

Supporting Information

A Turn-on Fluorescent Sensor for Selective Detection of Zn^{2+} , Cd^{2+} , and Hg^{2+} in Water

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Contents

1. The pH Responses of Receptor 1-----	S2
2. Job's Plot of Receptor 1 and Zn^{2+} -----	S2
3. Fluorescent Titrations of Receptor 1 with Zn^{2+} -----	S3
4. Job's Plot of Receptor 1 and Cd^{2+} -----	S3
5. Fluorescent Titrations of Receptor 1 with Cd^{2+} -----	S4
6. Job's Plot of Receptor 1 and Hg^{2+} -----	S4
7. Fluorescent Titrations of Receptor 1 with Hg^{2+} -----	S5
8. Absorption Titrations of Receptor 1 with Metal Ions -----	S6
9. ^1H NMR Titrations of Receptor 1 in the Presence of Zn^{2+} , Cd^{2+} -----	S7
10. ^1H NMR and ^{13}C NMR Spectra of Compounds 1 and 2-----	S8

1. The pH Responses of Receptor 1

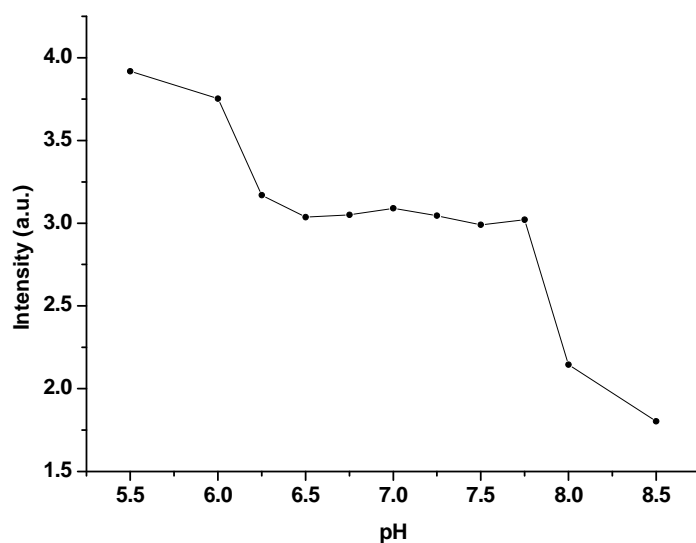


Figure S1. Effect of pH on the fluorescence intensity at 435 nm of receptor **1** (1.0×10^{-5} M) in buffer solution. The pH of solution was adjusted by aqueous solution of NaOH (1.0 M) and HCl (1.0 M). $\lambda_{\text{ex}} = 330$ nm, $\lambda_{\text{em}} = 435$ nm.

2. Job's Plot of Receptor 1 and Zn^{2+}

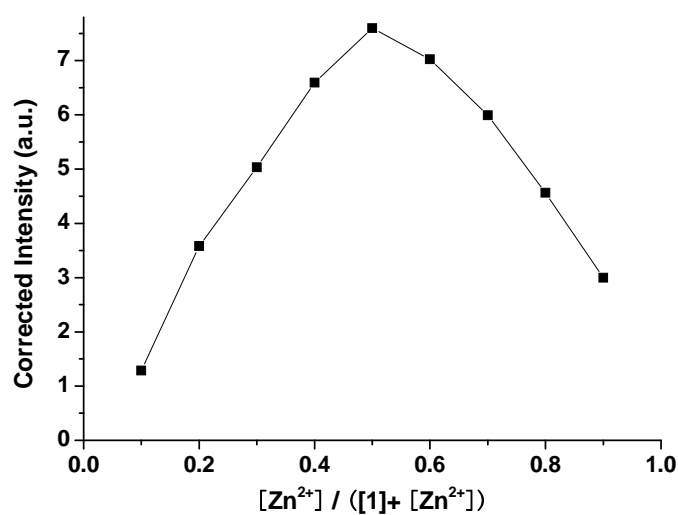


Figure S2. Job's plot of receptor **1** and Zn^{2+} . The total concentration of **1** and Zn^{2+} was kept at 10 μM in HEPES (10.0 mM, pH = 7.2). $\lambda_{\text{ex}} = 330$ nm, $\lambda_{\text{em}} = 435$ nm.

3. Fluorescent Titrations of Receptor 1 with Zn^{2+}

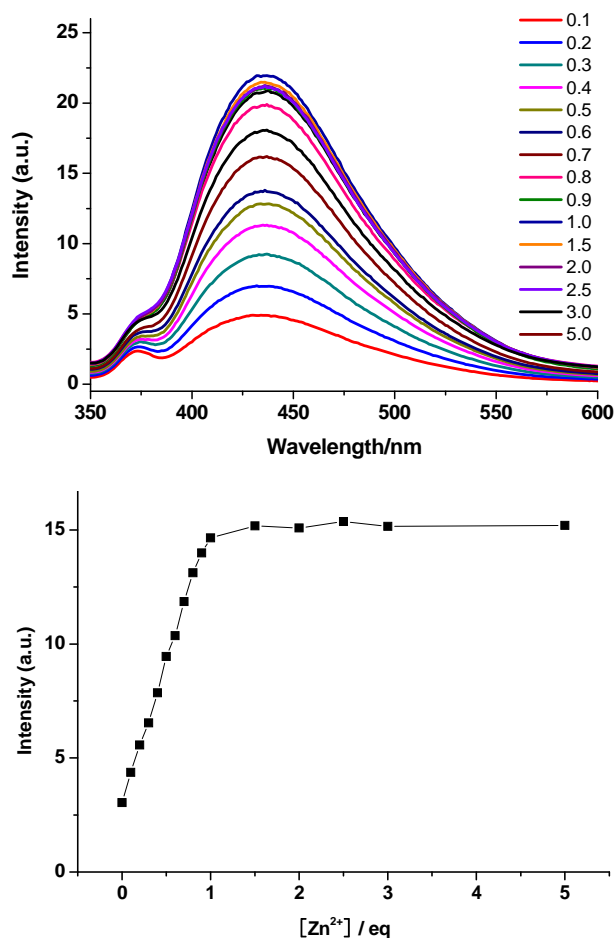


Figure S3. Up: emission spectra ($\lambda_{\text{ex}} = 330 \text{ nm}$) of **1** ($1.0 \times 10^{-5} \text{ M}$) in the presence of Zn^{2+} in HEPES (10.0 mM, pH = 7.2) at 25°C . Down: the fluorescence intensity of **1** at 435 nm vs. the number of equivalents of Zn^{2+} added.

4. Job's Plot of Receptor 1 and Cd^{2+}

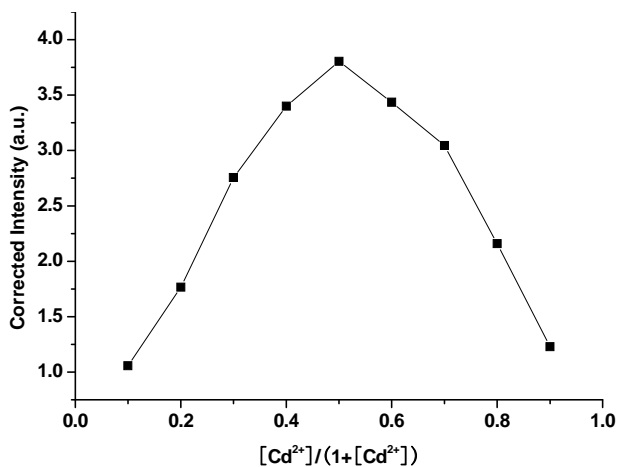


Figure S4. Job's plot of receptor **1** and Cd^{2+} . The total concentration of **1** and Cd^{2+} were kept at $10 \mu\text{M}$ in HEPES (10.0 mM, pH = 7.2). $\lambda_{\text{ex}} = 330 \text{ nm}$, $\lambda_{\text{em}} = 435 \text{ nm}$.

5. Fluorescent Titrations of Receptor 1 with Cd^{2+}

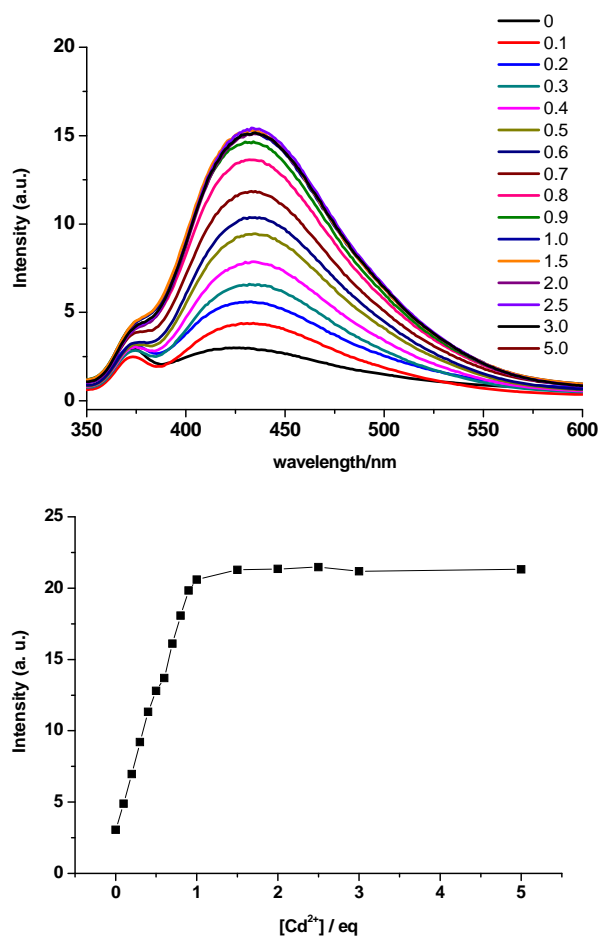


Figure S5. Up: emission spectra ($\lambda_{\text{ex}} = 330$ nm) of **1** (1.0×10^{-5} M) in the presence of Cd^{2+} in HEPES (10.0 mM, pH = 7.2) at 25°C. Down: the fluorescence intensity of **1** at 435 nm vs. the number of equivalents of Cd^{2+} added.

6. Job's Plot of Receptor 1 and Hg^{2+}

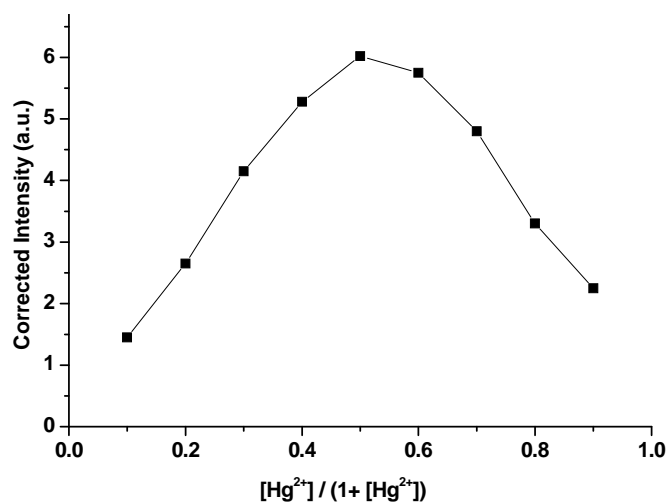


Figure S6. Job's plot of receptor **1** and Hg^{2+} . The total concentration of **1** and Hg^{2+} were kept at 10 μM in HEPES (10.0 mM, pH = 7.2). $\lambda_{\text{ex}} = 330$ nm, $\lambda_{\text{em}} = 435$ nm.

7. Fluorescent Titrations of Receptor 1 with Hg^{2+}

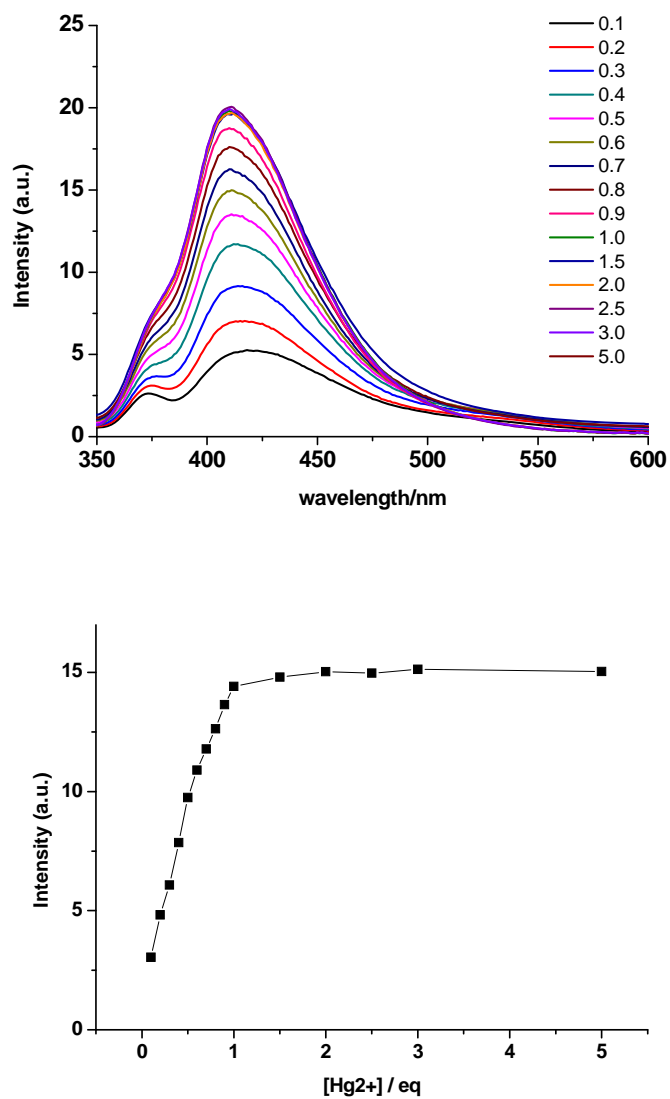


Figure S7. Up: emission spectra ($\lambda_{\text{ex}} = 330$ nm) of **1** (1.0×10^{-5} M) in the presence of Hg^{2+} in HEPES (10.0 mM, pH = 7.2) at 25°C. Down: the fluorescence intensity of **1** at 410 nm vs. the number of equivalents of Hg^{2+} added.

8. Absorption Titrations of Receptor 1 with Metal Ions

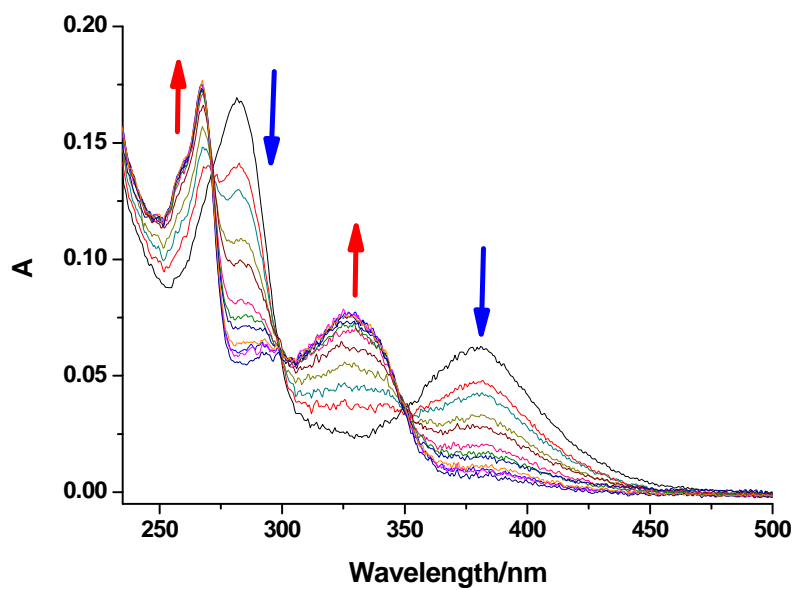


Figure S8. Absorption spectra of receptor **1** (1.0×10^{-5} M) in HEPES (10.0 mM, pH = 7.2) to various concentrations of Zn^{2+} .

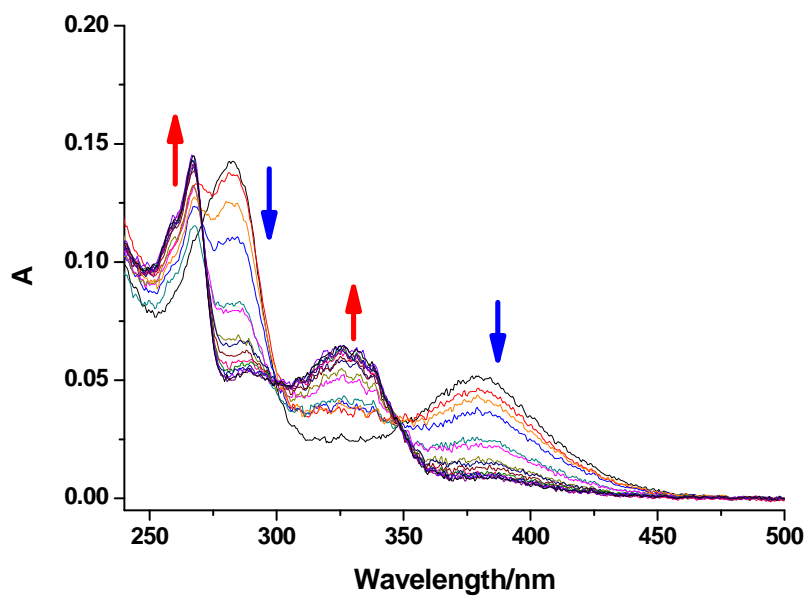


Figure S9. Absorption spectra of receptor **1** (1.0×10^{-5} M) in HEPES (10 mM, pH = 7.2) to various concentrations of Cd^{2+} .

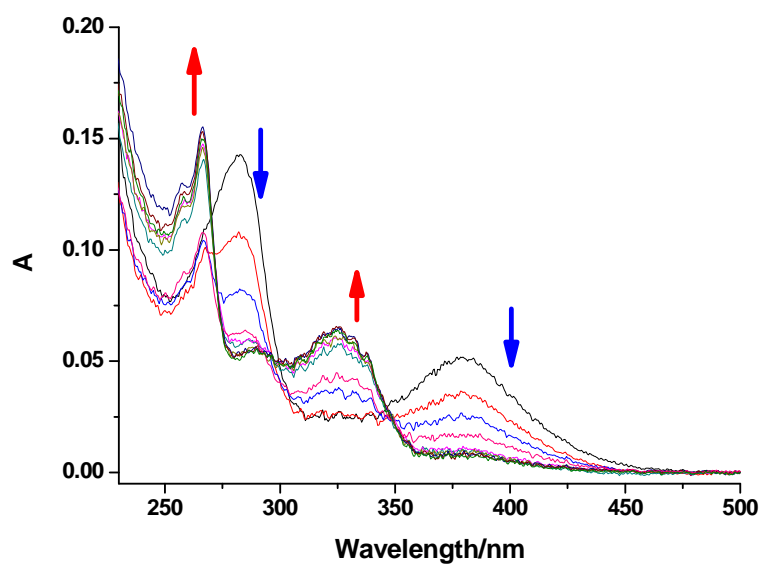


Figure S10. Absorption spectra of receptor **1** (1.0×10^{-5} M) in HEPES (10 mM, pH = 7.2) to various concentrations of Hg^{2+} .

9. ^1H NMR Titration of Receptor **1** in the Presence of Metal Ions

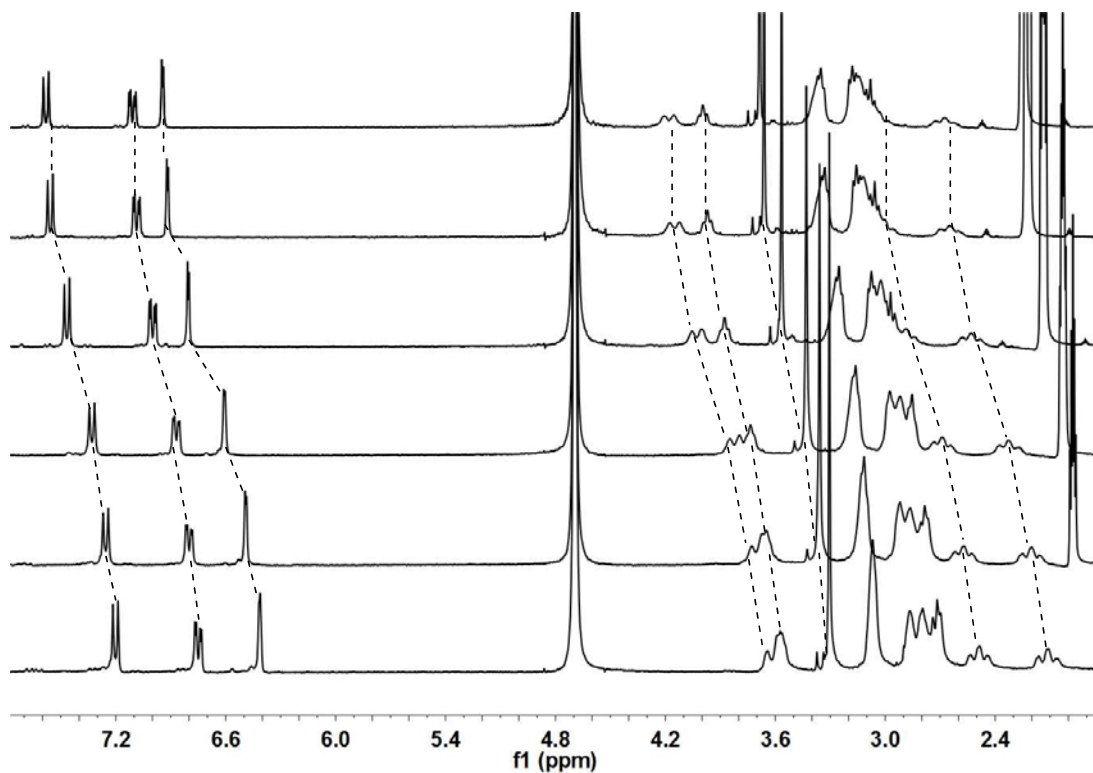


Figure S11. Partial ^1H NMR spectra of **1** in the presence of Cd^{2+} (from down to up: 0, 0.25, 0.5, 0.75, 1.0, and 2.0 equiv.) in D_2O .

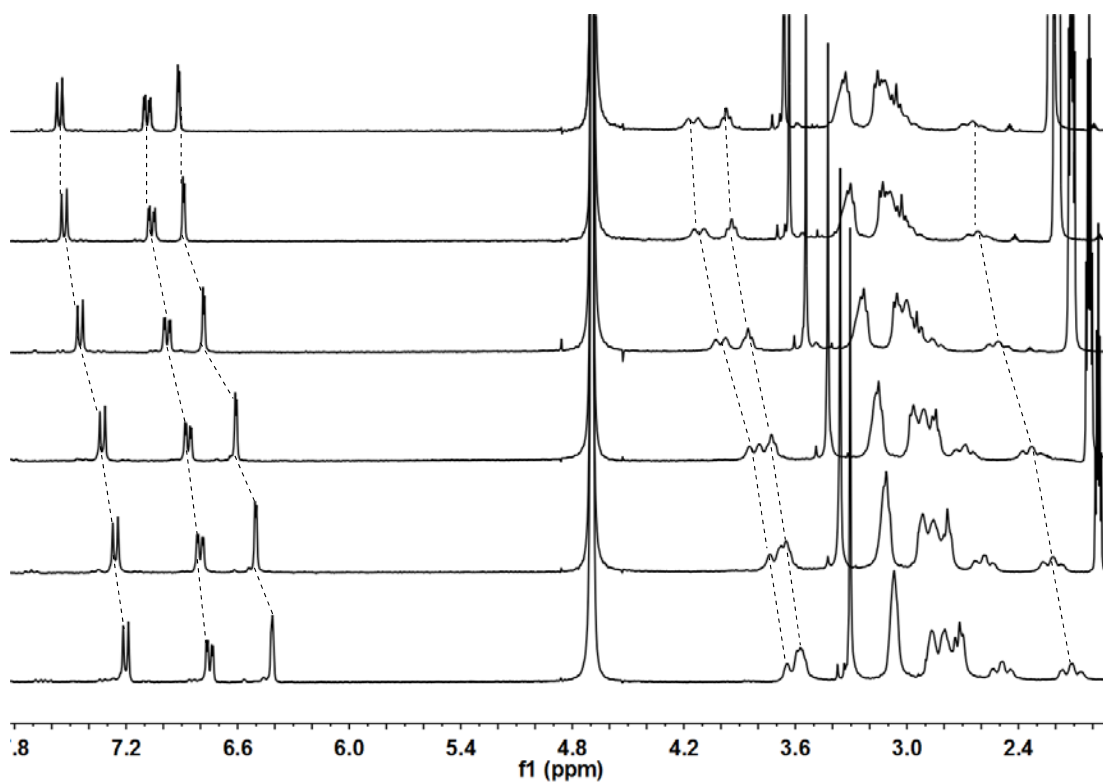


Figure S12. Partial ^1H NMR spectra of **1** in the presence of Zn^{2+} (from down to up: 0, 0.25, 0.5, 0.75, 1.0, and 2.0 equiv.) in D_2O .

10. Copies of ^1H NMR and ^{13}C NMR Spectra of New Compounds

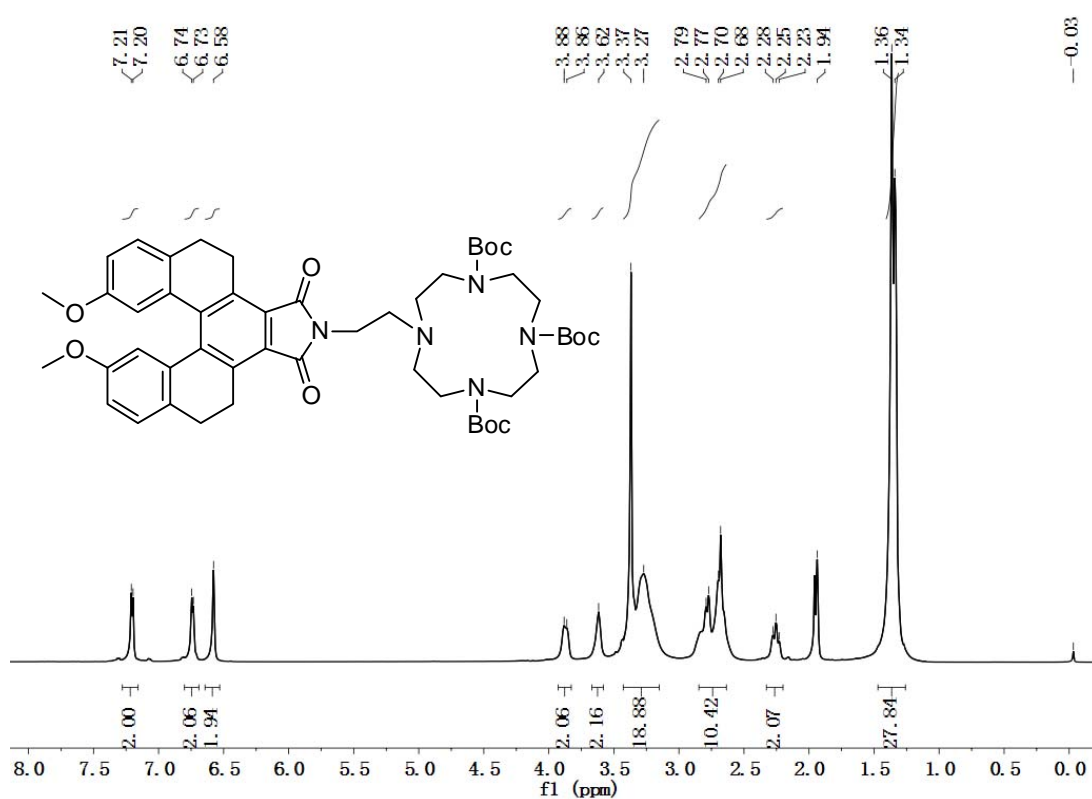


Figure S13. ^1H NMR spectrum (CD_3CN , 300 MHz) of **2**.

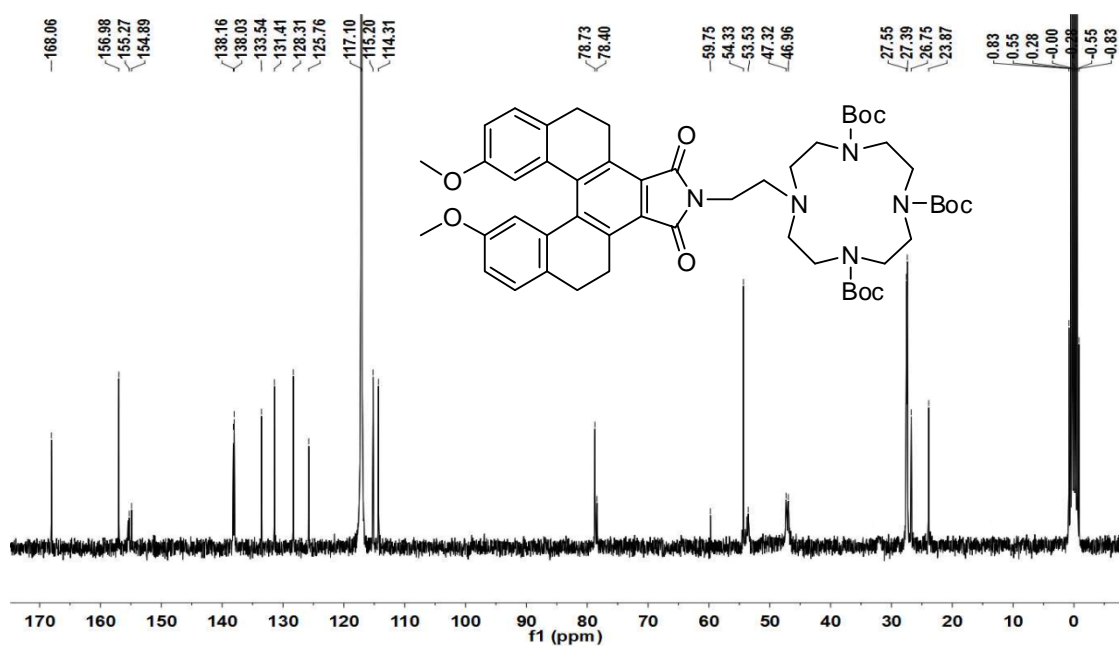


Figure S14. ¹³C NMR spectrum (CD₃CN, 75 MHz) of **2**.

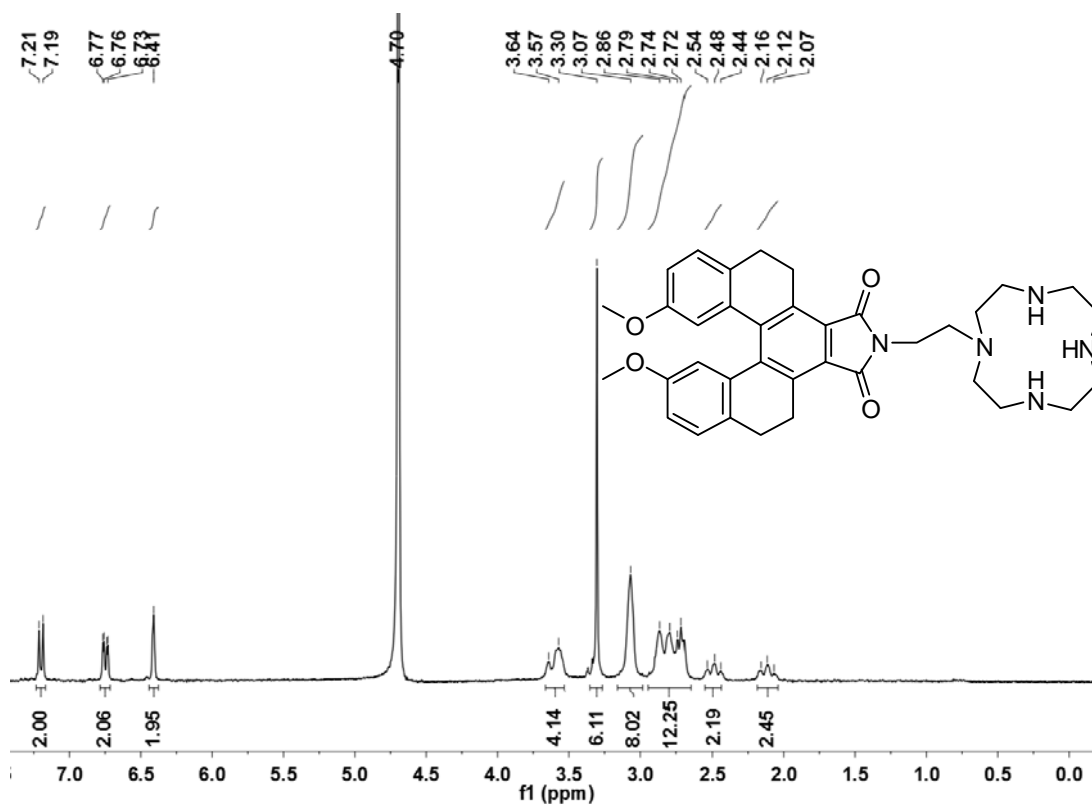


Figure S15. ¹H NMR spectrum (D₂O, 300 MHz) of **1**.

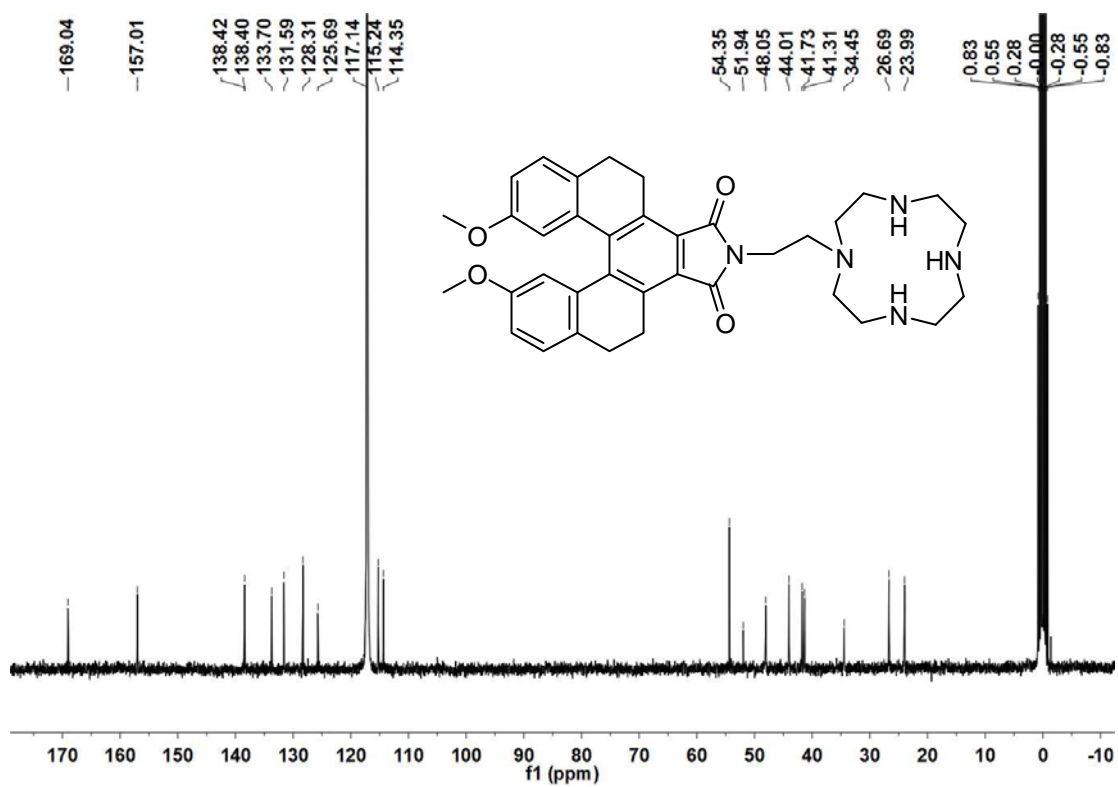


Figure S16. ^{13}C NMR spectrum (CD_3CN , 75 MHz) of **1**.