# High dual-state blue emission of functionalized pyrazoline derivative for picric acid detection

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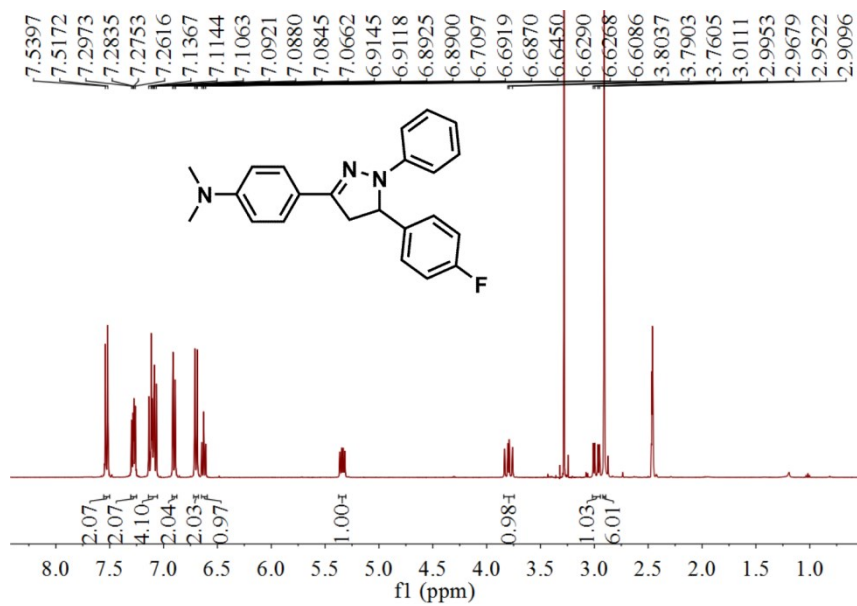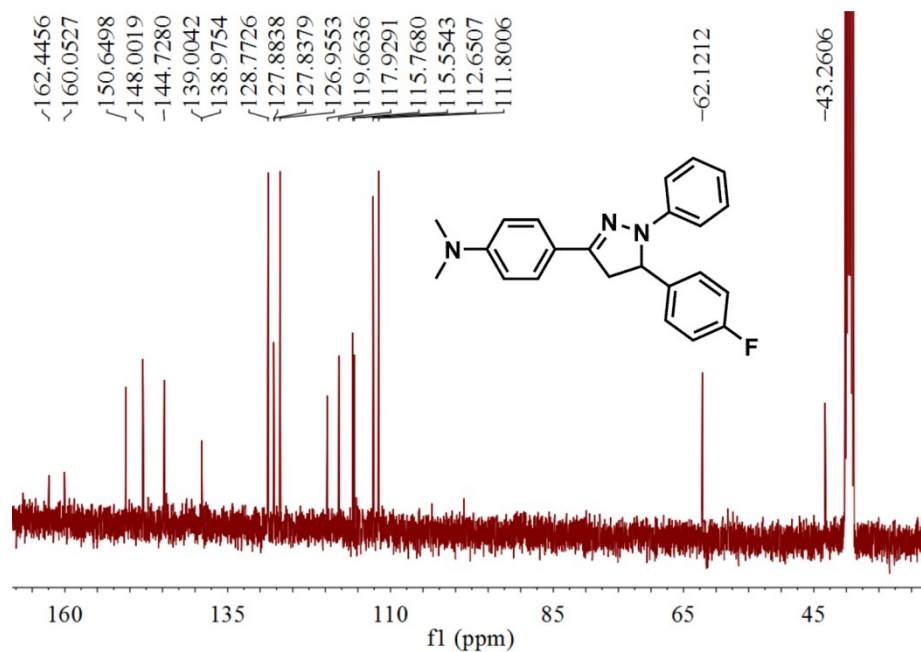
Fig. S1. ^{1}H NMR spectrum of **NF** in DMSO.

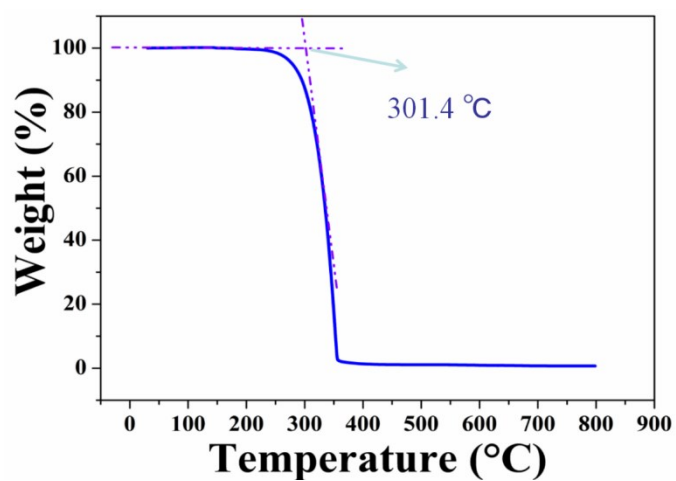**Fig. S2.** ^{13}C NMR spectrum of **NF** in DMSO.

Fig. S3. thermogravimetric (TG) analysis of **NF**

Table S1. Optical data of the compound **NF** in different solvents and solid state

Compound	solvents	λ_{ab}^a (nm)	λ_{em}^b (nm)	Δv^c (cm^{-1})	Φ_{PL}^d
	Benzene	369	439	4321	0.40

	DCM	369	439	4321	0.51
	THF	363	434	4507	0.58
	EA	362	433	4530	0.44
	EtOH	362	453	5549	0.25
	MeCN	362	438	4793	0.53
	DMF	362	437	4741	0.53
	Solid state	390	453	3566	0.43

[a] Peak position of the maximum absorption band. [b] Peak position of fluorescence emission, excited at the absorption maximum. [c] Stokes' shift in cm^{-1}. [d] fluorescence quantum yields (Φ_{PL}).
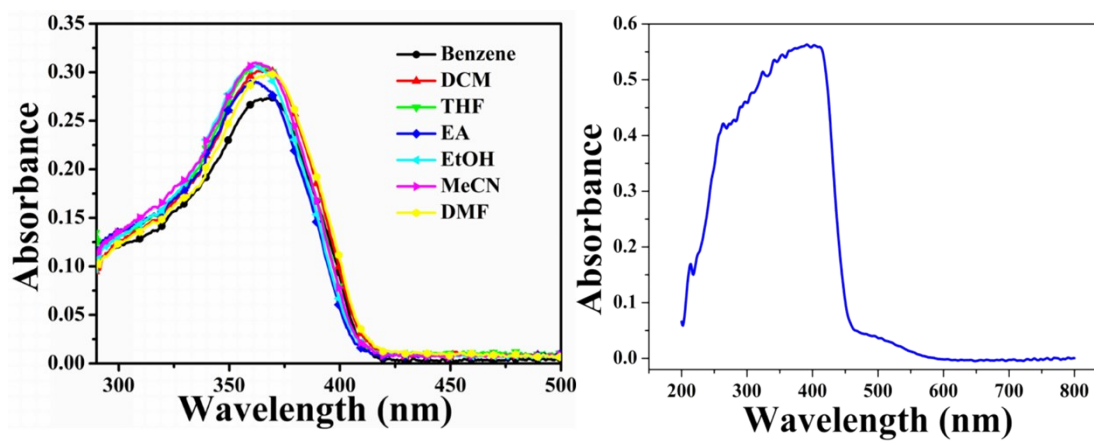

Fig. S4 the UV-vis absorption in different solvents (a) and solid state (b).
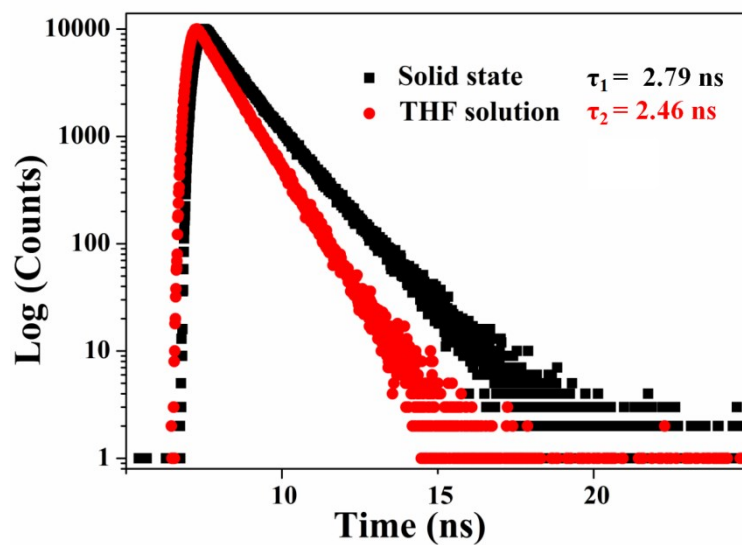
Fig. S5 Time-resolved emission decay curves of **NF** in THF solution and solid state.
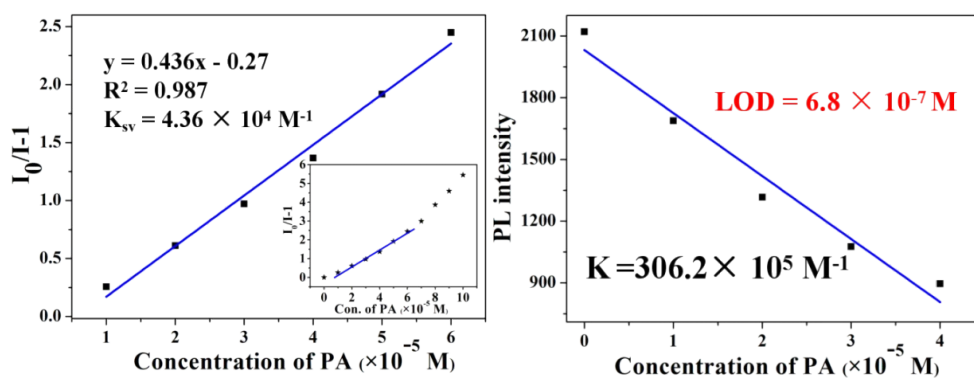

Fig. S6 (a) Corresponding Stern-Volmer plot for lower concentration of PA detection. Inset: Stern-Volmer plot obtained at concentration of PA. (b) The linear relationship of **NF** between the fluorescence intensity and the PA concentration
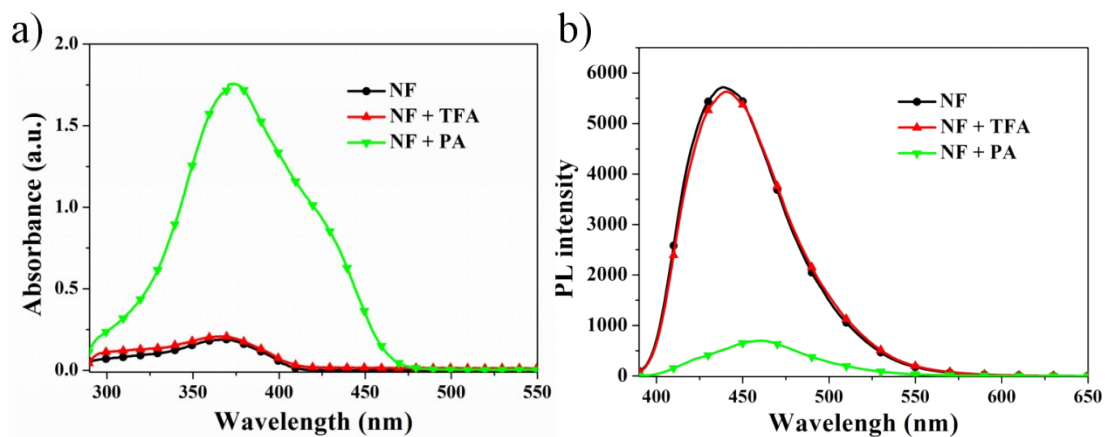
Fig. S7 the UV-vis absorption (a) and PL spectra (b) in THF/water (v/v = 8 : 2) containing PA and TFA.

Table S2. Summary of crystallographic data and structure refinement details for **NF**

Compounds	**NF**	Z, Calculated density	4, 1.238 (g/cm^{-3})
Formula	C$_{23}$H$_{22}$FN$_3$	Absorption coefficient	0.081 mm^{-1}
Mr	359.44	*Data/restraints/parameters*	3383/0/247
Temperature	293	*Goodness-of-fit on F^2*	1.120
Crystal system	orthorhombic	*Largest diff.peak and hole*	0.12 and -0.13 e.A^{-3}
Space group	*P*2$_1$2$_1$2$_1$	Theta range for data collection	2.24 to 49.98 deg.
a (Å)	5.9014		-7 ≤ h ≤ 6
b (Å)	8.9662	Limiting indices	-10 ≤ k ≤ 10
c (Å)	36.435		-43 ≤ l ≤ 37
β (°)	90	F(000)	760
α (°)	90	Reflection	2668 /3383 [R

		collected / unique	(int) = 0.0453]
Γ (°)	90	Final R indices [I>2σ(I)]	$R_1 = 0.0554$, $wR_2 = 0.1052$
Volume	1927.9	R indices (all)	$R_1 = 0.0769$, $wR_2 = 0.11128$

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