Electronic Supplementary Information (ESI)

A small-molecule chemosensor for the selective detection of 2,4,6-trinitrophenol (TNP)

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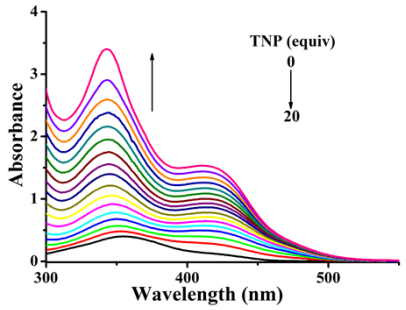

Figure S1. UV-Vis spectra of the probe **L** (10 μM) upon addition of TNP in THF. The arrow indicate the change in the absorption intensity with the increased TNP concentration.

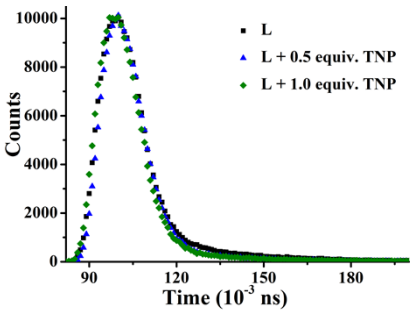

Figure S2. Time resolved fluorescence emission spectra of compound **L** for different concentrations of TNP. λ_{ex} = 350 nm.

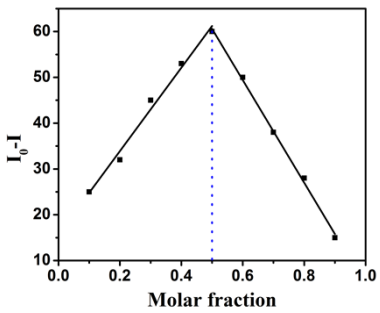

Figure S3. Job's plot of **L** with TNP shows 1:1 ratio.

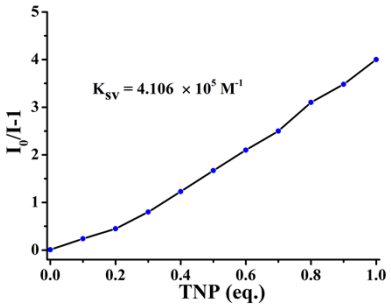

Figure S4. Stern-Volmer plot of (I_0/I-1) values versus TNP concentrations in THF for **L** (10 μM). I_0= peak intensity at [TNP] = 0. λ_{ex} = 350 nm.

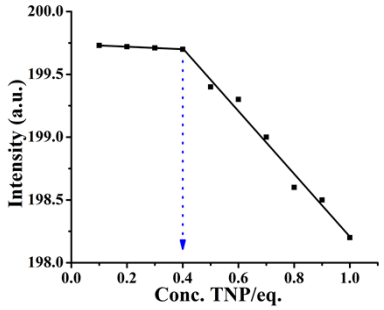

Figure S5. The fluorescence intensity at 440 nm as a function of TNP concentration.

Equation used for calculating detection limit (DL): DL= $C_L \times E_T$

C_L = Conc. of compound **L**; E_T = Conc. of titrant at which change observed.

Thus; detection limit for TNP:

DL = $1 \times 10^{-6} \times 0.4$ equiv = 4×10^{-7} or = 400 ppb

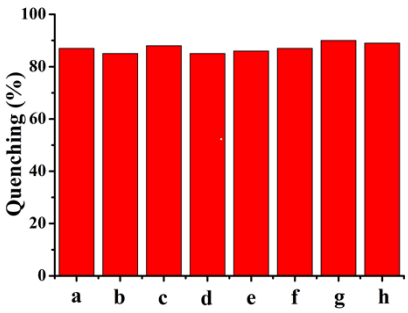

Figure S6. The interference experiment for **L** (10 μM) in THF with 5 equiv. of TNP in presence of other nitro aromatics in excess (10 equiv.).

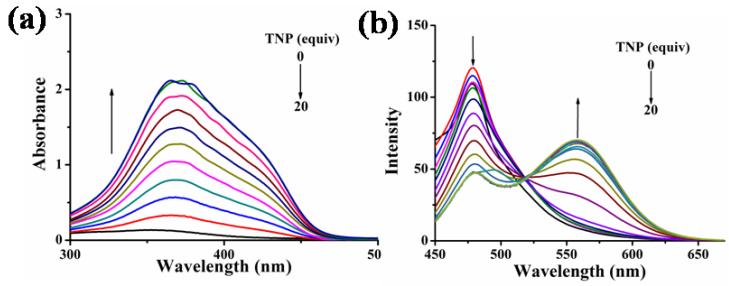

Figure S7. UV-Vis (a) and fluorescence (b) spectra of the probe **L** (10 μM) upon addition of TNP in THF/H_2O (1:9, v/v). The arrows indicate the changes in the absorption and fluorescence intensities with the increased TNP concentration (λ_{ex} = 400 nm).

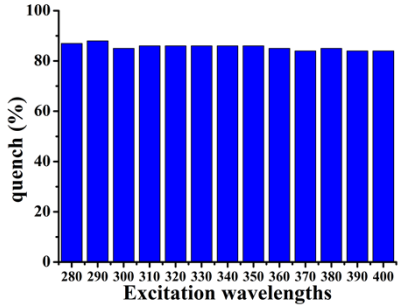

Figure S8. Comparison of fluorescence quenching of the probe **L** (10 μM) in THF after the addition of 20 equiv. TNP at various excitation wavelengths.

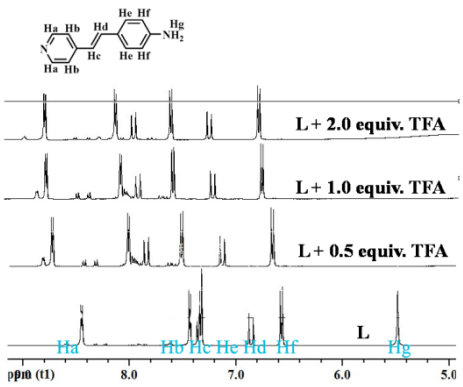

Figure S9. The whole ^{1}H NMR titration spectra (400 MHz) of the probe **L** with TFA (0, 0.5, 1.0, 2.0 equiv.) in DMSO-d_6.

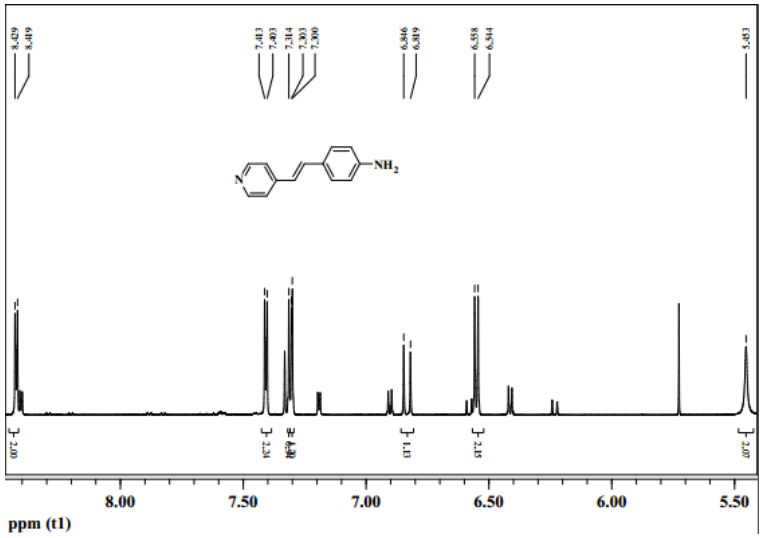

Figure S10. ^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of compound **L**.

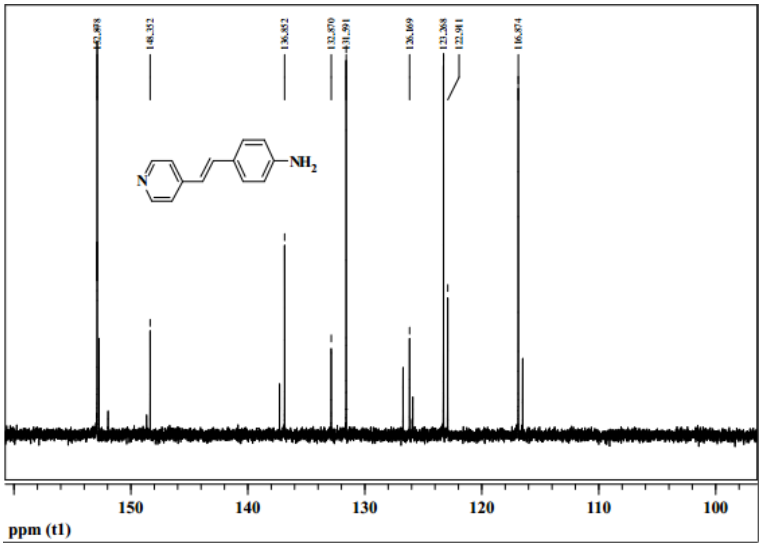

Figure S11. ^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of compound **L**.

The hydrogen-bonds data of L·TNP.

Table S1. Hydrogen bond lengths (Å) and bond angles (°)

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA
C(9)–H(9)···N(5)	0.931	2.646	3.563(3)	168.92
N(5)–H(5B)···O(4)	0.860	2.446	3.158(5)	140.65
C(7)–H(7)···O(2)	0.931	2.475	3.217(3)	136.77
C(10)–H(10)···O(3)	0.930	2.669	3.591(5)	171.29
N(4)–H(4A)···O(5)	0.859	2.277	2.791(5)	118.53
N(4)–H(4A)···O(7)	0.859	1.968	2.763(3)	153.28
N(5)–H(5A)···O(1)	0.860	2.265	3.080(3)	158.32
C(4)–H(4)···O(3)	0.930	2.609	3.386(5)	141.37
C(13)–H(13)···O(6)	0.931	2.614	3.486(5)	156.24