Electronic Supporting Information

Tripodal Supramolecular Sensor Successively Detect Picric Acid and CN⁻ through Guest Competitive Controlled AIE

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1. Characterization spectra of compound DN, TG.

Scheme S1. Synthesis of compound DN, TG.

Synthesis of DN: 1,8-naphthalic anhydride (0.19 g, 1.0 mmol) was added to a mixture of p-phenylenediamine (0.22 g, 2.0 mmol) in C₂H₅OH (60 mL), and the reaction mixture was stirred reflux 48 h. After reaction was finished, the solvent was filtered under reduced pressure. The crude product was elution with ethanol afforded DN as a yellow solid (0.28 g, 96%). Mp: > 280 °C. ¹H NMR (600 MHz, CDCl₃). δ 8.65-8.64 (m, 2H), 8.26-8.25 (m, 2H), 7.78 (m, 2H), 7.09–7.08 (m, 2H), 6.83–6.81 (m, 2H), 3.81 (t, 2H). ESI-MS m/z: [M + H]⁺ Calcd for C₁₈H₁₃O₂N₂ 289.0932, found 289.1392.
**Fig. S1** $^1$H NMR Spectrum of DN (CDCl$_3$, 600 MHz, 298 K).

**Fig. S2.** Mass Spectrum of DN.
**Synthesis of TG:** Compound trimesoyl chloride (0.26 g, 1.0 mmol) was added to a mixture of compound DN (0.86 g, 3.00 mmol) in DMF (50 mL), and the resulting mixture was stirred for 2-3 h. The solid was filtered and the solvent was removed. The crude product was purified by column chromatography using dichloromethane/ethyl acetate (v/v, 2:1) to give TG as a white solid (0.91 g, 89%). Mp: > 280 °C. $^1$H NMR (600 MHz, DMSO-$d_6$) δ (ppm): 10.93 (s, 3 H), 8.88 (s, 3 H), 8.50 (m, 12 H), 8.02 (m, 6 H), 7.88 (m, 6 H), 7.41 (m, 6 H). $^{13}$C NMR (DMSO-$d_6$, 150 MHz) δ/ppm 164.25, 139.16, 134.90, 131.23, 127.71, 123.09, 121.29. ESI-MS m/z: [M + Na]$^+$ Calcd for C$_{63}$H$_{59}$O$_{10}$N$_6$ 1043.2436, found 1043.2542.

**Fig. S3.** $^1$H NMR Spectrum of TG (DMSO-$d_6$, 600 MHz, 298 K).
Fig. S4. $^{13}$C NMR Spectrum of TG (DMSO-$d_6$, 150 MHz, 298 K).

Fig. S5. Mass Spectrum of TG.
2. Fluorescence emission of TG

Fig. S6. Fluorescence emission of TG in DMSO with different concentration.

3. S-TG detection of picric acid (PA) partial data.

Fig. S7. Fluorescence spectra of S-TG (1.0 × 10^{-4} M) in the presence of nitroaromatic compounds (10.0 equiv.), respectively.
Fig. S8. Fluorescence spectra of the S-TG (1.0 × 10^{-4} M) in the presence of different equivalent of \textit{PA} in DMSO (\(\lambda_{ex} = 370\) nm).

Fig. S9. Quenching percentage of S-TG emission after various nitroaromatic compounds (10.0 equiv.).
Fig. S10. Absorption spectrum of S-TG in the presence of different concentration of PA in DMSO solutions.

\[
\text{Linear Equation: } Y = -306.7857 X + 669 \quad R^2 = 0.9923
\]

\[
S = 3.0678 \times 10^8 \quad \delta = \sqrt{\frac{\sum (F - \bar{F})^2}{(N - 1)}} = 1.2143 \quad (N = 20) \quad K = 3
\]

\[
\text{LOD} = K \times \frac{\delta}{S} = 1.19 \times 10^{-8} \text{ M}
\]

Fig. S11. Plot of the fluorescence intensity at 435 nm for a mixture of the sensor S-TG and PA in DMSO solution.
Linear Equation: \( Y = 0.2835 \times X + (-0.1402) \quad R^2 = 0.9995 \)

\[
S = 2.835 \times 10^5 \quad \delta = \sqrt{\frac{\Sigma (F - \bar{F})^2}{(N - 1)}} = 0.0013 \quad (N = 20) \quad K = 3
\]

\[
LOD = K \times \delta/S = 1.38 \times 10^{-8} \text{M}
\]

**Fig. S12.** Plot of the absorbance for a mixture of the sensor S-TG and PA in DMSO solution.

**Table S1.** Comparative study of the Ksv and the detection limit (LOD) achieved in material used for the detection of PA.

<table>
<thead>
<tr>
<th>Publication</th>
<th>Material used</th>
<th>Ksv ( (M^{-1}) \times 10^4 )</th>
<th>LOD (M)</th>
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<tbody>
<tr>
<td>S1</td>
<td>Europium(III) based MOF</td>
<td>2.10</td>
<td>( 4.89 \times 10^{-6} )</td>
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<tr>
<td>S2</td>
<td>Cucurbit[8]uril based SOF</td>
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<td>( 3.58 \times 10^{-6} )</td>
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<td>S3</td>
<td>Polymer Nanoparticles</td>
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<td>( 2.60 \times 10^{-8} )</td>
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<tr>
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<td>Zn(II)-Coordination Polymer</td>
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<td>( 1.15 \times 10^{-7} )</td>
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<tr>
<td>S5</td>
<td>Nanoaggregates</td>
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<td>( 2.18 \times 10^{-6} )</td>
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<tr>
<td>S6</td>
<td>Zinc(II) based MOF</td>
<td>3.11</td>
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</tr>
<tr>
<td>---</td>
<td>This work</td>
<td>7.40</td>
<td>( 1.19 \times 10^{-8} )</td>
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</table>
4. TG detection of picric acid (PA) mechanism Partial data.

Fig. S13. Partial $^1$H NMR spectra of TG in DMSO–$d_6$ with different equivalent’s PA. (a) 0; (b) 0.1; (c) 0.2; (d) 0.5; (e) 1.0; (f) 1.5; (g) 2.0 equiv.

Fig. S14. IR spectra of sensor TG, TG-PA and TG-PA + CN$^-$, respectively.
Fig. S15. Mass Spectrum of mixture TG and PA, indicating the 1:1 stoichiometry for TG and PA.

5. TG-PA detection of CN⁻ Partial data.

Fig. S16. Fluorescent spectrum of TG-PA (10 μM) in the presence of different concentration of CN⁻ in DMSO solutions (λₑₓ = 370 nm).
Linear Equation: \( Y = 8.40995 \times 10^6 \)  

\[
S = 8.41 \times 10^6 \\
\delta = \sqrt{\frac{\sum (F - \bar{F})^2}{(N - 1)}} = 2.0891 \\
R^2 = 0.98902 \\
N = 20 \\
K = 3
\]

LOD = \( K \times \delta / S = 7.45 \times 10^{-7} \) M

**Fig. S17.** The photograph of the fluorescent spectrum linear range for \( \text{CN}^- \).

**Fig. S18.** Photographs of detection \( \text{CN}^- \) on silica gel plate treated by TG-PA.

**References**


