

Supporting Information

Triphenylamine based Lab-on-a-molecule for the highly selective and sensitive detection of Zn²⁺ and CN⁻ in aqueous solution

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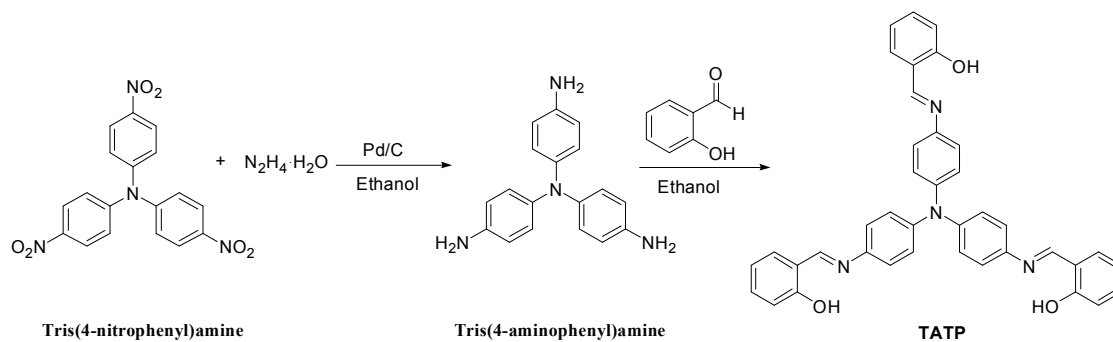


Fig. S1 The synthesis route of TATP.

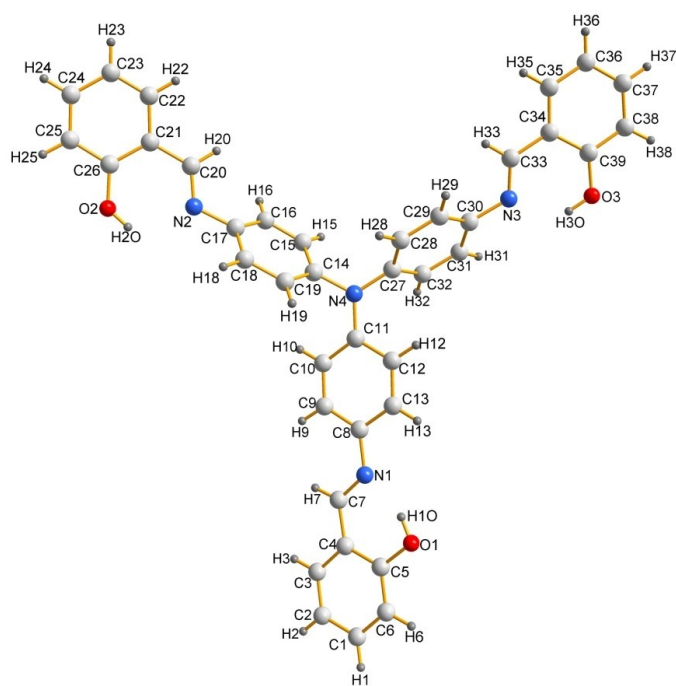


Fig. S2 Crystal structure of TATP and its unit cell. The deposit CCDC number: 1476312.

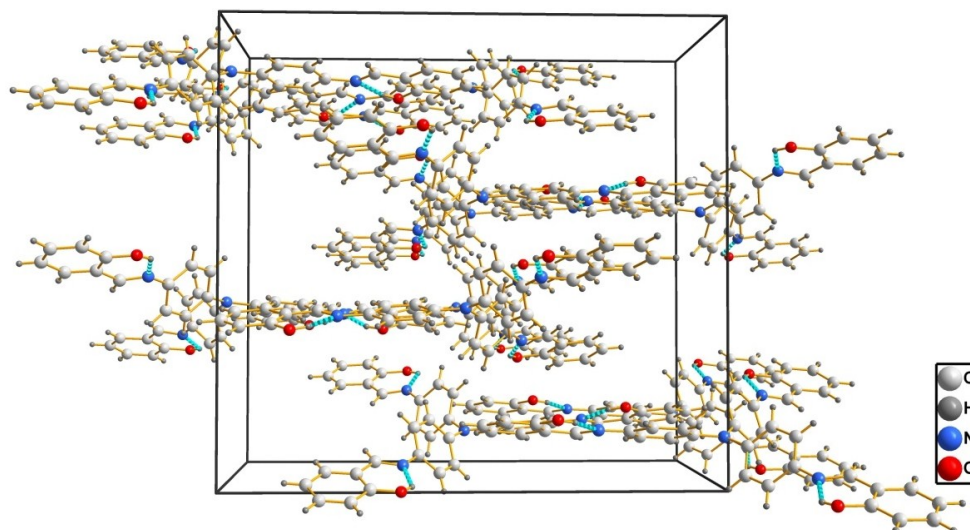


Fig. S3 Packing cell of the crystal structure of TATP.

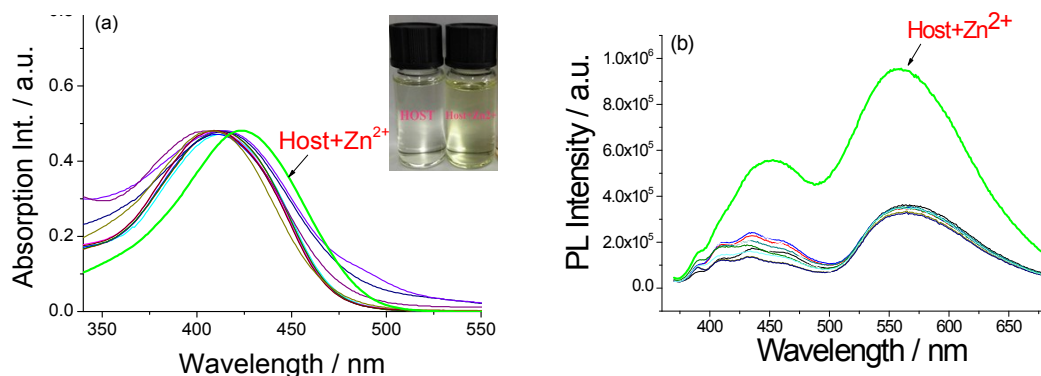


Fig. S4 (a) UV/vis spectra of TATP (10 μM) in 0.1 M Tris-ClO₄ buffer solution (pH = 7.24, DMF: buffer = 1 / 2, v / v) after addition of 50.0 equiv of various metal ions. Inset: The color changes of TATP (10 μM) upon addition of Zn²⁺; (b) Fluorescence emission spectra ($\lambda_{\text{ex}} = 350 \text{ nm}$) of TATP (10 μM) in the presence of 50.0 equiv of various metal ions in 0.1 M Tris-ClO₄ buffer solution (pH = 7.24, DMF: buffer = 1 / 2, v / v).

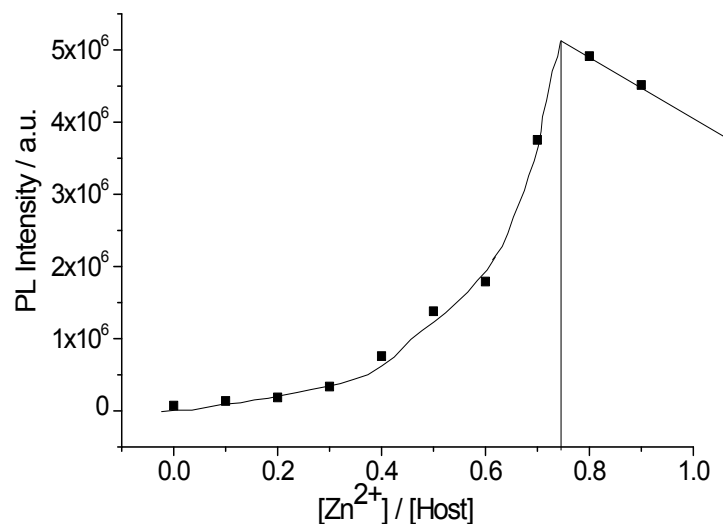


Fig. S5 Jobs plot of TATP and Zn²⁺ in 0.1 M Tris-ClO₄ buffer solution (pH = 7.24, DMF: buffer = 1 / 2, v / v). The total concentration of Zn²⁺ and TATP is $1 \times 10^{-4} \text{ M}$.

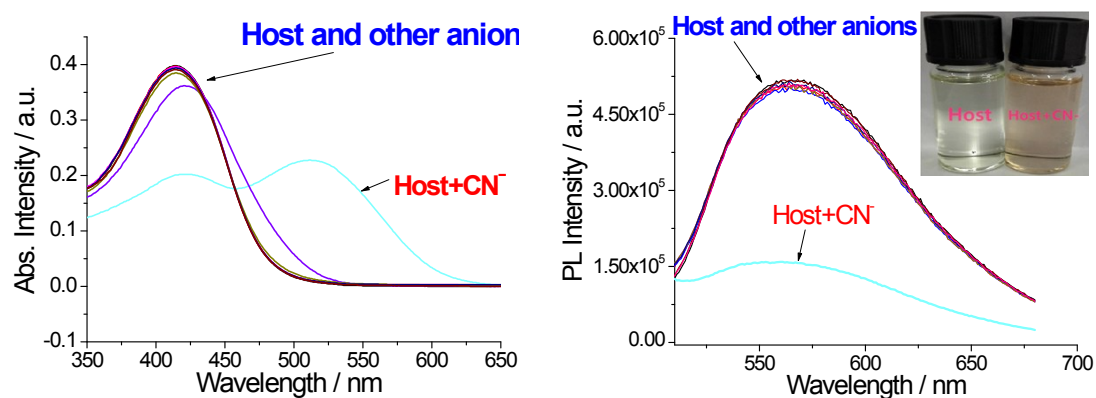


Fig. S6 UV/vis (a) and emission spectra (b, $\lambda_{\text{ex}} = 350 \text{ nm}$) of TATP (10 μM) in the presence of 50.0 equiv of various metal ions in 0.1 M Tris-ClO₄ buffer solution (pH = 7.24, DMF: buffer = 1 / 2, v / v); Inset: The solution

color changes of TATP (10 μ M) upon addition of CN^- .

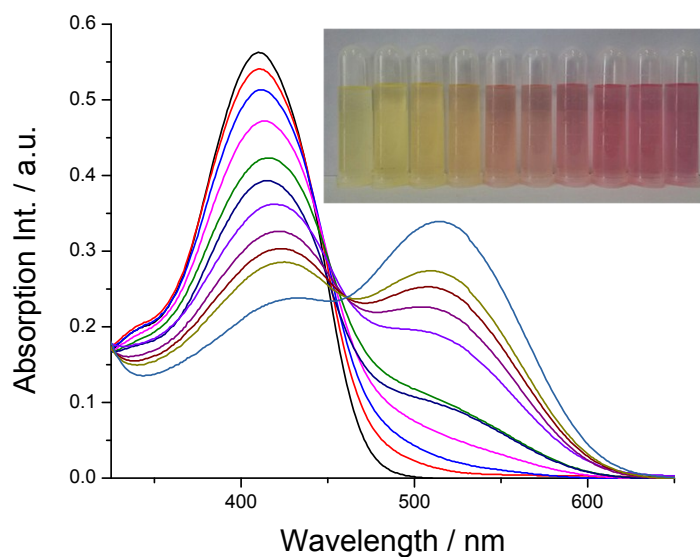


Fig. S7 UV/vis spectra of TATP (10 μ M) in 0.1 M Tris-ClO₄ buffer solution (pH = 7.24, DMF: buffer = 1 / 2, v / v) after addition of 0.5-50.0 equiv of CN^- .

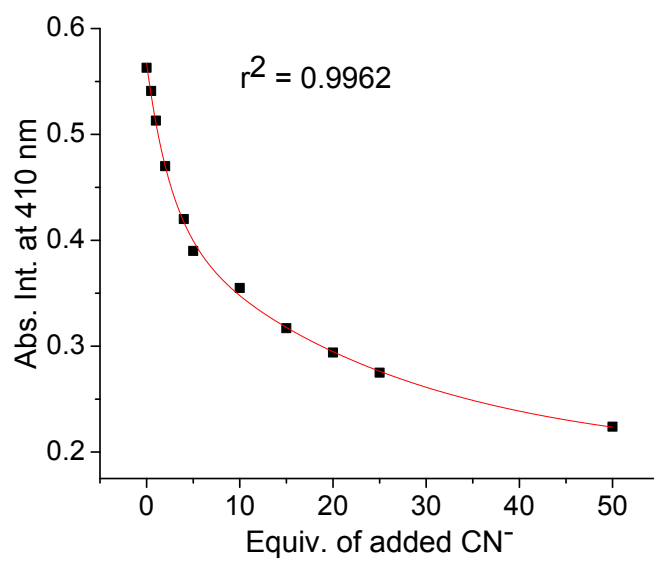


Fig. S8 The absorption intensity of TATP at 410 nm as a function of CN^- equivalent in 0.1 M Tris-ClO₄ buffer solution (pH = 7.24, DMF: buffer = 1 / 2, v / v).

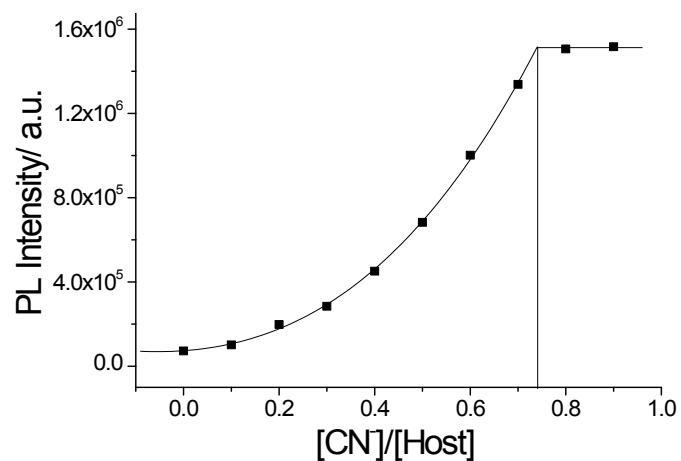


Figure S9 Jobs plot of **TATP** and **CN⁻** in 0.1 M Tris-ClO₄ buffer solution (pH = 7.24, DMF: buffer = 1 / 2, v / v). The total concentration of **CN⁻** and **TATP** is 1 × 10⁻⁴ M.

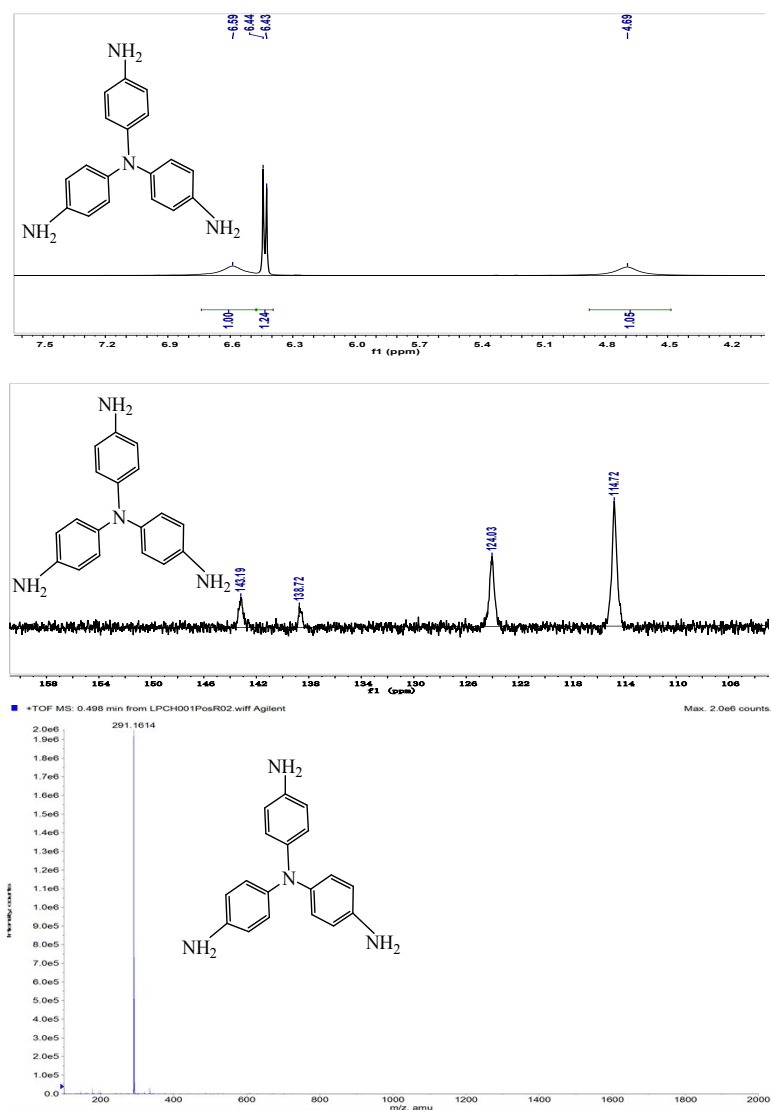


Fig. S10 ¹H-NMR, ¹³C-NMR and MS spectrogram (top to bottom) of Tris(4-aminophenyl)amine.

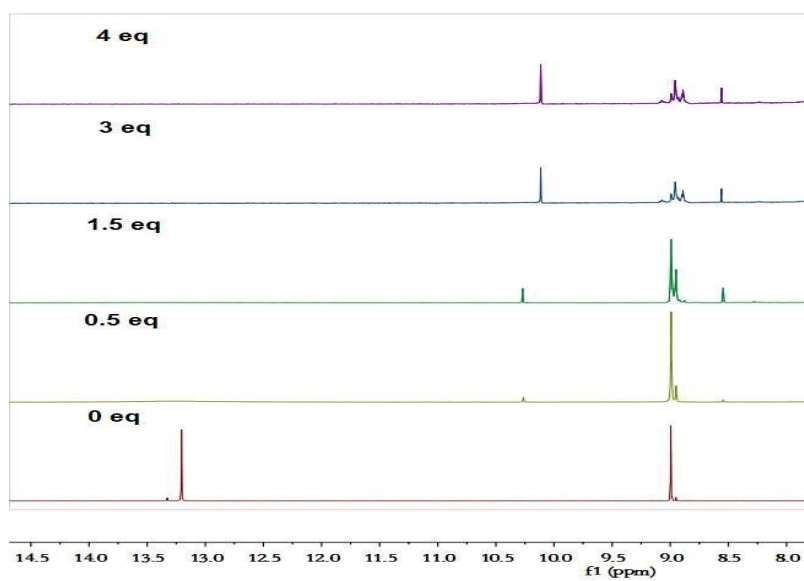


Fig. S13 ¹H NMR titration of TATP by adding different equivalents of CN⁻ into TATP solution in DMSO-d₆.