Supporting Information

Rational design of aggregation-induced emission sensor based on Rhodamine B for turn-on sensing trivalent metal cations, reversible data protection, and bioimaging

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Fig. S1 ^{1}H NMR spectrum (in CDCl$_3$) of **TPEThRB**.
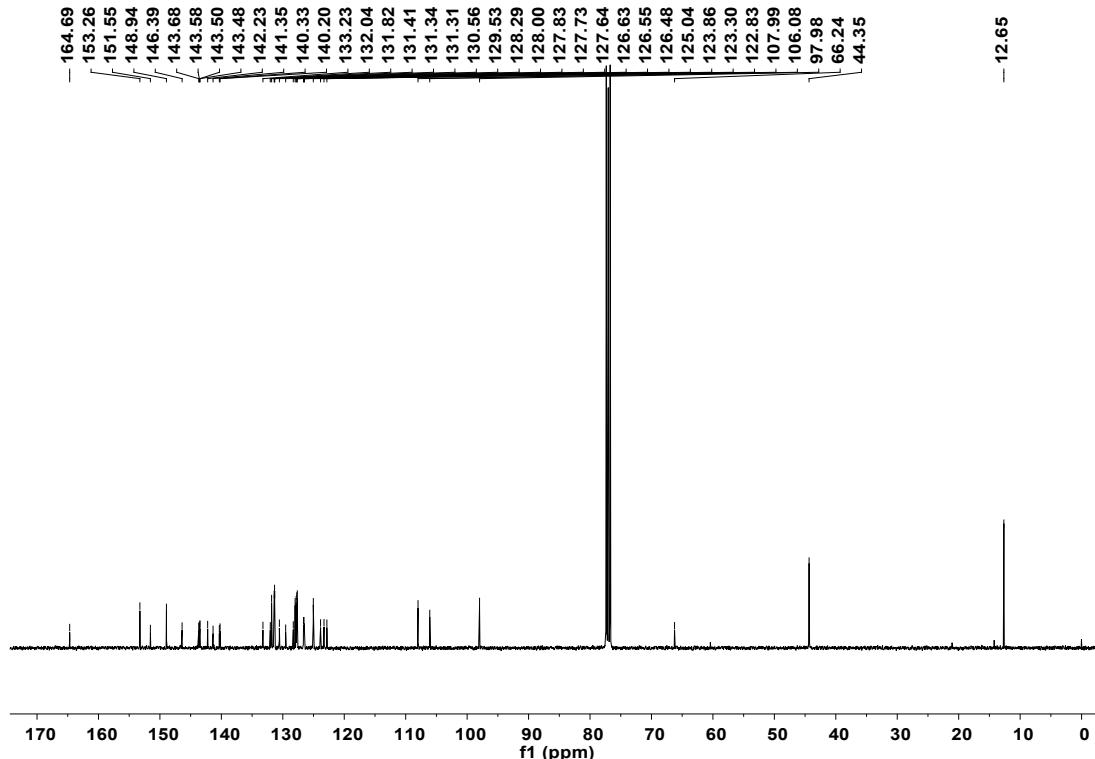
Fig. S2 ^{13}C NMR spectrum (in CDCl$_3$) of **TPEThRB**.
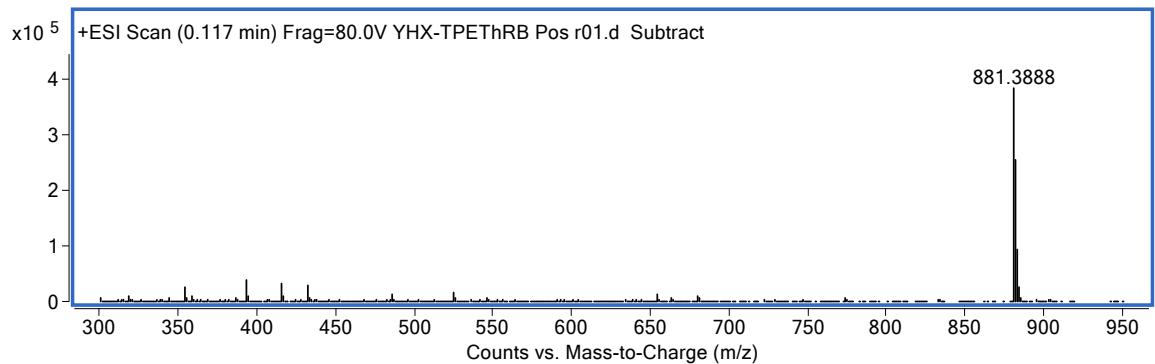
Fig. S3 Mass spectrum (ESI) of **TPEThRB**.
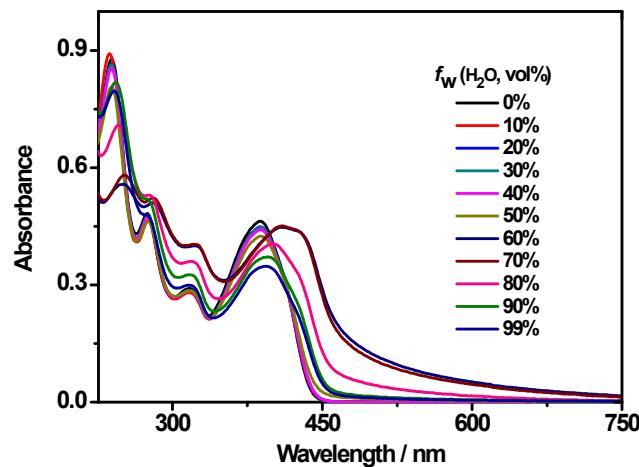
Fig. S4 Absorption spectra of **TPEThRB** (10 μM) in CH_3CN-H_2O mixtures (f_w = 0-99%).
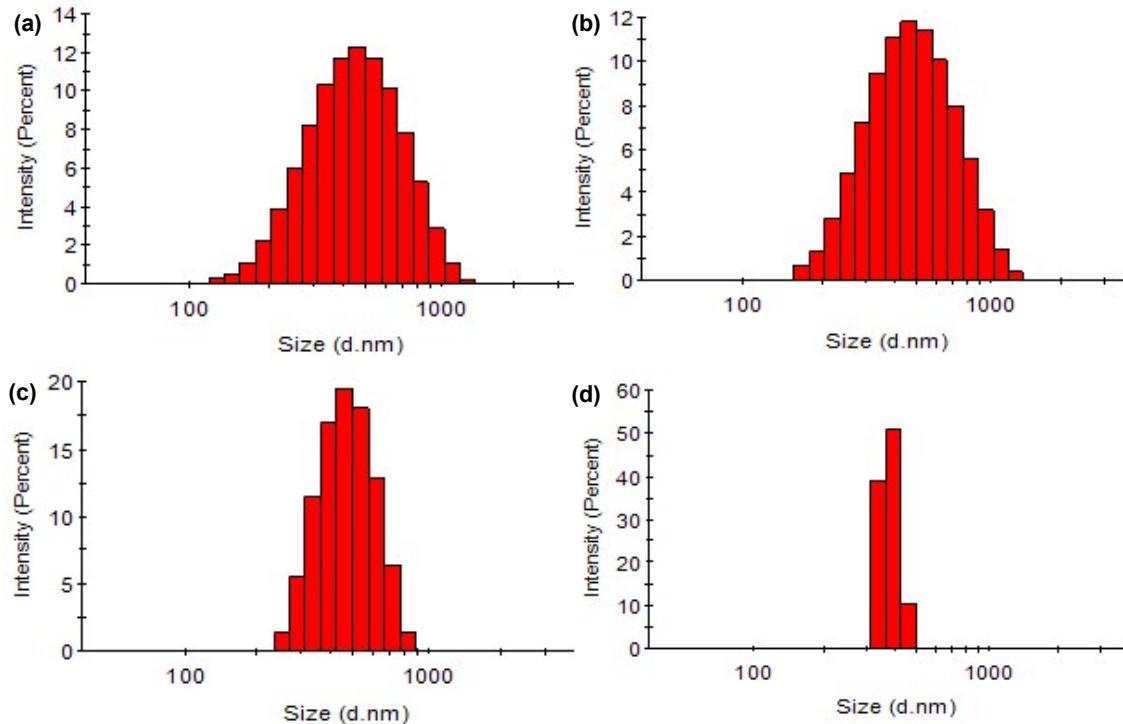
Fig. S5 Particle size distributions of **TPEThRB** in CH_3CN-H_2O mixtures with different water contents, (a) f_w = 60%, (b) f_w = 70%, (c) f_w = 80% and (d) f_w = 90%.
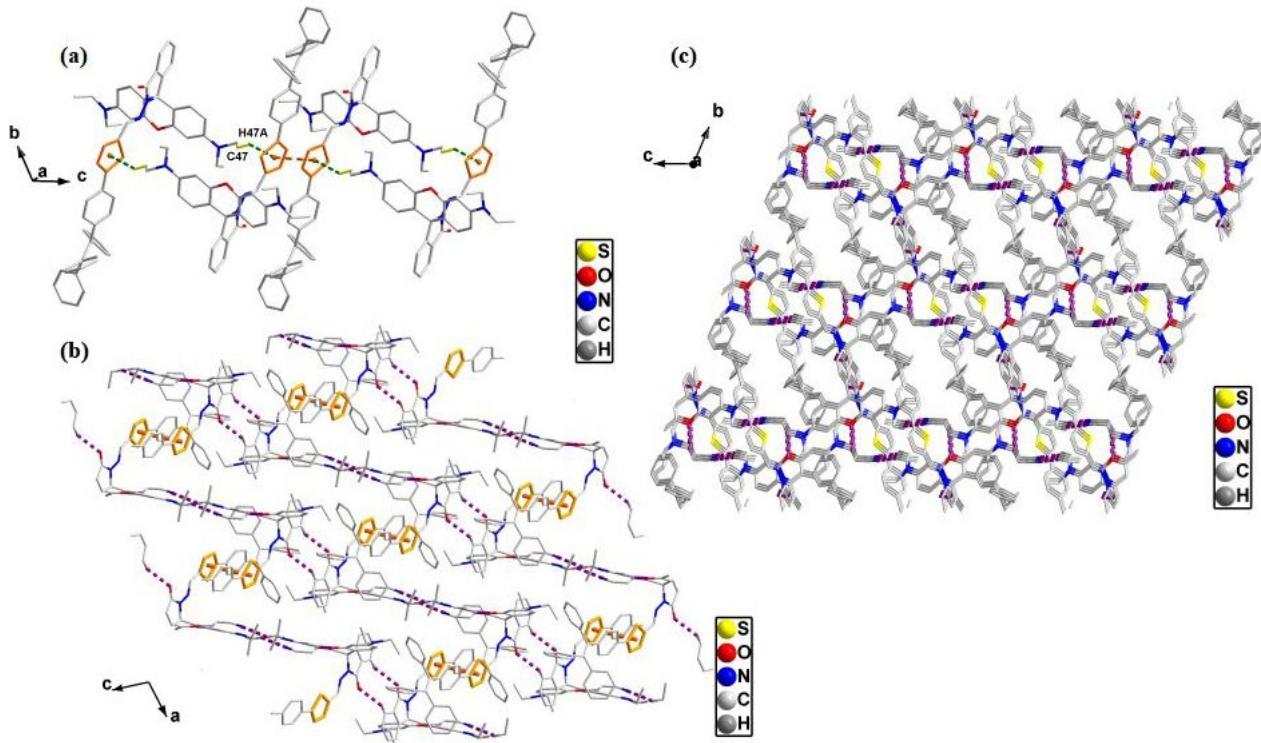
Fig. S6 The 2D stacking modes of **TPEThRB** along (a) a axis, (b) b axis and (c) 3D stacking mode.
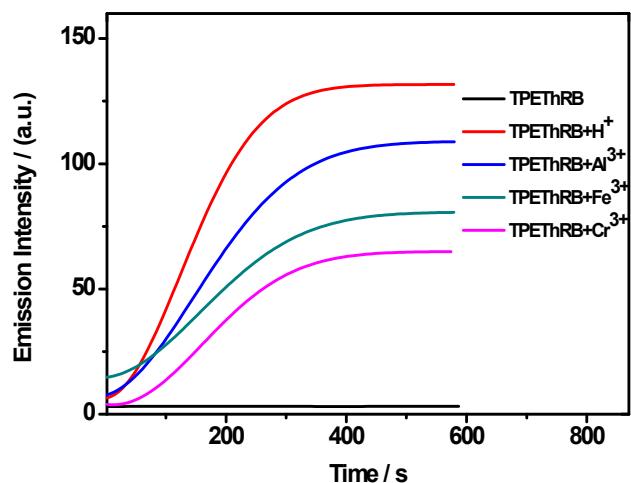
Fig. S7 Response time of **TPEThRB** (10 μM) in CH_3CN-H_2O (v:v 3:2) mixtures with Fe^{3+} (50 μM), Al^{3+} (150 μM), Cr^{3+} (150 μM), H^+ (150 μM).
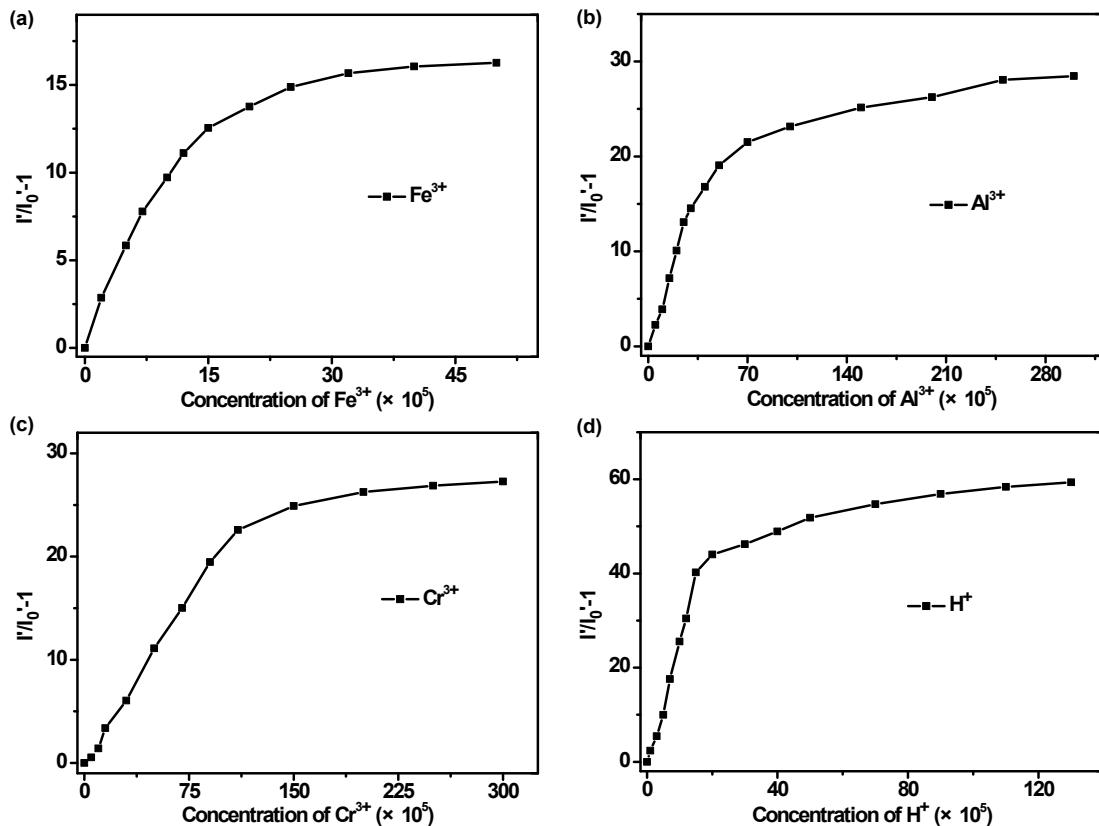
Fig. S8. Fluorescence titration plots of compound **TPEThRB** (10 μM) in CH_3CN-H_2O solution with different species (a) Fe^{3+}, (b) Al^{3+}, (c) Cr^{3+}, (d) H^+.
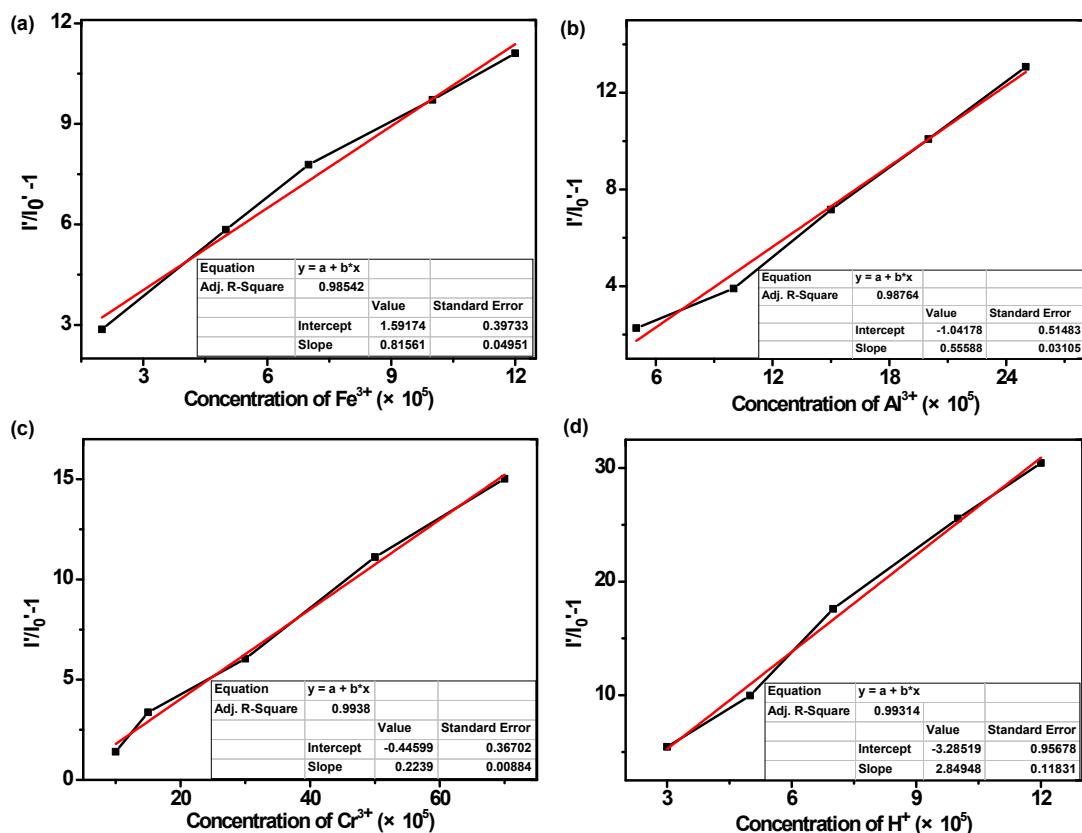
Fig. S9 The plots of $[I'/I_0'-1]$ versus the concentration of trivalent metal cations and H^+, (a) Fe^{3+}, (b) Al^{3+}, (c) Cr^{3+}, (d) H^+.
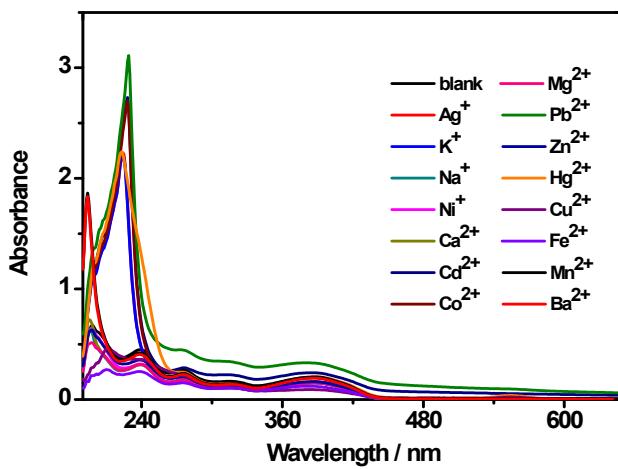
Fig. S10 UV-vis absorption spectra of **TPEThRB** with monovalent and divalent metal ions.
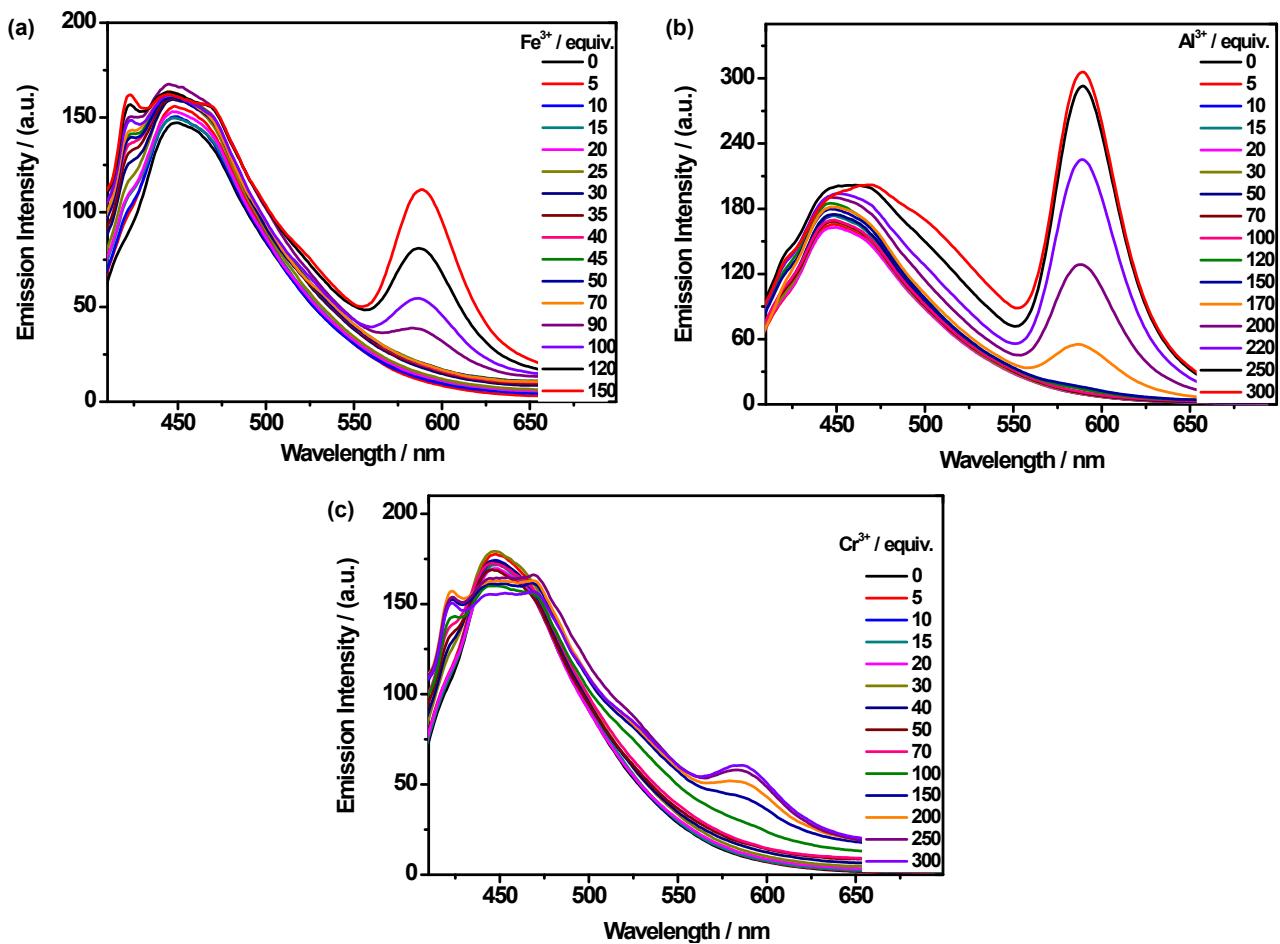
Fig. S11 Fluorescence spectra of compound **TPEThRB** with different species (a) Fe^{3+}, (b) Al^{3+}, (c) Cr^{3+} in CH_3CN-PBS (10 mM, pH = 7.4) mixture.
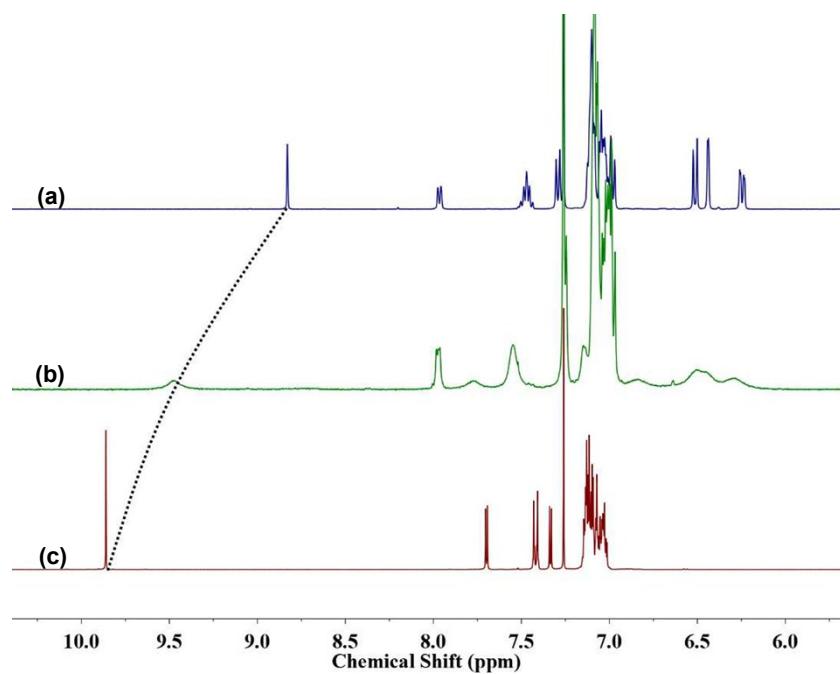
Fig. S12 ^{1}H NMR spectra (in CDCl$_3$) of (a) **TPEThRB**, (b) **TPEThRB** with H$^+$ ion and (c) compound **1.**
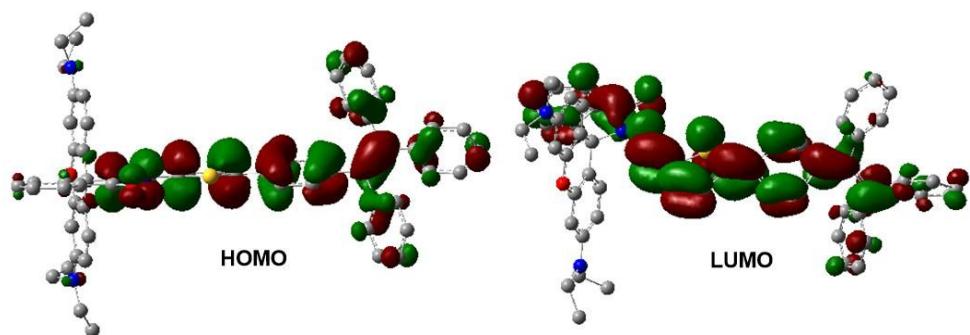
Fig. S13 Molecular orbitals of **TPEThRB** through DFT calculations with the B3LYP method.
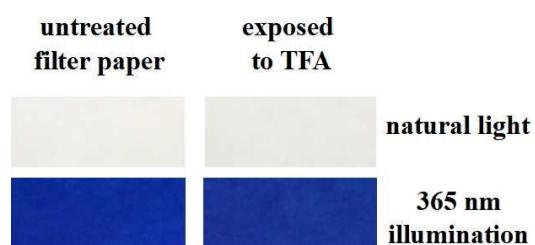
Fig. S14 The photographs of blank filter paper exposed to TFA vapor under natural light and the 365 nm UV lamp illumination.
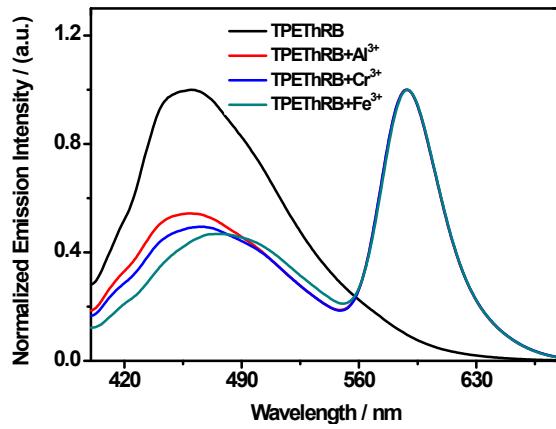
Fig. S15 Normalized fluorescence spectra of **TPEThRB** in the absence and presence of Fe^{3+}, Al^{3+} and Cr^{3+} ions.

Table S1 The summarizing list of detection limits of materials for sensing Fe^{3+}, Al^{3+} and Cr^{3+} ions.

| Material	LOD of Fe^{3+} (μM)	Material	LOD of Al^{3+} (μM)	Material	LOD of Cr^{3+} (μM)
bis(rhodamine)	50	6-thoxychomone-3-carbaldehyde-hydrazone	0.18	Pyrene derivative PB	0.23
Phenanthroimidazole derivative	5.26	naphtalimide and naphthaldehyde-based derivative	6.28	rhodamine-2-amino-5-bromopyrimidine	4.9
salicylaldehydeazine	9.5	Eu-BTB anionic framework	100	$\{[Zn_2(\mu_3\text{-}OH)(cpta)(4,4'\text{-}bipy)]\cdot H_2O\}_n$	5.55
Zn-MOF-74 nanodot	1.04	naphthalene-quinoline derivative	0.0367	2,7-disubstituted phenanthrene derivative	400
2D terbium(III) coordination polymer Tb-CP	0.05	copolymer-ATP supramolecular complex CP-ATP	3.7	Rhodamine capped gold nanoparticles	9.28
TPEThRB	3.2	**TPEThRB**	4.8	**TPEThRB**	11.9

Table S2 CheckCIF report of XRD data of single crystal of **TPEThRB** (CCDC 1814395).

Bond precision:	C-C = 0.0049 A	Wavelength=0.71073	
Cell:	a=13.5619(9)	b=13.7951(10)	c=15.3779(11)
	alpha=110.309(2)	beta=101.188(2)	gamma=97.849(2)
Temperature:	296 K		

	Calculated		Reported
Volume	2581.1(3)		2581.1(3)
Space group	P -1		P -1
Hall group	-P 1		-P 1
Moiety formula	$C_{59} H_{52} N_4 O_2 S$,	$C_2 H_3 N$	
Sum formula	$C_{61} H_{55} N_5 O_2 S$		$C_{61} H_{55} N_5 O_2 S$
Mr	922.16		922.16
Dx,g cm^{-3}	1.186		1.187
Z	2		2
Mu (mm-1)	0.111		0.111
F000	976.0		976.0
F000'	976.60		
h,k,lmax	16,16,18		16,16,18
Nref	9147		9139
Tmin,Tmax	0.982,0.989		0.980,0.989
Tmin'	0.980		

Data completeness= 0.999	Theta(max)= 25.048	
R(reflections)= 0.0572(5281)	wR2(reflections)= 0.1466 (9139)	
S = 1.019	Npar = 622	