

## 1 **Supplementary Information**

### 2 **A highly selective colorimetric fluorescence probe for** 3 **Cu<sup>2+</sup> in aqueous media: the synthesis, DFT** 4 **investigation and its application in living cells**

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14 Supplementary captions

15 **Fig. S1.** <sup>1</sup>H NMR spectrum of probe **POPH** in CDCl<sub>3</sub>.

16 **Fig. S2.** <sup>13</sup>C NMR spectrum of probe **POPH** in CDCl<sub>3</sub>.

17 **Fig. S3.** LC-MS spectrum of probe **POPH**.

18 **Fig. S4.** IR spectrum of probe **POPH** in KBr disk.

19 **Fig. S5.** IR spectrum of probe **POPH** and Cu<sup>2+</sup> complex in KBr disk.

20 **Fig. S6.** Determination of LOD for probe **POPH**.

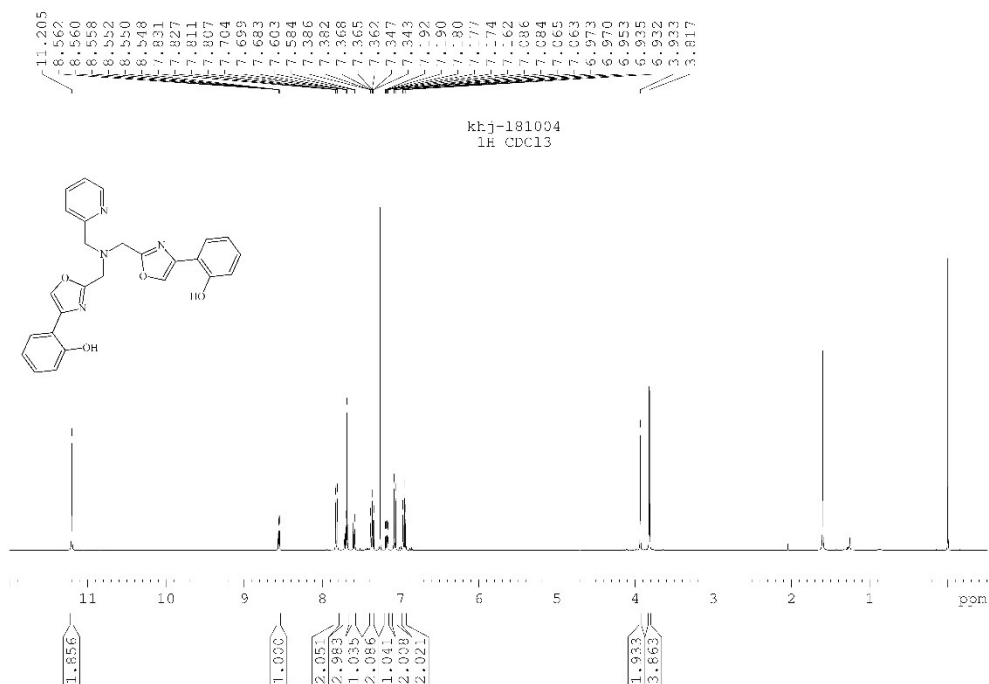
21 **Fig. S7.** Fluorescent quantum yield of probe **POPH** and **POPH-Cu<sup>2+</sup>**.

22 **Fig. S8.** FESEM and HRTEM images of probe **POPH**.

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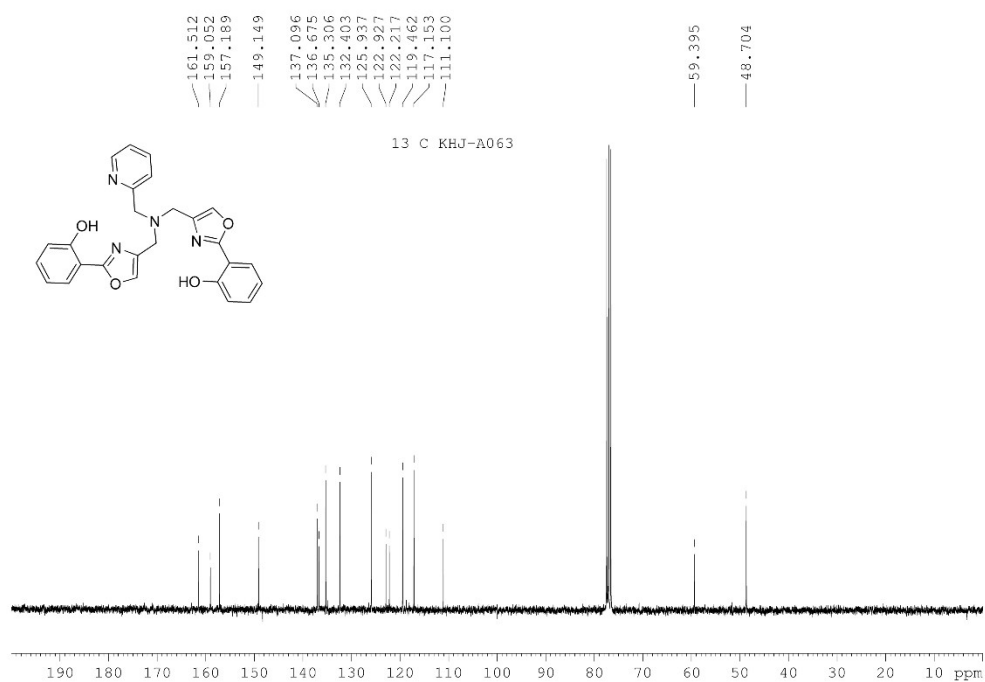
- 1 **Fig. S9.** FESEM and HRTEM images of probe **POPH** and Cu<sup>2+</sup> complex.
- 2 **Fig. S10.** Cytotoxicity assay of **POPH**.
- 3 **Table S1.** Comparison of LOD in this work with other works previously



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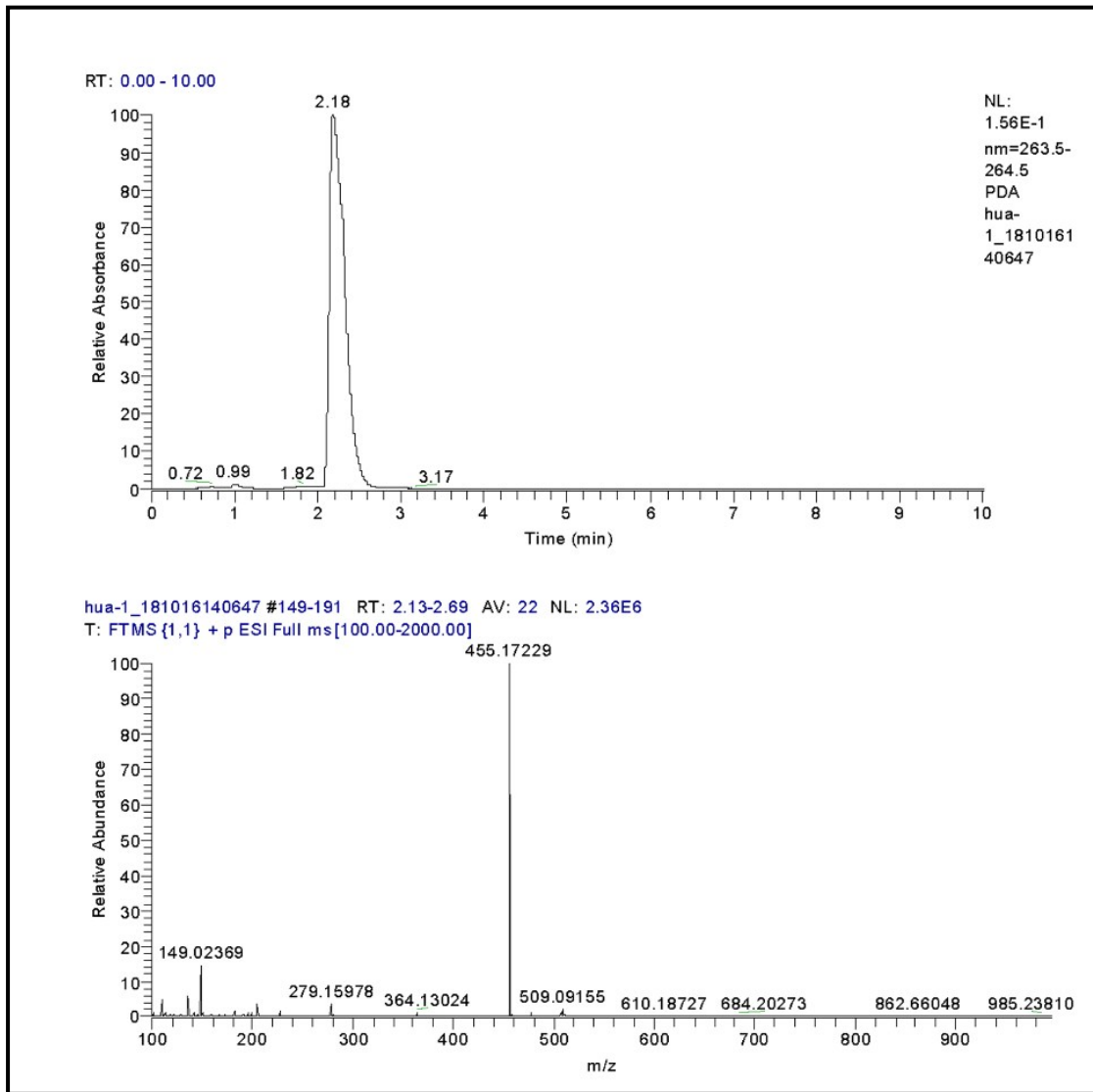
**Fig. S1** <sup>1</sup>H NMR spectrum of probe **POPH** in CDCl<sub>3</sub>



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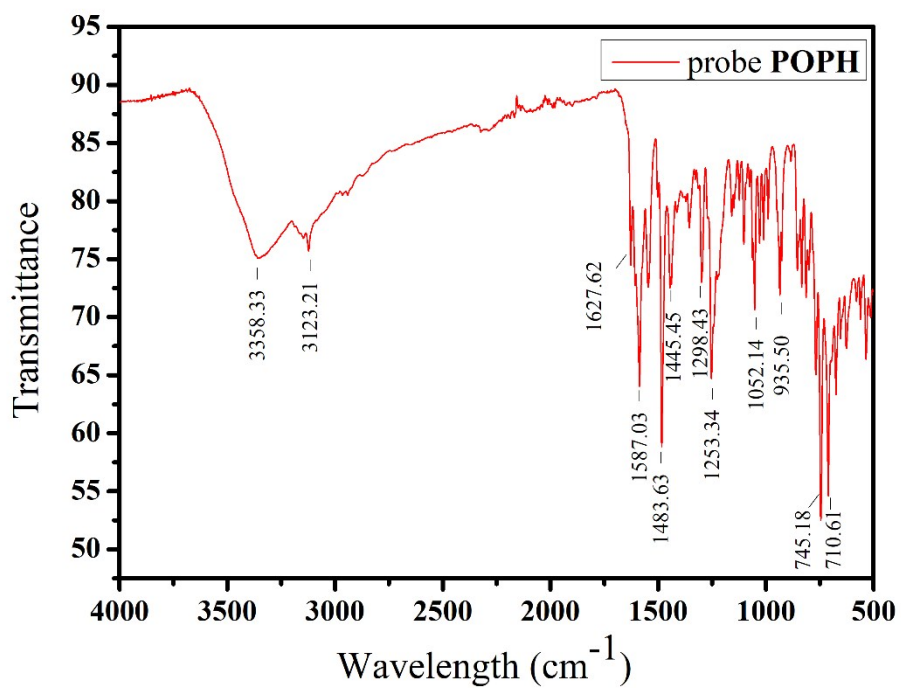
Fig. S2  $^{13}\text{C}$  NMR spectrum of probe **POPH** in  $\text{CDCl}_3$



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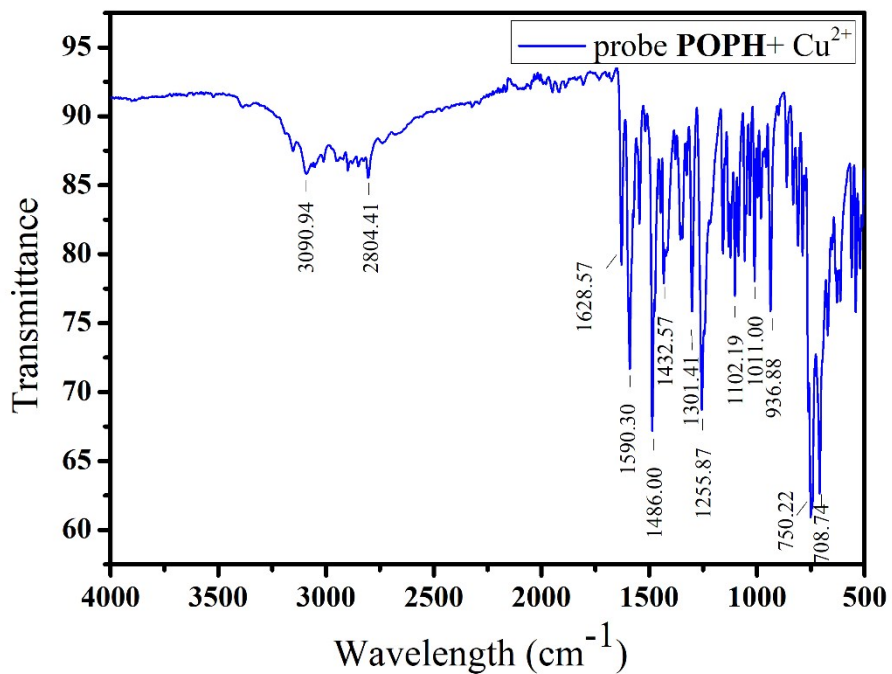
Fig. S3 LC-MS spectrum of probe **POPH**



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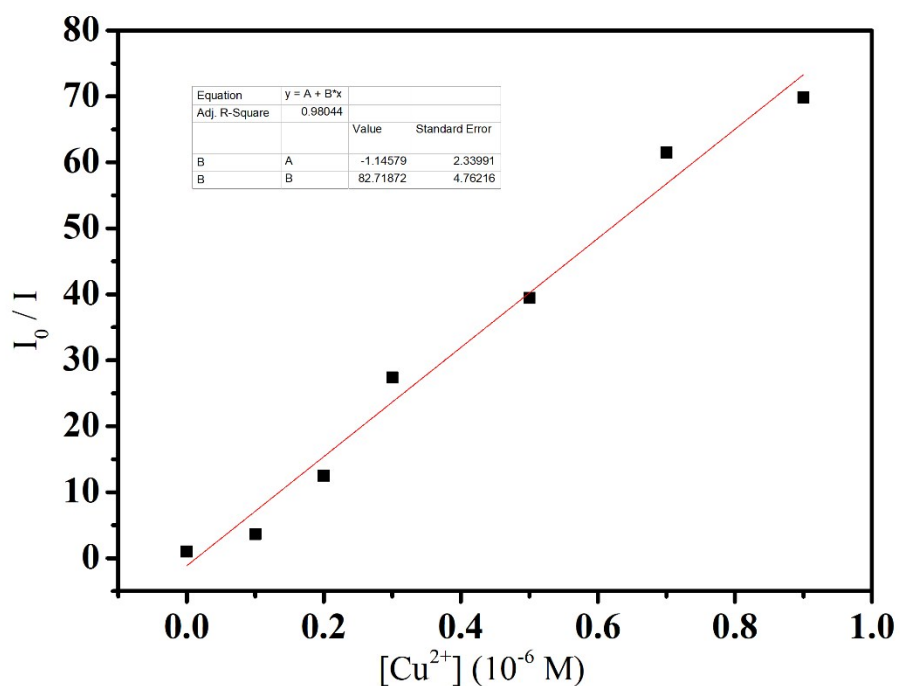
Fig. S4 IR spectrum of probe **POPH** in KBr disk



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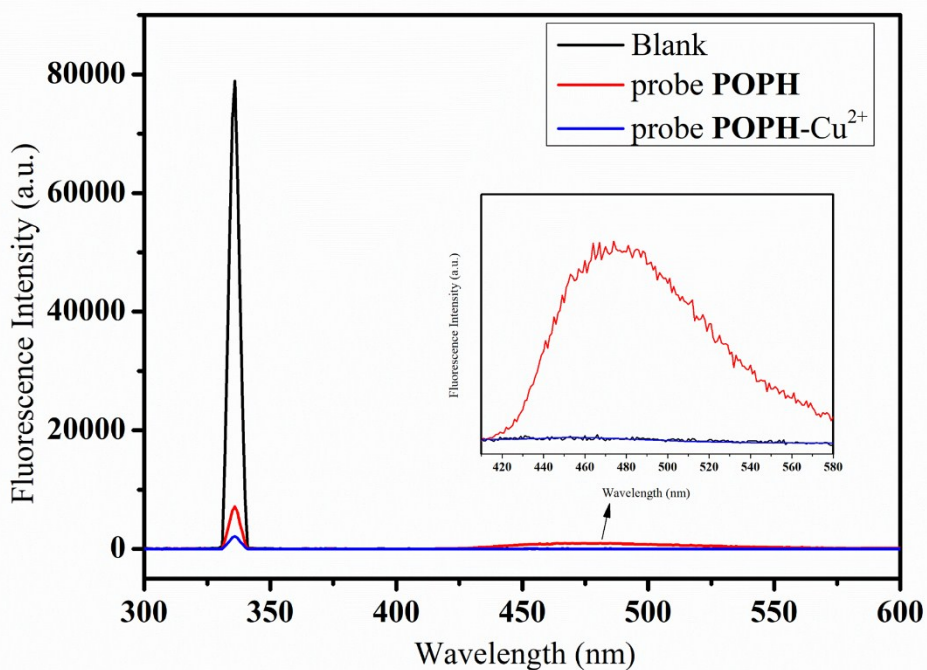
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Fig. S5 IR spectrum of probe **POPH** and **Cu<sup>2+</sup>** complex in KBr disk



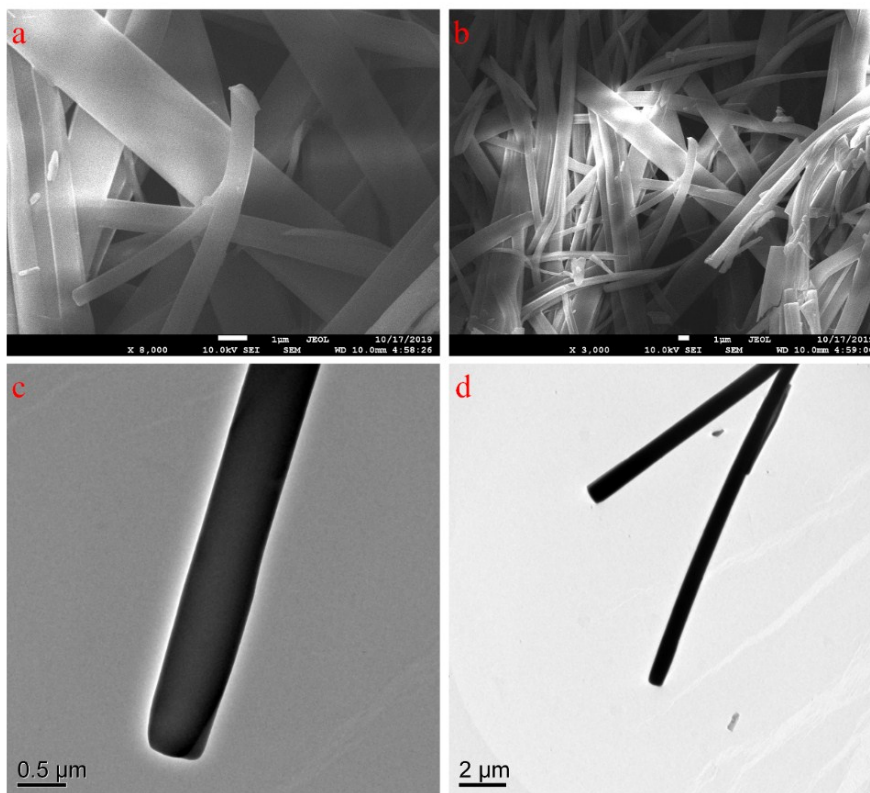
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2 Fig. S6 Fluorescence changes of POPH at 468 nm as a function of  
 3 aqueous  $\text{Cu}^{2+}$  ion concentration.  $S_d = 1.062 \times 10^{-6}$  (from experimental  
 4 data), and  $K = 82.72$ . Using the formula, we got  $\text{LOD} = 3.8 \times 10^{-8}$  M.



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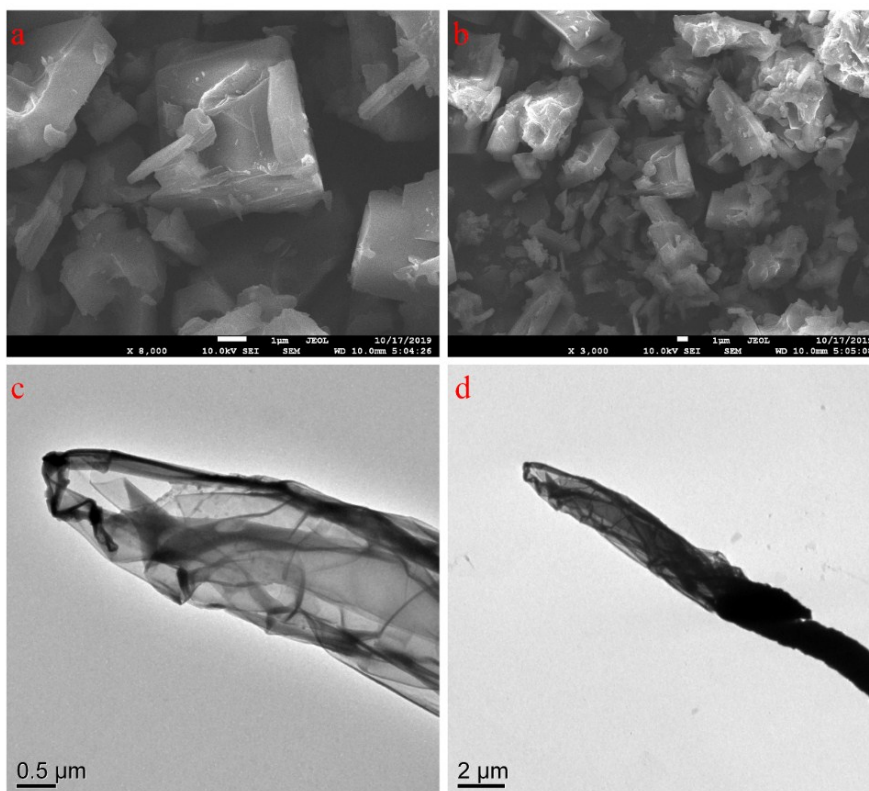
- 1 Fig. S7 Fluorescent quantum yield of probe **POPH** and probe **POPH-**
- 2  $\text{Cu}^{2+}$  under 336 nm excitation



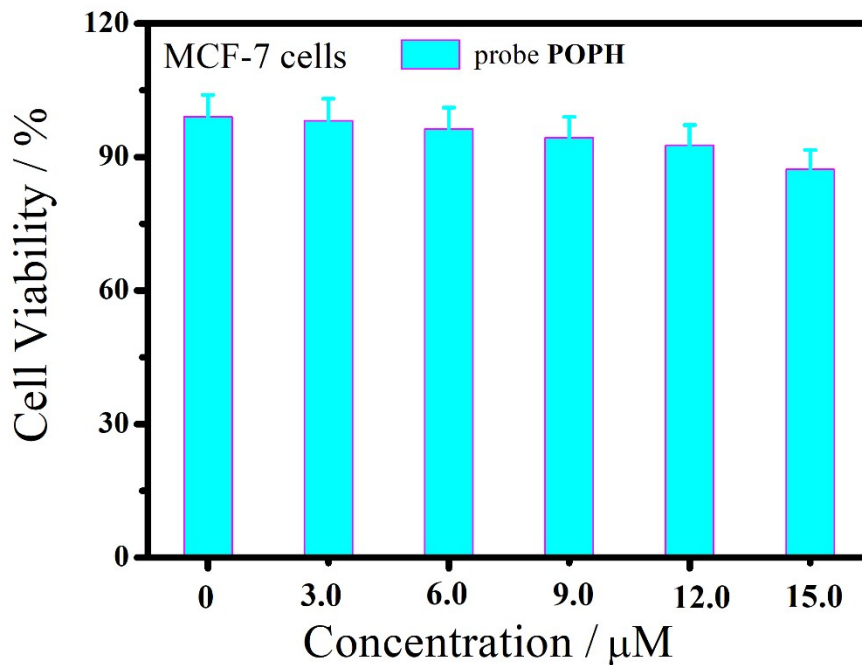
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Fig. S8 FESEM and HRTEM images of probe **POPH**



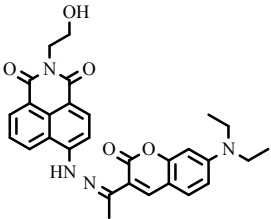
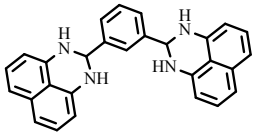
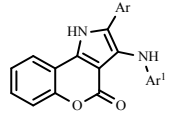
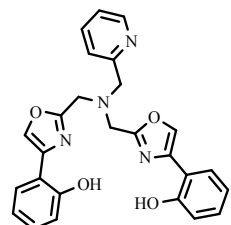
2 Fig. S9 FESEM and HRTEM images of probe **POPH** and  $\text{Cu}^{2+}$  complex



4 Fig. S10 Cytotoxicity assay of POPH after 4 h incubation

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Compound	Sensing method	LOD (M)	Ref.
	Turn - off	$3.9 \times 10^{-8}$	1
	Turn - off	$6.19 \times 10^{-8}$	2
	Turn - off	$1.13 \times 10^{-8}$	3
	Turn - off	$3.8 \times 10^{-8}$	This work

2 Table S1 Comparison of LOD in this work with other works previously

### 3 Reference

- 4 1 C. R. Li, Z. Y. Yang and S. L. Li, *J. Lumin.*, 2018, **198**, 327-336.
- 5 2 R. Debashis, C. Arijit and G. Rina, *RSC Adv.*, 2017, **7**, 40563-40570.
- 6 3 S. Mukherjee, S. Hazra, S. Chowdhury, S. Sarkar, K. Chattopadhyay, and A. Pramanik, *J. Photochem. Photobiol. A: Chem.*, 2018, **364**, 635-644.