Rhodamine basedSelective Turn-on Sensing of Picric acid.

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Electronic Supporting Information
**Materials and instrumental methods:**

All reagents and solvents were used without purification. Absorption measurements were carried out in JASCO V-550 UV-vis spectrophotometer. Fluorescence spectra were recorded in F-4500 Hitachi fluorescence spectrophotometer. The slit width was 5 nm for both excitation and emission. NMR spectra were recorded in Bruker (Avance) 300 MHz instrument using TMS as internal standard. ESI-MS spectral analysis was performed in positive ion as well as negative ion mode on a liquid chromatography-ion trap mass spectrometer (LCQ Fleet, Thermo Fisher Instruments Limited, US). Elemental analysis was carried out in a Perkin-Elmer 4100 elemental analyzer.

**Computational details:**

Density functional theory (DFT) calculations were carried out with B3LYP/ 6-311G basis set using Gaussian 09 program in order to understand the fluorescence enhancement of RDD-1 on addition of picric acid (PA) ions. The geometries of RDD-1 and RDD-1+PA were optimized by DFT-B3LYP using 6-311G basis sets. The TDDFT calculations on the optimized geometries of RDD-1 and RDD-1+PA complex using above basis sets were carried out to obtain the information about absorption change and corresponding transitions of RDD-1 and RDD-1 + PA. The MO’s were plotted using Gaussview 05 with the isosurface value 0.05.

**Preparation of test Strips:**

A filter paper was immersed in the probe RDD-1 (5.0 × 10^-3 M) dissolved in acetonitrile-water (8:2) for 10 seconds and then dried in air. The test papers was again immersed into the picric acid containing aqueous solution for 1 min then air-dried in order to detect picric acid in real samples.
Figure S1: $^1$H-nmr spectrum of RDD-1 in CDCl$_3$
Figure-S2: $^{13}$C-nmr spectrum of RDD-1 in CDCl$_3$.

Figure-S3: ESI-MS spectrum of RDD-1.
Figure-S4: UV-visible absorption spectra of RDD-1 in the presence of Nitro compounds (PA, BQ, NB, NT, NP, DNB, TNT, DNP) in aqueous solution.
Figure-S5: Job’s plot- (a) plot of Mole fraction of RDD-1 vs change of fluorescence intensity after addition of PA at $\lambda_{Emm} = 555\text{nm}$ (b) plot of Mole fraction of RDD-1 vs change of absorbance after addition of PA at $\lambda_{abs} = 535\text{ nm}$
Figure-S6: (a) observed ESI-MS spectrum of RDD-1 +PA. (b) stimulated ESI-MS spectrum of RDD-1 +PA
Figure-S7: plot of change of fluorescence intensity at $\lambda_{Emm} = 557$ vs concentration of PA added to the probe RDD-1.

Figure-S8: Time dependent Fluorescence response of 1 µM RDD-1 to PA.
Fig- S9: Fluorescence response of 1 µM RDD-1 to various NAC’s.

Figure-S10: Fluorescence response of RDD-1 (1 µM) various NAC’S (Brown bar) and to the mixture of 10 µM of tested NAC’S with 10 µM PA (Pink).
Figure-S11: Overlaid uv-Vis absorption spectra of RDD-1 with PA, TFA.

Figure-S12: Overlaid Fluorescence Emission spectra of RDD-1 with PA, TFA (1 Equivalents).
Figure-S13: pH dependent Fluorescence Emission spectra of RDD-1 and RDD-1 with PA in different pH values.

Figure-S14: Overlaid normalized Fluorescence Emission spectra of RDD-1 with PA in different solvents.
Table-S1: transitions and corresponding oscillator strengths calculated from RDD_1 and RDD-1 + PA using TDDFT/B3LYP-6-311G set.

**RDD-1:**

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<thead>
<tr>
<th>Transition</th>
<th>Oscillator strength (f)</th>
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<tbody>
<tr>
<td>HOMO-LUMO</td>
<td>0.4955</td>
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<tr>
<td>HOMO-1 to LUMO</td>
<td>0.0026</td>
</tr>
<tr>
<td>HOMO- LUMO+2</td>
<td>0.0124</td>
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**RDD-1+ PA-1:**

<table>
<thead>
<tr>
<th>Transition</th>
<th>Oscillator strength (f)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOMO - LUMO</td>
<td>0.7870</td>
</tr>
<tr>
<td>HOMO-1 - LUMO</td>
<td>0.0006</td>
</tr>
<tr>
<td>HOMO - LUMO+2</td>
<td>0.0004</td>
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