

## Supporting Information

**Fig. S1.**  $^1\text{H}$  NMR(600 MHz) of **QI** in DMSO - $d_6$ .

**Fig. S2.**  $^{13}\text{C}$  NMR(150 MHz) **QI** in DMSO - $d_6$ .

**Fig. S3.** HR-MS spectrum of **QI**.

**Fig. S4.** The Uv-vis spectra changes of **QI** and the normalized of Uv-vis spectra of **QI**, **QIO** and **1**.

**Fig. S5.** The fluorescence intensity of **QI**. toward HOCl under different pH conditions.

**Fig. S6.** Reaction time profile of **QI** with HOCl and **QI** at 520 nm in mixture solution.

**Fig. S7.** The HR-MS spectrum of [**QI**+HOCl].

**Fig. S8.** Viability of HeLa cells by treating with probe **QI**.

### 1. Materials and instruments

The materials and reagents used are commercially available and have not been further purified. The solution of compounds was prepared of deionized water. UV-vis spectroscopy was performed using HITACHI U-3900 spectrophotometer, and fluorescence spectroscopy was performed using HITACHI F-7000 spectrophotometer. All related compounds were characterized by  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR using a Bruker AVANCE-600 MHz spectrometer, followed by mass spectrometry using an AB Triple TOF 5600plus System (AB SCIEX, Framingham, USA). The final bioimaging application were measured the Zeiss LSM880 Airyscan confocal laser scanning microscope.

### 2. Bio-imaging

All the animal experiments were performed by following the protocols approved by Radiation Protection Institute of Drug Safety Evaluation Center in China (Production license: SYXK (Jin) 2018-0005). Balb/c type mouse (12-14 weeks, male) were purchased from Beijing Vital River Laboratory Animal Technology Co., Ltd. Experiments were conducted according to the National Institute of Health Guide for the Care and Use of Laboratory Animals. Imaging procedures were conducted with

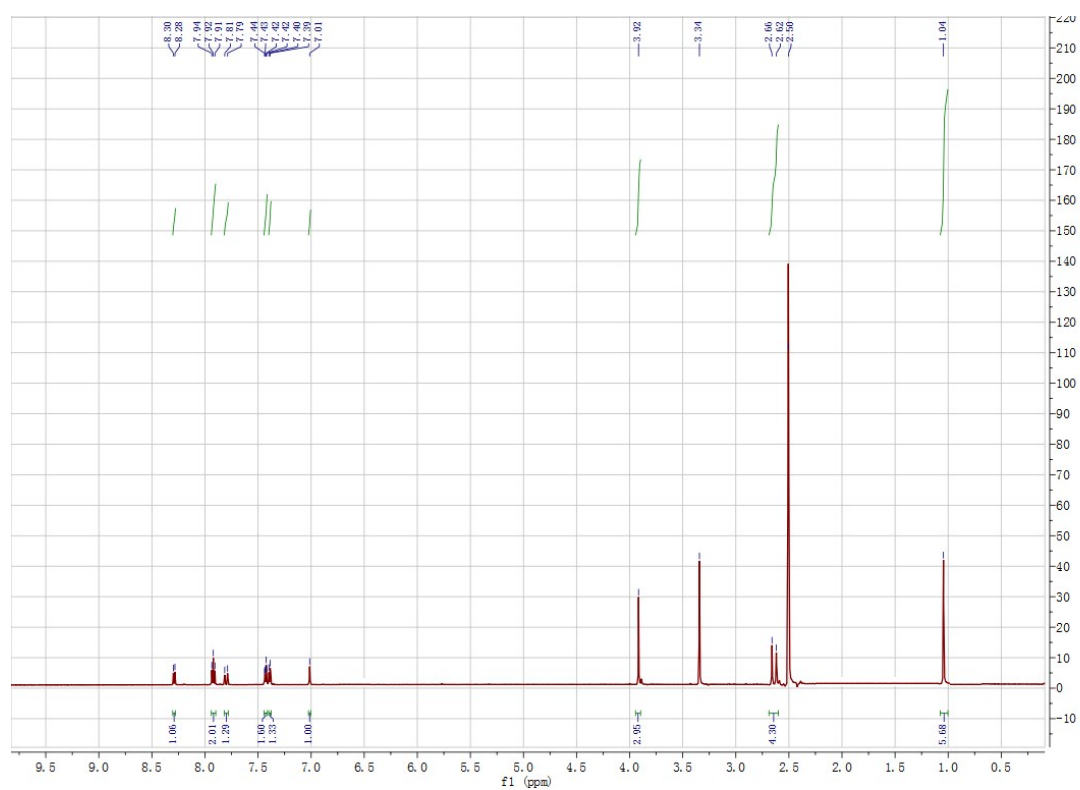
adult nude mice under general anesthesia by injection of sodium pentobarbital (0.5 mL/0.03 %). Then, probe **AI** and analytes (HOCl) was carefully injected into Balb/c type mouse according to designed experiment. Images were taken using an excitation laser of 405 nm and emission  $525\pm 20$  nm, respectively.

### 3. Experimental Section

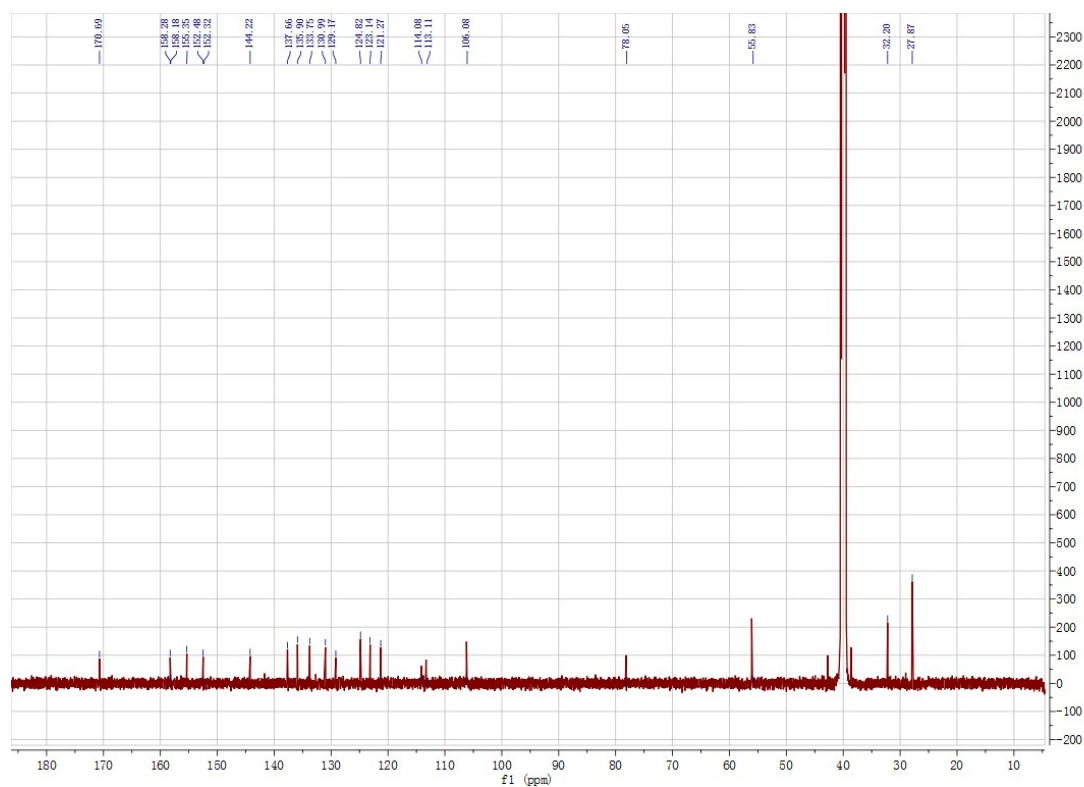
Precursors were synthesized using literature method . Synthesis of probe **QI** (Scheme 1). In a 25.0 mL round bottom flask, compound 1 (0.245 g, 1.00 mmol) and compound 2 (0.186 g, 1.00 mmol) were dissolved in ethanol (10.0 mL). Piperidine (0.150 mL) was added and the mixture was refluxed for 6 h. The reaction was cooled to room temperature, the crude product was purified by silica gel column chromatography using ethyl acetate and petroleum ether (1:8) as eluent to afford pure compound **QI** as an yellow solid (0.360 g, yield 68.5%).  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ ):  $\delta$  8.29 (d,  $J$  = 8.6 Hz, 1H), 7.92 (t,  $J$  = 8.9 Hz, 2H), 7.80 (d,  $J$  = 16.1 Hz, 1H), 7.43 (dd,  $J$  = 9.0, 2.9 Hz, 2H), 7.39 (d,  $J$  = 6.5 Hz, 1H), 7.01 (s, 1H), 3.92 (s, 3H), 2.64 (d,  $J$  = 24.6 Hz, 4H), 1.04 (s, 6H). (Fig. S1);  $^{13}\text{C}$  NMR (151 MHz, DMSO- $d_6$ ):  $\delta$  170.7, 164.6, 161.0, 159.9, 157.2, 156.9, 138.1, 132.2, 130.9, 130.0, 129.1, 127.6, 123.1, 122.2, 114.9, 114.5, 114.2, 113.7, 56.1, 32.1, 27.9, 27.5 (Fig. S2); HR-MS  $m/z$ : calcd for 355.16846; found:  $m/z$ : 356.17561 [**QI** +  $\text{H}^+$ ] (Fig. S3).

### 4. Spectral test preparation

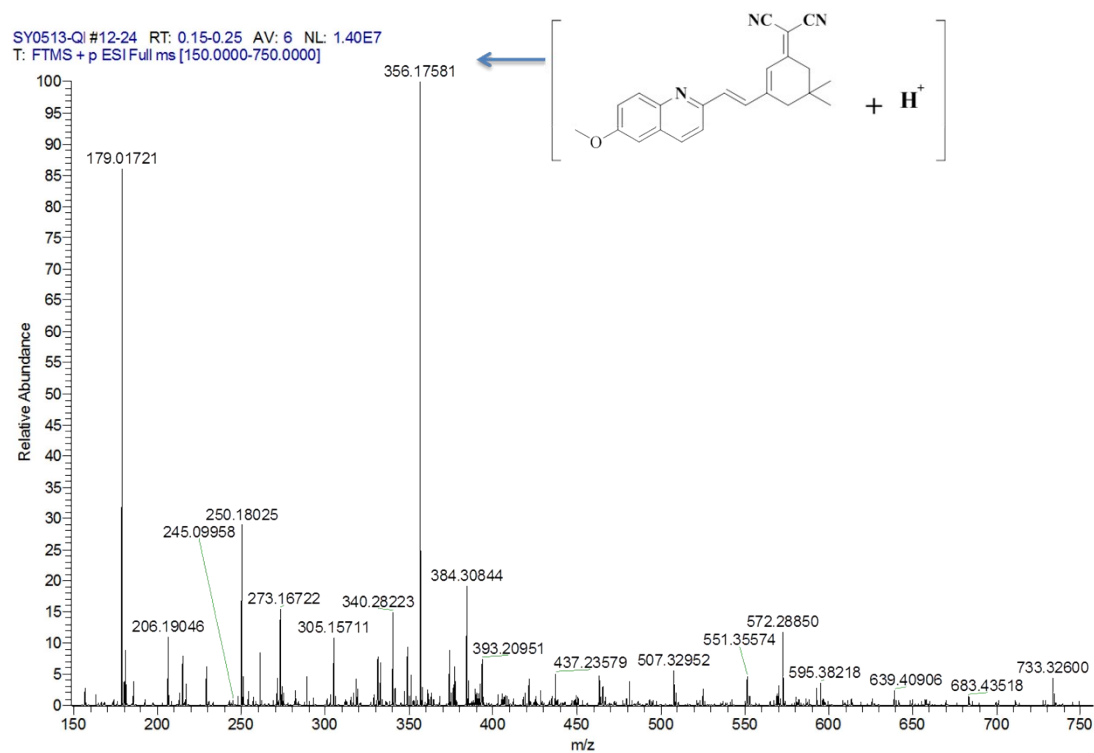
Probe **QI** was dissolved in DMSO to make a 2.0 mM stock solution. Through testing, we finally chose DMSO / PBS (1/1, v/v, pH = 7.4) as the test system, the probe concentration was 10.0  $\mu\text{M}$ . The concentration of interfering ions is 0.1M. Therein  $\text{NaNO}_2$  and  $\text{NaNO}_3$  are the donors of  $\text{NO}_2^-$  and  $\text{NO}_3^-$ .



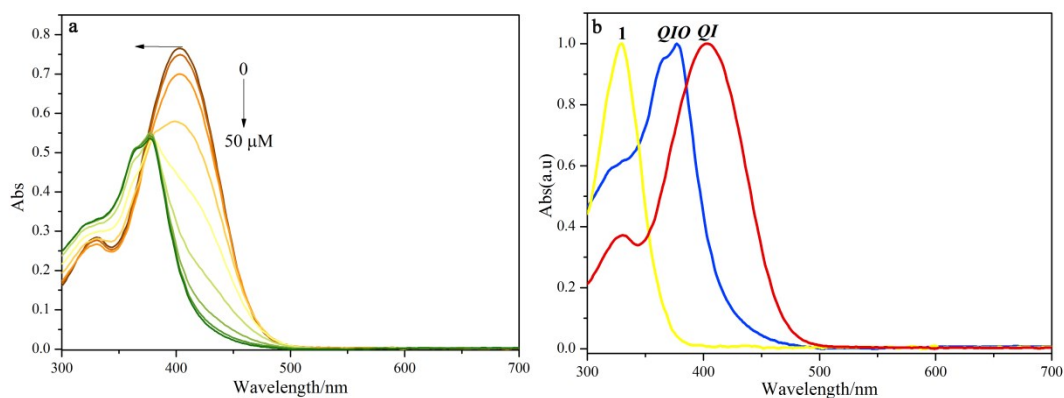
**Fig. S1.**  $^1\text{H}$  NMR(600 MHz) of **QI** in  $\text{DMSO}-d_6$ .



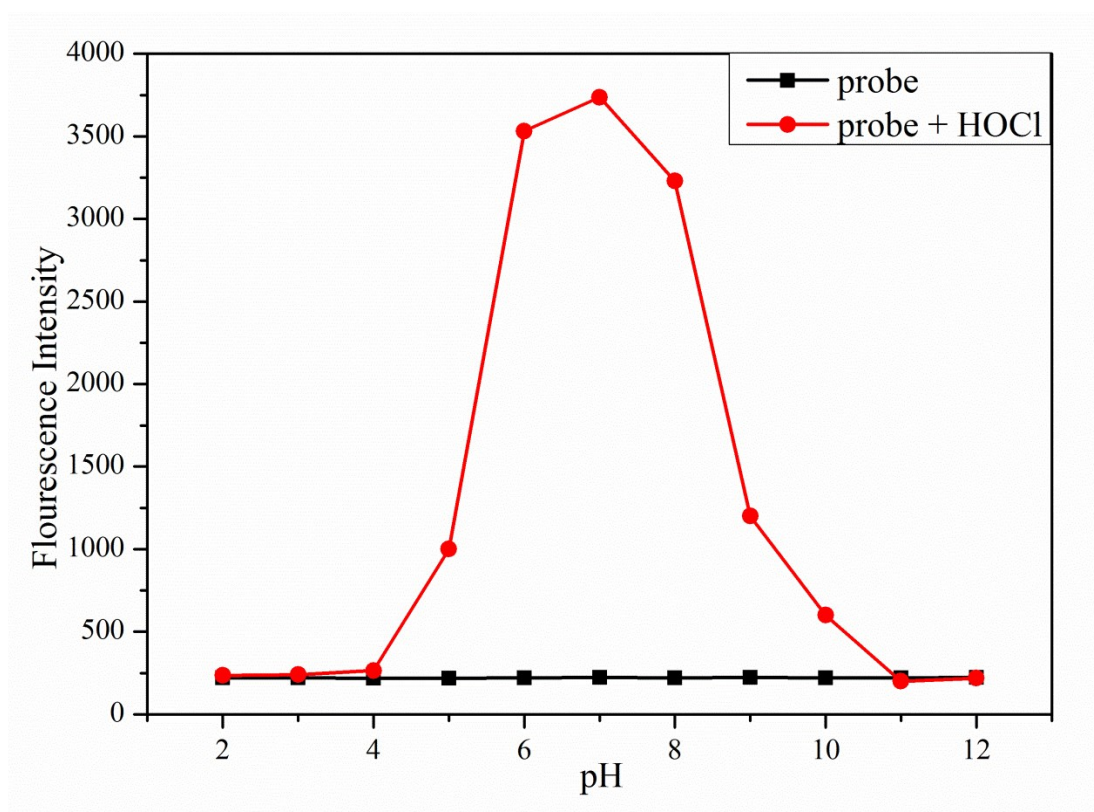
**Fig. S2.**  $^{13}\text{C}$  NMR(150 MHz) **QI** in  $\text{DMSO}-d_6$ .



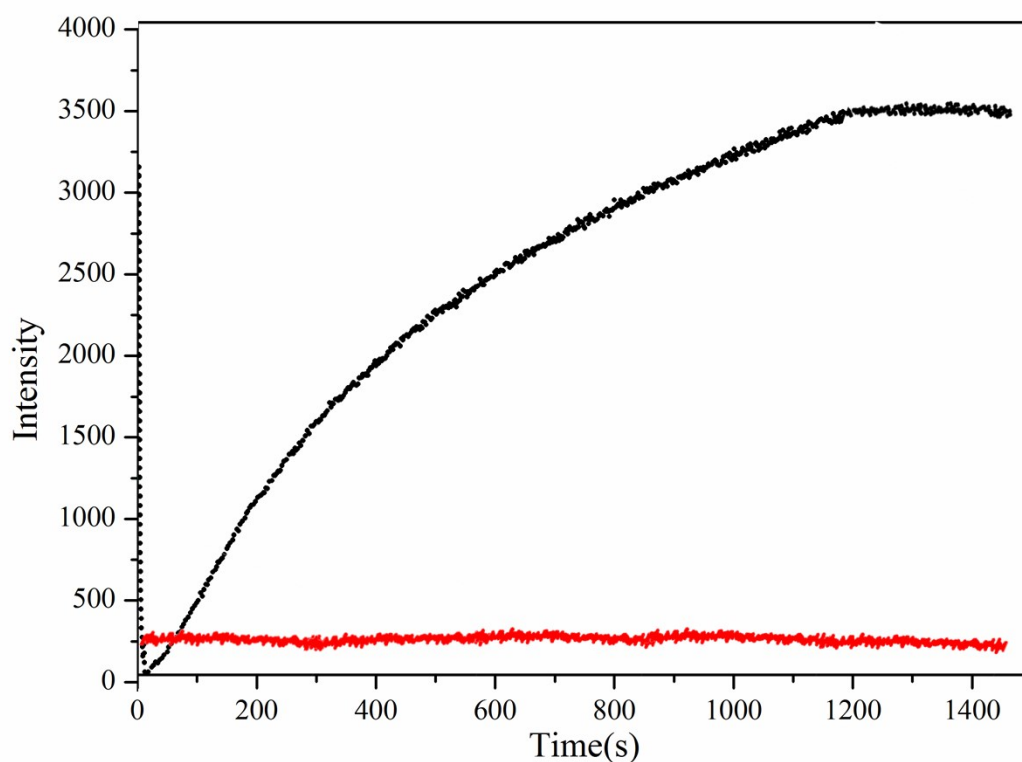
**Fig. S3.** HR-MS spectrum of **QI**.



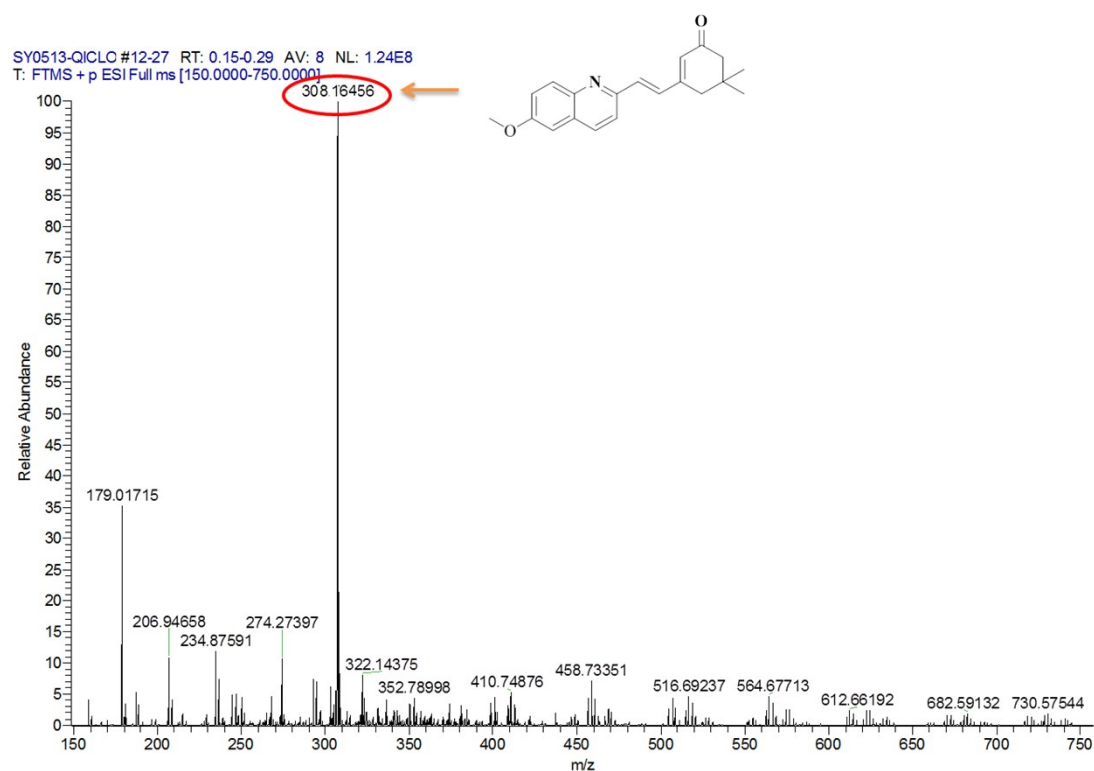
**Fig. S4.** (a) The Uv-vis spectra changes of **QI** (10  $\mu$ M) was reacted with different concentrations (0-50  $\mu$ M) of HOCl; (b) The normalized of Uv-vis spectra of **QI** (red line), **QIO** (blue line) and **1** (yellow line).



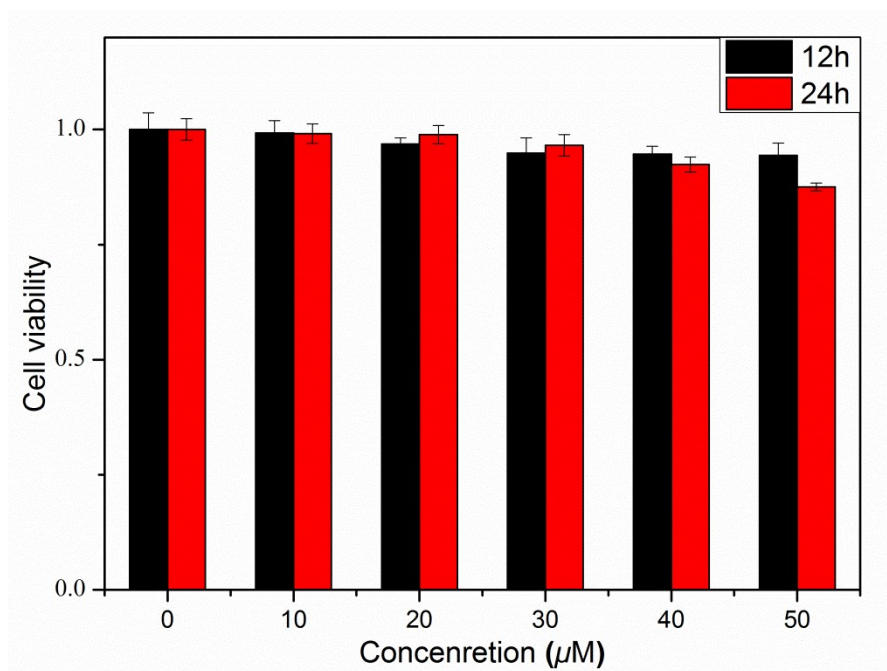
**Fig. S5.** The fluorescence intensity at 520 nm was obtained under different pH conditions in the presence and absence of HOCl. ( $\lambda_{\text{ex}} = 390 \text{ nm}$ ).



**Fig. S6.** Reaction time profile of **QI** (20  $\mu\text{M}$ ) with HOCl (50  $\mu\text{M}$ ) and **QI** (red line) at 520 nm in DMSO-PBS buffer (v/v, 1: 1, pH 7.4,) ( $\lambda_{\text{ex}} = 390 \text{ nm}$ ).



**Fig. S7.** The HR-MS spectrum of [*QI*+HOCl].



**Fig. S8.** Viability of HeLa cells by treating with probe *QI*.