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Supporting information for:

A Highly Specific Fluorescence Probe for Rapid Detection of Hypochlorous Acid *in vivo* and in Water Samples

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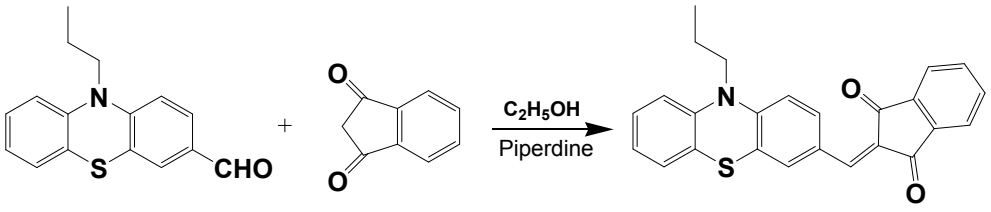

Scheme S1 Synthetic procedure of the fluorescence probe, **PI**.

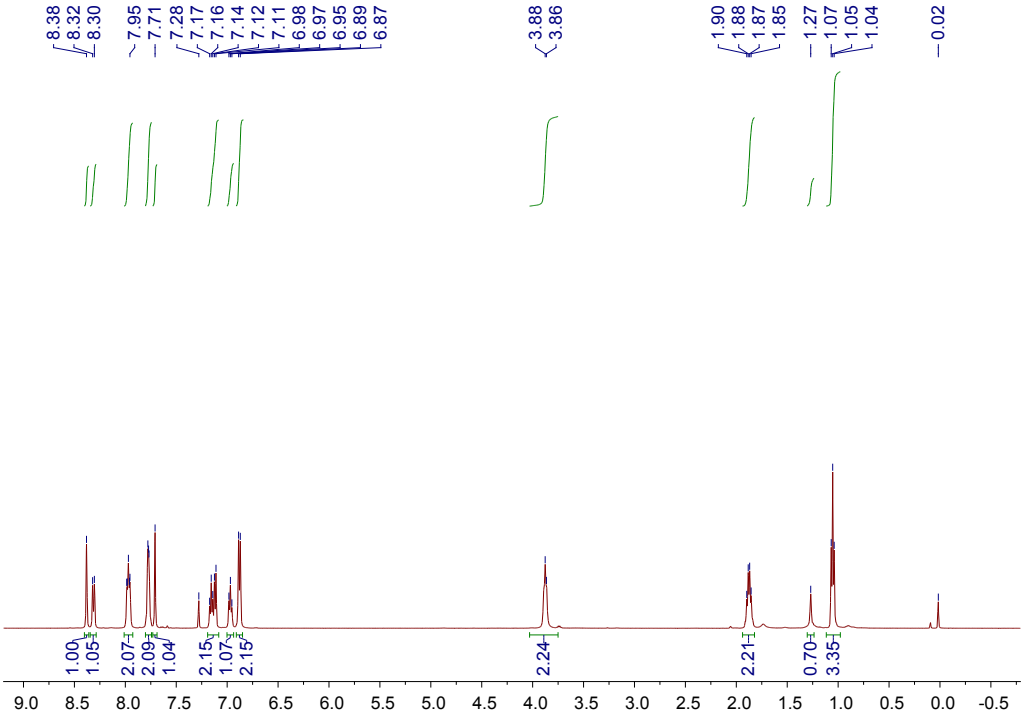

Fig. S1 ^{1}H NMR of **PI** ($CDCl_3$).

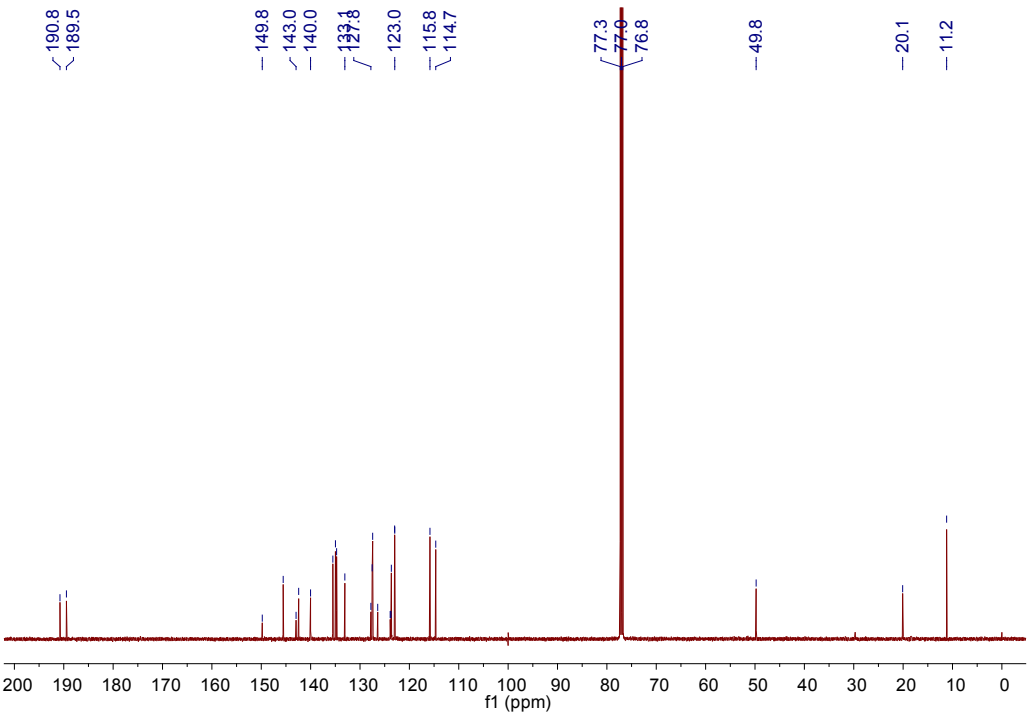

Fig. S2 ^{13}C NMR of **PI** ($CDCl_3$).

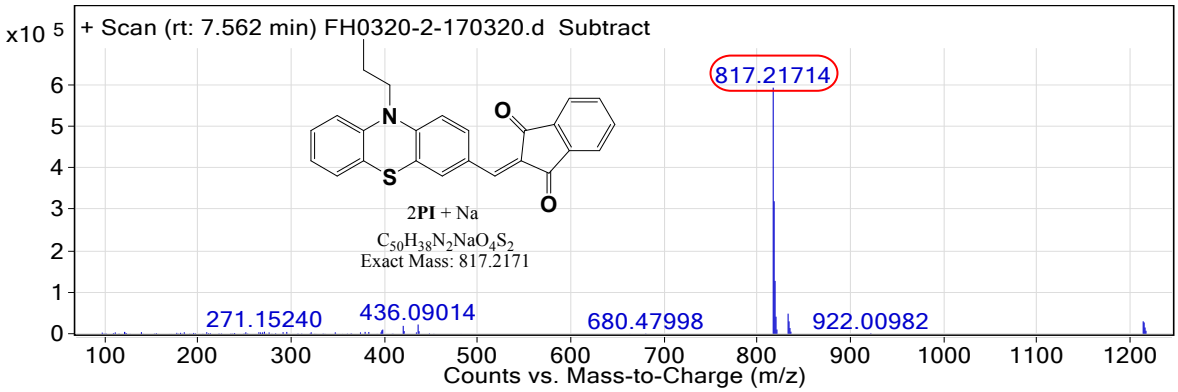

Fig. S3 HR MS of **PI**.

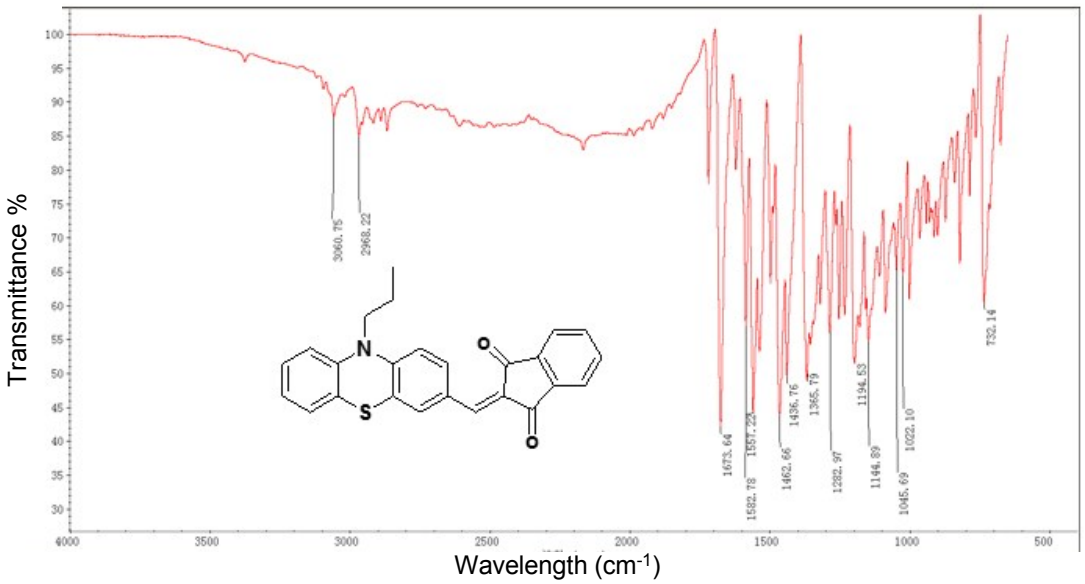

Fig. S4 FTIR spectrum of **PI**.

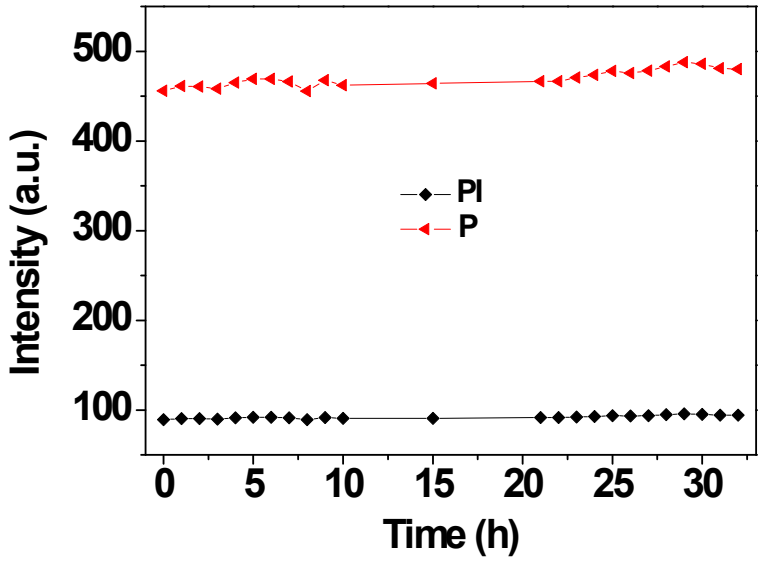

Fig. S5 Fluorescence intensities of **PI** (10 μM) and P (10 μM) at different time in PBS aqueous buffer (DMSO: H_2O = 9:1, 20 mM, pH = 7.4). Excitation at 440 nm.

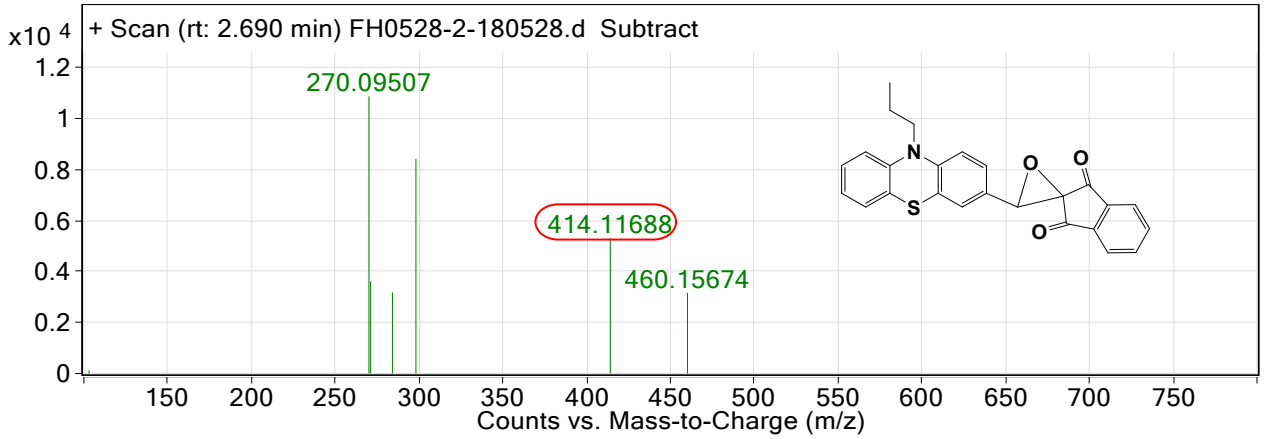

Fig. S6 HR MS of **PI** in the presence of HOCl.

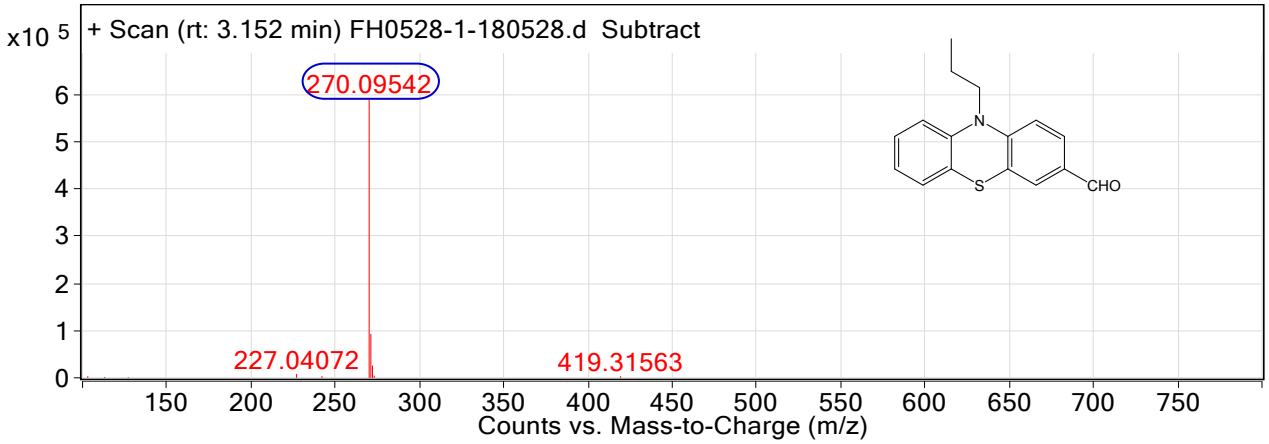

Fig. S7 HR MS of **PI** in the presence of more amount of HOCl.

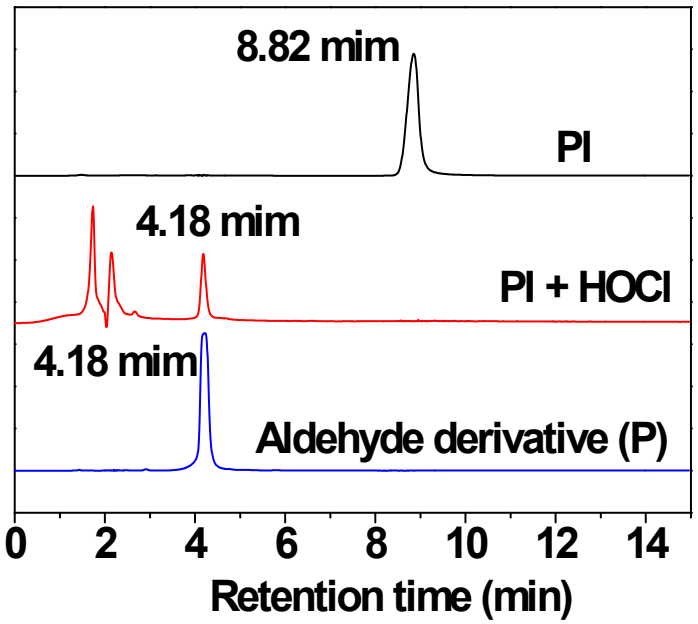

Fig. S8 HPLC chromatogram of **P**, **PI** in the (a) absence and (b) presence of HOCl.

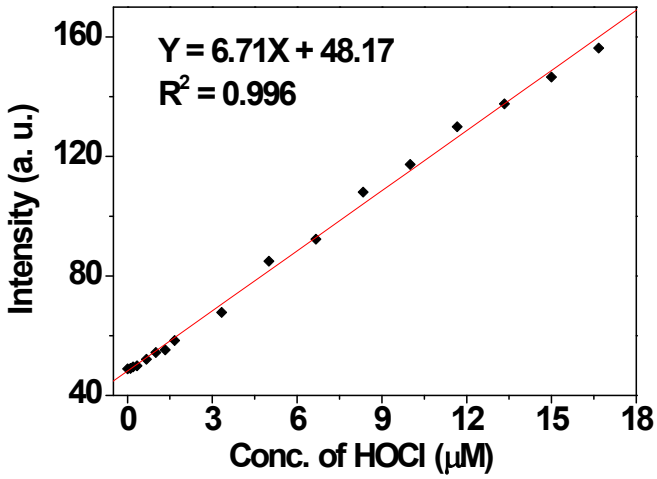

Fig. S9 The fluorescence intensity changes at 551 nm of **PI** (5 μM) as a function of HOCl concentration (0-17.0 μM). Excitation was performed at 440 nm.

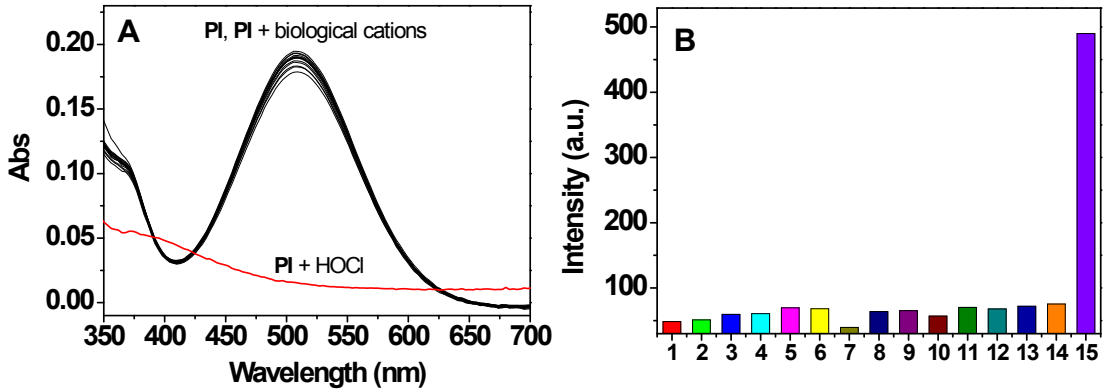

Fig. S10 (A) Absorption spectra and (B) fluorescence response of **PI** (10 μM) towards various biological cations (60 μM) in PBS buffer (DMSO:H_2O=9:1, v/v; pH 7.4). The cations include: 1. blank, 2. Al^{3+}, 3. Fe^{3+}, 4. Cr^{3+}, 5. Ag^{+}, 6. Li^{+}, 7. Co^{2+}, 8. Cu^{2+}, 9. Cd^{2+}, 10. Ca^{2+}, 11. Mg^{2+}, 12. Ba^{2+}, 13. K^{+}, 14. Na^{+}, 15. HOCl. The excitation and emission wavelength are 440/551 nm.

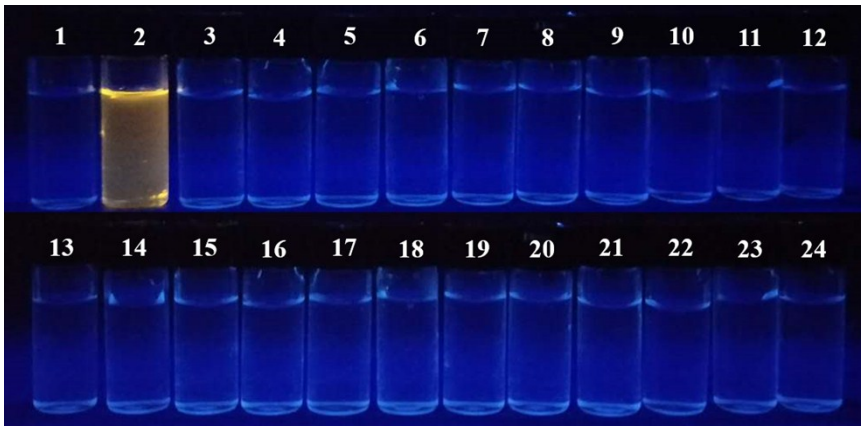

Fig. S11 Changes in fluorescence colour of **PI** (10 μM) in the presence of various analytes (60 μM) in PBS aqueous buffer (DMSO: H_2O = 9:1, 20 mM, pH = 7.4): (1) Free **PI**, (2) HOCl, (3) Br^{-}, (4) AcO^{-}, (5) Cl^{-}, (6) F^{-}, (7) HSO_3^{-}, (8) HSO_4^{-}, (9) S^{2-}, (10) NO_2^{-}, (11) NO_3^{-}, (12) $^1O_2$, (13) ·OH, (14) $ONOO^{-}$, (15) $P_2O_7^{4-}$, (16) PO_4^{3-}, (17) SO_3^{2-}, (18) HCO_3^{-}, (19) Pi, (20) PPi, (21) H_2O_2, (22) Cys, (23) Hcy and (24) GSH.

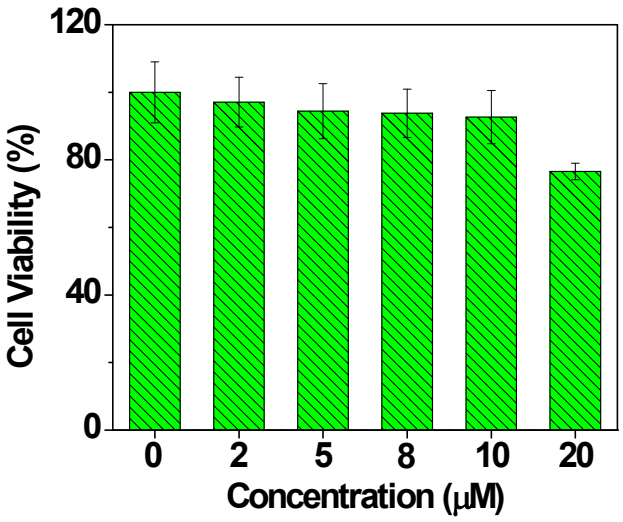

Fig. S12 Cytotoxicity of **PI** towards HeLa cells estimated by MTT assay.

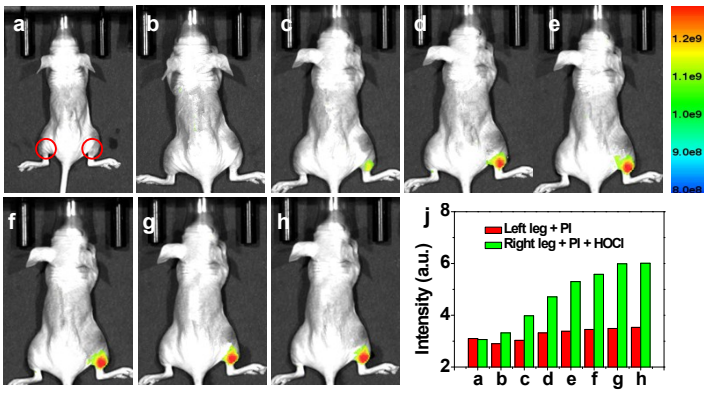

Fig. S13 Fluorescence imaging of exogenous HOCl in live nude mouse. (a) **PI** (50 μM, 125 μL) was subcutaneously injected into the right leg of mouse, followed by the injection of 20 μL HOCl (20 mM) to the area of interest. Images were recorded at different times: (b) 0 min; (c) 10 min; (d) 20 min; (e) 30 min; (f) 40 min; (g) 50 min and (h) 60 min, respectively. (j) The mean fluorescence intensities of areas of interest at different time showing in (a-h). The left hind limbs were injected with **PI** only as the control group. The mouse was imaged with excitation filter (465 nm) and emission filter (610 nm).

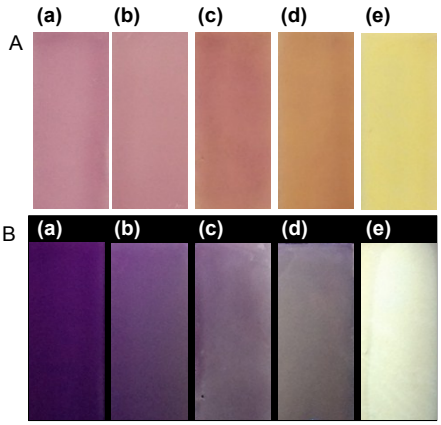

Fig. S14 Photographs of colour responses of the **PI**-based test papers exposured to different concentration of HOCl in pure water: (a) 0 mM, (b) 0.05 mM, (c) 0.1 mM, (d) 0.5 mM and (e) 1.0 mM. (A) Under visible light, (B) under UV light (365 nm).

Table S1. Some recently reported fluorescent probes for HOCl detection.

Probes	***Detection limit***	***Linearity range***	***Colour changes***	***Ex/Em (nm)***	***Response time***	***In vivo sensing***	***Preparation and application of probe-based chromatography plates or paper***	***Ref.***
SeCy7	0.31 μM	10-60 μM	No study	690/786	dozens of seconds	Exogenous and endogenous HOCl in nude mice	No study	1
HCTe	41.3 nM	1-10 μM	No study	480/531	< 200 s	No study	No study	2
FBS	0.2 μM	0−1.0 μM	No study	428/593	quickly (no data)	Detection of DUOX-dependent HOCl induction in the intestinal epithelia of Drosophila.	No study	3
complex 1	down to 1 *ppm*	No study	No study	346/587	No study	No study	naked-eye detectable under UV light (365 nm) irradiation by the test paper of 1	4
BRClO	1.95 μM and 0.59 μM for ratio measurement and intensity	0−100 μM	disappearance of the pink color	480/505,585	within 1 s	No study	Test strips for qualitative detection of HOCl in natural tap water	5
probe 1a	0.5 μM	0.5-5 μM	No study	480/532	Within 30 min	No study	No study	6
BDP-OX	0.85 μM	No study	No study	488/538,589	within 15s	No study	No study	7
Lyso-BHHBB-Eu3þ;Mito-BHHBB-	<15 nM	0−10 μM	No study	328/607; 333/6	within 5 s	Monitoring of HOCl uptake in Daphnia magna.	No study	8

Eu3þ				07				
Cy-HOCl	10 nM	0−45 μM	No study	543/625	about 15 min	In acute ischemia zebrafish and nude mice model	No study	9
RO610	2.88× 10^{-8} M	0−20 μM	No study	535/577	within 30 s	Exogenous and endogenous HOCl in nude mice	No study	10
TCBT-OMe	0.16 nM	0-0.7 μM	No study	310/472	within 10 s	No study	Test strips for qualitative detection of HOCl in natural tap water under UV light (365 nm).	11
MBTC	4.6 nM	0-1.0 μM	colorless to blue	620/690	In one minute	No study	No study	12
TPP-TCF	0.29 μM	0-10 μM	No study	488/660	within 30 seconds	endogenous HOCl in nude mice	No study	13
S-BODIPY	59 nM	0-70 μM	No study	540/587,619	within 30 s	Exogenous and endogenous HOCl in zebrafish; imaging of endogenous HOCl in an acute liver injury mouse model	No study	14
PL-HA	6.2× 10^{-8} M	0-25 μM	No study	365/525	100 s	No study	No study	15
QYMTC and QEMTC	29.3 nM and 17.8 nM	0–125 μM; 0–110μM	yellow to green; yellow to blue	580/700 630/720	within 30 seconds	No study	No study	16
QClO	89 nM	0.8–16.5 μM	No study	426/562,492	within 60 seconds	Tracking HOCl in wounded tissues of mice	No study	17
Gal-NPA	0.46 nM	0 to 1 μM	colorless to yellow	470/558	within 3 s.	No study	No study	18
PI	47 nM	3-34 μM	pink to pale yellow	440/551	within 1 minute	1) endogenous HOCl production in zebrafish; 2) exo-/endogenous HOCl in live nude mouse 3) visualisation of HOCl-mediated RA in mammals in live nude mouse	Quantitative analysis of HOCl in nature water samples by **PI**-based test chromatography plates with the naked eye	This work

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