

Supplementary Material

Design and Synthesis of a Dinuclear Copper(II) Probe for Selective Fluorescence Sensing of Pyrophosphate

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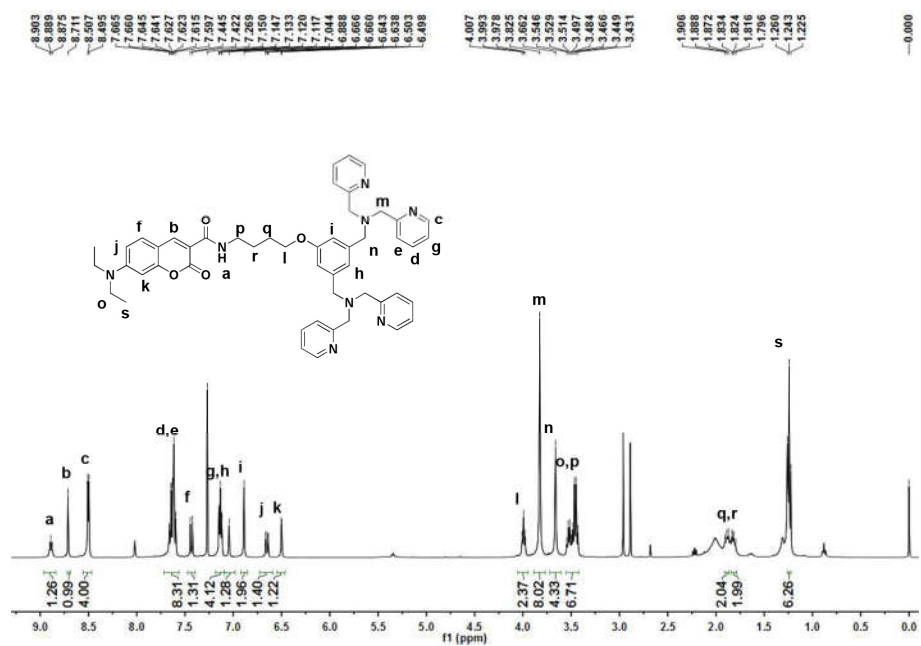


Figure S1. ¹H NMR of compound DPAC in CDCl₃.

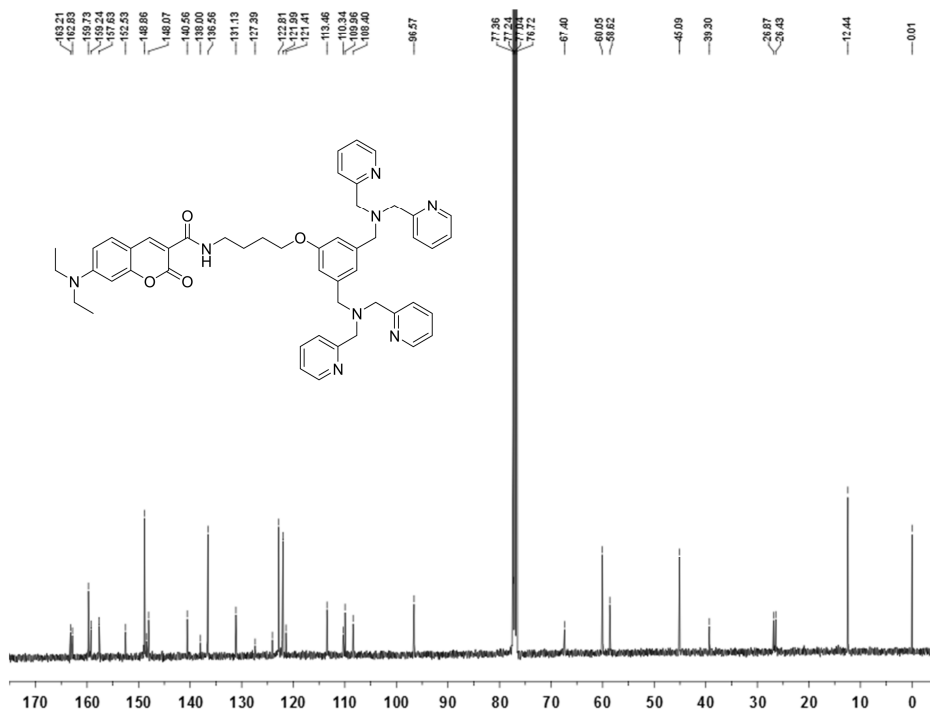


Figure S2. ¹³C NMR of compound DPAC in CDCl₃.

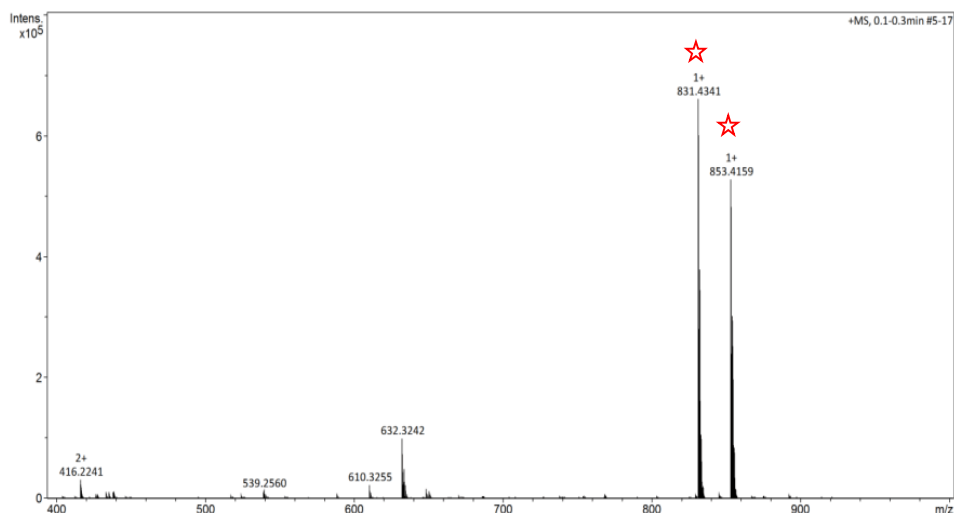


Figure S3. HRMS of compound **DPAC**.

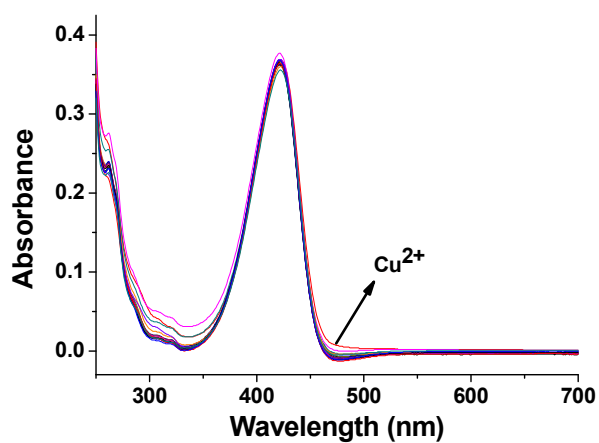


Figure S4. UV-vis absorption spectra of compound **DPAC** (10 μ M) upon addition of various metal ions (2 equivalents) in CH_3CN : HEPES (3: 2, v/v, $\text{pH}=7.2$) solutions.

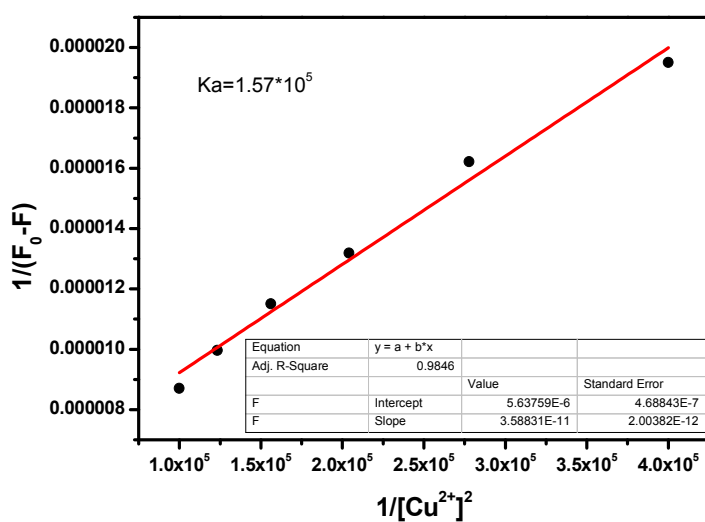


Figure S5. The Benesi-Hildebrand fitting of titration plots with the titration of Cu^{2+} assuming 1:2 stoichiometry with Cu^{2+} .

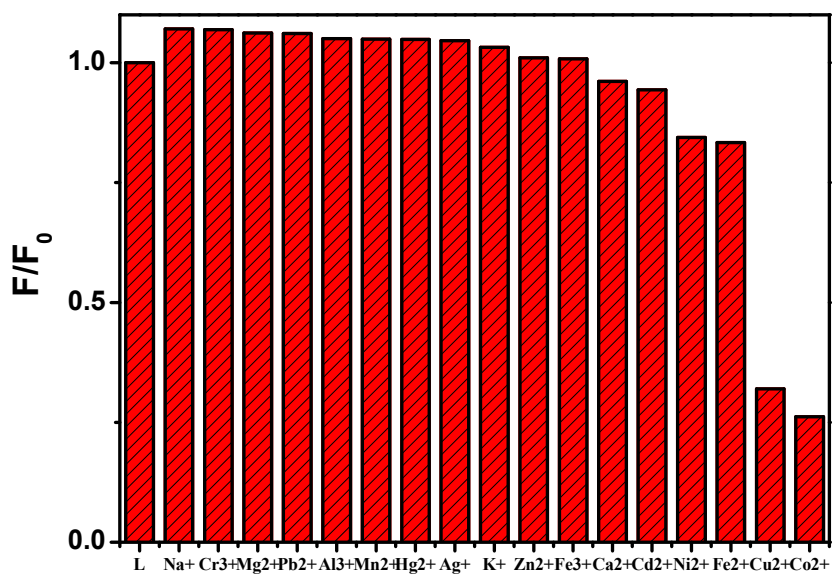


Figure S6. Emission responses of compound **DPAC** (10 μM) upon additions of various metal ions in CH_3CN : HEPES (3:2, v/v, pH=7.2) solution.

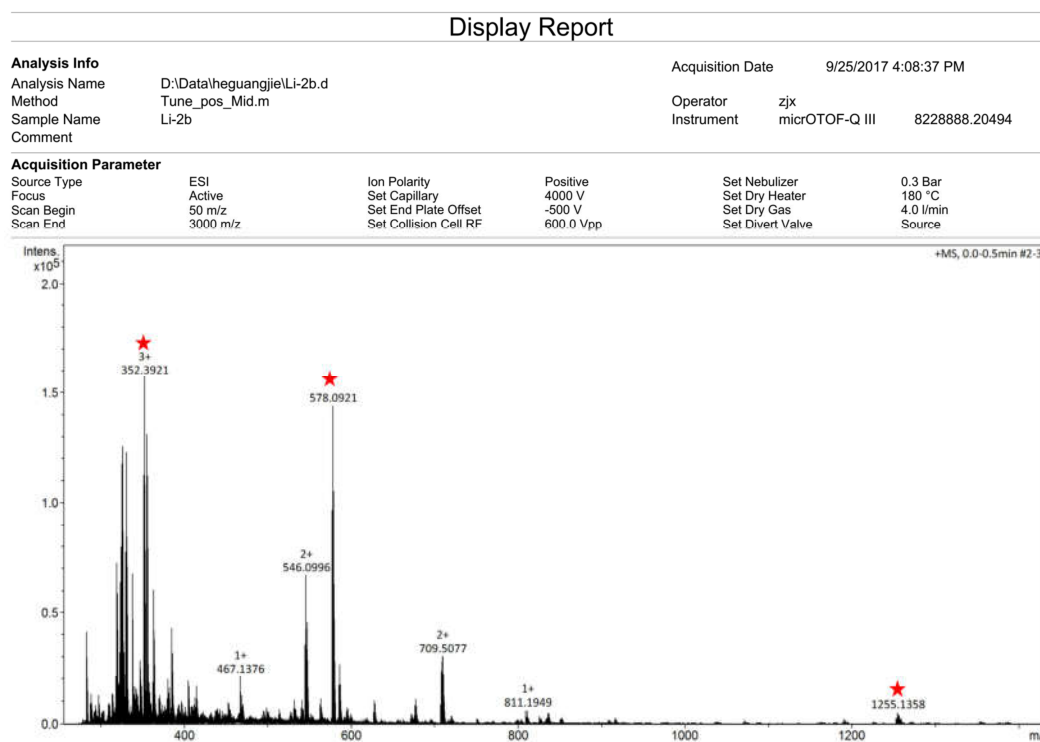


Figure S7. ESI-MS spectra of **DPAC** in the presence of Cu^{2+} in CH_3CN solution.

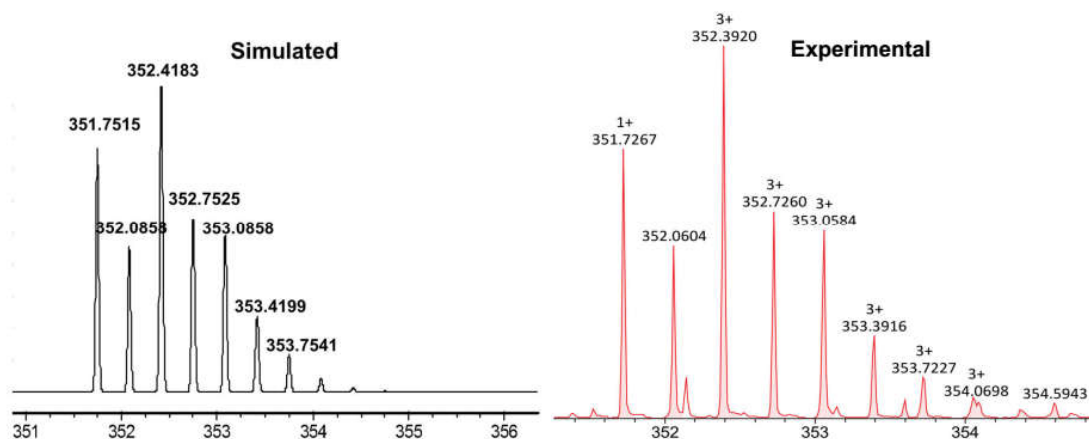


Figure S8. The simulated (left) and experimental (right) isotopic distributions of $[\text{Cu}_2(\text{DPAC})+\text{ClO}_4]^{3+}$ species.

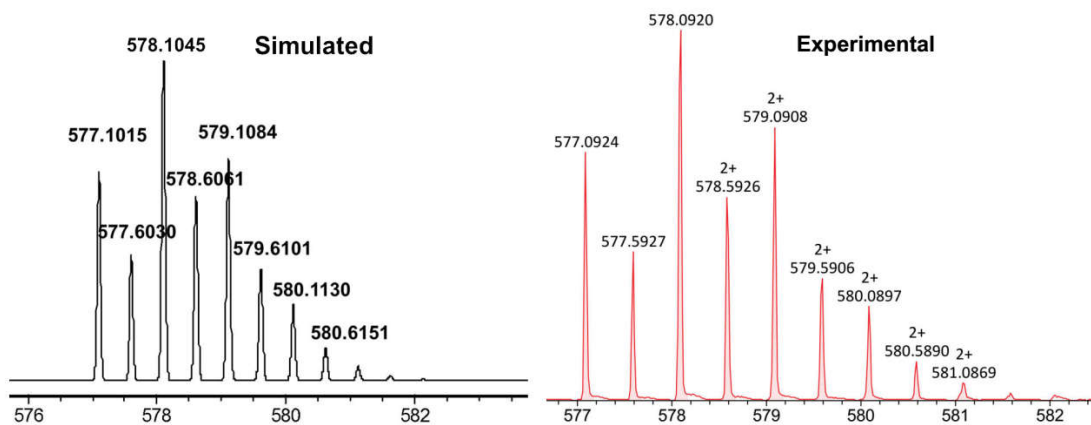


Figure S9. The simulated (left) and experimental (right) isotopic distributions of $[\text{Cu}_2(\text{DPAC})+2\text{ClO}_4]^{2+}$ species.

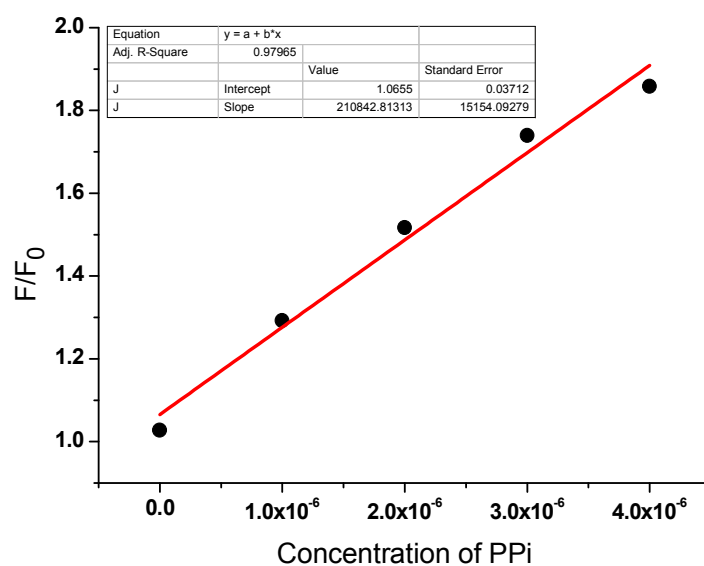


Figure S10. Fluorescence intensity of DPAC-Cu^{2+} ($10 \mu\text{M}$) in CH_3CN : HEPES (3:2, v/v, $\text{pH}=7.2$) solution upon additions of PPI in range of 1-4 μM .

Display Report

Analysis Info Analysis Name: D:\Data\heguangjie\Li-Cu-ppi.d Method: Tune_pos_Mid.m Sample Name: Li-Cu-ppi Comment:	Acquisition Date: 10/24/2017 4:20:54 PM Operator: zjx Instrument: micrOTOF-Q III 8228888.20494
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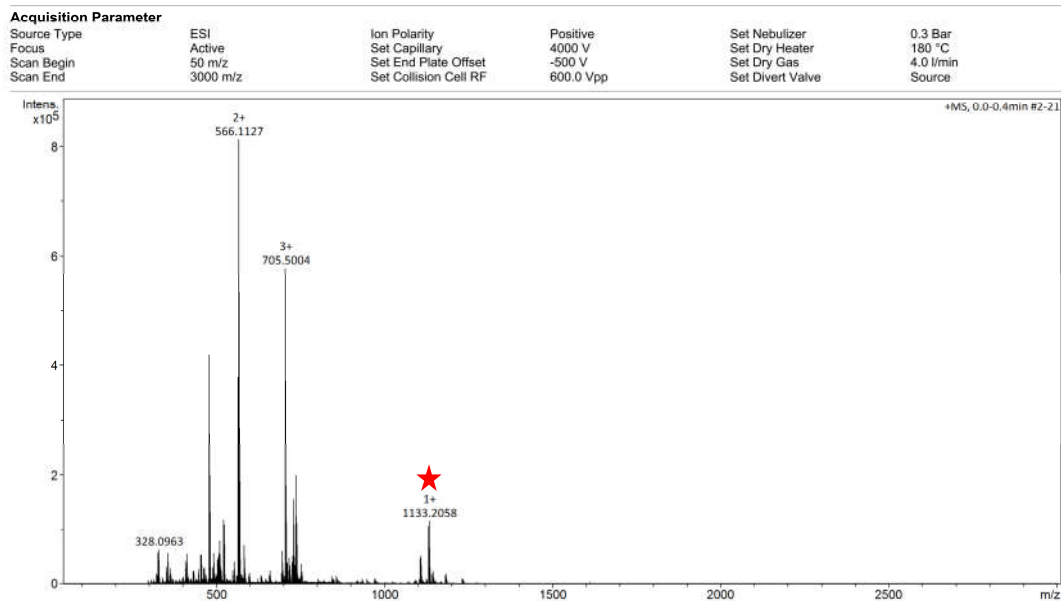


Figure S11. ESI-MS spectrum of **DPAC-Cu²⁺** with the addition of 1 equivalent of PPI.

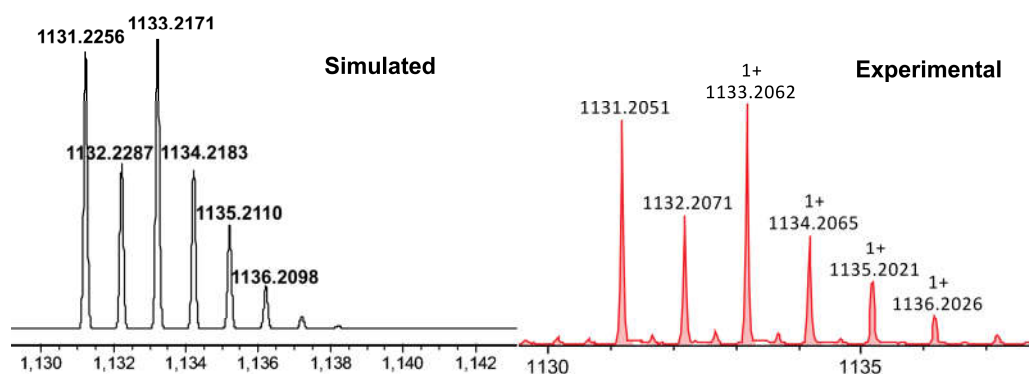


Figure S12. The simulated (left) and experimental (right) isotopic distributions of $[\text{Cu}_2(\text{DPAC})+\text{PPI}+\text{H}]^+$ species.

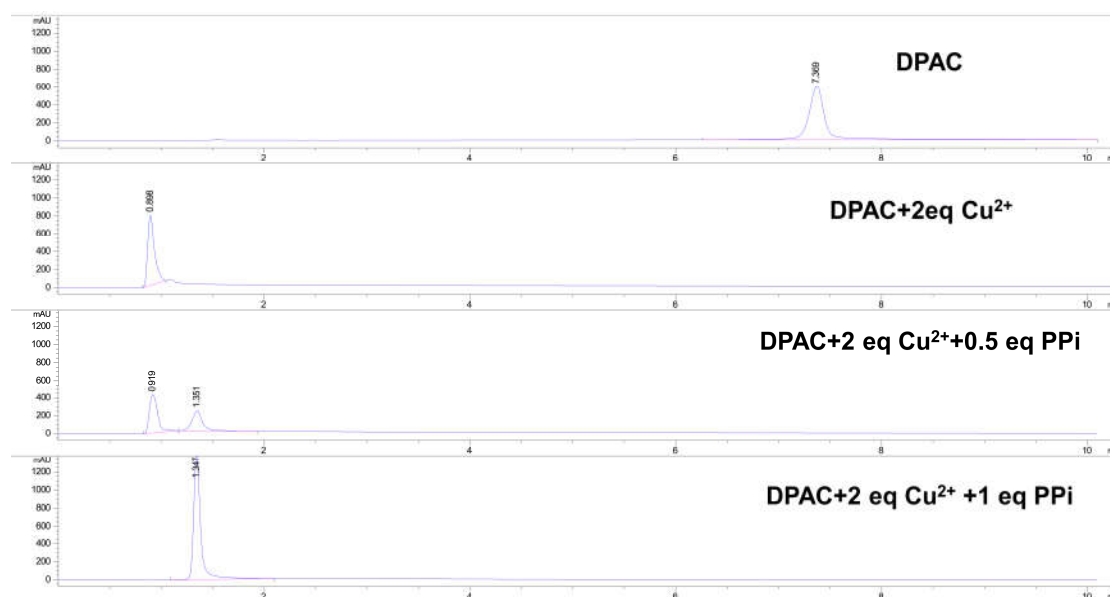


Figure S13. HPLC analyses of **DPAC**; **DPAC+2 equiv.Cu²⁺**; **DPAC+2 equiv.Cu²⁺+0.5 equiv. PPI**; **DPAC+2 equiv.Cu²⁺+1 equiv. PPI**. Liquid phase conditions: MeOH-water (8:2, v/v, mobile phase); 1.0 mL min⁻¹ (current velocity); ZORBAX SB-C18 (chromatographic column).

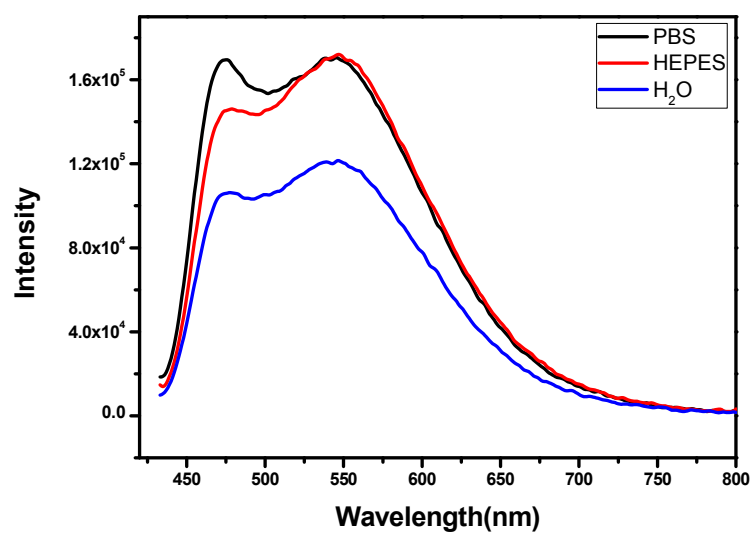


Figure S14. Fluorescence spectra of compound **DPAC** (10 μM) in different buffer solutions.