Supporting Information for

Imaging of Peroxynitrite in Drug-Induced Acute Kidney Injury with a Near-Infrared Fluorescence and Photoacoustic Dual-Modal Molecular Probe

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EXPERIMENTAL SECTION

Reagents and Apparatus. Water was purified and doubly distilled by a Milli-Q system (Millipore, USA). Photoluminescent spectra were recorded at room temperature with a HITACHI F4600 fluorescence spectrophotometer (1 cm standard quartz cell) with both excitation and emission slit set at 5.0 nm. Mass spectra were performed using an LCQ Advantage ion trap mass spectrometer (Thermo Finnigan). NMR spectra were recorded on a Bruker DRX-400 spectrometer using TMS as an internal standard. All chemical shifts are reported in the standard δ notation of parts per million. Thin layer chromatography (TLC) was conducted using silica gel 60 F254, and column chromatography was carried out over silica gel (200-300 mesh), both of them were obtained from Qingdao Ocean Chemicals (Qingdao, China). The pH was measured with a Mettler-Toledo Delta 320 pH meter. All photoacoustic images were analyzed and collected at various time points by an InVision 256-TF imaging system (iTheraMedical).

Mito-Tracker Green, lipopolysaccharide (LPS), and interferon-γ (IFN-γ) were purchased from *Beyotime Biotechnology*, 3-morpholinosydnonimine hydrochloride (SIN-1, $ONOO^-$ donor) was purchased from *Sigma-Aldrich*, 2, 2, 6, 6-tetramethylpiperidine-Noxyl (TEMPO), cisplatin and L-carnitine (LC) were purchased from *Chemical Energy*. Other chemicals used in the synthesis of probe were purchased from commercial suppliers and used without further purification.

Sources for different ROS/RNS are described as follows. H_2O_2 solution was purchased from Sigma-Aldrich and added into the probe solution directly. Superoxide ($O_2^{\bullet-}$) was generated from KO_2 was dissolved in dry DMSO. The source of NaOCl was commercial bleach. Hydroxyl radical (•OH) was generated by Fenton reaction. Briefly, ferrous chloride ($FeCl_2$) was added in the presence of 10 equiv. of H_2O_2. The concentration of •OH was equal to the Fe (II) concentration. Peroxynitrite ($ONOO^-$) solution was synthesized followed the procedure that 5 mL water solution of 0.3 mL 30 % H_2O_2 and 0.08 mL 96% H_2SO_4 was quickly poured into 5 mL water solution of $NaNO_2$ (0.2g) under -10 ℃, then NaOH (0.5 g in 10 mL water) solution was soon poured into above solution, followed with fast passing the solution through a short column of manganese dioxide, finally a pale yellow solution was obtained. The resulting solution was split into small aliquots and stored at -80 °C. The

aliquots were thawed immediately before use, and the concentration of $ONOO^-$ was determined by measuring the absorption of the solution at 302 nm. The extinction coefficient of peroxynitrite solution in 0.1 M NaOH is 1670 M^{-1} cm^{-1} at 302 nm. The initial concentration calculated to be 48 mM.

Spectrophotometric Experiments. Both the fluorescence and UV-Vis absorption measurement experiments were carried out in 100 mM phosphate buffer saline (PBS, pH 8.0) buffer solution containing 10% EtOH as the co-solvent. The fluorescence emission spectra were recorded at an excitation wavelength of 635 nm with emission wavelength ranged from 650 to 850 nm. The test solution of the **SiRho-HD** (2.5 μM) in 2 mL of 100 mM PBS buffer EtOH solution (pH 8.0) was prepared by placing 25 μL of the **SiRho-HD** stock solution (1.0×10^{-4} M in EtOH) in 2mL of the various analytes buffer/EtOH solution. The resulting solutions were kept at 37 ℃ for 10 min and then the fluorescence intensities were measured.

In Vitro PA imaging Experiments. 200 μL plastic tubes were filled with the reaction solution of **SiRho-HD** (5 μM) toward different concentrations of $OONO^-$ (0, 5, 10, 20, 30, 40, and 50 μM), respectively. Then, the photoacoustic imaging of those tubes was performed on an InVision 256-TF imaging system (iTheraMedical, Germany). For in vitro PA spectra, tube filled with **SiRho-HD** (5 μM) or **SiRho-HD** (5 μM) after reaction with $OONO^-$ (50 μM) were scanned from 680 nm to 800 nm with an interval of 5 nm. Tubes filled with PBS was used as the control for background deduction. All MSOT data were acquired with the MSOT imaging system with the following parameters, excitation (680 nm-980 nm), pulse frequency (10 Hz), pulse length (8 ns) and maximal optical parametric oscillator energy (120 mJ at 740 nm). The light was delivered to the sample via a ring-type fiber bundle. The generated acoustic signals were collected with a 256-element transducer array.

Cytotoxicity Study. To study the cytotoxicity, HeLa cells were seeded at 8×10^3 cells per well in 96-well plates and incubated for 24 h before treatment, followed by exposure to different concentrations (2-10 μM) of probe **SiRho-HD** or reaction solution of **SiRho-HD** with $ONOO^-$ for 1 h, then washed with Dulbecco's Phosphate Buffered Saline (DPBS) and incubated for further 24 h. And then the cytotoxic effects were determined by MTS assays. The absorbance value at 490 nm was measured by a microplate reader.

Fluorescence microscopy imaging in live cells. Live RAW264.7 and HK-2 cells were

cultured in 30-mm glass-bottom dish plated and grown to around 80% confluency for 24 h before the experiment. In the colocalization experiments, cells were washed with DPBS buffer (pH 7.4), followed by incubating with 2 μM **SiRho-HD** and Mito-Tracker Green (0.5 μM) for 30 min (1% DMSO) at 37 °C in 5% CO_2, then by washing with DPBS and imaged. In another group, the RAW264.7 macrophages were first incubated with 1 mM SIN-1 for 2 h, subsequently co-incubated with 2 μM **SiRho-HD** and Mito-Tracker Green (0.5 μM) for 30 min then by washing with DPBS and imaged.

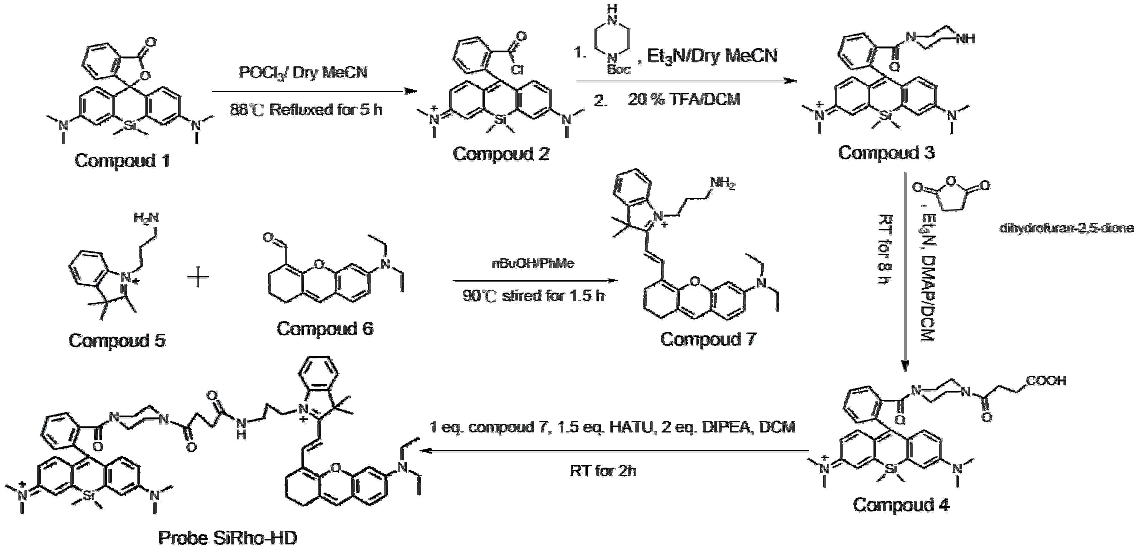
To investigate the capability of probe **SiRho-HD** for detection $ONOO^-$ in living cells, cells were first seeded in a 30 mm glass-bottom dish plated and grown to around 80% confluency for 24 h before the experiment. The cellular experiments can be divided into five groups. The first group is that RAW264.7 macrophages were incubated with 2 μM **SiRho-HD** for 30 min, then the cells were washed by DPBS buffer before imaging. In the second and third group, RAW264.7 macrophages were pre-incubated with 0.5 mM or 1 mM SIN-1 for 2 h respectively, and 2 μM **SiRho-HD** was further added for 30 min, then the cells were washed by DPBS prior to imaging. In the fourth group, RAW264.7 macrophages were pre-incubated with lipopolysaccharide (LPS, 1 μg/mL) and interferon-gamma (IFN-γ, 50 ng/mL) for 12 h, and 2 μM **SiRho-HD** was further added for 30 min, then the cells were washed by DPBS prior to imaging. In the fifth group, RAW264.7 macrophages were incubated with LPS (1 μg/mL) and IFN-γ (50 ng/mL) in the presence of 2, 2, 6, 6-tetramethylpiperidine-N-oxyl (TEMPO, 300 μM) for 12 h, respectively, and 2 μM **SiRho-HD** was further added for 30 min, then the cells were washed by DPBS prior to imaging.

For the cisplatin-induced nephrotoxicity model in HK-2 cells, the cellular experiment can be divided into four groups. The first group is that the HK-2 cells were treated with 2 μM **SiRho-HD**. The second and third group is that HK-2 cells were pre-treated with different concentrations of cispaltin (500 μM or 1000 μM) for 12 h, respectively, and then treated with 2 μM **SiRho-HD** for 30 min. Then the cells were washed by DPBS buffer before imaging. The fourth group, cells were pre-incubated with L-carnitine (LC) (3 mM) in the presence of cisplatin (1 mM) for 12 h, and then treated with 2 μM **SiRho-HD** for 30 min, then the cells were washed by DPBS buffer before imaging. Confocal fluorescence imaging of cells was performed using an Olympus FV1000 laser confocal microscopy (Japan).

Cisplatin-induced acute kidney injury and In Vivo dual model imaging. Cisplatin was dissolved in 0.9 % saline. BALB/c mice were intraperitoneally preinjected with cisplatin (20 mg/kg) or LC (200 mg/kg) /cisplatin (20 mg/kg) for 48 h, respectively, then intravenously injected with the probe **SiRho-HD** (50 μL, 200 μM). After 1.5 h, NIRF and PA imaging was observed under an IVIS Lumina XR (IS1241N6071) and InVision 256-TF imaging system (iTheraMedical, Germany) *in vivo* imaging system respectively. All live cells and live animal operations were in accord with institutional animal use and care regulations, according to protocol No. SYXK (Xiang) 2008-0001, approved by Laboratory Animal Center of Hunan.

Histopathological Studies. Renal tissues of BALB/c mice were fixed in 10% formaldehyde immediately following sacrifice, processed for histological examination according to a conventional method, and stained with hematoxylin and eosin (H&E).

Synthesis and Characterization



Scheme S1. Synthetic route for probe **SiRho-HD**.

Synthesis of compound 3. Si-rhodamine (compound **1**) was synthesized according to a literature procedure [1]. Compound 1 (0.428 g, 1 mmol) was dissolved in dry DCM, and then $POCl_3$ (0.5 mL) was added slowly through syringe, followed with a drop of dry DMF. The above solution was stirred at 60 ℃ for 5 h. After compound 1 was completely converted, the solvent was removed under vacuum and the residue was re-dissolved in dry MeCN, 1-boc-piperazine (0.186, 1mmol) and Et_3N (0.5 mL) in dry MeCN was added slowly through

syringe. The above solution was stirred at room temperature for 2 h. The solvent was removed under vacuum and the residue was re-dissolved in dry DCM (20 mL), and then 4 mL TFA was added. The above solution was stirred at room temperature for 2 h. And then the reaction solution was extracted with 100 mL DCM/CH_3OH (10:1, v/v) for three times. Then the combined organic solution was concentrated under reduced pressure. Because compound **3**, shows great polarity and is easily adsorbed on the silica gel column, so the crude product of compound **3** was not purified for next synthesis. Compound **3** was obtained as a blue solid (0.45 g, 90%).

Synthesis of compound 4. Compound **3** (0.25 g, 0.5 mmol), succinic anhydride (0.1 g, 1 mmol), DMAP (0.122g, 1 mmol) and Et_3N (0.5 mL) were dissolved in DCM, and reaction solution were stirred at room temperature for 5 h. The organic solution was concentrated under reduced pressure. After purified by the silica gel chromatography (CH_2Cl_2/CH_3OH, 10:1, v/v), compound **4** was obtained as a blue solid (0.23 g, 75%). ^{1}HNMR (DMSO-d6, 400 MHz) δ (ppm): 8.40 (s, 3 H), 8.28-8.26 (d, J = 8.27 Hz, 3H), 7.29-7.23 (m, 3H), 3.62-3.56 (m, 4H), 3.48-3.43 (dd, J = 3.46 Hz, 4H), 3.32 (s, 6 H), 3.13-3.07 (dd, J = 3.10 Hz, 4H), 1.30 (s, 6 H), 0.65 (s, 3 H), 0.46 (s, 3 H). MS (EI): m/z 597.32, $[M]^+$, calcd. 597.81.

Synthesis of compound 7. 1-(3-aminopropyl)-2,3,3-trimethyl-3H-indol-1-ium (compound **5**) and 6-(diethylamino)-2,3-dihydro-1H-xanthene-4-carbaldehyde (Compound **6**) were synthesized according to a literature procedure[2, 3], and used without purification. Compound **6** (0.28 g, 1 mmol) and indole salt (0.30 g, 1mmol) were dissolved in 20 mL n-BuOH/PhMe (1:1, v/v), and reaction solution were stirred at 90 ℃ for 1.5 h. The organic solution was concentrated under reduced pressure. After purified by the silica gel chromatography (CH_2Cl_2/CH_3OH, 10:1, v/v), compound **7** was obtained as a blue solid (0.35 g, 63%). ^{1}HNMR (DMSO-d6, 400 MHz) δ (ppm): δ 8.45-8.42 (m, 1H), 7.69-7.67 (m, 2H), 7.55-7.50 (t, J = 7.53, 2H), 7.47-7.44 (t, J = 7.46, 1H), 7.33-7.29 (t, J = 7.31, 1H), 6.94-6.92 (d, J = 6.93, 1H), 6.62 (s, 1H), 6.29-6.25 (d, J = 6.27, 1H), 4.33-4.29 (t, J = 4.31, 2H), 3.56-3.50 (m, 4H), 3.49-3.44 (q, J = 3.46, 2H), 3.24-3.19 (m, 2H), 2.72-2.68 (m, 4H), 1.88 (s, 6H), 1.84-1.81 (d, J = 1.83, 2H), 1.21-1.19 (t, J = 1.20, 6H). MS (EI): m/z, 482.7, $[M]^+$, calcd. 482.3.

Synthesis of probe SiRho-HD. Compound **4** (0.15 g, 0.25 mmol), Compound **7** (0.14 g, 0.25 mmol), HATU (0.19 g, 0.5 mmol) and DIPEA (0.5 mL) were dissolved in 20 mL DCM,

and reaction solution were stirred at room temperature for 3 h. Then, extracted with DCM (50 mL × 3), the combined organic solution was dried with Na_2SO_4, then concentrated under reduced pressure. After purified by the silica gel chromatography (CH_2Cl_2/CH_3CH_2OH, 10:1, v/v), compound **7** was obtained as a dark solid (0.35 g, 63%). ^{1}HNMR (DMSO-*d6*, 400 MHz) δ (ppm): δ 8.47-8.43 (m, 2H), 7.71-7.68 (m, 4H), 7.53-7.32 (m, 9H), 7.01-6.94 (m, 2H), 6.85-6.83 (d, J = 6.84 Hz, 1H), 6.65 (s, 1H), 6.28-6.25 (d, J = 6.27 Hz, 1H), 4.30 (m, 2H), 3.55 (s, 6H), 3.33 (m, 10H), 3.20 (m, 4H), 2.71 (m, 6H), 1.86 (m, 6H), 1.74 (s, 6H), 1.20 (m, 12H), 0.66 (s, 3H), 0.47 (s, 3H). ^{13}CNMR (DMSO-*d6*, 400 MHz) δ 173.84, 170.00, 169.87, 162.90, 156.16, 153.95, 152.17, 147.38, 142.36, 142.08, 141.71, 141.50, 138.51, 135.45, 130.71, 130.16, 129.31, 129.19, 129.06, 127.53, 127.25, 125.75, 123.28, 123.01, 121.68, 114.80, 114.32, 113.03, 112.68, 111.99, 110.67, 96.04, 60.23, 49.65, 44.86, 42.28, 40.94, 36.46, 29.45, 29.22, 28.47, 28.30, 27.52, 24.32, 23.04, 20.71, 14.55, 12.82. MS (EI): m/z, 524.32778, $[M]^{2+}$, calcd. 1048.4599 for $C_{65}H_{77}O_4Si^{2+}$.

probe	$\lambda_{ab}/\lambda_{em}$ (nm)	detection limit	Imaging model	Application	Ref.
PNCy3Cy5	530 nm/ 660 nm and 560 nm	0.65 nM	Ratiometric Fluorescence Imaging	Imaging of Endogenous OONO− in Stimulated RAW 264.7 cells	4
MITO-CC	420 nm/ 473 nm and 651 nm	11.30 nM	Two-photon Ratiometric Fluorescence Imaging	Visualization of the Endogenous OONO− in an Inflamed Mouse Model	5
NIR-$ONOO^-$	660 nm/ 703 nm	90 nM	Near-infrared Fluorescence Imaging	Evaluating Drug-Induced Hepatotoxicity	6
Rhod-$ONOO^-$	500 nm/ 558 nm	43 nM	Fluorescence Imaging	Investigation of Drug-Induced Hepatotoxicity	7
TPNIR-FP	570 nm/ 630 nm	34 nM	Two-Photon Fluorescence Imaging	Investigation of drug-induced cardiotoxicity	8
C-Py-1	425 nm/ 493 nm	150 nM	Fluorescence Imaging	Imaging of Endogenous OONO− in RAW264.7 cells	9
Gal-NIR	440 nm/ 720 nm and 500 nm	170 nM	Ratiometric Fluorescence Imaging	Monitoring Peroxynitrite During Drug-Induced Hepatotoxicity	10
Cy-NEt2	360 nm /487 nm 710 nm /742 nm	170 nM	Ratiometric Fluorescence Imaging	assessing the mitochondrial oxidative stress status	3
SiRho-HD This work	635 nm/ 680 nm and 750 nm	360 nM	Ratiometric Near-infrared Fluorescence Imaging/ Photoacoustic Imaging	Imaging of Peroxynitrite in Drug - Induced Acute Kidney Injury	

Table S1. Representative mitochondria-targeting $OONO^-$ probes.

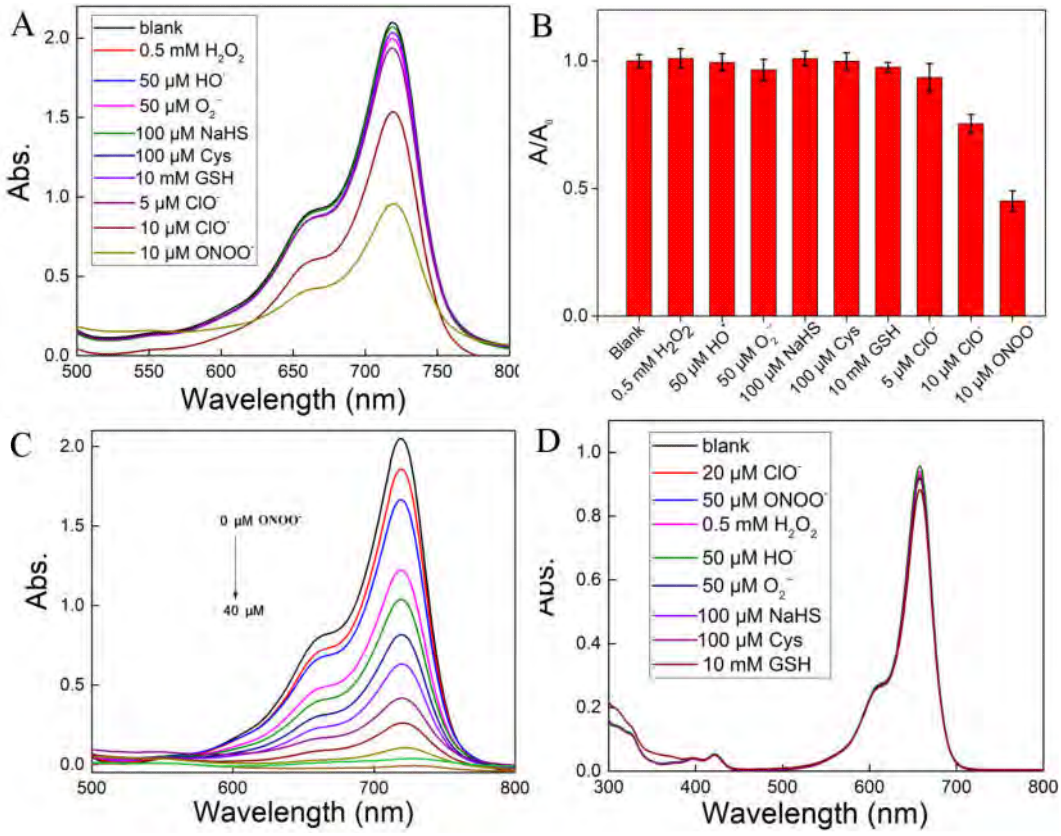


Fig. S1 (A) Absorption spectra of compound **7** (5 μM) treated with various agents. (B) The relative absorption intensity at 719 nm of compound **7** (5 μM) after treated with various agents, the absorption intensity of free compound **7** (5 μM) was defined as 1.0. (C) Absorption spectra of compound **7** (5 μM) treated with various concentration $OONO^-$. (D) Absorption spectra of compound **4** (5 μM) treated with various agents. The experiments were carried out in pH 8.0 PBS/EtOH (v/v, 9/1), data were recorded 10 min after the addition of analytes at 25 °C.

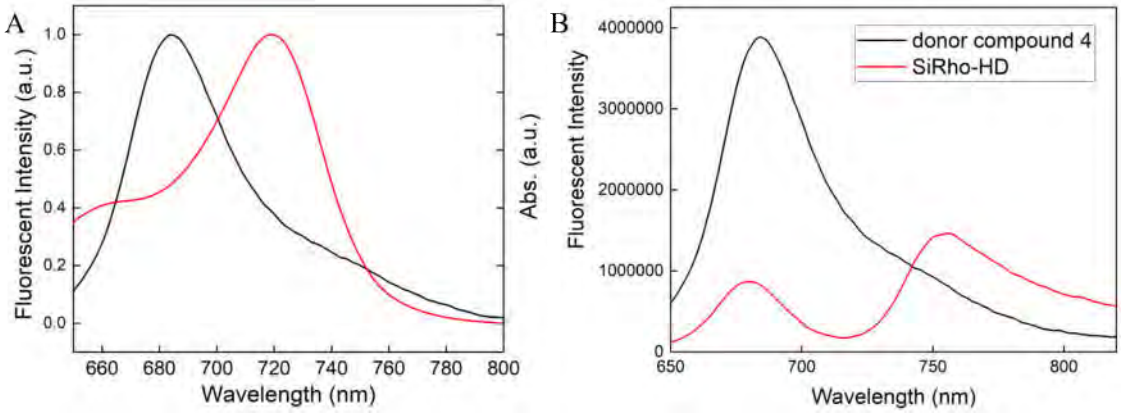


Fig. S2 (A) 1 (a) Normalized emission spectra of donor derivative **4** (black line) and normalized absorption spectra of acceptor **7** (red line). (B) Normalized emission spectra. The black and red lines represent donor derivative **4** (2 μM) and **SiRho-HD** (2 μM) respectively, as the respective fluorescence responses. The experiments were carried out in pH 7.4 PBS/EtOH (v/v, 9/1), data were recorded 10 min after the addition of analytes at 37 °C. **Energy Transfer Efficiency (ETE)** = [(fluorescence of donor-fluorescence of donor in cassette)/fluorescence of donor] × 100%; For **SiRho-HD** (2 μM), ETE=

(3739826 - 867177)/ 3739826 × 100% = 76.8%.

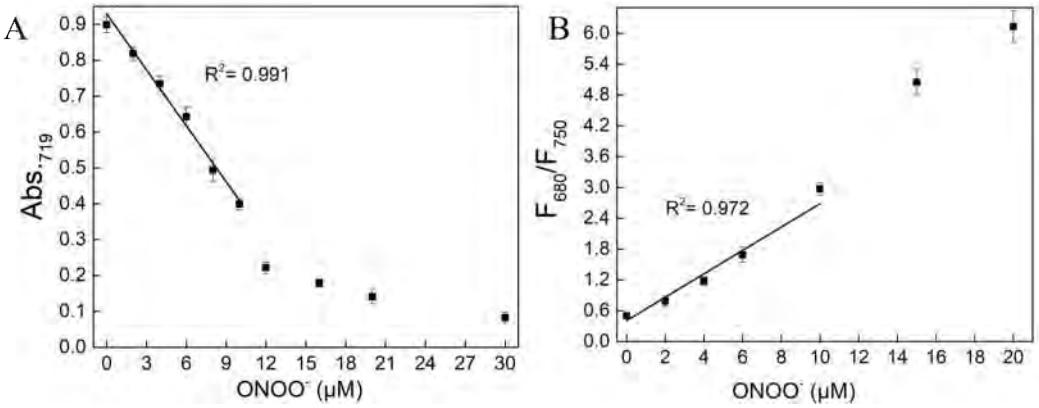


Fig. S3 (A) Plot of Abs_{719} of **SiRho-HD** against $OONO^-$ concentrations and linear relationship in 0-10 μM $OONO^-$ range. (B) Plot of F_{680}/F_{750} of **SiRho-HD** against $OONO^-$ concentrations and linear relationship in 0-10 μM $OONO^-$ range.

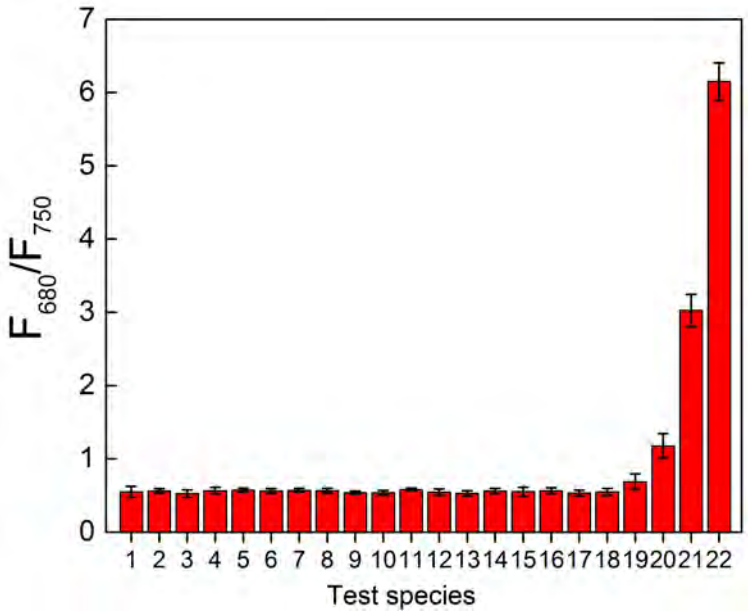


Fig. S4 Selective test in ph8.0 PBS/EtOH (9:1, v/v) solution, emission intensity ratio (F_{680}/F_{750}) of **SiRho-HD** (2 μM) in the presence of various metal ions and anion (1mM), sulfur compounds (1 mM) and RONSs: 1-22 (blank, Ca^{2+}, Mg^{2+}, Zn^{2+}, Fe^{3+}, NO_3^-, SO_4^{2-}, Cl^-, BSA (1 μg/mL), H_2S, Cys, 10 mM GSH, SO_3^{2-}, 200 μM H_2O_2, 200 μM tBuOOH, 100 μM $O_2^{\bullet-}$, 100 μM •OH, 50 μM NO, 5 μM ClO^-, 10 μM ClO^-, 10 μM $ONOO^-$, and 20 μM $ONOO^-$).

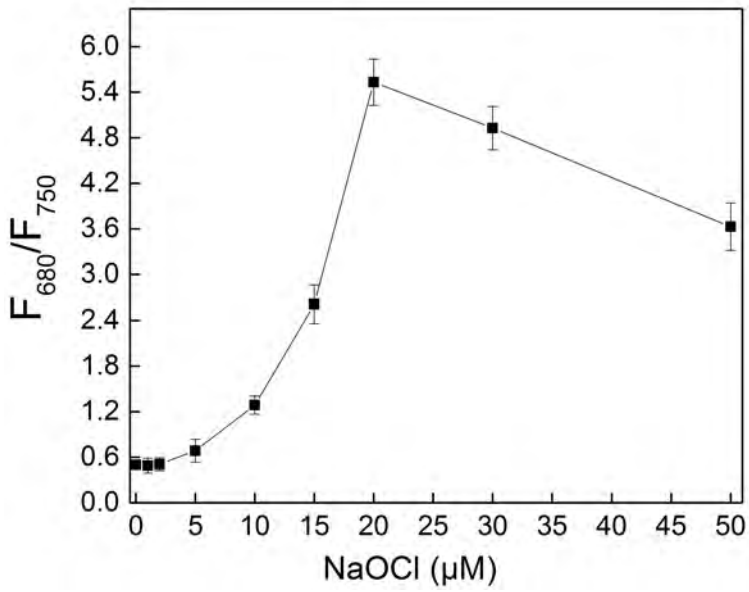


Fig. S5 Plot of F_{680}/F_{750} of **SiRho-HD** against NaOCl concentrations (0-50 μM NaOCl range). The experiment was conducted in ph8.0 PBS/EtOH (9:1, v/v) solution. The results clearly showed that the probe exhibited limited fluorescence change in the presence of 0-5 μM NaOCl, and when the concentration of NaOCl increased to 30 μM, the fluorescence intensity at 680 nm also showed decrease, probably because the destroy of **SiRho** by NaOCl.

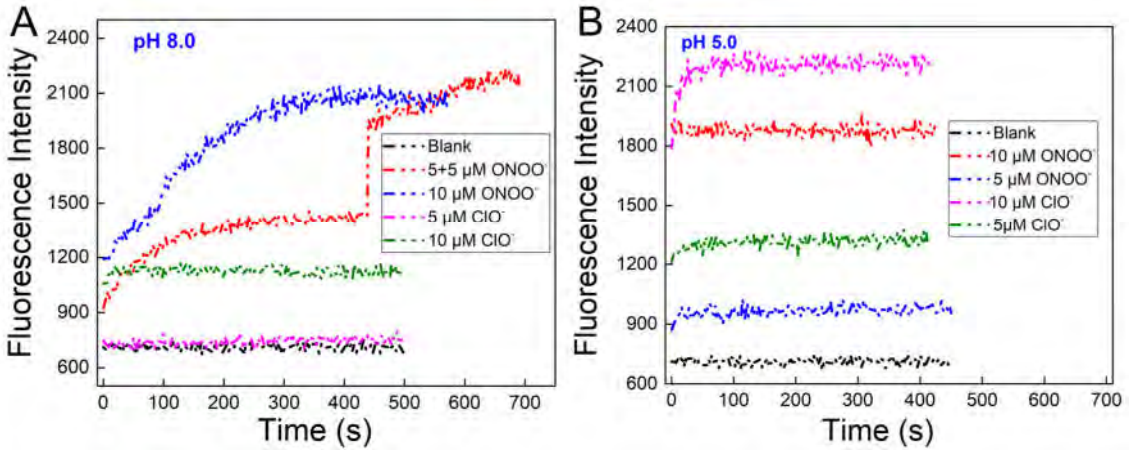


Fig. S6 Fluorescence intensity at 680 nm of **SiRho-HD** (2 μM) as a function of time in the presence of $ONOO^-$ or ClO^- in 100 mM PBS buffer, (A) pH 8.0, (B) pH 5.0. λ_{ex} = 635 nm.

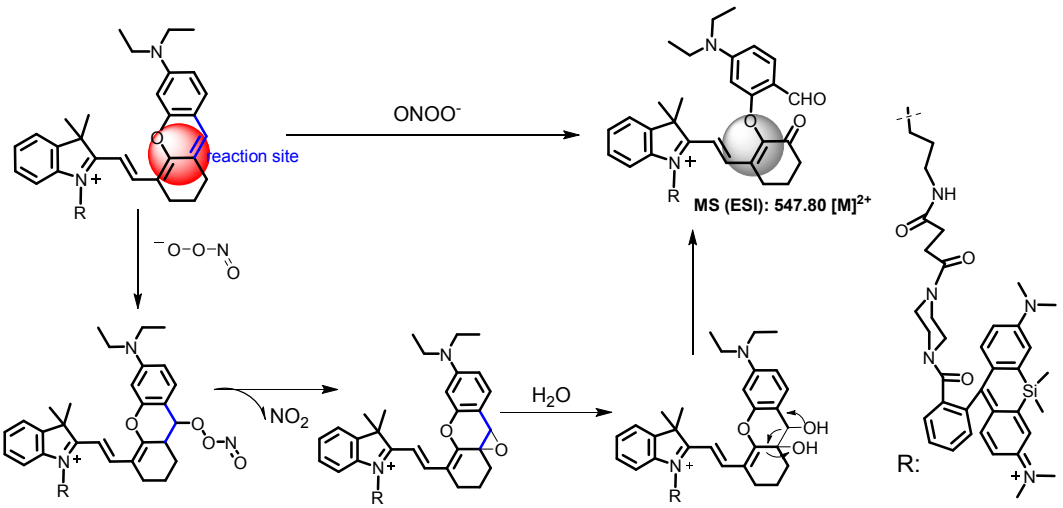


Fig. S7 The proposed reaction mechanism of probe **SiRho-HD** and $ONOO^-$.

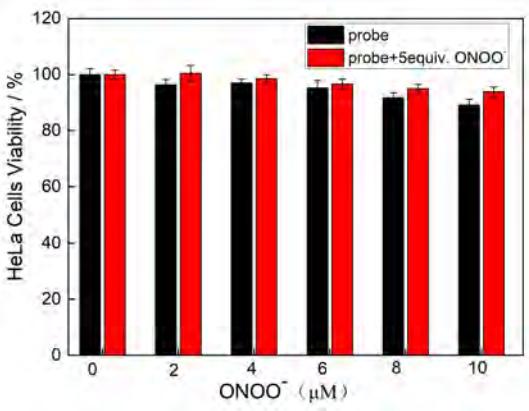


Fig. S8 Cytotoxicity of **SiRho-HD** against HeLa cells as determined by MTS assay. HeLa cells were treated with (black bar) **SiRho-HD** (0-10 μM) or (black bar) the solutions of **SiRho-HD** (0-10 μM) and 5 equiv. $ONOO^-$ for 24 h.

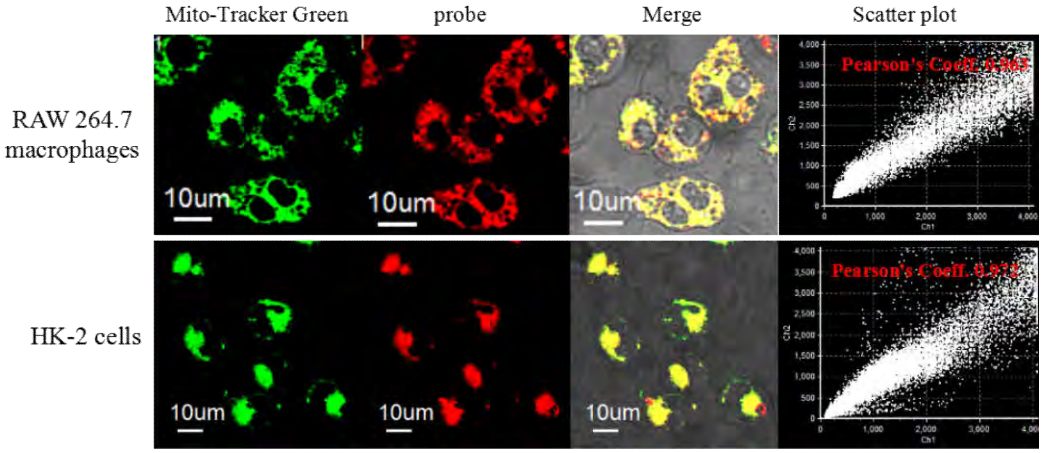


Fig. S9 Intracellular localization of **SiRho-HD** in RAW264.7 macrophages or HK-2 cells. Images of cells pretreated respectively with 2 μM SiRho-HD for 20 min and subsequently 0.5 μM Mito-Tracker Green for 10 min. Green channel: Mito-Tracker Green fluorescence (λ_{ex}= 488 nm, λ_{em} = 500−550 nm); Red channel: probe fluorescence (λ_{ex}= 635 nm, λ_{em} = 720−780 nm); yellow, merged signal. Scatter plot: Intensity correlation plot of stain. The Pearson correlation factor is 0.963 and 0.972 respectively. Scale bar: 10 μm.

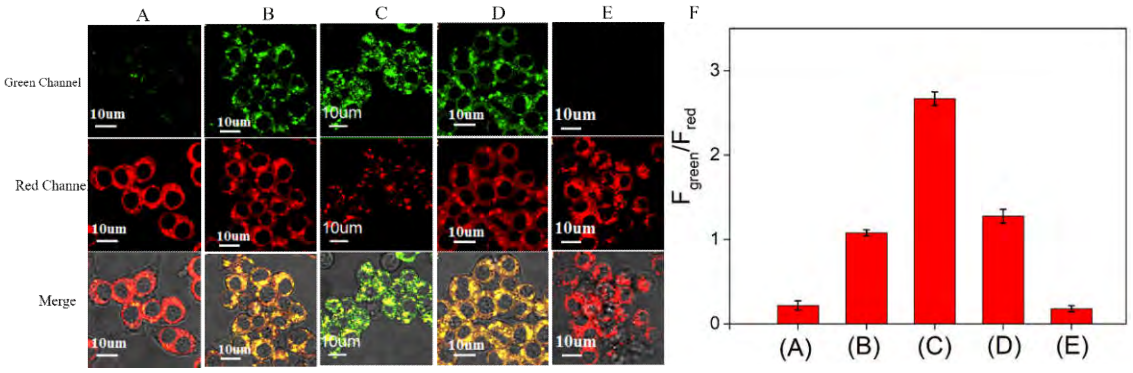


Fig. S10 Confocal fluorescence imaging of $ONOO^-$ using **SiRho-HD** (2 μM) in RAW264.7 macrophages. (A) Probe alone for 30 min; cells were stimulated with (B) 500 μM SIN-1 or (C) 1000 μM SIN-1 for 120 min, subsequently co-incubated with **SiRho-HD** for 30 min; (D) cells were pretreated with 1 μg/mL LPS and 50 ng/mL IFN-γ for 12 h, then co-incubated with **SiRho-HD** for 30 min; (E) cells simultaneously treated with 0.3 mM TEMPO during stimulation with 1 μg/mL LPS and 50 ng/mL IFN-γ for 12 h, then co-incubated with **SiRho-HD** for 0.5 h. (F) The normalized average fluorescence intensity of the ratio channel in above displayed imaging A-E. λ_{ex}= 635 nm, green channel at 650−700 nm; red channel at 720−780 nm. Error bars represent standard deviation.

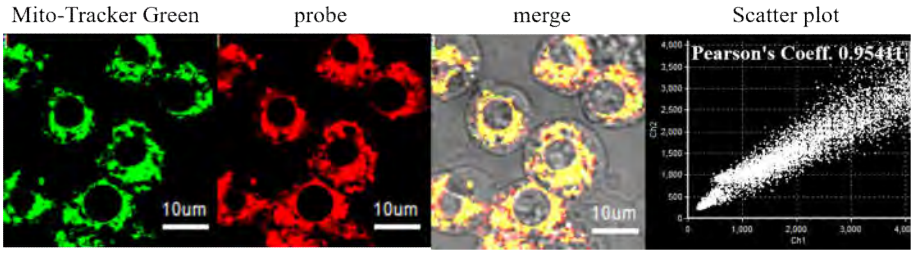


Fig. S11 Intracellular localization of **SiRho-HD** in 1 mM SIN-1 pretreated RAW264.7 macrophages. Images of cells pretreated respectively with 1 mM SIN-1 for 2 h, then washed with DPBS for twice, followed by incubating with 2 μM **SiRho-HD** for 20 min and subsequently 0.5 μM Mito-Tracker Green for 10 min. Green channel: Mito-Tracker Green fluorescence (λ_{ex}= 488 nm, λ_{em} = 500−550 nm); Red channel: probe fluorescence (λ_{ex}= 635 nm, λ_{em} = 650−700 nm); yellow, merged signal. Scatter plot: Intensity correlation plot of stain. The Pearson correlation factor is 0.954. Scale bar: 10 μm.

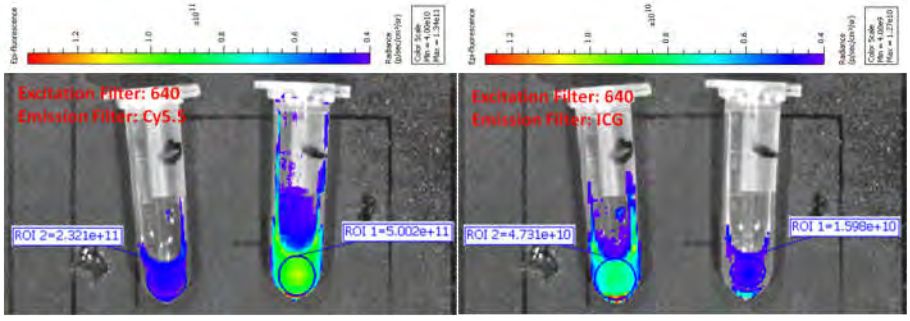


Fig. S12 Imaging of **SiRho-HD** (10 μM) before (marked as 0) or after (marked as 1) reaction with $ONOO^-$ (50 μM). The experiments were carried out in pH 8.0 PBS/EtOH (v/v, 9/1), data were recorded 10 min after the addition of analytes at 25 °C. Excitation filter 640, Emission filter Cy5.5 and ICG. The ratio of Cy5.5 channel / ICG channel is 4.906 and 31.30 for **SiRho-HD** before or after reaction with $ONOO^-$ respectively.

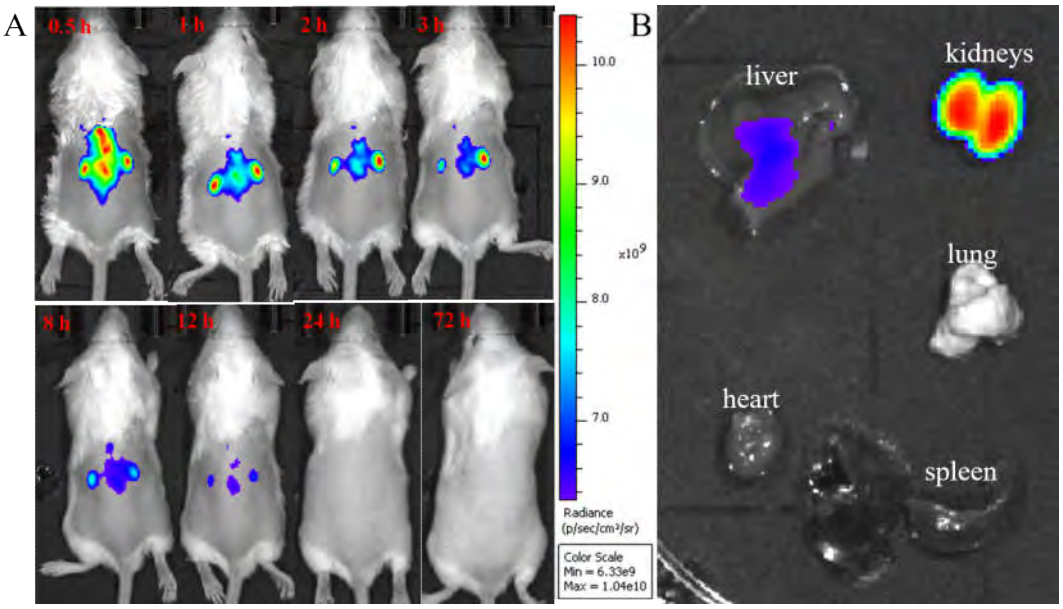


Fig. S13 (A) In vivo imaging of mice at various times after intravenous injection of **SiRho-HD** (50 μL, 100μM). (B) Fluorescence images of the internal organs at 1.5 h post injection of **SiRho-HD** after anatomy. Excitation filter 640, emission filter ICG.

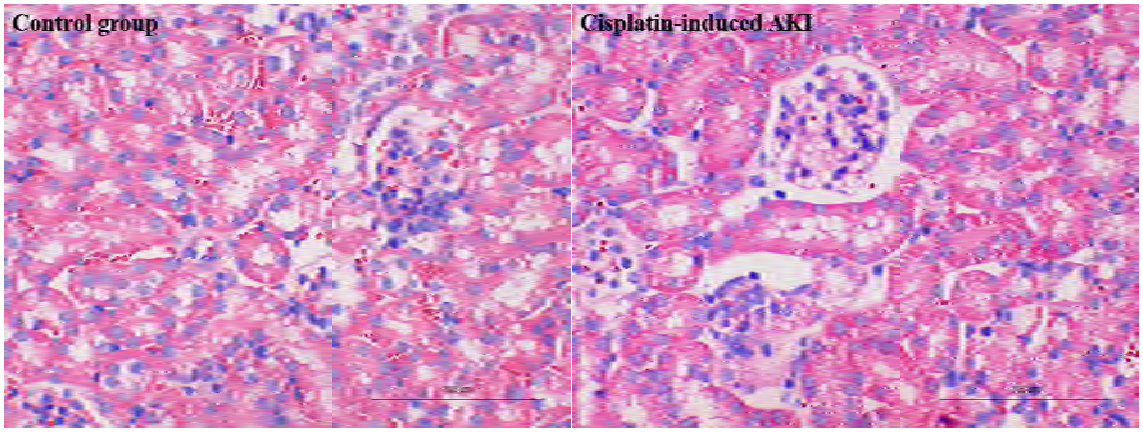


Fig. S14 Representative photomicrographs of H&E staining in paraffin-embedded kidney sections from normal mouse or mouse treated with cisplatin for 48 h.

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Mass Spectra and ^{1}HNMR

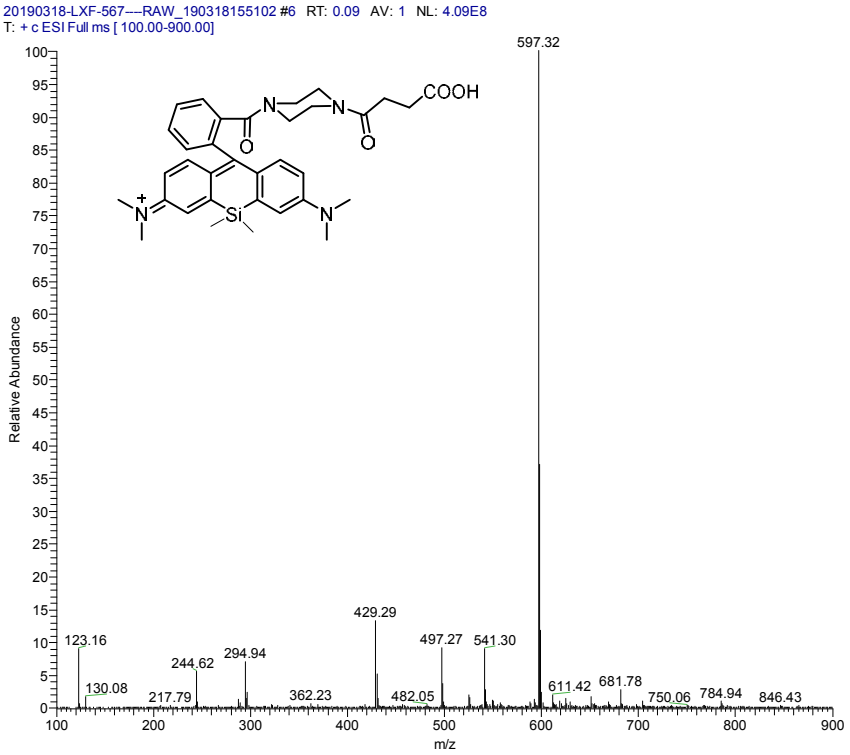

Fig. S15. EI mass spectrum of the compound **4**.

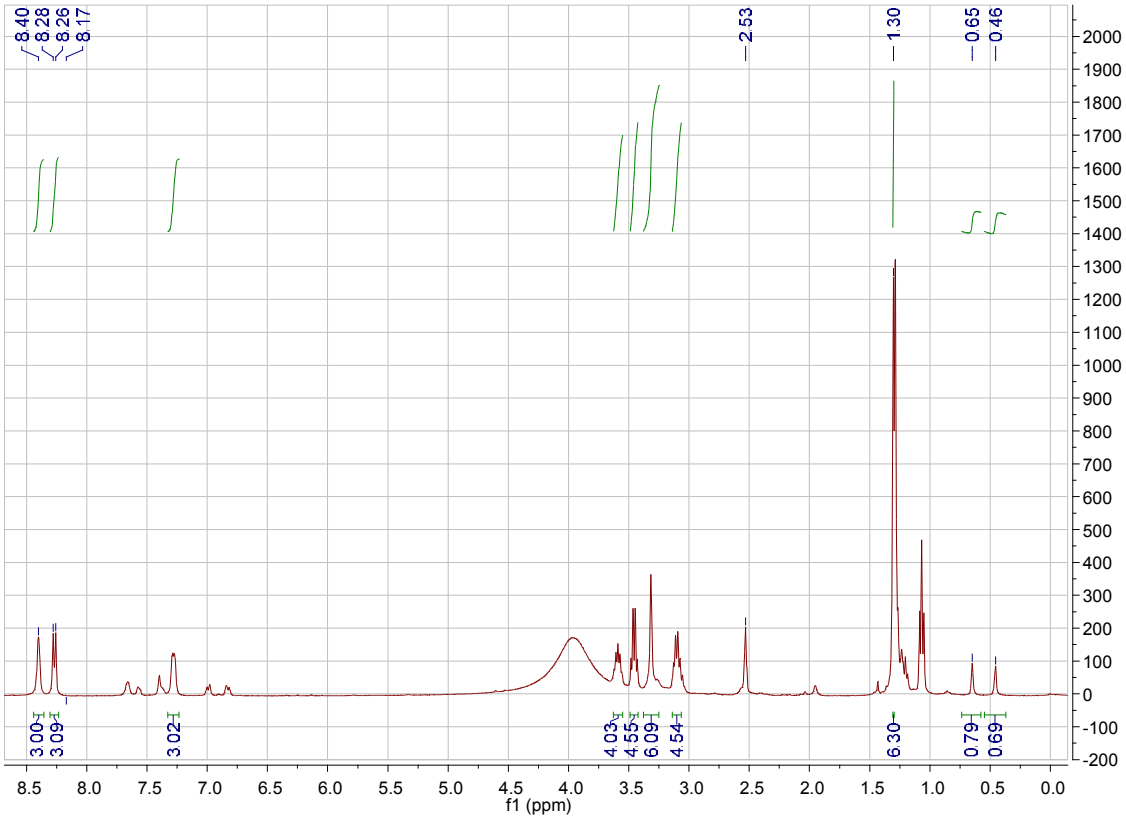

Fig. S16. ^{1}HNMR spectrum of the compound **4**.

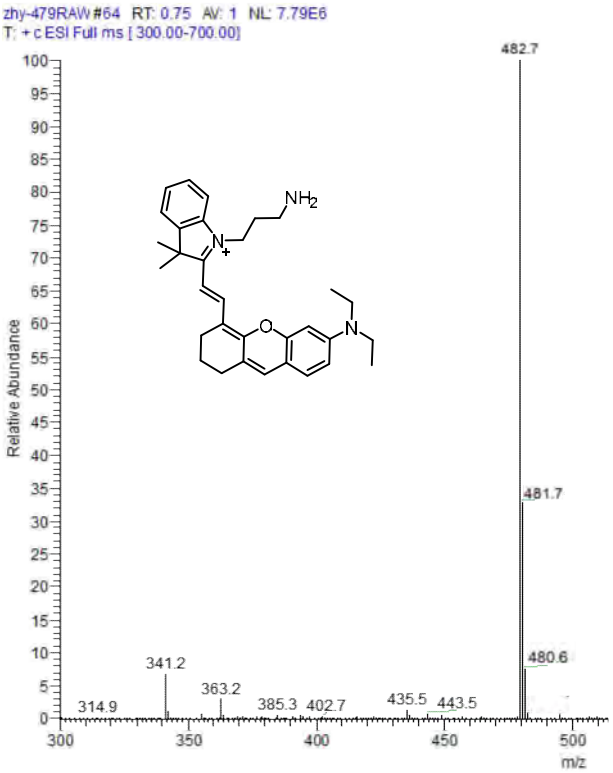

Fig. S17. ESI MS spectrum of the compound **7**.

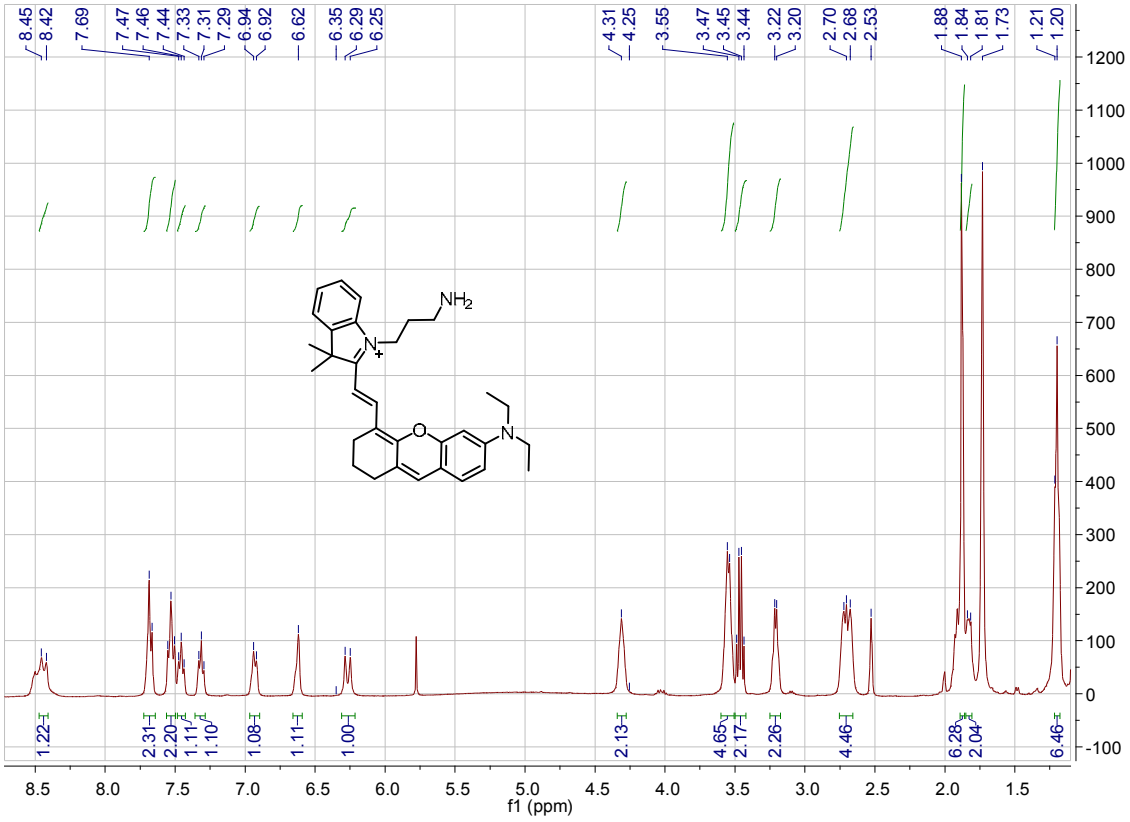

Fig. S18. [1]HNMR spectrum of the compound **7**.

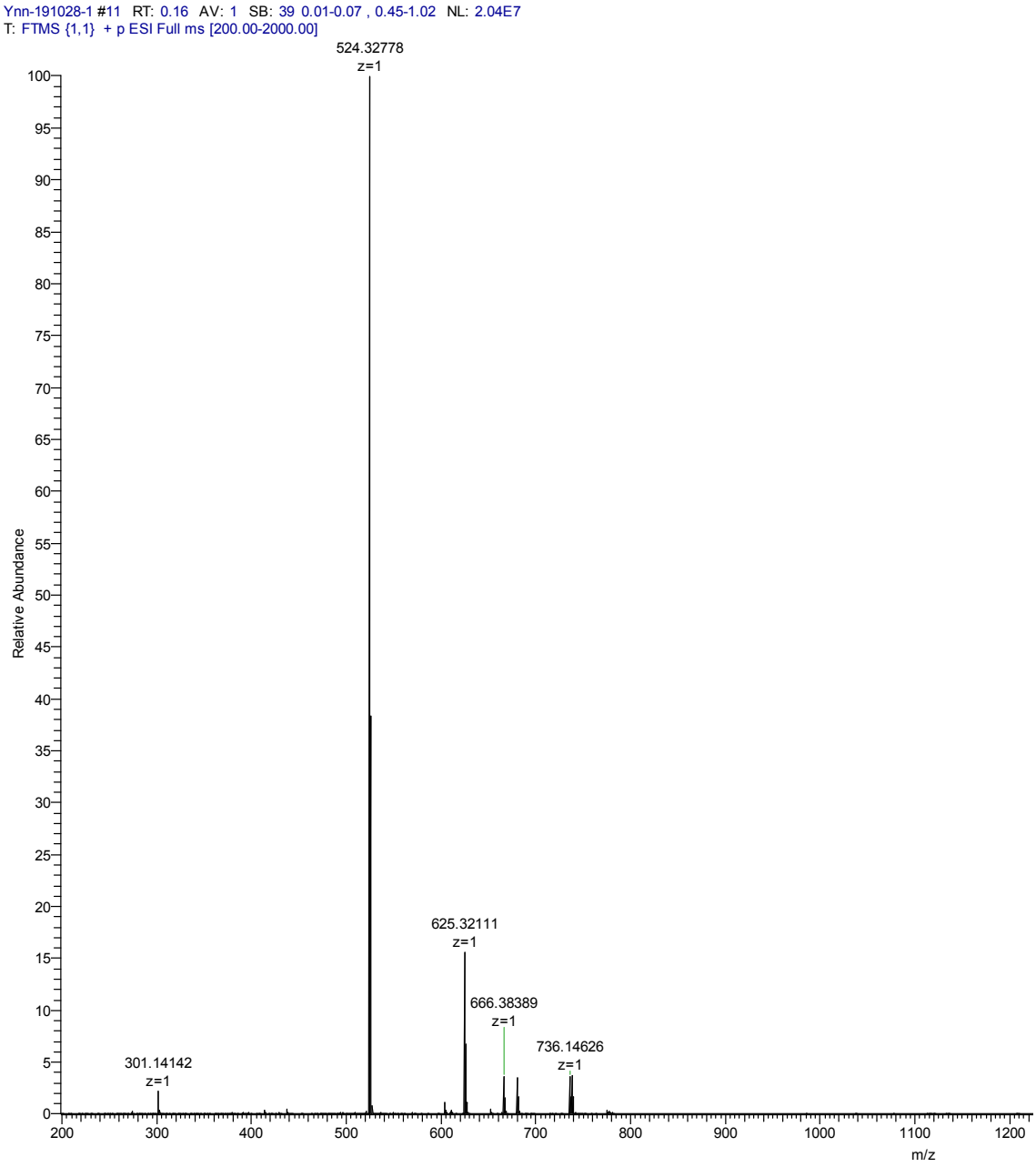

Fig. S19. HRMS-ESI mass spectrum of probe **SiRho-HD**.

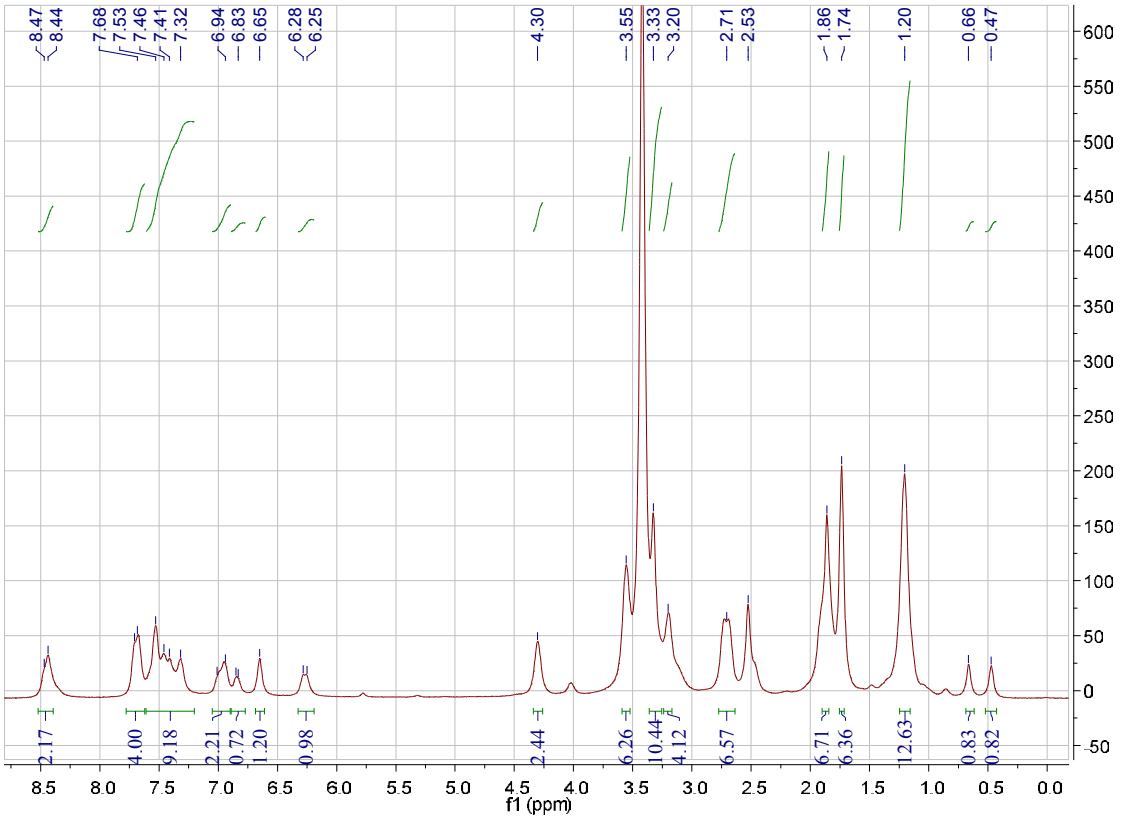

Fig. S20. [1]HNMR spectrum of **SiRho-HD**.

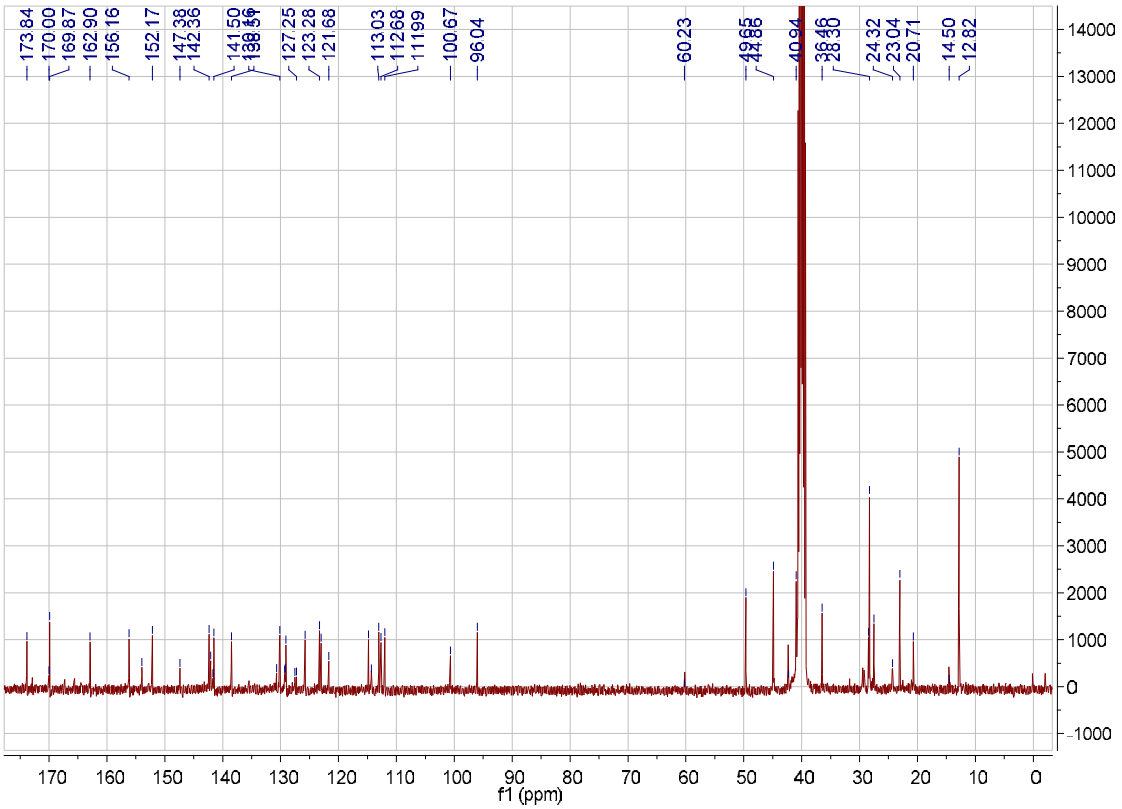

Fig. S21. [13]CNMR spectrum of **SiRho-HD**.

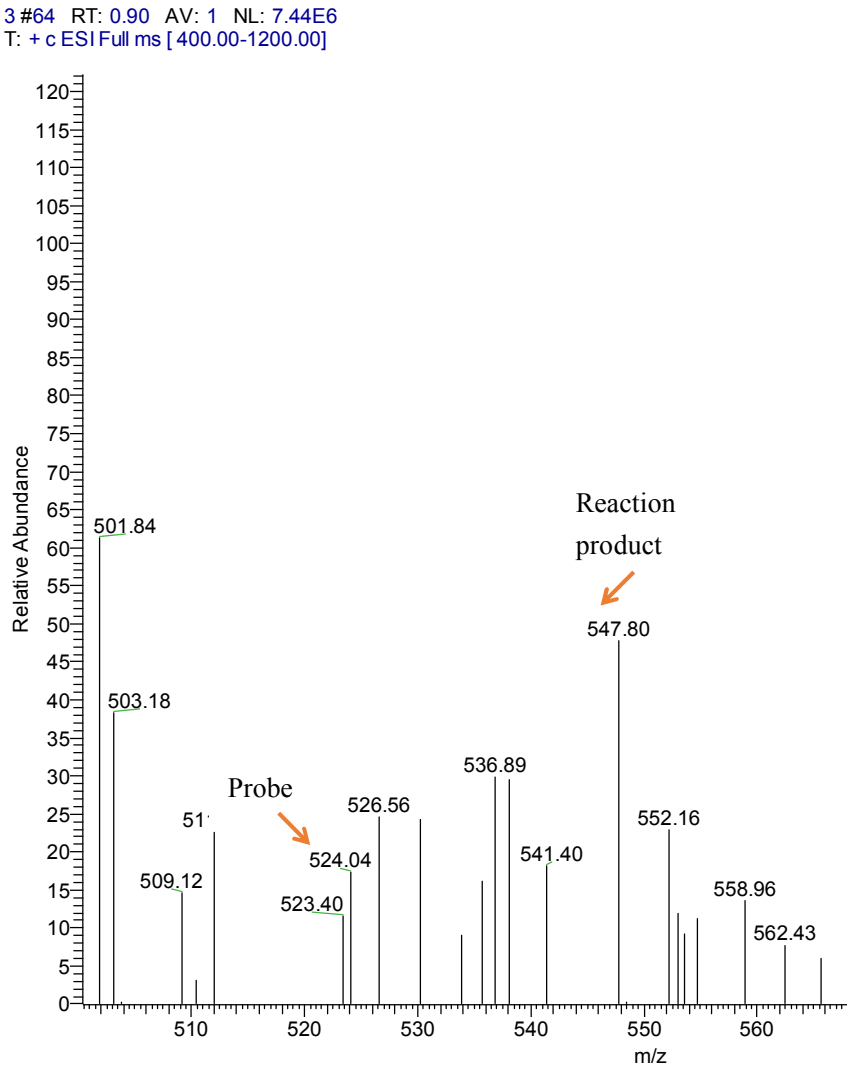

Fig. S22. MS spectrum of **SiRho-HD** after reaction with 10 μM $ONOO^-$.