Supporting information

Widely Applicable (Radio)dihalogenation of Alkynes and Alkenes using Two Different Nucleophilic Alkali Metal Halides

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1. General

1.1 Chemistry-General procedures and materials information

Commercial reagents and solvents were obtained from the commercial providers and used without further purification. The products were purified using a commercial flash chromatography system or a regular glass column. TLC was developed on silica gel 60 F254 glass plates. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on a Bruker NMR apparatus. Or alternatively, ^{1}H NMR chemical shifts were referenced to tetramethylsilane signal (0 ppm). The chemical shifts are reported in δ (ppm) values (^{1}H and ^{13}C NMR relative to $CHCl_3$, δ 7.26 ppm for ^{1}H NMR, and δ 77.0 ppm for ^{13}C NMR). Multiplicities are recorded by s (singlet), d (doublet), dd (doublet of doublets), dtd (doublet of triplet of doublets), t (triplet), td (triplet of doublets), m (multiplet) and br (broad), q (quartet). Coupling constants (J), are reported in Hertz (Hz). GC analyses were performed using a Shimadzu GC-2010-ultra gas chromatography-mass spectrometry instrument equipped with a Shimadzu AOC-20s autosampler.

2. Experimental Procedure and Characterization Data

2.1 Preparation of compound 1

All alkynes and alkenes were purchased from commercial providers unless otherwise noted below.

Procedure for the synthesis of compound 1ab, 1ac

Compound **1ab** and **1ac** were prepared according to the referenced literature.[1] To a suspension of aryl iodides (4.02 mmol), $Pd(PPh_3)_2Cl_2$ (0.120 mmol, 84.3 mg), CuI (0.240 mmol, 45.7 mg) and Et_3N (2.24 mL, 16.1 mmol) in DMF (6.8 mL) was added terminal alkynes (4.06 mmol). After stirring at 50 °C for 12 h, the reaction mixture was diluted with AcOEt and H_2O. The organic layer was washed with H_2O three times, washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel (eluant: petroleum ether/ethyl acetate).

Procedure for the synthesis of the compound 1ag

Compound **1ag** was prepared according to the referenced literature,[2] and the compounds' spectra data are in agreement with the reports.

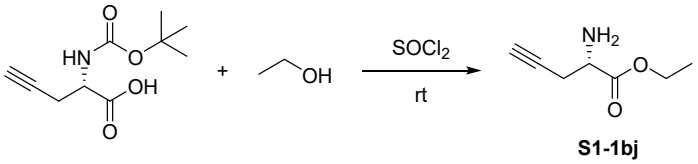
Procedure for the synthesis of compound 1ah, 1ai, 1aj

Compounds **1ah, 1ai, 1aj** were prepared according to the referenced literature.[3] To a solution of alcohol (10 mmol) and acid (12 mmol) in DCM (20 mL) at 0 °C, DCC (15 mmol, 15 mL of a 1 M solution in DCM) and DMAP (5 mmol, 611 mg) was added successively. The mixture was warmed to rt and stirred for 20 h. The suspension was filtered, and the solid was washed with DCM. The combined filtrate was evaporated, and the residue was purified by column chromatography on silica gel.

Procedure for the synthesis of 1bi

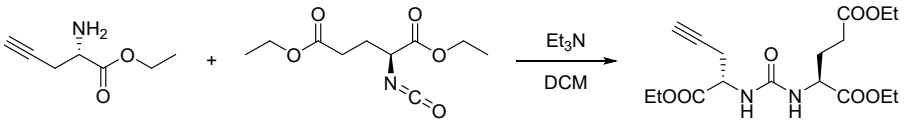
Compound **1bi** was prepared according to the referenced literature,[4] and the compounds' spectra data agree with the reports.

Procedure for the synthesis of 1bj



S1-1bj

To an oven-dried 100 mL flask, thionyl chloride (2.23 g, 19 mmol) was added dropwise to a solution of *N*-Boc-L-propargylglycine (1.0 g, 2.35 mmol) in ethanol (45 mL), and the mixture was stirred at room temperature for 14 hours. The reaction mixture was evaporated in vacuo, and the residue was dissolved in dichloromethane and washed with 1 M $NaHCO_3$ solution and brine. The organic layer was dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the intermediate compound **S1-1bj**(628 mg, 95%) as a yellow oil.



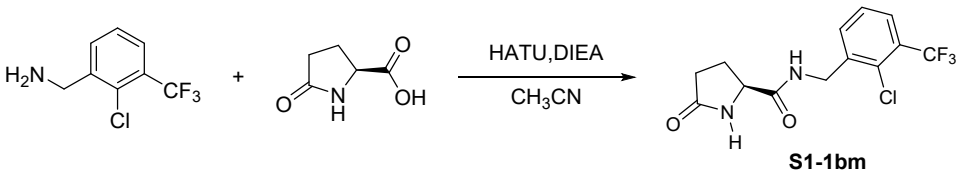
S1-1bj **1bj**

To a solution of **S1-1bj** compound in DCM(25 mL) were added diethyl (*S*)-2-isocyanatopentanedioate(1.03 mg, 4.48 mmol) and Triethylamine(3.68 mL) at room temperature. The reaction mixture was stirred at room temperature for 24 hours. Then the mixture was poured into a saturated aqueous solution of NH_4Cl (150 mL) and extracted by dichloromethane (150 mL). The organic layer was washed with brine, dried with $MgSO_4$, then concentrated under reduced pressure. The crude product was purified by chromatography on silica gel to afford compound **1bj** as a white solid (1.29 g, 78%).

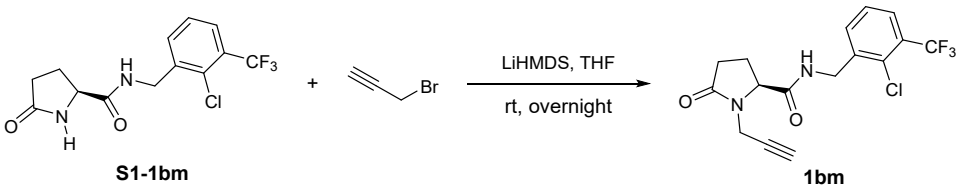
Procedure for the synthesis of 1bl

Compound **1bl** was prepared with two procedures according to the referenced literature,[5] and the compounds' spectra data are in agreement with the reports.

Procedure for the synthesis of 1bm



To an oven-dried 500 mL flask, 2-Chloro-3-(Trifluoromethyl) Benzylamine (1.68 g, 8.0 mmol), 2-Pyrrolidone-5-carboxylic acid (1.03 g, 8.0 mmol), DIEA (1.92 g, 10.0 mmol), HATU (3.80 g, 10.0 mmol) and CH_3CN (150 mL) were added sequentially and stirred at rt overnight. The reaction mixture was washed with HCl and $NaHCO_3$ solution. The organic layer was dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the intermediate compound **S1-1bm**(1.5 g, 60%) as a white solid[6].



To a solution of the **S1-1bm** in THF(15 mL) were added LiHMDS (4.5 mL), 3-Bromopropyne (714 mg, 6 mmol) at 0 ℃. The reaction mixture was gradually warmed to room temperature and was stirred overnight. The aqueous solution was extracted with EtOAc (3×25 mL), the organic layer washed with saturated NaCl solution (3×30 mL), dried with $MgSO_4$, and evaporated. The crude product was purified by chromatography on silica gel to afford compound **1bm** as a white solid (210 mg, 20%).

2.2 Preparation of iodochlorination of alkynes 3 or 4

Lithium iodide (0.24 mmol, 1.2 equiv), lithium chloride (0.24 mmol, 1.2 equiv) and alkynes (0.2 mmol) were added to a dried reaction vial equipped with a magnetic stir bar. Acetic acid (0.5 mL), DCM (0.25 mL) with or without HFIP (0.25 mL) were added, and the mixture was cooled to 0 ℃. Then *m*CPBA (0.24 mmol, 85%, 1.2 equiv) was added into the mixture and stirred for 2 h under air at 0 ℃. After the reaction was completed, the

saturated sodium thiosulfate solution was added into the mixture to quench the reaction (remove excess oxidants). The reaction mixture was extracted with DCM (15 mL×2). The combined organic layers were washed with brine, dried over Na_2SO_4, and then the excess solvent was removed under reduced pressure, the crude product was further purified by silica gel column chromatography to provide the corresponding product.

2.3 Preparation of iodobromination of alkenes 5

Lithium iodide (0.24 mmol, 32 mg, 1.2 equiv), lithium chloride (0.24 mmol, 10 mg, 1.2 equiv) were added to a dried reaction vial equipped with a magnetic stir bar. Acetic acid (0.5 mL), DCM (0.25 mL) were added, and the mixture was cooled to 0 °C. Then *m*CPBA (0.24 mmol, 48 mg, 85%, 1.2 equiv) was added to the mixture. After 10 min, 4-fluorostyrene (0.2 mmol, 24 mg) was introduced and stirred for 2 h under air at 0 °C. After the reaction was completed, the saturated sodium thiosulfate solution was added to the mixture to quench the reaction (remove excess oxidants). The reaction mixture was extracted with DCM (15 mL×2). The combined organic layers were washed with brine, dried over Na_2SO_4, and then the excess solvent was removed under reduced pressure; the residue was purified by silica gel column chromatography to provide the final products **5a**.

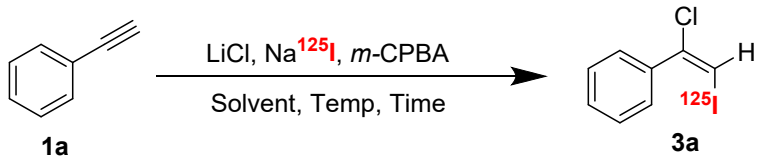
3. Radio-synthesis of ^{125}I-labeled alkenyl ioidide

3.1 General

Sodium[^{125}I] iodide was purchased from HTA Co., Ltd. as none carrier added [^{125}I]sodium iodide in 1×10^{-5} M NaOH. The crude radiolabelled product purification was performed by HPLC on UltiMate 3000 system (Thermo Fisher Scientific, USA) equipped with a Bioscan Flow-Count radio-HPLC detector under the following conditions: Agilent Eclipse XDB-C18, 5 μm, 4.6 × 250 mm, 75% acetonitrile in ammonium formate buffer (0.1 M, pH = 4.5) as mobile phase, the flow rate at 1.0 mL/min, UV wavelength at 254 and 220 nm. Glass backed thin layer chromatography (TLC) plates purchased from Merck coated with silica gel 60 F_{254} were used for radio-TLC analysis. Radio-TLC analyses were carried out on a Bioscan Mini-Scan TLC Scanner (Eckert & Ziegler). The data were recorded and processed by Chromatography Data System (Thermo Fisher Scientific, USA) for determination of radiochemical conversion. The activities of [^{125}I] radiolabeled samples were determined using a radioisotope dose calibrator CRC-55tR (Capintec Inc.).

3.2 Radioiodination condition screen

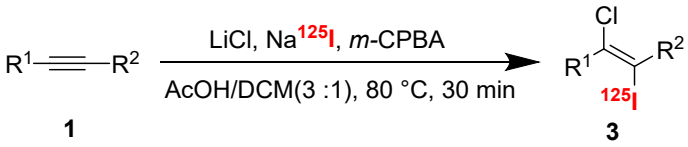
Table S1. Optimization of Radioiodination condition



1a 3a

Entry	mCPBA/μmol	DCM/μL	AcOH/μL	HFIP/μL	Temp/°C	Time/min	RCY/%
1	12	50	150	0	60	30	9
2	12	50	150	0	60	120	18
3	12	50	150	0	60	300	23
4	12	50	150	0	80	30	83
5	12	50	150	0	80	40	79
6	12	50	150	0	80	120	77
7	6	50	150	0	80	30	63
8	24	50	150	0	80	30	71
9	12	50	100	50	80	30	54
10	12	100	50	50	80	30	11

3.3 General procedure for the radio-iodization



1 3

Alkynes **1** (25 μmol) and lithium chloride (2 mg) were added to a 1.5 mL microcentrifuge tube, followed by the addition of acetic acid (100 μL), DCM (50 μL), and 3 - 9 MBq of $Na^{125}I$ in 2-5 μL aqueous solution. Finally, 12 μmol *m*-CPBA in 50 μL acetic acid was added to the mixture, and the reaction was kept at 80 °C for 30 min. The reaction was quenched by the addition of 10 mol% sodium thiosulfate (50 μL) and MeCN (50 μL). About 100 μL reaction mixture was analyzed by radio-HPLC to confirm the identity of the radiolabeled compound. The reaction mixture was eluted with acetonitrile and ammonium formate buffer (0.1 M, pH = 4.5), and the flow rate was 1.0 mL/min. Notedly, UV and radioactivity detectors were connected in series, giving a time delay of about 0.5-1.0 min. ^{125}I-labeled compounds were identified by co-injection of the unlabeled reference compounds.

3.4 Determinations of HPLC radiochemical yield (RCY)

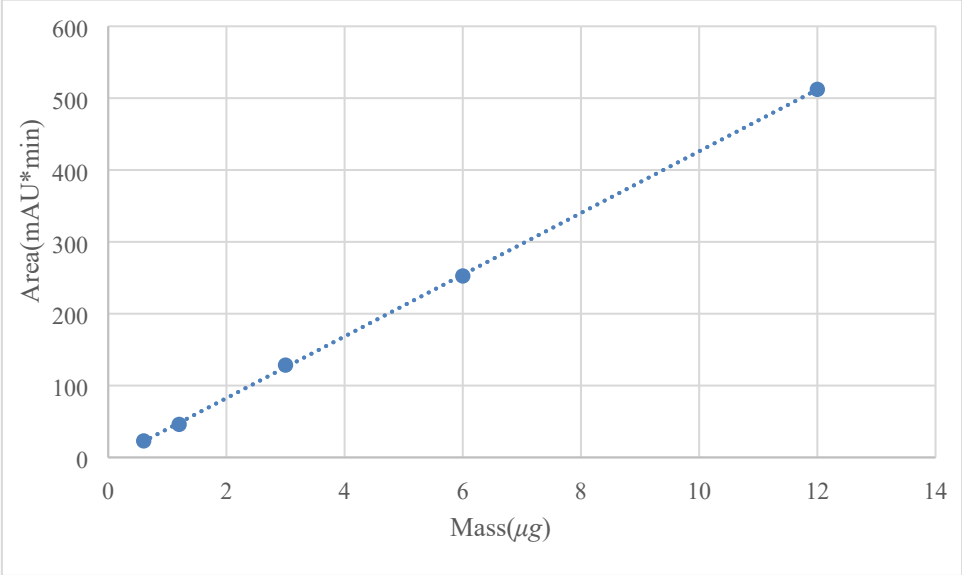
About 100 μL reaction mixture (typically containing 1.0-3.0 MBq) was injected into radio-HPLC for analysis. The activity injected into HPLC was measured (this activity was denoted by A), and the time of injection was recorded. The fraction was collected by automatic fraction collector. The activity orresponding to the radiolabeled product was measured (this activity was denoted by B). The decay-corrected RCY was calculated by dividing the decay-corrected B by A. The activities of [^{125}I] radiolabeled samples were determined using a radioisotope dose calibrator CRC-55tR (Capintec Inc.).

3.5 Specific activity calculation

The specific activities (GBq/mg) were calculated by dividing the radioactivity of the ^{125}I-labeled product by the amount of the unlabeled tracer determined from the peak area in UV-HPLC chromatograms (λ = 254 nm). The amounts of unlabeled compounds were determined from the UV absorbance/concentration calibration curve. The solution of ^{125}I-labeled product obtained after HPLC purification was concentrated through C-18 light SepPak, and then eluted by EtOH

The resulting solutions were completely injected into the HPLC system. The peak area was determined, and the amount of carrier was calculated according to the calibration curve. For 0.42 MBq of purified compound **3a**, UV absorbance (at 220 nm) of 21.19 was measured, corresponding to 0.57 μg for a specific activity of 7.53 GBq·mg^{-1} at time of injection (TOI).

Figure S1. Calibration curve for radio-iodization of (E)-(1-chloro-2-iodovinyl)benzene (**3a**).



4. Characterization data

diethyl (((*S*)-1-ethoxy-1-oxopent-4-yn-2-yl)carbamoyl)-*L*-glutamate(1bj). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). White solid (1.29 g, 78%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.75 (s, 1H), 4.40 (dd, J = 8.0, 4.9 Hz, 1H), 4.24 – 4.05 (m, 7H), 2.87 – 2.71 (m, 2H), 2.52 – 2.32 (m, 2H), 2.22 (dddd, J = 13.4, 8.4, 6.9, 4.9 Hz, 1H), 1.97 (dtd, J = 14.4, 8.3, 6.3 Hz, 1H), 1.30 – 1.22 (m, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 172.3, 171.7, 150.1, 149.6, 61.5, 61.3, 60.6, 57.8, 54.1, 53.4, 30.2, 29.6, 28.6, 27.5, 14.2 (d, J = 7.5 Hz). HRMS (ESI-ORBITRAP) Calculated for $C_{17}H_{26}N_2O_7$ $(M+H)^+$ 371.1813, found 371.1819.

(*S*)-*N*-(2-chloro-3-(trifluoromethyl)benzyl)-5-oxo-1-(prop-2-yn-1-yl)pyrrolidine-2-carboxamide (1bm). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). White solid (210 mg, 20%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, J = 7.9, 1.6 Hz, 1H), 7.62 (dd, J = 7.7, 1.6 Hz, 1H), 7.37 (t, J = 7.8 Hz, 1H), 6.56 (d, J = 6.2 Hz, 1H), 4.70 – 4.56 (m, 2H), 4.47 (dd, J = 17.7, 2.6 Hz, 1H), 4.33 – 4.21 (m, 1H), 3.69 (dd, J = 17.7, 2.5 Hz, 1H), 2.60 – 2.44 (m, 1H), 2.44 – 2.30 (m, 2H), 2.18 (t, J = 2.6 Hz, 1H), 2.14 – 2.00 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.2, 171.0, 137.5, 133.8, 131.7, 129.1, 127.2, 127.2, 127.2, 127.0, 121.8, 73.3, 60.5, 41.7, 31.5, 29.5, 23.4. HRMS (ESI-ORBITRAP) Calculated for $C_{16}H_{14}ClF_3N_2O_2$ $(M+H)^+$ 359.0769, found 359.0770.

(*E*)-(1-chloro-2-iodovinyl)benzene (3a). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (52 mg, 99%).[7] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.47 (m, 2H), 7.42 – 7.36 (m, 3H), 6.77 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.6, 134.1, 129.5, 129.0, 128.3, 73.0.

(*E*)-1-bromo-2-(1-chloro-2-iodovinyl)benzene (3b). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (62 mg, 91%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.1 Hz, 1H), 7.44 – 7.38 (m, 1H), 7.32 -7.27 (m, 2H), 6.89 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.5, 133.6, 133.2, 130.8, 130.5, 127.7, 122.0, 78.3. HRMS (EI-TOF) Calculated for C_8H_5BrClI (M^+) 341.8308, found 341.8301.

(*E*)-1-(1-chloro-2-iodovinyl)-2-ethylbenzene (3c). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (50 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.37 (m, 1H), 7.36 – 7.32 (m, 1H), 7.31 – 7.26 (m, 1H), 7.21 (dd, *J* = 7.6, 1.0 Hz, 1H), 6.84 (s, 1H), 2.73 (q, *J* = 7.6 Hz, 2H), 1.31

(t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.7, 137.7, 134.6, 129.7, 129.0, 128.7, 126.1, 76.8, 25.8, 14.8. HRMS (EI-TOF) Calculated for $C_{10}H_{10}ClI$ (M^+) 291.9516, found 291.9510.

(*E*)-1-(1-chloro-2-iodovinyl)-2-isopropylbenzene (3d). Purified by column chromatography on silica gel (eluant: petroleum ether = 9:1). Colorless oil (56 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.40 (m, 2H), 7.30 – 7.26 (m, 1H), 7.22 – 7.17 (m, 1H), 6.85 (s, 1H), 3.19 – 3.12 (m, 1H), 1.34 – 1.30 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.5, 137.2, 134.7, 129.9, 128.9, 126.1, 126.0, 76.9, 30.4, 24.2, 23.8. HRMS (EI-TOF) Calculated for $C_{11}H_{12}ClI$ (M^+) 305.9672, found 305.9678.

(*E*)-3-(1-chloro-2-iodovinyl)benzonitrile (3e). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 20:1). Colorless oil (46 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (s, 1H), 7.76 (d, J = 7.9 Hz, 1H), 7.68 (d, J = 7.8 Hz, 1H), 7.54 (t, J = 7.8 Hz, 1H), 6.90 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.0, 133.3, 132.9, 132.7, 131.6, 129.3, 118.0, 112.8, 75.4. HRMS (EI-TOF) Calculated for C_9H_5ClIN (M^+) 288.9155, found 288.9151.

(*E*)-1-(1-chloro-2-iodovinyl)-3-nitrobenzene (3f). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 15:1). Yellow oil (48 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 – 8.38 (m, 1H), 8.28 – 8.21 (m, 1H), 7.84 (d, J = 7.7 Hz, 1H), 7.59 (t, J = 8.0 Hz, 1H), 6.93 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.0, 139.2, 135.0, 131.4, 129.5, 124.3, 124.2, 75.7. HRMS (EI-TOF) Calculated for $C_8H_5ClINO_2$ (M^+) 308.9053, found 308.9048.

(*E*)-1-(1-chloro-2-iodovinyl)-3-fluorobenzene (3g). Purified by column chromatography on silica gel (eluant: petroleum ether = 10:1). Colorless oil (50 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.40 (m, 1H), 7.33 (d, J = 7.8 Hz, 1H), 7.27 – 7.22 (m, 1H), 7.14 – 7.07 (m, 1H), 6.83 (s, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -112.11 – -112.19 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2 (d, J = 246 Hz), 139.5 (d, J = 8.2 Hz), 132.6 (d, J = 2.5 Hz), 129.9 (d, J = 8.3 Hz), 124.8 (d, J = 3.1 Hz), 116.5 (d, J = 21 Hz), 116.1 (d, J = 23 Hz), 73.9. HRMS (EI-TOF) Calculated for C_8H_5ClFI (M^+) 281.9108, found 281.9103.

(*E*)-3-(1-chloro-2-iodovinyl)phenol (3h). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 10:1). Colorless oil (52 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, J = 7.9 Hz, 1H), 7.10 (d, J = 7.7 Hz, 1H), 7.02 – 6.95 (m, 1H), 6.91 – 6.85 (m, 1H), 6.76 (s, 1H), 5.01 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.2, 139.1, 133.5, 129.6, 121.5, 116.6, 115.8, 73.2. HRMS (ESI-ORBITRAP) Calculated for C_8H_5ClIO $(M-H)^-$ 278.9074, found 278.9068.

(*E*)-N-(3-(1-chloro-2-iodovinyl)phenyl)-*N*-,4-dimethylbenzenesulfonamide (3i). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 20:1). Colorless oil (76 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.1 Hz, 2H), 7.39 – 7.38 (m, 2H), 7.32 – 7.22 (m, 3H), 7.17 (s, 1H), 6.77 (s, 1H), 3.21 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 141.6, 138.3, 133.2, 133.0, 129.5, 128.9, 128.0, 127.9, 127.6, 126.3, 73.9, 37.9, 21.5. HRMS (ESI-ORBITRAP) Calculated for $C_{16}H_{16}ClINO_2S$ $(M+H)^+$ 447.9635, found 447.9629.

(*E*)-1-(4-(1-chloro-2-iodovinyl)phenyl)ethan-1-one (3j). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 30:1). Yellow oil (50 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.3 Hz, 2H), 7.62 (d, *J* = 8.3 Hz, 2H), 6.86 (s, 1H), 2.62 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.2, 142.0, 137.5, 132.9, 129.3, 128.3, 74.5, 26.7. HRMS (ESI-ORBITRAP) Calculated for $C_{10}H_9ClIO$ $(M+H)^+$ 306.9386, found 306.9381.

Methyl (*E*)-4-(1-chloro-2-iodovinyl)benzoate (3k). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 50:1). Colorless oil (54 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.2 Hz, 2H), 7.59 (d, *J* = 8.2 Hz, 2H), 6.85 (s, 1H), 3.93 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.3, 141.9, 133.0, 130.9, 129.6, 129.1, 74.4, 52.3. HRMS (ESI-ORBITRAP) Calculated for $C_{10}H_9ClIO_2$ $(M+H)^+$ 322.9336, found 322.9330.

(*E*)-1-(1-chloro-2-iodovinyl)-4-(trifluoromethyl)benzene (3l). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (50 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.62 (m, 4H), 6.88 (s, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -62.89 (s). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.1, 132.5, 131.3 (q, *J* = 33.3 Hz), 129.4, 125.4 (q, *J* = 4.0 Hz), 123.7 (q, *J* = 273.7 Hz), 74.6. HRMS (EI-TOF) Calculated for $C_9H_5ClF_3I$ (M^+) 331.9077, found 331.9070.

(*E*)-1-(1-chloro-2-iodovinyl)-4-(trifluoromethoxy)benzene (3m). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (68 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.7 Hz, 2H), 7.28 (d, *J* = 7.8 Hz, 2H), 6.85 (s, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.70 (s). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.6, 136.1, 132.7, 130.8, 120.5, 120.3 (q, *J* = 256 Hz), 73.9. HRMS (EI-TOF) Calculated for $C_9H_5ClF_3IO$ (M^+) 347.9026, found 347.9020.

(*E*)-1-chloro-4-(1-chloro-2-iodovinyl)benzene (3n). Purified by column chromatography on silica gel (eluant: petroleum ether = 9:1). Colorless oil (56 mg, 96%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.5 Hz, 2H),

7.38 (d, *J* = 8.5 Hz, 2H), 6.79 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.0, 135.4, 133.0, 130.4, 128.6, 73.6. HRMS (EI-TOF) Calculated for $C_8H_5Cl_2I$ (M^+) 297.8813, found 297.8819.

(*E*)-1-bromo-4-(1-chloro-2-iodovinyl)benzene (3o). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (64 mg, 94%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.52 (m, 2H), 7.41 (d, *J* = 8.5 Hz, 2H), 6.79 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.5, 133.0, 131.5, 130.6, 123.7, 73.7. HRMS (EI-TOF) Calculated for C_8H_5BrClI (M^+) 341.8308, found 341.8301.

(*E*)-1-(tert-butyl)-4-(1-chloro-2-iodovinyl)benzene (3p). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (63 mg, 98%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.6 Hz, 2H), 7.42 (d, *J* = 8.6 Hz, 2H), 6.73 (s, 1H), 1.35 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.7, 134.5, 134.2, 128.7, 125.1, 72.0, 34.8, 31.2.HRMS (EI-TOF) Calculated for $C_{12}H_{14}ClI$ (M^+) 319.9829, found 319.9833.

(*E*)-4-(1-chloro-2-iodovinyl)-1, 1'-biphenyl (3q). Purified by column chromatography on silica gel (eluant: petroleum ether = 7:1). Colorless oil (62 mg, 93%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.70 - 7.68 (m, 6H), 7.53 (t, *J* = 7.3 Hz, 2H), 7.46 - 7.43 (m, 1H), 6.85 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 140.2, 136.4, 133.9, 129.5, 128.9, 127.9, 127.2, 127.0, 73.0. HRMS (EI-TOF) Calculated for $C_{14}H_{10}ClI$ (M^+) 339.9516, found 339.9510.

(*E*)-1-(benzyloxy)-4-(1-chloro-2-iodovinyl)benzene (3r). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 50:1). Colorless oil (66 mg, 89%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.52 (m, 2H), 7.46 – 7.34 (m, 5H), 7.03 (d, *J* = 8.8 Hz, 2H), 6.72 (s, 1H), 5.13 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.5, 136.5, 134.0, 130.6, 130.0, 128.6, 128.1, 127.5, 114.4, 71.7, 70.1. HRMS (EI-TOF) Calculated for $C_{15}H_{12}ClIO$ (M^+) 369.9621, found 369.9620.

(*E*)-2-(1-chloro-2-iodovinyl)naphthalene (3s). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (56 mg, 89%). ^1H NMR (400 MHz, $CDCl_3$) δ 8.04 – 8.03 (m, 1H), 7.91 – 7.85 (m, 3H), 7.60 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.57 – 7.51 (m, 2H), 6.85 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.9, 134.2, 133.4, 132.5, 129.0, 128.4, 128.1, 127.8, 127.2, 126.6, 125.8, 73.2. HRMS (EI-TOF) Calculated for $C_{12}H_8ClI$ (M^+) 313.9359, found 313.9350.

(*E*)-2-(1-chloro-2-iodovinyl)benzofuran (3t). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (54 mg, 91%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.7 Hz, 1H), 7.57 (d, *J* = 8.3 Hz, 1H), 7.44 – 7.39 (m, 2H), 7.34 – 7.29 (m, 1H), 6.95 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$)

δ 154.7, 150.2, 127.5, 126.1, 124.2, 123.5, 121.8, 111.6, 110.3, 71.6. HRMS (EI-TOF) Calculated for $C_{10}H_6ClIO$ (M^+) 303.9152, found 303.9148.

(*E*)-2-(1-chloro-2-iodovinyl)benzo[*b*]thiophene (3u). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (60 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.82 (dd, *J* = 7.6, 1.5 Hz, 2H), 7.44 - 7.37 (m, 2H), 6.93 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.4, 138.2, 138.1, 128.3, 128.1, 125.9, 124.8, 124.5, 122.1, 72.7. HRMS (EI-TOF) Calculated for $C_{10}H_6ClIS$ (M^+) 319.8923, found 319.8917.

(*E*)-1-(1-chloro-2-iodovinyl)-9H-fluorene (3v). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (60 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 - 7.82 (m, 2H), 7.74 (s, 1H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.46 - 7.37 (m, 2H), 6.82 (s, 1H), 3.97 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 143.1, 143.0, 140.8, 135.8, 134.6, 128.0, 127.4, 126.9, 125.6, 125.1, 120.3, 119.5, 72.7, 36.9. HRMS (EI-TOF) Calculated for $C_{15}H_{10}ClI$ (M^+) 351.9516, found 351.9511.

(*E*)-(1-chloro-2-iodoprop-1-en-1-yl)benzene (3w). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (54 mg, 98%)[7]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.35 (m, 5H), 2.78 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.8, 129.2, 129.0, 128.8, 128.3, 92.0, 31.3.

(*E*)-(1-chloro-2-iodobut-1-en-1-yl)benzene (3x). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (56 mg, 97%)[7]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.28 (m, 5H), 2.88 (q, *J* = 7.4 Hz, 2H), 1.20 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.9, 129.2, 128.8, 128.3, 127.7, 102.8, 36.3, 13.1.

(*E*)-(1-chloro-2-iodopent-1-en-1-yl)benzene (3y). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (55 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.30 (m, 5H), 2.90 – 2.80 (m, 2H), 1.72 – 1.70 (m, 2H), 1.07– 1.03 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.1, 129.2, 128.7, 128.5, 128.3, 101.3, 43.9, 21.9, 12.9. HRMS (EI-TOF) Calculated for $C_{11}H_{12}ClI$ (M^+) 305.9672, found 305.9671.

(*E*)-3-chloro-2-iodo-3-phenylprop-2-en-1-ol (3z). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 8:1). Colorless oil (56 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.34 (m, 5H), 4.62 (d, *J* = 6.4 Hz, 2H), 2.15 (t, *J* = 6.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.9, 130.4, 129.3, 128.9, 128.4, 101.4, 67.8. HRMS (EI-TOF) Calculated for C_9H_8ClIO (M^+) 293.9308, found 293.9311.

(*E*)-(1-chloro-2-iodoethene-1,2-diyl)dibenzene (3aa).[8] Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (64 mg, 96%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.51 (m, 2H), 7.51 – 7.38 (m, 7H), 7.32 (t, *J* = 7.3 Hz, 1H).

(*E*)-4-(1, 6-dichloro-2-iodohex-1-en-1-yl)phenyl methanesulfonate (3ab). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 5:1). Colorless oil (74 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.7 Hz, 2H), 7.30 (d, *J* = 8.7 Hz, 2H), 3.62 (t, *J* = 6.4 Hz, 2H), 3.17 (s, 3H), 2.88 (t, *J* = 7.2 Hz, 2H), 1.94 – 1.77 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.1, 140.8, 131.1, 127.4, 121.9, 101.3, 44.6, 41.3, 37.6, 31.2, 25.8. HRMS (ESI-ORBITRAP) Calculated for $C_{13}H_{19}Cl_2IO_3SN$ $(M+NH_4)^+$ 465.9507, found 465.9502.

(*E*)-5-(1-chloro-2-iodo-5-phenylpent-1-en-1-yl)-1-tosyl-1H-indole (3ac). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 20:1). Colorless oil (100 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.6 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 3.7 Hz, 1H), 7.54 (d, *J* = 1.2 Hz, 1H), 7.37 – 7.30 (m, 3H), 7.30 – 7.24 (m, 5H), 6.69 – 6.68 (m, 1H), 2.97 – 2.89 (m, 2H), 2.81 – 2.73 (m, 2H), 2.39 (s, 3H), 2.09 – 1.98 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.2, 141.7, 137.1, 135.3, 134.5, 130.4, 130.0, 128.8, 128.5, 128.4, 127.1, 126.9, 125.9, 125.7, 122.4, 113.4, 109.0, 101.2, 41.9, 34.7, 30.2, 21.6. HRMS (ESI-ORBITRAP) Calculated for $C_{26}H_{24}ClINO_2S$ $(M+H)^+$ 576.0261, found 576.0262.

(*E*)-4-chloro-3-iodo-4-phenylbut-3-en-2-one (3ad). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 30:1). Colorless oil (49 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.46 (m, 2H), 7.43 – 7.41 (m, 3H), 2.57 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.0, 138.4, 131.1, 129.9, 128.9, 128.4, 92.3, 27.4. HRMS (ESI-ORBITRAP) Calculated for $C_{10}H_9ClIO$ $(M+H)^+$ 306.9386, found 306.9381.

(*E*)-3-chloro-2-iodo-3-phenylacrylaldehyde (3ae). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 40:1). Colorless oil (50 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.44 (s, 1H), 7.55 – 7.51 (m, 2H), 7.49 – 7.45 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.1, 149.1, 139.9, 130.8, 128.6, 128.5, 103.8. HRMS (ESI-ORBITRAP) Calculated for $C_9H_6ClIONa$ $(M+Na)^+$ 314.9050, found 314.9059.

(*E*)-3-chloro-2-iodo-3-phenylacrylonitrile (3af). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 20:1). Colorless oil (26 mg, 46%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.41 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 136.9, 131.3, 128.7, 128.6, 116.7, 52.5. HRMS (EI-TOF) Calculated for C_9H_5ClIN (M^+) 288.9155, found 288.9162.

(*8R, 9S, 13S, 14S*)-3-((*E*)-1-chloro-2-iodovinyl)-13-methyl-6, 7, 8, 9, 11, 12, 13, 14, 15, 16-decahydro-17*H*-cyclopenta[*a*]phenanthren-17-one (3ag). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 30:1). Colorless oil (66 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (s, 2H), 7.27 (s, 1H), 6.71 (s, 1H), 2.95 (dd, *J* = 8.5, 3.8 Hz, 2H), 2.52 (dd, *J* = 18.8, 8.6 Hz, 1H), 2.47 – 2.40 (m, 1H), 2.36 – 2.29 (m, 1H), 2.17 (dd, *J* = 18.4, 9.3 Hz, 1H), 2.11 – 2.02 (m, 2H), 2.01 – 1.95 (m, 1H), 1.69 – 1.61 (m, 2H), 1.60 –1.59 (m, 1H), 1.57 – 1.49 (m, 3H), 0.92 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.4, 136.6, 134.9, 134.1, 129.4, 126.4, 125.2, 72.1, 50.5, 47.9, 44.5, 37.9, 35.8, 31.6, 29.3, 26.4, 25.6, 21.6, 13.9. HRMS (ESI-ORBITRAP) Calculated for $C_{20}H_{23}ClIO$ $(M+H)^+$ 441.0482, found 441.0479.

(*1R, 2S, 5R*)-2-isopropyl-5-methylcyclohexyl 3-((*E*)-1-chloro-2-iodovinyl)benzoate (3ah). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 30:1). Colorless oil (72 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 1.5 Hz, 1H), 8.09 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.78 – 7.70 (m, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 6.86 (s, 1H), 5.01 –4.94 (m, 1H), 2.17–2.14 (m, 1H), 2.05 – 1.96 (m, 1H), 1.79 – 1.73 (m, 2H), 1.63 – 1.54 (m, 2H), 1.21 – 1.10 (m, 2H), 0.97– 0.94 (m, 7H), 0.82 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 137.9, 133.1, 131.1, 130.5, 130.3, 128.4, 75.3, 73.9, 47.3, 40.9, 34.3, 31.5, 26.5, 23.7, 22.1, 20.8, 16.6. HRMS (ESI-ORBITRAP) Calculated for $C_{19}H_{25}ClIO_2$ $(M+H)^+$ 447.0588, found 447.0582.

(*3aS, 5S, 6R, 6aS*)-5-((S)-2, 2-dimethyl-1,3-dioxolan-4-yl)-2, 2-dimethyltetrahydrofuro [2, 3-d][1, 3]dioxol-6-yl 3-((*E*)-1-chloro-2-iodovinyl)benzoate (3ai). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 10:1). Colorless oil (97 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (t, *J* = 1.5 Hz, 1H), 8.00 – 7.91 (m, 1H), 7.68 – 7.62 (m, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 6.75 (s, 1H), 5.86 (d, *J* = 3.7 Hz, 1H), 5.40 (d, *J* = 2.9 Hz, 1H), 4.55 (d, *J* = 3.7 Hz, 1H), 4.33 – 4.19 (m, 2H), 4.05 – 4.01 (m, 2H), 1.46 (s, 3H), 1.31 (s, 3H), 1.22 (s, 3H), 1.17 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.4, 138.2, 133.8, 132.8, 130.6, 130.4, 129.8, 128.7, 112.4, 109.5, 105.1, 83.4, 80.0, 74.4, 72.6, 67.4, 26.8, 26.7, 26.2, 25.2. HRMS (ESI-ORBITRAP) Calculated for $C_{21}H_{25}ClIO_7$ $(M+H)^+$ 551.0328, found 551.0325.

(*E*)-2-(1-chloro-2-iodovinyl)benzyl 2-(10-oxo-10,11-dihydrodibenzo[*b, f*]thiepin-2-yl)propanoate (3aj). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 20:1). Colorless oil (80 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 7.9 Hz, 1H), 7.55 (dd, *J* = 7.9, 4.0 Hz, 2H), 7.42 – 7.34 (m, 2H), 7.33 – 7.23 (m, 4H), 7.20 – 7.15 (m, 1H), 7.12 (dd, *J* = 8.0, 1.4 Hz, 1H), 6.72 (s, 1H), 5.14–5.04 (m, 2H), 4.31 (s, 2H), 3.75 (q, *J* = 7.1 Hz, 1H), 1.46 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.2,

173.5, 142.5, 140.2, 137.9, 137.8, 136.2, 133.3, 133.2, 132.5, 131.5, 131.5, 130.9, 129.8, 129.3, 129.1, 128.7, 128.7, 126.8, 126.5, 77.7, 64.1, 51.1, 45.1, 18.5. HRMS (ESI-ORBITRAP) Calculated for $C_{26}H_{21}ClIO_3S$ $(M+H)^+$ 574.9944, found 574.9935.

(*E*)-(1-chloro-2-iodovinyl)cyclopropane (3ak). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (36 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.27 (s, 1H), 2.23 – 2.16 (m, 1H), 0.98 – 0.90 (m, 2H), 0.85 – 0.80 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.7, 70.3, 18.4, 6.4. HRMS (EI-TOF) Calculated for C_5H_6ClI (M^+) 227.9203, found 227.9211.

(*E*)- (1-chloro-2-iodovinyl)cyclopentane (3al). Purified by column chromatography on silica gel (eluant: petroleum ether = 7:1). Colorless oil (42 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.25 (s, 1H), 3.46 – 3.36 (m, 1H), 1.88 – 1.75 (m, 4H), 1.72 – 1.62 (m, 4H). ^{13} NMR (101 MHz, $CDCl_3$) δ 142.3, 71.0, 46.4, 30.3, 25.9. HRMS (EI-TOF) Calculated for $C_7H_{10}ClI$ (M^+) 255.9516, found 255.9510.

(*E*)-2-chloro-1, 5-diiodopent-1-ene (3am). Purified by column chromatography on silica gel (eluant: petroleum ether = 5:1). Colorless oil (61 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (s, 1H), 3.57 (t, J = 6.5 Hz, 2H), 2.73 – 2.67 (m, 2H), 2.07 – 2.00 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 101.6, 80.6, 43.1, 42.4, 31.1. HRMS (EI-TOF) Calculated for $C_5H_7ClI_2$ (M^+) 355.8326, found 355.8321.

(*E*)-6-chloro-7-iodohept-6-en-1-ol (3an). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 5:1). Colorless oil (48 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.29 (s, 1H), 3.66 (t, J = 6.5 Hz, 2H), 2.61 – 2.56 (m, 2H), 1.64 – 1.58 (m, 4H), 1.46 – 1.39 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.0, 72.5, 62.8, 38.4, 32.5, 26.5, 24.6. HRMS (EI-TOF) Calculated for $C_7H_{12}ClIO$ (M^+) 273.9621, found 273.9616.

(*E*)-5-chloro-6-iodohex-5-en-1-yl 4-methylbenzenesulfonate (3ao). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 20:1). Colorless oil (66 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.3 Hz, 2H), 7.38 (d, J = 8.0 Hz, 2H), 6.33 (s, 1H), 4.09 (t, J = 6.0 Hz, 2H), 2.57 (t, J = 6.9 Hz, 2H), 2.48 (s, 3H), 1.74 – 1.64 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.8, 137.1, 133.1, 129.9, 127.9, 73.2, 70.0, 37.6, 27.5, 22.6, 21.7. HRMS (ESI-ORBITRAP) Calculated for $C_{13}H_{20}ClIO_3SN$ $(M+NH_4)^+$ 431.9897, found 431.9892.

(*E*)-6-chloro-7-iodohept-6-en-1-yl benzoate (3ap). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 30:1). Colorless oil (58 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J =

7.5 Hz, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 6.31 (s, 1H), 4.34 (t, *J* = 6.6 Hz, 2H), 2.61 (t, *J* = 7.3 Hz, 2H), 1.89 – 1.78 (m, 2H), 1.73 – 1.64 (m, 2H), 1.55 – 1.50 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 137.9, 132.8, 130.5, 129.6, 128.3, 72.6, 64.8, 38.4, 28.5, 26.3, 24.9. HRMS (ESI-ORBITRAP) Calculated for $C_{14}H_{17}ClIO_2$ $(M+H)^+$ 378.9962, found 378.9958.

(*E*)-2-(5-chloro-6-iodohex-5-en-1-yl)isoindoline-1,3-dione (3aq). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 10:1). Colorless oil (56 mg, 73%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.53 (m, 2H), 7.72 – 7.70 (m, 2H), 6.31 (s, 1H), 3.72 (t, *J* = 7.0 Hz, 2H), 2.62 (t, *J* = 7.1 Hz, 2H), 1.77 – 1.64 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.4, 137.5, 133.9, 132.1, 123.2, 72.9, 37.9, 37.7, 27.4, 23.9. HRMS (ESI-ORBITRAP) Calculated for $C_{14}H_{14}ClINO_2$ $(M+H)^+$ 389.9758, found 389.9751.

(*E*)-1, 2, 4-trichloro-3-iodobut-2-ene (3ar). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (50 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.57 (s, 2H), 4.50 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.5, 97.4, 52.1, 51.4. HRMS (EI-TOF) Calculated for $C_4H_4Cl_3I$ (M^{+}) 283.8430, found 283.8423.

(*E*)-4-chloro-5-iodooct-4-ene (3as). Purified by column chromatography on silica gel (eluant: petroleum ether). Colorless oil (47 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.70 – 2.61 (m, 4H), 1.64 – 1.53 (m, 4H), 0.97 –0.91 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 131.5, 99.2, 44.7, 43.6, 21.7, 20.5, 13.1, 12.8. HRMS (EI-TOF) Calculated for $C_8H_{14}ClI$ (M^+) 271.9829, found 271.9833.

(*E*)-1-(1-chloro-2-I odoprop-1-en-1-yl)cyclohexan-1-ol (3at). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 10:1). Colorless oil (48 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.79 (s, 1H), 2.54 (d, *J* = 1.4 Hz, 3H), 2.13 – 2.05 (m, 2H), 1.84 – 1.80 (m, 2H), 1.71 – 1.54 (m, 5H), 1.28 – 1.13 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 125.3, 113.6, 75.9, 36.9, 35.6, 25.1, 22.3. HRMS (ESI-ORBITRAP) Calculated for $C_9H_{15}ClIO$ $(M+H)^+$ 300.9856, found 300.9860.

(*E*)-(((3-chloro-2-iodonon-2-en-4-yl)oxy)methyl)benzene (3au). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 50:1). Colorless oil (58 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.27 (m, 5H), 4.52 – 4.18 (m, 2H), 3.99 (t, *J* = 6.7 Hz, 1H), 2.48 (s, 3H), 1.70 – 1.61 (m, 1H), 1.52 – 1.44 (m, 1H), 1.29 – 1.26 (m, 6H), 0.87 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.9, 129.5, 128.3, 128.2, 127.6, 107.9, 78.5, 70.3, 35.3, 31.6, 31.1, 24.3, 22.5, 14.0. HRMS (ESI-ORBITRAP) Calculated for $C_{16}H_{26}ClION$ $(M+NH_4)^+$ 410.0747, found 410.0742.

Methyl (E)-3-chloro-2-iodooct-2-enoate (3av). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 30:1). Colorless oil (42 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3H), 2.72 – 2.65 (m, 2H), 1.65 –1.56 (m, 2H), 1.36 –1.34 (m, 4H), 0.91 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4, 139.7, 79.5, 53.2, 41.7, 30.7, 26.4, 22.4, 13.8. HRMS (ESI-ORBITRAP) Calculated for $C_9H_{15}ClIO_2$ $(M+H)^+$ 316.9805, found 316.9800.

(*E*)-(2-chloro-1-iodo-2-phenylvinyl)(methyl)sulfane (3aw). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (51 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.31 (m, 4H), 7.31 –7.27 (m, 1H), 2.53 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6, 129.1, 128.9, 128.3, 128.2, 93.1, 18.5. HRMS (EI-TOF) Calculated for C_9H_8ClIS (M^+) 309.9081, found 309.9074.

(*E*)-(2,5-dichloro-1-iodopent-1-en-1-yl)(phenyl)sulfane (3ax). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (56 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.1 Hz, 2H), 7.18 (d, *J* = 7.9 Hz, 2H), 3.57 (t, *J* = 6.6 Hz, 2H), 2.97 – 2.92 (m, 2H), 2.36 (s, 3H), 2.12 – 2.04 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.9, 132.6, 130.0, 128.7, 127.9, 104.1, 43.3, 40.7, 31.5, 21.3. HRMS (EI-TOF) Calculated for $C_{12}H_{13}Cl_2IS$ (M^+) 385.9160, found 385.9166.

(*E*)-1-((2-chloro-1-iodohept-1-en-1-yl)oxy)-4-methylbenzene (3ay). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (60 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 2.64 – 2.56 (m, 2H), 2.32 (s, 3H), 1.66 – 1.58 (m, 2H), 1.40 – 1.37 (m, 4H), 0.95 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.0, 133.7, 130.2, 117.3, 104.1, 91.1, 43.9, 30.6, 28.3, 22.5, 20.8, 14.0. HRMS (EI-TOF) Calculated for $C_{14}H_{18}ClIO$ (M^+) 364.0087, found 364.0091.

(*E*)-(2-chloro-1-iodo-2-phenylvinyl)trimethylsilane (3az).[9] Purified by column chromatography on silica gel (eluant: petroleum ether = 10:1). Colorless oil (53 mg, 80%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37 - 7.35 (m, 3H), 7.32 (dd, *J* = 7.7, 1.7 Hz, 2H), -0.02 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.8, 139.7, 129.3, 128.7, 128.3, 109.4, 0.9.

(*E*)-(1,2-dichloro-2-iodovinyl)benzene (3ba). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (58 mg, 98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (s, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.3, 133.4, 129.6, 129.2, 128.6, 69.7. HRMS (EI-TOF) Calculated for $C_8H_5Cl_2I$ (M^+) 297.8813, found 297.8818.

(*E*)-(2-bromo-1-chloro-2-iodovinyl)benzene (3bb).[10] Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (64 mg, 94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (s, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.7, 136.0, 129.6, 128.8, 128.6, 51.8.

(1-chloro-2,2-diiodovinyl)benzene (3bc).[11] Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (70 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.9 Hz, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.7, 139.6, 129.4, 128.6, 128.5, 14.3.

(*E*)-1-(2-bromo-1-chloro-2-iodovinyl)-3-methylbenzene (3bd). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (70 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (t, *J* = 7.7 Hz, 1H), 7.19 (d, *J* = 7.5 Hz, 3H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.6, 138.4, 136.2, 130.3, 129.3, 128.5, 125.9, 51.6, 21.4. HRMS (EI-TOF) Calculated for C_9H_7BrClI (M^+) 355.8464, found 355.8466.

(*E*)-6-bromo-5-chloro-6-iodohex-5-enenitrile (3be). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 20:1). Colorless oil (54 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.83 (t, *J* = 7.4 Hz, 2H), 2.42 (t, *J* = 7.1 Hz, 2H), 2.02 (p, *J* = 7.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.4, 118.7, 51.3, 40.6, 23.2, 16.2. HRMS (ESI-ORBITRAP) Calculated for $C_6H_7BrClIN$ $(M+H)^+$ 333.8489, found 333.8490.

(*E*)-1-bromo-2-chloro-1-iodooct-1-ene (3bf). Purified by column chromatography on silica gel (eluant: petroleum ether = 20:1). Colorless oil (60 mg, 86%). 1H NMR (400 MHz, $CDCl_3$) δ 2.68 – 2.60 (m, 2H), 1.66 – 1.57 (m, 2H), 1.40 – 1.27 (m, 6H), 0.90 (t, J = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.4, 48.6, 41.9, 31.5, 28.2, 27.1, 22.5, 14.1. HRMS (EI-TOF) Calculated for $C_8H_{13}BrClI$ (M^+) 349.8934, found 349.8936.

(*E*)-1-chloro-3-(1-chloro-2-iodovinyl)benzene (3bg). Purified by column chromatography on silica gel (eluant: petroleum ether = 9:1). Light yellow oil (24 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.44 (m, 2H), 7.41 – 7.35 (m, 2H), 6.79 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.0, 135.5, 133.0, 130.4, 129.0. HRMS (EI-TOF) Calculated for $C_8H_5Cl_2I$ (M^+) 297.8813, found 297.8815.

(*E*)-3-(1-chloro-2-iodovinyl)quinoline (3bh). Purified by column chromatography on silica gel (eluant: petroleum ether = 9:1). Colorless oil (26 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (d, J = 2.3 Hz, 1H), 8.33 (d, J = 2.2 Hz, 1H), 8.14 (d, J = 8.4 Hz, 1H), 7.87 (dd, J = 8.2, 1.5 Hz, 1H), 7.81 – 7.74 (m, 1H), 7.65 – 7.56 (m, 1H), 6.97 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.9, 147.8, 136.8, 131.3, 131.0, 130.8, 129.4, 128.3, 128.1, 127.4, 126.9. HRMS (EI-TOF) Calculated for $C_{11}H_7ClIN$ (M^+) 314.9312, found 314.9314.

(*E*)-1-((2-chloro-1-iodoprop-1-en-1-yl)sulfonyl)-4-methylbenzene (3bi). Purified by column chromatography on silica gel (eluant: petroleum ether = 9:1). Brown solid (33 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 8.4 Hz, 2H), 2.57 (s, 3H), 2.45 (s, 3H), 1.25 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.0, 143.2, 136.1, 129.6, 128.8, 99.2, 34.9, 21.7. HRMS (ESI- ORBITRAP) Calculated for $C_{10}H_{10}ClIO_2S$ $(M+H)^+$ 356.9207, found 356.9212.

***(S,E)*-4-chloro-2-(3-((*S*)-1,5-diethoxy-1,5-dioxopentan-2-yl)ureido)-5-iodopent-4-enoic acid (3bj).** Purified by column chromatography on silica gel (eluant: petroleum ether = 5:5). Light yellow solid (31 mg, 42%).^{1}H NMR (400 MHz, $CDCl_3$) δ 5.75 (s, 1H), 4.40 (dd, J = 8.0, 4.9 Hz, 1H), 4.24 – 4.05 (m, 7H), 2.87 – 2.71 (m, 2H), 2.52 – 2.32 (m, 2H), 2.22 (dddd, J = 13.4, 8.4, 6.9, 4.9 Hz, 1H), 1.97 (dtd, J = 14.4, 8.3, 6.3 Hz, 1H), 1.30 – 1.22 (m, 9H).^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 172.3, 171.7, 150.1, 149.6, 61.5, 61.3, 60.6, 57.8, 54.1, 53.4, 30.2, 29.6, 28.6, 27.5, 14.2 (d, J = 7.5 Hz). HRMS (ESI-ORBITRAP) Calculated for Calculated for $C_{17}H_{26}IN_2O_7$ $(M-Cl)^+$ 497.07792, found 497.07784.

(8R,9S,13S,14S,17S)-17-((*E*)-1-chloro-2-iodovinyl)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene-3,17-diol (3bk). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:2). White solid (29 mg, 49%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.50 (m, 1H), 7.26 (s, 1H), 6.72 (s, 1H), 5.10 (s, 1H), 2.79 (dd, J = 8.7, 4.3 Hz, 2H), 2.61 (s, 1H), 2.40 – 2.22 (m, 2H), 2.19 (td, J = 10.9, 4.3 Hz, 1H), 2.09 – 1.97 (m, 1H), 1.96 – 1.63 (m, 4H), 1.56 – 1.22 (m, 4H), 0.88 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.5, 139.3, 135.1, 135.0, 114.9, 87.4, 82.4, 79.8, 74.1, 49.4, 47.0, 43.2, 39.1, 38.9, 32.6, 29.2, 27.0, 26.3, 22.8, 12.6. HRMS (ESI-ORBITRAP) Calculated for $C_{20}H_{25}ClIO_2$ $(M+H)^+$ 459.0582, found 459.0590.

methyl (*S,E*)-2-((tert-butoxycarbonyl)amino)-3-(4-(1-chloro-2-iodovinyl)phenyl)propanoate (3bl). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:2). Light yellow solid (33 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.44 (m, 2H), 7.18 (d, J = 7.9 Hz, 2H), 6.75 (s, 1H), 5.02 (d, J = 8.4 Hz, 1H), 4.62 (q, J = 6.9 Hz, 1H), 3.72 (s, 3H), 3.15 (dd, J = 13.7, 5.8 Hz, 1H), 3.06 (dd, J = 13.9, 6.4 Hz, 1H), 1.42 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 154.8, 137.8, 136.2, 133.8, 129.2, 129.2, 80.1, 72.8, 54.2, 52.3, 38.3, 28.3. HRMS (ESI-ORBITRAP) Calculated for $C_{17}H_{21}ClINO_4$ $(M+H)^+$ 466.0277, found 466.0279.

(*S,E*)-N-(2-chloro-3-(trifluoromethyl)benzyl)-1-(2-chloro-3-iodoallyl)-5-oxopyrrolidine-2-carboxamide (3bm). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:2). Light yellow solid (68 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (t, J = 7.9 Hz, 2H), 7.35 (t, J = 7.8 Hz, 1H), 7.11 (d, J = 1.2 Hz, 1H), 6.66 (t, J = 6.1 Hz, 1H), 4.66 – 4.61 (m, 2H), 4.61 – 4.57 (m, 1H), 4.04 – 3.90 (m, 2H), 2.63 – 2.49 (m, 1H), 2.52 – 2.32 (m, 2H), 2.08 (dtd, J = 11.7, 9.6, 8.5, 6.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 170.9, 137.5, 134.5, 132.0, 129.1 (q, *J* = 31.2 Hz), 127.2 (q, *J* = 1.4 Hz), 127.0, 122.7 (q, *J* = 274.5 Hz), 97.5, 83.7, 59.8, 52.6, 41.9, 29.4, 23.7. HRMS (ESI-ORBITRAP) Calculated for $C_{16}H_{15}Cl_2F_3IN_2O_2$ $(M+H)^+$ 520.9502, found 520.9508.

(*E*)-(1-bromo-2-iodoprop-1-en-1-yl)benzene (4a).[7] Purified by column chromatography on silica gel (eluant: petroleum ether = 20:1). Colorless oil (63 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.36 (m, 1H), 7.36 – 7.29 (m, 4H), 2.75 (s, 3H). ^{13}C NMR (101 MHz,$CDCl_3$) δ 143.8, 129.1, 128.7, 128.4, 118.3, 93.1, 34.5.

(*E*)-(1-bromo-2-iodopent-1-en-1-yl)benzene (4b). Purified by column chromatography on silica gel (eluant: petroleum ether = 8:1). Colorless oil (64 mg, 91%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.26 (m, 5H), 2.87 – 2.80 (m, 2H), 1.75 – 1.65 (m, 2H), 1.04 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.1, 129.1, 128.6, 128.4, 117.6, 102.2, 46.8, 21.8, 12.9. HRMS (EI-TOF) Calculated for $C_{11}H_{12}BrI$ (M^+) 349.9167, found 349.9166.

(*E*)-2-(1-bromo-2-iodovinyl)benzofuran (4c). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (60 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.8 Hz, 1H), 7.45 (d, *J* = 8.3 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.10 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.7, 150.8, 127.6, 126.2, 123.5, 121.8, 111.69, 111.3, 110.9, 74.1. HRMS (EI-TOF) Calculated for $C_{10}H_6BrIO$ (M^+) 347.8647, found 347.8641.

(*E*)-1-bromo-4-(1,2-diiodovinyl)benzene (4d).[12] Purified by column chromatography on silica gel (eluant: petroleum ether = 20:1). Colorless oil (68 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 6.79 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.5, 133.0, 131.6, 130.6, 123.8, 73.7.

(*E*)- (1, 2-diiodobut-1-en-1-yl)benzene (4e).[12] Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (53 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 - 7.33 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.1, 128.9, 128.5, 128.5, 96.2, 80.8.

(*E*)- (1, 2-dibromovinyl)benzene (4f).[13] Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (42 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.6 Hz, 2H), 7.43 - 7.35 (m, 3H), 6.81 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.1, 129.4, 129.2, 128.3, 121.3, 103.0.

(*E*)-2-(1-bromo-2-iodovinyl)benzofuran (4h). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (28 mg, 58%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.34 (m, 3H), 7.32 (d, *J* = 6.4 Hz, 2H), -0.05 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.5, 138.6, 134.7, 129.5, 129.4, 128.4, -0.65. HRMS (EI-TOF) Calculated for $C_{11}H_{14}Cl_2Si$ (M^+) 244.0242, found 244.0241.

(*E*)-(2-iodo-1-thiocyanatovinyl)benzene (4i).[14] Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 30:1). Colorless oil (37 mg, 66%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.52 – 7.44 (m, 5H), 7.28 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.9, 130.9, 130.3, 129.1, 129.0, 109.3, 81.3.

(*E*)-2-iodo-1-phenylvinyl acetate (4j).[15] Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 50:1). Colorless oil (24 mg, 43%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 - 7.59 (m, 2H), 7.39 -7.26 (m, 3H), 6.34 (s, 1H), 2.15 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.5, 151.2, 134.5, 129.5, 128.9, 128.2, 67.1, 20.8.

1-(1-chloro-2-iodoethyl)-4-fluorobenzene (5a). Purified by column chromatography on silica gel (eluant: petroleum ether = 20:1). Colorless oil (49 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.33 (m, 2H), 7.08 (t, *J* = 8.6 Hz, 2H), 5.06 (dd, *J* = 10.0, 5.5 Hz, 1H), 3.84 – 3.65 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.9 (d, *J* = 249.1 Hz), 135.0 (d, *J* = 3.3 Hz), 129.1 (d, *J* = 8.4 Hz), 115.8 (d, *J* = 22.6 Hz), 60.7, 9.9. HRMS (EI-TOF) Calculated for C_8H_7ClFI (M^+) 283.9365, found 283.9361.

1-bromo-4-(1-chloro-2-iodoethyl)benzene (5b). Purified by column chromatography on silica gel (eluant: petroleum ether = 20:1). Colorless oil (59 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.5 Hz, 2H), 7.26 (d, *J* = 8.5 Hz, 2H), 5.02 (dd, *J* = 10.0, 5.4 Hz, 1H), 3.84 – 3.63 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.1, 132.0, 128.9, 123.2, 60.6, 9.5. HRMS (EI-TOF) Calculated for C_8H_7BrClI (M^+) 343.8464, found 343.8469.

4-(1-chloro-2-iodoethyl)phenyl acetate (5c). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 50:1). Colorless oil (45 mg, 70%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.4 Hz, 2H), 5.17 - 5.15 (m, 1H), 4.13 – 3.98 (m, 2H), 2.33 (s, 3H). ^{13}C NMR (151

MHz, $CDCl_3$) δ 169.1, 151.0, 136.1, 128.9, 121.9, 50.1, 35.0, 21.2. HRMS (EI-TOF) Calculated for $C_{10}H_{10}ClIO_2$ (M^+) 323.9414, found 323.9411.

4-(1-chloro-2-iodoethyl)-1,1'-biphenyl (5d). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (52 mg, 76%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.58 (m, 4H), 7.47 – 7.44 (m, 4H), 7.40 – 7.35 (m, 1H), 5.13 (dd, *J* = 9.6, 5.8 Hz, 1H), 3.88 – 3.75 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.1, 140.3, 137.9, 128.8, 127.7, 127.7, 127.5, 127.2, 61.5, 9.8. HRMS (EI-TOF) Calculated for $C_{14}H_{12}ClI$ (M^+) 341.9672, found 341.9677.

1-(1-chloro-2-iodoethyl)-4-methylbenzene (5e). Purified by column chromatography on silica gel (eluant: petroleum ether = 50:1). Colorless oil (45 mg, 88%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 7.9 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 5.06 (dd, *J* = 9.7, 5.7 Hz, 1H), 3.84 – 3.69 (m, 2H), 2.37 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.2, 136.2, 129.5, 127.1, 61.6, 21.3, 10.1. HRMS (EI-TOF) Calculated for $C_9H_{10}ClI$ (M^+) 279.9516, found 279.9518.

1-(1-chloro-2-iodoethyl)-4-(trifluoromethyl)benzene (5f). Purified by column chromatography on silica gel (eluant: petroleum ether = 50:1). Colorless oil (44 mg, 66%). ^1H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 5.14 – 5.12 (m, 1H), 3.91 – 3.67 (m, 2H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -62.64 (s). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.9, 131.2 (q, *J* = 33.2 Hz), 127.8, 126.5, 125.8 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 271.8Hz), 60.3, 9.1. HRMS (EI-TOF) Calculated for $C_9H_7ClF_3I$ (M^+) 333.9233, found 333.9228.

1-(1-chloro-2-iodoethyl)-4-nitrobenzene (5g). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 15:1). Colorless oil (38 mg, 61%). ^1H NMR (600 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.6 Hz, 2H), 7.60 (d, *J* = 8.7 Hz, 2H), 5.16 – 5.13 (m, 1H), 3.87 – 3.67 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.2, 145.9, 128.5, 124.1, 59.5, 8.5. HRMS (EI-TOF) Calculated for $C_8H_7ClINO_2$ (M^+) 310.9210, found 310.9218.

Methyl-4-(1-chloro-2-iodoethyl)benzoate (5h). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 30:1). Colorless oil (47 mg, 73%). ^1H NMR (600 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.2 Hz, 2H), 7.48 (d, *J* = 8.2 Hz, 2H), 5.12 - 5.10 (m, 1H), 3.95 (s, 3H), 3.95 - 3.71 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.4, 143.8, 130.8, 130.1, 127.4, 60.6, 52.3, 9.1. HRMS (EI-TOF) Calculated for $C_{10}H_{10}ClIO_2$ (M^+) 323.9414, found 323.9218.

1-bromo-2-(1-chloro-2-iodoethyl)benzene (5i). Purified by column chromatography on silica gel (eluant: petroleum ether = 15:1). Colorless oil (53 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 –7.53 (m, 2H), 7.41 – 7.37 (m, 1H), 7.25 – 7.19 (m, 1H), 5.60 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.82 – 3.71 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.3, 133.1, 130.5, 128.2, 128.2, 123.8, 59.5, 8.5. HRMS (EI-TOF) Calculated for C_8H_7BrClI (M^+) 343.8464, found 343.8469.

1-bromo-3-(1-chloro-2-iodoethyl)benzene (5j). Purified by column chromatography on silica gel (eluant: petroleum ether = 20:1). Colorless oil (56 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.46 (m, 2H), 7.34 – 7.23 (m, 2H), 5.00 (dd, *J* = 9.8, 5.6 Hz, 1H), 3.81 – 3.63 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.3, 132.3, 130.4, 130.3, 125.9, 122.7, 60.5, 9.4. HRMS (EI-TOF) Calculated for C_8H_7BrClI (M^+) 343.8464, found 343.8469.

2-(1-chloro-2-iodoethyl)naphthalene (5k). Purified by column chromatography on silica gel (eluant: petroleum ether = 20:1). Colorless oil (45 mg, 71%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.6 Hz, 1H), 7.8 - 7.85 (m, 2H), 7.82 (d, *J* = 0.9 Hz, 1H), 7.54 – 7.49 (m, 3H), 5.27 - 5.24 (m, 1H), 3.92 – 3.83 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.2, 133.5, 132.9, 129.1, 128.2, 127.8, 127.2, 126.9, 126.7, 123.8, 62.0, 9.7. HRMS (EI-TOF) Calculated for $C_{12}H_{10}ClI$ (M^+) 315.9516, found 315.9521.

1-chloro-2-iodocyclooctane (5l). Purified by column chromatography on silica gel (eluant: petroleum ether = 5:1). Colorless oil (38 mg, 71%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 4.66 – 4.57 (m, 1H), 4.51 – 4.42 (m, 1H), 2.40 – 2.22 (m, 2H), 2.14 – 1.96 (m, 2H), 1.87 – 1.66 (m, 4H), 1.64 – 1.53 (m, 2H), 1.51 – 1.38 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 70.3, 41.9, 34.5, 33.3, 27.9, 25.6, 25.3, 25.2. HRMS (EI-TOF) Calculated for $C_8H_{14}ClI$ (M^+) 271.9829, found 271.9828.

(*4R*, *5R*)-4-chloro-5-iodooctane (5m). Purified by column chromatography on silica gel (eluant: petroleum ether = 5:1). Colorless oil (38 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.35 – 4.33 (m, 1H), 3.77–3.74 (m, 1H), 2.00 – 1.85 (m, 2H), 1.82 – 1.76 (m, 2H), 1.60 –1.57 (m, 2H), 1.46 – 1.35 (m, 2H), 1.03 – 0.86 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 66.4, 42.1, 38.8, 38.2, 22.8, 20.0, 13.5, 13.2. HRMS (EI-TOF) Calculated for $C_8H_{16}ClI$ (M^+) 273.9985, found 273.9991.

4-chloro-5-iodooctane (5m'). Purified by column chromatography on silica gel (eluant: petroleum ether = 5:1). Colorless oil (34 mg, 63%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 4.27 – 4.23 (m, 1H), 3.92 – 3.89 (m, 1H), 2.06 – 1.89 (m, 2H), 1.87 – 1.77 (m, 2H), 1.69 – 1.59 (m, 2H), 1.49 – 1.36 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 6H). ^{13}C NMR

(151 MHz, $CDCl_3$) δ 66.8, 42.3, 39.8, 39.1, 22.6, 19.4, 13.5, 13.2. HRMS (EI-TOF) Calculated for $C_8H_{16}ClI$ (M^+) 273.9985, found 273.9991.

2-(2-chloro-3-iodopropyl)isoindoline-1, 3-dione (5n). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 15:1). Colorless oil (58 mg, 83%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.76 (dd, *J* = 5.4, 3.1 Hz, 2H), 4.77 - 4.70 (m, 1H), 4.17 (d, *J* = 7.3 Hz, 2H), 4.05 - 3.87 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.7, 134.4, 131.7, 123.7, 48.3, 43.9, 26.3. HRMS (EI-TOF) Calculated for $C_{11}H_9ClINO_2$ (M^+) 348.9367, found 348.9371.

2-(2-chloro-3-iodopropoxy)benzaldehyde (5o). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 40:1). Colorless oil (41 mg, 63%). ^1H NMR (400 MHz, $CDCl_3$) δ 10.58 (s, 1H), 7.89 – 7.86 (m, 1H), 7.59 – 7.54 (m, 1H), 7.12 – 7.08 (m, 1H), 7.00 (t, *J* = 7.1 Hz, 1H), 4.59 – 4.37 (m, 3H), 4.15 – 3.67 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.4, 160.1, 136.0, 128.8, 125.2, 121.8, 112.8, 69.6, 46.2, 24.9. HRMS (EI-TOF) Calculated for $C_{10}H_{10}ClIO_2$ (M^+) 323.9414, found 323.9420.

4-(1-chloro-2-iodoethyl)-1, 3-dioxolan-2-one (5p). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 20:1). Colorless oil (37 mg, 68%). ^1H NMR (400 MHz, $CDCl_3$) δ 4.76 – 4.69 (m, 1H), 4.65 (t, *J* = 8.6 Hz, 1H), 4.28 – 4.19 (m, 2H), 4.12 – 3.98 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.7, 72.9, 69.5, 45.4, 31.8. HRMS (EI-TOF) Calculated for $C_5H_6ClIO_3$ (M^+) 275.9050, found 275.9058.

3-chloro-3-(iodomethyl)dihydrofuran-2(3*H*)-one (5q). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 40:1). Colorless oil (36 mg, 70%). ^1H NMR (400 MHz, $CDCl_3$) δ 4.45 (t, *J* = 8.8 Hz, 1H), 4.40 – 4.26 (m, 2H), 4.11 (d, *J* = 11.5 Hz, 1H), 2.87 – 2.78 (m, 1H), 2.41 (dd, *J* = 14.7, 5.3 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.7, 65.6, 48.6, 37.3, 33.8. HRMS (EI-TOF) Calculated for $C_5H_6ClIO_2$ (M^+) 259.9101, found 259.9105.

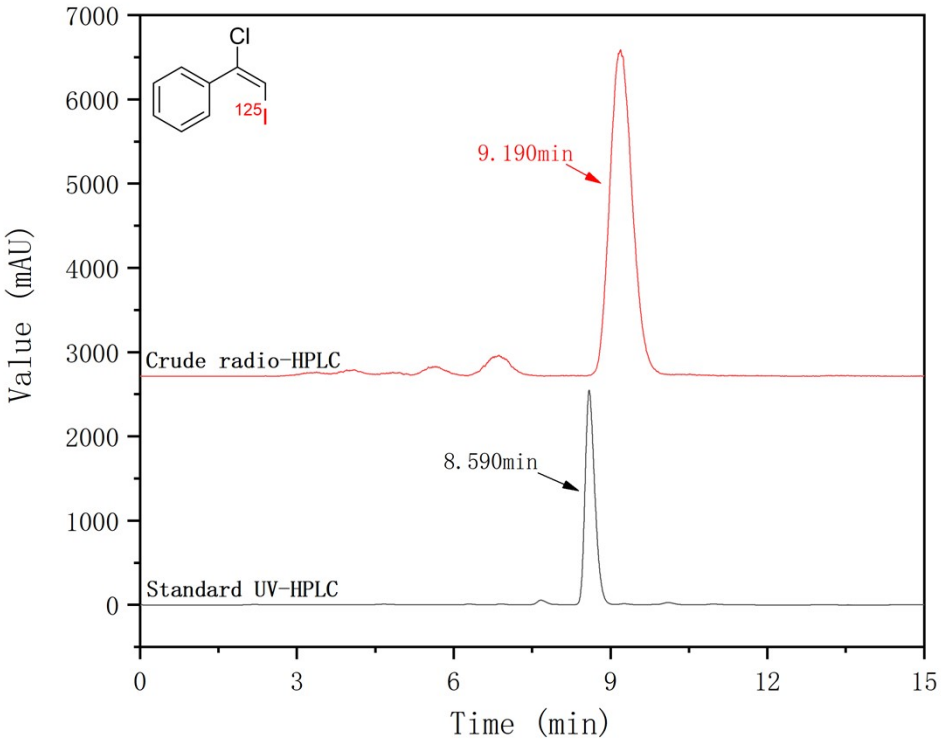
2-chloro-1-iododecane (5r). Purified by column chromatography on silica gel (eluant: petroleum ether). Colorless oil (40 mg, 66%). ^1H NMR (400 MHz, $CDCl_3$) δ 4.31 – 3.69 (m, 2H), 3.58 – 3.40 (m, 1H), 2.10 – 1.90 (m, 1H), 1.81 – 1.67 (m, 1H), 1.56 – 1.19 (m, 12H), 0.89 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 61.1, 50.0, 37.2, 36.4, 33.6, 31.8, 29.4, 29.4, 29.2, 29.2, 28.8, 28.7, 25.9, 22.7, 14.1, 11.1. HRMS (EI-TOF) Calculated for $C_{10}H_{20}ClI$ (M^+) 302.0298, found 302.0290.

4-(1-chloro-2-iodoethyl)phenyl acetate (5s). Purified by column chromatography on silica gel (eluant: petroleum ether/ethyl acetate = 50:1). Colorless oil (50 mg, 79%). ^1H NMR (600 MHz, $CDCl_3$) δ 7.49 – 7.34

(m, 2H), 7.22 – 7.07 (m, 2H), 5.10 - 5.08 (m, 1H), 3.88 – 3.58 (m, 2H), 2.33 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.2, 151.0, 136.6, 128.4, 121.9, 61.0, 21.2, 9.9. HRMS (EI-TOF) Calculated for $C_{10}H_{10}BrIO_2$ (M^+) 367.8909, found 367.8913.

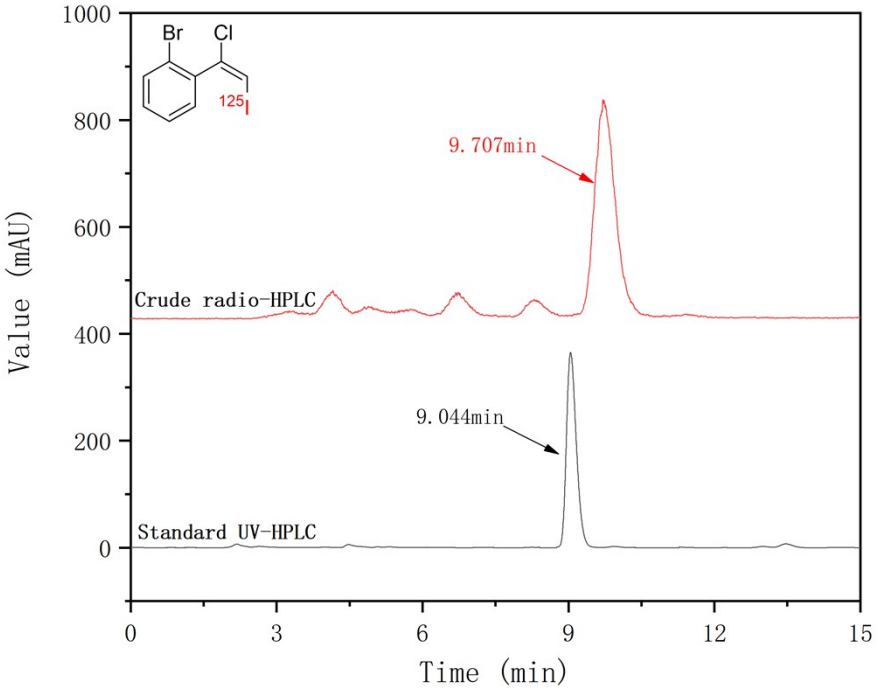
5. Radio-HPLC analysis and characterization for ^{125}I-labeled alkene

3a, tR = 8.59 min, RCY = 83±3%, n = 20



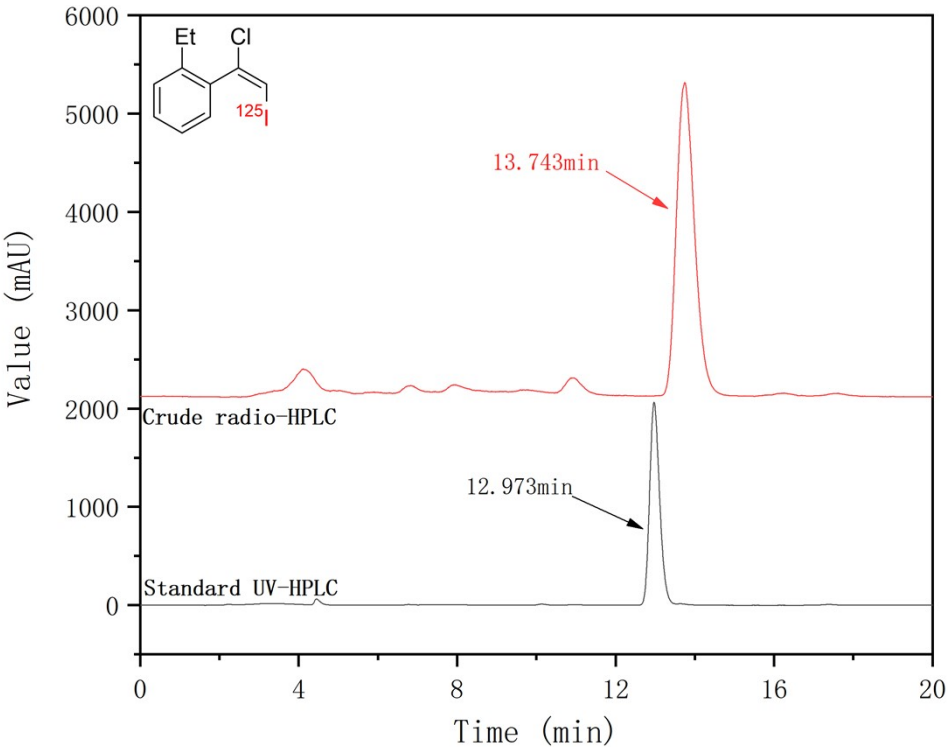
HPLC condition(SB-C18, MeCN/0.1 M ammonium formate buffer = 75/25, flow rate = 1 mL/min, λ = 254nm)

3b, tR = 9.04 min, RCY = 70±6%, n = 4



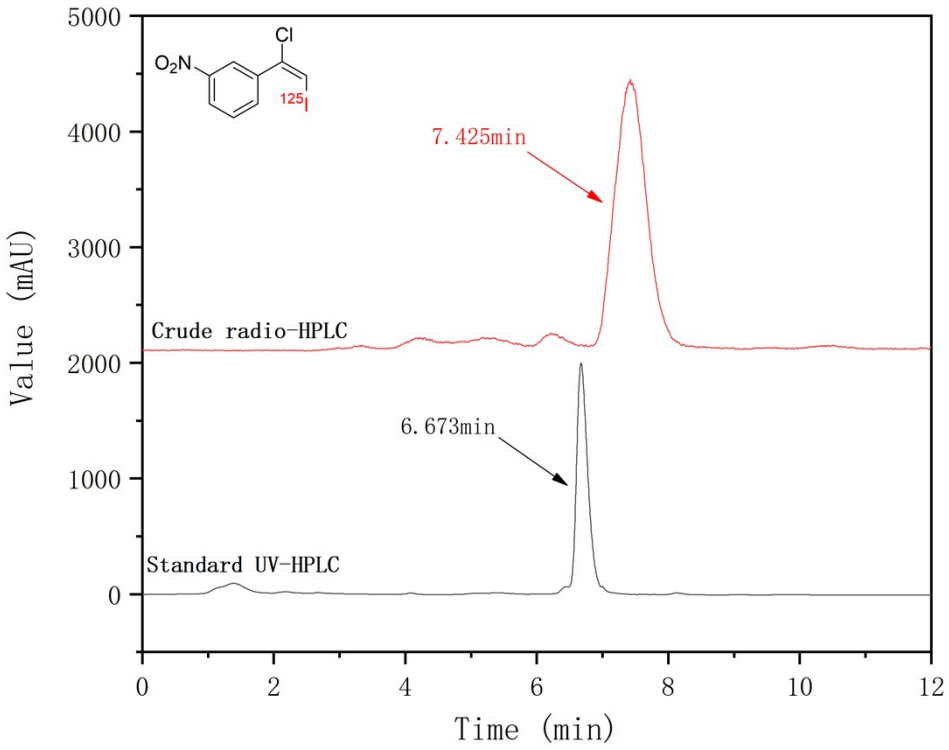
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer=75/25, flow rate = 1 mL/min, λ = 220 nm)

3c, tR = 12.97 min, RCY = 76±4%, n = 4



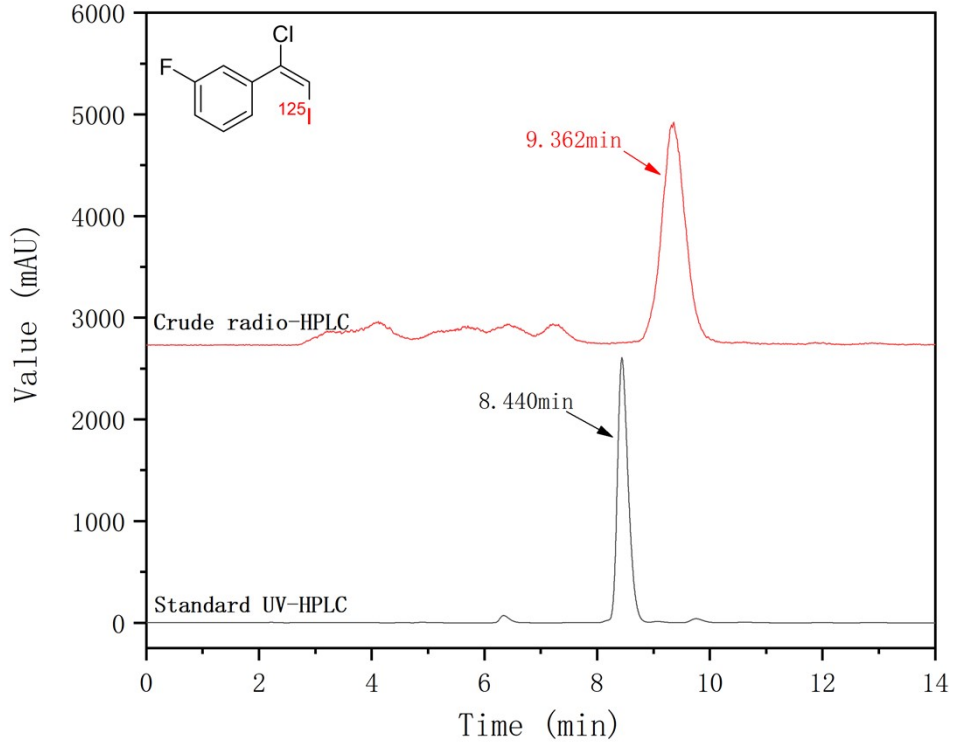
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 70/30, flow rate = 1 mL/min, λ = 254nm)

3f, tR = 6.67 min, RCY = 82±6 %, n = 4



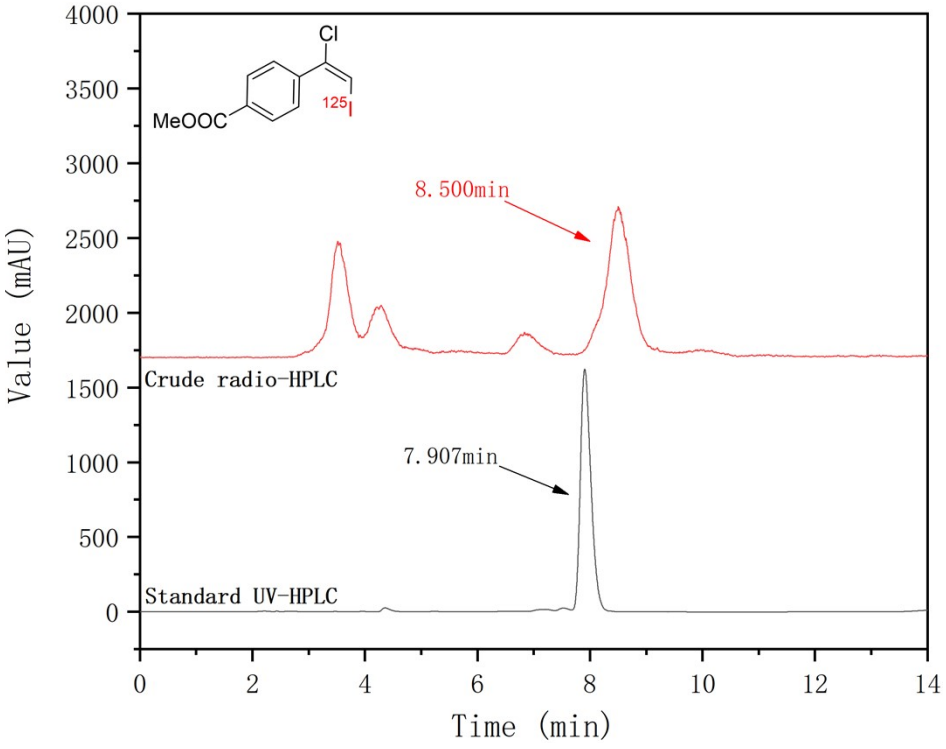
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 75/25, flow rate = 1 mL/min, λ = 220 nm)

3g, tR = 8.44 min, RCY = 69±8%, n = 4



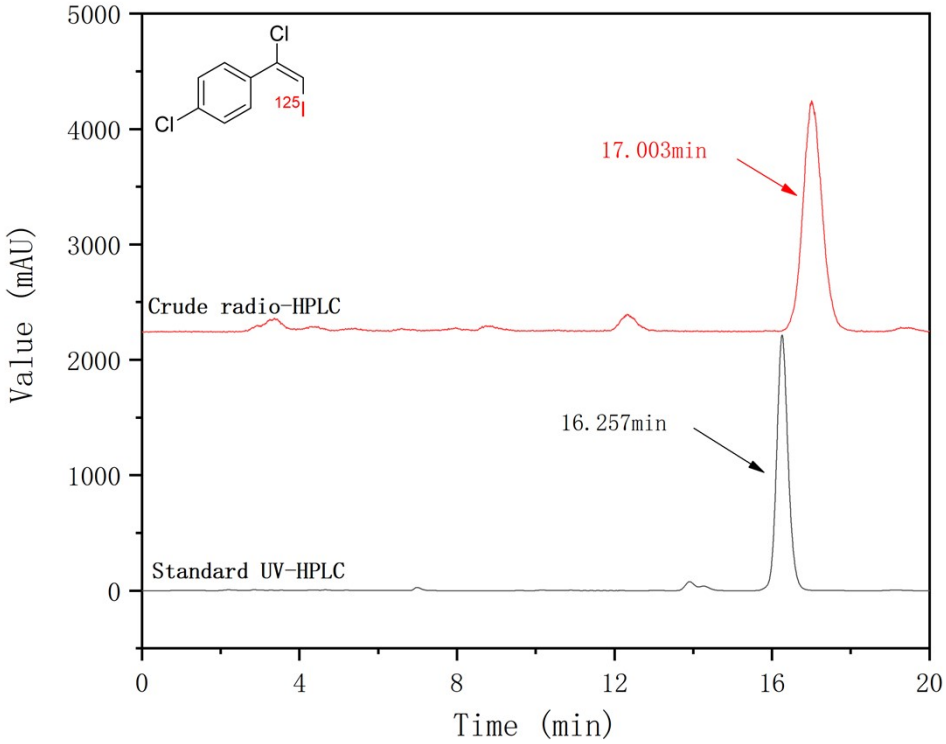
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 75/25, flow rate = 1 mL/min, λ = 220 nm)

3k, tR = 7.91 min, RCY = 40±6%, n = 4



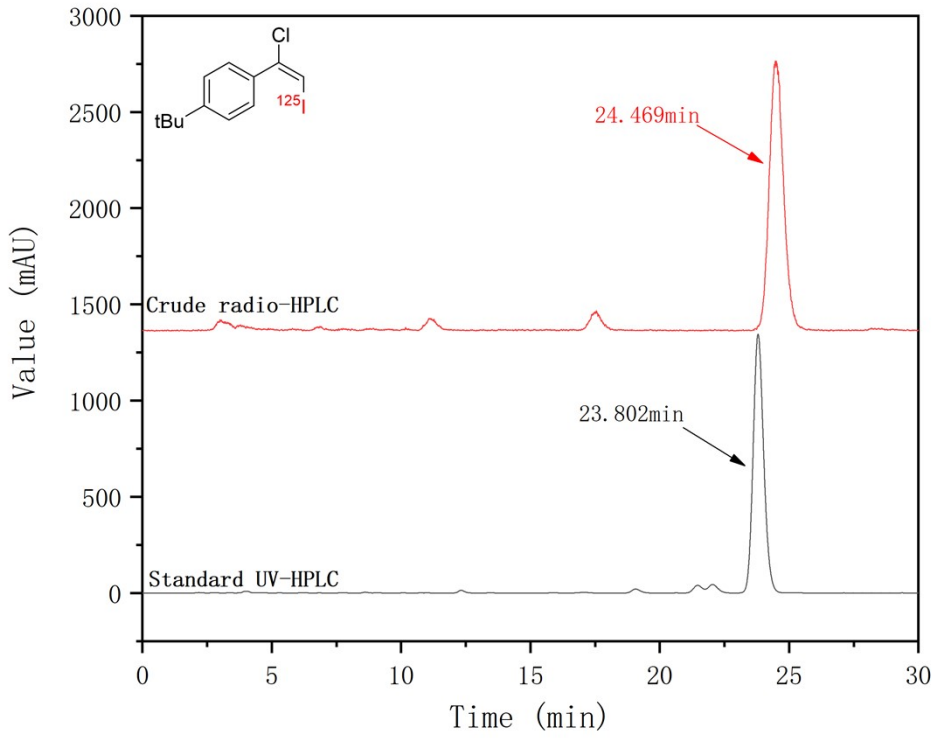
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 70/30, flow rate = 1 mL/min, λ = 220 nm)

3n, tR = 17.26 min, RCY = 82±3%, n = 4



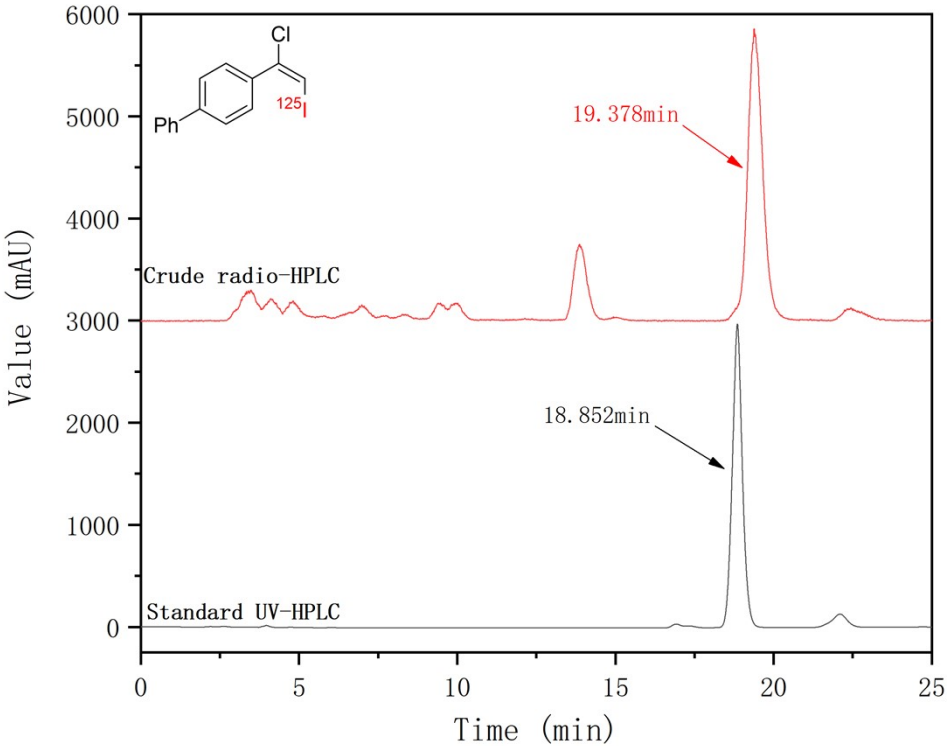
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 75/25, flow rate = 1 mL/min, λ = 220nm)

3p, tR =23.80 min, RCY = 85±2%, n = 3



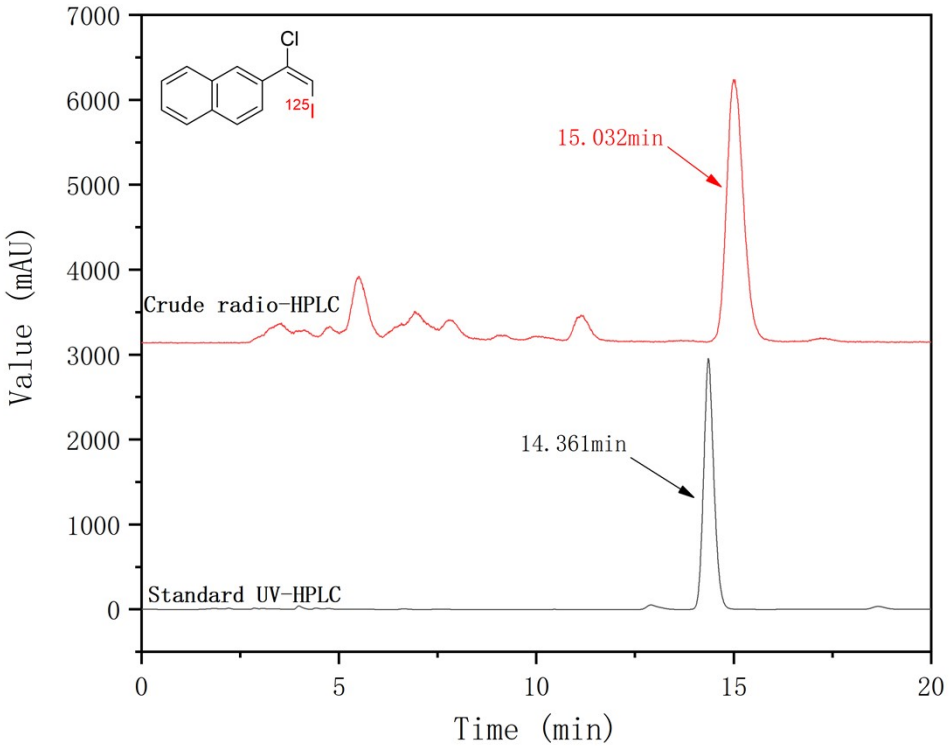
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 75/25, flow rate = 1 mL/min, λ = 220 nm)

3q, tR = 18.85 min, RCY = 60±7%, n = 3



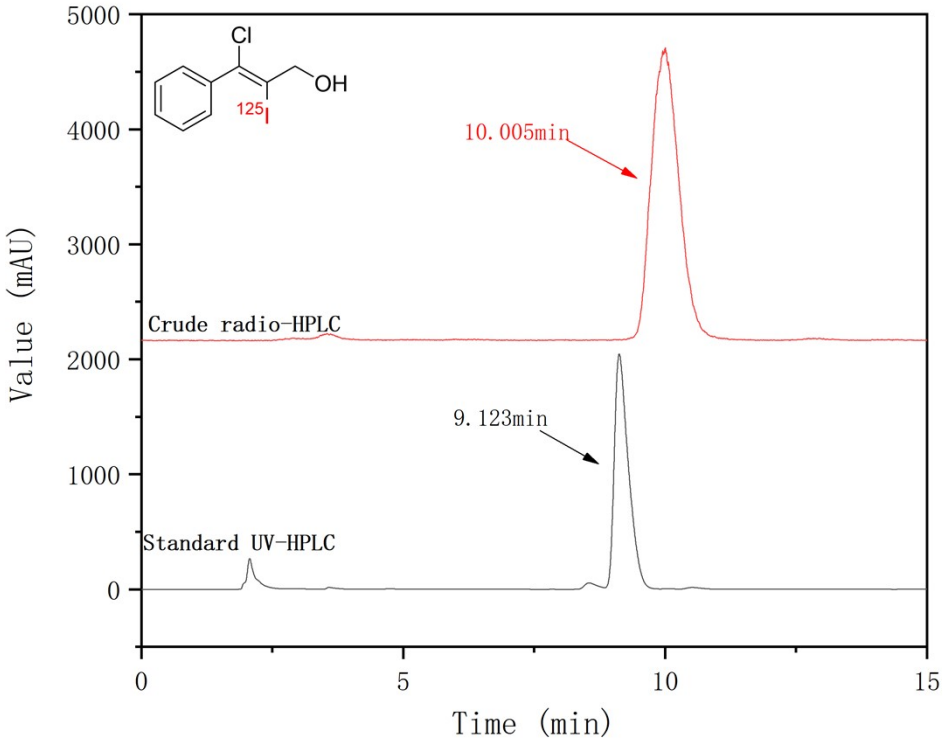
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer= 75/25, flow rate = 1 mL/min, λ = 220nm)

3s, tR = 14.36 min, RCY = 55±4%, n = 3



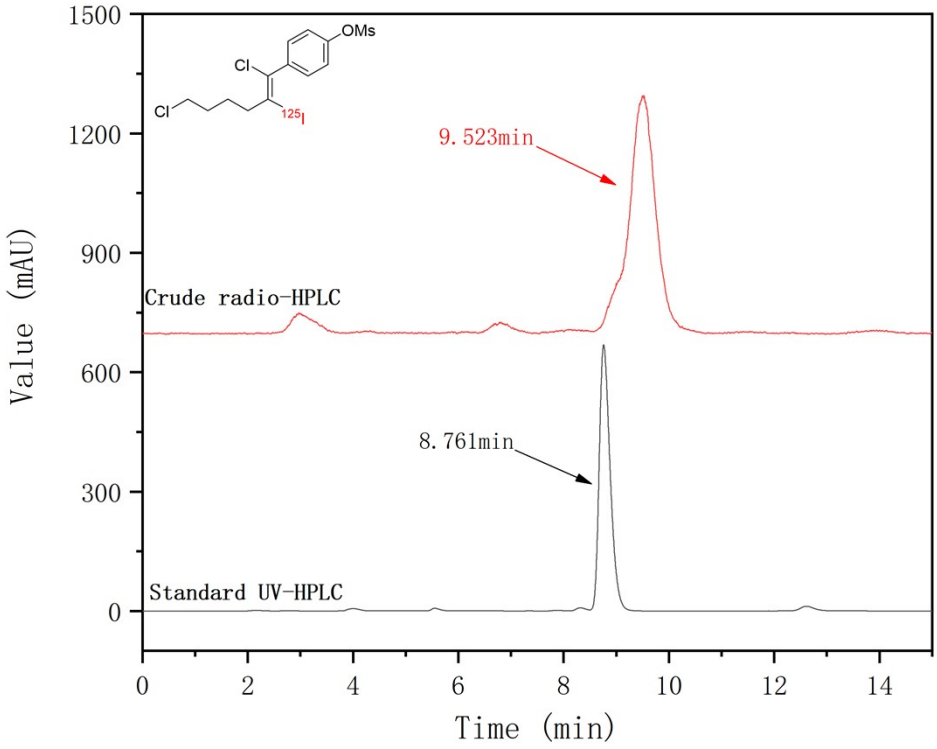
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 75/25, flow rate = 1 mL/min, λ = 220nm)

3z, tR = 9.12 min, RCY = 92±2%, n = 3



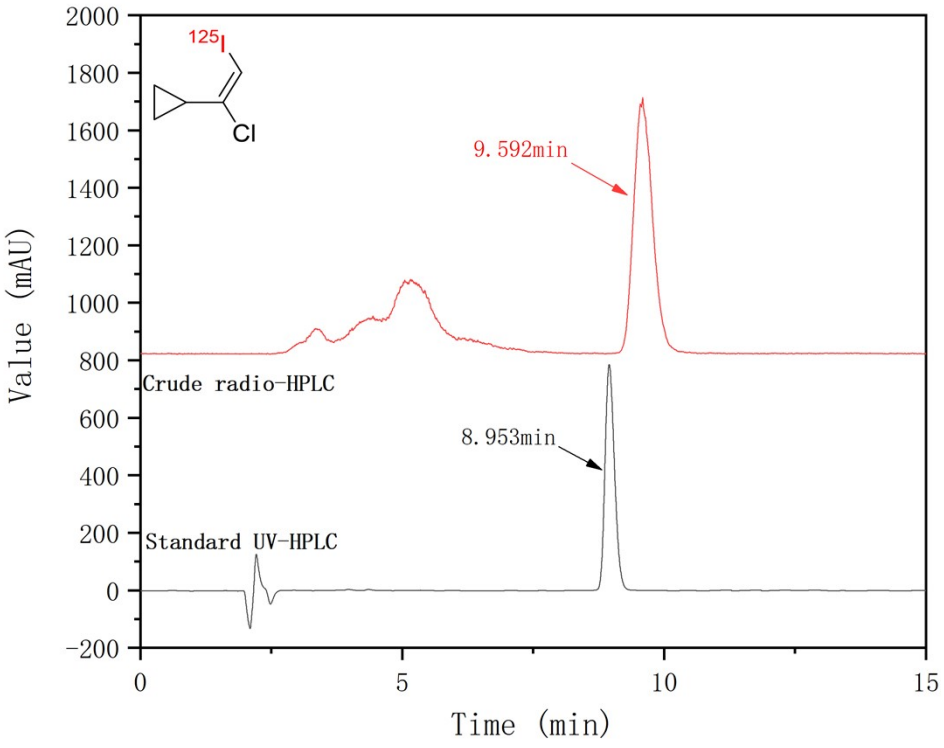
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 65/35, flow rate=1 mL/min, λ = 220nm)

3ab, tR = 8.76 min, RCY = 80±2%, n = 3



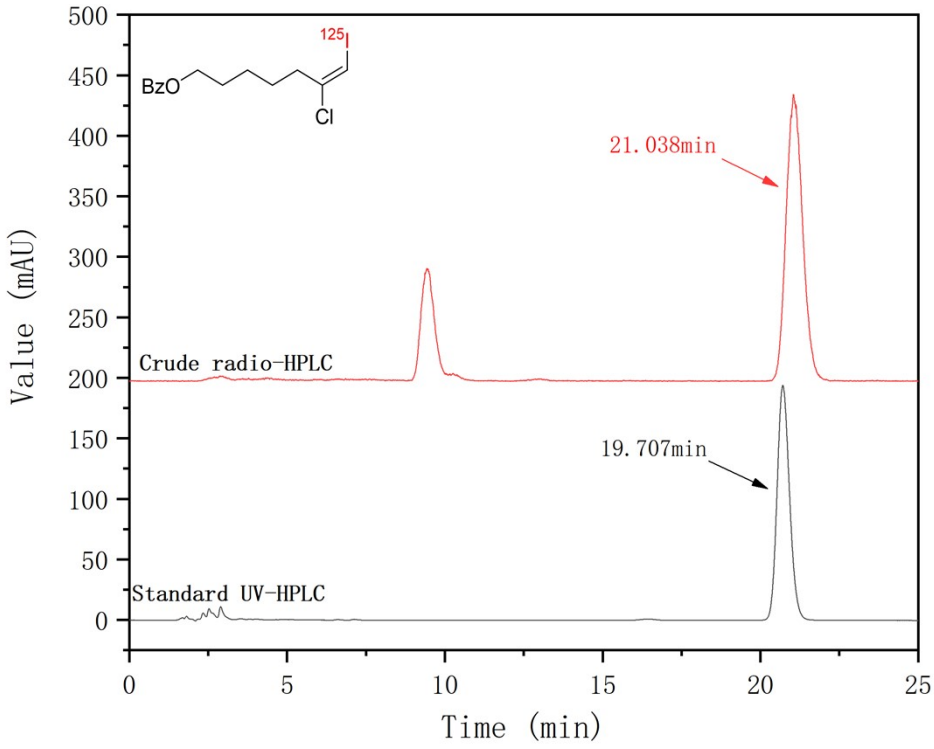
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer=75/25, flow rate = 1 mL/min, λ = 220nm)

3ak, tR = 8.95 min, RCY = 38±8%, n = 3



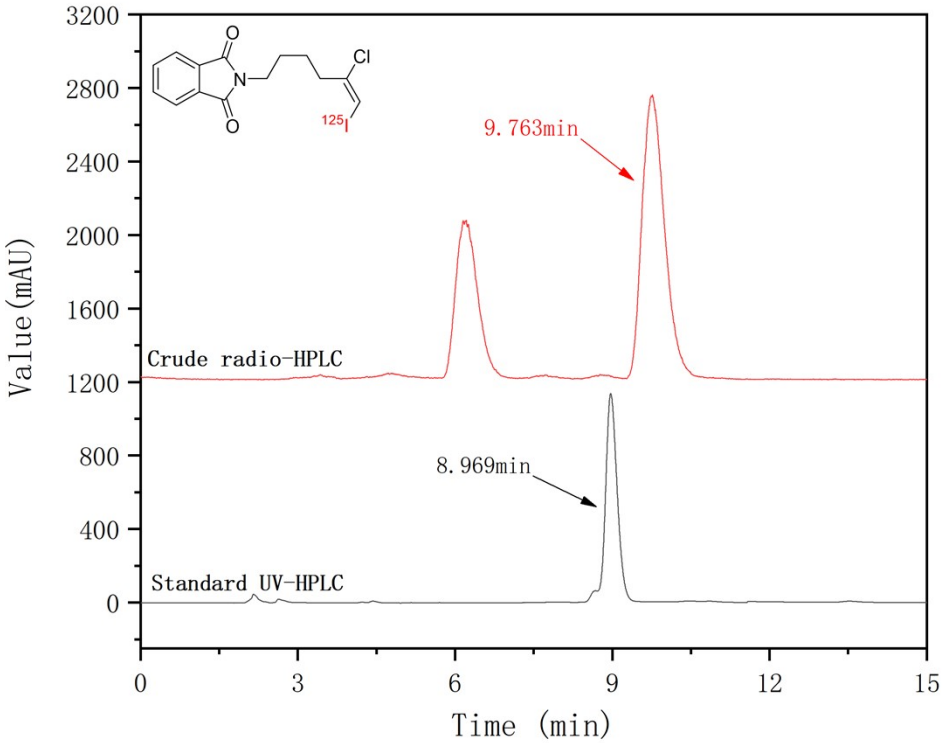
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer=75/25, flow rate=1 mL/min, λ =220nm)

3ap, tR = 17.71min, RCY = 70±3%, n = 3



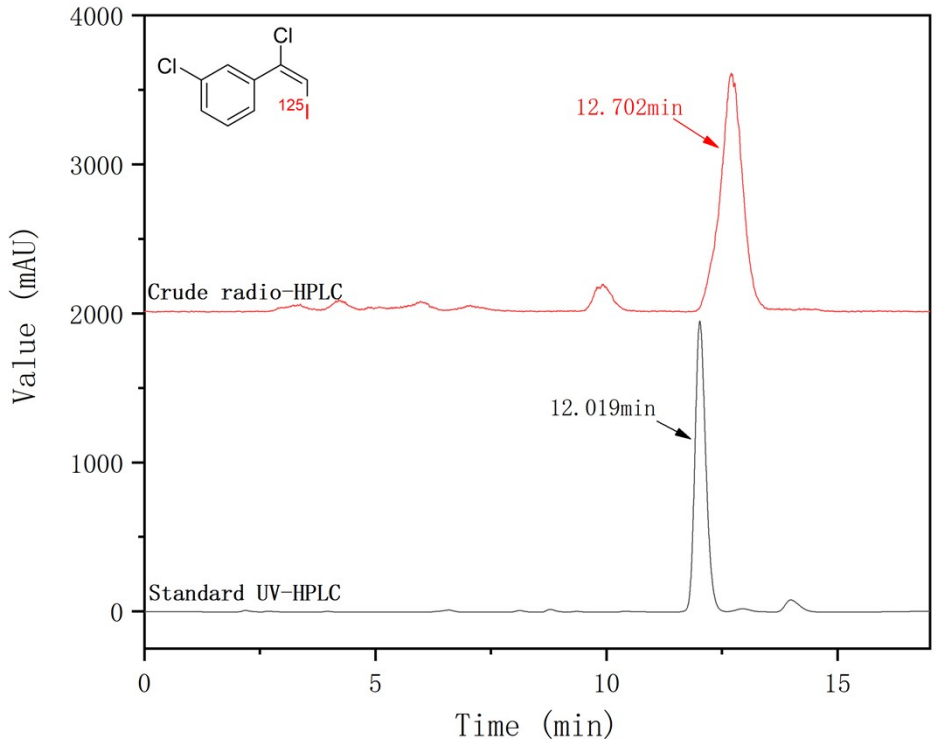
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 75/25, flow rate=1 mL/min, λ= 220 nm)

3aq, tR = 8.97 min, RCY = 51±5%, n = 3



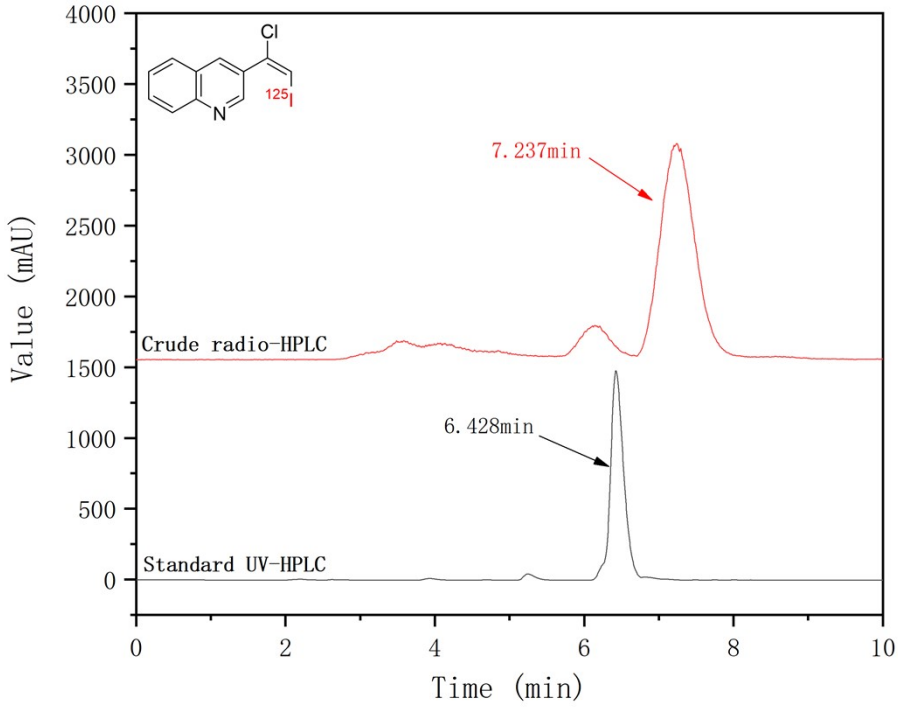
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer=75/25, flow rate=1 mL/min, λ =220nm)

3bg, tR = 12.02 min, RCY = 80±3%, n = 3



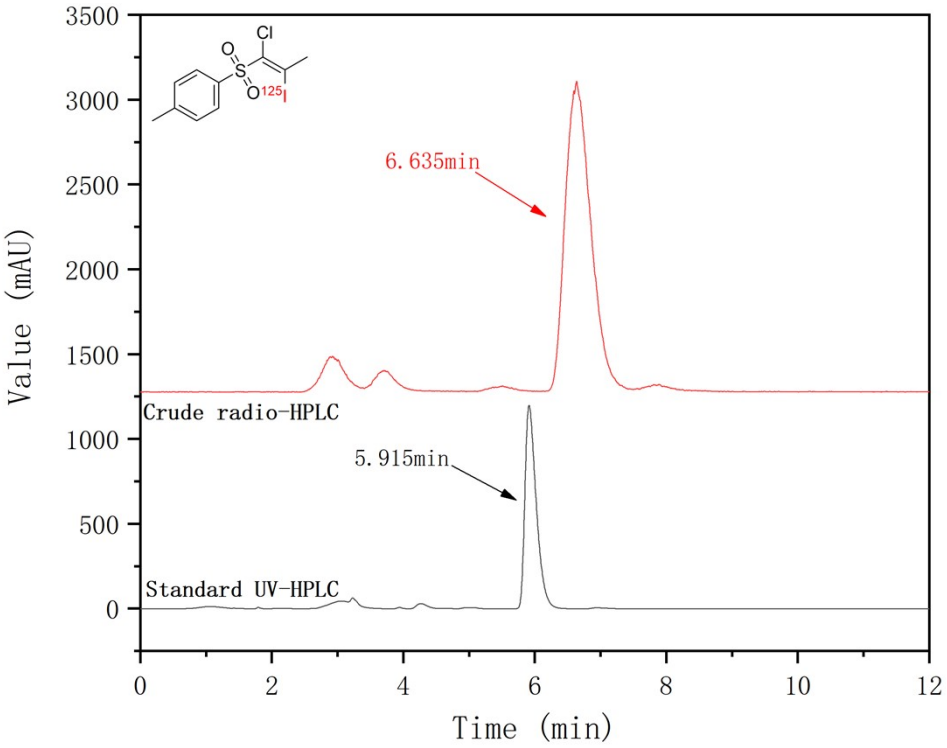
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 75/25, flow rate = 1 mL/min, λ= 220nm)

3bh, tR = 6.42 min, RCY = 65±5%, n = 3



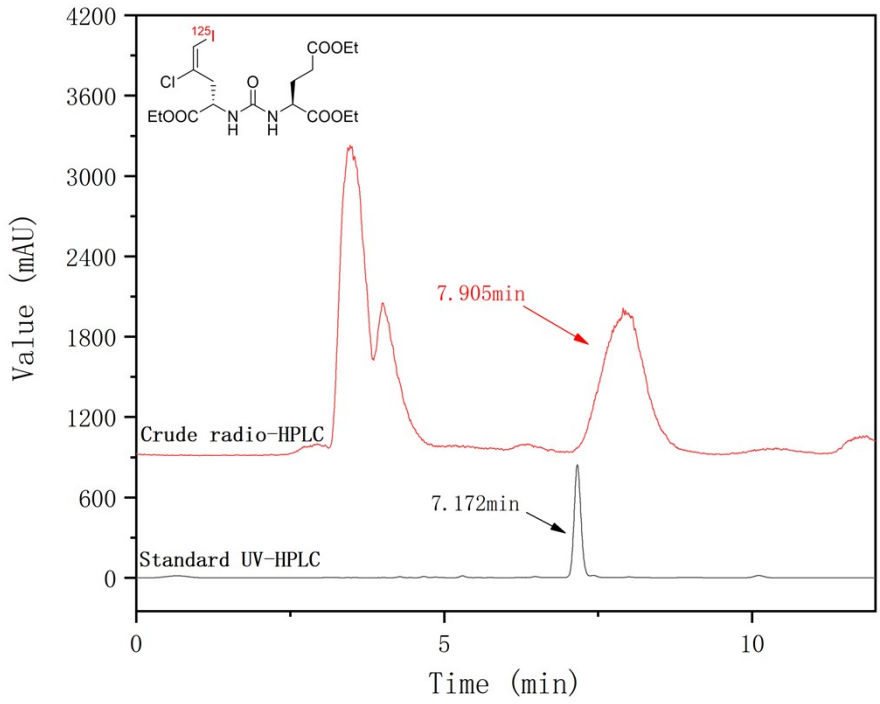
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer=75/25, flow rate = 1 mL/min, λ = 220 nm)

3bi, tR = 5.92 min, RCY = 76±4%, n = 3



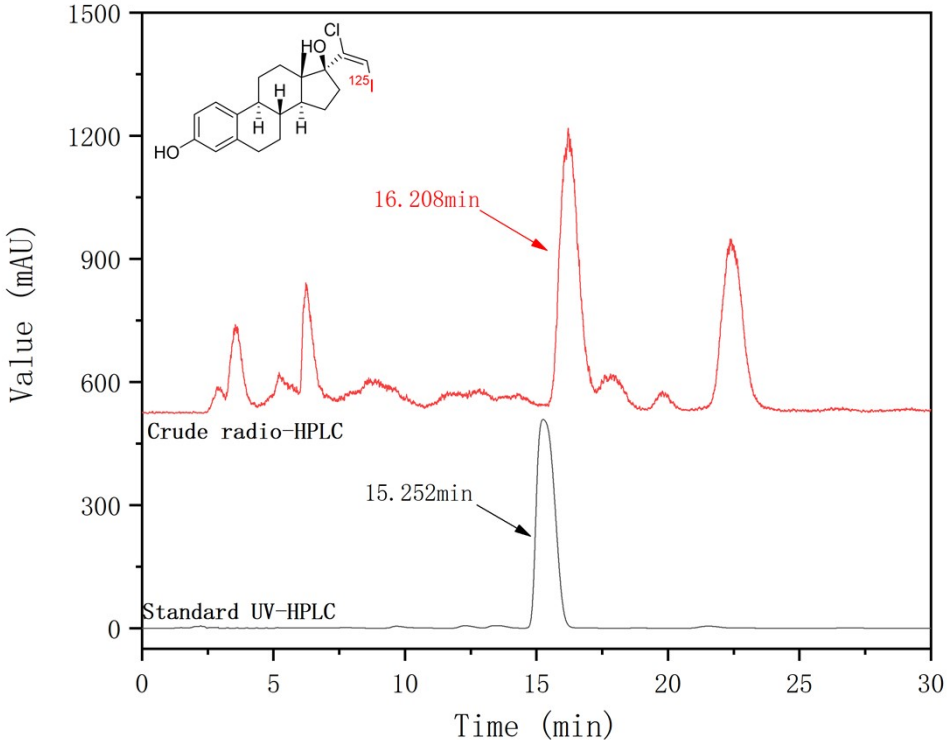
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 70/30, flow rate = 1 mL/min,λ = 220nm)

3bj, tR = 7.17 min, RCY = 30±7%, n = 3



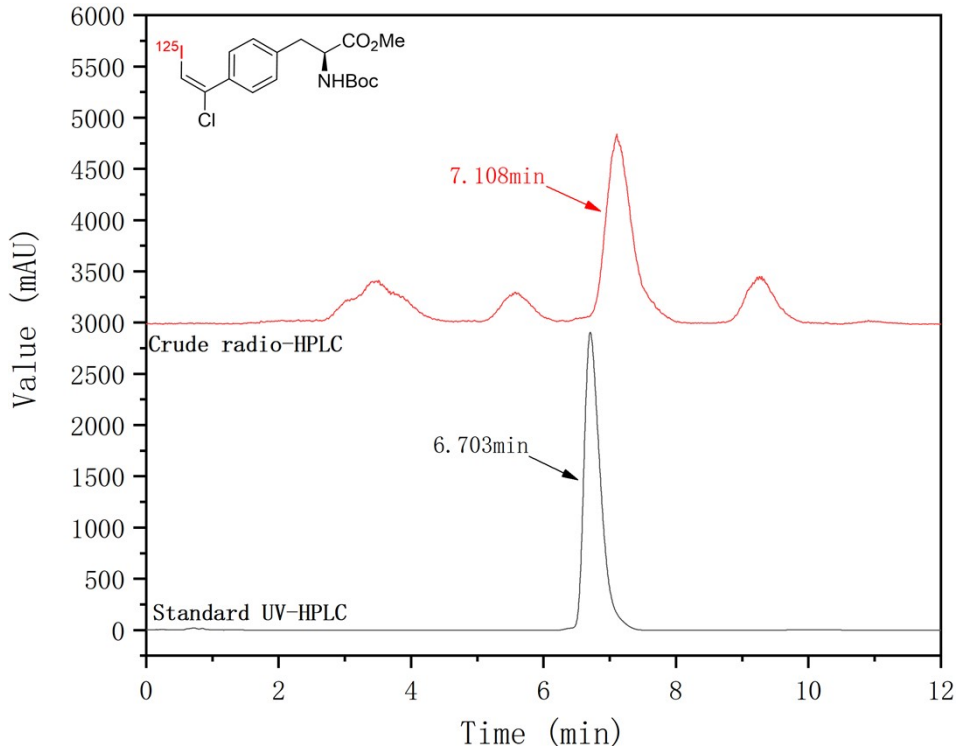
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 50/50, flow rate= 1 mL/min, λ = 220nm)

3bk, tR = 15.25 min, RCY = 28±10%, n = 3



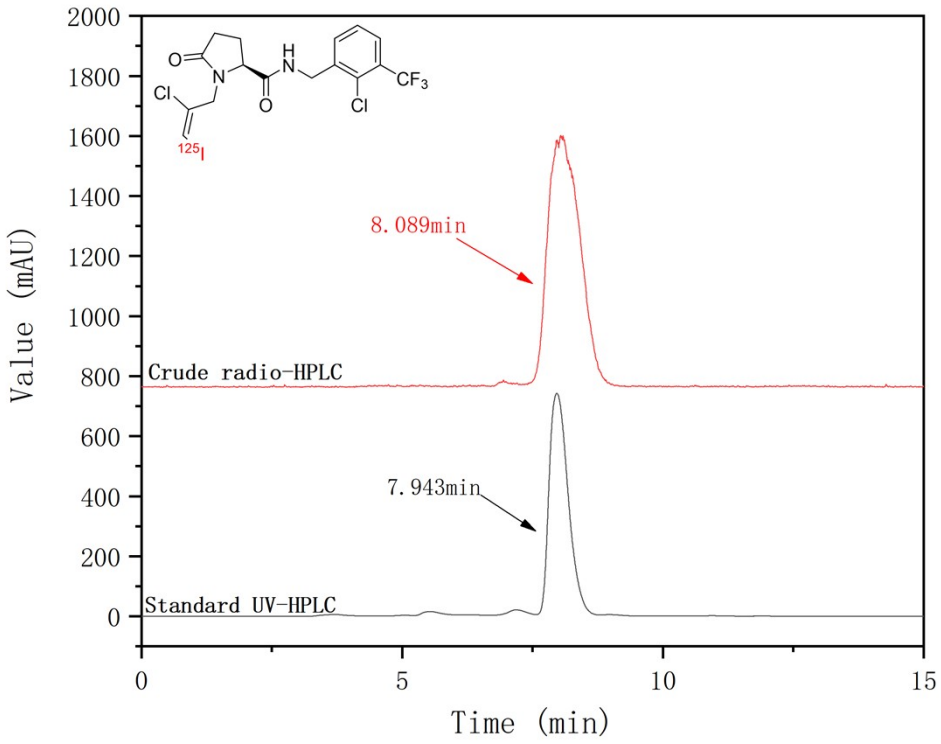
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 50/50, flow rate = 1 mL/min, λ = 220nm)

3bl, tR = 6.70 min, RCY = 45±7%, n = 5



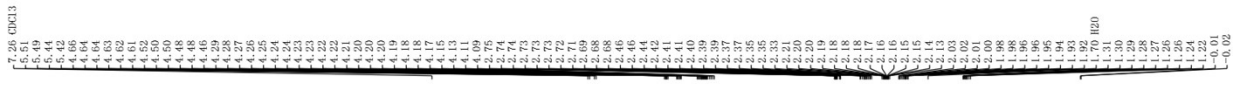
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 70/30, flow rate = 1 mL/min, λ = 220nm)

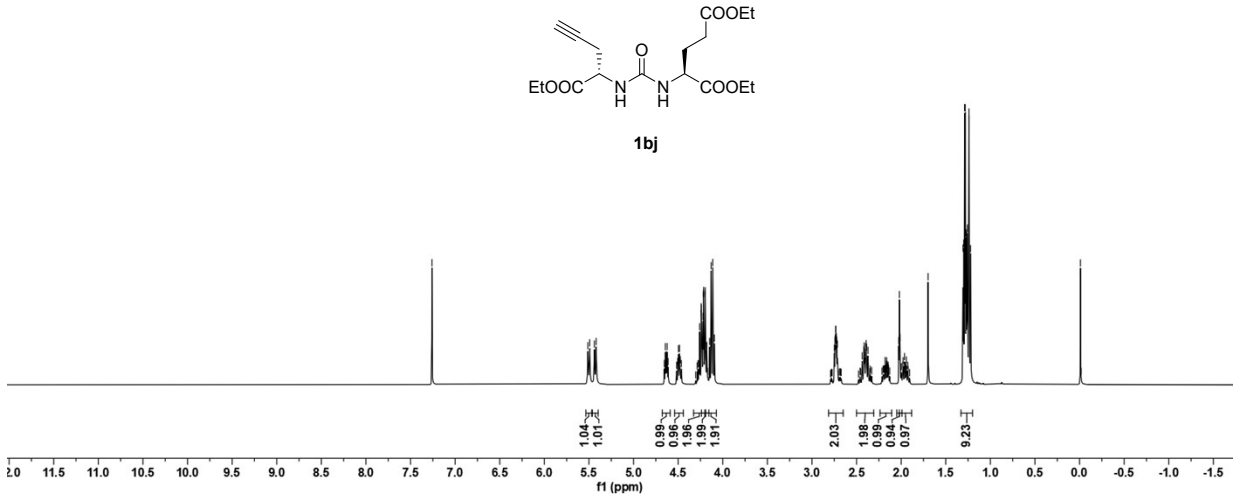
3bm, tR = 7.94 min, RCY = 93±3%, n = 6

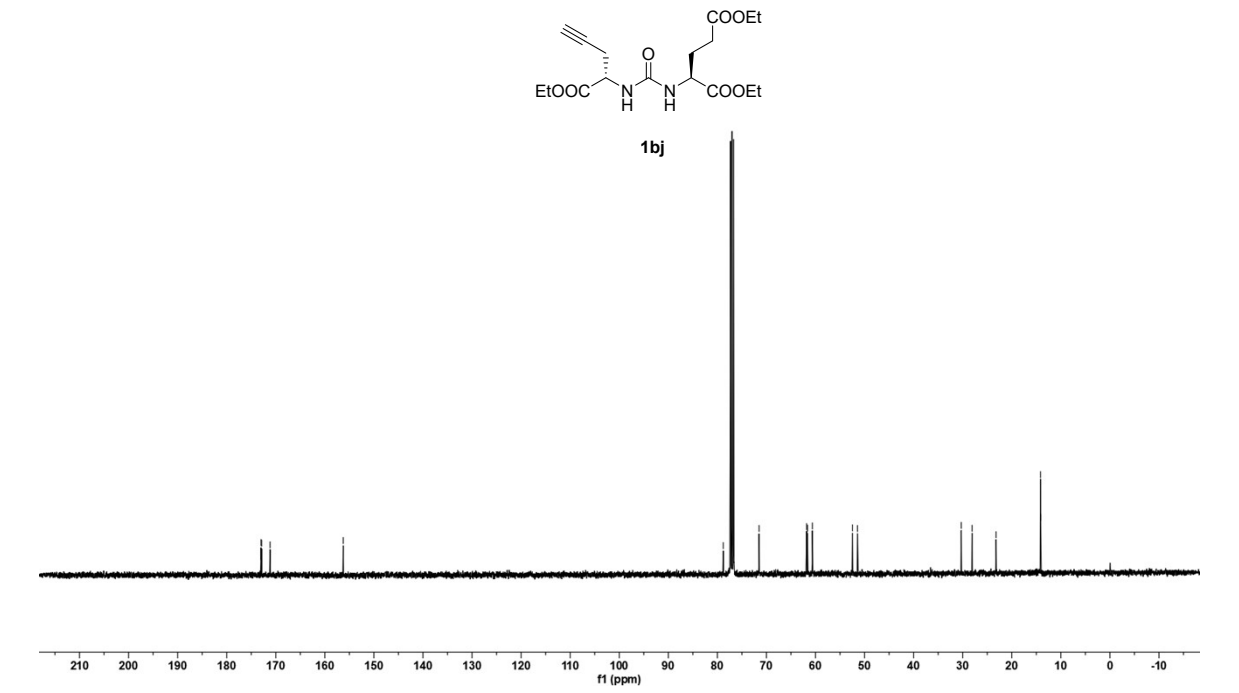


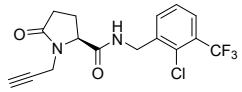
HPLC condition (SB-C18, MeCN/0.1 M ammonium formate buffer = 50/50, flow rate = 1 mL/min, λ = 220nm)

6. Copies of NMR Spectra

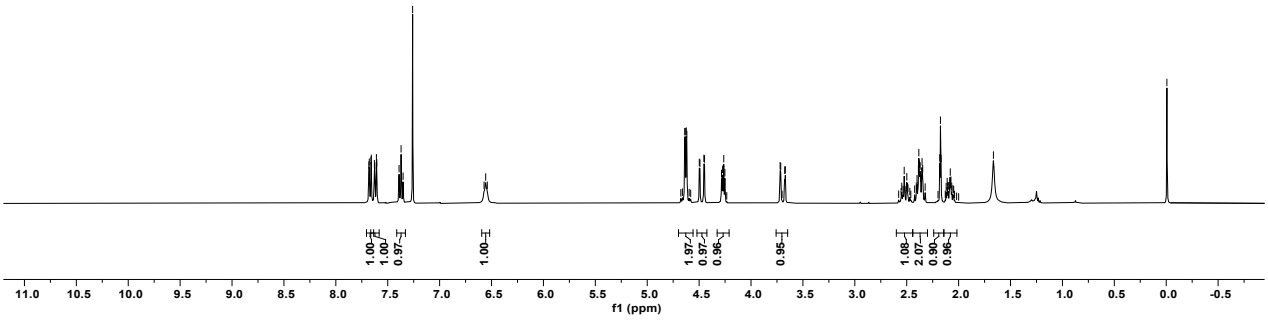


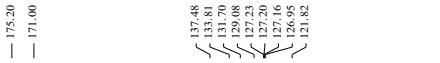


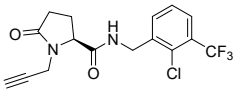




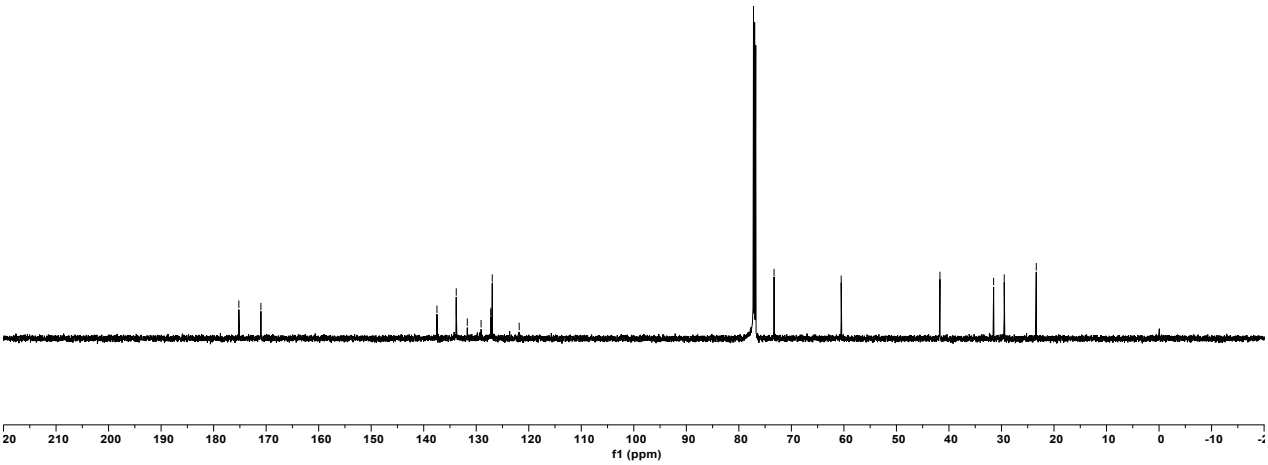
1bm



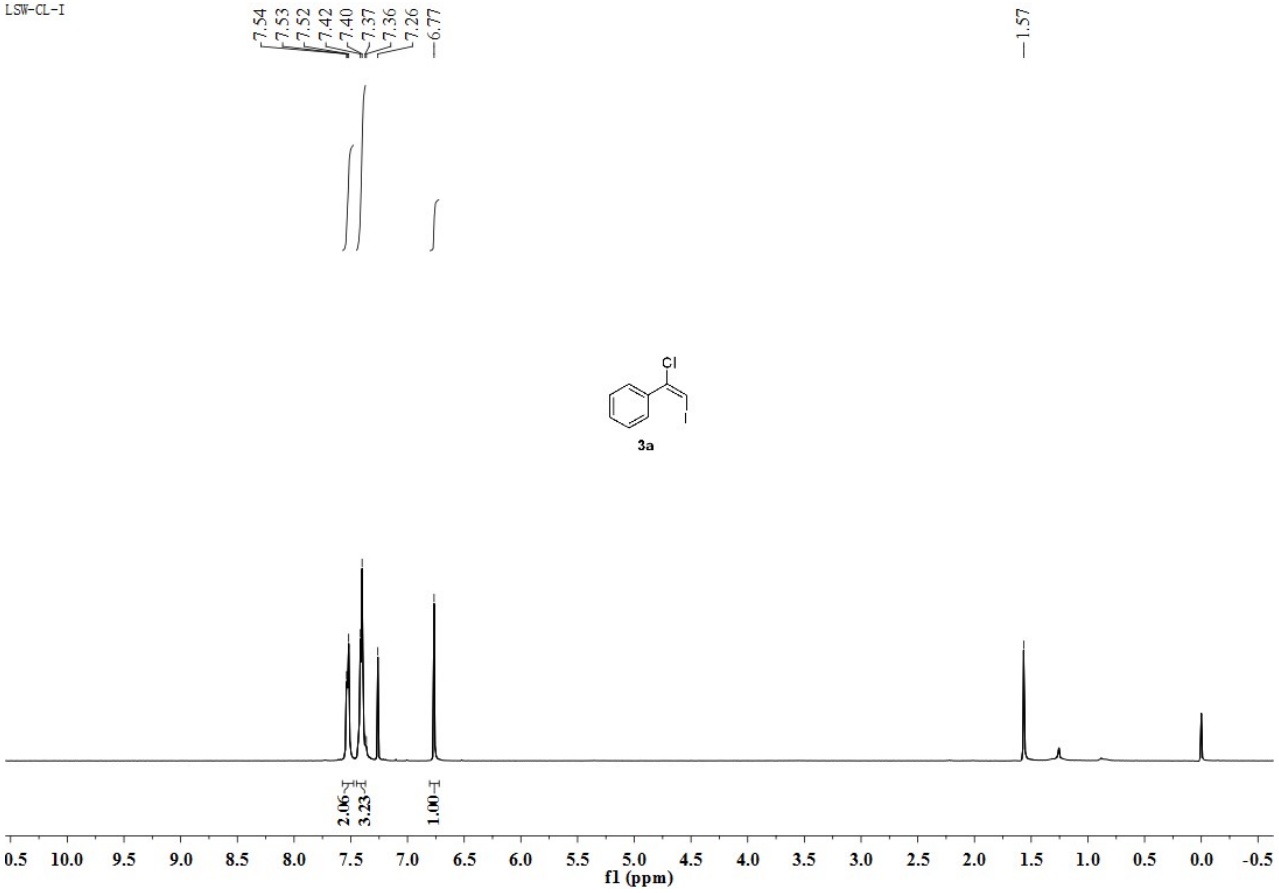




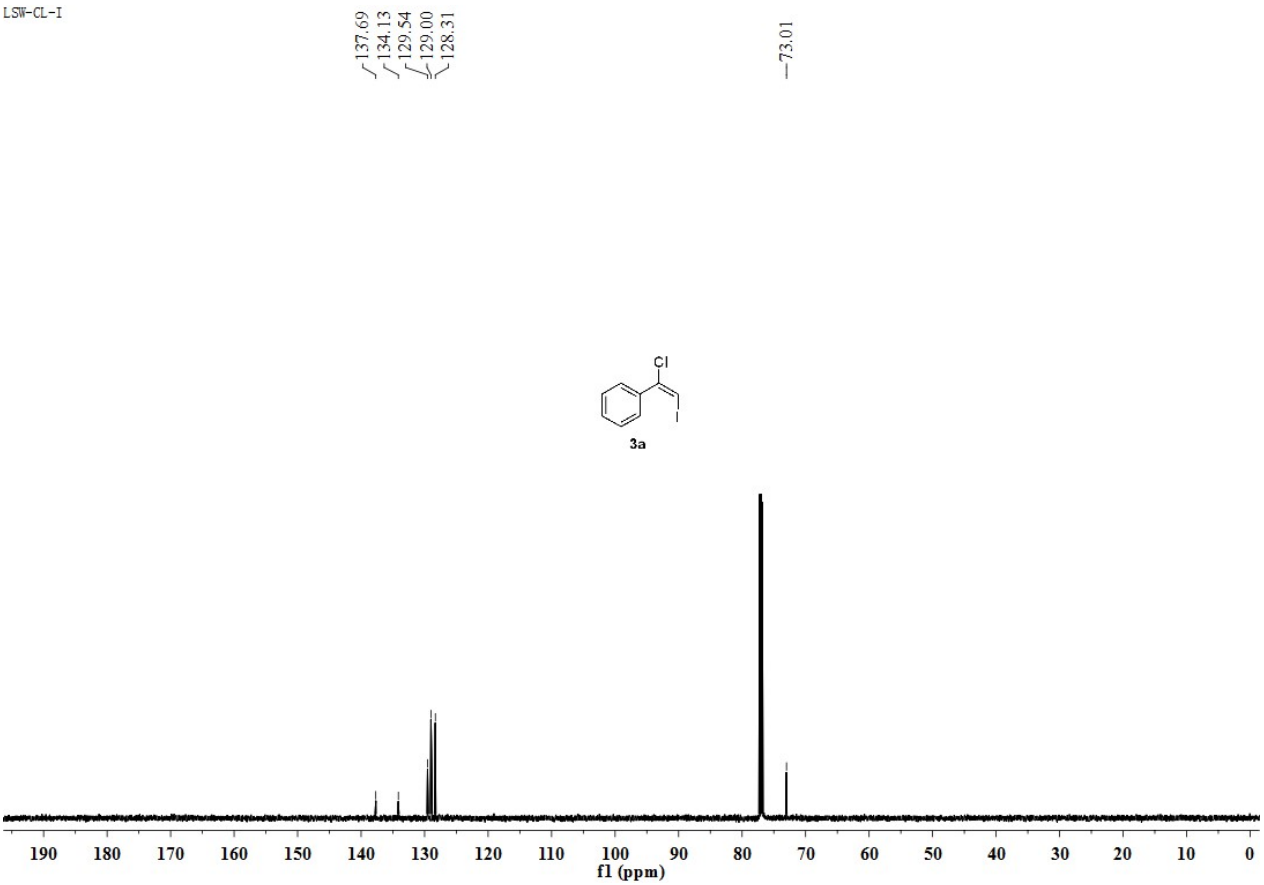
1bm



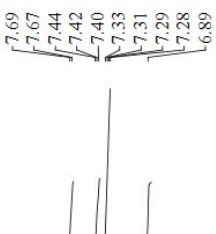
LSW-CL-I



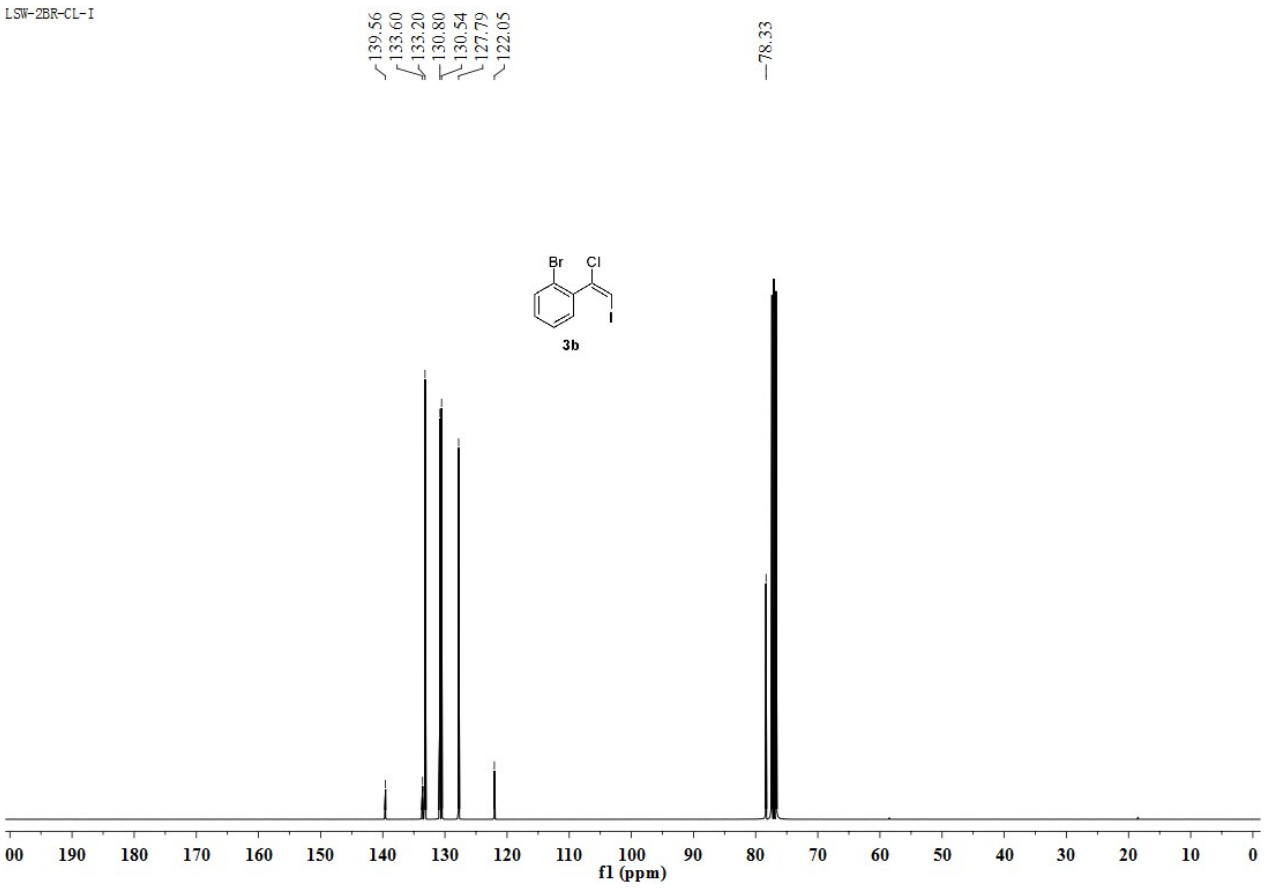
LSW-CL-I



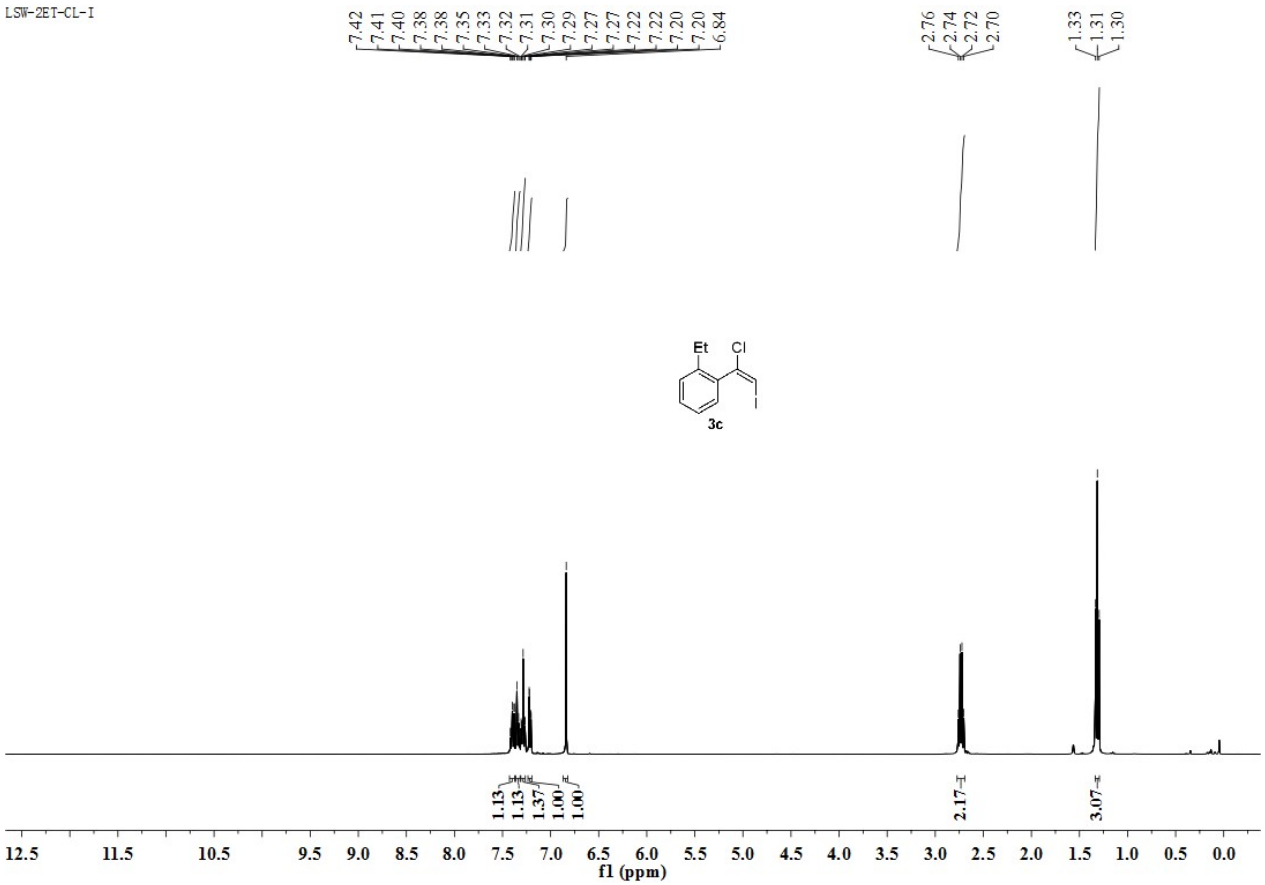
LSW-2BR-12233



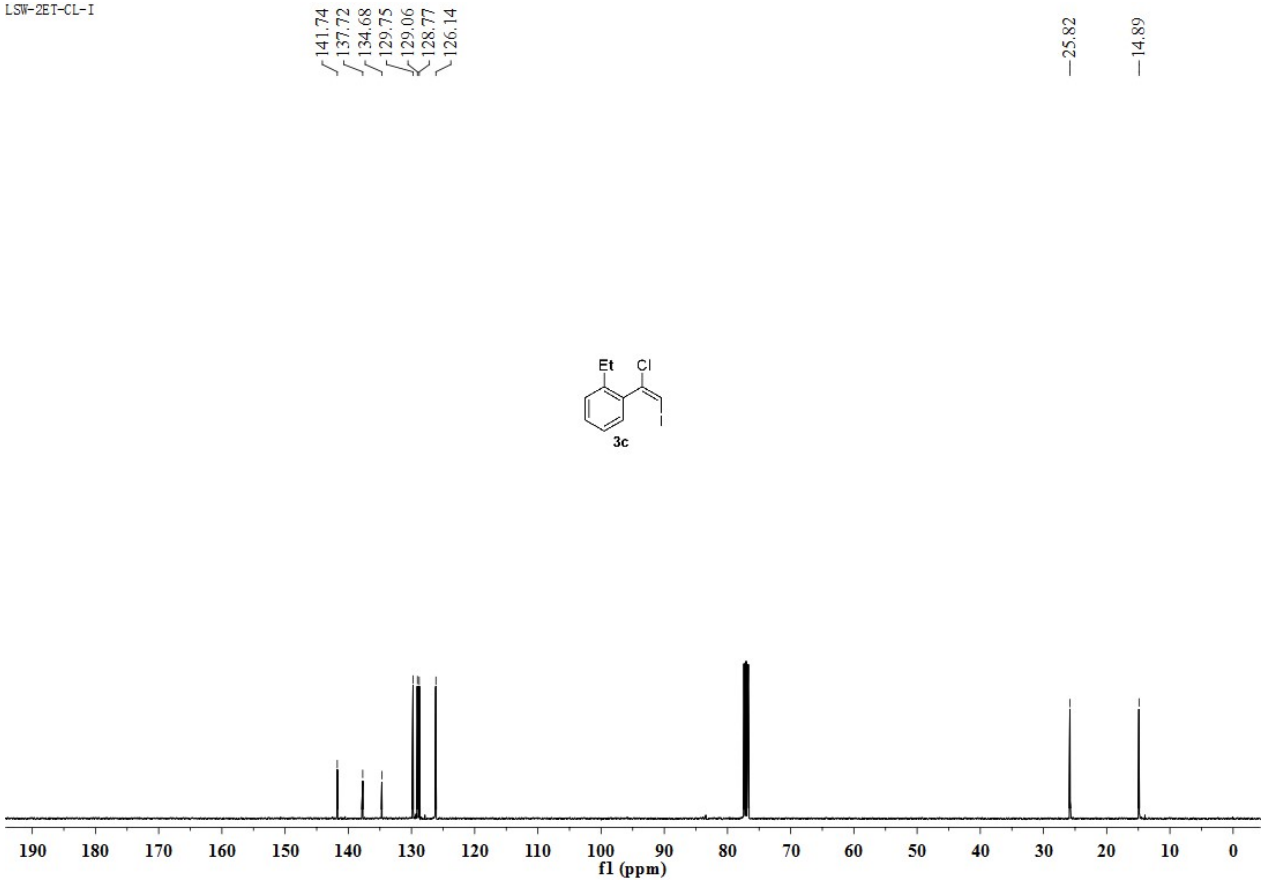
LSW-2BR-CL-I



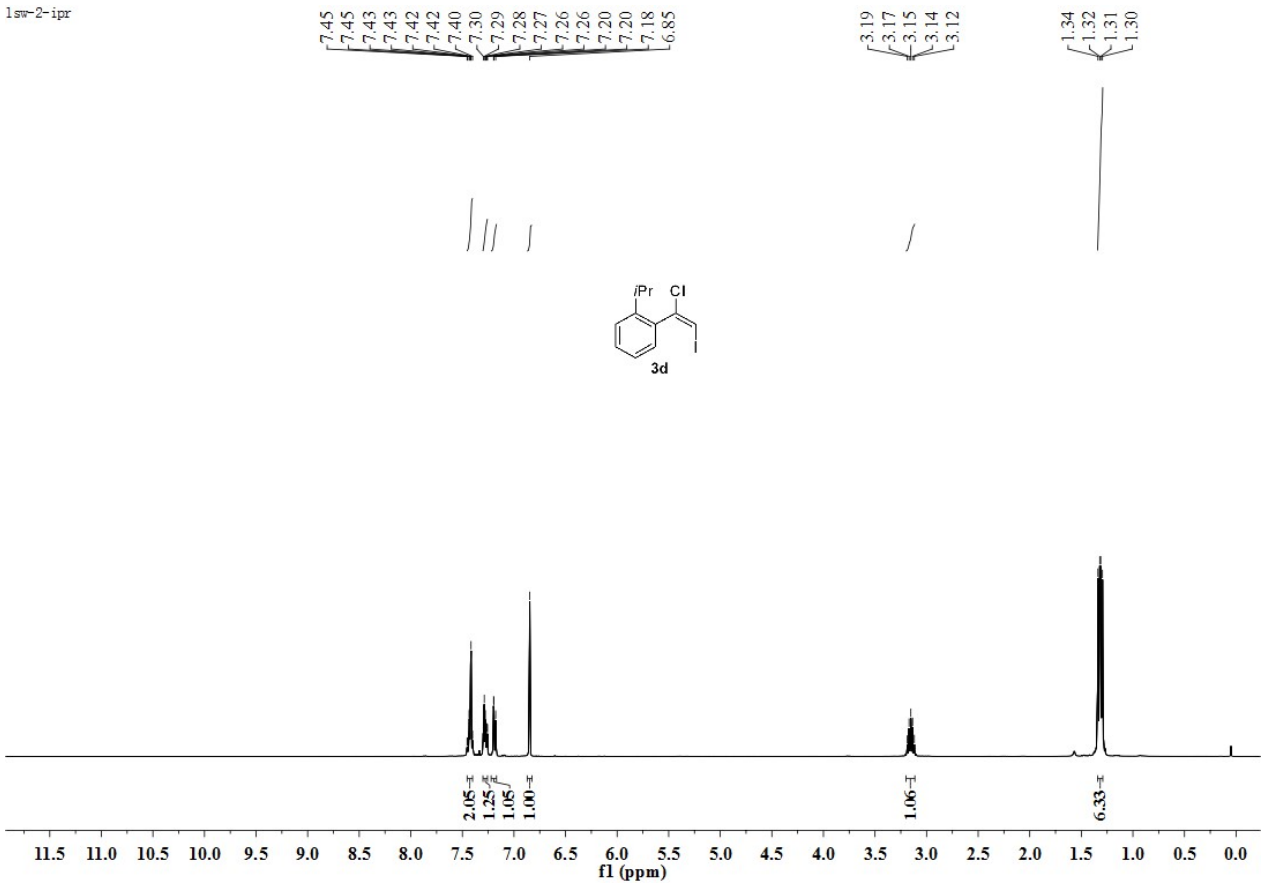
LSW-2ET-CL-I

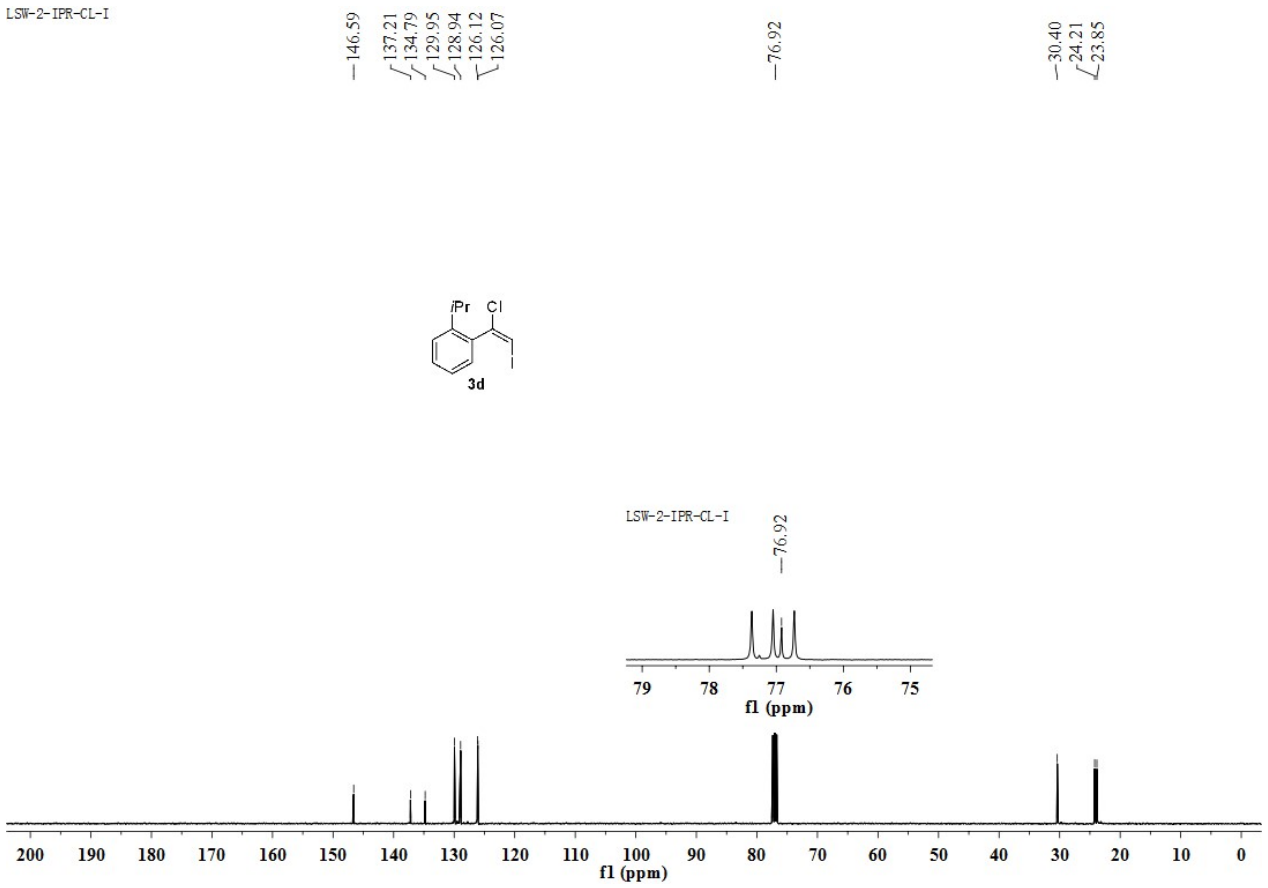


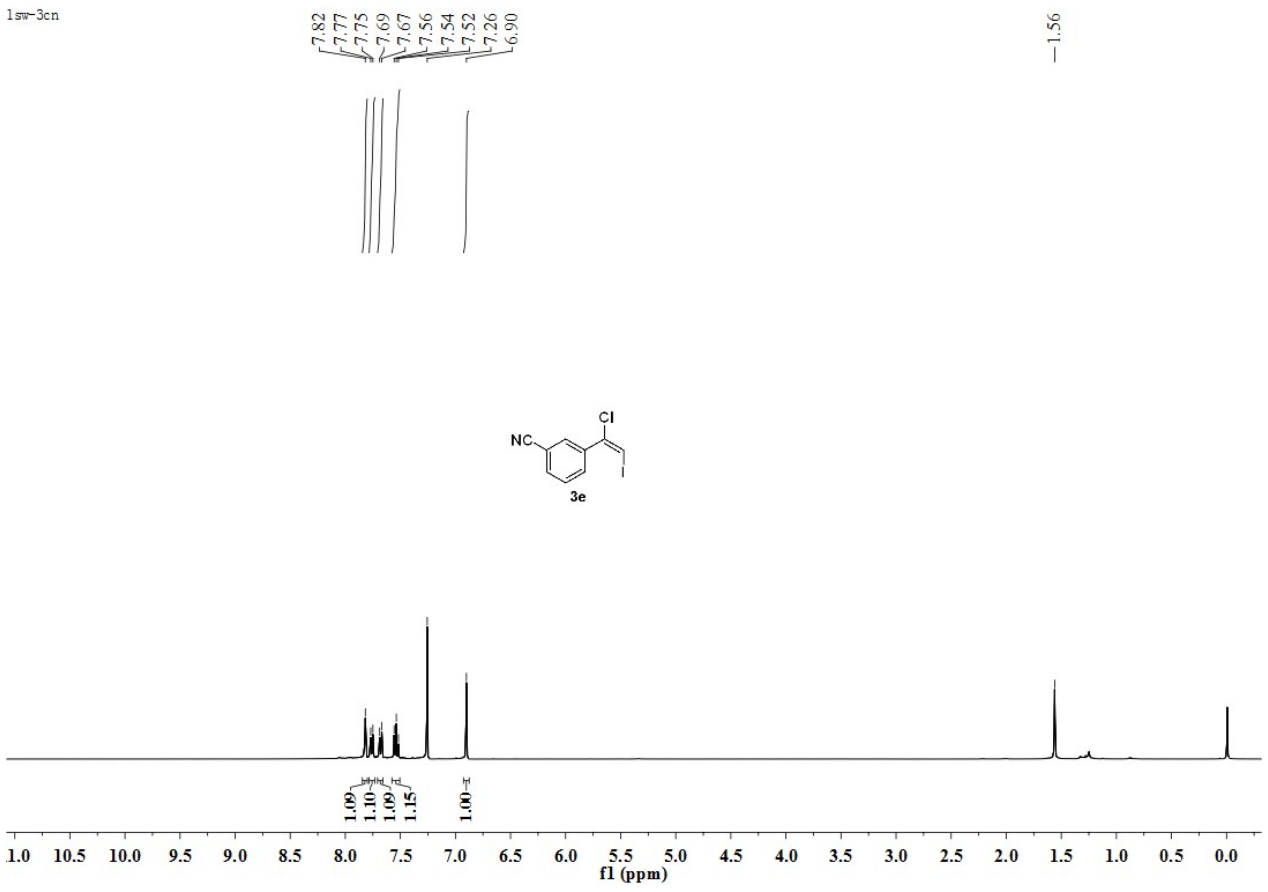
LSW-2ET-CL-I



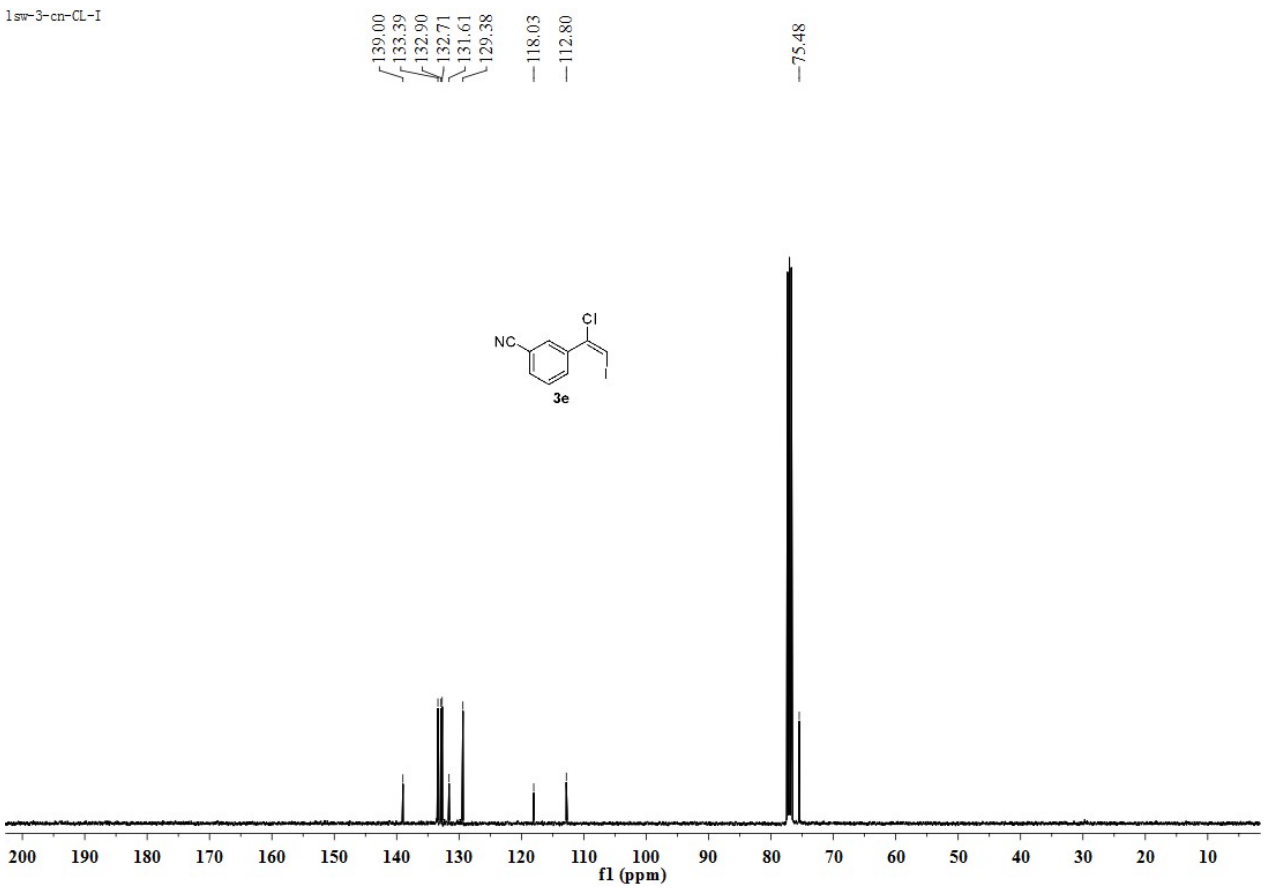
lsw-2-ipr



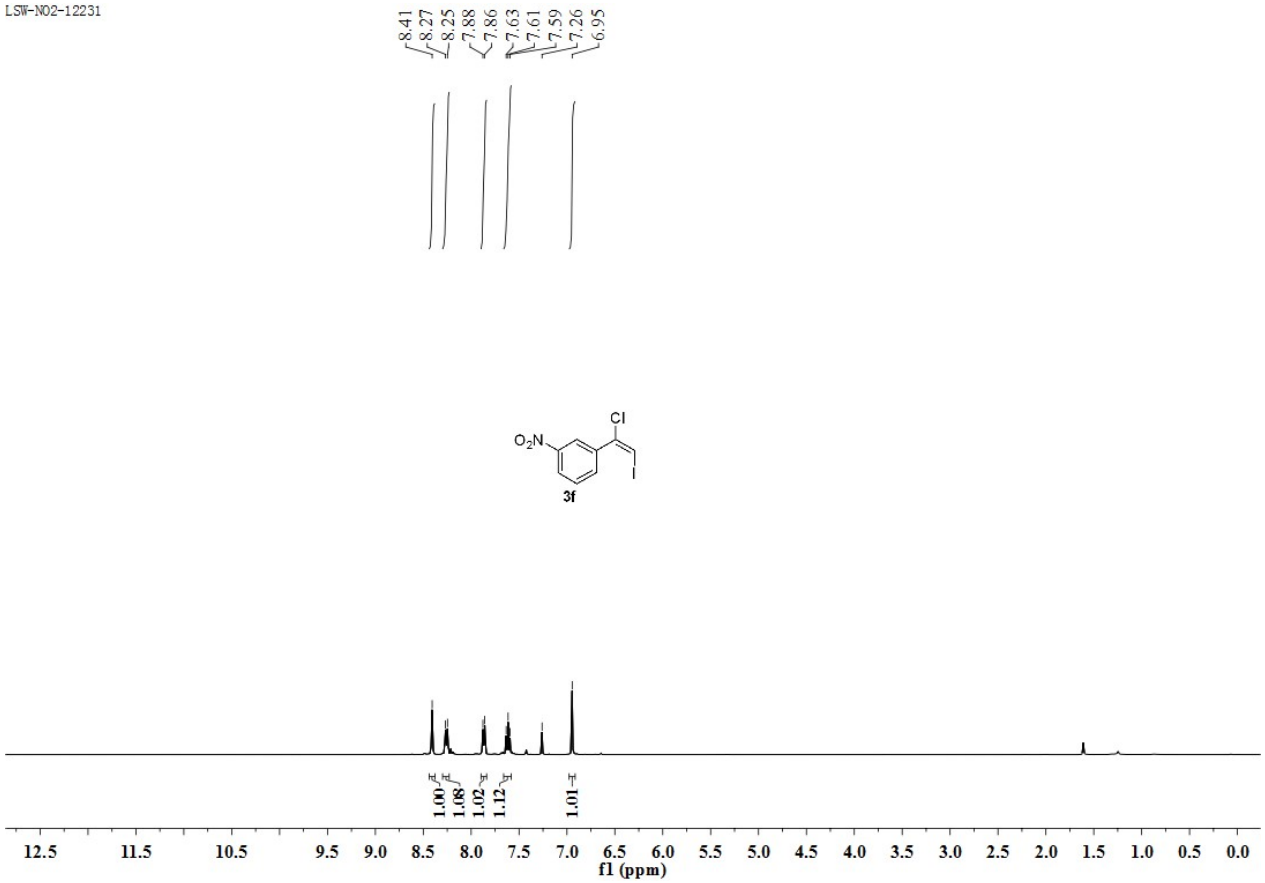

LSW-2-IPR-CL-I
146.59
137.21
134.79
129.95
128.94
126.12
126.07
76.92
30.40
24.21
23.85
iPr
Cl
3d
LSW-2-IPR-CL-I
76.92
79
78
77
76
75
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

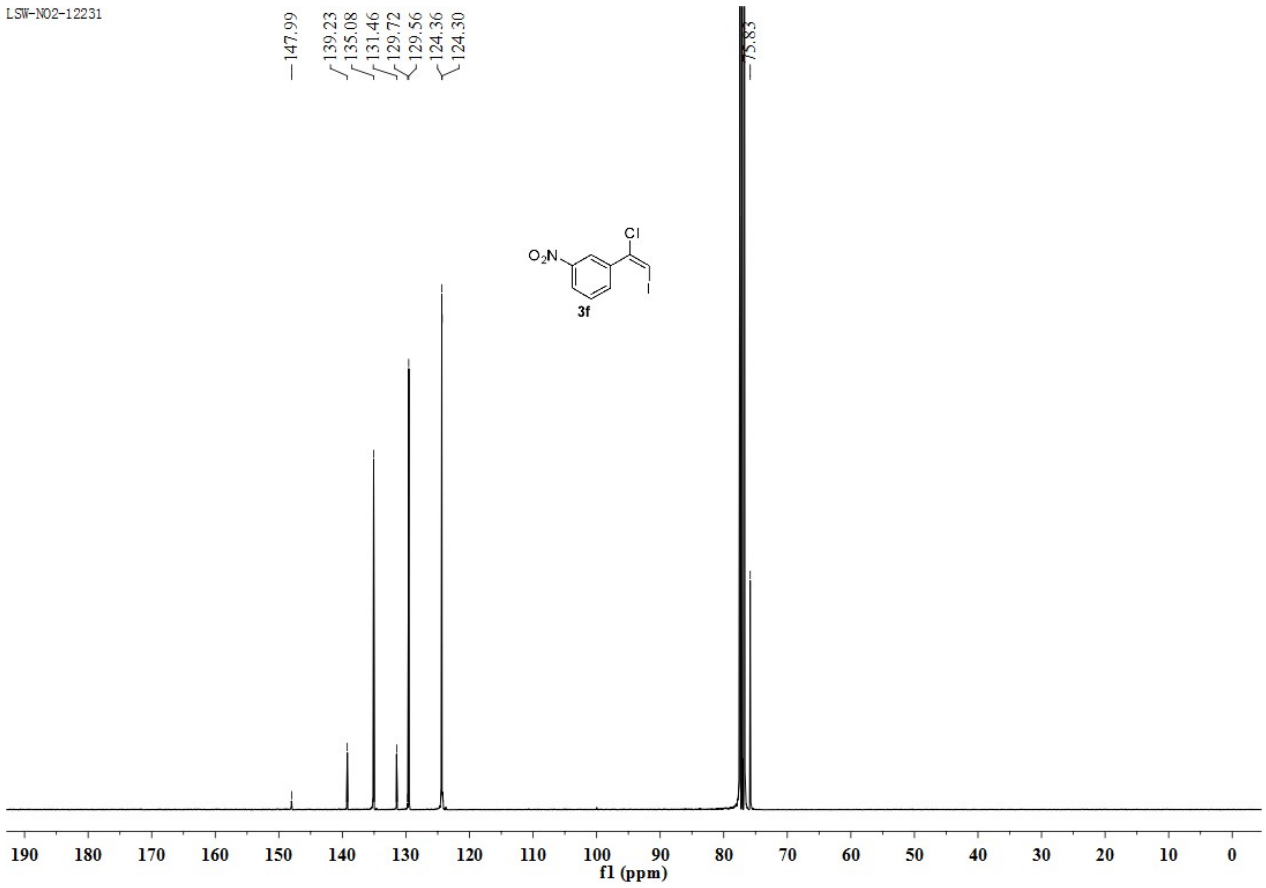

1sw-3cn
7.82
7.77
7.75
7.69
7.67
7.56
7.54
7.52
7.26
6.90
1.56
Cl
NC
3e
1.09
1.10
1.09
1.15
1.00
1.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

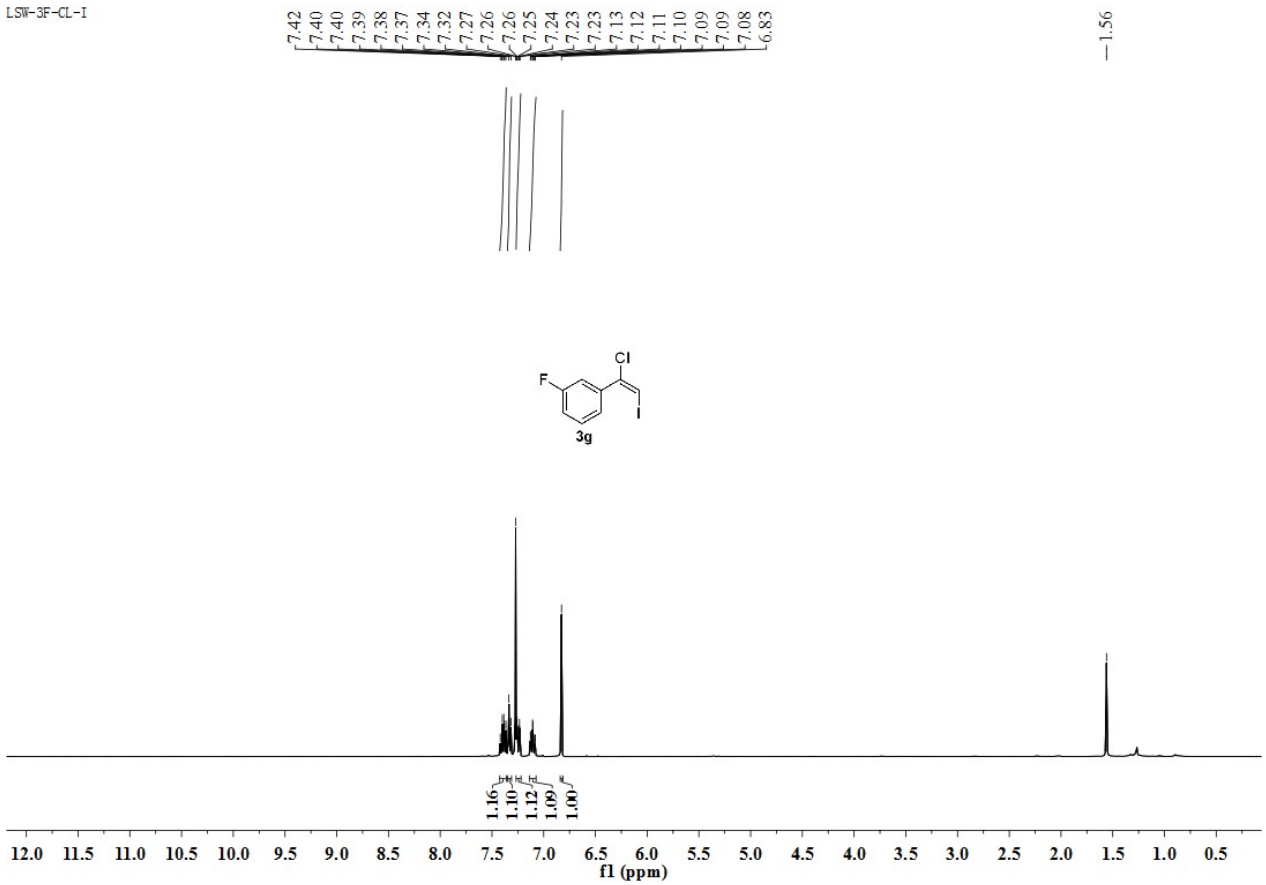
lsw-3-cn-CL-I



LSW-NO2-12231

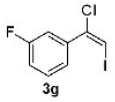



LSW-NO2-12231
147.99
139.23
135.08
131.46
129.72
129.56
124.36
124.30
75.83
Cl
O2N
I
3f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

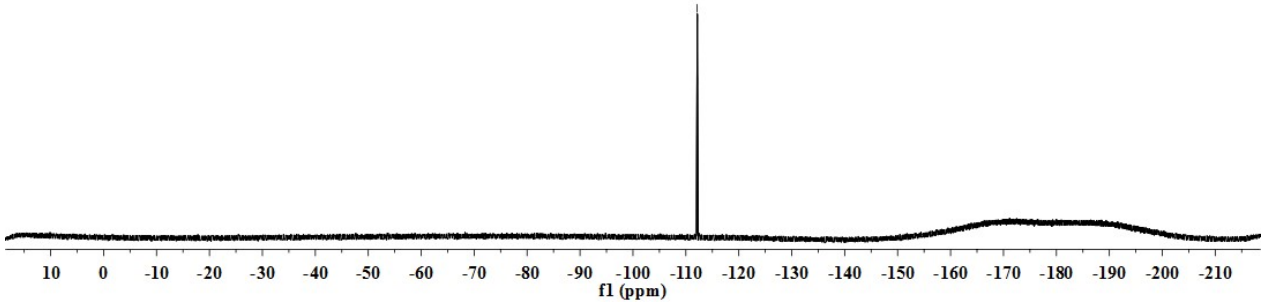

LSW-3F-CL-I
7.42
7.40
7.40
7.39
7.38
7.37
7.34
7.32
7.27
7.26
7.26
7.25
7.24
7.23
7.23
7.13
7.12
7.11
7.10
7.09
7.09
7.08
6.83
1.56
Cl
F
I
3g
1.16
1.10
1.12
1.09
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

LSW-3F-CL-I

-112.14
-112.15
-112.16

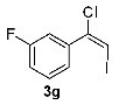


3g

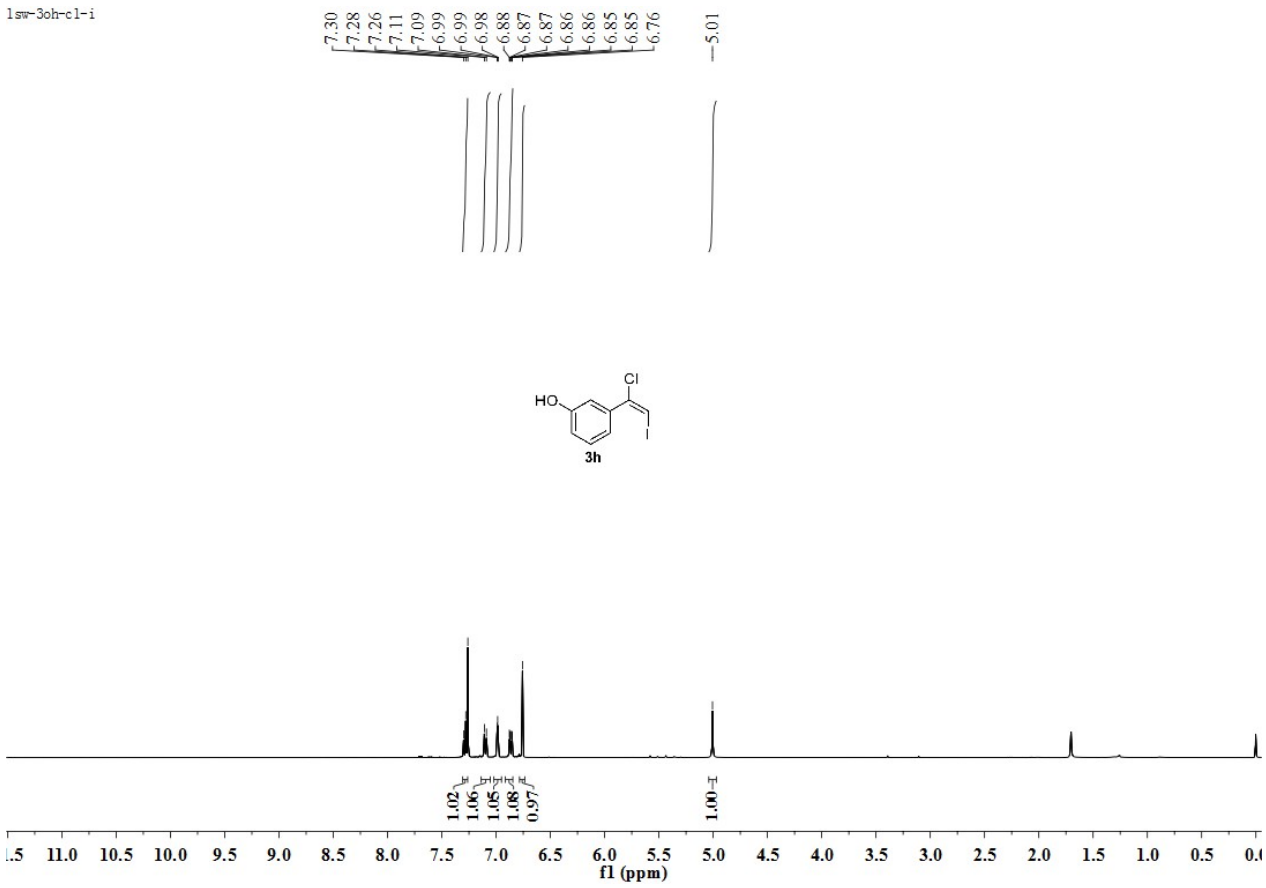


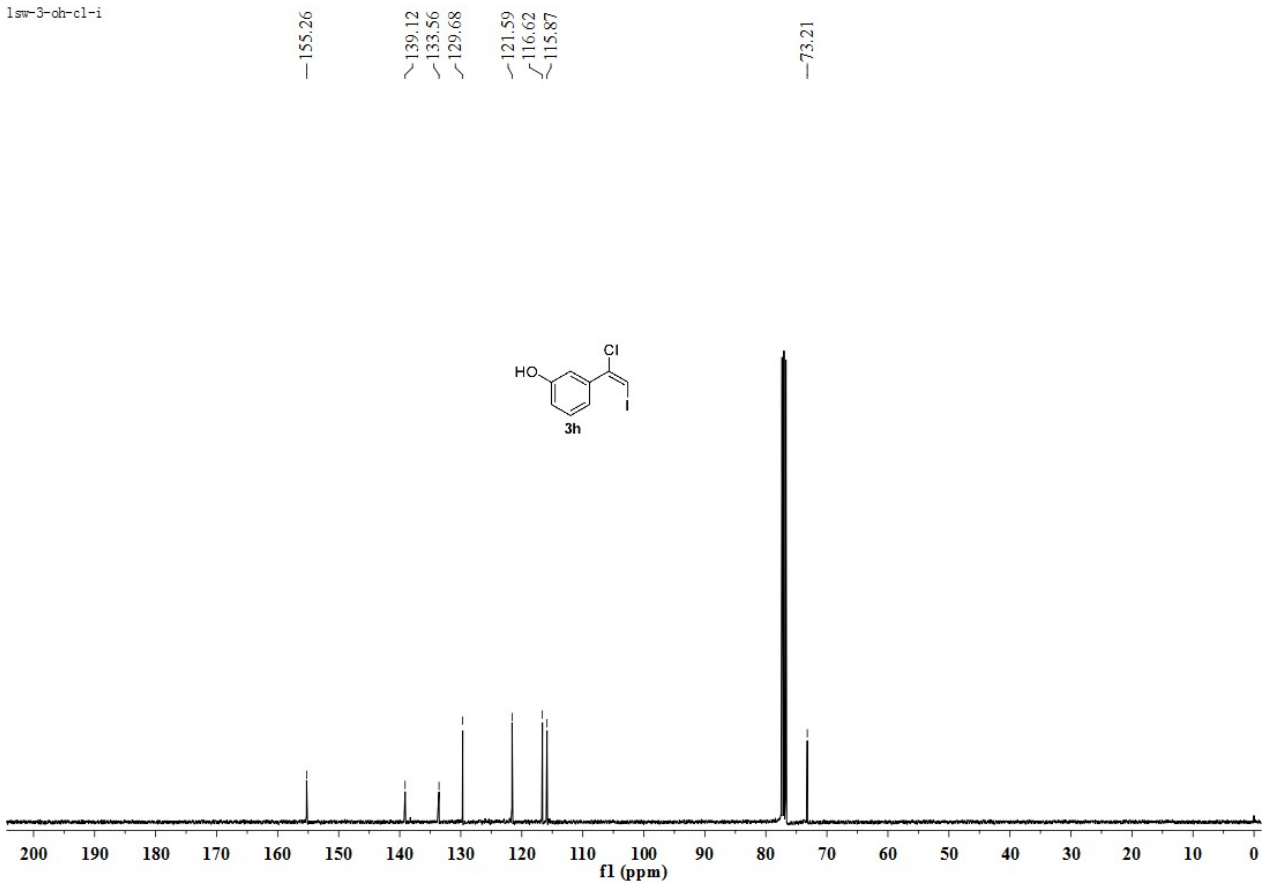
LSW-3F-CL-I

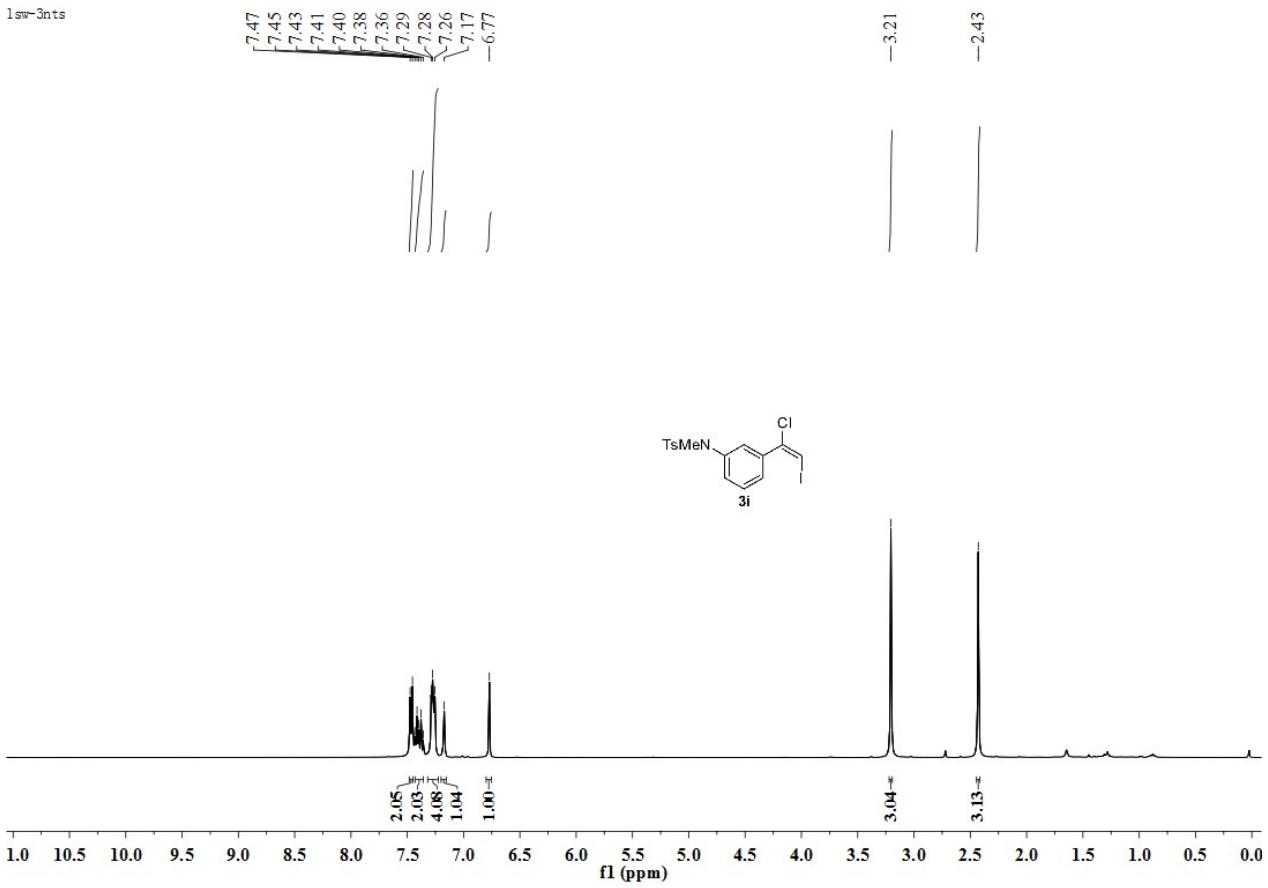
163.51
161.05
139.63
139.55
132.70
132.67
130.01
129.93
124.84
124.81
116.67
116.46
116.29
116.06
73.99

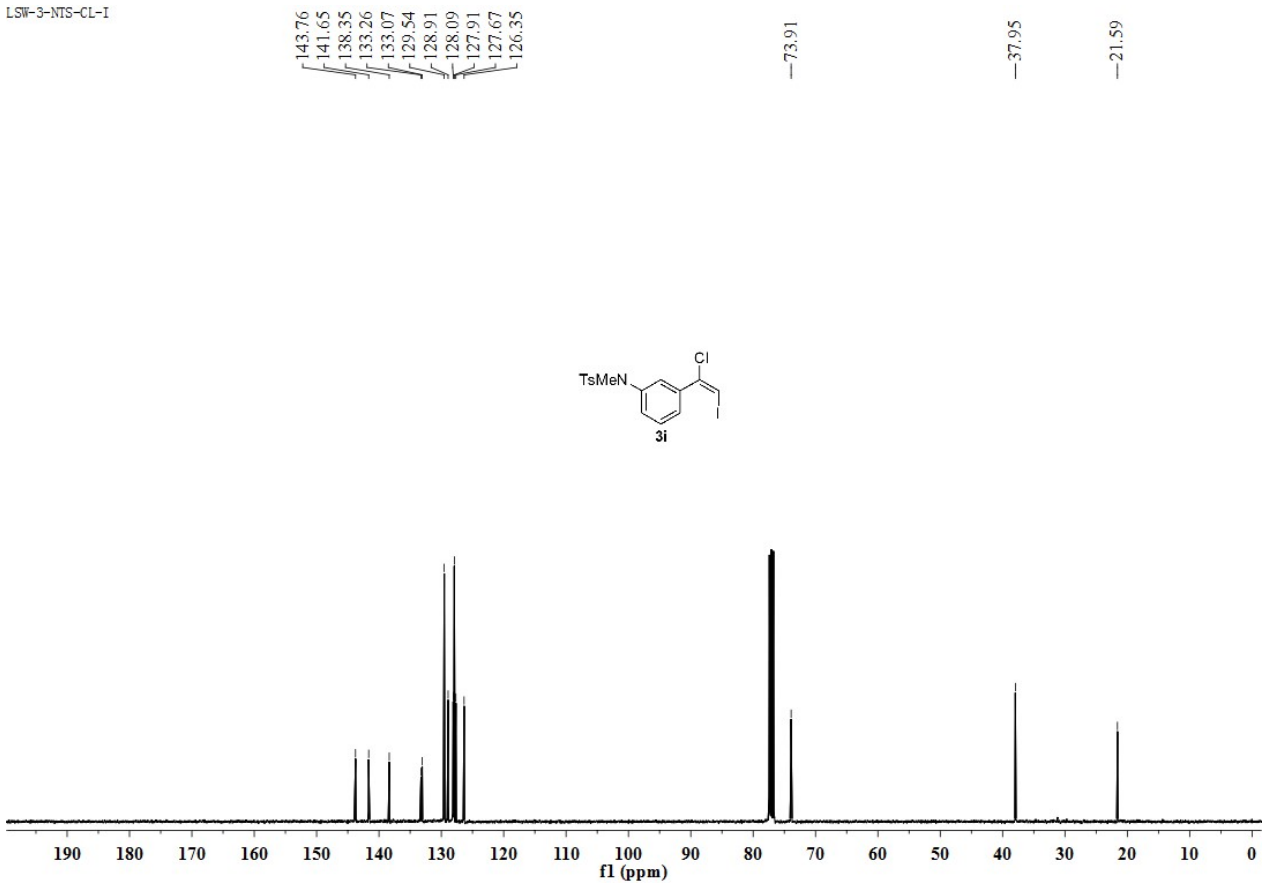


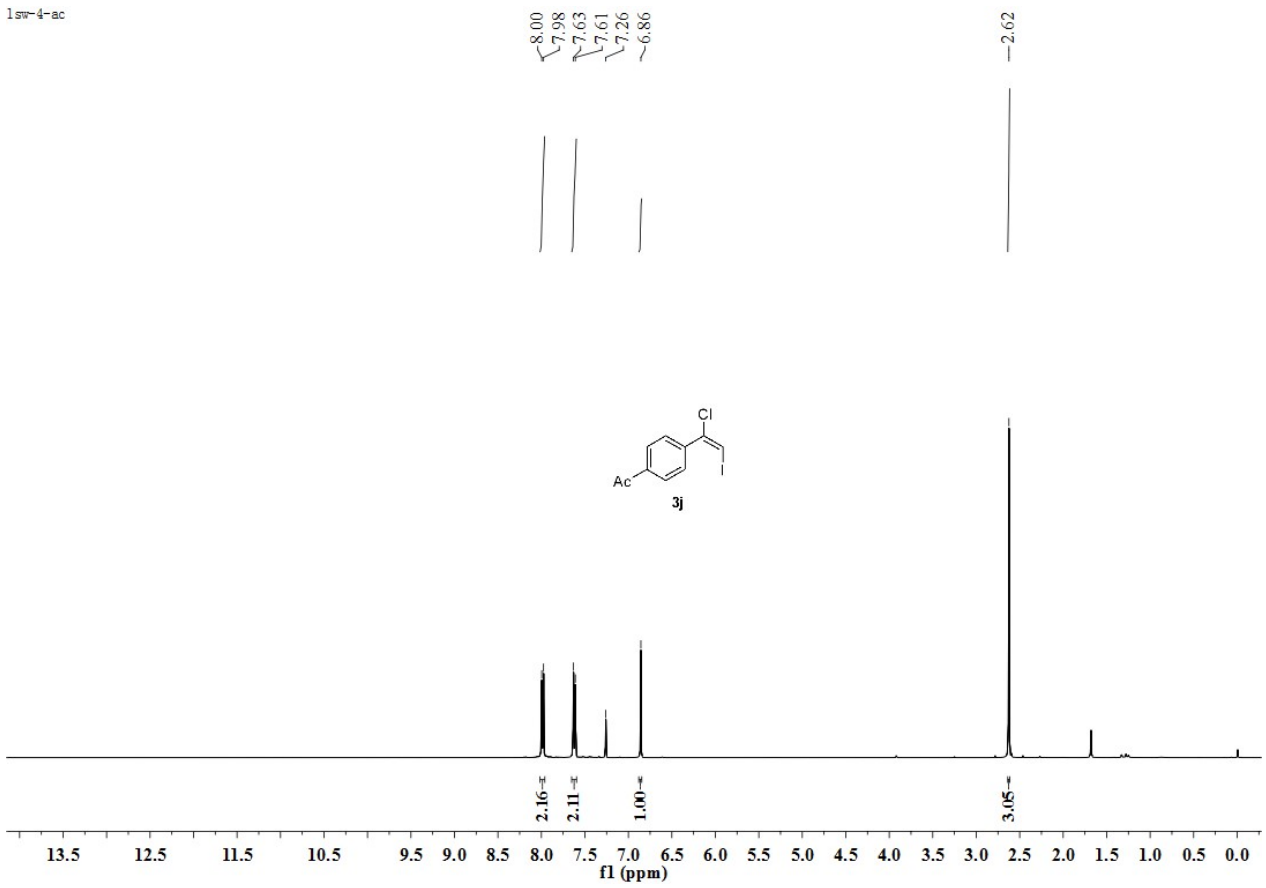
3g

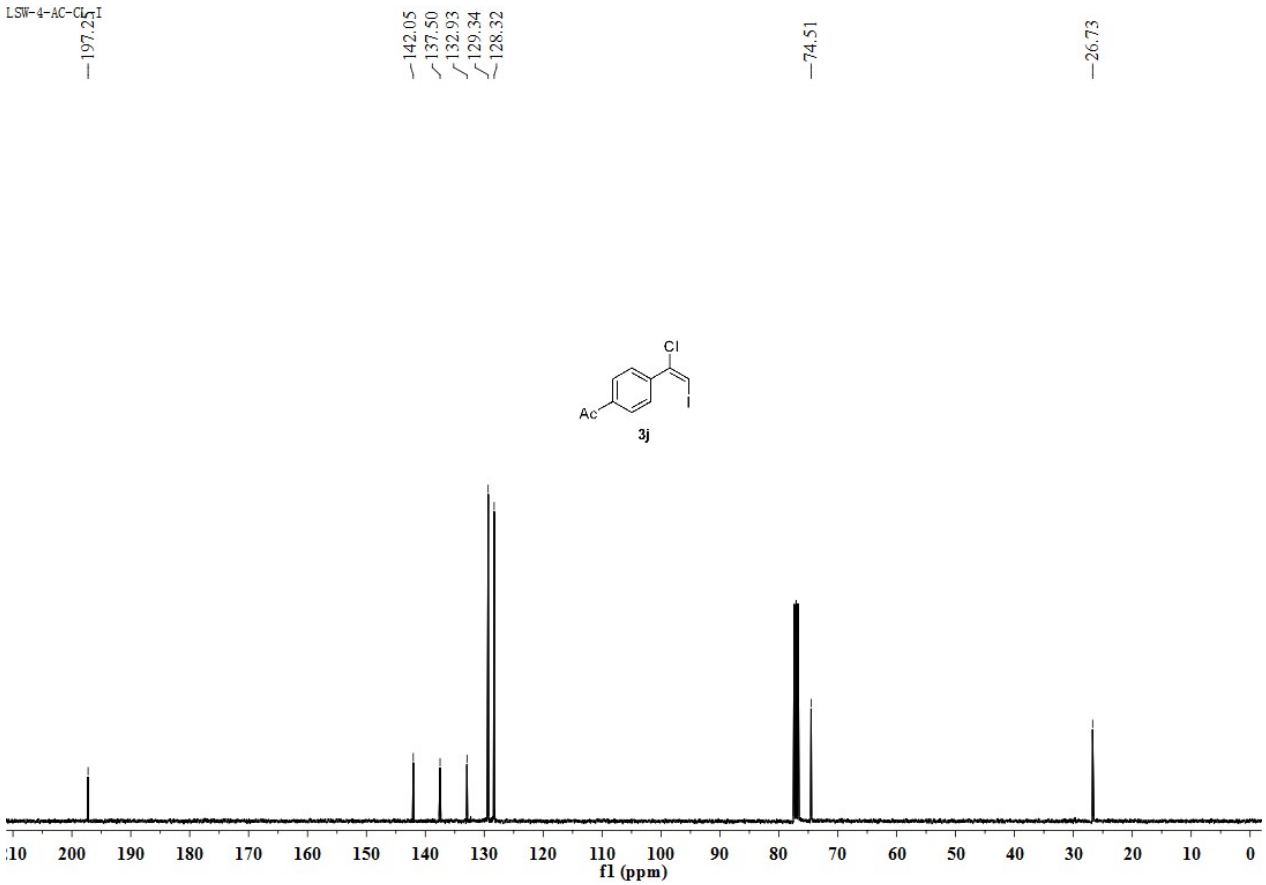

lsw-3oh-cl-i
7.30
7.28
7.26
7.11
7.09
6.99
6.99
6.98
6.88
6.87
6.87
6.86
6.86
6.85
6.85
6.76
5.01
HO
Cl
I
3h
1.02
1.06
1.05
1.08
0.97
1.00
f1 (ppm)

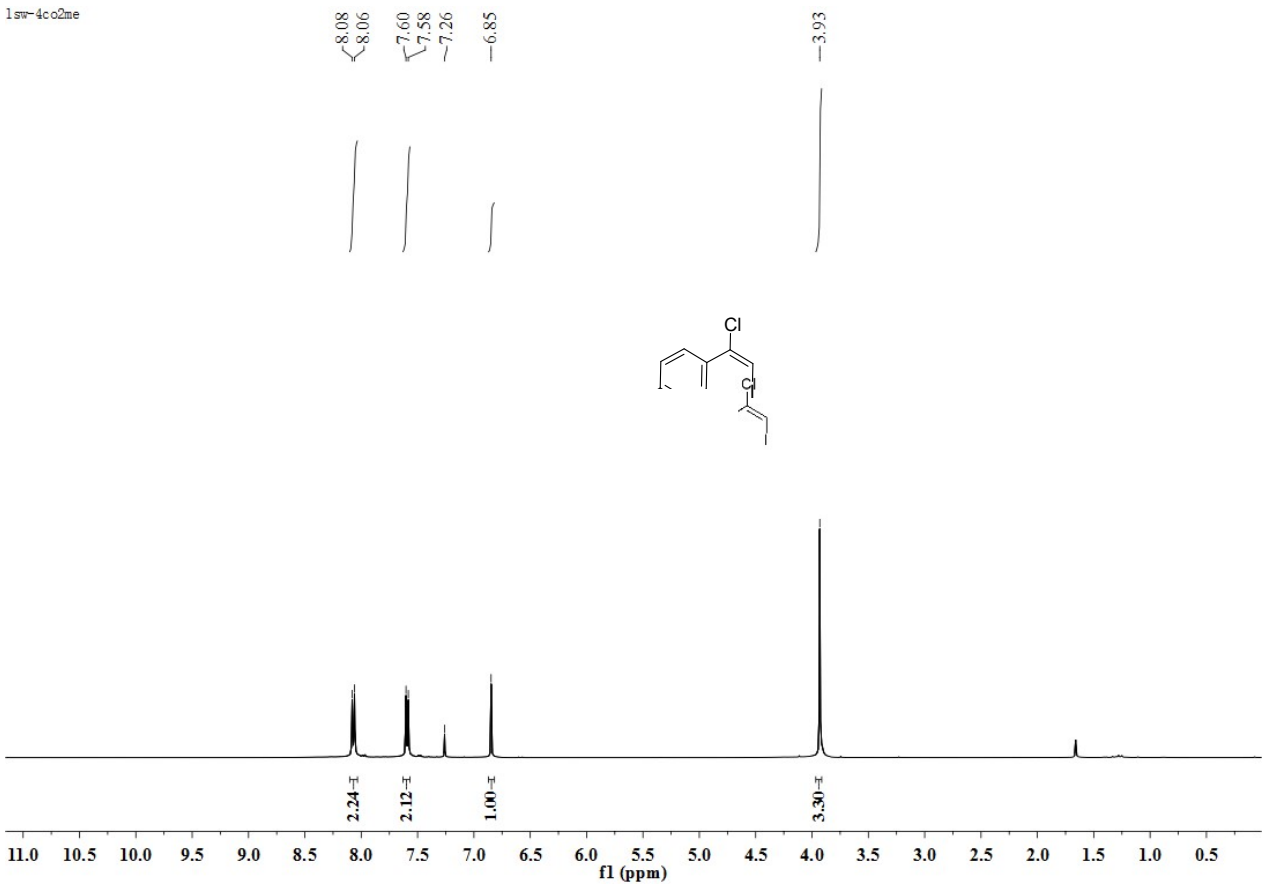

lsw-3-oh-cl-i
155.26
139.12
133.56
129.68
121.59
116.62
115.87
73.21
HO
Cl
I
3h
f1 (ppm)

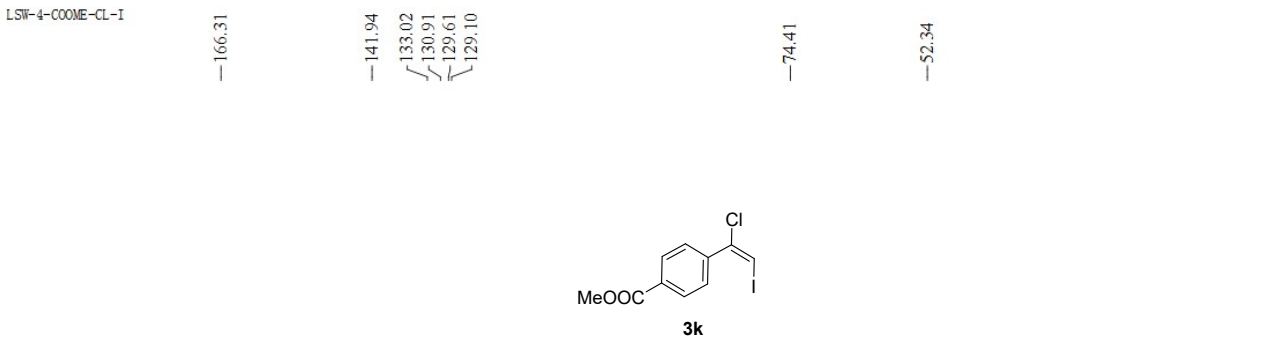

lsw-3nts
7.47
7.45
7.43
7.41
7.40
7.38
7.36
7.29
7.28
7.26
7.17
6.77
3.21
2.43
TsMeN
Cl
3i
2.05
2.03
4.08
1.04
1.00
3.04
3.13
f1 (ppm)


LSW-3-NTS-CL-I
143.76
141.65
138.35
133.26
133.07
129.54
128.91
128.09
127.91
127.67
126.35
73.91
37.95
21.59
TsMeN
Cl
3i
f1 (ppm)

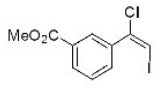

lsw-4-ac
8.00
7.98
7.63
7.61
7.26
6.86
2.62
Cl
Ac
I
3j
2.16
2.11
1.00
3.05
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


LSW-4-AC-CL-I
197.25
142.05
137.50
132.93
129.34
128.32
74.51
26.73
Cl
Ac
I
3j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

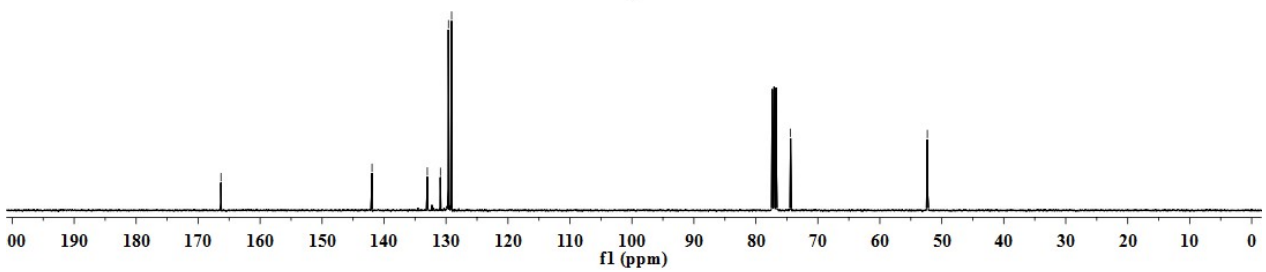

lsw-4co2me
8.08
8.06
7.60
7.58
7.26
6.85
3.93
Cl
Cl
2.24
2.12
1.00
3.30
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


LSW-4-COOME-CL-I
166.31
141.94
133.02
130.91
129.61
129.10
74.41
52.34
Cl
MeOOC
I

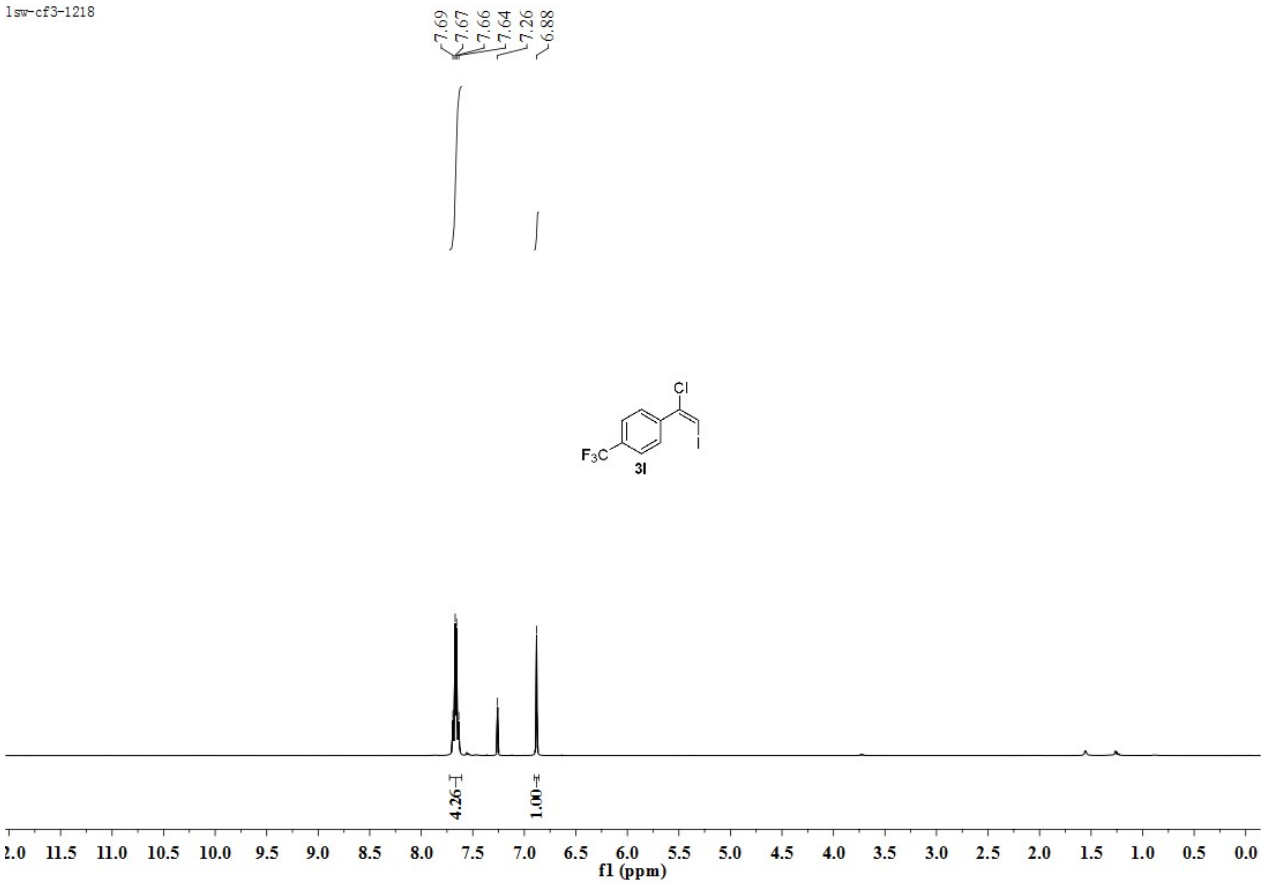
3k


MeO2C
Cl

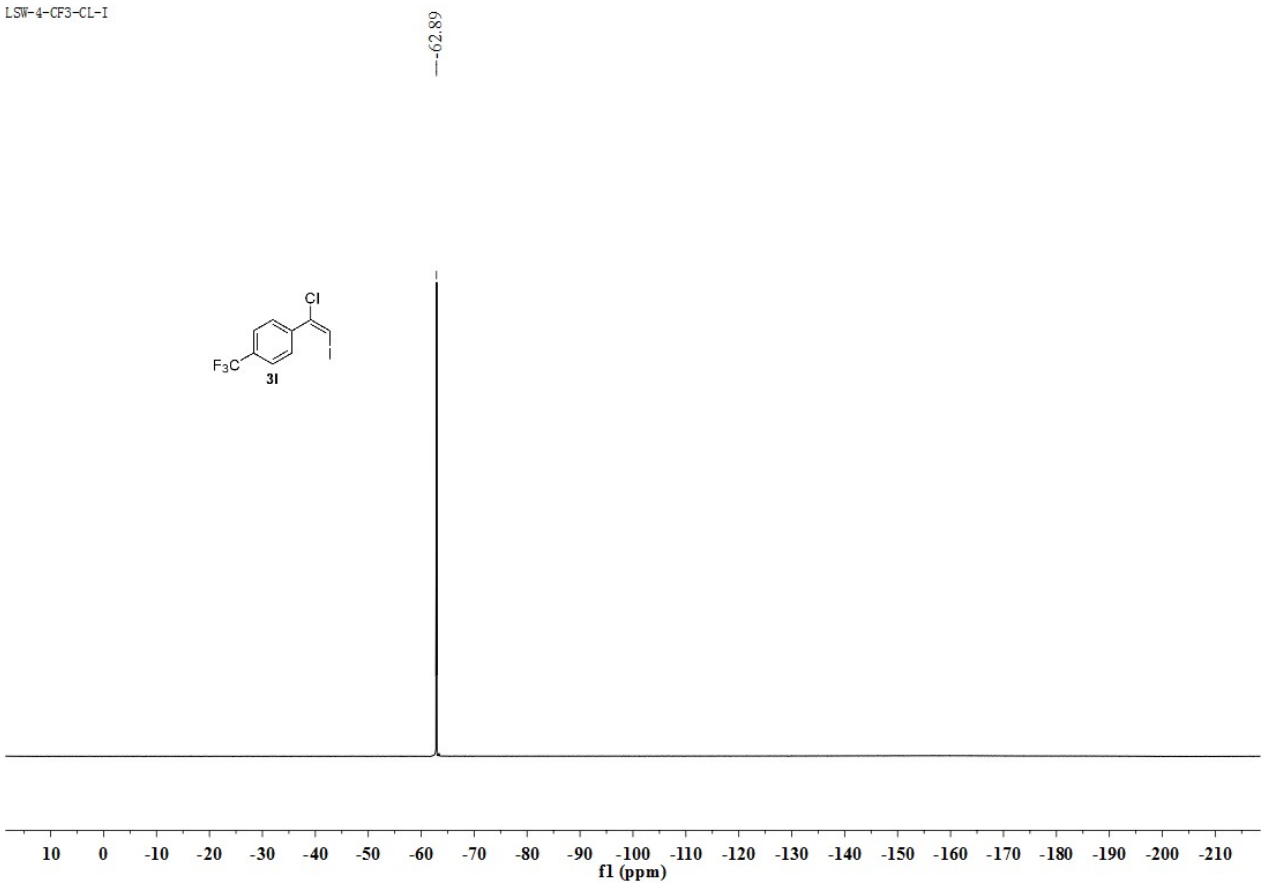
3k


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

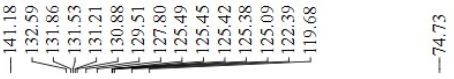
lsw-cf3-1218

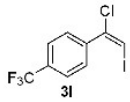


LSW-4-CF3-CL-I

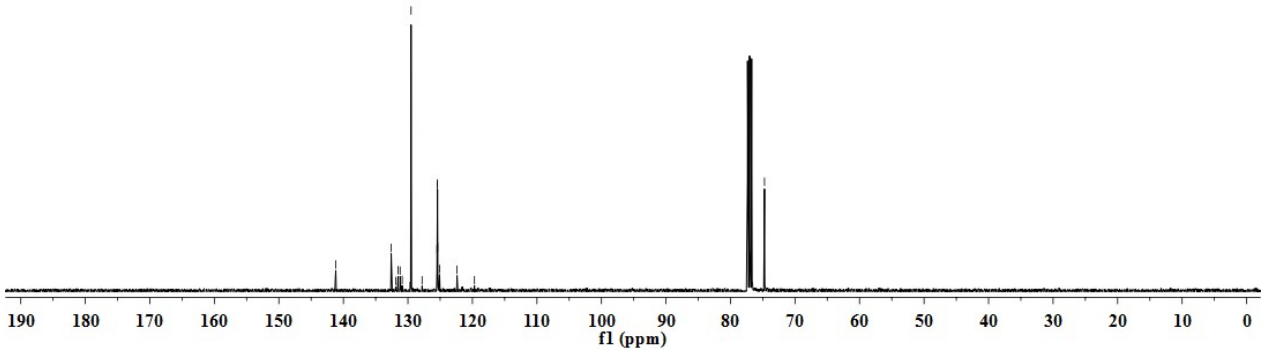


lsw-cf3-1218

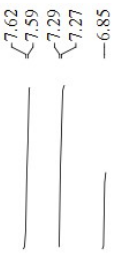


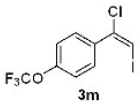


3l

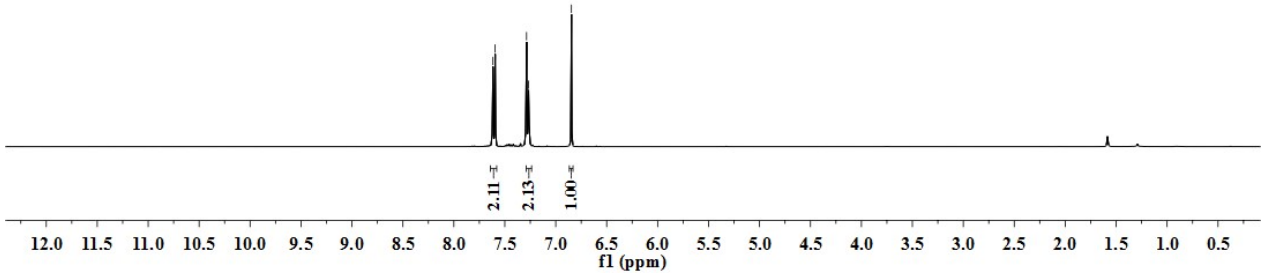


LSW-4-OCF3-CL-I

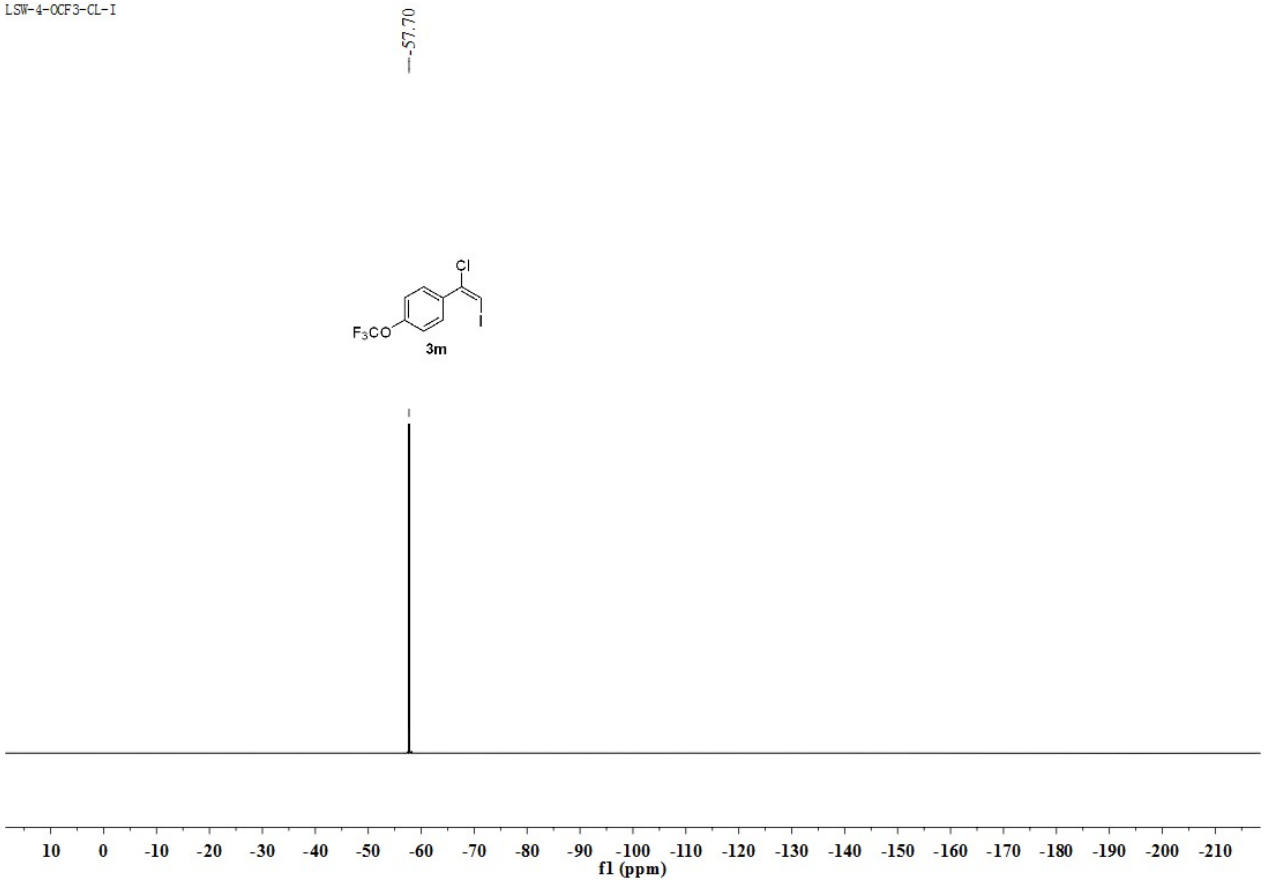




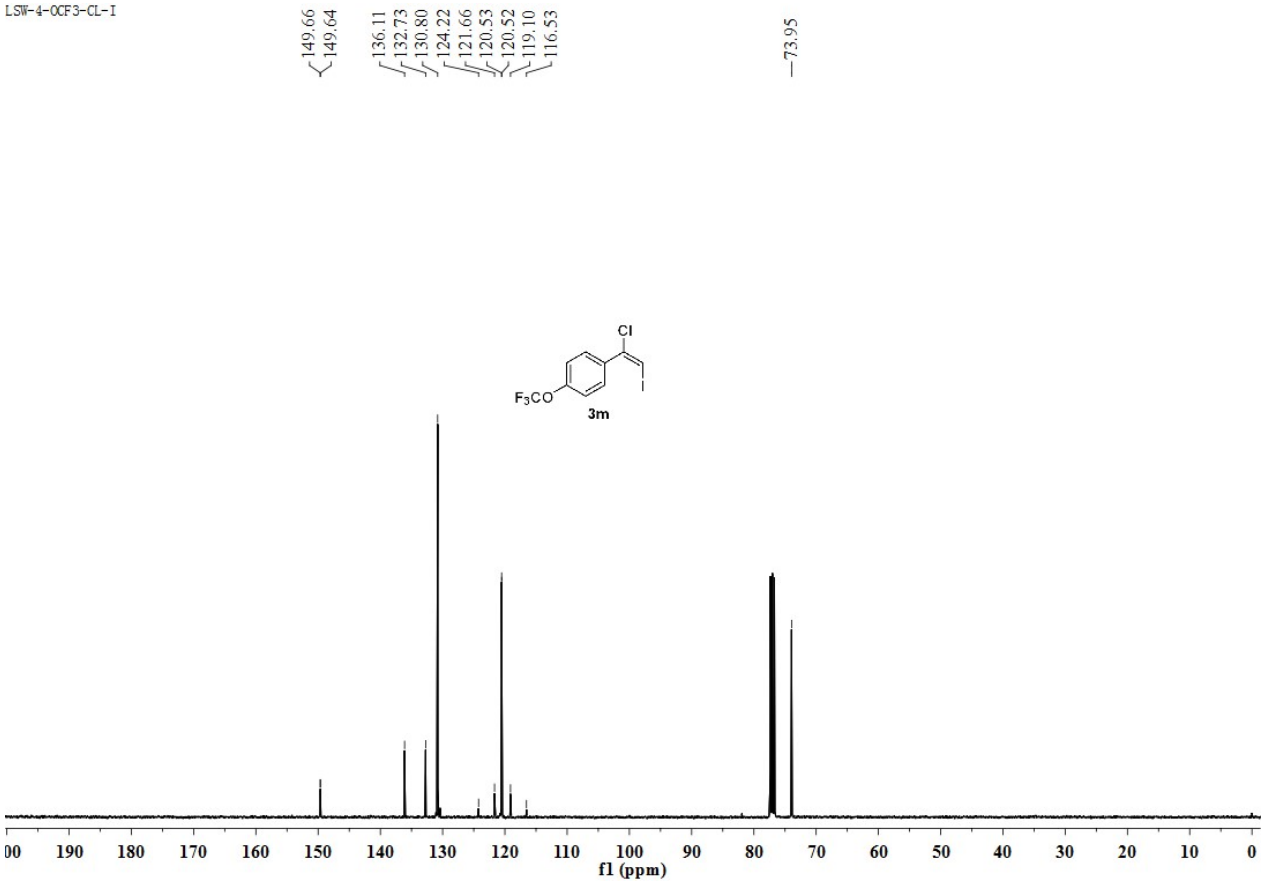
3m

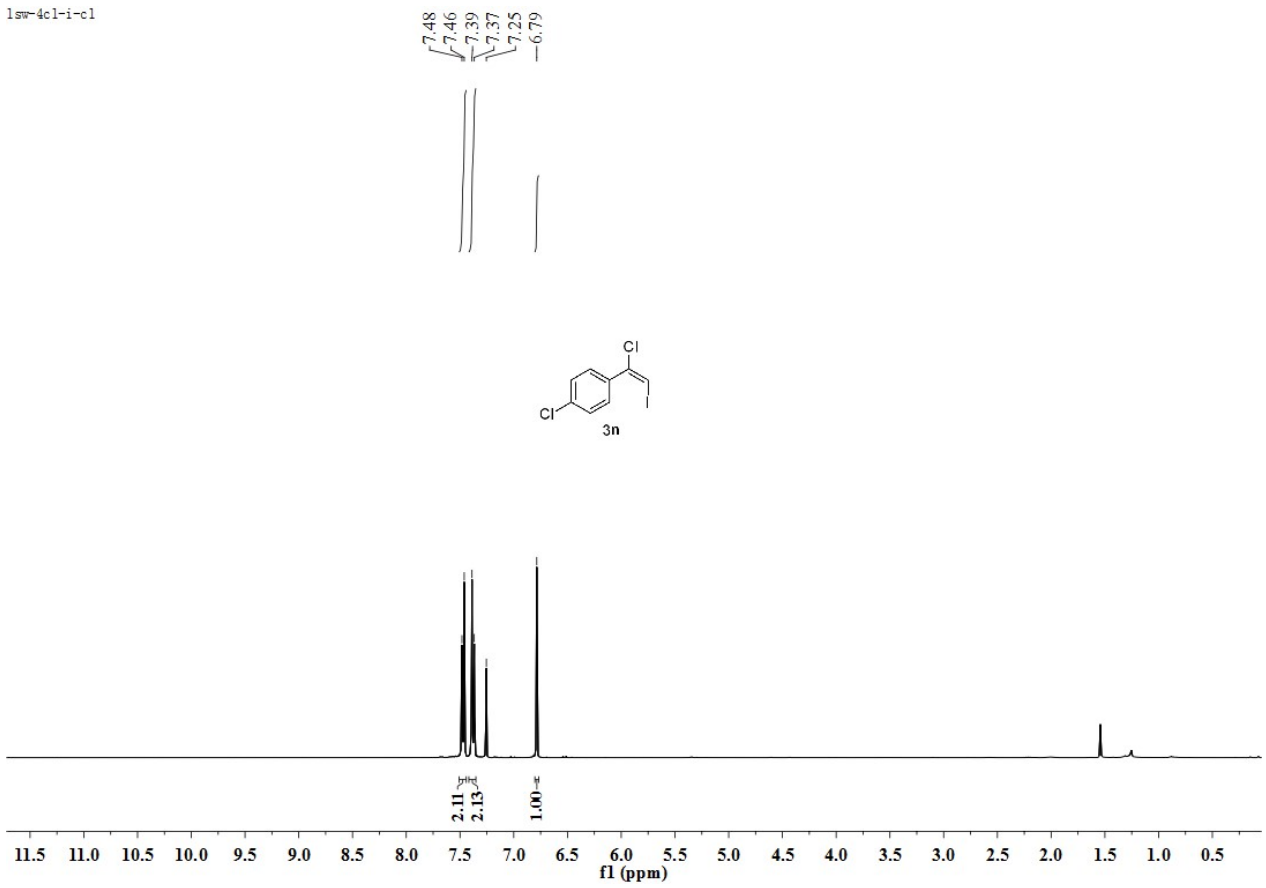


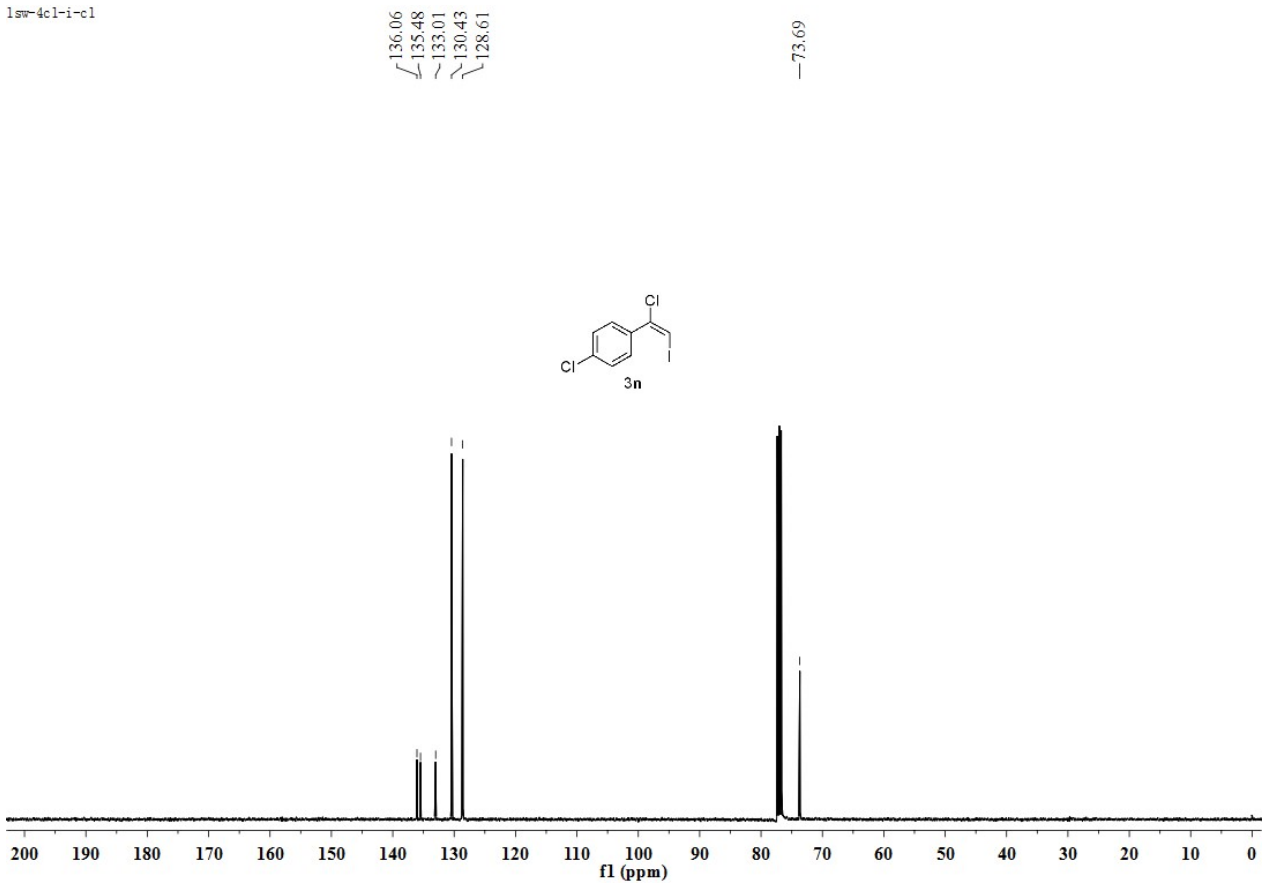
LSW-4-OCF3-CL-I



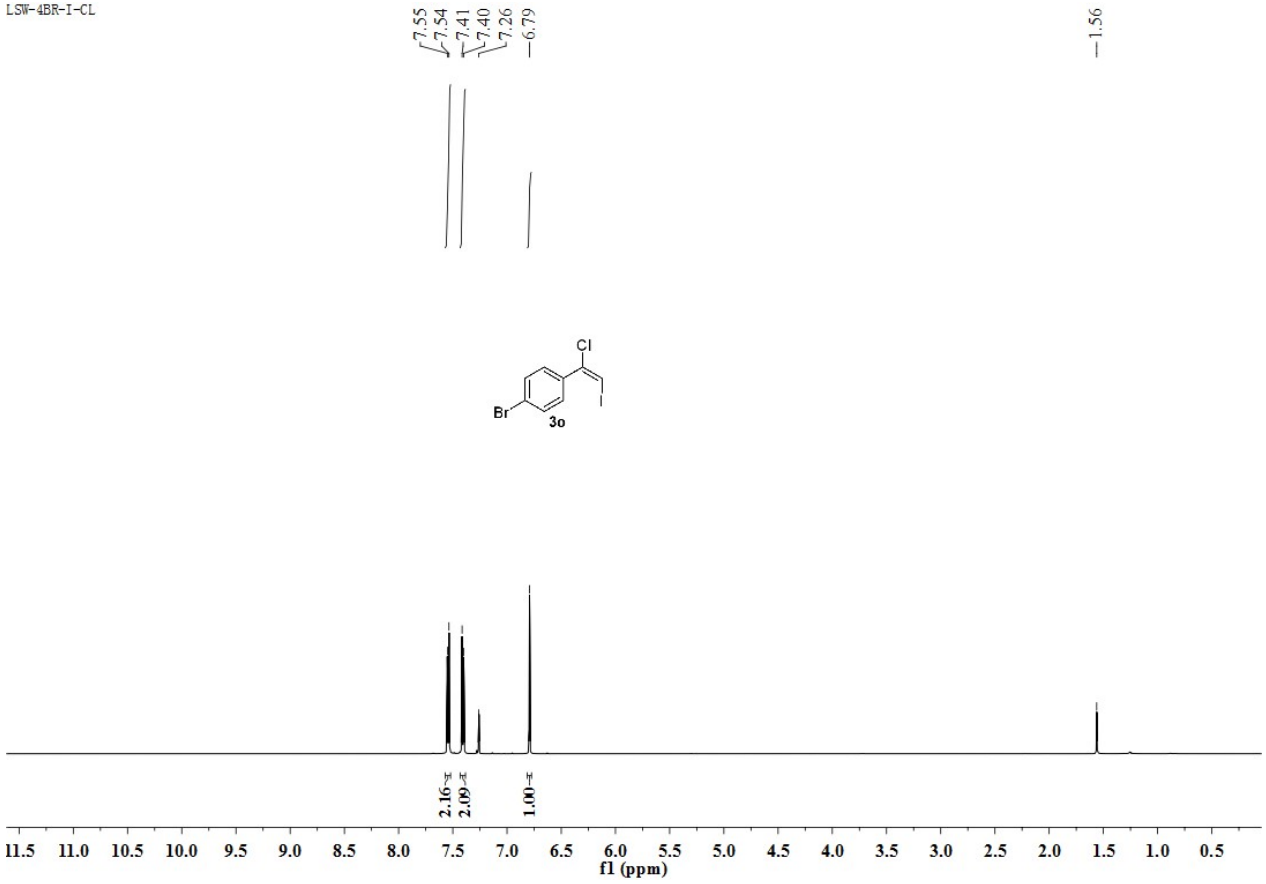
LSW-4-OCF3-CL-I



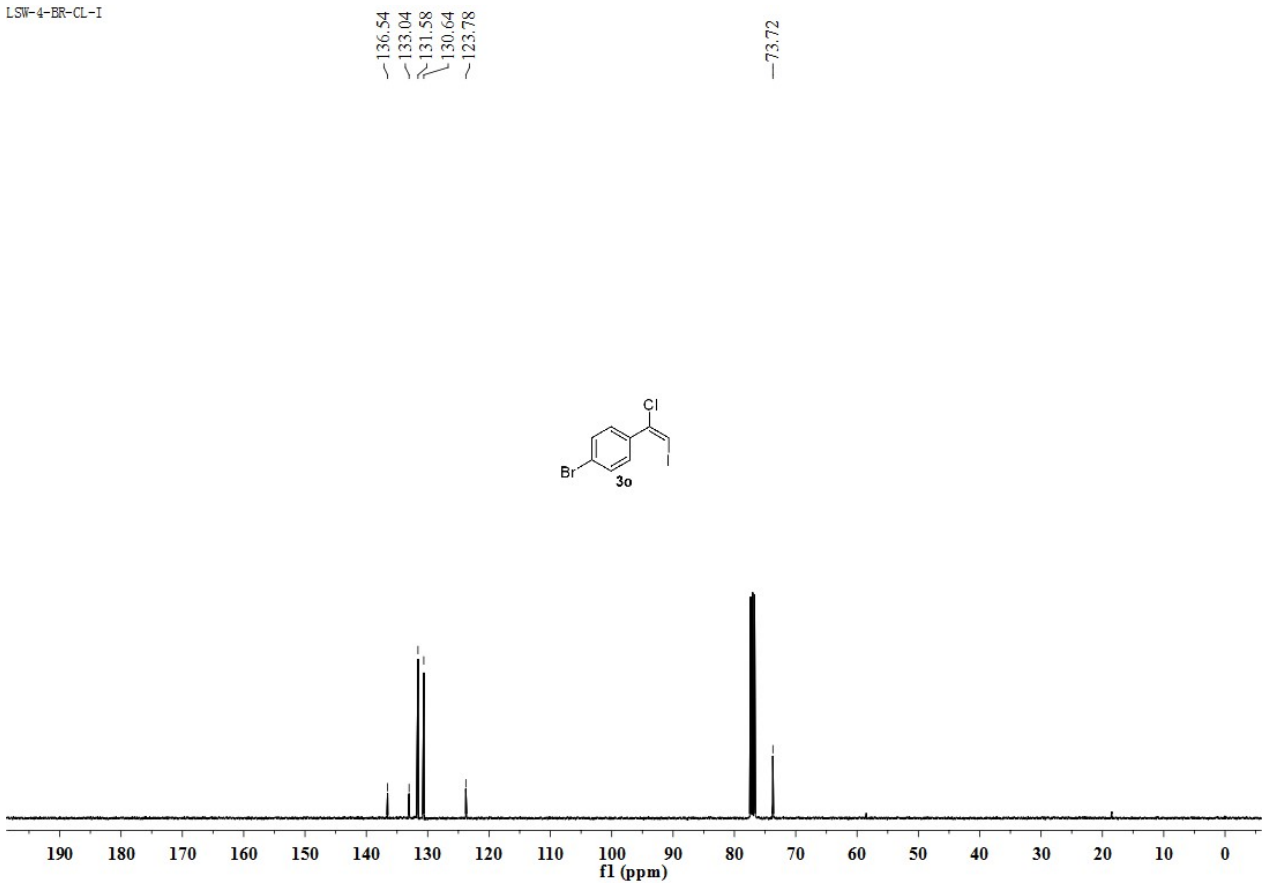

lsw-4cl-i-cl
7.48
7.46
7.39
7.37
7.25
6.79
Cl
Cl
I
3n
2.11
2.13
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

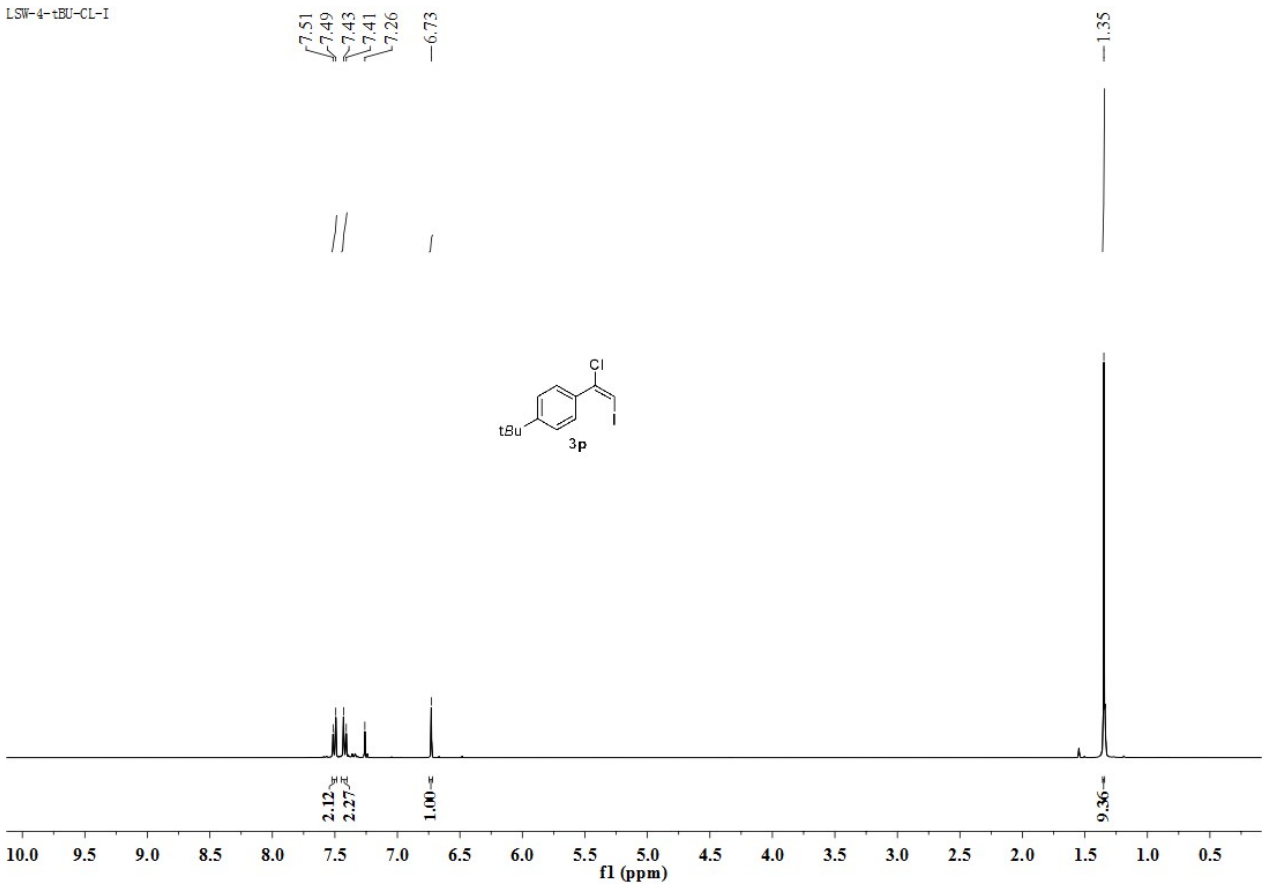

lsw-4cl-i-cl
136.06
135.48
133.01
130.43
128.61
73.69
Cl
Cl
I
3n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

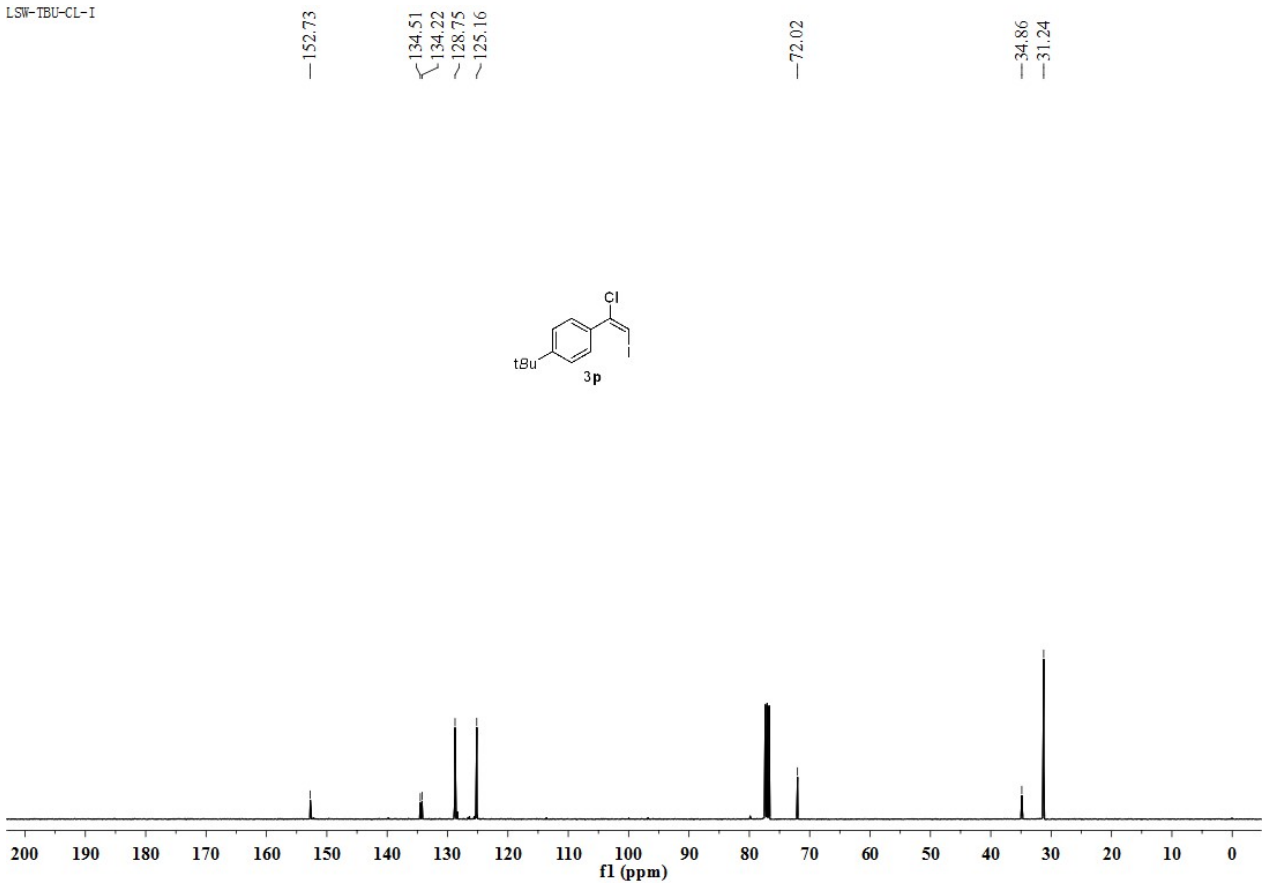
LSW-4BR-I-CL

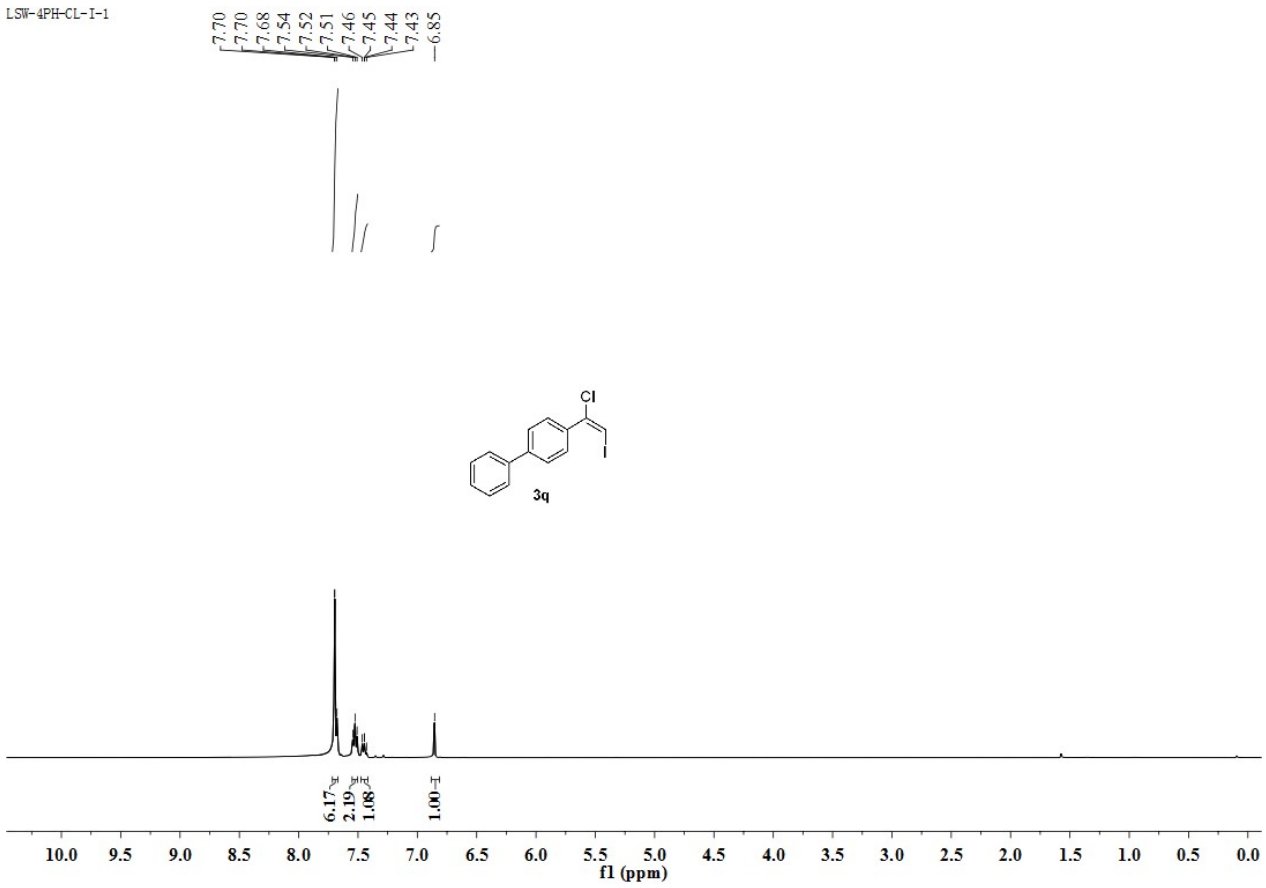


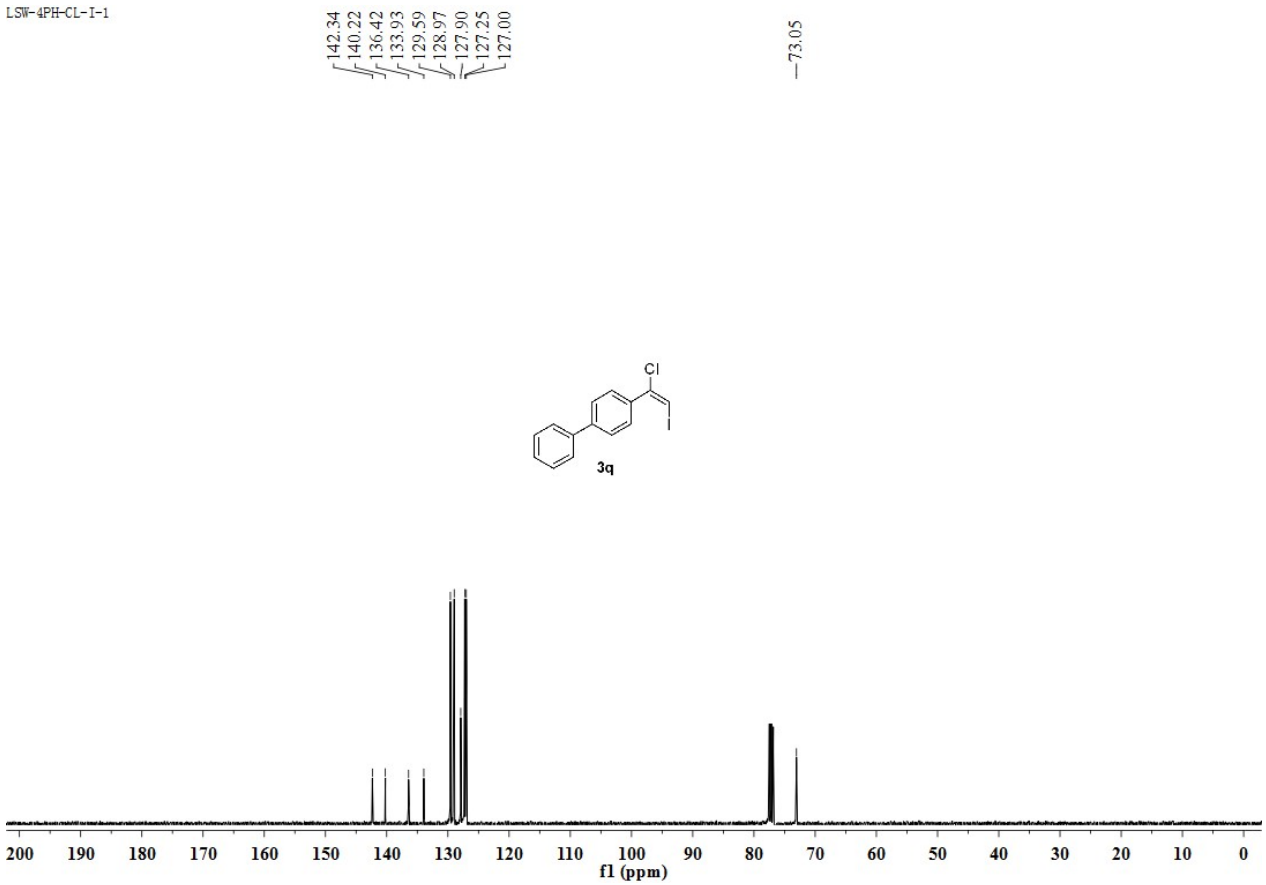
LSW-4-BR-CL-I

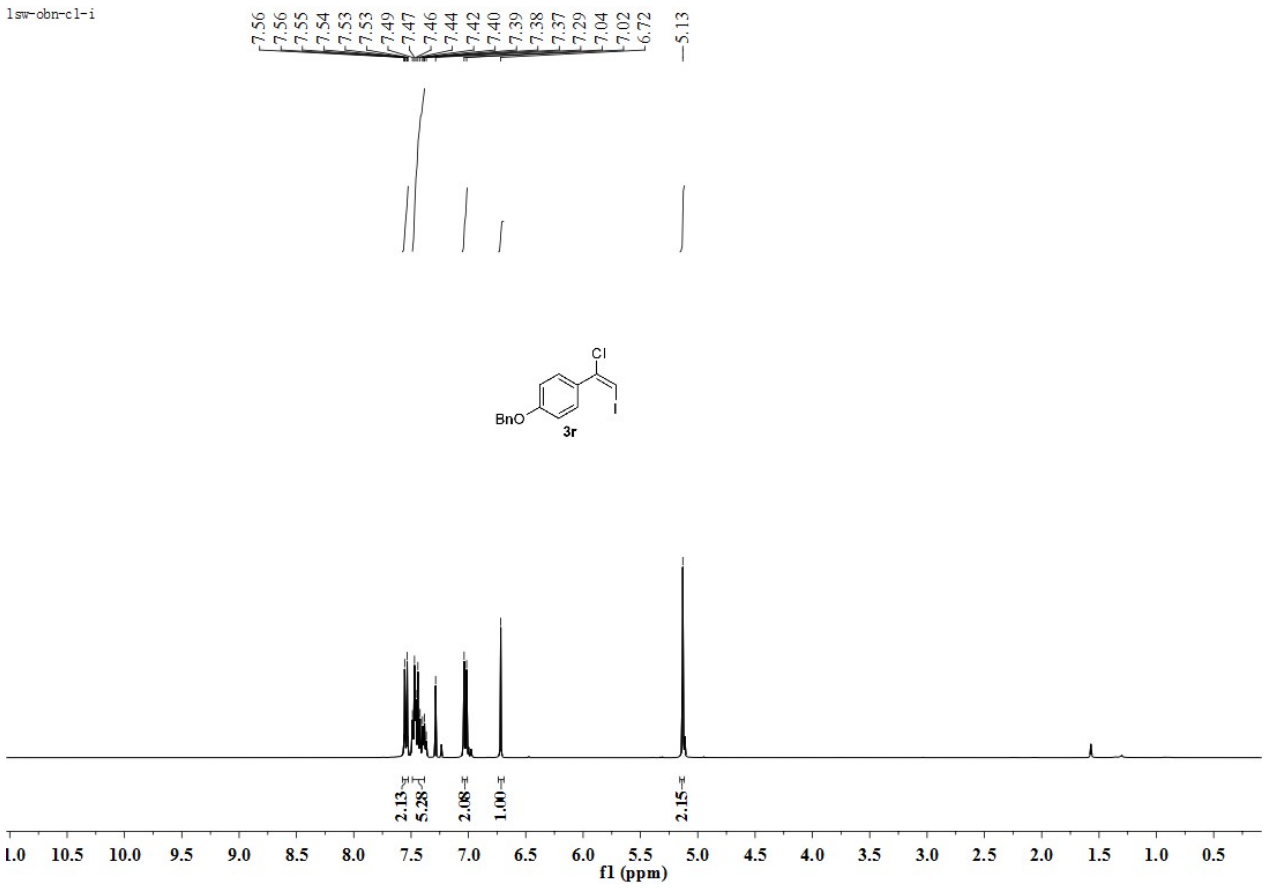


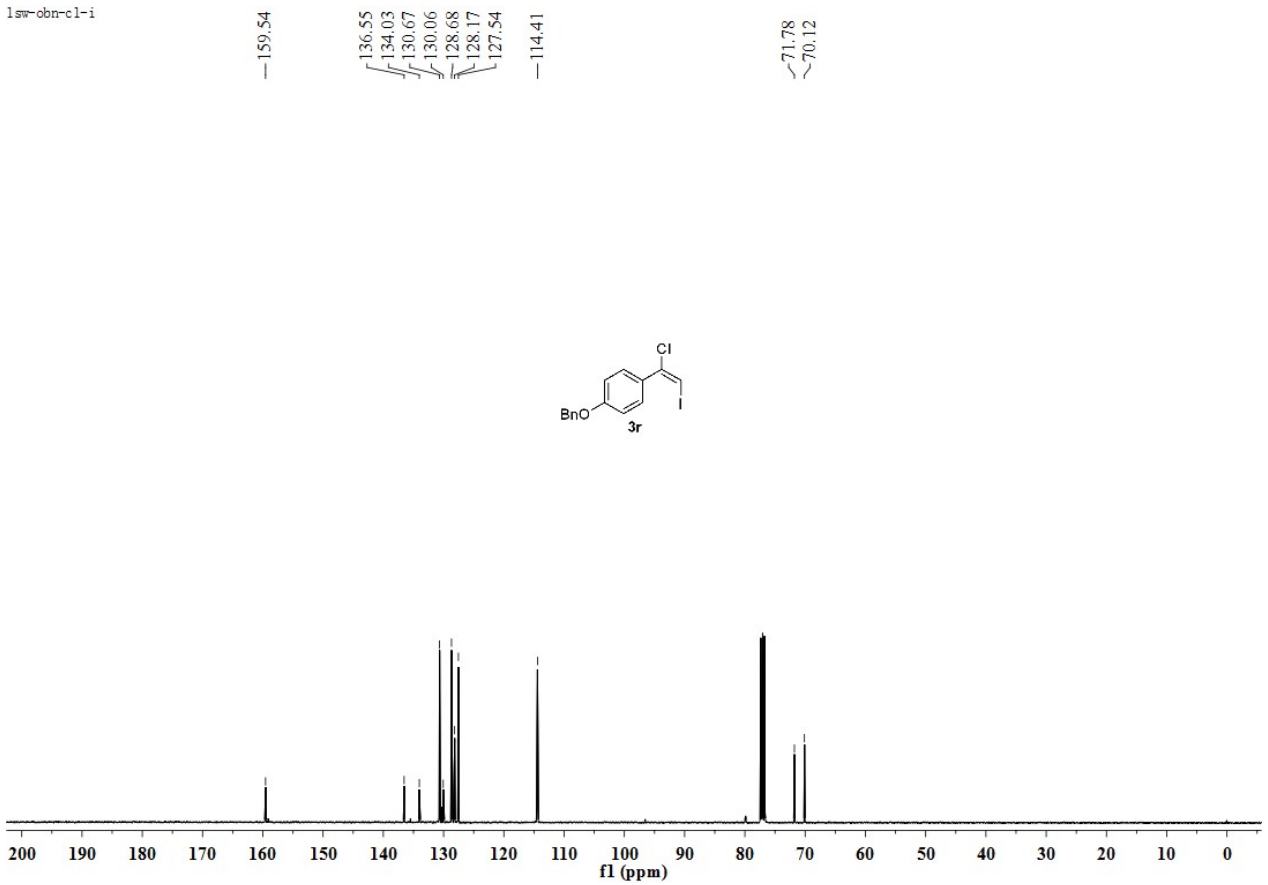

LSW-4-tBU-CL-I
7.51
7.49
7.43
7.41
7.26
6.73
1.35
Cl
tBu
3p
2.12
2.27
1.00
9.36
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

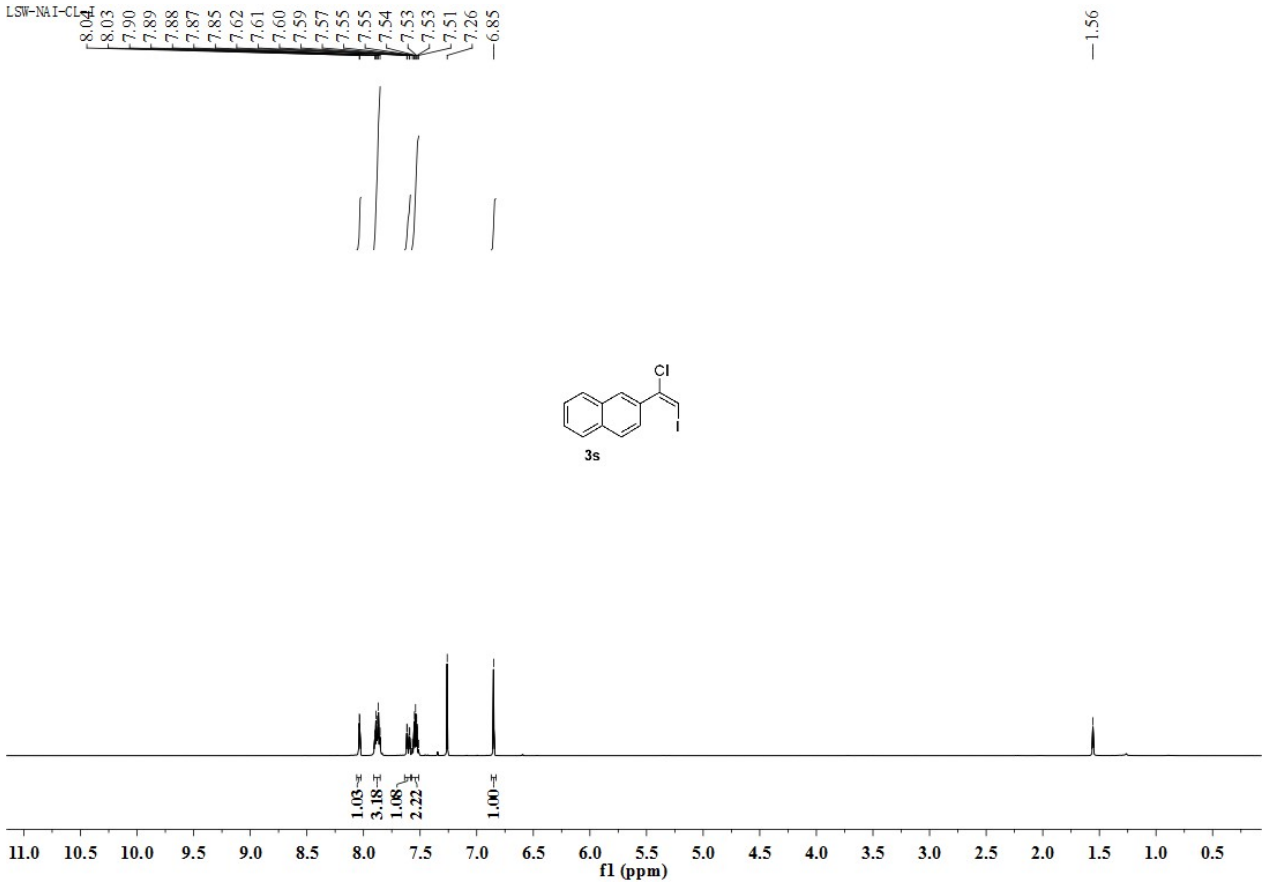

LSW-TBU-CL-I
152.73
134.51
134.22
128.75
125.16
72.02
34.86
31.24
Cl
tBu
3p
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

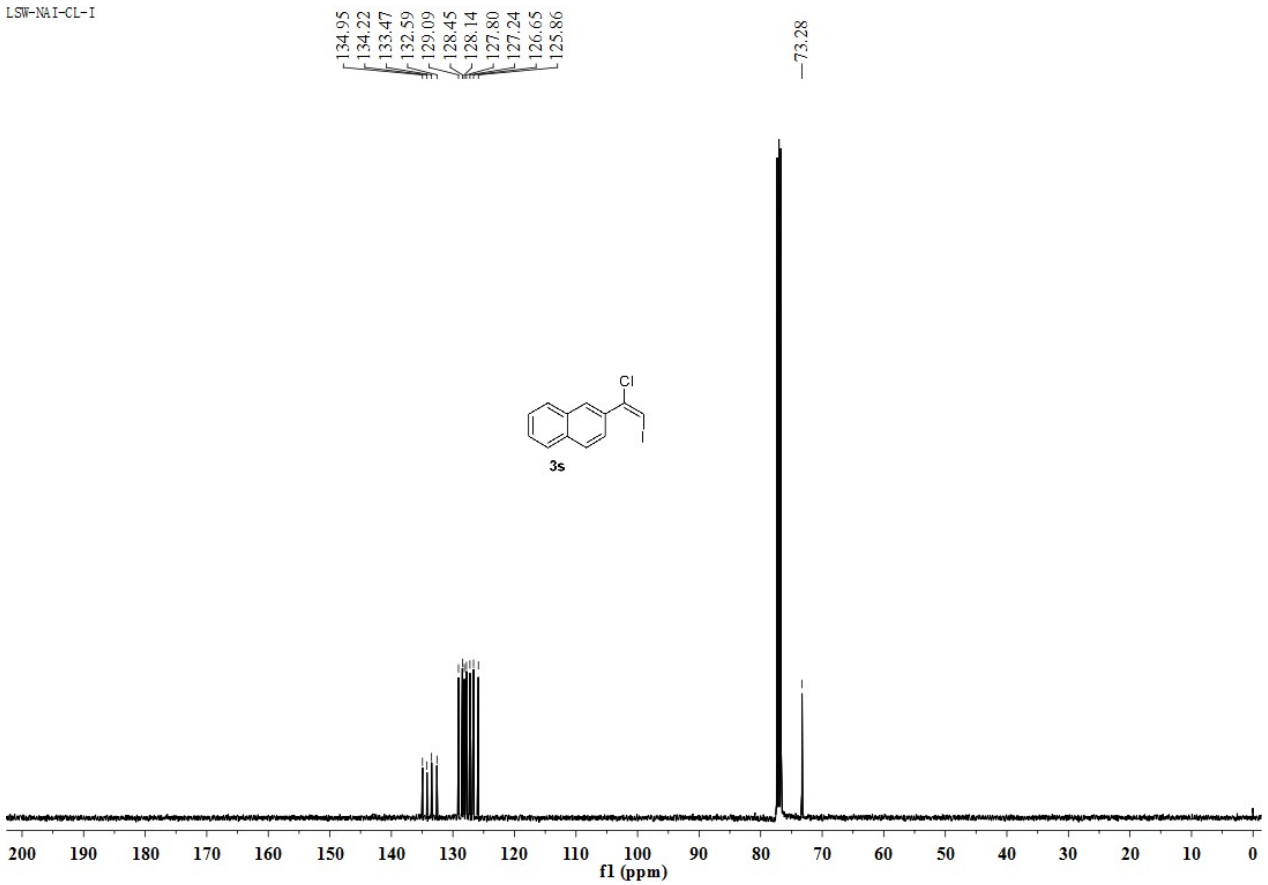

LSW-4PH-CL-I-1
7.70
7.70
7.68
7.54
7.52
7.51
7.46
7.45
7.44
7.43
6.85
Cl
I
3q
6.17
2.19
1.08
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


LSW-4PH-CL-I-1
142.34
140.22
136.42
133.93
129.59
128.97
127.90
127.25
127.00
73.05
Cl
I
3q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

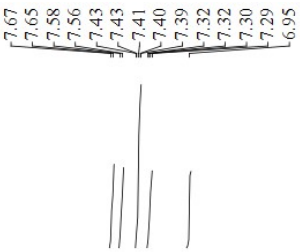

lsw-obn-cl-i
7.56
7.56
7.55
7.54
7.53
7.53
7.49
7.47
7.46
7.44
7.42
7.40
7.39
7.38
7.37
7.29
7.04
7.02
6.72
5.13
Cl
I
BnO
3r
2.13
5.28
2.08
1.00
2.15
f1 (ppm)

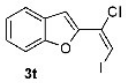

lsw-obn-cl-i
159.54
136.55
134.03
130.67
130.06
128.68
128.17
127.54
114.41
71.78
70.12
Cl
I
BnO
3r
f1 (ppm)


LSW-NAI-CL-H
8.04
8.03
7.90
7.89
7.88
7.87
7.85
7.62
7.61
7.60
7.59
7.57
7.55
7.55
7.54
7.53
7.53
7.51
7.26
6.85
1.56
Cl
I
3s
1.03
3.18
1.08
2.22
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

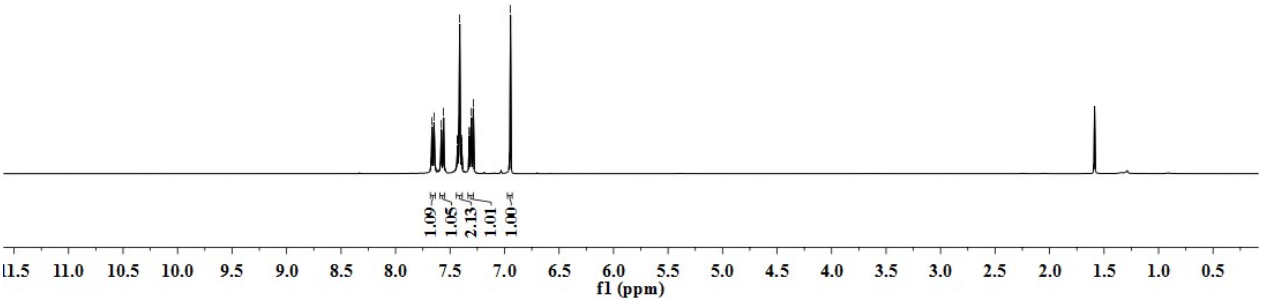

LSW-NAI-CL-I
134.95
134.22
133.47
132.59
129.09
128.45
128.14
127.80
127.24
126.65
125.86
73.28
Cl
I
3s
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

LSW-10-B-FUNAN-CI-I

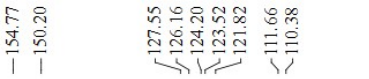


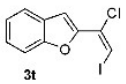


3t

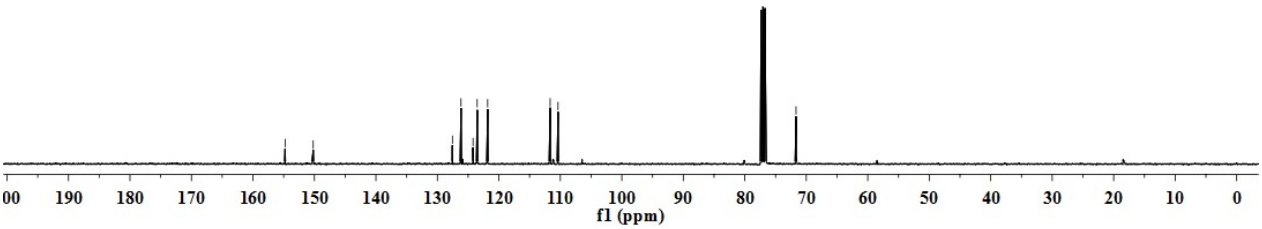


LSW-FUNAN-CL-I

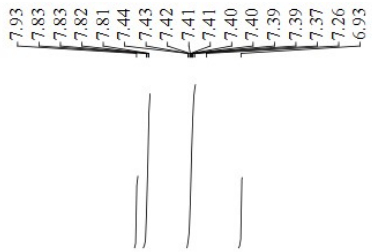


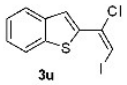


3t

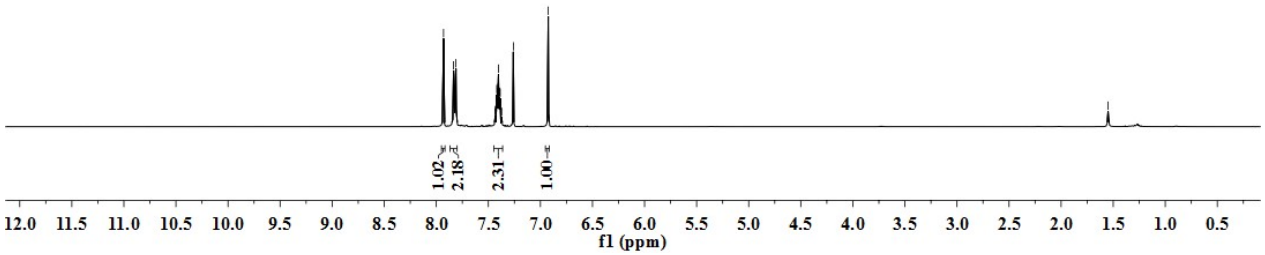


lsw-benbingsaifen

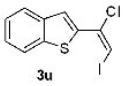




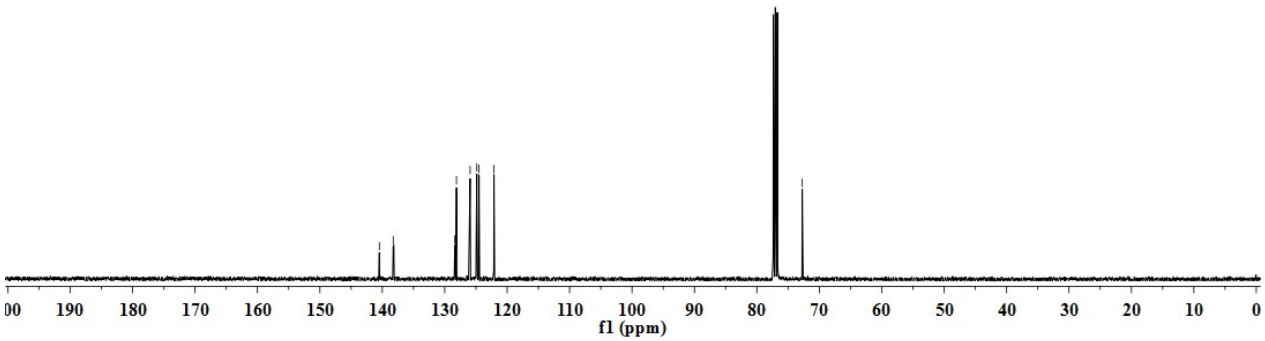
3u

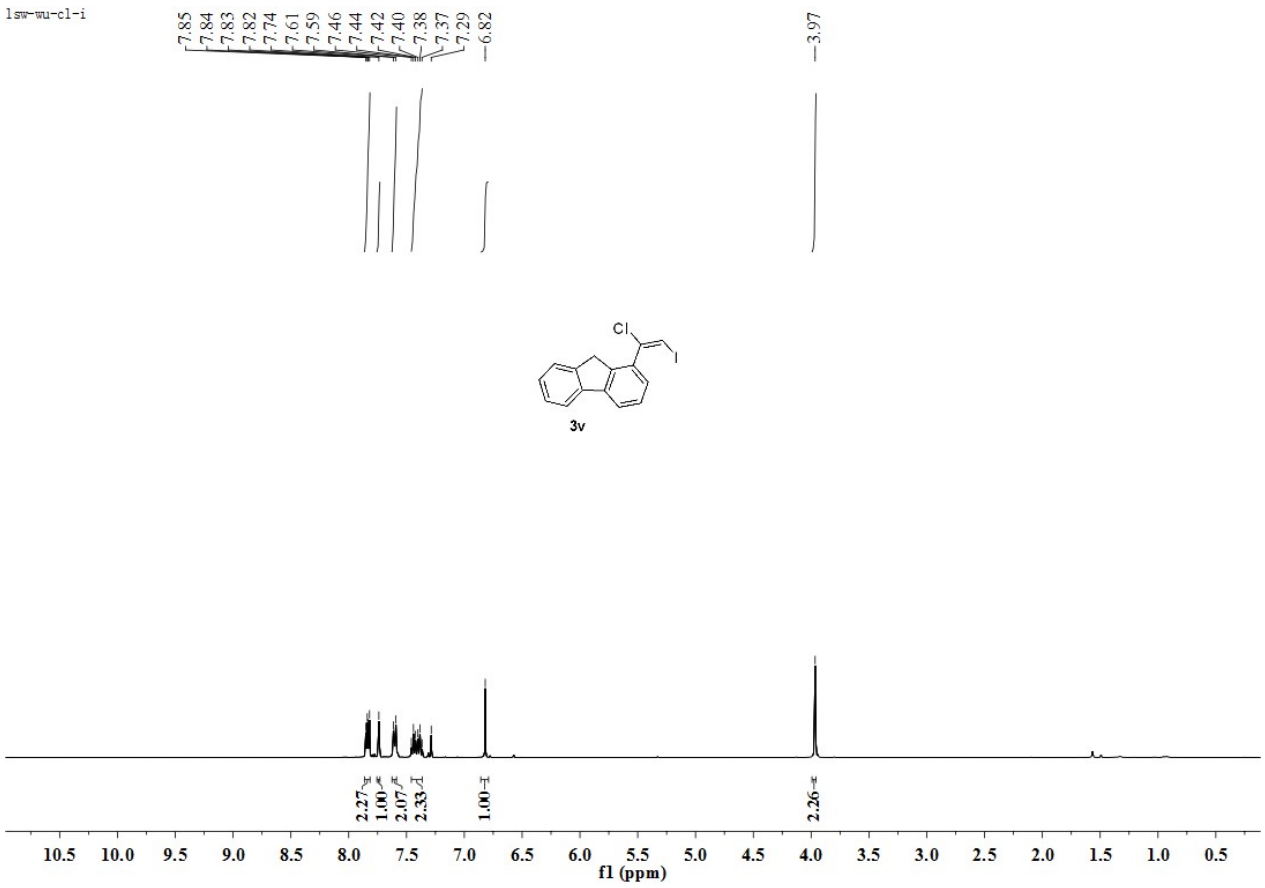


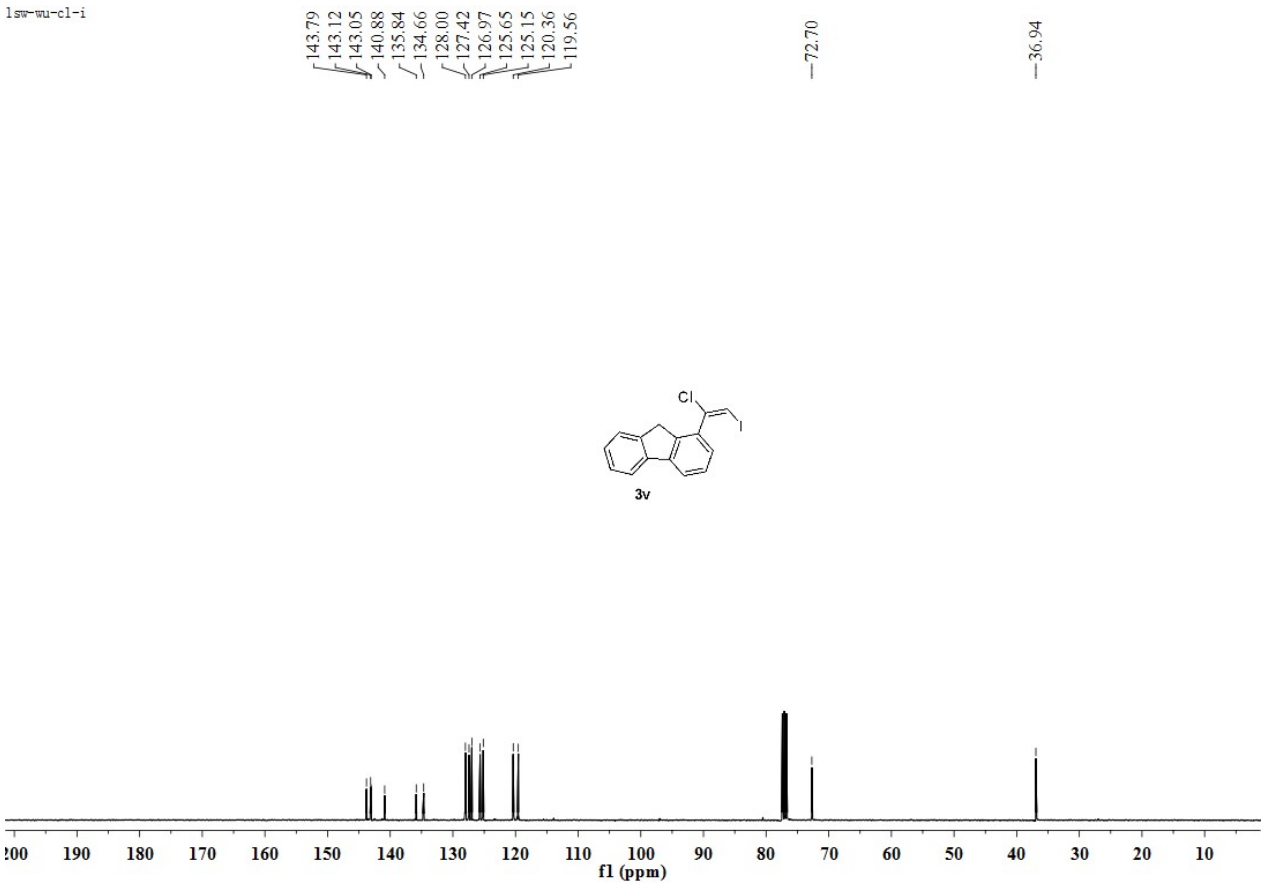
LSW-BBS-CL-I

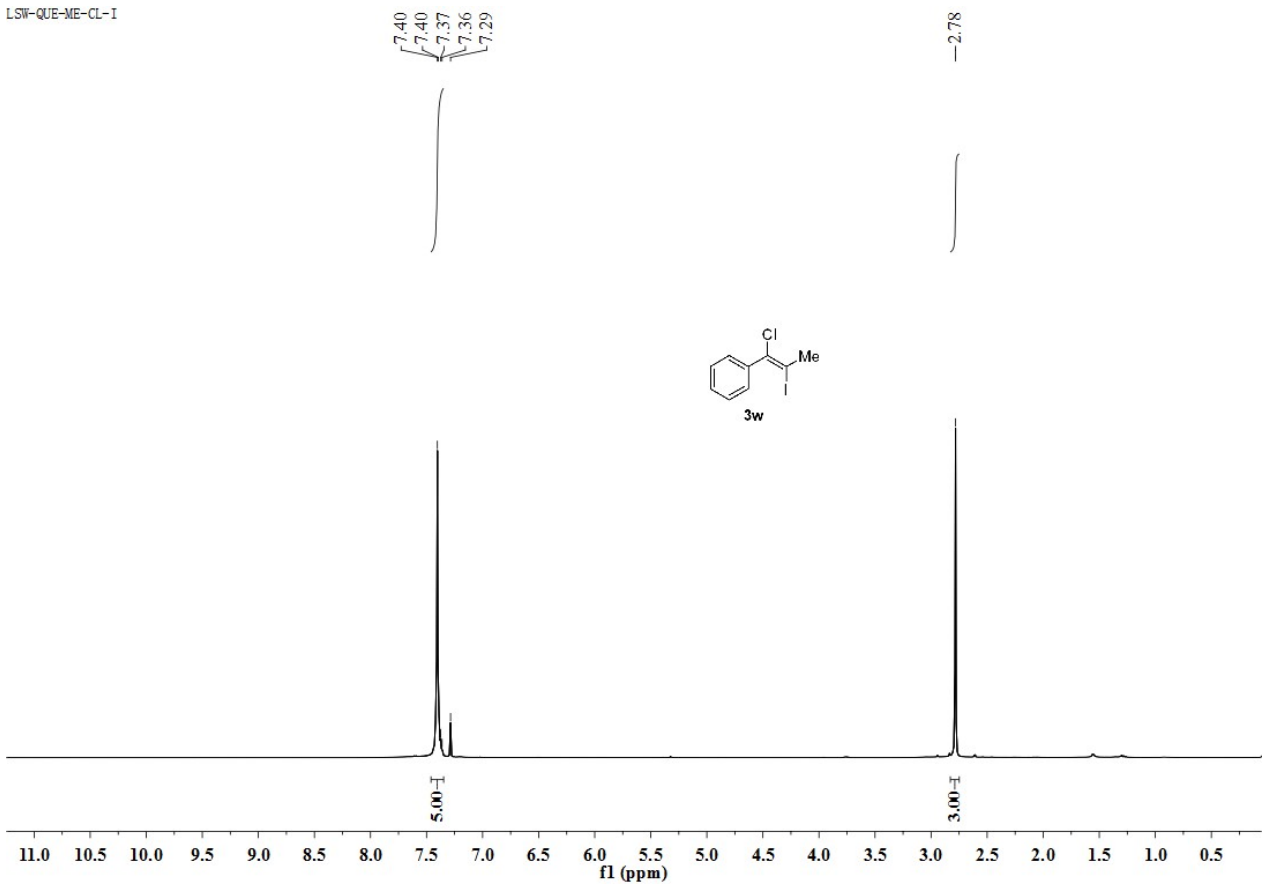


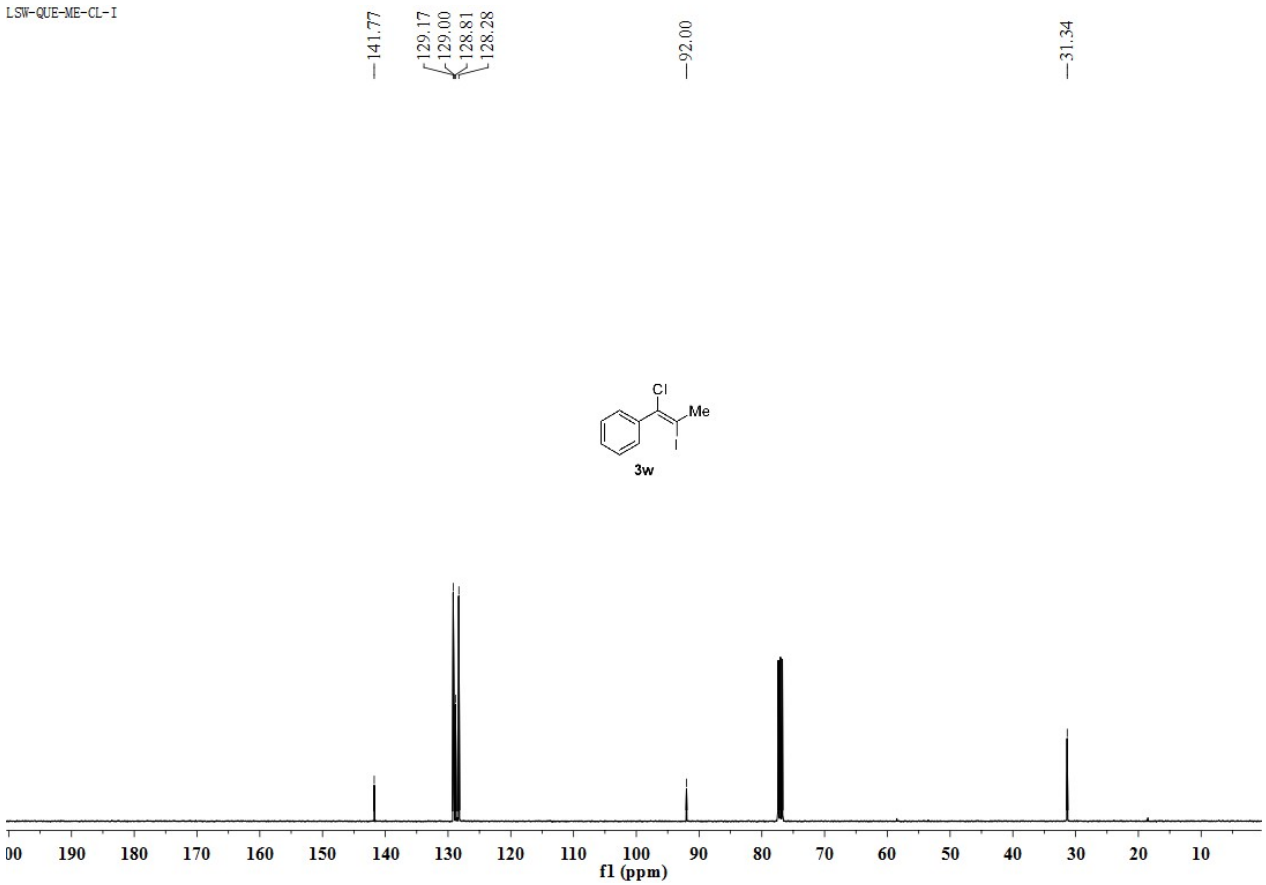
3u

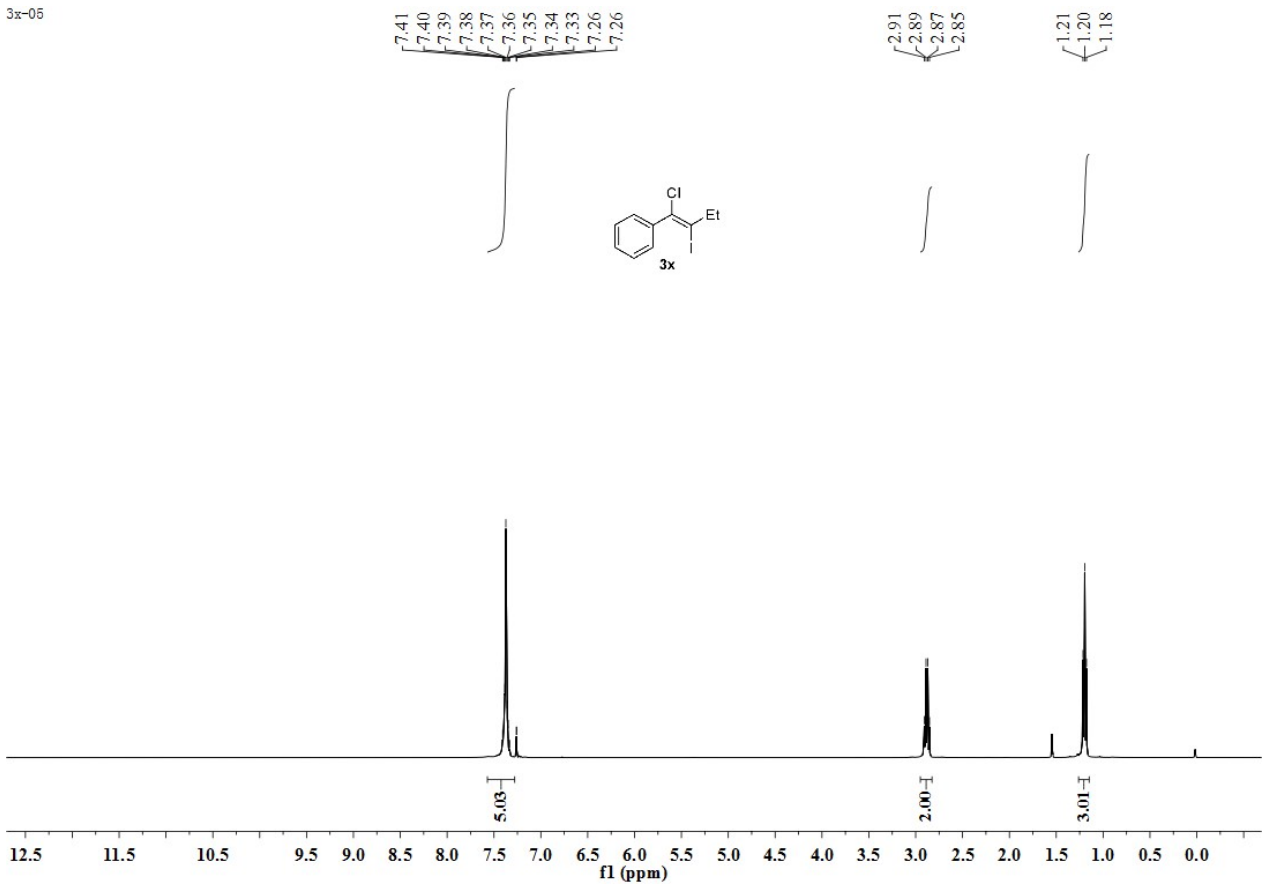


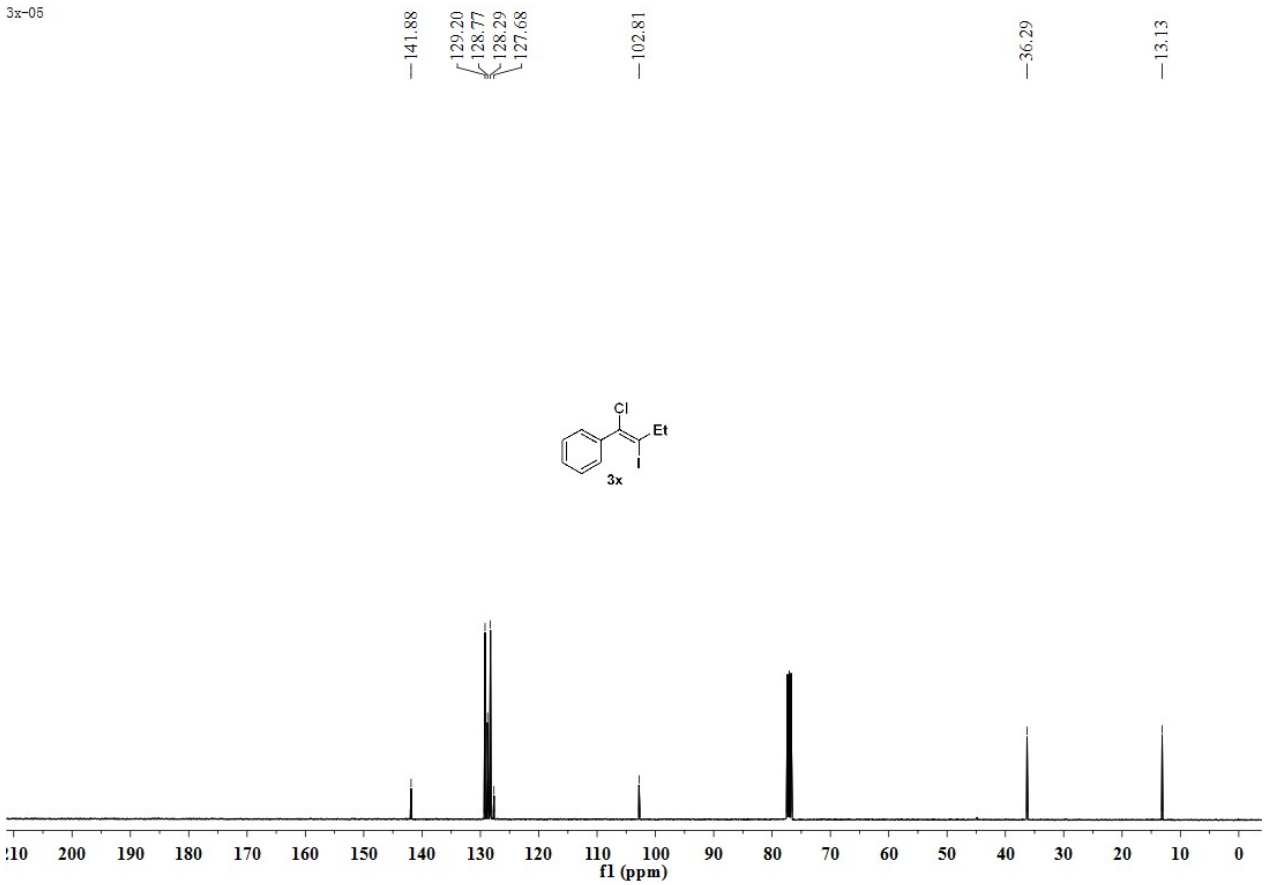

lsw-wu-cl-i
7.85
7.84
7.83
7.82
7.74
7.61
7.59
7.46
7.44
7.42
7.40
7.38
7.37
7.29
6.82
3.97
Cl
I
3v
2.27
1.00
2.07
2.33
1.00
2.26
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


lsw-wu-cl-i
143.79
143.12
143.05
140.88
135.84
134.66
128.00
127.42
126.97
125.65
125.15
120.36
119.56
72.70
36.94
Cl
I
3v
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

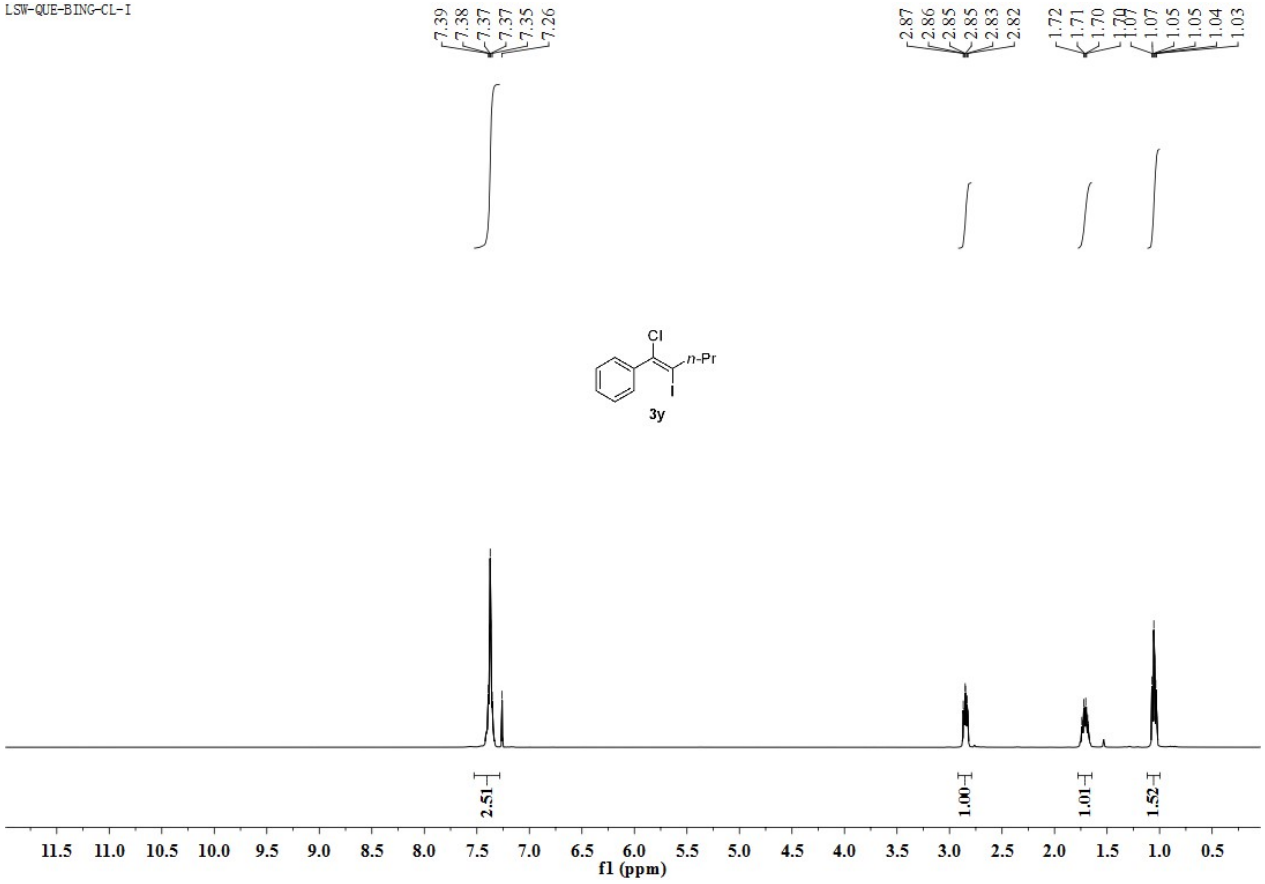

LSW-QUE-ME-CL-I
7.40
7.40
7.37
7.36
7.29
2.78
Cl
Me
I
3w
5.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


LSW-QUE-ME-CL-I
141.77
129.17
129.00
128.81
128.28
92.00
31.34
Cl
Me
I
3w
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

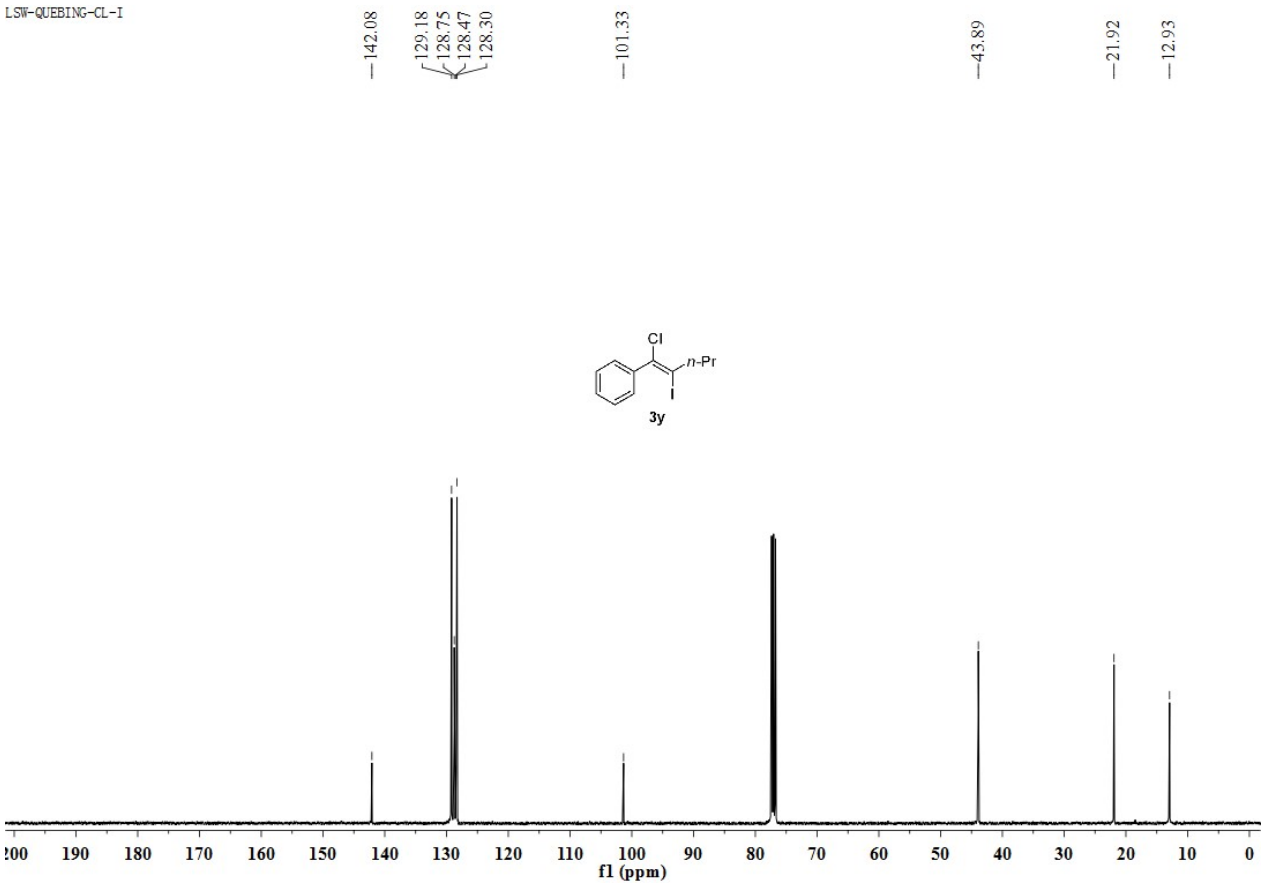

3x-05
7.41
7.40
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.26
7.26
2.91
2.89
2.87
2.85
1.21
1.20
1.18
Cl
Et
I
3x
5.03
2.00
3.01
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

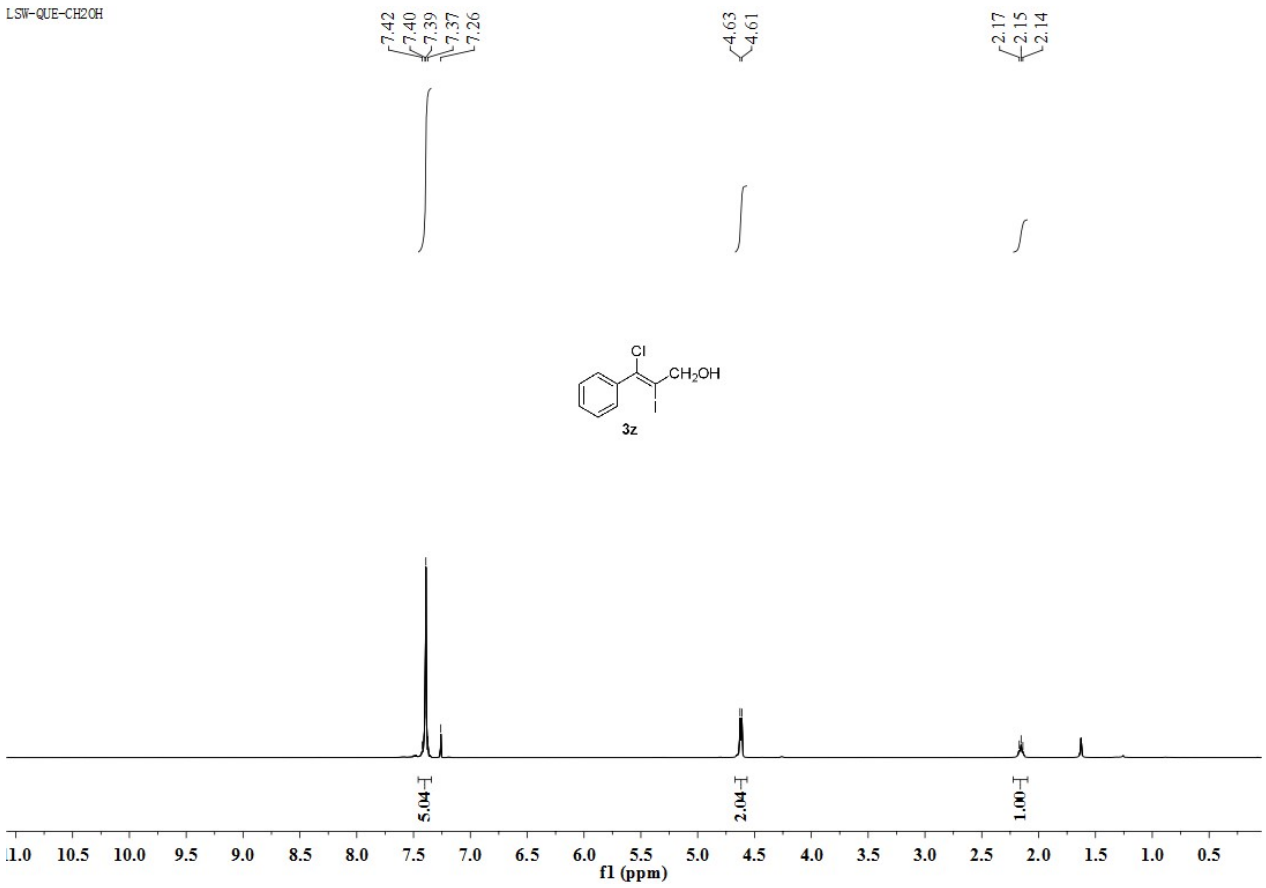

3x-05
141.88
129.20
128.77
128.29
127.68
102.81
36.29
13.13
Cl
Et
I
3x
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

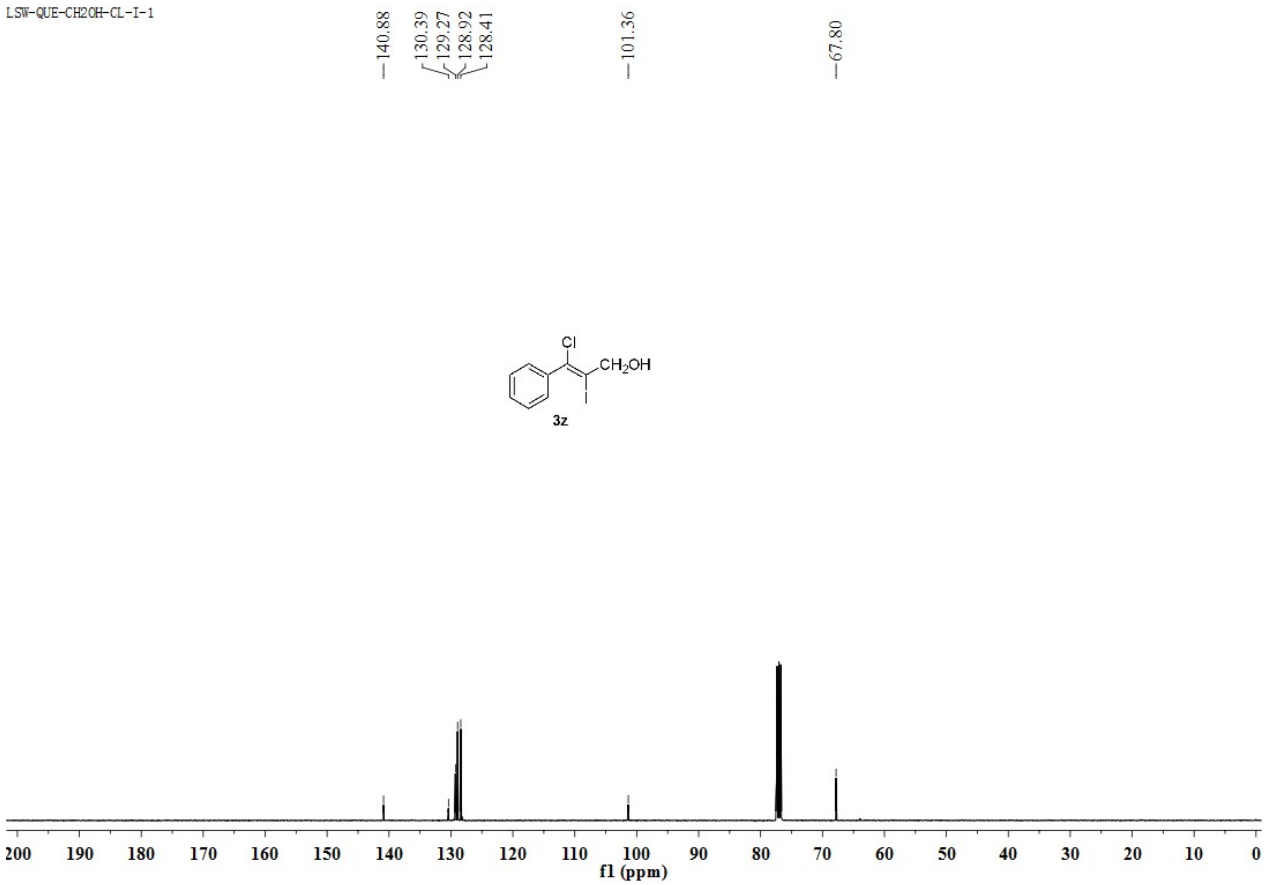
LSW-QUE-BING-CL-I

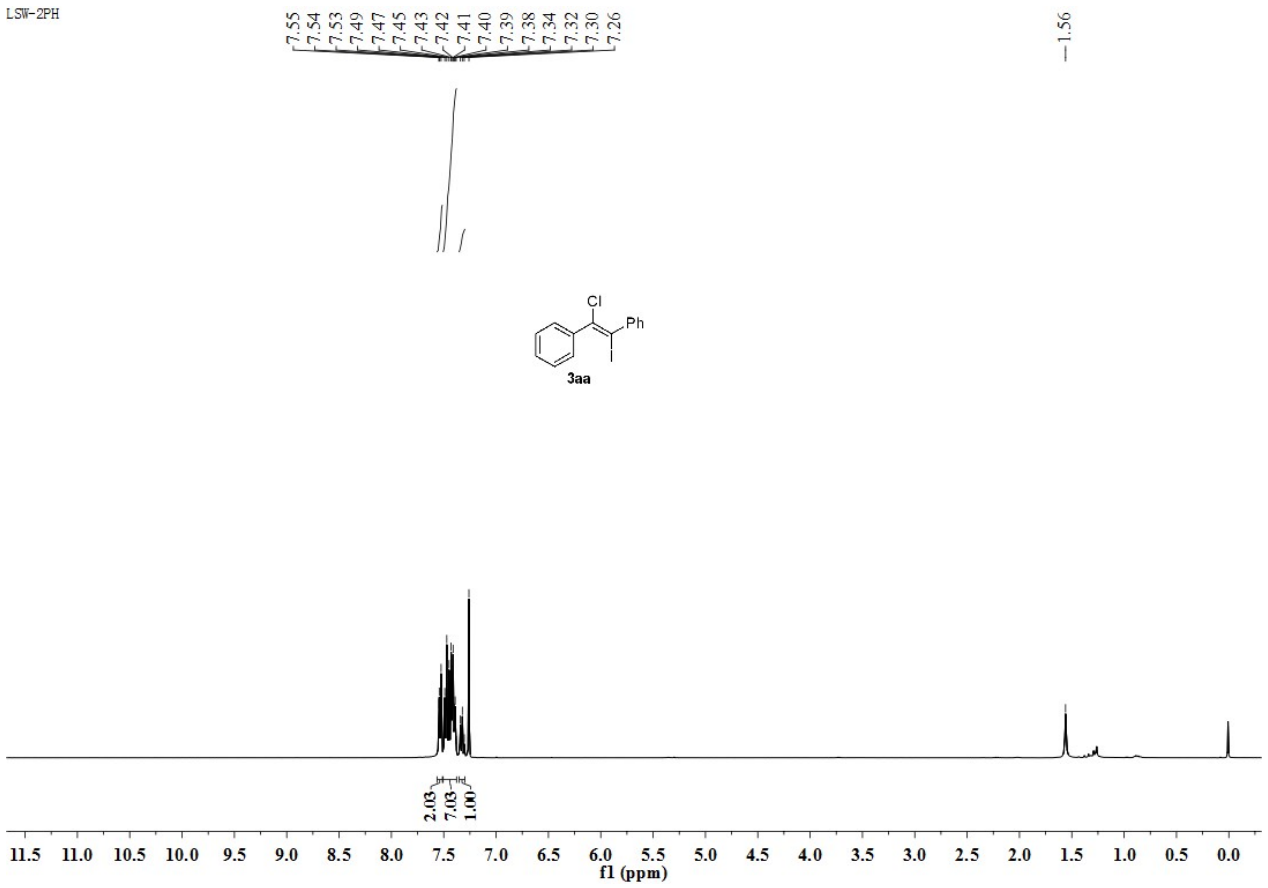


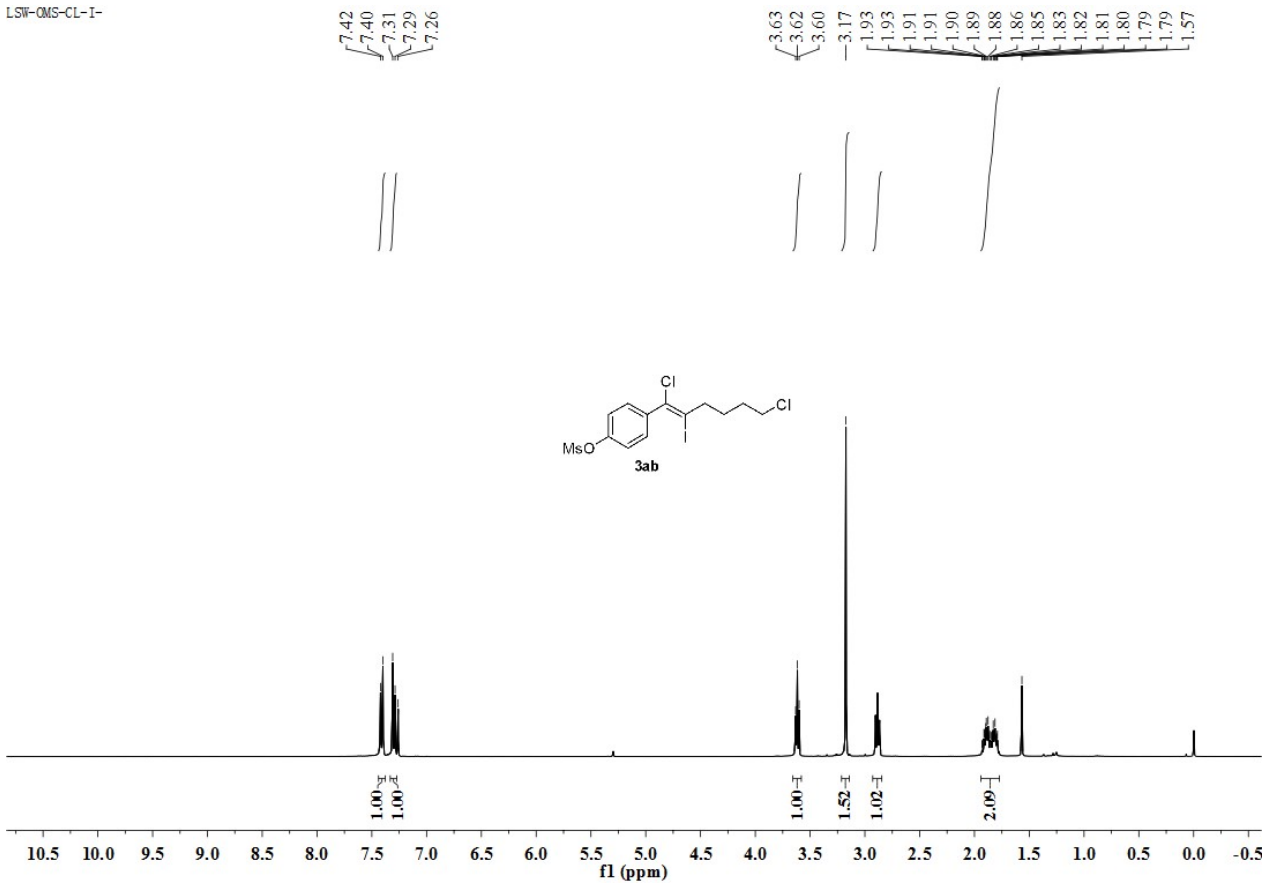
LSW-QUEBING-CL-I

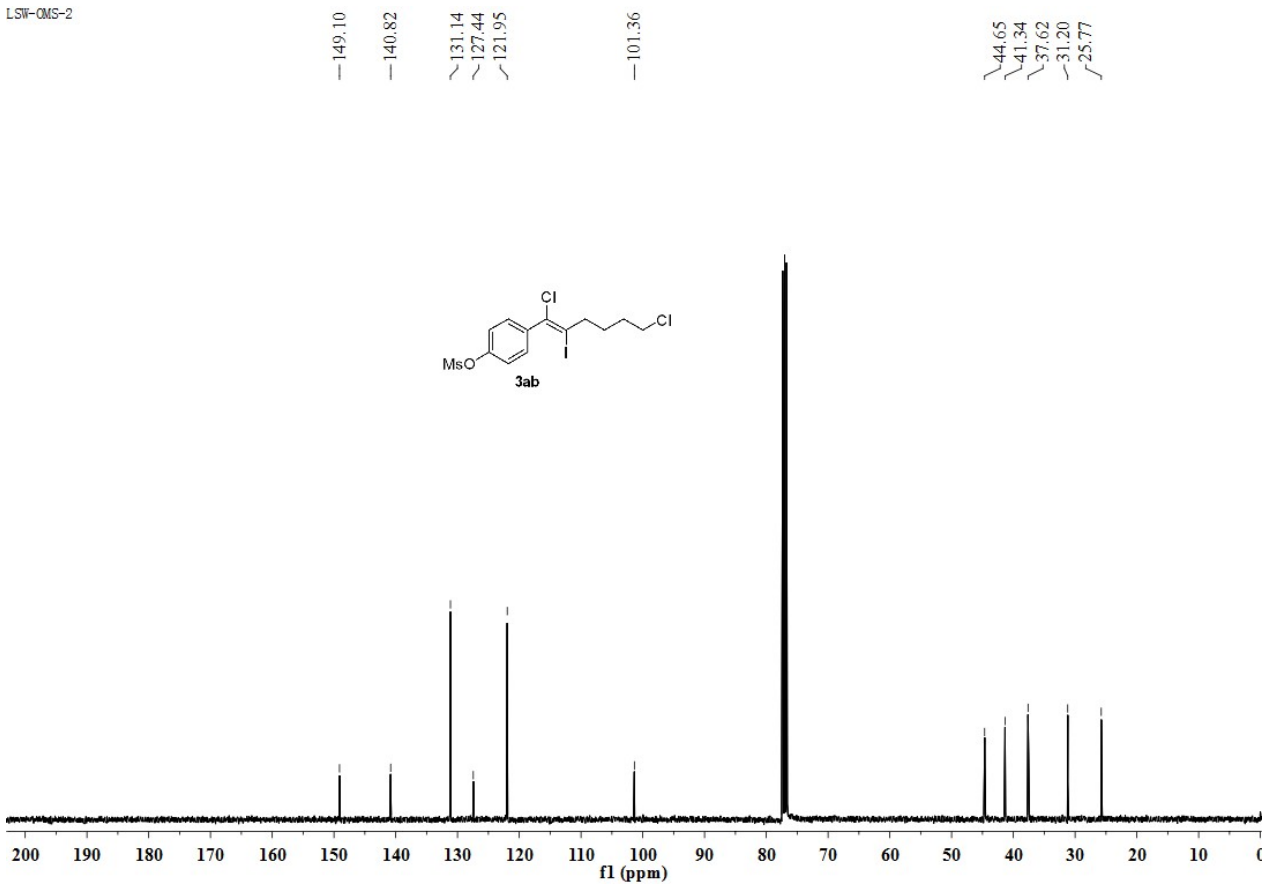


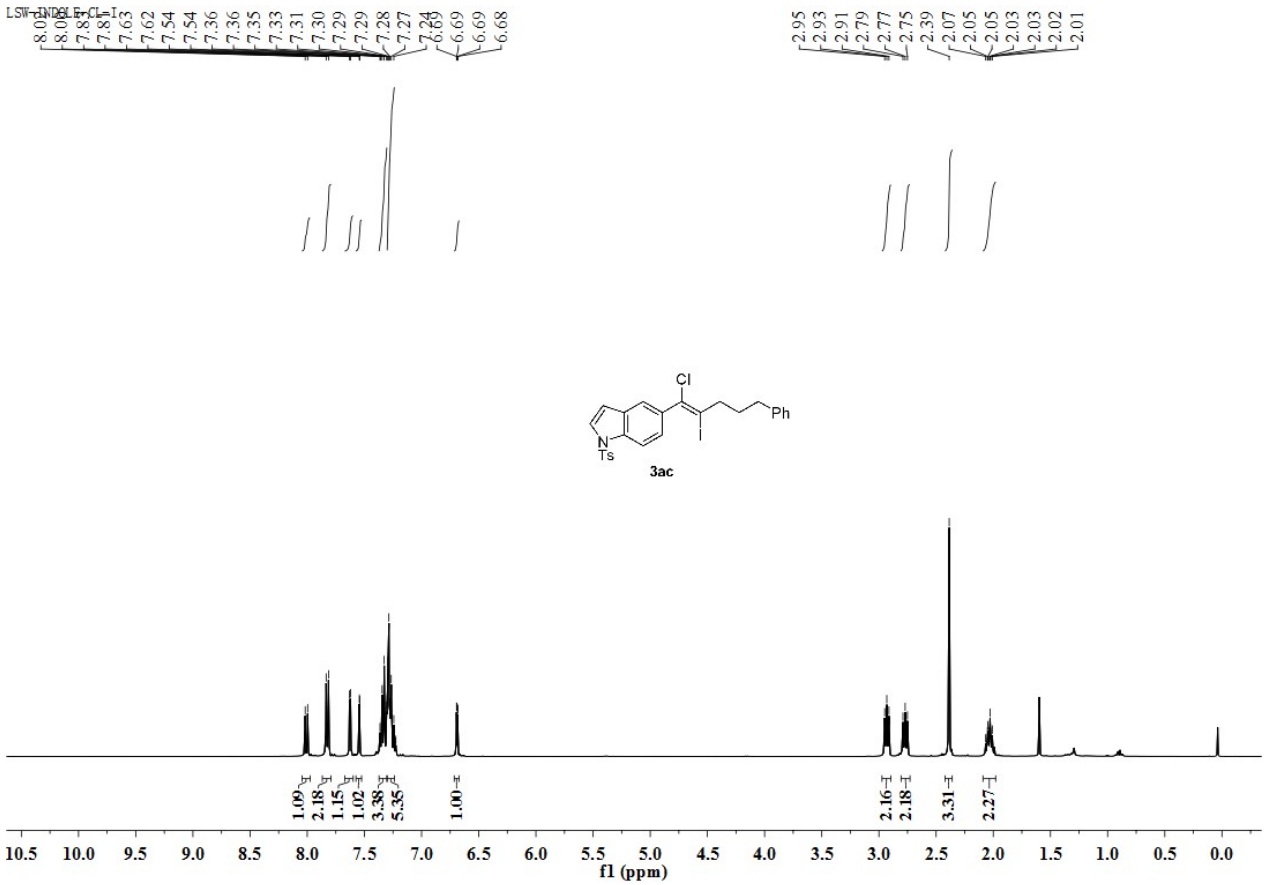

LSW-QUE-CH2OH
7.42
7.40
7.39
7.37
7.26
4.63
4.61
2.17
2.15
2.14
Cl
CH2OH
I
3z
5.04
2.04
1.00
f1 (ppm)


LSW-QUE-CH2OH-CL-I-1
140.88
130.39
129.27
128.92
128.41
101.36
67.80
Cl
CH2OH
I
3z
f1 (ppm)

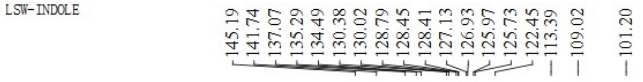

LSW-2PH
7.55
7.54
7.53
7.49
7.47
7.45
7.43
7.42
7.41
7.40
7.39
7.38
7.34
7.32
7.30
7.26
1.56
Cl
Ph
I
3aa
2.03
7.03
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

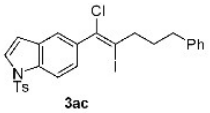

LSW-OMS-CL-I-
7.42
7.40
7.31
7.29
7.26
3.63
3.62
3.60
3.17
1.93
1.93
1.91
1.91
1.90
1.89
1.88
1.86
1.85
1.83
1.82
1.81
1.80
1.79
1.79
1.57
Cl
Cl
MsO
I
3ab
1.00
1.00
1.00
1.52
1.02
2.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


LSW-OMS-2
149.10
140.82
131.14
127.44
121.95
101.36
44.65
41.34
37.62
31.20
25.77
Cl
Cl
MsO
3ab
f1 (ppm)


8.02
8.00
7.85
7.83
7.63
7.62
7.54
7.54
7.36
7.35
7.33
7.31
7.30
7.29
7.29
7.28
7.27
7.24
6.69
6.69
6.68
2.95
2.93
2.91
2.79
2.77
2.75
2.39
2.07
2.05
2.05
2.03
2.03
2.02
2.01
Cl
Ph
N
Ts
3ac
1.09
2.18
1.15
1.02
3.38
5.35
1.00
2.16
2.18
3.31
2.27
f1 (ppm)

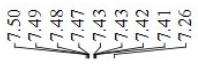
LSW-INDOLE

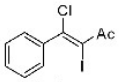




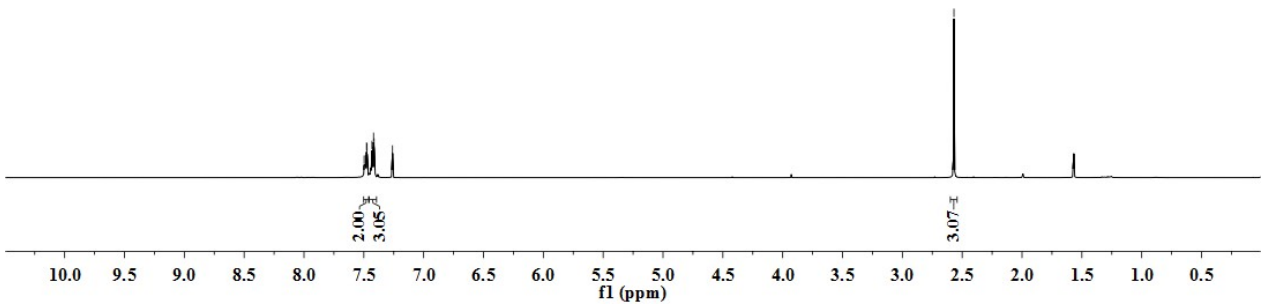
3ac

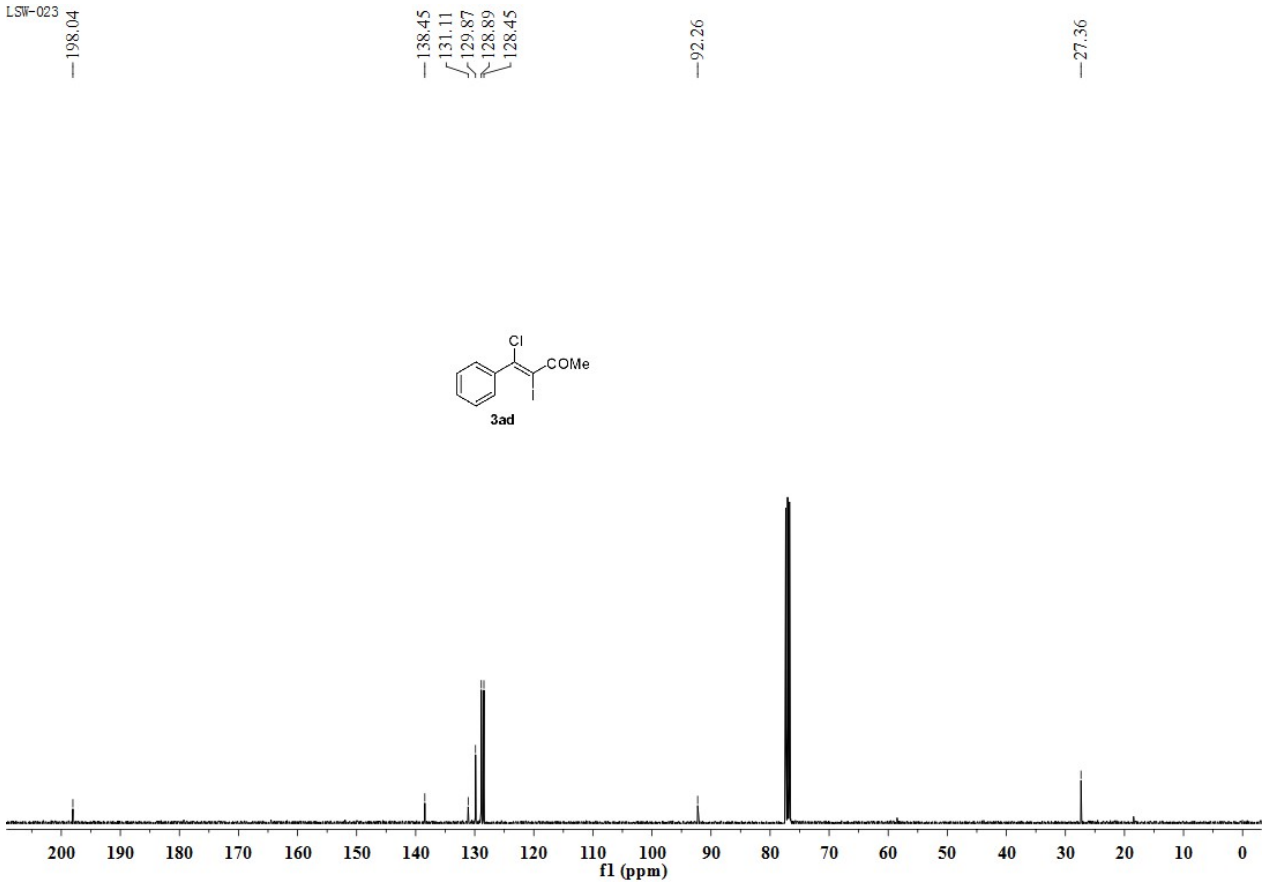
3ad-LSW-AC-2

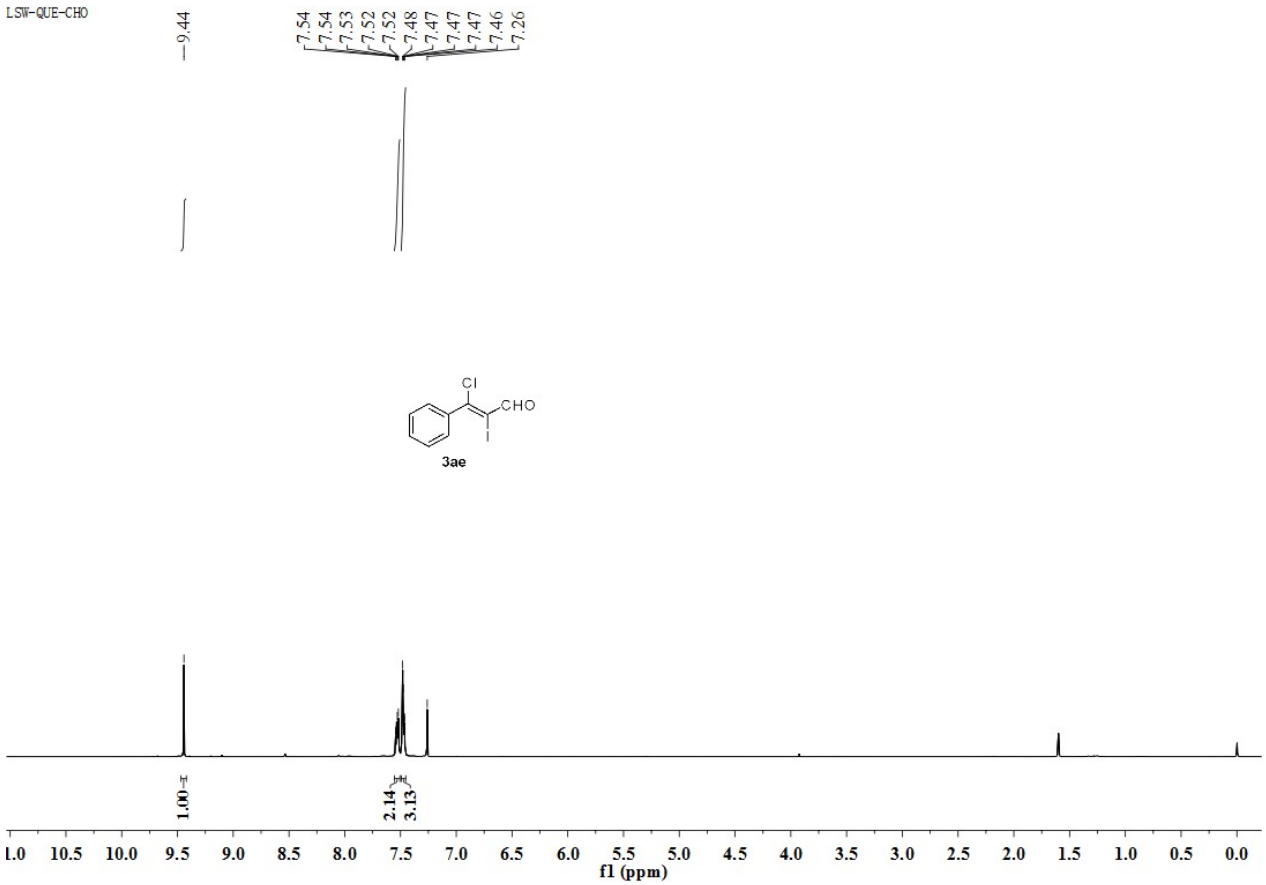


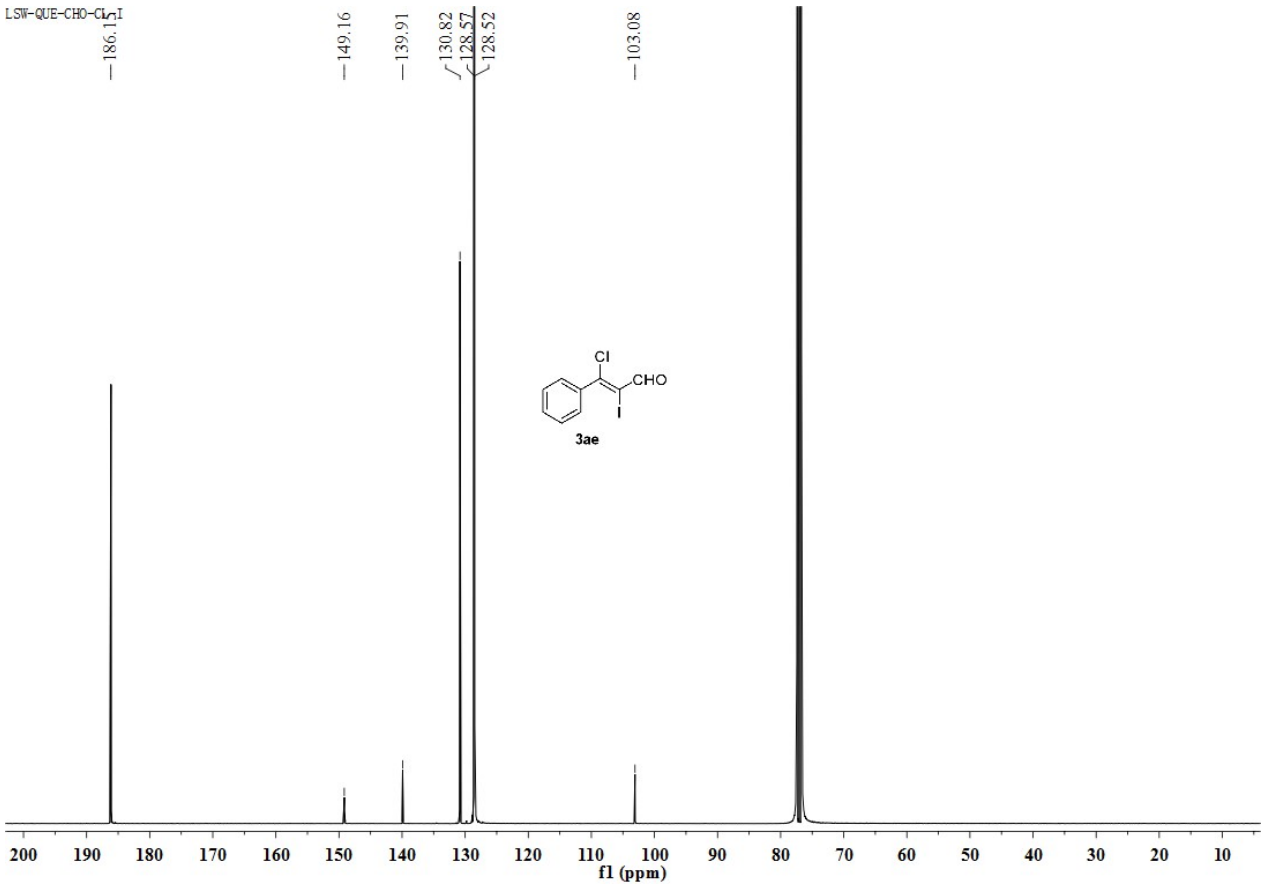


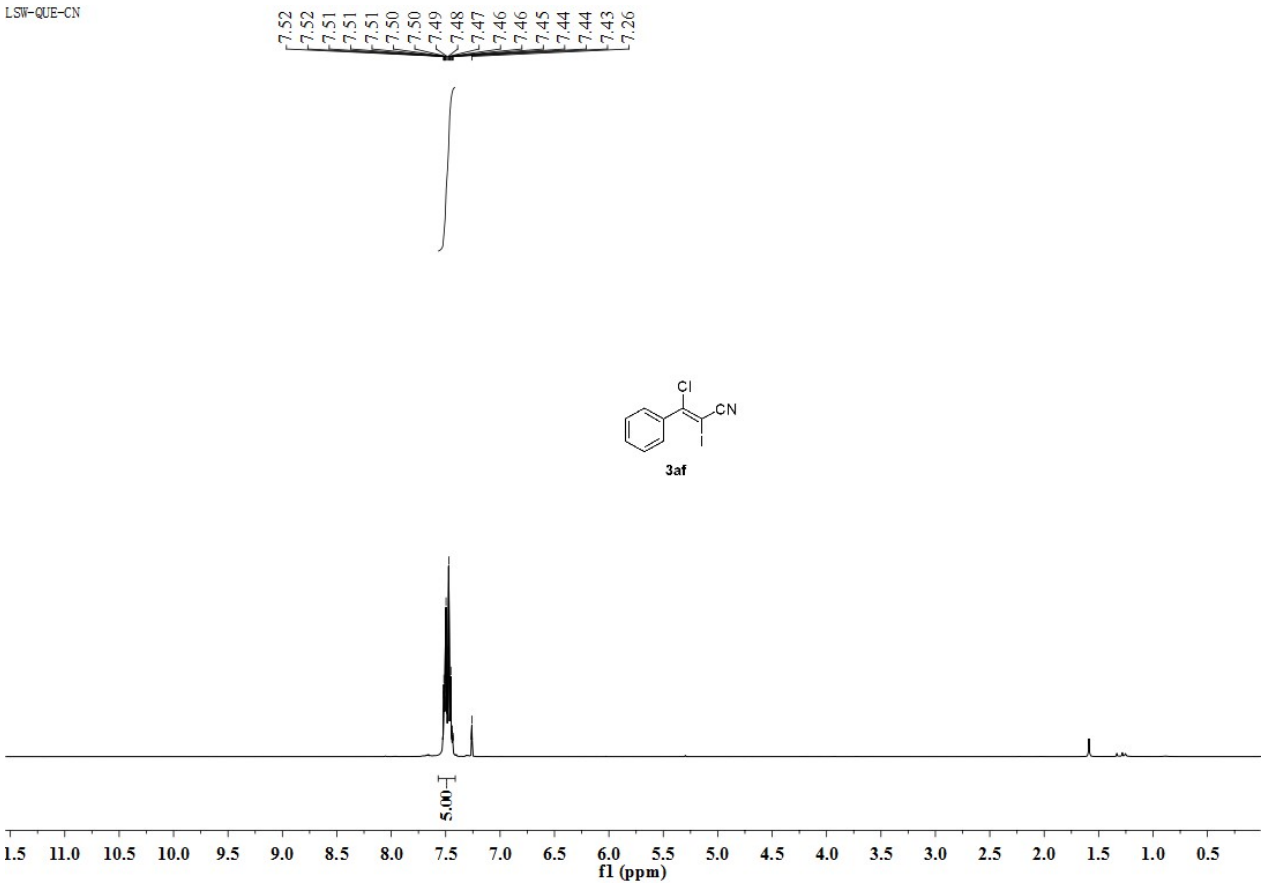
3ad

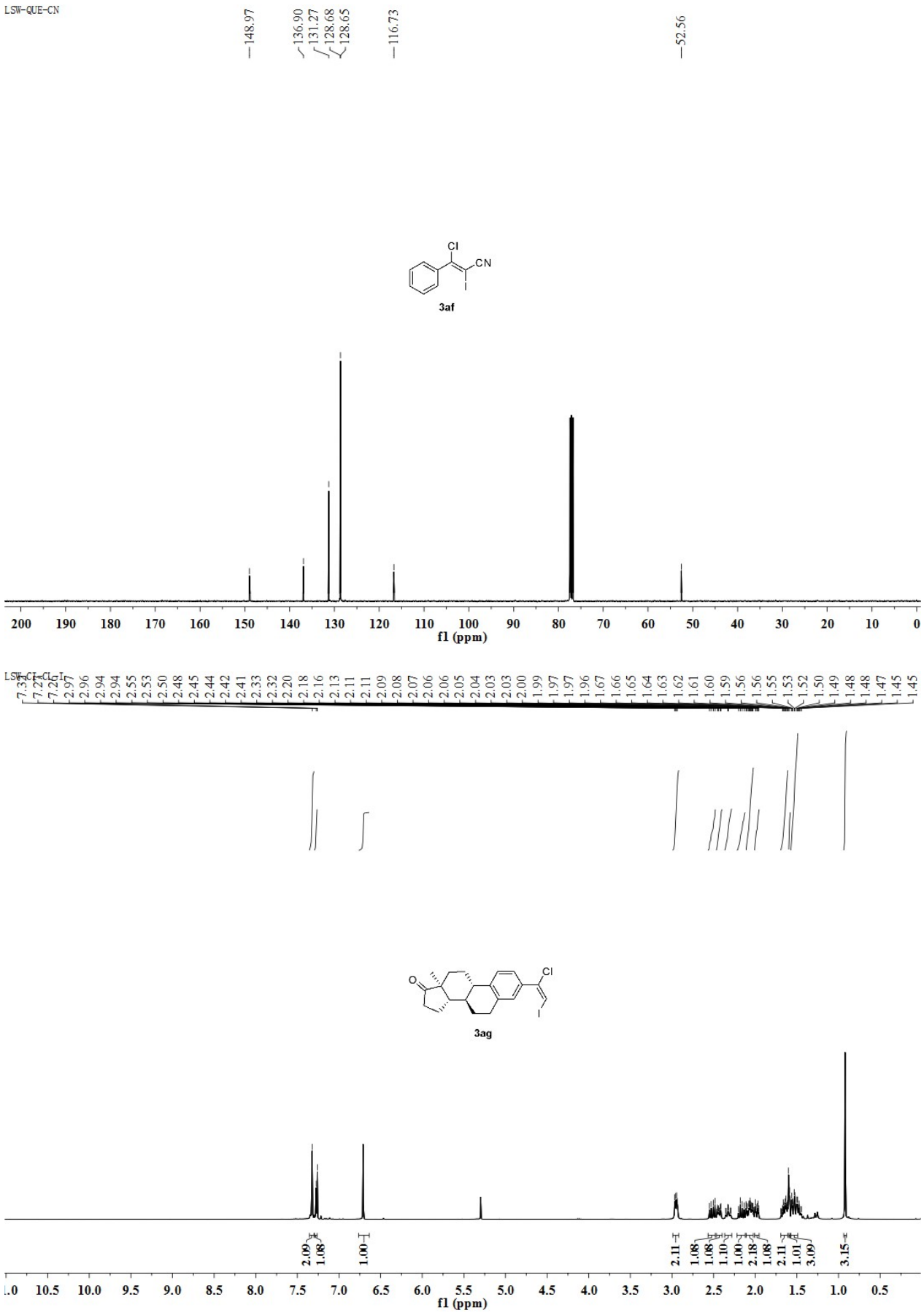


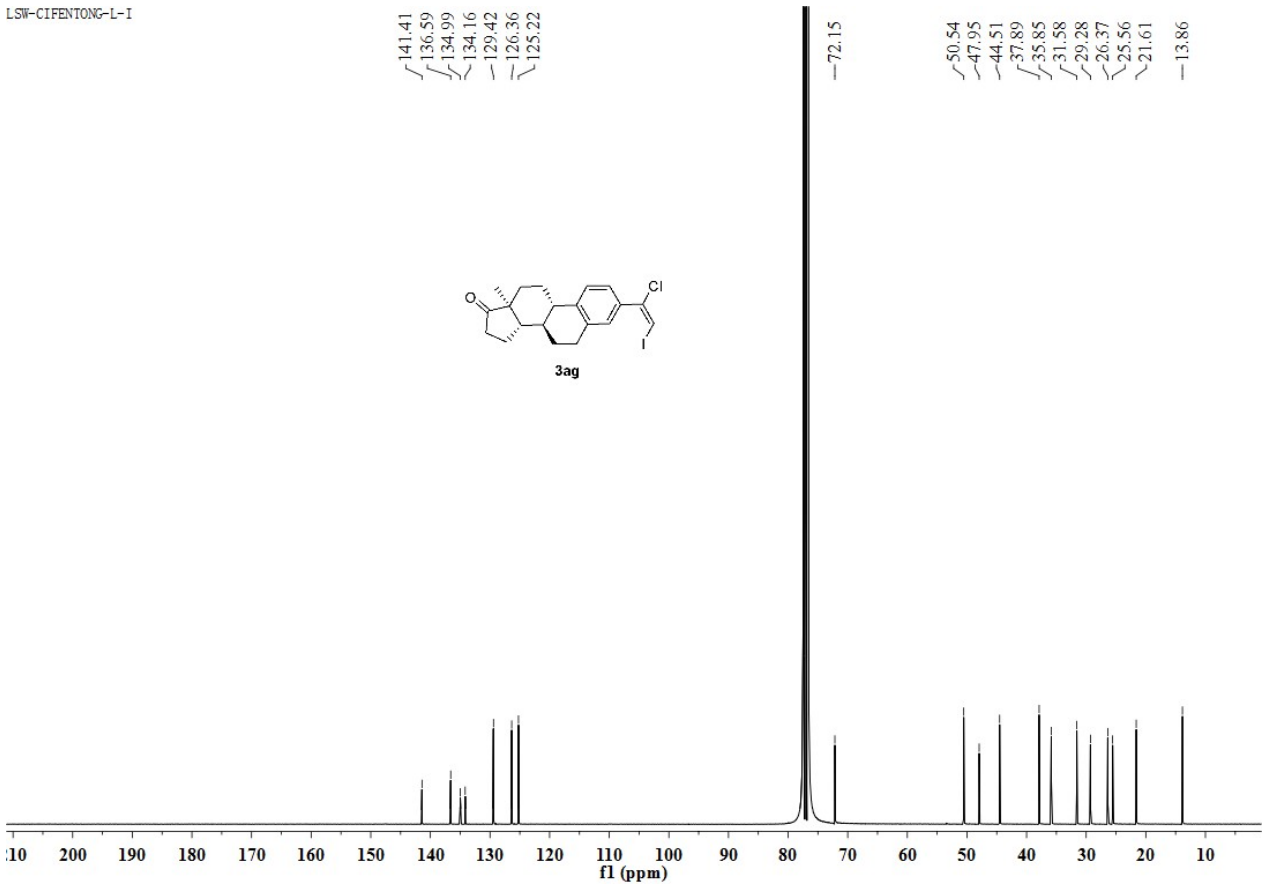

LSW-023
198.04
138.45
131.11
129.87
128.89
128.45
92.26
27.36
Cl
COMe
3ad
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

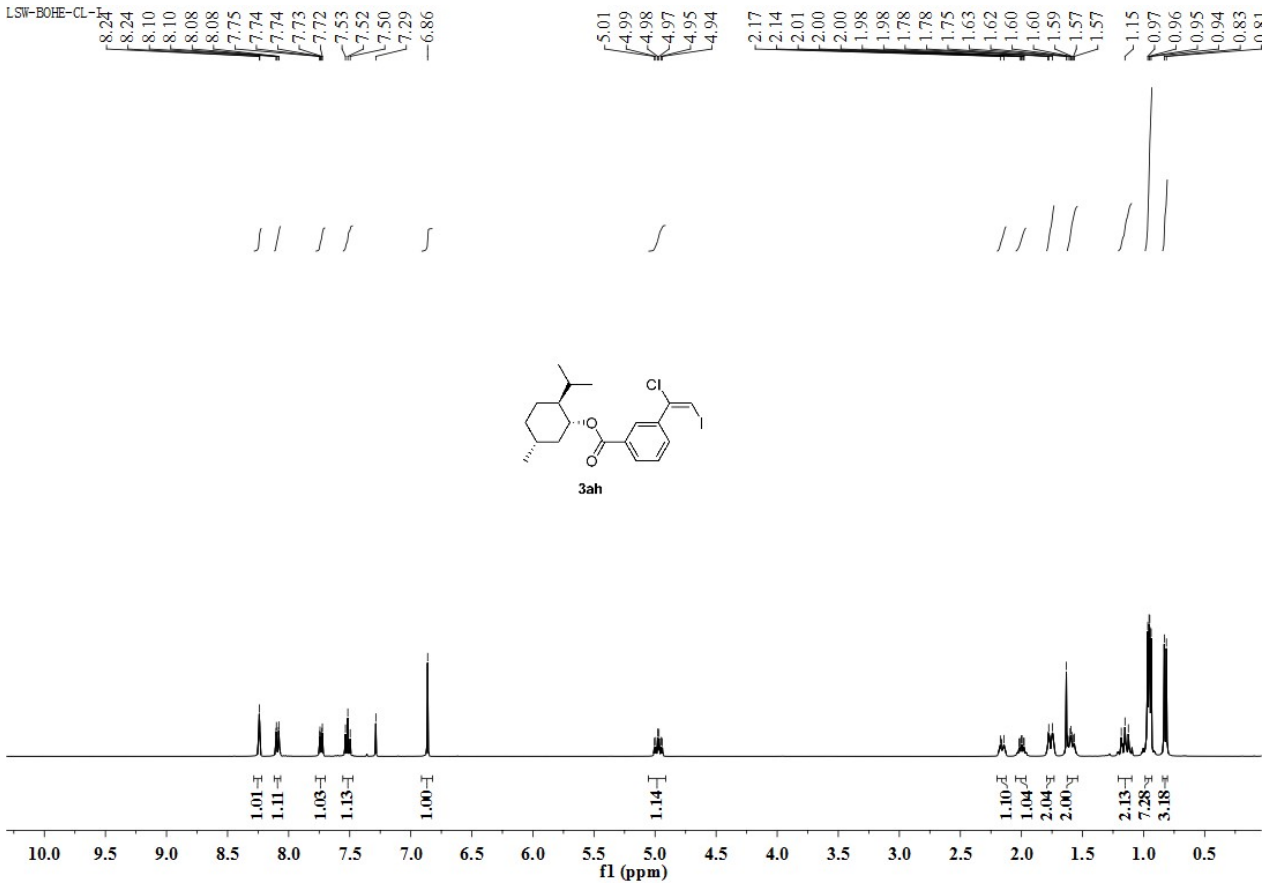

LSW-QUE-CHO
9.44
7.54
7.54
7.53
7.52
7.52
7.48
7.47
7.47
7.47
7.46
7.26
Cl
CHO
3ae
1.00
2.14
3.13
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

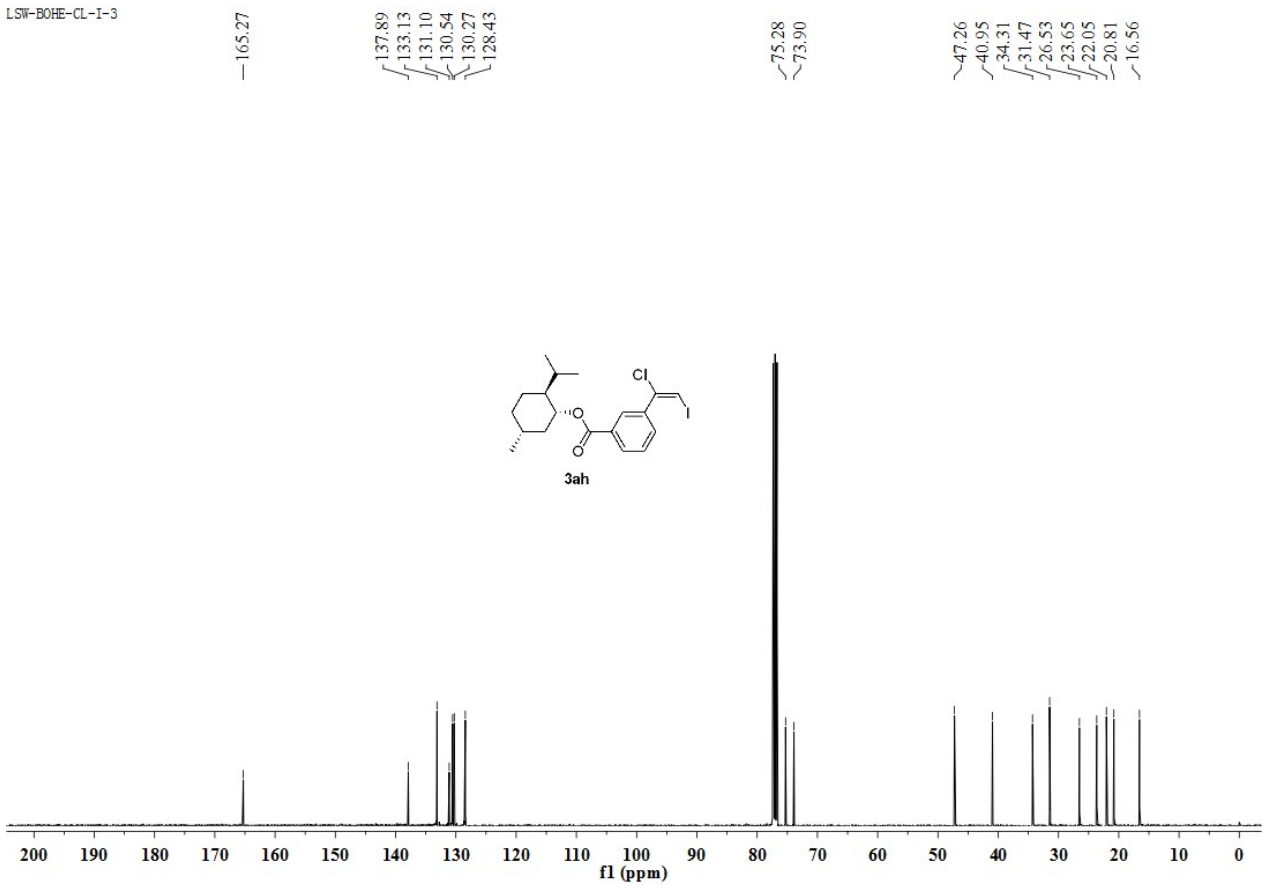

LSW-QUE-CHO-Cl-I
186.15
149.16
139.91
130.82
128.57
128.52
103.08
Cl
CHO
I
3ae
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

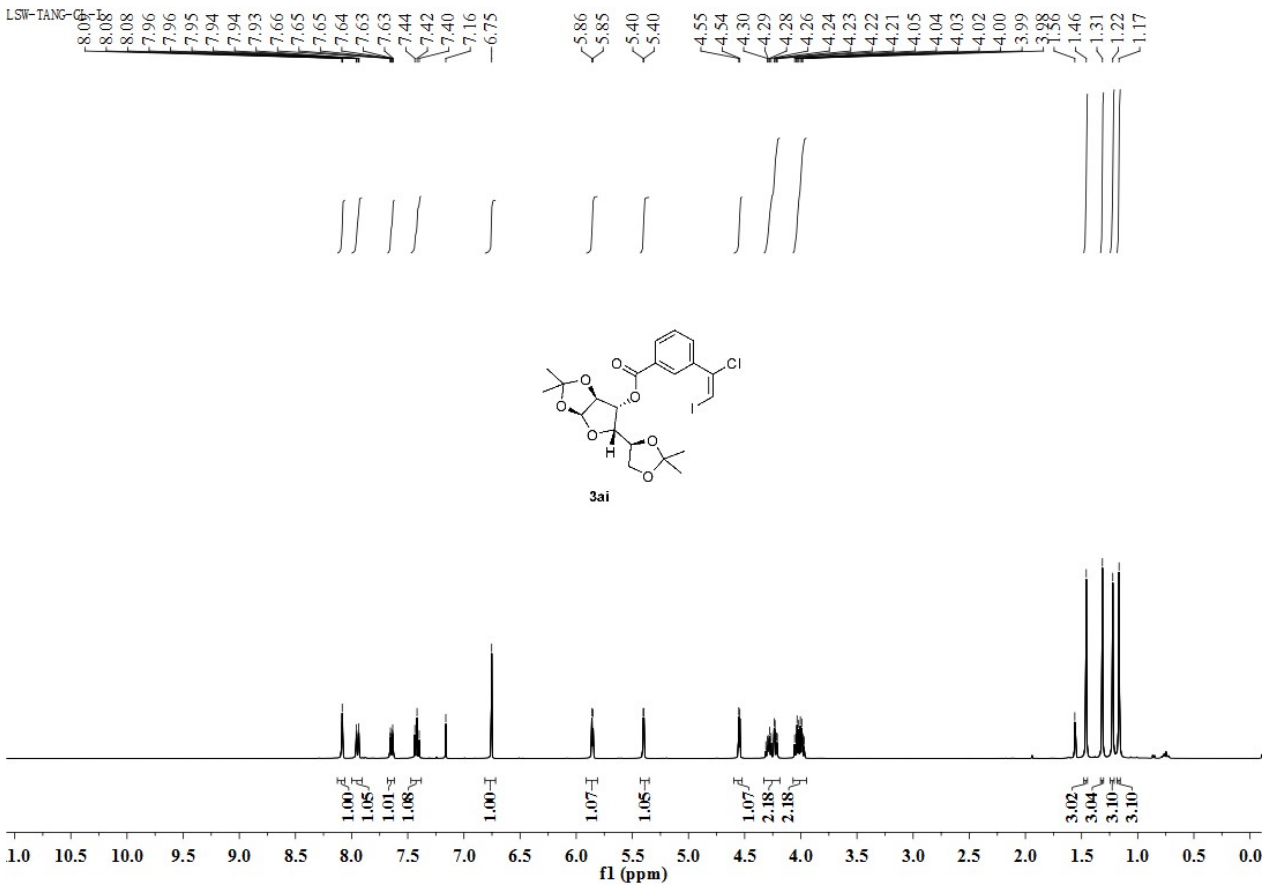

LSW-QUE-CN
7.52
7.52
7.51
7.51
7.51
7.50
7.50
7.49
7.48
7.47
7.46
7.46
7.45
7.44
7.44
7.43
7.26
Cl
CN
I
3af
5.00
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


LSW-QUE-CN
148.97
136.90
131.27
128.68
128.65
116.73
52.56
Cl
CN
3af
f1 (ppm)
Cl
O
3ag
f1 (ppm)

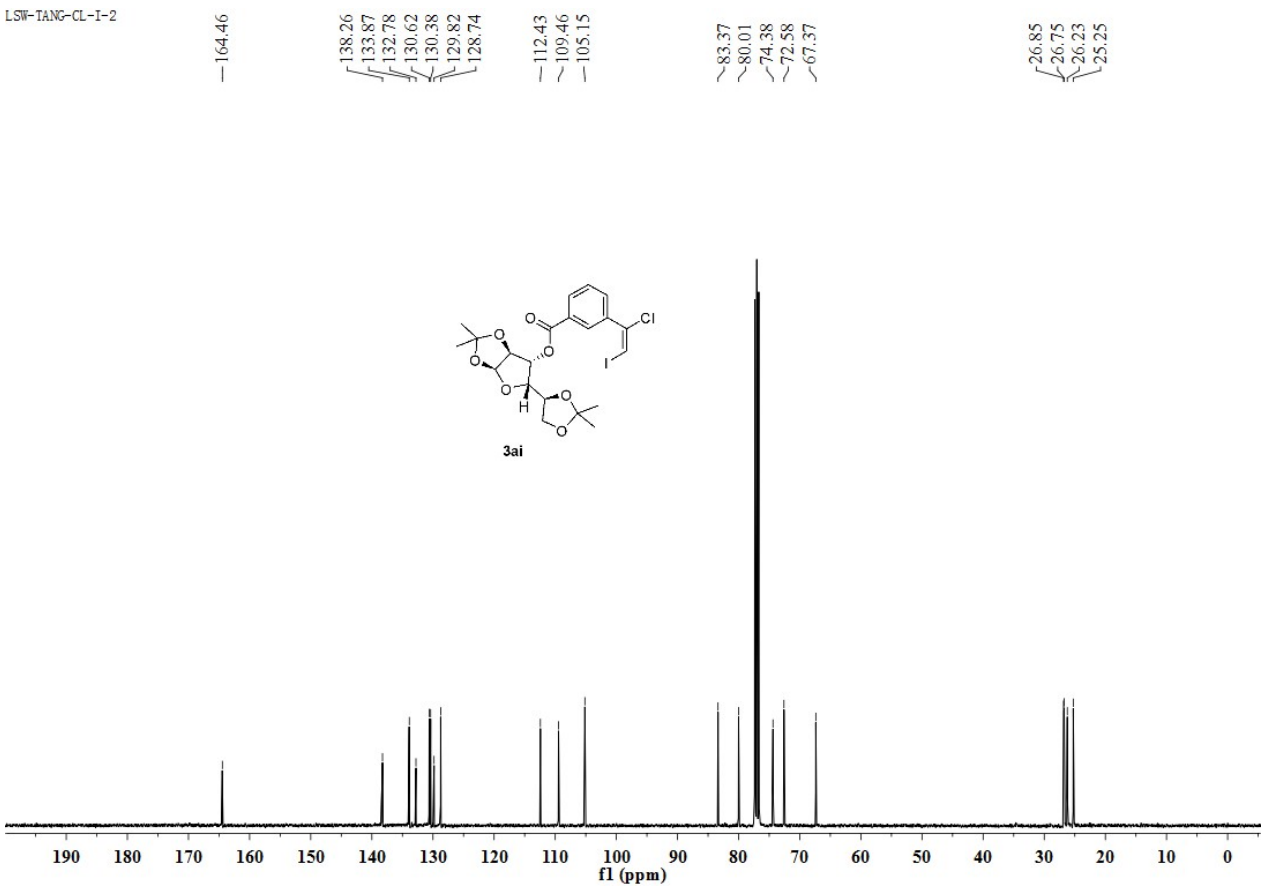

LSW-CIFENTONG-L-I
141.41
136.59
134.99
134.16
129.42
126.36
125.22
72.15
50.54
47.95
44.51
37.89
35.85
31.58
29.28
26.37
25.56
21.61
13.86
Cl
I
O
3ag
f1 (ppm)


LSW-BOHE-CL-I
8.24
8.24
8.10
8.10
8.08
8.08
7.75
7.74
7.74
7.73
7.72
7.53
7.52
7.50
7.29
6.86
5.01
4.99
4.98
4.97
4.95
4.94
2.17
2.14
2.01
2.00
2.00
1.98
1.98
1.78
1.78
1.75
1.63
1.62
1.60
1.60
1.59
1.57
1.57
1.15
0.97
0.96
0.95
0.94
0.83
Cl
I
O
O
3ah
1.01
1.11
1.03
1.13
1.00
1.14
1.10
1.04
2.04
2.00
2.13
7.28
3.18
f1 (ppm)

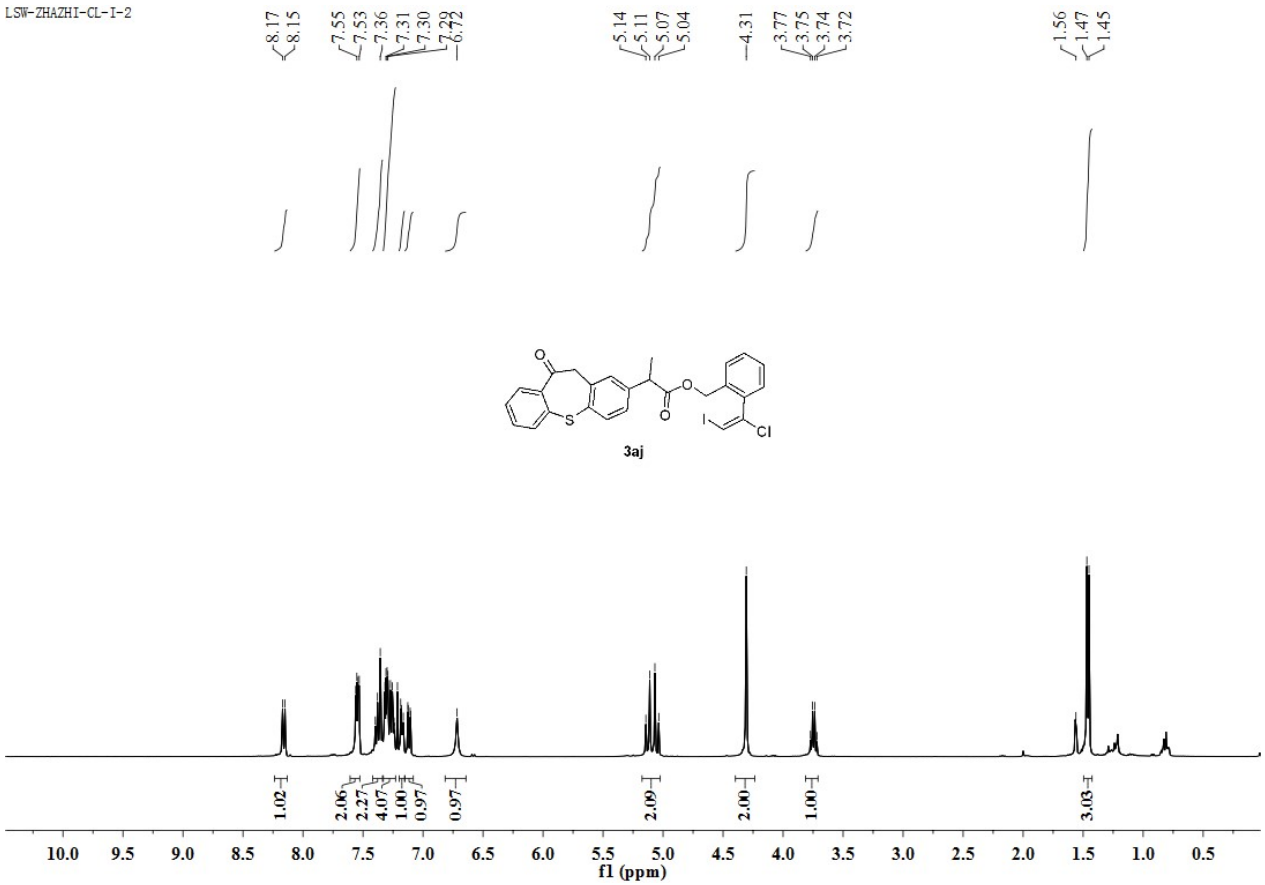

LSW-BOHE-CL-I-3
165.27
137.89
133.13
131.10
130.54
130.27
128.43
75.28
73.90
47.26
40.95
34.31
31.47
26.53
23.65
22.05
20.81
16.56
Cl
I
O
O
3ah
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

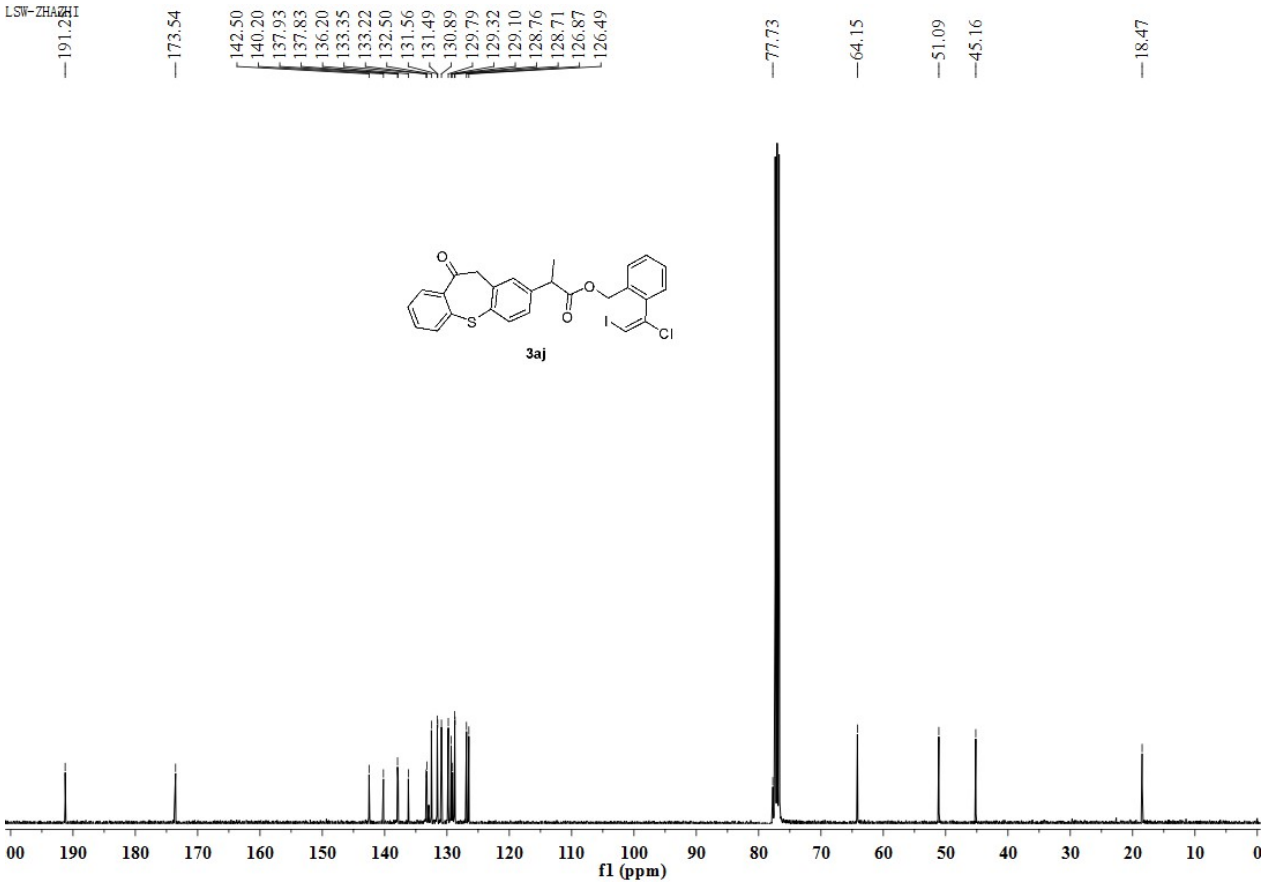

LSW-TANG-CL-I-
8.09
8.08
8.08
7.96
7.96
7.95
7.94
7.94
7.93
7.66
7.65
7.65
7.64
7.63
7.63
7.44
7.42
7.40
7.16
6.75
5.86
5.85
5.40
5.40
4.55
4.54
4.30
4.29
4.28
4.26
4.24
4.23
4.22
4.21
4.05
4.04
4.03
4.02
4.00
3.99
3.98
3.56
1.46
1.31
1.22
1.17
O
O
O
O
O
H
O
Cl
I
3ai
1.00
1.05
1.01
1.08
1.00
1.07
1.05
1.07
2.18
2.18
3.02
3.04
3.10
3.10
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

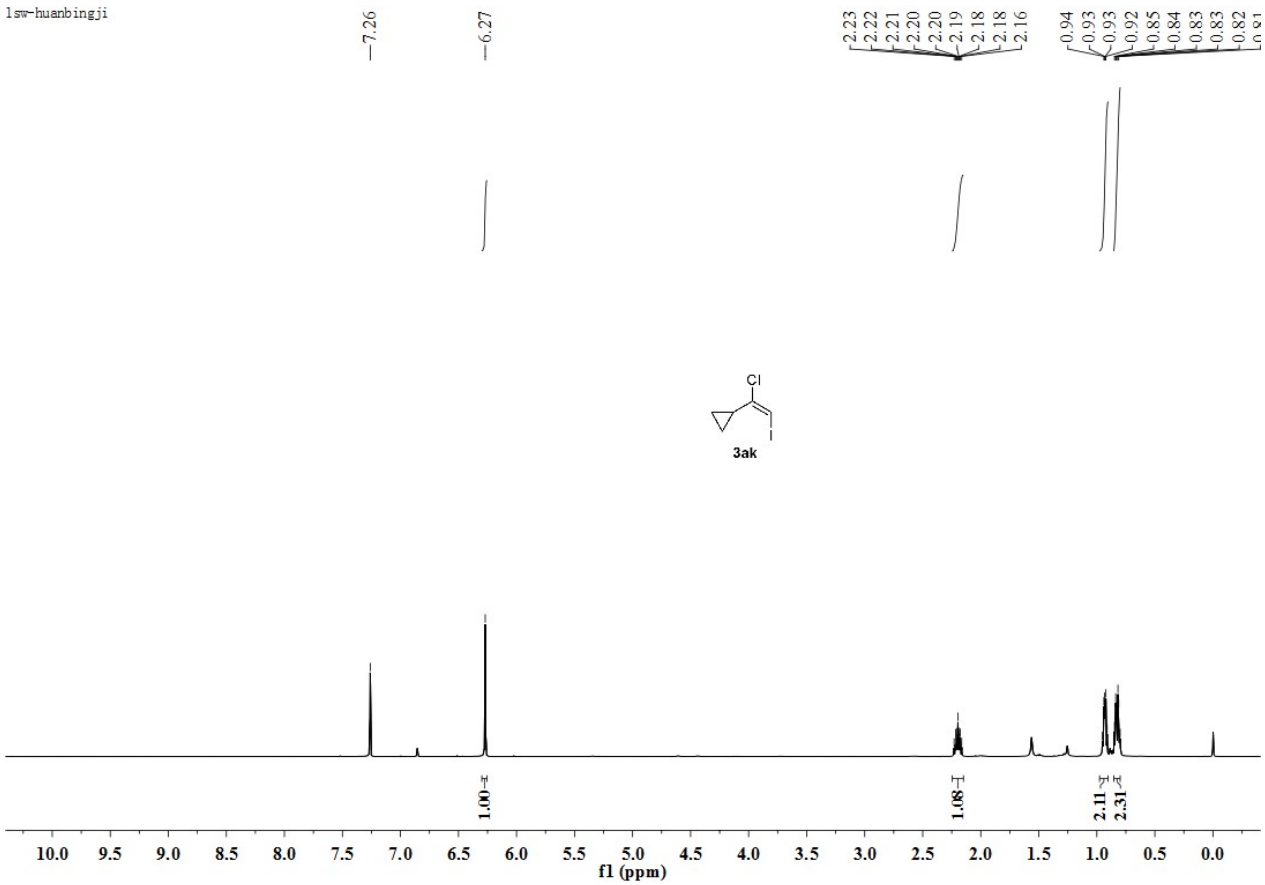
LSW-TANG-CL-I-2

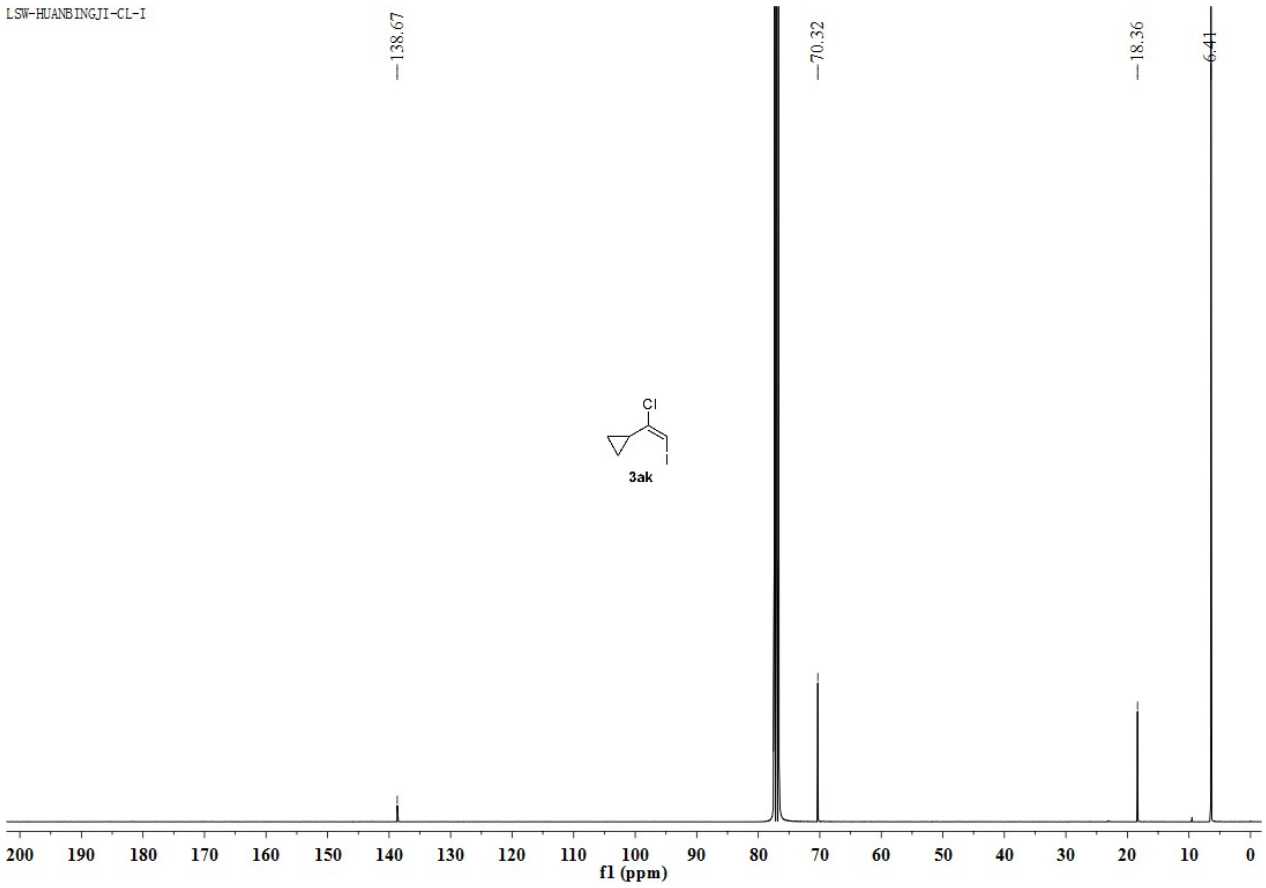


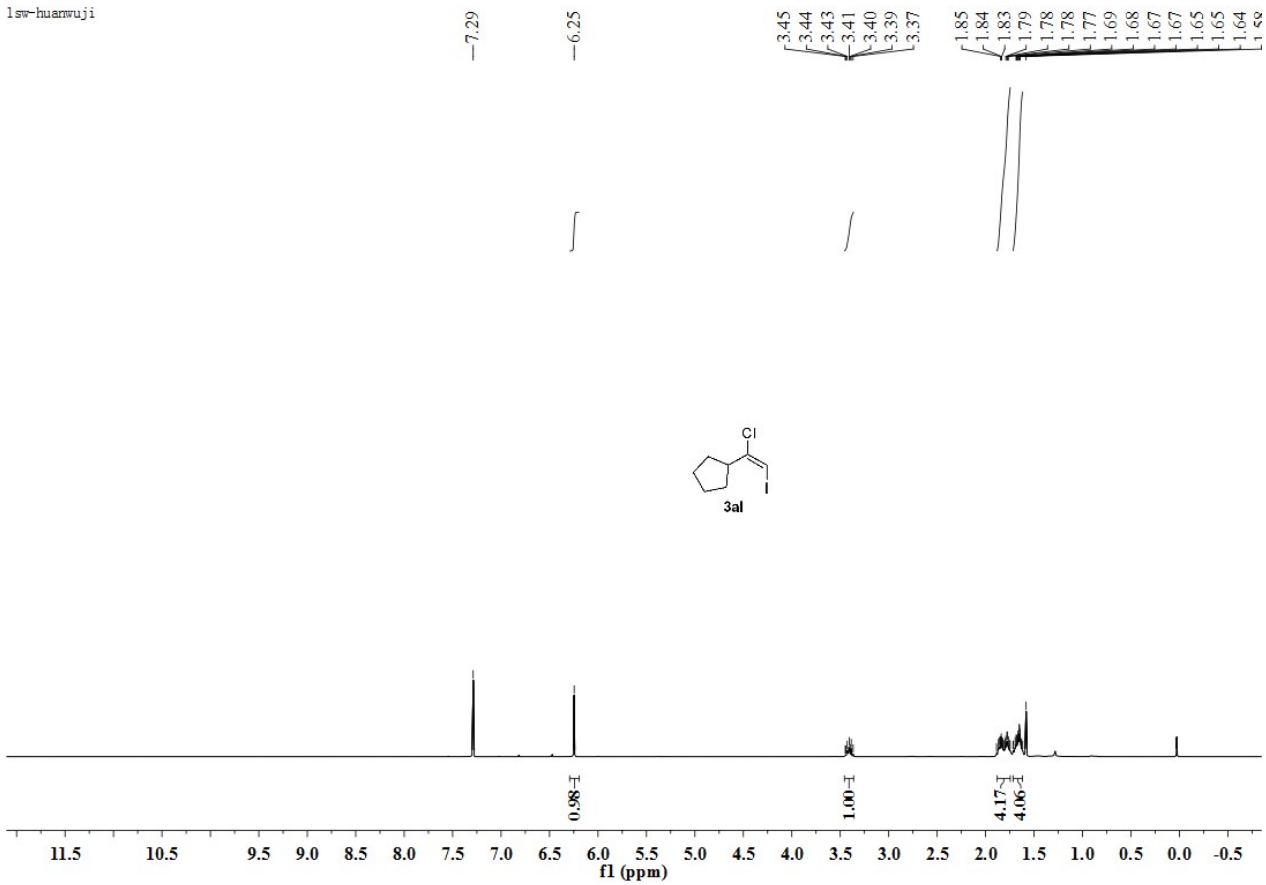
LSW-ZHAZHI-CL-I-2




LSW-ZHAZHI
191.28
173.54
142.50
140.20
137.93
137.83
136.20
133.35
133.22
132.50
131.56
131.49
130.89
129.79
129.32
129.10
128.76
128.71
126.87
126.49
77.73
64.15
51.09
45.16
18.47
3aj
f1 (ppm)


lsw-huanbingji
7.26
6.27
2.23
2.22
2.21
2.20
2.20
2.19
2.18
2.18
2.16
0.94
0.93
0.93
0.92
0.85
0.84
0.83
0.83
0.82
3ak
1.00
1.08
2.11
2.31
f1 (ppm)

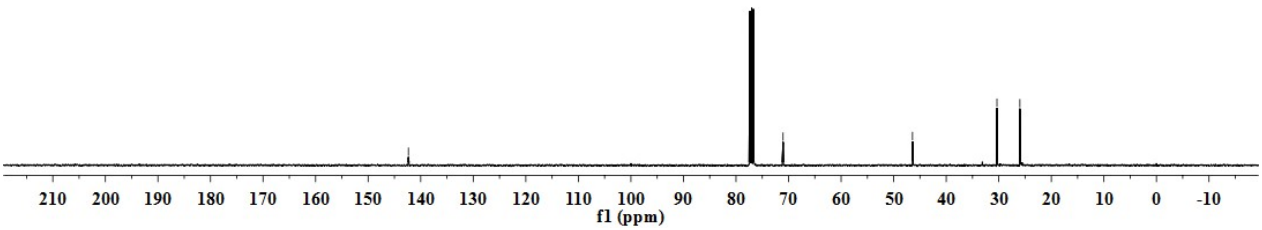

LSW-HUANBINGJI-CL-I
138.67
70.32
18.36
6.41
Cl
I
3ak
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


lsw-huanwuji
7.29
6.25
3.45
3.44
3.43
3.41
3.40
3.39
3.37
1.85
1.84
1.83
1.79
1.78
1.78
1.77
1.69
1.68
1.67
1.67
1.65
1.65
1.64
Cl
I
3al
0.98
1.00
4.17
4.06
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

LSW-HUANWUJI-CL-I

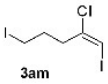
142.34
71.04
46.42
30.35
25.99

3al

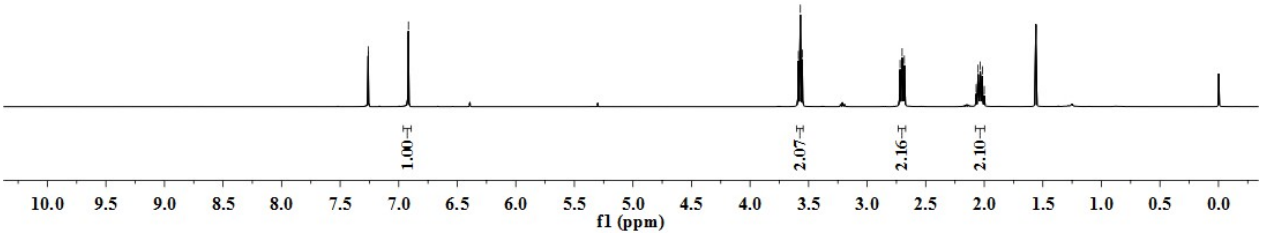


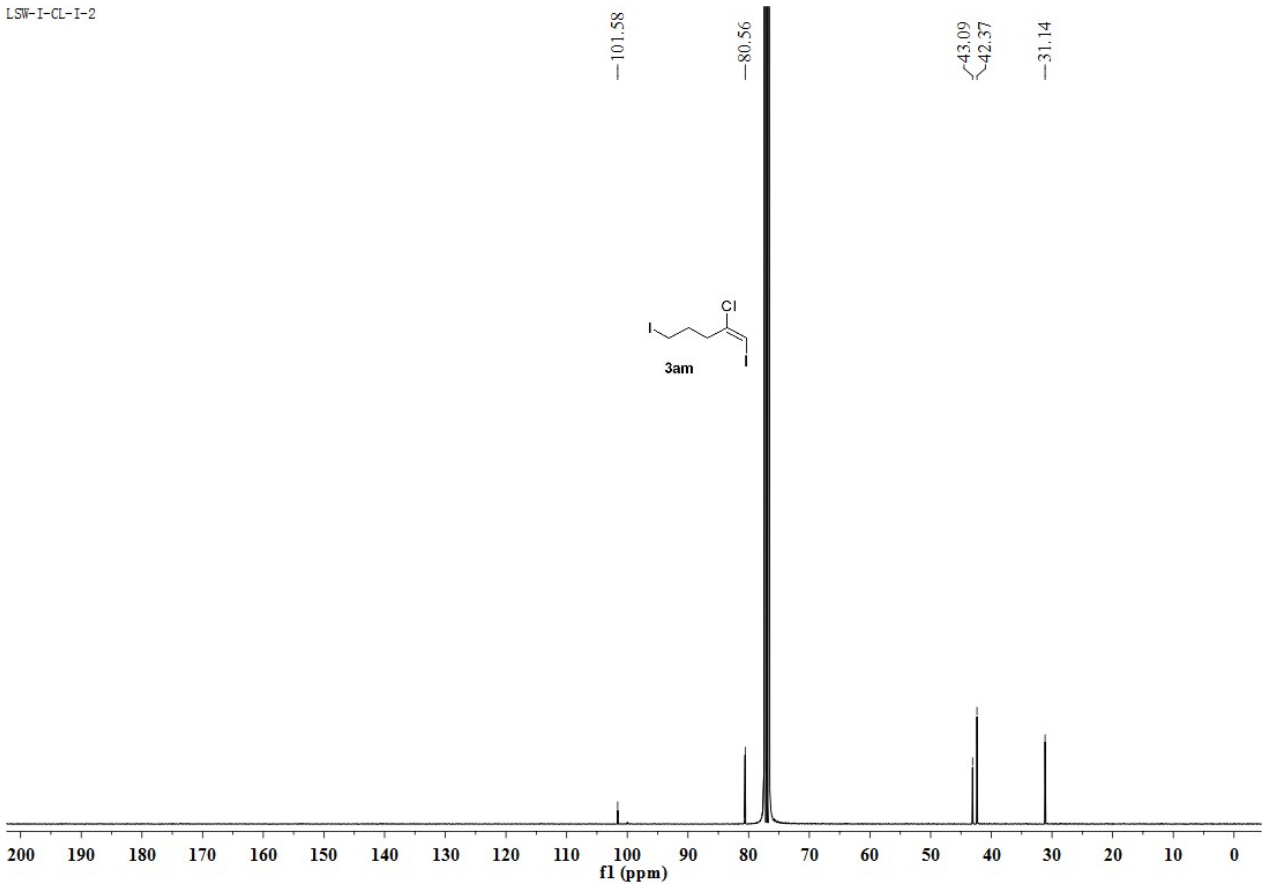
LSW-I-2

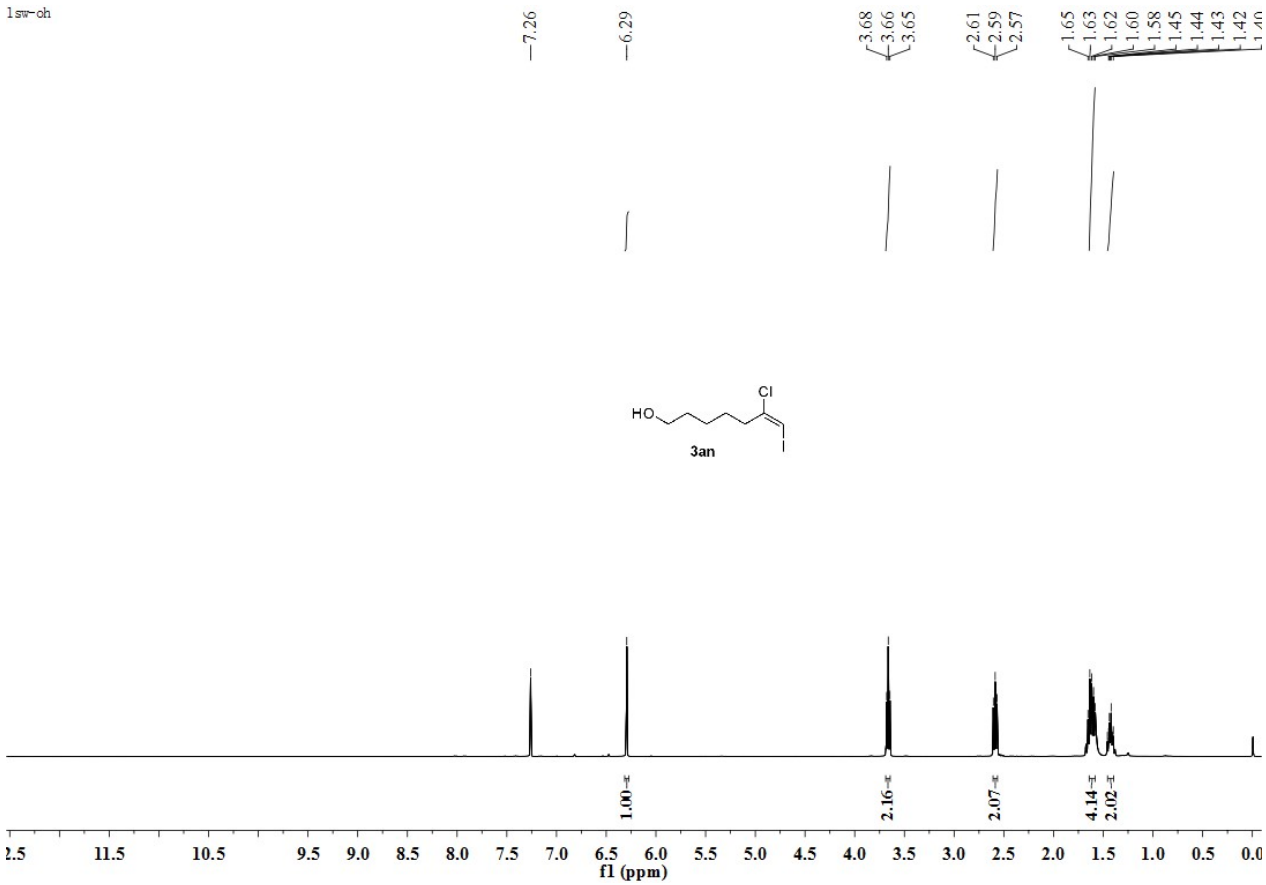
7.26
7.26
6.92
3.59
3.57
3.55
2.72
2.70
2.68
2.07
2.05
2.03
2.02
2.02
2.00



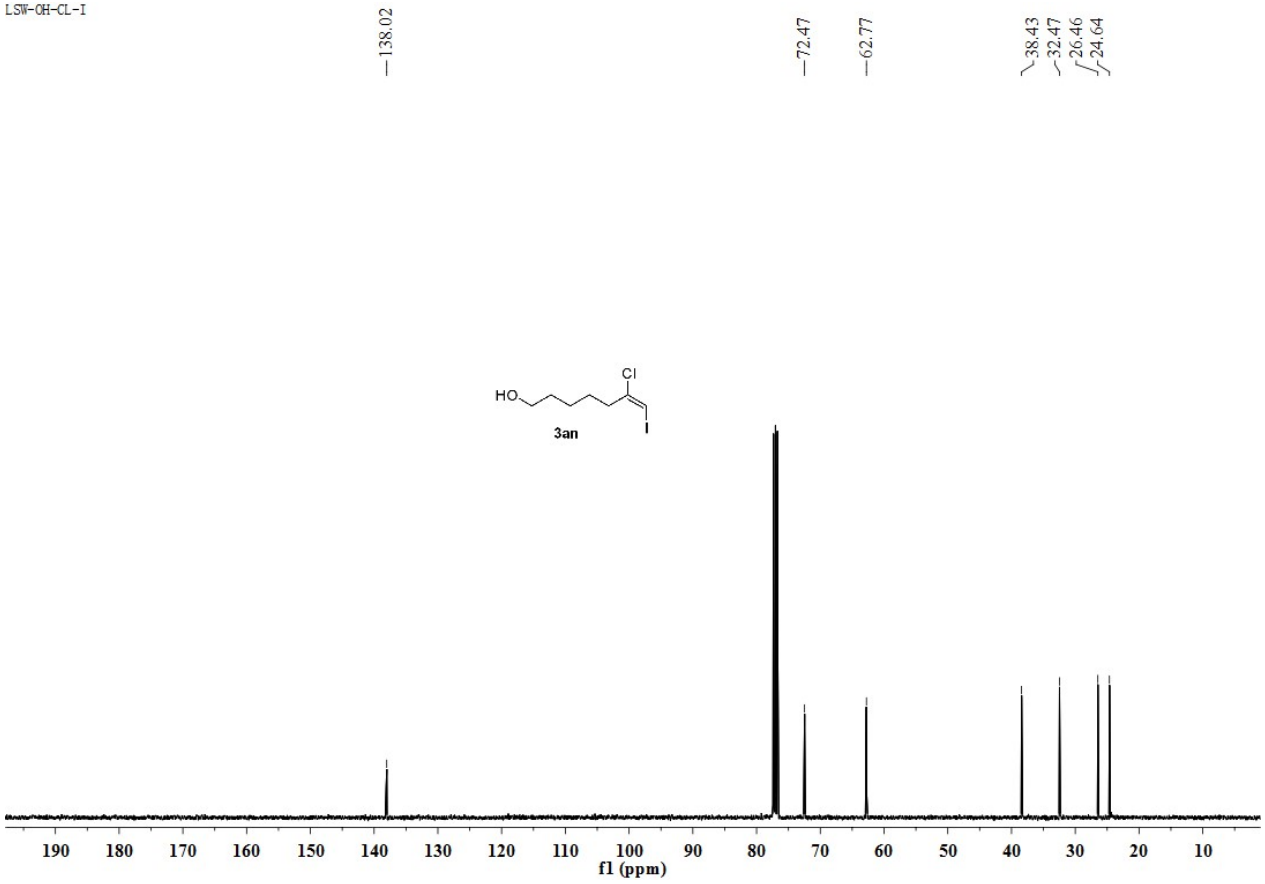
3am



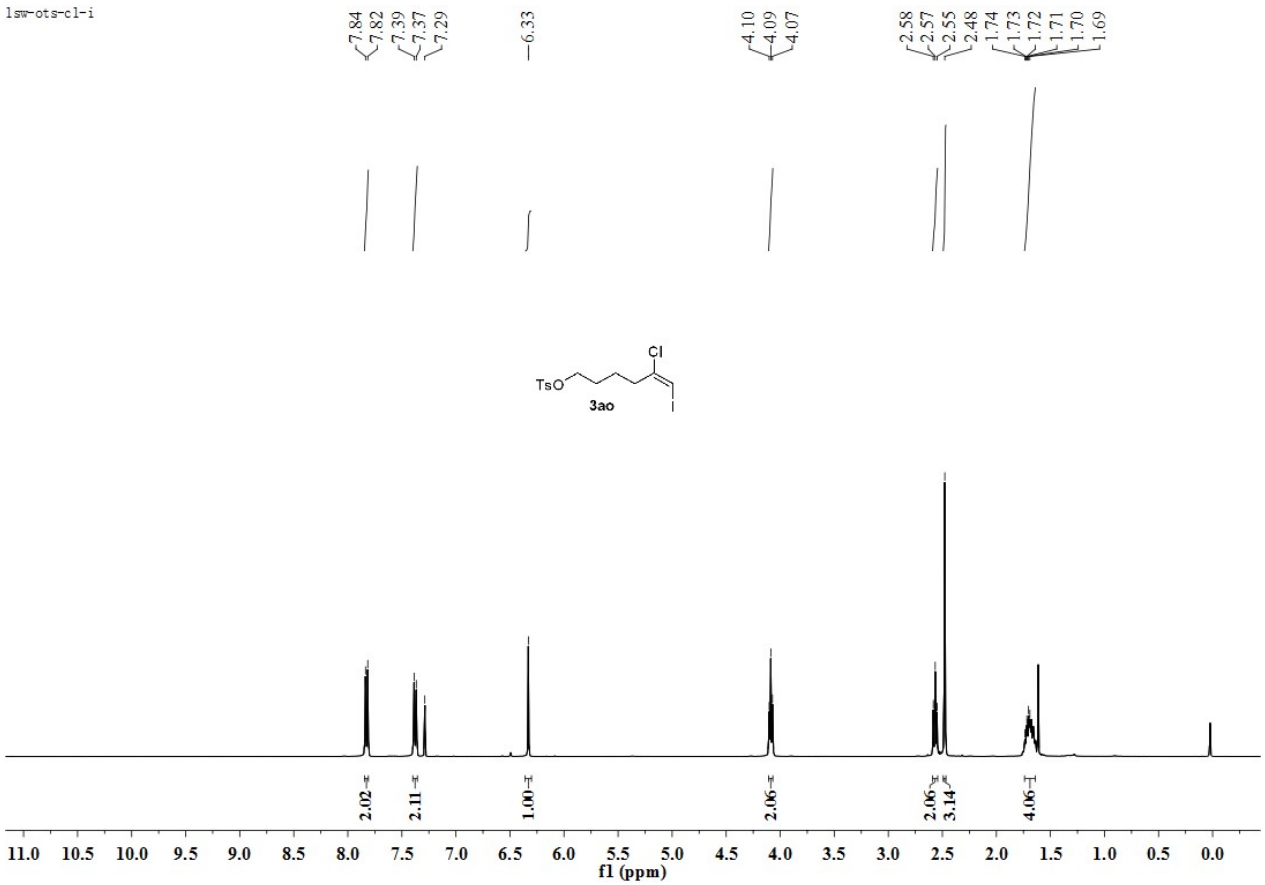

LSW-I-CL-I-2
101.58
80.56
43.09
42.37
31.14
Cl
I
3am
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


lsw-oh
7.26
6.29
3.68
3.66
3.65
2.61
2.59
2.57
1.65
1.63
1.62
1.60
1.58
1.45
1.44
1.43
1.42
Cl
HO
3an
1.00
2.16
2.07
4.14
2.02
f1 (ppm)

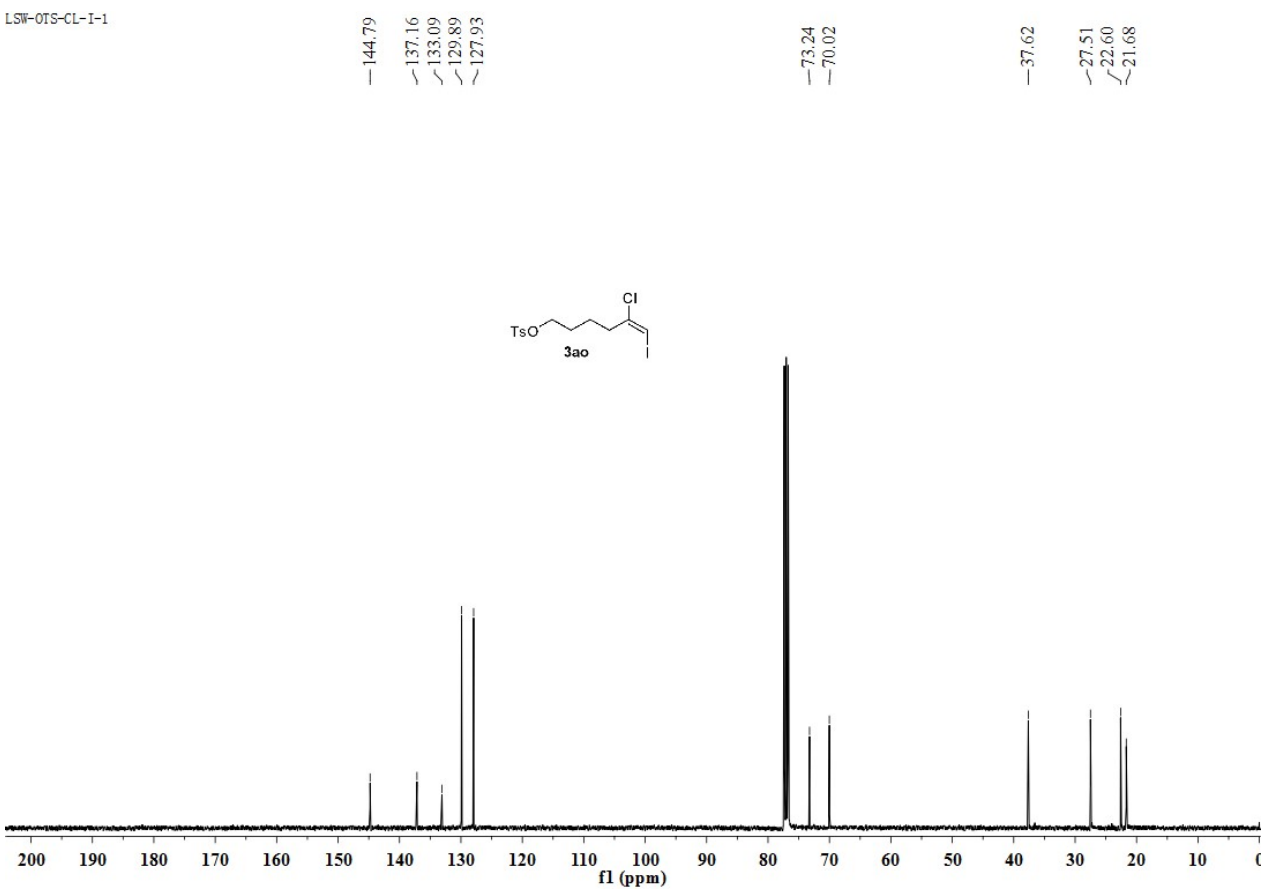
LSW-OH-CL-I



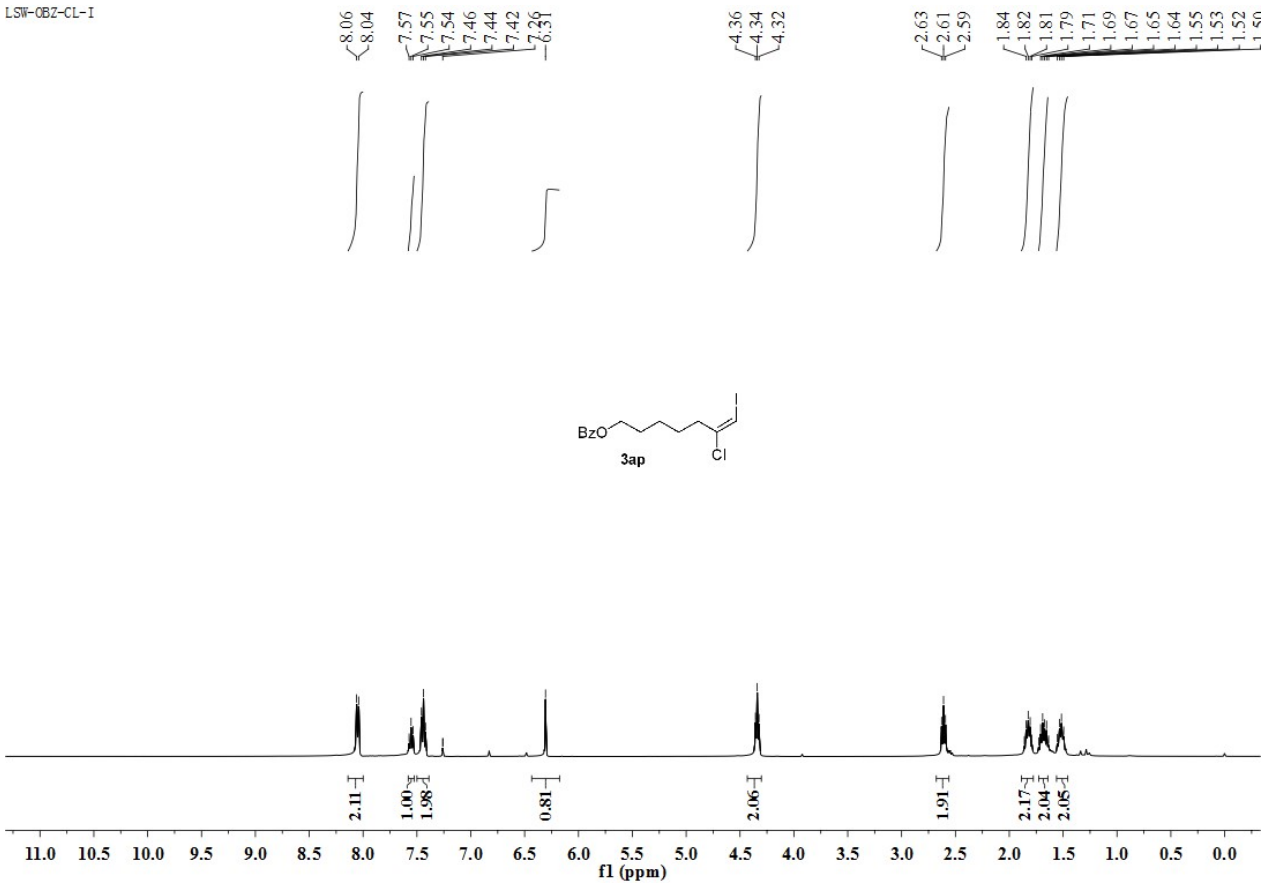
lsw-ots-cl-i



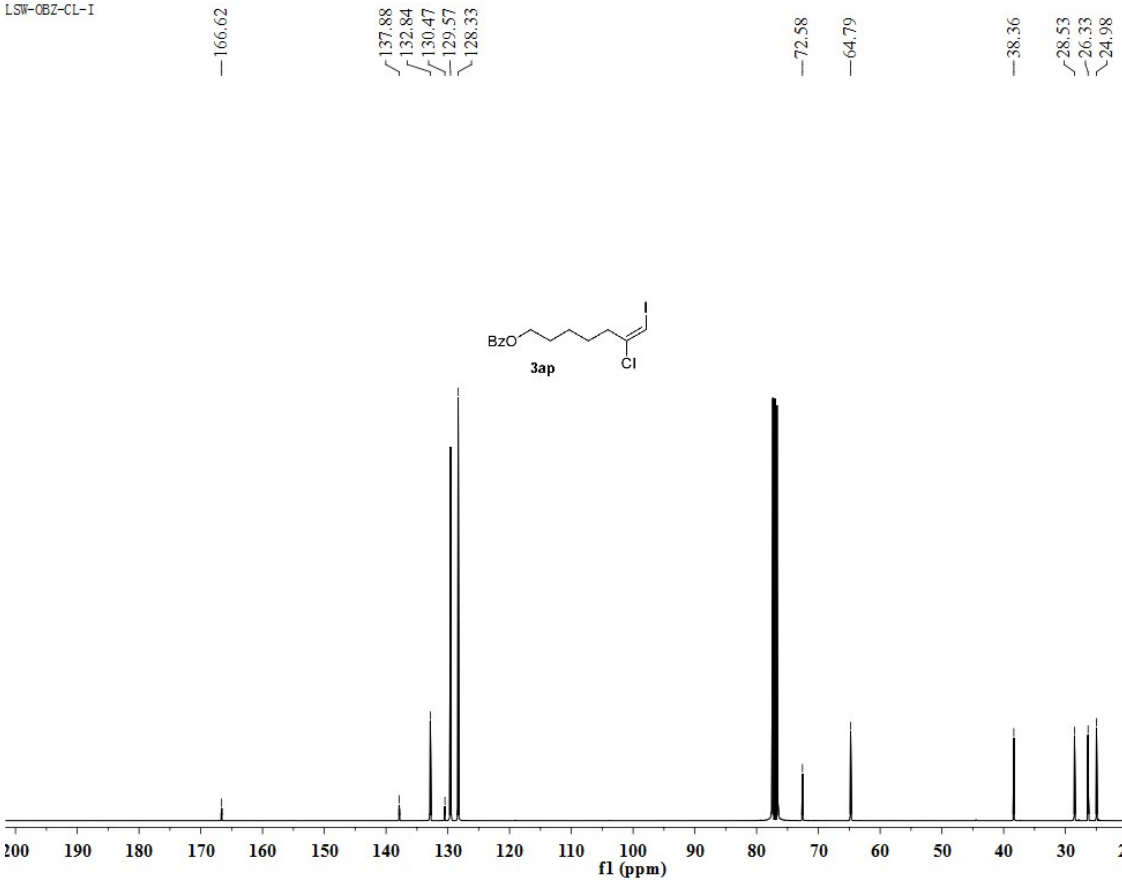
LSW-OTS-CL-I-1



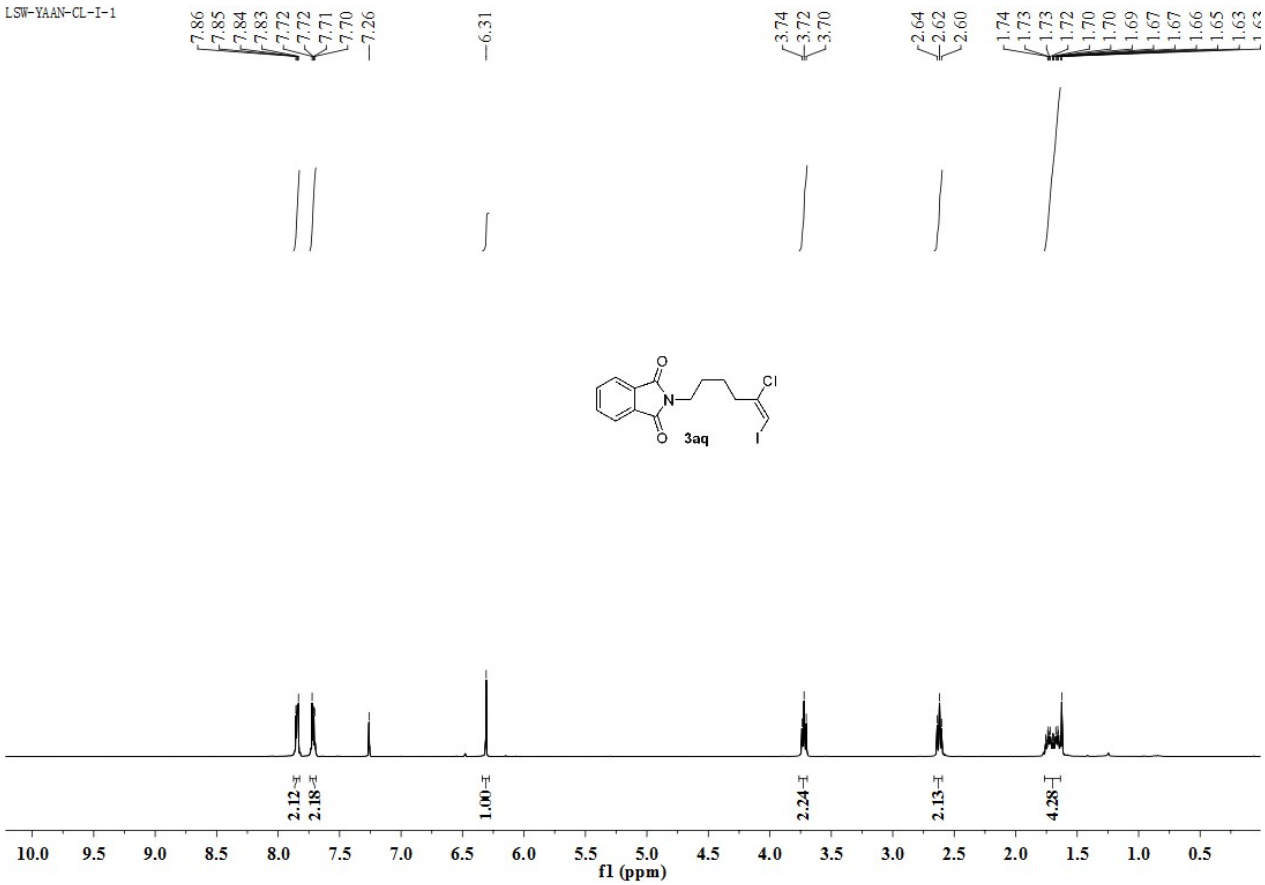
LSW-OBZ-CL-I



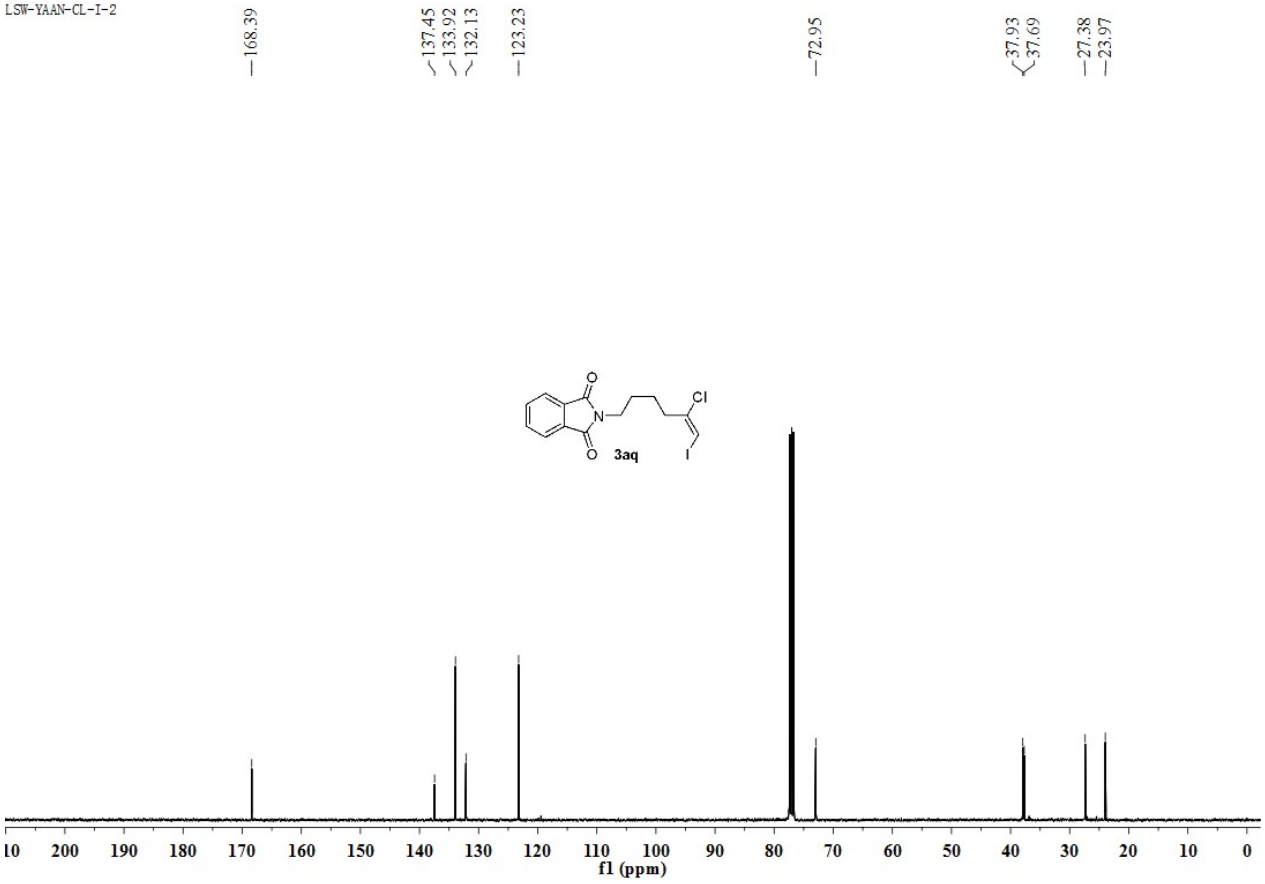
LSW-OBZ-CL-I



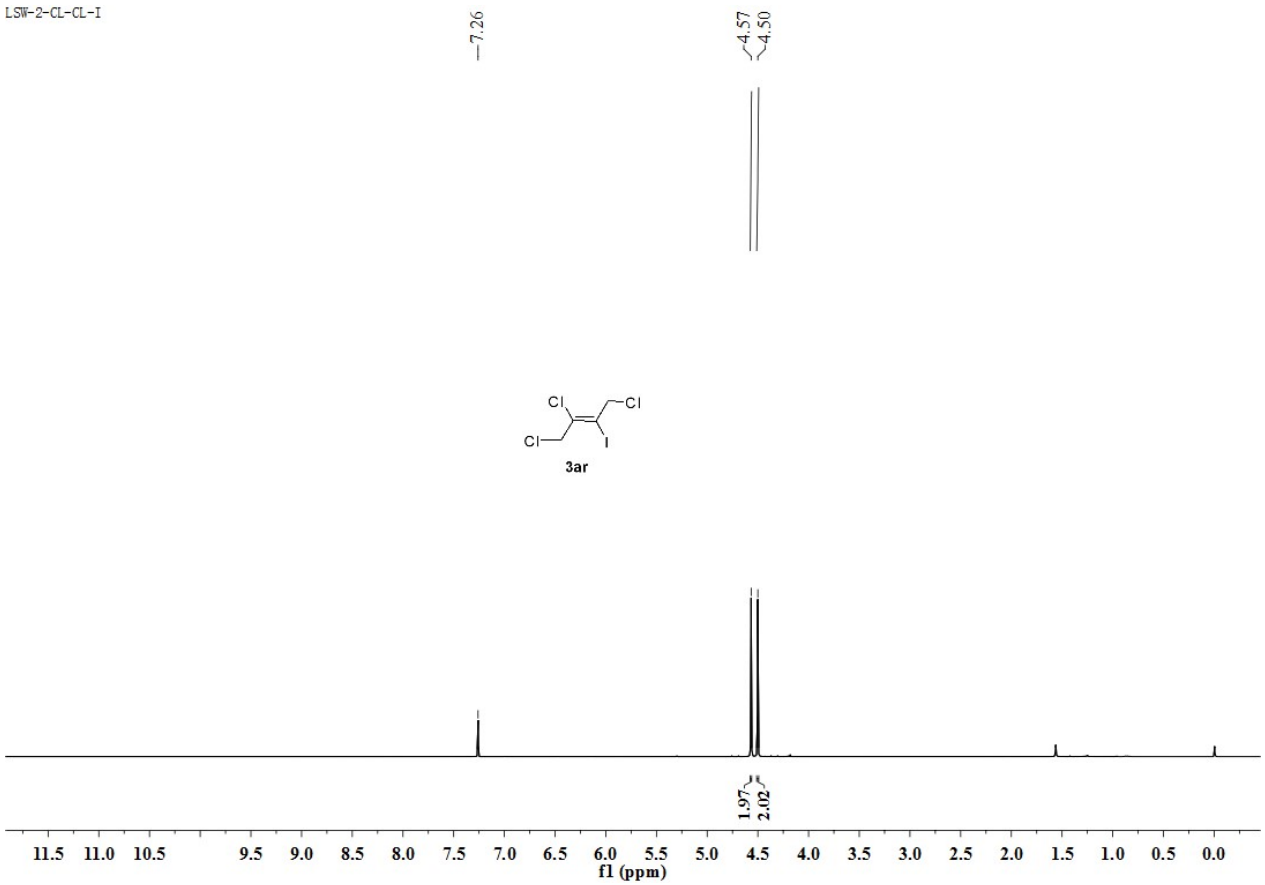
LSW-YAAN-CL-I-1



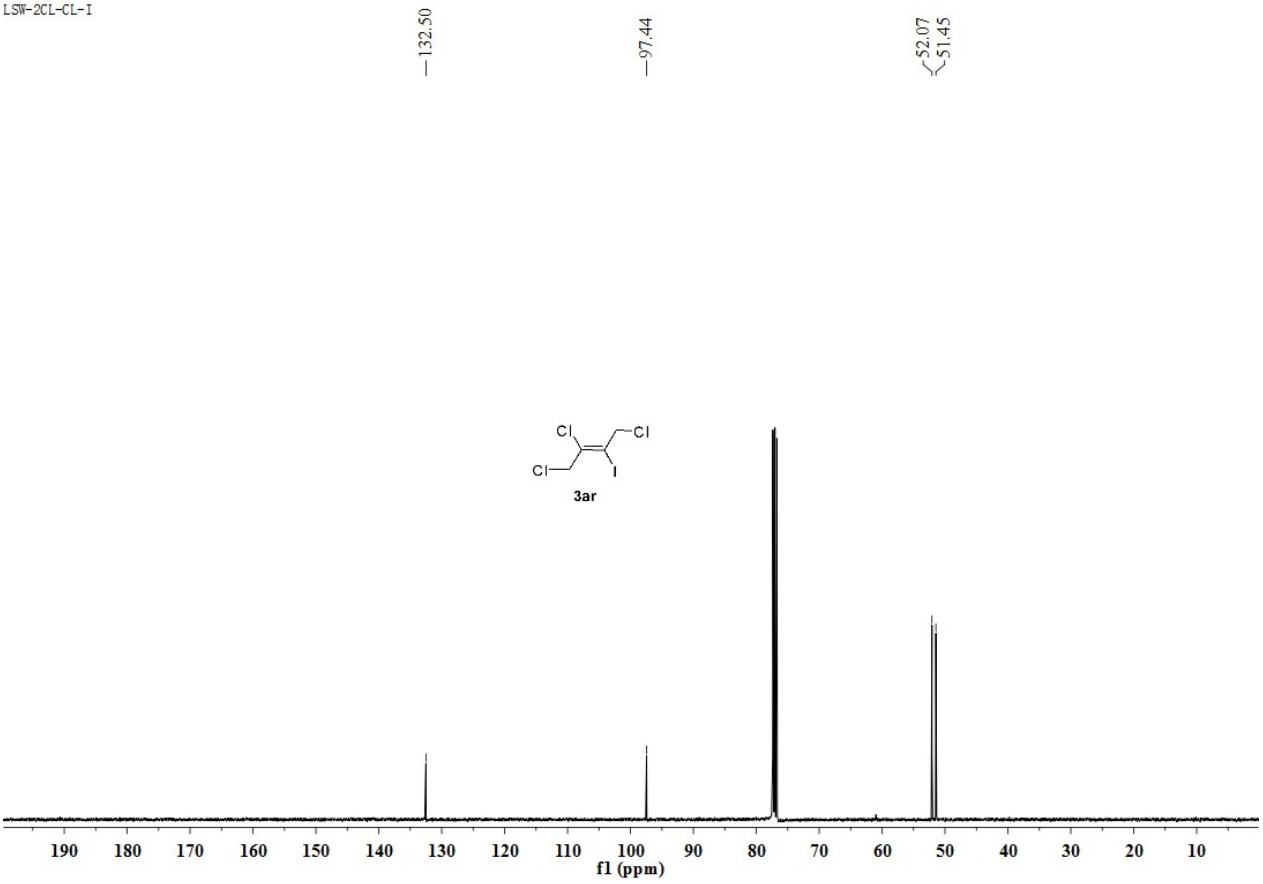
LSW-YAAN-CL-I-2



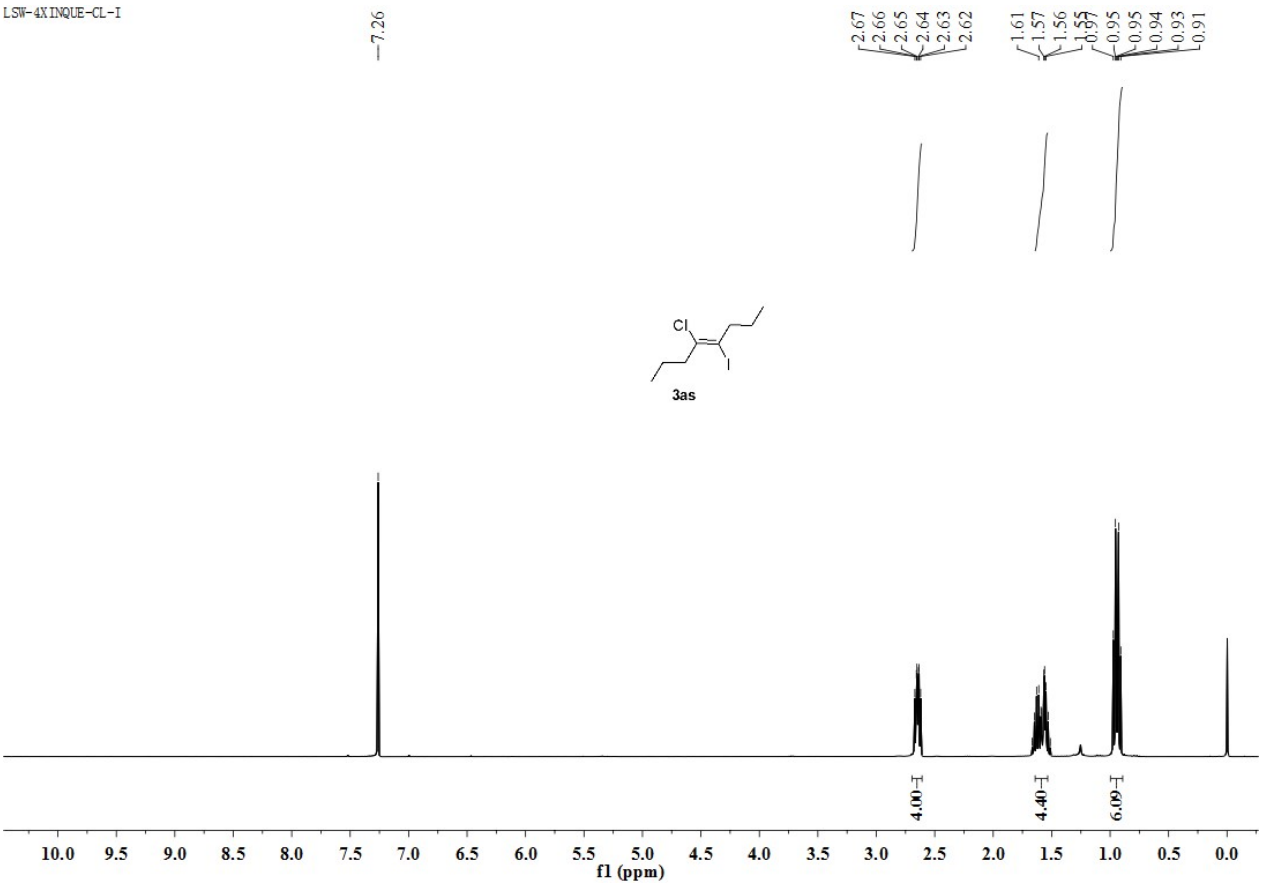
LSW-2-CL-CL-I



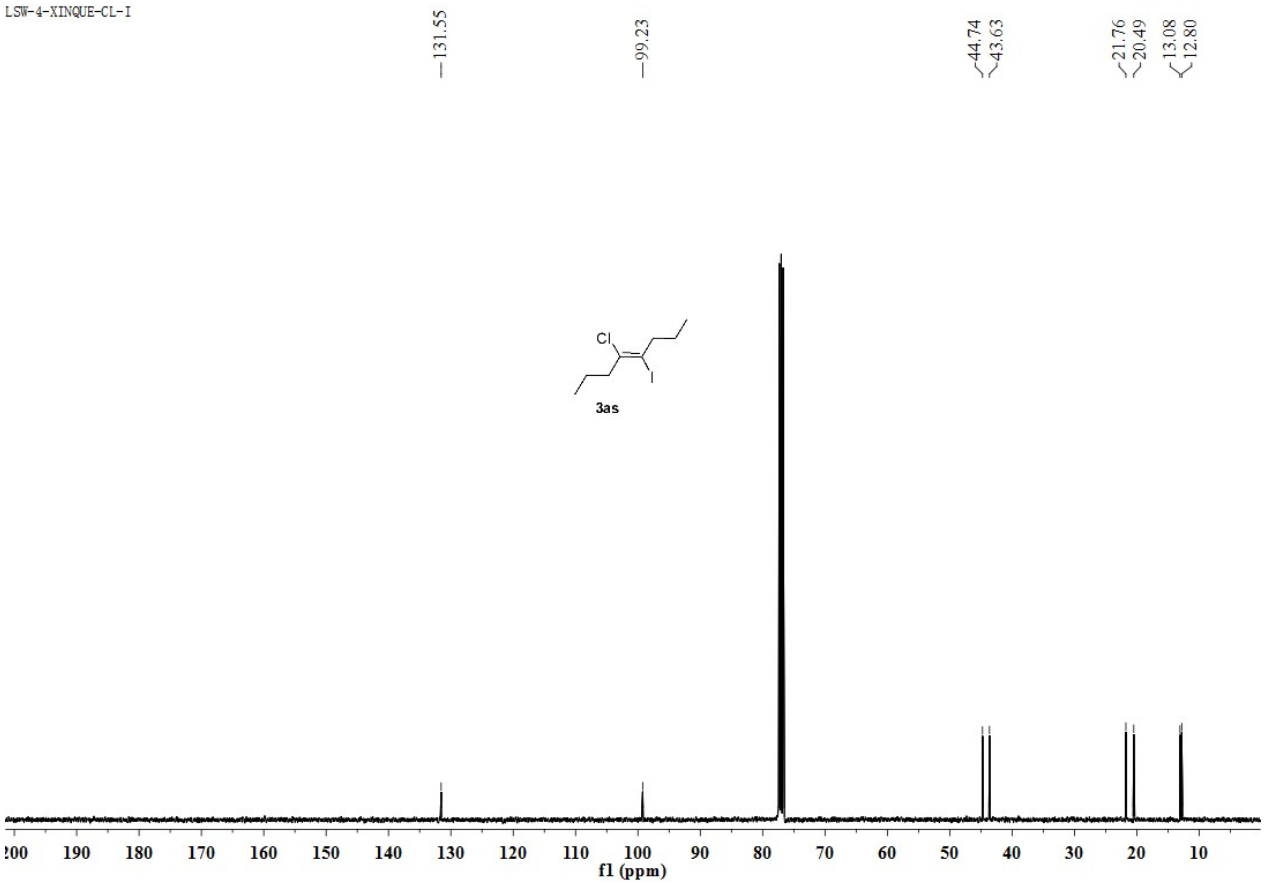
LSW-2CL-CL-I



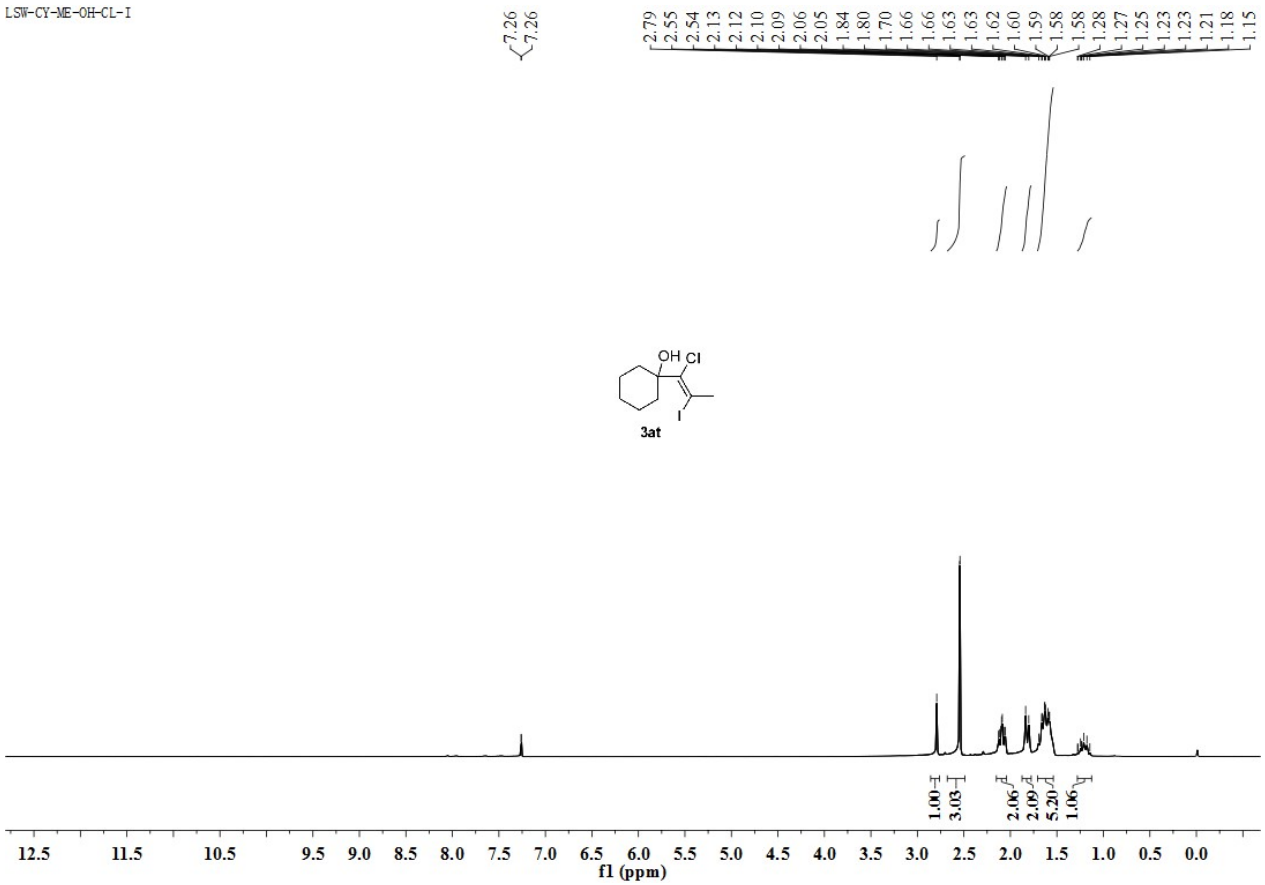
LSW-4XINQUE-CL-I



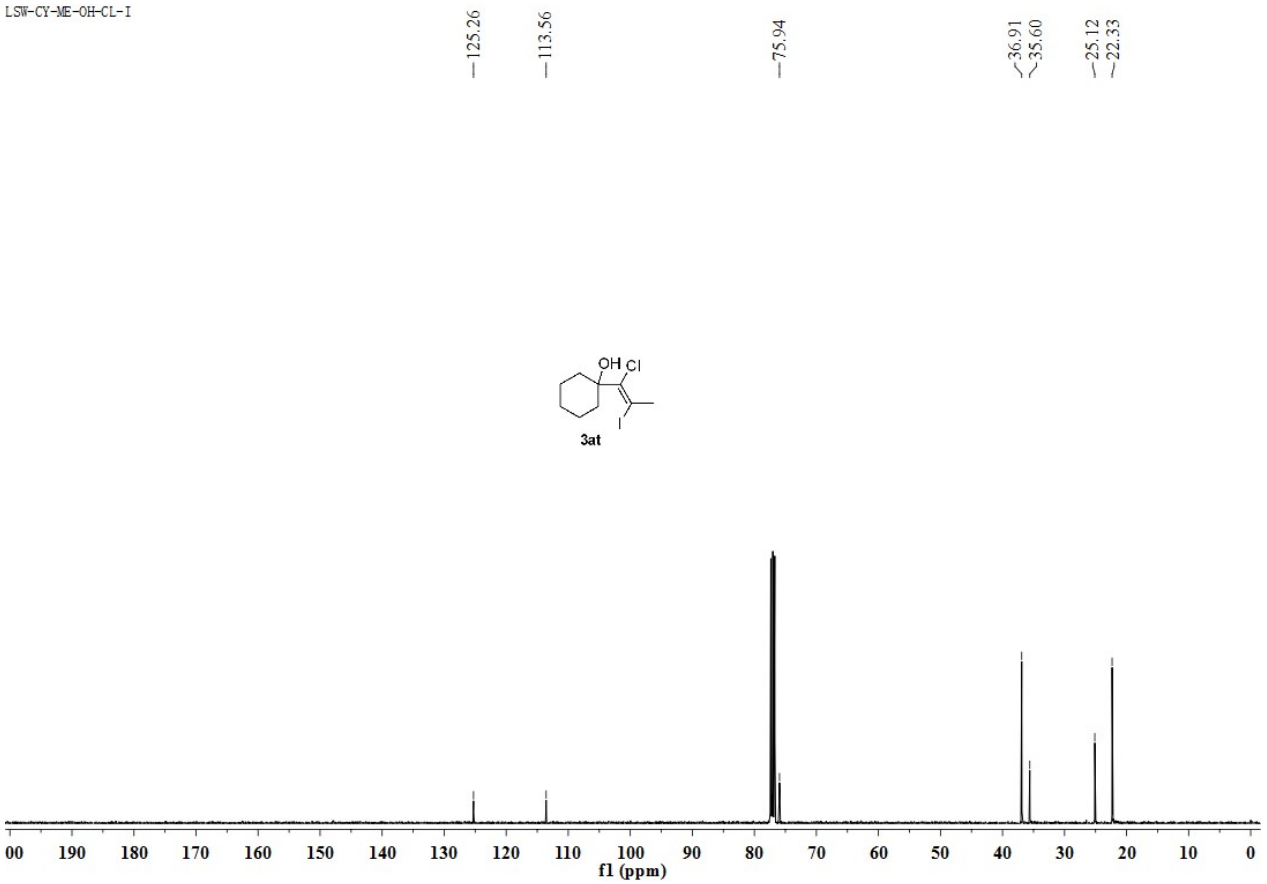
LSW-4-XINQUE-CL-I



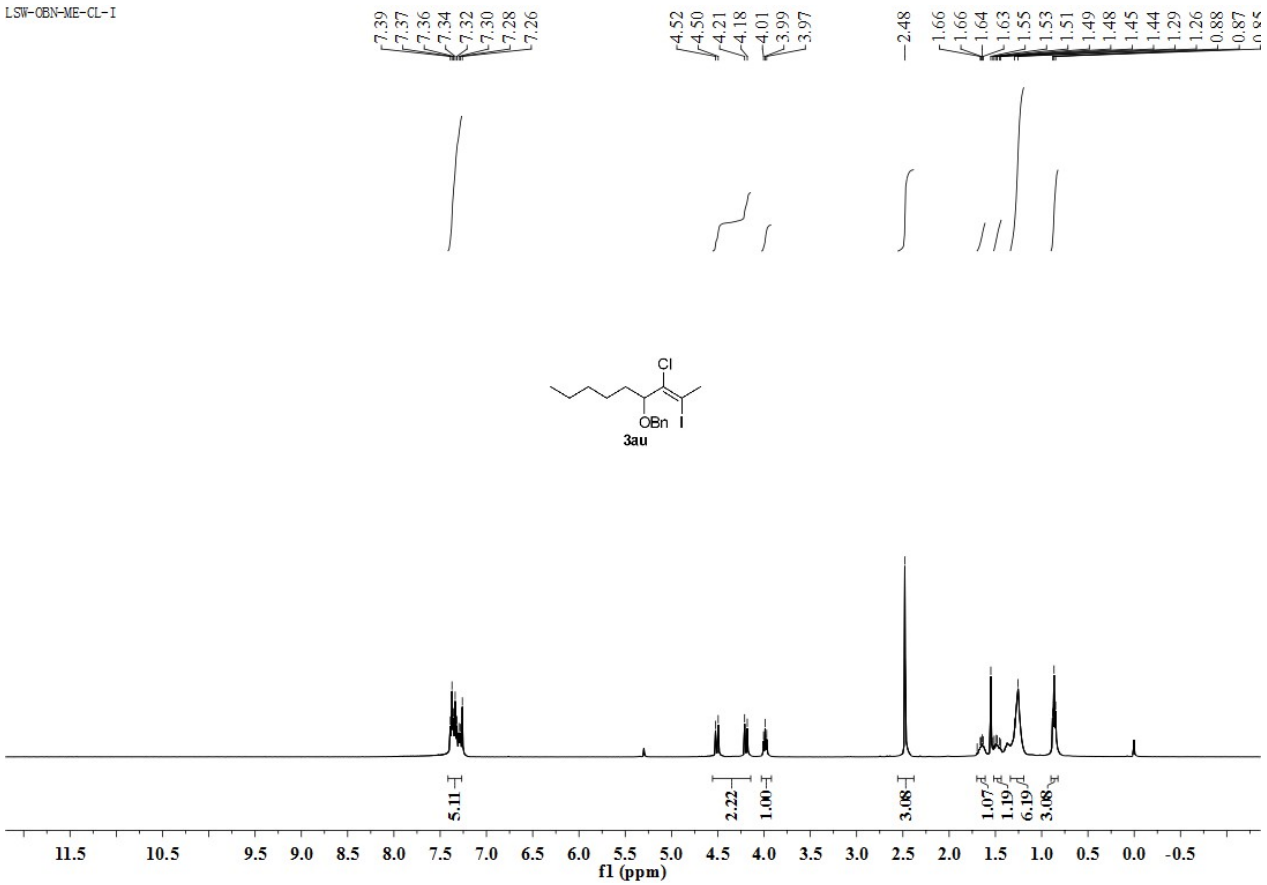
LSW-CY-ME-OH-CL-I



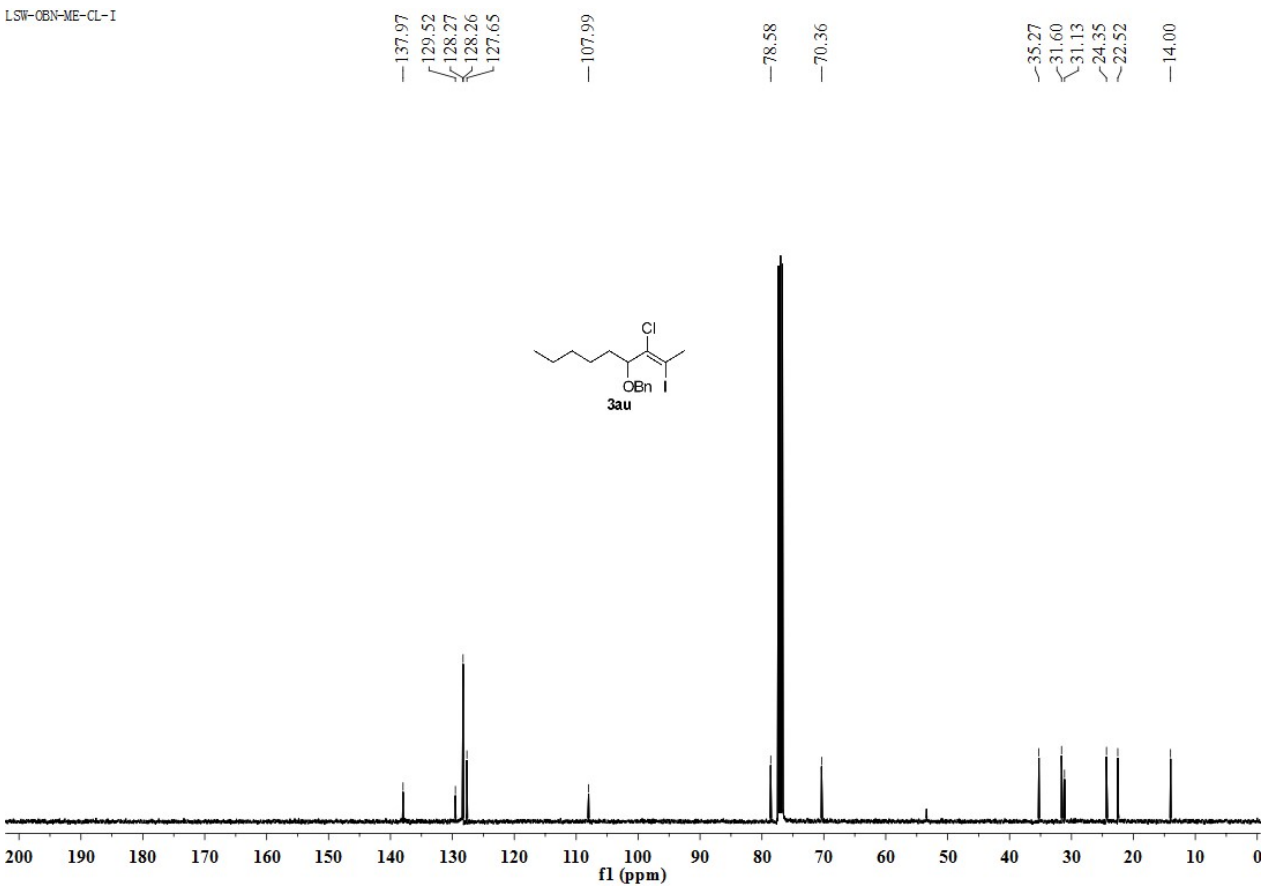
LSW-CY-ME-OH-CL-I



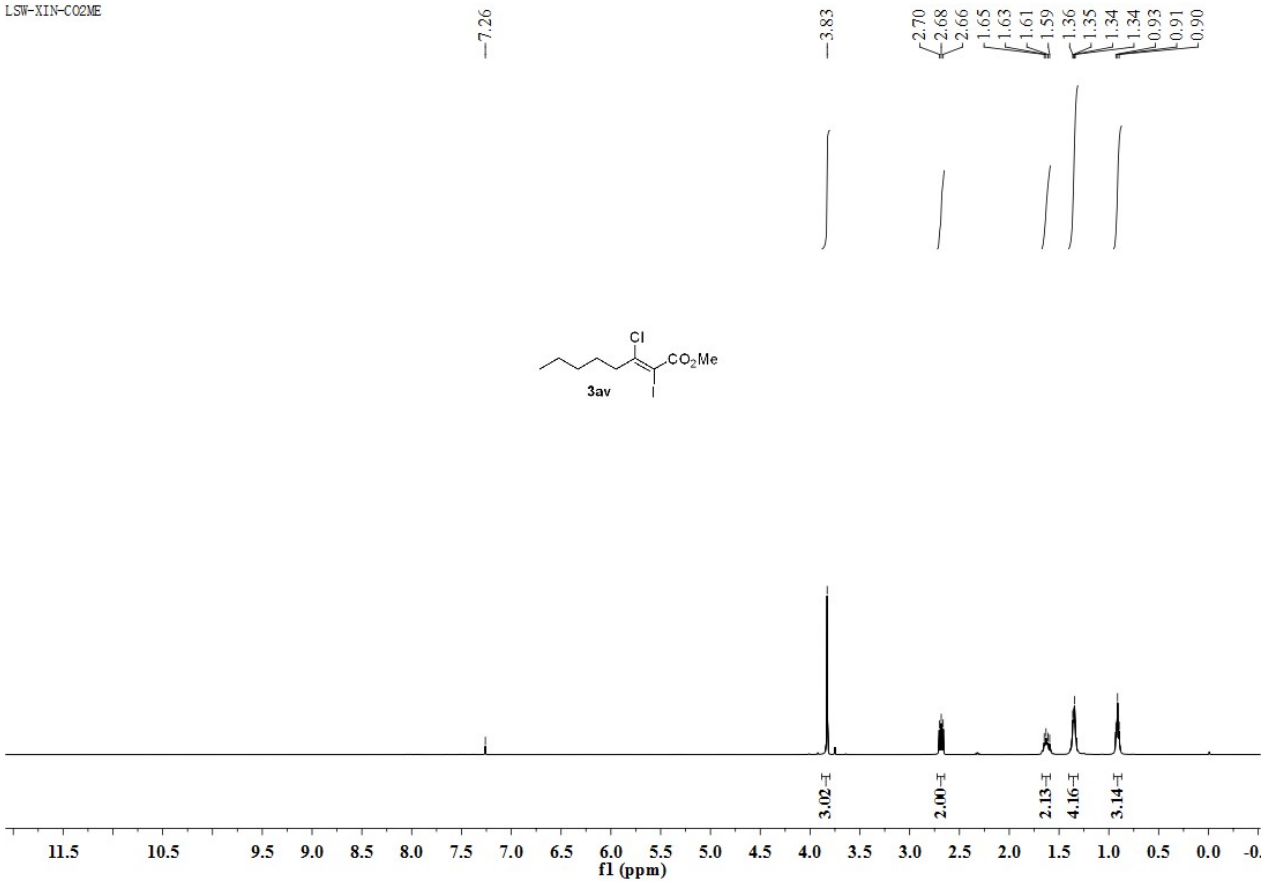
LSW-OBN-ME-CL-I



LSW-OBN-ME-CL-I

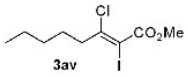


LSW-XIN-CO2ME

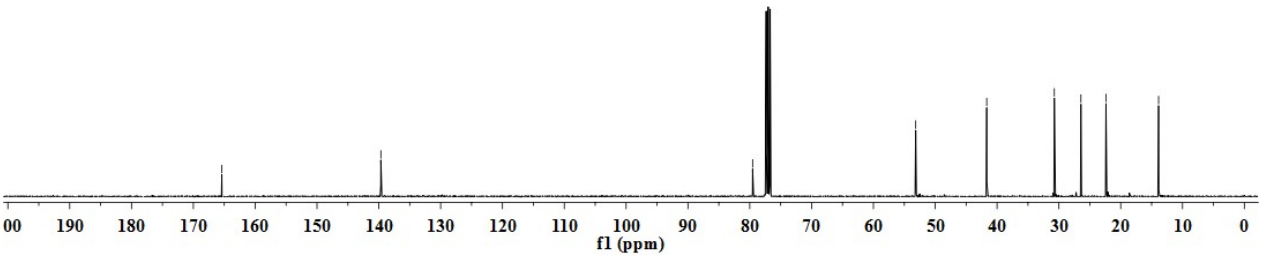


LSW-XIN-CO2ME

165.40
139.67
79.54
53.16
41.67
30.74
26.44
22.38
13.87

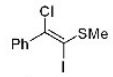


3av

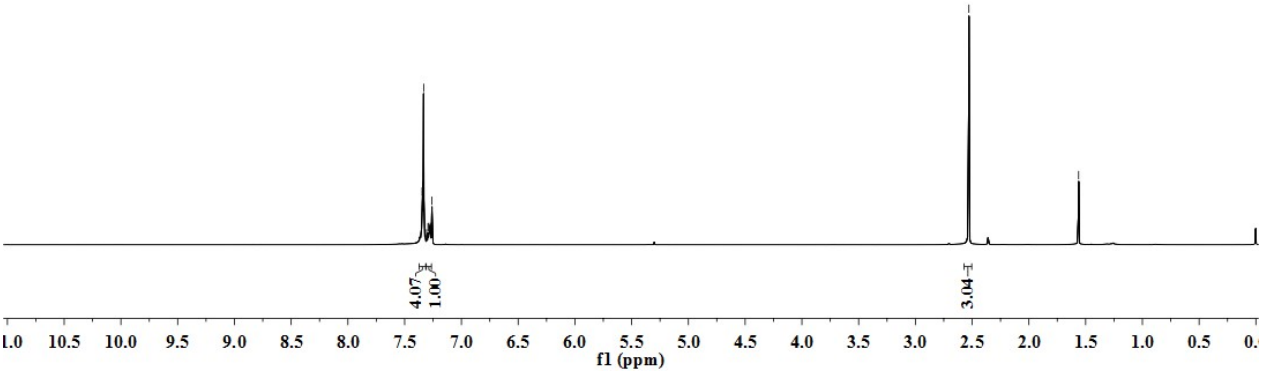


LSW-QUE-SME-CL-I-1

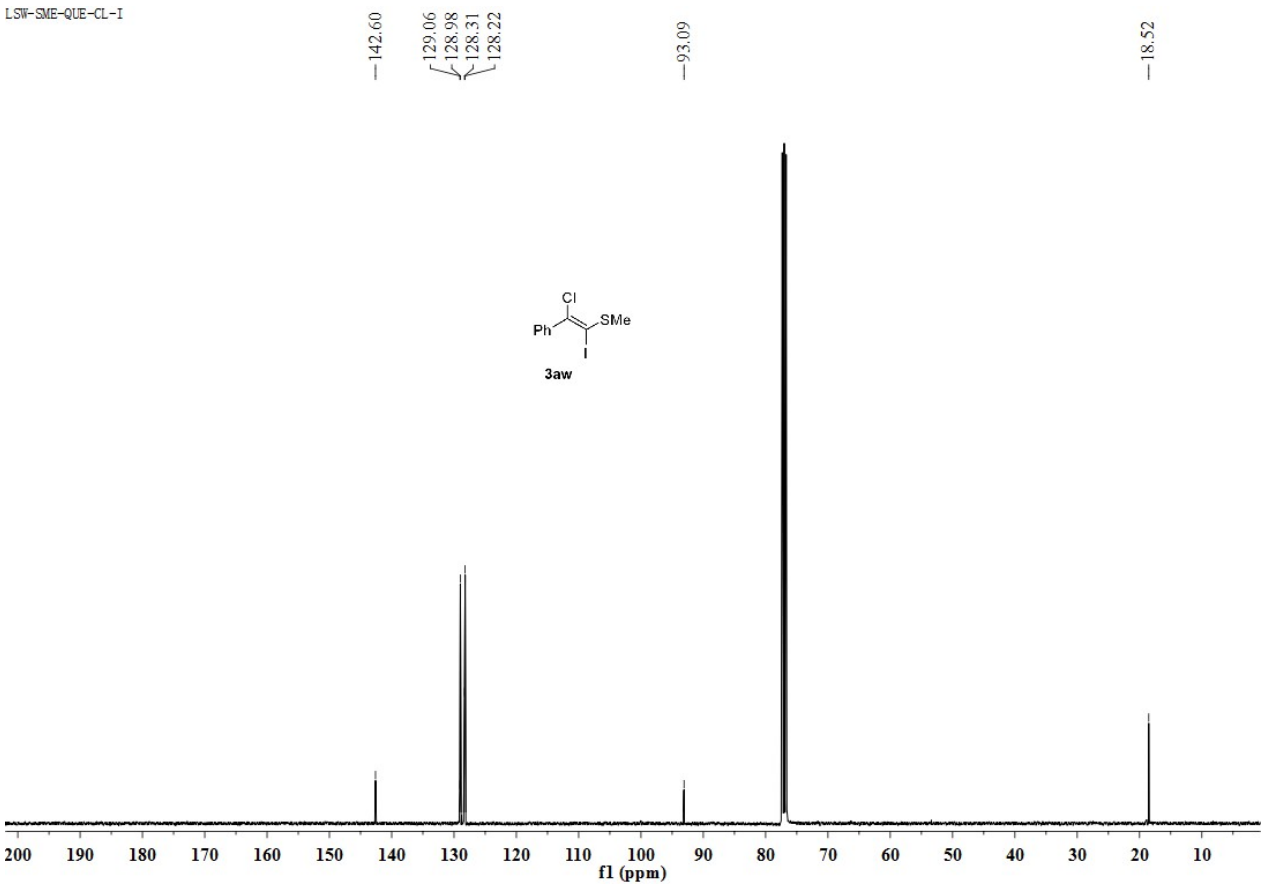
7.35
7.34
7.33
7.31
7.29
7.29
7.28
7.28
7.28
7.27
7.27
7.26
2.53
1.56



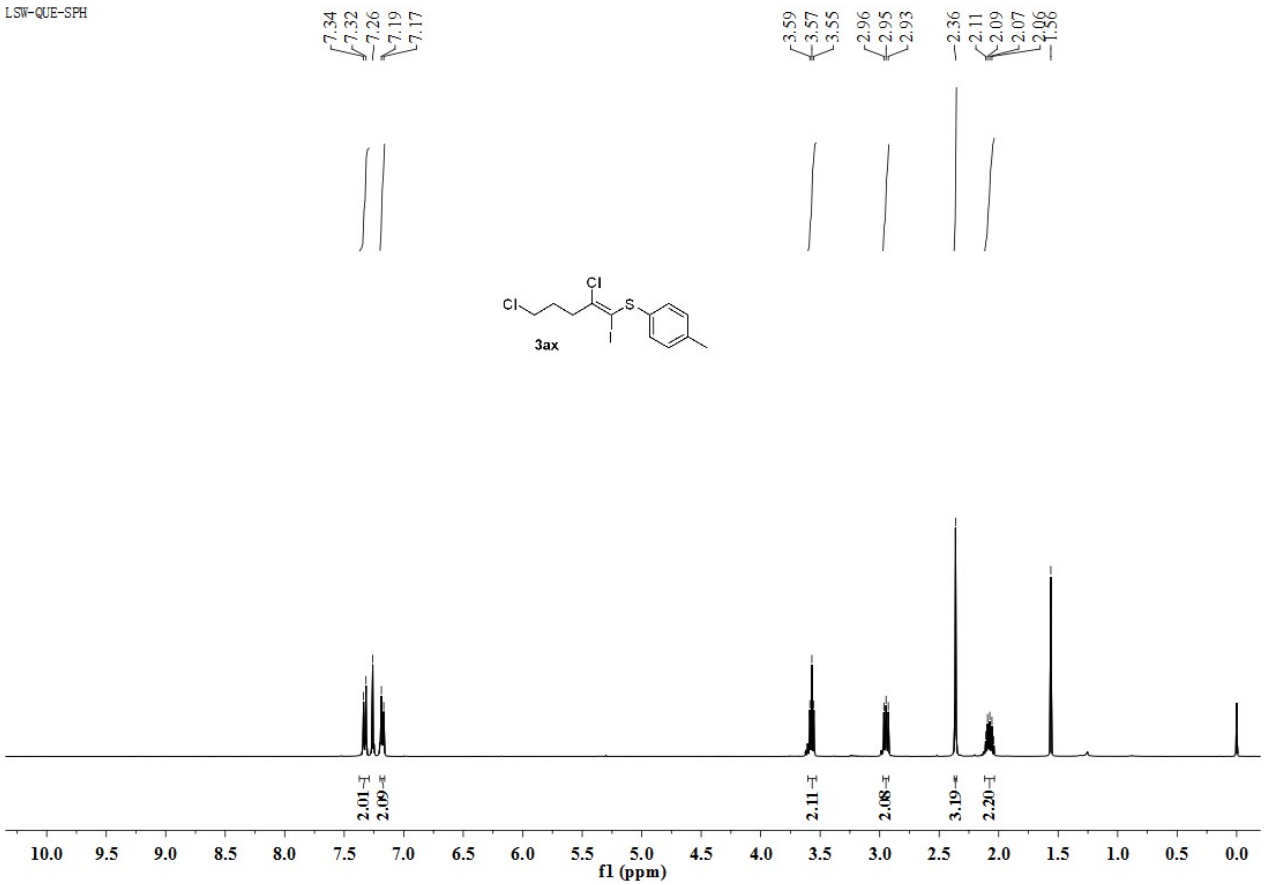
3aw



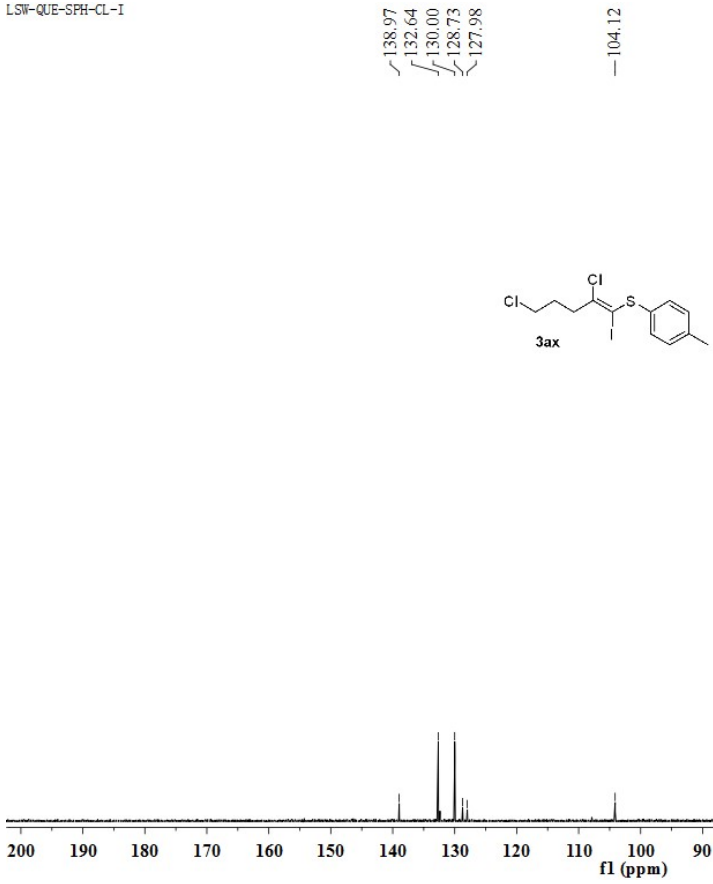
LSW-SME-QUE-CL-I



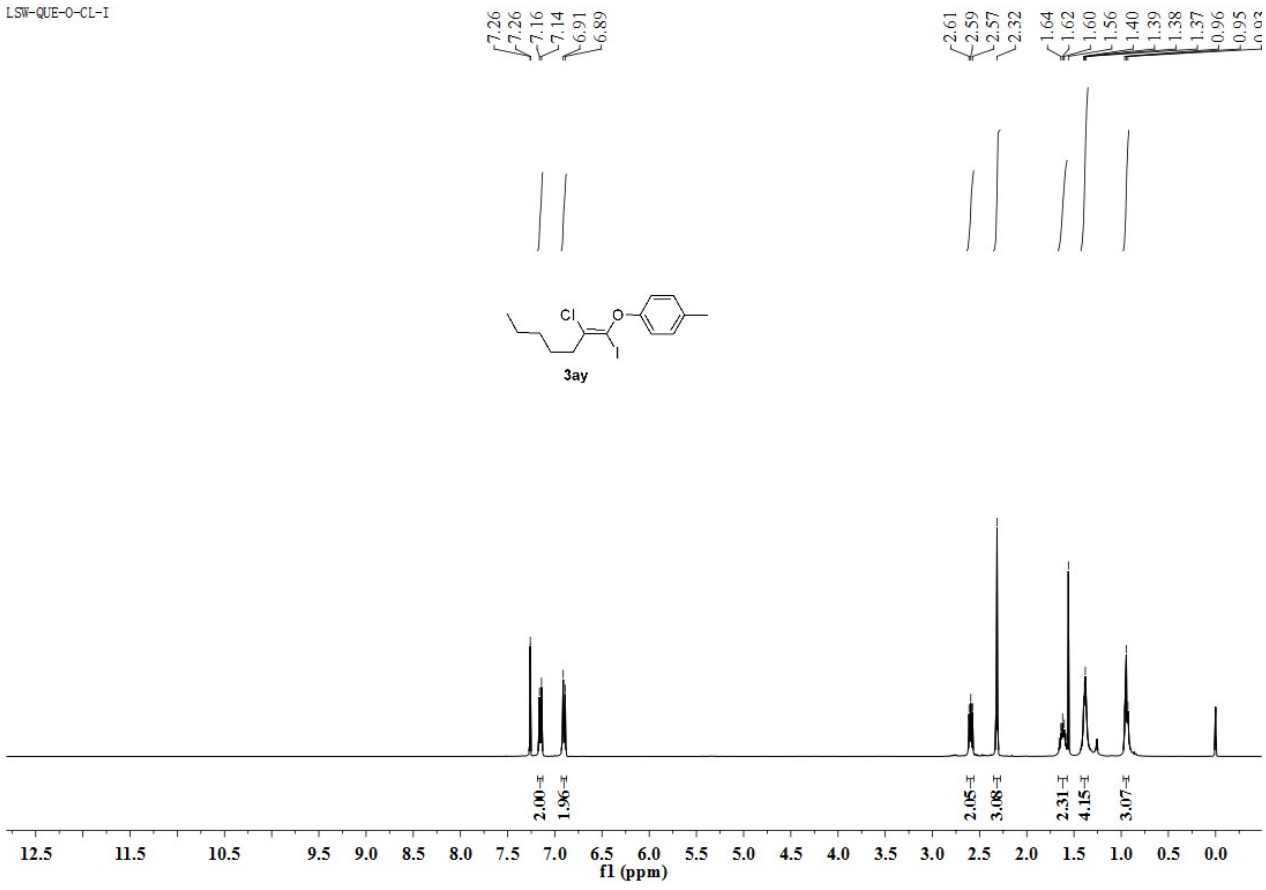
LSW-QUE-SPH

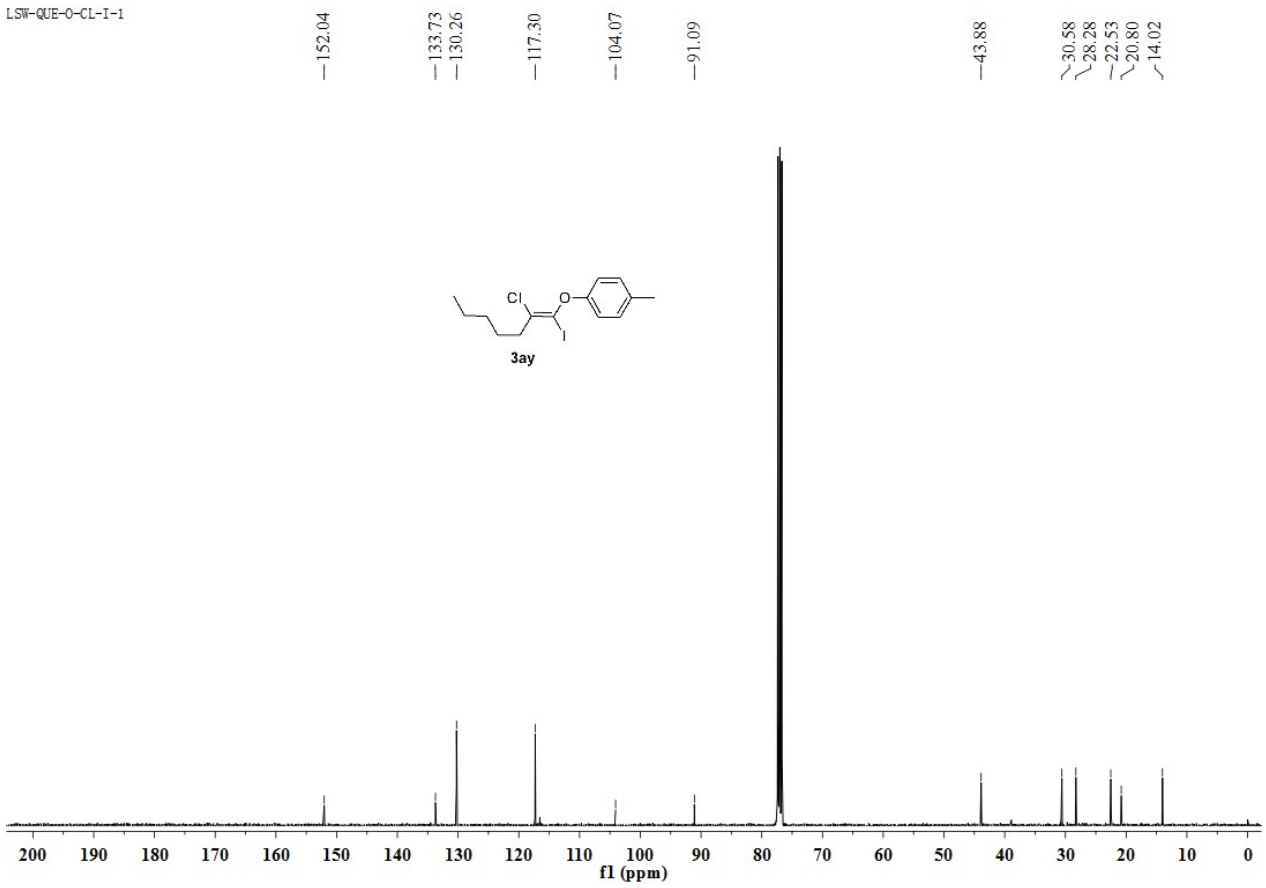


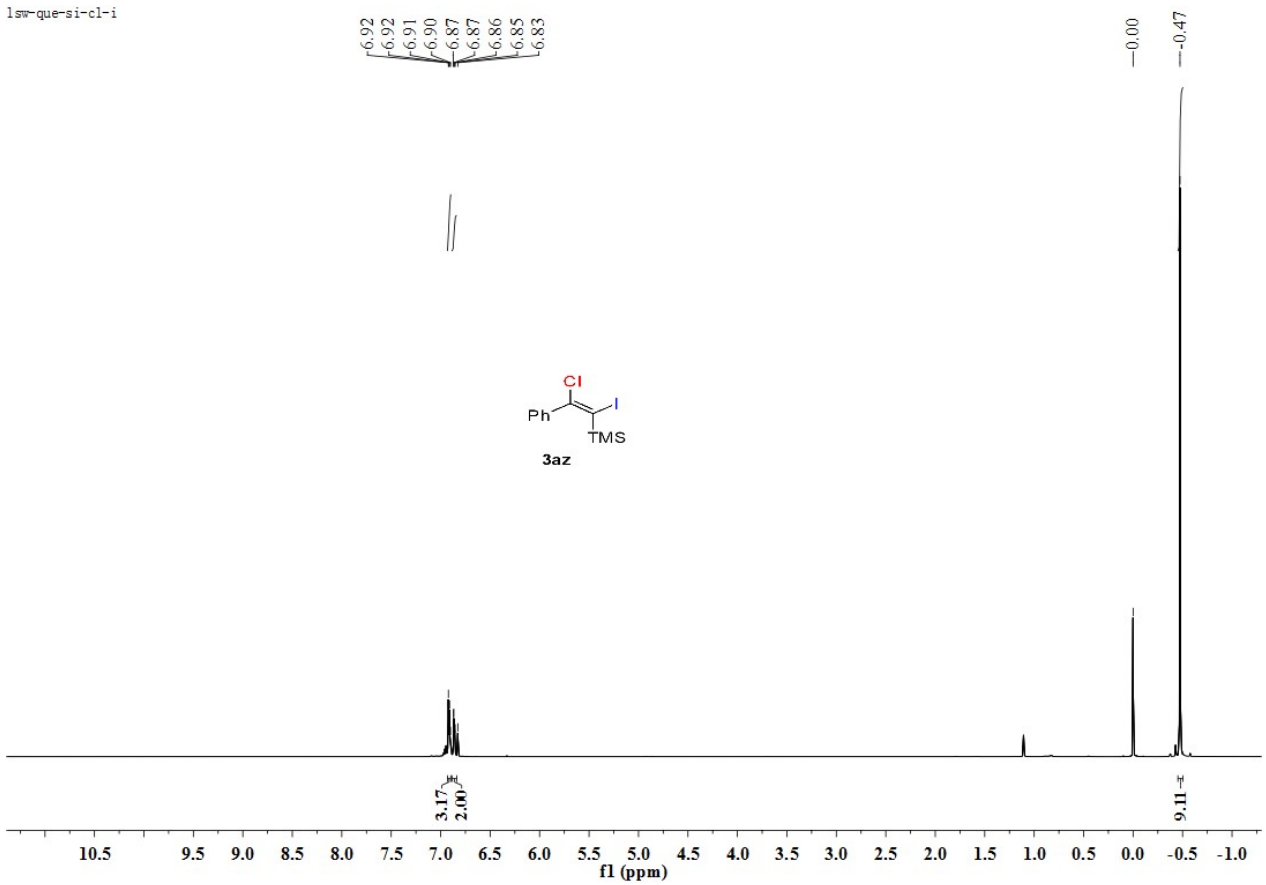
LSW-QUE-SPH-CL-I

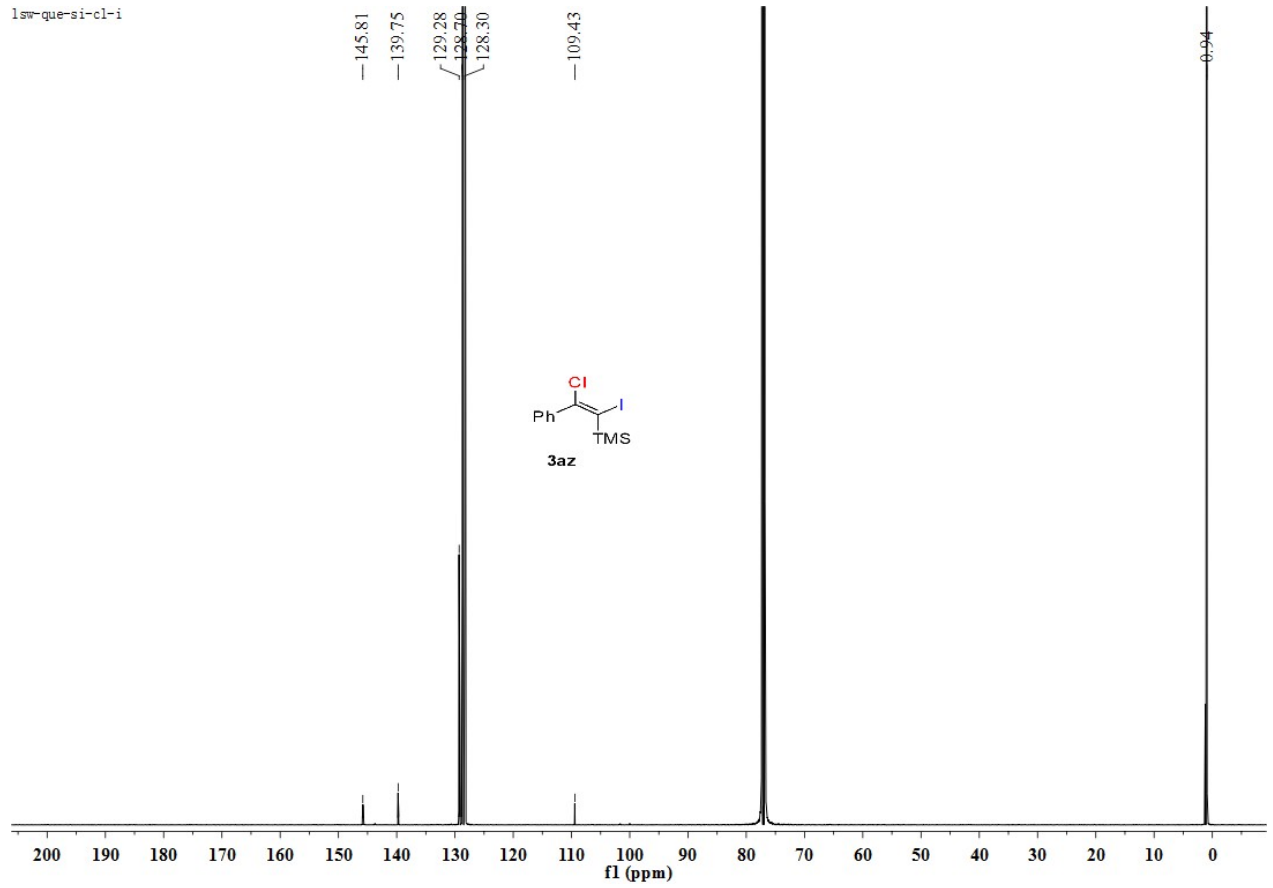


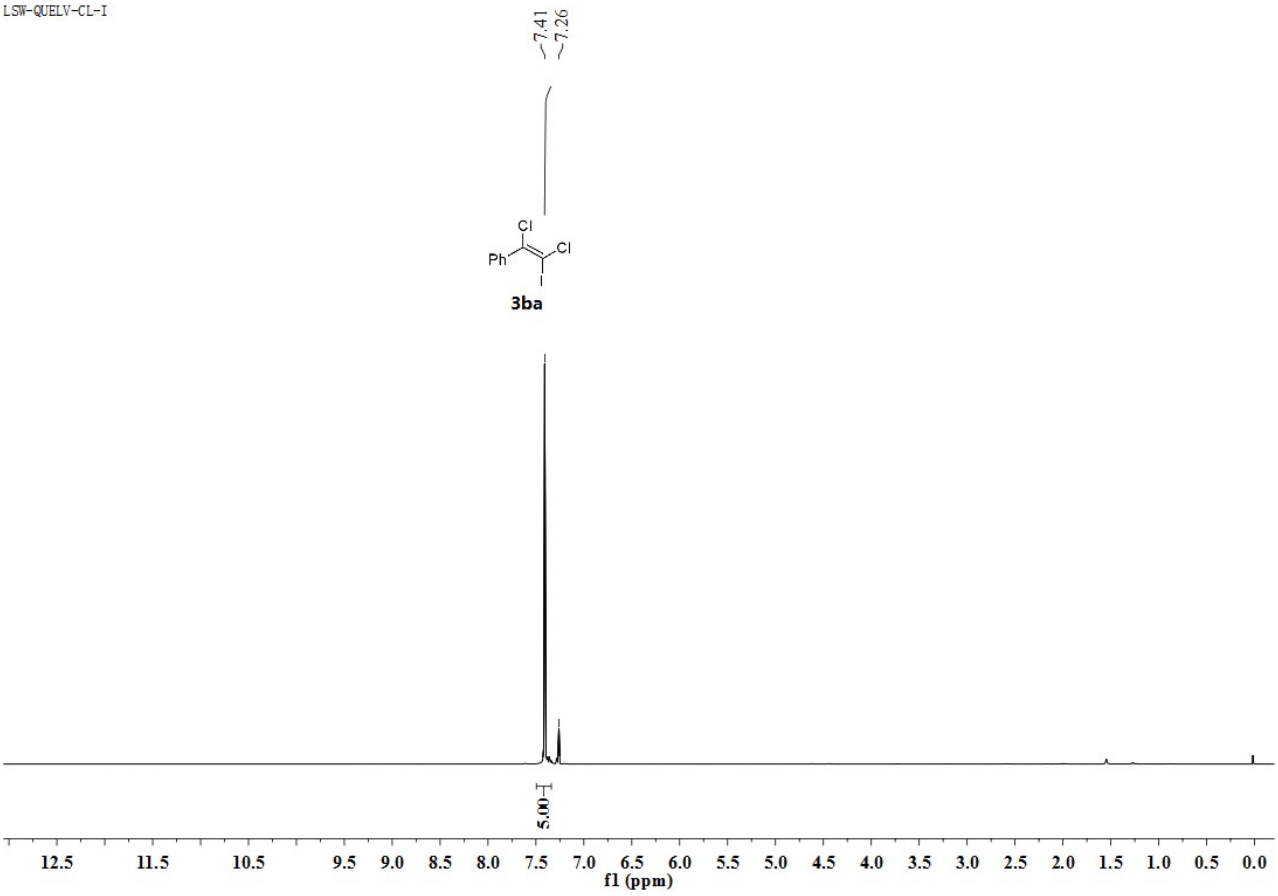
LSW-QUE-O-CL-I



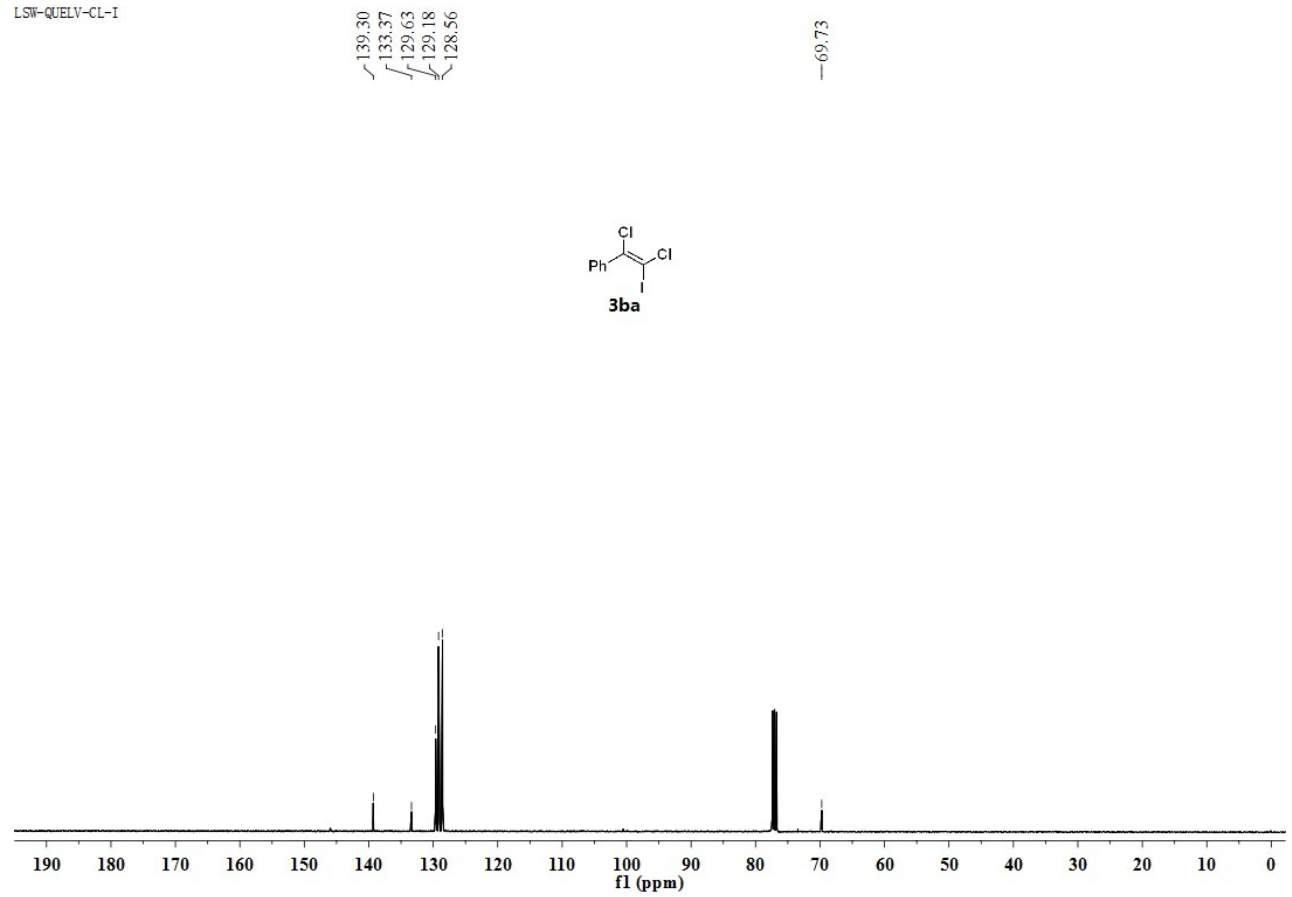

LSW-QUE-O-CL-I-1
152.04
133.73
130.26
117.30
104.07
91.09
43.88
30.58
28.28
22.53
20.80
14.02
Cl
O
I
3ay
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


lsw-que-si-cl-i
6.92
6.92
6.91
6.90
6.87
6.87
6.86
6.85
6.83
0.00
-0.47
Cl
Ph
I
TMS
3az
3.17
2.00
9.11
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

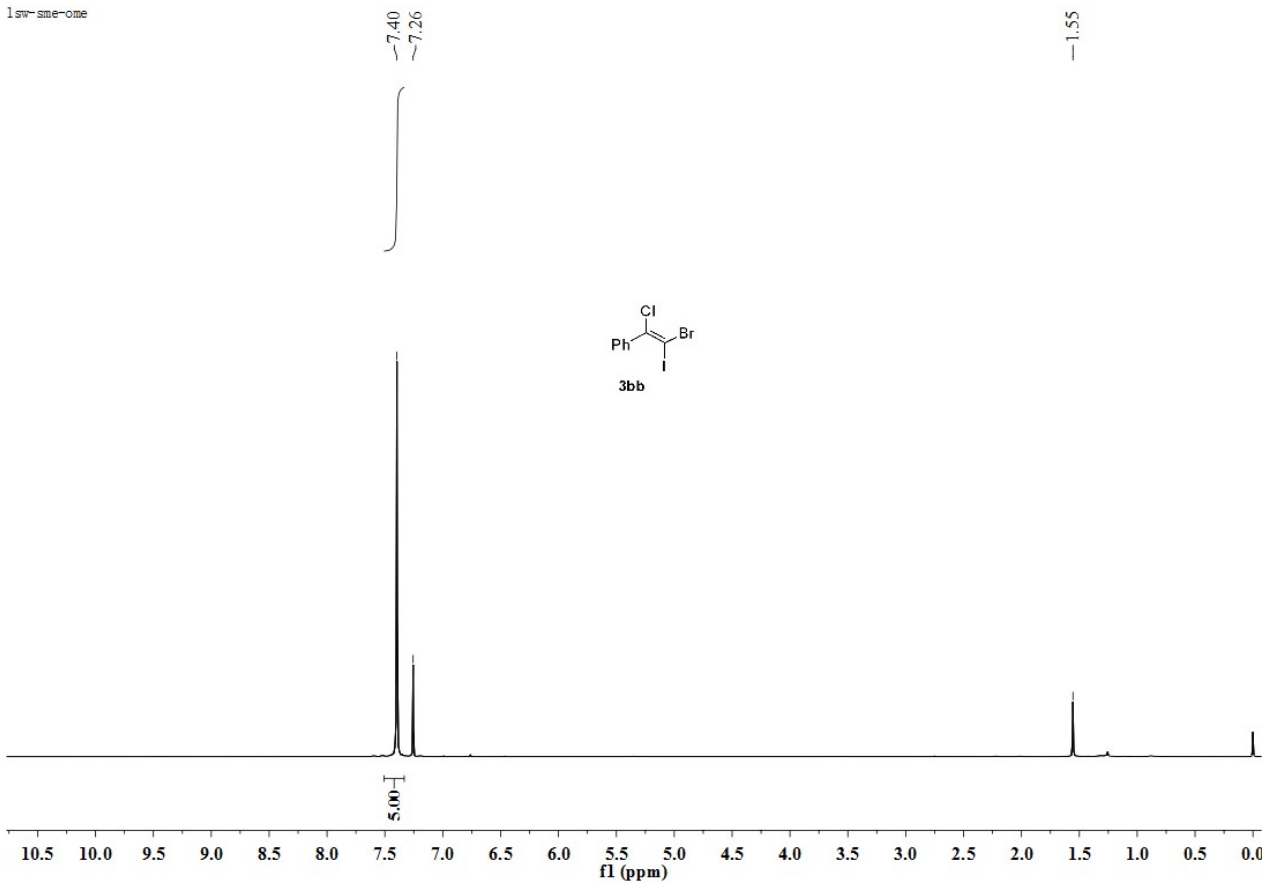

lsw-que-si-cl-i
145.81
139.75
129.28
128.70
128.30
109.43
0.94
Cl
I
Ph
TMS
3az
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


LSW-QUELV-CL-I
7.41
7.26
Cl
Ph
Cl
3ba
5.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

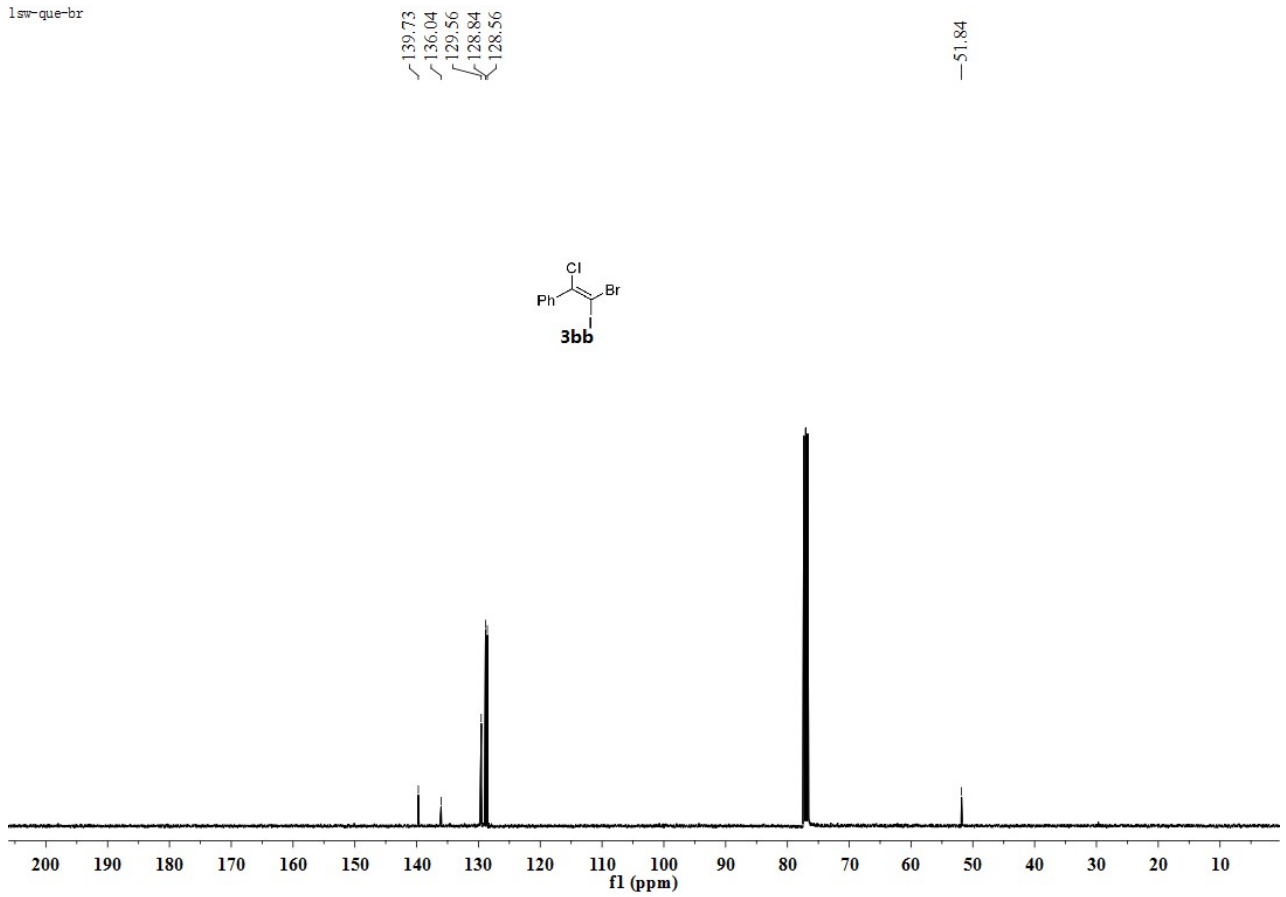
LSW-QUELV-CL-I



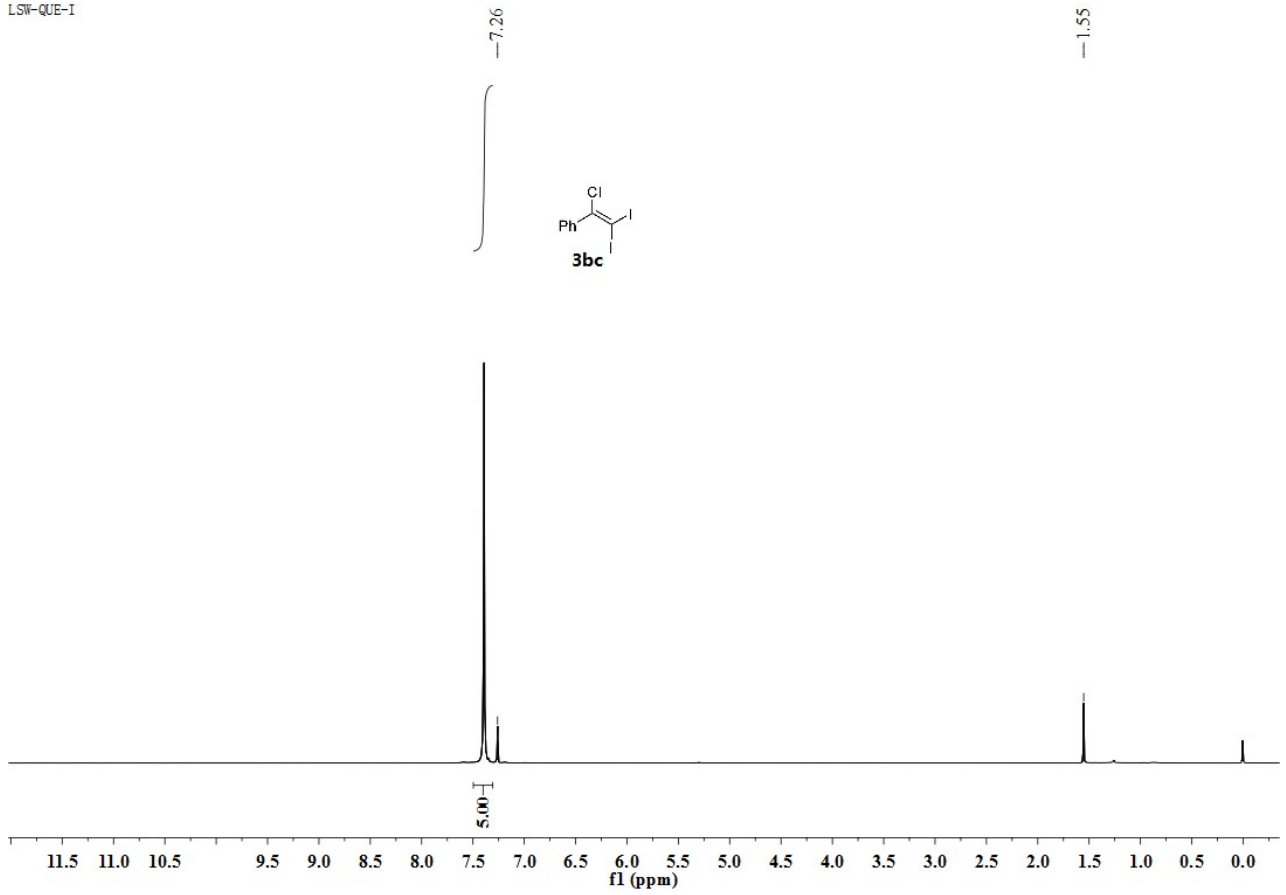
lsw-sme-ome



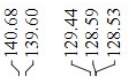
lsw-que-br



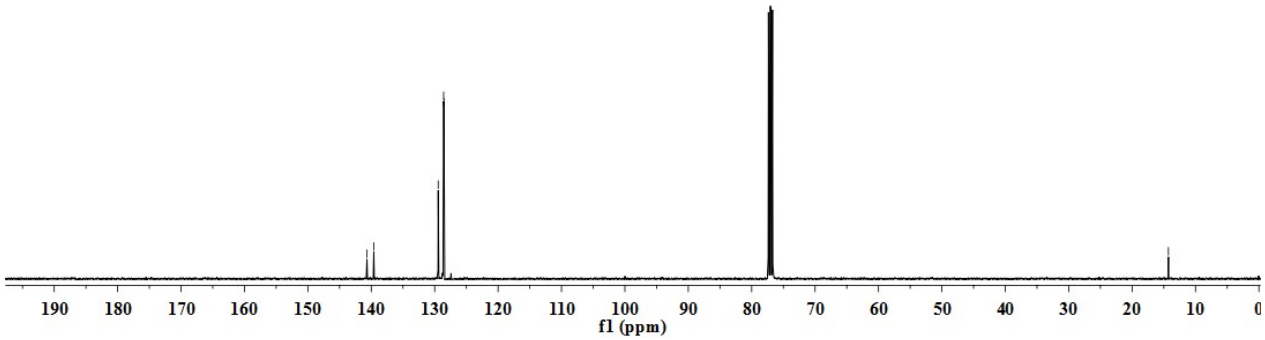
LSW-QUE-I



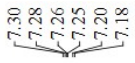
LSW-QUE-I-CL-I-2

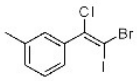


3bc

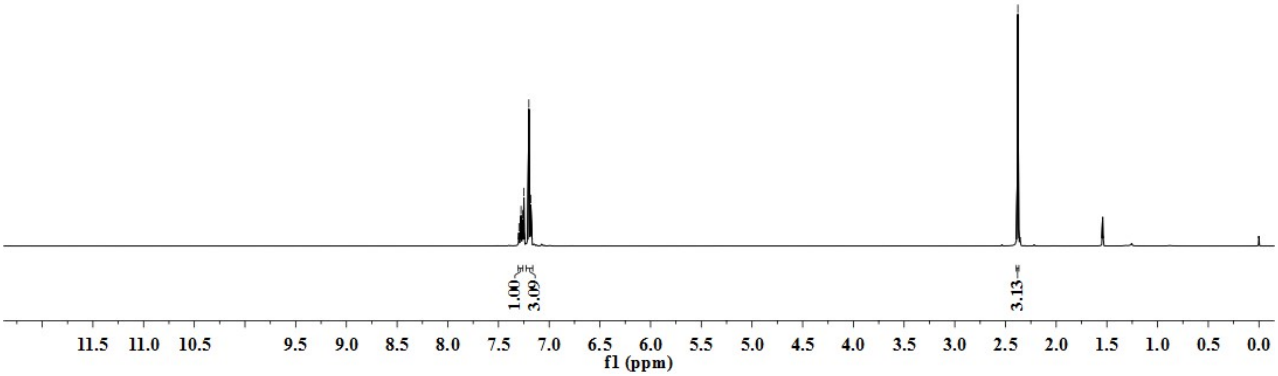


LSW-07-A



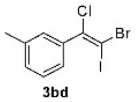


3bd

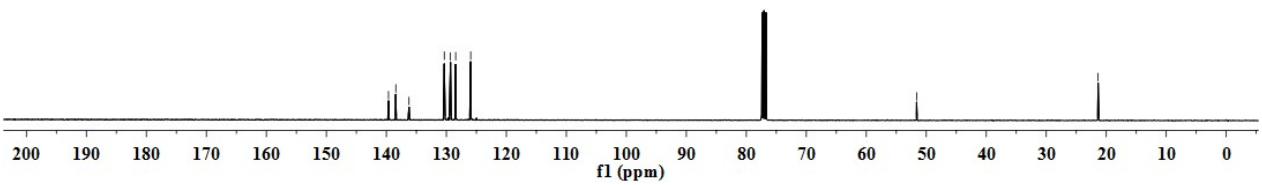


LSW-7A

139.64
138.42
136.22
130.34
129.31
128.45
125.94
51.61
21.37



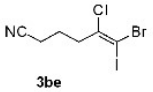
3bd



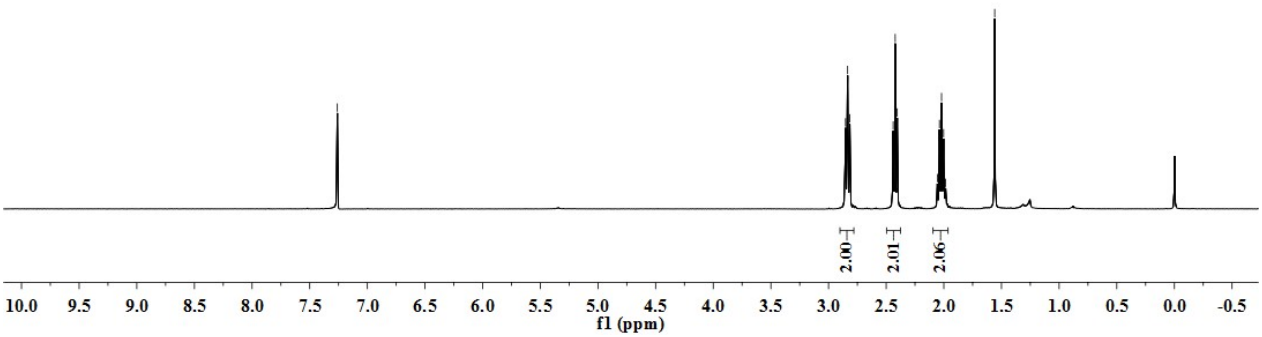
LSW-CN-BR-CL-I

7.26

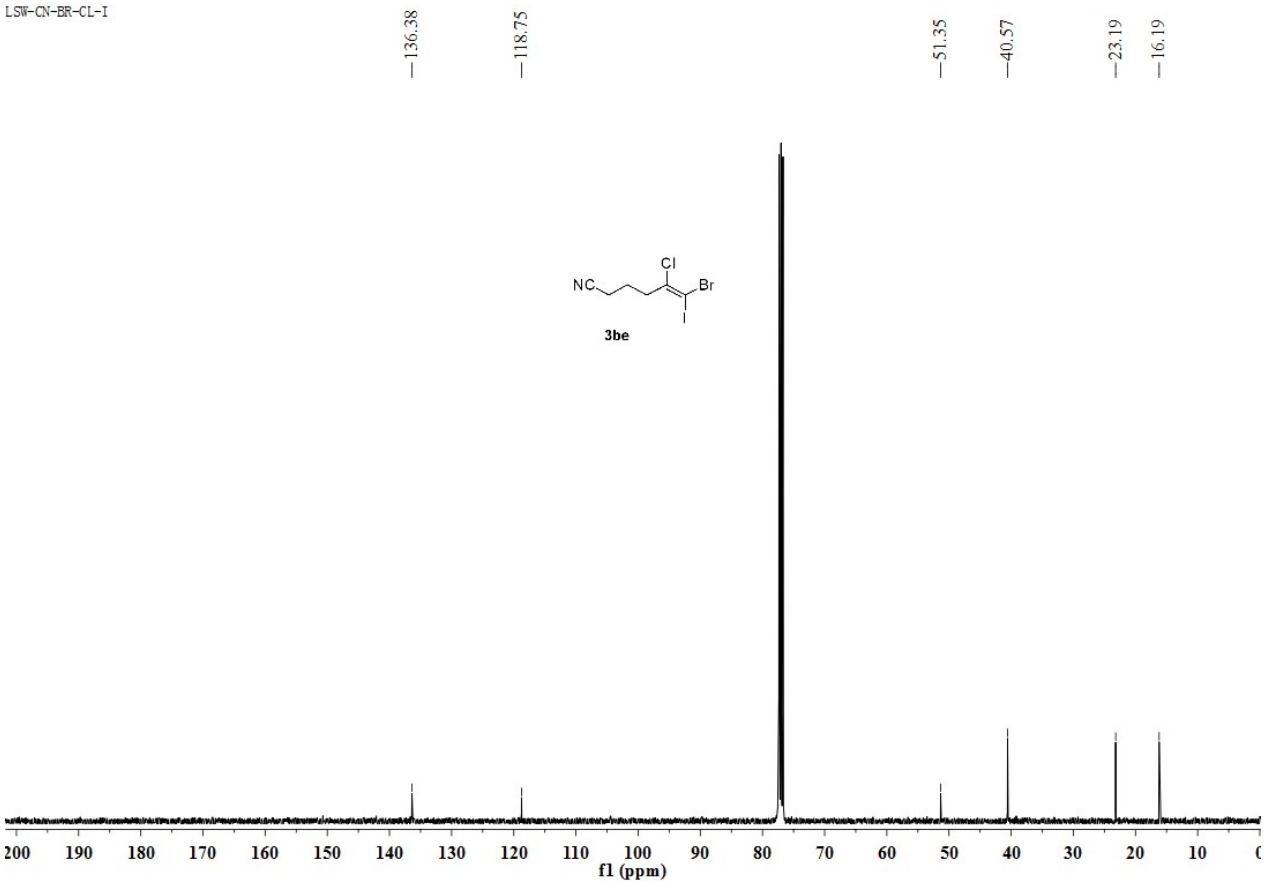
2.85
2.83
2.82
2.44
2.42
2.40
2.04
2.02
1.56



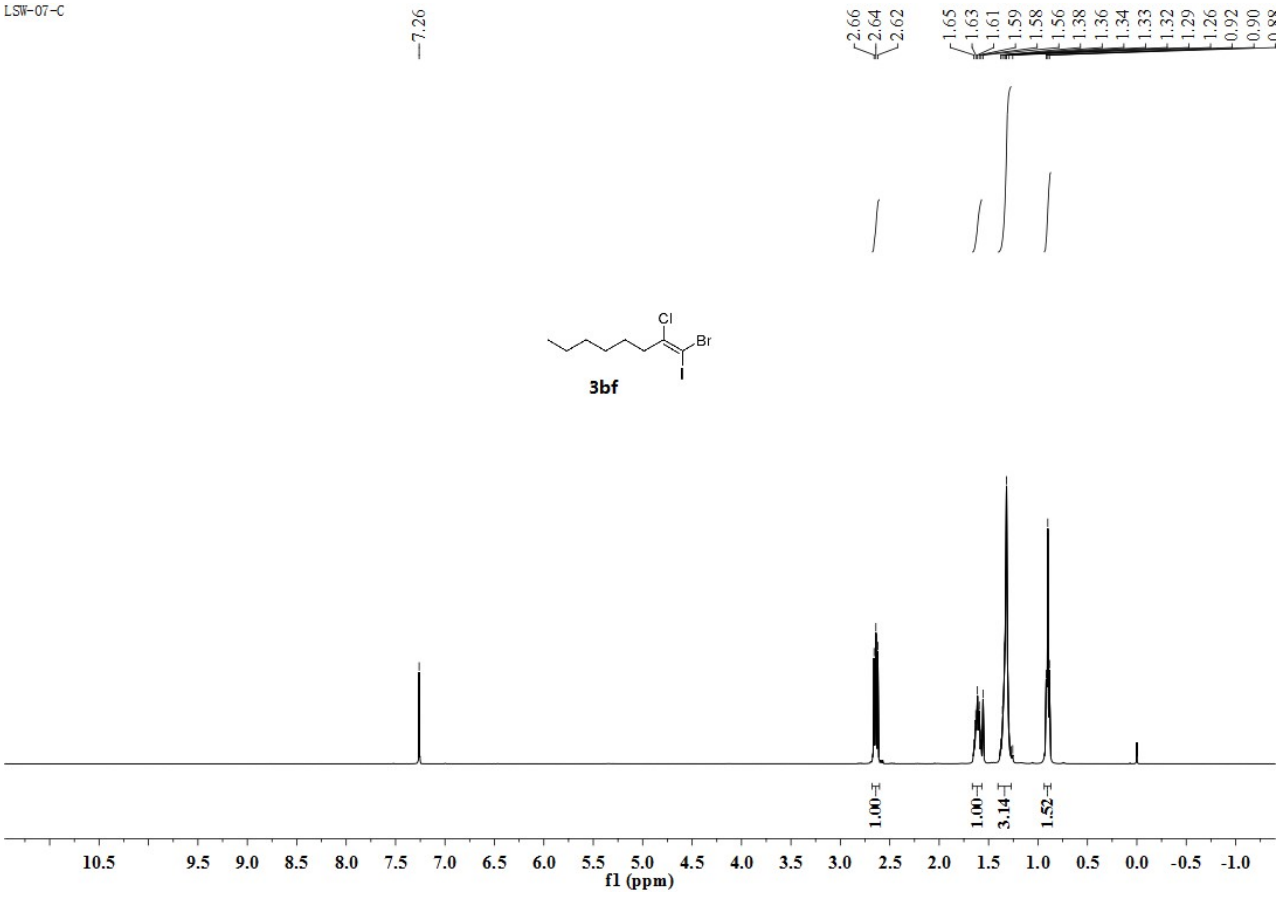
3be



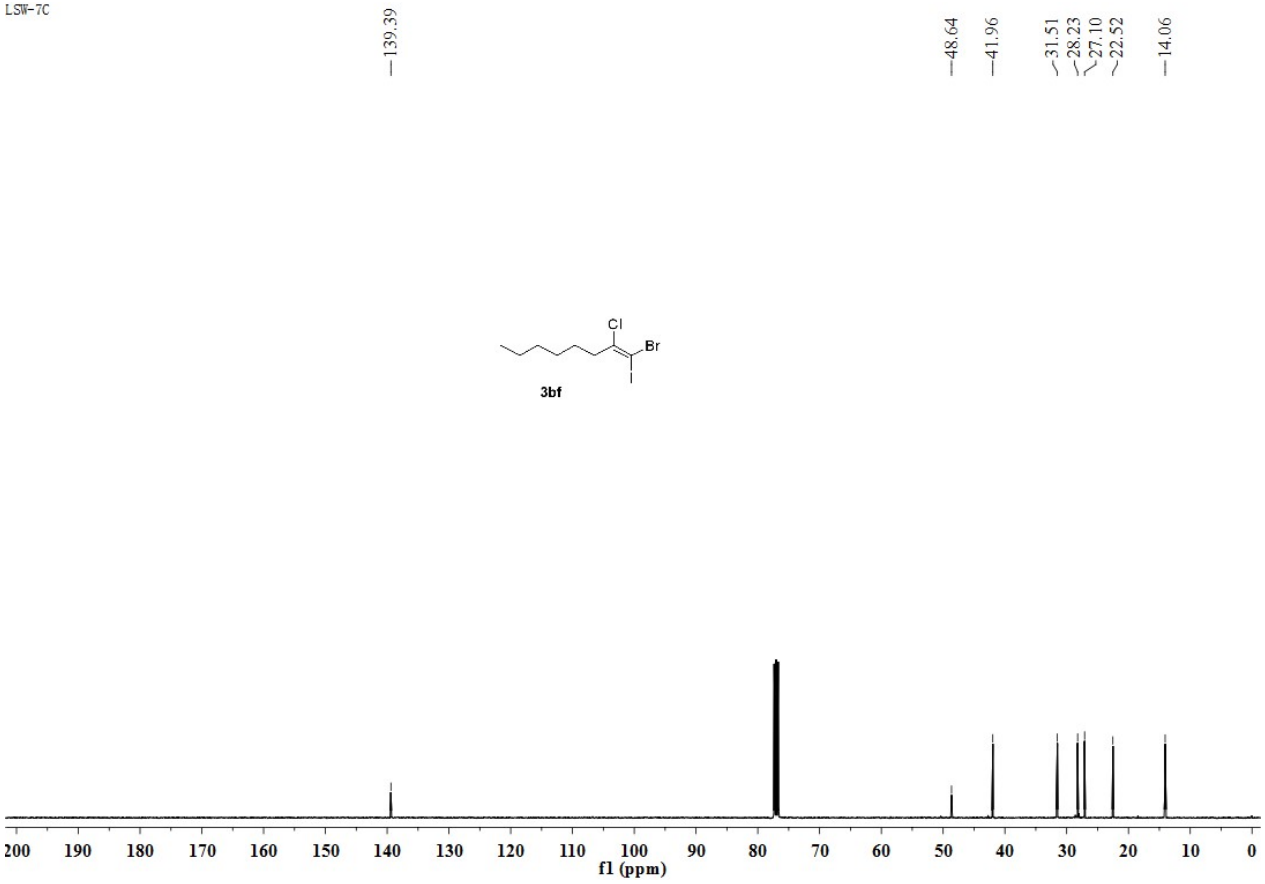
LSW-CN-BR-CL-I

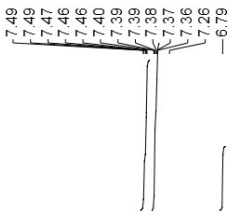


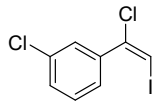
LSW-07-C



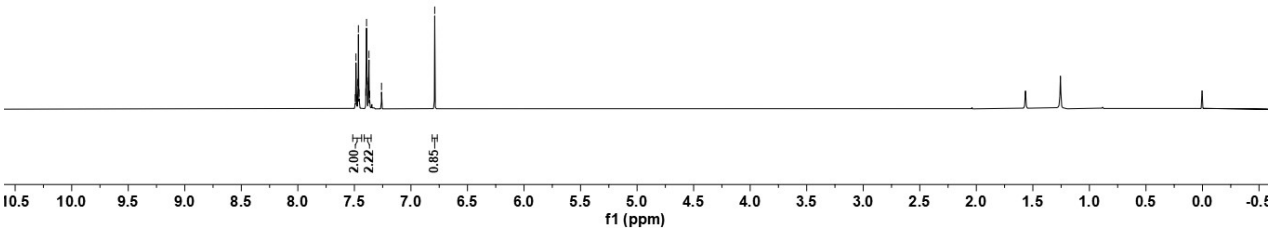
LSW-7C


139.39
48.64
41.96
31.51
28.23
27.10
22.52
14.06
Cl
Br
3bf
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

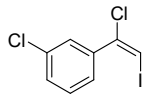

7.49
7.49
7.47
7.46
7.46
7.40
7.39
7.39
7.38
7.37
7.36
7.26
6.79


Cl
Cl
I

3bg

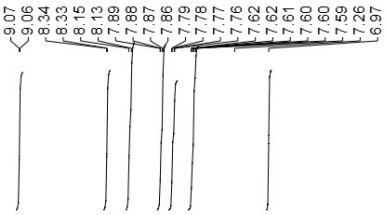

2.00
2.22
0.85
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

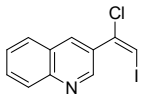

136.03
135.45
132.97
130.40
128.59
73.21


Cl
Cl
I

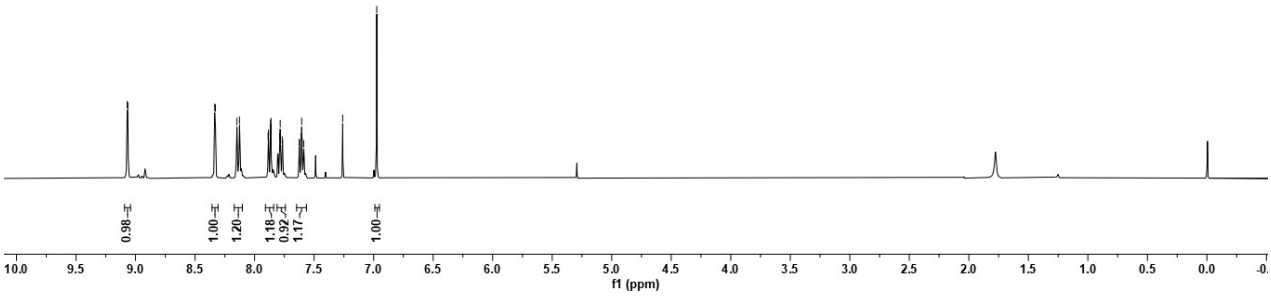
3bg

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


9.07
9.06
8.34
8.33
8.15
8.13
7.89
7.88
7.87
7.86
7.79
7.78
7.77
7.76
7.62
7.61
7.60
7.59
7.26
6.97


Cl
N
I

3bh

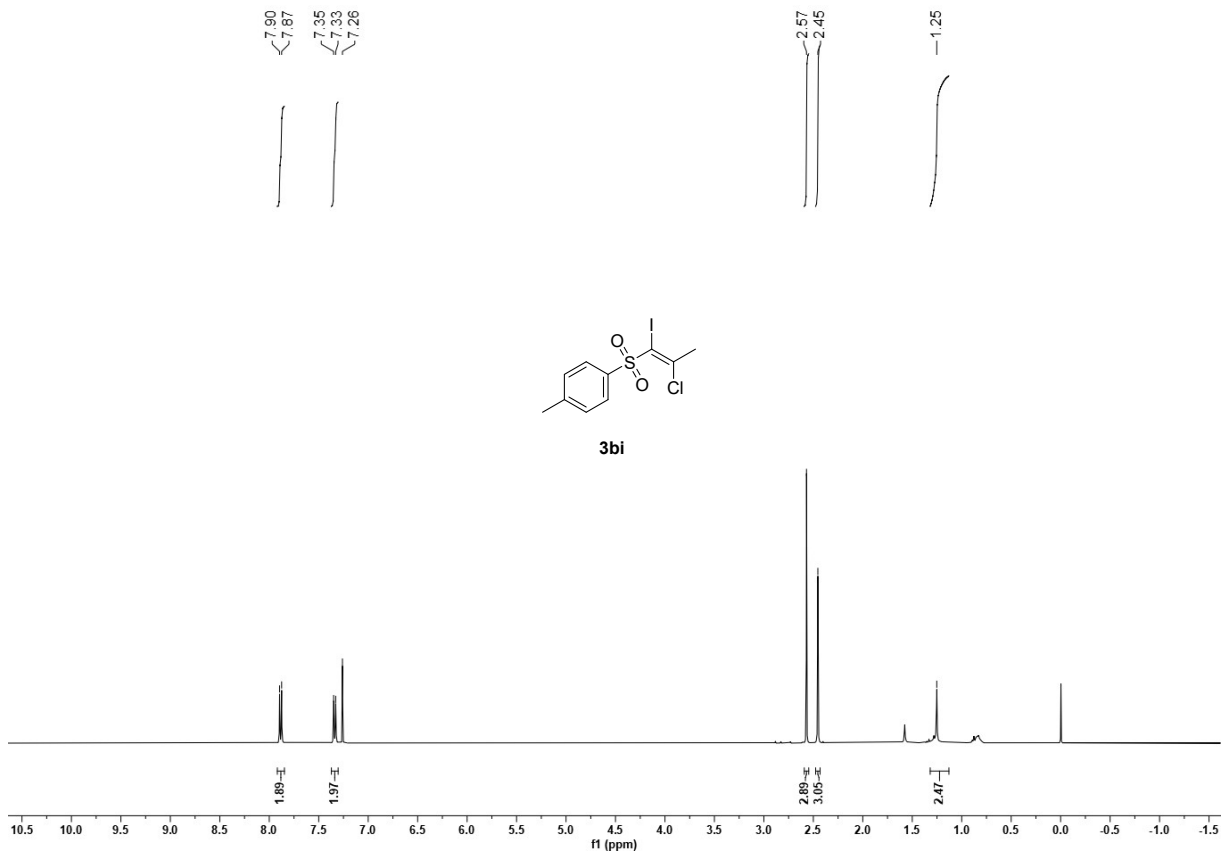

0.98
1.00
1.20
1.18
0.92
1.17
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


149.89
147.78
136.77
131.25
130.96
130.79
129.35
128.25
128.10
127.40
126.87

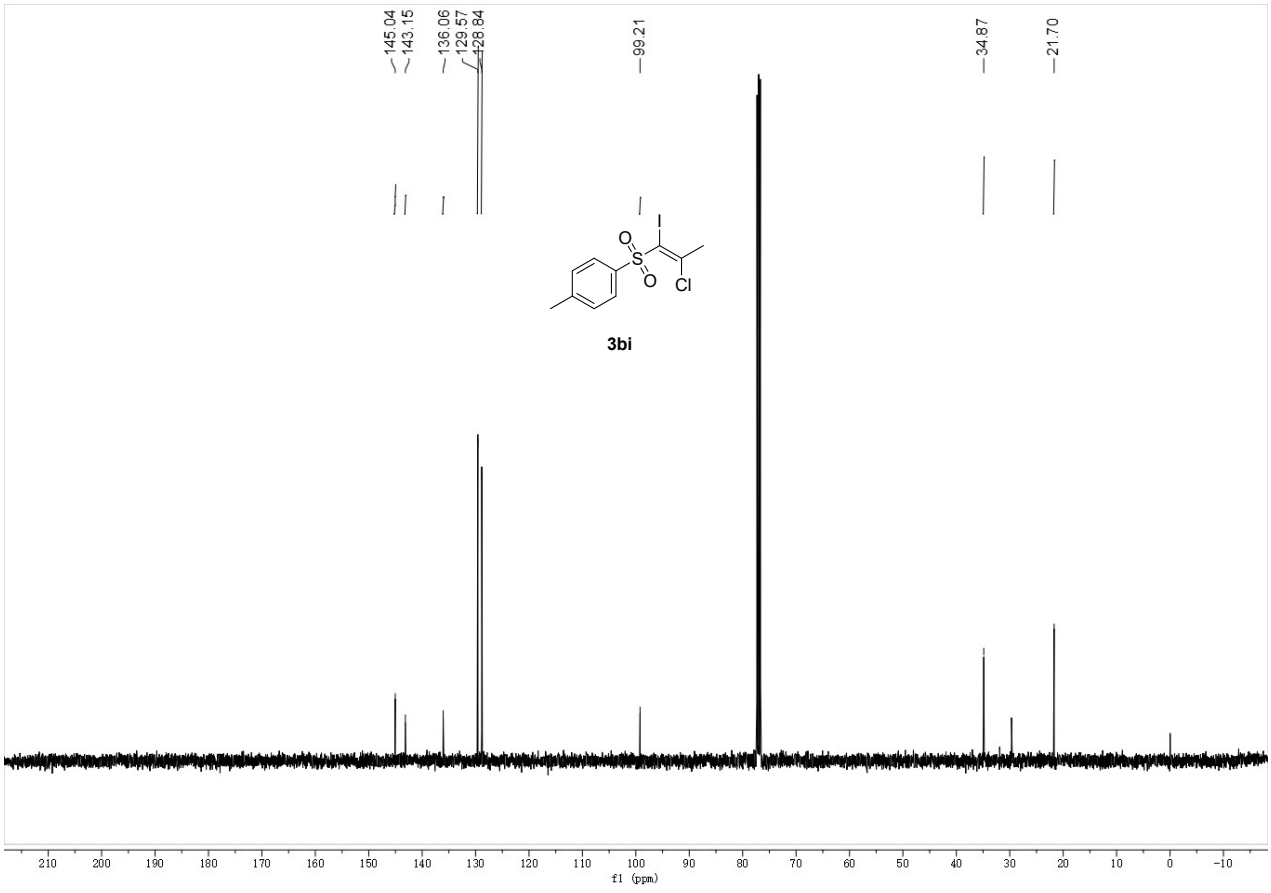
75.55
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Cl
N
I

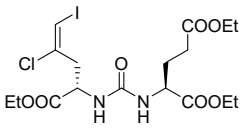
3bh


7.90
7.87
7.35
7.33
7.26
2.57
2.45
1.25
O
S
O
I
Cl
1.89
1.97
2.89
3.05
2.47
f1 (ppm)

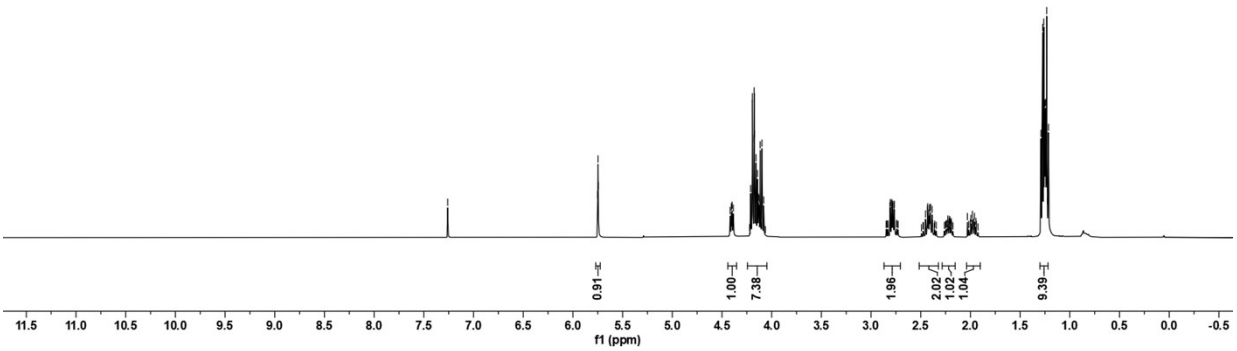
3bi

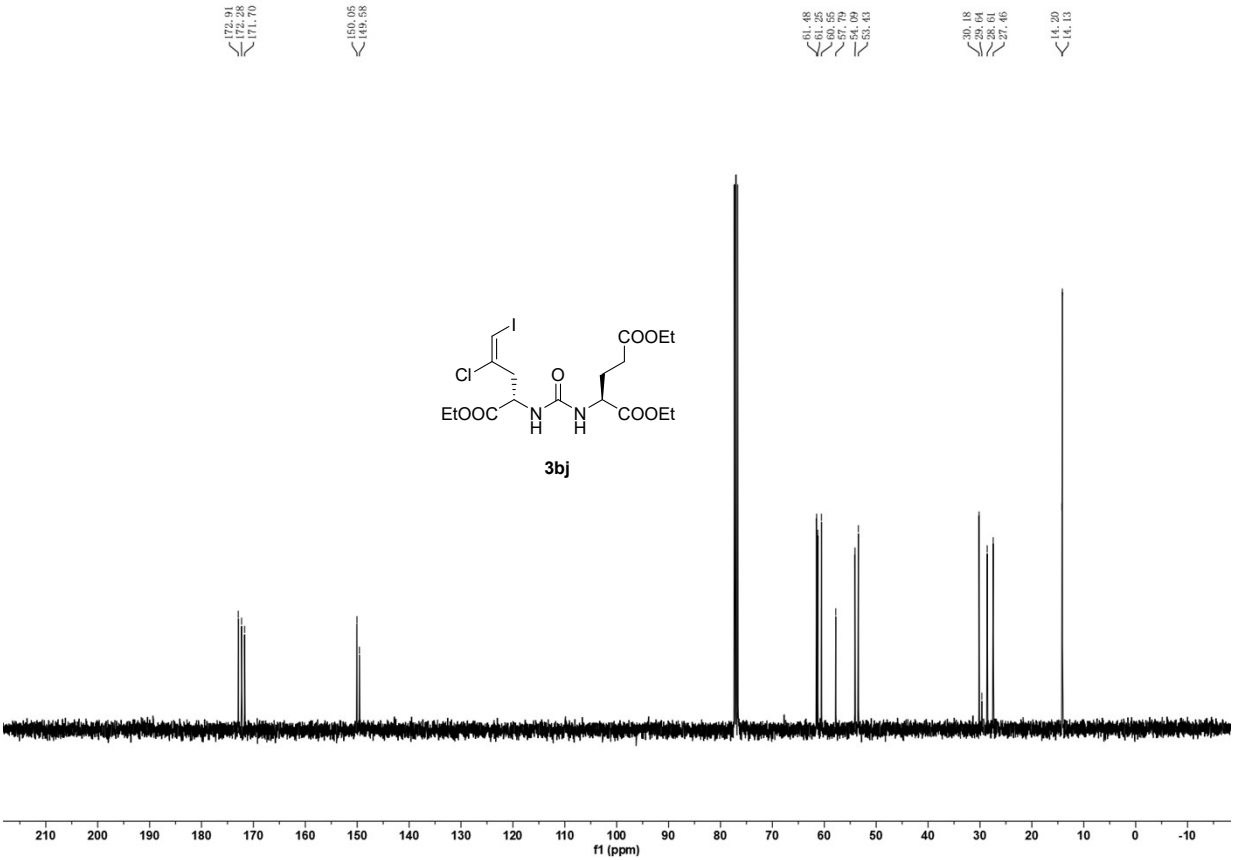

145.04
143.15
136.06
129.57
128.84
99.21
34.87
21.70
O
S
O
I
Cl
f1 (ppm)

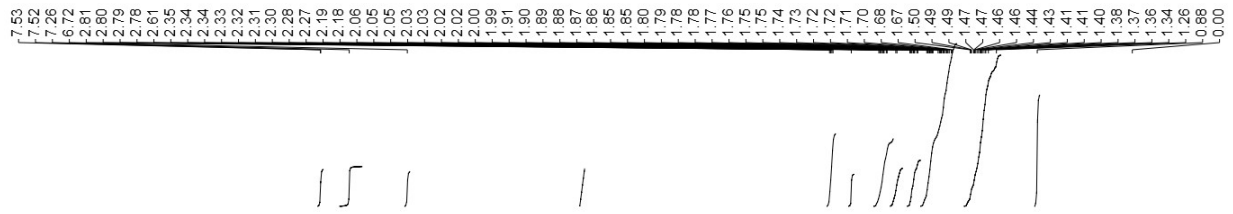
3bi

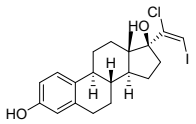


3bj

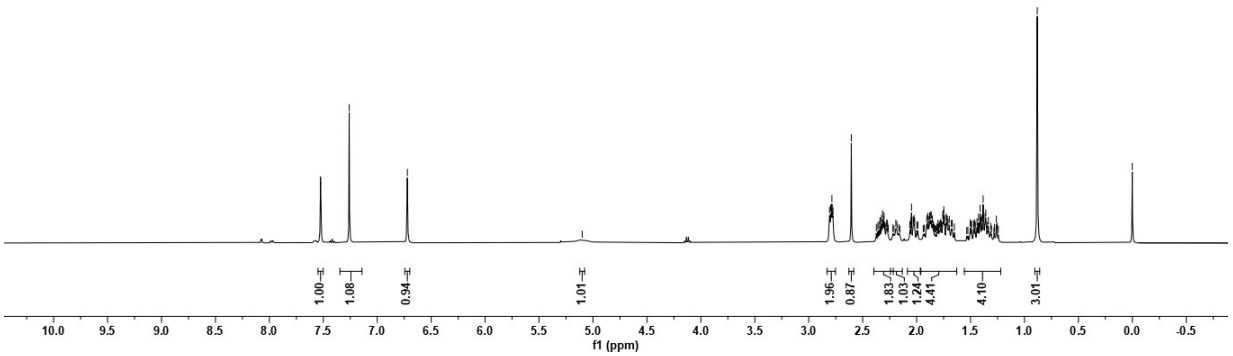


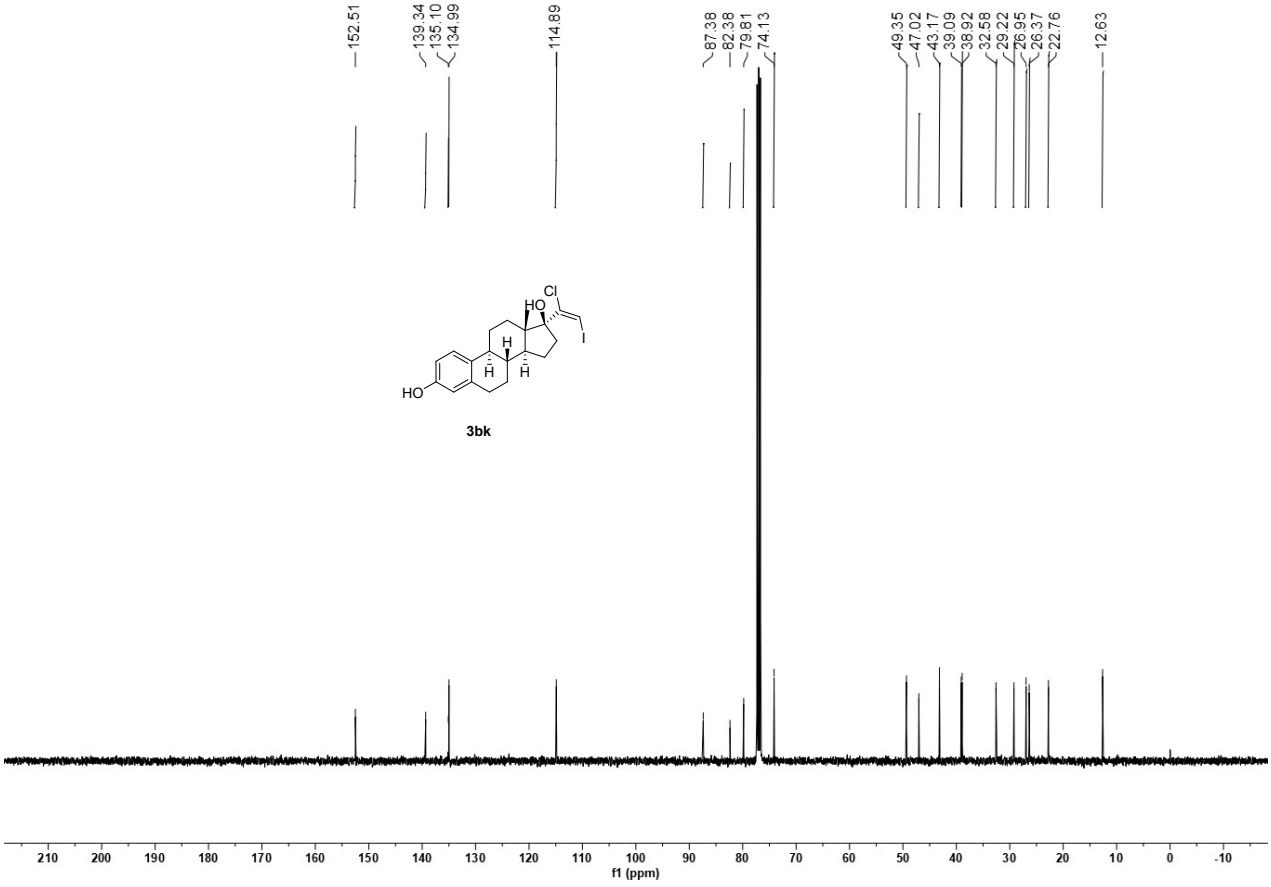



7.53
7.52
7.26
6.72
2.81
2.80
2.79
2.78
2.61
2.35
2.34
2.34
2.33
2.32
2.31
2.30
2.28
2.27
2.19
2.18
2.06
2.05
2.05
2.03
2.03
2.02
2.02
2.00
1.99
1.91
1.90
1.89
1.88
1.87
1.86
1.85
1.85
1.80
1.79
1.78
1.78
1.77
1.76
1.75
1.75
1.74
1.73
1.72
1.72
1.71
1.70
1.68
1.67
1.50
1.49
1.49
1.47
1.47
1.46
1.46
1.44
1.43
1.41
1.41
1.40
1.38
1.37
1.36
1.34
1.26
0.88
0.00

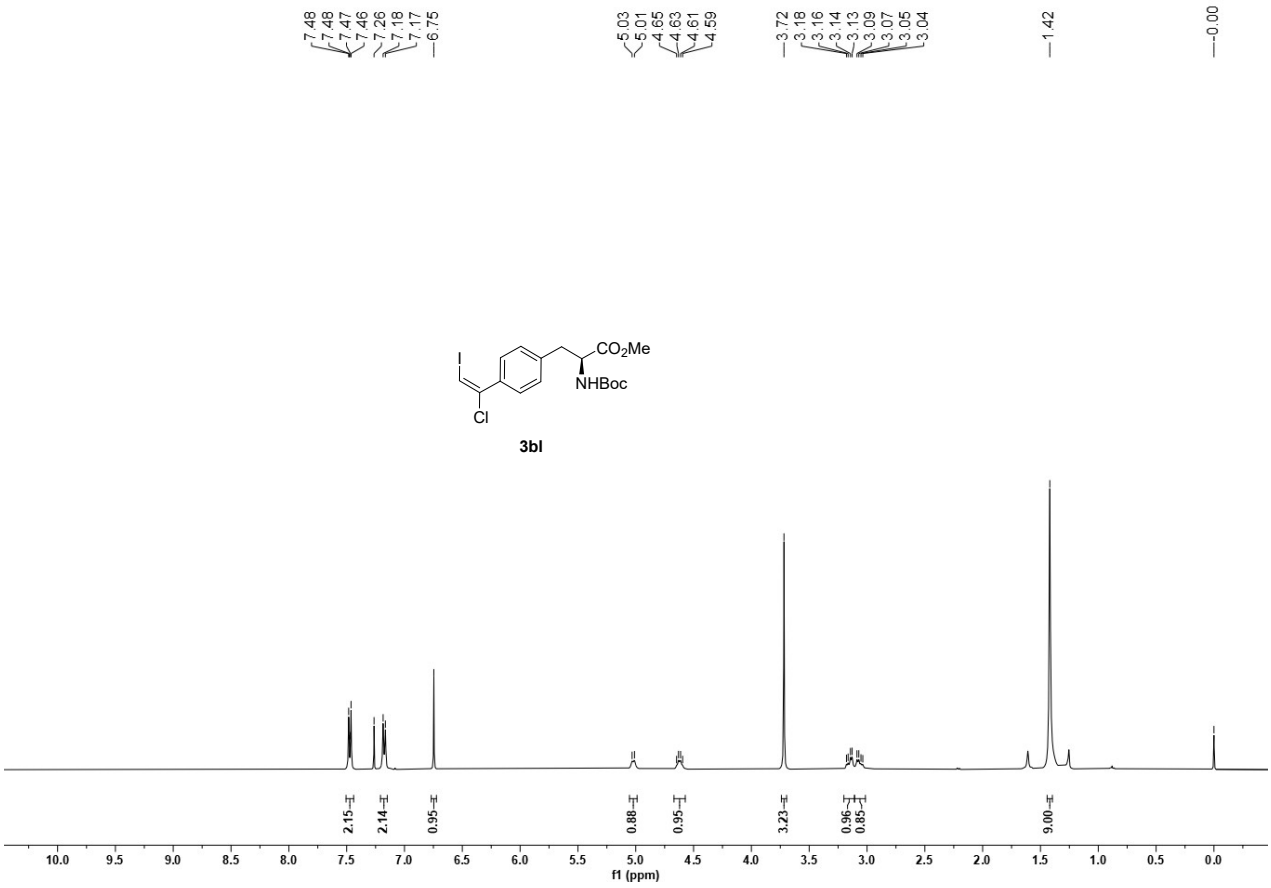

Cl
HO
I
H
H
HO

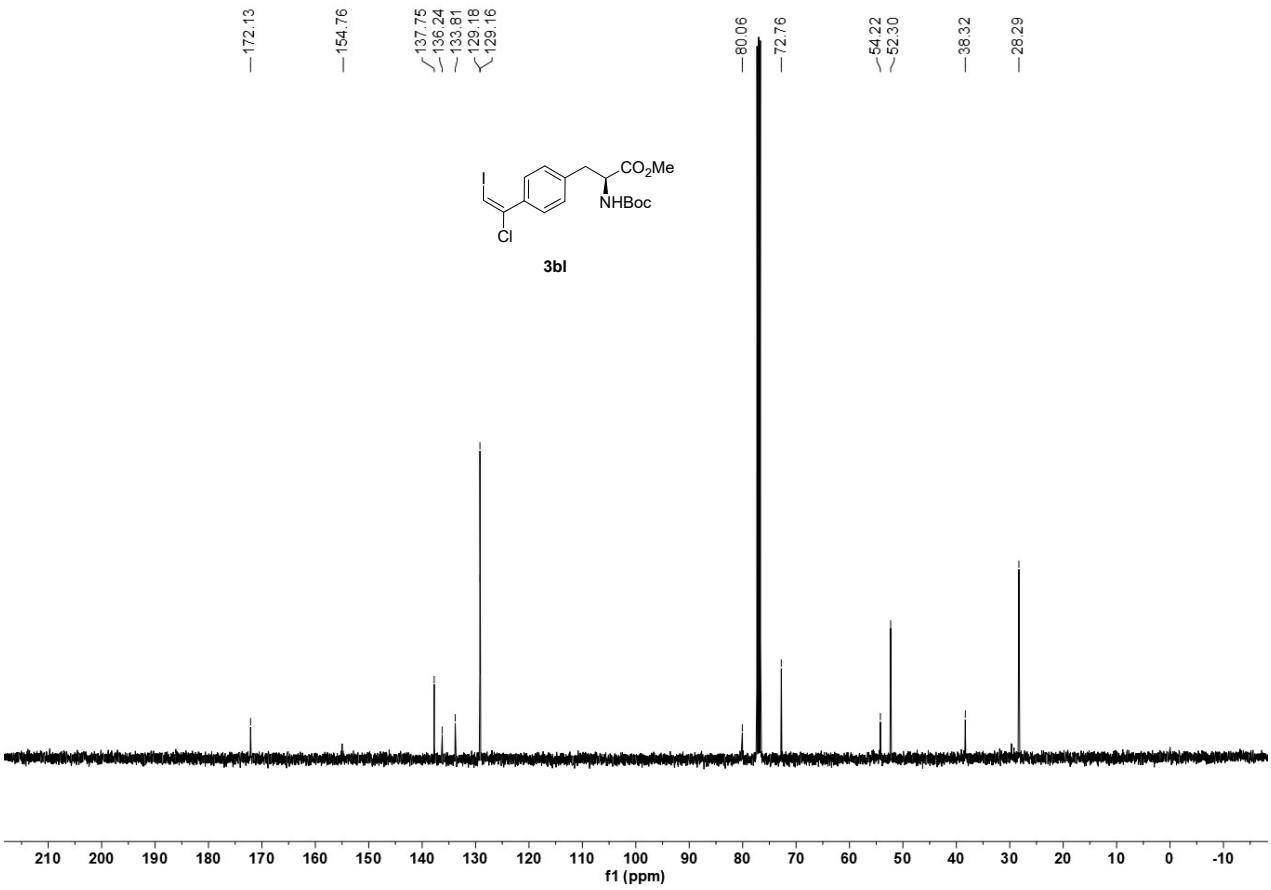
3bk

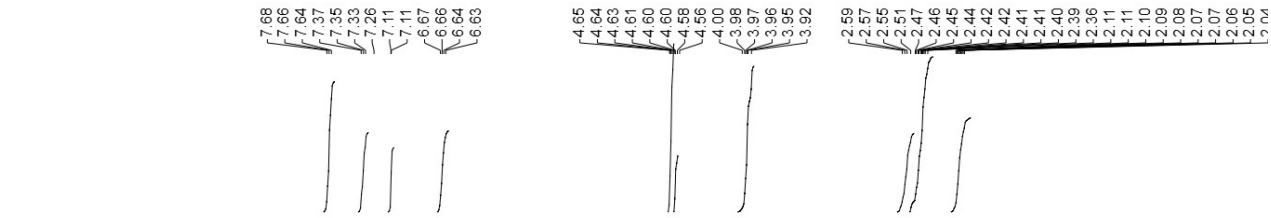

1.00
1.08
0.94
1.01
1.96
0.87
1.83
1.03
1.24
4.41
4.10
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

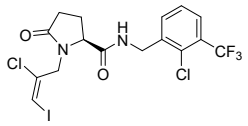

152.51
139.34
135.10
134.99
114.89
87.38
82.38
79.81
74.13
49.35
47.02
43.17
39.09
38.92
32.58
29.22
26.95
26.37
22.76
12.63
Cl
HO
I
H
H
HO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3bk

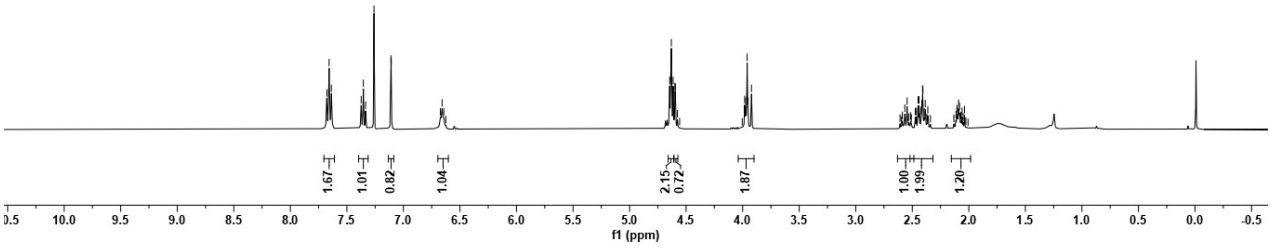

7.48
7.48
7.47
7.46
7.26
7.18
7.17
6.75
5.03
5.01
4.65
4.63
4.61
4.59
3.72
3.18
3.16
3.14
3.13
3.09
3.07
3.05
3.04
1.42
0.00
CO2Me
NHBoc
I
Cl
3bl
2.15
2.14
0.95
0.88
0.95
3.23
0.96
0.85
9.00
f1 (ppm)

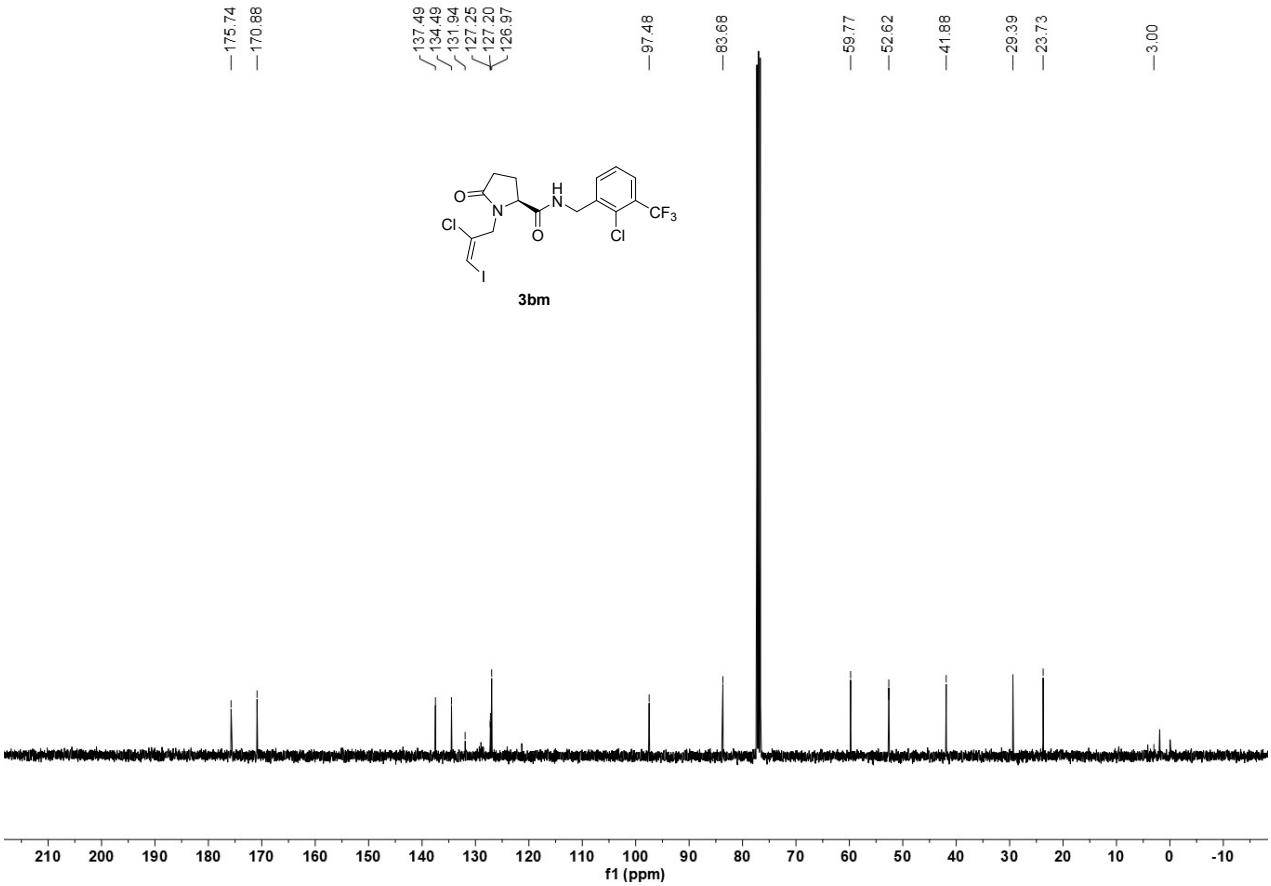

172.13
154.76
137.75
136.24
133.81
129.18
129.16
80.06
72.76
54.22
52.30
38.32
28.29
CO2Me
NHBoc
I
Cl
3bl
f1 (ppm)


7.68
7.66
7.64
7.37
7.35
7.33
7.26
7.11
7.11
6.67
6.66
6.64
6.63
4.65
4.64
4.63
4.61
4.60
4.60
4.58
4.56
4.00
3.98
3.97
3.96
3.95
3.92
2.59
2.57
2.55
2.51
2.47
2.46
2.45
2.44
2.42
2.42
2.41
2.41
2.40
2.39
2.36
2.11
2.11
2.10
2.09
2.08
2.07
2.07
2.06
2.05

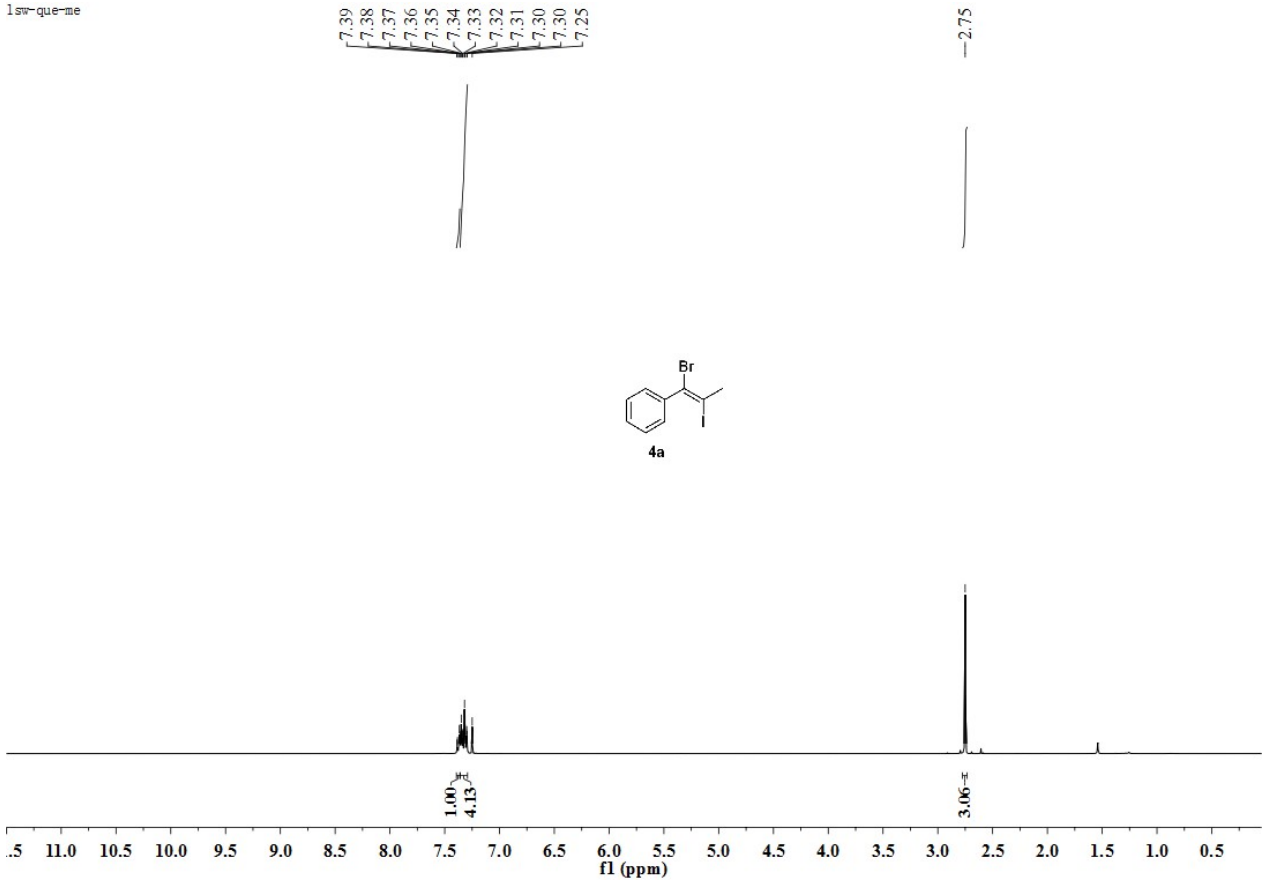


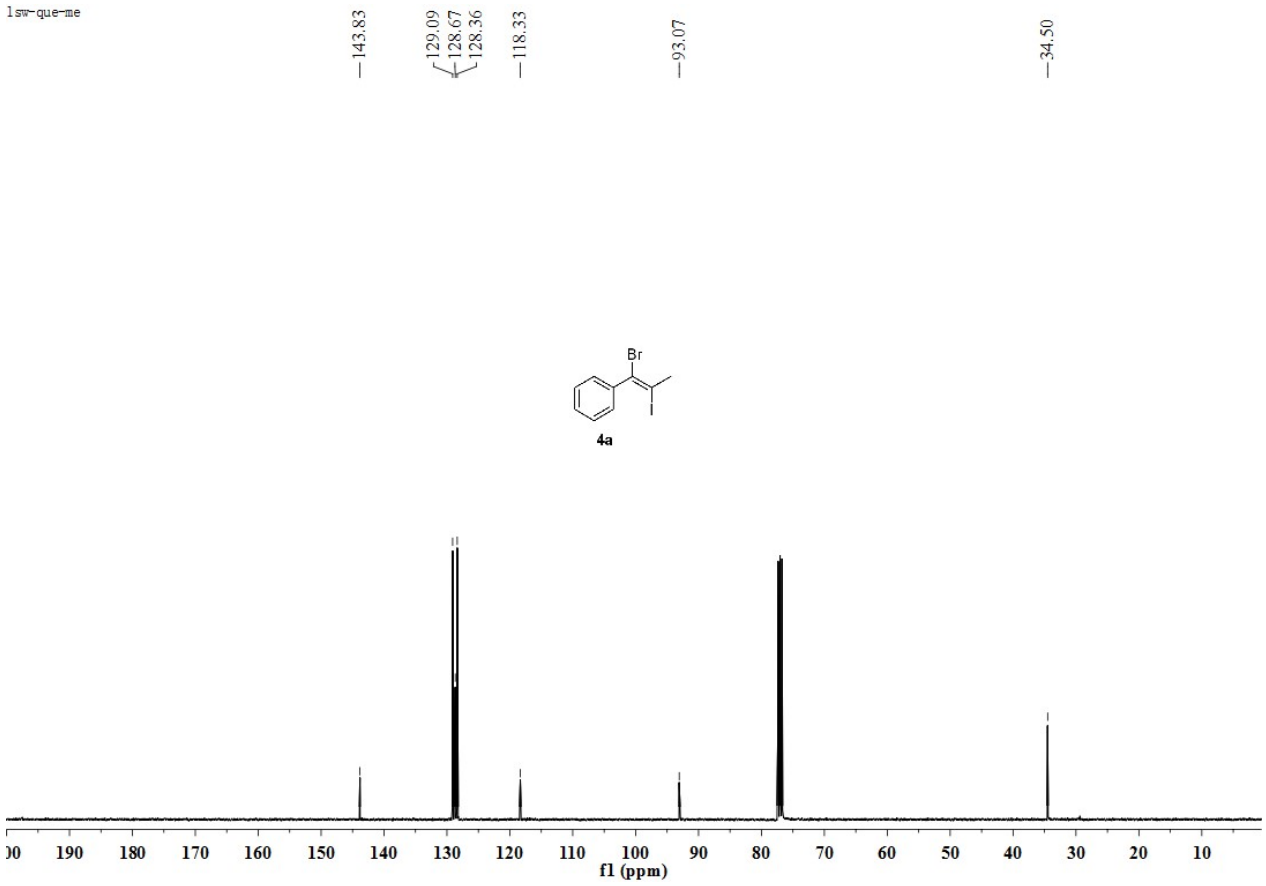
3bm

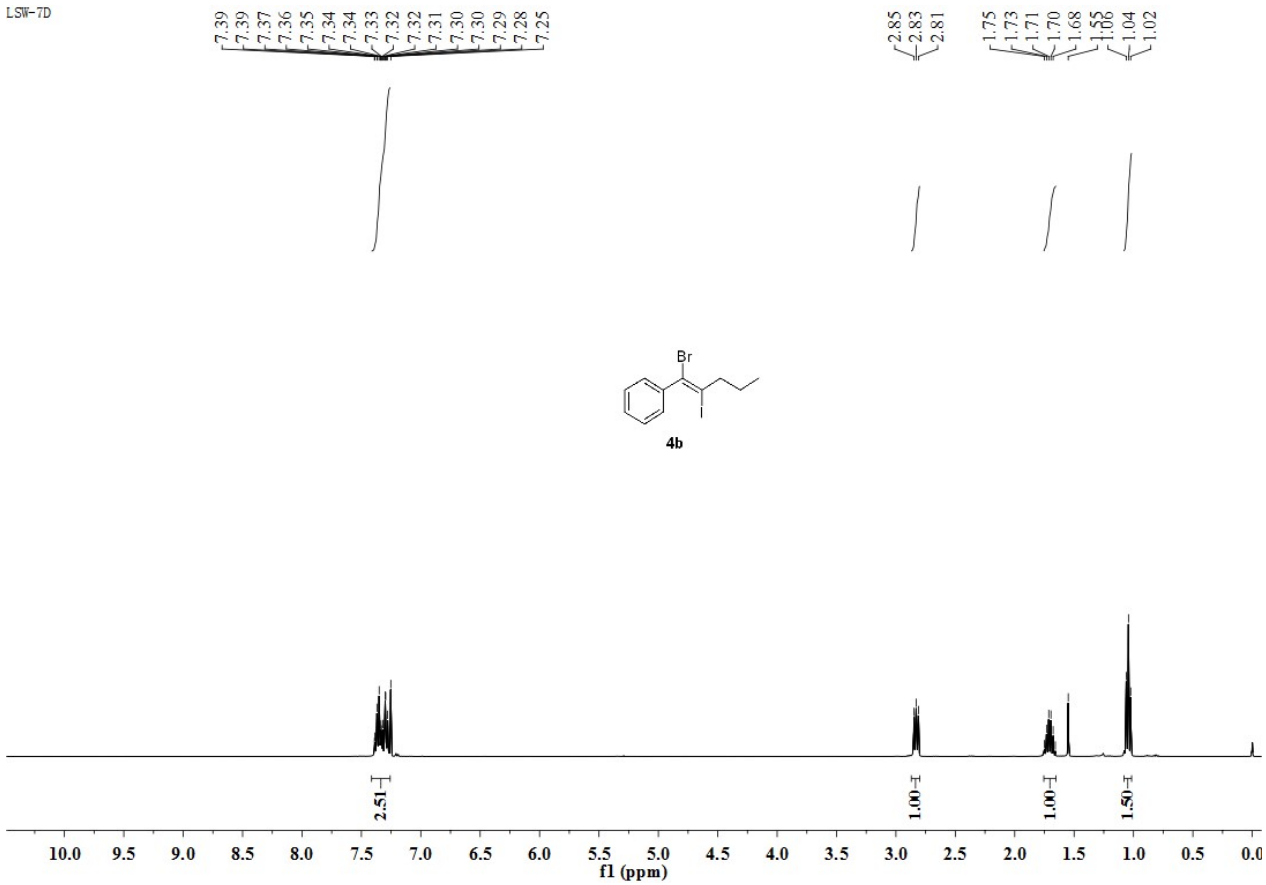

1.67
1.01
0.82
1.04
2.15
0.72
1.87
1.00
1.99
1.20
f1 (ppm)


175.74
170.88
137.49
134.49
131.94
127.25
127.20
126.97
97.48
83.68
59.77
52.62
41.88
29.39
23.73
3.00
f1 (ppm)

3bm

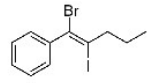

lsw-que-me
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.30
7.30
7.25
2.75
Br
4a
1.00
4.13
3.06
f1 (ppm)


lsw-que-me
143.83
129.09
128.67
128.36
118.33
93.07
34.50
Br
4a
f1 (ppm)

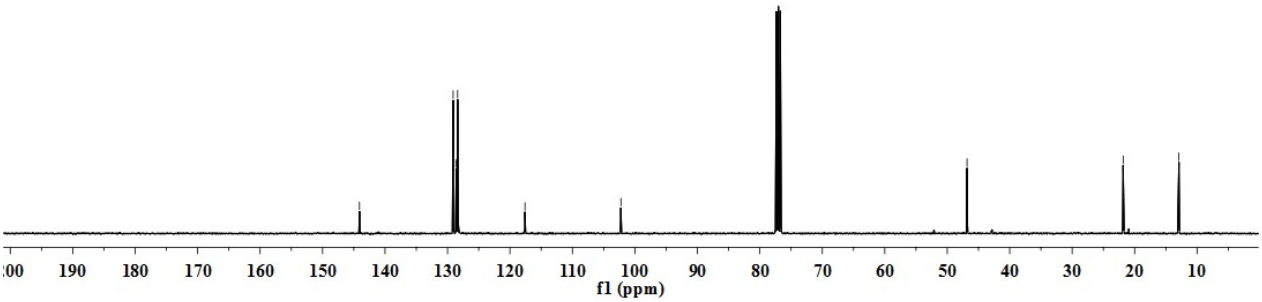

LSW-7D
7.39
7.39
7.37
7.36
7.35
7.34
7.34
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.28
7.25
2.85
2.83
2.81
1.75
1.73
1.71
1.70
1.68
1.55
1.04
1.02
Br
4b
2.51
1.00
1.00
1.50
f1 (ppm)

LSW-7D

144.09
129.10
128.61
128.38
117.60
102.24
46.83
21.83
12.91

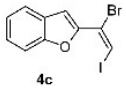


4b

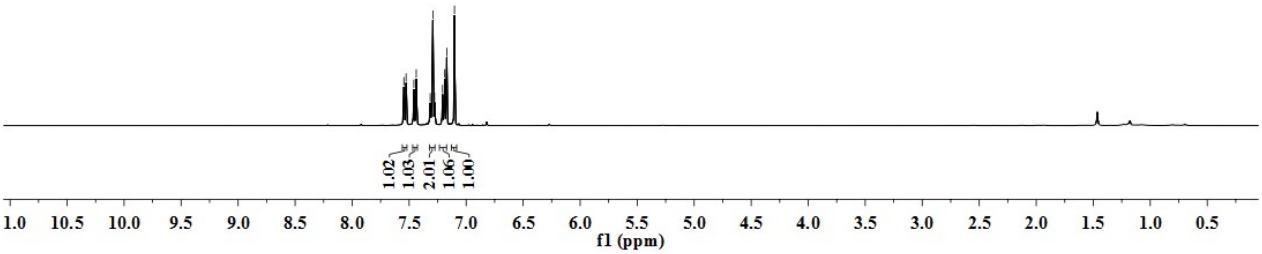


lsw-funan-br-i

7.55
7.53
7.46
7.44
7.32
7.29
7.28
7.21
7.19
7.17
7.10

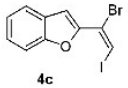


4c

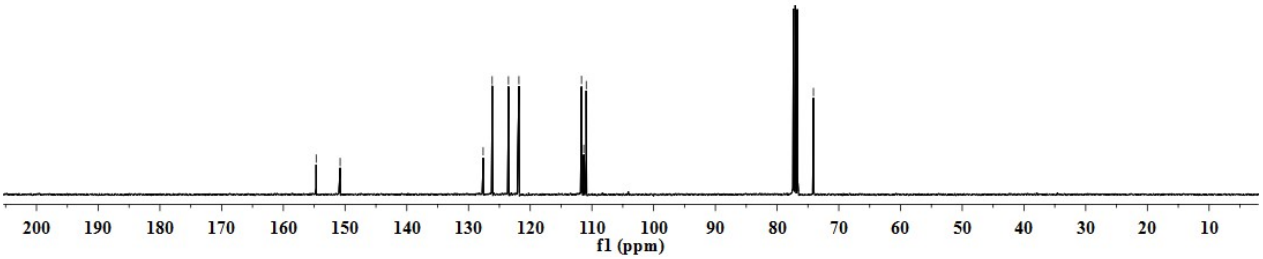


lsw-funan-br-i

154.68
150.80
127.63
126.16
123.52
121.83
111.69
111.32
110.92
74.11

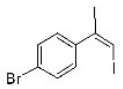


4c

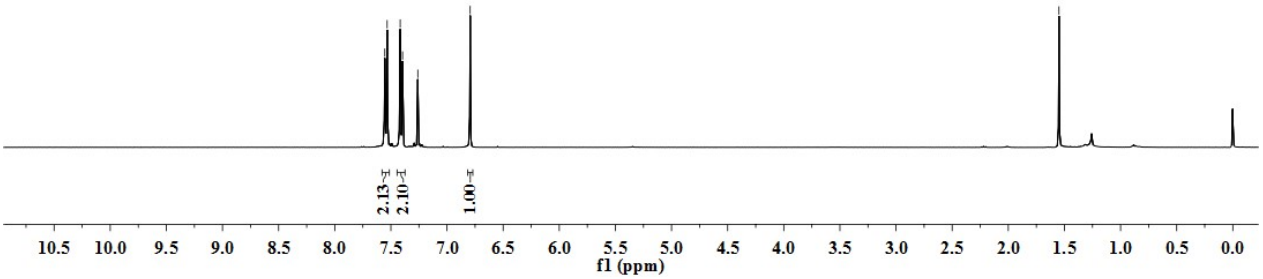


LSW-4BR-I-I

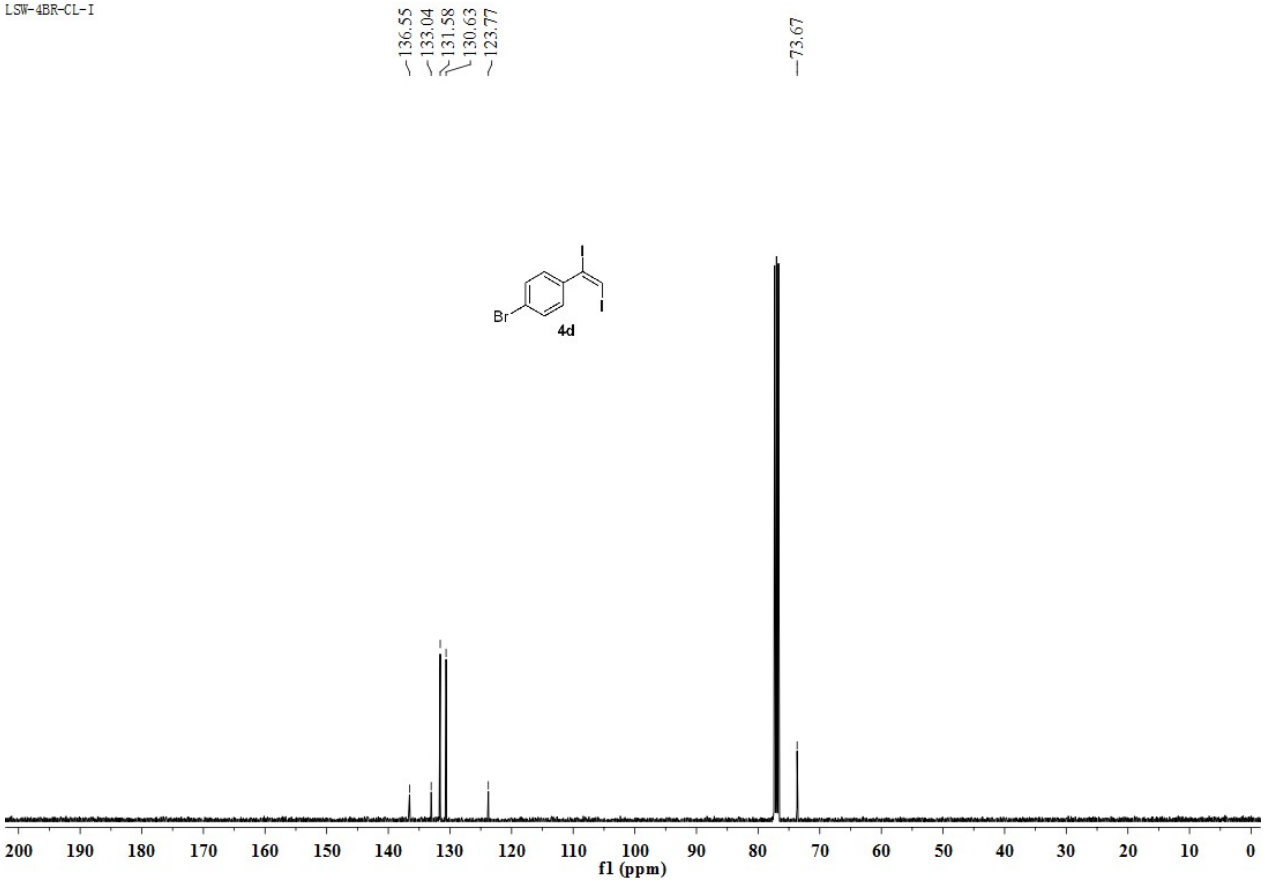
7.55
7.53
7.42
7.40
7.26
6.79
1.55



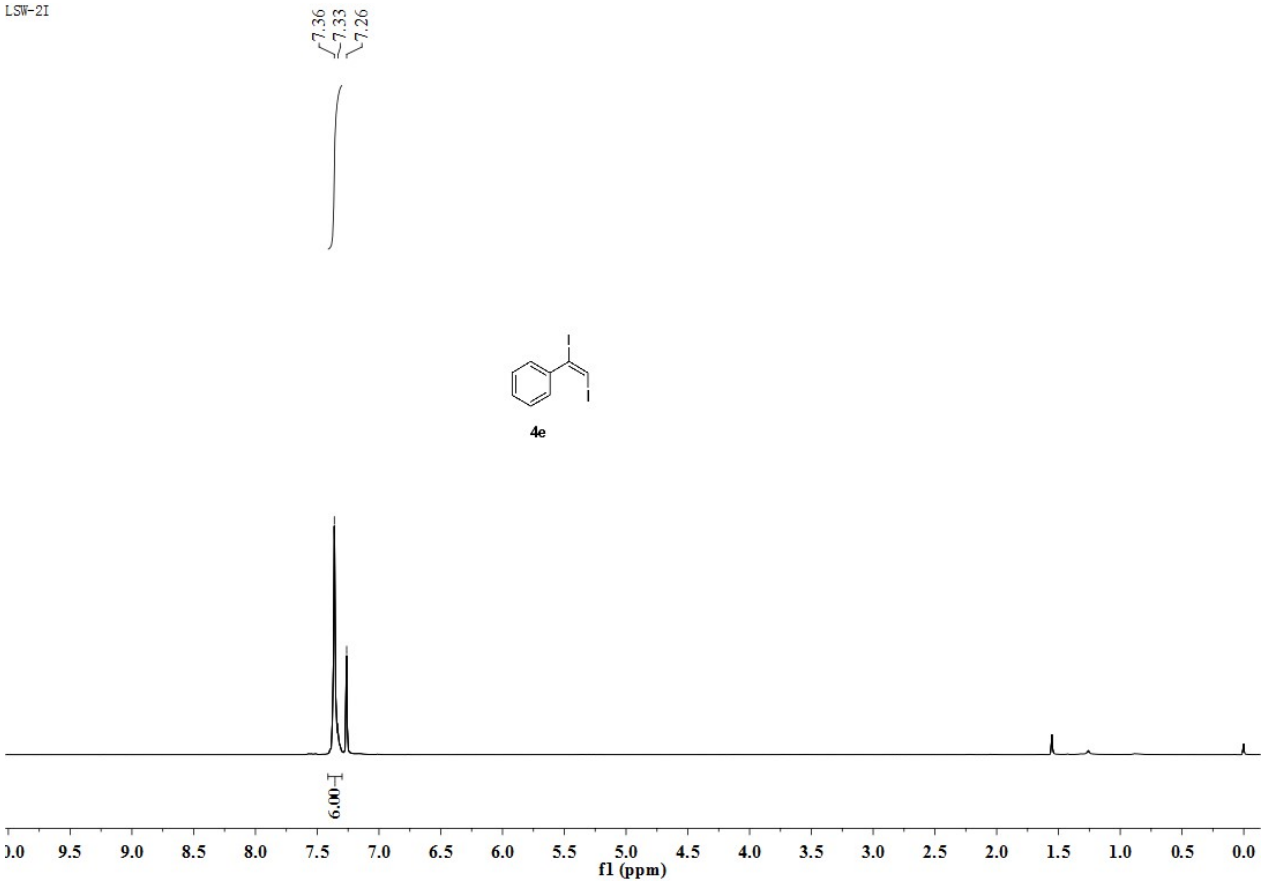
4d



LSW-4BR-CL-I

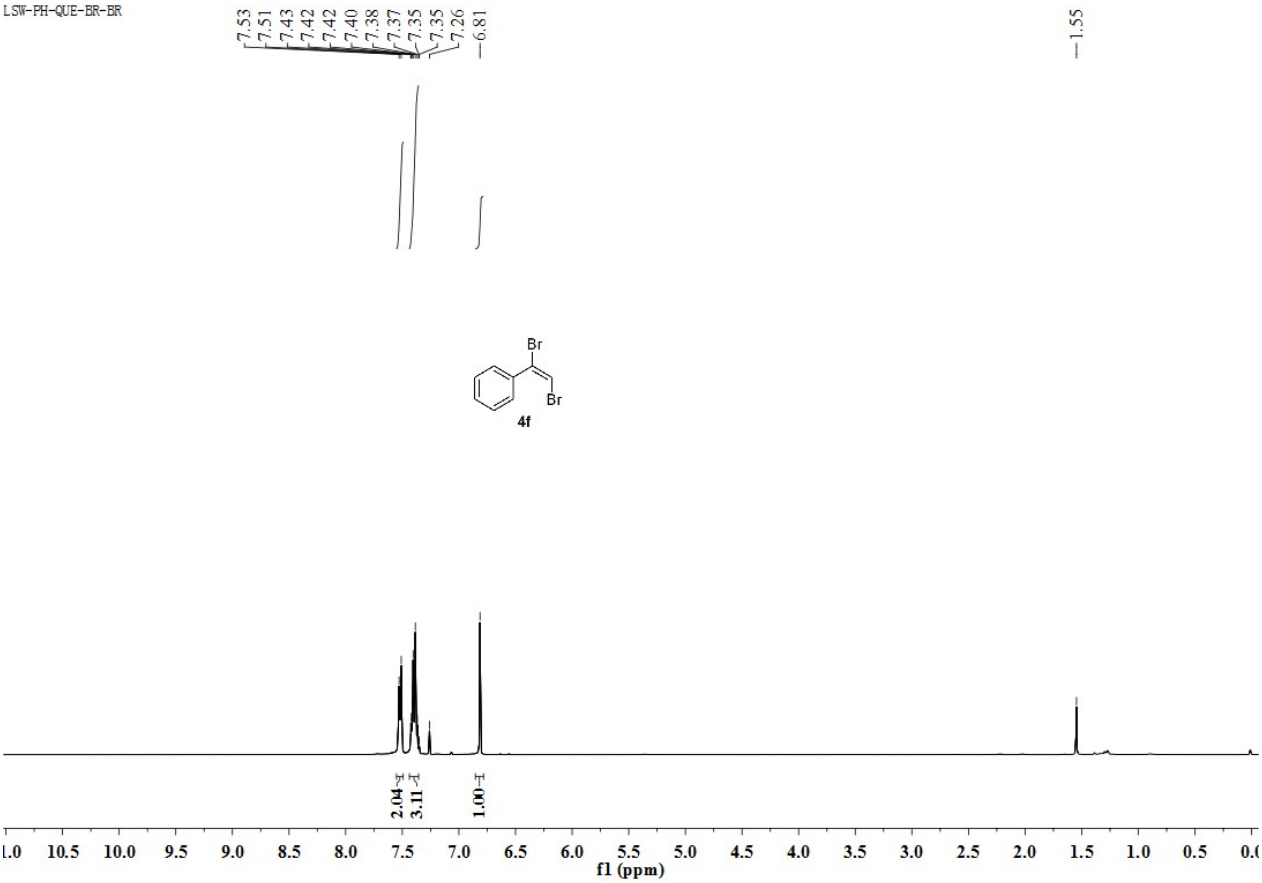


LSW-2I

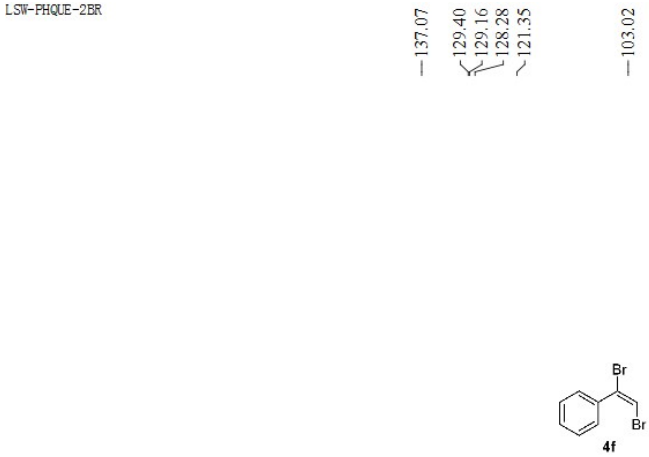


LSW-2I

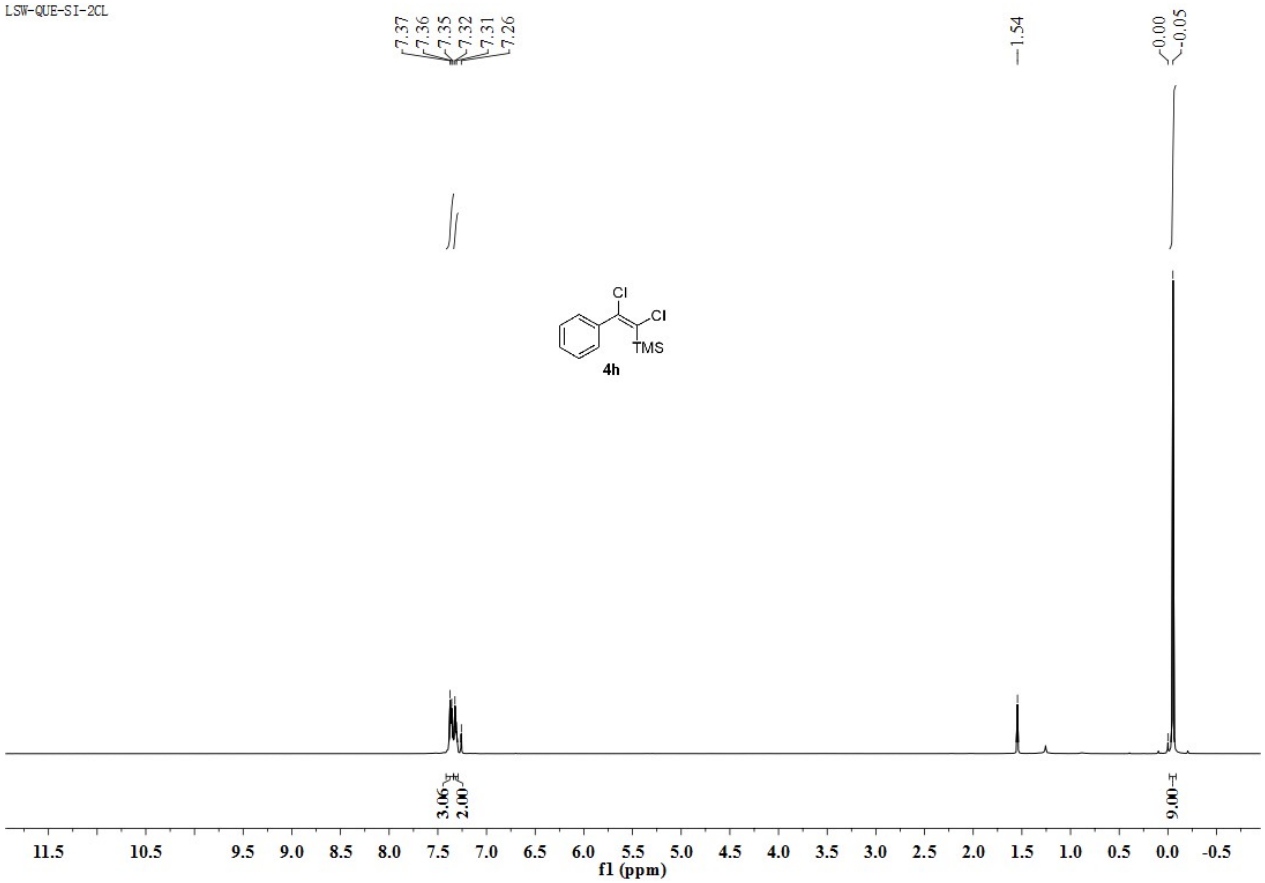
LSW-PH-QUE-BR-BR

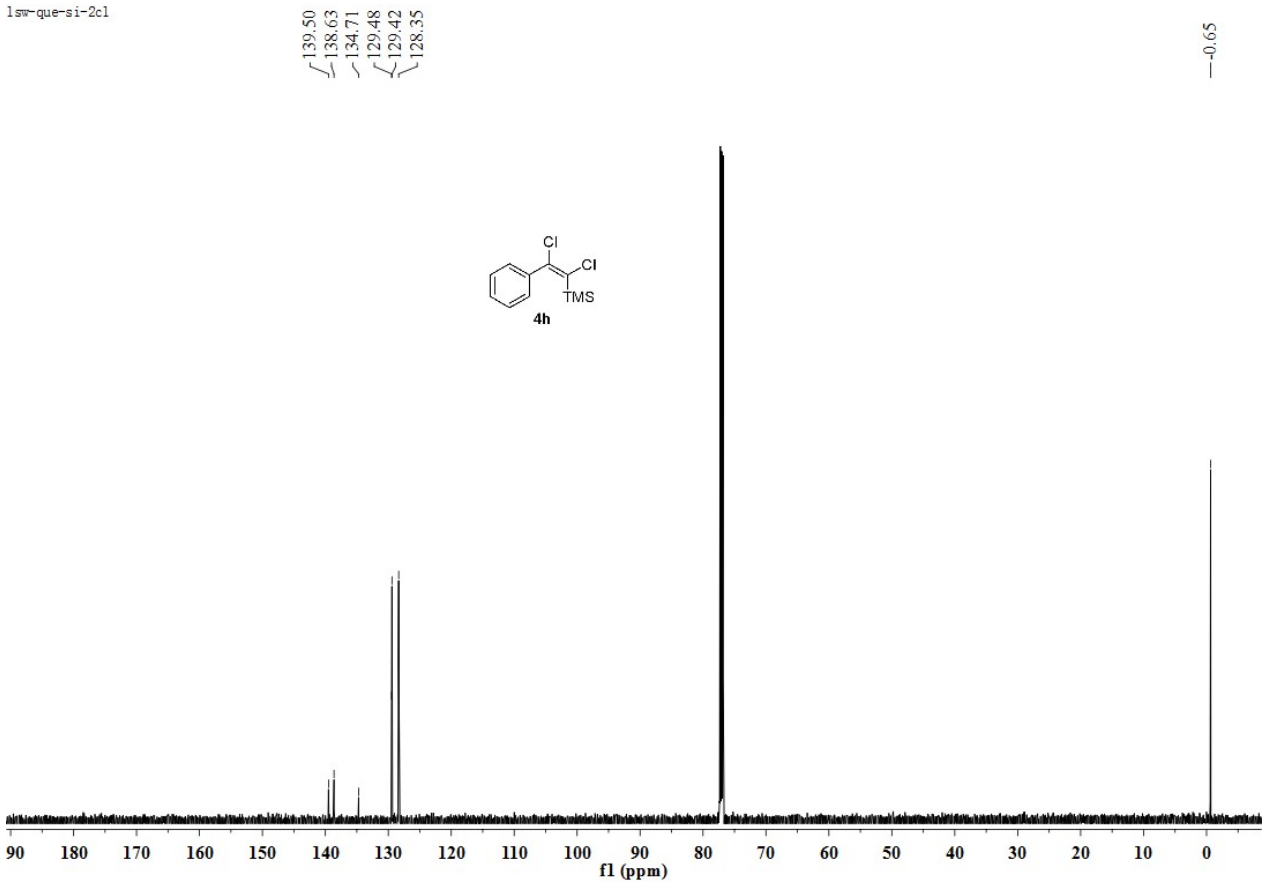


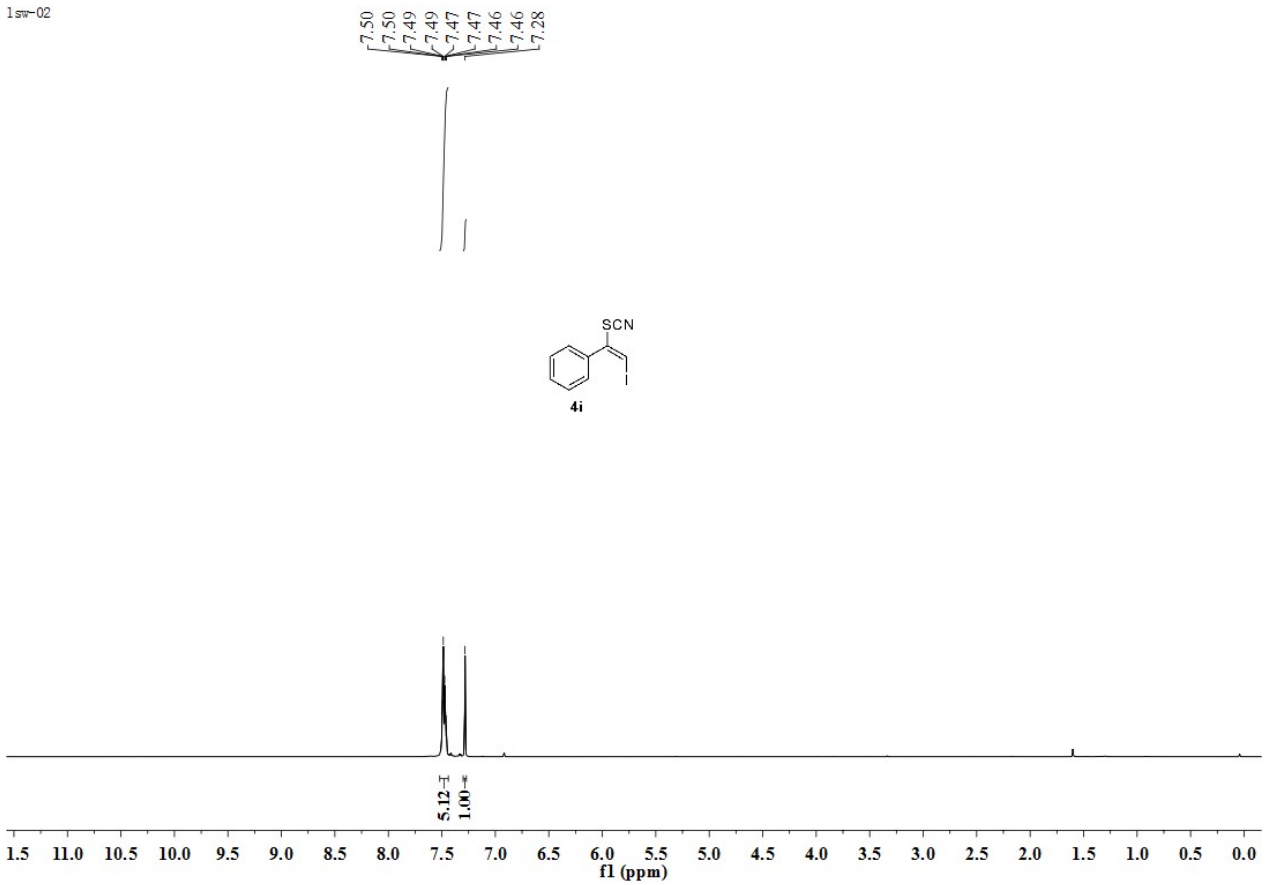
LSW-PHQUE-2BR



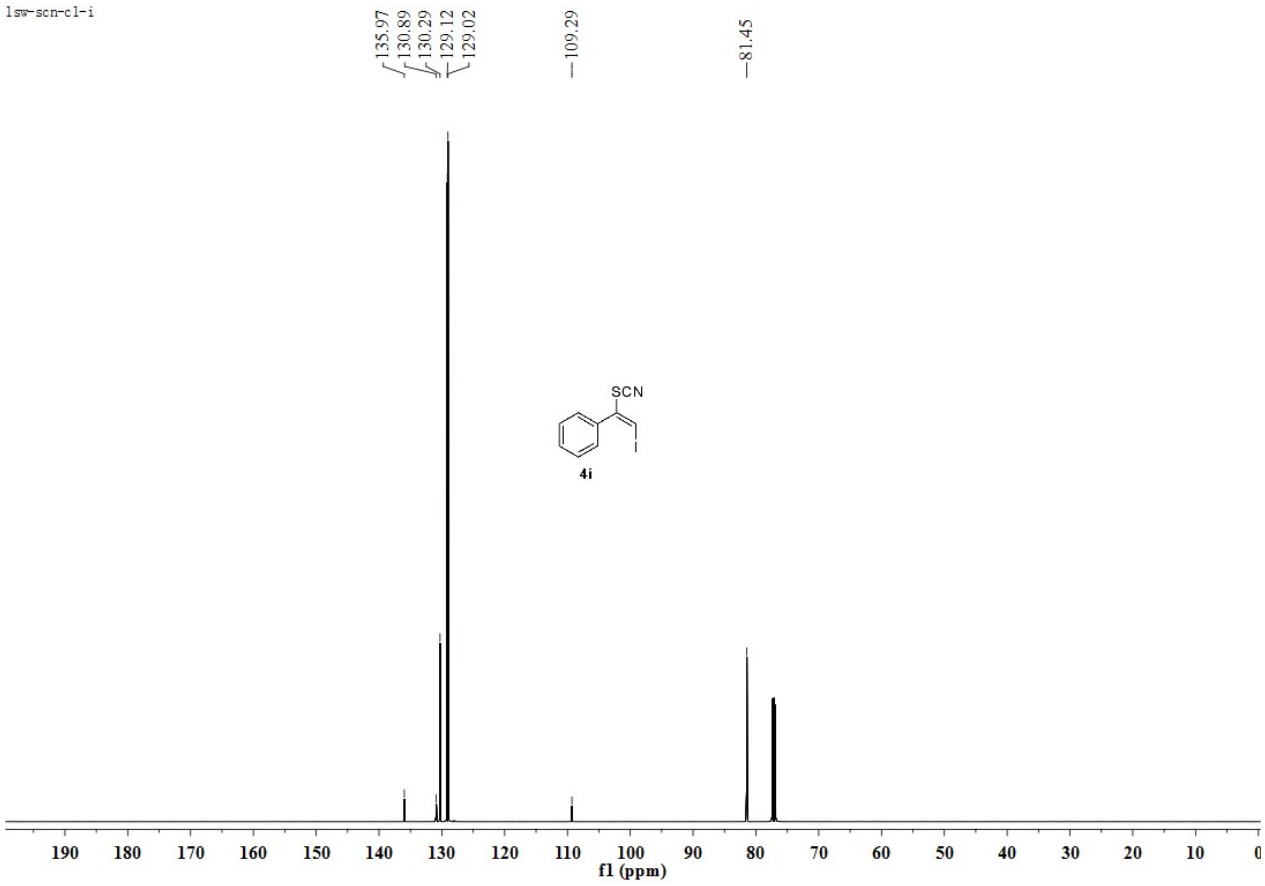
LSW-QUE-SI-2CL



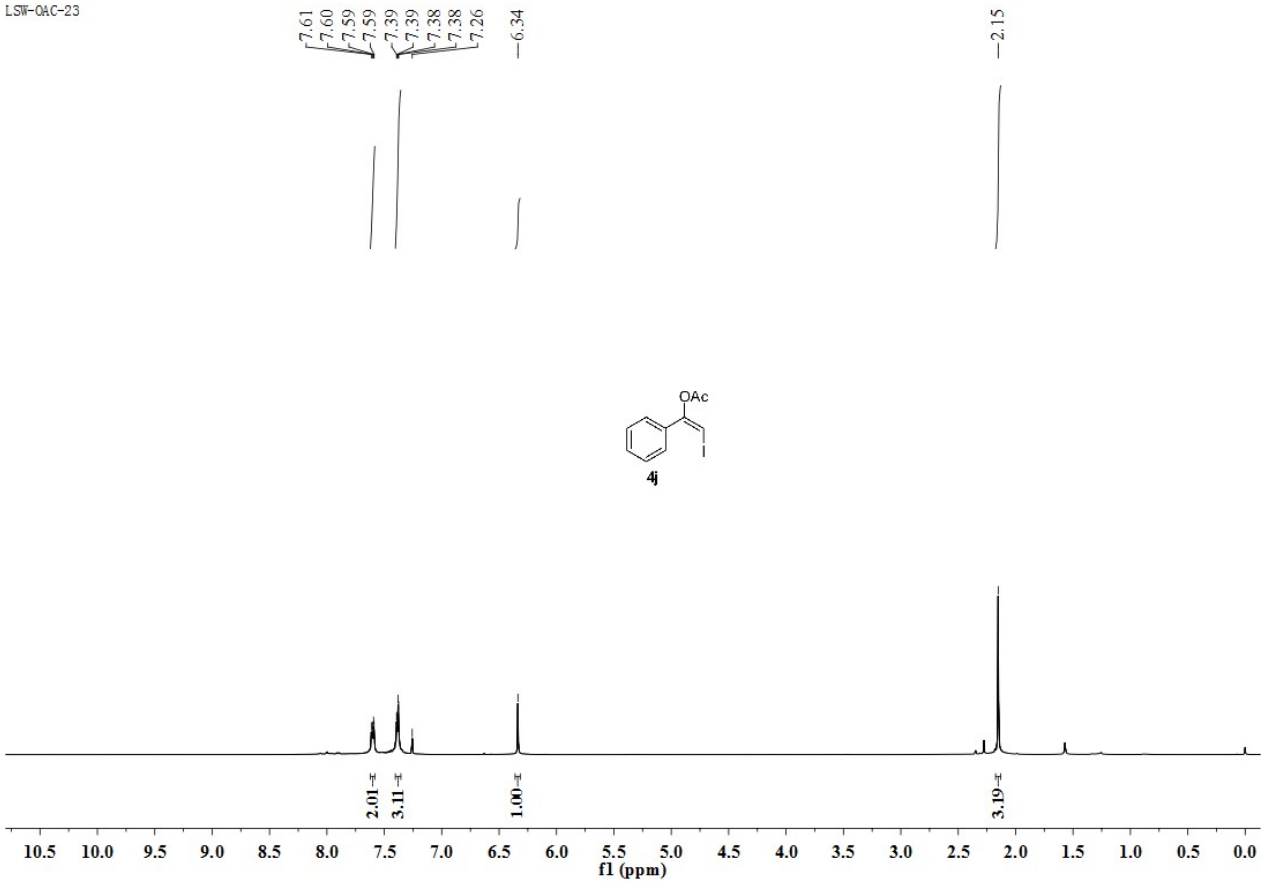

lsw-que-si-2cl
139.50
138.63
134.71
129.48
129.42
128.35
-0.65
Cl
Cl
TMS
4h
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


lsw-02
7.50
7.50
7.49
7.49
7.47
7.47
7.46
7.46
7.28
SCN
I
4i
5.12
1.00
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

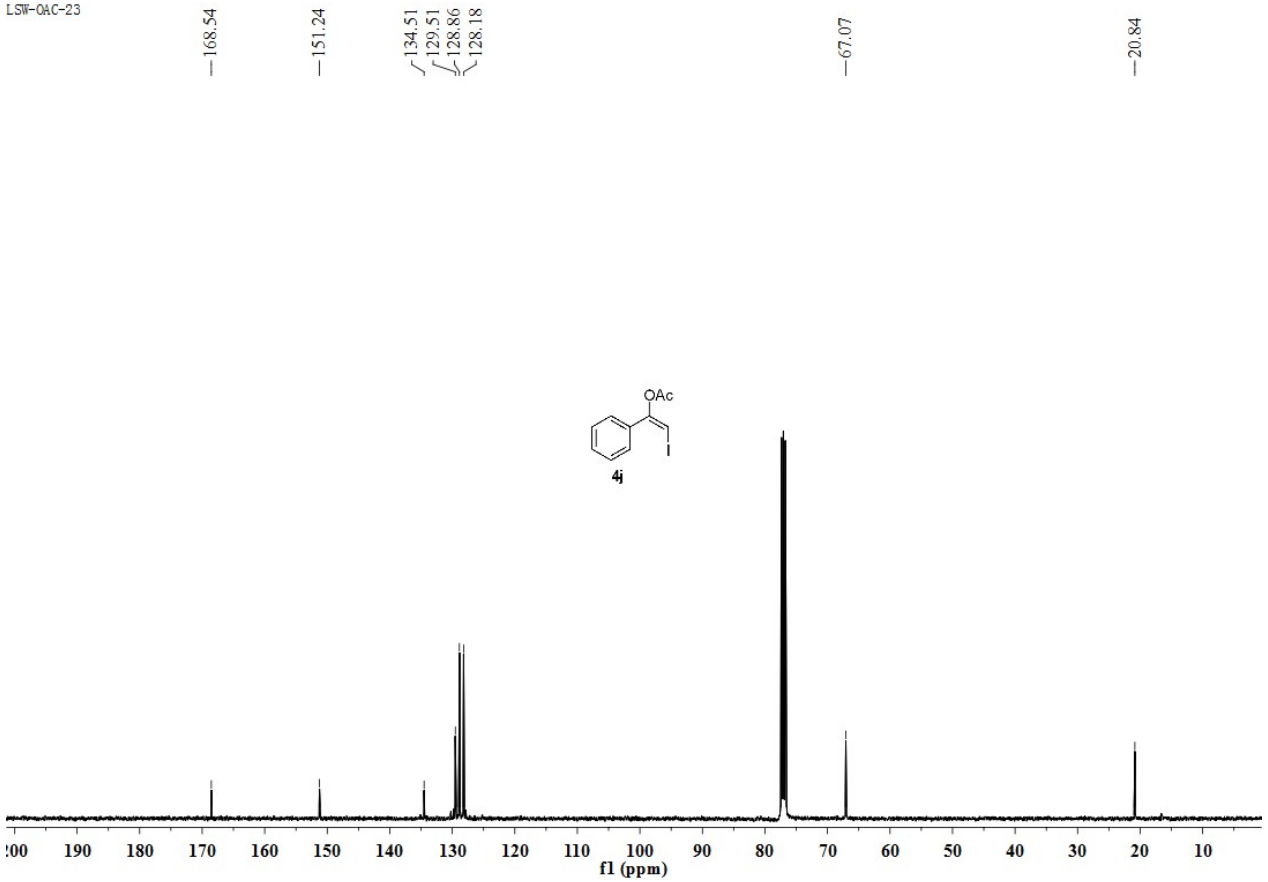
lsw-scn-cl-i



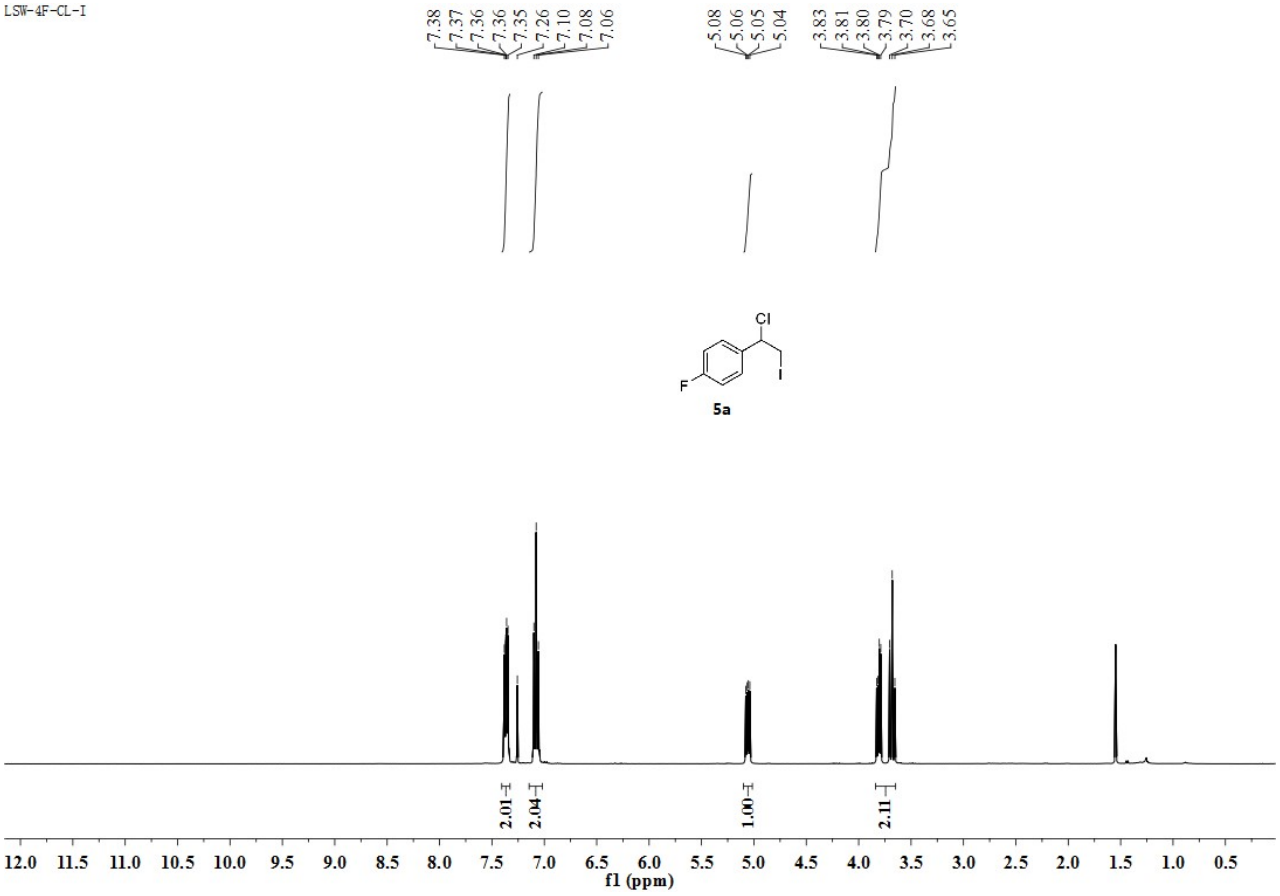
LSW-OAC-23

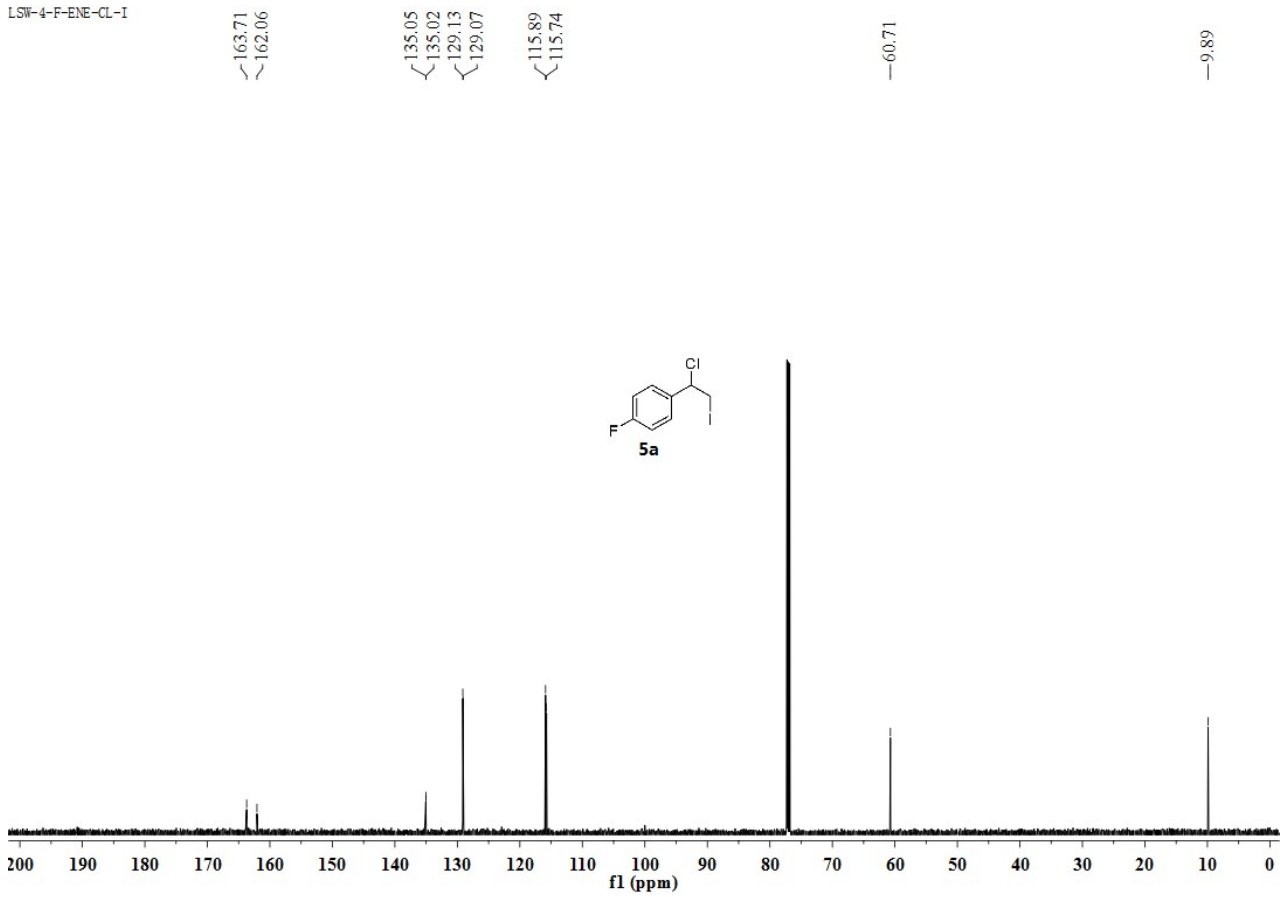


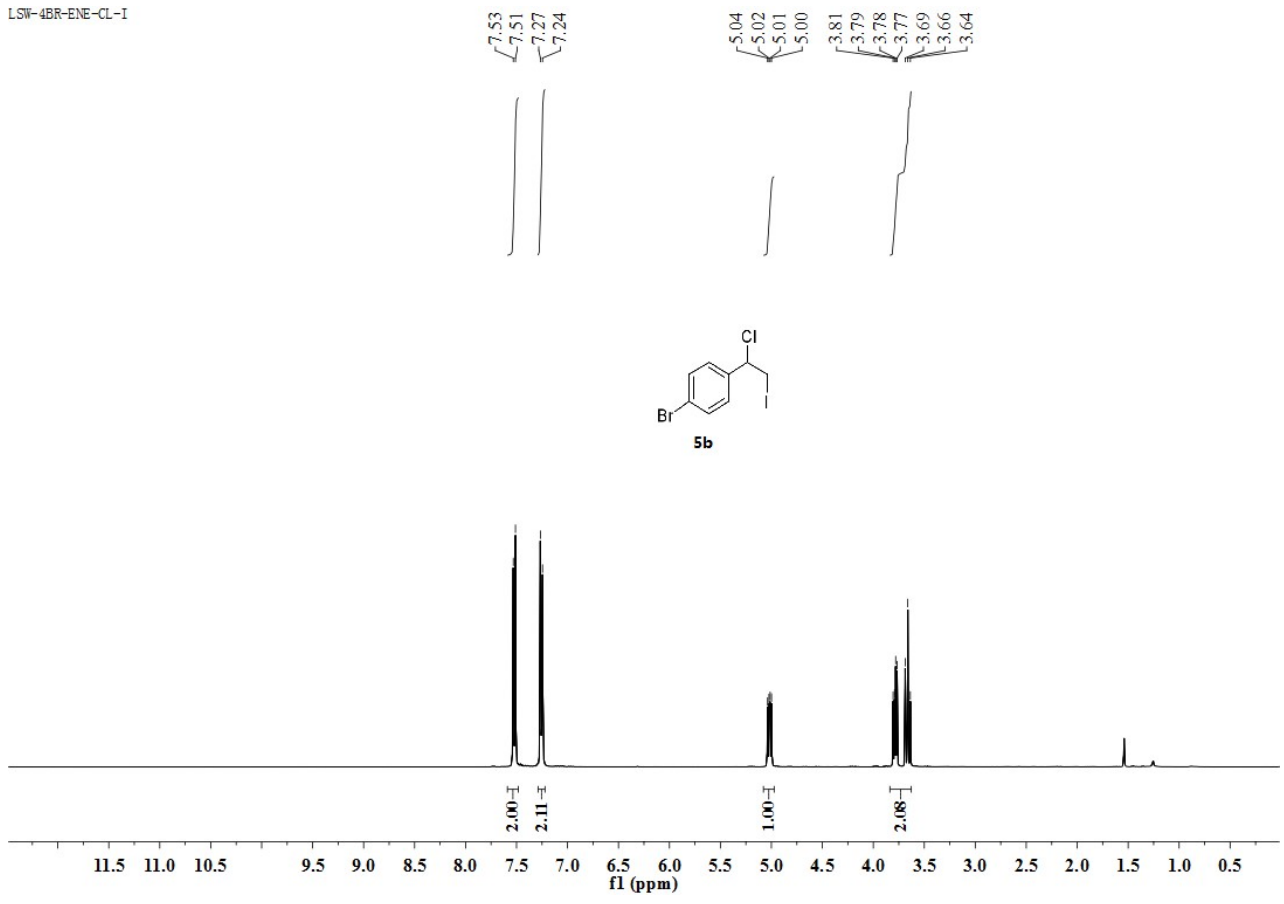
LSW-OAC-23



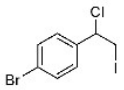
LSW-4F-CL-I



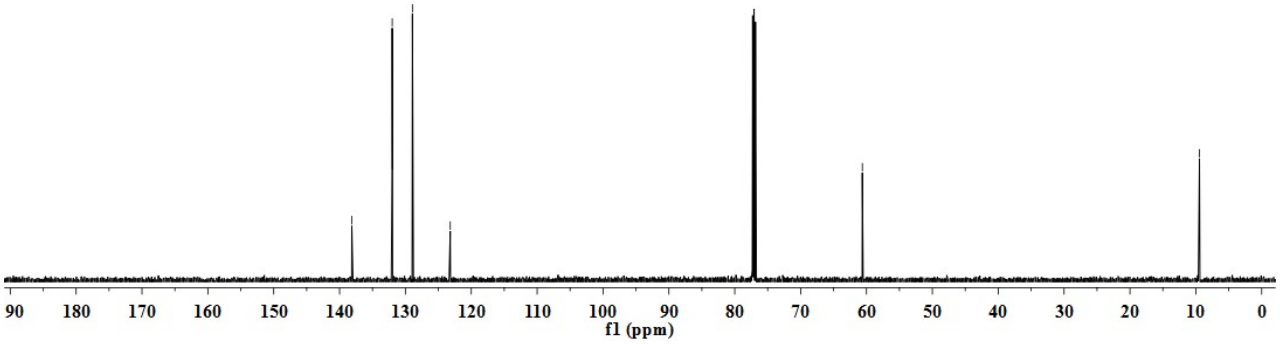

LSW-4-F-ENE-CL-I
163.71
162.06
135.05
135.02
129.13
129.07
115.89
115.74
60.71
9.89
Cl
F
I
5a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


LSW-4BR-ENE-CL-I
7.53
7.51
7.27
7.24
5.04
5.02
5.01
5.00
3.81
3.79
3.78
3.77
3.69
3.66
3.64
Cl
Br
I
5b
2.00
2.11
1.00
2.08
11.5 11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

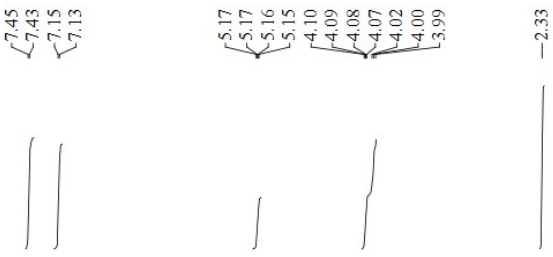
LSW-4-BR-ENE-CL-I

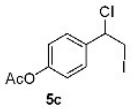


5b



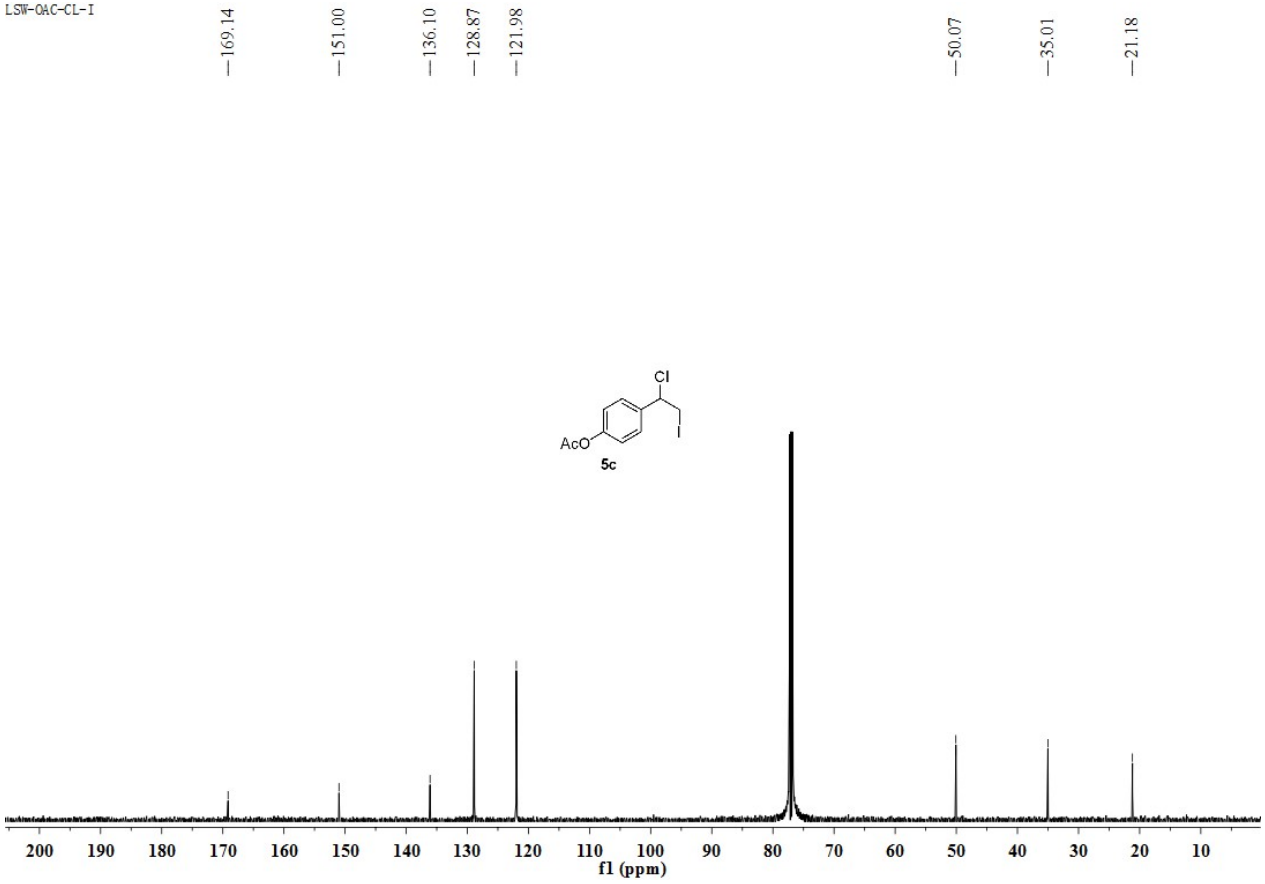
LSW-OAC-CL-I



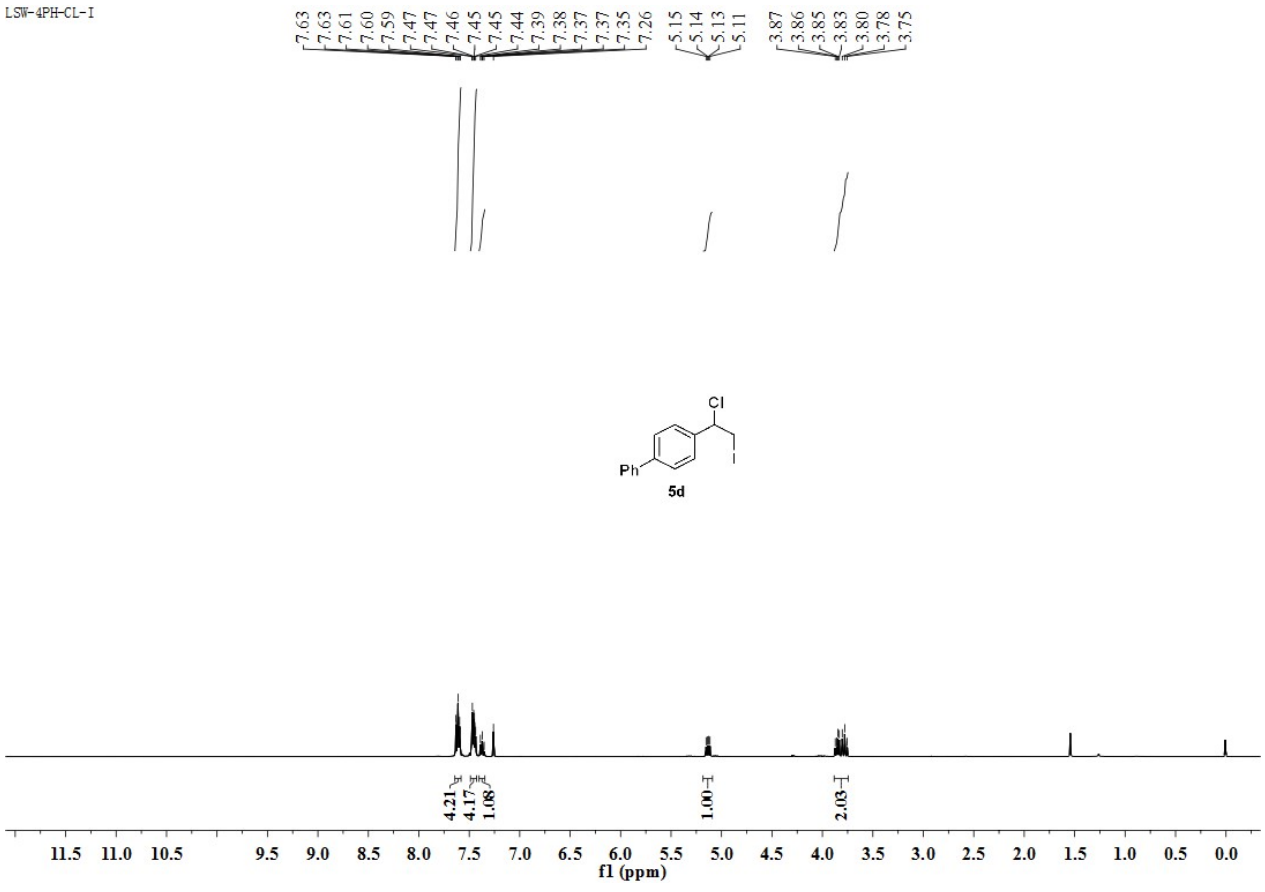


5c

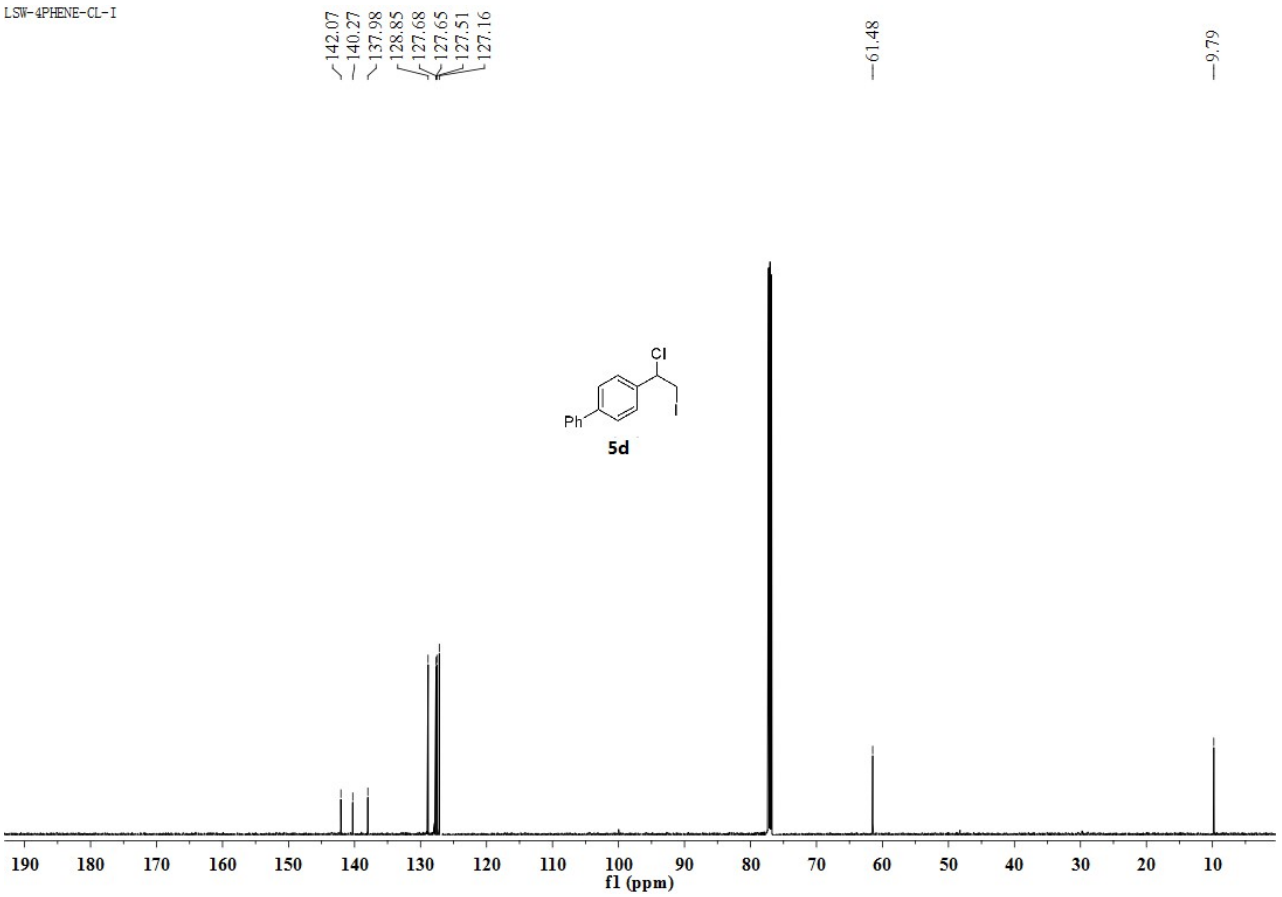
LSW-OAC-CL-I



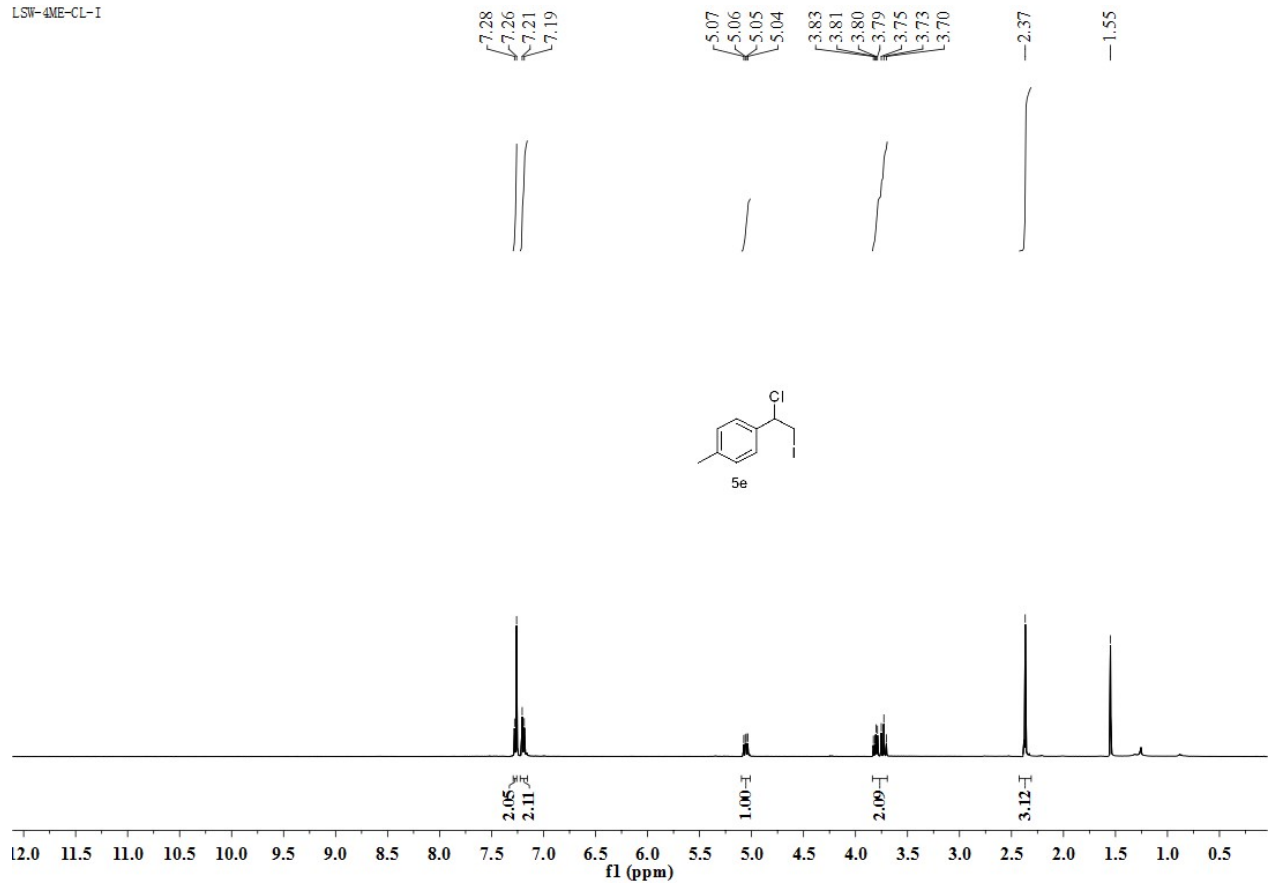
LSW-4PH-CL-I

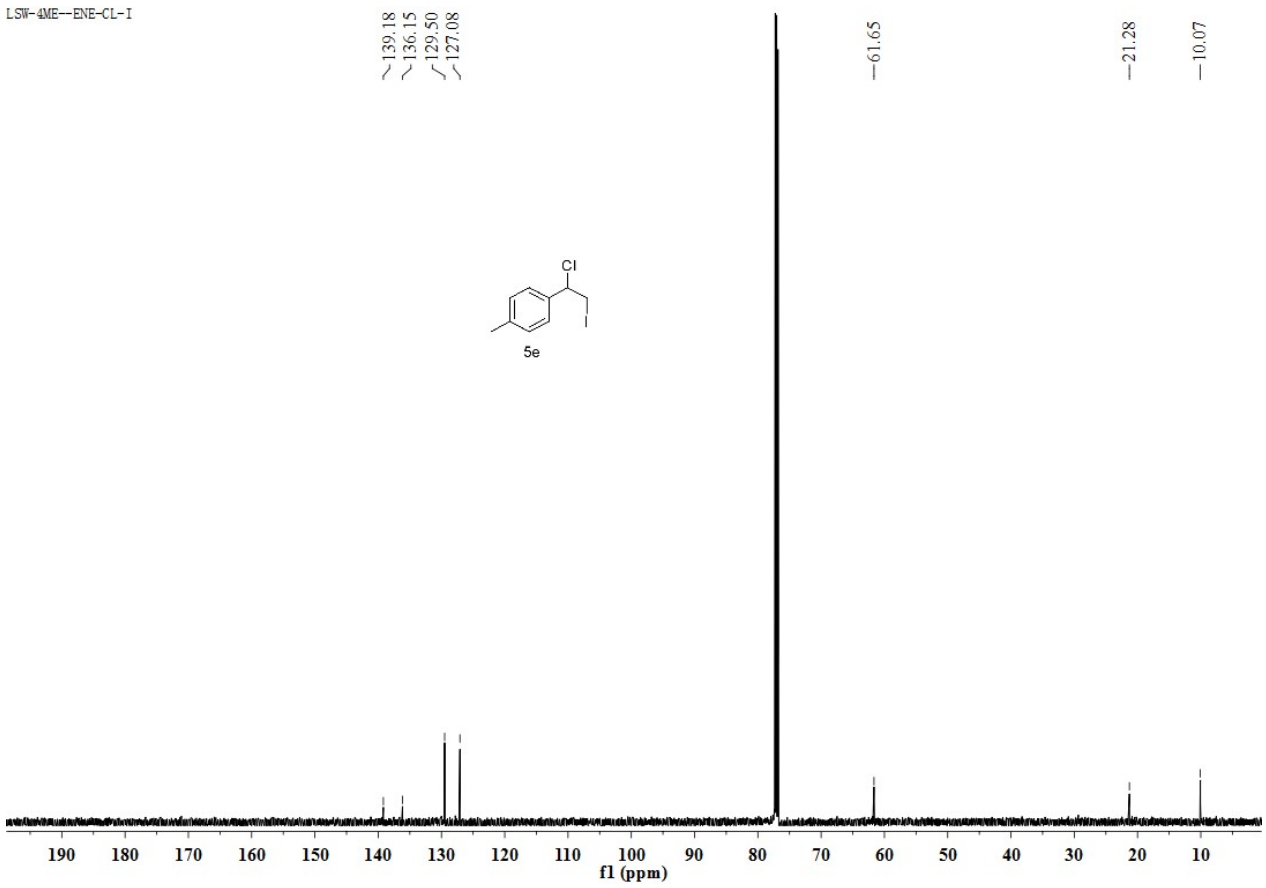


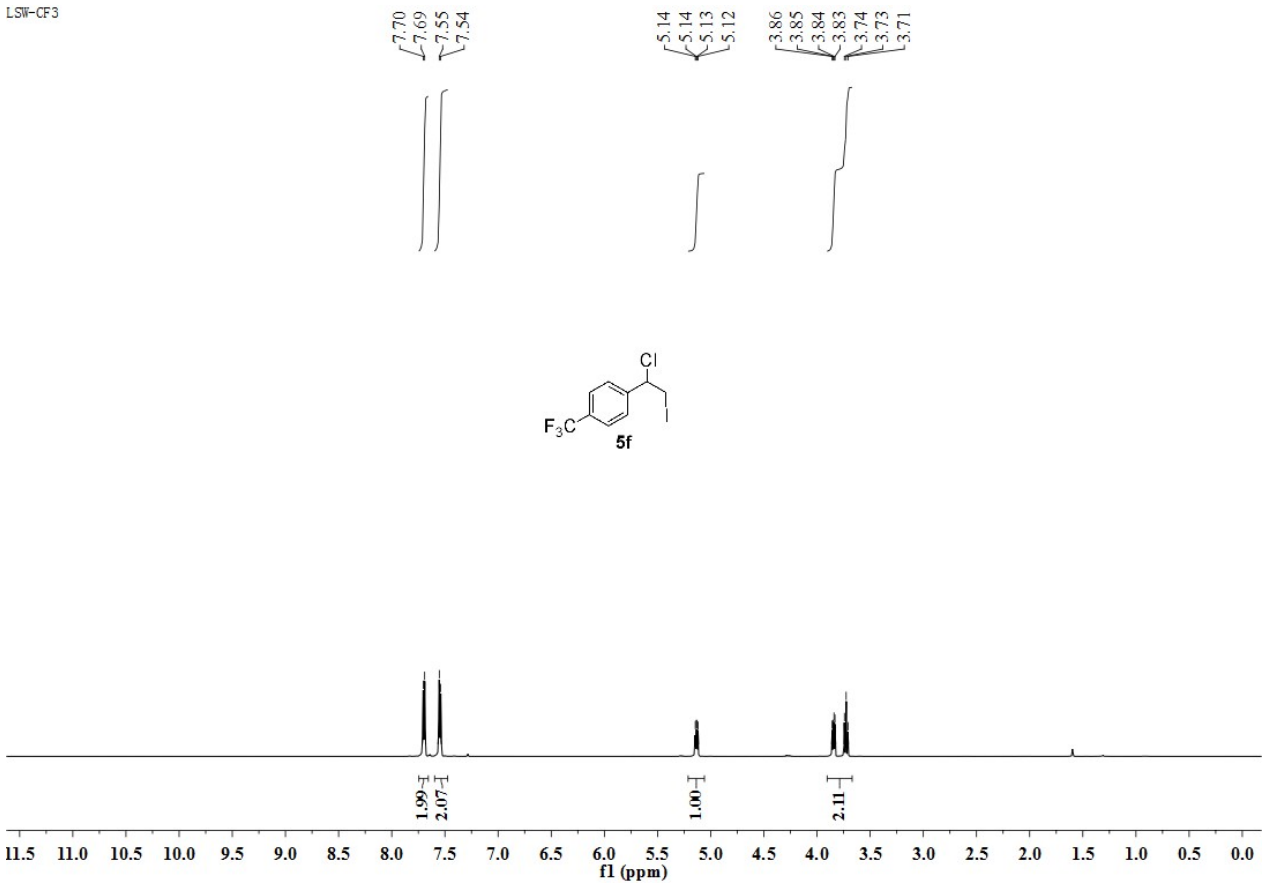
LSW-4PHENE-CL-I



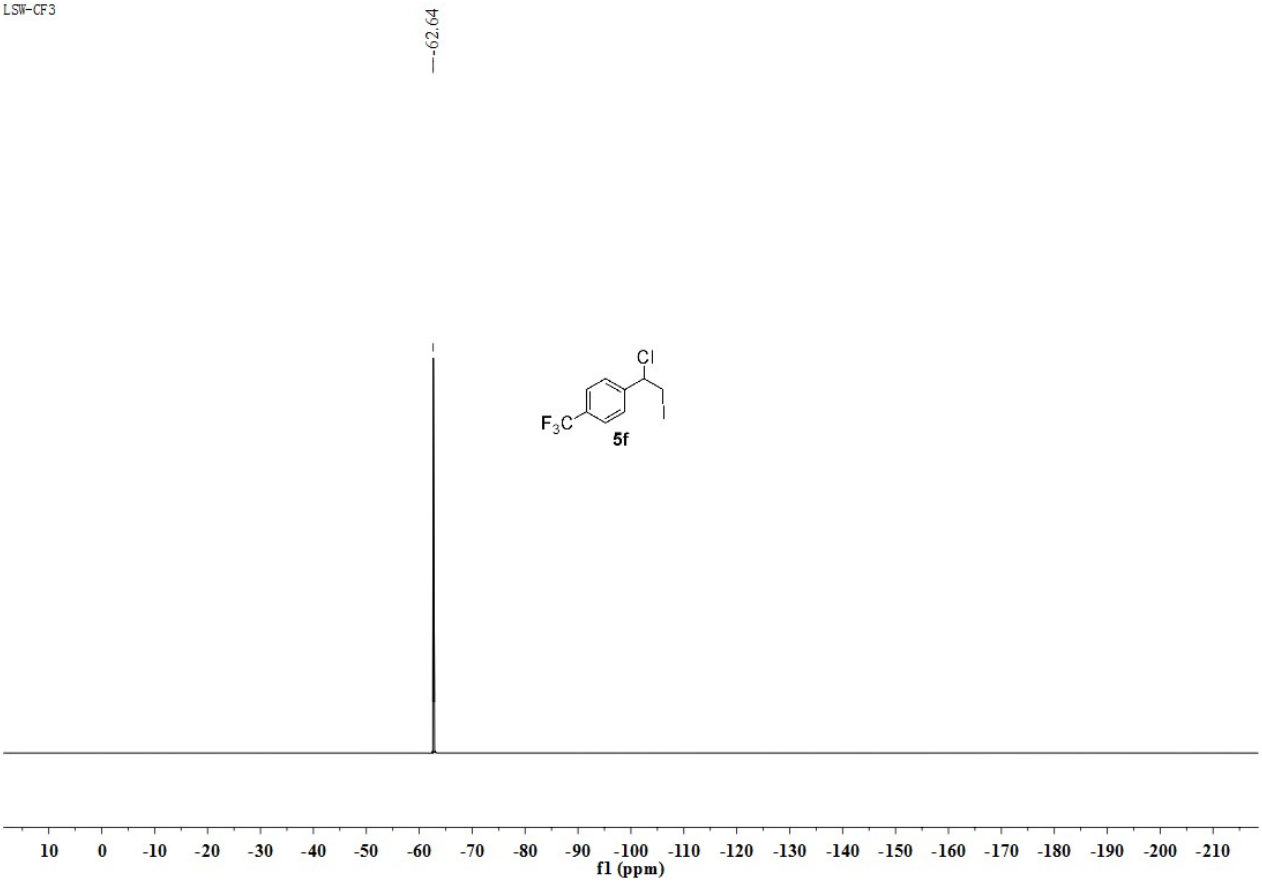
LSW-4ME-CL-I



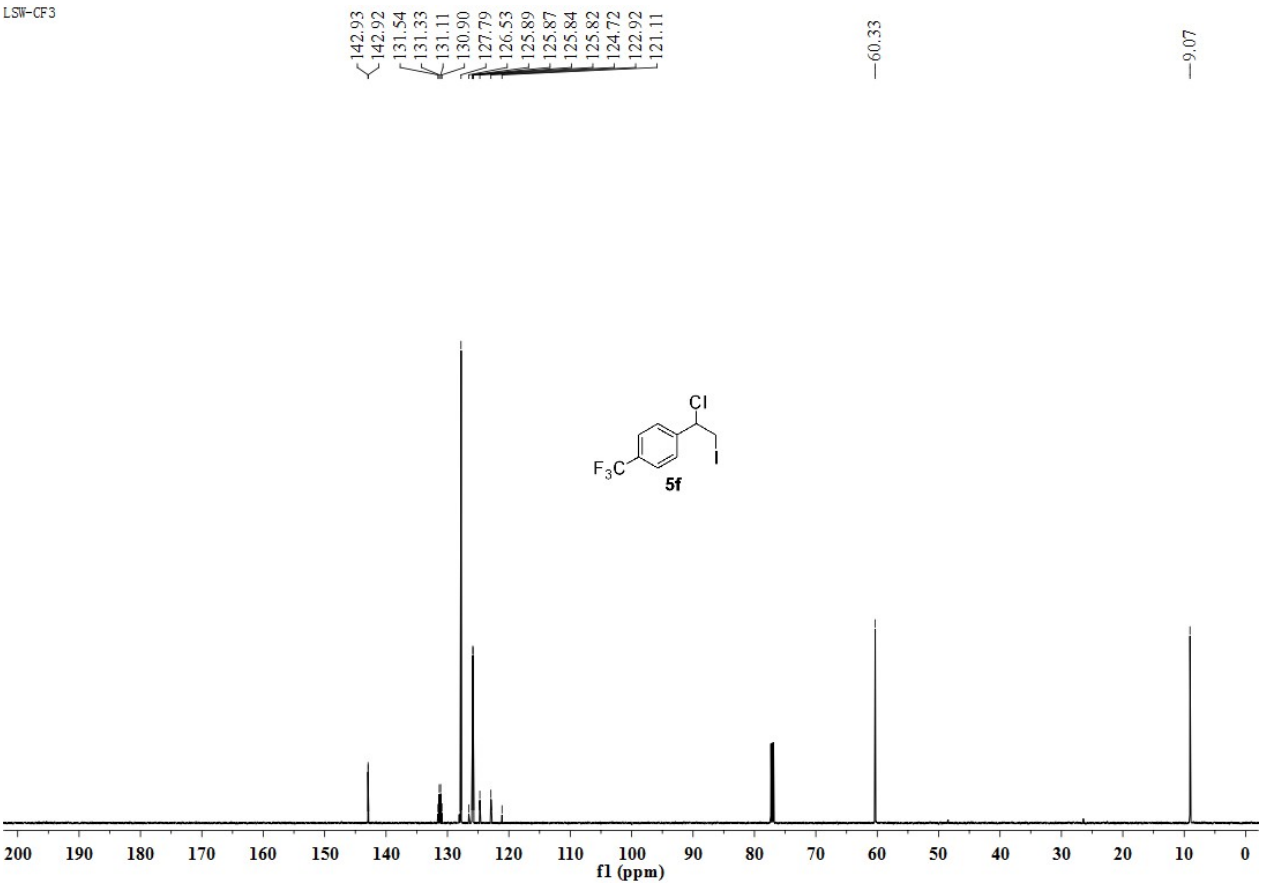

LSW-4ME--ENE-CL-I
139.18
136.15
129.50
127.08
61.65
21.28
10.07
Cl
I
5e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

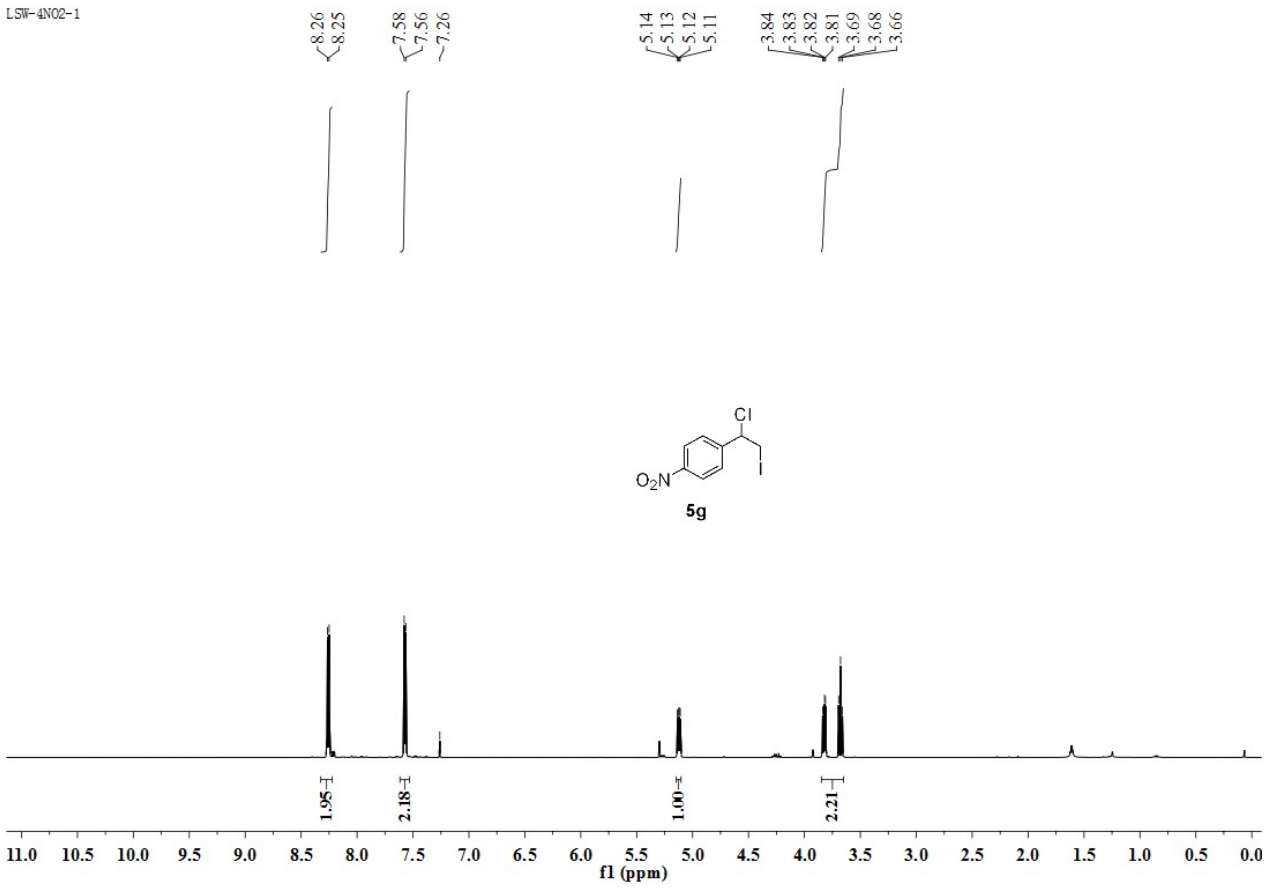

LSW-CF3
7.70
7.69
7.55
7.54
5.14
5.14
5.13
5.12
3.86
3.85
3.84
3.83
3.74
3.73
3.71
Cl
I
F3C
5f
1.99
2.07
1.00
2.11
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

LSW-CF3

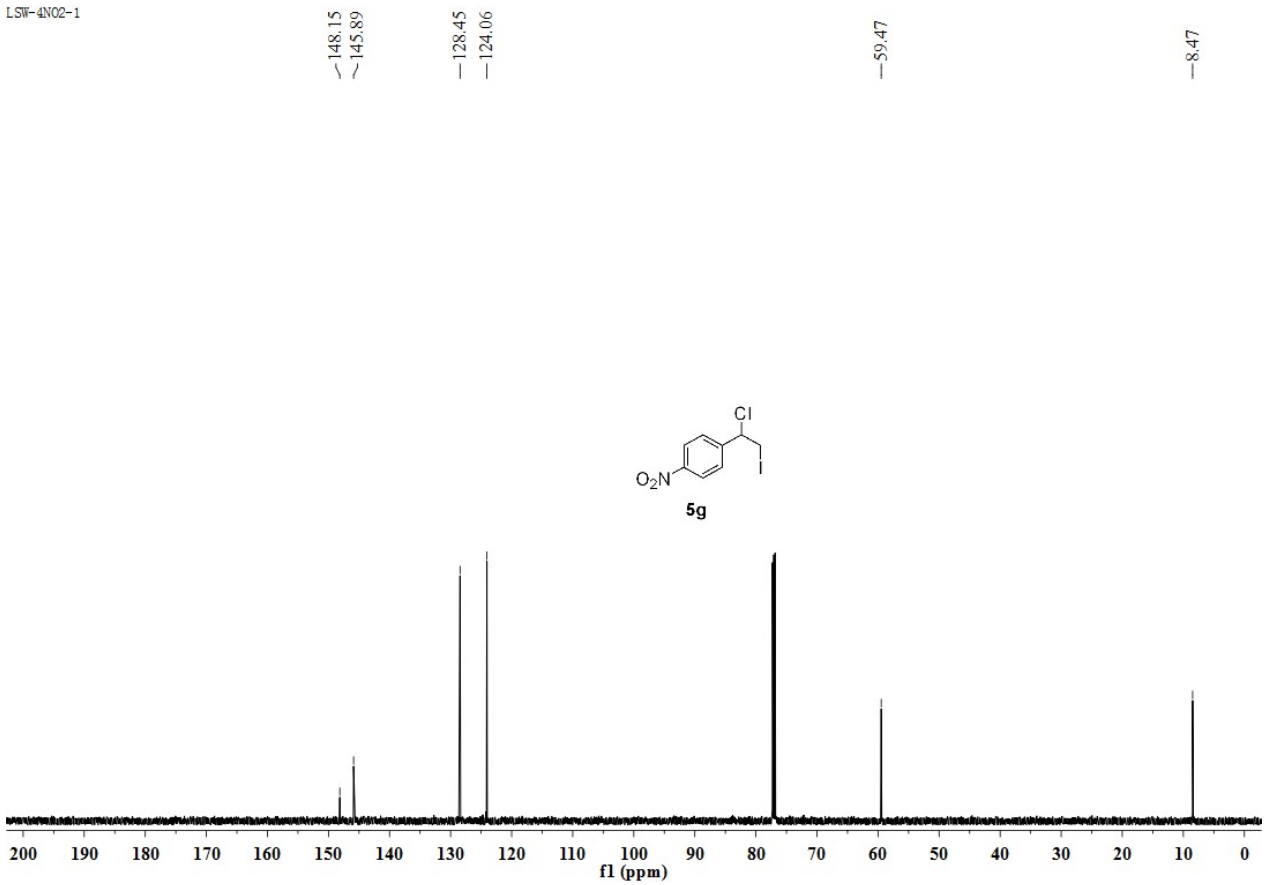


LSW-CF3



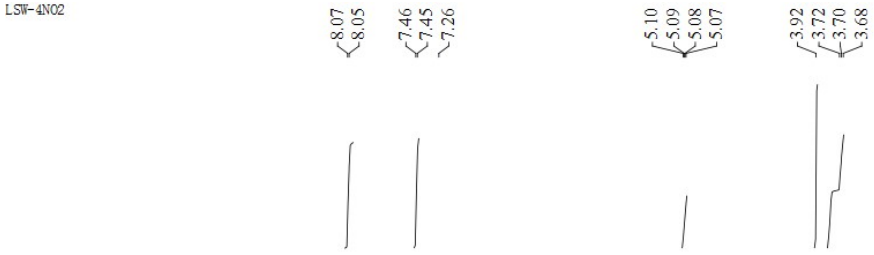

LSW-4NO2-1
8.26
8.25
7.58
7.56
7.26
5.14
5.13
5.12
5.11
3.84
3.83
3.82
3.81
3.69
3.68
3.66
Cl
O2N
1.95
2.18
1.00
2.21
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

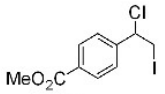
5g


LSW-4NO2-1
148.15
145.89
128.45
124.06
59.47
8.47
Cl
O2N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

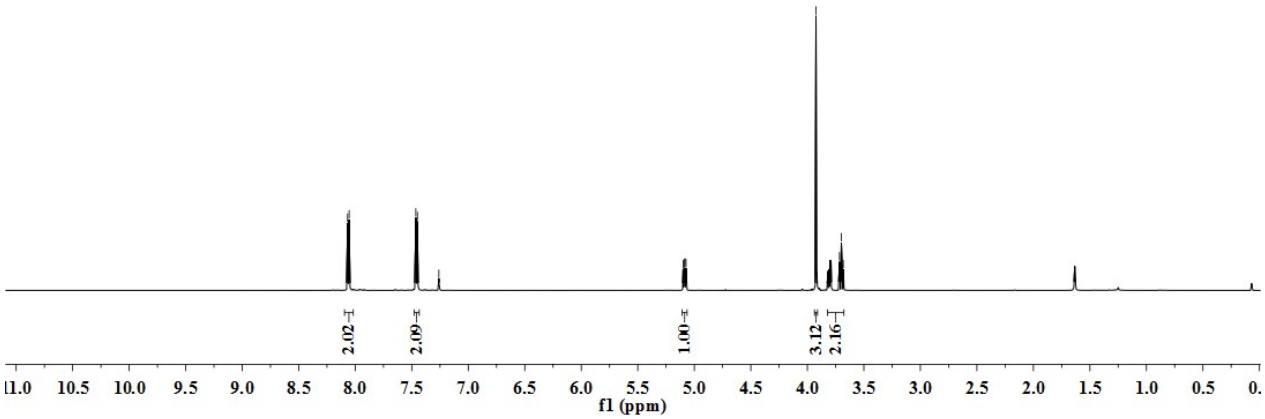
5g

LSW-4NO2

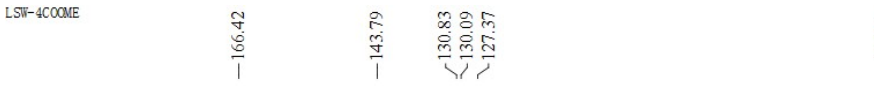


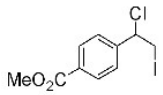


5h

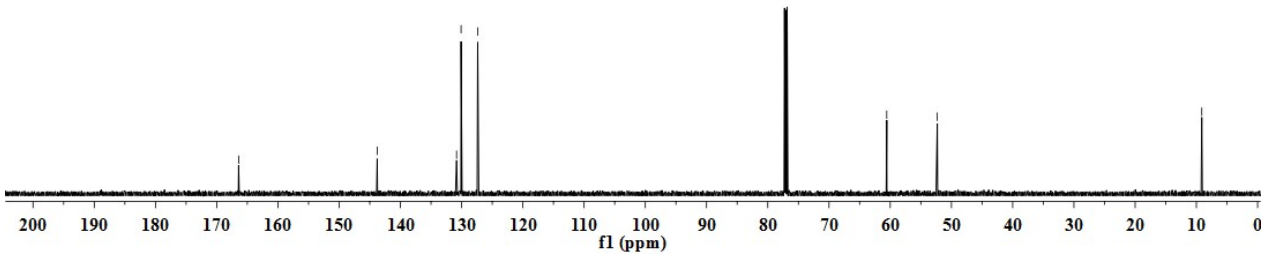


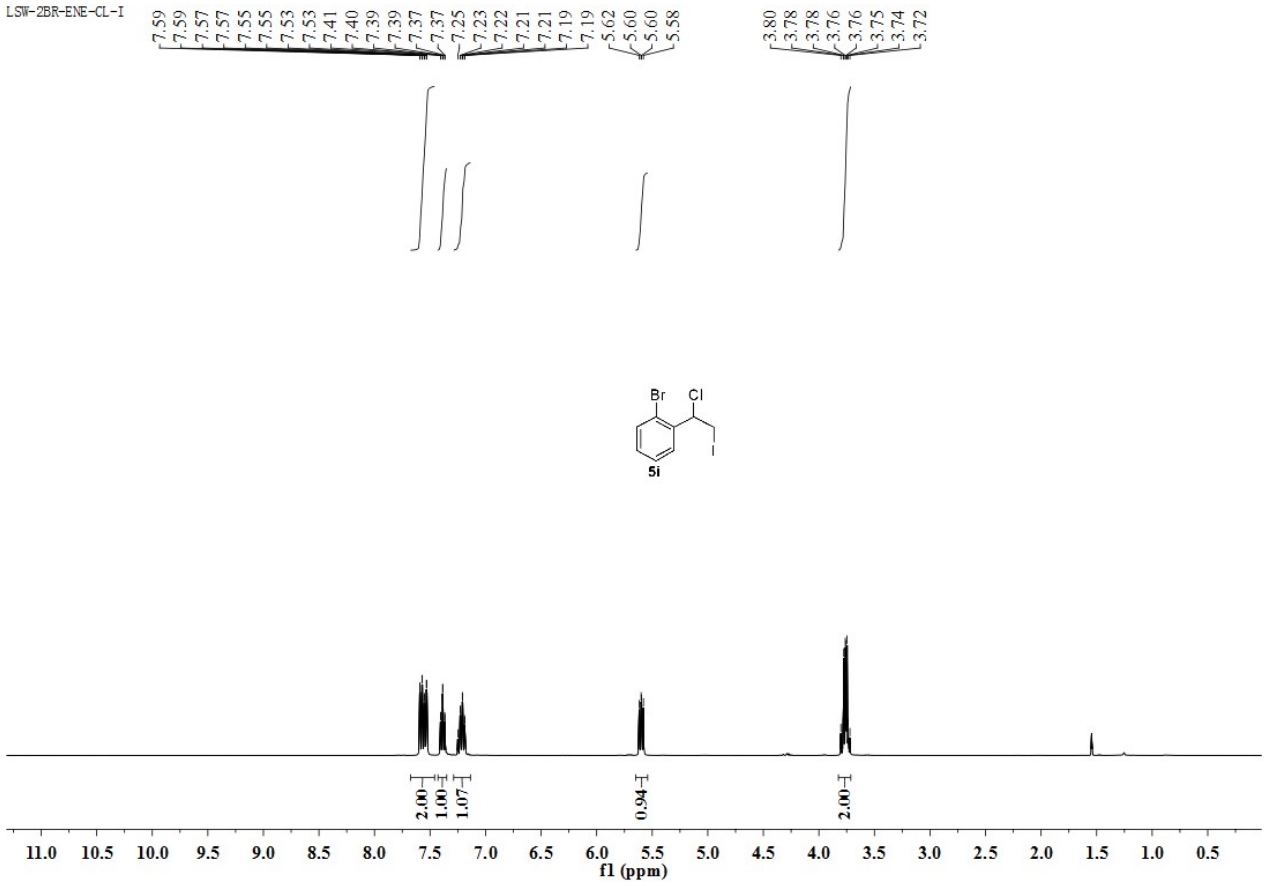
LSW-4COOME

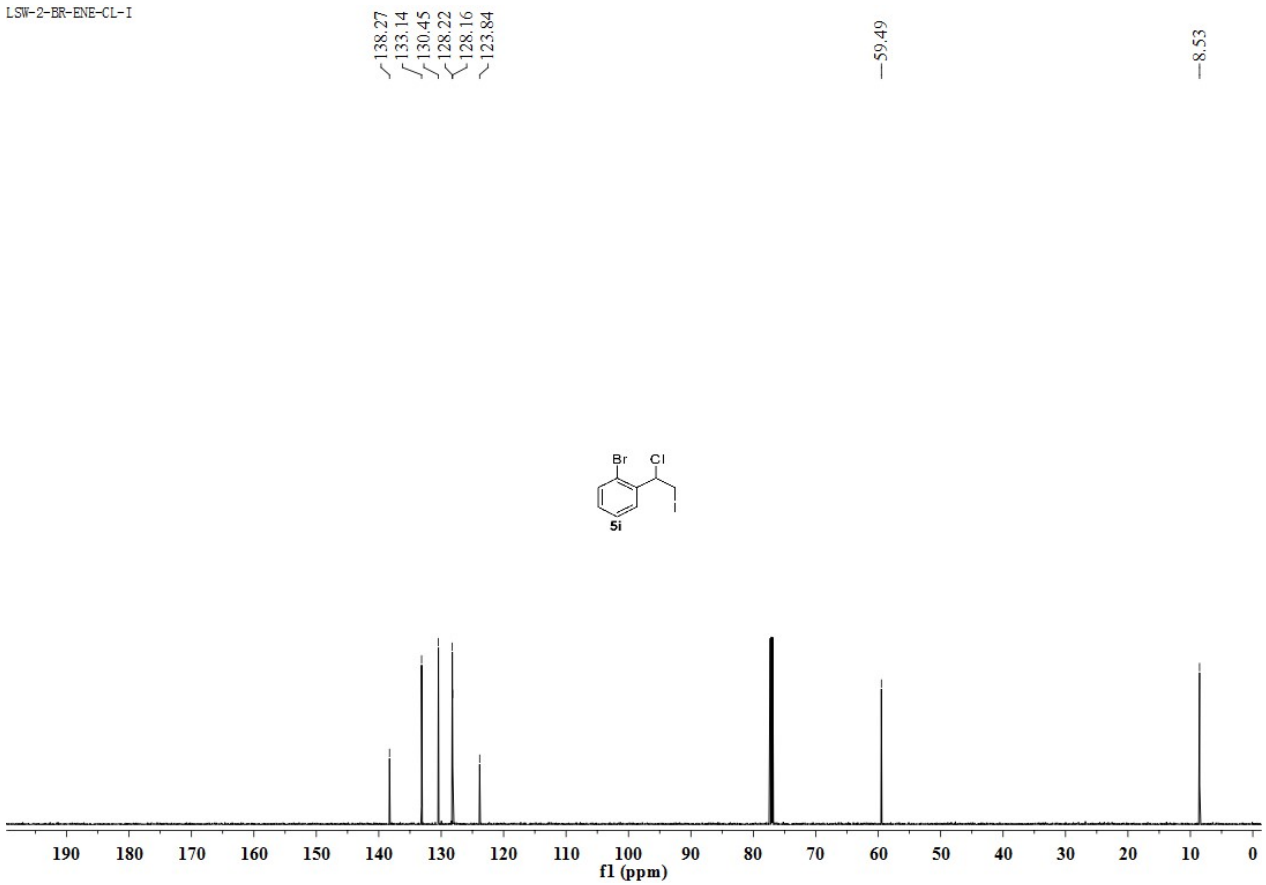




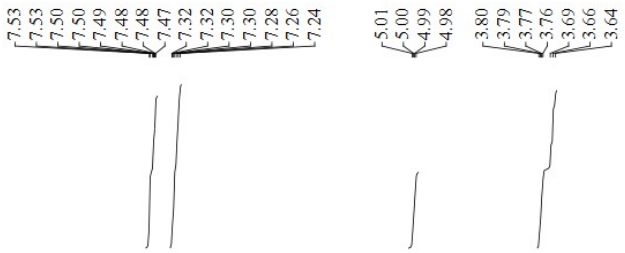
5h

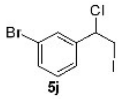



LSW-2BR-ENE-CL-I
7.59
7.59
7.57
7.57
7.55
7.55
7.53
7.53
7.41
7.40
7.39
7.39
7.37
7.37
7.25
7.23
7.22
7.21
7.21
7.19
7.19
5.62
5.60
5.60
5.58
3.80
3.78
3.78
3.76
3.76
3.75
3.74
3.72
Br
Cl
I
5i
2.00
1.00
1.07
0.94
2.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

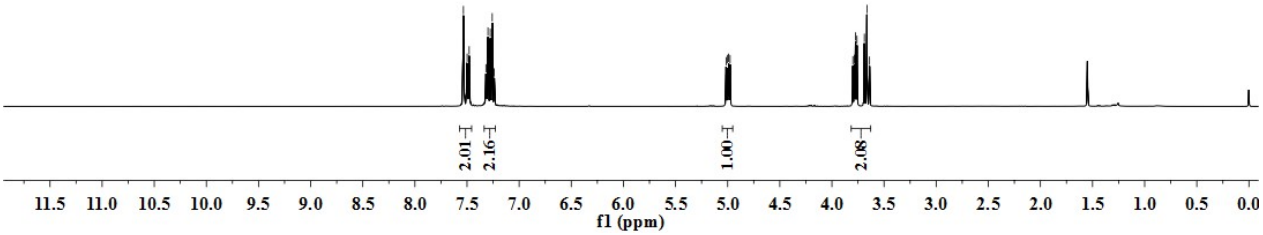

LSW-2-BR-ENE-CL-I
138.27
133.14
130.45
128.22
128.16
123.84
59.49
8.53
Br
Cl
I
5i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

LSW-3BR-ENE-CL-I

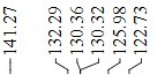


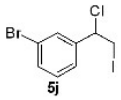


5j

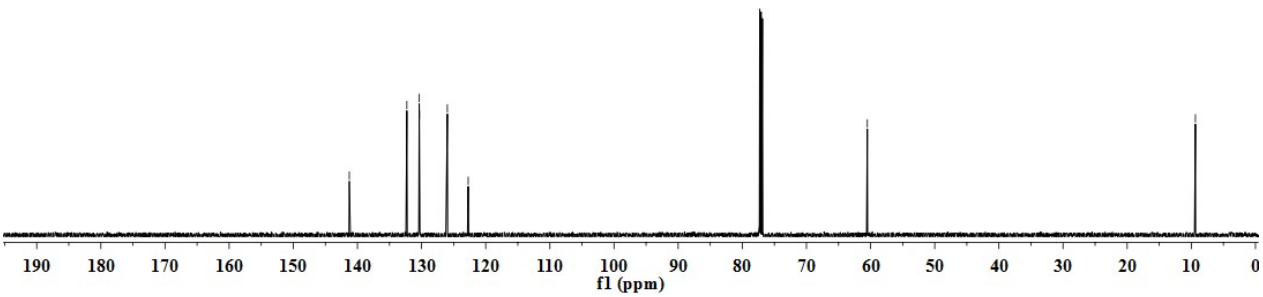


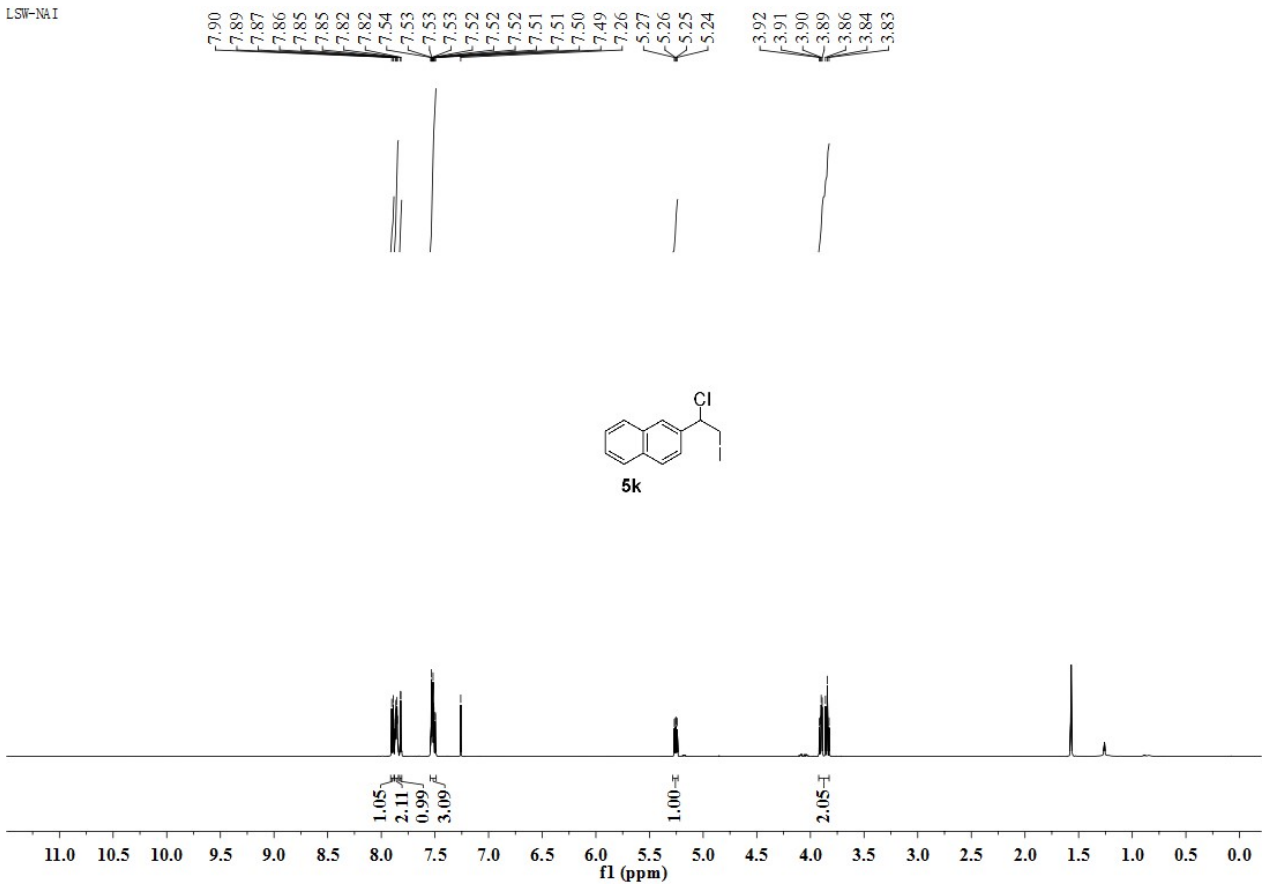
LSW-3-BR-ENE-CL-I

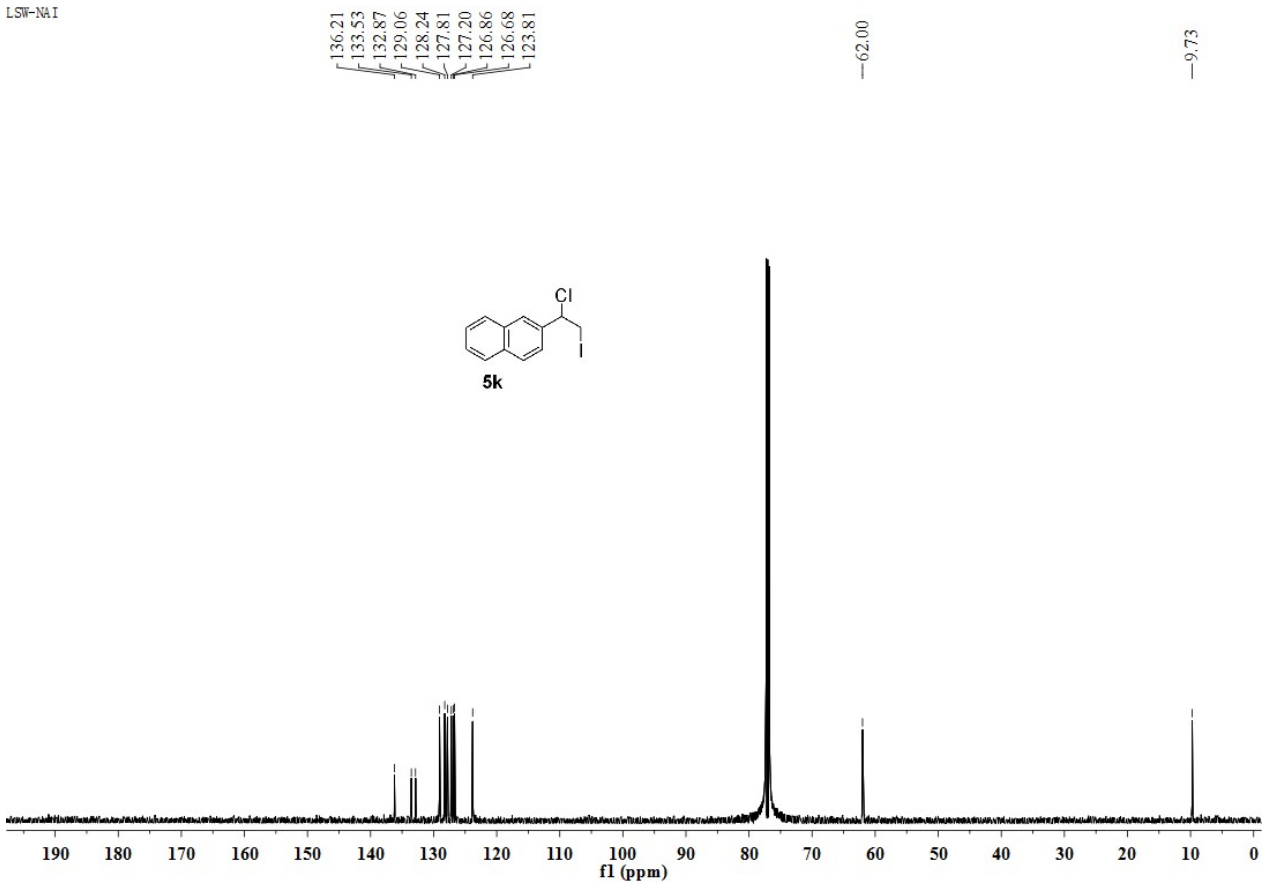


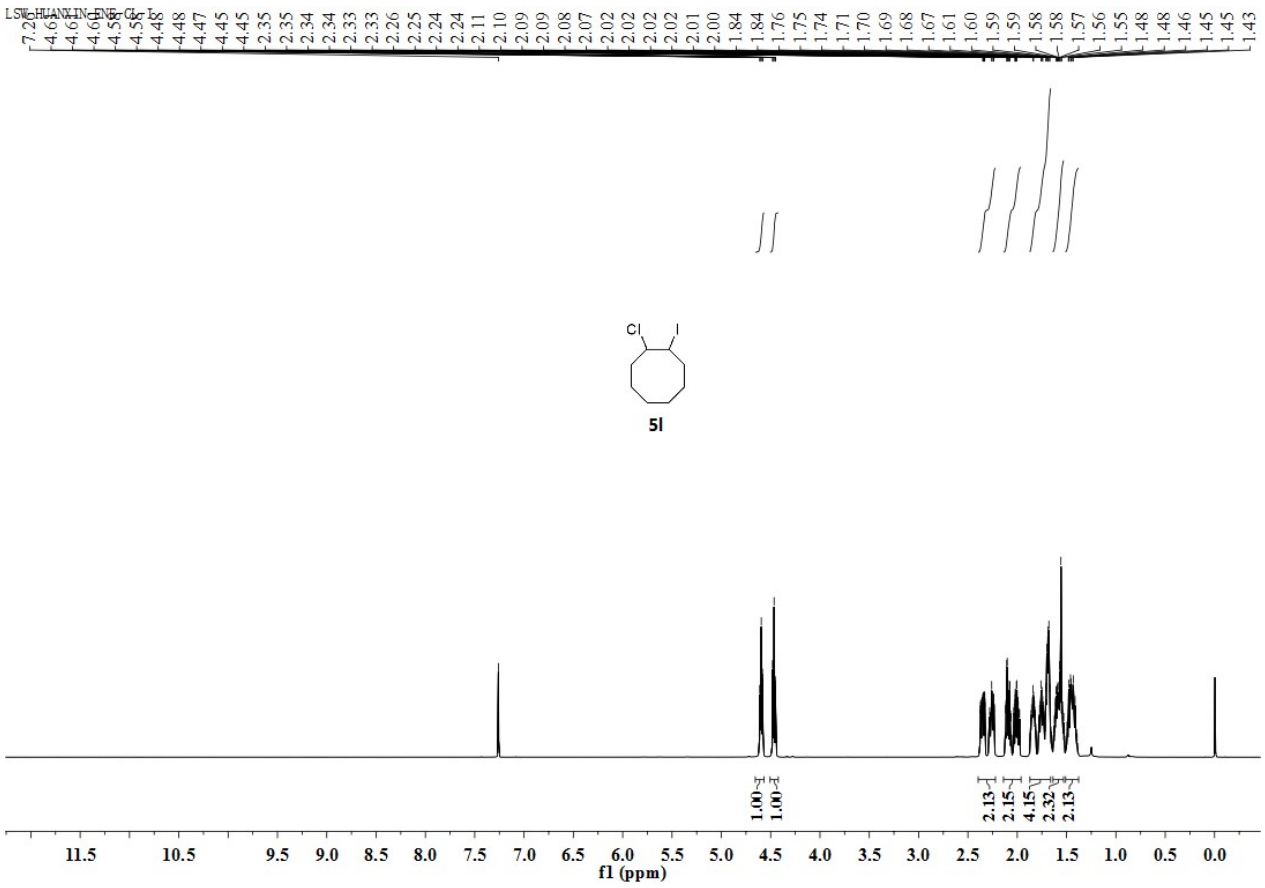


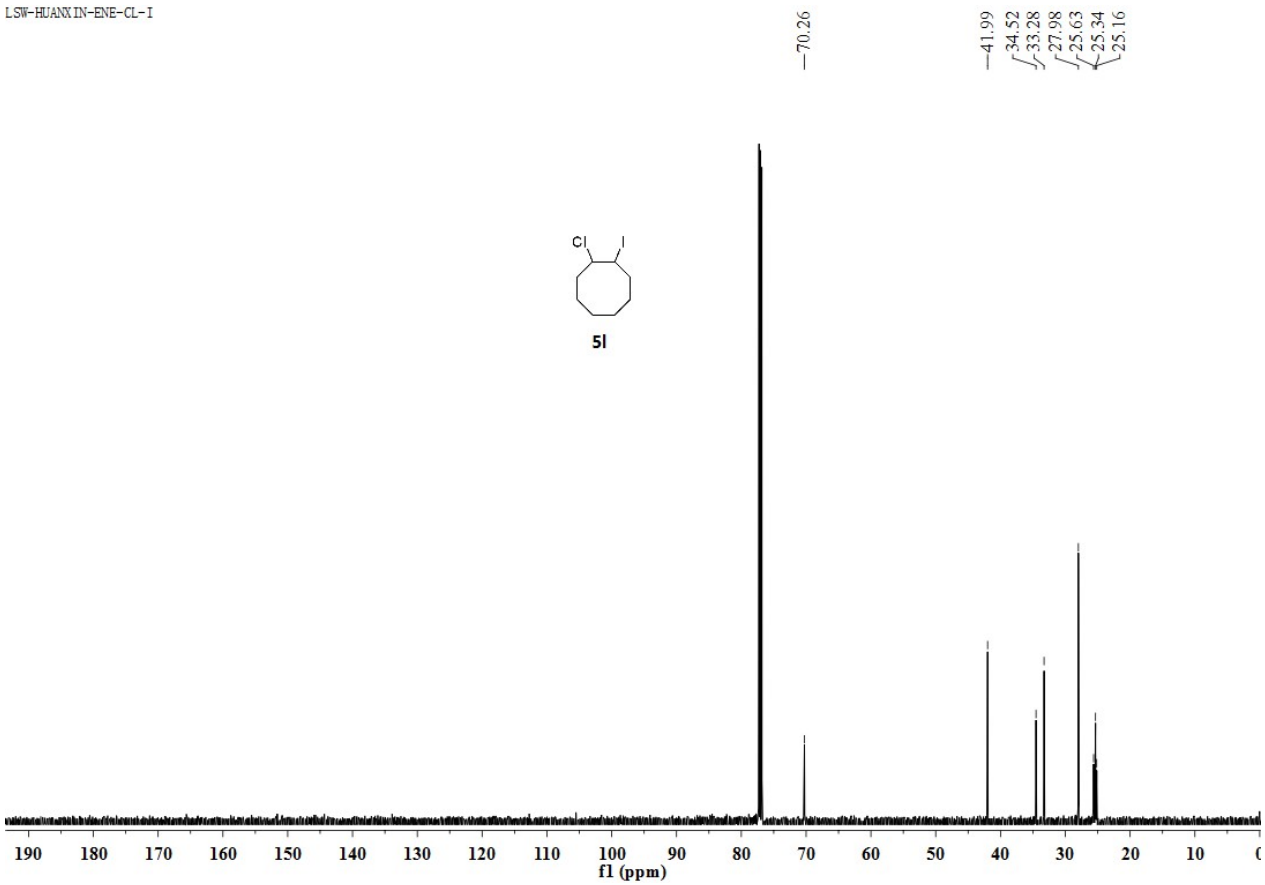
5j

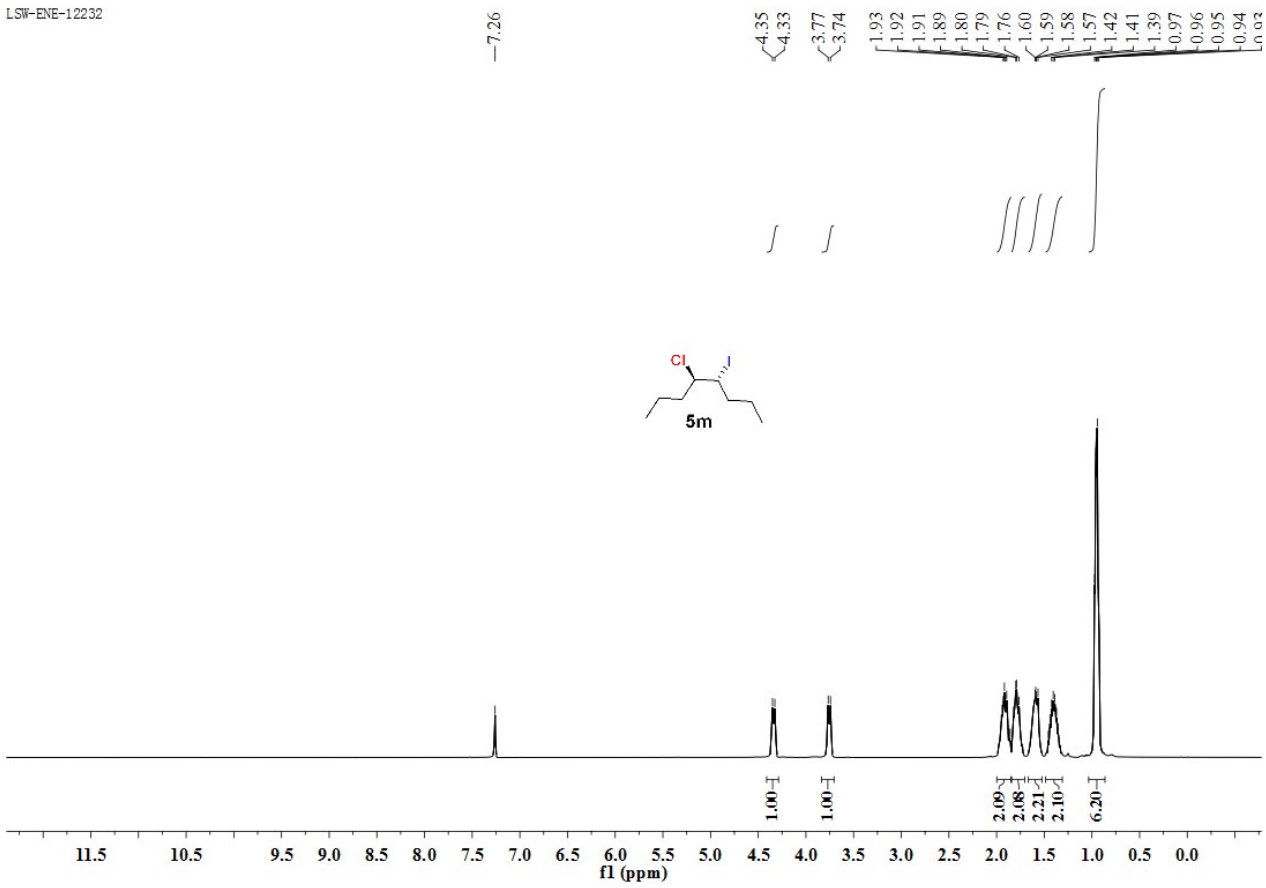


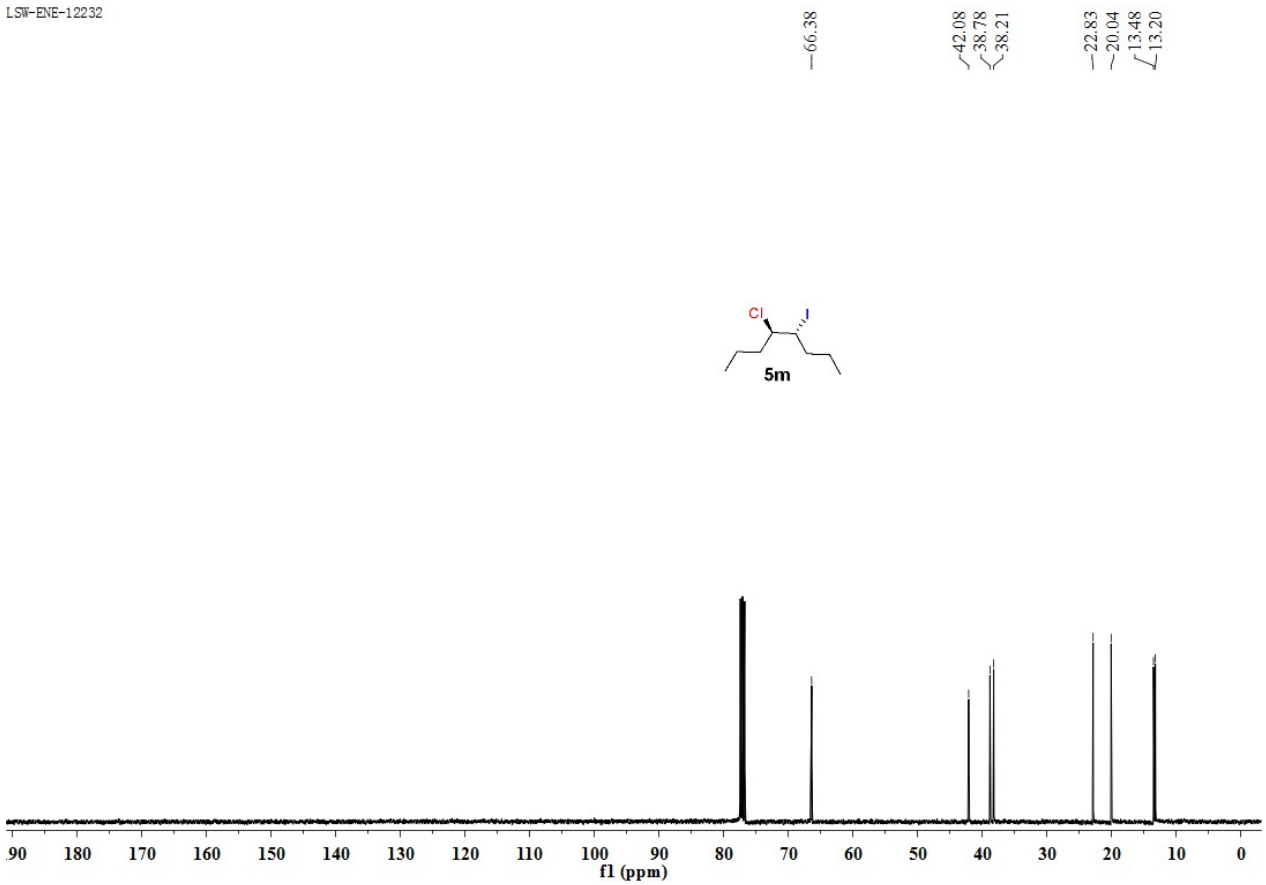

LSW-NAI
7.90
7.89
7.87
7.86
7.85
7.85
7.82
7.82
7.54
7.53
7.53
7.53
7.52
7.52
7.52
7.51
7.51
7.50
7.49
7.26
5.27
5.26
5.25
5.24
3.92
3.91
3.90
3.89
3.86
3.84
3.83
Cl
5k
1.05
2.11
0.99
3.09
1.00
2.05
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

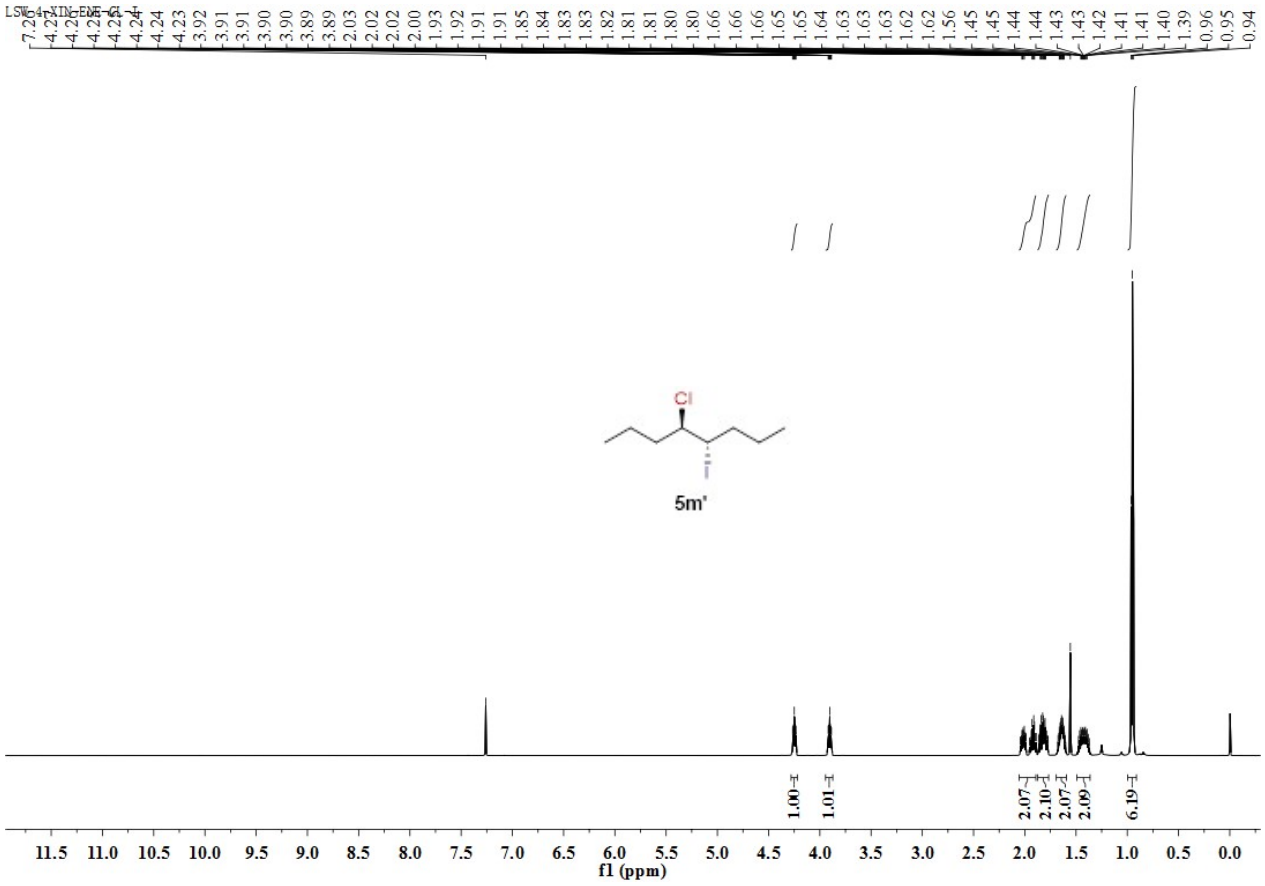

LSW-NAI
136.21
133.53
132.87
129.06
128.24
127.81
127.20
126.86
126.68
123.81
62.00
9.73
Cl
5k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

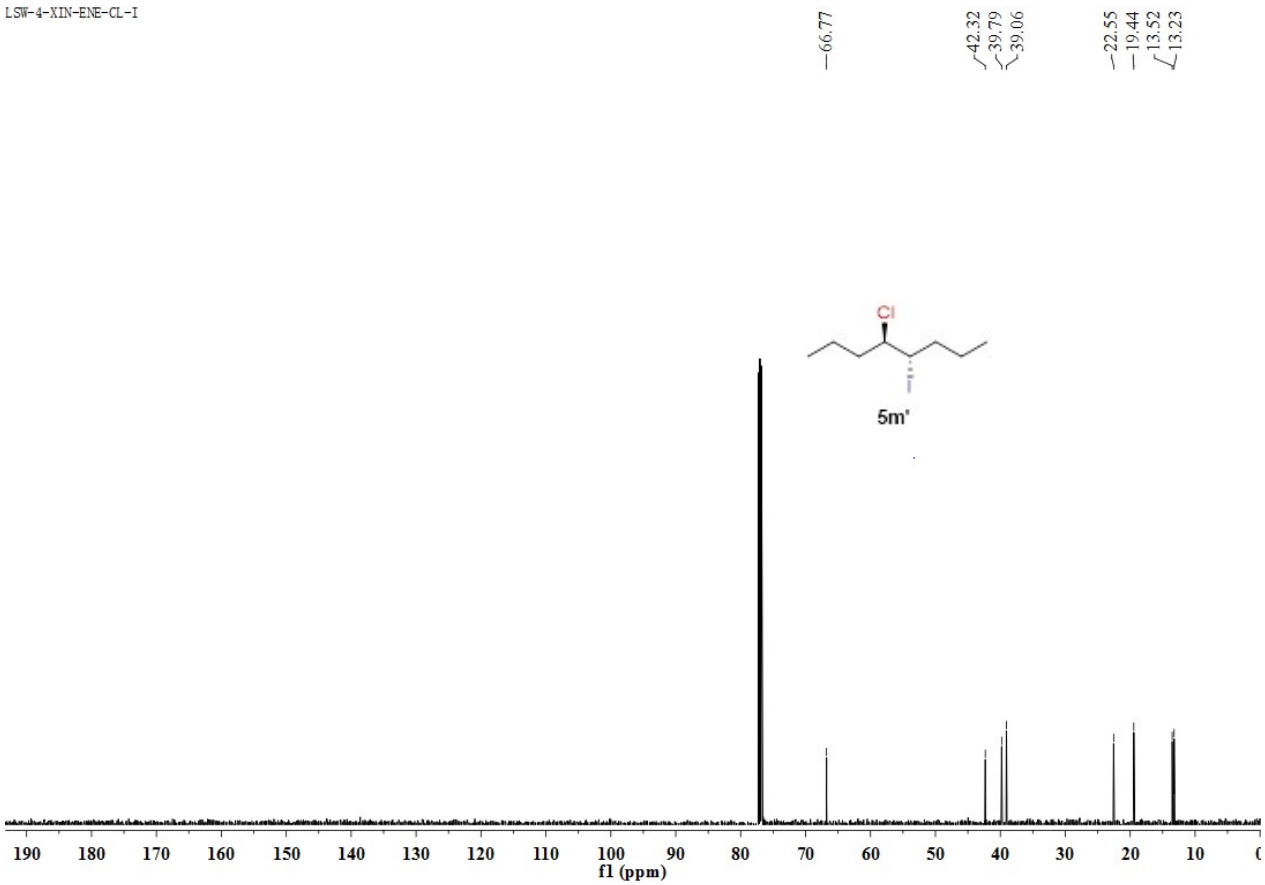

LSW-HUANXIN-ENE-CL-I
7.26
4.61
4.60
4.58
4.58
4.48
4.48
4.47
4.45
4.45
2.35
2.34
2.34
2.33
2.33
2.26
2.25
2.24
2.24
2.11
2.10
2.09
2.09
2.08
2.07
2.02
2.02
2.02
2.01
2.00
1.84
1.84
1.76
1.75
1.74
1.71
1.70
1.69
1.68
1.67
1.61
1.60
1.59
1.59
1.58
1.58
1.57
1.56
1.55
1.48
1.48
1.46
1.45
1.45
1.43
Cl
I
5l
1.00
1.00
2.13
2.15
4.15
2.32
2.13
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


LSW-HUANXIN-ENE-CL-I
70.26
41.99
34.52
33.28
27.98
25.63
25.34
25.16
Cl
I
5l
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

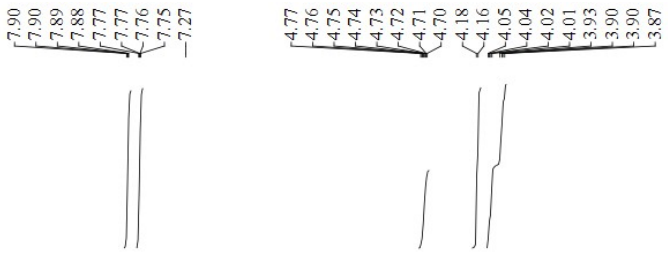

LSW-ENE-12232
7.26
4.35
4.33
3.77
3.74
1.93
1.92
1.91
1.89
1.80
1.79
1.76
1.60
1.59
1.58
1.57
1.42
1.41
1.39
0.97
0.96
0.95
0.94
Cl
I
5m
1.00
1.00
2.09
2.08
2.21
2.10
6.20
f1 (ppm)

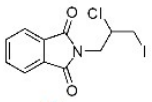

LSW-ENE-12232
66.38
42.08
38.78
38.21
22.83
20.04
13.48
13.20
Cl
I
5m
f1 (ppm)


LSW-4-XIN-ENE-CL-I
Cl
5m'
1.00
1.01
2.07
2.10
2.07
2.09
6.19
f1 (ppm)

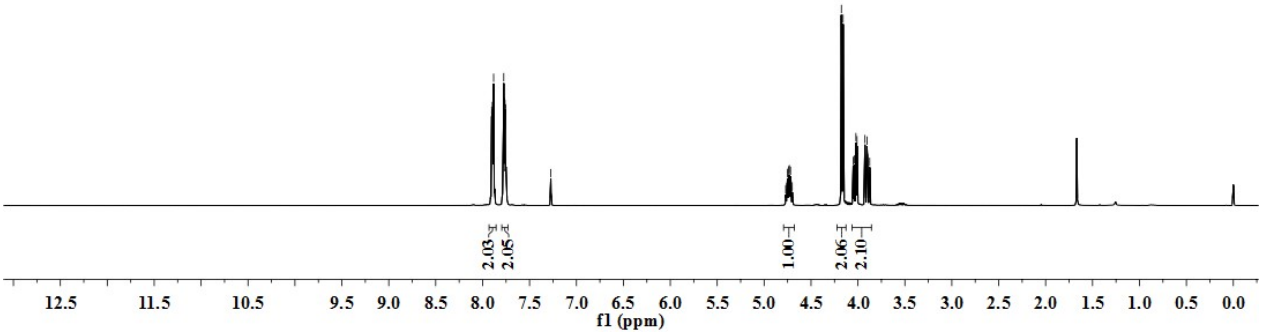

LSW-4-XIN-ENE-CL-I
66.77
42.32
39.79
39.06
22.55
19.44
13.52
13.23
Cl
5m'
f1 (ppm)

LSW-NCH2QUE-CL-I

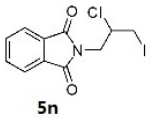




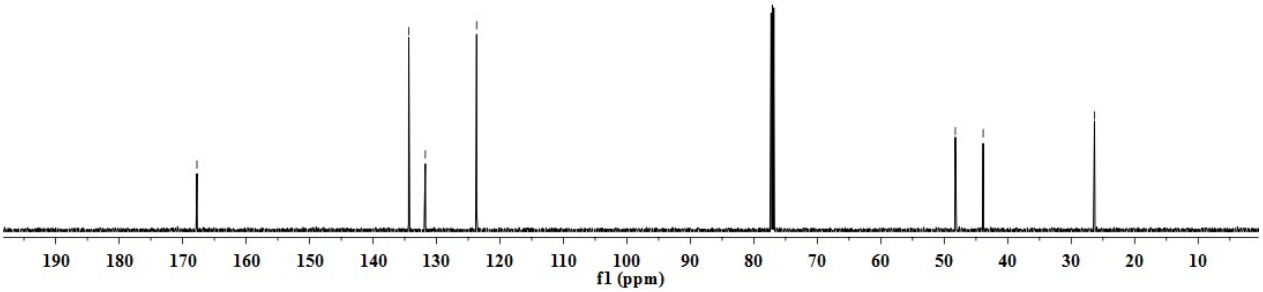
5n

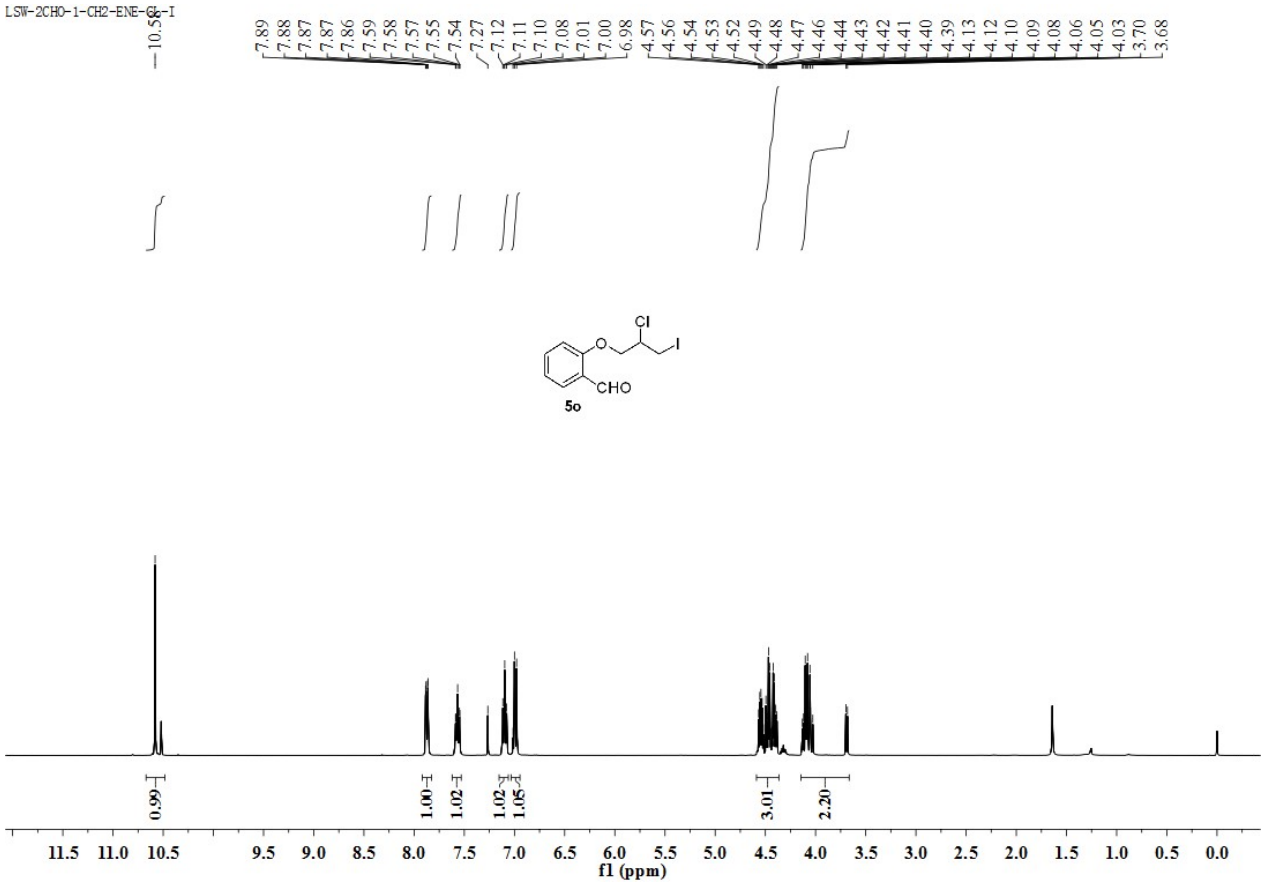


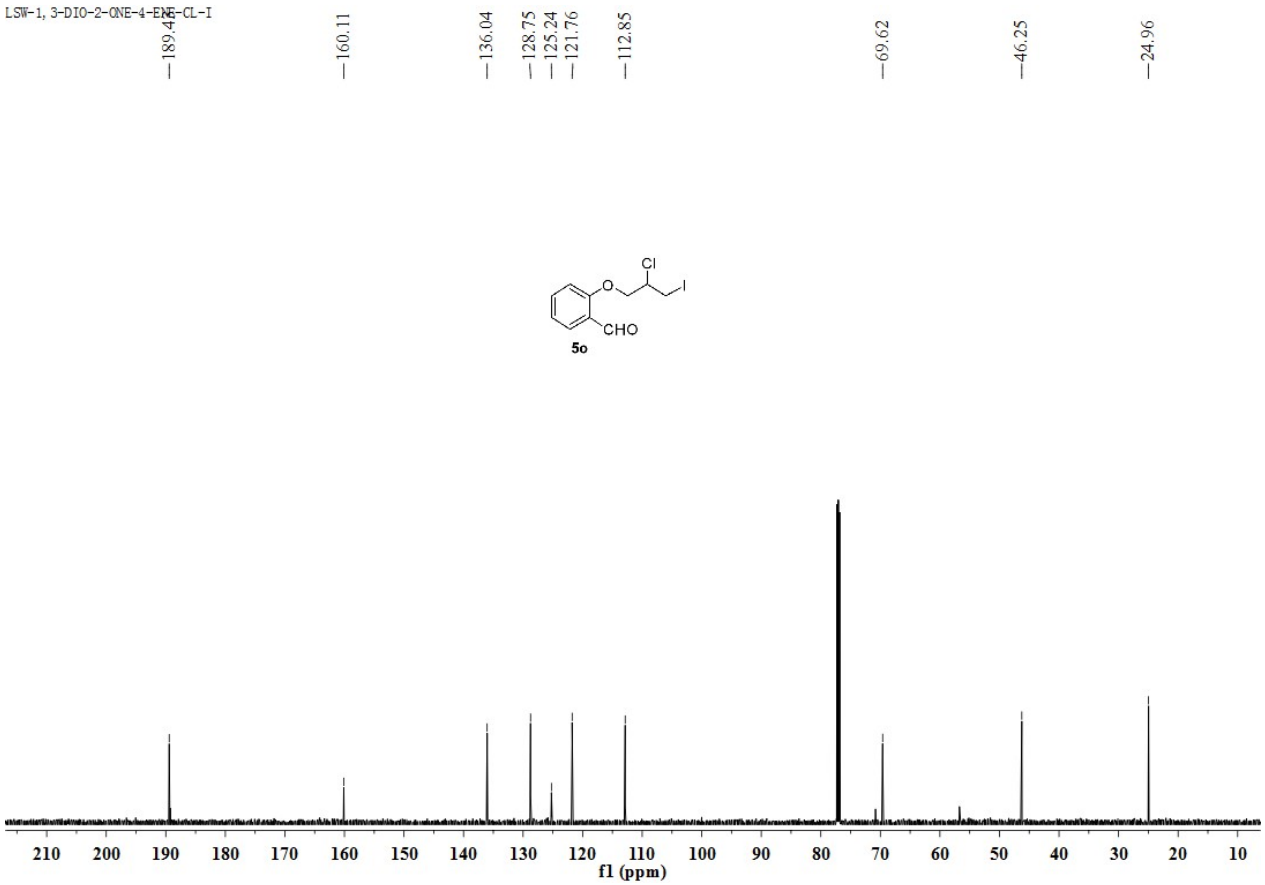
LSW-NCH2-ENE-CL-I



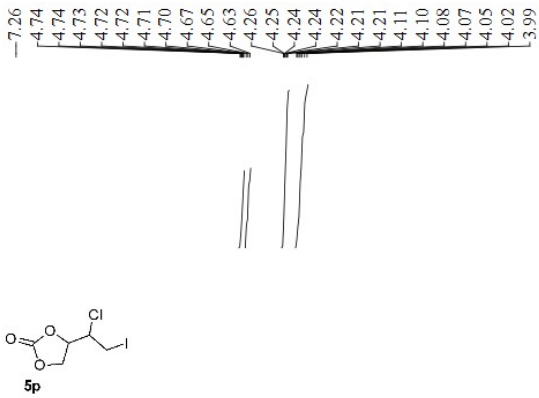
5n

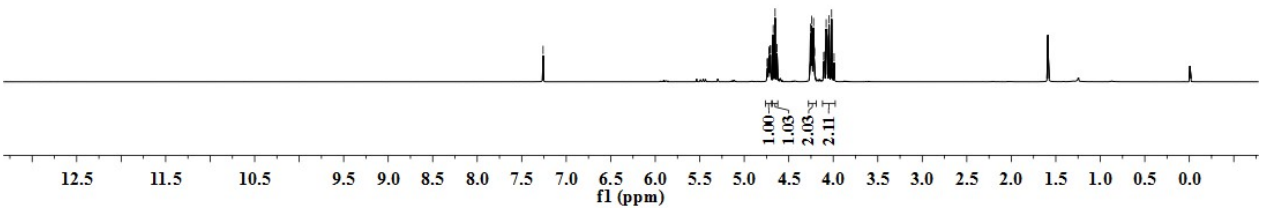



LSW-2CHO-1-CH2-ENE-CL-I
10.58
7.89
7.88
7.87
7.87
7.86
7.59
7.58
7.57
7.55
7.54
7.27
7.12
7.11
7.10
7.08
7.01
7.00
6.98
4.57
4.56
4.54
4.53
4.52
4.49
4.48
4.47
4.46
4.44
4.43
4.42
4.41
4.40
4.39
4.13
4.12
4.10
4.09
4.08
4.06
4.05
4.03
3.70
3.68
Cl
O
I
CHO
5o
0.99
1.00
1.02
1.02
1.05
3.01
2.20
11.5 11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

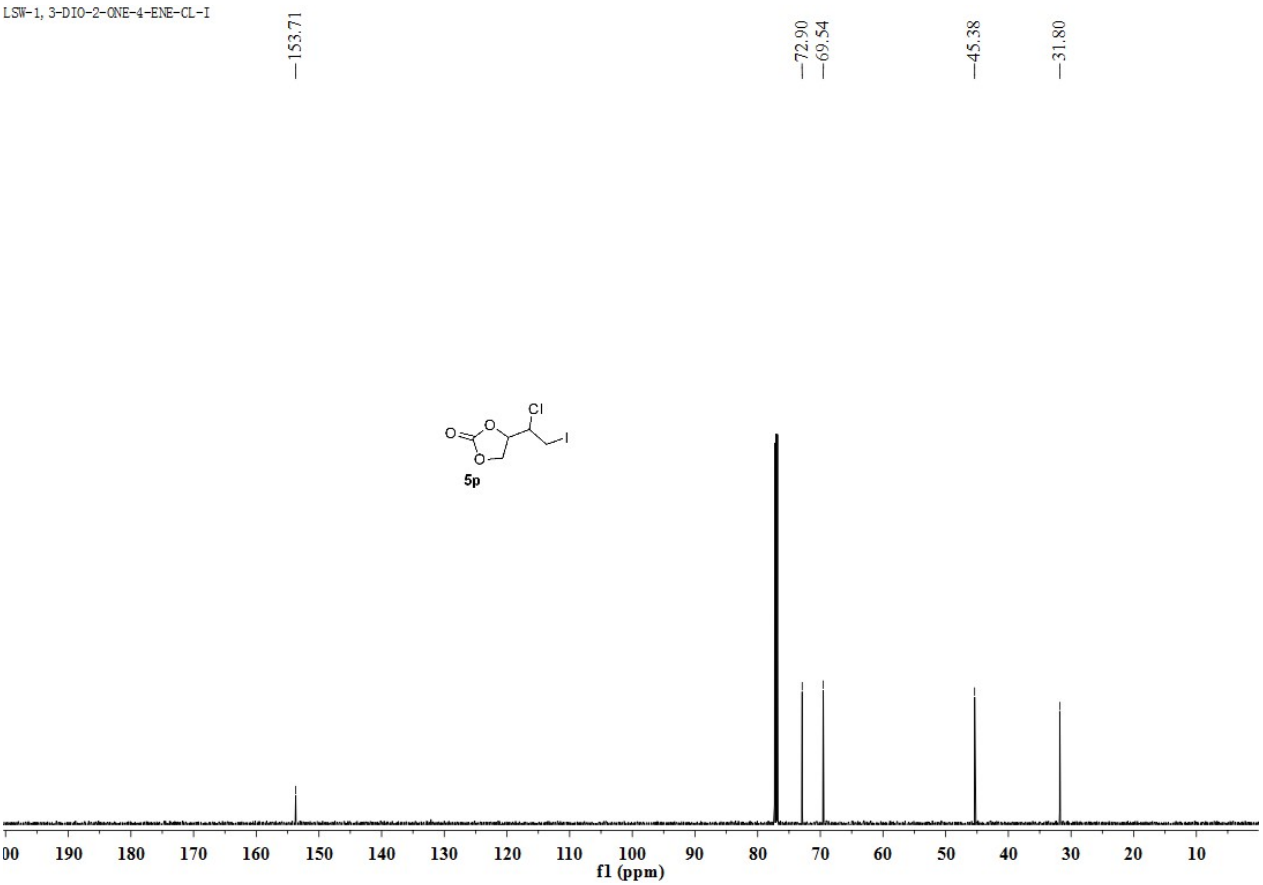

LSW-1, 3-DIO-2-ONE-4-ENE-CL-I
189.42
160.11
136.04
128.75
125.24
121.76
112.85
69.62
46.25
24.96
Cl
O
I
CHO
5o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

LSW-1, 3-DIO-6-ENE-CL-I



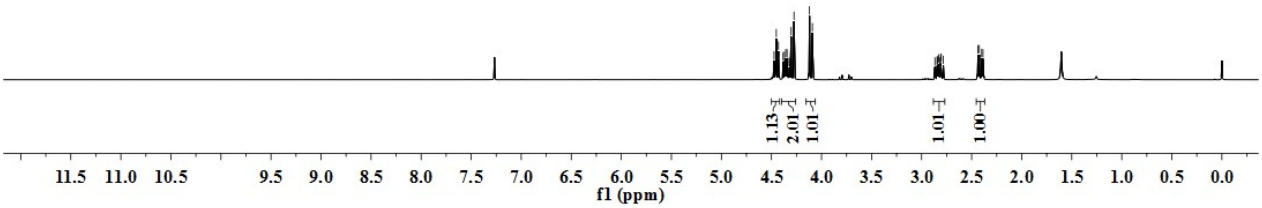


LSW-1, 3-DIO-2-ONE-4-ENE-CL-I

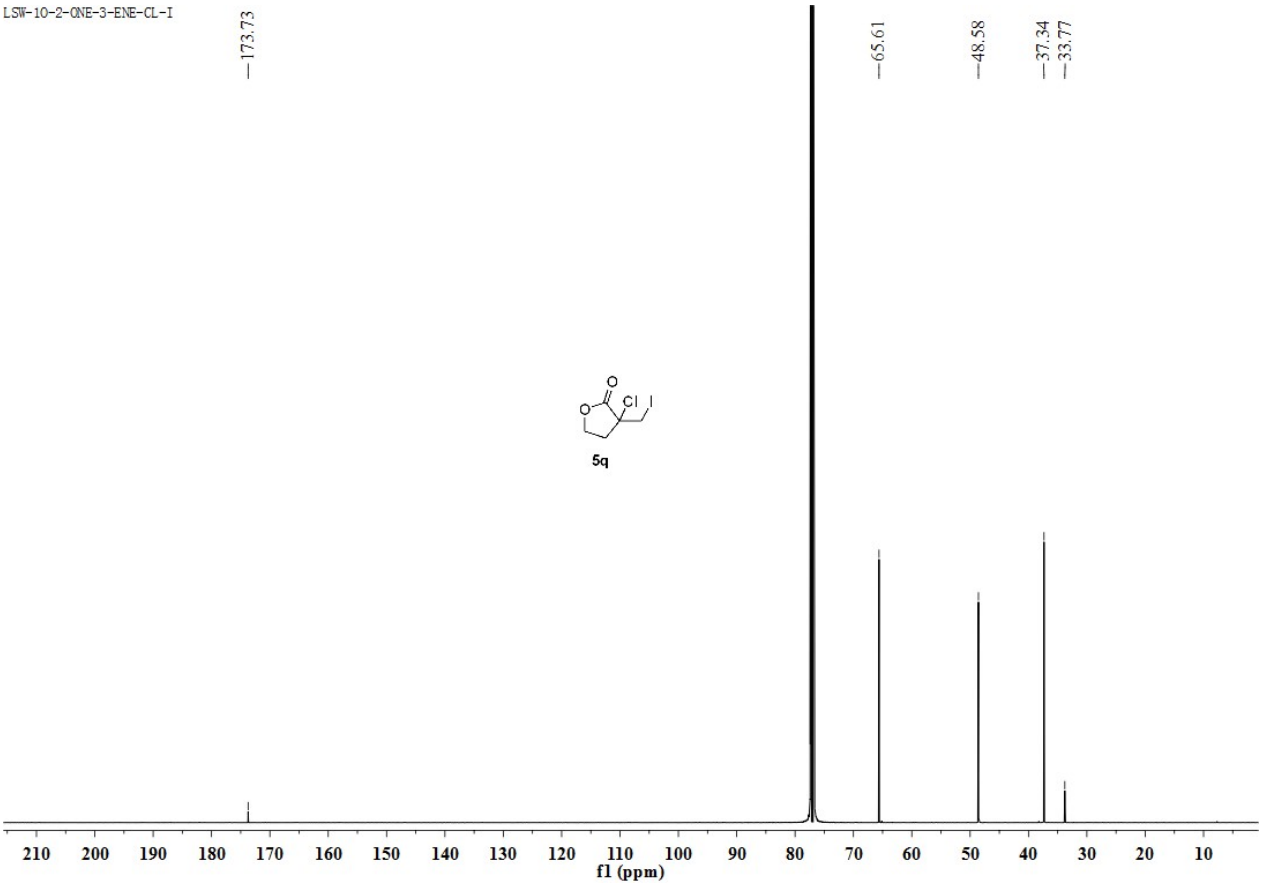


LSW-10-2ESTER-3-ENE-CL-I

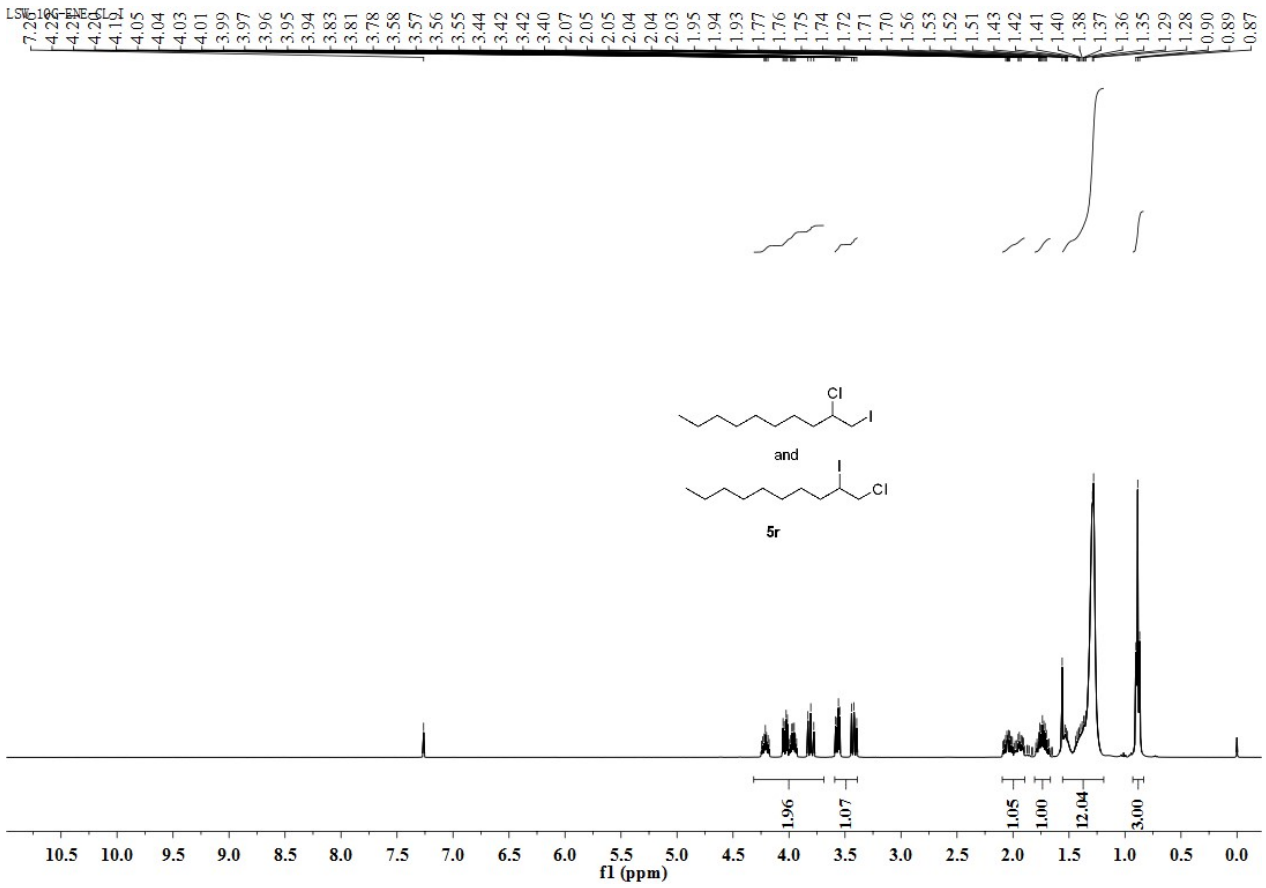
5q

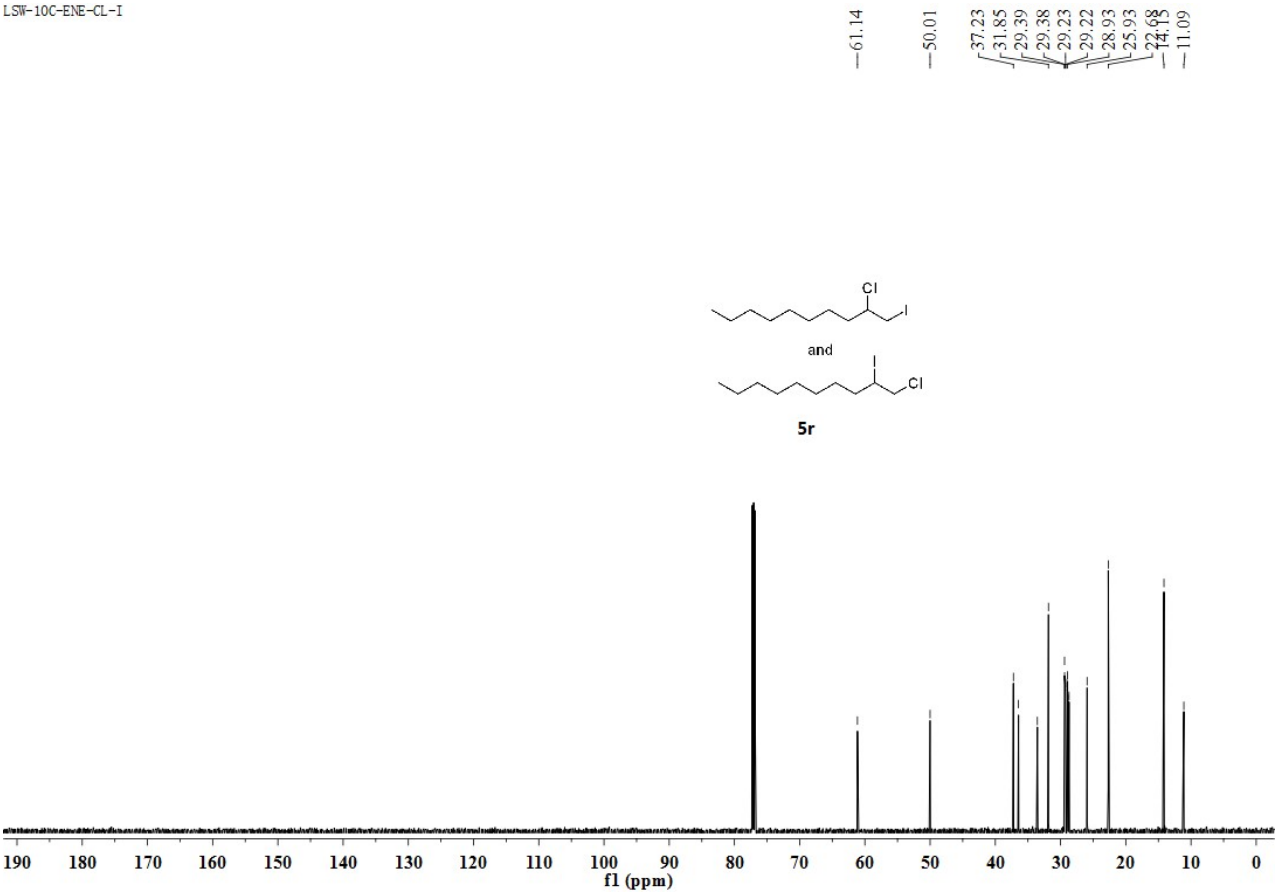


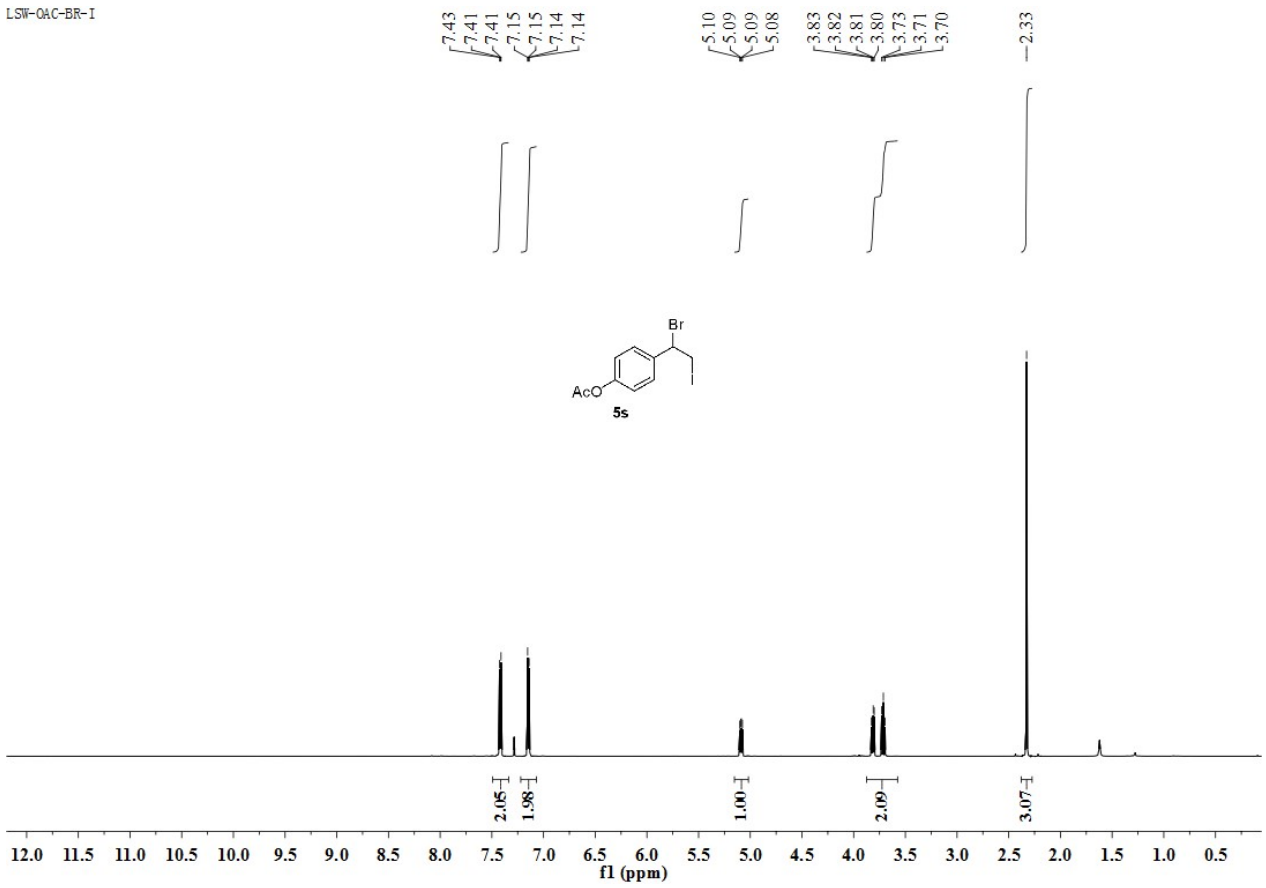
LSW-10-2-ONE-3-ENE-CL-I

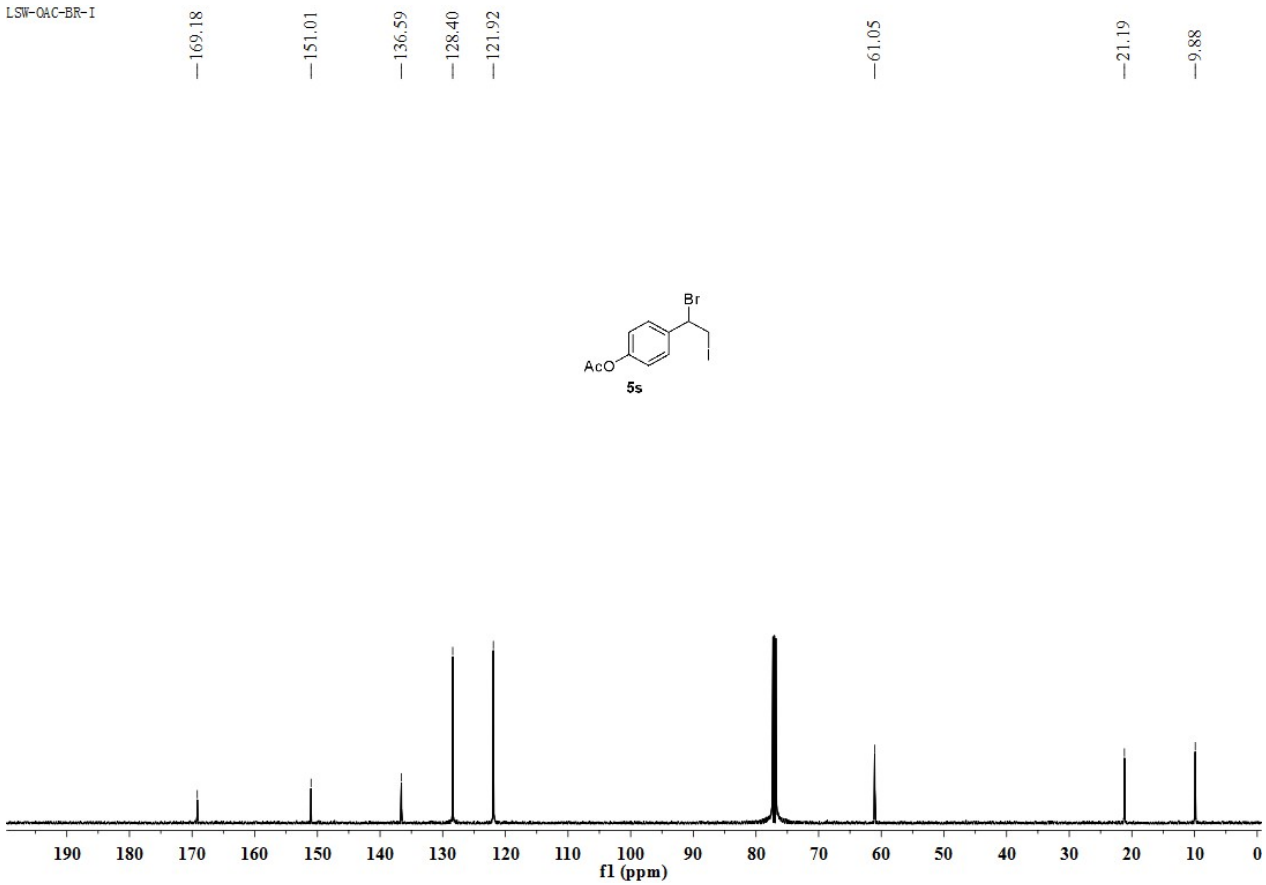


5q


LSW-10C-ENE-CL-I
7.26
4.23
4.22
4.20
4.15
4.05
4.04
4.03
4.01
3.99
3.97
3.96
3.95
3.94
3.83
3.81
3.78
3.58
3.57
3.56
3.55
3.44
3.42
3.42
3.40
2.07
2.05
2.05
2.04
2.04
2.03
1.95
1.94
1.93
1.77
1.76
1.75
1.74
1.72
1.71
1.70
1.56
1.53
1.52
1.51
1.43
1.42
1.41
1.40
1.38
1.37
1.36
1.35
1.29
1.28
0.90
0.89
0.87
Cl
I
and
I
Cl
5r
1.96
1.07
1.05
1.00
12.04
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


LSW-10C-ENE-CL-I
61.14
50.01
37.23
31.85
29.39
29.38
29.23
29.22
28.93
25.93
22.68
14.15
11.09
Cl
I
and
I
Cl
5r
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


LSW-OAC-BR-I
7.43
7.41
7.41
7.15
7.15
7.14
7.14
5.10
5.09
5.09
5.08
3.83
3.82
3.81
3.80
3.73
3.71
3.70
2.33
Br
AcO
5s
2.05
1.98
1.00
2.09
3.07
f1 (ppm)


LSW-OAC-BR-I
169.18
151.01
136.59
128.40
121.92
61.05
21.19
9.88
Br
AcO
5s
f1 (ppm)

7. X-ray crystallographic data of 3q

To a glass vial (2 mL) was added **3q** (CCDC 1912785) (0.2 g) and charged with DCM/hexane (1 mL : 0.5 mL) and then sealed with a septum. The crystal of 3q grew slowly with the volatilization of solvents within 1 week.

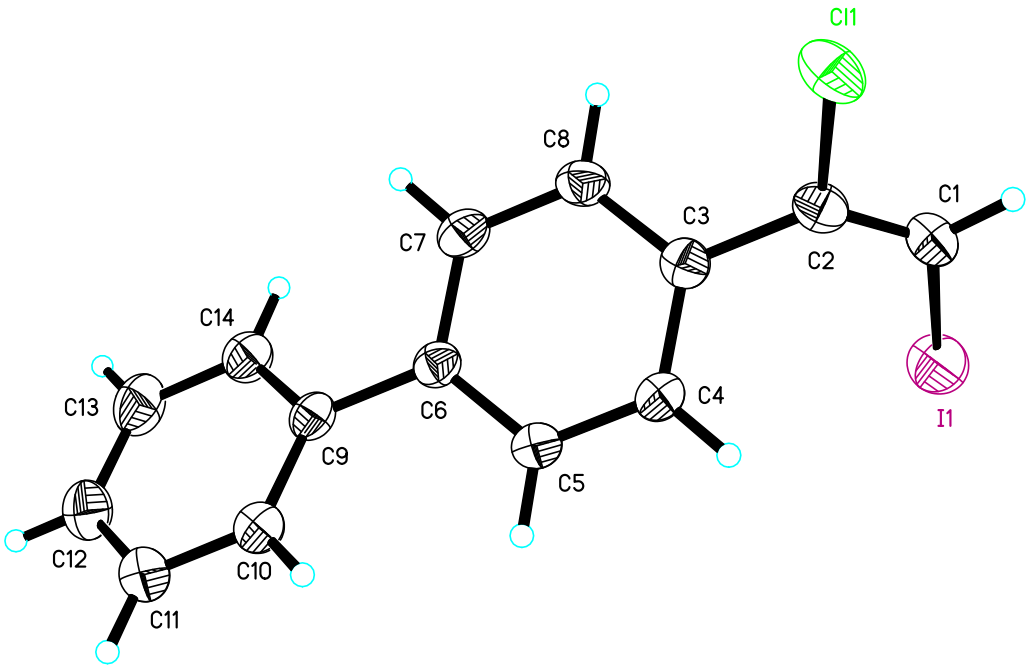


Figure S2. ORTEP drawing of 3q at the 50% probability level.

Table S2. Crystal data and structure refinement for mo_dd18319_0m.

Identification code mo_dd18319_0m

Empirical formula C14 H10 Cl I

Formula weight 340.57

Temperature 293(2) K

Wavelength 0.71073 Å

Crystal system Monoclinic

Space group P 21/c

Unit cell dimensions a = 9.7863(4) Å □= 90°.

b = 9.7114(3) Å □= 100.442(2)°.

c = 13.7154(5) Å □ = 90°.

Volume 1281.91(8) Å3

Z 4

Density (calculated) 1.765 Mg/m3

Absorption coefficient 2.676 mm-1

F(000) 656

Crystal size 0.170 x 0.150 x 0.110 mm3

Theta range for data collection 2.116 to 25.988°.

Index ranges -10<=h<=12, -11<=k<=10, -16<=l<=14

Reflections collected 6080

Independent reflections 2478 [R(int) = 0.0201]

Completeness to theta = 25.242° 98.7 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.7456 and 0.5529

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 2478 / 0 / 146

Goodness-of-fit on F2 1.050

Final R indices [I>2sigma(I)] R1 = 0.0397, wR2 = 0.0956

R indices (all data)R1 = 0.0474, wR2 = 0.1017

Extinction coefficient 0.0055(15)

Largest diff. peak and hole 1.069 and -0.788 e.Å-3

Table S3. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for mo_dd18319_0m. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
I(1)	7537(1)	10197(1)	3302(1)	78(1)
Cl(1)	8203(1)	7305(1)	722(1)	63(1)
C(1)	7781(4)	9237(5)	1995(3)	55(1)
C(2)	7857(4)	7890(4)	1879(3)	47(1)
C(3)	7684(4)	6774(4)	2581(3)	43(1)
C(4)	6471(4)	6649(4)	2952(3)	51(1)
C(5)	6295(4)	5596(4)	3591(3)	49(1)
C(6)	7339(4)	4628(4)	3894(3)	41(1)
C(7)	8554(4)	4758(4)	3504(3)	48(1)
C(8)	8719(4)	5803(4)	2862(3)	48(1)
C(9)	7159(4)	3508(4)	4593(3)	42(1)
C(10)	5864(4)	2960(4)	4629(3)	52(1)
C(11)	5697(5)	1921(5)	5286(4)	63(1)
C(12)	6827(5)	1410(5)	5927(4)	68(1)
C(13)	8114(5)	1929(5)	5894(4)	69(1)
C(14)	8298(4)	2968(4)	5239(3)	53(1)

Table S4. Anisotropic displacement parameters (Å2x 103) for mo_dd18319_0m. The anisotropic displacement factor exponent takes the form: -2□2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
I(1)	98(1)	57(1)	88(1)	-15(1)	38(1)	-5(1)
Cl(1)	74(1)	71(1)	47(1)	-2(1)	17(1)	-18(1)
C(1)	56(2)	54(2)	59(2)	8(2)	17(2)	-5(2)
C(2)	40(2)	53(2)	46(2)	-2(2)	6(2)	-8(2)
C(3)	44(2)	42(2)	43(2)	-4(2)	6(2)	-4(2)
C(4)	42(2)	47(2)	63(2)	8(2)	12(2)	9(2)
C(5)	43(2)	50(2)	57(2)	6(2)	16(2)	6(2)
C(6)	42(2)	40(2)	42(2)	-5(2)	8(2)	1(2)
C(7)	38(2)	52(2)	53(2)	-1(2)	3(2)	7(2)
C(8)	36(2)	54(2)	55(2)	-1(2)	11(2)	-2(2)
C(9)	48(2)	38(2)	41(2)	-6(2)	8(2)	5(2)
C(10)	49(2)	50(2)	59(2)	5(2)	10(2)	5(2)
C(11)	62(3)	53(3)	77(3)	10(2)	20(2)	2(2)
C(12)	78(3)	57(3)	72(3)	20(2)	17(3)	8(2)
C(13)	77(3)	62(3)	64(3)	16(2)	2(2)	17(3)
C(14)	52(2)	54(2)	52(2)	2(2)	6(2)	5(2)

Table S5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for mo_dd18319_0m.

	x	y	z	U(eq)
H(1)	7840	9793	1453	66
H(4)	5761	7286	2768	61
H(5)	5463	5528	3825	59
H(7)	9267	4124	3683	58
H(8)	9539	5861	2610	57
H(10)	5089	3298	4202	63
H(11)	4817	1566	5295	76
H(12)	6716	720	6377	82
H(13)	8883	1578	6320	83
H(14)	9184	3307	5230	63

Table S6. Torsion angles [°] for mo_dd18319_0m.

I(1)-C(1)-C(2)-C(3)	5.3(7)
I(1)-C(1)-C(2)-Cl(1)	-175.2(2)
C(1)-C(2)-C(3)-C(4)	58.2(6)
Cl(1)-C(2)-C(3)-C(4)	-121.4(4)
C(1)-C(2)-C(3)-C(8)	-123.7(5)
Cl(1)-C(2)-C(3)-C(8)	56.7(4)
C(8)-C(3)-C(4)-C(5)	0.6(6)
C(2)-C(3)-C(4)-C(5)	178.7(4)
C(3)-C(4)-C(5)-C(6)	0.7(7)
C(4)-C(5)-C(6)-C(7)	-1.4(6)
C(4)-C(5)-C(6)-C(9)	179.0(4)
C(5)-C(6)-C(7)-C(8)	0.9(6)
C(9)-C(6)-C(7)-C(8)	-179.6(4)
C(6)-C(7)-C(8)-C(3)	0.4(6)
C(4)-C(3)-C(8)-C(7)	-1.1(6)
C(2)-C(3)-C(8)-C(7)	-179.2(4)
C(7)-C(6)-C(9)-C(10)	-149.3(4)
C(5)-C(6)-C(9)-C(10)	30.2(5)
C(7)-C(6)-C(9)-C(14)	30.6(5)
C(5)-C(6)-C(9)-C(14)	-149.9(4)
C(14)-C(9)-C(10)-C(11)	0.5(6)
C(6)-C(9)-C(10)-C(11)	-179.6(4)
C(9)-C(10)-C(11)-C(12)	0.3(7)
C(10)-C(11)-C(12)-C(13)	-1.0(8)
C(11)-C(12)-C(13)-C(14)	0.9(8)

C(12)-C(13)-C(14)-C(9) -0.1(7)

C(10)-C(9)-C(14)-C(13) -0.6(6)

C(6)-C(9)-C(14)-C(13) 179.5(4)

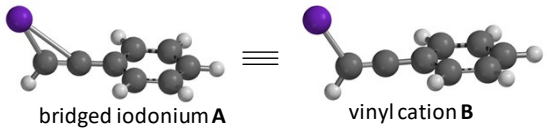
Symmetry transformations used to generate equivalent atoms:

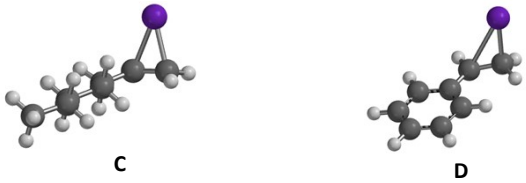
Table S7. Hydrogen bonds for mo_dd18319_0m [Å and °].

D-H...A d(D-H) d(H...A) d(D...A) <(DHA)

---

8. Calculated geometries of intermediates





Intermediate **A**

```
SPARTAN '14 Quantum Mechanics Driver: (Win/32b) Release 1.1.0
Job type: Geometry optimization.
Method: RDFTWB97X-D
Basis set: 6-311+G**
Number of shells: 96
Number of basis functions: 274
Charge : +1
Multiplicity: 1
Parallel Job: 8 threads

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization


Optimization:
Step Energy Max Grad. Max Dist.
1 -7227.758801 0.013729 0.155116
2 -7227.759158 0.005778 0.081724
3 -7227.759361 0.001178 0.008483
4 -7227.759373 0.000649 0.003919
5 -7227.759376 0.000244 0.003100
6 -7227.759376 0.000161 0.001631

Reason for exit: Successful completion
Quantum Calculation CPU Time : 14:31.38
Quantum Calculation Wall Time: 20:13.75
```

SPARTAN '14 Semi-Empirical Program: (Win/32b) Release 1.1.0
Semi-empirical Property Calculation

M0001
Memory Used: 557.62 Kb

Reason for exit: Successful completion
Semi-Empirical Program CPU Time : .31
Semi-Empirical Program Wall Time: .02

SPARTAN '14 Properties Program: (Win/32b) Release 1.1.0
Use of molecular symmetry disabled

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 H	H1	-1.8719746	-2.1596143	0.3832351
2 C	C1	-2.4071402	-1.2363950	0.1962588
3 C	C4	-3.7260106	1.2158294	-0.2680792
4 C	C2	-1.7402455	0.0110907	0.4000880
5 C	C6	-3.7108784	-1.2368777	-0.2332296
6 C	C5	-4.3611631	-0.0175480	-0.4622777
7 C	C3	-2.4220687	1.2438693	0.1599514
8 H	H6	-4.2352819	-2.1697948	-0.3954389
9 H	H5	-5.3914010	-0.0287605	-0.8017611
10 H	H3	-1.8983917	2.1786946	0.3194759
11 H	H4	-4.2621695	2.1369674	-0.4565310
12 C	C7	-0.4506261	0.0240168	0.8216612
13 C	C8	0.7758982	0.0328539	1.1846715
14 I	I1	2.2624152	0.0130282	-0.3020809
15 H	H9	1.0952716	0.0496949	2.2224296

Point Group = C1 Order = 1 Nsymop = 1

Intermediate **B** has identitical geometry as intermediate **A**

Intermediate **C**

SPARTAN '14 MECHANICS PROGRAM: (Win/32b) Release 1.1.0

Frequency Calculation

Warning: global charge (+0.00) does not match input file (+1)!
Adjusted 5 (out of 66) low frequency modes

Reason for exit: Successful completion
Mechanics CPU Time : .64
Mechanics Wall Time: .37

SPARTAN '14 Quantum Mechanics Driver: (Win/32b) Release 1.1.0

Job type: Geometry optimization.
Method: RB3LYP
Basis set: 6-31G* & LANL2DZ>Kr
Number of shells: 61
Number of basis functions: 147
Multiplicity: 1
Parallel Job: 4 threads

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

Optimization:
Step Energy Max Grad. Max Dist.
1 -286.266825 0.037863 0.175851
2 -286.271671 0.007064 0.141671
3 -286.271315 0.005188 0.118204
4 -286.271976 0.005218 0.244219
5 -286.272018 0.004271 0.165318
6 -286.271624 0.006251 0.058949
7 -286.272417 0.000997 0.015420
8 -286.272440 0.000752 0.023524
9 -286.272449 0.000236 0.036684
10 -286.272454 0.000653 0.005971
11 -286.272458 0.000195 0.003232

12 -286.272459 0.000108 0.002999

Reason for exit: Successful completion
Quantum Calculation CPU Time : 4:51.31
Quantum Calculation Wall Time: 11:29.53

SPARTAN '14 Semi-Empirical Program: (Win/32b) Release 1.1.0
Semi-empirical Property Calculation

M0001
Memory Used: 719.24 Kb

Reason for exit: Successful completion
Semi-Empirical Program CPU Time : .47
Semi-Empirical Program Wall Time: .02

SPARTAN '14 Properties Program: (Win/32b) Release 1.1.0
Use of molecular symmetry disabled

Cartesian Coordinates (Angstroms)
Atom X Y Z
--------- ------------- ------------- -------------

1 C C7 0.7714962 1.5603948 0.1744514
2 H H8 1.3646764 2.2228771 0.8047220
3 C C8 1.3675105 1.1902717 -1.0932171
4 H H2 0.7405063 0.7411031 -1.8588569
5 H H9 2.2304180 1.7492402 -1.4478873
6 I I1 2.1430833 -0.4359937 0.2151378
7 C C1 -0.6568557 1.3919660 0.5457428
8 H H3 -1.0464951 2.4206763 0.3888865
9 H H7 -0.7291649 1.2496575 1.6316511
10 C C2 -1.5222939 0.3854405 -0.2207840
11 H H1 -1.0843853 -0.6181323 -0.1326327
12 H H4 -1.5364847 0.6365075 -1.2897573
13 C C3 -2.9652771 0.3509430 0.3079300
14 H H5 -2.9523706 0.0964347 1.3772913
15 H H10 -3.4078331 1.3542134 0.2336756
16 C C4 -3.8458008 -0.6557162 -0.4448534

17 H H6 -3.3831902 -1.6512895 -0.3905844
18 H H11 -3.8728205 -0.3865884 -1.5098637
19 C C5 -5.2728802 -0.7239448 0.1063305
20 H H12 -5.2783273 -1.0282086 1.1596338
21 H H13 -5.8728466 -1.4492760 -0.4520201
22 H H14 -5.7756172 0.2477434 0.0363862

Intermediate **D**

SPARTAN '14 Quantum Mechanics Driver: (Win/32b) Release 1.1.0
Job type: Geometry optimization.
Method: RB3LYP
Basis set: 6-31G* & LANL2DZ>Kr
Number of shells: 53
Number of basis functions: 150
Multiplicity: 1
Parallel Job: 4 threads

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

Optimization:
Step Energy Max Grad. Max Dist.
1 -320.698706 0.035062 0.207173
2 -320.713781 0.025046 0.212035
3 -320.724588 0.020347 0.230662
4 -320.732822 0.016244 0.224955
5 -320.739334 0.013545 0.215704
6 -320.744848 0.011728 0.204188
7 -320.749800 0.010649 0.198502
8 -320.754394 0.009755 0.192977
9 -320.758774 0.009014 0.188802
10 -320.763063 0.008115 0.189877
11 -320.767001 0.006593 0.191244
12 -320.770414 0.006646 0.181636
13 -320.773179 0.006515 0.168861
14 -320.775130 0.005086 0.174281

```
15 -320.776095 0.005308 0.202812
16 -320.776928 0.006898 0.099844
17 -320.777349 0.006860 0.075329
18 -320.778046 0.002153 0.062140
19 -320.778114 0.002566 0.028765
20 -320.778228 0.000520 0.009730
21 -320.778233 0.000399 0.014025
22 -320.778237 0.000313 0.008093
23 -320.778239 0.000164 0.003170
24 -320.778240 0.000081 0.002034

Reason for exit: Successful completion
Quantum Calculation CPU Time : 9:27.30
Quantum Calculation Wall Time: 25:36.73


SPARTAN '14 Semi-Empirical Program: (Win/32b) Release 1.1.0
Semi-empirical Property Calculation

M0001
Memory Used: 622.27 Kb

Reason for exit: Successful completion
Semi-Empirical Program CPU Time : .61
Semi-Empirical Program Wall Time: .04


SPARTAN '14 Properties Program: (Win/32b) Release 1.1.0
Use of molecular symmetry disabled

Cartesian Coordinates (Angstroms)
Atom X Y Z
--------- ------------- ------------- -------------

1 H H1 -0.6551815 -1.0715584 -1.3137798
2 C C1 -1.4755613 -0.6269607 -0.7604824
3 C C4 -3.6104503 0.5181705 0.6970624
4 C C2 -1.3012695 0.6244506 -0.0890517
5 C C6 -2.6903004 -1.2771095 -0.6981492
6 C C5 -3.7549121 -0.7067655 0.0267874
7 C C3 -2.3976082 1.1777440 0.6464324
```

8 H H6 -2.8301411 -2.2262071 -1.2049148
9 H H5 -4.7072598 -1.2280689 0.0681840
10 H H3 -2.2635927 2.1251400 1.1611959
11 H H4 -4.4433201 0.9387049 1.2504664
12 C C7 -0.1100984 1.3601429 -0.1347166
13 H H8 -0.0997193 2.3107509 0.3971284
14 C C8 1.1355208 1.0152343 -0.8163804
15 H H2 1.1077202 0.1852841 -1.5170706
16 H H9 1.6742198 1.8747555 -1.2127405
17 I I1 2.2888321 0.3721624 0.9475240

Point Group = C1 Order = 1 Nsymop = 1

Closed-Shell Molecular Orbital Coefficients
MO: 1 2 3 4 5
Eigenvalues: -10.44549 -10.41629 -10.39679 -10.38900 -10.38819
(ev) -284.23632 -283.44177 -282.91121 -282.69928 -282.67711

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