Supporting information

Fluoralbumin, an engineered vehicle for drug analysis

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Materials and Methods

Materials. Bovine serum albumin was purchased from Innochem. Albumin was purchased from Psaitong. The 4-12% SDS-PAGE Precast Gel, 8% Native-PAGE Precast Gel, Prestained Color Protein Marker (15-120 kD, 10-170 kD), Coomassie Blue Super-Fast Staining Solution and 12% SDS-PAGE Gel Super-Quick Preparation Kit and the related materials were all purchased from Beyotime. DL-dithiothreitol, iodoacetamide and formic acid were purchased from Sigma (St. Louis, MO, USA), trypsin and chymotrypsin were purchased from Promega (Madison, WI, USA). All chemicals were purchased from commercial suppliers and used without further purification. All solvents were purified prior to use. Distilled water was used after passing through a water ultra-purification system. TLC analysis was performed using precoated silica plates.

Hitachi F-7000 fluorescence spectrophotometer was employed to measure fluorescence spectra. Hitachi U-3900 UV-vis spectrophotometer was employed to measure UV-vis spectra. Shanhai Huamei Experiment Instrument Plants provided a PO-120 quartz cuvette (10 mm). ^{1}H NMR and ^{13}C NMR experiments were performed with a BRUKER AVANCE II HD 600 MHz and151 MHz NMR spectrometer, respectively (Bruker, Billerica, MA). Coupling constants (J values) are reported in hertz. HR-MS determinations were carried out on a Thermo Scientific Q Exactive Instrument. Ultimate 3000 system coupled with a Q Exactive™ Hybrid Quadrupole-Orbitrap™ Mass Spectrometer (Thermo Fisher Scientific, USA) with an ESl nano-spray source were used in the protein modification site analysis experiment, The BlO-RAD Mini-PROTEAN Tetra Cell was used in the electrophoresis experiments. The corresponding fluorescent images and Coomassie blue staining images were obtained by a BlO-RAD ChemiDoc XRS+ Imaging System. Cell imaging experiments were performed with a ZEISS LSM-710 Confocal Fluorescence Microscopy.

Preparation of solutions of probes and analytes. Stock solution of the dyes (2 mM) were prepared in DMSO. Stock solutions of other analytes were prepared by direct dissolution in deionized water. All chemicals used were of analytical grade.

General fluorescence spectra measurements. The detection experiments were measured in PBS (pH 7.4, 10 mM). The procedure was as follows: into a PBS solution, containing 5 μM Dyes, an analyte sample was added. The process was monitored by fluorescence spectrometer. All of the fluorescent spectra were obtained 10 min after analytes added.

Cell culture and imaging. The HCT-116 cells were grown in 1640 medium supplemented with 12% FBS and 1% antibiotics at 37 °C in humidified environment of 5% CO_2. Cells were plated on a 6-well plate with slides and allowed to adhere for 24 h. Before the experiments, cells were washed with PBS 3 times. The fluorescent images were obtained by a ZEISS LSM-710 Confocal Fluorescence Microscopy.

In-gel digestion. Gel pieces were destained in 50 mM NH_4HCO_3 in 50% acetonitrile (v/v) until clear. Gel pieces were dehydrated with acetonitrile (100 μL) for 5 min. After the liquid removed, the gel pieces were rehydrated in 10 mM dithiothreitol and incubated at 56 °C for 1 h. Gel pieces were then dehydrated in acetonitrile again. After removing the liquid, gel pieces were rehydrated with 55 mM iodoacetamide and incubated for 45 min at room temperature in the dark. The gel pieces

were washed with 50 mM NH_4HCO_3 and dehydrated with acetonitrile. Finally, resuspend the gel block with 50 mM ammonium bicarbonate containing 10 ng/μL trypsin, and incubate on ice for 1 h. After removing the excess solution from the sample, the gel block was digested overnight at 37 °C. The peptides after enzymatic hydrolysis were used to extract the gel pieces with 50% acetonitrile/5% formic acid and acetonitrile in turn, and the peptide solution was freeze-dried and resuspended in 2% acetonitrile/0.1% formic acid.

LC-MS/MS analysis. The peptides were dissolved in the mobile phase A of liquid chromatography and then separated using the EASY-nLC 1000 ultra-high performance liquid system. Mobile phase A is an aqueous solution containing 0.1% formic acid and 2% acetonitrile; mobile phase B is an aqueous solution containing 0.1% formic acid and 90% acetonitrile. Liquid phase gradient setting: 0-16min, 9%~25% phase B; 16-22min, 25%~40% phase B; 22-26min, 40%~80% phase B; 26-30min, 80% phase B. The flow rate is maintained at 450 nL/min.

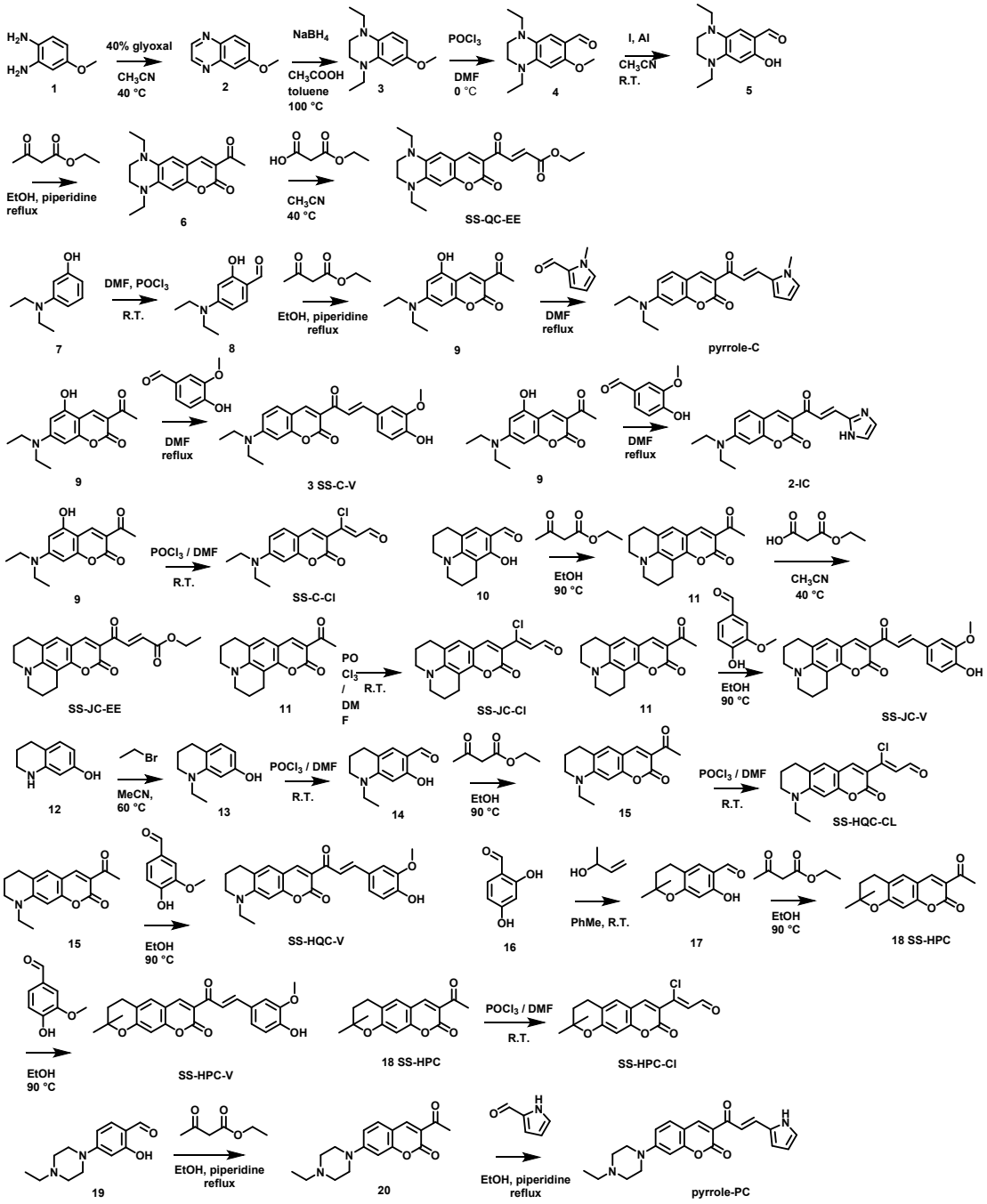
The peptides were separated by the ultra-high performance liquid system and injected into the NSI ion source for ionization and then analyzed by Thermo Scientific ^{TM}Q Exactive mass spectrometry. The ion source voltage was set to 2.2 kV, and the peptide precursor ions and their secondary fragments were detected and analyzed by high-resolution Orbitrap. The scanning range of the primary mass spectrometer was set to 350-1800 m/z, the scanning resolution was set to 70,000; the secondary scanning resolution was set to 17,500. The data acquisition mode uses the data-dependent scanning (DDA) program, that was, after the first-level scan, the first 20 peptide precursor ions with the highest signal intensity were selected to enter the HCD collision cell and use 28% of the fragmentation energy for fragmentation. Same parameters were used for the secondary mass spectrometry analysis. A data-dependent procedure that alternated between one MS scan followed by 20 MS/MS scans with 15.0 s dynamic exclusion. Automatic gain control (AGC) was set at $5e^4$.

Data processing. The resulting MS/MS data were processed using Proteome Discoverer 1.3. Tandem mass spectra were searched against Homo Sapiens (SwissProt, 20366 sequences) data base. Trypsin/p was specified as cleavage enzyme allowing up to 2 missing cleavages. Mass error was set to 10 ppm for precursor ions and 0.02 Da for fragment ions. Carbamidomethyl on Cys was specified as fixed modification. Oxidation on Met and protein N-terminal acetylation were specified as variable modification. Peptide confidence was set at high, and peptide ion score was set > 20. Fluorescence imaging was performed using a laser confocal microscope - Zeiss 880, and post-processing was carried out using ImageJ.

Synthesis of the probes

Scheme S1. **SS-1** and **SS-QC-ACl** was synthesized based on the reported procedure.[1]

Scheme S2. Synthesis of dyes.



SS-QC-EE: SS-QC-EE was synthesized based on the reported procedure with minor modification.[2]

SS-JC-V: In details, 0.5 mmol compound **11** and 0.7 mmol vaniline was dissolved in 20 ml EtOH. 3 drops piperidine was then added. The resulting mixture was refluxed for 70 h under Argon atmosphere. After cooling to room temperature, the solvent was removed under reduced pressure and the residue was separated by column chromatography using EtOAc/PE (1/1) as eluent to obtain SS-JC-V. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.46 (s, 1H), 8.06 (d, *J* = 15.6 Hz, 1H), 7.77 (d, *J* = 15.6 Hz, 1H), 7.22 (d, *J* = 1.9 Hz, 1H), 7.19 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.01 (s, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 3.95 (s, 3H), 3.35 (q, *J* = 5.9 Hz, 4H), 2.91 (t, *J* = 6.4 Hz, 2H), 2.77 (t, *J* = 6.3 Hz, 2H),

1.99 (q, *J* = 6.1 Hz, 5H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.59, 161.43, 153.66, 148.66, 148.58, 148.00, 146.74, 143.23, 128.30, 127.68, 124.24, 122.89, 119.54, 114.59, 109.57, 108.65, 105.72, 56.00, 50.37, 49.98, 27.44, 21.19, 20.25, 20.07.

SS-JC-Cl: Add 1.0 mL of $POCl_3$ dropwise into 1.0 mL of DMF while keeping the mixture in an ice bath, and stir at 0 °C for 15 minutes. Then, add compound **11** (0.30 mmol). After reacting at room temperature for 3 hours, quench the reaction by adding 20 mL of water. Adjust the pH of the mixture to neutral using sodium bicarbonate, extract with CH_2Cl_2, and dry the organic layer over anhydrous sodium sulfate. Perform column chromatography using ethyl acetate/petroleum ether (V/V = 1:1) as the eluent to obtain compound **SS-JC-Cl**. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 10.26 (d, *J* = 6.9 Hz, 1H), 8.27 (s, 1H), 7.68 (d, *J* = 6.9 Hz, 1H), 6.98 (s, 1H), 3.35 (dt, *J* = 8.5, 5.9 Hz, 4H), 2.88 (t, *J* = 6.4 Hz, 2H), 2.79 – 2.75 (m, 2H), 1.98 (dtt, *J* = 8.4, 6.3, 2.5 Hz, 4H). ^{13}C NMR (151 MHz, CDCl3) δ 192.54, 158.67, 151.95, 148.45, 145.77, 144.85, 126.92, 125.65, 119.62, 111.77, 108.32, 105.67, 50.32, 49.94, 27.45, 21.16, 20.17, 20.04.

SS-HQC-V: SS-HQC-V was synthesized based on a similar procedure with **SS-JC-V.** ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.49 (s, 1H), 8.03 (d, *J* = 15.6 Hz, 1H), 7.78 (d, *J* = 15.6 Hz, 1H), 7.21 (d, *J* = 8.6 Hz, 2H), 7.11 (s, 1H), 6.93 (d, *J* = 7.9 Hz, 1H), 6.42 (s, 1H), 5.89 (s, 1H), 3.96 (s, 3H), 3.46 – 3.40 (m, 4H), 2.77 (t, *J* = 6.3 Hz, 2H), 1.98 (t, *J* = 6.1 Hz, 2H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.47, 161.17, 157.85, 150.82, 148.31, 148.05, 146.74, 143.50, 129.45, 128.23, 124.13, 122.76, 120.87, 116.52, 114.63, 109.85, 108.63, 95.38, 56.07, 48.83, 46.24, 27.47, 21.45, 10.92.

SS-HQC-CI: SS-HQC-CI was synthesized based on a similar procedure with **SS-JC--Cl.** ^{1}H NMR (600 MHz, Chloroform-*d*) δ 10.27 (d, *J* = 6.9 Hz, 1H), 8.31 (s, 1H), 7.68 (d, *J* = 6.9 Hz, 1H), 7.10 (s, 1H), 6.41 (s, 1H), 3.43 (dd, *J* = 6.9, 4.7 Hz, 4H), 2.78 (t, *J* = 6.3 Hz, 2H), 2.02 – 1.94 (m, 2H), 1.23 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 192.43, 158.54, 156.07, 150.65, 145.44, 144.55, 128.74, 125.96, 121.00, 112.59, 108.30, 95.24, 48.80, 46.26, 27.49, 21.43, 10.89.

SS-HPC: Compound **17** (6.0 mmol), ethyl acetoacetate (9.0 mmol), and 0.2 mL of piperidine were dissolved in 40 mL of anhydrous ethanol. The mixture was refluxed for 10 hours and then cooled to room temperature. The solvent was removed under reduced pressure, and the resulting solid precipitate was collected. The final product, compound **SS-HPC**, was obtained by recrystallization from anhydrous ethanol. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.44 (s, 1H), 7.32 (s, 1H), 6.72 (s, 1H), 2.85 (t, *J* = 6.7 Hz, 2H), 2.69 (s, 3H), 1.87 (t, *J* = 6.7 Hz, 2H), 1.38 (s, 6H). ^{13}C NMR (151 MHz, CDCl3) δ 195.78, 160.71, 160.08, 155.85, 147.79, 131.06, 120.35, 119.59, 111.74, 104.27, 76.76, 32.24, 30.66, 26.99, 21.83.

SS-HPC-Cl: SS-HPC-V was synthesized based on a similar procedure with **SS-JC- Cl** ^{1}H NMR (600 MHz, Chloroform-*d*) δ 10.30 (d, *J* = 6.8 Hz, 1H), 8.44 (s, 1H), 7.69 (d, *J* = 6.8 Hz, 1H), 7.36 (s, 1H), 6.76 (s, 1H), 2.89 (t, *J* = 6.7 Hz, 2H), 1.90 (t, *J* = 6.7 Hz, 2H), 1.41 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 192.20, 160.50, 157.85, 154.10, 144.87, 144.17, 130.20, 127.86, 119.77, 117.41, 111.87, 104.17, 32.24, 26.98, 21.88.

SS-HPC-V: **SS-HPC-V** was synthesized based on a similar procedure with **SS-JC-V**. ^{1}H NMR

(600 MHz, Chloroform-*d*) δ 8.53 (s, 1H), 7.90 (d, *J* = 15.6 Hz, 1H), 7.80 (d, *J* = 15.6 Hz, 1H), 7.35 (s, 1H), 7.21 (dd, *J* = 8.2, 1.9 Hz, 1H), 7.20 (d, *J* = 1.9 Hz, 1H), 6.94 (d, *J* = 8.1 Hz, 1H), 6.75 (s, 1H), 5.91 (s, 1H), 3.96 (s, 3H), 2.86 (t, *J* = 6.7 Hz, 2H), 1.88 (t, *J* = 6.7 Hz, 2H), 1.40 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.44, 160.51, 160.24, 155.69, 148.42, 148.35, 146.77, 144.69, 130.83, 127.81, 124.51, 122.02, 121.27, 119.54, 114.70, 112.16, 109.74, 104.27, 76.71, 56.05, 32.28, 27.00, 21.86.

Additional figures

Fig. S1. Fluorescence modulation of HSA and **SS-HQC-V**, **SS-JC-V**, **SS-JV-Cl**, **SS-QC-Cl**. Fluorescence spectrum changes of **SS-HQC-V** (A), **SS-JC-V** (B), **SS-JV-Cl** (C) and **SS-QC-Cl** (D) (5 μM) reaction with 1 mg/mL HSA in the presence of NEM (800 μM).

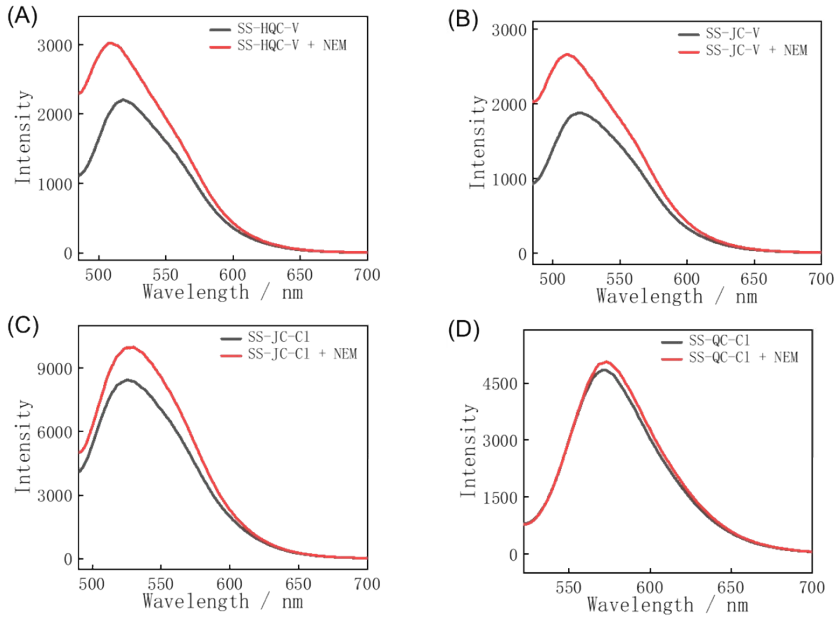


Fig. S2 Optical responses of **SS-JC-Cl** toward HSA. (A) UV-vis absorption changes upon addition of 1 mg mL^{-1} HSA into a 10 μM SS-JC-Cl containing PBS system. (B) The corresponding changes in the fluorescence spectra. (C) UV-vis absorption changes upon addition of 1 mg mL^{-1} HSA into a 10 μM SS-JC-Cl containing Different polar solvents. (D) K_a evaluation obtained by the area of fluorescence spectra (500-600 nm). Error bars represent standard deviations obtained from three independent experiments. λ_{ex} = 475 nm; λ_{em} = 500-700 nm; slit 5/5 nm; 600 V. (E) The change of fluorescence intensity with time at 522 nm. (F) The corresponding changes in the fluorescence spectra about (C). λ_{ex} = 475 nm; λ_{em} = 500-700 nm; slit 2.5/2.5 nm; 600 V.

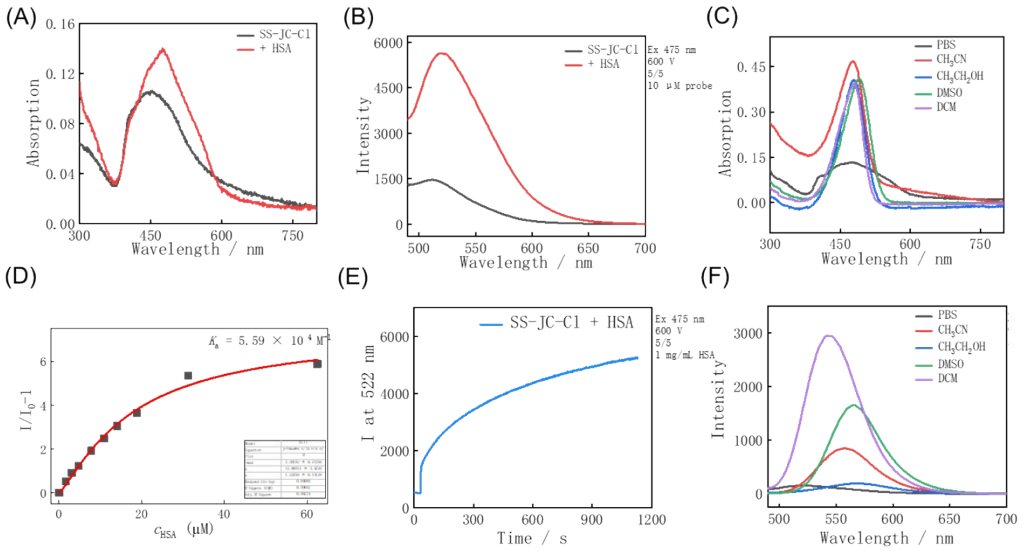


Fig. S3 Optical responses of **SS-JC-V** toward HSA. (A) UV-vis absorption changes upon addition of 1 mg mL^{-1} HSA into a 10 μM **SS-JC-V** containing PBS system. (B) The corresponding changes in the fluorescence spectra. (C) UV-vis absorption changes upon addition of 1 mg mL^{-1} HSA into a 10 μM **SS-JC-V** containing Different polar solvents. (D) Ka evaluation obtained by the area of fluorescence spectra (500-600 nm). Error bars represent standard deviations obtained from three independent experiments. λ_{ex} = 495 nm; λ_{em} = 500-700 nm; slit 5/5 nm; 600 V. (E) The change of fluorescence intensity with time at 550 nm. (F) The corresponding changes in the fluorescence spectra about (C). λ_{ex} = 495 nm; λ_{em} = 500-700 nm; slit 2.5/5 nm; 600 V.

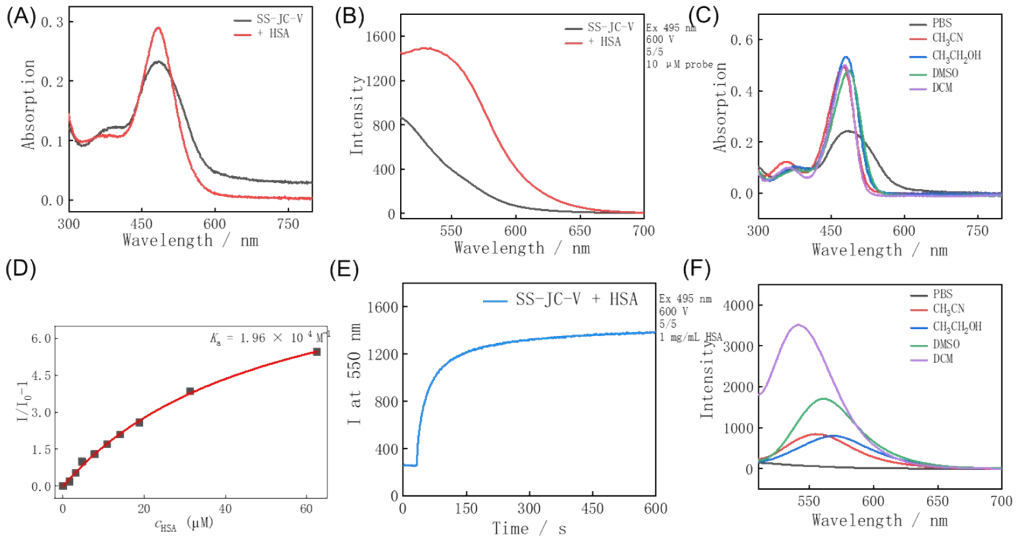


Fig. S4 **SS-JC-V** + **SS-1** Response to Drug Concentration Dependence. (A) UV-vis absorption changes upon addition of 1 mg mL^{-1} HSA into a 10 μM **SS-JC-V** + **SS-1** containing the presence of ibuprofen (100 μM). (B) The corresponding changes in the fluorescence spectra. **SS-JC-V** + **SS-1** Response to Drug Concentration Dependence Fluorescence spectra of **SS-JC-V** + **SS-1** in the presence of ibuprofen (0-100 μM) in the HSA labeling system, showing induced fluorescent spectral changes. Concentration-dependent fluorescent intensity changes of the mixture containing 1 mg/mL $^{-1}$HSA and 10 μM **SS-JC-V** + **SS-1** in response to varying concentrations of ibuprofen. λ_{ex} = 495 nm; λ_{em} = 500-700 nm; slit 5/5 nm; 600 V. (C) (D) Optical responses of **SS-JC-V** + **SS-1** in the presence of Warfarin (0-100 μM) in the HSA labeling system.

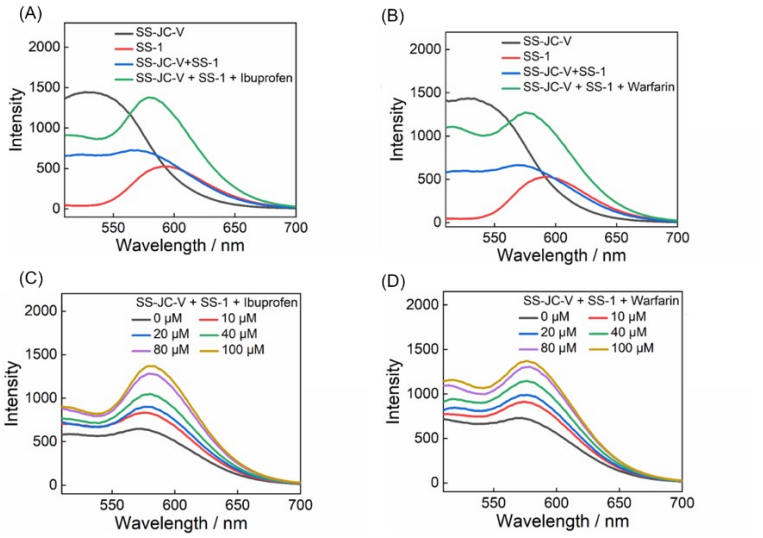


Fig. S5 Fragment Mass results of K [+275.095] C [+57.021] ASLQK and the corresponding calculated mass data. The signals labeled b6 and y2 were found in the experimental result.

PID=264534: KCASLQKF

#	a calc.	b calc.	b-18 calc.	Seq.	y calc.	y++ calc.	#
1	376.2020	404.1969	386.1864	K			8
2	536.2327	**564.2276**	546.2170	C	853.4236	427.2155	7
3	**607.2698**	**635.2647**	617.2541	A	693.3930	347.2001	6
4	694.3018	**722.2967**	**704.2862**	S	622.3559	311.6816	5
5	**807.3859**	**835.3808**	817.3702	L	535.3239	268.1656	4
6	**935.4444**	**963.4394**	945.4288	Q	**422.2398**	211.6235	3
7	1063.5394	1091.5343	1073.5238	K	**294.1812**	147.5942	2
8				F	**166.0863**	83.5468	1

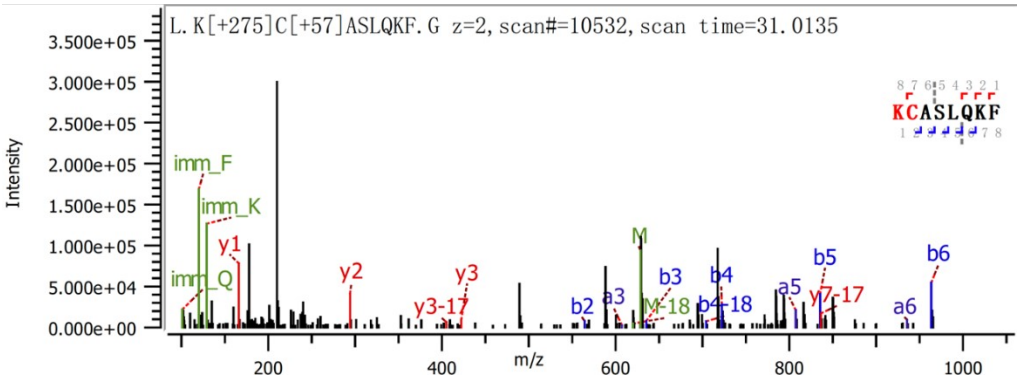


Fig. S6 Evaluation of Cell Viability Using CCK-8 Assay: At a concentration of 0-50 μM over 24 hours, the cytotoxicity of SS-1, SS-JC-Cl, and SS-1-SS-JC-Cl-HSA was measured. Error bars indicate the standard deviations from three independent experiments.

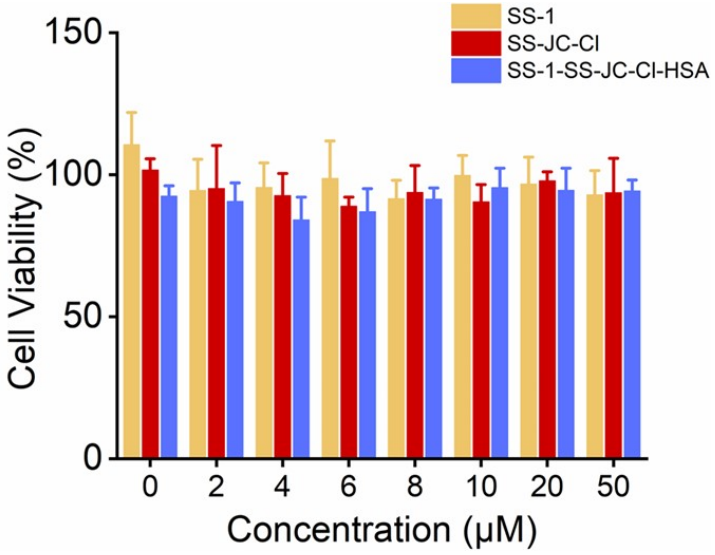


Fig. S7 (A) Fluorescence imaging of HSA in HCT-116 cells by SS-1-SS-JC-Cl-HSA with different concentrations of ibuprofen. Fluorescence image in the green channel and red channel; (B) Histogram analysis of fluorescence intensity of (A). Green channel: λ_{Ex} = 405 nm, λ_{Em} = 450–500 nm; Red channel: λ_{Ex} = 561 nm, λ_{Em} = 580–600 nm. Error bars represent standard deviations obtained from three independent experiments. Statistical analyses were performed with Student's t-test, *P < 0.05.

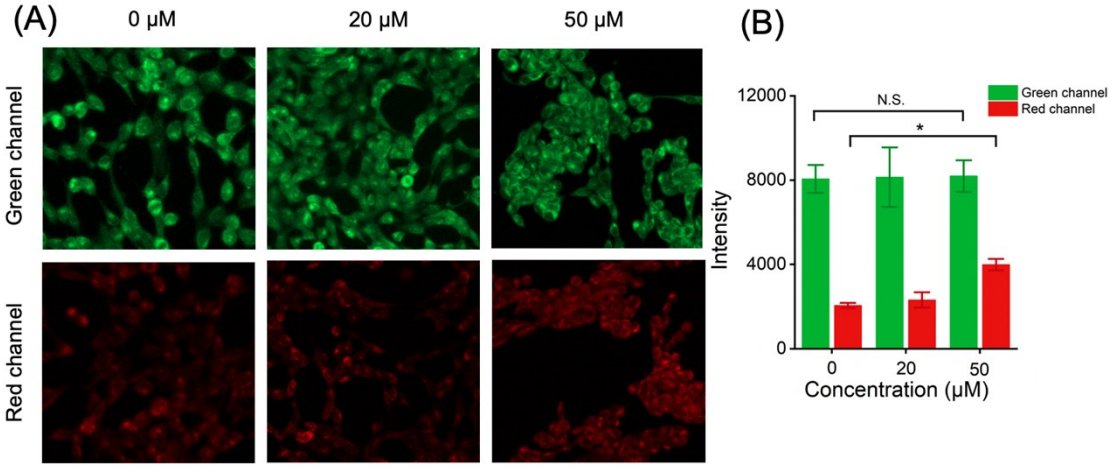


Fig. S8. (A) The fluorescence intensity was determined by flow cytometry of HSA in HCT-116 cells by SS-1-SS-JC-Cl-HSA with different concentrations of ibuprofen. (B) Histogram analysis of fluorescence intensity of (A). Error bars represent standard deviations obtained from three independent experiments. Statistical analyses were performed with Student's t-test, *P < 0.05, **P < 0.01.

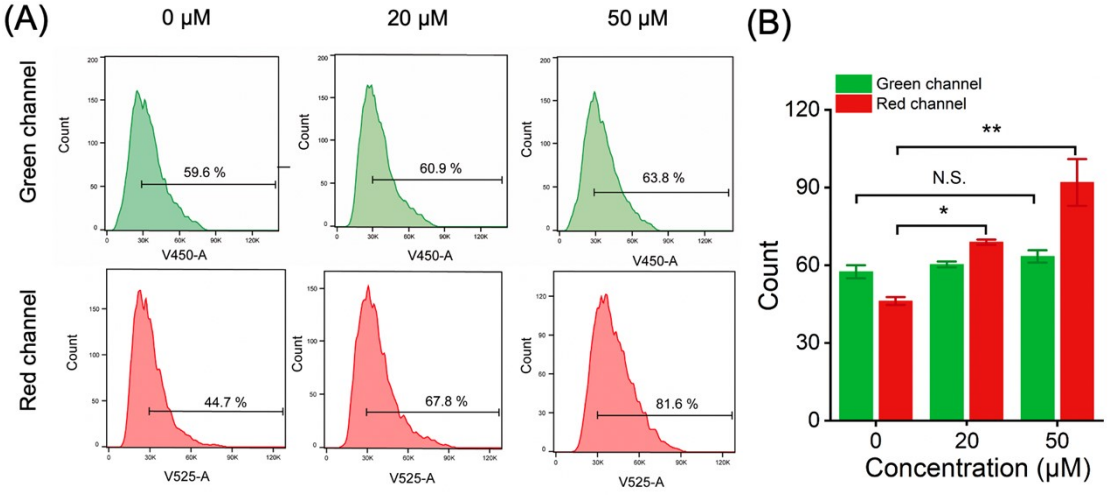


Fig. S9. Specificity evaluation of the SS-1-SS-JC-Cl-HSA system for ibuprofen analysis. The representative biological molecules including Glu, Ser, Arg, Cys KCl, Na_2SO_3 and $NaHCO_3$ with a concentration of 50 μM was added into the detection system, respectively.

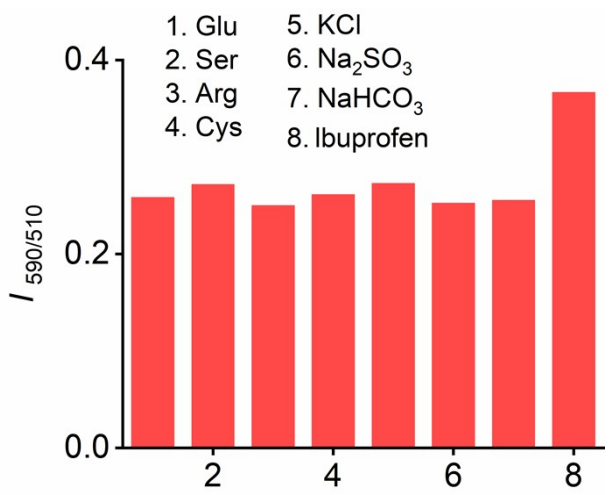
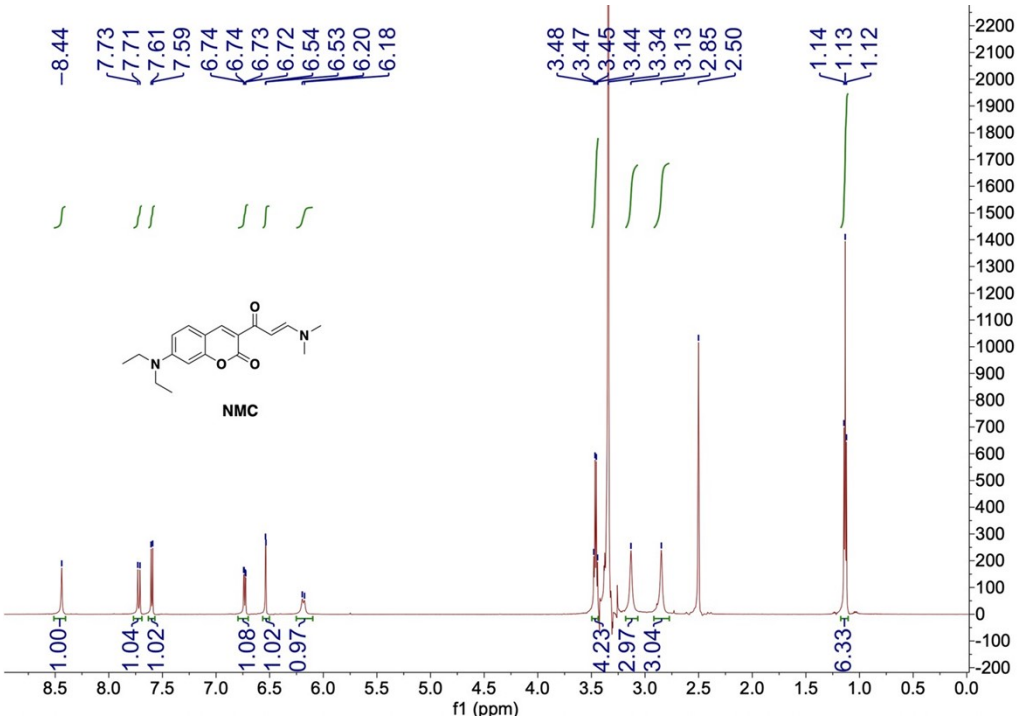
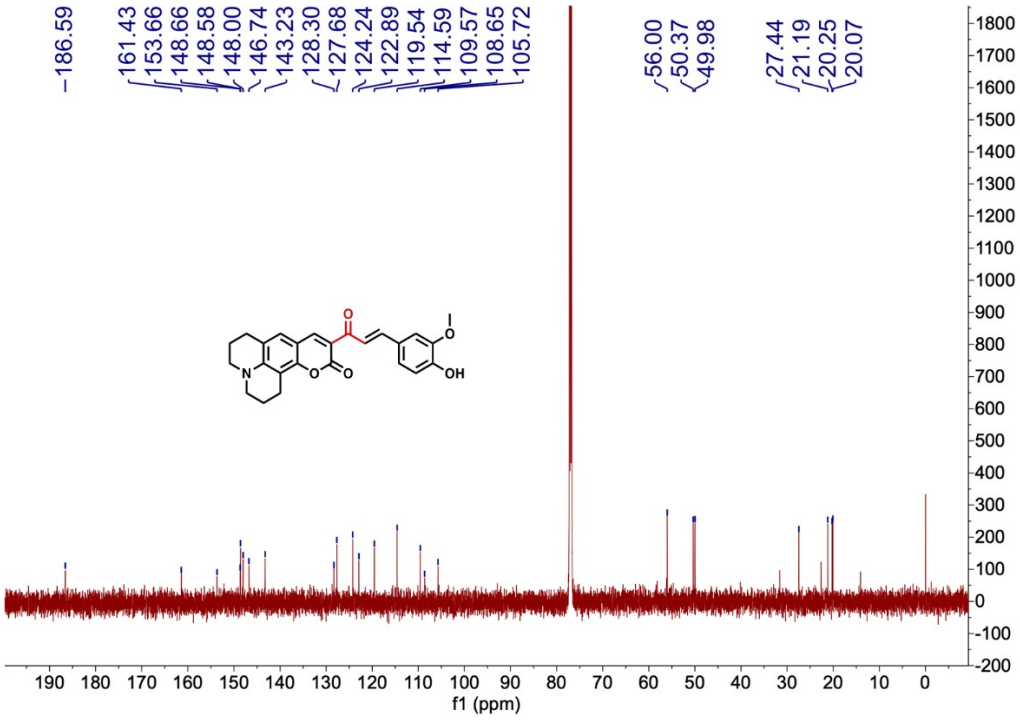

1. Glu
2. Ser
3. Arg
4. Cys
5. KCl
6. Na_2SO_3
7. $NaHCO_3$
8. Ibuprofen
$I_{590/510}$
0.4
0.2
0.0
2
4
6
8

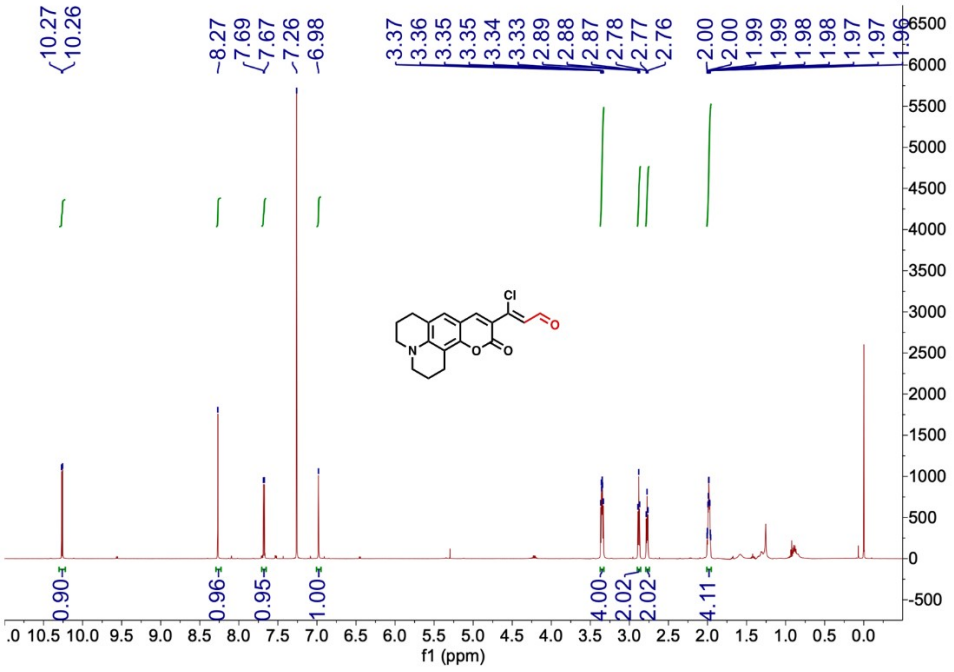
Table S1. Peptide mass spectra of SS-JC-Cl modified HSA.

Position	Peptide < ProteinMetrics Confidential >	Modification Type(s)	Observed m/z	z	Observed (M+H)	Calc. mass (M+H)	Mass error (ppm)	Starting position	Score	Scan Time	intensity
219	K.ASSAK[+275.095]QR.L	K[+275]	511.763	2	1022.518	1022.506	12.3	215	483.7	17.8368	2910100
214	R.DEGK[+275.095]ASSAK.Q	K[+275]	584.276	2	1167.545	1167.532	11.0	211	469.9	20.3432	11883000
214	R.DEGK[+275.095]ASSAKQR.L	K[+275]	484.573	3	1451.704	1451.691	8.6	211	356.7	17.5291	10188000
223	R.LK[+275.095]C[+57.021]ASLQK.F	C[+57], K[+275]	611.824	2	1222.640	1222.629	8.8	222	349.7	25.8388	0
214	K.LDELRDEGK[+275.095]ASSAK.Q	K[+275]	598.633	3	1793.885	1793.871	8.1	206	309.9	25.82	18094000
223	R.LK[+275.095]C[+57.021]ASLQKFGER.A	C[+57], K[+275]	571.300	3	1711.886	1711.863	13.9	222	258.5	30.3981	9611200
236	R.AFK[+275.095]AWAVAR.L	K[+275]	432.237	3	1294.695	1294.673	17.2	234	234.2	40.9546	2049600
214	K.LDELRDEGK[+275.095]ASSAKQR.L	K[+275]	520.270	4	2078.056	2078.030	12.6	206	196.3	21.4951	24847000
598	K.K[+275.095]LVAASQAALGL.-	K[+275]	708.911	2	1416.814	1416.789	18.0	598	157.5	49.1854	3599000
221	K.ASSAKQR[+275.095]LK.C	R[+275]	421.905	3	1263.700	1263.685	11.9	215	112.0	19.4697	8835600

Characterization






10.27
10.26
8.27
7.69
7.67
7.26
6.98
3.37
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3.35
3.35
3.34
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2.89
2.88
2.87
2.78
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2.76
2.00
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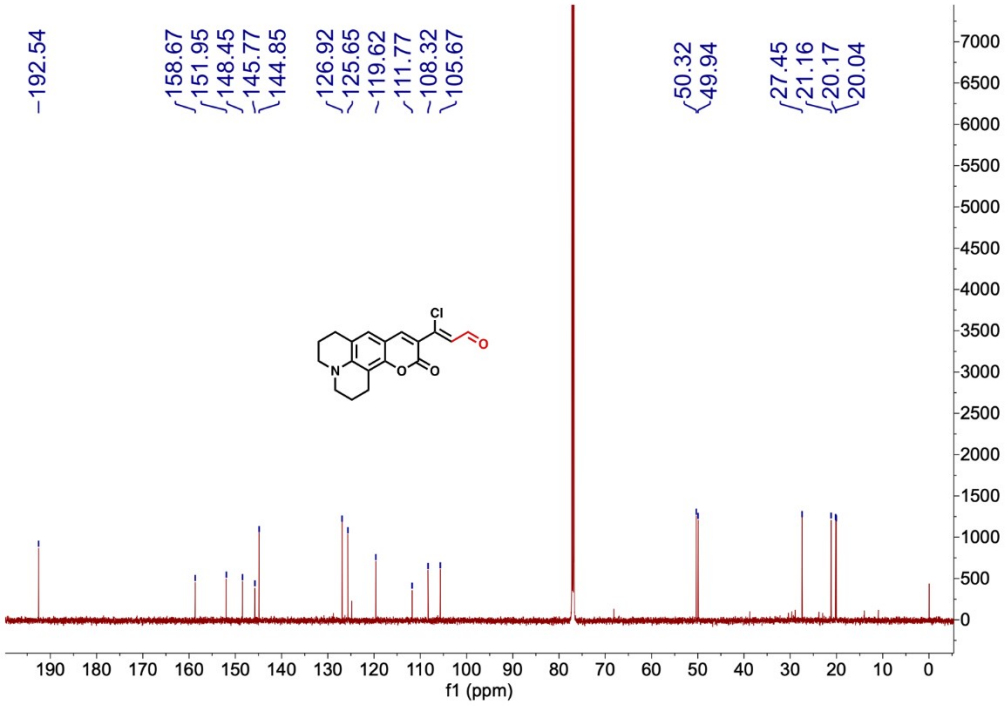
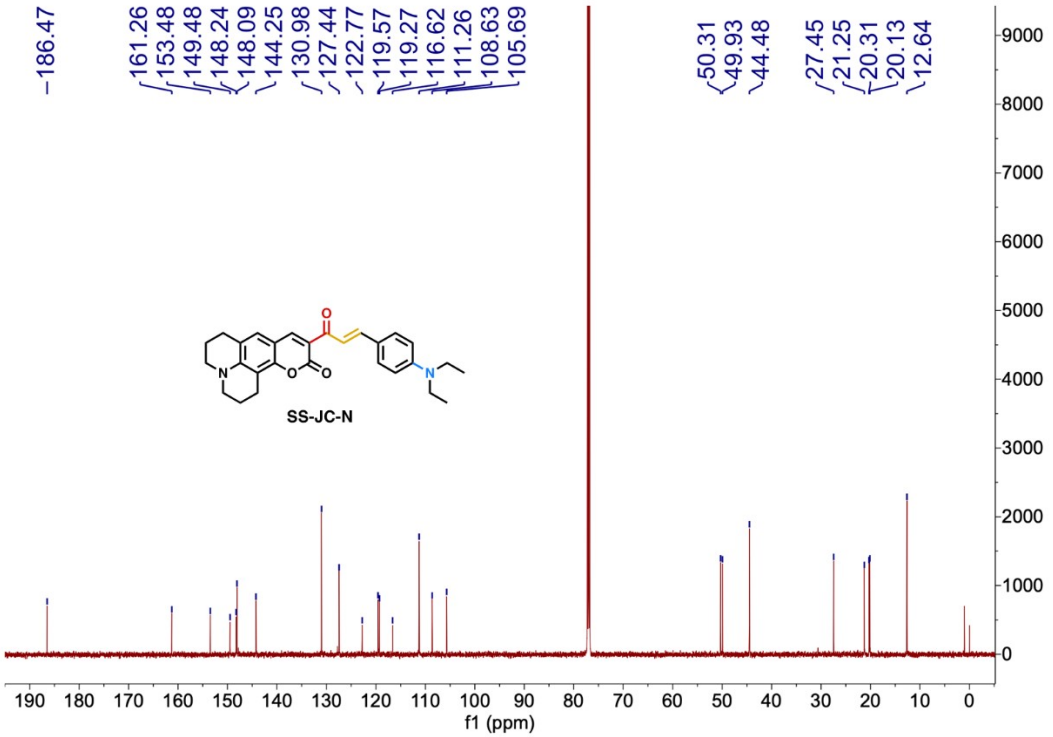
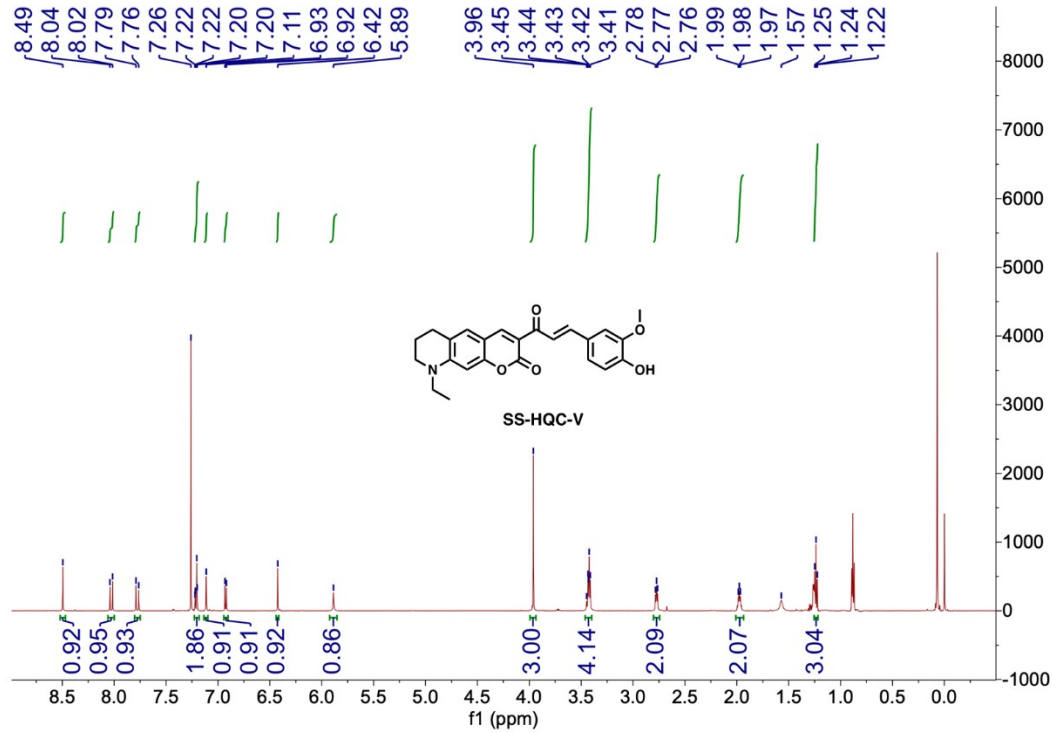
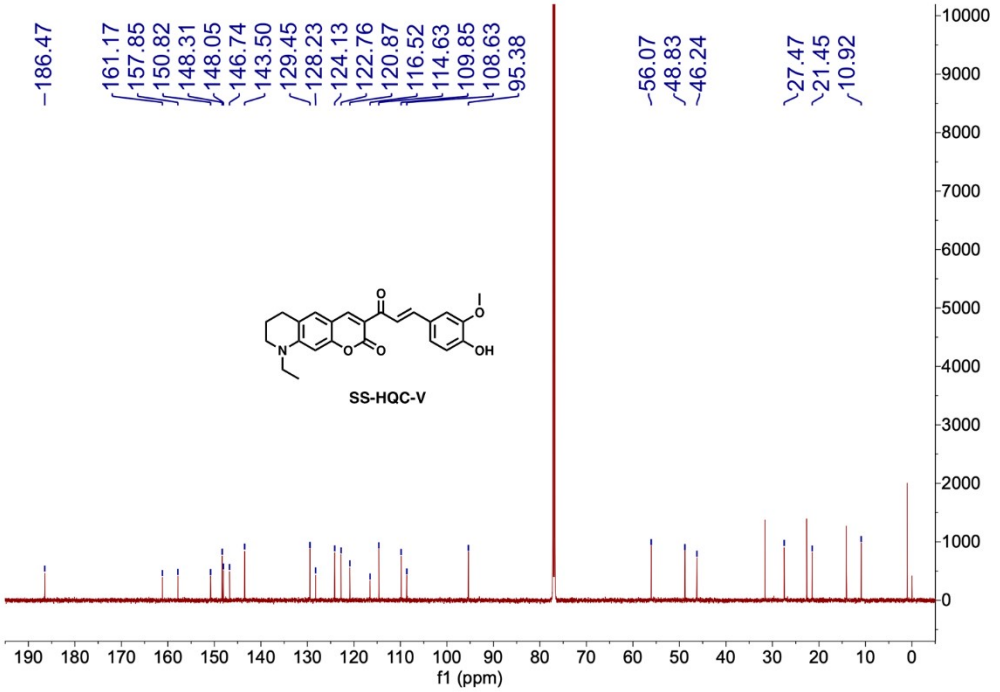
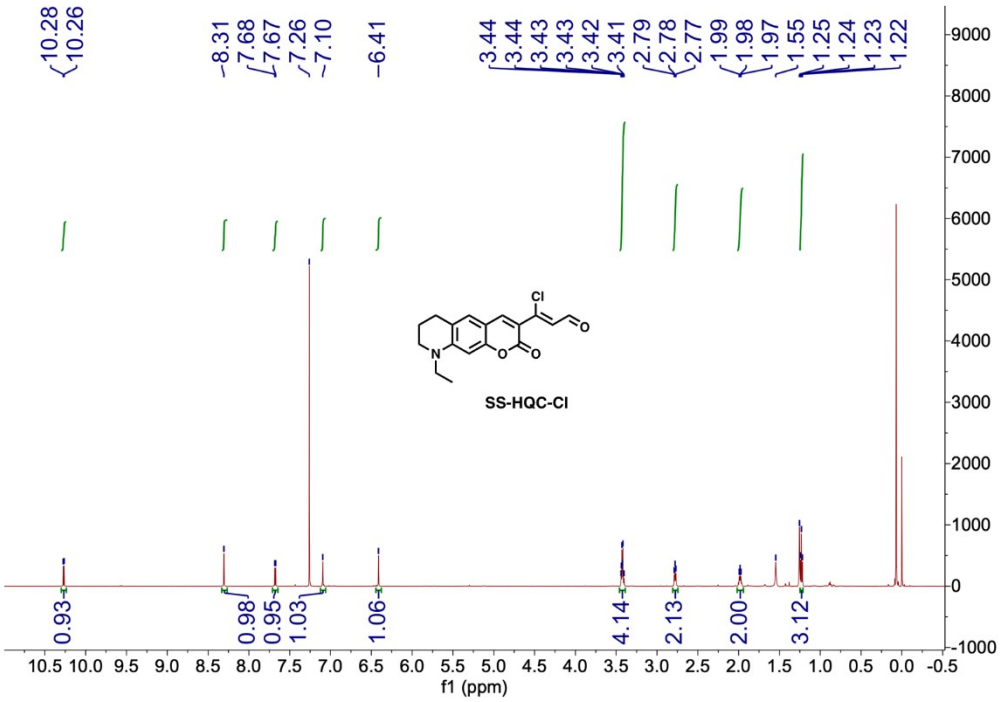
0.90
0.96
0.95
1.00
4.00
2.02
2.02
4.11
f1 (ppm)

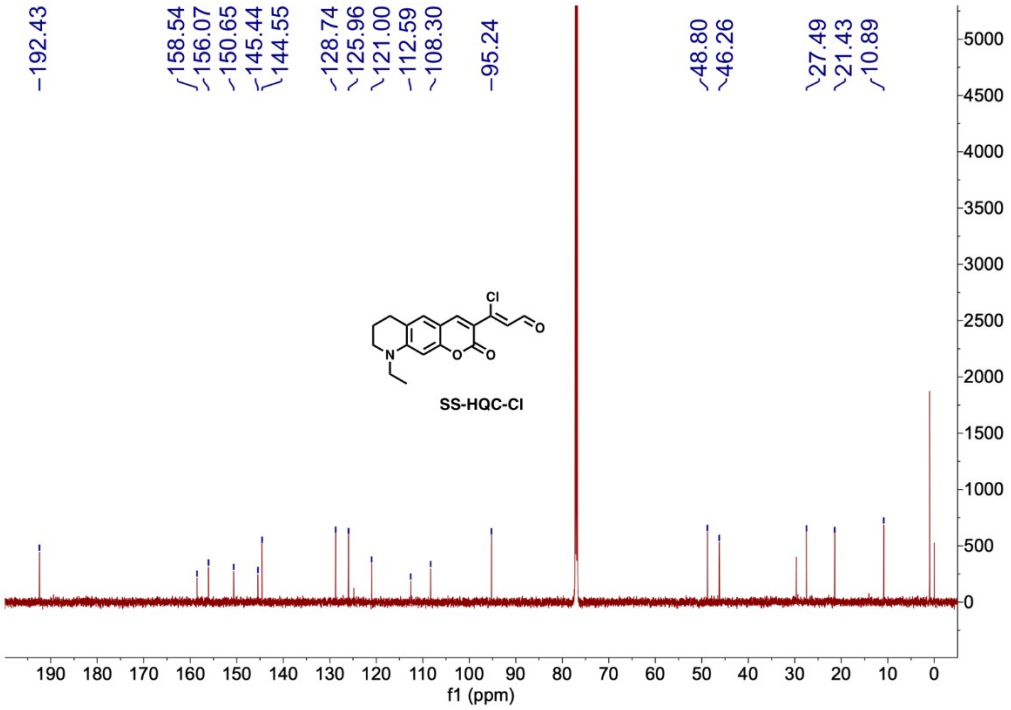

192.54
158.67
151.95
148.45
145.77
144.85
126.92
125.65
119.62
111.77
108.32
105.67
50.32
49.94
27.45
21.16
20.17
20.04
f1 (ppm)


186.47
161.26
153.48
149.48
148.24
148.09
144.25
130.98
127.44
122.77
119.57
119.27
116.62
111.26
108.63
105.69
50.31
49.93
44.48
27.45
21.25
20.31
20.13
12.64
SS-JC-N
f1 (ppm)


8.49
8.04
8.02
7.79
7.76
7.26
7.22
7.22
7.20
7.20
7.11
6.93
6.92
6.42
5.89
3.96
3.45
3.44
3.43
3.42
3.41
2.78
2.77
2.76
1.99
1.98
1.97
1.57
1.25
1.24
1.22
SS-HQC-V
0.92
0.95
0.93
1.86
0.91
0.91
0.92
0.86
3.00
4.14
2.09
2.07
3.04
f1 (ppm)


186.47
161.17
157.85
150.82
148.31
148.05
146.74
143.50
129.45
128.23
124.13
122.76
120.87
116.52
114.63
109.85
108.63
95.38
56.07
48.83
46.24
27.47
21.45
10.92
SS-HQC-V
f1 (ppm)


10.28
10.26
8.31
7.68
7.67
7.26
7.10
6.41
3.44
3.44
3.43
3.43
3.42
3.41
2.79
2.78
2.77
1.99
1.98
1.97
1.55
1.25
1.24
1.23
1.22
0.93
0.98
0.95
1.03
1.06
4.14
2.13
2.00
3.12
SS-HQC-Cl
f1 (ppm)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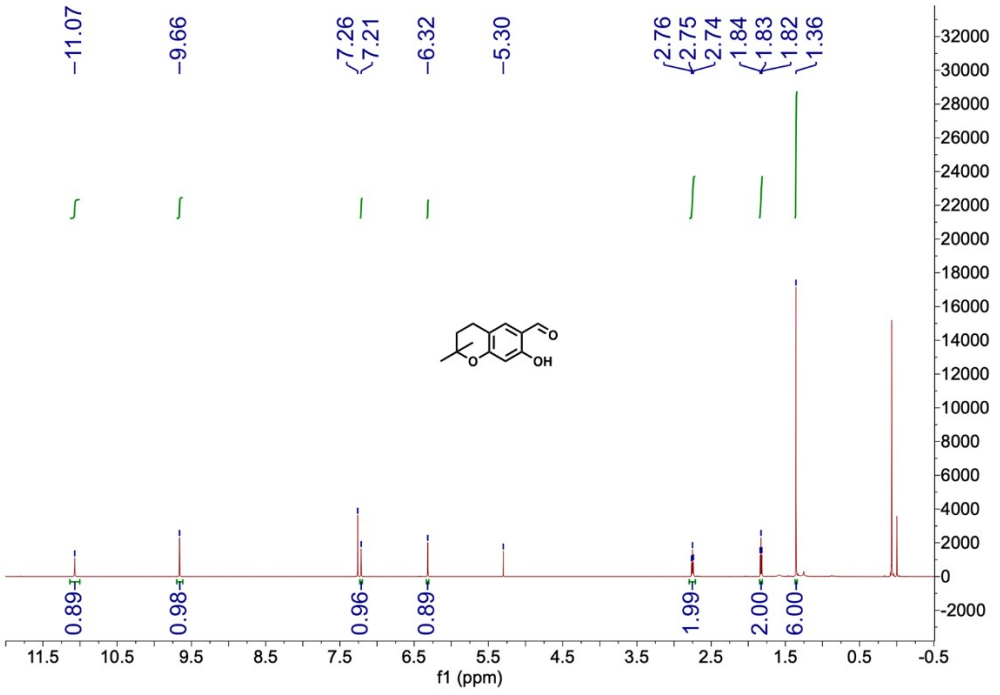
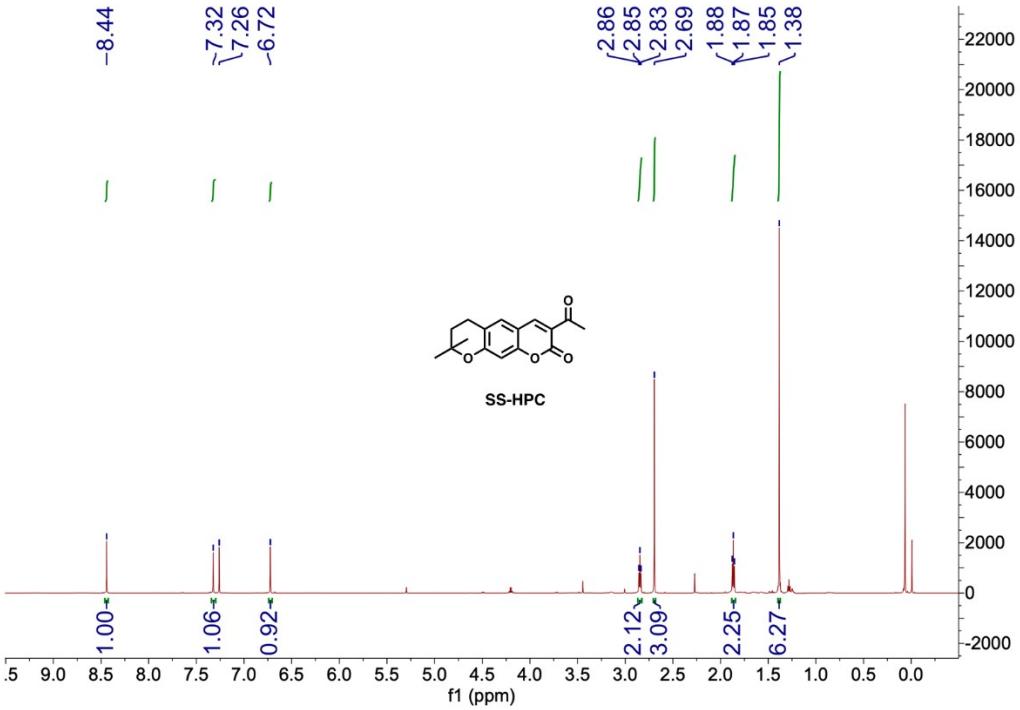
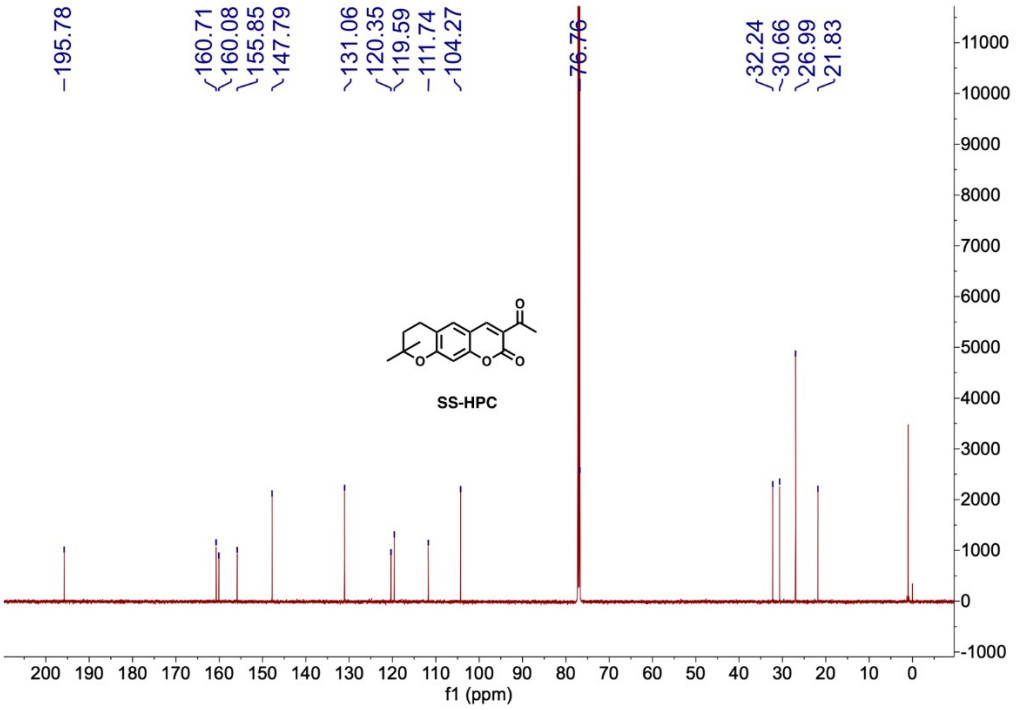
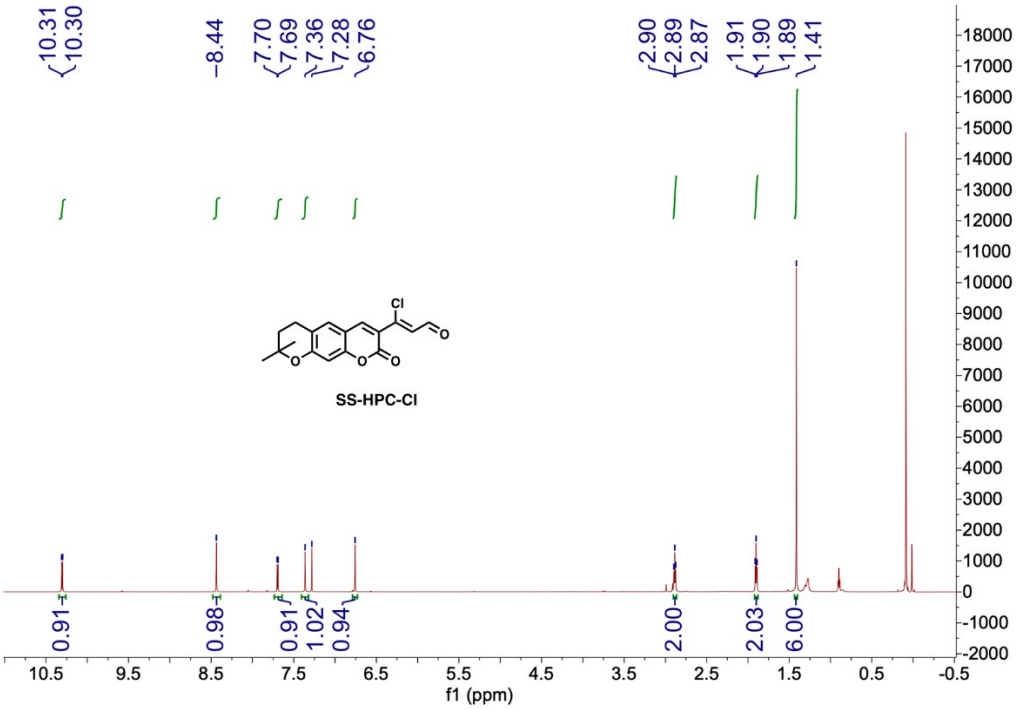
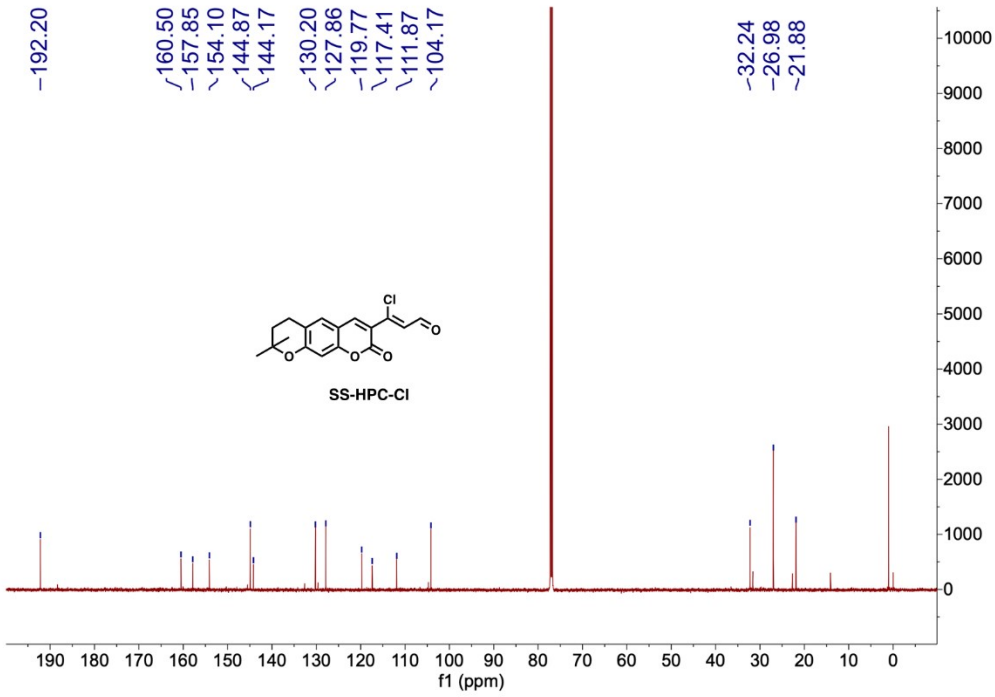
158.54
156.07
150.65
145.44
144.55
128.74
125.96
121.00
112.59
108.30
95.24
48.80
46.26
27.49
21.43
10.89
Cl
O
N
O
O
SS-HQC-CI
f1 (ppm)


11.07
9.66
7.26
7.21
6.32
5.30
2.76
2.75
2.74
1.84
1.83
1.82
1.36
O
O
OH
0.89
0.98
0.96
0.89
1.99
2.00
6.00
f1 (ppm)


8.44
7.32
7.26
6.72
2.86
2.85
2.83
2.69
1.88
1.87
1.85
1.38
SS-HPC
1.00
1.06
0.92
2.12
3.09
2.25
6.27
f1 (ppm)


195.78
160.71
160.08
155.85
147.79
131.06
120.35
119.59
111.74
104.27
76.76
32.24
30.66
26.99
21.83
SS-HPC
f1 (ppm)


10.31
10.30
8.44
7.70
7.69
7.36
7.28
6.76
2.90
2.89
2.87
1.91
1.90
1.89
1.41
Cl
O
O
O
SS-HPC-Cl
0.91
0.98
0.91
1.02
0.94
2.00
2.03
6.00
f1 (ppm)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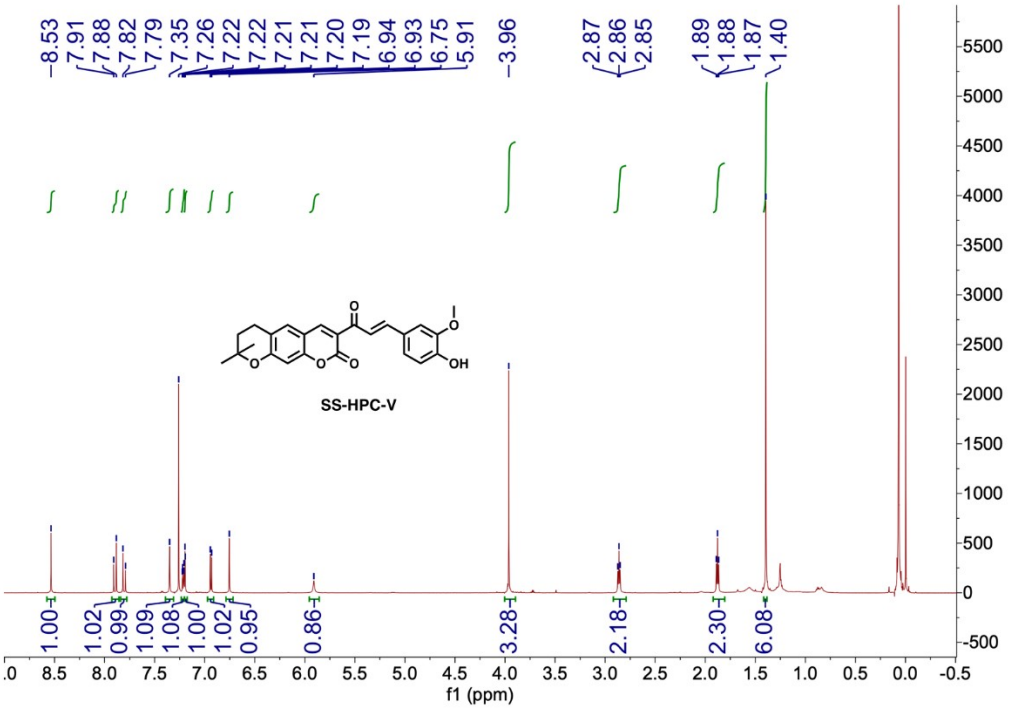
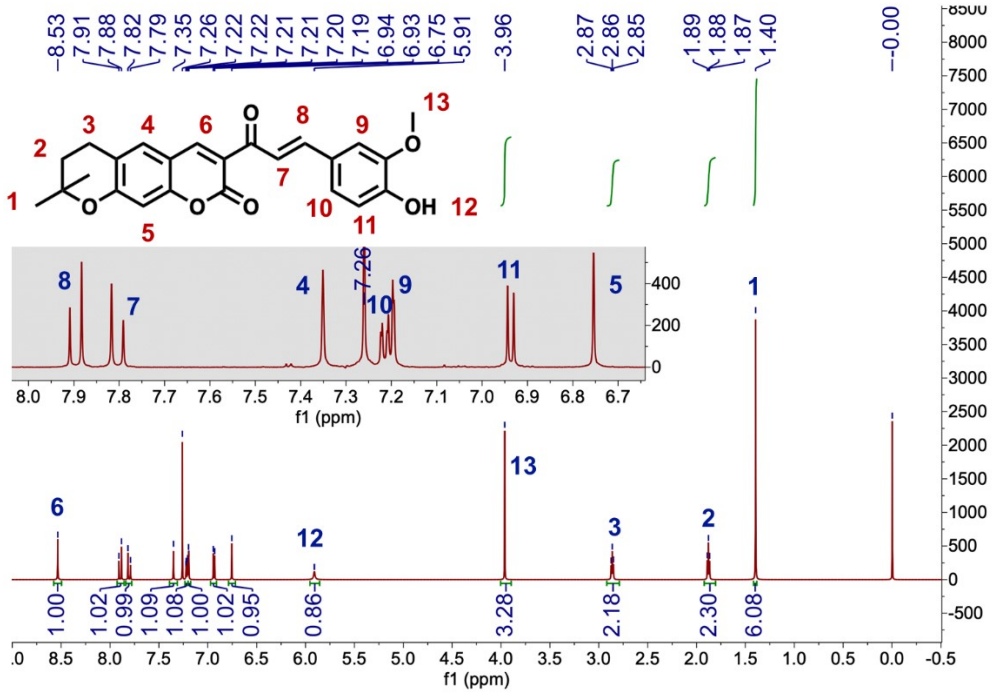
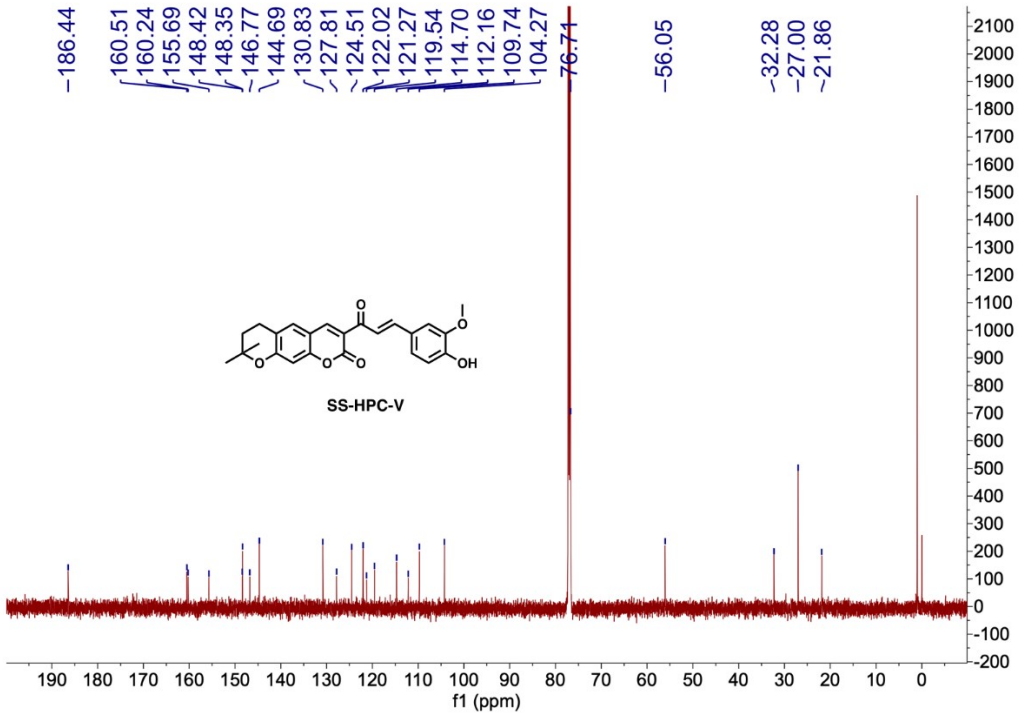
157.85
154.10
144.87
144.17
130.20
127.86
119.77
117.41
111.87
104.17
32.24
26.98
21.88
Cl
O
O
O
SS-HPC-Cl
f1 (ppm)


SS-HPC-V
f1 (ppm)


f1 (ppm)
f1 (ppm)



References

1. Y. Yue, T. Zhao, Y. Wang, K. Ma, X. Wu, F. Huo, F. Cheng and C. Yin, *Chemical Science*, 2022, **13**, 218-224.

2. Y. Yue, F. Huo, X. Li, Y. Wen, T. Yi, J. Salamanca, J. O. Escobedo, R. M. Strongin and C. Yin, *Org Lett*, 2017, **19**, 82-85.