

## Supporting Information

### Synthesis and optical properties of aggregation-induced emission (AIE) molecules based on ESIPT mechanism as pH- and Zn<sup>2+</sup>-Responsive fluorescent sensors

Liqiang Yan,<sup>a</sup> Tingting Qing,<sup>a</sup> Renjie Li,<sup>a</sup> Zhongwei Wang and Zhengjian Qi <sup>\*ab</sup>

<sup>a</sup>College of Chemistry and Chemical engineering, Southeast University, Nanjing, Jiangsu, 210096, P. R. China..

<sup>b</sup>qizhengjian@seu.edu.cn; liqiangyan2014@163.com;

#### Contents

1. Fig.S1 Compound **1** <sup>1</sup>H-NMR (DMSO-d<sub>6</sub>, 300MHz).
2. Fig.S2 Compound **2** <sup>1</sup>H-NMR (DMSO-d<sub>6</sub>, 300MHz).
3. Fig.S3 Compound **3** <sup>1</sup>H-NMR (DMSO-d<sub>6</sub>, 300MHz).
4. Fig.S4 IR spectra of compound **1**.
5. Fig.S5 IR spectra of compound **2**.
6. Fig.S6 IR spectra of compound **3**.
7. Fig.S7 Positive ESI mass spectra of **1** in CH<sub>3</sub>CN.
8. Fig.S8 Positive ESI mass spectra of **2** in CH<sub>3</sub>CN.
9. Fig.S9 Positive ESI mass spectra of **3** in CH<sub>3</sub>CN.
10. Fig.S10 Positive ESI mass spectra of **3** in CH<sub>3</sub>CN after the addition of a drop of hydrochloric acid.
11. Fig.S11 Absorption spectra of **1-3** in pure EtOH and in EtOH/H<sub>2</sub>O mixtures (f<sub>w</sub>=90%).
12. Fig.S12 Fluorescent spectra of compound **1** (10.0 μM) in EtOH/H<sub>2</sub>O solution (fw=80%, pH=7.4) with 1 equiv. of Zn<sup>2+</sup>.
13. Fig.S13 Fluorescent spectra of compound **3** (10.0 μM) in EtOH/H<sub>2</sub>O solution (fw=80%, pH=7.4) with 1 equiv. of Zn<sup>2+</sup>.

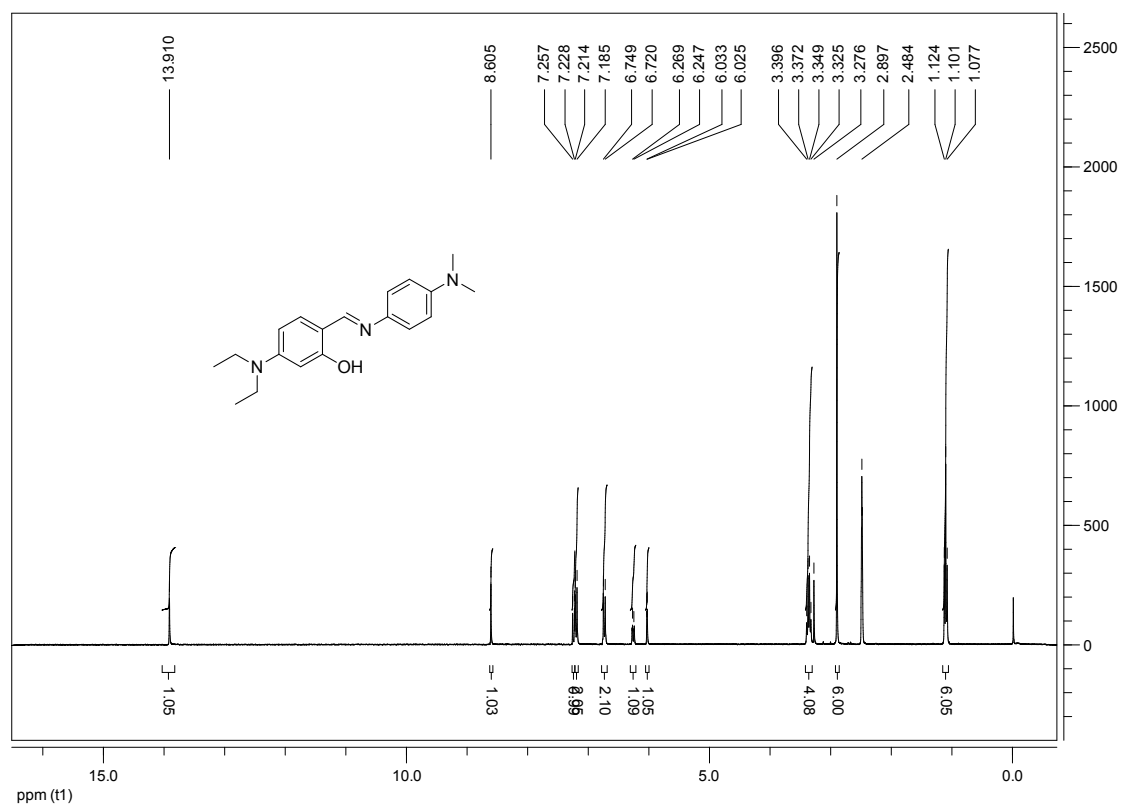


Fig.S1 Compound 1 <sup>1</sup>H-NMR (DMSO-d<sub>6</sub>, 300MHz).

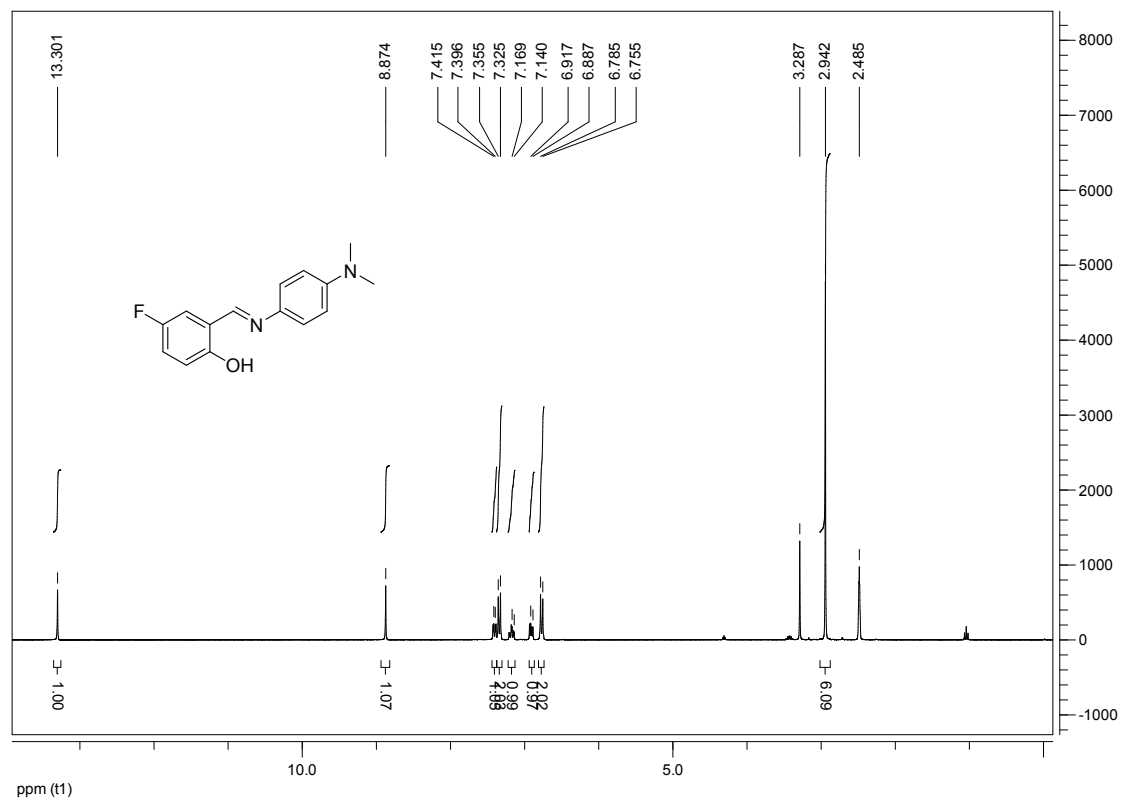


Fig.S2 Compound 2 <sup>1</sup>H-NMR (DMSO-d<sub>6</sub>, 300MHz).

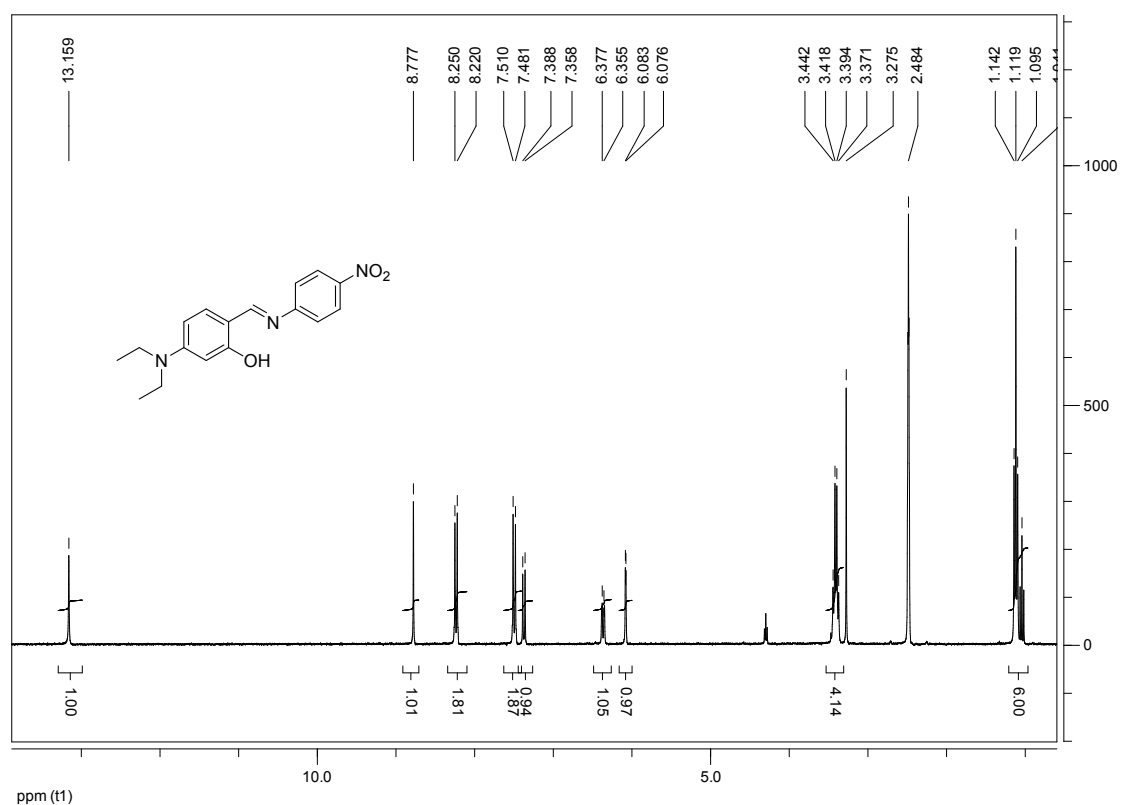


Fig.S3 Compound 3 <sup>1</sup>H-NMR (DMSO-d<sub>6</sub>, 300MHz).

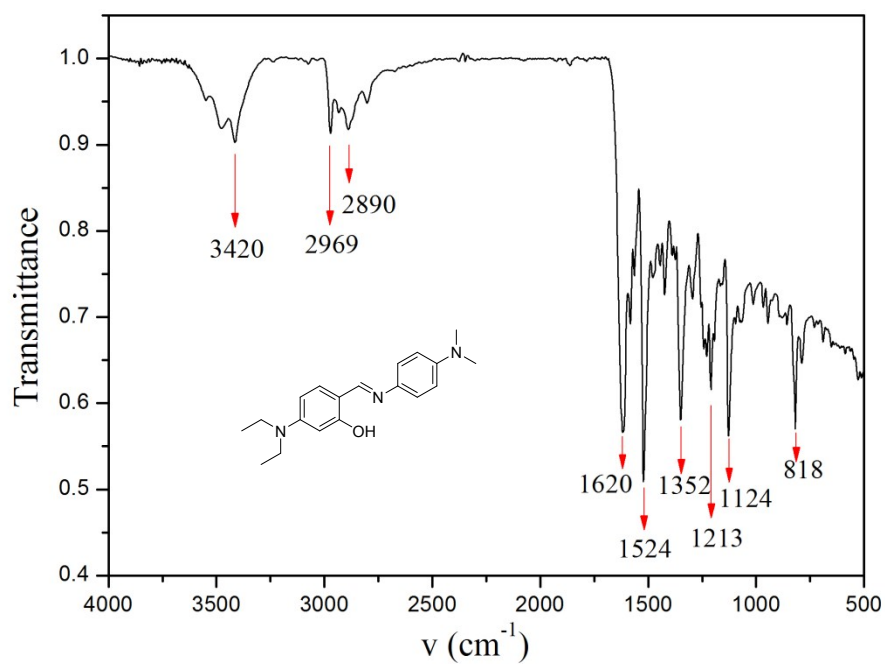


Fig.S4 IR spectra of compound 1.

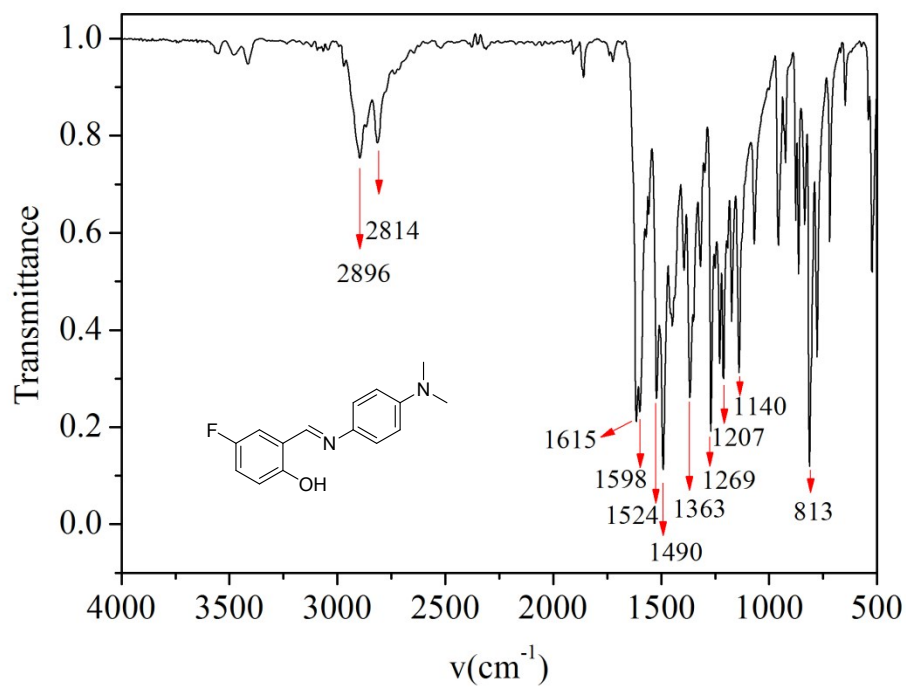


Fig.S5 IR spectra of compound 2.

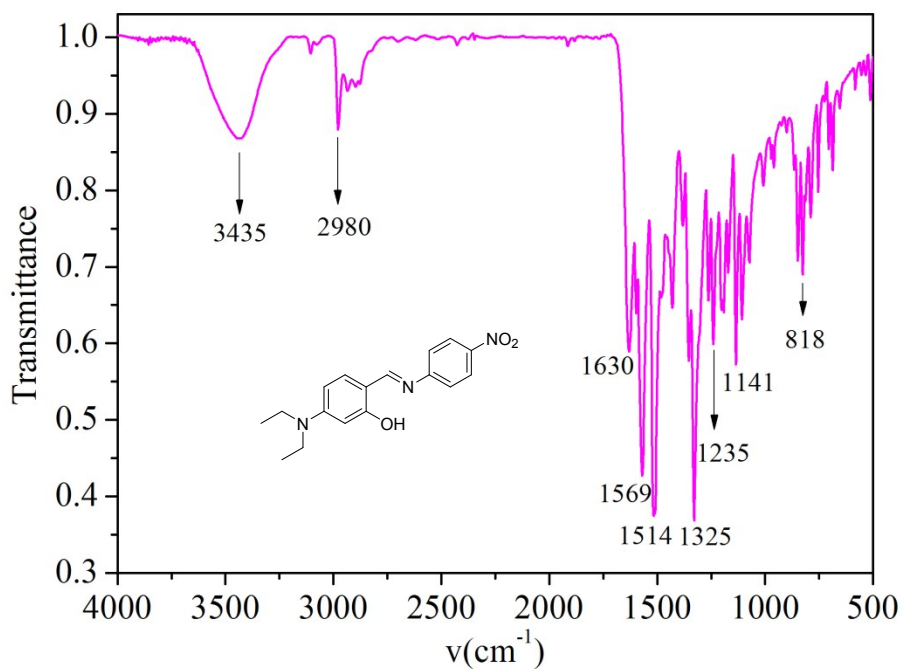


Fig.S6 IR spectra of compound 3.

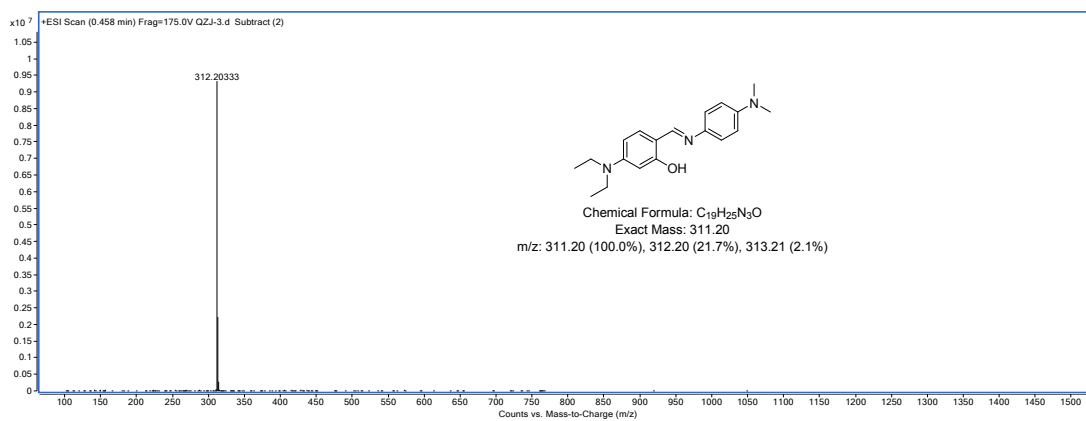


Fig.S7 Positive ESI mass spectra of **1** in CH<sub>3</sub>CN.

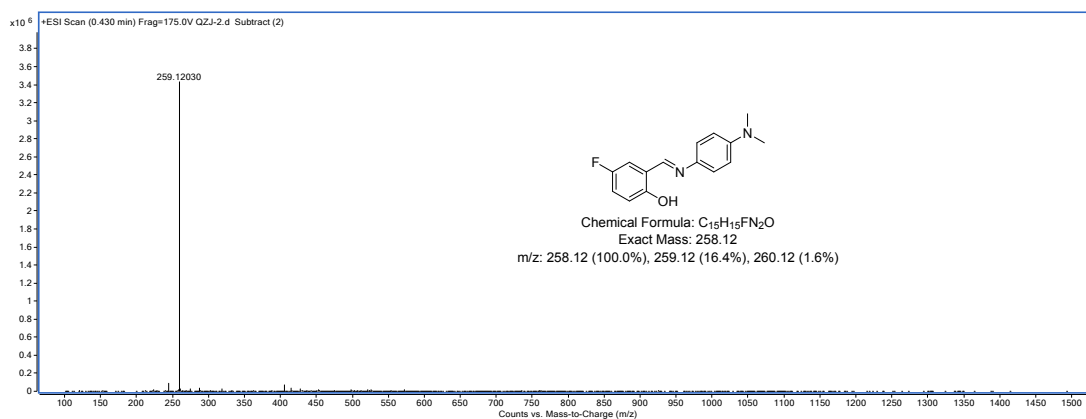


Fig.S8 Positive ESI mass spectra of **2** in CH<sub>3</sub>CN.

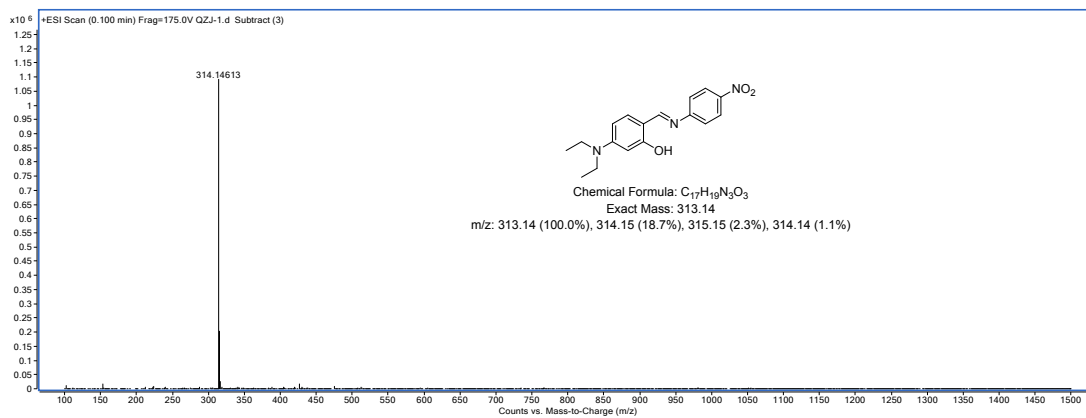


Fig.S9 Positive ESI mass spectra of **3** in CH<sub>3</sub>CN.

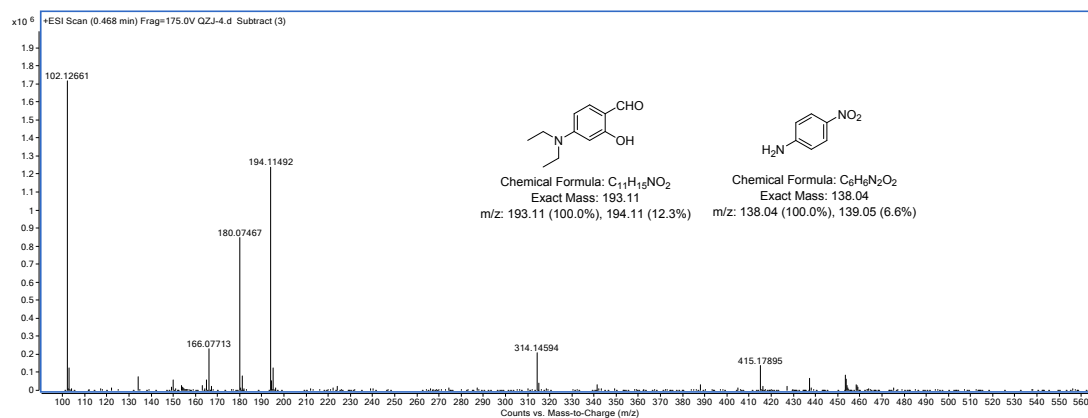


Fig.S10 Positive ESI mass spectra of **3** in  $CH_3CN$  after the addition of a drop of hydrochloric acid.

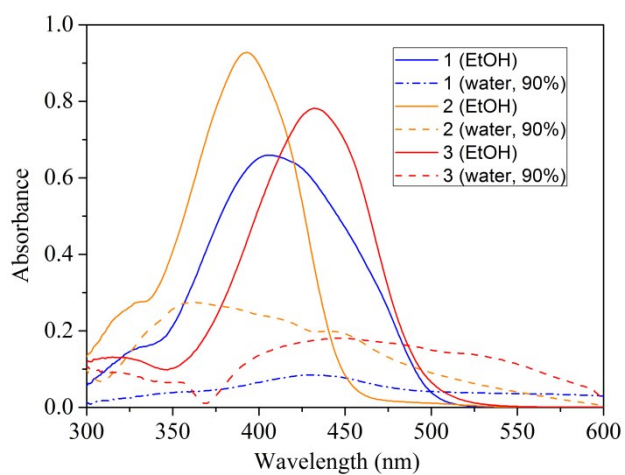


Fig.S11 Absorption spectra of **1-3** in pure EtOH (solid line) and in EtOH/ $H_2O$  mixtures ( $f_w=90\%$ ) (dash line). Condition: The concentration of **1-3** is  $1.0 \mu\text{mol/L}$ , respectively.

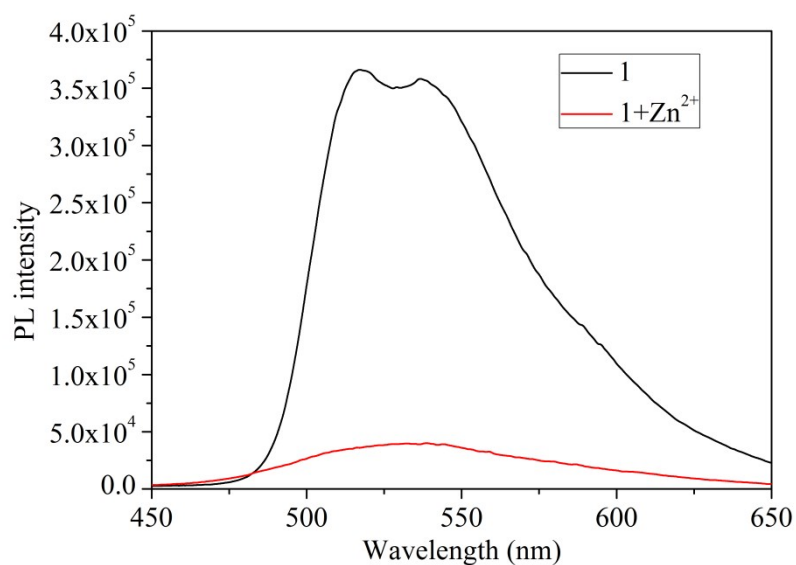


Fig.S12 Fluorescent spectra of compound **1** (10.0  $\mu\text{M}$ ) in EtOH/H<sub>2</sub>O solution (fw=80%, pH=7.4) with 1 equiv. of Zn<sup>2+</sup>.

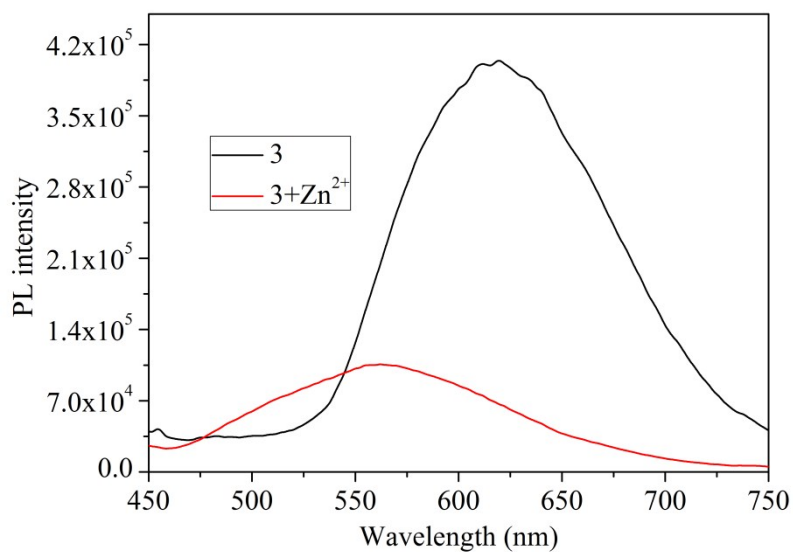


Fig.S13 Fluorescent spectra of compound **3** (10.0  $\mu\text{M}$ ) in EtOH/H<sub>2</sub>O solution (fw=80%, pH=7.4) with 1 equiv. of Zn<sup>2+</sup>.