"Phenothiazine-Functionalized Pyridine-Based AIEE- Active Molecule: A Versatile Molecular Probe for Highly Sensitive Detection of Hypochlorite and Picric Acid"

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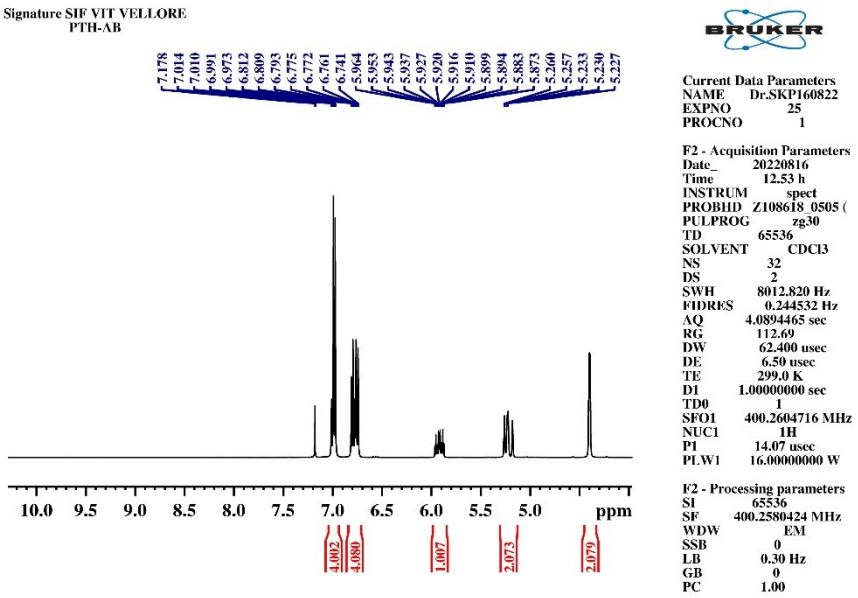

Fig S1. ^{1}H NMR of **PTH-AB** in $CDCl_3$ (400 MHz)

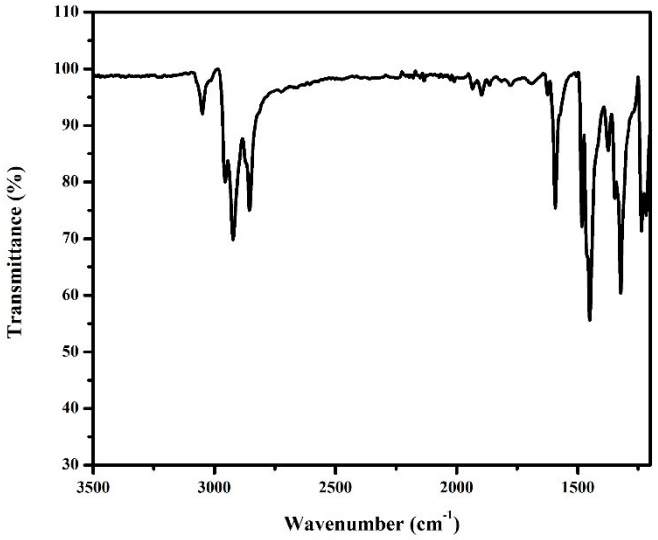

Fig S2. FT-IR data of **PTH-AB**

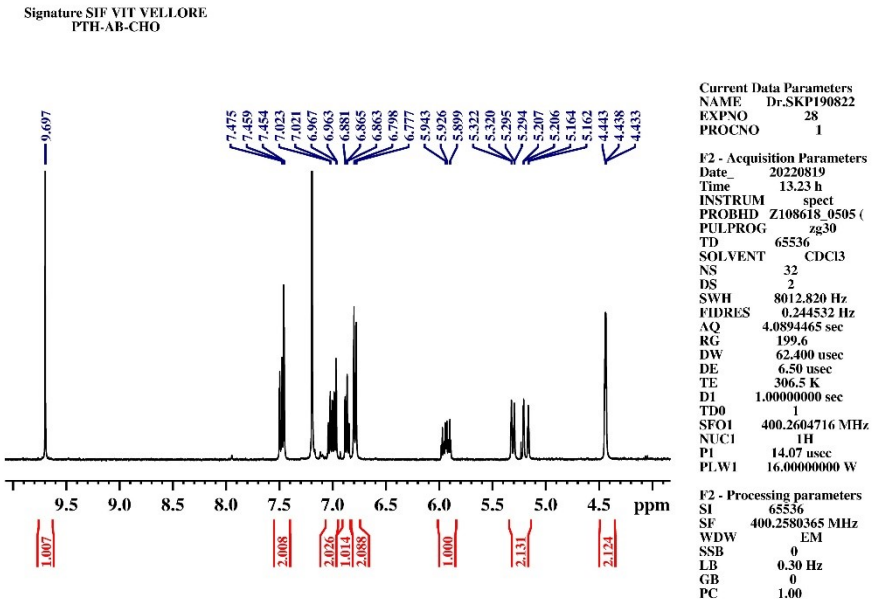

Fig S3. ^{1}H NMR of **PTH-AB-1CHO** in $CDCl_3$ (400 MHz)

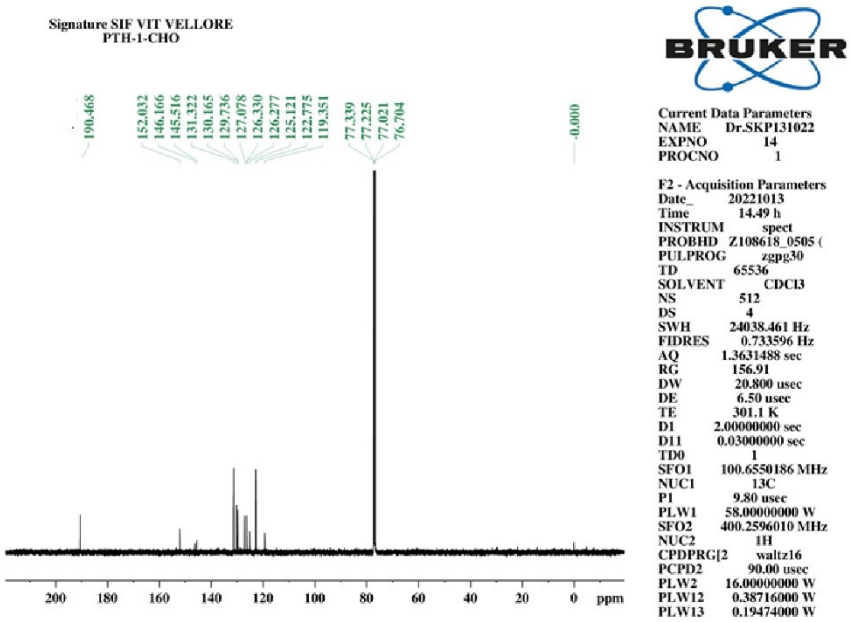

Fig S4. ^{13}C NMR of **PTH-AB-1CHO** in $CDCl_3$ (400 MHz)

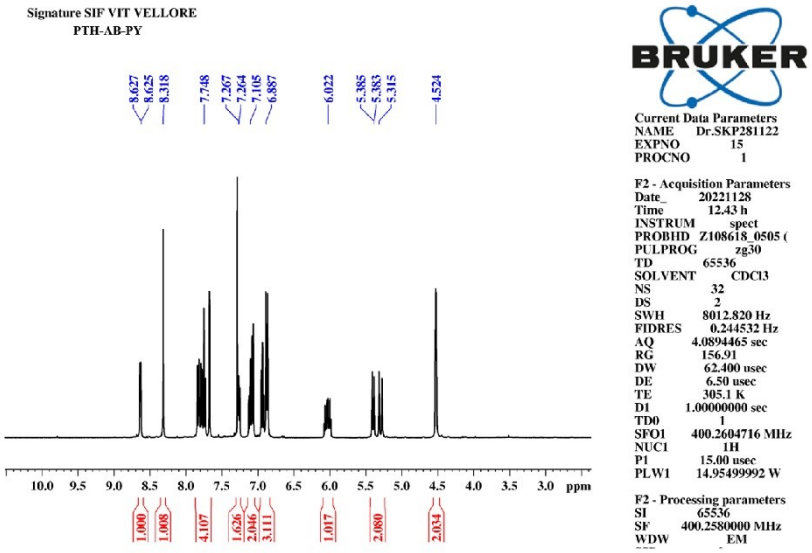

Fig S5. ^{1}H NMR of **PTH-AB-PY** in $CDCl_3$ (400 MHz)

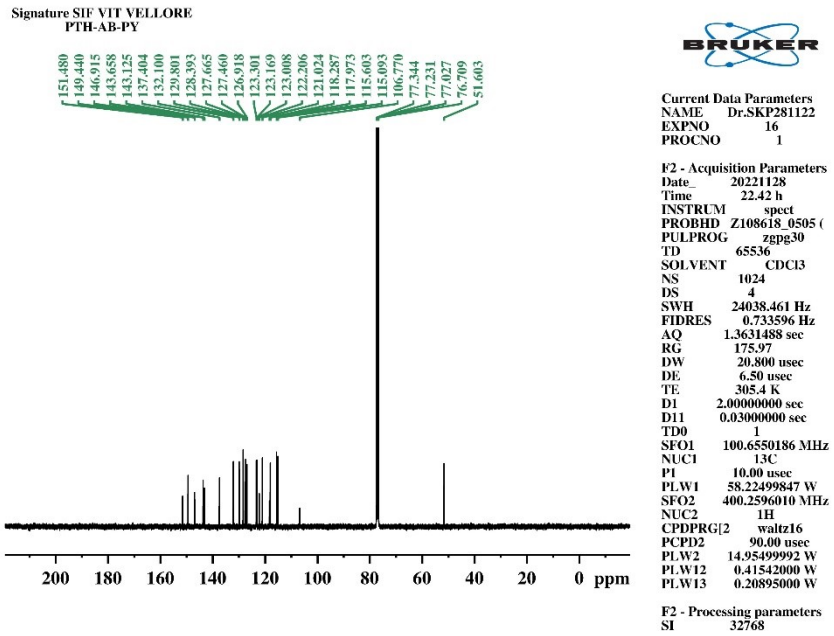

Fig S6. ^{13}C NMR of **PTH-AB-PY** in $CDCl_3$ (400 MHz)

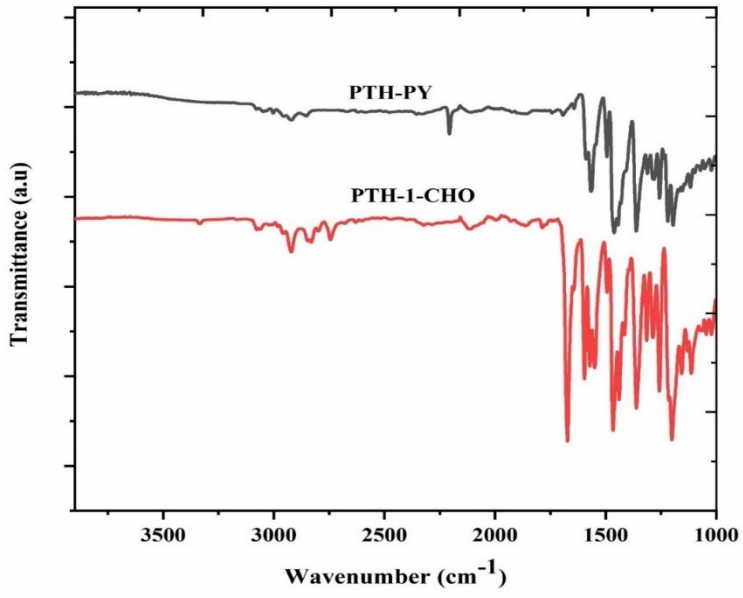

Fig S7. FT-IR spectrum of **PTH-AB-PY**

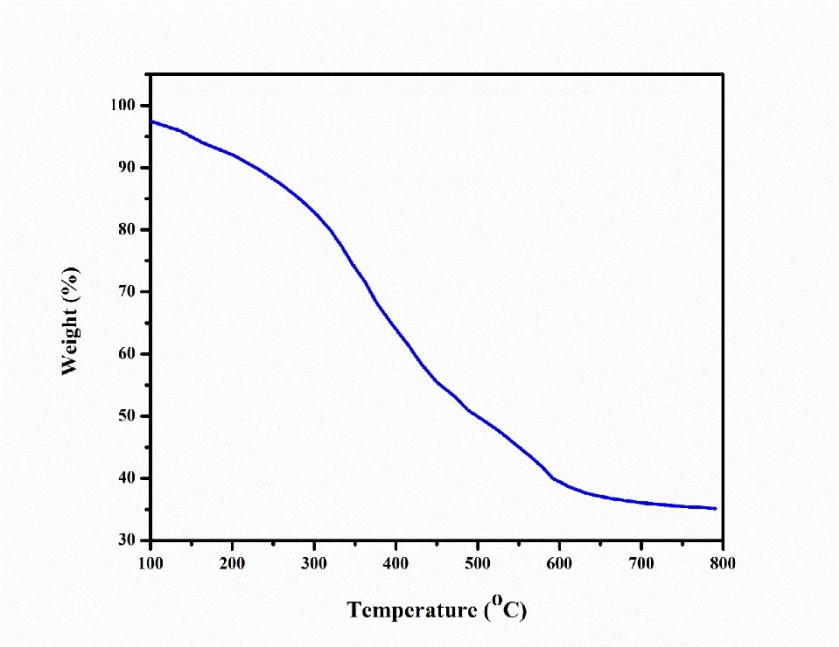

Fig S8. TGA data of **PTH-AB-PY**

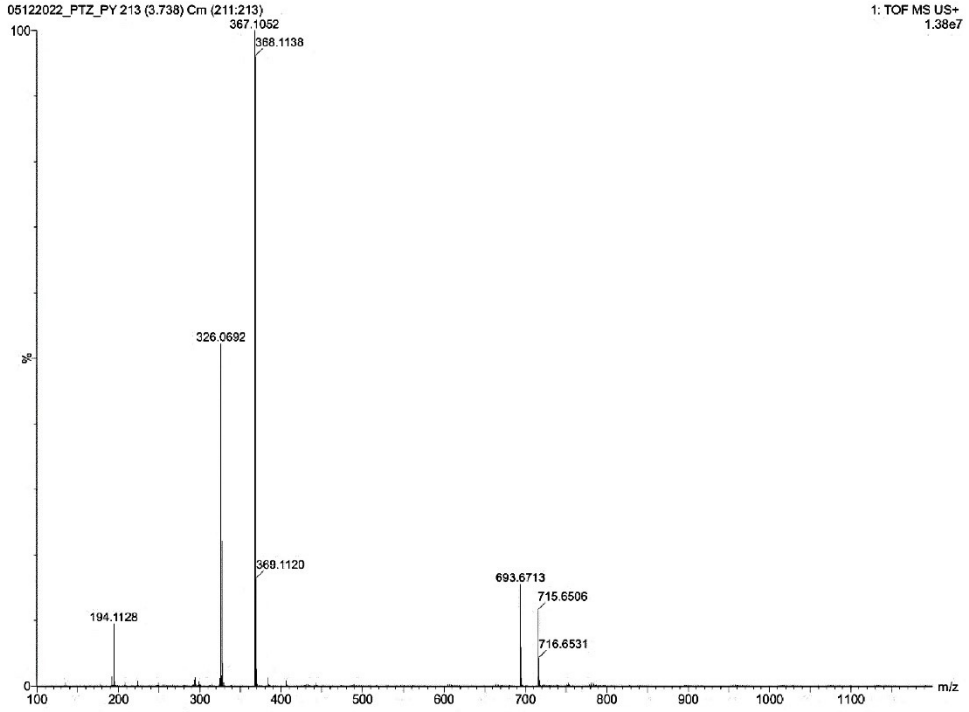

Fig S9. HRMS spectrum of **PTH-AB-PY**

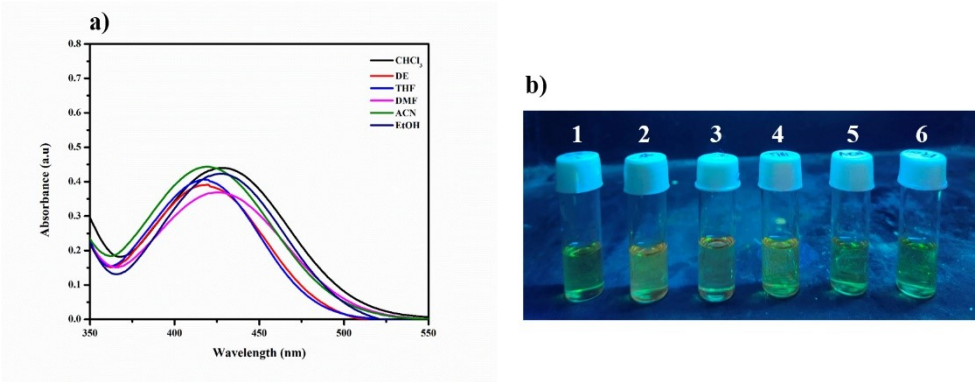

Fig S10. (a) Solvent effect of PTH-AB-PY in UV-vis region. (b) Visual changes of PTH-AB-PY in various solvents

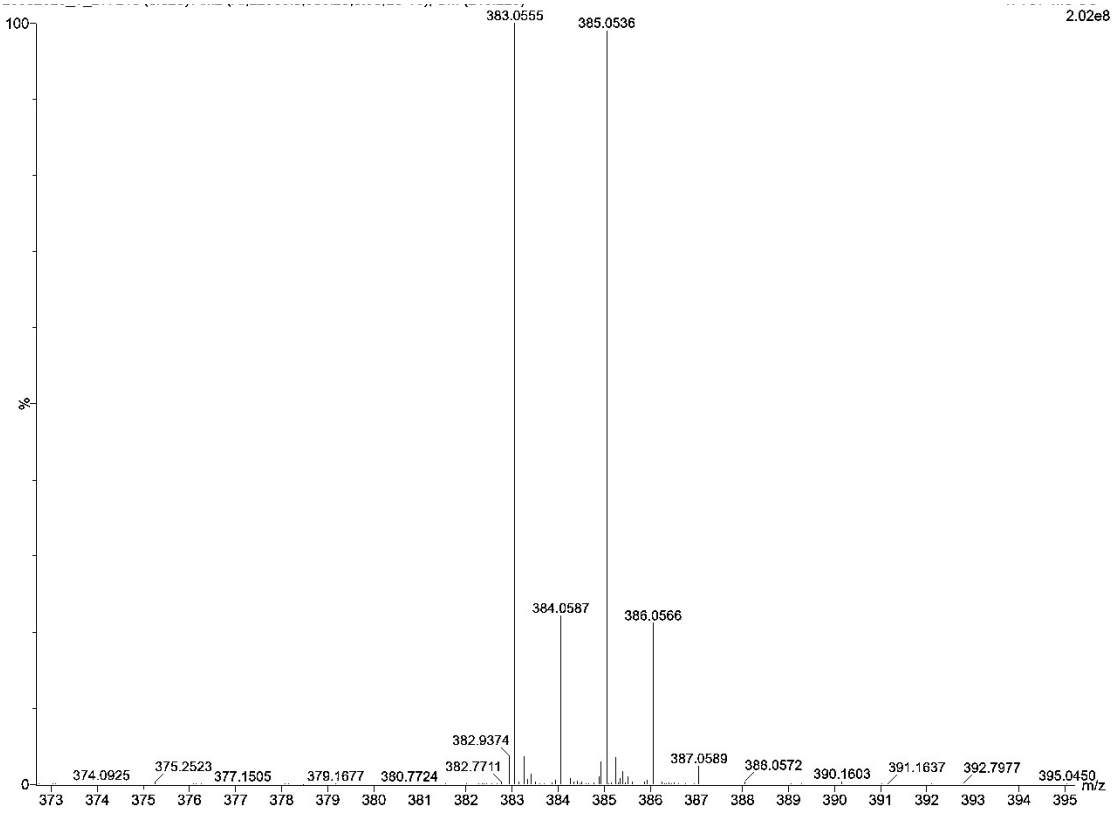

Fig S11. HRMS Data of PTH-AB-PY with hypochlorite

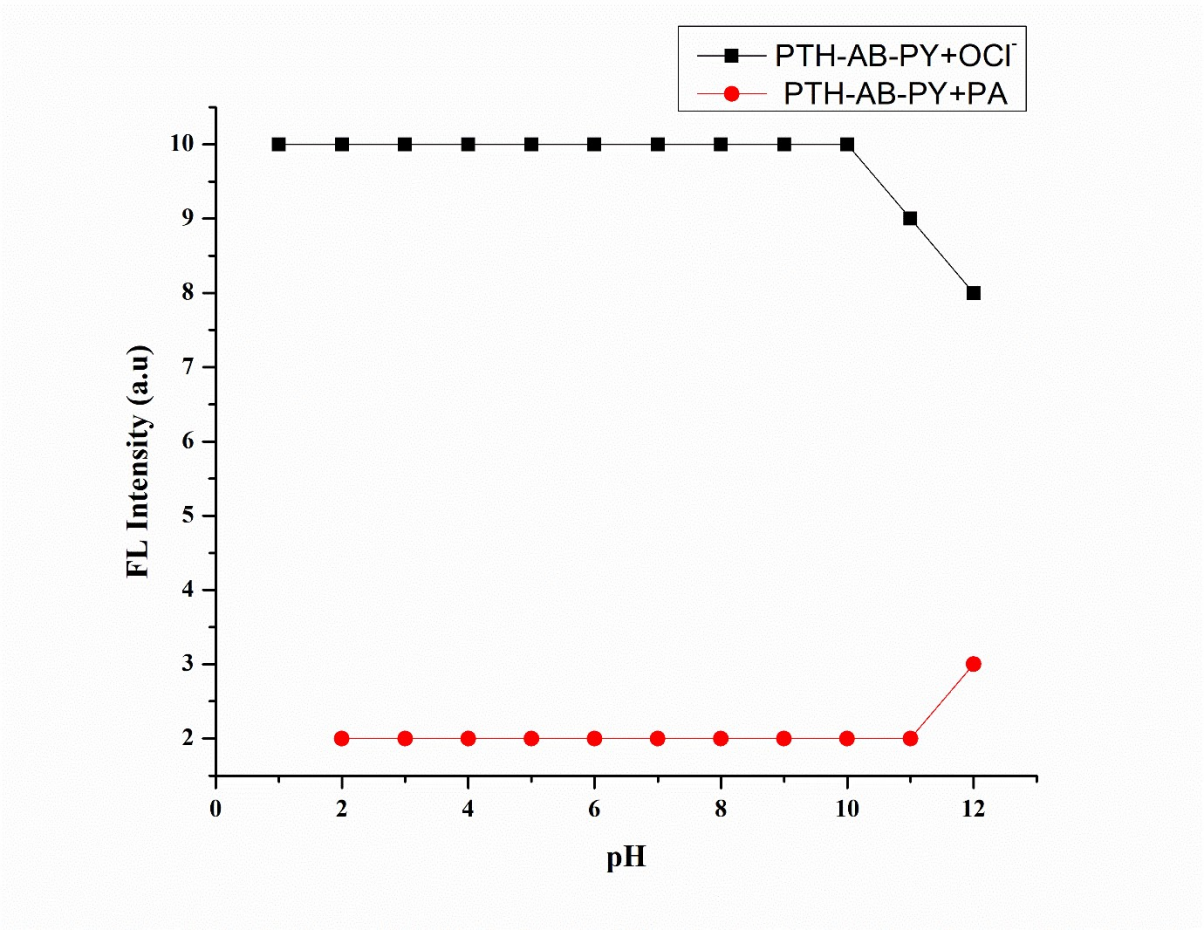

Fig S12. pH plot of both hypochlorite and picric acid with PTH-AB-PY

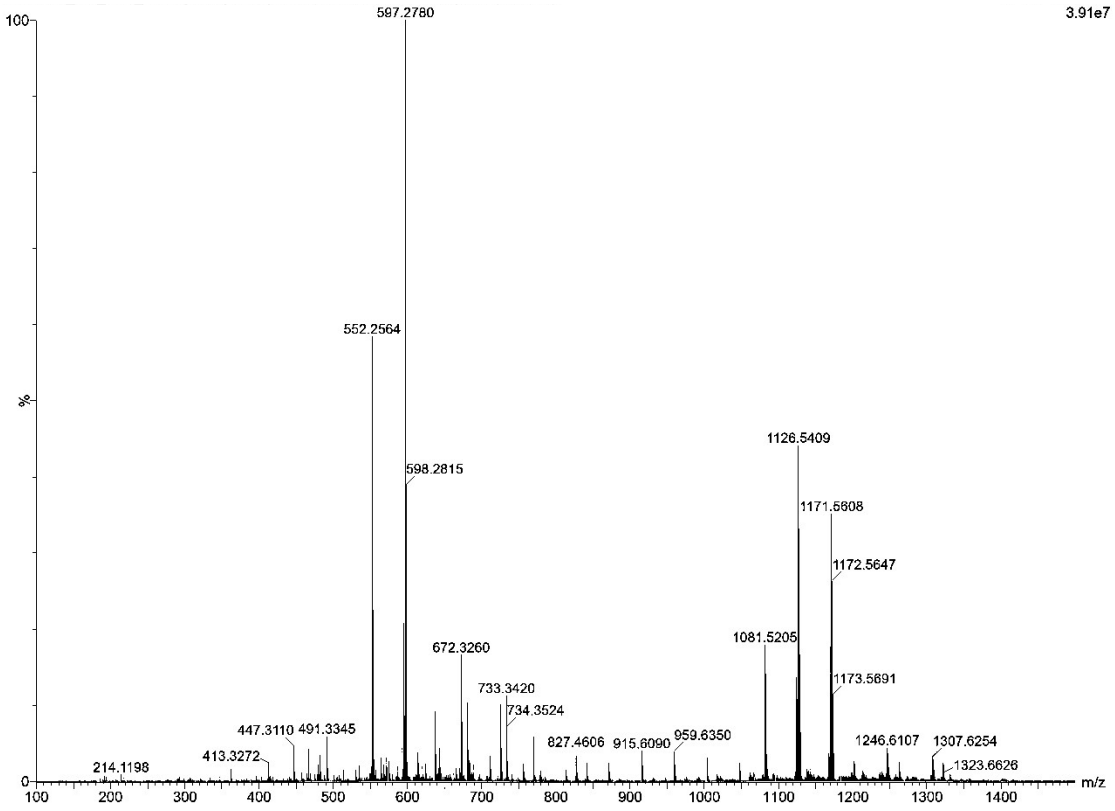

Fig S13. HRMS Data of PTH-AB-PY with picric acid

Table S1. The crystallographic data and parameters for the refinement of the PTH-AB-PY	
Compound	PTH-AB-PY
CCDC Number	2278692
Molecular formula	$C_{23}H_{17}N_3S$
Crystal system	Monoclinic
Point group	P21/n
a (Å)	9.3292 (16)
b (Å)	14.298 (2)
c (Å)	14.191 (3)
Temperature (K)	300
Wavelength (Å)	0.71073
α (deg)	90
β (deg)	96.460(6)
γ (deg)	90
V (Å)	1880.9(6)
Z	4
μ (mm-1)	0.184
Dcalc (g/cm3)	1.298
R1	0.0547
wR2	0.1283

Table S2. Bond Lengths for **PTH-AB-PY**					
Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C11	1.756(2)	C9	C1	1.446(3)
S1	C23	1.756(2)	C9	C14	1.396(3)
N3	C12	1.401(2)	C23	C18	1.391(3)
N3	C18	1.417(2)	C23	C22	1.384(3)
N3	C15	1.465(2)	C4	C5	1.384(3)
N1	C4	1.332(2)	C18	C19	1.394(3)
N1	C8	1.326(3)	C16	C15	1.498(3)
C12	C11	1.401(3)	C16	C17	1.294(3)
C12	C13	1.392(3)	C19	C20	1.379(3)
C11	C10	1.376(3)	C3	N2	1.146(3)
C13	C14	1.375(3)	C22	C21	1.376(3)
C2	C1	1.349(3)	C21	C20	1.369(3)
C2	C4	1.479(3)	C5	C6	1.366(3)
C2	C3	1.432(3)	C7	C8	1.375(3)
C9	C10	1.398(3)	C7	C6	1.365(3)

Table S3. Bond Angles for **PTH-AB-PY**								
Atom	Atom	Atom	Angle/˚		Atom	Atom	Atom	Angle/˚
C23	S1	C11	100.15(9)		C22	C23	C18	120.83(19)
C12	N3	C18	121.40(16)		C2	C1	C9	132.66(19)
C12	N3	C15	118.71(16)		N1	C4	C2	116.38(17)
C18	N3	C15	118.87(16)		N1	C4	C5	121.62(19)
C8	N1	C4	117.74(18)		C5	C4	C2	121.94(19)
C11	C12	N3	120.66(17)		C23	C18	N3	120.94(18)
C13	C12	N3	121.59(17)		C23	C18	C19	117.79(19)
C13	C12	C11	117.74(18)		C19	C18	N3	121.27(19)
C12	C11	S1	120.24(15)		C13	C14	C9	122.24(19)
C10	C11	S1	118.32(14)		C17	C16	C15	126.7(2)
C10	C11	C12	121.07(18)		N3	C15	C16	116.97(18)
C14	C13	C12	120.69(18)		C20	C19	C18	120.6(2)
C1	C2	C4	122.00(18)		N2	C3	C2	177.2(2)
C1	C2	C3	122.33(19)		C21	C22	C23	120.5(2)
C3	C2	C4	115.59(17)		C20	C21	C22	119.1(2)
C10	C9	C1	125.86(18)		C6	C5	C4	119.2(2)
C14	C9	C10	116.70(18)		C21	C20	C19	121.1(2)
C14	C9	C1	117.42(18)		C6	C7	C8	117.3(2)
C11	C10	C9	121.52(17)		N1	C8	C7	124.2(2)
C18	C23	S1	120.29(16)		C7	C6	C5	119.8(2)
C22	C23	S1	118.78(16)					

Table S4: Comparison of previously reported phenothiazine probe

S. No	Probe	Test media	Operation mode	LOD (M)	Response time (s)	Ref
1	ERC-Ctrl	ACN : H_2O = 3 : 7	Ratiometric	0.44 x 10^{-4}	6	37
2	CPD	DMSO : H_2O = 1 :5	Ratiometric	0.012 x 10^{-4}	10	38
3	**PTH-AB-PY**	ACN : H_2O = 1:1	Ratiometric	6.8 x 10^{-4}	3	This work

Table S5: Results for the Detection of ClO^- in water samples

Analyte	Water samples	Spiked level (M)	Found level (M)	Recovery (%)
Hypochlorite	River water	2.00 x 10^{-4}	1.98 x 10^{-4}	99
		4.00 x 10^{-4}	3.97 x 10^{-4}	99.2
	Tap water	2.00 x 10^{-4}	1.99 x 10^{-4}	99.5
		4.00 x 10^{-4}	3.92 x 10^{-4}	98
Picric acid	River water	2.00 x 10^{-4}	2.01 x 10^{-4}	100
		4.00 x 10^{-4}	3.8 x 10^{-4}	95
	Tap water	2.00 x 10^{-4}	1.98 x 10^{-4}	99
		4.00 x 10^{-4}	3.86 x 10^{-4}	96.5

Table S6: Results for the Detection of ClO^- in Vegetable Samples

Analyte	Water samples	Spiked level (M)	Found level (M)	Recovery (%)
Hypochlorite	Tomato	3.00 x 10^{-4}	3.00 x 10^{-4}	100
	Carrot	3.00 x 10^{-4}	2.9 x 10^{-4}	96.6
Picric acid	Tomato	3.00 x 10^{-4}	2.8 x 10^{-4}	93.33
	Carrot	3.00 x 10^{-4}	2.98 x 10^{-4}	99.33