

Supplementary Material

Construction of a Luminescent Cadmium-Based Metal–Organic Framework for Highly Selective Discrimination of Ferric Ions

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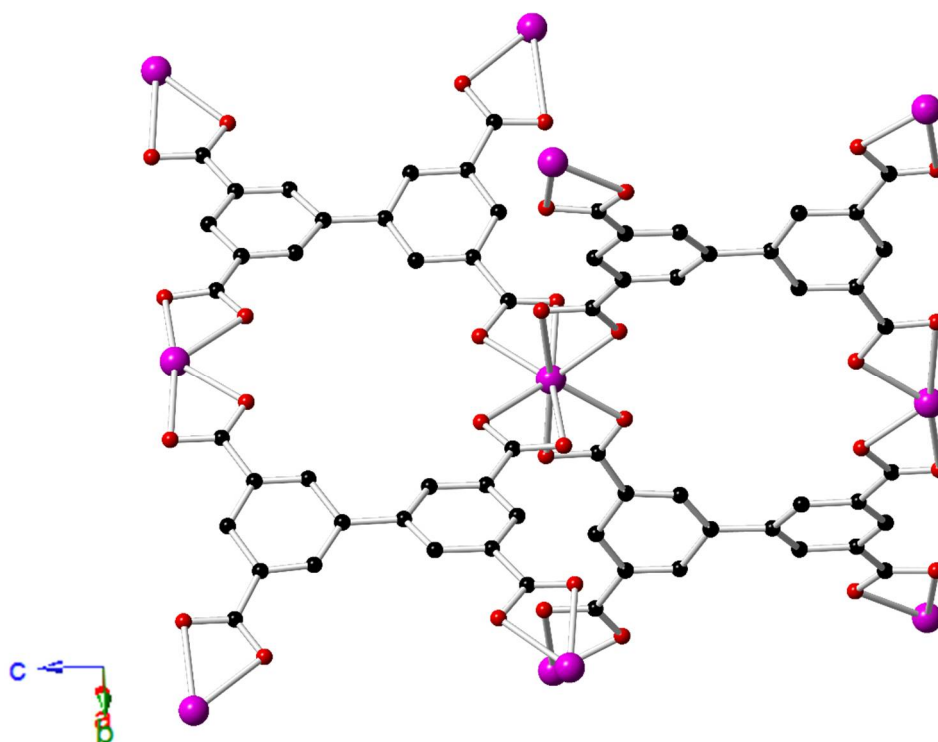


Figure S1. Ball-and-stick view of the coordination environments of Cd^{2+} and BPTC^{4-} in CdBPTC .

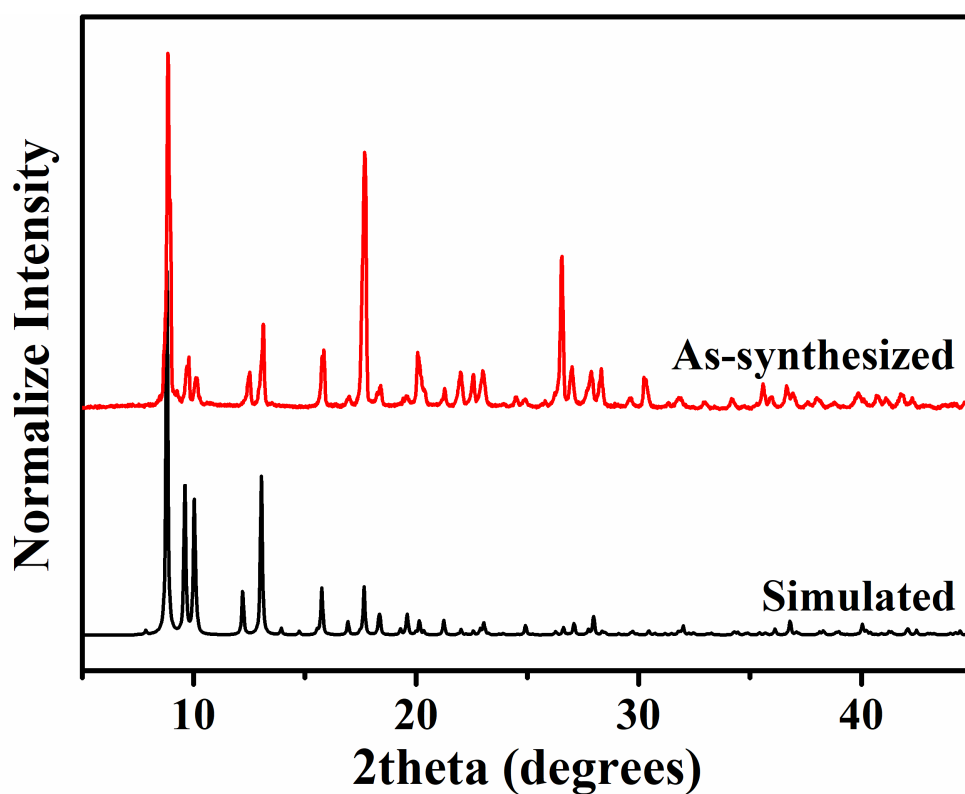
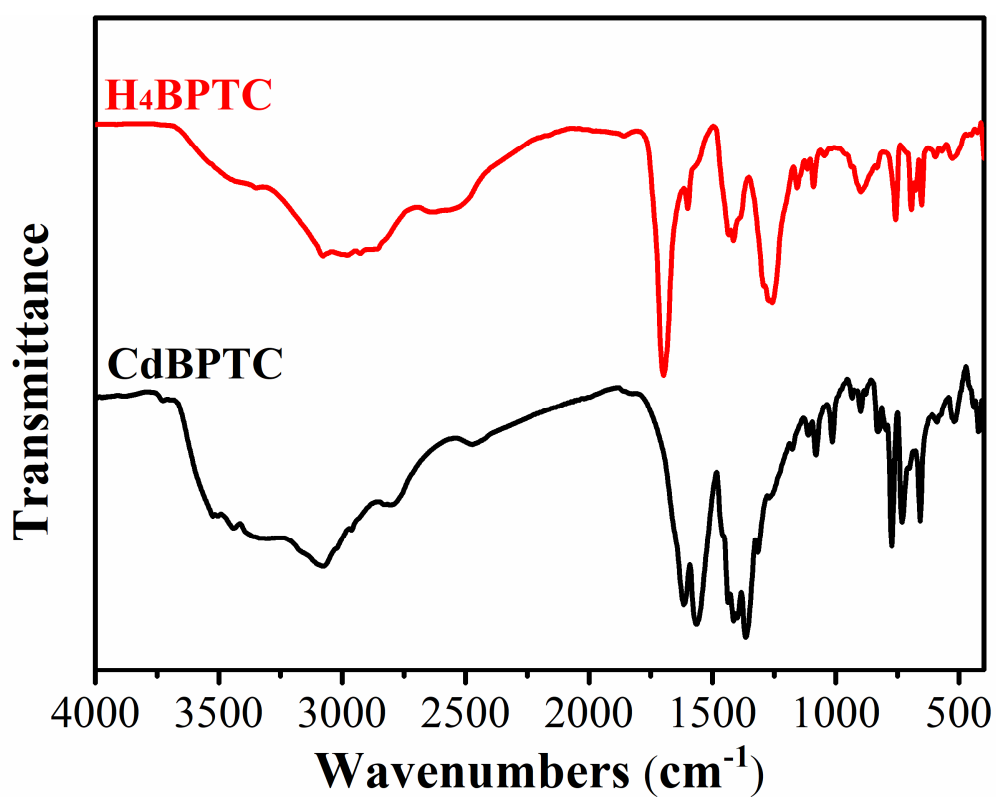


Figure S2. PXRD patterns of CdBPTC.

Figure S3. IR spectra of CdBPTC and H₄BPTC ligand.

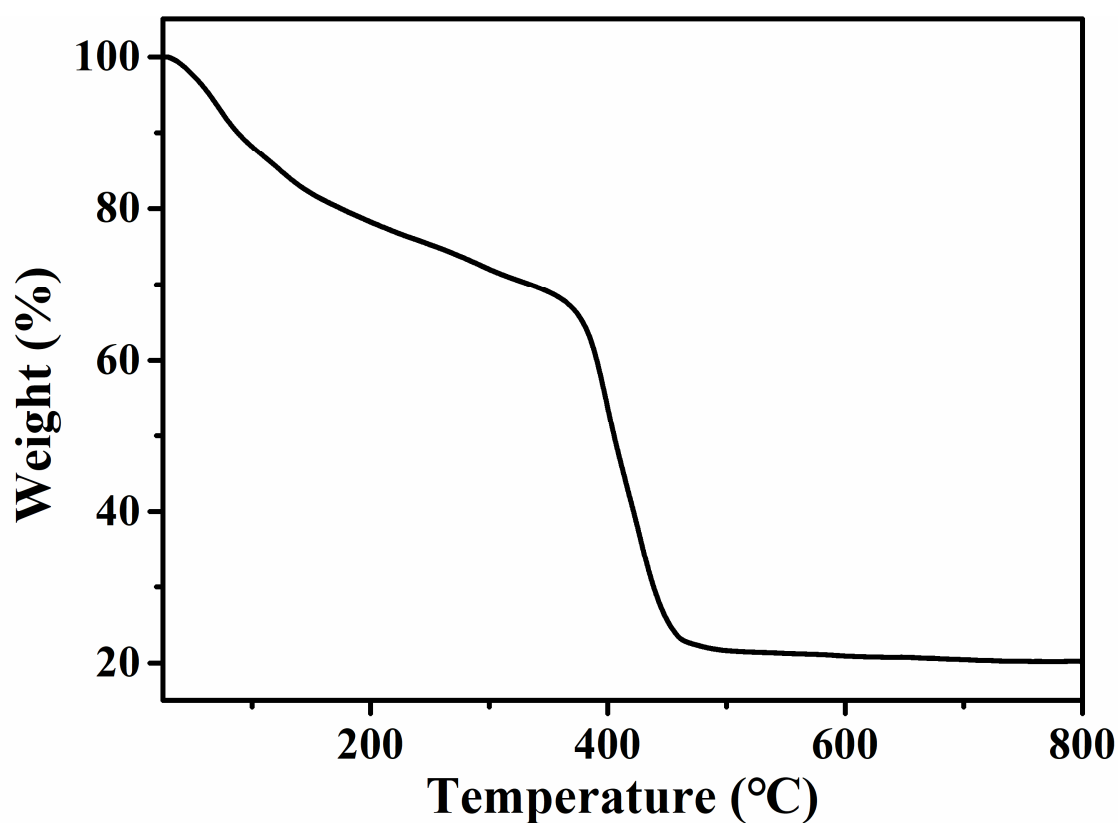


Figure S4. TGA curve of CdBPTC.

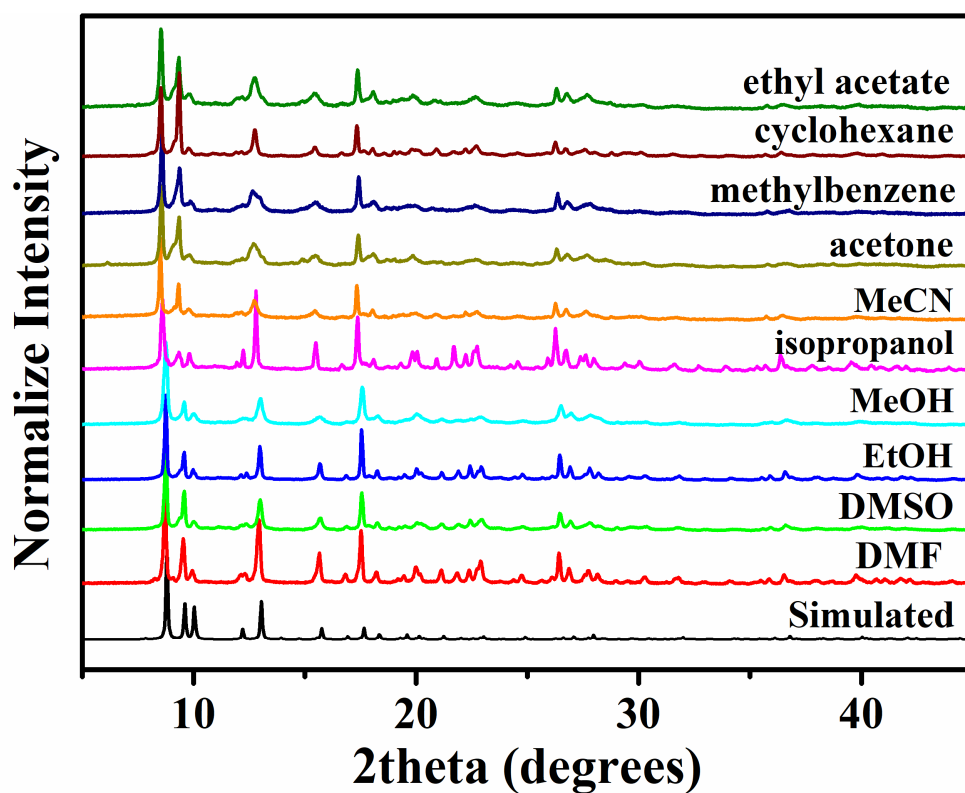


Figure S5. PXRD patterns of CdBPTC soaked in different organic solvents.

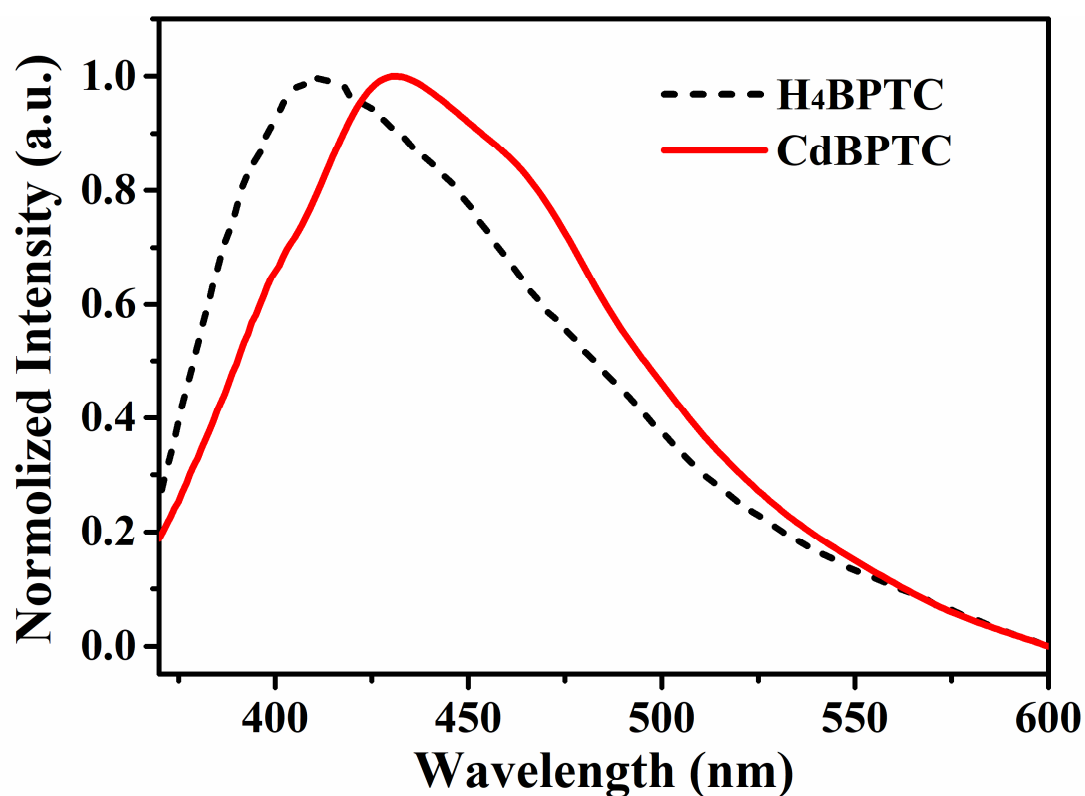


Figure S6. The emission spectra of CdBPTC and H₄BPTC ligand in solid state at room temperature.

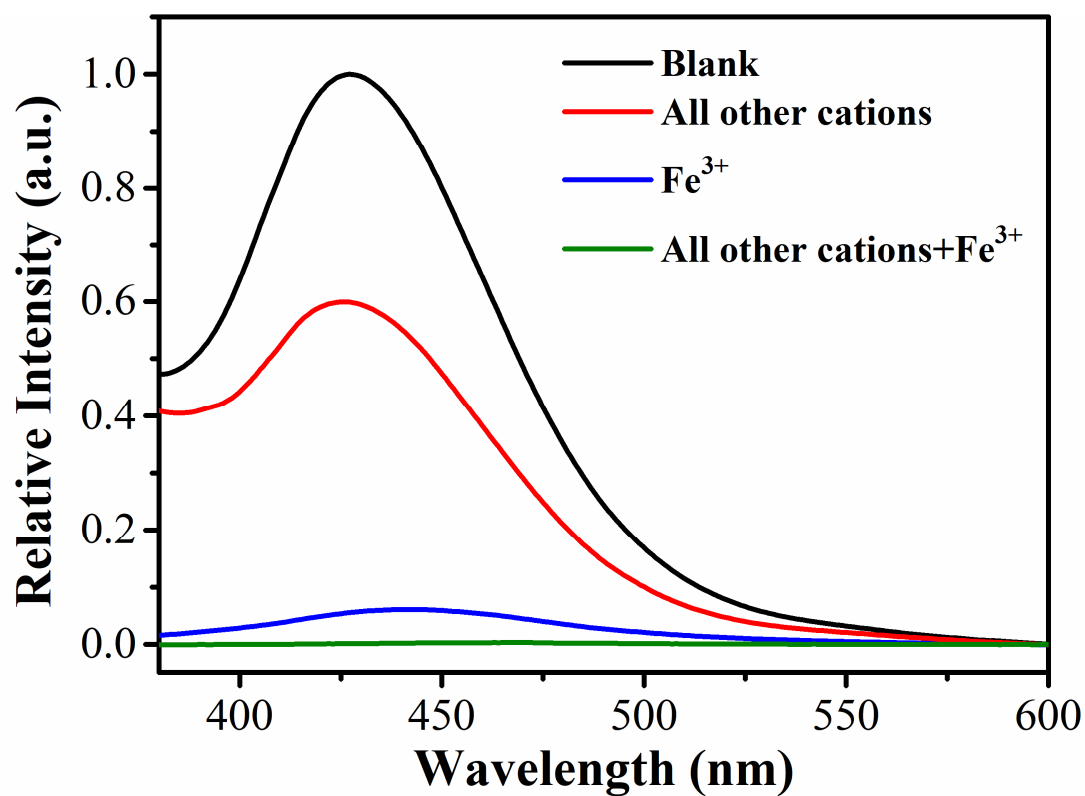


Figure S7. Photoluminescence spectra of CdBPTC in DMF and aqueous solution containing different metal ions ($1.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$) when excited at 337 nm.

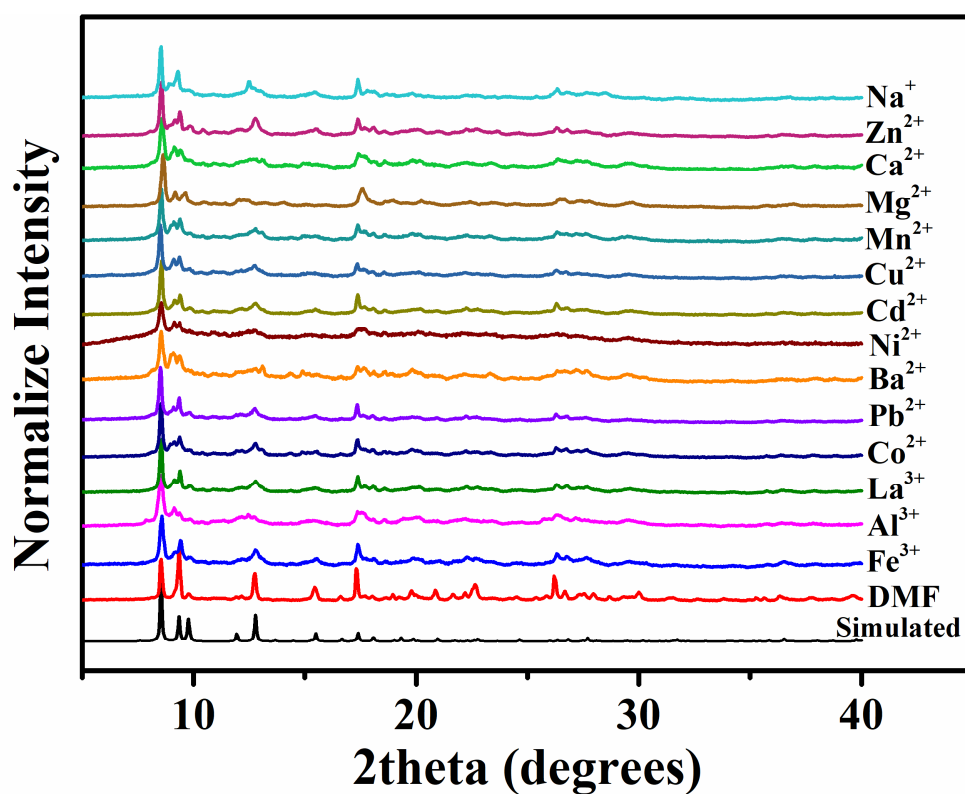


Figure S8. PXRD patterns of CdBPTC after being dispersed in DMF and different metal ions solutions for 72 hours.



Figure S9. Images of CdBPTC powder soaked in DMF solutions of different metal salts ($1.0 \times 10^{-2} \text{ mol} \cdot \text{L}^{-1}$) for 0 hours (a) and 72 hours (b).

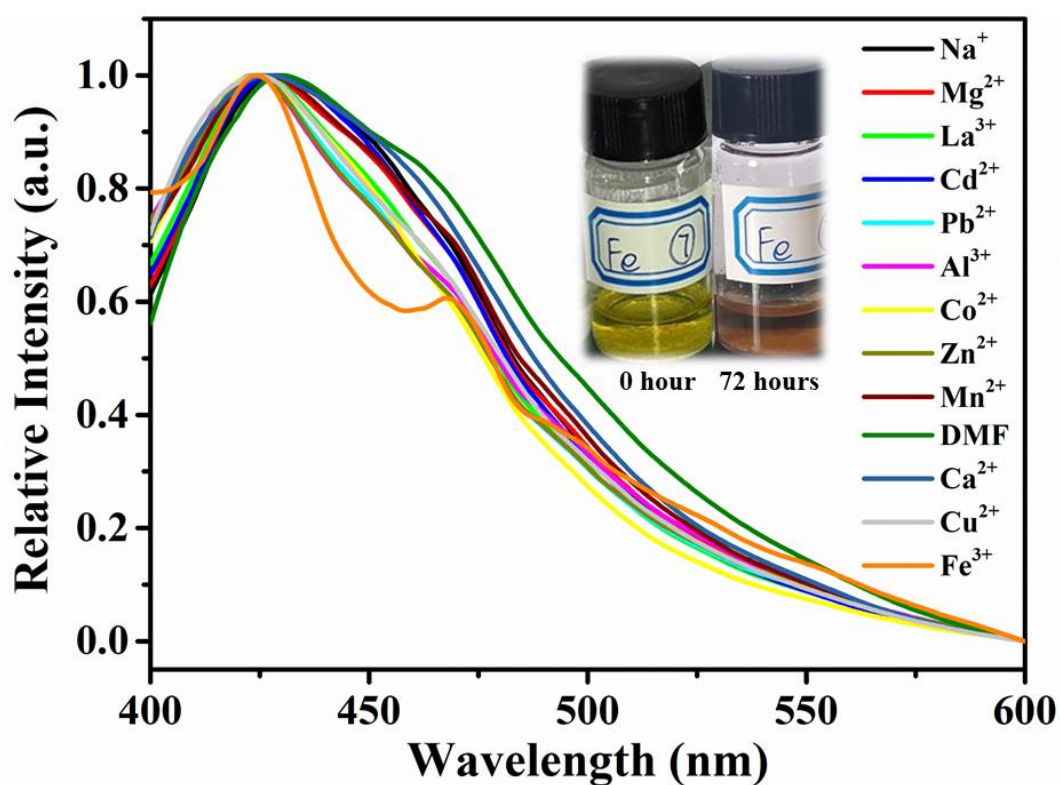


Figure S10. Solid emission spectra of CdBPTC after being soaked in pure DMF, DMF solution of Fe^{3+} ion, and other cations ($1.0 \times 10^{-2} \text{ mol}\cdot\text{L}^{-1}$) for 72 hours. The inset shows the darker color of the CdBPTC sample after immersion in the solution of ferric ions.

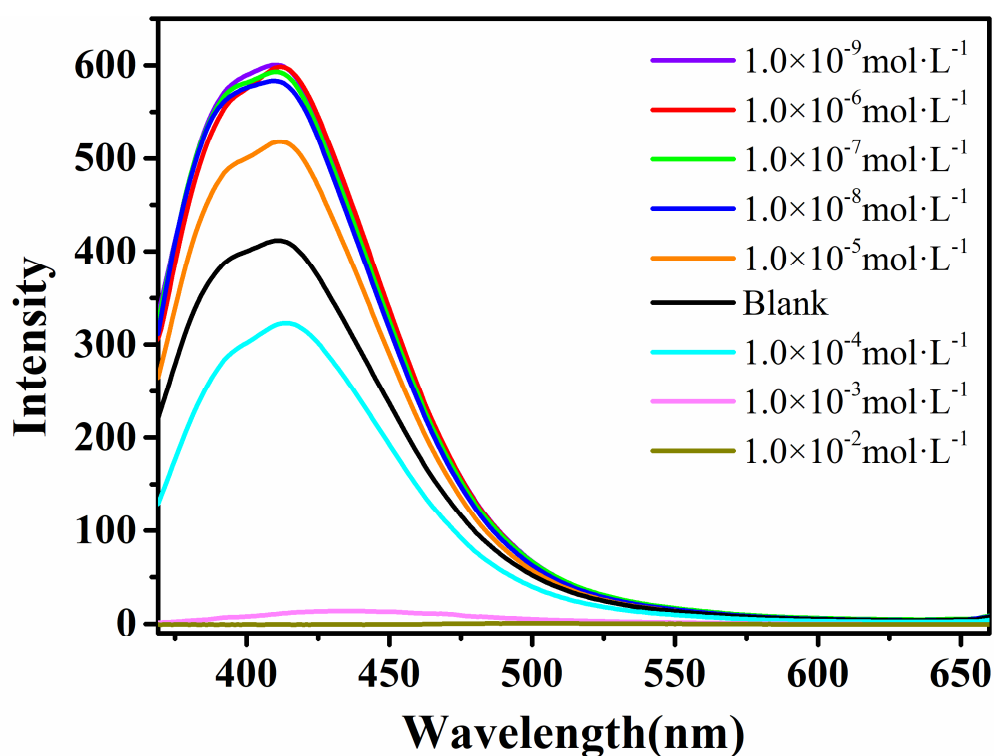


Figure S11. Liquid luminescence spectra of CdBPTC presenting turn on and turn off fluorescence signals with different concentrations of Fe^{3+} DMF solution at room temperature, $\lambda_{\text{ex}} = 337 \text{ nm}$.

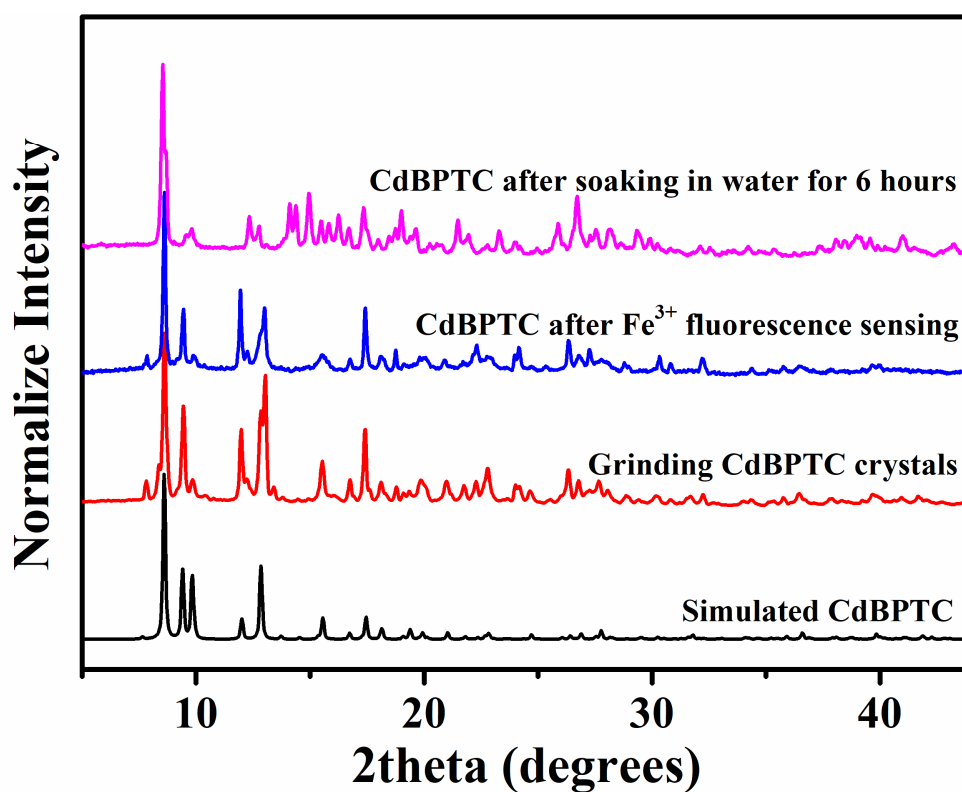


Figure S12. PXRD patterns of CdBPTC after grinding, sensing, or soaking in water.

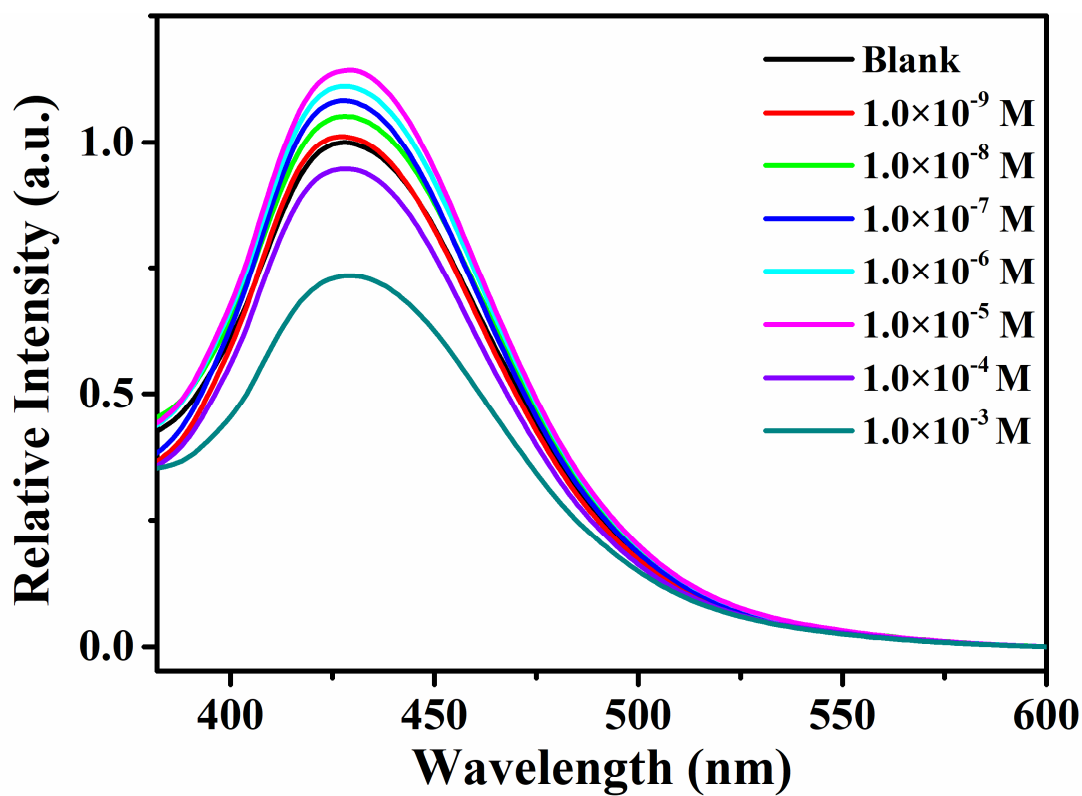


Figure S13. Liquid luminescence spectra of CdBPTC/DMF suspensions with different concentrations of Cr³⁺ at room temperature, $\lambda_{\text{ex}} = 337$ nm.

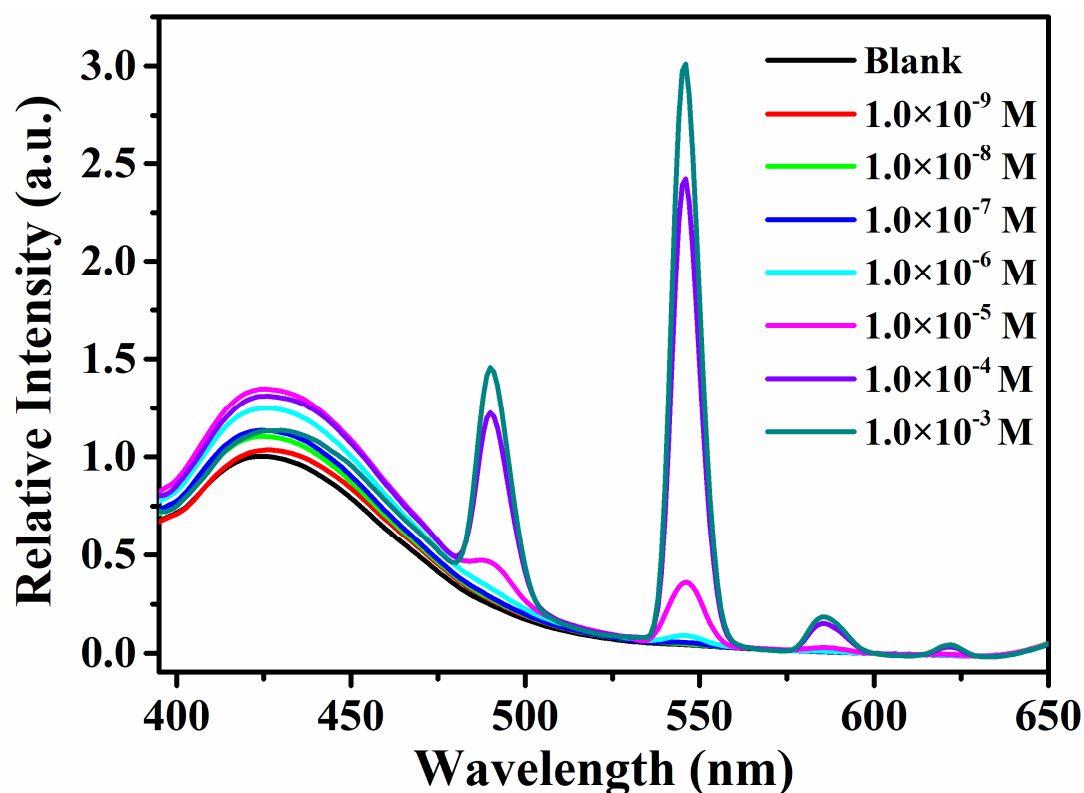


Figure S14. Liquid luminescence spectra of CdBPTC/DMF suspensions with different concentrations of Tb³⁺ at room temperature, $\lambda_{\text{ex}} = 337$ nm.

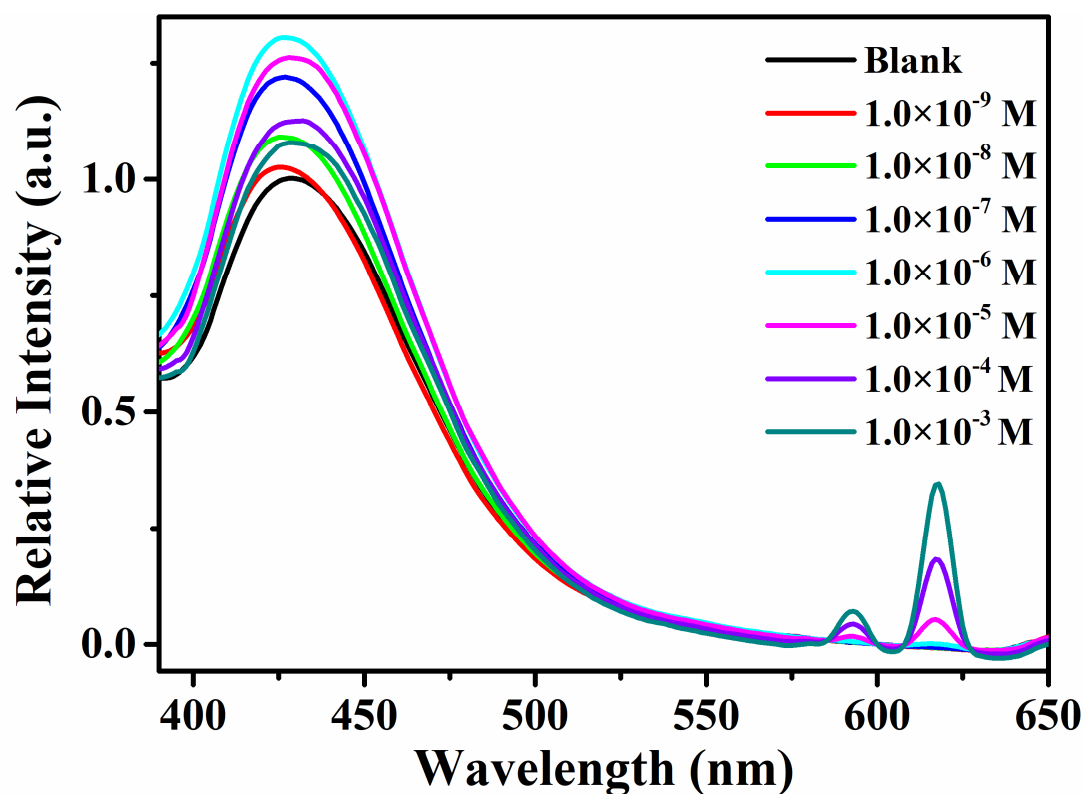


Figure S15. Liquid luminescence spectra of CdBPTC/DMF suspensions with different concentrations of Eu³⁺ at room temperature, $\lambda_{\text{ex}} = 337$ nm.

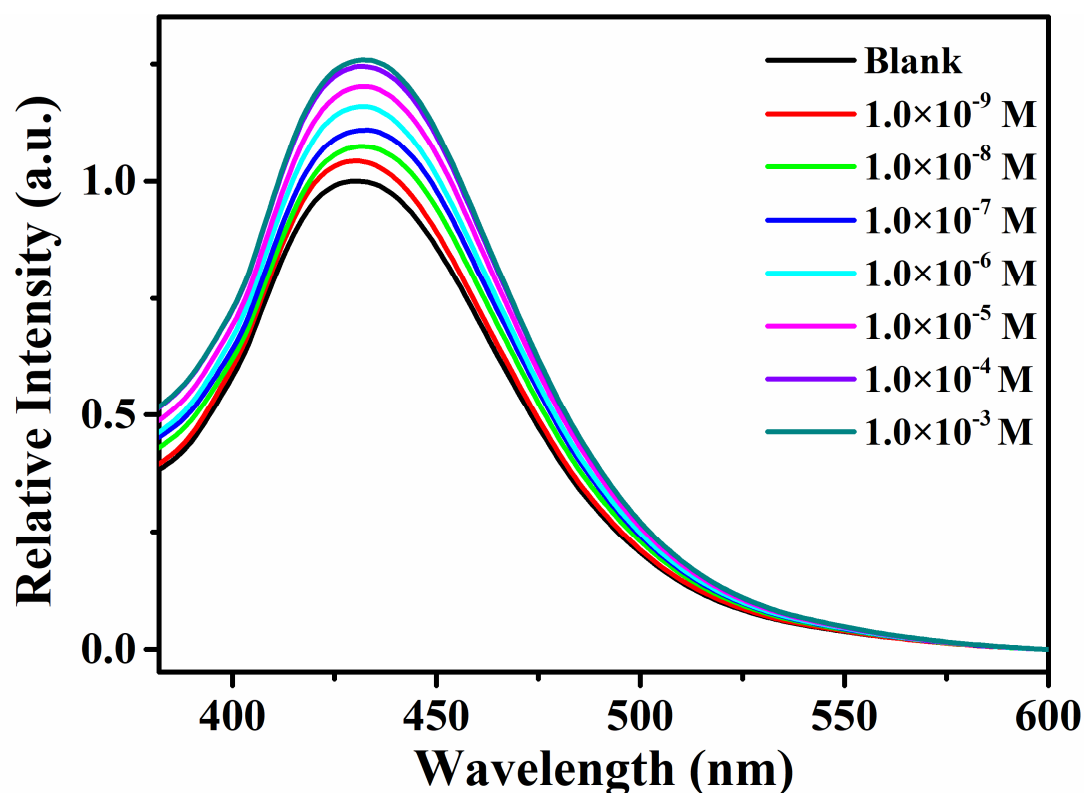


Figure S16. Liquid luminescence spectra of CdBPTC/DMF suspensions with different concentrations of La^{3+} at room temperature, $\lambda_{\text{ex}} = 337$ nm.

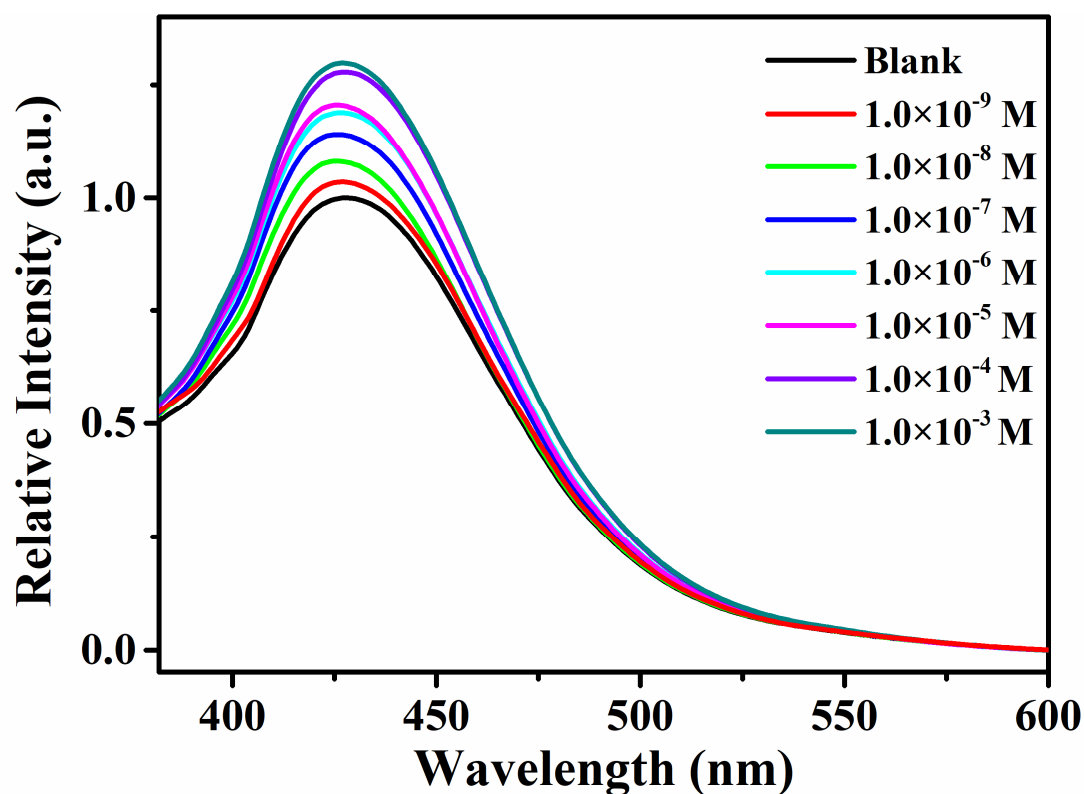


Figure S17. Liquid luminescence spectra of CdBPTC/DMF suspensions with different concentrations of Mn^{2+} at room temperature, $\lambda_{\text{ex}} = 337$ nm.

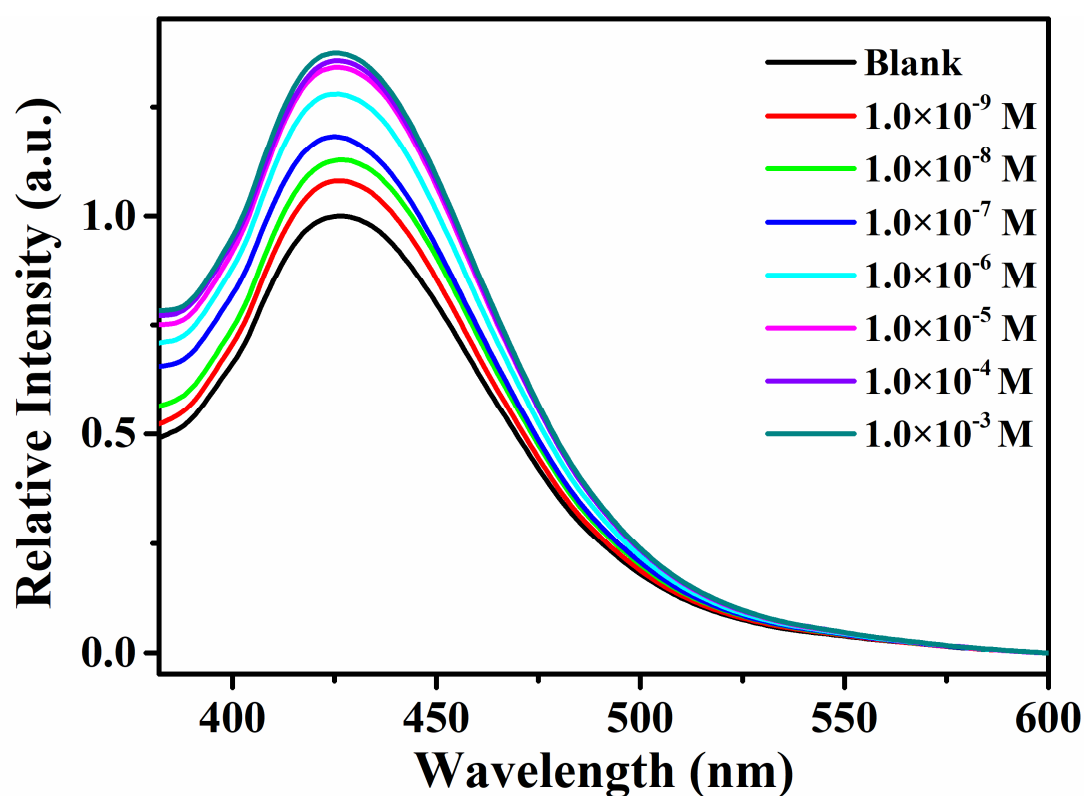


Figure S18. Liquid luminescence spectra of CdBPTC/DMF suspensions with different concentrations of Zn²⁺ at room temperature, $\lambda_{\text{ex}} = 337$ nm.

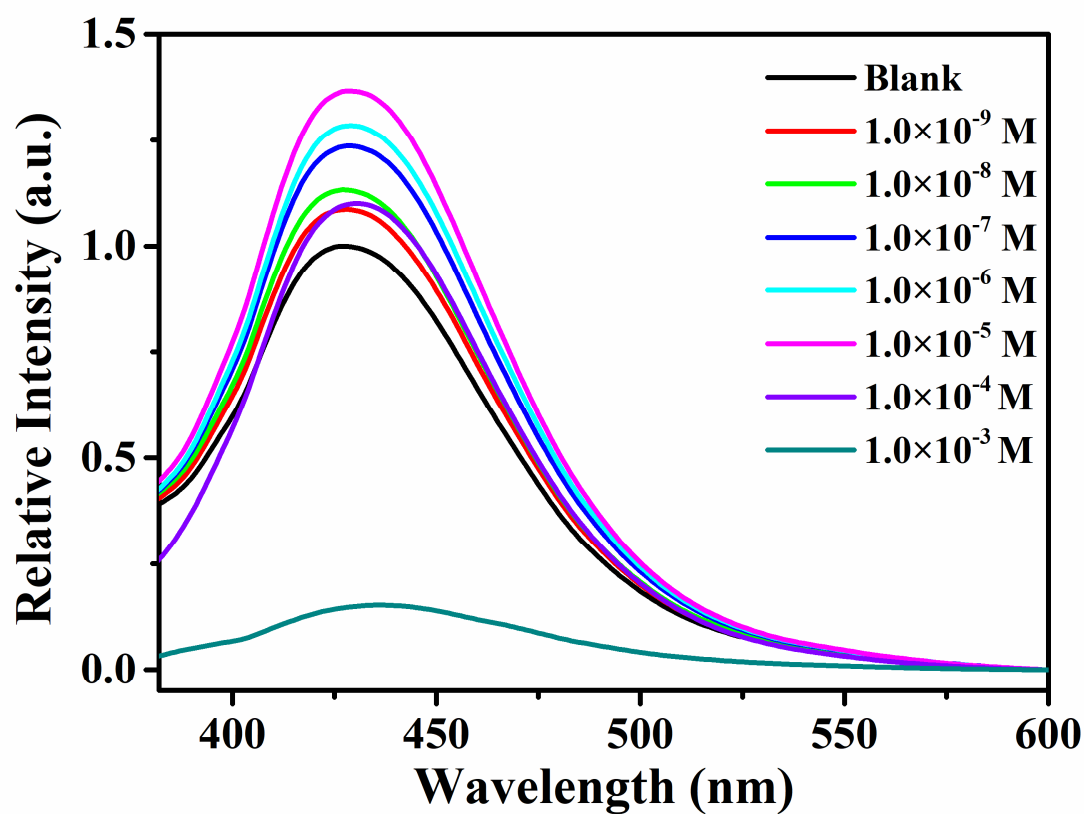


Figure S19. Liquid luminescence spectra of CdBPTC/DMF suspensions with different concentrations of Fe²⁺ at room temperature, $\lambda_{\text{ex}} = 337$ nm.

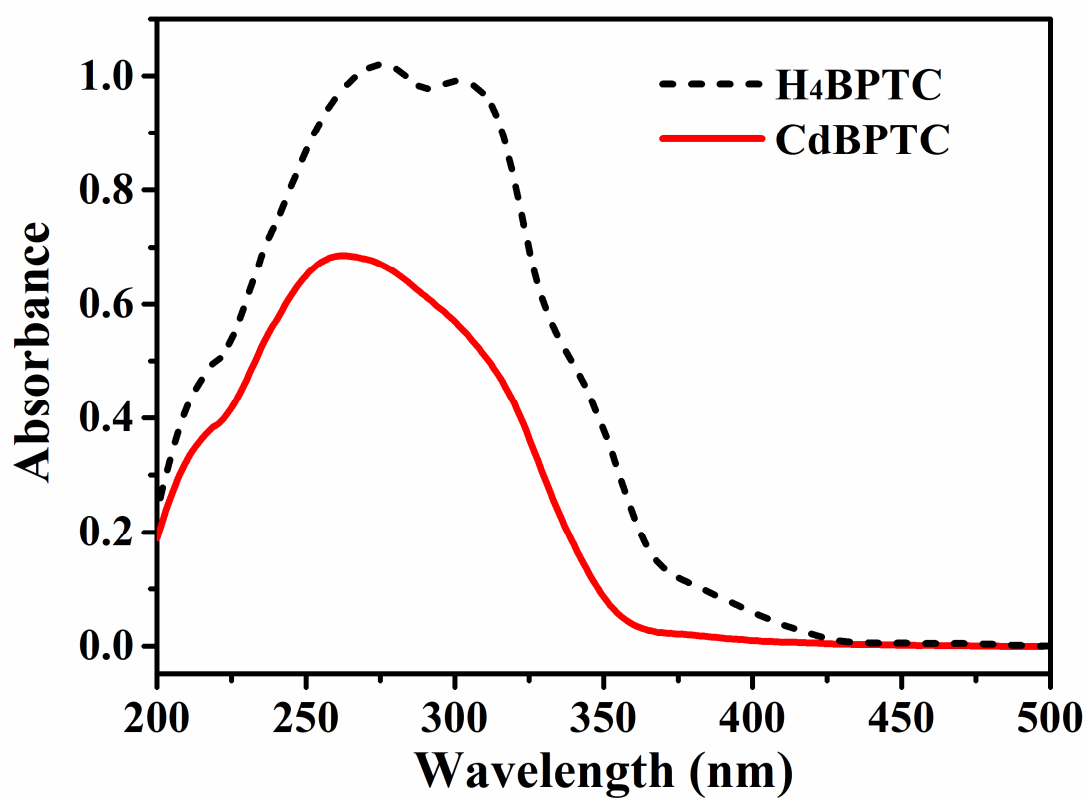


Figure S20. Solid UV-Vis spectra of CdBPTC and H₄BPTC ligand.

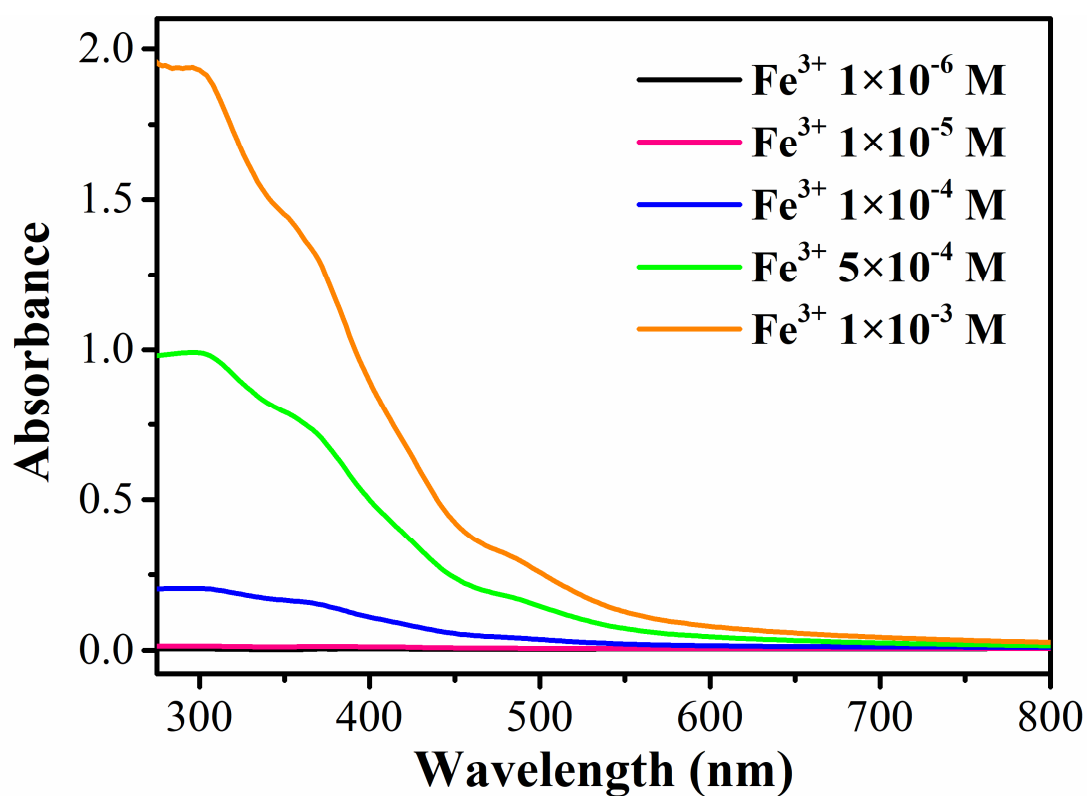


Figure S21. UV-Vis absorption spectra of Fe³⁺ aqueous solutions with different concentrations.

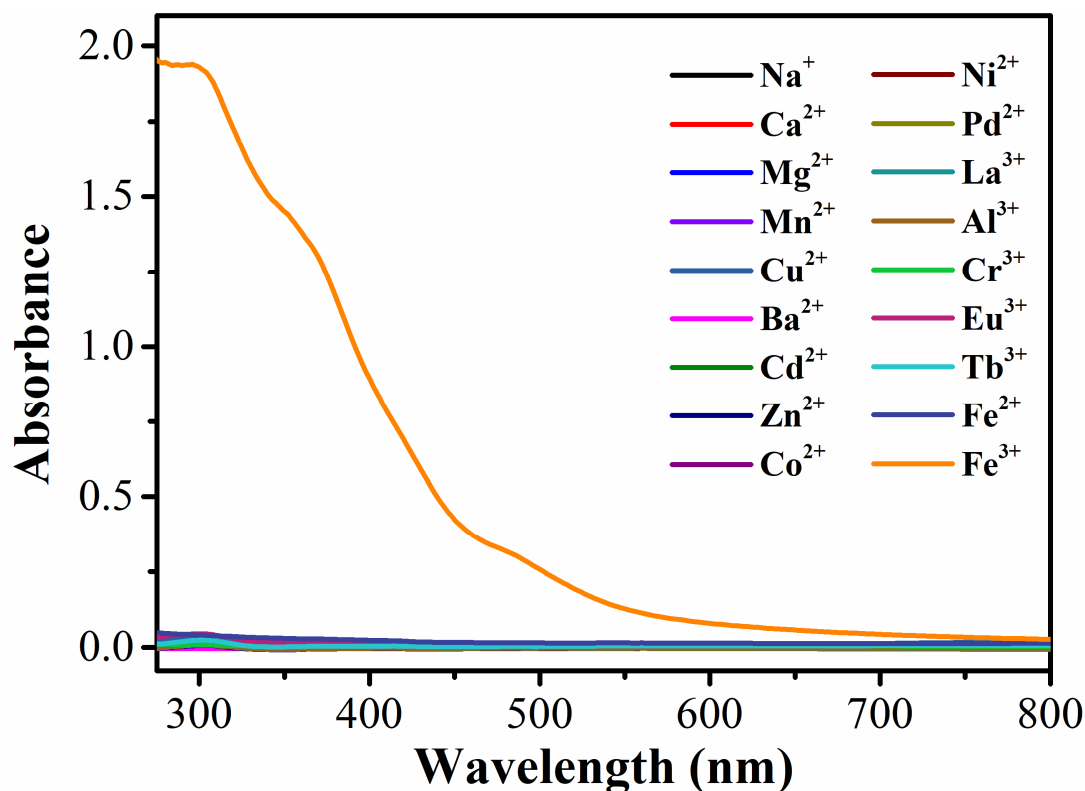


Figure S22. UV-Vis absorption spectra of different metal cations in aqueous solutions ($1 \times 10^{-3} \text{ mol} \cdot \text{L}^{-1}$).

Table S1. Selected bond lengths (Å) and bond angles (°) of CdBPTC.

| CdBPTC | | | |
|---------------------------------------|------------|---------------------------------------|------------|
| Cd1-O5 ¹ | 2.313(7) | Cd1-O6 ¹ | 2.592(6) |
| Cd1-O8 ² | 2.271(6) | Cd1-O3 ³ | 2.590(5) |
| Cd1-O7 ² | 2.533(4) | Cd1-O1 | 2.330(7) |
| Cd1-O2 | 2.461(4) | Cd1-O4 ³ | 2.290(7) |
| O5 ¹ -Cd1-O7 ² | 135.1(2) | O2-Cd1-O6 ¹ | 90.76(19) |
| O5 ¹ -Cd1-O2 | 86.1(2) | O2-Cd1-C15 ² | 98.12(17) |
| O5 ¹ -Cd1-O6 ¹ | 54.4(2) | O2-Cd1-O3 ³ | 168.0(2) |
| O5 ¹ -Cd1-C15 ² | 110.1(3) | O6 ¹ -Cd1-C15 ² | 161.7(2) |
| O5 ¹ -Cd1-O3 ³ | 81.99(19) | O3 ³ -Cd1-O6 ¹ | 81.39(18) |
| O5 ¹ -Cd1-O1 | 127.64(19) | O3 ³ -Cd1-C15 ² | 87.09(16) |
| O8 ² -Cd1-O5 ¹ | 82.6(3) | O1-Cd1-O7 ² | 88.35(17) |
| O8 ² -Cd1-O7 ² | 52.87(19) | O1-Cd1-O2 | 53.8(2) |
| O8 ² -Cd1-O2 | 92.34(19) | O1-Cd1-O6 ¹ | 90.2(2) |
| O8 ² -Cd1-O6 ¹ | 136.6(2) | O1-Cd1-C15 ² | 107.9(2) |
| O8 ² -Cd1-C15 ² | 27.8(2) | O1-Cd1-O3 ³ | 134.7(2) |
| O8 ² -Cd1-O3 ³ | 87.27(17) | O4 ³ -Cd1-O5 ¹ | 123.41(17) |
| O8 ² -Cd1-O1 | 125.44(18) | O4 ³ -Cd1-O7 ² | 82.08(19) |
| O8 ² -Cd1-O4 ³ | 120.7(2) | O4 ³ -Cd1-O2 | 136.1(3) |
| O7 ² -Cd1-O6 ¹ | 166.1(2) | O4 ³ -Cd1-O3 ³ | 52.4(3) |
| O7 ² -Cd1-C15 ² | 25.1(2) | O4 ³ -Cd1-O6 ¹ | 84.04(19) |
| O7 ² -Cd1-O3 ³ | 89.82(15) | O4 ³ -Cd1-C15 ² | 100.1(2) |
| O4 ³ -Cd1-O1 | 82.6(3) | O2-Cd1-O7 ² | 99.51(17) |

¹ 1/2-Y, 1-X, 1/4+Z; ² +Y, 1/2-X, 1/4+Z; ³ -1/2+X, 1/2-Y, +Z.