Supplementary Information

A mitochondria-anchored dual-lock probe for sequential detection of HOCl and viscosity during oxidative stress and ferroptosis

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1. General Experimental Section

All chemical/biological reagents and solvents were obtained commercially and used as supplied. Bruker 400NMR spectrometers were used for NMR. High-resolution mass spectrometry (HR-MS, ESI) spectra were obtained on a Bruker maxis UHRTOF instrument. Melting points of substances were determined in open capillaries and are uncorrected. A Shimadzu UV-1700 vis spectrophotometer and a HITACHI F-4600 fluorescence spectrophotometer were used to record absorption and fluorescence spectra. Cell imaging and in vivo imaging experiments were measured on a Leica SP8 confocal fluorescence spectrophotometer. HeLa cells, and HeLa cells were purchased from the Cell Bank of the Chinese Academy of Sciences (Shanghai, China).

Quantum calculations

All quantum chemical calculations were performed using Gaussian 16. The ground-state geometry was optimized and confirmed as a minimum via frequency analysis at the B3LYP-D3/6-31G(d) level to describe long-range interactions accurately [1, 2]. Subsequently, the excited-state structure was optimized using Time-Dependent Density Functional Theory (TDDFT). Based on the TDDFT results, the electron-hole analysis for the target excitation was conducted using Multiwfn 3.8 to characterize the excitation nature [3]. All molecular orbitals and electron-hole distribution maps were rendered using VMD 1.9.3 for visualization [4].

Fluorescence Properties of the Probe in Solvents of Different Viscosities

A glycerol-PBS system was employed to investigate the viscosity sensitivity of the probe. Solutions with varying viscosities (ranging from 0% to 80% glycerol) were prepared by mixing PBS and glycerol at different volume ratios. The glycerol volume fractions were 60%, 65%, 70%, 72%, 75%, 77%, and 80%. The probe **DHX -HOCl-V** stock solution was added to each viscosity solution, thoroughly mixed, and the fluorescence spectra were recorded using a fluorescence spectrophotometer. Measurements were conducted with an excitation wavelength of 660 nm and a probe **DHX-HOCl-V** concentration of 10 μM.

Selectivity Assay of the Probe DHX-V-HOCl Toward Interfering Species

To validate the stability and specificity of probe **DHX-HOCl-V**, a series of interfering substances including metal ions, reducing agents, amino acids, halide ions and oxidizing agents were selected. The fluorescence emission spectra of probe **DHX - HOCl-V** were measured in PBS buffer and 80% (v/v) glycerol solutions. Specifically, aliquots of the probe stock solution were mixed with PBS buffer or 80% glycerol, followed by the addition of different interfering ion solutions. The final probe concentration was consistently maintained at 10 μM, with interfering substances at the following concentrations: 1 mM: GSH, Cys, Hcy, DTT; 200 μM: Glu, NaHS, Na_2SO_3, H_2O_2, HClO, KO_2, metal ions (Fe^{3+}, Fe^{2+}, Na^+, K^+, Cu^{2+}, Ca^{2+}, Mg^{2+}, Zn^{2+}, Ni^{2+}, Ag^+, Mn^{2+}), and halide anions (I^-, Br^-, F^-). After thorough mixing, the solutions were incubated at 37°C for 30 minutes in a constant-temperature incubator. Fluorescence emission spectra were then recorded for each interference group in both PBS and 80% glycerol systems, using an excitation wavelength of 660 nm and a probe concentration of 10 μM.

pH Stability Assay of the Probe DHX-HOCl-V

The pH stability of the probe **DHX-HOCl-V** was evaluated by measuring its fluorescence properties in PBS and 80% (v/v) glycerol-PBS solutions at varying pH levels. First, PBS or glycerol solutions (80% v/v) were adjusted to pH values across the range of 6-9 using HCl/NaOH under pH meter monitoring. The probe stock solution was then dissolved in these pre-adjusted solutions. After vortex mixing, the solutions were incubated at 37°C for 30 minutes in a constant-temperature incubator. Fluorescence spectra were subsequently recorded at each pH value with an excitation wavelength of 725 nm and probe **DHX -HOCl-V** concentration of 10 μM.

Cell Culture

This study utilized HeLa and HepG2 cancer cell lines for cellular experiments. Cells were cultured in DMEM medium supplemented with 10% fetal bovine serum (FBS) and 1% penicillin/streptomycin. Culture flasks were maintained at 37°C in a

humidified incubator with 5% CO_2. Upon reaching 80-90% confluency, cells were passaged using trypsinization. For imaging experiments, cells were seeded in glass-bottom dishes 24 hours prior, incubated with probes or drugs, and rinsed three times with PBS before analysis.

MTT Cytotoxicity Assay

An *in vitro* cytotoxicity analysis of the probe was performed using HeLa cells and HepG2 cells. Confluent cells were trypsinized, diluted in culture medium to a density of 1×10^5 cells/mL, and seeded into 96-well plates for 24-hour incubation. After adherence, cells were treated with probe solutions at concentrations of 0, 5, 10, 15, 20, 25, and 30 μM for 24 hours. The supernatant was then aspirated, and 100 μL of MTT solution (0.5 mg/mL) was added to each well for 4 hours. Following MTT removal, 100 μL of DMSO was introduced to dissolve the formed purple formazan crystals. Absorbance at 490 nm was measured using a microplate reader. Cell viability was calculated as:

Cell viability (%) = $(A_1 / A_2) \times 100$

where A_1 = absorbance of probe-treated groups and A_2 = absorbance of control groups.

Co-localization Experiment

The mitochondrial-targeting performance of probe **DHX-HOCl-V** was tested with the colocalization experiments by co-staining the HeLa cells with Mito-Tracker Green (a typical commercially available mitochondrial tracker) and the probe. The HeLa cells were incubated with MitoTracker Green (150 nM) for 30 min and **DHX-HOCl-V** (10 μM) for 20 min. Emission from the red channel (**DHX-HOCl-V**). λ_{ex} = 633 nm, collected 660-795 nm. Emission from the green channel (Mito-Tracker Green). λ_{ex} = 488 nm, collected 500-560 nm. At the same time, lysosomes were localized using Lysotracker Green (2 μM, incubated for 2 h), λ_{ex} = 488 nm, harvesting wavelength of 508-580 nm, Nile red (3 μM, incubated for 30min) (λ_{ex} = 561 nm, collected 585-650 nm), cells were rapidly imaged under a sp8 confocal microscope with Hoechst 33342 (10 μg /mL, incubated for 30min) localization of nuclei, λ_{ex} = 405 nm, collection

wavelength 410-450 nm. HeLa cells costained with probe **DHX-HOCl-V** (10 μM, 30 min) and MitoTracker Green (150 nM, 30 min) upon treatment with CCCP (20 μM, 30 min).

Simultaneous Fluorescence Imaging of HOCl and Viscosity in Nys and HOCl - Stimulated HeLa Cells

This experiment included four treatment groups, and the specific procedures were as follows: **Group 1 (Blank Control):** HeLa cells cultured in confocal dishes were incubated with medium containing the **DHX-HOCl-V** probe (10 μM) in a cell culture incubator for 30 min, washed with PBS, and then replaced with DMEM medium for later use. **Group 2 (Nystatin Treatment)**: HeLa cells cultured in confocal dishes were first treated with medium containing nystatin (10 μM) and incubated for 8 h in a cell culture incubator. Then, the medium was replaced with one containing the **DHX-HOCl-V** probe (10 μM) and incubated for another 30 min, followed by PBS washing and replacement with DMEM medium for later use. **Group 3 (HOCl Treatment):** HeLa cells cultured in confocal dishes were first incubated with medium containing sodium hypochlorite (100 μM) for 30 min, washed with PBS, and then incubated with medium containing the **DHX-HOCl-V** probe (10 μM) for another 30 min. After washing with PBS, the medium was replaced with DMEM for later use. **Group 4 (Nystatin + HOCl Treatment)**: HeLa cells cultured in confocal dishes were treated sequentially as follows: first with medium containing nystatin (10 μM) for 8 h; then with medium containing sodium hypochlorite (100 μM) for 30 min, followed by PBS washing; next with medium containing the **DHX-HOCl-V** probe (10 μM) for 30 min, washed again with PBS, and finally replaced with DMEM medium for later use. After completing the above treatments, the cells from all four groups were subjected to fluorescence imaging using a Leica SP8 laser scanning confocal microscope. Probe **DHX-HOCl-V** was excited at 633 nm, and emission was collected at 660-795 nm.

Simultaneous Fluorescence Imaging of HOCl and Viscosity in APAP and NAC - Stimulated HeLa Cells

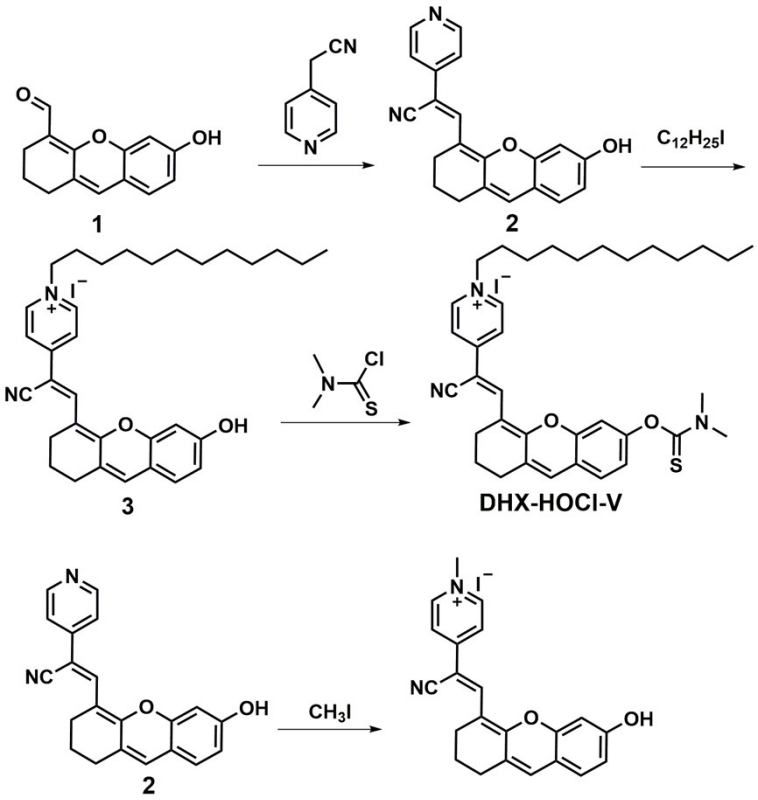
In this study, HepG2 cells were used and divided into four treatment groups. The specific procedures were as follows: **Group 1 (Blank Control)**: Cells without any pretreatment were directly incubated with culture medium containing the **DHX-HOCl-V** probe (10 μM) in a cell culture incubator for 0.5 h, followed by PBS washing and replacement with DMEM medium for later use. **Group 2 (NAC Treatment):** Cells were first incubated with culture medium containing NAC (1 mM) for 2 h in a cell culture incubator, washed with PBS, and then incubated with medium containing the **DHX-HOCl-V** probe (10 μM) for another 0.5 h. After a second PBS wash, the medium was replaced with DMEM for later use. **Group 3 (APAP Treatment)**: Cells were first incubated with culture medium containing APAP (500 μM) for 8 h, washed with PBS, and then further incubated with medium containing the **DHX-HOCl-V** probe (10 μM) for 0.5 h. After PBS washing, the medium was replaced with DMEM for later use. **Group 4 (APAP + NAC Treatment)**: Cells were treated sequentially as follows: incubation with APAP (500 μM) for 8 h, PBS wash; incubation with NAC (1 mM) for 2 h, PBS wash; incubation with the **DHX-HOCl-V** probe (10 μM) for 0.5 h, PBS wash; and replacement with DMEM medium for later use. After the above treatments, all four groups of cells were subjected to fluorescence imaging using a Leica SP8 laser scanning confocal microscope. Probe **DHX-HOCl-V** was excited at 633 nm, and emission was collected at 660-795 nm.

Fluorescence Imaging of Hypochlorous Acid and Viscosity during Ferroptosis in Cells

This experiment utilized HeLa cells and included five treatment groups. The specific procedures were as follows: **Group 1 (Blank Control)**: Cells without any pretreatment were directly incubated with culture medium containing the **DHX-HOCl-V** probe (10 μM) in a cell culture incubator for 0.5 h, then the medium was replaced with DMEM for later use. **Group 2 (Erastin Treatment):** Cells were incubated with culture medium containing Erastin (10 μM) for 8 h in a cell culture

incubator, followed by replacement with medium containing the **DHX-HOCl-V** probe (10 μM) for another 0.5 h. The medium was then replaced with fresh culture medium for later use. **Group 3 (Erastin + NAC Treatment):** Cells were treated sequentially as follows: incubated with Erastin (10 μM) for 8 h, then with NAC (1 mM) for 2 h, followed by the **DHX-HOCl-V** probe (10 μM) for 0.5 h, and finally the medium was replaced with fresh culture medium for later use. **Group 4 (Erastin + Ferrostatin-1 Treatment)**: Cells were incubated with culture medium containing both Erastin (10 μM) and Ferrostatin-1 (15 μM, abbreviated as Fer-1) for 8 h, then with the **DHX-HOCl-V** probe (10 μM) for 0.5 h, after which the medium was replaced with fresh culture medium for later use. After completing the above treatments, all five groups of cells were subjected to fluorescence imaging using a Leica SP8 laser scanning confocal microscope. Probe **DHX-HOCl-V** was excited at 633 nm, and emission was collected at 660-795 nm.

2. Synthesis of probe DHX-HOCl-V



Scheme S1. The synthesis route of probe **DHX-HOCl-V** and N-methylated derivative

of **compound 2.**

Synthesis of Compound 2

To a reaction flask were added compound 1 (410 mg, 1.8 mmol), 4-pyridineacetonitrile (425 mg, 3.6 mmol), a catalytic amount of piperidine, and ethanol (15 mL). The mixture was stirred at room temperature for 20 minutes under nitrogen atmosphere. Then, the reaction system was heated to 80 °C and stirred for 12 hours. After completion of the reaction, the mixture was concentrated under vacuum to afford a brown-black oil. Purification by column chromatography (eluent: ethyl acetate/petroleum ether = 2:1) yielded compound 2 as a brown-black solid (206 mg) in 35% yield. mp. > 300 °C. IR $\tilde{\nu}$ 2193, 1602,1524, 1314, 1114, 834 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 10.16 (s, 1H), 8.58-8.60 (d, *J* = 8Hz, 2H), 8.24 (s, 1H), 7.59-7.61(d, *J* = 8Hz, 2H), 7.18-7.20 (d, *J* = 8Hz, 1H), 6.91 (s, 1H), 6.82 (s, 1H), 6.60-6.62 (d, *J* = 8Hz, 1H), 2.88-2.91 (m, 2H), 2.55-2.58 (m, 2H), 1.75-1.78 (m, 2H). ^{13}C NMR (101 MHz, C_5D_5N) δ: 161.20, 155.20, 154.43, 150.52, 144.18, 144.11, 138.71, 127.99, 126.89, 125.75, 119.41, 114.16, 112.66, 109.24, 103.03, 99.98, 29.75, 29.16, 26.08, 23.25, 21.00.

Synthesis of N-methylated derivative of compound 2.

Into a reaction flask were added 33 mg of **compound 2** (1 mmol), 107 mg of iodomethane (5 mmol), and 5 mL of DMF. The reaction mixture was stirred at 80 °C under an argon atmosphere overnight. After completion, the mixture was concentrated in vacuo to give a blue crude product, which was purified by column chromatography (ethyl acetate/petroleum ether = 1:1) to afford 40 mg of a blue solid in 85% yield. mp. > 300 °C. IR $\tilde{\nu}$ 2938, 2199, 1637, 1525, 12754, 1186 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 10.62 (br,1H), 8.68-8.67 (d, *J* = 8 Hz, 2H), 8.51 (s,1H), 8.11-8.09 (d, *J* = 8Hz, 2H), 7.39- -7.35 (m, 3H), 7.04 (s,1H), 6.79-6.77(d, *J* = 8 Hz, 2H), 4.22 (s,3H), 2.94(s, 2H), 2.65 (s, 2H), 1.80 (s,2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.65, 160.68, 154.58, 153.95, 151.76, 150.69, 144.78, 142.47, 133.12, 129.23, 125.80, 120.84, 119.38, 118.93, 114.46, 110.80, 103.05, 93.71, 46.88, 28.65, 25.59, 20.79.

HR MS (ESI): m/z calculated for $[C_{22}H_{19}N_2O_2]^+$ 343.1441, found 343.1400.

Synthesis of Compound 3

To a reaction flask were added compound 2 (330 mg, 1.0 mmol), 1-iododododecane (600 mg, 2.0 mmol), and acetonitrile (12 mL). The mixture was stirred under nitrogen atmosphere at room temperature for 30 minutes, then heated to 80 °C and stirred for 6 hours. After the reaction was complete, the mixture was concentrated under reduced vacuum to afford a brown-black oil. Purification by column chromatography (eluent: ethyl acetate/petroleum ether = 3:1) gave compound 3 as a brown-black solid (230 mg) in 46% yield. mp. 127-129 °C. IR $\tilde{\nu}$ 2920, 2851, 2177, 1620, 1518, 1445, 1255, 1129, 840. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 8.61-8.61 (d, *J* = 8Hz, 2H), 8.35 (s, 1H), 7.92-7.94 (d, *J* = 8Hz, 2H), 7.34-7.36 (d, *J* = 8Hz, 2H), 6.91 (s, 1H), 6.70-6.72 (d, *J* = 8Hz, 1H), 4.38-4.41 (m, 2H), 2.91-2.94 (m, 2H), 2.62-2.65 (m, 2H), 1.76-1.87 (m, 4H), 1.25-1.27 (m, 18H), 0.81-0.86(m, 3H). ^{13}C NMR (101 MHz, C_5D_5N) δ: 160.16, 157.20, 152.07, 150.18, 149.10, 140.98, 136.79, 135.79, 134.76, 129.64, 123.77, 122.73, 120.24, 117.66, 115.44, 103.65, 58.43, 53.35, 31.87, 31.12, 29.63, 29.54, 29.43, 29.35, 29.08, 28.14, 26.13, 26.02, 22.69, 21.28, 14.04. HR MS (ESI): m/z calculated for $[C_{33}H_{41}N_2O_2]^+$ 497.3162, found 497.3170.

Synthesis of probe DHX-HOCl-V

To a reaction flask were added compound 3 (75 mg, 0.15 mmol), dichloromethane (8 mL), dimethylcarbamothioic chloride (185 mg, 1.5 mmol), and N, N-diisopropylethylamine (0.1 mL). The reaction mixture was stirred under a nitrogen atmosphere at room temperature for 24 hours, and the progress was monitored by TLC. After completion, the mixture was quenched with water (10 mL) and extracted with dichloromethane. The organic layer was washed with water (10 mL × 3) and concentrated under reduced pressure to give a brown oil. Purification by column chromatography (eluent: ethyl acetate/petroleum ether = 3:1) afforded **DHX-HOCl-V** as a brown solid (43 mg) in 49 % yield. mp. 89-91 °C. IR $\tilde{\nu}$ 2921, 2850, 2220, 1636, 1471, 1273,1122. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.92 (s, 2H), 8.47 (s, 1H), 8.07 (s,

2H), 7.71 (s, 1H), 7.32-7.34 (d, J = 8 Hz, 1H), 7.05 (s, 1H), 6.99-7.01(d, J = 8 Hz, 1H), 4.70 (s, 1H), 3.45-3.50 (m, 6H), 3.05-3.08 (m, 2H), 2.70-2.72 (m, 2H), 1.90-1.97(m, 6H), 1.23-1.26 (m, 18H), 0.86-0.89 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 186.70, 160.10, 156.18, 153.04, 152.20, 143.75, 142.93, 130.98, 129.34, 127.24, 121.64, 120.57, 119.33, 117.84, 112.34, 112.09, 95.66, 60.96, 43.57, 39.58, 34.70, 31.91, 31.75, 29.60, 29.52, 29.39, 29.34, 29.13, 26.20, 25.51, 22.70, 20.62, 17.41, 14.15. HR MS (ESI): m/z calculated for $[C_{36}H_{46}N_3O_2S]^+$ 584.3305, found 584.3164.

3. Supplemental figures

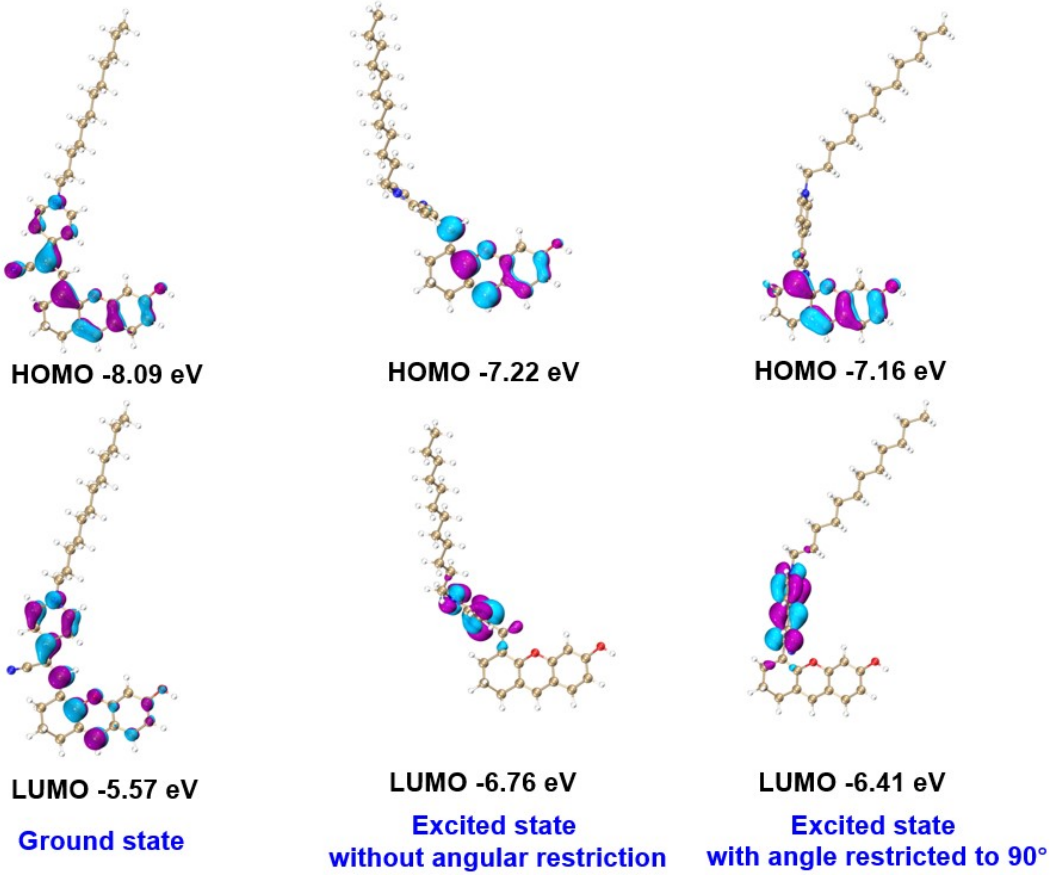


Fig. S1 HOMO and LUMO of **compound 3** at the minimum energy structures of compound 3 in electronic ground and excited states. Geometries were optimized at the B3LYP-D3/6-31G(d) level.

DFT calculations indicate that photoexcitation of **compound 3** (the product after reaction of probe **DHX-HOCl-V** with HOCl) from the S_0 to the S_1 state is primarily governed by electron transitions from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO). The HOMO is largely localized

on the dihydroxanthene group, whereas the LUMO is mainly situated on the pyridinium unit. The frontier molecular orbital diagram reveals a distinct charge transfer from the dimethylaniline moiety to the pyridinium unit, indicative of a typical twisted intramolecular charge transfer (TICT) process. Based on the discussion above, it can be concluded that **compound 3** functions as an excellent viscosity-sensitive fluorescent probe operating via the TICT mechanism.

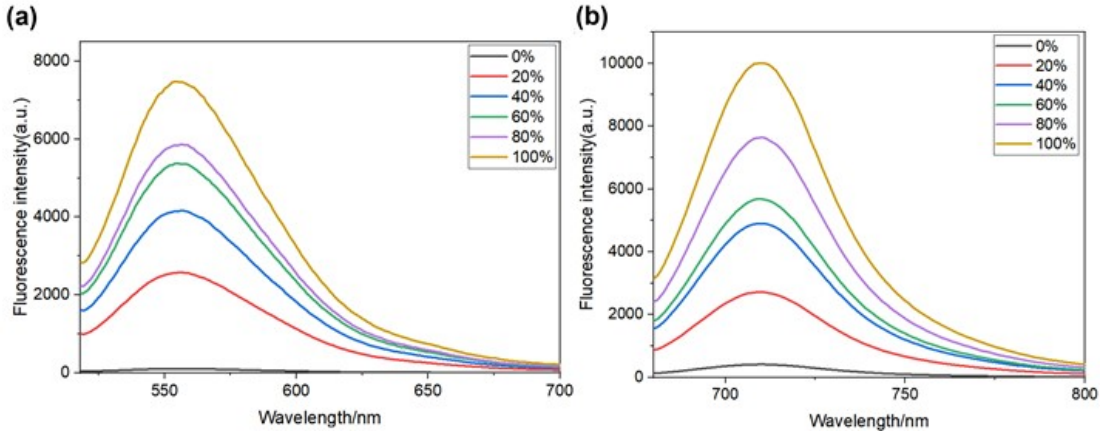


Fig. S2 (a) Fluorescence spectra of **compound 2** (10 μM) in mixed solvents with different proportions of PBS and glycerol. λ_{ex} = 490 nm. (b) Fluorescence spectra of **N-methylated compoud 2** (10 μM) in mixed solvents with different proportions of PBS and glycerol. λ_{ex} = 660 nm.

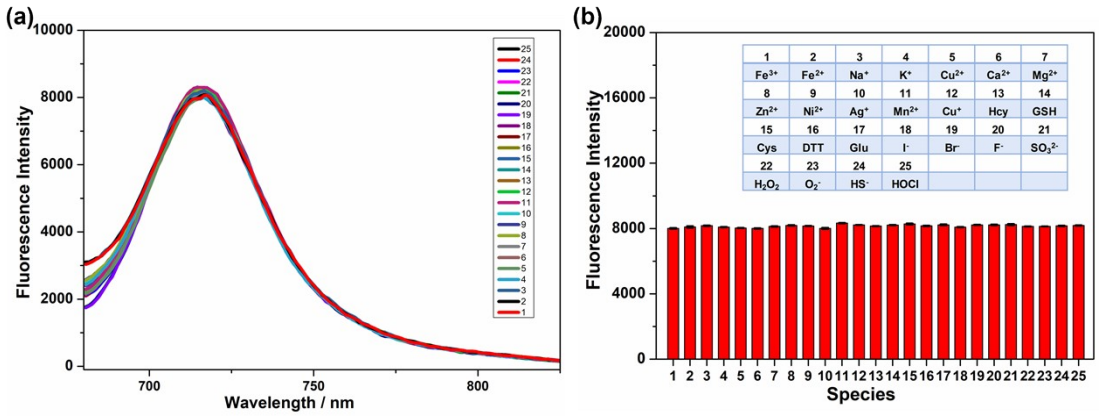


Fig. S3. Fluorescence response of **DHX-HOCl-V** (10 μM) with addition of HOCl (60 μM) in the presence of various analytes in 80 % glycerol. λ_{ex} = 660 nm. Interfering substances at the following concentrations: 200 μM: Glu, NaHS, Na_2SO_3, H_2O_2, HClO, KO_2, metal ions (Fe^{3+}, Fe^{2+}, Na^+, K^+, Cu^{2+}, Ca^{2+}, Mg^{2+}, Zn^{2+}, Ni^{2+}, Ag^+, Mn^{2+}), and halide anions (I^-, Br^-, F^-).1 mM: GSH, Cys, Hcy, DTT;

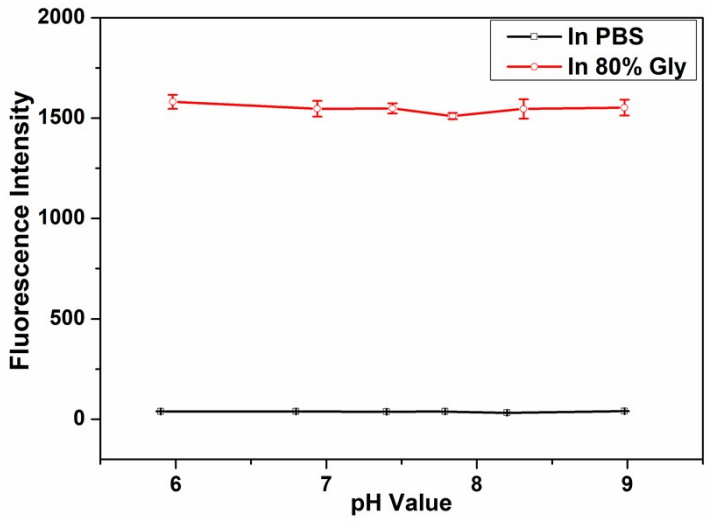


Fig. S4. Stability of **DHX-HOCl-V** (10 μM) with the addition of HOCl (60 μM) at different pH.

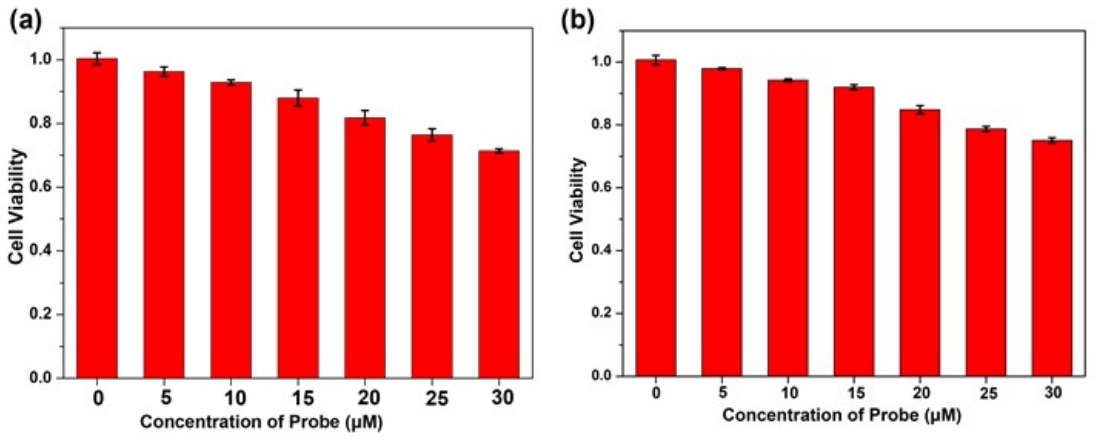


Fig. S5. MTT assay of HeLa cells (a) and HepG2 cells (b) in the presence of different concentrations of **DHX-HOCl-V**

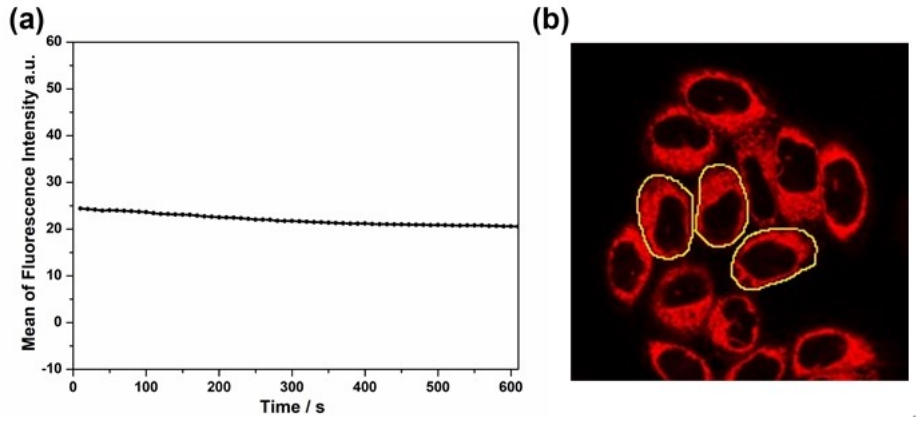


Fig. S6. Test of photostability of **DHX-HOCl-V** in HeLa cells. Confocal fluorescence images (0-600 s) were achieved by means of time-sequential scanning of the **DHX-**

HOCl-V (10 μM)-loaded HeLa cells.

4. References

[1] M. J. Frisch, et al., Gaussian 16, Revision C.01, Gaussian, Inc., Wallingford, CT, 2016.

[2] S. Grimme, et al., A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu, *J. Chem. Phys.*, 2010, **132**, 154104.

[3] T. Lu, F. Chen, Multiwfn: A multifunctional wavefunction analyzer, *J. Comput. Chem.*, 2012, **33**, 580-592.

[4] W. Humphrey, et al., VMD: Visual molecular dynamics, *J. Mol. Graph.*, 1996, **14**, 33-38.

5. ^{1}H NMR, ^{13}C NMR and HR MS spectra

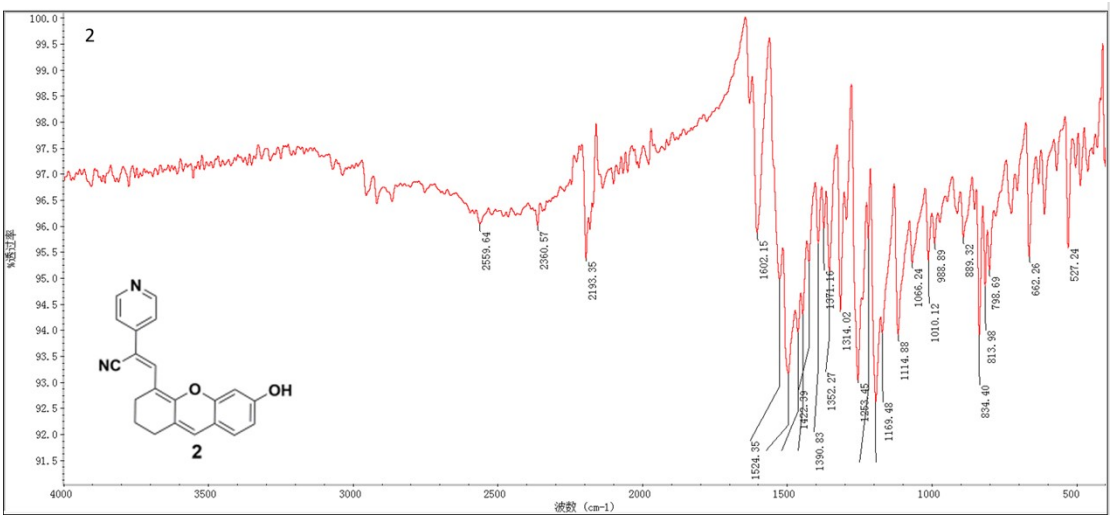


Fig. S7 IR spectrum of compound **2**

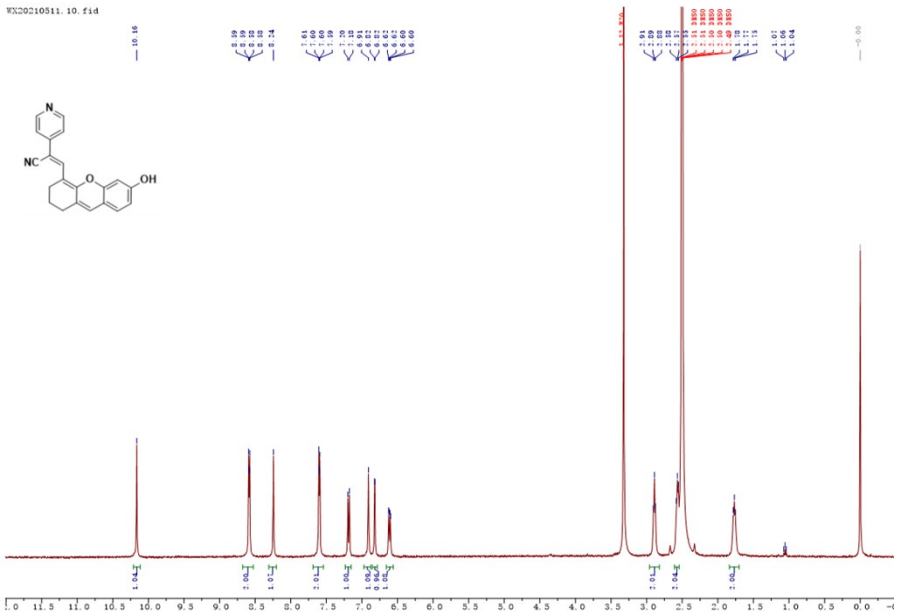


Fig. S8 ^{1}H NMR spectrum of **compound 2** in DMSO-d_6 (400 MHz).

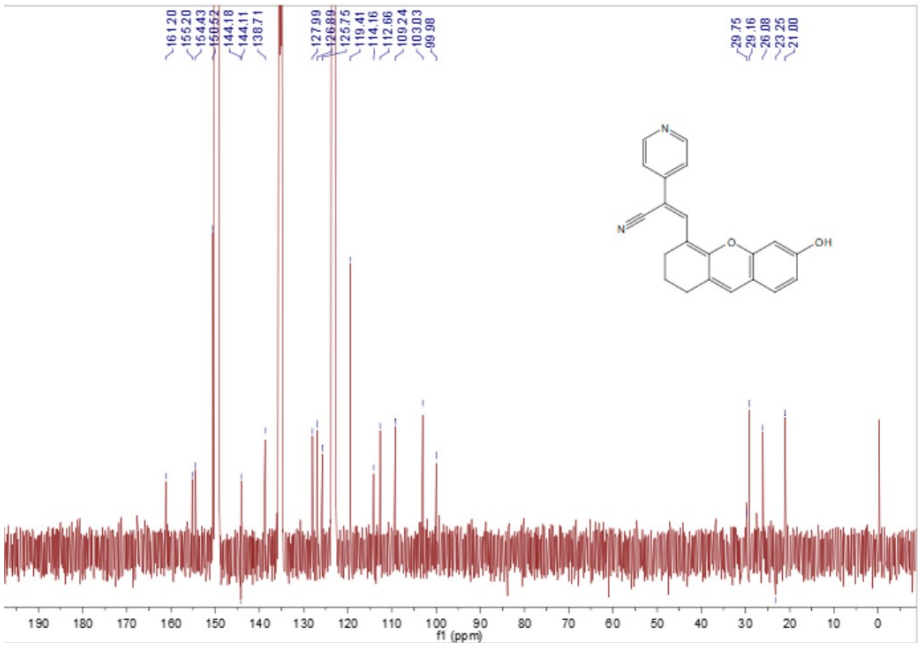


Fig. S9 ^{13}C NMR spectrum of **compound 2** in C_5D_5N (101 MHz)

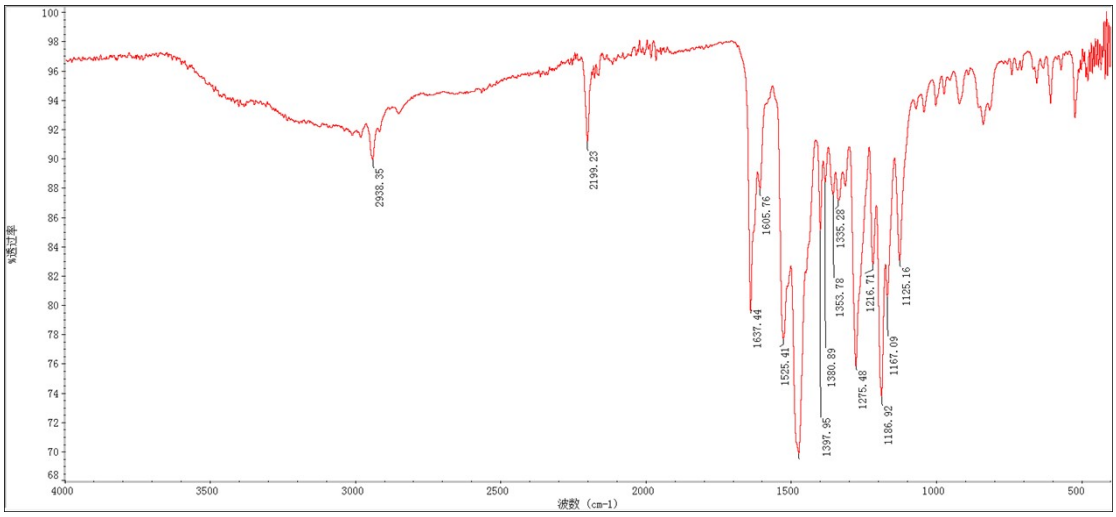


Fig. S10 IR spectrum of **N-methylated compound 2**

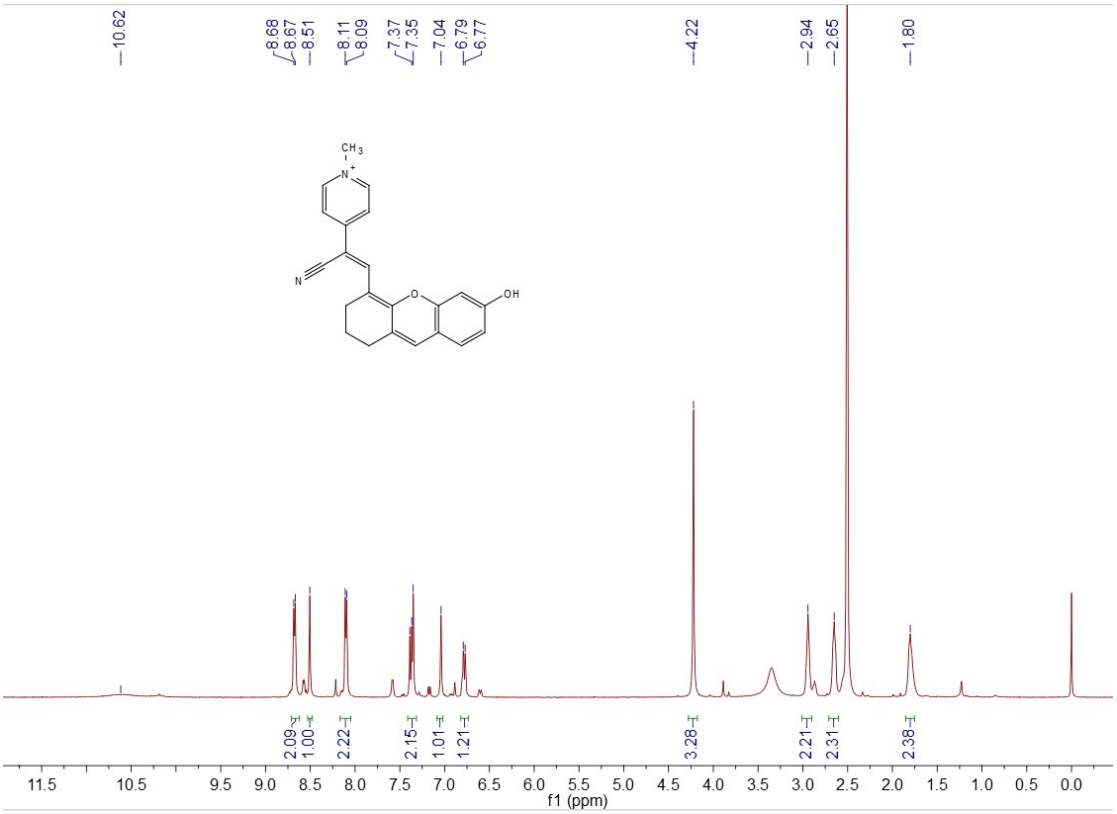


Fig. S11 ^{1}H NMR spectrum of **N-methylated compound 2** in DMSO-d_6 (400 MHz)

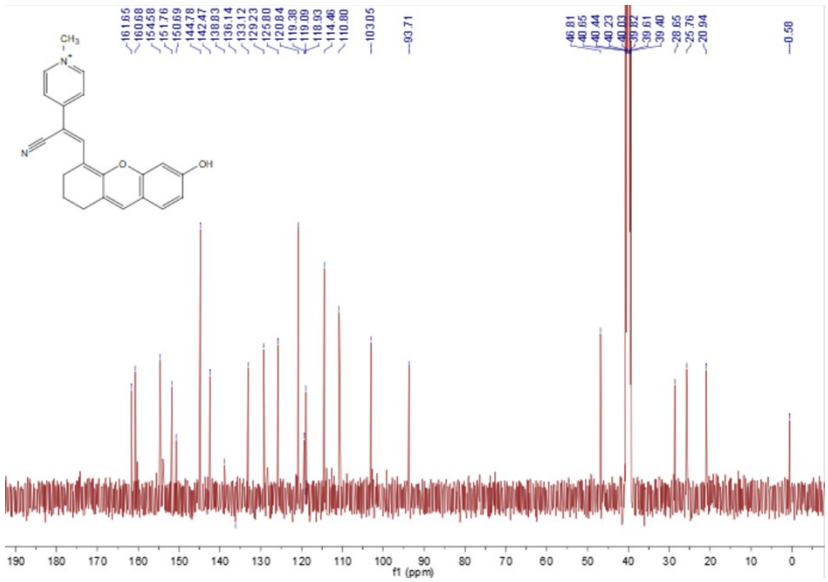


Fig. S12 ^{13}C NMR spectrum of **N-methylated compound 2** in DMSO-d_6 (101MHz)

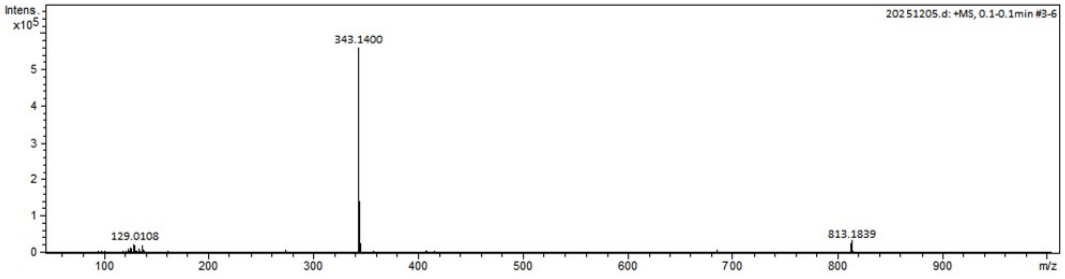


Fig. S13 HR MS spectrum of **N-methylated derivative of compound 2**

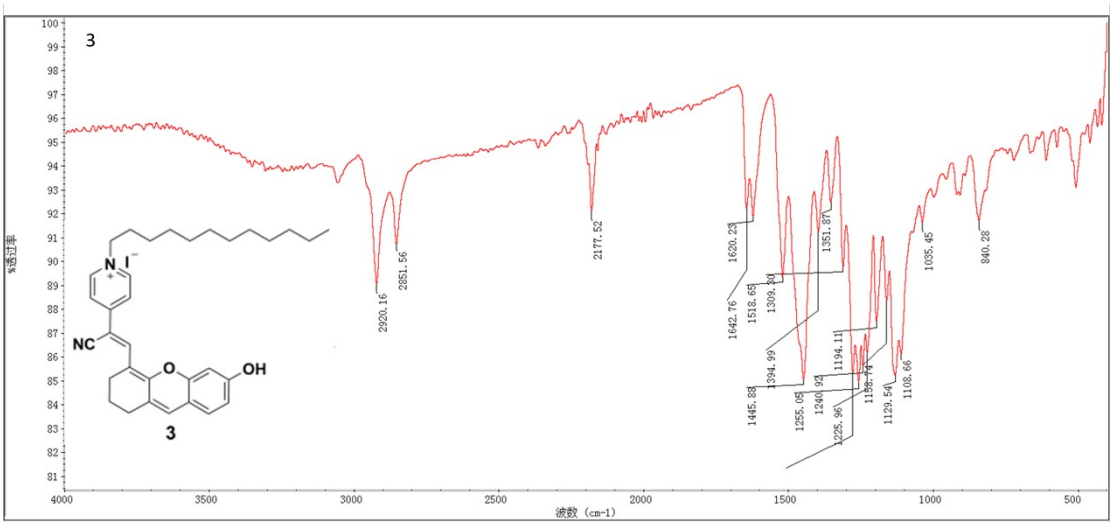


Fig. S14 IR spectrum of **compound 3**

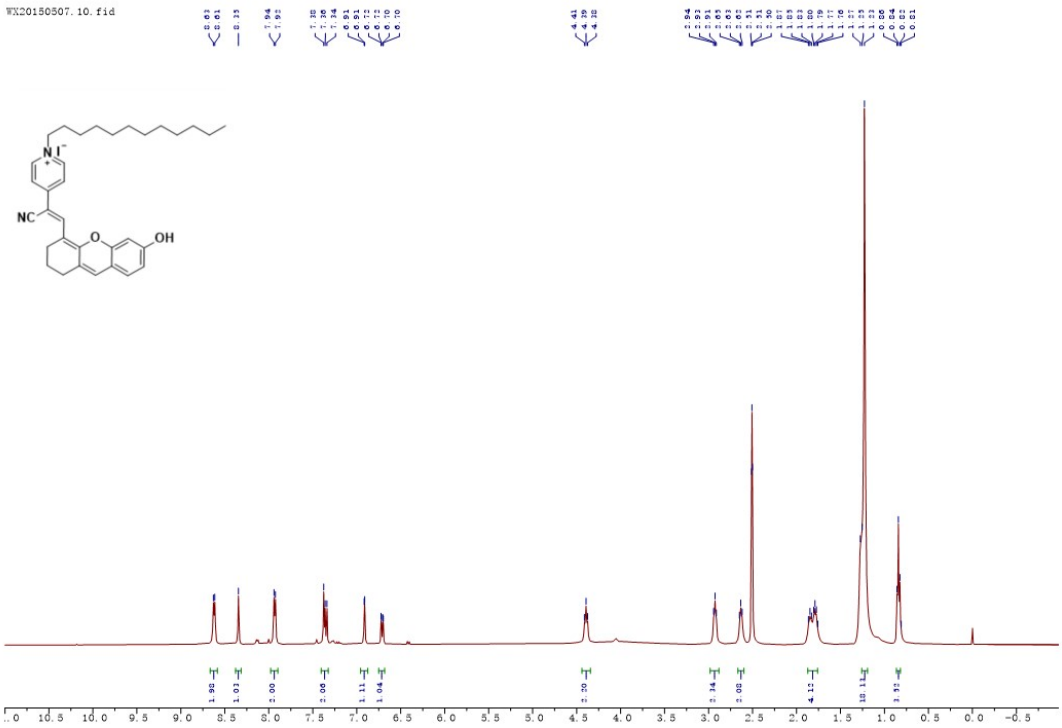


Fig. S15 ^{1}H NMR spectrum of **compound 3** in DMSO-d_6 (400 MHz).

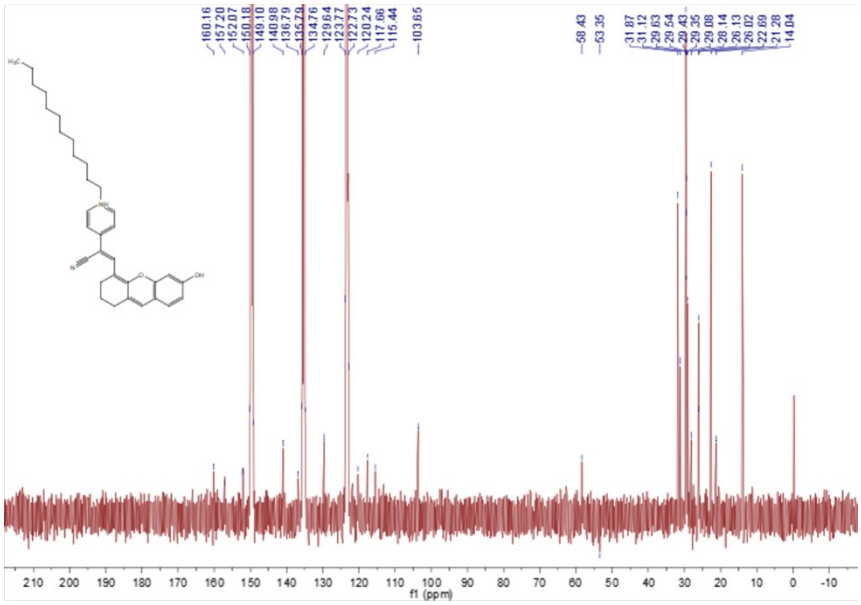
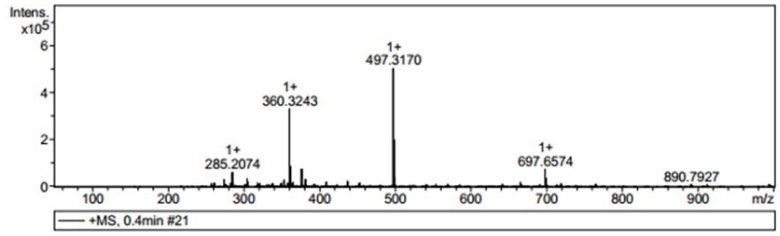


Fig. S16 ^{13}C NMR spectrum of **compound 3** in C_5D_5N (101 MHz)



#	m/z	I	I %	S/N	Res.	FWHM
1	261.1310	16787	3.3	1526.1	20932	0.0125
2	274.2741	31407	6.3	2855.2	20118	0.0136
3	285.2074	62334	12.4	5666.7	23164	0.0123
4	304.2613	34275	6.8	3115.9	22233	0.0137
5	305.1564	22563	4.5	2051.2	21316	0.0143
6	318.3003	18205	3.6	1655.0	22674	0.0140
7	321.1314	14523	2.9	1320.3	22262	0.0144
8	338.3416	15027	3.0	1366.1	24066	0.0141
9	349.1810	15884	3.2	1444.0	20003	0.0175
10	353.2656	28699	5.7	2609.0	21656	0.0163
11	358.3078	17122	3.4	1556.5	20111	0.0178
12	360.3243	330525	65.8	30047.7	24596	0.0146
13	361.3272	88183	17.6	8016.6	22880	0.0158
14	362.3302	17538	3.5	1594.4	18389	0.0197
15	365.1573	19050	3.8	1731.8	20607	0.0177
16	376.2982	75663	15.1	6878.5	22957	0.0164
17	377.3013	19671	3.9	1788.3	21702	0.0174
18	381.2975	33876	6.7	3079.6	21953	0.0174
19	409.1833	20561	4.1	1869.2	21328	0.0192
20	437.1930	23463	4.7	2133.0	14928	0.0293
21	453.1705	15411	3.1	1401.0	20843	0.0217
22	453.2069	17142	3.4	1558.4	19981	0.0227
23	497.2359	15811	3.1	1437.4	21120	0.0235
24	497.3170	502414	100.0	45674.0	27930	0.0178
25	498.3196	200392	39.9	18217.5	25101	0.0199
26	499.3222	39714	7.9	3610.4	20883	0.0239
27	665.5033	19250	3.8	1750.0	21246	0.0313
28	697.6574	75968	15.1	6906.2	23663	0.0295
29	698.6607	39002	7.8	3545.6	22004	0.0304
30	718.6308	14316	2.8	1301.5	22390	0.0321

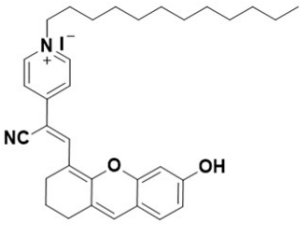


Fig. S17 HR MS spectrum of **compound 3**

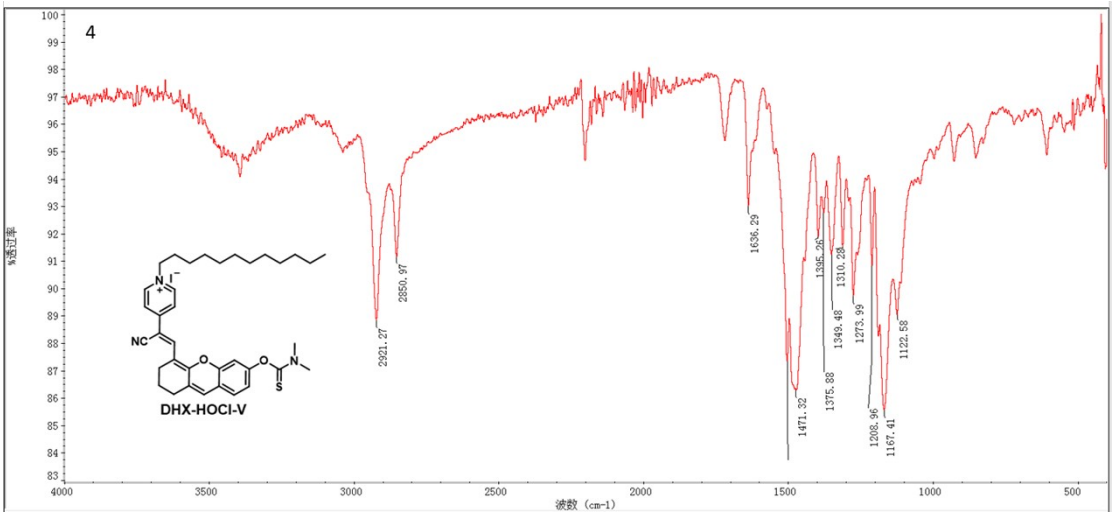


Fig. S18 IR spectrum of compound **DHX-HOCl-V**

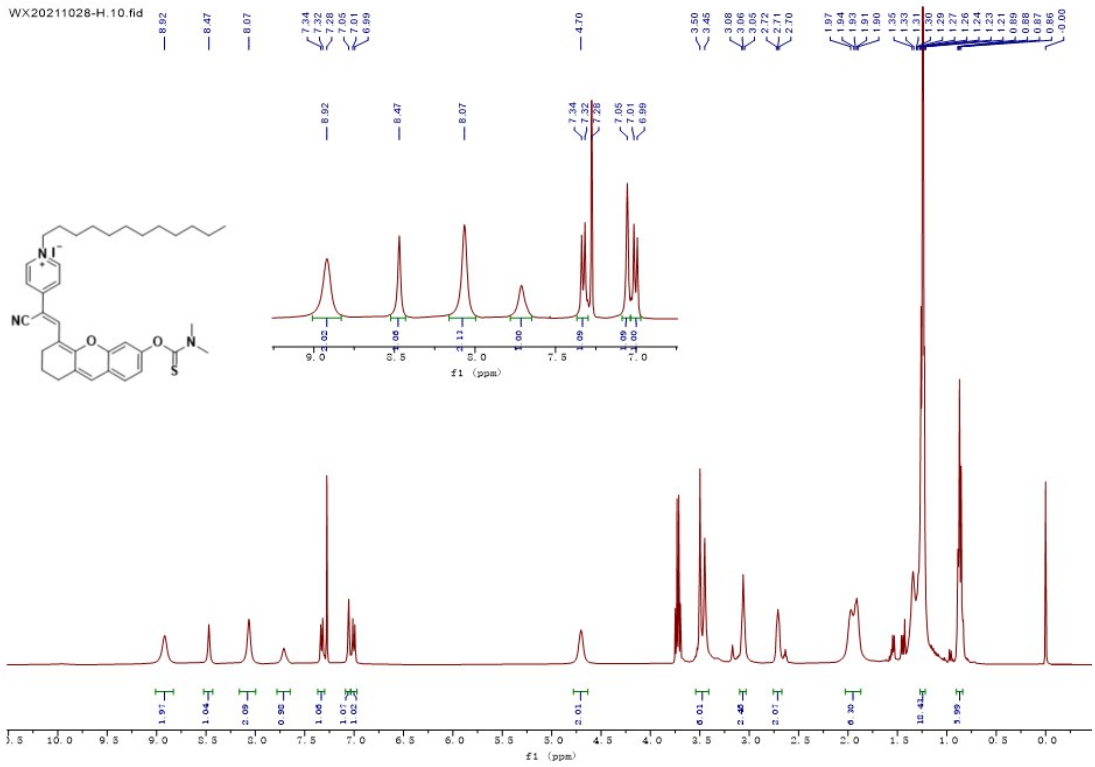


Fig. S19 ^{1}H NMR spectrum of compound **DHX-HOCl-V** in $CDCl_3$ (400 MHz).

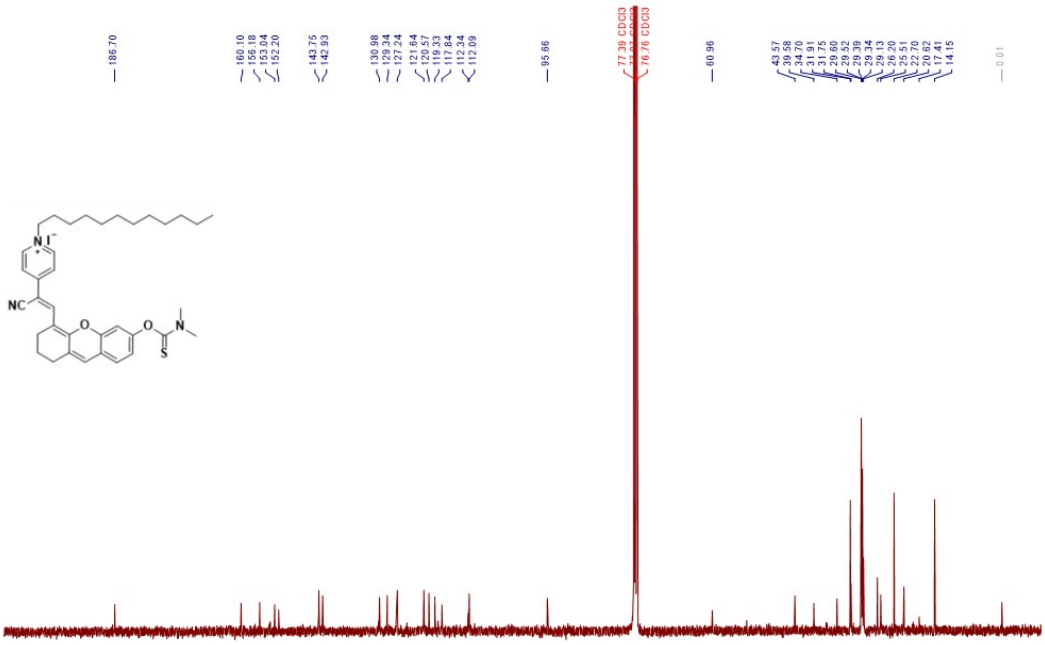
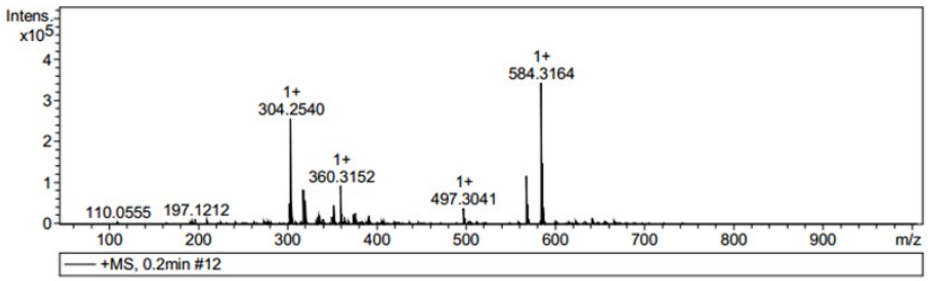


Fig. S20 ^{13}C NMR spectrum of compound **DHX -HOCl-V** in $CDCl_3$ (100 MHz).



#	m/z	I	I %	Area	A %	S/N	Res.
1	197.1212	11756	3.4	148	1.6	246.0	17542
2	302.2384	49565	14.4	807	8.9	672.7	21649
3	304.2540	255900	74.5	3954	43.7	3468.8	22037
4	305.2572	53258	15.5	929	10.3	721.6	19972
5	318.2323	84589	24.6	1543	17.0	1108.7	20569
6	319.2353	17286	5.0	366	4.0	226.3	19073
7	320.2462	58225	16.9	1420	15.7	760.8	18333
8	321.2491	12992	3.8	323	3.6	169.7	17687
9	334.2218	17879	5.2	510	5.6	227.7	13351
10	336.2400	21695	6.3	552	6.1	274.9	21303
11	350.2571	16521	4.8	361	4.0	203.1	18749
12	352.2368	45165	13.1	957	10.6	552.5	21305
13	360.3152	92817	27.0	1702	18.8	1122.0	23459
14	361.3181	23605	6.9	463	5.1	285.3	21624
15	364.2363	17338	5.0	391	4.3	209.3	19013
16	374.2939	24726	7.2	535	5.9	292.7	20883
17	376.3067	26566	7.7	657	7.2	313.6	20186
18	391.3191	19584	5.7	424	4.7	227.1	21582
19	392.3044	14803	4.3	501	5.5	171.4	16958
20	497.3041	39322	11.4	1185	13.1	387.6	20420
21	498.3068	15054	4.4	469	5.2	148.3	19623
22	568.3394	117989	34.3	3371	37.2	1034.1	23164
23	569.3426	48636	14.2	1542	17.0	426.1	22791
24	570.3453	12771	3.7	410	4.5	111.9	22251
25	584.3164	343657	100.0	9057	100.0	2945.4	26739
26	585.3195	148605	43.2	4624	51.1	1272.2	23030
27	585.5176	30679	8.9	1141	12.6	262.6	19865
28	586.3190	41250	12.0	1648	18.2	353.2	17669
29	586.5215	12835	3.7	491	5.4	109.9	20640
30	641.5799	16018	4.7	538	5.9	130.4	22548

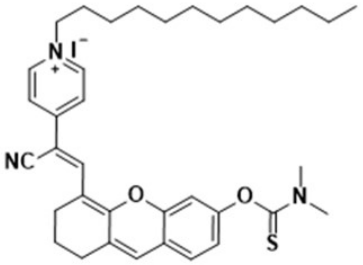


Fig. S21 HR MS spectrum of **DHX -HOCl-V**