One-Step Synthesis of a pH Switched Pyrene-Based Fluorescent Probe for Ratiometric Detection of HS^- in real water samples

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Supplementary data

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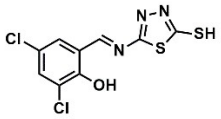
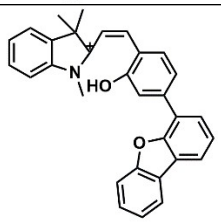
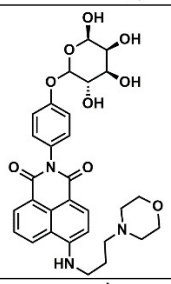
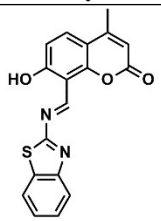
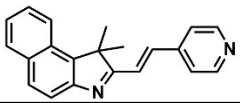
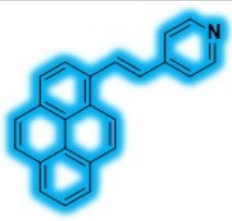
Table S1. Comparison of proposed probe with recently reported pH responsive fluorescent probe.

S.NO	Probe	pH range	Emission (λ_{max})	Solvent	Stoke shift	Reversibility with specific analyte	Reference
1.		7.2	579 nm	50 % aq. MeOH	-	-	[1]
2.		4.0-8.0	570 nm	Hexane, THF, EtOH, MeCN, And DMSO	87,95,106 ,111, and 122nm	-	[2]
3.		4.5-6.0	550 nm	Tris buffer-HCl	100 nm	-	[3]
4.		12.0	560 nm	EtOH	107 nm	-	[4]
5.		3.0-6.0	510 nm	H_2O	-	-	[5]
6.		2.0	595 nm	70 % aq. ACN	113 nm	HS^-	This work

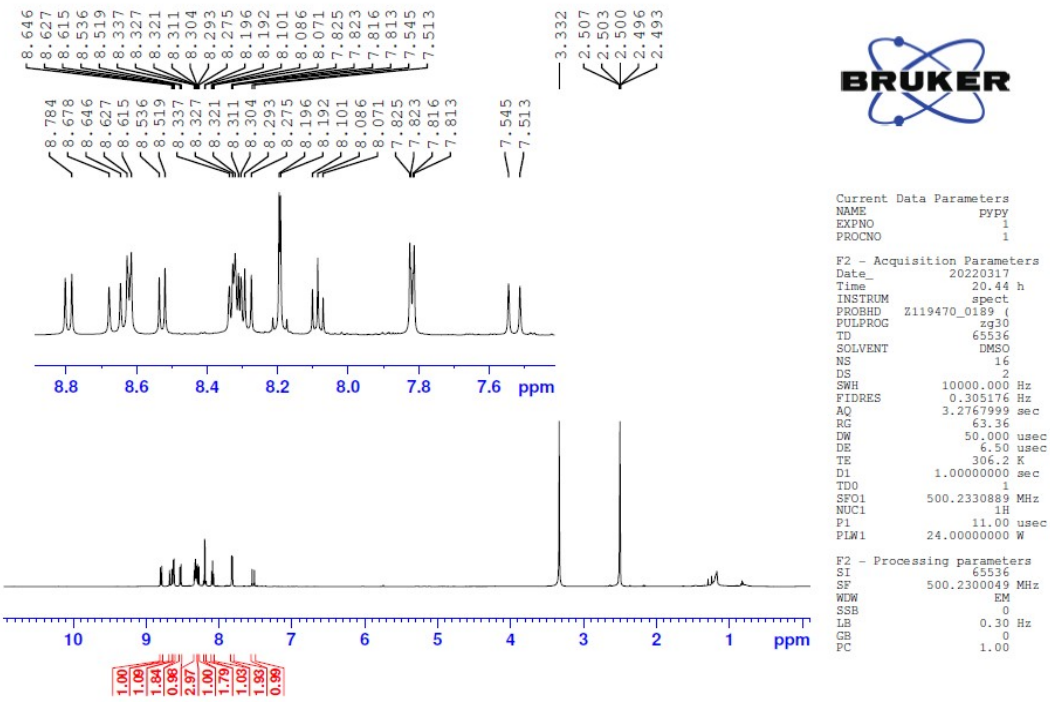


Figure. S1. [1]H NMR Spectrum of Pyr

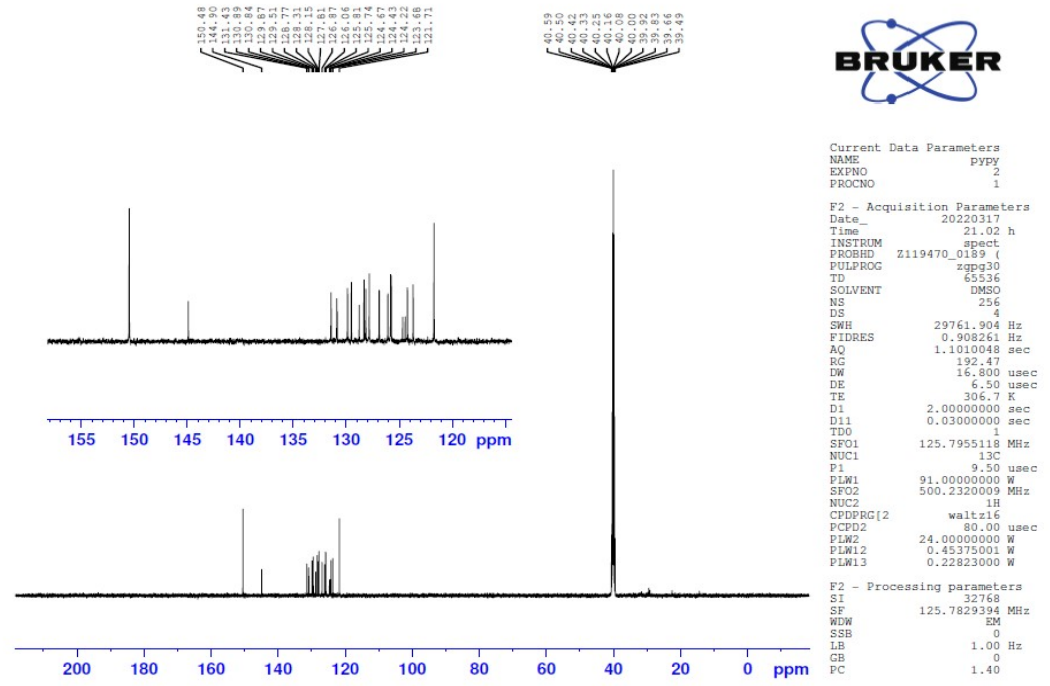


Figure. S2. [13]C NMR Spectrum of Pyr

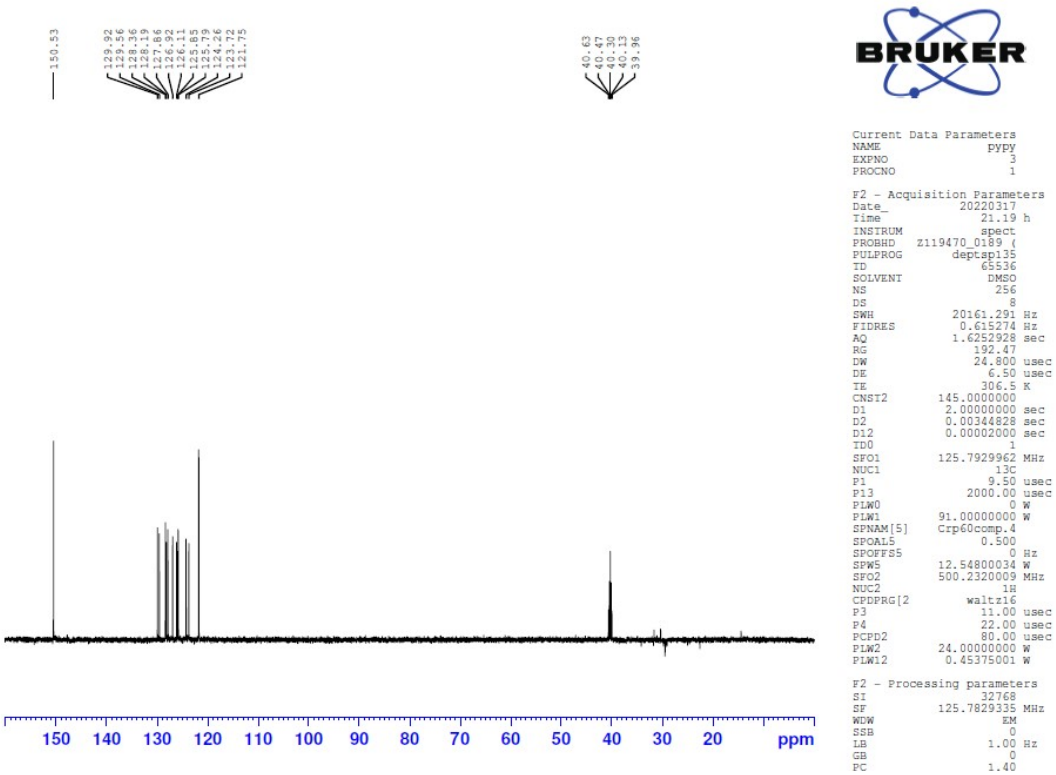


Figure S3. DEPT 135 NMR spectrum of Pyr

Figure S4. LR-Mass spectrum of Pyr

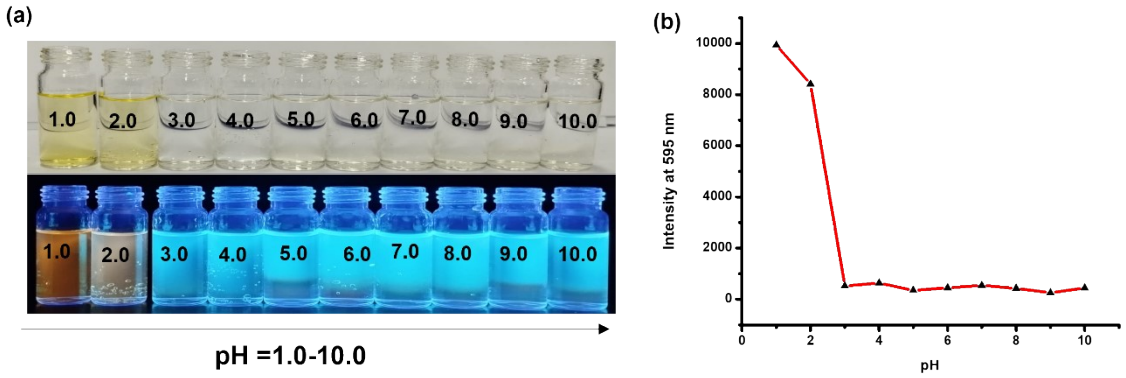


Figure S5. (a) Colorimetric and fluorescence changes of Pyr in 10 mM PBS containing 30% ACN of pH values from 1.0 to 10.0 (b) Fluorescence intensities of Pyr in 10 mM PBS containing 30% ACN of pH values from 1.0 to 10.0

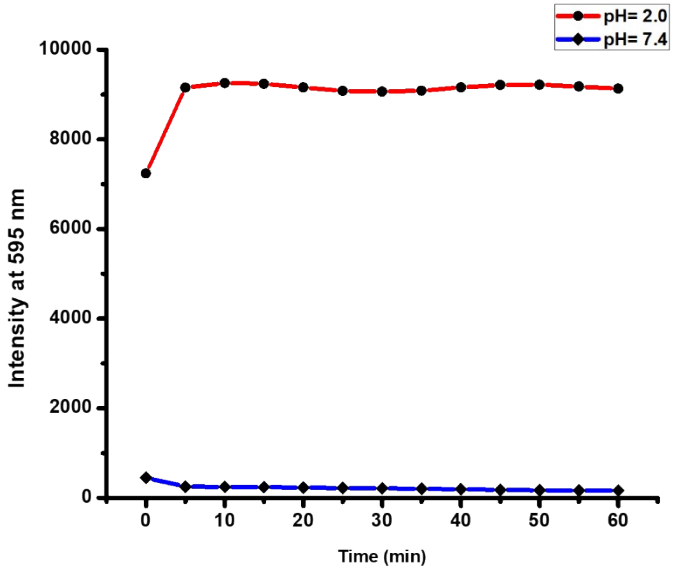


Figure S6. Time-dependent fluorescence intensity of Pyr at 595 nm from 0 to 60 minutes in 10 mM PBS with 30% ACN and pH values of 2.0 (red line) and 7.4 (blue line).

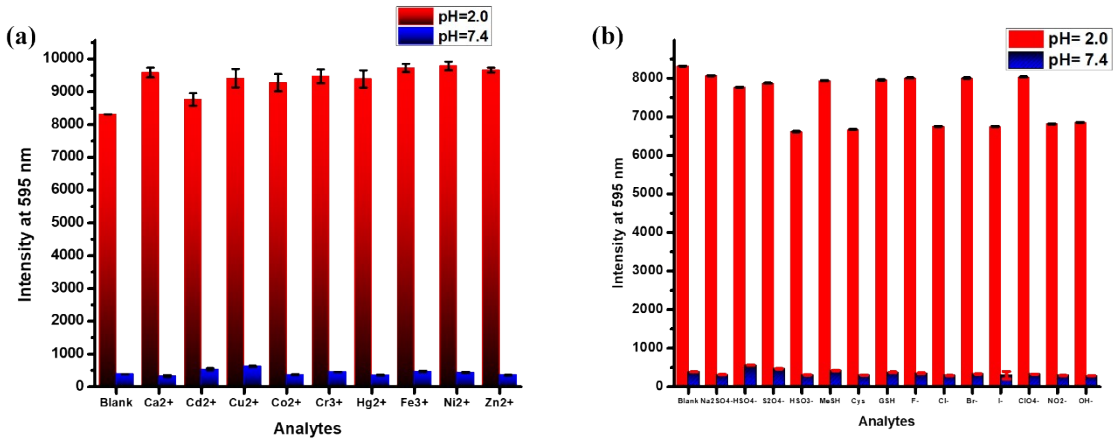


Figure S7. Fluorescence intensity of Pyr at 595 nm in 10 mM PBS containing 30% ACN of pH 2.0 (red bars) and 7.4 (blue bars) upon treatment with 400 μM series of different cations, anions, and amino acids.

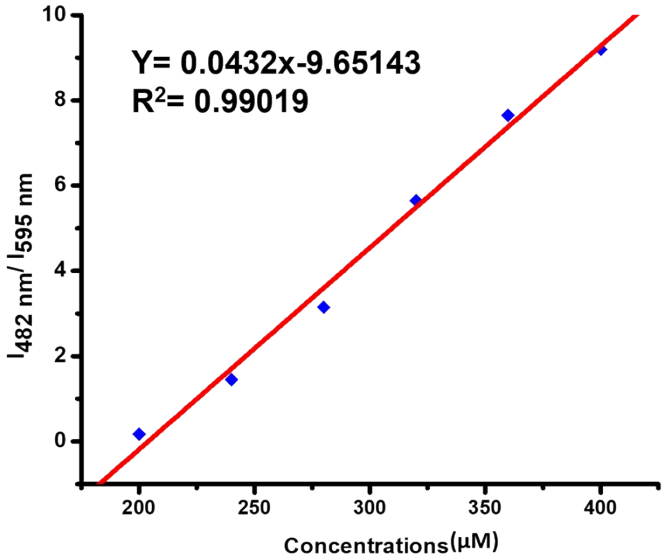


Figure S8. Linear relationship of $I_{482\ nm}/I_{595\ nm}$ vs HS^- from 0-400 μM.

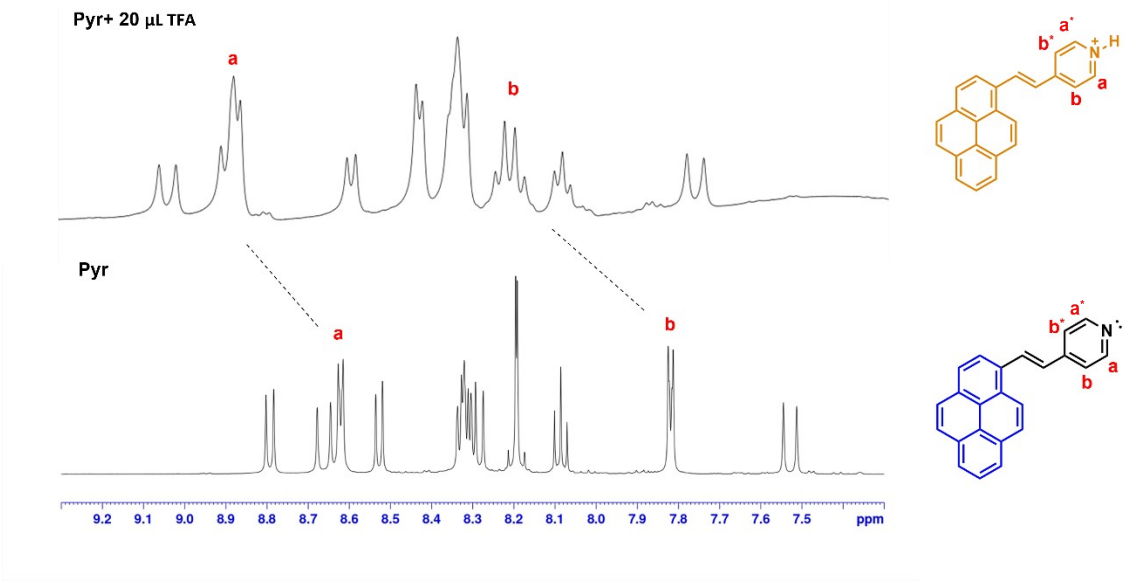


Figure S9. ^{1}H NMR spectrum of probe before and after addition of TFA (20 µL)

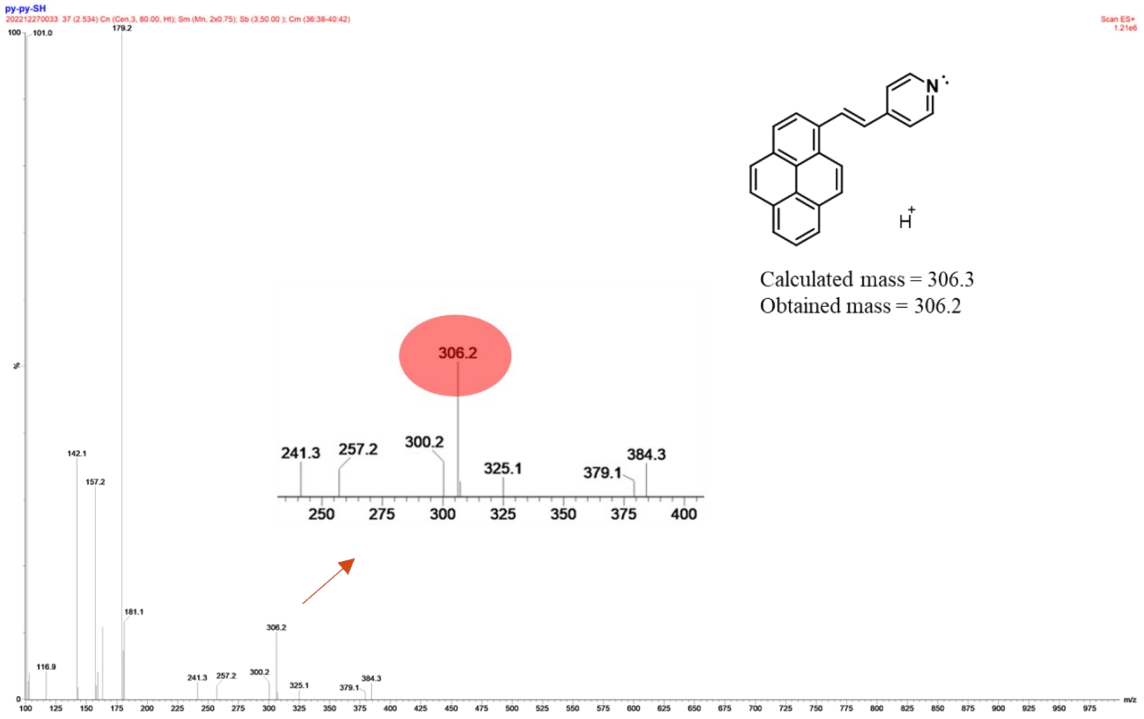


Figure S10. ESI mass spectrum of PyrH after reacted with HS^-

ESI 1. Detection limit and quantum yield calculation

Based on the IUPAC definition, the detection limit was determined based on the formula and the fluorescence titration data

LOD = 3Sb/m

Where Sb is the standard deviation of blank measurement and 'm' represents the slop between intensity and ion concentrations.

Quantum yield

$\Phi_S = \Phi_R I_S / I_R * A_R / A_S$

Φ_S- Quantum yield of sample; Φ_R- Quantum yield of reference (RhB = 0.32)

I_S- Integrated fluorescent area of sample; I_R- Integrated fluorescent area of reference

A_R- Absorbance of reference; A_S- Absorbance of sample

Table S2. Quantum yield data

Sample	Absorbance	Fluorescence (I_A)	Solutions	Φ
Rhodamine-B	1.0144	462259.3705	Water	0.32
PyrH	0.4409	140629.6275	30 % ACN in PBS	0.22
PyrH+HS^-	0.6149	64434.694	30 % ACN in PBS	0.07

Reference

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4 D. Singh, S. Tomar, S. Singh, G. Chaudhary, A. P. Singh and R. Gupta, *J. Photochem. Photobiol. A Chem.*, 2023, **435**, 114334.

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