Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting information

Practical Fluorothiolation and Difluorothiolation of Alkenes using Pyridine-HF and N-thiosuccinimides

Shiwen Liu[a, b], Xiaojun Zeng[b, *], Bo Xu[b, *]

[a] College of Textiles and Clothing, Yancheng Institute of Technology, Yancheng, 224051, China.

[b] Key Laboratory of Science and Technology of Eco-Textiles, Ministry of Education, College of Chemistry, Chemical Engineering and Biotechnology, Donghua University, Shanghai 201620, China.

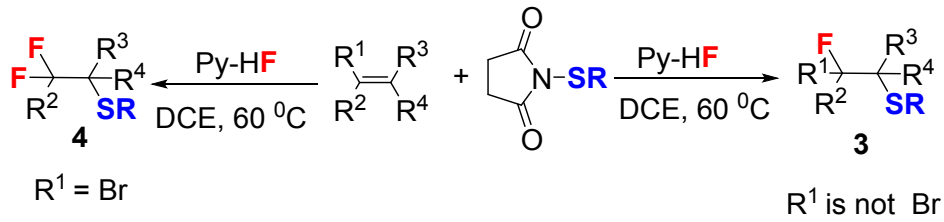
1. General

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

2. General procedure for the preparation of *N*-thiosuccinimides[1]

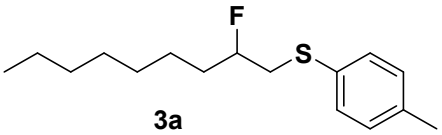
Sulfuryl chloride (1.0 equivalent) was added dropwise to a solution of thiol (1.0 equivalent) and triethylamine (0.1 equivalents) in dichloromethane (1M) at 0 °C. After stirring for 15 minutes, the mixture was warmed to room temperature and stirred for 30 minutes and then cooled to 0 °C. The resulting solution was transferred dropwise via cannula to a solution of succinimide (1.0 equivalent) in dichloromethane (1M) and triethylamine (1.3 equivalents) at 0 °C, and the mixture was then warmed to room temperature over 1 hour. The solution was diluted with water and extracted with an equal volume of dichloromethane before being dried over sodium sulfate. Evaporation of the solvent gave the crude product which could be purified by flash column chromatography.

3. General procedure for preparation of products 3 and 4



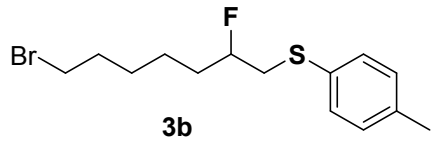
N-thiosuccinimide (0.12 mmol) and alkene (0.1 mmol) were added to a dried polypropylene tube equipped with a magnetic stirring bar. DCE (1 mL) was added and the mixture was stirred for 10 mins. Then, HF-Py (70 wt/wt%, 0.5 mmol) was added into the mixture and stirred for 6-12 h under air at 60 °C. Upon completion, a saturated sodium bicarbonate aqueous solution was added to quench the reaction, and the resulting aqueous mixture was extracted with DCM (3 x 5 mL). The combined organic layers were dried over Na_2SO_4 and concentrated. The crude product was further purified by silica gel column chromatography.

4. Characterization data for compounds 3 and 4



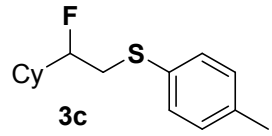
3a

(2-fluorononyl)(p-tolyl)sulfane (3a). Colorless oil (24 mg, 91%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 4.67 – 4.47 (m, 1H), 3.21 – 2.94 (m, 2H), 2.32 (s, 3H), 1.79 – 1.63 (m, 2H), 1.48 – 1.23 (m, 12H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -175.73 – -178.33 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.78, 131.98, 130.74, 129.80, 92.65 (d, *J* = 173.1 Hz), 39.26 (d, *J* = 24.2 Hz), 34.15 (d, *J* = 20.2 Hz), 31.85, 29.41, 29.35, 29.20, 24.85 (d, *J* = 3.9 Hz), 22.65, 21.01, 14.09. HRMS (EI) Calculated for $C_{16}H_{25}FS$ (M^+) 268.1661, found 268.1663.



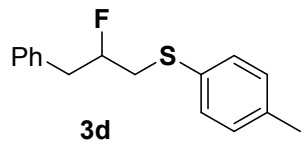
3b

(7-bromo-2-fluoroheptyl)(p-tolyl)sulfane (3b). Colorless oil (26 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 4.66 – 4.47 (m, 1H), 3.39 (t, *J* = 6.8 Hz, 2H), 3.20 – 2.95 (m, 2H), 2.33 (s, 3H), 1.90 – 1.65 (m, 4H), 1.53 – 1.35 (m, 4H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.63 – -177.39 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.91, 131.79, 130.81, 129.85, 92.42 (d, *J* = 173.7 Hz), 39.18 (d, *J* = 23.2 Hz), 33.87 (d, *J* = 22.7 Hz), 33.61, 32.56, 27.87, 24.07 (d, *J* = 3.7 Hz), 21.03. HRMS (EI) Calculated for $C_{14}H_{20}BrFS$ (M^+) 318.0453, found 318.0450.



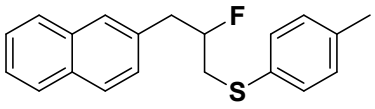
3c

(2-cyclohexyl-2-fluoroethyl)(p-tolyl)sulfane (3c). Colorless oil (18 mg, 72%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.1 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.43 – 4.32 (m, 1H), 3.17 – 3.09 (m, 2H), 2.34 (s, 3H), 1.86 – 1.62 (m, 6H), 1.29 – 1.21 (m, 2H), 1.20 – 1.13 (m, 2H), 1.10 – 1.06 (m, 1H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -184.46 – -184.84 (m). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.68, 132.13, 130.64, 129.79, 96.06 (d, *J* = 173.6 Hz), 41.12 (d, *J* = 19.4 Hz), 37.09 (d, *J* = 24.1 Hz), 28.77 (d, *J* = 4.6 Hz), 26.96 (d, *J* = 5.2 Hz), 26.21, 25.96 , 25.71, 21.05. HRMS (EI) Calculated for $C_{15}H_{21}FS$ (M^+) 252.1348, found 252.1352.



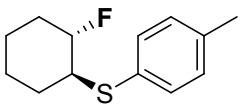
3d

(2-fluoro-3-phenylpropyl)(p-tolyl)sulfane (3d). Colorless oil (21 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.09 (m, 7H), 7.01 (d, *J* = 8.0 Hz, 2H), 4.81 – 4.60 (m, 1H), 3.10 – 2.87 (m, 4H), 2.24 (s, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -174.68 – -176.89 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.92, 136.45 (d, J = 2.1 Hz), 131.63, 130.79, 129.88, 129.53, 128.52, 126.79, 92.67 (d, J = 176.3 Hz), 40.16 (d, J = 21.3 Hz), 38.49 (d, J = 24.3 Hz), 21.03. HRMS (EI) Calculated for $C_{16}H_{17}FS$ (M^+) 260.1035, found 260.1030.



3e

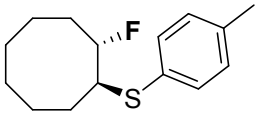
(2-fluoro-3-(naphthalen-2-yl)propyl)(p-tolyl)sulfane (3e). Colorless oil (23 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.88 (m, 1H), 7.82 – 7.74 (m, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.45 – 7.37 (m, 2H), 7.36 – 7.27 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 6.99 (d, *J* = 8.0 Hz, 2H), 4.97 – 4.78 (m, 1H), 3.61–3.49 (m, 1H), 3.38 – 3.30 (m, 1H), 3.21–2.99 (m, 2H), 2.23 (s, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -172.47 – -173.28 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.91, 133.94, 132.74 (d, *J* = 4.1 Hz), 132.06, 131.62, 130.67, 129.87, 128.86, 127.92, 127.69, 126.13, 125.64, 125.47, 123.64, 92.31 (d, *J* = 4.1 Hz), 38.91(d, *J* = 23.1 Hz), 37.37 (d, *J* = 21.1 Hz), 21.02. HRMS (EI) Calculated for $C_{20}H_{19}FS$ (M^+) 310.1191, found 310.1199.



3f

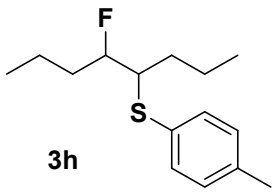
((1S, 2S)-2-fluorocyclohexyl)(p-tolyl)sulfane (3f). Colorless oil (17 mg, 88%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 7.9 Hz, 2H), 4.40 – 4.28 (m, 1H), 3.08–3.03 (m, 1H), 2.30 (s, 3H), 2.15 – 2.01 (m, 2H), 1.73 – 1.60 (m, 2H), 1.43 – 1.23 (m, 4H). ^{19}F NMR (565 MHz,

$CDCl_3$) δ -170.46 – -175.65 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.65, 133.71, 129.99, 129.64, 92.54 (d, *J* = 176.2 Hz), 51.00 (d, *J* = 18.6 Hz), 31.17, 30.87 (d, *J* = 21.2 Hz), 24.23, 22.77 (d, *J* = 8.4 Hz), 21.09. HRMS (EI) Calculated for $C_{13}H_{17}FS$ (M^+) 224.1035, found 224.1041.



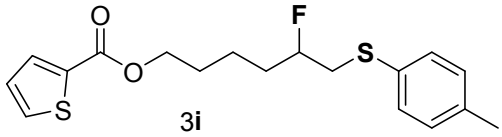
3g

((1S, 2S)-2-fluorocyclooctyl)(p-tolyl)sulfane (3g). Colorless oil (22 mg, 90 %). ^1H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.73 – 4.57 (m, 1H), 3.46 – 3.35 (m, 1H), 2.33 (s, 3H), 2.07 – 1.93 (m, 3H), 1.84 – 1.59 (m, 5H), 1.56 – 1.28 (m, 4H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -158.48 – -159.57 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.35, 133.22, 131.10, 129.65, 96.66 (d, *J* = 171.2 Hz), 53.20 (d, *J* = 21.2 Hz), 31.81 (d, *J* = 23.1 Hz), 28.60 (d, *J* = 6.0 Hz), 26.12, 25.42, 25.27, 24.14 (d, *J* = 6.8 Hz), 21.11. HRMS (EI) Calculated for $C_{15}H_{21}FS$ (M^+) 252.1348, found 252.1355.



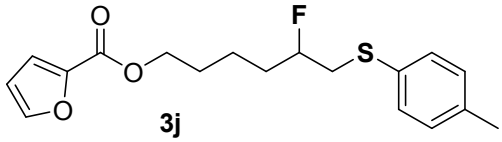
3h

(5-fluorooctan-4-yl)(p-tolyl)sulfane (3h). Colorless oil (21 mg, 84 %). ^1H NMR (600 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 4.53 – 4.42 (m, 1H), 3.07 – 3.00 (m, 1H), 2.33 (s, 3H), 1.78 – 1.65 (m, 4H), 1.52 – 1.35 (m, 4H), 0.94 – 0.89 (m, 6H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -182.21 – -182.67 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.34, 132.96, 131.31, 129.70, 95.31 (d, *J* = 175.1 Hz), 53.59 (d, *J* = 20.1 Hz), 34.50 (d, *J* = 21.2 Hz), 32.25 (d, *J* = 5.1 Hz), 21.08, 20.23, 18.61 (d, *J* = 3.7 Hz), 13.92, 13.83. HRMS (EI) Calculated for $C_{15}H_{23}FS$ (M^+) 254.1504, found 254.1500.



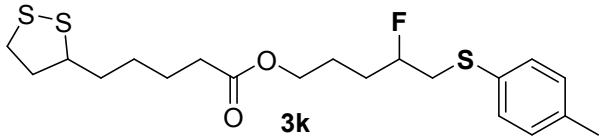
3i

5-fluoro-6-(p-tolylthio)hexyl thiophene-2-carboxylate (3i). Colorless oil (34 mg, 97 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.82 (m, 1H), 7.58 –7.57 (m, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.14 –7.12 (m, 3H), 4.72 – 4.53 (m, 1H), 4.31 (t, *J* = 6.5 Hz, 2H), 3.24 –2.99 (m, 2H), 2.35 (s, 3H), 1.92 – 1.73 (m, 4H), 1.63 – 1.49 (m, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.91 – -177.43 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.26, 136.92, 133.94, 133.34, 132.27, 131.75, 130.81, 129.86, 127.73, 93.24 (d, *J* = 172.8 Hz), 64.81, 39.15 (d, *J* = 23.2 Hz), 33.67 (d, *J* = 20.1 Hz), 28.44, 21.53 (d, *J* = 3.8 Hz), 21.02. HRMS (EI) Calculated for $C_{18}H_{21}FO_2S_2$ (M^+) 352.0967, found 352.0966.



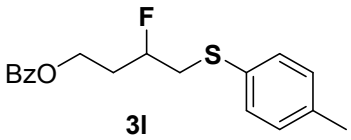
3j

5-fluoro-6-(p-tolylthio)hexyl furan-2-carboxylate (3j). Colorless oil (31 mg, 92 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.53 (m, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.16 (m, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.53 – 6.47 (m, 1H), 4.68 – 4.48 (m, 1H), 4.29 (t, *J* = 6.5 Hz, 2H), 3.20 – 2.96 (m, 2H), 2.32 (s, 3H), 1.85 – 1.69 (m, 4H), 1.67 – 1.59 (m, 1H), 1.54 – 1.45 (m, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.92 – -177.49 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.76, 146.25, 144.78, 136.93, 131.73, 130.80, 129.85, 117.83, 111.80, 92.36 (d, *J* = 172.2 Hz), 64.62, 39.15 (d, *J* = 23.7 Hz), 33.66 (d, *J* = 20.1 Hz), 28.43, 21.48 (d, *J* = 3.7 Hz), 21.02. HRMS (EI) Calculated for $C_{18}H_{21}FO_3S$ (M^+) 336.1195, found 336.1191.



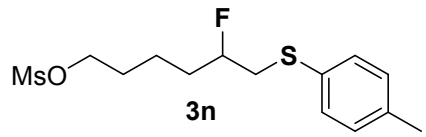
3k

4-fluoro-5-(p-tolylthio)pentyl 5-(1,2-dithiolan-3-yl)pentanoate (3k). Colorless oil (22 mg, 53 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.66 –4.51 (m, 1H), 4.14 – 4.02 (m, 2H), 3.60 – 3.53 (m, 1H), 3.26 – 2.92 (m, 4H), 2.50 – 2.44 (m, 1H), 2.38 – 2.25 (m, 5H), 1.95 – 1.86 (m, 1H), 1.86 – 1.59 (m, 8H), 1.53 –1.41 (m, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.49 – -179.92 (m). ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.47, 137.01, 131.59, 130.84, 129.89, 92.11 (d, *J* = 173.5 Hz), 63.82, 56.35, 40.24, 39.13 (d, *J* = 22.6 Hz), 38.50, 34.62, 34.05, 30.68 (d, *J* = 21.1 Hz), 28.78, 24.70, 24.30 (d, *J* = 3.5 Hz), 21.05. HRMS (EI) Calculated for $C_{20}H_{29}FO_2S_3$ (M^+) 416.1314, found 416.1311.



3l

3-fluoro-4-(p-tolylthio)butyl benzoate (3l). Colorless oil (21 mg, 68 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.5 Hz, 2H), 7.57 – 7.53 (m, 1H), 7.43 – 7.39 (m, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 4.87 – 4.67 (m, 1H), 4.52 – 4.36 (m, 2H), 3.27 – 3.18 (m, 2H), 2.32 – 2.03 (m, 5H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -178.99 – -179.81 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.37, 137.18, 133.02, 131.24, 131.18, 130.08, 129.90, 129.60, 128.37, 89.46 (d, *J* = 173.4 Hz), 60.76 (d, *J* = 4.4 Hz), 39.17 (d, *J* = 23.4 Hz), 33.28 (d, *J* = 21.4 Hz), 21.03. HRMS (EI) Calculated for $C_{18}H_{19}FO_2S$ (M^+) 318.1090, found 318.1095.

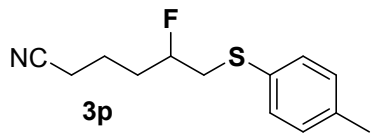


3n

5-fluoro-6-(p-tolylthio)hexyl methanesulfonate (3n). Colorless oil (24 mg, 76 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.65 – 4.59 (m, 1H), 4.21 (t, *J* = 6.4 Hz, 2H), 3.22 – 2.93 (m, 5H), 2.32 (s, 3H), 1.87 – 1.67 (m, 4H), 1.61 – 1.43 (m, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.81 – -177.59 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.01, 131.61, 130.83, 129.90, 92.24 (d, *J* = 172.4 Hz), 69.58, 39.19 (d, *J* = 24.4 Hz), 37.40, 33.35 (d, *J* = 21.1 Hz), 28.85, 21.08, 21.04 (d, *J* = 3.0 Hz). HRMS (EI) Calculated for $C_{14}H_{21}FO_3S_2$ (M^+) 320.0916, found 320.0921.

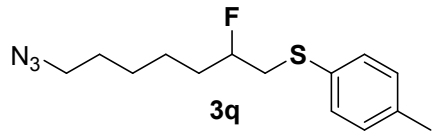
3o

4-fluoro-5-(p-tolylthio)pentyl-4-methylbenzenesulfonate (3o). Colorless oil (23 mg, 61 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.59 – 4.41 (m, 1H), 4.14 – 3.96 (m, 2H), 3.16 – 2.89 (m, 2H), 2.45 (s, 3H), 2.32 (s, 3H), 1.87 – 1.63 (m, 4H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -177.80 – -178.32 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.82, 137.08, 133.11, 131.49, 130.89, 129.91, 129.88, 127.89, 91.85 (d, *J* = 172.5 Hz), 69.88, 39.80 (d, *J* = 23.5 Hz), 30.10 (d, *J* = 21.1 Hz), 24.64 (d, *J* = 3.5 Hz), 21.63, 21.02. HRMS (ESI) Calculated for $C_{19}H_{23}FO_3S_2Na$ (M+Na) 405.0970, found 405.0961.



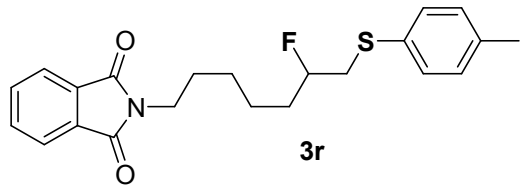
3p

5-fluoro-6-(p-tolylthio)hexanenitrile (3p). Colorless oil (19 mg, 80 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 4.65 – 4.46 (m, 1H), 3.23 – 2.91 (m, 2H), 2.36 (t, *J* = 6.4 Hz, 2H), 2.31 (s, 3H), 1.97 – 1.69 (m, 4H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -177.38 – -177.97 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.24, 131.28, 131.02, 129.96, 119.16, 91.77 (d, *J* = 173.3 Hz), 39.00 (d, *J* = 24.3 Hz), 32.78 (d, *J* = 20.1 Hz), 21.28 (d, *J* = 3.3 Hz), 21.04, 16.99. HRMS (EI) Calculated for $C_{13}H_{16}FNS$ (M^+) 237.0987, found 237.0982.



3q

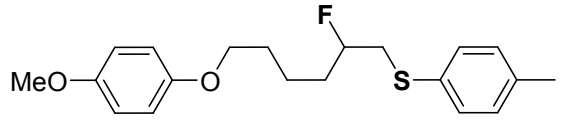
(7-azido-2-fluoroheptyl)(p-tolyl)sulfane (3q). Colorless oil (21 mg, 75 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.66 – 4.47 (m, 1H), 3.25 (t, *J* = 6.9 Hz, 2H), 3.20 – 2.94 (m, 2H), 2.32 (s, 3H), 1.82 – 1.57 (m, 4H), 1.52 – 1.36 (m, 4H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.63 – -177.46 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.91, 131.80, 130.80, 129.85, 92.47 (d, *J* = 172.3 Hz), 51.32, 39.17 (d, *J* = 24.1 Hz), 33.89 (d, *J* = 21.1 Hz), 28.69, 26.46, 24.45 (d, *J* = 3.7 Hz), 21.01. HRMS (EI) Calculated for $C_{14}H_{20}FN_3S$ (M^+) 281.1362, found 281.1367.



3r

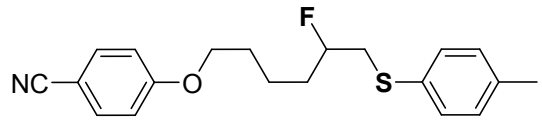
2-(6-fluoro-7-(p-tolylthio)heptyl)isoindoline-1,3-dione (3r). Colorless oil (26 mg, 69 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.76 (m, 2H), 7.76 – 7.56 (m, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 4.64 – 4.44 (m, 1H), 3.67 (t, *J* = 7.2 Hz, 2H), 3.17 – 2.94 (m, 2H), 2.31 (s, 3H), 1.75–1.62 (m, 4H), 1.56 – 1.30 (m, 4H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -175.52 – -177.29 (m). ^{13}C NMR

(101 MHz, $CDCl_3$) δ 168.43, 136.84, 133.88, 132.18, 131.83, 130.81, 129.82, 123.19, 93.30 (d, *J* = 172.1 Hz), 91.58, 39.19 (d, *J* = 24.1 Hz), 37.86, 33.93 (d, *J* = 20.1 Hz), 28.44, 26.60, 24.46 (d, *J* = 3.8 Hz), 21.02. HRMS (EI) Calculated for $C_{22}H_{24}FNO_2S$ (M^+) 385.1512, found 385.1516.



3s

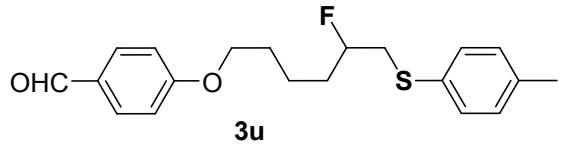
(2-fluoro-6-(4-methoxyphenoxy)hexyl)(p-tolyl)sulfane (3s). Colorless oil (33 mg, 96 %). ^1H NMR (400 MHz, $CDCl_3$) δ 7.23 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.77 – 6.75 (m, 4H), 4.61 – 4.43 (m, 1H), 3.82 (t, *J* = 6.3 Hz, 2H), 3.69 (s, 3H), 3.13 – 2.89 (m, 2H), 2.25 (s, 3H), 1.77 – 1.63 (m, 4H), 1.75 –1.66 (m, 1H), 1.59 –1.45 (m, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.66 – -177.53 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.80, 153.18, 136.88, 131.82, 130.79, 129.85, 115.48, 114.68, 92.47 (d, *J* = 172.1 Hz), 68.28, 55.76, 39.20 (d, *J* = 23.1 Hz), 33.85 (d, *J* = 20.0 Hz), 29.10, 21.63 (d, *J* = 3.8 Hz), 21.03. HRMS (EI) Calculated for $C_{20}H_{25}FO_2S$ (M^+) 348.1559, found 348.1556.



3t

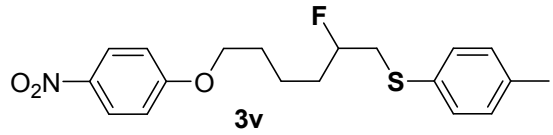
4-((5-fluoro-6-(p-tolylthio)hexyl)oxy)benzonitrile (3t). Colorless oil (32 mg, 95 %). ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.7 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.91 (d, *J* = 8.7 Hz, 2H), 4.69 – 4.50 (m, 1H), 3.99 (t, *J* = 6.3 Hz, 2H), 3.22 – 3.13 (m, 2H), 2.32 (s, 3H), 1.91 – 1.72 (m, 4H), 1.71 – 1.62 (m, 1H), 1.57 – 1.52 (m, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.62 – -177.53 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.30, 136.95, 133.98, 131.73, 130.76, 129.87, 119.25, 115.19, 103.86, 92.38 (d, *J* = 172.1 Hz), 68.01, 39.12 (d, *J* = 23.0 Hz), 33.69 (d, *J* = 20.0 Hz), 28.71,

21.55 (d, J = 3.7 Hz), 21.03. HRMS (EI) Calculated for $C_{20}H_{22}FNOS$ (M^+) 343.1406, found 343.1410.



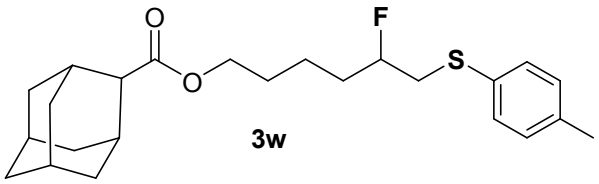
3u

4-((5-fluoro-6-(p-tolylthio)hexyl)oxy)benzaldehyde (3u). Colorless oil (31 mg, 90 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 7.82 (d, J = 8.6 Hz, 2H), 7.30 (d, J = 8.1 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 6.97 (d, J = 8.6 Hz, 2H), 4.70 – 4.50 (m, 1H), 4.03 (t, J = 6.3 Hz, 2H), 3.25 – 2.95 (m, 2H), 2.32 (s, 3H), 1.90 – 1.72 (m, 4H), 1.71 – 1.64 (m, 1H), 1.61 – 1.51 (m, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.60 – -177.54 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.78, 164.09, 136.94, 132.00, 131.74, 130.77, 129.91, 129.87, 114.76, 92.80 (d, J = 172.1 Hz), 68.01, 39.14 (d, J = 23.0 Hz), 33.73 (d, J = 3.7 Hz), 28.78, 21.57 (d, J = 3.7 Hz), 21.03. HRMS (EI) Calculated for $C_{20}H_{23}FO_2S$ (M^+) 346.1403, found 346.1400.



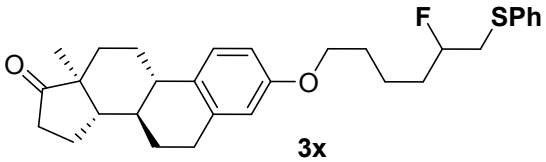
3v

(2-fluoro-6-(4-nitrophenoxy)hexyl)(p-tolyl)sulfane (3v). Colorless oil (31 mg, 87 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 9.1 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 6.92 (d, J = 9.2 Hz, 2H), 4.70 – 4.51 (m, 1H), 4.04 (t, J = 6.3 Hz, 2H), 3.25 – 2.96 (m, 2H), 2.32 (s, 3H), 1.91 – 1.58 (m, 6H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.62 – -178.97 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.06, 141.46, 136.97, 131.71, 130.76, 129.87, 125.92, 114.41, 92.37 (d, J = 172.1 Hz), 68.48, 39.11 (d, J = 23.7 Hz), 33.67 (d, J =20.1 Hz), 28.70, 21.53 (d, J = 3.7 Hz), 21.03. HRMS (EI) Calculated for $C_{19}H_{22}FNO_3S$ (M^+) 363.1304, found 363.1310.



3w

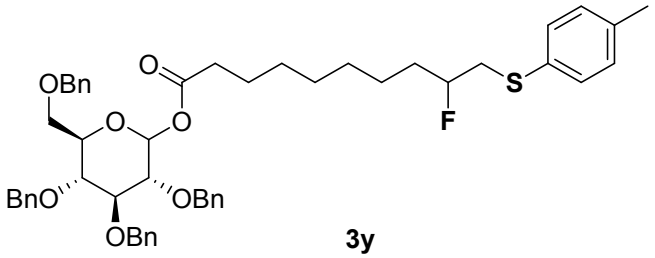
5-fluoro-6-(p-tolylthio)hexyl-adamantane-2-carboxylate (3w). Colorless oil (31 mg, 84 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.67 – 4.45 (m, 1H), 4.04 (t, *J* = 6.4 Hz, 2H), 3.20 – 2.95 (m, 2H), 2.32 (s, 3H), 2.06 (s, 2H), 1.96 (s, 3H), 1.74 – 1.60 (m, 14H), 1.57 – 1.38 (m, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.72 – -177.55 (m). ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.89, 136.89, 131.75, 130.77, 129.86, 92.35 (d, *J* = 174.2 Hz), 63.62, 49.02, 42.43, 39.13 (d, *J* = 24.7 Hz), 36.76, 33.67 (d, *J* = 21.1 Hz), 32.76, 28.63, 28.44, 21.56 (d, *J* = 3.7 Hz), 21.04. HRMS (EI) Calculated for $C_{24}H_{33}FO_2S$ (M^+) 404.2185, found 404.2187.



3x

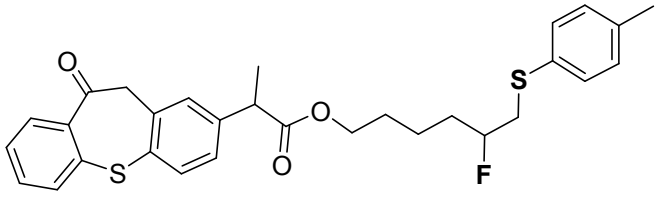
(8R, 9S, 13S, 14S)-3-((5-fluoro-6-(phenylthio)hexyl)oxy)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[a]phenanthren-17-one (3x). Colorless oil (33 mg, 70 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.23 – 7.18 (m, 2H), 6.70 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.64 –6.63 (m, 1H), 4.75 – 4.49 (m, 1H), 3.93 (t, *J* = 6.2 Hz, 2H), 3.26–3.03 (m, 2H), 2.91–2.87 (m, 2H), 2.54 –2.47 (m, 1H), 2.44 – 2.34 (m, 1H), 2.27 – 2.22 (m, 1H), 2.20 – 1.92 (m, 4H), 1.90 – 1.73 (m, 4H), 1.68 – 1.57 (m, 4H), 1.56 – 1.43 (m, 4H), 0.91 (s, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.37 – -177.40 (m). ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.02, 137.75, 135.63, 132.01, 129.90, 129.08, 126.60, 126.34, 114.57, 112.12, 92.41 (d, *J* = 171.1 Hz), 67.49, 50.43, 48.04, 44.00, 38.56, 38.40, 35.90, 33.95 (d, *J* = 19.6 Hz), 31.61, 29.68, 29.04, 26.58, 25.95, 21.65 (d, *J* =

21.1 Hz), 21.61, 13.88. HRMS (EI) Calculated for $C_{30}H_{37}FO_2SNa$ (M+Na) 503.2391, found 503.2388.



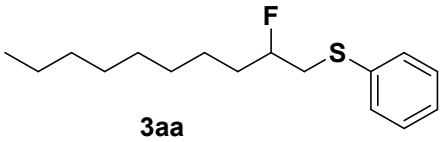
3y

(3R, 4S, 5R, 6R)-3,4,5-tris(benzyloxy)-6-((benzyloxy)methyl)tetrahydro-2H-pyran-2-yl 9-fluoro-10-(p-tolylthio)decanoate (3y). Colorless oil (50 mg, 61 %). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.31 – 7.23 (m, 20H), 7.10 (dd, *J* = 7.3, 2.0 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.37 – 6.36 (m, 1H), 4.92 – 4.91 (m, 1H), 4.84 – 4.76 (m, 2H), 4.70 – 4.63 (m, 1H), 4.60 – 4.56 (m, 2H), 4.48 – 4.43 (m, 2H), 3.90 – 3.87 (m, 1H), 3.85 – 3.78 (m, 1H), 3.72 – 3.68 (m, 2H), 3.67 – 3.65 (m, 1H), 3.61 – 3.59 (m, 1H), 3.12 – 2.69 (m, 2H), 2.35– 2.28 (m, 2H), 2.28 (s, 3H), 1.67 – 1.57 (m, 4H), 1.43 – 1.18 (m, 9H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -176.37 – -177.71 (m). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.2, 138.6, 138.04, 137.84, 137.67, 136.79, 131.92, 130.71, 129.83, 128.45,128.43, 128.11, 128.04, 127.97, 127.93, 127.89, 127.85, 127.77, 127.71, 127.68, 92.56(d, *J* = 172.1 Hz), 89.78, 81.72, 78.99, 76.96, 75.69, 75.34, 73.56, 73.13, 72.88, 68.14, 39.22 (d, *J* = 22.6 Hz), 34.36, 34.10 (d, *J* = 21.1 Hz), 29.17, 29.11, 28.90, 24.86, 24.83 (d, *J* = 4.5 Hz), 21.04. HRMS (ESI) Calculated for $C_{51}H_{59}FO_7SNa$ (M+Na) 857.3858, found 857.3853.



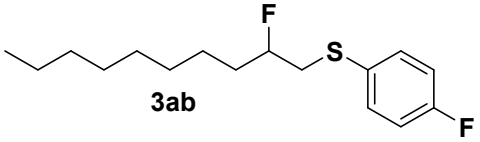
3z

5-fluoro-6-(p-tolylthio)hexyl 2-(10-oxo-10,11-dihydrodibenzo *[b, f]* thiepin-2-yl)propanoate (3z). Colorless oil (47 mg, 90 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 – 8.10 (m, 1H), 7.52 – 7.49 (m, 2H), 7.36 – 7.30 (m, 2H), 7.25 – 7.18 (m, 3H), 7.10 – 6.99 (m, 3H), 4.52 – 4.32 (m, 1H), 4.26 (s, 2H), 3.96 (t, *J* = 6.5 Hz, 2H), 3.62 (q, *J* = 7.2 Hz, 1H), 3.06 – 2.80 (m, 2H), 2.23 (s, 3H), 1.58 – 1.46 (m, 4H), 1.39 (d, *J* = 7.2 Hz, 3H), 1.33 – 1.19 (m, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.97 – -177.48 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.30, 173.89, 142.78, 140.24, 137.94, 136.86, 136.18, 133.23, 132.51, 131.81, 131.53, 131.47, 130.85, 130.73, 129.85, 128.64, 126.84, 126.34, 92.27 (d, *J* = 172.1 Hz), 64.63, 51.05, 45.23, 39.05 (d, *J* = 23.7 Hz), 33.54 (d, *J* = 21.0 Hz), 28.22, 21.32 (d, *J* = 3.7 Hz), 21.02, 18.38.HRMS (ESI) Calculated for $C_{30}H_{31}FO_3S_2Na$ (M+Na) 545.1591, found 545.1588.



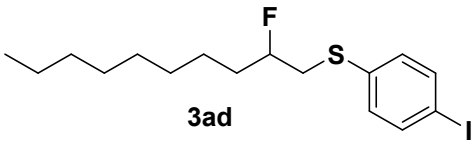
3aa

(2-fluorodecyl)(phenyl)sulfane (3aa). Colorless oil (23 mg, 86 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.5 Hz, 2H), 7.31 – 7.26 (m, 2H), 7.22 – 7.19 (m, 1H), 4.69 – 4.51 (m, 1H), 3.24 –3.01 (m, 2H), 1.81 – 1.62 (m, 2H), 1.49 – 1.25 (m, 12H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.37 – -177.24 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.79, 129.88, 129.02, 126.51, 92.59 (d, *J* = 172.1 Hz), 38.57 (d, *J* = 24.1 Hz), 34.20 (d, *J* = 21.1 Hz), 31.83, 29.40, 29.34, 29.18, 24.84 (d, *J* = 4.1 Hz), 22.65, 14.08. HRMS (EI) Calculated for $C_{16}H_{25}FS$ (M^+) 268.1661, found 268.1667.



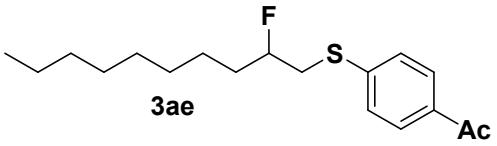
3ab

2-fluorodecyl-4-fluorophenyl sulfane (3ab). Colorless oil (23 mg, 80 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.31 (m, 2H), 7.02 – 6.98 (m, 2H), 4.65 – 4.47 (m, 1H), 3.16 – 2.96 (m, 2H), 1.76 – 1.60 (m, 2H), 1.48 – 1.25 (m, 12H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -114.79 – -114.89 (m), -176.09 – -178.74 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.09 (d, *J* = 246.2 Hz), 133.06 (d, *J* = 8.9 Hz), 130.67 (d, *J* = 3.6 Hz), 116.25 (d, *J* = 22.1 Hz), 93.44 (d, *J* = 172.1 Hz), 39.91 (d, *J* = 24.1 Hz), 34.15 (d, *J* = 21.0 Hz), 31.83, 29.40, 29.33, 29.18, 24.84 (d, *J* = 4.2 Hz), 22.64, 14.08. HRMS (EI) Calculated for $C_{16}H_{24}F_2S$ (M^+) 286.1567, found 286.1563.



3ad

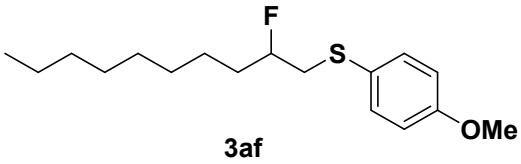
(2-fluorodecyl)(4-iodophenyl)sulfane (3ad). Colorless oil (30 mg, 77 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.2 Hz, 2H), 7.12 – 7.10 (m, 2H), 4.67 – 4.49 (m, 1H), 3.20 –3.00 (m, 2H), 1.77 – 1.60 (m, 2H), 1.49 – 1.25 (m, 12H), 0.88 (t, *J* = 6.7 Hz, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.70 – -177.06 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.97, 136.03, 131.36, 91.46 (d, *J* = 172.1 Hz), 91.31, 38.46 (d, *J* = 24.0 Hz), 34.22 (d, *J* = 20.0 Hz), 31.84, 29.40, 29.33, 29.18, 24.85 (d, *J* = 4.0 Hz), 22.65, 14.09. HRMS (EI) Calculated for $C_{16}H_{24}FIS$ (M^+) 394.0627, found 394.0621.



3ae

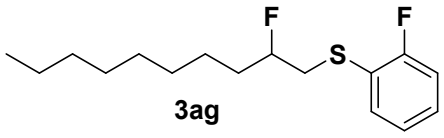
1-(4-((2-fluorodecyl)thio)phenyl)ethan-1-one (3ae). Colorless oil (16 mg, 53 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.6 Hz, 2H), 7.36 (d, *J* = 8.6 Hz, 2H), 4.75 – 4.56 (m, 1H), 3.31 – 3.11 (m, 2H), 2.57 (s, 3H), 1.81 – 1.63 (m, 2H), 1.39 – 1.19 (m, 12H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.38 – -177.19 (m). ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.14, 143.38, 134.41,

128.87, 127.11, 92.34 (d, J = 175.1 Hz), 36.93 (s), 36.85 (d, J = 24.1 Hz), 34.41 (d, J = 21.0 Hz), 31.83, 29.40, 29.33, 29.19, 26.47, 24.88 (d, J = 4.0 Hz), 22.65, 14.10.HRMS (EI) Calculated for $C_{18}H_{27}FOS$ (M^+) 310.1767, found 310.1763.



3af

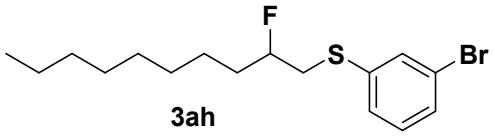
(2-fluorodecyl)(4-methoxyphenyl)sulfane (3af). Colorless oil (25 mg, 83 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, J = 8.5 Hz, 2H), 6.85 (d, J = 8.6 Hz, 2H), 4.63 – 4.44 (m, 1H), 3.80 (s, 3H), 3.17 – 2.86 (m, 2H), 1.78 – 1.60 (m, 2H), 1.48 – 1.24 (m, 12H), 0.88 (t, J = 6.7 Hz, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.92 – -177.75 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.27, 133.77, 125.88, 114.69, 92.67 (d, J = 172.1 Hz), 55.34, 40.55 (d, J = 21.1 Hz), 34.10 (d, J = 20.0 Hz), 31.84, 29.41, 29.36, 29.19, 24.84 (d, J = 3.8 Hz), 22.65, 14.08. HRMS (EI) Calculated for $C_{17}H_{27}FOS$ (M^+) 298.1767, found 298.1763.



3ag

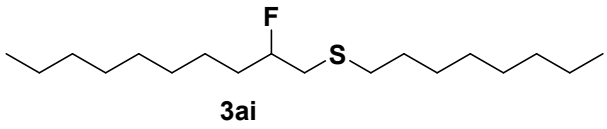
(2-fluorodecyl)(2-fluorophenyl)sulfane (3ag). Colorless oil (23 mg, 82 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.39 (m, 1H), 7.28 – 7.19 (m, 1H), 7.12 – 7.01 (m, 2H), 4.66 – 4.47 (m, 1H), 3.19 – 2.98 (m, 2H), 1.75 – 1.62 (m, 2H), 1.49 – 1.23 (m, 12H), 0.86 (t, J = 6.8 Hz, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -108.57 – -108.89 (m), -176.71 – -177.74 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.35 (d, J = 244.1 Hz) 133.12, 129.08 (d, J = 8.1 Hz), 124.52 (d, J = 4.1 Hz), 122.41 (d, J = 18.2 Hz) 115.97 (d, J = 23.1 Hz), 92.73 (d, J =171.1 Hz), 38.13 (d, J = 24.1 Hz), 34.15 (d, J = 21.1 Hz),

31.83, 29.39, 29.32, 29.18, 24.81 (d, J = 4.2 Hz), 22.64, 14.08. HRMS (EI) Calculated for $C_{16}H_{24}F_2S$ (M^+) 286.1567, found 286.1560.



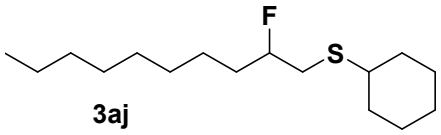
3ah

(3-bromophenyl)(2-fluorodecyl)sulfane (3ah). Colorless oil (23 mg, 71 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.34 – 7.28 (m, 2H), 7.17 – 7.13 (m, 1H), 4.70 – 4.52 (m, 1H), 3.23 – 3.03 (m, 2H), 1.77 – 1.64 (m, 2H), 1.49 – 1.26 (m, 12H), 0.88 (t, J = 6.7 Hz, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.66 – -177.02 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.38, 131.89, 130.27, 129.43, 127.94, 122.86, 92.41 (d, J = 172.1 Hz), 38.34 (d, J = 24.1 Hz), 34.22 (d, J = 21.1 Hz), 31.83, 29.39, 29.33, 29.18, 24.84 (d, J = 4.1 Hz), 22.64, 14.08.HRMS (EI) Calculated for $C_{16}H_{24}BrFS$ (M^+) 346.0766, found 346.0771.



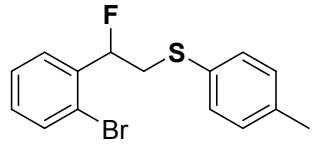
3ai

(2-fluorodecyl)(octyl)sulfane (3ai). Colorless oil (20 mg, 67 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.69 – 4.49 (m, 1H), 2.82 – 2.51 (m, 4H), 1.74 – 1.42 (m, 6H), 1.39 – 1.24 (m, 20H), 0.88 (t, J = 6.7 Hz, 6H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -176.02 – -176.76 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 92.05 (d, J = 170.0 Hz), 36.51 (d, J = 23.0 Hz), 34.29 (d, J = 20.1 Hz), 33.12, 31.85, 31.81, 29.68, 29.68, 29.44, 29.40, 29.21, 29.18, 28.84, 24.95 (d, J = 4.1 Hz), 22.65, 14.08. HRMS (EI) Calculated for $C_{18}H_{37}FS$ (M^+) 304.2600, found 304.2610.



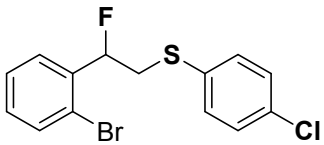
3aj

Cyclohexyl(2-fluorodecyl)sulfane (3aj). Colorless oil (20 mg, 62 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.66 – 4.47 (m, 1H), 2.84 – 2.63 (m, 3H), 2.04 – 1.92 (m, 2H), 1.83 – 1.56 (m, 6H), 1.52 – 1.22 (m, 16H), 0.88 (t, *J* = 6.7 Hz, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -175.67 – -176.04 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 92.12 (d, *J* = 170.2 Hz), 44.21, 34.43 (d, *J* = 24.2 Hz), 34.31 (d, *J* = 20.2 Hz), 33.72, 33.68, 31.85, 29.44, 29.39, 29.21, 26.09, 26.05, 25.80, 24.95 (d, *J* = 4.2 Hz), 22.65, 14.08. HRMS (EI) Calculated for $C_{16}H_{31}FS$ (M^+) 274.2130, found 274.2136.



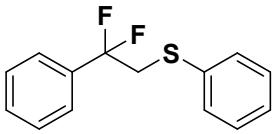
3ak

(2-(2-bromophenyl)-2-fluoroethyl)(p-tolyl)sulfane (3ak). Colorless oil (13 mg, 41 %). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.51 – 7.48 (m, 2H), 7.35 –7.33 (m, 3H), 7.18 – 7.15 (m, 1H), 7.09 (d, *J* = 8.0 Hz, 2H), 5.88 – 5.79 (m, 1H), 3.43 – 3.18 (m, 2H), 2.31 (s, 3H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -180.63 – -180.85 (m). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.10 (d, *J* = 22.6 Hz), 138.03, 137.12, 132.73, 131.57, 131.39, 129.97 (d, *J* = 1.6 Hz), 129.75, 127.76, 127.24 (d, *J* = 9.9 Hz), 120.80 (d, *J* = 6.0 Hz), 92.12 (d, *J* = 176.6 Hz), 40.60 (d, *J* = 25.6 Hz), 21.09. HRMS (EI) Calculated for $C_{15}H_{14}BrFS$ (M^+) 323.9984, found 323.9978.



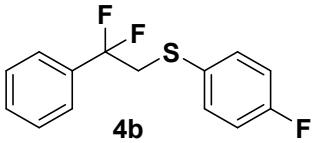
3al

(2-(2-bromophenyl)-2-fluoroethyl)(4-chlorophenyl)sulfane (3al). Colorless oil (14 mg, 42 %). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 – 7.48 (m, 2H), 7.39 – 7.33 (m, 3H), 7.26 – 7.23 (m, 2H), 7.21 – 7.18 (m, 1H), 5.91 – 5.81 (m, 1H), 3.46 –3.23 (m, 2H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -180.68 – -180.84 (m). ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.78 (d, J = 21.1 Hz), 133.73, 132.99, 132.75, 132.19, 130.10 (d, J = 1.0 Hz), 129.08, 127.81, 127.25 (d, J = 10.0 Hz), 120.70 (d, J = 5.8 Hz), 91.45 (d, J = 178.2 Hz), 40.11 (d, J = 25.6 Hz). HRMS (EI) Calculated for $C_{14}H_{11}BrClFS$ (M^+) 343.9437, found 343.9430.



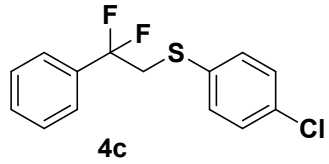
4a

(2, 2-difluoro-2-phenylethyl)(phenyl)sulfane (4a). Colorless oil (14 mg, 51 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.46 (m, 2H), 7.44 – 7.37 (m, 3H), 7.34 – 7.30 (m, 2H), 7.25 – 7.16 (m, 3H), 3.57 (t, J = 14.4 Hz, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -94.53 (t, J = 14.3 Hz). ^{13}C NMR (151 MHz, $CDCl_3$) δ 135.84 (t, J = 25.6 Hz), 135.26, 130.80, 130.11, 128.98, 128.41, 127.06, 125.38 (t, J = 6.1 Hz), 121.15 (t, J = 244. 6Hz), 43.39 (t, J = 31.7 Hz). HRMS (EI) Calculated for $C_{14}H_{12}F_2S$ (M^+) 250.0628, found 250.0633.



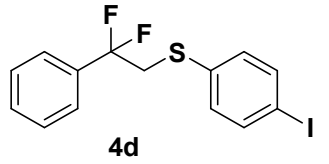
4b

(2, 2-difluoro-2-phenylethyl)(4-fluorophenyl)sulfane (4b). Colorless oil (11 mg, 44 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.44 (m, 2H), 7.43 – 7.39 (m, 3H), 7.34 – 7.29 (m, 2H), 6.93 (t, *J* = 8.7 Hz, 2H), 3.50 (t, *J* = 14.3 Hz, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -94.66 (t, *J* = 14.3 Hz), -113.97 – -114.05 (m). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.35 (d, *J* = 249.1 Hz), 135.76 (t, *J* = 26.3 Hz), 134.06 (t, *J* = 7.5 Hz), 130.17 (d, *J* = 3.1 Hz),130.13 (t, *J* = 26.3 Hz) 128.42, 125.37 (d, *J* = 21.1 Hz), 121.13 (d, *J* = 244.6 Hz), 116.14 (d, *J* = 22.6 Hz), 44.47 (d, *J* = 33.2 Hz). HRMS (EI) Calculated for $C_{14}H_{11}F_3S$ (M^+) 268.0534, found 268.0533.



4c

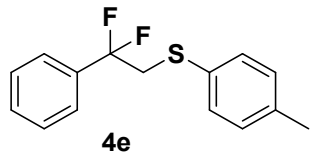
(4-chlorophenyl)(2, 2-difluoro-2-phenylethyl)sulfane (4c). Colorless oil (11 mg, 47 %). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 – 7.44 (m, 2H), 7.42 – 7.38 (m, 3H), 7.24 – 7.22 (m, 2H), 7.21 – 7.18 (m, 2H), 3.51 (t, *J* = 14.3 Hz, 2H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -94.67 (t, *J* = 14.3 Hz). ^{13}C NMR (151 MHz, $CDCl_3$) δ 135.66 (t, *J* = 27.1 Hz), 133.69, 133.31, 132.34, 130.19, 129.10, 128.45, 125.34 (t, *J* = 6.1 Hz), 121.04 (t, *J* = 244.6 Hz), 43.61 (t, *J* = 244.6 Hz). HRMS (EI) Calculated for $C_{14}H_{11}ClF_2S$ (M^+) 284.0238, found 284.0241.



4d

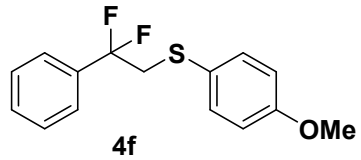
(2, 2-difluoro-2-phenylethyl)(4-iodophenyl)sulfane (4d). Colorless oil (14 mg, 39 %). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 – 7.53 (m, 2H), 7.46 (d, *J* = 7.1 Hz, 2H), 7.44 – 7.38 (m, 3H), 7.05 – 7.02 (m, 2H), 3.53 (t, *J* = 14.2 Hz, 2H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -94.66 (t, *J* = 14.3 Hz). ^{13}C NMR

(151 MHz, $CDCl_3$) δ 137.95, 135.30, 132.38, 130.20, 128.47, 125.32 (t, *J* = 6.3 Hz), 92.30, 43.17 (t, *J* = 31.7 Hz). HRMS (EI) Calculated for $C_{14}H_{11}F_2IS$ (M^+) 375.9594, found 375.9602.



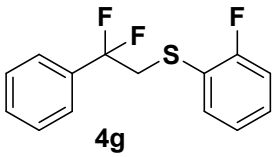
4e

(2, 2-difluoro-2-phenylethyl)(p-tolyl)sulfane (4e). Colorless oil (14 mg, 53 %). ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 2H), 7.45 – 7.37 (m, 3H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 3.52 (t, *J* = 14.5 Hz, 2H), 2.31 (s, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -94.56 (t, *J* = 14.4 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.33, 135.96 (t, *J* = 26.1 Hz), 131.64, 131.55, 130.03, 129.74, 128.37, 125.39 (t, *J* = 6.1 Hz), 123.63, 121.21 (t, *J* = 242.2 Hz), 44.04 (t, *J* = 31.2 Hz), 21.04. HRMS (EI) Calculated for $C_{15}H_{14}F_2S$ (M^+) 264.0784, found 264.0781.



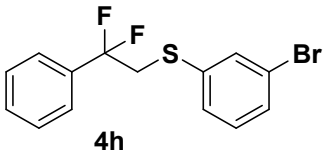
4f

(2, 2-difluoro-2-phenylethyl)(4-methoxyphenyl)sulfane (4f). Colorless oil (11 mg, 41 %). ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.35 (m, 5H), 7.32 – 7.27 (m, 2H), 6.84 – 6.71 (m, 2H), 3.78 (s, 3H), 3.46 (t, *J* = 14.5 Hz, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -94.57 (t, *J* = 14.6 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.52, 136.00 (t, *J* = 26.2 Hz), 134.44, 130.01, 128.35, 125.66, 125.41 (t, *J* = 9.1 Hz), 123.70, 118.85 (t, *J* = 243.1 Hz), 55.34, 45.10 (t, *J* = 31.1 Hz). HRMS (EI) Calculated for $C_{15}H_{14}F_2OS$ (M^+) 280.0733, found 280.0771.



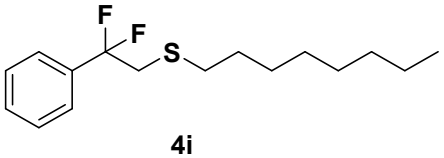
4g

(2, 2-difluoro-2-phenylethyl)(2-fluorophenyl)sulfane (4g). Colorless oil (11 mg, 36 %). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.51 – 7.46 (m, 2H), 7.46 – 7.37 (m, 3H), 7.36 – 7.33 (m, 1H), 7.25 – 7.21 (m, 1H), 7.09 – 7.00 (m, 2H), 3.58 (t, *J* = 14.2 Hz, 2H). ^{19}F NMR (565 MHz, $CDCl_3$) δ -94.73 (t, *J* = 14.9 Hz), -108.04 – -108.80 (m). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.98 (d, *J* = 247.6 Hz), 134.02, 130.10 (t, *J* = 1.7 Hz), 129.68 (d, *J* = 8.2 Hz), 128.36, 125.31 (t, *J* = 6.4 Hz), 124.44 (d, *J* = 4.1 Hz), 121.63, 121.12, 115.76 (d, *J* = 22.6 Hz), 42.10 (d, *J* = 4.0 Hz). HRMS (EI) Calculated for $C_{14}H_{11}F_3S$ (M^+) 268.0534, found 268.0531.



4h

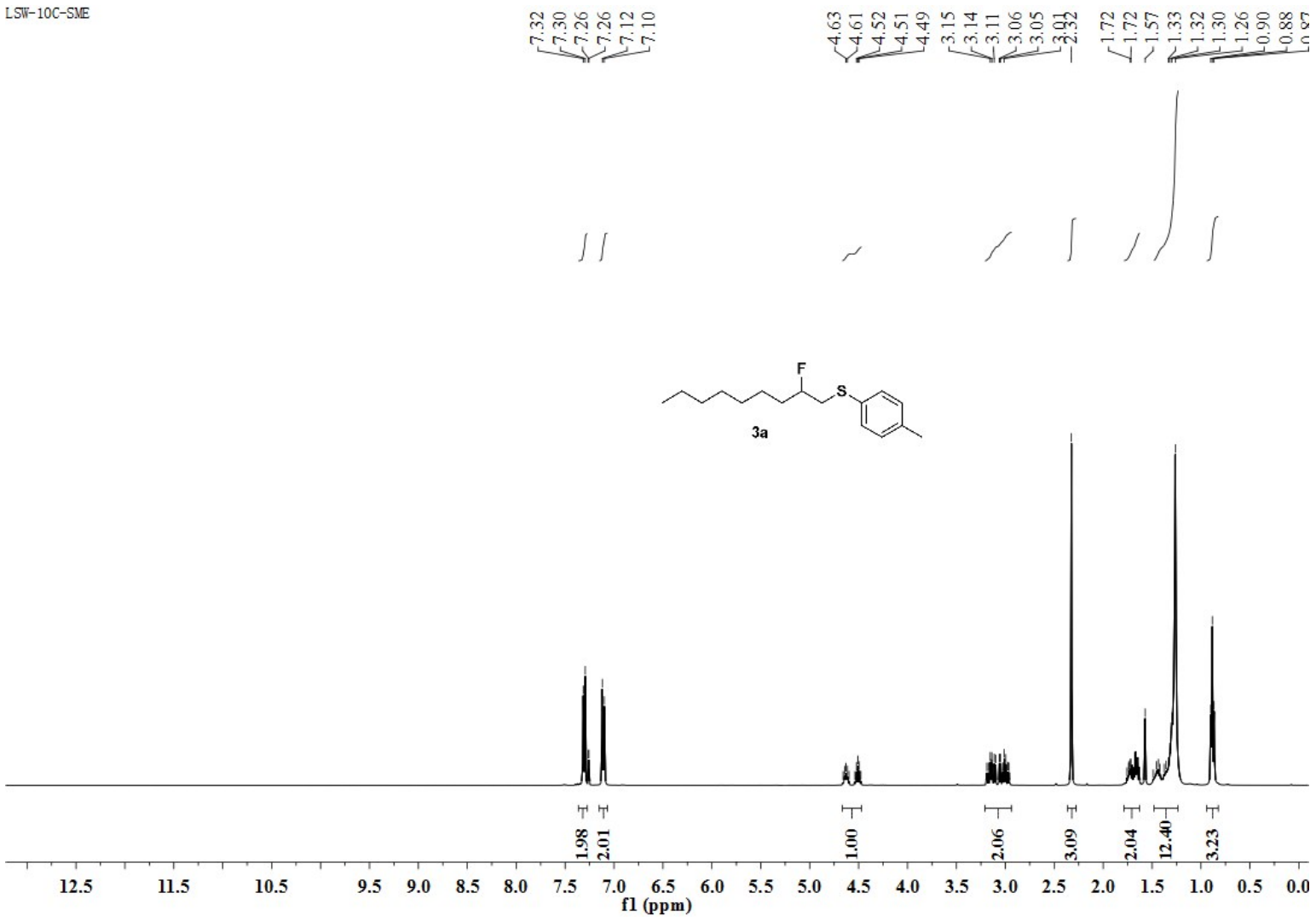
(3-bromophenyl)(2, 2-difluoro-2-phenylethyl)sulfane (4h). Colorless oil (15 mg, 46 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.45 (m, 2H), 7.43 – 7.37 (m, 4H), 7.32 – 7.30 (m, 1H), 7.25 – 7.21 (m, 1H), 7.09 (t, *J* = 7.9 Hz, 1H), 3.56 (t, *J* = 14.1 Hz, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -94.62 (t, *J* = 14.1 Hz). ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.46, 135.51 (t, *J* = 25.6 Hz), 133.03, 130.28, 130.22, 130.07, 129.04, 128.45, 125.35 (t, *J* = 6.1 Hz), 122.65, 120.98 (t, *J* = 246.1 Hz), 43.11 (d, *J* = 31.7 Hz). HRMS (EI) Calculated for $C_{14}H_{11}BrF_2S$ (M^+) 327.9733, found 327.9731.



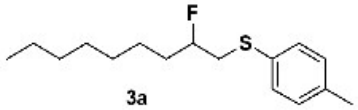
4i

(2, 2-difluoro-2-phenylethyl)(octyl)sulfane (4i). Colorless oil (5 mg, 20 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.48 (m, 2H), 7.44 – 7.43 (m, 3H), 3.15 (t, *J* = 14.6 Hz, 2H), 2.47 (t, *J* = 7.4 Hz, 2H), 1.54 – 1.48 (m, 2H), 1.36 – 1.26 (m, 6H), 1.23 (s, 4H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -94.37 (t, *J* = 14.6 Hz). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.21 (t, *J* = 25.6 Hz), 129.99, 128.36, 125.36 (t, *J* = 6.1 Hz), 121.89 (t, *J* = 243.1 Hz), 40.11 (t, *J* = 31.7 Hz), 33.49, 31.81, 29.29, 29.15, 29.12, 28.70, 22.65, 14.11. HRMS (EI) Calculated for $C_{16}H_{24}F_2S$ (M^+) 286.1567, found 286.1560.

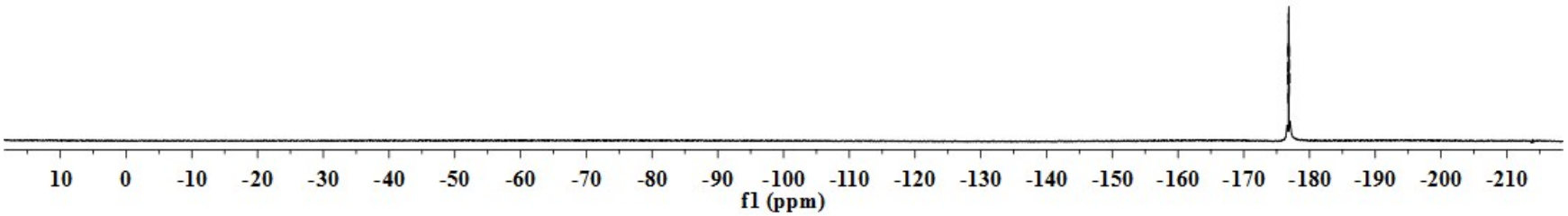
5. Copies of NMR Spectra



LSW-10C-SME



3a



LSW-10C-SME-C

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129.80
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91.79
39.38
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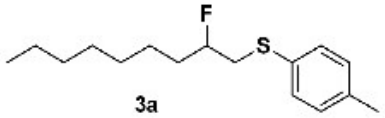
29.20
24.86
24.83
22.65
21.01
14.09



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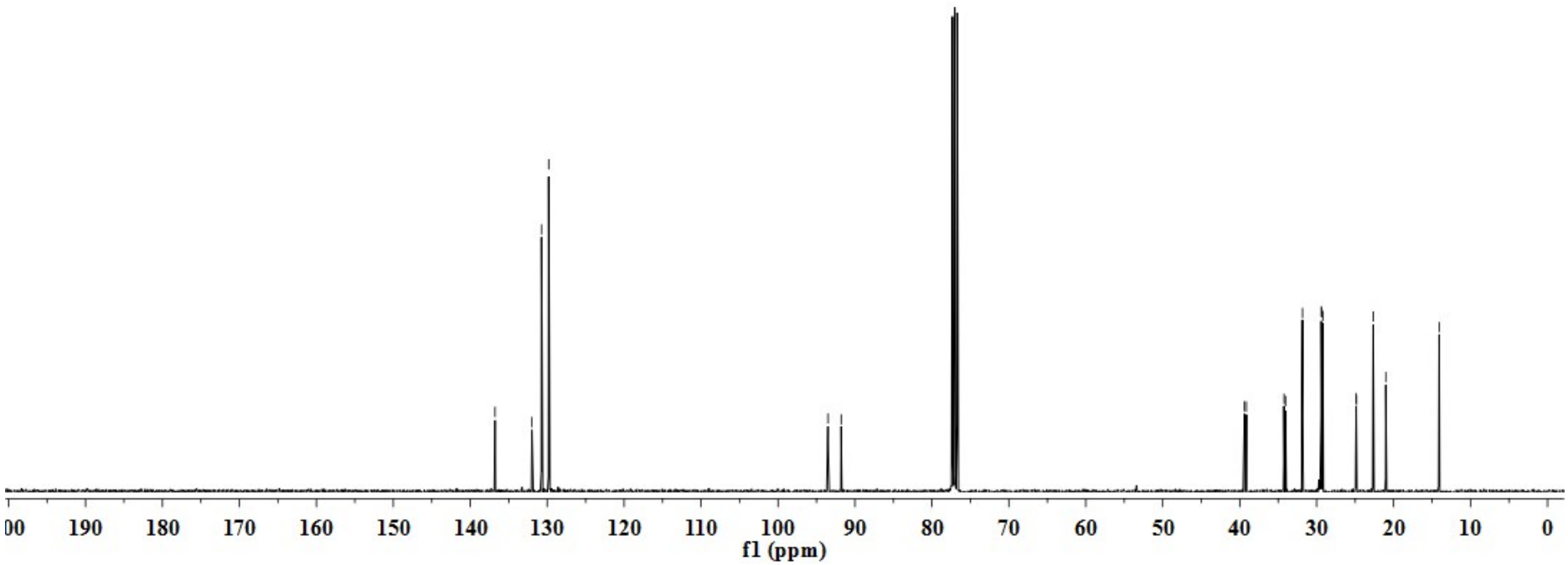
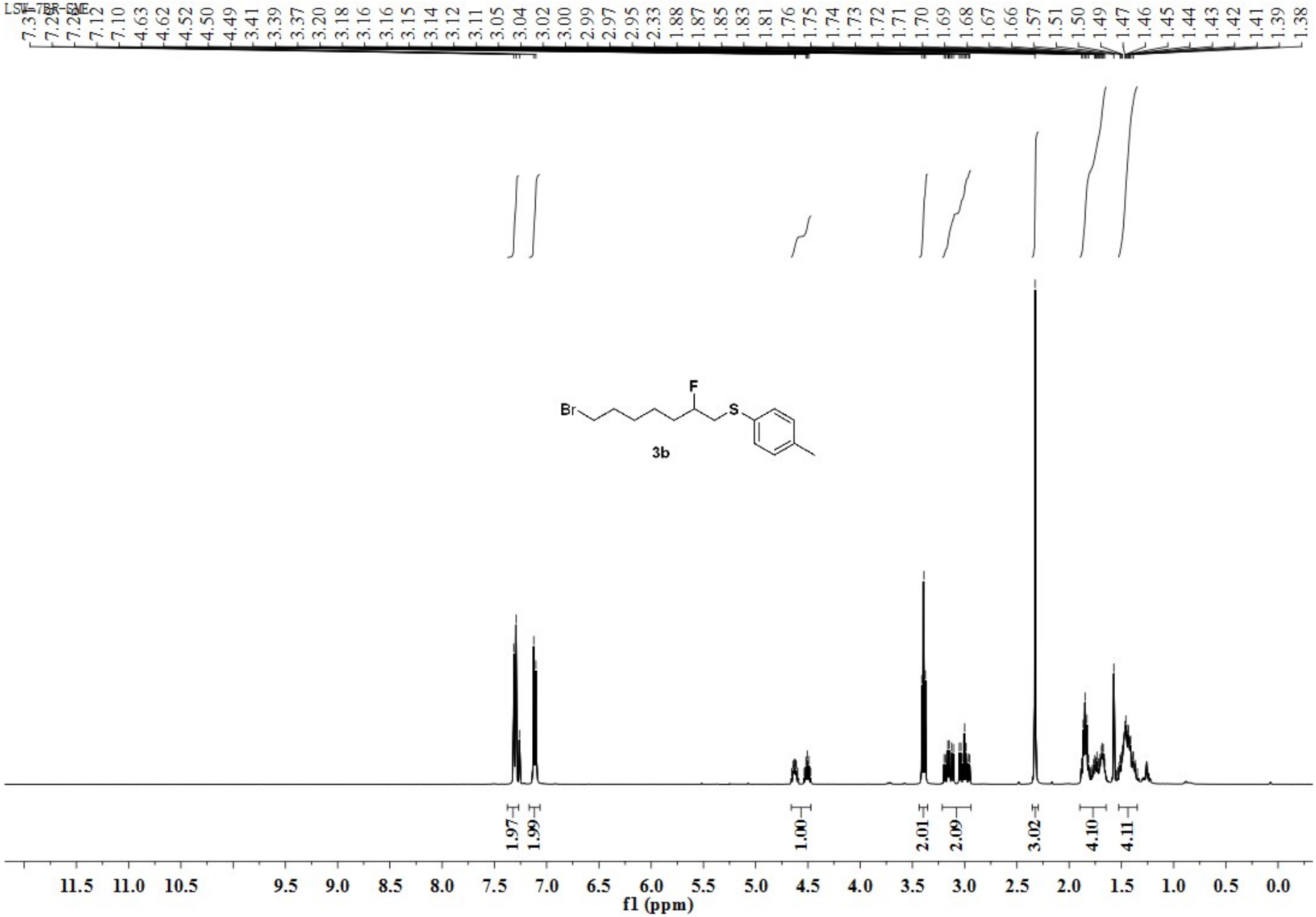
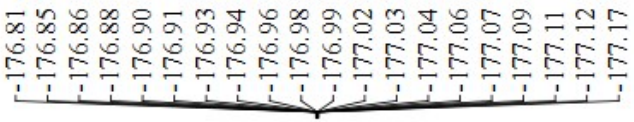
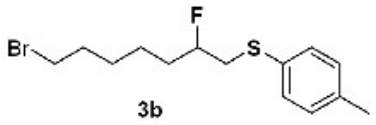


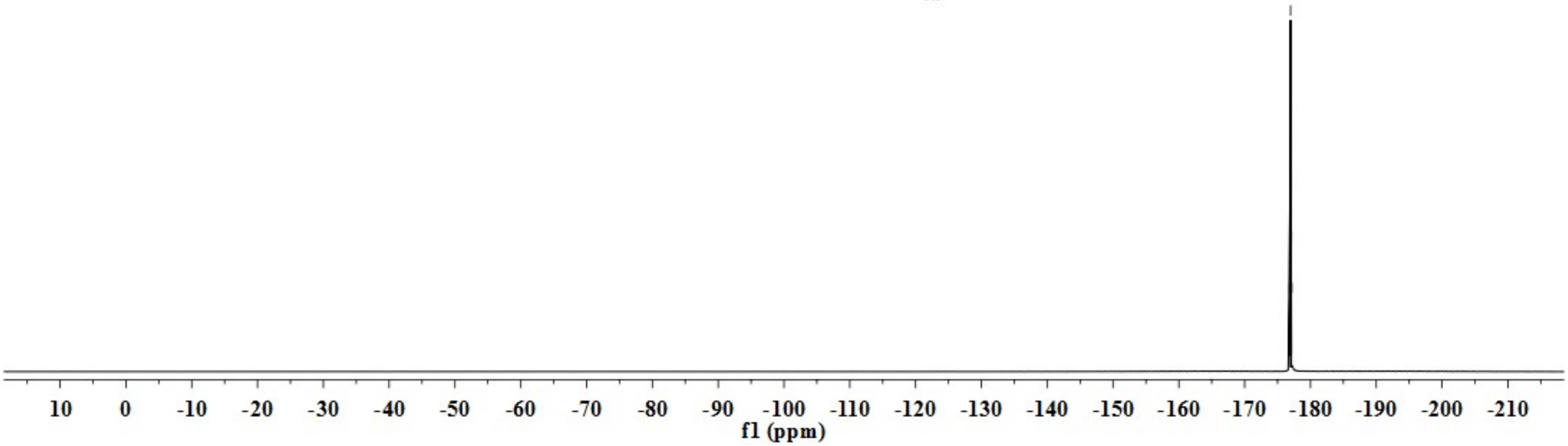

7.31
7.25
7.12
7.10
4.63
4.62
4.52
4.50
4.49
3.41
3.39
3.37
3.20
3.18
3.16
3.16
3.15
3.14
3.12
3.11
3.05
3.04
3.02
3.00
2.99
2.97
2.95
2.33
1.88
1.87
1.85
1.83
1.81
1.76
1.75
1.74
1.73
1.72
1.71
1.70
1.69
1.68
1.67
1.66
1.57
1.51
1.50
1.49
1.47
1.46
1.45
1.44
1.43
1.42
1.41
1.39
1.38
F
Br
S
3b
1.97
1.99
1.00
2.01
2.09
3.02
4.10
4.11
11.5
11.0
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-7BR-SME

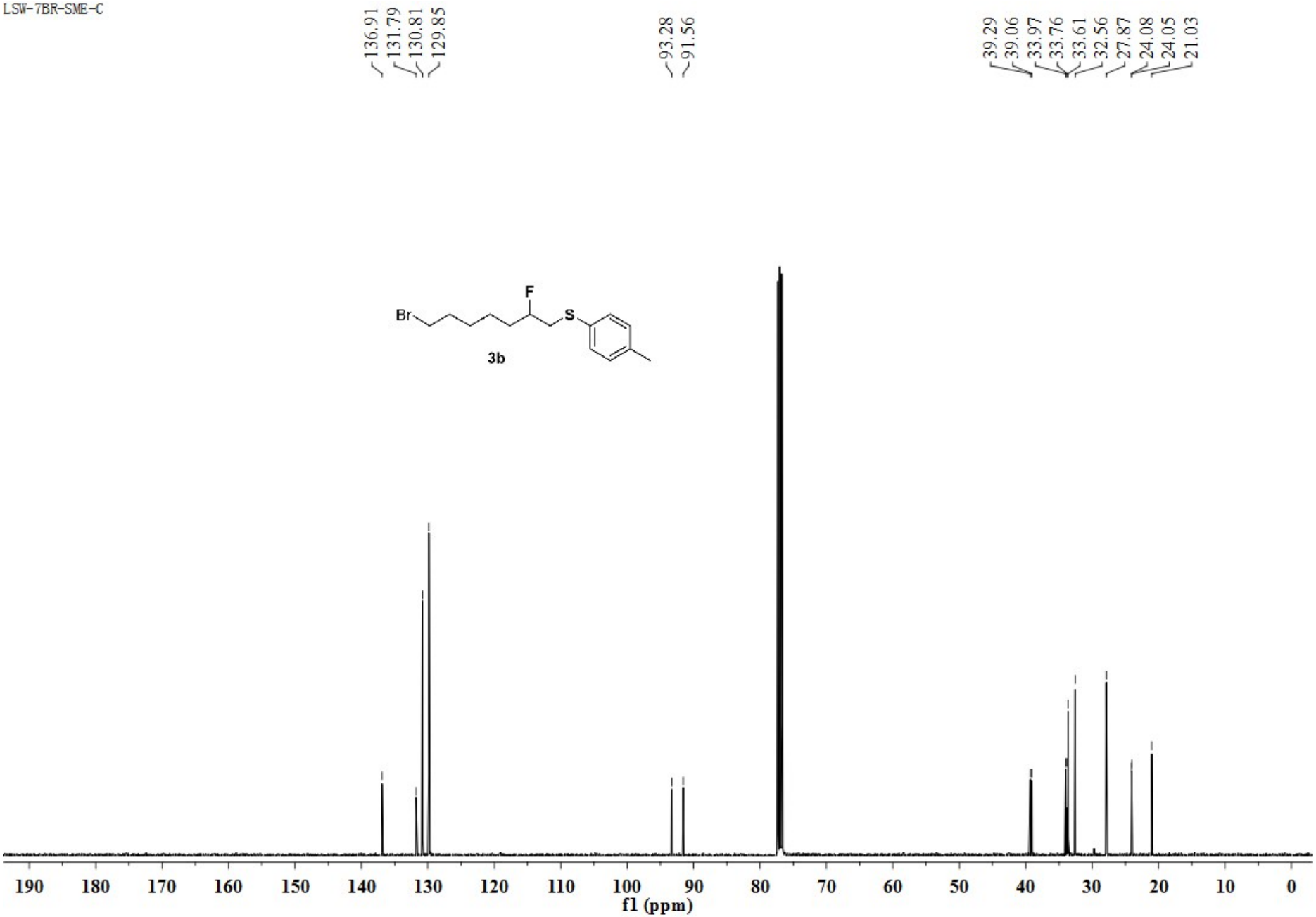


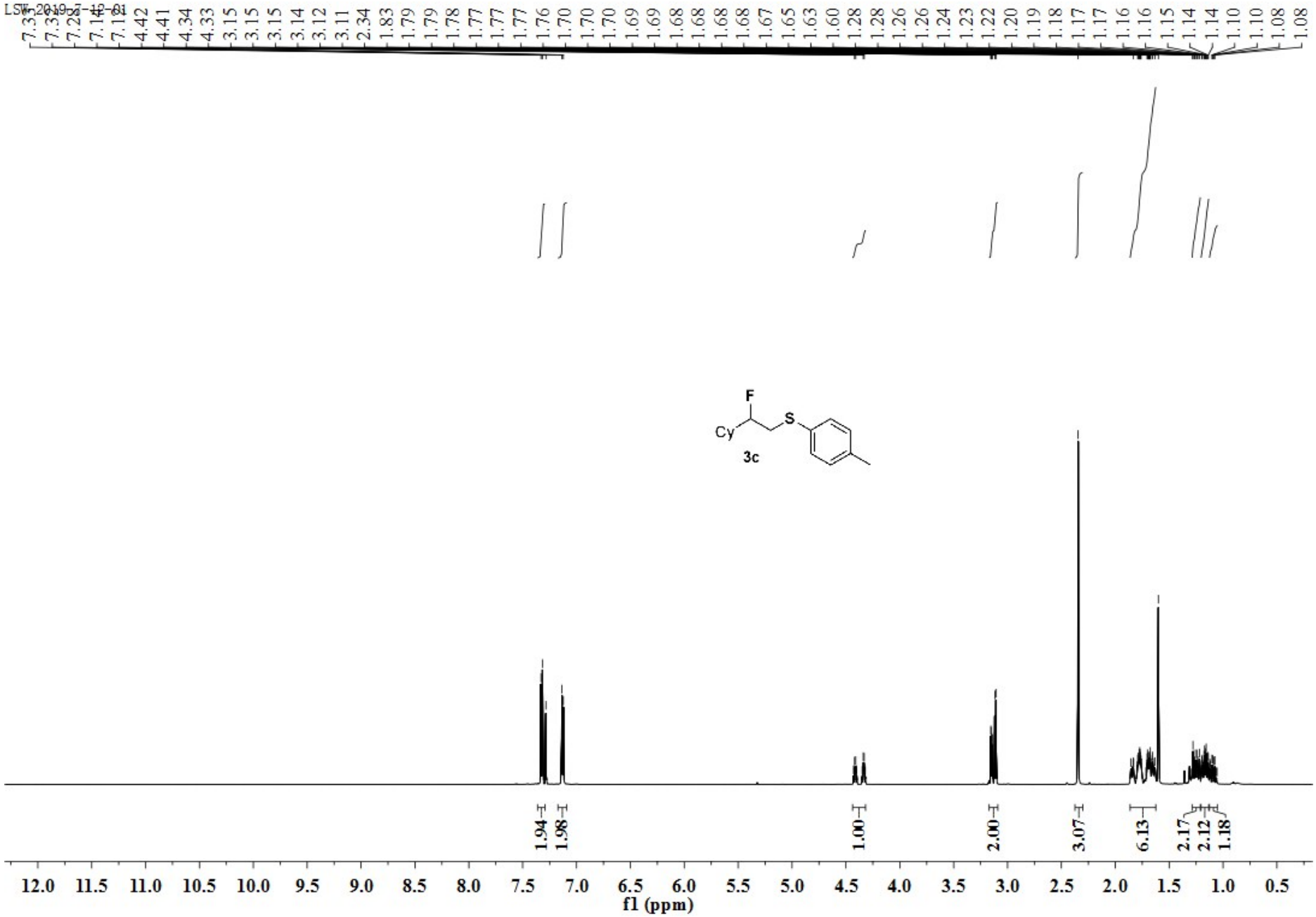


3b



LSW-7BR-SME-C

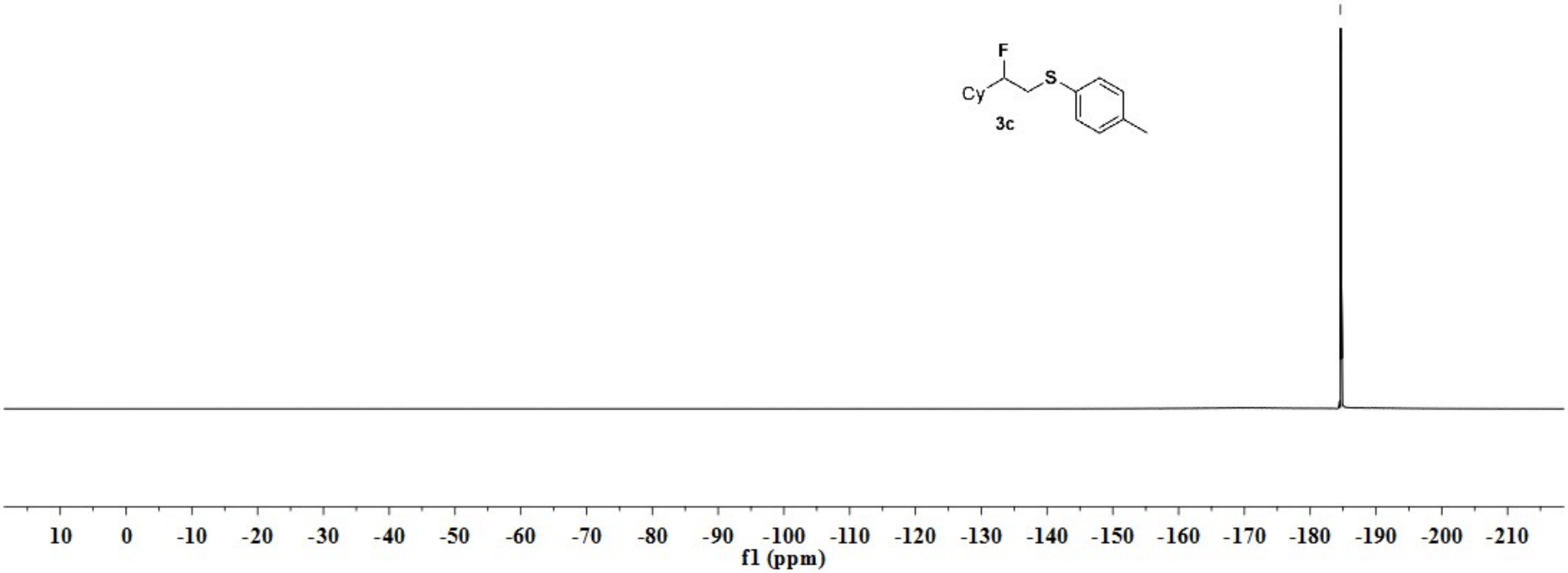

136.91
131.79
130.81
129.85
93.28
91.56
39.29
39.06
33.97
33.76
33.61
32.56
27.87
24.08
24.05
21.03
Br
F
S
3b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


LSW-2019-15-01
7.33
7.32
7.28
7.14
7.13
4.42
4.41
4.34
4.33
3.15
3.15
3.15
3.14
3.12
3.11
2.34
1.83
1.79
1.79
1.78
1.77
1.77
1.77
1.76
1.70
1.70
1.70
1.69
1.69
1.68
1.68
1.68
1.68
1.67
1.65
1.63
1.60
1.28
1.28
1.26
1.26
1.24
1.23
1.22
1.20
1.19
1.18
1.17
1.17
1.16
1.16
1.15
1.14
1.14
1.10
1.10
1.08
1.08
F
Cy
S
3c
1.94
1.98
1.00
2.00
3.07
6.13
2.17
2.12
1.18
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

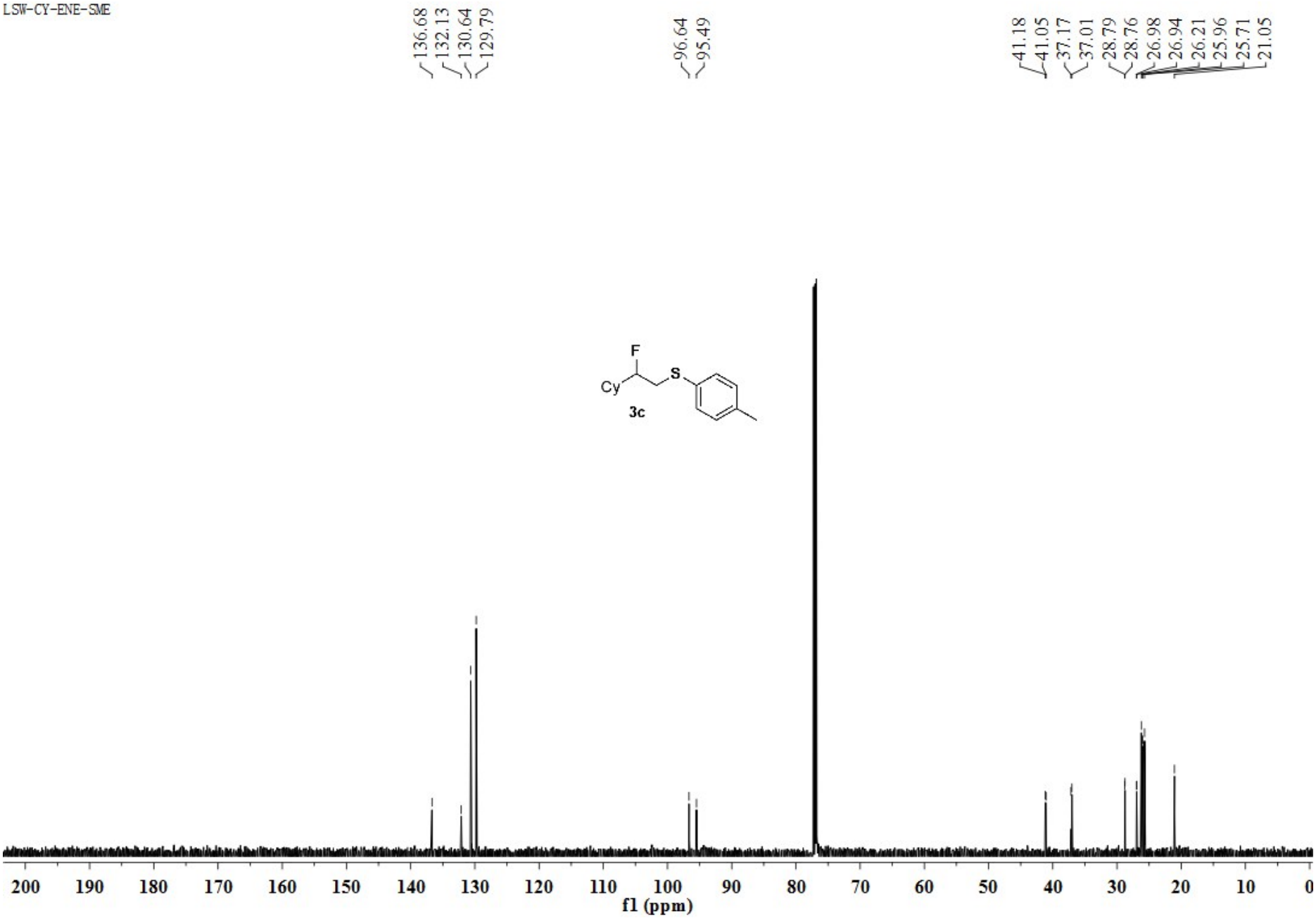
LSW-2019-7-12-01

184.53
184.56
184.57
184.60
184.61
184.64
184.65
184.66
184.68
184.69
184.73

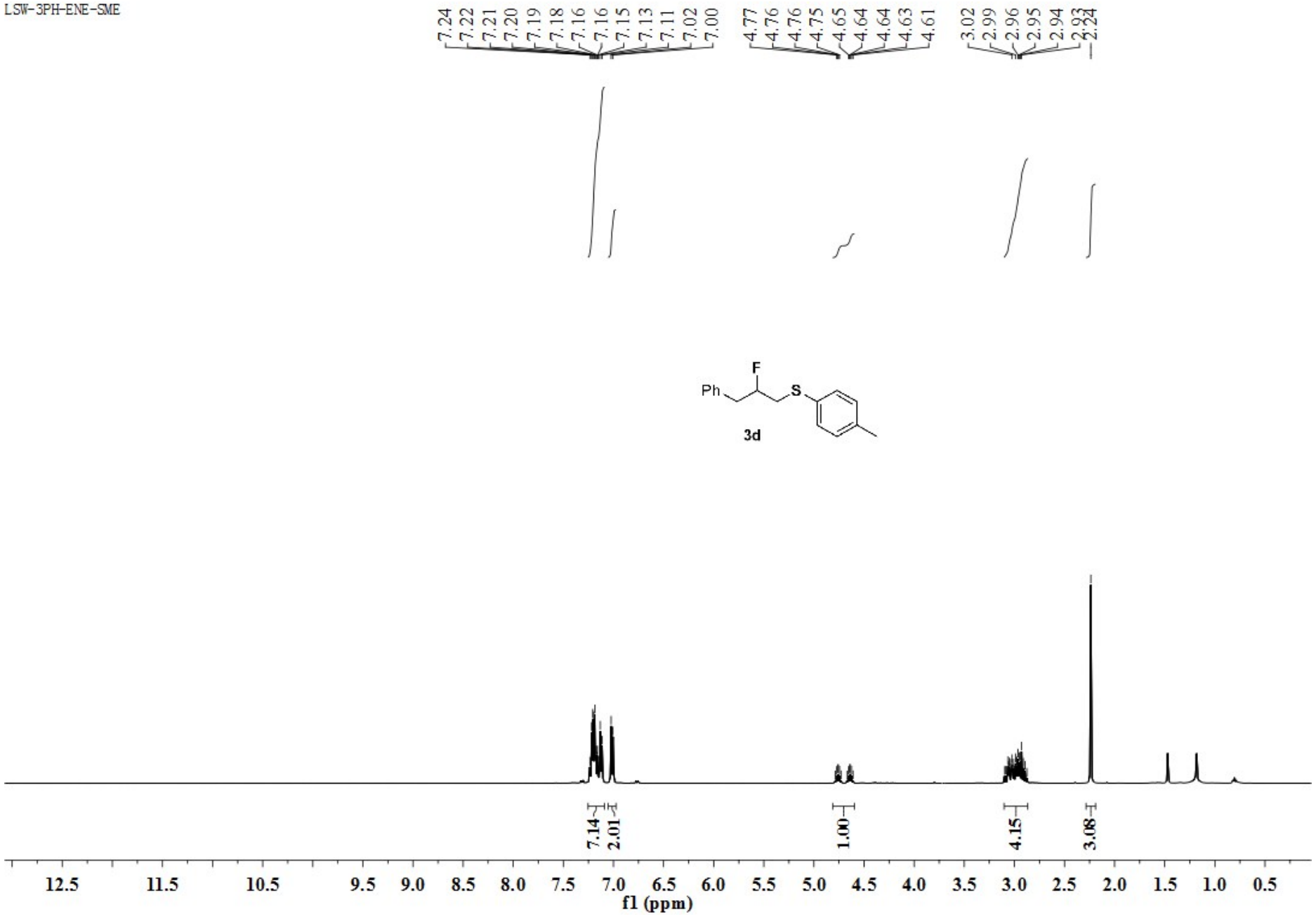
3c



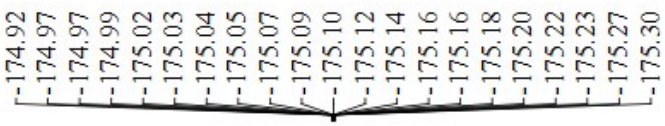
LSW-CY-ENE-SME

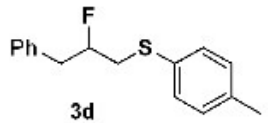


LSW-3PH-ENE-SME

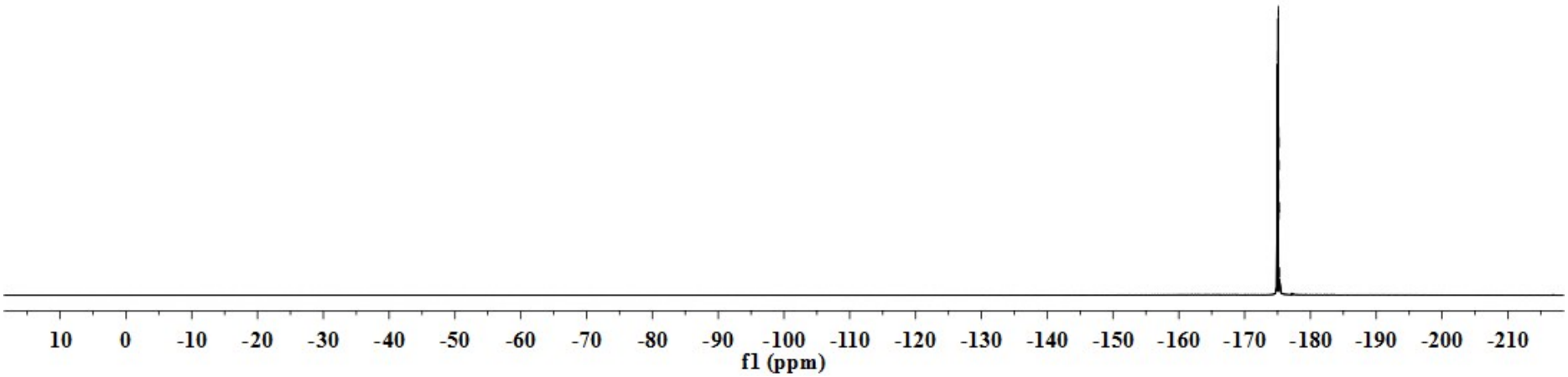


LSW-3PH-ENE-SME

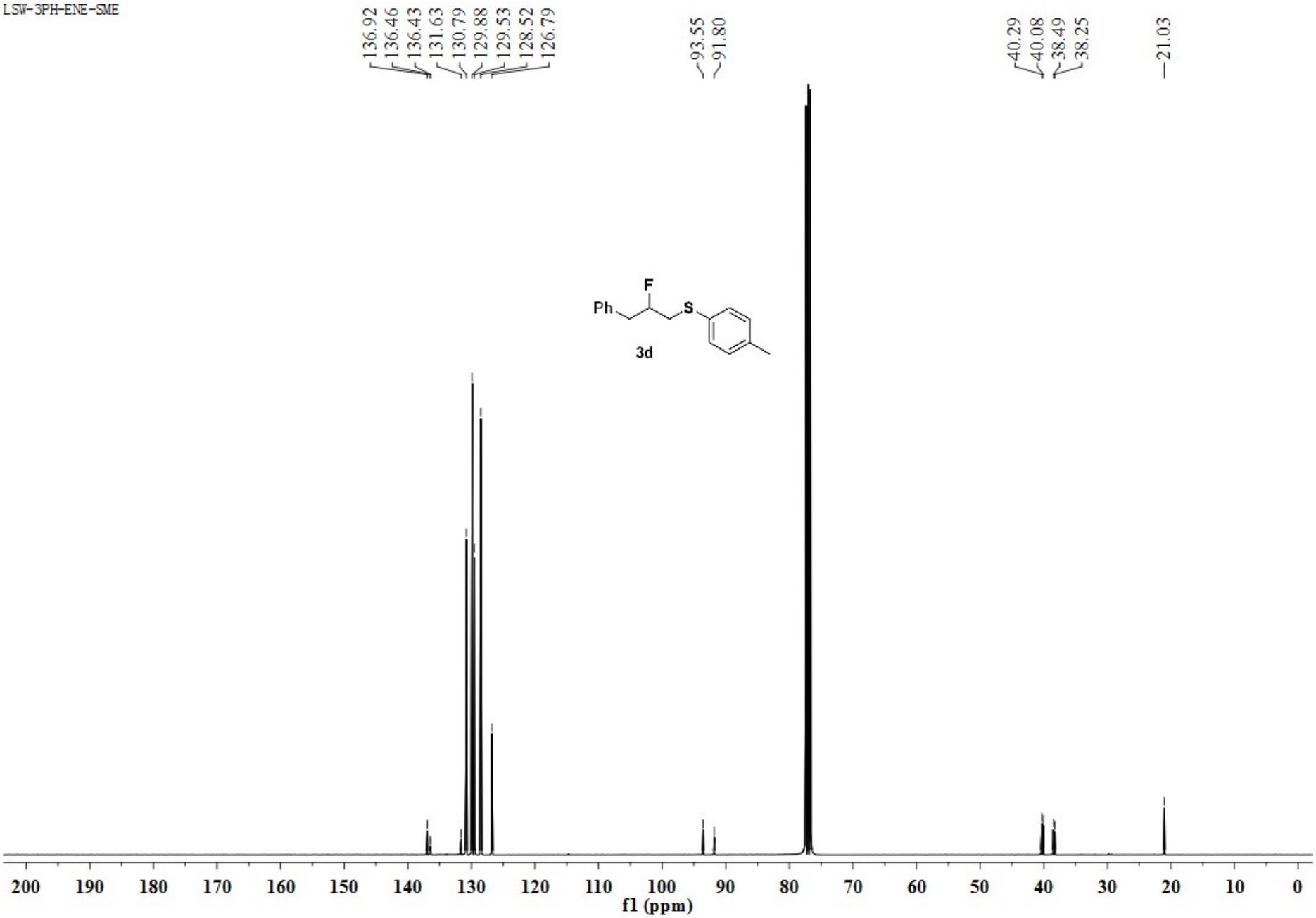


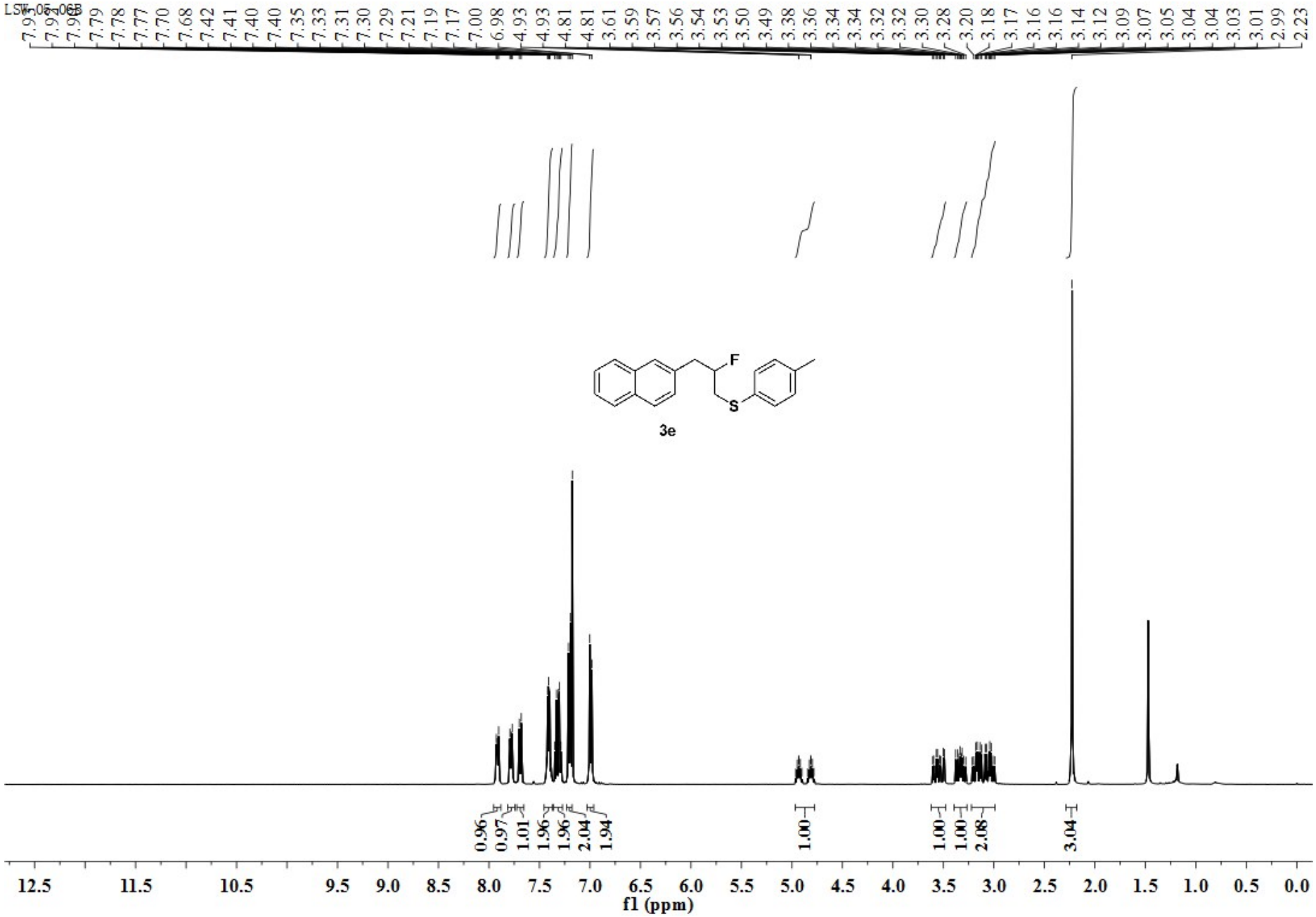


3d



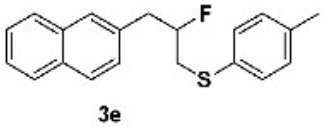
LSW-3PH-ENE-SME



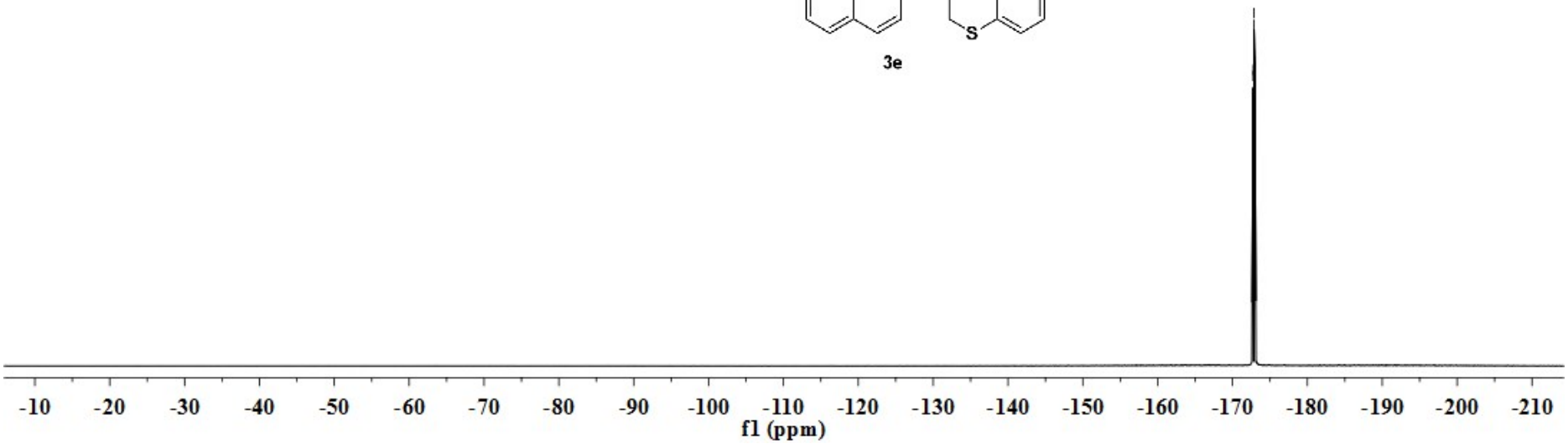

7.93
7.92
7.92
7.98
7.79
7.78
7.77
7.70
7.68
7.42
7.41
7.40
7.40
7.35
7.33
7.31
7.30
7.29
7.21
7.19
7.17
7.00
6.98
4.93
4.93
4.81
4.81
3.61
3.59
3.57
3.56
3.54
3.53
3.50
3.49
3.38
3.36
3.34
3.34
3.32
3.32
3.30
3.28
3.20
3.18
3.17
3.16
3.16
3.14
3.12
3.09
3.07
3.05
3.04
3.04
3.03
3.01
2.99
2.23
F
S
3e
0.96
0.97
1.01
1.96
1.96
2.04
1.94
1.00
1.00
1.00
2.08
3.04
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-05-06B


172.69
172.74
172.76
172.78
172.81
172.82
172.83
172.86
172.86
172.89
172.90
172.91
172.94
172.96
172.98
173.03


F
S

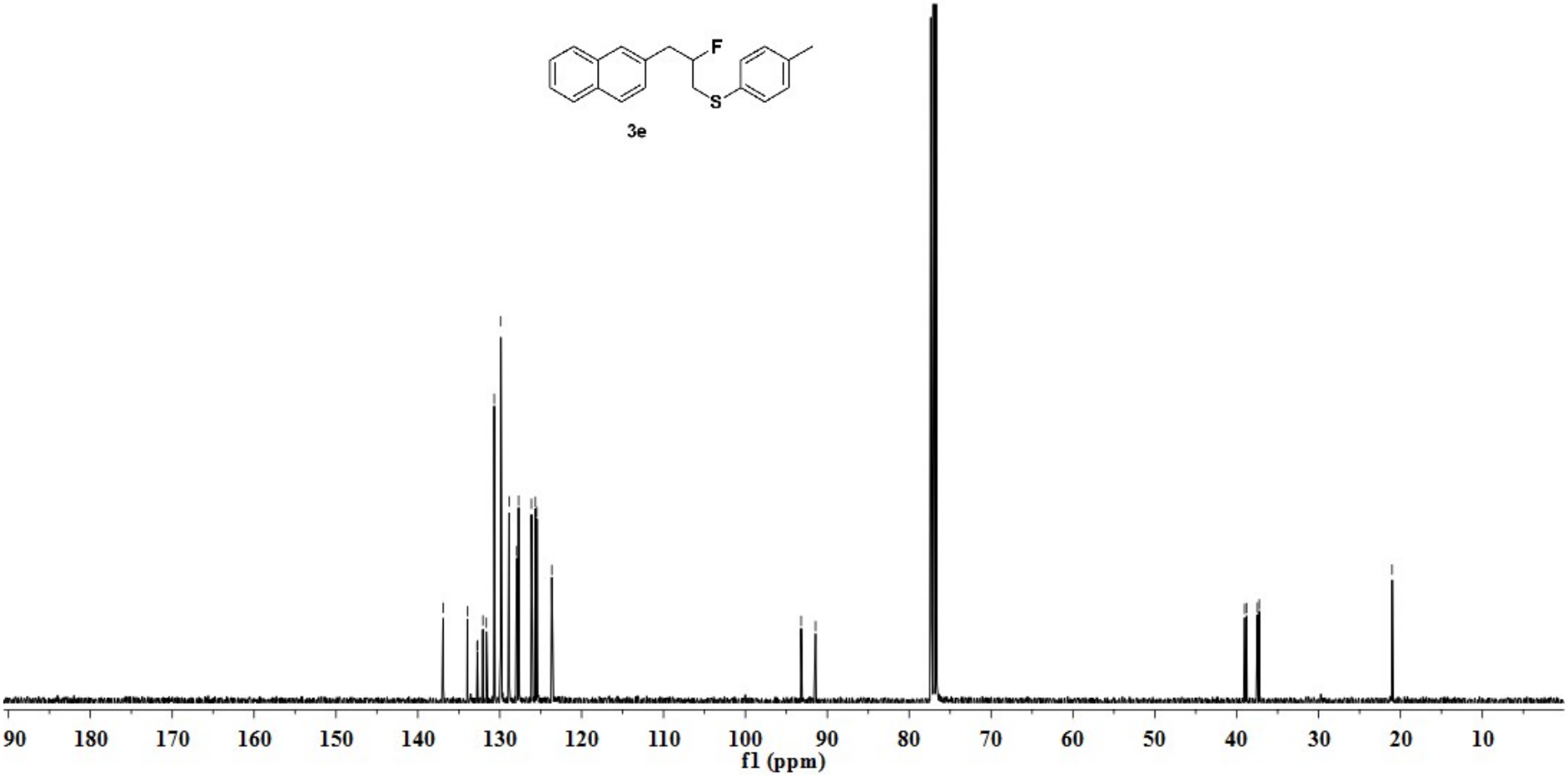
3e

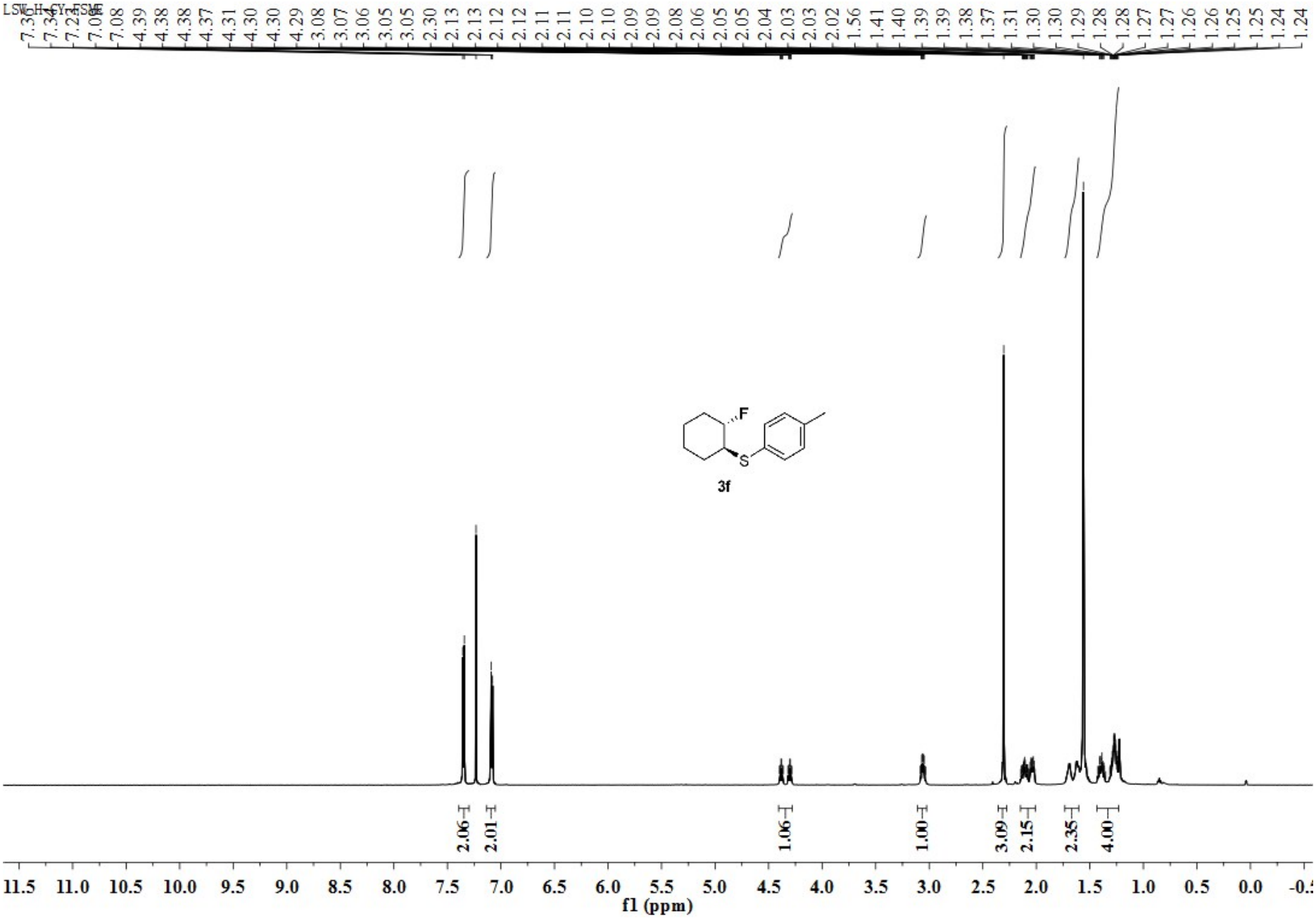

-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

LSW-6B

136.91
133.94
132.76
132.72
132.06
131.62
130.67
129.87
128.86
127.92
127.69
126.13
125.64
125.47
123.64
93.19
91.43
39.03
38.80
37.47
37.26
21.02

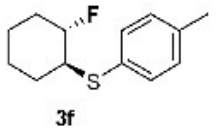
3e



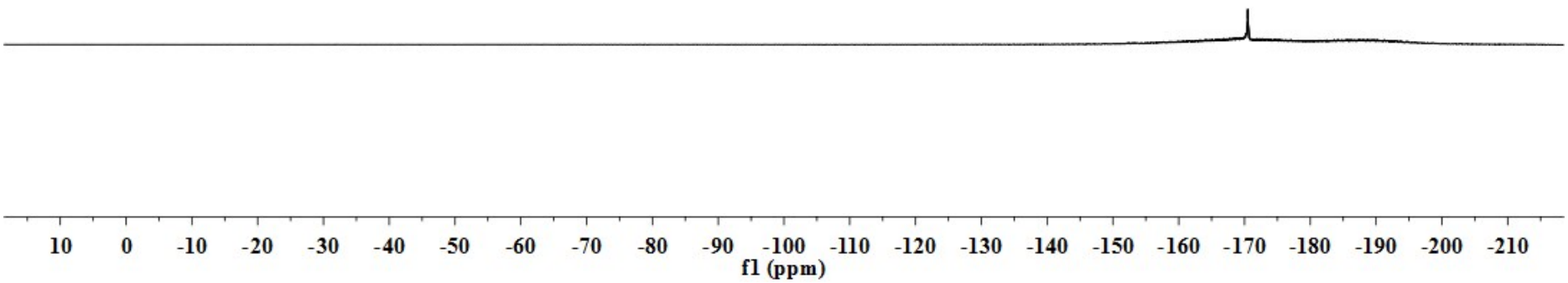

7.30 7.34 7.23 7.08 7.08 4.39 4.38 4.38 4.37 4.31 4.30 4.30 4.29 3.08 3.07 3.06 3.05 3.05 2.30 2.13 2.13 2.12 2.12 2.11 2.11 2.10 2.10 2.09 2.09 2.08 2.06 2.05 2.05 2.04 2.03 2.03 2.02 1.56 1.41 1.40 1.39 1.39 1.38 1.37 1.31 1.30 1.30 1.29 1.28 1.28 1.27 1.27 1.26 1.26 1.25 1.25 1.24 1.24
F
S
3f
2.06
2.01
1.06
1.00
3.09
2.15
2.35
4.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

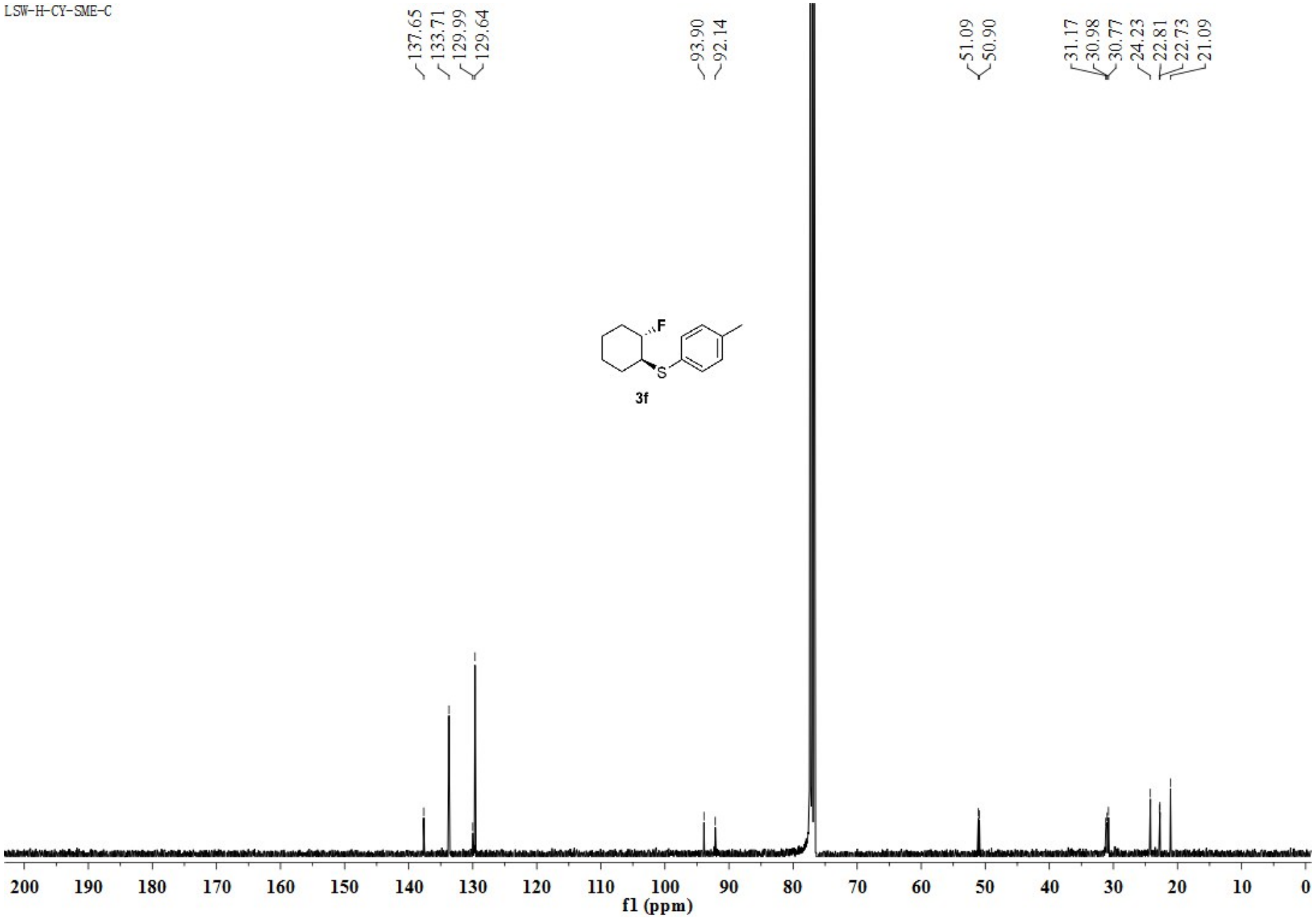
LSW-H-CY-FSME

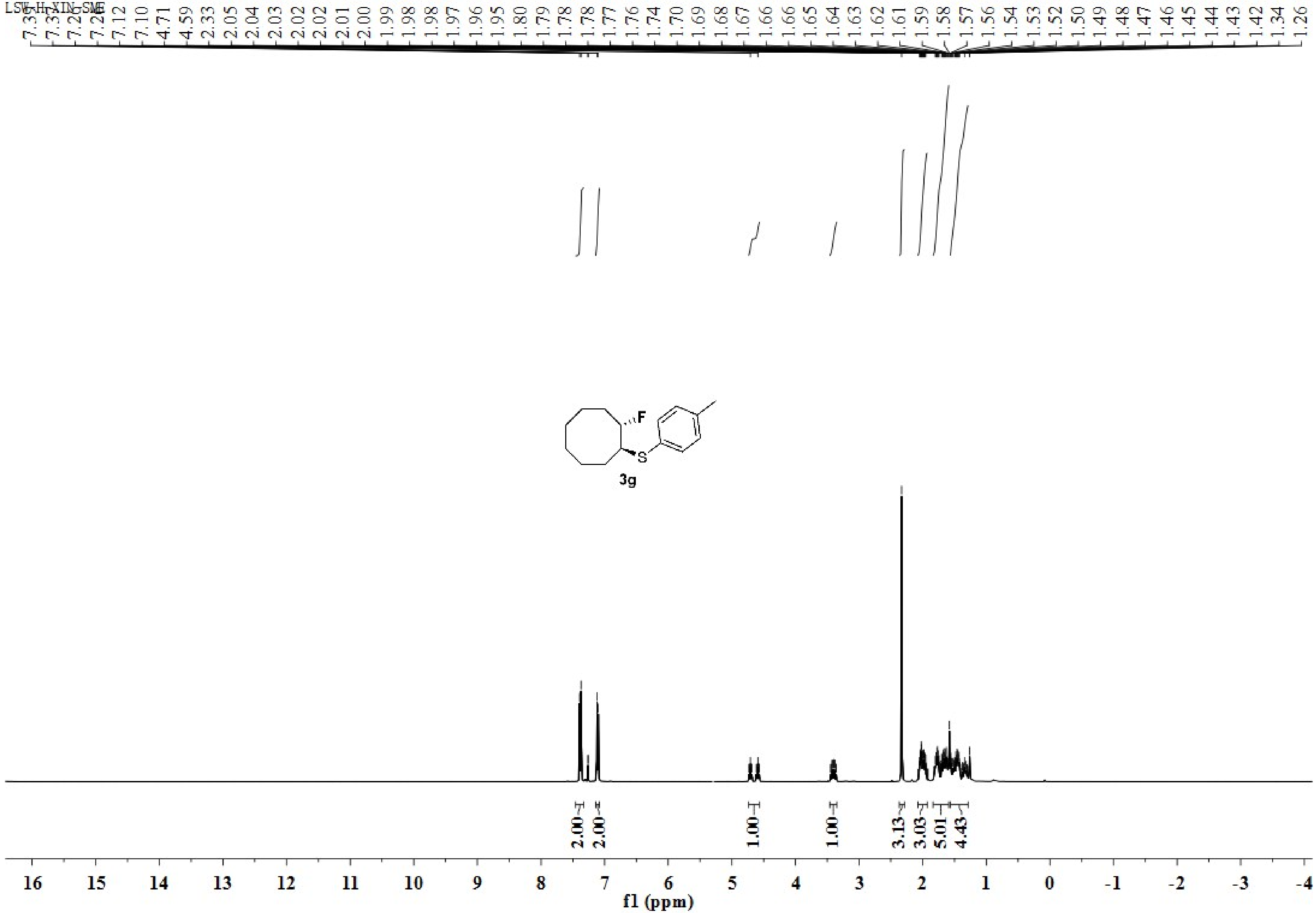
-170.47
-170.49
-170.49
-170.50
-170.50
-170.51



3f

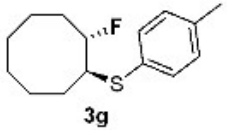



LSW-H-CY-SME-C
137.65
133.71
129.99
129.64
93.90
92.14
51.09
50.90
31.17
30.98
30.77
24.23
22.81
22.73
21.09
F
S
3f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.12
7.10
4.71
4.59
2.33
2.05
2.04
2.03
2.02
2.02
2.01
2.00
1.99
1.98
1.98
1.97
1.96
1.95
1.80
1.79
1.78
1.78
1.77
1.76
1.74
1.70
1.69
1.68
1.67
1.66
1.66
1.65
1.64
1.63
1.62
1.61
1.59
1.58
1.57
1.56
1.54
1.53
1.52
1.50
1.49
1.48
1.47
1.46
1.45
1.44
1.43
1.42
1.34
1.26
F
S
3g
2.00
2.00
1.00
1.00
3.13
3.03
5.01
4.43
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

LSW-H-XIN-SME

158.52
158.53
158.54
158.55
158.61
158.62
158.62
158.63
158.66
158.66
158.69
158.74
158.78
158.79
158.83
158.86
158.89
158.91
158.91



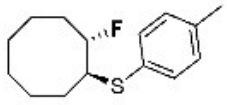
3g

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

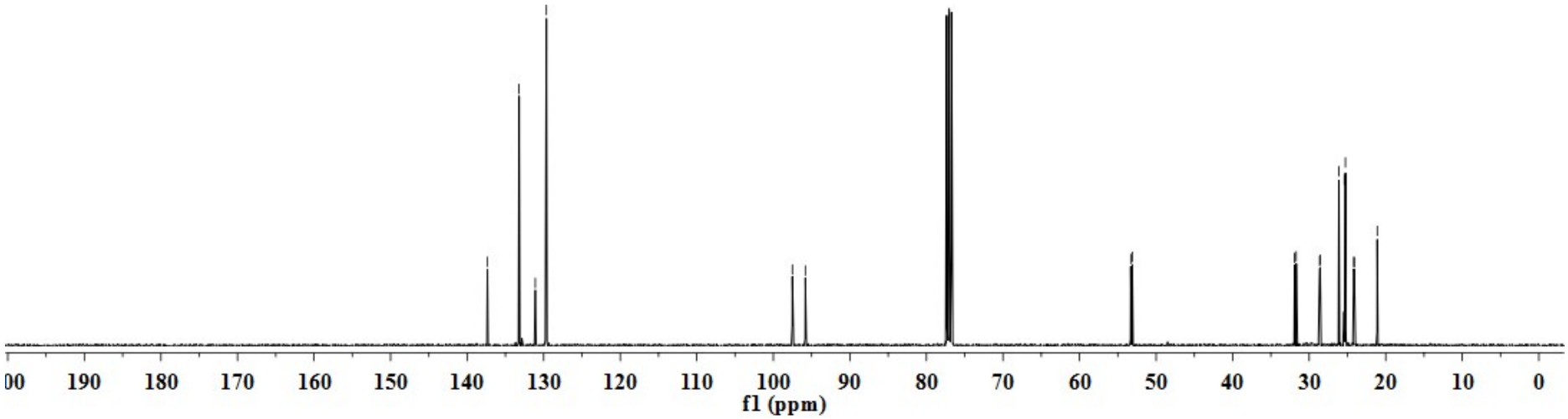
f1 (ppm)

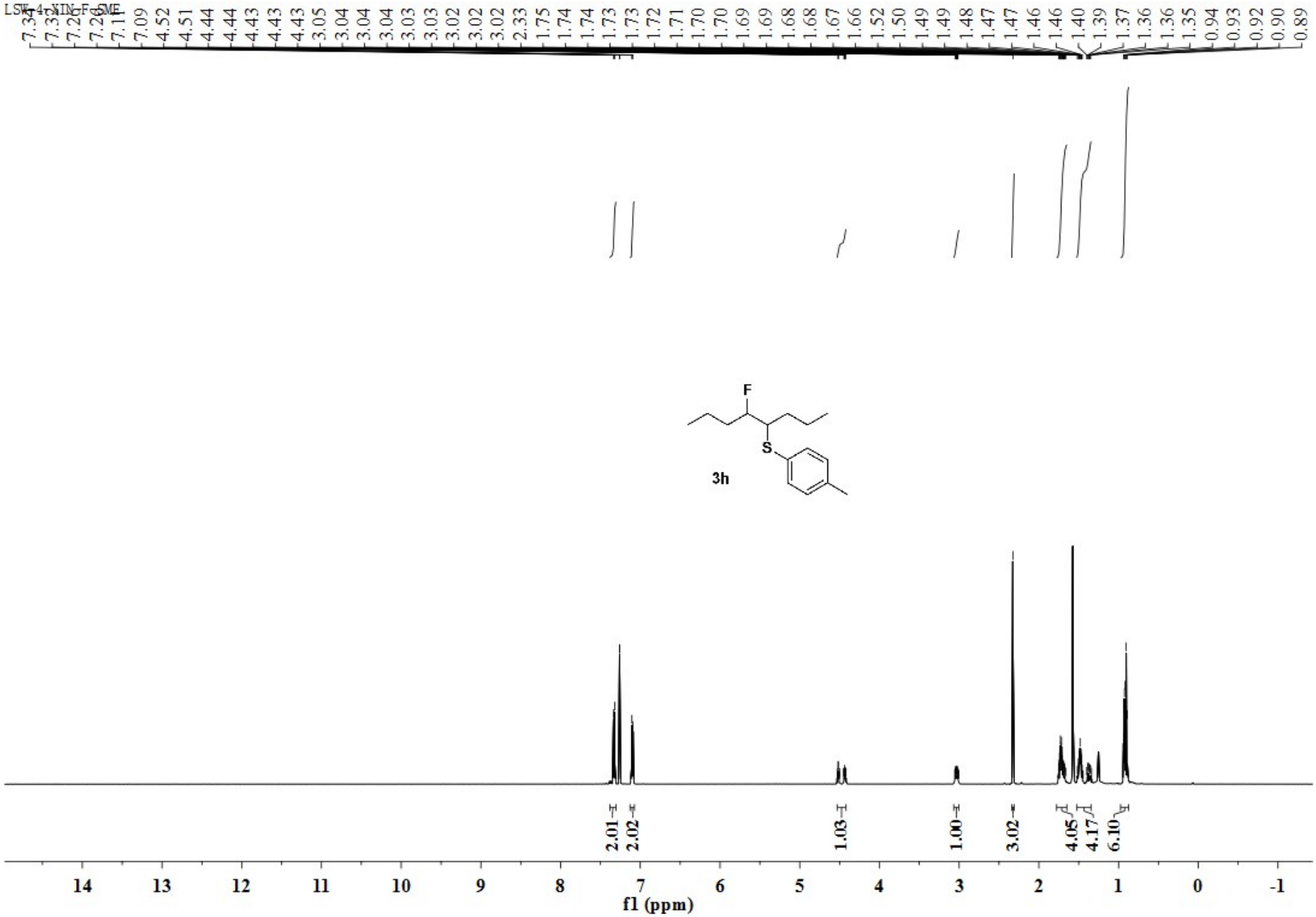
LSW-H-XIN-SME

137.35
133.22
131.10
129.65
97.52
95.81
53.31
53.10
31.92
31.69
28.63
28.57
26.12
25.42
25.27
24.18
24.11
21.11



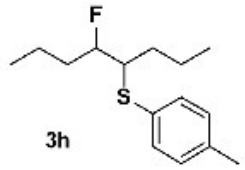
3g



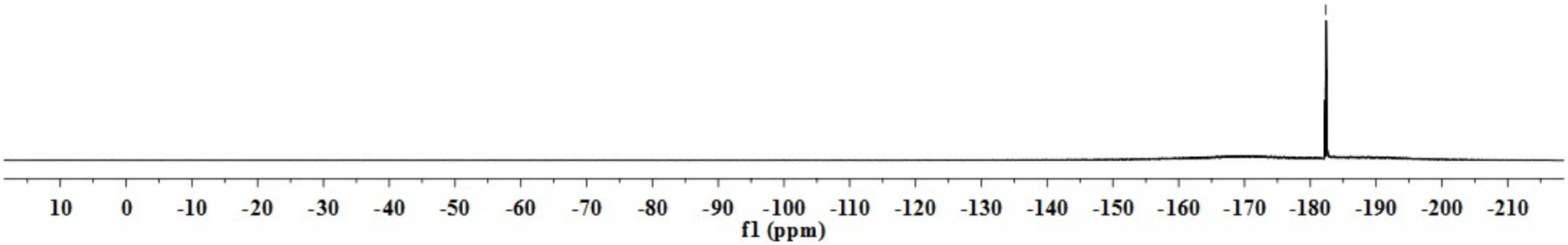

F
S
3h
2.01
2.02
1.03
1.00
3.02
4.05
4.17
6.10
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

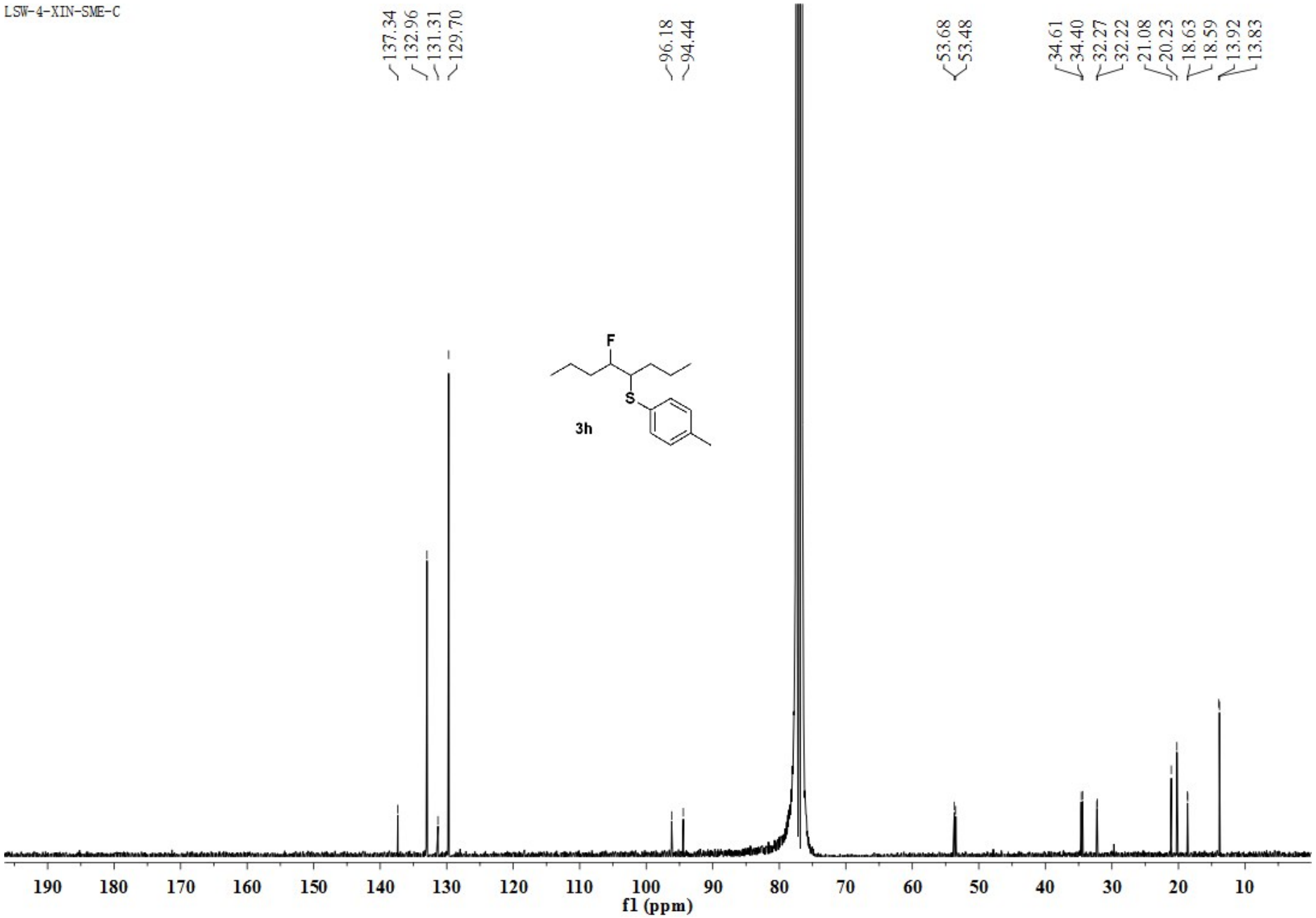
LSW-4-XIN-F-SME

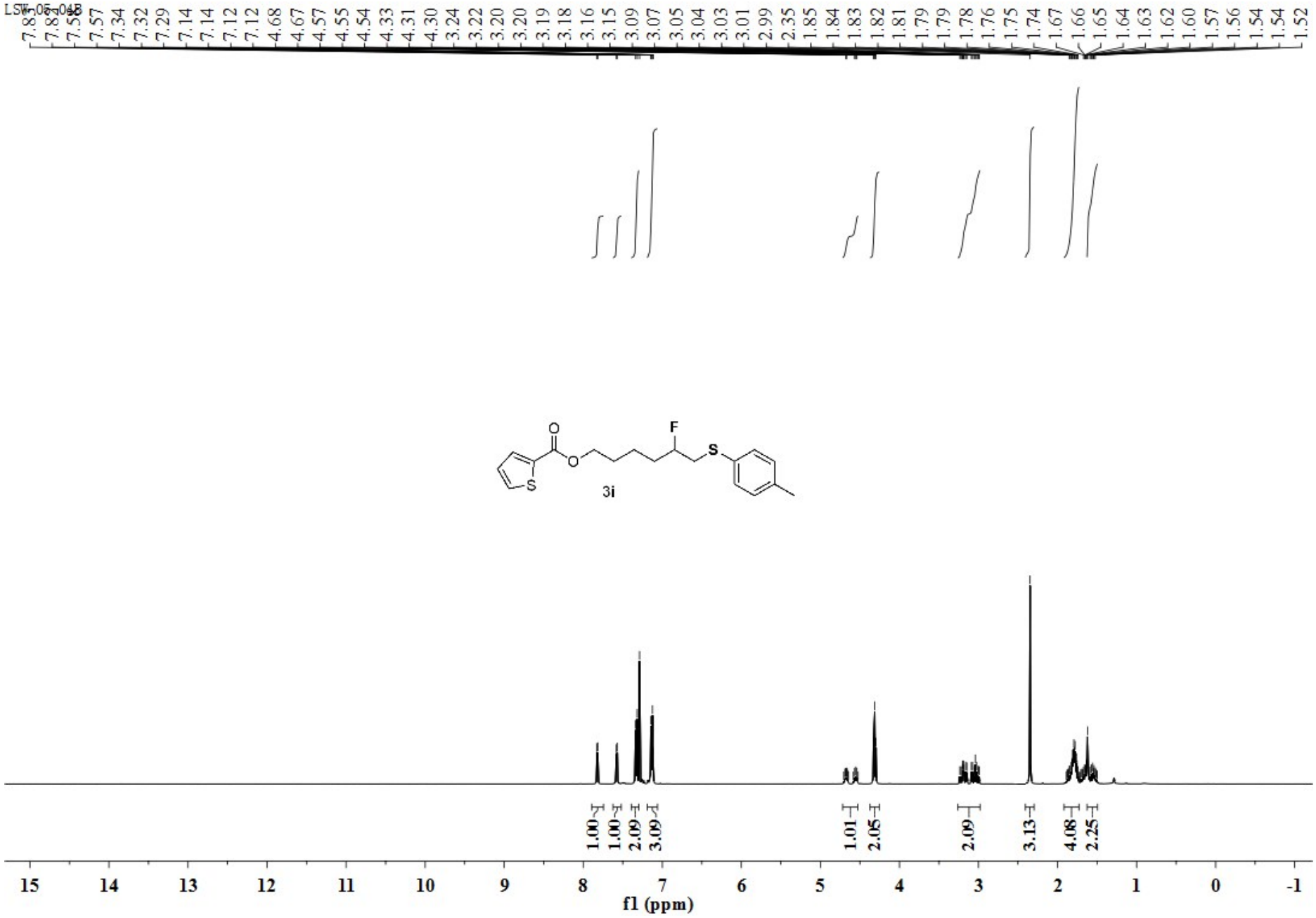
182.28
182.31
182.32
182.34
182.37
182.37
182.39
182.40
182.41
182.42
182.43
182.45
182.46
182.49



3h




LSW-4-XIN-SME-C
137.34
132.96
131.31
129.70
96.18
94.44
53.68
53.48
34.61
34.40
32.27
32.22
21.08
20.23
18.63
18.59
13.92
13.83
F
S
3h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

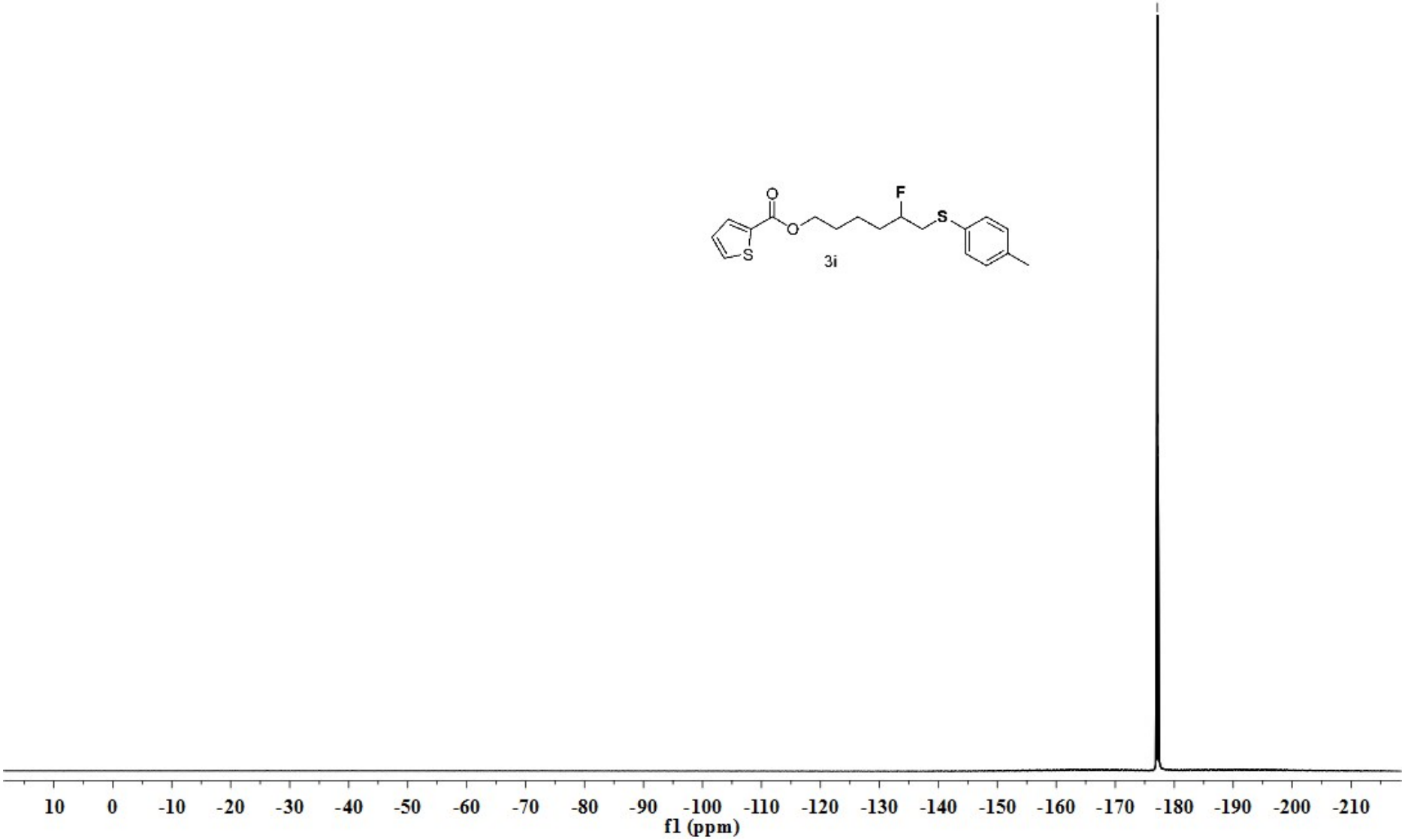

LSW-05-04B
7.83
7.82
7.58
7.57
7.34
7.32
7.29
7.14
7.14
7.12
7.12
4.68
4.67
4.57
4.55
4.54
4.33
4.31
4.30
3.24
3.22
3.20
3.20
3.19
3.18
3.16
3.15
3.09
3.07
3.05
3.04
3.03
3.01
2.99
2.35
1.85
1.84
1.83
1.82
1.81
1.79
1.79
1.78
1.76
1.75
1.74
1.67
1.66
1.65
1.64
1.63
1.62
1.60
1.57
1.56
1.54
1.54
1.52
O
F
S
O
O
S
3i
1.00
1.00
2.09
3.09
1.01
2.05
2.09
3.13
4.08
2.25
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

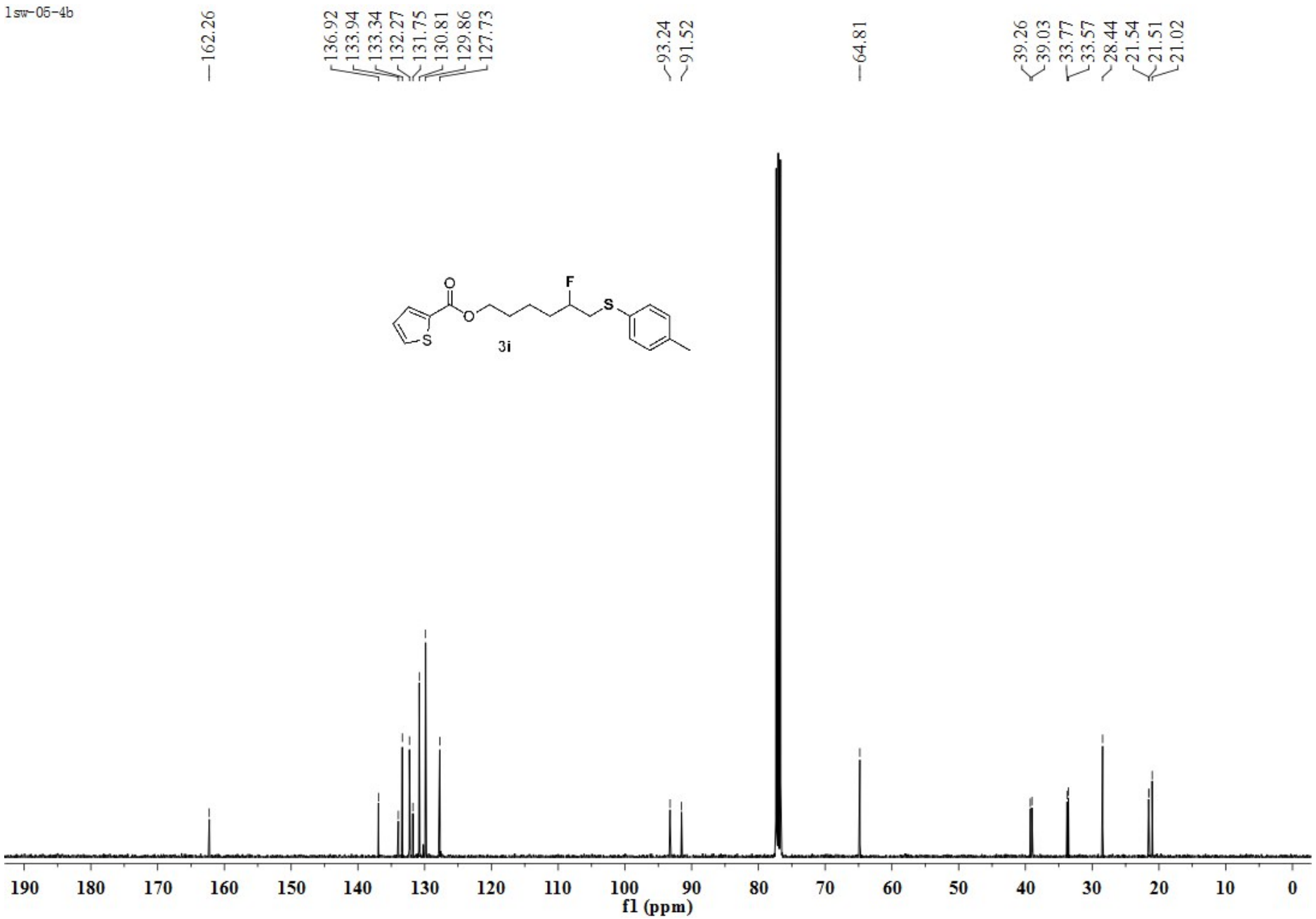
LSW-05-04B

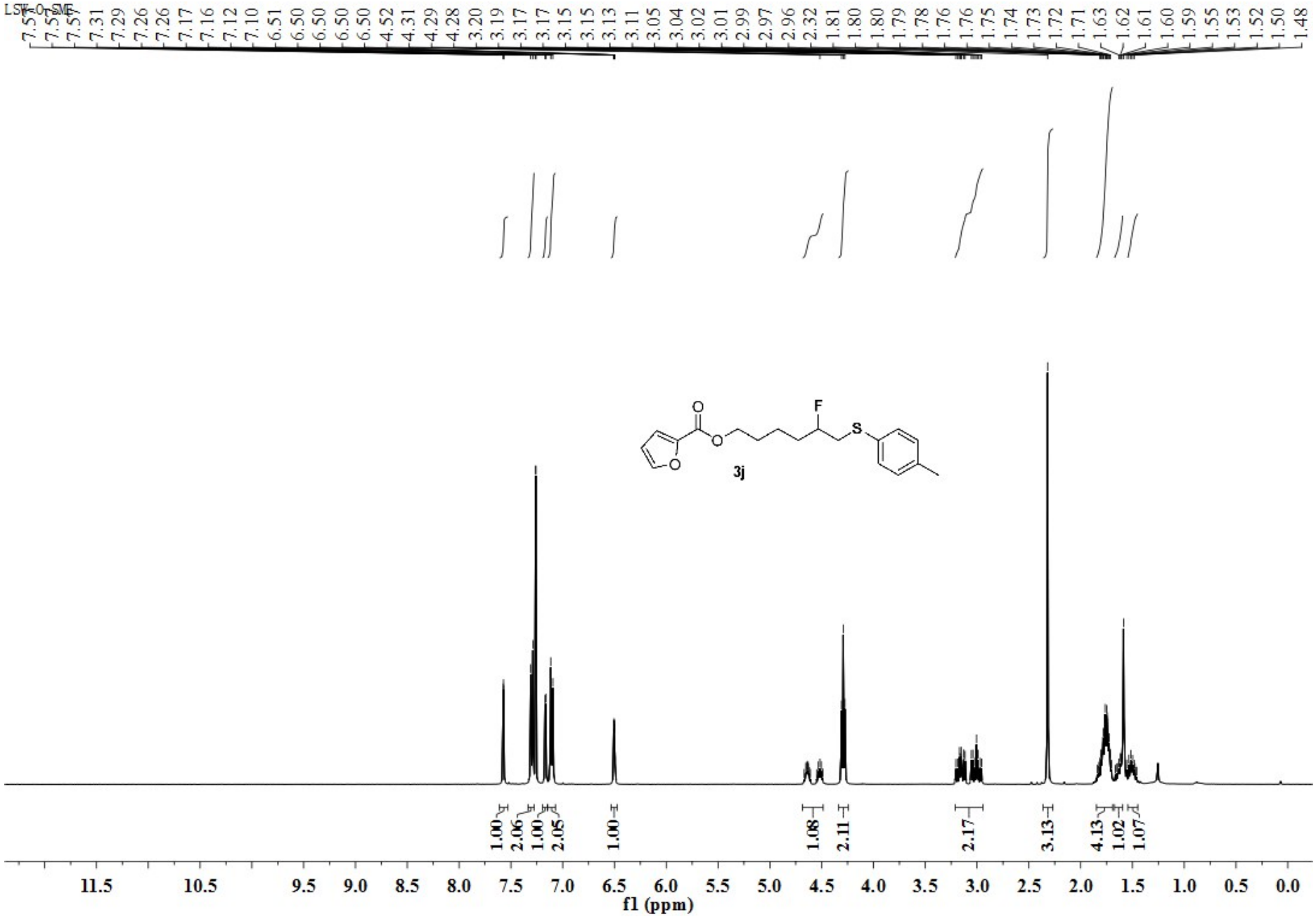

176.94
176.97
177.02
177.03
177.05
177.07
177.08
177.10
177.11
177.12
177.15
177.16
177.19
177.20
177.23
177.24
177.25
177.28
177.29
177.33
177.35
177.36
177.37
177.38
177.39
177.40
177.41

O
F
O
S
S

3i


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


1sw-05-4b
162.26
136.92
133.94
133.34
132.27
131.75
130.81
129.86
127.73
93.24
91.52
64.81
39.26
39.03
33.77
33.57
28.44
21.54
21.51
21.02
O
F
S
O
S
3i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

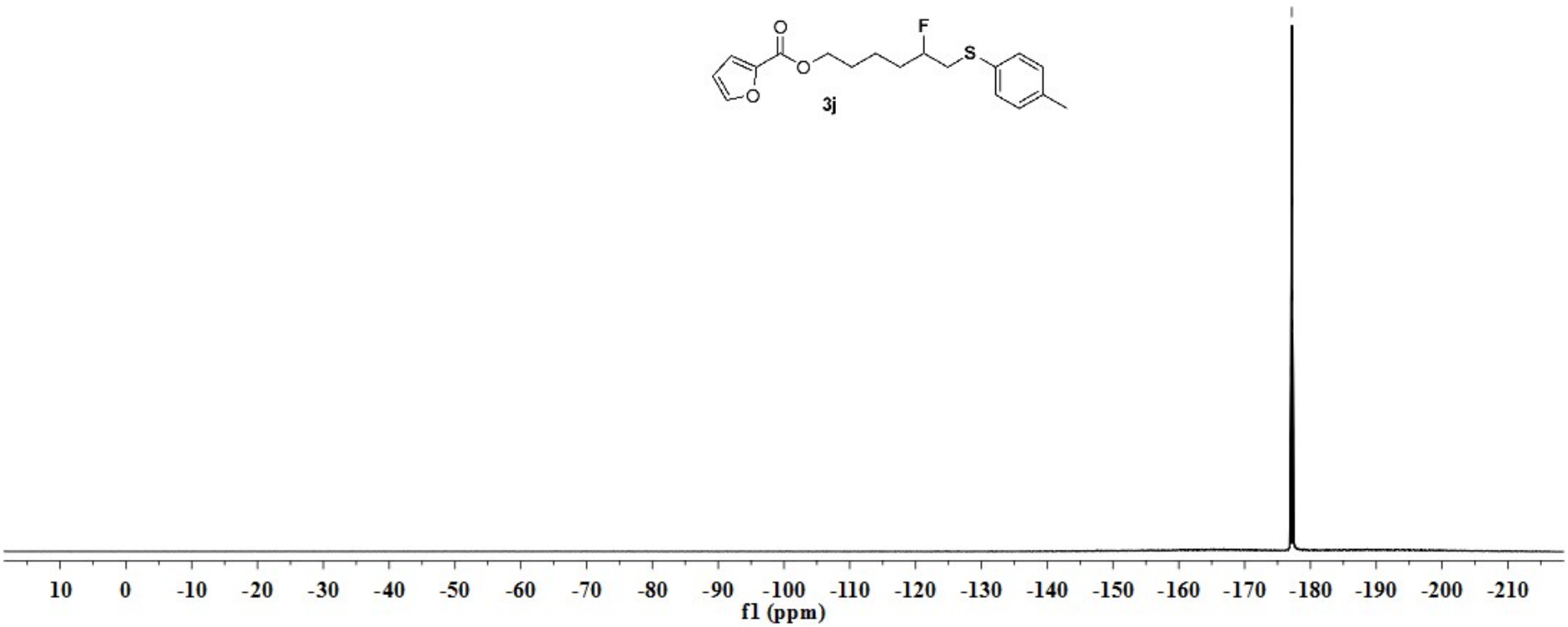

LSF-0-SME
7.57
7.57
7.57
7.31
7.29
7.26
7.26
7.17
7.16
7.12
7.10
6.51
6.50
6.50
6.50
6.50
4.52
4.31
4.29
4.28
3.20
3.19
3.17
3.17
3.15
3.15
3.13
3.11
3.05
3.04
3.02
3.01
2.99
2.97
2.96
2.32
1.81
1.80
1.80
1.79
1.78
1.76
1.76
1.75
1.74
1.73
1.72
1.71
1.63
1.62
1.61
1.60
1.59
1.55
1.53
1.52
1.50
1.48
O
O
O
F
S
3j
1.00
2.06
1.00
2.05
1.00
1.08
2.11
2.17
3.13
4.13
1.02
1.07
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

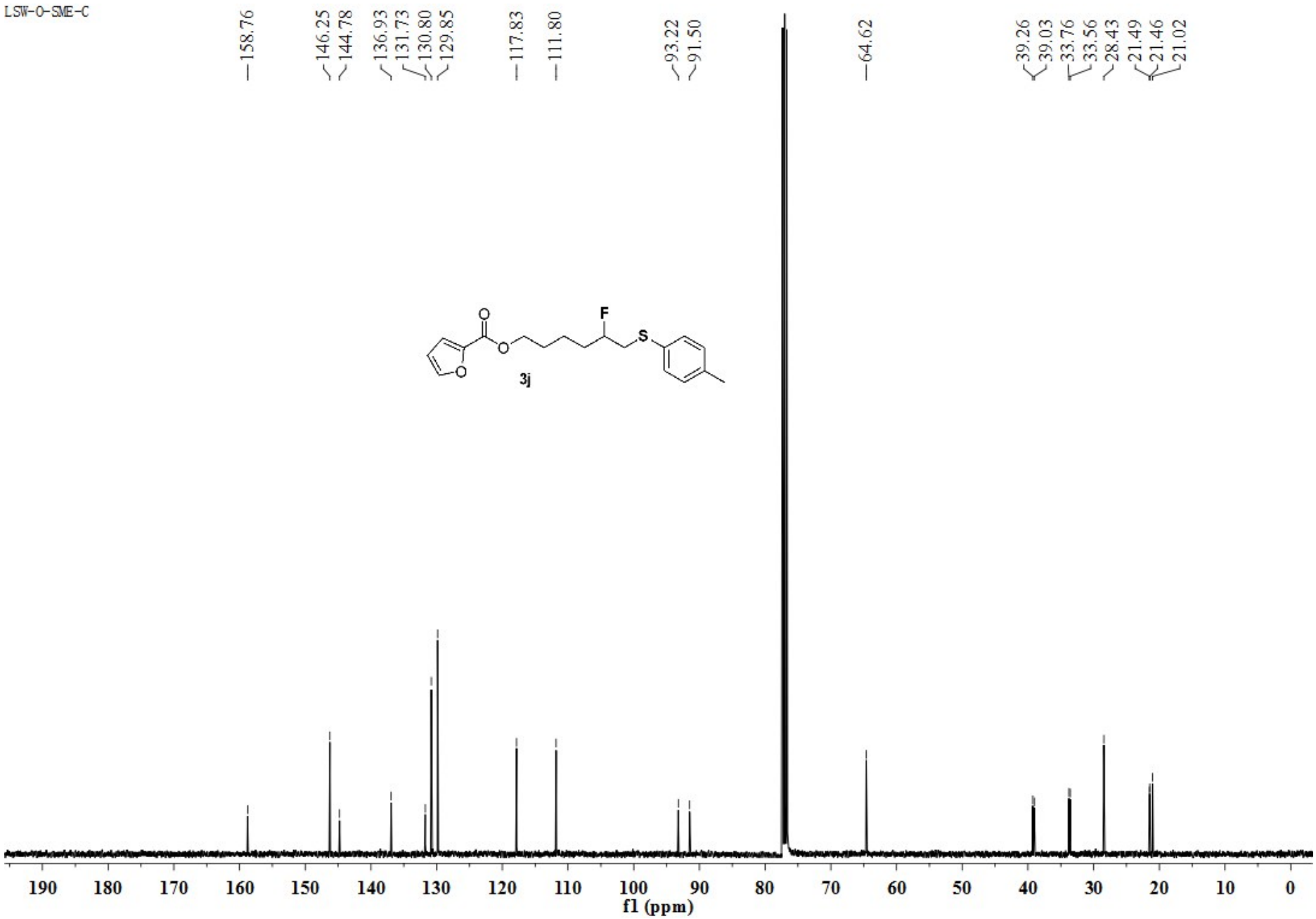
LSW-O-SME

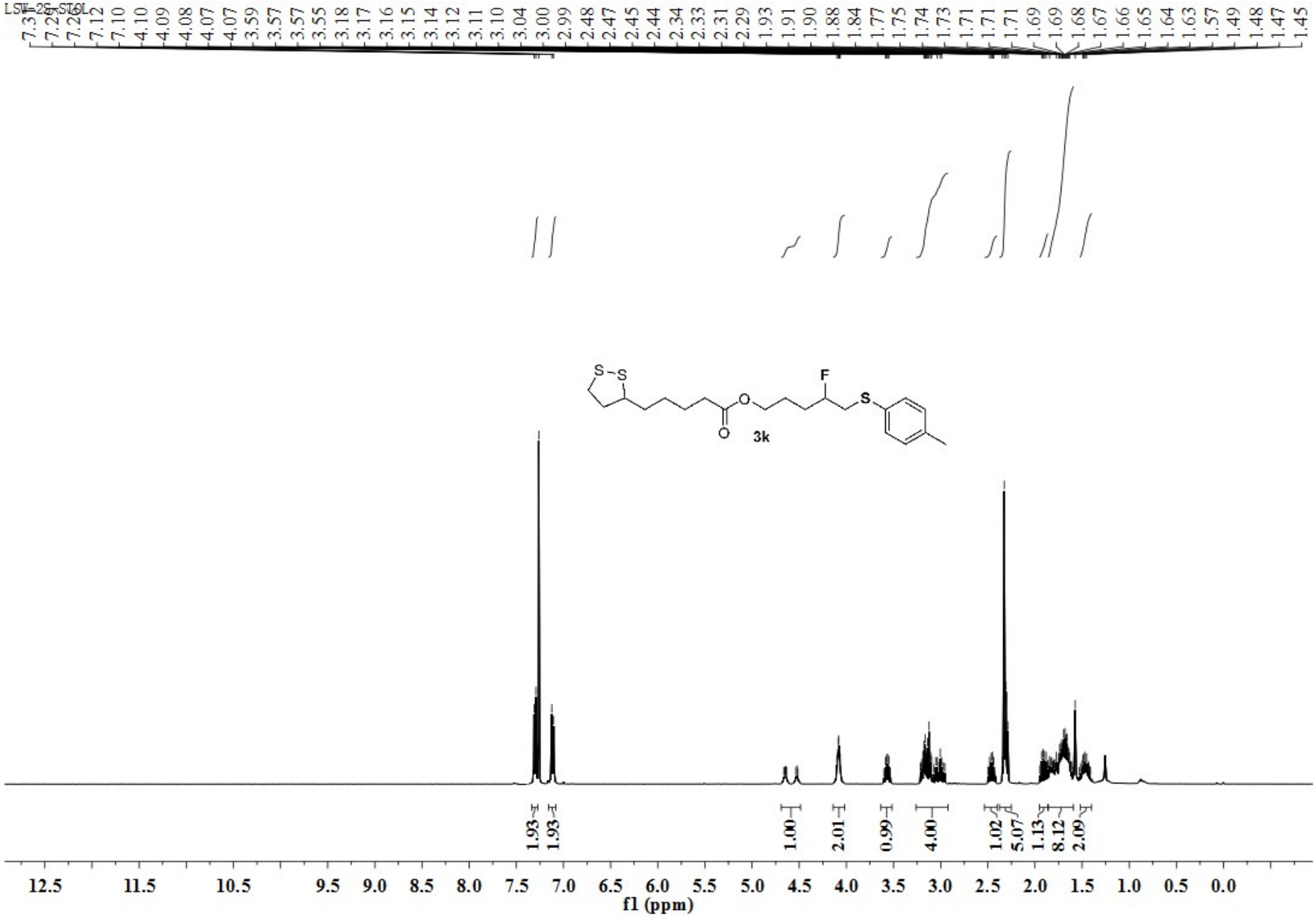

176.95
176.98
177.00
177.04
177.05
177.08
177.09
177.10
177.12
177.13
177.14
177.17
177.18
177.21
177.22
177.25
177.26
177.27
177.30
177.31
177.35
177.38
177.38
177.39
177.40
177.41
177.42
177.42
177.43
177.45
177.46

O
F
S
O
O

3j

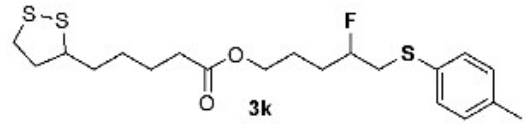

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


LSW-O-SME-C
158.76
146.25
144.78
136.93
131.73
130.80
129.85
117.83
111.80
93.22
91.50
64.62
39.26
39.03
33.76
33.56
28.43
21.49
21.46
21.02
O
F
S
O
O
3j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.31
7.29
7.28
7.26
7.12
7.10
4.10
4.09
4.08
4.07
4.07
4.07
3.59
3.57
3.57
3.55
3.18
3.17
3.16
3.15
3.14
3.12
3.11
3.10
3.04
3.00
2.99
2.48
2.47
2.45
2.44
2.34
2.33
2.31
2.29
1.93
1.91
1.90
1.88
1.84
1.77
1.75
1.74
1.73
1.71
1.71
1.71
1.69
1.69
1.68
1.67
1.66
1.65
1.64
1.63
1.57
1.49
1.48
1.47
1.45
S
S
O
O
F
S
3k
1.93
1.93
1.00
2.01
0.99
4.00
1.02
5.07
1.13
8.12
2.09
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-2S-STOL

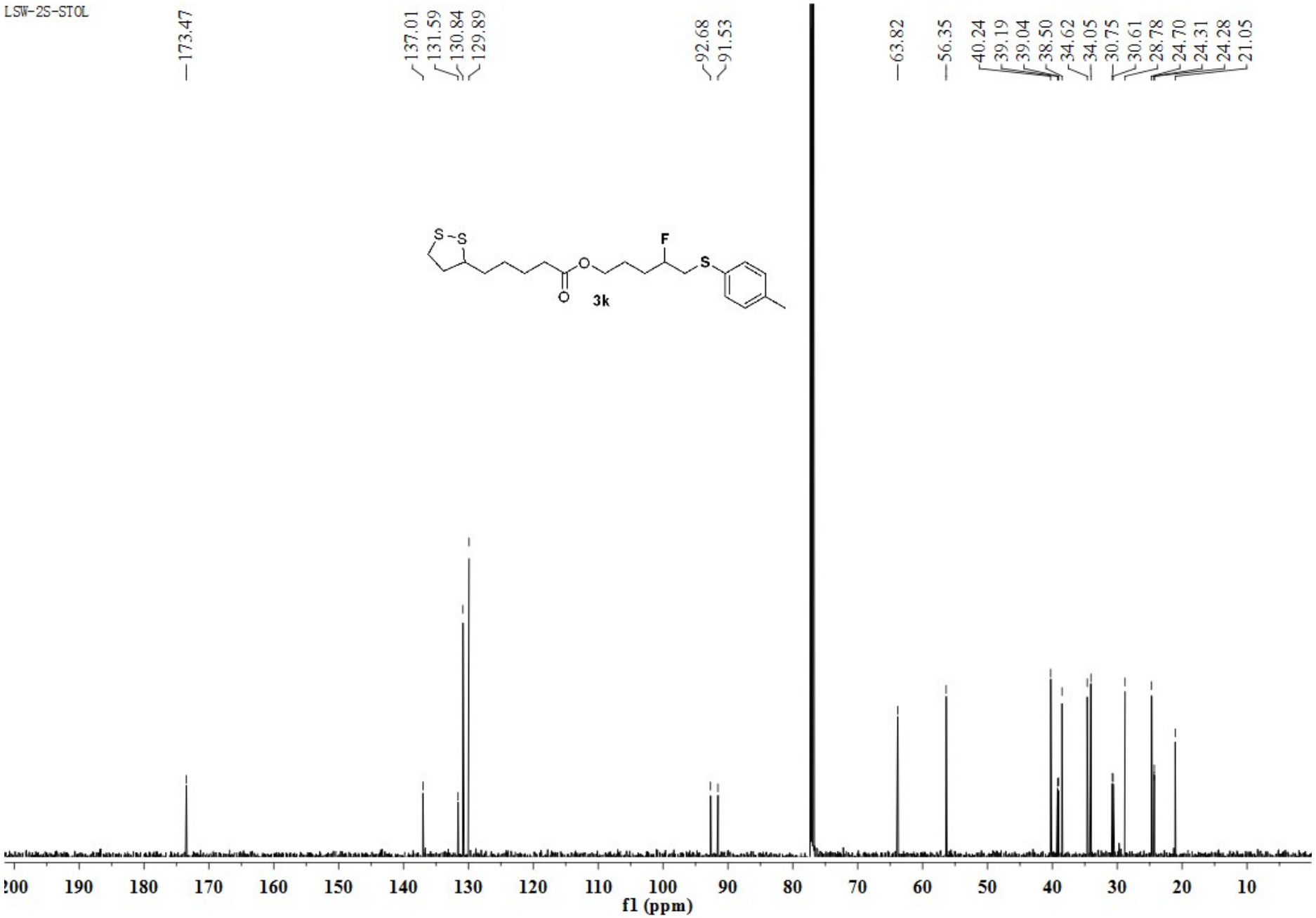
177.22
177.23
177.24
177.27
177.28
177.29
177.30
177.31
177.32
177.33
177.36
177.38
177.39
177.40
177.41
177.42
177.43
177.43
177.45
177.46
177.47
177.49
177.50
177.51
177.51
177.52
177.53
177.54
177.55
177.56
177.57
177.57
177.58
177.59
177.60
177.61
177.62
177.62

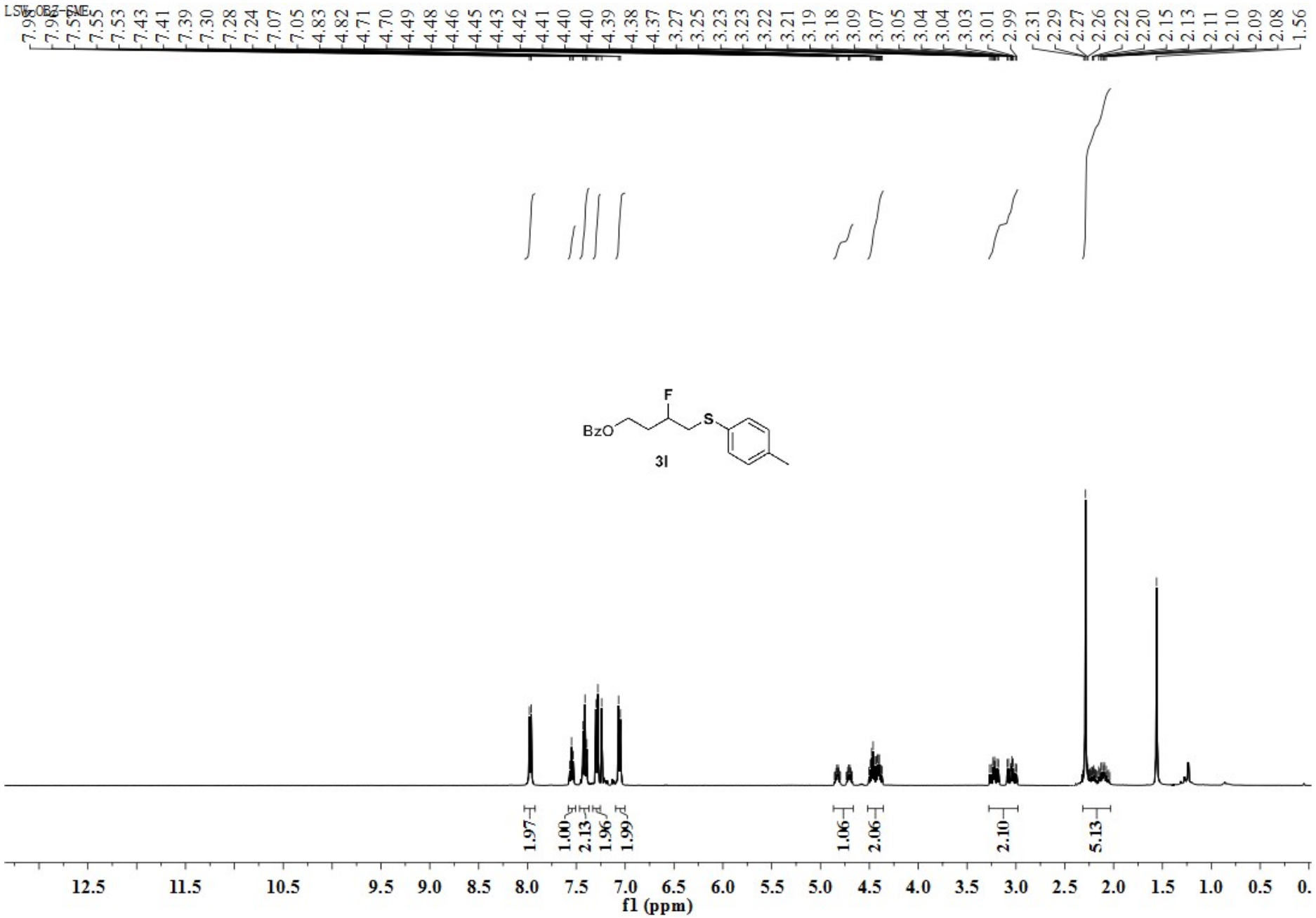


3k

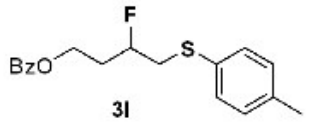
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210

f1 (ppm)

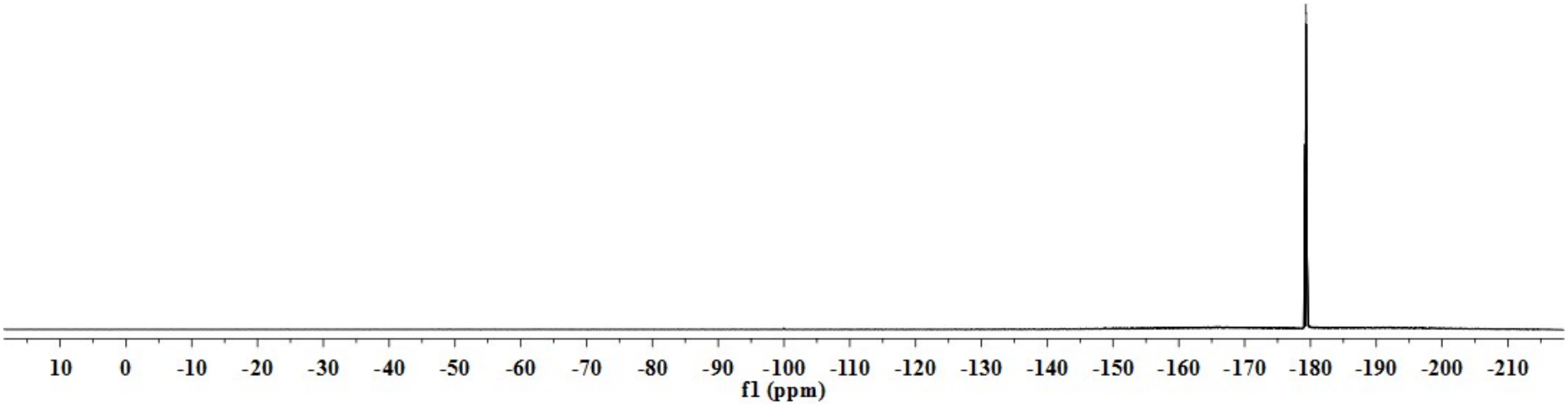

LSW-2S-STOL
173.47
137.01
131.59
130.84
129.89
92.68
91.53
63.82
56.35
40.24
39.19
39.04
38.50
34.62
34.05
30.75
30.61
28.78
24.70
24.31
24.28
21.05
S
S
O
O
F
S
3k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

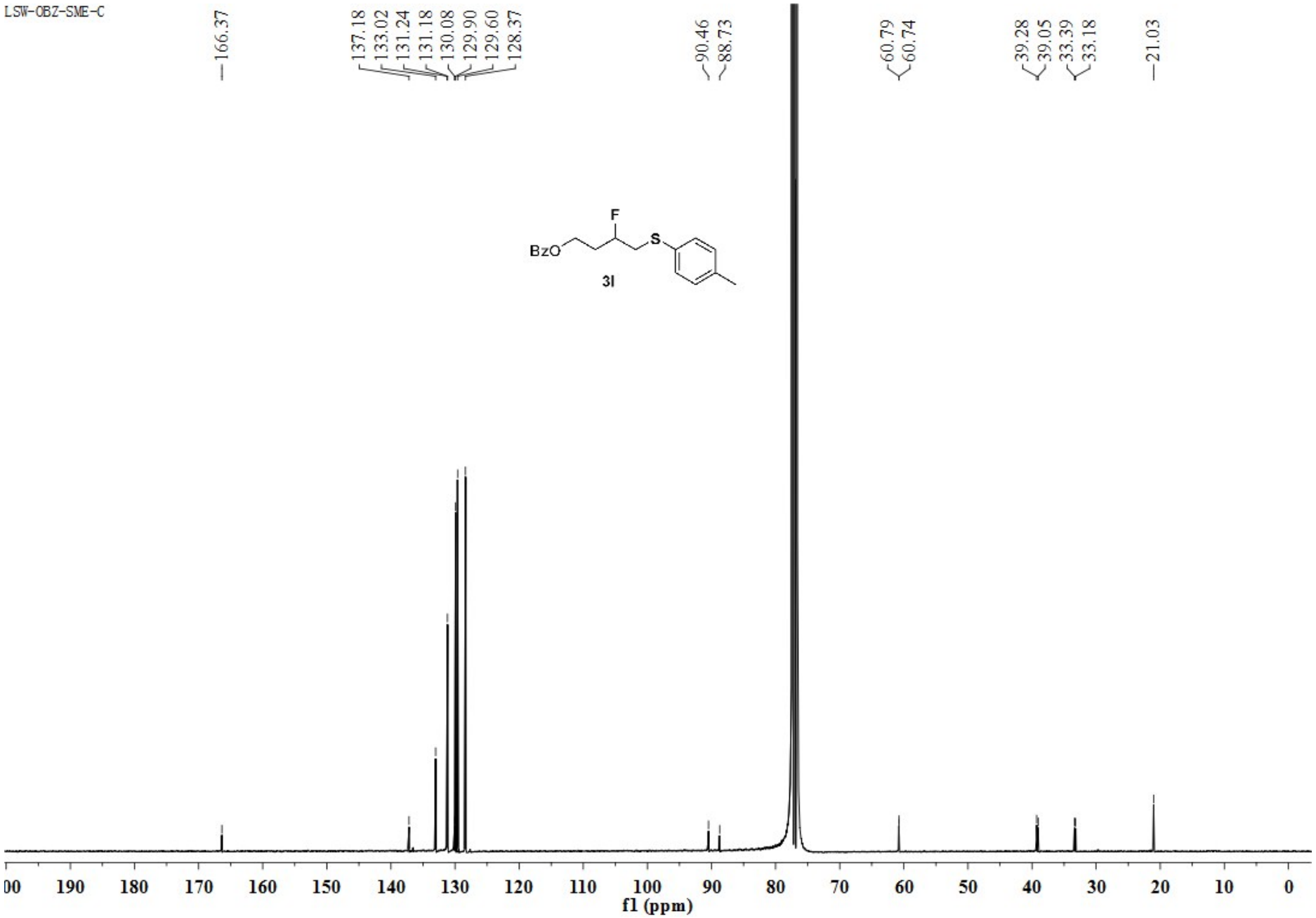

LSW-OBz-EME
7.98
7.96
7.55
7.53
7.43
7.41
7.39
7.30
7.28
7.24
7.07
7.05
4.83
4.82
4.71
4.70
4.49
4.48
4.46
4.45
4.43
4.42
4.41
4.40
4.40
4.39
4.38
4.37
3.27
3.25
3.23
3.23
3.22
3.21
3.19
3.18
3.09
3.07
3.05
3.04
3.04
3.03
3.01
2.99
2.31
2.29
2.27
2.26
2.22
2.20
2.15
2.13
2.11
2.10
2.09
2.08
1.56
F
BzO
S
3l
1.97
1.00
2.13
1.96
1.99
1.06
2.06
2.10
5.13
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

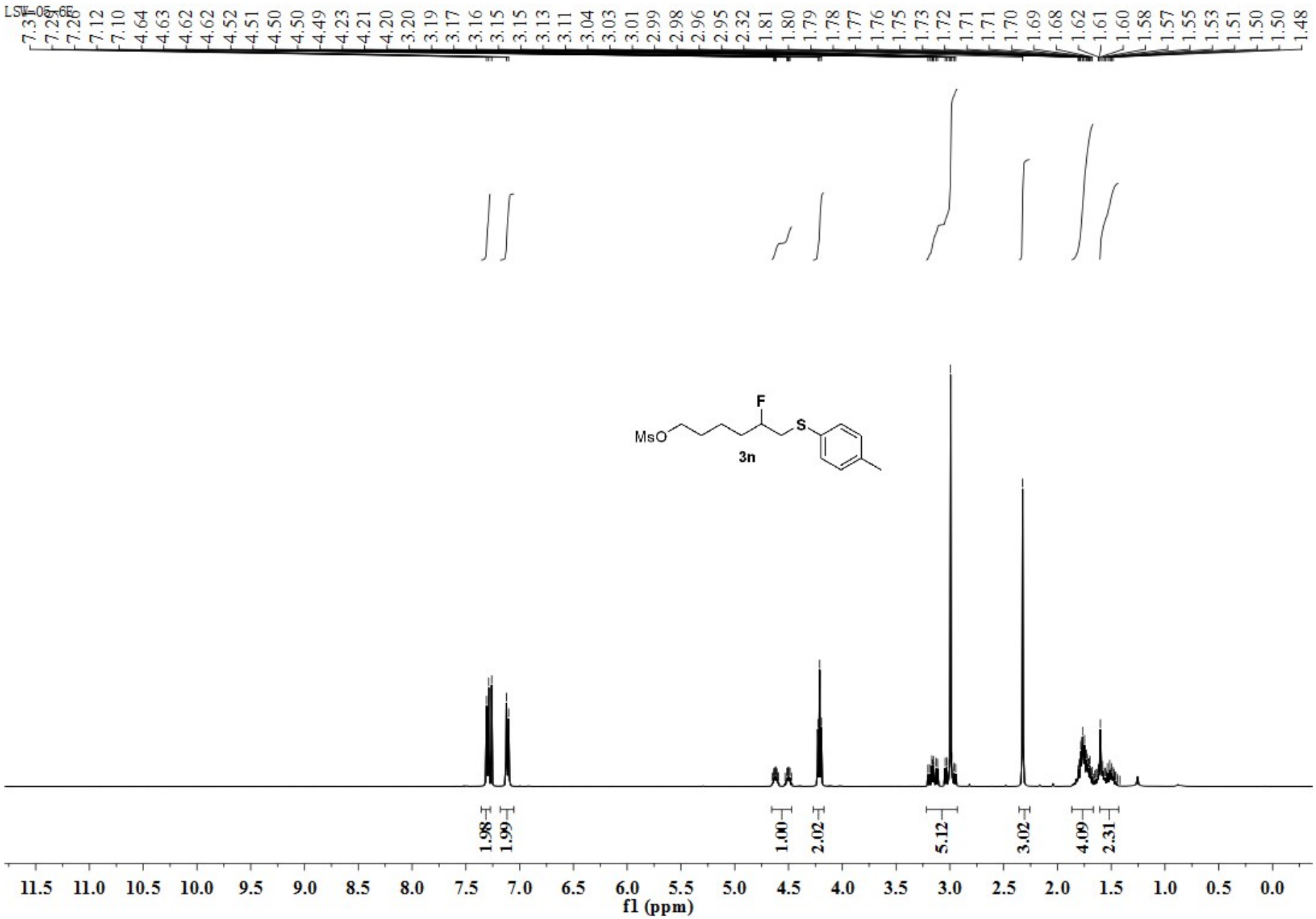
LSW-OBZ-SME



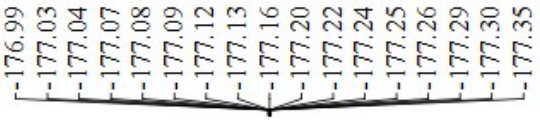
3l




LSW-OBZ-SME-C
166.37
137.18
133.02
131.24
131.18
130.08
129.90
129.60
128.37
90.46
88.73
60.79
60.74
39.28
39.05
33.39
33.18
21.03
F
BzO
S
3l
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

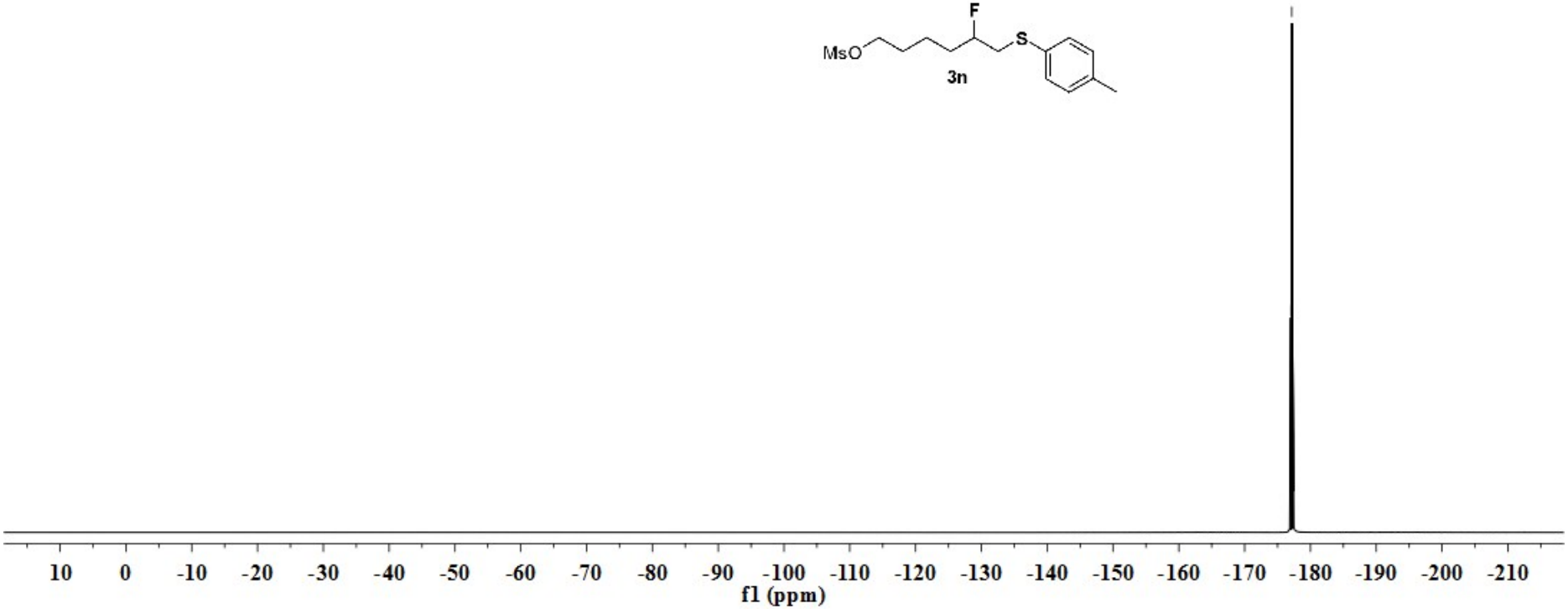

7.31
7.29
7.28
7.12
7.10
4.64
4.63
4.62
4.62
4.52
4.51
4.50
4.50
4.49
4.23
4.21
4.20
3.20
3.19
3.17
3.16
3.15
3.15
3.13
3.11
3.04
3.03
3.01
2.99
2.98
2.96
2.95
2.32
1.81
1.80
1.79
1.78
1.77
1.76
1.75
1.73
1.72
1.71
1.71
1.70
1.69
1.68
1.62
1.61
1.60
1.58
1.57
1.55
1.53
1.51
1.50
1.50
1.48
F
S
MsO
3n
1.98
1.99
1.00
2.02
5.12
3.02
4.09
2.31
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-05-6E


176.99
177.03
177.04
177.07
177.08
177.09
177.12
177.13
177.16
177.20
177.22
177.24
177.25
177.26
177.29
177.30
177.35

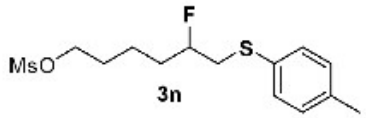
F
MsO
S

3n

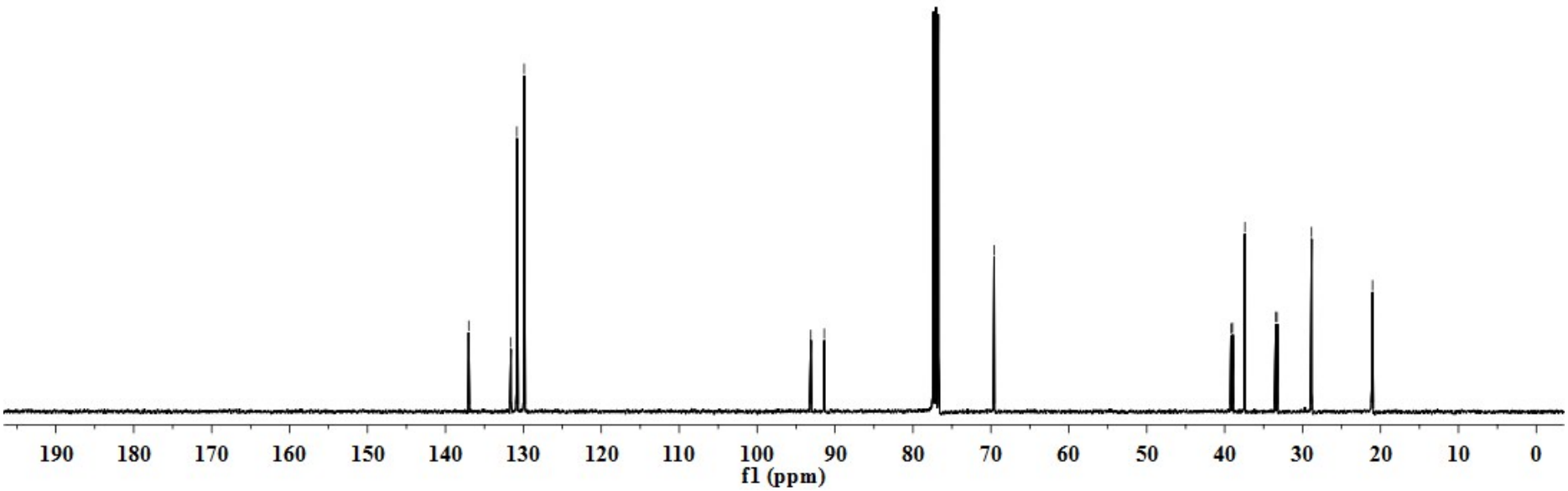

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

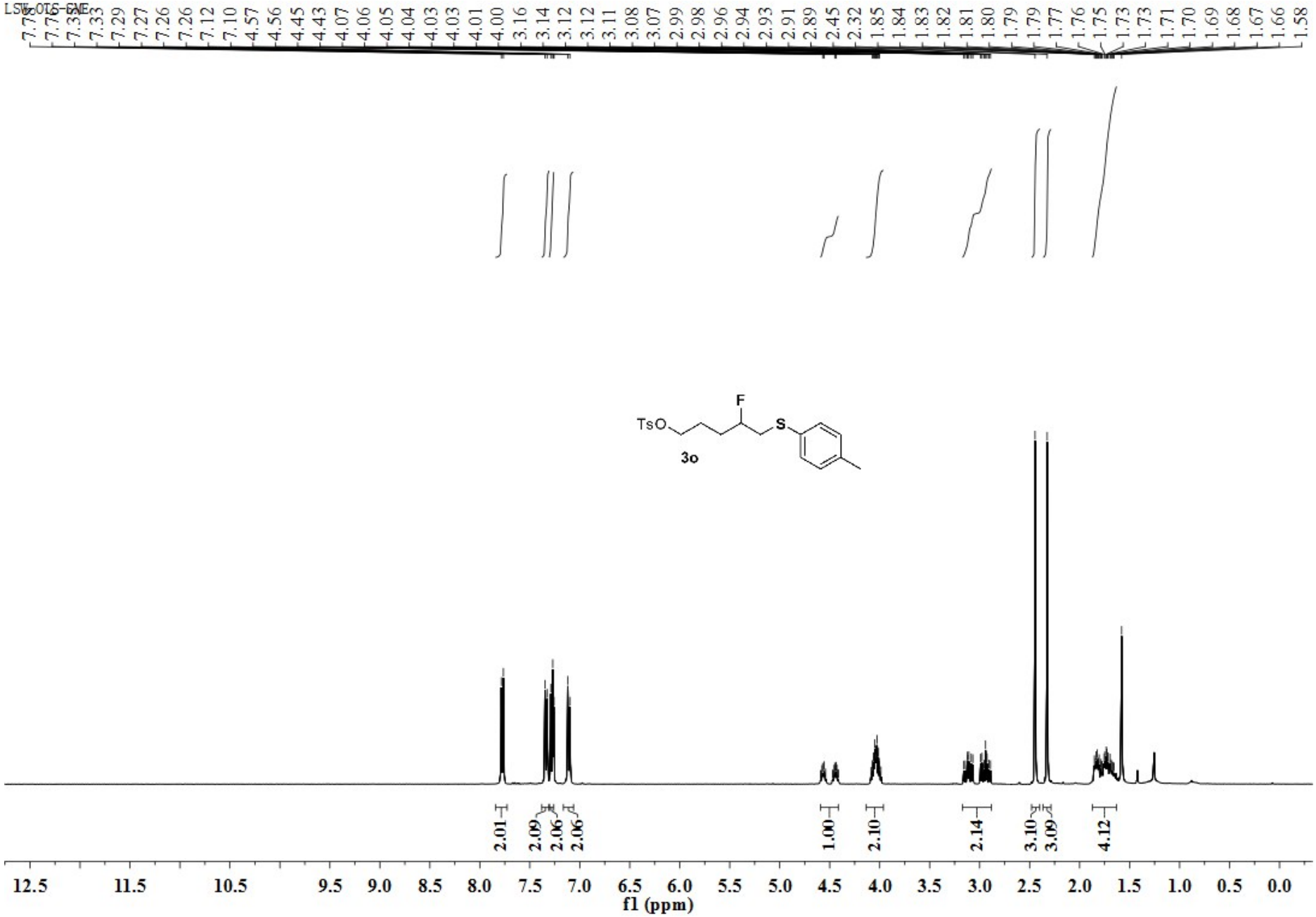
LSW-6E

137.01
131.61
130.83
129.90
93.10
91.38
69.58
39.19
38.95
37.40
33.45
33.24
28.85
21.08
21.05
21.02



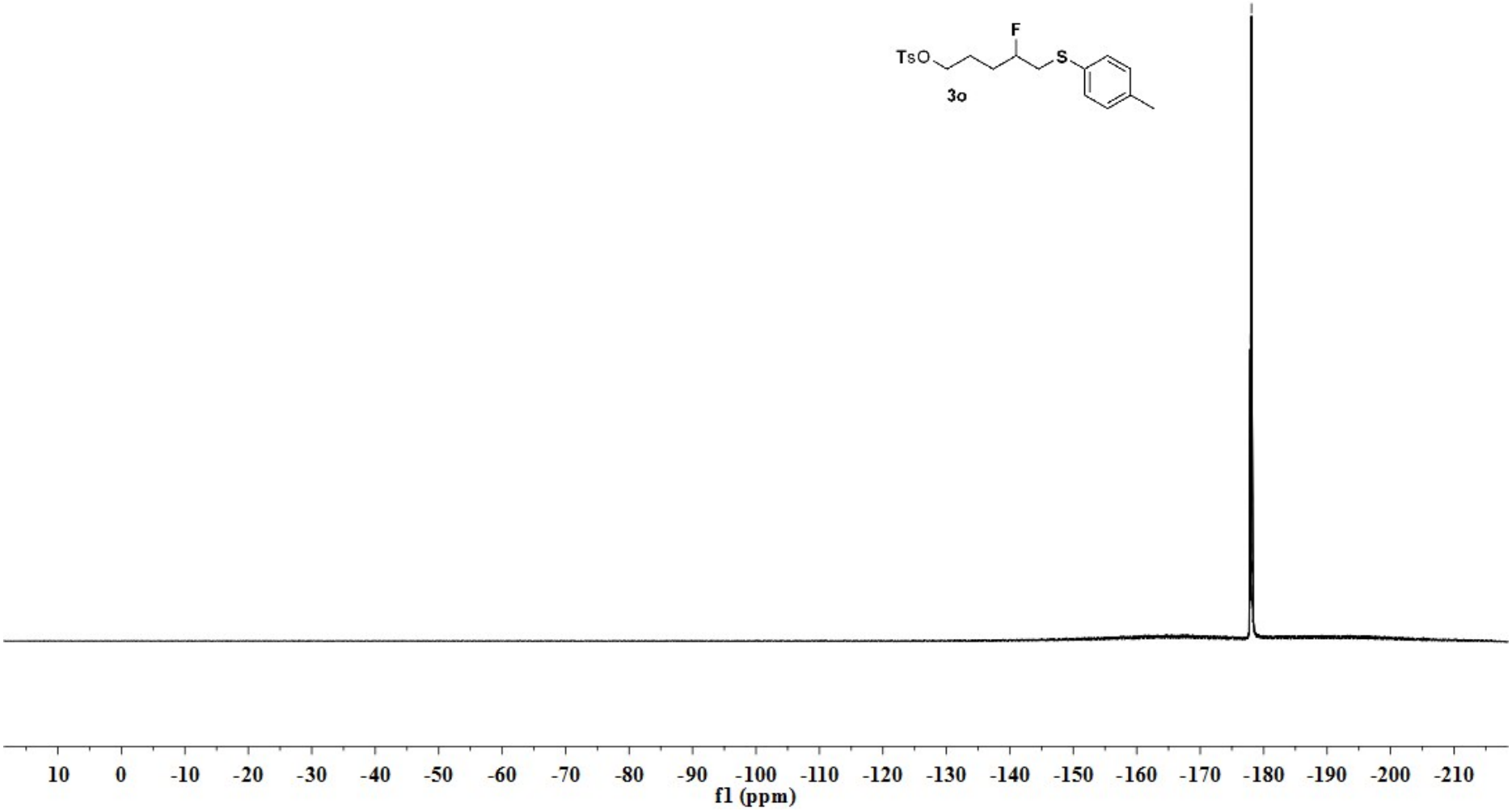
3n

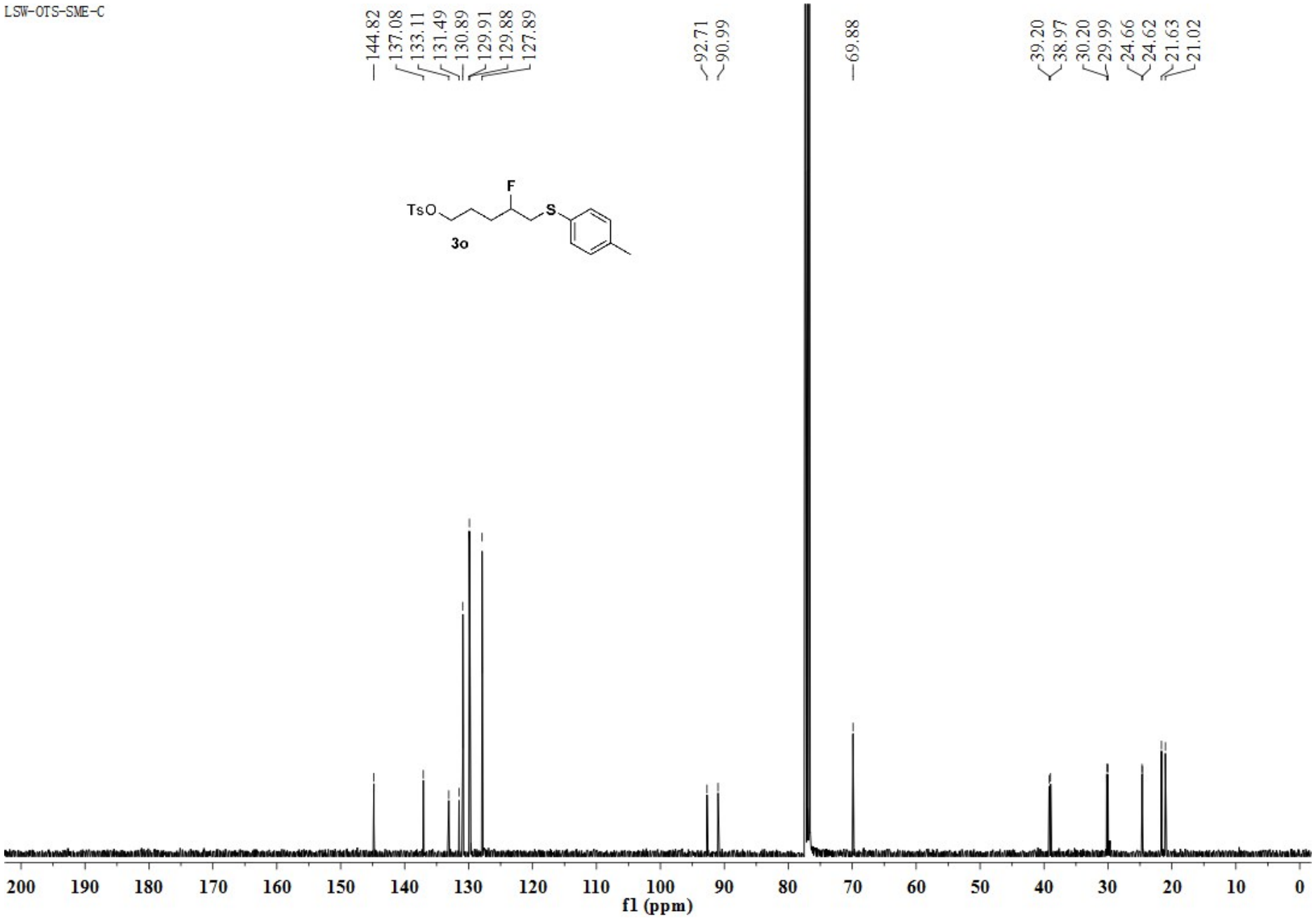


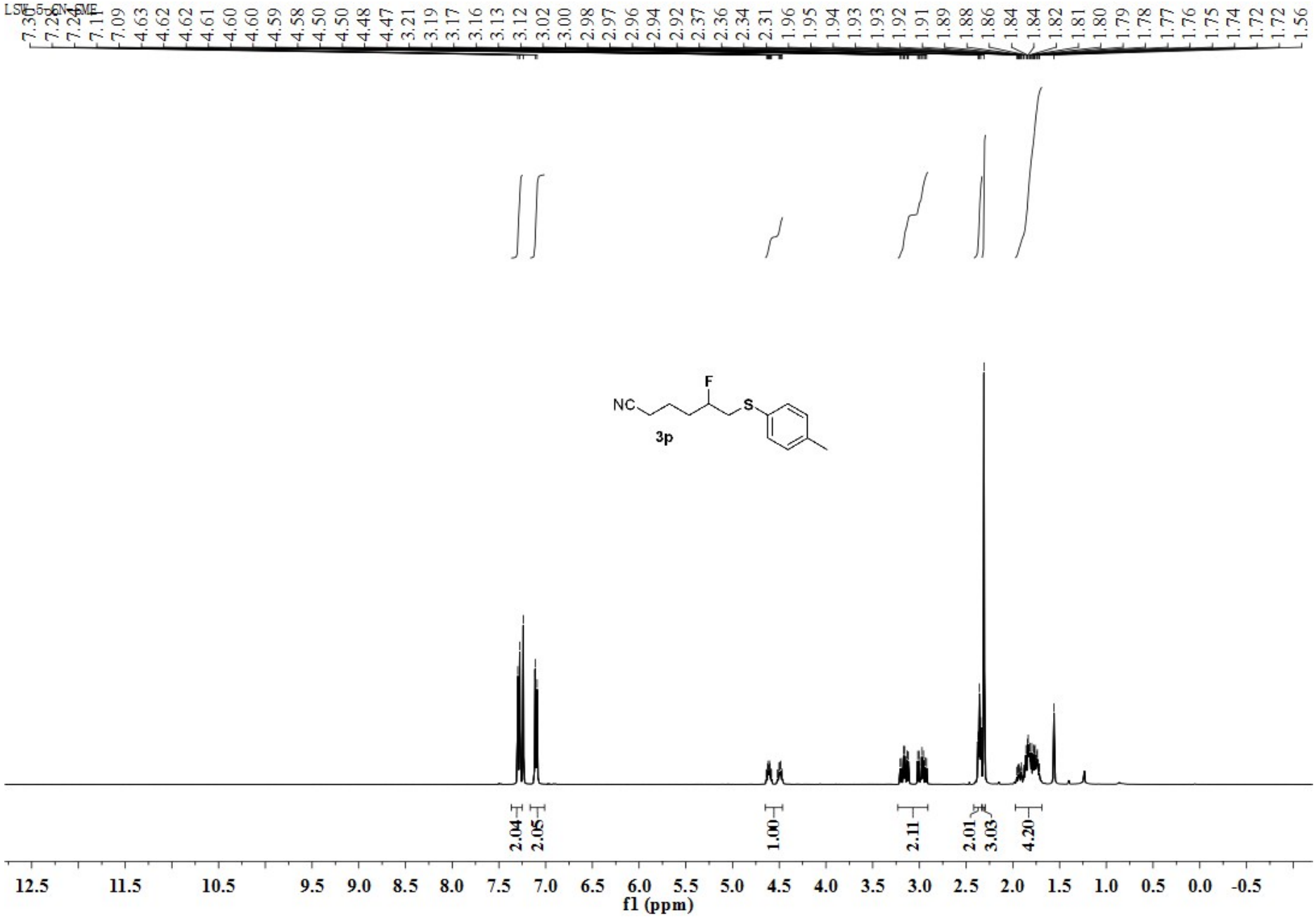

LSW-OTS-CME
7.78
7.76
7.35
7.33
7.29
7.27
7.26
7.26
7.12
7.10
4.57
4.56
4.45
4.43
4.07
4.06
4.05
4.04
4.03
4.03
4.01
4.00
3.16
3.14
3.12
3.12
3.11
3.08
3.07
2.99
2.98
2.96
2.94
2.93
2.91
2.89
2.45
2.32
1.85
1.84
1.83
1.82
1.81
1.80
1.79
1.79
1.77
1.76
1.75
1.73
1.73
1.71
1.70
1.69
1.68
1.67
1.66
1.58
TsO
F
S
3o
2.01
2.09
2.06
2.06
1.00
2.10
2.14
3.10
3.09
4.12
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-OTS-SME

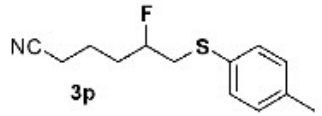
3o



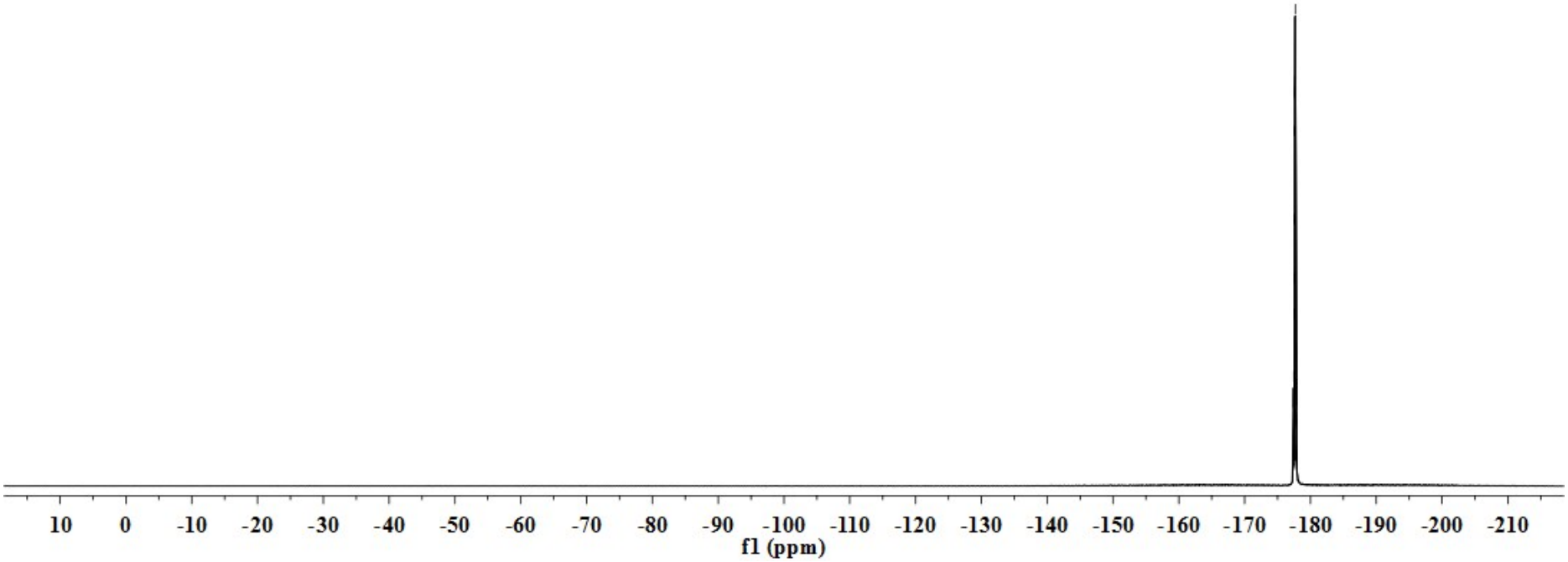

LSW-OTS-SME-C
144.82
137.08
133.11
131.49
130.89
129.91
129.88
127.89
92.71
90.99
69.88
39.20
38.97
30.20
29.99
24.66
24.62
21.63
21.02
F
TsO
S
3o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

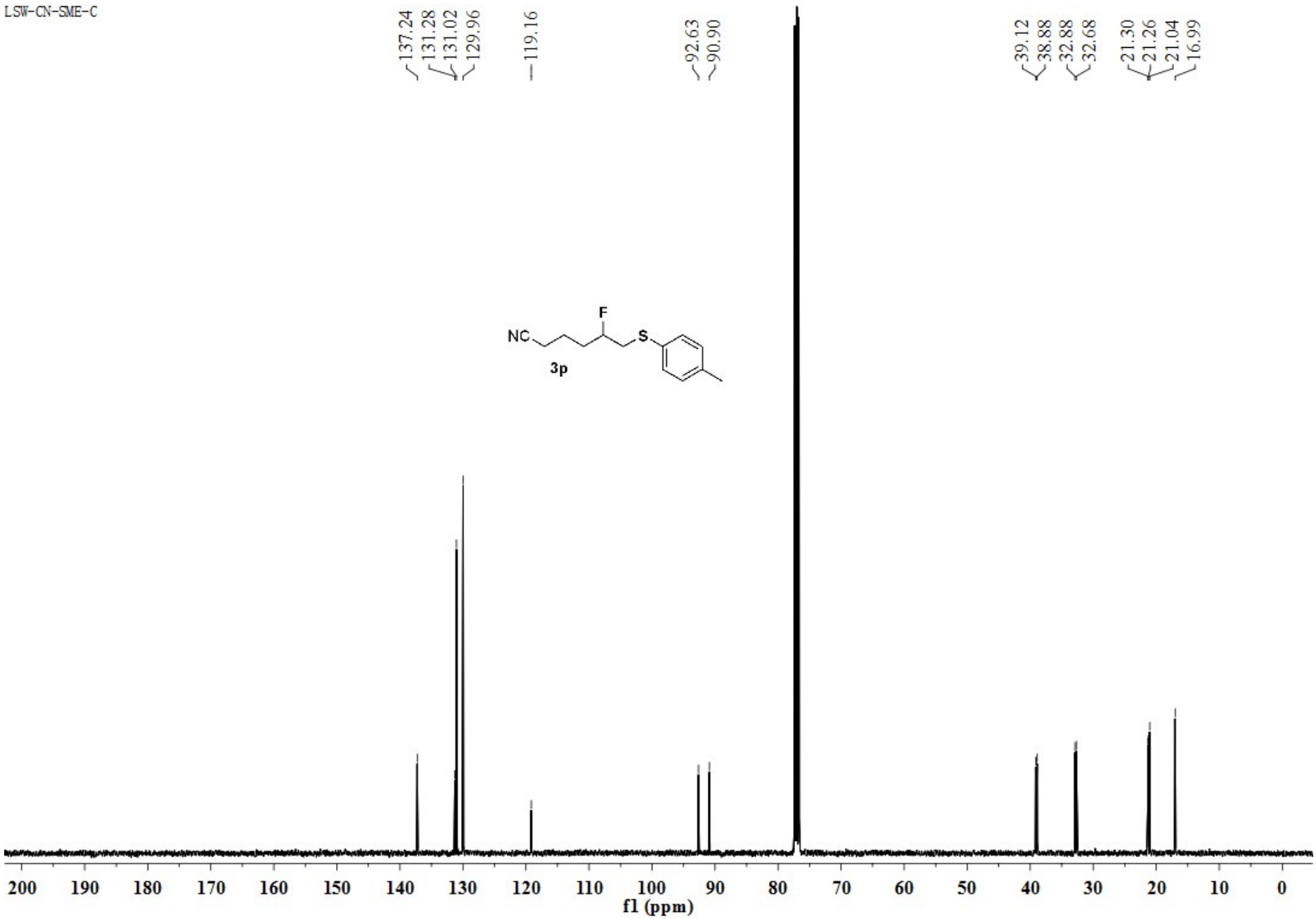

LSW-5-CN-EME
7.30
7.28
7.24
7.11
7.09
4.63
4.62
4.62
4.61
4.60
4.60
4.59
4.58
4.50
4.50
4.48
4.47
3.21
3.19
3.17
3.16
3.13
3.12
3.02
3.00
2.98
2.97
2.96
2.94
2.92
2.37
2.36
2.34
2.31
1.96
1.95
1.94
1.93
1.93
1.92
1.91
1.89
1.88
1.86
1.84
1.84
1.82
1.81
1.80
1.79
1.78
1.77
1.76
1.75
1.74
1.72
1.72
1.56
F
NC
S
3p
2.04
2.05
1.00
2.11
2.01
3.03
4.20
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

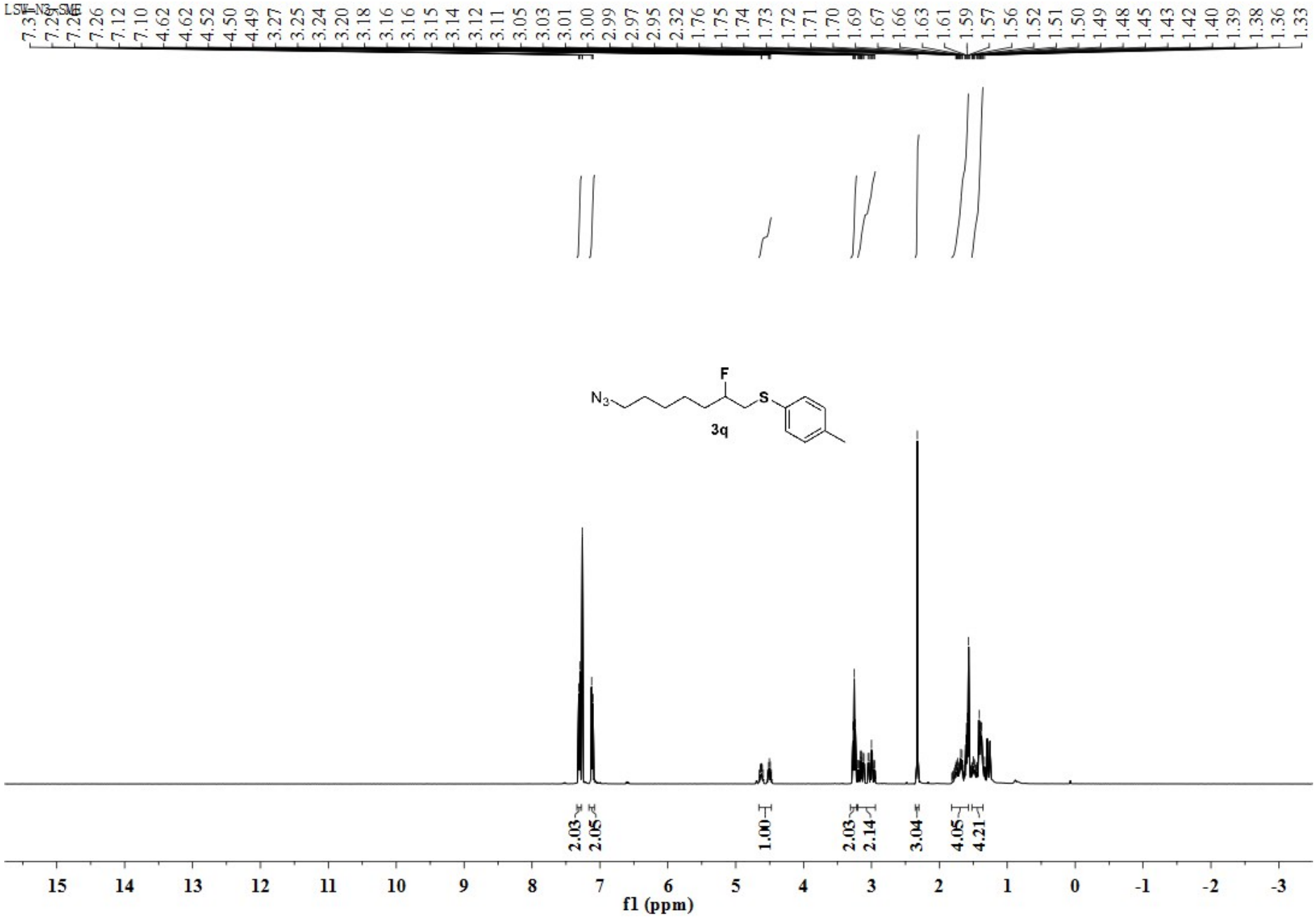
LSW-6-CN-SME



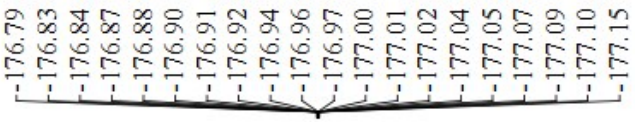
3p

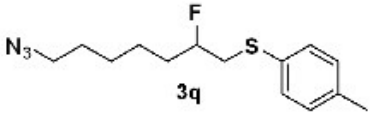



LSW-CN-SME-C
137.24
131.28
131.02
129.96
119.16
92.63
90.90
39.12
38.88
32.88
32.68
21.30
21.26
21.04
16.99
F
NC
S
3p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

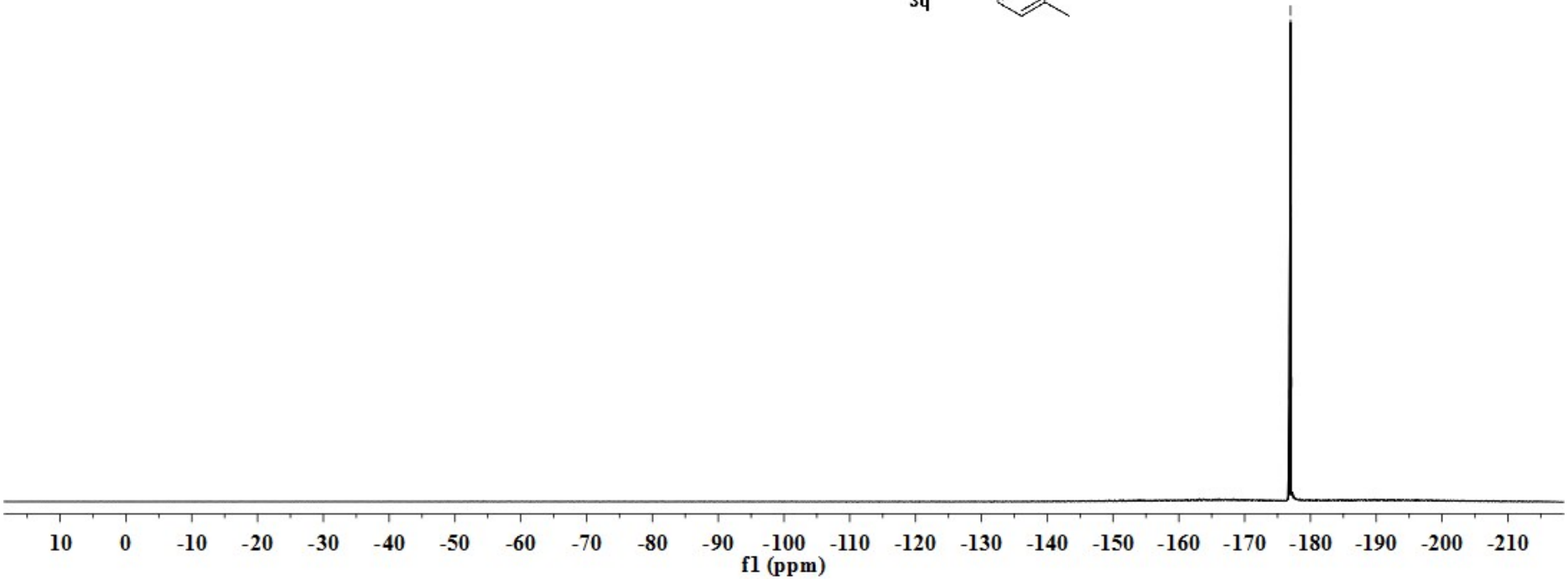

LSW-N3-SM5
7.31
7.26
7.26
7.12
7.10
4.62
4.62
4.52
4.50
4.49
3.27
3.25
3.24
3.20
3.18
3.16
3.16
3.15
3.14
3.12
3.11
3.05
3.03
3.01
3.00
2.99
2.97
2.95
2.32
1.76
1.75
1.74
1.73
1.72
1.71
1.70
1.69
1.67
1.66
1.63
1.61
1.59
1.57
1.56
1.52
1.51
1.50
1.49
1.48
1.45
1.43
1.42
1.40
1.39
1.38
1.36
1.33
F
N3
S
3q
2.03
2.05
1.00
2.03
2.14
3.04
4.05
4.21
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

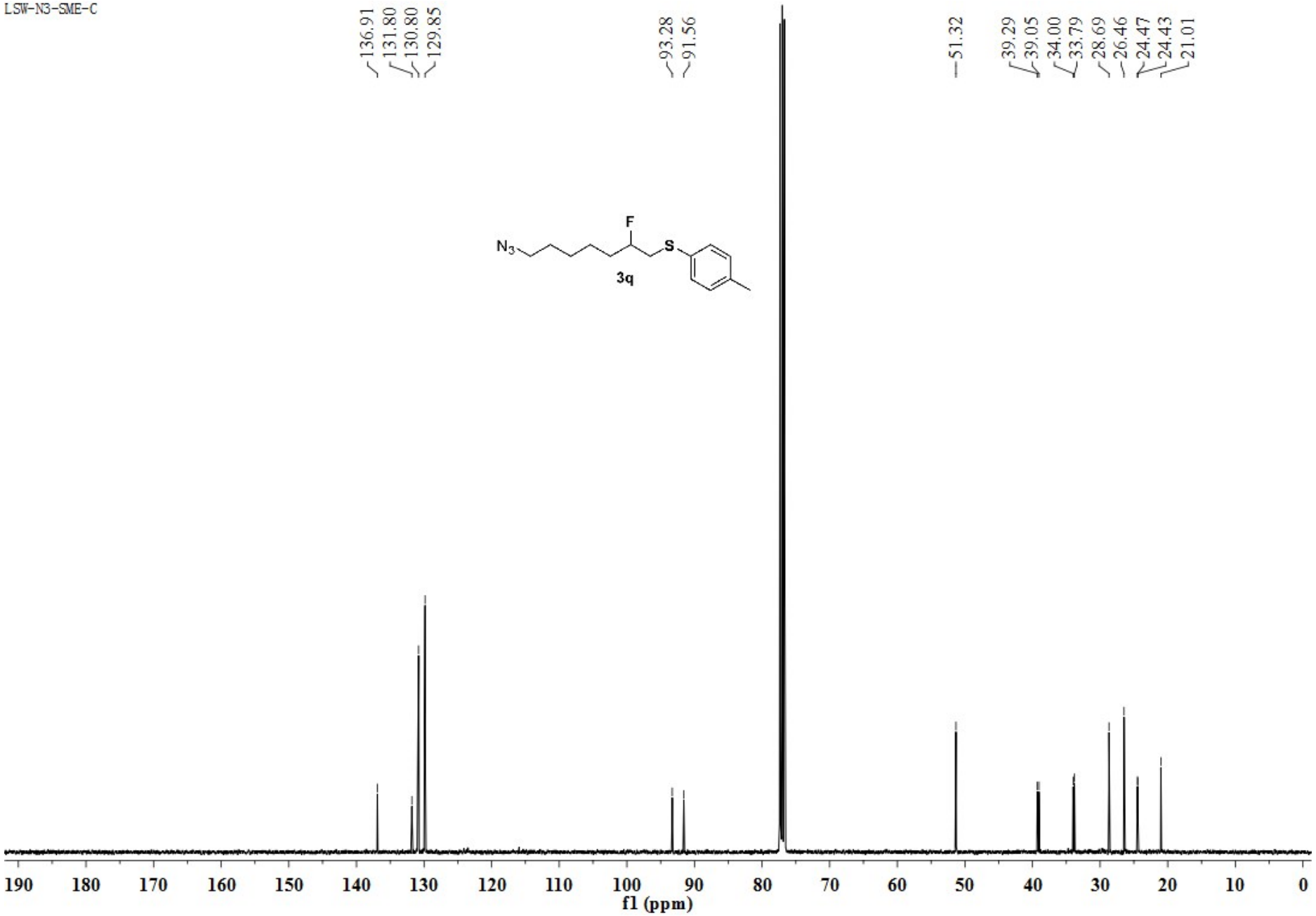
LSW-N3-SME

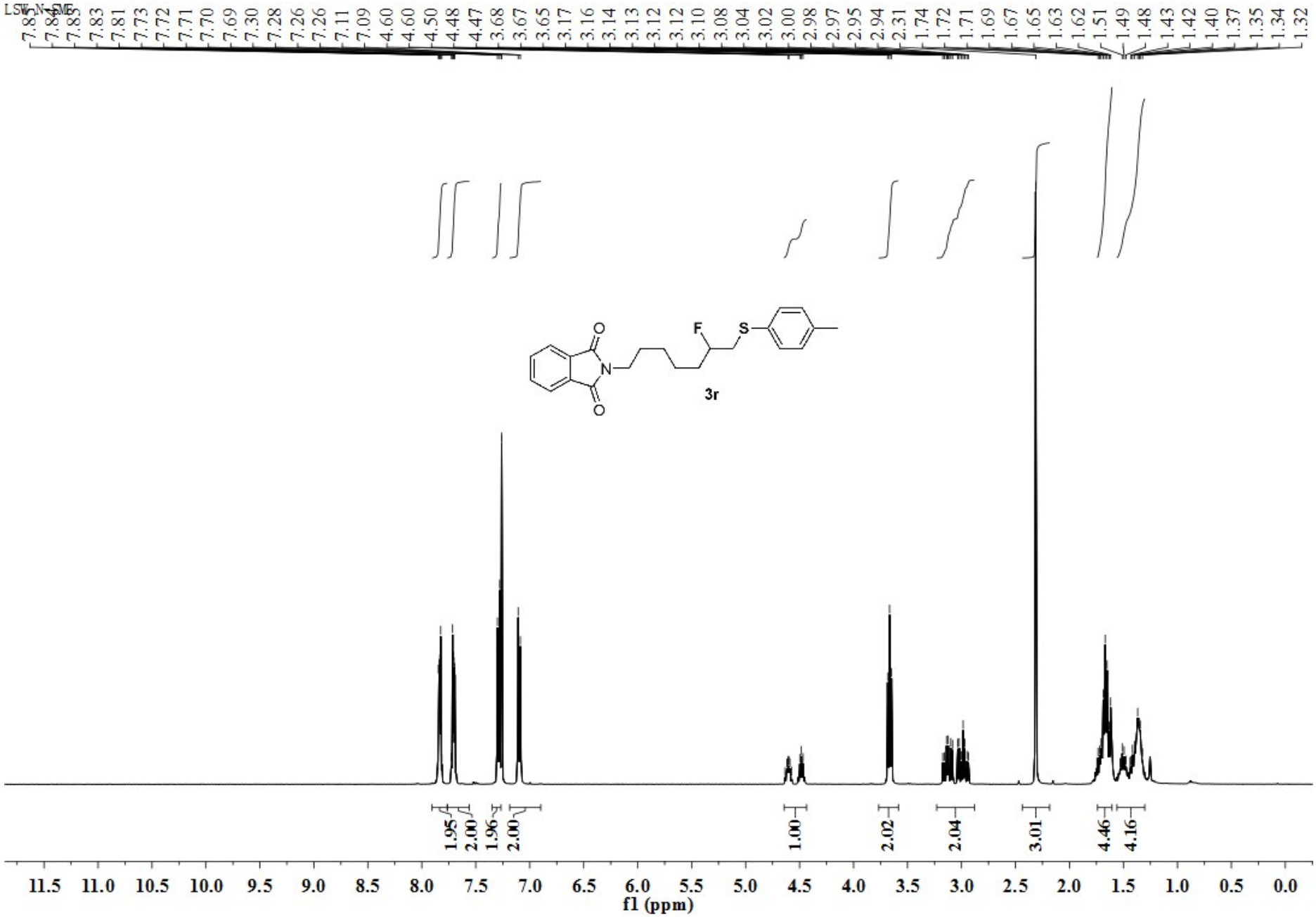

176.79
176.83
176.84
176.87
176.88
176.90
176.91
176.92
176.94
176.96
176.97
177.00
177.01
177.02
177.04
177.05
177.07
177.09
177.10
177.15


F
N3
S

3q


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

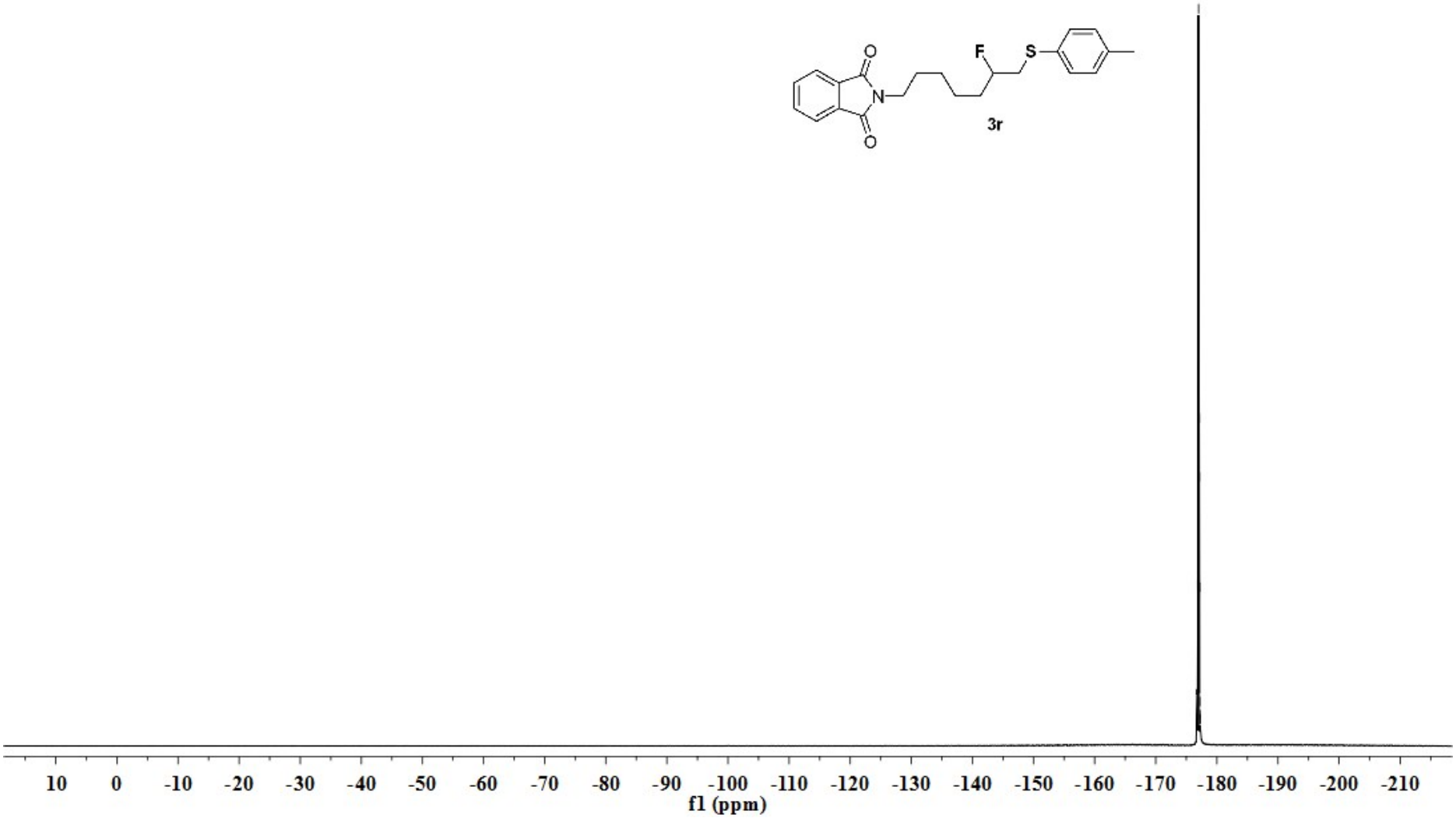

LSW-N3-SME-C
136.91
131.80
130.80
129.85
93.28
91.56
51.32
39.29
39.05
34.00
33.79
28.69
26.46
24.47
24.43
21.01
F
N3
S
3q
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


LSW-N-SME
7.85
7.84
7.85
7.83
7.81
7.73
7.72
7.71
7.70
7.69
7.30
7.28
7.26
7.26
7.11
7.09
4.60
4.60
4.50
4.48
4.47
3.68
3.67
3.65
3.17
3.16
3.14
3.13
3.12
3.12
3.10
3.08
3.04
3.02
3.00
2.98
2.97
2.95
2.94
2.31
1.74
1.72
1.71
1.69
1.67
1.65
1.63
1.62
1.51
1.49
1.48
1.43
1.42
1.40
1.37
1.35
1.34
1.32
O
N
O
F
S
3r
1.95
2.00
1.96
2.00
1.00
2.02
2.04
3.01
4.46
4.16
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-N-SME

176.79
176.80
176.83
176.88
176.89
176.91
176.93
176.94
176.95
176.96
176.99
177.01
177.02
177.04
177.06
177.09
177.10
177.11
177.14
177.15
177.19
177.22
177.25
177.26
177.26

3r



LSW-N-SME-C

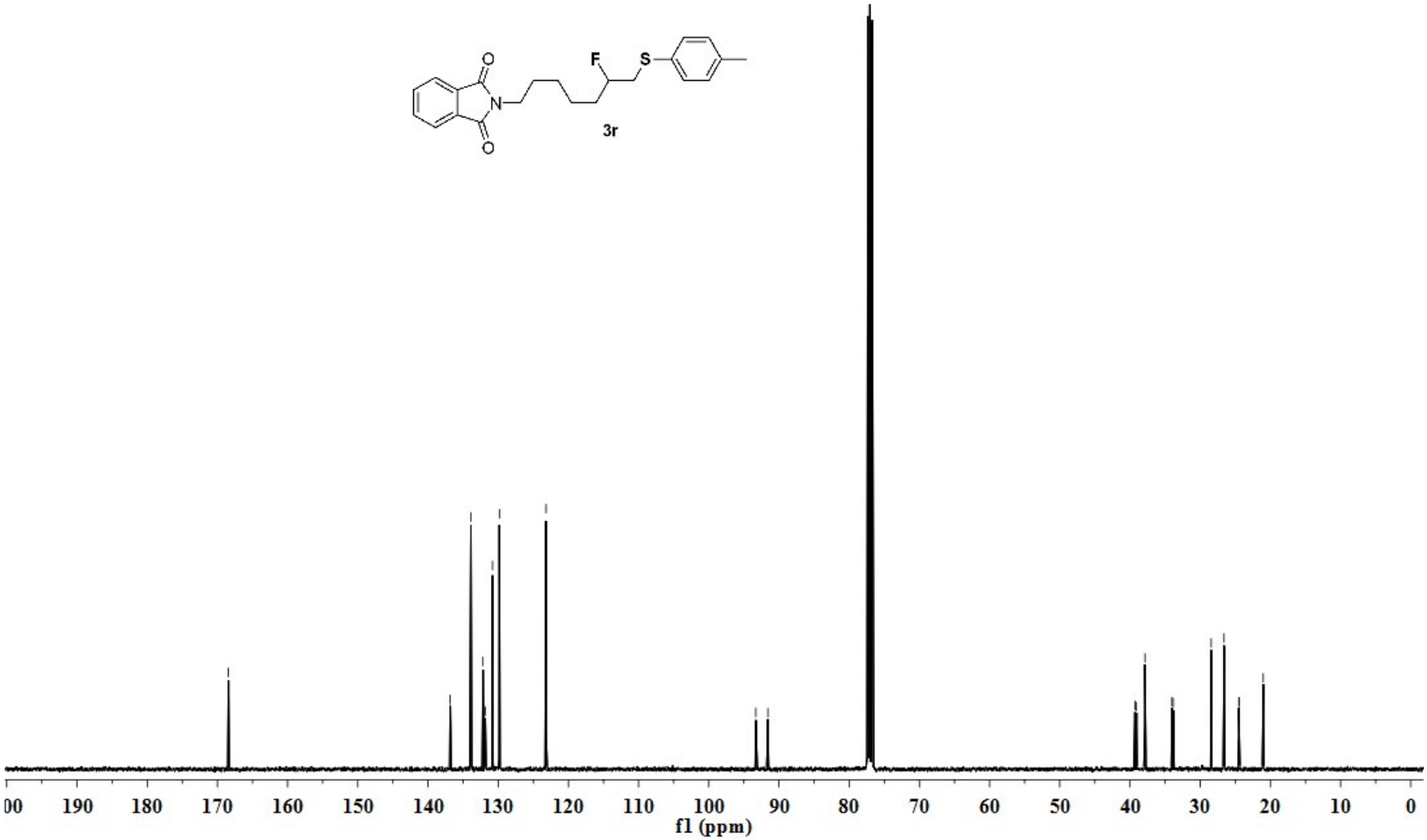
168.43

136.84
133.88
132.18
131.83
130.81
129.82
123.19

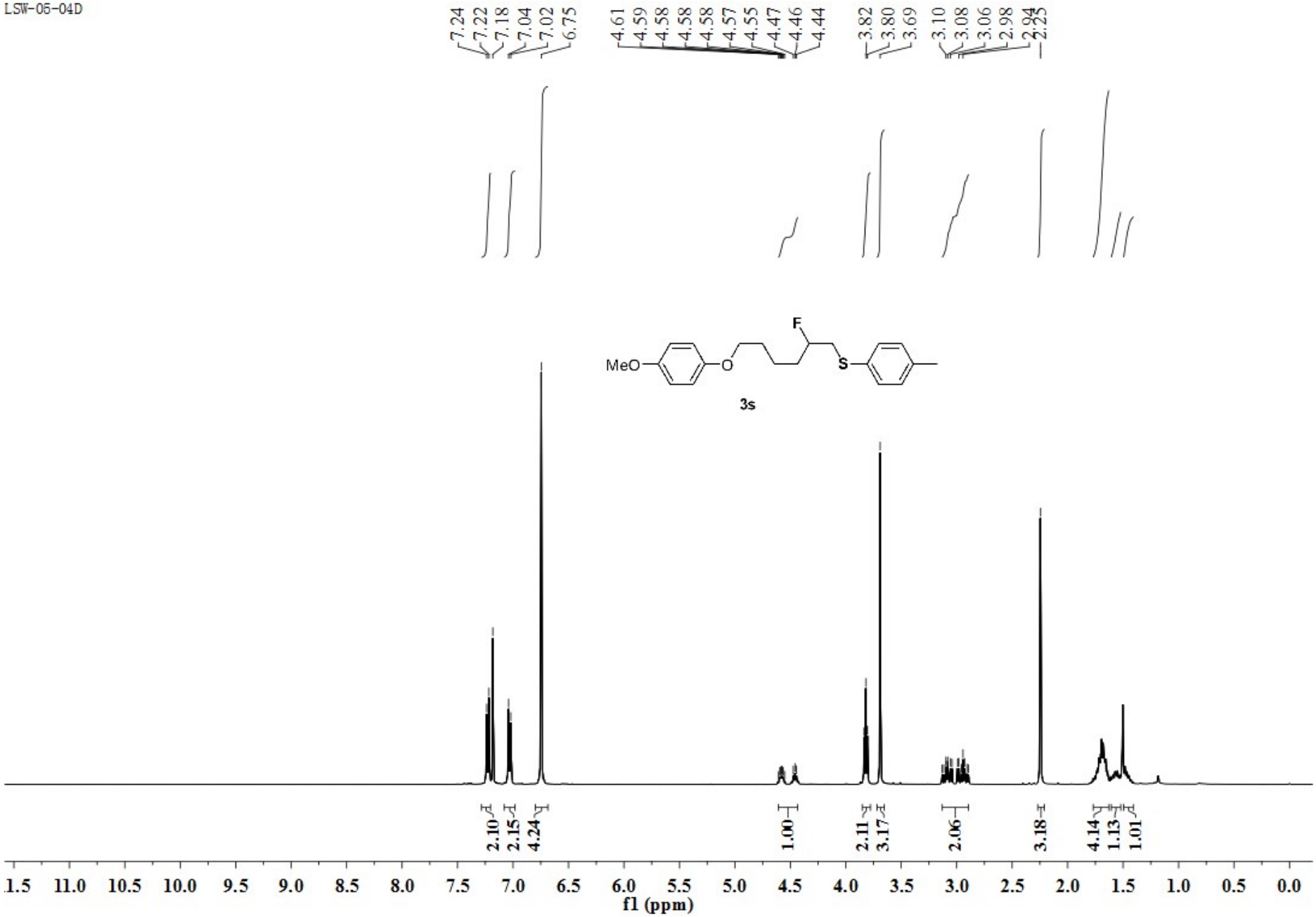
93.30
91.58

39.31
39.07
37.86
34.03
33.83
28.44
26.60
24.48
24.45
21.02

3r



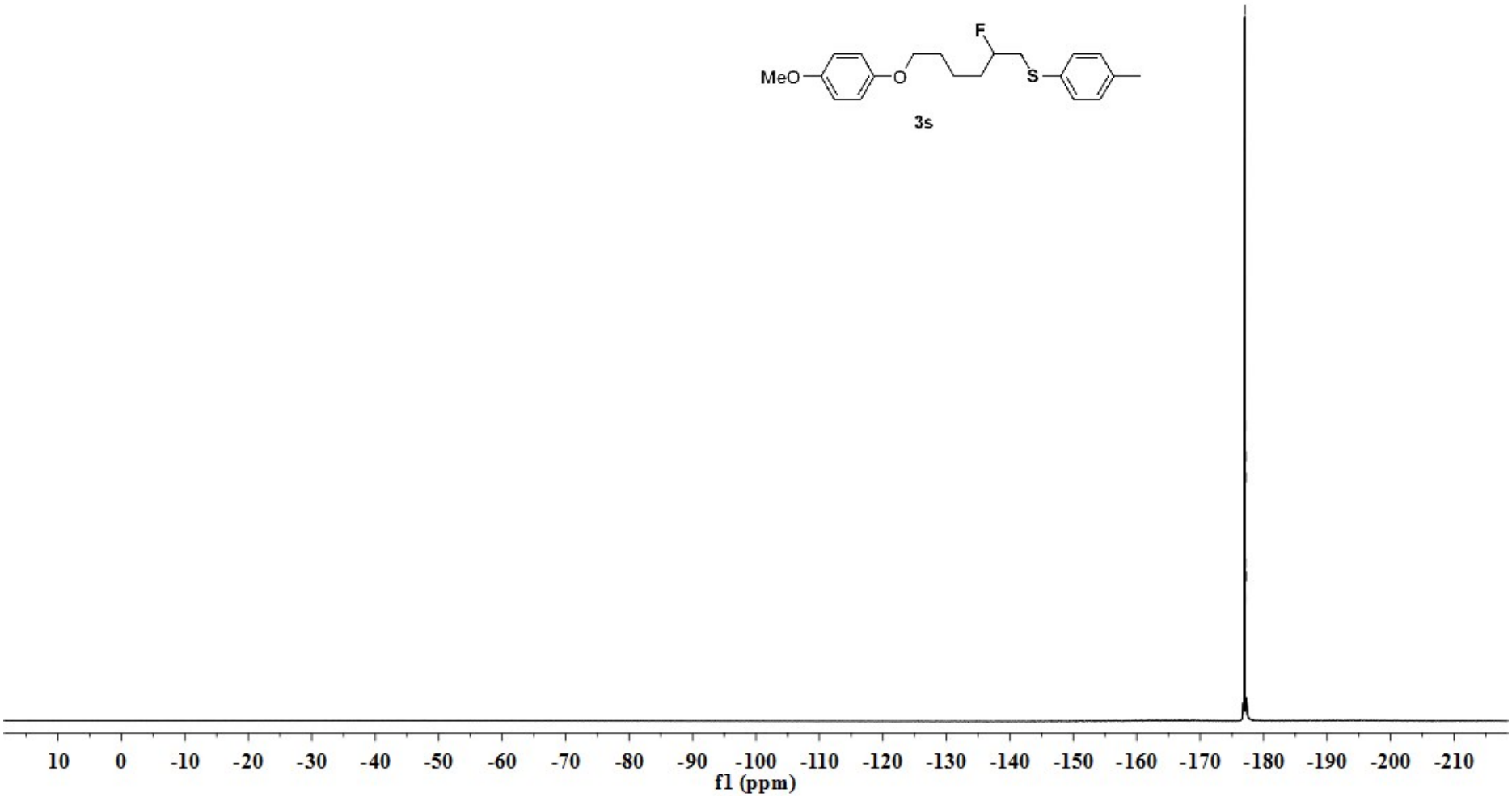
LSW-05-04D


7.24
7.22
7.18
7.04
7.02
6.75
4.61
4.59
4.58
4.58
4.58
4.57
4.55
4.47
4.46
4.44
3.82
3.80
3.69
3.10
3.08
3.06
2.98
2.94
2.25
F
MeO
O
S
3s
2.10
2.15
4.24
1.00
2.11
3.17
2.06
3.18
4.14
1.13
1.01
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

LSW-05-04D

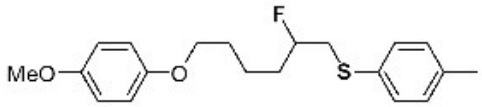
176.86
176.91
176.92
176.94
176.96
176.97
176.99
177.00
177.01
177.04
177.05
177.07
177.09
177.12
177.13
177.14
177.17
177.18
177.22

3s

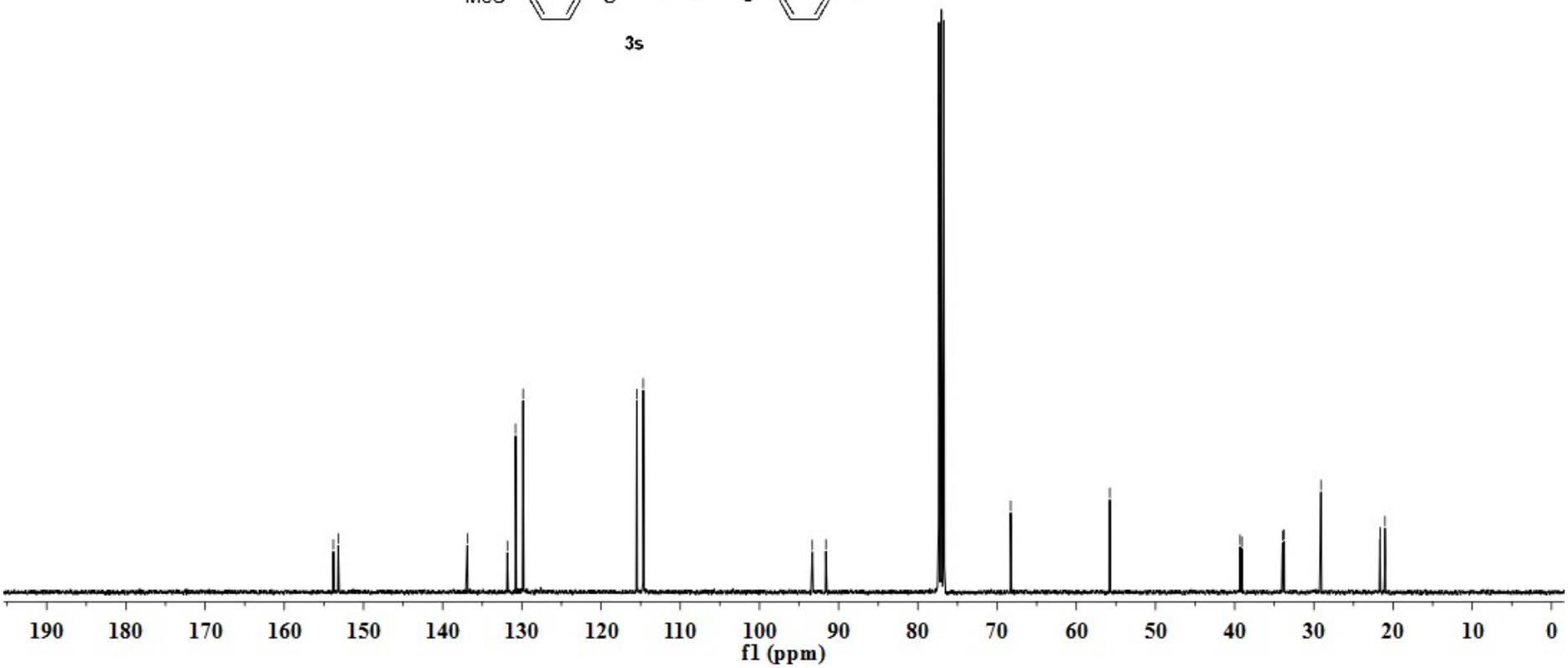


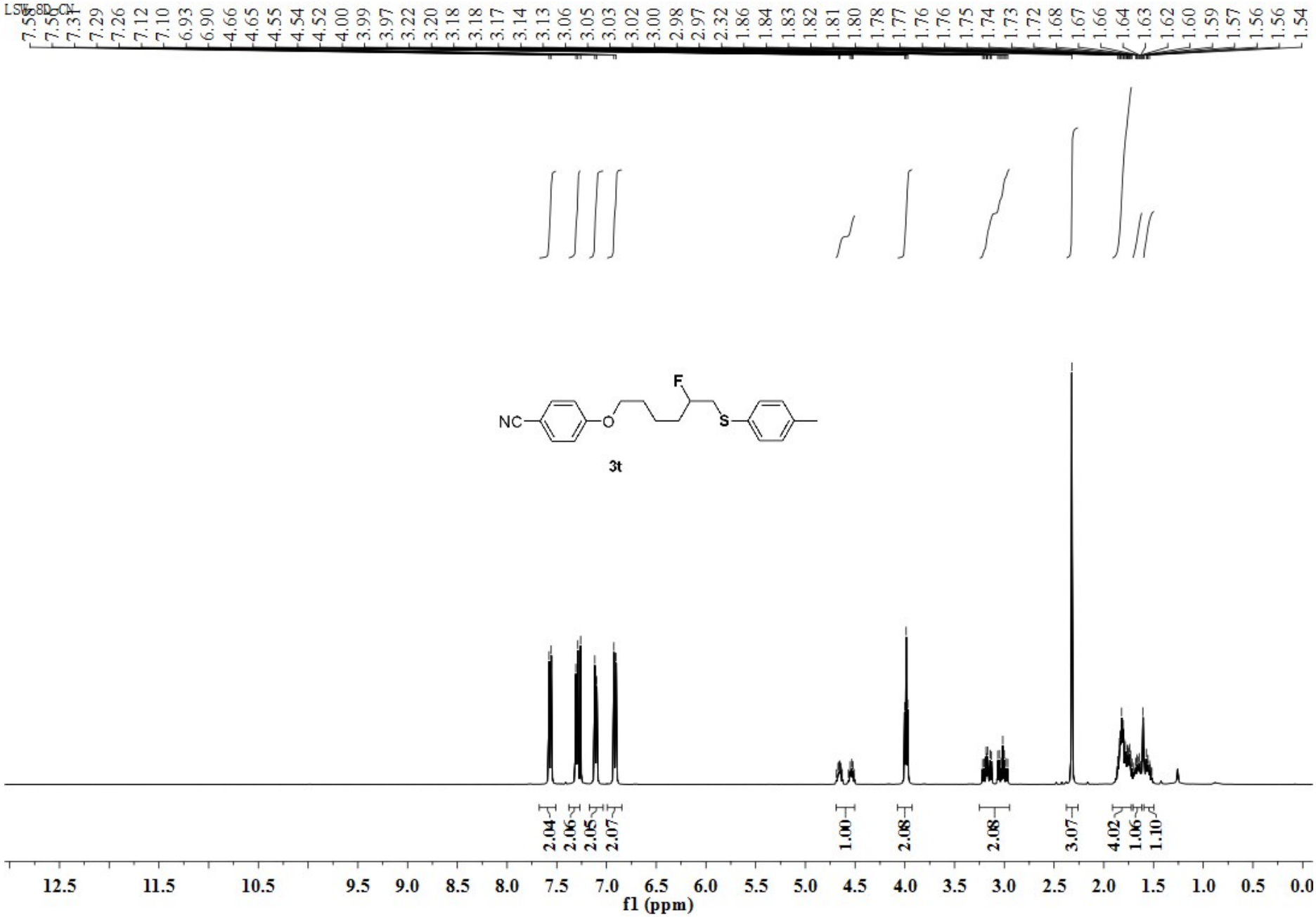
LSW-05-4D

153.80
153.18
136.88
131.82
130.79
129.85
115.48
114.68
93.33
91.61
68.28
55.76
39.31
39.08
33.95
33.75
29.10
21.64
21.61
21.03



3s



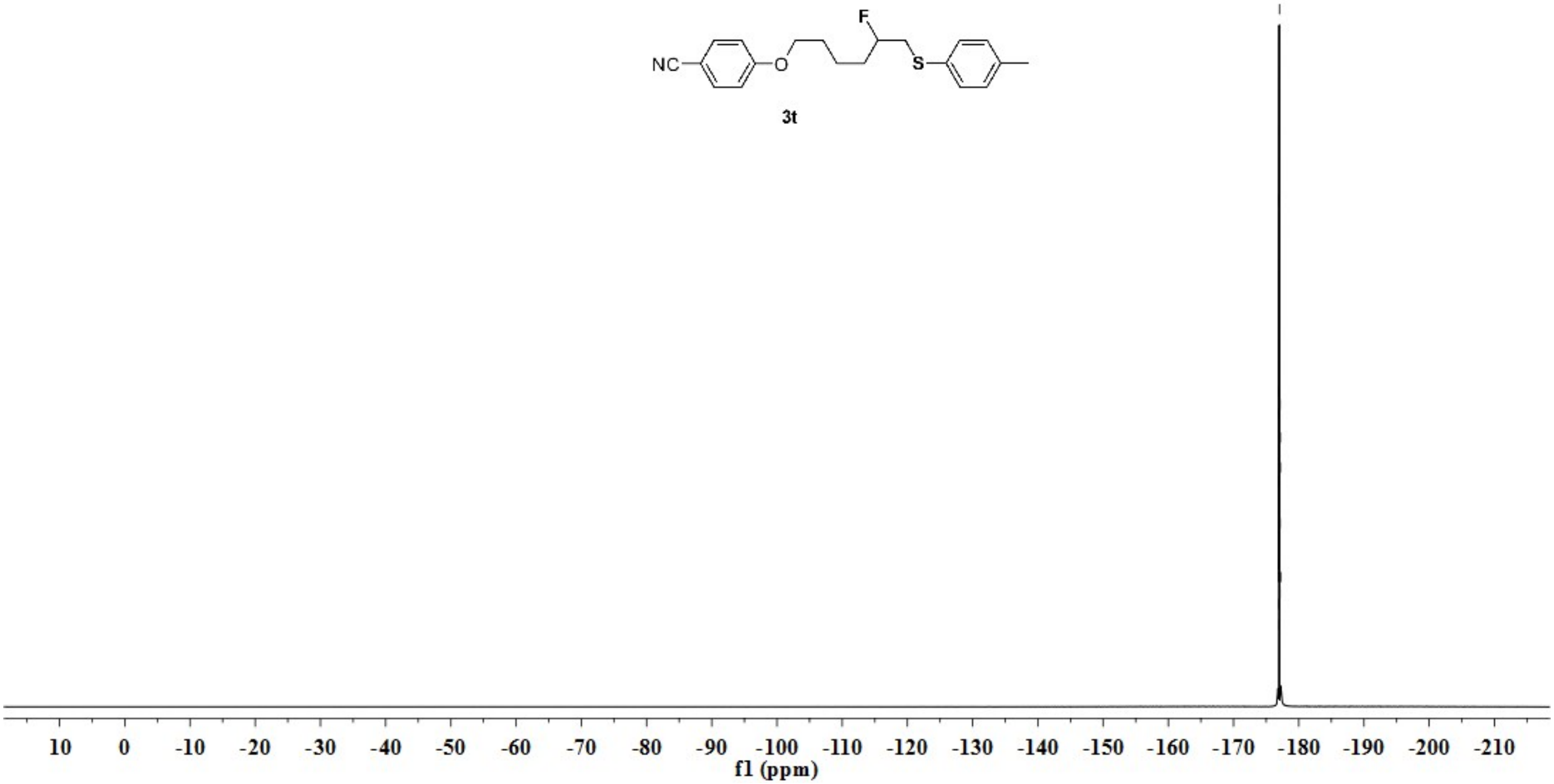

LSW-8D-CN
7.58
7.56
7.31
7.29
7.26
7.12
7.10
6.93
6.90
4.66
4.65
4.55
4.54
4.52
4.00
3.99
3.97
3.22
3.20
3.18
3.18
3.17
3.14
3.13
3.06
3.05
3.03
3.02
3.00
2.98
2.97
2.32
1.86
1.84
1.83
1.82
1.81
1.80
1.78
1.77
1.76
1.76
1.75
1.74
1.73
1.72
1.68
1.67
1.66
1.64
1.63
1.62
1.60
1.59
1.57
1.56
1.56
1.54
F
NC
O
S
3t
2.04
2.06
2.05
2.07
1.00
2.08
2.08
3.07
4.02
1.06
1.10
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-8D-CN


176.87
176.91
176.92
176.95
176.96
176.97
177.00
177.01
177.04
177.05
177.08
177.09
177.12
177.13
177.14
177.17
177.18
177.22

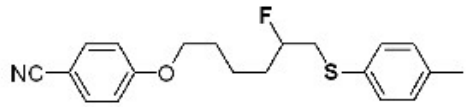
F
NC
O
S

3t

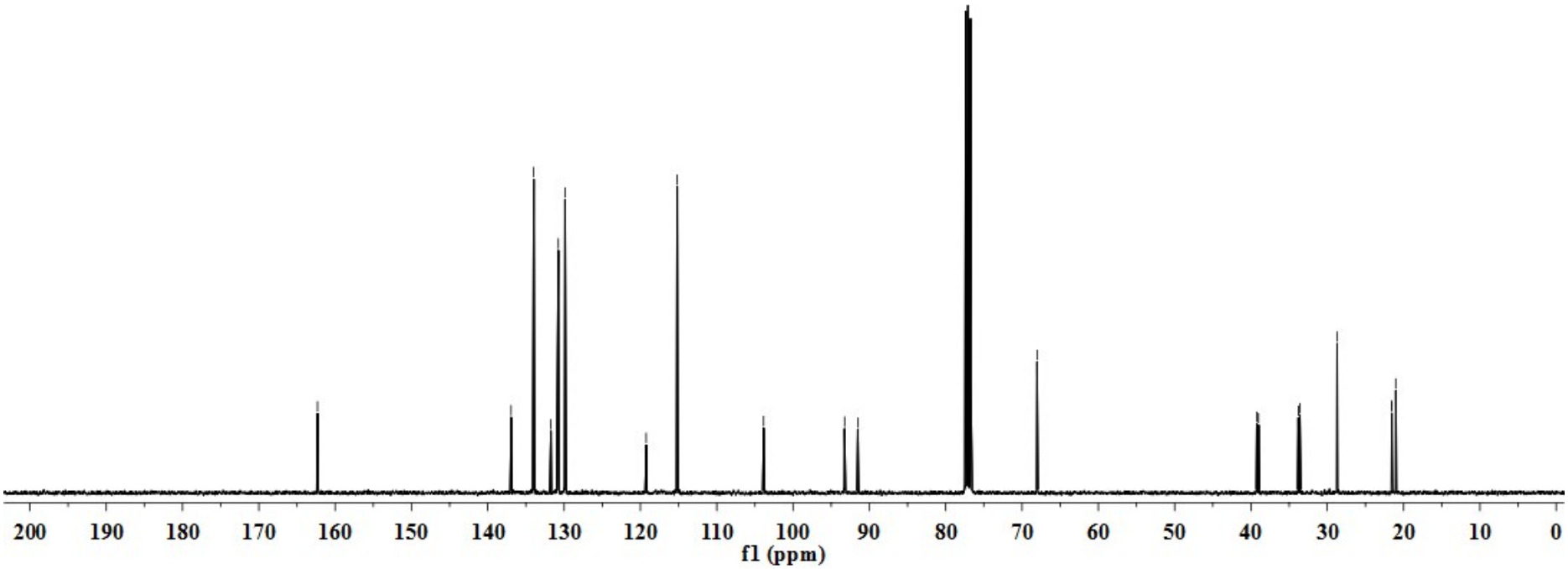

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

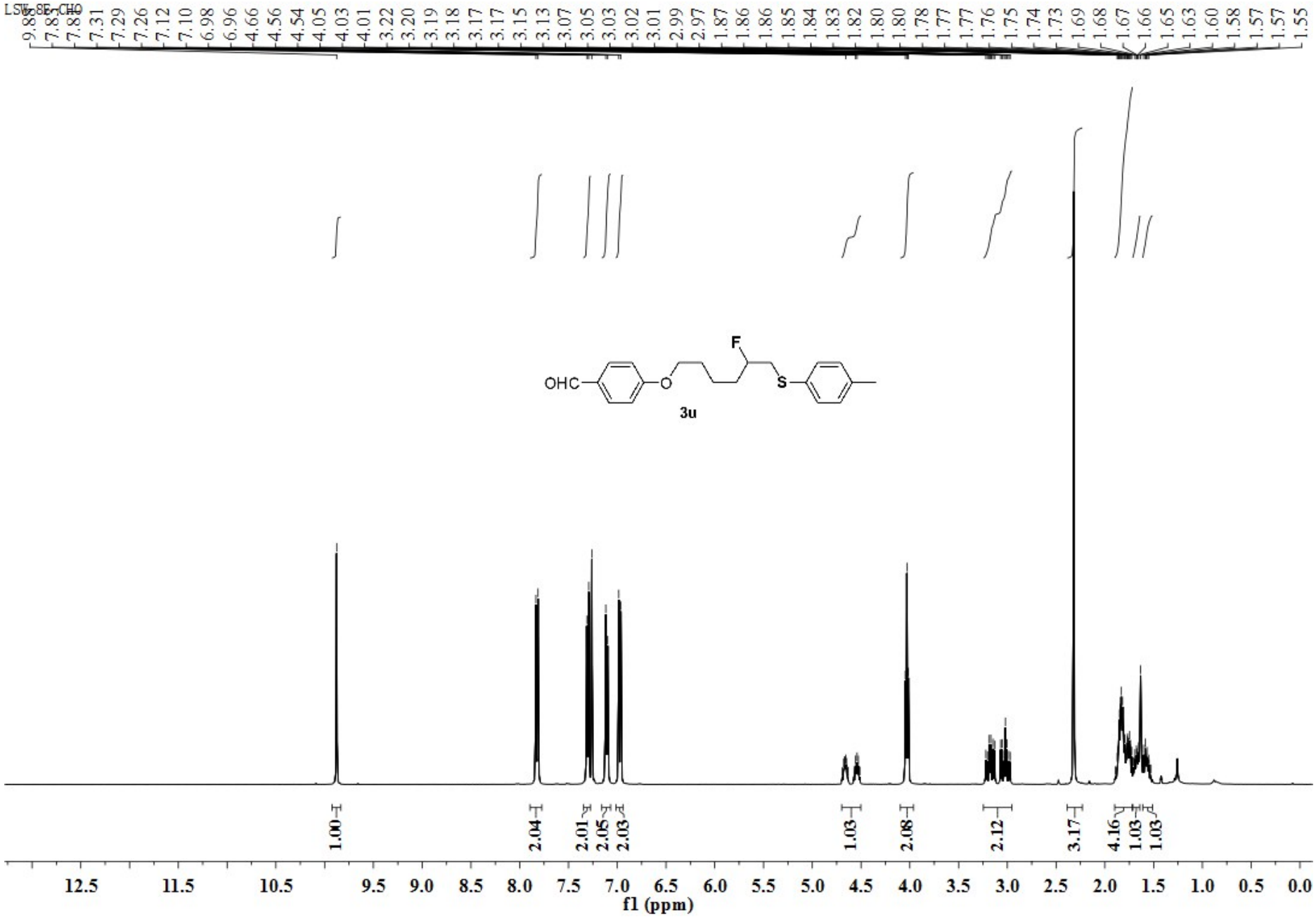
LSW-8D

162.30
136.95
133.98
131.73
130.76
129.87
119.25
115.19
103.86
93.24
91.52
68.01
39.23
39.00
33.79
33.59
28.71
21.56
21.53
21.03

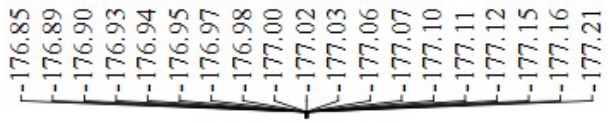


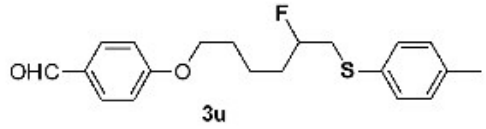
3t



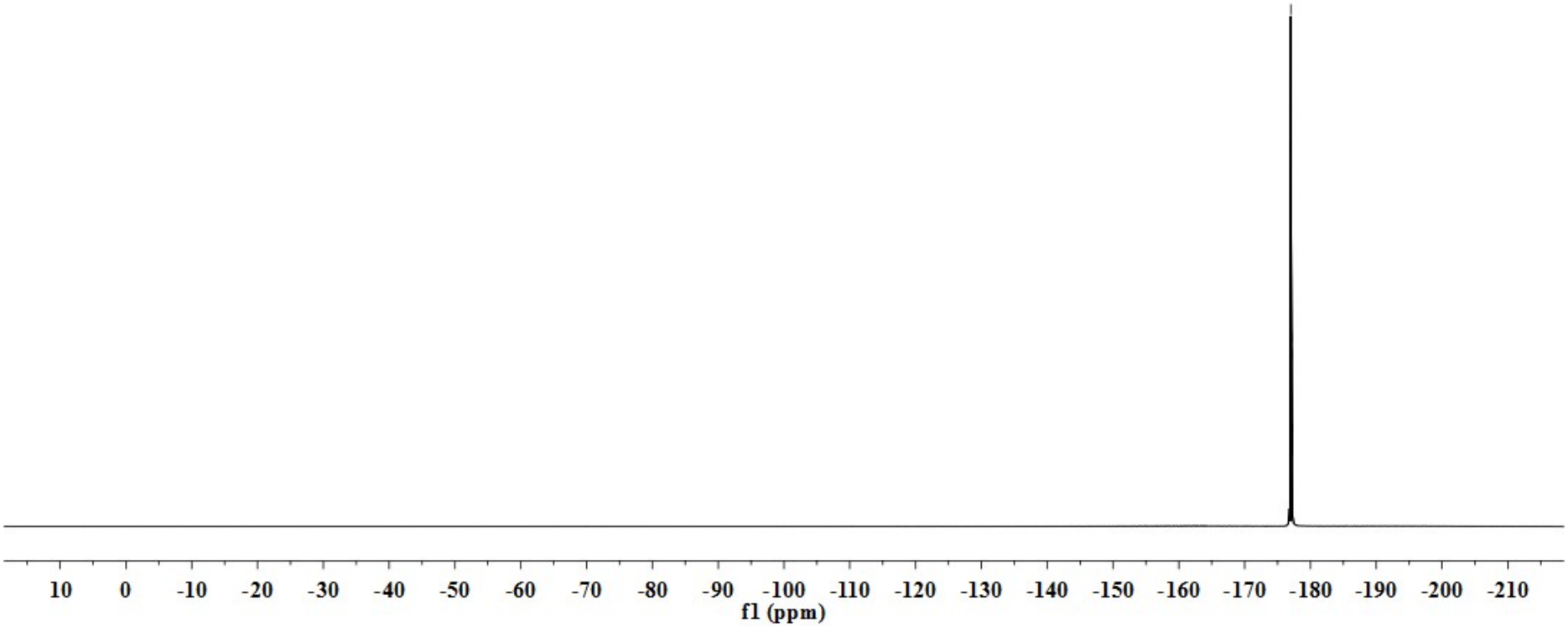

LSW-8F-CHO
9.88
7.85
7.84
7.31
7.29
7.26
7.12
7.10
6.98
6.96
6.66
4.56
4.54
4.05
4.03
4.01
3.22
3.20
3.19
3.18
3.17
3.17
3.15
3.13
3.07
3.05
3.03
3.02
3.01
2.99
2.97
1.87
1.86
1.86
1.85
1.84
1.83
1.82
1.80
1.80
1.78
1.77
1.77
1.76
1.75
1.74
1.73
1.69
1.68
1.67
1.66
1.65
1.63
1.60
1.58
1.57
1.57
1.55
F
OHC
O
S
3u
1.00
2.04
2.01
2.05
2.03
1.03
2.08
2.12
3.17
4.16
1.03
1.03
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-8E-CHO


176.85
176.89
176.90
176.93
176.94
176.95
176.97
176.98
177.00
177.02
177.03
177.06
177.07
177.10
177.11
177.12
177.15
177.16
177.21

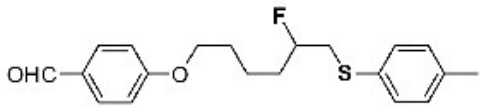

F
OHC
O
S

3u

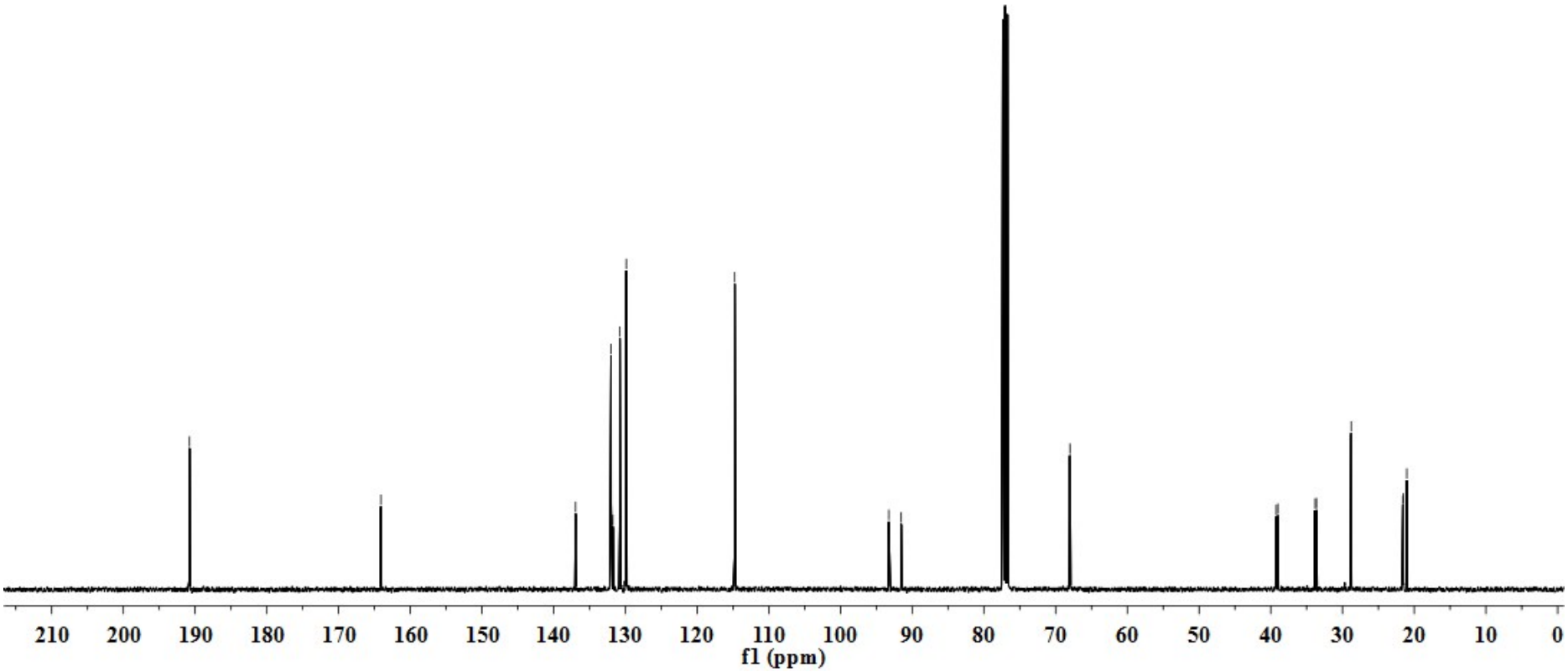

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

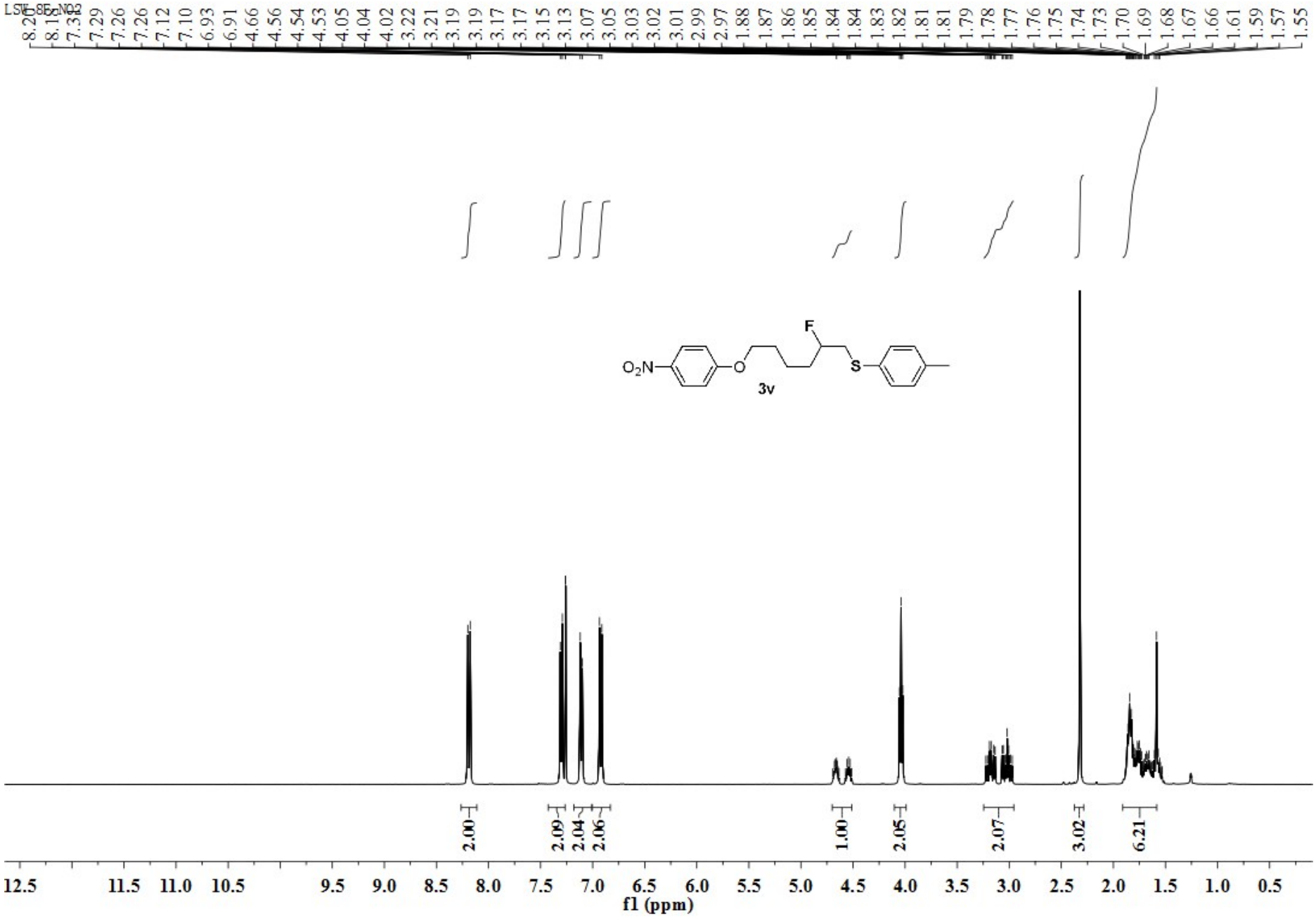
LSW-8E

190.78
164.09
136.94
132.00
131.74
130.77
129.91
129.87
114.76
93.26
91.54
68.01
39.25
39.02
33.83
33.62
28.78
21.59
21.55
21.03

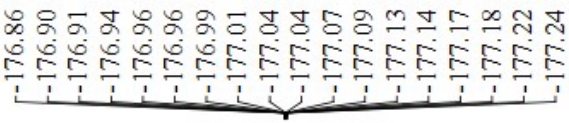


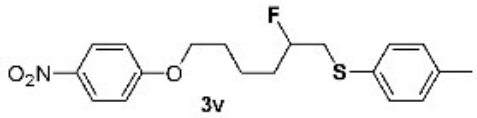
3u



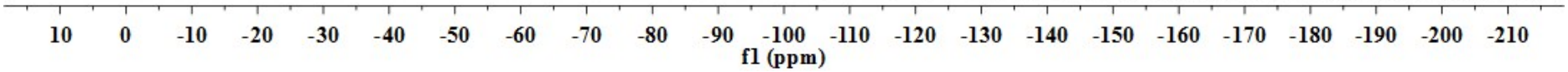

LSW-8E-NO2
8.20
8.18
7.32
7.29
7.26
7.26
7.12
7.10
6.93
6.91
4.66
4.56
4.54
4.53
4.05
4.04
4.02
3.22
3.21
3.19
3.19
3.17
3.17
3.15
3.13
3.07
3.05
3.03
3.02
3.01
2.99
2.97
1.88
1.87
1.86
1.85
1.84
1.84
1.83
1.82
1.81
1.81
1.79
1.78
1.77
1.76
1.75
1.74
1.73
1.70
1.69
1.68
1.67
1.66
1.61
1.59
1.57
1.55
F
O2N
O
S
3v
2.00
2.09
2.04
2.06
1.00
2.05
2.07
3.02
6.21
12.5
11.5
11.0
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

LSW-8F-NO2


176.86
176.90
176.91
176.94
176.96
176.96
176.99
177.01
177.04
177.04
177.07
177.09
177.13
177.14
177.17
177.18
177.22
177.24

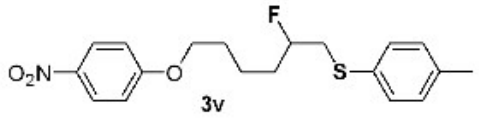

F
O2N
O
S

3v

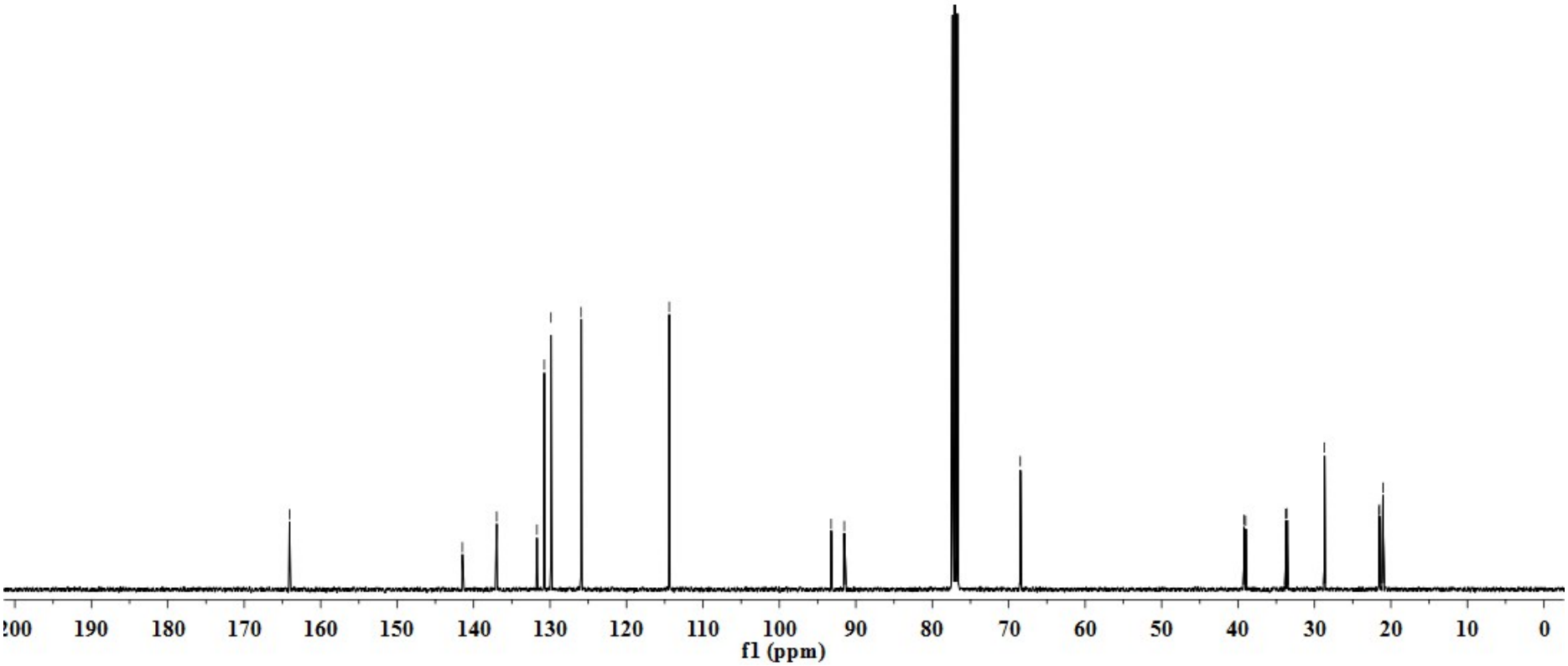

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

LSW-8F

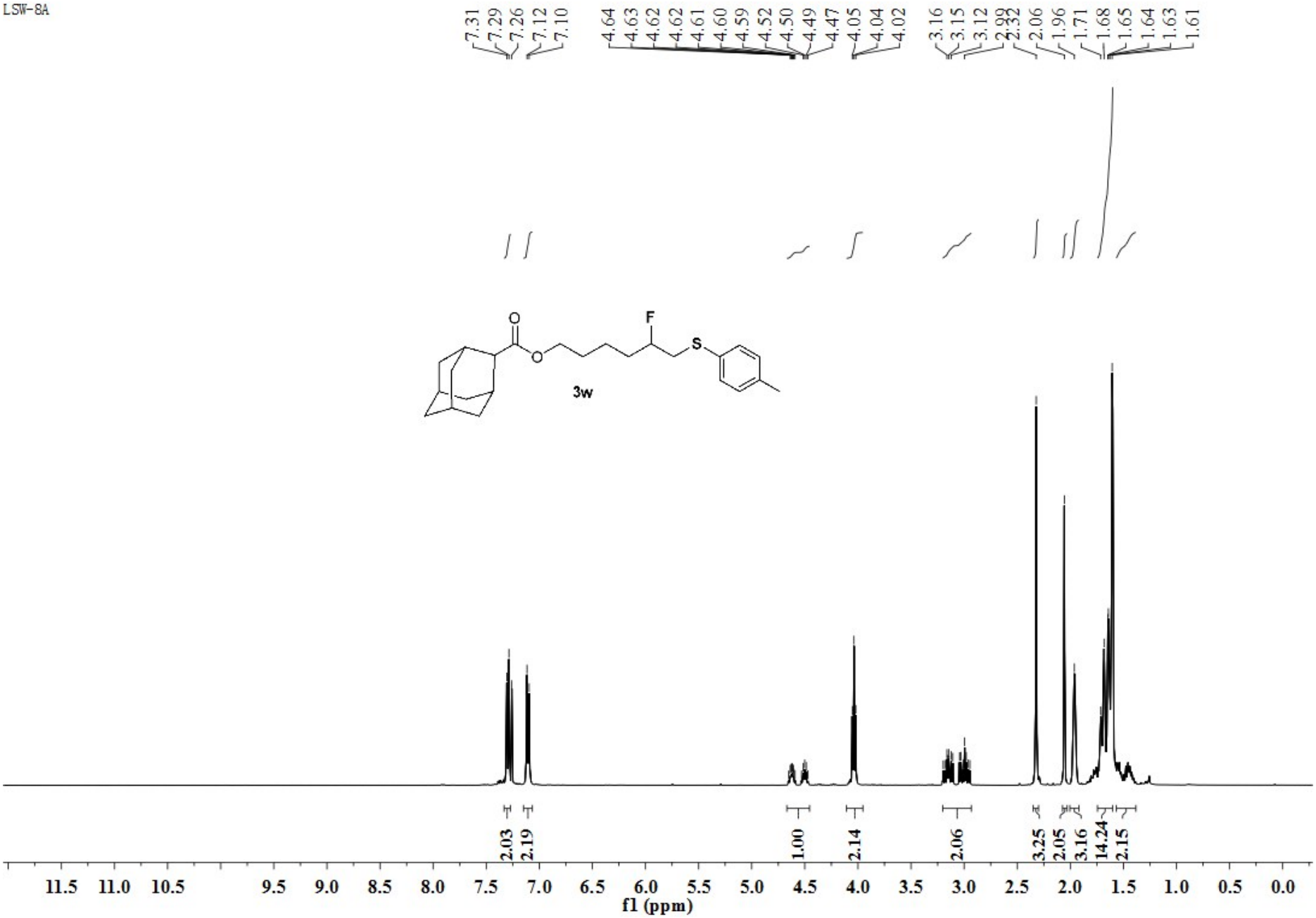
164.06
141.46
136.97
131.71
130.76
129.87
125.92
114.41
93.23
91.51
68.48
39.22
38.99
33.78
33.57
28.70
21.55
21.52
21.03



3v

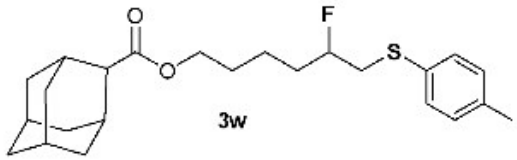


LSW-8A

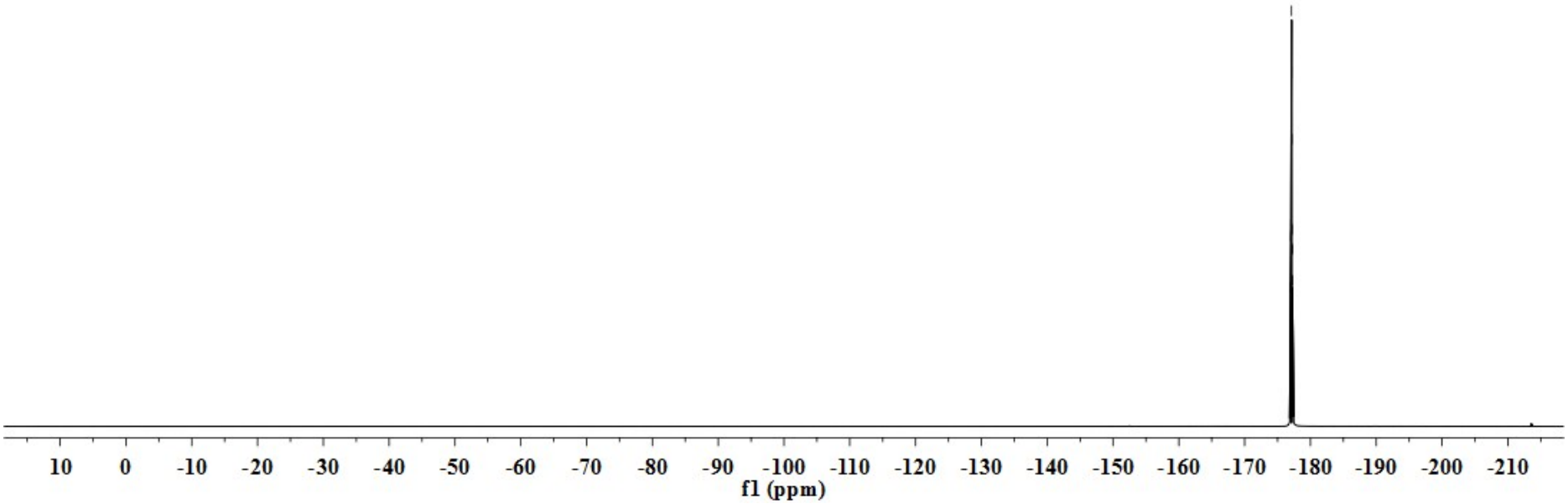

7.31
7.29
7.26
7.12
7.10
4.64
4.63
4.62
4.62
4.61
4.60
4.59
4.52
4.50
4.49
4.47
4.05
4.04
4.02
3.16
3.15
3.12
2.32
2.06
1.96
1.71
1.68
1.65
1.64
1.63
1.61
O
O
F
S
3w
2.03
2.19
1.00
2.14
2.06
3.25
2.05
3.16
14.24
2.15
11.5
11.0
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-8A

176.95
176.99
177.00
177.02
177.04
177.05
177.07
177.08
177.09
177.12
177.13
177.16
177.17
177.20
177.21
177.22
177.25
177.26
177.30

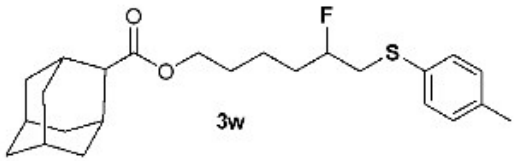


3w

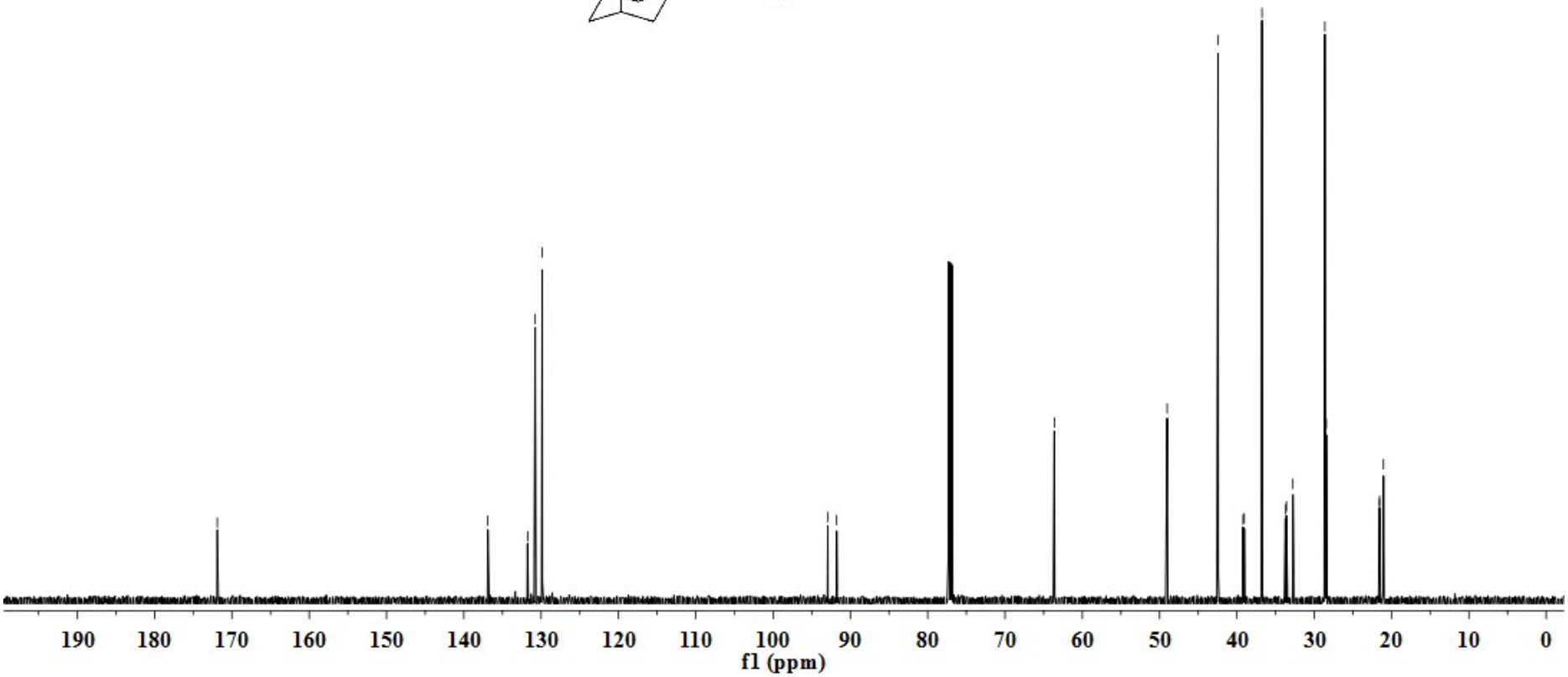


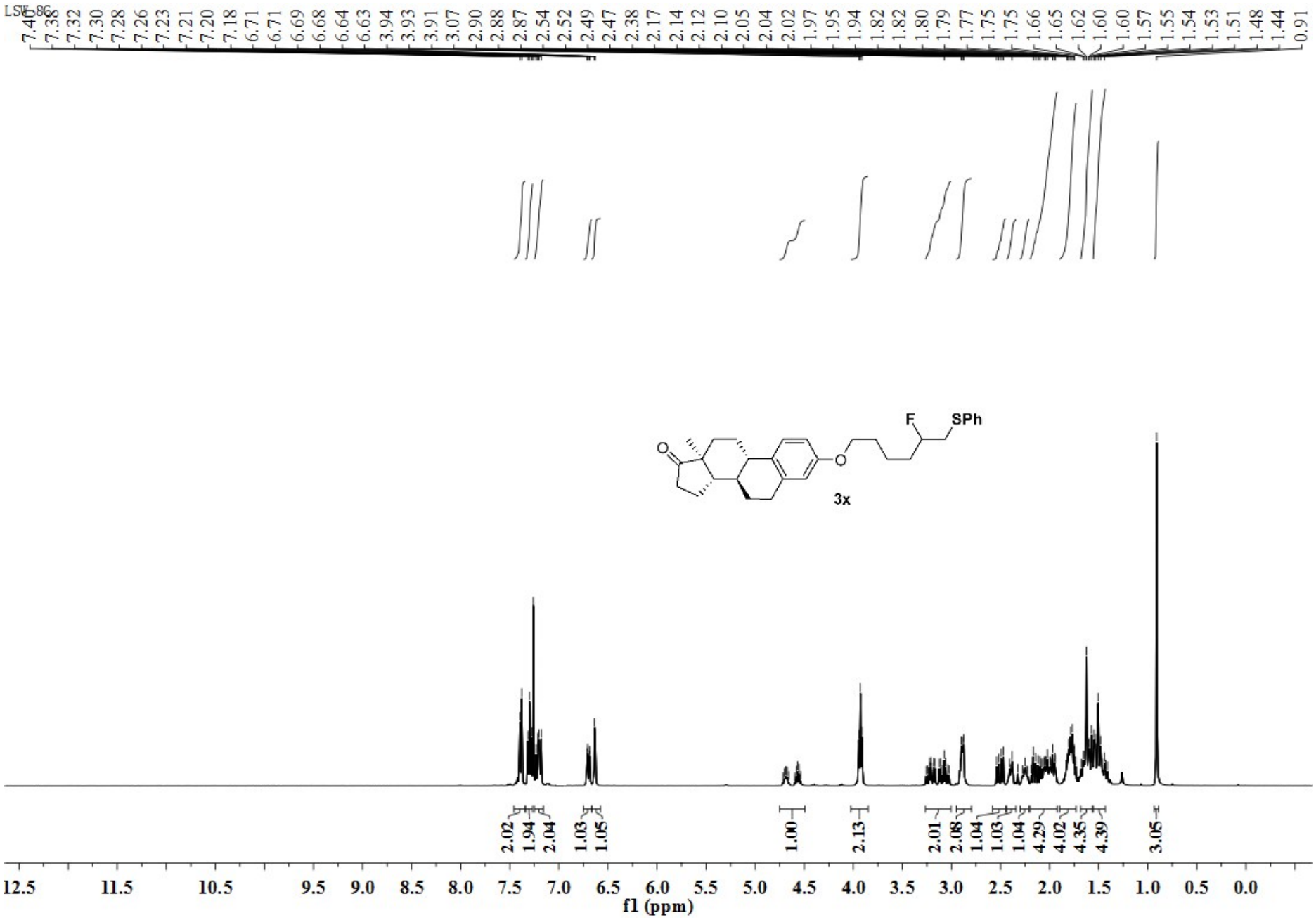
LSW-8B-JIN

171.89
136.89
131.75
130.77
129.86
92.92
91.78
63.62
49.02
42.43
39.21
39.05
36.76
33.74
33.60
32.76
28.63
28.44
21.57
21.55
21.04



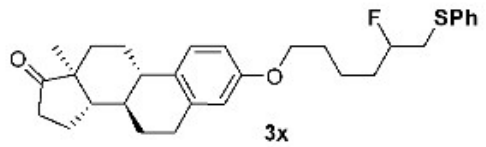
3w



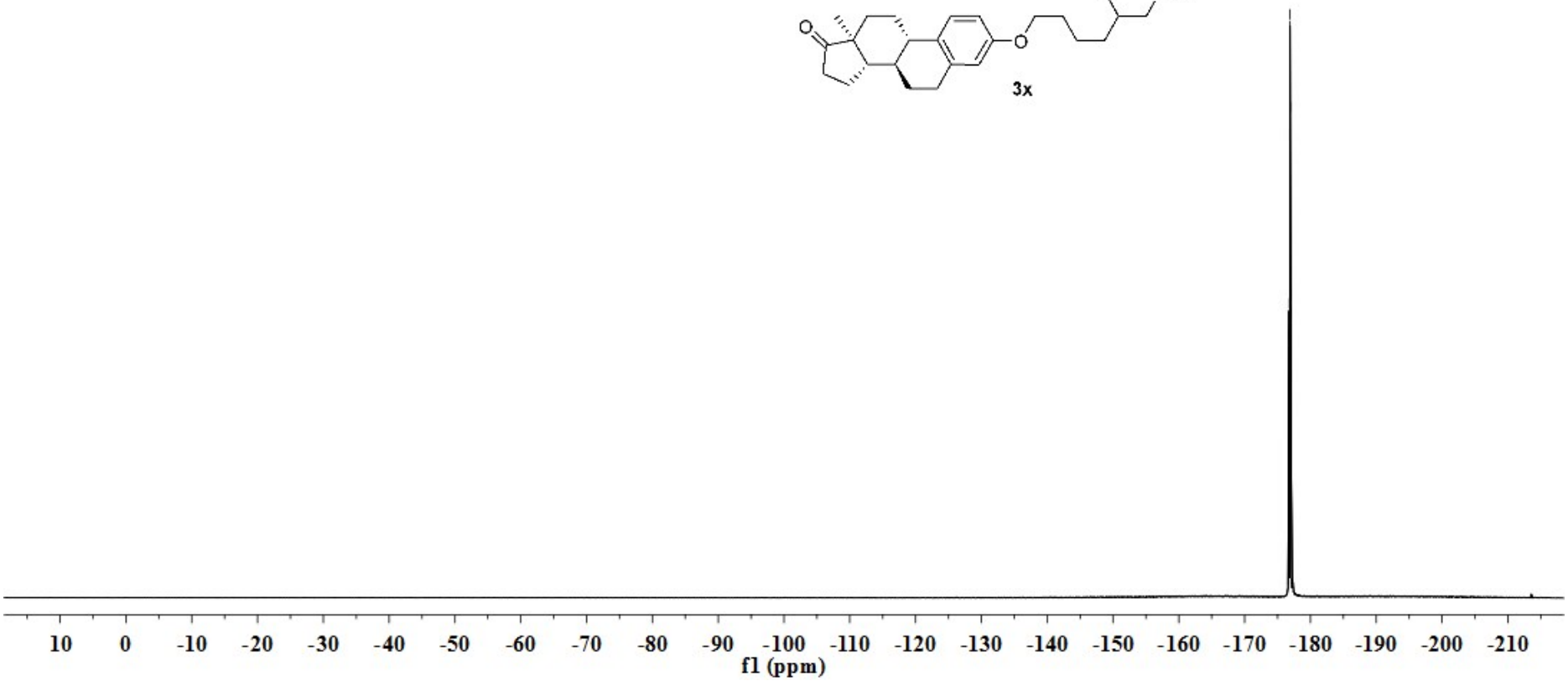

7.40
7.38
7.32
7.30
7.28
7.26
7.23
7.21
7.20
7.18
6.71
6.71
6.69
6.68
6.64
6.63
3.94
3.93
3.91
3.07
2.90
2.88
2.87
2.54
2.52
2.49
2.47
2.38
2.17
2.14
2.12
2.10
2.05
2.04
2.02
1.97
1.95
1.94
1.82
1.82
1.80
1.79
1.77
1.75
1.75
1.66
1.65
1.62
1.60
1.60
1.57
1.55
1.54
1.53
1.51
1.48
1.44
0.91
F
SPh
O
O
3x
2.02
1.94
2.04
1.03
1.05
1.00
2.13
2.01
2.08
1.04
1.03
1.04
4.29
4.02
4.35
4.39
3.05
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-8C

176.70
176.75
176.76
176.78
176.80
176.81
176.82
176.84
176.86
176.88
176.89
176.91
176.93
176.96
176.97
176.99
177.01
177.02
177.06



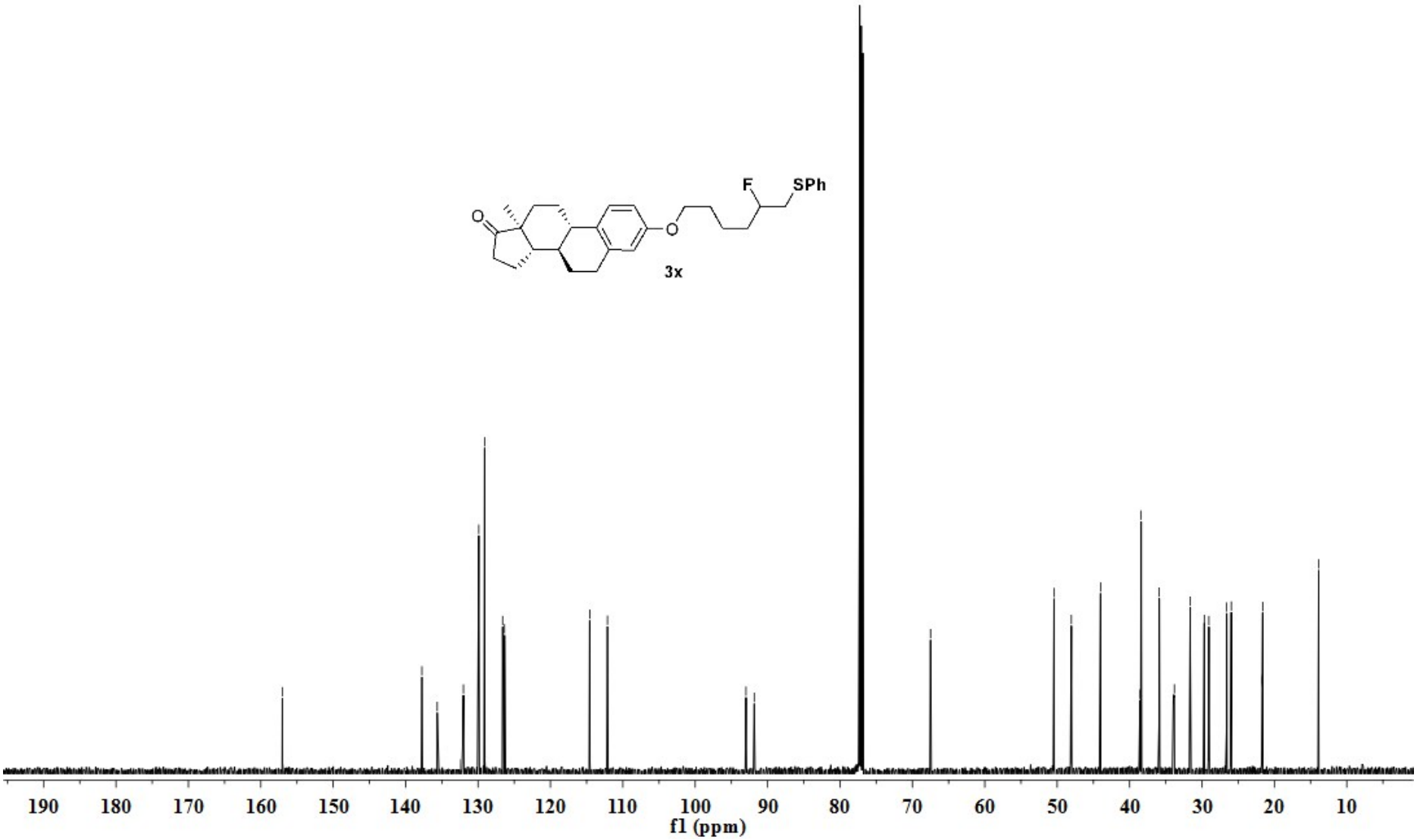
3x

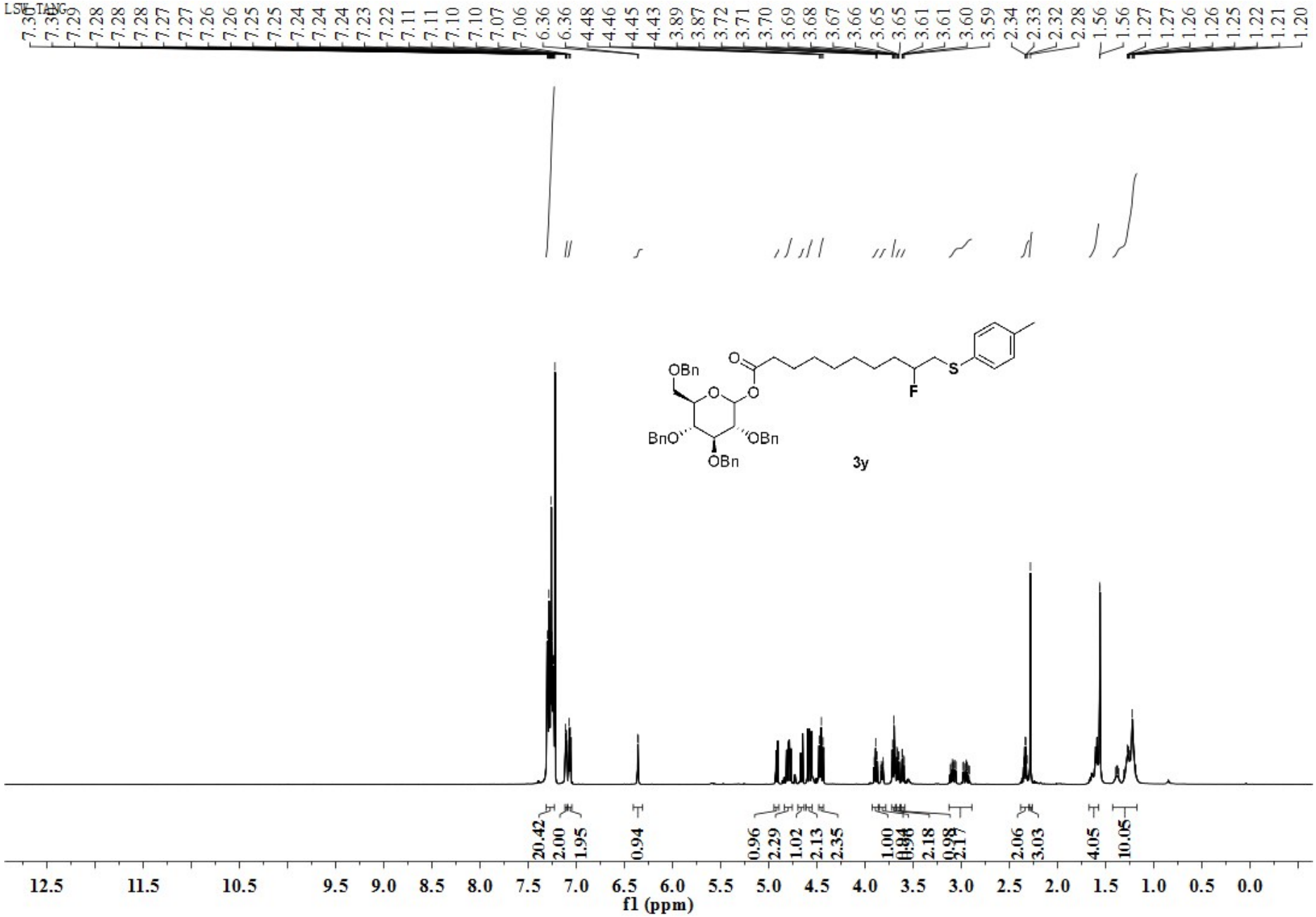


LSW-CI

157.02
137.75
135.63
132.01
129.90
129.08
126.60
126.34
114.57
112.12
92.98
91.84
67.49
50.43
48.04
44.00
38.56
38.40
35.90
33.82
31.61
29.68
29.04
26.58
25.95
21.67
21.64
21.61
13.88

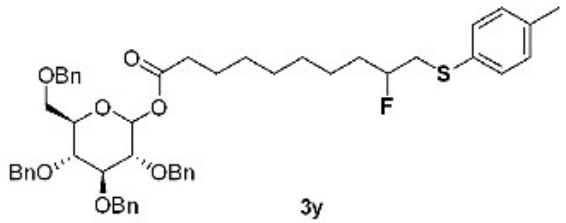
3x



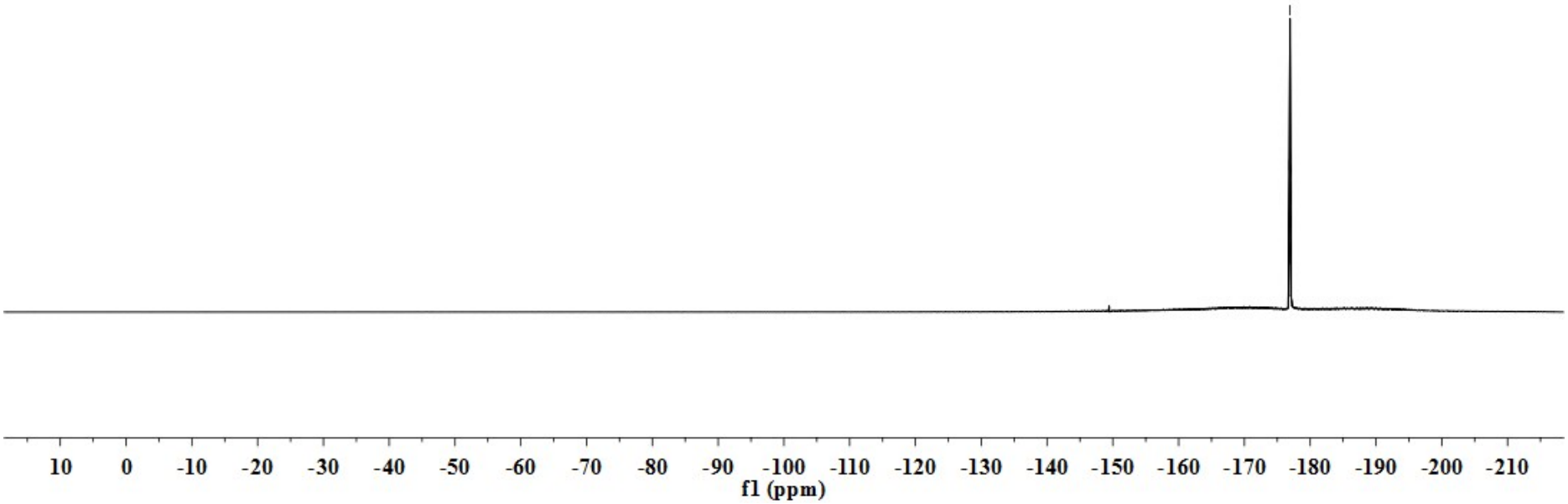

LSW-TANG
7.30 7.30 7.29 7.28 7.28 7.28 7.27 7.27 7.26 7.26 7.25 7.25 7.24 7.24 7.24 7.23 7.22 7.11 7.11 7.10 7.10 7.07 7.06 6.36 6.36 4.48 4.46 4.45 4.43 3.89 3.87 3.72 3.71 3.70 3.69 3.68 3.67 3.66 3.65 3.65 3.61 3.61 3.60 3.59 2.34 2.33 2.32 2.28 1.56 1.56 1.27 1.27 1.26 1.26 1.25 1.22 1.21 1.20
OBn
O
O
O
S
F
BnO
OBn
OBn
3y
20.42
2.00
1.95
0.94
0.96
2.29
1.02
2.13
2.35
1.00
2.18
0.98
2.06
3.03
4.05
10.05
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

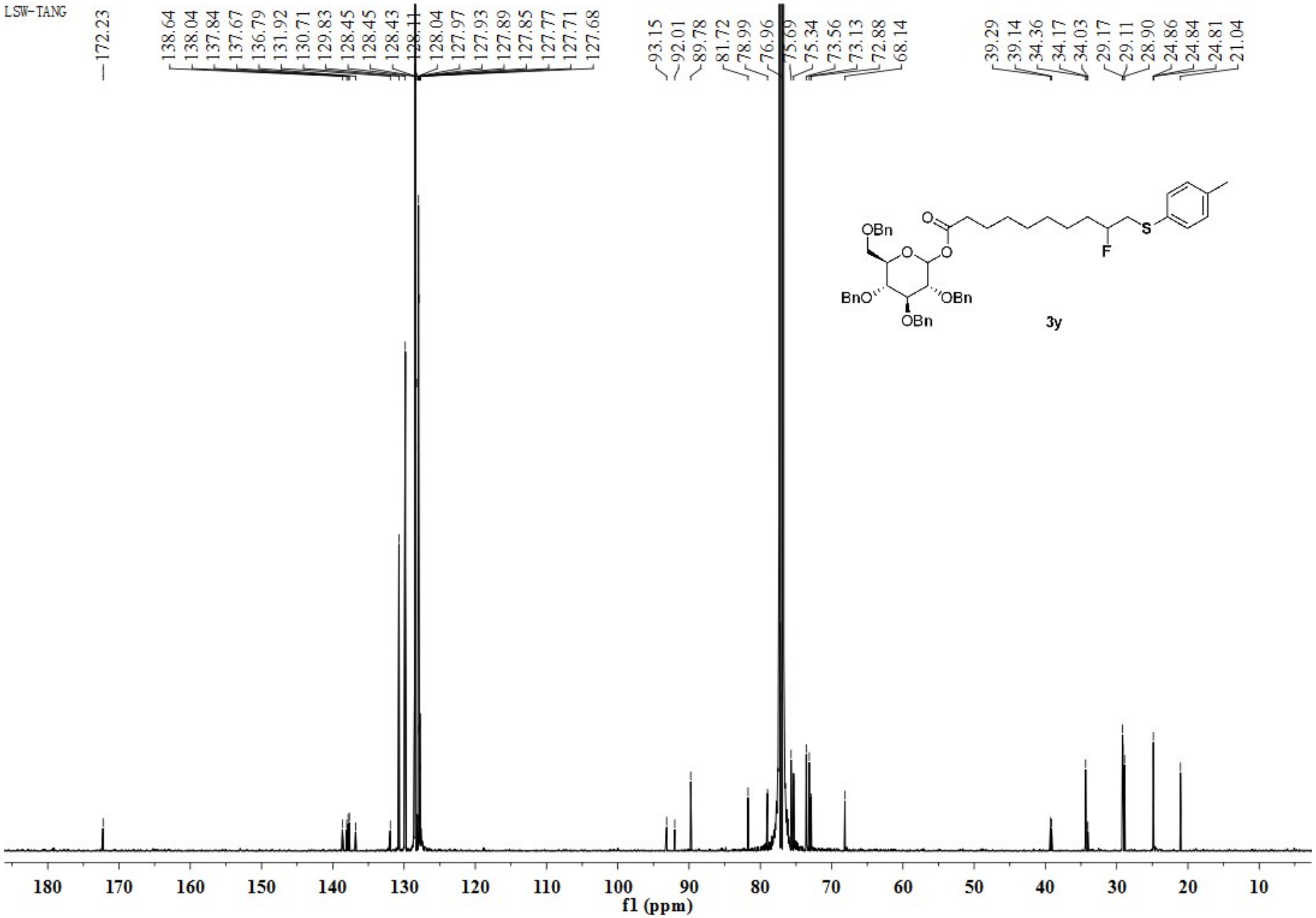
LSW-TANG

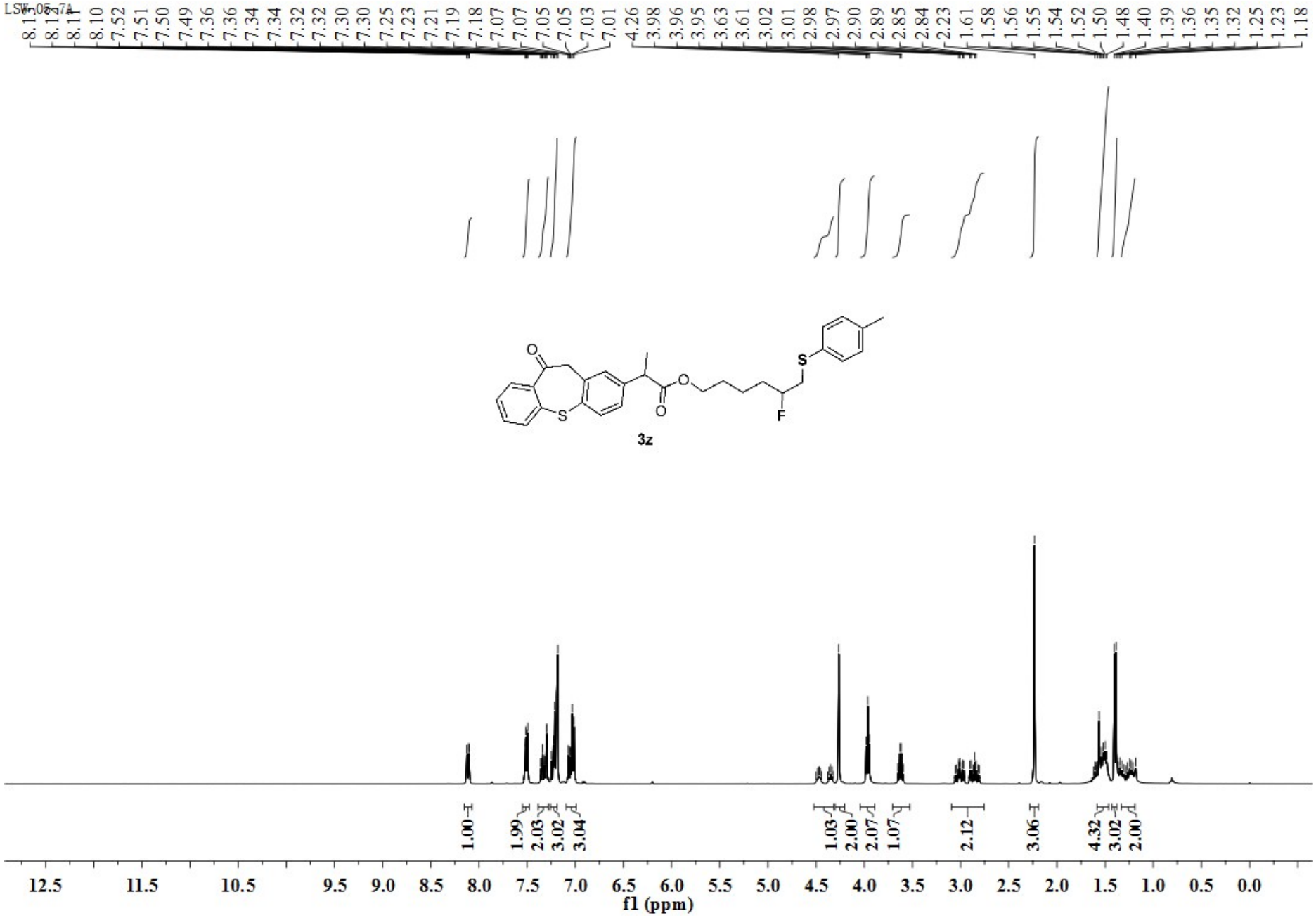

176.80
176.81
176.83
176.83
176.84
176.86
176.87
176.88
176.89
176.91
176.92
176.93
176.95
176.96
176.96
176.97
176.98
176.99
177.00
177.01
177.02
177.04
177.05


OBn
O
O
O
S
F
BnO
OBn
OBn

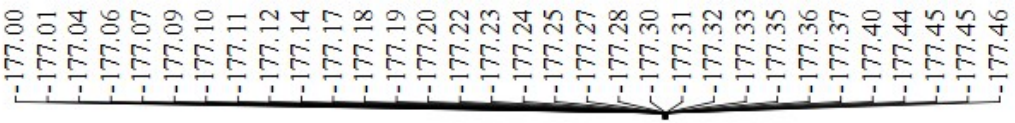
3y

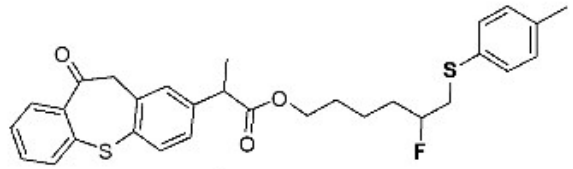

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


LSW-TANG
172.23
138.64
138.04
137.84
137.67
136.79
131.92
130.71
129.83
128.45
128.45
128.43
128.11
128.04
127.97
127.93
127.89
127.85
127.77
127.71
127.68
93.15
92.01
89.78
81.72
78.99
76.96
75.69
75.34
73.56
73.13
72.88
68.14
39.29
39.14
34.36
34.17
34.03
29.17
29.11
28.90
24.86
24.84
24.81
21.04
OBn
O
O
O
S
F
BnO
OBn
OBn
3y
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

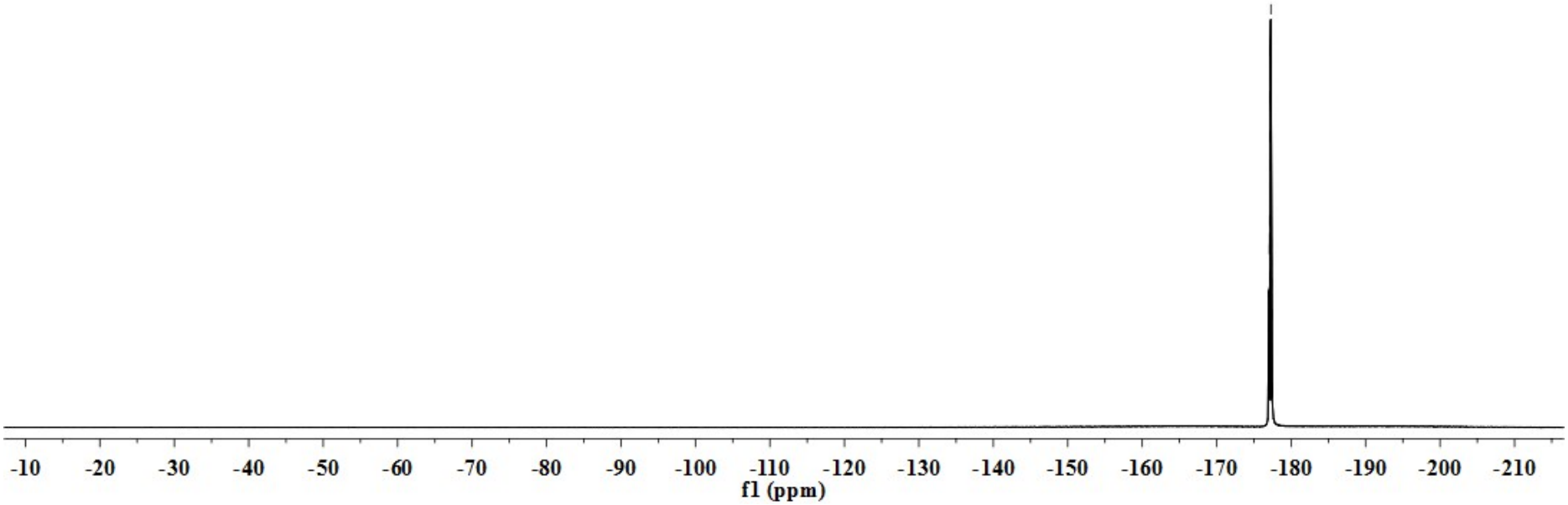

8.13
8.12
8.11
8.10
7.52
7.51
7.50
7.49
7.36
7.36
7.34
7.34
7.32
7.32
7.30
7.30
7.25
7.23
7.21
7.19
7.18
7.07
7.07
7.05
7.05
7.03
7.01
4.26
3.98
3.96
3.95
3.63
3.61
3.02
3.01
2.98
2.97
2.90
2.89
2.85
2.84
2.23
1.61
1.58
1.56
1.55
1.54
1.52
1.50
1.48
1.40
1.39
1.36
1.35
1.32
1.25
1.23
1.18
O
O
O
S
S
F
3z
1.00
1.99
2.03
3.02
3.04
1.03
2.00
2.07
1.07
2.12
3.06
4.32
3.02
2.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-05-7A


177.00
177.01
177.04
177.06
177.07
177.09
177.10
177.11
177.12
177.14
177.17
177.18
177.19
177.20
177.22
177.23
177.24
177.25
177.27
177.28
177.30
177.31
177.32
177.33
177.35
177.36
177.37
177.40
177.44
177.45
177.45
177.46

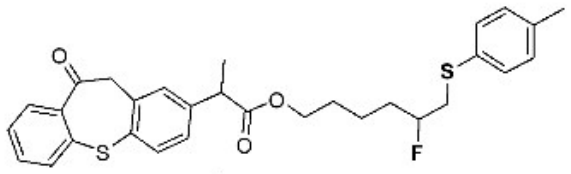

O
S
O
O
S
F

3z

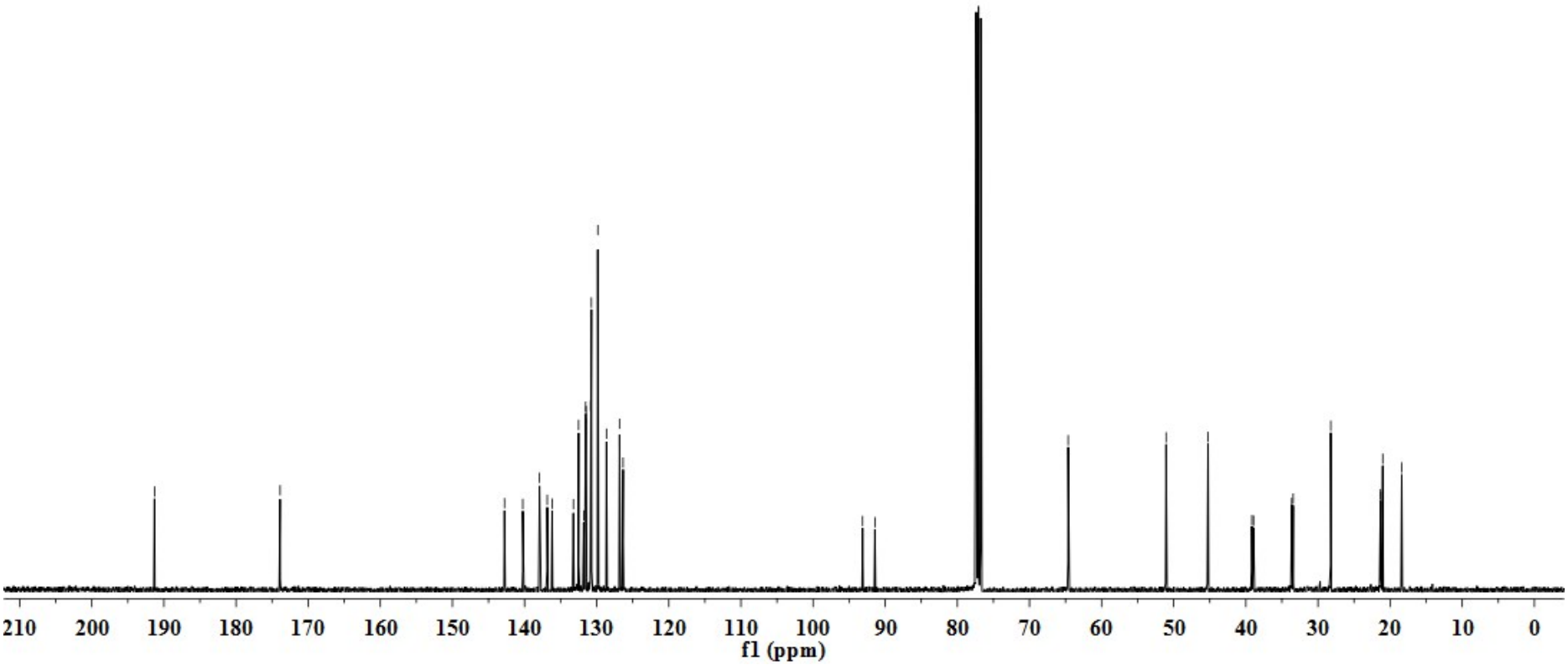

-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

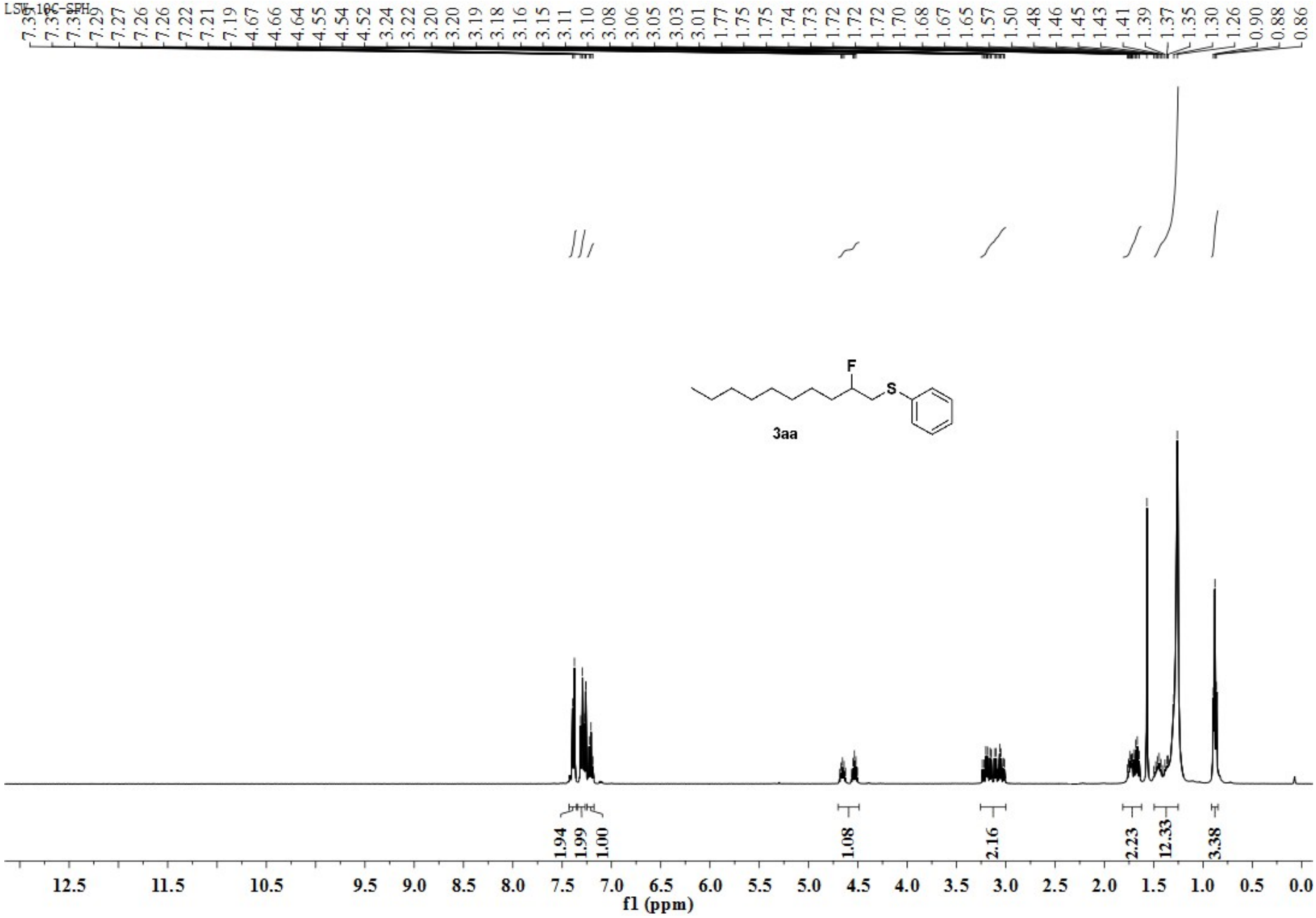
LW-7A

191.30
173.89
142.78
140.24
137.94
136.86
136.18
133.23
132.51
131.81
131.53
131.47
130.85
130.73
129.85
128.64
126.84
126.34
93.14
91.42
64.63
51.05
45.23
39.17
38.94
33.64
33.43
28.22
21.33
21.30
21.02
18.38

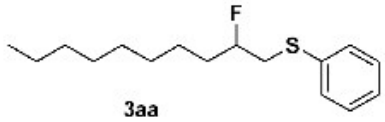


3z

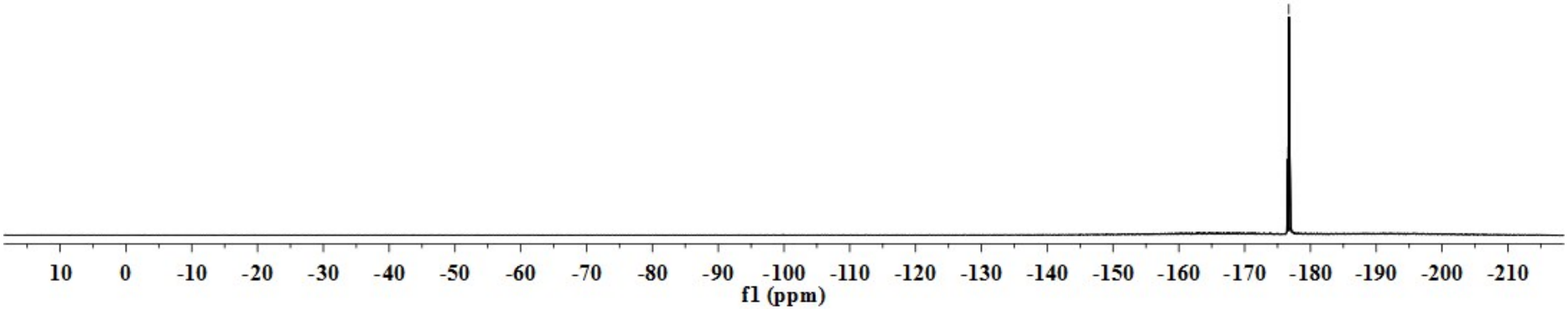


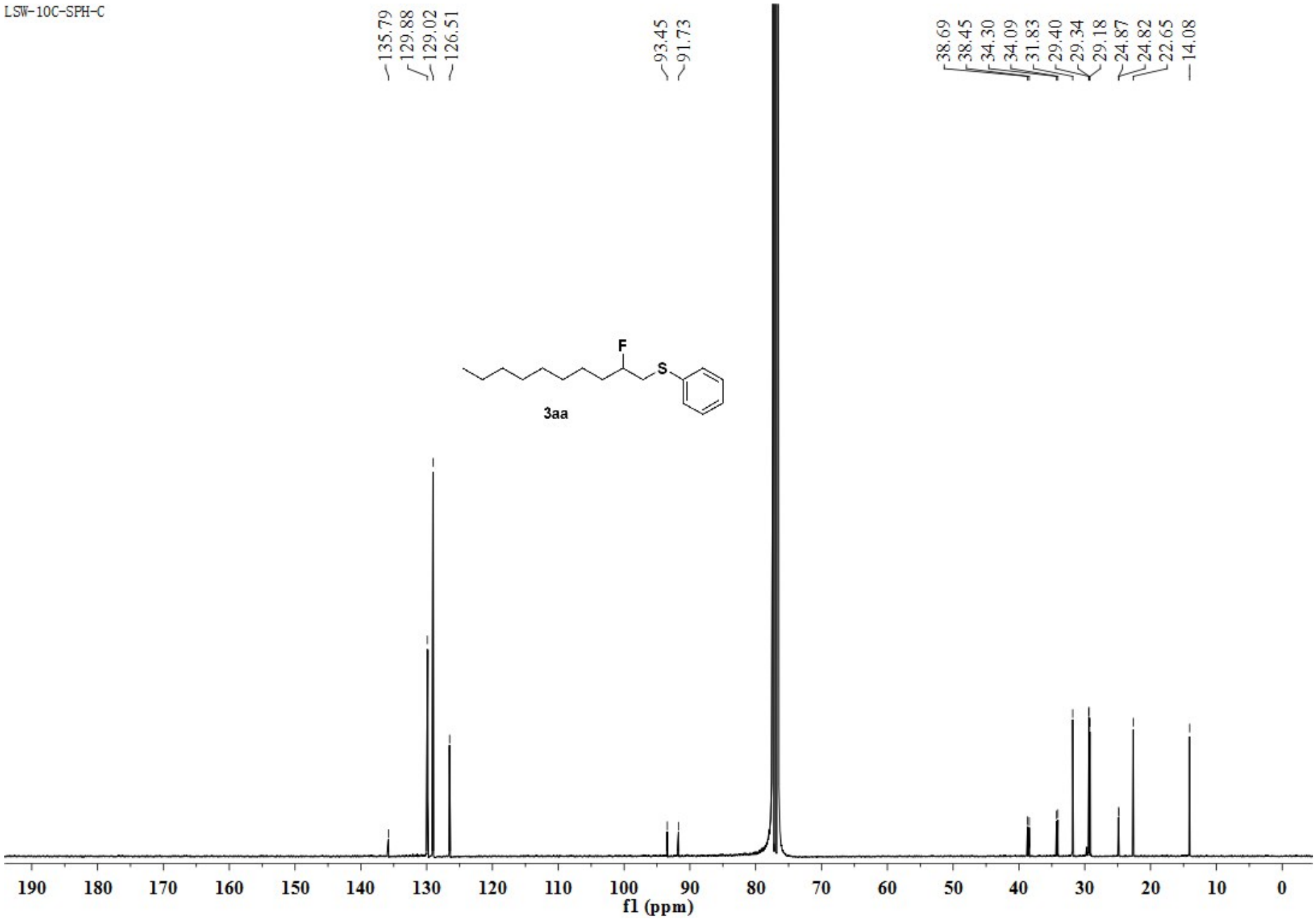

LSW-10C-SPH
7.39
7.38
7.38
7.29
7.27
7.26
7.26
7.22
7.21
7.19
4.67
4.66
4.64
4.55
4.54
4.52
3.24
3.22
3.20
3.20
3.19
3.18
3.16
3.15
3.11
3.10
3.08
3.06
3.05
3.03
3.01
1.77
1.75
1.75
1.74
1.73
1.72
1.72
1.72
1.70
1.68
1.67
1.65
1.57
1.50
1.48
1.46
1.45
1.43
1.41
1.39
1.37
1.35
1.30
1.26
0.90
0.88
0.86
F
S
3aa
1.94
1.99
1.00
1.08
2.16
2.23
12.33
3.38
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

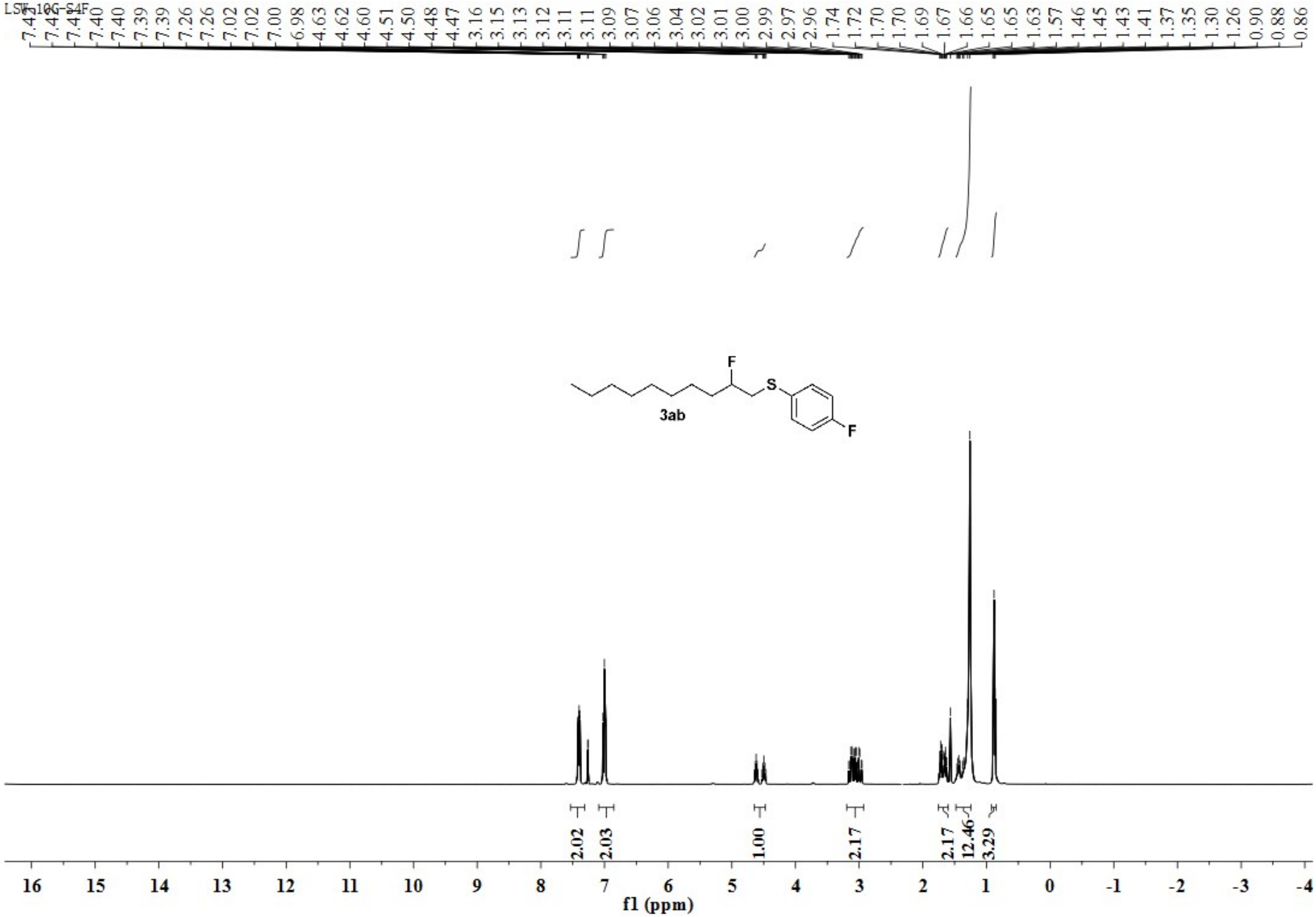
LSW-10C-SPH



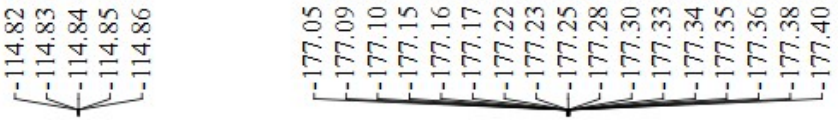
3aa

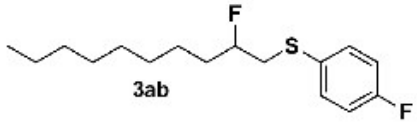



LSW-10C-SPH-C
135.79
129.88
129.02
126.51
93.45
91.73
38.69
38.45
34.30
34.09
31.83
29.40
29.34
29.18
24.87
24.82
22.65
14.08
F
S
3aa
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

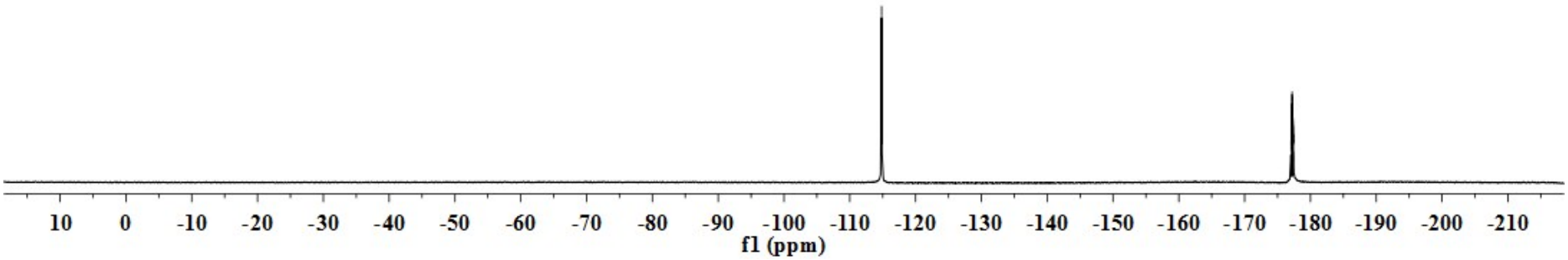

LSW-10G-S4F
7.42
7.40
7.40
7.40
7.39
7.39
7.26
7.26
7.02
7.02
7.00
6.98
4.63
4.62
4.60
4.51
4.50
4.48
4.47
3.16
3.15
3.13
3.12
3.11
3.11
3.09
3.07
3.06
3.04
3.02
3.01
3.00
2.99
2.97
2.96
1.74
1.72
1.70
1.70
1.69
1.67
1.66
1.65
1.65
1.63
1.57
1.46
1.45
1.43
1.41
1.37
1.35
1.30
1.26
0.90
0.88
0.86
F
S
F
3ab
2.02
2.03
1.00
2.17
2.17
12.46
3.29
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

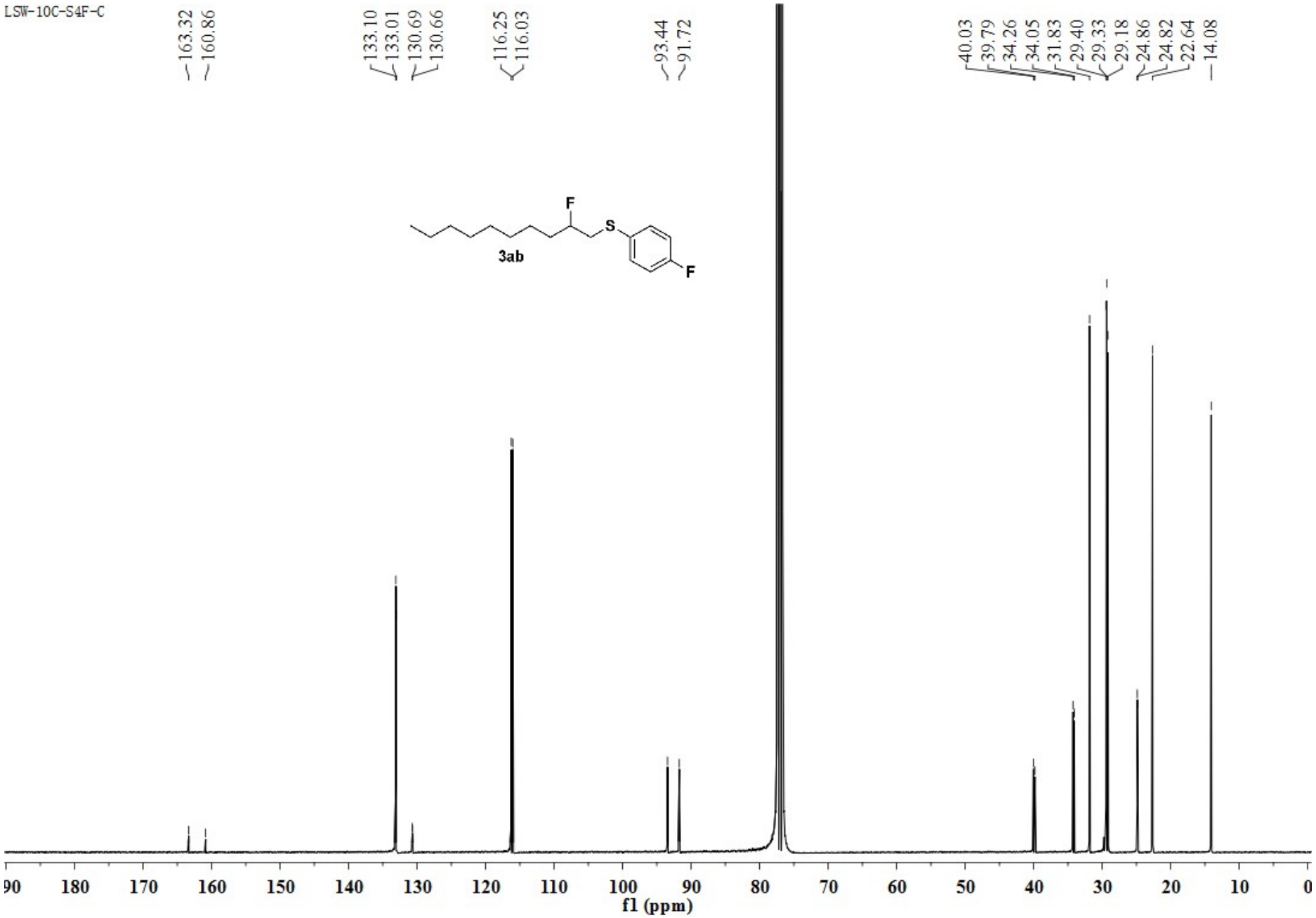
LSW-10C-S4F



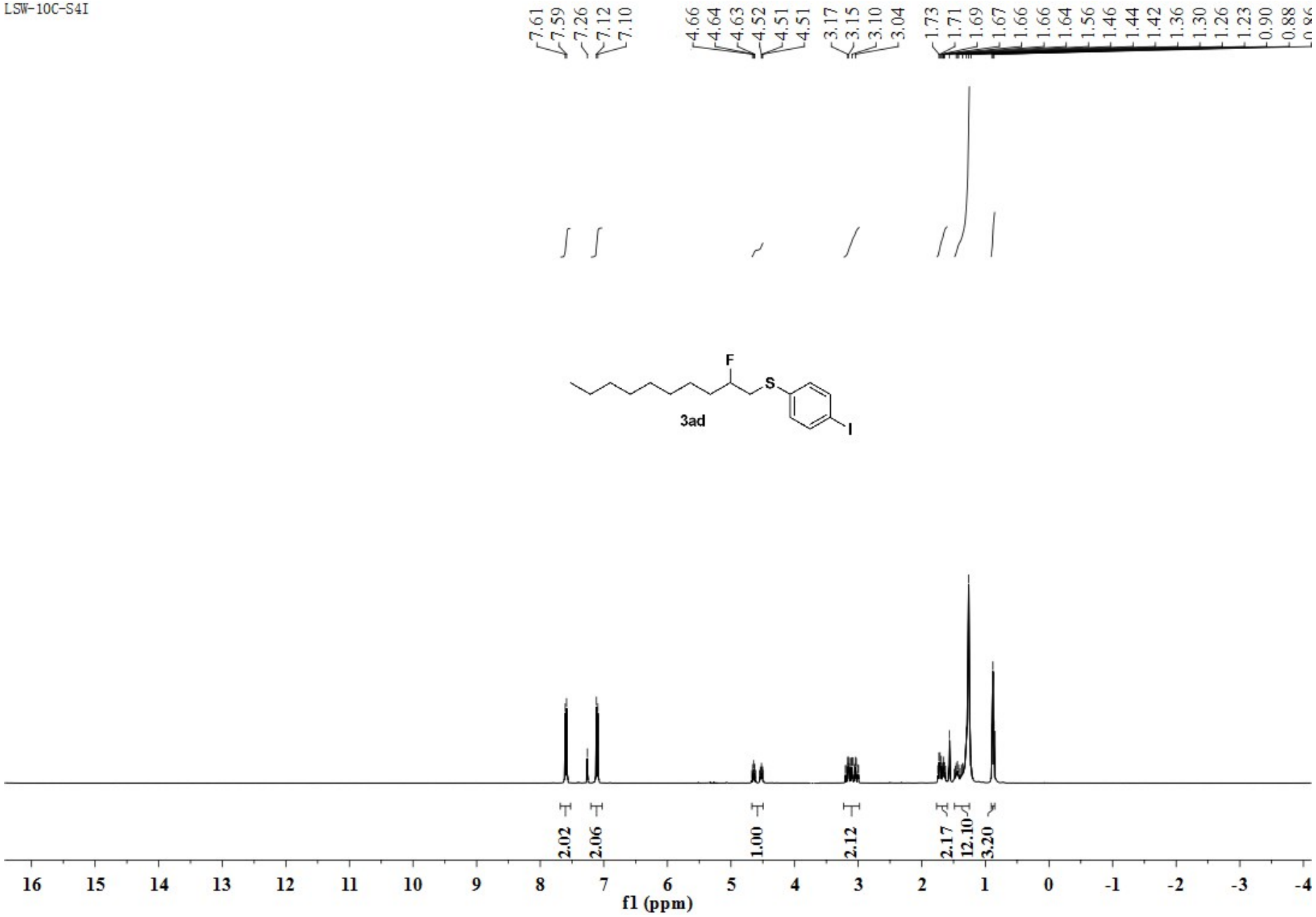


3ab

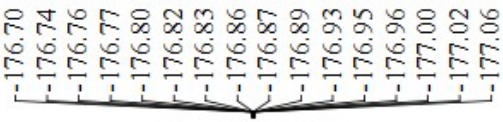


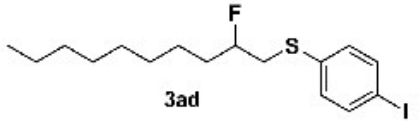

LSW-10C-S4F-C
163.32
160.86
133.10
133.01
130.69
130.66
116.25
116.03
93.44
91.72
40.03
39.79
34.26
34.05
31.83
29.40
29.33
29.18
24.86
24.82
22.64
14.08
F
S
F
3ab
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

LSW-10C-S4I

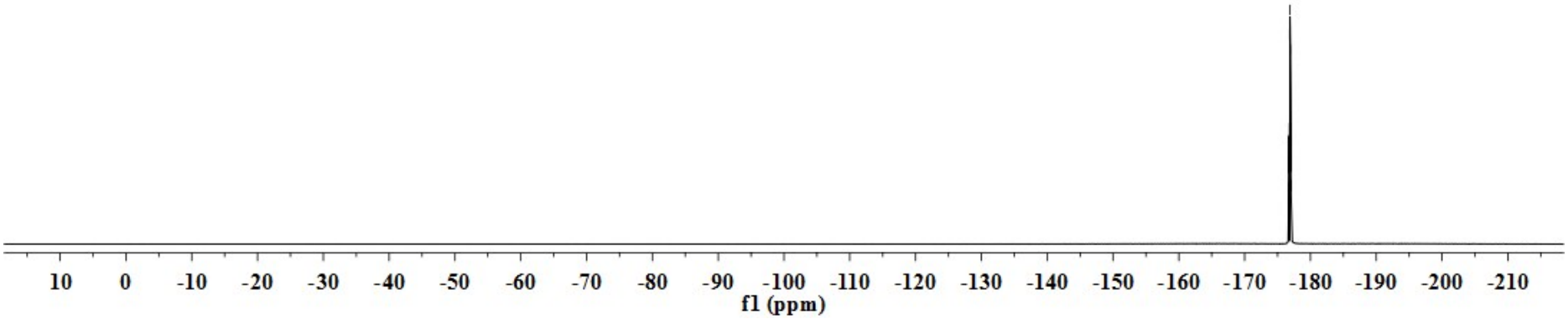

7.61
7.59
7.26
7.12
7.10
4.66
4.64
4.63
4.52
4.51
4.51
3.17
3.15
3.10
3.04
1.73
1.71
1.69
1.67
1.66
1.66
1.64
1.56
1.46
1.44
1.42
1.36
1.30
1.26
1.23
0.90
0.88
F
S
I
3ad
2.02
2.06
1.00
2.12
2.17
12.10
3.20
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

LSW-10C-S4I



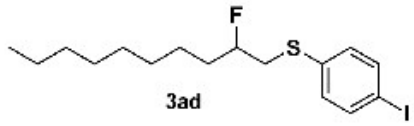


3ad

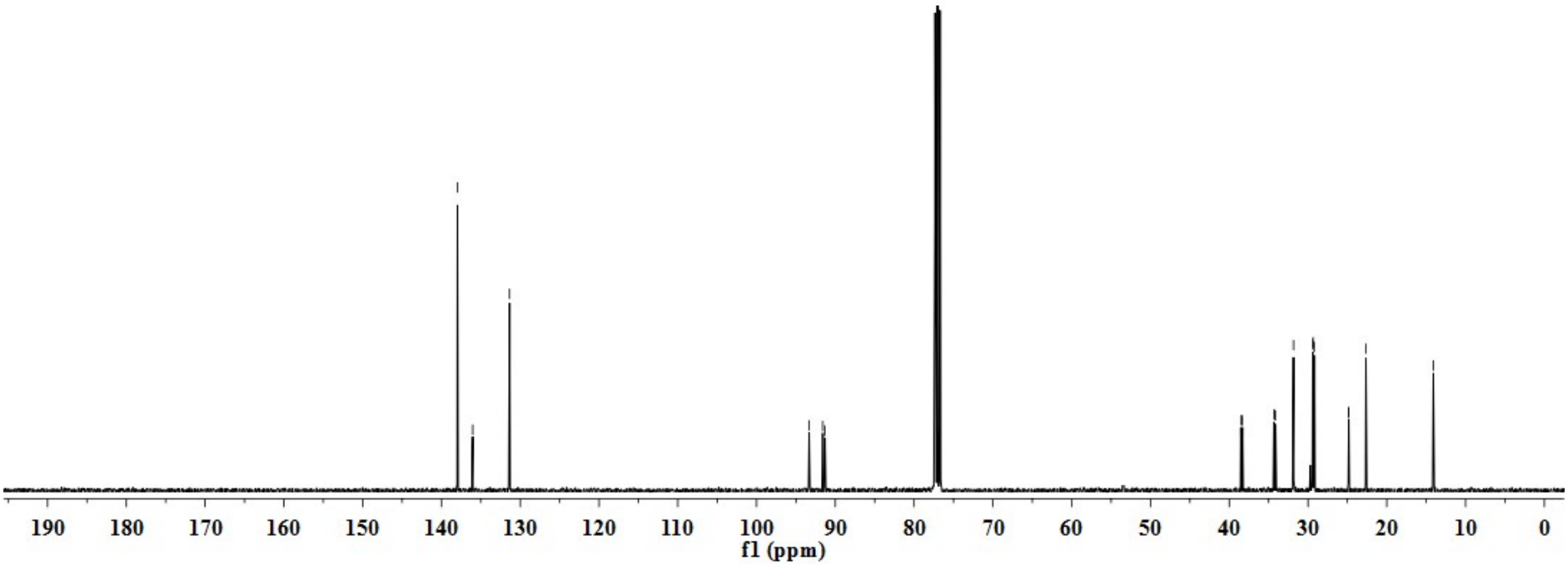


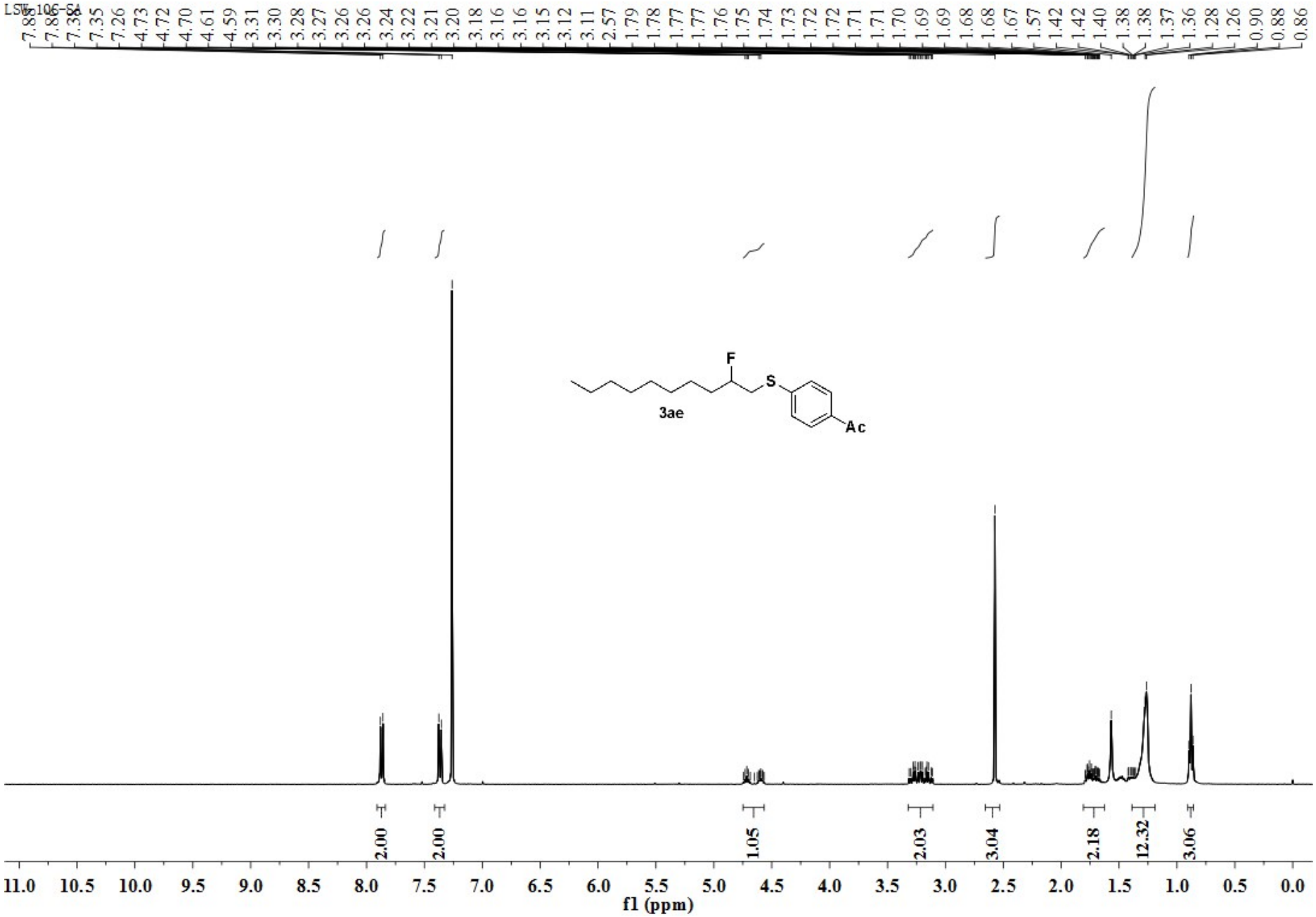
LSW-10C-S4I-C

137.97
136.03
131.36
93.32
91.60
91.31
38.53
38.29
34.32
34.12
31.84
29.40
29.33
29.18
24.86
24.83
22.65
14.09

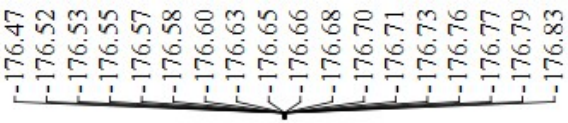


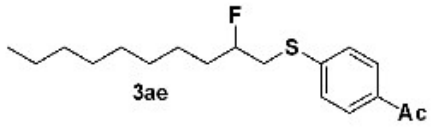
3ad

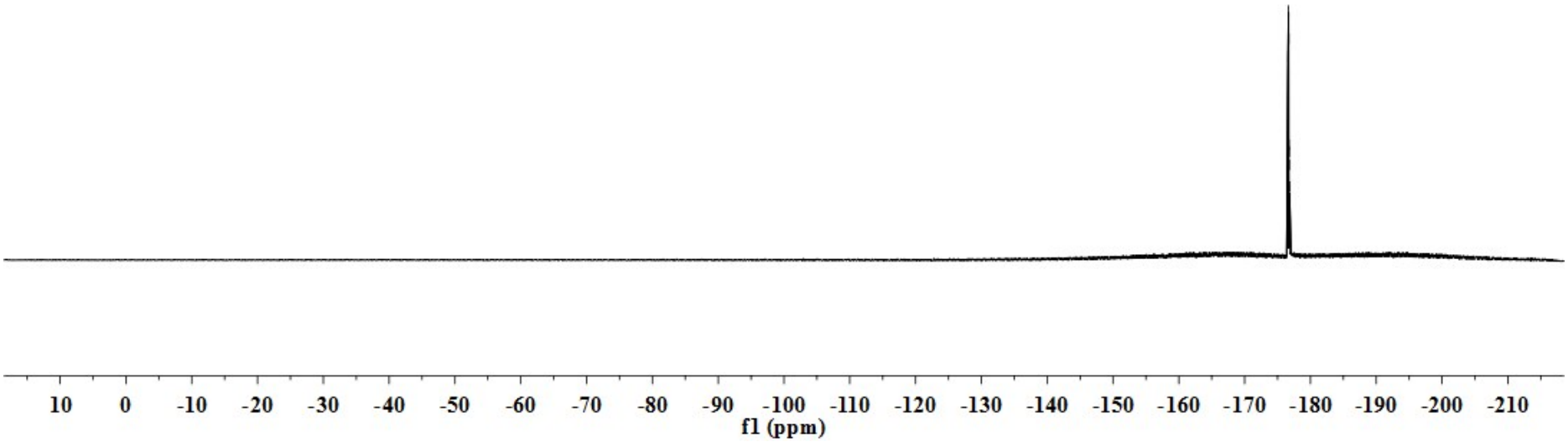


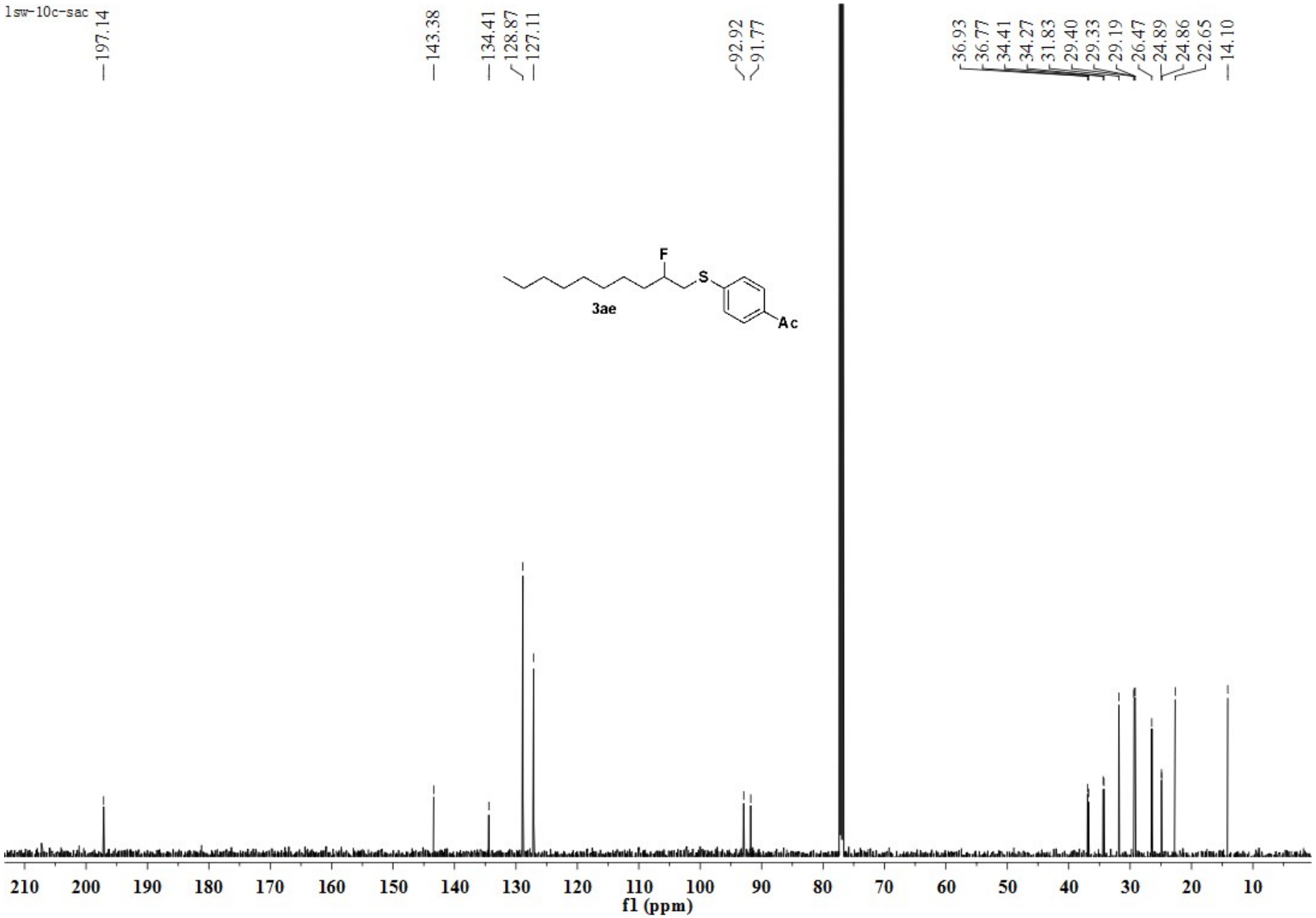

LSW-106-C1
7.88
7.86
7.38
7.35
7.26
4.73
4.72
4.70
4.61
4.59
3.31
3.30
3.28
3.27
3.26
3.26
3.24
3.22
3.21
3.20
3.18
3.16
3.16
3.15
3.12
3.11
2.57
1.79
1.78
1.77
1.77
1.76
1.75
1.74
1.73
1.72
1.72
1.71
1.71
1.70
1.69
1.69
1.68
1.68
1.67
1.57
1.42
1.42
1.40
1.38
1.38
1.37
1.36
1.28
1.26
0.90
0.88
0.86
F
S
3ae
Ac
2.00
2.00
1.05
2.03
3.04
2.18
12.32
3.06
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-10C-SA

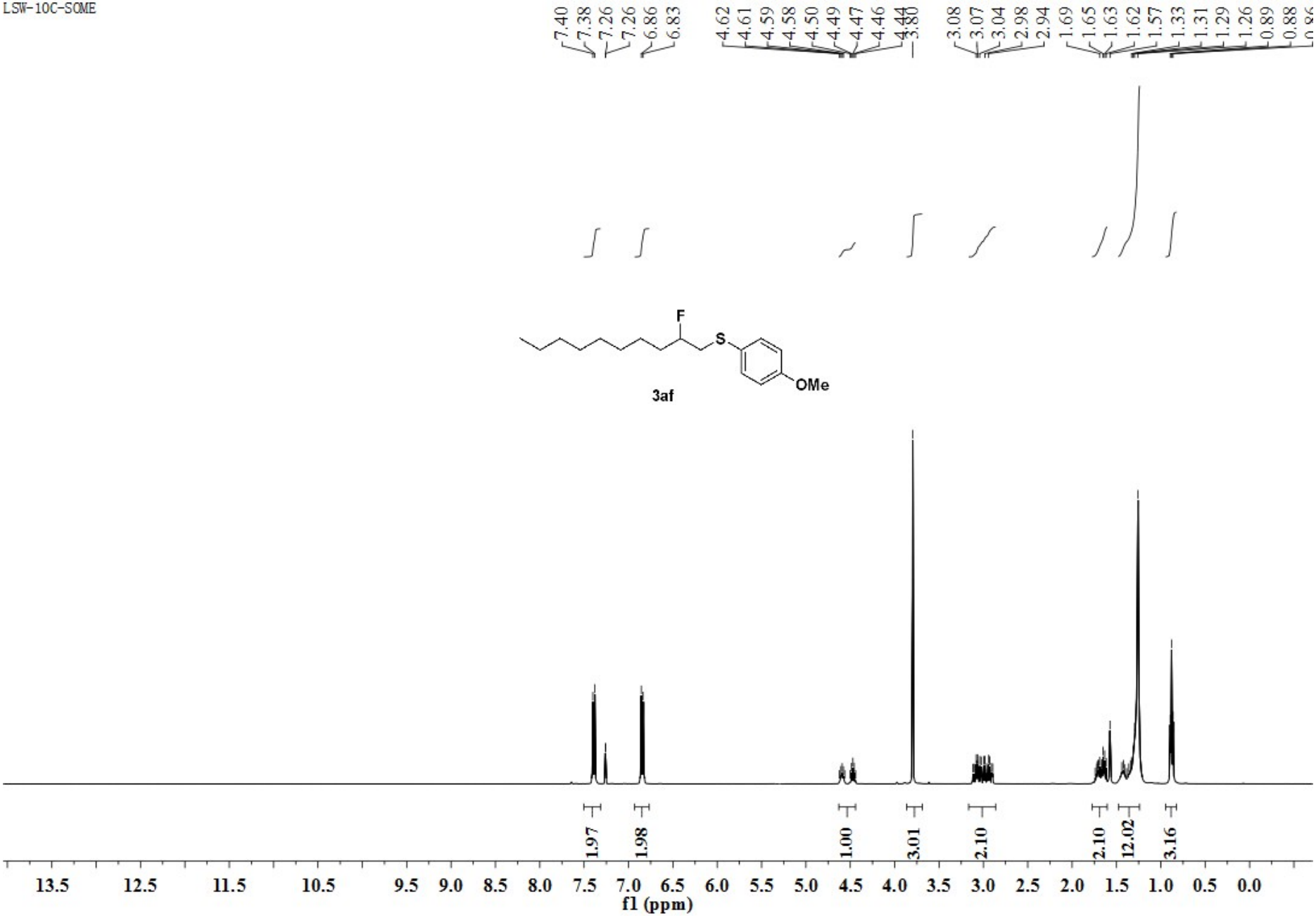

176.47
176.52
176.53
176.55
176.57
176.58
176.60
176.63
176.65
176.66
176.68
176.70
176.71
176.73
176.76
176.77
176.79
176.83


F
S
3ae
Ac

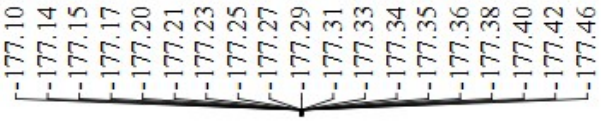

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

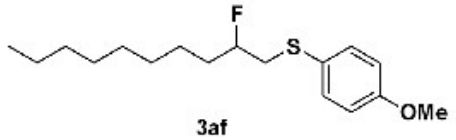

1sw-10c-sac
197.14
143.38
134.41
128.87
127.11
92.92
91.77
36.93
36.77
34.41
34.27
31.83
29.40
29.33
29.19
26.47
24.89
24.86
22.65
14.10
F
S
Ac
3ae
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

LSW-10C-SOME

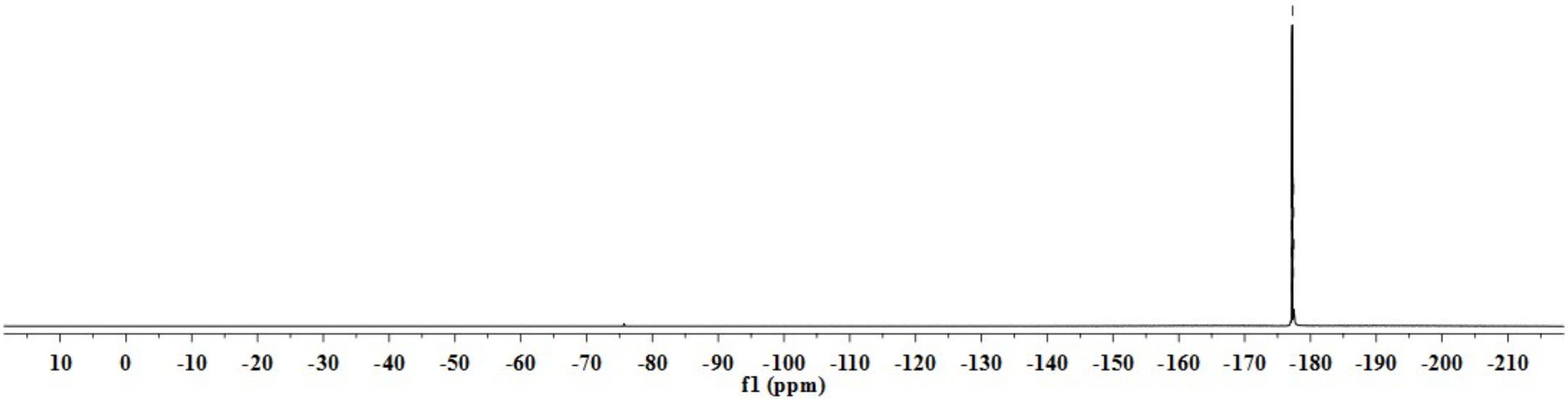

7.40
7.38
7.26
7.26
6.86
6.83
4.62
4.61
4.59
4.58
4.50
4.49
4.47
4.46
4.44
3.80
3.08
3.07
3.04
2.98
2.94
1.69
1.65
1.63
1.62
1.57
1.33
1.31
1.29
1.26
0.89
0.88
F
S
OMe
3af
1.97
1.98
1.00
3.01
2.10
2.10
12.02
3.16
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-10C-SOME





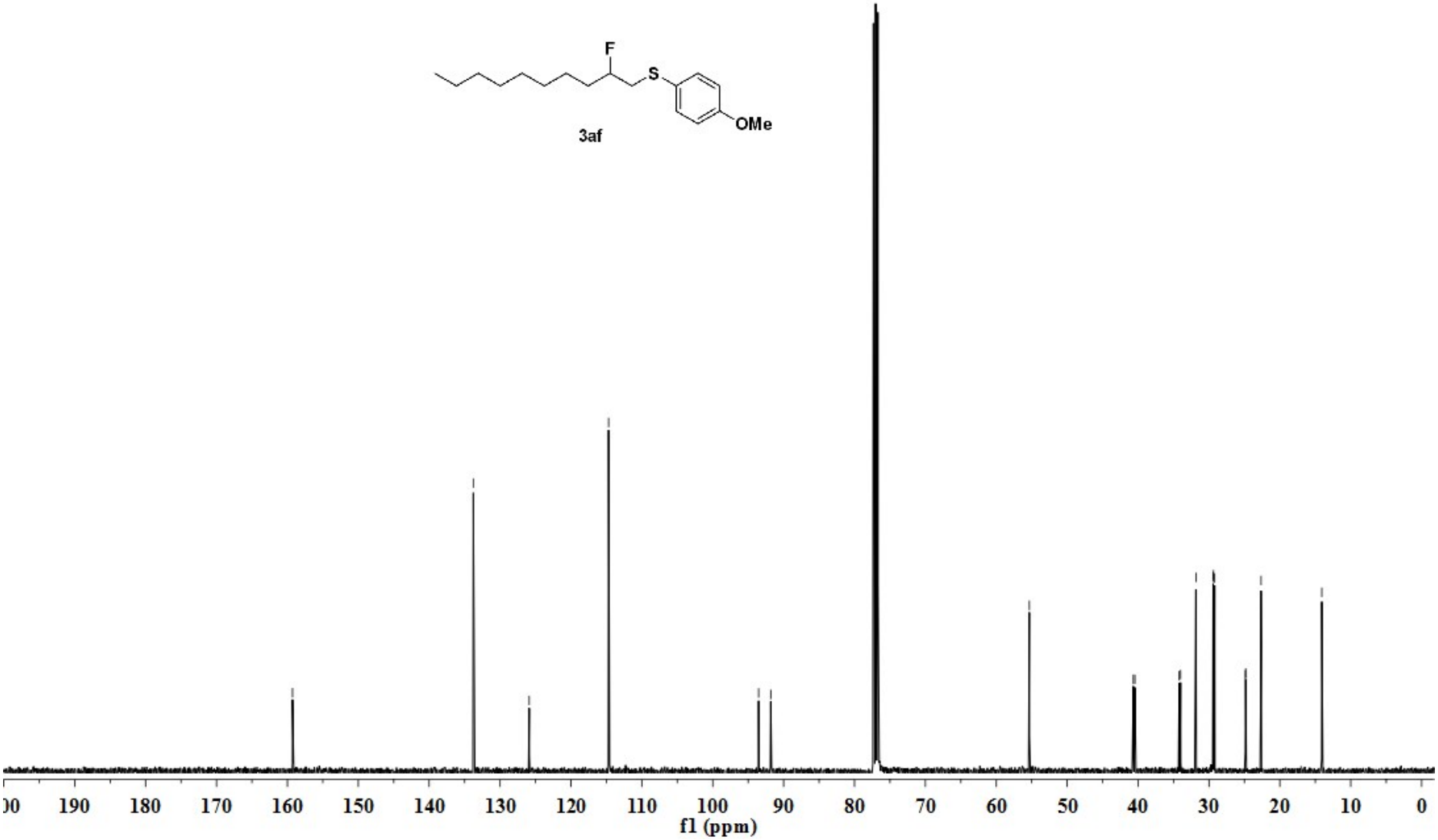
3af

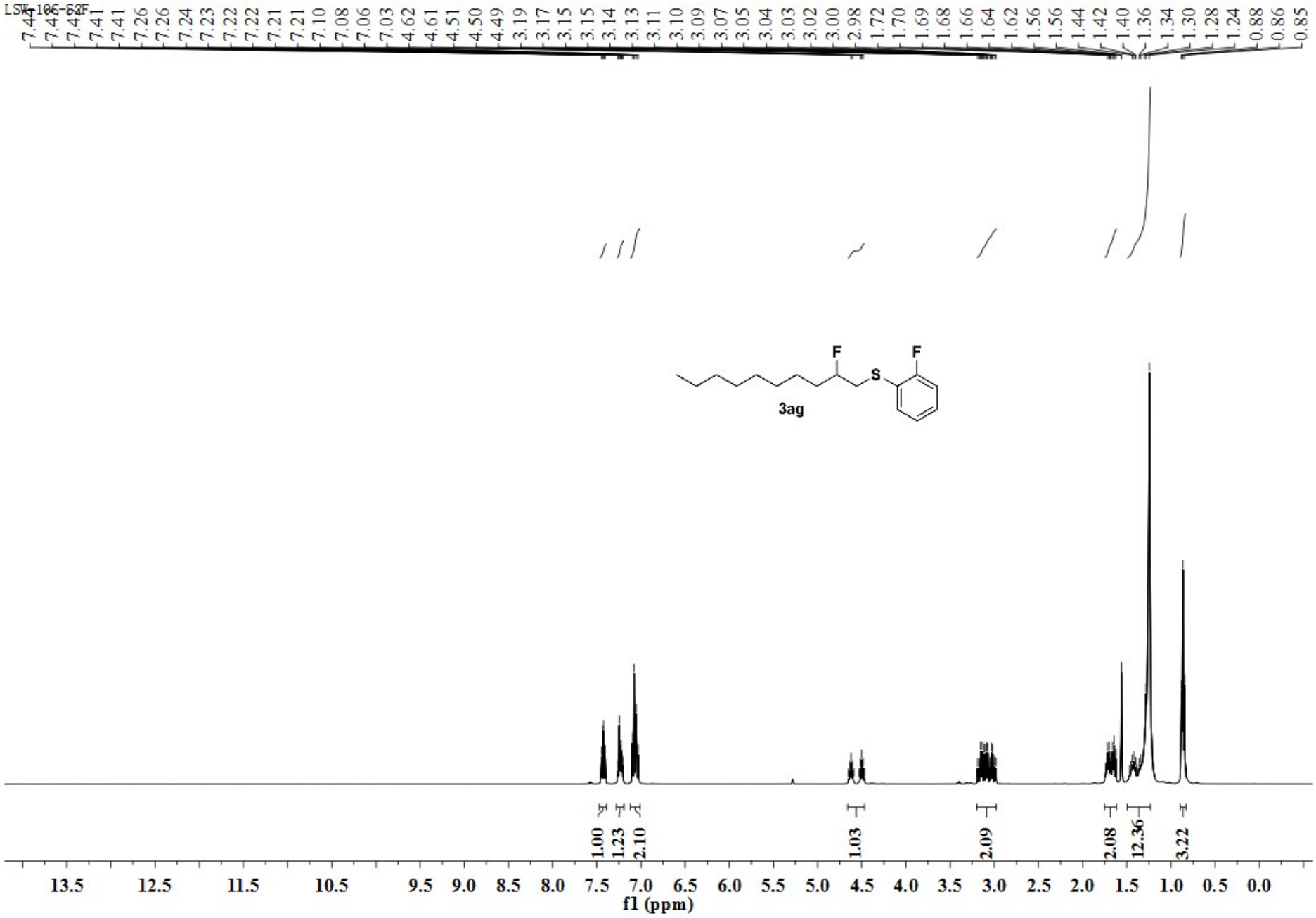


LSW-10C-SOME-C

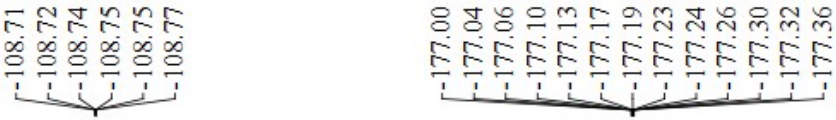
159.27
133.77
125.88
114.69
93.53
91.81
55.34
40.67
34.20
34.00
31.84
29.41
29.36
29.19
24.86
24.83
22.65
14.08

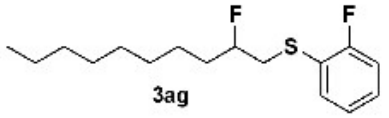
3af



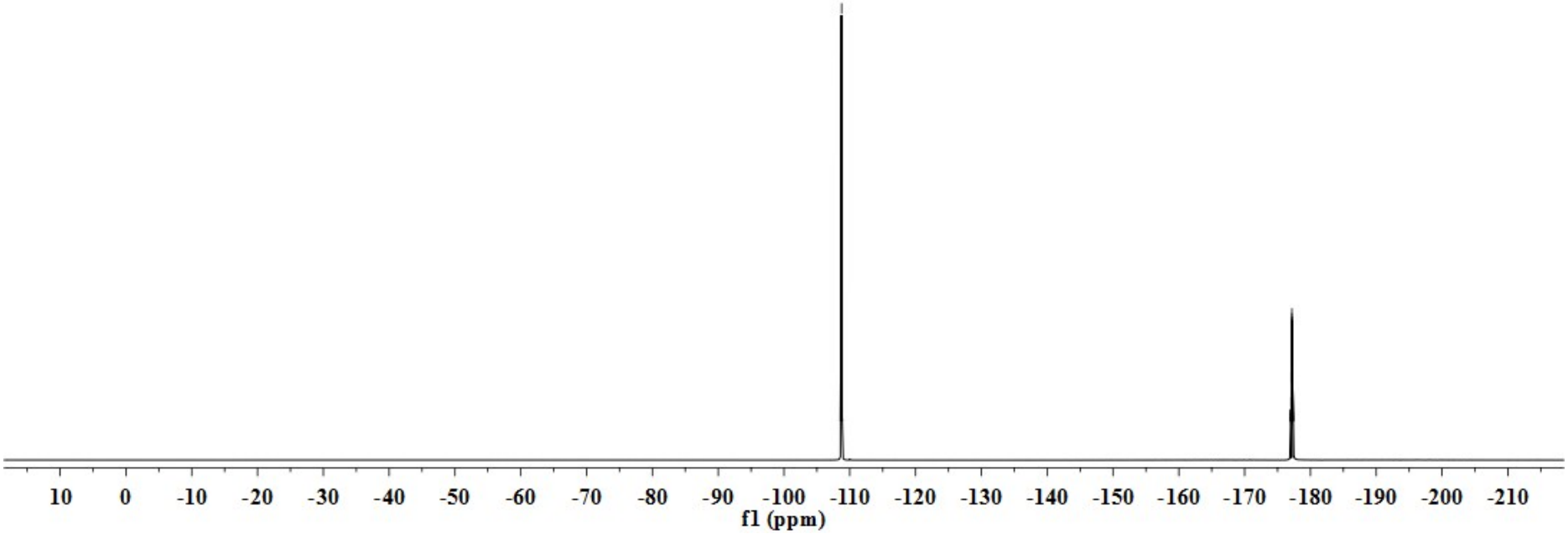

LSW-106-S2F
7.44 7.43 7.41 7.41 7.41 7.26 7.26 7.24 7.23 7.22 7.22 7.21 7.21 7.10 7.08 7.06 7.03 4.62 4.61 4.51 4.50 4.49 3.19 3.17 3.15 3.15 3.14 3.13 3.11 3.10 3.09 3.07 3.05 3.04 3.03 3.02 3.00 2.98 1.72 1.70 1.69 1.68 1.66 1.64 1.62 1.56 1.56 1.44 1.42 1.40 1.36 1.34 1.30 1.28 1.24 0.88 0.86 0.85
F
F
S
3ag
1.00
1.23
2.10
1.03
2.09
2.08
12.36
3.22
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

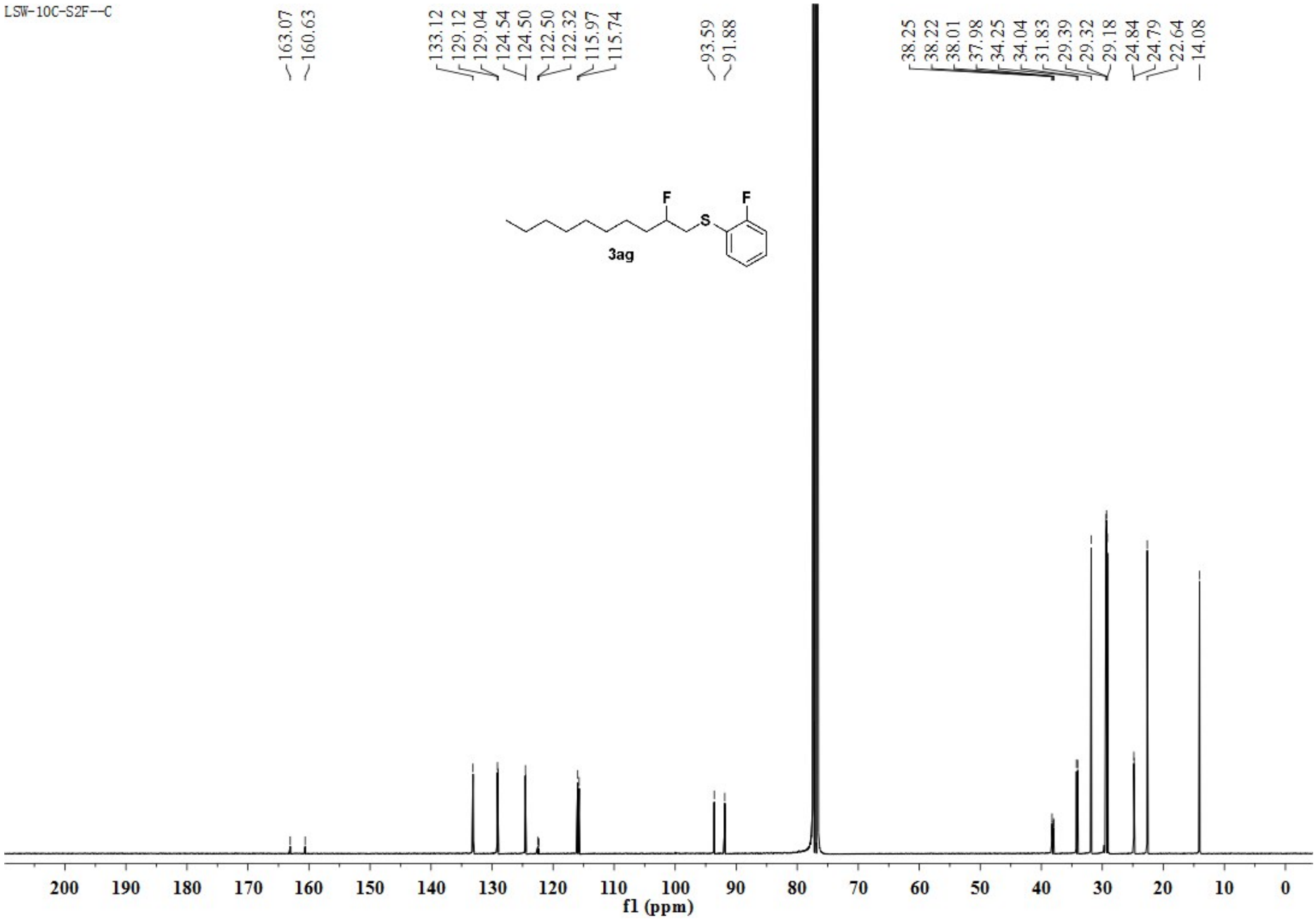
LSW-10C-S2F

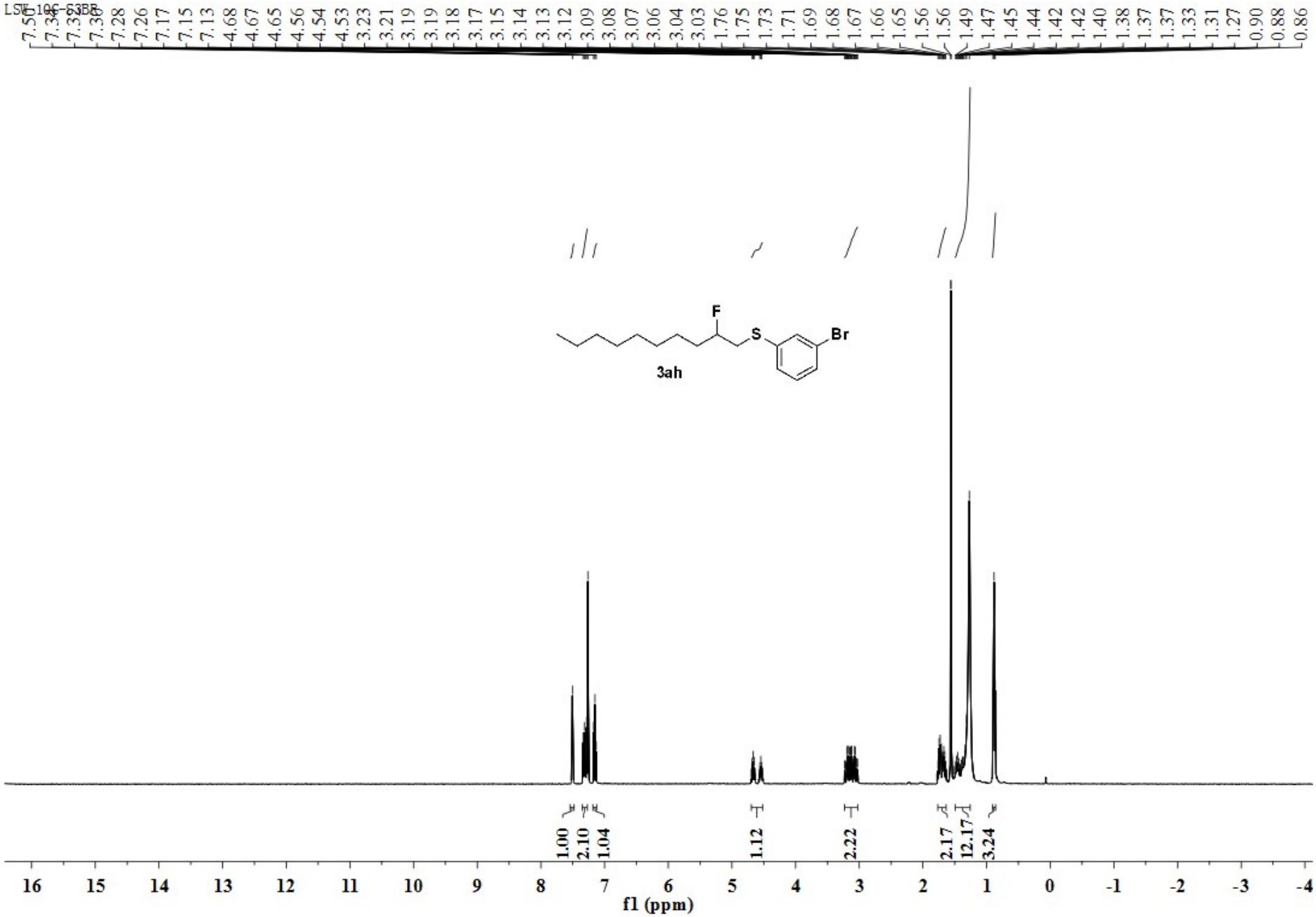




3ag

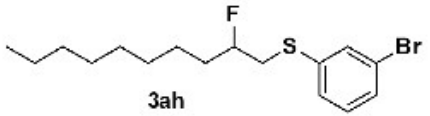



LSW-10C-S2F--C
163.07
160.63
133.12
129.12
129.04
124.54
124.50
122.50
122.32
115.97
115.74
93.59
91.88
38.25
38.22
38.01
37.98
34.25
34.04
31.83
29.39
29.32
29.18
24.84
24.79
22.64
14.08
F
S
F
3ag
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

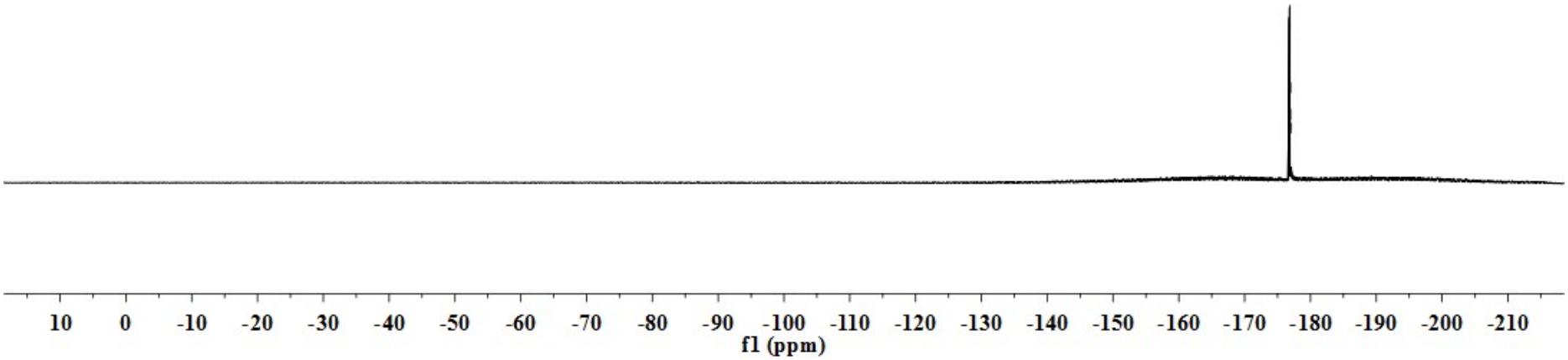

7.50
7.34
7.33
7.30
7.28
7.26
7.17
7.15
7.13
4.68
4.67
4.65
4.56
4.54
4.53
3.23
3.21
3.19
3.19
3.18
3.17
3.15
3.14
3.13
3.12
3.09
3.08
3.07
3.06
3.04
3.03
1.76
1.75
1.73
1.71
1.69
1.68
1.67
1.66
1.65
1.56
1.56
1.49
1.47
1.45
1.44
1.42
1.42
1.40
1.38
1.37
1.37
1.33
1.31
1.27
0.90
0.88
0.86
F
S
Br
3ah
1.00
2.10
1.04
1.12
2.22
2.17
12.17
3.24
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

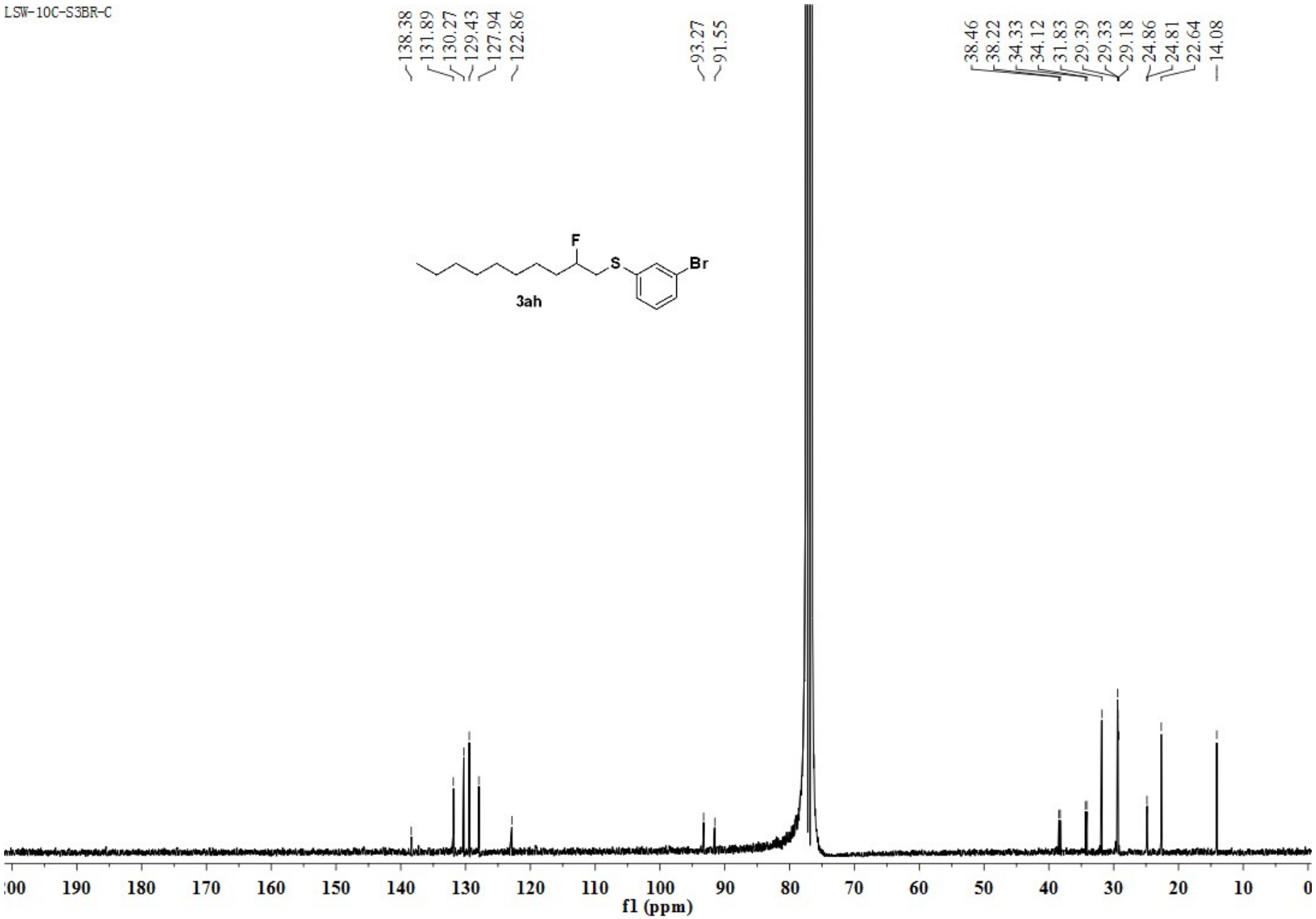
LSW-10C-S3BR

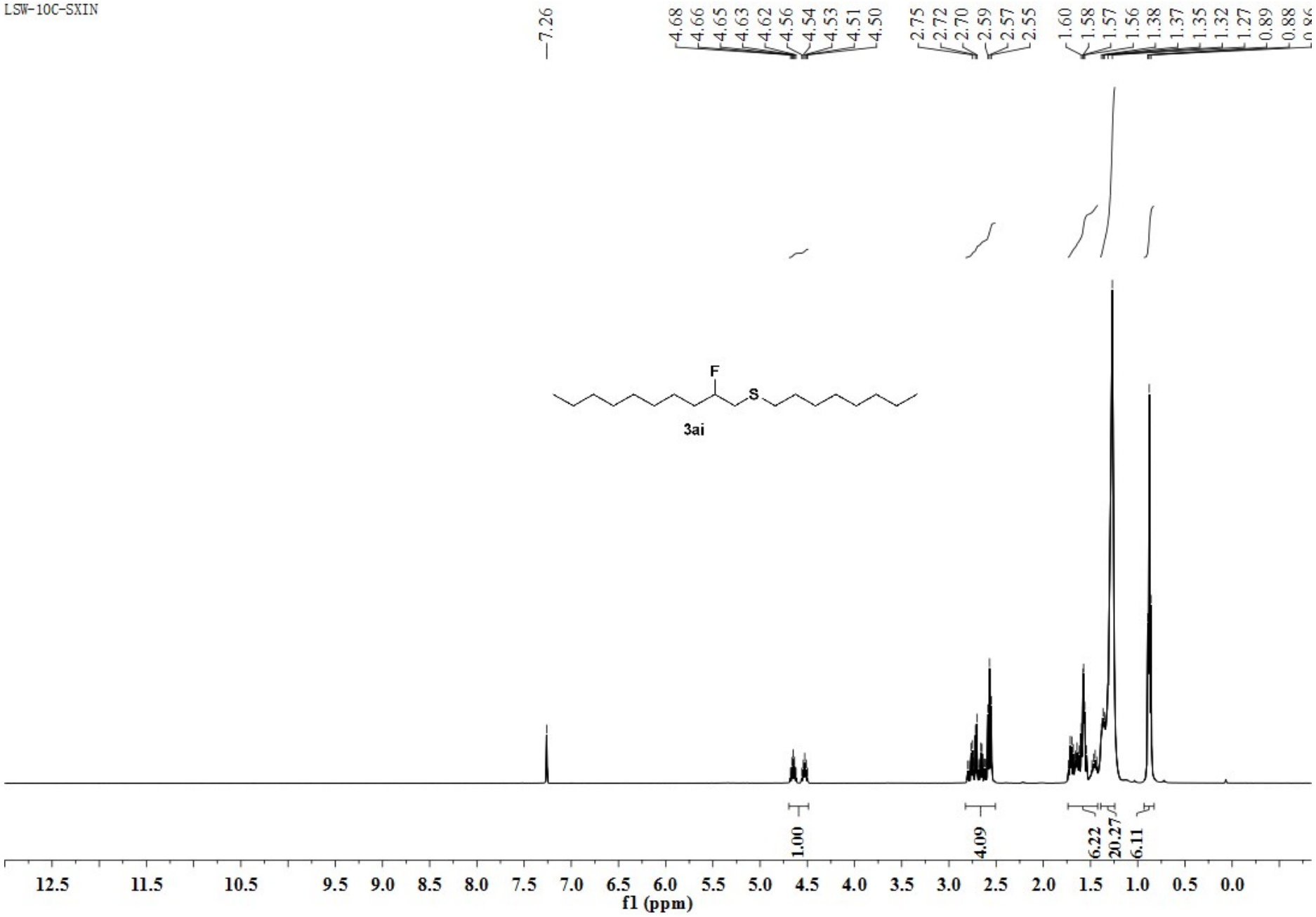
176.66
176.71
176.72
176.76
176.78
176.79
176.82
176.84
176.85
176.89
176.91
176.91
176.92
176.97
176.98
177.02



3ah

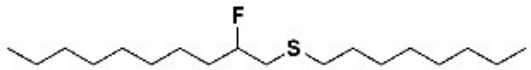



LSW-10C-S3BR-C
138.38
131.89
130.27
129.43
127.94
122.86
93.27
91.55
38.46
38.22
34.33
34.12
31.83
29.39
29.33
29.18
24.86
24.81
22.64
14.08
F
S
Br
3ah
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

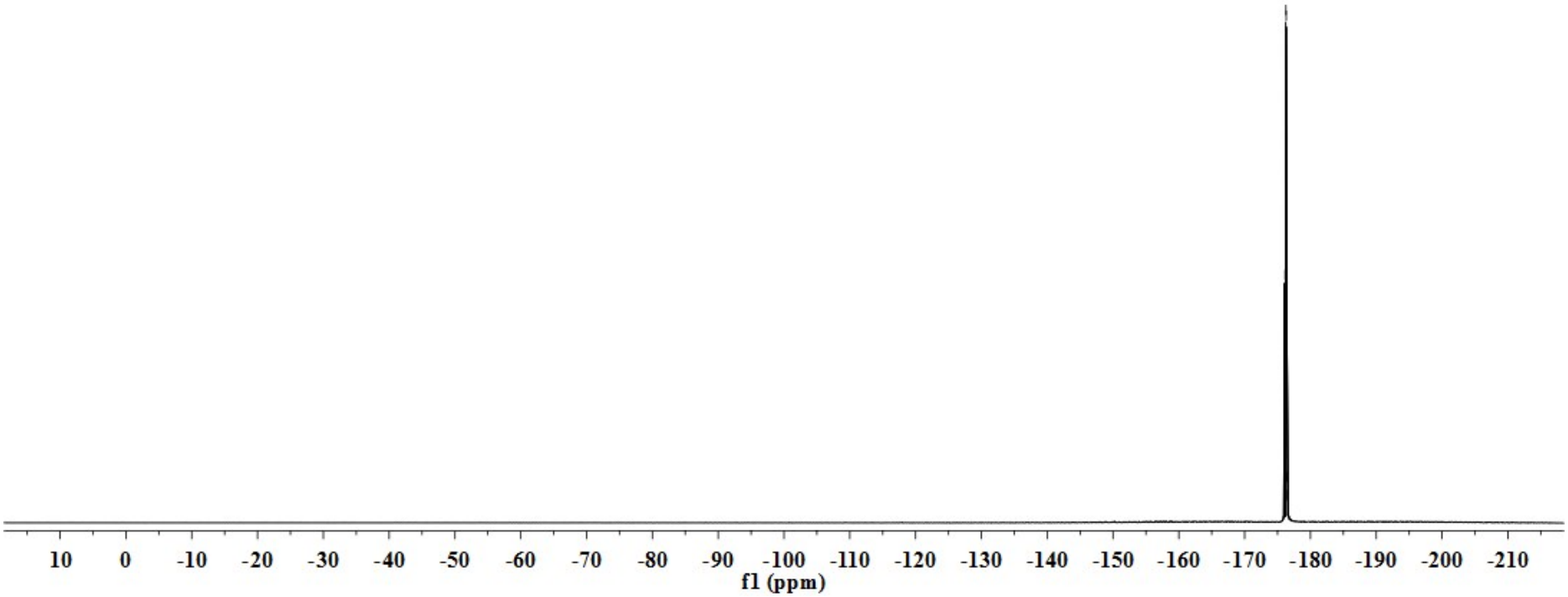

LSW-10C-SXIN
7.26
4.68
4.66
4.65
4.63
4.62
4.56
4.54
4.53
4.51
4.50
2.75
2.72
2.70
2.59
2.57
2.55
1.60
1.58
1.57
1.56
1.38
1.37
1.35
1.32
1.27
0.89
0.88
F
S
3ai
1.00
4.09
6.22
20.27
6.11
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

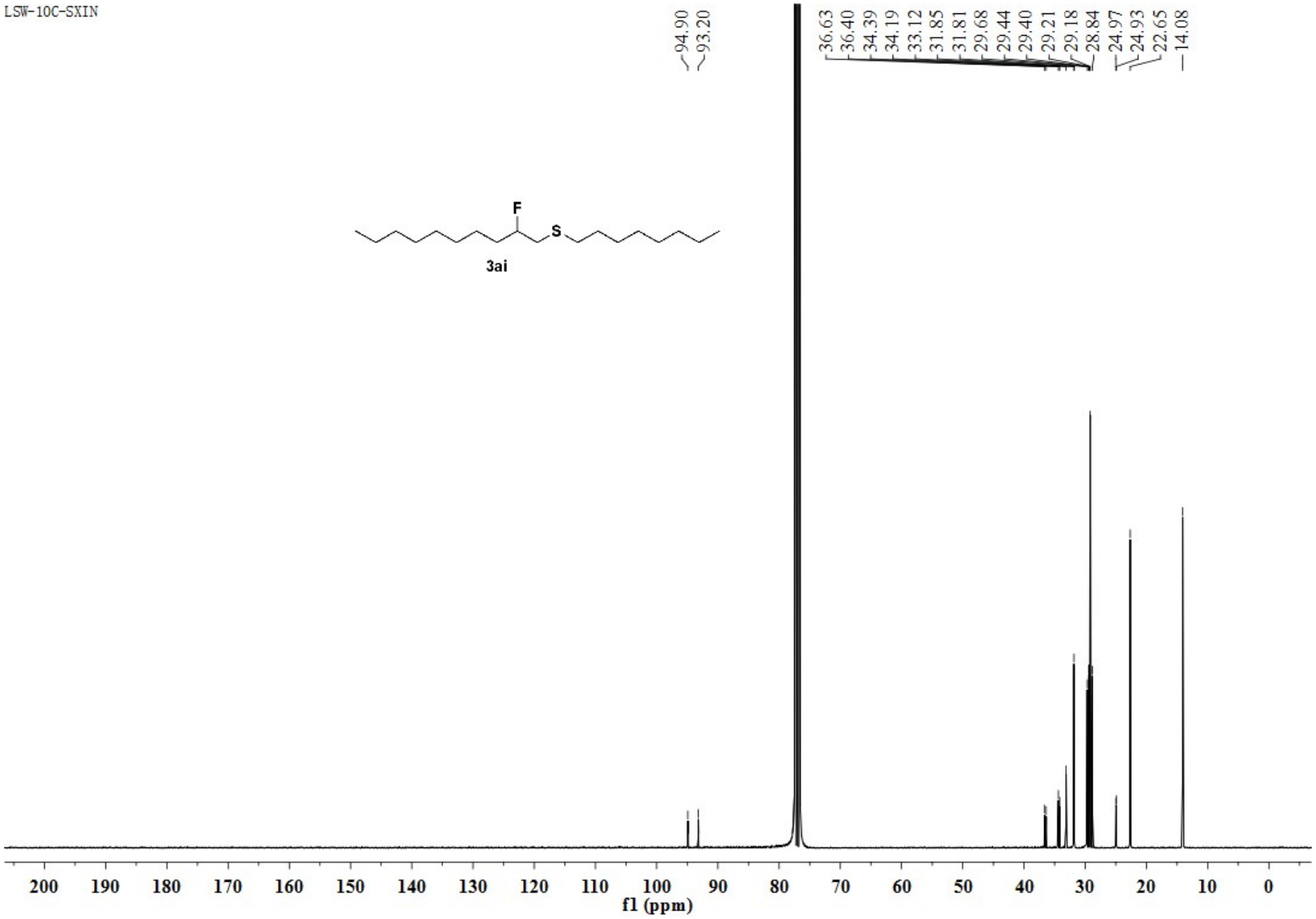
LSW-10C-SXIN

-176.05
-176.08
-176.10
-176.13
-176.14
-176.18
-176.20
-176.21
-176.25
-176.27
-176.31
-176.34
-176.36
-176.38
-176.40
-176.42
-176.44

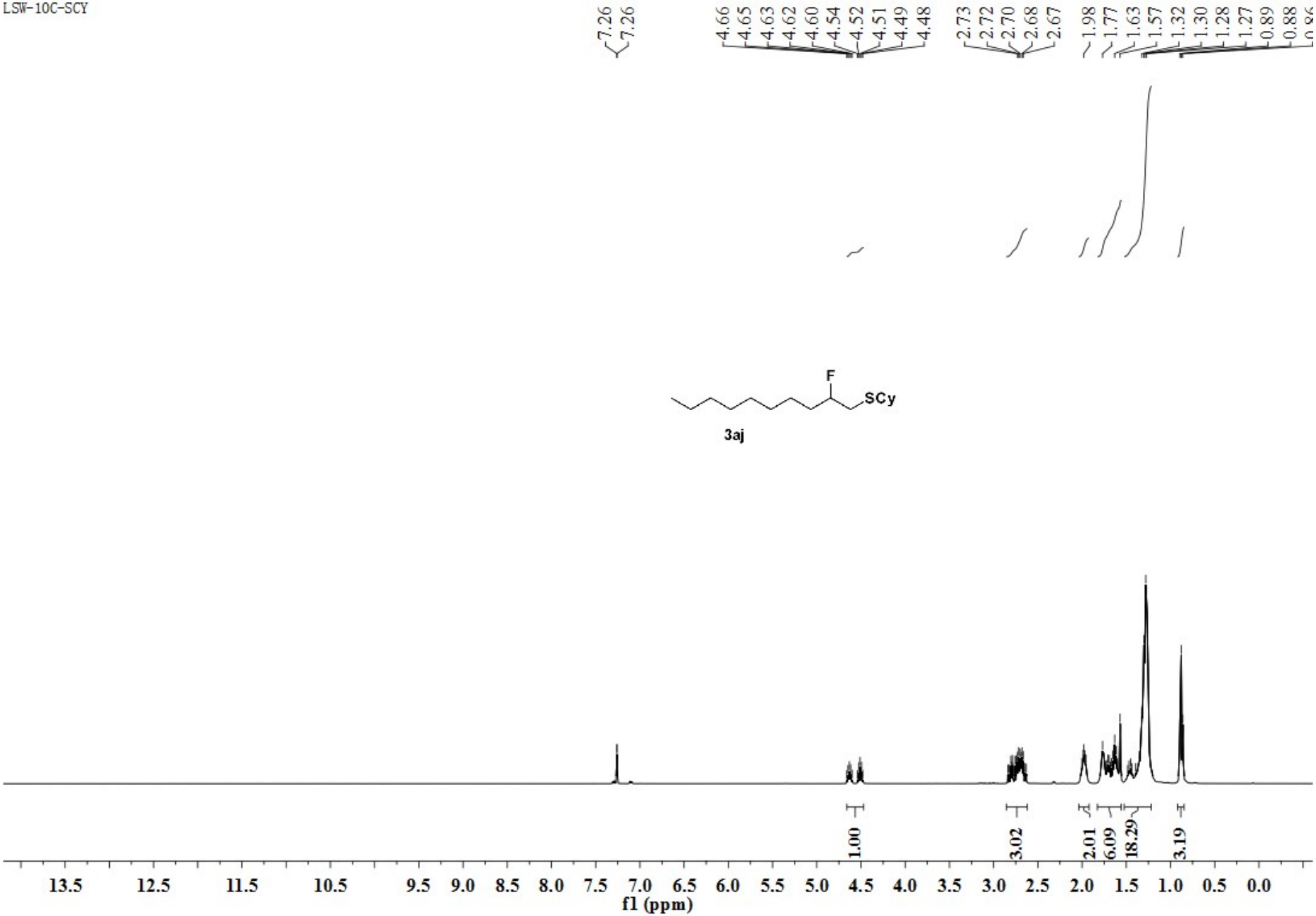


3ai

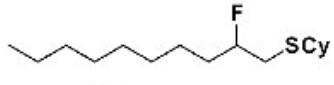



LSW-10C-SXIN
94.90
93.20
36.63
36.40
34.39
34.19
33.12
31.85
31.81
29.68
29.44
29.40
29.21
29.18
28.84
24.97
24.93
22.65
14.08
F
S
3ai
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

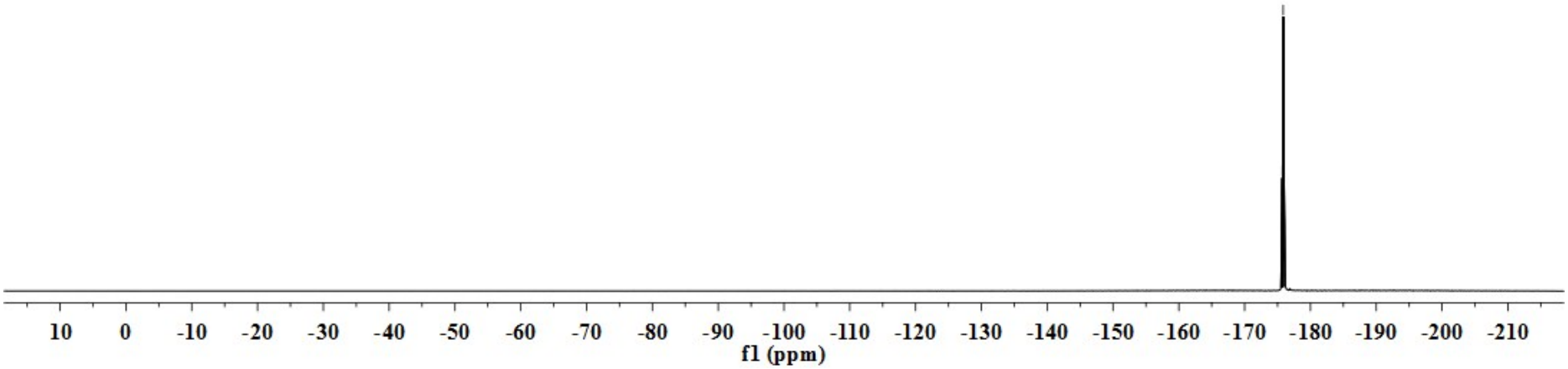
LSW-10C-SCY

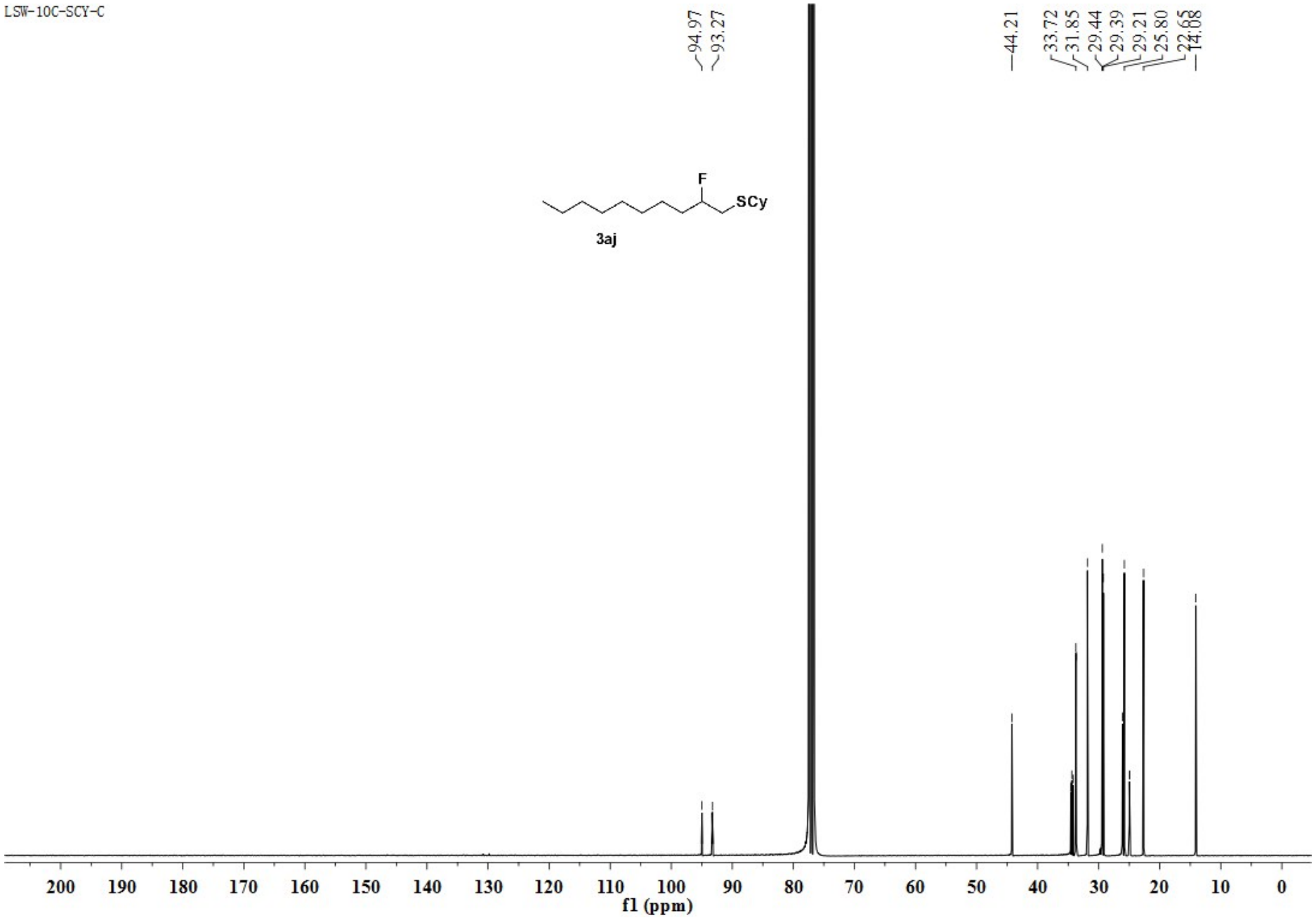

7.26
7.26
4.66
4.65
4.63
4.62
4.60
4.54
4.52
4.51
4.49
4.48
2.73
2.72
2.70
2.68
2.67
1.98
1.77
1.63
1.57
1.32
1.30
1.28
1.27
0.89
0.88
F
SCy
3aj
1.00
3.02
2.01
6.09
18.29
3.19
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

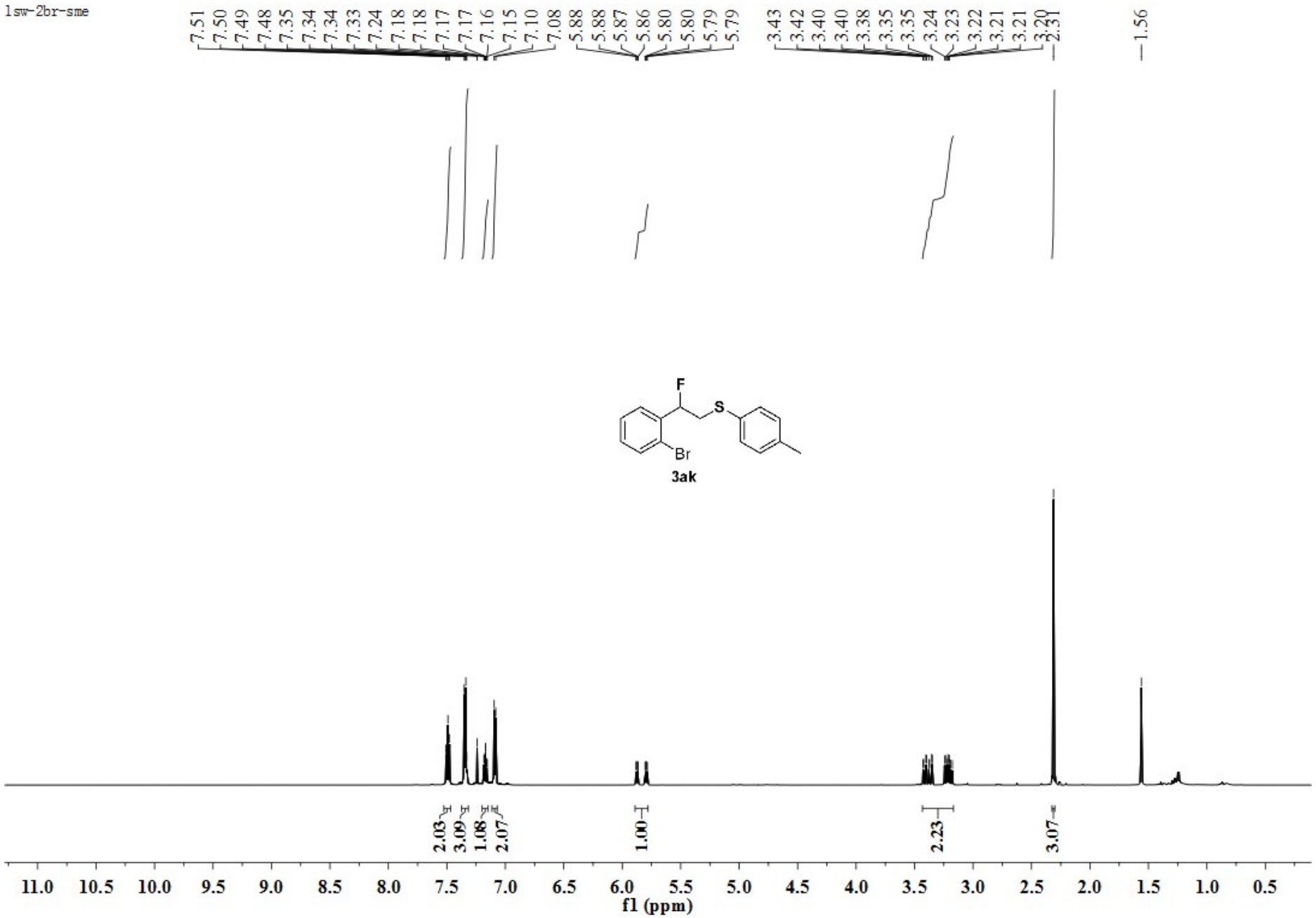
LSW-10C-SCY



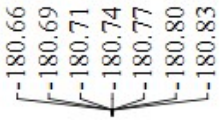
3aj

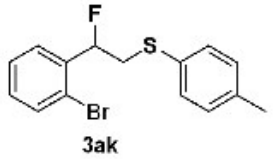



LSW-10C-SCY-C
94.97
93.27
44.21
33.72
31.85
29.44
29.39
29.21
25.80
22.65
14.08
F
SCy
3aj
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

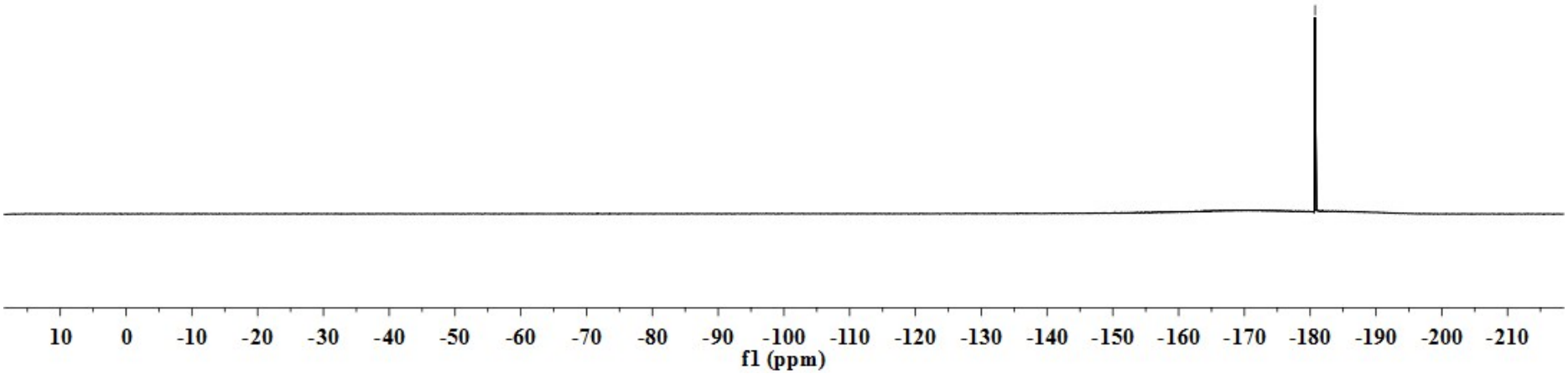

1sw-2br-sme
7.51
7.50
7.49
7.48
7.35
7.34
7.34
7.33
7.24
7.18
7.18
7.17
7.17
7.16
7.15
7.10
7.08
5.88
5.88
5.87
5.86
5.80
5.80
5.79
5.79
3.43
3.42
3.40
3.40
3.38
3.35
3.35
3.24
3.23
3.22
3.21
3.21
3.20
2.31
1.56
F
S
Br
3ak
2.03
3.09
1.08
2.07
1.00
2.23
3.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

1sw-2br-sme





3ak



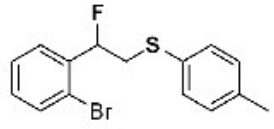
1sw-2br-sme

138.18
138.03
137.12
132.73
131.57
131.39
129.97
129.96
129.75
127.76
127.27
127.21
120.82
120.78

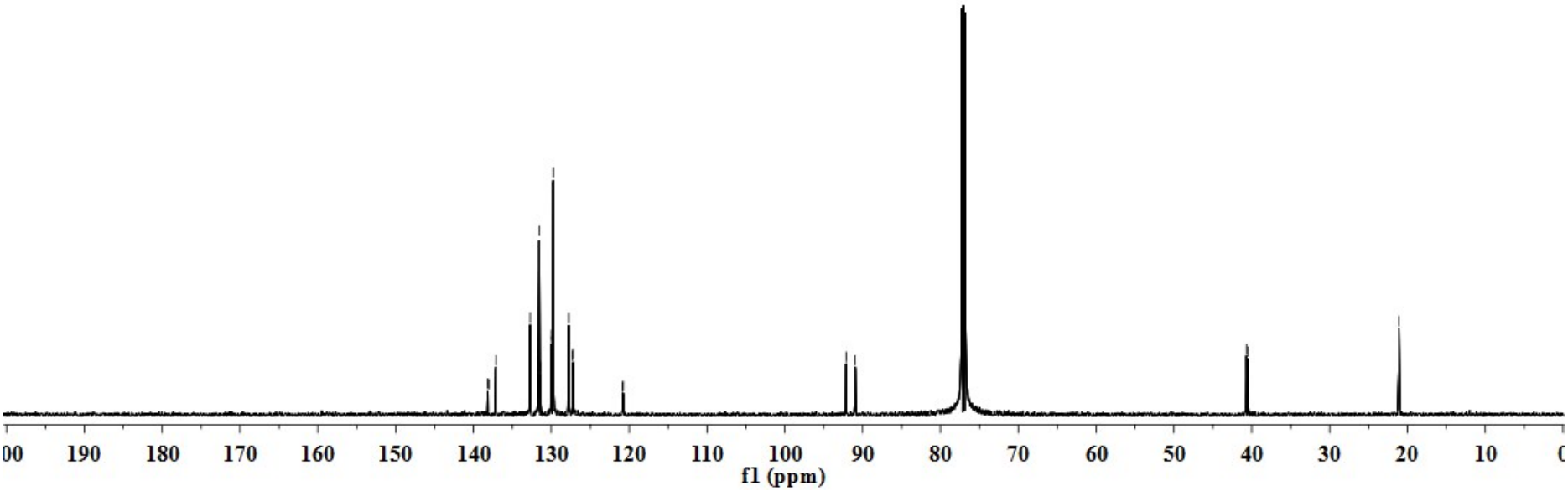
92.12
90.95

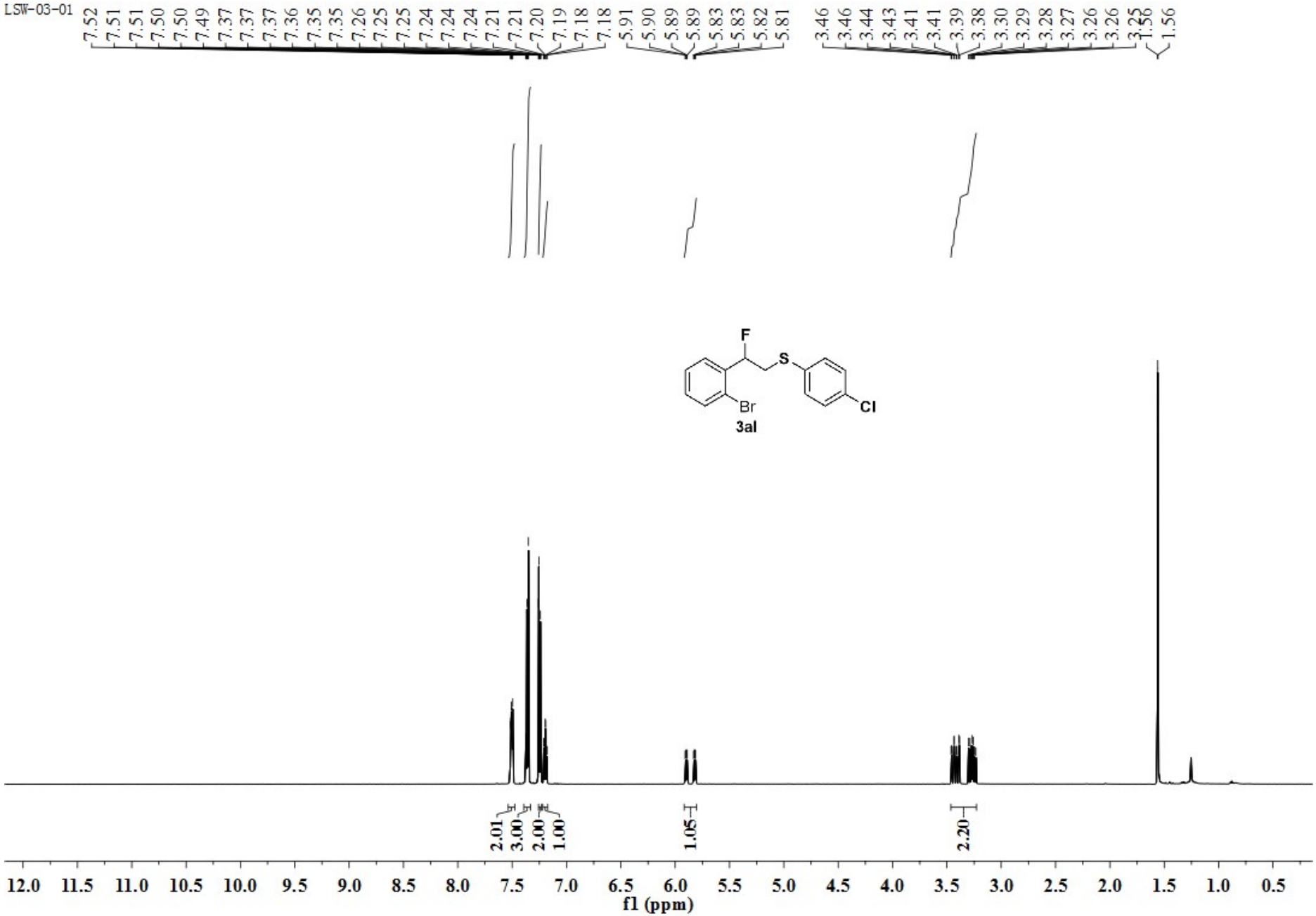
40.68
40.51

21.09

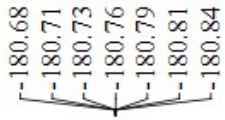


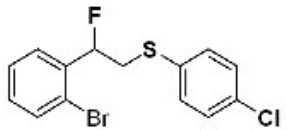
3ak



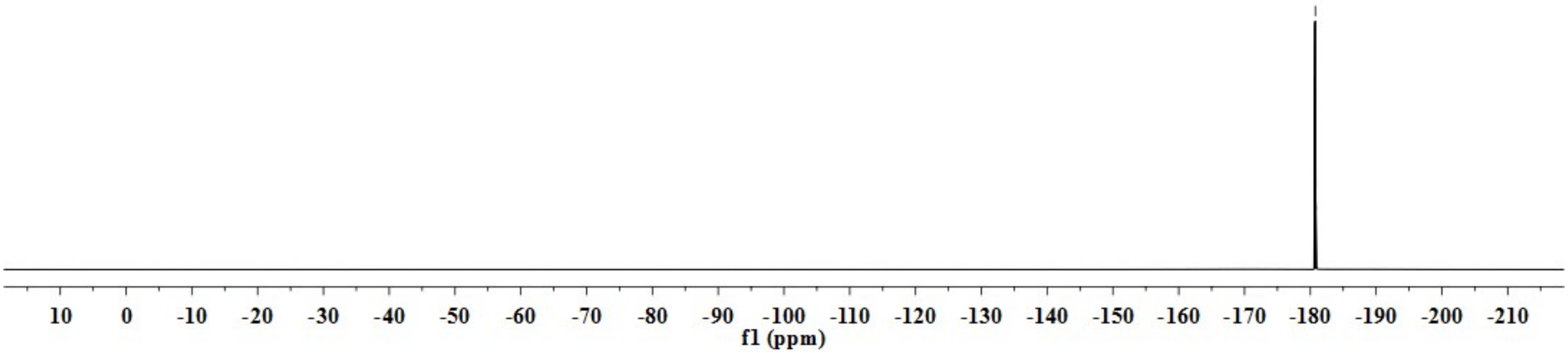

LSW-03-01
7.52
7.51
7.51
7.50
7.50
7.49
7.37
7.37
7.37
7.36
7.35
7.35
7.26
7.25
7.25
7.24
7.24
7.24
7.21
7.21
7.20
7.19
7.18
7.18
5.91
5.90
5.89
5.89
5.83
5.83
5.82
5.81
3.46
3.46
3.44
3.43
3.41
3.41
3.39
3.38
3.30
3.29
3.28
3.27
3.26
3.26
3.25
1.56
1.56
F
S
Br
Cl
3al
2.01
3.00
2.00
1.00
1.05
2.20
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

LSW-03-01

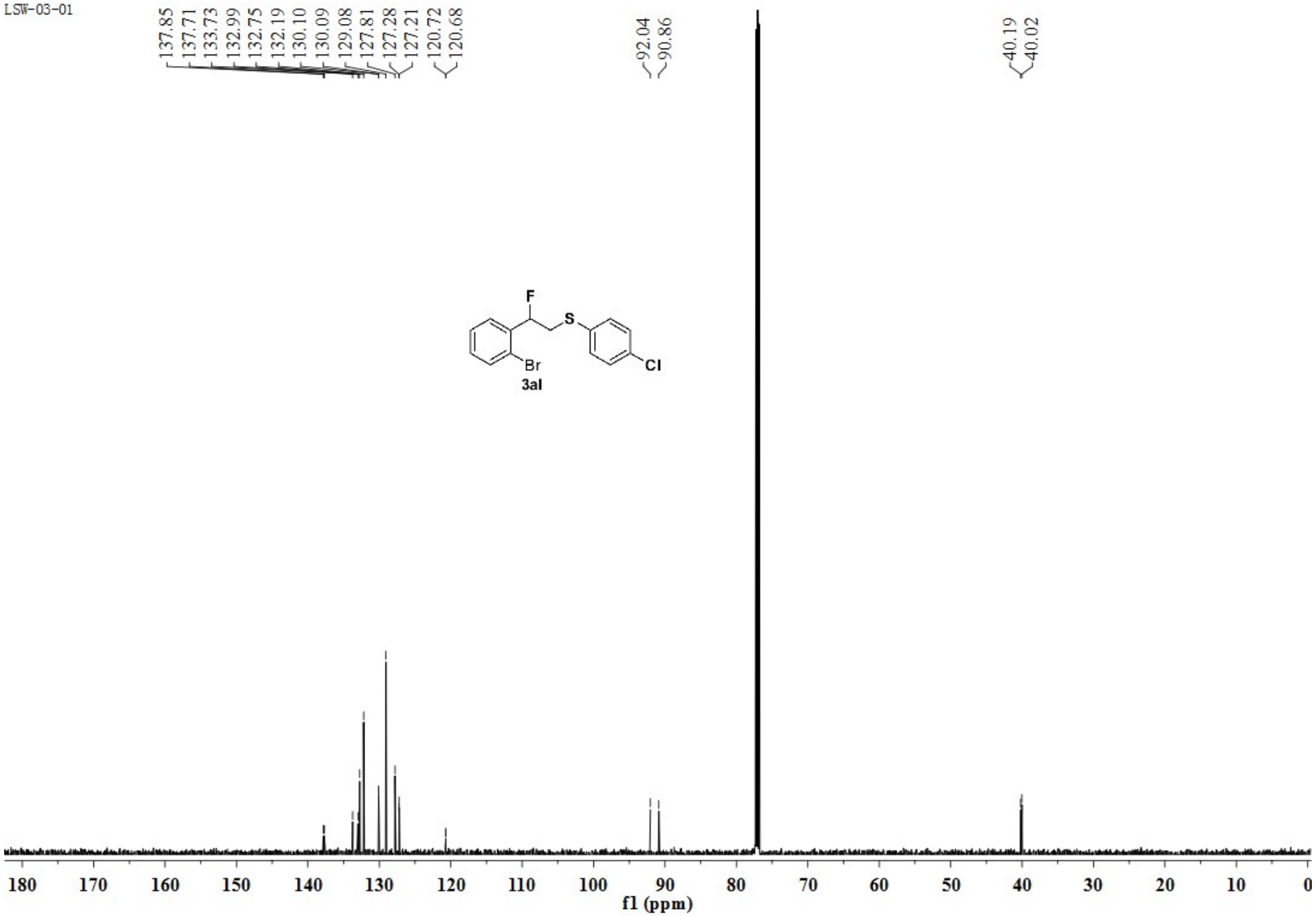

180.68
180.71
180.73
180.76
180.79
180.81
180.84

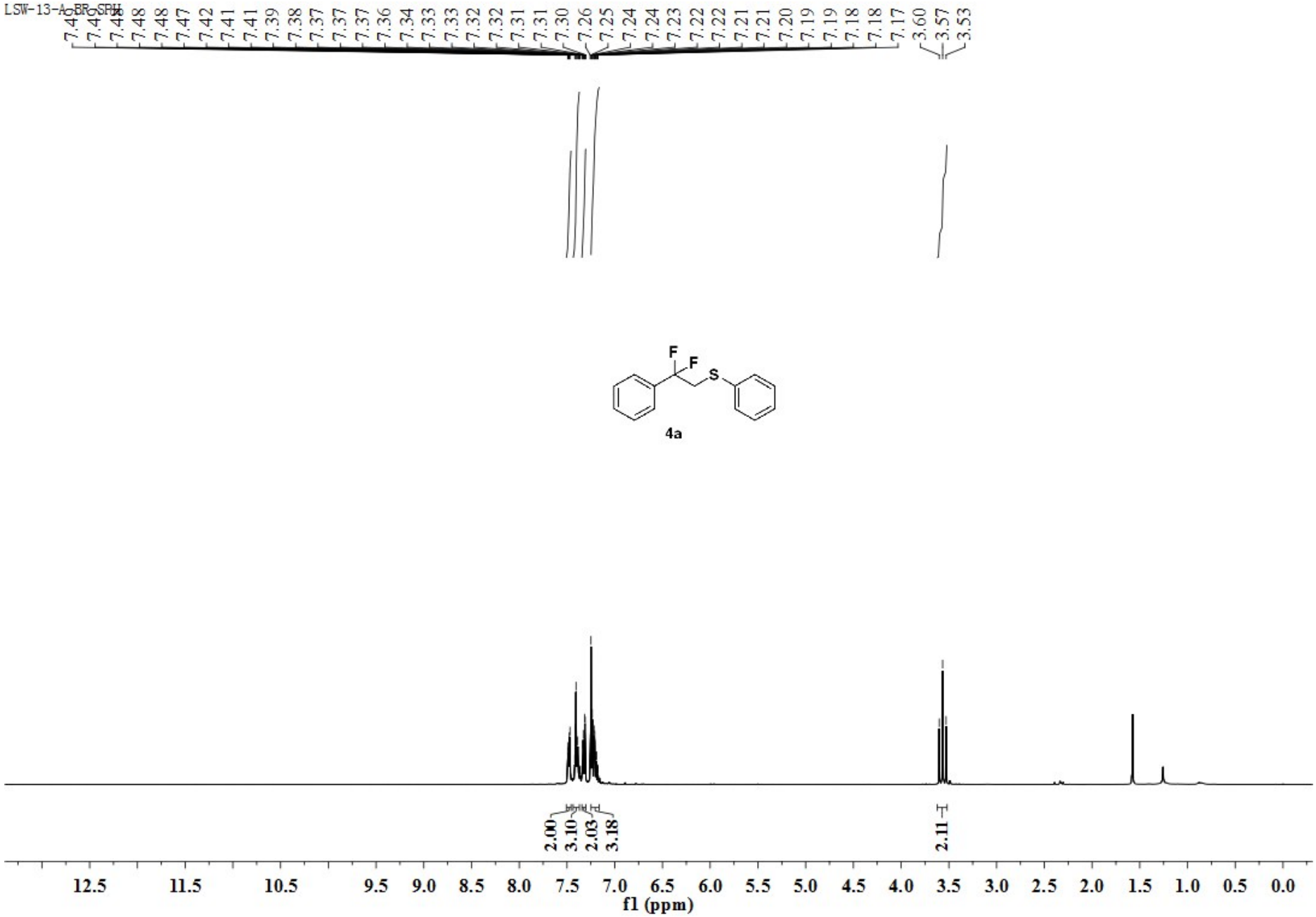

F
S
Br
Cl

3al


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

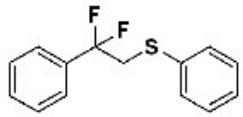
LSW-03-01


137.85
137.71
133.73
132.99
132.75
132.19
130.10
130.09
129.08
127.81
127.28
127.21
120.72
120.68
92.04
90.86
40.19
40.02
F
S
Br
Cl
3al
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

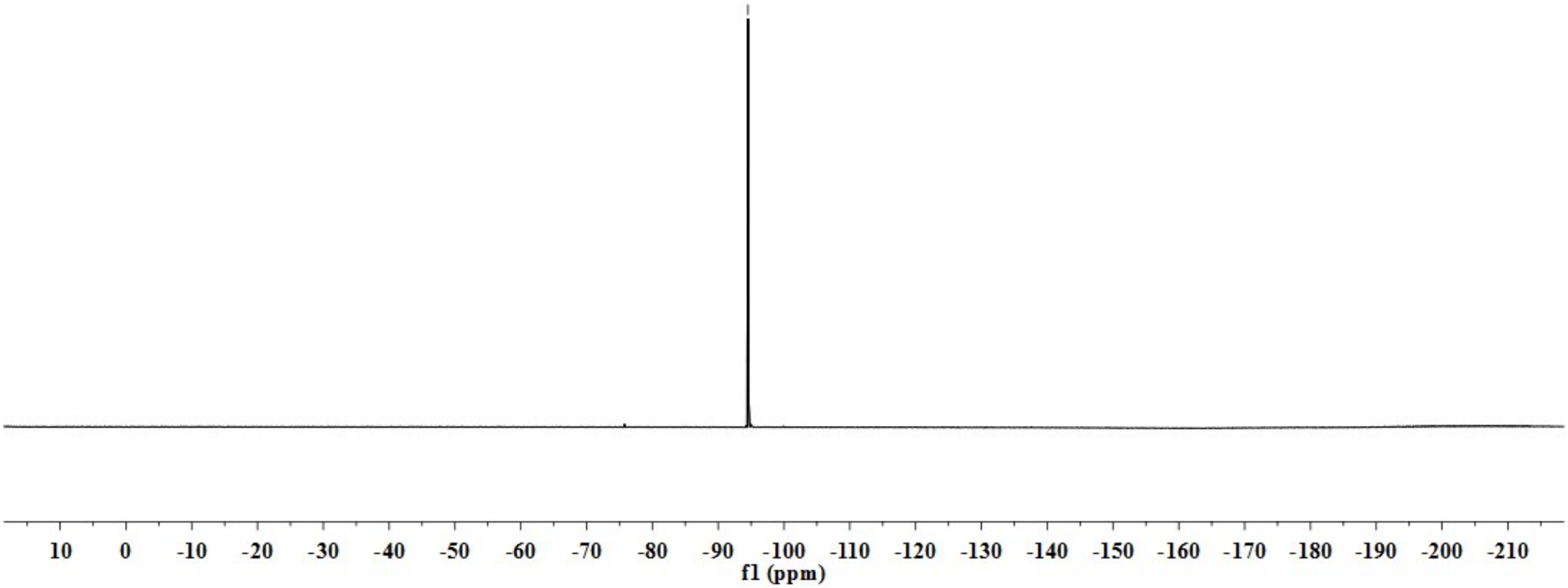

LSW-13-A-BR-SPH
7.48
7.48
7.47
7.42
7.41
7.41
7.39
7.38
7.37
7.37
7.37
7.36
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.26
7.25
7.24
7.24
7.23
7.22
7.22
7.21
7.21
7.20
7.19
7.19
7.18
7.18
7.17
3.60
3.57
3.53
F
F
S
4a
2.00
3.10
2.03
3.18
2.11
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-13-A-BR-SPH

-94.49
-94.53
-94.56



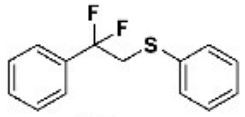
4a



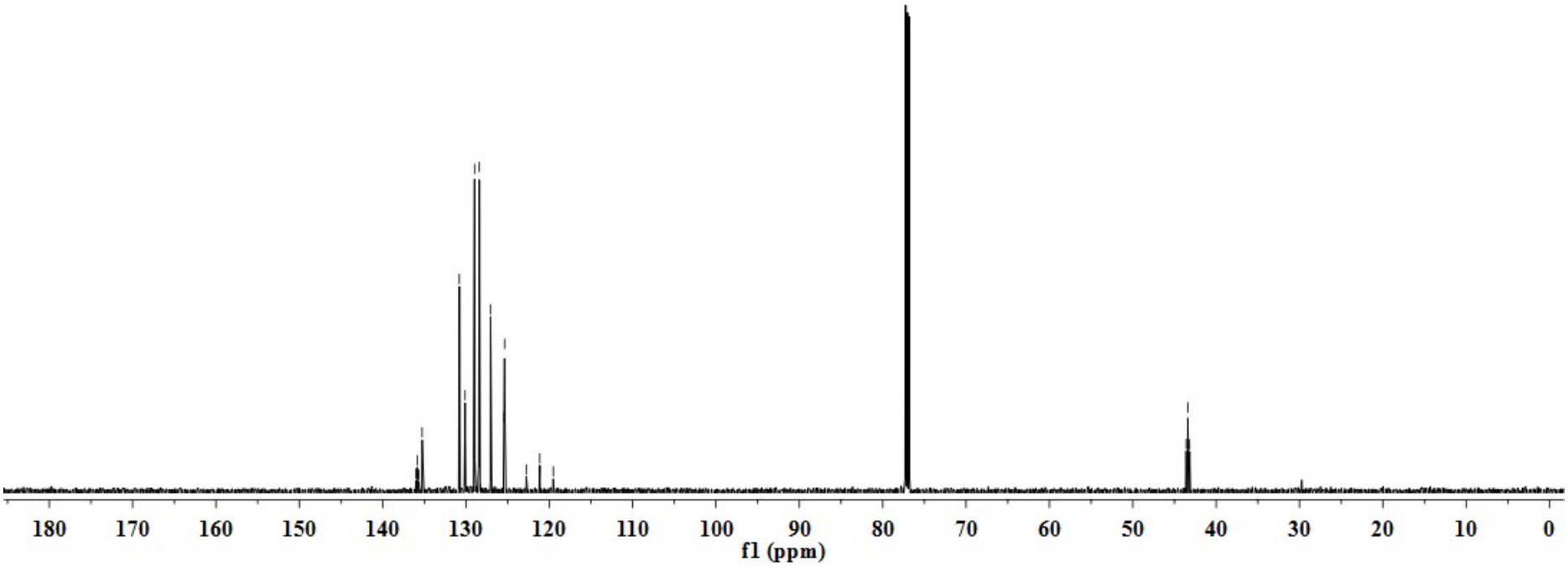
LSW-11-D

136.01
135.84
135.67
135.26
130.80
130.11
128.98
128.41
127.06
125.42
125.38
125.34
122.77
121.15
119.53

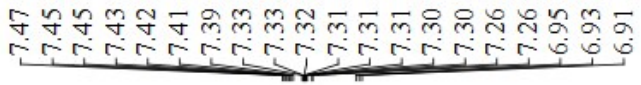
43.60
43.39
43.18

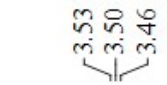


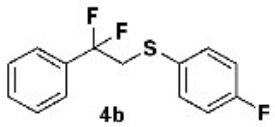
4a



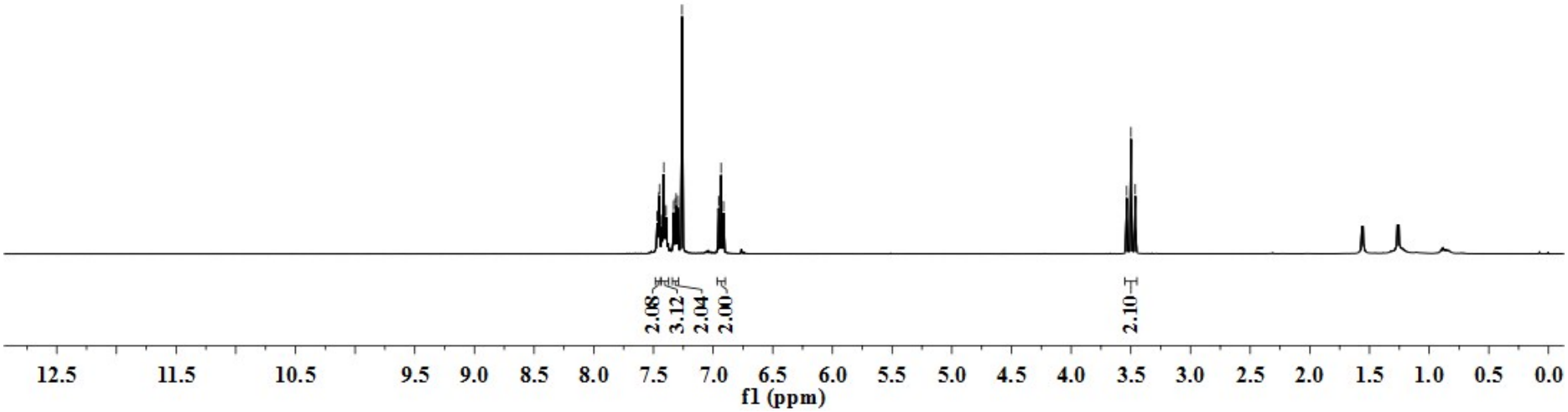
LSW-12-A-A-BR-4F





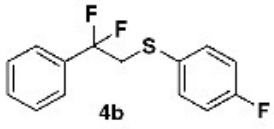


4b

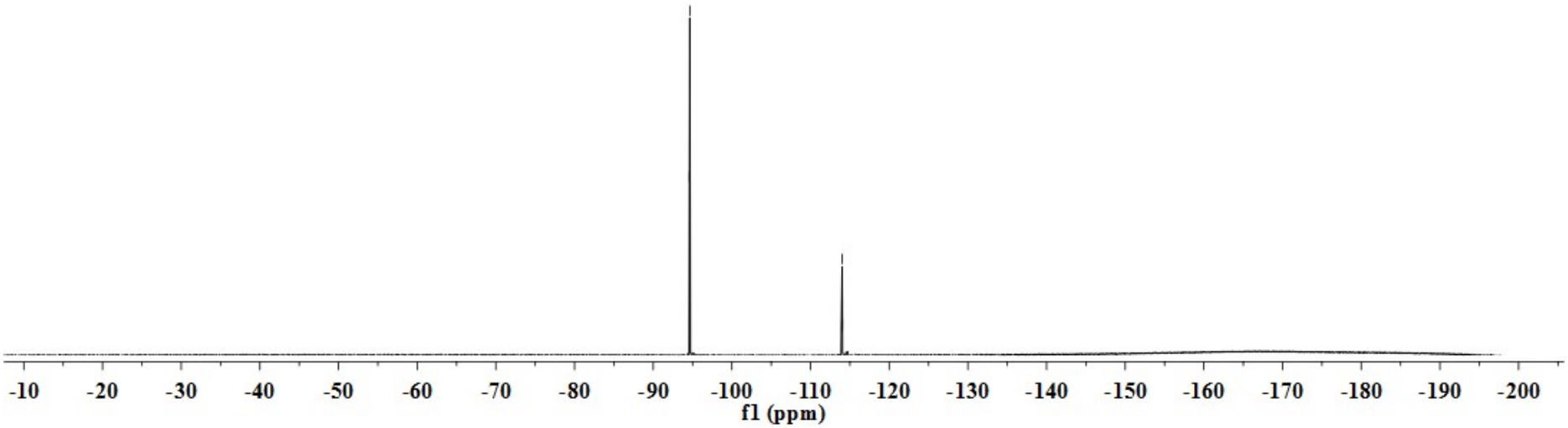


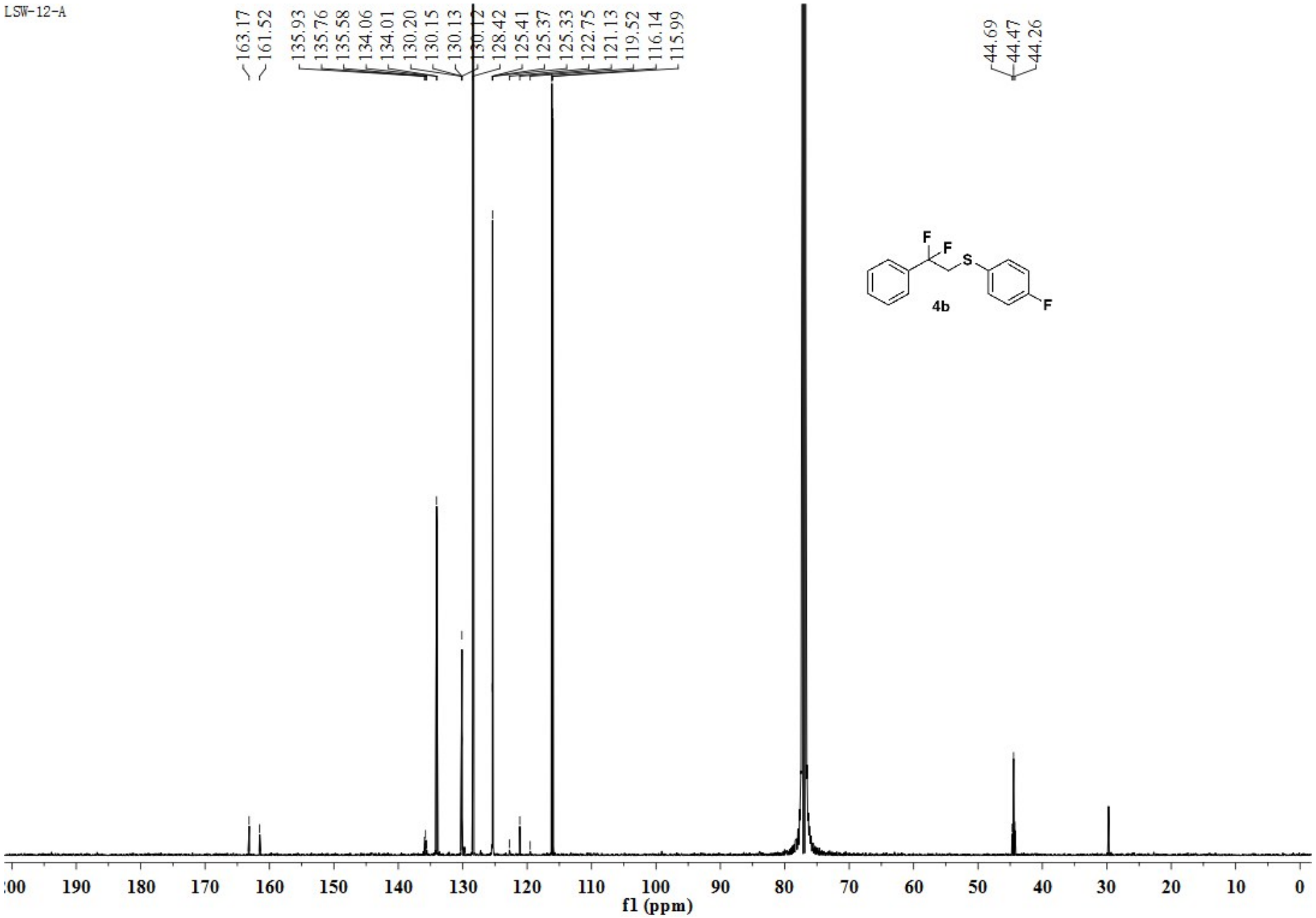
LSW-12-A-A-BR-4F

-94.62
-94.65
-94.69
-113.97
-113.99
-114.00
-114.00
-114.01
-114.02
-114.03
-114.03
-114.05



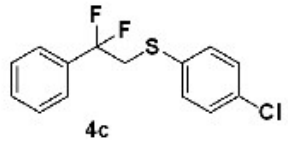
4b



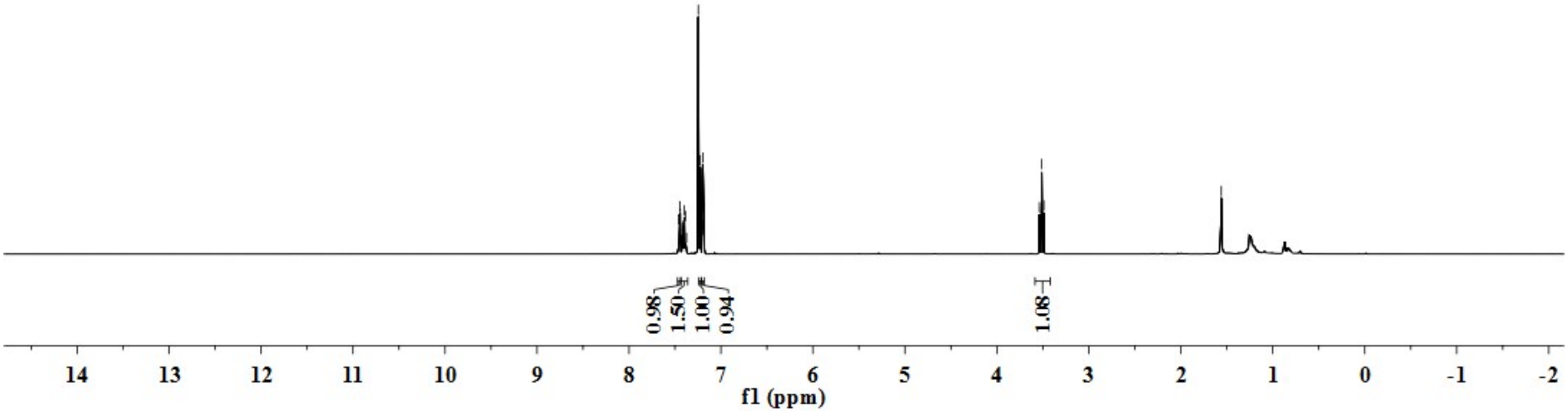

LSW-12-A
163.17
161.52
135.93
135.76
135.58
134.06
134.01
130.20
130.15
130.13
130.12
128.42
125.41
125.37
125.33
122.75
121.13
119.52
116.14
115.99
44.69
44.47
44.26
F
F
S
F
4b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

LSW-9D

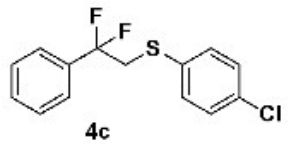
7.46 7.46 7.44 7.44 7.42 7.41 7.41 7.41 7.41 7.40 7.39 7.38 7.25 7.24 7.24 7.23 7.22 7.22 7.20 7.20 7.19 7.19 7.18 3.54 3.51 3.49 1.56



4c



LSW-9D

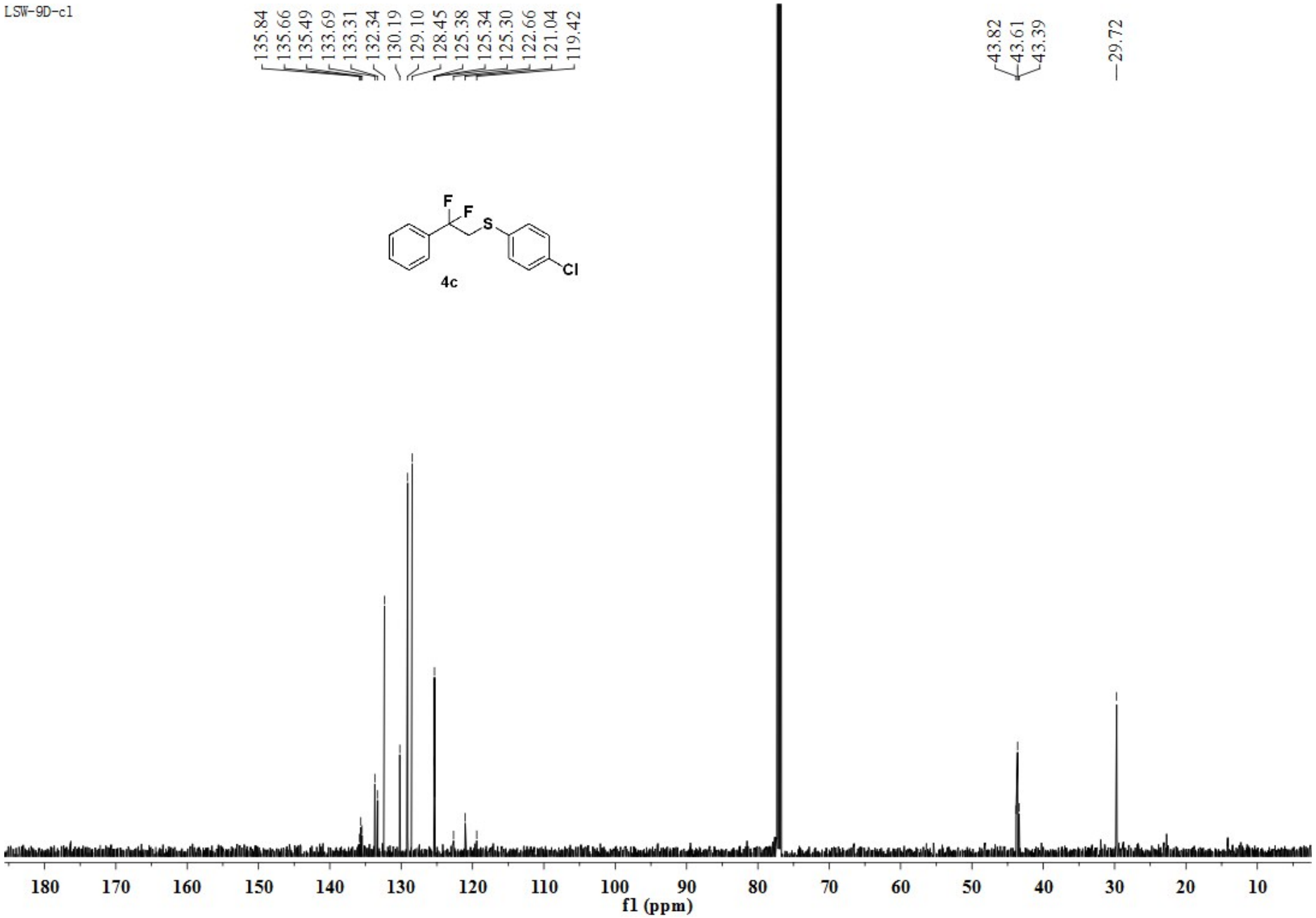


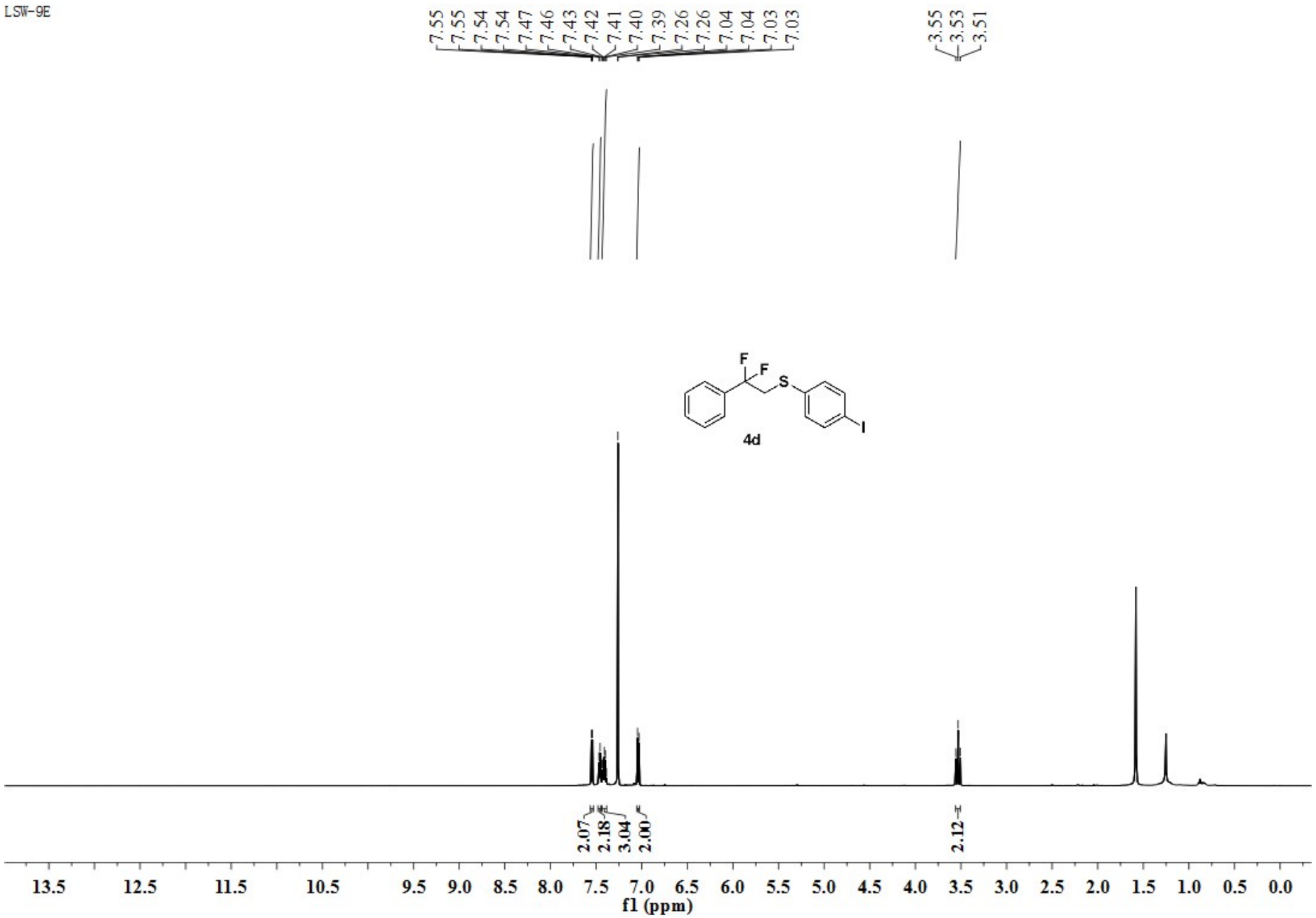
4c

-94.65
-94.67
-94.70

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

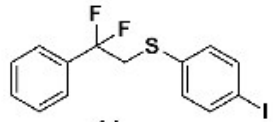
f1 (ppm)


LSW-9D-cl
135.84
135.66
135.49
133.69
133.31
132.34
130.19
129.10
128.45
125.38
125.34
125.30
122.66
121.04
119.42
43.82
43.61
43.39
29.72
F
F
S
Cl
4c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


LSW-9E
7.55
7.55
7.54
7.54
7.47
7.46
7.43
7.42
7.41
7.40
7.39
7.26
7.26
7.04
7.04
7.03
7.03
3.55
3.53
3.51
F
F
S
I
4d
2.07
2.18
3.04
2.00
2.12
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

LSW-9E

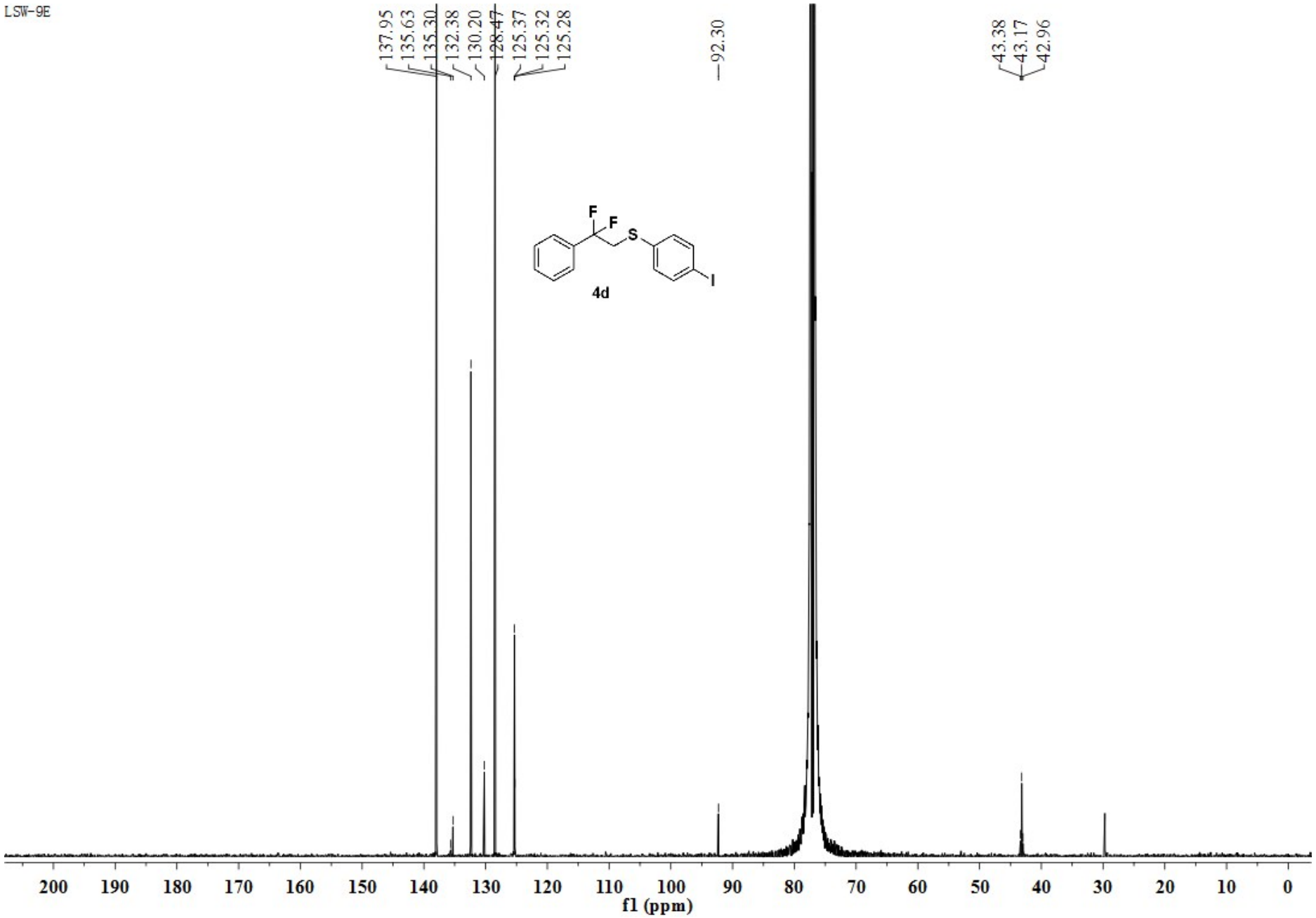
-94.63
-94.66
-94.68

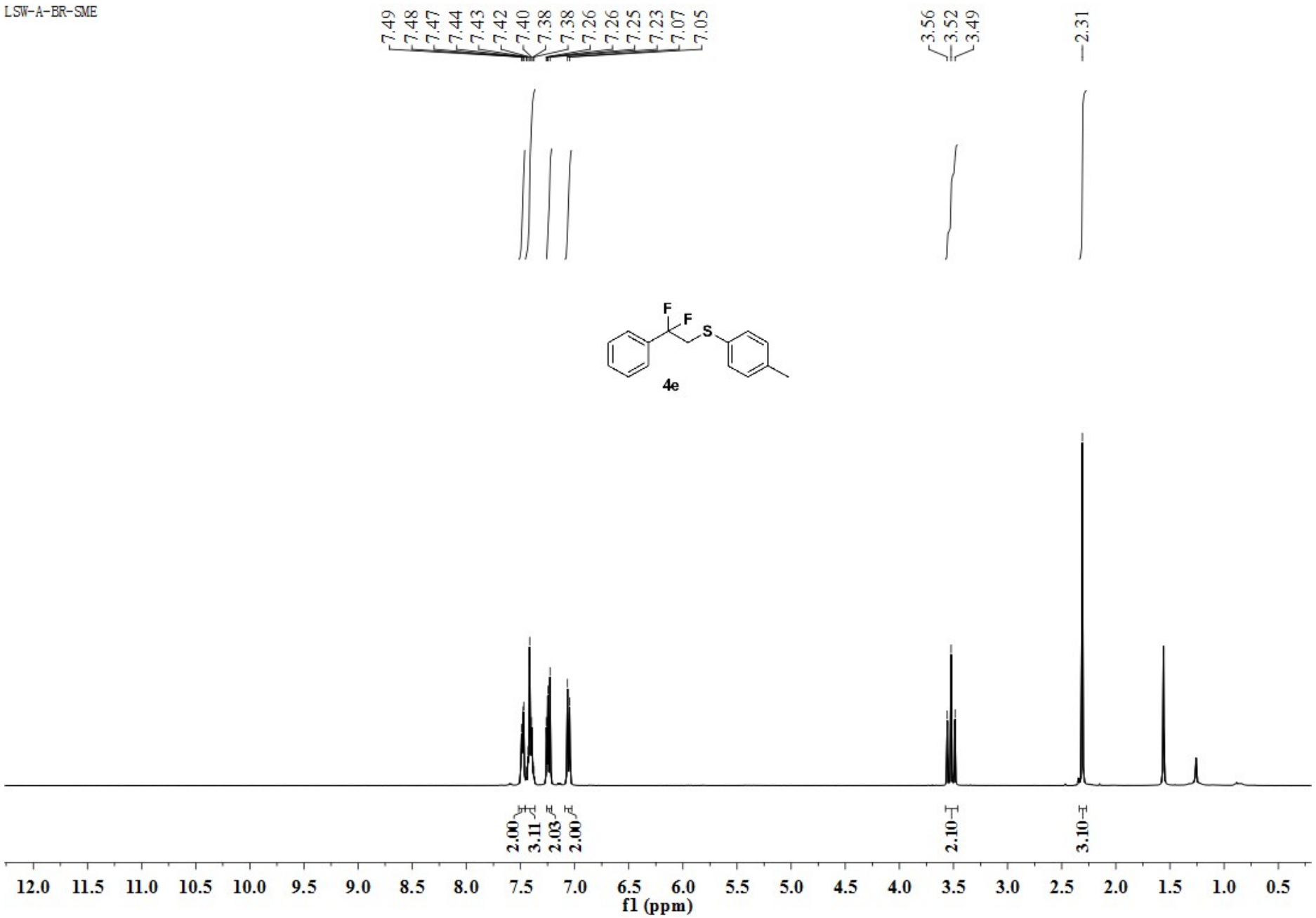


4d

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

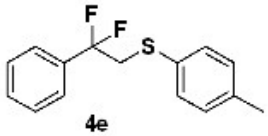
f1 (ppm)


LSW-9E
137.95
135.63
135.30
132.38
130.20
128.47
125.37
125.32
125.28
92.30
43.38
43.17
42.96
F
F
S
I
4d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

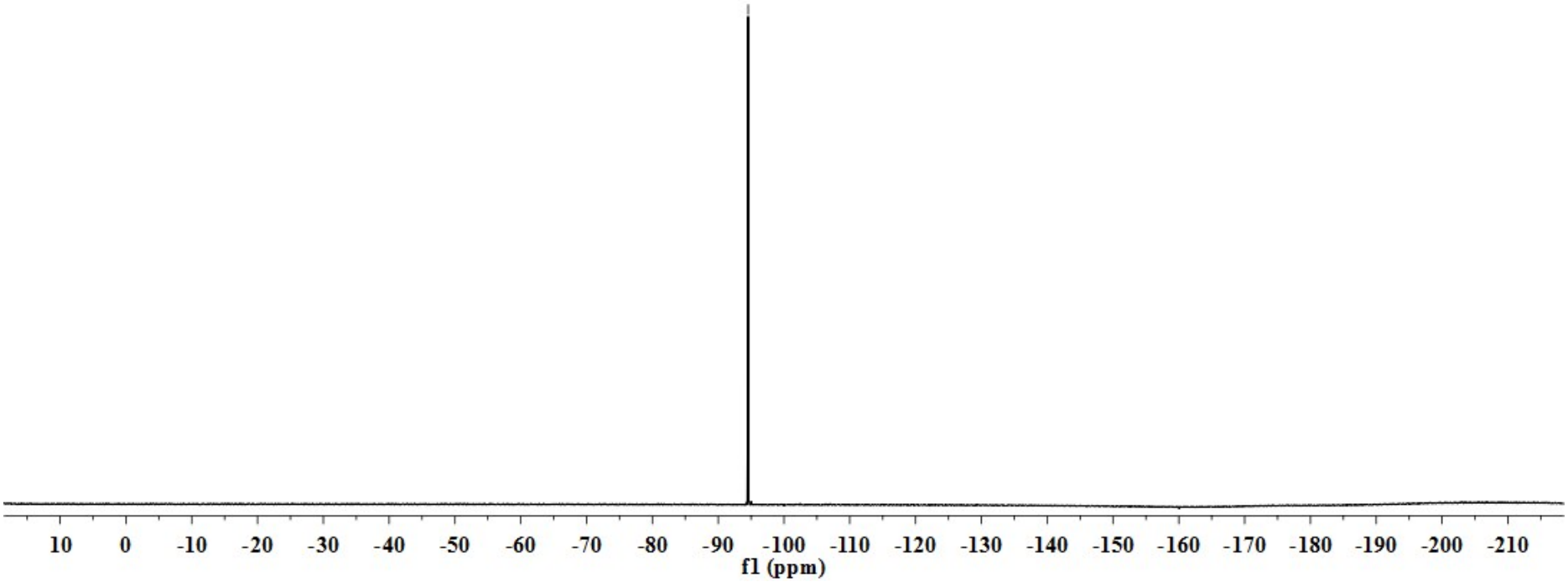

LSW-A-BR-SME
7.49
7.48
7.47
7.44
7.43
7.42
7.40
7.38
7.38
7.26
7.26
7.25
7.23
7.07
7.05
3.56
3.52
3.49
2.31
F
F
S
4e
2.00
3.11
2.03
2.00
2.10
3.10
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

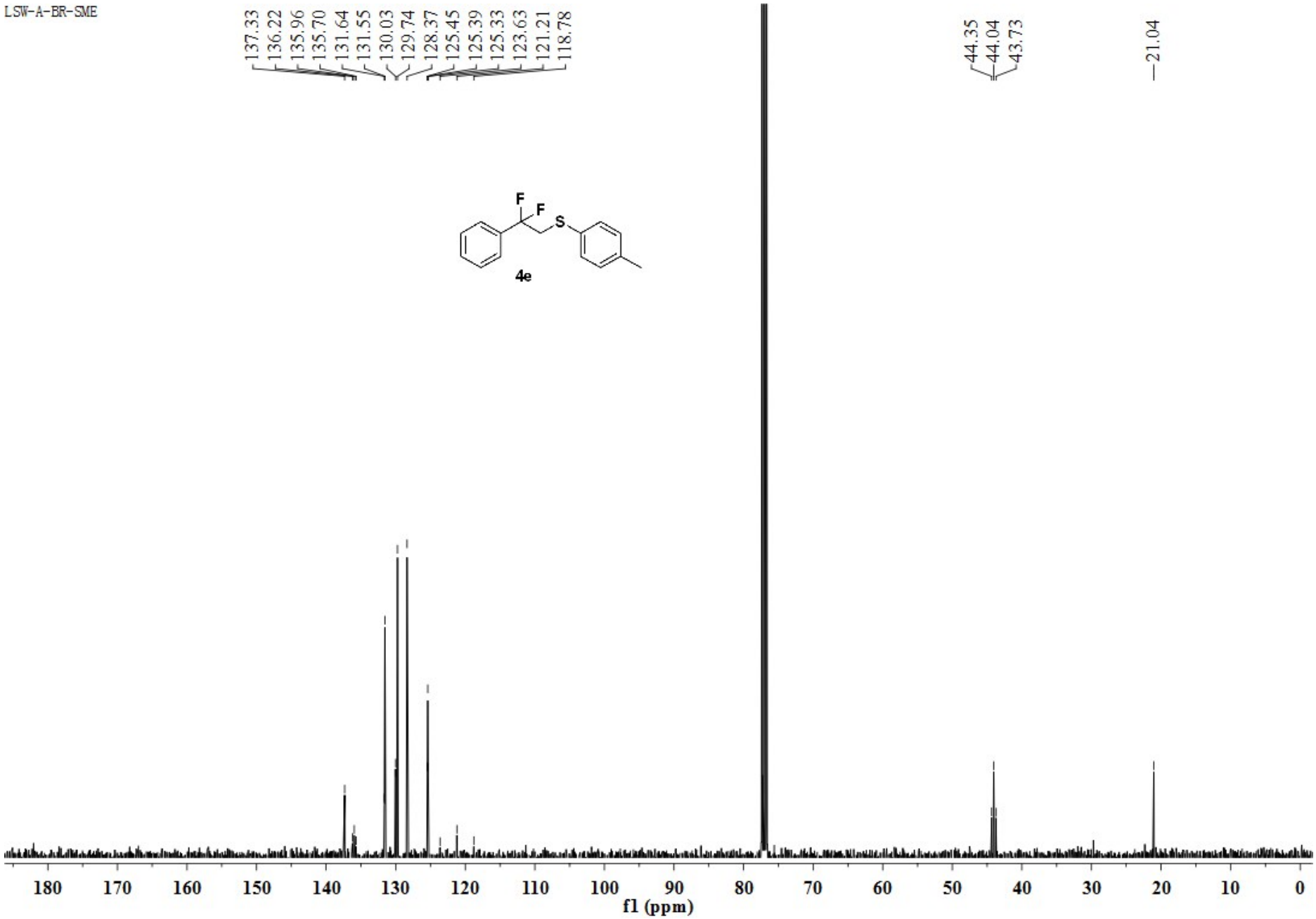
LSW-A-BR-SME

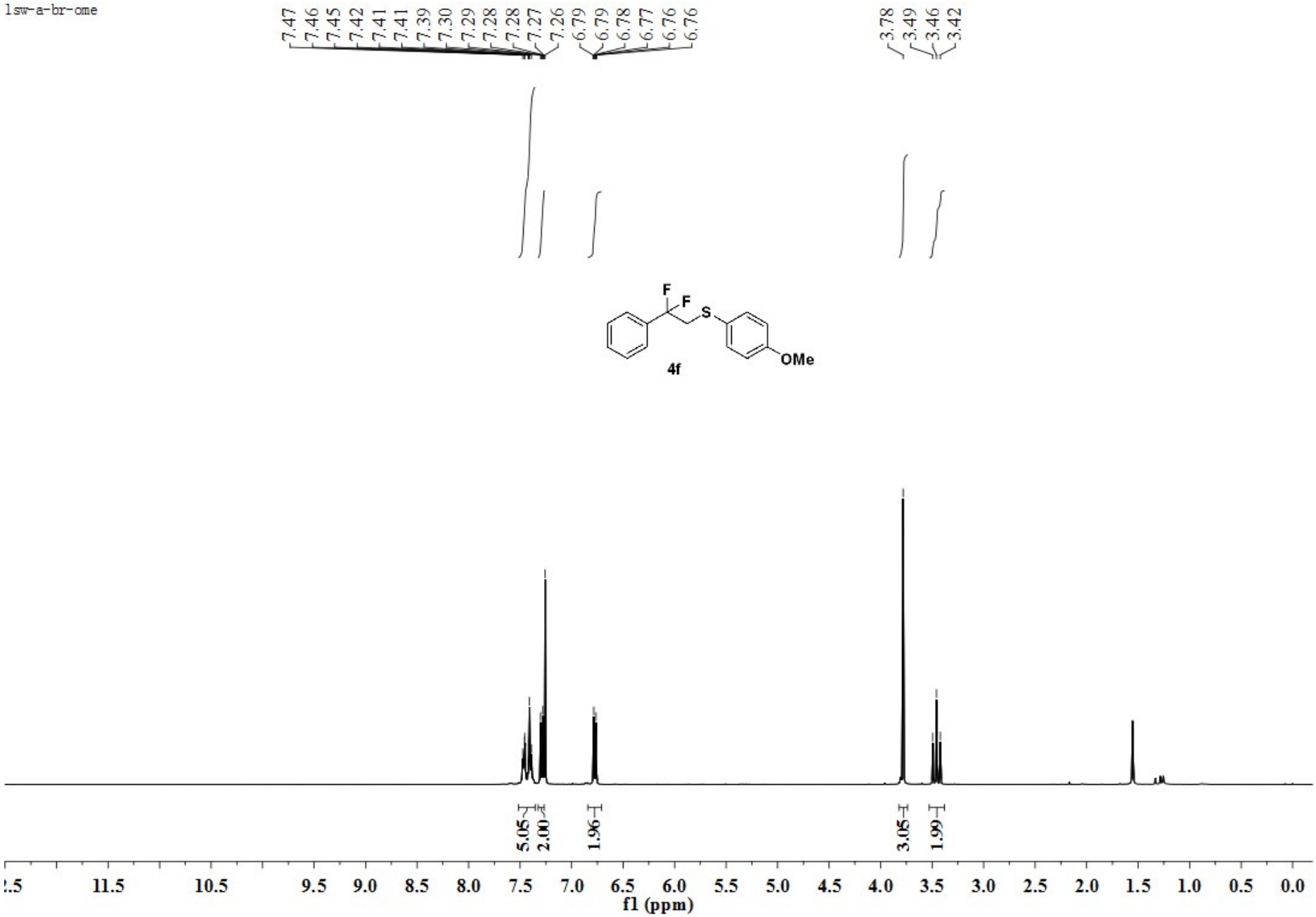
-94.52
-94.56
-94.60



4e

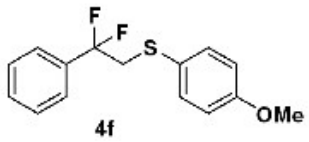



LSW-A-BR-SME
137.33
136.22
135.96
135.70
131.64
131.55
130.03
129.74
128.37
125.45
125.39
125.33
123.63
121.21
118.78
44.35
44.04
43.73
21.04
F
F
S
4e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

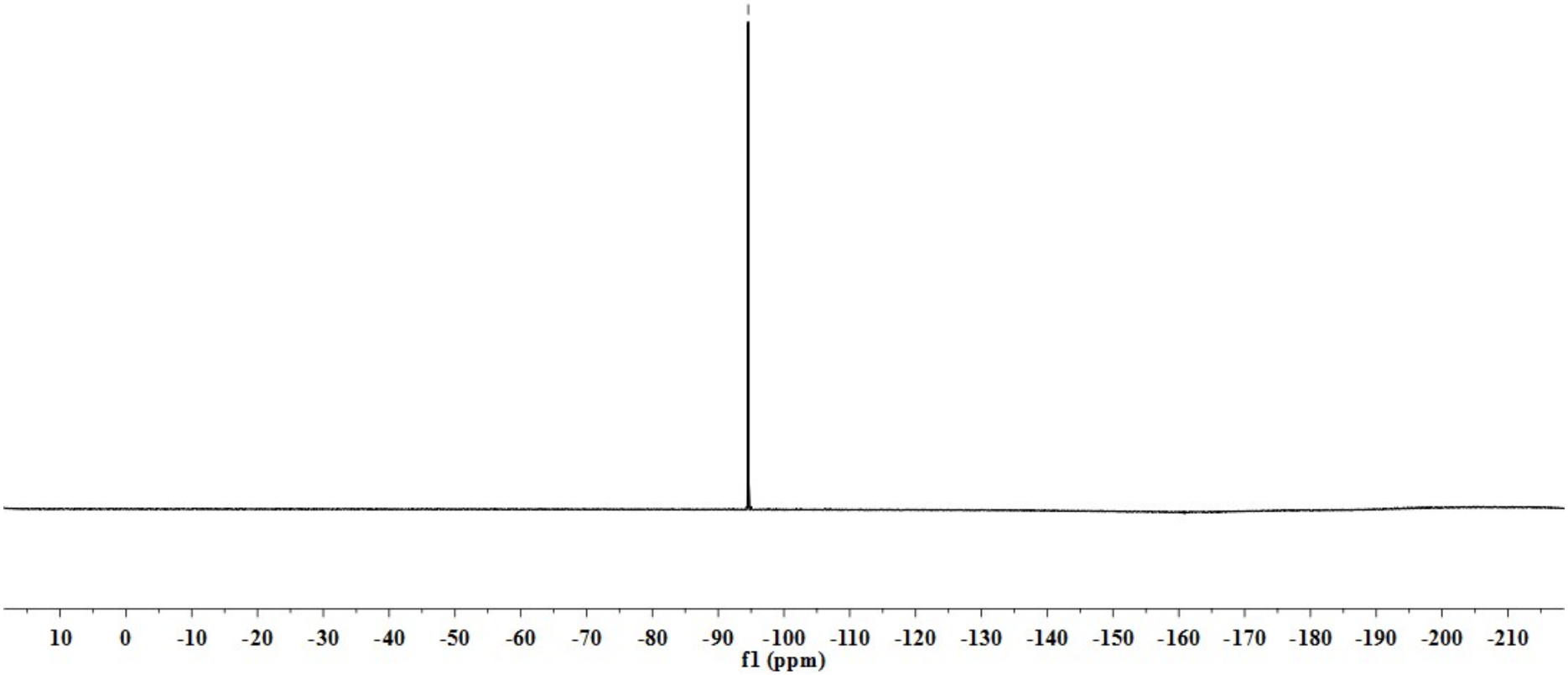

lsw-a-br-ome
7.47
7.46
7.45
7.42
7.41
7.41
7.39
7.30
7.29
7.28
7.28
7.27
7.26
6.79
6.79
6.78
6.77
6.76
6.76
3.78
3.49
3.46
3.42
F
F
S
OMe
4f
5.05
2.00
1.96
3.05
1.99
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

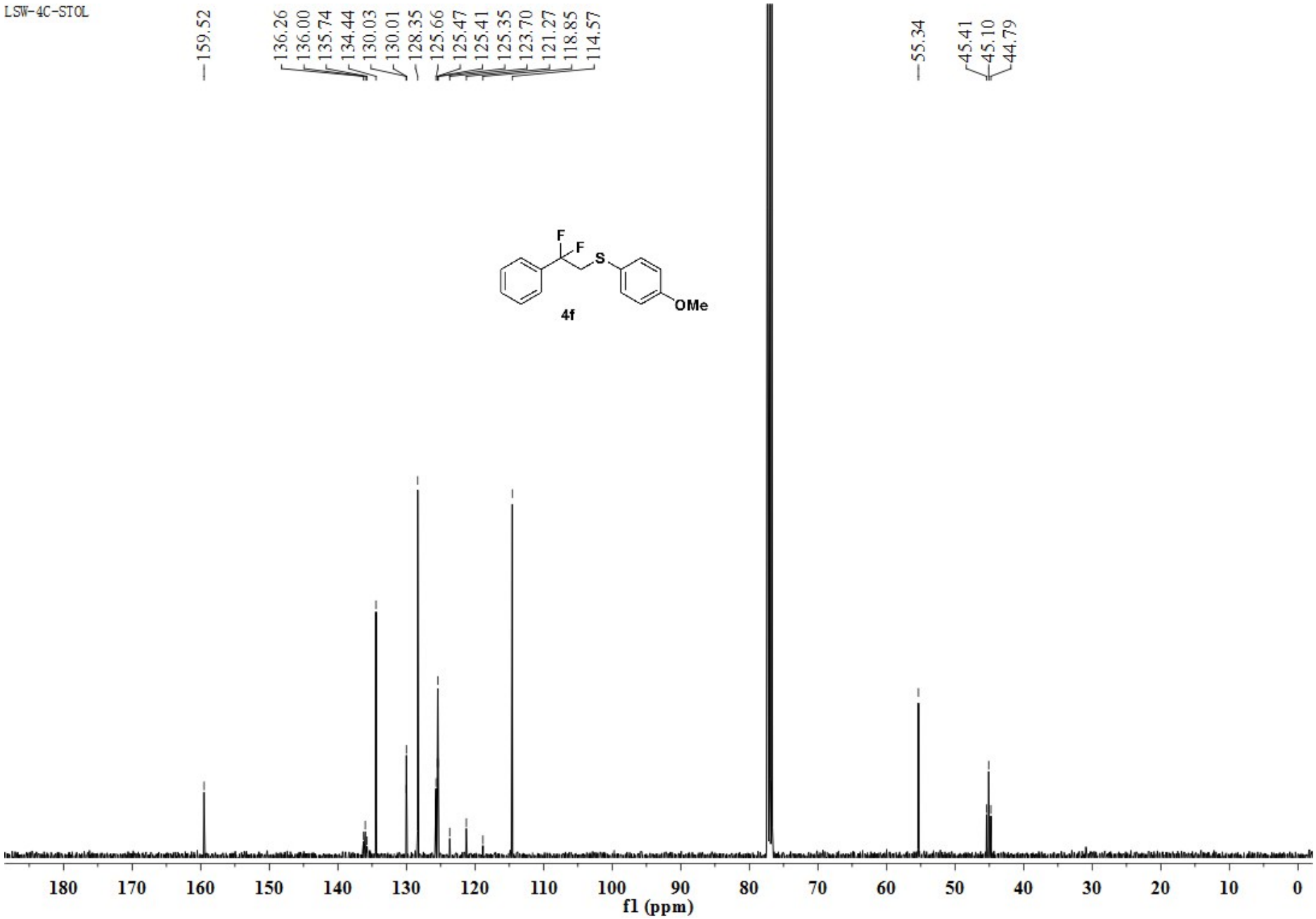
lsw-a-br-ome

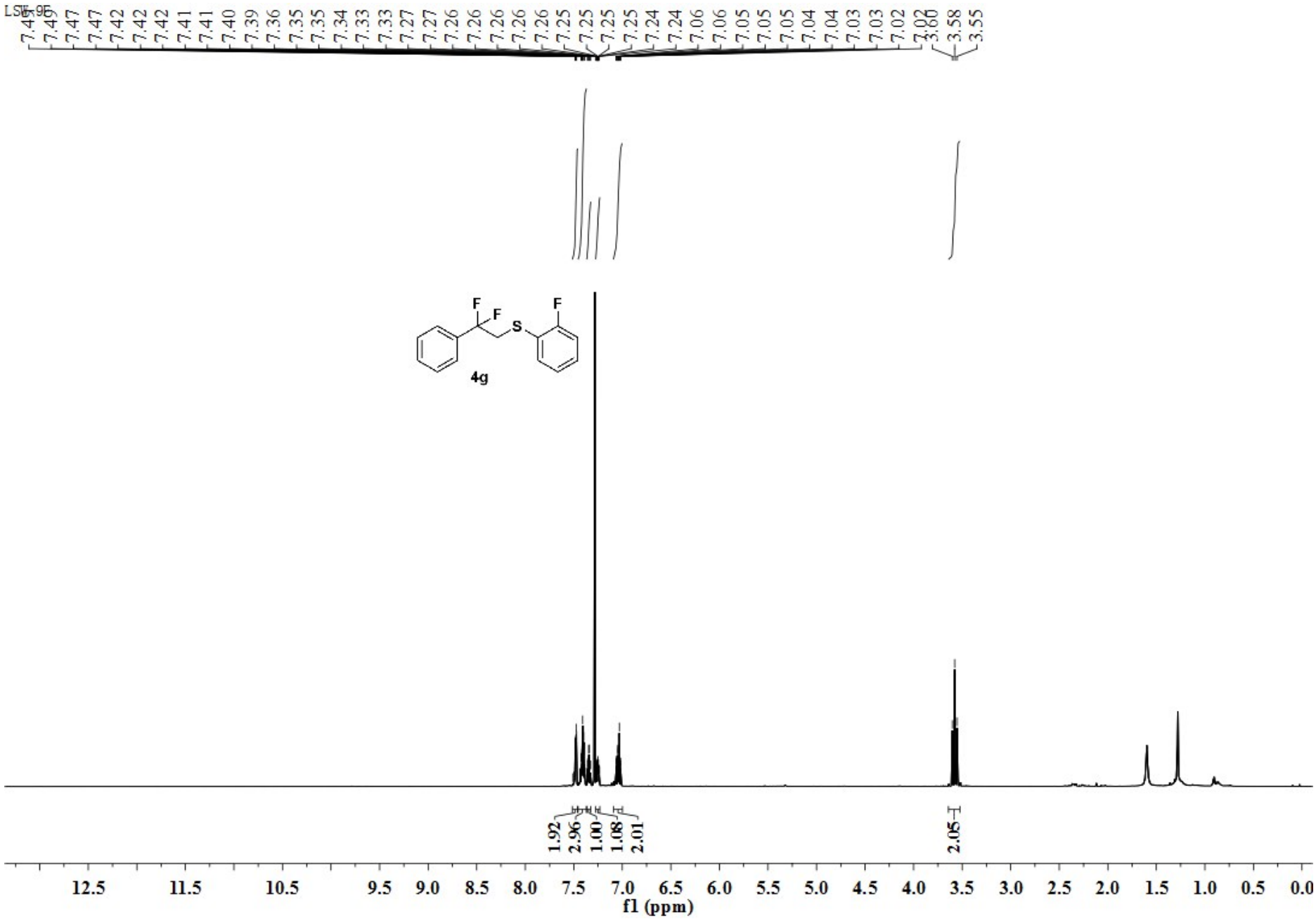
-94.53
-94.57
-94.61



4f

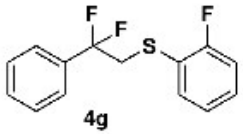



LSW-4C-STOL
159.52
136.26
136.00
135.74
134.44
130.03
130.01
128.35
125.66
125.47
125.41
125.35
123.70
121.27
118.85
114.57
55.34
45.41
45.10
44.79
F
F
S
OMe
4f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

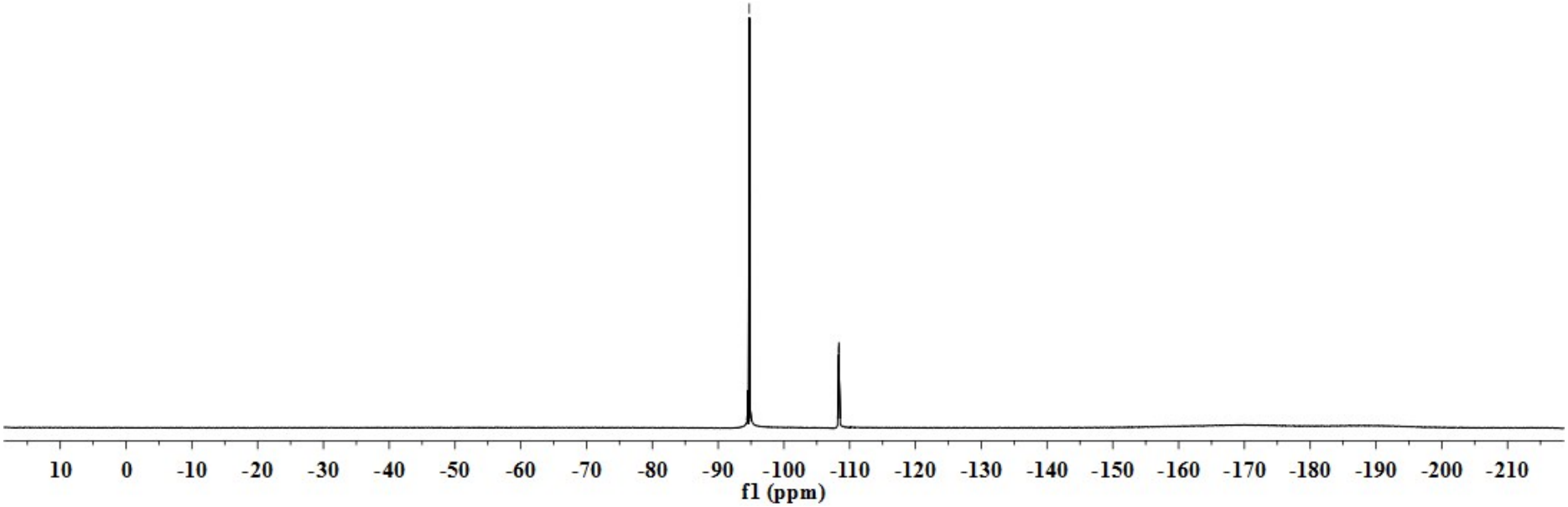

7.49
7.47
7.47
7.42
7.42
7.42
7.41
7.41
7.40
7.39
7.36
7.35
7.35
7.34
7.33
7.33
7.27
7.27
7.26
7.26
7.26
7.26
7.25
7.25
7.25
7.25
7.24
7.24
7.06
7.06
7.05
7.05
7.05
7.04
7.04
7.03
7.03
7.02
3.60
3.58
3.55
F
F
S
F
4g
1.92
2.96
1.00
1.08
2.01
2.05
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

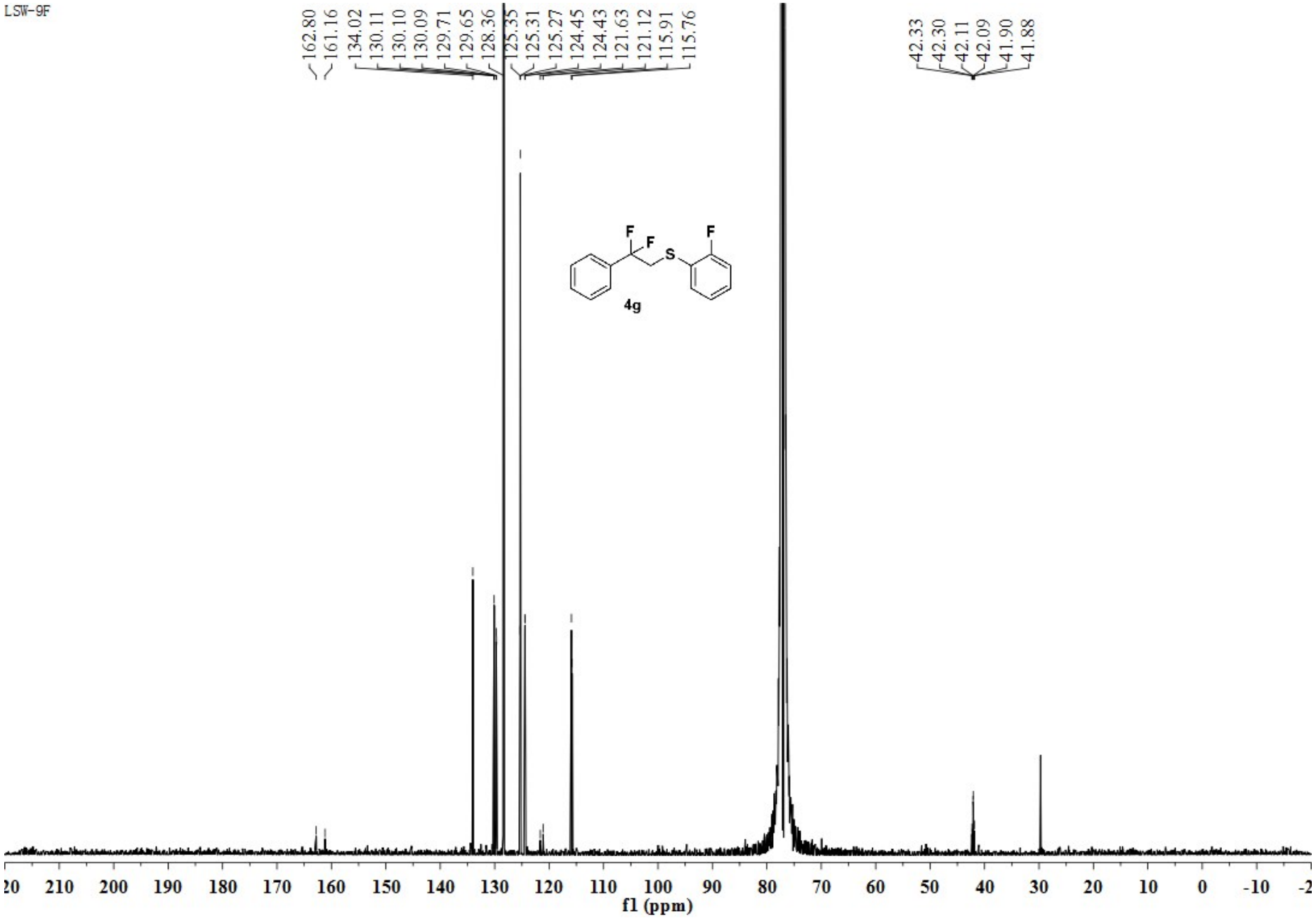
LSW-9F

-94.71
-94.73
-94.76
-108.35
-108.35
-108.36
-108.37
-108.38

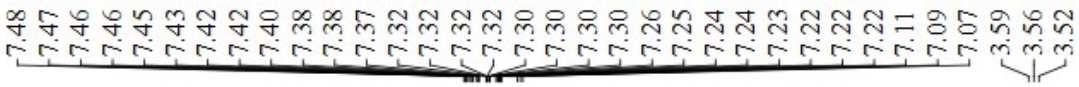


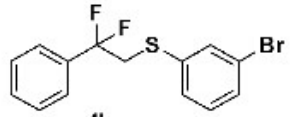
4g



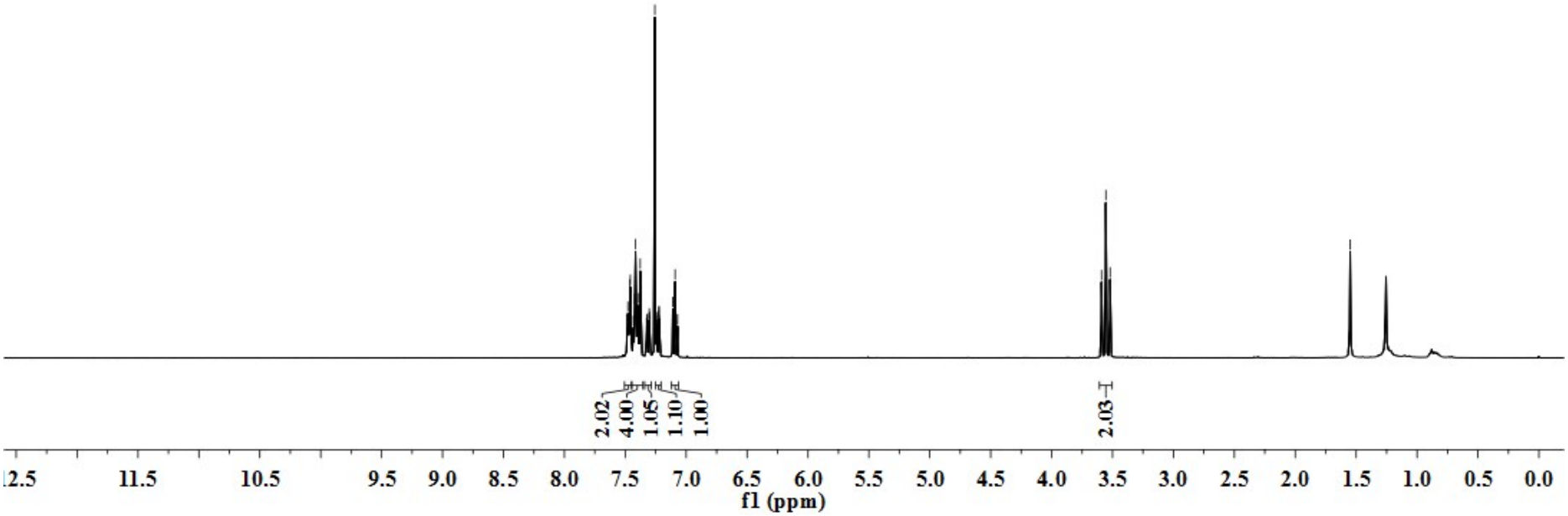

LSW-9F
162.80
161.16
134.02
130.11
130.10
130.09
129.71
129.65
128.36
125.35
125.31
125.27
124.45
124.43
121.63
121.12
115.91
115.76
42.33
42.30
42.11
42.09
41.90
41.88
F
F
S
F
4g
f1 (ppm)

LSW-12-B--BR-S3BR



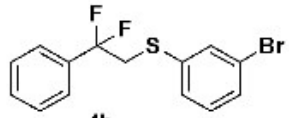


4h

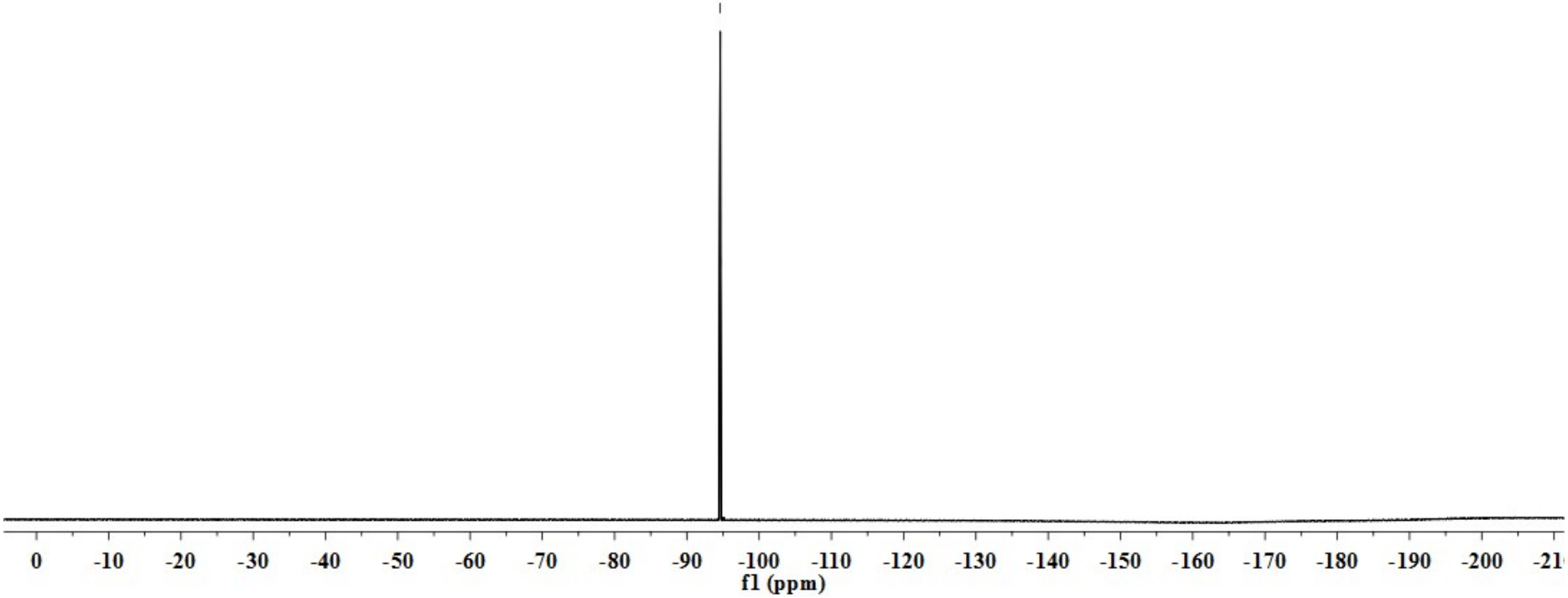


LSW-12-B--BR-S3BR

-94.58
-94.62
-94.65



4h

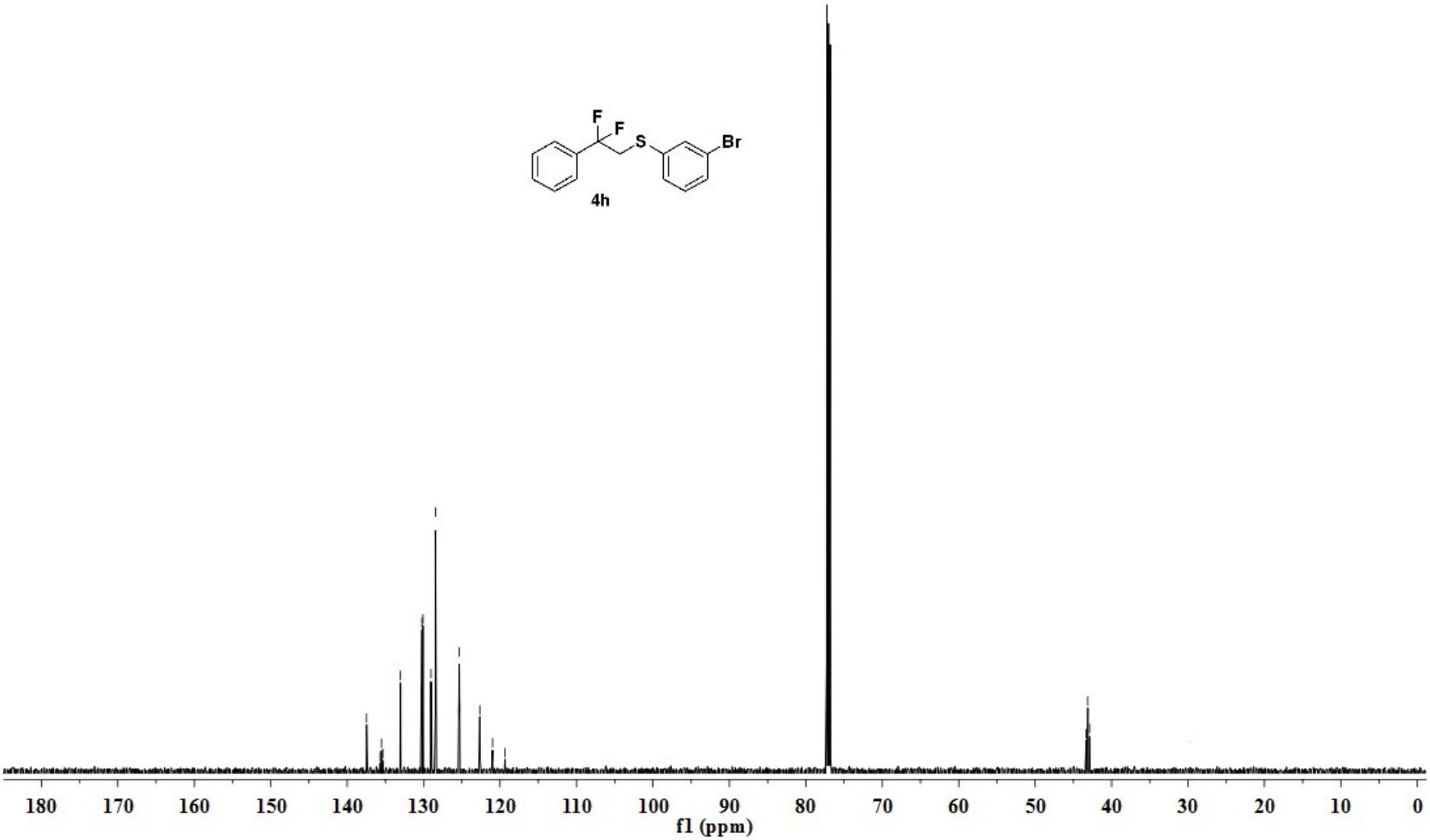


LSW-12-B

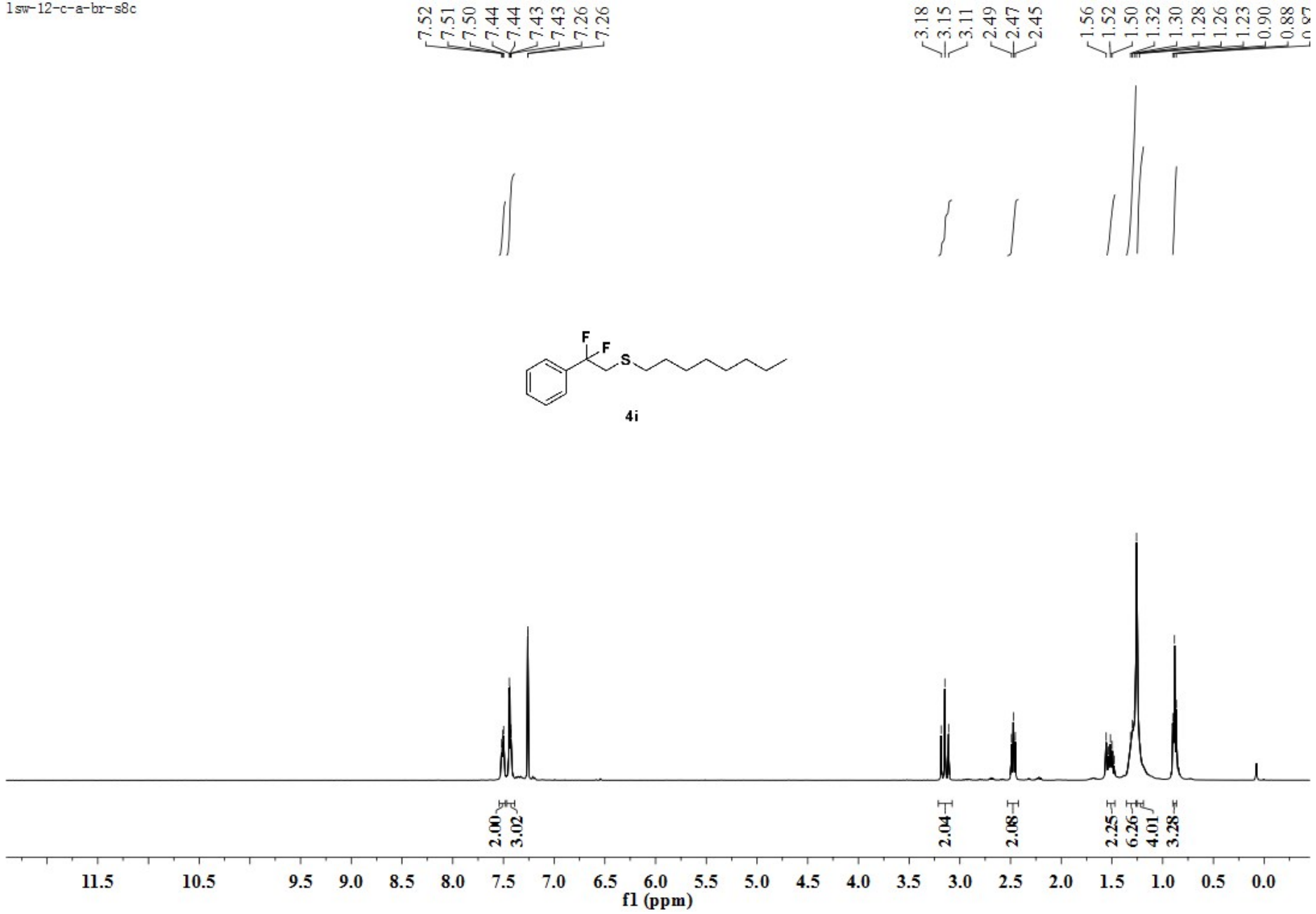
137.46
135.68
135.51
135.34
133.03
130.28
130.22
130.07
129.04
128.45
125.39
125.35
125.31
122.65
122.60
120.98
119.35

43.32
43.11
42.90

4h

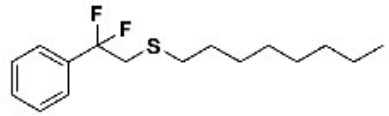


1sw-12-c-a-br-s8c

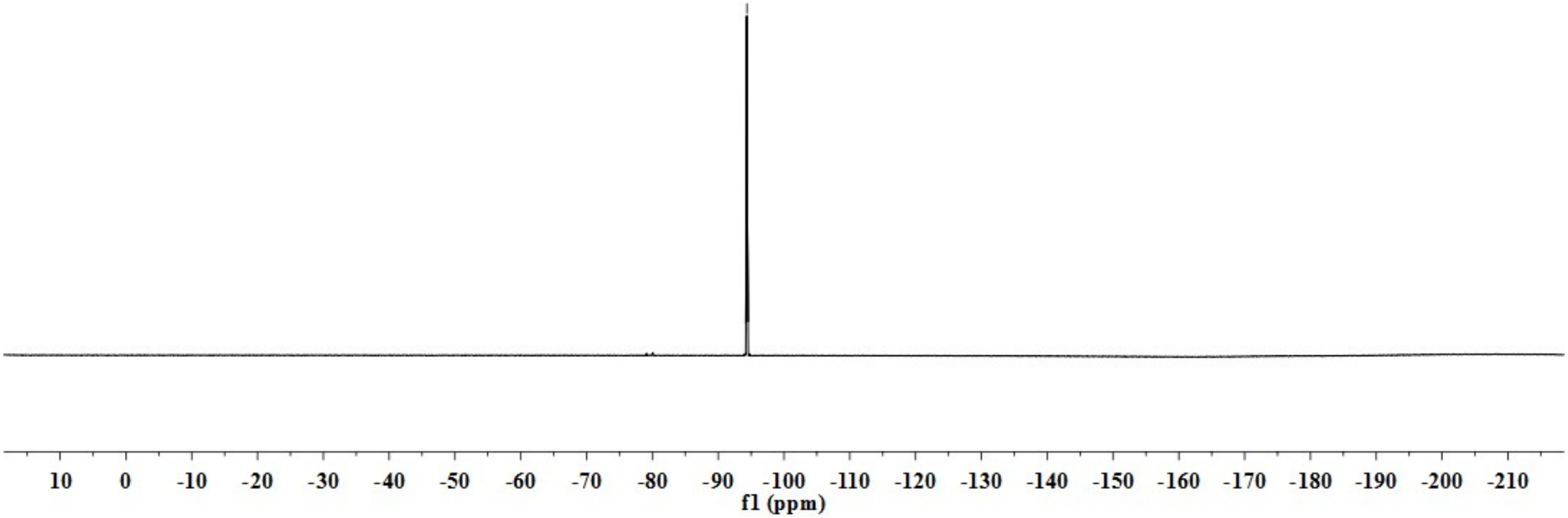


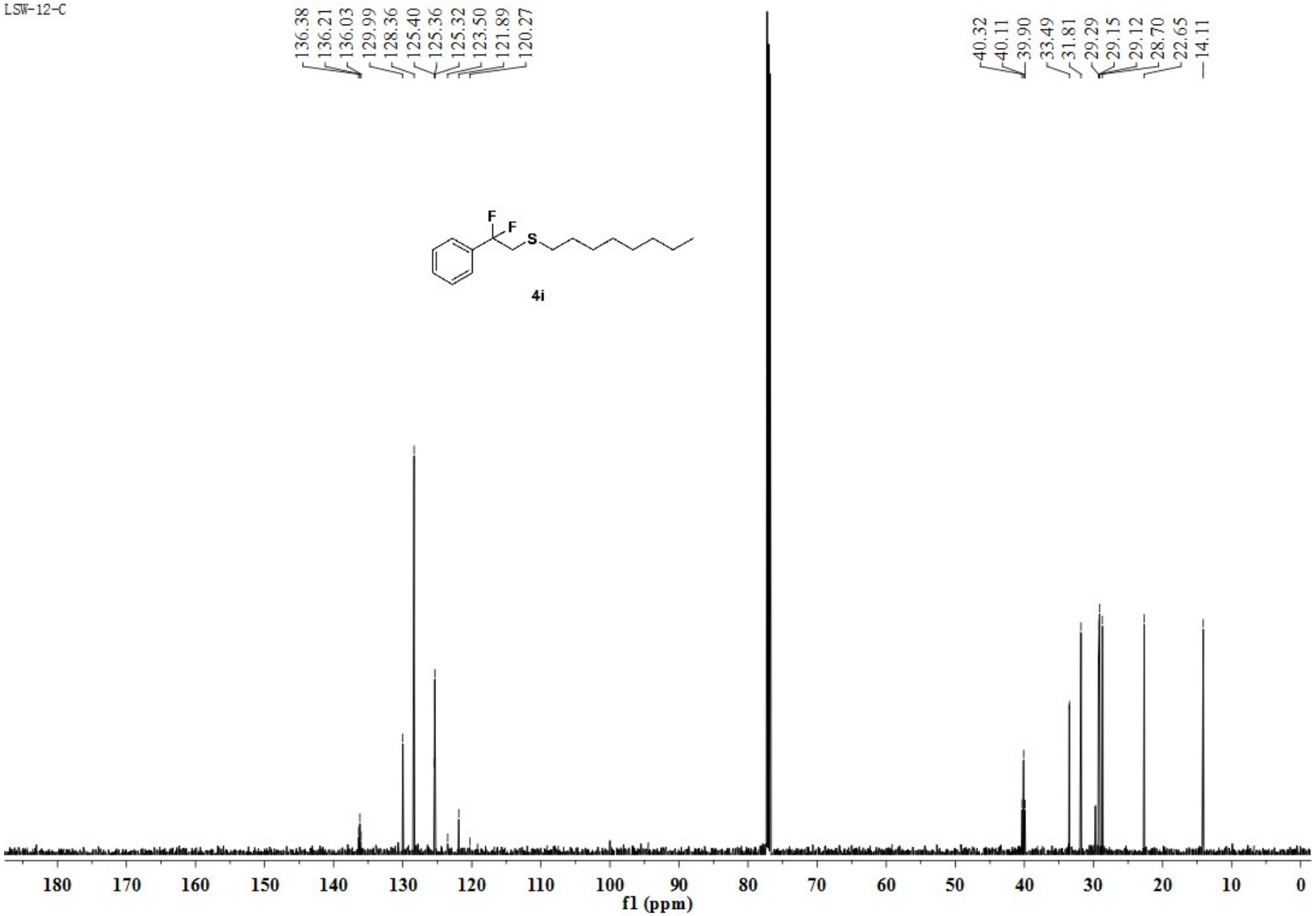
lsw-12-c-a-br-s8c

-94.33
-94.37
-94.40



4i




LSW-12-C
136.38
136.21
136.03
129.99
128.36
125.40
125.36
125.32
123.50
121.89
120.27
40.32
40.11
39.90
33.49
31.81
29.29
29.15
29.12
28.70
22.65
14.11
F
F
S
4i
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

6. References

1. Nalbandian, C. J.; Miller, E. M.; Toenjes, S. T.; Gustafson, J. L. *Chem. Commun.* **2017,** *53*, 1494-1497.