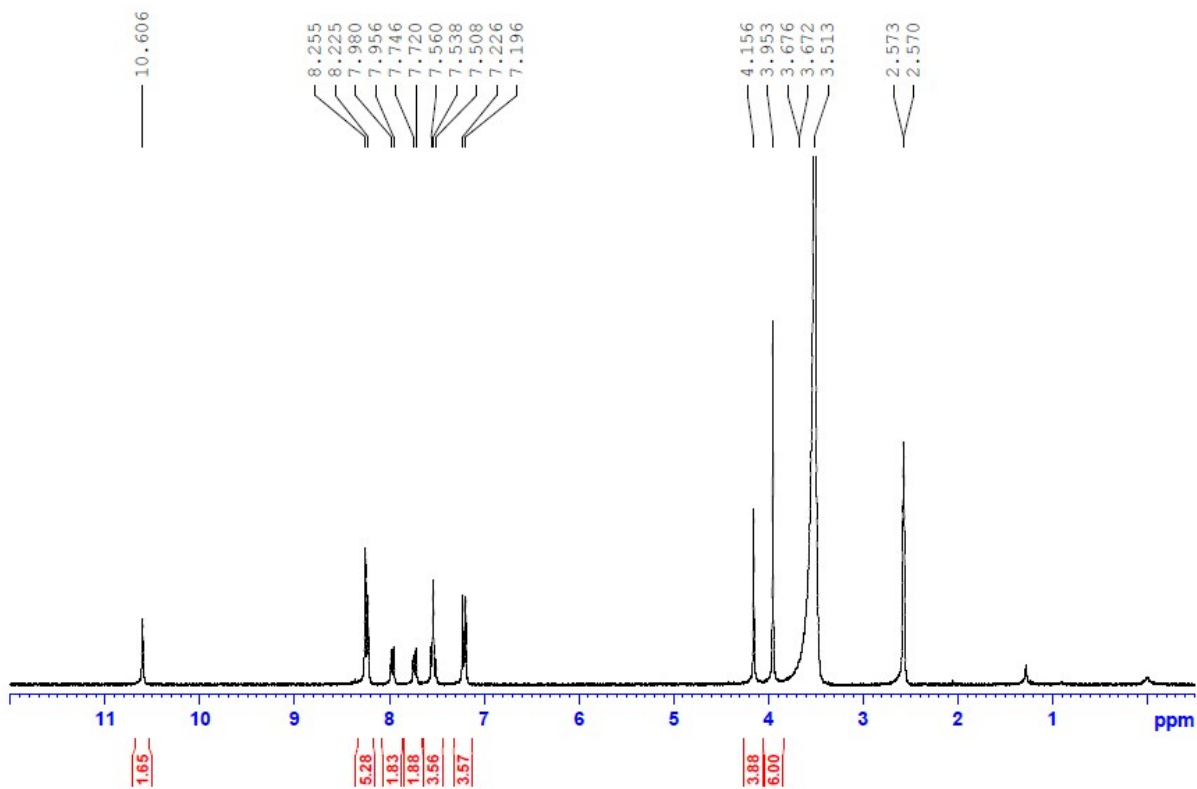


Fig. S2 <sup>1</sup>H NMR spectrum of compound **2** in DMSO-d<sub>6</sub> (300 MHz).

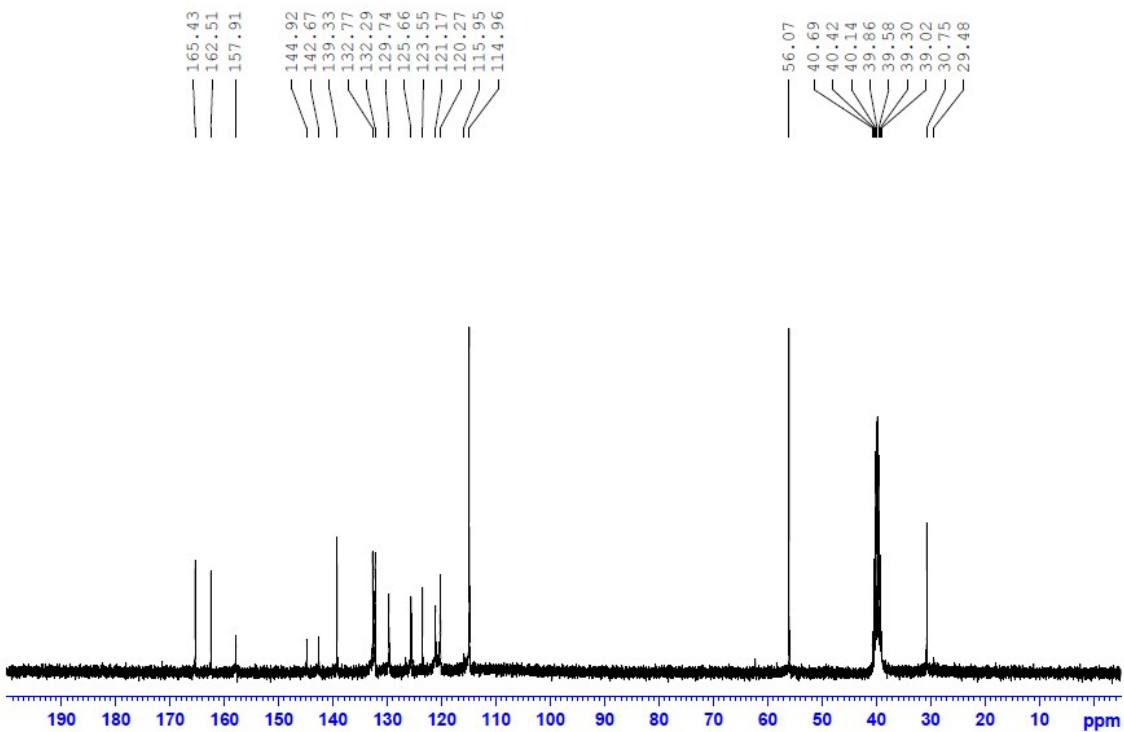


Fig. S3  $^{13}\text{C}$  NMR spectrum of compound **2** in  $\text{DMSO-d}_6$  (75 MHz).

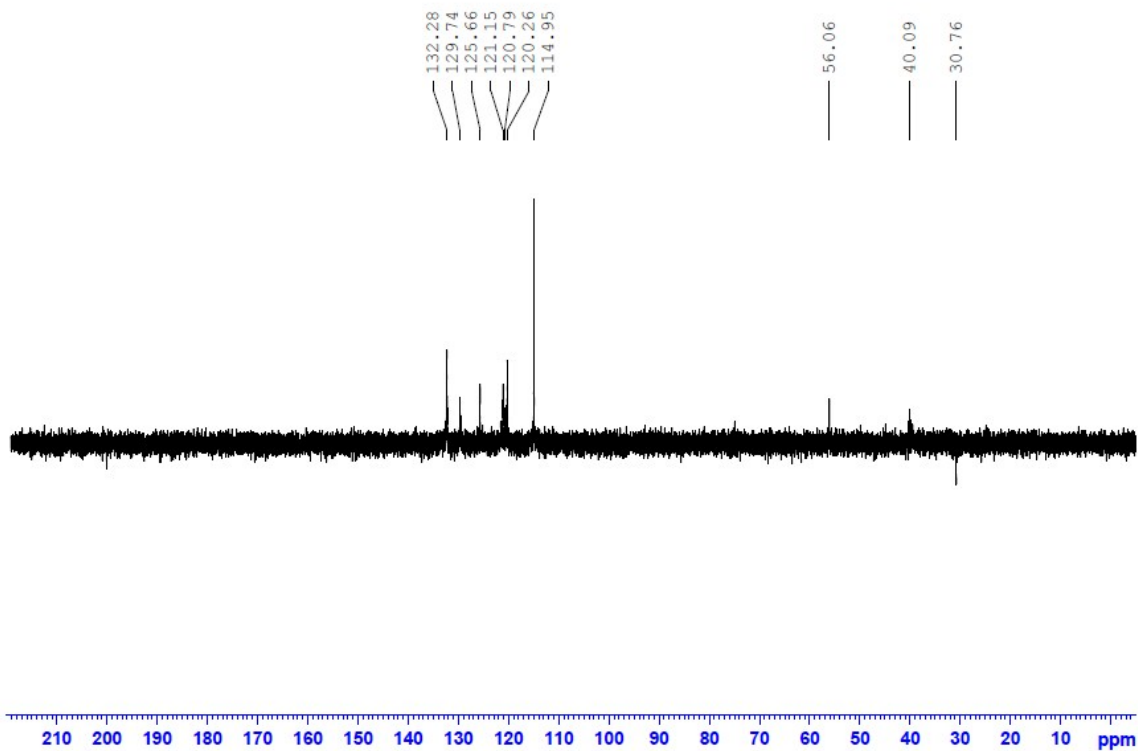


Fig. S4 DEPT-135 NMR spectrum of compound **2** in  $\text{DMSO-d}_6$  (75 MHz).

## Mass Spectrum List Report

### Analysis Info

Analysis Name OSSUYT590307004.d  
Method esi\_tune\_wide\_pos\_20150911.m  
Sample Name aza\_BDP\_DPA  
aza\_BDP\_DPA

Acquisition Date 3/7/2016 4:24:51 PM  
Operator Administrator  
Instrument micrOTOF 72

### Acquisition Parameter

Source Type ESI  
Scan Range n/a  
Scan Begin 50 m/z  
Scan End 3000 m/z

Ion Polarity Positive  
Capillary Exit 300.0 V  
Hexapole RF 600.0 V  
Skimmer 1 70.0 V  
Hexapole 1 25.0 V

Set Corrector Fill 50 V  
Set Pulsar Pull 337 V  
Set Pulsar Push 337 V  
Set Reflector 1300 V  
Set Flight Tube 9000 V  
Set Detector TOF 2295 V

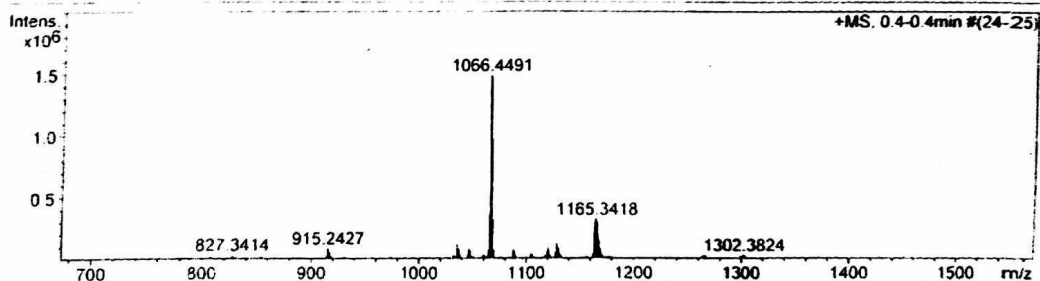


Fig. S5 HR-ESI MS of **1**: C<sub>62</sub>H<sub>55</sub>BF<sub>2</sub>N<sub>11</sub>O<sub>4</sub><sup>+</sup> calcd. 1066.4494; m/z [M+H]<sup>+</sup> found 1066.4491.

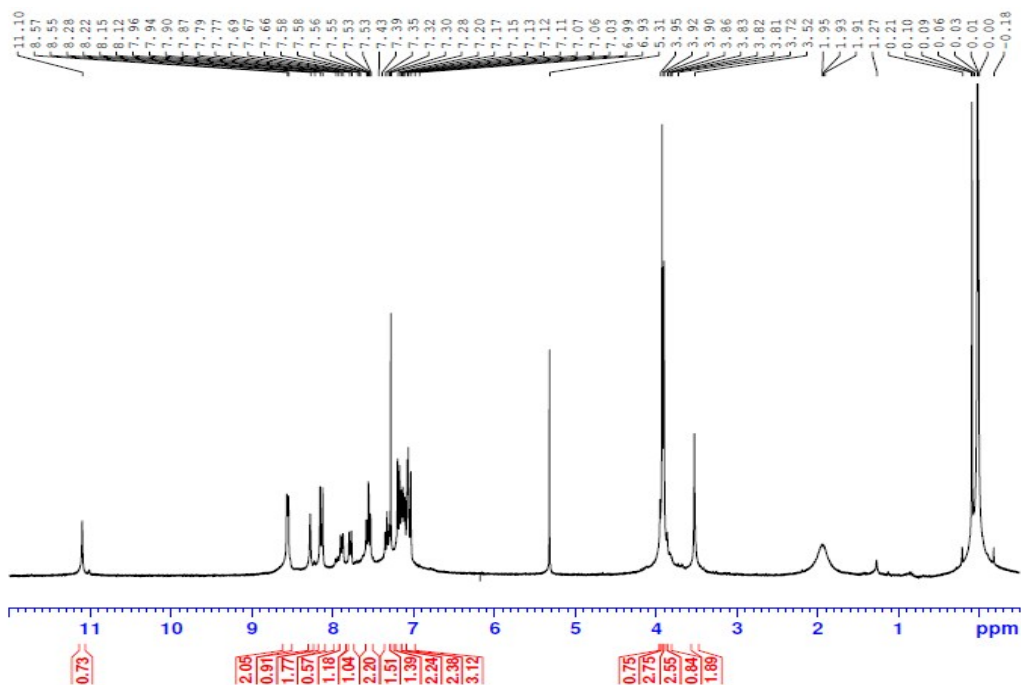


Fig. S6 <sup>1</sup>H NMR spectrum of **1** in CDCl<sub>3</sub> (300 MHz).

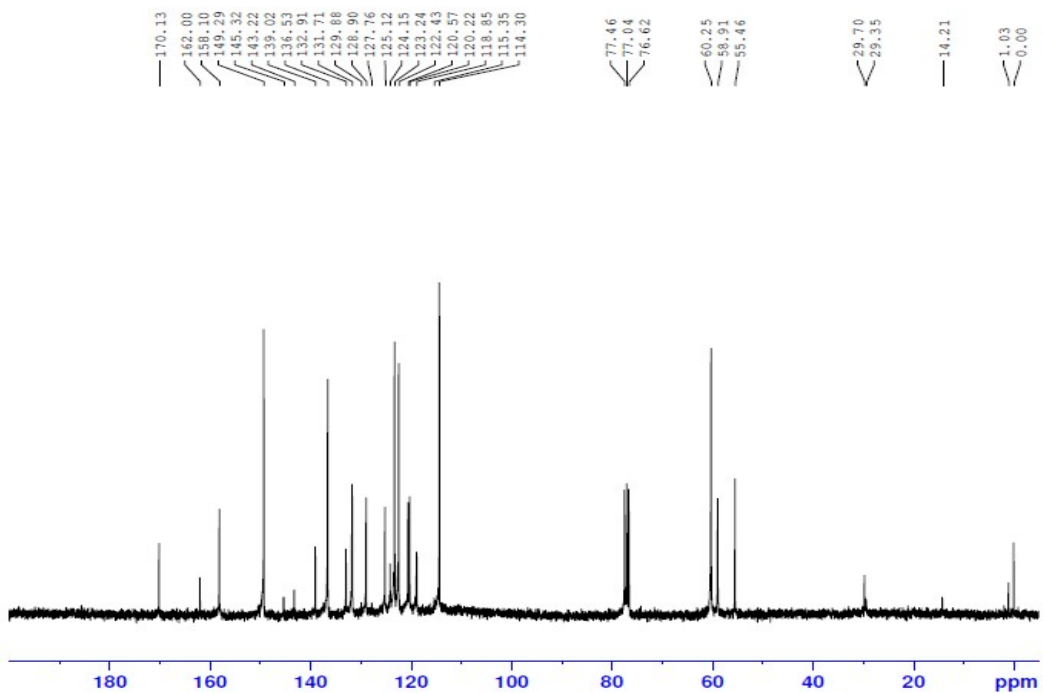


Fig. S7  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{CDCl}_3$  (75 MHz).

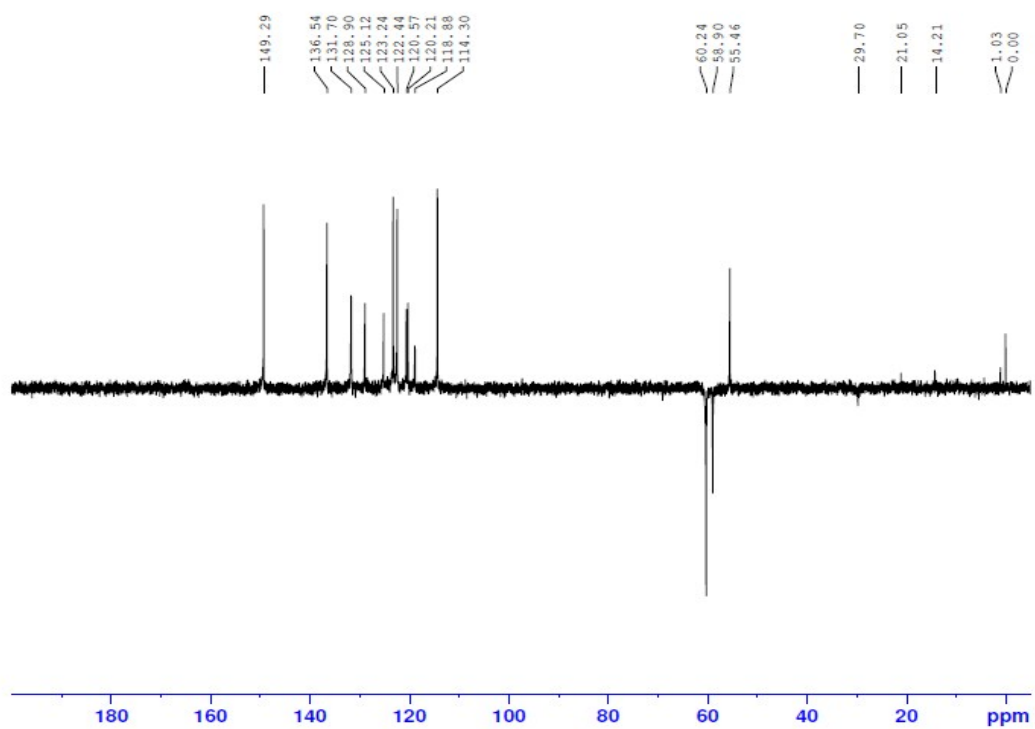
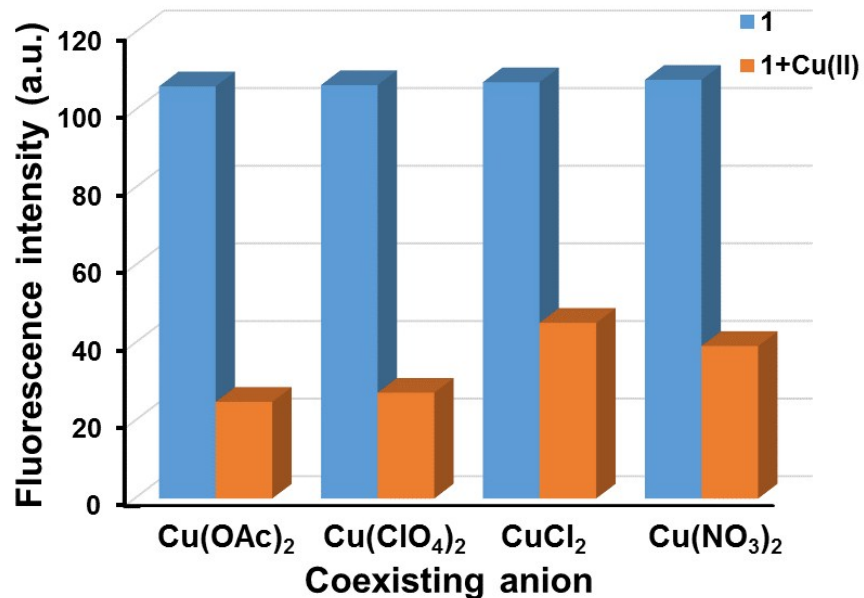
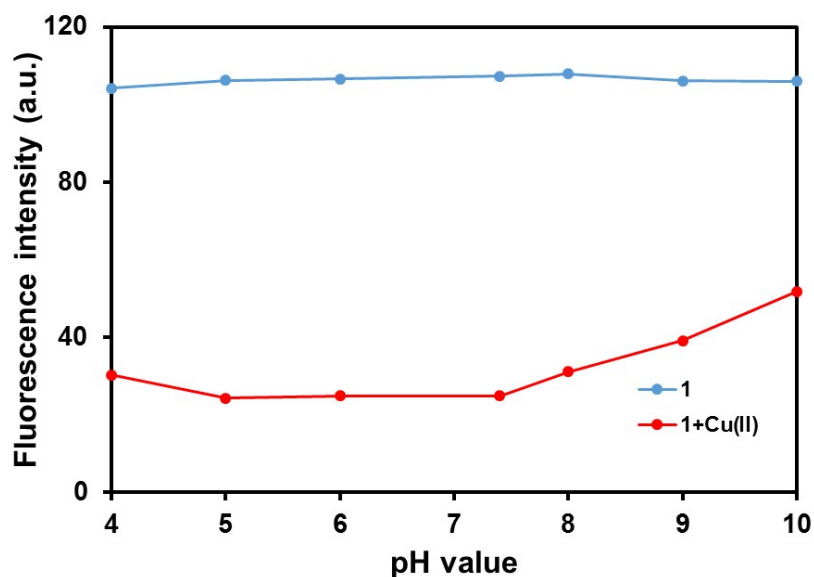


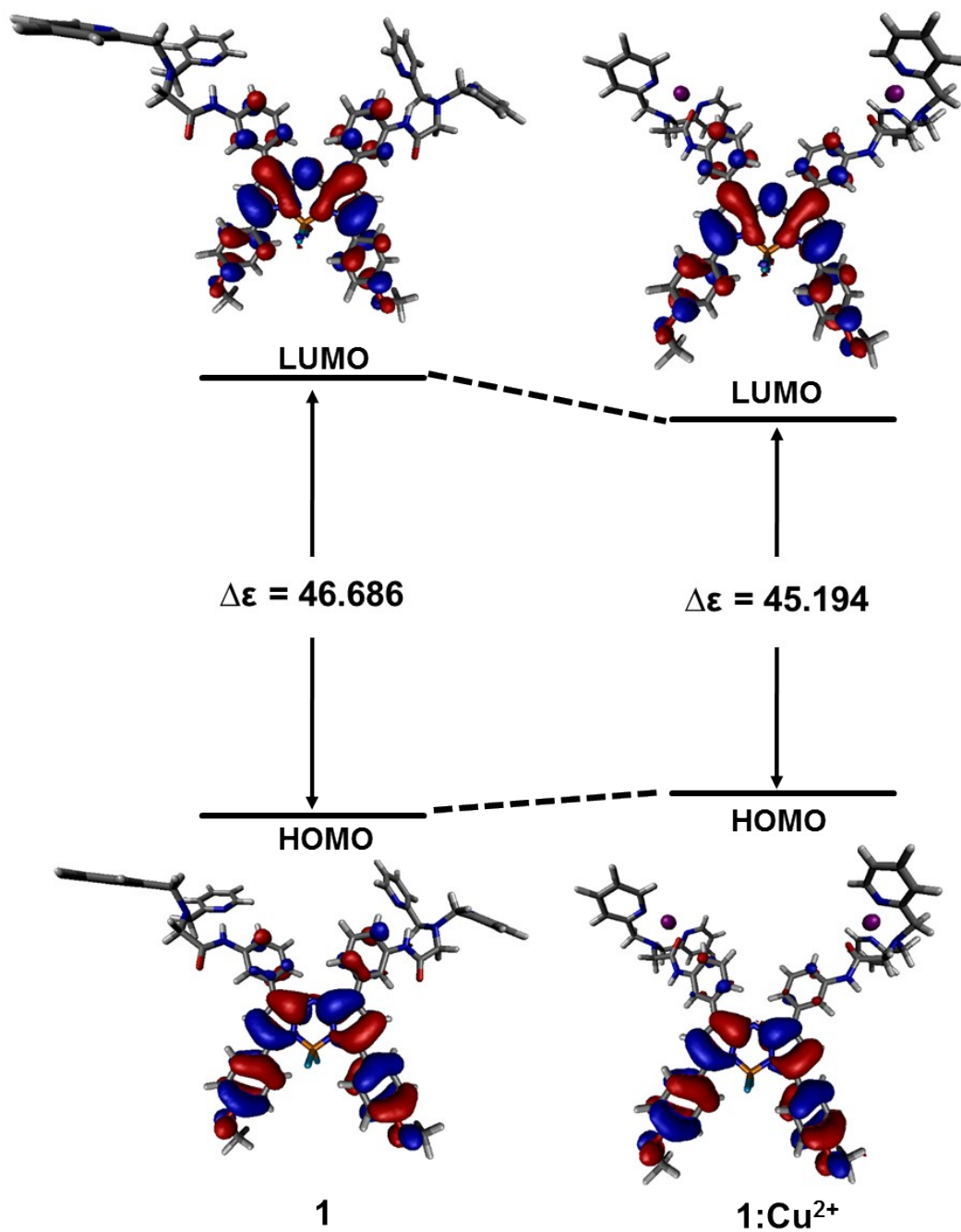
Fig. S8 DEPT-135 NMR spectrum of **1** in  $\text{CDCl}_3$  (75 MHz).



**Fig. S9** The effect of coexisting anion in fluorescence emissions ( $\lambda_{em} = 717$  nm) of **1** (5.0  $\mu$ M) in the absence and present of  $\text{Cu}^{2+}$  (5.0  $\mu$ M) in 5 mM PBS buffer (pH 7.4): acetonitrile (95:5 v/v) with 0.5% triton X-100 ( $\lambda_{ex} = 650$  nm).



**Fig. S10** The effect of pH on the fluorescence intensity ( $\lambda_{em} = 717$  nm) of **1** (5.0  $\mu$ M) in the absence and present of  $\text{Cu}^{2+}$  (5.0  $\mu$ M) in 5 mM PBS buffer (pH 7.4): acetonitrile (95:5 v/v) with 0.5% triton X-100 ( $\lambda_{ex} = 650$  nm).



**Fig. S11** The calculated HOMOs, LUMOs distribution and energy gaps of the **1** and **1:Cu<sup>2+</sup>** complexation.