Electronic Supplementary Material (ESI) for RSC Advances.

Rhodamine based Selective 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.

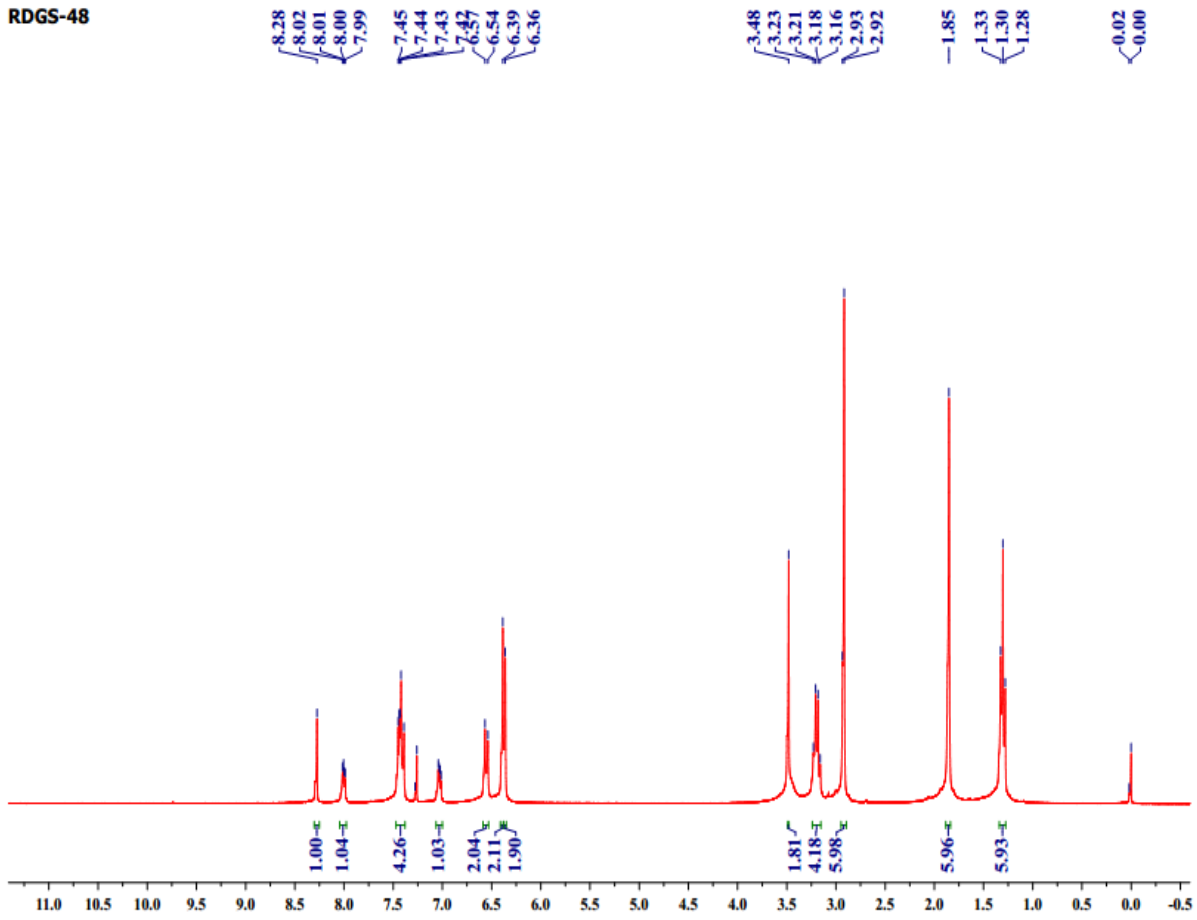


Figure S1:^{1}H-nmr spectrum of RDD-1in $CDCl_3$

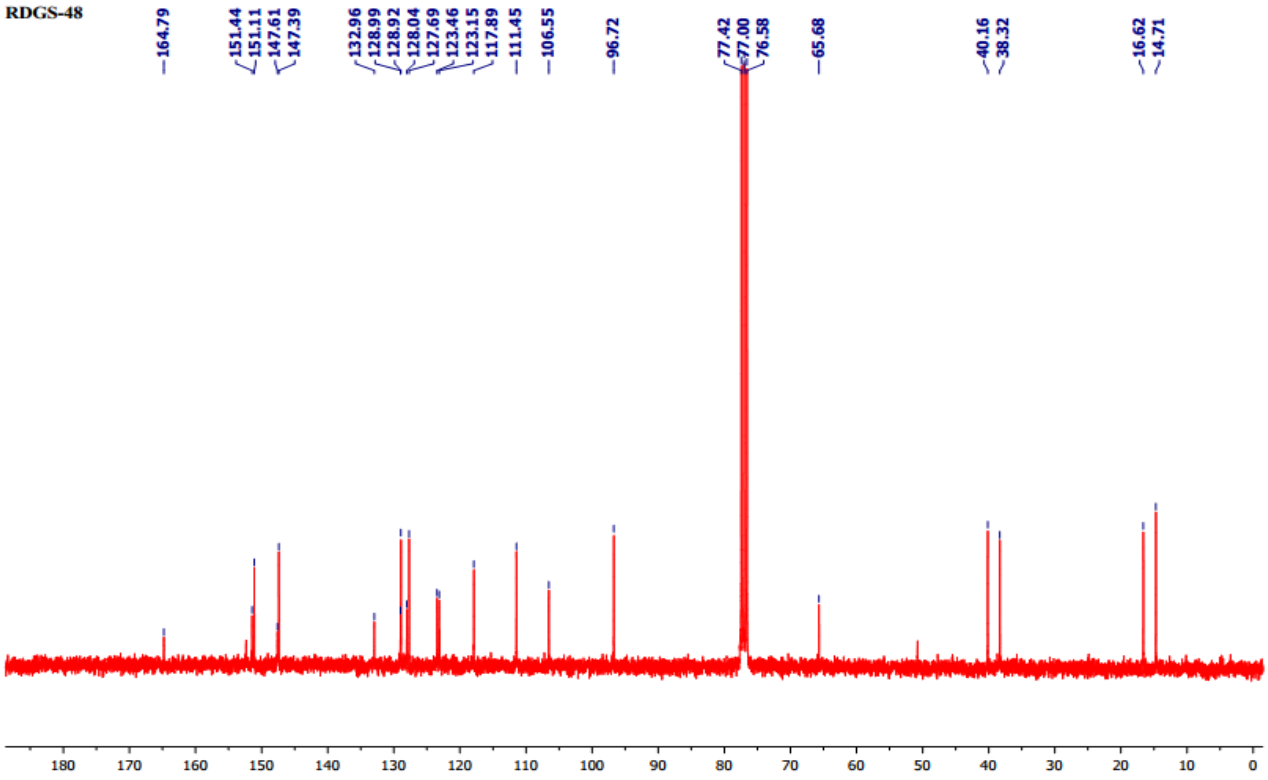


Figure-S2 :^{13}C-nmr spectrum of RDD-1in $CDCl_3$.

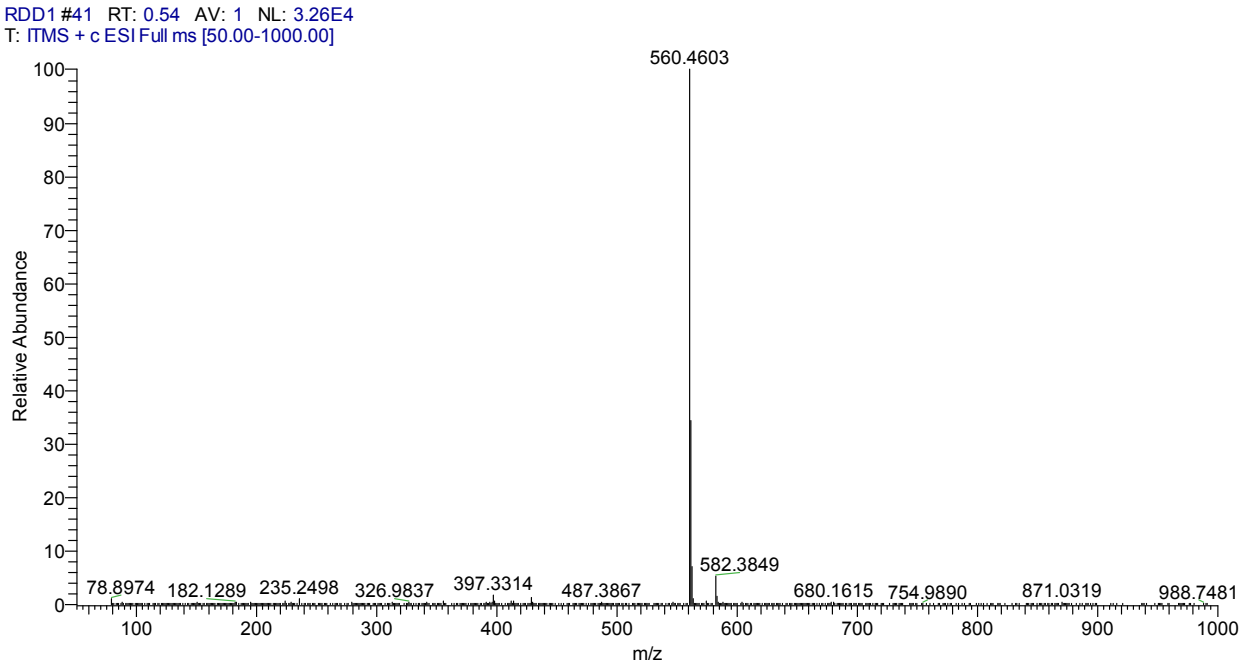


Figure-S3: ESI-MS spectrum of RDD-1.

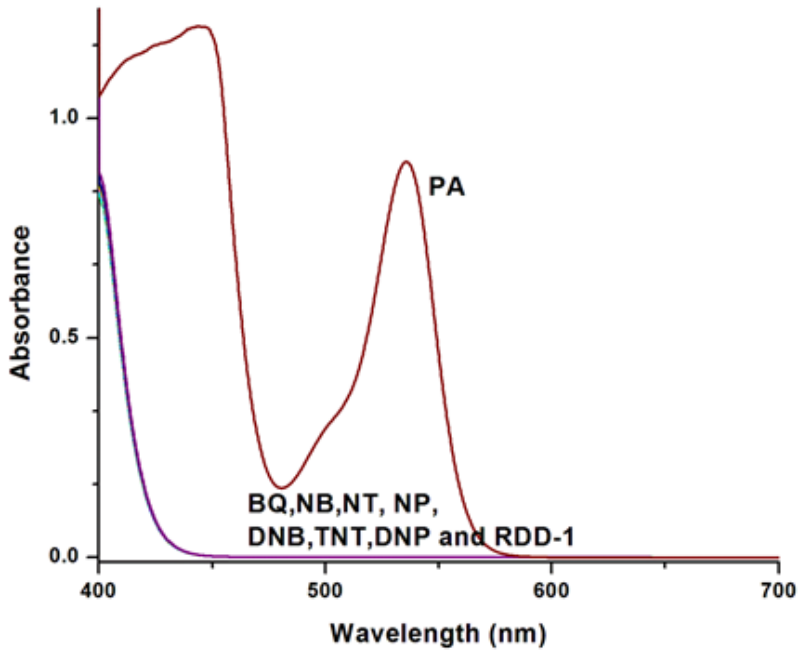
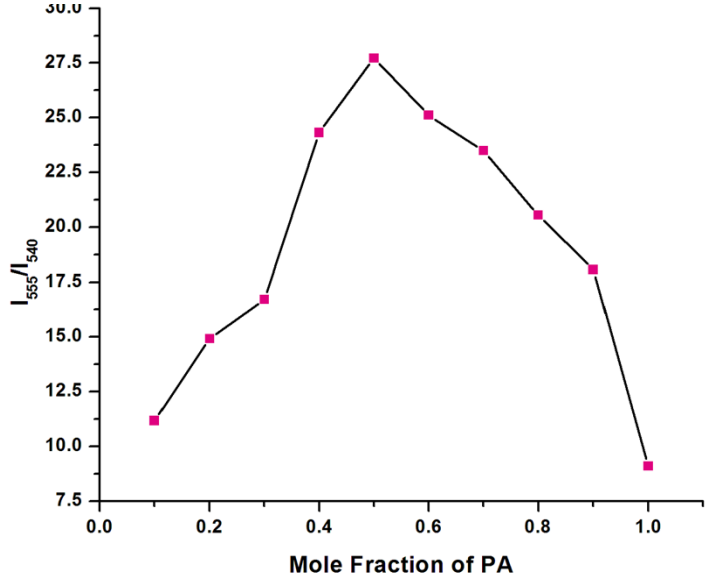


Figure-S4: UV-visible absorption spectra of RDD-1 in the presence of Nitro compounds (PA, BQ, NB, NT, NP, DNB, TNT, DNP) in aqueous solution .



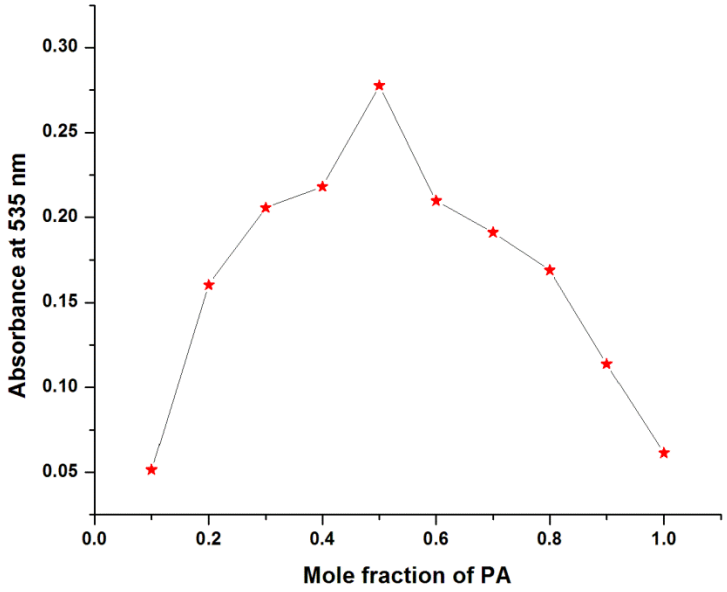
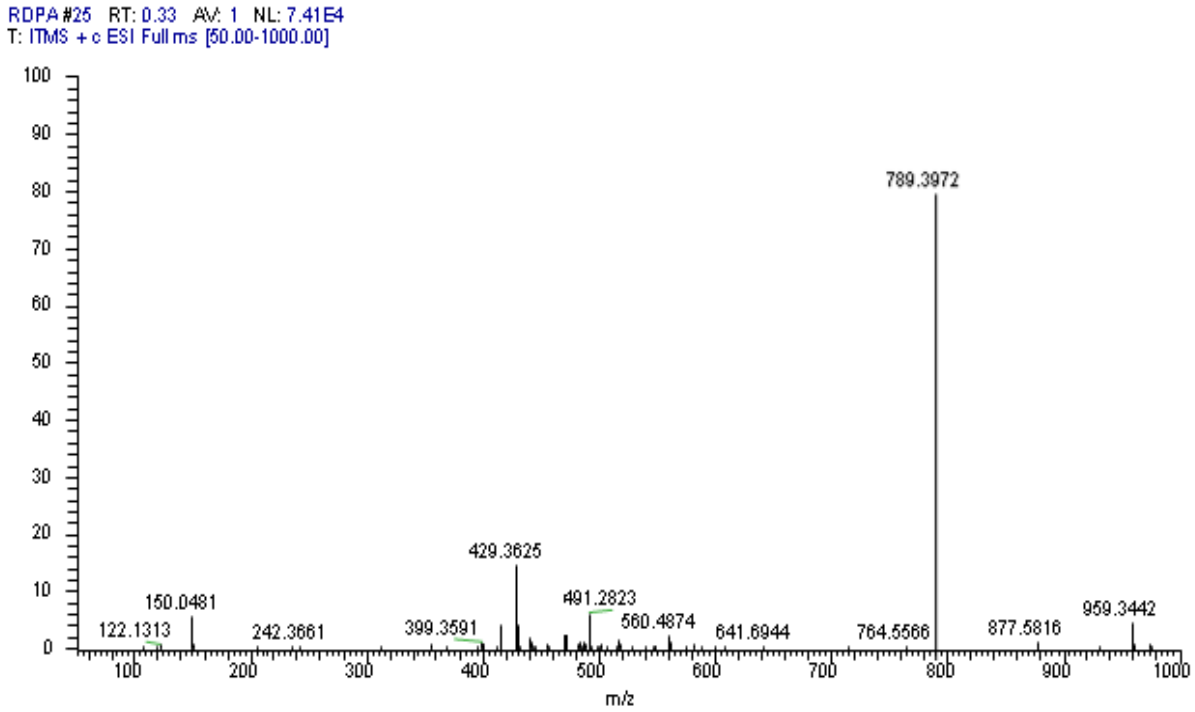


Figure-S5: Job's plot- (a) plot of Mole fraction of RDD-1 *vs* change of fluorescence intensity after addition of PA at λ_{Emm} = 555nm (b) plot of Mole fraction of RDD-1 *vs* change of absorbance after addition of PA at λ_{abs} = 535 nm



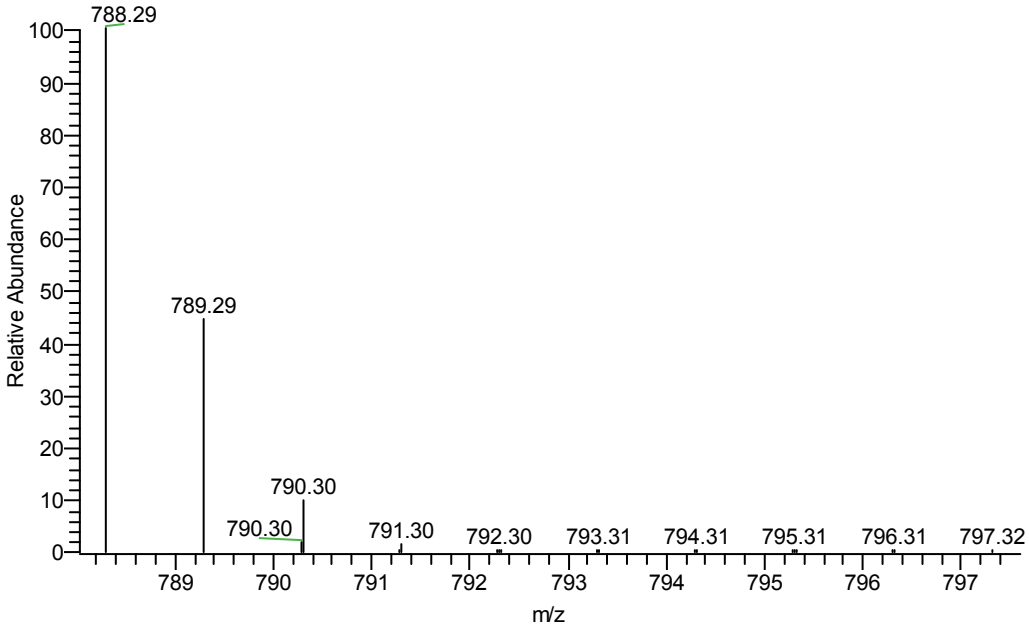


Figure-S6: (a) observed ESI-MS spectrum of RDD-1 +PA . (b) stimulated ESI-MS spectrum of RDD-1 +PA

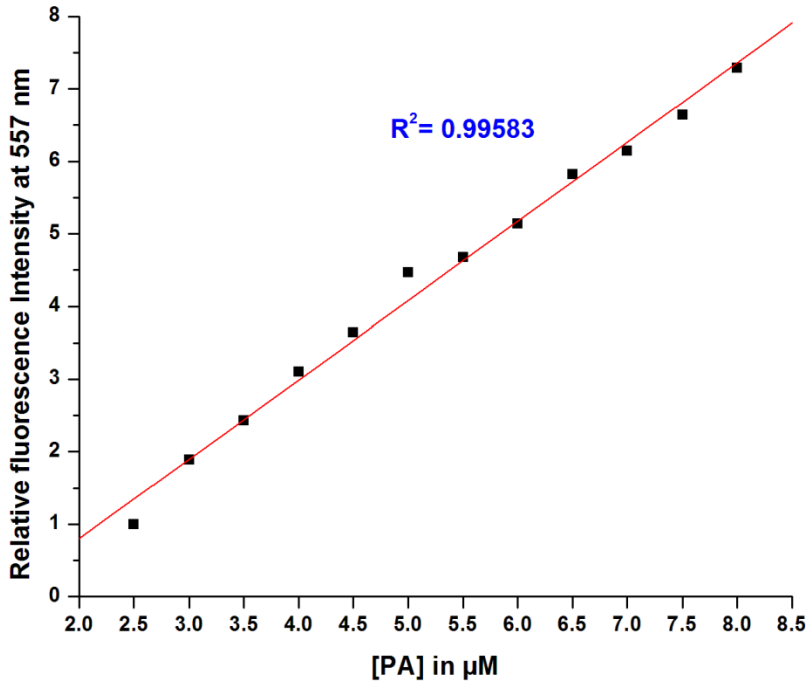


Figure-S7: plot of change of fluorescence intensity at λ_{Emm} = 557 *vs* concentration of PA added to the probe RDD-1.

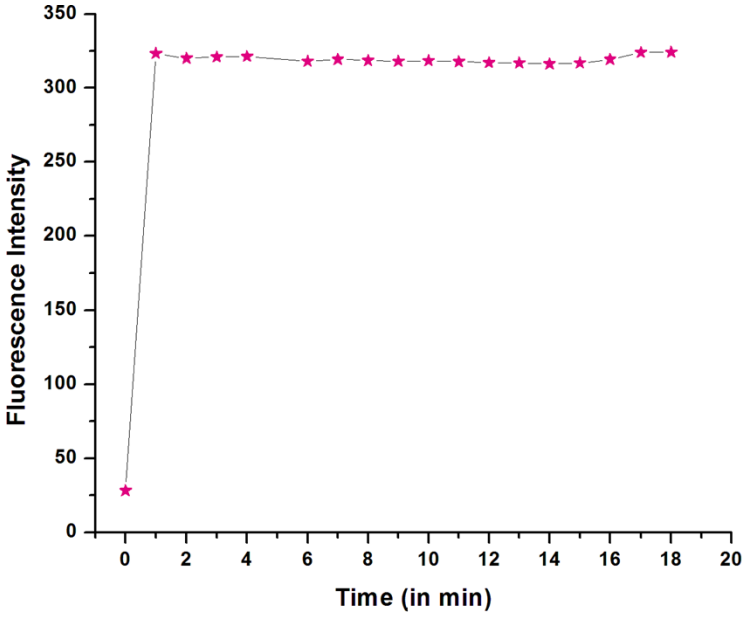


Figure- S8: Time dependent Fluorescence response of 1 μM RDD-1 to PA.

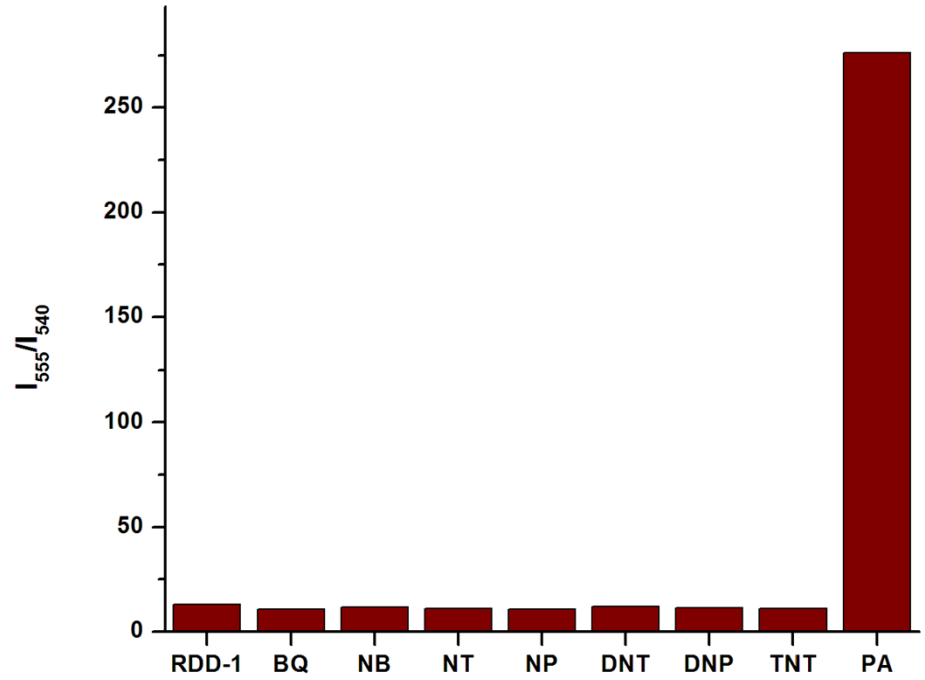


Fig- S9: Fluorescence response of 1 µM RDD-1 to various NAC's.

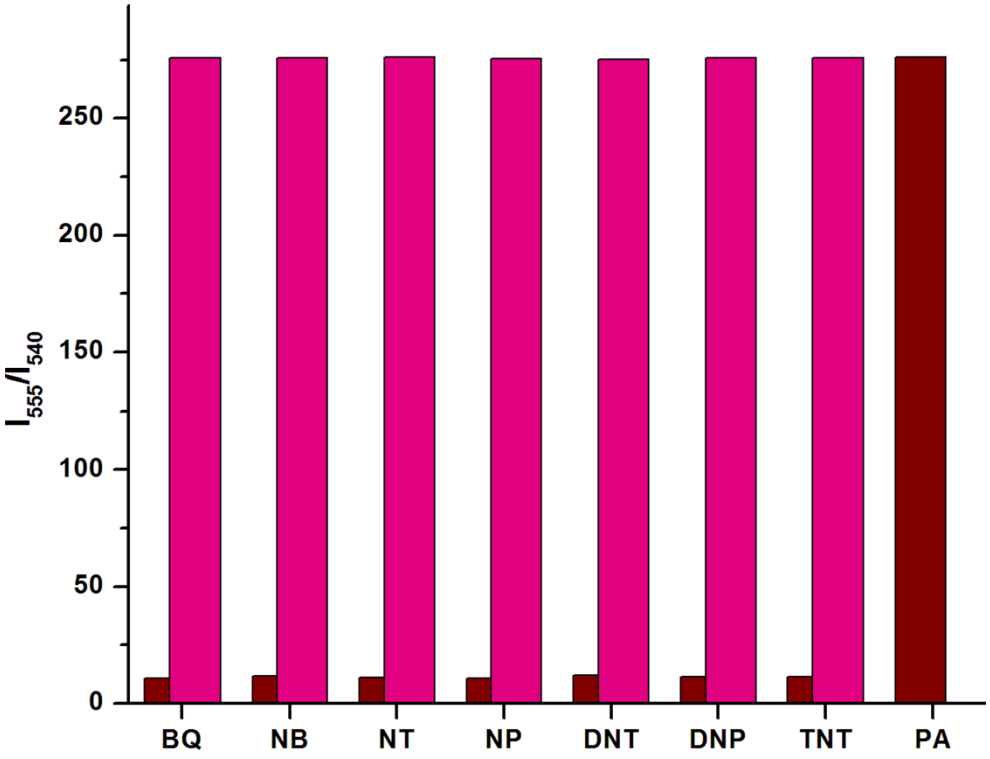


Figure-S10: Fluorescence response of RDD-1 (1 µM) various NAC'S (Brown bar) and to the mixture of 10 µM of tested NAC'S with 10 µM PA (Pink).

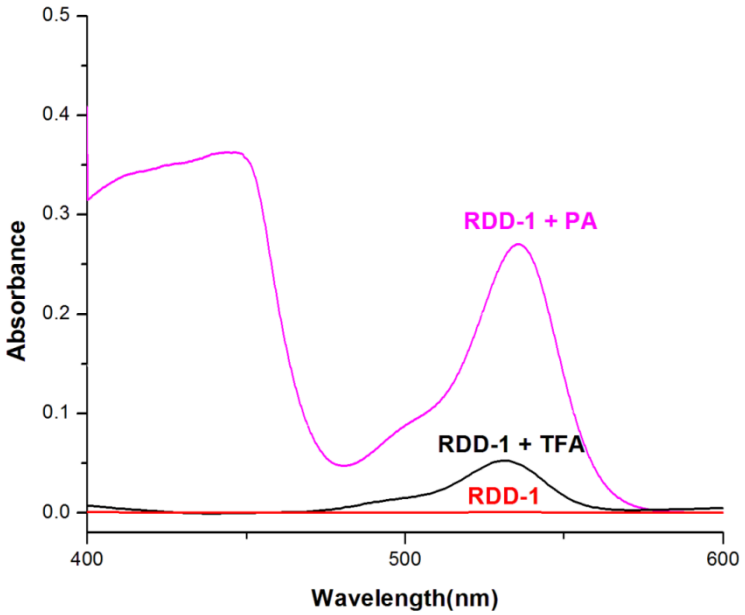


Figure-S11: Overlaid uv-Vis absorption spectra of RDD-1 with PA, TFA.

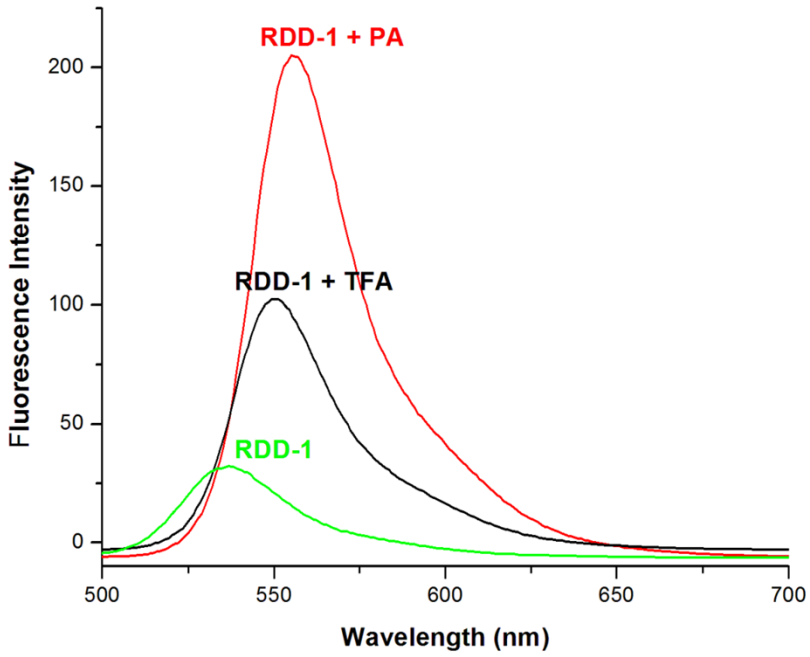


Figure-S12 : Overlaid Fluorescence Emission spectra of RDD-1 with PA, TFA (1 Equivalents) .

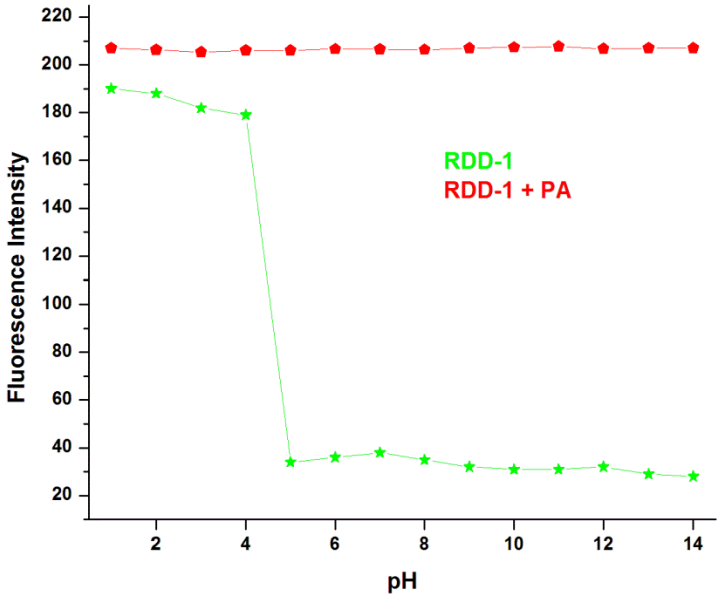


Figure-S13 : pH dependent Fluorescence Emission spectra of RDD-1 and RDD-1 with PA in different pH values.

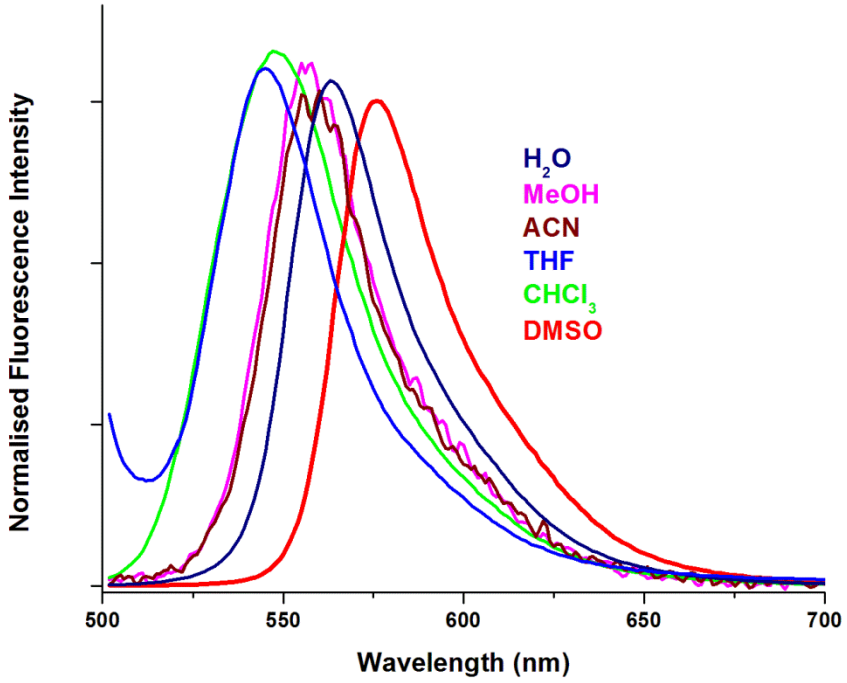


Figure-S14 : Overlaid normalized Fluorescence Emission spectra of RDD-1 with PA in different solvents.

Table-S1: transitions and corresponding oscillator strengths calculated from RDD_1 and RDD-1 + PA using TDDFT/B3LYP-6-311G set.

RDD-1:

Transition	**Oscillator strength (f)**
HOMO-LUMO	0.4955
HOMO-1 to LUMO	0.0026
HOMO- LUMO+2	0.0124
RDD-1+ PA-1:	
HOMO - LUMO	0. 7870
HOMO-1 - LUMO	0.0006
HOMO - LUMO+2	0.0004