Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Far-red to NIR emitting ultra-sensitive probe to detect the endogenous HOCl in zebrafish and Raw 264.7 cell line

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Supporting information

Figure S1. ^{1}H NMR spectrum of Isophorone with malononitrile

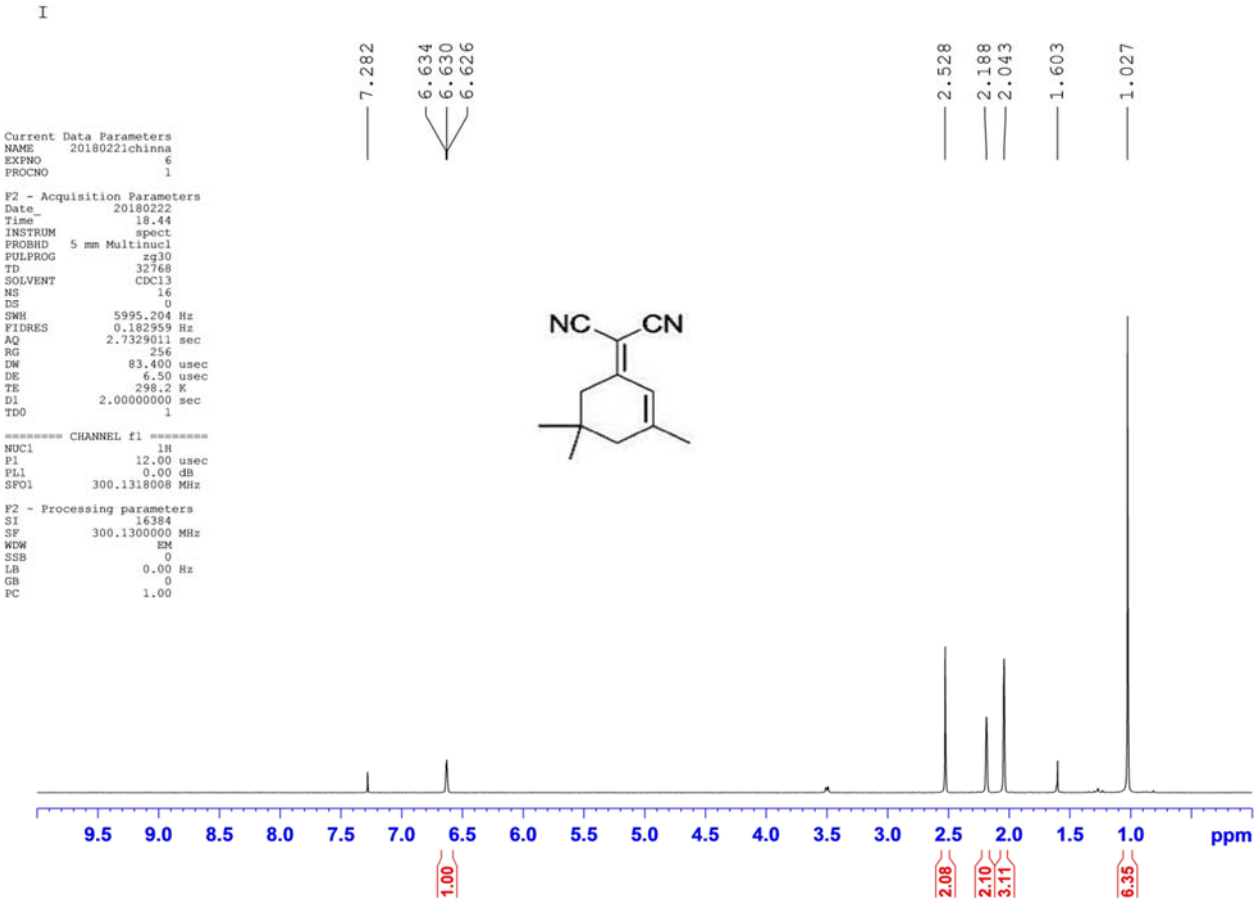

Figure S2. ^{1}H NMR spectrum of n-butylated phenothiazine

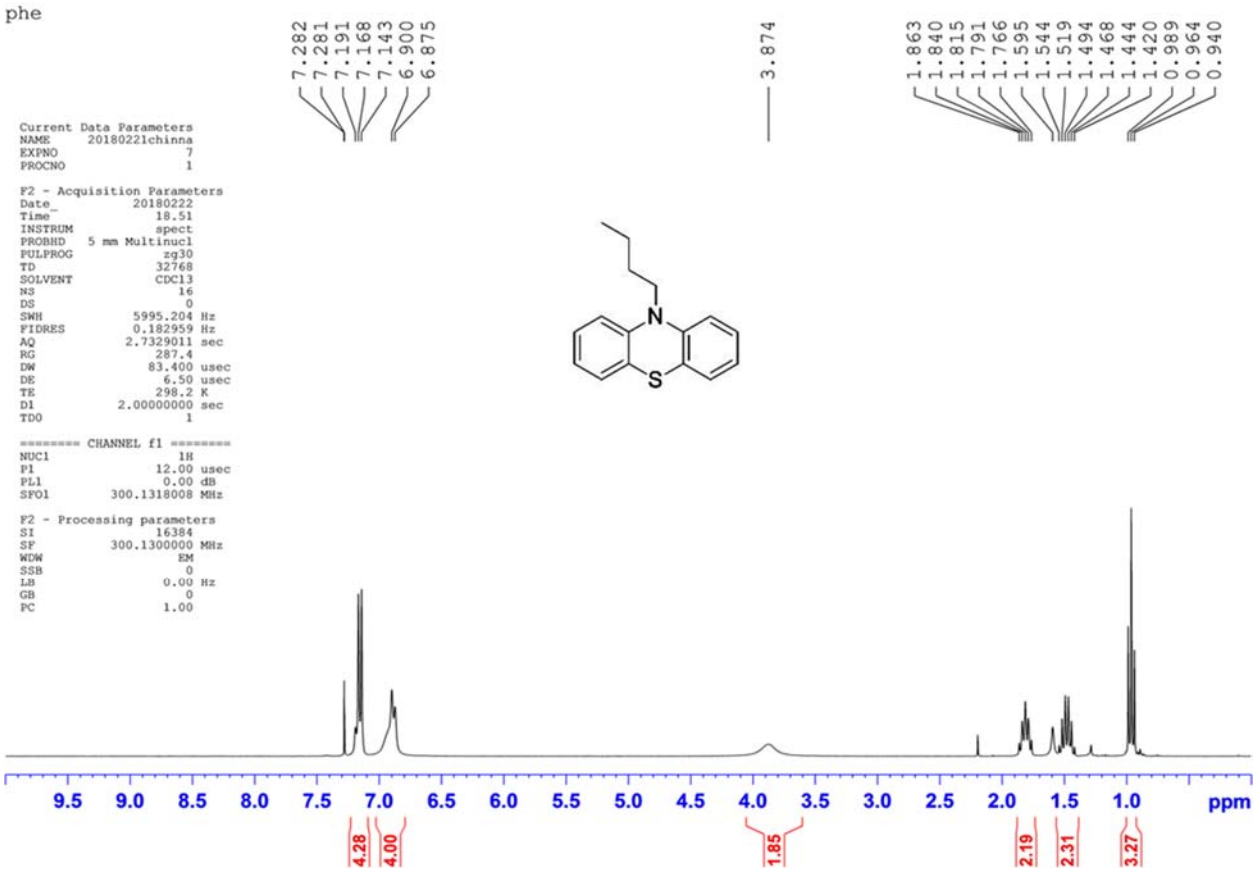

Figure S3. ^{1}H NMR spectrum of formyl phenothiazine

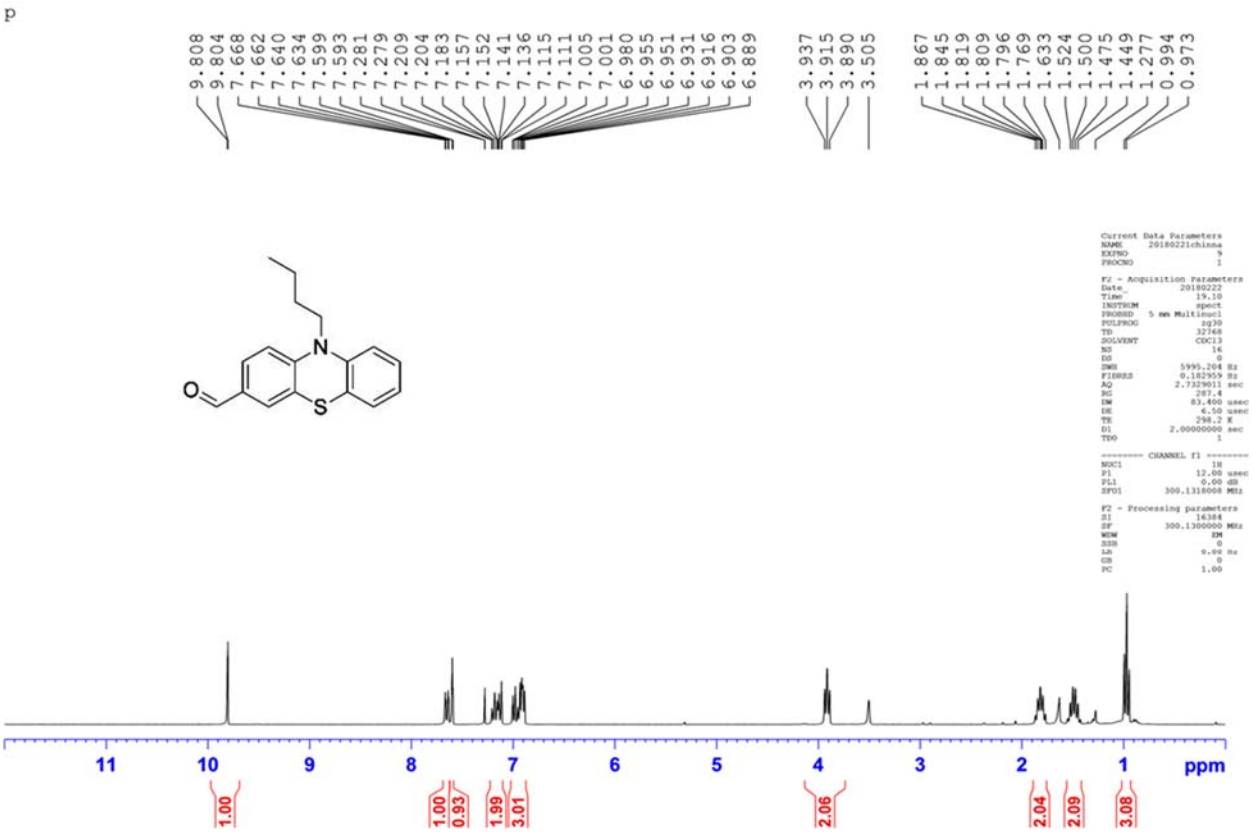

Figure S4. ^{1}H NMR spectrum of **PI**

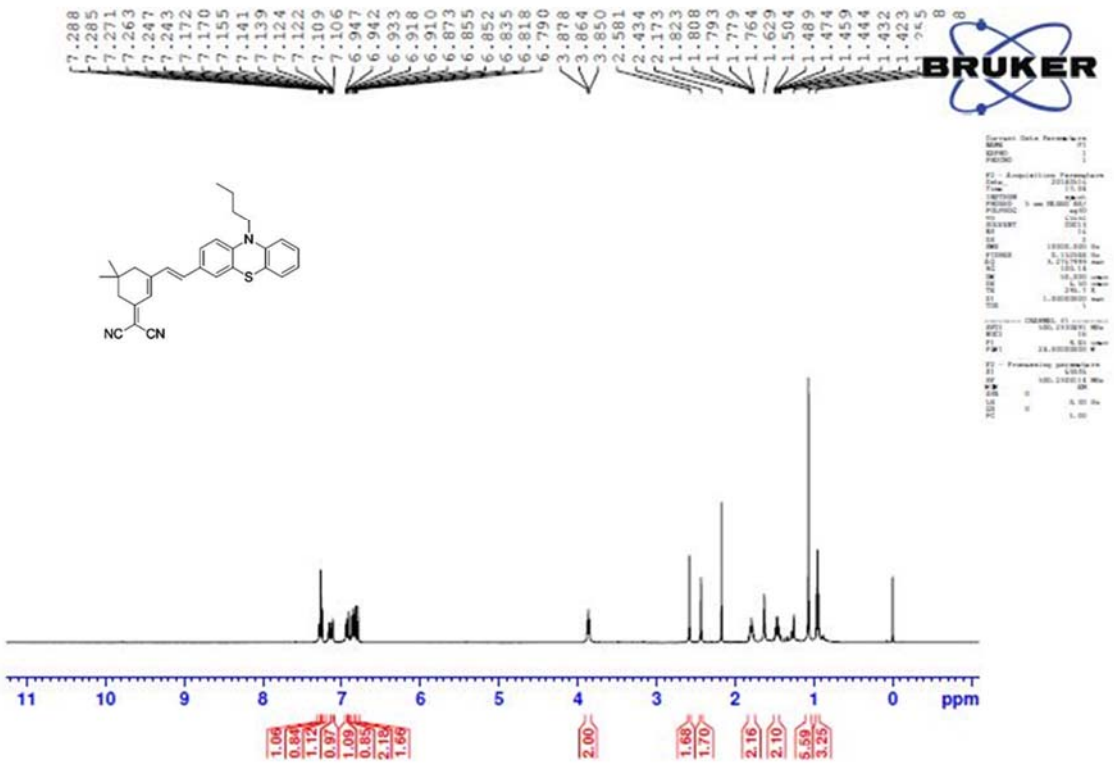

Figure S5. ^{1}H NMR spectrum (expansion) of PI

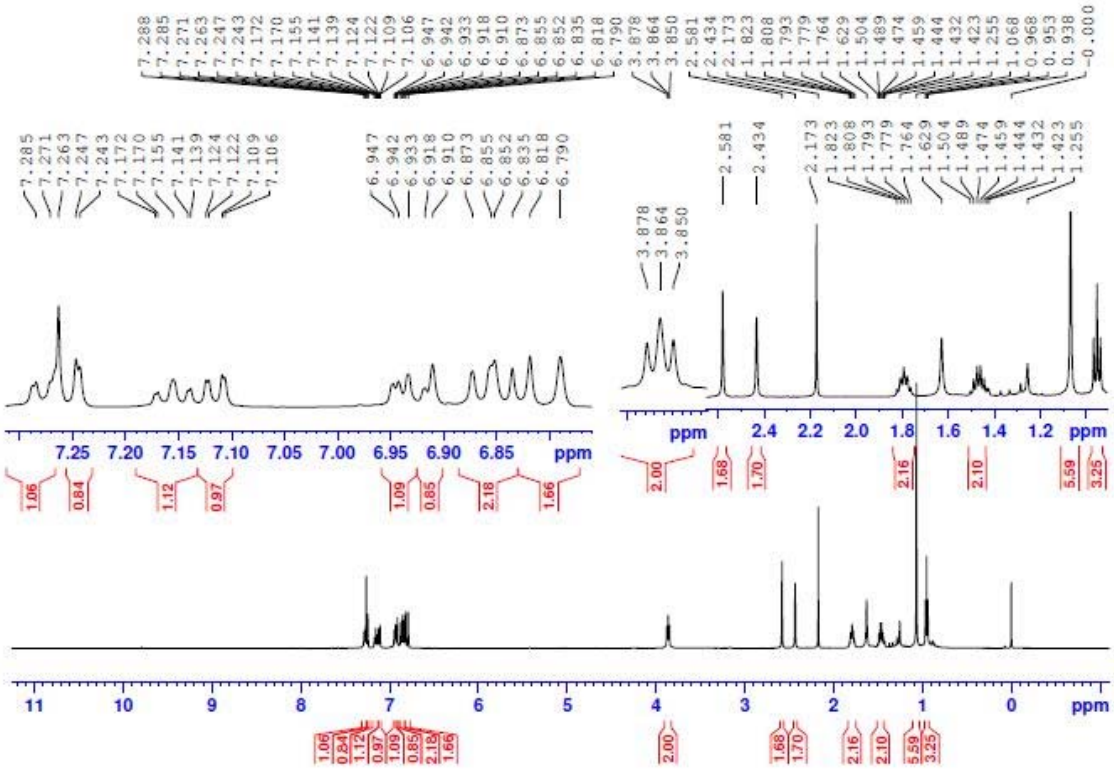

Figure S6. ^{13}C NMR spectrum of PI

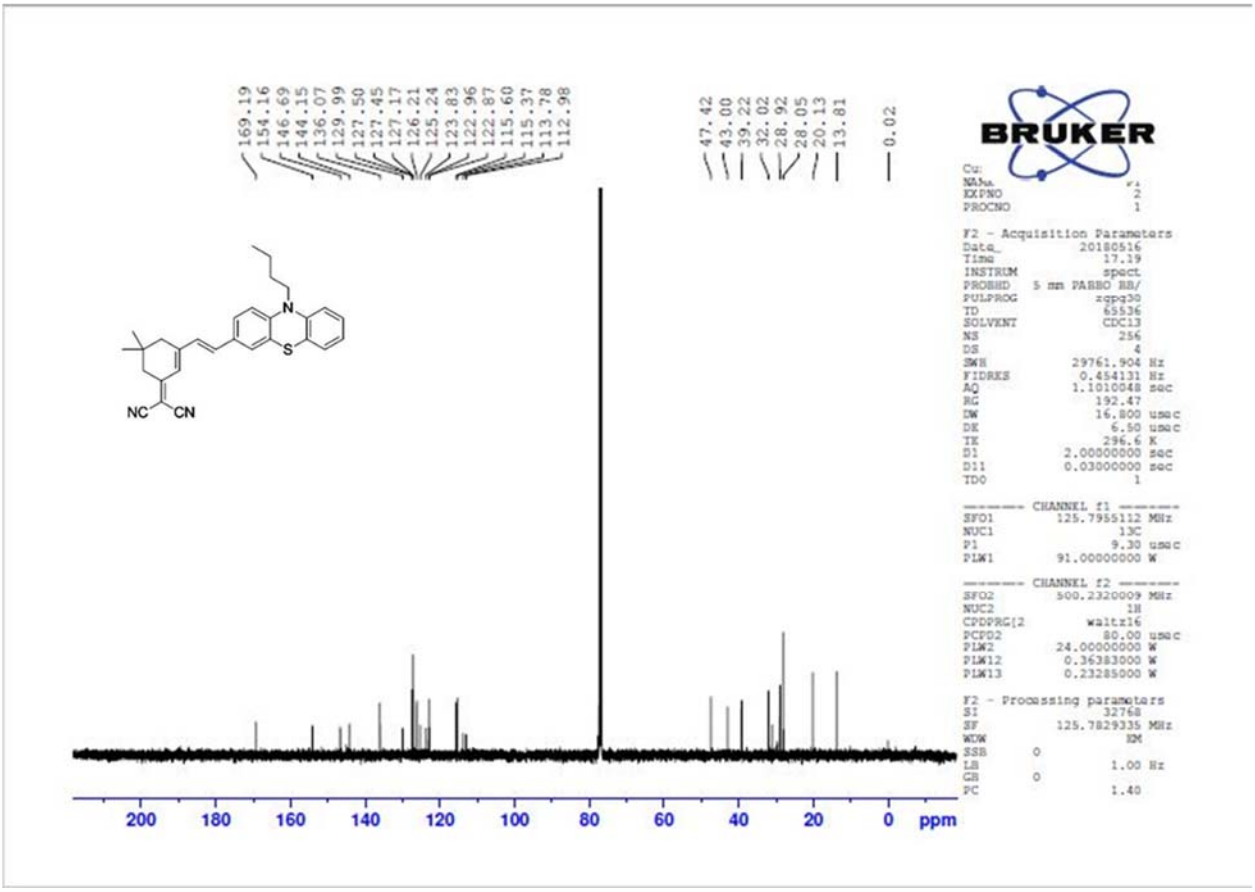

Figure S7. DEPT 135 ^{13}CNMR spectrum of PI

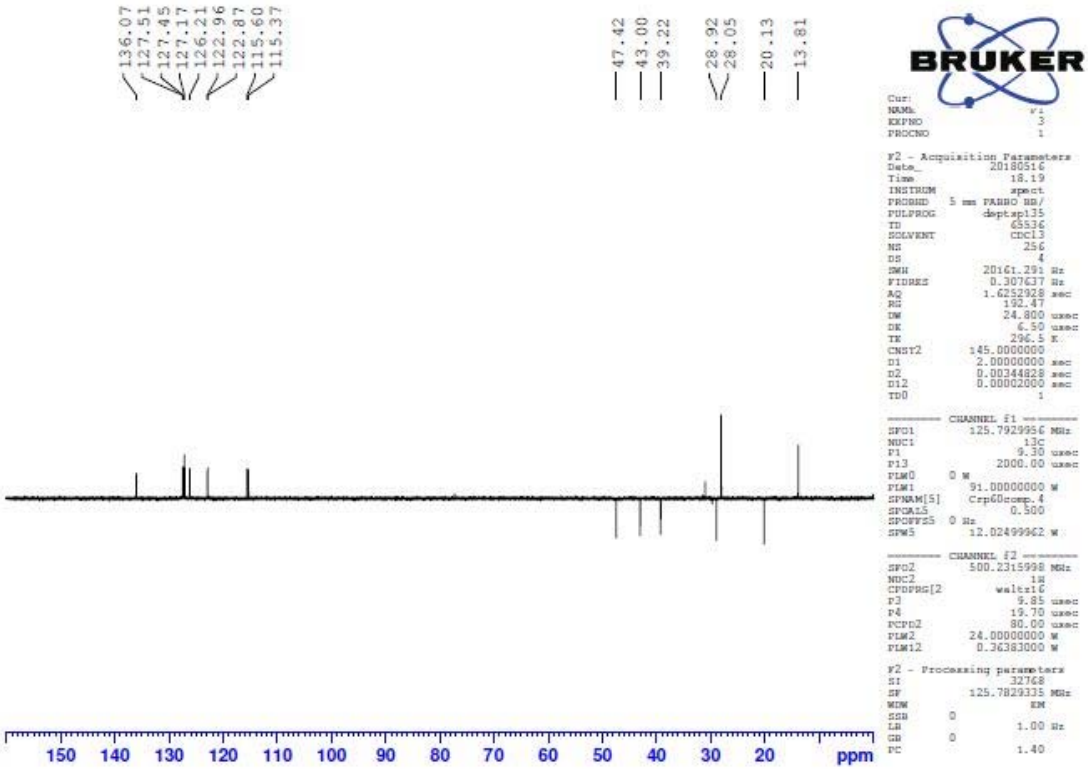

Figure S8. MeOH/water solvent ratio with 100 μM HOCl

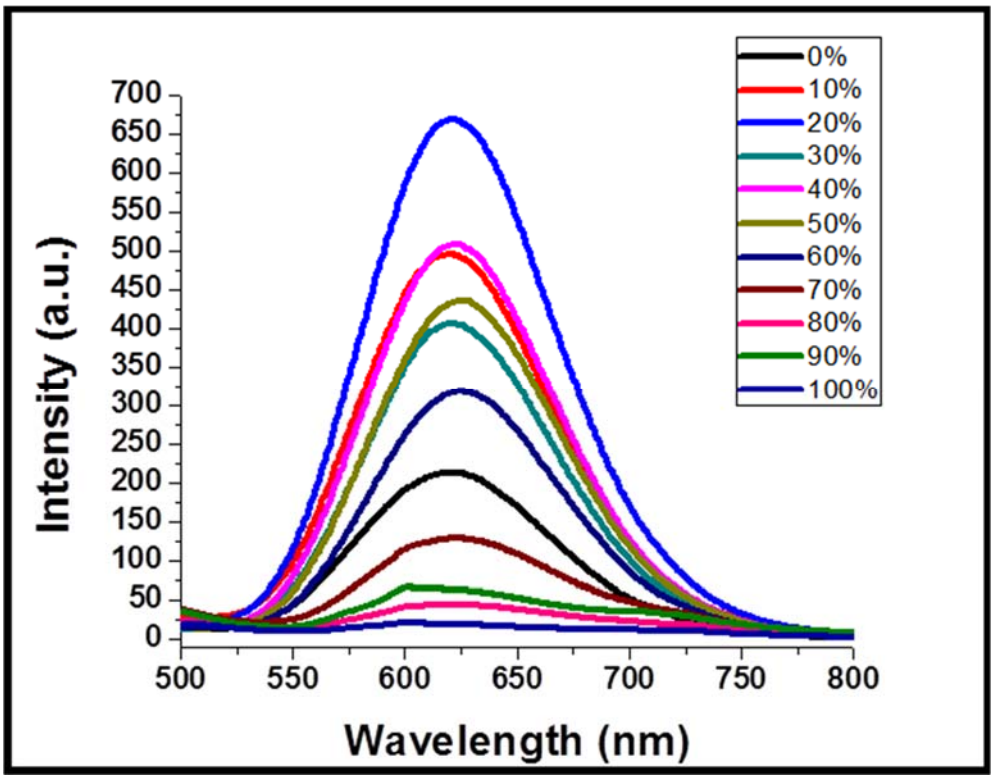

Figure S9. Fluorescence intensity of PI (20 μM) with HOCl (100 μM) at 620 nm in 20% aq. MeOH in various pH.

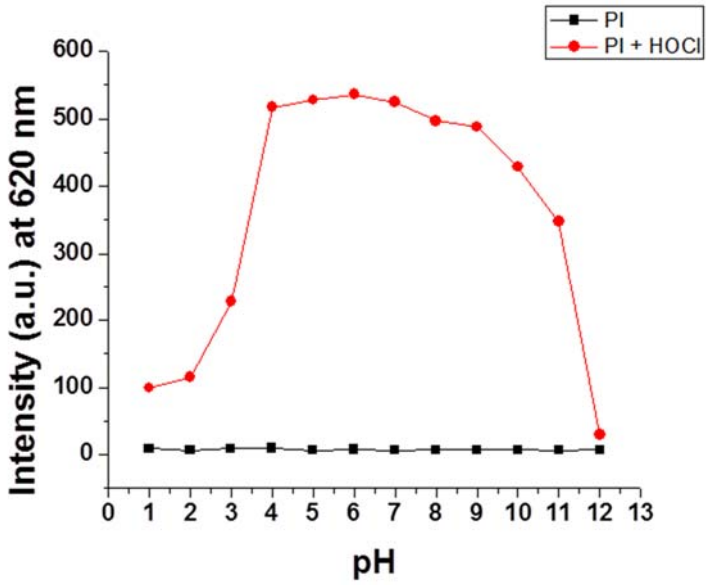

Figure S10. Detection limit plot

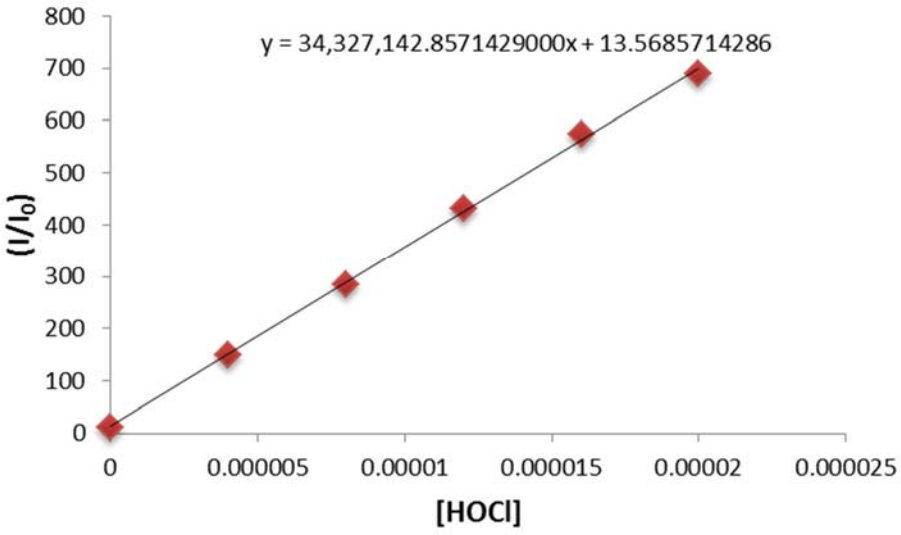

Figure S11. ESI mass spectrum of PI

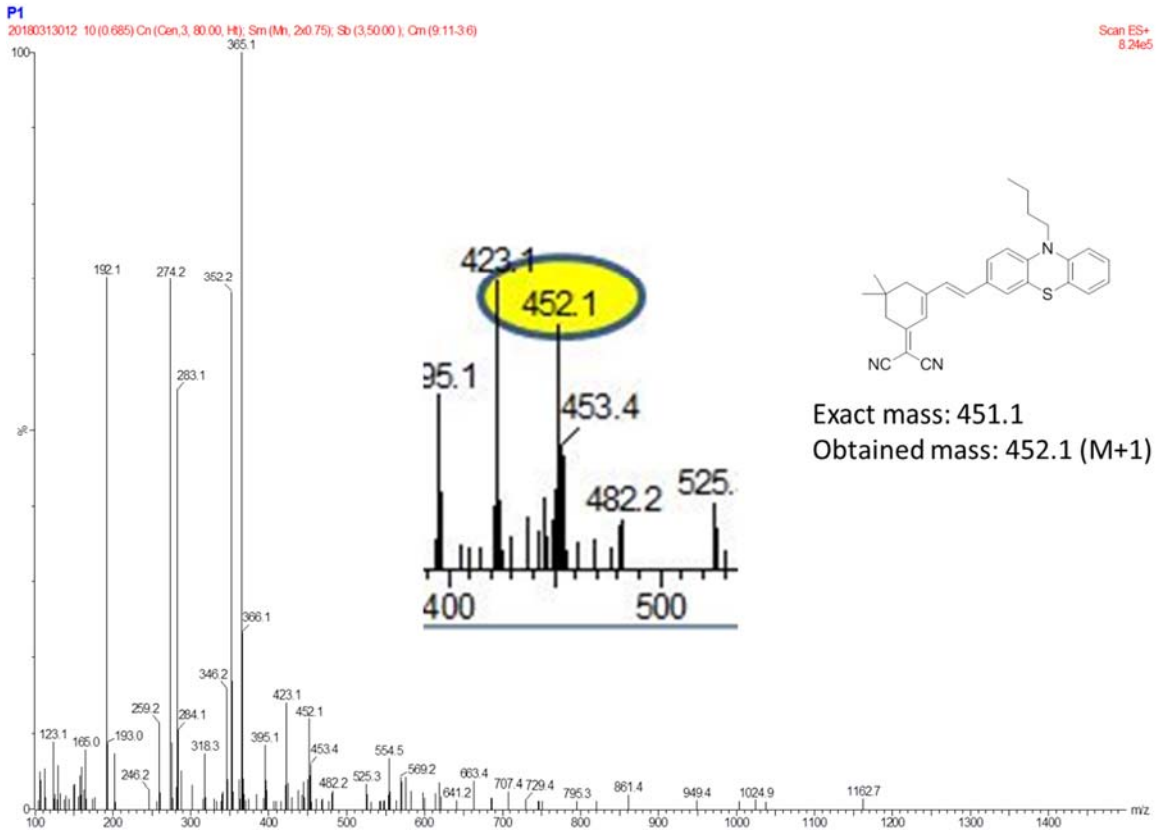

Figure S12. ESI massspectrum of PI with HOCl

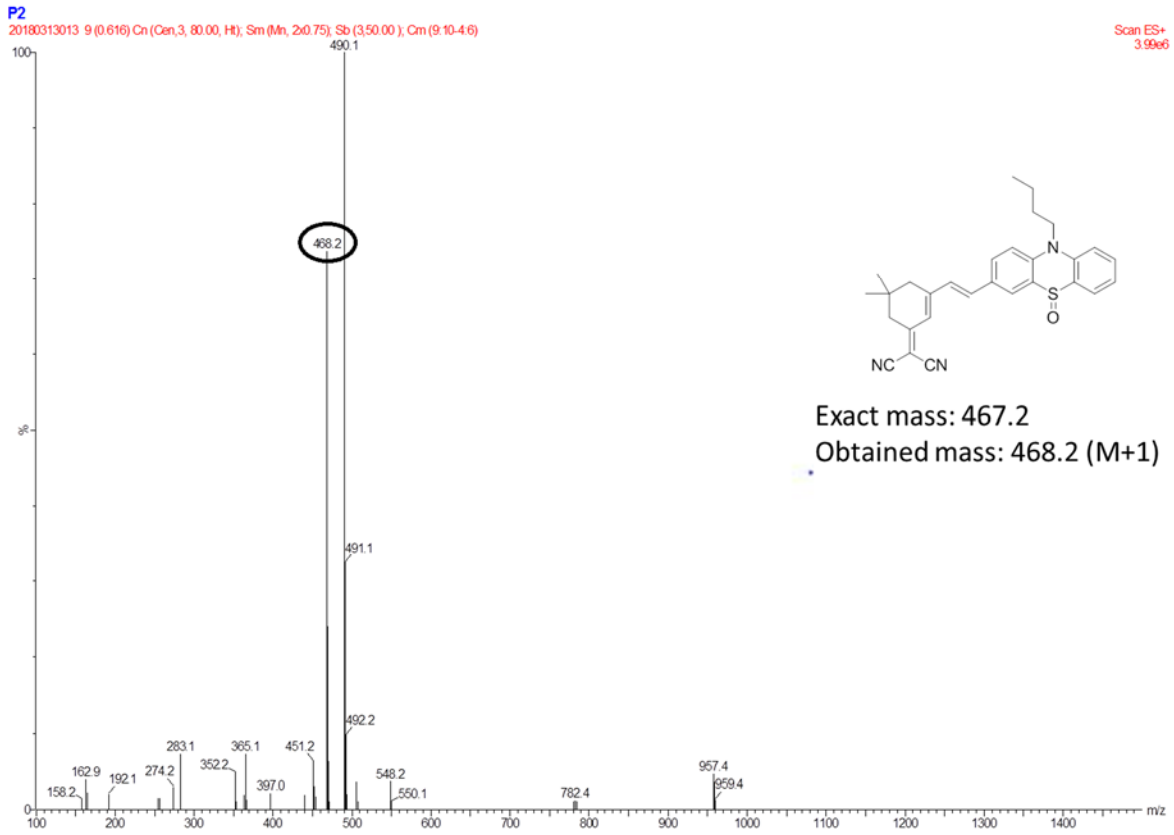

Figure S13. GSH interference with oxidized probe (20 μM probe in 20% aqueous methanol added with 100 μM HOCl and GSH)

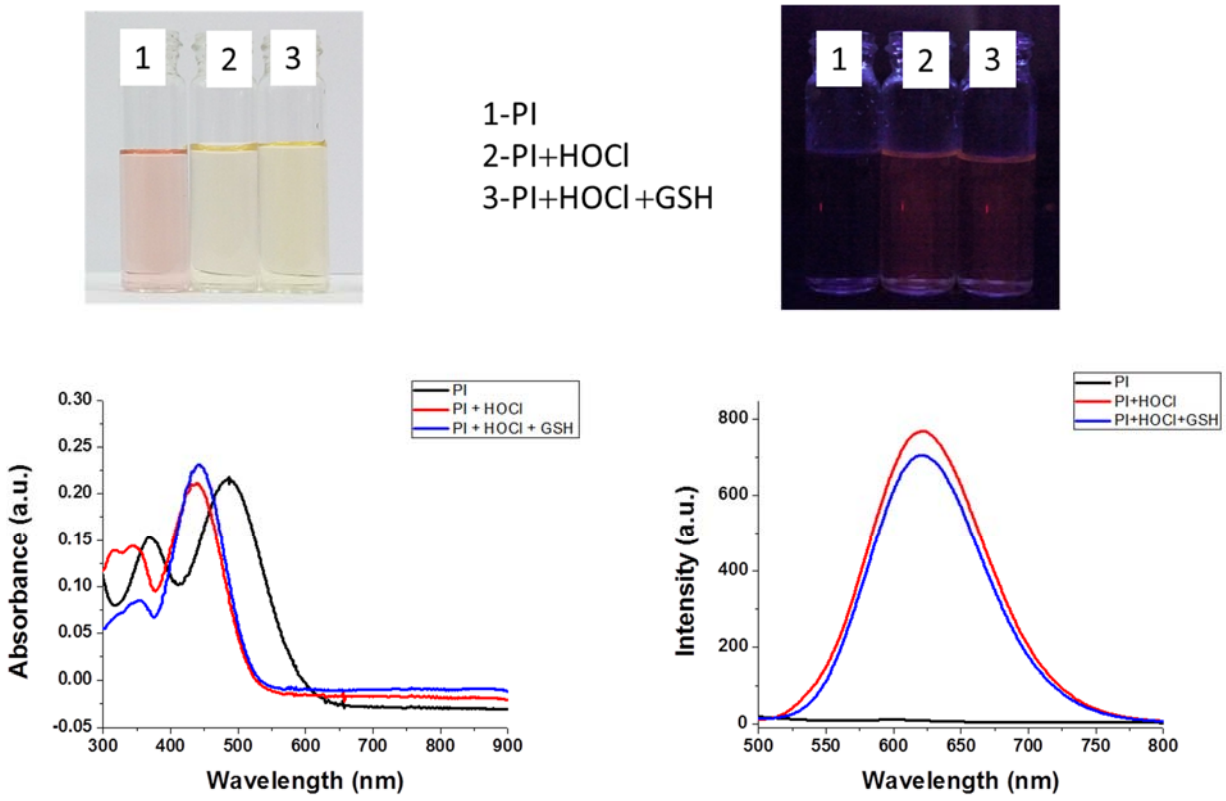

Table S1. A comparison of the detection limit with some other previously reported HOCl probes

PROBE FOR HOCl	DETECTION LIMIT
Probe reported by Suhua Wang[1]	0.13 and 0.70μM
Probe reported by Bao-Xiang Zhao[2]	0.19 μM
Probe reported by Bao-Xiang Zhao[3]	0.21 μM
Our probe PI	**42 nM (0.042μM)**

Table S2. Quantum yield calculation for the probe PI 20 μM with 100 μM HOCl

S.NO	Compound	Area of Fluorescence spectrum	Absorbance	Reference quantum yield	Quantum yield
1.	PI	19	207	**0.95**	0.0156
2.	PI + HOCl	**462**	**214**		**0.3679**
3.	Rhodamine B	11466	2.057		0.95

Quantum yield is calculated using the following formula:

$$\Phi_S / \Phi_R = (I_S / I_R) \text{ X } [(1\text{-}10^{-AR}) / (1\text{-}10^{-AS})] \text{ X } (n_S^2 / n_R^2)$$

Φ_S – Quantum yield of the sample; Φ_R – Quantum yield of reference
I - Fluorescence intensity of sample (S) and reference (R); A- Absorbance of sample (S) and reference (R); n- Refractive index of the solvent used ; As quantum yield is temperature dependent, in both the cases temperature maintained same.

1. **M. Sun, H. Yu, H. Zhu, F. Ma, S. Zhang, D. Huang and S. Wang, *Anal. Chem.*, 2013, 86, 671-677.**
2. **L.-L. Xi, X.-F. Guo, C.-L. Wang, W.-L. Wu, M.-F. Huang, J.-Y. Miao and B.-X. Zhao, *Sensors Actuators B: Chem.*, 2018, 255, 666-671.**
3. **Y.-R. Zhang, Z.-M. Zhao, L. Su, J.-Y. Miao and B.-X. Zhao, *RSC Adv.*, 2016, 6, 17059-17063.**