# Supporting Information for

## A Novel Lysosome-targeted Fluorogenic Probe Based on 5-Triazole-quinoline for the Rapid Detection of Hydrogen Sulfide in Living Cells

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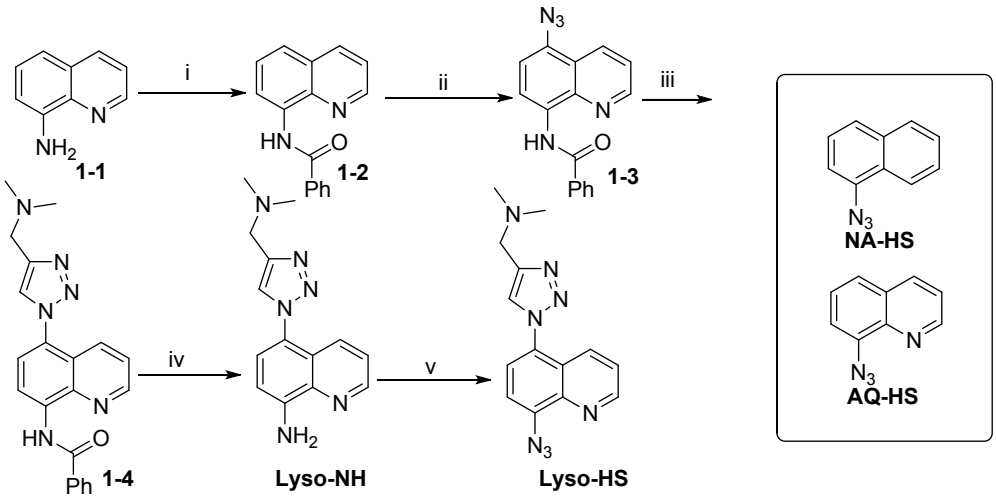
## General Methods

All reactions were performed at air atmosphere. All chemicals were obtained from commercial sources and used directly without further purification. Solvents used in the experiment have been prior treated following standard procedure. The reaction process was monitored by TLC. The NMR was recorded in 500 MHz apparatus using $CDCl_3$ or DMSO as solvent, and the frequencies for measuring $^{1}H$, $^{13}C$ NMR were 126 MHz Chemical shifts were recorded in ppm by employing TMS (for 1H NMR) or the solvent peak of CDCl3 (77.0 ppm, for $^{13}C$ NMR) as internal standard. HRMS data were obtained under ESI model.

## Experimental Section

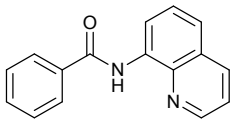
Synthetic procedures




Scheme S1. Synthesis of Probe Lyso-HS and AQ-HS, NA-HS

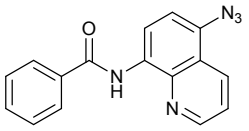
**N-(quinolin-8-yl)benzamide (1-2)** To a 100 mL schlenk flask charged with $CH_2Cl_2$

(30 mL) were added 8-aminoquinoline (10 mmol) and triethylamine (15 mmol). After stirring at room temperature for 5 min, the reaction solution was cooled in an ice bath. An acid chloride (11 mmol) was added dropwise. Note that the solidified acid chloride reagent needs to be dissolved firstly with $CH_2Cl_2$. Then the reaction solution was stirred overnight to improve the yield. The mixture was filtered through a pad of Celite, and the residue was washed with $CH_2Cl_2$ (25 mL) subsequently. The collected $CH_2Cl_2$ solution was washed with 1 M $NaHCO_3$ aqueous solution for three times. After that, the organic layer was collected and dried over $Na_2SO_4$. The solvent was removed by rotary-evaporation. The raw product was then purified by silica gel column with a mixture solvent of PE/EtOAc (v/v; 10:1) to afford the pure product **1a** [1]. $^1$H NMR (500 MHz, $CDCl_3$) δ 10.61 (s, 1H), 8.90 (dd, *J* = 7.6, 1.1 Hz, 1H), 8.68 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.03 (dd, *J* = 3.7, 2.1 Hz, 2H), 7.95 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.48 (m, 4H), 7.36 (dgd, *J* = 8.2, 1.1 Hz, 1H), 7.26 (dd, *J* = 8.2, 4.2 Hz, 1H).$^{13}$C NMR (126 MHz, $CDCl_3$) δ 164.74, 147.81, 138.20, 135.83, 134.64, 134.09, 131.42, 128.37, 127.47, 126.84， 126.80, 121.26， 121.18, 116.00. HRMS ($ESI^+$): Calculated for $C_{16}H_{12}N_2O$: $[M+H]^+$ 249.0950，found 249.0957.

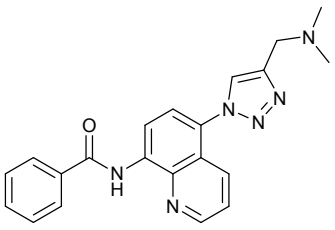



**N-(5-azidoquinolin-8-yl)benzamide（1-3）** A 25 mL schlenk tube was equipped with a magnetic stir bar and charged with *N*-(quinolin-8-yl)benzamide **1-2** (0.2 mmol), $NaN_3$(0.4 mmol, 2 equiv), $K_2S_2O_8$ (0.4 mmol, 3 equiv), DUB(0.2 mmol,1 equ.), TBAB(0.2 mmol, 1 equ.), $Cu(OAc)_2$ (0.05 mmol, 25mol %), and DMF(5 mL), $H_2O$(5mL). The resulting mixture was heated at 40 $^0$C for 12 h, and cooled to room temperature. The mixture was poured into water(10ml), Then the mixture was extracted with $CH_2Cl_2$ for three times, extracted with $H_2O$ for 5 times.Then combined organic layer was dried over anhydrous $Mg_2SO_4$ and filtered.After evaporation of the solvent undervacuum, the residue was purified by column chromatography on silica gel (100–200 mesh) using Petroleum ether-EtOAc as an eluent (10:1, V/V) to afford the pure product **2a** of a white solid. $^1$H NMR (500 MHz, $CDCl_3$) δ 10.56 (s, 1H), 8.93 (dd, *J* = 10.2, 5.4 Hz, 1H), 8.84 (dd, *J* = 4.1, 1.2 Hz, 1H), 8.39 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.07 (dd, *J* = 13.8, 6.9 Hz, 2H), 7.62 – 7.50 (m, 3H), 7.45 (dd, *J* = 8.4, 4.1

Hz, 1H), 7.28 (dd, *J* = 7.7, 5.3 Hz, 1H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 165.11, 149.08, 138.99, 134.88, 131.84, 131.52， 131.56, 130.32, 128.76, 127.18, 121.50, 121.33, 116.36, 114.84. HRMS ($ESI^+$): Calculated for $C_{16}H_{11}N_5O$: $[M+H]^+$ 290.0963. found 290.1036.

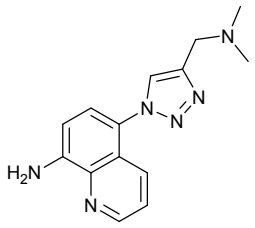


**N-(5-(4-((dimethylamino)methyl)-1H-1,2,3-triazol-1-yl)quinolin-8-yl)benzamide（1-4）：** To a 100 mL single-neck flask charged with tetrahydrofuran (15 mL) and water (15mL). was added **1-3** (10 mmol) and nanometer CuI (10 mmol). After stirring at room temperature for 5 hour, the mixture was removed by rotary-evaporation., and the residue was washed with $CH_2Cl_2$ for three times. The collected $CH_2Cl_2$ solution was washed with NaCl aqueous solution for three times. After that, the organic layer was collected and dried over $Na_2SO_4$. The solvent was removed by rotary-evaporation. The raw product was then purified by silica gel column with a mixture solvent of PE/EtOAc (v/v; 3:1) as the eluent. And afforded product **5b**(76%) of a white solid. $^1$H NMR (500 MHz, $CDCl_3$) δ 10.87 (s, 1H), 9.06 (d, *J* = 8.3 Hz, 1H), 8.95 (dd, *J* = 4.1, 1.5 Hz, 1H), 8.20 (dd, *J* = 8.6, 1.5 Hz, 1H), 8.15 – 8.06 (m, 2H), 7.93 (s, 1H), 7.69 (d, *J* = 8.3 Hz, 1H), 7.64 – 7.56 (m, 4H), 3.81 (s, 2H), 2.42 (s, 6H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 165.64, 149.22, 145.17, 138.51, 136.31, 134.64, 132.23, 128.93, 127.47, 127.34 – 127.28, 125.15, 124.36, 123.73, 123.13, 115.15, 54.22, 45.16. HRMS ($ESI^+$): Calculated for $C_{21}H_{20}N_6O$: $[M+H]^+$ 373.1699， found 373.1703.

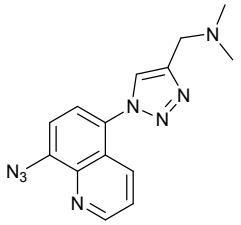


**5-(4-((dimethylamino)methyl)-1H-1,2,3-triazol-1-yl)quinolin-8-amine（Lyso-NH）**: To a 100 mL single-neck flask charged with methanol, was added 1-4 (10 mmol) and nanometer KOH (20 mmol). The resulting mixture was heated at 80 $^0$C for 12 h, and cooled to room temperature, the mixture was removed by rotary-

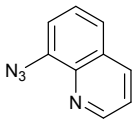
evaporation., and the residue was washed with $CH_2Cl_2$ for three times. The collected $CH_2Cl_2$ solution was washed with NaCl aqueous solution for three times. After that, the organic layer was collected and dried over $Na_2SO_4$. The solvent was removed by rotary-evaporation. The raw product was then purified by silica gel column with a mixture solvent of PE/EtOAc (v/v; 2:1) as the eluent. And afforded product **5b** (75%) of a white solid. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.79 (dd, *J* = 4.1, 1.6 Hz,1H), 7.87 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.84 (s, 1H), 7.41 (dd, *J* = 8.3, 4.9 Hz, 2H), 6.90 (d, *J* = 8.1 Hz, 1H), 5.36 (s, 2H), 3.80 (s, 2H), 2.41 (s, 6H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 148.04, 145.94, 144.33, 137.31, 131.00, 125.57, 125.00, 124.59, 122.79, 122.11, 107.46, 54.15, 44.99. HRMS ($ESI^+$): Calculated for $C_{14}H_{16}N_6$: $[M+H]^+$ 269.1436，found 269.1501.




**1-(1-(8-azidoquinolin-5-yl)-1H-1,2,3-triazol-4-yl)-N,N-dimethylmethanamine**（**Lyso-HS**）: The appropriate (180 mg, 0.65mmol) was dissolved in 18 mL of dry $CH_3CN$. After cooling the solution to 0 °C, 0.12 mL (0.91 mol) of tert-butyl nitrite (tert-BuONO) was added dropwise. The reaction mixture was stirred for about 1 h, and then, 0.12 mL (1.04 mmol) of azidotrimethylsilane (TMS-$N_3$) was added. The reaction mixture was transferred to room temperature and stirred overnight. After the completion of reaction by TLC monitoring (ethyl acetate/methanol 5:1), the solvent was evaporated, and the residue was further purified by the silica gel chromatography to afford azidoluciferin as a yellow solid. $^1$H NMR (500 MHz, $CDCl_3$) δ 9.05 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.55 (s, 1H), 8.04 (dd, *J* = 8.6, 1.4 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 1H), 7.76 (dd, *J* = 8.7, 4.1 Hz, 1H), 7.56 (d, *J* = 8.1 Hz, 1H), 3.66 (s, 2H), 2.25 (s, 6H). $^{13}$C NMR (126 MHz, DMSO) δ 150.13, 144.21, 141.25, 137.41, 131.94, 129.68, 126.44, 124.30 (d, *J* = 12.9 Hz), 123.83, 118.45, 53.47, 44.68. HRMS ($ESI^+$): Calculated for $C_{14}H_{14}N_8$: [M+H]+ 295.1341，found 269.1301.

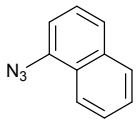


**8-azidoquinoline (AQ-HS)**: The appropriate 8-AQ (180 mg, 0.65mmol) was dissolved in 18 mL of dry $CH_3CN$. After cooling the solution to 0 °C, 0.12 mL (0.91 mol) of tert-butyl nitrite (tert-BuONO) was added dropwise. The reaction mixture was stirred for about 1 h, and then, 0.12 mL (1.04 mmol) of azidotrimethylsilane (TMS-$N_3$) was added. The reaction mixture was transferred to room temperature and stirred overnight. After the completion of reaction by TLC monitoring (ethyl acetate/methanol 5:1), the solvent was evaporated, and the residue was further purified by the silica gel chromatography to afford azidoluciferin as a yellow solid. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.85 (dd, *J* = 4.1, 1.6 Hz, 1H), 8.08 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.38 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.31 (dd, *J* = 7.5, 1.0 Hz, 1H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 149.28, 141.33, 136.96, 135.97, 129.14, 126.34, 124.02, 121.77, 118.05. HRMS ($ESI^+$): Calculated for $C_9H_6N_4$: $[M+H]^+$ 171.0592，found 171.0602.



**1-azidonaphthalene (NA-HS)**: The appropriate naphthalene (180 mg, 0.65mmol) was dissolved in 18 mL of dry $CH_3CN$. After cooling the solution to 0 °C, 0.12 mL (0.91 mol) of tert-butyl nitrite (tert-BuONO) was added dropwise. The reaction mixture was stirred for about 1 h, and then, 0.12 mL (1.04 mmol) of azidotrimethylsilane (TMS-$N_3$) was added. The reaction mixture was transferred to room temperature and stirred overnight. After the completion of reaction by TLC monitoring (ethyl acetate/methanol 5:1), the solvent was evaporated, and the residue was further purified by the silica gel chromatography to afford azidoluciferin as a yellow solid. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 8.2, 1.4 Hz, 5H), 7.86 (dd, *J* = 6.8, 2.6 Hz, 6H), 7.67 (s, 3H), 7.57 – 7.52 (m, 10H), 7.48 (d, *J* = 8.2 Hz, 5H), 7.28 (dd, *J* = 7.4, 0.8 Hz, 5H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 136.51, 134.34, 127.70, 126.92 (d, *J* =

14.9 Hz), 126.11, 125.63, 124.67, 122.54, 113.89. HRMS ($ESI^+$): Calculated for $C_{10}H_7N_3$: [M+H]+ 170.0640，found 170.0639.




## Fluorescence Quantum Yield Measurement

Fluorescence quantum yield of probe and probe after reaction with $Na_2S$ was determined in the reference of fluorescein ($\Phi$ = 0.98) in 0.1 M aqueous NaOH. The quantum yield of probe and probe with $Na_2S$ are calculated according to following equation.

$\Phi_x=\Phi_s(A_sS_x)/(A_xS_s)$

$\Phi$s is the fluorescence quantum yield of fluorescein, $A_x$ is the absorbance of Lyso-HS and Lyso-HS with $Na_2S$. As is the absorbance of the standard. $S_x$ is integrated fluorescence emission of Lyso-HS and Lyso-HS with $Na_2S$ while the Ss is integrated fluorescence emission corresponding to the standard.

## Cell Viability Assay.

MTT assay was performed to assess the viability of HeLa cells. The cells were seeded at a density of 10,000 cells per well and grown overnight at 37°C incubator with 5% $CO_2$. The cells were then exposed to different concentrations of **Lyso-HS** for 48h. After the stipulated time of probe exposure, 10 μL of MTT [3-(4, 5-dimethylthiazol-2-yl)-2, 5-diphenyltetrazolium bromide] was added at a concentration of 5 mg/mL and solubilized using 100 μL of MTT solubilizing agent (DMSO) after 2h. The readings were taken at 590 nm with a reference filter of 620 nm using Synergy HT Multi-Mode Microplate reader (Biotek).The same procedure was followed to assess the viability of probe treated **HePG-2, RTE** and **A-549** cells.

**Cell Culture, Reagent Preparation and Fluorescence Imaging.** Human cervical cancer cells(HeLa), A549, H293K cells were cultured in DMEM high glucose media supplemented with 10% fetal bovineserum, 1% Penstrep, 0.2% Amphotericin B. The cells were grown overnight at 37°C incubator with 5% $CO_2$. HeLa, A549, H293K were seeded at a density of $0.3x10^6$ cells in 35 mm dish and kept

overnight. The cells were treated with 5 μM of **Lyso- HS** for 15 min. Images were acquired using Zeiss Fluorescence Microscope (A1 Axiovert) with x40 objective lens.

## Supporting figures

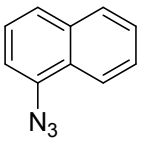
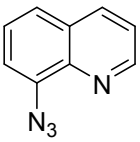
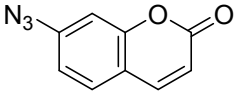
| Structure |  |  |  |
|---|---|---|---|
| Time/min | **15** | **1.5** | **30** |

**Figure S1**. Time of three probes(10 μM) with 10 equiv $H_2S$ in PBS solution (10 mM, pH 7.4, 10% DMSO) at 25 °C for 40 min.

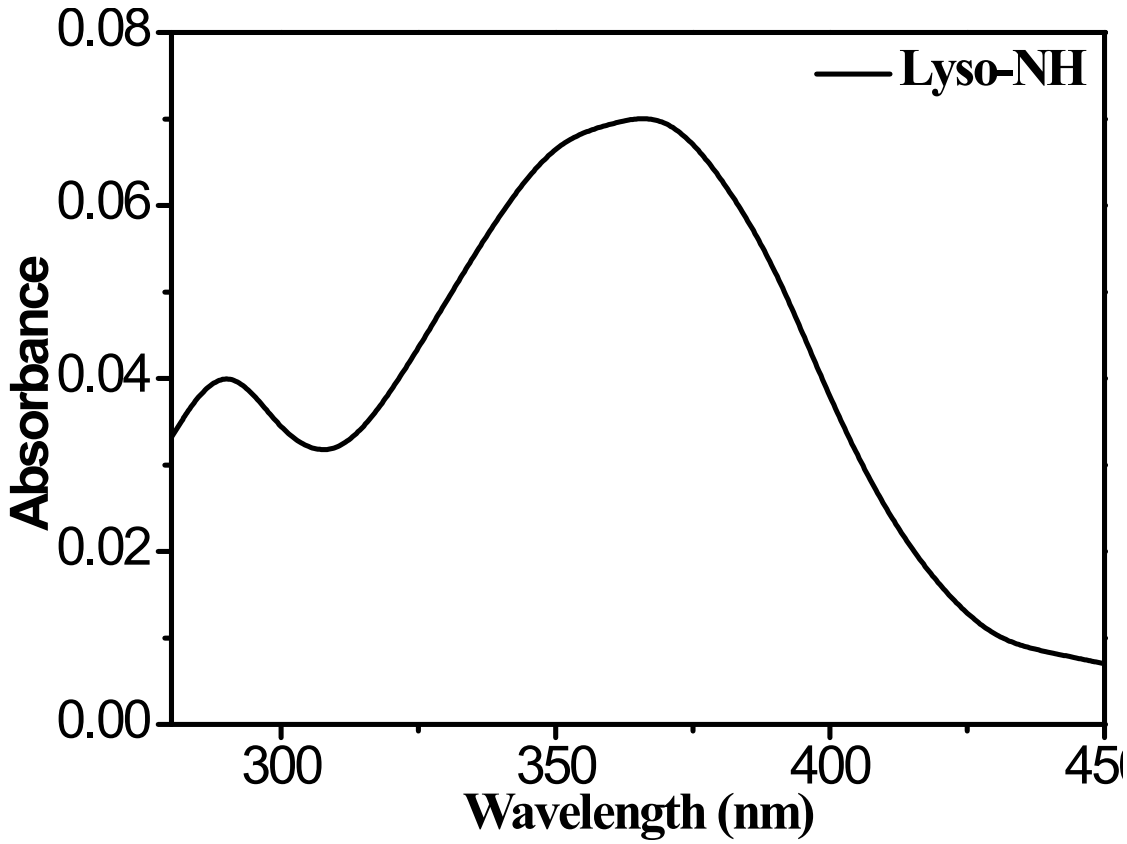



**Figure S2**. UV-Vis absorption of Lyso-NH(10 μM) with 10 equiv $H_2S$ in PBS solution (10 mM, pH 7.4, 10% DMSO) at 25 °C for 40 min.

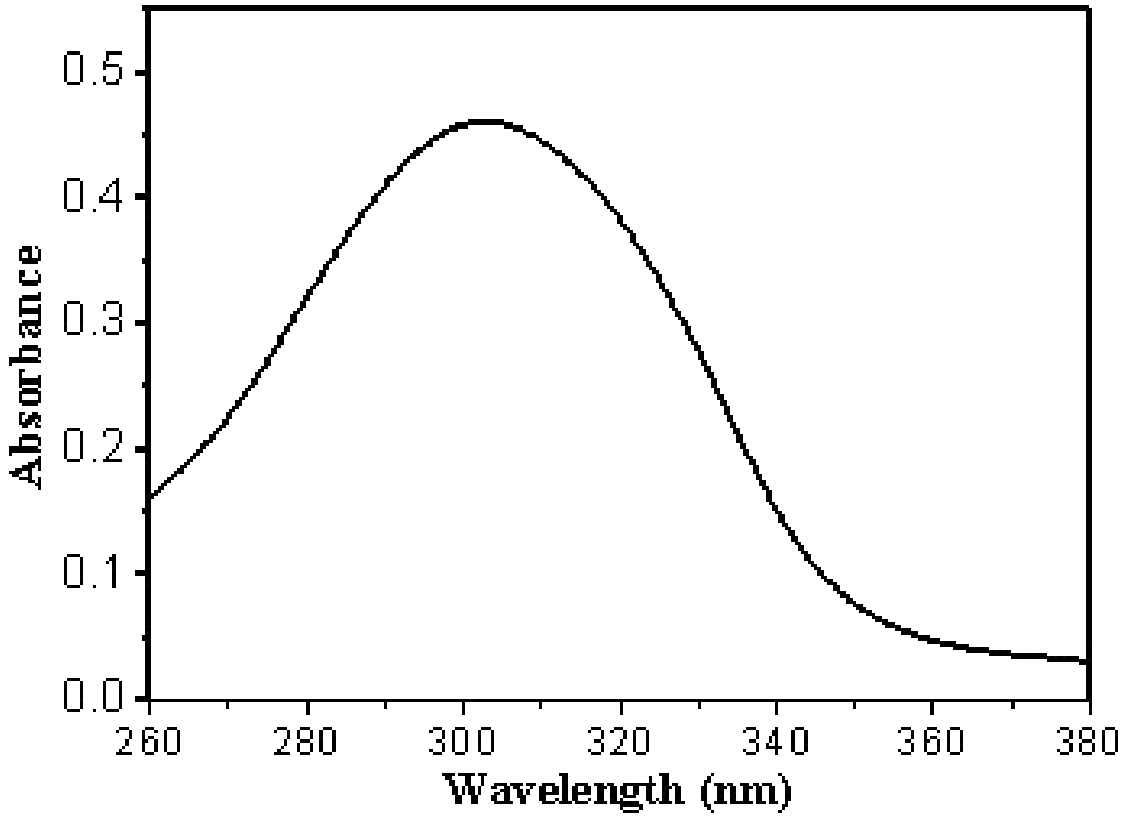



**Figure S3**. UV-Vis absorption of NA-HS(10 μM) with 10 equiv $H_2S$ in PBS solution (10 mM, pH 7.4, 10% DMSO) at 25 °C for 40 min.

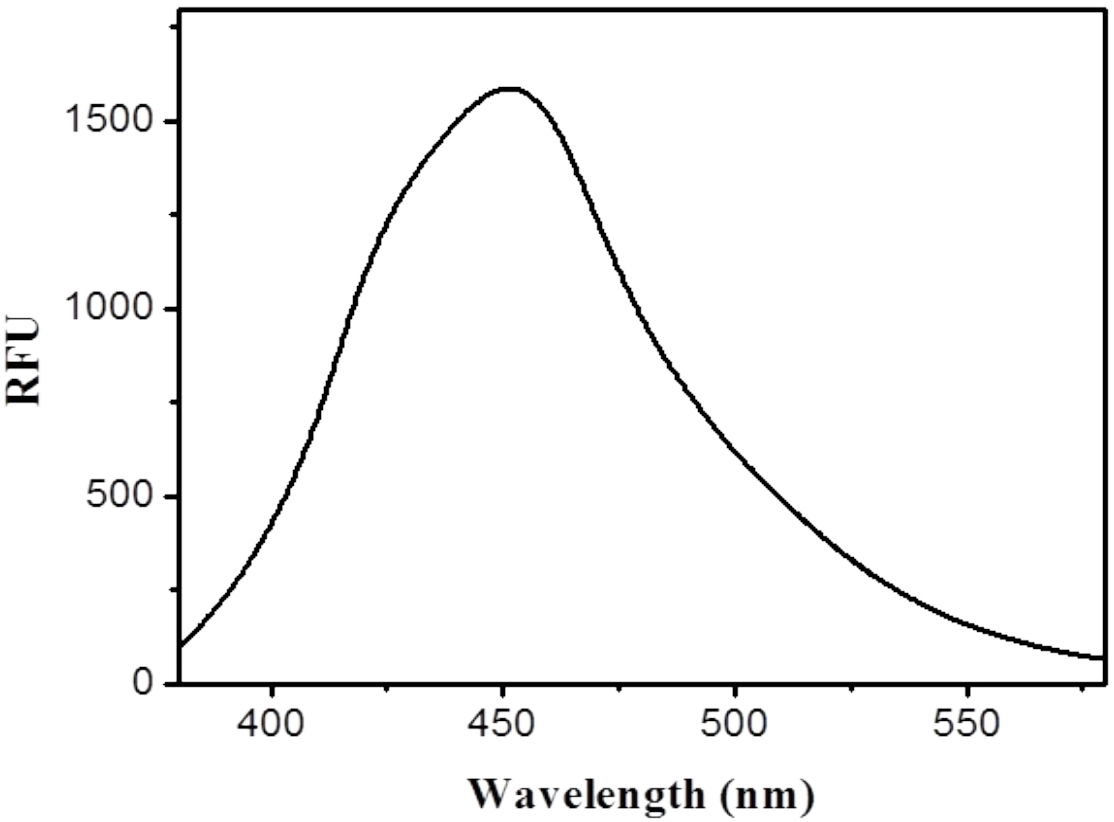



**Figure S4**. Emission of NA-HS(10 μM) with 10 equiv $H_2S$ in PBS solution (10 mM, pH 7.4, 10% DMSO) at 25 °C for 40 min.

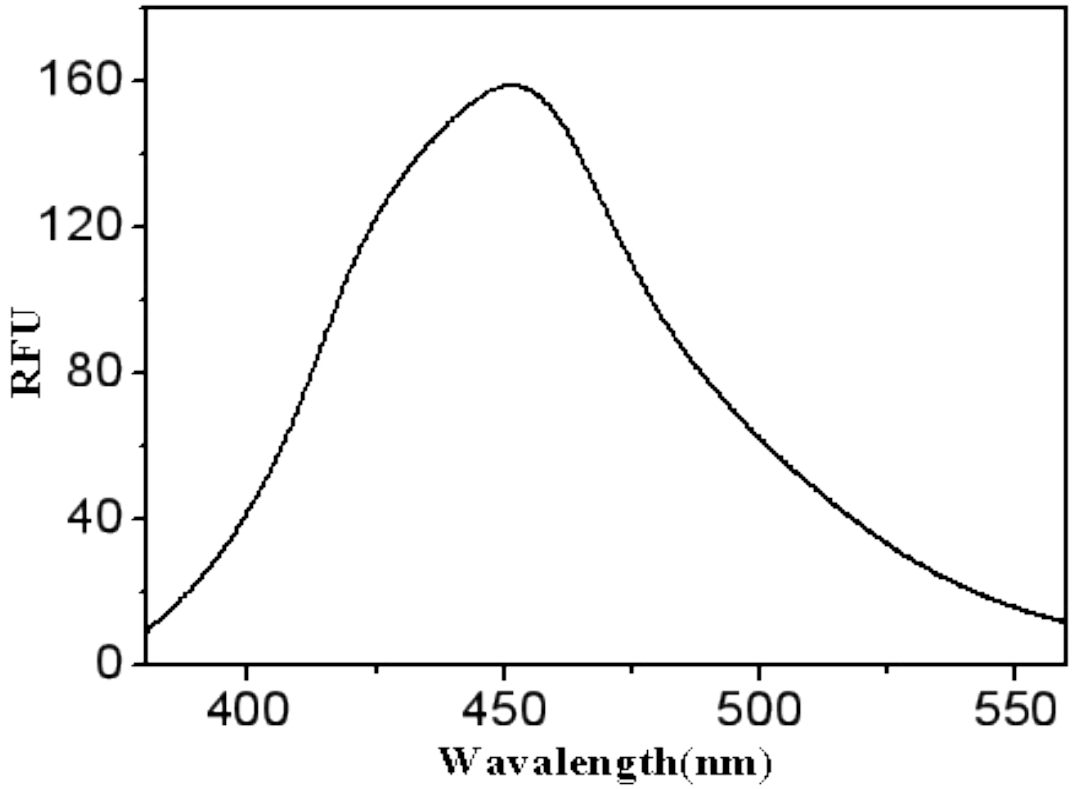



**Figure S5.** Emission of AQ-HS(10 μM) with 10 equiv $H_2S$ in PBS solution (10 mM, pH 7.4, 10% DMSO) at 25 °C for 40 min.

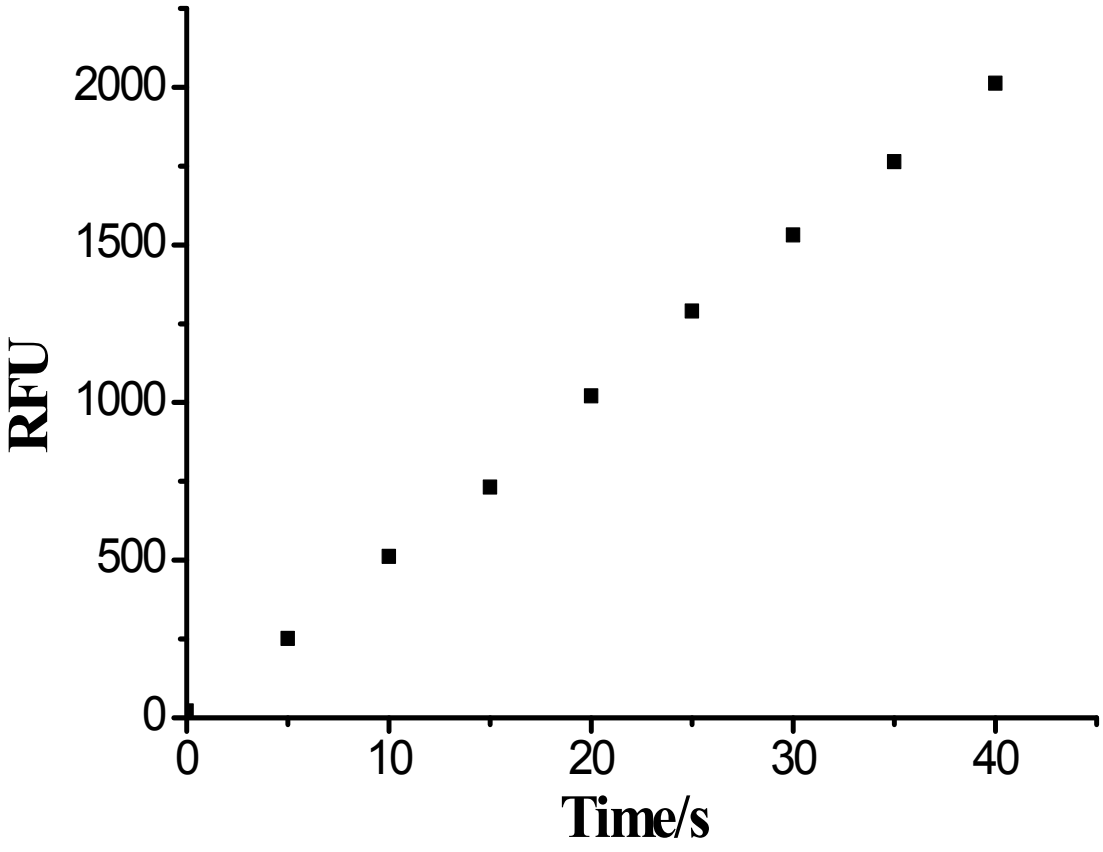



**Figure S6.** The stability of time dependence of **probe Lyso-HS** (10 μM) with 10 equiv $H_2S$ in PBS solution (10 mM, pH 7.4, 10% DMSO).

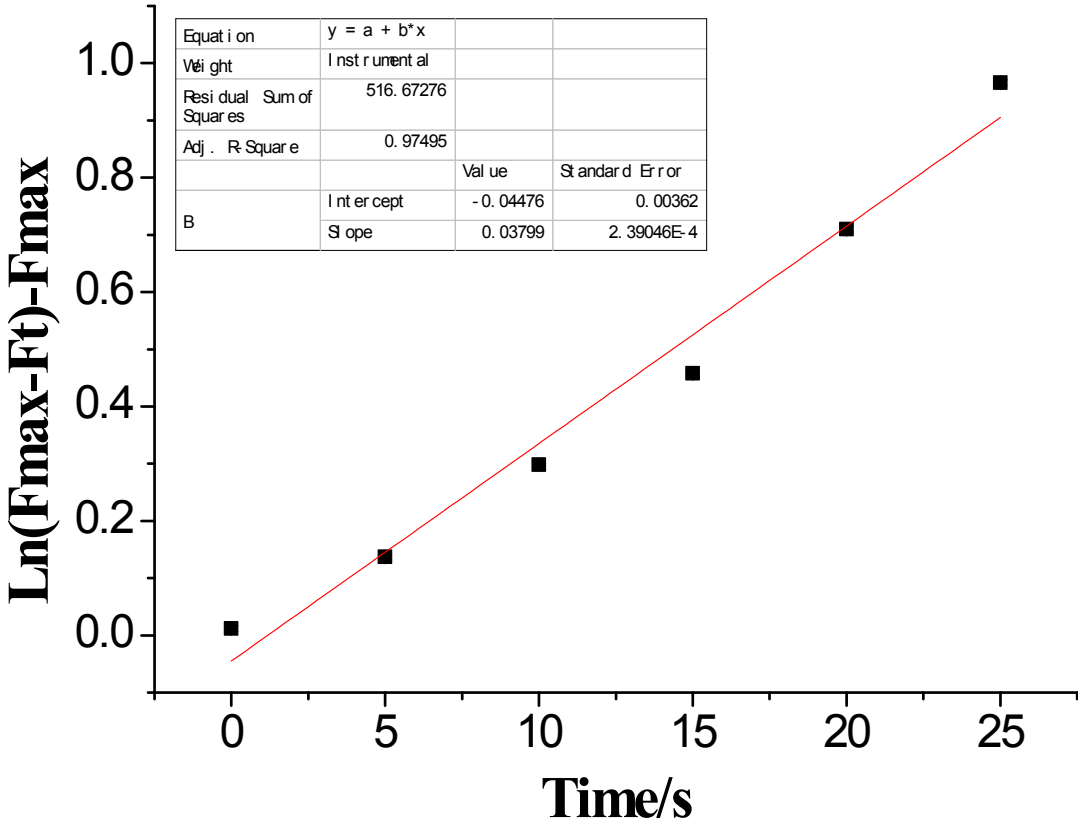



**Figure S7.** Line fitting of time dependence of **probe Lyso-HS**(10 μM) with 10 equiv $H_2S$ in PBS solution (10 mM, pH 7.4, 10% DMSO).

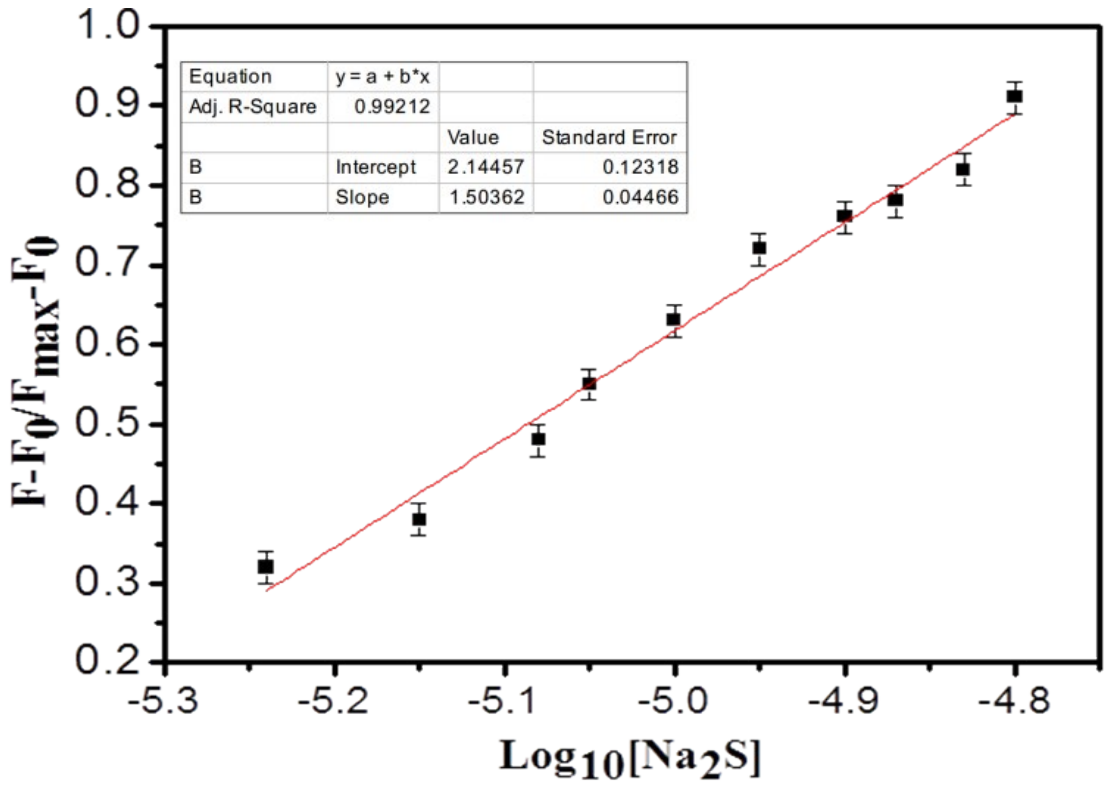



**Figure S8.** The Detection limit of Lyso-HS with $Na_2S$ with $H_2S$ in PBS solution (10 mM, pH 7.4, 10% DMSO).

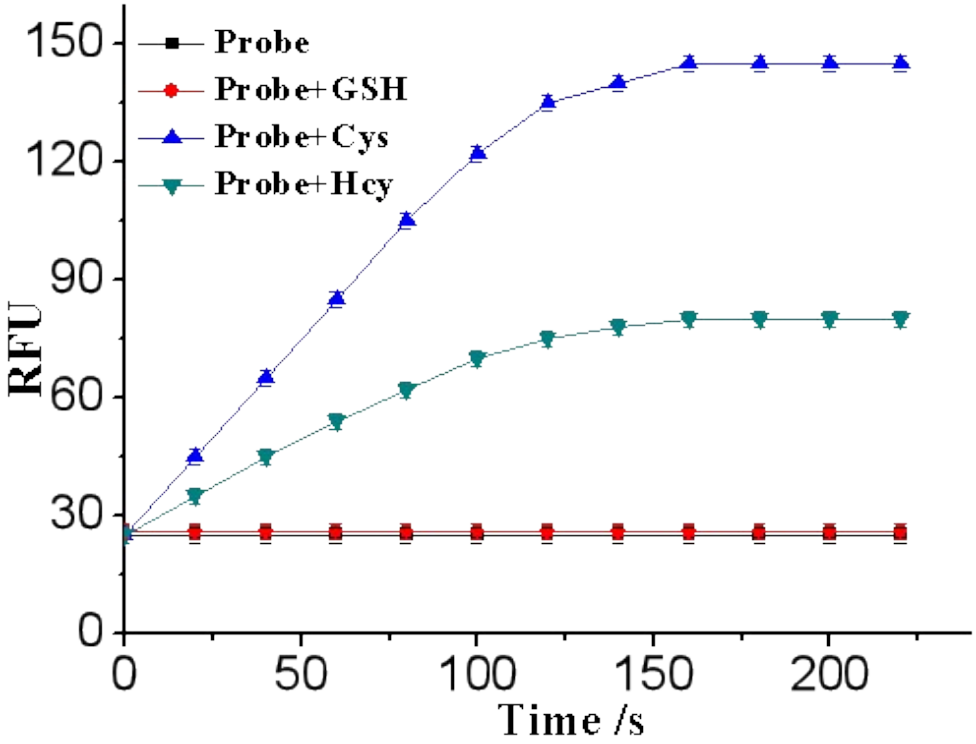



**Figure S9.** Time course experiment of **Lyso-HS** (10 μM ) with GSH, Cys and Hcy in the presence of various biologically relevant analytes at their biological concentrations (GSH, 10 mM; Cys, 200μM; Hcy, 50μM)

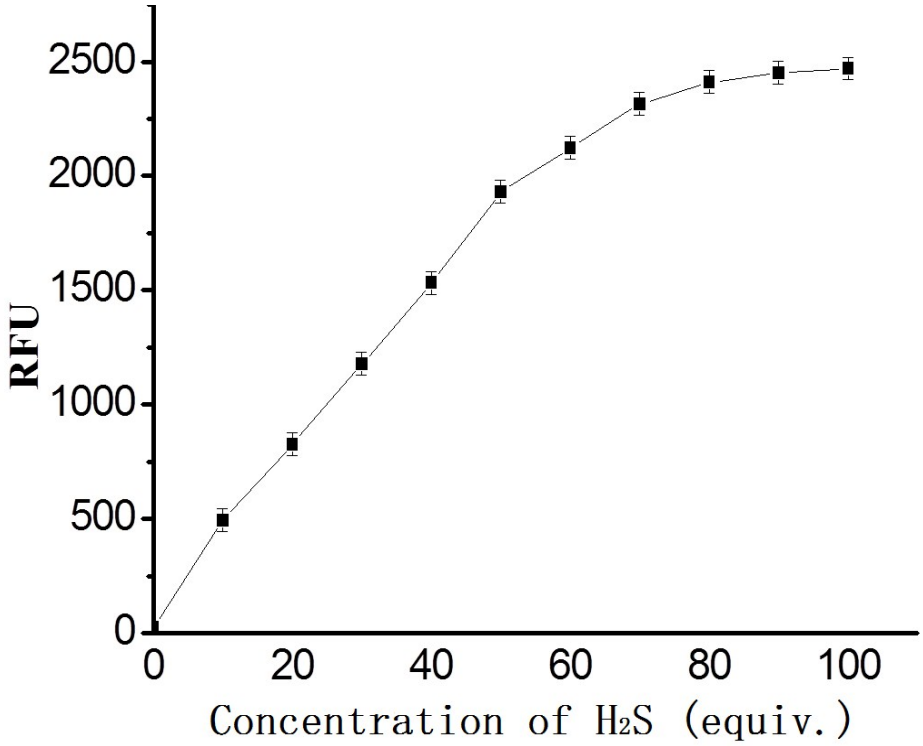



**Figure S10.** Fluorescence response of the probe **Lyso-HS** (10 μM) in PBS solution (20 mM, pH 7.4, 10% DMSO) with the addition of increasing concentrations of $H_2S$ (0–10 equiv. $H_2S$), λex= 365 nm, λem= 400–650 nm after 10 min of incubation

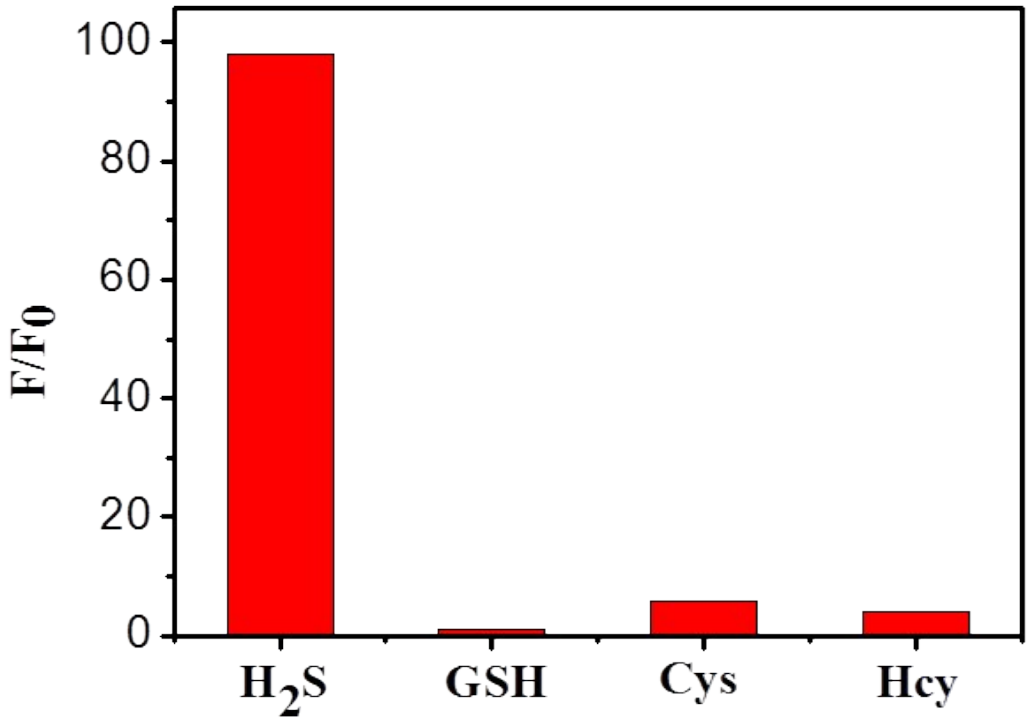



**Figure S11** Fluorescence responses of probe Lyso-HS (10 μM) in the presence of various biologically relevant analytes at their biological concentrations ($Na_2S$, 100 uM; GSH, 10 mM; Cys, 200μM; Hcy, 50μM).

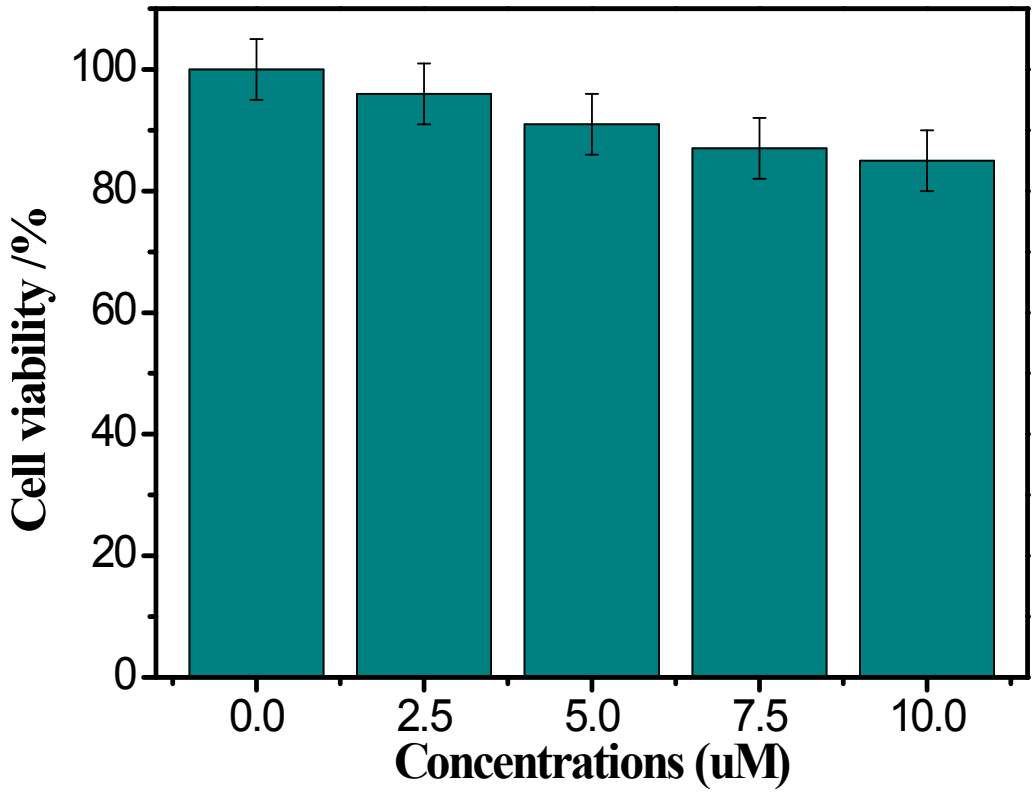



**Figure S12** Cell viability of Lyso-HS by a standard MTT assay, the experiment was repeated five times and the data are shown as mean (±S.D.).( HePG-2)

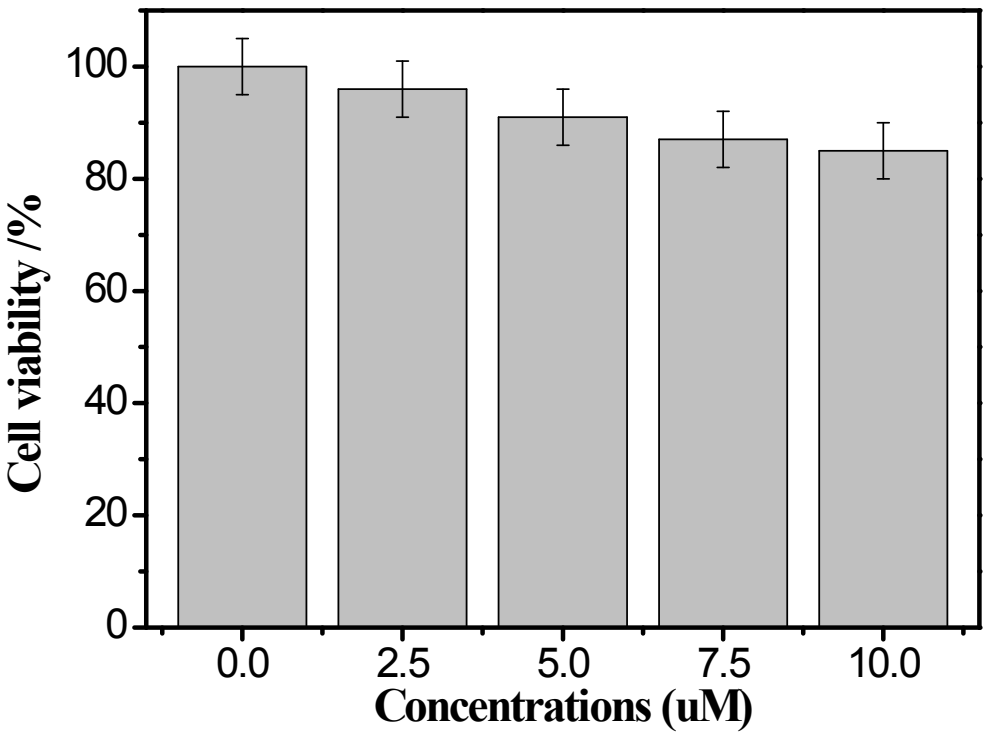



**Figure S13 C**ell viability of Lyso-HS by a standard MTT assay, the experiment was repeated five times and the data are shown as mean (±S.D.). （A549）

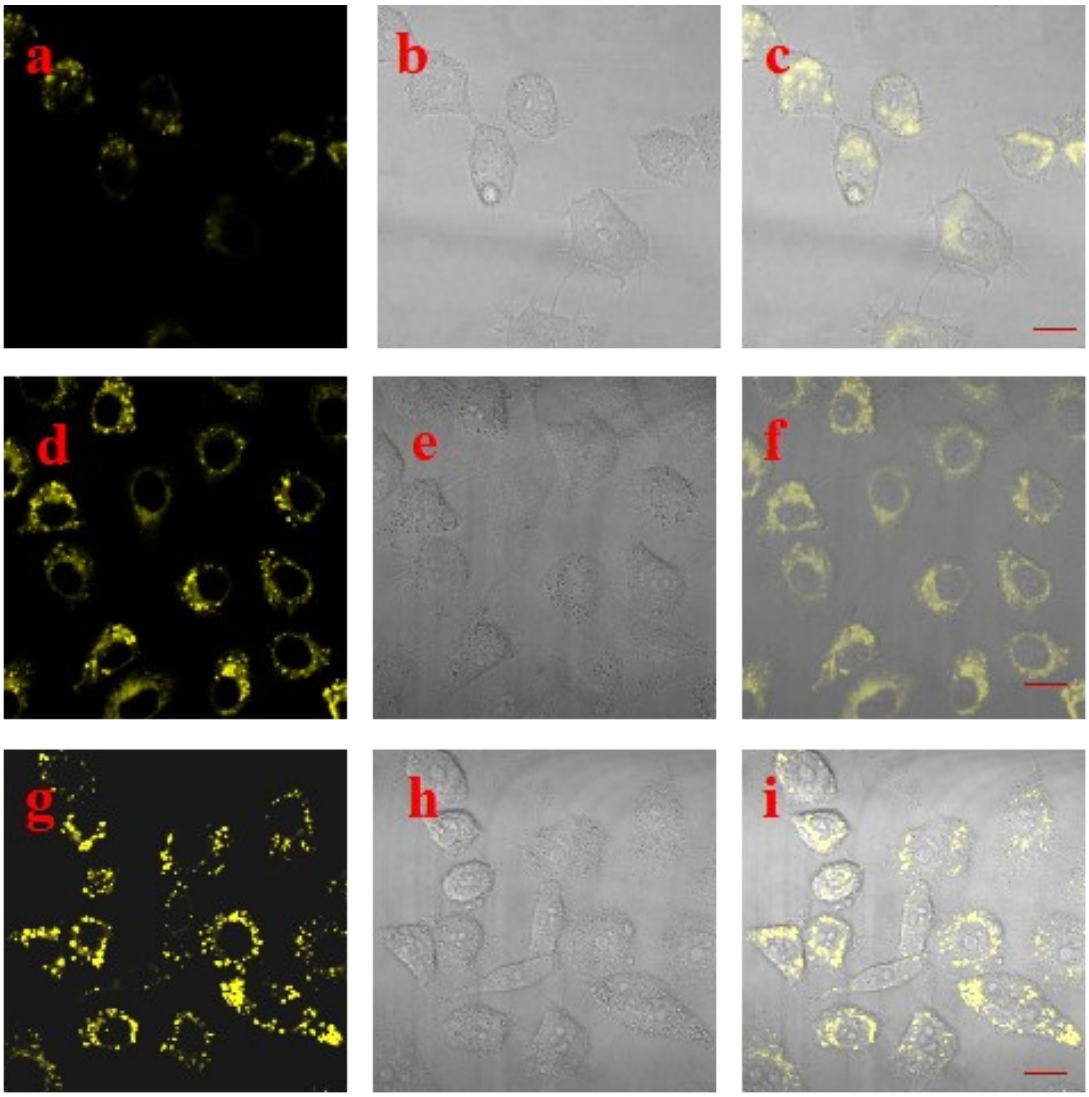



**Figure S 14** A549 cells were incubated with 10 μM Lyso-HS for 10 min and further incubated with 0, 100, and 300 μM $H_2S$ for another 30 min. λEx= 405 nm, λEm=480–530 nm. c, f, i)Merged images of Bright field image and UV. (Microscopic multiple 60X)

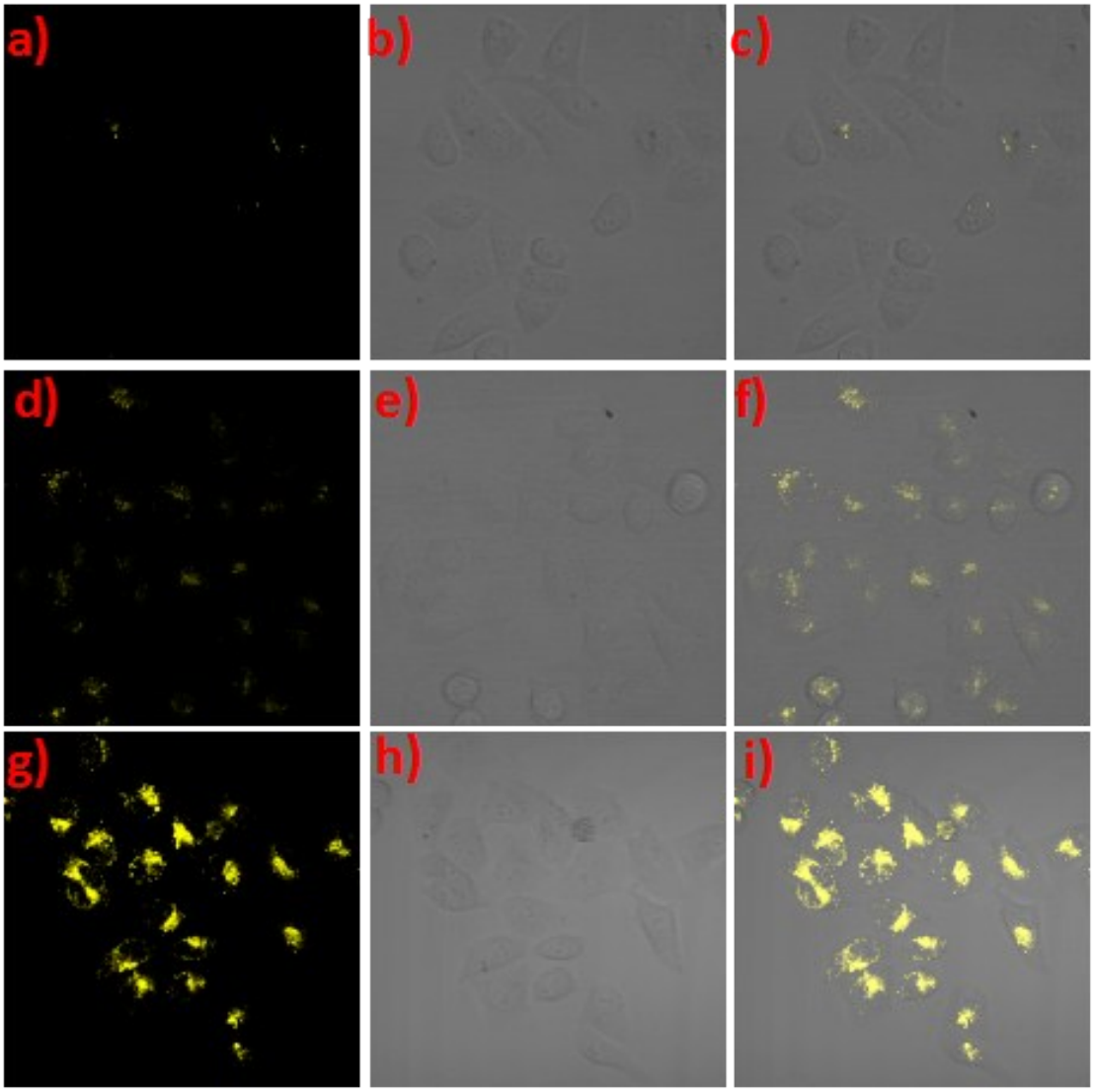



**Figure S 15** a, b, c) Cells were preincubated with 1 mM PAG (DL-propargylglycine) for 1 h and incubated with 10 μM Lyso-HS; d, e, f) HeLa cells were incubated with 10 μM Lyso-HS for 10 min and washed with PBS; g, h, i) Cells were preincubated with 1 mM cystathionine-β-synthase for 1 h and incubated with 10 μM Lyso-HS. λEx= 405 nm, λEm=480–530 nm. (Microscopic multiple 40X)

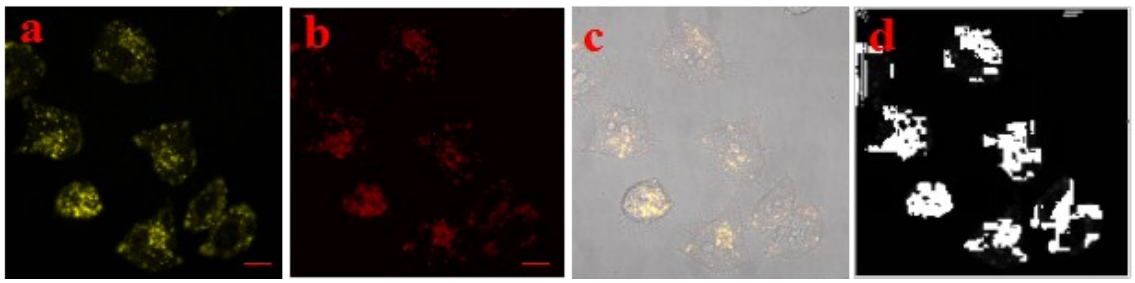



**Figure S 16** Fluorescence and co-localization images of **Lyso-H**S and DND-99 red. HePG-2 cells were co-treated with **Lyso-HS** (10 μM) and DND-99 Red (250 nM) for 15 min. The images were collected at (a) Ex = 405 nm, Em = 480–530 nm and (b) λEx = 545 nm, λEm = 570–620 nm. (c) colocalization graph Lyso-HS and DND-99 (Microscopic multiple 60X)red.

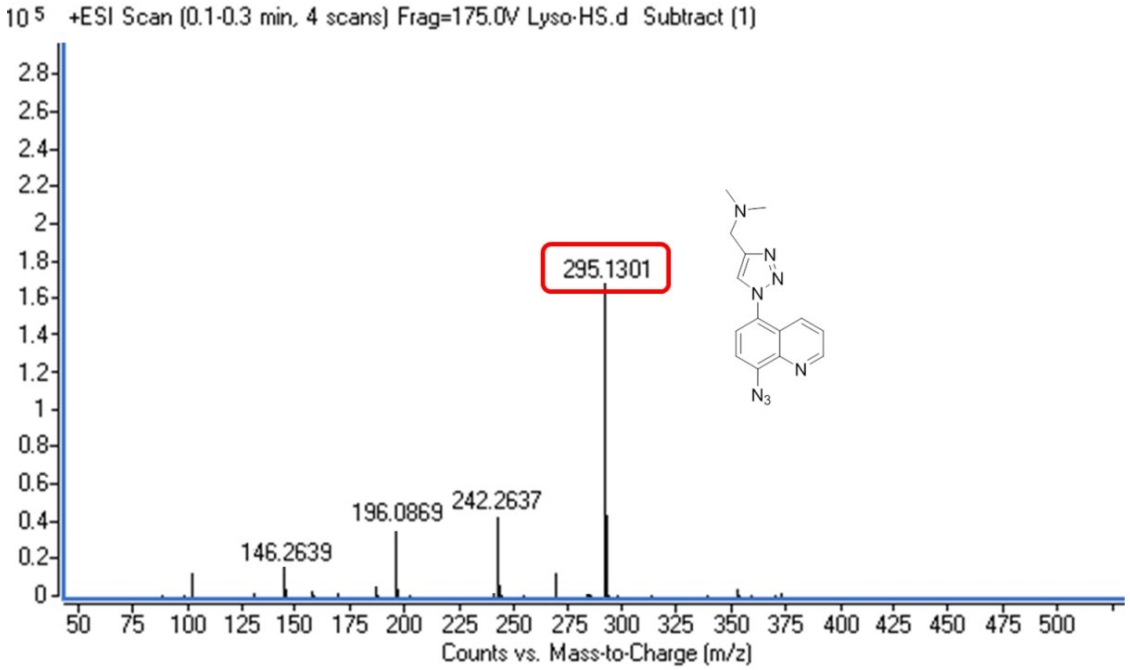



**Figure S17**. Mass spectrum of **Lyso-HS**

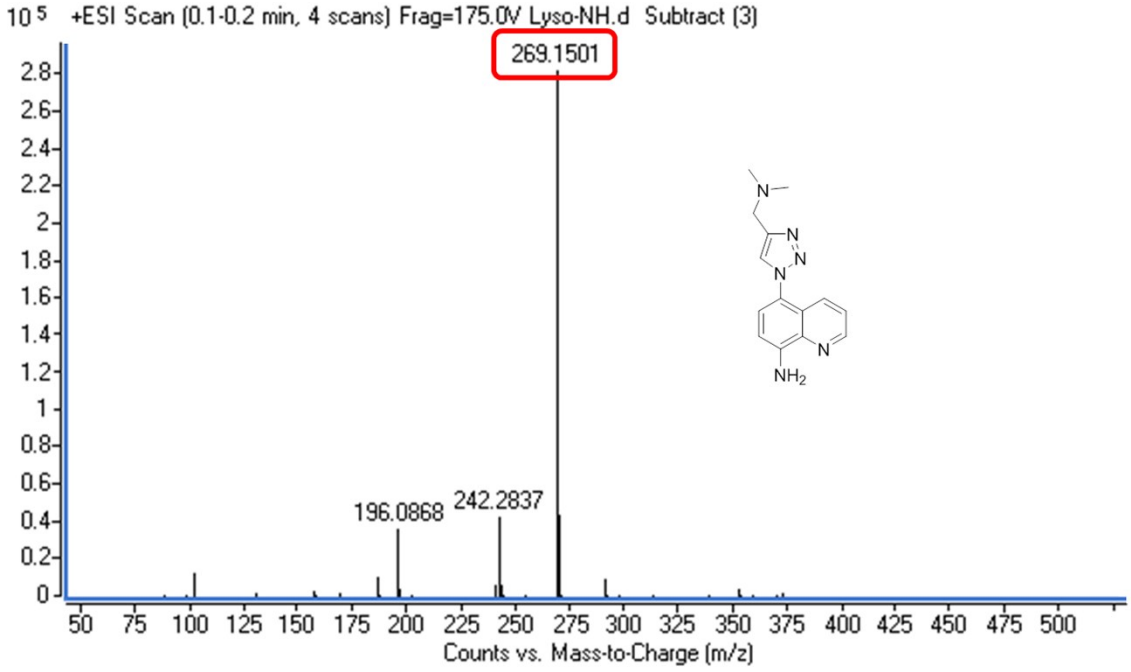



**Figure S18**. Mass spectrum after 10 μM of **Lyso-HS** reacted with 100 μM of $Na_2S$

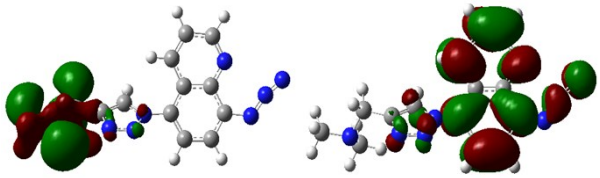
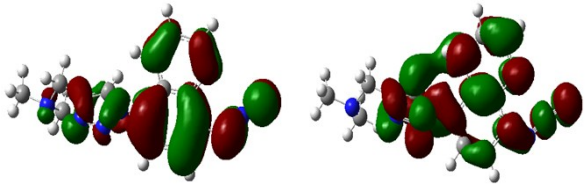
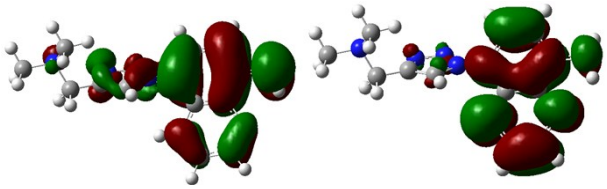
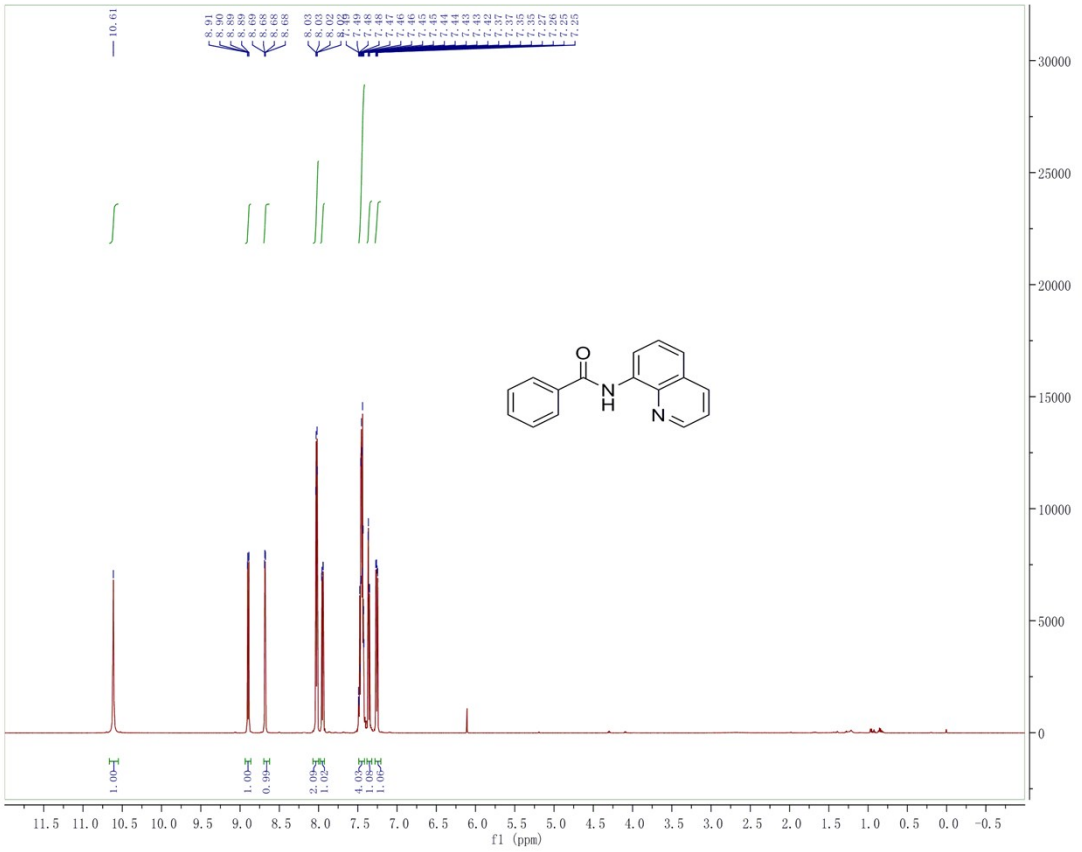
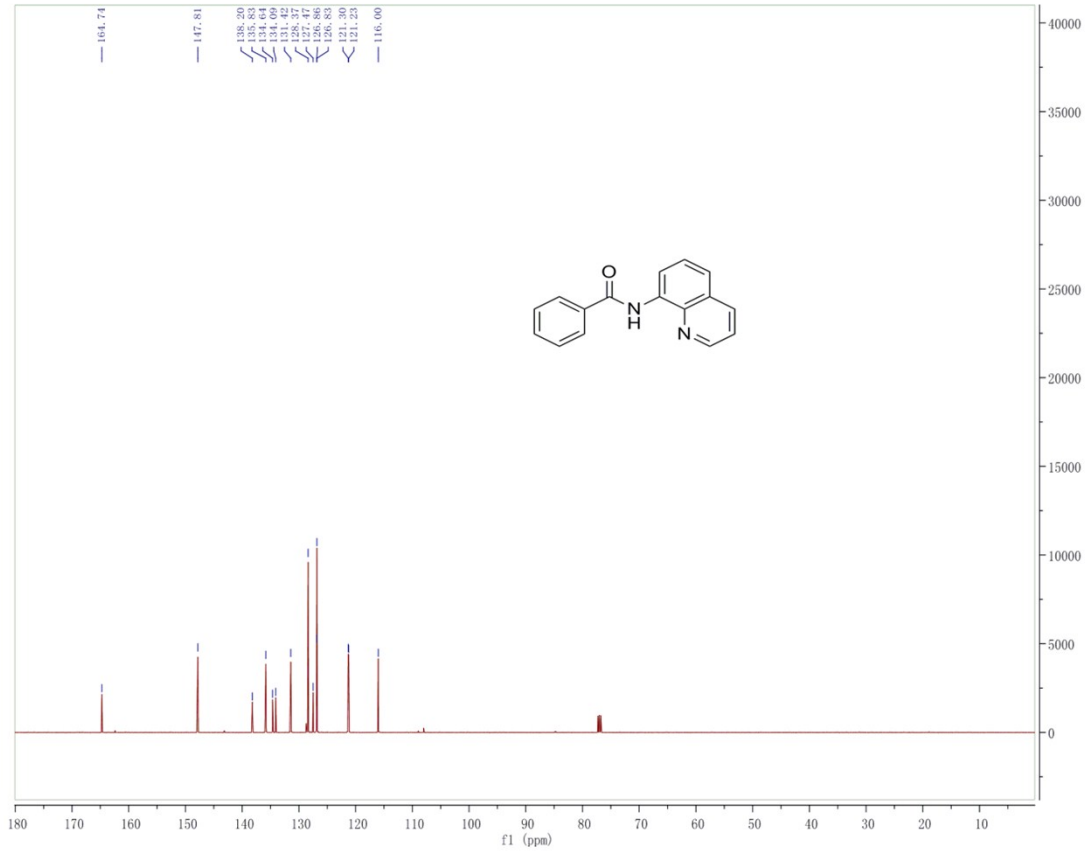
| Probe | Molecular orbitals | Contributions of orbital transitions |
|---|---|---|
| Lyso-HS |  HOMO LUMO  HOMO-1 LUMO+3 | Excited State 2: 362.57 nm<br>Singlet 3.5166 eV<br>Oscitallr strength =0.2057<br>HOMO-1->LUMO 95%<br>HOMO-1->LUMO+3 2.6% |
| Lyso-NH |  HOMO LUMO | Excited State 1:<br>Singlet 3.4125 eV<br>363.32nm<br>Oscitallr strength =0.0888<br>HOMO -> LUMO 96% |

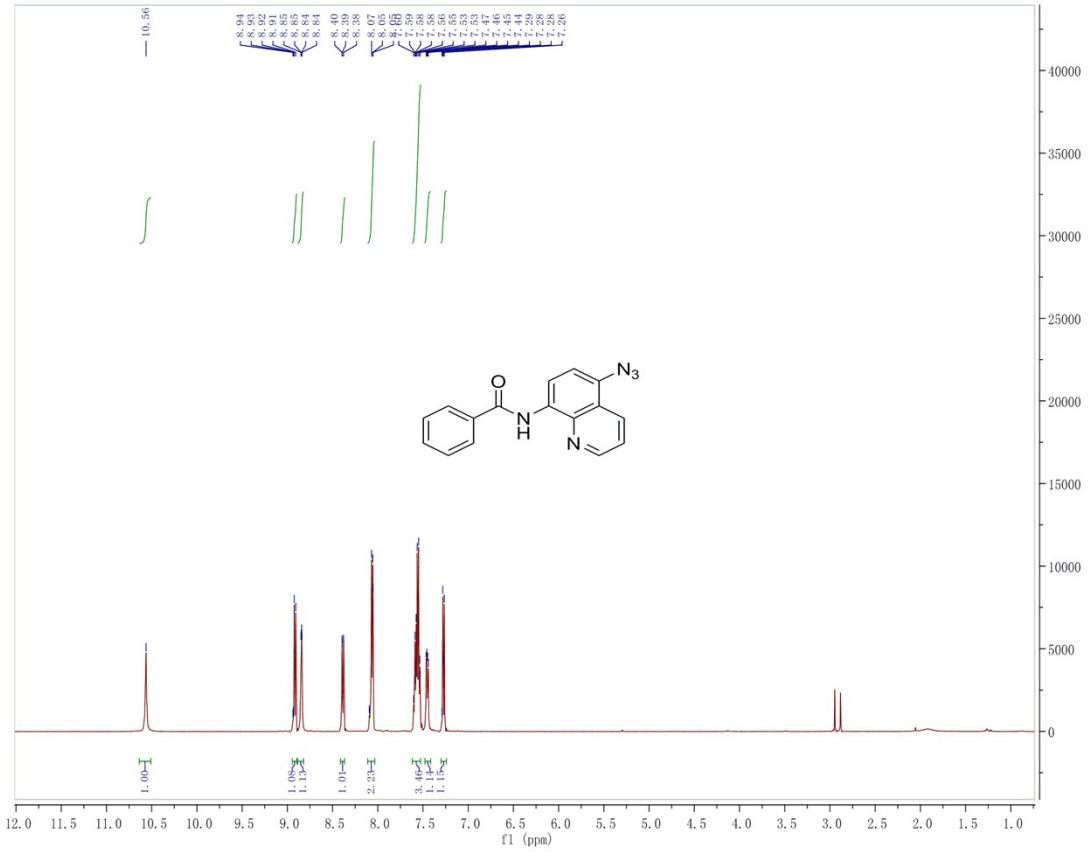
**Figure S19**. Calculated molecular orbitals and the contributions of orbital transitions for the excitation of probe Lyso-HS and Lyso-NH corresponding to experimental excitation energy (362 nm) at B3LYP/6-31G(d) level of theory.

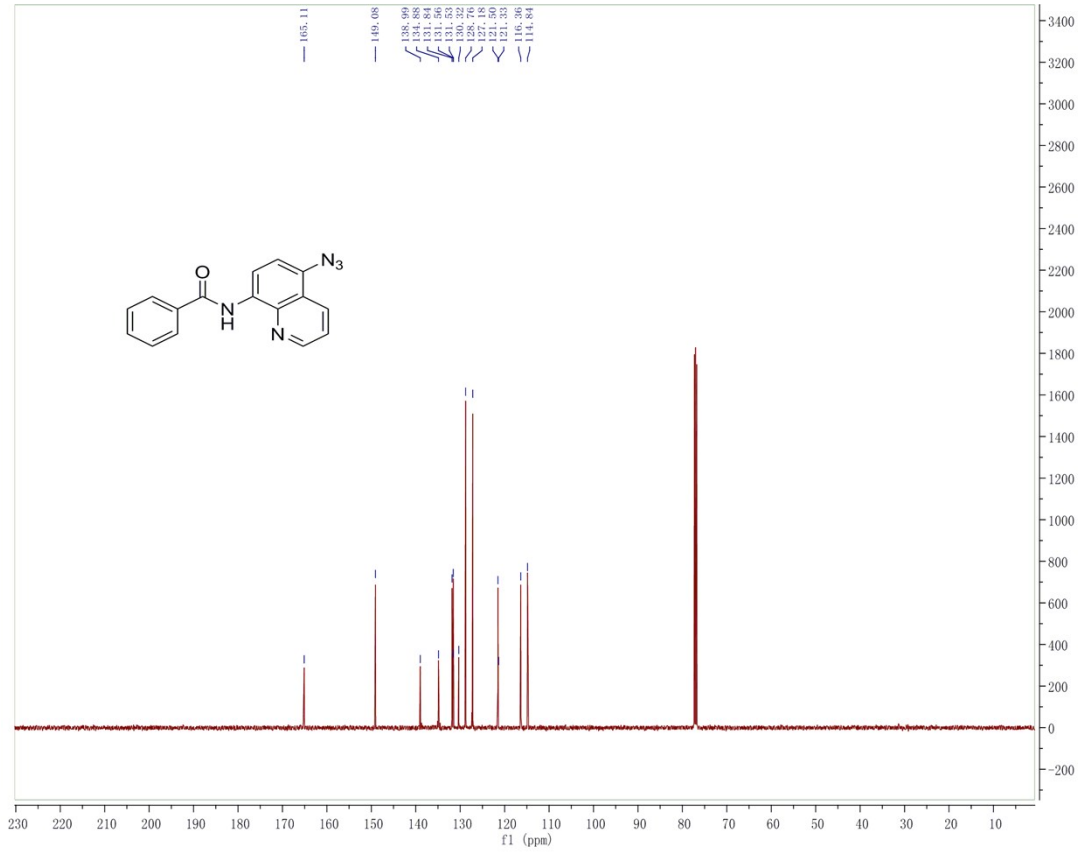
## $^{1}H$ and $^{13}C$ NMR spectra of 1-2



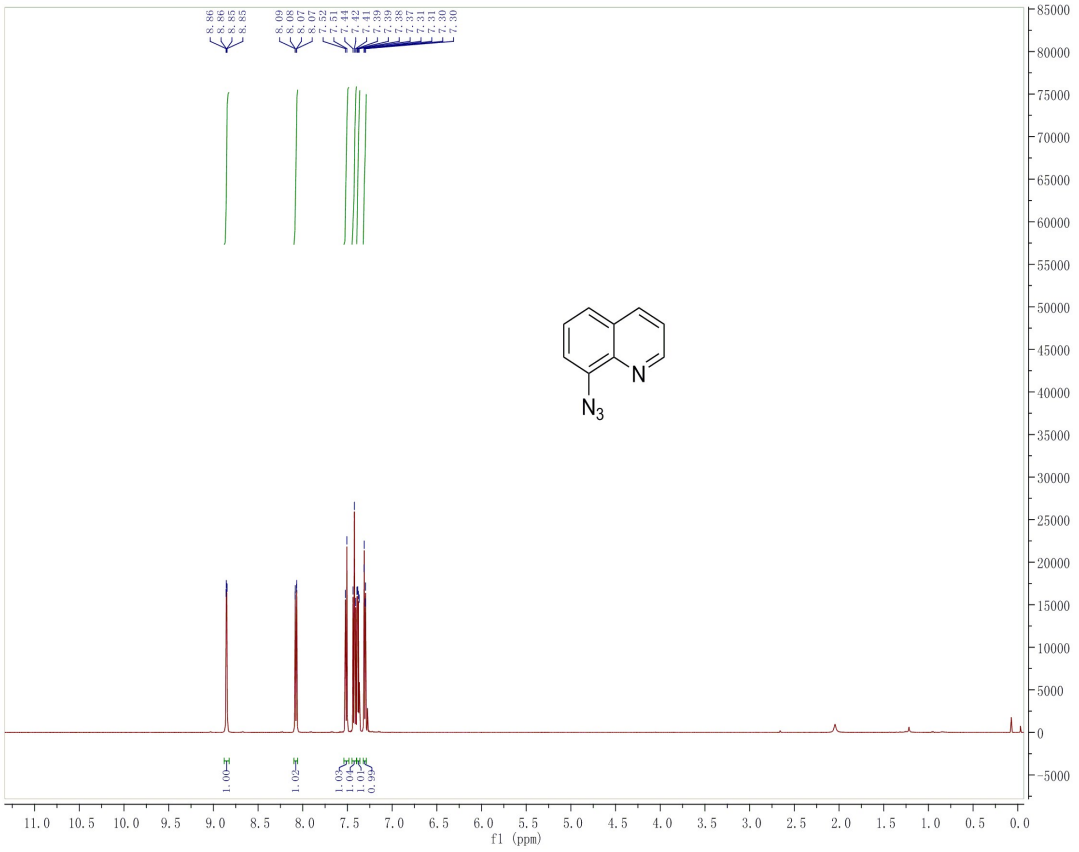



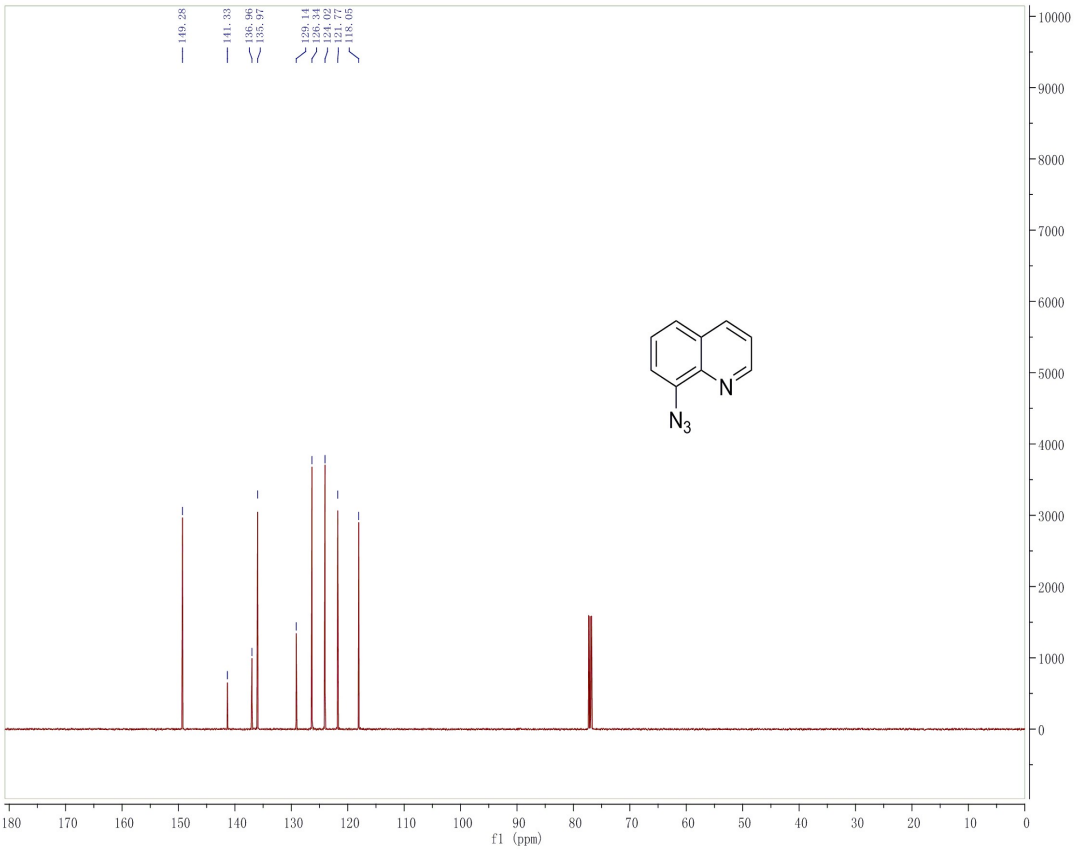
## $^{1}H$ and $^{13}C$ NMR spectra of 1-3



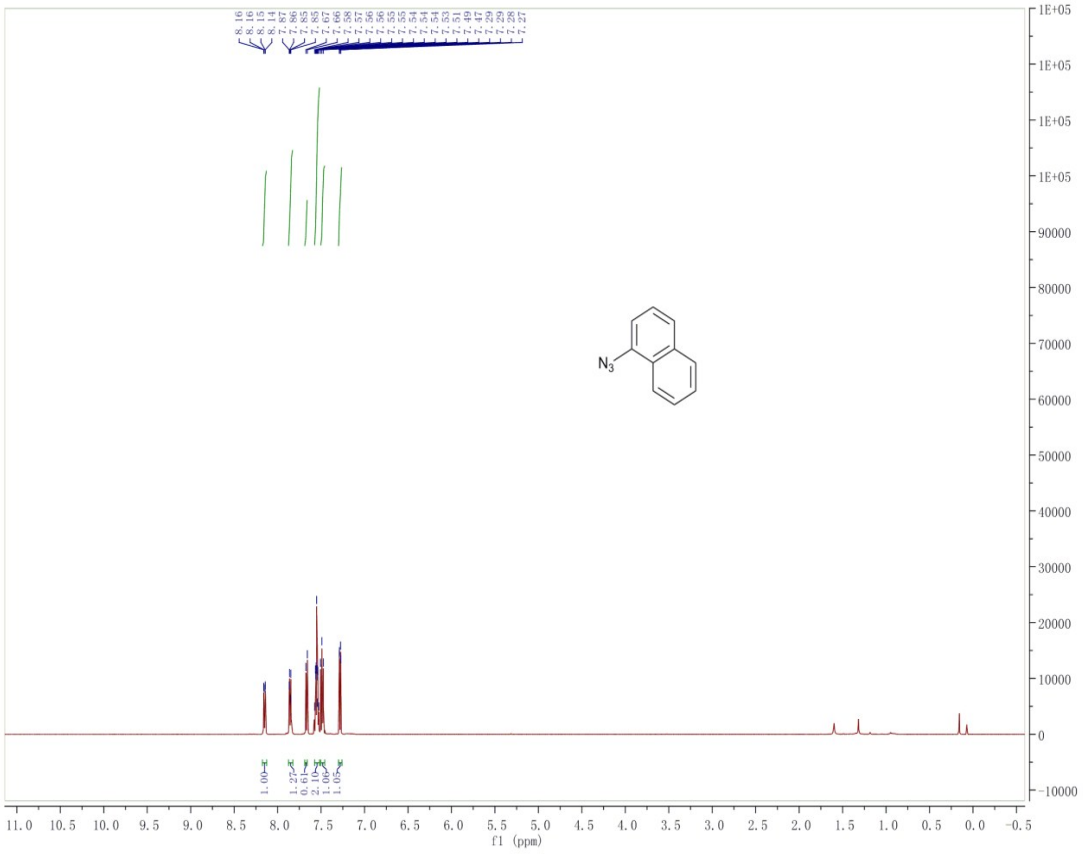



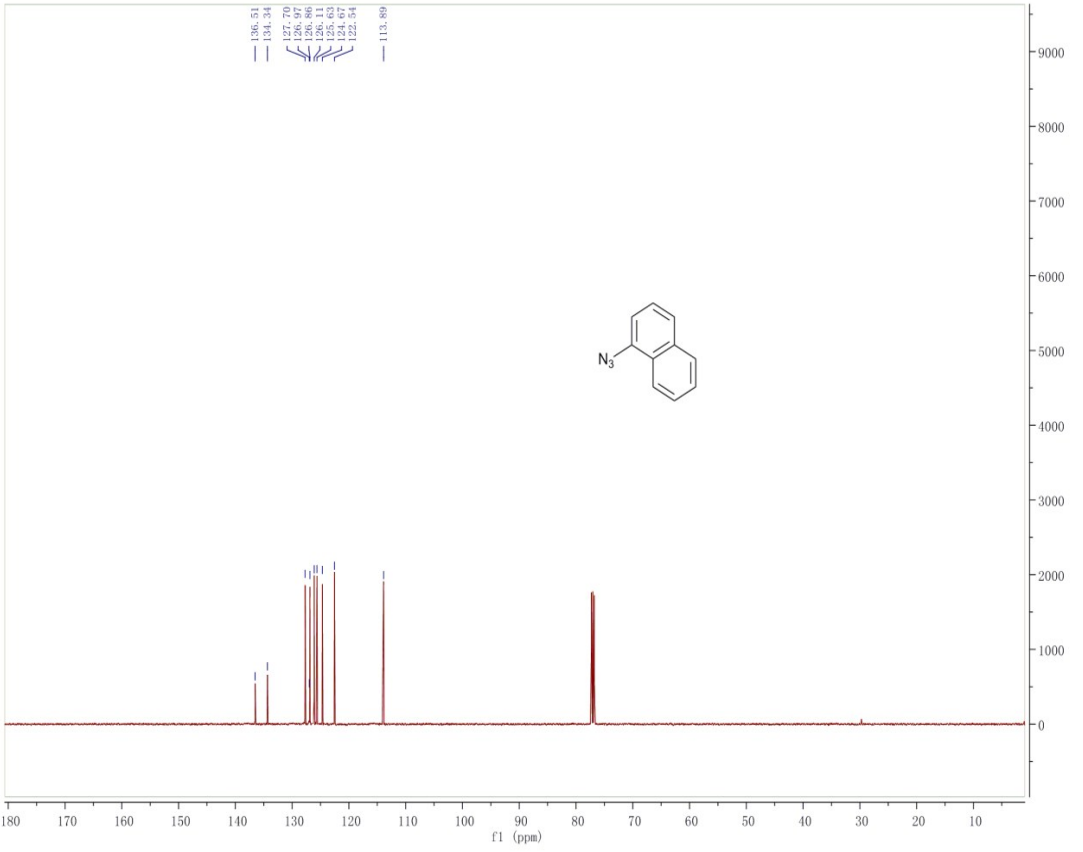
## $^{1}H$ and $^{13}C$ NMR spectra of NA-HS



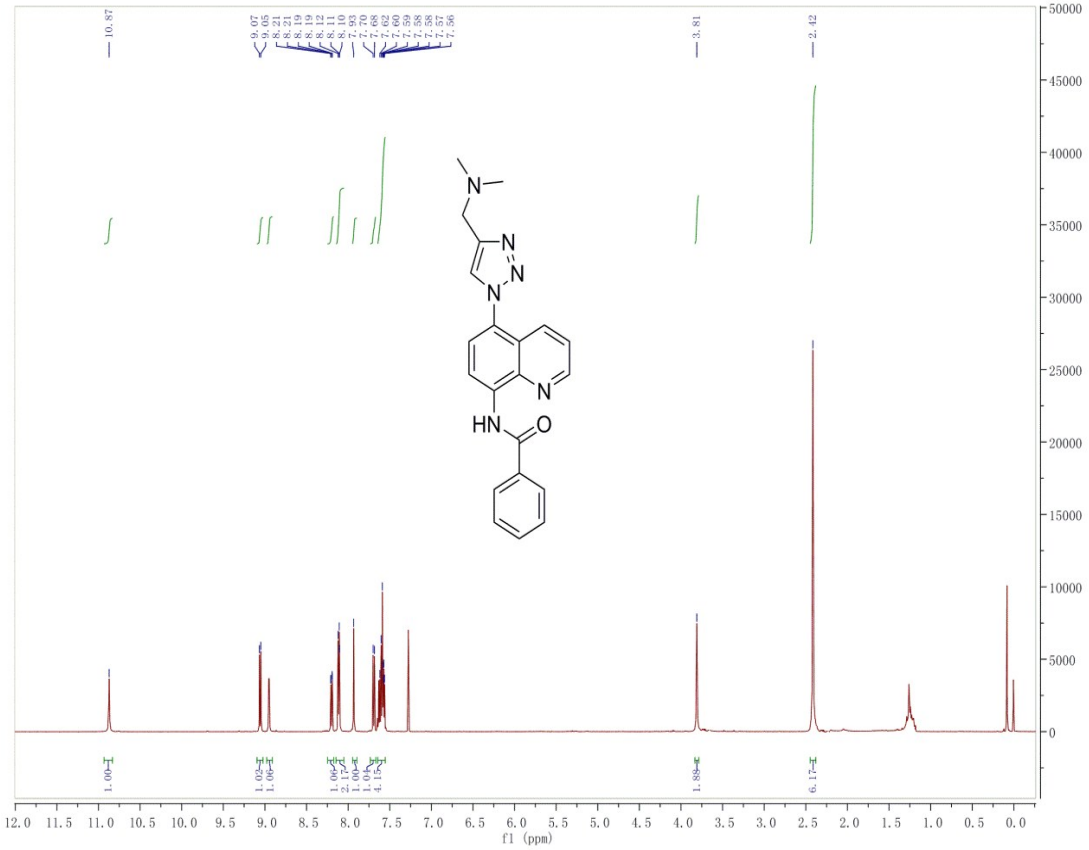



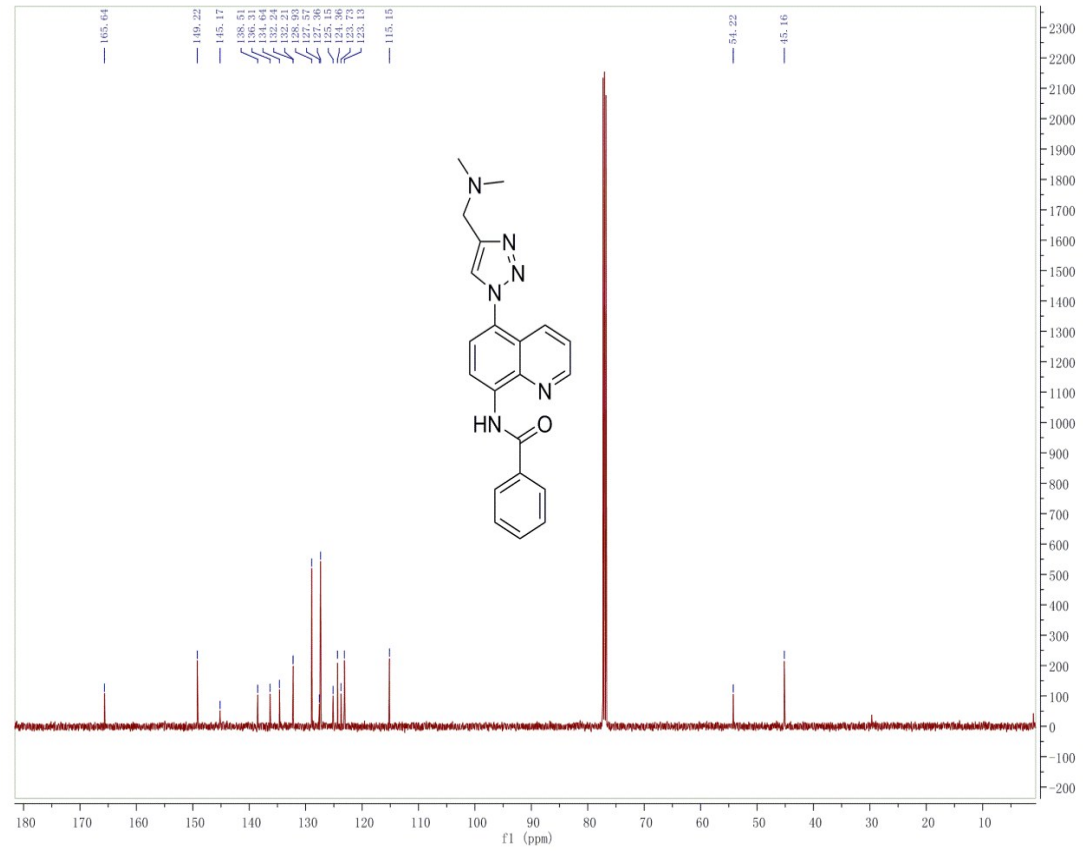
## $^{1}H$ and $^{13}C$ NMR spectra of NA-HS



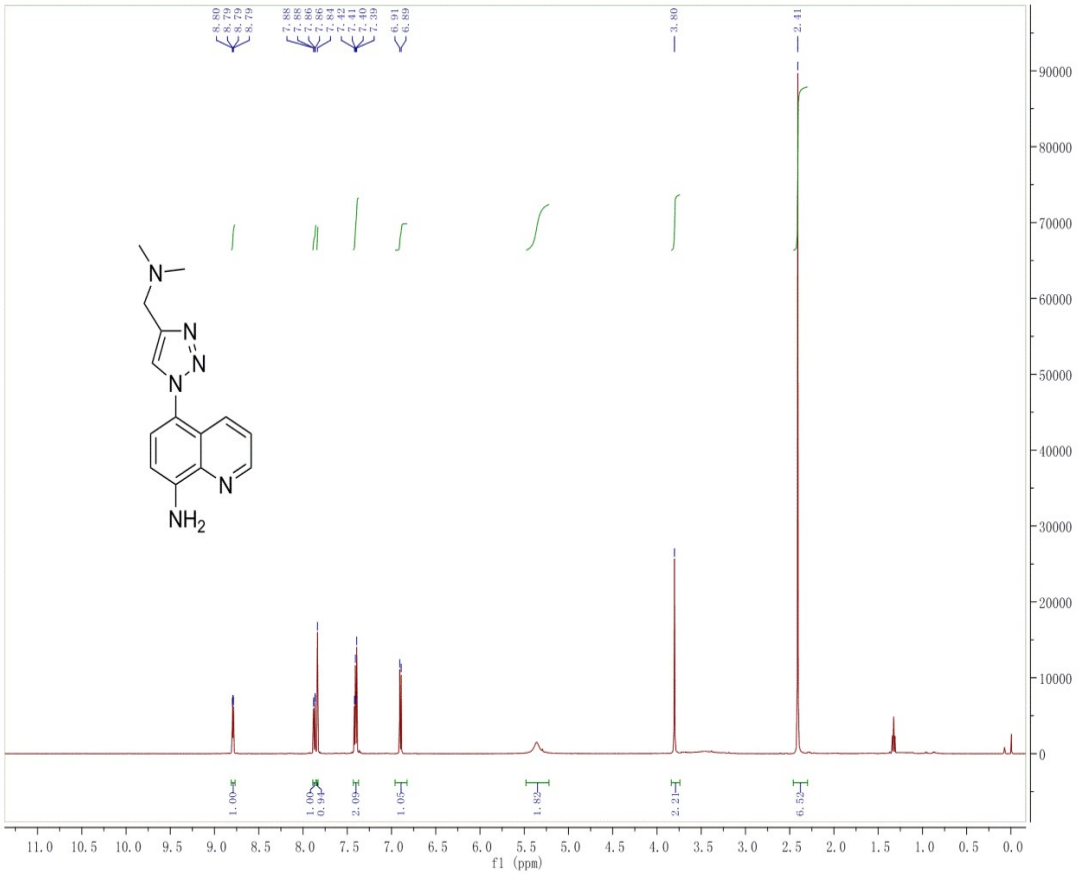



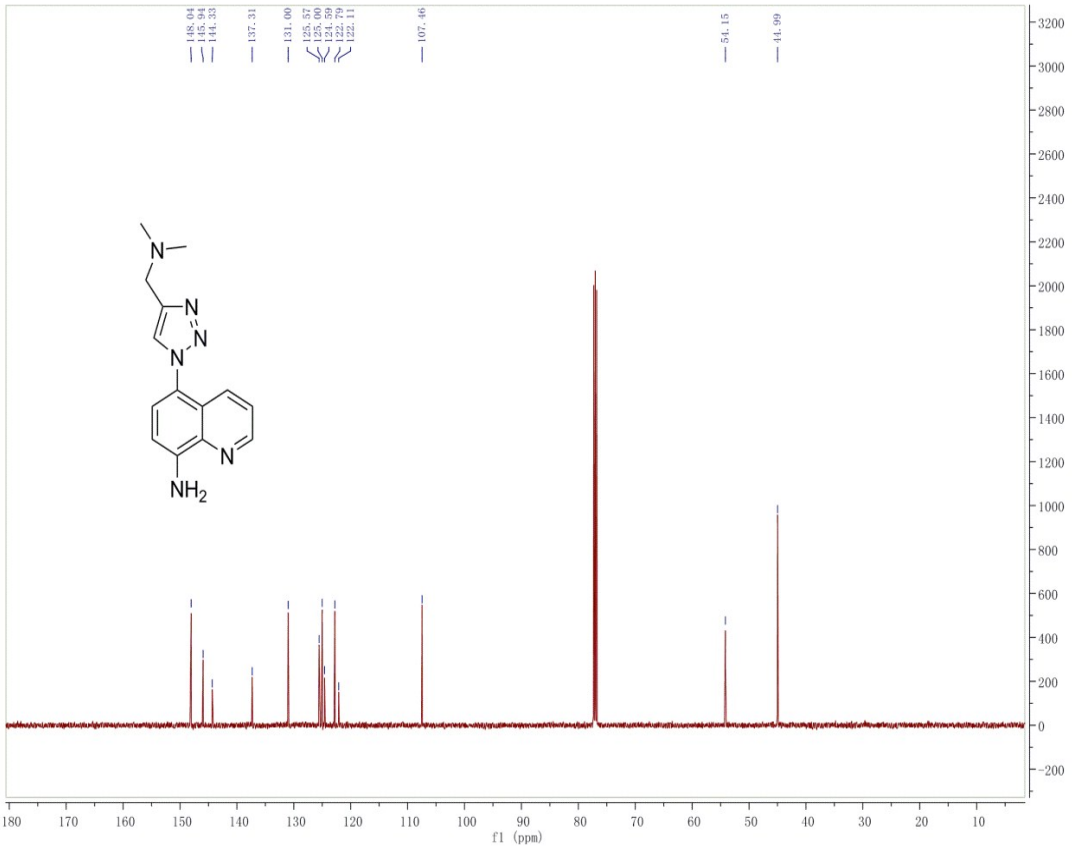
## $^{1}H$ and $^{13}C$ NMR spectra of 1-4



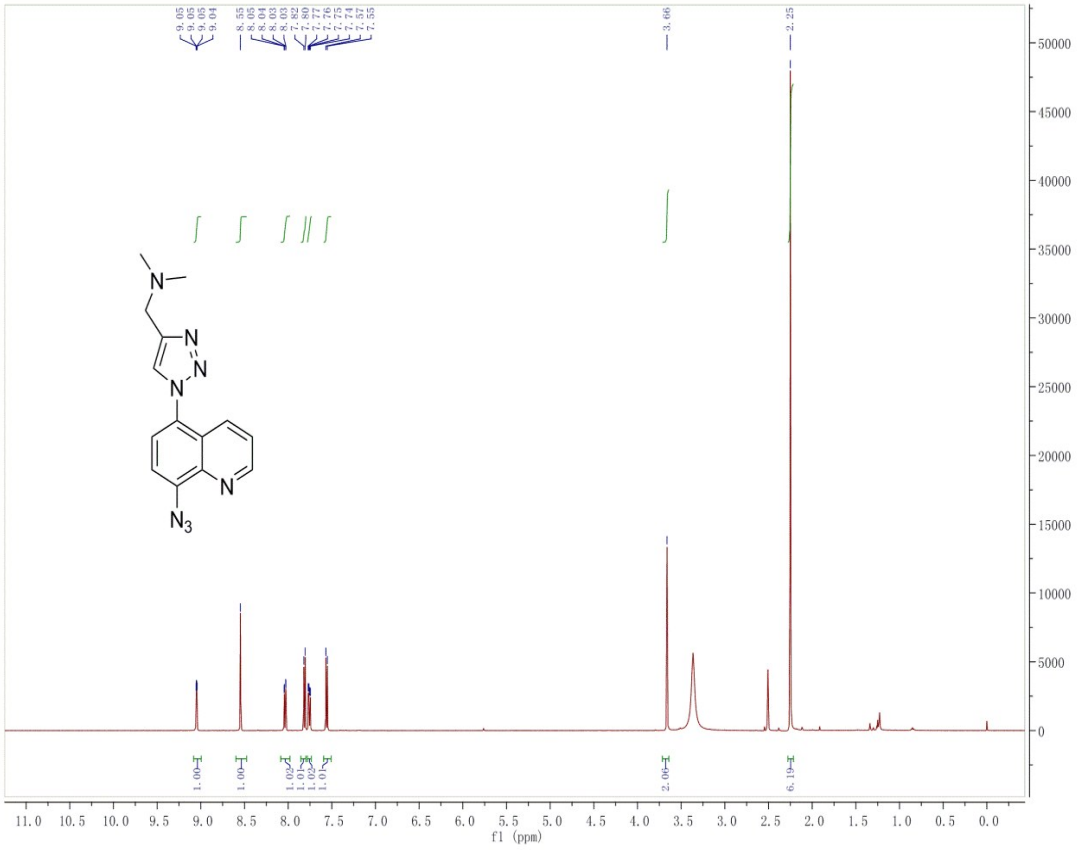



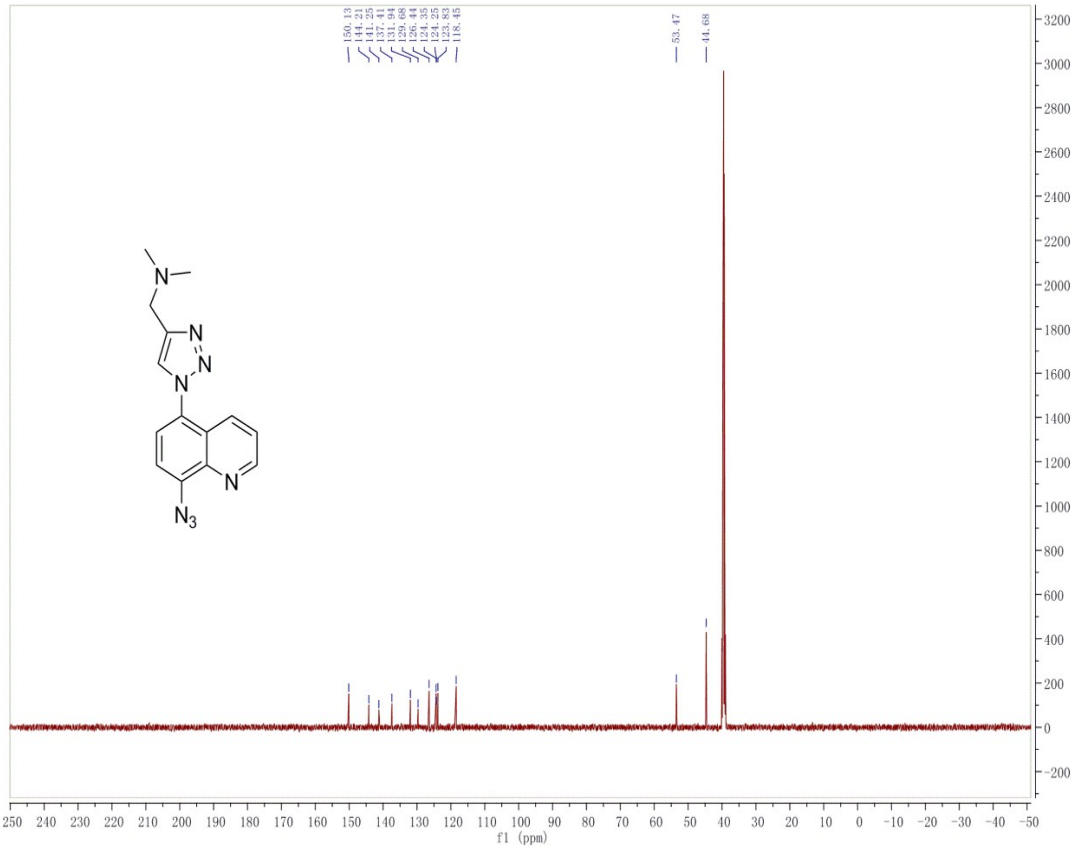
## $^{1}H$ and $^{13}C$ NMR spectra of Lyso-NH



## $^{1}H$ and $^{13}C$ NMR spectra of Lyso-HS



## Geometry-optimized structure of the probe Lyso-HS and Lyso-NH.

%chk=Lyso-NS-S0.chk
%mem=20GB
%nprocshared=28
#p opt freq b3lyp/6-31g(d)
S0 opt
0 1

| | | | |
|---|---|---|---|
| C | 2.22714100 | -2.15628000 | 0.07570400 |
| C | 3.14445600 | -1.13330100 | -0.10947100 |
| C | 2.69892400 | 0.22933600 | -0.03847300 |
| C | 1.31582900 | 0.50824100 | 0.21853100 |
| C | 0.40749500 | -0.58193300 | 0.35343400 |
| C | 0.86783600 | -1.88197500 | 0.29711700 |
| H | 2.57541600 | -3.18231100 | 0.02999900 |
| C | 0.95692800 | 1.87538900 | 0.35214600 |
| H | 0.16294800 | -2.69594600 | 0.42461800 |
| C | 1.91320700 | 2.85163300 | 0.19744400 |
| C | 3.24168800 | 2.46543300 | -0.09393500 |
| H | -0.06727600 | 2.14126900 | 0.59149100 |
| H | 1.66311100 | 3.90271300 | 0.30258700 |
| H | 4.01426600 | 3.21983800 | -0.23361400 |
| N | 3.62270100 | 1.20861200 | -0.19994400 |
| N | -0.97909700 | -0.35450500 | 0.57998300 |
| C | -1.87139600 | 0.36974300 | -0.15333500 |
| C | -3.08203100 | 0.18661500 | 0.47744900 |
| H | -1.58562700 | 0.91200600 | -1.04154100 |
| N | -2.87423900 | -0.63501700 | 1.55403400 |
| N | -1.62060900 | -0.96541000 | 1.62175700 |
| C | -4.43588000 | 0.74344200 | 0.14687200 |
| H | -4.89856700 | 1.08052000 | 1.08094200 |
| H | -4.31039500 | 1.64065100 | -0.49412800 |
| N | -5.33771200 | -0.23743100 | -0.45922600 |
| C | -4.90628800 | -0.64770600 | -1.78685900 |
| H | -5.58210300 | -1.42095400 | -2.16685000 |
| H | -4.89497200 | 0.18668000 | -2.51870600 |
| H | -3.89965500 | -1.07351600 | -1.73965300 |
| C | -6.70880400 | 0.25172200 | -0.47512100 |
| H | -6.84490900 | 1.16064400 | -1.09591300 |
| H | -7.36930900 | -0.52709600 | -0.87086000 |
| H | -7.03149000 | 0.48441500 | 0.54537300 |
| N | 4.46206700 | -1.53410400 | -0.35090600 |
| N | 5.39679500 | -0.73322800 | -0.53269900 |
| N | 6.39494300 | -0.22192600 | -0.72482400 |

%chk=Lyso-NH-S0-opt.chk
%mem=20GB
%nprocshared=28
#p opt freq b3lyp/6-31g(d)
S0 opt
0 1

| | | | |
|---|---|---|---|
| C | -2.67624400 | 2.26634800 | -0.07725700 |
| C | -3.62226300 | 1.27107800 | -0.29441200 |
| C | -3.20823800 | -0.10580700 | -0.19590900 |
| C | -1.84520500 | -0.43121100 | 0.08871600 |
| C | -0.90873400 | 0.63083800 | 0.25134800 |
| C | -1.33462600 | 1.94241800 | 0.18552000 |
| H | -2.97048000 | 3.31076300 | -0.13360700 |
| C | -1.53590900 | -1.81033600 | 0.22079800 |
| H | -0.60966500 | 2.73487500 | 0.33952300 |
| C | -2.52590400 | -2.75118400 | 0.05339700 |
| C | -3.83926100 | -2.31911200 | -0.24137500 |
| H | -0.52320800 | -2.11304800 | 0.46671700 |
| H | -2.31364000 | -3.81106700 | 0.15580300 |
| H | -4.63754600 | -3.04764800 | -0.37531800 |
| N | -4.17427900 | -1.04892300 | -0.35674900 |
| N | -4.92748100 | 1.52884800 | -0.63217400 |
| H | -5.54667000 | 0.73076800 | -0.55854200 |
| H | -5.31679700 | 2.42266700 | -0.36954100 |
| N | 0.46429700 | 0.35887000 | 0.52272400 |
| C | 1.36909100 | -0.33181700 | -0.22514200 |
| C | 2.55322700 | -0.24121300 | 0.47384000 |
| H | 1.10724900 | -0.79380600 | -1.16481400 |
| N | 2.31796200 | 0.49719100 | 1.60275500 |
| N | 1.06966100 | 0.85921500 | 1.63961900 |
| C | 3.90336500 | -0.81803000 | 0.16375400 |
| H | 4.30915800 | -1.24382900 | 1.08810800 |
| H | 3.78167800 | -1.65712500 | -0.55246800 |
| N | 4.86786500 | 0.17220400 | -0.31979600 |
| C | 4.51368300 | 0.70574500 | -1.62610400 |
| H | 5.23491000 | 1.47867400 | -1.91202000 |
| H | 4.50482600 | -0.06574000 | -2.42427100 |
| H | 3.52230600 | 1.16645100 | -1.58652200 |
| C | 6.21877200 | -0.36908100 | -0.31707400 |
| H | 6.35024200 | -1.23073900 | -1.00328500 |
| H | 6.92578900 | 0.41114900 | -0.61892800 |
| H | 6.48517100 | -0.69601900 | 0.69389500 |