

Supplementary Information for

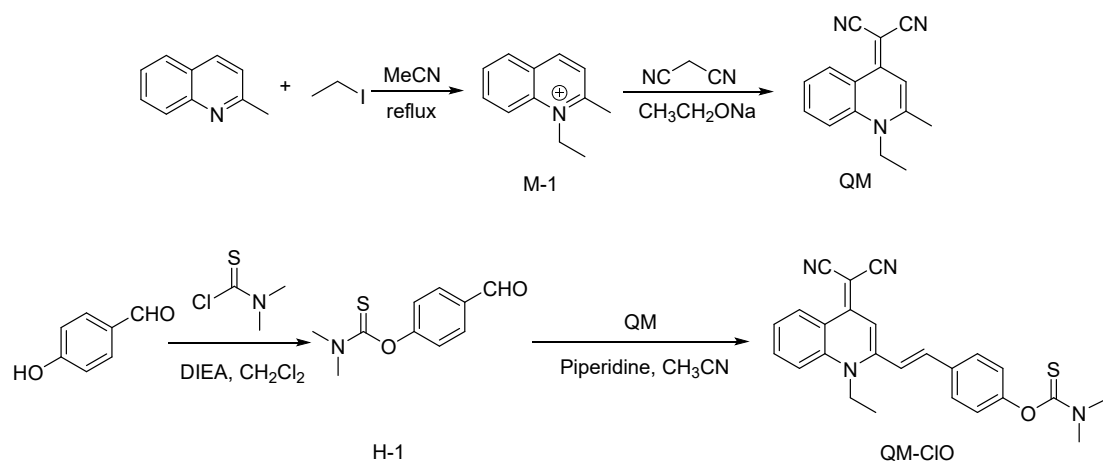
A long-wavelength activable AI-Egen fluorescent probe for HClO and cell apoptosis imaging

Mengyun Wang^a, Xiaojing Han^a, Xiaopeng Yang^a, Jianfei Liu^a, Xiangzhi Song^b, Weimin Zhu^{a*}, Yong Ye^{a*}

^aGreen Catalysis Center, and College of Chemistry, Zhengzhou University, Zhengzhou 450001, China

^bCollege of Chemistry & Chemical Engineering, Central South University, Changsha 410083, China

EXPERIMENTAL SECTION



Scheme S1. Synthetic route of QM-CIO.

Synthesis of M-1. Under N₂ atmosphere, 2-methylquinoline (1.43 g, 10 mmol) and iodoethane (4.71 g, 30 mmol) were dissolved in acetonitrile (20 mL) and refluxed for 12 h. Then the reaction product was concentrated under reduced pressure to obtain a light yellow solid M-1 as a crude product, which can be used in the next reaction without further purification.

Synthesis of QM. Under ice-water bath conditions, compound M-1 (1.74 g, 6 mmol) and malononitrile (1.00 g, 15 mmol) were dissolved in absolute ethanol (20 mL), and sodium ethoxide solution (20 mL anhydrous Ethanol, 0.97 g sodium). After 4 hours of

reaction, the mixture was poured into 500 mL ice water, and the pH was adjusted to 7-8 with 1 M hydrochloric acid solution. The resulting precipitate was filtered, washed with distilled water and dried in vacuum to obtain the desired product QM: yellow solid (1.06 g, 78%).

Synthesis of H-1. P-Hydroxybenzaldehyde (2 mmol, 0.12 g) and dimethylthiocarbamoyl chloride (10 mmol, 1.24 g) were dissolved in 10 mL of anhydrous dichloromethane, then 400 μ L DIEA was added, and the mixture was stirred at room temperature for 4 hours. Concentrated under reduced pressure to remove dichloromethane, and then purified by column chromatography(0.17 g, 40%).

Apparatus. Absorption and fluorescence emission spectra were measured using HP-8453 UV/Vis spectrometer and F-4600 FL spectrophotometer. The slit width is 5 nm/5 nm, excitation voltage is 700V. Nuclear magnetic resonance (NMR) spectra were carried out by using Bruker DTX-400 spectrometer. High-resolution mass spectrometry (HRMS) was performed on Agilent ESI-Q-TOF mass instrument. ESI mass spectra were implemented on the HPLCQ-ToF HR-MS. The fluorescence imaging of cells were tested by confocal laser-scanning microscope (Leica TCS SP8). Dynamic light scattering (DLS) was performed using NanoPlus-3 DLS particle size/zeta potential analyzer.

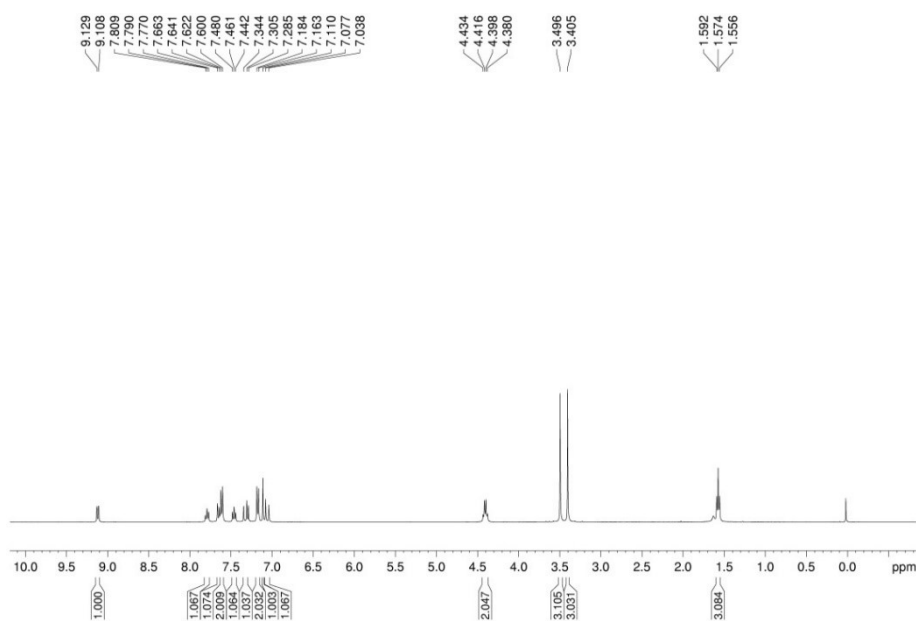


Fig S1. ¹H NMR spectrum of QM-C10 in CDCl₃.

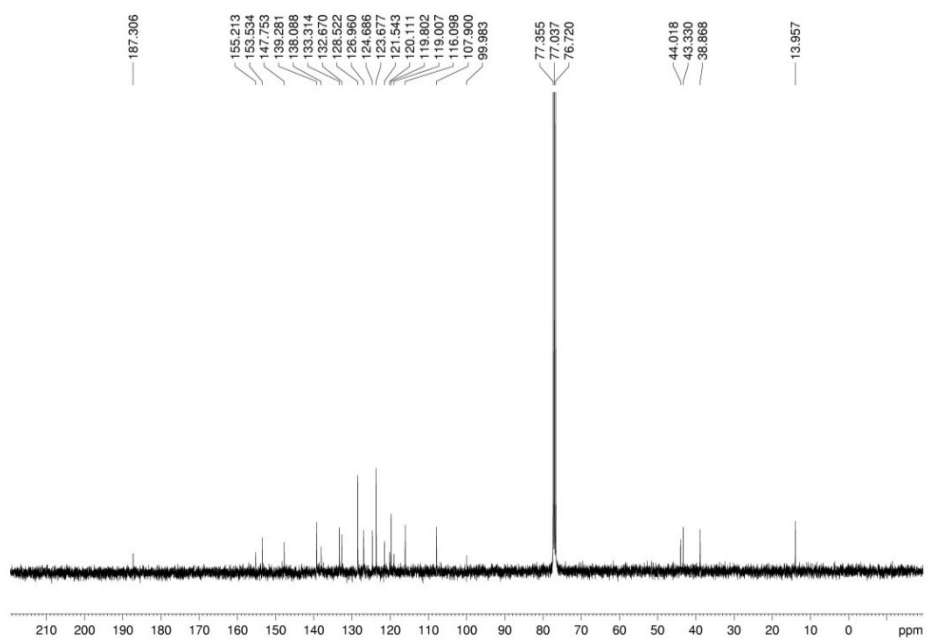


Fig S2. ^{13}C NMR spectrum of QM-C10 in CDCl_3 .

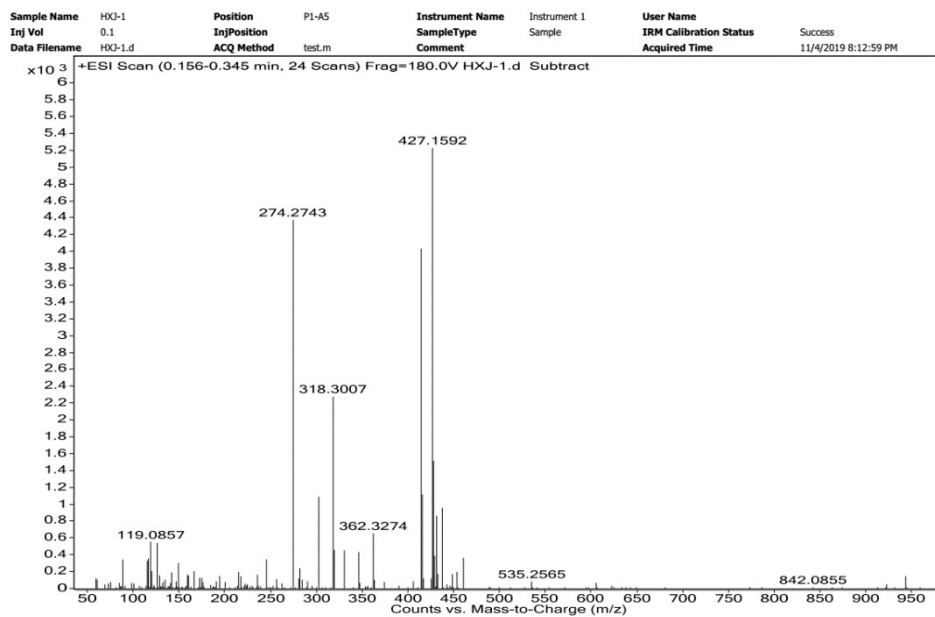


Fig S3. HR-MS spectra of QM-C10.

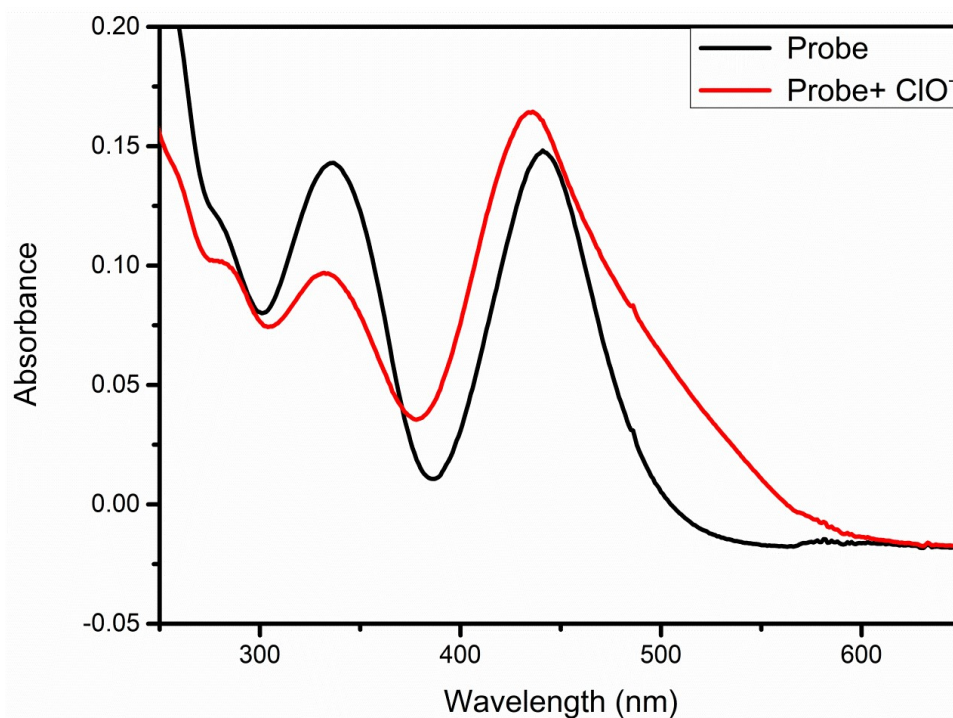


Fig S4. The UV-vis spectra of probe QM-CIO (10.0 μM) in the presence of ClO^- .

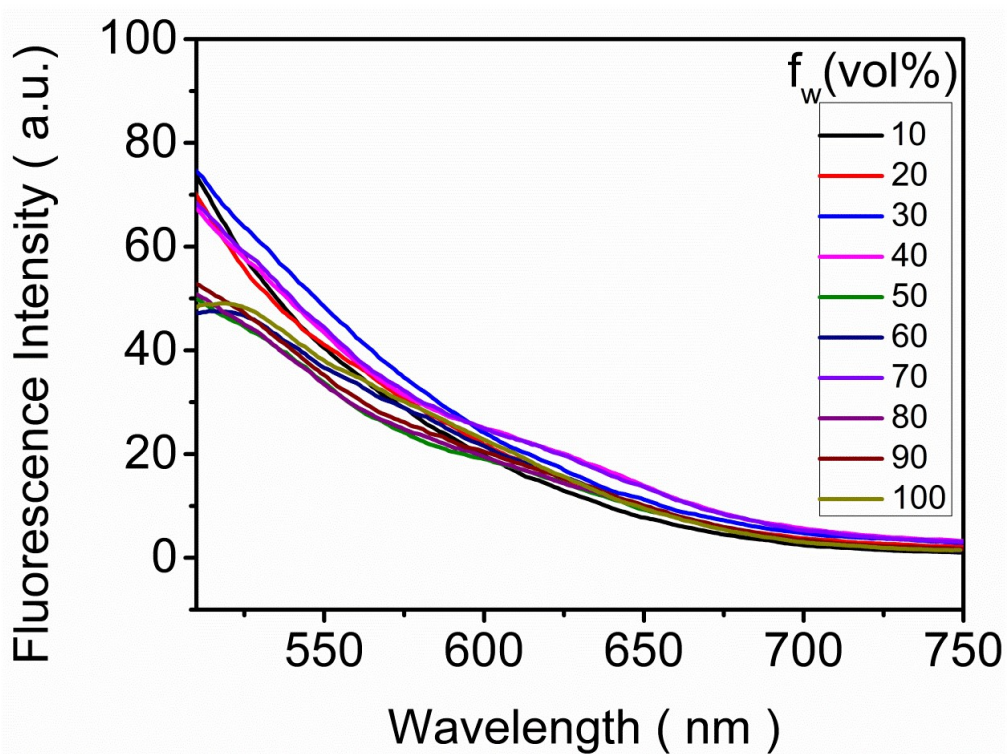


Fig S5 Spectrum character and diameter of QM-CIO (f_w) in a different ratios of PBS/DMSO.

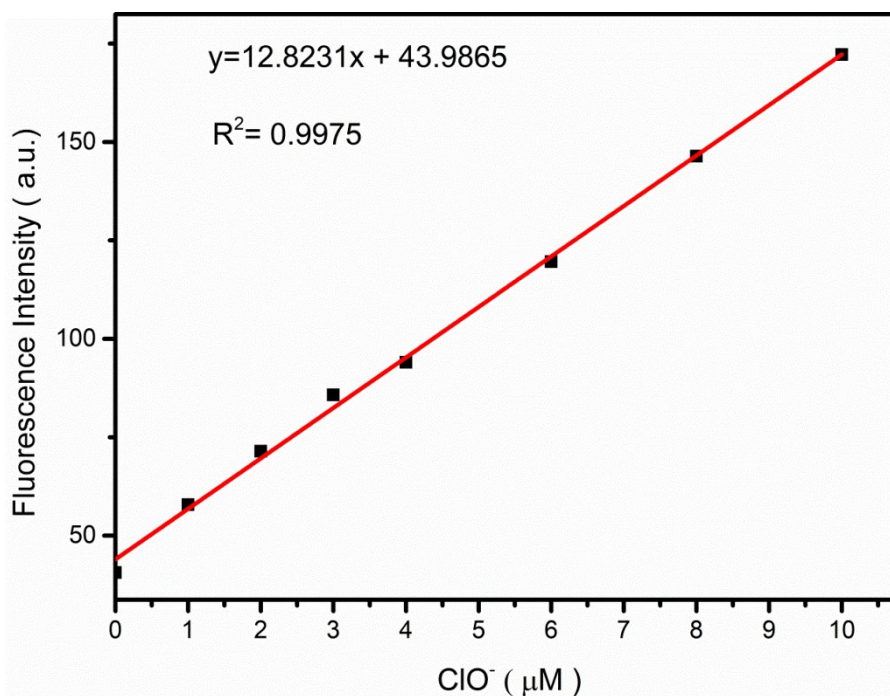


Fig S6. Linear plot of the fluorescence emission against ClO^- concentrations. ($\lambda_{\text{ex}} = 430 \text{ nm}$).

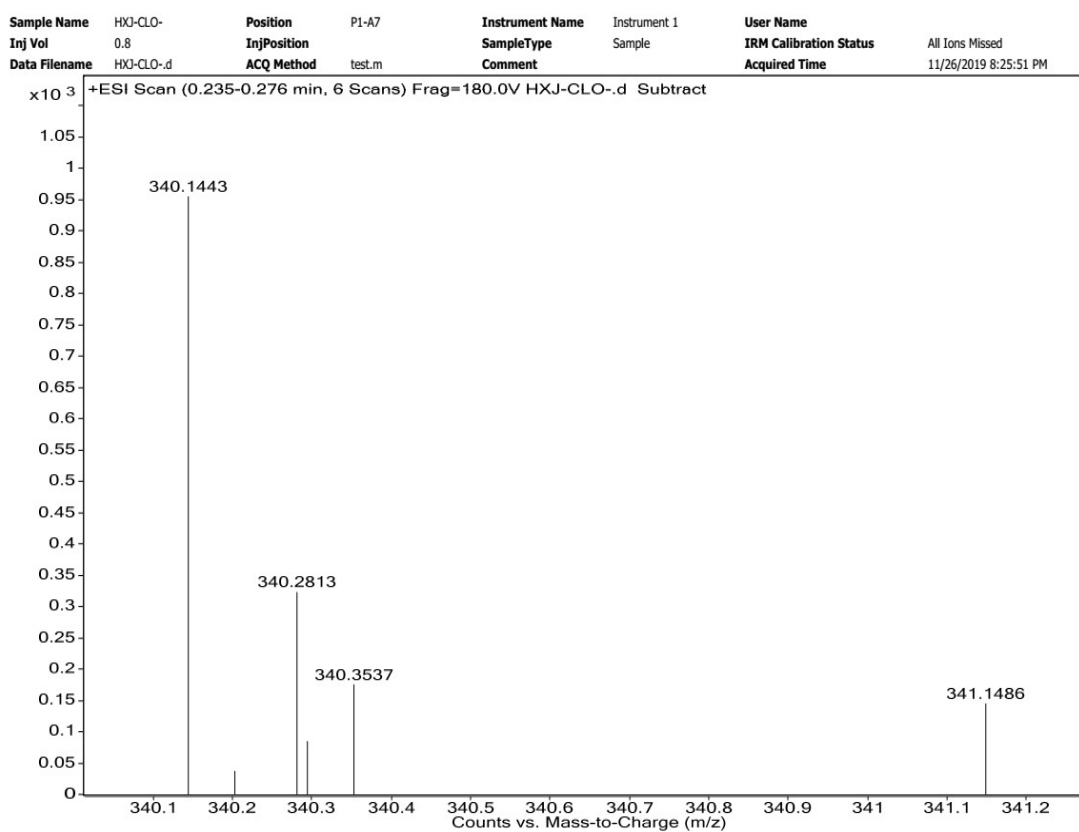
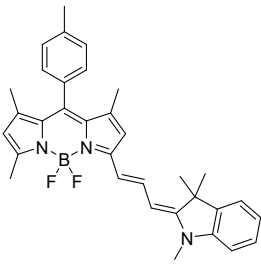
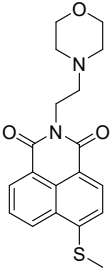
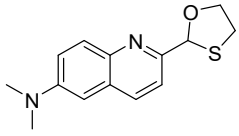
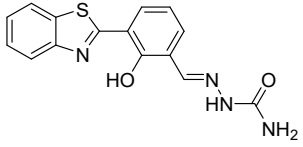
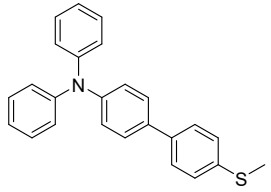
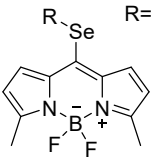
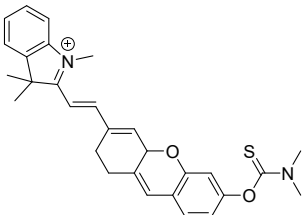
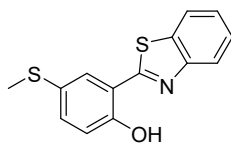
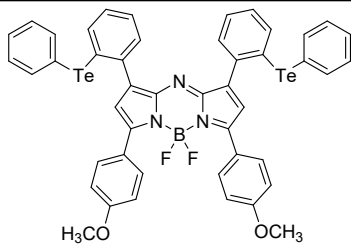
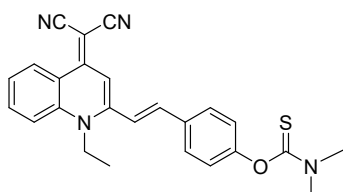


Fig S7. HR-MS spectra of QM-CIO in the presence of ClO^- (10 equiv.)

Table S1. Comparison of reported probes for recognition of HClO.

Structure	$\lambda_{\text{ex}}/\lambda_{\text{em}}$ (nm)	Response time	Detection limit	AIE	Cell imaging
 <p>Sensors and Actuators B: Chemical 2017246 293-299</p>	488/511 635/713	10 s	10.6nM	NO	Endogenous and exogenous hypochlorous acid in cell lysosomes.
 <p>Anal. Chem. 2017, 89, 10384-10390</p>	405/505	150 s	0.674 μM	NO	Detection of HClO in intracellular lysosomes.
 <p>Chem. Sci., 2018, 9, 6035</p>	426/492, 562	60 s	89 nM	NO	The production of HClO during wound healing in mice.
 <p>Sensors and Actuators B 2018260 832-840</p>	360/465	20 min	8.2×10^{-9} M	NO	Membrane permeability and low toxicity
 <p>Chem. Commun., 2019, 55, 12912</p>	365/437, 497	60 s	16 nM	NO	Production of hypochlorous acid during alcohol-induced liver injury

 <p>R-Se R=Et, PhCH₂ or Ph</p> <p>J. Mater. Chem. B, 2019, 7, 6861</p>	532/548 530/545 532/550	2 s 5 s 100 s	0.3 nM 0.8 nM 9.2 nM	NO	Exogenous and endogenous hypochlorous acid, and localized in mitochondria
 <p>Sensors and Actuators: B. Chemical 2021327 128884</p>	680/710	5s	0.09 μM	NO	Fluctuations in endogenous hypochlorous acid produced by the immune system during Staphylococcus aureus infection and muscle tissue injury in live mice
 <p>Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 2020 239 118515</p>	365/450, 580	3 min	4.2×10^{-7} M	NO	Cellular imaging of hypochlorous acid
 <p>Talanta2021 233 122581</p>	630/738	immediate	0.09 μM	NO	Exogenous and endogenous detection HClO
 <p>This work</p>	430/620	100 s	30.8 nM	Yes	Changes of hypochlorous acid content during CCCP-induced cell apoptosis