Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Phthalimide-Based-$SSCF_3$ Reagent for Enantioselective Dithiotrifluoromethylation

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1. General Information

NMR

^{1}H and ^{13}C spectra were collected on 300 M, 400 M or 500 M Hz NMR spectrometers (Bruker AVANCE). Chemical shifts for protons are reported in parts per million (ppm) downfield and are referenced to residual protium in the NMR solvent. ($CHCl_3$ = δ 7.26, DMSO = δ 2.50). Chemical for carbon are reported in parts per million downfield and are referenced to the carbon resonances of solvent ($CHCl_3$ = δ 77.0, DMSO = δ 39.52). Date are represented as follows: chemical shift, multiplicity (br = broad, s = singlet, d = double, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz), integration.

MS

High-resolution mass spectra (HRMS) were performed on a micrOTOF-Q II instrument with an ESI or EI source.

IR

IR spectra were measured using SHIMADZU IR Tracer-100 Spectrometers. Wavenumbers are quoted in cm^{-1}. All compounds were measured neat directly on the crystal of the IR machine.

HPLC

The HPLC measurements were carried out on a Thermo UltiMate 3000 apparatus. The used solvents were hexane and 2-propanol and were bought from Titan® and Energy® as HPLC grade. The chiral columns used for the separation of the enantiomers were Daicel Chiralcel AD-H (0.46 cm i.d. x 25 cm), Daicel Chiralcel OD-H (0.46 cm Ø x 25 cm), and Chiralcel AS-H (0.46 cm i.d. x 25 cm).

Rotation

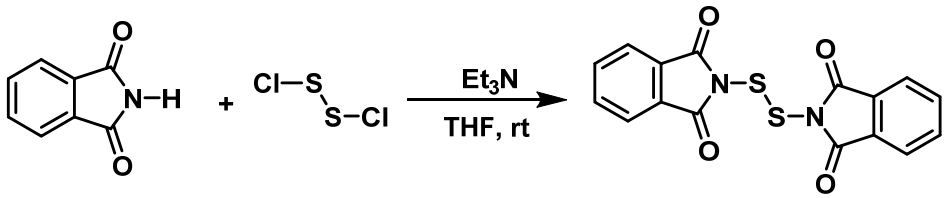
Optical rotations were measured on an Anton Paar MCP 5500 polarimeter.

Chromatography

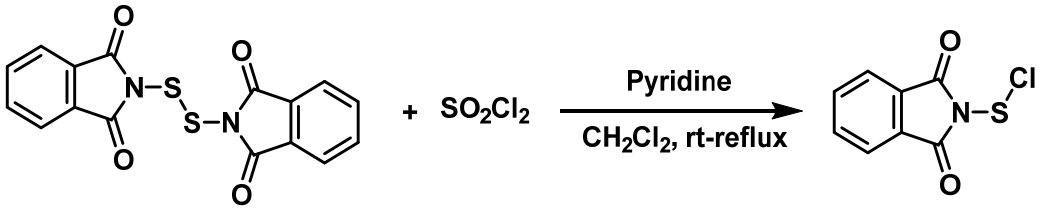
All solvents were obtained from commercial sources and were purified according to standard procedures. Petroleum ether (PE), where used, has the boiling point range 60-90 ^{o}C. Column chromatography was performed with silica gel (300-400 mesh).

2 Experimental procedure

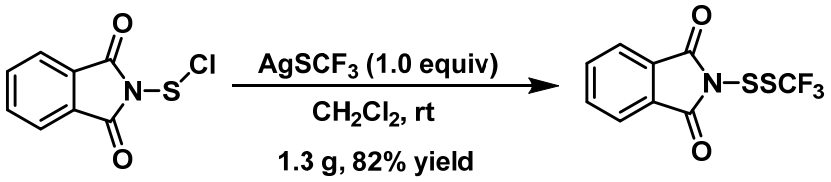
2.1 General Procedure for the synthesis of *N*-trifluoromethyldithio phthalimide



Phthalimide (2.9 g, 19.7 mmol) was dissolved in THF (40 mL) and triethylamine (4.1 mL, 30 mmol). The mixture was cooled in a salt ice bath, and then sulfur monochloride (0.8 mL, 10 mmol) was added dropwise to the cooled mixture. The solution was stirred for 2 h, and then quenched with 60 mL of H_2O. The resulting precipitate was filtered and washed with diethyl ether. The resulting precipitate was collected and dissolved in the solvent of $CHCl_3$:CH_3OH [2:1 (v:v), 45 mL], and reflux for 0.5-1 h. The insoluble solid was removed, and the filtrate was concentrated under vacuum to give 2,2'-disulfanediylbis(isoindoline-1,3-dione) as white crystal (3.5 g, yield: 98%). The NMR spectra are consistent with literature reports.[S1]



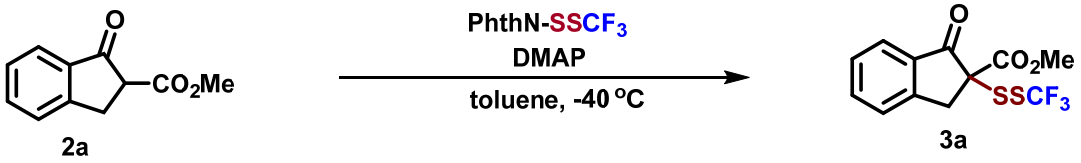
Synthesis of N-(chlorosulfenyl)phthalimide. Following a slightly modified procedure described in literatures,[S2] to a solution of di(1-phthalimidyl)disulfane (750 mg, 2 mmol) and anhydrous pyridine (0.1 mL, 1.2 mmol) in 10 mL of CH_2Cl_2 was added sulfuryl chloride (2 mL, 25 mmol) dropwise at room temperature. The yellow mixture was stirred at room temperature for 24 h, and reflux for 4 h (Note: Please ensure no water come inside during this period!). The solvent and excess sulfuryl chloride were removed under vacuum, and the resulting solid was dissolved in 15 mL of CCl_4 at reflux for 0.5 h. The insoluble precipitate was removed, and the filtrate was concentrated to give a yellow solid (380 mg, yield: 90%).



*Synthesis of N-Trifluoromethyldithio phthalimide **1***. To a 100 mL round-bottomed flask charged

with *N*-(chlorosulfenyl)phthalimide (1.21 g, 5.67 mmol) and $AgSCF_3$ (1.18 g, 5.67 mmol) was added dichloromethane (20 mL). The mixture was stirred vigorously at room temperature for 10 min and then filtered through a pad of Celite and washed with dichloromethane (50 mL). The filtrate was concentrated in vacuo and purified by chromatography (PE:EtOAc = 1:10) to give **1** (1.3 g, 82%) as white solid.

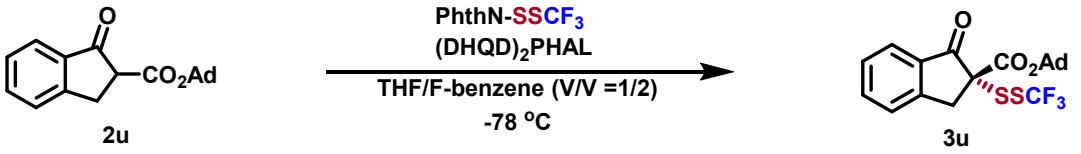
2.2 General procedure for the α-trifluoromethyldithiolation of β-keto esters



$SSCF_3$-Incorporation. To a solution of **1** (0.1 mmol) and **2a** (0.12 mmol) in 2 mL of toluene was added DMAP (20 mol%) at -40 °C. The reaction was stirred at -40 °C until **1** was completely consumed (TLC monitoring). The crude mixture was directly charged on silica gel and purified by column chromatography to give **3a** as colorless oil (29.6 mg, 92%).

Reuse of Phthalimide. The mixture of **1** (0.5 mol), **2a** (0.5 mmol) and DMAP (20 mol%) in 5 mL of toluene was stirred at -40 °C until **1** was completely consumed. The precipitate was immediately collected by filtration, and washed 3 times with hexane. The white solid could be used for the synthesis of *N*-Trifluoromethyldithio phthalimide without further purification.

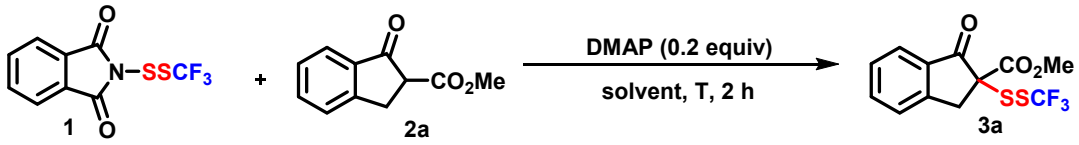
2.3 General procedure for the enantioselective trifluoromethyldithiolation



In a screw capped reaction tube, a mixture of phthN-$SSCF_3$ **1** (0.12 mmol), β-keto ester **2u** (0.12 mmol, 1.0 eq), and $(DHQD)_2PHAL$ (20 mol%) was dissolved in THF (0.5 mL) and fluorobenzene (1.5 mL) was added. The resulting solution was stirred at -78 °C until **2u** was fully consumed (TLC monitoring). The crude reaction mixture was directly subjected to silica gel and purified by column chromatography to give **3u** as pale yellow oil (35.4 mg, 80% yield, 92% *ee*).

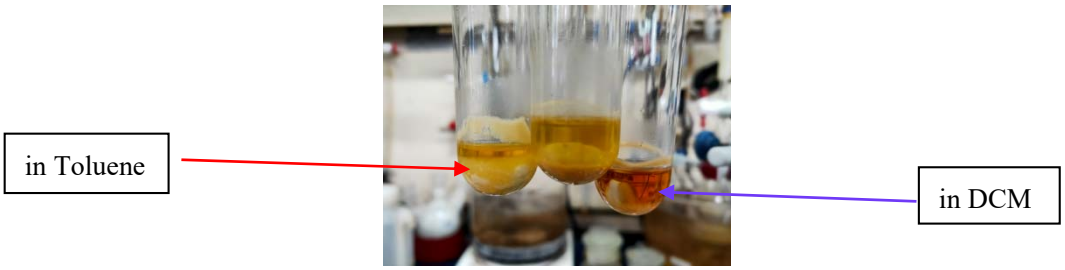
3. Tables of reaction optimization

3.1 Table S1. Reaction Optimization of Trifluoromethylthioation[a]



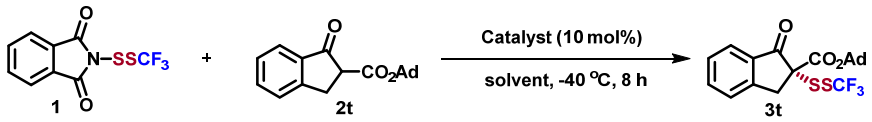
Entry	Solvent	T (°C)	Yield (%)[b]
1	DCM	rt	49%
2	toluene	rt	45%
3	MeCN	rt	41%
4	THF	rt	23%
5	DCE	rt	7%
6	1,4-dioxane	rt	17%
7	THF	0 °C	60%
8	THF	- 40 °C	83%
9	THF	-78 °C	73%
10	toluene	- 40 °C	89%

[a] Condiitions: **1** (0.1 mmol), **2a** (0.12 mmol) and DMAP (0.02 mmol) in 2 mL of solvent were stirred at indicated temperature for 2 h. [b] Isolated yield.

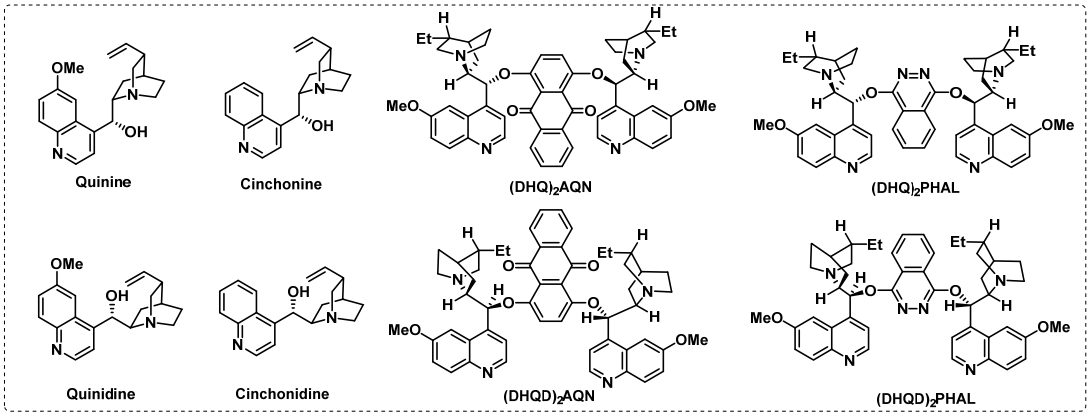


The precipitation of phthalimide in toluene promoted the reaction equilibrium.

3.2 Table S2. Catalyst Screening for Asymmetric Trifluoromethylthioation[a]

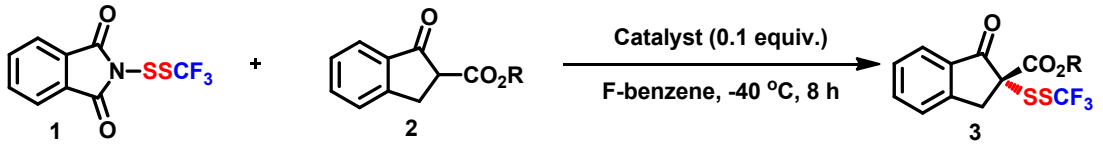


Entry	Catalyst	Solvent	Yield(%)[b]	ee(%)[c]
1	Cinchonine	Toluene	48	-29
2	Cinchonidine	Toluene	67	35
3	Quinine	Toluene	27	20
4	Quinidine	Toluene	32	-7
5	$(DHQ)_2AQN$	Toluene	38	-58
6	$(DHQN)_2AQN$	Toluene	45	75
7	$(DHQ)_2PHAL$	Toluene	70	-81
8	$(DHQD)_2PHAL$	Toluene	74	79



[a] Reaction conditions: **1** (0.1 mmol), **2t** (0.12 mmol), catalyst (10 mol%) in 1.5 mL of solvent at indicated temperature for 8 h. [b] Yield of isolated product. [c] Determined by HPLC analysis on a chiral stationary phase.

3.3 Table 3. Effect of Ester Group on the Asymmetric Trifluoromethylthioation[a]

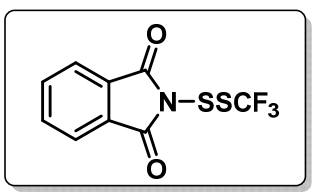


Entry	Catalyst	R	Yield (%)[b]	ee (%)[c]
1	$(DHQD)_2PHAL$	Me	90	52
2	$(DHQD)_2PHAL$	*i*-Pr	73	66
3	$(DHQD)_2PHAL$	Bn	73	59
4	$(DHQD)_2PHAL$	*t*-Bu	71	81
5	$(DHQD)_2PHAL$	Ad	57	91

[a] Reaction conditions: **1** (0.1 mmol), **2** (0.12 mmol), catalyst (10 mol%) in 1.5 mL of solvent at indicated temperature for 8 h. [b] Yield of isolated product. [c] Determined by HPLC analysis on a chiral stationary phase.

4. Characterization of products

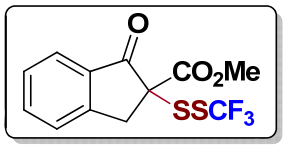
2-((Trifluoromethyl)sulfinothioyl)isoindoline-1,3-dione



Yield: 82%; white solid; m.p. 89.5-91.5 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ 8.0-7.95 (m, 2H), 7.87-7.81 (m, 2H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -45.2 (s, 3 F); ^{13}C NMR (125 MHz; $CDCl_3$): δ 165.8, 135.2, 131.8, 128.3 (q, J = 318 Hz) 124.5; IR (KBr): 2365, 1710,

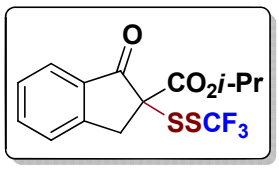
1148, 1093, 1030, 864, 710 cm^{-1}; HRMS (EI) $C_{12}H_{10}O_3F_3S_2$ $[M]^+$: calcd: 278.9637, found: 278.9637.

Methyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3a)



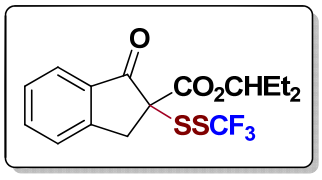
Yield: 92%; pale yellow solid; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.80 (d, J = 8.0 Hz, 1H), 7.68 (t, J = 8.0 Hz 1H), 7.50 – 7.42 (m, 2H), 4.05 (d, J = 20.0 Hz, 1H), 3.80 (s, 3H), 3.48 (d, J = 16.0 Hz, 1H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 195.0, 167.9, 150.8, 136.2, 133.8, , 128.6, 128.3 (q, J = 313.0 Hz), 126.8, , 125.5, 64.3, 53.9, 38.6; IR (KBr): 1735, 1712, 1699, 1602, 1587, 1467, 1434, 1275, 1257, 1155, 1128, 1042, 1026, 964, 821, 589, 742 cm^{-1}; HRMS (ESI) $C_{12}H_{10}O_3F_3S_2$ $[M+H]^+$: calcd: 323.0018, found: 323.0017.

Isopropyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3b)



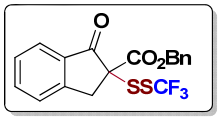
Yield: 91%; colorless oil;; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.81 (d, J = 8.0 Hz, 1H), 7.67 (t, J = 4.0 Hz, 1H), 7.51 - 7.45 (m, 2H), 5.12 – 5.06 (m, 1H), 4.00 (d, J = 16.0 Hz, 1H), 3.49 (d, J = 20.0 Hz, 1H), 1.26 (d, J = 8.0 Hz, 1H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 195.2, 166.9, 151.0, 136.0, 134.0, 128.3 (q, J = 313.0 Hz), 128.5, 126.1 125.4; IR (KBr) 2984, 1718, 1606, 1465, 1272, 1146, 1098, 920, 752 cm^{-1}; HRMS (ESI) $C_{14}H_{14}O_3F_3S_2$ $[M+H]^+$: calcd: 351.0331, found: 351.0331.

Pentan-3-yl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-caboxylate (3c)



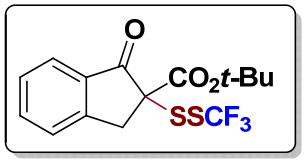
Yield: 80%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.81 (d, J = 8.0 Hz, 1H), 7.67 (t, J = 4.0 Hz, 1H), 7.51 - 7.43 (m, 2H), 4.87 - 4.81 (m, 1H), 4.01 (d, J = 16.0 Hz, 1H), 3.51 (d, J = 16.0 Hz, 1H), 1.64 - 1.52 (m, 4H), 0.89 – 0.79 (m, 6 H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 195.3, 167.3, 151.0, 136.0, 134.1, 128.3 (q, J = 313.0 Hz), 126.1, 125.4, 80.5, 64.9, 38.5, 26.2, 9.4; IR (KBr): 2972, 2938, 1717, 1605, 1465, 1301, 1211, 1145, 1097, 917, 893, 752 cm^{-1}; HRMS (ESI) $C_{16}H_{18}O_3F_3S_2$ $[M+H]^+$: calcd 379.0644, found 379.0643.

Benzyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3d)



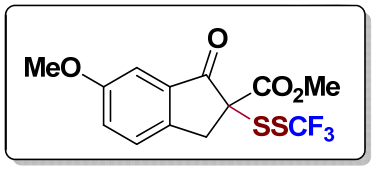
Yield: 78%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.82 (d, J = 8.0 Hz, 1H), 7.67 (t, J = 8.0 Hz, 1H), 7.49 - 7.45 (m, 2H), 7.37 – 7.30 (m, 5 H), 5.28 – 5.21 (m, 2H), 4.03 (d, J = 20.0 Hz, 1H), 3.49 (d, J = 20.0 Hz, 1H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.8, 167.2, 150.7, 136.1, 134.7, 133.9, 128.6, 128.5, 128.3 (q, J = 313.0 Hz), 128.0, 126.1, 125.5, 68.6, 64.3, 38.4; IR (KBr): 1717, 1684, 1605, 1476, 1429, 1329, 1257, 1168, 1048, 751, 695 cm^{-1}; HRMS (ESI) $C_{18}H_{14}O_3F_3S_2$ $[M+H]^+$: calcd 399.0331, found 399.0331.

Tert-butyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3e)



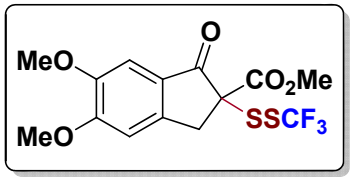
Yield: 92%; pale yellow oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.80 (d, J = 8.0 Hz, 1H), 7.65 (t, J = 8.0 Hz, 1H), 7.50 – 7.44 (m, 2H), 3.96 (d, J = 20.0 Hz, 1H), 3.48 (d, J = 20.0 Hz, 1H), 1.46 (s, 9H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 195.7, 166.3, 151.2, 135.9, 134.1, 128.4, 128.3 (q, J = 313.0 Hz), 126.0, 125.3, 84.7, 65.3, 38.6, 27.7; IR (KBr): 2981, 1714, 1606, 1591, 1476, 1370, 1271, 1254, 1144, 1095, 905, 837, 794 cm^{-1}; HRMS (ESI) $C_{15}H_{15}O_3F_3NaS_2$ $[M+Na]^+$: calcd 387.0307, found 387.0303.

Methyl-6-methoxy-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3f)



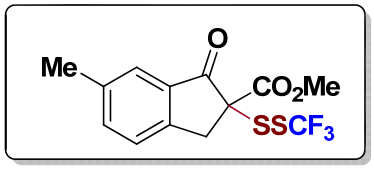
Yield: 90%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.31 (d, J = 8.0 Hz, 1H), 7.21 - 7.18 (m, 1H), 7.15 (d, J = 4.0 Hz, 1H), 3.89 (d, J = 20.0 Hz, 1H), 3.77 (s, 3H), 3.74 (s, 3H), 3.34 (d, J = 20.0 Hz, 1H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 195.0, 167.9, 160.2, 143.7, 138.3 (q, J = 313.0 Hz), 135.1, 126.8, 125.7, 106.3, 64.9, 55.7, 53.8, 38.0; IR (KBr) 1737, 1713, 1616, 1491, 1433, 1341, 1227, 1096, 1024, 852, 827, 752 cm^{-1} HRMS (ESI) $C_{13}H_{12}O_4F_3S_2$ $[M+H]^+$: calcd 353.0124, found 353.0124.

2-((4-Methoxybenzyl)disulfanyl)isoindoline-1,3-dione (3g)



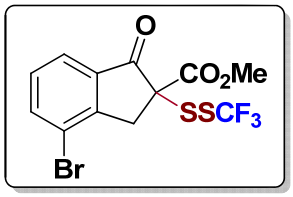
Yield: 93%; white solid; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.18 (s, 1H), 6.89 (s, 1H), 3.99 (s, 3H), 3.96 (d, J = 20.0 Hz, 1H), 3.90 (s, 3H), 3.80 (s, 3H), 3.41 (d, J = 20.0 Hz, 1H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 193.6, 168.0, 156.8, 150.2, 147.0, 128.3 (q, J = 313.0 Hz), 126.5, 106.8, 105.2, 65.2, 56.4, 56.2, 53.9, 38.4; IR (KBr): 2987, 1734, 1701, 1590, 1503, 1436, 1310, 1249, 1222, 1097, 863, 752 cm^{-1}; HRMS (ESI) $C_{14}H_{13}O_5F_3S_2$ $[M]^+$: calcd 382.0157, found 382.0154.

Methyl-6-methyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3h)



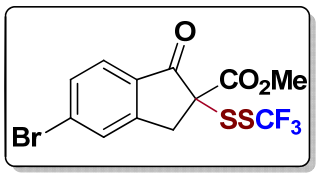
Yield: 83%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.60 (s, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.38 (d, J = 4.0 Hz, 1H), 3.99 (q, J = 20.0 Hz, 1H), 3.80 (s, 3H), 3.43 (d, J = 16.0 Hz, 1H), 2.41 (s, 3H),; ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 195.0, 167.9, 148.2, 138.7, 137.5, 134.0, 128.3 (d, J = 313.0 Hz), 125.7, 125.3, 106.3, 64.6, 53.8, 38.3, 21.0; IR (KBr): 1738, 1714, 1617, 1585, 1493, 1433, 1278, 1247, 1145, 1095, 968, 817, 752 cm^{-1}; HRMS (ESI) $C_{13}H_{12}O_3F_3S_2$ $[M+H]^+$: calcd 337.0174, found 337.0177.

Methyl-4-bromo-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3i)



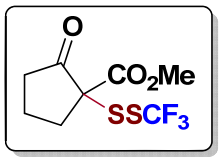
Yield: 86%; pale yellow oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.85 (d, J = 8.0 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.37 (t, J = 8.0 Hz, 1H), 3.96 (d, J = 20.0 Hz, 1H), 3.83 (s, 3H), 3.43 (d, J = 20.0 Hz, 1H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.3, 167.4, 150.4, 138.8, 135.8, 130.3, 128.3 (q, J = 313.0 Hz), 124.3, 121.4, 63.9, 54.0, 39.5; IR (KBr): 2957, 2359, 1724, 1598, 1458, 1327, 1256, 1126, 1098, 959, 804, 753 cm^{-1}; HRMS (EI) $C_{12}H_8O_3F_3S_2Br$ $[M]^+$: calcd 399.9050, found 399.9052.

Methyl-5-bromo-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3j)



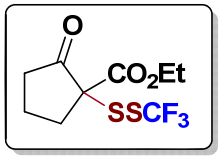
Yield: 84%; pale yellow oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.69 (d, J = 4.0 Hz, 1H), 7.66 (s, 1H), 7.60 (d, J = 12.0 Hz, 1H), 4.04 (d, J = 20.0 Hz, 1H), 3.82 (s, 3H), 3.47 (d, J = 20.0 Hz, 1H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 193.9, 167.4, 152.2, 132.6, 132.3, 131.8, 129.5, 128.2 (q, J = 314.0 Hz), 126.6, 64.2, 54.0, 38.0; IR (KBr): 2955, 1718, 1595, 1580, 1434, 1315, 1261, 1207, 1142, 1095, 1057, 953, 888, 752, 590 cm^{-1}; HRMS (EI) $C_{12}H_8O_3F_3S_2Br$ $[M]^+$: calcd 399.9050, found 399.9046.

Methyl-2-oxo-1-((trifluoromethyl)sulfinothioyl)cyclopentanecarboxylate (3k)



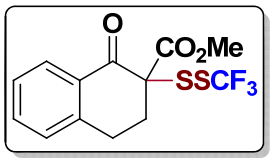
Yield: 73%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 3.78(s, 3H), 2.81 – 2.73 (m, 1H), 2.55 – 2.38 (m, 2H), 2.35 – 2.28 (m, 1H), 2.12 - 2.05 (m, 2H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -45.0 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 205.7, 168.0, 128.6 (q, J = 313.0 Hz), 64.8, 53.6, 36.7, 33.8, 19.0; IR (KBr): 2958, 1751, 1731, 1436, 1275, 1139, 1093, 993, 828, 752 cm^{-1}; HRMS (EI) $C_8H_9O_3F_3S_2$ $[M]^+$: calcd 273.9945, found 273.9946.

Ethyl-2-oxo-1-((trifluoromethyl)sulfinothioyl)cyclopentanecarboxylate (3l)



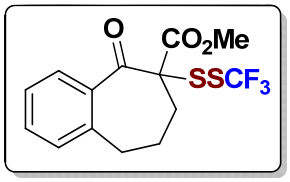
Yield: 76%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 4.25 – 4.20 (m, 2H), 2.80 – 2.72 (m, 1H), 2.54 – 2.38 (m, 2H), 2.35 – 2.28 (m, 1H), 2.12 - 2.05 (m, 2H), 1.29 – 1.26 (m, 3H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -45.0 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 205.9, 167.6, 128.6 (q, J = 313.0 Hz), 65.0, 62.9, 36.8, 33.8, 19.0, 13.7; IR (KBr): 2985, 1726, 1447, 1367, 1244, 1141, 1092, 1018, 918, 752 cm^{-1}; HRMS (EI) $C_9H_{11}O_3F_3S_2$ $[M]^+$: calcd 288.0102, found 288.0100.

Methyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-1,2,3,4-tetrahydronaphthalene-2-carboxylate (3m)



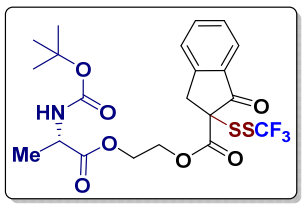
Yield: 52%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 8.05 (d, J = 8.0 Hz, 1H), 7.55 – 7.51 (m, 1H), 7.35 (t, J = 8.0 Hz 1H), 7.25 (d, J = 4.0 Hz, 1H), 3.74 (s, 3H), 3.14 – 3.10 (m, 2H), 3.08 – 3.02 (m, 1H), 2.39 – 2.32 (m, 1H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.7 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 190.1, 167.5, 142.7, 130.8, 128.9, 128.6 (d, J = 313.0 Hz), 128.4, 127.2, 65.0, 53.3, 31.6, 26.3; IR (KBr): 2934, 1734, 1680, 1600, 1455, 1434, 1298, 1219, 1141, 1094, 1019, 981, 888, 805, 752, 736, 576 cm^{-1}; HRMS (ESI) $C_{13}H_{12}O_3F_3S_2$ $[M+H]^+$: calcd 337.0174, found 337.0177.

Methyl-5-oxo-6-((trifluoromethyl)sulfinothioyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulene-6-carboxylate (3n)



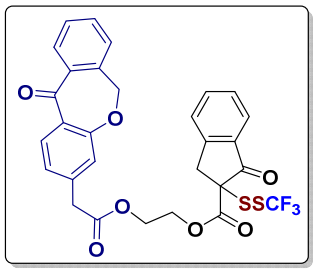
Yield: 47%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.50 (d, J = 12.0 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.29 (t, 1H), 7.15 (d, J = 8.0 Hz, 1H), 3.62 (s, 3H), 2.92 – 2.86 (m, 2H), 2.84 – 2.79 (m, 1H), 2.17 – 1.97 (m, 3H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 199.5, 167.6, 138.9, 138.0, 132.1, 132.1, 129.8, 129.6, 128.4 (d, J = 313.0 Hz), 126.7, 70.3, 53.0, 33.8, 33.6, 24.3; IR (KBr): 2866, 1741, 1683, 1598, 1436, 1349, 1094, 972, 846, 751, 615 cm^{-1}; HRMS (EI) $C_{14}H_{13}O_3F_3S_2$ $[M]^+$: calcd 350.0258, found 350.0255.

2-(((S)-2-((tert-butoxycarbonyl)amino)propanoyl)oxy)ethyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3o)



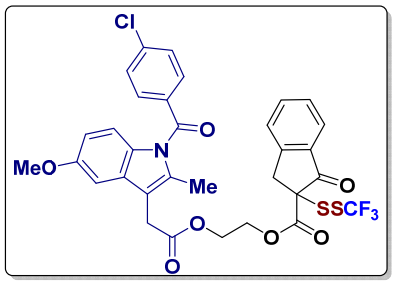
Yield: 95%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.80 (d, J = 8 Hz, 1H), 7.68 (t, J = 8 Hz, 1H), 7.51 – 7.44(m, 2H), 5.05 (brs, 1H), 4.43 – 4.28 (m, 5H), 4.05 – 4.03 d, J = 16 Hz, 1H), 3.48 (t, J = 16 Hz, 1H), 1.43 (s, 9H) 1.33 (d, J = 8.0 Hz, 3H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.6, 173.0, 167.2, 155.1, 150.7, 136.2, 133.7, 128.6, 128.3 (q, J = 31.3Hz), 126.2, 125.5, 79.8, 64.3, 62.6, 62.2, 49.1, 38.4, 29.7, 28.3, 18.4; IR (KBr): 2866, 1741, 1683, 1598, 1436, 1349, 1094, 972, 846, 751, 615 cm^{-1}; HRMS (ESI) $C_{21}H_{24}O_7NF_3S_2Na$ $[M+Na]^+$: calcd 546.0838, found 546.0825.

2-(2-(11-oxo-6,11-dihydrodibenzo[b,e]oxepin-3-yl)acetoxy)ethyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3p)



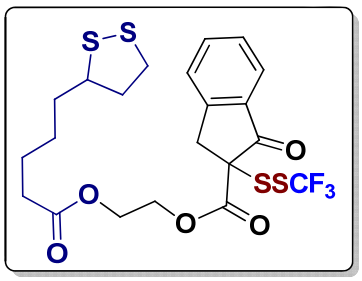
Yield: 97%; yellow oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 8.09 (s, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.66 (t, 1H), 7.56 (t, 1H), 7.48 – 7.35 (m, 5H), 7.01 (d, J = 8.0 Hz, 1H), 5.17 (s, 2H), 4.47 – 4.27 (m, 4H), 3.98 (d, J = 20.0 Hz, 1H), 3.63 (s, 2H), 3.44 (d, J = 20.0 Hz, 1H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.6, 190.7, 171.0, 167.2, 160.5, 150.6, 140.3, 136.3, 136.1, 135.5, 133.7, 132.7, 132.4, 129.4, 129.2, 128.5, 128.3 (d, J = 313.0 Hz), 127.8, 127.3, 126.2, 125.4, 125.1, 121.1, 73.6, 64.4, 64.0, 61.9, 39.8, 38.3; IR (KBr): 2359, 1735, 1647, 1491, 1413, 1300, 1138, 1097, 1015, 908, 830, 730, 641, 623 cm^{-1}; HRMS (ESI) $C_{31}H_{18}O_7F_3S_2$ $[M+H]^+$: calcd 603.0754, found 603.0758.

2-(2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)acetoxy)ethyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3q)



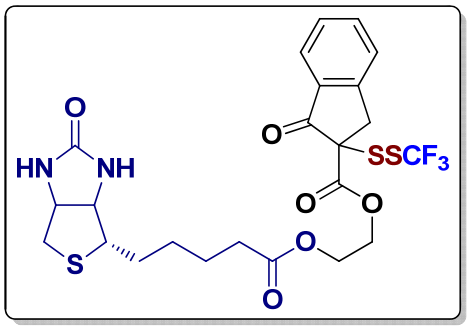
Yield: 95%; yellow oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.78 (d, J = 4.0 Hz, 1H), 7.68 – 7.65 (m, 3H), 7.47 – 7.42 (m, 4H), 6.96 (d, J = 4.0 Hz, 1H), 6.91 (d, J = 8.0 Hz, 1H), 6.67 (dd, J = 8.8 Hz, J = 2.4 Hz, 1H), 4.48 – 4.27 (m, 4H), 3.88 (d, J = 20.0 Hz, 1H), 3.83 (s, 3H), 3.68 (s, 2H), 3.35 (d, J = 20.0 Hz, 1H), 2.34 (s, 3H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (125 MHz; $CDCl_3$): δ 194.6, 170.4, 168.2, 167.2, 156.1, 150.6, 139.1, 136.1, 136.0, 134.2, 133.8, 133.6, 132.6, 131.1, 130.7, 130.6, 129.1, 128.6 (q, J = 314.0 Hz), 128.5, 126.1, 125.4, 123.5, 114.9, 112.1, 111.7, 101.2, 64.3, 63.9, 62.0, 55.6, 38.2, 30.0, 13.3; IR (KBr): 1737, 1680, 1590, 1477, 1401, 1356, 1321, 1271, 1098, 1034, 1014, 993, 909, 833, 752, 729, 648 cm^{-1}; HRMS (ESI) $C_{32}H_{26}O_7ClF_3S_2$ $[M+H]^+$: calcd 692.0786, found 692.0780.

2-((5-(1,2-dithiolan-3-yl)pentanoyl)oxy)ethyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3r)



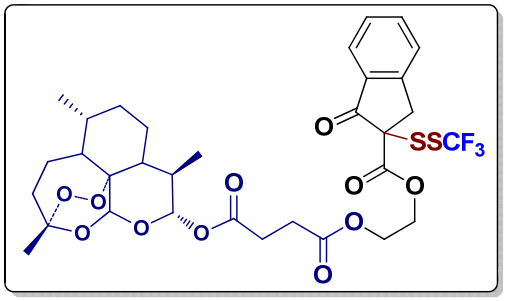
Yield: 52%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.81 (d, J = 8.0 Hz, 1H), 7.69 (t, J = 6.0 Hz, 1H), 7.52 – 7.45 (m, 2H), 4.46 – 4.36 (m, 2H), 4.34 – 4.24 (m, 2H), 4.05 (d, J = 20.0 Hz, 1H), 3.60 – 3.53 (m, 1H), 3.49 (d, J = 16.0 Hz, 1H), 3.21 – 3.08 (m, 2H), 2.50 - 2.42 (m, 1H), 2.30 (t, J = 8.0 Hz, 2H), 1.94 – 1.86 (m, 1H), 1.73 – 1.58 (m, 4H), 1.51 – 1.37 (m, 2H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 193.6, 172.1, 166.3, 149.7, 135.1, 127.6, 127.3 (q, J = 313.0 Hz), 125.2, 124.5, 63.5, 63.1, 60.3, 55.3, 39.2, 37.5, 37.4, 33.5, 32.7, 28.7, 27.7, 23.5; IR (KBr): 2961, 1718, 1258, 1086, 1010, 866, 789, 703, 686, 668, 660 cm^{-1}; HRMS (ESI) $C_{21}H_{23}O_5F_3NaS_4$ $[M+Na]^+$: calcd 563.0273, found 563.0274.

2-((5-((4S)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl)pentanoyl)oxy)ethyl 1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3s)



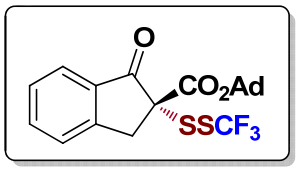
Yield: 97%; yellow oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.75 (td, J = 4.0 Hz, 1H), 7.63 (t, J = 8.0 Hz, 1H), 7.46 – 7.38 (m, 2H), 6.08 (brs, 1H), 5.61 (brs, 1H), 4.43 (brs, 1H), 4.36 – 4.15 (m, 5H), 3.98 (d, J = 20.0 Hz, 1H), 3.43 (d, J = 20.0 Hz, 1H), 3.09 (brs, 1H), 2.83 (m, 1H), 2.68 (d, J = 12.0 Hz, 1H), 2.26 - 2.16 (m, 2H), 1.62 – 1.55 (m, 4H), 1.39 – 1.33 (m, 2H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.7, 173.3, 167.3, 163.8, 150.6, 136.2, 133.6, 128.6, 128.2 (d, J = 313.0 Hz), 126.2, 125.5, 124.2, 64.5, 64.1, 61.9, 61.3, 60.1, 55.4, 40.5, 38.4, 33.5, 28.2, 28.1, 24.5; IR (KBr): 2934, 1735, 1700, 1604, 1590, 1464, 1330, 1269, 1211, 1097, 991, 867, 732, 668 cm^{-1}; HRMS (ESI) $C_{23}H_{26}O_6N_2F_3S_3$ $[M+H]^+$: calcd 579.0900, found 579.0885.

2-((1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carbonyl)oxy)ethyl ((3R, 6R, 9R, 10S, 12aR)-3,6,9-trimethyldecahydro-3H-3,12-epoxy[1,2]dioxepino[4,3-i]-isochromen-10-yl) succinate (3t)



Yield: 94%; pale yellow oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.80 (d, J = 8 Hz, 1H), 7.68 (t, J = 8.0 Hz, 1H), 7.53 – 7.44 (m, 2H), 5.77 – 5.74 (m, 1H), 5.41 (s, 1H), 4.44 – 4.22 (m, 4H), 4.03 (d, J = 16.0 Hz, 1H), 3.48 (d, J = 20 .0Hz, 1H), 2.69 – 2.50 (m, 5H), 2.39 – 2.32 (m, 1H), 2.04 – 2.00 (m, 1H), 1.90 – 1.86 (m, 1H), 1.78 – 1.68 (m, 2H), 1.63 – 1.57 (m, 1H), 1.51 – 1.43 (m, 1H), 1.41 (s, 3H), 1.38 – 1.22 (m, 3H), 1.03 – 0.94 (m, 4H), 0.84 – 0.81 (m, 3H); two diastereoisomers could be detected in ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.57 (-44.58) (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.63 (194.58), 171.72 (171.70), 170.93 (170.91), 167.25 (167.21), 150.68 (150.62), 136.1, 133.7, 128.58 (128.56), 128.3 (q, J = 313.0 Hz), 126.19 (126.16), 125.44 (125.42), 104.4, 92.1, 91.4, 80.0, 64.3, 64.03 (64.00), 61.6, 51.5, 45.1, 38.38 (38.34), 37.2, 36.1, 34.0, 31.7, 29.0, 28.60 (28.57), 25.9, 24.5, 21.9, 20.1, 12.0; IR (KBr): 2951, 1738, 1604, 1465, 1433, 1377, 1329, 1272, 1211, 1148, 1098, 1033, 910, 875, 844, 730, 648 cm^{-1}; HRMS (ESI) $C_{32}H_{37}O_{11}F_3NaS_2$ $[M+Na]^+$: calcd 741.1622, found 741.1617.

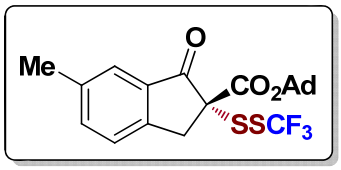
(2R)-adamantan-1-yl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3u)



Yield: 80%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.80 (d, J = 8.0 Hz, 1H), 7.66 (t, J = 8.0 Hz, 1H), 7.50 - 7.42 (m, 2H), 3.96 (d, J = 20.0 Hz, 1H), 3.49 – 3.45 (d, J = 16.0 Hz, 1H), 2.16 (s, 3H), 2.09 (s, 6H), 1.63 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 195.7, 165.9, 151.2, 135.8, 134.2, 128.4 (q, J = 313.0 Hz), 128.3, 126.0, 125.3, 84.8, 65.4, 41.0, 38.6, 35.9, 30.9; IR (KBr): 2912, 2853, 1716, 1607, 1269, 1243, 1211, 1145, 1097, 1045, 963, 789, 752 cm^{-1}; HRMS (ESI) $C_{21}H_{22}O_3F_3S_2$ $[M+H]^+$: calcd 443.0957, found 443.0962; the enantioselectivity (92% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 7.7 min, T_R (minor) = 8.4 min; $[\alpha]_D^{20}$ = -90.9 (c = 0.29, $CHCl_3$).

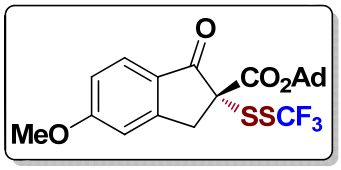
(2R)-adamantan-1-yl-6-methyl-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-

1H-indene-2-carboxylate (3v)



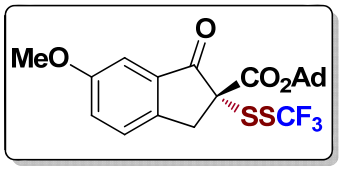
Yield: 76%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.52 (s, 1H), 7.40 (d, J = 4.0 Hz, 1H), 7.30 (d, J = 8.0 Hz, 2H), 3.82 (d, J = 16.0 Hz, 1H), 3.35 (d, J = 20.0 Hz, 1H), 2.35 (s, 3H), 2.09 (s, 3H), 2.02 (s, 6H), 1.56 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 195.8, 166.1, 148.6, 138.4, 137.5, 137.1, 134.4, 128.4 (d, J = 313.0 Hz), 125.7, 125.3, 125.1, 84.7, 65.7, 41.0, 40.7, 38.4, 35.9, 30.9, 21.1; IR (KBr): 2912, 2852, 1714, 1617, 1585, 1493, 1277, 1242, 1220, 1149, 1097, 1046, 963, 861, 814, 752 cm^{-1}; HRMS (ESI) $C_{22}H_{24}O_3F_3S_2$ $[M+H]^+$: calcd 457.1113, found 457.1115; the enantioselectivity (98% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 5.4 min, T_R (minor) = 6.8 min; $[\alpha]_D^{20}$ = -104.1 (c = 0.38, $CHCl_3$).

(2R)-adamantan-1-yl-5-methoxy-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3w)



Yield: 67%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.72(d, J = 12.0 Hz, 1H), 6.95 (d, J = 12.0 Hz, 1H), 6.90 (s, 1H), 3.92 - 3.88 (m, 4H), 3.43 (d, J = 16.0 Hz, 1H), 2.15 (s, 3H), 2.08 (s, 6H), 1.62 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 193.9, 166.2, 166.1, 154.6, 128.4 (d, J = 313.0 Hz), 127.2, 127.0, 116.4, 109.1, 84.6, 66.1, 55.8, 40.9, 38.6, 35.9, 30.9; IR (KBr): 2914, 2853, 1711, 1599, 1491, 1301, 1262, 1241, 1146, 1096, 1047, 1025, 963, 873, 752, 665 cm^{-1}; HRMS (ESI) $C_{22}H_{24}O_4F_3S_2$ $[M+H]^+$: calcd 473.1063, found 473.1062; the enantioselectivity (98% ee) was determined by HPLC analysis: Daicel Chiralcel OD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 7.6 min, T_R (minor) = 8.5 min; $[\alpha]_D^{20}$ = -77.6 (c = 0.22, $CHCl_3$).

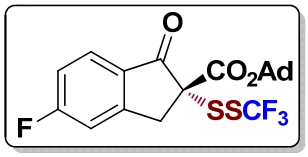
(2R)-adamantan-1-yl-6-methoxy-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3x)



Yield: 72%; colorless solid; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.37(d, J = 8.0 Hz, 1H), 7.25 – 7.23 (m, 1H), 7.21 (s, 1H), 3.87 - 3.83 (m, 4H), 3.38 (d, J = 16.0 Hz, 1H), 2.16 (s, 3H), 2.08 (s, 6H), 1.63 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 195.8, 166.0,

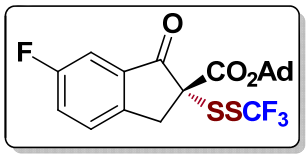
160.0, 144.1, 135.4, 128.4 (d, J = 313.0 Hz), 126.7, 125.4, 106.1, 84.7, 66.1, 55.6, 41.0, 38.1, 35.9, 30.9; IR (KBr): 2927, 2904, 2856, 1727, 1713, 1436, 1290, 1275, 1147, 1095, 1048, 1020, 963, 928, 861, 828, 750, 744 cm^{-1}; HRMS (ESI) $C_{22}H_{24}O_4F_3S_2$ $[M+H]^+$: calcd 473.1063, found 473.1062; the enantioselectivity (97% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 6.5 min, T_R (minor) = 7.8 min; $[\alpha]_D^{20}$ = -75.8 (c = 0.37, $CHCl_3$).

(2R)-adamantan-1-yl-5-fluoro-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3y)



Yield: 65%; colorless oil; ^1H NMR (400 MHz; $CDCl_3$): δ 7.83 – 7.79(m, 1H), 7.17 – 7.12 (m, 2H), 3.95 (d, J = 20.0 Hz, 1H), 3.47 (d, J = 20.0 Hz, 1H), 2.17 (s, 3H), 2.08 (s, 6H), 1.64 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F), -100.0 (s, 1F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.0, 167.7 (d, J = 257.0 Hz), 165.6, 154.2 (d, J = 10.0 Hz), 130.6, 128.3 (d, J = 313.0 Hz), 127.7 (d, J = 11.0 Hz), 116.8 (d, J = 24.0 Hz), 112.9 (d, J = 23.0 Hz), 85.1, 65.7, 41.0, 38.4, 35.9, 30.9; IR (KBr): 2912, 2854, 1718, 1615, 1595, 1483, 1241, 1146, 1097, 1046, 963, 940, 874, 826, 813, 752 cm^{-1}; HRMS (ESI) $C_{21}H_{21}O_3F_4S_2$ $[M+H]^+$: calcd 461.0863, found 461.0870; the enantioselectivity (97% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 8.5 min, T_R (minor) = 9.5 min; $[\alpha]_D^{20}$ = -98.3 (c = 0.22, $CHCl_3$).

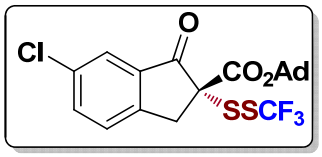
(2R)-adamantan-1-yl-6-fluoro-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3z)



Yield: 87%; colorless oil; ^1H NMR (400 MHz; $CDCl_3$): δ 7.48 – 7.35(m, 3H), 3.91 (d, J = 16.0 Hz, 1H), 3.43 (d, J = 20.0 Hz, 1H), 2.17 (s, 3H), 2.08 (s, 6H), 1.64 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.6 (s, 3F), -112.7 (s, 1F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.8, 165.6, 162.7 (d, J = 250.0 Hz), 146.6 (d, J = 2.0 Hz), 136.0 (d, J = 80.0 Hz), 128.3 (q, J = 313.0 Hz), 127.5 (d, J = 8.0 Hz), 123.5 (d, J = 23.6 Hz), 111.0 (d, J = 22.6 Hz), 85.1, 66.0, 41.0, 38.1, 35.9, 30.9; IR (KBr): 2912, 2854, 1719, 1490, 1287, 1244, 1220, 1148, 1097, 1044, 963, 864, 752 cm^{-1}; HRMS (ESI) $C_{21}H_{21}O_3F_4S_2$ $[M+H]^+$: calcd 461.0863, found 461.0868; the enantioselectivity (97% ee) was determined by HPLC

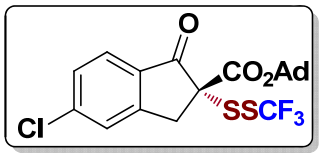
analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 7.1 min, T_R (minor) = 9.0 min; $[\alpha]_D^{20}$ = -84.7 (c = 0.53, $CHCl_3$).

(2R)-adamantan-1-yl-6-chloro-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3aa)



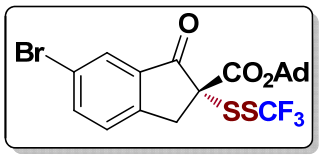
Yield: 70%; pale yellow oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.75(s, 1H), 7.63 – 7.60 (m, 1H), 7.44 (d, J = 8.0 Hz, 1H), 3.91 (d, J = 16.0 Hz, 1H), 3.43 (d, J = 20.0 Hz, 1H), 2.16 (s, 3H), 2.08 (s, 6H), 1.63 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.6, 165.5, 149.2, 135.9, 135.6, 134.8, 128.3 (q, J = 313.0 Hz), 127.2, 124.9, 85.1, 65.7, 41.0, 38.2, 35.9, 30.9; IR (KBr): 2913, 2853, 1719, 1473, 1249, 1199, 1182, 1097, 1044, 963, 752, 710 cm^{-1}; HRMS (ESI) $C_{21}H_{21}O_3ClF_3S_2$ $[M+H]^+$: calcd 477.0567, found 477.0568; the enantioselectivity (94% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 6.5 min, T_R (minor) = 8.7 min; $[\alpha]_D^{20}$ = -78.7 (c = 0.59, $CHCl_3$).

(2R)-adamantan-1-yl-5-chloro-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3ab)



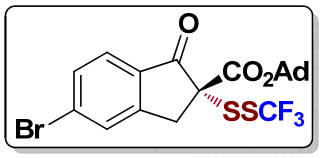
Yield: 68%; yellow solid; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.73 (d, J = 8.0 Hz, 1H), 7.49 (s, 1H), 7.42 (d, J = 8.0 Hz, 1H), 3.87 (d, J = 16.0 Hz, 1H), 3.38 (d, J = 16.0 Hz, 1H), 2.10 (s, 3H), 2.02 (s, 6H), 1.57 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.4, 165.5, 152.6, 142.6, 132.6, 129.2, 128.3 (q, J = 313.0 Hz), 126.3, 85.1, 65.5, 41.0, 38.2, 35.9, 30.9; IR (KBr): 2910, 2850, 1733, 1712, 1599, 1417, 1318, 1241, 1208, 1153, 1094, 1048, 996, 963, 895, 870, 863, 844, 786, 751, 657 cm^{-1}; HRMS (EI) $C_{21}H_{20}O_3ClF_3S_2$ $[M]^+$: calcd 476.0495, found 476.0488; the enantioselectivity (96% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 9.1 min, T_R (minor) = 9.7 min; $[\alpha]_D^{20}$ = -72.4 (c = 0.31, $CHCl_3$).

(2R)-adamantan-1-yl-6-bromo-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3ac)



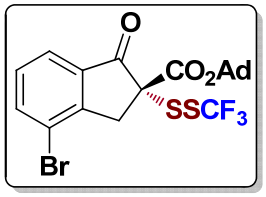
Yield: 86%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.91(s, 1H), 7.76 (d, J = 8.0 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 3.89 (d, J = 20.0 Hz, 1H), 3.40 (d, J = 16.0 Hz, 1H), 2.16 (s, 3H), 2.08 (s, 6H), 1.63 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.4, 165.5, 149.7, 138.6, 135.9, 128.3 (d, J = 313.0 Hz), 128.0, 127.6, 122.5, 85.1, 65.5, 41.0, 38.2, 35.9, 30.9; IR (KBr): 2913, 2853, 1718, 1599, 1469, 1457, 1251, 1197, 1181, 1146, 1097, 1044, 963, 817, 752, 704 cm^{-1}; HRMS (ESI) $C_{21}H_{21}O_3{}^{81}BrF_3S_2$ $[M+H]^+$: calcd 523.0042, found 523.0048; the enantioselectivity (96% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 6.9 min, T_R (minor) = 9.7 min; $[\alpha]_D^{20}$ = -85.4 (c = 0.45, $CHCl_3$).

(2R)-adamantan-1-yl-5-bromo-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3ad)



Yield: 86%; colorless solid; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.68 (s, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.58 (d, J = 8.0 Hz, 1H), 3.94 (d, J = 12.0 Hz, 1H), 3.45 (d, J = 16.0 Hz, 1H), 2.17 (s, 3H), 2.08 (s, 6H), 1.63 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 194.7, 165.6, 152.7, 133.1, 132.2, 131.5, 129.4, 128.7 (d, J = 313.0 Hz), 126.4, 85.2, 65.4, 41.0, 38.2, 35.9, 31.0; IR (KBr): 2853, 1718, 1596, 1457, 1314, 1260, 1242, 1206, 1146, 1097, 1045, 963, 860, 813, 785, 752 cm^{-1}; HRMS (ESI) $C_{21}H_{21}O_3{}^{81}BrF_3S_2$ $[M+H]^+$: calcd 523.0042, found 523.0048; the enantioselectivity (94% ee) was determined by HPLC analysis: Daicel Chiralcel OD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 4.8 min, T_R (minor) = 5.2 min; $[\alpha]_D^{20}$ = -62.3 (c = 0.21, $CHCl_3$).

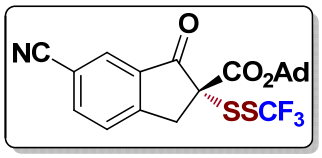
(2R)-adamantan-1-yl-4-bromo-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3ae)



Yield: 86%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.83 (d, J = 8.0 Hz, 1H), 7.75 (d, J = 4.0 Hz, 1H), 7.35 (t, J = 6.0 Hz, 1H), 3.86 (d, J = 20.0 Hz, 1H), 3.40 (d, J = 16.0 Hz, 1H), 2.17 (s, 3H), 2.09 (s, 6H), 1.64 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100

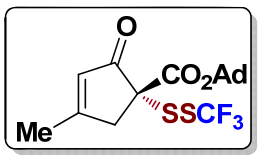
MHz; $CDCl_3$): δ 195.1, 165.5, 150.8, 138.5, 136.1, 130.1, 128.3 (q, J = 313.0 Hz), 124.1, 121.3, 85.2, 65.0, 41.0, 39.7, 35.9, 30.9; IR (KBr): 2911, 2853, 1718, 1598, 1457, 1240, 1146, 1126, 1096, 1044, 962, 803, 752, 728 cm^{-1} HRMS (ESI) $C_{21}H_{21}O_3BrF_3S_2$ $[M+H]^+$: calcd 523.0000, found 523.0000; the enantioselectivity (86% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 5.6 min, T_R (minor) = 6.3 min; $[\alpha]_D^{20}$ = -44.1 (c = 0.50, $CHCl_3$).

(2R)-adamantan-1-yl-6-cyano-1-oxo-2-((trifluoromethyl)sulfinothioyl)-2,3-dihydro-1H-indene-2-carboxylate (3af)



Yield: 88%; white solid; ^1H NMR (400 MHz; $CDCl_3$): δ 8.07 (s, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.65 (d, J = 8.0 Hz, 1H), 4.03 (d, J = 16.0 Hz, 1H), 3.53 (d, J = 16.0 Hz, 1H), 2.17 (s, 3H), 2.08 (s, 6H), 1.63 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.5 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 193.9, 165.0, 154.9, 138.2, 134.8, 129.3, 127.7 (q, J = 313.0 Hz), 127.3, 117.4, 112.9, 85.6, 65.0, 41.0, 38.7, 35.8, 30.9; IR (KBr): 2912, 2855, 2233, 1720, 1615, 1486, 1457, 1428, 1243, 1146, 1097, 1043, 962, 862, 752 cm^{-1}; HRMS (ESI) $C_{22}H_{21}O_3NF_3S_2$ $[M+H]^+$: calcd 468.0909, found 468.0911; the enantioselectivity (81% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/10, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 7.5 min, T_R (minor) = 10.3 min; $[\alpha]_D^{20}$ = -83.9 (c = 0.42, $CHCl_3$).

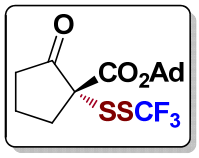
`(1R)-adamantan-1-yl-4-methyl-2-oxo-1-((trifluoromethyl)sulfinothioyl)cyclopent-3-enecarboxylate (3ag)



Yield: 50%; colorless oil; ^1H NMR (400 MHz; $CDCl_3$): δ 5.96 (s, 1H), 3.37 (d, J = 20.0 Hz, 1H), 2.90 (d, J = 16.0 Hz, 1H), 2.20 (s, 3H), 2.17 (s, 3H), 2.09 (s, 6H), 1.64 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.4 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 198.4, 177.5, 165.6, 128.4 (q, J = 313.0 Hz), 128.0, 84.8, 65.0, 44.9, 41.0, 35.9, 30.9, 19.2; IR (KBr): 2911, 2854, 1710, 1626, 1423, 1247, 1163, 1096, 1045, 963, 849, 790, 752 cm^{-1}; HRMS (ESI) $C_{18}H_{22}O_3F_3S_2$ $[M+H]^+$: calcd 407.0957, found 407.0955; the enantioselectivity (97% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 4.9 min, T_R (minor) = 6.1 min; $[\alpha]_D^{20}$ = -

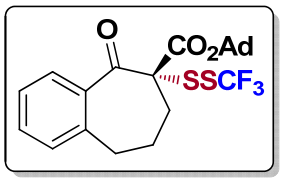
106.5 (c = 0.25, $CHCl_3$).

(1R)-adamantan-1-yl-2-oxo-1-((trifluoromethyl)sulfinothioyl)cyclopentanecarboxylate (3ah)



Yield: 67%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 2.69 – 2.61 (m, 1H), 2.39 – 2.35 (m, 2H), 2.28 - 2.21 (m, 1H), 2.11 (s, 3H), 2.04 – 2.00 (m, 8H), 1.59 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.9 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 206.5, 166.3, 128.7 (q, J = 312.0 Hz), 84.3, 65.8, 41.1, 36.8, 36.0, 33.9, 30.9, 19.2; IR (KBr): 2912, 2853, 1718, 1249, 1228, 1141, 1096, 1047, 965, 875, 752 cm^{-1}; HRMS (ESI) $C_{17}H_{22}O_3F_3S_2$ $[M+H]^+$: calcd 395.0957, found 395.0957; the enantioselectivity (92% ee) was determined by HPLC analysis: Daicel Chiralcel OD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 5.1 min, T_R (minor) = 4.7 min; $[\alpha]_D^{20}$ = -165.4 (c = 0.30, $CHCl_3$).

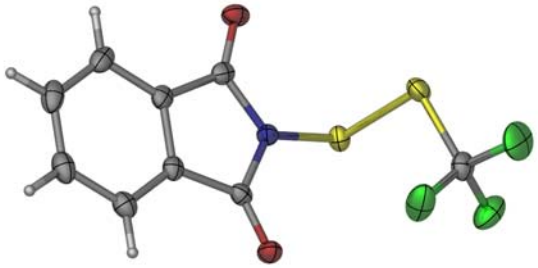
(6R)-adamantan-1-yl-5-oxo-6-((trifluoromethyl)sulfinothioyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulene-6-carboxylate (3ai)



Yield: 48%; colorless oil; ^{1}H NMR (400 MHz; $CDCl_3$): δ 7.54 (d, J = 8.0 Hz, 1H), 7.40 (t, J = 8.0 Hz, 1H), 7.29 (t, J = 8.0 Hz, 1H), 7.16 (d, J = 8.0 Hz, 1H), 3.04 – 2.97 (m, 1H), 2.91 – 2.80 (m, 2H), 2.18 – 2.06(m, 5H), 2.00 - 1.92 (m, 1H), 1.89 – 1.86 (m, 3H) 1.74 (d, J = 12.0 Hz, 3H), 1.55 (s, 6H); ^{19}F NMR (375 MHz, $CDCl_3$): δ -44.2 (s, 3F); ^{13}C NMR (100 MHz; $CDCl_3$): δ 199.6, 165.6, 139.7, 138.2, 131.9, 130.4, 129.7, 128.4 (d, J = 313.0 Hz), 126.3, 83.8, 71.0, 40.6, 35.9, 33.8, 33.6, 30.7, 24.8; IR (KBr): 2911, 2853, 1732, 1447, 1254, 1221, 1143, 1097, 1049, 964, 790, 752, 735, 619 cm^{-1}; HRMS (ESI) $C_{23}H_{25}O_3F_3NaS_2$ $[M+Na]^+$: calcd 493.1089, found 493.1081; the enantioselectivity (50% ee) was determined by HPLC analysis: Daicel Chiralcel AD-H, hexane/*i*-PrOH: 95/2.5, 1.0 mL/min, 30 °C, 254 nm, T_R (major) = 5.1 min, T_R (minor) = 5.8 min; $[\alpha]_D^{20}$ = +31.1 (c = 0.22, $CHCl_3$).

5. X-Ray crystal data

5.1 Crystal data of 1 (CCDC 2052954)

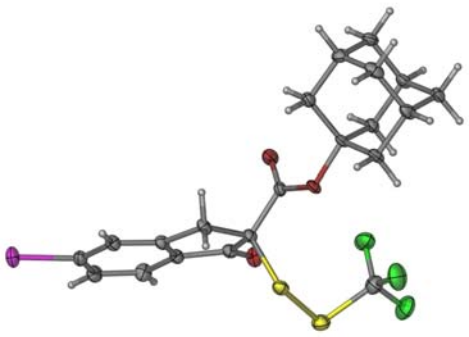


	exp_1116
Crystal data	
Chemical formula	$C_9H_4F_3NO_2S_2$
M_r	279.25
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	9.2185 (3), 4.9869 (2), 23.6764 (8)
β (°)	97.301 (3)
V (Å^3)	1079.62 (7)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.83
Crystal size (mm)	0.26 × 0.22 × 0.14
Data collection	
Diffractometer	XtaLAB AFC12 (RINC): Kappa dual home/near
Absorption correction	Multi-scan *CrysAlis PRO* 1.171.39.28b (Rigaku Oxford Diffraction, 2015) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.167, 1.000
No. of measured, independent and	19219, 1905, 1799

observed [$I > 2\sigma(I)$] reflections	
R_{int}	0.056
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.076, 1.06
No. of reflections	1905
No. of parameters	154
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.27, −0.20

Computer programs: *CrysAlis PRO* 1.171.39.28b (Rigaku OD, 2015), ShelXT (Sheldrick, 2015), *SHELXL* (Sheldrick, 2015), Olex2 (Dolomanov *et al.*, 2009).

5.2 Crystal data of 3ad (CCDC 2052955)



	exp_1642
Crystal data	
Chemical formula	$C_{21}H_{20}BrF_3O_3S_2$
M_r	521.40
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	170
a, b, c (Å)	6.8887 (1), 7.4921 (1), 39.5436 (3)
V (Å^3)	2040.88 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	5.11
Crystal size (mm)	0.45 × 0.12 × 0.08
Data collection	
Diffractometer	XtaLAB AFC12 (RINC): Kappa dual home/near
Absorption correction	Multi-scan *CrysAlis PRO* 1.171.39.32a (Rigaku Oxford Diffraction, 2017) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.339, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41991, 3625, 3545
R_{int}	0.086
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.066, 1.03
No. of reflections	3625
No. of parameters	271
H-atom treatment	H-atom parameters constrained

$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.32
Absolute structure	Flack x determined using 1422 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	−0.016 (9)

Computer programs: *CrysAlis PRO* 1.171.39.32a (Rigaku OD, 2017), ShelXT (Sheldrick, 2015), XL (Sheldrick, 2008), Olex2 (Dolomanov *et al.*, 2009).

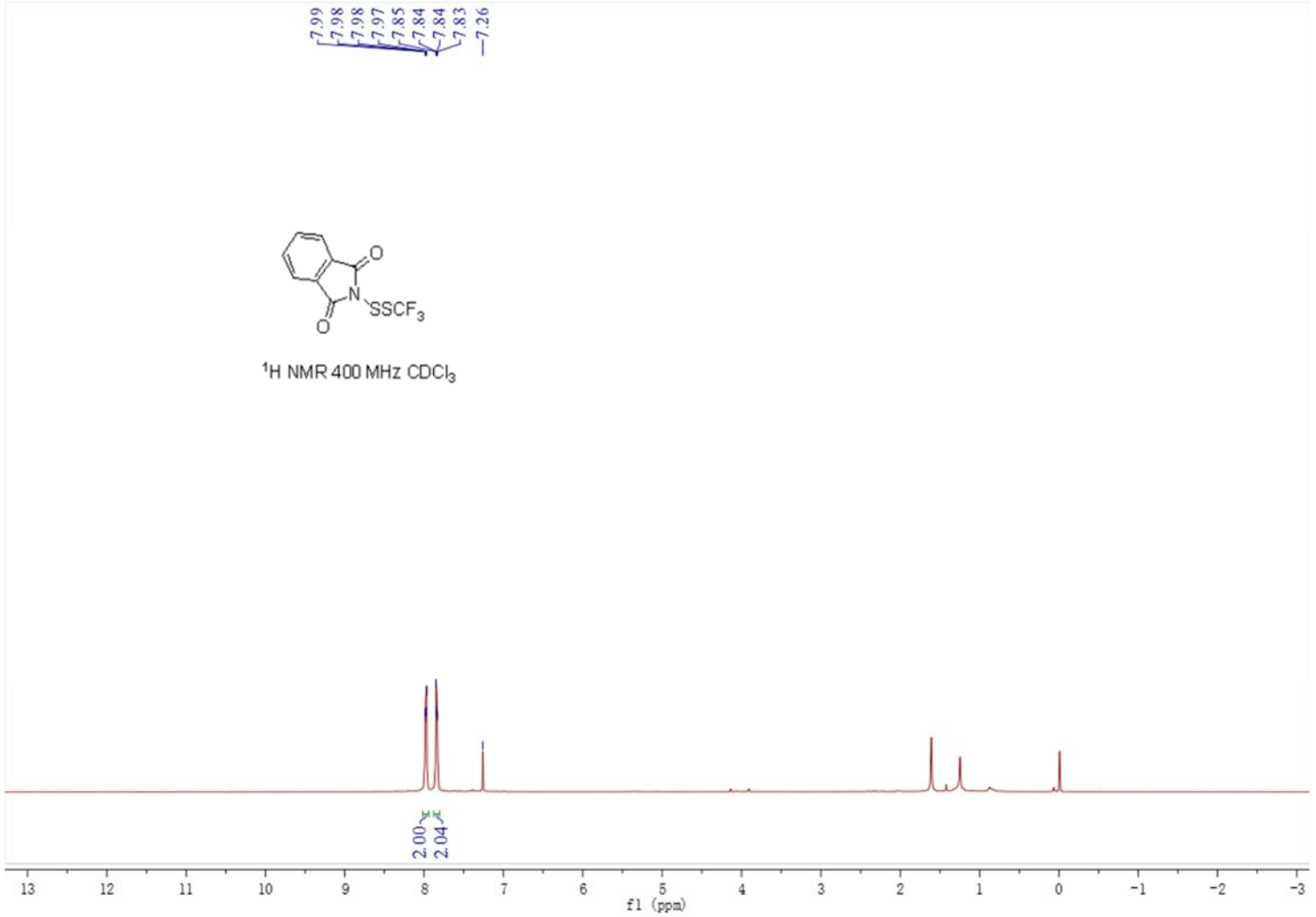
6. References:

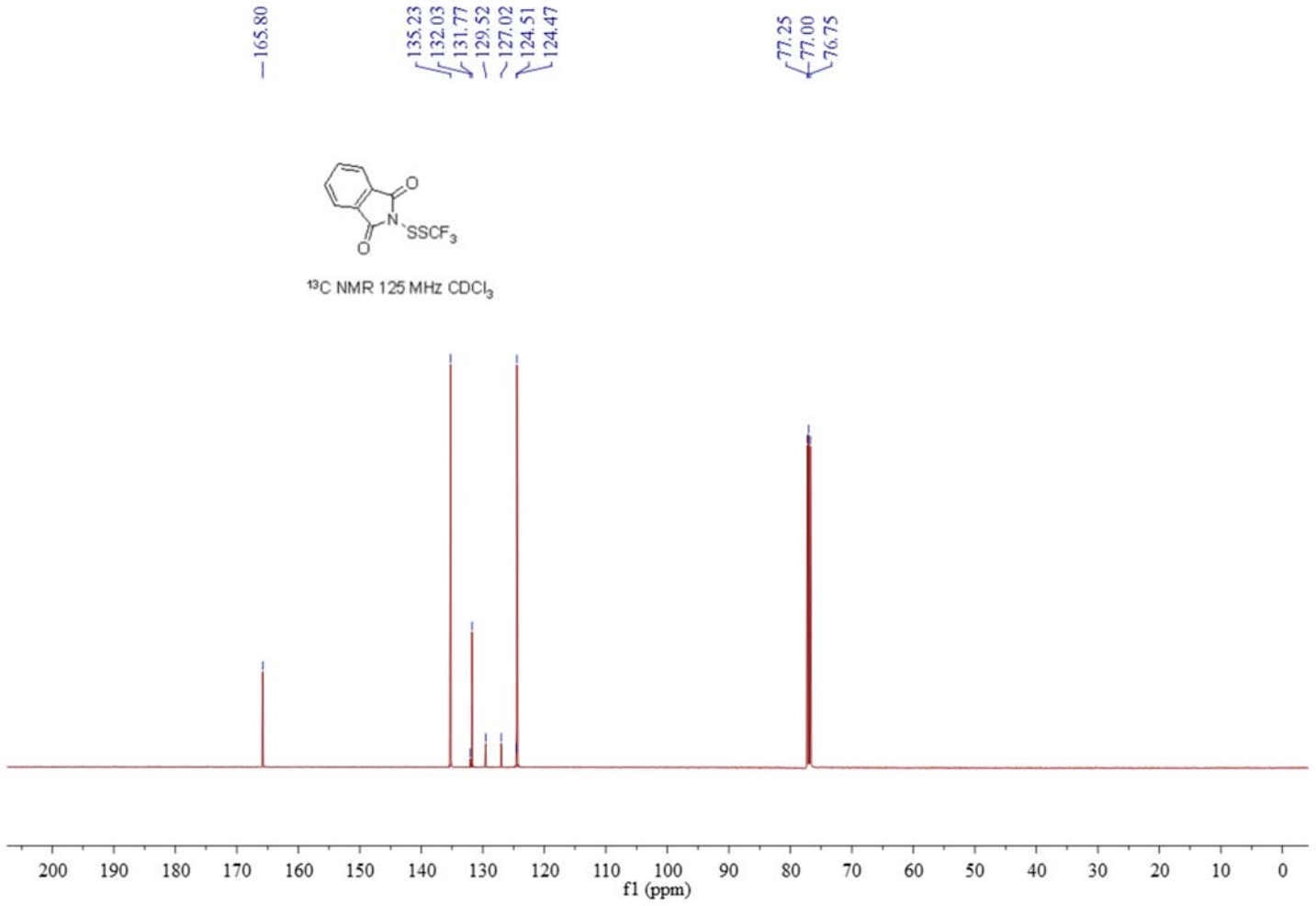
[S1] T. A. Graf, J. Yoo, A. B. Brummett, R. Lin, M. Wohlgenannt, D. Quinn, and N. B. Bowden, *Macromolecules* **2012**, *45*, 8193

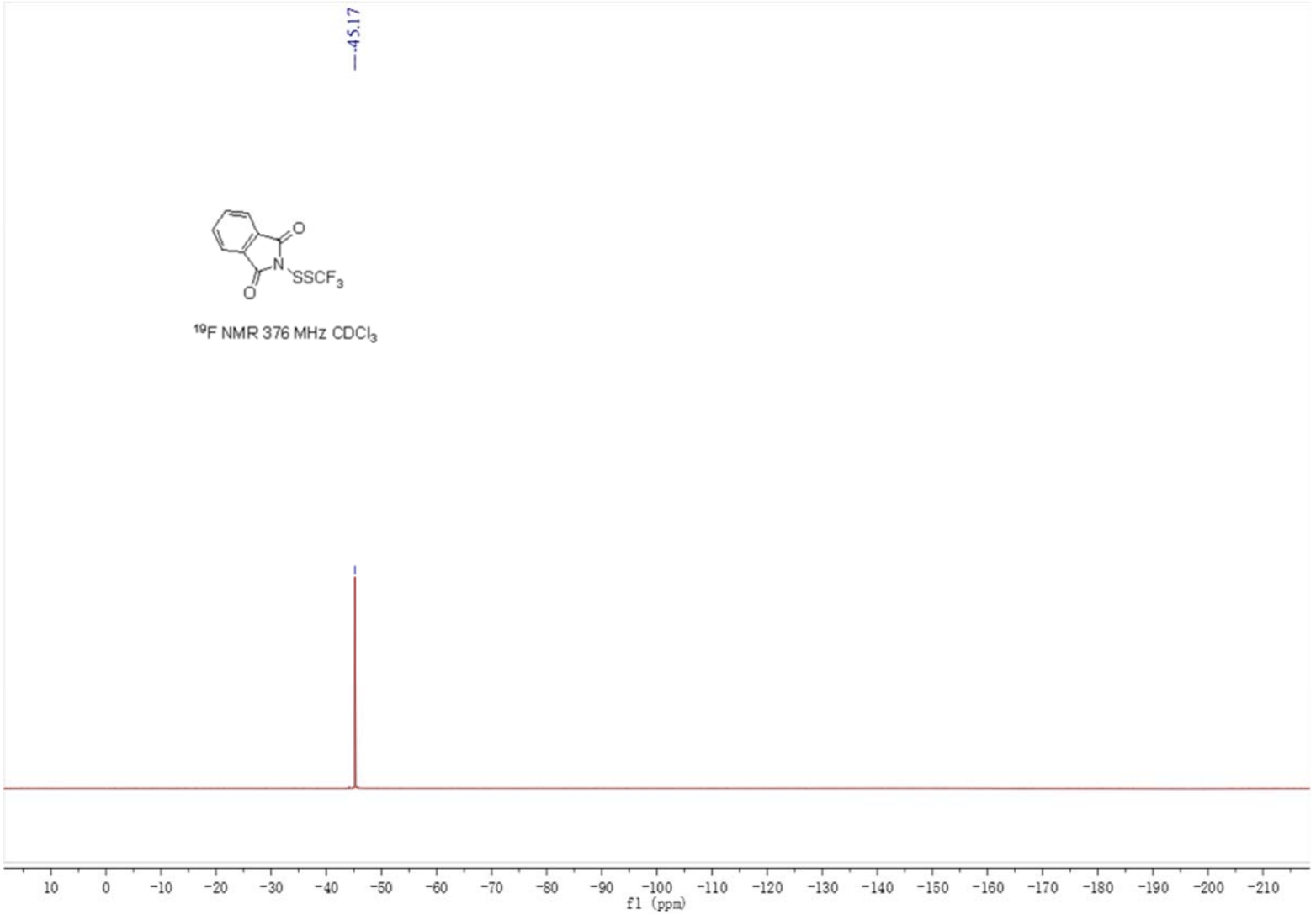
[S2] D. Zhu, Y. Gu, L. Lu, and Q. Shen, *J. Am. Chem. Soc.* **2015**, *137*, 10547.

7. Copies of NMR and HPLC spectra

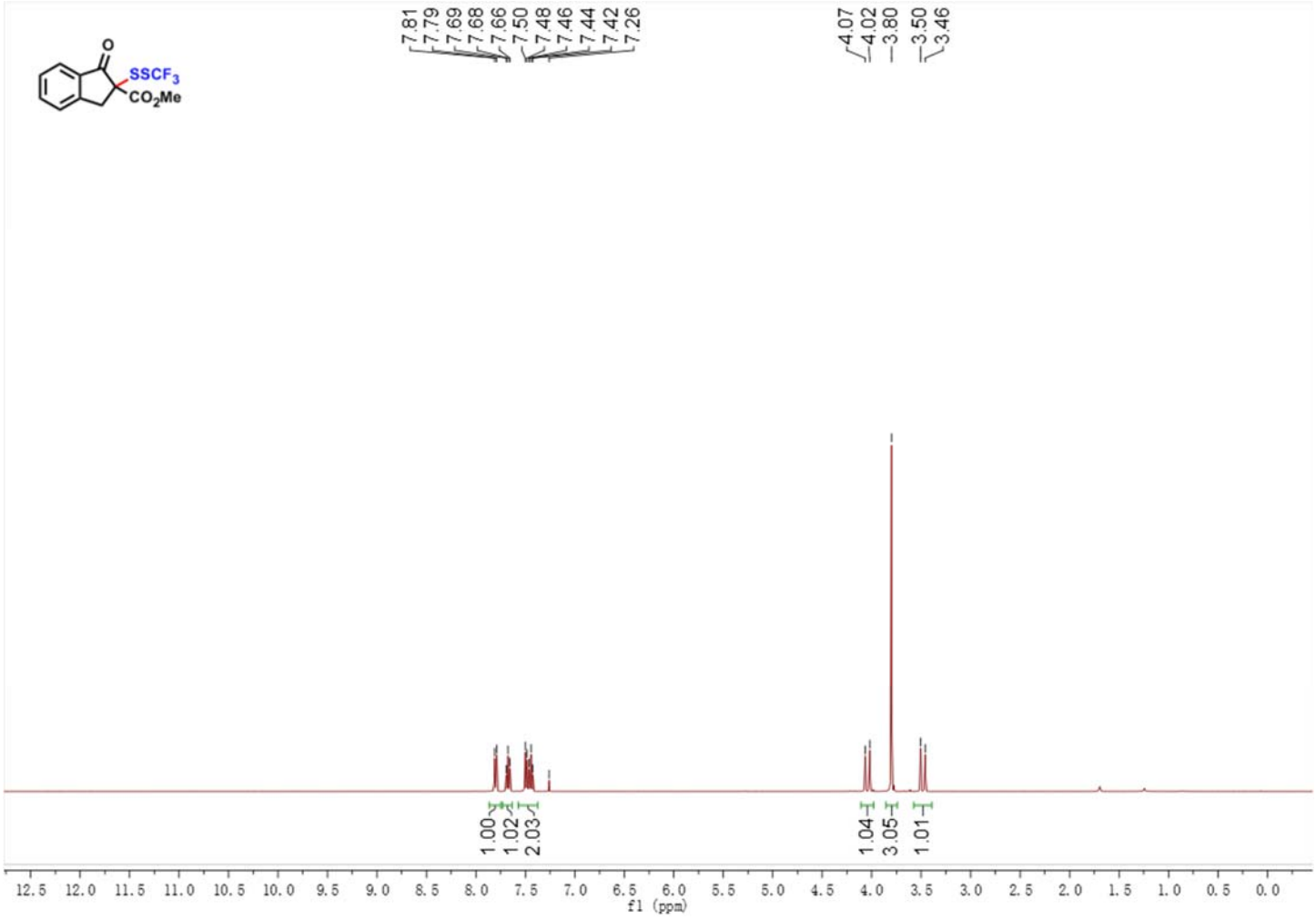
1

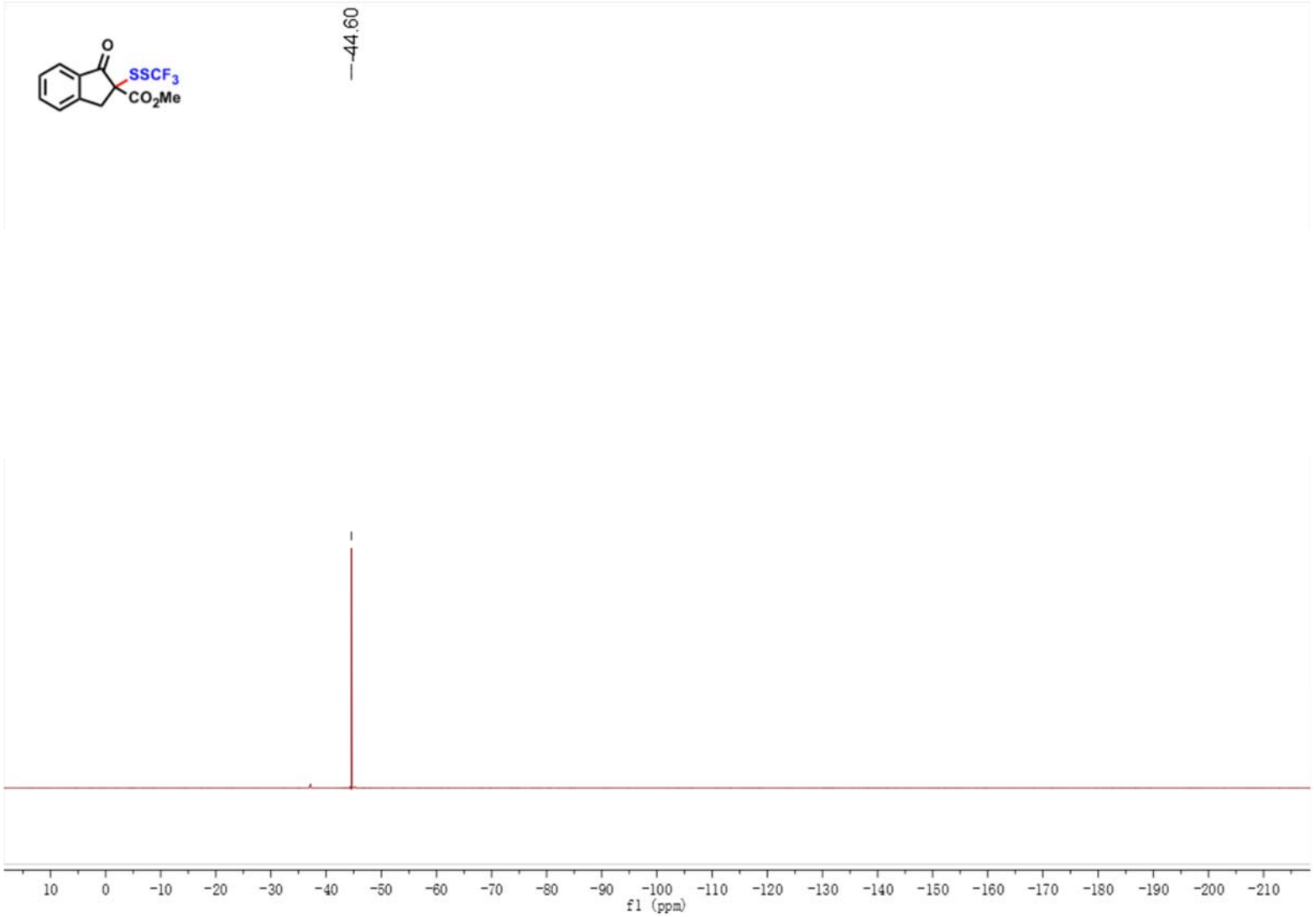

7.99
7.98
7.98
7.97
7.85
7.84
7.84
7.83
7.26
O
N
SSCF3
O
1H NMR 400 MHz CDCl3
2.00
2.04
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


165.80
135.23
132.03
131.77
129.52
127.02
124.51
124.47
77.25
77.00
76.75
O
N
SSCF3
O
13C NMR 125 MHz CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-45.17
O
N
SSCF3
O
19F NMR 376 MHz CDCl3
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)

3a


O
SSCF3
CO2Me
7.81
7.79
7.69
7.68
7.66
7.50
7.48
7.46
7.44
7.42
7.26
4.07
4.02
3.80
3.50
3.46
1.00
1.02
2.03
1.04
3.05
1.01
f1 (ppm)


O
SSCF3
CO2Me
-44.60
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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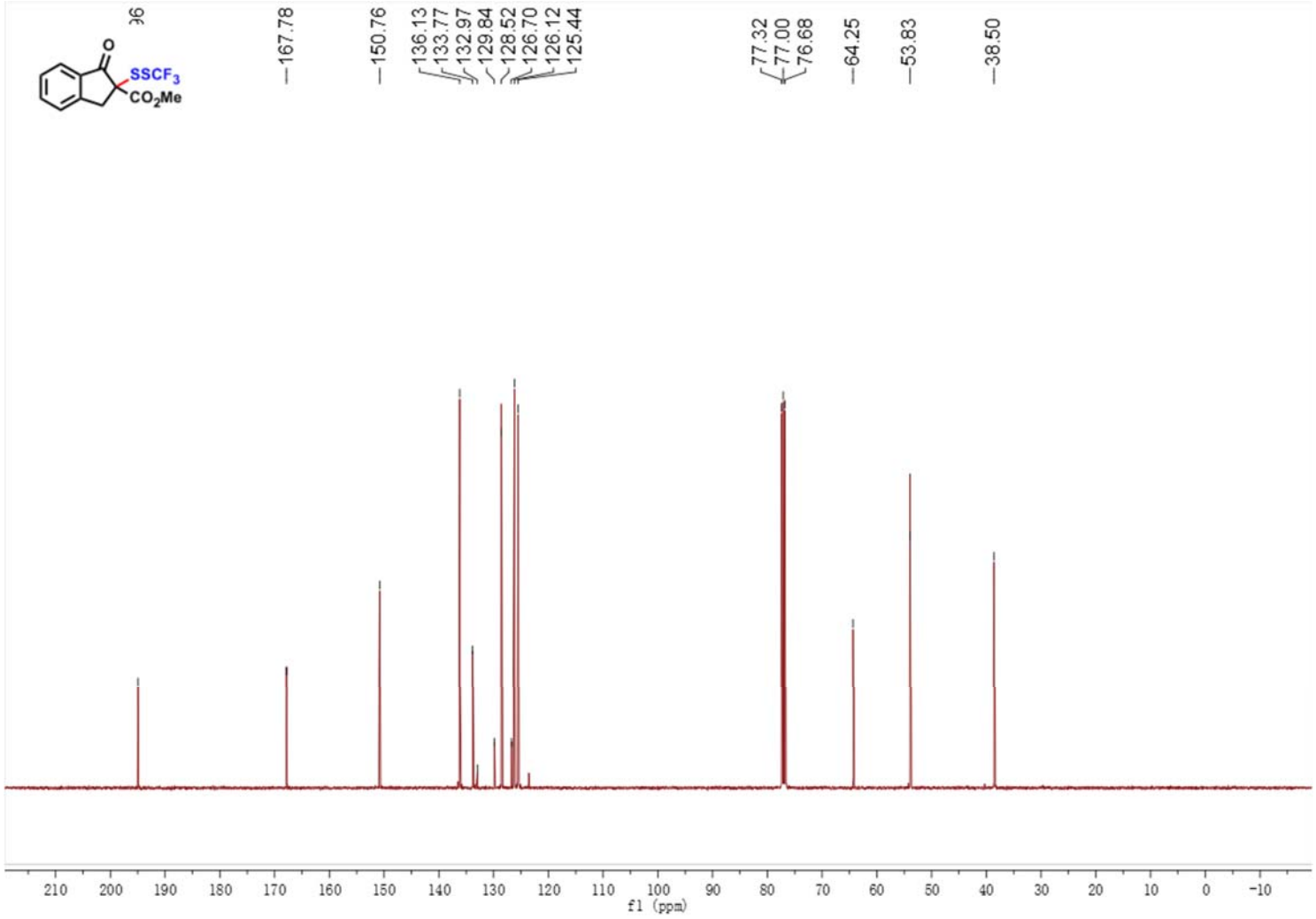
-170
-180
-190
-200
-210
f1 (ppm)


SSCF3
CO2Me
167.78
150.76
136.13
133.77
132.97
129.84
128.52
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125.44
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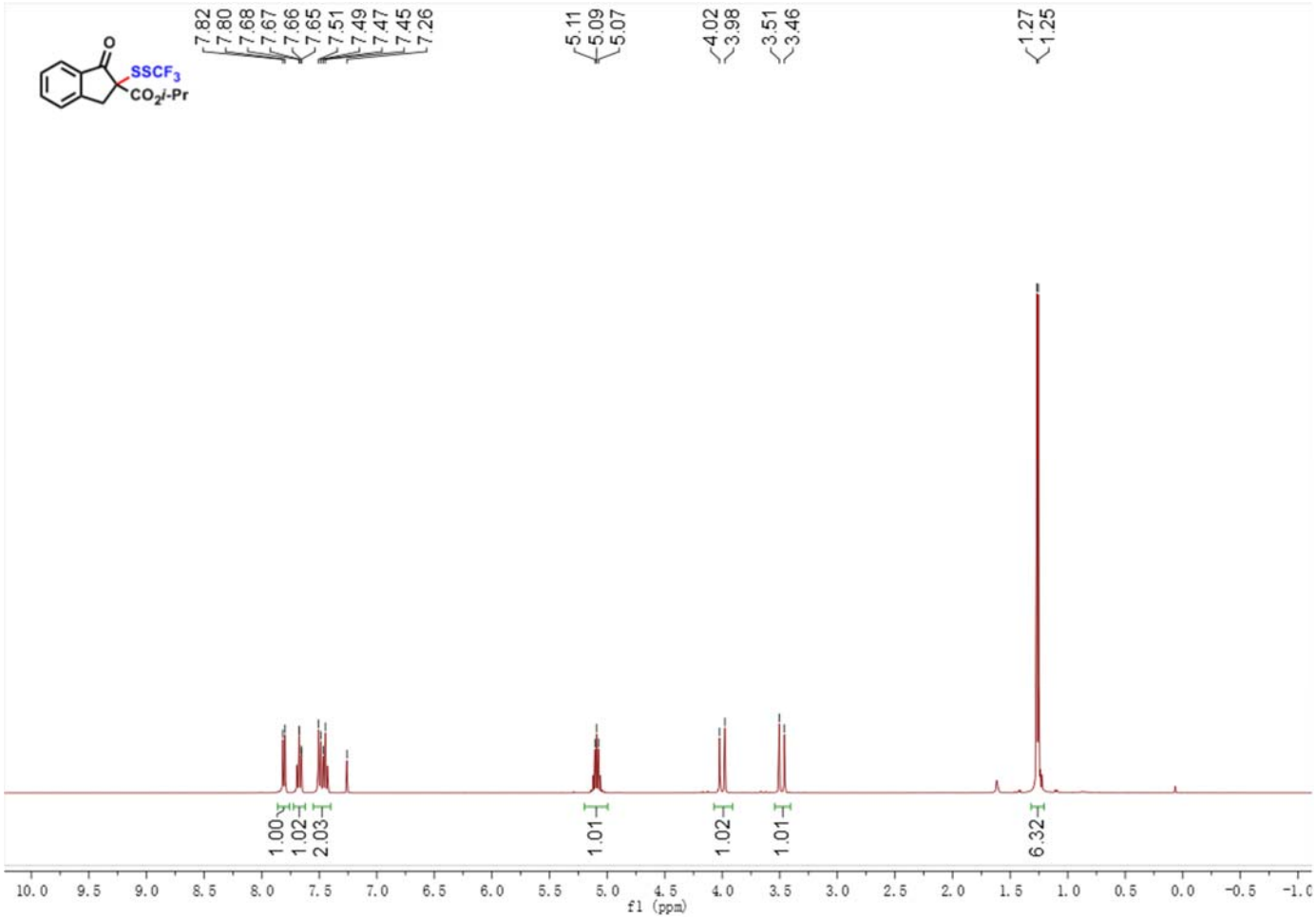
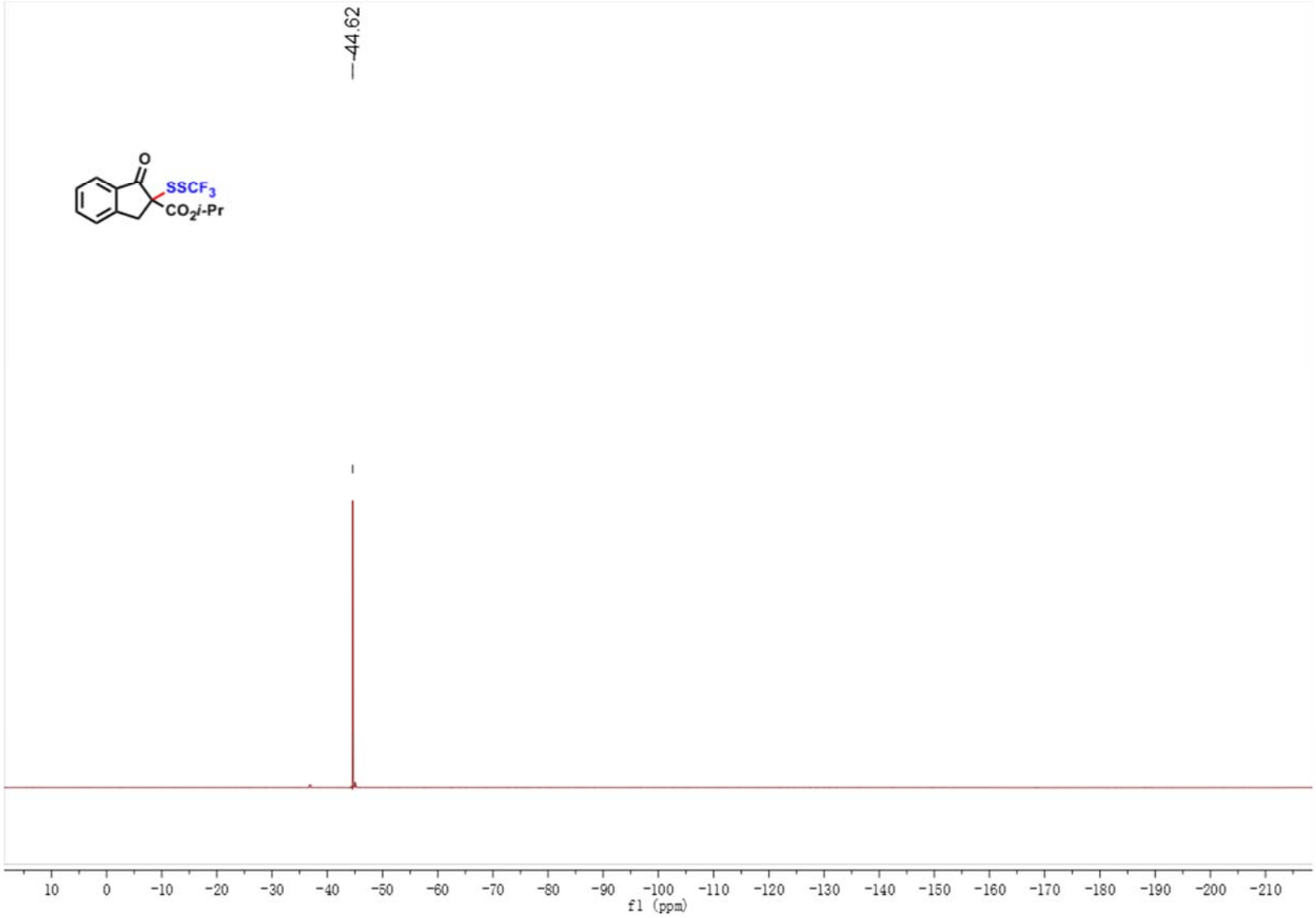
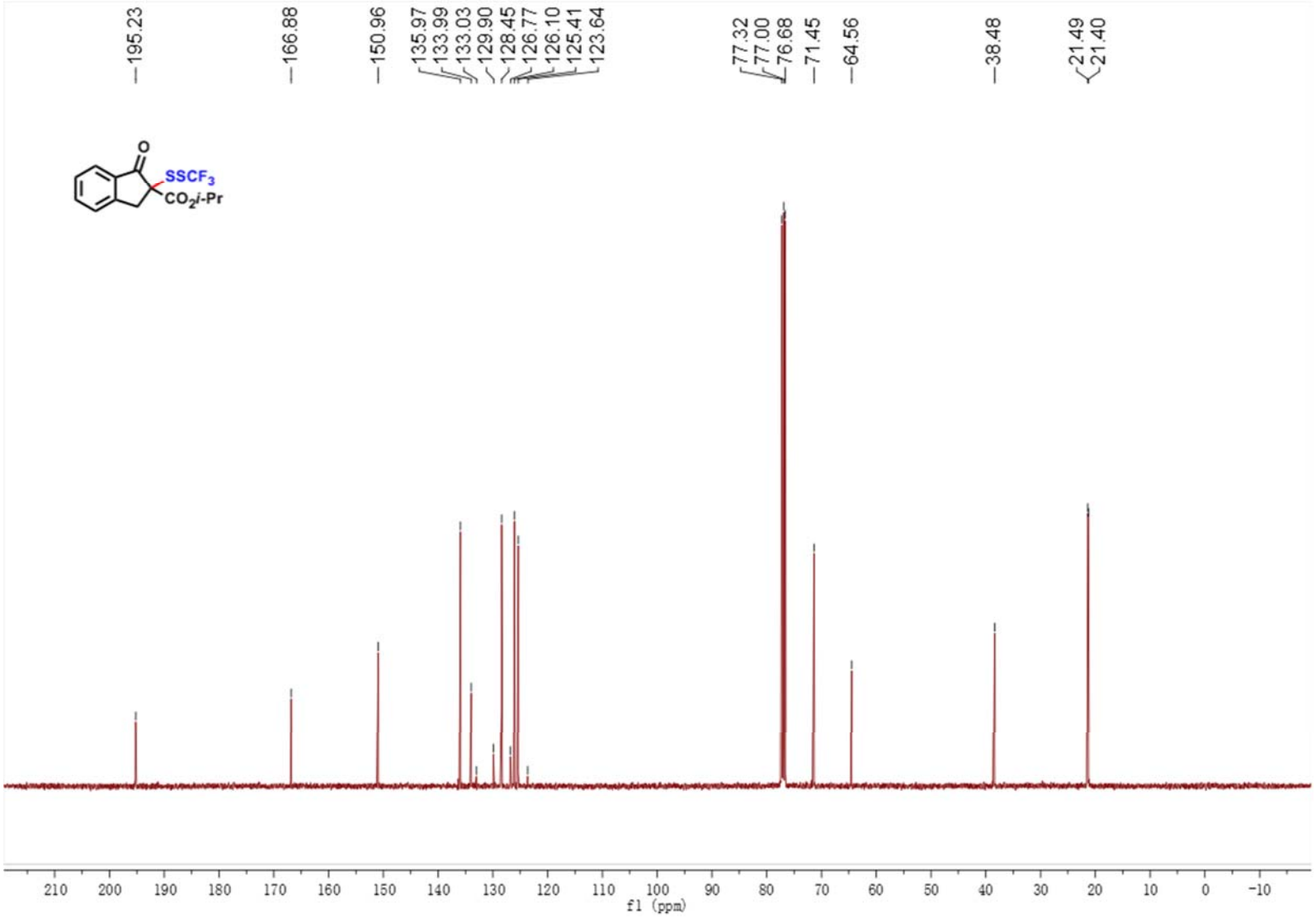
64.25
53.83
38.50
f1 (ppm)

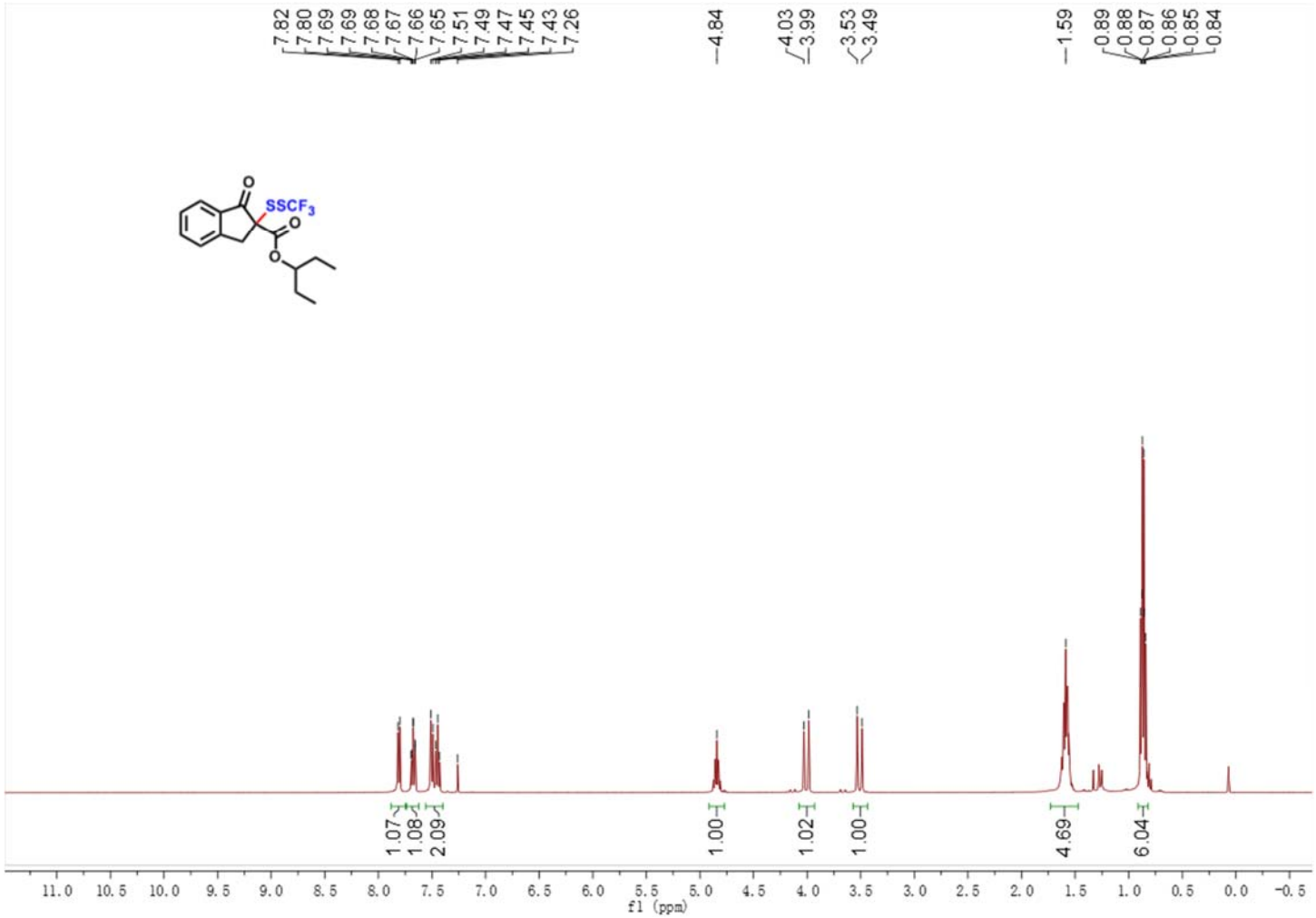
3b


7.82
7.80
7.68
7.67
7.66
7.65
7.51
7.49
7.47
7.45
7.26
5.11
5.09
5.07
4.02
3.98
3.51
3.46
1.27
1.25
SSCF3
CO2i-Pr
1.00
1.02
2.03
1.01
1.02
1.01
6.32
f1 (ppm)


-44.62
O
SSCF3
CO2i-Pr
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)


195.23
166.88
150.96
135.97
133.99
133.03
129.90
128.45
126.77
126.10
125.41
123.64
77.32
77.00
76.68
71.45
64.56
38.48
21.49
21.40
O
SSCF3
CO2i-Pr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3c


7.82
7.80
7.69
7.69
7.68
7.67
7.66
7.65
7.51
7.49
7.47
7.45
7.43
7.26
4.84
4.03
3.99
3.53
3.49
1.59
0.89
0.88
0.87
0.86
0.85
0.84
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1.07
1.08
2.09
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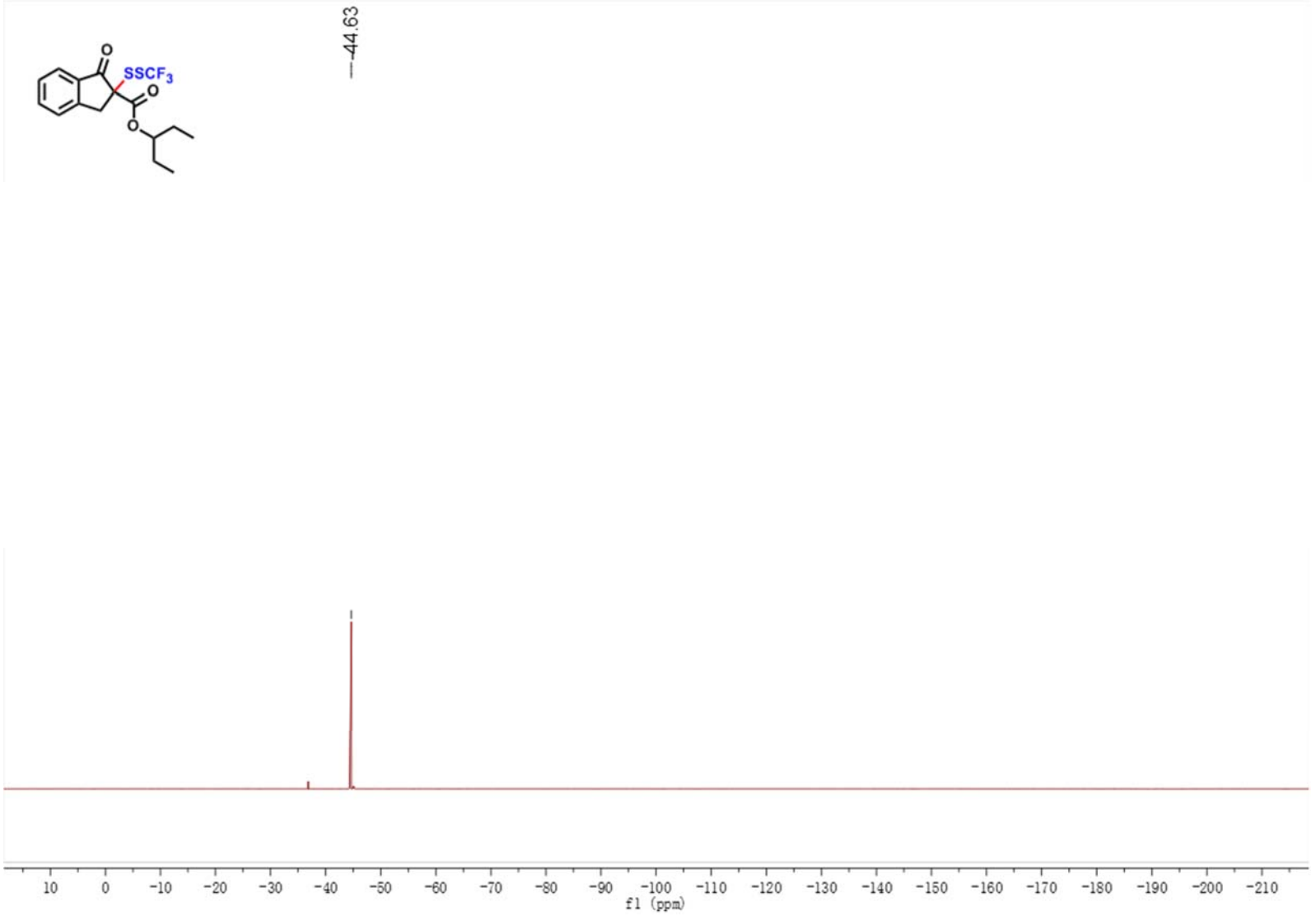
1.02
1.00
4.69
6.04
f1 (ppm)


SSCF3
O
O
O
-44.63
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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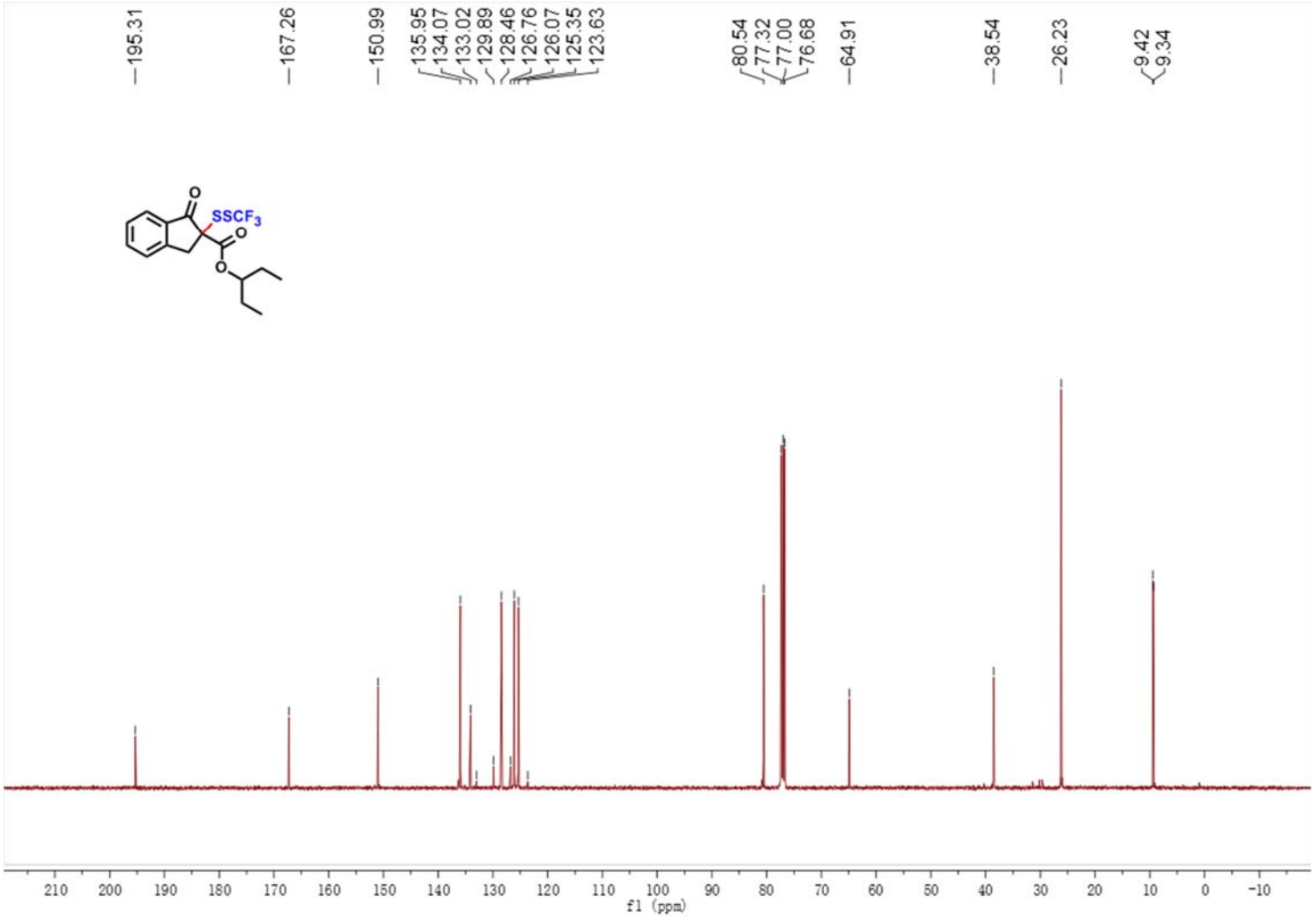
-170
-180
-190
-200
-210
f1 (ppm)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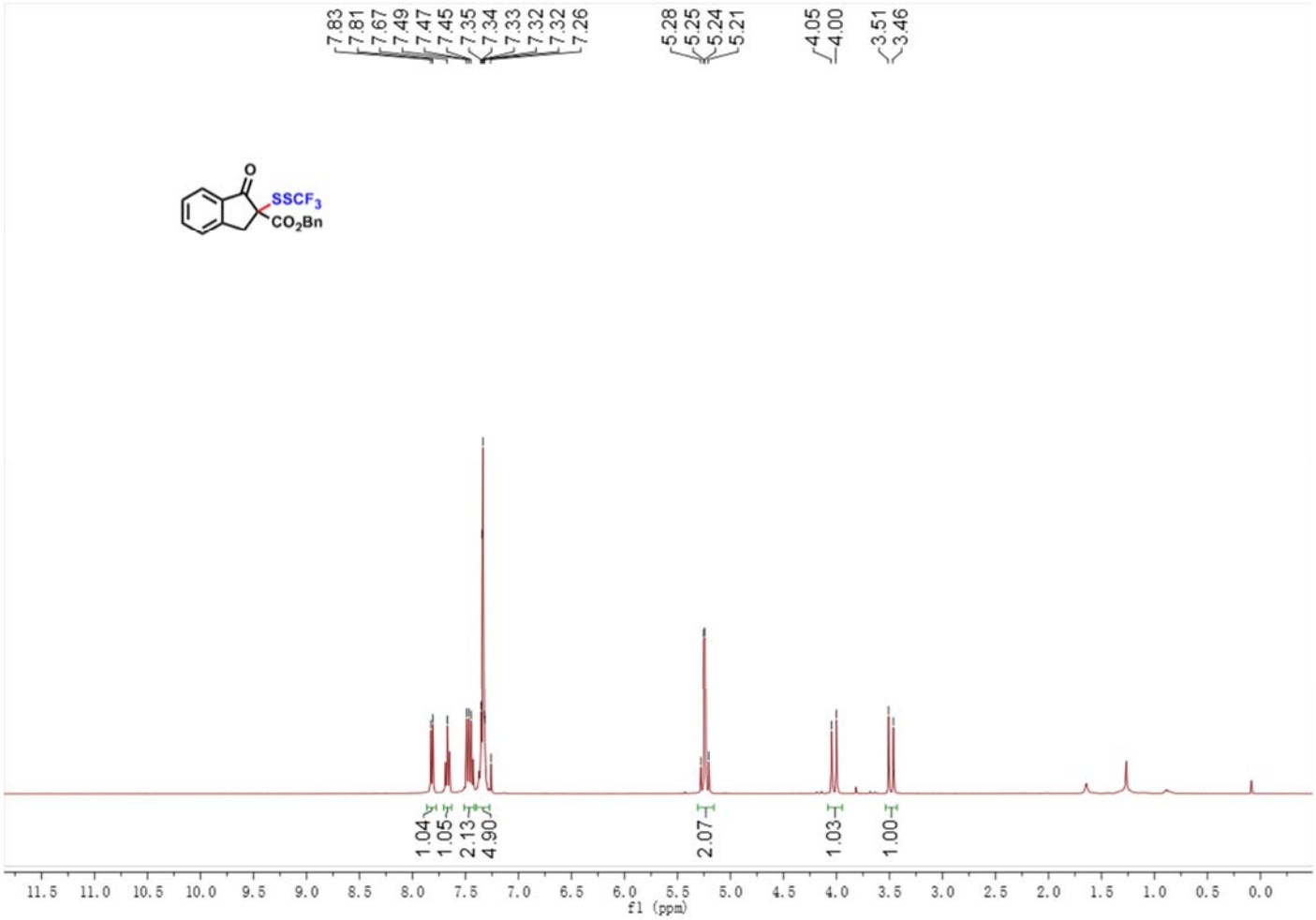
167.26
150.99
135.95
134.07
133.02
129.89
128.46
126.76
126.07
125.35
123.63
80.54
77.32
77.00
76.68
64.91
38.54
26.23
9.42
9.34
SSCF3
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3d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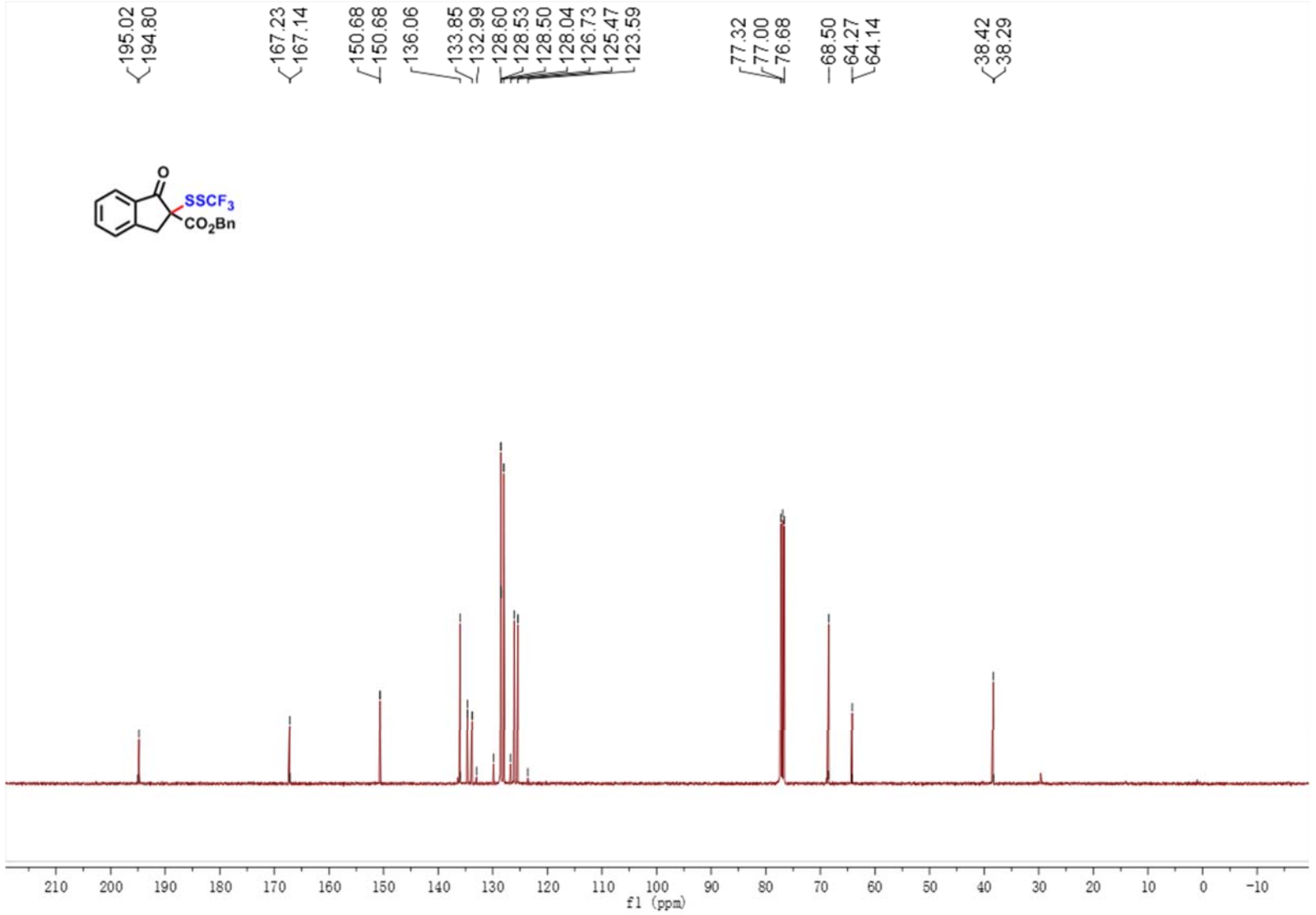
7.45
7.35
7.34
7.33
7.32
7.32
7.26
5.28
5.25
5.24
5.21
4.05
4.00
3.51
3.46
O
SSCF3
CO2Bn
1.04
1.05
2.13
4.90
2.07
1.03
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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194.80
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128.04
126.73
125.47
123.59
77.32
77.00
76.68
68.50
64.27
64.14
38.42
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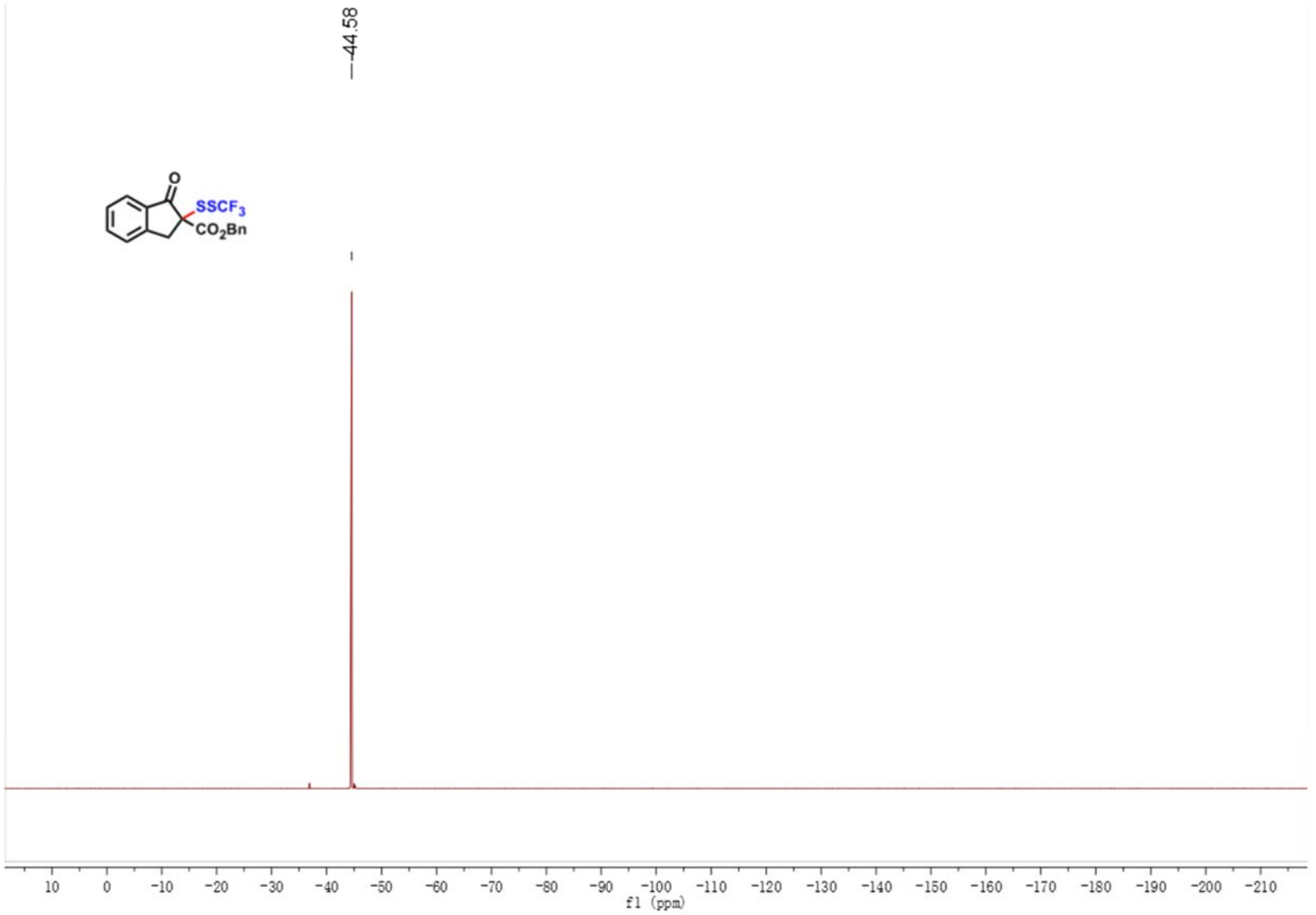
O
SSCF3
CO2Bn
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-44.58
O
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CO2Bn
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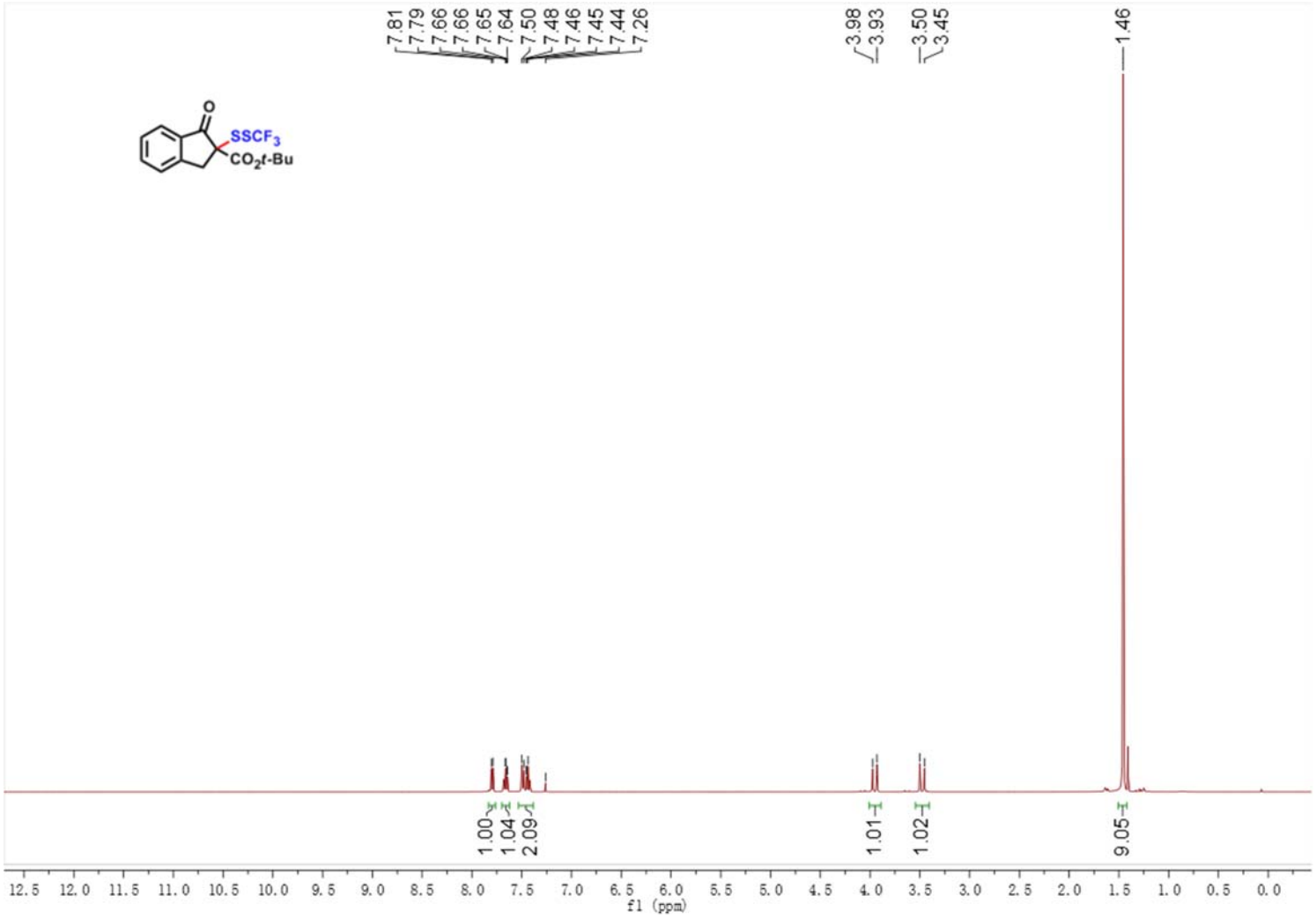
f1 (ppm)

3e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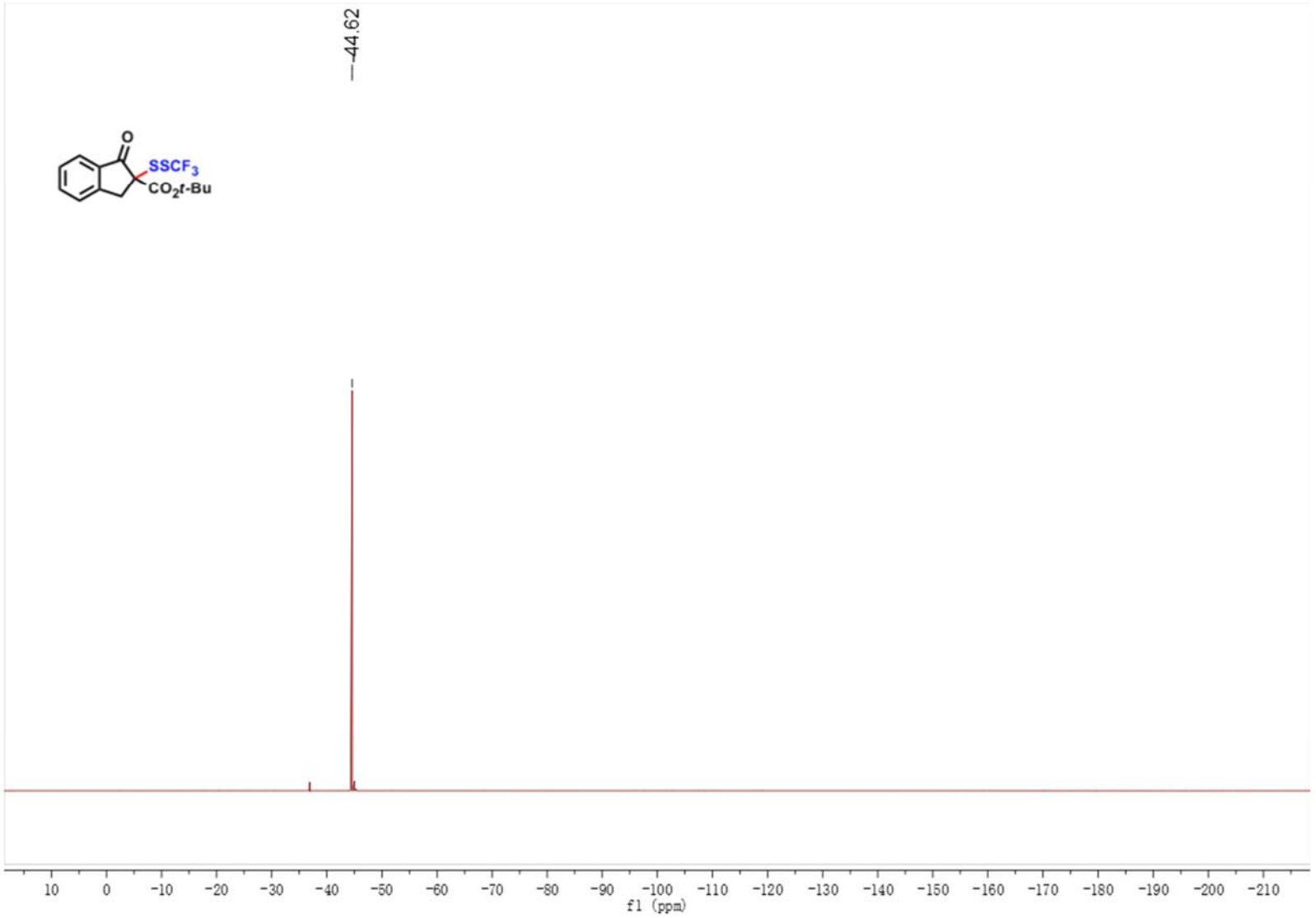
7.66
7.65
7.64
7.50
7.48
7.46
7.45
7.44
7.26
3.98
3.93
3.50
3.45
1.46
SSCF3
CO2t-Bu
1.00
1.04
2.09
1.01
1.02
9.05
f1 (ppm)


-44.62
O
SSCF3
CO2t-Bu
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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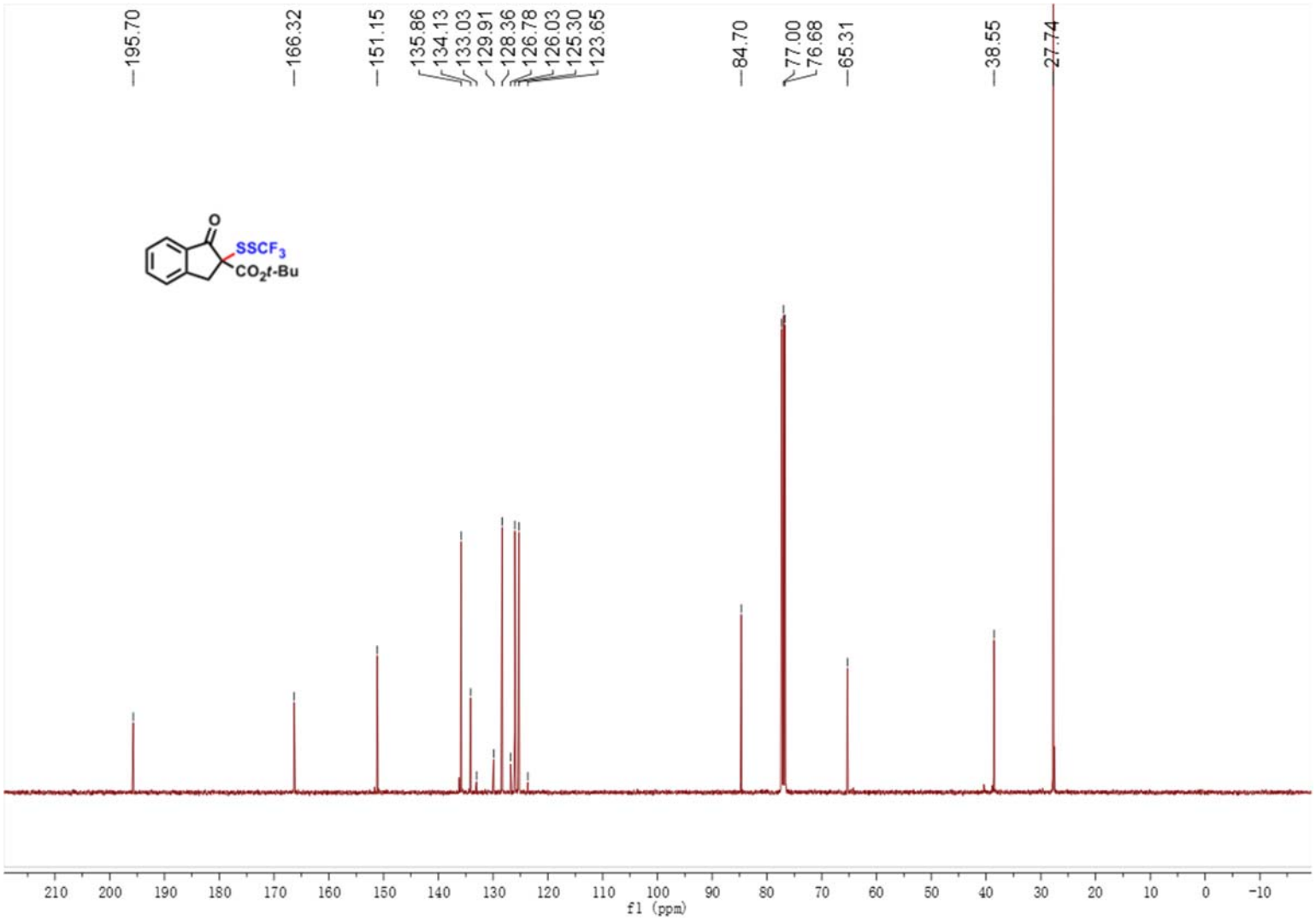
-170
-180
-190
-200
-210
f1 (ppm)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151.15
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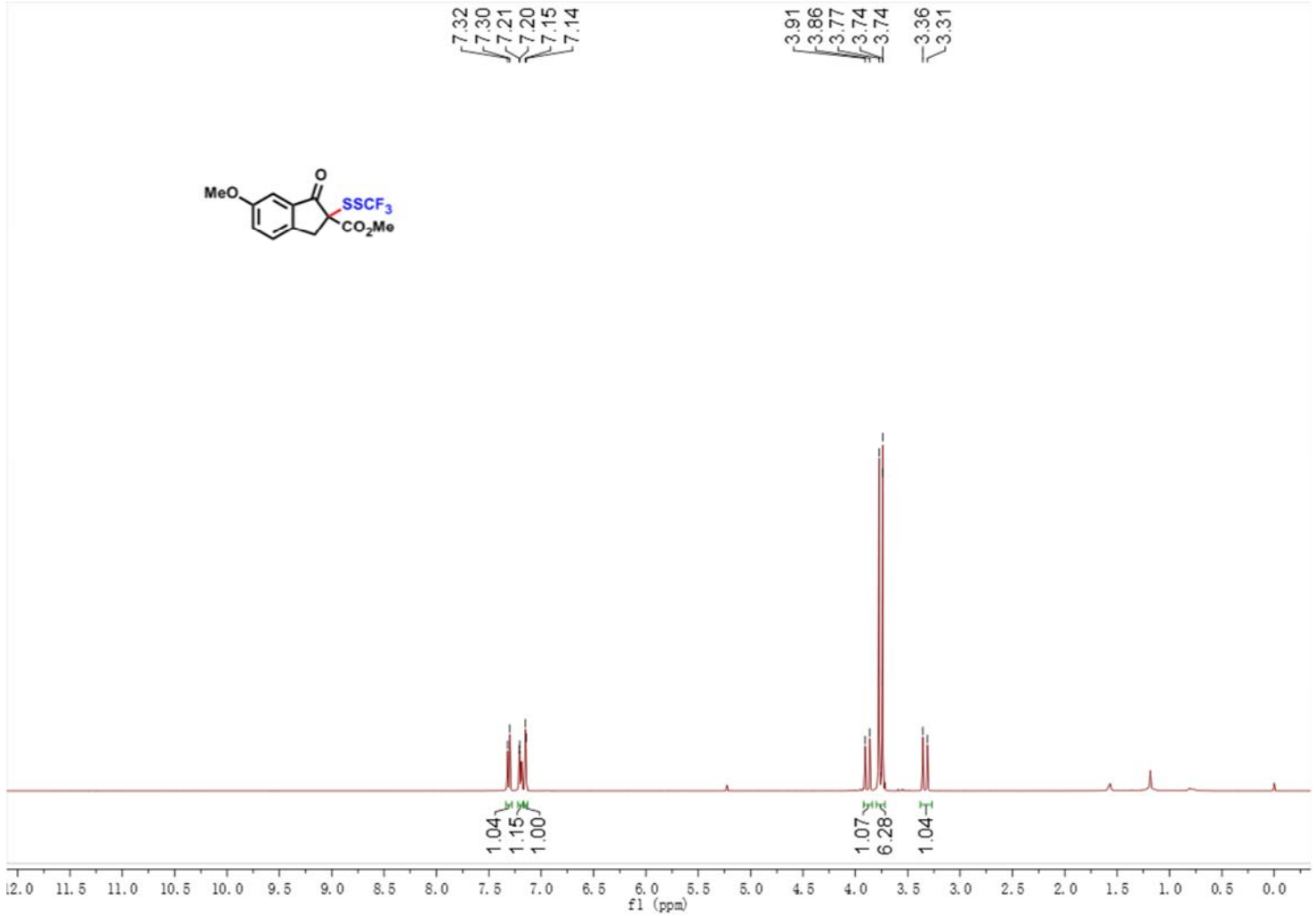
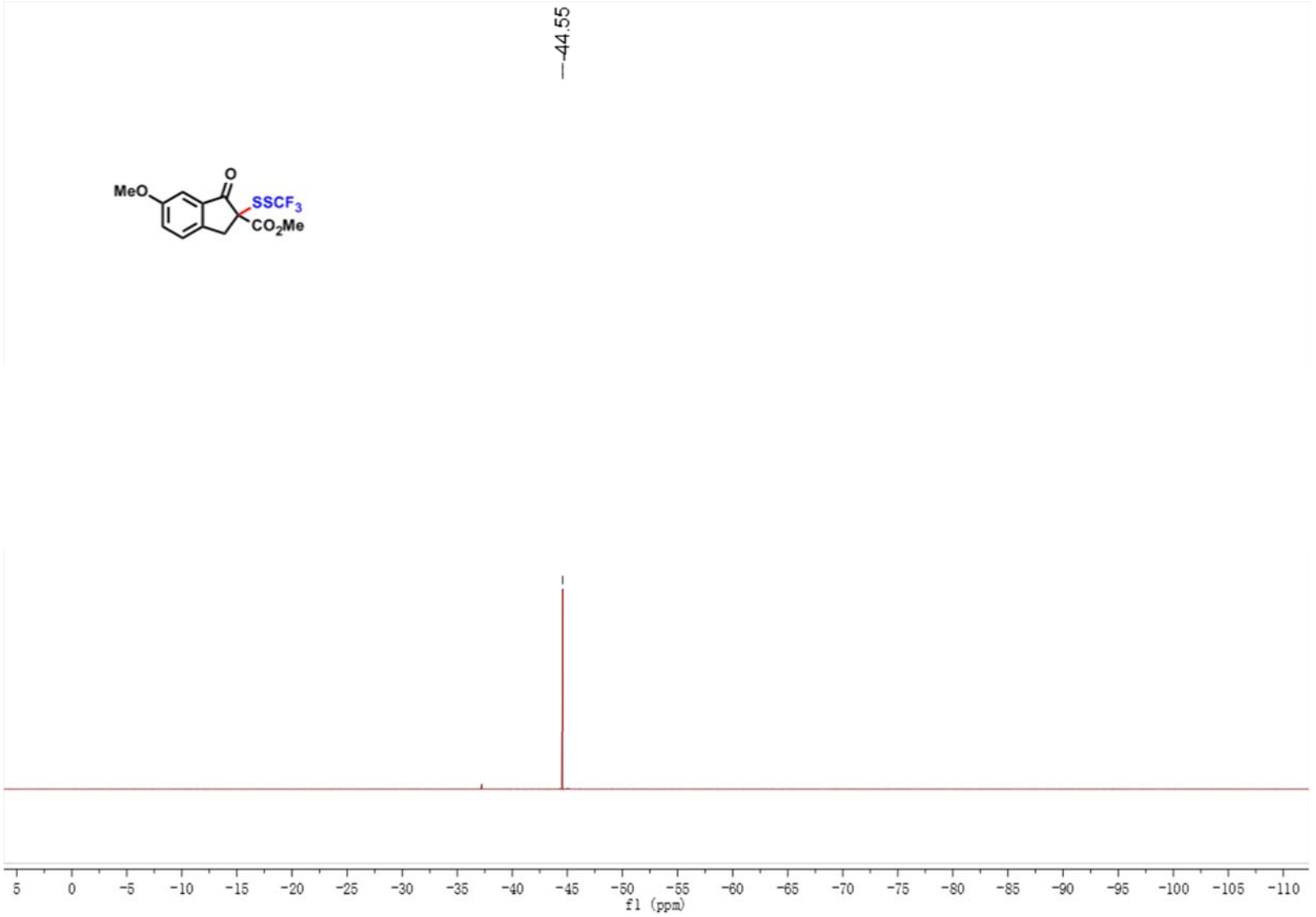
134.13
133.03
129.91
128.36
126.78
126.03
125.30
123.65
84.70
77.00
76.68
65.31
38.55
27.74
O
SSCF3
CO2t-Bu
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3f


7.32
7.30
7.21
7.20
7.15
7.14
3.91
3.86
3.77
3.74
3.74
3.36
3.31
MeO
O
SSCF3
CO2Me
1.04
1.15
1.00
1.07
6.28
1.04
f1 (ppm)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MeO
O
SSCF3
CO2Me
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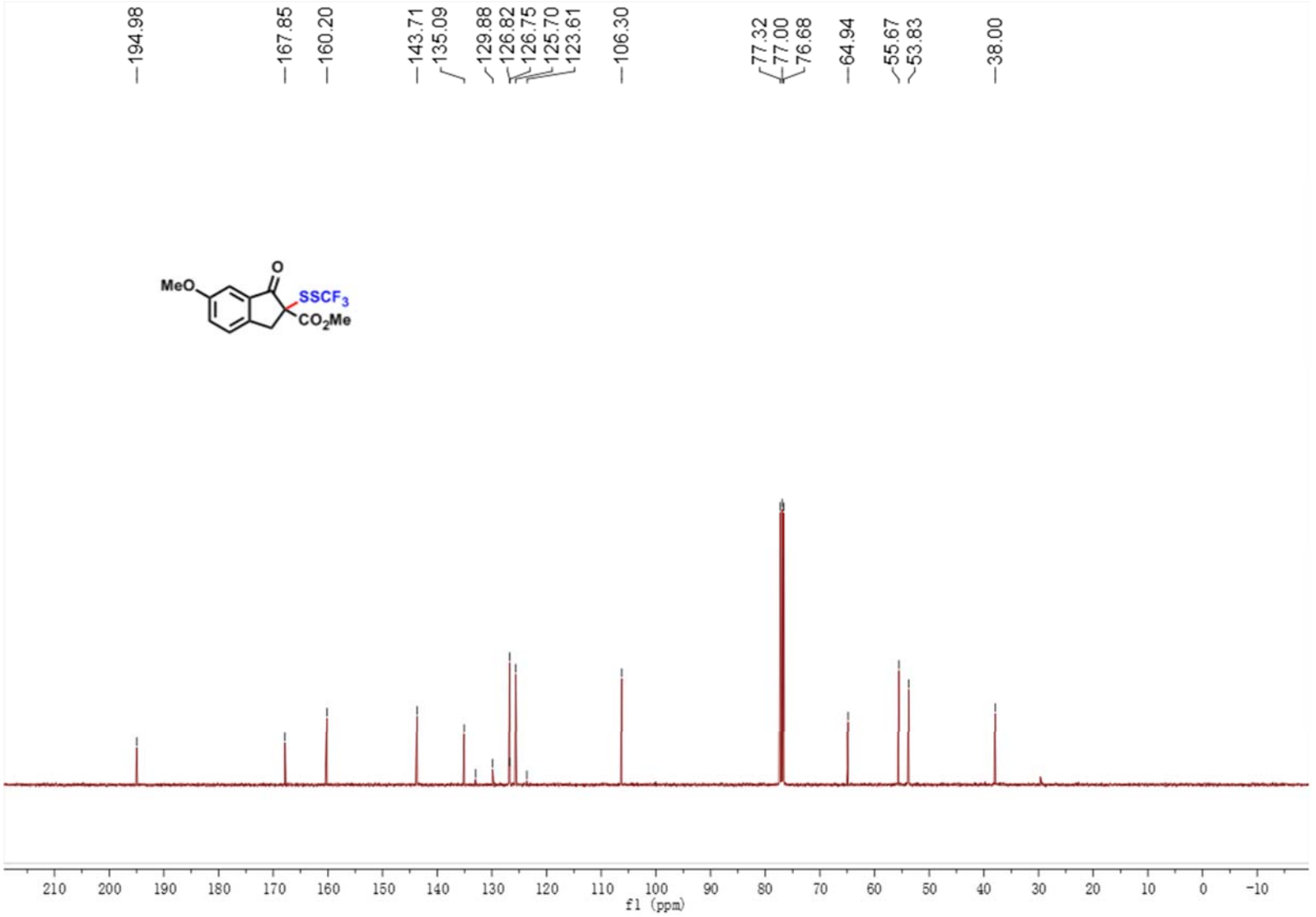
-110
f1 (ppm)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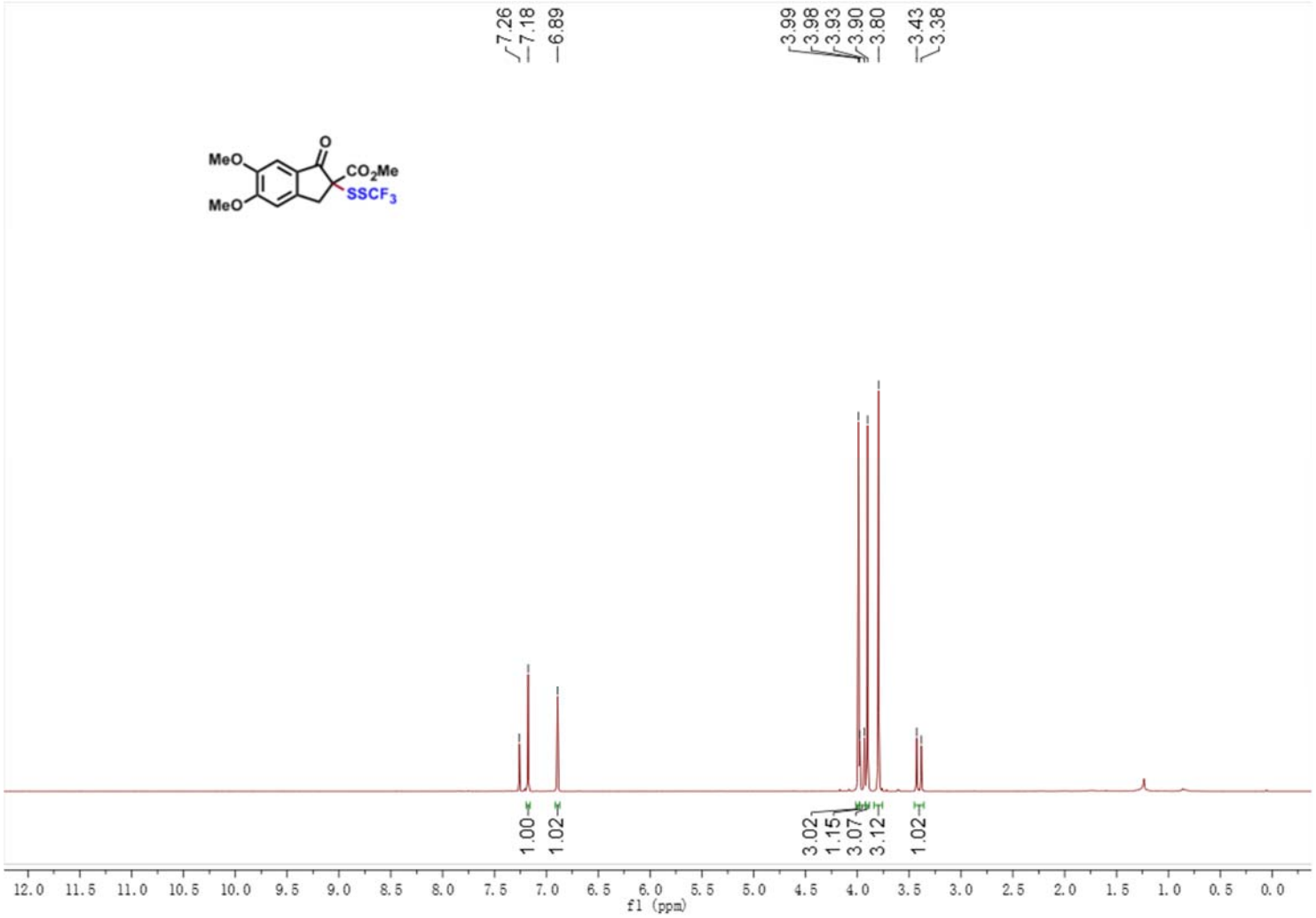
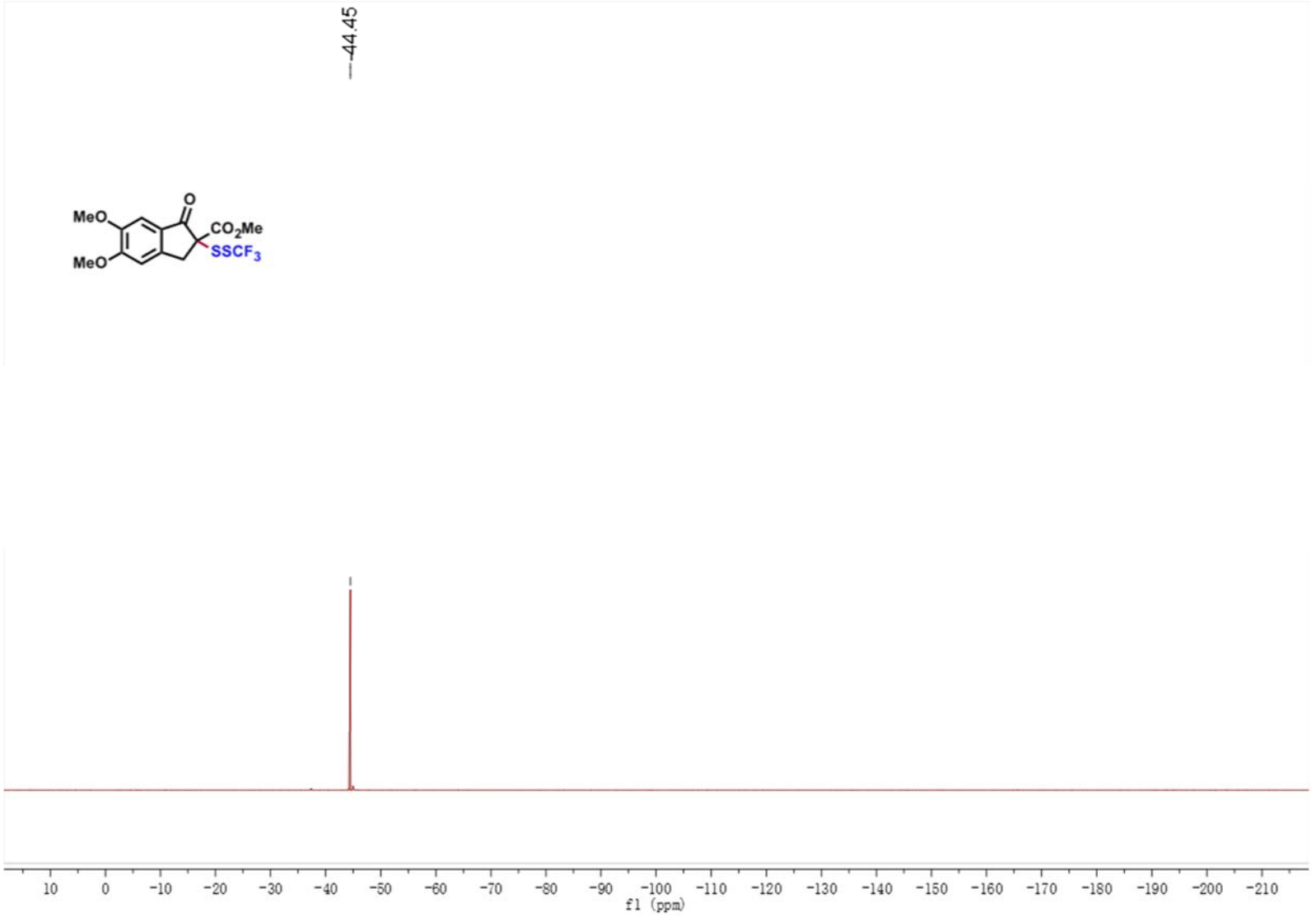
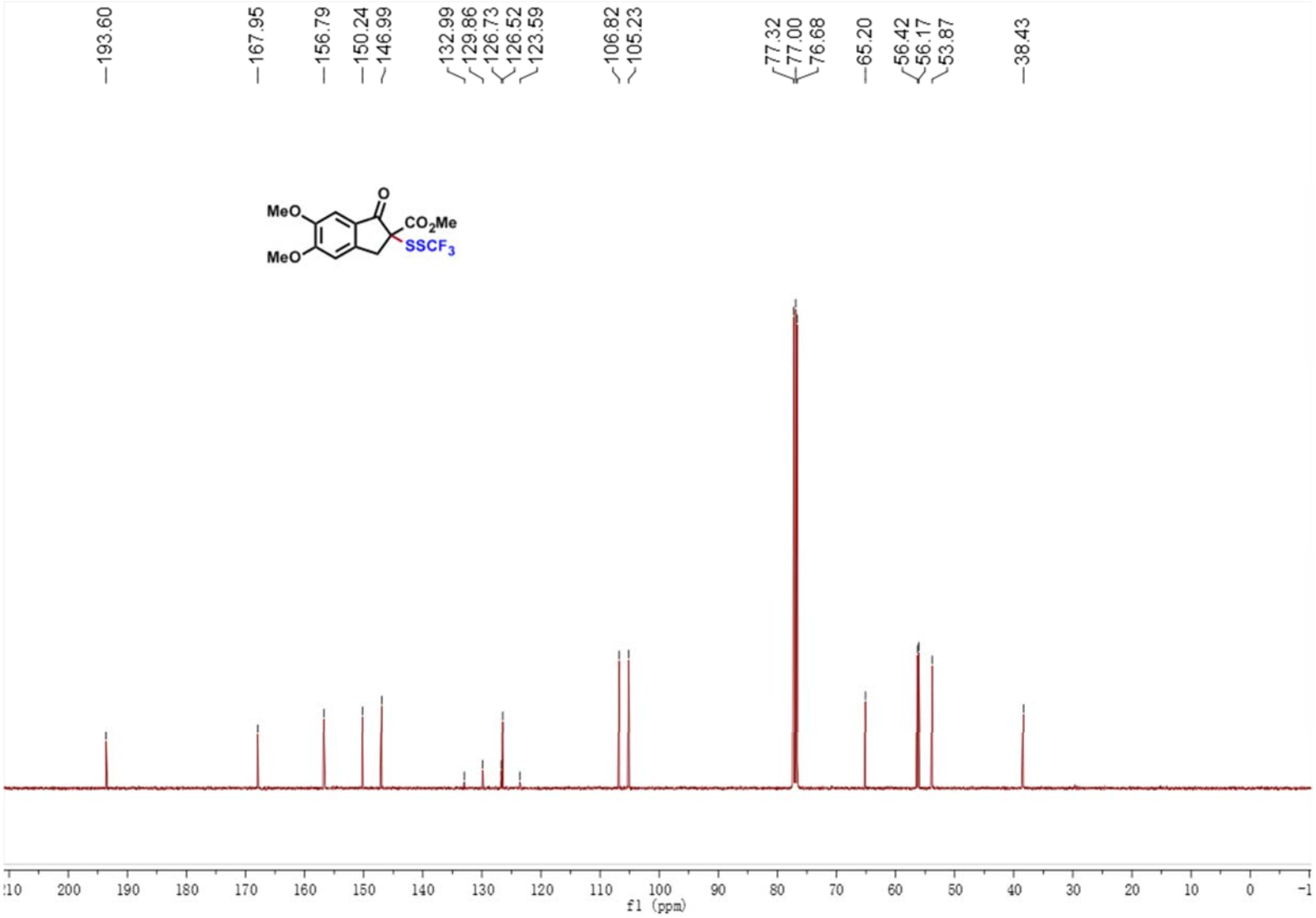
126.75
125.70
123.61
106.30
77.32
77.00
76.68
64.94
55.67
53.83
38.00
MeO
O
SSCF3
CO2Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

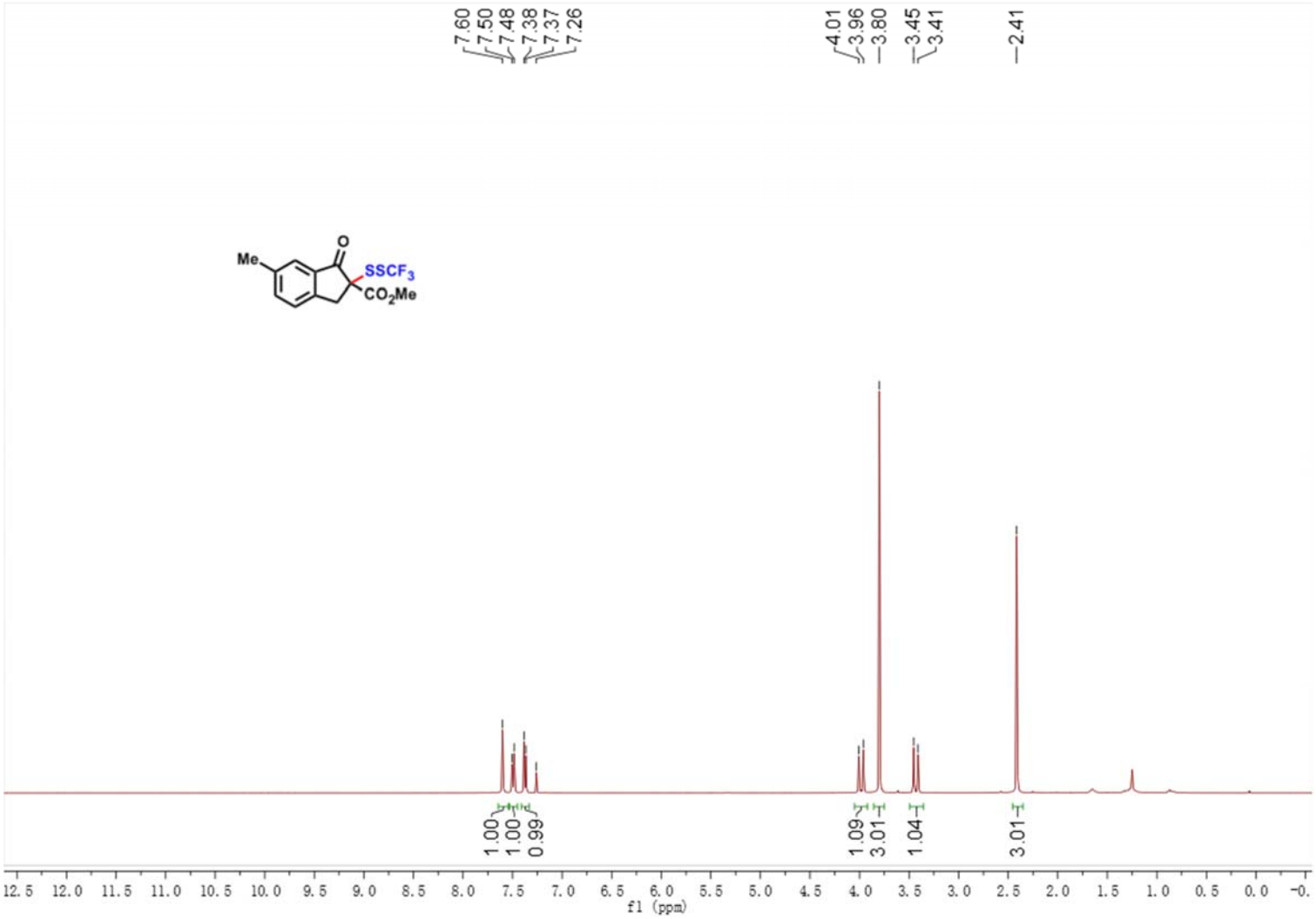
3g

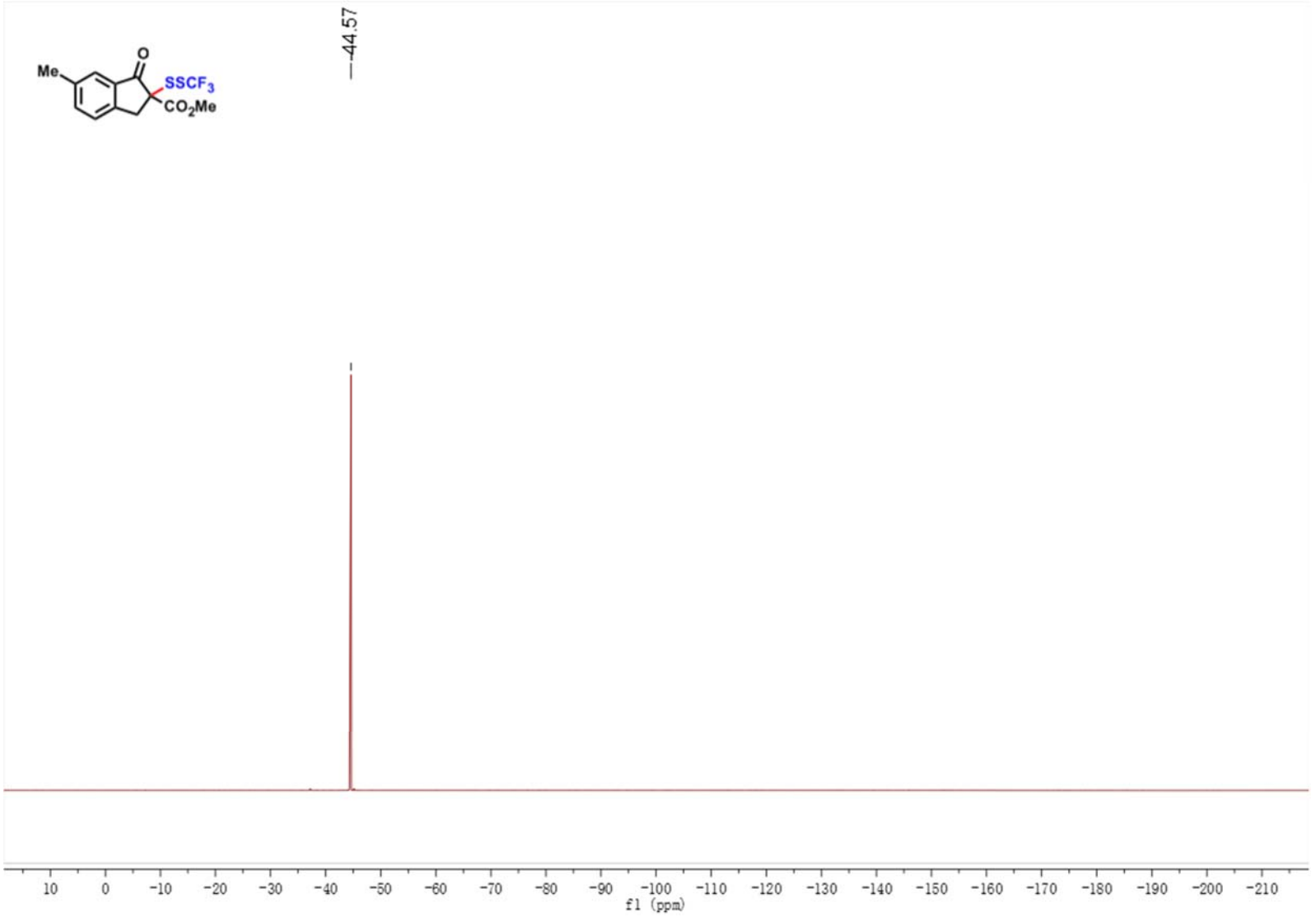

7.26
7.18
6.89
3.99
3.98
3.93
3.90
3.80
3.43
3.38
MeO
MeO
O
CO2Me
SSCF3
1.00
1.02
3.02
1.15
3.07
3.12
1.02
f1 (ppm)

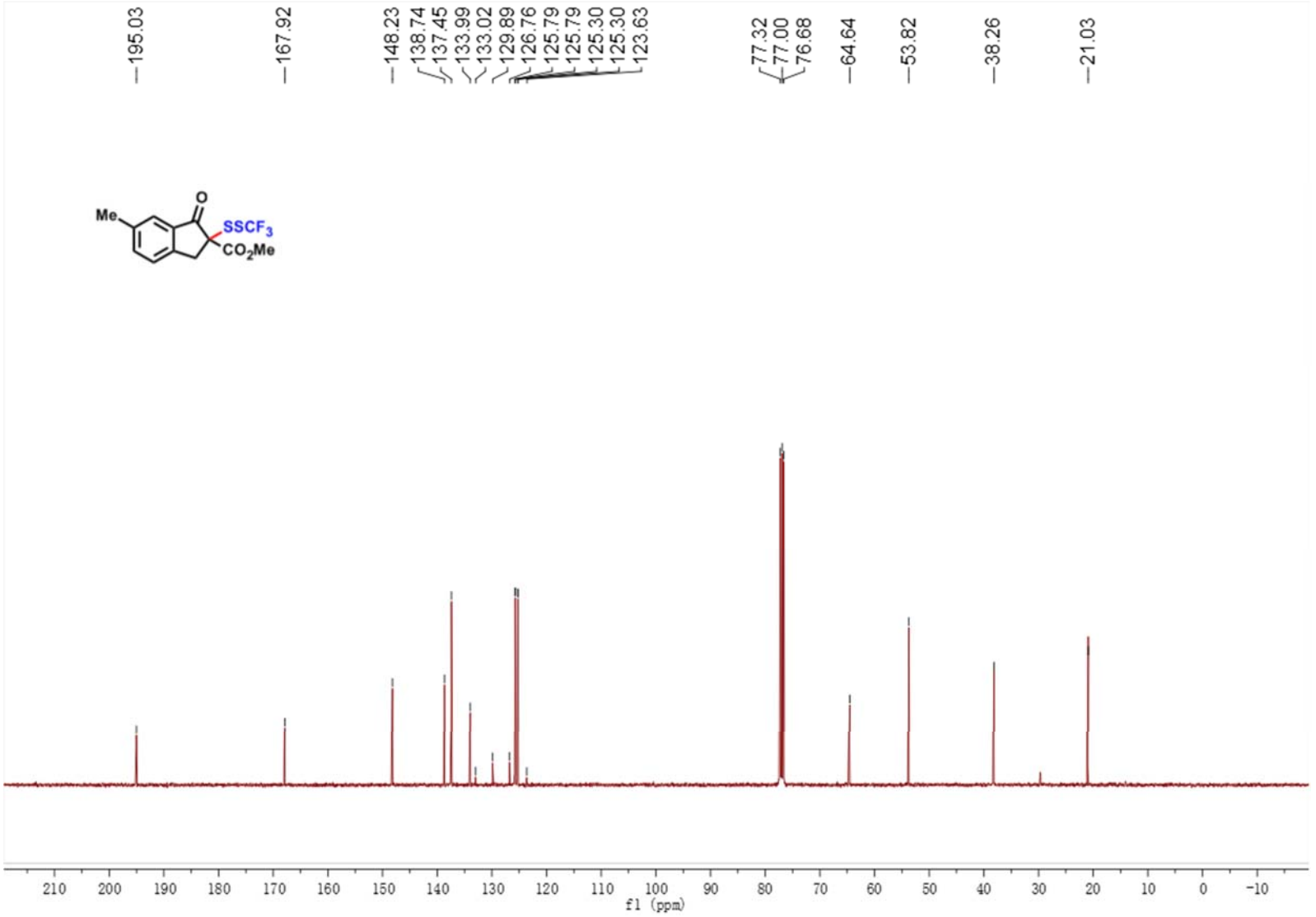

-44.45
MeO
MeO
O
CO2Me
SSCF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


193.60
167.95
156.79
150.24
146.99
132.99
129.86
126.73
126.52
123.59
106.82
105.23
77.32
77.00
76.68
65.20
56.42
56.17
53.87
38.43
MeO
MeO
O
CO2Me
SSCF3
f1 (ppm)

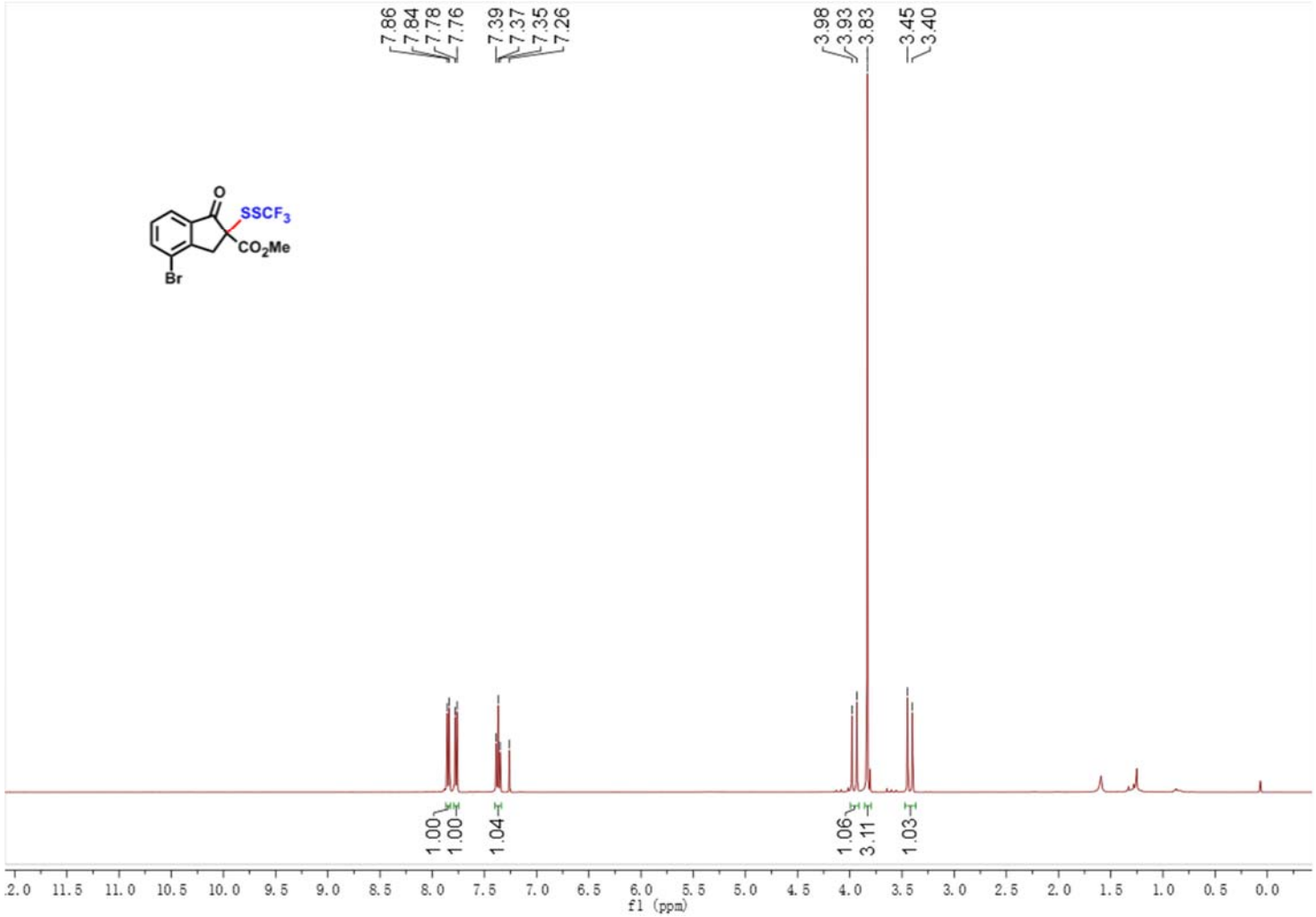
3h

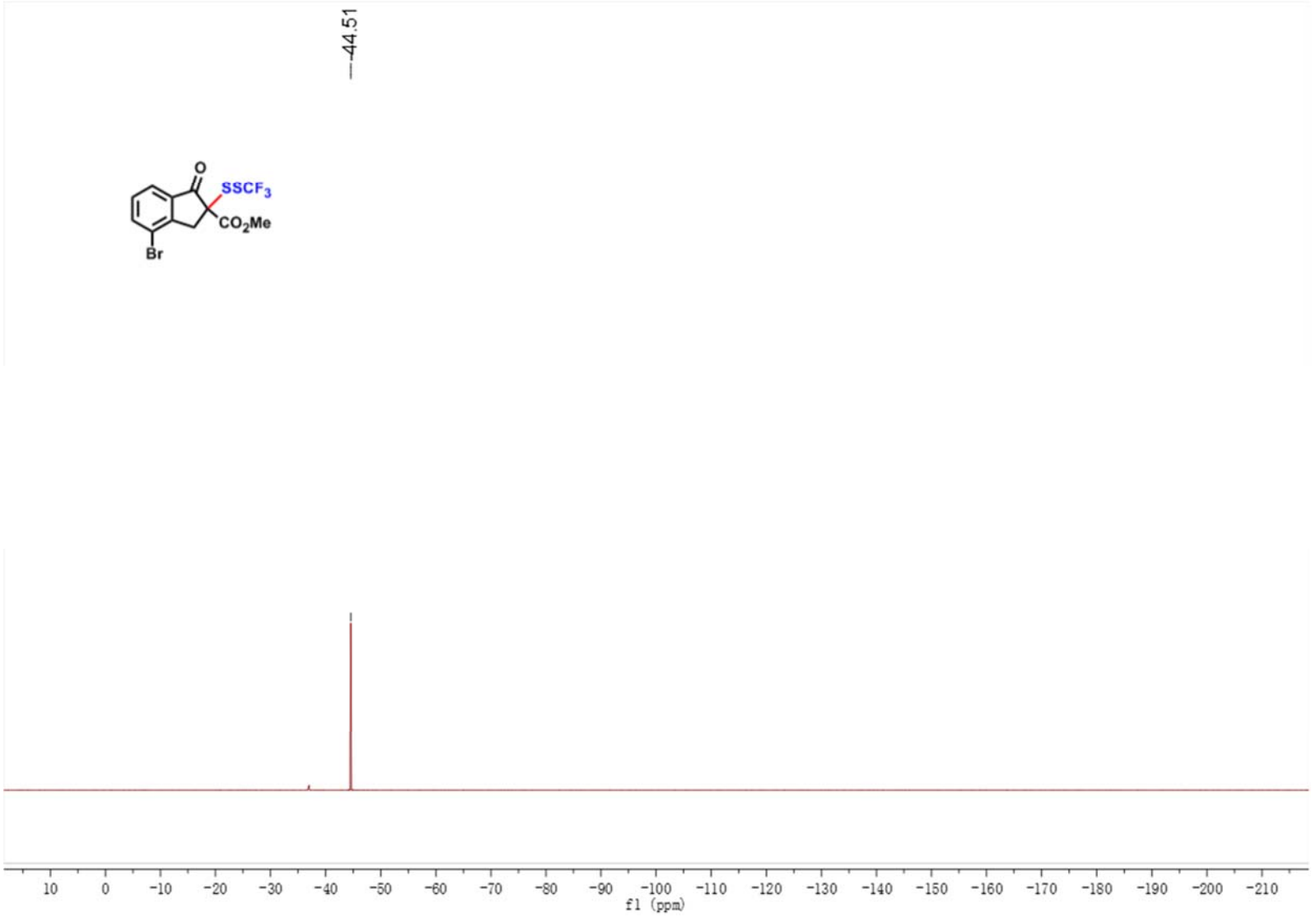

7.60
7.50
7.48
7.38
7.37
7.26
4.01
3.96
3.80
3.45
3.41
2.41
Me
O
SSCF3
CO2Me
1.00
1.00
0.99
1.09
3.01
1.04
3.01
f1 (ppm)


Me
O
SSCF3
CO2Me
-44.57
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)


195.03
167.92
148.23
138.74
137.45
133.99
133.02
129.89
126.76
125.79
125.79
125.30
125.30
123.63
77.32
77.00
76.68
64.64
53.82
38.26
21.03
Me
O
SSCF3
CO2Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3i


7.86
7.84
7.78
7.76
7.39
7.37
7.35
7.26
3.98
3.93
3.83
3.45
3.40
O
SSCF3
CO2Me
Br
1.00
1.00
1.04
1.06
3.11
1.03
f1 (ppm)


-44.51
O
SSCF3
CO2Me
Br
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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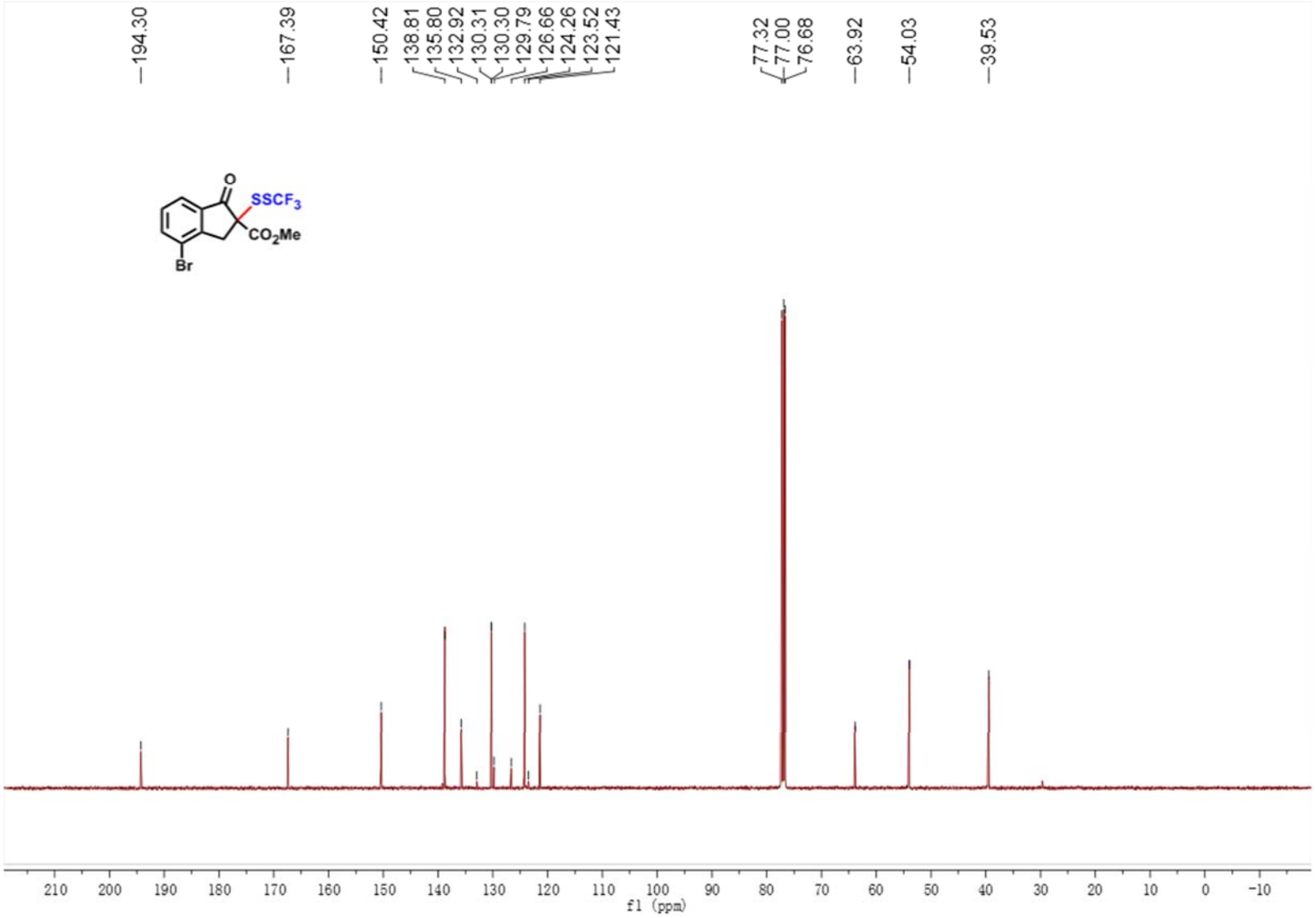
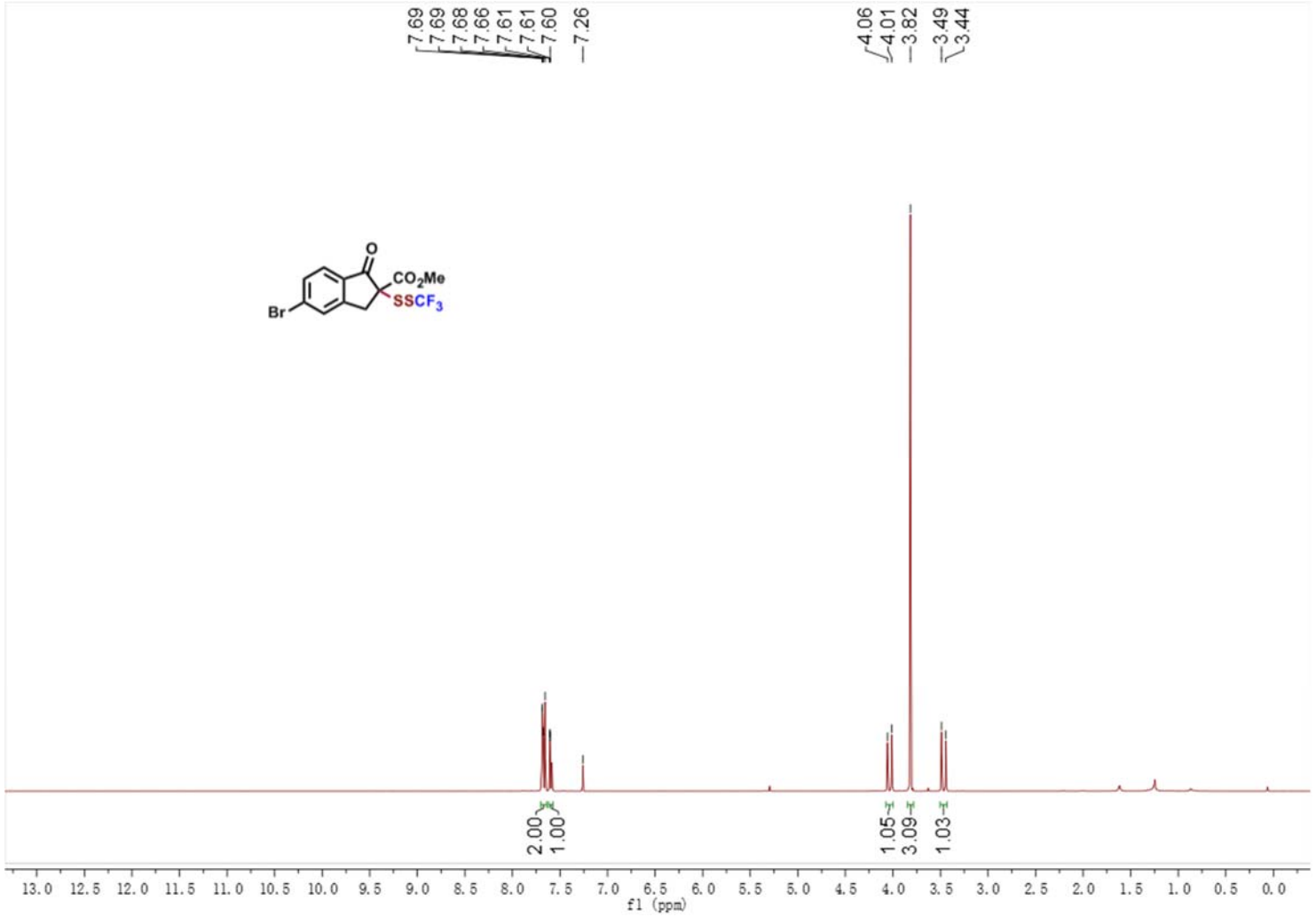
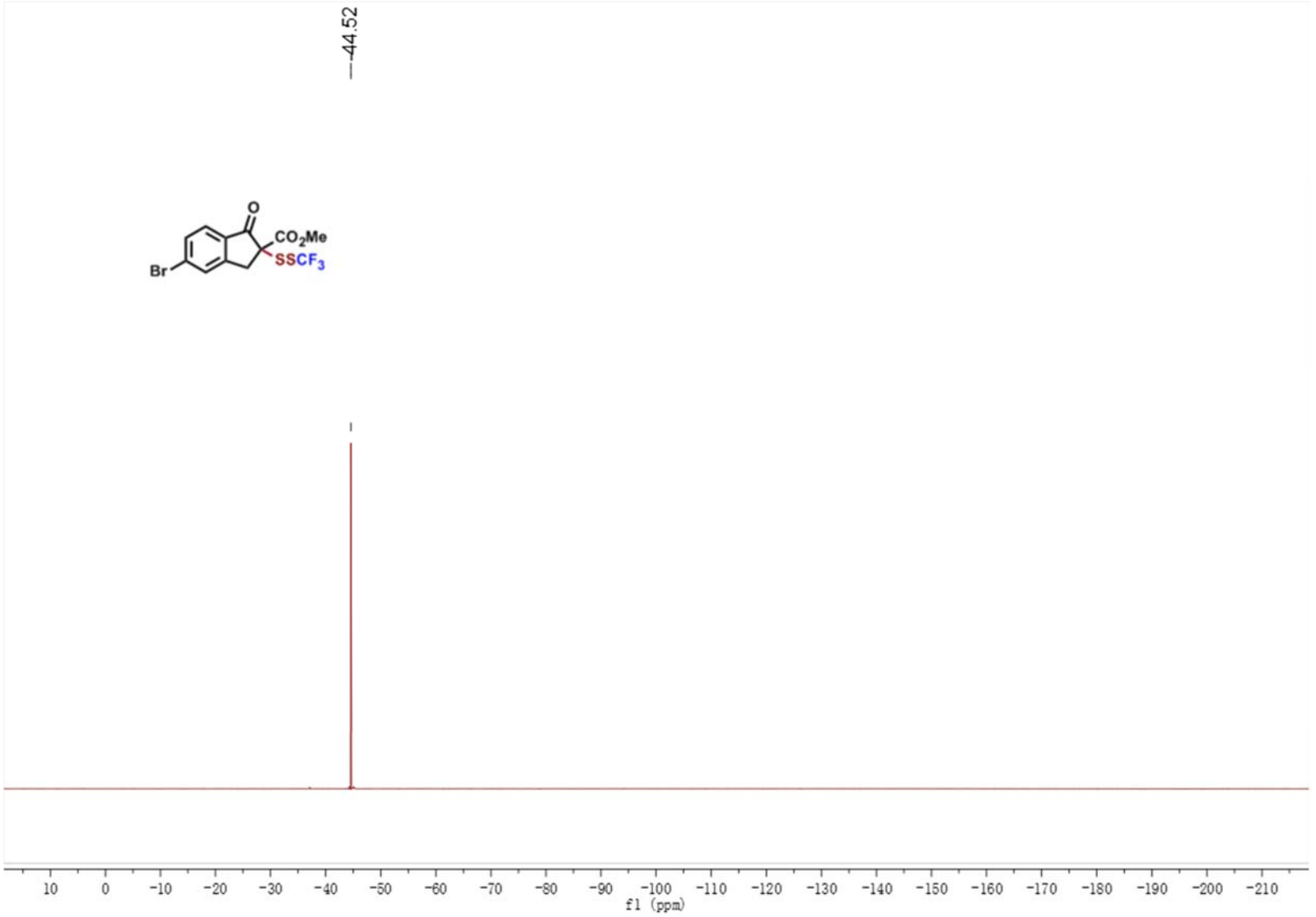
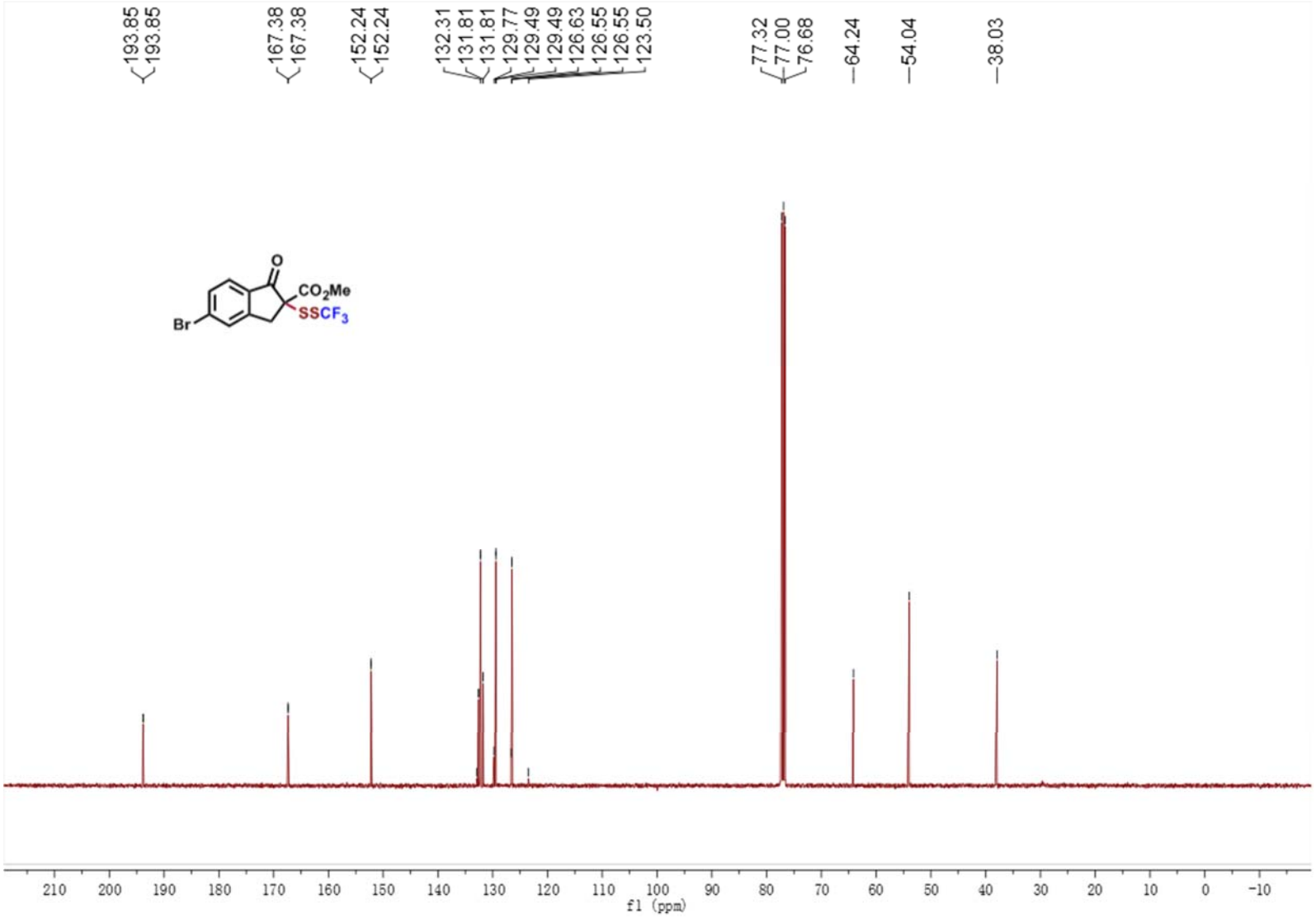
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


194.30
167.39
150.42
138.81
135.80
132.92
130.31
130.30
129.79
126.66
124.26
123.52
121.43
77.32
77.00
76.68
63.92
54.03
39.53
O
SSCF3
CO2Me
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

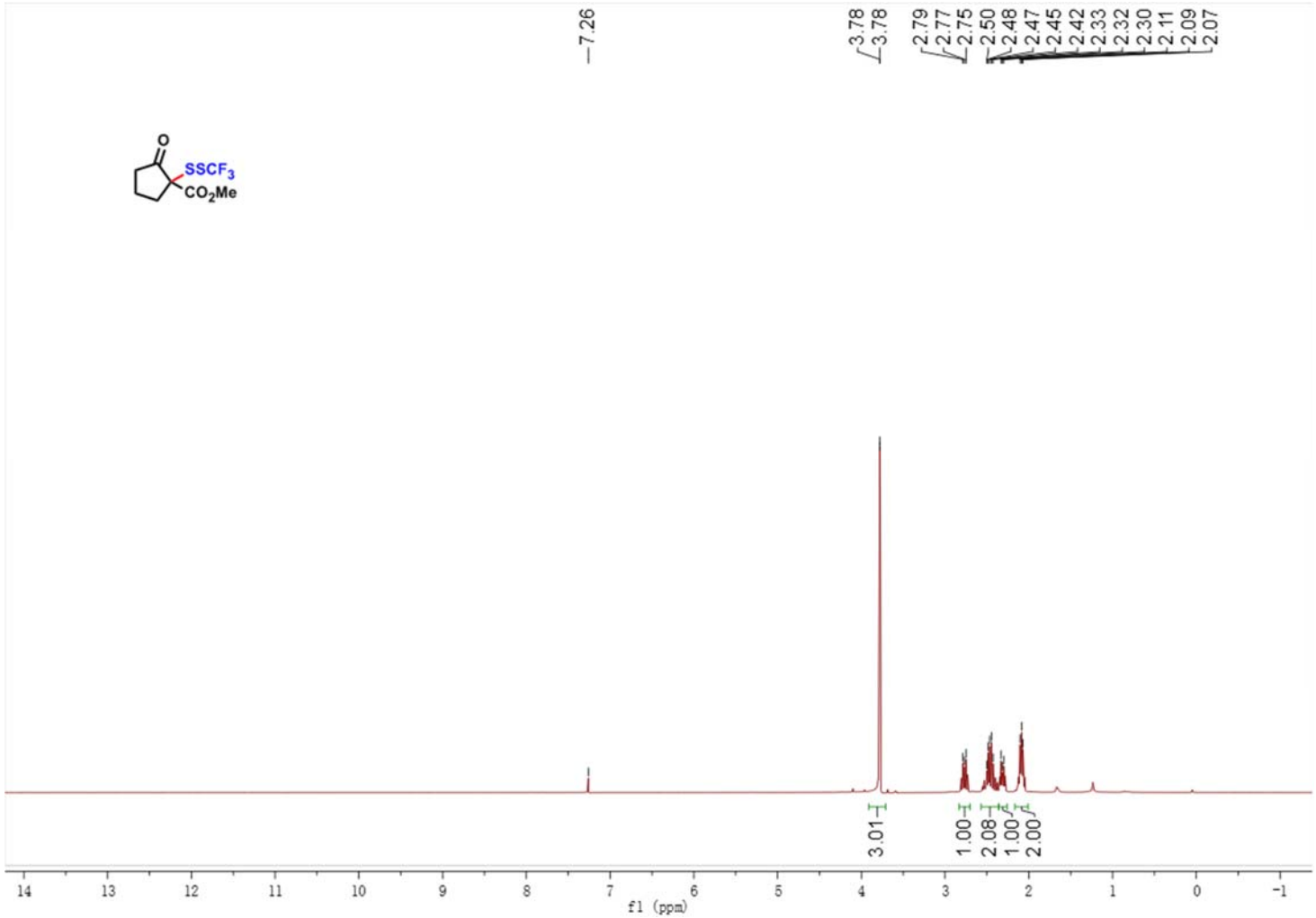
3j

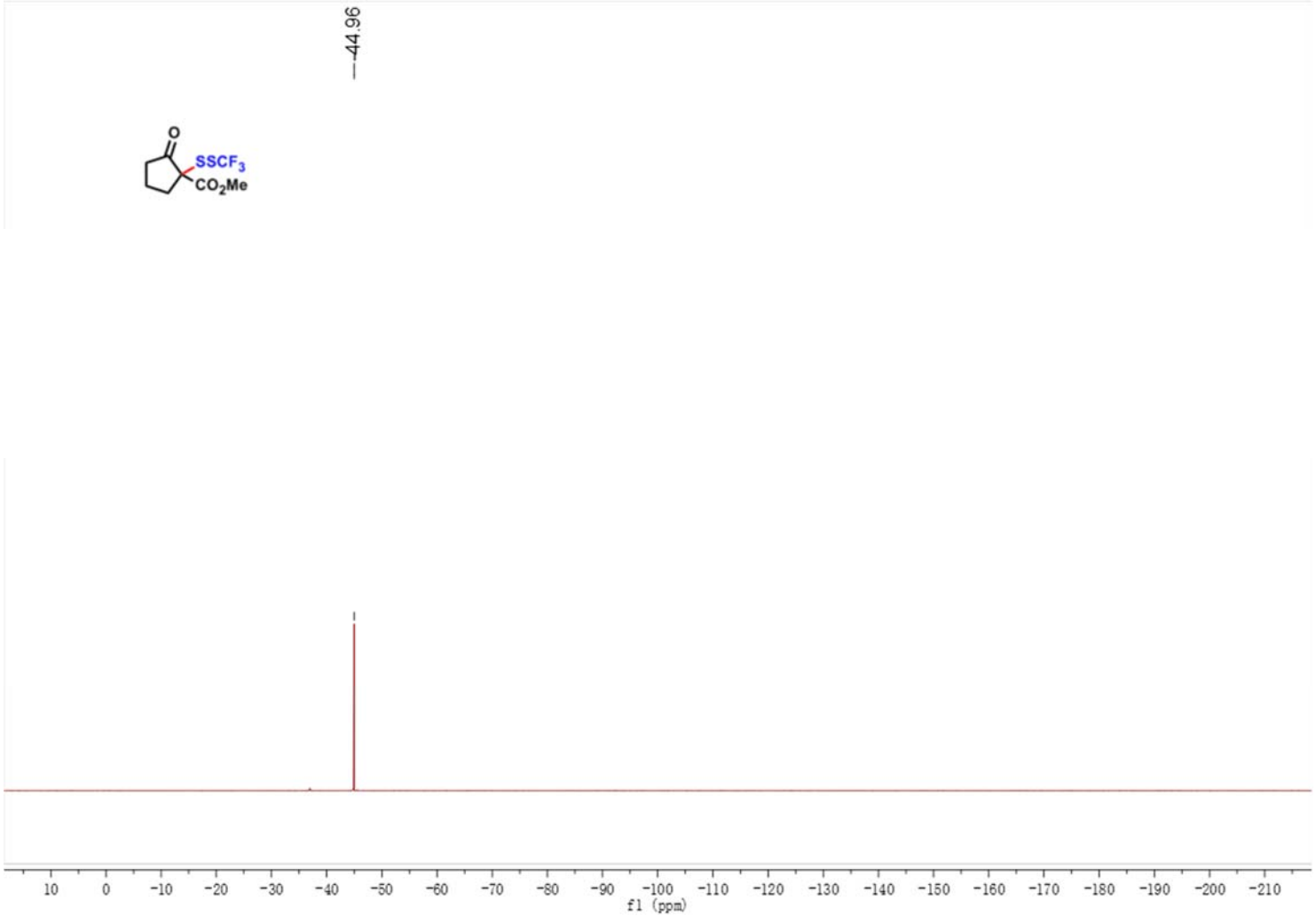

7.69
7.69
7.68
7.66
7.61
7.61
7.60
7.26
4.06
4.01
3.82
3.49
3.44
O
CO2Me
SSCF3
Br
2.00
1.00
1.05
3.09
1.03
f1 (ppm)

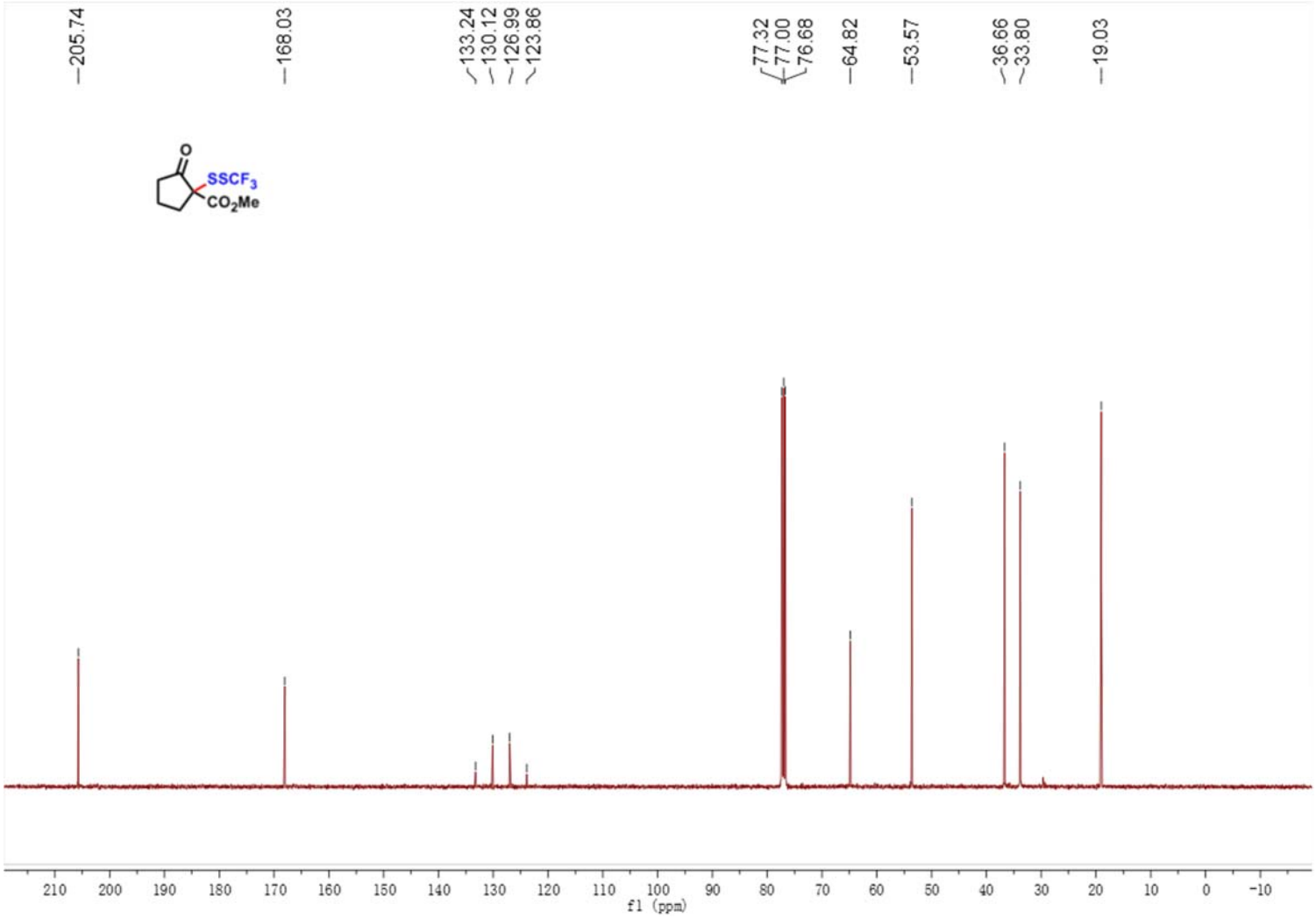

-44.52
O
CO2Me
SSCF3
Br
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


193.85
193.85
167.38
167.38
152.24
152.24
132.31
131.81
131.81
129.77
129.49
129.49
126.63
126.55
126.55
123.50
77.32
77.00
76.68
64.24
54.04
38.03
O
CO2Me
SSCF3
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

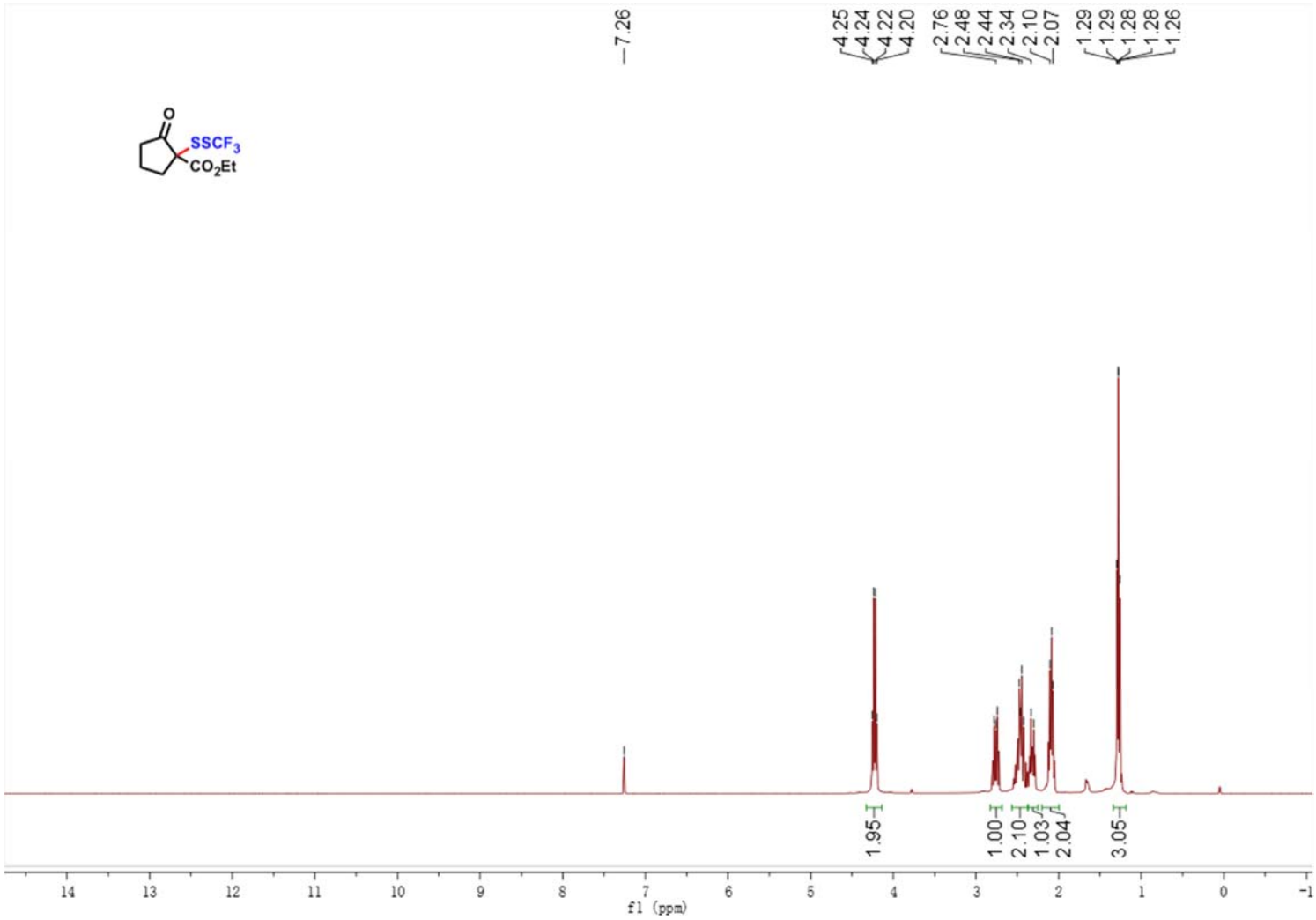
3k

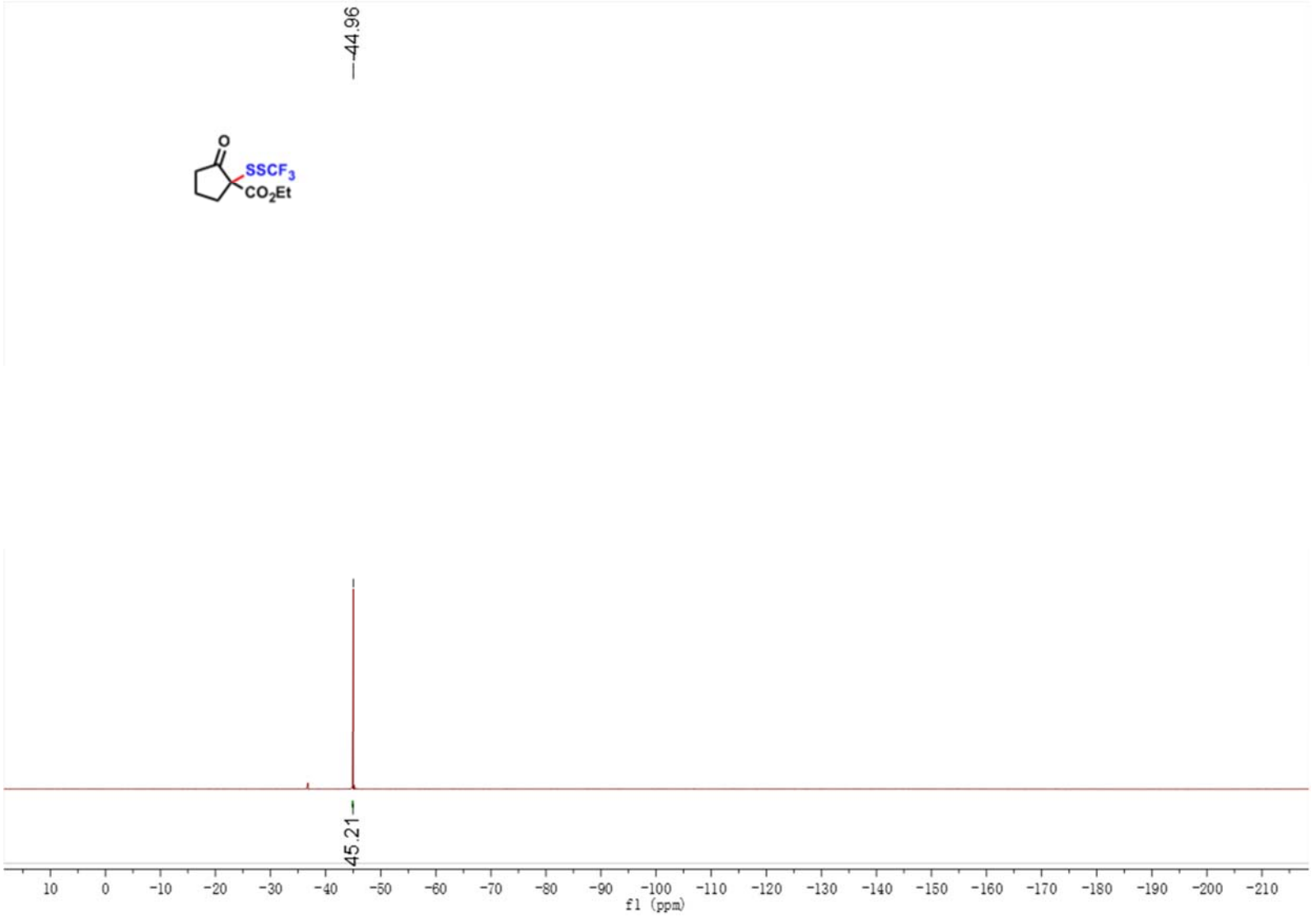

7.26
3.78
3.78
2.79
2.77
2.75
2.50
2.48
2.47
2.45
2.42
2.33
2.32
2.30
2.11
2.09
2.07
O
SSCF3
CO2Me
3.01
1.00
2.08
1.00
2.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

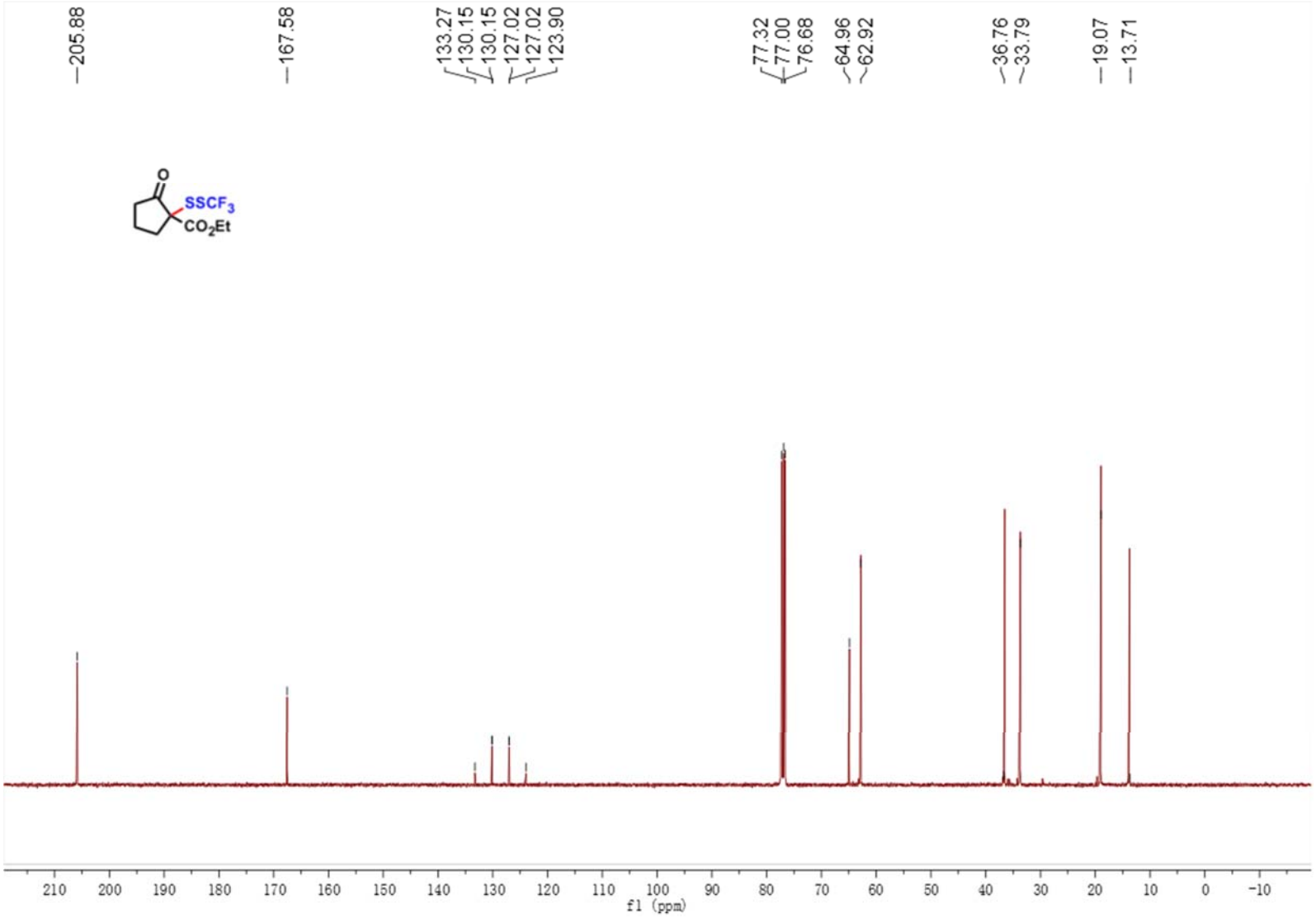

-44.96
O
SSCF3
CO2Me
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


205.74
168.03
133.24
130.12
126.99
123.86
77.32
77.00
76.68
64.82
53.57
36.66
33.80
19.03
O
SSCF3
CO2Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

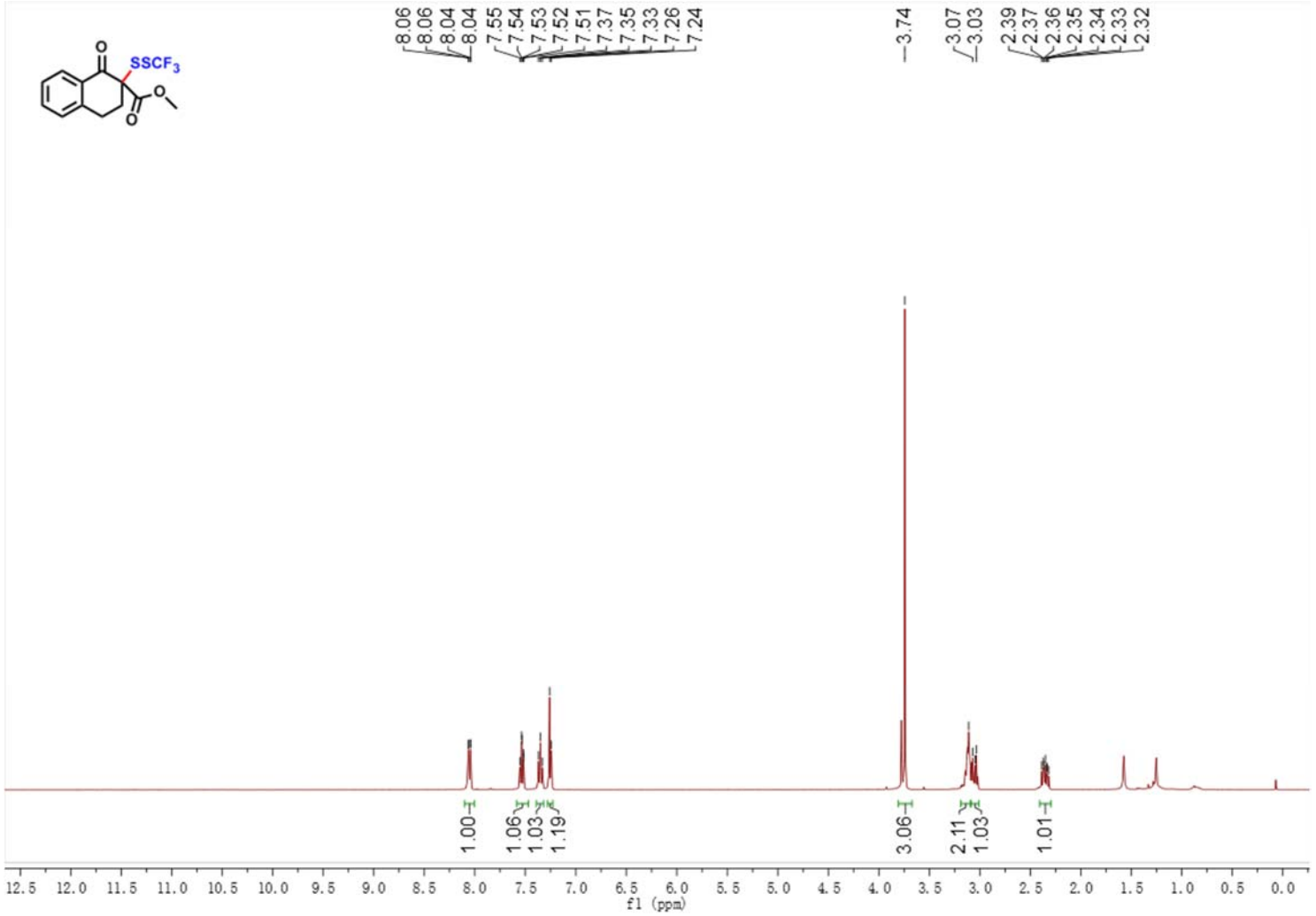
3l

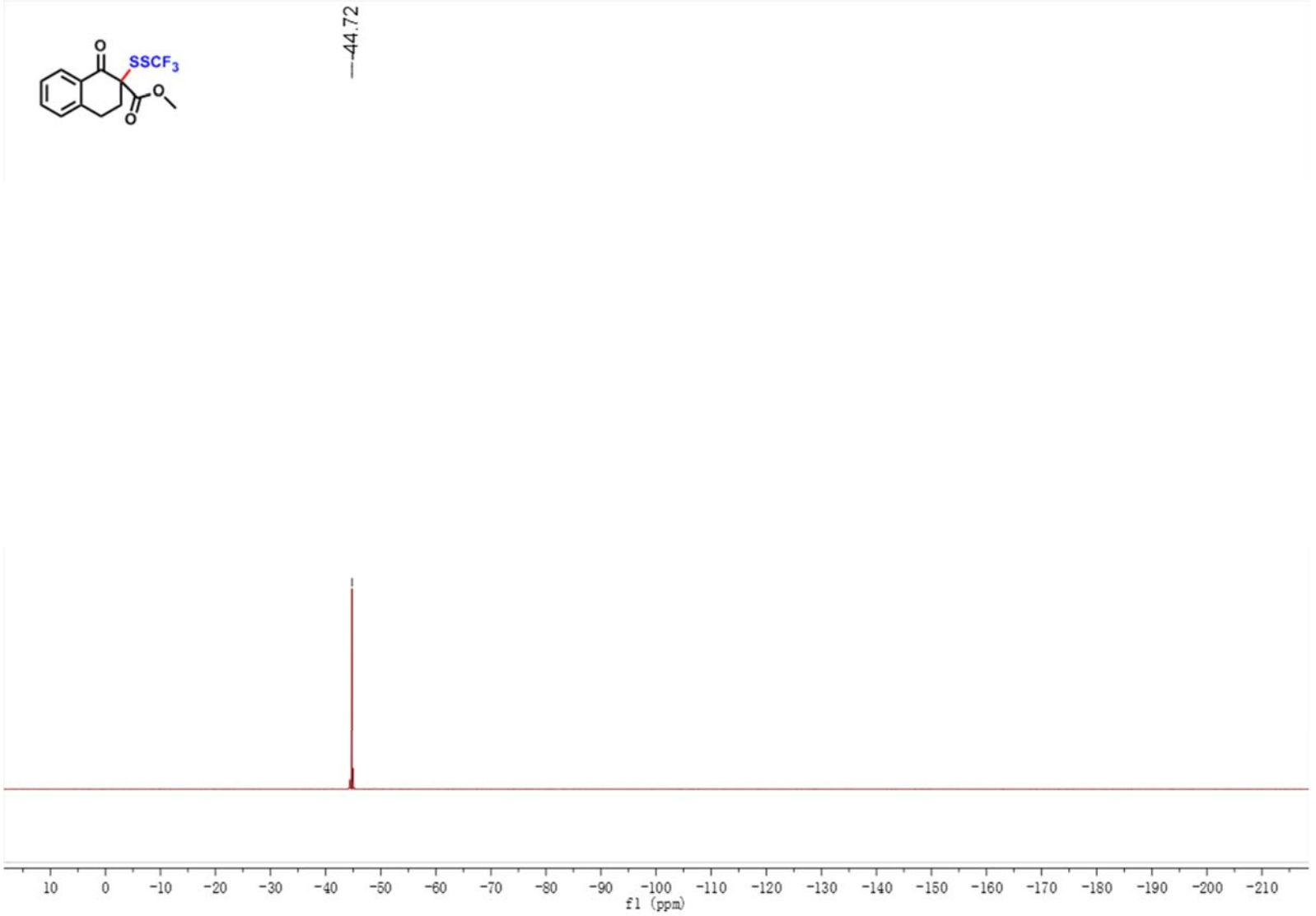

7.26
4.25
4.24
4.22
4.20
2.76
2.48
2.44
2.34
2.10
2.07
1.29
1.29
1.28
1.28
1.26
SSCF3
CO2Et
1.95
1.00
2.10
1.03
2.04
3.05
f1 (ppm)

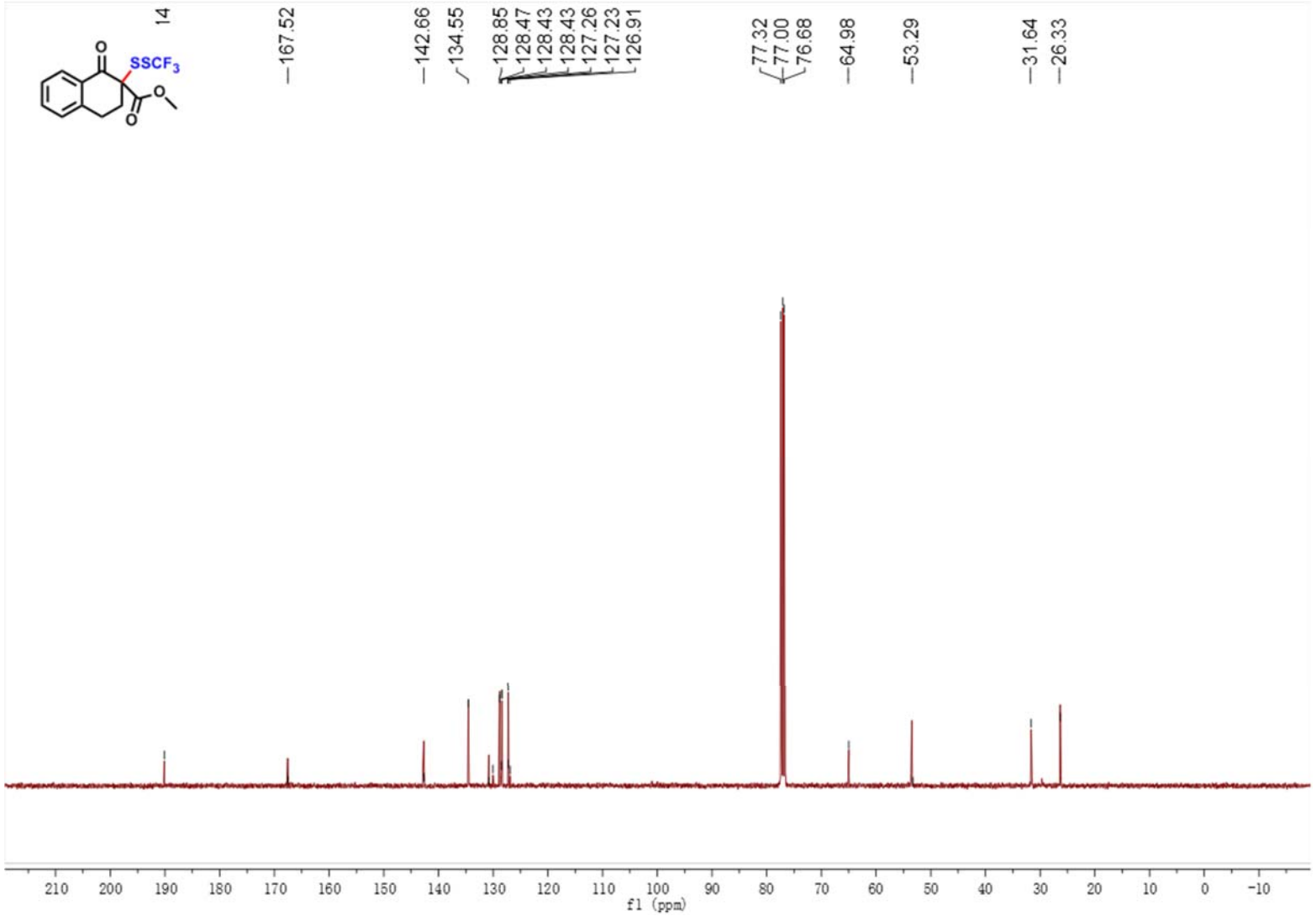

-44.96
O
SSCF3
CO2Et
45.21
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


205.88
167.58
133.27
130.15
130.15
127.02
127.02
123.90
77.32
77.00
76.68
64.96
62.92
36.76
33.79
19.07
13.71
O
SSCF3
CO2Et
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

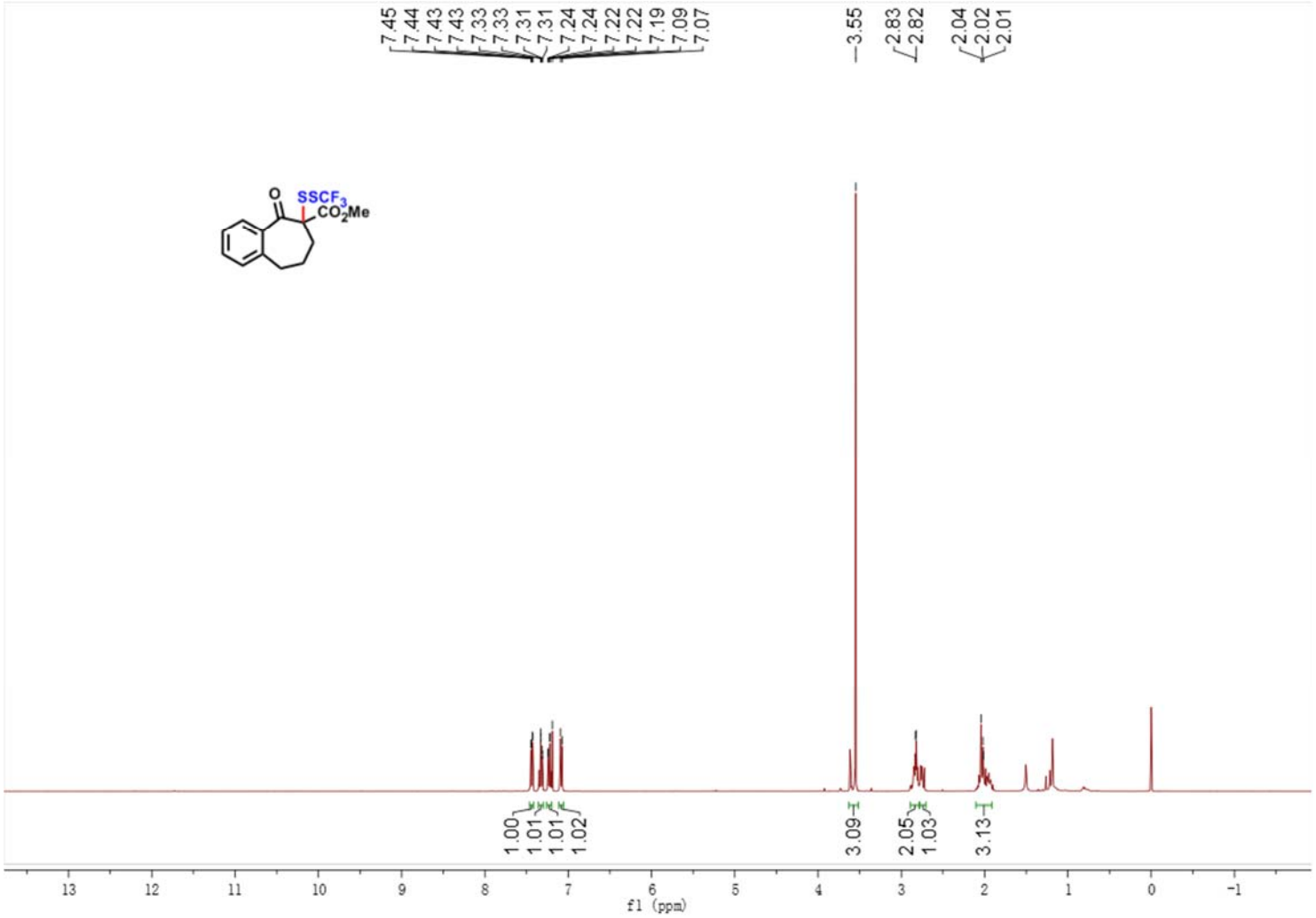
3m

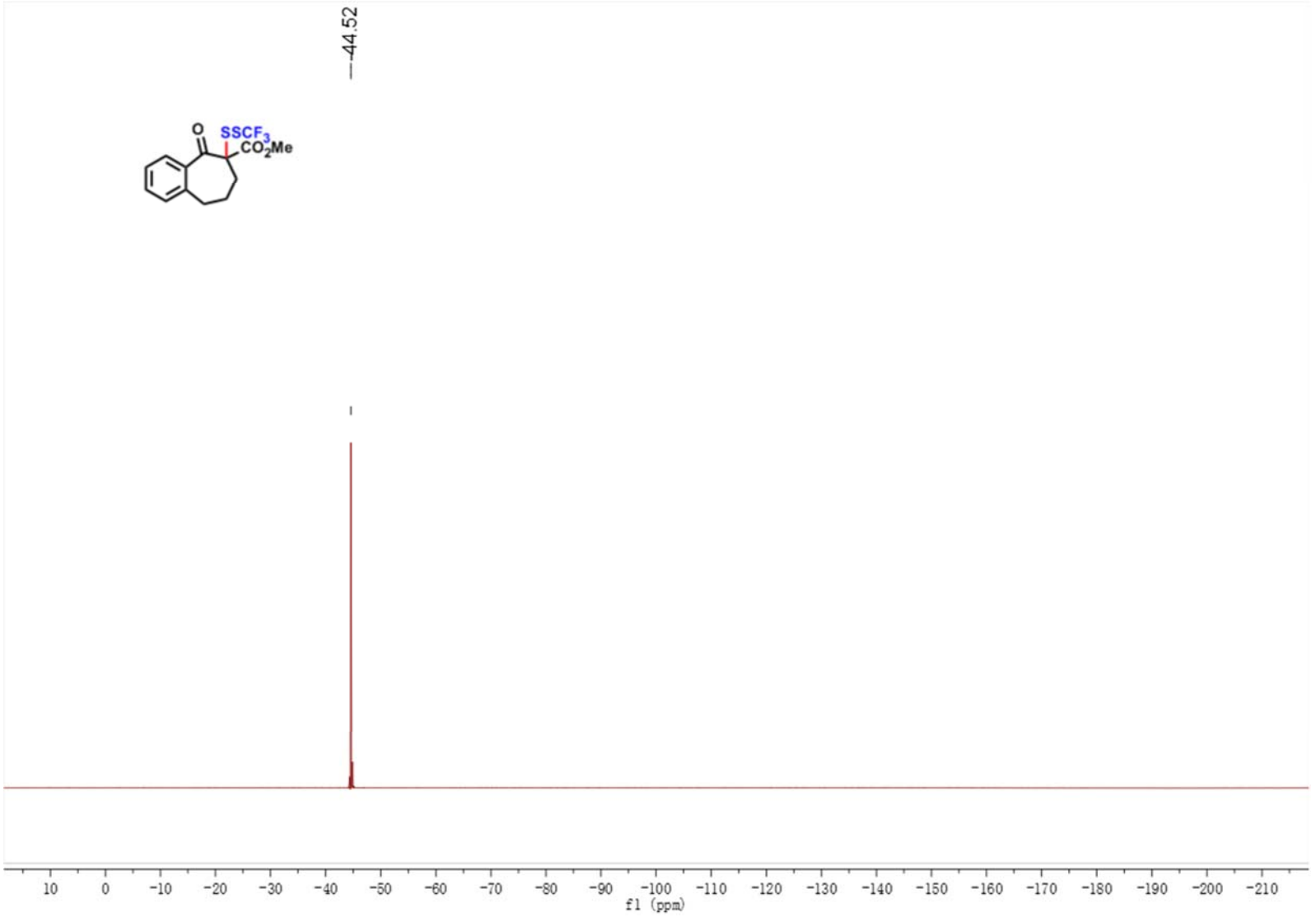

SSCF3
8.06
8.06
8.04
8.04
7.55
7.54
7.53
7.52
7.51
7.37
7.35
7.33
7.26
7.24
3.74
3.07
3.03
2.39
2.37
2.36
2.35
2.34
2.33
2.32
1.00
1.06
1.03
1.19
3.06
2.11
1.03
1.01
f1 (ppm)


SSCF3
-44.72
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)


14
SSCF3
167.52
142.66
134.55
128.85
128.47
128.43
128.43
127.26
127.23
126.91
77.32
77.00
76.68
64.98
53.29
31.64
26.33
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3n


7.45
7.44
7.43
7.43
7.33
7.33
7.31
7.31
7.24
7.24
7.22
7.22
7.19
7.09
7.07
3.55
2.83
2.82
2.04
2.02
2.01
SSCF3
CO2Me
1.00
1.01
1.01
1.02
3.09
2.05
1.03
3.13
f1 (ppm)


-44.52
O
SSCF3
CO2Me
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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-100
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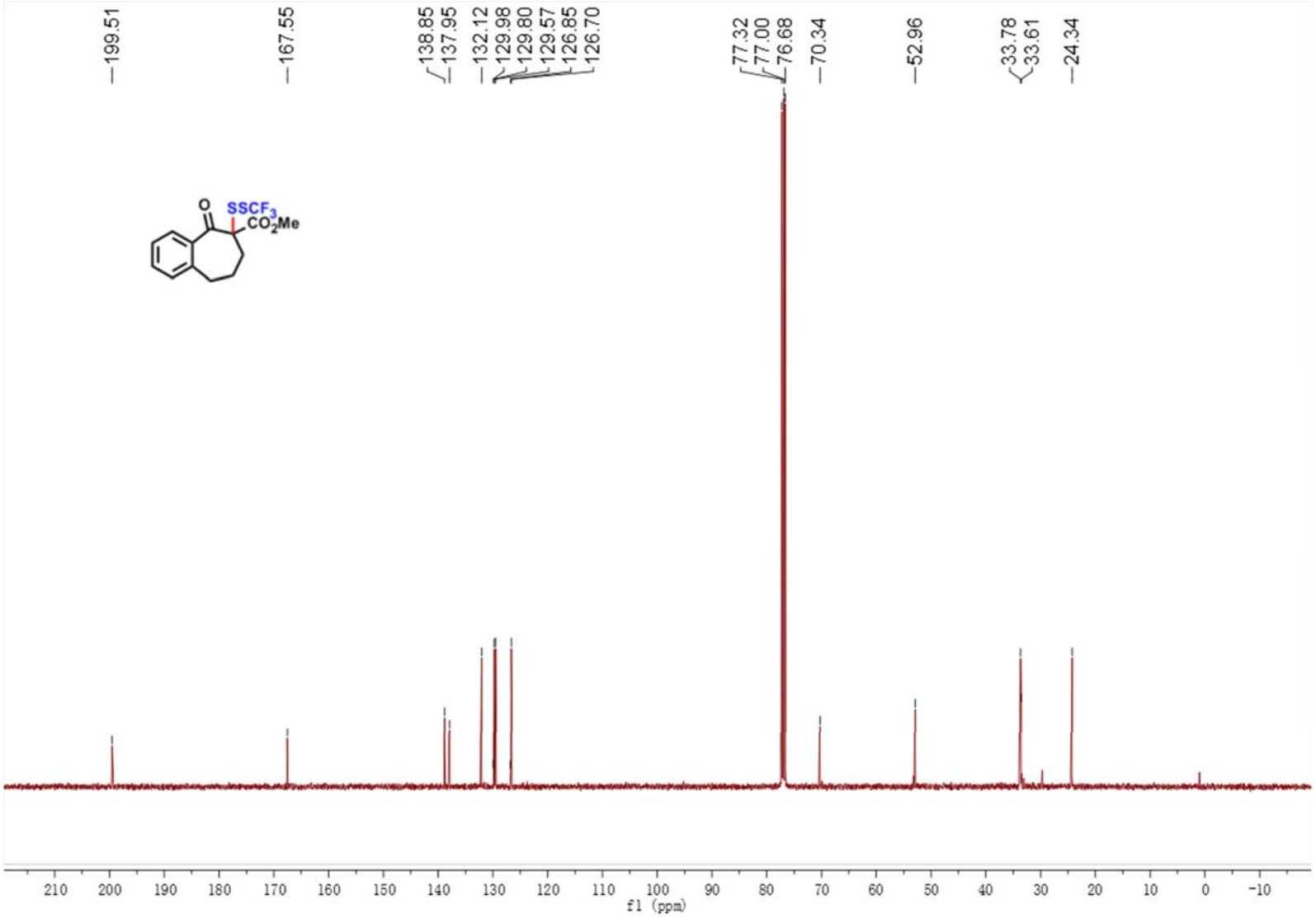
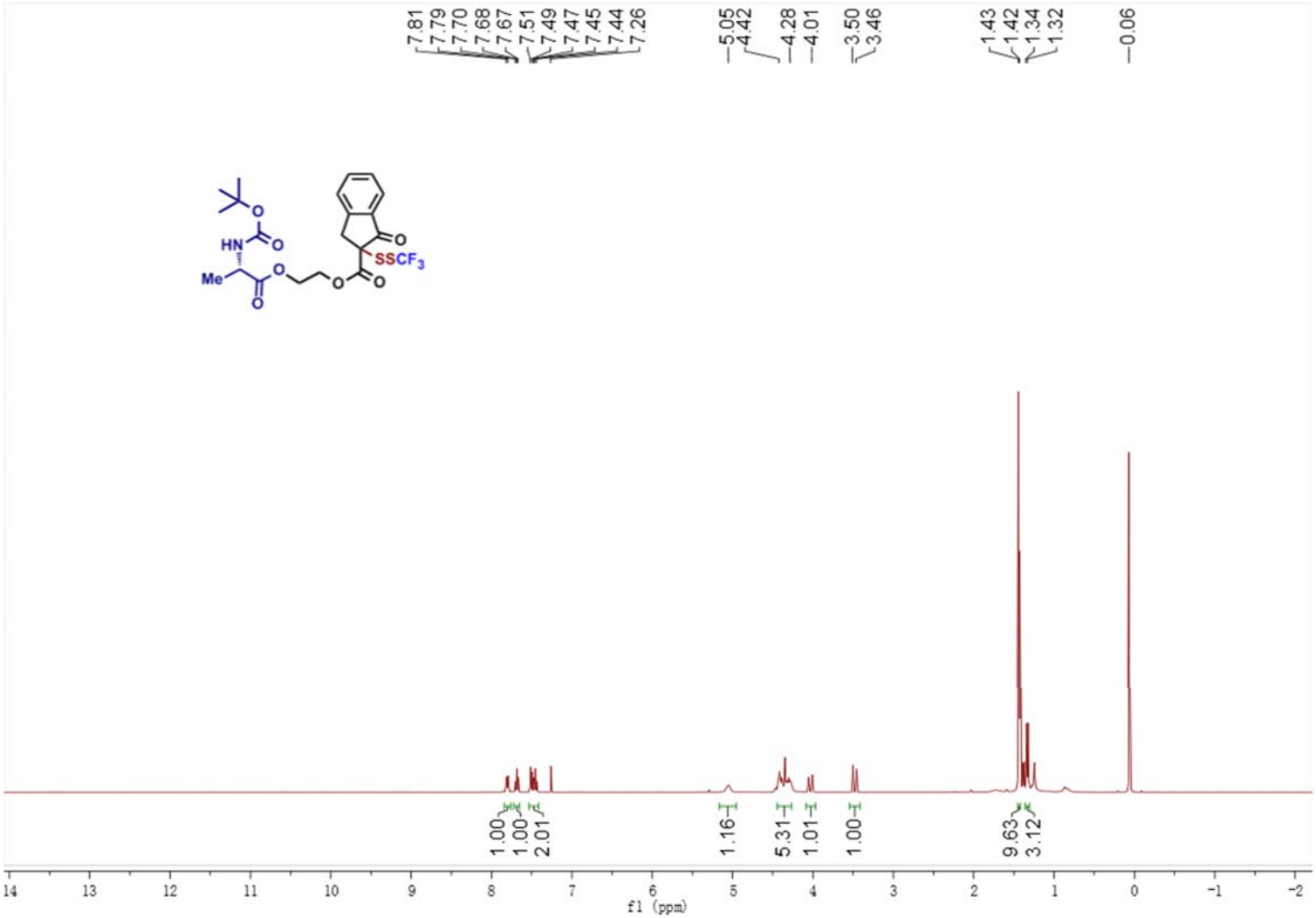
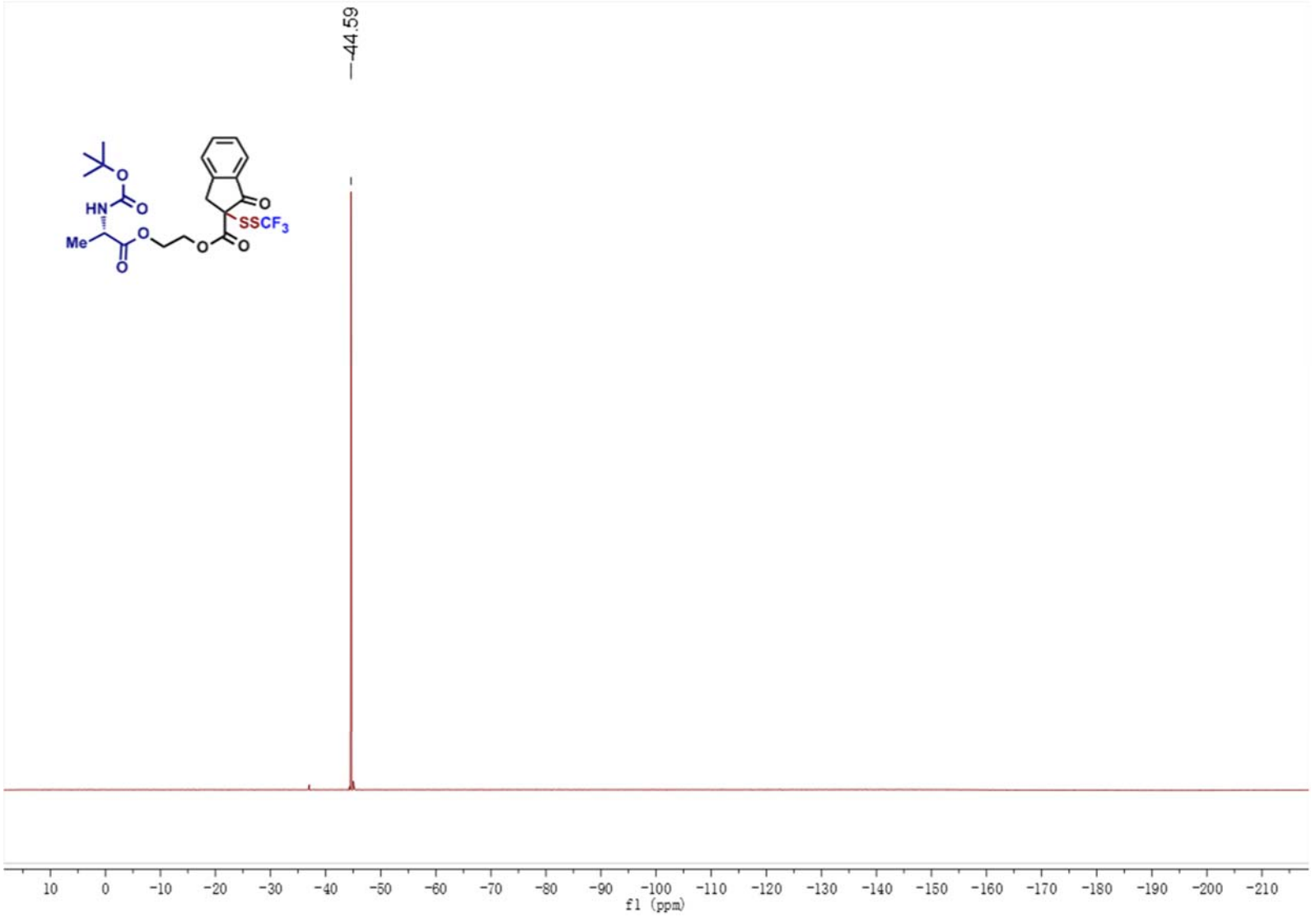
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


199.51
167.55
138.85
137.95
132.12
129.98
129.80
129.57
126.85
126.70
77.32
77.00
76.68
70.34
52.96
33.78
33.61
24.34
SSCF3
CO2Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3o


7.81
7.79
7.70
7.68
7.67
7.51
7.49
7.47
7.45
7.44
7.26
5.05
4.42
4.28
4.01
3.50
3.46
1.43
1.42
1.34
1.32
0.06
HN
Me
SSCF3
1.00
1.00
2.01
1.16
5.31
1.01
1.00
9.63
3.12
f1 (ppm)


-44.59
HN
Me
SSCF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
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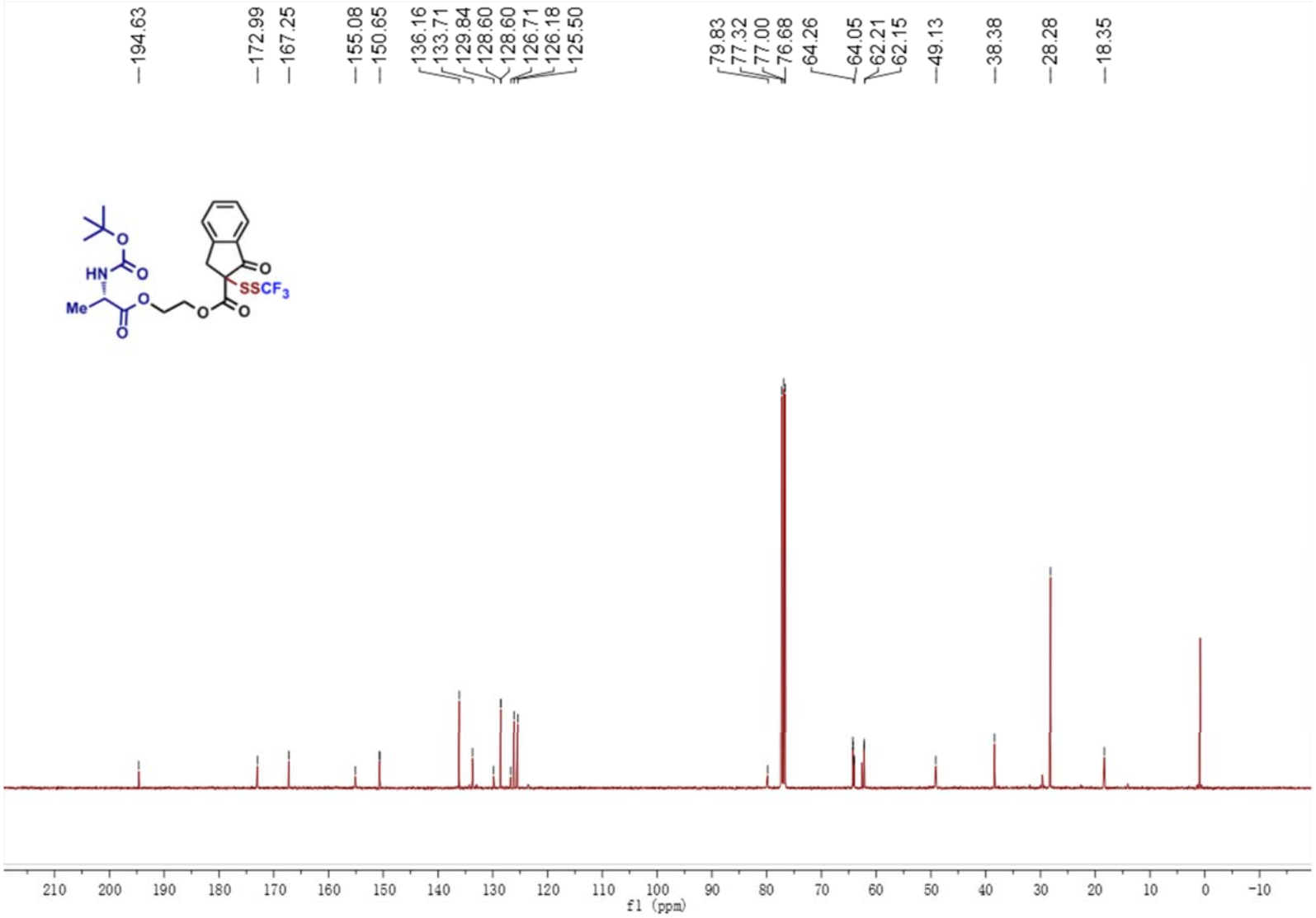
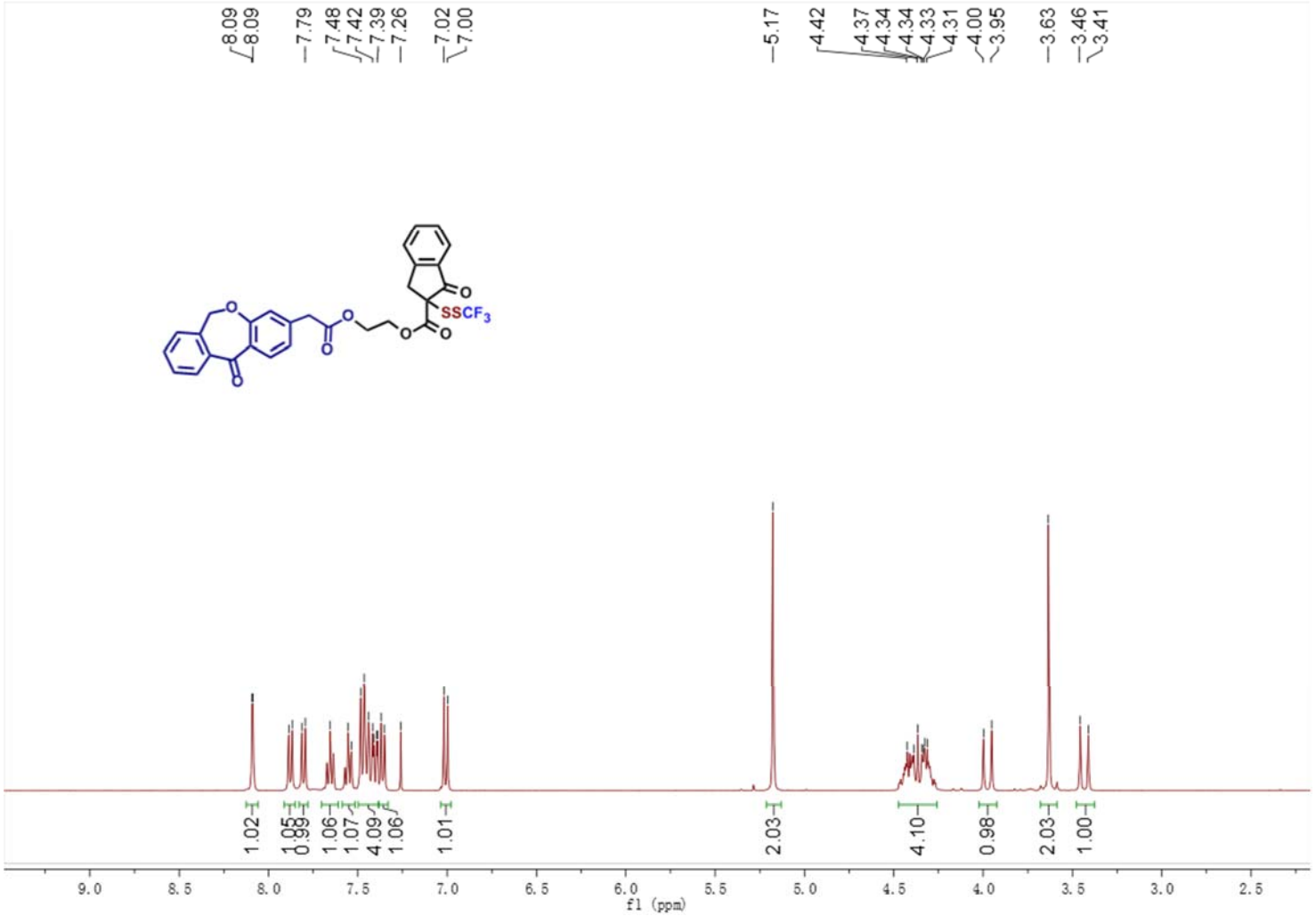
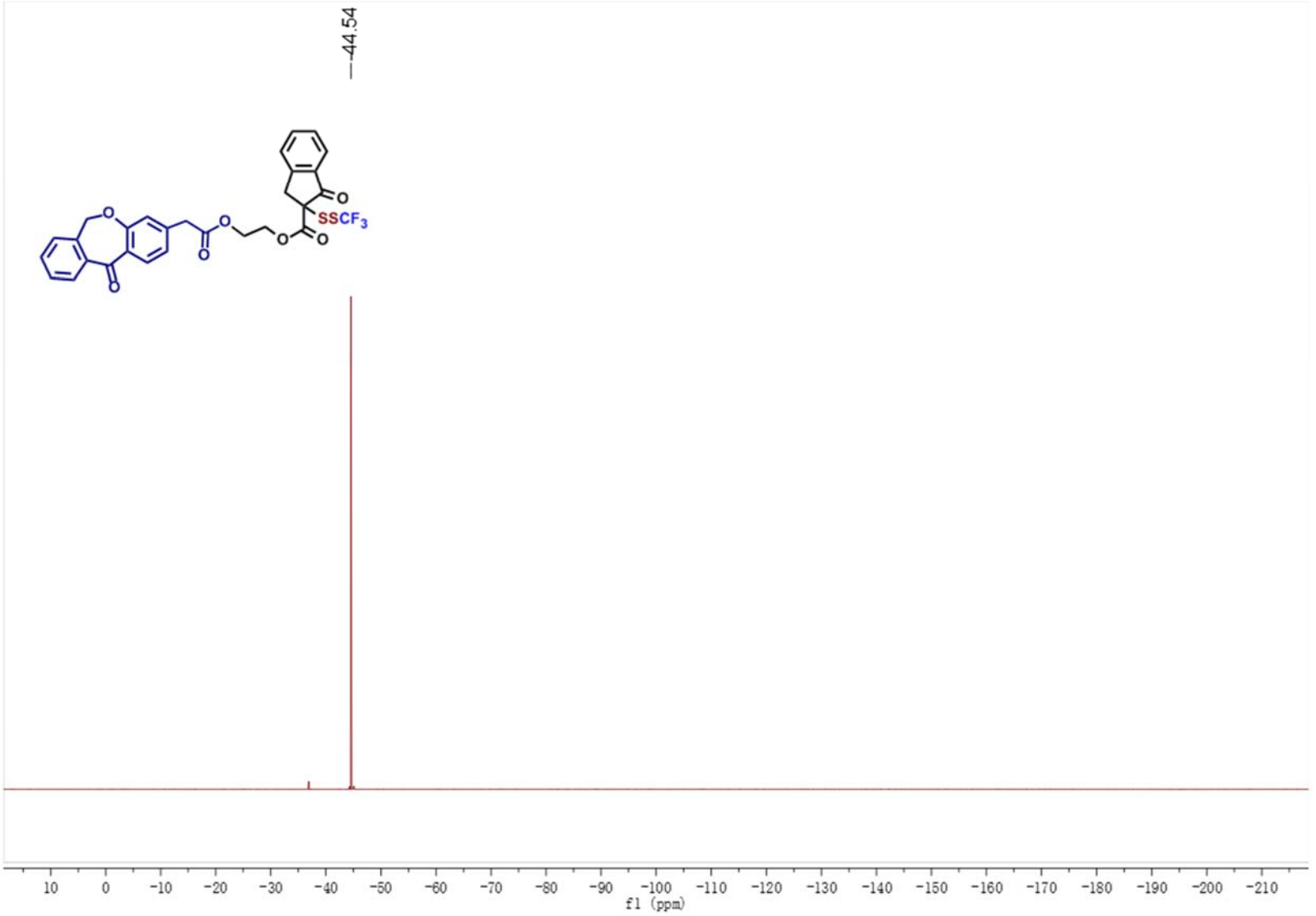
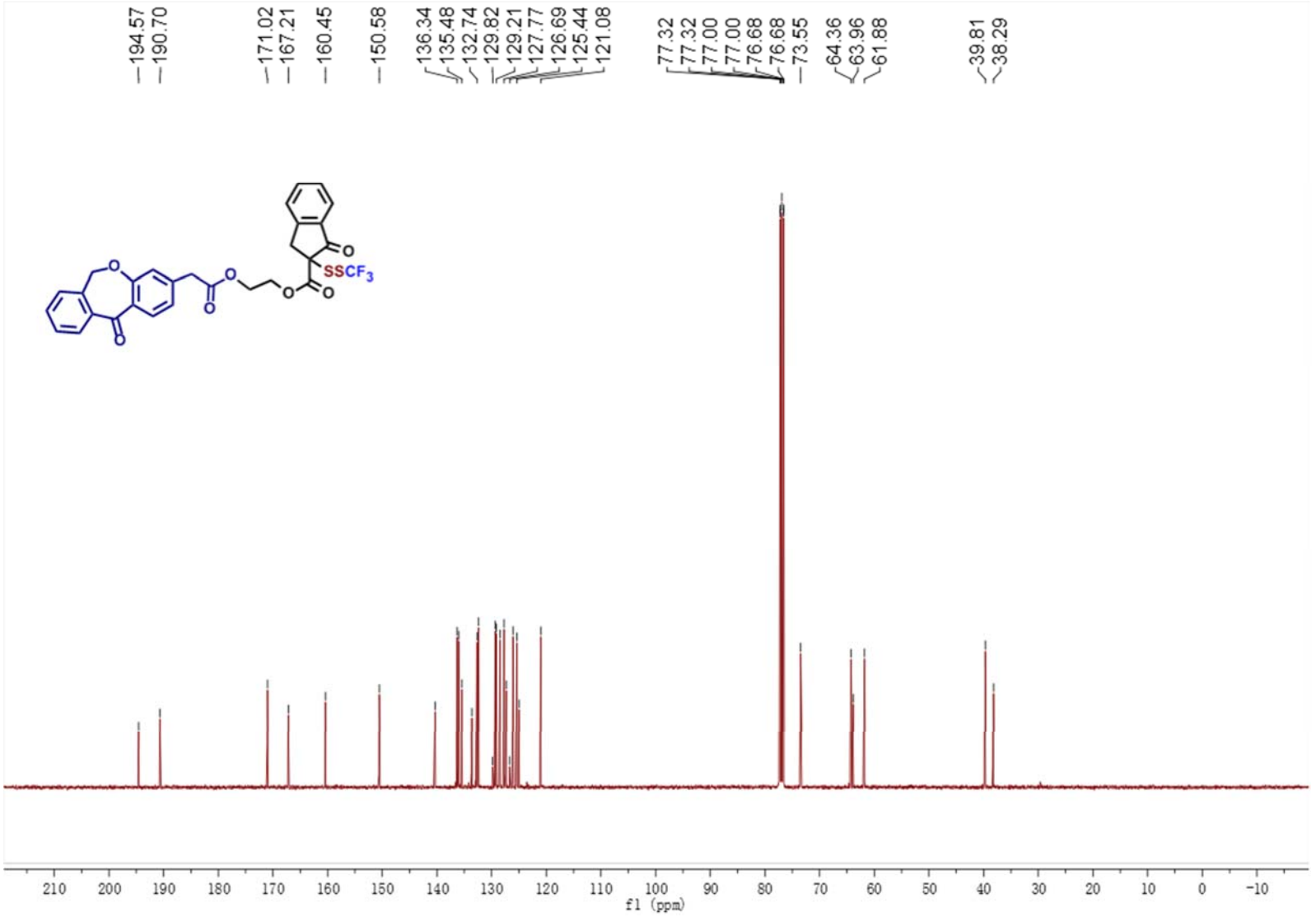
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


194.63
172.99
167.25
155.08
150.65
136.16
133.71
129.84
128.60
128.60
126.71
126.18
125.50
79.83
77.32
77.00
76.68
64.26
64.05
62.21
62.15
49.13
38.38
28.28
18.35
HN
Me
SSCF3
f1 (ppm)

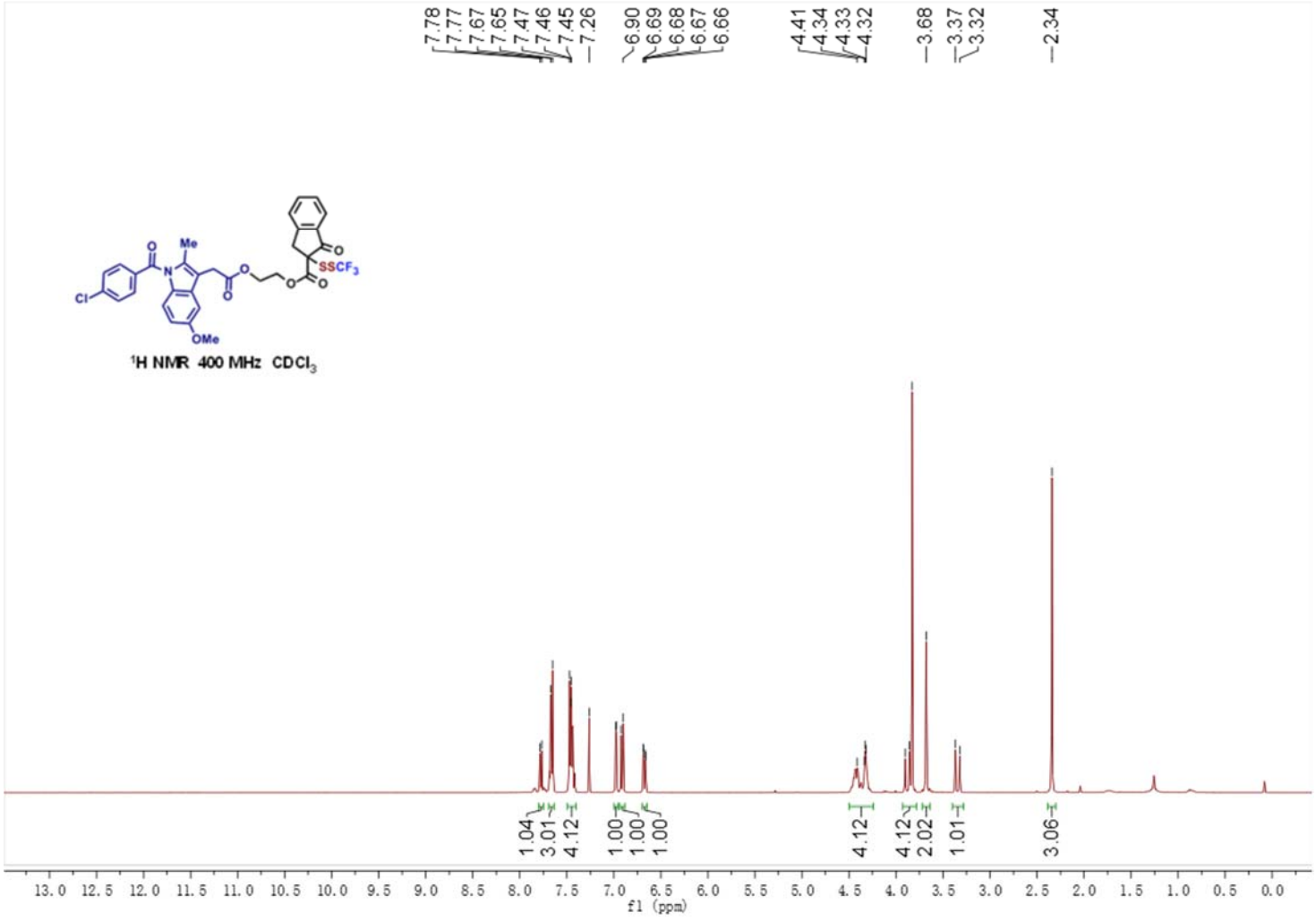
3p

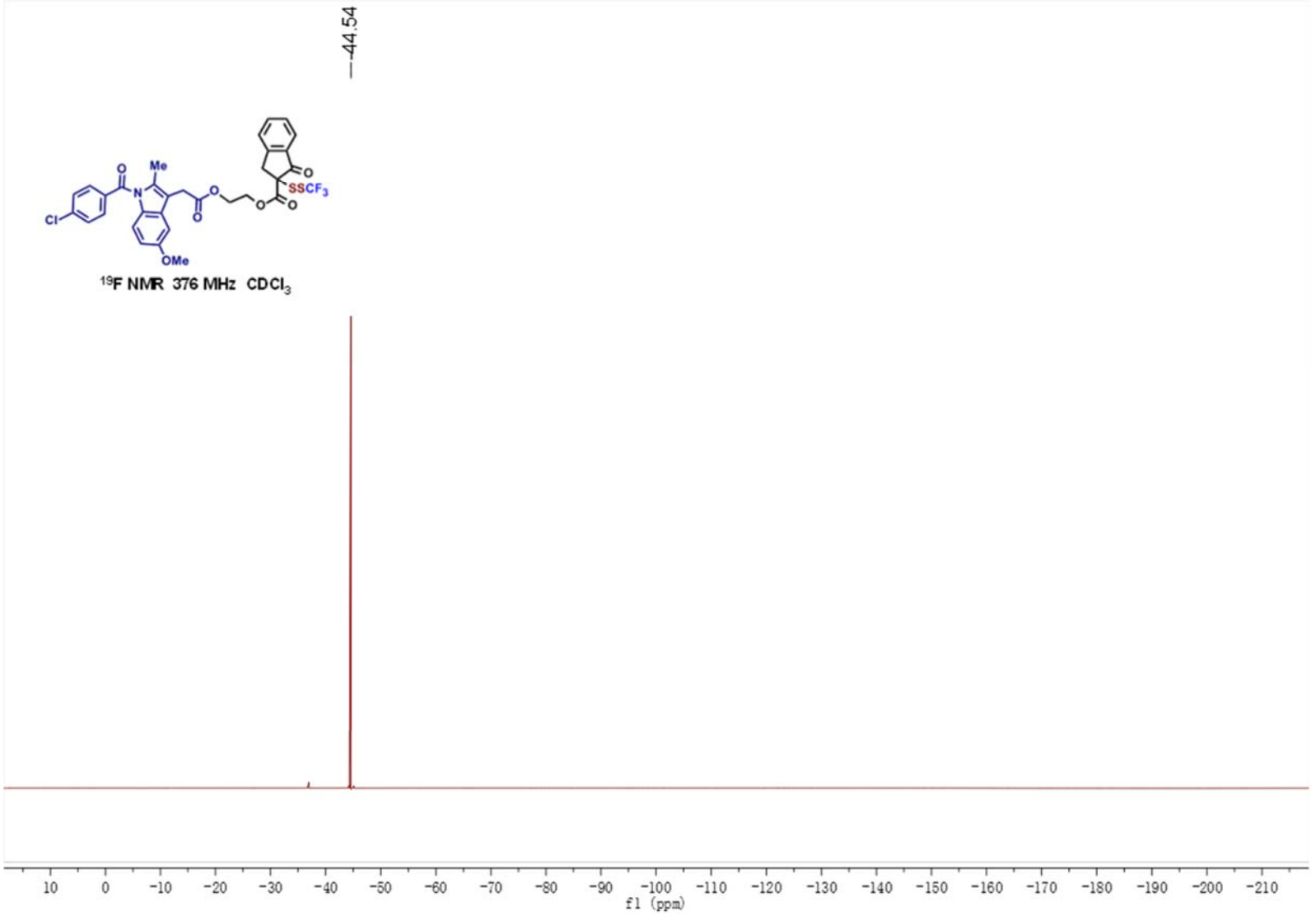

8.09
8.09
7.79
7.48
7.42
7.39
7.26
7.02
7.00
5.17
4.42
4.37
4.34
4.34
4.33
4.31
4.00
3.95
3.63
3.46
3.41
SSCF3
1.02
1.05
0.99
1.06
1.07
4.09
1.06
1.01
2.03
4.10
0.98
2.03
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f1 (ppm)

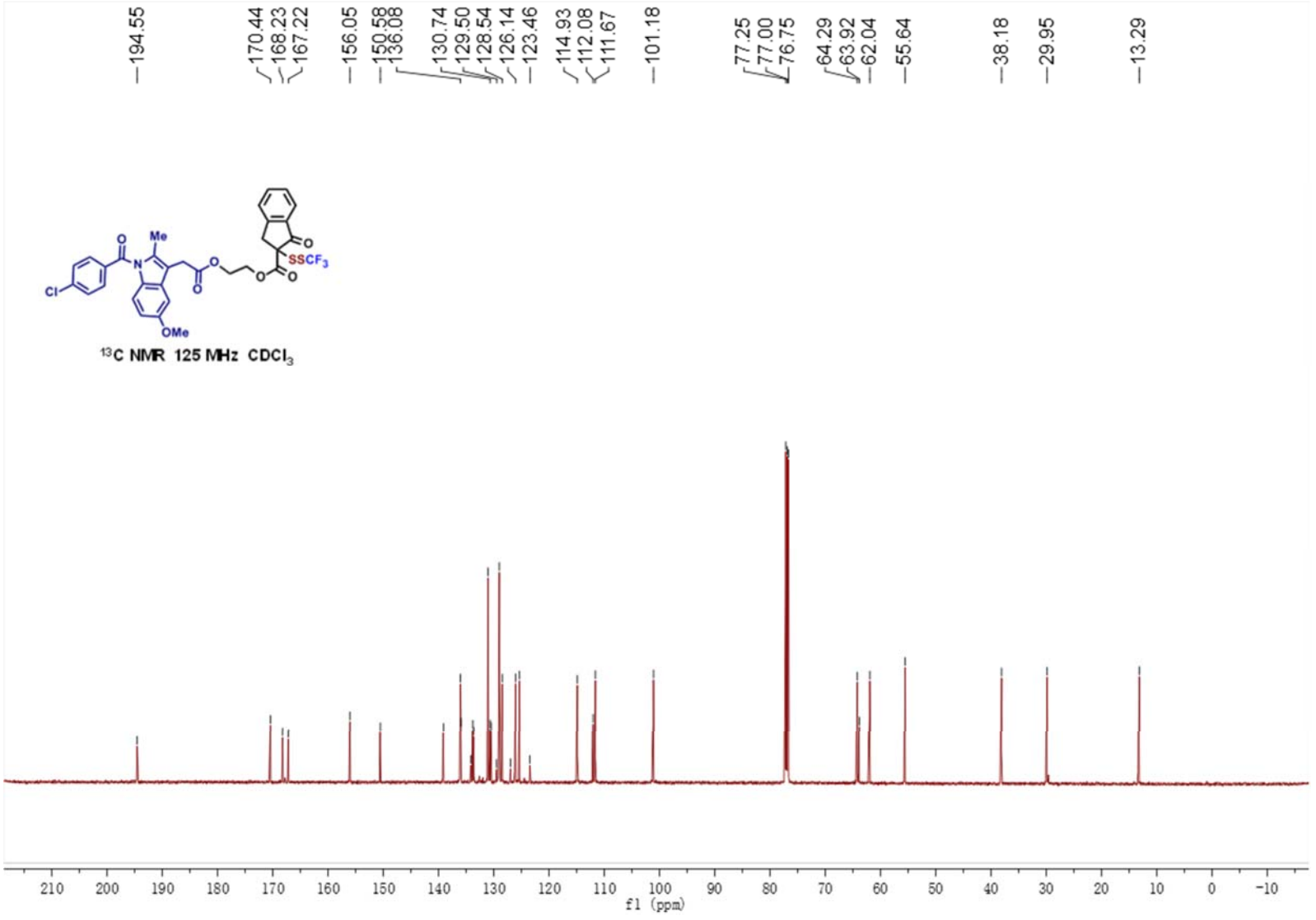

-44.54
SSCF3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


194.57
190.70
171.02
167.21
160.45
150.58
136.34
135.48
132.74
129.82
129.21
127.77
126.69
125.44
121.08
77.32
77.32
77.00
77.00
76.68
76.68
73.55
64.36
63.96
61.88
39.81
38.29
SSCF3
f1 (ppm)

3q


7.78
7.77
7.67
7.65
7.47
7.46
7.45
7.26
6.90
6.69
6.68
6.67
6.66
4.41
4.34
4.33
4.32
3.68
3.37
3.32
2.34
Me
SSCF3
Cl
OMe
1H NMR 400 MHz CDCl3
1.04
3.01
4.12
1.00
1.00
1.00
4.12
4.12
2.02
1.01
3.06
f1 (ppm)


-44.54
Me
O
N
O
O
O
O
O
SSCF3
Cl
OMe
19F NMR 376 MHz CDCl3
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)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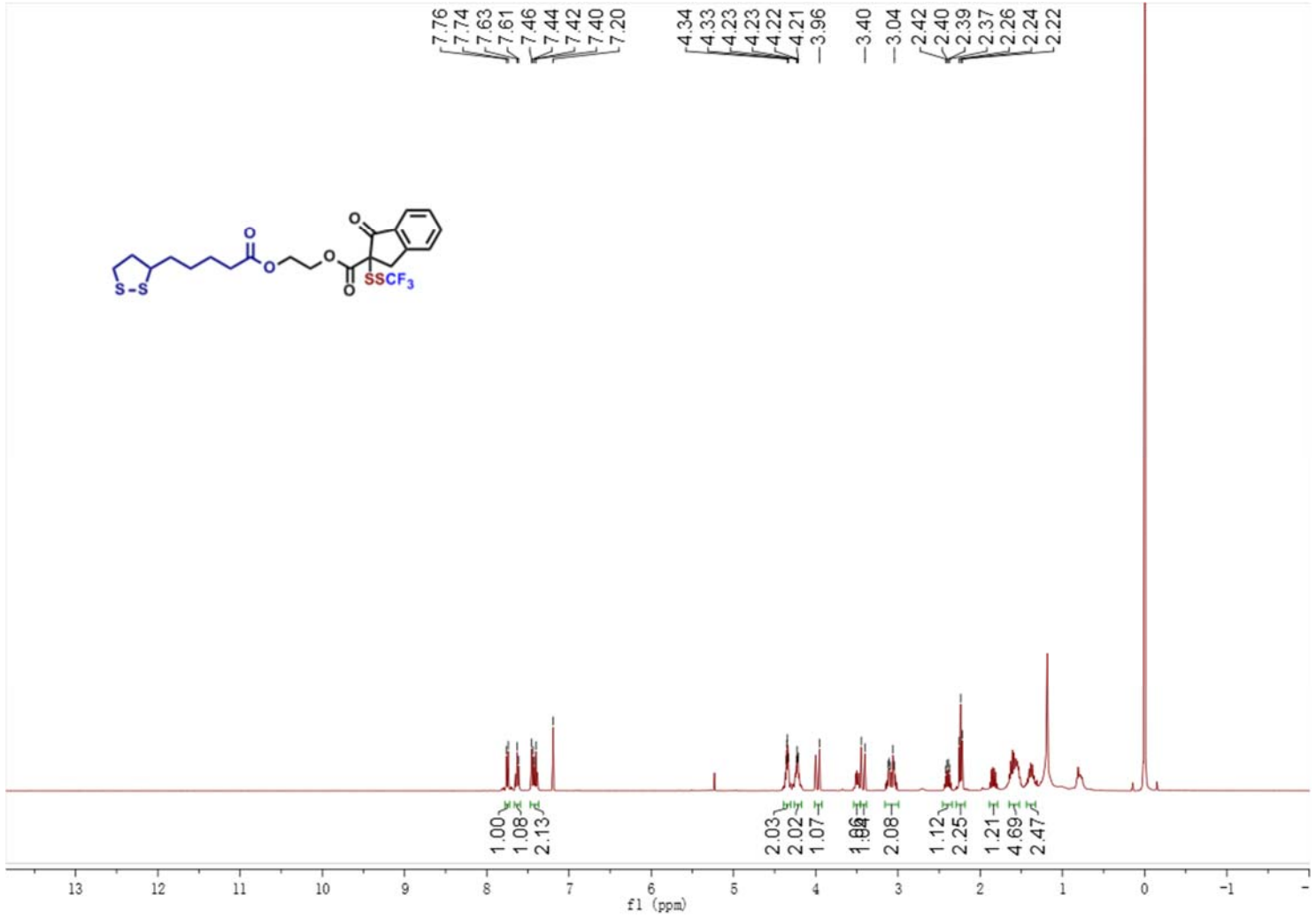
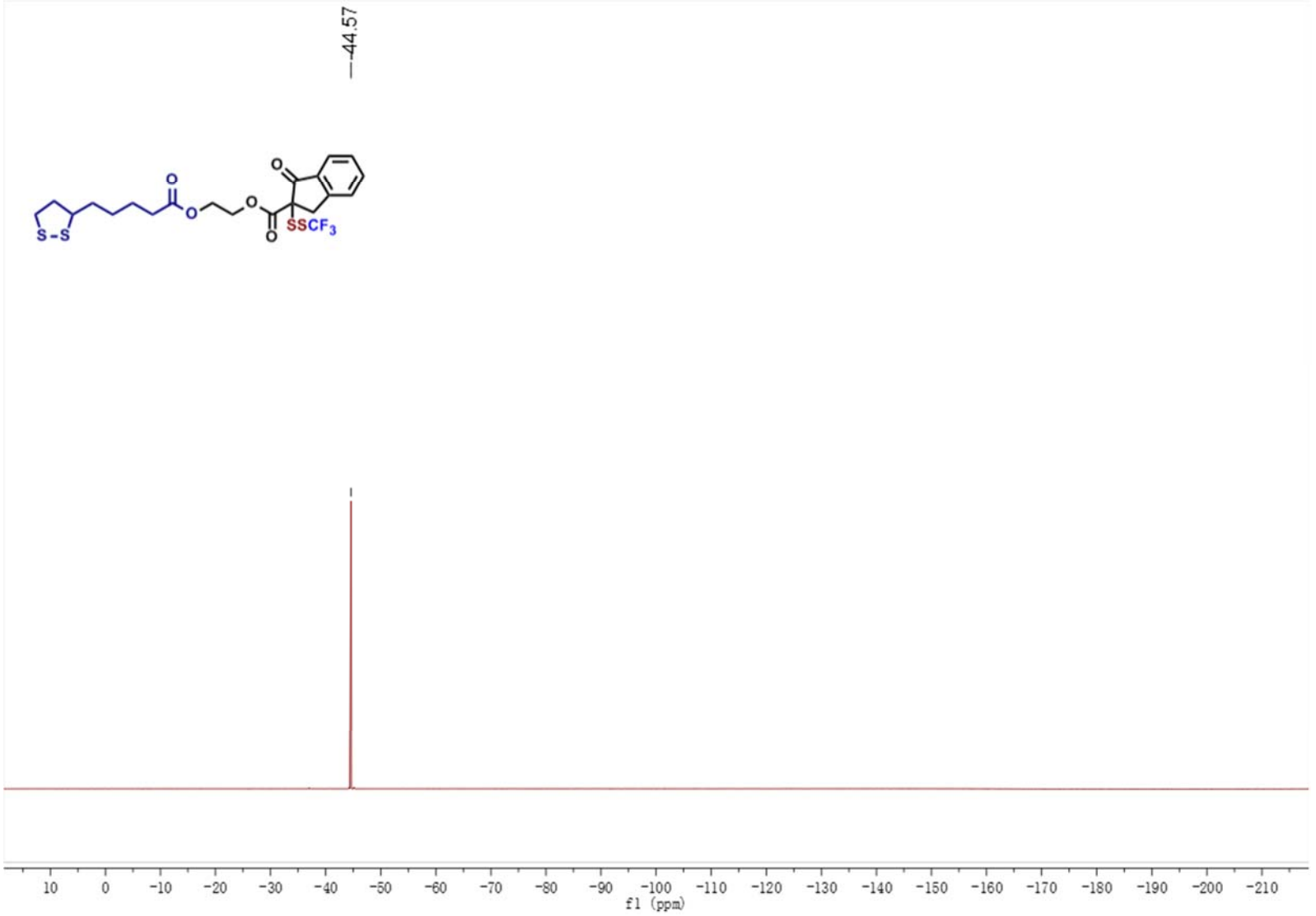
170.44
168.23
167.22
156.05
150.58
136.08
130.74
129.50
128.54
126.14
123.46
114.93
112.08
111.67
101.18
77.25
77.00
76.75
64.29
63.92
62.04
55.64
38.18
29.95
13.29
Me
SSCF3
Cl
OMe
O
N
O
O
O
O
O
O
13C NMR 125 MHz CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3r


7.76
7.74
7.63
7.61
7.46
7.44
7.42
7.40
7.20
4.34
4.33
4.23
4.23
4.22
4.21
3.96
3.40
3.04
2.42
2.40
2.39
2.37
2.26
2.24
2.22
S-S
SSCF3
1.00
1.08
2.13
2.03
2.02
1.07
2.08
1.12
2.25
1.21
4.69
2.47
f1 (ppm)


-44.57
S-S
SSCF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
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-130
-140
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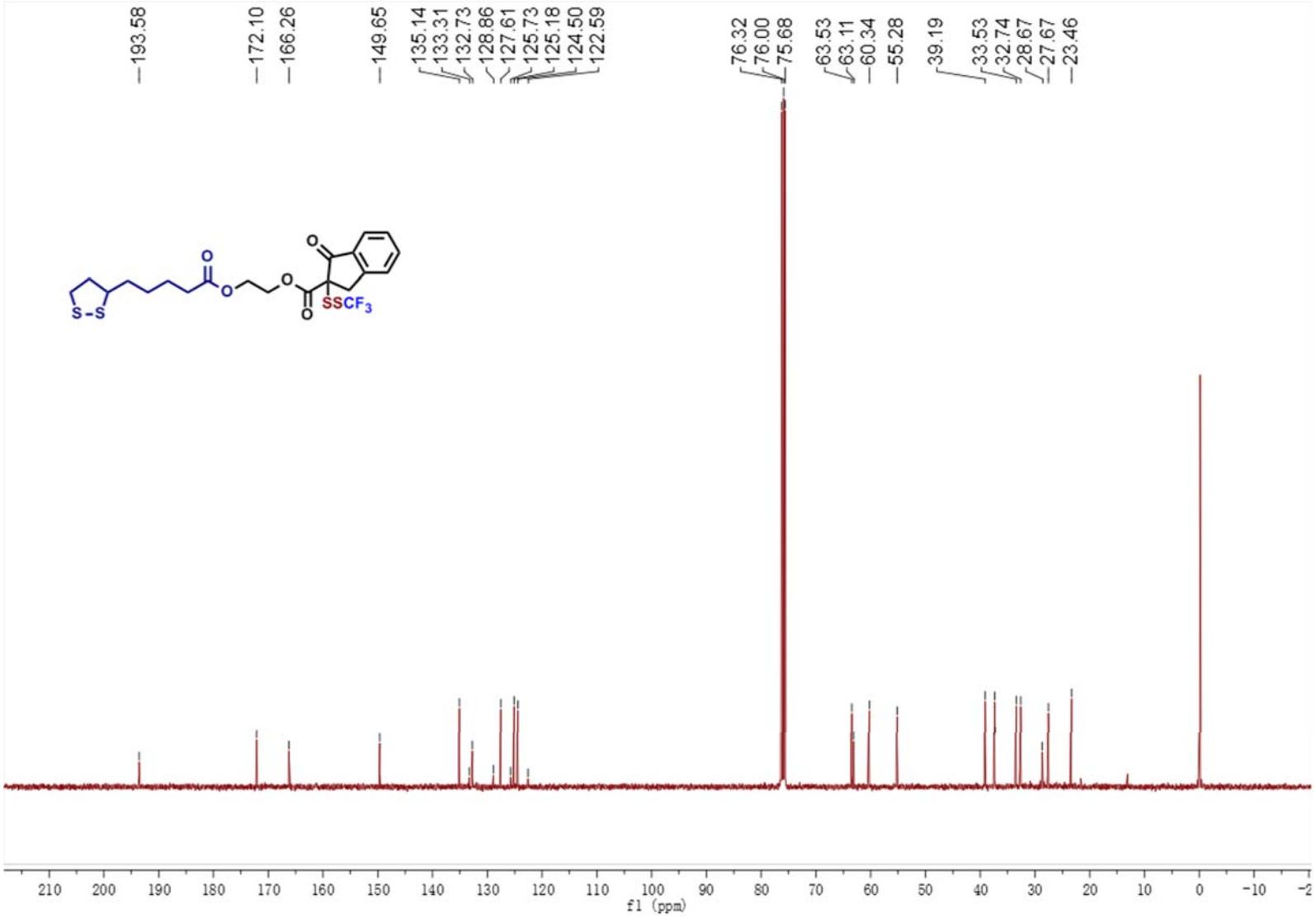
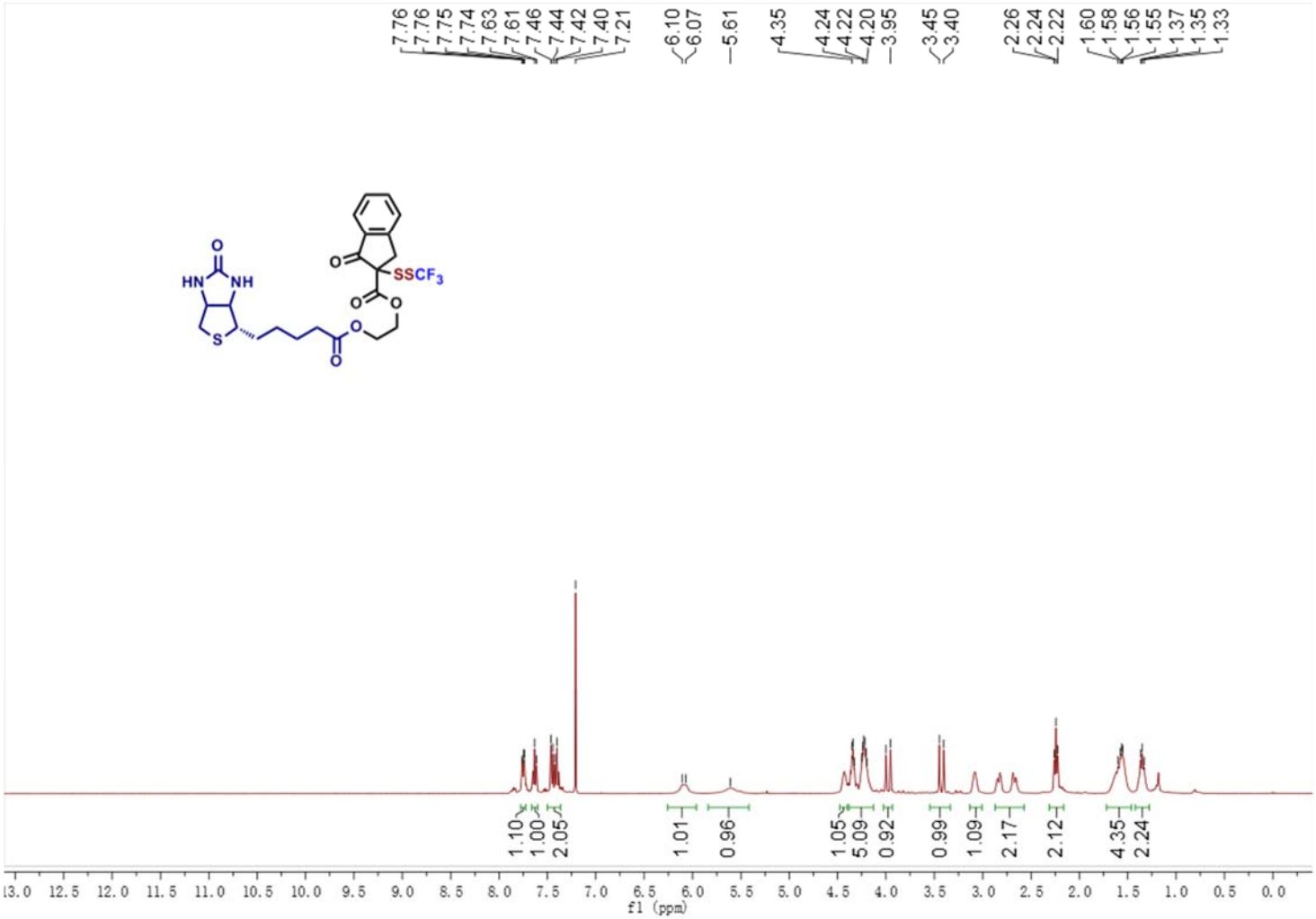
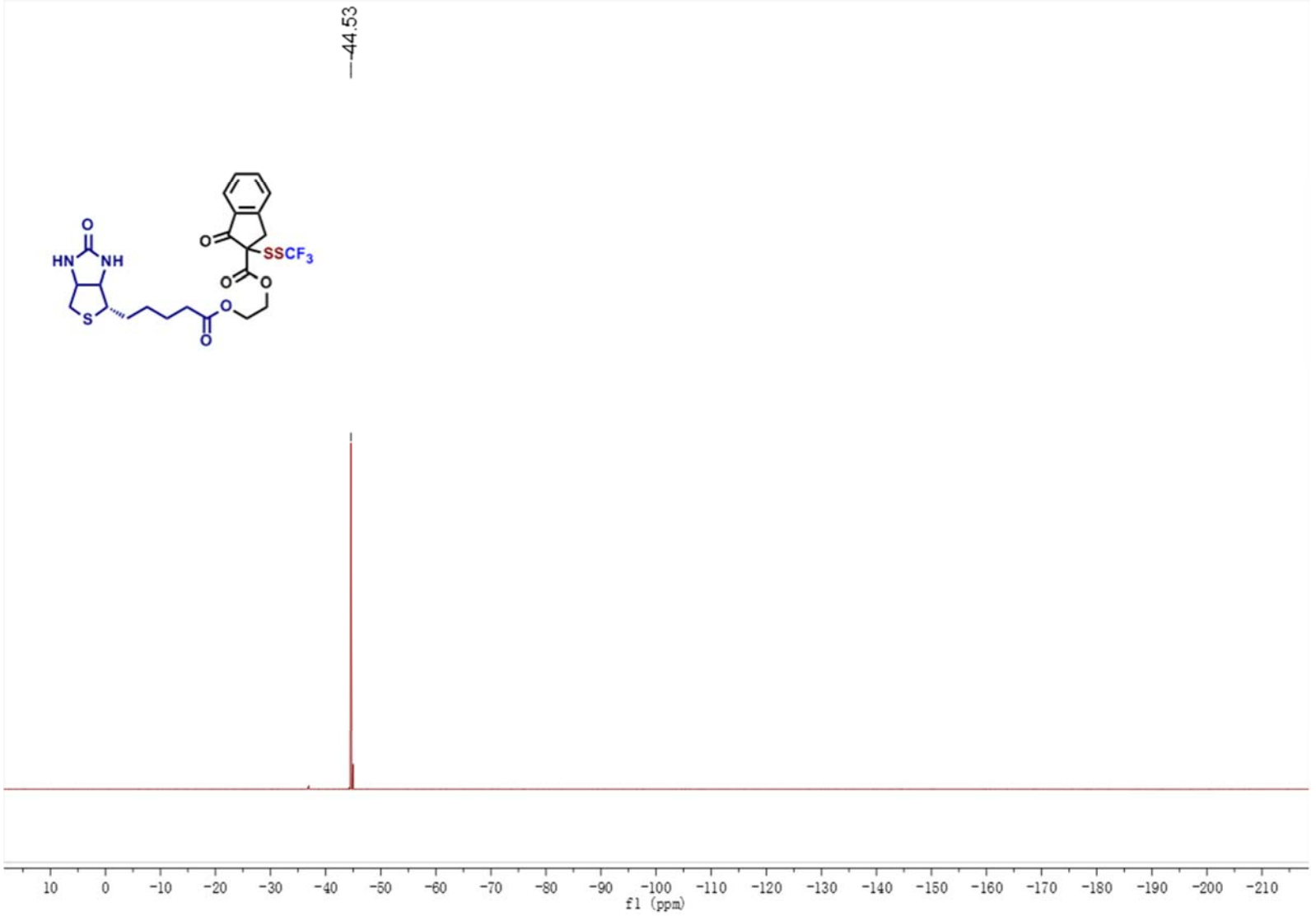
-160
-170
-180
-190
-200
-210
f1 (ppm)


193.58
172.10
166.26
149.65
135.14
133.31
132.73
128.86
127.61
125.73
125.18
124.50
122.59
76.32
76.00
75.68
63.53
63.11
60.34
55.28
39.19
33.53
32.74
28.67
27.67
23.46
S-S
SSCF3
f1 (ppm)

3s


7.76
7.76
7.75
7.74
7.63
7.61
7.46
7.44
7.42
7.40
7.21
6.10
6.07
5.61
4.35
4.24
4.22
4.20
3.95
3.45
3.40
2.26
2.24
2.22
1.60
1.58
1.56
1.55
1.37
1.35
1.33
HN
NH
O
S
SSCF3
1.10
1.00
2.05
1.01
0.96
1.05
5.09
0.92
0.99
1.09
2.17
2.12
4.35
2.24
f1 (ppm)


-44.53
HN
NH
O
S
SSCF3
10
0
-10
-20
-30
-40
-50
-60
-70
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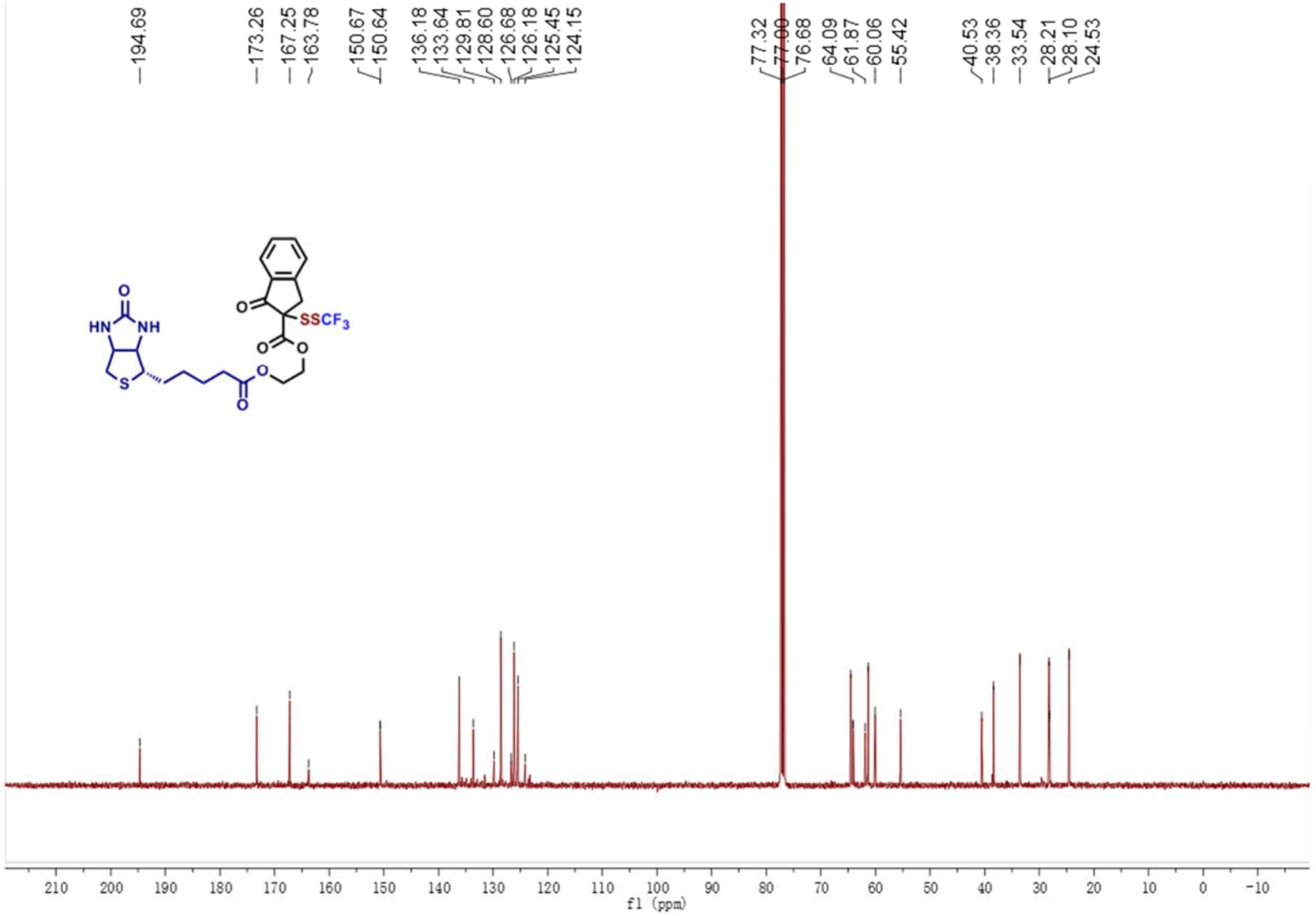
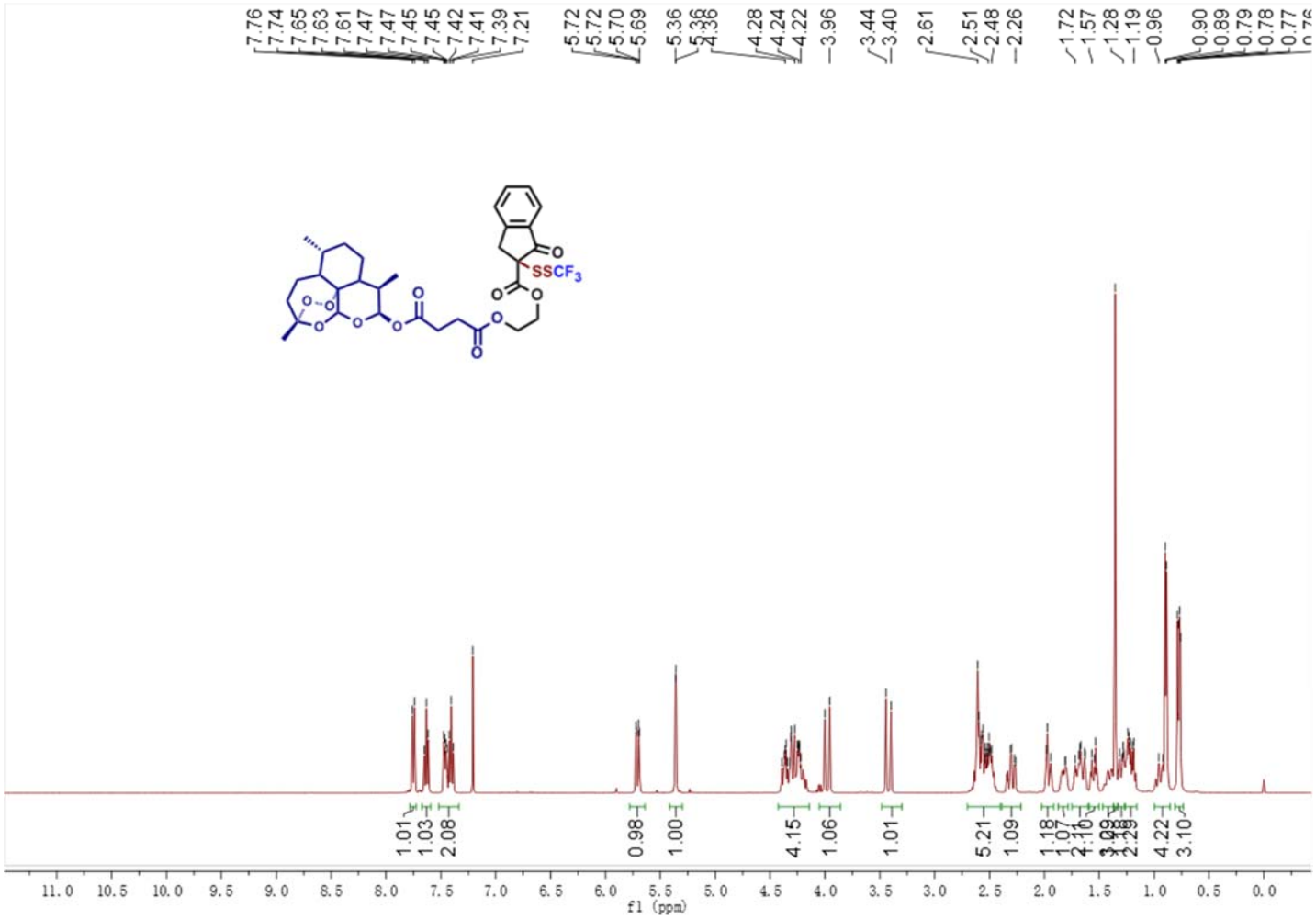
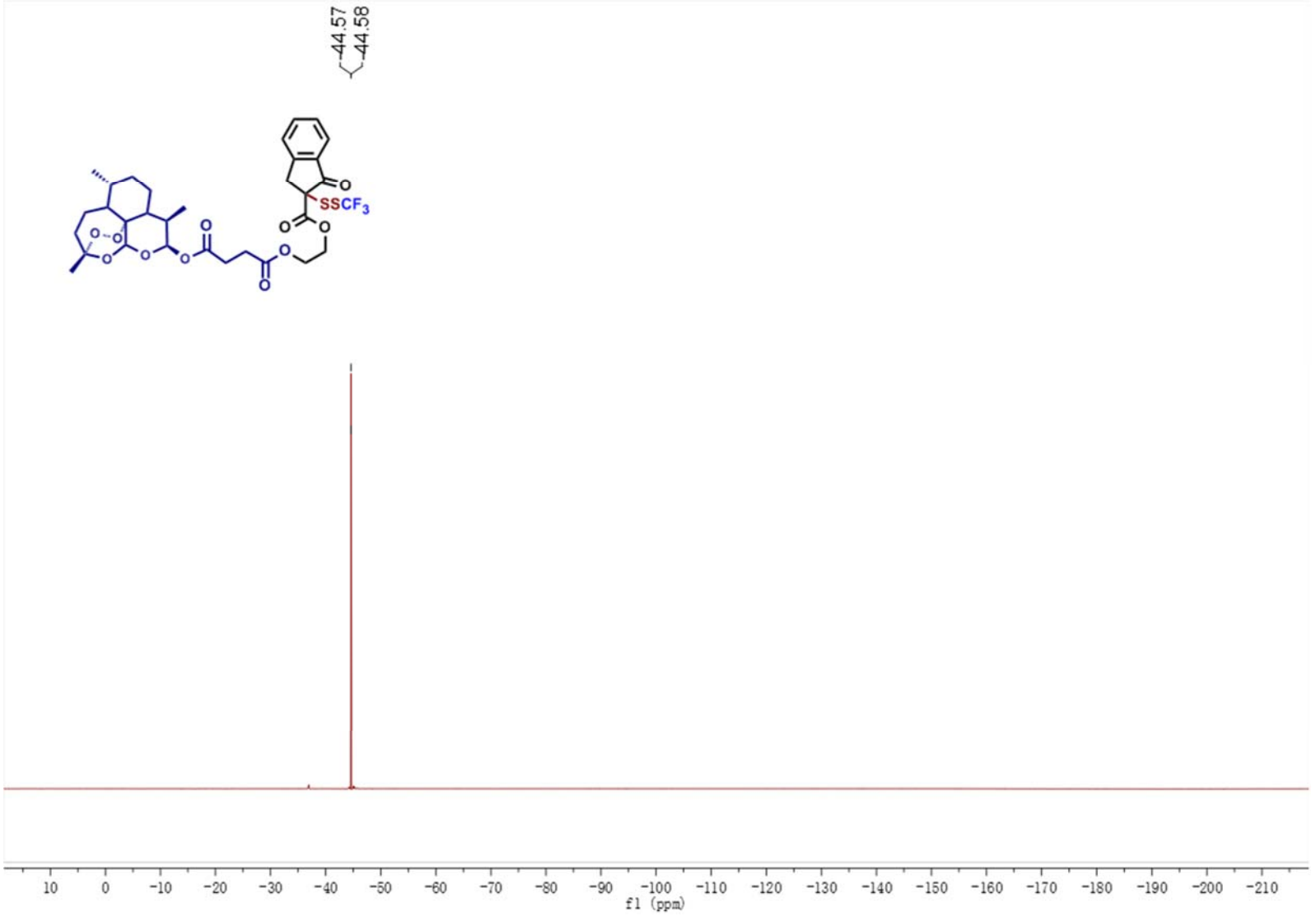
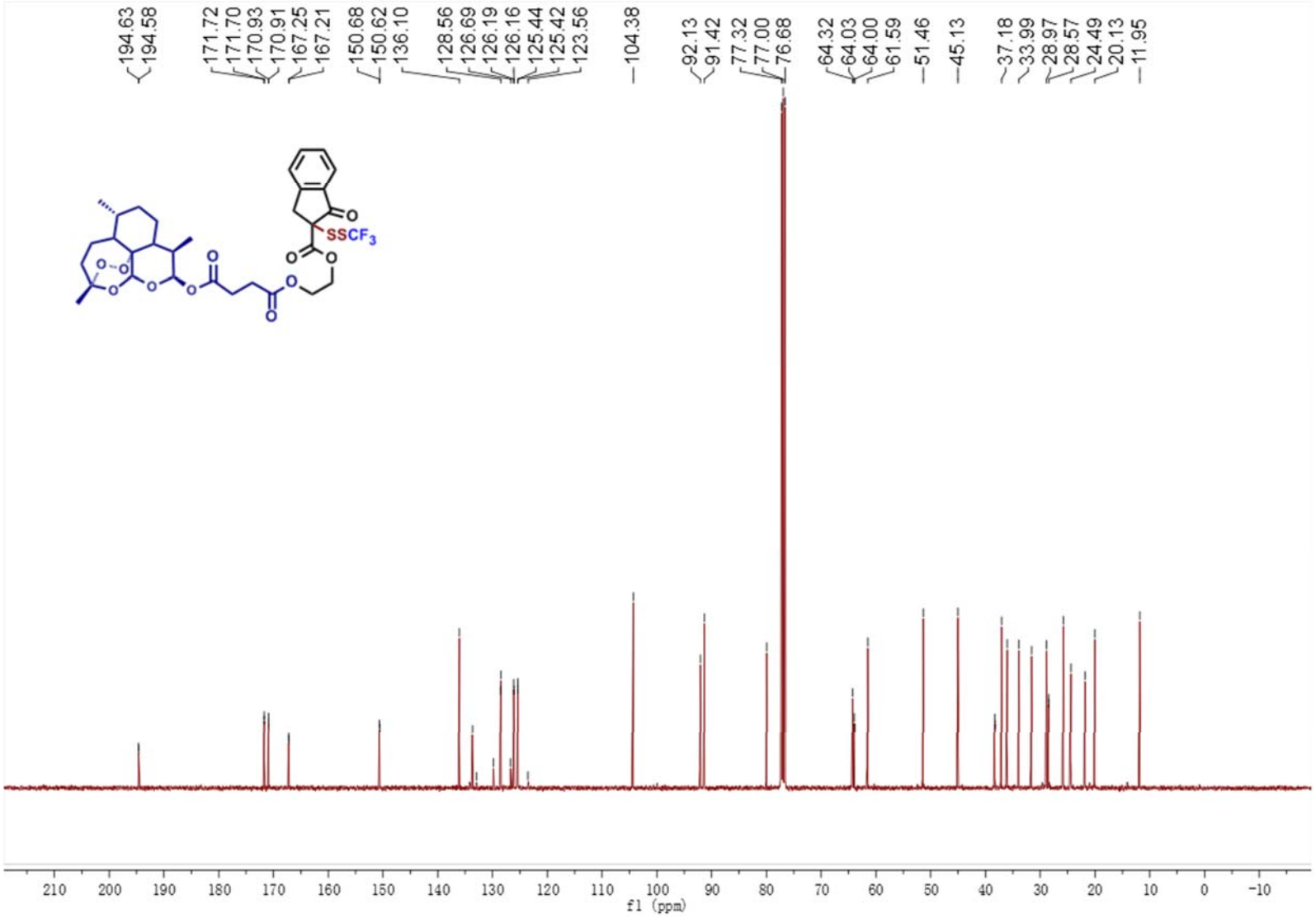
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


194.69
173.26
167.25
163.78
150.67
150.64
136.18
133.64
129.81
128.60
126.68
126.18
125.45
124.15
77.32
77.00
76.68
64.09
61.87
60.06
55.42
40.53
38.36
33.54
28.21
28.10
24.53
SSCF3
f1 (ppm)

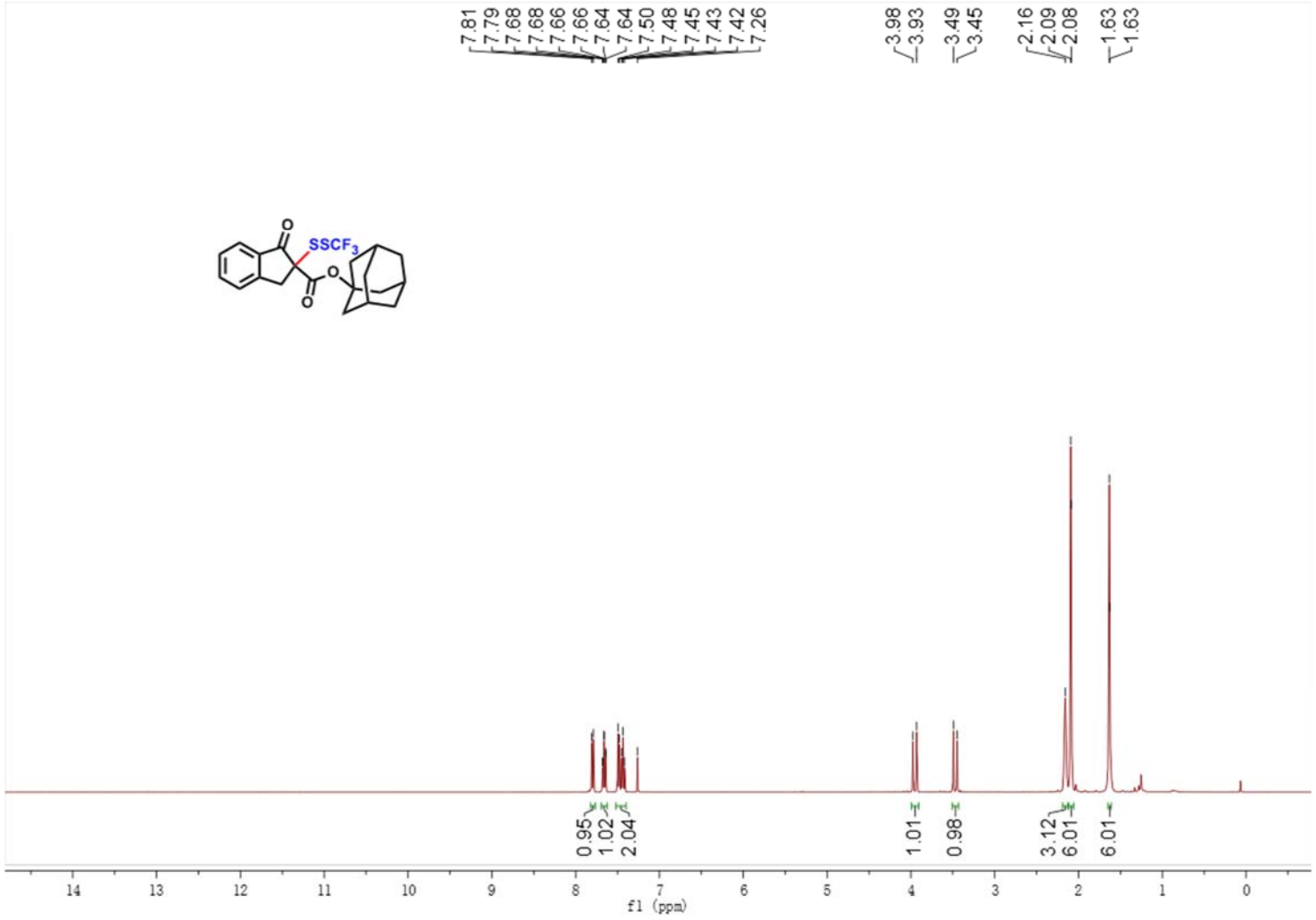
3t

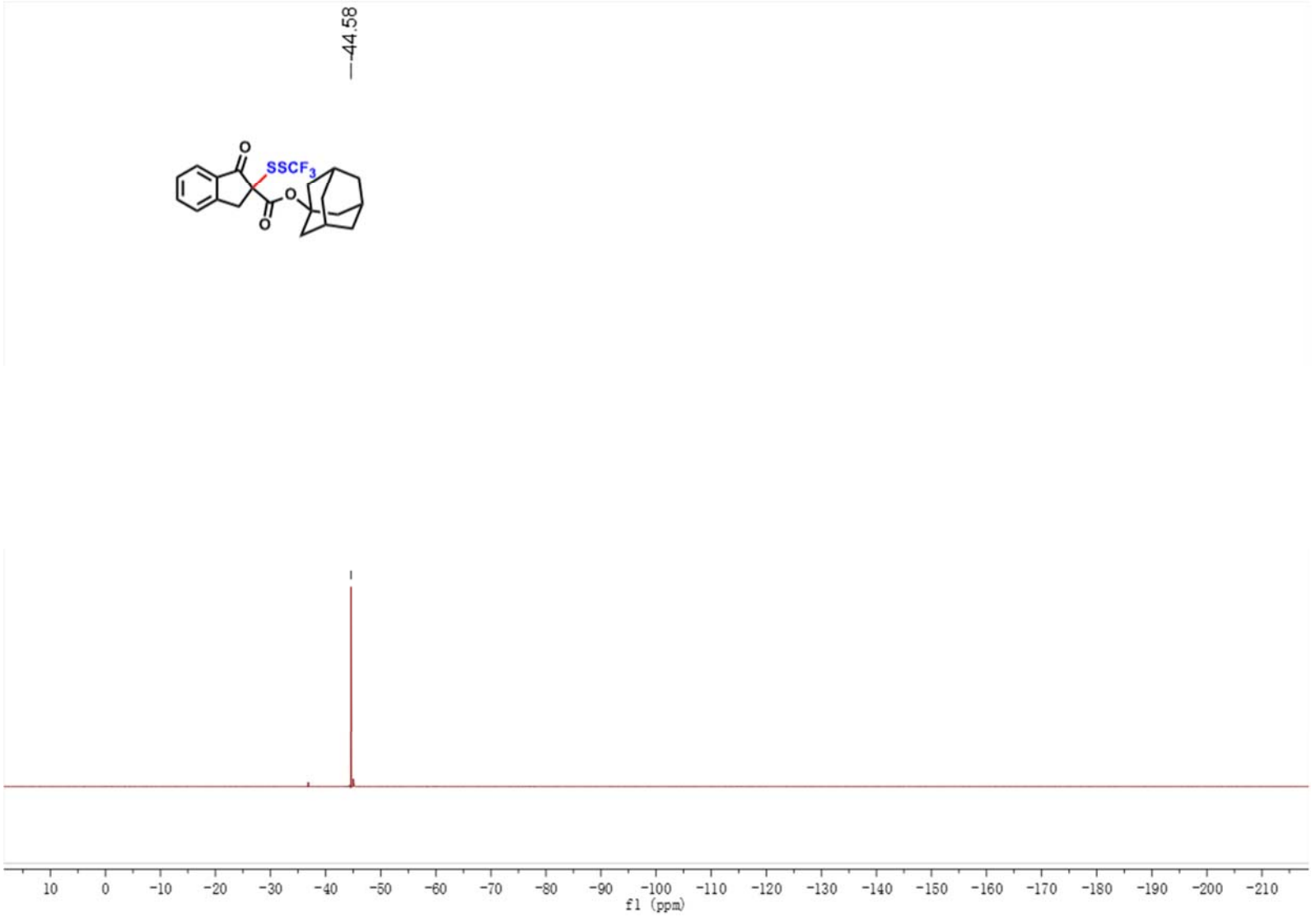

7.76
7.74
7.65
7.63
7.61
7.47
7.47
7.45
7.45
7.42
7.41
7.39
7.21
5.72
5.72
5.70
5.69
5.36
5.36
4.36
4.28
4.24
4.22
3.96
3.44
3.40
2.61
2.51
2.48
2.26
1.72
1.57
1.28
1.19
0.96
0.90
0.89
0.79
0.78
0.77
SSCF3
1.01
1.03
2.08
0.98
1.00
4.15
1.06
1.01
5.21
1.09
1.18
1.07
4.22
3.10
11.0 10.5 10.0 9.5 9.0 8.5 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)


-44.57
-44.58
SSCF3
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)


194.63
194.58
171.72
171.70
170.93
170.91
167.25
167.21
150.68
150.62
136.10
128.56
126.69
126.19
126.16
125.44
125.42
123.56
104.38
92.13
91.42
77.32
77.00
76.68
64.32
64.03
64.00
61.59
51.46
45.13
37.18
33.99
28.97
28.57
24.49
20.13
11.95
SSCF3
f1 (ppm)

3u


7.81
7.79
7.68
7.68
7.66
7.66
7.64
7.64
7.50
7.48
7.45
7.43
7.42
7.26
3.98
3.93
3.49
3.45
2.16
2.09
2.08
1.63
1.63
SSCF3
O
O
O
0.95
1.02
2.04
1.01
0.98
3.12
6.01
6.01
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


-44.58
SSCF3
O
O
O
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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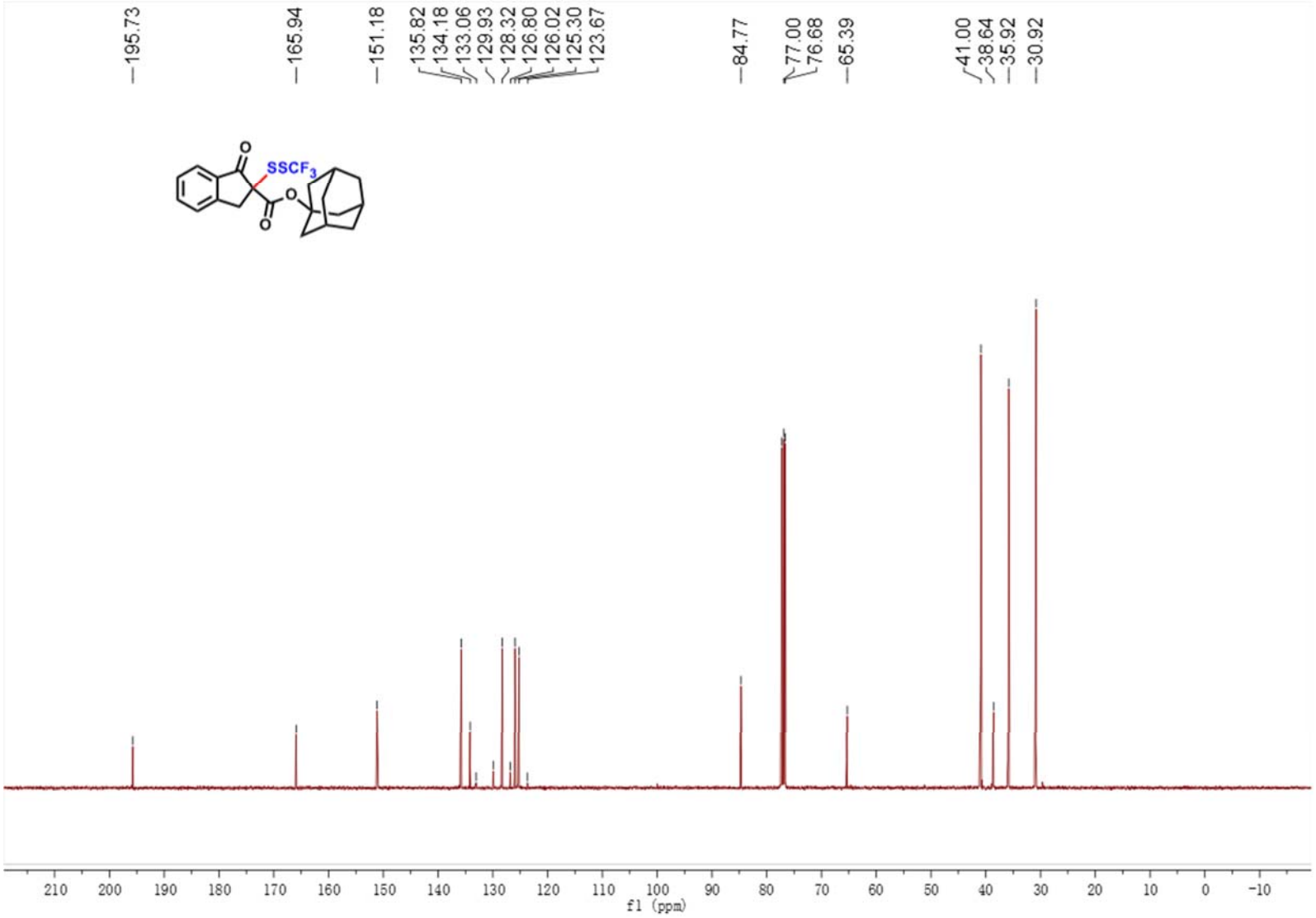
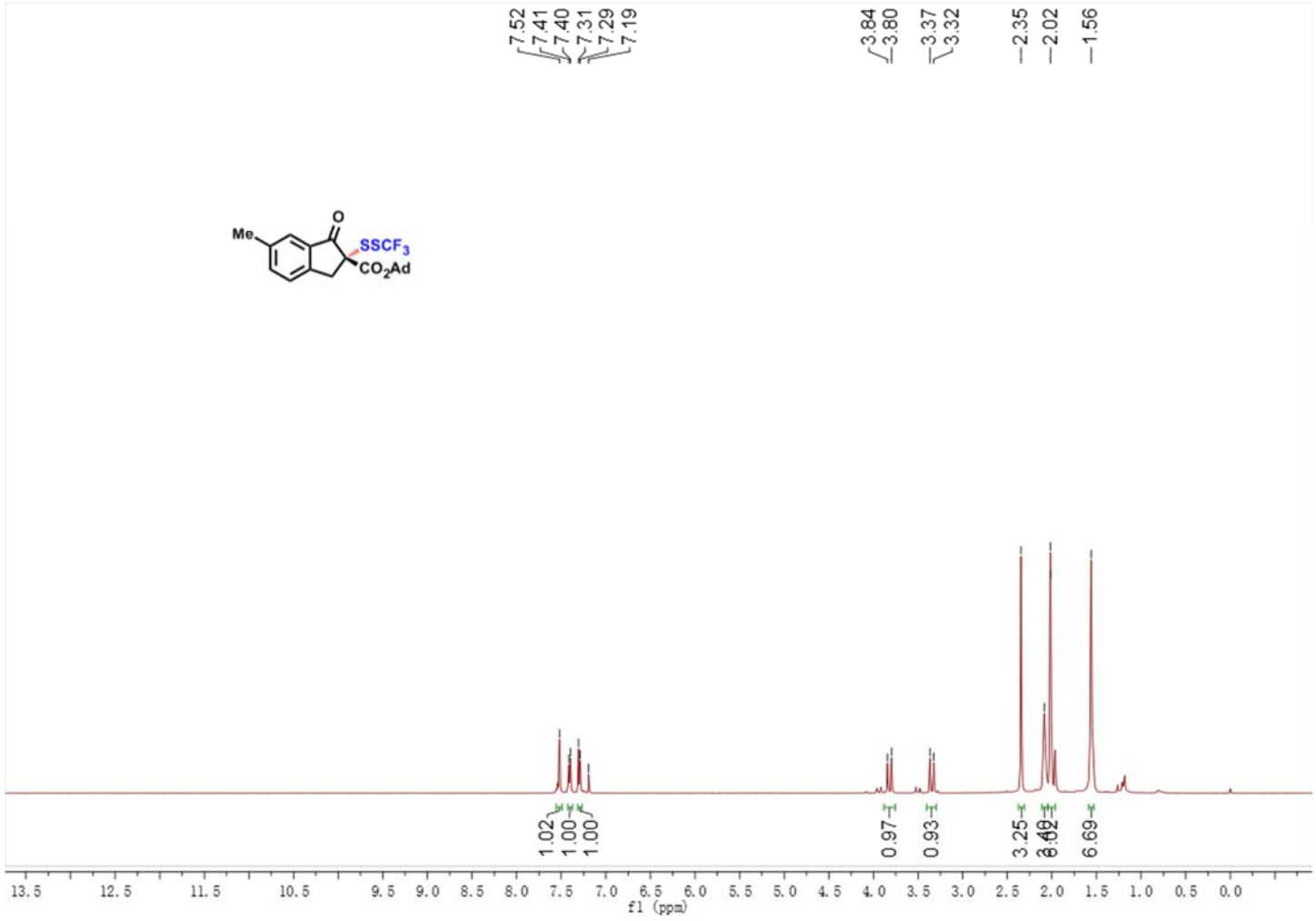
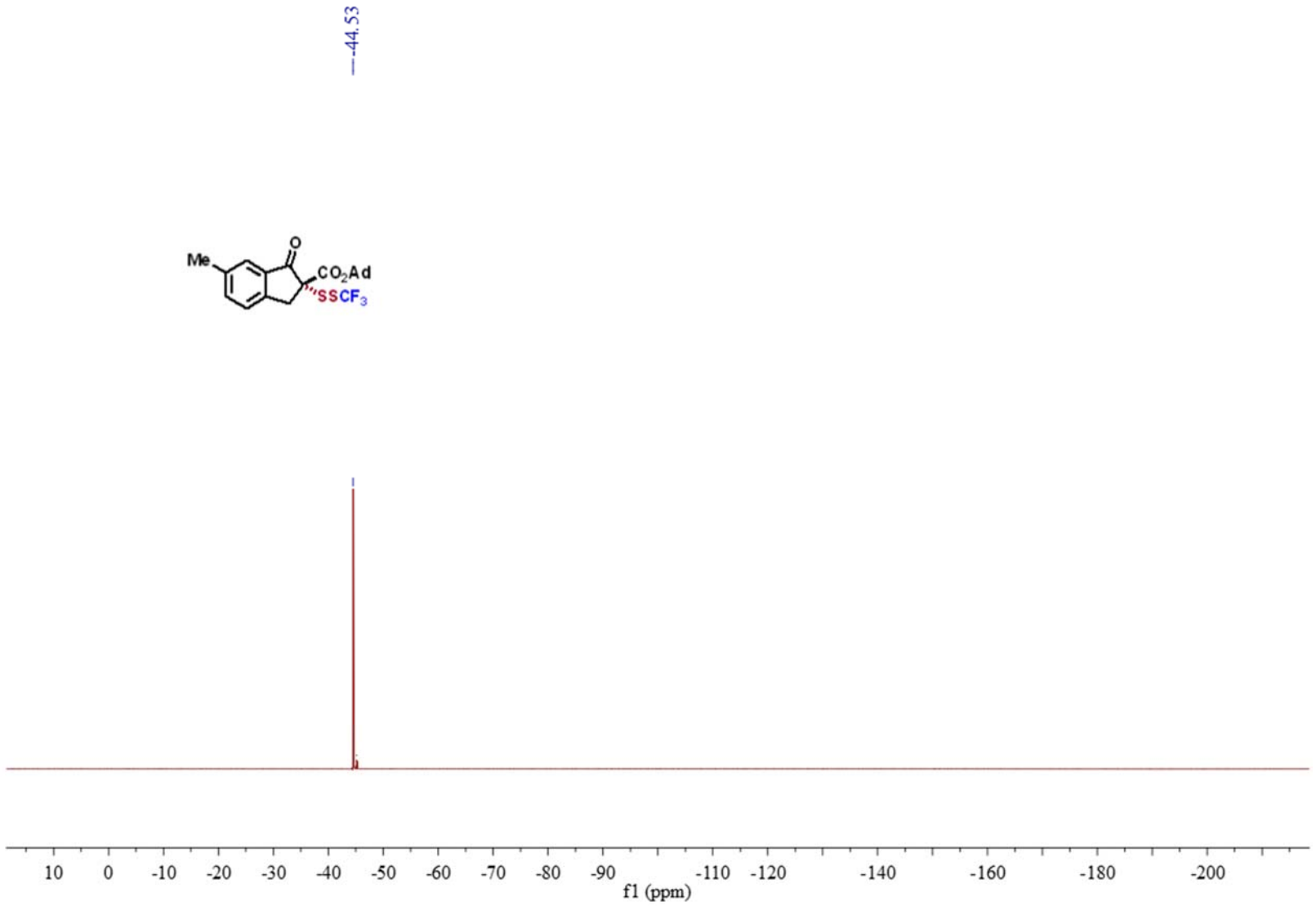
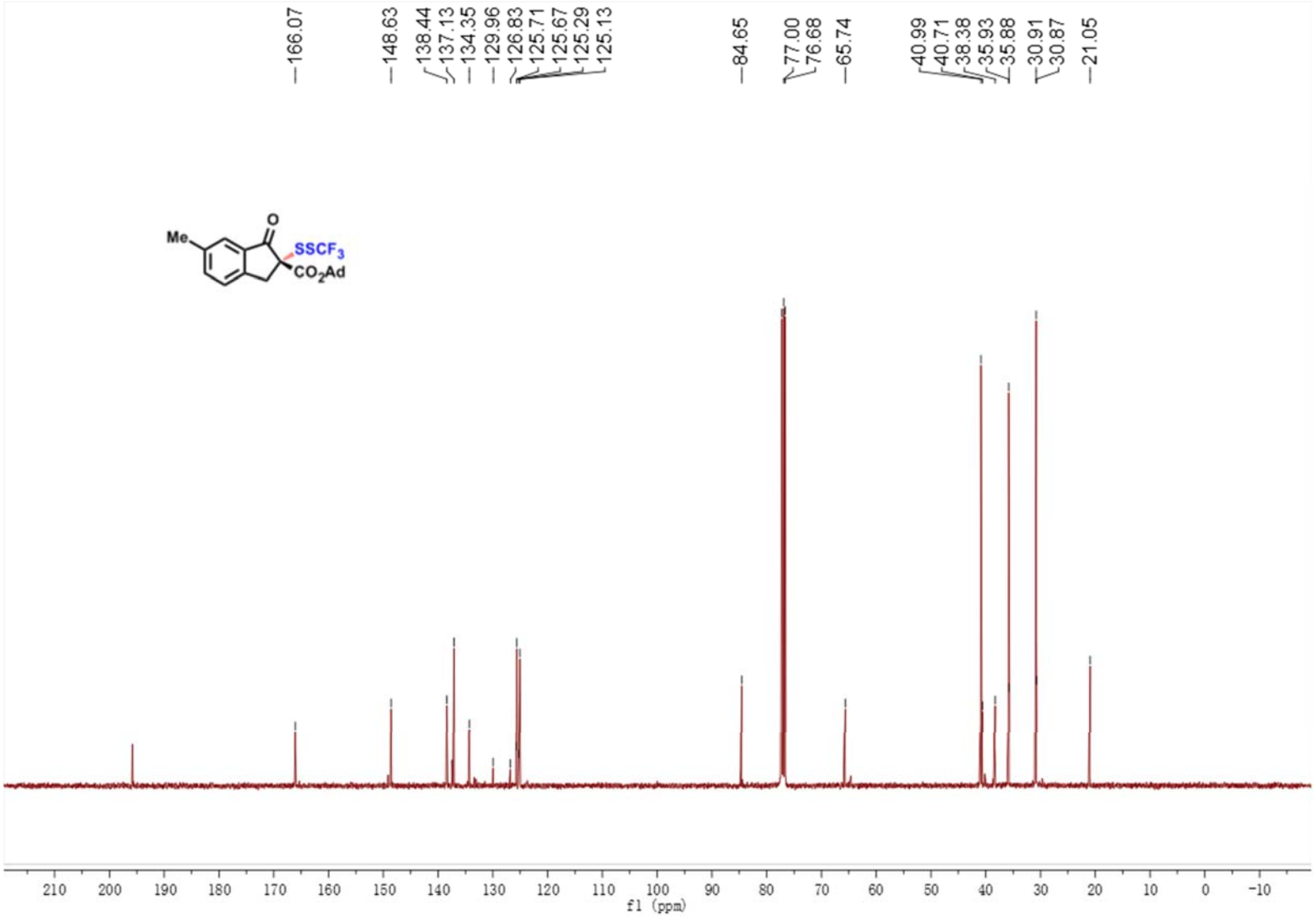
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


195.73
165.94
151.18
135.82
134.18
133.06
129.93
128.32
126.80
126.02
125.30
123.67
84.77
77.00
76.68
65.39
41.00
38.64
35.92
30.92
SSCF3
O
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

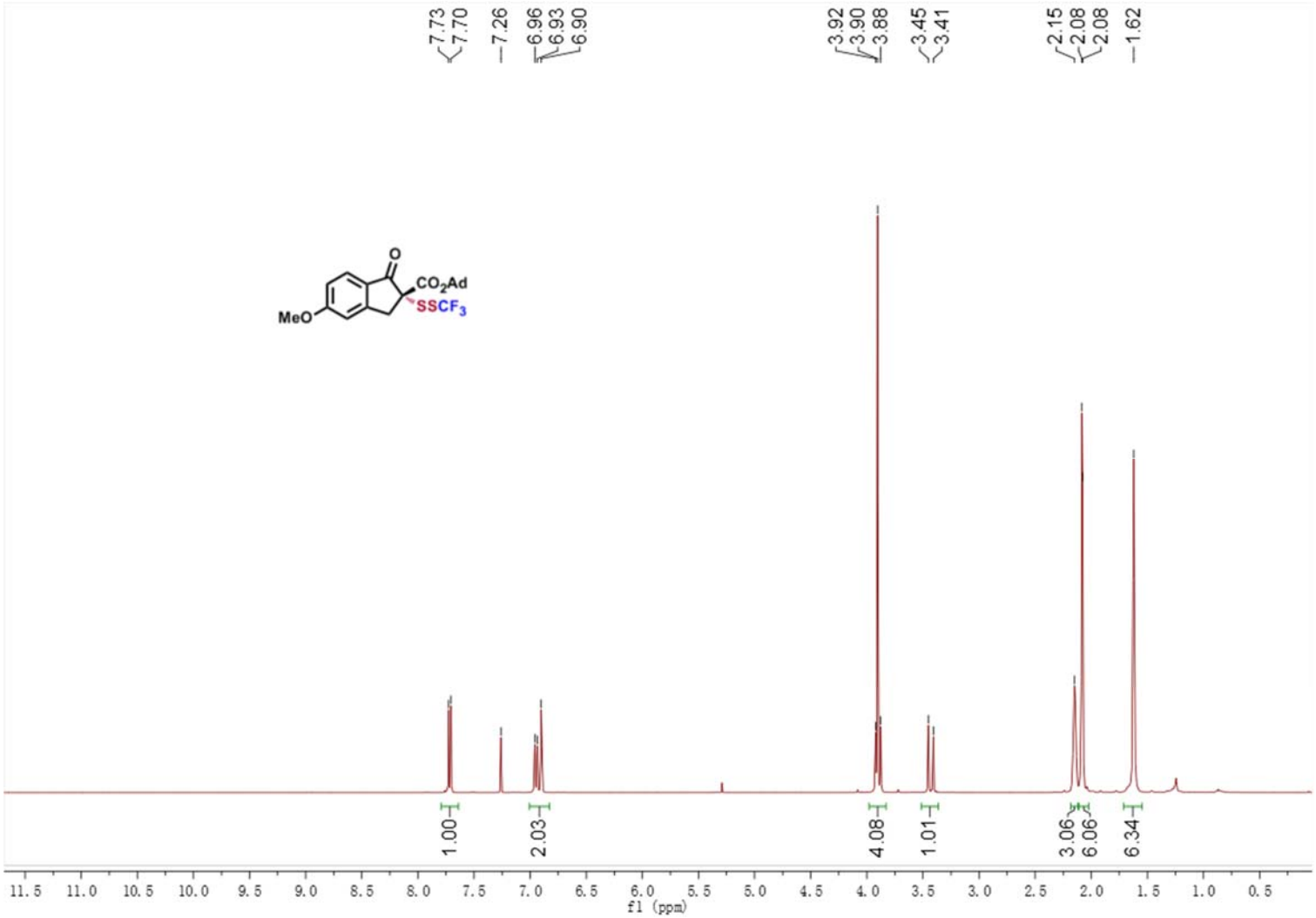
3v

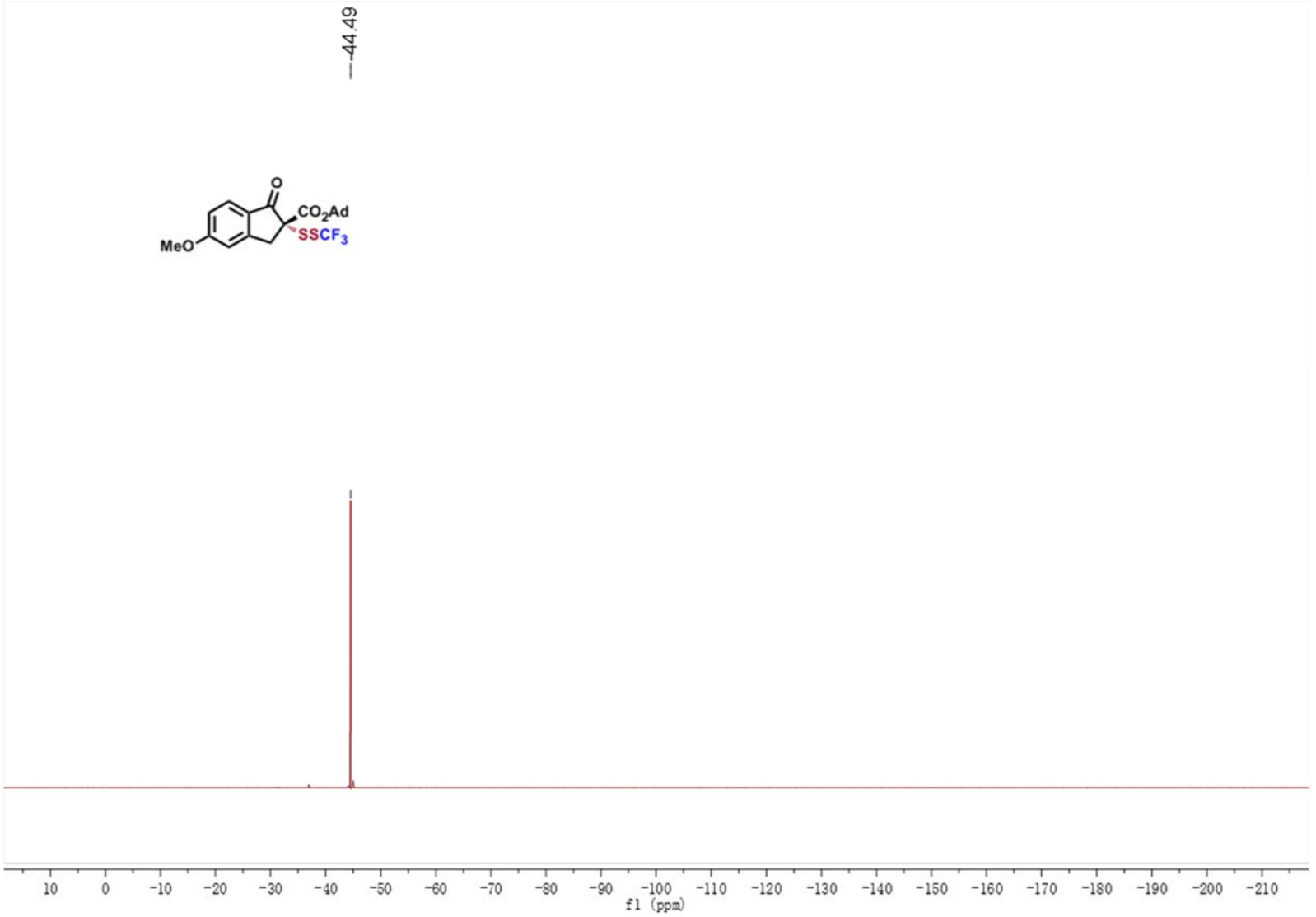

7.52
7.41
7.40
7.31
7.29
7.19
3.84
3.80
3.37
3.32
2.35
2.02
1.56
Me
O
SSCF3
CO2Ad
1.02
1.00
1.00
0.97
0.93
3.25
6.69
f1 (ppm)

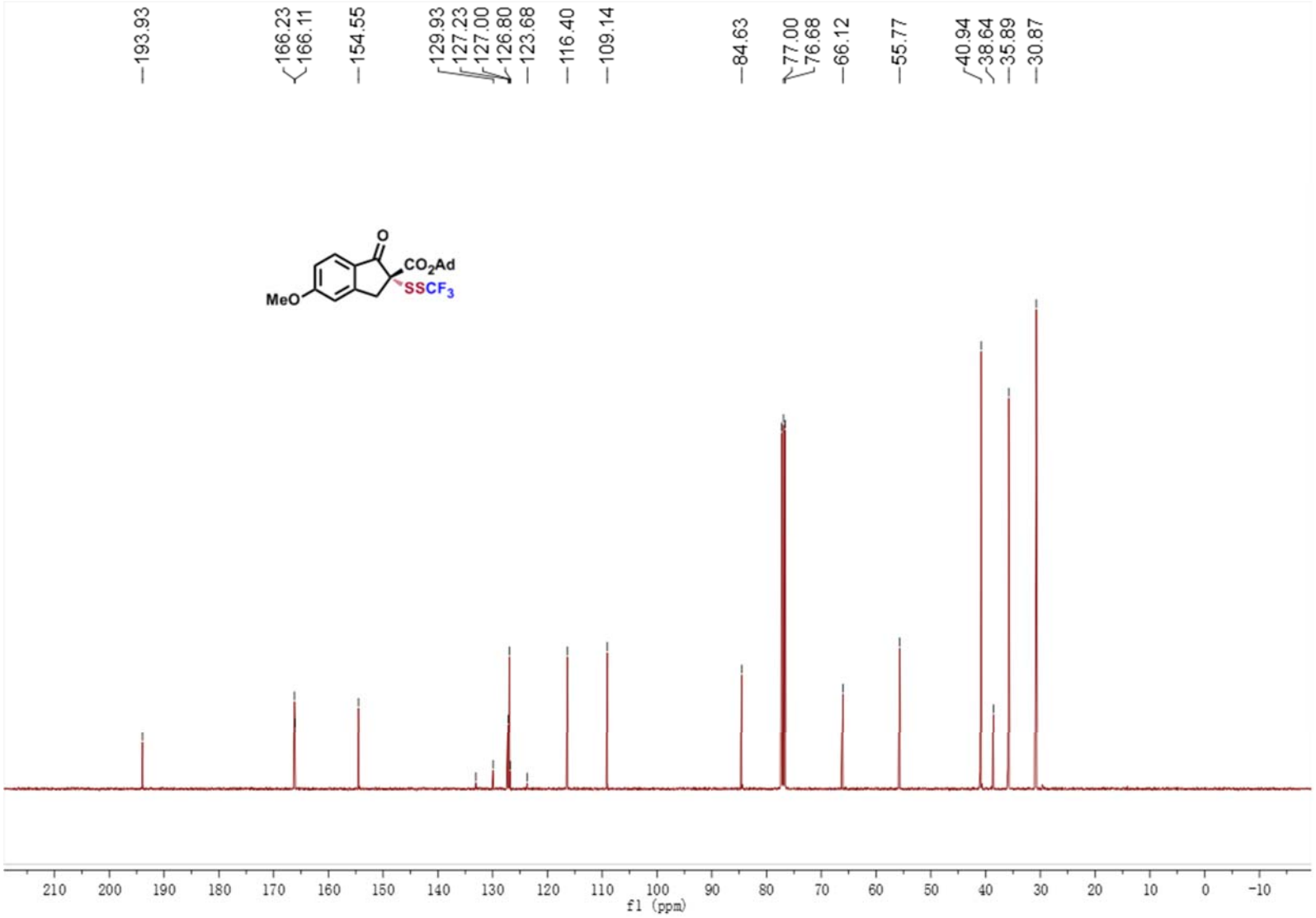

-44.53
Me
O
CO2Ad
SSCF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)


166.07
148.63
138.44
137.13
134.35
129.96
126.83
125.71
125.67
125.29
125.13
84.65
77.00
76.68
65.74
40.99
40.71
38.38
35.93
35.88
30.91
30.87
21.05
Me
O
SSCF3
CO2Ad
f1 (ppm)

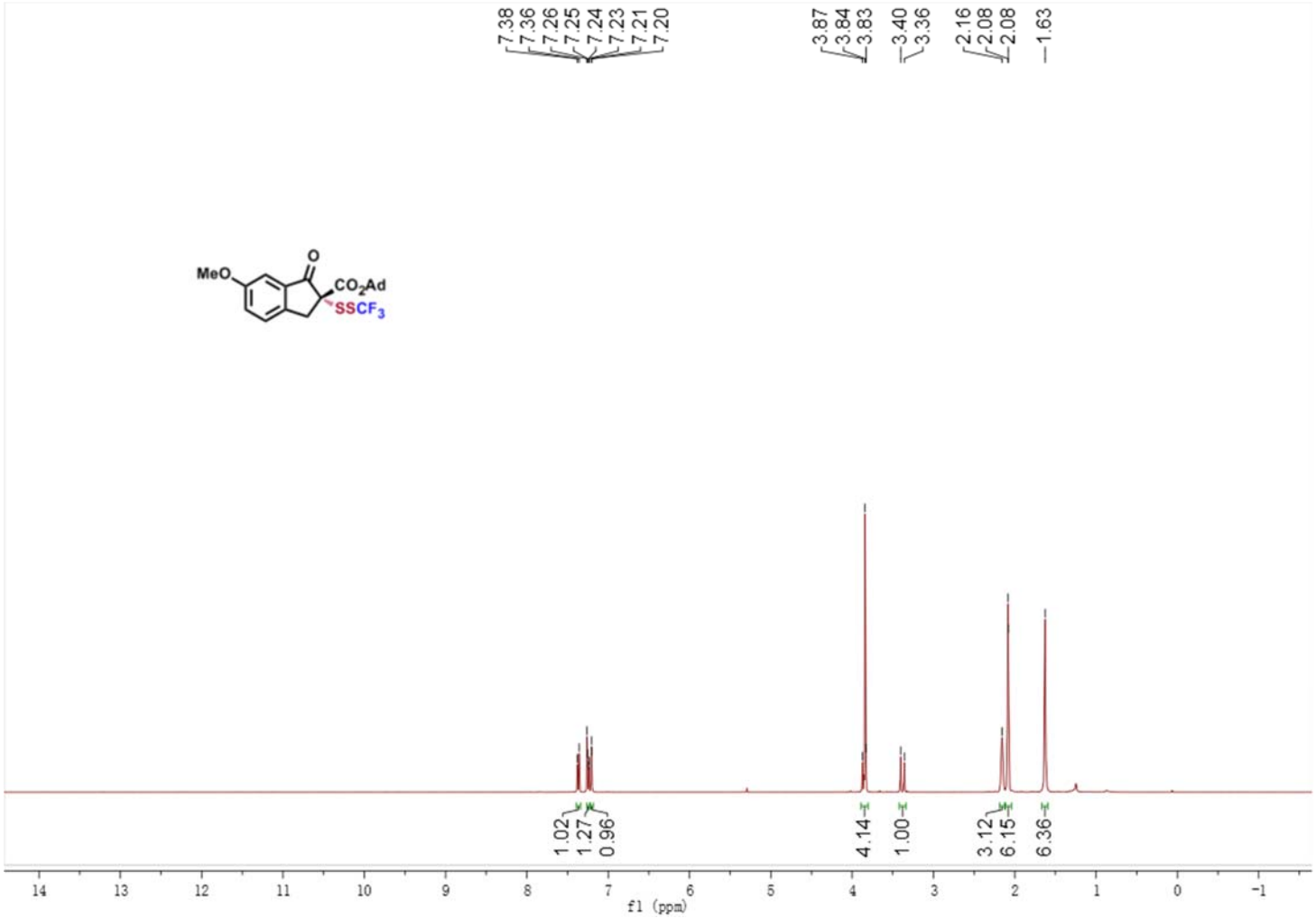
3w

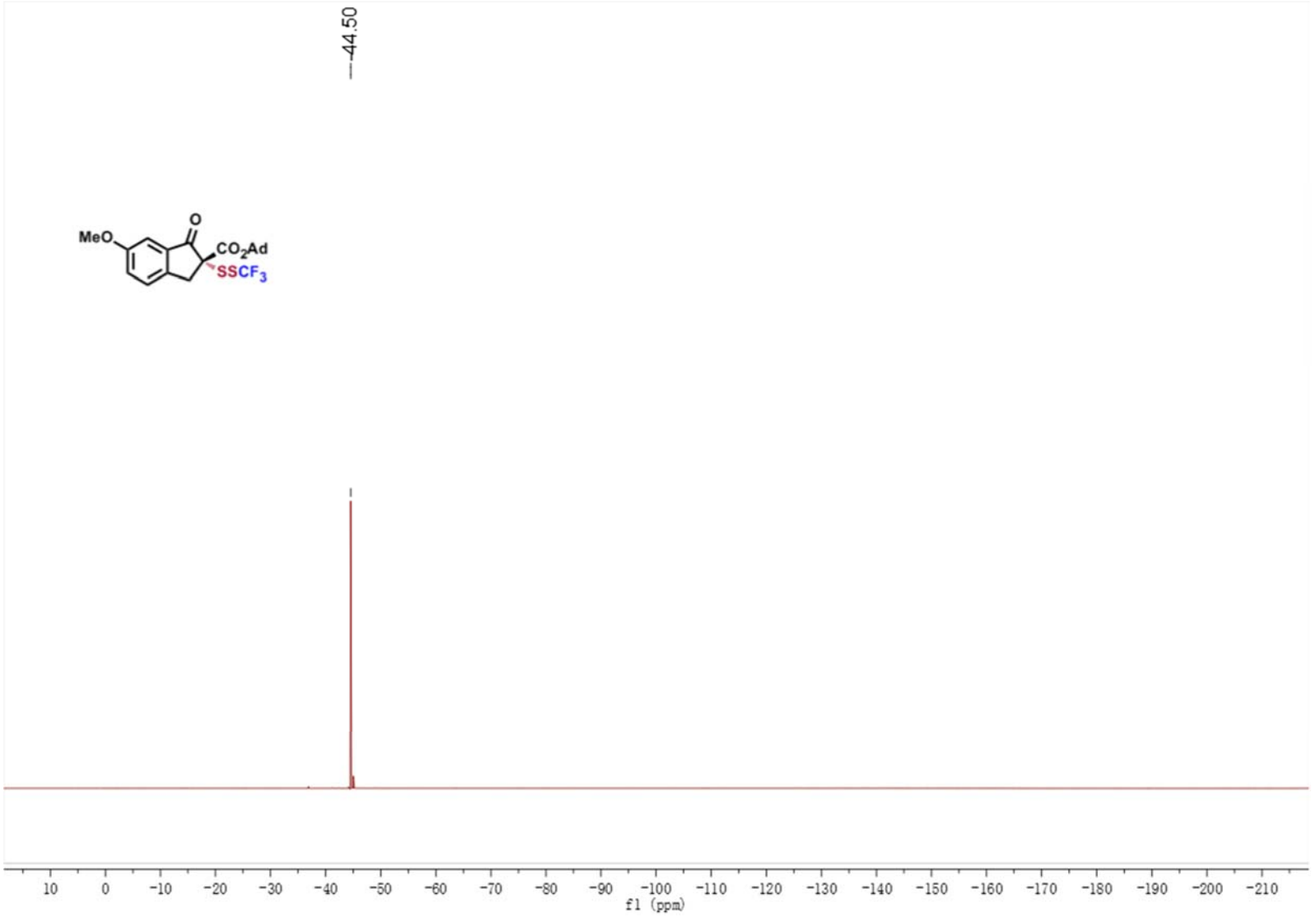

7.73
7.70
7.26
6.96
6.93
6.90
3.92
3.90
3.88
3.45
3.41
2.15
2.08
2.08
1.62
O
CO2Ad
SSCF3
MeO
1.00
2.03
4.08
1.01
3.06
6.06
6.34
f1 (ppm)

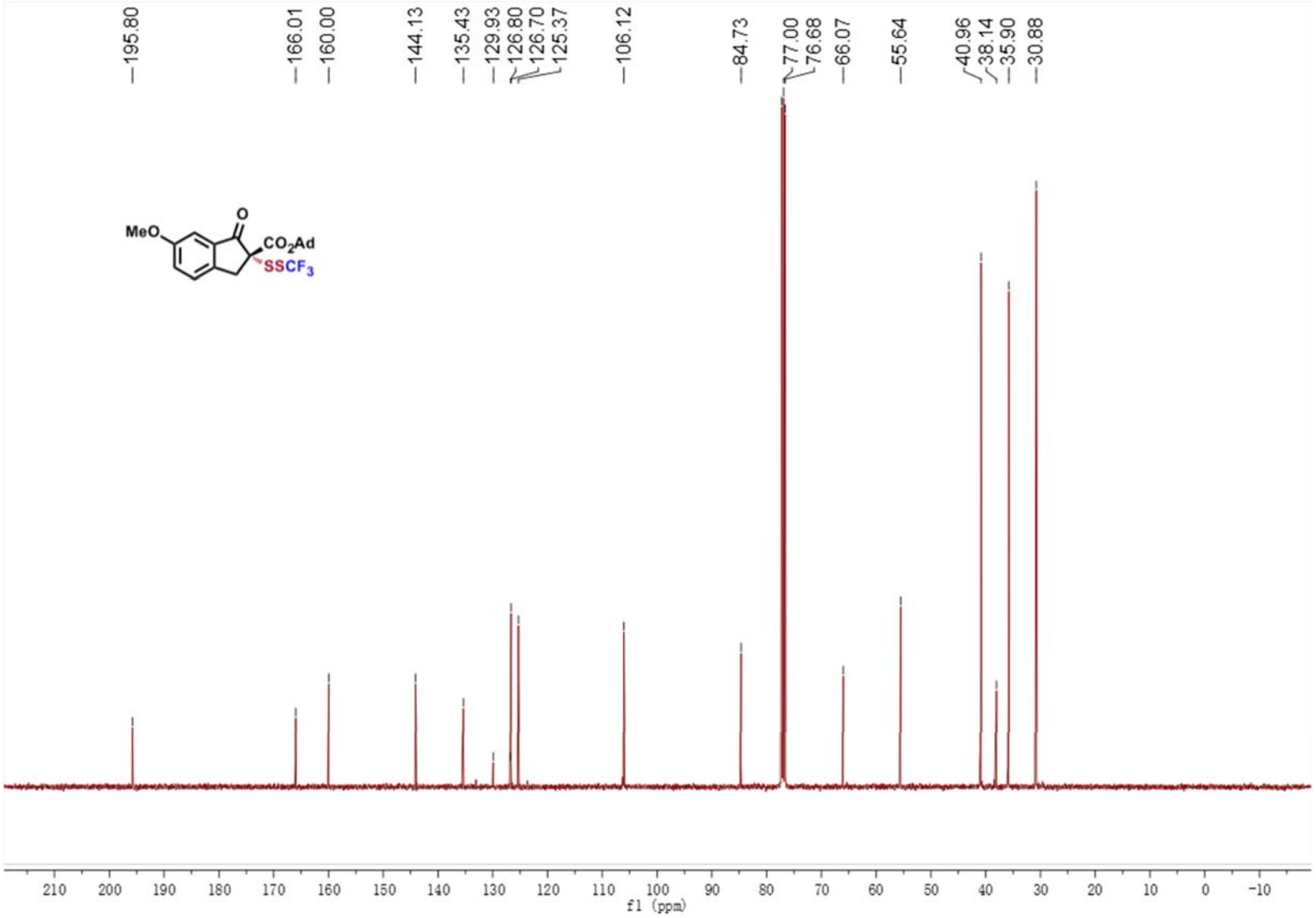

-44.49
O
CO2Ad
SSCF3
MeO
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


193.93
166.23
166.11
154.55
129.93
127.23
127.00
126.80
123.68
116.40
109.14
84.63
77.00
76.68
66.12
55.77
40.94
38.64
35.89
30.87
O
CO2Ad
SSCF3
MeO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

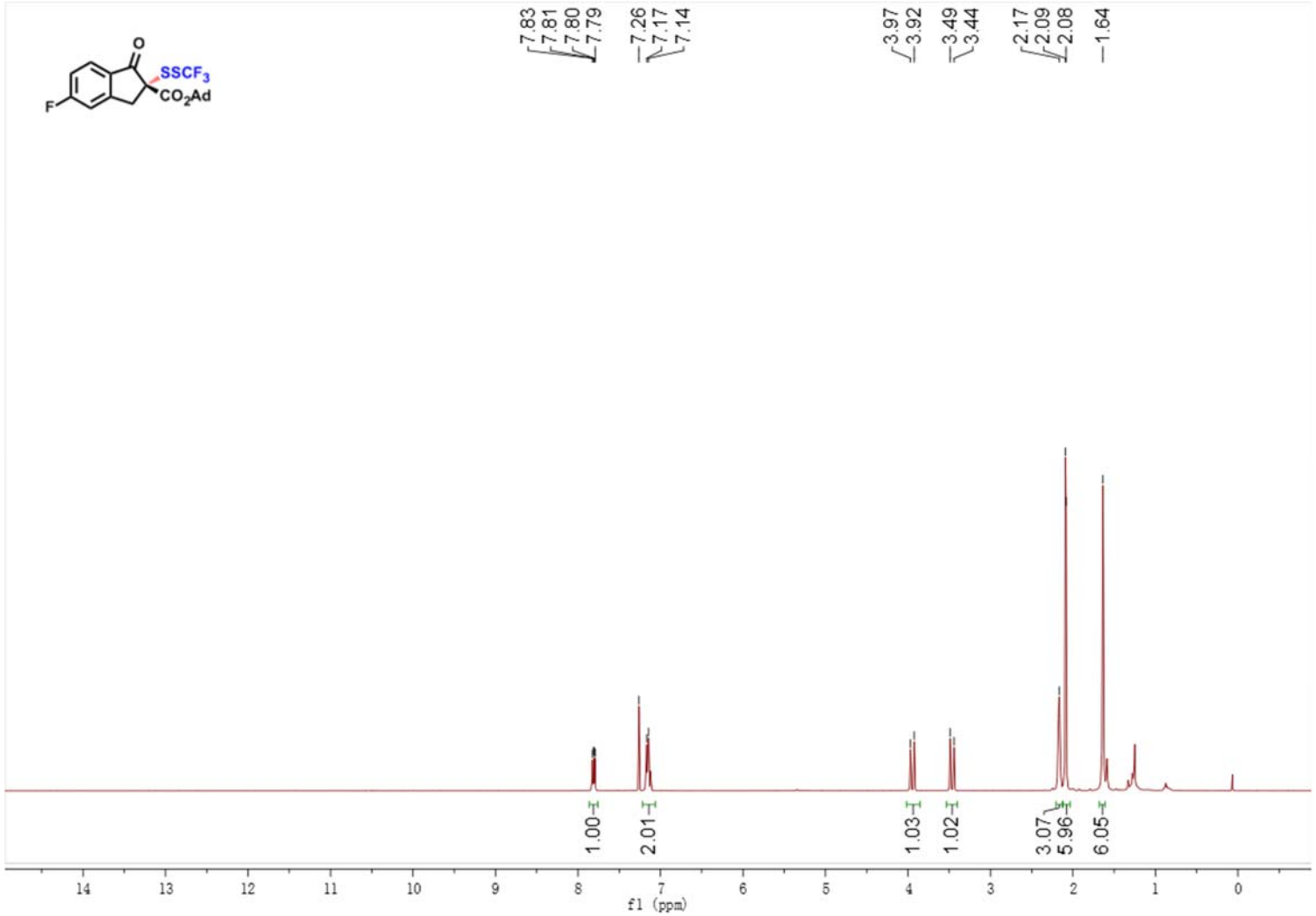
3x

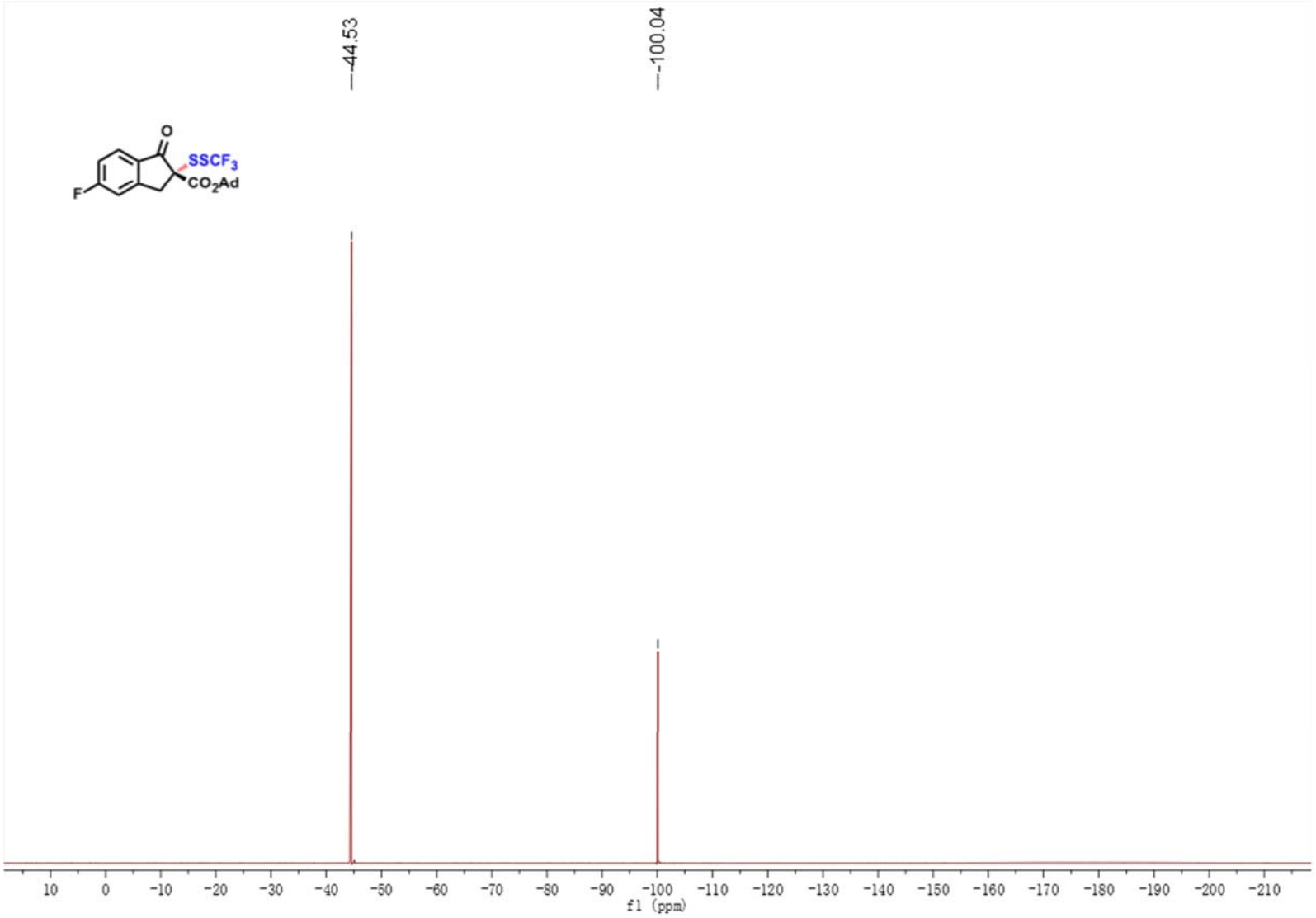

7.38
7.36
7.26
7.25
7.24
7.23
7.21
7.20
3.87
3.84
3.83
3.40
3.36
2.16
2.08
2.08
1.63
MeO
O
CO2Ad
SSCF3
1.02
1.27
0.96
4.14
1.00
3.12
6.15
6.36
f1 (ppm)

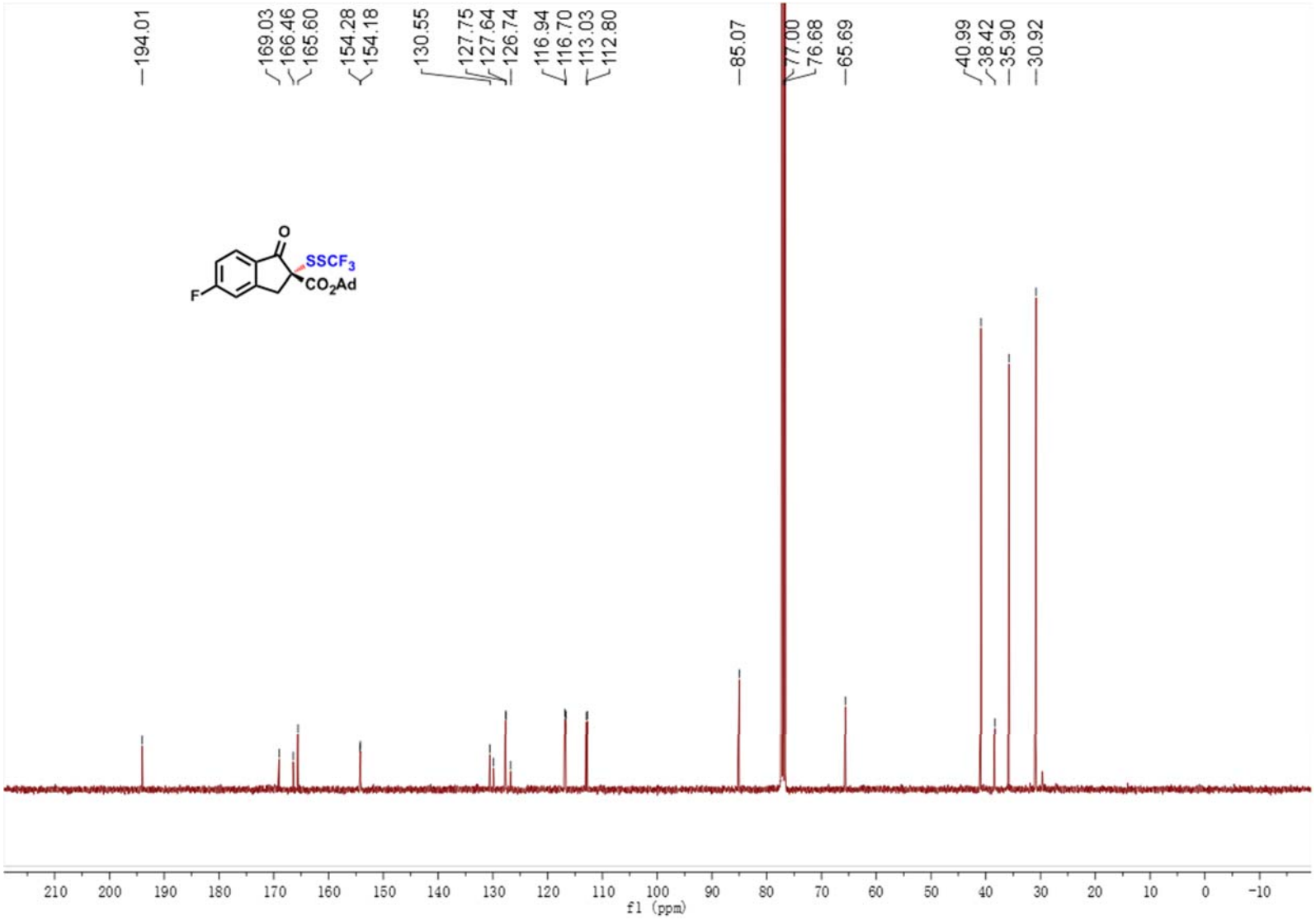

-44.50
MeO
O
CO2Ad
SSCF3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


195.80
166.01
160.00
144.13
135.43
129.93
126.80
126.70
125.37
106.12
84.73
77.00
76.68
66.07
55.64
40.96
38.14
35.90
30.88
MeO
O
CO2Ad
SSCF3
f1 (ppm)

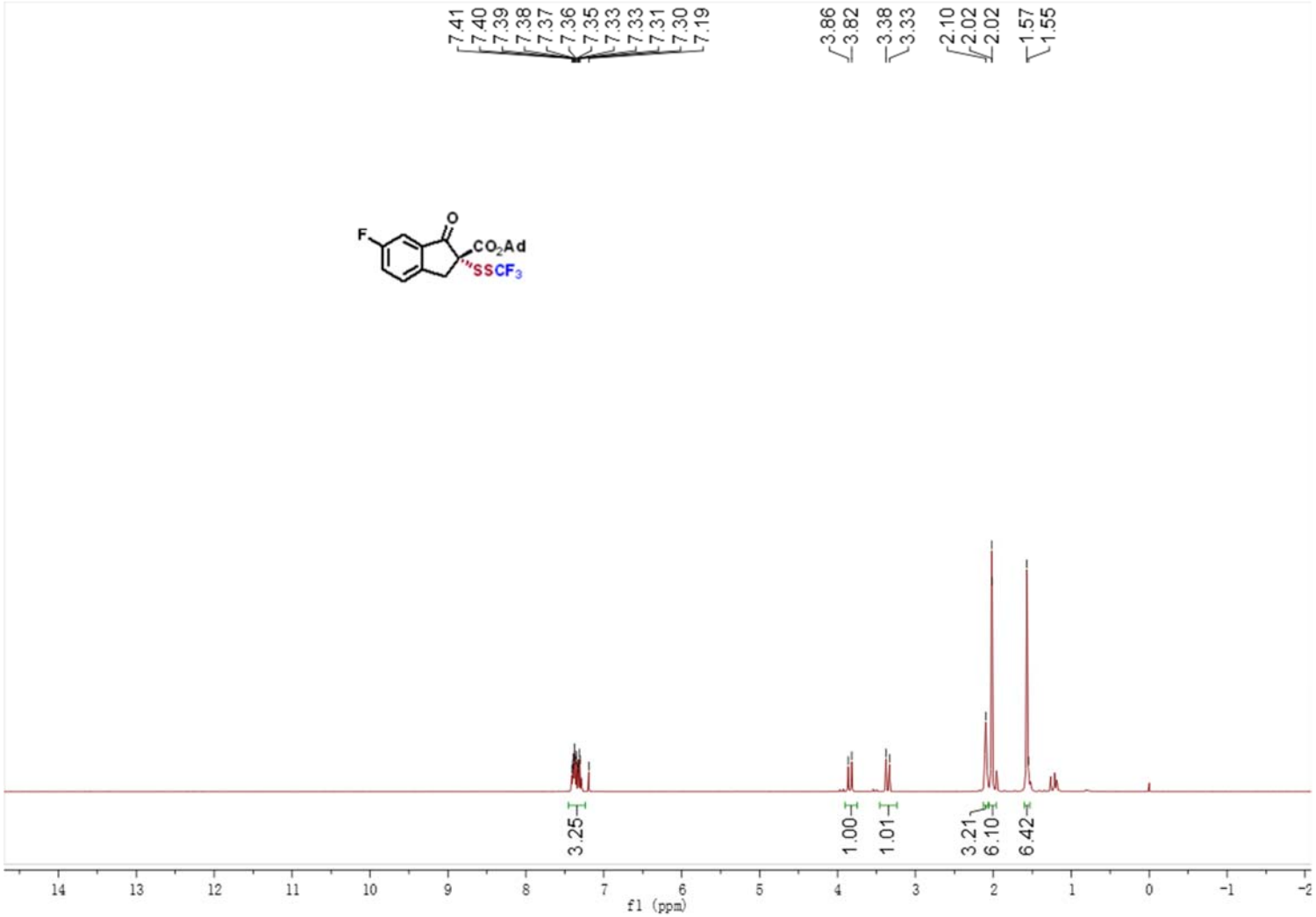
3y


7.83
7.81
7.80
7.79
7.26
7.17
7.14
3.97
3.92
3.49
3.44
2.17
2.09
2.08
1.64
1.00
2.01
1.03
1.02
3.07
5.96
6.05
f1 (ppm)


-44.53
-100.04
O
SSCF3
CO2Ad
F
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)


194.01
169.03
166.46
165.60
154.28
154.18
130.55
127.75
127.64
126.74
116.94
116.70
113.03
112.80
85.07
77.00
76.68
65.69
40.99
38.42
35.90
30.92
O
SSCF3
CO2Ad
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3z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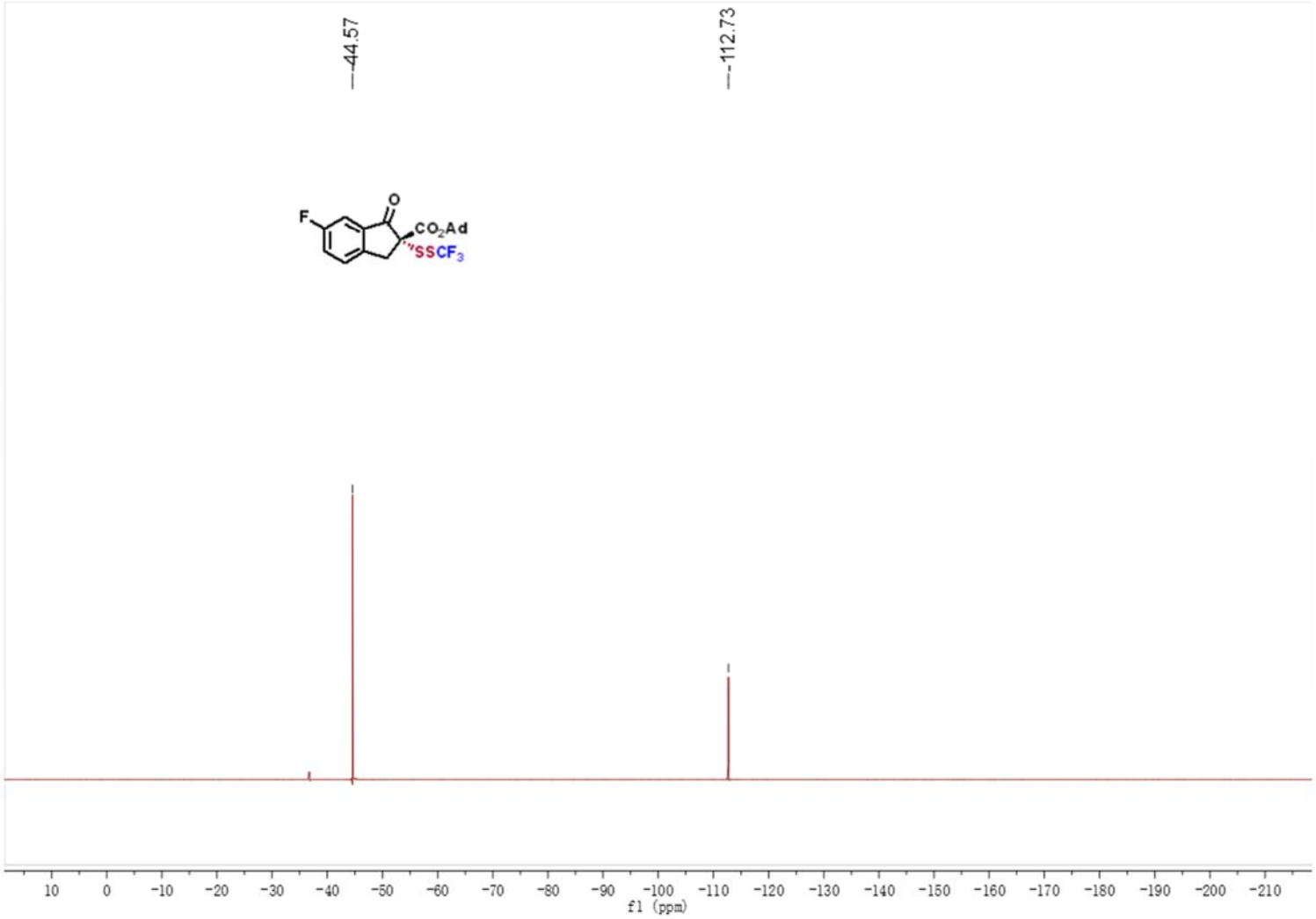
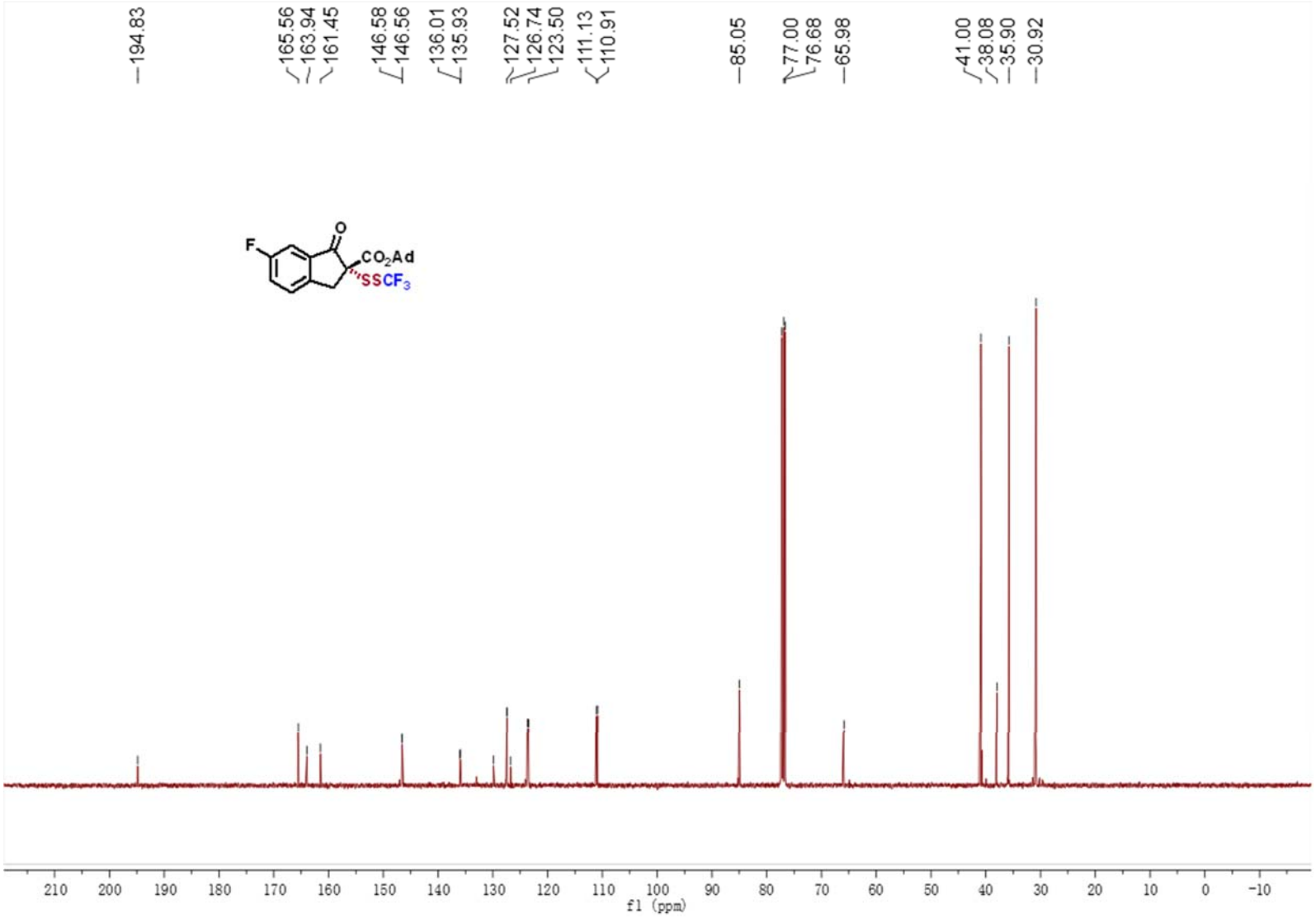
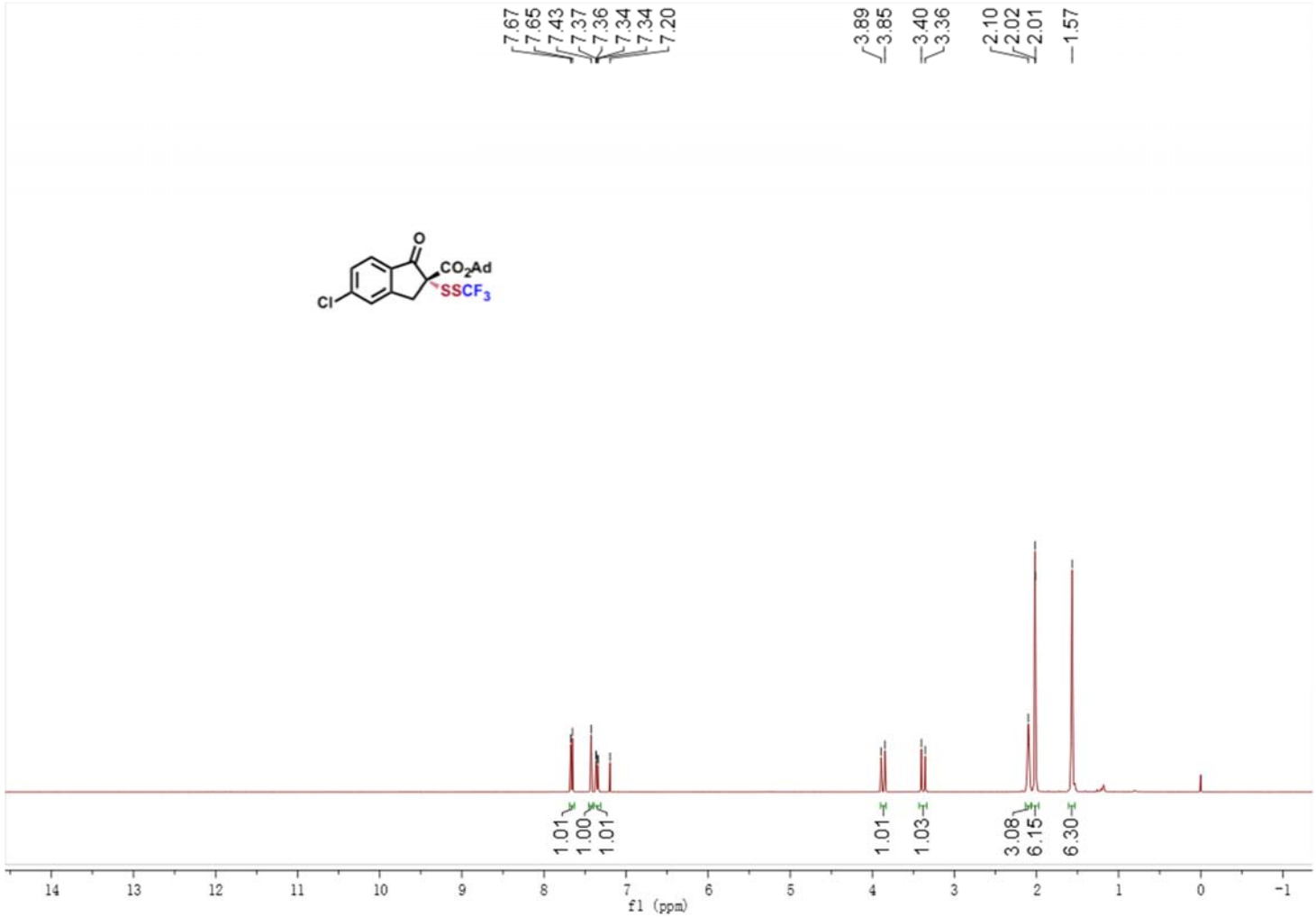
7.36
7.35
7.33
7.33
7.31
7.30
7.19
3.86
3.82
3.38
3.33
2.10
2.02
2.02
1.57
1.55
F
O
CO2Ad
SSCF3
3.25
1.00
1.01
3.21
6.10
6.42
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

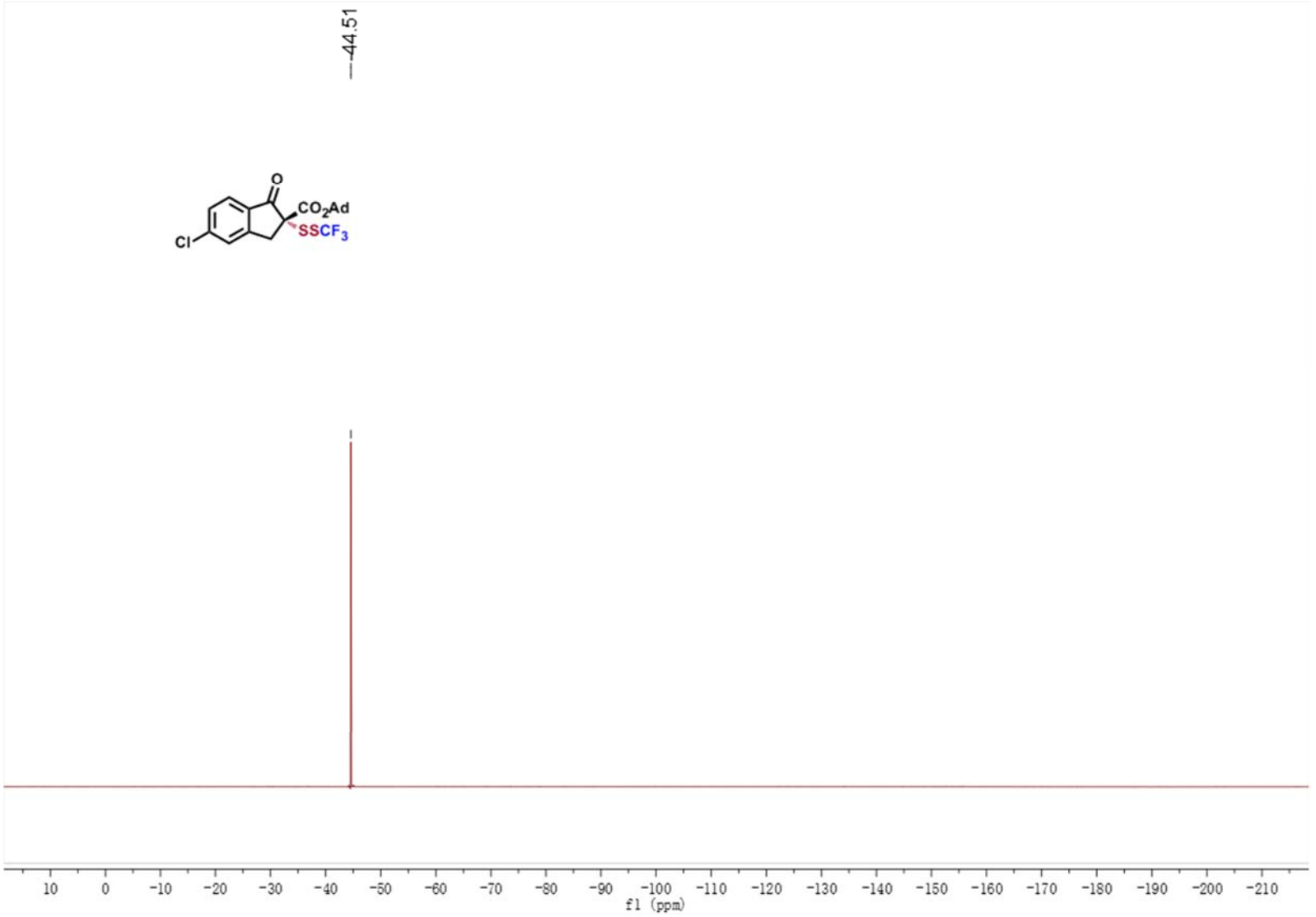
3z

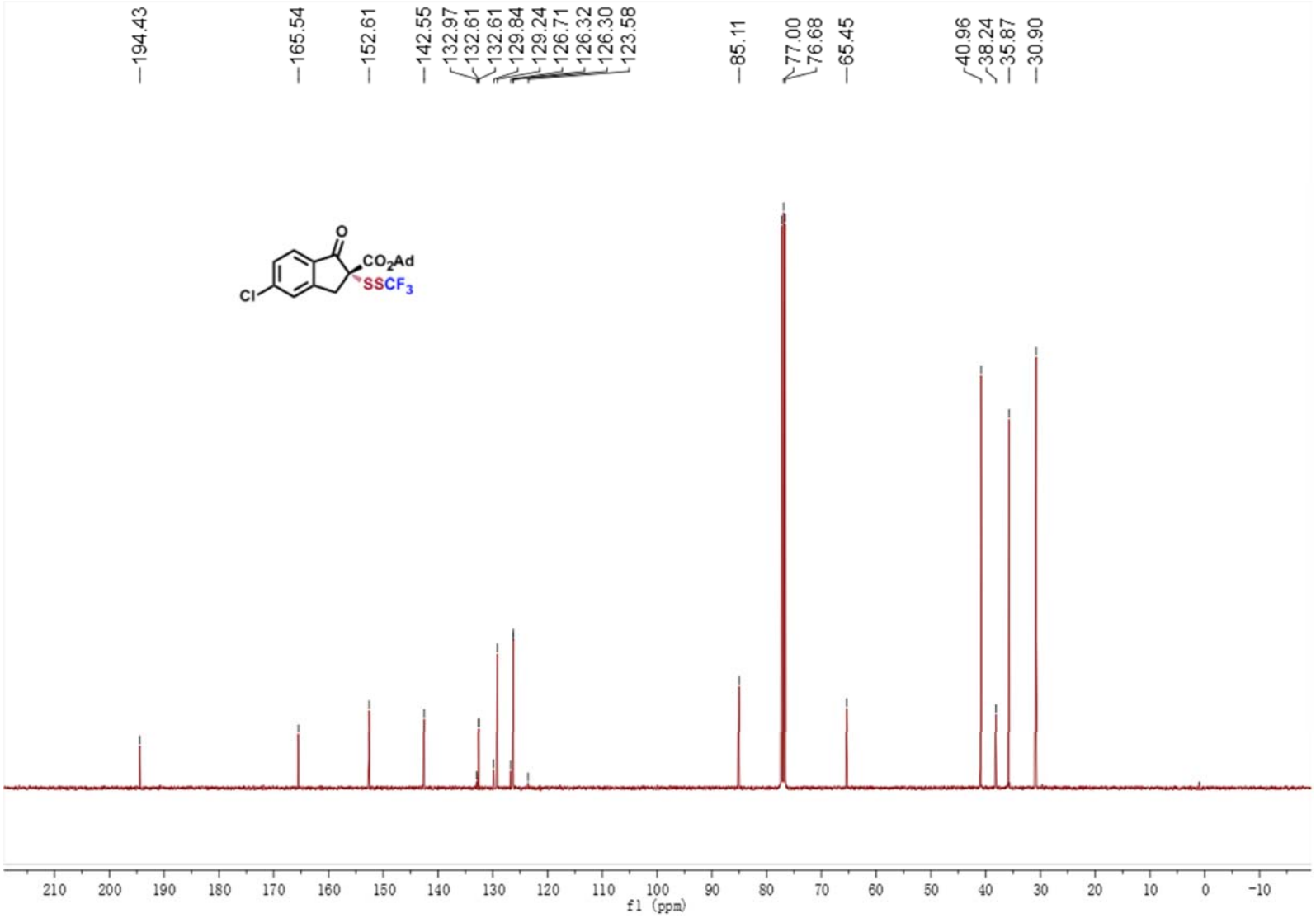

-44.57
-112.73
F
O
CO2Ad
SSCF3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


194.83
165.56
163.94
161.45
146.58
146.56
136.01
135.93
127.52
126.74
123.50
111.13
110.91
85.05
77.00
76.68
65.98
41.00
38.08
35.90
30.92
F
O
CO2Ad
SSCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

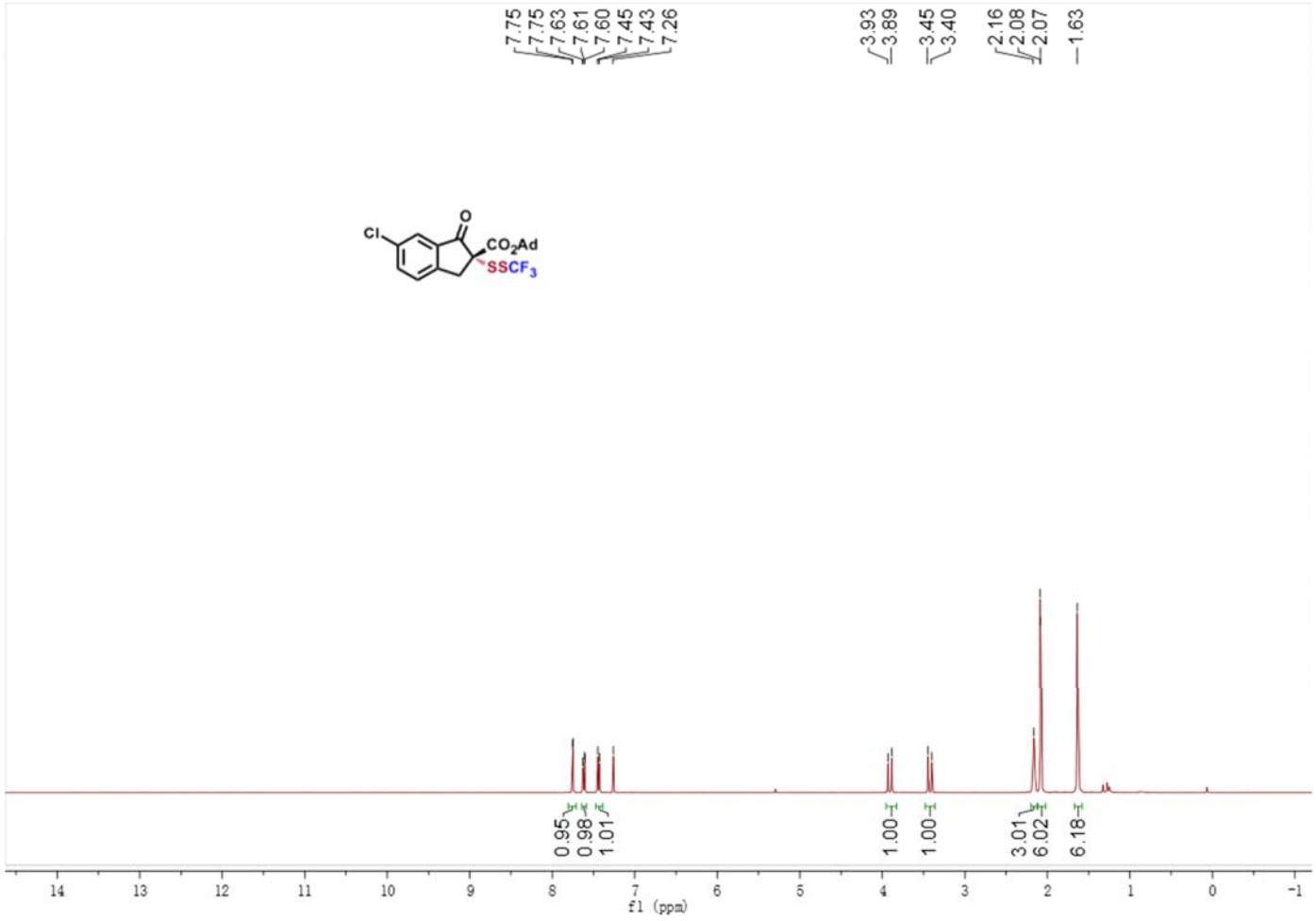
3aa

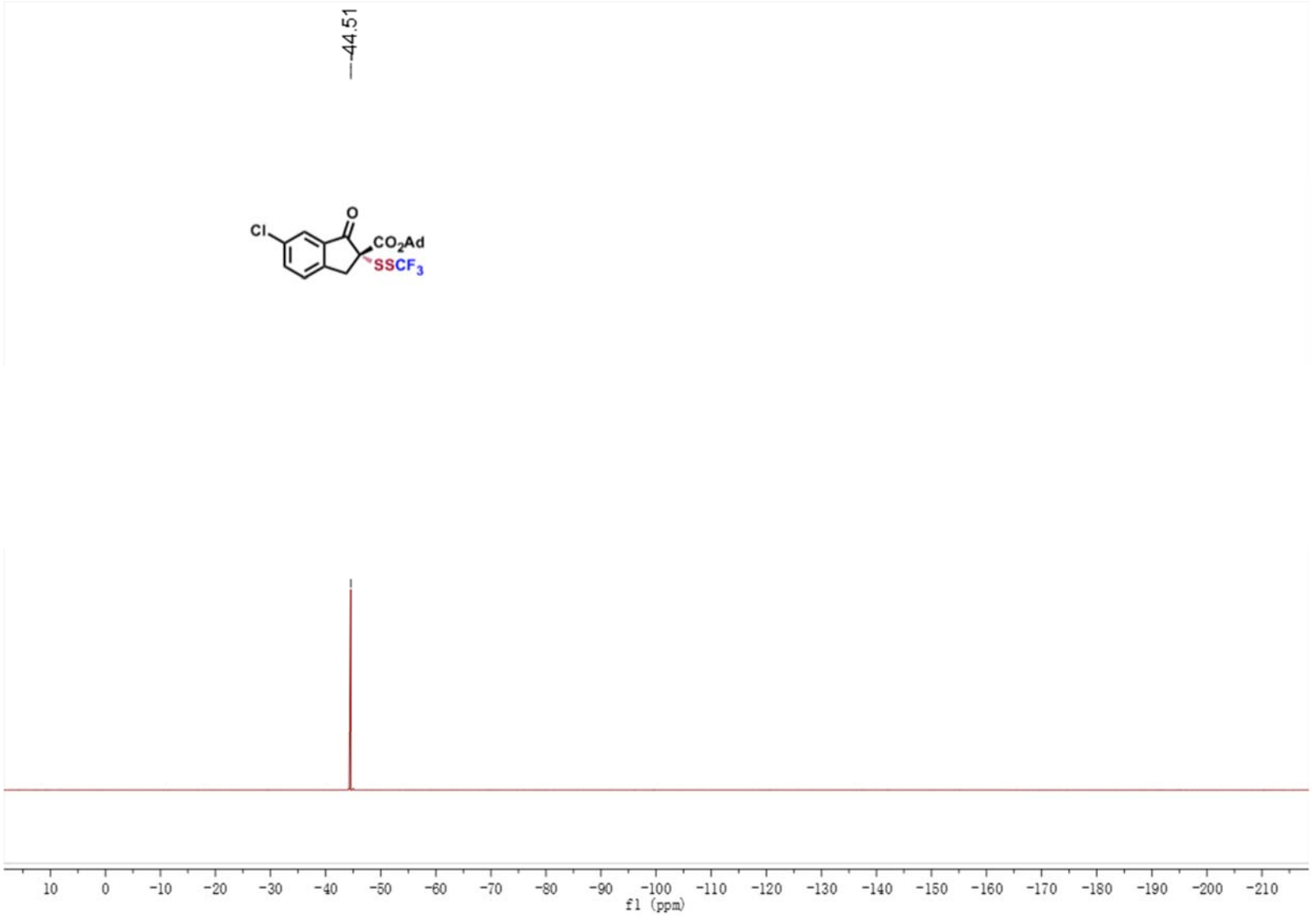

7.67
7.65
7.43
7.37
7.36
7.34
7.34
7.20
3.89
3.85
3.40
3.36
2.10
2.02
2.01
1.57
O
CO2Ad
SSCF3
Cl
1.01
1.00
1.01
1.01
1.03
3.08
6.15
6.30
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

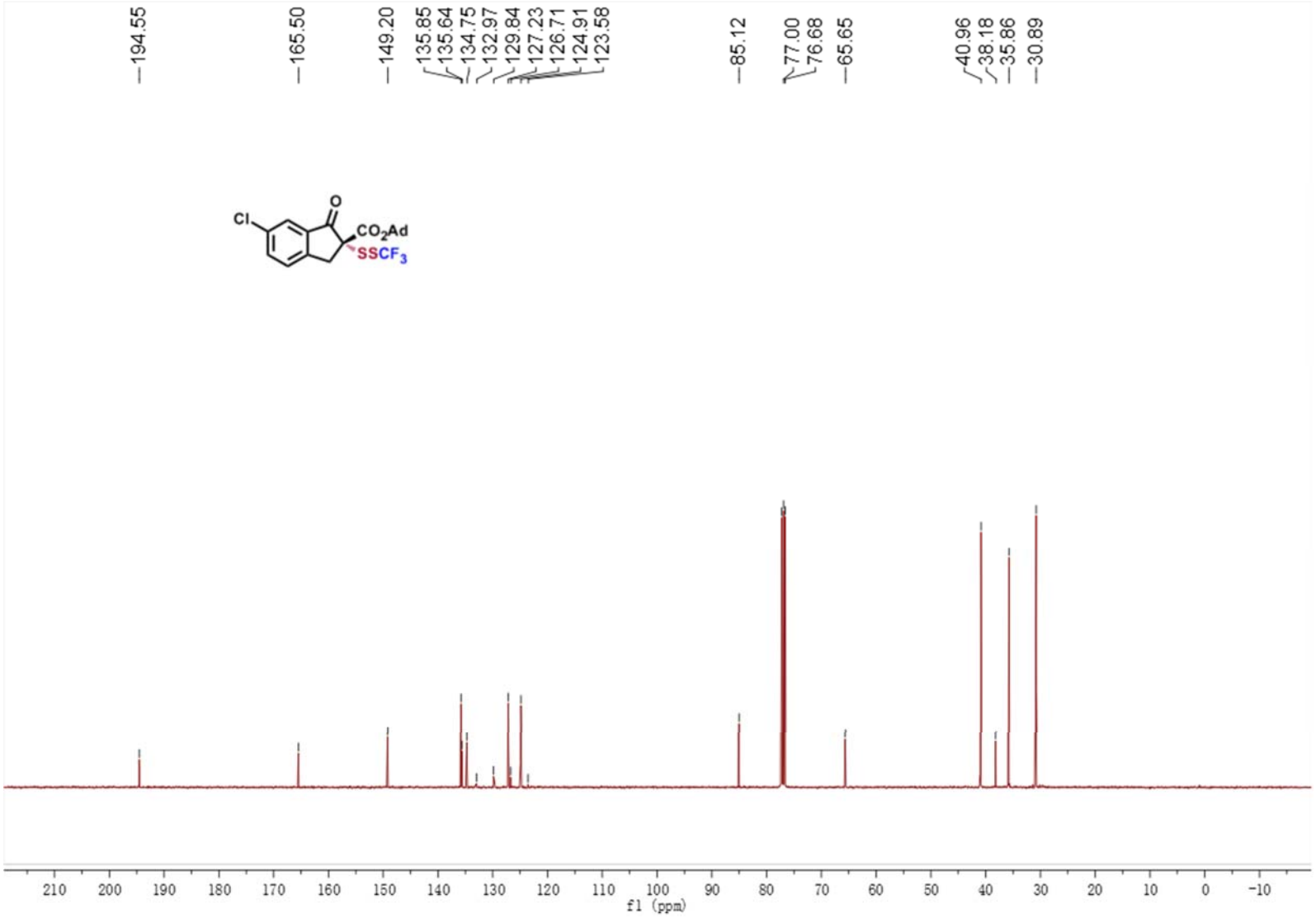

-44.51
O
CO2Ad
SSCF3
Cl
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


194.43
165.54
152.61
142.55
132.97
132.61
132.61
129.84
129.24
126.71
126.32
126.30
123.58
85.11
77.00
76.68
65.45
40.96
38.24
35.87
30.90
O
CO2Ad
SSCF3
Cl
f1 (ppm)

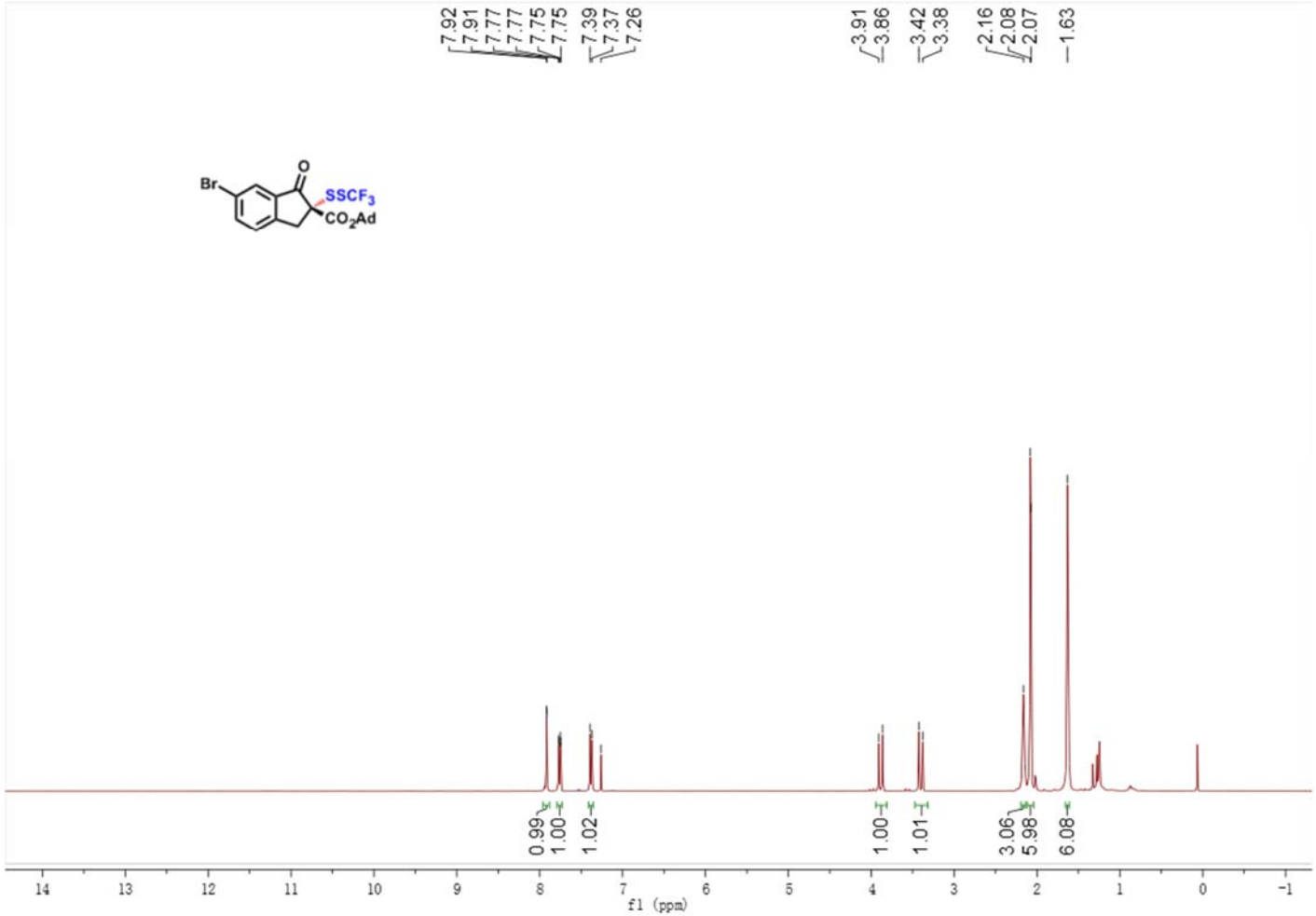
3ab

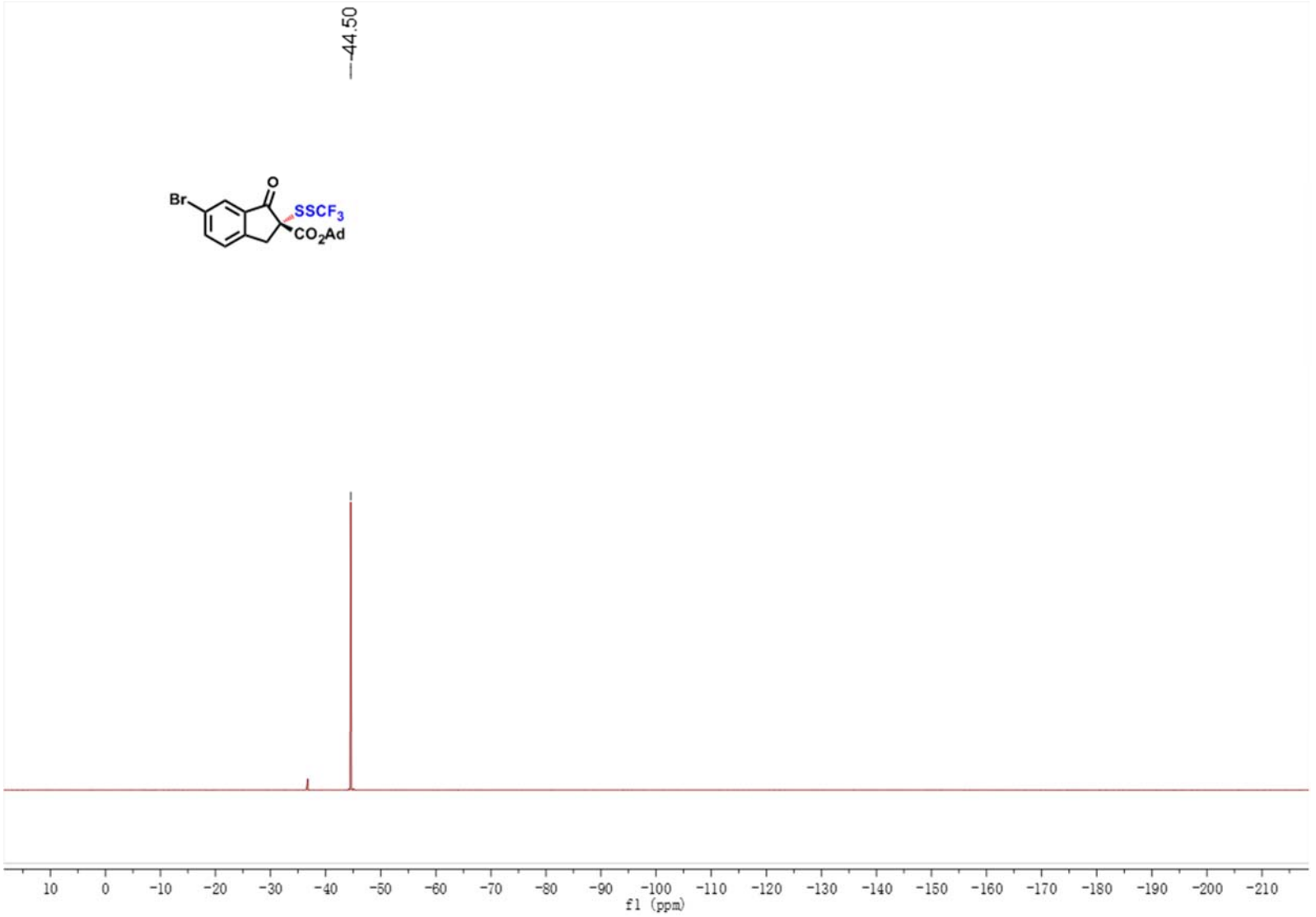

7.75
7.75
7.63
7.61
7.60
7.45
7.43
7.26
3.93
3.89
3.45
3.40
2.16
2.08
2.07
1.63
Cl
O
CO2Ad
SSCF3
0.95
0.98
1.01
1.00
1.00
3.01
6.02
6.18
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

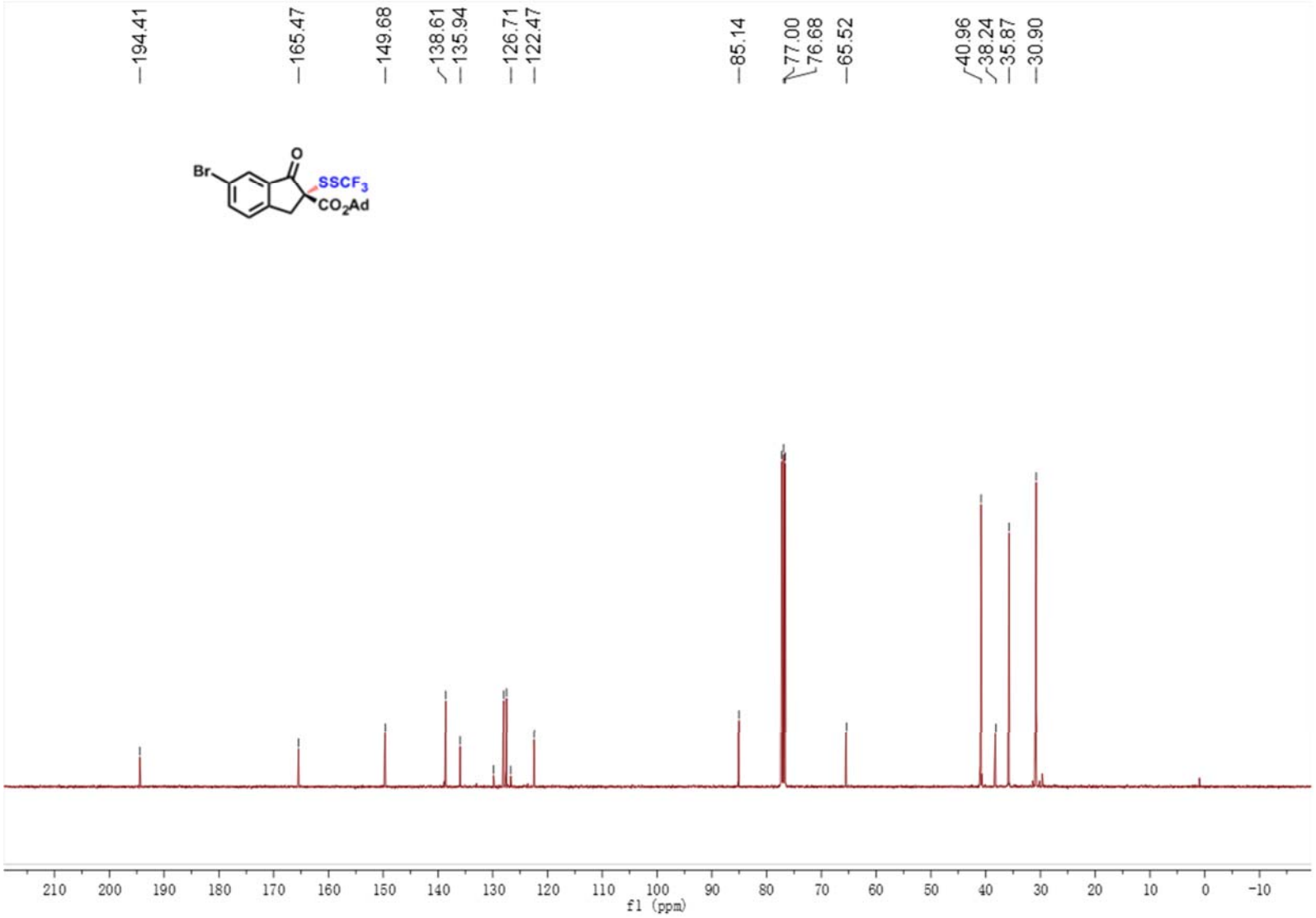

-44.51
Cl
O
CO2Ad
SSCF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


194.55
165.50
149.20
135.85
135.64
134.75
132.97
129.84
127.23
126.71
124.91
123.58
85.12
77.00
76.68
65.65
40.96
38.18
35.86
30.89
Cl
O
CO2Ad
SSCF3
f1 (ppm)

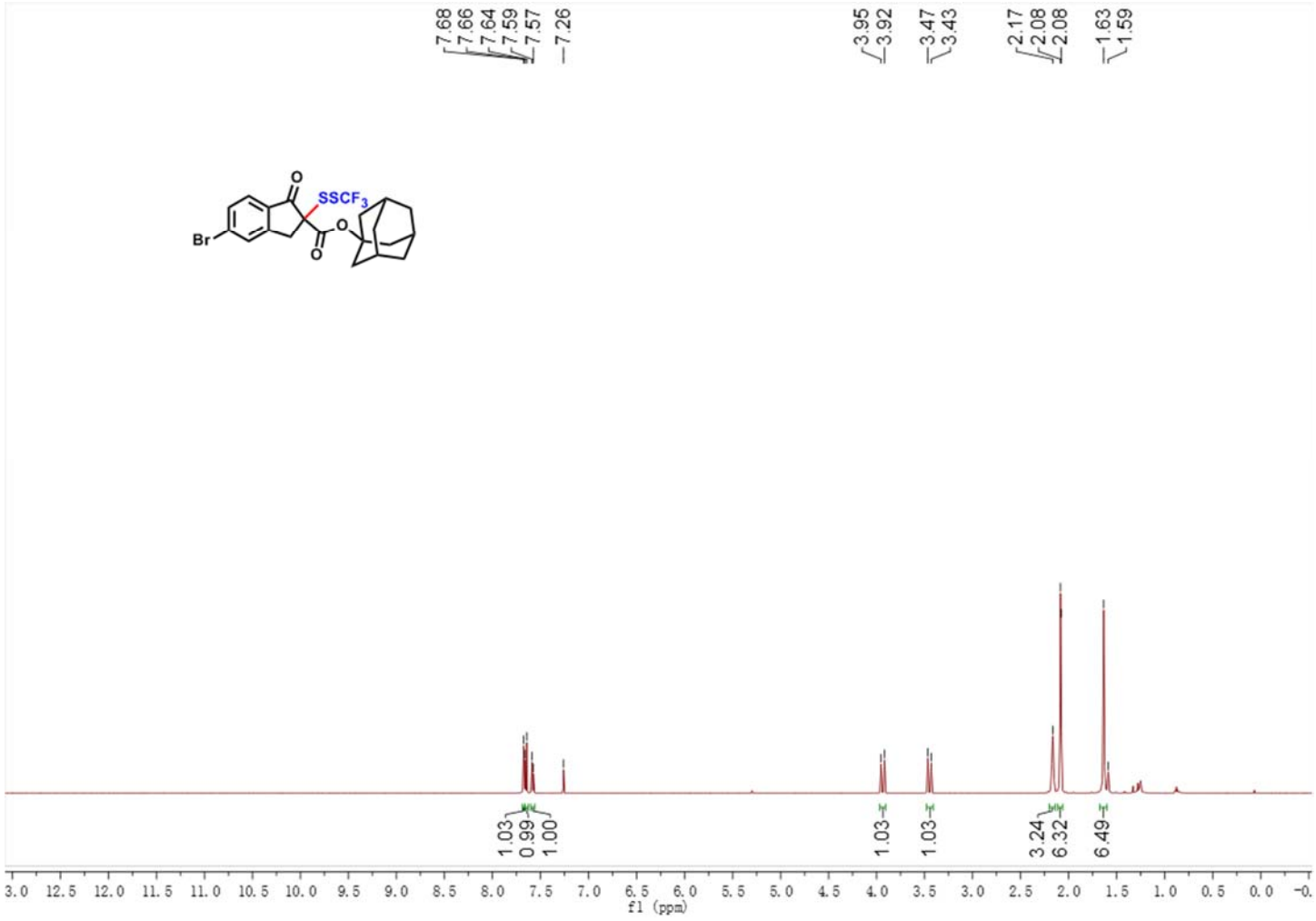
3ac

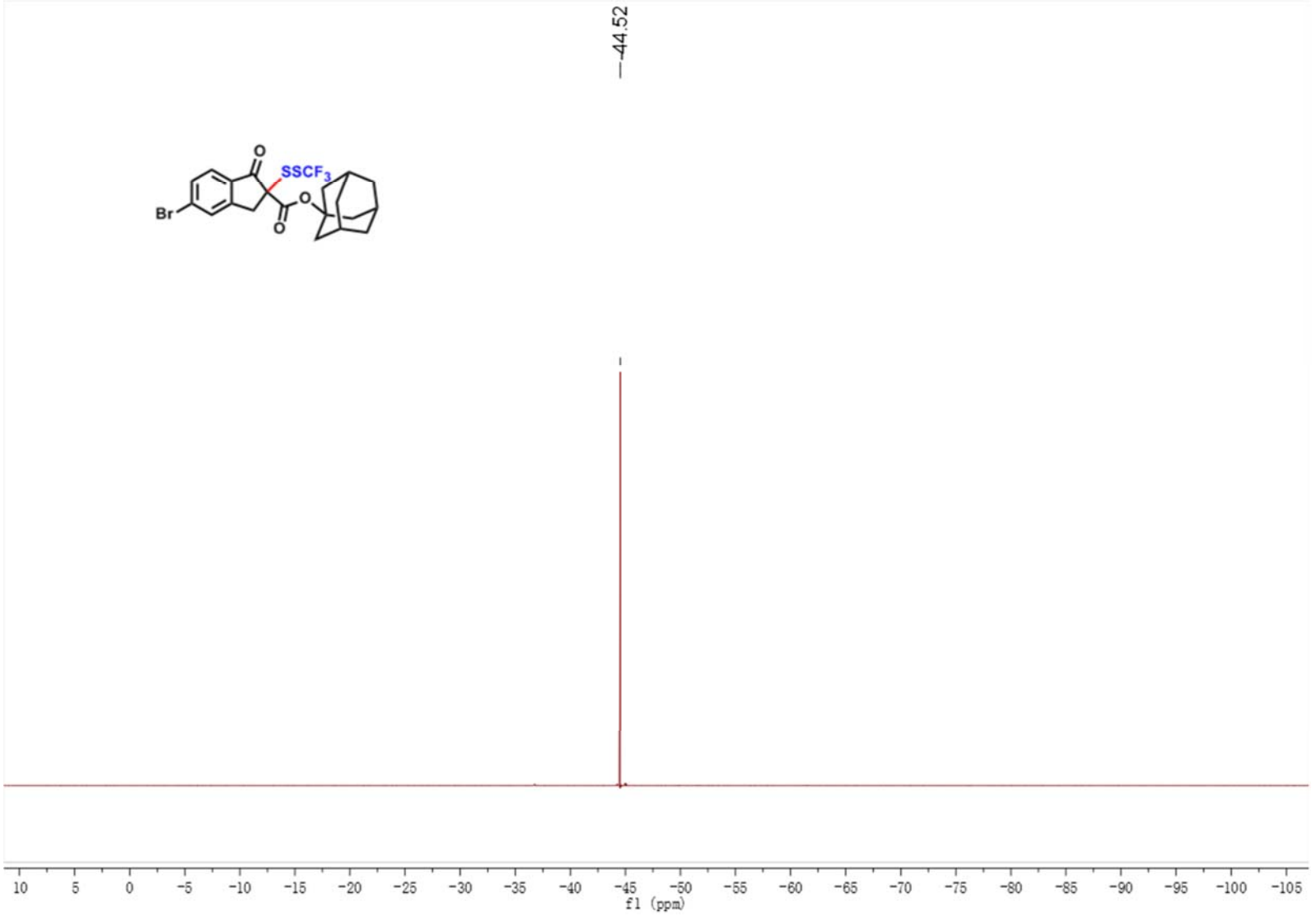

7.92
7.91
7.77
7.77
7.75
7.75
7.39
7.37
7.26
3.91
3.86
3.42
3.38
2.16
2.08
2.07
1.63
Br
O
SSCF3
CO2Ad
0.99
1.00
1.02
1.00
1.01
3.06
5.98
6.08
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

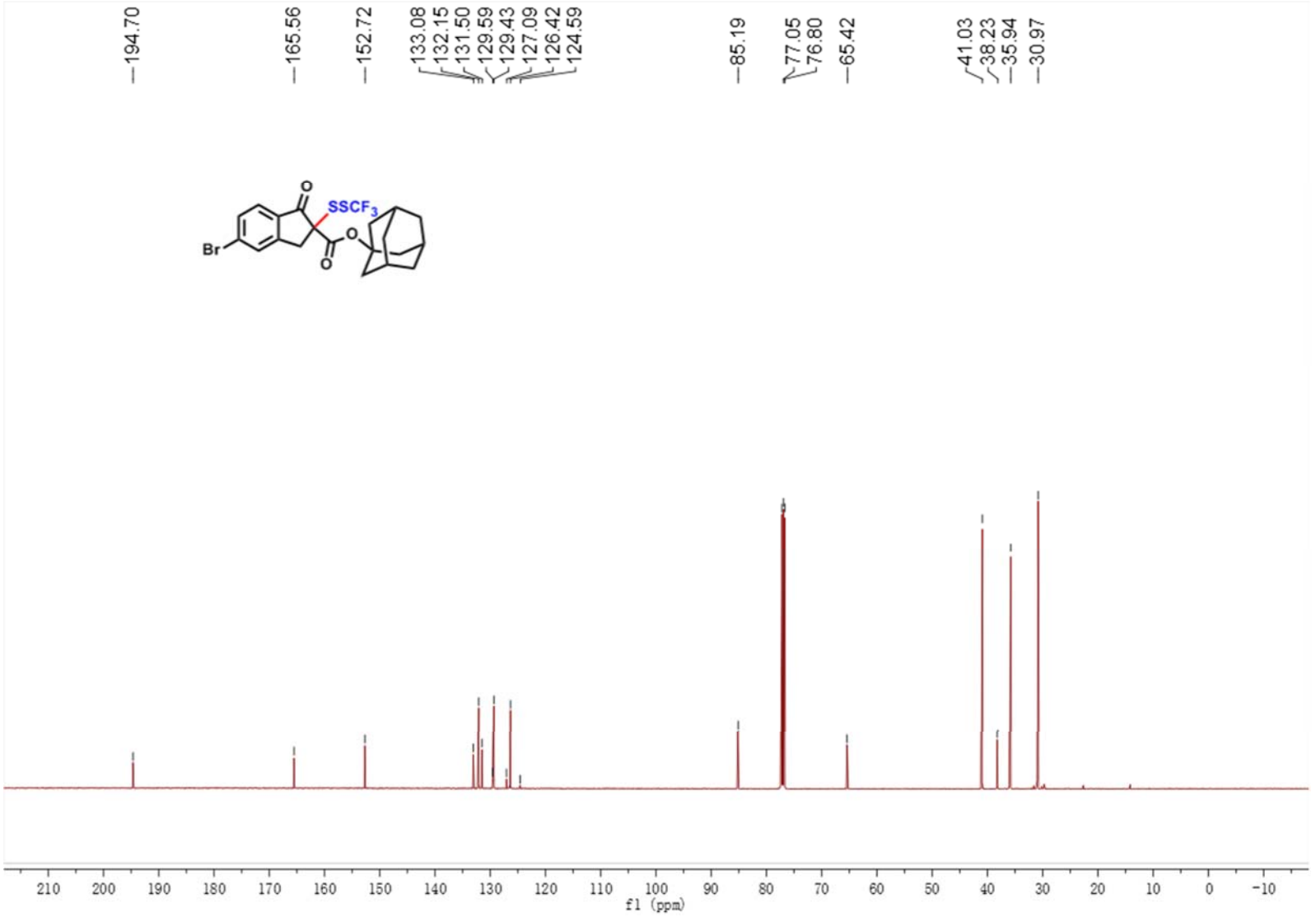

-44.50
Br
O
SSCF3
CO2Ad
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


194.41
165.47
149.68
138.61
135.94
126.71
122.47
85.14
77.00
76.68
65.52
40.96
38.24
35.87
30.90
Br
O
SSCF3
CO2Ad
f1 (ppm)

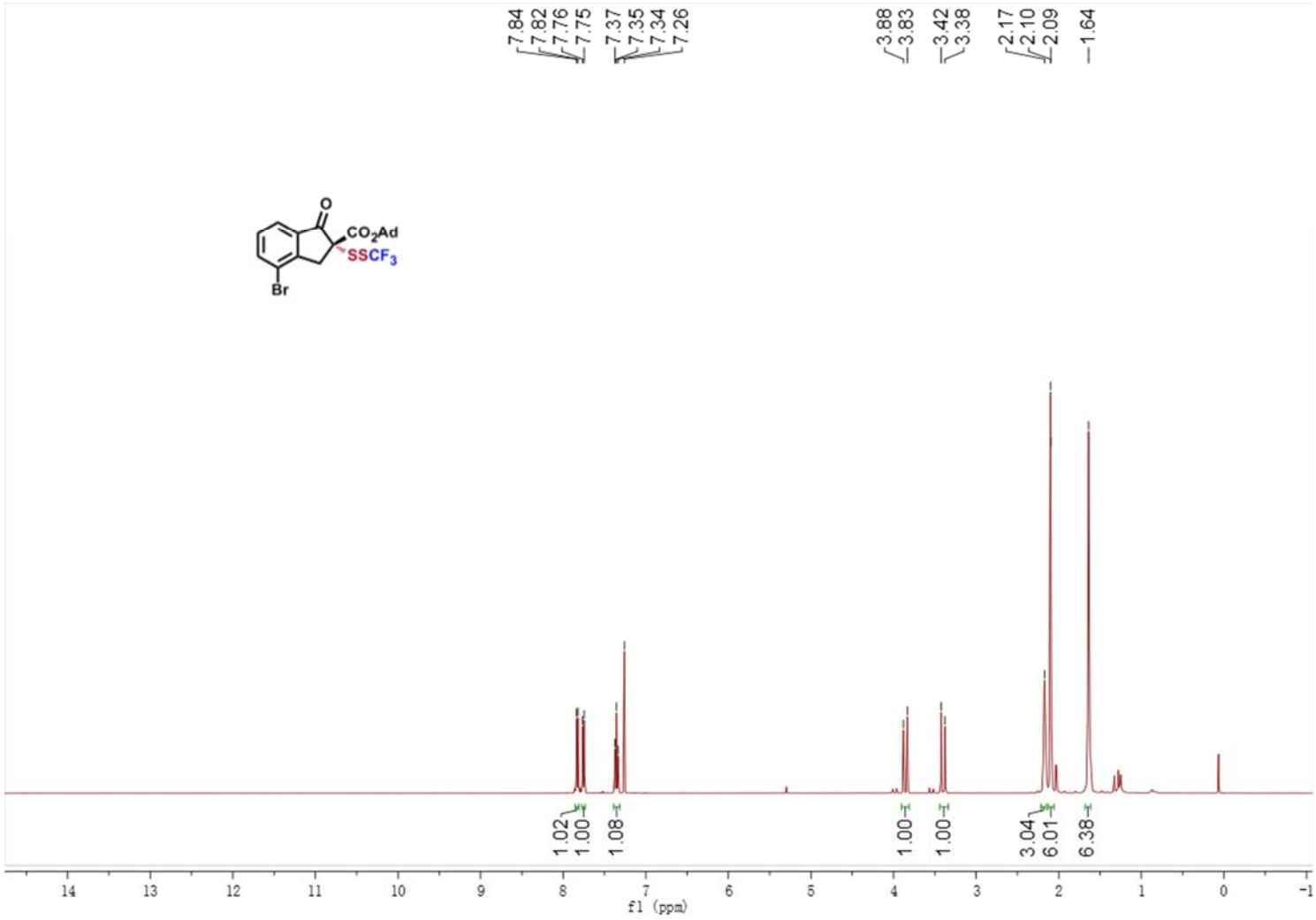
3ad

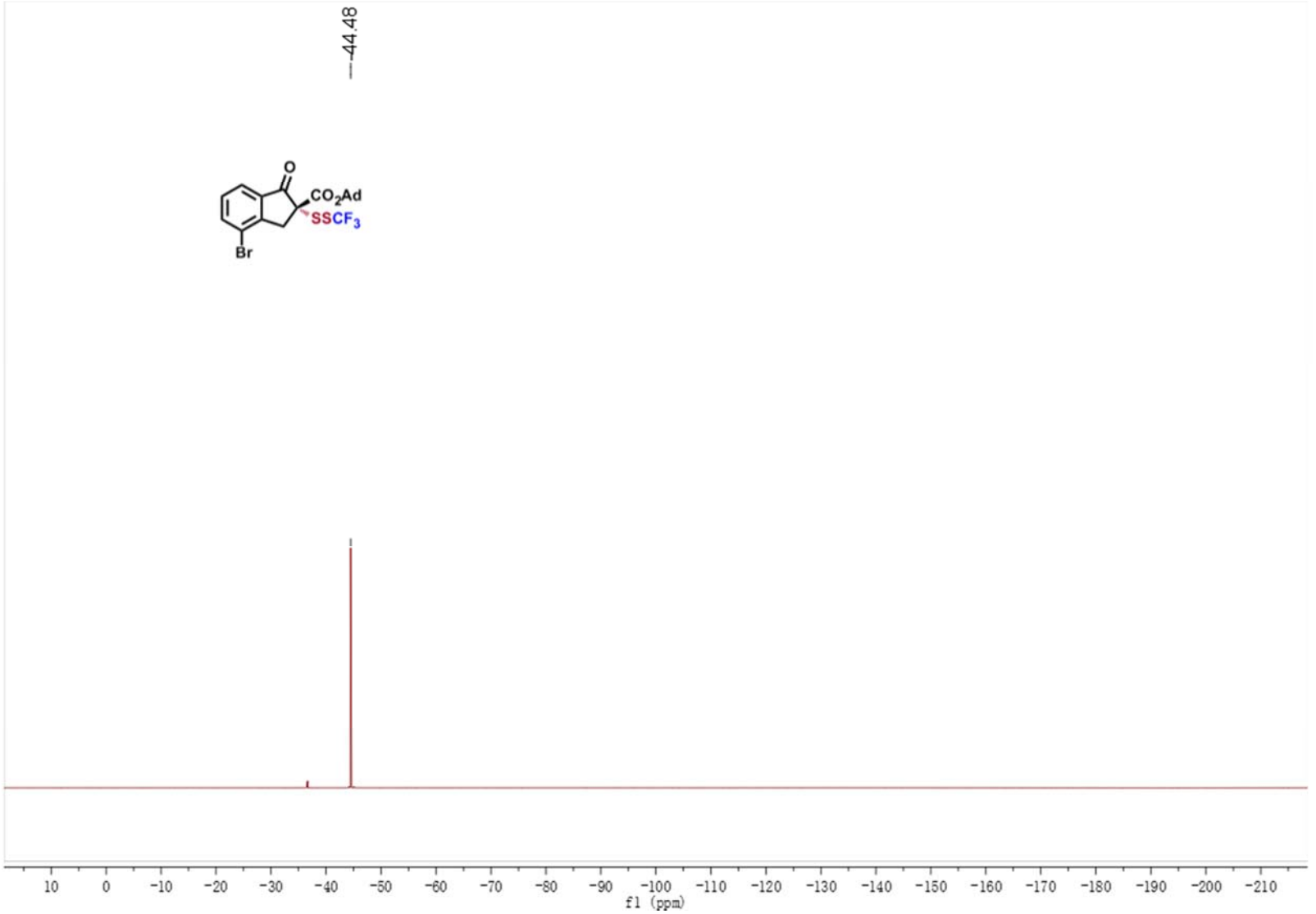

7.68
7.66
7.64
7.59
7.57
7.26
3.95
3.92
3.47
3.43
2.17
2.08
2.08
1.63
1.59
SSCF3
Br
O
O
O
O
1.03
0.99
1.00
1.03
1.03
3.24
6.32
6.49
f1 (ppm)

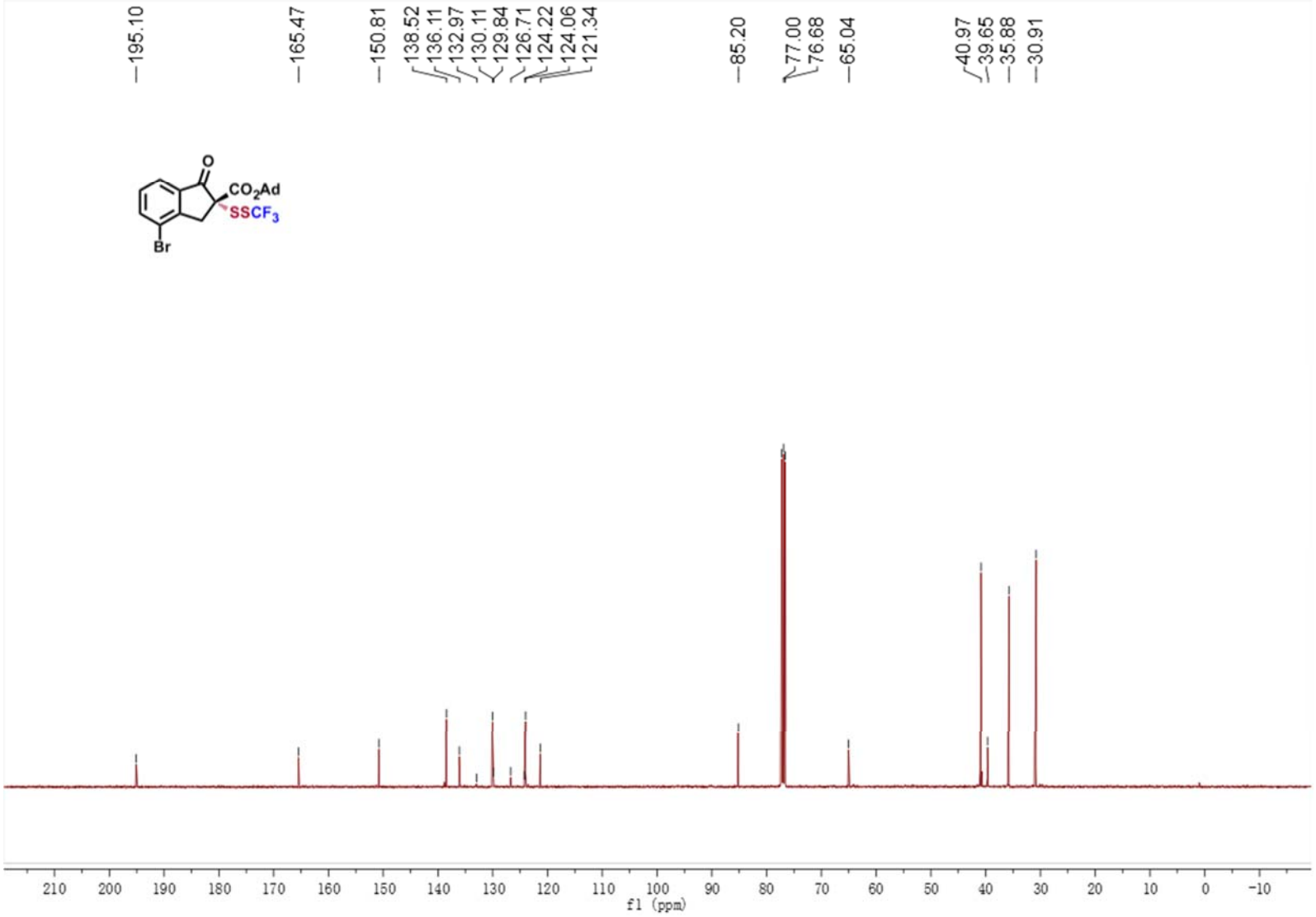

-44.52
O
SSCF3
Br
O
O
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
f1 (ppm)


194.70
165.56
152.72
133.08
132.15
131.50
129.59
129.43
127.09
126.42
124.59
85.19
77.05
76.80
65.42
41.03
38.23
35.94
30.97
O
SSCF3
Br
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

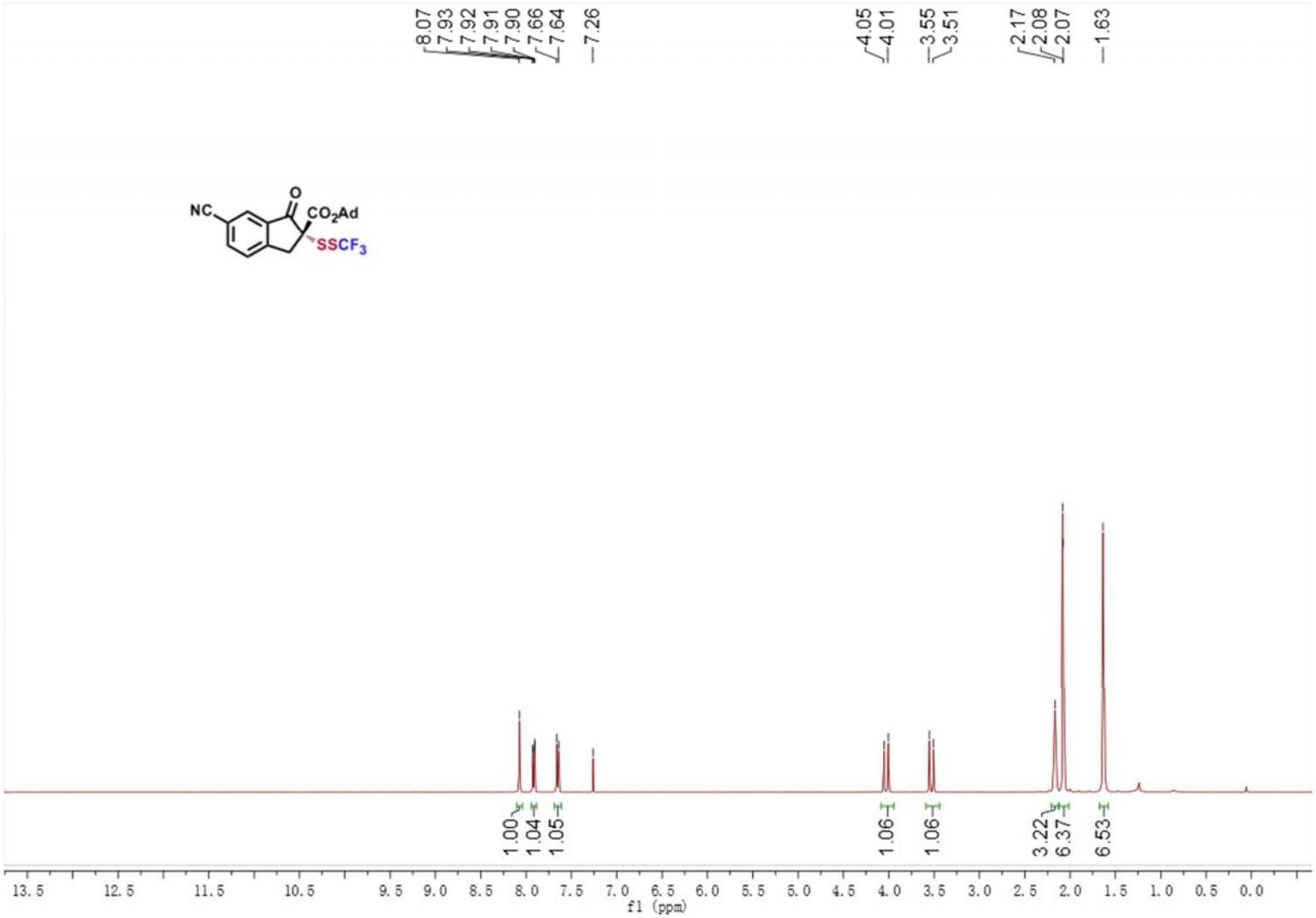
3ae

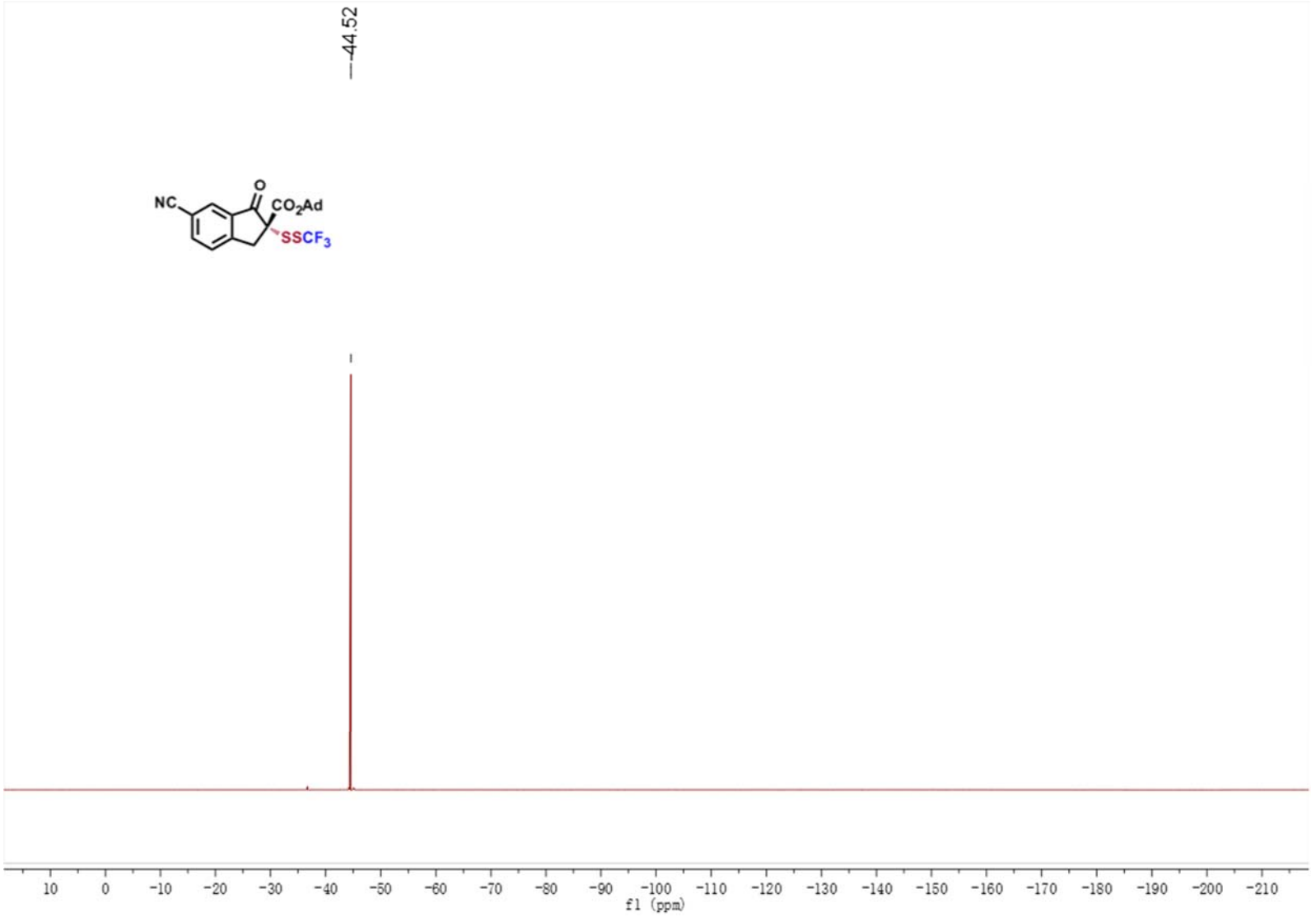

7.84
7.82
7.76
7.75
7.37
7.35
7.34
7.26
3.88
3.83
3.42
3.38
2.17
2.10
2.09
1.64
O
CO2Ad
SSCF3
Br
1.02
1.00
1.08
1.00
1.00
3.04
6.01
6.38
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

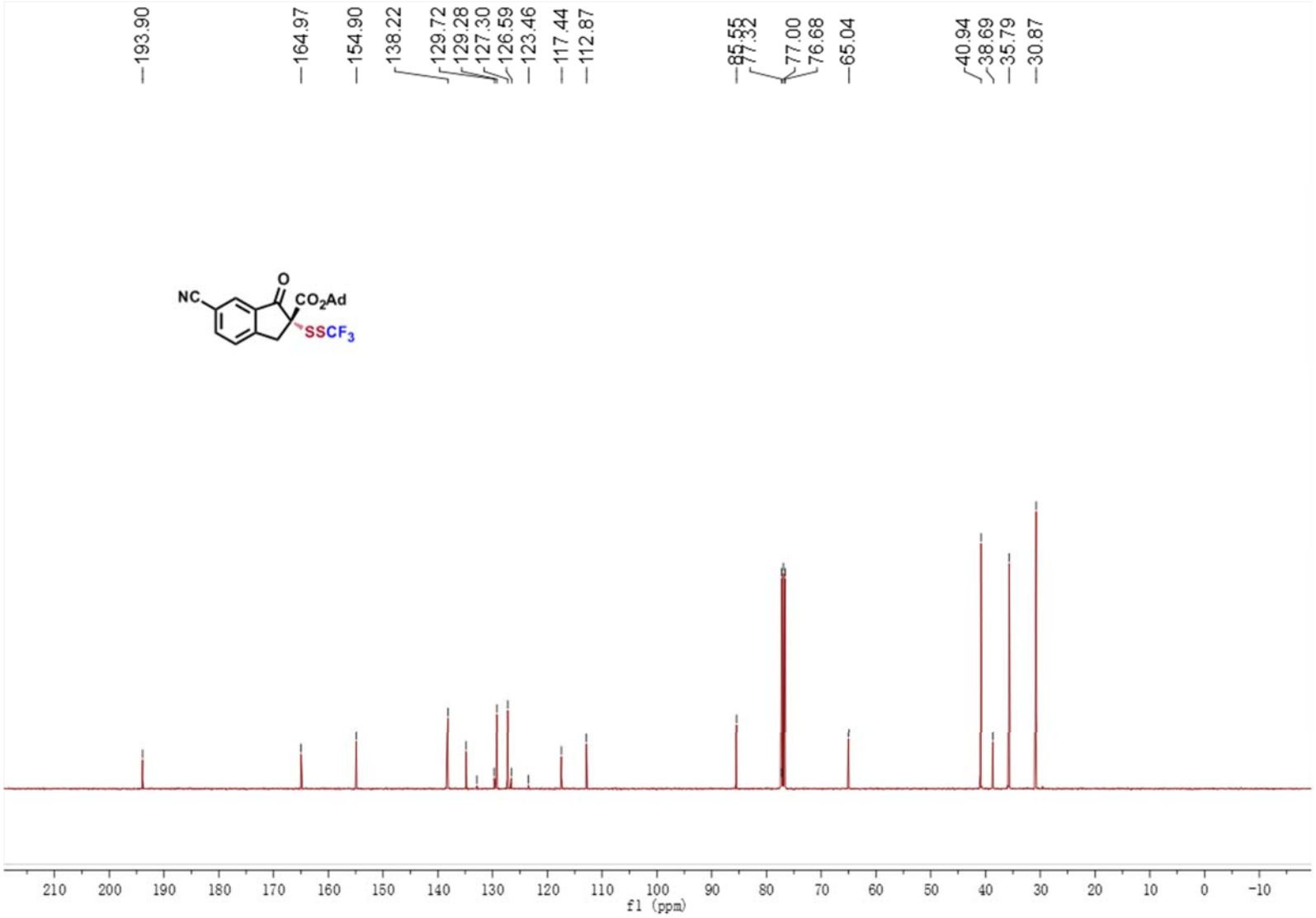

-44.48
O
CO2Ad
SSCF3
Br
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


195.10
165.47
150.81
138.52
136.11
132.97
130.11
129.84
126.71
124.22
124.06
121.34
85.20
77.00
76.68
65.04
40.97
39.65
35.88
30.91
O
CO2Ad
SSCF3
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

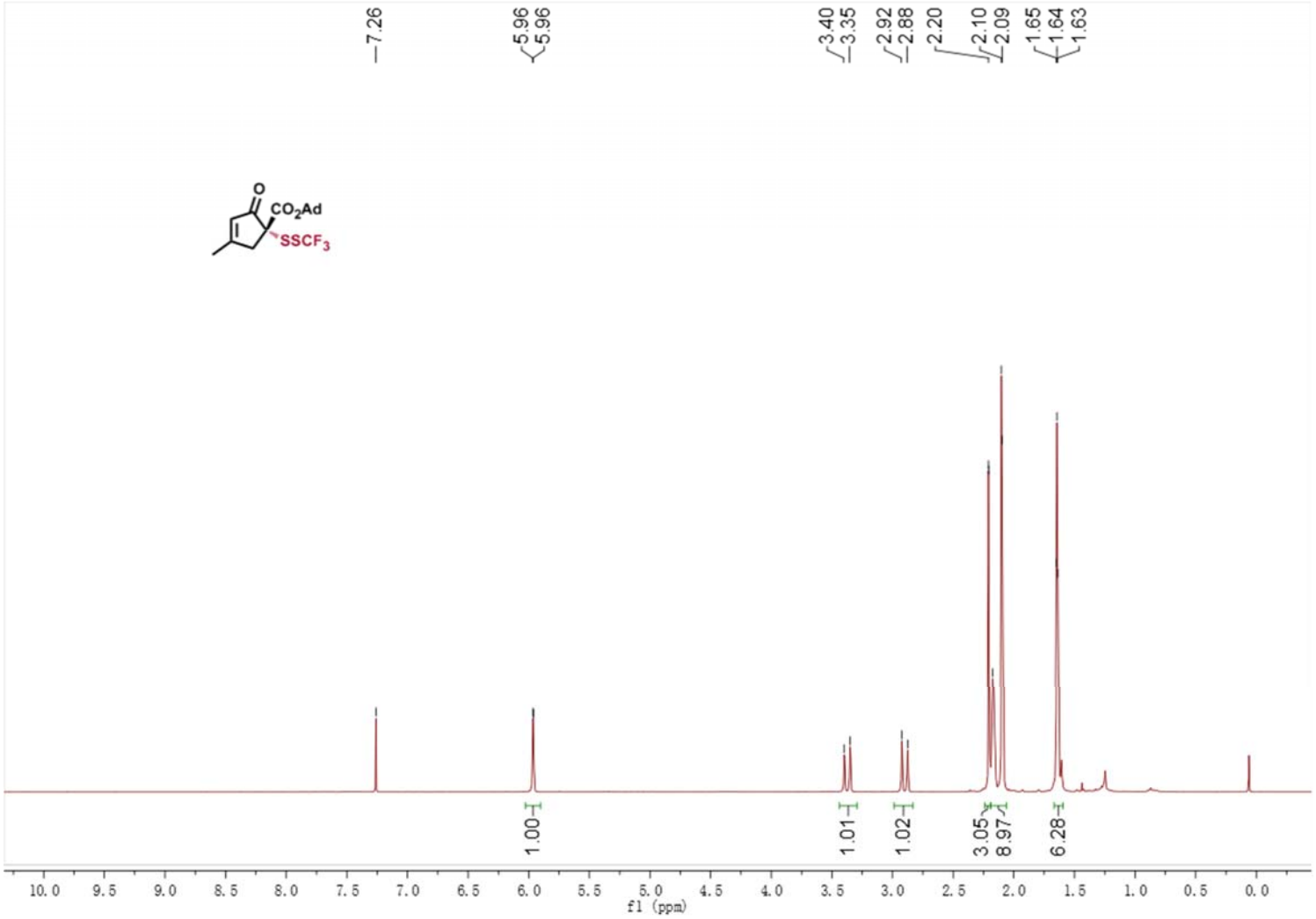
3af

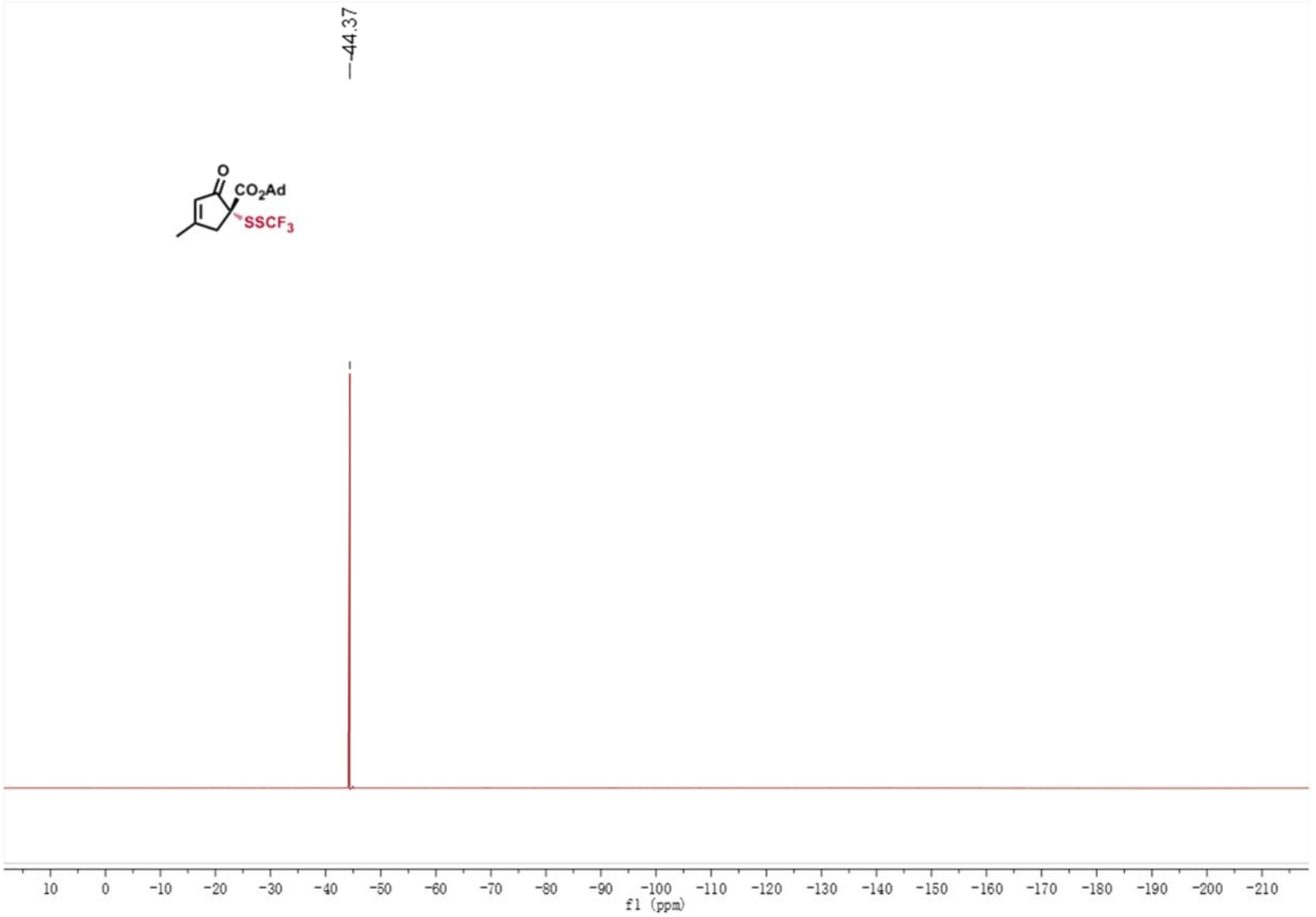

8.07
7.93
7.92
7.91
7.90
7.66
7.64
7.26
4.05
4.01
3.55
3.51
2.17
2.08
2.07
1.63
NC
O
CO2Ad
SSCF3
1.00
1.04
1.05
1.06
1.06
3.22
6.37
6.53
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

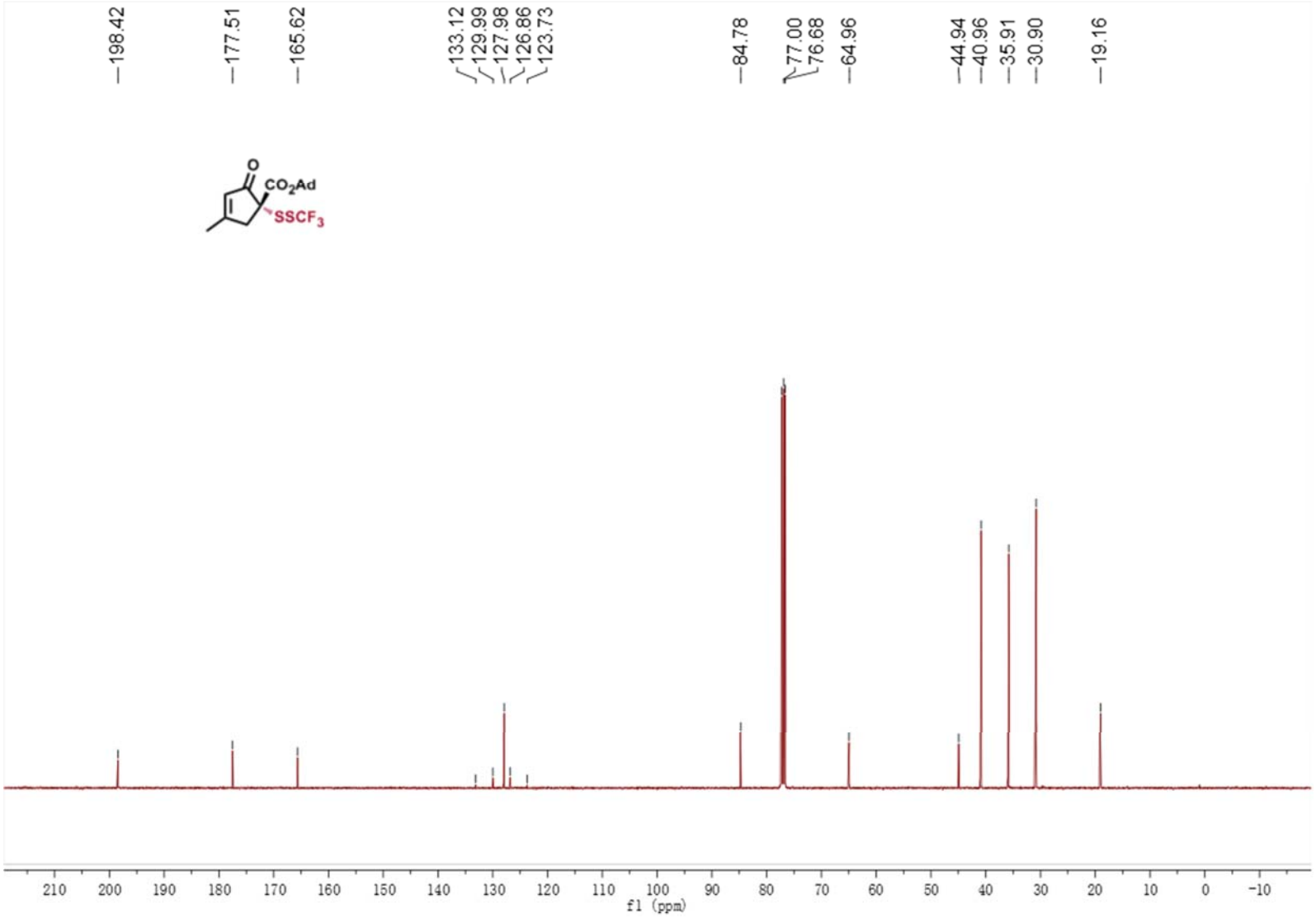

-44.52
NC
O
CO2Ad
SSCF3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


193.90
164.97
154.90
138.22
129.72
129.28
127.30
126.59
123.46
117.44
112.87
85.55
77.32
77.00
76.68
65.04
40.94
38.69
35.79
30.87
NC
O
CO2Ad
SSCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

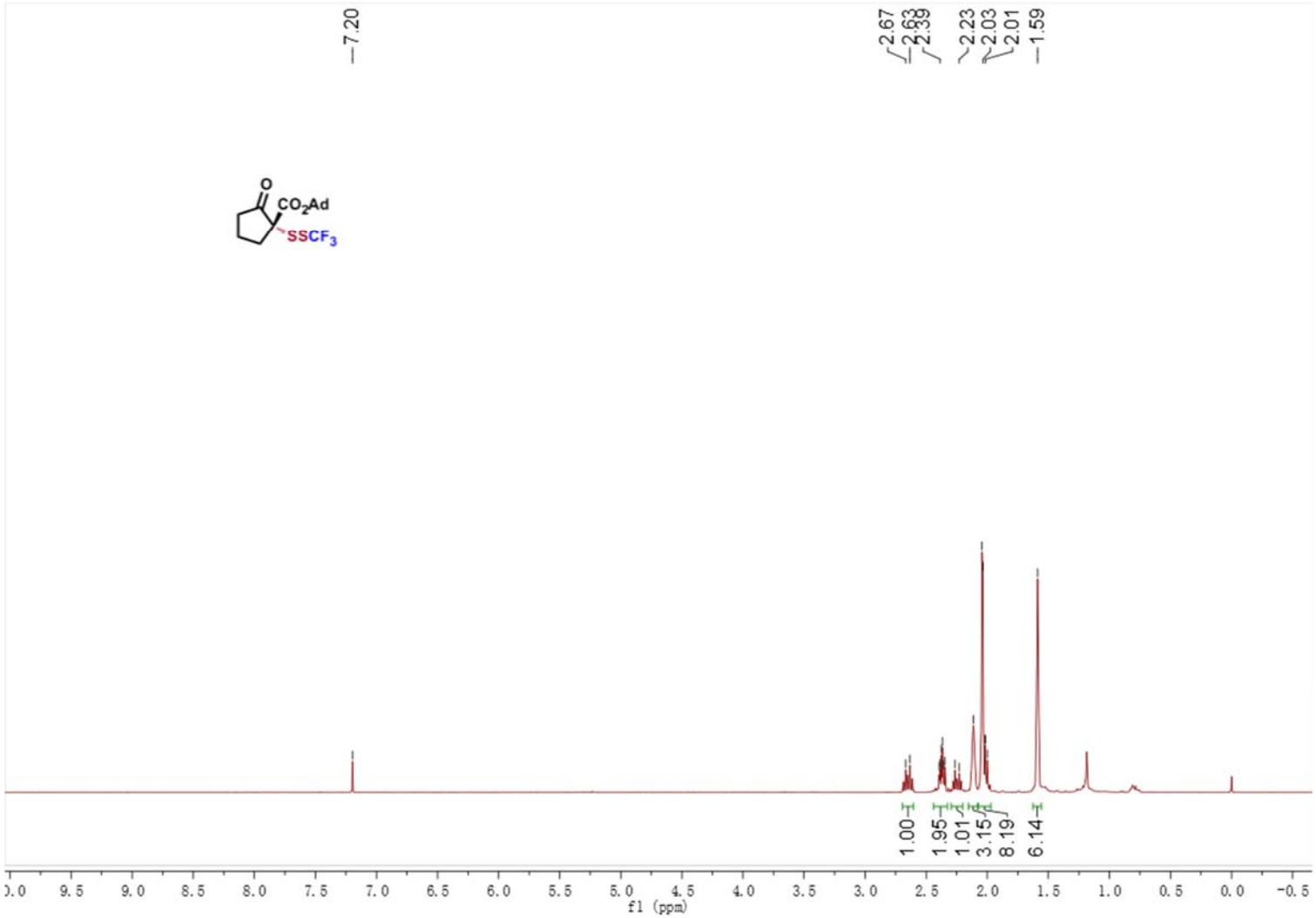
3ag

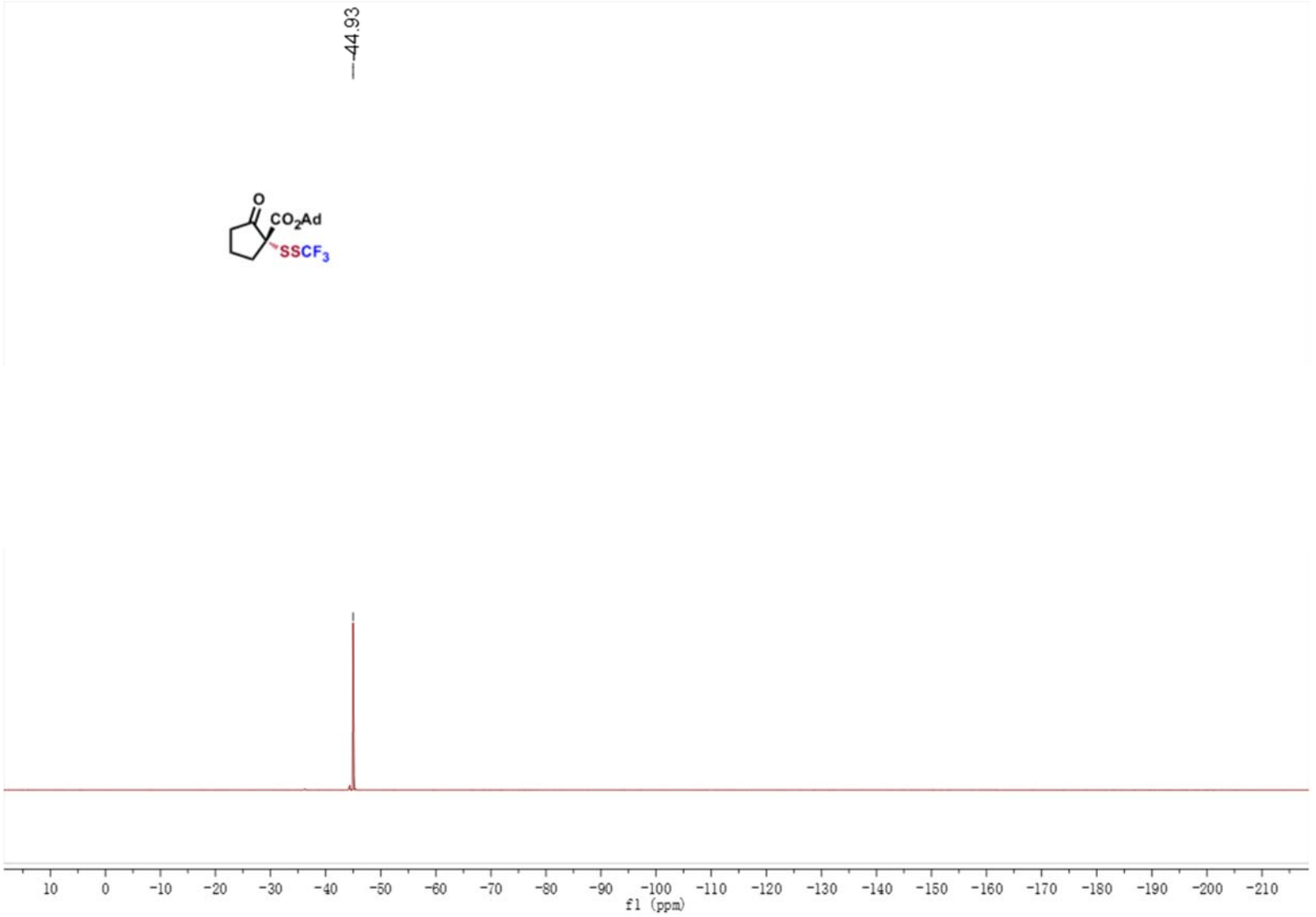

7.26
5.96
5.96
3.40
3.35
2.92
2.88
2.20
2.10
2.09
1.65
1.64
1.63
O
CO2Ad
SSCF3
1.00
1.01
1.02
3.05
8.97
6.28
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

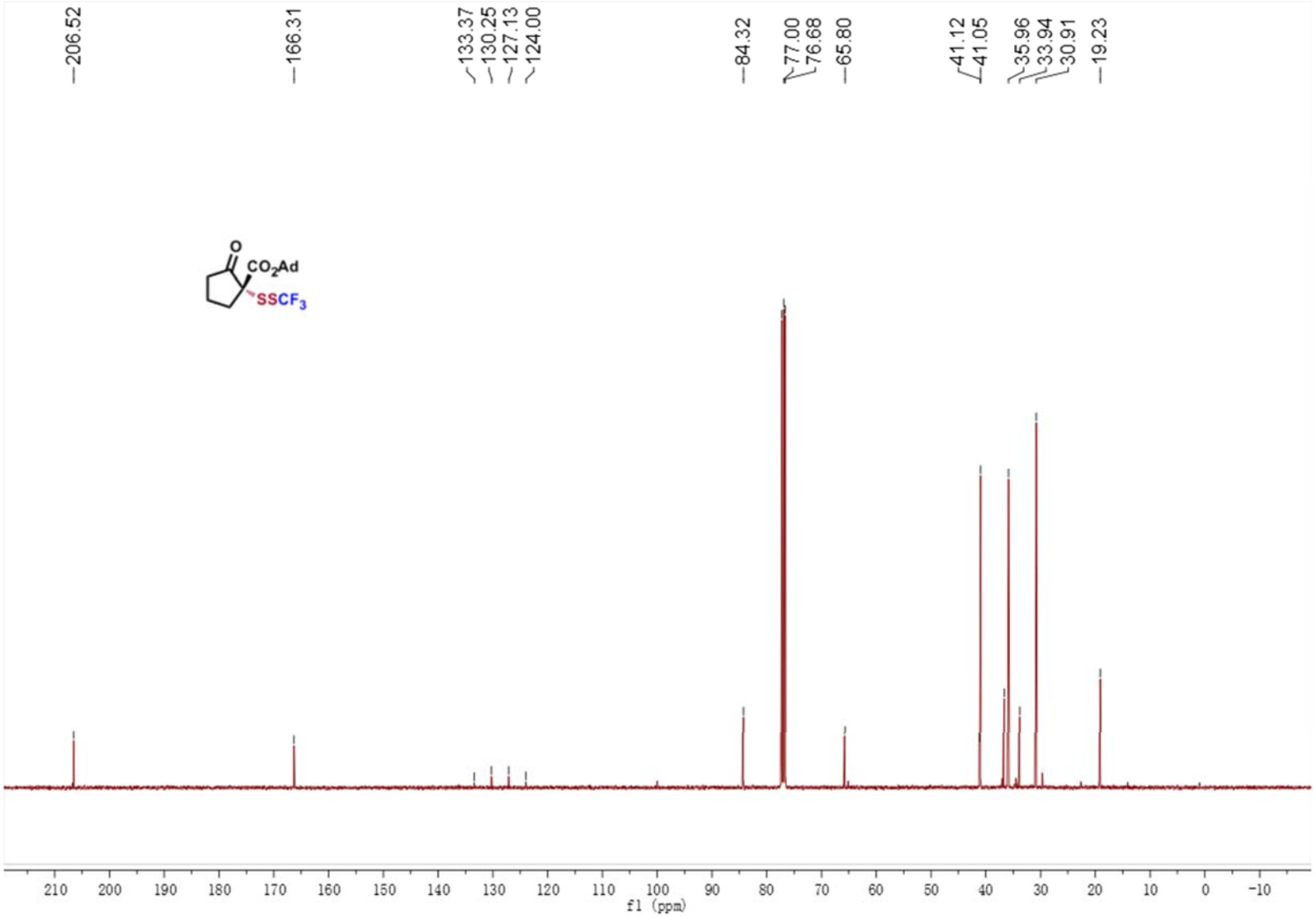

-44.37
O
CO2Ad
SSCF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


198.42
177.51
165.62
133.12
129.99
127.98
126.86
123.73
84.78
77.00
76.68
64.96
44.94
40.96
35.91
30.90
19.16
O
CO2Ad
SSCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

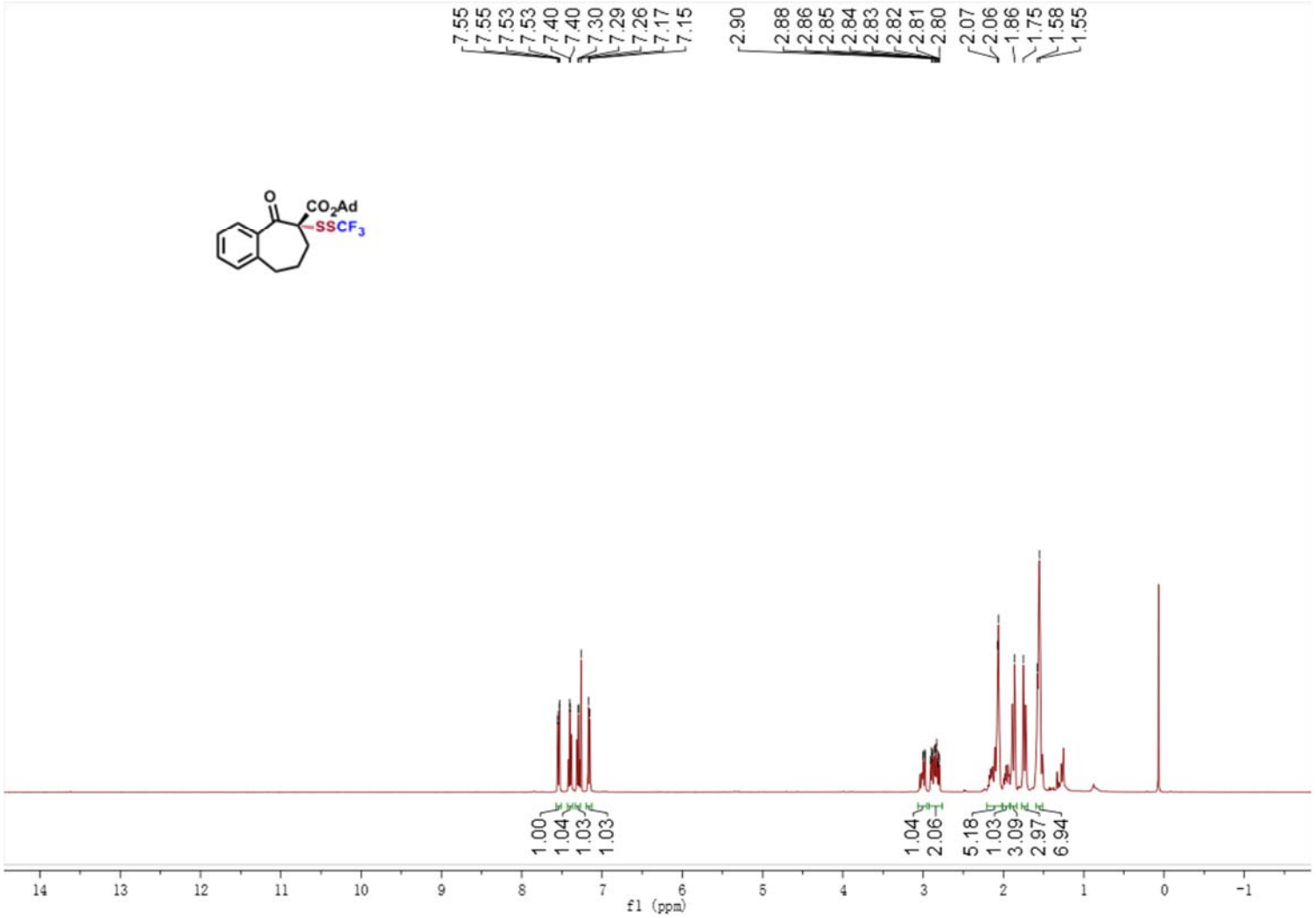
3ah

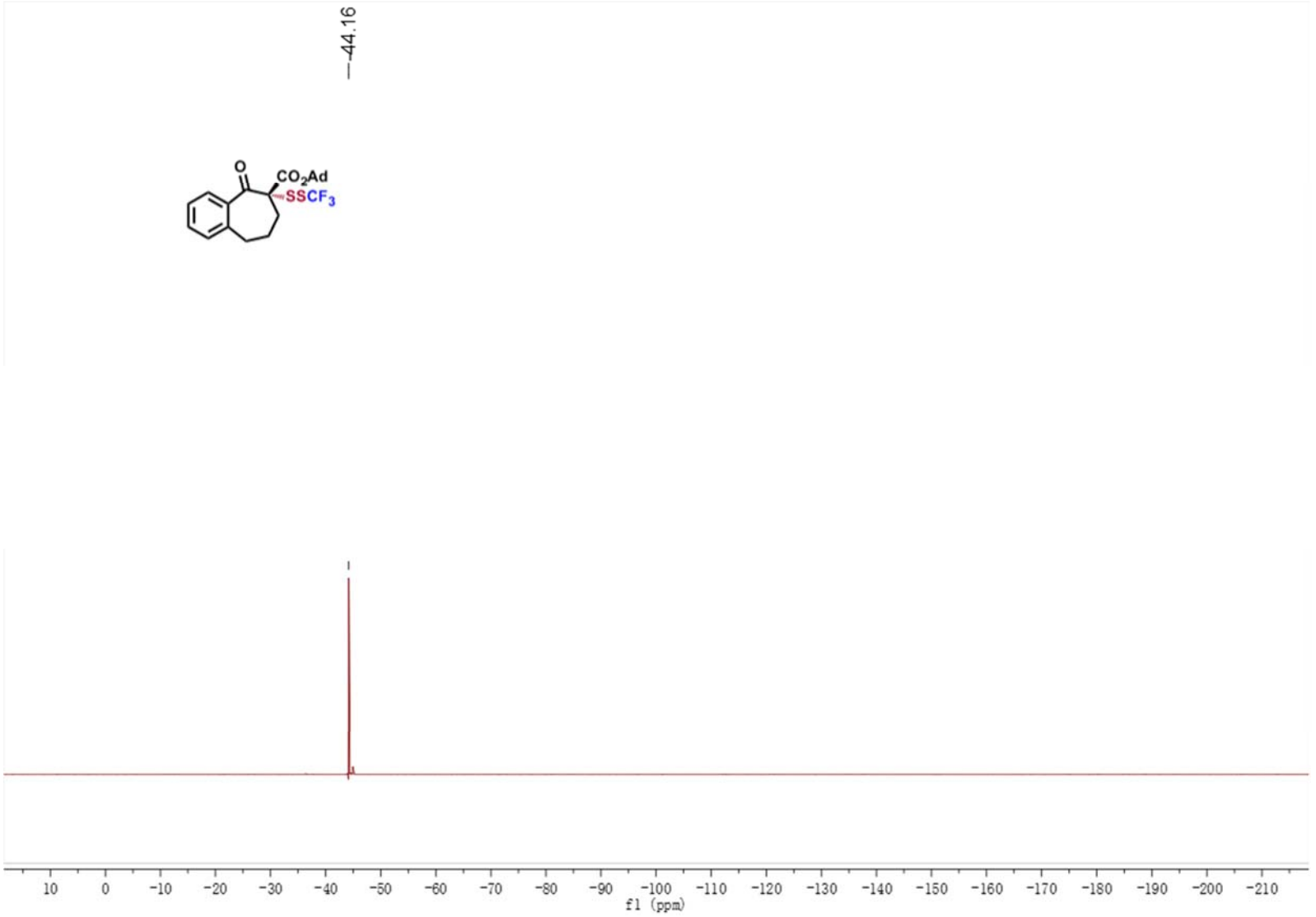

7.20
2.67
2.63
2.39
2.23
2.03
2.01
1.59
O
CO2Ad
SSCF3
1.00
1.95
1.01
3.15
8.19
6.14
f1 (ppm)


-44.93
O
CO2Ad
SSCF3
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)


206.52
166.31
133.37
130.25
127.13
124.00
84.32
77.00
76.68
65.80
41.12
41.05
35.96
33.94
30.91
19.23
O
CO2Ad
SSCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ai


7.55
7.55
7.53
7.53
7.40
7.40
7.30
7.29
7.26
7.17
7.15
2.90
2.88
2.86
2.85
2.84
2.83
2.82
2.81
2.80
2.07
2.06
1.86
1.75
1.58
1.55
O
CO2Ad
SSCF3
1.00
1.04
1.03
1.03
1.04
2.06
5.18
1.03
3.09
2.97
6.94
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


-44.16
O
CO2Ad
SSCF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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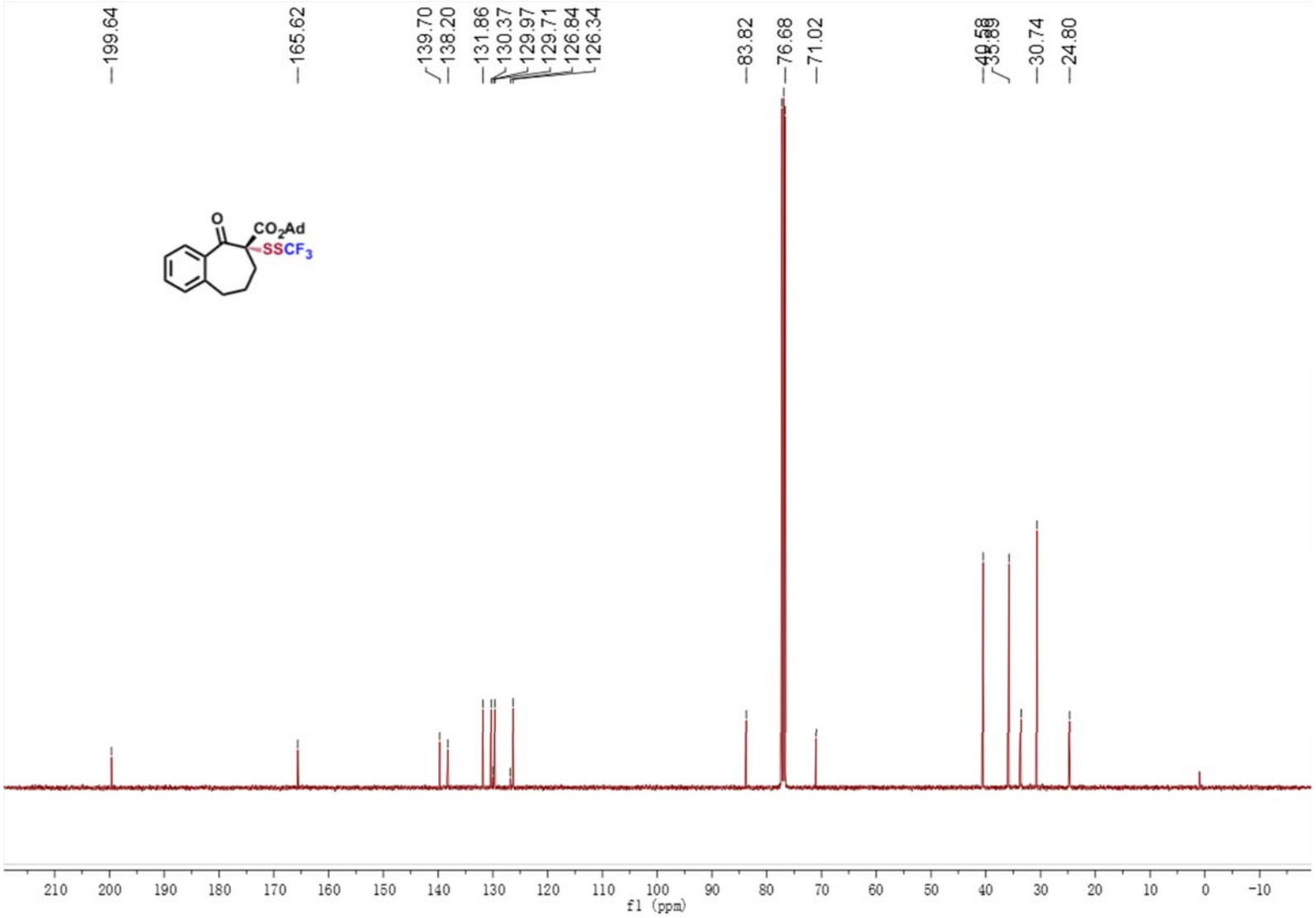
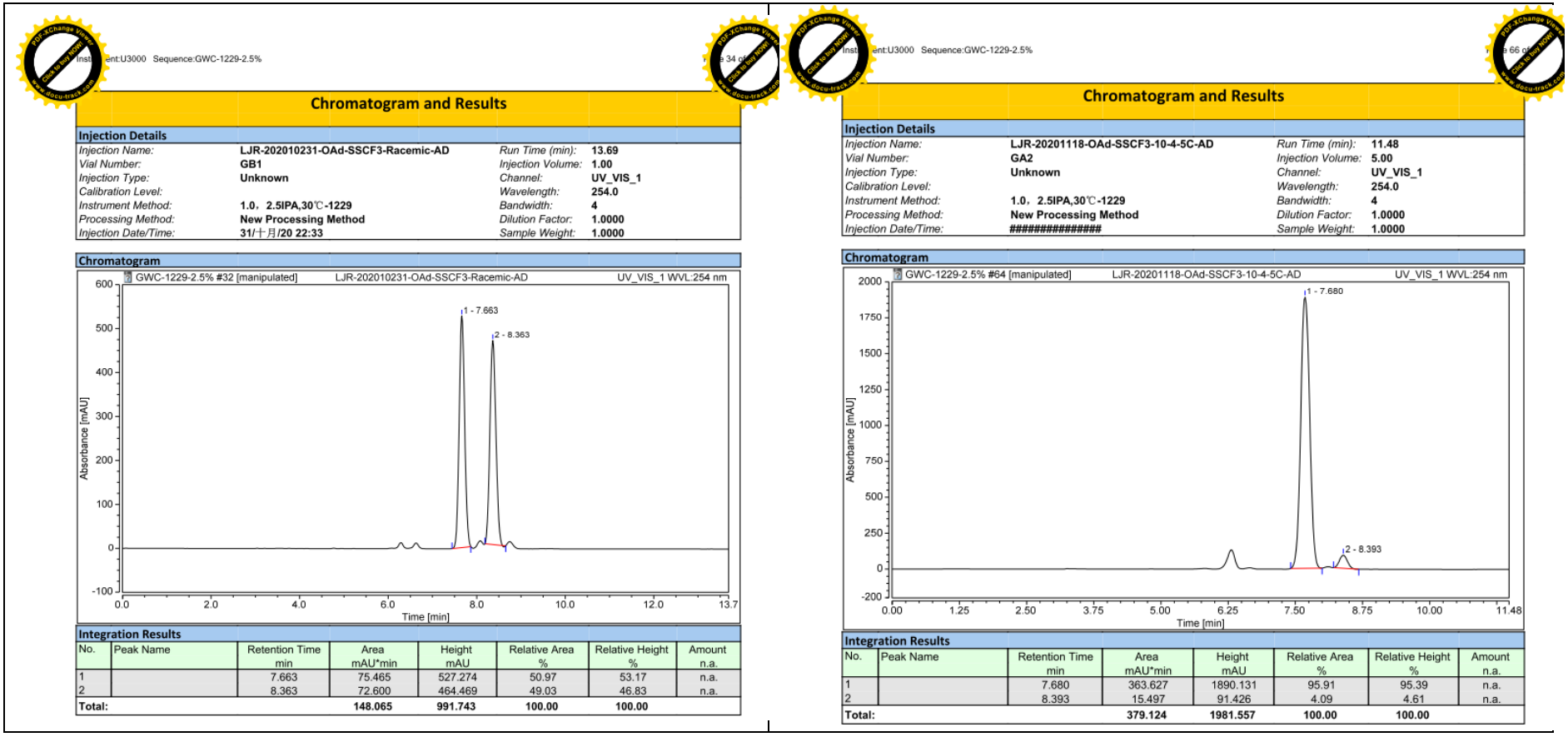
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


199.64
165.62
139.70
138.20
131.86
130.37
129.97
129.71
126.84
126.34
83.82
76.68
71.02
40.58
35.89
30.74
24.80
O
CO2Ad
SSCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

HPLC spectra of 3u



Chromatogram and Results

Injection Details

Injection Name:	LJR-202010231-OAd-SSCF3-Racemic-AD	Run Time (min):	13.69
Vial Number:	GB1	Injection Volume:	1.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	31/十月/20 22:33	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.663	75.465	527.274	50.97	53.17	n.a.
2		8.363	72.600	464.469	49.03	46.83	n.a.
Total:			148.065	991.743	100.00	100.00	

Chromatogram and Results

Injection Details

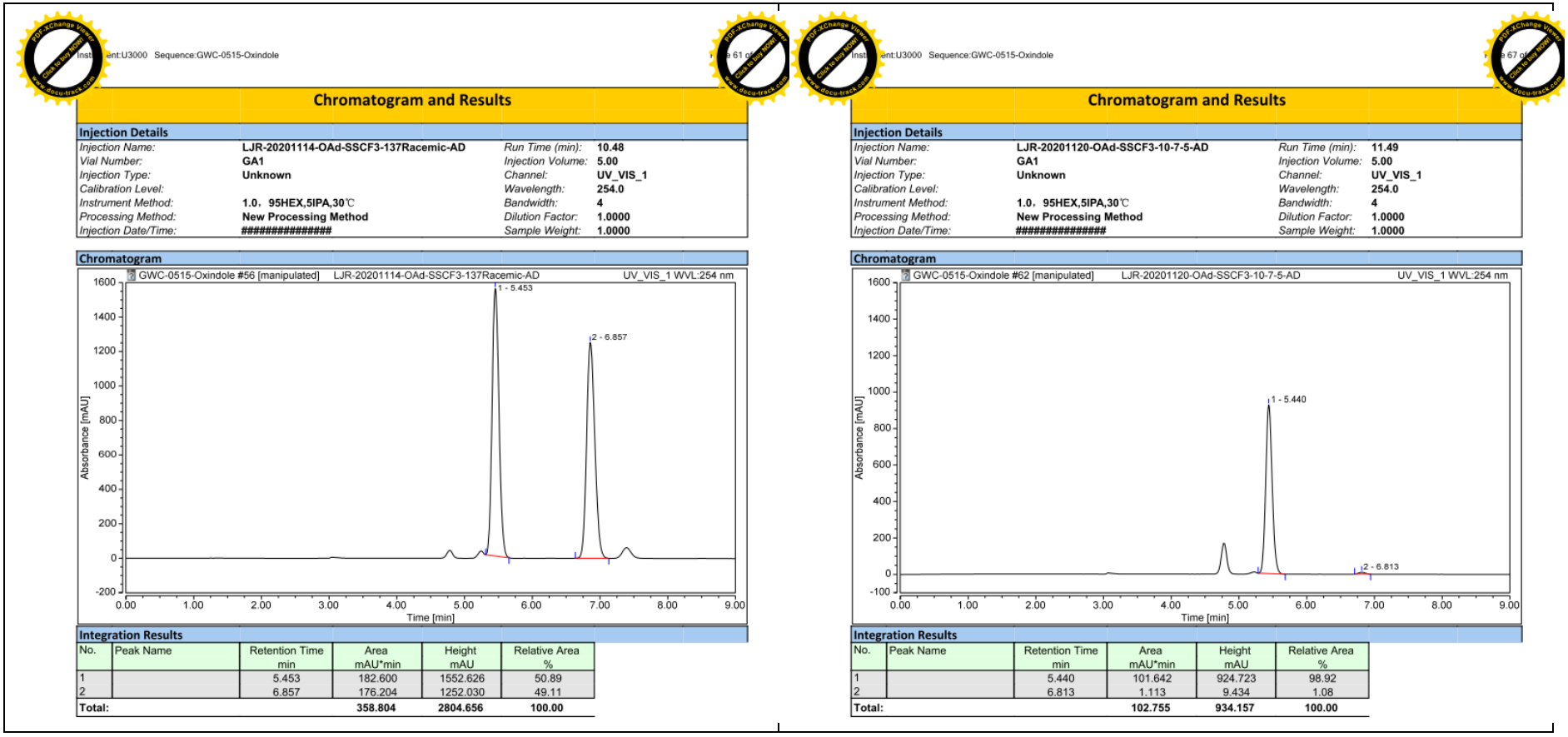
Injection Name:	LJR-20201118-OAd-SSCF3-10-4-5C-AD	Run Time (min):	11.48
Vial Number:	GA2	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.680	363.627	1890.131	95.91	95.39	n.a.
2		8.393	15.497	91.426	4.09	4.61	n.a.
Total:			379.124	1981.557	100.00	100.00	

HPLC spectra of 3v



Chromatogram and Results

Injection Details

Injection Name:	LJR-20201114-OAd-SSCF3-137Racemic-AD	Run Time (min):	10.48
Vial Number:	GA1	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，95HEX,5IPA,30℃	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %
1		5.453	182.600	1552.626	50.89
2		6.857	176.204	1252.030	49.11
Total:			358.804	2804.656	100.00

Chromatogram and Results

Injection Details

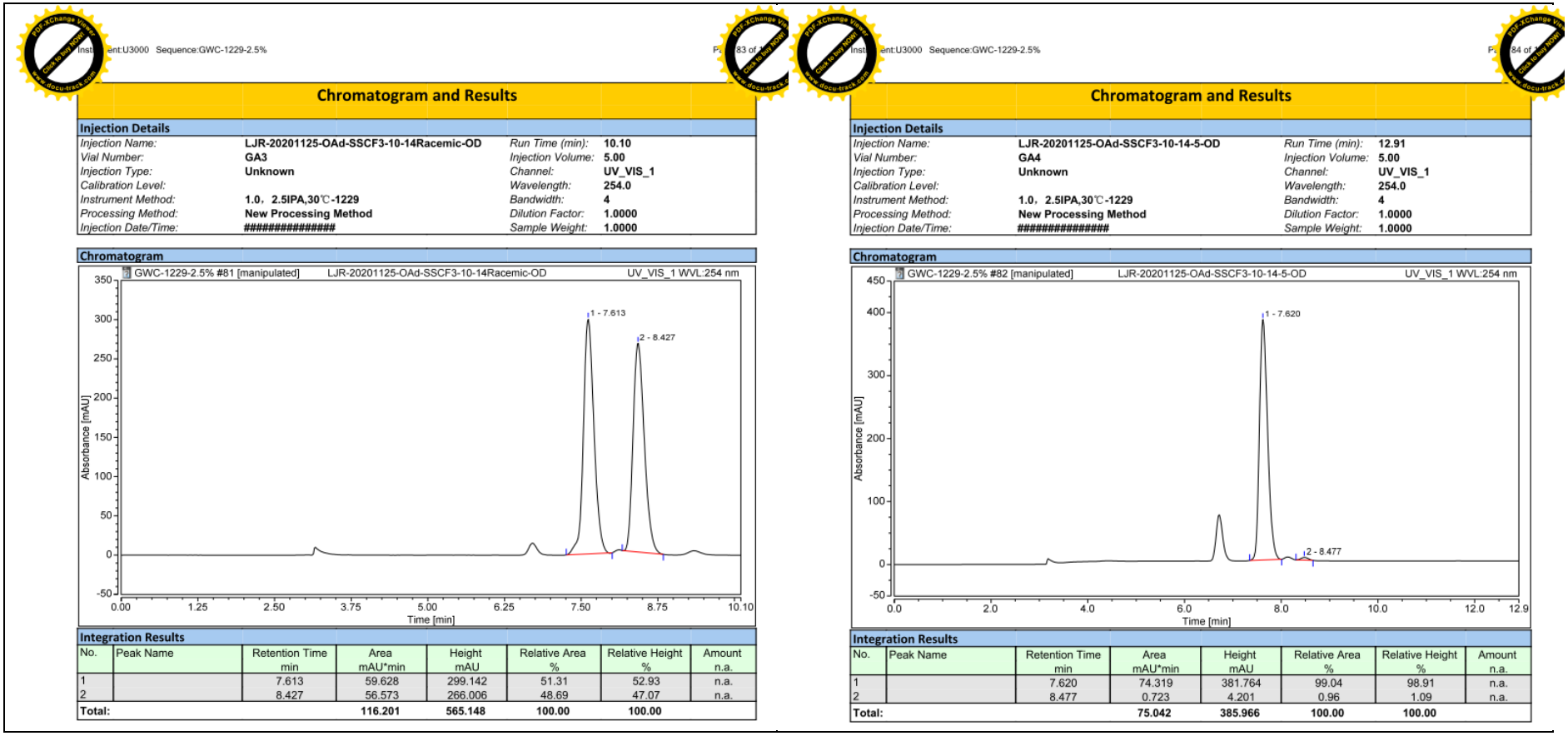
Injection Name:	LJR-20201120-OAd-SSCF3-10-7-5-AD	Run Time (min):	11.49
Vial Number:	GA1	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，95HEX,5IPA,30℃	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %
1		5.440	101.642	924.723	98.92
2		6.813	1.113	9.434	1.08
Total:			102.755	934.157	100.00

HPLC spectra of 3w



Chromatogram and Results

Injection Details

Injection Name:	LJR-20201125-OAd-SSCF3-10-14Racemic-OD	Run Time (min):	10.10
Vial Number:	GA3	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.613	59.628	299.142	51.31	52.93	n.a.
2		8.427	56.573	266.006	48.69	47.07	n.a.
Total:			116.201	565.148	100.00	100.00	

Chromatogram and Results

Injection Details

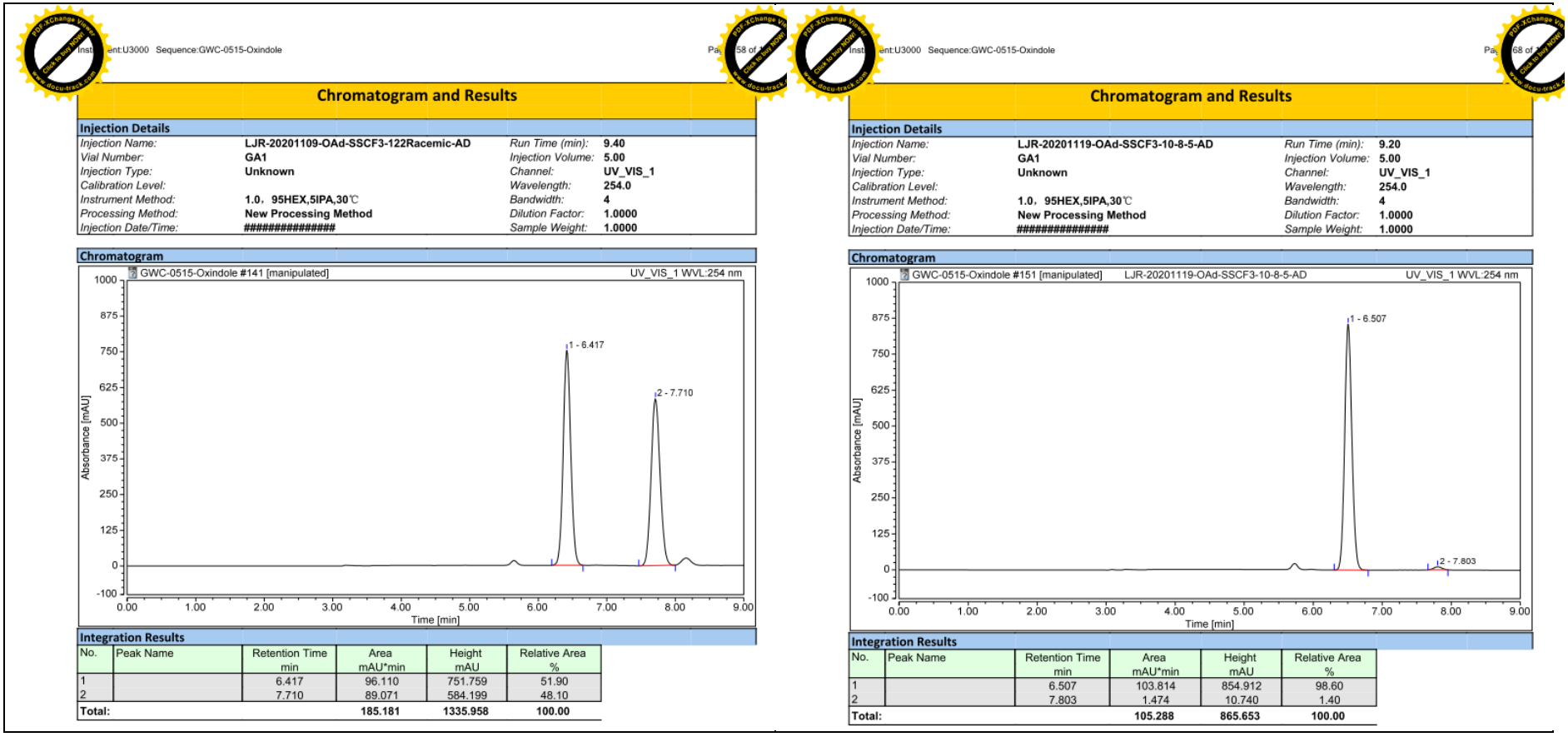
Injection Name:	LJR-20201125-OAd-SSCF3-10-14-5-OD	Run Time (min):	12.91
Vial Number:	GA4	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.620	74.319	381.764	99.04	98.91	n.a.
2		8.477	0.723	4.201	0.96	1.09	n.a.
Total:			75.042	385.966	100.00	100.00	

HPLC spectra of 3x



Chromatogram and Results

Injection Details

Injection Name:	LJR-20201109-OAd-SSCF3-122Racemic-AD	Run Time (min):	9.40
Vial Number:	GA1	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，95HEX,5IPA,30℃	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %
1		6.417	96.110	751.759	51.90
2		7.710	89.071	584.199	48.10
Total:			185.181	1335.958	100.00

Chromatogram and Results

Injection Details

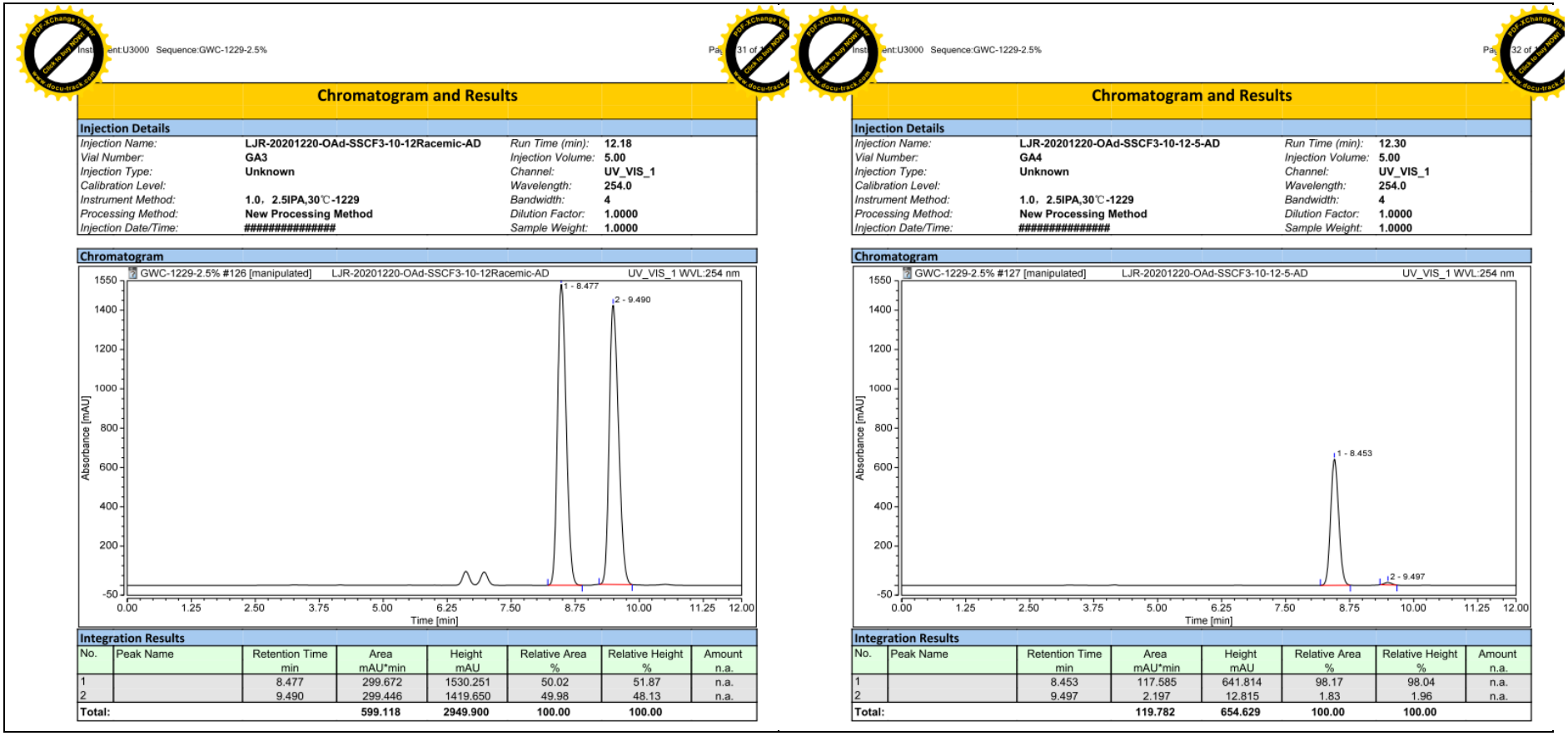
Injection Name:	LJR-20201119-OAd-SSCF3-10-8-5-AD	Run Time (min):	9.20
Vial Number:	GA1	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，95HEX,5IPA,30℃	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %
1		6.507	103.814	854.912	98.60
2		7.803	1.474	10.740	1.40
Total:			105.288	865.653	100.00

HPLC spectra of 3y



Chromatogram and Results

Injection Details

Injection Name:	LJR-20201220-OAd-SSCF3-10-12Racemic-AD	Run Time (min):	12.18
Vial Number:	GA3	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.477	299.672	1530.251	50.02	51.87	n.a.
2		9.490	299.446	1419.650	49.98	48.13	n.a.
Total:			599.118	2949.900	100.00	100.00	

Chromatogram and Results

Injection Details

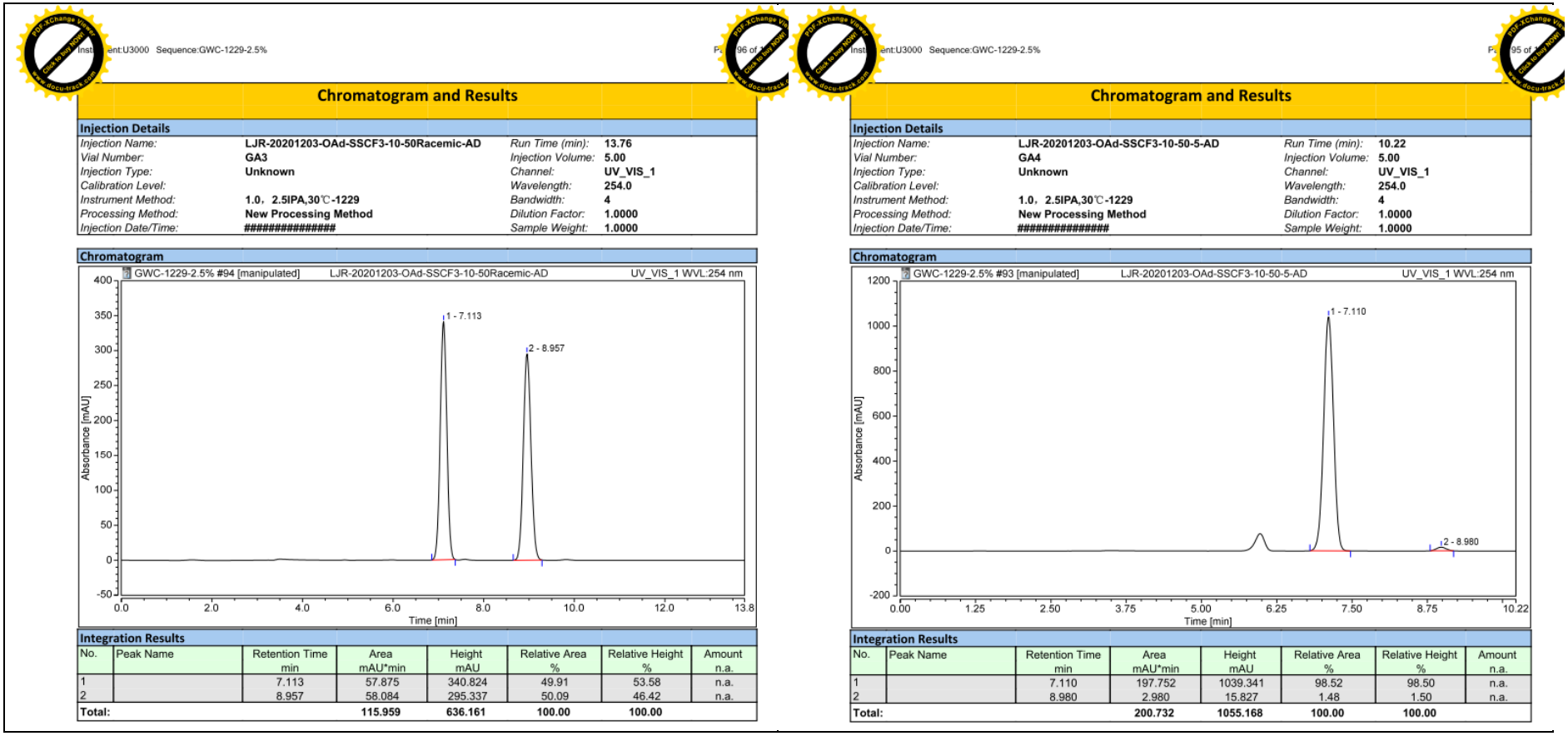
Injection Name:	LJR-20201220-OAd-SSCF3-10-12-5-AD	Run Time (min):	12.30
Vial Number:	GA4	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.453	117.585	641.814	98.17	98.04	n.a.
2		9.497	2.197	12.815	1.83	1.96	n.a.
Total:			119.782	654.629	100.00	100.00	

HPLC spectra of 3z



Chromatogram and Results

Injection Details

Injection Name:	**LJR-20201203-OAd-SSCF3-10-50Racemic-AD**	*Run Time (min):*	**13.76**
Vial Number:	**GA3**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，2.5IPA,30℃-1229**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.113	57.875	340.824	49.91	53.58	n.a.
2		8.957	58.084	295.337	50.09	46.42	n.a.
Total:			**115.959**	**636.161**	**100.00**	**100.00**	

Chromatogram and Results

Injection Details

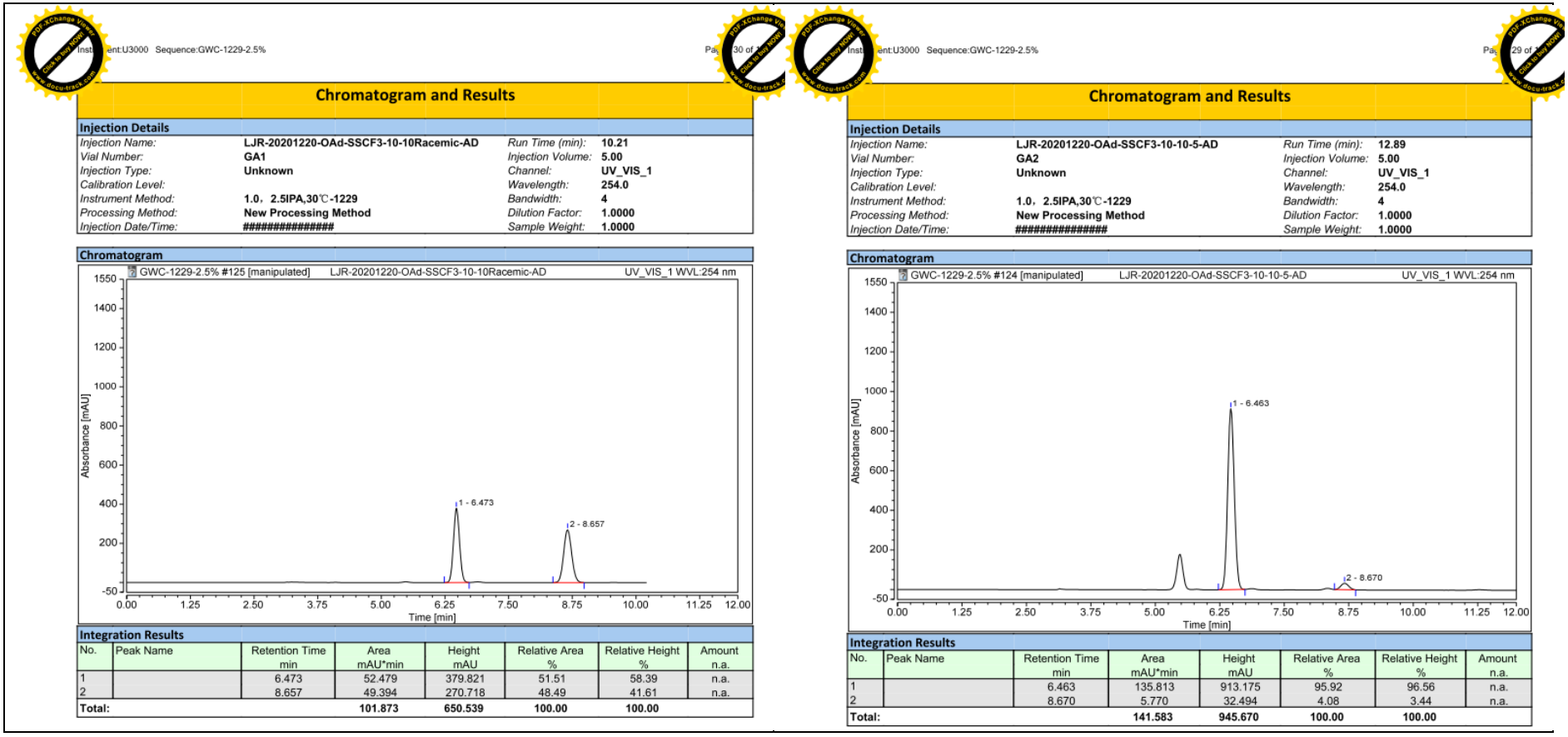
Injection Name:	**LJR-20201203-OAd-SSCF3-10-50-5-AD**	*Run Time (min):*	**10.22**
Vial Number:	**GA4**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，2.5IPA,30℃-1229**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.110	197.752	1039.341	98.52	98.50	n.a.
2		8.980	2.980	15.827	1.48	1.50	n.a.
Total:			**200.732**	**1055.168**	**100.00**	**100.00**	

HPLC spectra of 3aa



Chromatogram and Results

Injection Details

Injection Name:	LJR-20201220-OAd-SSCF3-10-10Racemic-AD	Run Time (min):	10.21
Vial Number:	GA1	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.473	52.479	379.821	51.51	58.39	n.a.
2		8.657	49.394	270.718	48.49	41.61	n.a.
Total:			101.873	650.539	100.00	100.00	

Chromatogram and Results

Injection Details

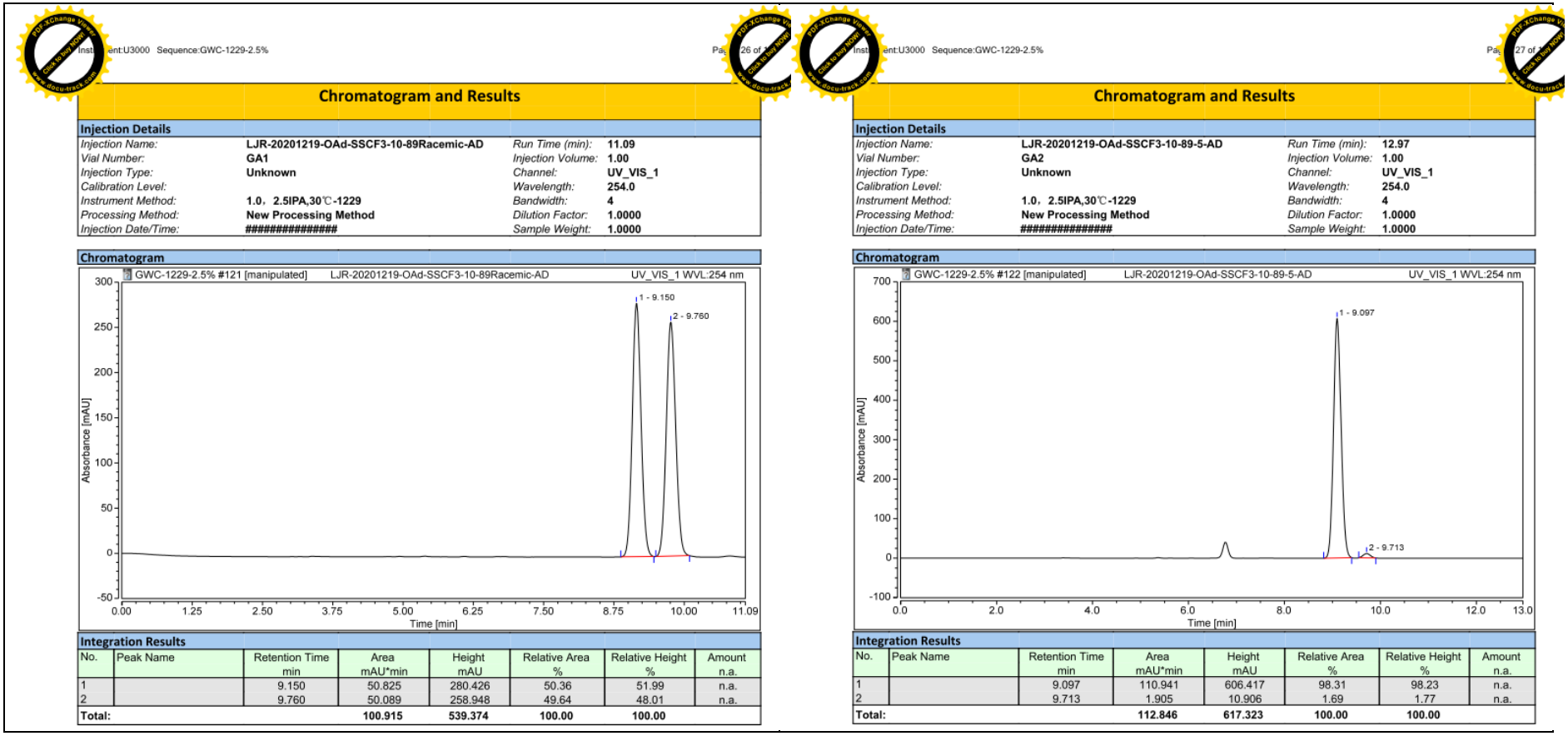
Injection Name:	LJR-20201220-OAd-SSCF3-10-10-5-AD	Run Time (min):	12.89
Vial Number:	GA2	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.463	135.813	913.175	95.92	96.56	n.a.
2		8.670	5.770	32.494	4.08	3.44	n.a.
Total:			141.583	945.670	100.00	100.00	

HPLC spectra of 3ab



Chromatogram and Results

Injection Details

Injection Name:	LJR-20201219-OAd-SSCF3-10-89Racemic-AD	Run Time (min):	11.09
Vial Number:	GA1	Injection Volume:	1.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.150	50.825	280.426	50.36	51.99	n.a.
2		9.760	50.089	258.948	49.64	48.01	n.a.
Total:			100.915	539.374	100.00	100.00	

Chromatogram and Results

Injection Details

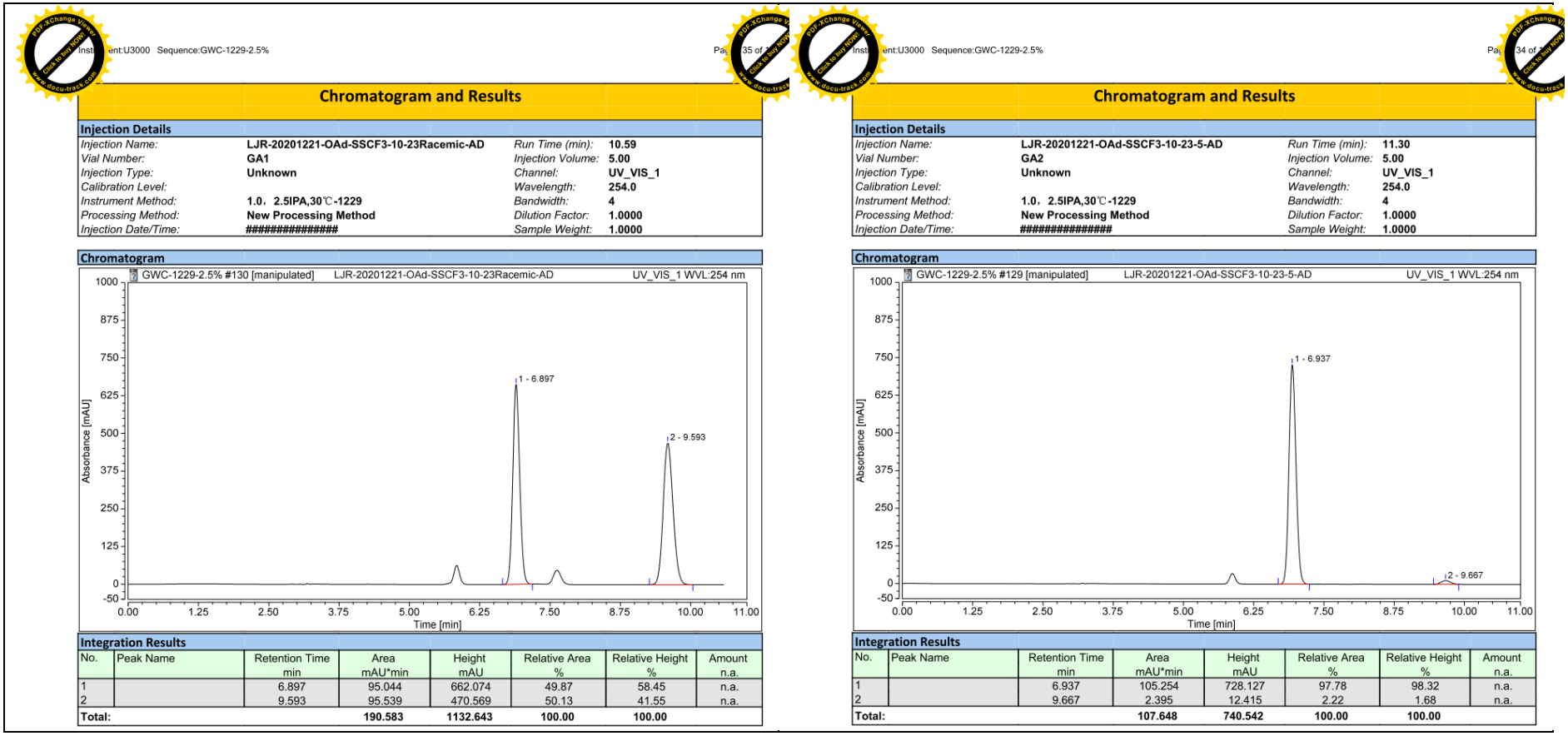
Injection Name:	LJR-20201219-OAd-SSCF3-10-89-5-AD	Run Time (min):	12.97
Vial Number:	GA2	Injection Volume:	1.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.097	110.941	606.417	98.31	98.23	n.a.
2		9.713	1.905	10.906	1.69	1.77	n.a.
Total:			112.846	617.323	100.00	100.00	

HPLC spectra of 3ac



Inst ent:U3000 Sequence:GWC-1229-2.5%

Pa 35 of

Chromatogram and Results

Injection Details

Injection Name:	**LJR-20201221-OAd-SSCF3-10-23Racemic-AD**	*Run Time (min):*	**10.59**
Vial Number:	**GA1**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，2.5IPA,30℃-1229**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

Chromatogram

GWC-1229-2.5% #130 [manipulated] LJR-20201221-OAd-SSCF3-10-23Racemic-AD UV_VIS_1 WVL:254 nm

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.897	95.044	662.074	49.87	58.45	n.a.
2		9.593	95.539	470.569	50.13	41.55	n.a.
Total:			**190.583**	**1132.643**	**100.00**	**100.00**	

Inst ent:U3000 Sequence:GWC-1229-2.5%

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Chromatogram and Results

Injection Details

Injection Name:	**LJR-20201221-OAd-SSCF3-10-23-5-AD**	*Run Time (min):*	**11.30**
Vial Number:	**GA2**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，2.5IPA,30℃-1229**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

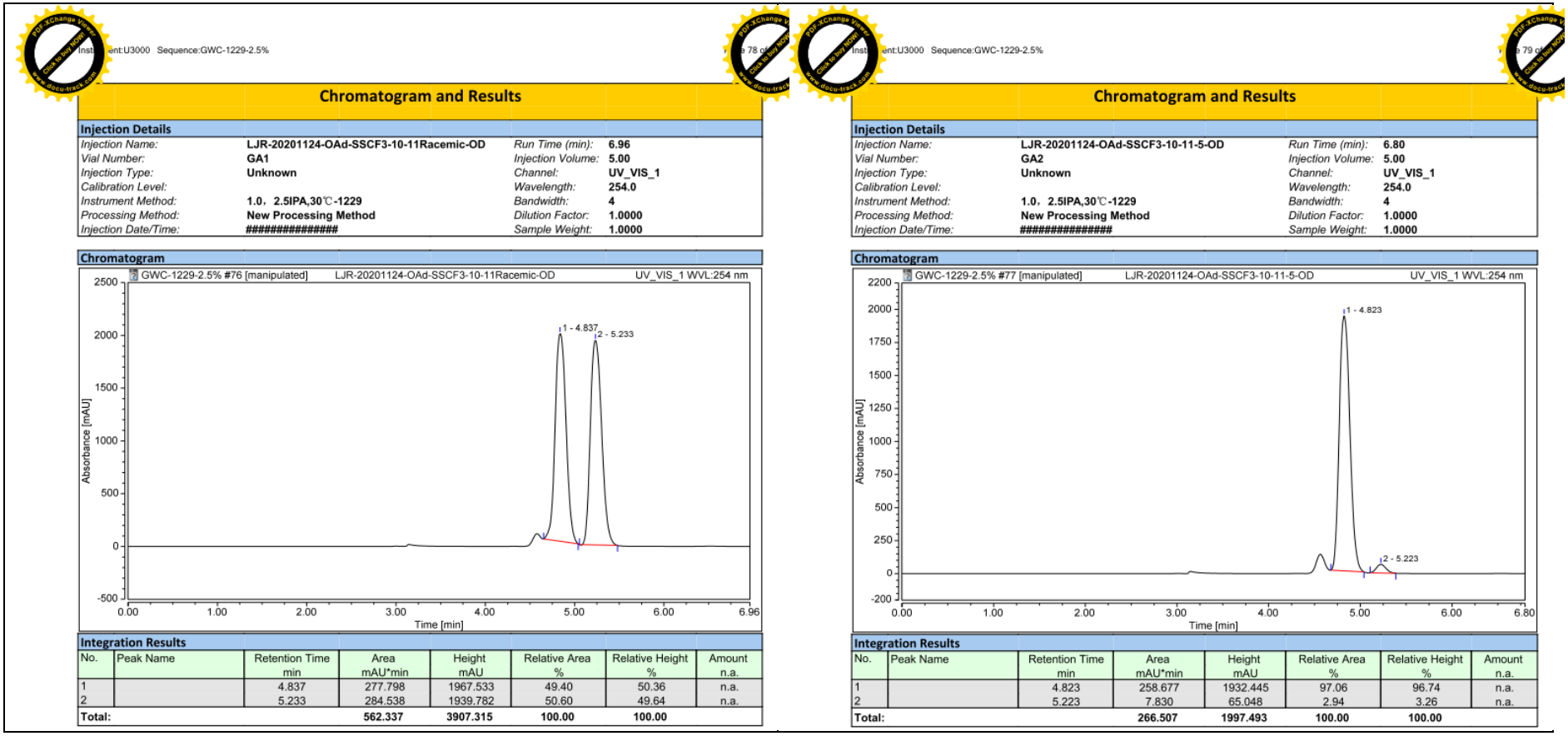
Chromatogram

GWC-1229-2.5% #129 [manipulated] LJR-20201221-OAd-SSCF3-10-23-5-AD UV_VIS_1 WVL:254 nm

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.937	105.254	728.127	97.78	98.32	n.a.
2		9.667	2.395	12.415	2.22	1.68	n.a.
Total:			**107.648**	**740.542**	**100.00**	**100.00**	

HPLC spectra of 3ad



ent:U3000 Sequence:GWC-1229-2.5%

Chromatogram and Results

Injection Details

Injection Name:	**LJR-20201124-OAd-SSCF3-10-11Racemic-OD**	*Run Time (min):*	**6.96**
Vial Number:	**GA1**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，2.5IPA,30℃-1229**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

Chromatogram

GWC-1229-2.5% #76 [manipulated] LJR-20201124-OAd-SSCF3-10-11Racemic-OD UV_VIS_1 WVL:254 nm

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.837	277.798	1967.533	49.40	50.36	n.a.
2		5.233	284.538	1939.782	50.60	49.64	n.a.
Total:			**562.337**	**3907.315**	**100.00**	**100.00**	

ent:U3000 Sequence:GWC-1229-2.5%

Chromatogram and Results

Injection Details

Injection Name:	**LJR-20201124-OAd-SSCF3-10-11-5-OD**	*Run Time (min):*	**6.80**
Vial Number:	**GA2**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，2.5IPA,30℃-1229**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

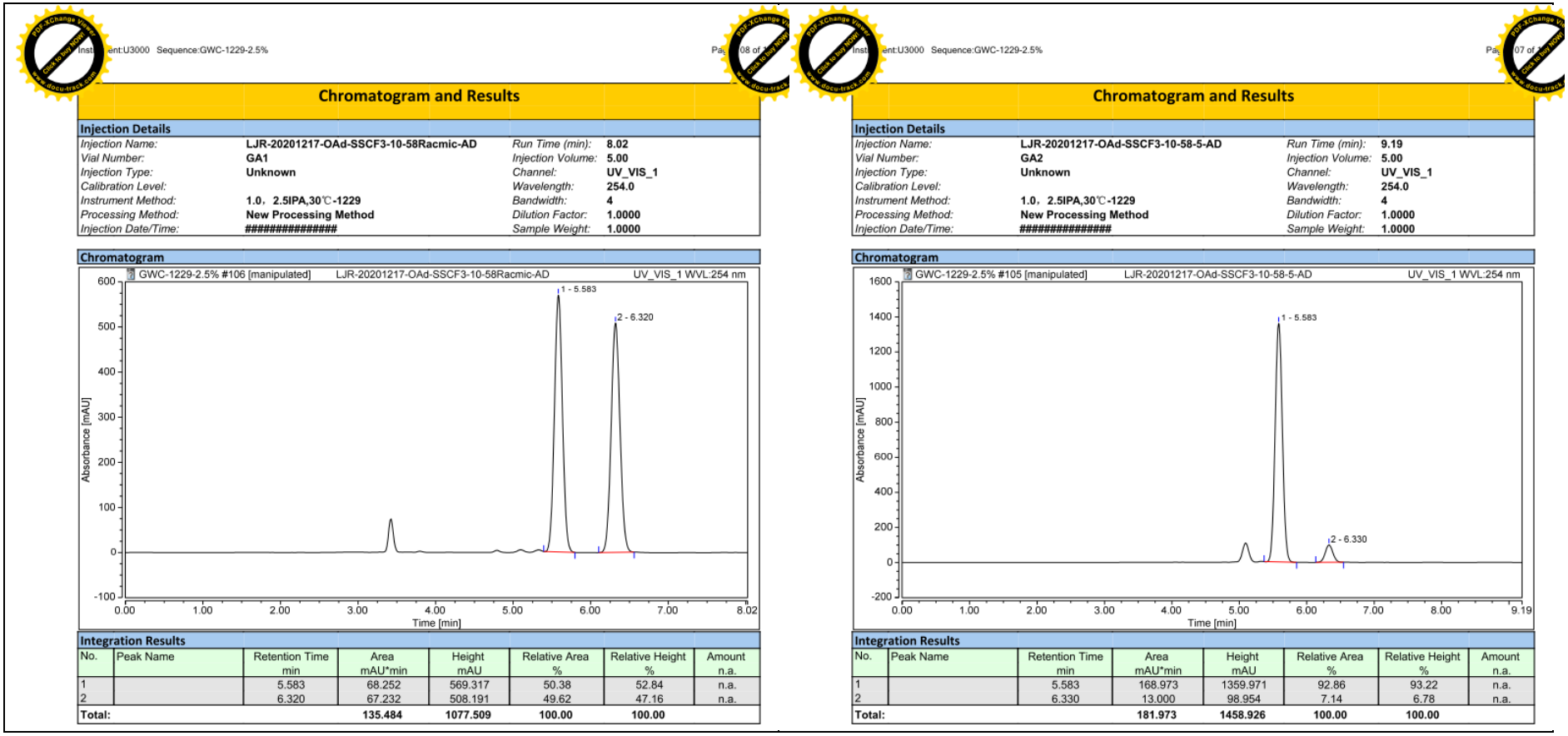
Chromatogram

GWC-1229-2.5% #77 [manipulated] LJR-20201124-OAd-SSCF3-10-11-5-OD UV_VIS_1 WVL:254 nm

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.823	258.677	1932.445	97.06	96.74	n.a.
2		5.223	7.830	65.048	2.94	3.26	n.a.
Total:			**266.507**	**1997.493**	**100.00**	**100.00**	

HPLC spectra of 3ae



Chromatogram and Results

Injection Details			
Injection Name:	LJR-20201217-OAd-SSCF3-10-58Racmic-AD	Run Time (min):	8.02
Vial Number:	GA1	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.583	68.252	569.317	50.38	52.84	n.a.
2		6.320	67.232	508.191	49.62	47.16	n.a.
Total:			135.484	1077.509	100.00	100.00	

Chromatogram and Results

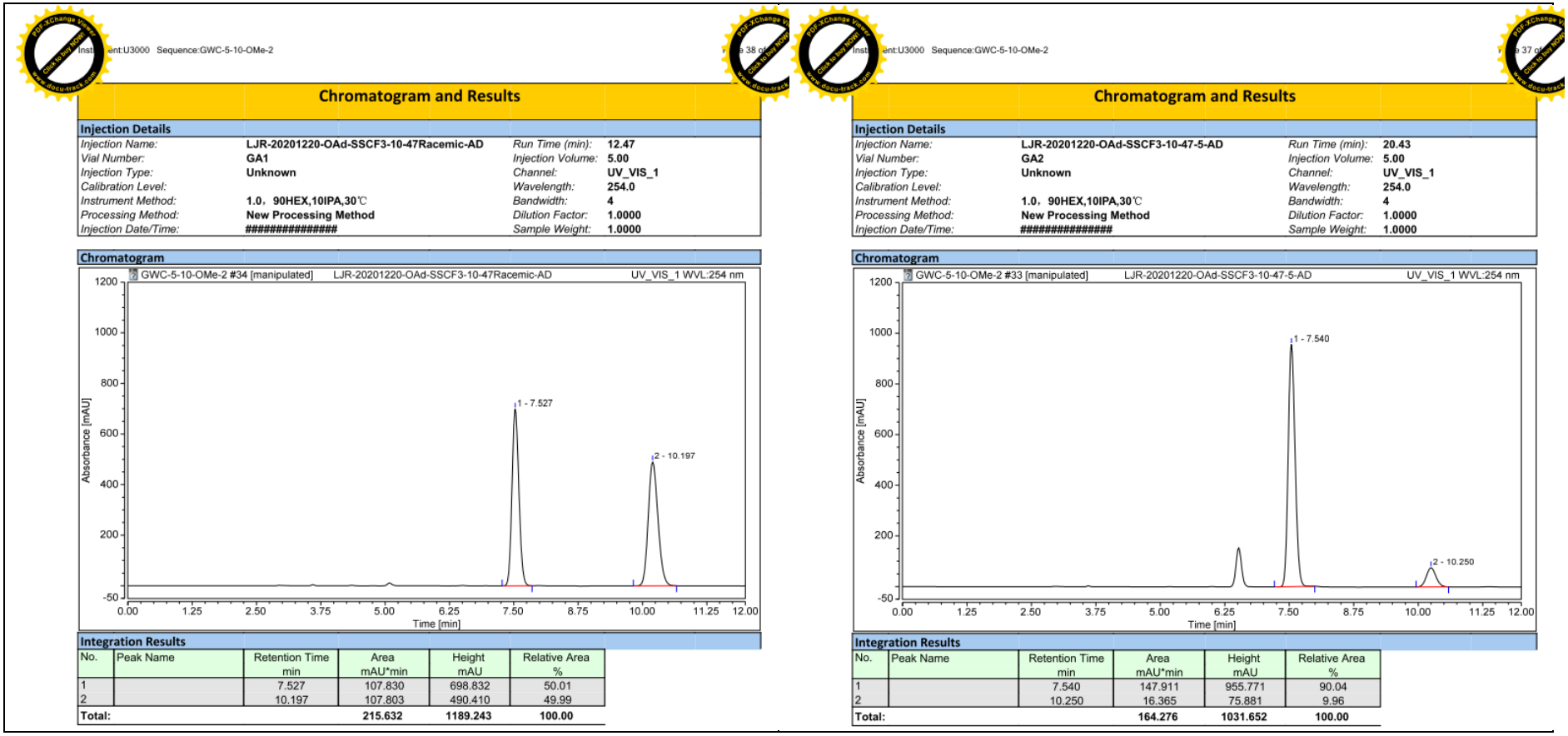
Injection Details			
Injection Name:	LJR-20201217-OAd-SSCF3-10-58-5-AD	Run Time (min):	9.19
Vial Number:	GA2	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，2.5IPA,30℃-1229	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.583	168.973	1359.971	92.86	93.22	n.a.
2		6.330	13.000	98.954	7.14	6.78	n.a.
Total:			181.973	1458.926	100.00	100.00	

HPLC spectra of 3af



Chromatogram and Results

Injection Details

Injection Name:	LJR-20201220-OAd-SSCF3-10-47Racemic-AD	Run Time (min):	12.47
Vial Number:	GA1	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，90HEX,10IPA,30℃	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %
1		7.527	107.830	698.832	50.01
2		10.197	107.803	490.410	49.99
Total:			215.632	1189.243	100.00

Chromatogram and Results

Injection Details

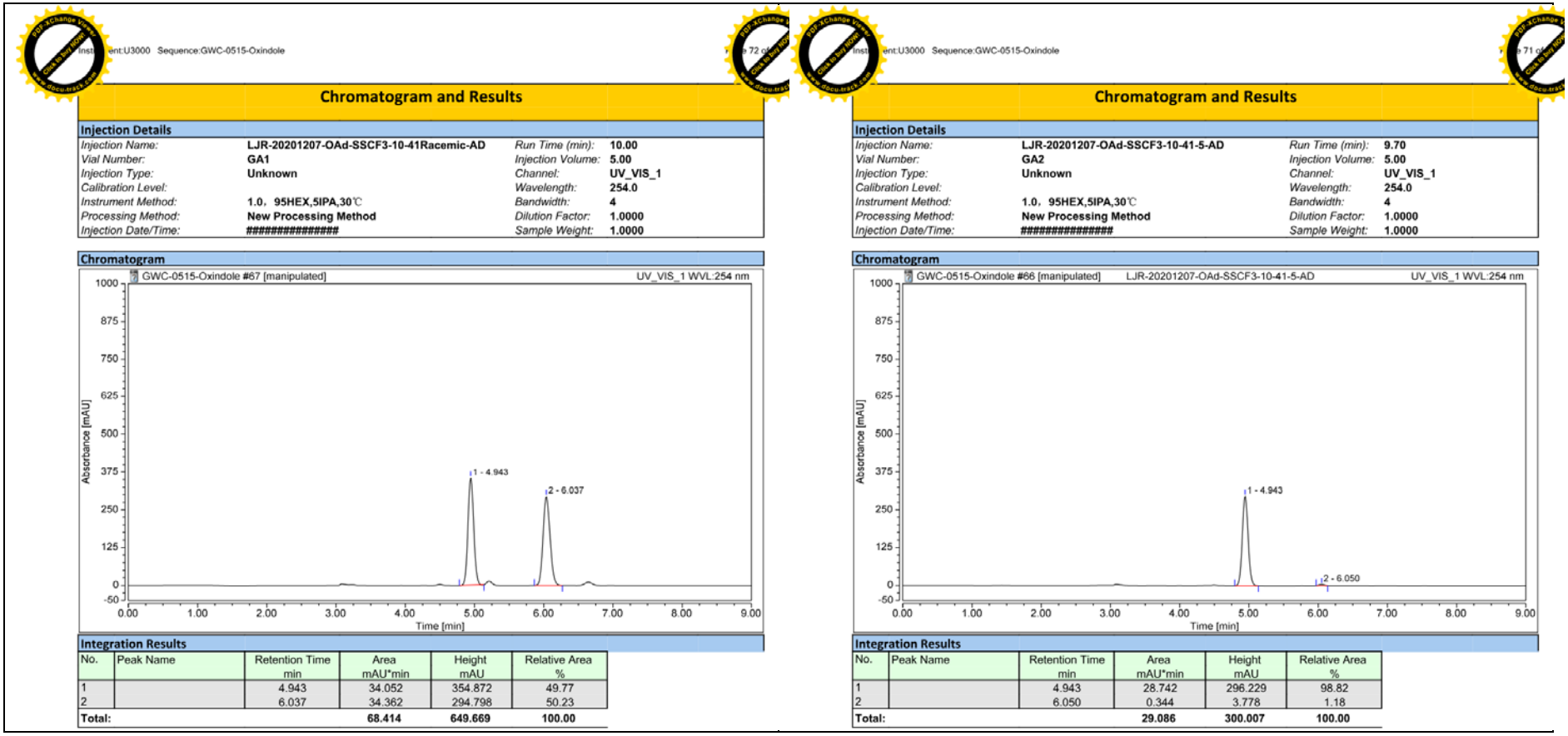
Injection Name:	LJR-20201220-OAd-SSCF3-10-47-5-AD	Run Time (min):	20.43
Vial Number:	GA2	Injection Volume:	5.00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	254.0
Instrument Method:	1.0，90HEX,10IPA,30℃	Bandwidth:	4
Processing Method:	New Processing Method	Dilution Factor:	1.0000
Injection Date/Time:	################	Sample Weight:	1.0000

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %
1		7.540	147.911	955.771	90.04
2		10.250	16.365	75.881	9.96
Total:			164.276	1031.652	100.00

HPLC spectra of 3ag



ent:U3000 Sequence:GWC-0515-Oxindole

Chromatogram and Results

Injection Details

Injection Name:	**LJR-20201207-OAd-SSCF3-10-41Racemic-AD**	*Run Time (min):*	**10.00**
Vial Number:	**GA1**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，95HEX,5IPA,30℃**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %
1		4.943	34.052	354.872	49.77
2		6.037	34.362	294.798	50.23
Total:			**68.414**	**649.669**	**100.00**

ent:U3000 Sequence:GWC-0515-Oxindole

Chromatogram and Results

Injection Details

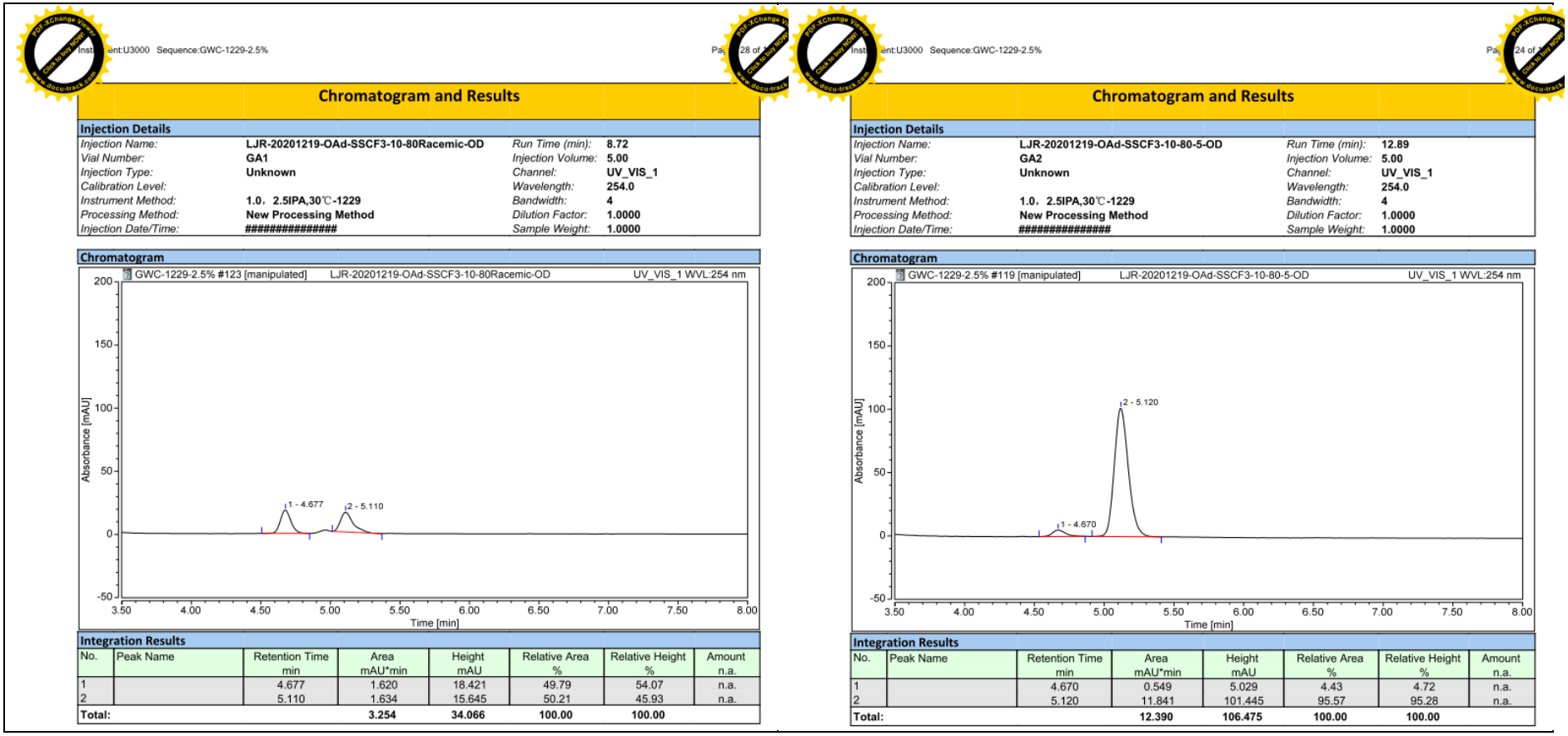
Injection Name:	**LJR-20201207-OAd-SSCF3-10-41-5-AD**	*Run Time (min):*	**9.70**
Vial Number:	**GA2**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，95HEX,5IPA,30℃**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %
1		4.943	28.742	296.229	98.82
2		6.050	0.344	3.778	1.18
Total:			**29.086**	**300.007**	**100.00**

HPLC spectra of 3ah



ent:U3000 Sequence:GWC-1229-2.5%

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Chromatogram and Results

Injection Details

Injection Name:	**LJR-20201219-OAd-SSCF3-10-80Racemic-OD**	*Run Time (min):*	**8.72**
Vial Number:	**GA1**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，2.5IPA,30℃-1229**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.677	1.620	18.421	49.79	54.07	n.a.
2		5.110	1.634	15.645	50.21	45.93	n.a.
Total:			**3.254**	**34.066**	**100.00**	**100.00**	

ent:U3000 Sequence:GWC-1229-2.5%

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Chromatogram and Results

Injection Details

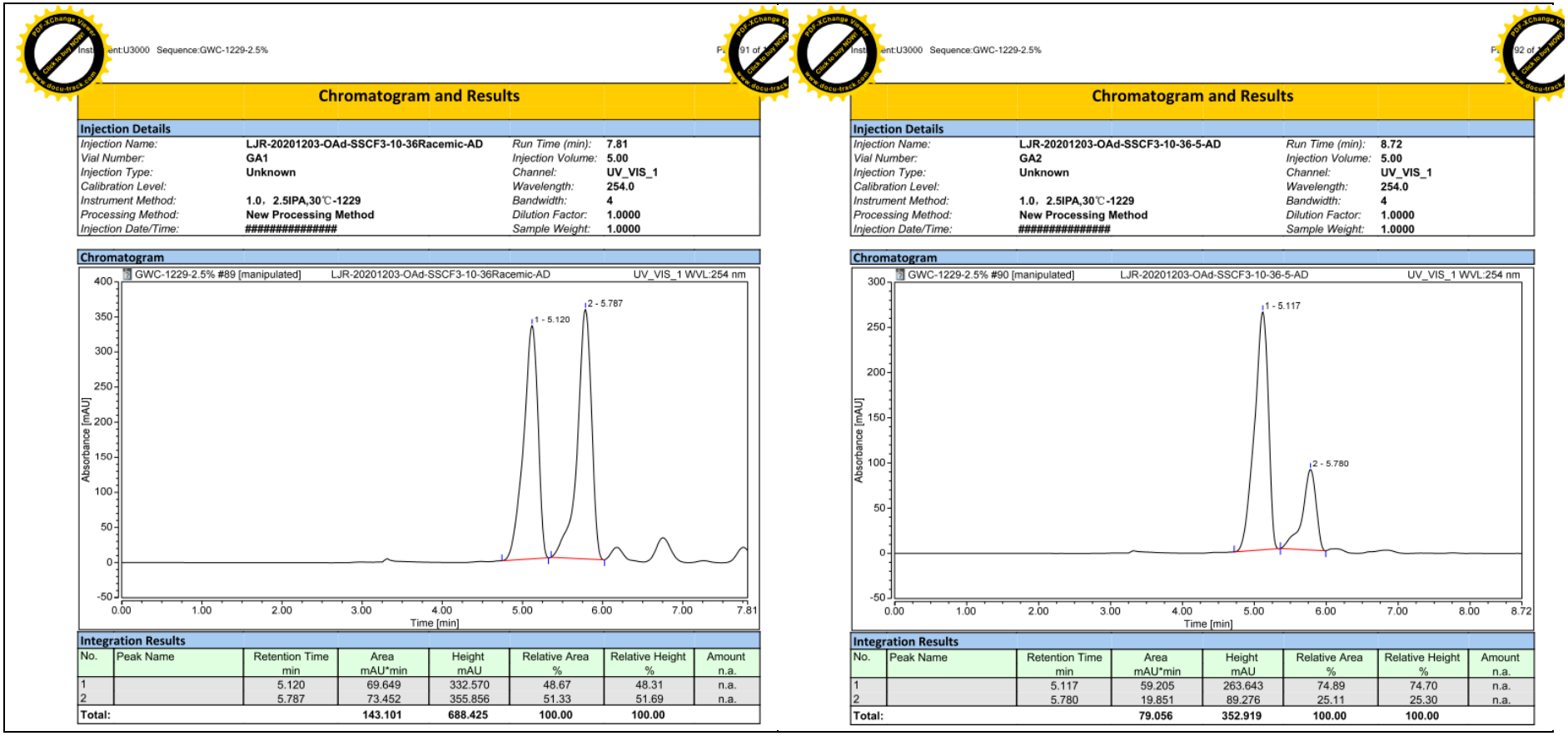
Injection Name:	**LJR-20201219-OAd-SSCF3-10-80-5-OD**	*Run Time (min):*	**12.89**
Vial Number:	**GA2**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，2.5IPA,30℃-1229**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.670	0.549	5.029	4.43	4.72	n.a.
2		5.120	11.841	101.445	95.57	95.28	n.a.
Total:			**12.390**	**106.475**	**100.00**	**100.00**	

HPLC spectra of 3ai



ent:U3000 Sequence:GWC-1229-2.5%

Chromatogram and Results

Injection Details

Injection Name:	**LJR-20201203-OAd-SSCF3-10-36Racemic-AD**	*Run Time (min):*	**7.81**
Vial Number:	**GA1**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，2.5IPA,30℃-1229**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.120	69.649	332.570	48.67	48.31	n.a.
2		5.787	73.452	355.856	51.33	51.69	n.a.
Total:			**143.101**	**688.425**	**100.00**	**100.00**	

ent:U3000 Sequence:GWC-1229-2.5%

Chromatogram and Results

Injection Details

Injection Name:	**LJR-20201203-OAd-SSCF3-10-36-5-AD**	*Run Time (min):*	**8.72**
Vial Number:	**GA2**	*Injection Volume:*	**5.00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**254.0**
Instrument Method:	**1.0，2.5IPA,30℃-1229**	*Bandwidth:*	**4**
Processing Method:	**New Processing Method**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**################**	*Sample Weight:*	**1.0000**

Chromatogram

Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.117	59.205	263.643	74.89	74.70	n.a.
2		5.780	19.851	89.276	25.11	25.30	n.a.
Total:			**79.056**	**352.919**	**100.00**	**100.00**	