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Supporting Information

Engineering dithiobenzoic acid lactone decorated Si-rhodamine as highly selective near-infrared HOCl fluorescent probe for imaging drug-induced acute nephrotoxicity

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1. Reported representative fluorescent probes for HOCl

Probes	□λ_{ex}/nm	□λ_{em}/nm	LOD/nM	Sensitivity[a]	Detection time	Bioimaging application
HKOCl-3[1]	490	527	0.33	358-fold (2.0 equiv)	Within 1 min	Cell Zebrafish
FCN2[2]	415	485	6.68	1643.4-fold (3.3 equiv)	Within 30 min	Cell Zebrafish
1[3]	394	509/439	～	9.8-fold (30.0 equiv)	Within seconds	～
Flu-1[4]	454	530	～	61-fold (20.0 equiv)	Within seconds	Cell
STP-HOCl[5]	420	520/470	～	ca. 10-fold (30.0 equiv)	1 min	Cell Liver tissue
CY-FPA[6]	700	774	700	0.1-fold (30 equiv)	～	Cell
1[7]	465	520/629	500	ca. 760-fold	ca. 10 min	Cell
ClO1[8]	530	605/760	100	69-fold (2.8 equiv)	～	Cell Mouse inflamed lung
SeCy7[9]	690	786	310	19.4-fold (2.0 equiv)	Within dozen of seconds	Living mice
NI-Se[10]	450	523	586	> 10 fold (10.0 equiv)	Several minutes	Cell Living mice
FO-PSe[11]	415	520	350	> 10 fold (1.0 equiv)	Within seconds	Cell Mouse peritonitis Zebrafish
1[12]	492	507	30.9	ca. 18-fold (3.0 equiv)	Within seconds	Cell
2[12]	511	526	4.5	ca. 50-fold (4.0 equiv)	Within seconds	Cell
MPhSe-BOD[13]	460	510	～	ca. 5-fold (10.0 equiv)	20 min	Cell
HCSe[14]	510	526	7.98	138-fold (1.0 equiv)	ca. 6 min	Cell
CM1[15]	405	480	10	> 50-fold (7.0 equiv)	Within seconds	Cell
2[16]	337	392	～	～	1 h	～
Coum-Se[17]	475	618/495	4.6	241-fold (5.0 equiv)	Within seconds	Cell Liver and Kidney tissues
HySO3H[18]	555	575	～	> 50-fold (2.5 equiv)	Within seconds	Cell
MMSiR[19]	620	675	～	> 50-fold	Within	Cell

				(1.0 equiv)	seconds	Mouse peritonitis
MITO-TP[20]	375	500	17.2	634-fold (20.0 equiv)	Within seconds	Cell Inflamed tissues
LYSO-TP[20]	375	500	19.6	610-fold (20.0 equiv)	Within seconds	Cell Inflamed tissues
PIS[21]	378	505	71	> 5-fold (5.0 equiv)	ca. 10 min	Cell Hippocampal slice
rTP-HOCl 1[22]	460	633/598	34.8	> 70-fold (3.6 equiv)	Within seconds	Cell Mouse brain tissues
FDOCl-1[23]	620	686	2.62	2068-fold (2.5 equiv)	30 s	Cell Inflamed tissues Living mice
FBS[24]	498	523	200	> 50-fold (3.6 equiv)	Within seconds	Intestinal epithelia of *Drosophila*
Lyso-NIR-HClO[25]	620	680	20	Ca. 35-fold (6.0 equiv)	4 min	Cell Liver tissue Mouse peritonitis
QClO[26]	426	562/492	89	ca. 16-fold (5.0 equiv)	1 min	Cell Mouse wounded tissues
Lyso-SiR-2S (this work)	**616**	**677**	**25**	**83-fold (12.0 equiv)**	**Within seconds**	**Cell Kidney organ Living mice**

[a]Fluorescence intensity or emission ratio changes before and after treated with HOCl.

Table S1 Some reported representative fluorescent probes for HOCl and our probe **Lyso-SiR-2S**.

2. Materials and instruments

All reagents were purchased from commercial suppliers and used without further purification. Some organic solvents were redistilled and dried by standard methods if necessary. Silica gel 60 F254 plates were employed for thin layer chromatography (TLC), and silica gel (200−300 mesh) for column chromatography. Both were obtained from the Qingdao Ocean Chemicals. Hypochlorous acid (HOCl) was from commercial bleach NaOCl solution. The solution of *tert*-butyl hydroperoxide (*t*BuOOH) and Hydrogen peroxide (H_2O_2) was prepared by diluting commercial aqueous solution, respectively. Tertbutoxy radical *(t*BuO·*)* andHydroxyl radical (·OH) were generated *in situ* by reaction of Fe^{2+} with *t*BuOOH or H_2O_2, respectively. Superoxide solution ($O_2^{\bullet-}$) was prepared by dissolving KO_2 in DMSO. Peroxynitrite ($ONOO^-$) solution was prepared from SIN-1.[27]

NMR spectra were recorded on a Bruker-400 spectrometer, and high-resolution electronspray (ESI-HRMS) spectra were obtained from The Thermo Fisher Scientific LTQ FT Ultra (Shanghai Institute of Organic Chemistry Chinese Academic of Sciences). Mass spectra were performed using an LCQ Advantage ion trap mass spectrometer (Thermo Finnigan). Phosphate buffers were prepared using twice-distilled water by a Milli-Q system (Millipore, USA). Fluorescence spectra

were recorded on Hitachi F-7000 fluorescence spectrometer (1 cm standard quartz cell). Absorption spectra were taken on a UV 1800 ultraviolet and visible spectrophotometer. The pH values were measured on a Mettler-Toledo Delta 320 pH meter. The fluorescence images were acquired with one-photo confocal laser scanning microscope (Nikon, Japan) or Olympus FV1000 equipped with a CCD camera. The fluorescence imaging of kidneys was carried out using an IVIS Lumina XR (IS1241N6071) *in vivo* imaging system.

3. Illustration for background and selectivity of SiR-2S

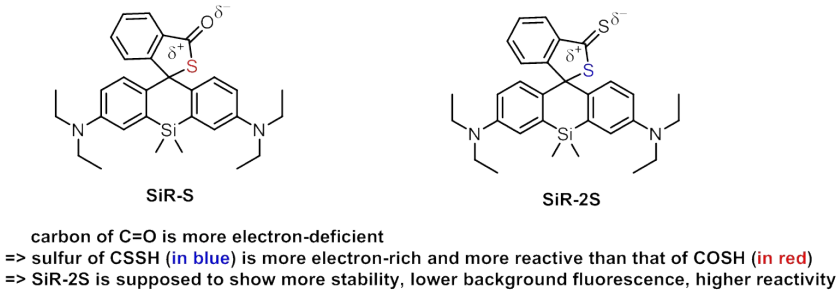


Fig. S1 Illustration for lower background fluorescence and higher selectivity of Si-rhodamine B dithiolactone (**SiR-2S**).

4. Spectrometric studies of SiR-S and SiR-2S

For measurement of photophysical properties, the compounds (**SiR-S**, **SiR-2S**) were dissolved in EtOH to make the stock solutions (500 μM), which were diluted to 5 μM with PBS buffer solution (25 mM, 30% EtOH, pH 4.5) when tested.

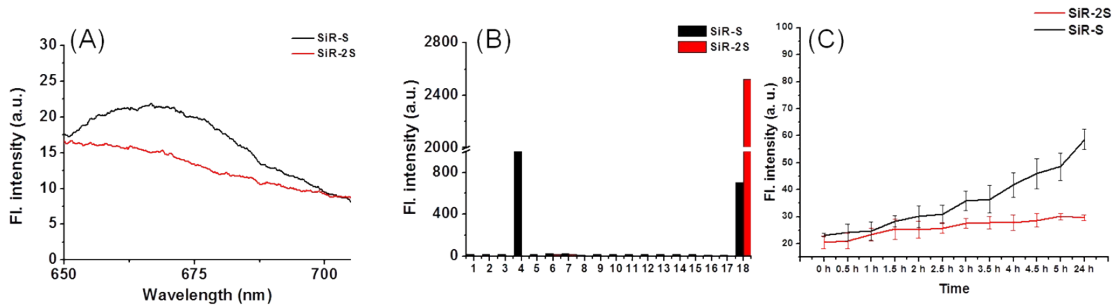


Fig. S2 (A) Background fluorescence of **SiR-S** and **SiR-2S** (5 μM) in PBS (30% EtOH, pH 4.5). (B) Selective response of **SiR-S** and **SiR-2S** (5 μM) toward analytes (100 μM). (1) blank; (2)-(7) in order: H_2O_2; $O_2^{\bullet-}$; $ONOO^-$; *t*BuOOH; $HO\cdot$; *t*BuOO·; (8) Cys; (9) H_2S; (10)-(17) in order: Cu^{2+}; Fe^{3+}; Mg^{2+}; Mn^{2+}; Pb^{2+}; Zn^{2+}; K^+; Na^+; (18) HOCl. The excitation wavelength was 616 nm. (C) Time profile of fluorescence for probes **SiR-S** and **SiR-2S** (5 μM) in PBS buffer solution (25 mM, 30% EtOH, pH 4.5).

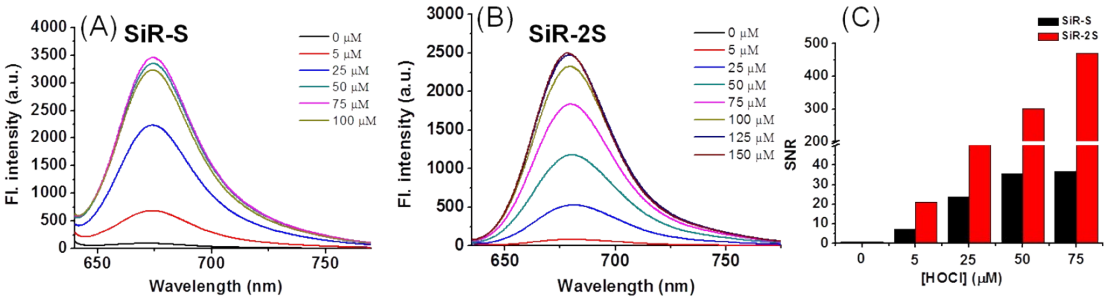


Fig.S3 Fluorescence spectra of **SiR-2S** (5 μM) (A) and **SiR-2S** (5 μM) (B) in PBS buffer solution (25 mM, 30% EtOH, pH 4.5) upon titration of HOCl. (C) The ratio of the signal divided by noise during the titration of **SiR-S** and **SiR-2S** (5 μM) with HOCl.

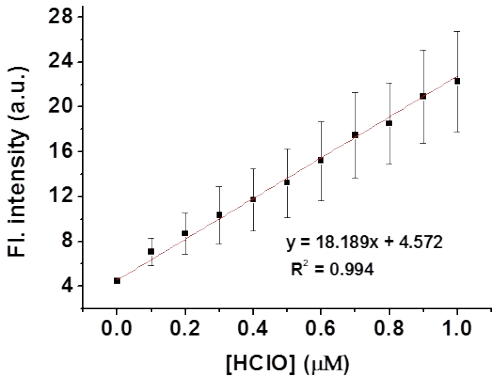
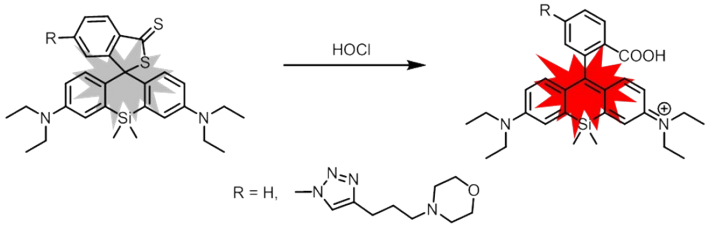
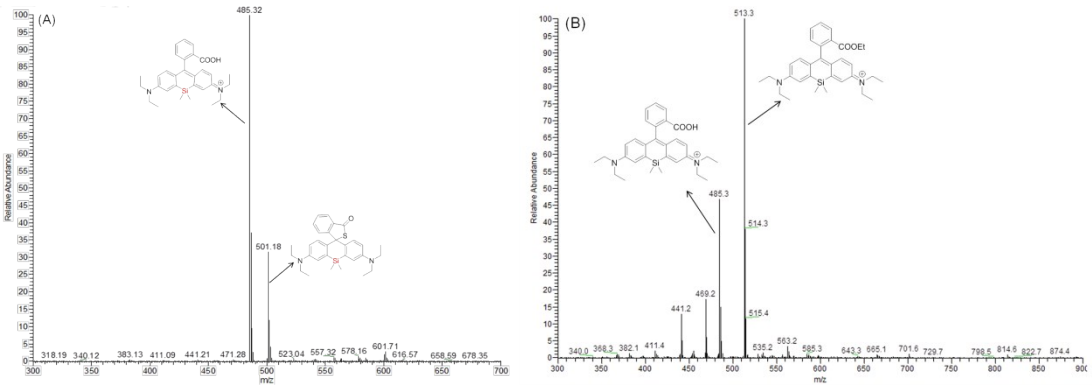


Fig. S4 Linear relationship between the fluorescence of **SiR-2S** (5 μM) and low concentration of HOCl.

5. Mechanism of the probes responding to HOCl





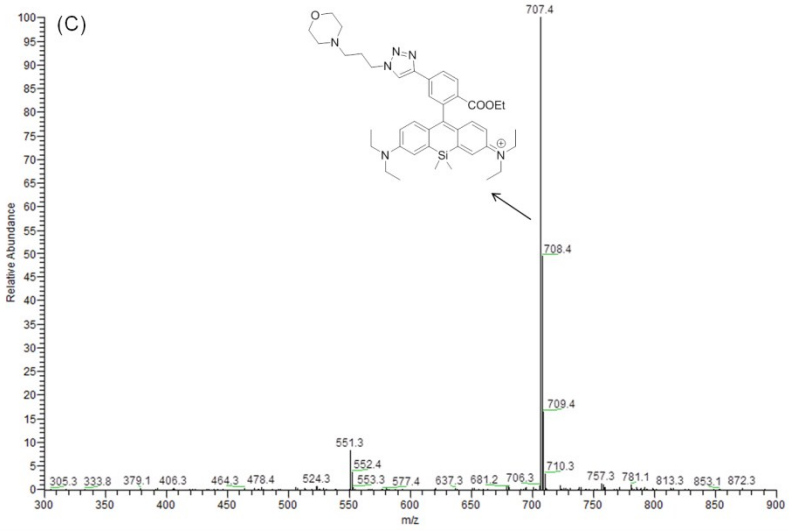


Fig. S5 Mass spectra for the probes **SiR-S** (A), **SiR-2S** (B) and **Lyso-SiR-2S** (C) in the presence of HOCl.

6. Spectrometric studies of Lyso-SiR-2S

The compound **Lyso-SiR-2S** was dissolved in EtOH to make the stock solutions (500 μM), which were diluted to 5 μM with PBS buffer solution (25 mM, 15% EtOH, pH 4.5) when tested.

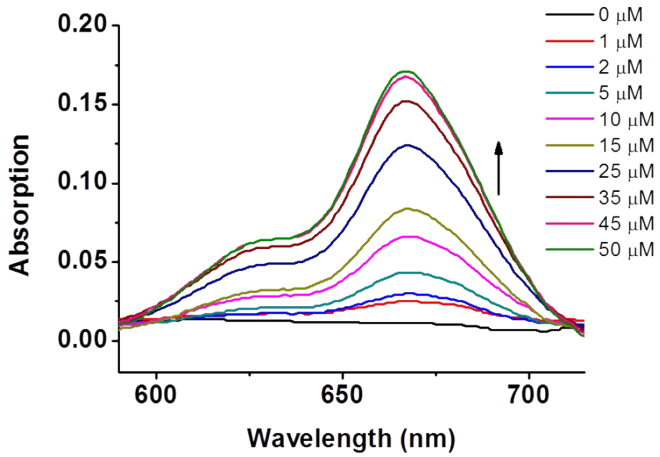


Fig. S6 Absorption spectra of the probe **Lyso-SiR-2S** (5 μM) in PBS buffer solution (25 mM, 15% EtOH, pH 4.5) upon addition of HOCl.

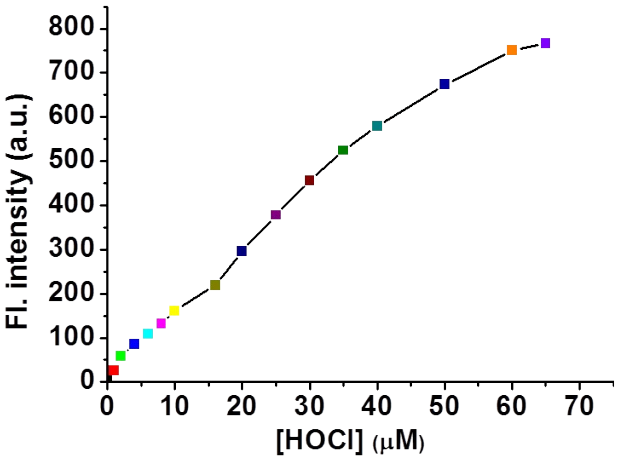


Fig. S7 Fluorescence intensity of **Lyso-SiR-2S** (5 μM) in PBS solution (25 mM, 15% EtOH, pH 4.5) upon HOCl addition (0–65 μM) at emission wavelength 677 nm. The excitation wavelength was 616 nm.

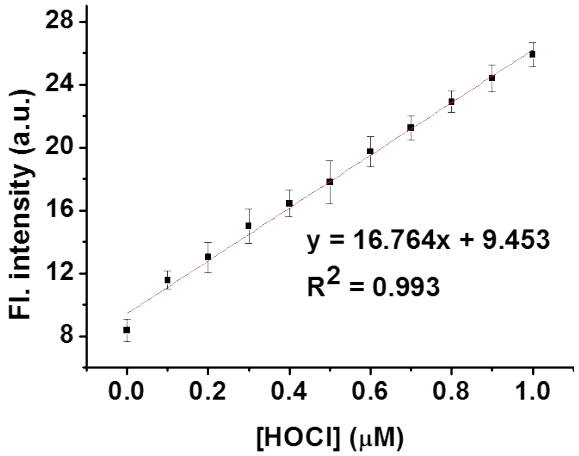


Fig. S8 Linear relationship between the fluorescence of **Lyso-SiR-2S** (5 μM) and low concentration of HOCl. λ_{ex} = 616 nm.

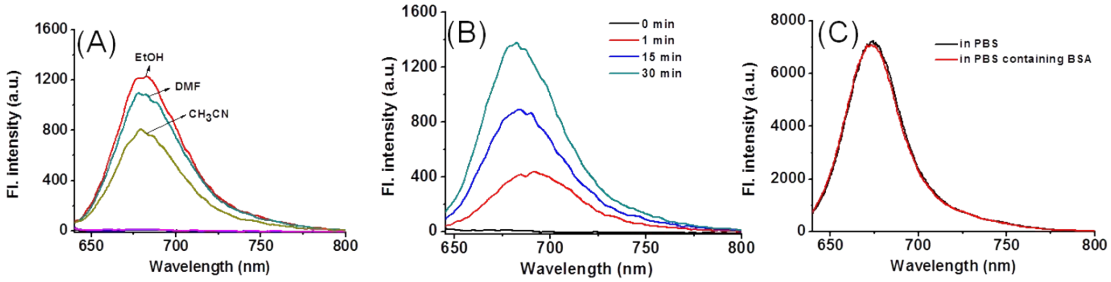


Fig. S9 (A) the response of the probe **Lyso-SiR-2S** (5 μM) to HOCl (50 μM) in PBS (25 mM, pH 4.5) by using 15% EtOH, DMF or CH_3CN as co-solvent. (B) The fluorescence of **Lyso-SiR-2S** (5 μM) in the presence of HOCl (50 μM) in PBS (25 mM, pH 4.5, 15% EtOH) containng 0.5 mg mL^{-1} BSA. (C) the fluorescence of the dye Si-rhodamine B (5μM) in PBS (25 mM, pH 4.5, 15% EtOH) with or without BSA (0.5 mg mL^{-1}).

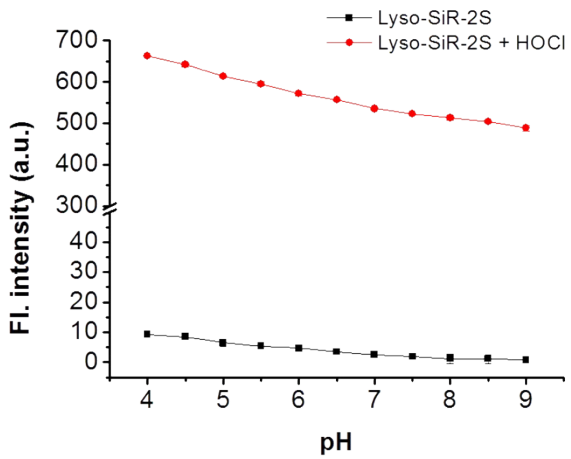


Fig. S10 pH-dependent fluorescence intensity changes of the probe **Lyso-SiR-2S** (5 μM) in PBS buffer solution (25 mM, 15% EtOH) after addition of 50 Mm HOCl, λ_{ex} = 616 nm, λ_{ex} = 677 nm.

7. Cytotoxicitymeasurement

HeLa cells were seeded into a 96-well flat-bottomed plate at 1×10^5 cells per well and incubated at 37 °C and 5% CO_2 for 24 h. Then cells were exposed different concentrations of the probe **Lyso-SiR-2S** and incubated for additional 12 h. After the MTT (0.5 mg mL^{-1}) reagent was added, cells were incubated for 4 h at 37°C. Subsequently DMSO (100 μL per well) was added to dissolve the precipitated formazan violet crystals and cells were incubated at 37 °C for 15 min. The absorbance at 490 nm was measured by a multidetection microplate reader. The viability of cell growth was calculated according to the formula: Cell viability (%) = (mean of *A* value of treatment group/mean of *A* value of control) ×100.

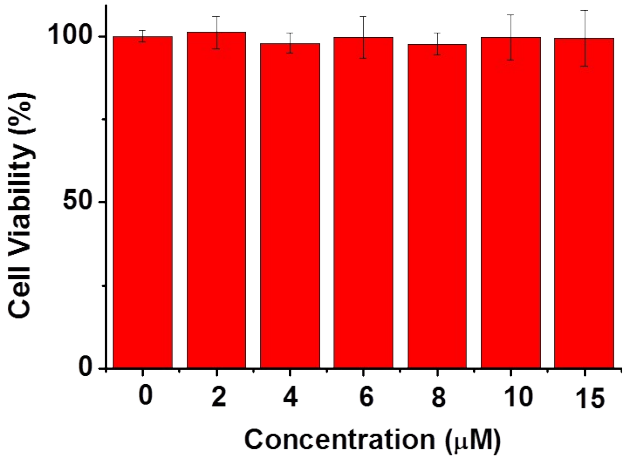


Fig. S11 Cytotoxicity of **Lyso-SiR-2S** for HeLa cells. Cells were incubated with the probe at corresponding concentrations for 12 h. Cell viability was measured by MTT assay and the results were reported as percentage relative to untreated cells (mean ± SD).

8. Cell culture and imaging

HeLa cells were cultured in RPMI-1640 medium, RAW264.7 macrophages and HK-2 cells were cultured in Dulbecco's modified Eagle's medium (DMEM, Hyclone) at 37°C and 5% CO_2. Both two kinds of medium were supplemented with 10% fetal bovine serum (FBS, BI), and 1%

antibiotics (100 U mL^{-1} penicillin and 100 μg mL^{-1} streptomycin, Hyclone). Cells were carefully harvested and split when they reached 80% confluence to maintain exponential growth. One day before imaging, the cells were detached and replanted on glass-bottomed dishes. All the fluorescence microscopic imaging experiments were conducted in live cells.

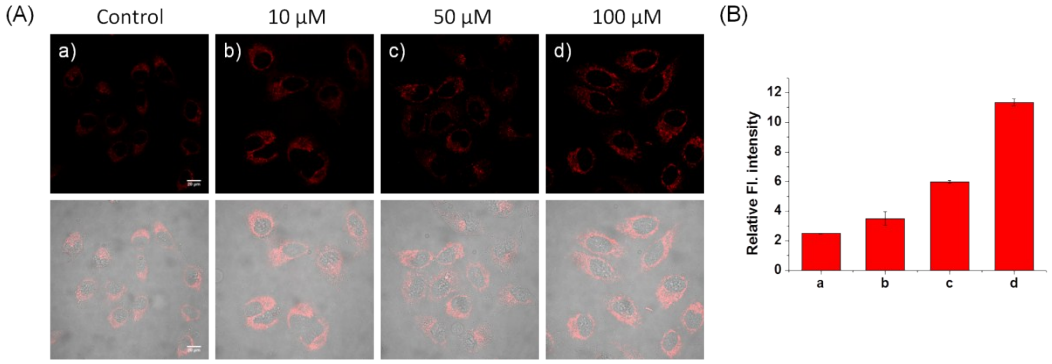


Fig. S12 (A) Confocal fluorescence imaging of HeLa cells pretreated with 10 μM probe **Lyso-SiR-2S** for 1 h then treated with NaOCl (0, 10, 50, 100 μM) for another 30 min. (B) Average intensity in A (a–d), respectively. Data are expressed as mean ± SD of three parallel experiments. The excitation wavelength was 635 nm. Scale bar: 20 μm.

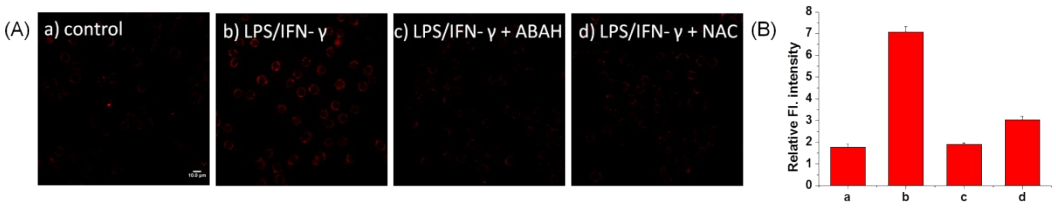


Fig. S13 (A) Confocal fluorescence imaging of RAW264.7 macrophages cells. (a) the probe **Lyso-SiR-2S** (10 μM) was incubated with cells for 1 h. (b) cells were prestimulated with LPS (1 μg mL^{-1}) and IFN-γ (50 ng mL^{-1}) for 12 h, subsequently incubated with probe (10 μM, 1 h), then imaged. (c, d) cells were pretreated with HOCl scavenger ABAH (500 μM) or NAC (3 mM) during stimulation with LPS (1 mg mL^{-1}) and IFN-γ (50 ng mL^{-1}) for 12 h, subsequently incubated with probe (10 μM, 1 h) then imaged. (B) Average intensity in A (a–d), respectively. Data are expressed as mean ± SD of three parallel experiments. The excitation wavelength was 635 nm. Scale bar: 10 μm.

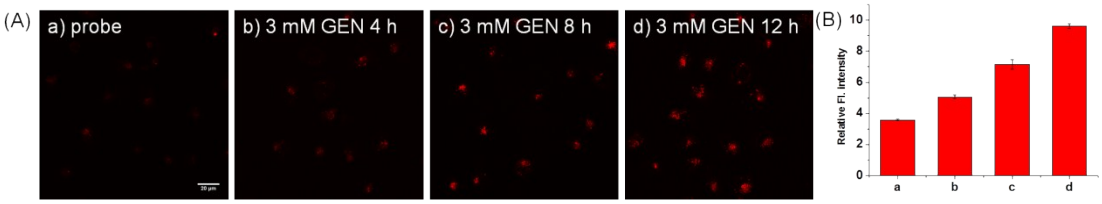


Fig. S14 (A) Confocal fluorescence images of HK-2 cells. cells were pre-treated without GEN (a) or with GEN 3 mM for different time (4 h (b), 8 h (c), 12 h (d)), then treated with the probe **Lyso-SiR-2S** (10 μM) for 1 h. (B) Average intensity in A (a–d), respectively. Data are expressed as mean ± SD of three parallel experiments. The excitation wavelength was 635 nm. The emission band was at 650–750 nm. Scale bar: 20 μm

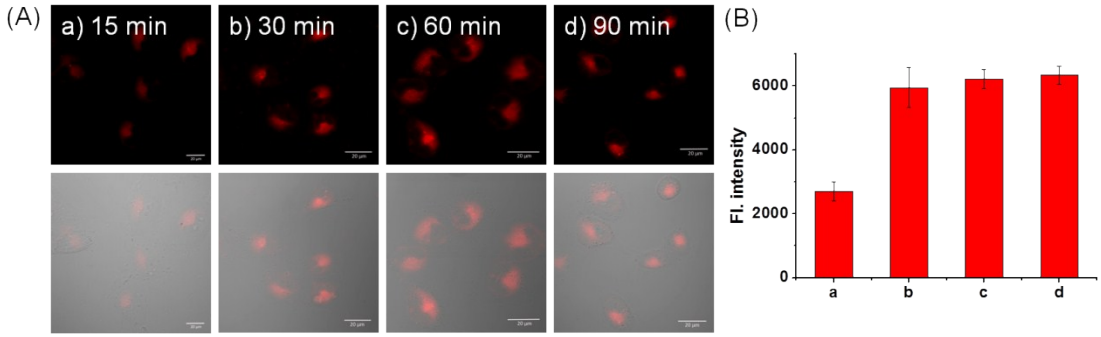


Fig. S15 (A) Confocal fluorescence imaging of HK-2 cells. The cells were pretreated with GEN 3 mM for 8 h, then treated with the probe **Lyso-SiR-2S** (10 μM) for different time (15 min (a), 30 min (b), 60 min (c), 90 min (d)). (B) Average intensity in A (a–d), respectively. Data are expressed as mean ± SD of three parallel experiments. The excitation wavelength was 635 nm. The emission band was at 650–750 nm. Scale bar: 20 μm.

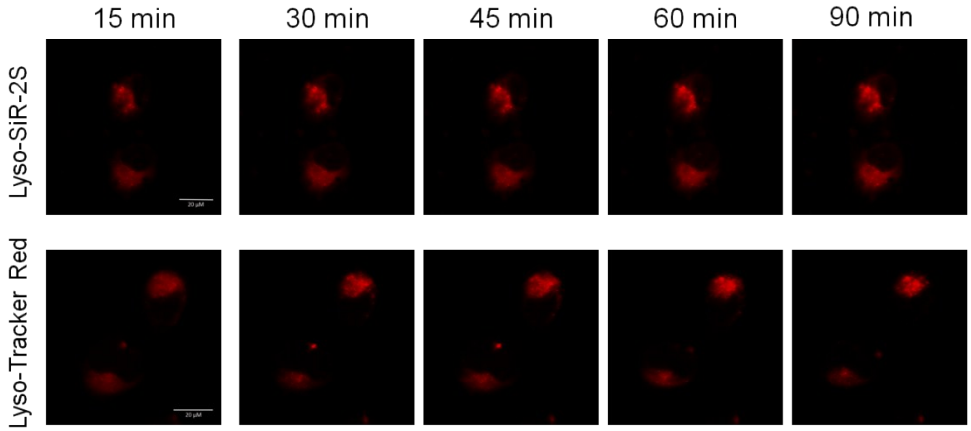


Fig. S16 (A) Confocal fluorescence imaging of HK-2 cells. The first row: the cells were co-incubated with GEN 3 mM for 8 h, then with the probe **Lyso-SiR-2S** (10 μM) for 15 min and imaged. Subsequently the dish was kept still at room temperature for other time (30, 60, 90 min) to obtain images under consistent parameters of the microscope. The excitation wavelength was 635 nm. The emission band was at 650–750 nm. The second row: the cells were directly co-incubated with Lyso-Tracker Red (1 μM) for 15 min, then images were obtained in the same way with the first row. The excitation wavelength was 543 nm. The emission band was at 550–650 nm. Scale bar: 20 μm.

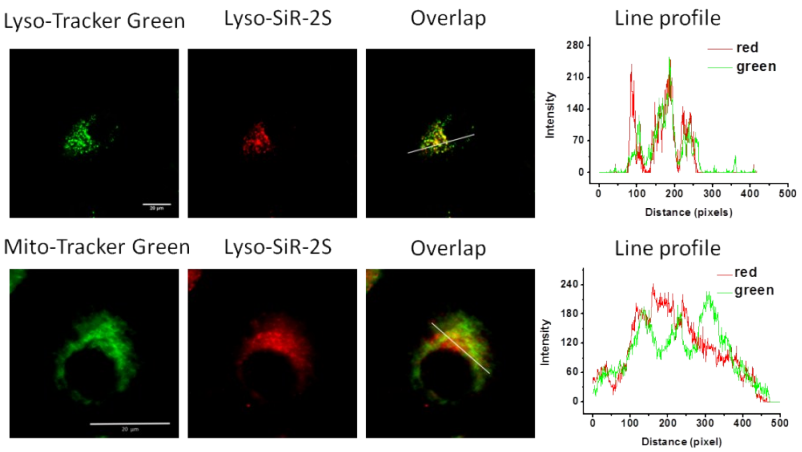


Fig. S17 Intracellular localization of probe **Lyso-SiR-2S** in HK-2 cells. Cells were cocultured successively with 3 mM GEN for 8 h, the probe for 1 h, and 1 μM subcellular organell tracker for 10 min. First-Forth Column in order: Fluorescence of Lyso-Tracker Green or Mito-Tracker green (λ_{ex} = 488 nm, λ_{em} = 500–550 nm); Fluorescence of the probe (λ_{ex} = 635 nm, λ_{em} = 650–750 nm); Merged images; Profile of the white line in merged images. Scale bar: 20 μm. The Pearson's correlation coefficient is 0.81 and 0.52, respectively.

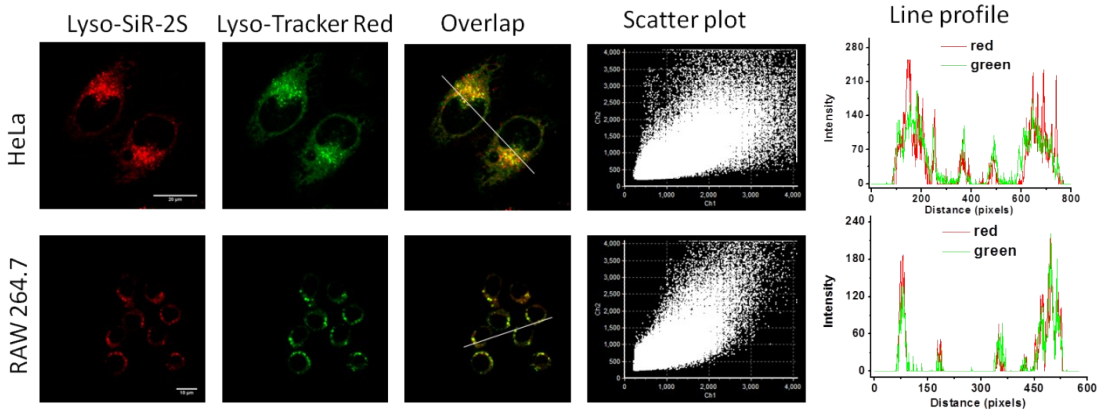


Fig. S18 Intracellular localization of **Lyso-SiR-2S** in HeLa cells (first row) and in RAW 264.7 cells (second row). HeLa cells were pretreated with 10 μM probe for 1 h and subsequently 1 μM Lyso-Tracker Red for 30 min. Then cells were treated with 50 μM HOCl for another 30 min, imaged. Scale bar: 20 μm; RAW 264.7 cells were stimulated with LPS (1 μg mL^{-1}) and IFN-γ (50 ng mL^{-1}) for 12 h, subsequently incubated with probe (10 μM) for 1 h, then 1 μM Lyso-Tracker Red for 30 min, imaged. Scale bar: 10 μm; First Column: Red channel of the probe (λ_{ex} = 635 nm, λ_{em} = 650–750 nm); Second column: Green channel of Lyso-Tracker Red (λ_{ex} = 543 nm, λ_{em} = 550–650 nm); Third column: Merged signal; Forth column: Scatter plot: the overlap of green and red channel images.

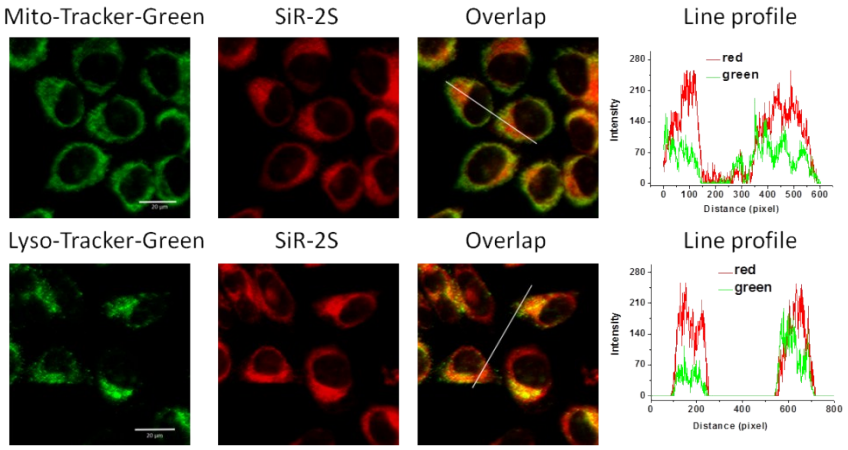


Fig. S19 Intracellular localization of probe **SiR-2S** in HeLa cells. Cells were pretreated with 10 μM probe for 1 h and subsequently 1 μM Mito-tracker-green or Lyso-Tracker Green for 30 min. Then cells were treated with 50 μM HOCl for another 30 min, imaged. Scale bar: 20 μm First-Forth Column in order: Fluorescence of Mito-Tracker Green or Lyso-Tracker Green (λ_{ex} = 488 nm, λ_{em} = 500–550 nm); Fluorescence of the probe (λ_{ex} = 635 nm, λ_{em} = 650–750 nm); Merged images; Profile of the white line in merged images. The Pearson's correlation coefficient is 0.62 and 0.67, respectively.

9. Mouse model

All animal procedures were carried out according to the Guidelines for Care and Use of Laboratory Animals of Hunan University and experiments were approved by the Animal Ethics Committee of College of Biology (Hunan University).

Fluorescence imaging of kidneys in mice with GEN-induced acute kidney injury. The solution of GEN was prepared by dissolving GEN in 0.9% saline. BALB/c mice were randomly divided into three groups, and every group composed of three mice. The intact mice were imaged as the blank group. For the control and experimental group, PBS or GEN (50 mg kg^{-1}) was pre-injected intraperitoneally in BALB/c mice for consecutive eight days, then the probe **Lyso-SiR-2S** (100 μL, 200 μM) was injected via tail vein. After 1.5 h, all the mice were anaesthetized and performed a simple laparotomy to expose the kidney, then imaged using an IVIS Lumina XR (IS1241N6071) *in vivo* imaging system.

GEN at different concentrations (0, 50, 100 mg kg^{-1}) was intraperitoneally pre-injected in BALB/c mice for different times (2, 5, 8, 10 d), then the probe **Lyso-SiR-2S** (100 μL, 100 μM) was injected via tail vein. After 3 h, the mice were dissected and kidneys were transferred to glass-bottomed dishes. Finally, the kidneys were imaged using an IVIS Lumina XR (IS1241N6071) *in vivo* imaging system.

Measurements of serum creatinine and blood urea. The mice were administrated with PBS or GEN (100 mg kg^{-1}) by intraperitoneal injection for 8 d, subsequently the probe was injected via the tail vein for 3 h. Afterwards blood was taken by removing eyeballs, and the values of serum creatinine and blood urea were measured.

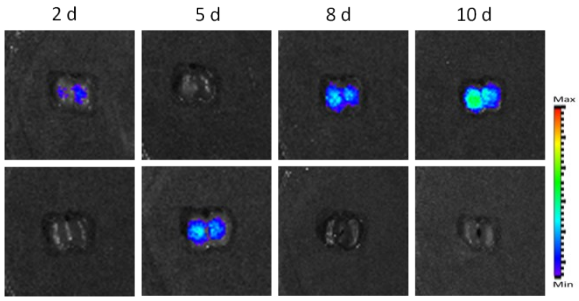
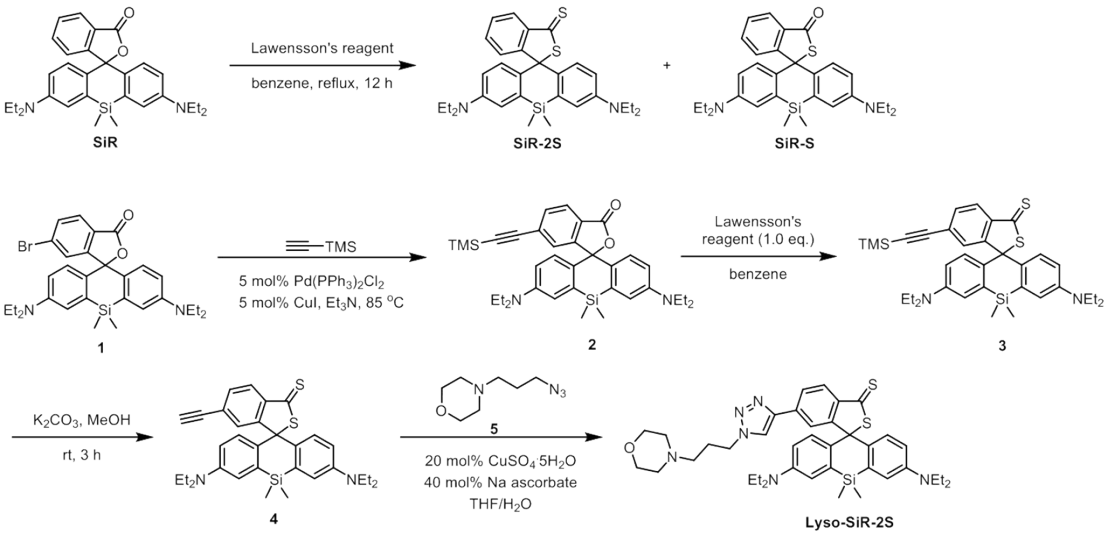


Fig. S20 The partially representative control images from the mice without GEN injection.

10. Synthesis



Scheme S1 Synthetic routes of compounds **SiR-S**, **SiR-2S**, **Lyso-SiR-2S**

Compounds **SiR**,[28] **SiR-S**,[29,30] **1**,[28] and **5**[31] were synthesized according to the literatures.

*Compound **SiR-2S*** The mixture of **SiR** (96.9 mg, 0.20 mmol) and Lawensson's reagent (58.5 mg, 0.12 mmol) in 3 mL dry benzene was refluxed for 16 h. TLC showed **SiR** was completely consumed. After removal of benzene under reduced pressure, the residue was purified by silica gel chromatography to give white solid (30.2 mg, 30% yield) as the product **SiR-S**, and brown oil (39.2 mg, 38% yield) as the product **SiR-2S**, which was solidified in the fridge. Characterization of **SiR-2S** is following: ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 8.07 (d, J = 7.8 Hz, 1H), 7.52 - 7.56(m, 1H), 7.44 - 7.47 (m, 1H), 7.16 (d, J = 7.8 Hz, 1H), 6.76 (s, 2H), 6.55 (d, J = 8.7 Hz, 2H), 6.39 (d, J = 8.4 Hz, 2H), 3.25 (q, J = 6.8 Hz, 8H), 1.06 (t, J = 6.6 Hz, 12H), 0.55 (s, 3H), 0.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 184.58, 157.00, 146.10, 144.52, 136.33, 133.13, 132.61, 129.14, 128.44, 127.92, 124.61, 115.23, 113.50, 75.82, 44.31, 12.74, 1.11, 2.19; HRMS (ESI): calculated for $[C_{30}H_{37}N_2S_2Si]^+$ ($M+H^+$) 517.2167, found 517.2165.

*Compound **2*** The mixture of Compound **1** (112 mg, 0.2 mmol), trimethylsilylacetylene (39.3 mg, 0.40 mmol), $Pd(PPh_3)_2Cl_2$ (7.0 mg, 0.01 mmol), CuI (1.9 mg, 0.01 mmol) and 2 mL Et_3N was stirred at 85 °C for 12 h under N_2 atmosphere. TLC showed the starting material was completely

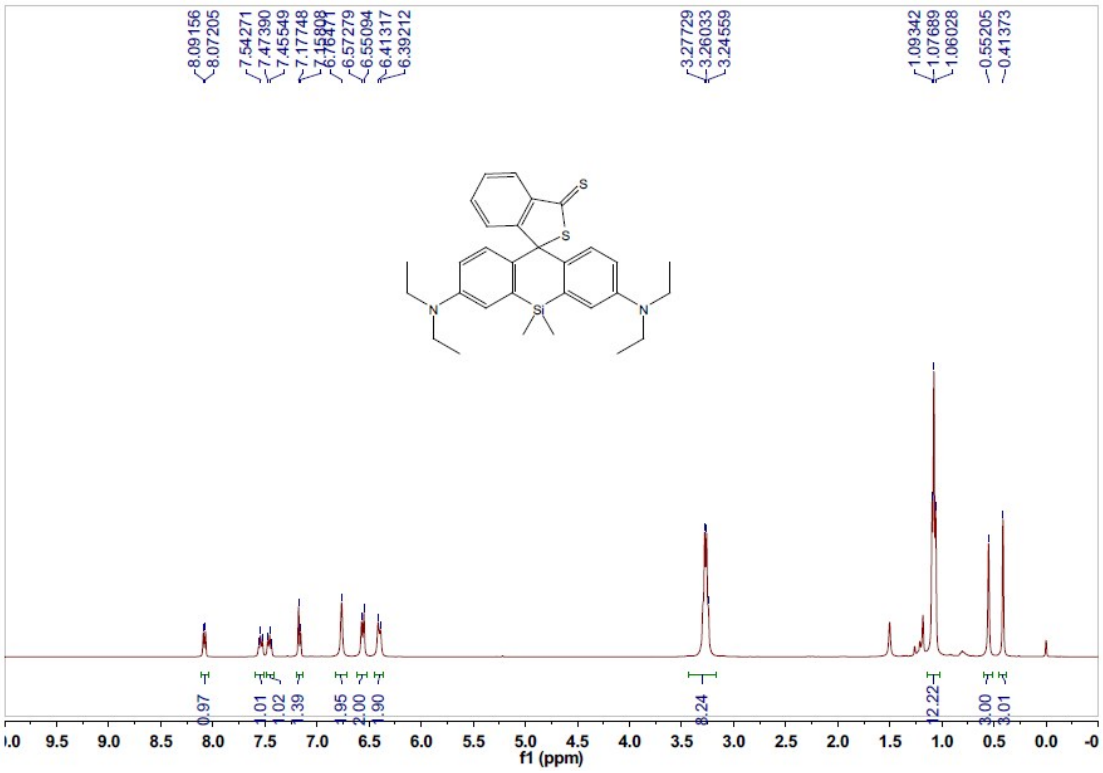
consumed. Then it was quenched with water (5 mL), and the aqueous layer was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic layers were washed with brine, dried with anhydrous Na_2SO_4, concentrated under vacuum. The obtained residue was purified by silica gel chromatography to give yellow oil (107 mg, 92% yield) as the product **2**. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 7.89 (d, J = 7.9 Hz, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.39 (s, 1H), 6.92 (s, 2H), 6.72 (d, J = 8.8 Hz, 2H), 6.51 (d, J = 8.7 Hz, 2H), 3.35 (q, J = 6.7 Hz, 8H), 1.15 (t, J = 6.8 Hz, 12H), 0.64 (s, 3H), 0.60 (s, 3H), 0.24 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 170.18, 154.76, 146.69, 137.08, 132.35, 130.20, 128.81, 128.69, 128.11, 126.85, 125.34, 115.79, 112.73, 104.04, 98.55, 92.18, 44.35, 12.66, 0.42, -0.15, -1.47; HRMS (ESI): calculated for $[C_{35}H_{45}N_2O_2Si_2]^+$ ($M+H^+$) 581.3020, found 581.3019.

*Compound **3*** It was made using the same protocol with **SiR-2S** in 37% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 7.82 (d, J = 7.9 Hz, 1H), 7.59 (d, J = 7.9 Hz, 1H), 7.35 (s, 1H), 6.83 (s, 2H), 6.60 (d, J = 8.8 Hz, 2H), 6.51 (d, J = 8.8 Hz, 2H), 3.35 (q, J = 6.8 Hz, 8H), 1.16 (t, J = 6.6 Hz, 12H), 0.63 (s, 3H), 0.47 (s, 3H), 0.20 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 197.03, 158.05, 145.89, 136.77, 136.11, 133.90, 131.83, 131.62, 129.71, 128.73, 122.97, 114.77, 113.62, 103.95, 98.81, 69.48, 44.28, 12.78, 0.99, -0.14, -2.14; HRMS (ESI): calculated for $[C_{35}H_{45}N_2S_2Si_2]^+$ ($M+H^+$) 613.2563, found 613.2564.

*Compound **4*** To the solution of Compound **3** (30.7 mg, 0.05 mmol) in MeOH was added K_2CO_3 (34.6 mg, 0.25 mmol), and the mixture was stirred at room temperature upon completion (3 h). The mixture was diluted with ethyl acetate (20 mL), then successively washed with saturated aqueous NH_4Cl, water, and brine. The organic layer was dried over anhydrous Na_2SO_4, and concentrated under vacuum to give the crude product **4** (27.0 mg, 99% yield). It was used for the next step without further purification.

*Compound **Lyso-SiR-2S*** Under N_2 atmosphere, to a mixture of compound **4** (27.0 mg, 0.05 mmol) and 4-(3-azidopropyl)morpholine in THF (3 mL) was added a solution of $CuSO_4{\cdot}5H_2O$ (2.5 mg, 0.01 mmol) and sodium ascorbate (4.0 mg, 0.02 mmol) in water (1 mL). The reaction mixture was stirred at room temperature for 16 h upon completion, and the solvent was mostly removed under reduced pressure. Water (5 mL) was added and the aqueous layer was extracted with dichloromethane (3 × 15 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated under vacuum. The residue was purified by silica gel column chromatography to give brown solid (26.6 mg, 75% yield) as the product **Lyso-SiR-2S**. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 8.20 (d, J = 8.3 Hz, 1H), 8.12 (d, J = 8.3 Hz, 1H), 7.78 (s, 1H), 7.58 (s, 1H), 6.84 (s, 2H), 6.69 (d, J = 9.0 Hz, 2H), 6.47 (d, J = 6.8 Hz, 2H), 4.42 (t, J = 6.8 Hz, 2H), 3.67 (s, 4H), 3.31 (q, J = 6.9 Hz, 8H), 2.41 (s, 4H), 2.34 (t, J = 6.6 Hz, 2H), 2.21 (t, J = 6.7 Hz, 2H), 1.13 (t, J = 6.9 Hz, 12H), 0.64 (s, 3H), 0.48 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 157.95, 146.46, 146.07, 144.14, 136.25, 135.43, 132.49, 129.30, 125.81, 125.29, 124.42, 121.52, 115.12, 113.66, 75.60, 66.94, 55.10, 53.61, 48.41, 44.28, 27.11, 12.72, 1.11, 2.25; HRMS (ESI): calculated for $[C_{39}H_{51}N_6OS_2Si]^+$ ($M+H^+$) 711.3335, found 711.3337.

11. NMR spectra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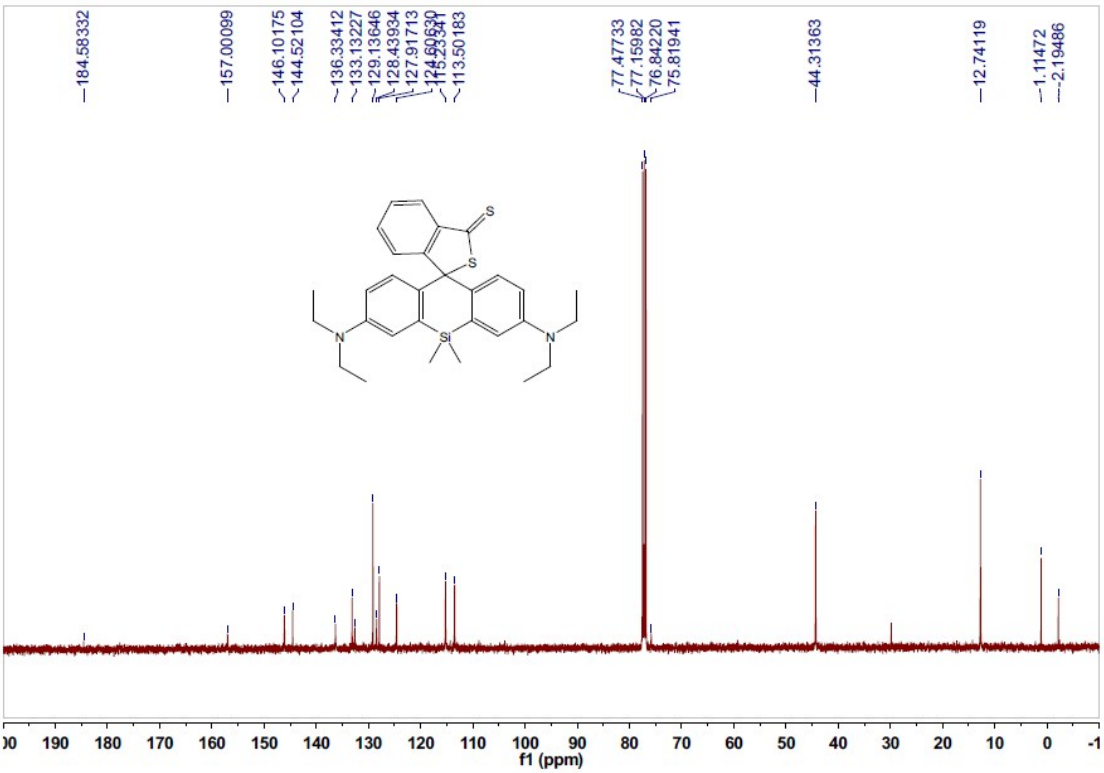
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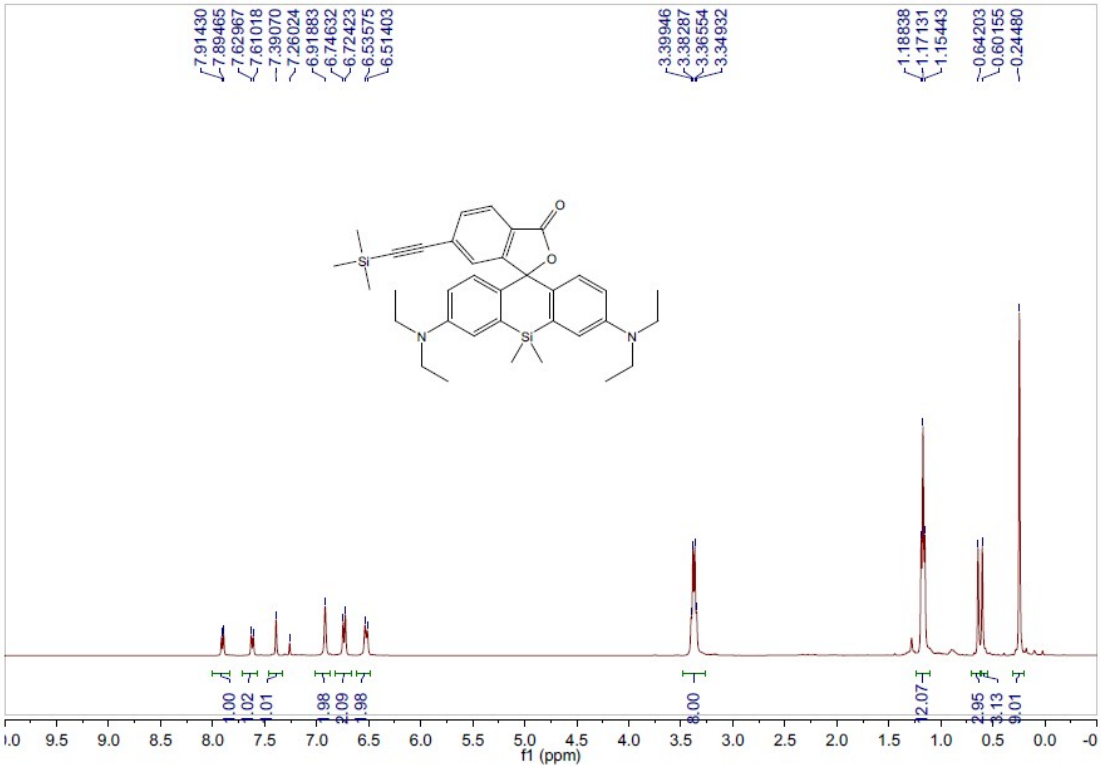
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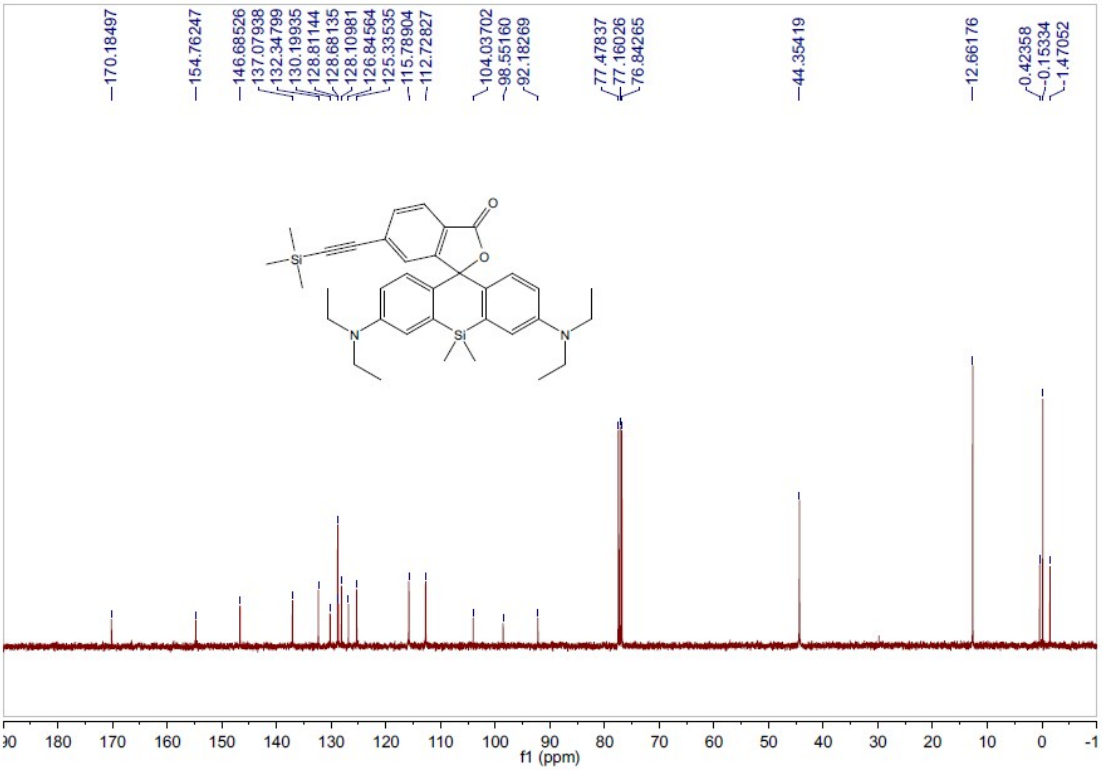
f1 (ppm)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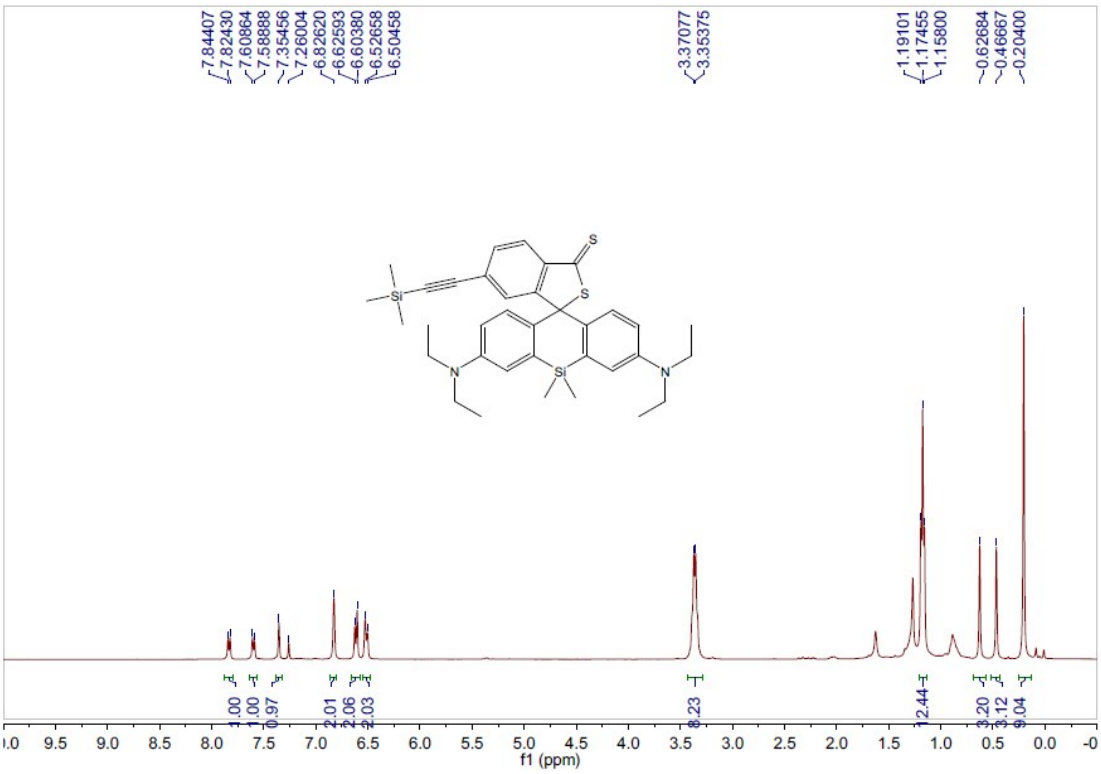
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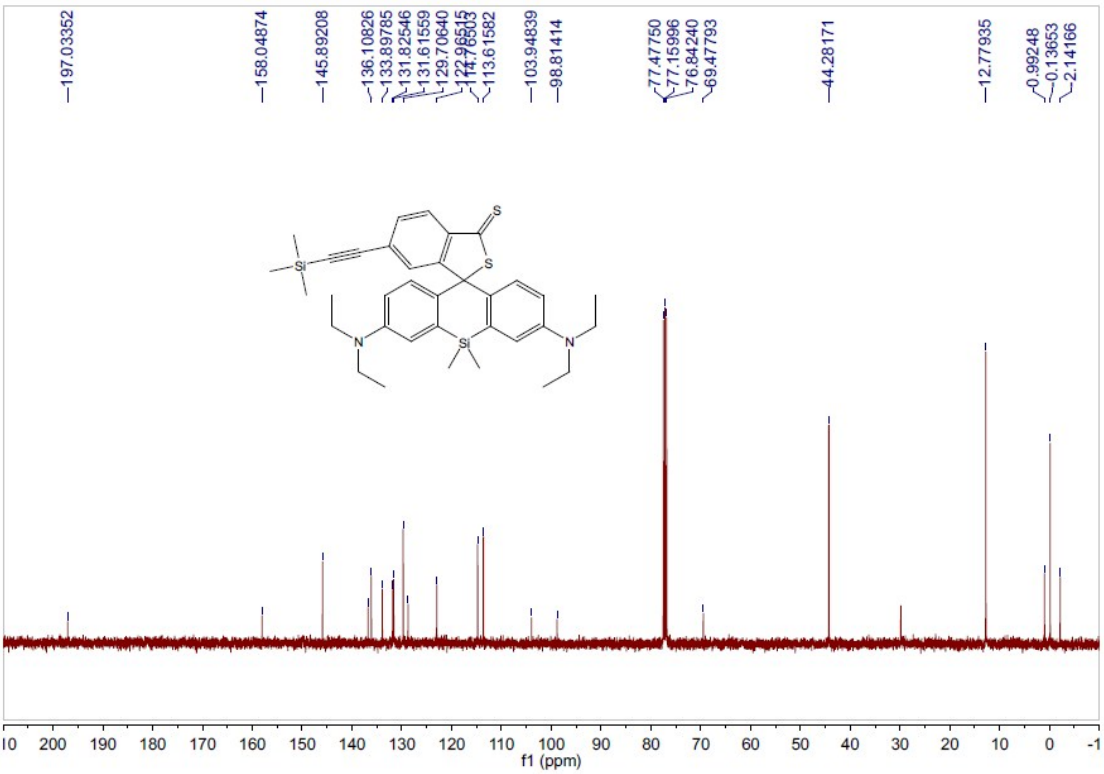
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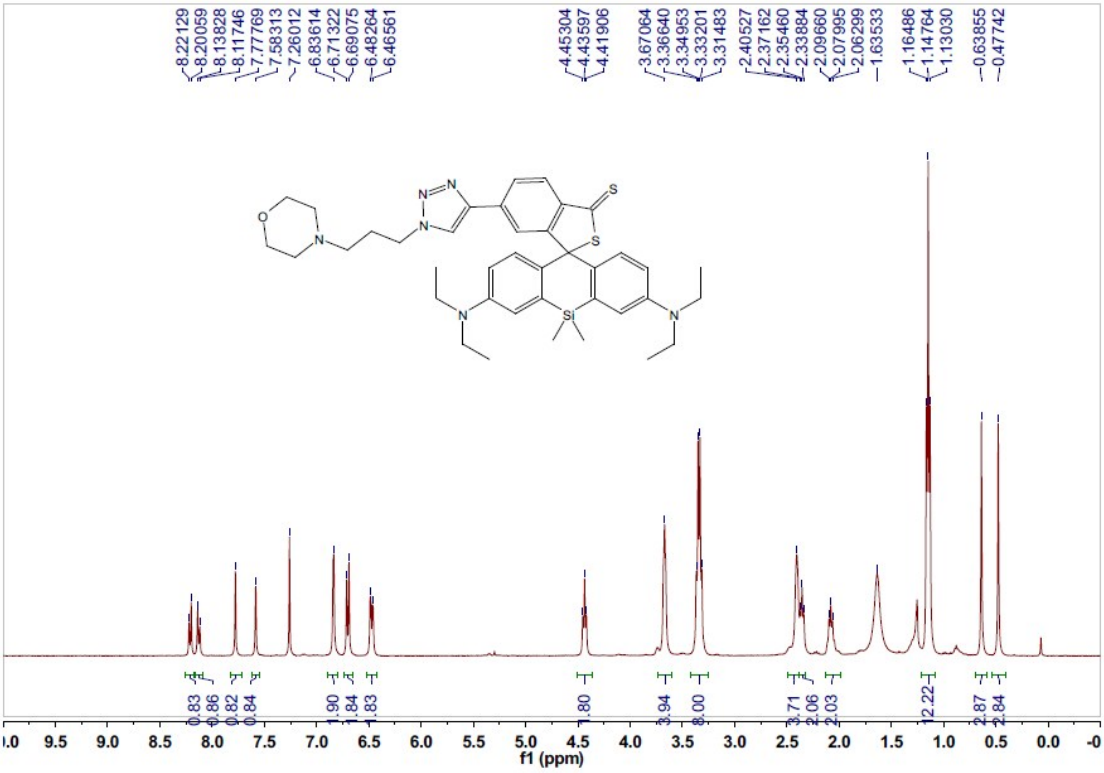

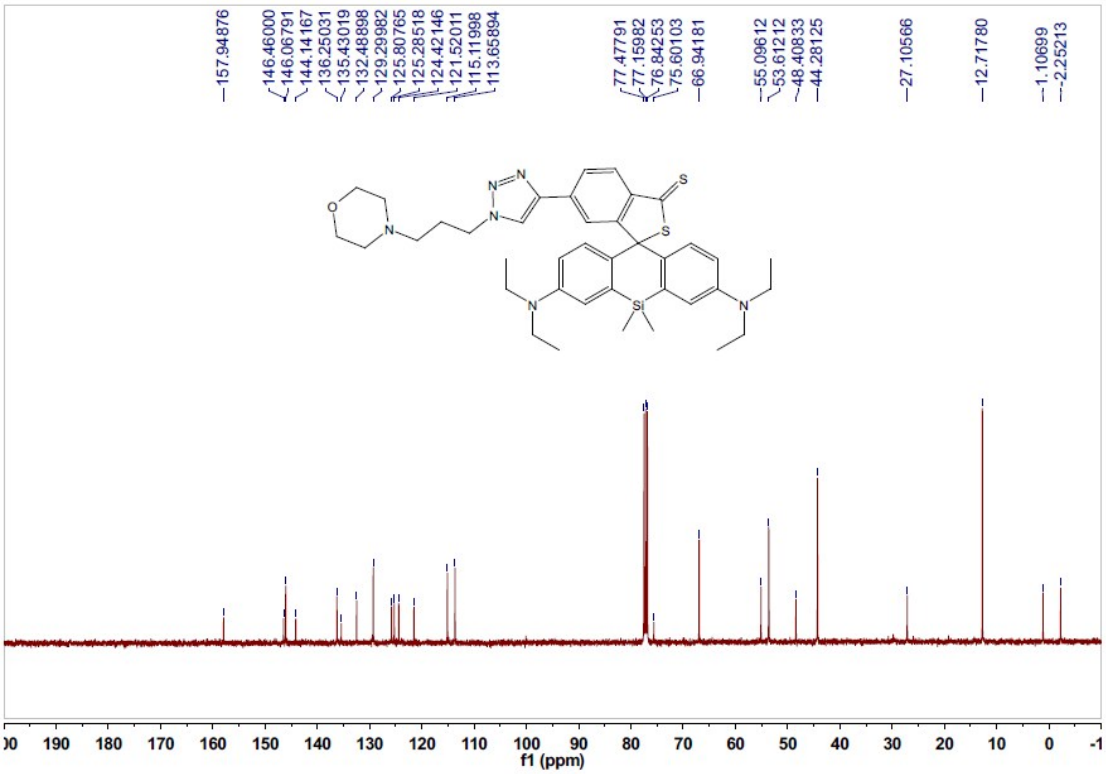

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