Supporting Information

Sulfinyl Isobutyramide as an Auxiliary for Palladium(II)-Catalyzed C–H Arylation and Iodination of Benzylamine Derivatives

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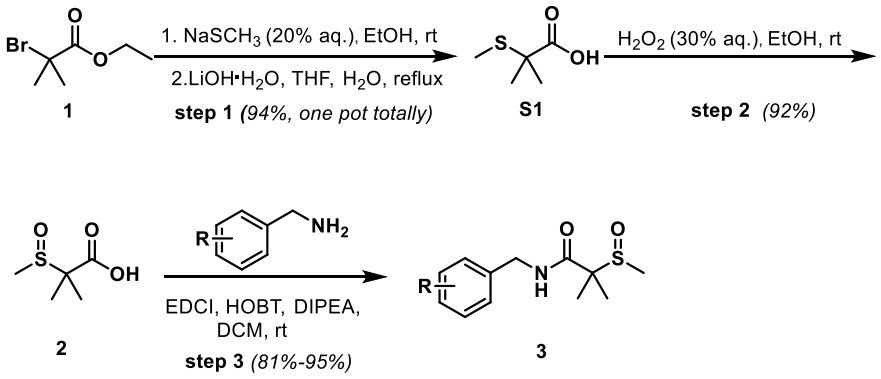
1. General Information

Unless otherwise noted, the commercial available reagents were purchased from commercial suppliers (such as Strem, J&K Chemical Co., Energy Chemical and Sinopharm,), and used as received. Solvents were dried over 4 Å molecular sieves. Hexafluoroisopropanol (HFIP) was distilled before use. Unless otherwise noted, all reactions were run under air and the indicated reaction temperature was that of the oil bath. The reaction vessels used for C–H functionalization were 38 mL sealed tube (Synthware). Purification of products was performed by flash chromatography (FC) using silica gel or preparative thin layer chromatography. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE III spectrometer (400 MHz and 101 MHz, respectively). Chemical shifts are reported parts per million (ppm) referenced to $CDCl_3$ (δ 7.26 ppm) for ^{1}H NMR, $CDCl_3$ (δ 77.16 ppm) for ^{13}C NMR or tetramethylsilane (TMS, δ 0.00 ppm for 1H NMR), MeOD (δ 49.00 ppm) for ^{13}C NMR. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet and br = broad. High-resolution mass spectra (HRMS) were obtained on Impact II UHR-TOF from Bruker with an ESI source at Fujian Institute of Research on the Structure of Matter.

2. Experimental Section

2.1 Preparation and characterization of substrates.



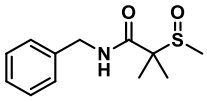
Scheme S1. General procedure for preparing substrates

Step 1: A round-bottom flask was charged with ethyl 2-bromo-2-methylpropanoate **1** (9.75 g, 50 mmol) and $NaSCH_3$ (20% aq., 31 mL, 100 mmol). Then ethanol (50 mL) was added, the mixture was stirred for 12 hours at room temperature. Then THF (50 mL), H_2O (15 mL) and $LiOH·H_2O$ (6.30 g, 150 mmol) were added, the mixture were stirred at 90 °C under reflux for 4 hours. Then the reaction mixture was cooled to 0 °C, and an aqueous

solution of hydrochloric acid was added dropwise till the pH was adjusted to 2. The solvent was removed under reduced pressure, and the residue was washed with brine and extracted with EtOAc (70 mL × 5). The combined organic phase was dried on Na_2SO_4, filtered and concentrated *in vacuo* to afford compound 2-methyl-2-methylthiopropanoic acid **S1** (6.28 g, 94%) as a light yellow oil. **S1**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.77 (brs, 1H), 2.17 (s, 3H), 1.52 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 180.3, 46.1, 24.8, 13.2.

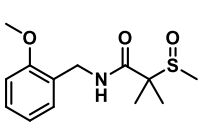
Step 2: To a solution of product **S1** (without purification, 47 mmol) from Step 1 stirred in EtOH (12 mL) was added H_2O_2 (30% aq., 5.11 mL, 50 mmol) dropwise at 0 °C. The mixture was stirred for another 3 hours at room temperature and quenched with Pd/C (10%, 35 mg) for 0.5 h.[S1] Then the mixture was filtered with Celite pad and the filtrate concentrated *in vacuo*. The residue could be easily purified by silica gel chromatography with EtOAc to afford compound 2-methyl-2-(methylsulfinyl) propanoic acid **2** (6.46 g, 92%) as a white solid. **2:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (brs, 1H), 2.64 (s, 3H), 1.61 (s, 3H), 1.47 (s, 3H); ^{13}C NMR (101 MHz, MeOD) δ 173.7, 63.5, 33.5, 20.6, 16.6; HRMS (m/z, ESI-TOF): Calcd for $C_5H_{10}NaO_3S^+$ [M+Na$^+$] 173.0243, found 173.0243.

Step 3: To a solution of **2** (1.55 g, 10.3 mmol) and benzylamine (1.1 mL, 10.1 mmol) in CH_2Cl_2 (15 mL) at room temperature was added 1-Hydroxybenzotriazole (1.46 g, 10.8 mmol), *N*,*N*-Diisopropylethylamine (1.9 mL, 10.8 mmol) and EDCI (2.07 g, 10.8 mmol). The mixture was stirred for 5 hours at room temperature. Then the mixture was washed with diluted solution of sodium bicarbonate and extracted with CH_2Cl_2 (60 mL × 3). The combined organic phase was dried on Na_2SO_4, filtered and concentrated *in vacuo.* The residue can be purified by silica gel chromatography with petroleum ether/EtOAc (4:1) to afford compound *N*-benzyl-2-methyl-2-(methylsulfinyl)propanamide **3a** (2.11 g, 86%).



3a

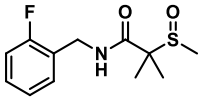
***N*-benzyl-2-methyl-2-(methylsulfinyl)propanamide:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.35-7.24 (m, 5H), 4.55-4.45 (ABm, J_{AB} = 14.8 Hz, 2H), 2.41 (s, 3H), 1.64 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 138.3, 128.8, 128.0, 127.6, 59.3, 43.7, 33.0, 23.0, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{18}NO_2S^+$ [M+H$^+$] 240.1053, found 240.1056.



3b

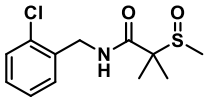
***N*-(2-methoxybenzyl)-2-methyl-2-(methylsulfinyl)propanamide:** From 2-methoxybenzylamine (1 equiv, 411 mg, 3 mmol) following the **Step 3** for 6 hours

yielded the title compound (702.3 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (s, 1H), 7.30-7.26 (m, 2H), 6.92-6.85 (m, 2H), 4.48 (ABqd, J_{AB} = 14.3 Hz, J_d = 5.7 Hz, 2H), 3.85 (s, 3H), 2.33 (s, 3H), 1.59 (s, 3H), 1.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 157.6, 129.9, 129.0, 126.2, 120.6, 110.3, 59.4, 55.4, 39.6, 32.8, 22.6, 18.8. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{20}NO_3S^+$ [M+H$^+$] 270.1158, found 270.1160.



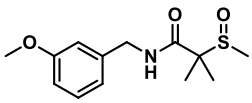
3c

***N*-(2-fluorobenzyl)-2-methyl-2-(methylsulfinyl)propanamide:** From 2-fluorobenzylamine (1 equiv, 375 mg, 3 mmol) following the **Step 3** for 7 hours yielded the title compound (647.9 mg, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.38-7.35 (m, 1H), 7.28-7.24 (m, 1H), 7.12-7.08 (m, 1H), 7.07-7.03 (m, 1H), 4.60-4.50 (ABm, J_{AB} = 16.0 Hz, 2H), 2.41 (s, 3H), 1.63 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 161.0 (d, $J_{C\text{-}F}$ = 247.7 Hz), 130.4 (d, $J_{C\text{-}F}$ = 4.2 Hz), 129.5 (d, $J_{C\text{-}F}$ = 8.1 Hz), 125.2 (d, $J_{C\text{-}F}$ = 14.9 Hz), 124.4 (d, $J_{C\text{-}F}$ = 3.7 Hz), 115.6 (d, $J_{C\text{-}F}$ = 21.3 Hz), 59.3, 37.7 (d, $J_{C\text{-}F}$ = 4.0 Hz), 33.0, 22.9, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{17}FNO_2S^+$ [M+H$^+$] 258.0959, found 258.0960.



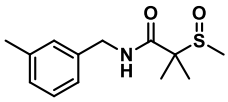
3d

***N*-(2-chlorobenzyl)-2-methyl-2-(methylsulfinyl)propanamide:** From 2-chlorobenzylamine (1 equiv, 708 mg, 5 mmol) following the **Step 3** for 6 hours yielded the title compound (1.22 g, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (s, 1H), 7.43-7.41 (m, 1H), 7.38-7.36 (m, 1H), 7.26-7.20 (m, 2H), 4.59 (ABqd, J_{AB} = 14.8 Hz, J_d = 5.6 Hz, 2H), 2.41 (s, 3H), 1.64 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 135.6, 133.8, 130.4, 129.7, 129.1, 127.1, 59.4, 41.7, 33.0, 22.9, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{16}ClNNaO_2S^+$ [M+Na$^+$] 296.0482, found 296.0487.



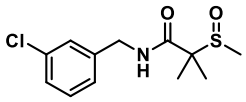
3e

***N*-(3-methoxybenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** From 3-methoxybenzylamine (1 equiv, 343 mg, 2.5 mmol) following the **Step 3** for 7 hours yielded the title compound (639 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.25-7.21 (m, 1H), 6.89 (d, J = 7.1 Hz, 1H), 6.85 (s, 1H), 6.79 (d, J = 7.8 Hz, 1H), 4.52-4.42 (ABm, 2H), 3.79 (s, 3H), 2.43 (s, 3H), 1.64 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 159.9, 139.8, 129.8, 120.1, 113.3, 113.0, 59.3, 55.3, 43.5, 33.0, 22.8, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{19}NNaO_3S^+$ [M+Na$^+$] 292.0978, found 292.0982.



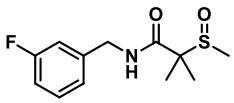
3f

2-methyl-*N*-(3-methylbenzyl)-2-(methylsulfinyl)propanamide: From 3- methylbenzylamine (1 equiv, 424 mg, 3.5 mmol) following the **Step 3** for 7 hours yielded the title compound (769 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.23-7.19 (m, 1H), 7.15-7.02 (m, 3H), 4.46 (ABqd, J_{AB} = 14.7 Hz, J_d = 5.8 Hz, 2H), 2.42 (s, 3H), 2.33 (s, 3H), 1.63 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 138.4, 138.2, 128.7, 128.7, 128.3, 124.9, 59.3, 43.6, 33.0, 22.9, 21.5, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{19}NNaO_2S^+$ [M+Na$^+$] 276.1029, found 276.1029.



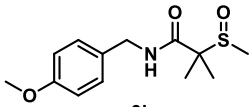
3g

***N*-(3-chlorobenzyl)-2-methyl-2-(methylsulfinyl)propanamide:** From 3- chlorobenzylamine (1 equiv, 427 mg, 3 mmol) following the **Step 3** for 7 hours yielded the title compound (698 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.31 (s, 1H), 7.28-7.17 (m, 3H), 4.47 (ABqd, J_{AB} = 15.0 Hz, J_d = 6.0 Hz, 2H), 2.43 (s, 3H), 1.65 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 140.4, 134.6, 130.1, 128.1, 127.7, 126.0, 59.3, 43.1, 33.0, 23.0, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{16}ClNNaO_2S^+$ [M+Na$^+$] 296.0482, found 296.0480.



3h

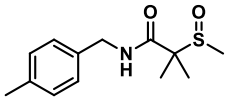
***N*-(3-fluorobenzyl)-2-methyl-2-(methylsulfinyl)propanamide:** From 3- fluorobenzylamine (1 equiv, 440 mg, 3.5 mmol) following the **Step 3** for 6 hours yielded the title compound (790.2 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.33-7.27 (m, 1H), 7.09 (d, J = 7.5 Hz, 1H), 7.02 (d, J = 9.6 Hz, 1H), 6.96 (t, J = 8.4 Hz, 1H), 4.49 (ABqd, J_{AB} = 15.0 Hz, J_d = 5.9 Hz, 2H), 2.43 (s, 3H), 1.65 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 163.0 (d, $J_{C\text{-}F}$ = 247.5 Hz), 140.9 (d, $J_{C\text{-}F}$ = 7.1 Hz), 130.3 (d, $J_{C\text{-}F}$ = 8.3 Hz), 123.5 (d, $J_{C\text{-}F}$ = 2.9 Hz), 114.8 (d, $J_{C\text{-}F}$ = 21.8 Hz), 114.5 (d, $J_{C\text{-}F}$ = 21.1 Hz), 59.3, 43.1 (d, J = 1.7 Hz), 33.0, 23.1, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{17}FNO_2S^+$ [M+H$^+$] 258.0959, found 258.0957.



3i

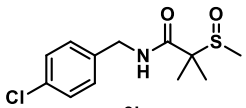
***N*-(4-methoxybenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** From 4- methoxybenzylamine (1 equiv, 412 mg, 3 mmol) following the **Step 3** for 7

hours yielded the title compound (653 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (s, 1H), 7.24 (d, *J* = 8.4 Hz, 2H), 6.85 (d, *J* = 8.4 Hz, 2H), 4.49-4.38 (ABm, 2H), 3.79 (s, 3H), 2.40 (s, 3H), 1.62 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 159.0, 130.5, 129.4, 114.1, 59.3, 55.4, 43.2, 33.0, 22.9, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{20}NO_3S^+$ [M+H$^+$] 270.1158, found 270.1156.



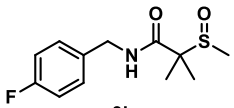
3j

2-methyl-*N*-(4-methylbenzyl)-2-(methylsulfinyl)propanamide: From 4- methylbenzylamine (1 equiv, 316 mg, 2.6 mmol) following the **Step 3** for 7 hours yielded the title compound (546 mg, 83%).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (s, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 7.9 Hz, 2H), 4.45(ABqd, J_{AB} = 14.8 Hz, J_d = 5.8 Hz, 2H), 2.41 (s, 3H), 2.32 (s, 3H), 1.62 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 137.2, 135.3, 129.5, 128.0, 59.3, 43.5, 33.1, 22.9, 21.2, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{19}NNaO_2S^+$ [M+Na$^+$] 276.1029, found 276.1029.



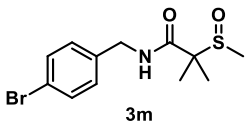
3k

***N*-(4-chlorobenzyl)-2-methyl-2-(methylsulfinyl)propanamide:** From 4- chlorobenzylamine (1 equiv, 354 mg, 2.5 mmol) following the **Step 3** for 7 hours yielded the title compound (560 mg, 82%).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.31-7.24 (m, 4H), 4.50-4.40 (ABm, J_{AB} = 15.2 Hz, 2H), 2.40 (s, 3H), 1.63 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 136.9, 133.4, 129.4, 128.9, 59.3, 43.0, 33.0, 23.1, 18.6. Calcd for $C_{12}H_{17}ClNO_2S^+$ [M+H$^+$] 274.0663, found 274.0662.



3l

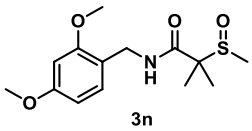
***N*-(4-fluorobenzyl)-2-methyl-2-(methylsulfinyl)propanamide:** From 4- fluorobenzylamine (1 equiv, 313 mg, 2.5 mmol) following the **Step 3** for 7 hours yielded the title compound (553 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.32-7.27 (m, 2H), 7.07-6.94 (m, 2H), 4.50-4.41 (ABm, 2H), 2.39 (s, 3H), 1.63 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 162.3 (d, *J* = 246.5 Hz), 134.2 (d, *J* = 3.3 Hz), 129.8 (d, *J* = 8.2 Hz), 115.6 (d, *J* = 21.6 Hz), 59.3, 43.0, 33.0, 23.1, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{17}FNO_2S^+$ [M+H$^+$] 258.0959, found 258.0961.



3m

***N*-(4-bromobenzyl)-2-methyl-2-(methylsulfinyl)propanamide**

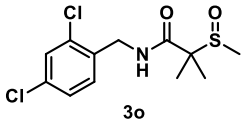
From 4- bromobenzylamine (1 equiv, 518 mg, 2.8 mmol) following the **Step 3** for 7 hours yielded the title compound (719.3 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.45 (d, J = 8.3 Hz, 2H), 7.20 (d, J = 8.3 Hz, 2H), 4.50-4.38 (ABm, J_{AB} = 15.2 Hz, 2H), 2.40 (s, 3H), 1.63 (s, 3H), 1.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 137.5, 131.9, 129.7, 121.4, 59.3, 43.1, 33.0, 23.1, 18.5. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{16}BrNNaO_2S^+$ [M+Na$^+$] 339.9977, found 339.9979.



3n

***N*-(2,4-dimethoxybenzyl)-2-methyl-2-(methylsulfinyl)**

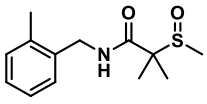
propanamide: From 2,4-dimethoxybenzylamine (1 equiv, 518 mg, 3.1 mmol) following the **Step 3** for 7 hours yielded the title compound (778 mg, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (s, 1H), 7.20 (d, J = 8.1 Hz, 1H), 6.44-6.40 (m, 2H), 4.45 (ABqd, J_{AB} = 14.2 Hz, J_d = 6.0 Hz, 1H), 4.35 (ABqd, J_{AB} = 14.2 Hz, J_d = 5.4 Hz, 1H), 3.82 (s, 3H), 3.79 (s, 3H), 2.32 (s, 3H), 1.58 (s, 3H), 1.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 160.6, 158.6, 130.6, 118.9, 103.9, 98.6, 59.4, 55.5, 55.4, 39.2, 32.9, 22.5, 18.8. HRMS (m/z, ESI-TOF): Calcd for $C_{14}H_{21}NNaO_4S^+$ [M+Na$^+$] 322.1083, found 322.1086.



3o

***N*-(2,4-dichlorobenzyl)-2-methyl-2-(methylsulfinyl) propanamide:**

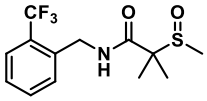
From 2,4-dichlorobenzylamine (1 equiv, 440 mg, 2.5 mmol) following the **Step 3** for 7 hours yielded the title compound (675.5 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (s, 1H), 7.38-7.36 (m, 2H), 7.23-7.21 (m, 1H), 4.58-4.49 (ABm, 2H), 2.41 (s, 3H), 1.63 (s, 3H), 1.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 134.4, 134.3, 134.1, 131.2, 129.5, 127.4, 59.3, 41.2, 33.0, 23.0, 18.5. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{16}Cl_2NO_2S^+$ [M+H$^+$] 308.0273, found 308.0275.



3p

2-methyl-*N*-(2-methylbenzyl)-2-(methylsulfinyl)propanamide: From 2- methylbenzylamine (1 equiv, 605 mg, 5 mmol) following the **Step 3** for 7 hours yielded the title compound (1.16 g, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (s, 1H), 7.33-7.27 (m, 1H), 7.22-7.11 (m, 3H), 4.54 (ABqd, J_{AB} = 14.8 Hz, J_d = 5.9 Hz, 1H), 4.45

(ABqd, J_{AB} = 14.8 Hz, J_d =5.4 Hz, 1H), 2.40 (s, 3H), 2.36 (s, 3H), 1.63 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 136.2, 135.8, 130.5, 128.7, 127.7, 126.2, 59.3, 41.7, 32.9, 22.8, 19.2, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{19}NNaO_2S^+$ [M+Na$^+$] 276.1029, found 276.1029.



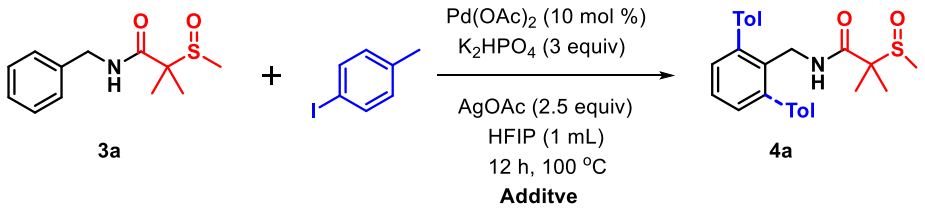
3q

2-methyl-2-(methylsulfinyl)-*N*-(2-(trifluoromethyl)benzyl) propanamide: From (2-(trifluoromethyl)phenyl)methanamine (1 equiv, 525 mg, 3 mmol) following the **Step 3** for 7 hours yielded the title compound (819 mg, 90%).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 7.8 Hz, 1H), 7.61-7.46 (m, 3H), 7.38 (t, J = 7.3 Hz, 1H), 4.75 (ABqd, J_{AB} = 15.3 Hz, J_d = 5.3 Hz, 1H), 4.64 (ABqd, J_{AB} = 15.4, J_d = 5.2 Hz, 1H), 2.43 (s, 3H), 1.63 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 136.5, 132.3, 130.3, 128.3 (q, J_{C-F} = 31.3 Hz), 127.7, 126.2 (q, J_{C-F} = 5.6 Hz), 124.4 (q, J_{C-F} = 274.8 Hz), 59.3, 40.2, 33.0, 22.7, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{17}F_3NO_2S^+$ [M+H$^+$] 308.0927, found 308.0927.

2.2 Reaction conditions optimization for *ortho*-C–H bond arylation.

General optimization procedure: A 38 mL Schlenk sealed tube (with a Teflon cap) equipped with a magnetic stir bar was charged with amide **3a** (23.9 mg, 0.10 mmol, 1.0 equiv), *p-iodotoluene* (65.5mg, 0.30 mmol, 3.0 equiv), $Pd(OAc)_2$ (2.3 mg, 0.01 mmol, 10 mol %), AgOAc (41.8 mg, 0.25 mmol, 2.5 equiv), K_2HPO_4 (52.2 mg, 0.30 mmol, 3.0 equiv) and Additives (20 mol %). Then HFIP (1 mL) was added along the inside wall of the tube. The tube was then capped and submerged into a preheated set temperature oil bath. The reaction was stirred for 24 h and cooled to room temperature. The crude reaction mixture was diluted with EtOAc (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 30 mL of EtOAc. The filtrate was concentrated *in vacuo*, crude ^{1}H NMR spectrum was taken using CH_2Br_2 as internal standard.

Table S1. Screening of the ligands or other additives effecting arylation process.[a]



3a 4a

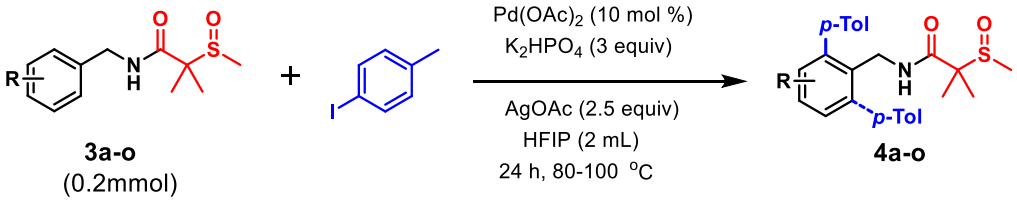
Entry	Additive (20 mol %)	Yield[%][b](product)
1	PivOH	5(**4a**$_{mono}$), 71(**4a**$_{di}$)
2	TsOH·H_2O	2(**4a**$_{mono}$), 88(**4a**$_{di}$)
3	TFA	5(**4a**$_{mono}$), 67(**4a**$_{di}$)

4	2,4,6-Trimethylbenzoic acid	7(**4a**$_{mono}$), 69(**4a**$_{di}$)
5	$(BnO)_2PO_2$	5(**4a**$_{mono}$), 71(**4a**$_{di}$)
6	DMF	3(**4a**$_{mono}$), 80(**4a**$_{di}$)
7	DMSO	3(**4a**$_{mono}$), 74(**4a**$_{di}$)
8	**2**	6(**4a**$_{mono}$), 43(**4a**$_{di}$)
9	Ac-Phe-OH	5(**4a**$_{mono}$), 87(**4a**$_{di}$)
10	Ac-Leu-OH	4(**4a**$_{mono}$), 86(**4a**$_{di}$)
11	Ac-Gly-OH	4(**4a**$_{mono}$), 85(**4a**$_{di}$)
12	Formyl-Gly-OH	7(**4a**$_{mono}$), 69(**4a**$_{di}$)
13[c]	Formyl-Gly-OH	4(**4a**$_{mono}$), 40(**4a**$_{di}$)
14[c]	CH_3CN	4(**4a**$_{mono}$), 12(**4a**$_{di}$)
15	2-Chloropyridine	trace(**4a**$_{mono}$), 17(**4a**$_{di}$)
16	2-(Trifluoromethyl)pyridine	5(**4a**$_{mono}$), 71(**4a**$_{di}$)
17	2,6-Dichloropyridine	3(**4a**$_{mono}$), 66(**4a**$_{di}$)

[a)]Reaction conditions: amide **3a** (0.10 mmol), *p-iodotoluene* (0.30 mmol, 3 equiv), $Pd(OAc)_2$ (0.01 mmol, 10 mol %), K_2HPO_4 (0.30 mmol, 3 equiv), AgOAc (0.25 mmol, 2.5 equiv) and additives (0.02 mmol, 20 mol %) in HFIP (1.0 mL), 100 °C, 12 h. [b)]Yield was determined by ^1H NMR with CH_2Br_2 as internal standard. [c)] Additive (0.06 mmol, 60 mol %) was used.

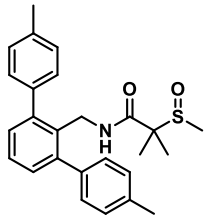
2.3 *ortho*-Arylation of benzylamine.

2.3.1 General procedure for *ortho*-arylation of benzylamine derivatives with *p*-iodotoluene.



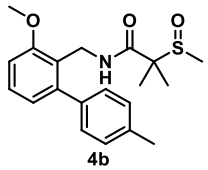
3a-o (0.2mmol) **4a-o**

A 38 mL Schlenk sealed tube (with a Teflon cap) equipped with a magnetic stir bar was charged with amide **3** (0.20 mmol, 1.0 equiv), *p*-iodotoluene (130.8 mg, 0.60 mmol, 3.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol %), AgOAc (83.5 mg, 0.50 mmol, 2.5 equiv) and K_2HPO_4 (104.4 mg, 0.6 mmol, 3.0 equiv). Then HFIP (2 mL) was added along the inside wall of the tube. The tube was then capped and submerged into a preheated set temperature oil bath. The reaction was stirred for 12 h and cooled to room temperature. The crude reaction mixture was diluted with EtOAc (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 50 mL of EtOAc. The filtrate was concentrated *in vacuo*, crude ^1H NMR spectrum was taken using CH_2Br_2 as internal standard. The resulting residue was purified by preparative thin layer chromatography or flash chromatography using petroleum ether/EtOAc as the eluent.



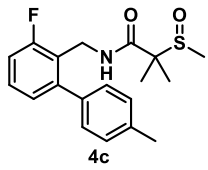
4a$_{di}$

***N*-((4,4''-dimethyl-[1,1':3',1''-terphenyl]-2'-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 68.9 mg, 82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (t, *J* = 7.6 Hz, 1H), 7.27-7.17 (m, 10H), 6.82 (s, 1H), 4.35 (dd, *J* = 13.8, 5.4 Hz, 1H), 4.20 (dd, *J* = 13.8, 2.3 Hz, 1H), 2.38 (s, 6H), 2.22 (s, 3H), 1.34 (s, 3H), 1.13 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9, 143.9, 138.4, 137.0, 131.6, 129.8, 129.1, 128.9, 127.7, 59.2, 40.0, 32.8, 21.9, 21.3, 18.8. HRMS (m/z, ESI-TOF): Calcd for $C_{26}H_{30}NO_2S^+$ [M+H$^+$] 420.1992, found 420.1996.



4b

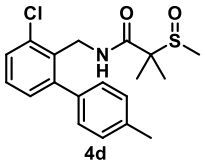
***N*-((3-methoxy-4'-methyl-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 44.5 mg, 62%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (brs, 1H), 7.29 (t, *J* = 8.0 Hz, 1H), 7.24-7.18 (m, 4H), 6.91-6.88 (m, 1H), 6.88-6.85 (m, 1H), 4.42 (d, *J* = 4.8 Hz, 2H), 3.89 (s, 3H), 2.41 (s, 3H), 2.38 (s, 3H), 1.53 (s, 3H), 1.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.4, 158.5, 144.1, 137.7, 137.0, 129.2, 129.0, 128.5, 123.2, 122.7, 109.3, 59.5, 55.7, 37.2, 32.9, 22.2, 21.3, 18.9. HRMS (m/z, ESI-TOF): Calcd for $C_{20}H_{26}NO_3S^+$ [M+H$^+$] 360.1628, found 360.1630.



4c

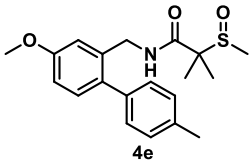
***N*-((3-fluoro-4'-methyl-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 55.1 mg, 79%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (td, *J* = 8.0, 5.8 Hz, 1H), 7.23-7.20 (m, 5H), 7.10-7.02 (m, 2H), 4.52-4.40 (ABm, 2H), 2.41 (s, 3H), 2.40 (s, 3H), 1.52 (s, 3H), 1.25 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 161.9 (d, $J_{C\text{-}F}$ = 248.5 Hz), 144.8 (d, $J_{C\text{-}F}$ = 3.7 Hz), 137.5, 136.6 (d, $J_{C\text{-}F}$ = 2.6 Hz), 129.1, 129.1 (d, $J_{C\text{-}F}$ = 9.8 Hz), 129.0, 126.1 (d, $J_{C\text{-}F}$ = 3.0 Hz), 122.3 (d, $J_{C\text{-}F}$ = 14.6 Hz), 114.4

(d, $J_{C\text{-}F}$ = 22.4 Hz), 59.3, 35.9 (d, $J_{C\text{-}F}$ = 4.1 Hz), 32.9, 22.5, 21.3, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{19}H_{22}FNNaO_2S^+$ [M+Na^+] 370.1247, found 370.1248.



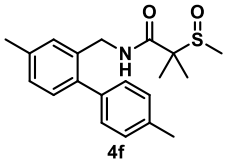
4d

***N*-((3-chloro-4'-methyl-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 63.4 mg, 87%; 1.12 g, 77% in a 4 mmol (1.10 gram) scale. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.9 Hz, 1H), 7.31-7.15 (m, 7H), 4.50 (ABqd, J_{AB} = 13.7 Hz, J_d = 5.4 Hz, 1H), 4.40 (ABqd, J_{AB} = 13.7 Hz, J_d = 3.5 Hz, 1H), 2.46 (s, 3H), 2.39 (s, 3H), 1.57 (s, 3H), 1.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.6, 145.5, 137.5, 137.3, 135.7, 132.4, 129.1, 129.1, 129.0, 128.9, 59.3, 40.1, 33.1, 22.7, 21.3, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{19}H_{22}ClNNaO_2S^+$ [M+Na^+] 386.0952, found 386.0948.



4e

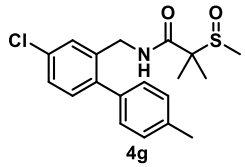
***N*-((4-methoxy-4'-methyl-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 61.0 mg, 85%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.18 (m, 5H), 7.16 (d, *J* = 8.4 Hz, 1H), 6.98 (d, *J* = 2.7 Hz, 1H), 6.85 (dd, *J* = 8.4, 2.7 Hz, 1H), 4.49 (ABqd, J_{AB} = 15.0 Hz, J_d = 5.9 Hz, 1H), 4.37 (ABqd, J_{AB} = 15.0 Hz, J_d = 5.3 Hz, 1H), 3.82 (s, 3H), 2.39 (s, 3H), 2.38 (s, 3H), 1.54 (s, 3H), 1.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.0, 159.1, 137.6, 136.7, 136.6, 134.3, 131.5, 129.3, 129.1, 113.9, 113.0, 59.4, 55.4, 41.9, 33.0, 22.4, 21.2, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{20}H_{25}NNaO_3S^+$ [M+Na^+] 382.1447, found 382.1449.



4f

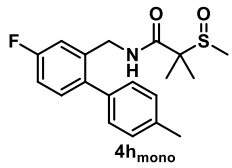
***N*-((4,4'-dimethyl-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 62.3 mg, 91%; 61 mg, 89% at 80 °C for 48 h. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (s, 1H), 7.23-7.18 (m, 4H), 7.18-7.07 (m, 3H), 4.49 (ABqd, J_{AB} = 14.8 Hz, J_d = 5.9 Hz, 1H), 4.35 (ABqd, J_{AB} = 14.8 Hz, J_d = 5.1 Hz, 1H), 2.38 (s, 3H), 2.37 (s, 3H), 2.37 (s, 3H), 1.52 (s, 3H), 1.26 (s, 3H);^{13}C NMR (101 MHz,

$CDCl_3$) δ 169.9, 139.0, 137.9, 137.3, 136.8, 135.0, 130.4, 129.6, 129.2, 129.1, 128.3, 59.4, 41.8, 33.0, 22.3, 21.3, 21.2, 18.8. HRMS (m/z, ESI-TOF): Calcd for $C_{20}H_{25}NNaO_2S^+$ [M+Na^+] 366.1498, found 366.1498.



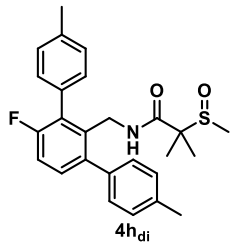
4g

***N*-((4-chloro-4'-methyl-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 64.1 mg, 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 2.1 Hz, 1H), 7.36-7.29 (m, 1H), 7.26 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.25-7.17 (m, 4H), 7.16 (d, *J* = 8.2 Hz, 1H), 4.47 (ABqd, J_{AB} = 15.2 Hz, J_d = 6.0 Hz, 1H), 4.34 (ABqd, J_{AB} = 15.2 Hz, J_d = 5.5 Hz, 1H), 2.40 (s, 3H), 2.39 (s, 3H), 1.56 (s, 3H), 1.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 140.2, 137.5, 137.4, 136.7, 133.4, 131.6, 129.2, 129.0, 128.5, 127.5, 59.3, 41.3, 33.0, 22.6, 21.2, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{19}H_{22}ClNNaO_2S^+$ [M+Na^+] 386.0952, found 386.0949.



$4h_{mono}$

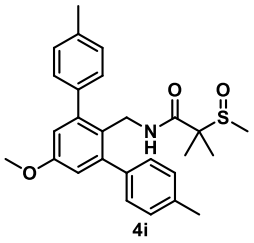
***N*-((4-fluoro-4'-methyl-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 40.3 mg, 58%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (s, 1H), 7.25-7.17 (m, 5H), 7.14 (dd, *J* = 9.7, 2.7 Hz, 1H), 6.99 (td, *J* = 8.3, 2.7 Hz, 1H), 4.49 (ABqd, J_{AB} = 15.2 Hz, J_d = 6.0 Hz, 1H), 4.33 (ABqd, J_{AB} = 15.2 Hz, J_d = 5.5 Hz, 1H), 2.40 (s, 3H), 2.39 (s, 3H), 1.57 (s, 3H), 1.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 162.2 (d, J_{C-F} = 247.1 Hz), 137.9 (d, J_{C-F} = 7.2 Hz), 137.7 (d, J_{C-F} = 3.2 Hz), 137.2, 136.9, 131.9 (d, J_{C-F} = 8.1 Hz), 129.2 , 129.2, 115.1 (d, J_{C-F} = 22.2 Hz), 114.3 (d, J_{C-F} = 21.1 Hz), 59.4, 41.5, 33.0, 22.7, 21.3, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{19}H_{23}FNO_2S^+$ [M+H^+] 348.1428, found 348.1431.



$4h_{di}$

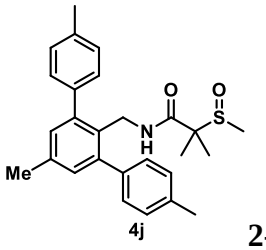
***N*-((4'-fluoro-4,4''-dimethyl-[1,1':3',1''-terphenyl]-2'-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with

standard conditions for 24 h in 0.2 mmol scale; 19.2 mg, 22%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.16 (m, 9H), 7.13 (t, *J* = 8.6 Hz, 1H), 6.87 (s, 1H), 4.24 (dd, *J* = 13.6, 5.5 Hz, 1H), 4.08 (dd, *J* = 13.6, 2.6 Hz, 1H), 2.38 (s, 3H), 2.37 (s, 3H), 2.23 (s, 3H), 1.37 (s, 3H), 1.12 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 159.4 (d, J_{C-F} = 245.6 Hz), 139.7 (d, J_{C-F} = 3.7 Hz), 137.8, 137.6, 137.2, 134.5 (d, J_{C-F} = 2.4 Hz), 131.0 (d, J_{C-F} = 8.4 Hz), 131.0 (d, J_{C-F} = 17.0 Hz), 130.9 (d, J_{C-F} = 0.6 Hz), 129.9, 129.2, 129.2, 129.0, 115.1 (d, J_{C-F} = 23.1 Hz), 59.2, 40.0 (d, J_{C-F} = 2.6 Hz), 32.9, 22.3, 21.4, 21.2, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{26}H_{29}FNO_2S^+$ [M+H$^+$] 438.1898, found 438.1899.



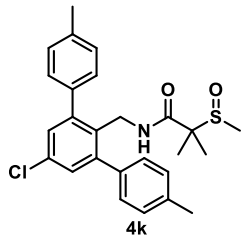
4i

***N*-((5'-methoxy-4,4''-dimethyl-[1,1':3',1''-terphenyl]-2'-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 74.6 mg, 83%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.0 Hz, 4H), 7.18 (d, *J* = 7.9 Hz, 4H), 6.79 (s, 2H), 6.77 (brs, 1H), 4.24 (ABqd, J_{AB} = 13.9 Hz, J_d = 5.3 Hz, 1H), 4.11 (ABqd, J_{AB} = 13.9 Hz, J_d = 2.8 Hz, 1H), 3.80 (s, 3H), 2.37 (s, 6H), 2.21 (s, 3H), 1.35 (s, 3H), 1.12 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9, 158.4, 145.3, 138.4, 137.1, 129.0, 128.9, 124.1, 115.2, 59.2, 55.4, 39.5, 32.8, 21.9, 21.2, 18.8. HRMS (m/z, ESI-TOF): Calcd for $C_{27}H_{31}NNaO_3S^+$ [M+Na$^+$] 472.1917, found 472.1911.



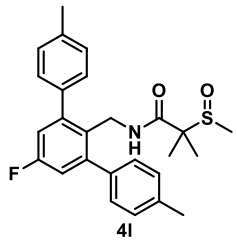
4j

2-methyl-2-(methylsulfinyl)-*N*-((4,4'',5'-trimethyl-[1,1':3',1''-terphenyl]-2'-yl)methyl)propanamide: The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 68.0 mg, 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 7.9 Hz, 4H), 7.17 (d, *J* = 7.9 Hz, 4H), 7.06 (s, 2H), 6.74 (brs, 1H), 4.30 (ABqd, J_{AB} = 13.8 Hz, J_d = 5.3 Hz, 1H), 4.17 (ABqd, J_{AB} = 13.8 Hz, J_d = 2.8 Hz, 1H), 2.37 (s, 9H), 2.20 (s, 3H), 1.33 (s, 3H), 1.12 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9, 143.8, 138.5, 137.4, 136.9, 130.6, 129.1, 128.9, 128.7, 59.3, 39.8, 32.9, 21.8, 21.3, 21.1, 18.8. HRMS (m/z, ESI-TOF): Calcd for $C_{27}H_{32}NO_2S^+$ [M+H$^+$] 434.2148, found 434.2147.



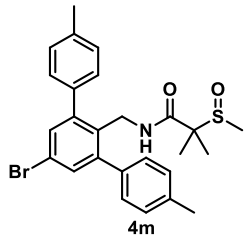
4k

***N*-((5'-chloro-4,4''-dimethyl-[1,1':3',1''-terphenyl]-2'-yl) methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 83.0 mg, 92%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.18 (m, 10H), 6.84 (s, 1H), 4.30 (dd, *J* = 13.8, 5.5 Hz, 1H), 4.14 (dd, *J* = 13.8, 2.8 Hz, 1H), 2.38 (s, 6H), 2.21 (s, 3H), 1.34 (s, 3H), 1.12 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 145.6, 137.6, 137.2, 133.2, 130.5, 129.6, 129.1, 128.9, 59.2, 39.5, 32.8, 22.1, 21.3, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{26}H_{29}ClNO_2S^+$ [M+H$^+$] 454.1602, found 454.1604.



4l

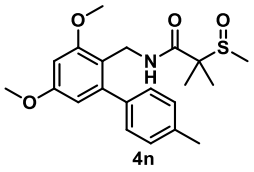
***N*-((5'-fluoro-4,4''-dimethyl-[1,1':3',1''-terphenyl]-2'-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 76.3 mg, 87%. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.25 (d, *J* = 8.2 Hz, 4H), 7.19 (d, *J* = 8.0 Hz, 4H), 6.96 (d, *J* = 9.0 Hz, 2H), 6.85 (brs, 1H), 4.28 (dd, *J* = 13.9, 5.5 Hz, 1H), 4.13 (dd, *J* = 13.9, 2.7 Hz, 1H), 2.38 (s, 6H), 2.22 (s, 3H), 1.36 (s, 3H), 1.12 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 161.3 (d, $J_{C\text{-}F}$ = 249.5 Hz), 146.1 (d, $J_{C\text{-}F}$ = 8.3 Hz), 137.5, 137.4 (d, $J_{C\text{-}F}$ = 1.7 Hz), 129.1, 128.9, 127.8 (d, $J_{C\text{-}F}$ = 3.2 Hz), 116.5 (d, $J_{C\text{-}F}$ = 21.1 Hz), 59.1, 39.5, 32.8, 22.2, 21.3, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{26}H_{28}FNNaO_2S^+$ [M+Na$^+$] 460.1717, found 460.1716.



4m

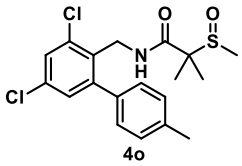
***N*-((5'-bromo-4,4''-dimethyl-[1,1':3',1''-terphenyl]-2'-yl) methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 85.5 mg, 86%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (s, 2H), 7.24 (d, *J* = 8.1 Hz, 4H), 7.19 (d, *J* = 8.0 Hz, 4H), 6.84 (brs,

1H), 4.29 (dd, J = 13.8, 5.5 Hz, 1H), 4.13 (dd, J = 13.9, 2.8 Hz, 1H), 2.37 (s, 6H), 2.21 (s, 3H), 1.34 (s, 3H), 1.11 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 145.8, 137.6, 137.0, 132.5, 131.0, 129.1, 129.0, 121.5, 59.1, 39.6, 32.8, 22.1, 21.3, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{26}H_{28}BrNNaO_2S^+$ [M+Na$^+$] 520.0916, found 520.0921.



4n

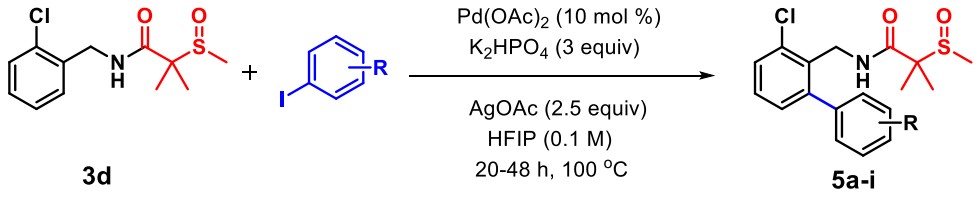
***N*-((3,5-dimethoxy-4'-methyl-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 39.6 mg, 51%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23-7.17 (m, 5H), 6.47 (d, J = 2.4 Hz, 1H), 6.39 (d, J = 2.4 Hz, 1H), 4.34 (ABqd, J_{AB} = 13.9 Hz, J_d = 4.6 Hz, 1H), 4.30 (ABqd, J_{AB} = 13.6 Hz, J_d = 5.2 Hz, 1H), 3.85 (s, 3H), 3.80 (s, 3H), 2.40 (s, 3H), 2.38 (s, 3H), 1.52 (s, 3H), 1.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.4, 159.8, 159.6, 144.7, 138.0, 137.2, 129.1, 129.0, 116.0, 106.3, 97.7, 59.5, 55.7, 55.5, 36.9, 33.0, 22.2, 21.3, 19.0. HRMS (m/z, ESI-TOF): Calcd for $C_{21}H_{27}NNaO_4S^+$ [M+H$^+$] 412.1553, found 412.1549.



4o

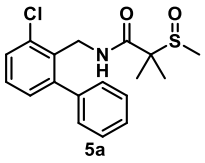
***N*-((3,5-dichloro-4'-methyl-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 68.0 mg, 86%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, J = 2.2 Hz, 1H), 7.29 (brs, 1H), 7.22-7.17 (m, 5H), 4.47 (ABqd, J_{AB} = 13.8 Hz, J_d = 5.5 Hz, 1H), 4.36 (ABqd, J_{AB} = 13.8 Hz, J_d = 3.8 Hz, 1H), 2.44 (s, 3H), 2.39 (s, 3H), 1.56 (s, 3H), 1.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 146.5, 138.1, 136.4, 136.2, 134.0, 131.3, 129.2, 129.2, 128.8, 128.6, 59.3, 39.5, 33.1, 22.8, 21.3, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{19}H_{22}Cl_2NO_2S^+$ [M+H$^+$] 398.0743, found 398.0748.

2.3.2 General procedure for *ortho*-arylation of 3d with aryl iodides



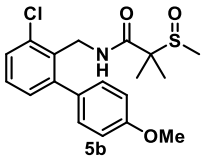
3d **5a-i**

A 38 mL Schlenk sealed tube (with a Teflon cap) equipped with a magnetic stir bar was charged with amide **3d** (27.3 mg, 0.10 mmol, 1.0 equiv), aryl iodides (0.30 mmol, 3.0 equiv), $Pd(OAc)_2$ (2.3 mg, 0.01 mmol, 10 mol %), AgOAc (41.8 mg, 0.25 mmol, 2.5 equiv) and K_2HPO_4 (52.2 mg, 0.3 mmol, 3.0 equiv). Then HFIP (1 mL) was added along the inside wall of the tube. The tube was then capped and submerged into a preheated 100 °C oil bath. The reaction was stirred for 20-48 h and cooled to room temperature. The crude reaction mixture was diluted with EtOAc (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 30 mL of EtOAc. The filtrate was concentrated *in vacuo*, crude ^{1}H NMR spectrum was taken using CH_2Br_2 as internal standard. The resulting residue was purified by preparative thin layer chromatography preparative chromatography using petroleum ether/EtOAc as the eluent.



5a

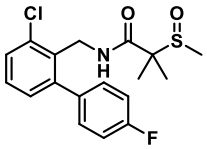
***N*-((3-chloro-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 20 h in 0.1 mmol scale; 30.3 mg, 87%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.28 (m, 7H), 7.23 (brs, 1H), 7.18 (dd, J = 7.6, 1.3 Hz, 1H), 4.52 (ABqd, J_{AB} = 13.7 Hz, J_d = 5.5 Hz, 1H), 4.39 (ABqd, J_{AB} = 13.7 Hz, J_d = 3.7 Hz, 1H), 2.44 (s, 3H), 1.56 (s, 3H), 1.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.6, 145.4, 140.2, 135.7, 132.4, 129.1, 129.1, 129.0, 129.0, 128.4, 127.8, 59.3, 39.9, 33.1, 22.8, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{18}H_{20}ClNNaO_2S^+$ [M+Na$^+$] 372.0795, found 372.0798.



5b

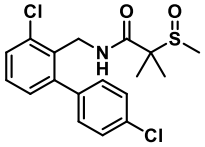
***N*-((3-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, J = 7.9 Hz, 1H), 7.28-7.23 (m, 4 H),

7.16 (d, J = 7.0 Hz, 1H), 6.93 (d, J = 8.6 Hz, 2H), 4.51 (ABqd, J_{AB} = 13.6 Hz, J_d = 5.2 Hz, 1H), 4.41 (ABqd, J_{AB} = 13.6 Hz, J_d = 3.6 Hz, 1H), 3.84 (s, 3H), 2.46 (s, 3H), 1.57 (s, 3H), 1.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.6, 159.2, 145.1, 135.7, 132.5, 132.5, 130.2, 129.2, 128.8, 128.8, 113.7, 59.3, 55.3, 40.0, 33.0, 22.7, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{19}H_{22}ClNNaO_3S^+$ [M+Na^+] 402.0901, found 402.0901.



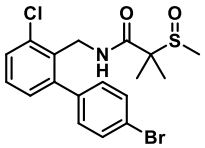
5c

***N*-((3-chloro-4'-fluoro-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propenamide:** The corresponding reaction was run with standard conditions for 48 h in 0.1 mmol scale; 33.8 mg, 92%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (dd, J = 8.0, 1.1 Hz, 1H), 7.32-7.26 (m, 4H), 7.16 (dd, J = 7.6, 1.1 Hz, 1H), 7.13-7.03 (m, 2H), 4.50 (ABqd, J_{AB} = 13.7 Hz, J_d = 5.6 Hz, 1H), 4.36 (ABqd, J_{AB} = 13.8 Hz, J_d = 3.7 Hz, 1H), 2.45 (s, 3H), 1.57 (s, 3H), 1.27 (s, 3H)； ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 162.5 (d, $J_{C\text{-}F}$ = 248.2 Hz), 144.3, 136.2 (d, $J_{C\text{-}F}$ = 3.4 Hz), 135.8, 132.6, 130.8 (d, $J_{C\text{-}F}$ = 8.2 Hz), 129.3, 129.1, 129.0, 115.4 (d, $J_{C\text{-}F}$ = 21.6 Hz), 59.3, 39.9, 33.1, 22.9, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{18}H_{19}ClFNNaO_2S^+$ [M+Na^+] 390.0701, found 390.0705.



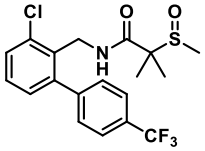
5d

***N*-((3,4'-dichloro-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.1 mmol scale; 35.8 mg, 93%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, J = 8.0, 1.2 Hz, 1H), 7.40-7.36 (m, 2H), 7.31-7.24 (m, 4H), 7.15 (dd, J = 7.6, 1.2 Hz, 1H), 4.50 (ABqd, J_{AB} = 13.8 Hz, J_d = 5.6 Hz, 1H), 4.36 (ABqd, J_{AB} = 13.8 Hz, J_d = 3.7 Hz, 1H), 2.45 (s, 3H), 1.58 (s, 3H), 1.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 144.1, 138.6, 135.9, 134.0, 132.4, 130.5, 129.5, 129.1, 129.0, 128.6, 59.3, 39.9, 33.1, 22.9, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{18}H_{19}Cl_2NNaO_2S^+$ [M+Na^+] 406.0406, found 406.0402.



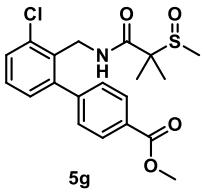
5e

***N*-((4'-bromo-3-chloro-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.1 mmol scale; 38.8 mg, 91%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.51 (m, 2H), 7.43 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.34-7.27 (m, 2H), 7.21-7.18 (m, 2H), 7.14 (dd, *J* = 7.6, 1.1 Hz, 1H), 4.50 (ABqd, J_{AB} = 13.8 Hz, J_d = 5.6 Hz, 1H), 4.36 (ABqd, J_{AB} = 13.8 Hz, J_d = 3.6 Hz, 1H), 2.45 (s, 3H), 1.57 (s, 3H), 1.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 144.1, 139.1, 135.9, 132.3, 131.5, 130.8, 129.5, 129.1, 128.9, 122.2, 59.3, 39.9, 33.1, 22.9, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{18}H_{19}BrClNNaO_2S^+$ [M+Na^+] 449.9901, found 449.9901.



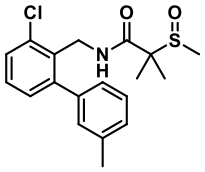
5f

***N*-((3-chloro-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 48 h in 0.1 mmol scale; 38.3 mg, 92%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.0 Hz, 2H), 7.46 (d, *J* = 8.1 Hz, 3H), 7.38-7.29 (m, 2H), 7.16 (dd, *J* = 7.6, 1.1 Hz, 1H), 4.50 (dd, *J* = 13.9, 5.7 Hz, 1H), 4.35 (dd, *J* = 13.9, 3.6 Hz, 1H), 2.44 (s, 3H), 1.57 (s, 3H), 1.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 143.9, 136.0, 132.4, 130.1 (q, J_{C-F} = 32.7 Hz), 129.8, 129.6, 129.2, 128.9, 125.4 (q, J_{C-F} = 3.7 Hz), 124.2 (q, J_{C-F} = 274.2 Hz), 59.3, 39.9, 33.1, 22.9, 18.5. HRMS (m/z, ESI-TOF): Calcd for $C_{19}H_{19}ClF_3NNaO_2S^+$ [M+Na^+] 440.0669, found 440.0671.



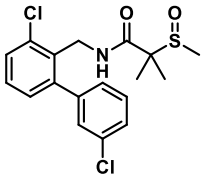
5g

methyl 3'-chloro-2'-((2-methyl-2-(methylsulfinyl)propanamido) methyl)-[1,1'-biphenyl]-4-carboxylate: The corresponding reaction was run with standard conditions for 24 h in 0.2 mmol scale; 50.0 mg, 61%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-8.06 (m, 2H), 7.45 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.43-7.39 (m, 2H), 7.35-7.27 (m, 2H), 7.18 (dd, *J* = 7.7, 1.2 Hz, 1H), 4.49 (ABqd, J_{AB} = 13.8 Hz, J_d = 5.6 Hz, 1H), 4.36 (ABqd, J_{AB} = 13.8 Hz, J_d = 3.6 Hz, 1H), 3.95 (s, 3H), 2.45 (s, 3H), 1.58 (s, 3H), 1.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 166.8, 144.9, 144.3, 136.0, 132.3, 129.7, 129.6, 129.3, 129.1, 128.8, 59.3, 52.3, 39.9, 33.1, 22.9, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{20}H_{22}ClNNaO_4S^+$ [M+Na^+] 430.0850, found 430.0852.



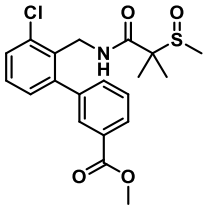
5h

***N*-((3-chloro-3'-methyl-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.1 mmol scale; 26.1 mg, 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 8.0 Hz, 1H), 7.34-7.15 (m, 2H), 7.10 (brs, 2H), 4.51 (ABqd, J_{AB} = 13.6 Hz, J_d = 5.3 Hz, 1H), 4.40 (ABqd, J_{AB} = 13.6 Hz, J_d = 2.7 Hz, 1H), 2.46 (s, 3H), 2.38 (s, 3H), 1.57 (s, 3H), 1.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 145.6, 140.2, 138.0, 135.7, 132.4, 129.8, 129.0, 129.0, 128.9, 128.6, 128.3, 126.2, 59.3, 40.0, 33.1, 22.8, 21.6, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{19}H_{22}ClNNaO_2S^+$ [M+Na$^+$] 386.0952, found 386.0948.



5i

***N*-((3,3'-dichloro-[1,1'-biphenyl]-2-yl)methyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 24 h in 0.1 mmol scale; 35.6 mg, 93%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (dd, J = 8.0, 1.2 Hz, 1H), 7.37-7.27 (m, 5H), 7.23-7.19 (m, 1H), 7.16 (dd, J = 7.6, 1.2 Hz, 1H), 4.49 (ABqd, J_{AB} = 13.8 Hz, J_d = 5.6 Hz, 1H), 4.36 (ABqd, J_{AB} = 13.8 Hz, J_d = 3.5 Hz, 1H), 2.48 (s, 3H), 1.60 (s, 3H), 1.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 143.9, 141.9, 135.9, 134.2, 132.3, 129.7, 129.6, 129.2, 129.1, 128.9, 128.1, 127.3, 59.3, 39.9, 33.1, 23.0, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{18}H_{19}Cl_2NNaO_2S^+$ [M+Na$^+$] 406.0406, found 406.0407.



5j

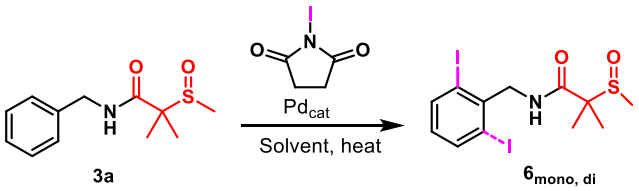
methyl 3'-chloro-2'-((2-methyl-2-(methylsulfinyl)propanamido)methyl)-[1,1'-biphenyl]-3-carboxylate: The corresponding reaction was run with standard conditions for 48 h in 0.1 mmol scale; 37.0 mg, 91%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, J = 7.4, 1.6 Hz, 1H), 7.97 (t, J = 1.4 Hz, 1H), 7.54 (dt, J = 7.6, 1.6 Hz,

1H), 7.50 (t, J = 7.5 Hz, 1H), 7.45 (dd, J = 8.0, 1.2 Hz, 1H), 7.33-7.29 (m, 2H), 7.18 (dd, J = 7.6, 1.2 Hz, 1H), 4.47 (ABqd, J_{AB} = 13.8 Hz, J_d = 5.4 Hz, 1H), 4.40 (ABqd, J_{AB} = 13.8 Hz, J_d = 3.9 Hz, 1H), 3.92 (s, 3H), 2.45 (s, 3H), 1.58 (s, 3H), 1.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 166.8, 144.2, 140.5, 135.9, 133.6, 132.5, 130.4, 130.1, 129.6, 129.1, 129.1, 129.1, 128.6, 59.3, 52.3, 39.9, 33.1, 22.8, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{20}H_{22}ClNNaO_4S^+$ [M+Na$^+$] 430.0850, found 430.0853.

2.4 Reaction conditions optimization for *ortho*-C–H bond iodination.

General optimization procedure: A 38 mL Schlenk sealed tube (with a Teflon cap) equipped with a magnetic stir bar was charged with amide **3a** (23.9 mg, 0.10 mmol, 1.0 equiv), *N*-Iodosuccinimide (49.5 mg, 0.22 mmol, 2.2 equiv), $Pd(OAc)_2$ (2.3 mg, 0.01 mmol, 10 mol %). Then (combined) solvent (1 mL) was added along the inside wall of the tube. The tube was then capped and submerged into a preheated 100 ℃ oil bath. The reaction was stirred for 12 h and cooled to room temperature. The crude reaction mixture was diluted with EtOAc (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 30 mL of EtOAc. The filtrate was concentrated *in vacuo*, crude ^{1}H NMR spectrum was taken using CH_2Br_2 as internal standard.

Table S2. Screening of the optimal iodination reaction conditions.[a]

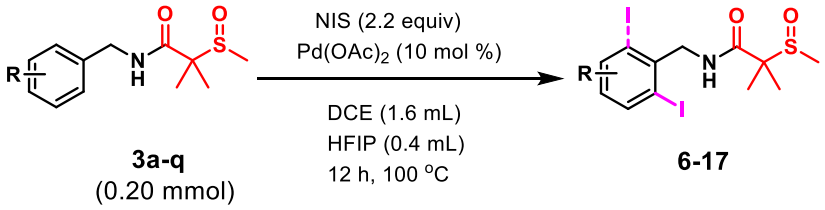


3a **6$_{mono, di}$**

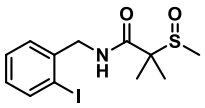
Entry	Solvent (v/v)	T (℃)	Yield [%][b]	
			6$_{mono}$	**6$_{di}$**
1	Dioxane	100	27	33
2	Toluene	100	27	34
3	DCE	100	24	39
4	HFIP	100	50	9
5	Toluene	90	37	28
6	Toluene/HFIP (9/1)	90	42	27
7	DCE/HFIP (9/1)	90	43	34
8	DCE/HFIP (8/2)	90	33	49
9	**DCE/HFIP (8/2)**	**100**	**32**	**62**

[a] Reaction conditions: substrate amide **3a** (0.10 mmol), *N*-Iodosuccinimide (0.22 mmol, 2.2 equiv), $Pd(OAc)_2$ (0.01 mmol, 10 mol %) in solvent (1.0 mL), heat, 12 h. [b] Yield was determined by ^{1}H NMR with CH_2Br_2 as internal standard.

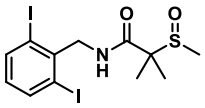
2.5 General procedure for *ortho*-iodination of benzylamine.



A 38 mL Schlenk sealed tube (with a Teflon cap) equipped with a magnetic stir bar was charged with amide **3** (0.20 mmol, 1.0 equiv), *N*-Iodosuccinimide (99 mg, 0.44 mmol, 2.2 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol %) and HFIP (0.4 mL). Then DCE (1.6 mL) was added along the inside wall of the tube. The tube was then capped and submerged into a preheated 100 °C oil bath. The reaction was stirred for 12 h and cooled to room temperature. The crude reaction mixture was diluted with EtOAc (10 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 60 mL of EtOAc. The filtrate was concentrated *in vacuo*, crude ^{1}H NMR spectrum was taken using CH_2Br_2 as internal standard. The resulting residue was purified (10% NaOH aqueous solution could be used to remove pyrrolidine-2,5-dione before purification) by preparative thin layer chromatography or preparative chromatography using petroleum ether/EtOAc as the eluent.

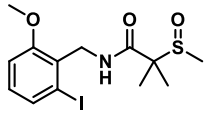


6_{mono} ***N*-(2-iodobenzyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 22.6 mg, 31%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.61 (brs, 1H), 7.40 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.32 (td, *J* = 7.5, 1.1 Hz, 1H), 6.97 (td, *J* = 7.6, 1.7 Hz, 1H), 4.58 (ABqd, J_{AB} = 14.9 Hz, J_d = 5.9 Hz, 1H), 4.48 (ABqd, J_{AB} = 14.9 Hz, J_d = 5.8 Hz, 1H), 2.44 (s, 3H), 1.64 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 140.3, 139.7, 129.9, 129.4, 128.6, 99.2, 59.5, 48.5, 33.1, 22.8, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{17}INO_2S^+$ [M+H$^+$] 366.0019, found 366.0018.

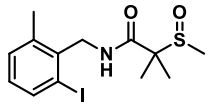


6_{di} ***N*-(2,6-diiodobenzyl)-2-methyl-2-(methylsulfinyl)propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 53.8

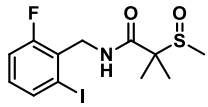
mg, 55%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 7.9 Hz, 2H), 7.35 (brs, 1H), 6.62 (t, J = 7.9 Hz, 1H), 4.92 (ABqd, J_{AB} = 14.0 Hz, J_d = 5.4 Hz, 1H), 4.82 (ABqd, J_{AB} = 14.0 Hz, J_d = 4.1 Hz, 1H), 2.56 (s, 3H), 1.64 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 141.3, 140.5, 131.4, 100.1, 59.5, 55.0, 33.4, 23.0, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{16}I_2NO_2S^+$ [M+H$^+$] 491.8986, found 491.8982.



7 ***N*-(2-iodo-6-methoxybenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 62.7 mg, 79%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58-7.52 (m, 3H), 6.63 (d, J = 8.6 Hz, 1H), 4.45 (ABqd, J_{AB} = 14.6 Hz, J_d = 6.2 Hz, 1H), 4.38 (ABqd, J_{AB} = 14.6 Hz, J_d = 5.7 Hz, 1H), 3.82 (s, 3H), 2.36 (s, 3H), 1.60 (s, 3H), 1.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 157.5, 138.2, 137.7, 129.0, 112.7, 82.7, 59.4, 55.6, 38.9, 32.9, 22.8, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{19}INO_3S^+$ [M+H$^+$] 396.0125, found 396.0127.

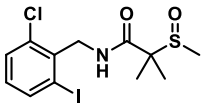


8 ***N*-(2-iodo-6-methylbenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 58.0 mg, 77%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 7.9 Hz, 1H), 7.34 (brs, 1H), 7.15 (d, J = 7.5 Hz, 1H), 6.88 (t, J = 7.7 Hz, 1H), 4.70 (ABqd, J_{AB} = 14.1 Hz, J_d = 5.7 Hz, 1H), 4.59 (ABqd, J_{AB} = 14.1 Hz, J_d = 4.5 Hz, 1H), 2.49 (s, 3H), 2.48 (s, 3H), 1.60 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 139.1, 138.0, 137.9, 131.0, 129.8, 102.3, 59.5, 46.2, 33.2, 22.7, 21.1, 18.8. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{19}INO_2S^+$ [M+H$^+$] 380.0176, found 380.0173.

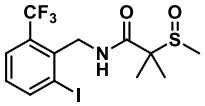


9 ***N*-(2-fluoro-6-iodobenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 66.3 mg, 87%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, J = 7.8 Hz, 1H), 7.49 (brs, 1H), 7.07 (t, J = 8.5 Hz, 1H), 6.99 (td, J = 8.0, 5.8 Hz, 1H), 4.71-4.59 (ABm, 2H), 2.46 (s, 3H), 1.60 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 160.7 (d, J_{C-F} = 253.6 Hz), 135.5 (d, J_{C-F} = 3.7 Hz), 131.1 (d, J_{C-F} = 9.0 Hz), 128.2 (d, J_{C-F} = 16.3 Hz), 116.1 (d, J_{C-F} = 23.1 Hz), 100.8 (d, J_{C-F} = 2.8 Hz), 59.5, 42.2 (d, J_{C-F} = 3.7 Hz), 33.2, 22.8, 18.7.

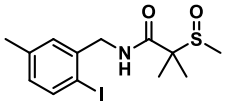
HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{15}FINNaO_2S^+$ [M+Na^+] 405.9744, found 405.9747.



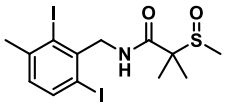
10 ***N*-(2-chloro-6-iodobenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 65.9 mg, 83%; 864 mg, 72% in a 3 mmol (0.821 gram) scale. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, *J* = 7.9, 0.9 Hz, 1H), 7.44 (brs, 1H), 7.38 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.93 (t, *J* = 8.0 Hz, 1H), 4.84 (ABqd, J_{AB} = 14.0 Hz, J_d = 5.4 Hz, 1H), 4.78 (ABqd, J_{AB} = 14.0 Hz, J_d = 4.8 Hz, 1H), 2.50 (s, 3H), 1.61 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 138.8, 137.5, 134.9, 130.8, 130.3, 101.6, 59.5, 47.3, 33.2, 22.9, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{16}ClINO_2S^+$ [M+H^+] 399.9630, found 399.9626.



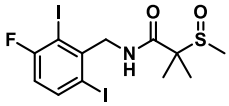
11 ***N*-(2-iodo-6-(trifluoromethyl)benzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 79.0 mg, 91%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.9 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.29 (brs, 1H), 7.14 (t, *J* = 7.9 Hz, 1H), 4.80 (ABqd, J_{AB} = 14.3 Hz, J_d = 5.5 Hz, 1H), 4.70 (ABqd, J_{AB} = 14.3 Hz, J_d = 2.6 Hz, 1H), 2.54 (s, 3H), 1.63 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 144.1, 137.5, 131.2 (q, $J_{C\text{-}F}$ = 30.4 Hz), 129.8, 126.6 (q, $J_{C\text{-}F}$ = 5.7 Hz), 123.5 (q, $J_{C\text{-}F}$ = 275.6 Hz), 104.1, 59.2, 45.7 (d, $J_{C\text{-}F}$ = 2.2 Hz), 33.1, 23.0, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{16}F_3INO_2S^+$ [M+H^+] 433.9893, found 433.9895.



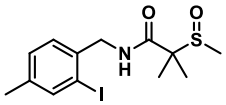
12$_{mono}$ ***N*-(2-iodo-5-methylbenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 56.0 mg, 74%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.0 Hz, 1H), 7.56 (brs, 1H), 7.21 (d, *J* = 1.4 Hz, 1H), 6.80 (dd, *J* = 8.0, 1.6 Hz, 1H), 4.54 (ABqd, J_{AB} = 14.8 Hz, J_d = 6.0 Hz, 1H), 4.43 (ABqd, J_{AB} = 14.8 Hz, J_d = 5.7 Hz, 1H), 2.45 (s, 3H), 2.28 (s, 3H), 1.64 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 140.0, 139.4, 138.6, 130.9, 130.4, 95.1, 59.5, 48.4, 33.1, 22.7, 21.1, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{18}INNaO_2S^+$ [M+Na^+] 401.9995, found 401.9998.



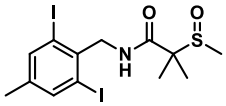
12$_{di}$ ***N*-(2,6-diiodo-3-methylbenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 13.0 mg, 13%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.0 Hz, 1H), 7.27 (brs, 1H), 6.86 (d, J = 8.0 Hz, 1H), 5.02 (ABqd, J_{AB} = 14.0 Hz, J_d = 5.4 Hz, 1H), 4.94 (ABqd, J_{AB} = 14.0 Hz, J_d = 3.9 Hz, 1H), 2.58 (s, 3H), 2.45 (s, 3H), 1.64 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 143.9, 141.4, 139.6, 131.0, 107.9, 96.1, 59.5, 56.1, 33.4, 30.2, 23.0, 18.8. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{17}I_2NNaO_2S^+$ [M+Na$^+$] 527.8962, found 527.8963.



13 ***N*-(3-fluoro-2,6-diiodobenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 90.2 mg, 89%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, J = 8.6, 5.5 Hz, 1H), 7.44 (brs, 1H), 6.75 (dd, J = 8.6, 7.2 Hz, 1H), 4.98 (ABqd, J_{AB} = 13.9 Hz, J_d = 5.5 Hz, 1H), 4.86 (ABqd, J_{AB} = 14.0 Hz, J_d = 4.2 Hz, 1H), 2.56 (s, 3H), 1.63 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 162.3 (d, $J_{C\text{-}F}$ = 247.5 Hz), 143. 5 (d, $J_{C\text{-}F}$ = 0.6 Hz), 141.0 (d, $J_{C\text{-}F}$ = 7.6 Hz), 116.9 (d, $J_{C\text{-}F}$ = 25.7 Hz), 93.2 (d, $J_{C\text{-}F}$ = 3.5 Hz), 89.0 (d, $J_{C\text{-}F}$ = 26.1 Hz), 59.5, 54.4 (d, $J_{C\text{-}F}$ = 2.4 Hz), 33.4, 23.1, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{15}FI_2NO_2S^+$ [M+H$^+$] 509.8892, found 509.8892.



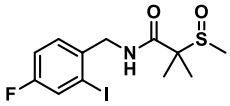
14$_{mono}$ ***N*-(2-iodo-4-methylbenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 16.5 mg, 22%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 0.7 Hz, 1H), 7.54 (brs, 1H), 7.27 (d, J = 7.7 Hz, 1H), 7.11 (dd, J = 7.7, 0.8 Hz, 1H), 4.53 (ABqd, J_{AB} = 14.8 Hz, J_d = 5.9 Hz, 1H), 4.45 (ABqd, J_{AB} = 14.8 Hz, J_d = 5.7 Hz, 1H), 2.43 (s, 3H), 2.28 (s, 3H), 1.63 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 140.1, 139.6, 137.4, 129.7, 129.4, 99.2, 59.5, 48.1, 33.1, 22.7, 20.6, 18.7. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{19}INO_2S^+$ [M+H$^+$] 380.0176, found 380.0178.



14_{di}

***N*-(2,6-diiodo-4-methylbenzyl)-2-methyl-2-(methylsulfinyl)**

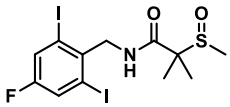
propanamide: The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 69.6 mg, 69%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 2H), 7.27 (brs, 1H), 4.87 (ABqd, J_{AB} = 14.0 Hz, J_d = 5.3 Hz, 1H), 4.79 (ABqd, J_{AB} = 14.0 Hz, J_d = 4.2 Hz, 1H), 2.55 (s, 3H), 2.24 (s, 3H), 1.63 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 141.9, 141.0, 138.2, 99.6, 59.5, 54.5, 33.4, 22.9, 19.8, 18.8. HRMS (m/z, ESI-TOF): Calcd for $C_{13}H_{18}I_2NHO_2S^+$ [M+H$^+$] 505.9142, found 505.9146.



15_{mono}

***N*-(4-fluoro-2-iodobenzyl)-2-methyl-2-(methylsulfinyl)**

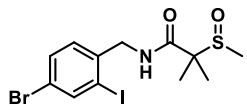
propanamide: The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 25.8 mg, 34%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (brs, 1H), 7.56 (dd, J = 8.0, 2.6 Hz, 1H), 7.38 (dd, J = 8.5, 5.9 Hz, 1H), 7.04 (td, J = 8.3, 2.6 Hz, 1H), 4.54 (ABqd, J_{AB} = 14.9 Hz, J_d = 5.9 Hz, 1H), 4.46 (ABqd, J_{AB} = 14.9 Hz, J_d = 5.9 Hz, 1H), 2.43 (s, 3H), 1.64 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 161.4 (d, $J_{C\text{-}F}$ = 252.5 Hz), 136.5 (d, $J_{C\text{-}F}$ = 3.4 Hz), 130.8 (d, $J_{C\text{-}F}$ = 8.2 Hz), 126.6 (d, $J_{C\text{-}F}$ = 23.8 Hz), 115.6 (d, $J_{C\text{-}F}$ = 20.9 Hz), 98.3 (d, $J_{C\text{-}F}$ = 8.2 Hz), 59.4, 47.6, 33.1, 22.9, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{16}FINO_2S^+$ [M+H$^+$] 383.9925, found 383.9923.



15_{di}

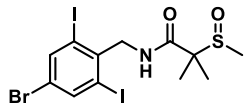
***N*-(4-fluoro-2,6-diiodobenzyl)-2-methyl-2-(methylsulfinyl)**

propanamide: The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 51.8 mg, 51%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, J = 7.5 Hz, 2H), 7.38 (brs, 1H), 4.92 (ABqd, J_{AB} = 14.2 Hz, J_d = 5.5 Hz, 1H), 4.81 (ABqd, J_{AB} = 14.2 Hz, J_d = 4.2 Hz, 1H), 2.55 (s, 3H), 1.63 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 160.7 (d, $J_{C\text{-}F}$ = 259.1 Hz), 137.6 (d, $J_{C\text{-}F}$ = 3.8 Hz), 127.5 (d, $J_{C\text{-}F}$ = 23.1 Hz), 98.3 (d, $J_{C\text{-}F}$ = 8.0 Hz), 59.5, 53.8, 33.4, 23.0, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{15}FI_2NO_2S^+$ [M+H$^+$] 509.8892, found 509.8893.



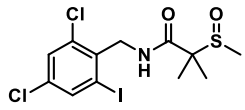
16_{mono}

***N*-(4-bromo-2-iodobenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 21.0 mg, 24%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 1.9 Hz, 1H), 7.68 (brs, 1H), 7.45 (dd, J = 8.2, 1.9 Hz, 1H), 7.28 (d, J = 5.4 Hz, 1H), 4.52 (ABqd, J_{AB} = 15.0 Hz, J_d = 5.9 Hz, 1H), 4.42 (ABqd, J_{AB} = 15.0 Hz, J_d = 5.9 Hz, 1H), 2.44 (s, 3H), 1.64 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 141.5, 139.5, 131.7, 130.9, 122.0, 99.4, 59.4, 47.9, 33.1, 22.9, 18.5. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{15}BrINNaO_2S^+$ [M+Na^+] 465.8944, found 465.8946.



16_{di}

***N*-(4-bromo-2,6-diiodobenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 76.8 mg, 68%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 2H), 7.44 (brs, 1H), 4.89 (ABqd, J_{AB} = 14.1 Hz, J_d = 5.5 Hz, 1H), 4.76 (ABqd, J_{AB} = 14.1 Hz, J_d = 4.3 Hz, 1H), 2.55 (s, 3H), 1.63 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 142.4, 140.5, 123.1, 99.7, 59.5, 54.1, 33.4, 23.1, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{14}BrI_2NNaO_2S^+$ [M+Na^+] 591.7910, found 591.7908.

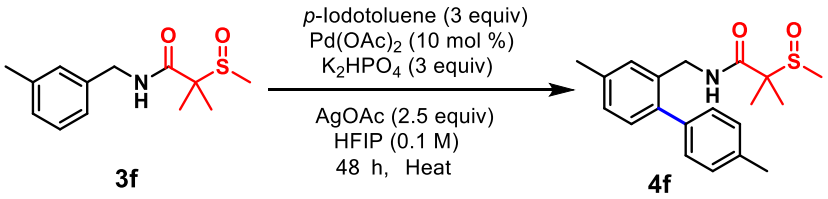


17

***N*-(2,4-dichloro-6-iodobenzyl)-2-methyl-2-(methylsulfinyl) propanamide:** The corresponding reaction was run with standard conditions for 12 h in 0.2 mmol scale; 76.0 mg, 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 2.1 Hz, 1H), 7.50 (brs, 1H), 7.41 (d, J = 2.1 Hz, 1H), 4.76 (ABqd, J_{AB} = 14.1 Hz, J_d = 5.1 Hz, 2H), 2.49 (s, 3H), 1.61 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 138.2, 136.3, 135.1, 134.8, 130.1, 101.1, 59.4, 46.5, 33.2, 22.9, 18.6. HRMS (m/z, ESI-TOF): Calcd for $C_{12}H_{14}Cl_2INNaO_2S^+$ [M+Na^+] 455.0959, found 455.0960.

2.6 Arylation at a lower temperature

Table S3. Screening of the lower-temperature arylation[a]

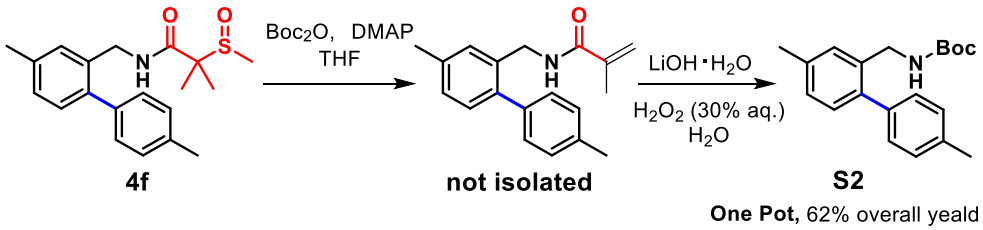


Entry	Temperature (℃)	Yield [%]
1	60	23
2	70	61
3	80	96 (89)[b]

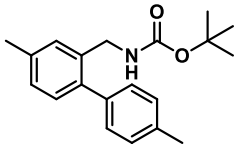
[a)] General reaction conditions: amide **3f** (0.10 mmol), *p*-iodotoluene (0.30 mmol), $Pd(OAc)_2$ (0.01 mmol), K_2HPO_4 (0.30 mmol) and AgOAc (0.25 mmol) in HFIP (1.0 mL), heat, 48 h. Yield was determined by ^1H NMR with CH_2Br_2 as internal standard. [b)] 0.2 mmol, scale, isolated yield.

General procedure: A 38 mL Schlenk sealed tube (with a Teflon cap) equipped with a magnetic stir bar was charged with amide **3f** (25.3 mg, 0.10 mmol, 1.0 equiv), *p*-iodotoluene (65.5mg, 0.30 mmol, 3.0 equiv), $Pd(OAc)_2$ (2.3 mg, 0.01 mmol, 10 mol %), AgOAc (41.8 mg, 0.25 mmol, 2.5 equiv), K_2HPO_4 (52.2 mg, 0.30 mmol, 3.0 equiv) and Additives (0.02 mmol, 20 mol %). Then HFIP (1 mL) was added along the inside wall of the tube. The tube was then capped and submerged into a preheated set temperature oil bath. The reaction was stirred for 48 h and cooled to room temperature. The crude reaction mixture was diluted with EtOAc (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 30 mL of EtOAc. The filtrate was concentrated *in vacuo*, crude ^1H NMR spectrum was taken using CH_2Br_2 as internal standard.

2.7 Removal of the directing group



A mixture of arylation product **4f** (102.9 mg, 0.30 mmol, 1.0 equiv), $(Boc)_2O$ (124 μL, 0.54 mmol, 1.8 equiv) and DMAP (7.3 mg, 0.06 mmol, 0.2 equiv) in anhydrous tetrahydrofuran (0.65 mL) in a sealed tube was stirred at 100 °C for 16 h. Then $LiOH·H_2O$ (63 mg, 1.50 mmol, 5.0 equiv), 30% H_2O_2 (120 μL, 1.20 mmol, 4.0 equiv) and H_2O (0.20 mL) were added in the same system. The mixture was stirred at 100 °C for 2 h, followed by stirring at room temperature for 12 h. The reaction mixture was diluted with water (10 mL) and extracted with EtOAc (25 mL × 3). The combined organic phase was dried on Na_2SO_4, filtered and concentrated *in vacuo* to afford crude products as orange oil. The resulting residue was purified by silica-gel flash chromatography (petroleum ether/EtOAc: 25:1) to give the product **S2** as a white solid (57.6 mg, 62%).

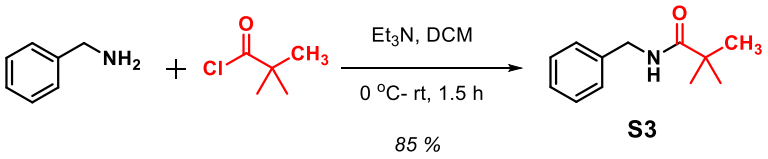


S2

***tert*-butyl ((4,4'-dimethyl-[1,1'-biphenyl]-2-yl)methyl)carbamate:** The corresponding reaction was run with standard conditions in 0.3 mmol scale; 57.6 mg, 62%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.08 (m, 7H), 4.60 (brs, 1H), 4.25 (d, J = 5.4 Hz, 2H), 2.39 (s, 3H), 2.38 (s, 3H), 1.42 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8, 138.8, 137.9, 137.3, 136.8, 136.0, 130.2, 129.1, 129.1, 129.0, 128.0, 79.4, 42.6, 28.5, 21.3, 21.2. HRMS (m/z, ESI-TOF): Calcd for $C_{20}H_{25}NNaO_2^+$ [M+Na$^+$] 334.1777, found 334.1778.

2.8 Control experiment.

2.8.1 Procedures for preparing substrate *N*-benzyl-pivalamide S3 [S2]

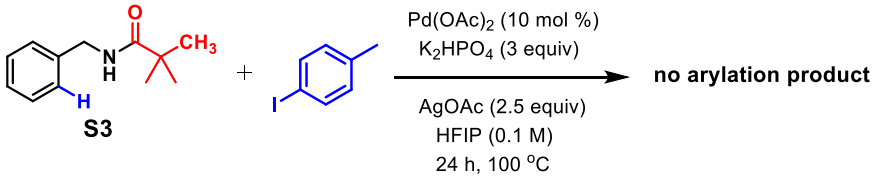


S3

To a solution of benzylamine (218.3 μL, 2.0 mmol, 1.0 equiv) and trimethylamine (278 μL, 2.0 mmol, 1.0 equiv) stirred in anhydrous dichloromethane (10 mL), pivaloyl chloride (246.3 μL, 2.0 mmol, 1.0 equiv) was added dropwise at 0 °C. The mixture was stirred for another 80 min at room temperature. After addition of H_2O (20 mL), the resulting aqueous extracted with DCM (20 mL × 3). The combined organic phase were dried on Na_2SO_4, filtered and concentrated *in vacuo* to afford crude products as yellow oil. The resulting residue was purified by silica gel chromatography with petroleum

ether/EtOAc (12:1) to afford compound *N*-benzyl-pivalamide **S3** (323.8 mg, 85%) as clear oil. Substrate **S3** (CAS 26209-45-0): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.24 (m, 5H), 5.89 (brs, 1H), 4.44 (d, *J* = 5.6 Hz, 2H), 1.23 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.4, 138.8, 128.9, 127.8, 127.6, 43.8, 38.9, 27.8.

2.8.2 Control arylation reaction



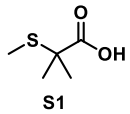
A 38 mL Schlenk sealed tube (with a Teflon cap) equipped with a magnetic stir bar was charged with amide **S3** (38.2 mg, 0.20 mmol, 1.0 equiv), aryl iodides (130.8 mg, 0.60 mmol, 3.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol %), AgOAc (83.5 mg, 0.5 mmol, 2.5 equiv) and K_2HPO_4 (104.4 mg, 0.6 mmol, 3.0 equiv). Then HFIP (2 mL) was added along the inside wall of the tube. The tube was then capped and submerged into a preheated 100 °C oil bath. The reaction was stirred for 24 h and cooled to room temperature. The crude reaction mixture was diluted with EtOAc (5 mL) and filtered through a short pad of Celite. The sealed tube and Celite pad were washed with an additional 50 mL of EtOAc. The filtrate was concentrated *in vacuo*, crude ^{1}H NMR spectrum was taken using CH_2Br_2 as internal standard. The resulting residue was also determined by GC-MS. No desired arylation products was observed.

2.9 References

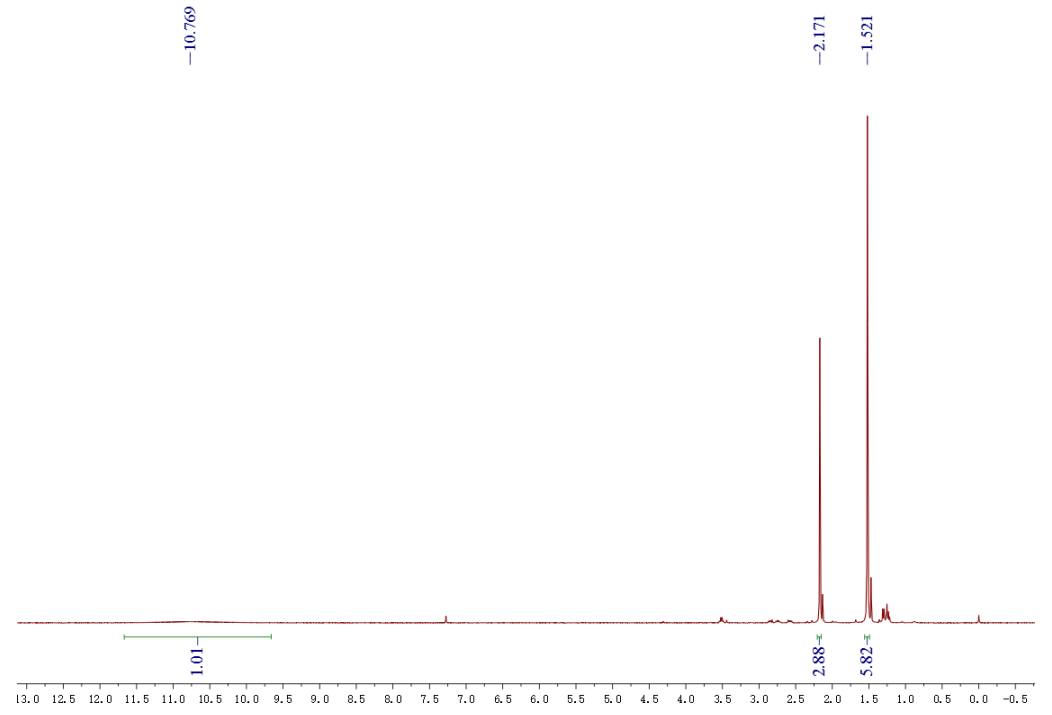
[S1] C. A. Gandolfi, R. D. Domenico, S. Spinelli, L. Gallico, L. Fiocchi, A. Lotto, E. Menta, A. Borghi, C. D. Rosa and S. Tognella, *J. Med. Chem*., 1995, **38**, 508.

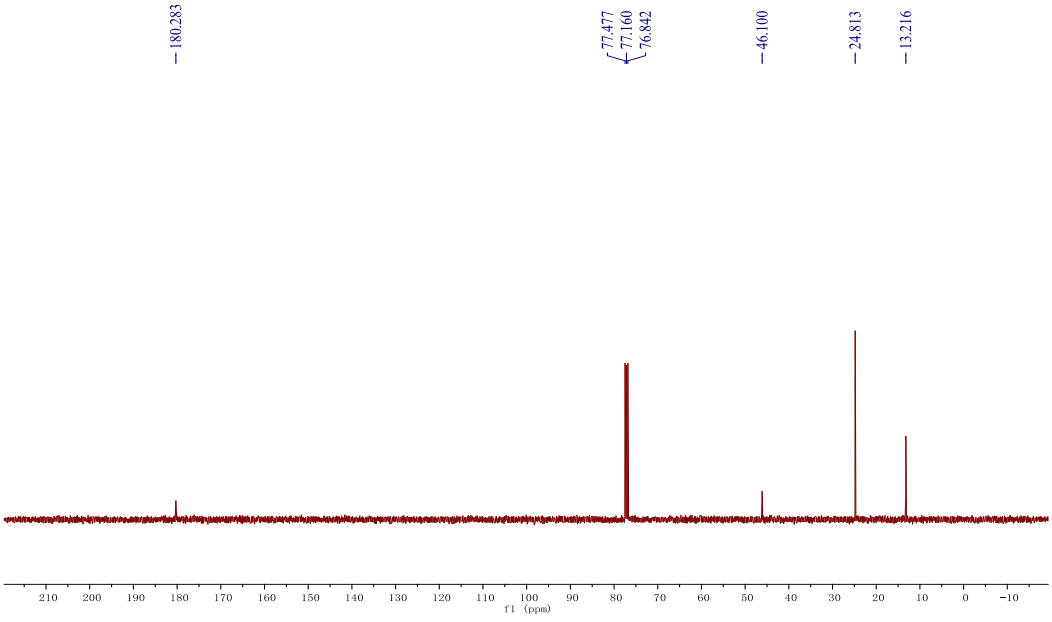
[S2] L. Zhou and W. Lu, *Org. Lett*., 2014, **16**, 508.

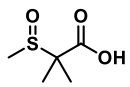
3. NMR Spectra of New Compounds



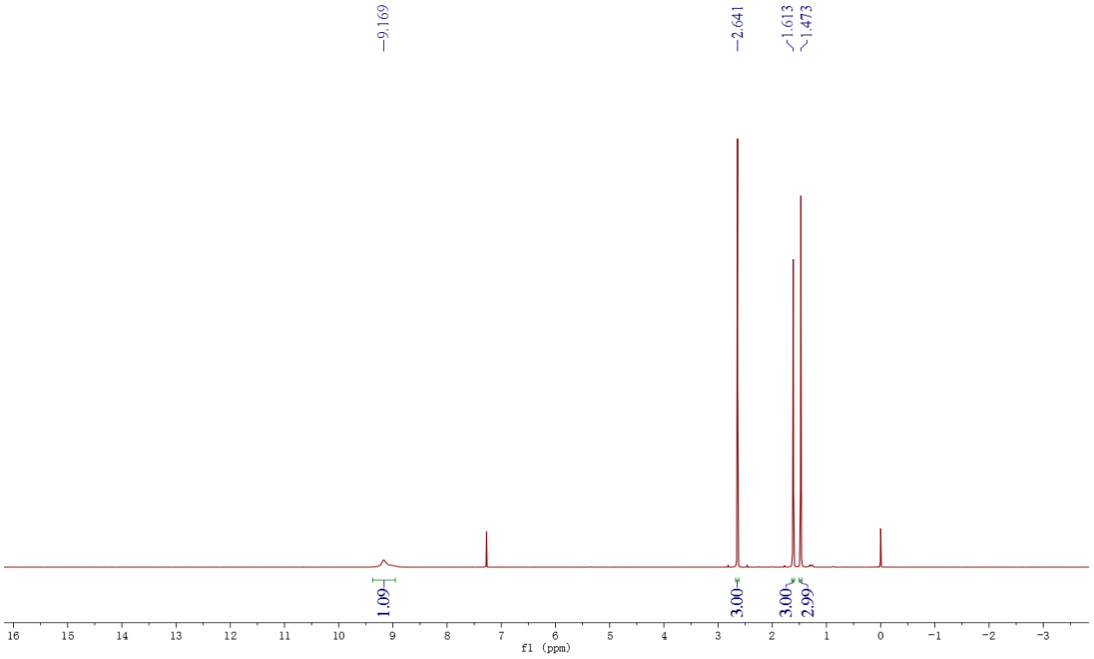
S1






O
O
S
OH

2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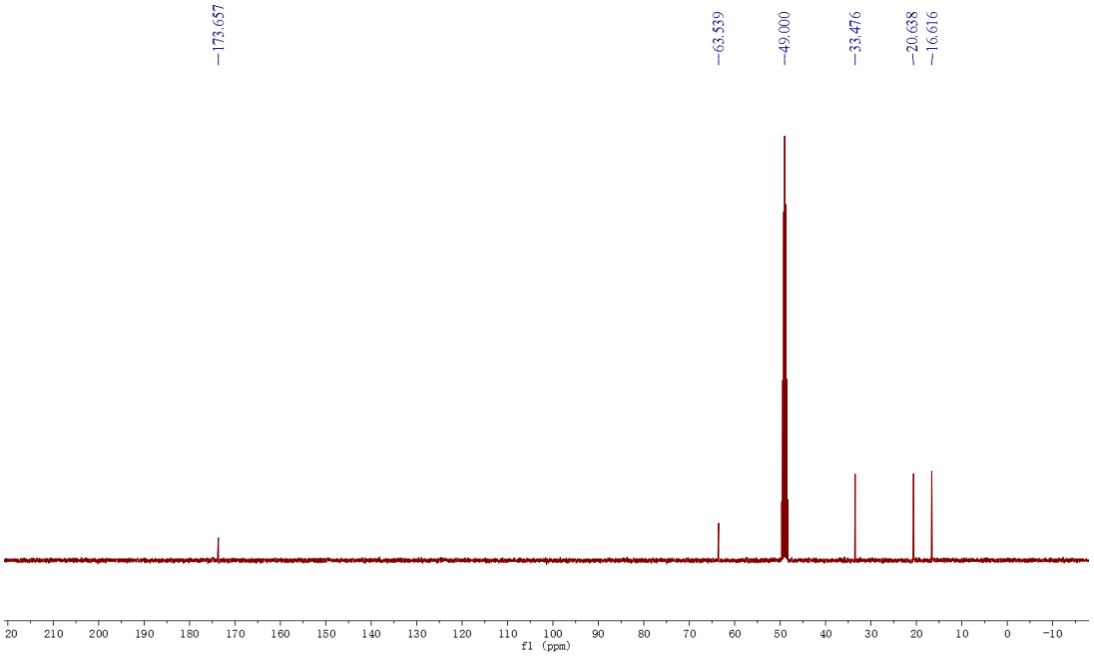
1.473
1.09
3.00
3.00
2.99
f1 (ppm)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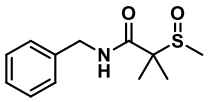
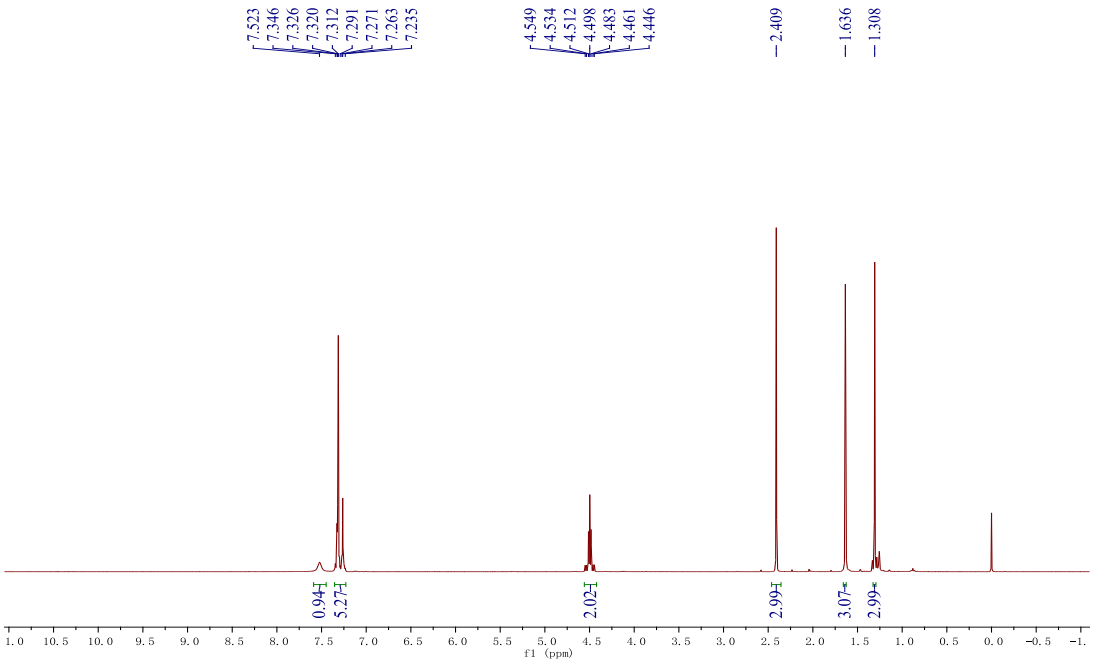
63.539
49.000
33.476
20.638
16.616
f1 (ppm)



3a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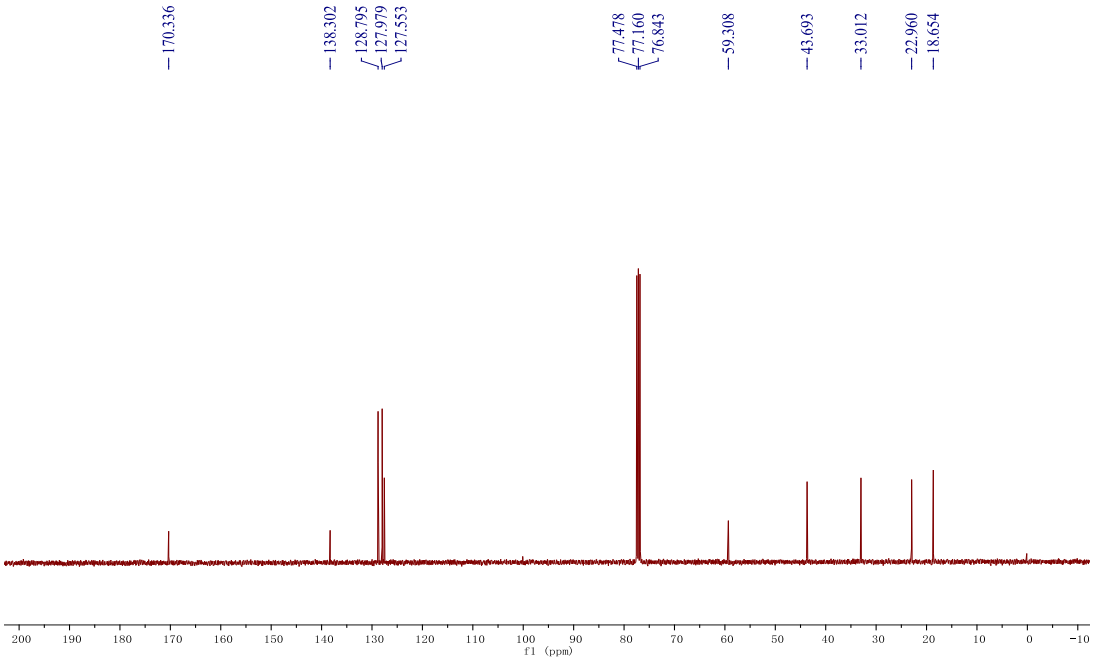
7.271
7.263
7.235
4.549
4.534
4.512
4.498
4.483
4.461
4.446
2.409
1.636
1.308
0.94
5.27
2.02
2.99
3.07
2.99
f1 (ppm)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127.979
127.553
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43.693
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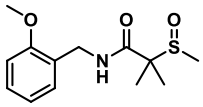
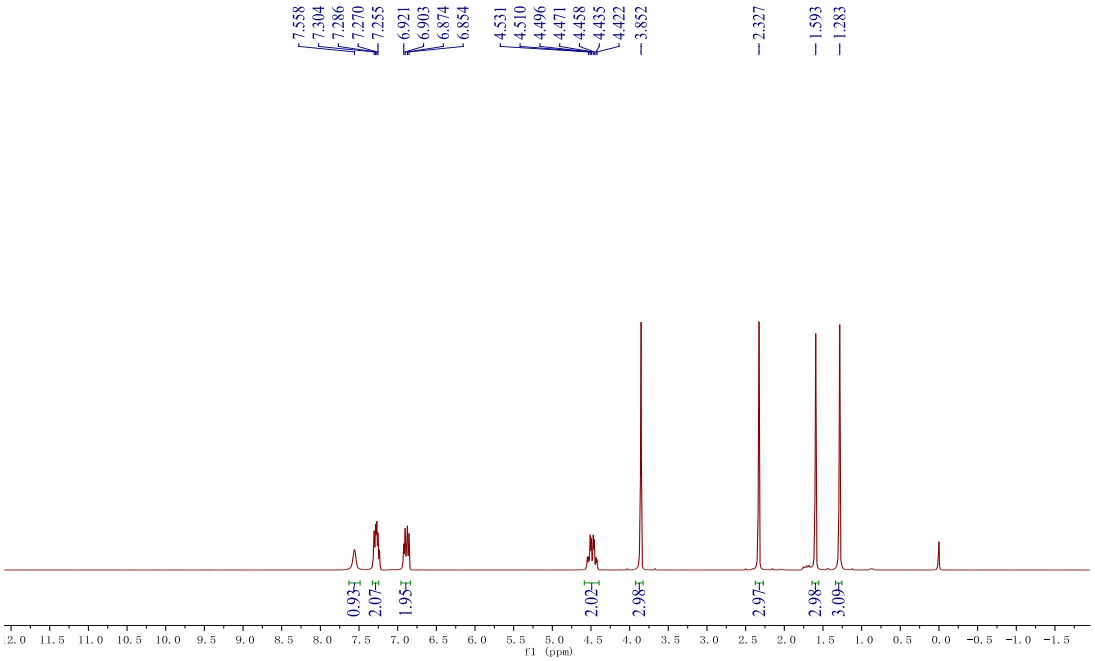
22.960
18.654
f1 (ppm)



3b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7.255
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6.903
6.874
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4.531
4.510
4.496
4.471
4.458
4.435
4.422
3.852
2.327
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1.95
2.02
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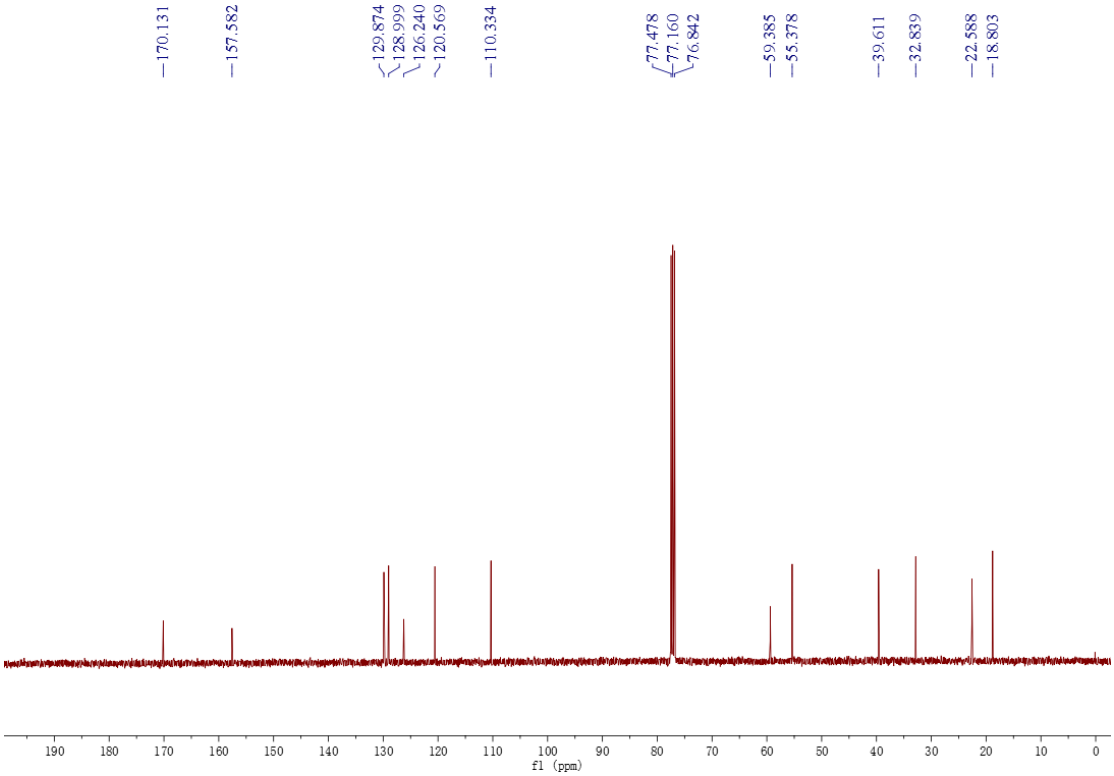
2.97
2.98
3.09
f1 (ppm)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128.999
126.240
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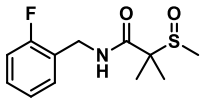
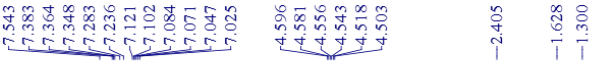
18.803
f1 (ppm)


F
O
O
N
H
S

3c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4.518
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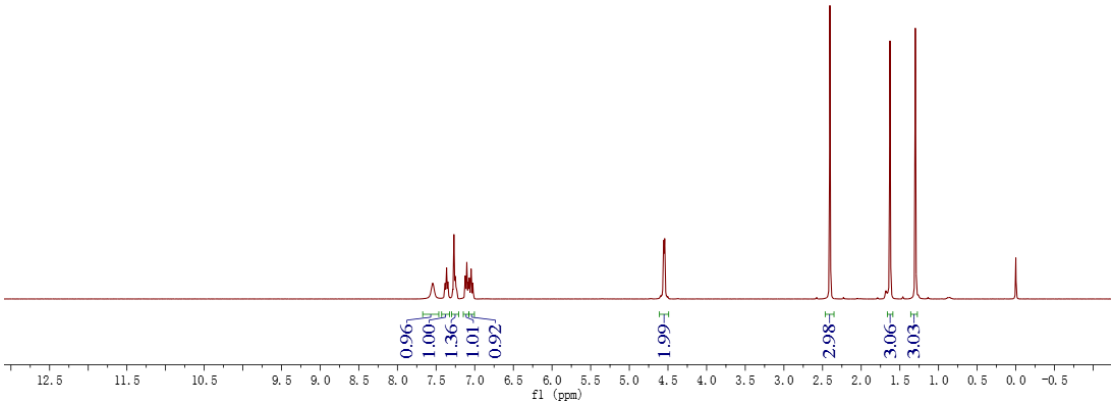
1.300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0.92
1.99
2.98
3.06
3.03
f1 (ppm)


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130.370
130.328
129.509
129.428
124.329
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77.478
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76.843
59.315
37.731
37.691
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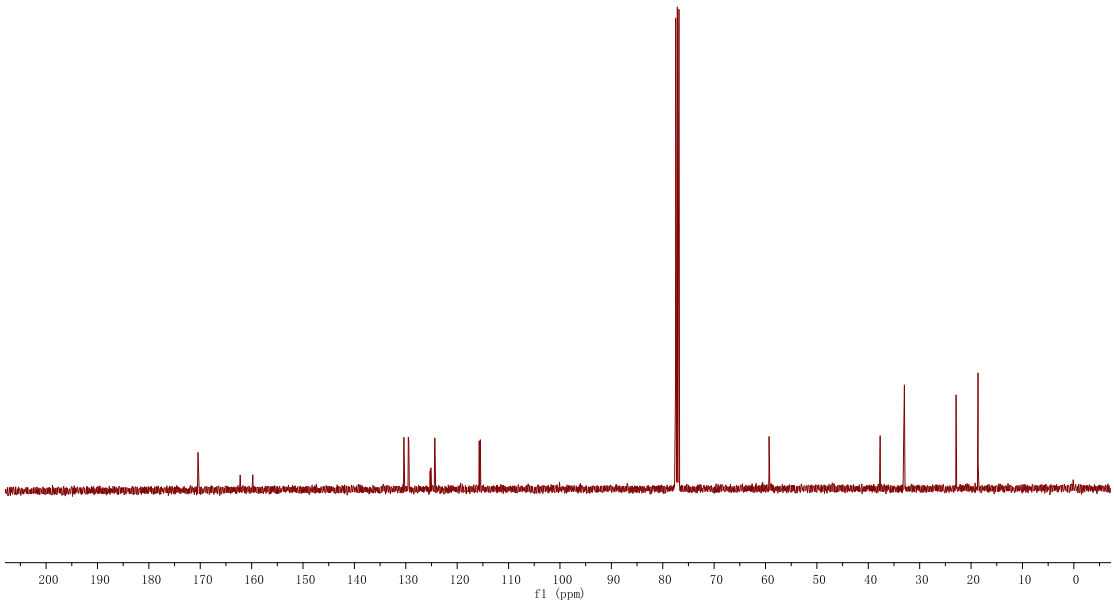
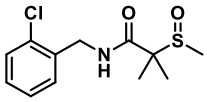
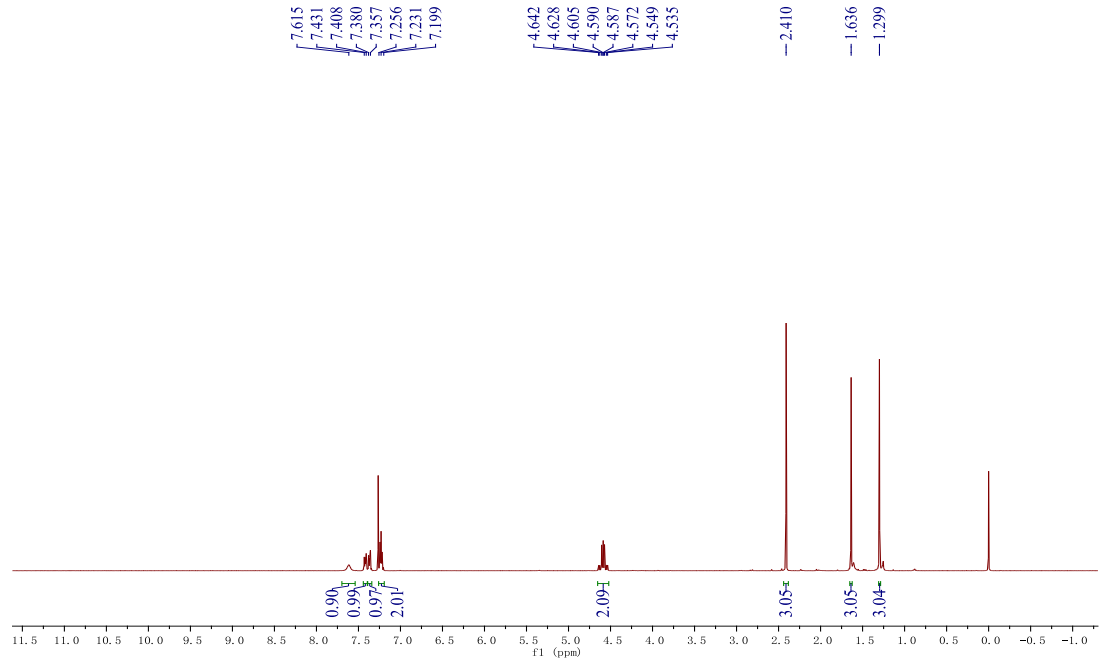
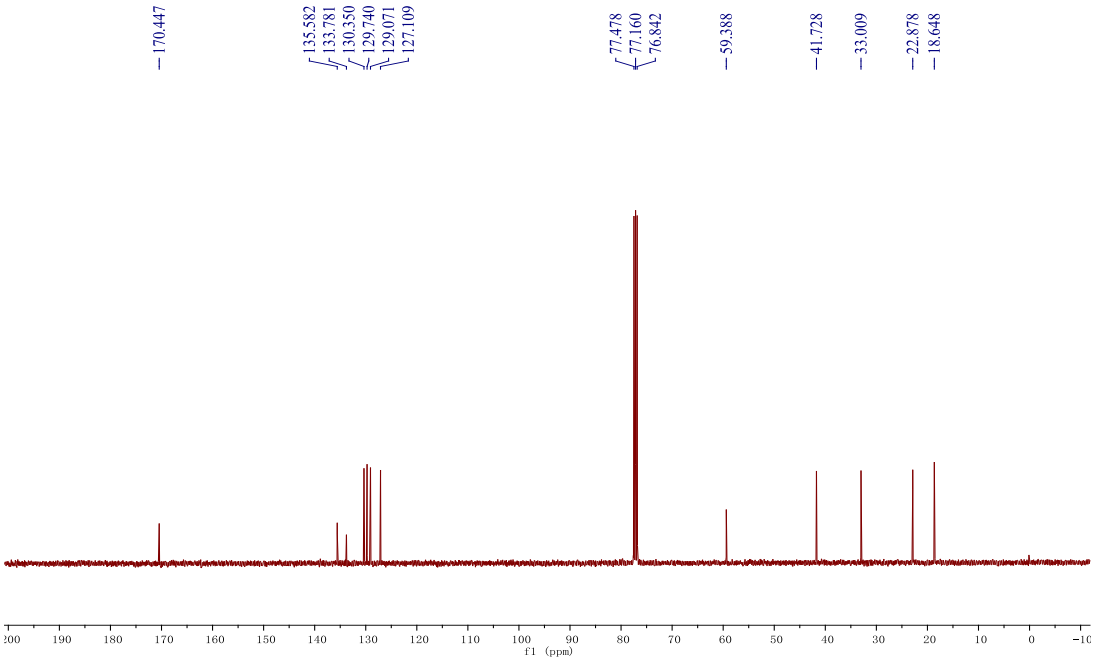
22.920
18.642

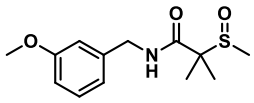

f1 (ppm)


Cl
O
O
S
N
H

3d

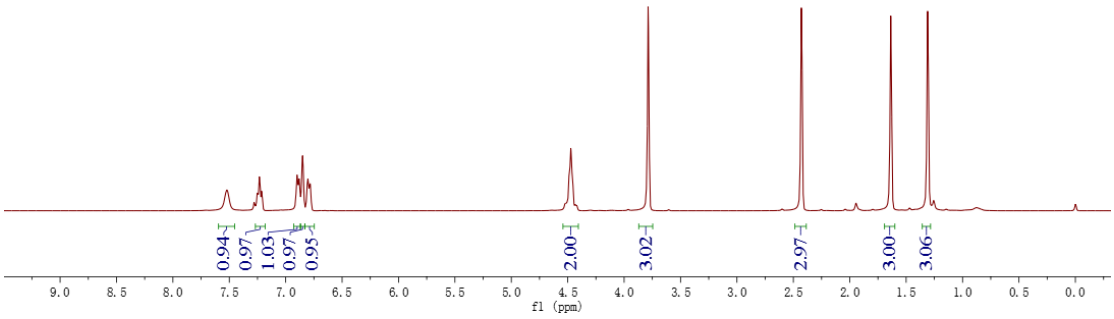

7.615
7.431
7.408
7.380
7.357
7.256
7.231
7.199
4.642
4.628
4.605
4.590
4.587
4.572
4.549
4.535
2.410
1.636
1.299
0.90
0.99
0.97
2.01
2.09
3.05
3.05
3.04
f1 (ppm)


170.447
135.582
133.781
130.350
129.740
129.071
127.109
77.478
77.160
76.842
59.388
41.728
33.009
22.878
18.648
f1 (ppm)

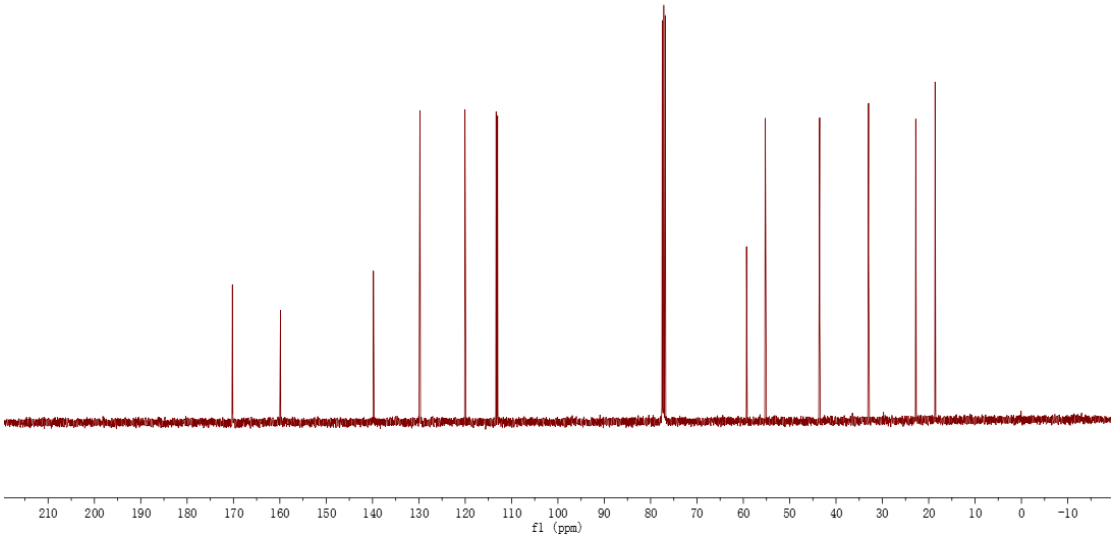


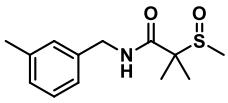
3e


7.521
7.253
7.233
7.214
6.899
6.881
6.850
6.803
6.784
4.521
4.509
4.473
4.436
4.422
3.788
2.429
1.637
1.310

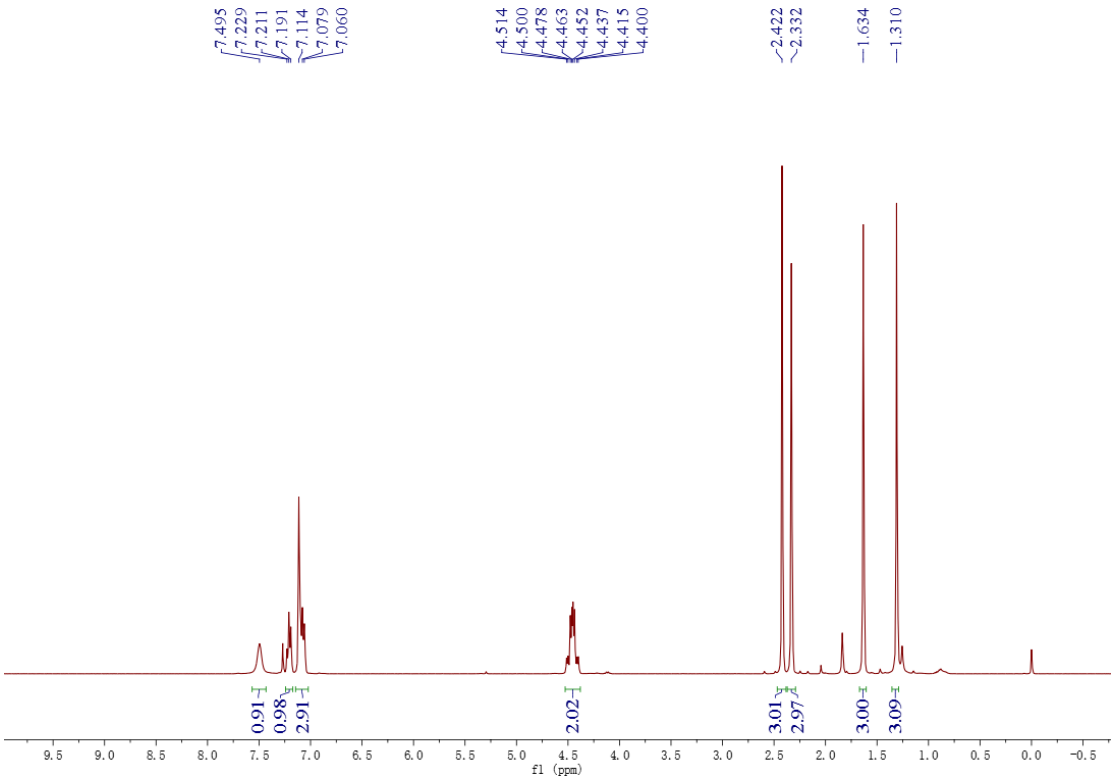

0.94
0.97
1.03
0.97
0.95
2.00
3.02
2.97
3.00
3.06
f1 (ppm)

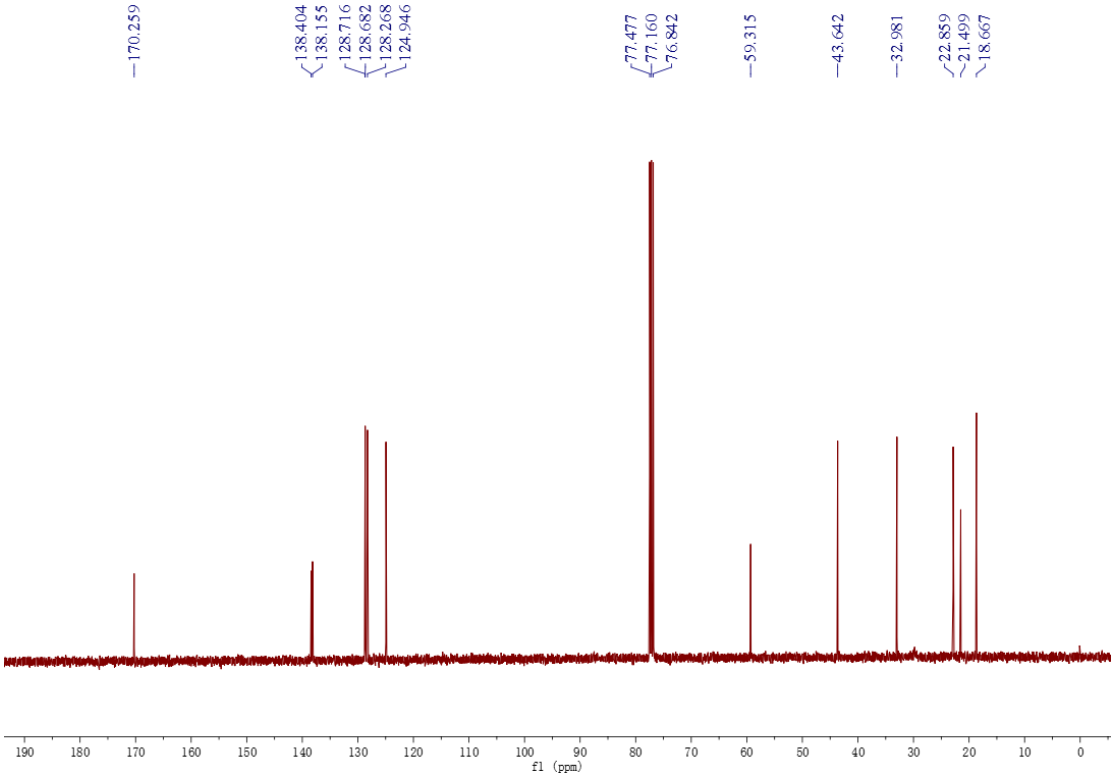

170.232
159.865
139.808
129.768
120.056
113.324
113.012
77.478
77.160
76.842
59.299
55.268
43.530
32.977
22.791
18.620

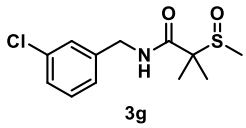

f1 (ppm)



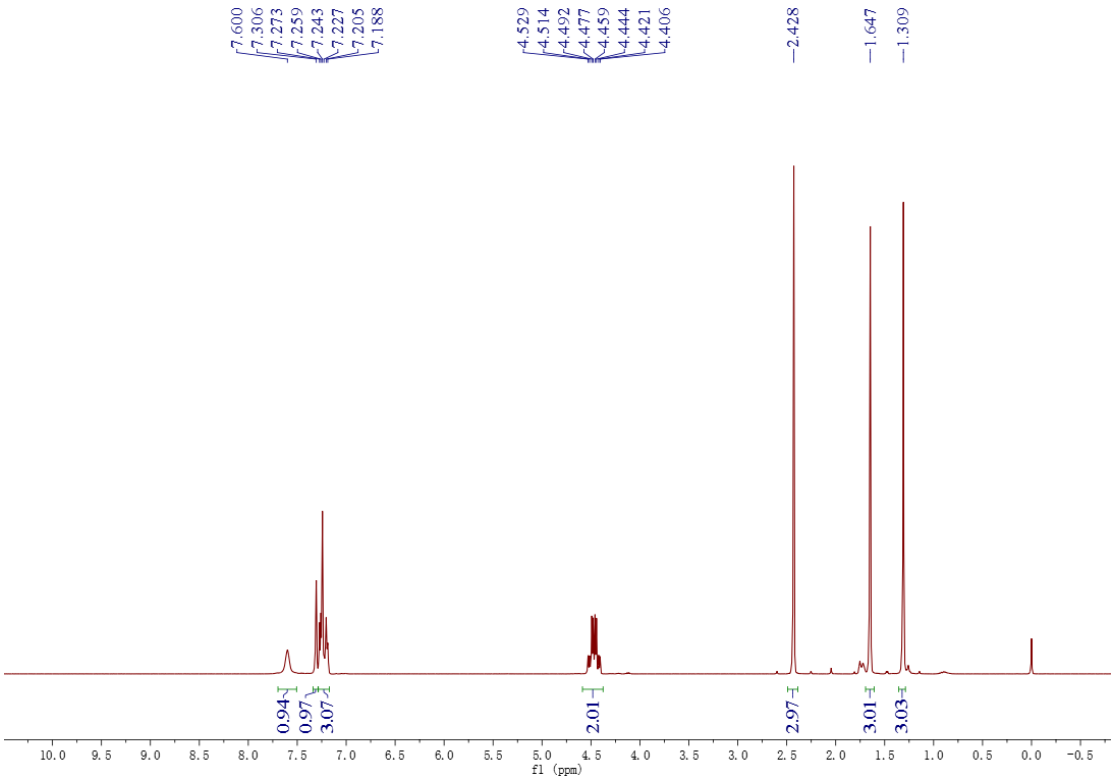
3f

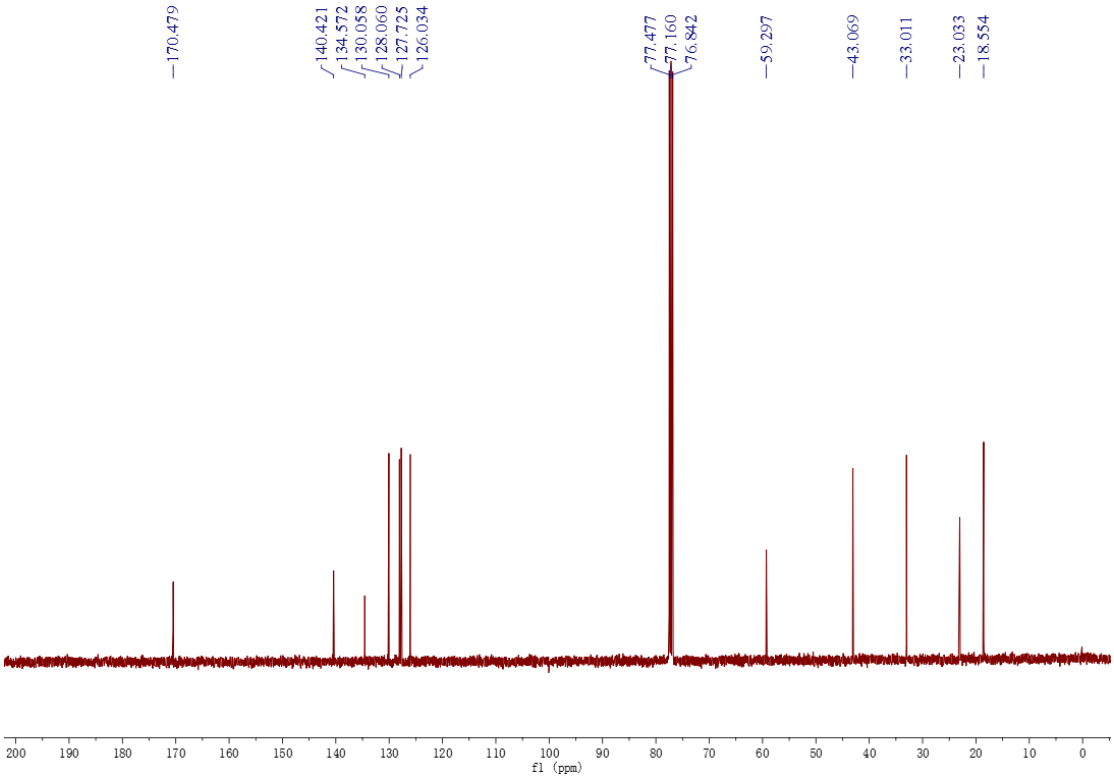

7.495
7.229
7.211
7.191
7.114
7.079
7.060
4.514
4.500
4.478
4.463
4.452
4.437
4.415
4.400
2.422
2.332
1.634
1.310
0.91
0.98
2.91
2.02
3.01
2.97
3.00
3.09
f1 (ppm)

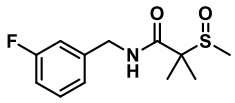

170.259
138.404
138.155
128.716
128.682
128.268
124.946
77.477
77.160
76.842
59.315
43.642
32.981
22.859
21.499
18.667
f1 (ppm)


Cl
N
H
O
O
S

3g

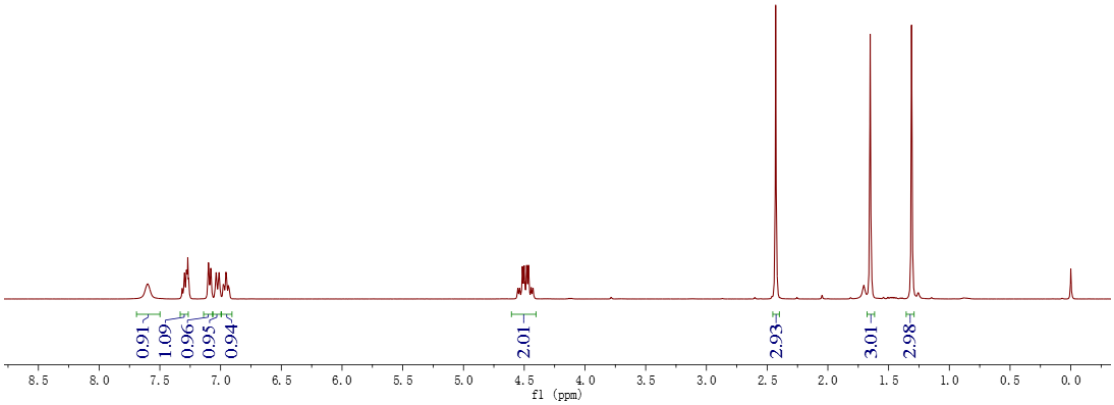

7.600
7.306
7.273
7.259
7.243
7.227
7.205
7.188
4.529
4.514
4.492
4.477
4.459
4.444
4.421
4.406
2.428
1.647
1.309
0.94
0.97
3.07
2.01
2.97
3.01
3.03
f1 (ppm)


170.479
140.421
134.572
130.058
128.060
127.725
126.034
77.477
77.160
76.842
59.297
43.069
33.011
23.033
18.554
f1 (ppm)

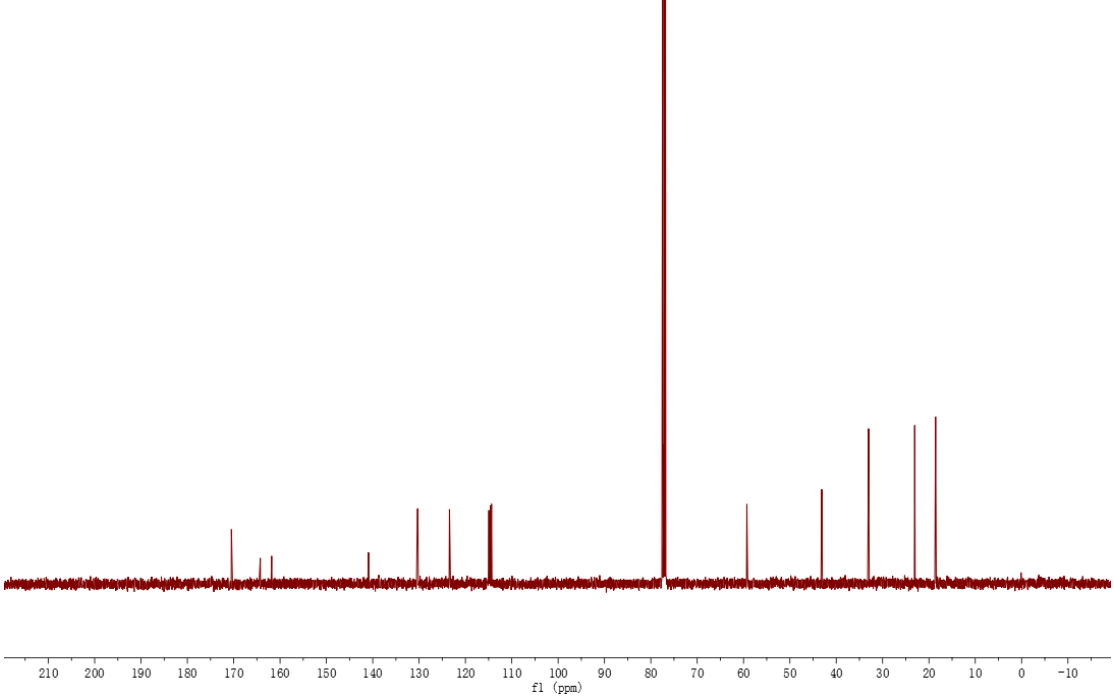

F
O
N
H
O
S

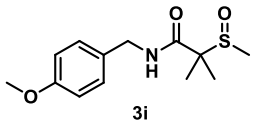
3h


7.601
7.316
7.297
7.282
7.277
7.270
7.099
7.081
7.036
7.013
6.978
6.957
6.936
4.553
4.538
4.515
4.500
4.480
4.465
4.442
4.428
2.430
1.652
1.311

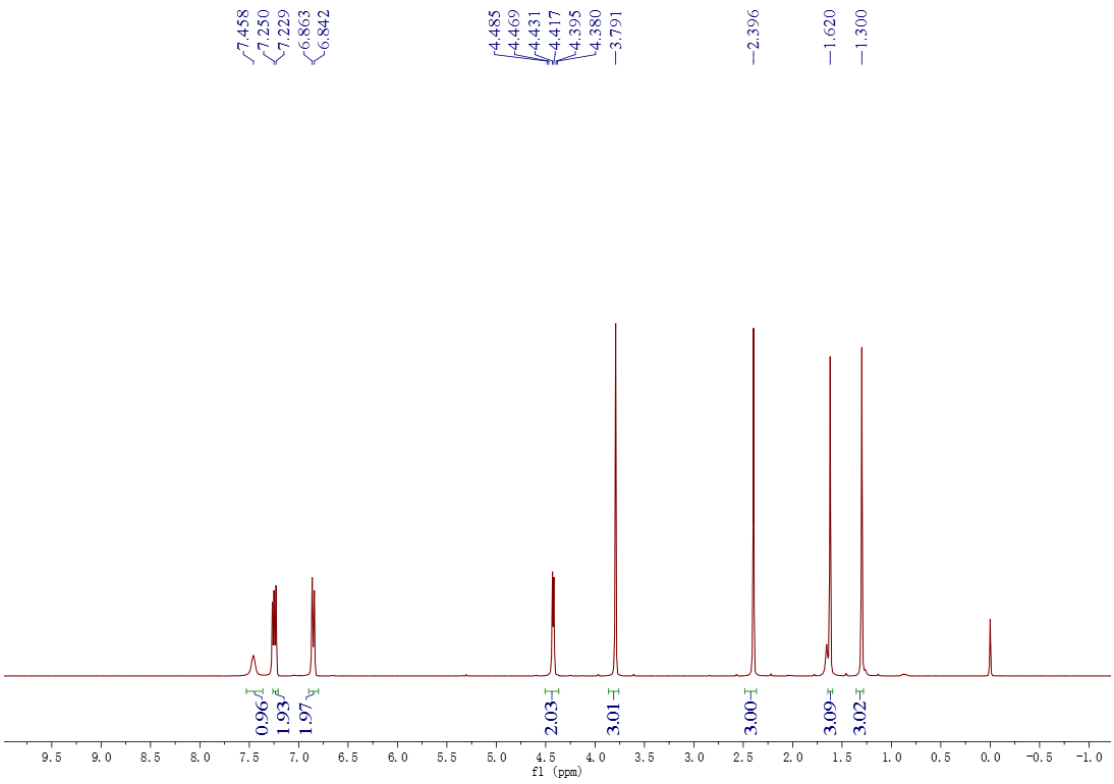

0.91
1.09
0.96
0.95
0.94
2.01
2.93
3.01
2.98
f1 (ppm)

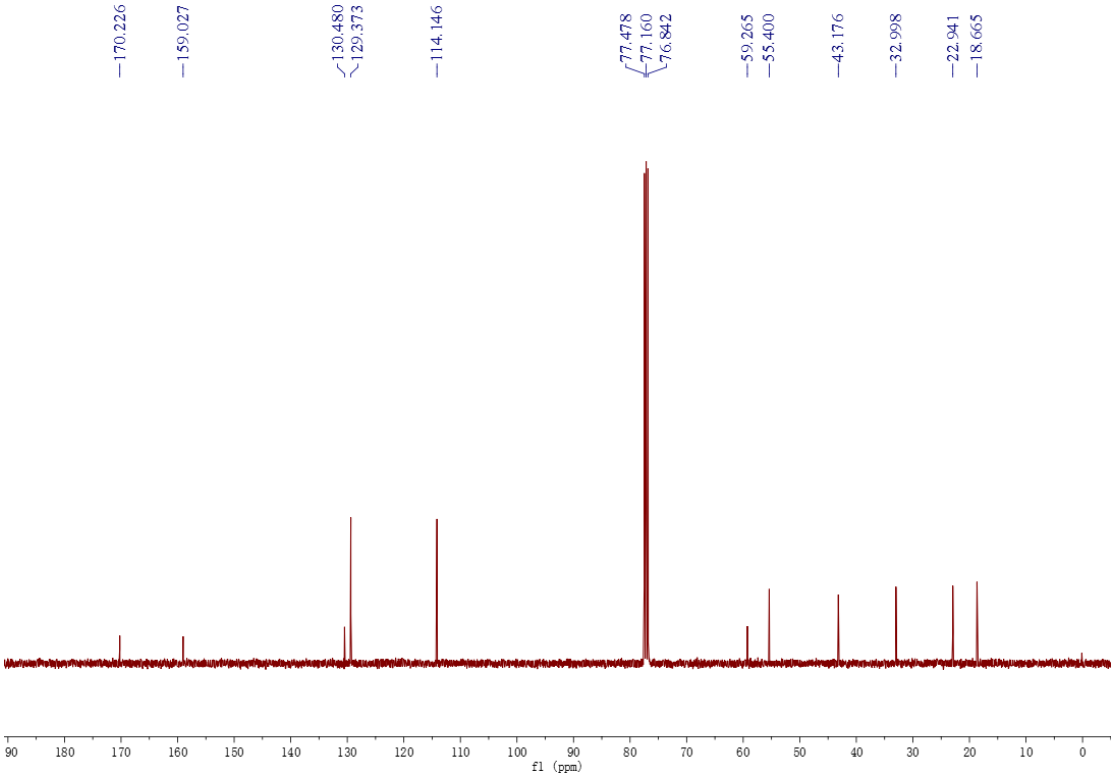

170.495
164.263
161.813
140.943
140.873
130.362
130.280
123.475
123.447
114.944
114.728
114.584
114.375
77.477
77.160
76.842
59.287
43.131
43.114
33.016
23.072
18.565

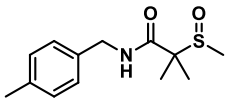

f1 (ppm)



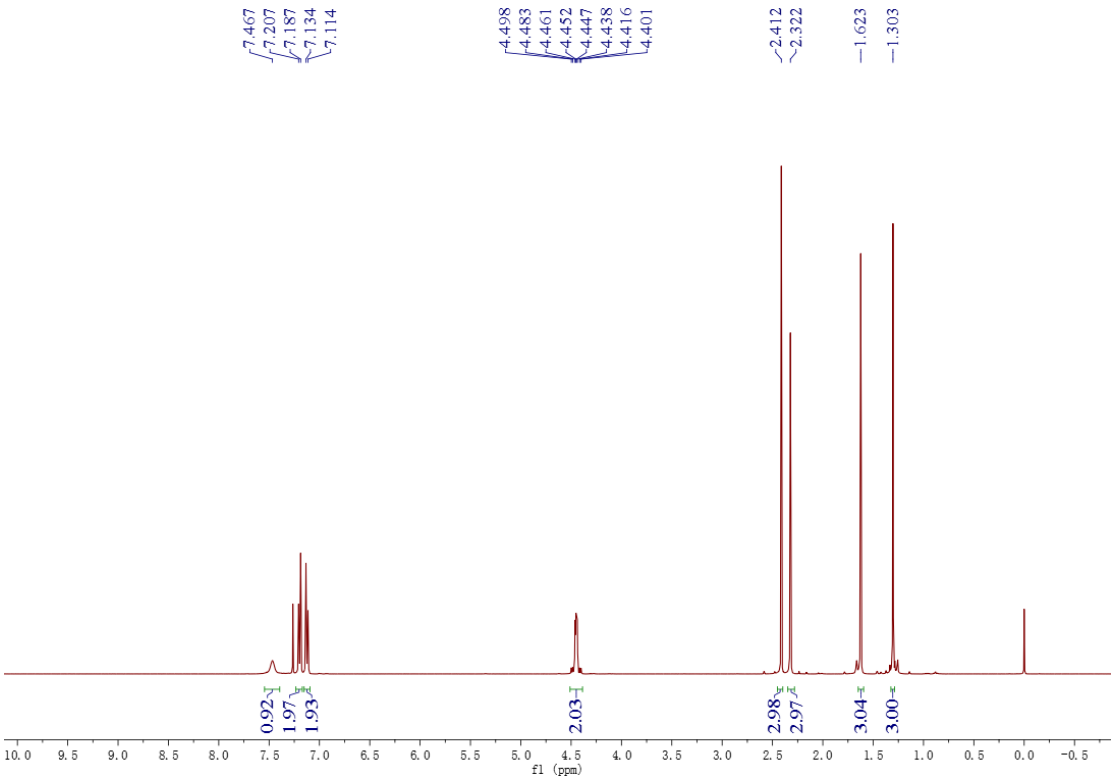
3i

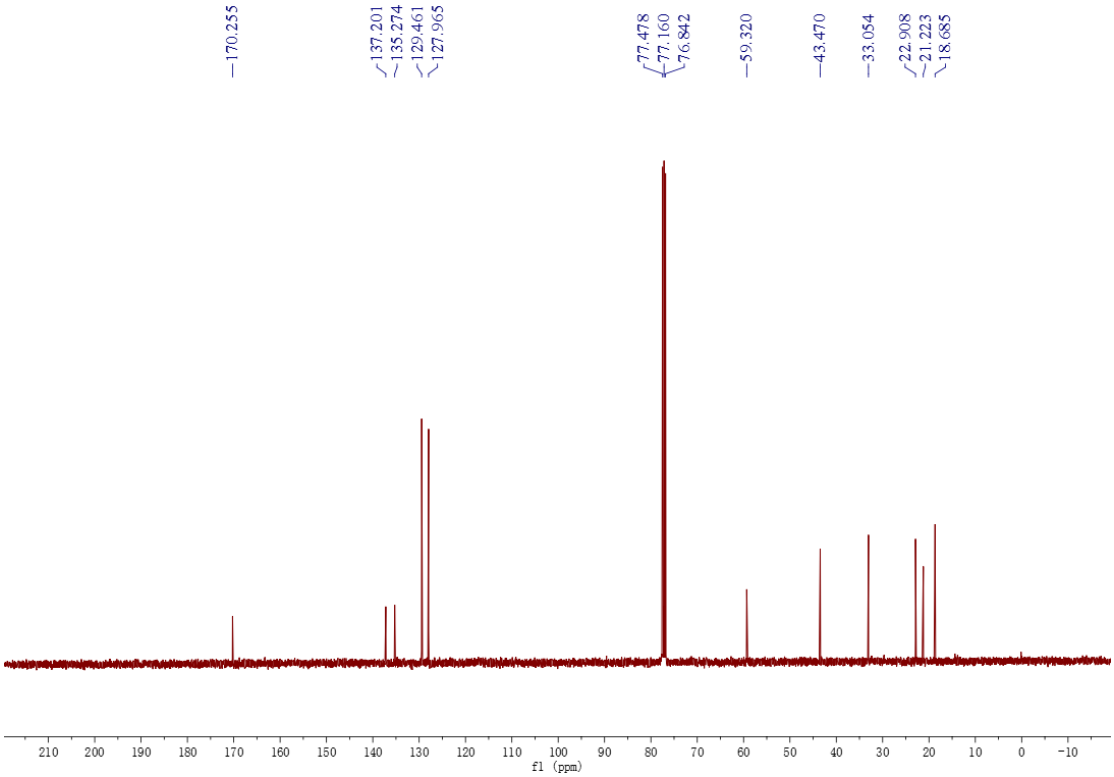

7.458
7.250
7.229
6.863
6.842
4.485
4.469
4.431
4.417
4.395
4.380
3.791
2.396
1.620
1.300
0.96
1.93
1.97
2.03
3.01
3.00
3.09
3.02
f1 (ppm)

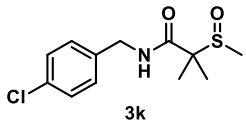

170.226
159.027
130.480
129.373
114.146
77.478
77.160
76.842
59.265
55.400
43.176
32.998
22.941
18.665
f1 (ppm)



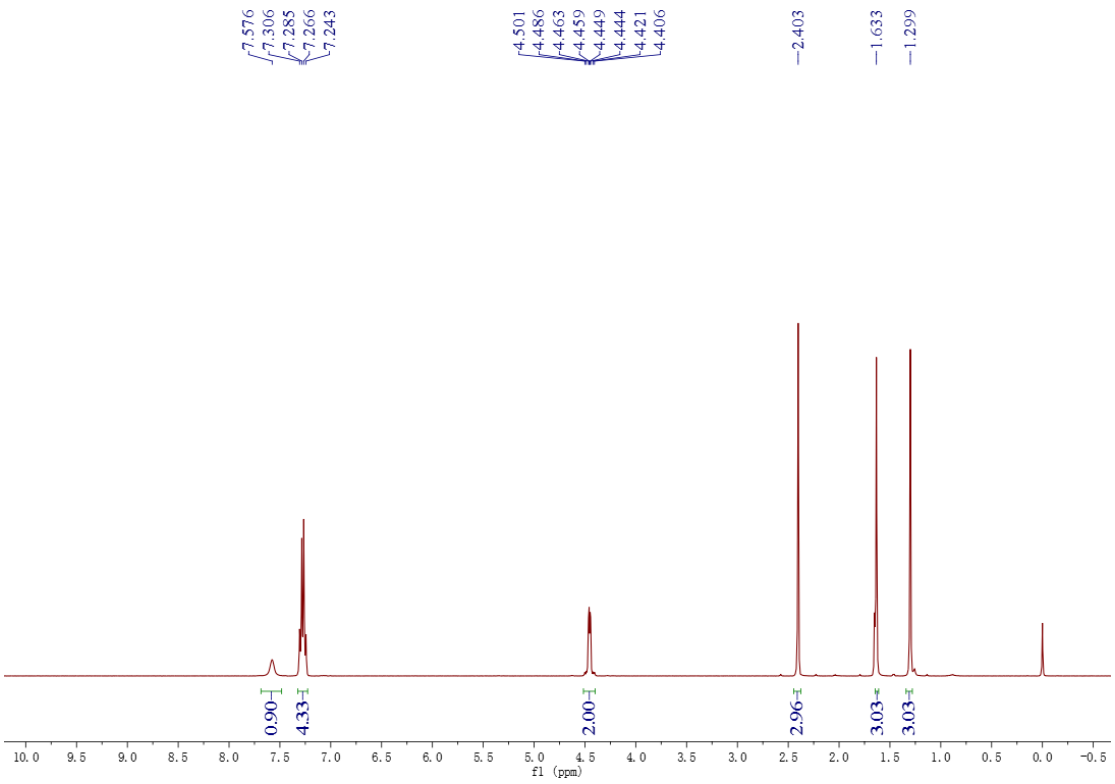
3j

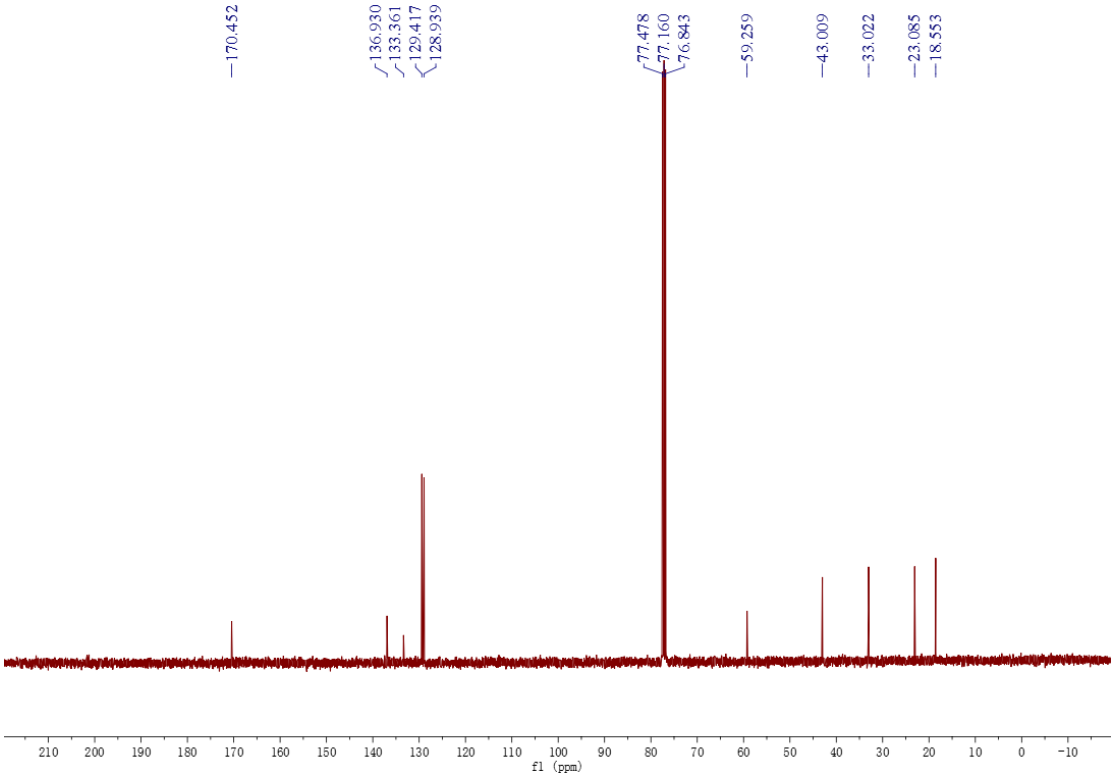

7.467
7.207
7.187
7.134
7.114
4.498
4.483
4.461
4.452
4.447
4.438
4.416
4.401
2.412
2.322
1.623
1.303
0.92
1.97
1.93
2.03
2.98
2.97
3.04
3.00
f1 (ppm)

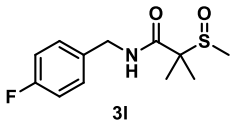

170.255
137.201
135.274
129.461
127.965
77.478
77.160
76.842
59.320
43.470
33.054
22.908
21.223
18.685
f1 (ppm)


O
O
S
N
H
Cl

3k

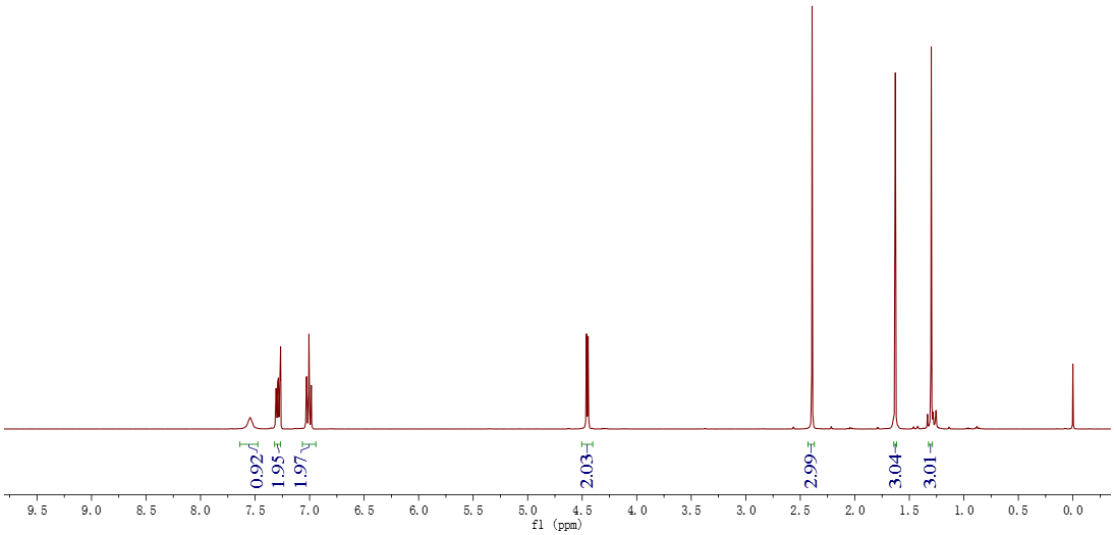

7.576
7.306
7.285
7.266
7.243
4.501
4.486
4.463
4.459
4.449
4.444
4.421
4.406
2.403
1.633
1.299
0.90
4.33
2.00
2.96
3.03
3.03
f1 (ppm)


170.452
136.930
133.361
129.417
128.939
77.478
77.160
76.843
59.259
43.009
33.022
23.085
18.553
f1 (ppm)

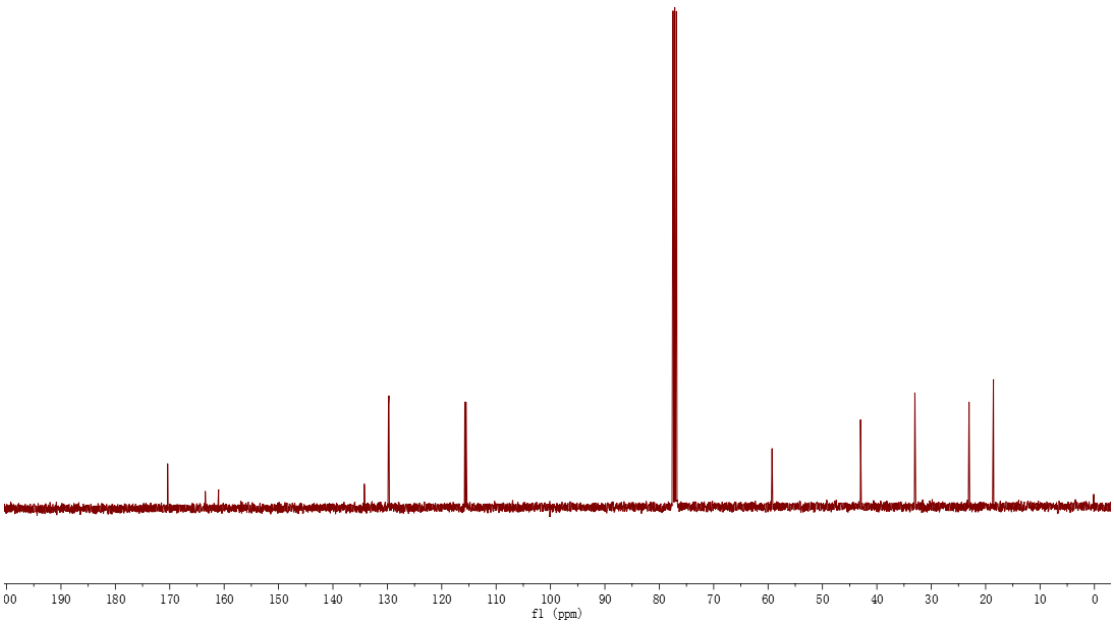


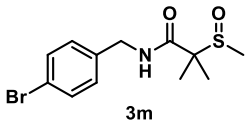
3l


7.545
7.314
7.307
7.294
7.286
7.277
7.273
7.035
7.028
7.006
6.985
6.977
4.498
4.481
4.461
4.446
4.424
4.409
2.392
1.629
1.299

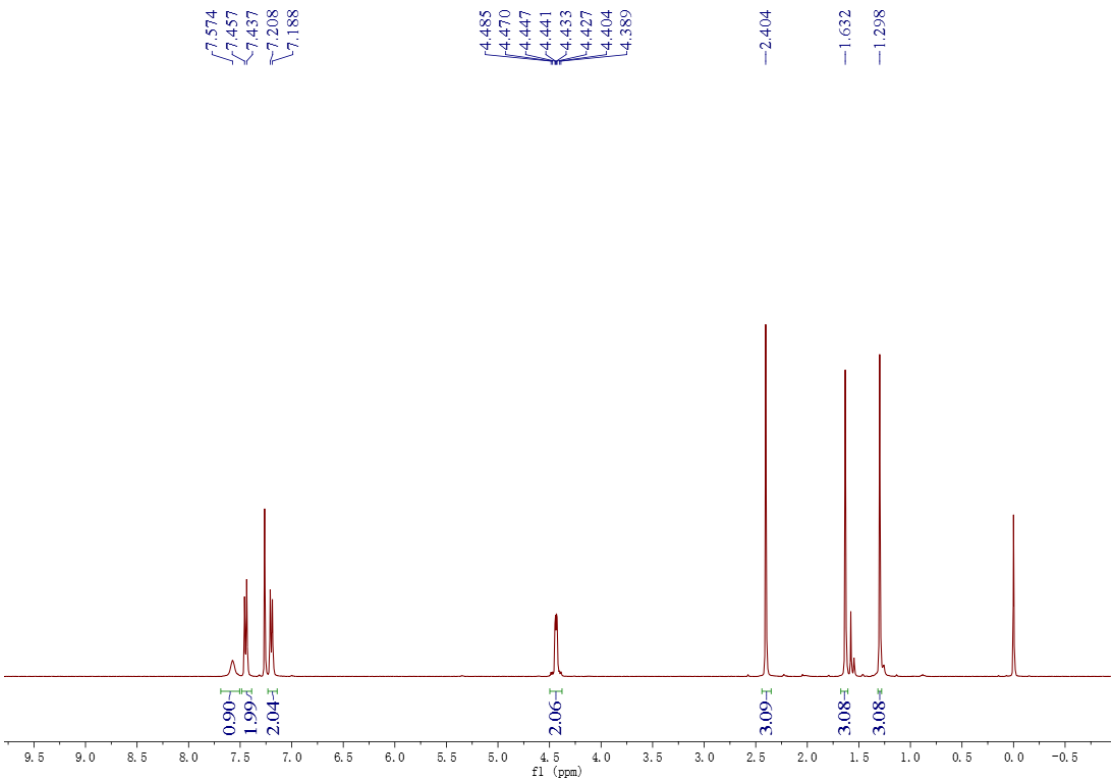

0.92
1.95
1.97
2.03
2.99
3.04
3.01
f1 (ppm)

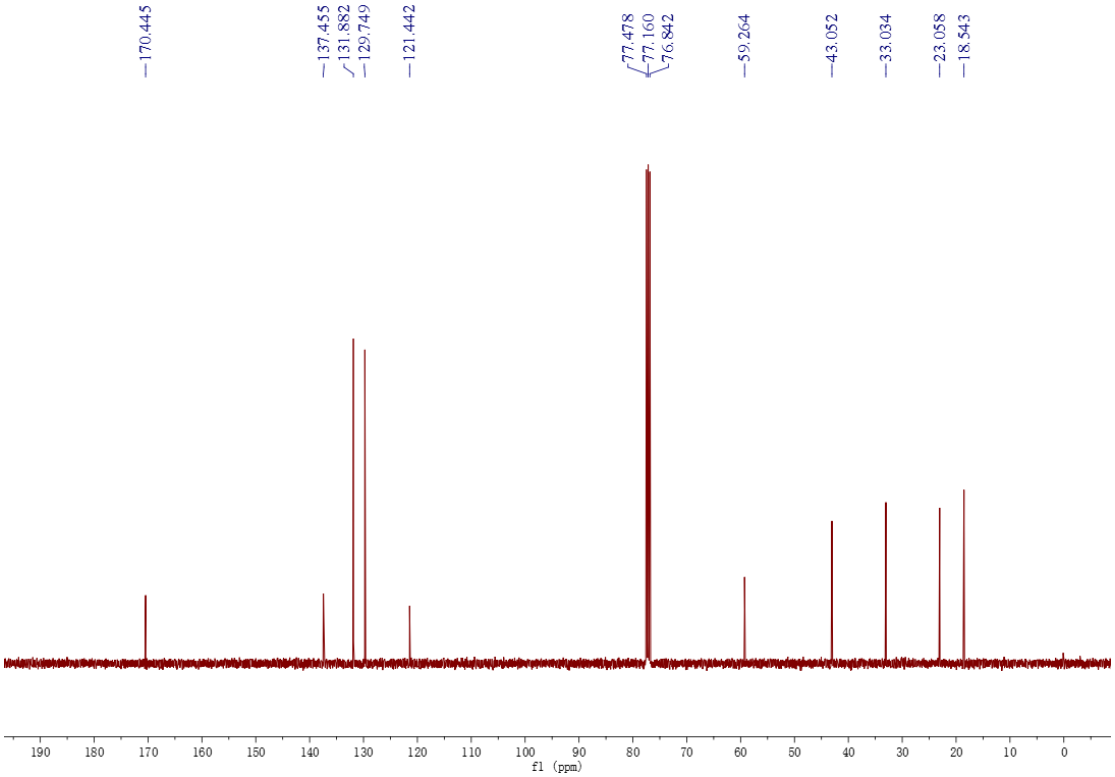

170.392
163.471
161.030
134.240
134.207
129.791
129.710
115.751
115.537
77.478
77.160
76.843
59.267
42.998
33.007
23.053
18.573

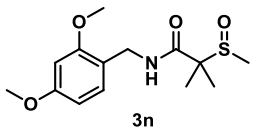

f1 (ppm)


O
O
N
H
S
Br

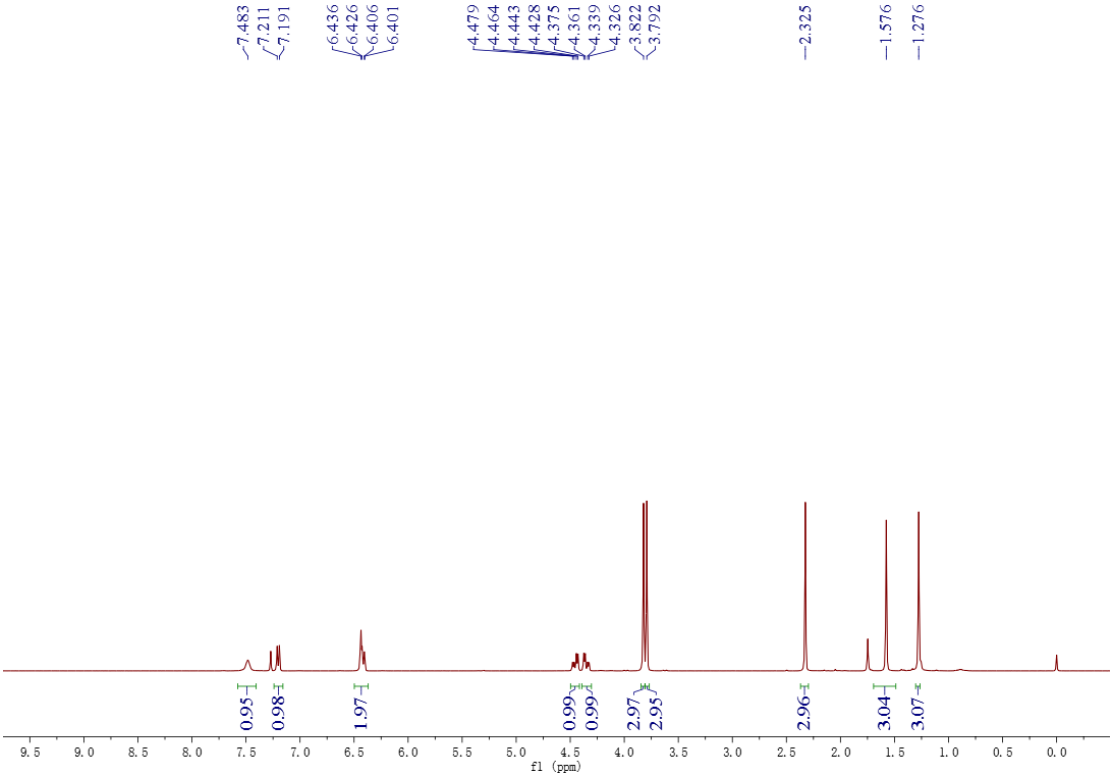
3m

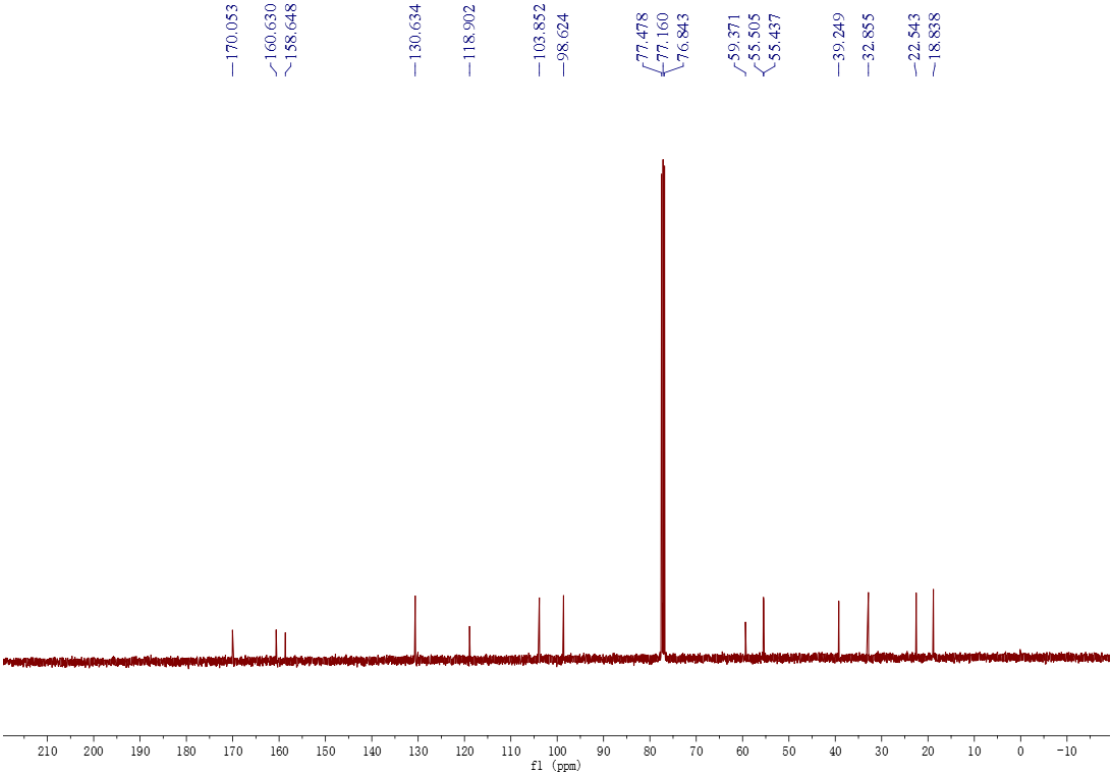

7.574
7.457
7.437
7.208
7.188
4.485
4.470
4.447
4.441
4.433
4.427
4.404
4.389
2.404
1.632
1.298
0.90
1.99
2.04
2.06
3.09
3.08
3.08
f1 (ppm)

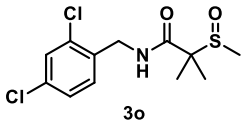

170.445
137.455
131.882
129.749
121.442
77.478
77.160
76.842
59.264
43.052
33.034
23.058
18.543
f1 (ppm)



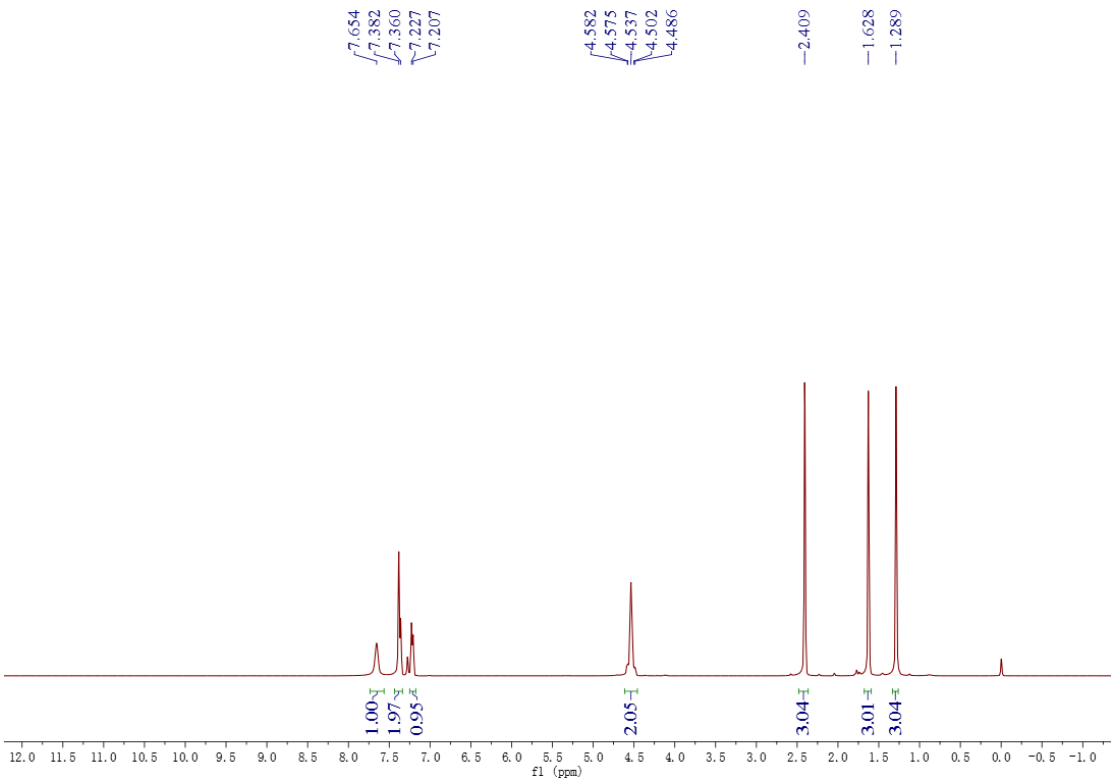
3n

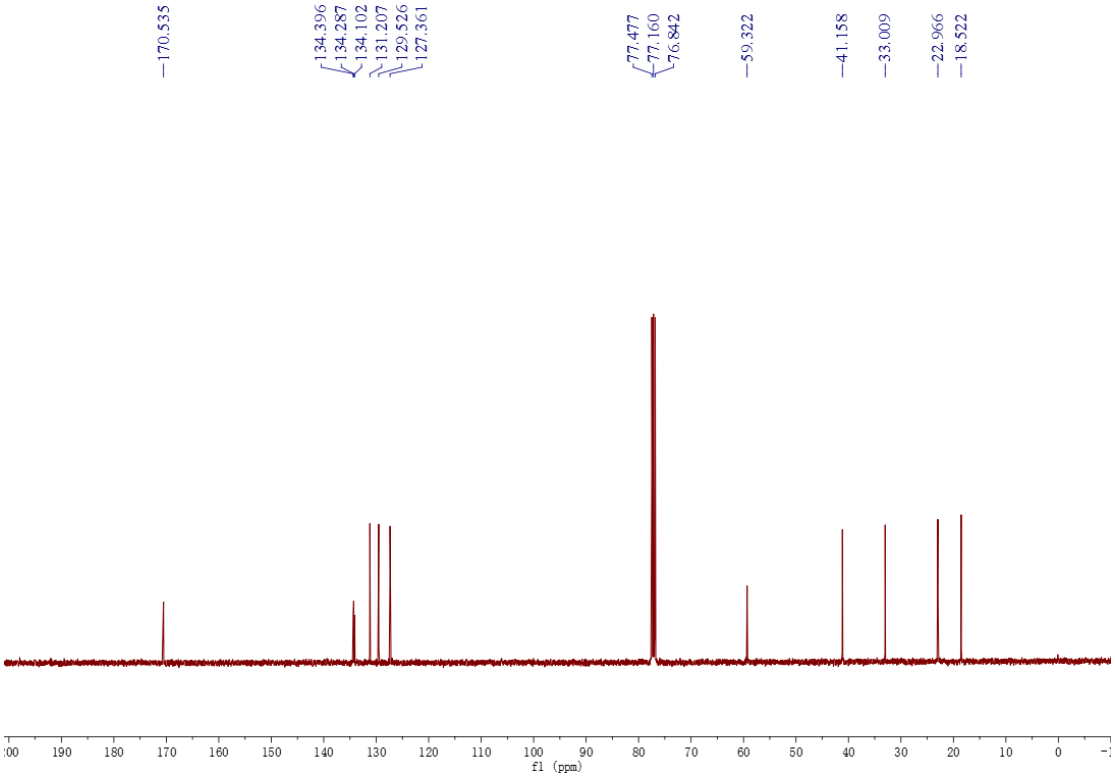

7.483
7.211
7.191
6.436
6.426
6.406
6.401
4.479
4.464
4.443
4.428
4.375
4.361
4.339
4.326
3.822
3.792
2.325
1.576
1.276
0.95
0.98
1.97
0.99
0.99
2.97
2.95
2.96
3.04
3.07
f1 (ppm)

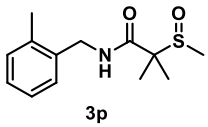

170.053
160.630
158.648
130.634
118.902
103.852
98.624
77.478
77.160
76.843
59.371
55.505
55.437
39.249
32.855
22.543
18.838
f1 (ppm)


Cl
O
O
N
H
S
Cl

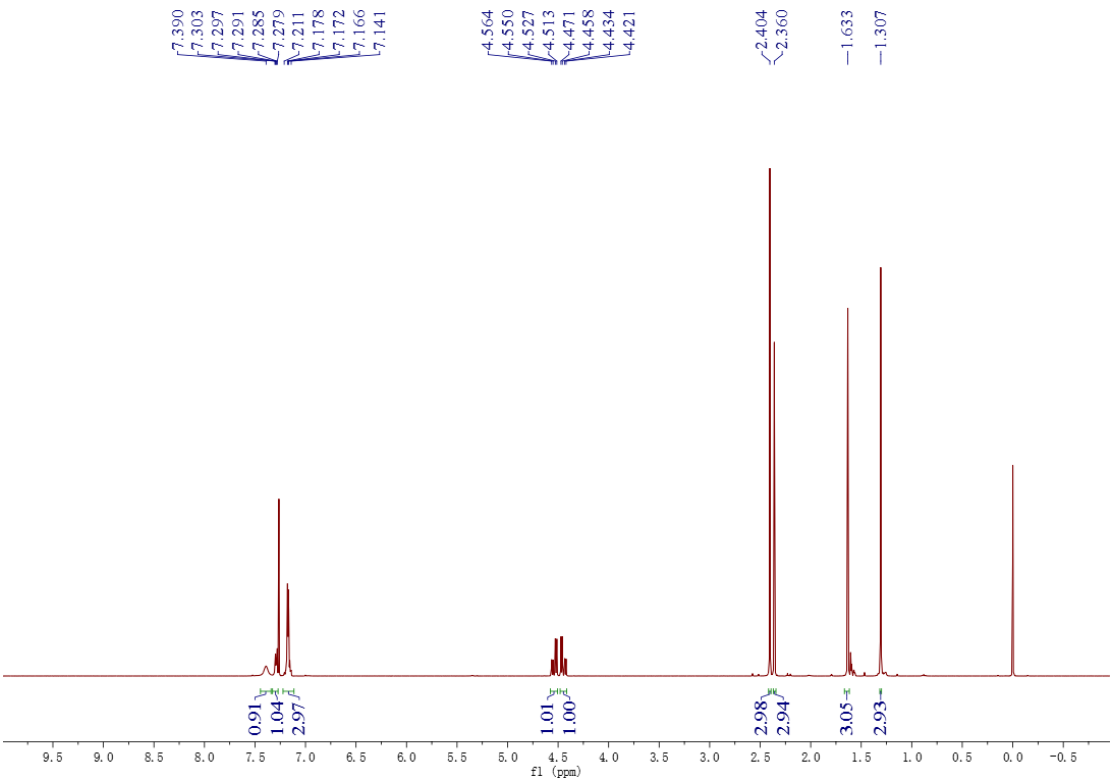
3o

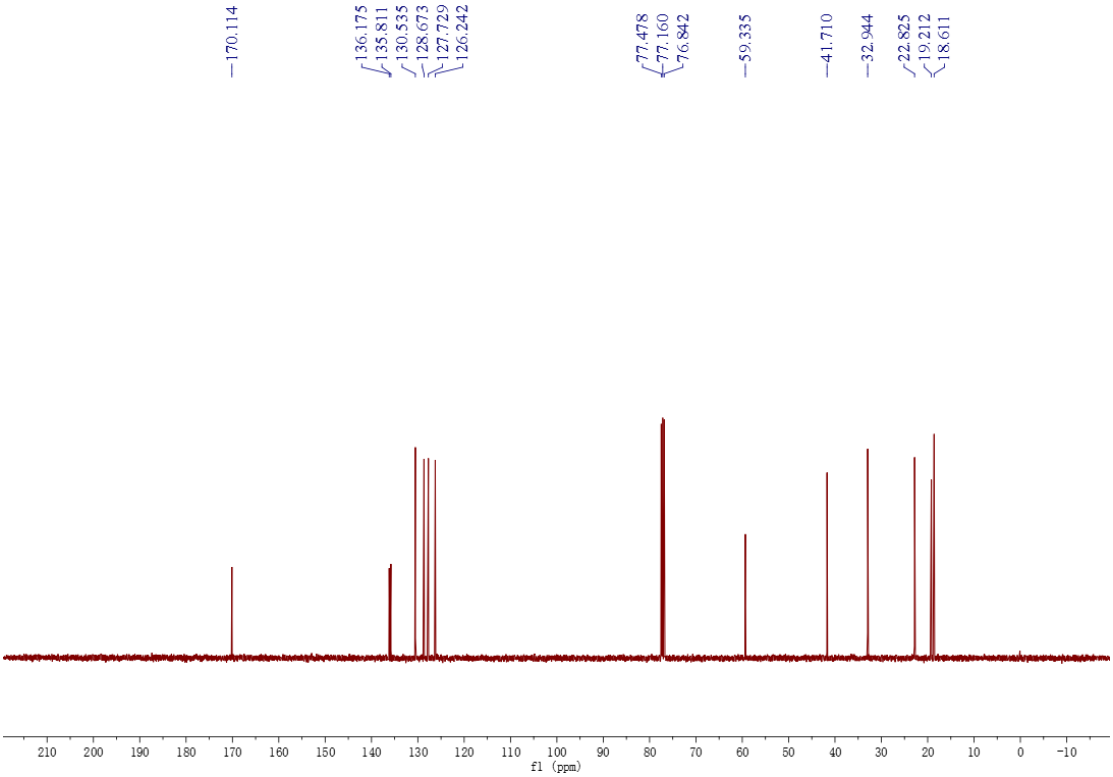

7.654
7.382
7.360
7.227
7.207
4.582
4.575
4.537
4.502
4.486
2.409
1.628
1.289
1.00
1.97
0.95
2.05
3.04
3.01
3.04
f1 (ppm)

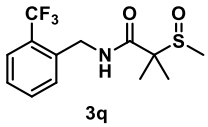

170.535
134.396
134.287
134.102
131.207
129.526
127.361
77.477
77.160
76.842
59.322
41.158
33.009
22.966
18.522
f1 (ppm)



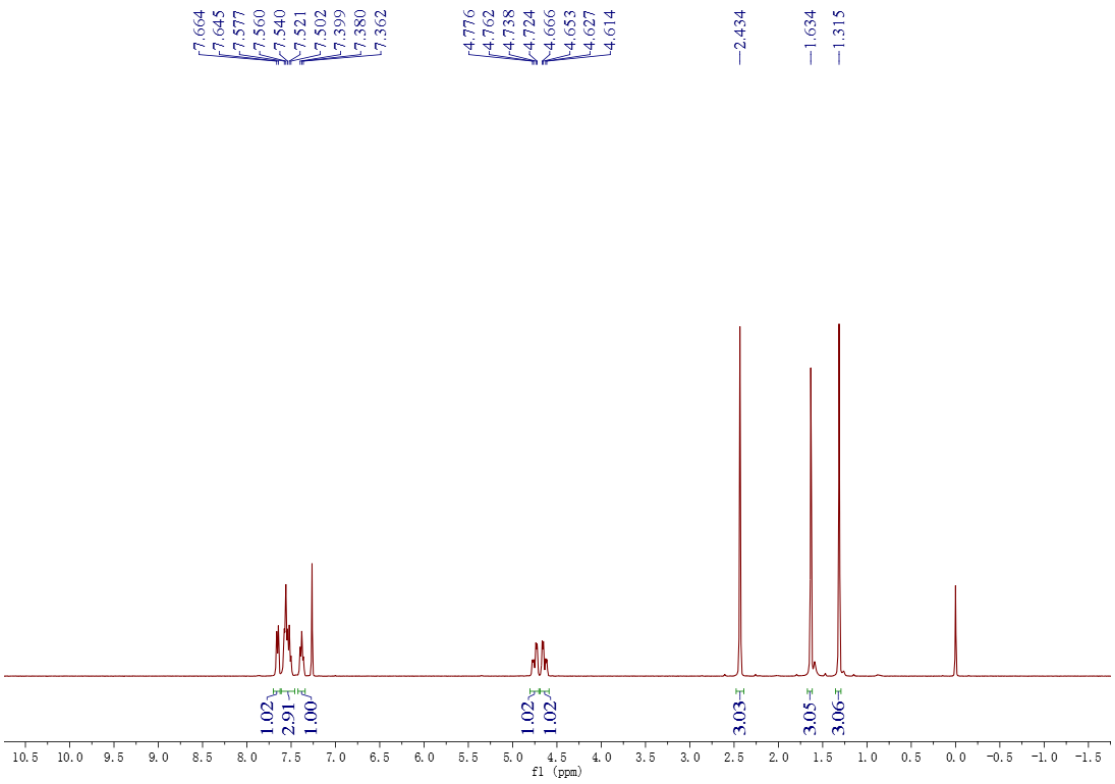
3p

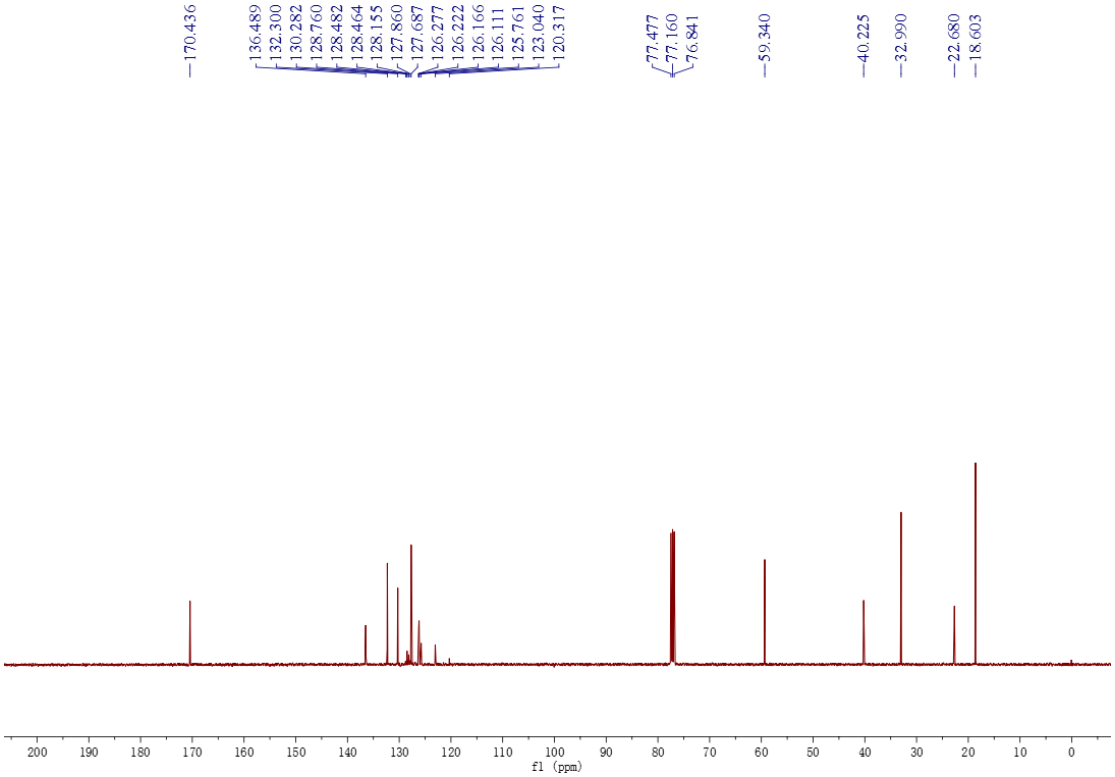

7.390
7.303
7.297
7.291
7.285
7.279
7.211
7.178
7.172
7.166
7.141
4.564
4.550
4.527
4.513
4.471
4.458
4.434
4.421
2.404
2.360
1.633
1.307
0.91
1.04
2.97
1.01
1.00
2.98
2.94
3.05
2.93
f1 (ppm)

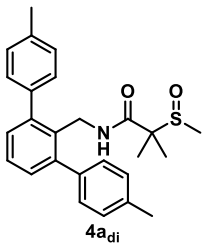

170.114
136.175
135.811
130.535
128.673
127.729
126.242
77.478
77.160
76.842
59.335
41.710
32.944
22.825
19.212
18.611
f1 (ppm)



3q

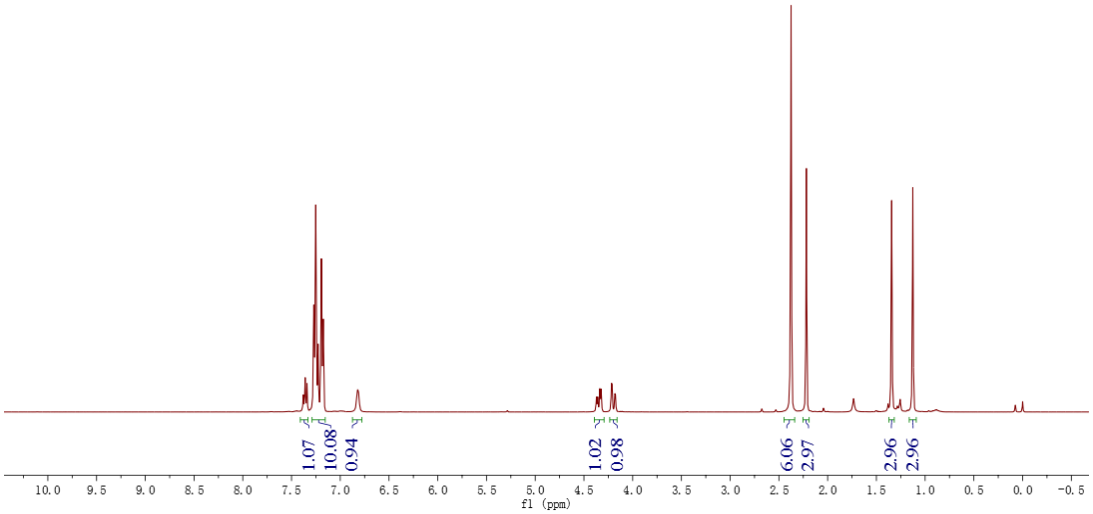

7.664
7.645
7.577
7.560
7.540
7.521
7.502
7.399
7.380
7.362
4.776
4.762
4.738
4.724
4.666
4.653
4.627
4.614
2.434
1.634
1.315
1.02
2.91
1.00
1.02
1.02
3.03
3.05
3.06
f1 (ppm)


170.436
136.489
132.300
130.282
128.760
128.482
128.464
128.155
127.860
127.687
126.277
126.222
126.166
126.111
125.761
123.040
120.317
77.477
77.160
76.841
59.340
40.225
32.990
22.680
18.603
f1 (ppm)

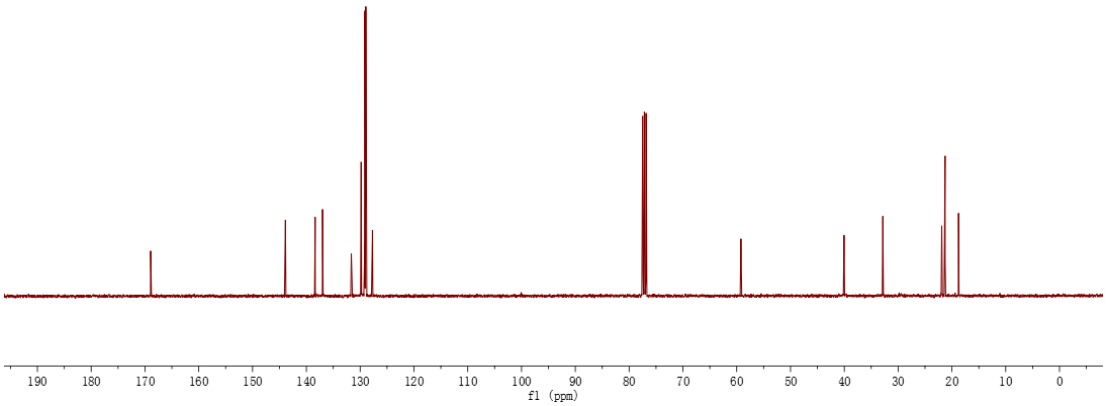

O
O
S
N
H

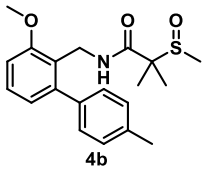
4a$_{di}$


7.379
7.360
7.341
7.272
7.252
7.194
7.174
6.820
4.372
4.358
4.337
4.324
4.217
4.211
4.183
4.177
2.375
2.219
1.343
1.127

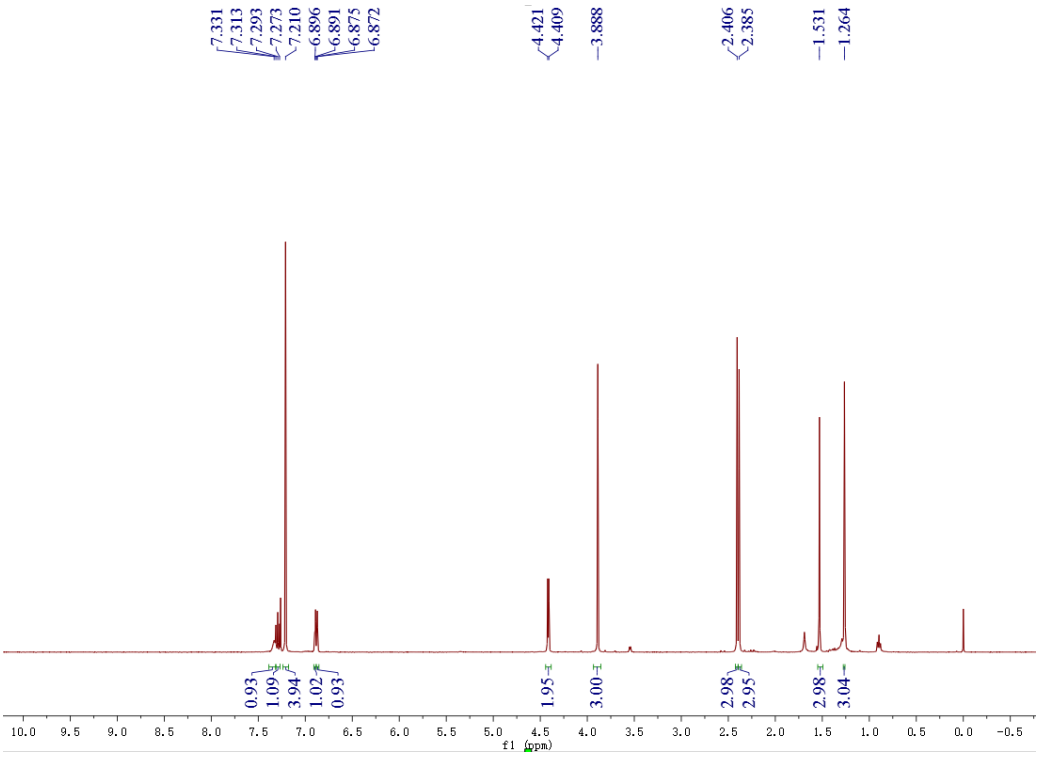

1.07
10.08
0.94
1.02
0.98
6.06
2.97
2.96
2.96
f1 (ppm)

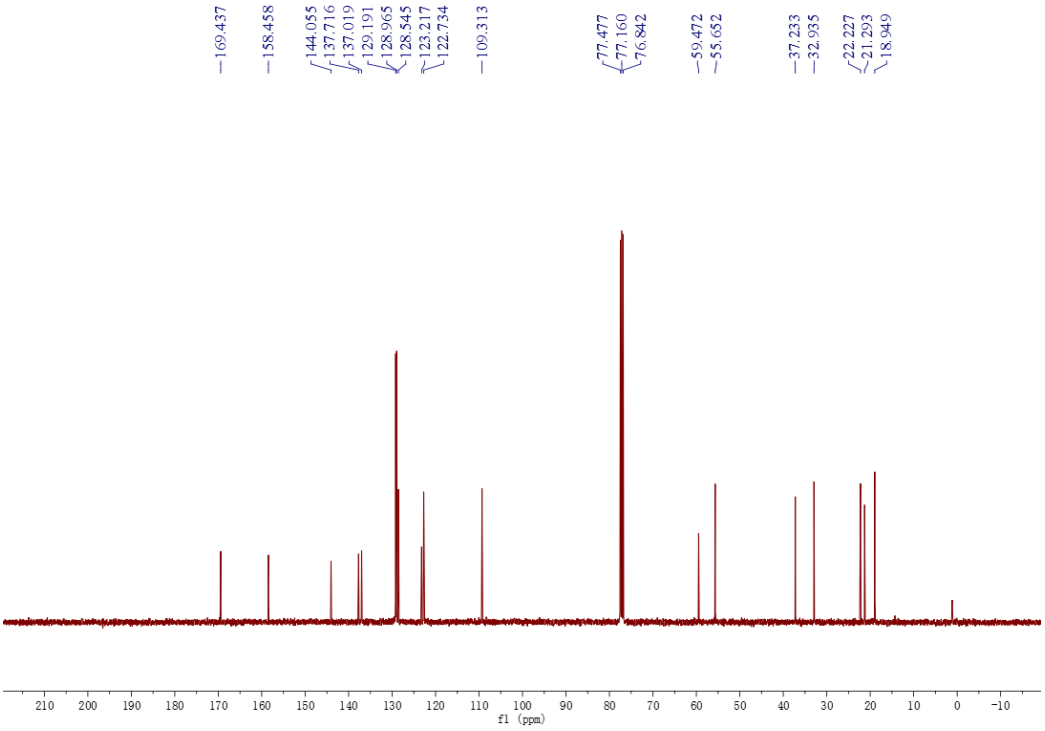

168.939
143.889
138.361
136.986
131.641
129.813
129.110
128.939
127.709
77.477
77.160
76.842
59.220
40.049
32.841
21.890
21.267
18.761

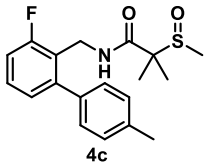

f1 (ppm)



4b

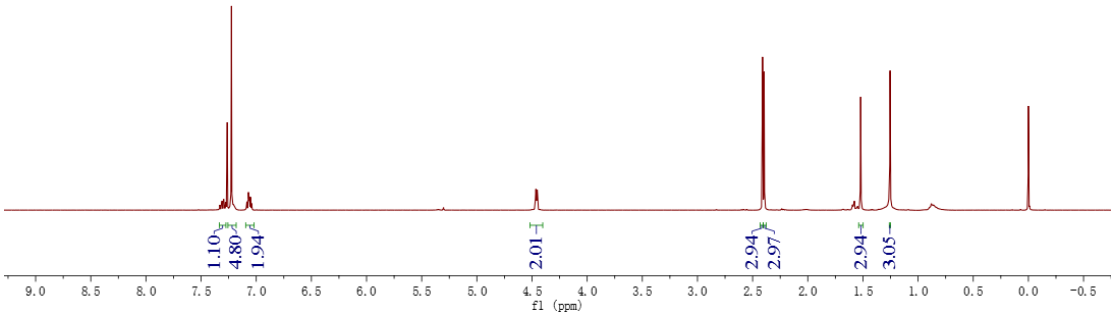

7.331
7.313
7.293
7.273
7.210
6.896
6.891
6.875
6.872
4.421
4.409
3.888
2.406
2.385
1.531
1.264
0.93
1.09
3.94
1.02
0.93
1.95
3.00
2.98
2.95
2.98
3.04
f1 (ppm)


169.437
158.458
144.055
137.716
137.019
129.191
128.965
128.545
123.217
122.734
109.313
77.477
77.160
76.842
59.472
55.652
37.233
32.935
22.227
21.293
18.949
f1 (ppm)

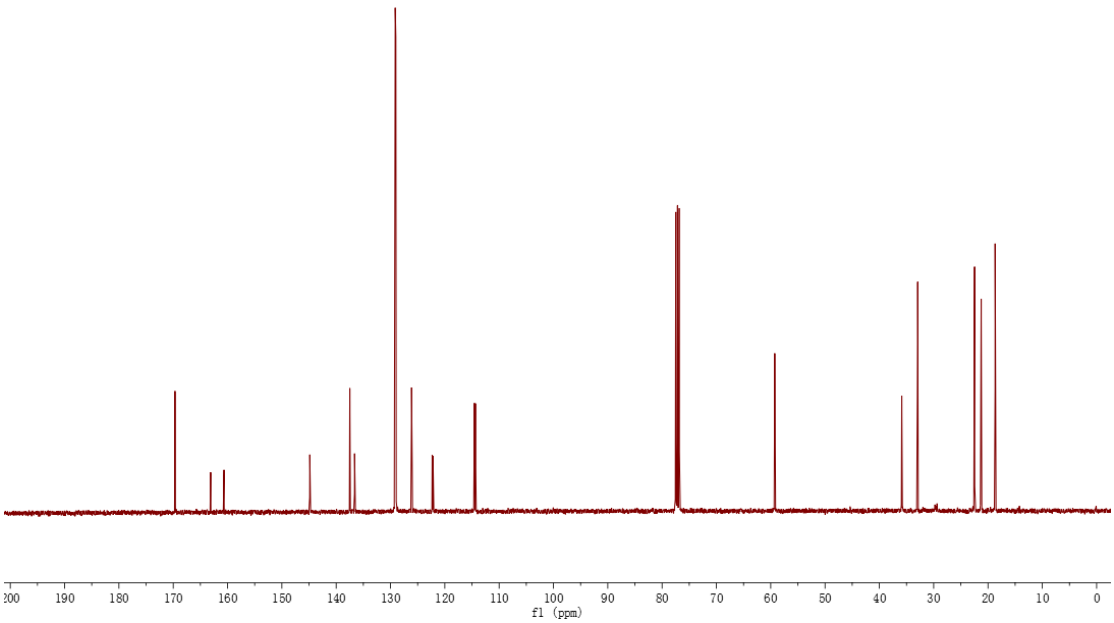

F
O
O
N
H
S

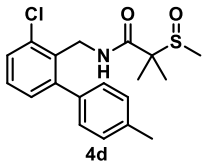
4c


7.329
7.315
7.309
7.295
7.290
7.275
7.225
7.204
7.085
7.071
7.063
7.052
7.042
4.503
4.500
4.491
4.487
4.465
4.453
4.430
4.427
4.418
4.415
2.410
2.396
1.521
1.254


1.10
4.80
1.94
2.01
2.94
2.97
2.94
3.05
f1 (ppm)

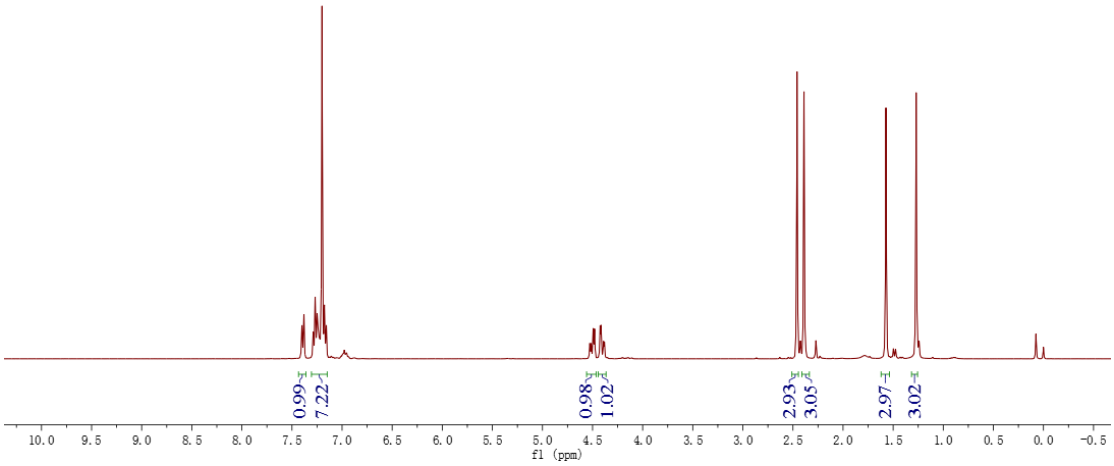

169.672
163.107
160.647
144.858
144.822
137.491
136.610
136.585
129.128
129.056
129.016
114.346
114.324
77.478
77.160
76.842
59.254
35.878
35.837
32.941
22.470
21.253
18.686


f1 (ppm)

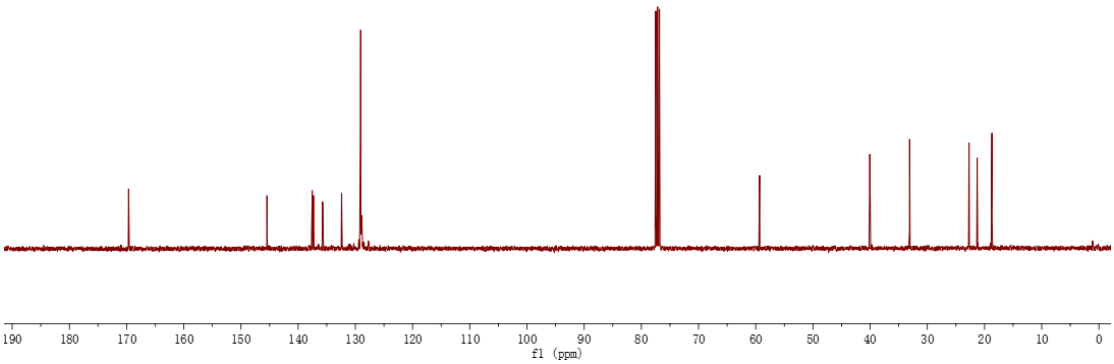

Cl
O
O
S
N
H

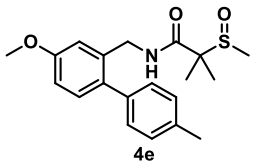
4d


7.400
7.380
7.288
7.268
7.249
7.176
7.157
4.528
4.514
4.493
4.480
4.424
4.415
4.390
4.381
2.460
2.390
1.572
1.270


0.99
7.22
0.98
1.02
2.93
3.05
2.97
3.02
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)

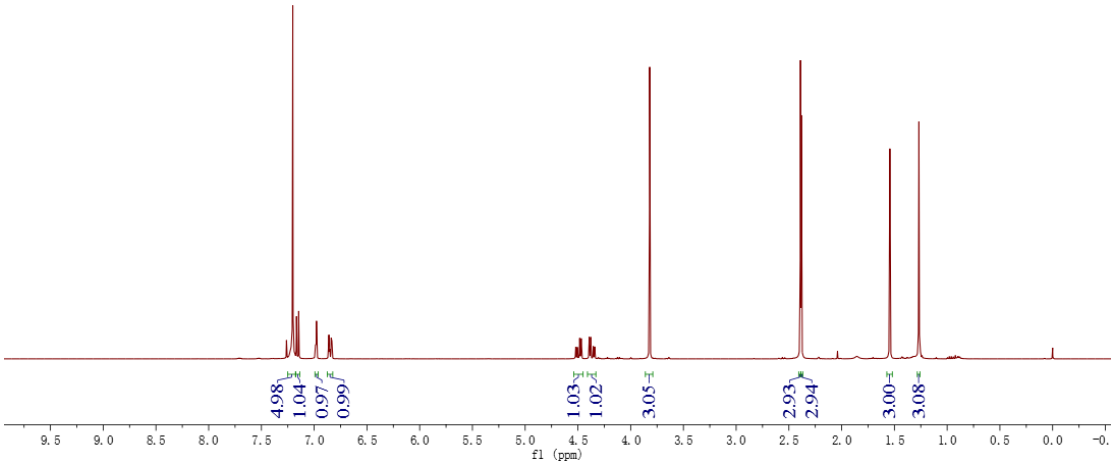

169.644
145.455
137.545
137.321
135.726
132.412
129.113
129.073
128.975
128.927
77.478
77.160
76.842
59.328
40.056
33.095
22.711
21.289
18.702


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

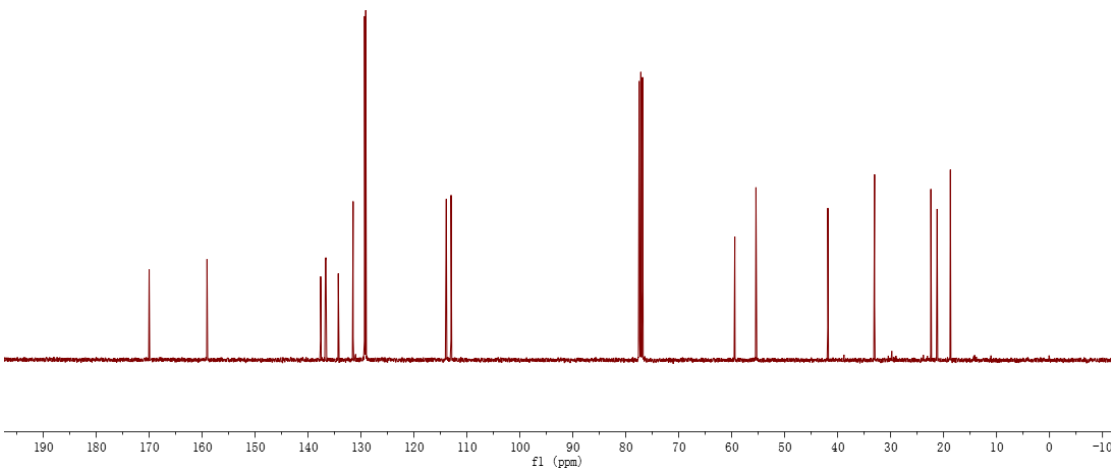


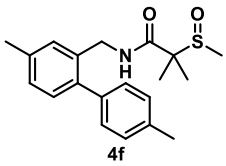
4e


7.225
7.222
7.203
7.185
7.182
7.168
7.147
6.985
6.978
6.860
6.854
6.839
6.833
4.521
4.506
4.483
4.468
4.392
4.379
4.355
4.342
3.820
2.390
2.383
1.543
1.268

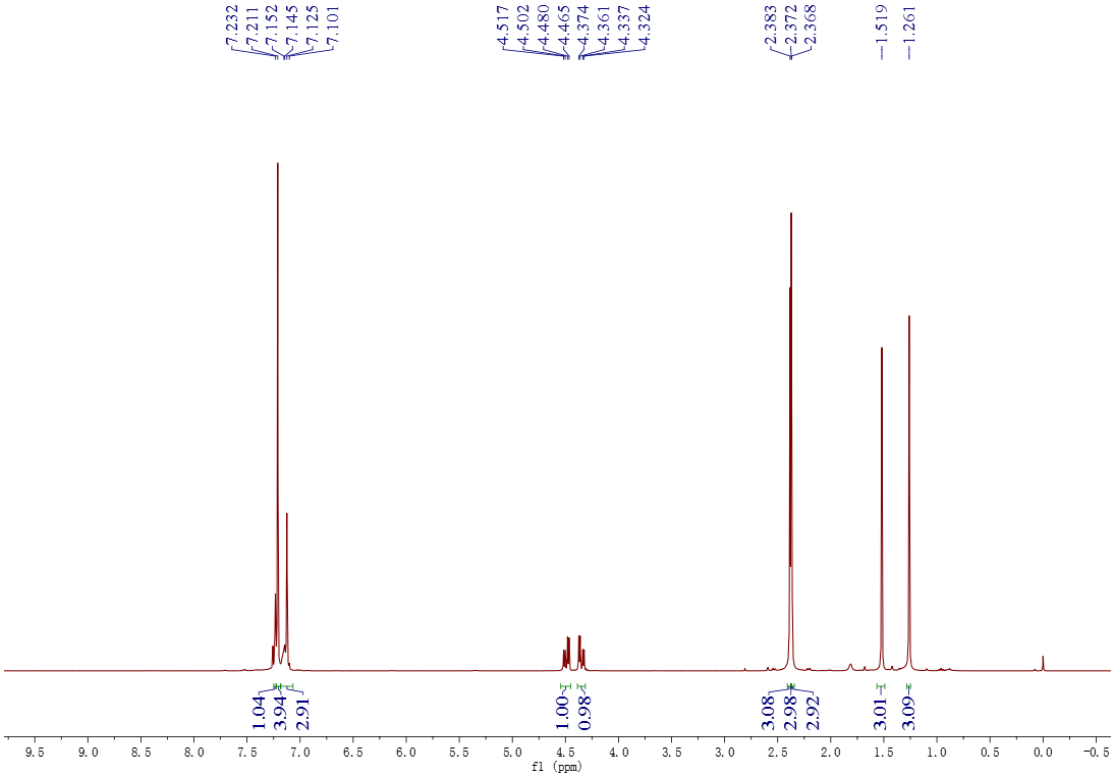

4.98
1.04
0.97
0.99
1.03
1.02
3.05
2.93
2.94
3.00
3.08
f1 (ppm)

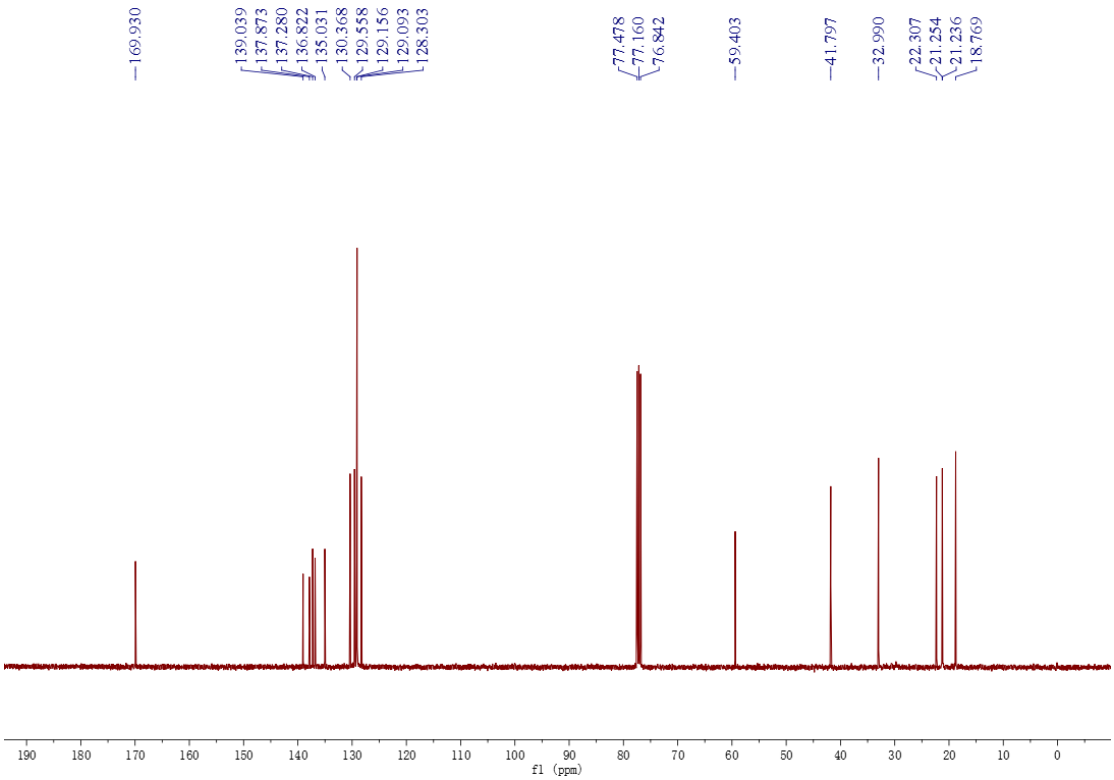

169.990
159.063
137.607
136.707
136.621
134.279
131.481
129.317
129.094
113.888
112.985
77.478
77.160
76.842
59.419
55.426
41.851
33.032
22.402
21.222
18.721

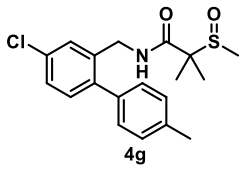

f1 (ppm)


O
O
S
N
H

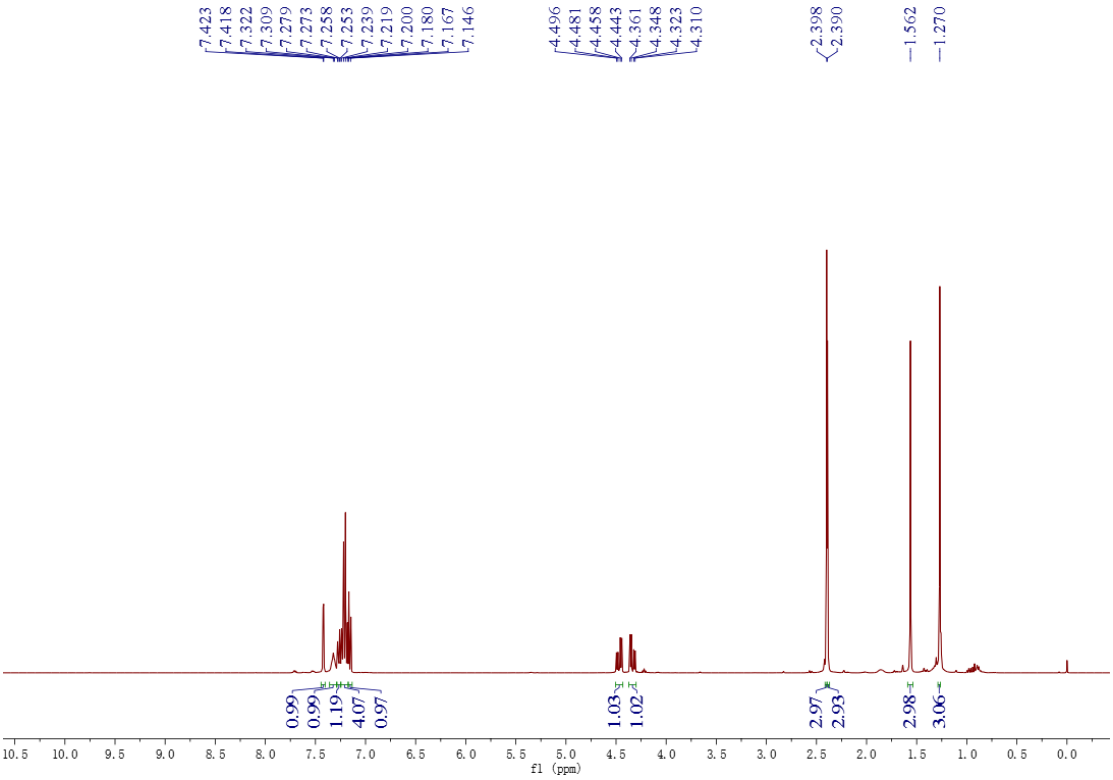
4f

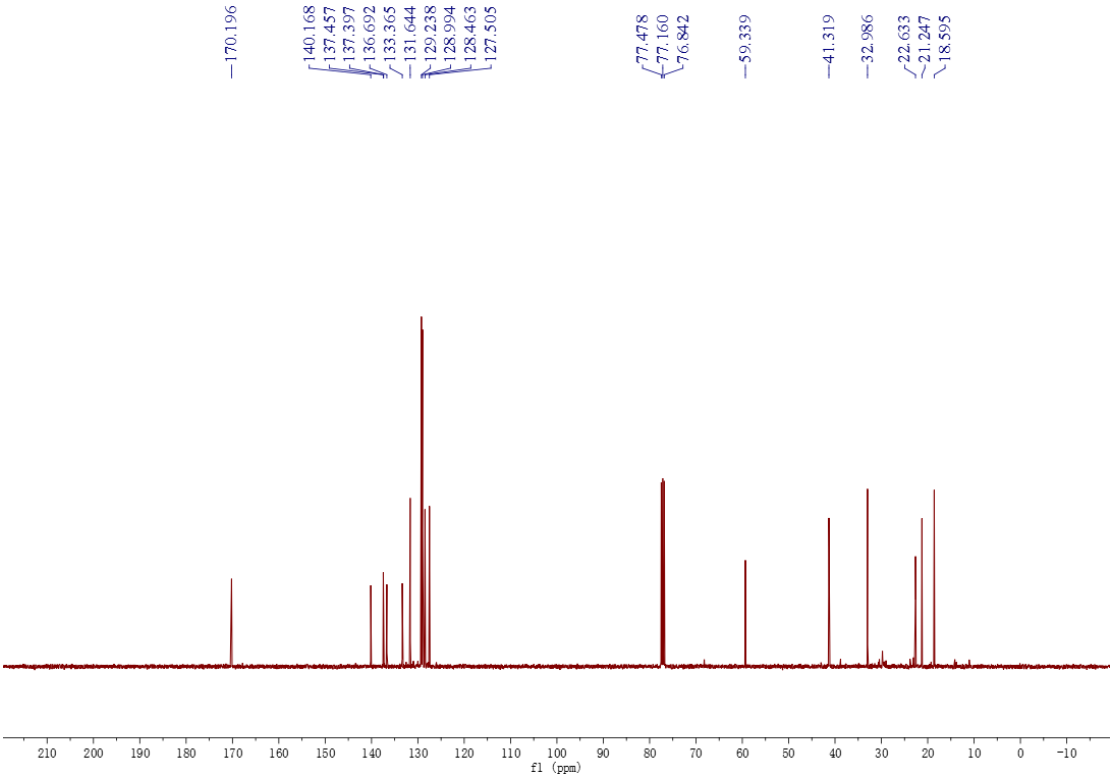

7.232
7.211
7.152
7.145
7.125
7.101
4.517
4.502
4.480
4.465
4.374
4.361
4.337
4.324
2.383
2.372
2.368
1.519
1.261
1.04
3.94
2.91
1.00
0.98
3.08
2.98
2.92
3.01
3.09
f1 (ppm)

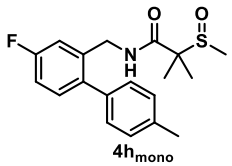

169.930
139.039
137.873
137.280
136.822
135.031
130.368
129.558
129.156
129.093
128.303
77.478
77.160
76.842
59.403
41.797
32.990
22.307
21.254
21.236
18.769
f1 (ppm)

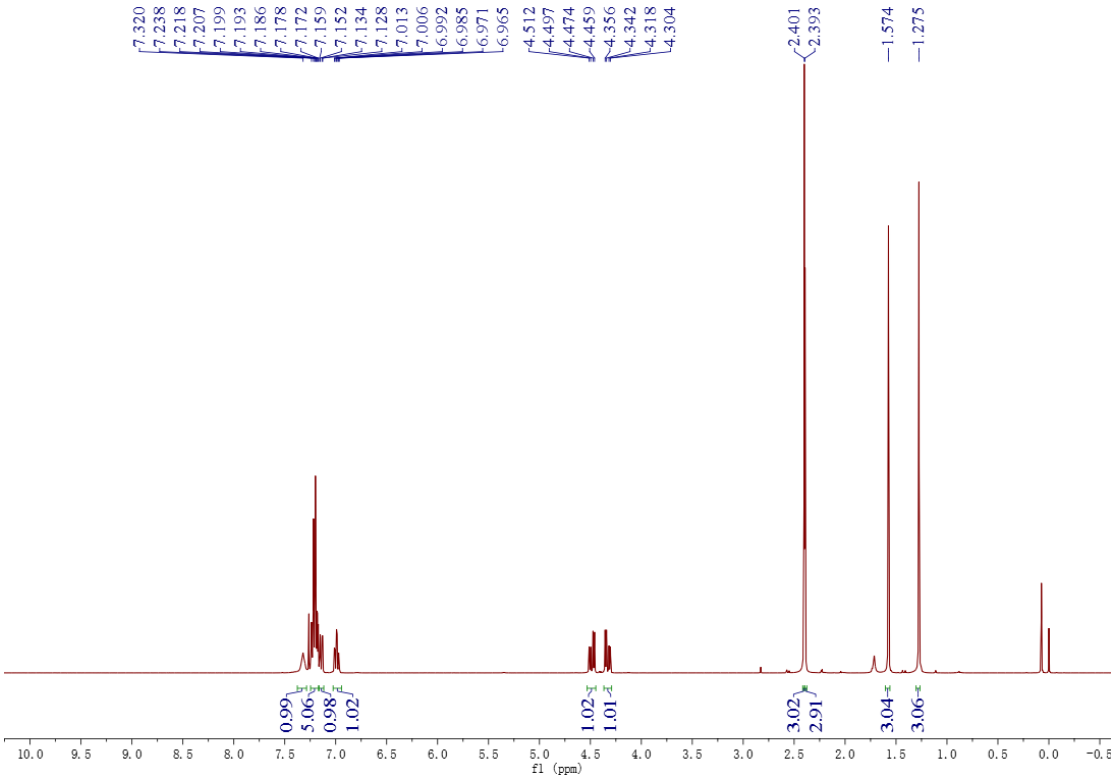

Cl
O
O
S
N
H

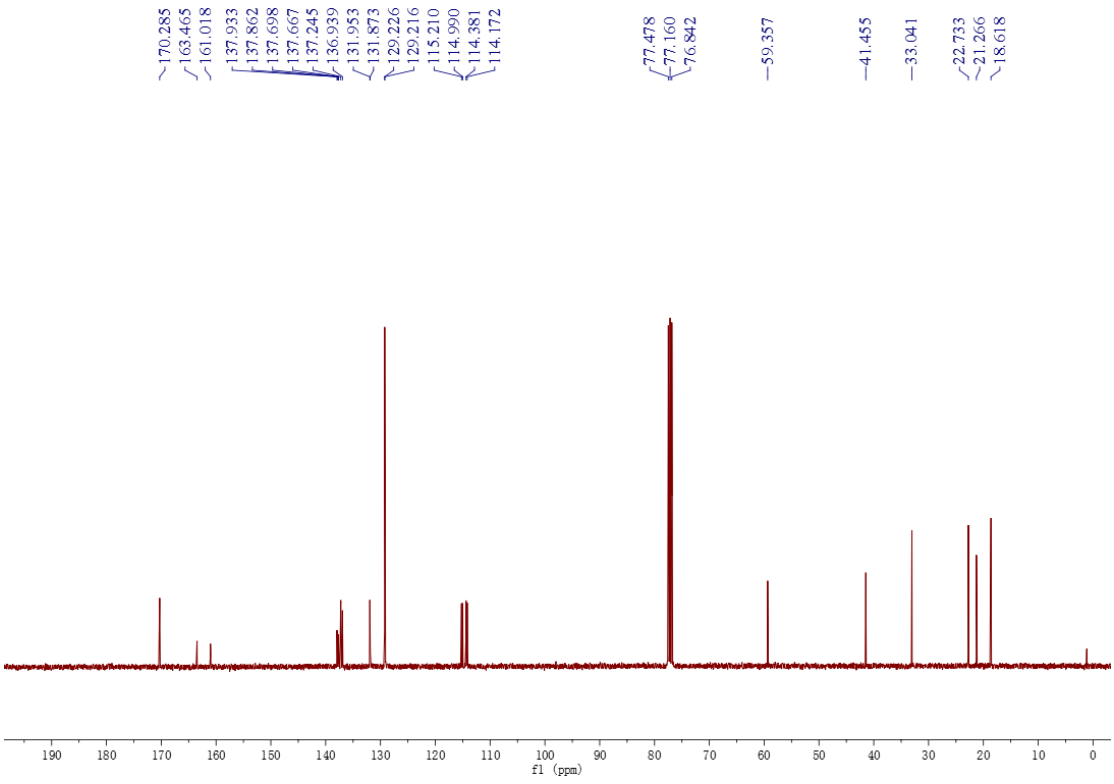
4g

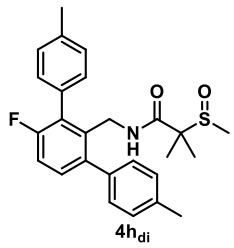

7.423
7.418
7.322
7.309
7.279
7.273
7.258
7.253
7.239
7.219
7.200
7.180
7.167
7.146
4.496
4.481
4.458
4.443
4.361
4.348
4.323
4.310
2.398
2.390
1.562
1.270
0.99
0.99
1.19
4.07
0.97
1.03
1.02
2.97
2.93
2.98
3.06
f1 (ppm)


170.196
140.168
137.457
137.397
136.692
133.365
131.644
129.238
128.994
128.463
127.505
77.478
77.160
76.842
59.339
41.319
32.986
22.633
21.247
18.595
f1 (ppm)


F
O
N
H
O
S
4h$_{mono}$

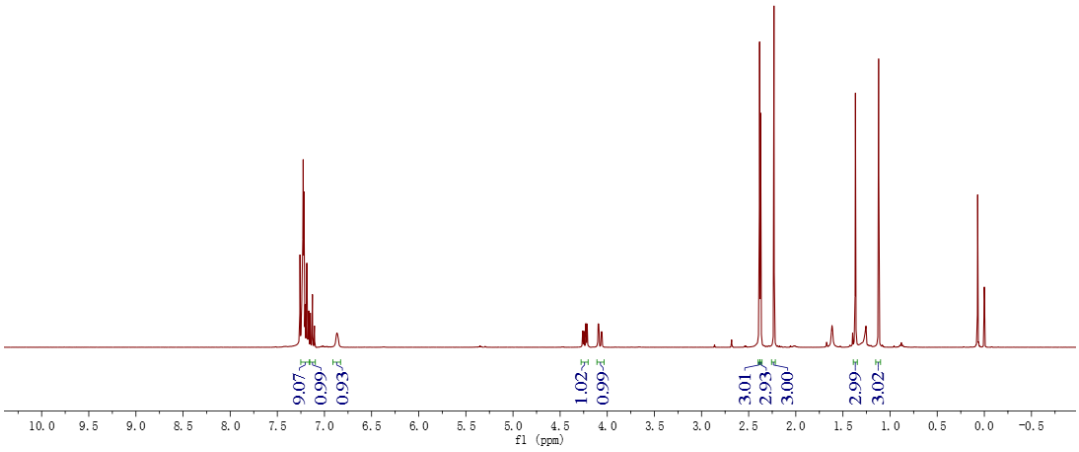

7.320
7.238
7.218
7.207
7.199
7.193
7.186
7.178
7.172
7.159
7.152
7.134
7.128
7.013
7.006
6.992
6.985
6.971
6.965
4.512
4.497
4.474
4.459
4.356
4.342
4.318
4.304
2.401
2.393
1.574
1.275
0.99
5.06
0.98
1.02
1.02
1.01
3.02
2.91
3.04
3.06
f1 (ppm)

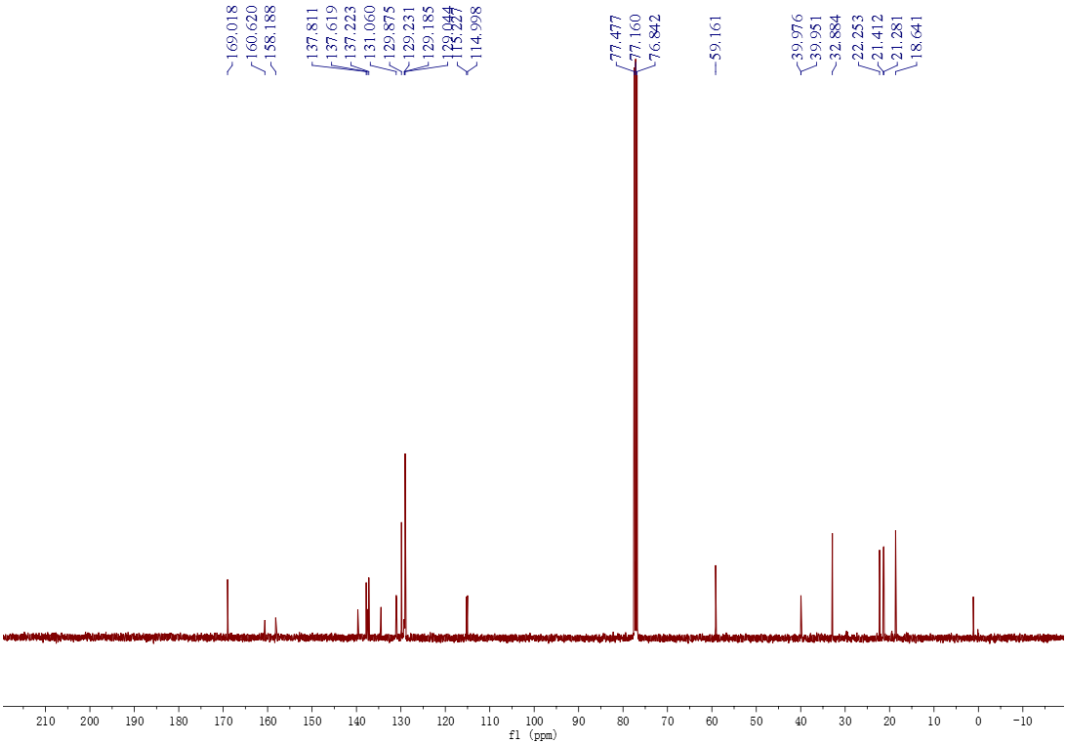

170.285
163.465
161.018
137.933
137.862
137.698
137.667
137.245
136.939
131.953
131.873
129.226
129.216
115.210
114.990
114.381
114.172
77.478
77.160
76.842
59.357
41.455
33.041
22.733
21.266
18.618
f1 (ppm)

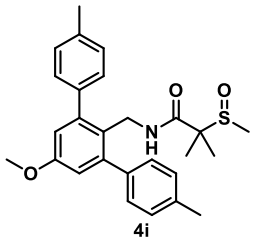

F
O
O
S
N
H

$4h_{di}$

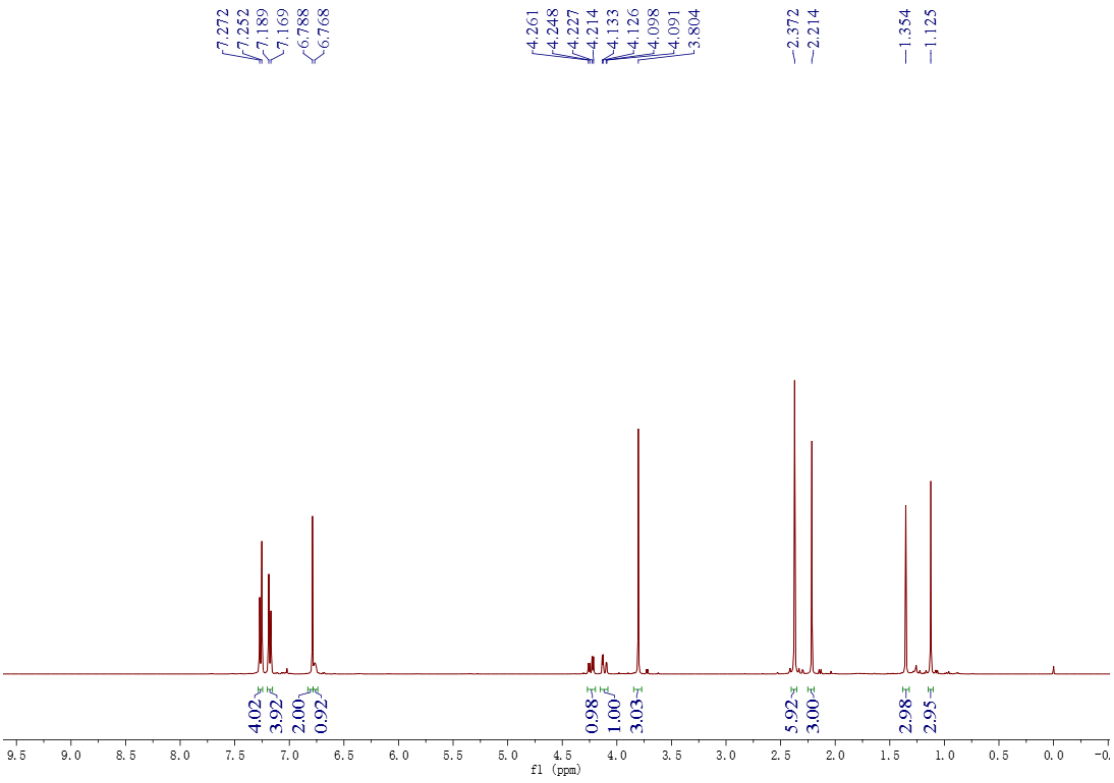

7.237
7.226
7.217
7.204
7.187
7.167
7.149
7.128
7.106
6.868
4.261
4.247
4.227
4.213
4.097
4.090
4.063
4.056
2.384
2.373
2.231
1.367
1.121

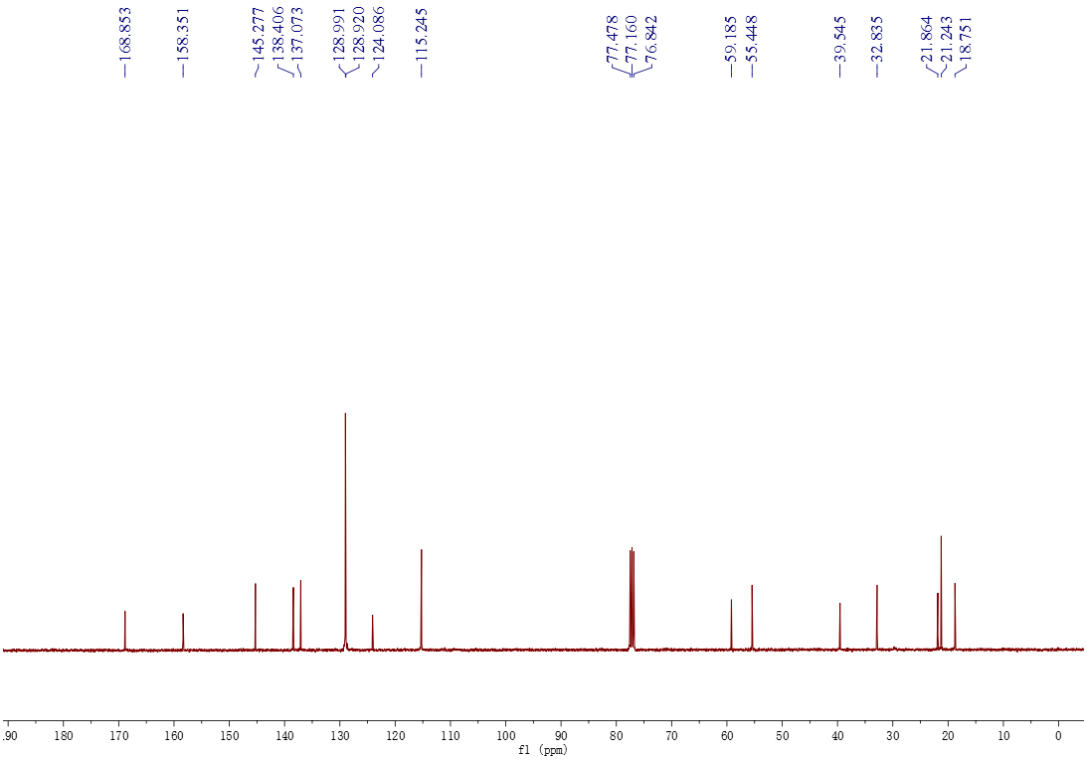

9.07
0.99
0.93
1.02
0.99
3.01
2.93
3.00
2.99
3.02
f1 (ppm)

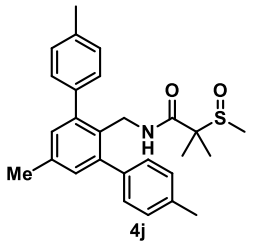

169.018
160.620
158.188
137.811
137.619
137.223
131.060
129.875
129.231
129.185
129.044
115.227
114.998
77.477
77.160
76.842
59.161
39.976
39.951
32.884
22.253
21.412
21.281
18.641
f1 (ppm)


O
O
S
N
H
O

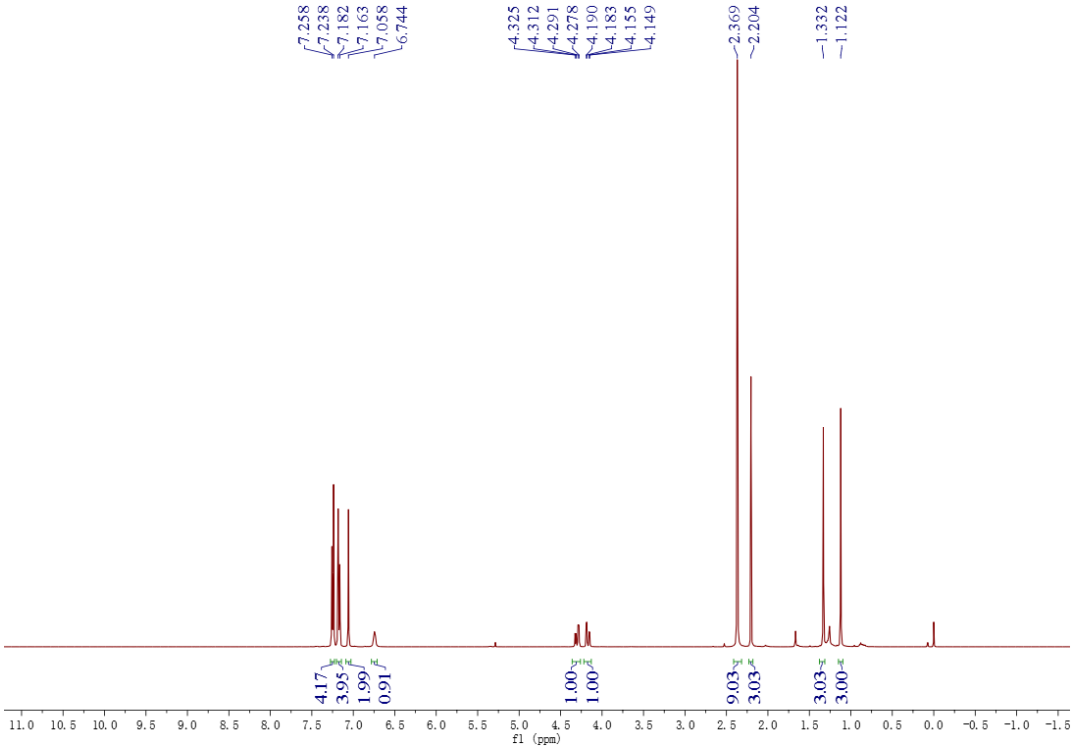
4i

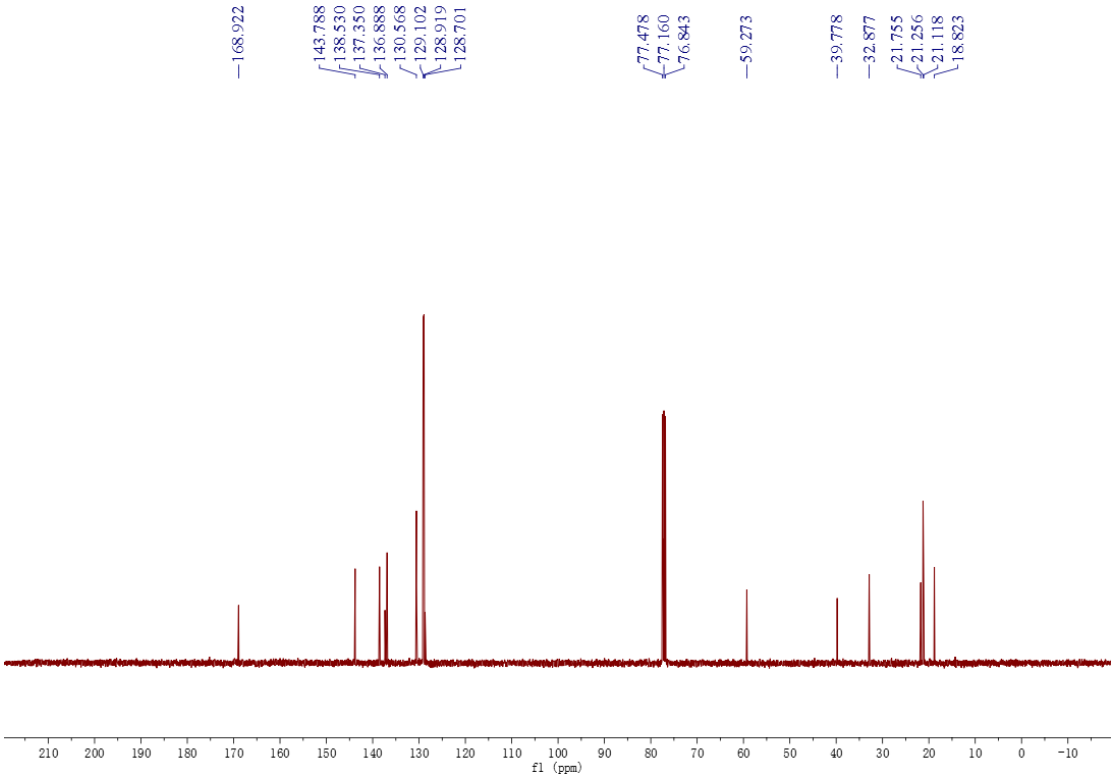

7.272
7.252
7.189
7.169
6.788
6.768
4.261
4.248
4.227
4.214
4.133
4.126
4.098
4.091
3.804
2.372
2.214
1.354
1.125
4.02
3.92
2.00
0.92
0.98
1.00
3.03
5.92
3.00
2.98
2.95
f1 (ppm)

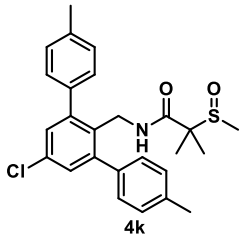

168.853
158.351
145.277
138.406
137.073
128.991
128.920
124.086
115.245
77.478
77.160
76.842
59.185
55.448
39.545
32.835
21.864
21.243
18.751
f1 (ppm)


O
O
S
N
H
Me

4j

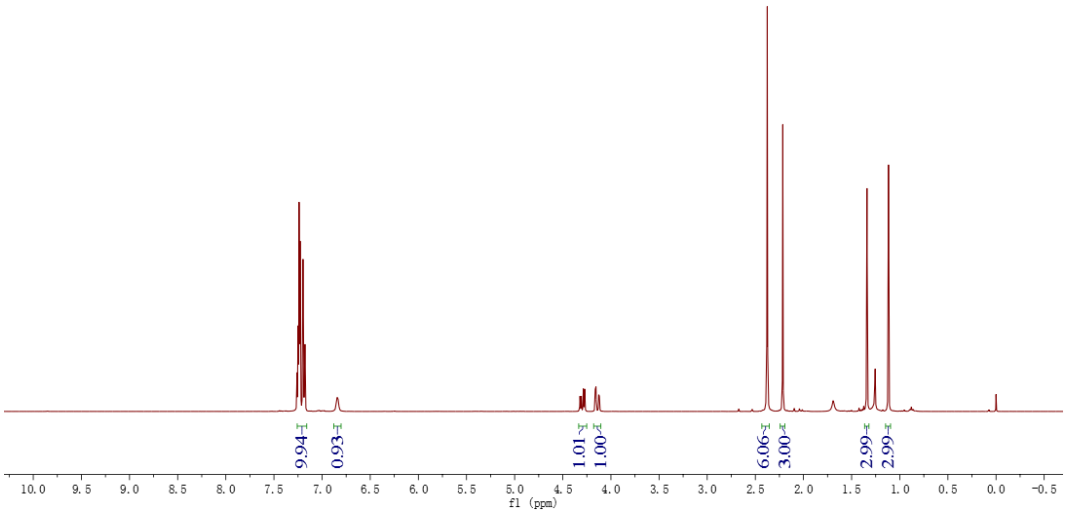

7.258
7.238
7.182
7.163
7.058
6.744
4.325
4.312
4.291
4.278
4.190
4.183
4.155
4.149
2.369
2.204
1.332
1.122
4.17
3.95
1.99
0.91
1.00
1.00
9.03
3.03
3.03
3.00
f1 (ppm)


168.922
143.788
138.530
137.350
136.888
130.568
129.102
128.919
128.701
77.478
77.160
76.843
59.273
39.778
32.877
21.755
21.256
21.118
18.823
f1 (ppm)


O
O
S
N
H
Cl

4k


7.249
7.239
7.234
7.229
7.198
7.178
6.843
4.321
4.307
4.287
4.273
4.162
4.155
4.127
4.120
2.376
2.215
1.340
1.117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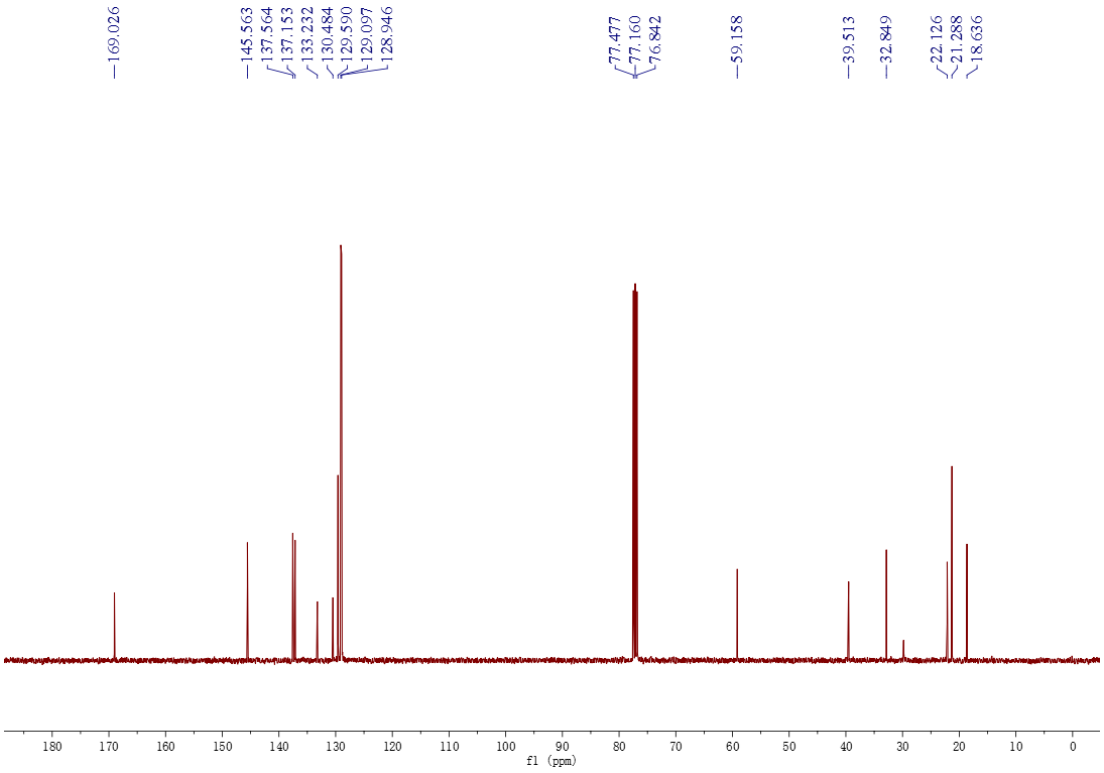
0.93
1.01
1.00
6.06
3.00
2.99
2.99
f1 (ppm)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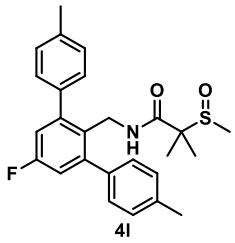
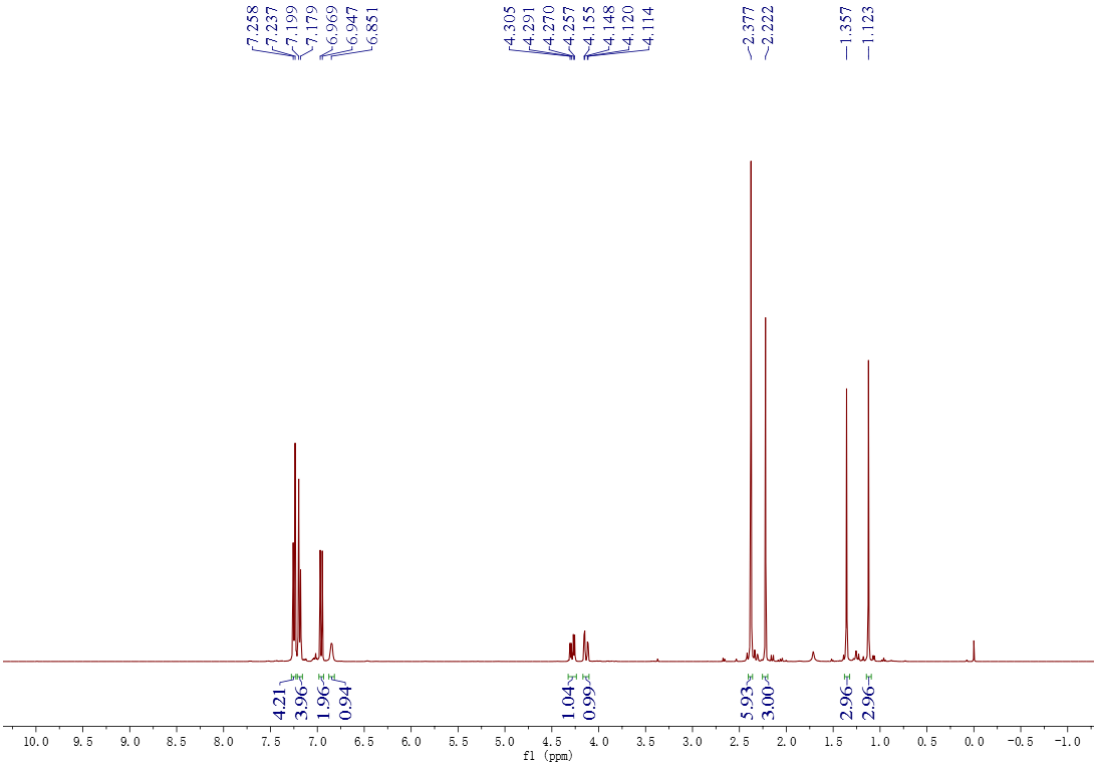
137.564
137.153
133.232
130.484
129.590
129.097
128.946
77.477
77.160
76.842
59.158
39.513
32.849
22.126
21.288
18.636
f1 (ppm)


O
O
S
N
H
F

4l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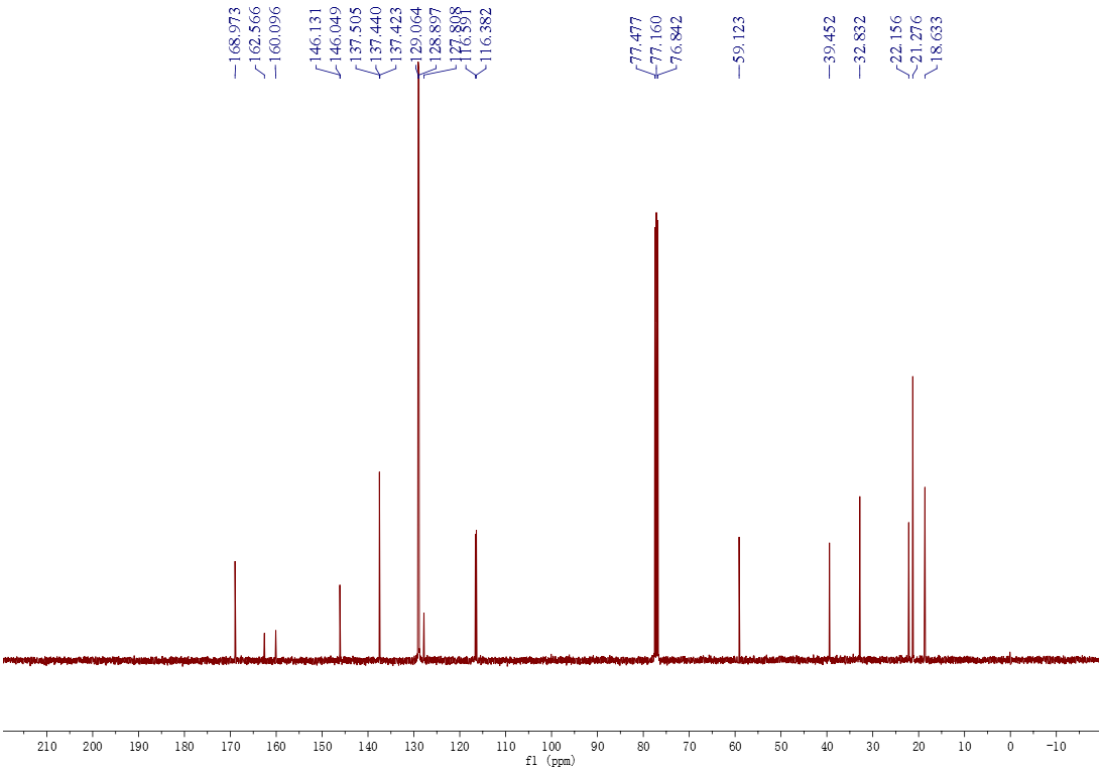
7.237
7.199
7.179
6.969
6.947
6.851
4.305
4.291
4.270
4.257
4.155
4.148
4.120
4.114
2.377
2.222
1.357
1.123
4.21
3.96
1.96
0.94
1.04
0.99
5.93
3.00
2.96
2.96
f1 (ppm)


168.973
162.566
160.096
146.131
146.049
137.505
137.440
137.423
129.064
128.897
127.808
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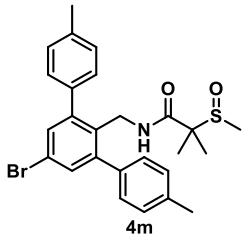
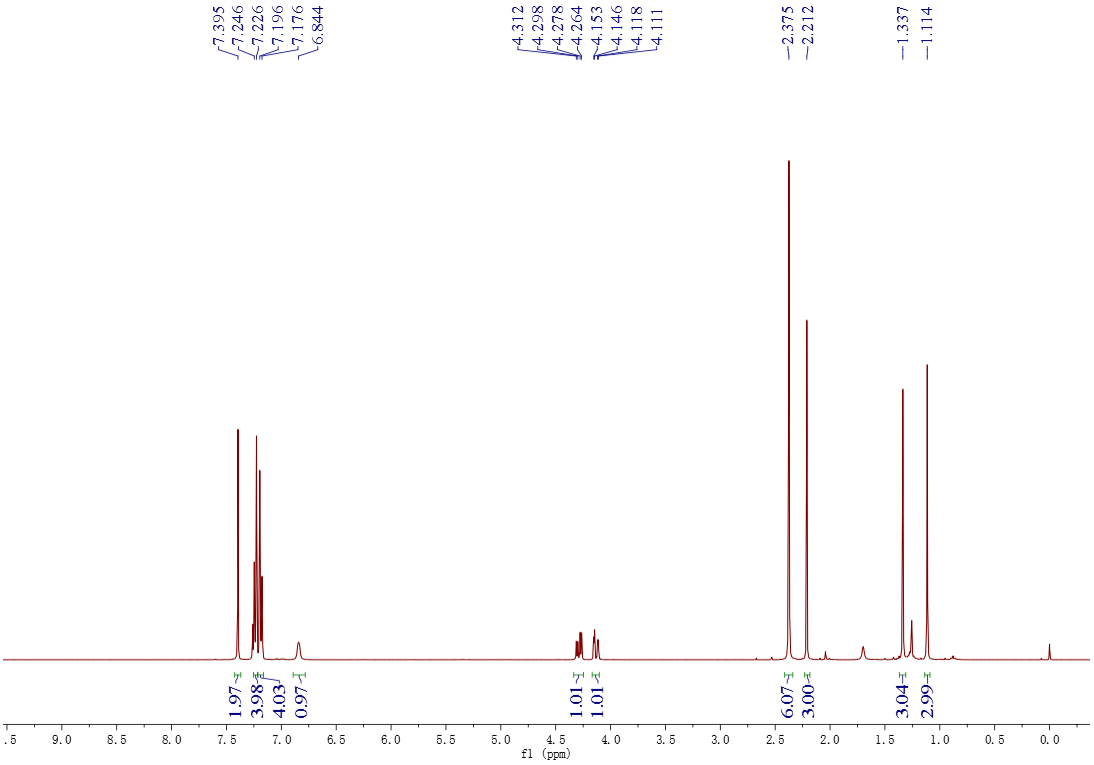
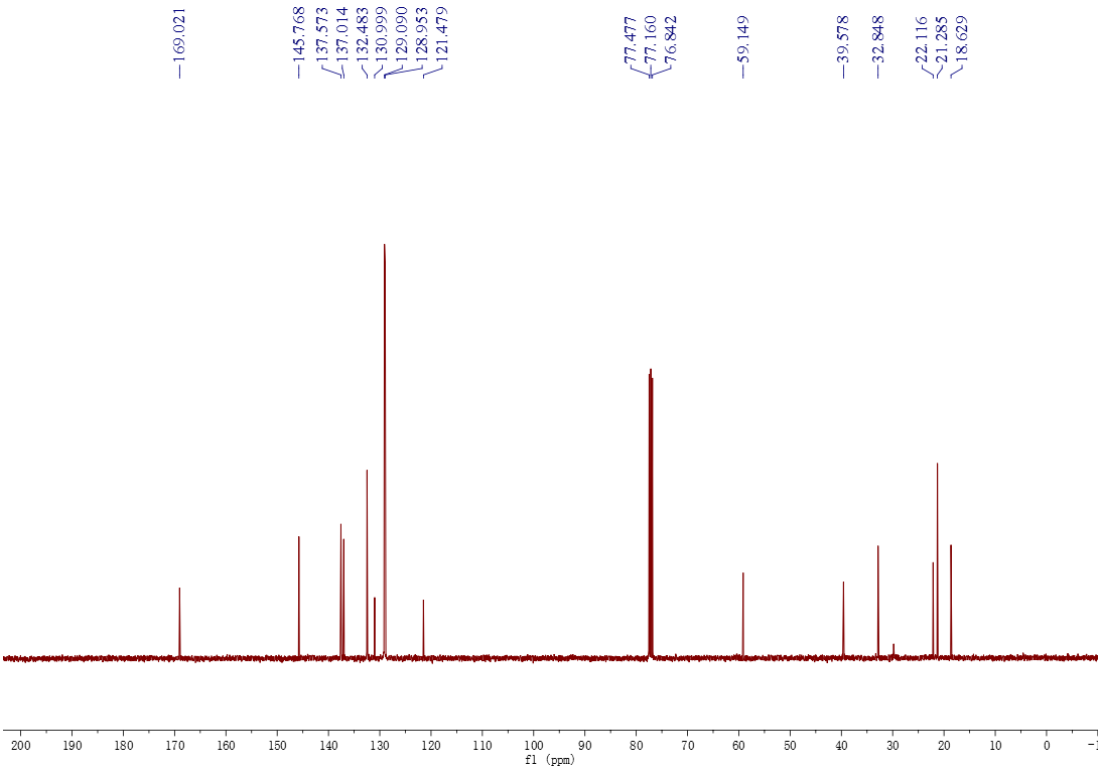
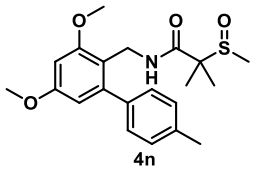
32.832
22.156
21.276
18.633
f1 (ppm)


O
O
S
N
H
Br

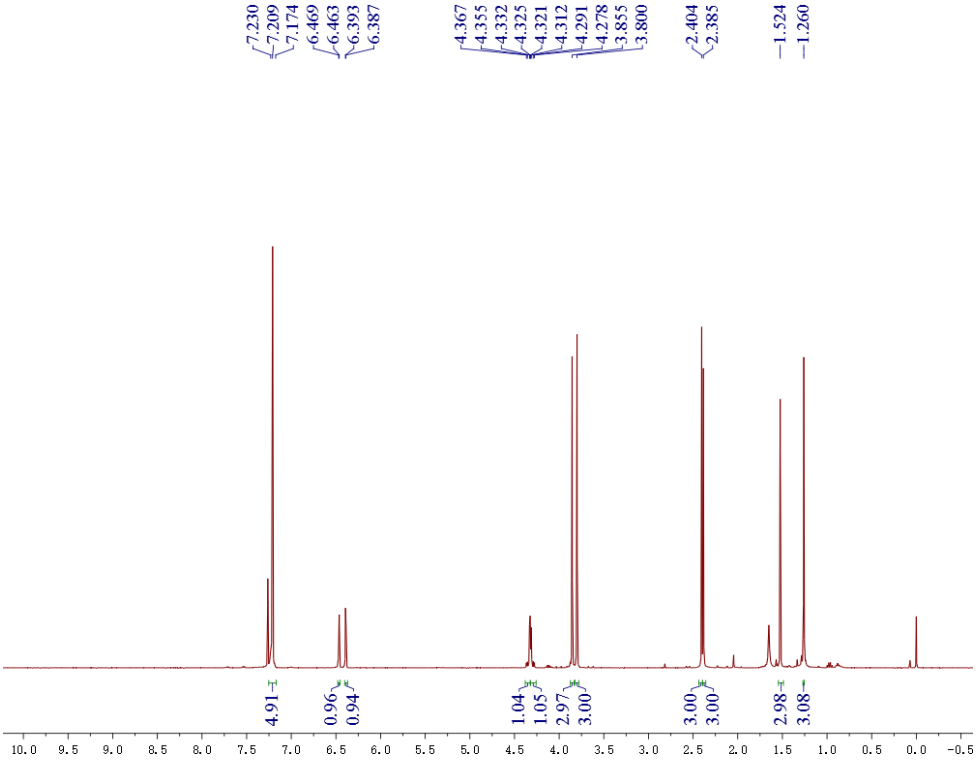
4m

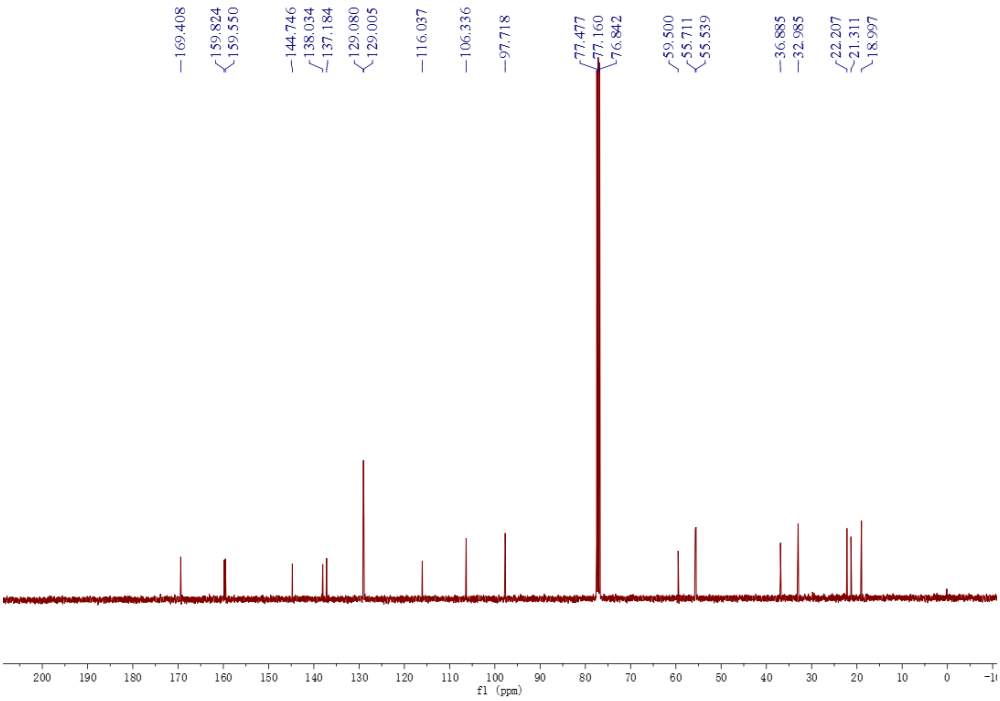

7.395
7.246
7.226
7.196
7.176
6.844
4.312
4.298
4.278
4.264
4.153
4.146
4.118
4.111
2.375
2.212
1.337
1.114
1.97
3.98
4.03
0.97
1.01
1.01
6.07
3.00
3.04
2.99
f1 (ppm)


169.021
145.768
137.573
137.014
132.483
130.999
129.090
128.953
121.479
77.477
77.160
76.842
59.149
39.578
32.848
22.116
21.285
18.629
f1 (ppm)



4n


7.230
7.209
7.174
6.469
6.463
6.393
6.387
4.367
4.355
4.332
4.325
4.321
4.312
4.291
4.278
3.855
3.800
2.404
2.385
1.524
1.260
4.91
0.96
0.94
1.04
1.05
2.97
3.00
3.00
3.00
2.98
3.08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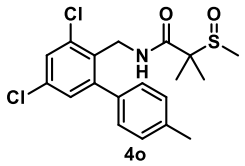
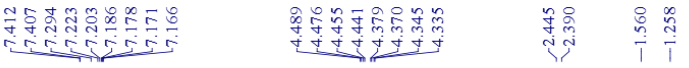
159.824
159.550
144.746
138.034
137.184
129.080
129.005
116.037
106.336
97.718
77.477
77.160
76.842
59.500
55.711
55.539
36.885
32.985
22.207
21.311
18.997
f1 (ppm)


Cl
O
O
S
N
H
Cl

4o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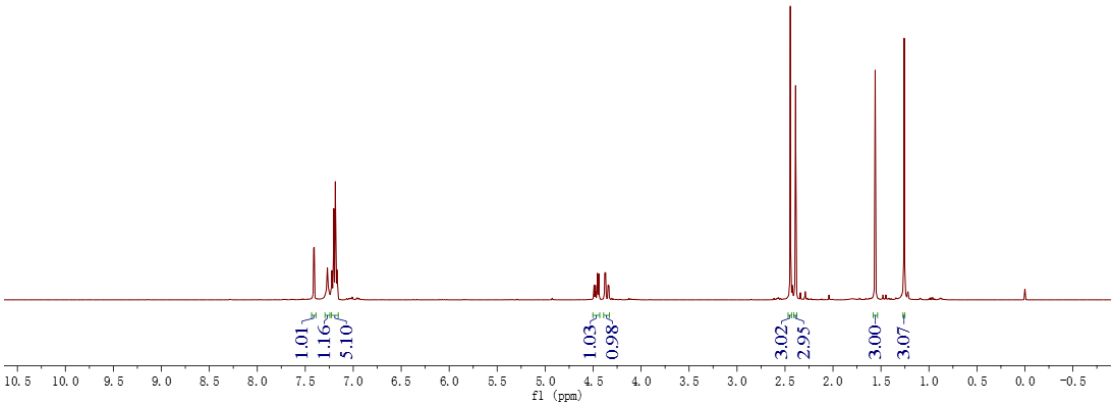
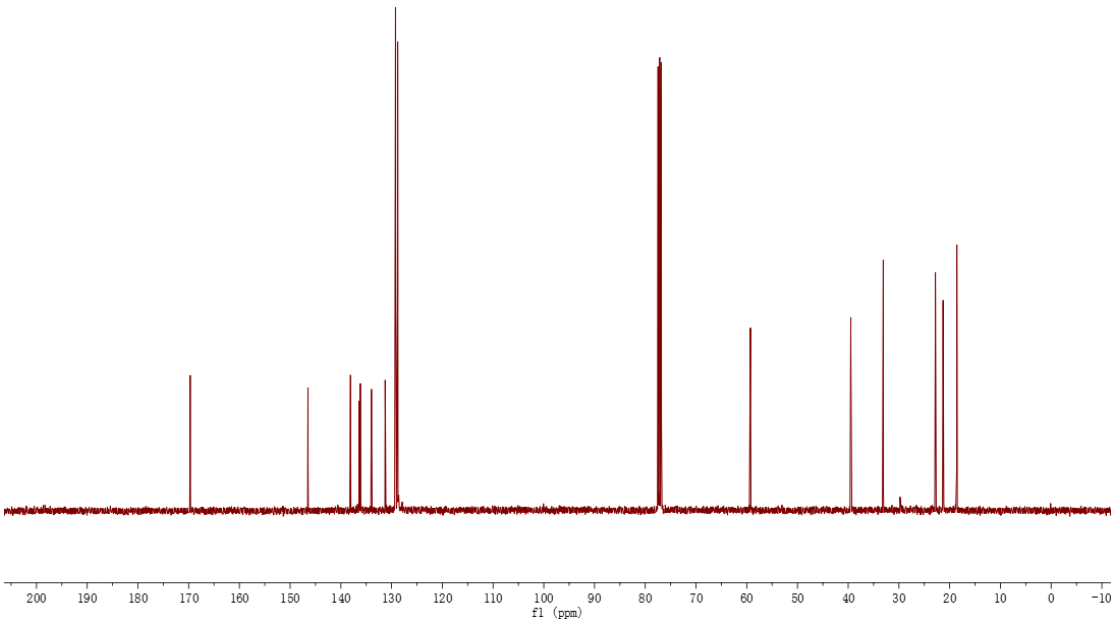
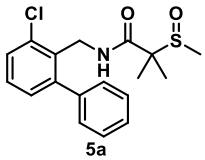
7.407
7.294
7.223
7.203
7.186
7.178
7.171
7.166
4.489
4.476
4.455
4.441
4.379
4.370
4.345
4.335
2.445
2.390
1.560
1.258


1.01
1.16
5.10
1.03
0.98
3.02
2.95
3.00
3.07
f1 (ppm)

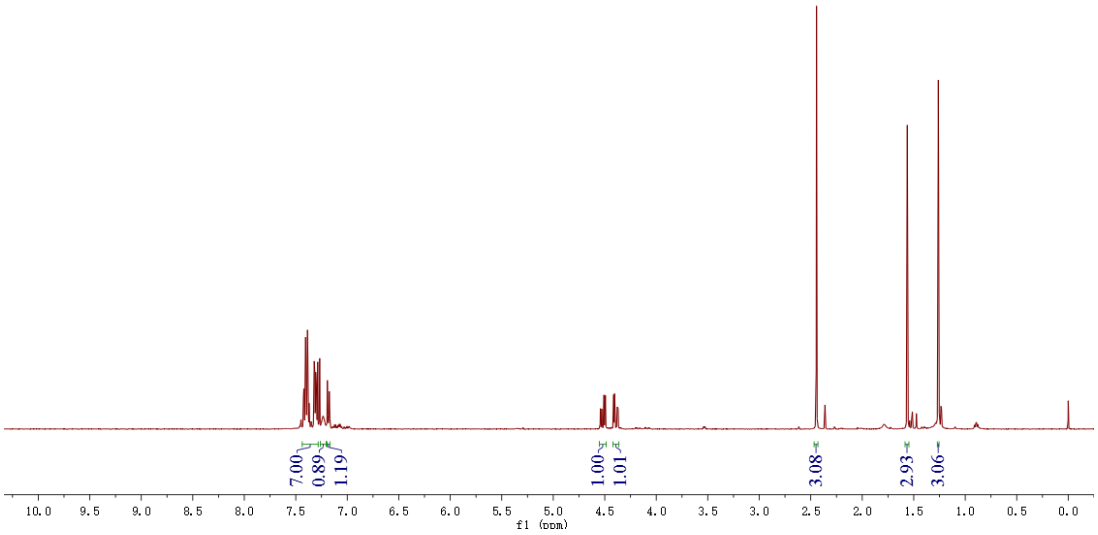

169.695
146.479
138.096
136.356
136.161
133.971
131.266
129.224
129.202
128.800
128.637
77.478
77.160
76.842
59.271
39.487
33.085
22.821
21.297
18.593

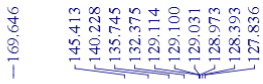

f1 (ppm)

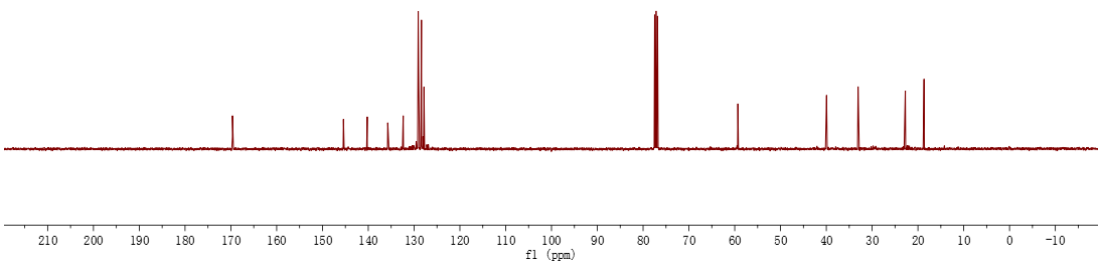

Cl
O
O
S
N
H

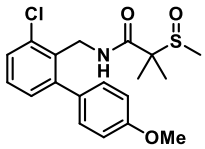
5a


7.424
7.421
7.405
7.401
7.386
7.321
7.316
7.306
7.301
7.297
7.287
7.234
7.193
7.190
7.174
7.171
4.542
4.528
4.508
4.494
4.413
4.404
4.379
4.370
2.444
1.563
1.261

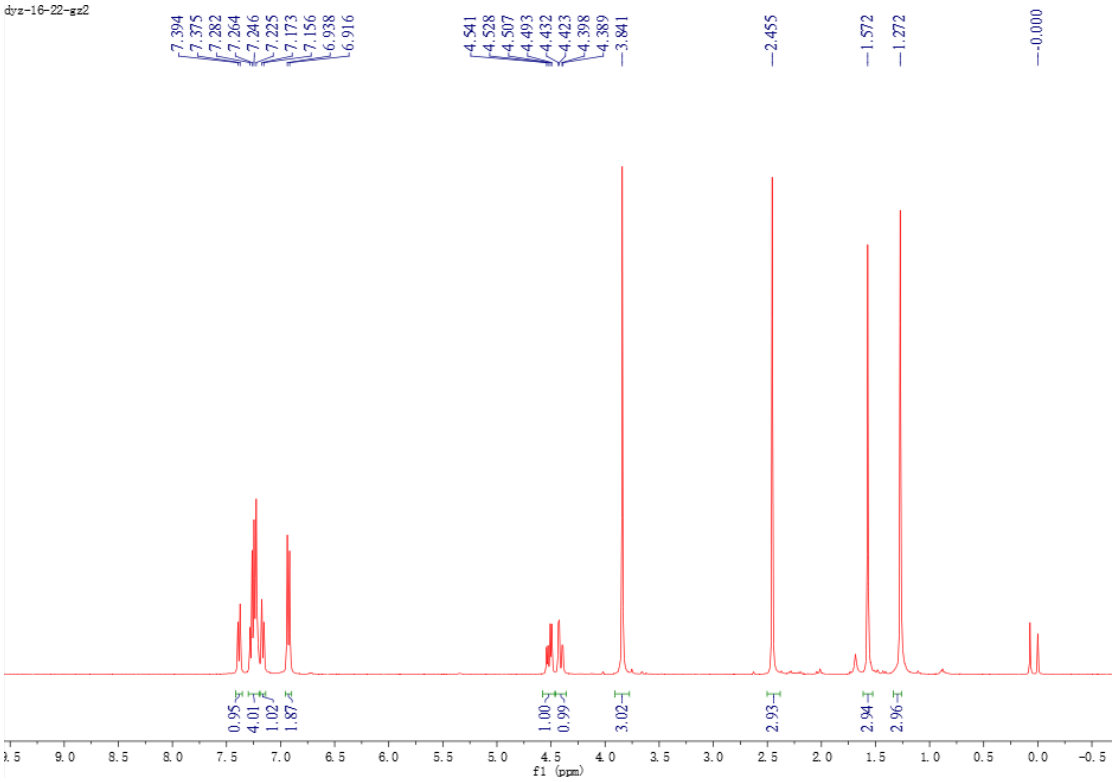

7.00
0.89
1.19
1.00
1.01
3.08
2.93
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


169.646
145.413
140.228
135.745
132.375
129.114
129.100
129.031
128.973
128.393
127.836
77.478
77.160
76.842
59.308
39.946
33.072
22.753
18.663


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
O
O
S
N
H
OMe

5b


dyz-16-22-gz2
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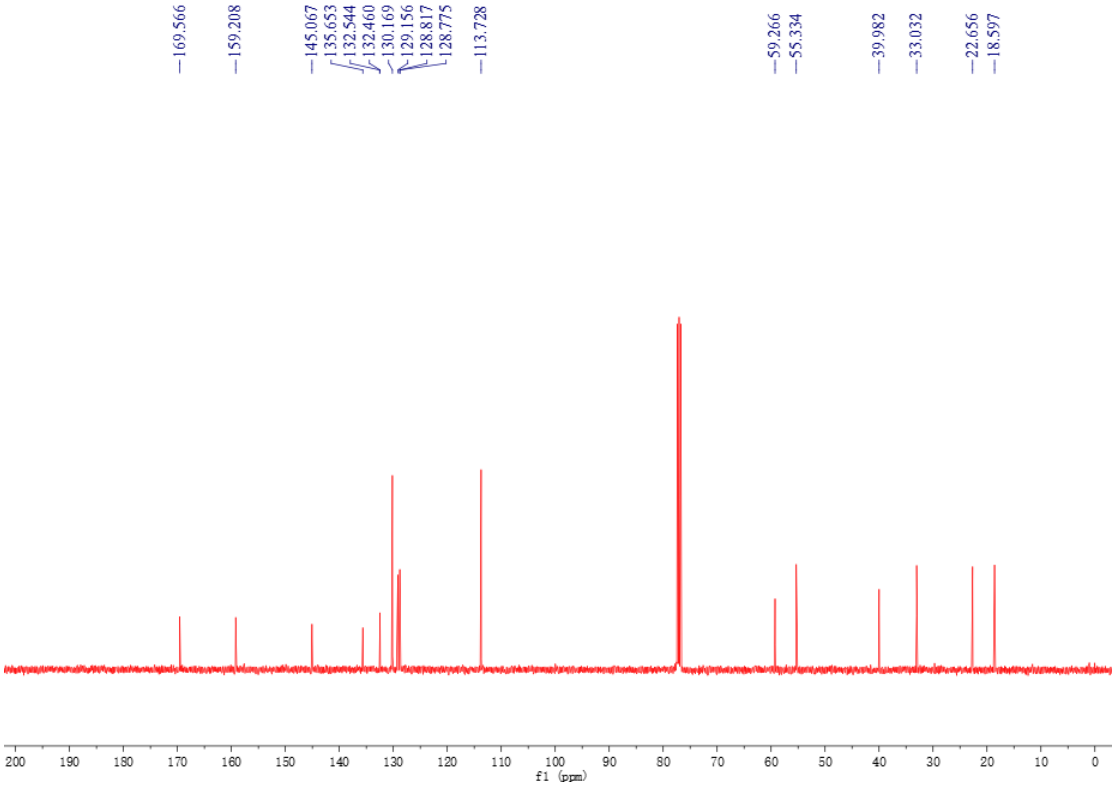
7.282
7.264
7.246
7.225
7.173
7.156
6.938
6.916
4.541
4.528
4.507
4.493
4.432
4.423
4.398
4.389
3.841
2.455
1.572
1.272
0.000
0.95
4.01
1.02
1.87
1.00
0.99
3.02
2.93
2.94
2.96
f1 (ppm)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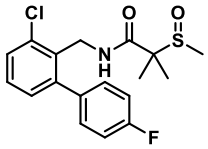
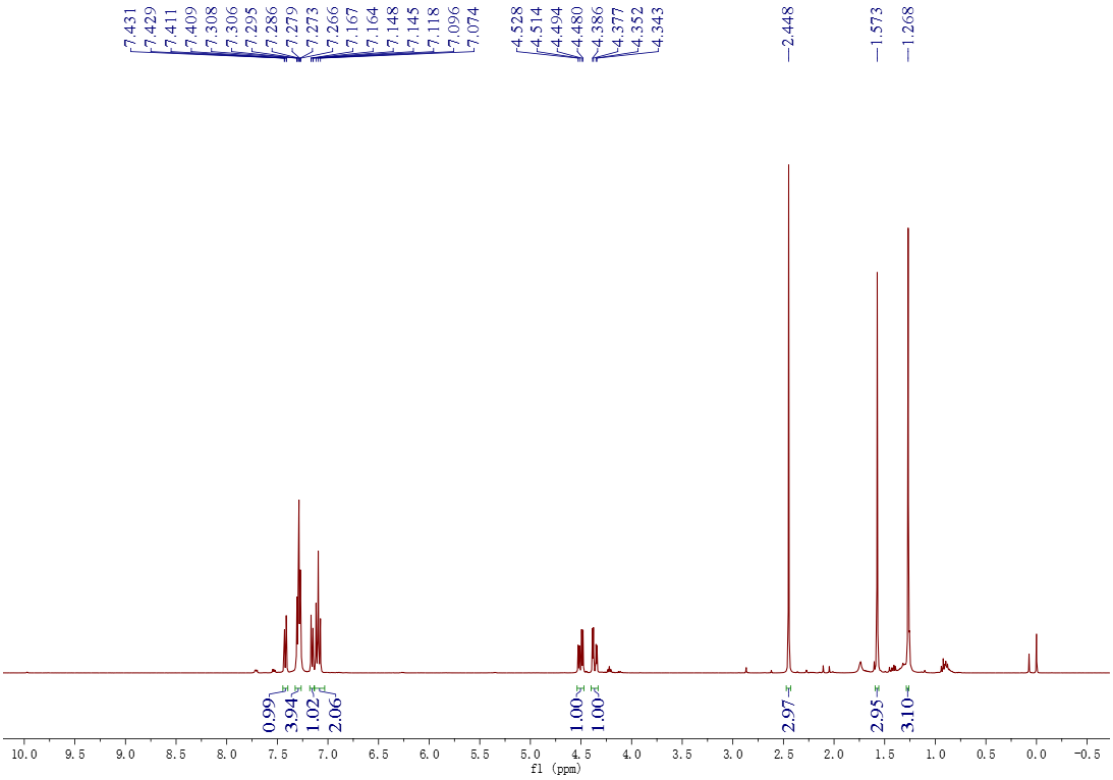
159.208
145.067
135.653
132.544
132.460
130.169
129.156
128.817
128.775
113.728
59.266
55.334
39.982
33.032
22.656
18.597
f1 (ppm)


Cl
O
O
S
N
H
F

5c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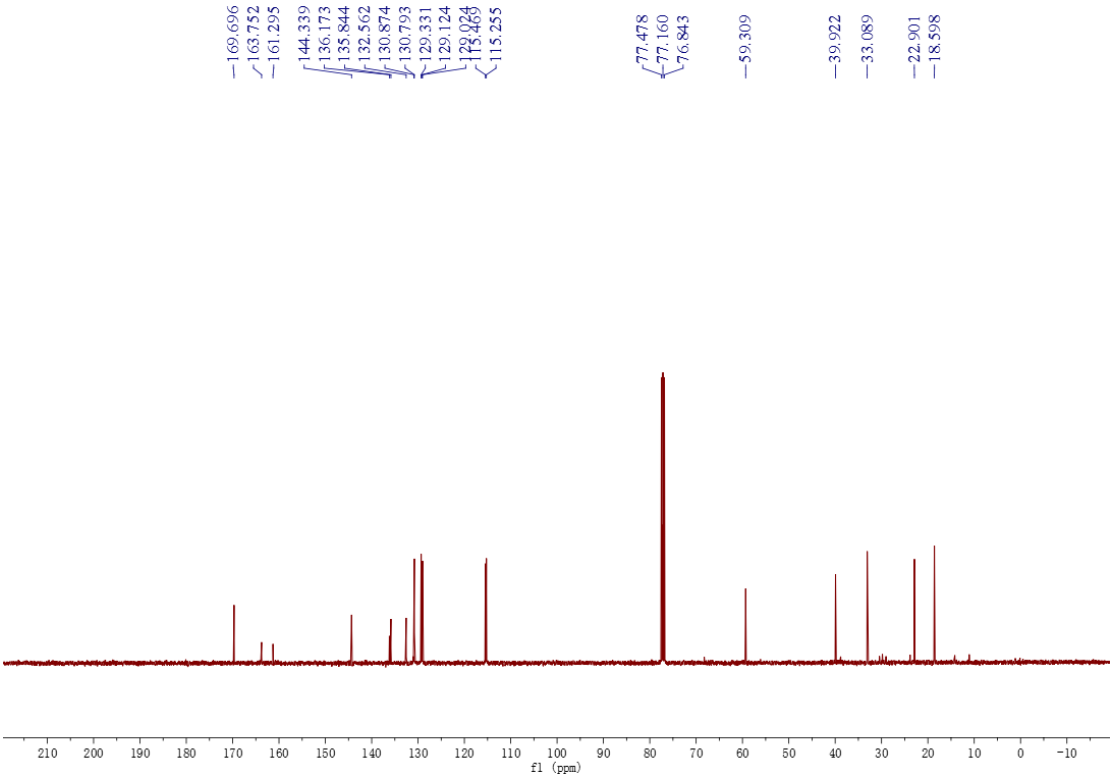
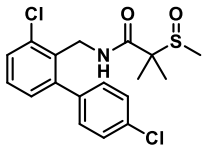
7.411
7.409
7.308
7.306
7.295
7.286
7.279
7.273
7.266
7.167
7.164
7.148
7.145
7.118
7.096
7.074
4.528
4.514
4.494
4.480
4.386
4.377
4.352
4.343
2.448
1.573
1.268
0.99
3.94
1.02
2.06
1.00
1.00
2.97
2.95
3.10
f1 (ppm)


169.696
163.752
161.295
144.339
136.173
135.844
132.562
130.874
130.793
129.331
129.124
77.478
77.160
76.843
59.309
39.922
33.089
22.901
18.598
f1 (ppm)



5d


7.438
7.435
7.418
7.415
7.399
7.393
7.388
7.377
7.372
7.366
7.312
7.292
7.278
7.272
7.255
7.250
7.244
7.159
7.156
7.140
7.137
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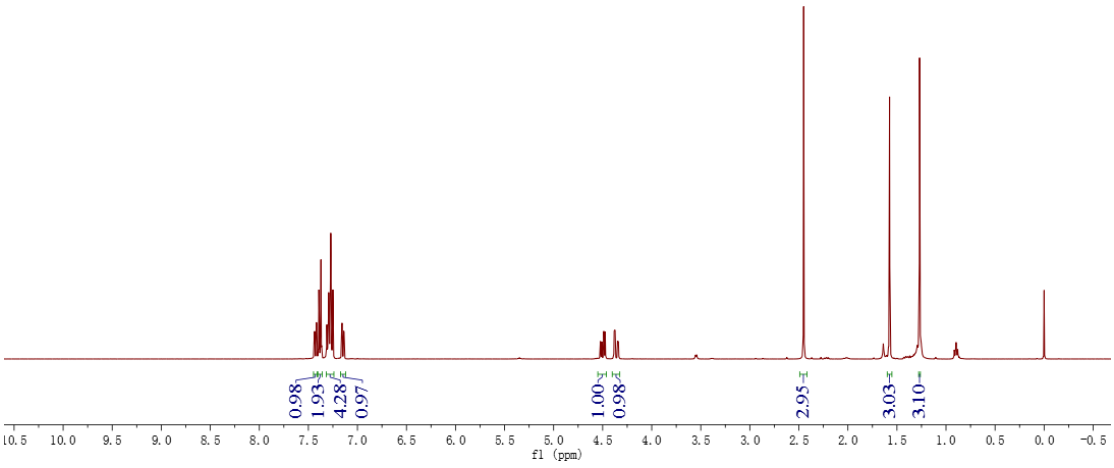
4.488
4.474
4.383
4.374
4.348
4.339
2.451
1.575
1.270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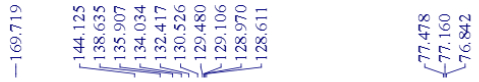
1.00
0.98
2.95
3.03
3.10
f1 (ppm)


169.719
144.125
138.635
135.907
134.034
132.417
130.526
129.480
129.106
128.970
128.611
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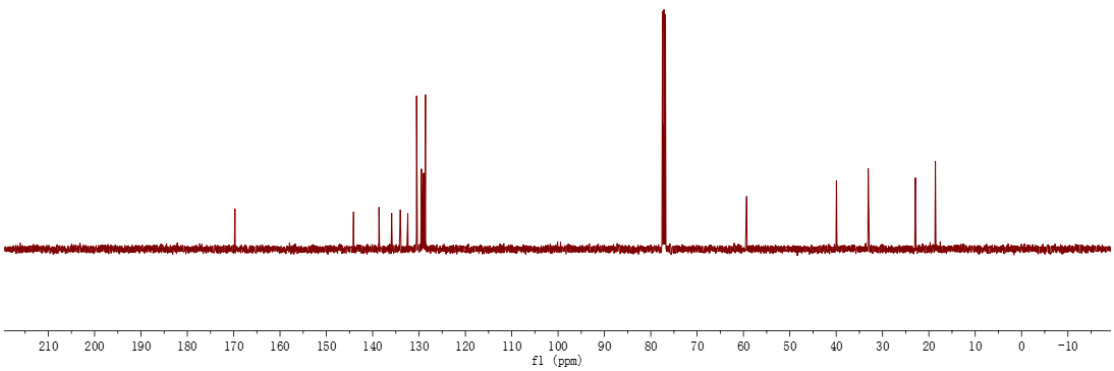
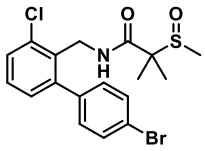
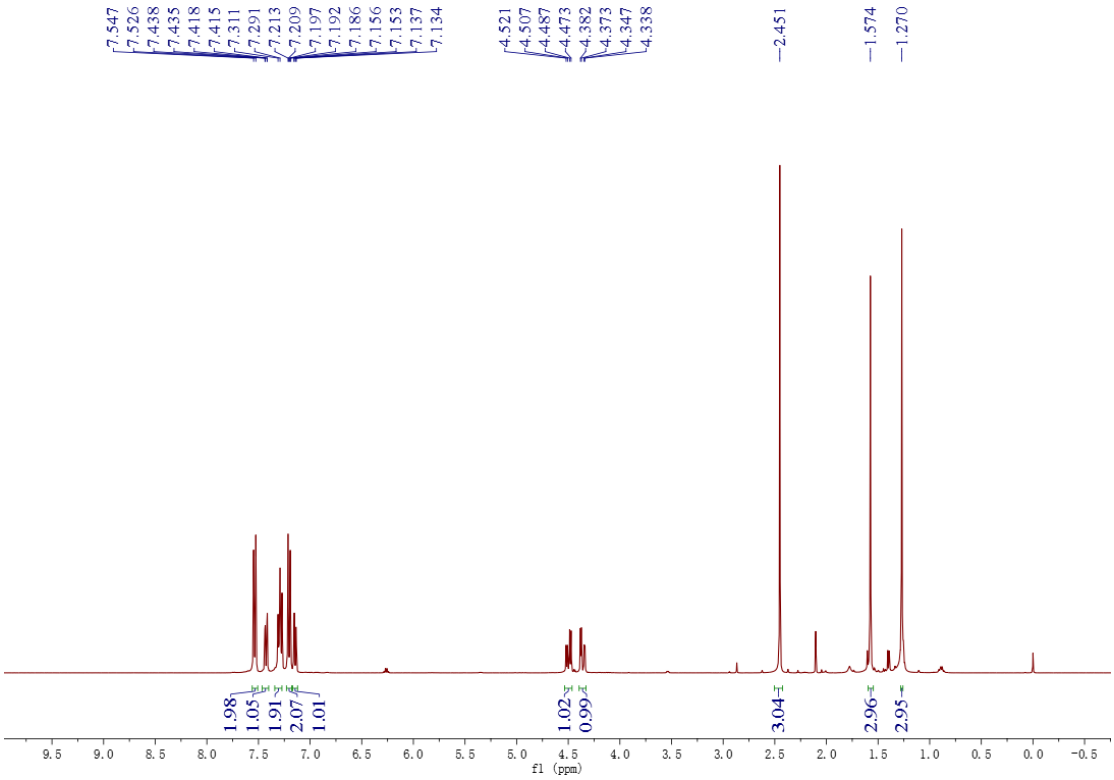
59.321
39.939
33.091
22.902
18.598


f1 (ppm)


Cl
O
O
N
H
S
Br

5e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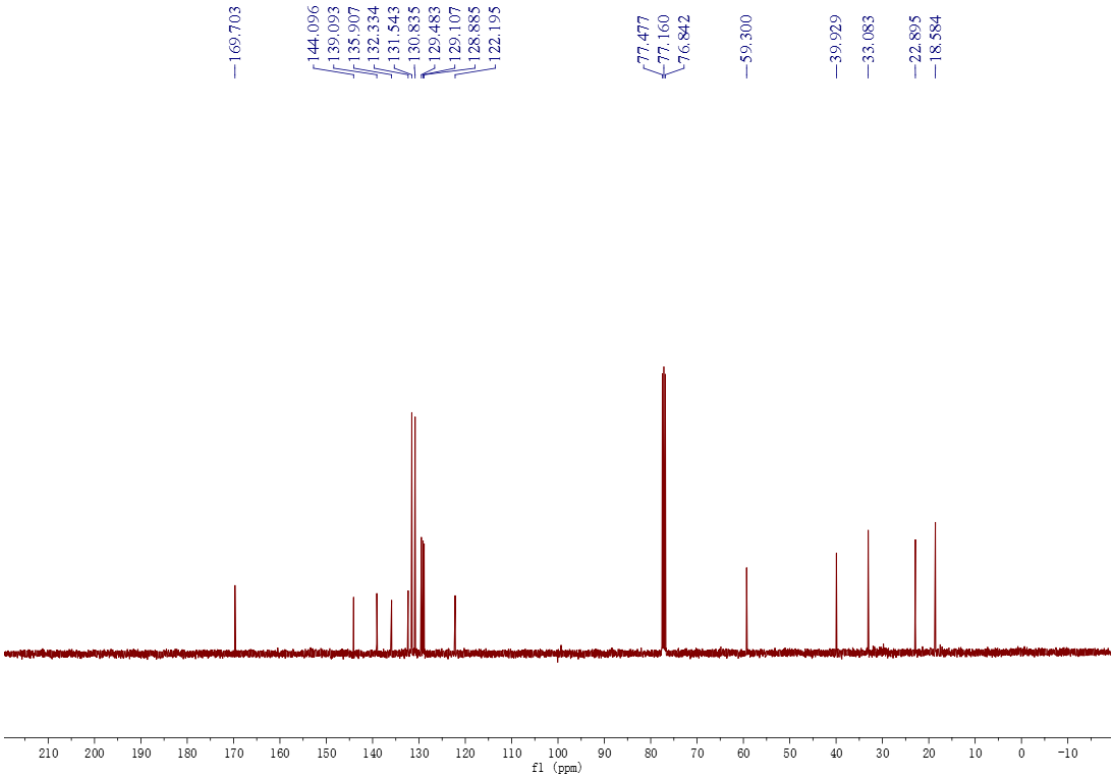
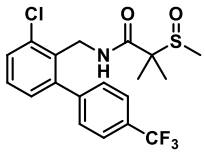
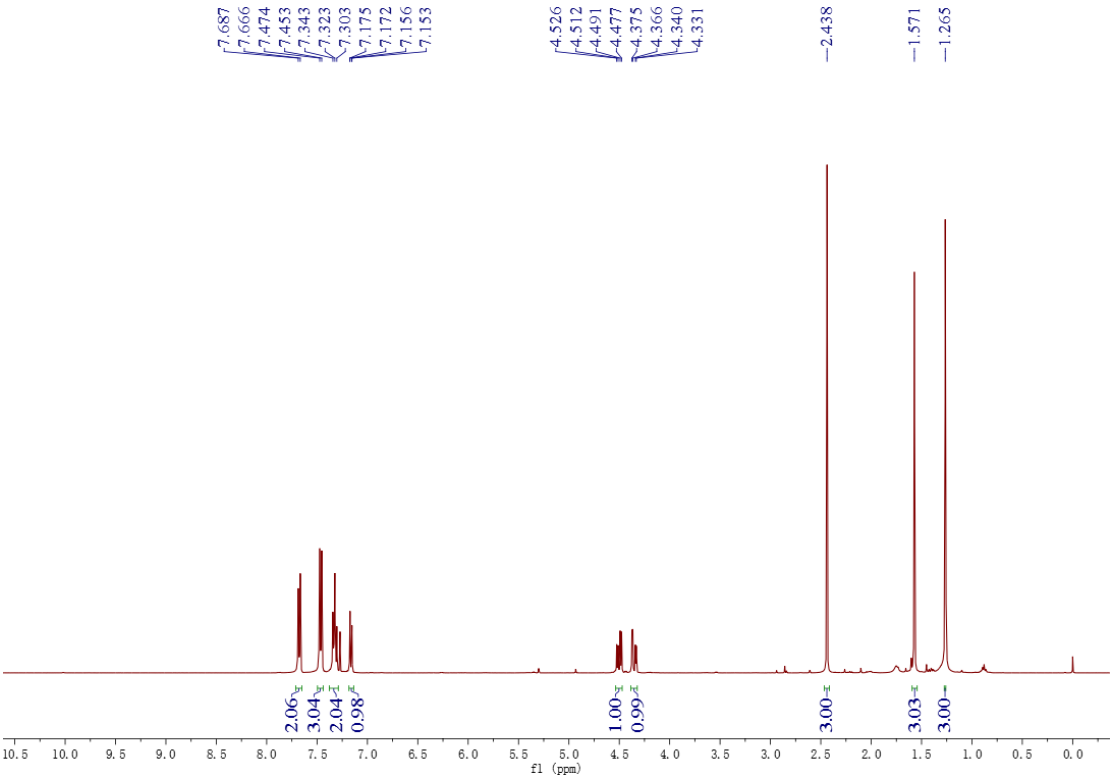
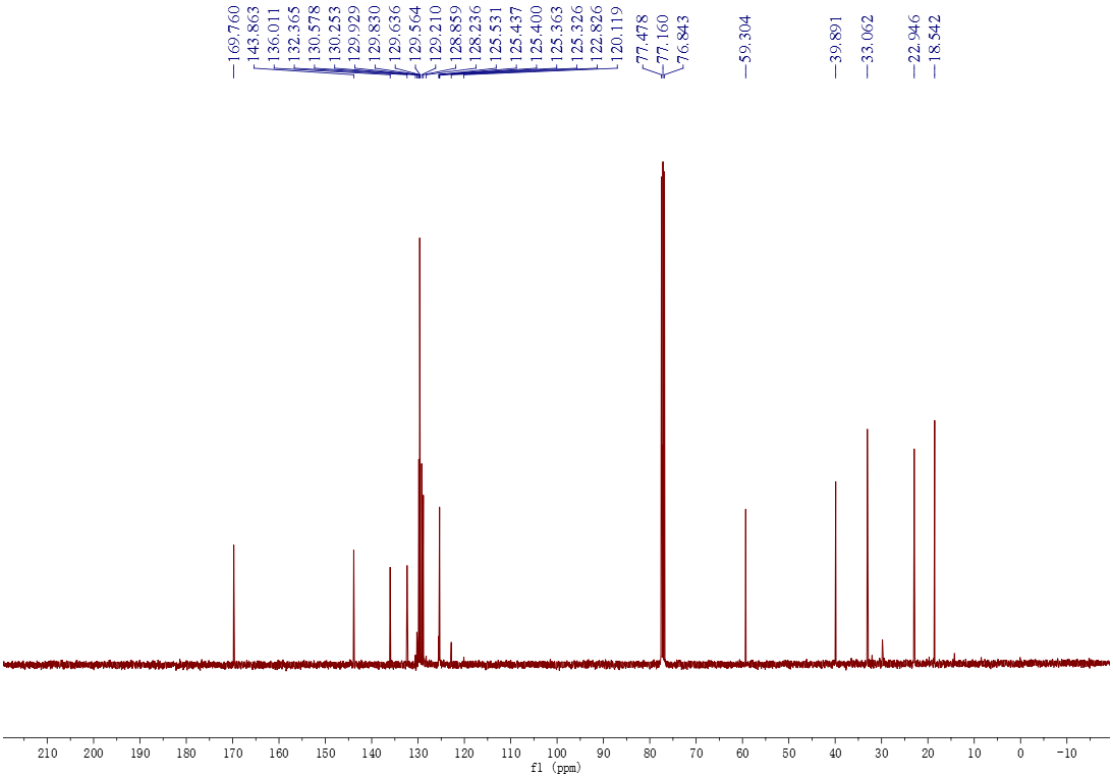
7.526
7.438
7.435
7.418
7.415
7.311
7.291
7.213
7.209
7.197
7.192
7.186
7.156
7.153
7.137
7.134
4.521
4.507
4.487
4.473
4.382
4.373
4.347
4.338
2.451
1.574
1.270
1.98
1.05
1.91
2.07
1.01
1.02
0.99
3.04
2.96
2.95
f1 (ppm)

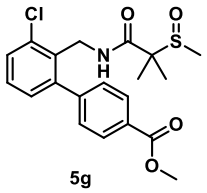

169.703
144.096
139.093
135.907
132.334
131.543
130.835
129.483
129.107
128.885
122.195
77.477
77.160
76.842
59.300
39.929
33.083
22.895
18.584
f1 (ppm)


Cl
O
O
S
N
H
CF3

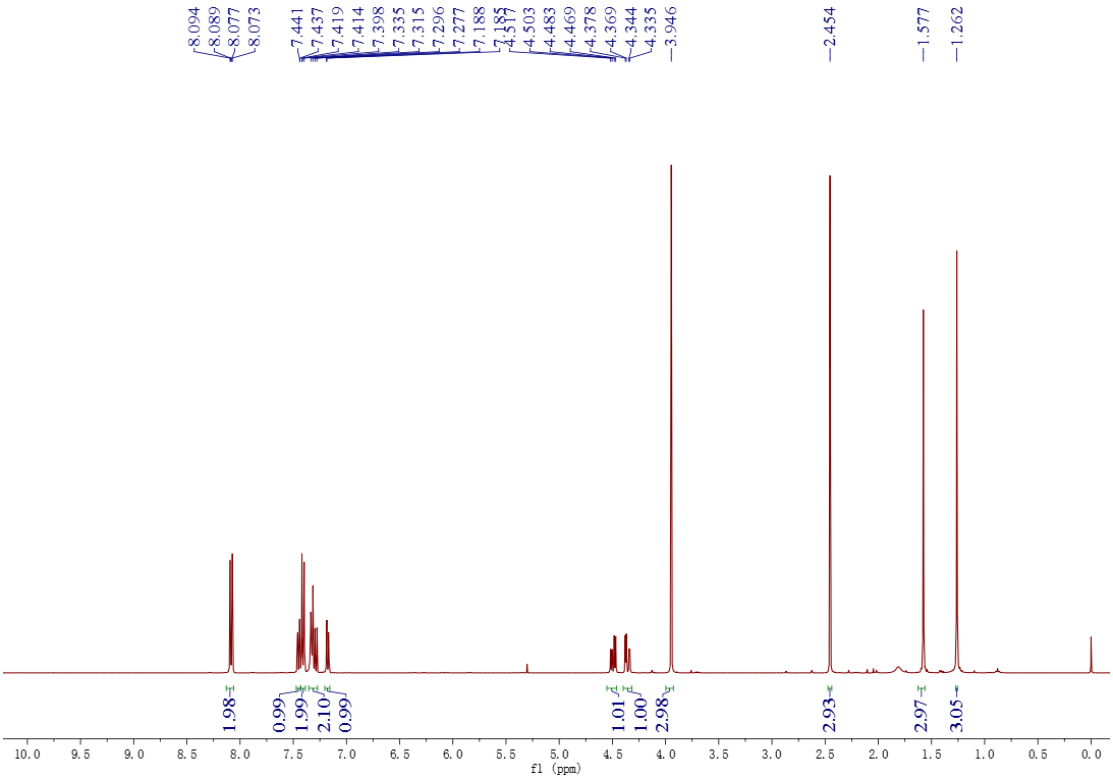
5f

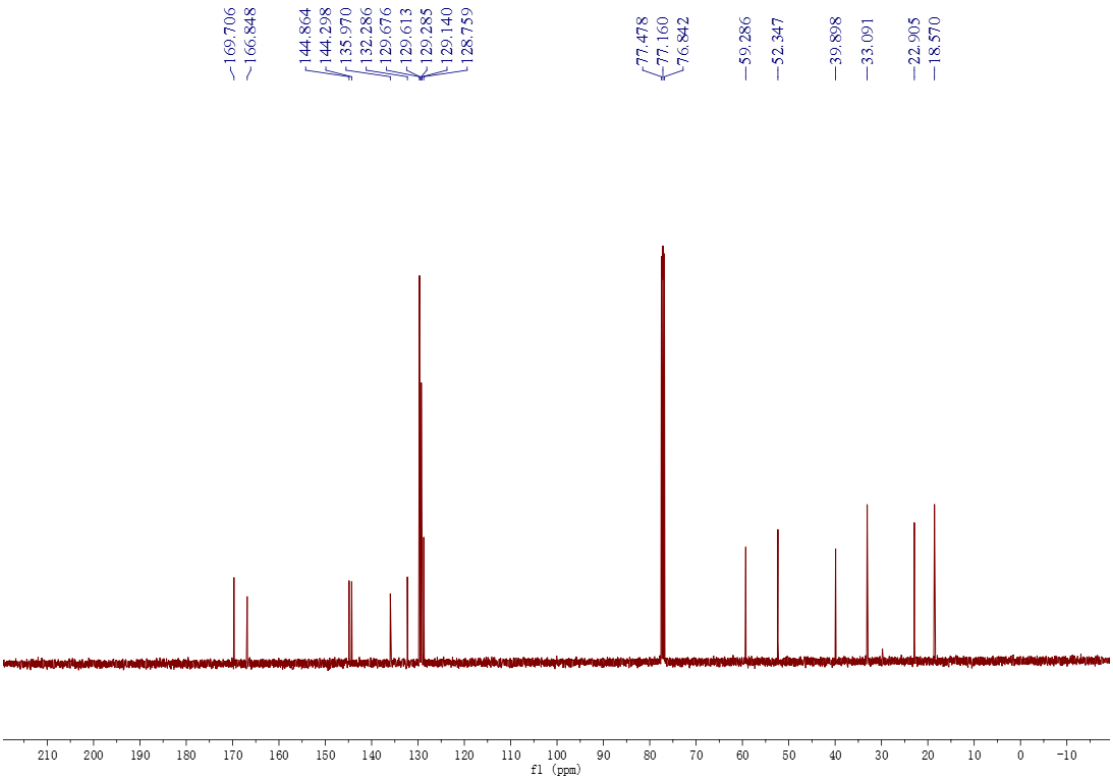

7.687
7.666
7.474
7.453
7.343
7.323
7.303
7.175
7.172
7.156
7.153
4.526
4.512
4.491
4.477
4.375
4.366
4.340
4.331
2.438
1.571
1.265
2.06
3.04
2.04
0.98
1.00
0.99
3.00
3.03
3.00
f1 (ppm)

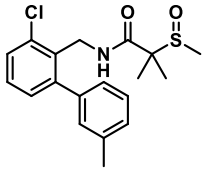

169.760
143.863
136.011
132.365
130.578
130.253
129.929
129.830
129.636
129.564
129.210
128.859
128.236
125.531
125.437
125.400
125.363
125.326
122.826
120.119
77.478
77.160
76.843
59.304
39.891
33.062
22.946
18.542
f1 (ppm)


Cl
O
O
S
N
H
O
O

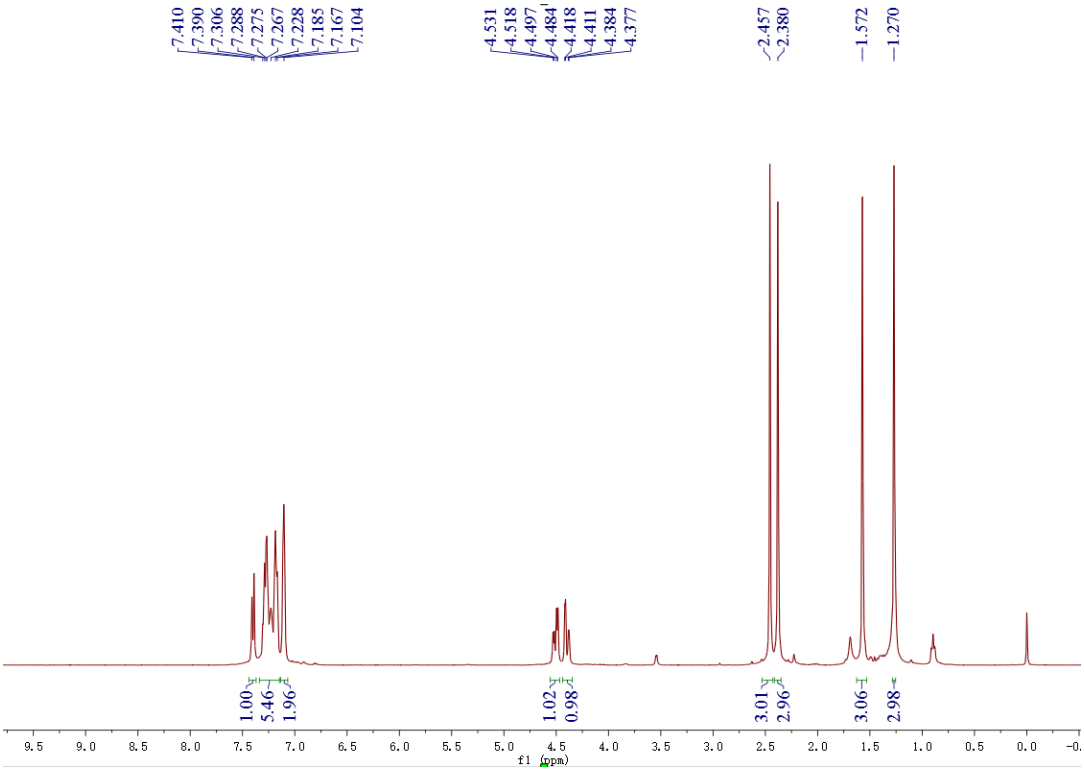
5g

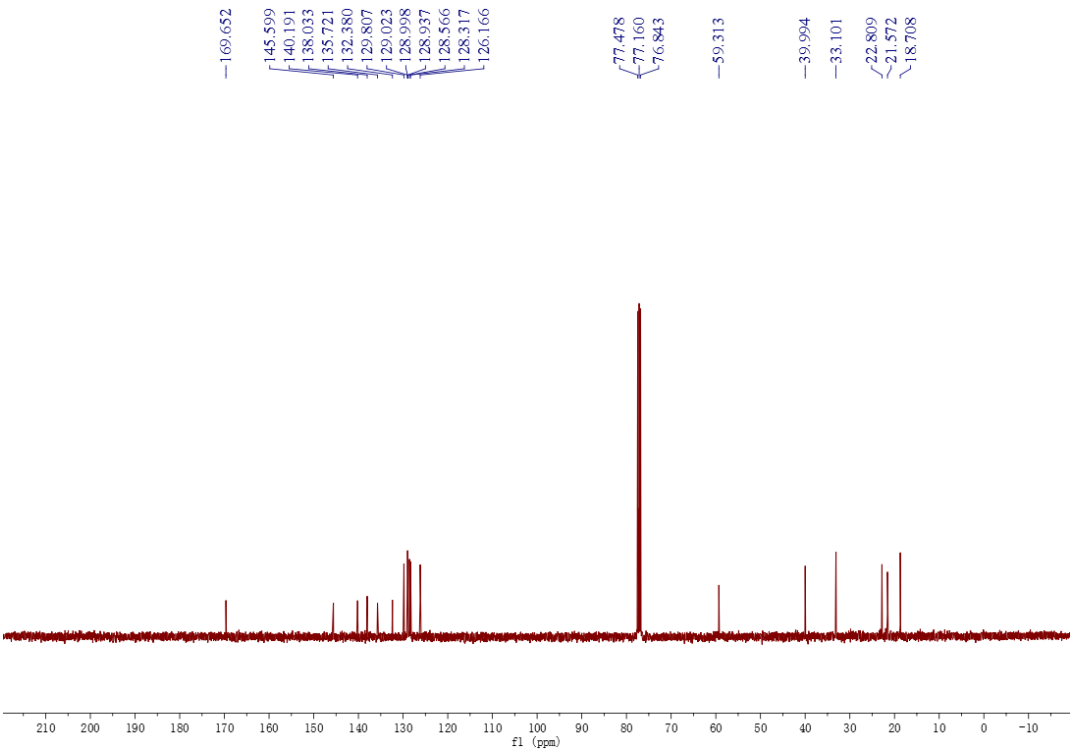

8.094
8.089
8.077
8.073
7.441
7.437
7.419
7.414
7.398
7.335
7.315
7.296
7.277
7.188
7.185
4.517
4.503
4.483
4.469
4.378
4.369
4.344
4.335
3.946
2.454
1.577
1.262
1.98
0.99
1.99
2.10
0.99
1.01
1.00
2.98
2.93
2.97
3.05
f1 (ppm)

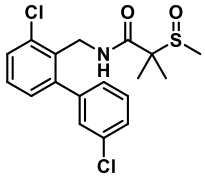

169.706
166.848
144.864
144.298
135.970
132.286
129.676
129.613
129.285
129.140
128.759
77.478
77.160
76.842
59.286
52.347
39.898
33.091
22.905
18.570
f1 (ppm)


Cl
O
O
N
H
S

5h

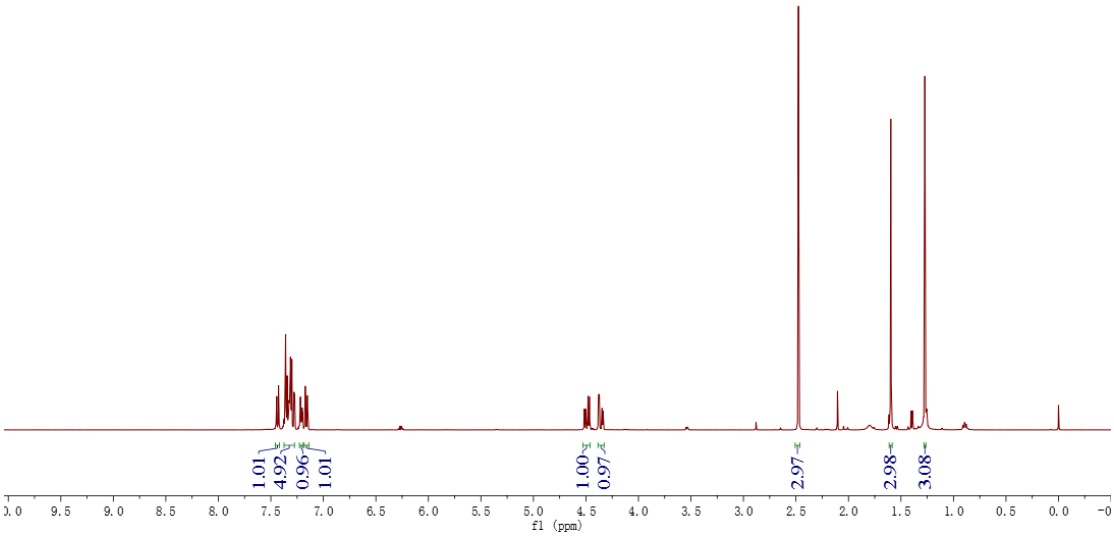

7.410
7.390
7.306
7.288
7.275
7.267
7.228
7.185
7.167
7.104
4.531
4.518
4.497
4.484
4.418
4.411
4.384
4.377
2.457
2.380
1.572
1.270
1.00
5.46
1.96
1.02
0.98
3.01
2.96
3.06
2.98
f1 (ppm)


169.652
145.599
140.191
138.033
135.721
132.380
129.807
129.023
128.998
128.937
128.566
128.317
126.166
77.478
77.160
76.843
59.313
39.994
33.101
22.809
21.572
18.708
f1 (ppm)

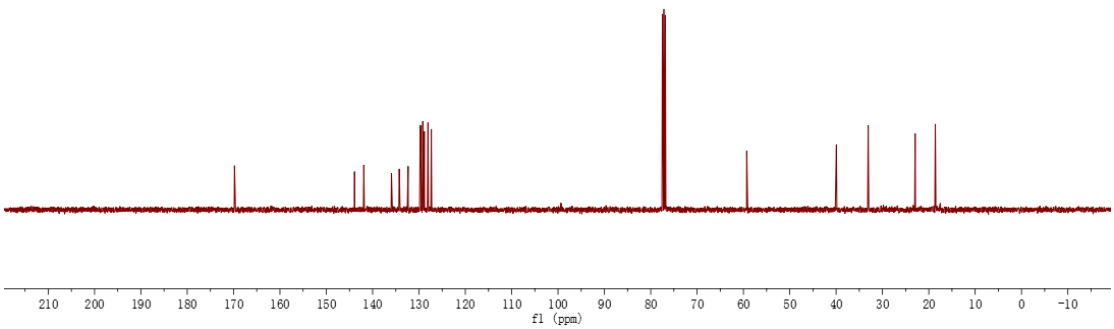

Cl
O
O
N
H
S
Cl

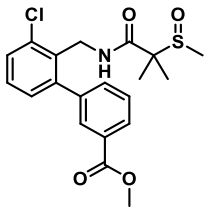
5i


7.447
7.444
7.427
7.424
7.362
7.359
7.353
7.344
7.313
7.300
7.280
7.223
7.218
7.212
7.207
7.203
7.201
7.197
4.514
4.500
4.480
4.466
4.381
4.372
4.346
4.338
2.476
1.597
1.273


1.01
4.92
0.96
1.01
1.00
0.97
2.97
2.98
3.08
f1 (ppm)

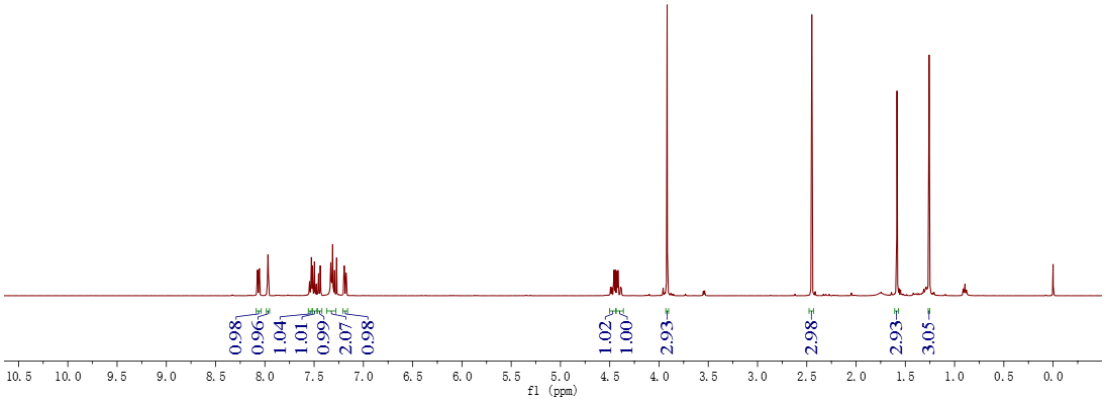

169.798
143.896
141.903
135.934
134.244
132.344
129.727
129.607
129.184
129.138
128.851
128.054
127.342
77.478
77.160
76.842
59.284
39.941
33.082
22.952
18.599


f1 (ppm)

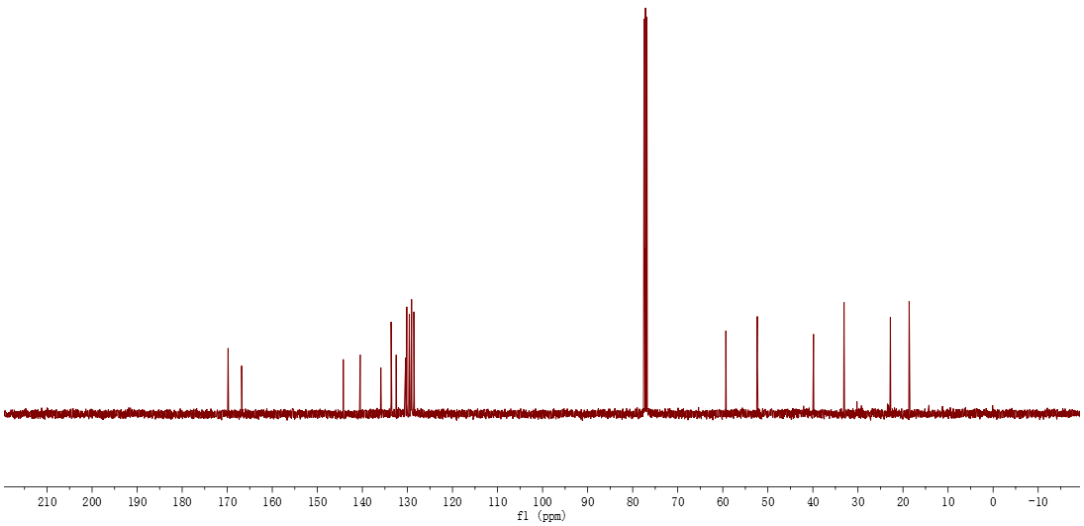

Cl
O
O
S
N
H
O
O

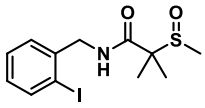
5j


8.079
8.075
8.071
8.060
8.056
8.052
7.972
7.969
7.965
7.528
7.515
7.497
7.438
7.435
7.331
7.312
7.292
7.196
7.193
4.491
4.478
4.457
4.443
4.426
4.416
4.391
4.382
3.917
2.449
1.585
1.259

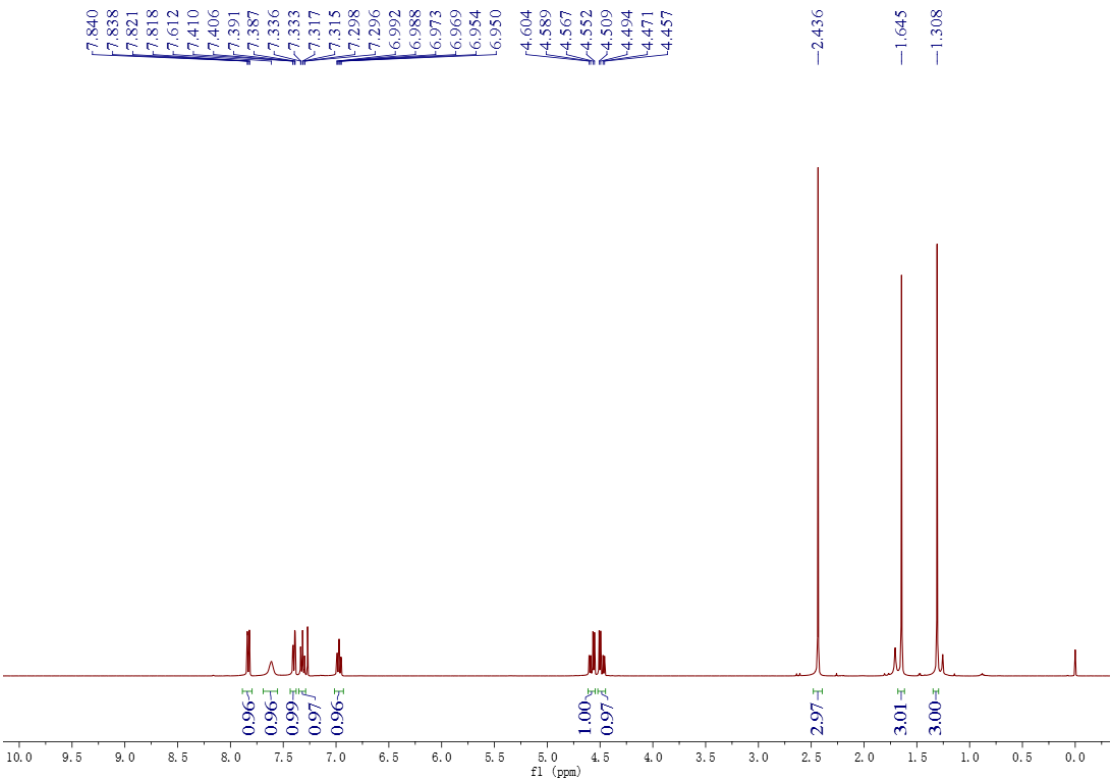

0.98
0.96
1.04
1.01
0.99
2.07
0.98
1.02
1.00
2.93
2.98
2.93
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

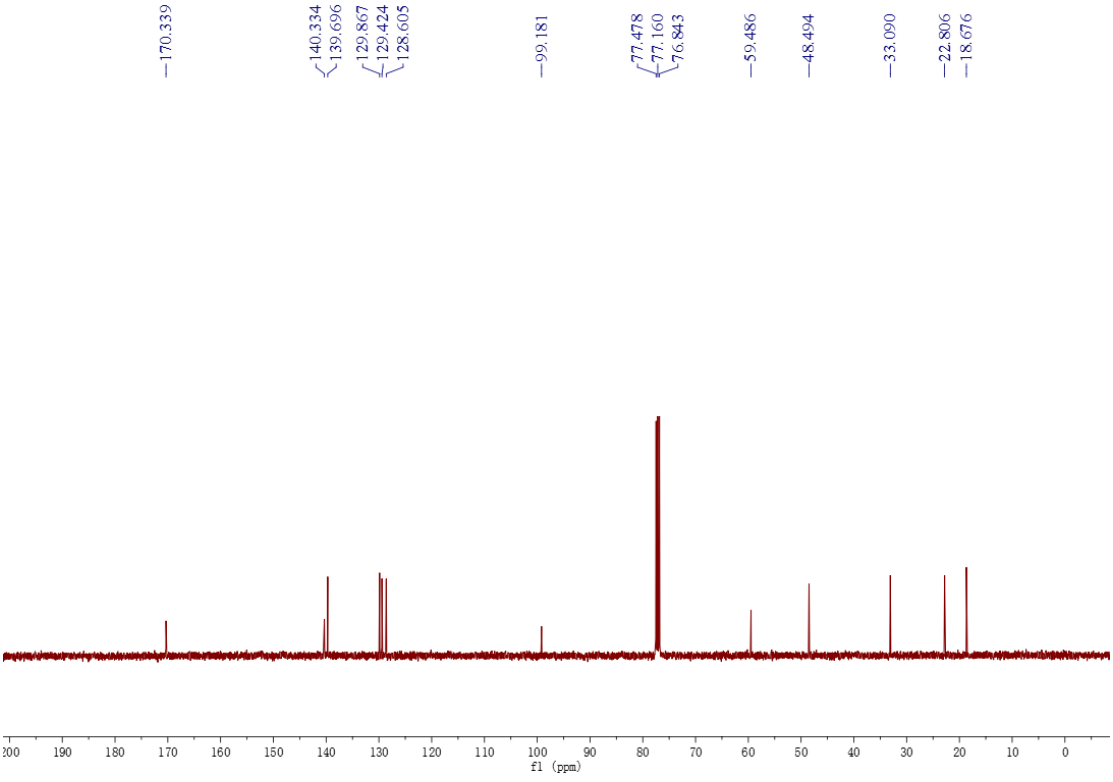

169.805
166.794
144.243
140.469
135.907
133.618
132.491
130.394
130.149
129.577
129.140
129.081
129.062
128.571
77.477
77.160
76.842
59.318
52.347
39.870
33.090
22.804
18.633

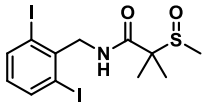

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



6$_{mono}$

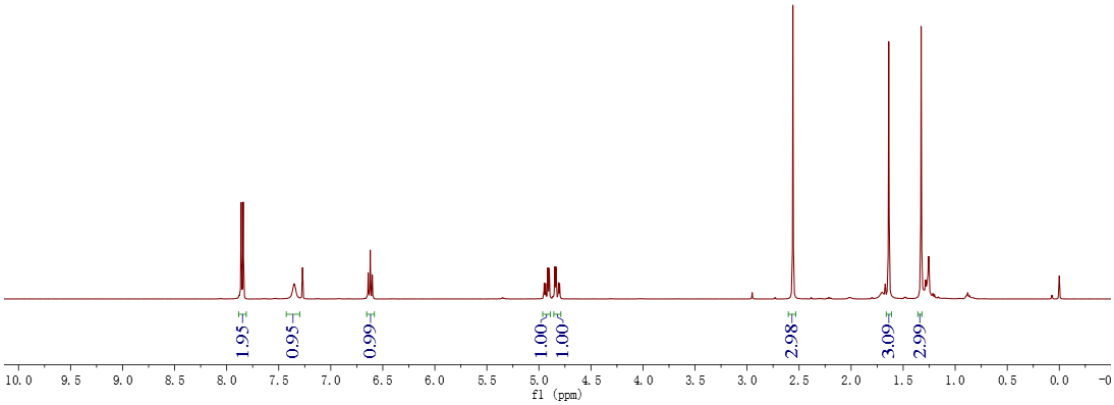

7.840
7.838
7.821
7.818
7.612
7.410
7.406
7.391
7.387
7.336
7.333
7.317
7.315
7.298
7.296
6.992
6.988
6.973
6.969
6.954
6.950
4.604
4.589
4.567
4.552
4.509
4.494
4.471
4.457
2.436
1.645
1.308
0.96
0.96
0.99
0.97
0.96
1.00
0.97
2.97
3.01
3.00
f1 (ppm)


170.339
140.334
139.696
129.867
129.424
128.605
99.181
77.478
77.160
76.843
59.486
48.494
33.090
22.806
18.676
f1 (ppm)

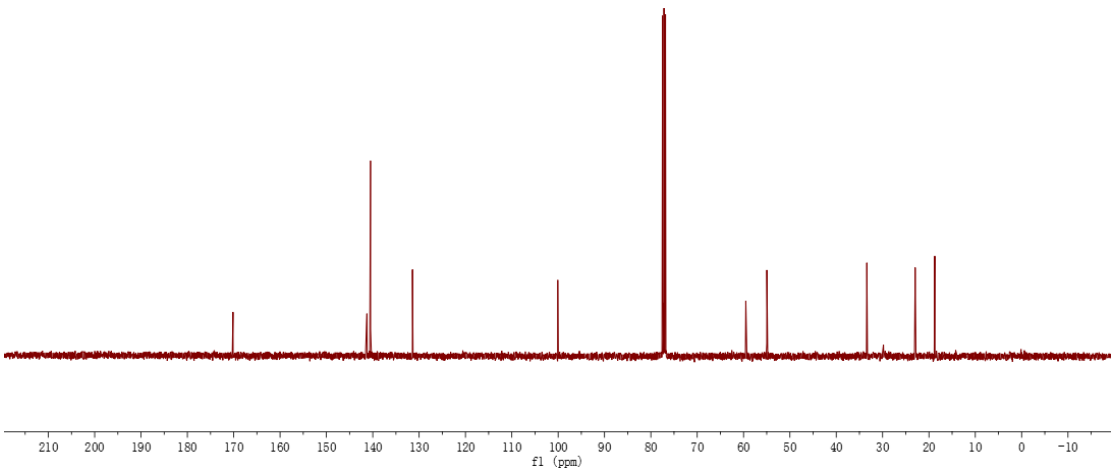


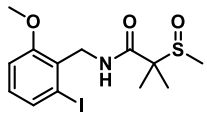
6_{di}


7.861
7.841
7.351
6.640
6.620
6.601
4.949
4.935
4.914
4.900
4.846
4.836
4.811
4.801
2.559
1.639
1.327

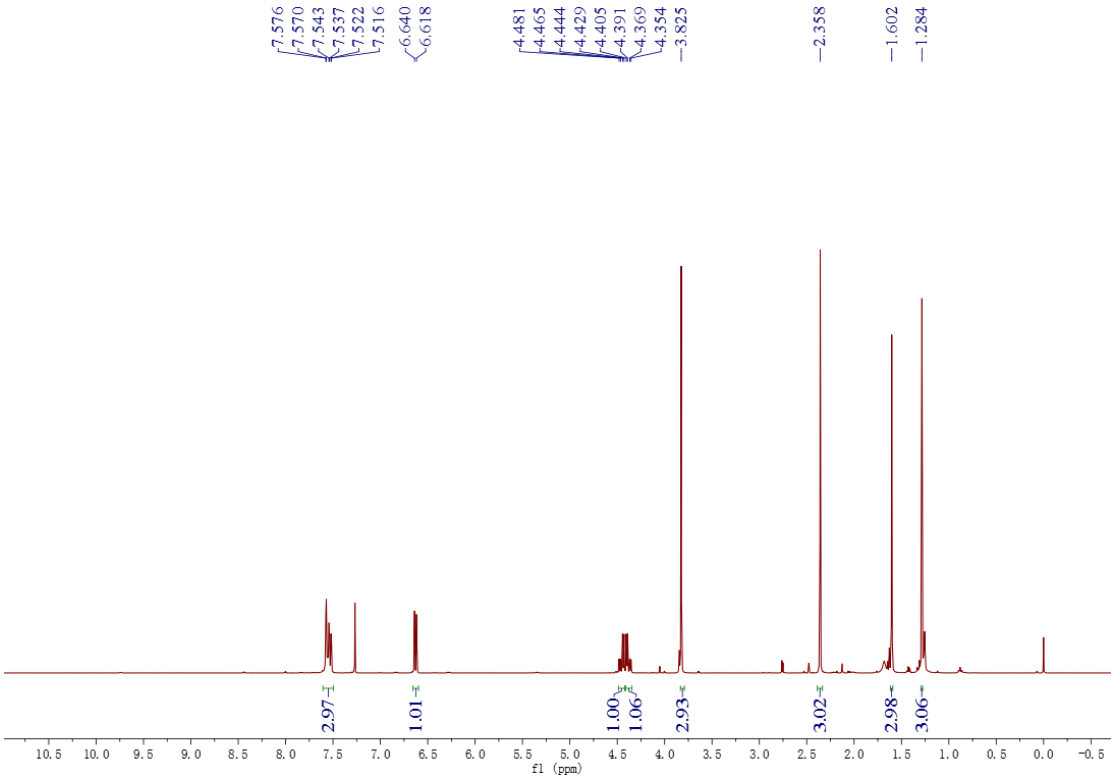

1.95
0.95
0.99
1.00
1.00
2.98
3.09
2.99
f1 (ppm)

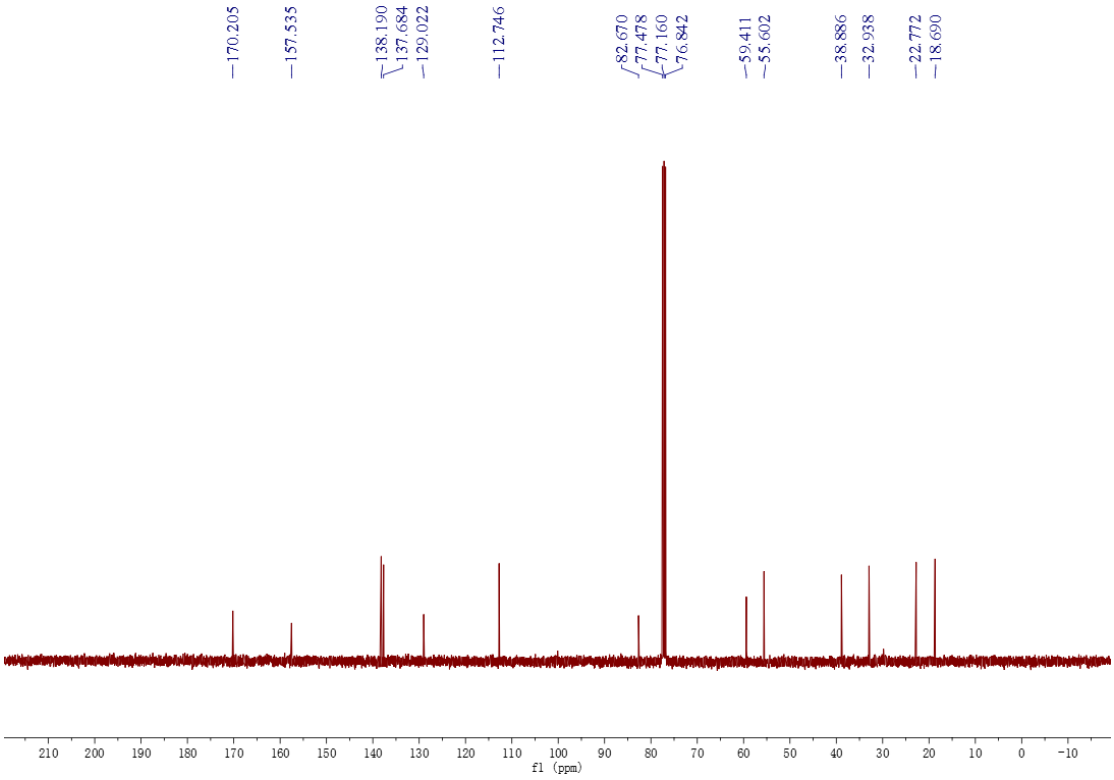

170.152
141.257
140.481
131.425
100.077
77.477
77.160
76.842
59.512
54.969
33.397
22.970
18.742

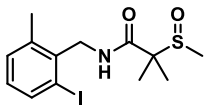

f1 (ppm)



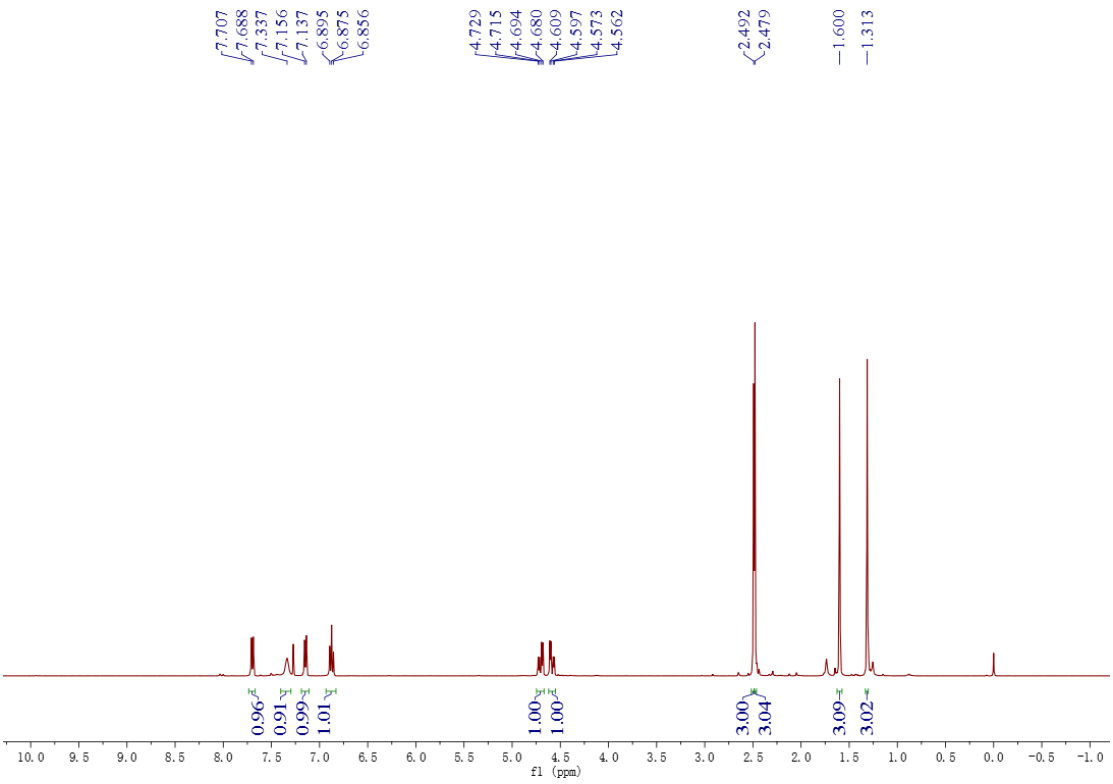
7


7.576
7.570
7.543
7.537
7.522
7.516
6.640
6.618
4.481
4.465
4.444
4.429
4.405
4.391
4.369
4.354
3.825
2.358
1.602
1.284
2.97
1.01
1.00
1.06
2.93
3.02
2.98
3.06
f1 (ppm)


170.205
157.535
138.190
137.684
129.022
112.746
82.670
77.478
77.160
76.842
59.411
55.602
38.886
32.938
22.772
18.690
f1 (ppm)



8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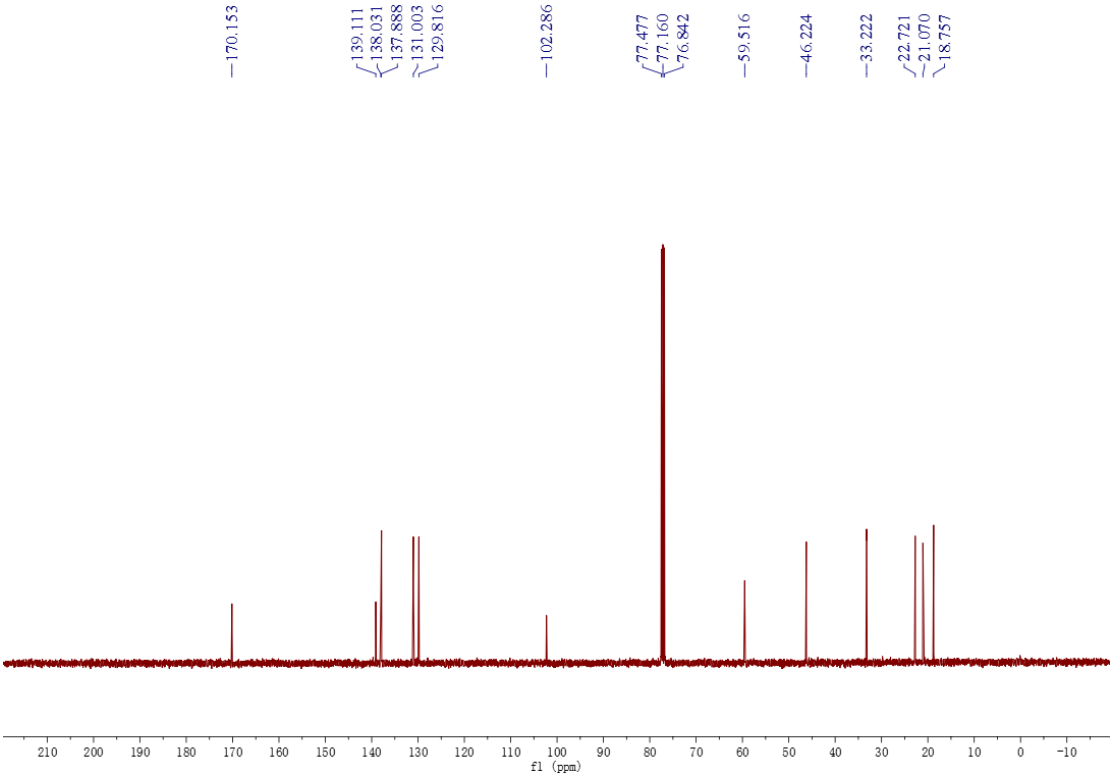
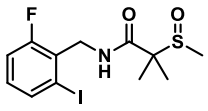
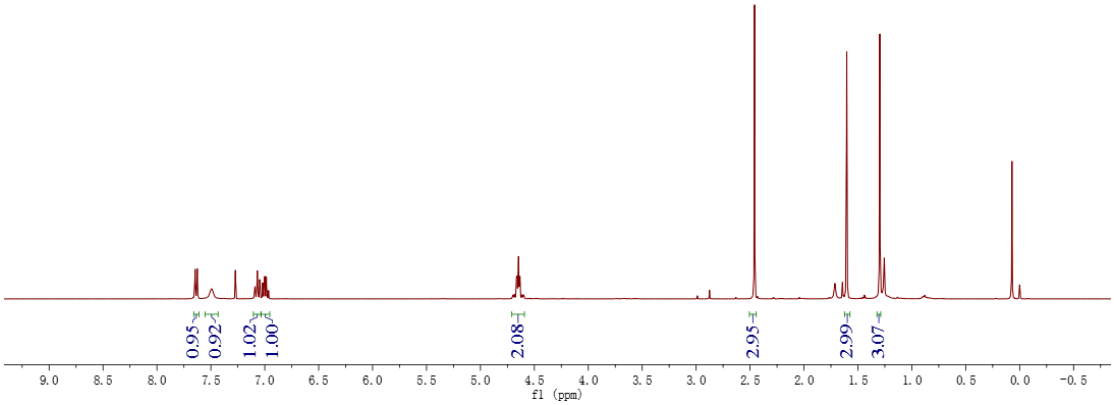
7.688
7.337
7.156
7.137
6.895
6.875
6.856
4.729
4.715
4.694
4.680
4.609
4.597
4.573
4.562
2.492
2.479
1.600
1.313
0.96
0.91
0.99
1.01
1.00
1.00
3.00
3.04
3.09
3.02
f1 (ppm)


170.153
139.111
138.031
137.888
131.003
129.816
102.286
77.477
77.160
76.842
59.516
46.224
33.222
22.721
21.070
18.757
f1 (ppm)

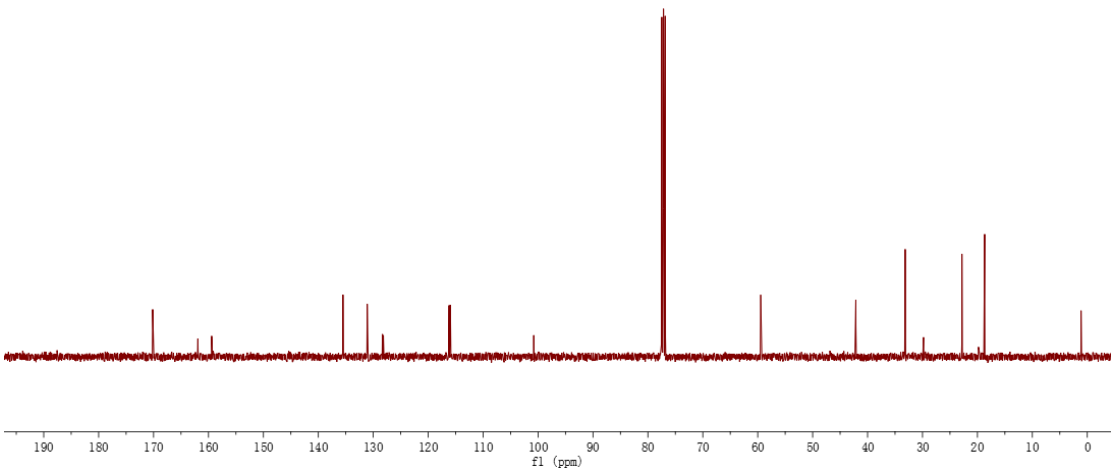


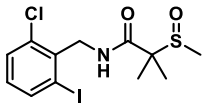
9


7.646
7.626
7.493
7.090
7.069
7.047
7.020
7.005
7.000
6.985
4.701
4.696
4.687
4.683
4.665
4.661
4.651
4.647
4.638
4.633
4.615
4.611
4.602
4.598
2.459
1.604
1.297

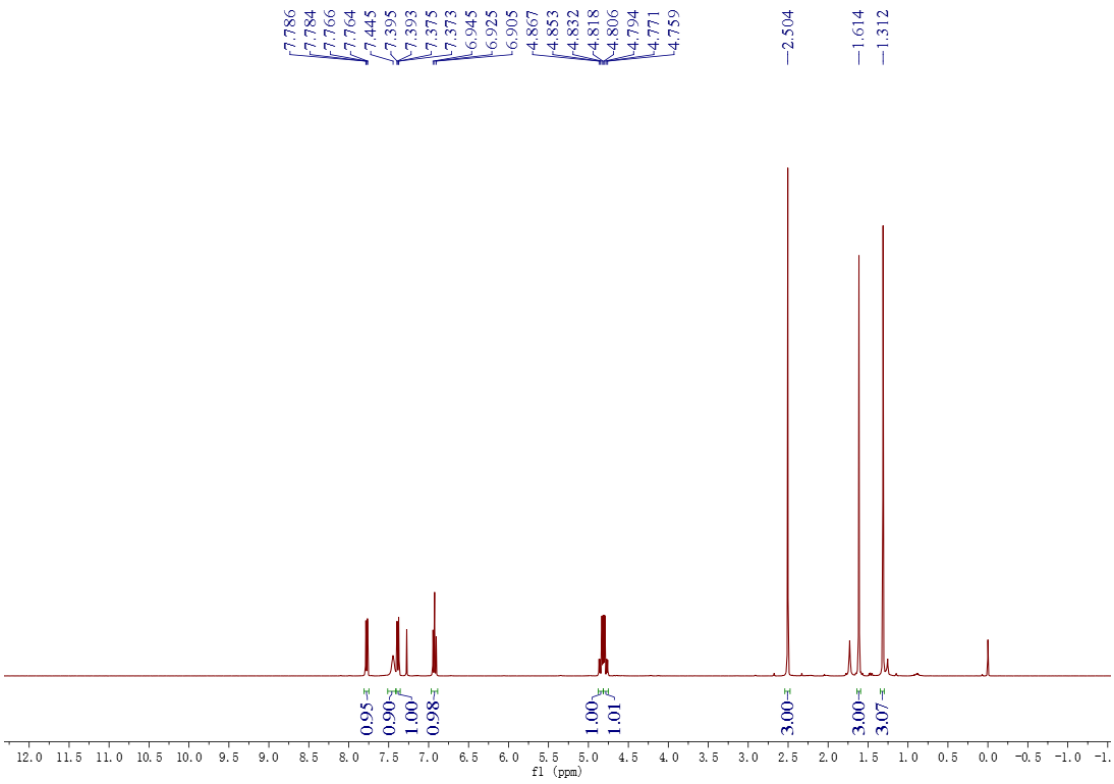

0.95
0.92
1.02
1.00
2.08
2.95
2.99
3.07
f1 (ppm)

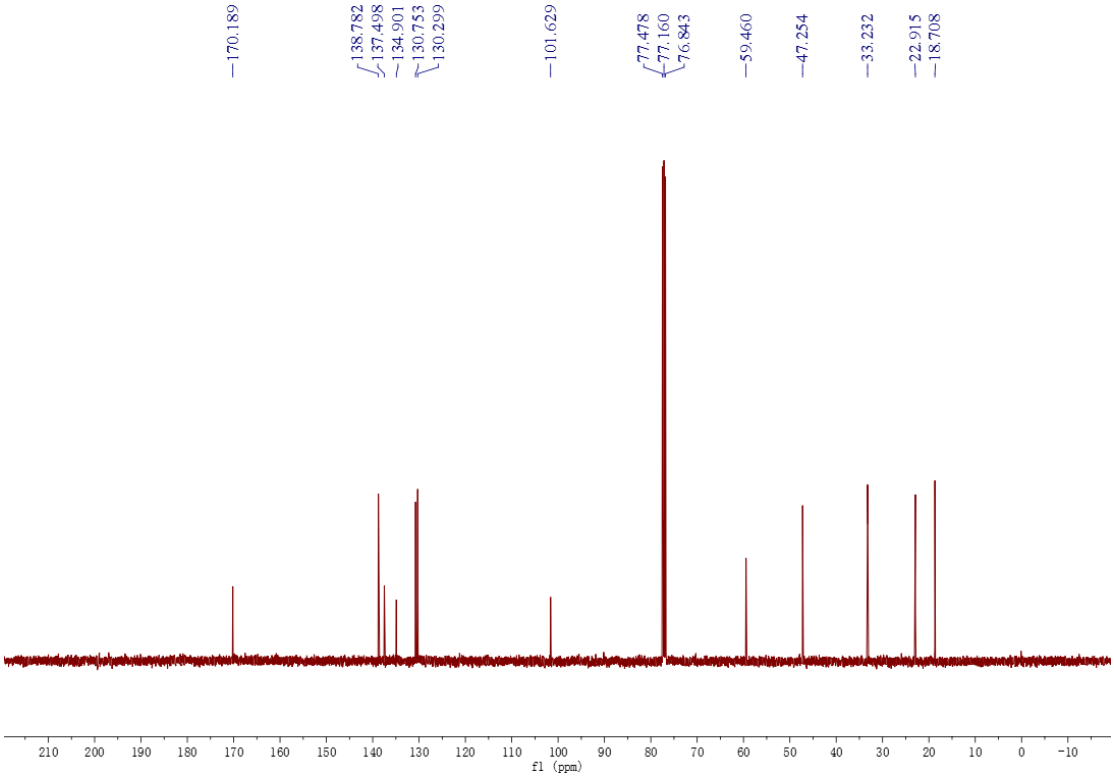

170.162
161.931
159.420
135.553
135.516
131.101
131.012
128.325
128.164
116.192
115.963
100.778
100.751
77.478
77.160
76.842
59.459
42.173
42.137
33.153
22.820
18.685

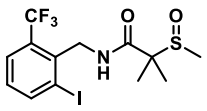

f1 (ppm)


Cl
O
O
S
N
H
I

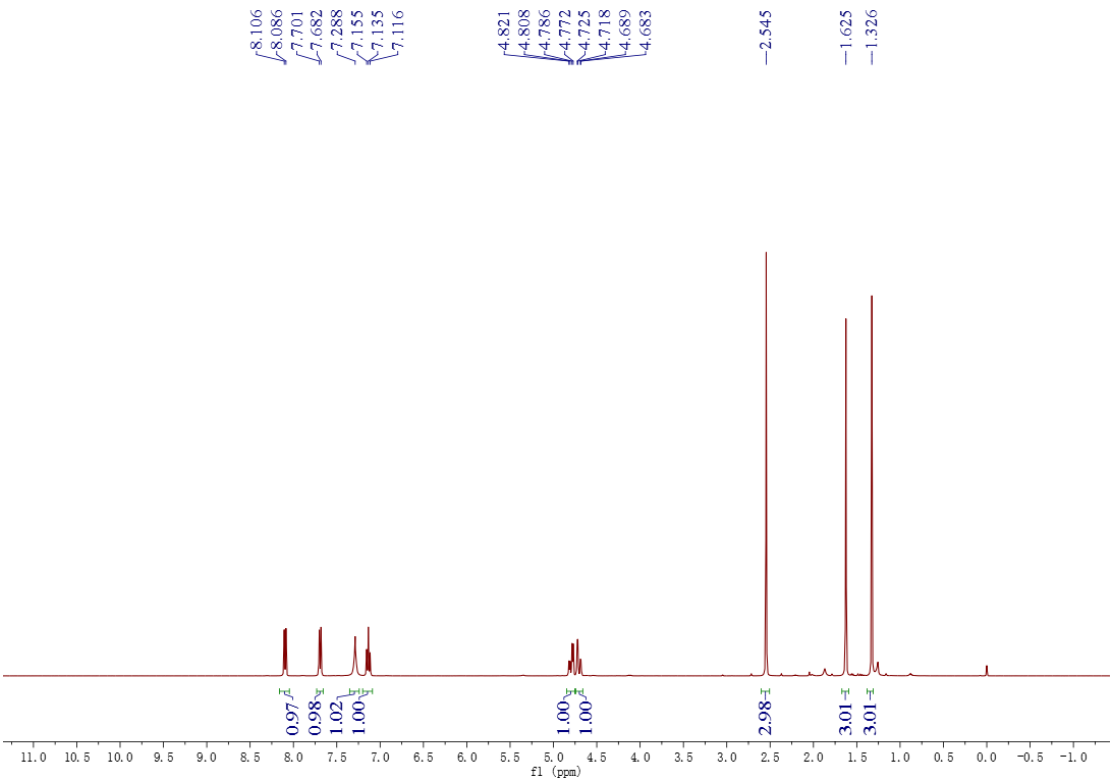
10

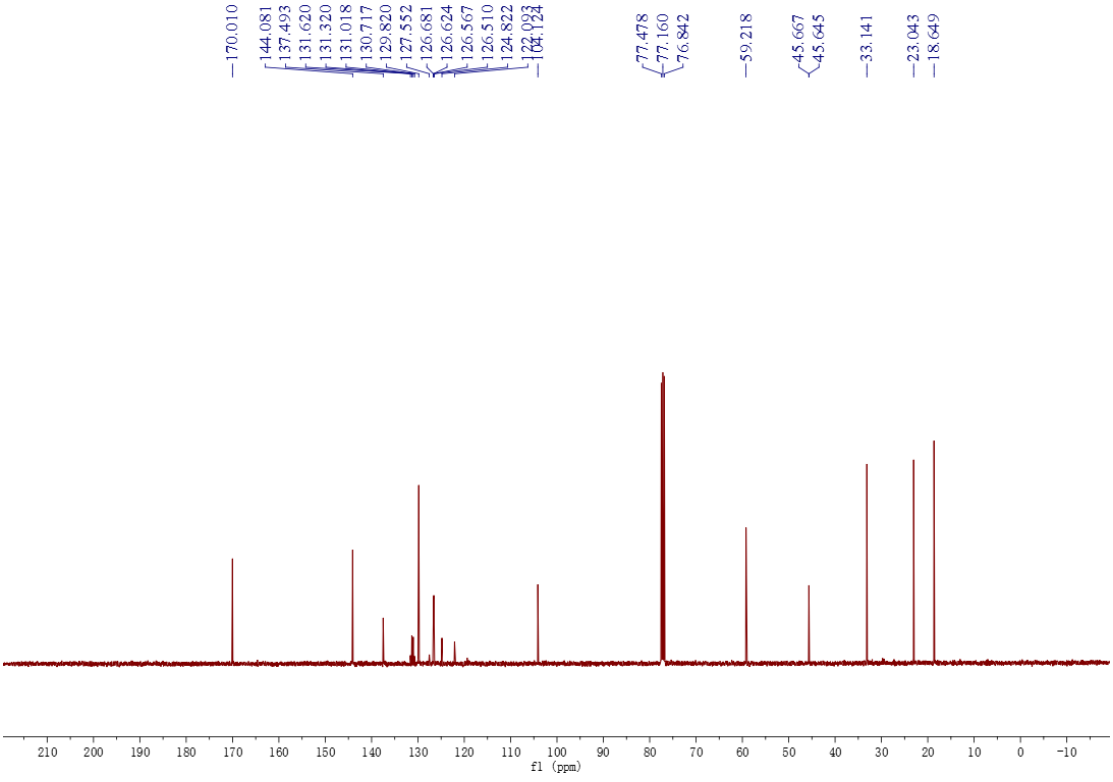

7.786
7.784
7.766
7.764
7.445
7.395
7.393
7.375
7.373
6.945
6.925
6.905
4.867
4.853
4.832
4.818
4.806
4.794
4.771
4.759
2.504
1.614
1.312
0.95
0.90
1.00
0.98
1.00
1.01
3.00
3.00
3.07
f1 (ppm)

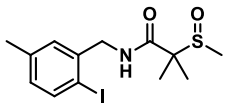

170.189
138.782
137.498
134.901
130.753
130.299
101.629
77.478
77.160
76.843
59.460
47.254
33.232
22.915
18.708
f1 (ppm)



11

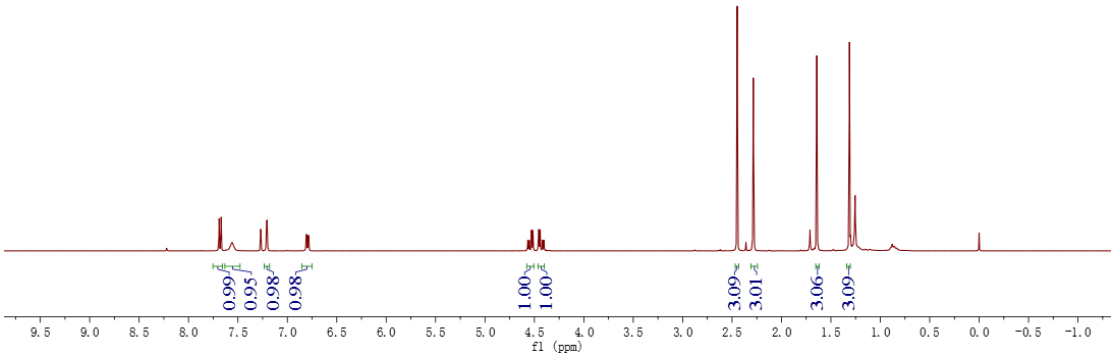

8.106
8.086
7.701
7.682
7.288
7.155
7.135
7.116
4.821
4.808
4.786
4.772
4.725
4.718
4.689
4.683
2.545
1.625
1.326
0.97
0.98
1.02
1.00
1.00
1.00
2.98
3.01
3.01
f1 (ppm)


170.010
144.081
137.493
131.620
131.320
131.018
130.717
129.820
127.552
126.681
126.624
126.567
126.510
124.822
122.093
104.124
77.478
77.160
76.842
59.218
45.667
45.645
33.141
23.043
18.649
f1 (ppm)

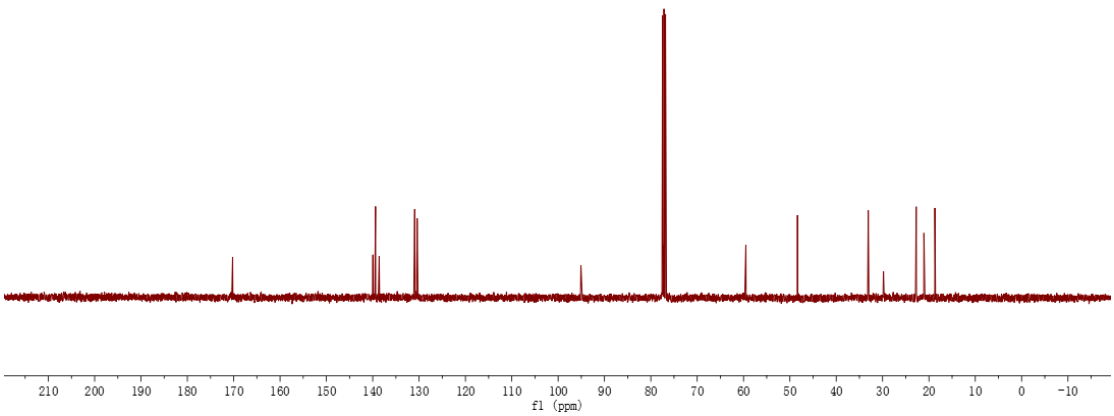


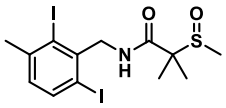
12$_{mono}$


7.690
7.670
7.559
7.209
7.205
6.808
6.804
6.788
6.784
4.567
4.552
4.530
4.515
4.456
4.442
4.419
4.405
2.448
2.285
1.643
1.312


0.99
0.95
0.98
0.98
1.00
1.00
3.09
3.01
3.06
3.09
f1 (ppm)

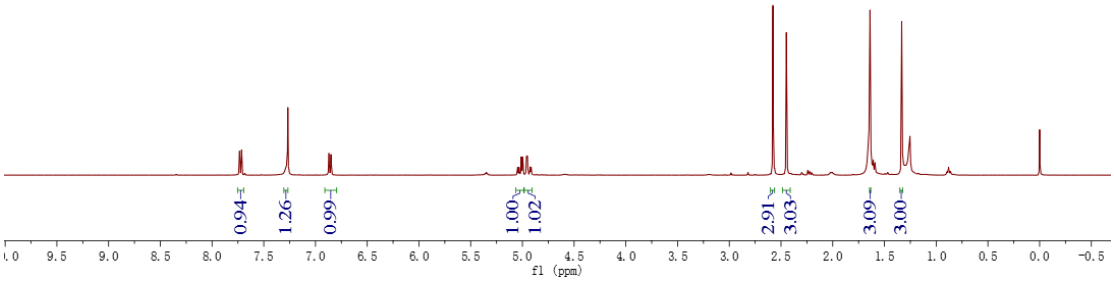

170.232
139.963
139.400
138.609
130.946
130.420
95.086
77.478
77.160
76.842
59.496
48.354
33.094
22.741
21.078
18.713


f1 (ppm)

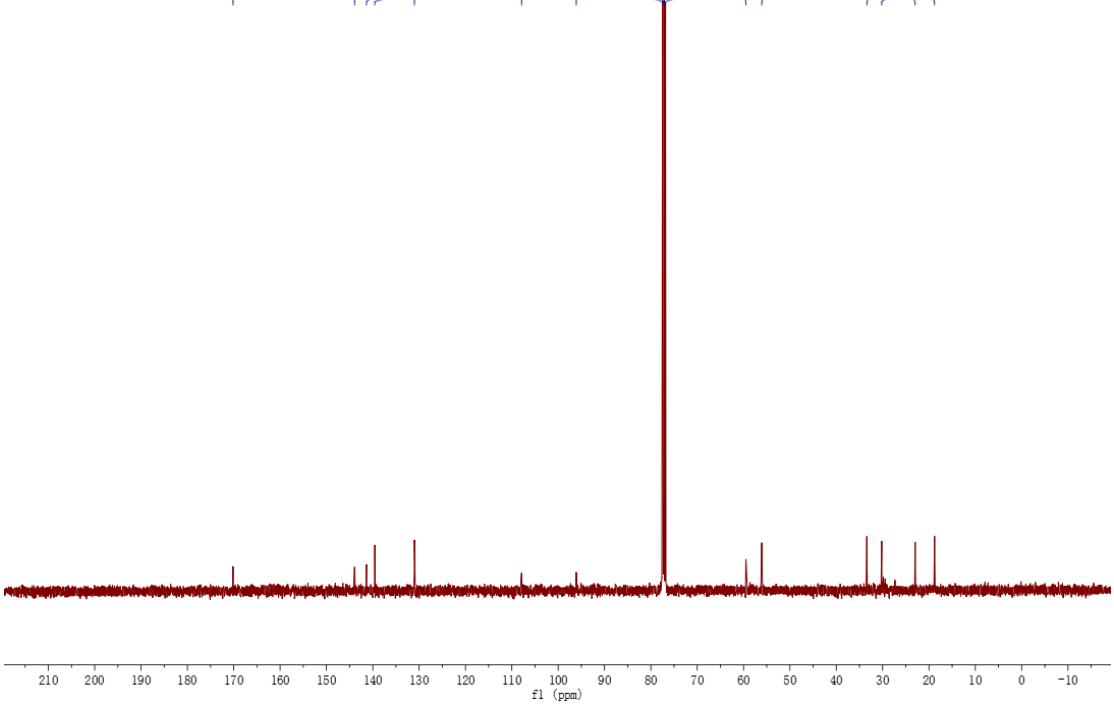


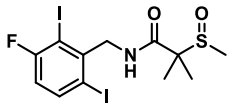
12$_{di}$


7.734
7.714
7.267
6.870
6.850
5.045
5.032
5.011
4.997
4.961
4.951
4.926
4.916
2.578
2.448
1.640
1.334

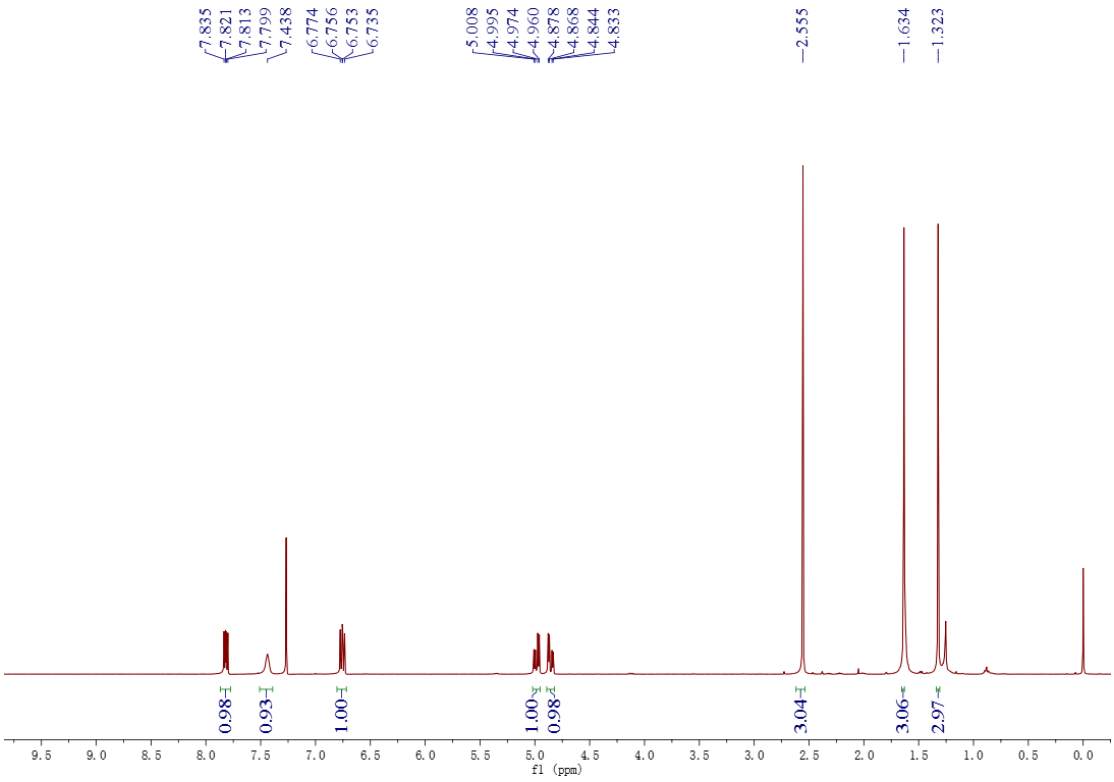

0.94
1.26
0.99
1.00
1.02
2.91
3.03
3.09
3.00
f1 (ppm)

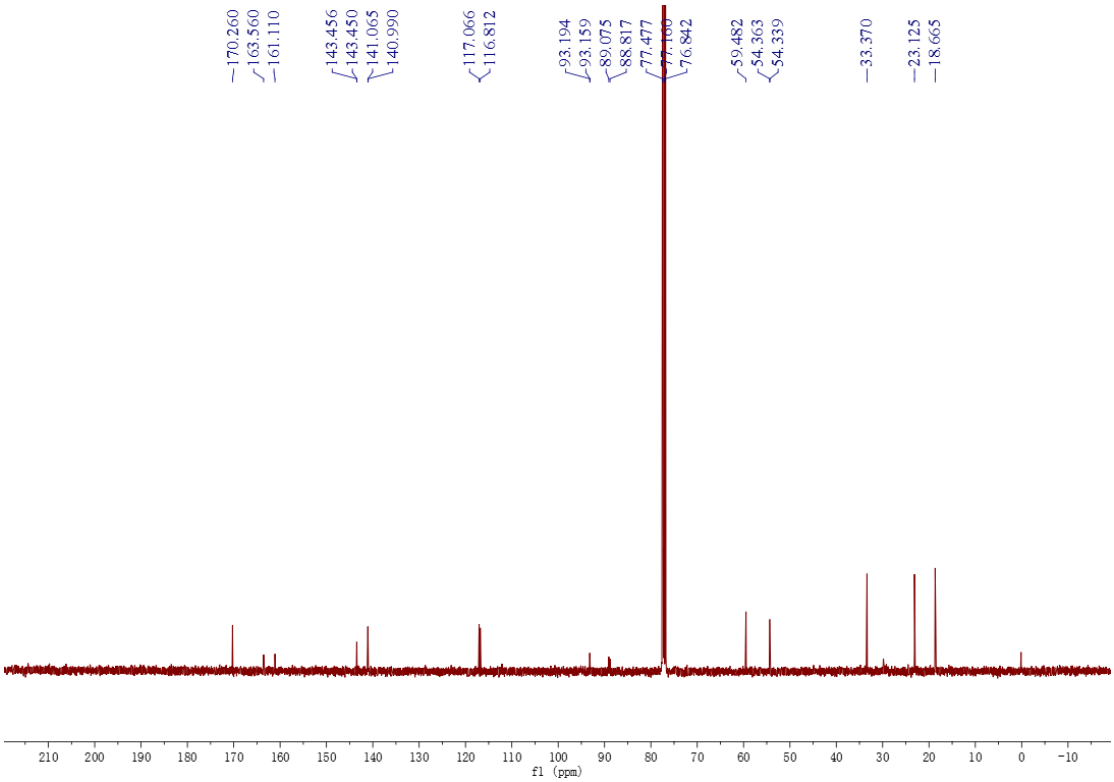

170.150
143.927
141.364
139.563
131.012
107.895
96.095
77.477
77.160
76.842
59.500
56.075
33.404
30.194
22.979
18.794

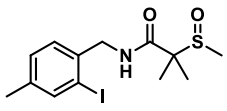

f1 (ppm)



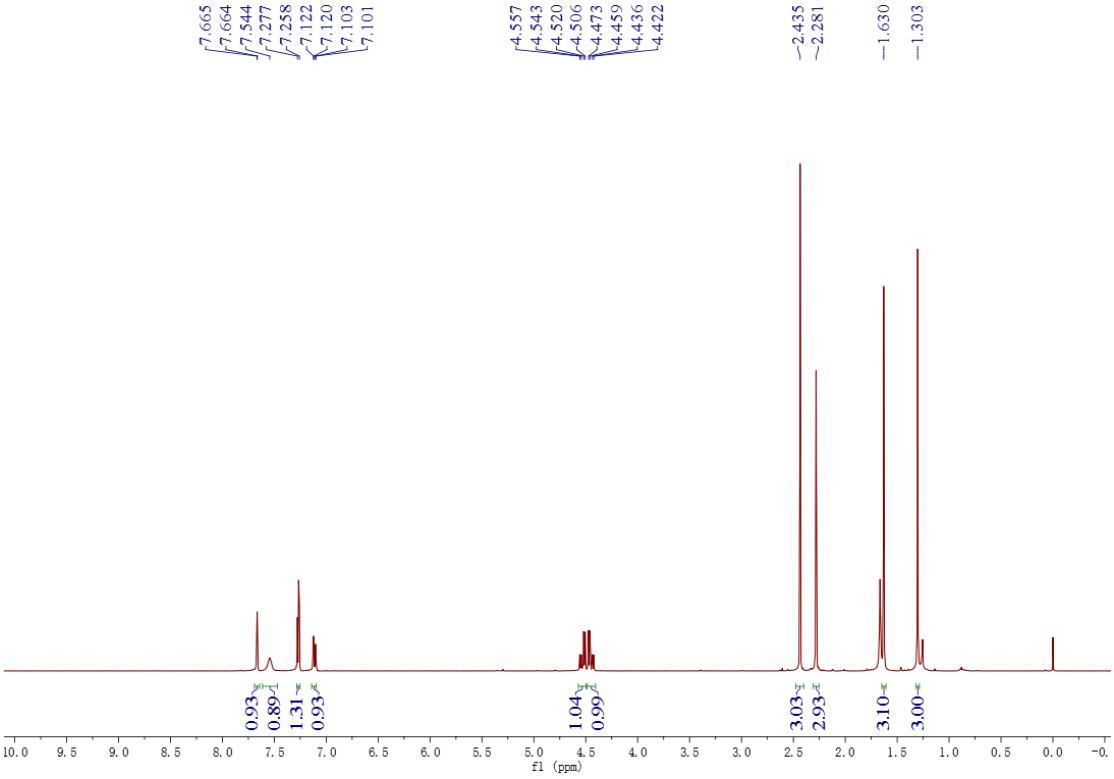
13

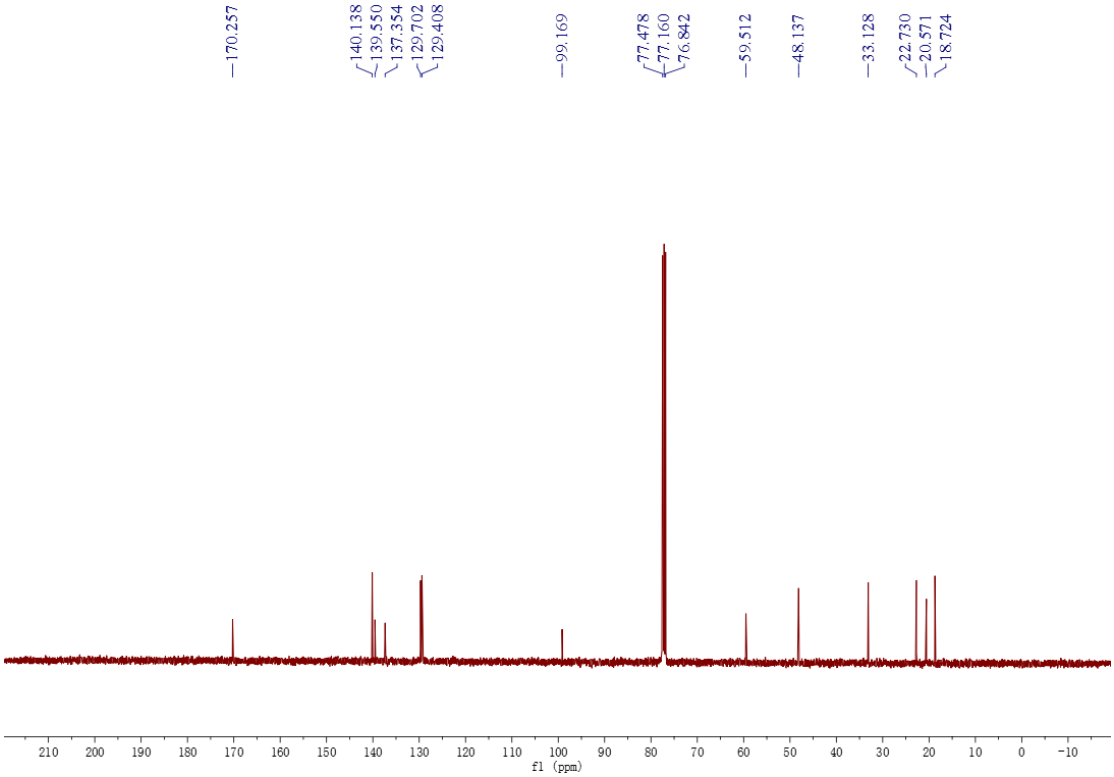

7.835
7.821
7.813
7.799
7.438
6.774
6.756
6.753
6.735
5.008
4.995
4.974
4.960
4.878
4.868
4.844
4.833
2.555
1.634
1.323
0.98
0.93
1.00
1.00
0.98
3.04
3.06
2.97
f1 (ppm)

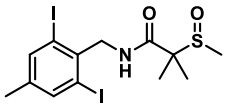

170.260
163.560
161.110
143.456
143.450
141.065
140.990
117.066
116.812
93.194
93.159
89.075
88.817
77.477
77.160
76.842
59.482
54.363
54.339
33.370
23.125
18.665
f1 (ppm)



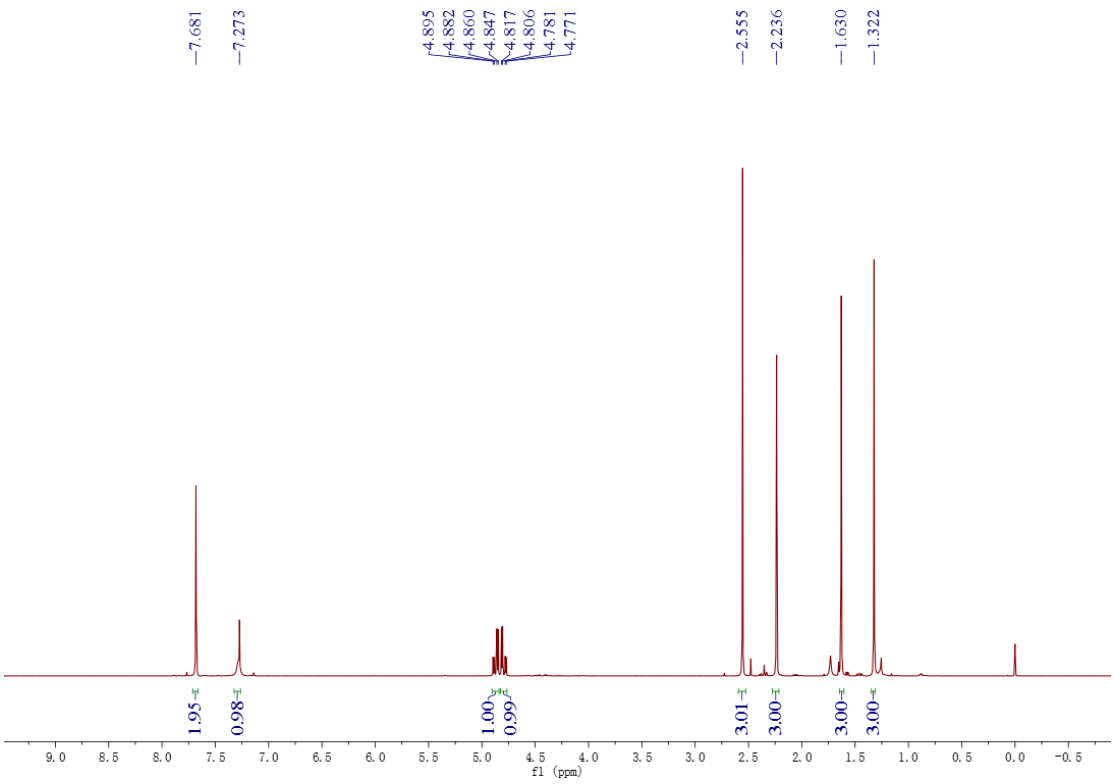
14$_{mono}$

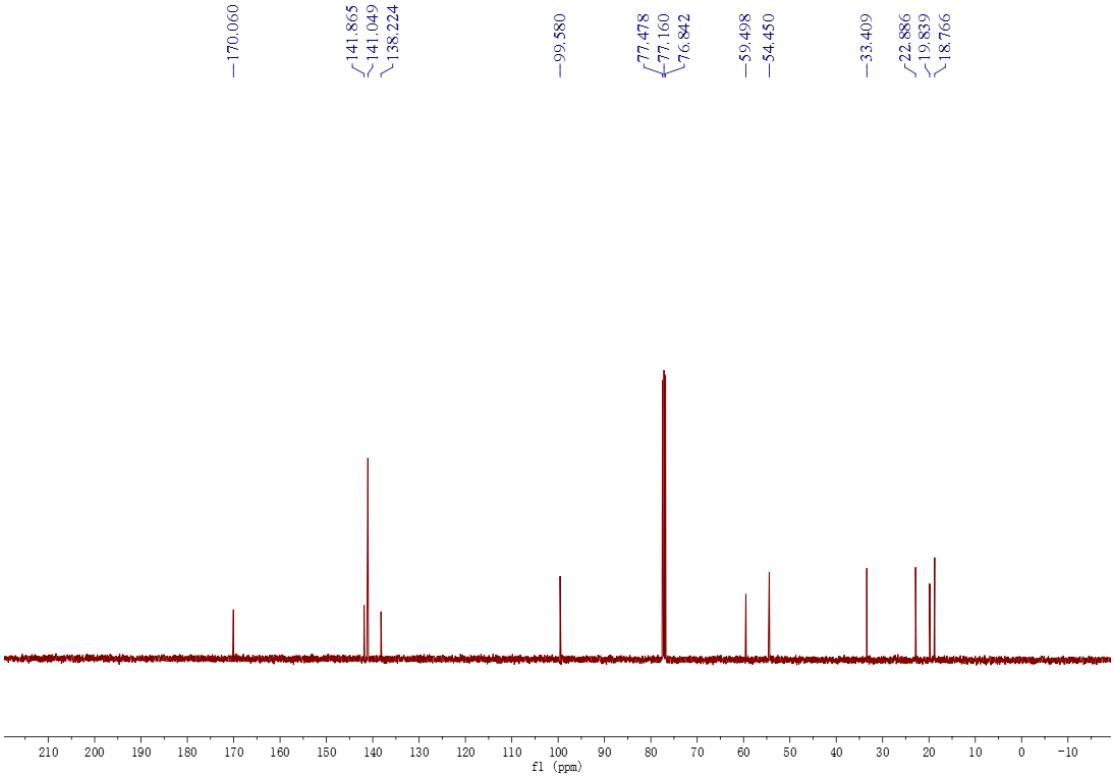

7.665
7.664
7.544
7.277
7.258
7.122
7.120
7.103
7.101
4.557
4.543
4.520
4.506
4.473
4.459
4.436
4.422
2.435
2.281
1.630
1.303
0.93
0.89
1.31
0.93
1.04
0.99
3.03
2.93
3.10
3.00
f1 (ppm)

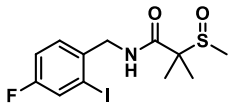

170.257
140.138
139.550
137.354
129.702
129.408
99.169
77.478
77.160
76.842
59.512
48.137
33.128
22.730
20.571
18.724
f1 (ppm)



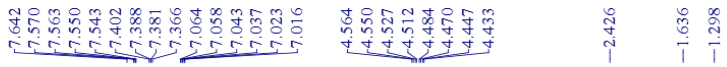
14_{di}

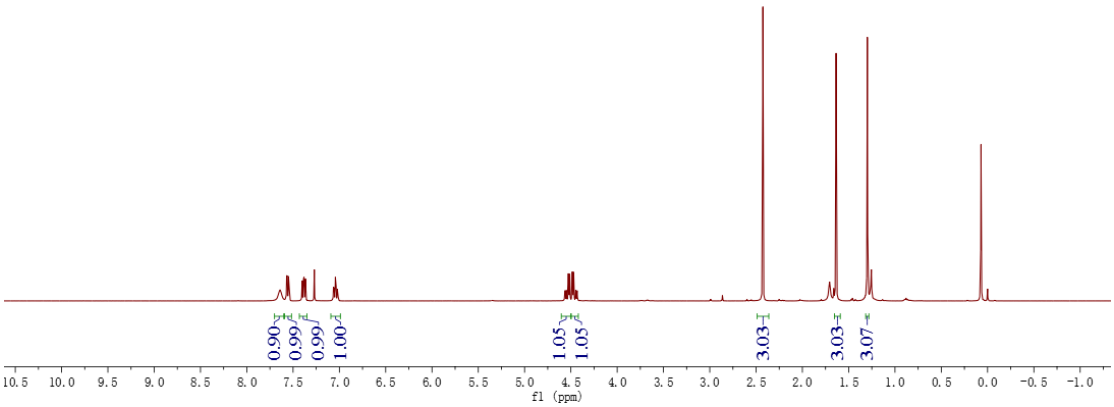

7.681
7.273
4.895
4.882
4.860
4.847
4.817
4.806
4.781
4.771
2.555
2.236
1.630
1.322
1.95
0.98
1.00
0.99
3.01
3.00
3.00
3.00
f1 (ppm)


170.060
141.865
141.049
138.224
99.580
77.478
77.160
76.842
59.498
54.450
33.409
22.886
19.839
18.766
f1 (ppm)

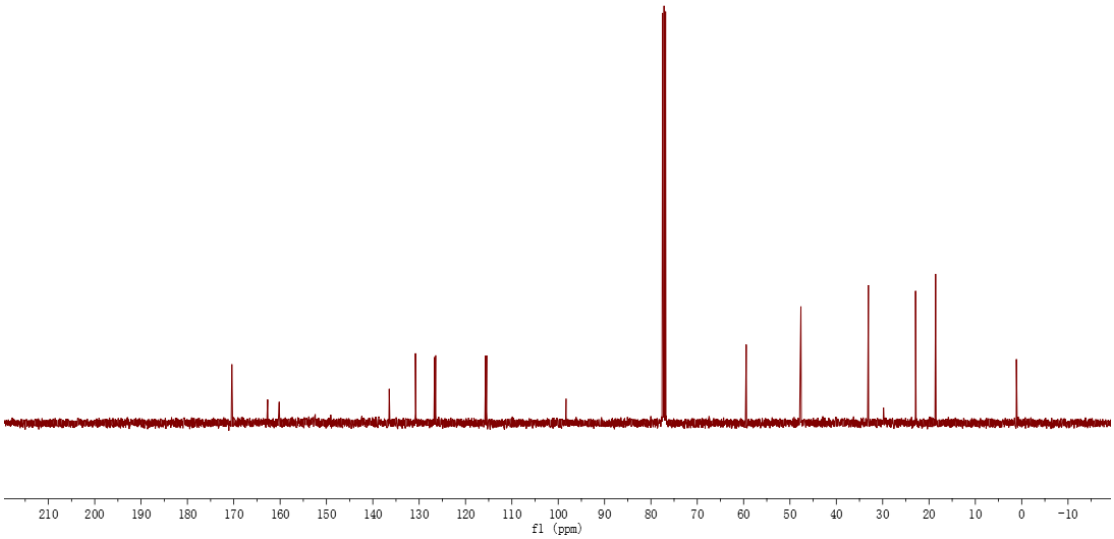

O
O
N
H
S
F
I

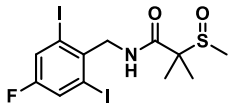
15$_{mono}$


7.642
7.570
7.563
7.550
7.543
7.402
7.388
7.381
7.366
7.064
7.058
7.043
7.037
7.023
7.016
4.564
4.550
4.527
4.512
4.484
4.470
4.447
4.433
2.426
1.636
1.298

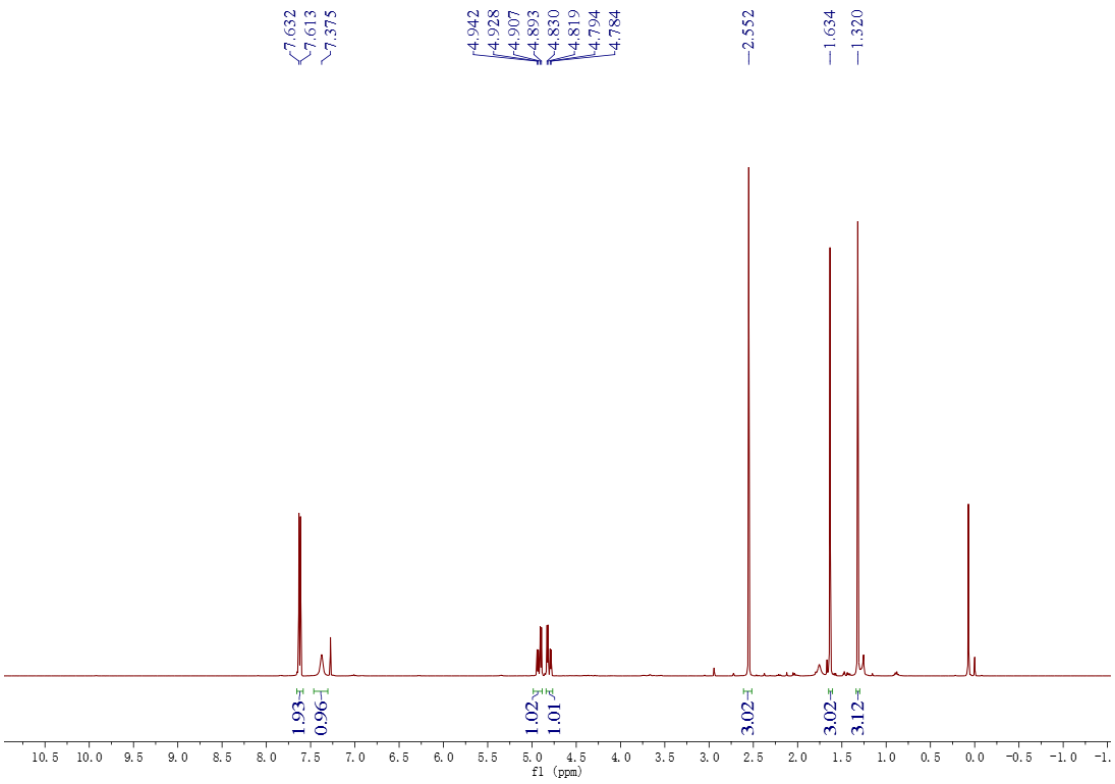

0.90
0.99
0.99
1.00
1.05
1.05
3.03
3.03
3.07
f1 (ppm)

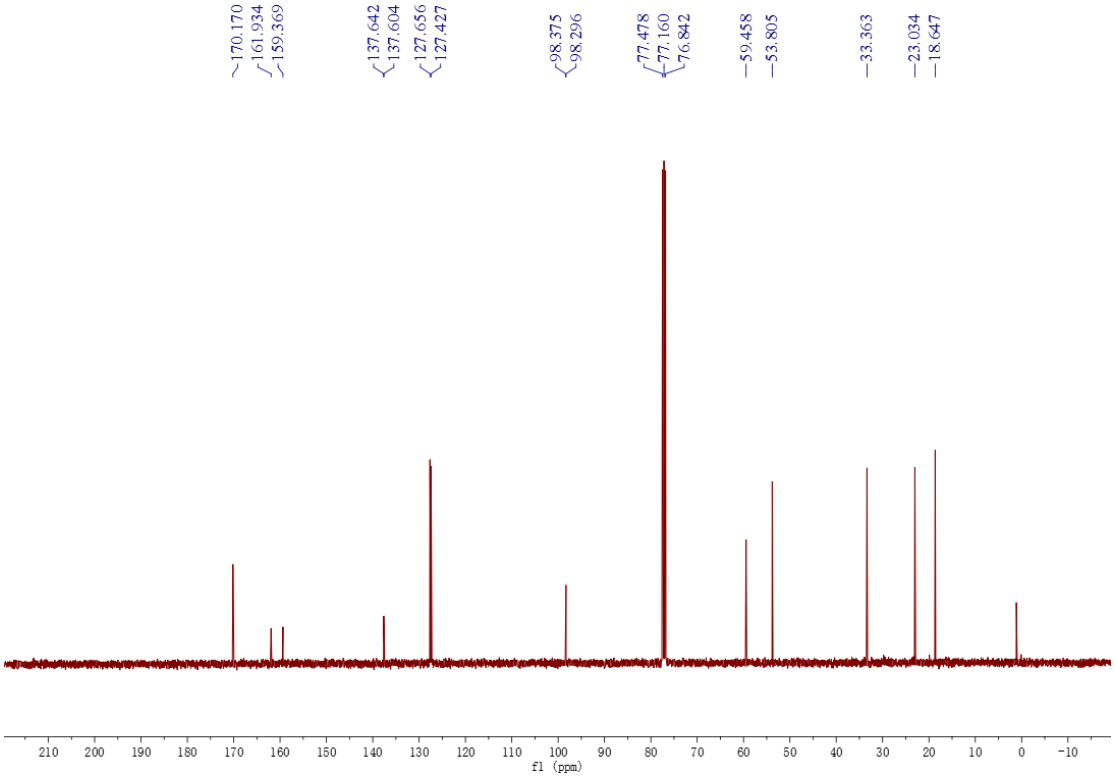

170.408
162.693
160.193
136.489
136.455
130.796
130.715
126.671
126.435
115.652
115.445
98.383
98.302
77.477
77.160
76.842
59.439
47.639
33.078
22.894
18.580

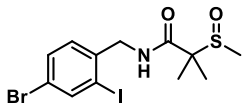

f1 (ppm)



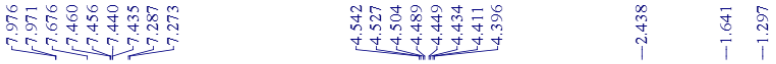
15_{di}

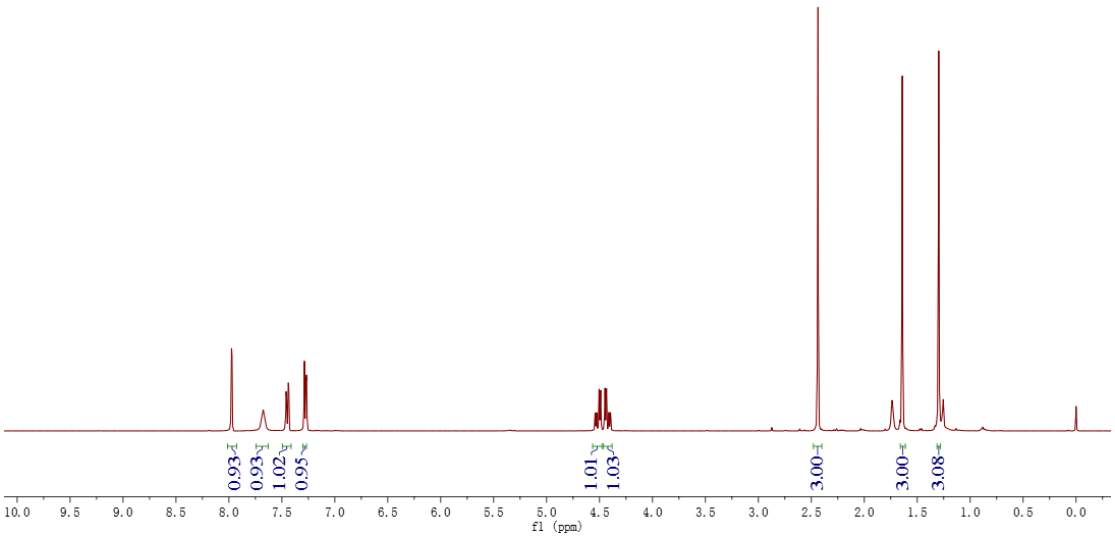

7.632
7.613
7.375
4.942
4.928
4.907
4.893
4.830
4.819
4.794
4.784
2.552
1.634
1.320
1.93
0.96
1.02
1.01
3.02
3.02
3.12
f1 (ppm)


170.170
161.934
159.369
137.642
137.604
127.656
127.427
98.375
98.296
77.478
77.160
76.842
59.458
53.805
33.363
23.034
18.647
f1 (ppm)

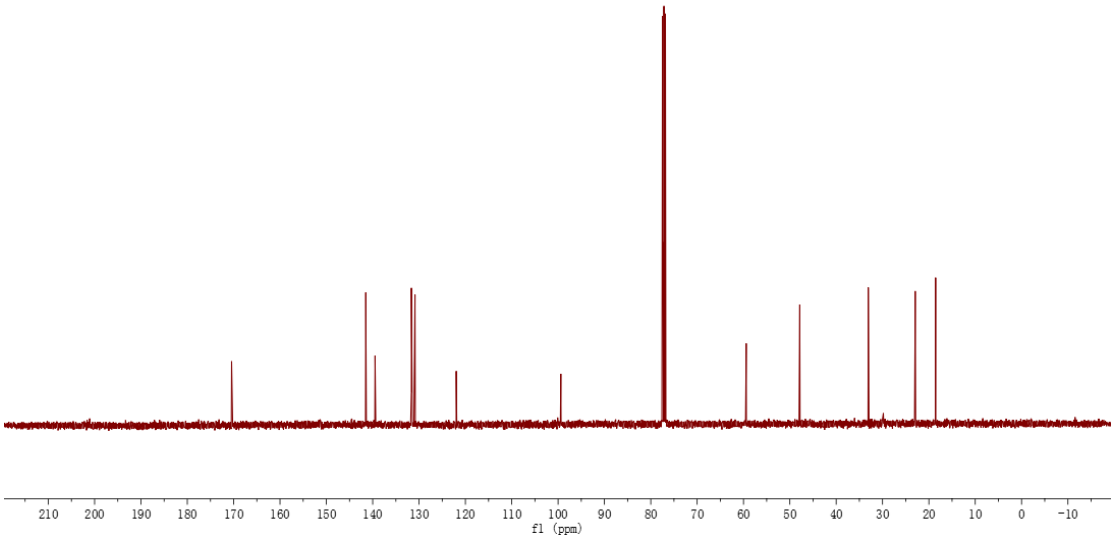

O
O
S
N
H
Br
I

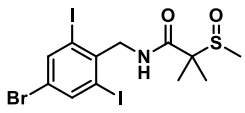
16$_{mono}$


7.976
7.971
7.676
7.460
7.456
7.440
7.435
7.287
7.273
4.542
4.527
4.504
4.489
4.449
4.434
4.411
4.396
2.438
1.641
1.297

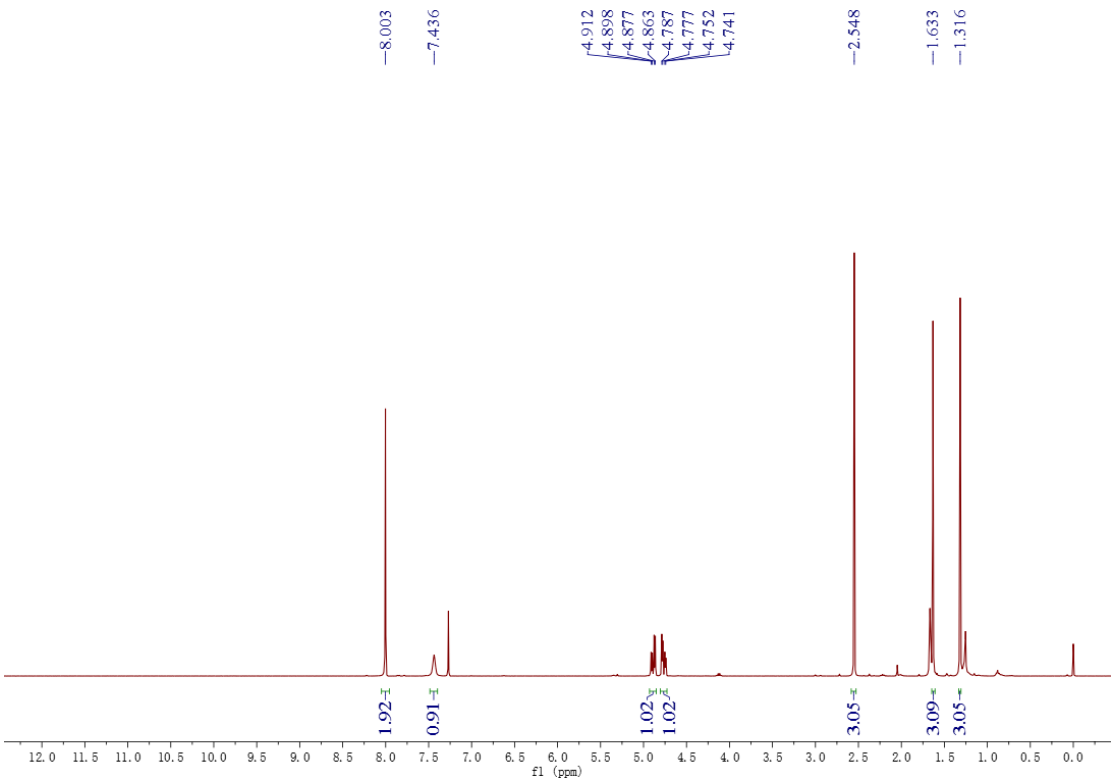

0.93
0.93
1.02
0.95
1.01
1.03
3.00
3.00
3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

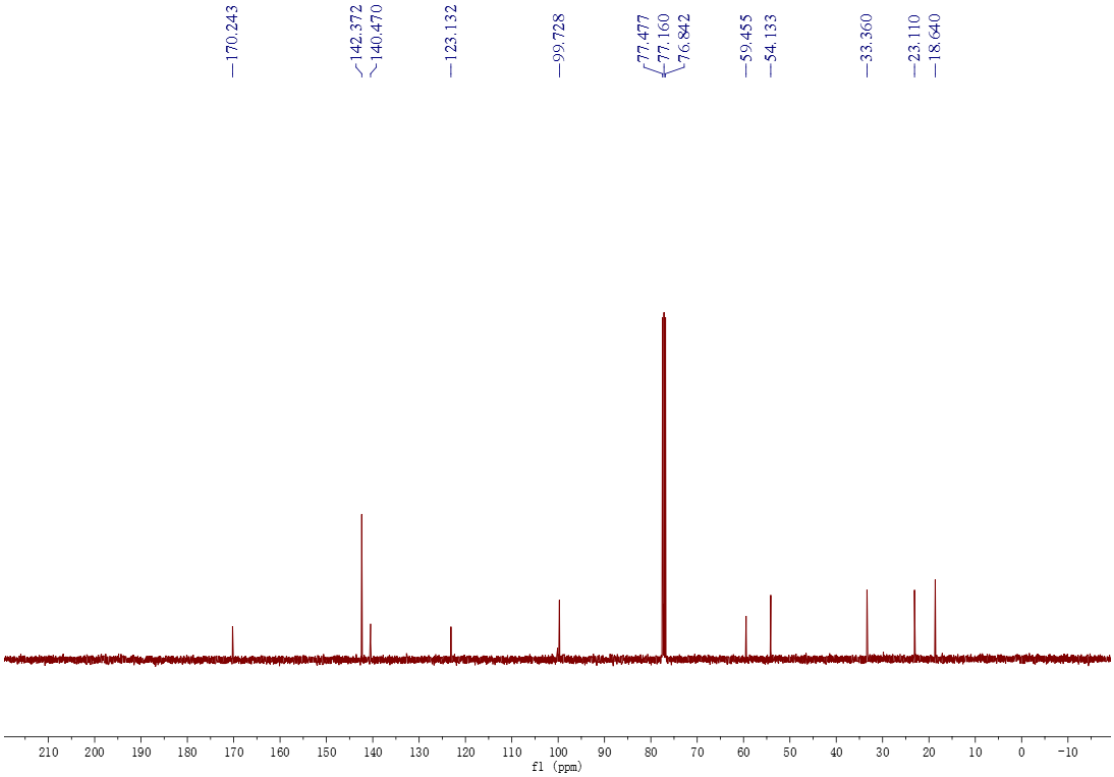

170.446
141.490
139.490
131.652
130.874
121.974
99.406
77.478
77.160
76.842
59.408
47.859
33.075
22.943
18.546

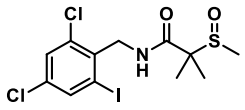

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



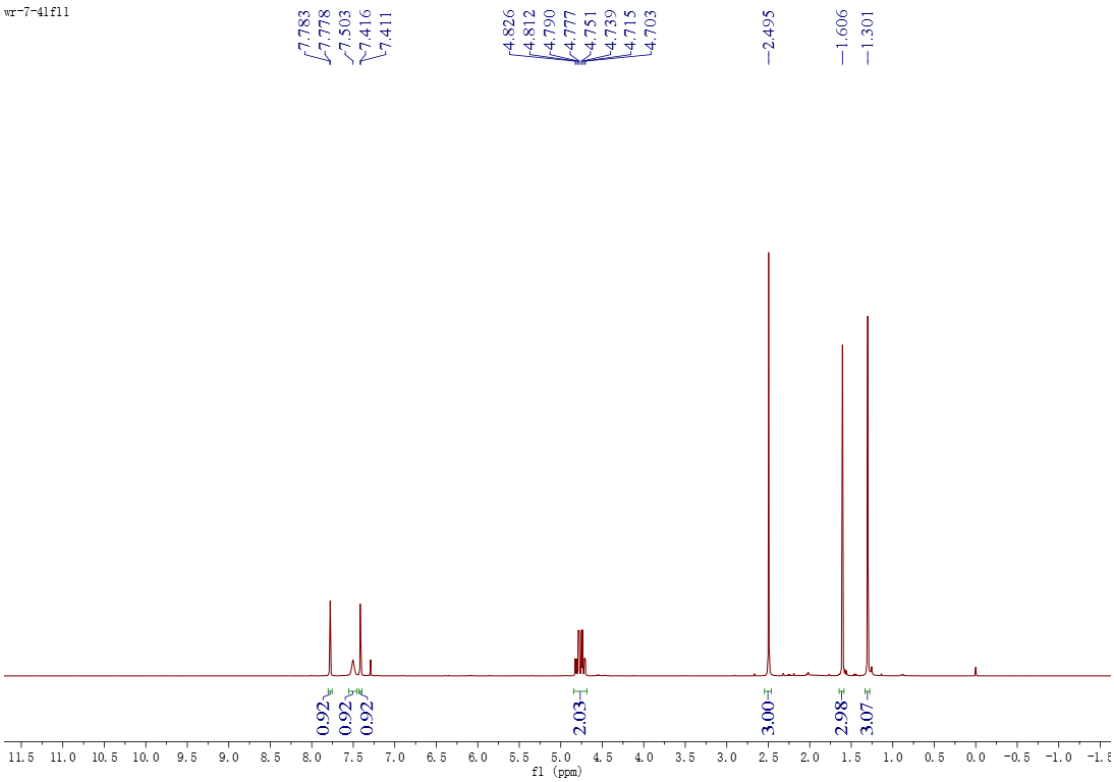
16$_{di}$

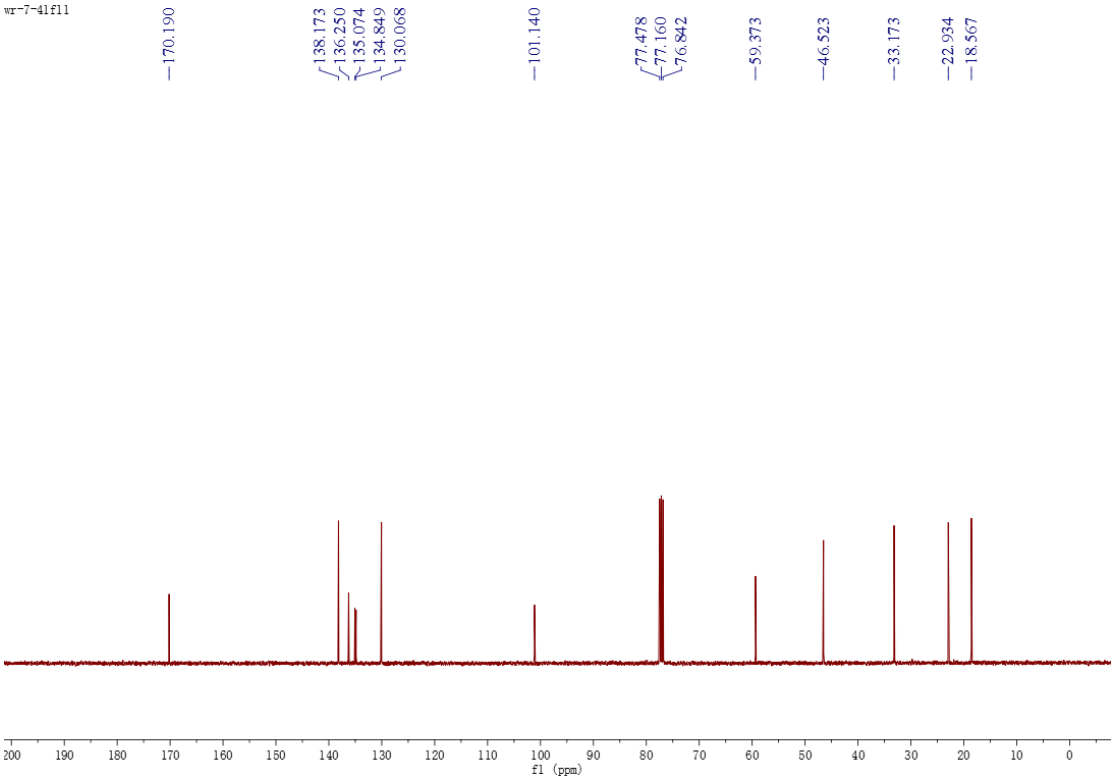

8.003
7.436
4.912
4.898
4.877
4.863
4.787
4.777
4.752
4.741
2.548
1.633
1.316
1.92
0.91
1.02
1.02
3.05
3.09
3.05
f1 (ppm)

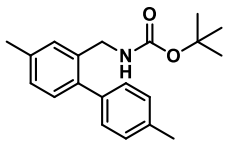

170.243
142.372
140.470
123.132
99.728
77.477
77.160
76.842
59.455
54.133
33.360
23.110
18.640
f1 (ppm)


Cl
O
O
S
N
H
Cl
I

17

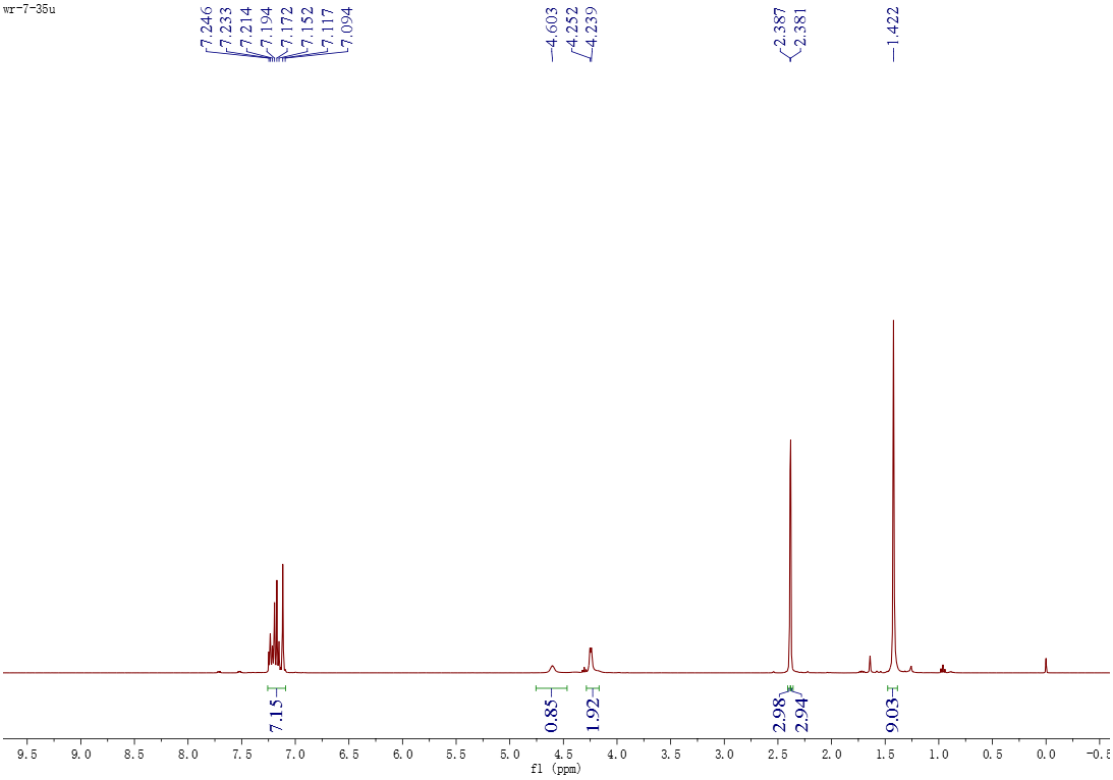

wr-7-41f11
7.783
7.778
7.503
7.416
7.411
4.826
4.812
4.790
4.777
4.751
4.739
4.715
4.703
2.495
1.606
1.301
0.92
0.92
0.92
2.03
3.00
2.98
3.07
f1 (ppm)


wr-7-41f11
170.190
138.173
136.250
135.074
134.849
130.068
101.140
77.478
77.160
76.842
59.373
46.523
33.173
22.934
18.567
f1 (ppm)



S2

wr-7-35u



wr-7-37u