Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Divergent Access to *N*-Hydroxypyrroles and Isoxazoles via Gold(I)- or Brønsted Acid- Catalysed Regioselective Cyclization of *N*-(2-trifluoromethyl-3-Alkynyl) Oximes

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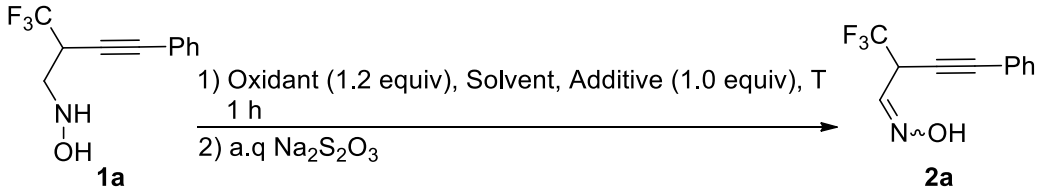
1. General information.

^{1}H NMR spectra, ^{13}C NMR spectra were recorded on a Bruker 400 MHz spectrometer in chloroform-d3. All signals are reported in ppm with the internal TMS signal at 0 ppm as a standard. The data is being reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad signal, coupling constant(s) in Hz, integration). All reactions were carried out under an atmosphere of Argon in flame-dried glassware with magnetic stirring. $ClCH_2CH_2Cl$ (DCE), CH_2Cl_2 (DCM), CH_3CN, DMSO, DMF were freshly distilled from CaH_2; toluene and THF was freshly distilled from sodium metal prior to use. 4 Å molecular sieves were powdered and dried at 300 ºC in muffle furnace for 8-10 hours prior to use. hydroxylamines **1** were prepared in good yields according to the literature.[1]

2. Table S1. Optimization of reaction conditions for 4-phenyl-2-

(trifluoromethyl)but-3-ynal oxime **2a** synthesis from corresponding hydroxylamine **1a**.[a]

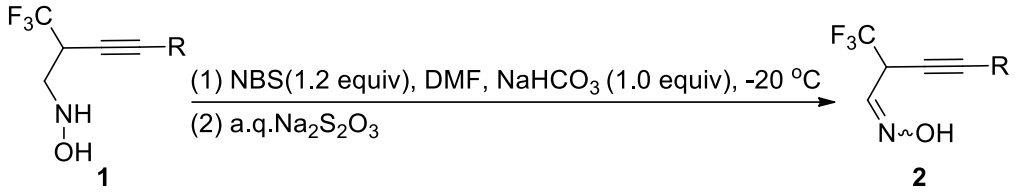


Entry	Oxidant	Solvent	T[°C]	Additive	**2a** [%][b]
1	NIS	DMF	-20	--	72
2	DDQ	DMF	-20	--	70
3	DTBP	DMF	-20	--	--
4	TBHP	DMF	-20	--	--
5	TEMPO	DMF	-20	--	--
6	BQ	DMF	-20	--	--
7	NIS	THF	-20	--	trace
8	NIS	DCE	-20	--	trace
9	NIS	DCM	-20	--	trace
10	NIS	Toluent	-20	--	trace
11	NIS	CH_3CN	-20	--	trace
12	NBS	DMF	-20	--	73
13	**NBS**	**DMF**	**-20**	**$NaHCO_3$**	**78(81)**
14	NBS	DMF	0	$NaHCO_3$	47
15	NBS	DMF	-20	Et_3N	--
16	NBS	DMF	-20	K_2CO_3	--
17	NBS	DMF	-20	DBU	38

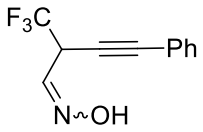
[a] Reactions were conducted on a 0.1 mmol scale, oxidant (1.2 equiv) in 1.0 mL of solvent. [b] NMR yields using CH_2Br_2 as the internal reference, yields of isolated product are shown in parentheses.

3. General procedure for the synthesis of *N*-(2-trifluoromethyl-3-

Alkynyl) oximes 2



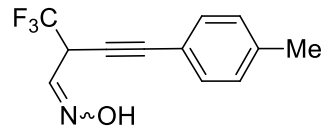
To the solution of *N*-(2–(trifluoromethyl)-3-alkynyl)hydroxylamines **1** (1.0 mmol), Sodium bicarbonate (1.0 mmol) in DMF (10 mL) at -20 °C was added NBS(1.2 mmol, 213.6 mg), the reaction was stirred at -20 °C for 15 min～1h. After the hydroxylamines **1** was completely consumed, which was determined by TLC analysis, saturated aqueous sodium thiosulfate (10 mL) was then added at -20 °C. The reaction mixture was extracted with ethyl acetate (3×15 mL) and the combined organic extracts were dried (Na_2SO_4). After filtration and evaporation, the residue was purified by flash column chromatography on silica gel [eluent: petroleum ether: ether=10:1] to give 2-(trifluoromethyl)but-3-ynal oxime **2** in 60%～91% yield.



2a

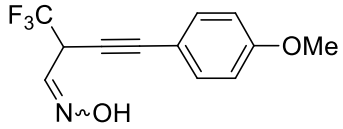
yellow oil, 81% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ [9.54 (brs, 0.69H), 9.12 (brs, 0.31H)]; [7.56 – 7.45(m, 1.38H), 7.56 – 7.45 (m, 0.62H)]; [7.42 – 7.29(m, 2.07H), 7.42 – 7.29 (m, 0.93H)]; [7.56 – 7.45 (m, 0.31H), 6.98 – 6.90 (m, 0.69H)]; [5.25 – 5.05 (m, 0.69H), 4.35 – 4.24(m, 0.31H)]. ^{19}F NMR (377 MHz, $CDCl_3$) δ -69.49, -69.55. ^{13}C NMR (126 MHz, $CDCl_3$) δ (142.61, 140.60), 131.99, (129.17, 129.08), 128.33, [123.45 (q, *J* = 280.9 Hz), 123.40 (q, *J* = 280.4 Hz)], (121.49, 121.34), (87.28, 87.22), 85.17, [39.92 (q, *J* = 32.7 Hz), 33.91 (q, *J* = 33.5 Hz)]. MS (70 eV): m/z (%): 227

(M+, 62.80), 91(100). HRMS calcd for $C_{11}H_8F_3NO$: 227.0558, found: 227.0556.



2b

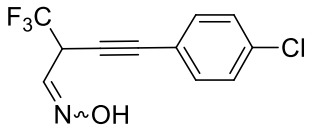
White solid, 80% isolated yield. 1H NMR (500 MHz, CDCl3) δ [9.23 (brs, 0.6H), 8.85 (brs, 0.4H)]; [7.51 (d, *J* = 6.6 Hz, 0.4H), 6.92 (d, *J* = 7.1 Hz, 0.6H)]; [7.38 (d, *J* = 8.4 Hz, 1.2H), 7.38 (d, *J* = 8.4 Hz, 0.8H)]; [7.17 – 7.10 (m, 1.2H), 7.17 – 7.10 (m, 0.8H)] ; [5.16-5.07 (m, 0.6H), 4.31 – 4.23 (m, 0.4H)]; [2.36 (s, 1.8H),2.36 (s, 1.2H)]. ^{19}F NMR (377 MHz, CDCl3) δ -69.56, -69.60. ^{13}C NMR (125 MHz, $CDCl_3$) δ (142.71, 140.74), (139.41, 139.30), 131.87, 129.07, [123.49 (q, *J* = 280.7 Hz), 123.43 (q, *J* = 280.3 Hz)], (118.44, 118.29), 87.40, 85.33, [39.94 (q, J = 32.6 Hz), 33.89 (q, *J* = 33.2 Hz)], 21.45.



2c

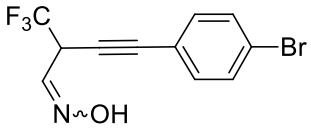
Yellow solid, 91% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) [8.78 (brs, 0.2H), 8.44 (brs, 0.8H)]; [7.47 (d, *J* = 6.9 Hz, 0.8H), 6.88 (d, *J* = 7.4 Hz, 0.2H)]; [7.40 (d, *J* = 8.8 Hz, 1.6H), 7.40 (d, *J* = 8.8 Hz, 0.4H)]; [6.84 (d, *J* = 8.8 Hz, 1.6H), 6.84 (d, *J* = 8.8 Hz, 0.4H)]; [5.15-5.05 (m, 0.2H), 4.27 – 4.18 (m, 0.8H)]; [3.81 (s, 1.2H, 3.81 (s, 1.8H)]. ^{19}F NMR (377 MHz, $CDCl_3$) δ -69.63, -69.69. ^{13}C NMR (100 MHz, $CDCl_3$) δ (160.20, 160.13), (142.77, 140.75), 133.49, [123.56 (q, *J* = 280.7 Hz), 123.48 (q, *J* = 280.7 Hz)], 113.98, 113.50, 87.05, 75.90(q, *J* = 3.3 Hz), 55.29 (d, *J* = 2.1 Hz),

[39.94 (q, *J* = 33.6 Hz), 33.83 (q, *J* = 33.0 Hz)]. HRMS-ESI calcd for $C_{12}H_9NO_2F_3$[M-H$^+$]: 256.0591, found:256.0587.



2d

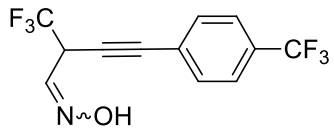
Yellow solid, 88% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ [7.85 (brs, 0.59H), 7.49 (brs, 0.41H)]; [7.48 (d, *J* = 6.6 Hz , 0.41H), 6.89(d, *J* = 7.1 Hz , 0.59H)]; [7.41 (d, *J* = 8.5 Hz , 0.82H), 7.39(d, *J* = 8.5 Hz , 1.18H)]; [7.30 (d, *J* = 8.5 Hz , 0.82H), 7.30 (d, *J* = 8.5 Hz , 1.18H)]; [5.15-5.05 (m, 0.59H), 4.31 – 4.20 (m, 0.41H)]. ^{19}F NMR (377 MHz, $CDCl_3$) δ -69.46, -69.49. ^{13}C NMR (100 MHz, $CDCl_3$) δ (142.41, 140.31), (135.35, 135.25), 133.22, 128.72, [123.37 (q, *J* = 280.9 Hz), 123.31 (q, *J* = 280.4 Hz)], (119.98, 119.83), 86.02, 83.99, [39.92 (q, *J* = 32.4 Hz), 33.84 (q, *J* = 33.4 Hz)]. HRMS calcd for $C_{11}H_6NOF_3Cl$: 260.0095, found: 260.0099.



2e

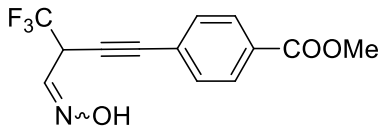
Yellow solid, 60% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ [9.13 (brs, 0.44H), 8.75 (brs, 0.56H)]; [7.53-7.45 (m, 0.88H), 7.53-7.45 (m, 1.12H)]; [7.34 (d, *J* = 7.4 Hz , 0.56H), 6.92(d, *J* = 7.1 Hz , 0.44H)]; [7.40 – 7.28 (m, 0.88H), 7.40 – 7.28 (m, 1.12H)]; [5.17-5.06 (m, 0.44H), 4.32 – 4.22 (m, 0.56H)]. ^{19}F NMR (377 MHz, $CDCl_3$) δ -69.50, -69.54. ^{13}C NMR (100 MHz, $CDCl_3$) δ [142.56 (q, *J* = 1.9 Hz), 140.54], 131.98, (129.16, 129.06), 128.33, [123.45 (q, *J* = 280.6 Hz), 123.39 (q, *J* = 280.1 Hz)], (121.50, 121.35), 87.16, 85.10, [39.91 (q, *J* = 32.6 Hz), 33.85 (q, *J* = 33.4 Hz)]. HRMS-ESI calcd for

$C_{11}H_6NOF_3Br$: 303.9590, found: 303.9587.



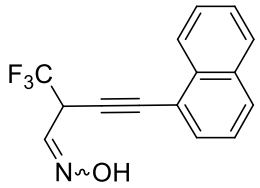
2f

Yellow oil ,76% isolated yield, unstable. ^{1}H NMR (400 MHz, $CDCl_3$) δ [8.58 (s, 0.73H), 8.33 (s, 0.27H)]; [7.64 (d, *J* = 8.2 Hz, 1.46H), 7.58 (d, *J* = 6.6 Hz, 0.54H)]; [7.49 (d, *J* = 6.6Hz, 0.54H), 7.43 (d, *J* = 8.1 Hz, 1.46H)]; [6.98 (q, *J* = 2.4 Hz, 0.73H), 6.90 (d, *J* = 7.0 Hz, 0.27H)]; [5.18-5.07 (m, 0.27H), 4.34 – 4.22 (m, 0.73H)]. ^{19}F NMR (377 MHz, $CDCl_3$) δ -61.53, -62.89, -63.04, -69.44. HRMS-ESI calcd for $C_{12}H_6NF_6O$[M-H+]: 294.0359, found: 294.0355.



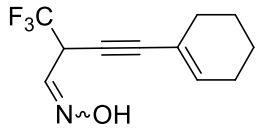
2g

Yellow oil, 67% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) [9.00 (brs, 0.57H), 8.61 (brs, 0.43H)]; [7.99 (d, *J* = 8.4 Hz, 1.14H), 7.99 (d, *J* = 8.4 Hz, 0.86H)]; [7.53 (d, *J* = 8.4 Hz, 0.86H), 7.52 (d, *J* = 8.4 Hz, 1.14H)]; [7.48 (d, *J* = 7.0 Hz, 0.43H), 6.89 (d, *J* = 7.0 Hz, 0.57H)]; [5.19-5.08 (m, 0.57H), 4.34-4.24 (m, 0.43H)]; [3.92 (s, 1.71H) , 3.92 (s, 1.27H)].^{19}F NMR (377 MHz, $CDCl_3$) δ -69.38, -69.42. ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.50, (142.11, 139.91), 131.95, 130.24, 129.47, 126.16, [123.35 (d, *J* = 280.8 Hz), 123.29 (d, *J* = 280.4 Hz)], 86.12, 84.13, 52.37, [39.94 (q, *J* = 32.9 Hz), 33.84 (q, *J* = 33.2 Hz)]. HRMS-ESI calcd for $C_{13}H_9NO_3F_3$[M-H$^+$]: 284.0540, found: 284.0539.



2j

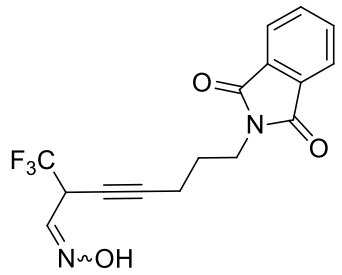
Yellow oil, 89% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ [9.33 (brs, 0.62H), 8.86 (brs, 0.38H)]; [8.29 (d, *J* = 8.3 Hz, 1.24H), 8.29 (d, *J* = 8.3 Hz, 0.76H)]; [7.76 (dd, *J* = 7.2, 0.9Hz, 0.76H), 7.73 (dd, *J* = 7.2, 0.9Hz, 1.24H)]; [7.67-7.59 (m, 0.62H), 7.67-7.59 (m, 0.38H)]; [7.62 (d, *J* = 7.0 Hz, 0.38H), 7.07 (d, *J* = 7.0 Hz, 0.62H)]; [7.58 – 7.51 (m, 0.62H), 7.58 – 7.51 (m, 0.38H)]; [7.47 – 7.40 (m, 0.62H), 7.47 – 7.40 (m, 0.38H)]; [5.36 – 5.25 (m, 0.62H), 4.52 – 4.43 (m, 0.38H)]. ^{19}F NMR (377 MHz, $CDCl_3$) δ -69.33, -69.36. ^{13}C NMR (100 MHz, $CDCl_3$) δ [142.73 (q, *J* = 2.0 Hz), 140.65], (133.36, 133.31), 133.07, (131.19, 131.13), (129.70, 129.59), 128.33, 127.13, 126.54, 125.71, 125.02, [124.10 (q, *J* = 280.8 Hz), 124.05 (q, *J* = 280.4 Hz)], (119.08, 118.94), (85.51, 83.49), [81.95 (q, *J* = 3.8 Hz), 81.85 (q, *J* = 3.8 Hz)], [40.24 (q, *J* = 32.7 Hz), 34.27 (q, *J* = 33.3 Hz)]. HRMS-ESI calcd for $C_{15}H_9NOF_3$[M-H^+]: 276.0642, found: 276.0637.



2l

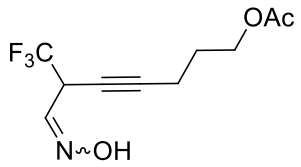
White solid, 80% isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ [9.39 (s, 0.71H), 8.98 (s, 0.29H)]; [7.41 (d, *J* = 6.6 Hz, 0.29H), 6.81 (d, *J* = 7.2 Hz, 0.71H)]; [6.19 (d, *J* = 1.6 Hz, 0.71H), 6.19 (d, *J* = 1.6 Hz, 0.29H)]; [5.03-4.94 (m, 0.71H), 4.18-4.09 (m, 0.29H)]; [2.15-2.05 (m, 2.84H), 2.15-2.05 (m, 1.16H)]; [1.68 – 1.53 (m, 2.84H), 1.68 – 1.53 (m, 1.16H)]. ^{19}F NMR (377 MHz, $CDCl_3$) δ -69.88, -69.90. ^{13}C NMR (126 MHz, $CDCl_3$) δ

[142.91 (q, *J* = 1.9 Hz), 141.02 (q, *J* = 0.8 Hz)], (137.21,137.06), [123.48 (q, *J* = 280.6 Hz), 123.42 (q, *J* = 280.3 Hz)], (119.43, 119.34), (89.05, 87.00), [74.33 (q, *J* = 3.7 Hz), 74.18 (q, *J* = 3.4 Hz)]; [39.80(q, *J* = 32.6 Hz), 33.77 (q, *J* = 33.2 Hz)], (28.73,28.65), 25.56, 22.07, 21.30. HRMS-ESI calcd for $C_{11}H_{11}NOF_3$[M-H^+]: 230.0798, found: 230.0805.



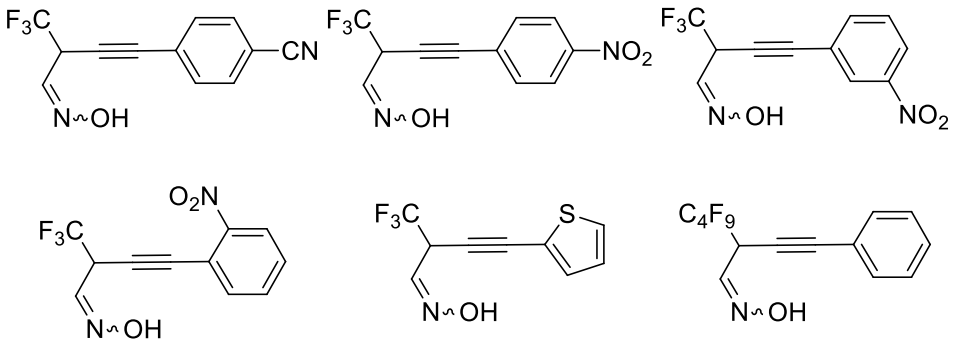
2m

White Solid, 83% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ [9.13 (s,0.43H), 8.81 (s, 0.57H)]; [7.87 – 7.80 (m, 1.14H), 7.87 – 7.80 (m, 0.86H)]; [7.74 – 7.67 (m, 1.14H), 7.74 – 7.67 (m, 0.86H)]; [7.32 (d, *J* = 6.6 Hz, 0.57H), 6.72 (d, *J* = 7.0 Hz, 0.43H)]; [4.82 – 4.71 (m, 0.43H), 3.97 – 3.85 (m, 0.57H)]; [3.81 – 3.73 (m, 0.86H), 3.81 – 3.73 (m, 1.14H)]; [2.35-2.25 (m, 0.86H), 2.35-2.25 (m, 1.14H)]; [1.97 – 1.86 (m, 0.86H), 1.97 – 1.86 (m, 1.14H)]. ^{19}F NMR (377 MHz, $CDCl_3$) δ -70.01, -70.03. ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.45, (142.59, 140.78), 134.01, 131.98, [123.53 (q, *J* = 280.6 Hz), 123.50 (q, *J* =280.1 Hz)], 123.29, (86.59, 84.44), [69.49 (q, 1.6 Hz), 69.43 (q, 1.5 Hz)], [39.24 (q, *J* = 32.8 Hz), 33.24 (q, *J* = 33.0 Hz)], 37.12, (27.09, 27.02), 16.45. HRMS-ESI calcd for $C_{16}H_{12}N^2F_3O_3$[M-H^+]: 337.0806, found: 337.0802.



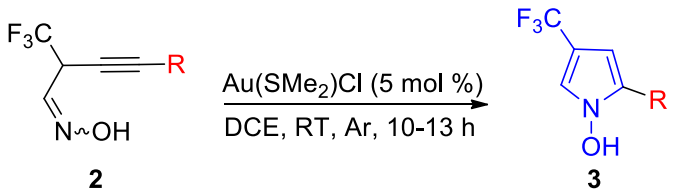
2n

Colorless oil, 64% isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ [9.56 (brs, 0.70H), 9.14 (brs, 0.30H)]; [7.35 (d, *J* = 6.6 Hz, 0.30H), 6.75 (d, *J* = 7.0 Hz, 0.70H)]; [4.88 – 4.78 (m, 0.70H), 4.03 – 3.94 (m, 0.30H)]; [4.18-4.10 (m, 1.4H), 4.18-4.10 (m, 0.6H)]; [2.35 – 2.26 (m, 1.4H), 2.35 – 2.26 (m, 0.6H)]; [2.04 (s, 2.1H), 2.04 (s, 0.9H)]; [1.88 – 1.79 (m, 1.4H), 1.88 – 1.79 (m, 0.6H)]. ^{19}F NMR (377 MHz, $CDCl_3$) δ -70.12, -70.12. ^{13}C NMR (126 MHz, $CDCl_3$) δ (171.68, 171.67), [142.57 (q, *J* = 2.0 Hz), 140.63 (q, *J* = 0.9 Hz)], [123.54 (q, *J* = 280.6 Hz), 123.51 (q, *J* = 280.0 Hz)], (86.52, 84.33), [69.41 (q, *J* = 3.7 Hz), 69.43 (q, *J* = 3.7 Hz)], (63.10, 63.08), [39.24 (q, *J* = 32.4 Hz), 33.22 (q, *J* = 33.1 Hz)], (27.18, 27.13), 20.82, (15.35, 15.33). HRMS-ESI calcd for $C_{10}H_{11}NO_3F_3$[M-H$^+$]: 250.0697, found: 250.0727.

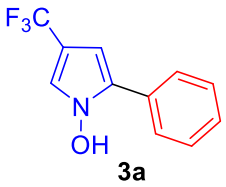


The above six oximes compounds are very unstable, we could not obtain their clean NMR spectra

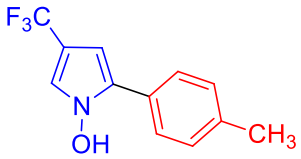
4. General procedure for the synthesis of 4-trifluoromethyl substituted *N*-hydroxypyrroles 3



To the solution of *N*-(2–(trifluoromethyl)-3-alkynyl) oximes **2** (0.1 mmol) in 1, 2-dichloroethane (1.0 mL) at room temperature was added $Au(SMe_2)Cl$ (1.5mg. 5mol %), the reaction mixture was stirred at room temperature for 10-13 h under argon atmosphere. After oximes **2** were completely consumed, which was determined by TLC analysis, the solvent was evaporated under reduced pressure and the residue was purified by silica gel flash column chromatography [eluent: petroleum ether: ether=10:1~5:1] to give the desired *N*-hydroxypyrroles **3**.

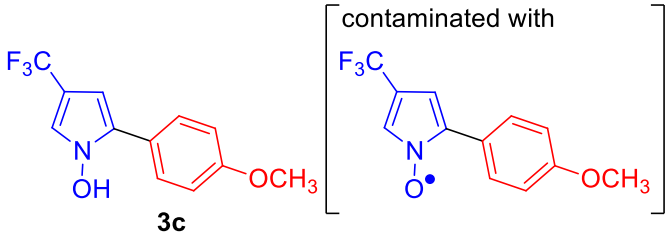


Colorless oil, 80% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.57 (m, 2H), 7.45-7.39 (m, 2H), 7.37 – 7.31 (m, 1H), 7.19 (d, *J* = 1.1 Hz, 1H), 6.73 (s, 1H), 6.38 (d, *J* = 2.2 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.47. ^{13}C NMR (100 MHz, $CDCl_3$) δ 130.49, 129.66, 128.65, 127.76, 127.54, 123.45 (q, *J* = 266.0 Hz), 117.52 (q, *J* = 4.7 Hz), 110.17 (q, *J* = 38.1 Hz), 101.47 (d, *J* = 3.0 Hz). MS (70 eV): m/z (%): 229 (M^+, 100). HRMS-ESI calcd for $C_{11}H_7F_3NO$ [M-H^+]: 226.0485, found: 226.0488.



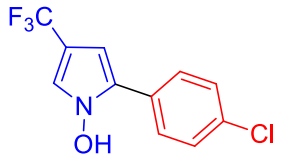
3b

White solid, 82% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.13 (q, *J* = 1.0 Hz, 1H), 6.96 (s, 1H), 6.34 (d, *J* = 2.1 Hz, 1H), 2.39 (s, 3H).^{19}F NMR (377 MHz, $CDCl_3$) δ -57.44 (s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.75, 130.58, 129.34, 127.47, 126.85, 123.53 (q, *J* = 266.0 Hz), 117.22 (q, *J* = 4.7 Hz), 110.05 (q, *J* = 38.0 Hz), 101.03 (q, *J* = 3.0 Hz), 21.18 (q, *J* = 1.7 Hz). MS (70 eV): m/z (%): 243(M^+, 100). HRMS-ESI calcd for $C_{12}H_9NOF_3$[M-H^+]: 240.0642, found: 240.0653.



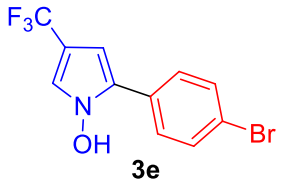
3c

White solid, 69% isolated yield. This compound is unstable. ^{1}H NMR (400 MHz, $CDCl_3$) δ [7.55-7.46 (m, 2H)], [7.15 (q, *J* = 1.1 Hz, 1H)], 6.96 (brs, 1H), [6.94 – 6.86 (m, 2H)], [6.29 (s, 1H)], [3.82 (s, 1.6H), 3.79 (s, 1.4H)]. ^{19}F NMR (377 MHz, $CDCl_3$) δ [-57.46, -57.49]. ^{13}C NMR (100 MHz, $CDCl_3$) δ (159.12, 158.92), (130.44, 130.40), (129.07, 129.03), [123.55 (q, *J* = 266.0 Hz)], (122.54, 122.44), [116.90 (q, *J* = 4.6 Hz), 116.94 (q, *J* = 4.6 Hz)], 114.15, 110.05 (q, *J* = 38.0 Hz), 100.70 (q, *J* = 2.9 Hz), (55.43, 55.40). HRMS-ESI calcd for $C_{12}H_9NO_2F_3$[M-H^+]: 256.0591, found: 256.0596.



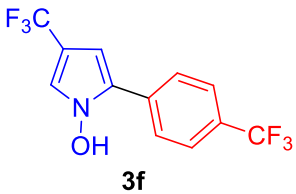
3d

3d yellow oil, 88% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.5 Hz, 2H), 7.37 (d, *J* = 8.5 Hz, 2H), 7.18 (s, 1H), 7.11 (s, 1H), 6.38 (d, *J* = 2.0 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.54. ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.64, 129.43, 128.85, 128.67, 128.14, 123.34 (q, *J* = 266.2 Hz), 117.85 (q, *J* = 4.7 Hz), 110.37 (q, *J* = 38.2 Hz), 101.69 (q, *J* = 3.0 Hz). HRMS-ESI calcd for $C_{11}H_6NOF_3Cl[M\text{-}H^+]$: 260.0095, found: 260.0105.



3e

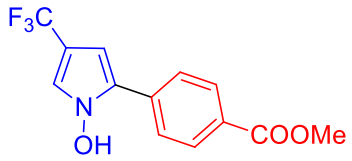
Yellow oil, 89% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.8 Hz, 2H), 7.49 (d, *J* = 8.8 Hz, 2H), 7.39 (s, 1H), 7.18 (q, *J* = 1.1 Hz, 1H), 6.39 (d, *J* = 2.1 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.53. ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.79, 129.41, 128.92, 128.66, 123.34 (q, *J* = 266.1 Hz), 121.74, 117.92 (q, *J* = 4.6 Hz), 110.37 (q, *J* = 38.1 Hz), 101.70 (d, *J* = 3.0 Hz). HRMS-ESI calcd for $C_{11}H_6NOF_3Br[M\text{-}H^+]$: 303.9590, found: 303.9598



3f

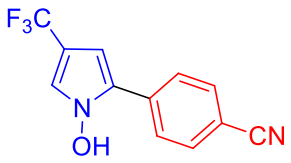
White solid, 61% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.2 Hz,2H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.28 (s, 1H), 7.24 (q, *J* = 1.1 Hz, 1H),

6.48 (d, J = 2.0 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.69, -62.68. ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.19, 129.50 (q, J = 32.6 Hz), 129.10, 127.46, 125.62 (q, J = 3.8 Hz), 124.05 (q, J = 272.0 Hz), 123.25 (q, J = 266.2 Hz), 118.52 (q, J = 4.6 Hz), 110.74 (q, J = 38.3 Hz), 102.66 (d, J = 3.0 Hz). HRMS-ESI calcd for $C_{12}H_6NF_6O$[M-H$^+$]: 294.0359, found: 294.0369.



3g

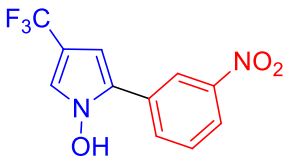
White solid, 72% isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.65 (s, 1H), 7.72 (d, J = 7.6 Hz, 2H), 7.57 (d, J = 7.4 Hz, 2H), 7.29 (s, 1H), 6.46 (s, 1H), 3.70 (s, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.52. ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.47, 134.61, 129.86, 129.16, 127.41, 126.76, 123.34 (q, J = 266.0 Hz), 119.05 (q, J = 4.6 Hz), 110.46 (q, J = 38.0 Hz), 102.61 (q, J = 2.9 Hz), 52.45. HRMS-ESI calcd for $C_{13}H_9NO_3F_3$[M-H$^+$]: 284.0540, found: 284.0541.



3h

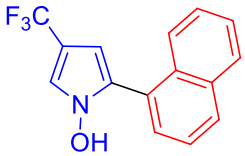
White solid, 35% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.72 (d, J = 8.5 Hz, 2H), 7.50 (d, J = 8.5 Hz, 2H), 7.20 – 7.16 (m, 1H), 6.45 (d, J = 1.9 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.62. ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.98, 132.41, 128.26, 127.31, 123.20 (q, J = 266.2 Hz), 119.53 (q, J = 4.6 Hz), 118.84, 110.77 (q, J = 38.3 Hz), 109.39, 103.32 (q, J

= 3.0 Hz). HRMS-ESI calcd for $C_{12}H_6N_2F_3O[M\text{-}H^+]$: 251.0438, found: 251.0451.



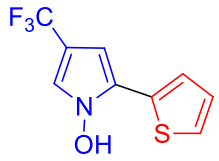
3i

Yellow solid, 76% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (t, *J* = 1.9 Hz, 1H), 8.08 (d, *J* = 8.2 Hz,1H), 8.00 (brs, 1H), 7.96 (d, *J* = 7.9 Hz,1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.26 (s, 1 H), 6.50 (d, *J* = 1.9 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.64. ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.15, 133.21, 131.55, 129.65, 127.93, 123.17 (q, *J* = 266.3 Hz), 122.03, 121.81, 118.97 (q, *J* = 4.6 Hz),110.69 (q, *J* = 38.3 Hz), 102.79 (q, *J* = 3.0 Hz). HRMS-ESI calcd for $C_{12}H_6N_2F_3O_3[M\text{-}H^+]$: 271.0366, found: 271.0334.



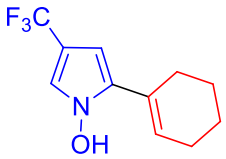
3j

Yellow oil, 94% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 6.7 Hz, 1H), δ 7.86 (d, *J* = 7.2 Hz, 1H), 7.76 (d, *J* = 7.5 Hz, 1H), 7.51 – 7.41 (m, 4H), 7.17 (s, 1H), 7.07 (s, 1H), 6.35 (d, *J* = 2.1 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.02. ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.60, 132.28, 129.22, 129.02, 128.91, 128.53, 127.12, 126.91, 126.18, 125.24, 125.19, 123.66 (q, *J* = 266.0 Hz), 116.64 (q, *J* = 4.7 Hz), 109.96 (q, *J* = 37.9 Hz), 103.61 (q, *J* = 2.9 Hz). HRMS-ESI calcd for $C_{15}H_9NOF_3[M\text{-}H^+]$: 276.0642, found: 276.0646.



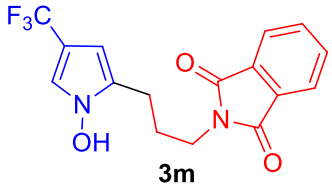
3k

Brown oil, 73% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (brs, 1H), 7.29 (d, *J* = 3.5 Hz, 1H), 7.28 (d, *J* = 5.0 Hz, 1H), 7.11 (s, 1H), 7.06 (dd, *J* = 5.1, 3.7 Hz, 1H), 6.41 (d, *J* = 2.1 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.53. ^{13}C NMR (100 MHz, $CDCl_3$) δ 130.91, 127.43, 125.10, 124.98, 124.80, 123.27 (d, *J* = 266.2 Hz), 117.26 (q, *J* = 4.7 Hz), 110.40 (q, *J* = 38.2 Hz), 100.87 (q, *J* = 3.0 Hz). HRMS-ESI calcd for $C_9H_5NF_3OS[M\text{-}H^+]$: 232.0049, found: 232.0055.



3l

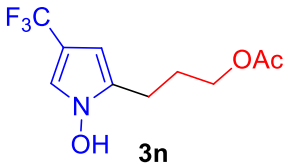
White solid, 73% isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.06 (brs, 1H), 7.04 (dd, J = 2.3, 1.2 Hz, 1H), 6.31-6.27 (m, 1H), 6.08 (d, *J* = 1.8 Hz, 1H), 2.34-2.28 (m, 2H), 2.23-2.16 (m, 2H), 1.76-1.71 (m, 2H), 1.68 – 1.61 (m, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.46. ^{13}C NMR (126 MHz, $CDCl_3$) δ 131.87, 126.84, 126.77, 123.63 (d, *J* = 265.8 Hz), 117.11 (q, *J* = 4.7 Hz), 109.16 (q, *J* = 37.9 Hz), 99.89 (q, *J* = 2.9 Hz), 27.48, 25.51, 22.63, 21.85. HRMS-ESI calcd for $C_{11}H_{11}NOF_3[M\text{-}H^+]$: 230.0798, found: 230.0815.



3m

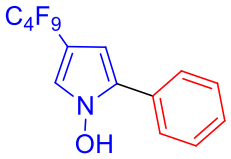
White solid, 94% isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) 8.42 (brs, 1H),

δ 7.77-7.73 (m, 2H), 7.72 – 7.68 (m, 2H), 6.90 (d, *J* = 1.0 Hz, 1H), 5.91 (d, *J* = 1.6 Hz, 1H), 3.68 (t, *J* = 6.7 Hz, 2H), 2.71 (t, *J* = 6.7 Hz, 2H), 2.09 – 2.02 (m, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.33. ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.36, 134.32, 131.55, 129.47, 123.55 (q, *J* = 265.7 Hz), 123.33, 115.70 (q, *J* = 4.8 Hz), 109.17 (q, *J* = 37.6 Hz), 99.49 (q, *J* = 2.9 Hz), 37.36, 27.30, 21.64. HRMS-ESI calcd for $C_{16}H_{12}N_2F_3O_3$[M-H$^+$]: 337.0806, found: 337.0804.



3n

Colorless oil, 98% isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.66 (s, 1H), 6.99 (s, 1H), 5.93 (d, *J* = 1.4 Hz, 1H), 4.06 (t, *J* = 6.4 Hz, 2H), 2.65 (t, *J* = 7.3 Hz, 2H), 2.00 (s,3H), 1.98 – 1.90 (m, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.14. ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.26, 129.58, 123.74 (q, *J* = 265.6 Hz), 115.60 (q, *J* = 4.8 Hz), 109.00 (d, *J* = 37.6 Hz), 99.47 (q, *J* = 2.9 Hz), 64.25, 27.52, 21.00, 20.87. HRMS-ESI calcd for $C_{10}H_{11}NO_3F_3$[M-H$^+$]: 250.0633, found: 250.0624.

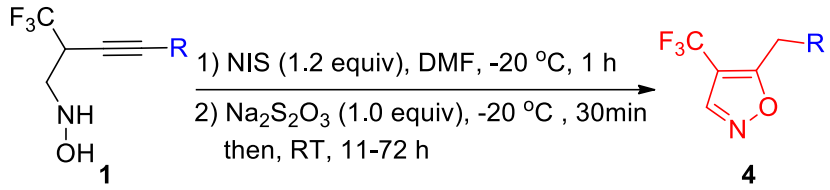


3o

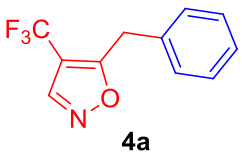
Light yellow solid, 34% isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.23 (d, *J* = 1.5 Hz, 1H), 7.51 – 7.50 (m, 2H), 7.42 – 7.35 (m, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -80.38 – -80.79 (m, 3F), -115.75 – -115.82 (m, 2F), -116.77 – -116.84 (m, 2F), -127.02 – -127.00 (m, 2F). HRMS-ESI

calcd for $C_{14}H_7NOF_9[M\text{-}H^+]$: 376.0389, found: 376.0380.

5. General procedure for the one-pot synthesis of 4-trifluoromethyl-5-akylisoxazoles 4



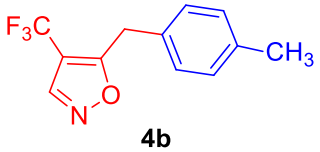
To the solution of *N*-(2–(trifluoromethyl)-3-alkynyl) hydroxylamine **1** (0.2 mmol) in DMF (2.0 mL) at -20℃ was added NIS (45.0 mg. 0.24 mol), the reaction mixture was stirred at -20℃for nearly 1 h. After the hydroxylamine **1** was completely consumed, which was determined by TLC analysis, $Na_2S_2O_3$(32.0 mg, 0.2 mmol) was added and the reaction mixture was stirred at -20℃ for about 30 mins till the brown colour of reaction mixture disappeared. The reaction mixture was subsequently warmed up to room temperature and stirred for 11-72 h. After the complete consumption of oxime intermediate **2,** water (2.0 mL) was added and the reaction mixture was extracted with ethyl acetate (3x4.0 mL). The combined organic extracts were washed with brine (4.0 mL) and dried over $MgSO_4$. After filtration and evaporation, the residue was purified by flash column chromatography on silica gel to afford 4-trifluoromethyl-5-alkylisoxazole **4**. [Eluent: petroleum ether : ethyl acetate = 50:1～5:1].



4a

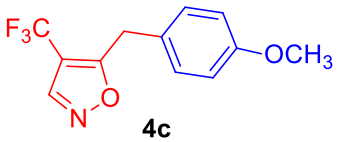
Colorless oil, 72%isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.36 – 7.23 (m, 5H), 4.23 (s, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.74. ^{13}C

NMR (100 MHz, $CDCl_3$) δ 170.92 (q, *J* = 3.1 Hz), 147.67 (q, *J* = 2.1 Hz), 134.05, 128.95, 128.67, 127.55, 121.46 (q, *J* = 267.0 Hz), 108.54 (q, *J* = 38.9 Hz), 32.04. MS (70 eV):m/z (%): 227 (M^+, 73.71), 91 (100). HRMS calcd for $C_{11}H_8F_3NO$: 227.0558, found: 227.0557.



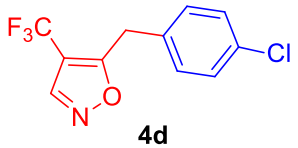
4b

Colorless oil, 78%isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.15 (s, 4H), 4.21 (s, 2H), 2.34 (s, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.73 (s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.19 (q, *J* = 3.2 Hz), 147.63 (d, *J* = 2.2 Hz), 137.27, 131.01, 129.61, 128.54, 121.50 (q, *J* = 266.9 Hz), 108.36 (q, *J* = 39.1 Hz), 31.64, 20.98. MS (70 eV):m/z (%): 241 (M^+, 98.25), 105 (100). HRMS calcd for $C_{12}H_{10}F_3NO$: 241.0714, found: 241.0712.



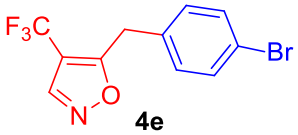
4c

Colorless oil, 66% isolated yield.^1H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.18 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 4.18 (s, 2H), 3.79 (s, 3H).^{19}F NMR (377 MHz, $CDCl_3$) δ -56.71. ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.32 (q, *J* = 3.1 Hz), 159.00 (s), 147.63 (q, *J* = 2.2 Hz), 129.76, 126.04, 121.49 (q, *J* = 266.9 Hz), 114.34, 108.21 (q, *J* = 39.0 Hz), 55.23, 31.21. MS (70 eV):m/z (%): 257 (M^+, 73.88),121 (100). HRMS calcd for C12H10F3NO2: 257.0664, found: 257.0663.



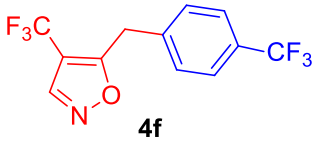
4d

Colorless oil, 76% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 4.21 (s, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.78. ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.32 (q, *J* = 3.1 Hz), 147.70 (q, *J* = 1.8 Hz), 133.67, 132.47, 130.01, 129.15, 121.39 (q, *J* = 267.0 Hz), 108.71 (q, *J* = 39.1 Hz), 31.40. MS (70 eV):m/z (%): 261 (M^+, 51.37), 226(100). HRMS calcd for $C_{11}H_7F_3NOCl$: 261.0168, found: 261.0169.



4e

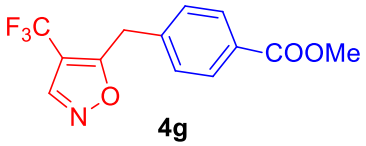
White solid, 81% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.13 (d, *J* = 8.4 Hz, 2H), 4.20 (s, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.76.^{13}C NMR (100 MHz, $CDCl_3$) δ 170.21 (q, *J* = 3.2 Hz), 147.72 (q, *J* = 2.1 Hz), 132.98, 132.12, 130.36, 121.71, 121.37 (q, *J* = 266.9 Hz), 108.73 (q, *J* = 39.1 Hz), 31.48. MS (70 eV):m/z (%): 305 (M^+, 50.20), 226 (100). HRMS calcd for $C_{11}H_7F_3NOBr$: 304.9663, found: 304.9662.



4f

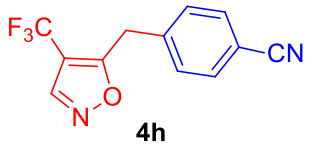
Colorless oil, 65% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.60 (d, J = 8.1 Hz, 2H), 7.38 (d, J = 8.1 Hz, 2H), 4.31 (s, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.83, -62.74. ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.78 (q, *J* = 3.2 Hz), 147.77 (q, *J* = 2.1 Hz)， 137.95, 130.06 (q, *J* = 32.7 Hz),

129.07, 125.96 (q, *J* = 3.8 Hz), 123.91 (q, *J* = 272.1 Hz)，121.33 (q, *J* = 267.0 Hz), 109.02 (q, *J* = 39.1 Hz), 31.78. MS (70 eV):m/z (%): 295 (M^+, 79.54), 159 (100). HRMS calcd for $C_{12}H_7F_6NO$: 295.0432, found: 295.0431.



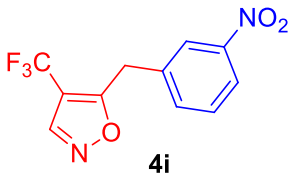
4g

Yellow oil, 49% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.00 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 4.30 (s, 2H), 3.91 (s, 3H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.80. ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.96 (q, *J* = 3.1 Hz), 166.55, 147.75 (q, *J* = 2.1 Hz), 139.00, 130.26, 129.60, 128.71, 121.34 (q, *J* = 267.0 Hz), 108.95 (q, *J* = 39.2 Hz), 52.15, 31.96. MS (70 eV):m/z (%): 285 (M^+, 36.11), 254 (100). HRMS calcd for $C_{13}H_{10}F_3NO_3$: 285.0613, found: 285.0611.



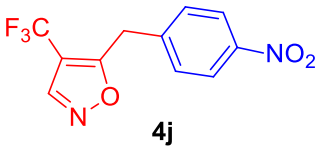
4h

Yellow solid, 65% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.64 (d, *J* = 8.2 Hz, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 4.31 (s, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.81.^{13}C NMR (100 MHz, $CDCl_3$) δ 169.19 (q, *J* = 3.1 Hz), 147.78 (q, *J* = 2.1 Hz), 139.19, 132.76, 129.48, 121.23 (q, *J* = 267.1 Hz), 118.25, 111.87, 109.22 (q, *J* = 39.2 Hz), 31.97. MS (70 eV):m/z (%): 252 (M^+, 72.18), 116 (100). HRMS calcd for $C_{12}H_7F_3N_2O$: 252.0510, found: 252.0508.



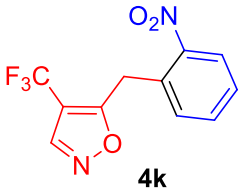
4i

Colorless oil, 69% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 8.19 – 8.13 (m, 1H), 8.15 (s, 1 H), 7.63-7.50 (m, 2H), 4.37 (s, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.76. ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.18 (q, *J* = 3.1 Hz), 148.54, 147.82 (q, *J* = 2.1 Hz), 135.86, 134.74, 130.03, 123.71, 122.80, 121.23 (q, *J* = 267.1 Hz)，，109.25 (q, *J* = 39.2 Hz), 31.57. MS (70 eV):m/z (%): 272 (M^+, 100), 272 (100). HRMS calcd for $C_{11}H_7F_3N_2O_3$: 272.0409, found: 272.0407.



4j

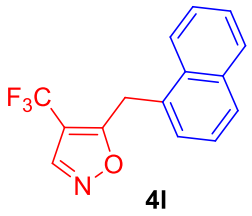
Yellow solid, 60% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 8.20 (d, *J* = 8.6 Hz, 2H), 7.43 (d, *J* = 8.6 Hz, 2H), 4.36 (s, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.81. ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.03 (q, *J* = 3.1 Hz), 147.82 (q, *J* = 2.1 Hz)，147.48, 141.11, 129.63, 124.19, 121.21 (q, *J* = 267.1 Hz), 109.29 (q, *J* = 39.2 Hz), 31.71. MS (70 eV):m/z (%): 272 (M^+, 100.00), 272(100). HRMS calcd for $C_{11}H_7F_3N_2O_3$: 272.0409, found: 272.0411.



4k

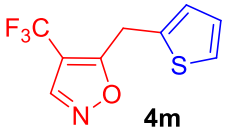
Yellow solid, 79% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.14 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.66-7.60 (m, 1H), 7.56 – 7.49 (m, 1H), 7.32

(d, *J* = 7.7 Hz, 1H), 4.67 (s, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -57.01.^{13}C NMR (100 MHz, $CDCl_3$) δ 168.94 (q, *J* = 3.2 Hz), 148.40, 147.88 (q, *J* = 2.1, Hz), 133.90, 132.29, 129.14, 128.89, 125.63, 121.25 (q, *J* = 267.1 Hz), 109.10 (d, *J* = 39.3 Hz), 30.16. MS (70 eV):m/z (%): 272 (M^+, 44.80), 164(100). HRMS calcd for $C_{11}H_7F_3N_2O_3$: 272.0409, found: 272.0410.



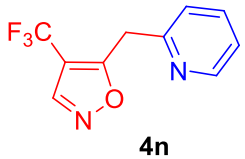
4l

Yellow solid, 54% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 8.04 (d, *J* = 8.3 Hz, 1H), 7.90 (d, *J* = 7.7 Hz, 1H), 7.84 (d, *J* = 8.3 Hz, 1H), 7.63 – 7.50 (m, 2H), 7.48 – 7.41 (m, 1H), 7.33 (d, *J* = 7.0 Hz, 1H), 4.70 (s, 2H). ^{19}F NMR (377 MHz, CDCl3) δ -56.74. ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.83 (q, *J* = 3.2 Hz), 147.77 (q, *J* = 2.2 Hz), 133.84, 131.48, 129.96, 128.90, 128.56, 127.28, 126.72, 126.01, 125.44, 123.01, 121.48 (q, *J* = 267.0 Hz, 108.87 (q, *J* = 39.1 Hz), 29.43. MS (70 eV):m/z (%): 277 (M^+,80.71), 141 (100). HRMS calcd for $C_{15}H_{10}F_3NO$: 277.0714, found: 277.0715.



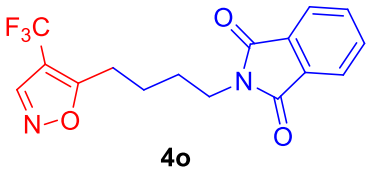
4m

Yellow oil, 67% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.22 (dd, *J* = 4.9, 1.4 Hz, 1H), 6.98-6.92 (m, 2H), 4.45 (s, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.88. ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.72 (q, *J* = 3.2 Hz), 147.71 (q, *J* = 2.1 Hz), 135.05, 127.21, 126.91, 125.43, 121.28 (q, *J* = 267.1 Hz), 108.45 (q, *J* = 39.1 Hz), 26.22. MS (70 eV):m/z (%):233 (M^+, 96.24), 97 (100). HRMS calcd for $C_9H_6F_3NOS$: 233.0122, found: 233.0120.



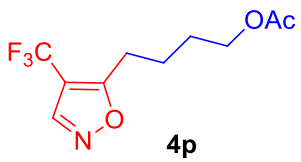
4n

Yellow oil, 42% isolated yield.^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 (d, *J* = 3.1 Hz, 1H), 8.38 (s, 1H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 7.2 Hz, 2H), 4.46 (s, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.97. ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.58 (q, *J* = 3.2 Hz), 154.16, 149.85, 147.77 (q, *J* = 2.1 Hz), 137.01, 122.93, 122.49, 121.35 (q, *J* = 267.0 Hz), 109.35 (q, *J* = 39.1 Hz), 34.76. MS (70 eV):m/z (%): 228 (M^+, 1.52), 201 (100). HRMS calcd for $C_{10}H_7F_3N_2O$: 228.0510, found: 228.0509.



4o

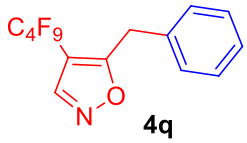
White solid, 43% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.83 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.71 (dd, *J* = 5.4, 3.1 Hz, 2H), 3.72 (t, *J* = 6.6 Hz, 2H), 2.97 (t, *J* = 7.0 Hz, 2H), 1.85-1.70 (m, 4H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.92. ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.35 (q, *J* = 3.2 Hz), 168.31, 147.55 (q, *J* = 2.1 Hz), 133.97, 131.96, 123.24, 121.46 (q, *J* = 266.7 Hz), 108.42 (q, *J* = 38.9 Hz), 37.11, 27.86, 25.39, 24.55. MS (70 eV):m/z (%): 338(M^+, 9.64), 160 (100). HRMS calcd for $C_{16}H_{13}F_3N_2O_3$: 338.0878, found: 338.0876.



4p

Colorless oil, 38% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 4.08 (t, *J* = 6.3 Hz, 2H), 2.96 (t, *J* = 7.5 Hz, 2H), 2.04 (s, 3H), 1.88-1.77 (m,

2H), 1.74 – 1.64 (m, 2H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -56.99. ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.50 (q, *J* = 3.1 Hz), 171.01, 147.59 (q, *J* = 2.2 Hz), 121.52 (q, *J* = 266.8 Hz), 108.44 (q, *J* = 39.0 Hz)，63.47, 27.88, 25.54, 23.94, 20.83. MS (70 eV):m/z (%): 251 (M^+, 0.26), 43 (100). HRMS calcd for $C_{10}H_{12}F_3NO_3$: 251.0769, found: 251.0768.



4q

Yellow oil, 35% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.37 – 7.22 (m, 5H), 4.22 (s, 2H).^{19}F NMR (377 MHz, $CDCl_3$) δ -80.77 – -80.32 (m, 3F), -106.43 – -107.12 (m, 2F), -122.91 – -123.45 (m, 2F), -125.46 – -126.12 (m, 2F).^{13}C NMR (100 MHz, $CDCl_3$) δ 172.12 (t, *J* = 3.2 Hz), 148.37, 134.01, 128.91, 128.73, 127.54, 120.69-108.53 (m, 4C), 106.25 (t, *J* = 29.4 Hz), 32.18. MS (70 eV):m/z (%): 377 (M^+, 38.89), 91 (100). HRMS calcd for $C_{14}H_8F_9NO$: 377.0460, found: 377.0462.

6. X-ray structures of 3g and 4h.

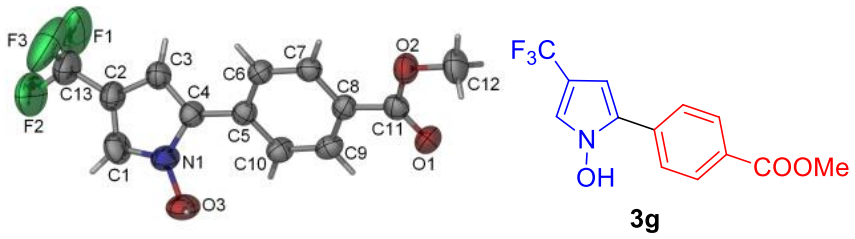


Figure 1. ORTEP depiction of compound **3g**, CCDC 1575114

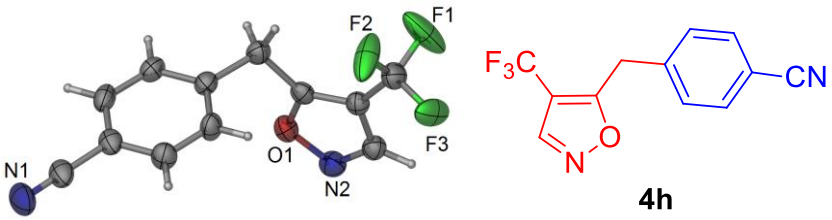
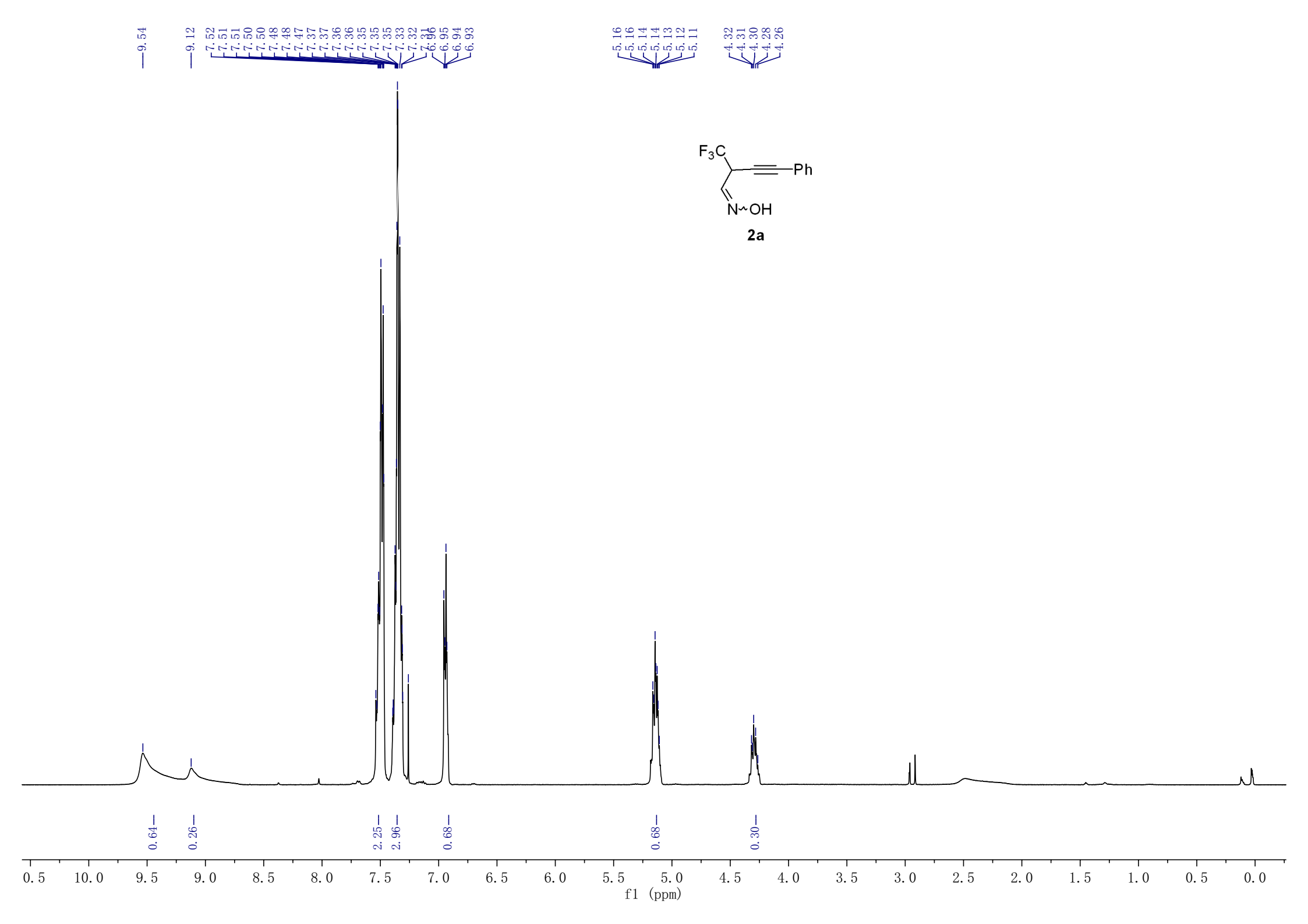


Figure 2. ORTEP depiction of compound **4h**, CCDC 1575115

7. References

[1] Q. Zeng, L. Zhang, J. Yang, B. Xu, Y. Xiao, J. Zhang, *Chem. Commun.*, **2014**, *50*, 4203.

8. NMR Spectra.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7.50
7.50
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7.37
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6.93
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5.14
5.14
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5.12
5.11
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4.31
4.30
4.28
4.26
F3C
Ph
N~OH
2a
0.64
0.26
2.25
2.96
0.68
0.68
0.30
0.5
10.0
9.5
9.0
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
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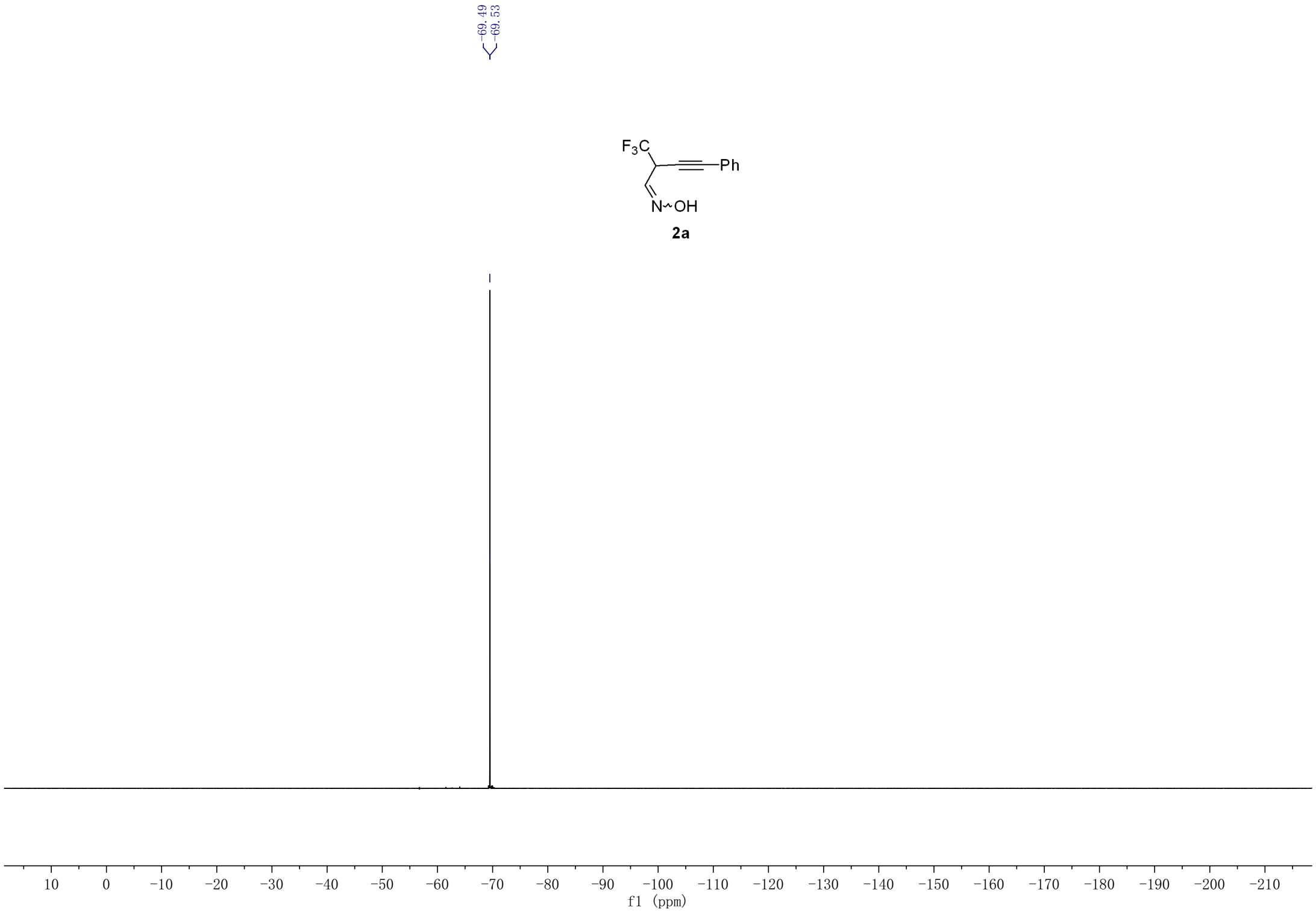
0.5
0.0
f1 (ppm)


-69.49
-69.53
F3C
Ph
N~OH
2a
10
0
-10
-20
-30
-40
-50
-60
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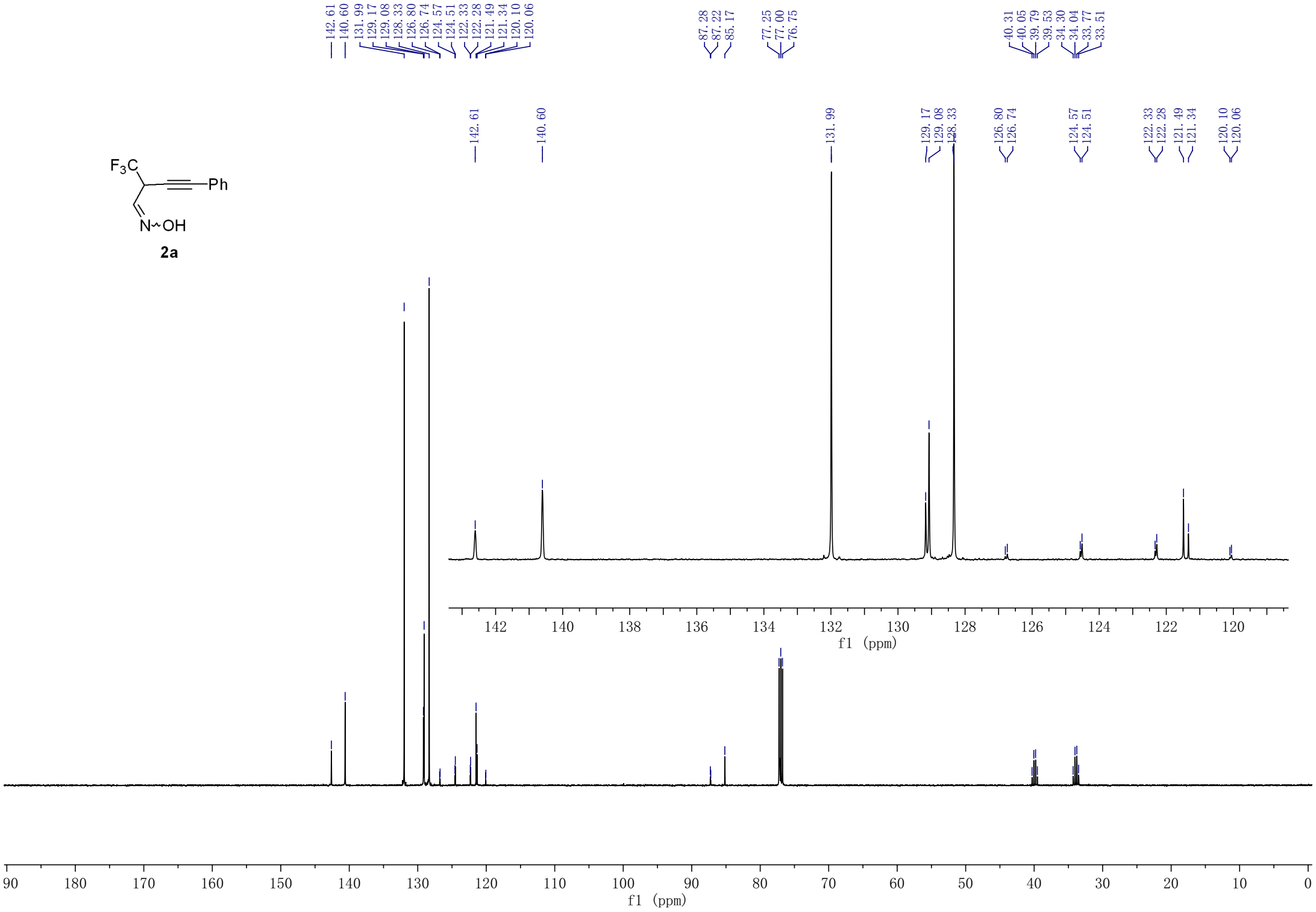
-170
-180
-190
-200
-210
f1 (ppm)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121.34
120.10
120.06
87.28
87.22
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77.00
76.75
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40.05
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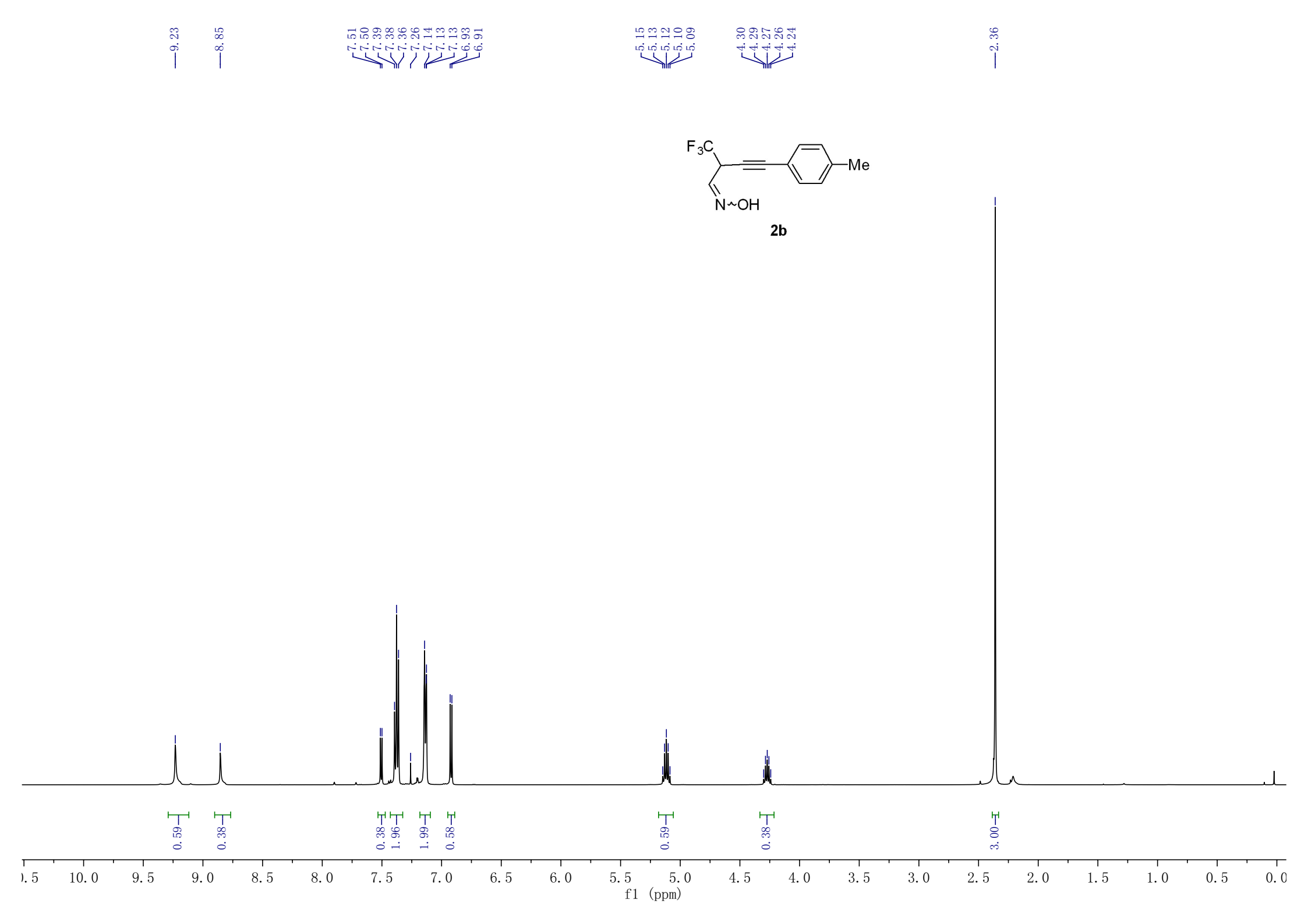
Ph
N~OH
2a
f1 (ppm)
f1 (ppm)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4.27
4.26
4.24
2.36
F3C
Me
N~OH
2b
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1.99
0.58
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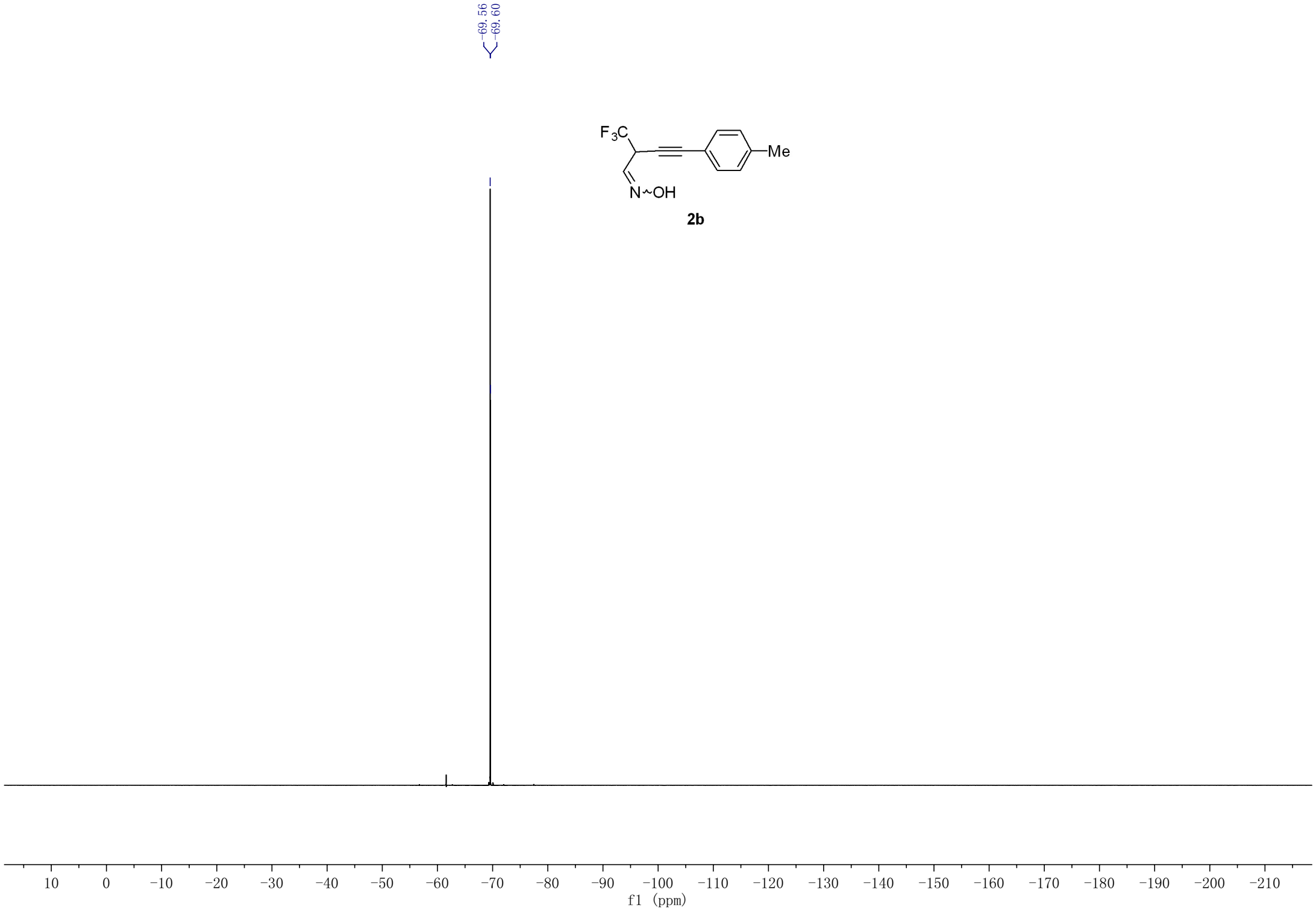
0.38
3.00
f1 (ppm)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-69.60
F3C
Me
N~OH
2b
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-10
-20
-30
-40
-50
-60
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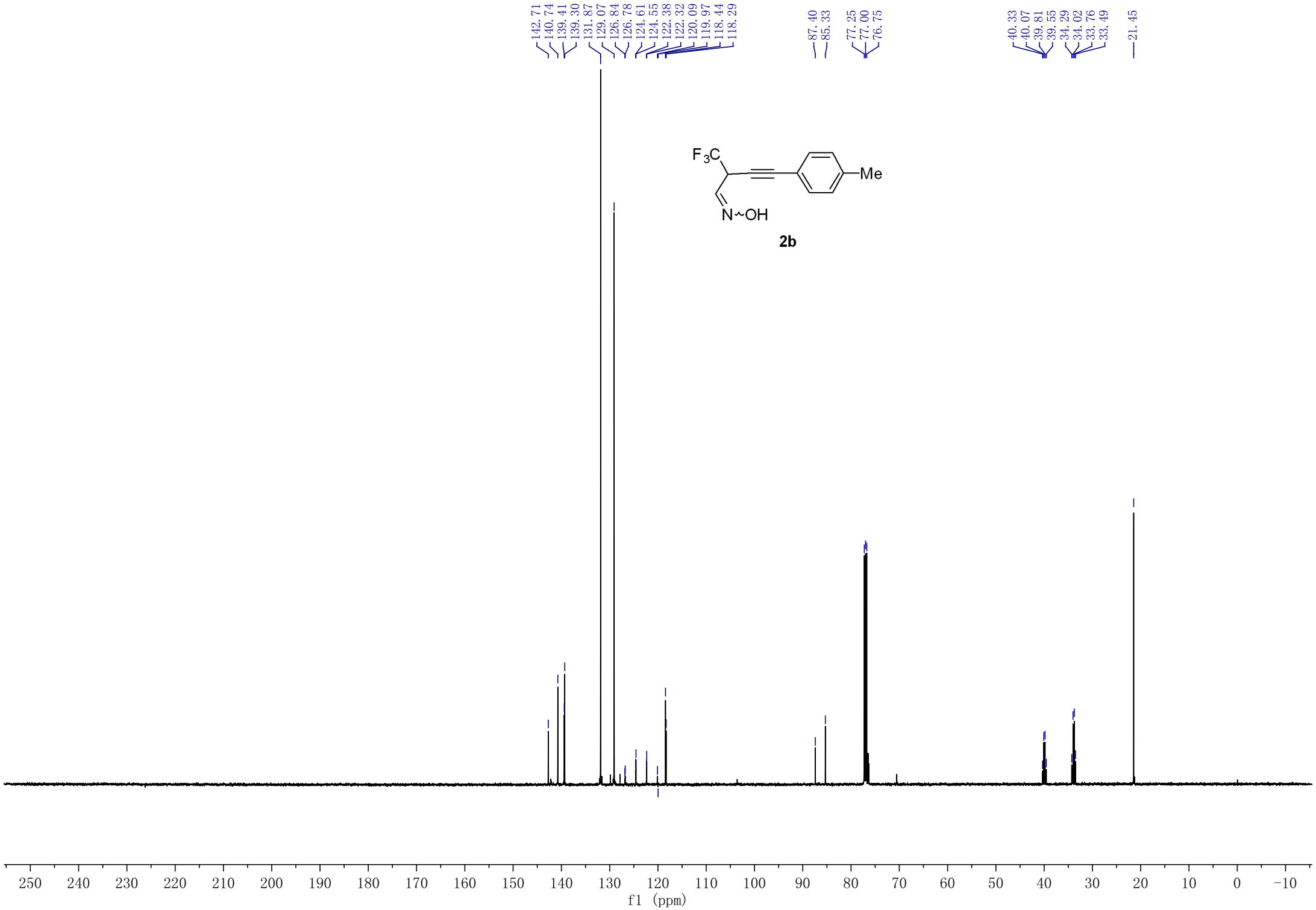
-170
-180
-190
-200
-210
f1 (ppm)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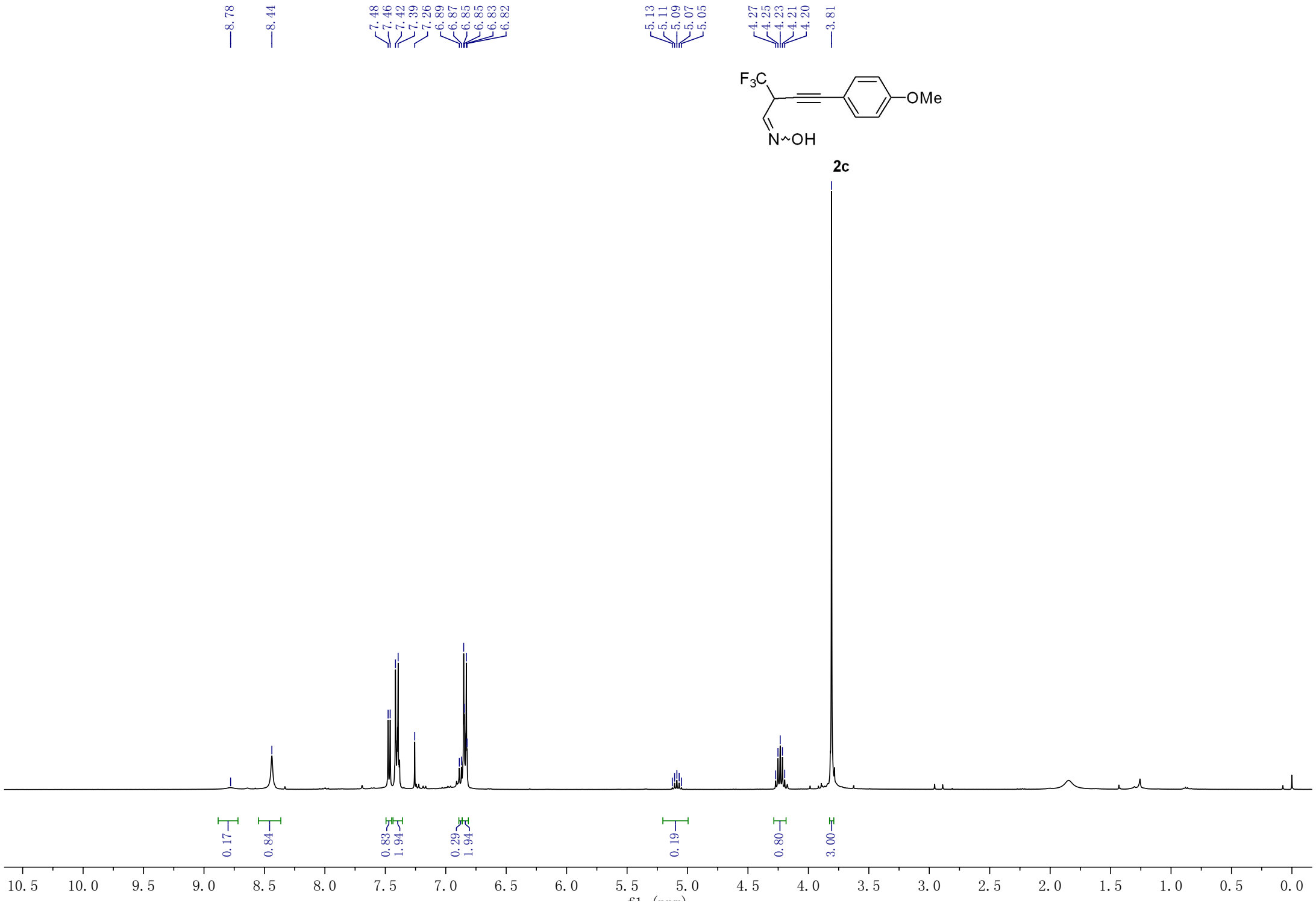
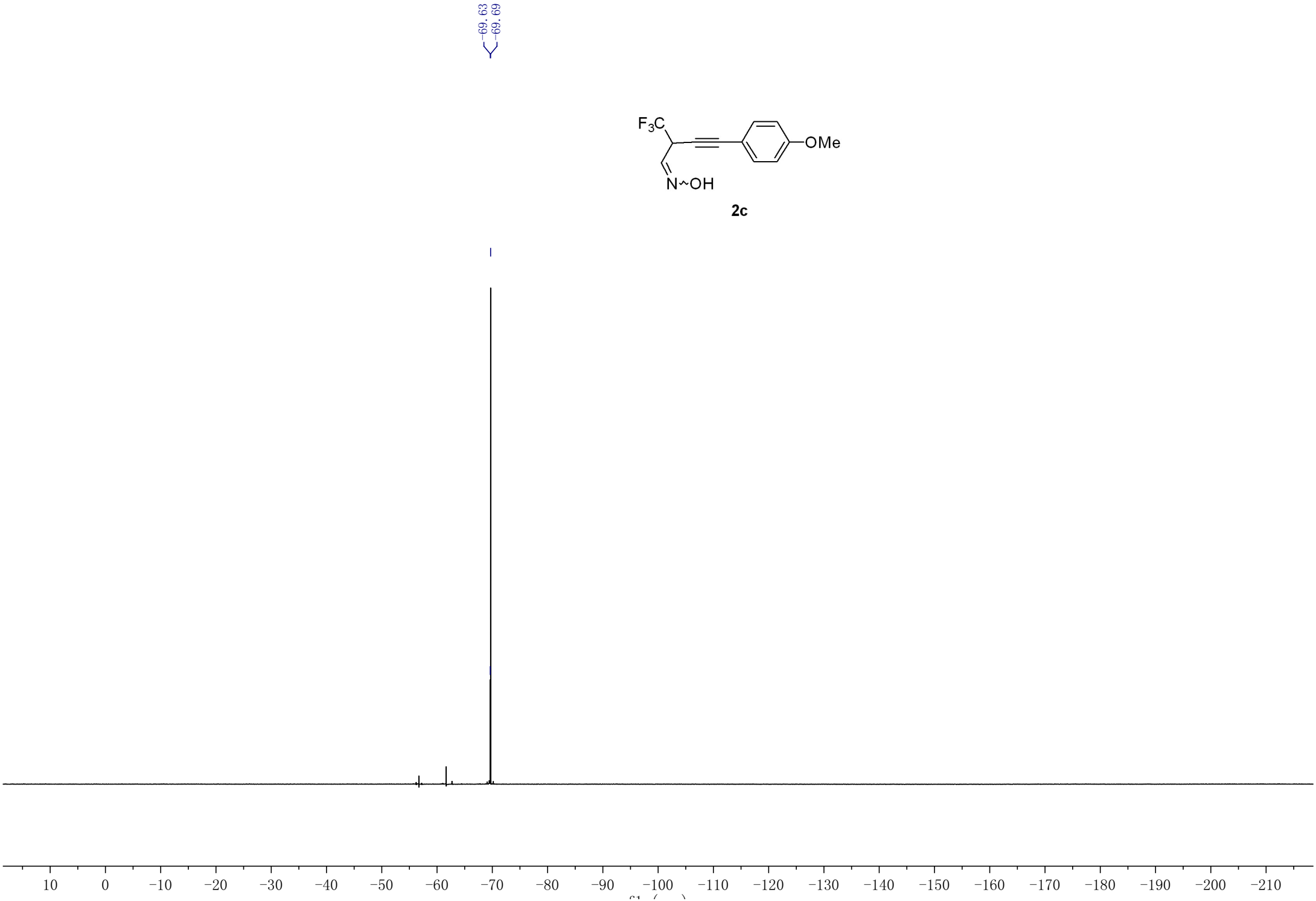
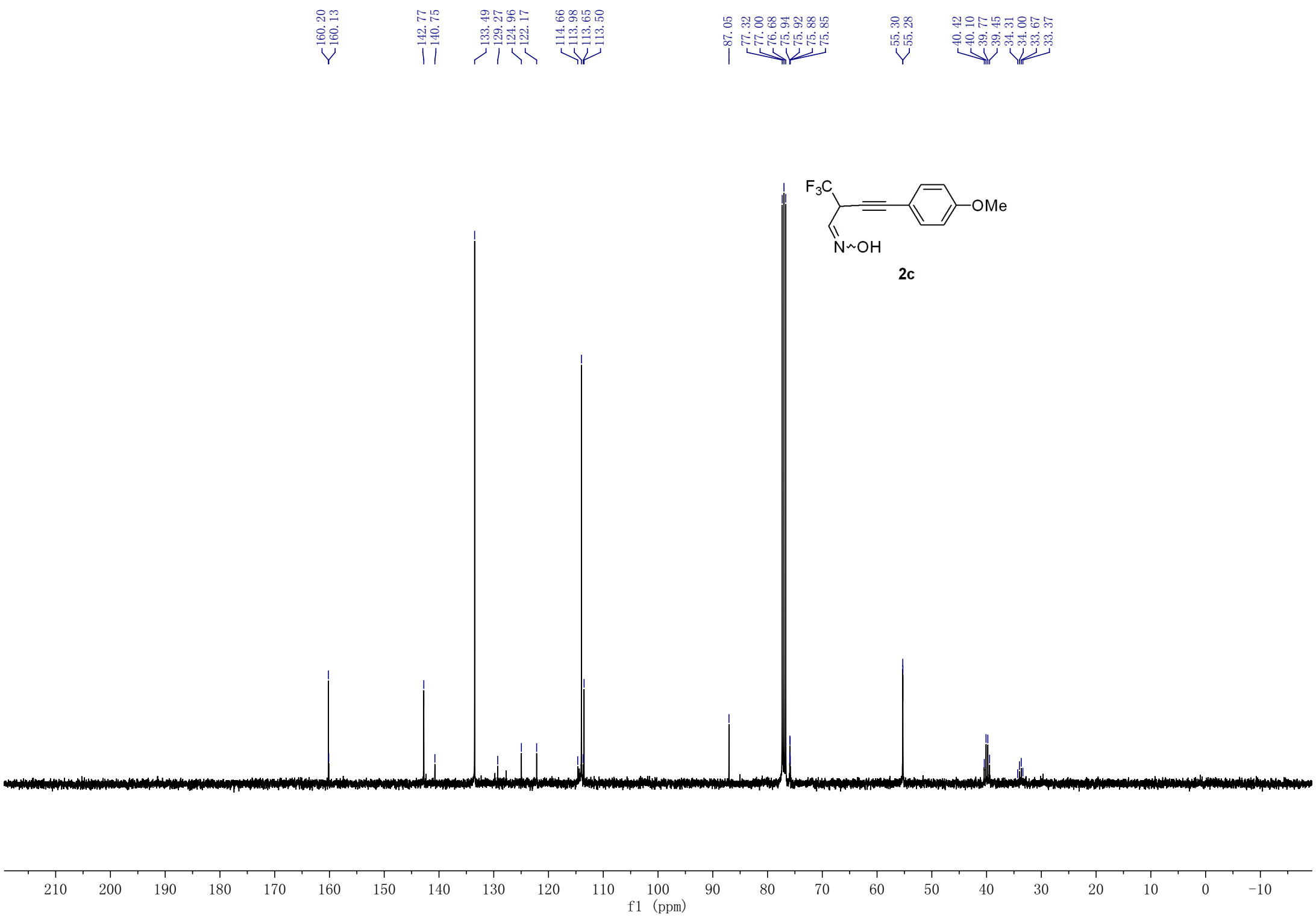
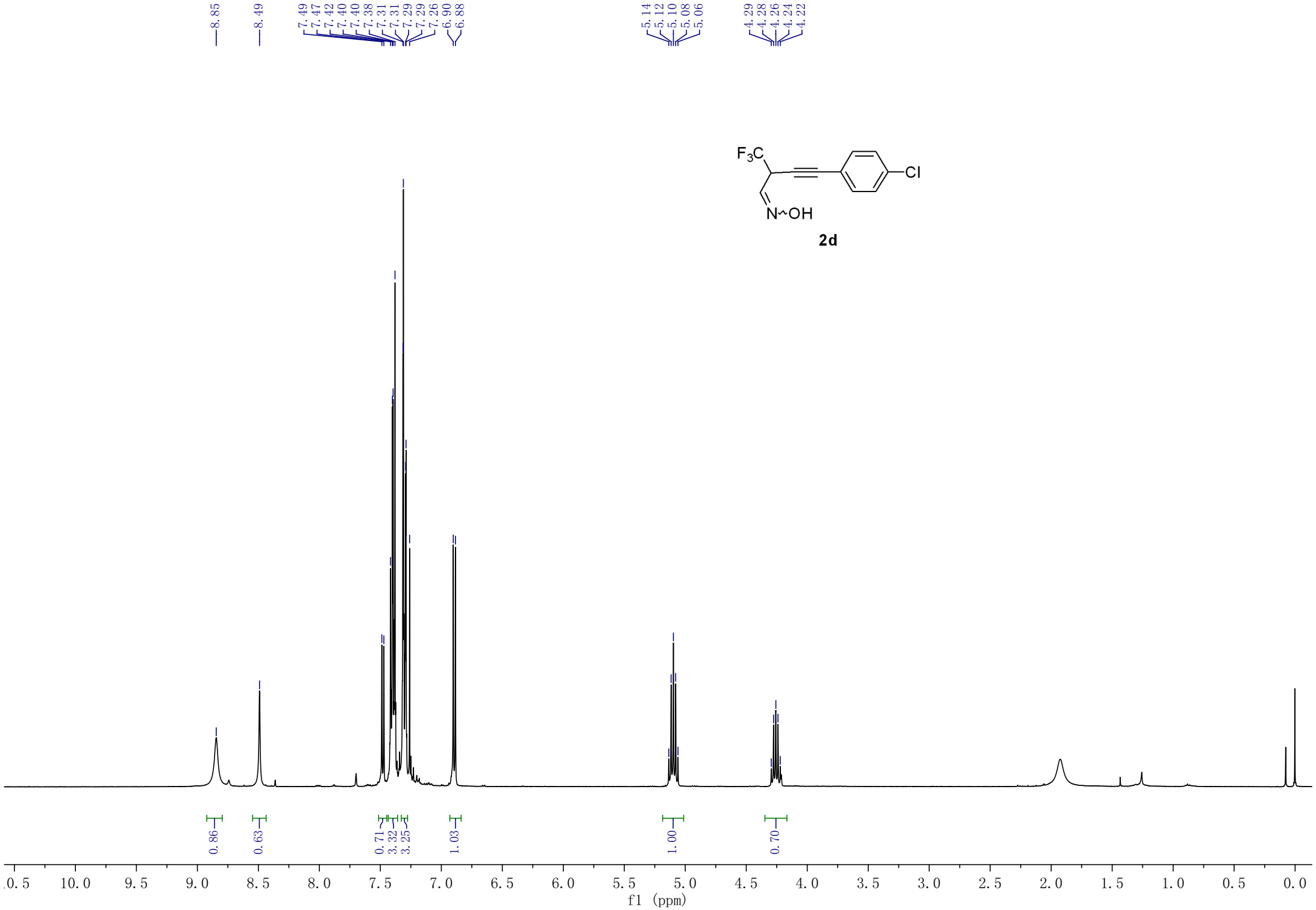
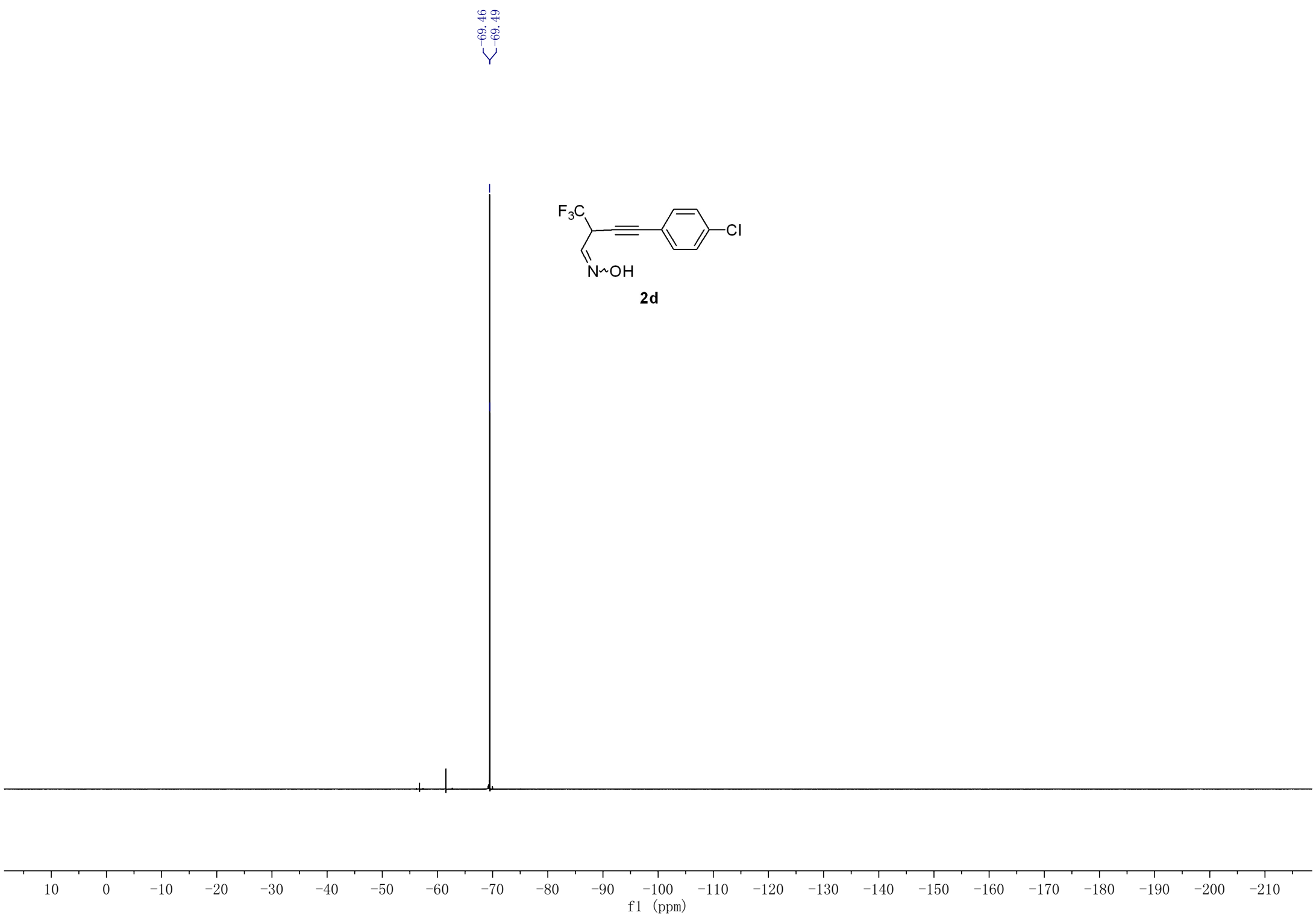
122.32
120.09
119.97
118.44
118.29
87.40
85.33
77.25
77.00
76.75
40.33
40.07
39.81
39.55
34.29
34.02
33.76
33.49
21.45
F3C
Me
N~OH
2b
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

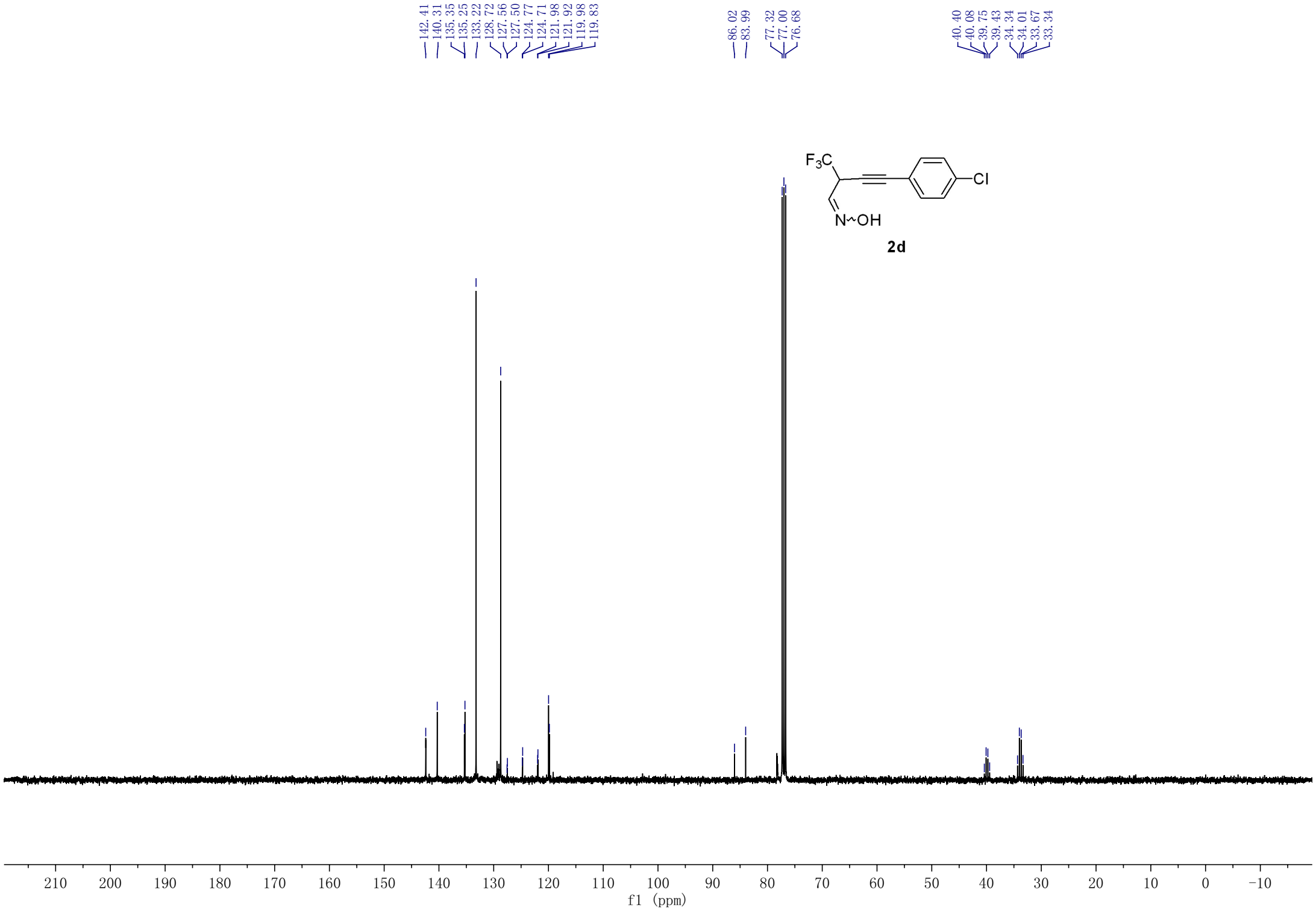

8.78
8.44
7.48
7.46
7.42
7.39
7.26
6.89
6.87
6.85
6.85
6.83
6.82
5.13
5.11
5.09
5.07
5.05
4.27
4.25
4.23
4.21
4.20
3.81
F3C
OMe
N~OH
2c
0.17
0.84
0.83
1.94
0.29
1.94
0.19
0.80
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

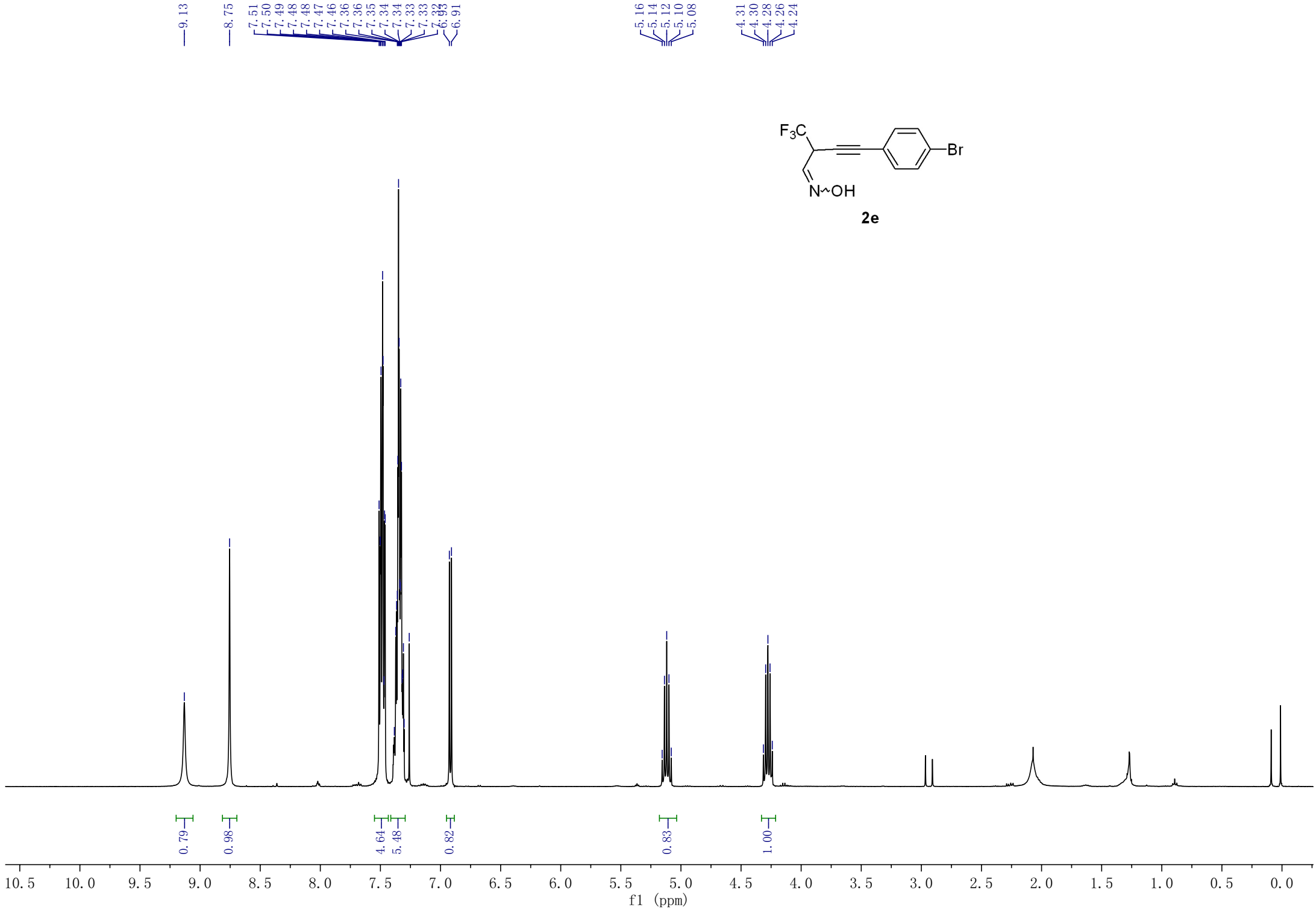

-69.63
-69.69
F3C
OMe
N~OH
2c
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210

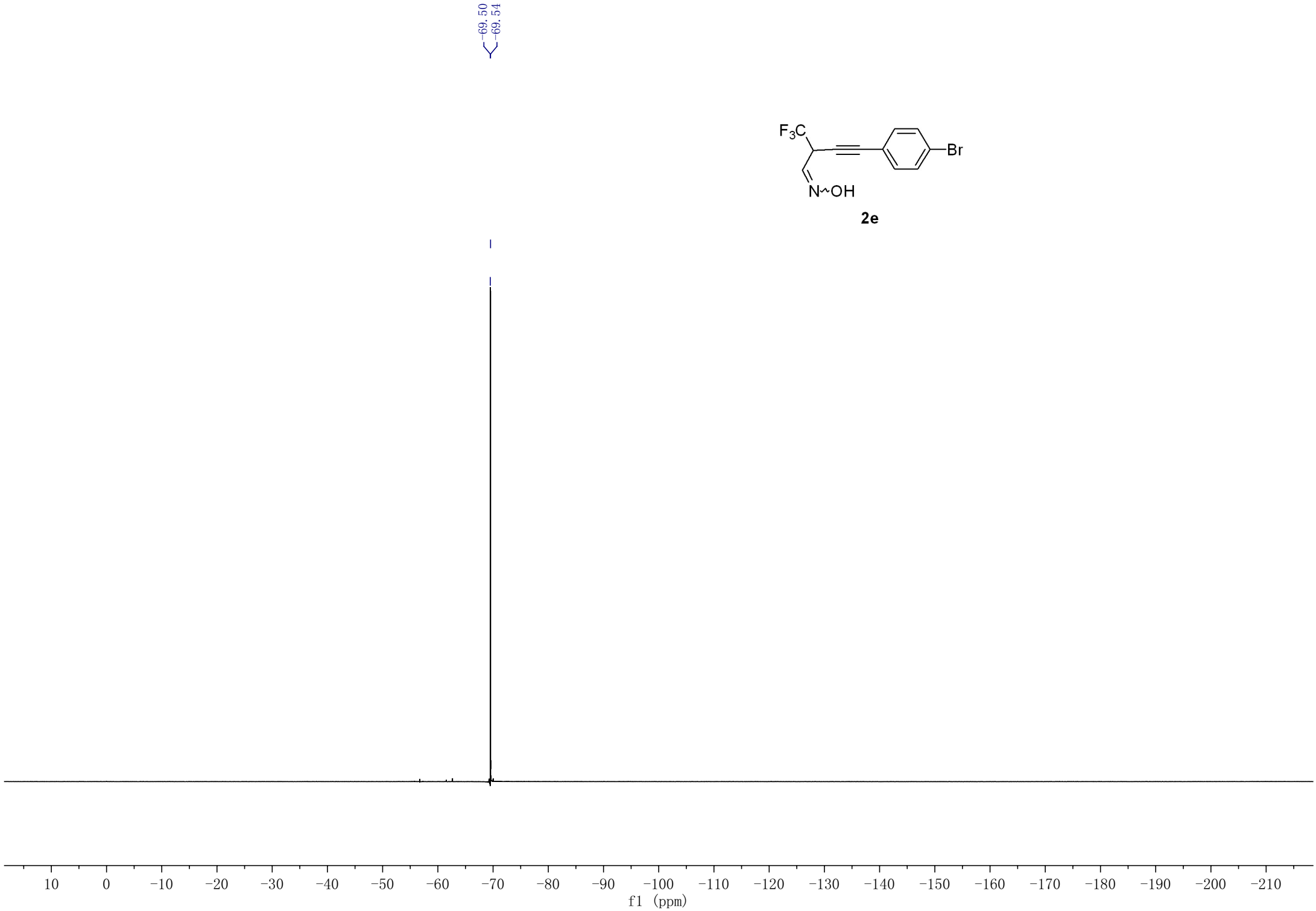

160.20
160.13
142.77
140.75
133.49
129.27
124.96
122.17
114.66
113.98
113.65
113.50
87.05
77.32
77.00
76.68
75.94
75.92
75.88
75.85
55.30
55.28
40.42
40.10
39.77
39.45
34.31
34.00
33.67
33.37
F3C
OMe
N~OH
2c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

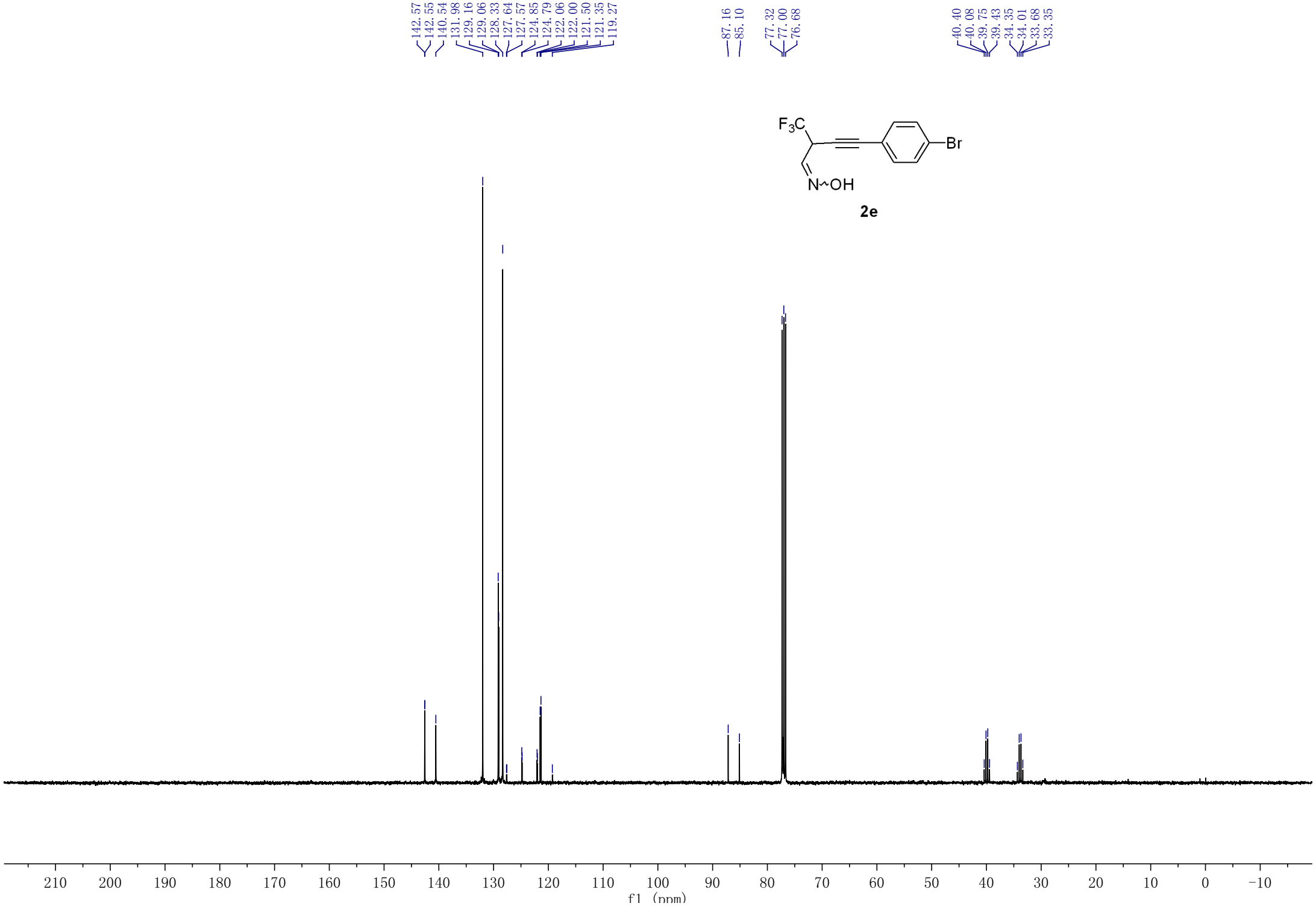

8.85
8.49
7.49
7.47
7.42
7.40
7.40
7.38
7.31
7.31
7.29
7.29
7.26
6.90
6.88
5.14
5.12
5.10
5.08
5.06
4.29
4.28
4.26
4.24
4.22
F3C
Cl
N~OH
2d
0.86
0.63
0.71
3.32
3.25
1.03
1.00
0.70
f1 (ppm)

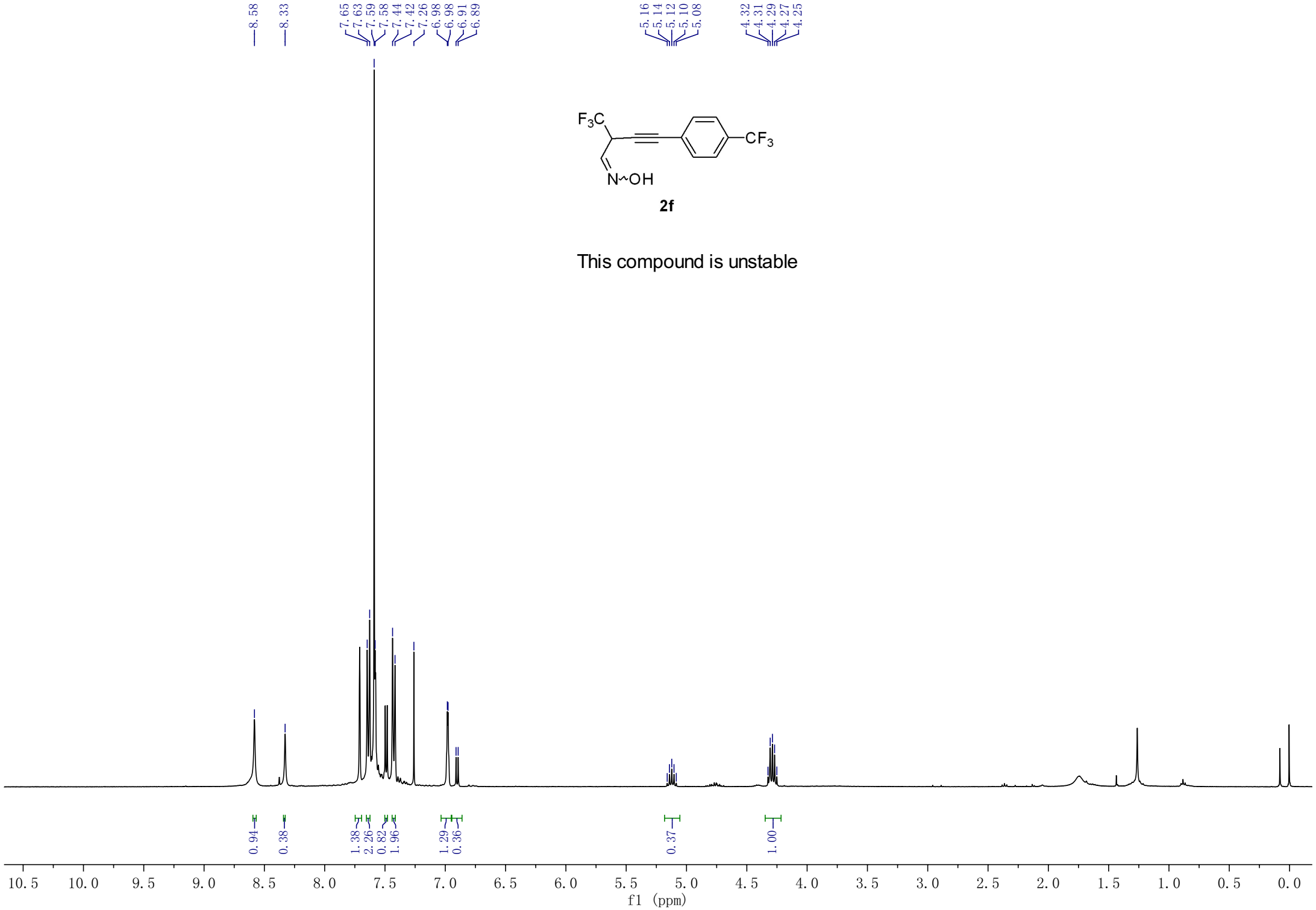

-69.46
-69.49
F3C
Cl
N~OH
2d
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

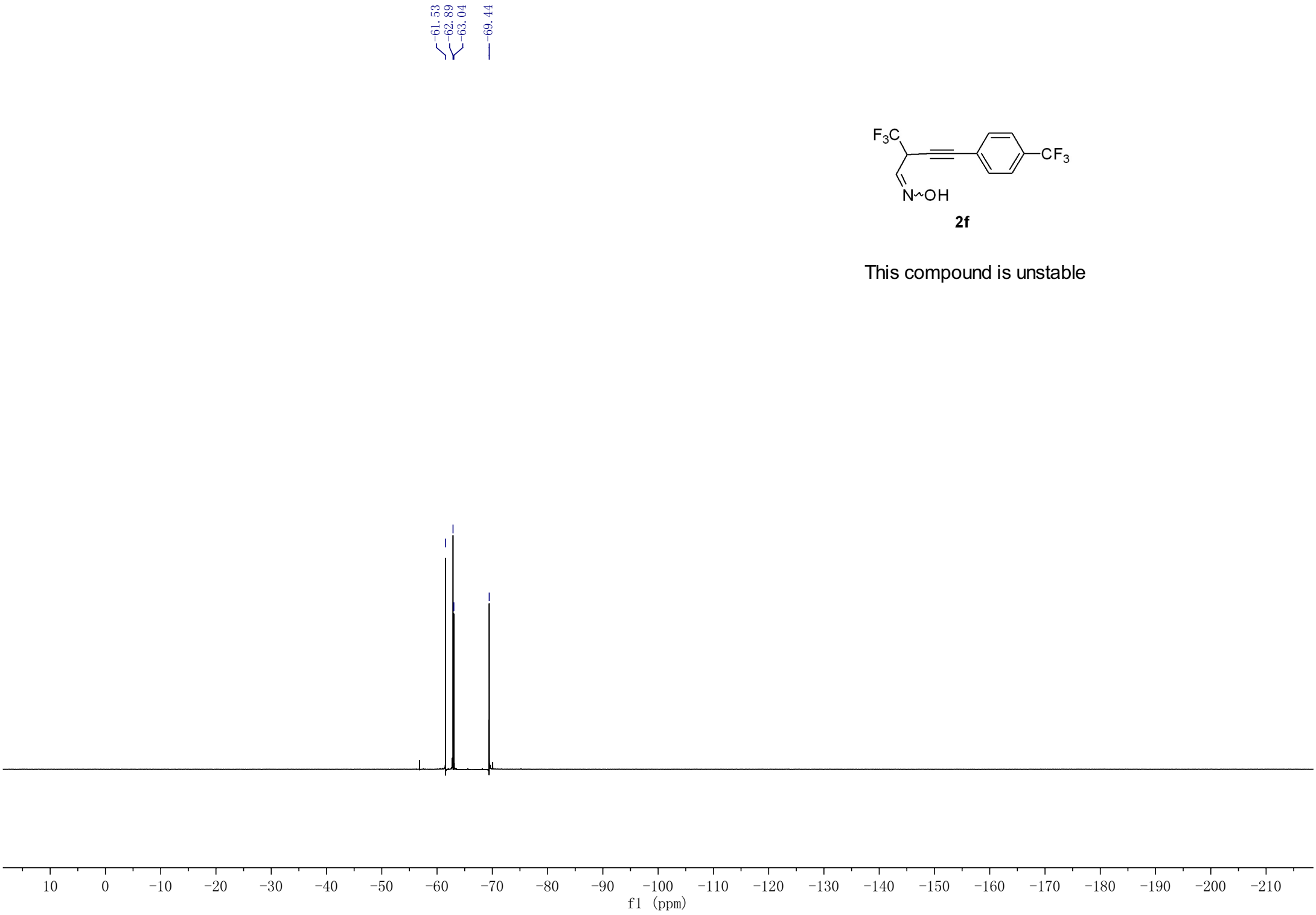

142.41
140.31
135.35
135.25
133.22
128.72
127.56
127.50
124.77
124.71
121.98
121.92
119.98
119.83
86.02
83.99
77.32
77.00
76.68
40.40
40.08
39.75
39.43
34.34
34.01
33.67
33.34
F3C
Cl
N~OH
2d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

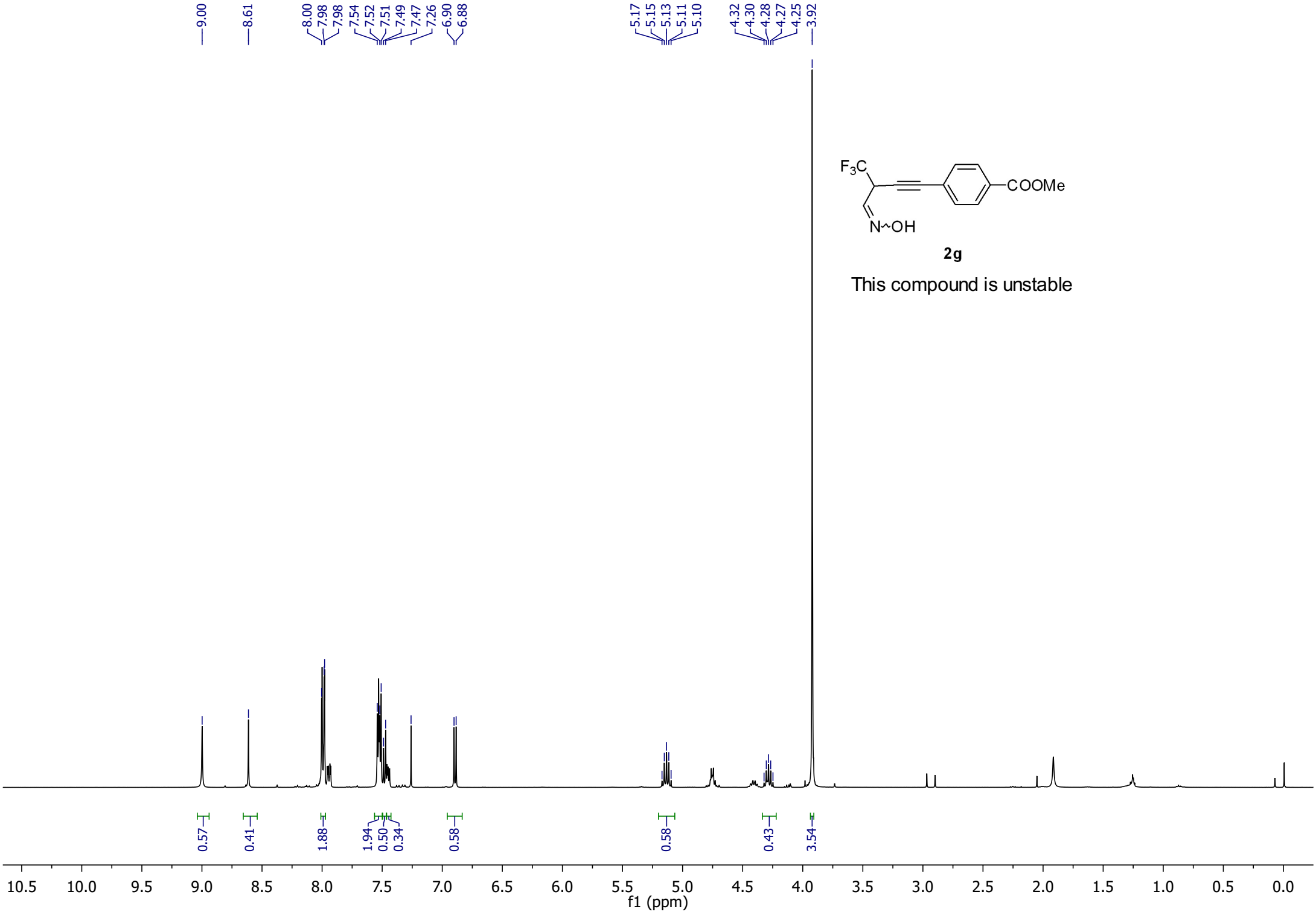

9.13
8.75
7.51
7.50
7.49
7.48
7.48
7.47
7.46
7.36
7.35
7.34
7.34
7.33
7.32
6.93
6.91
5.16
5.14
5.12
5.10
5.08
4.31
4.30
4.28
4.26
4.24
F3C
Br
N~OH
2e
0.79
0.98
4.64
5.48
0.82
0.83
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

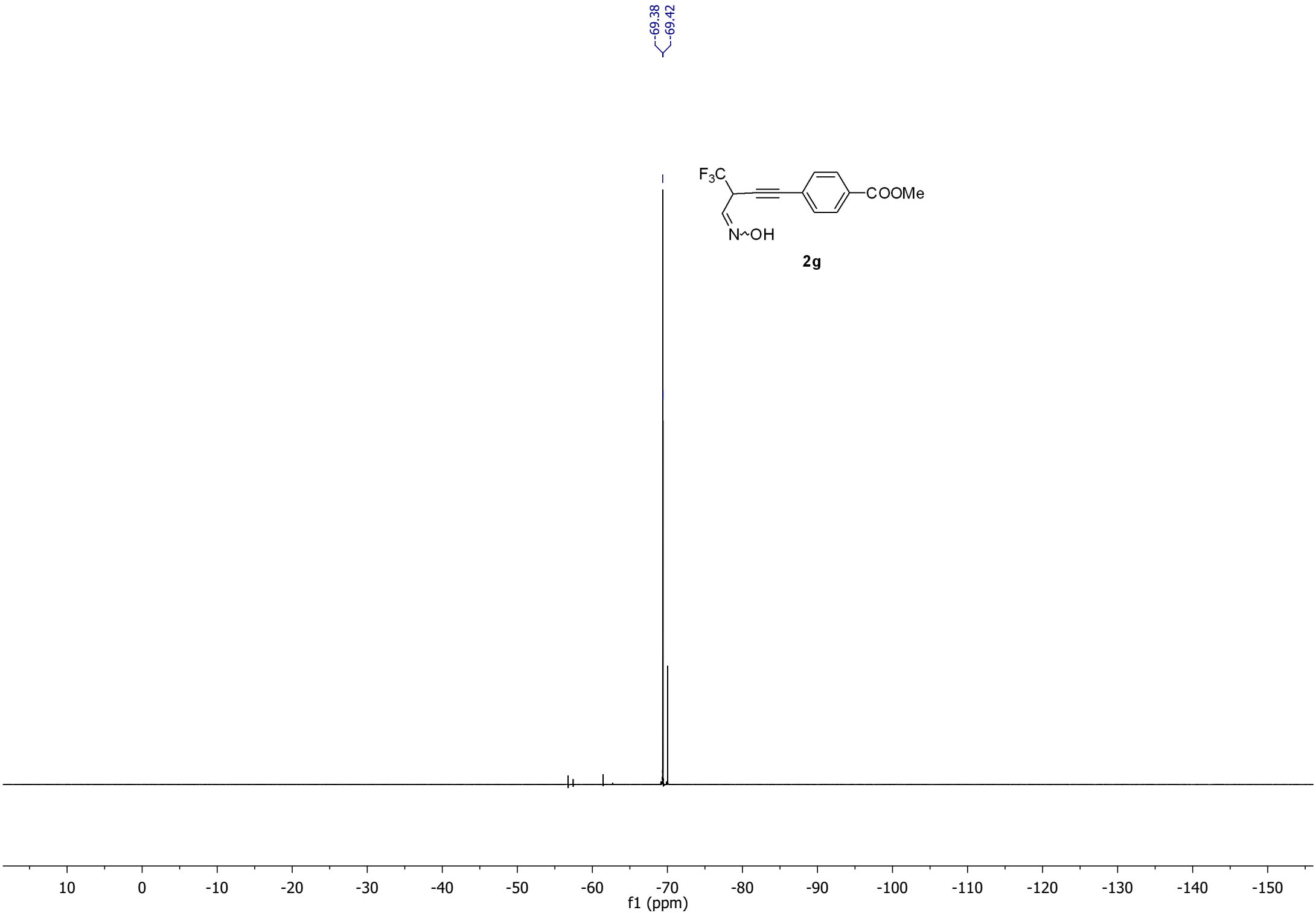

-69.50
-69.54
F3C
Br
N~OH
2e
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

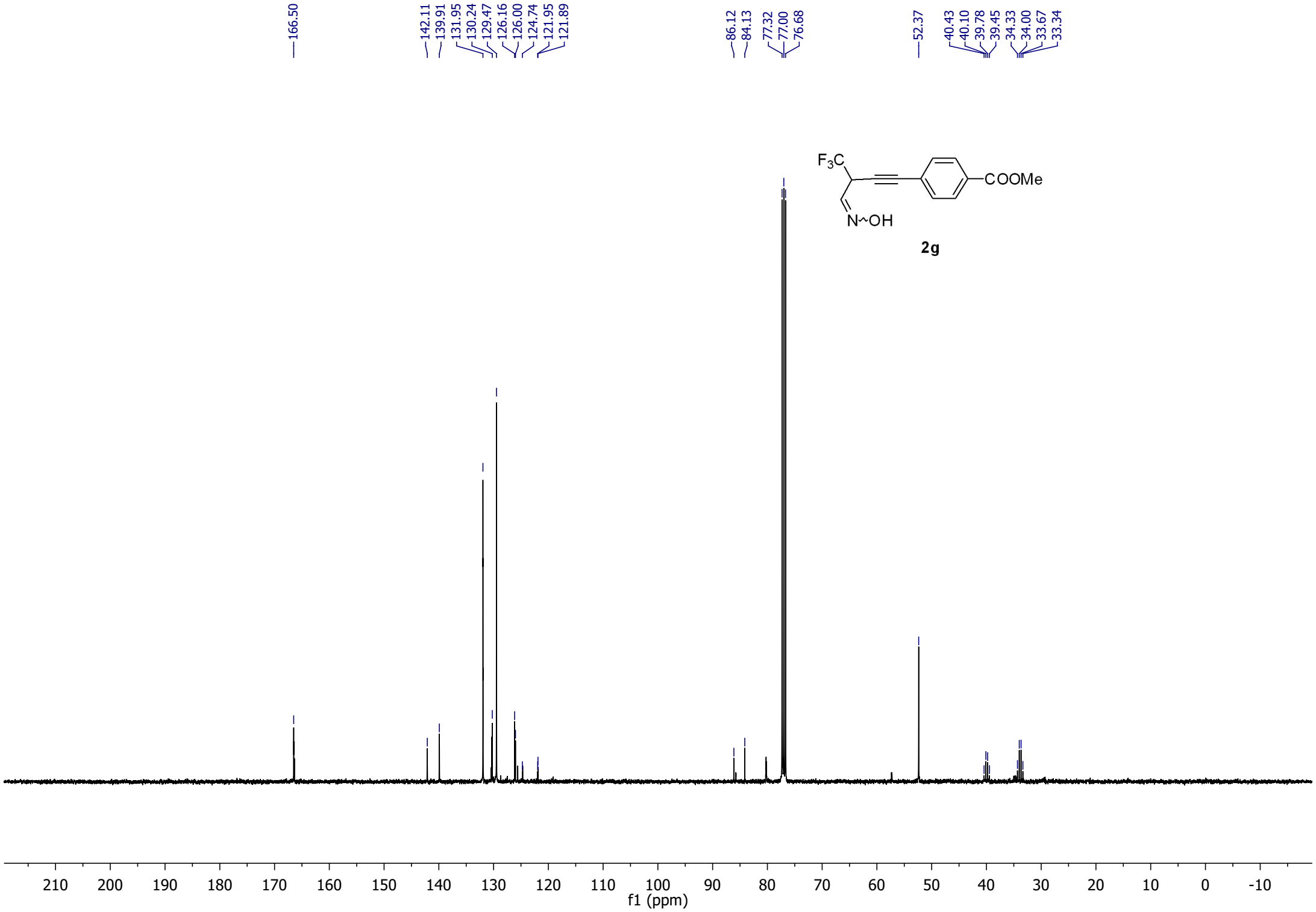

142.57
142.55
140.54
131.98
129.16
129.06
128.33
127.64
127.57
124.85
124.79
122.06
122.00
121.50
121.35
119.27
87.16
85.10
77.32
77.00
76.68
40.40
40.08
39.75
39.43
34.35
34.01
33.68
33.35
F3C
Br
N~OH
2e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

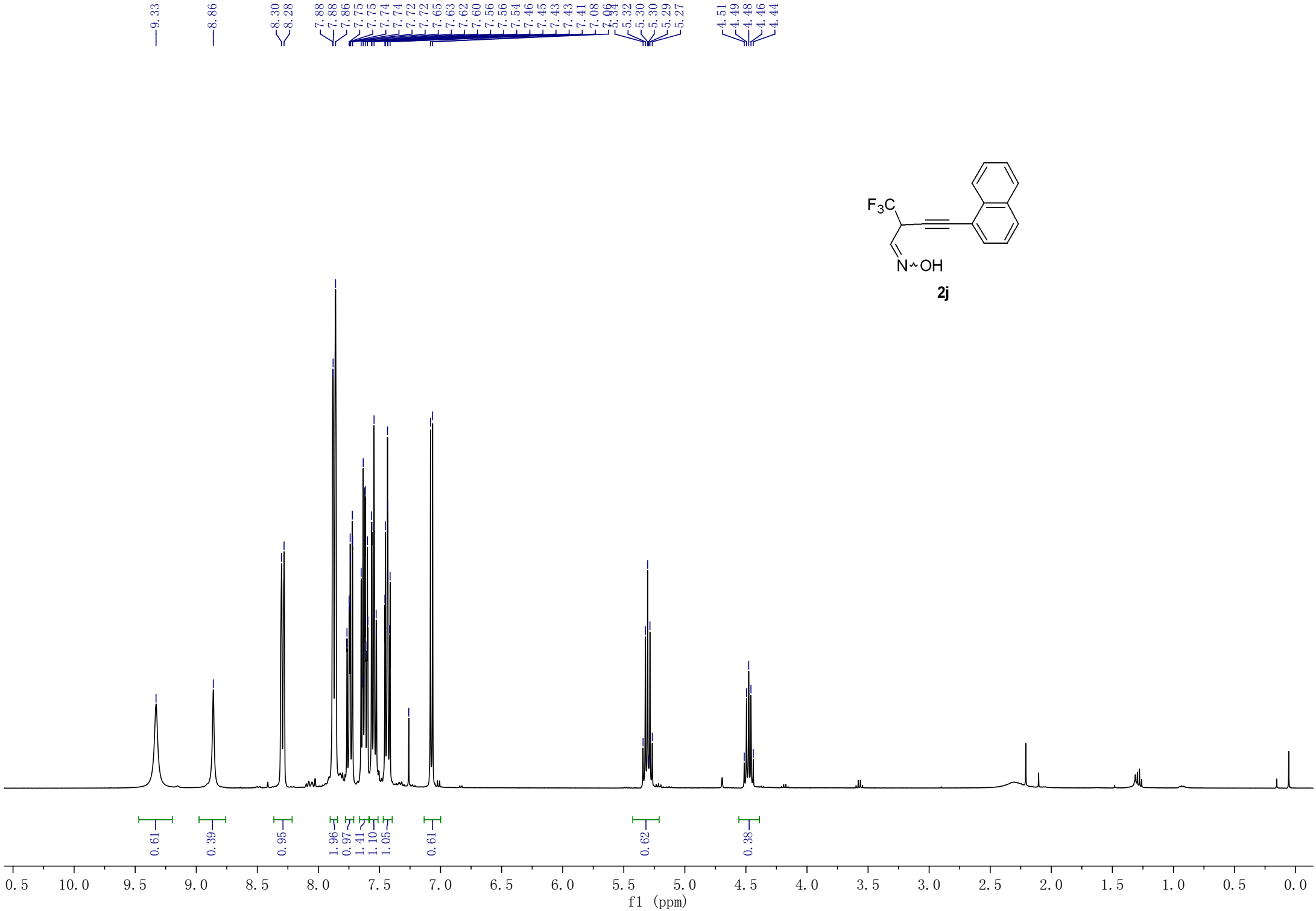

8.58
8.33
7.65
7.63
7.59
7.58
7.44
7.42
7.26
6.98
6.98
6.91
6.89
5.16
5.14
5.12
5.10
5.08
4.32
4.31
4.29
4.27
4.25
F3C
CF3
N~OH
2f
This compound is unstable
0.94
0.38
1.38
2.26
0.82
1.96
1.29
0.36
0.37
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

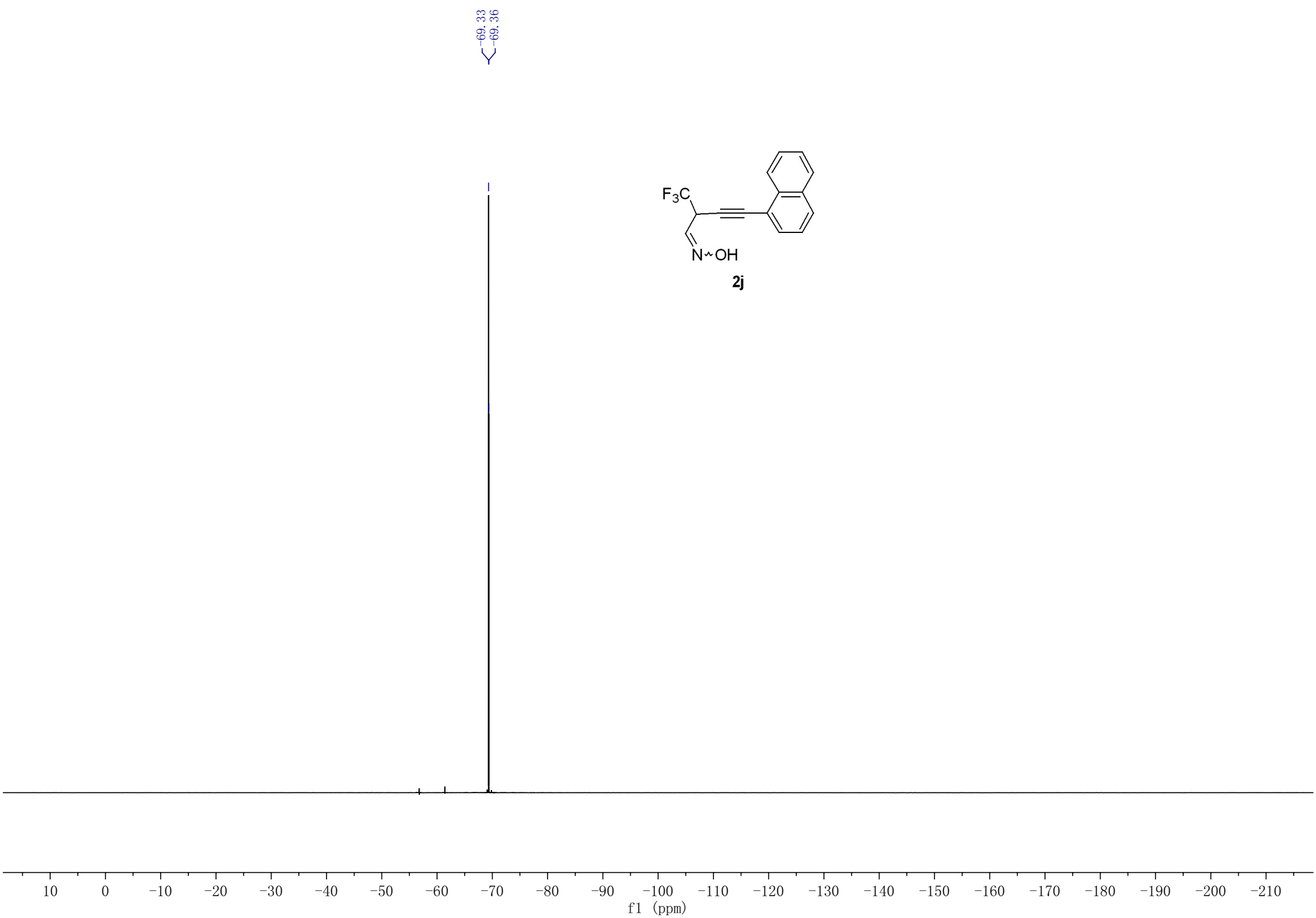

-61.53
-62.89
-63.04
-69.44
F3C
CF3
N~OH
2f
This compound is unstable
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

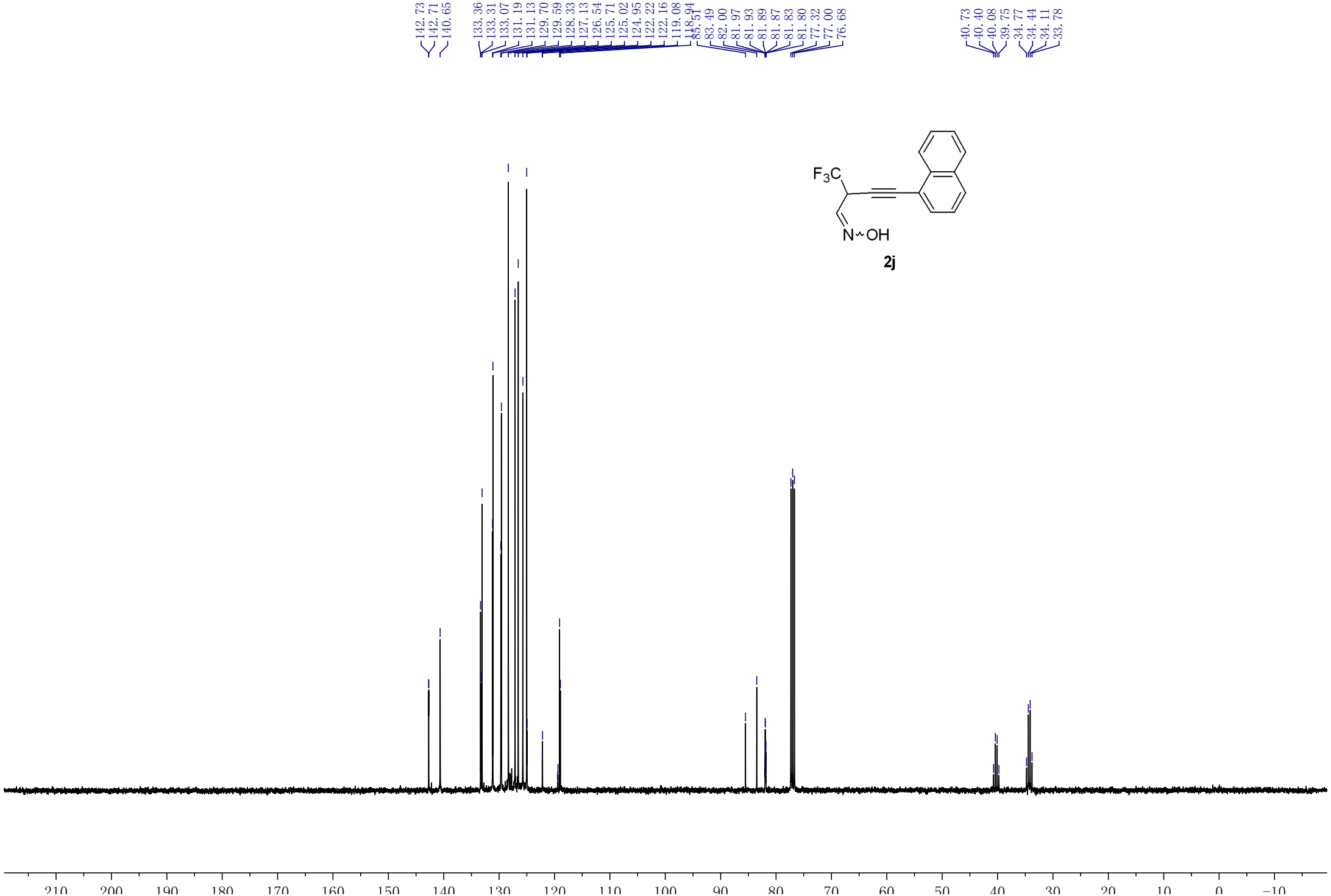

9.00
8.61
8.00
7.98
7.98
7.54
7.52
7.51
7.49
7.47
7.26
6.90
6.88
5.17
5.15
5.13
5.11
5.10
4.32
4.30
4.28
4.27
4.25
3.92
F3C
COOMe
N~OH
2g
This compound is unstable
0.57
0.41
1.88
1.94
0.50
0.34
0.58
0.58
0.43
3.54
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

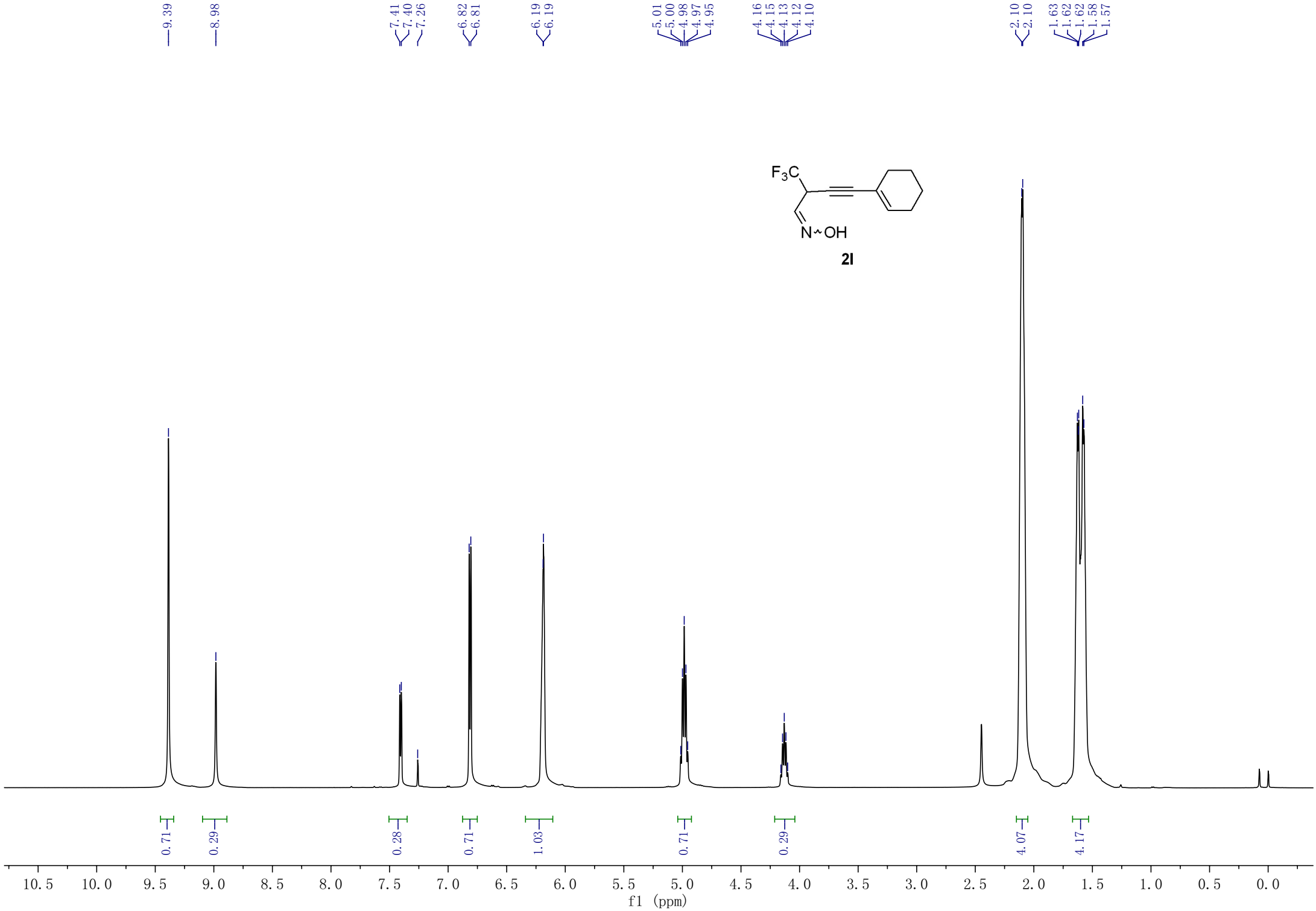

-69.38
-69.42
F3C
COOMe
N~OH
2g
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

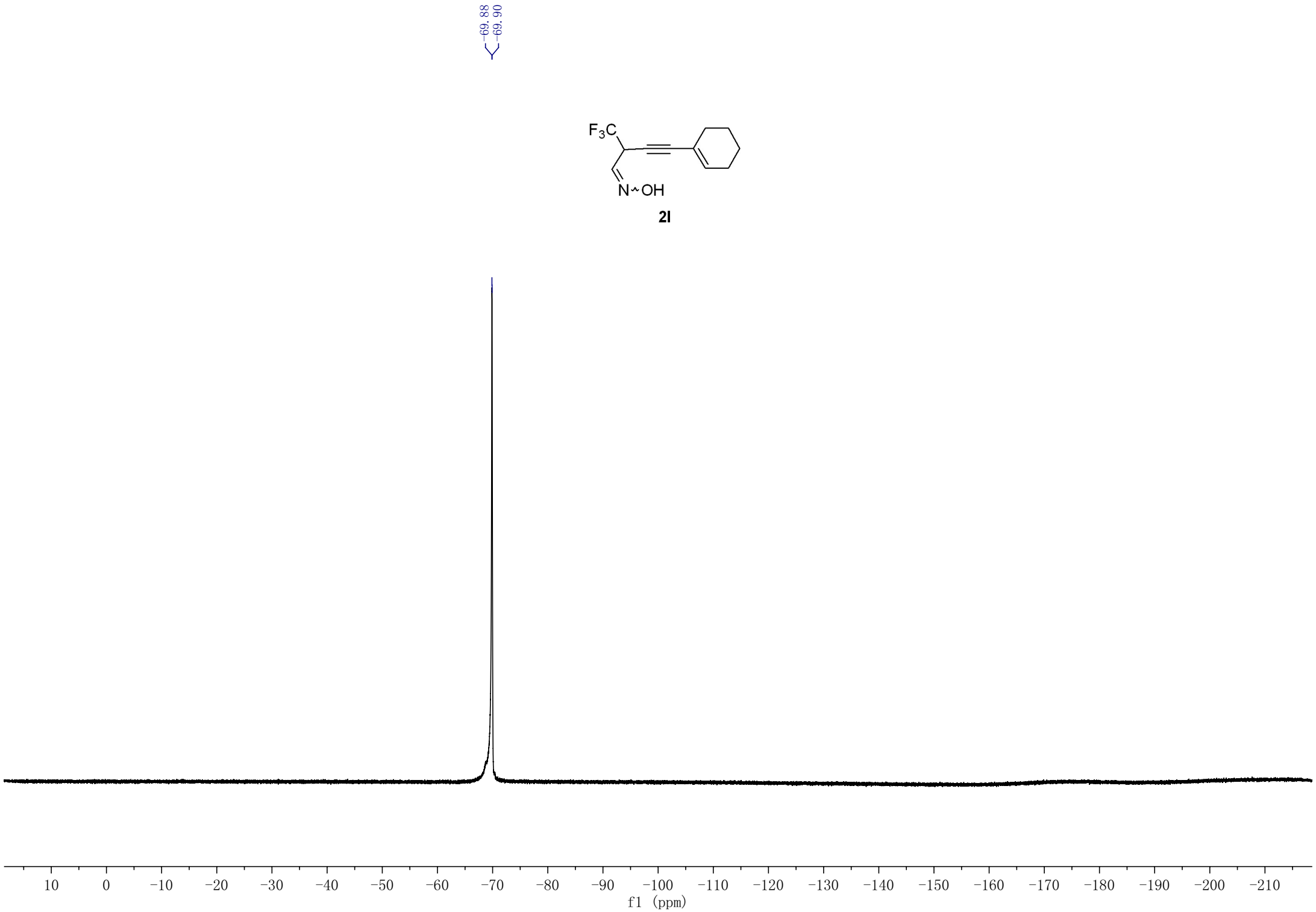

166.50
142.11
139.91
131.95
130.24
129.47
126.16
126.00
124.74
121.95
121.89
86.12
84.13
77.32
77.00
76.68
52.37
40.43
40.10
39.78
39.45
34.33
34.00
33.67
33.34
F3C
COOMe
N~OH
2g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

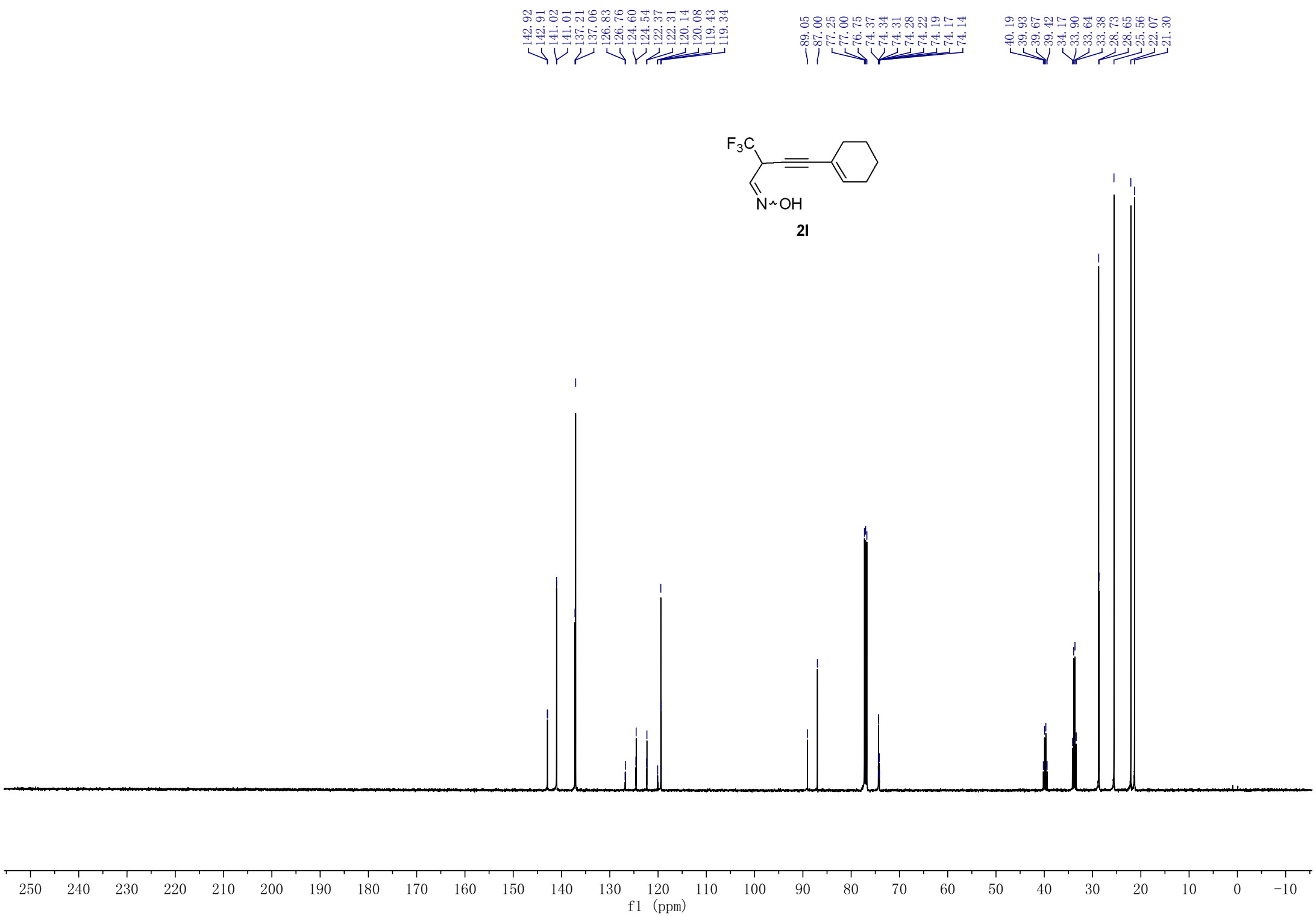

9.33
8.86
8.30
8.28
7.88
7.88
7.86
7.75
7.75
7.74
7.74
7.72
7.72
7.65
7.63
7.62
7.60
7.56
7.56
7.54
7.46
7.45
7.43
7.43
7.41
7.08
5.34
5.32
5.30
5.30
5.29
5.27
4.51
4.49
4.48
4.46
4.44
F3C
N~OH
2j
0.61
0.39
0.95
1.96
0.97
1.41
1.10
1.05
0.61
0.62
0.38
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

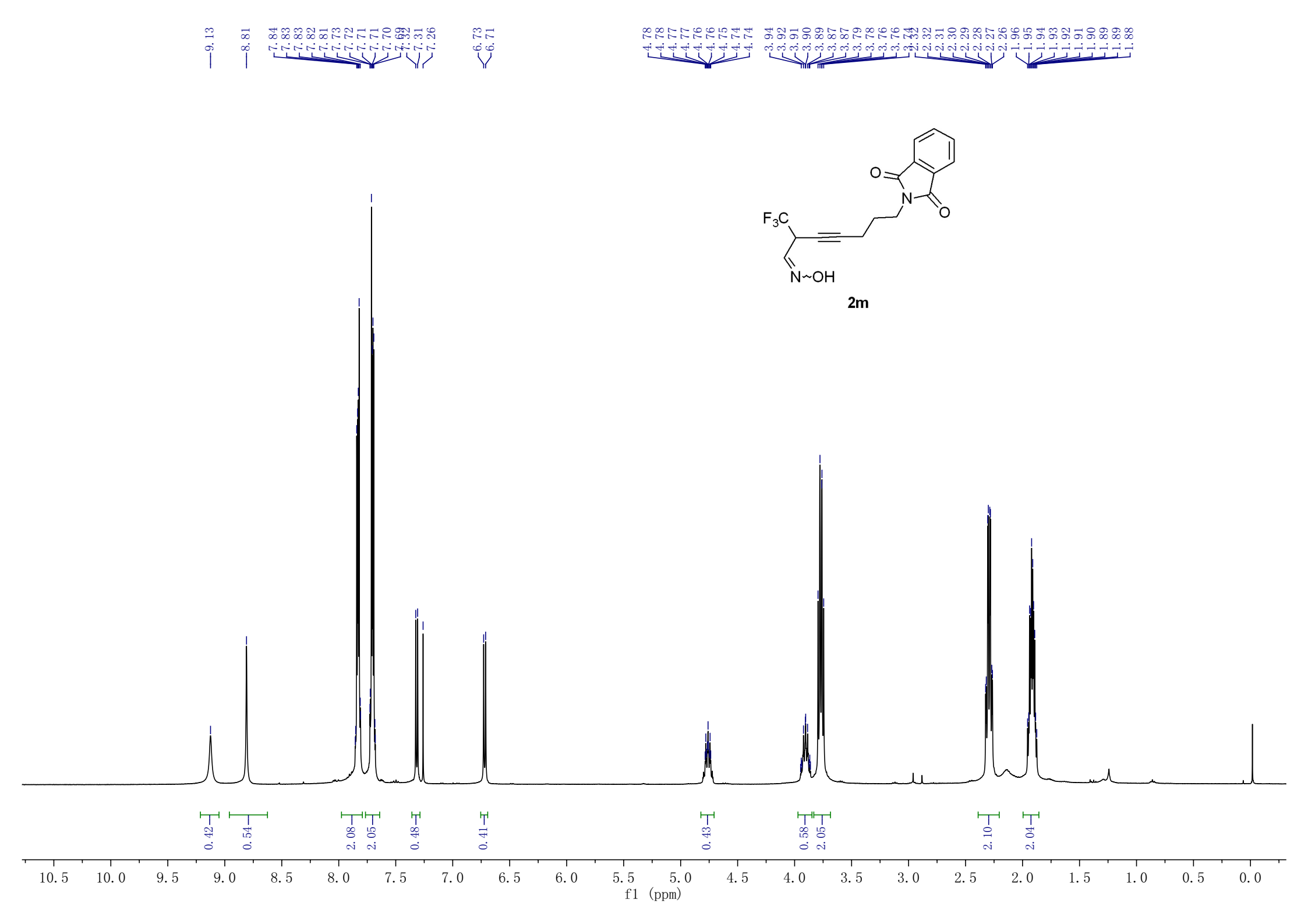

-69.33
-69.36
F3C
N~OH
2j
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

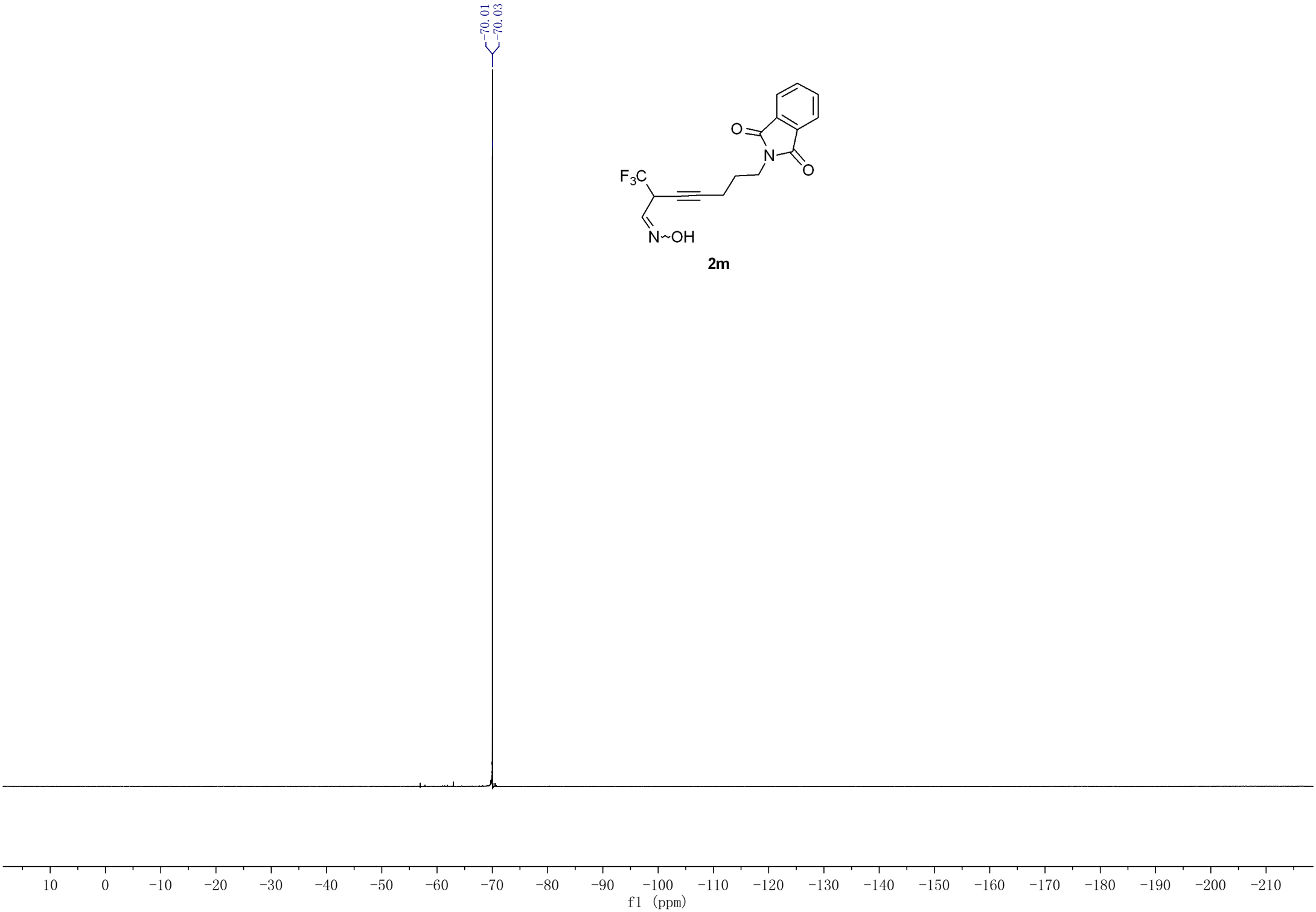

142.73
142.71
140.65
133.36
133.31
133.07
131.19
131.13
129.70
129.59
128.33
127.13
126.54
125.71
125.02
124.95
122.22
122.16
119.08
118.94
85.51
83.49
82.00
81.97
81.93
81.89
81.87
81.83
81.80
77.32
77.00
76.68
40.73
40.40
40.08
39.75
34.77
34.44
34.11
33.78
F3C
N~OH
2j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

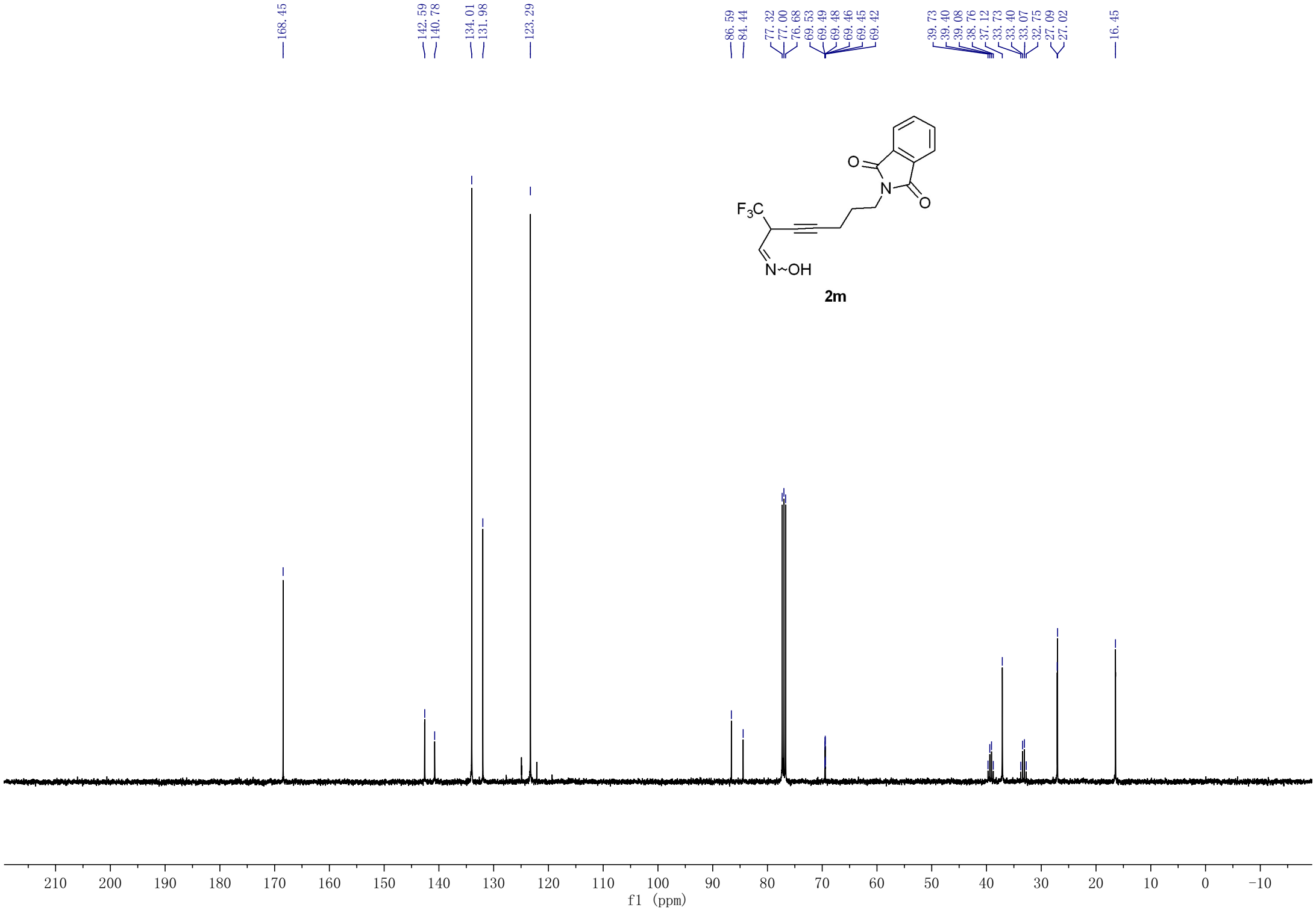

9.39
8.98
7.41
7.40
7.26
6.82
6.81
6.19
6.19
5.01
5.00
4.98
4.97
4.95
4.16
4.15
4.13
4.12
4.10
2.10
2.10
1.63
1.62
1.62
1.58
1.57
F3C
N~OH
2l
0.71
0.29
0.28
0.71
1.03
0.71
0.29
4.07
4.17
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

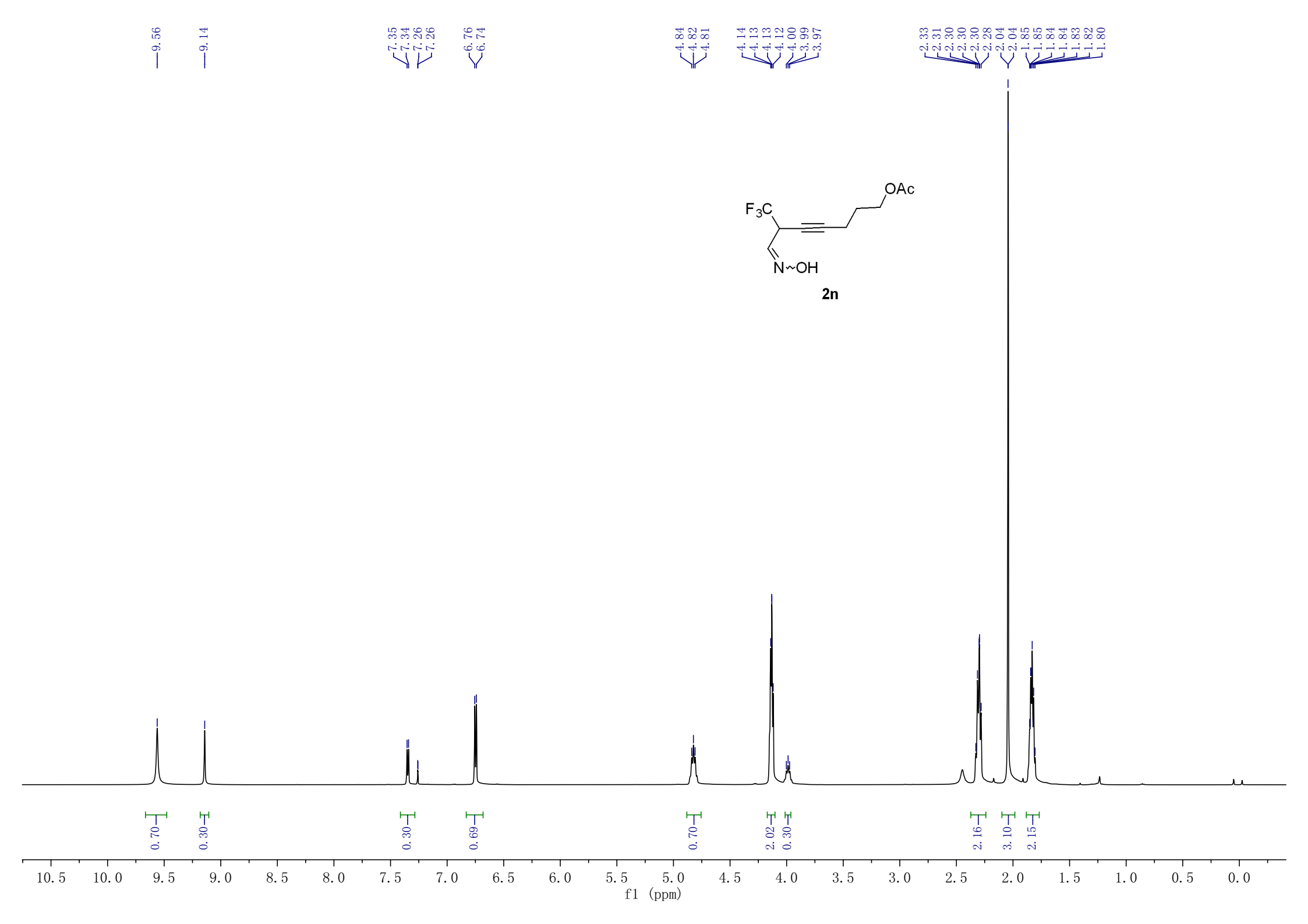

-69.88
-69.90
F3C
N~OH
2l
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

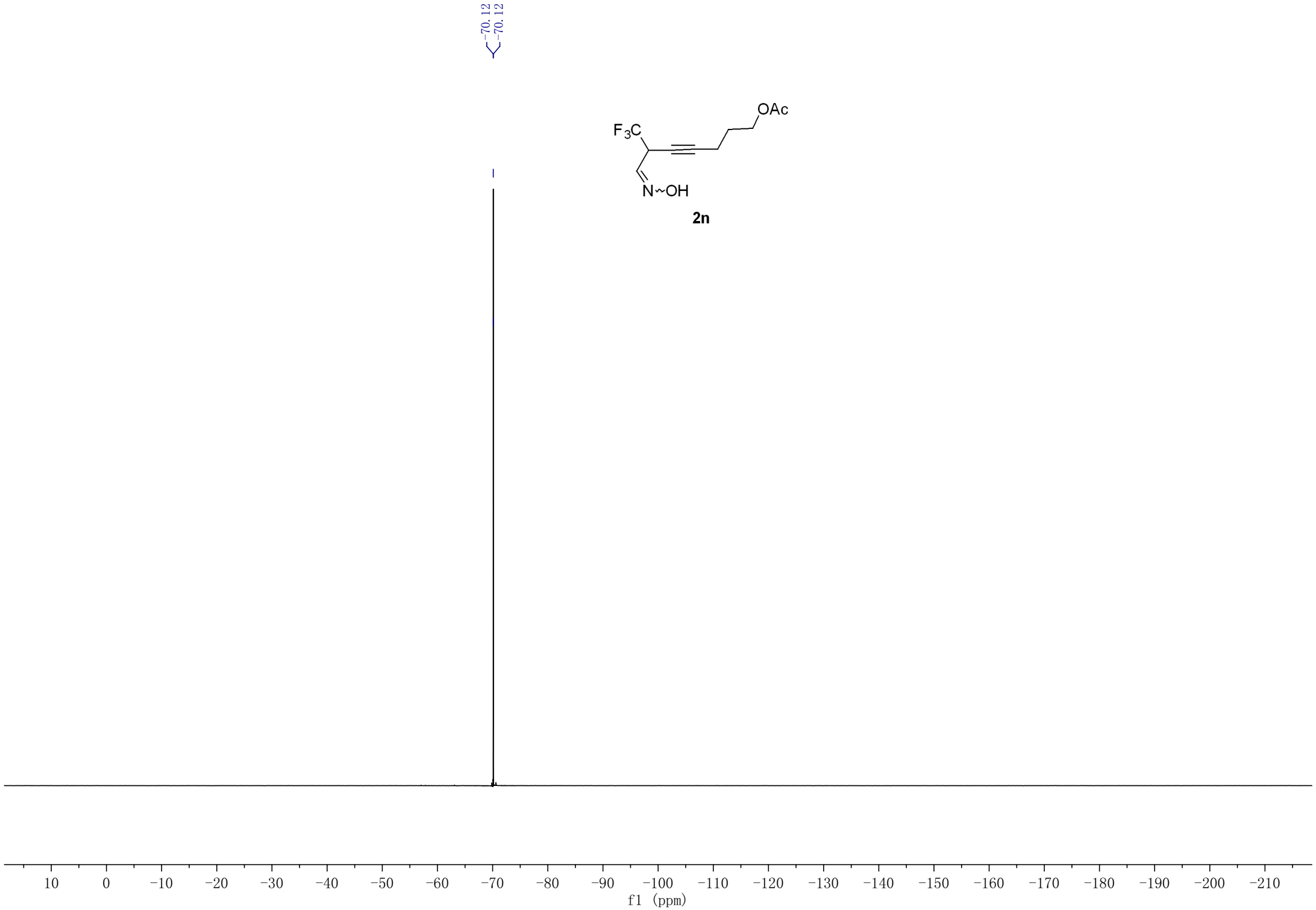

142.92
142.91
141.02
141.01
137.21
137.06
126.83
126.76
124.60
124.54
122.37
122.31
120.14
120.08
119.43
119.34
89.05
87.00
77.25
77.00
76.75
74.37
74.34
74.31
74.28
74.22
74.19
74.17
74.14
40.19
39.93
39.67
39.42
34.17
33.90
33.64
33.38
28.73
28.65
25.56
22.07
21.30
F3C
N~OH
2l
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

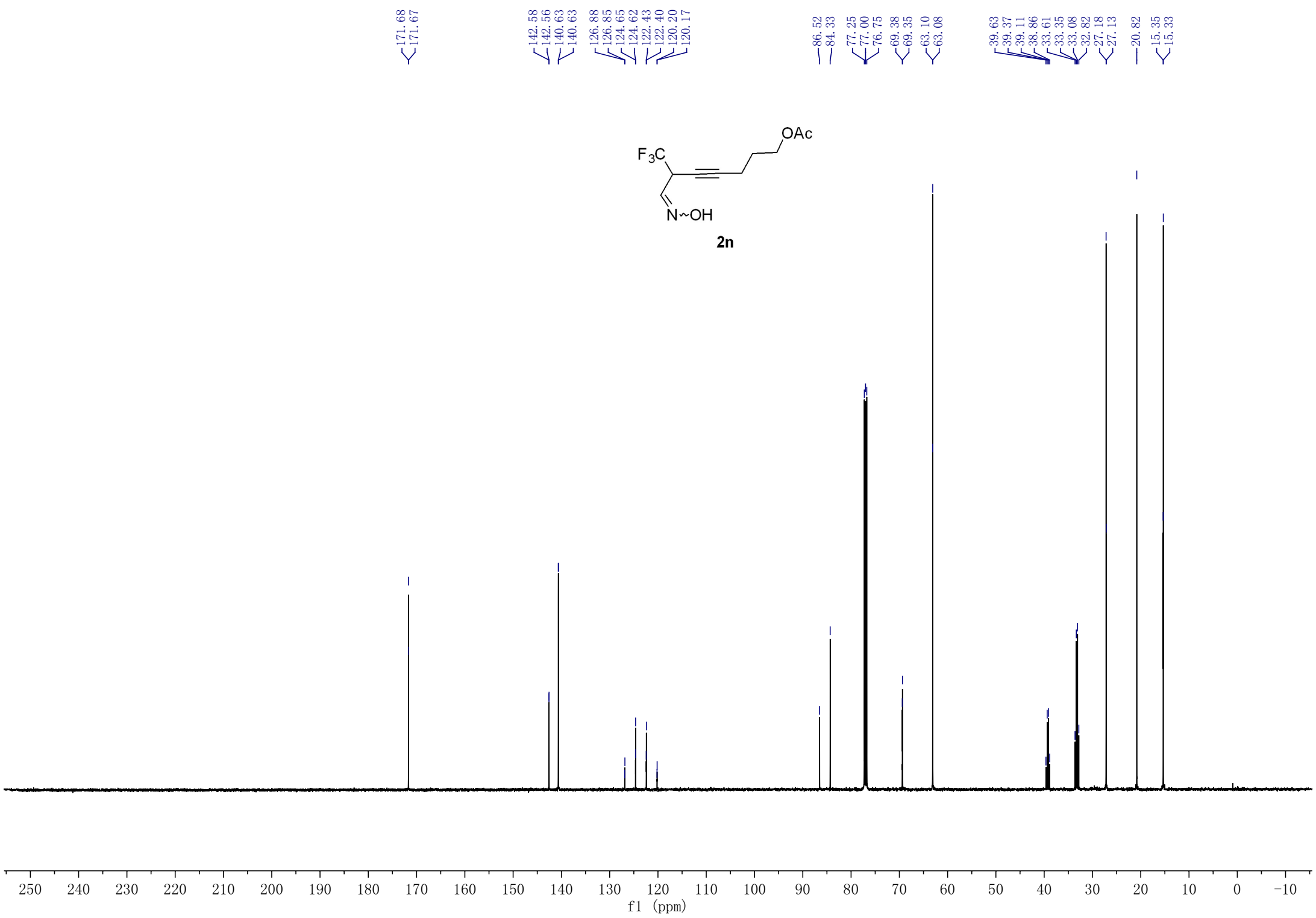

9.13
8.81
7.84
7.83
7.83
7.82
7.81
7.73
7.72
7.71
7.71
7.70
7.69
7.32
7.31
7.26
6.73
6.71
4.78
4.78
4.77
4.77
4.76
4.76
4.75
4.74
4.74
3.94
3.92
3.91
3.90
3.89
3.87
3.87
3.79
3.78
3.76
3.76
2.32
2.32
2.31
2.30
2.29
2.28
2.27
2.26
1.96
1.95
1.94
1.93
1.92
1.91
1.90
1.89
1.89
1.88
O
N
O
F3C
N~OH
2m
0.42
0.54
2.08
2.05
0.48
0.41
0.43
0.58
2.05
2.10
2.04
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)

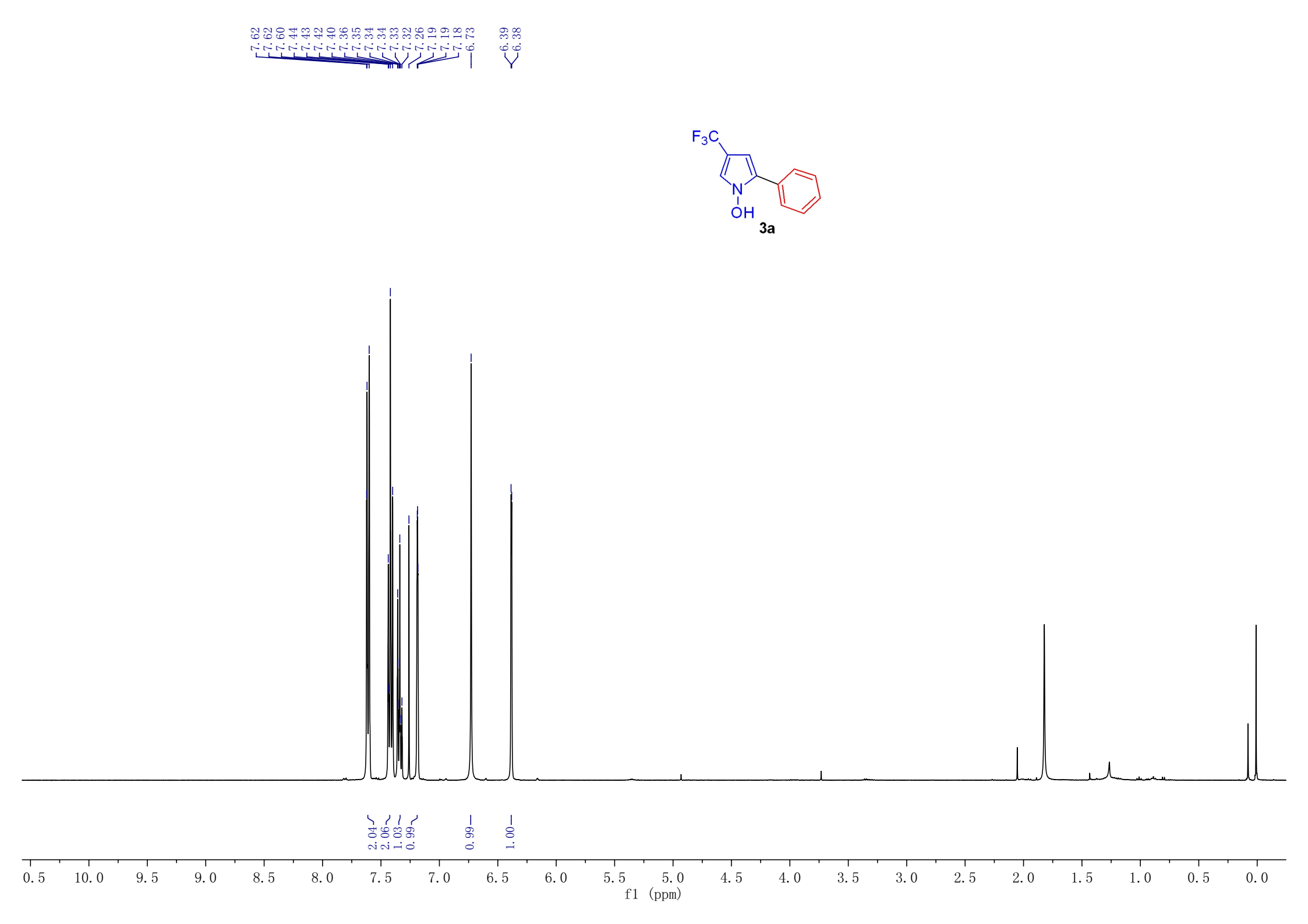

-70.01
-70.03
O
N
O
F3C
N~OH
2m
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

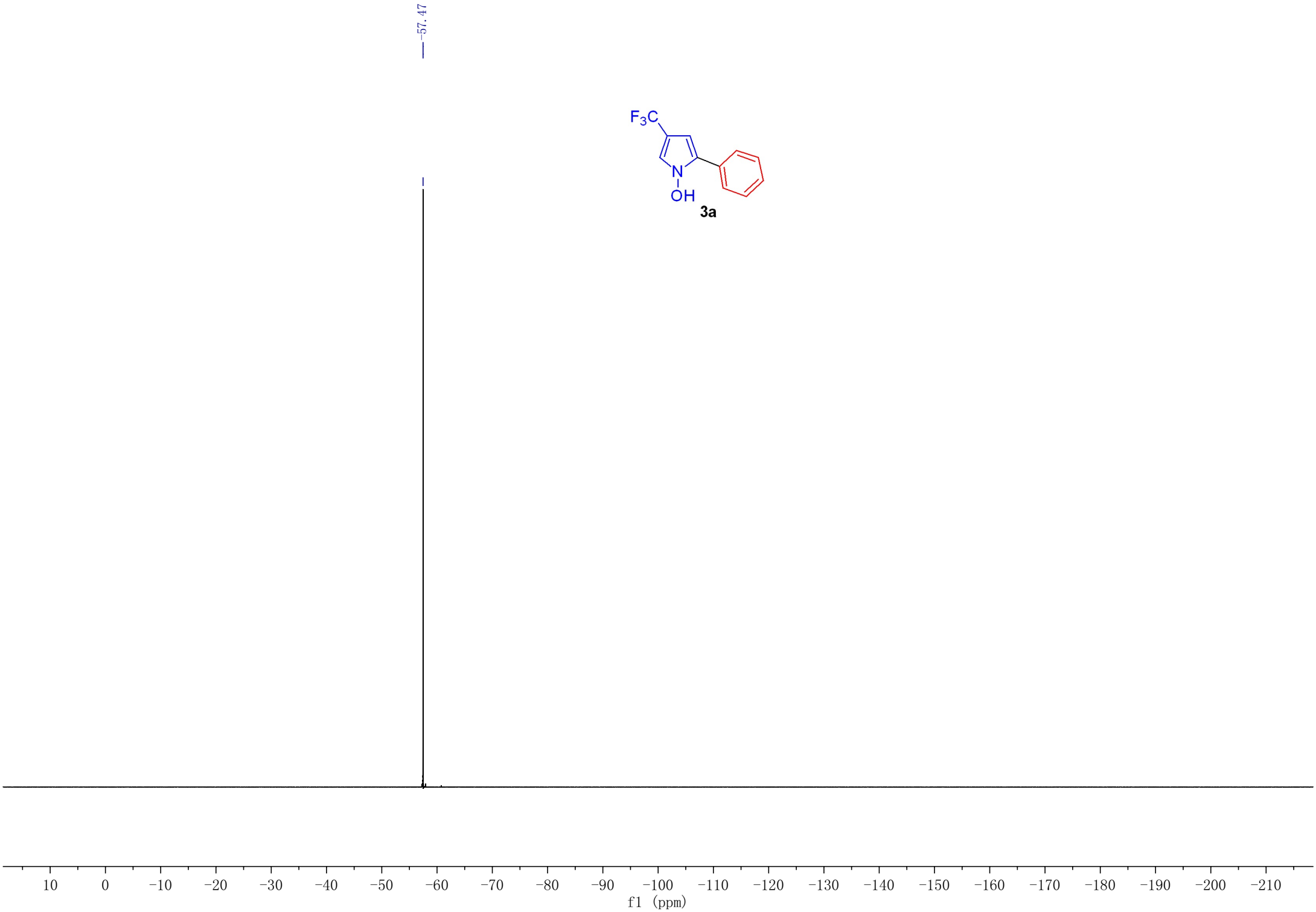

168.45
142.59
140.78
134.01
131.98
123.29
86.59
84.44
77.32
77.00
76.68
69.53
69.49
69.48
69.46
69.45
69.42
39.73
39.40
39.08
38.76
37.12
33.73
33.40
33.07
32.75
27.09
27.02
16.45
O
N
O
F3C
N~OH
2m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


9.56
9.14
7.35
7.34
7.26
7.26
6.76
6.74
4.84
4.82
4.81
4.14
4.13
4.13
4.12
4.00
3.99
3.97
2.33
2.31
2.30
2.30
2.30
2.28
2.04
2.04
1.85
1.85
1.84
1.84
1.83
1.82
1.80
OAc
F3C
N~OH
2n
0.70
0.30
0.30
0.69
0.70
2.02
0.30
2.16
3.10
2.15
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)


-70.12
-70.12
OAc
F3C
N~OH
2n
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)


171.68
171.67
142.58
142.56
140.63
140.63
126.88
126.85
124.65
124.62
122.43
122.40
120.20
120.17
86.52
84.33
77.25
77.00
76.75
69.38
69.35
63.10
63.08
39.63
39.37
39.11
38.86
33.61
33.35
33.08
32.82
27.18
27.13
20.82
15.35
15.33
OAc
F3C
N~OH
2n
250
240
230
220
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)


7.62
7.62
7.60
7.44
7.43
7.42
7.40
7.36
7.35
7.34
7.34
7.33
7.32
7.26
7.19
7.19
7.18
6.73
6.39
6.38
F3C
N
OH
3a
2.04
2.06
1.03
0.99
0.99
1.00
0.5
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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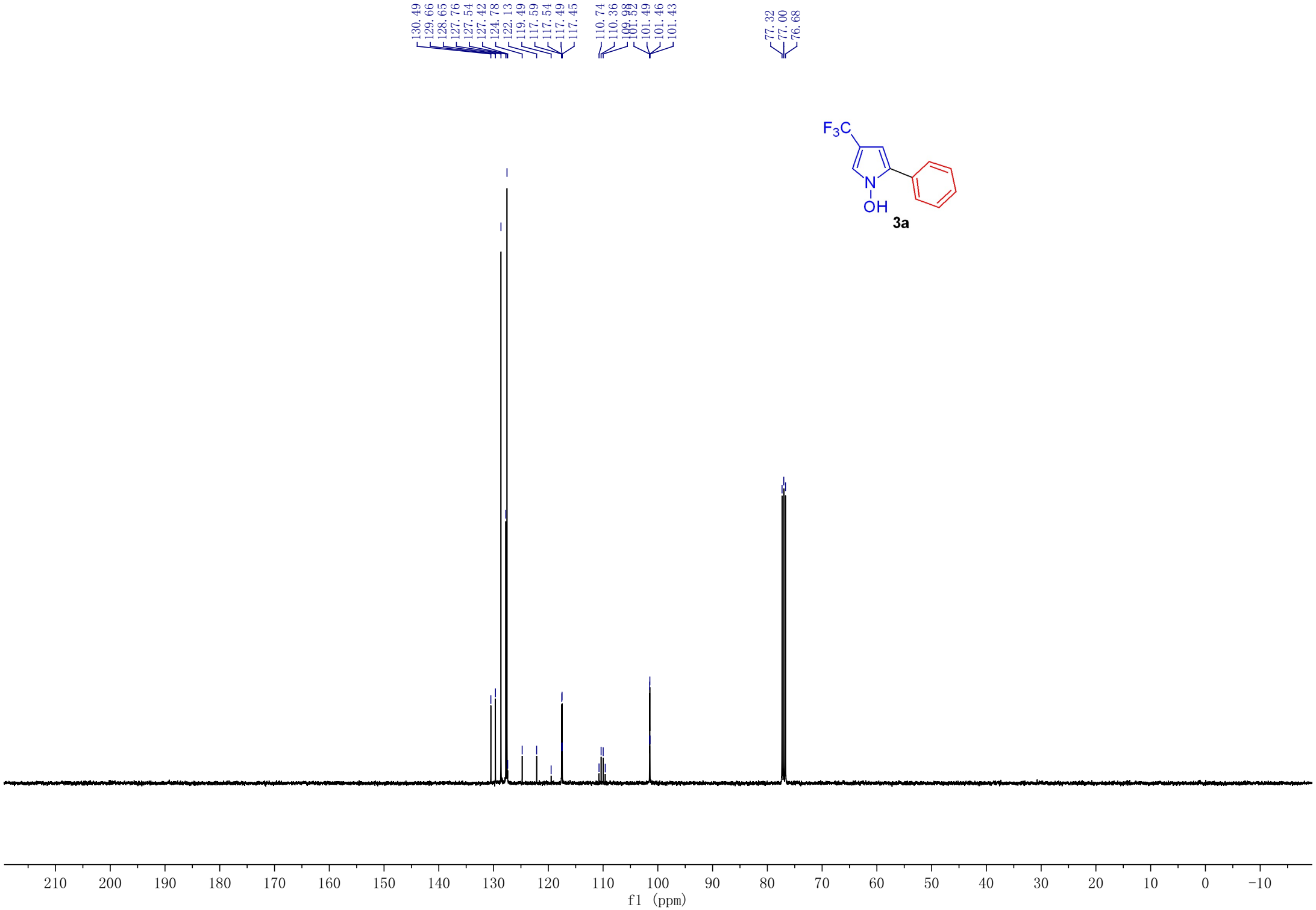
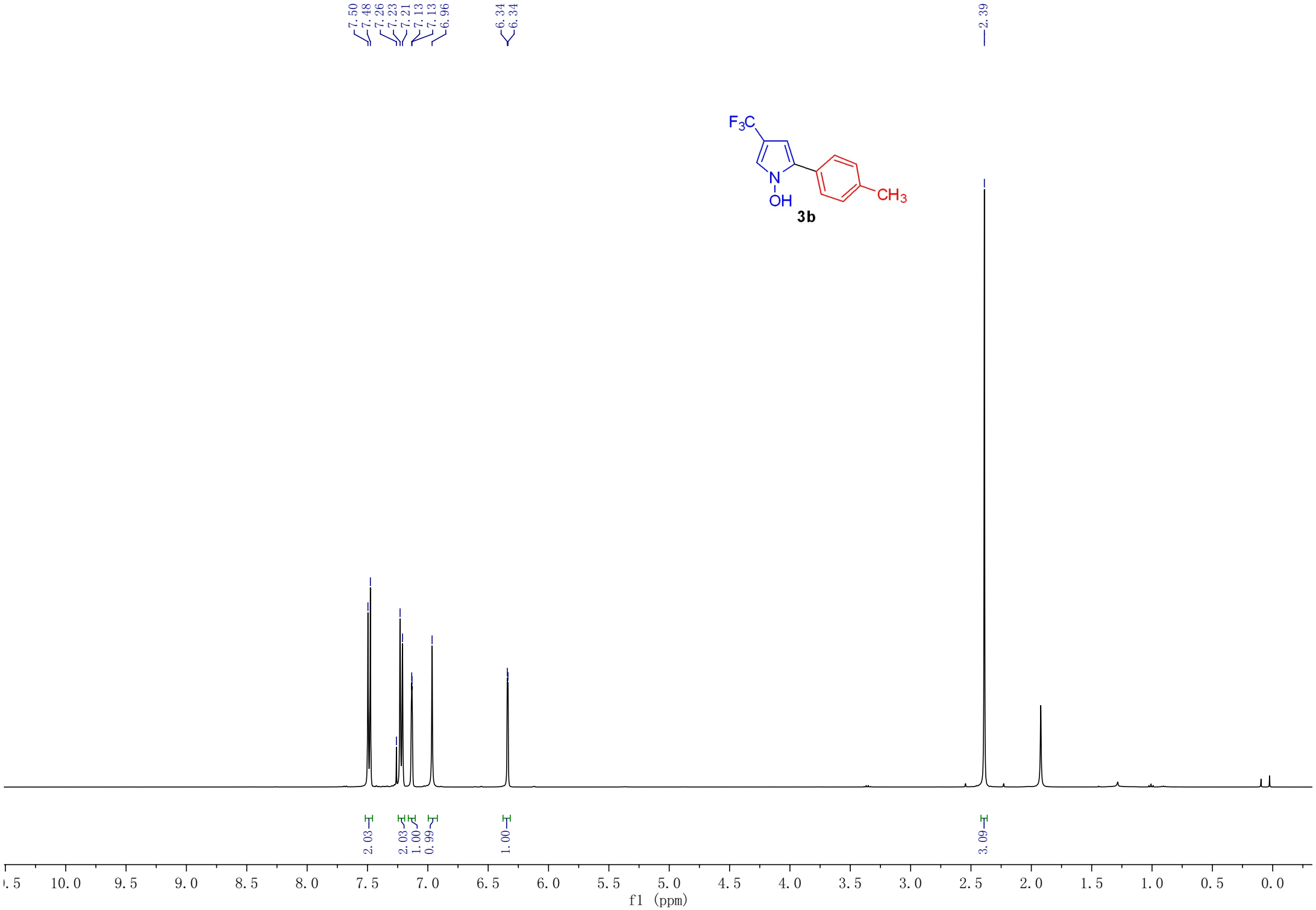
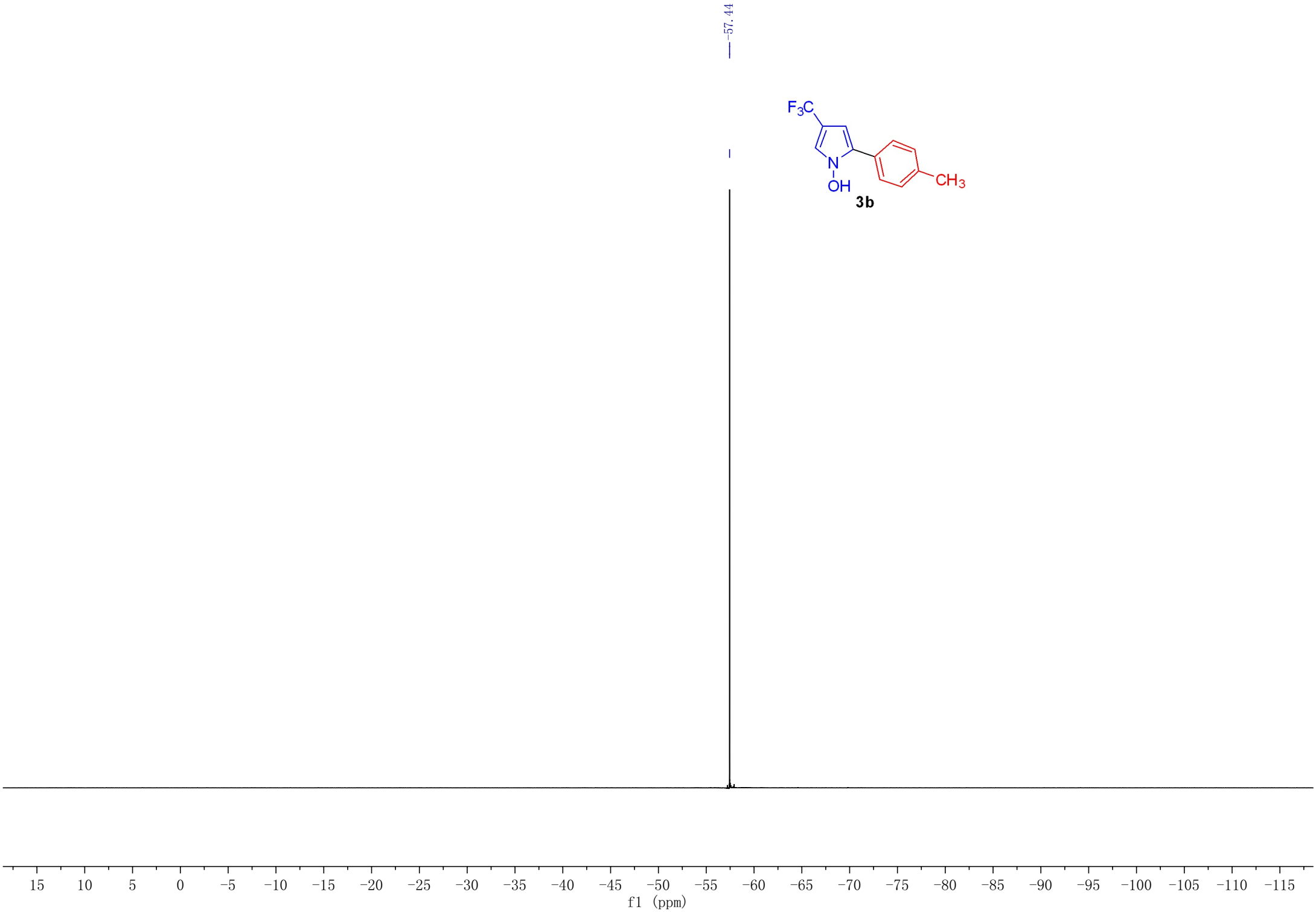
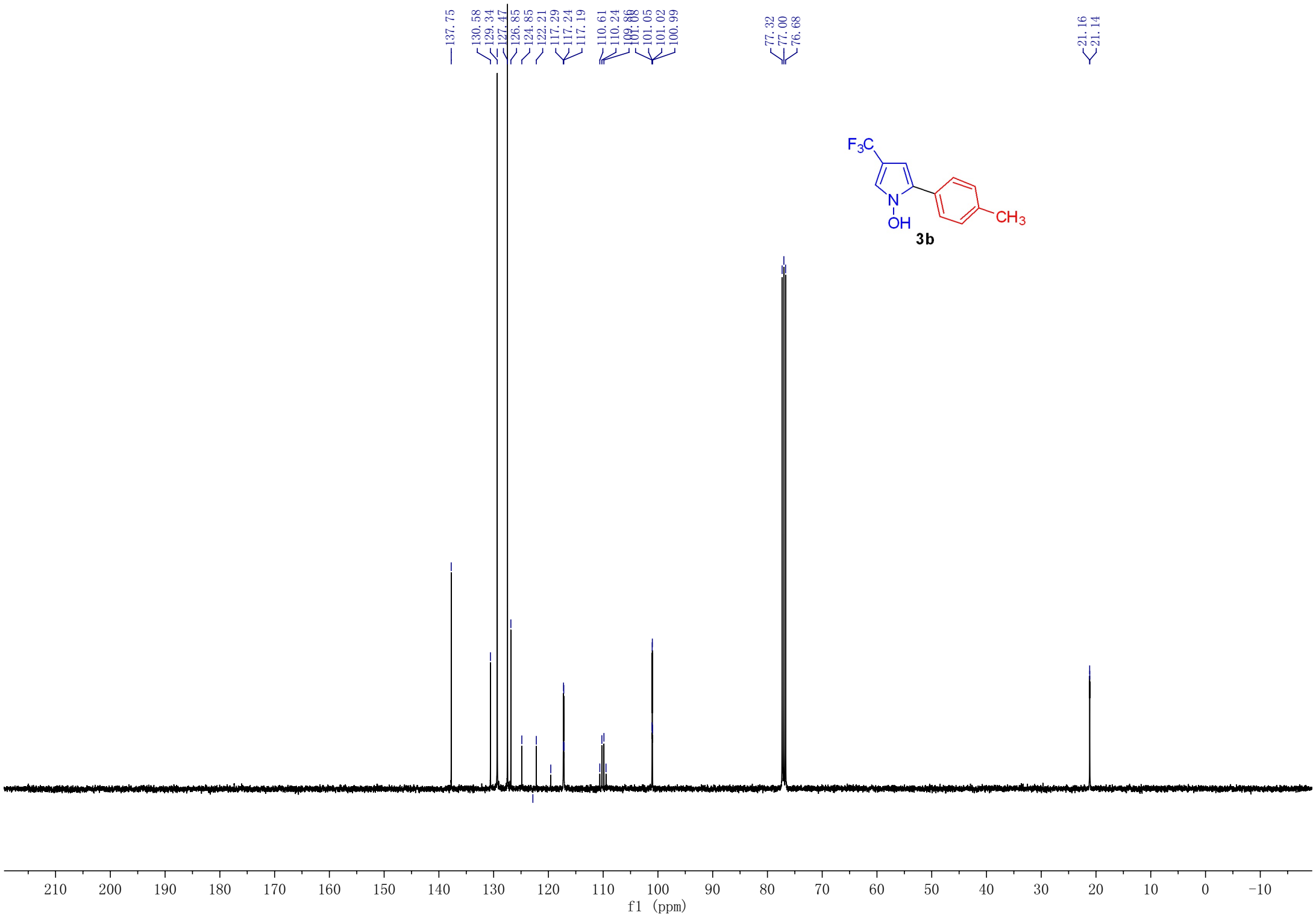
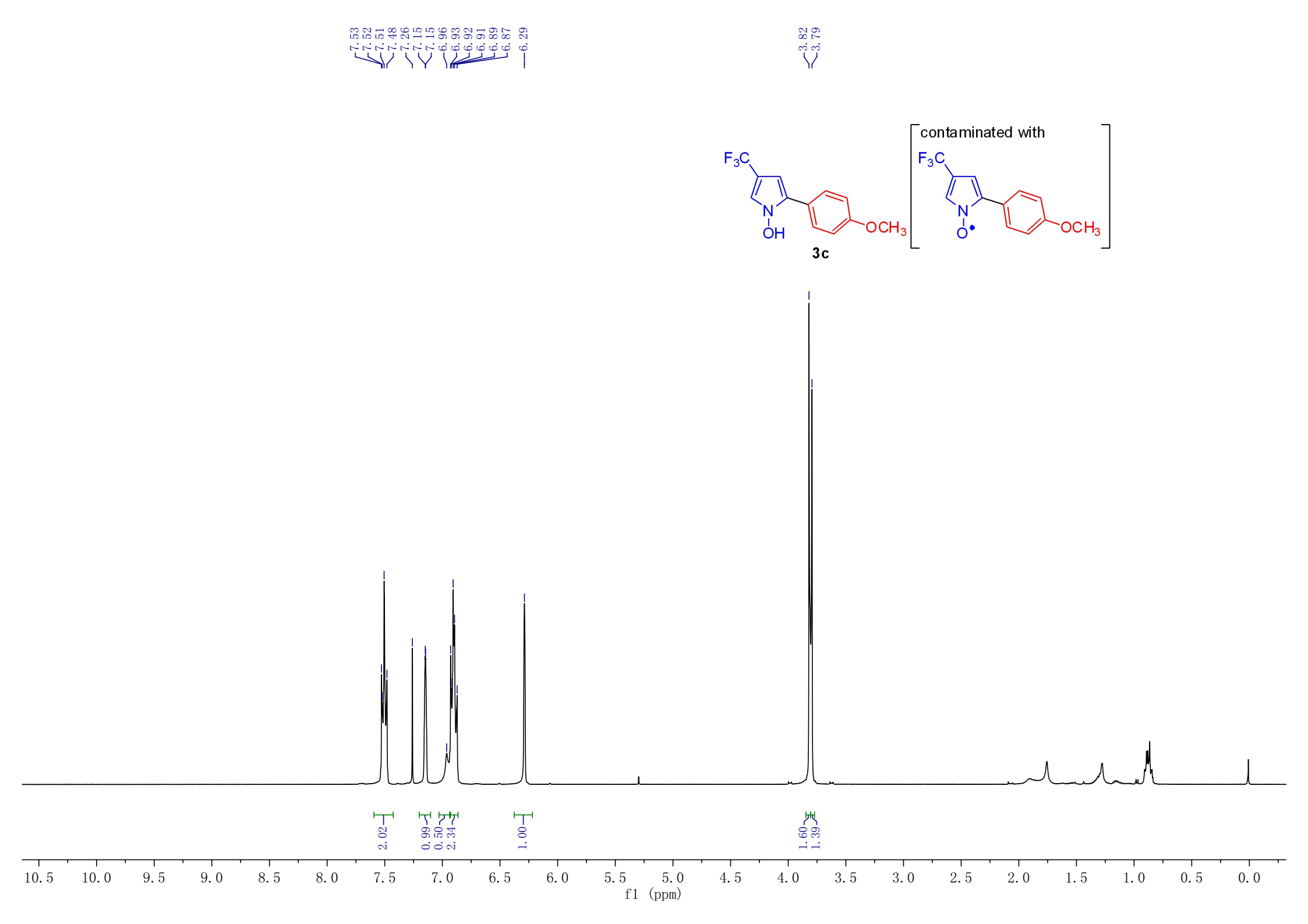
N
OH
3a
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

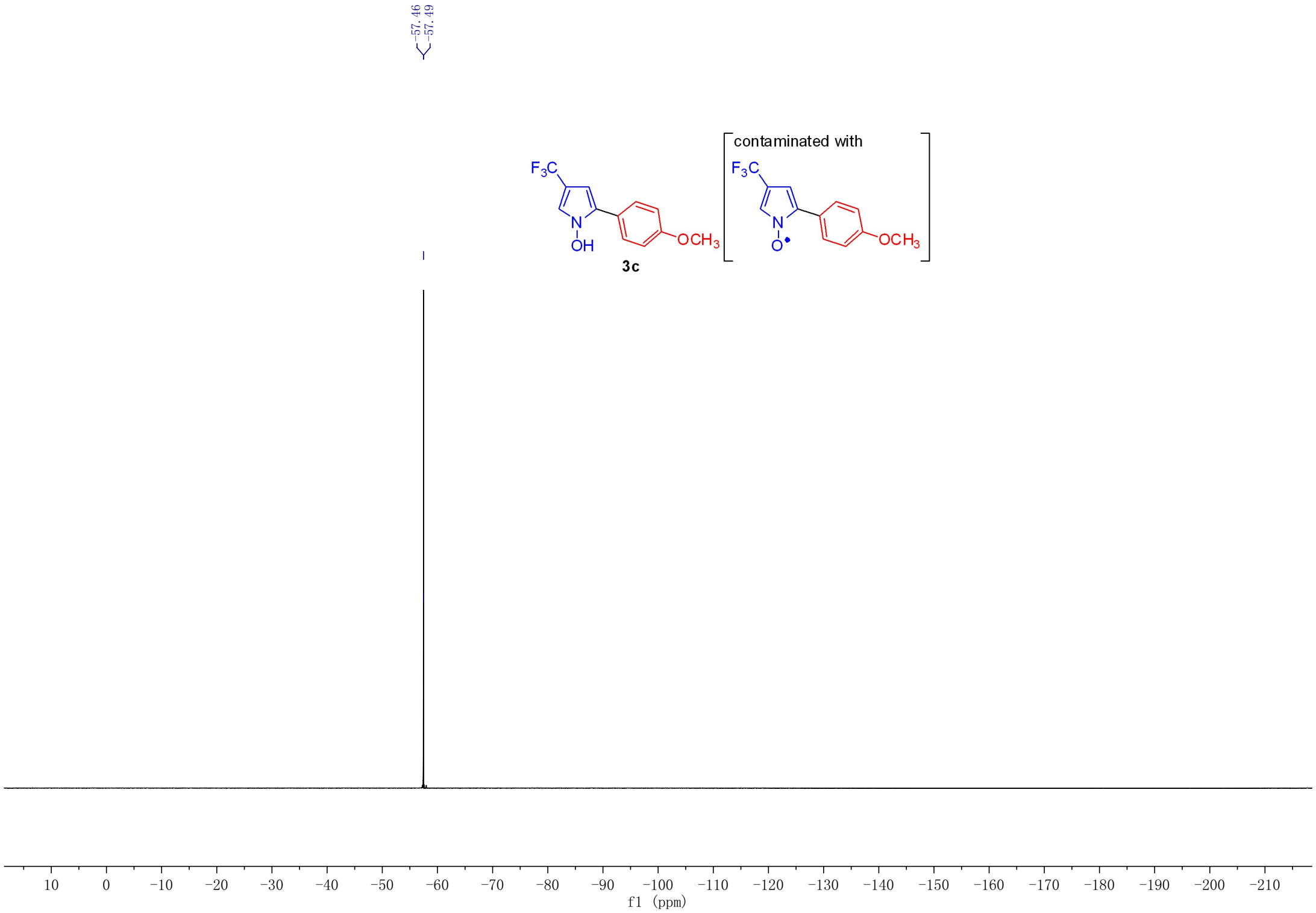

130.49
129.66
128.65
127.76
127.54
127.42
124.78
122.13
119.49
117.59
117.54
117.49
117.45
110.74
110.36
101.49
101.46
101.43
77.32
77.00
76.68
F3C
N
OH
3a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

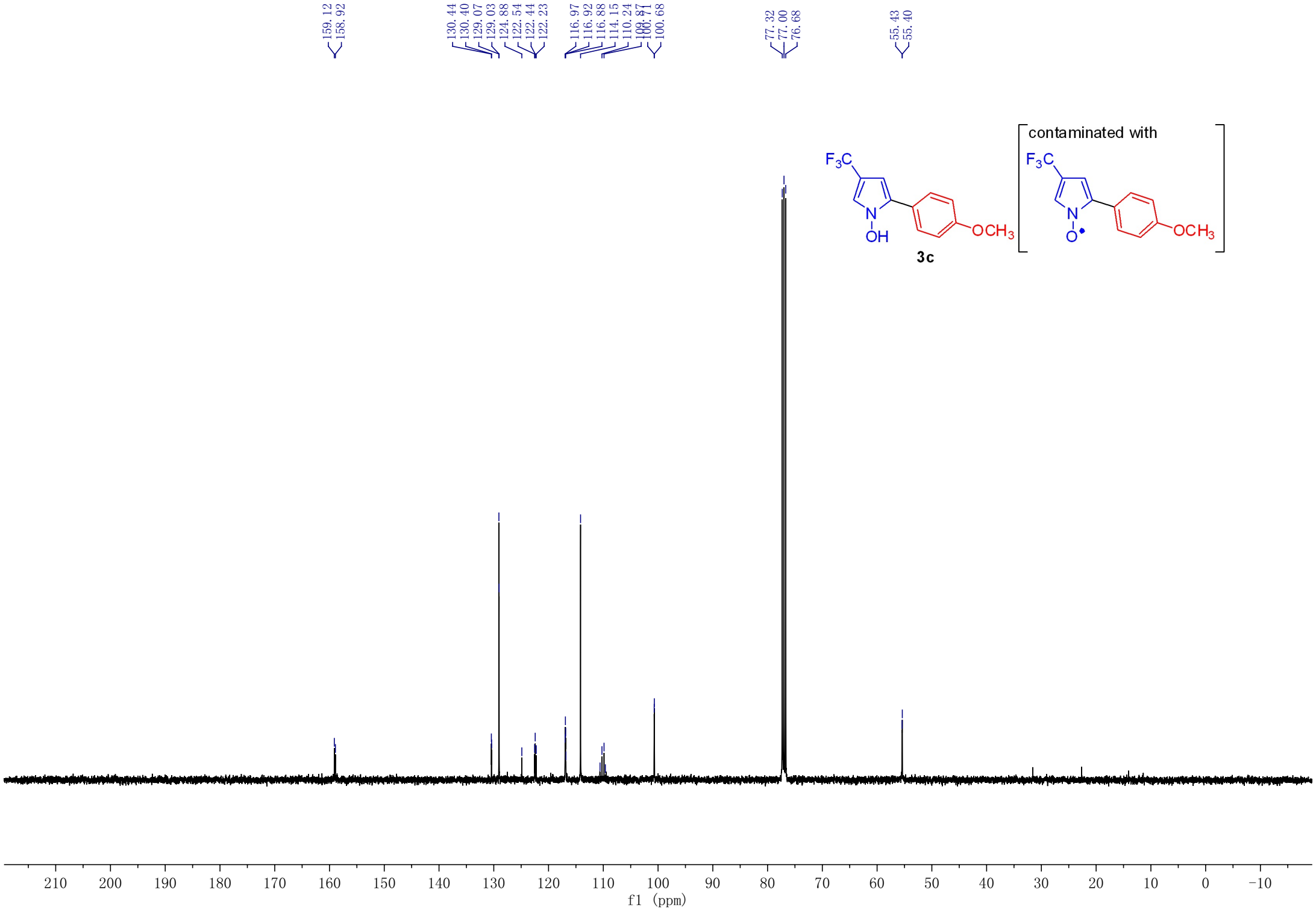

7.50
7.48
7.26
7.23
7.21
7.13
7.13
6.96
6.34
6.34
2.39
F3C
N
OH
CH3
3b
2.03
2.03
1.00
0.99
1.00
3.09
f1 (ppm)

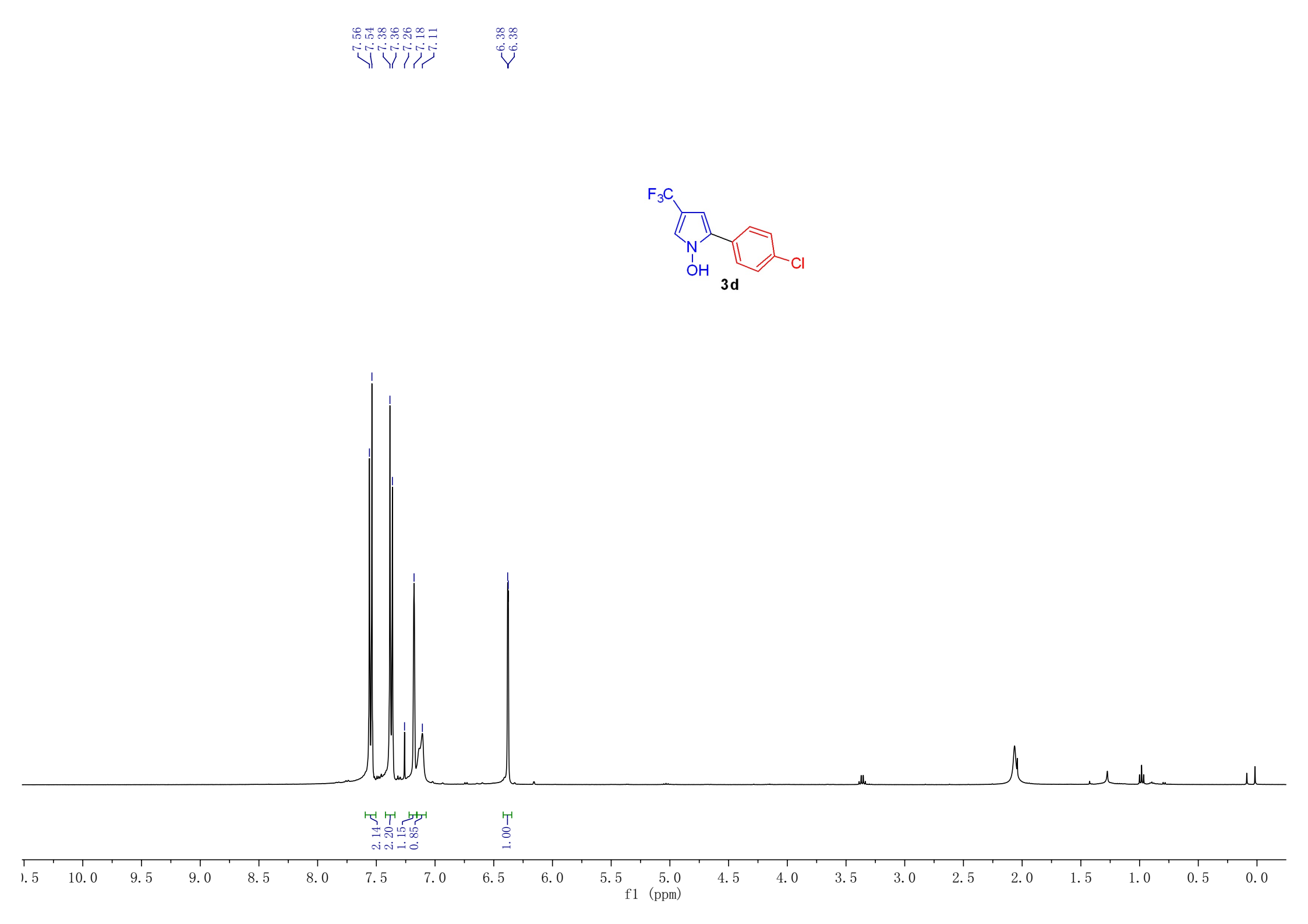

-57.44
F3C
N
OH
CH3
3b
15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115
f1 (ppm)

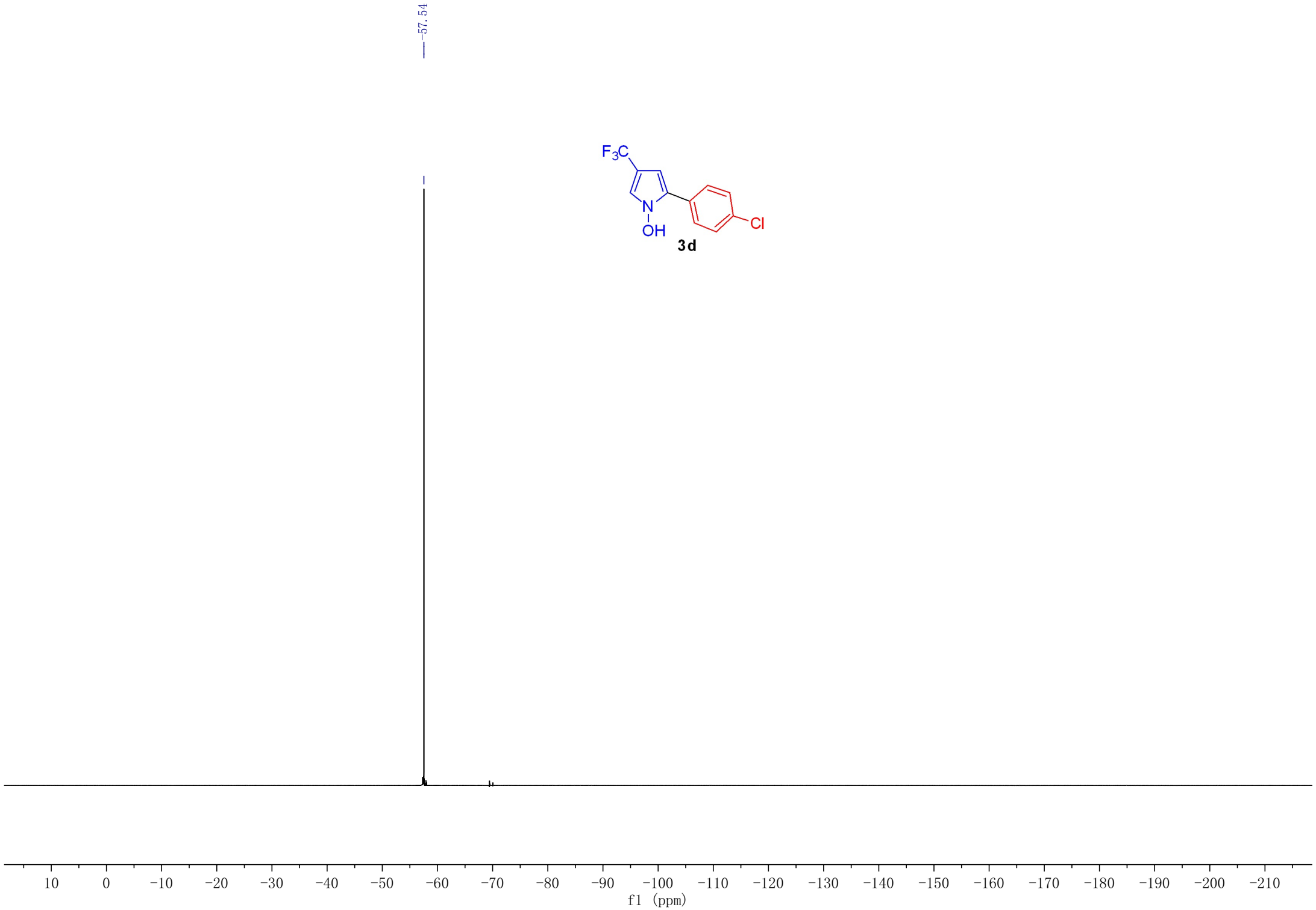

137.75
130.58
129.34
127.47
126.85
124.85
122.21
117.29
117.24
117.19
110.61
110.24
101.05
101.02
100.99
77.32
77.00
76.68
21.16
21.14
F3C
N
OH
CH3
3b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

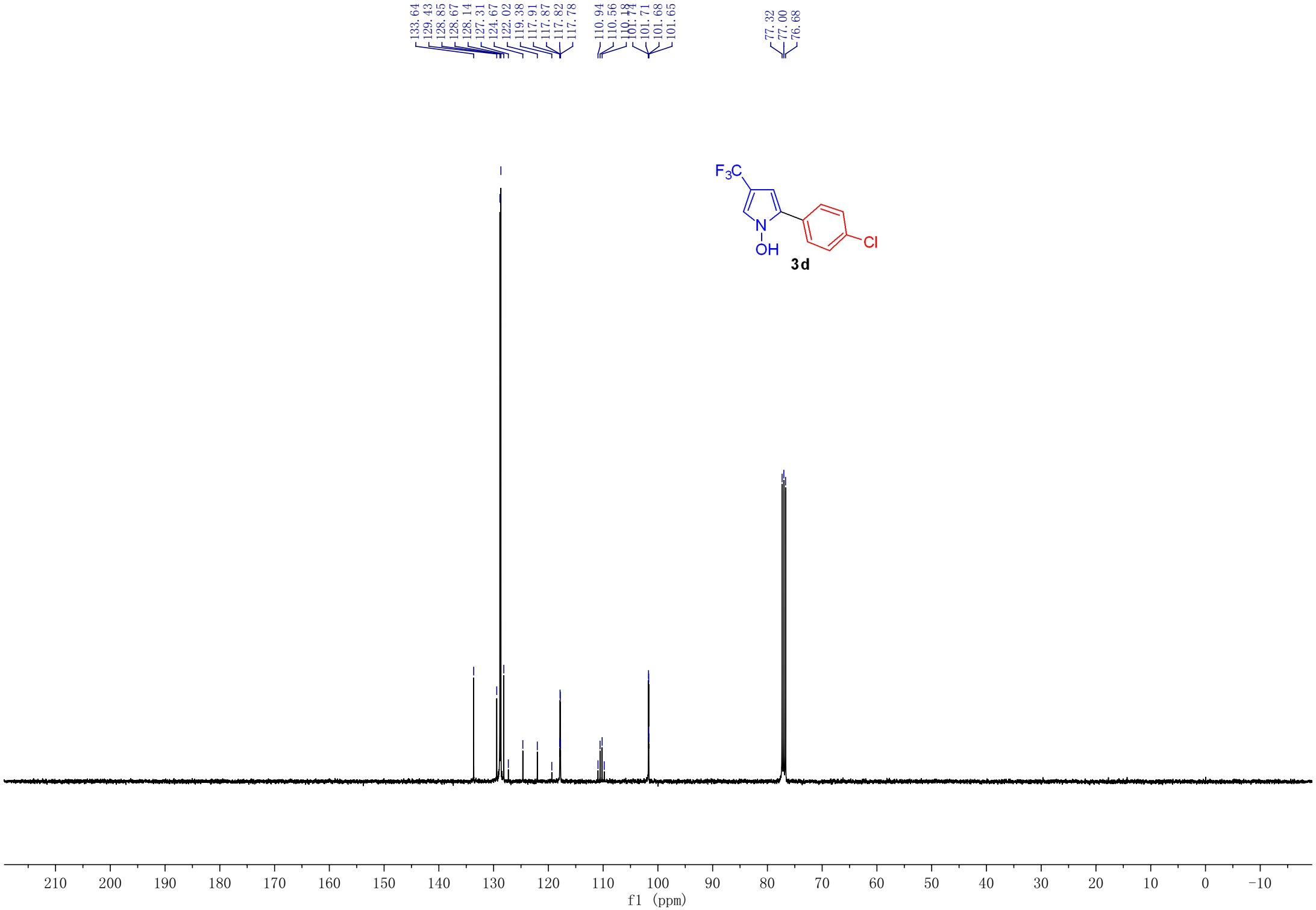

7.53
7.52
7.51
7.48
7.26
7.15
7.15
6.96
6.93
6.92
6.91
6.89
6.87
6.29
3.82
3.79
contaminated with
F3C
N
OH
OCH3
3c
F3C
N
O•
OCH3
2.02
0.99
0.50
2.34
1.00
1.60
1.39
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

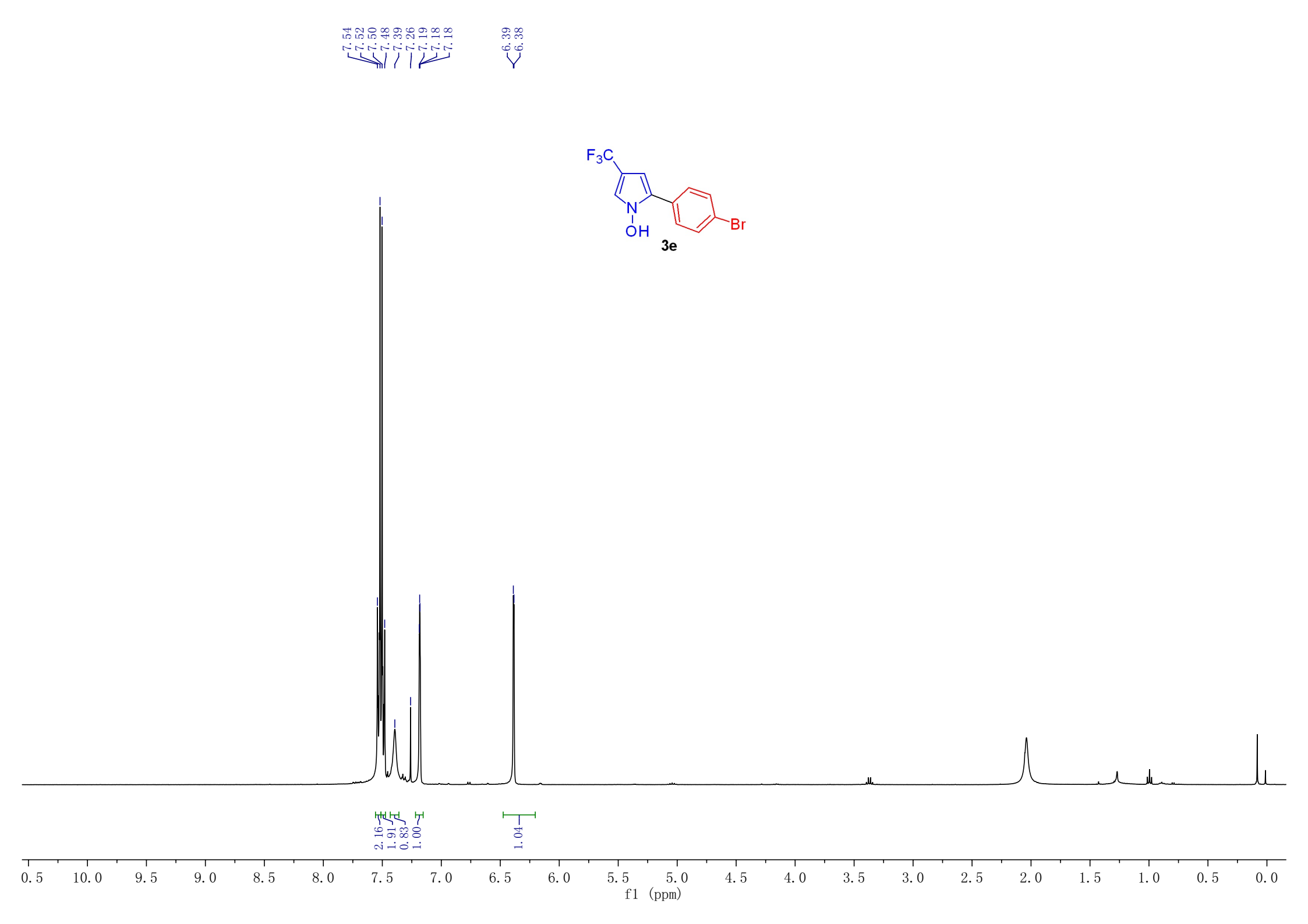

-57.46
-57.49
F3C
N
OH
OCH3
3c
contaminated with
F3C
N
O
OCH3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

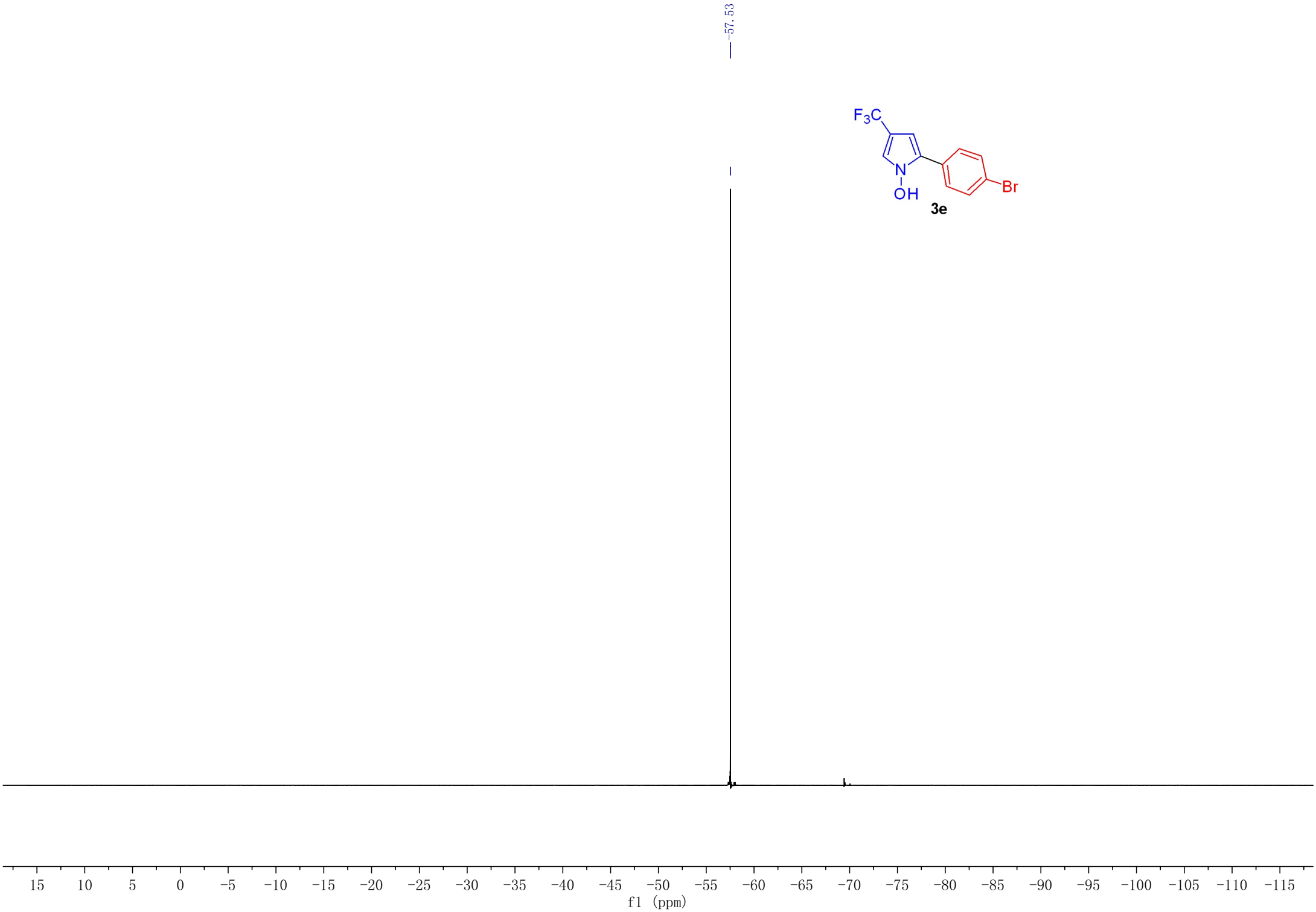

159.12
158.92
130.44
130.40
129.07
129.03
124.88
122.54
122.44
122.23
116.97
116.92
116.88
114.15
110.24
100.71
100.68
77.32
77.00
76.68
55.43
55.40
contaminated with
F3C
N
OH
OCH3
3c
F3C
N
O
OCH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

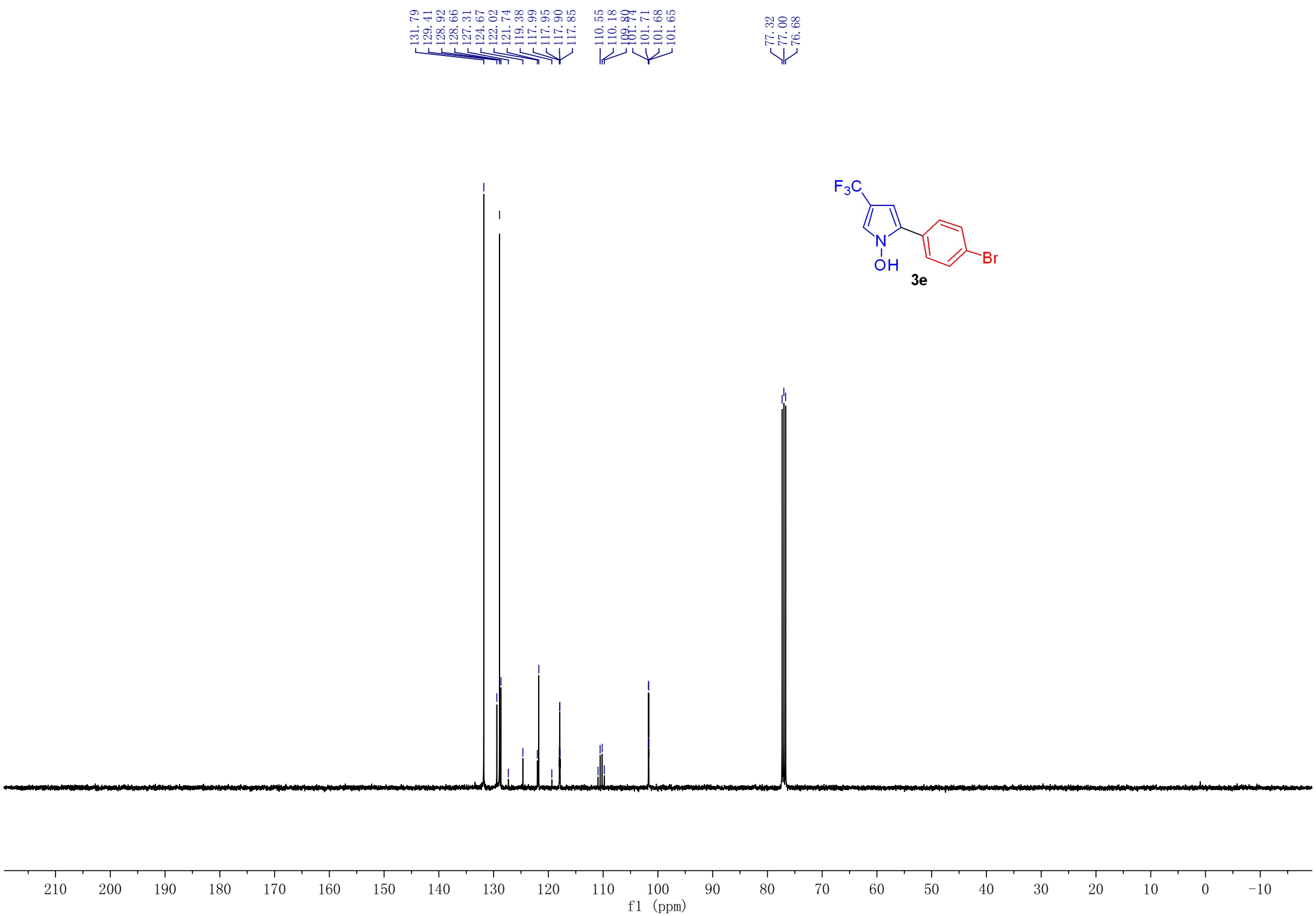

7.56
7.54
7.38
7.36
7.26
7.18
7.11
6.38
6.38
F3C
N
OH
Cl
3d
2.14
2.20
1.15
0.85
1.00
f1 (ppm)

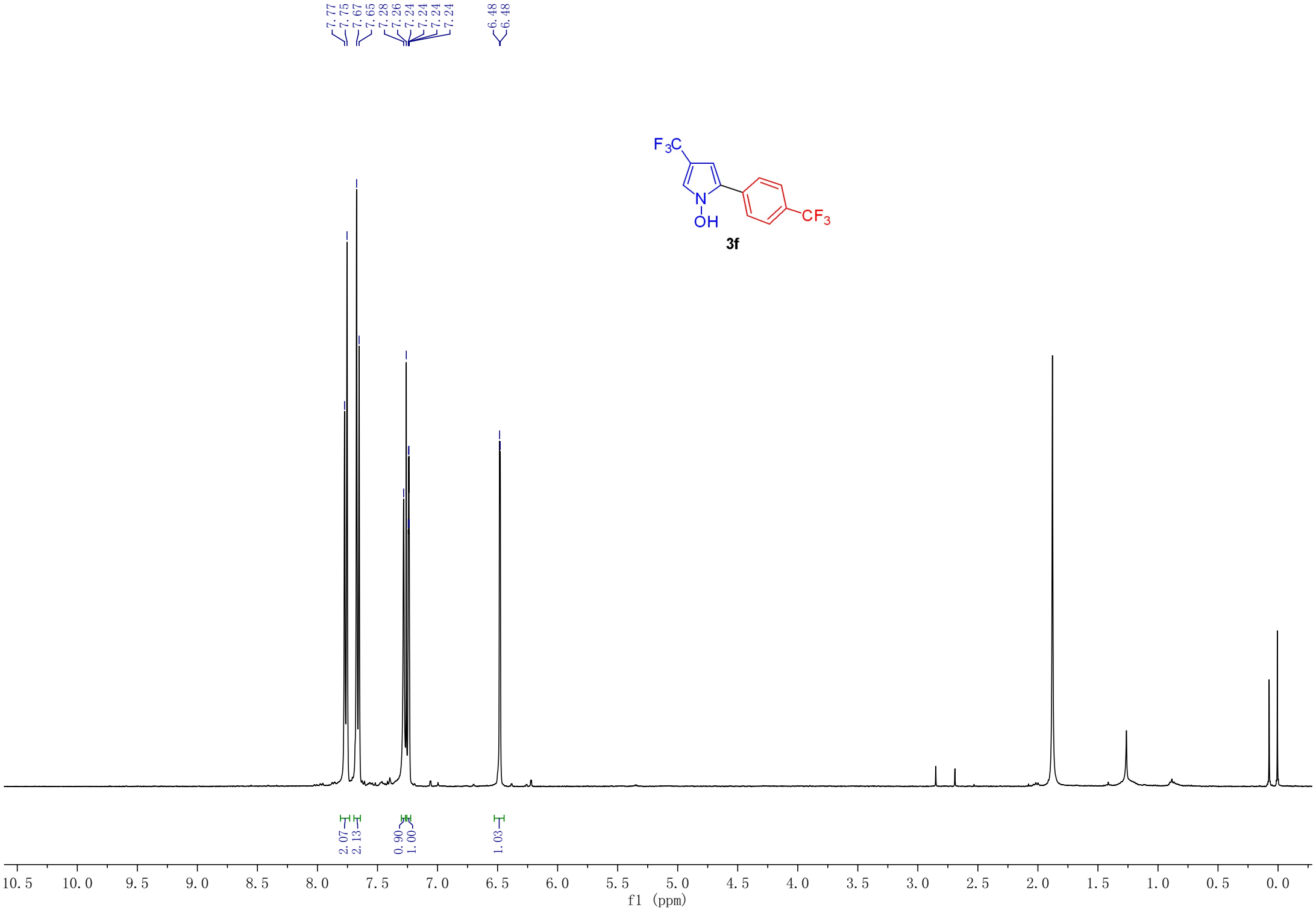

-57.54
F3C
N
OH
Cl
3d
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

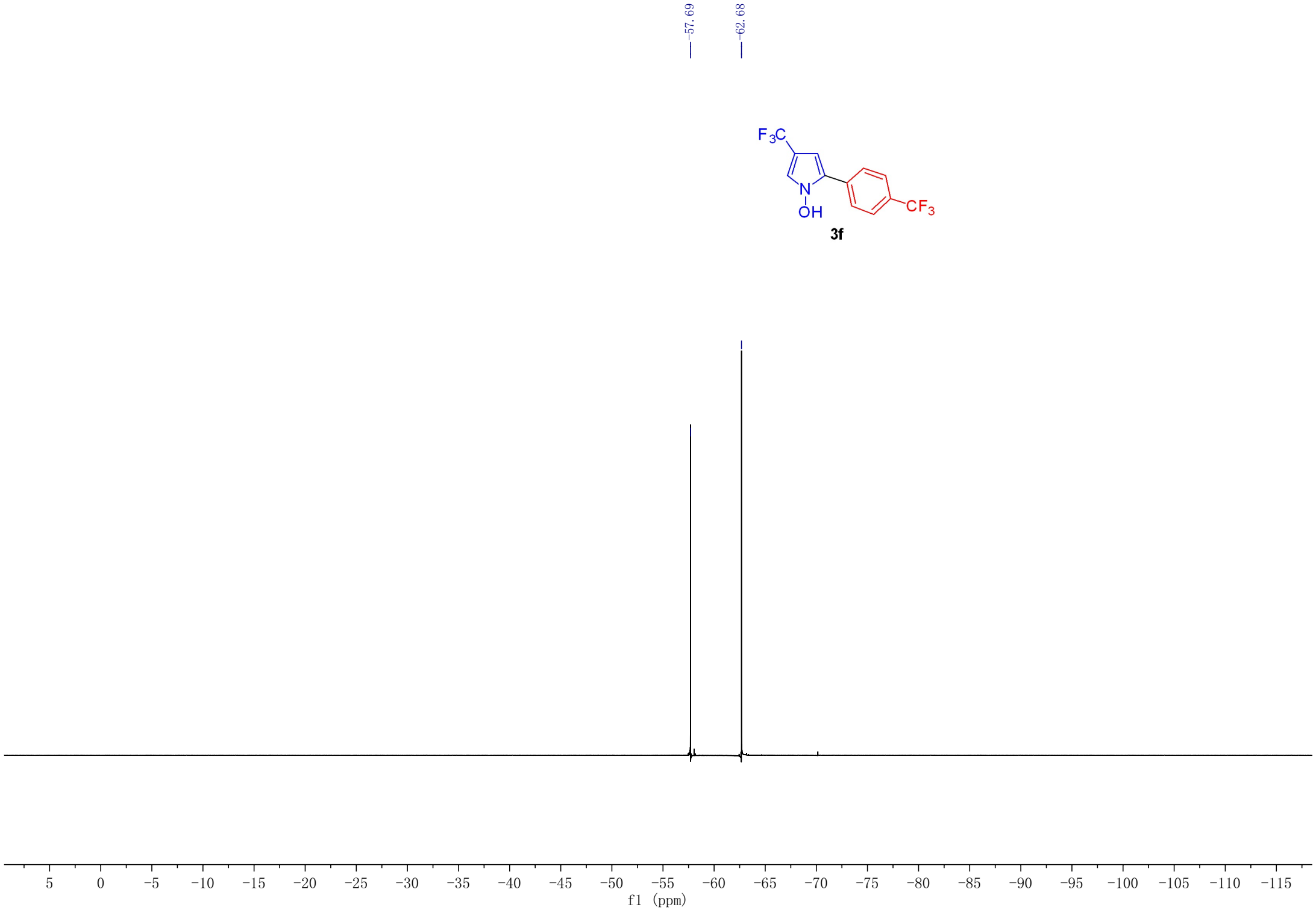

133.64
129.43
128.85
128.67
128.14
127.31
124.67
122.02
119.38
117.91
117.87
117.82
117.78
110.94
110.56
101.74
101.71
101.68
101.65
77.32
77.00
76.68
F3C
N
OH
Cl
3d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

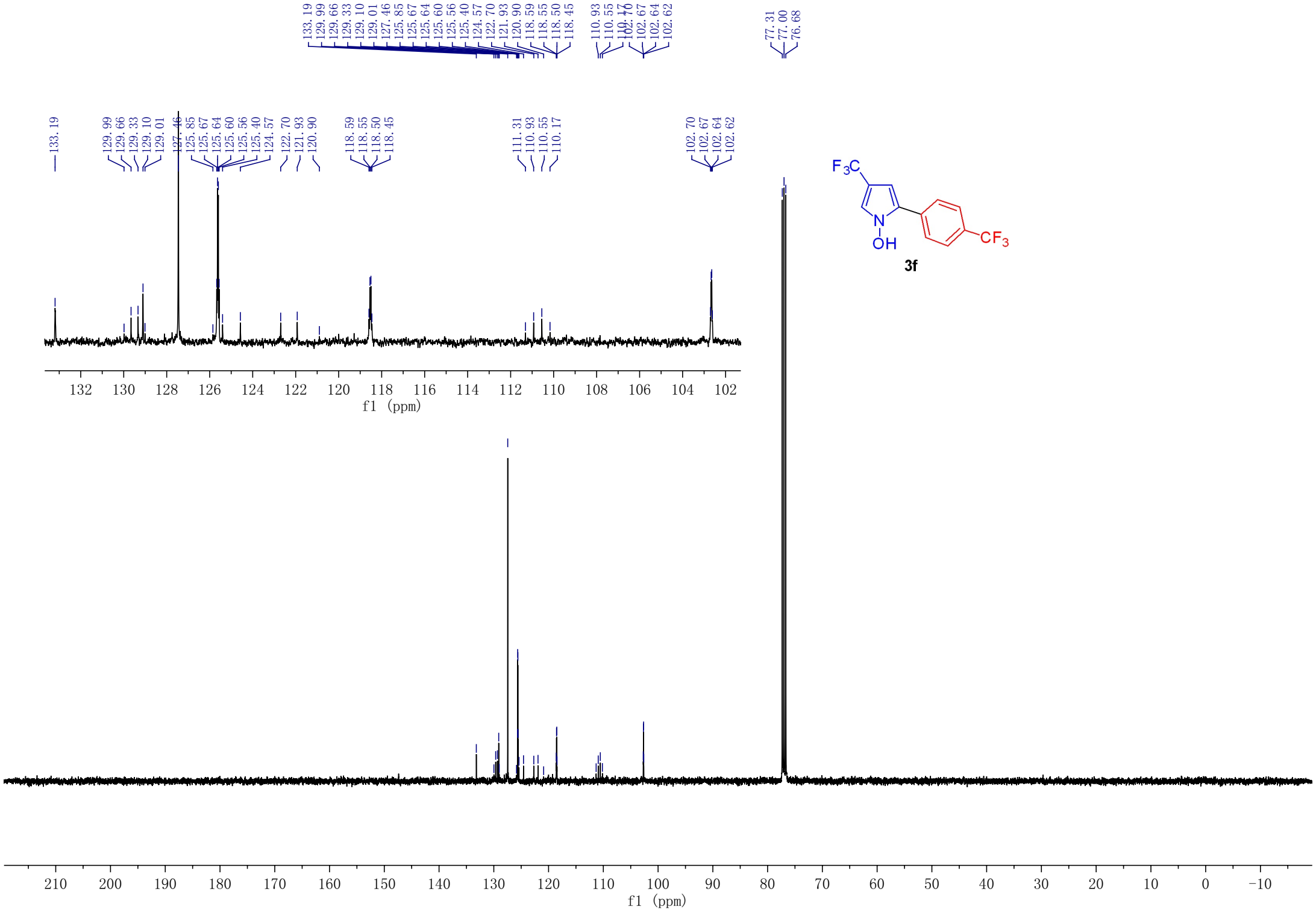

7.54
7.52
7.50
7.48
7.39
7.26
7.19
7.18
7.18
6.39
6.38
F3C
N
OH
Br
3e
2.16
1.91
0.83
1.00
1.04
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

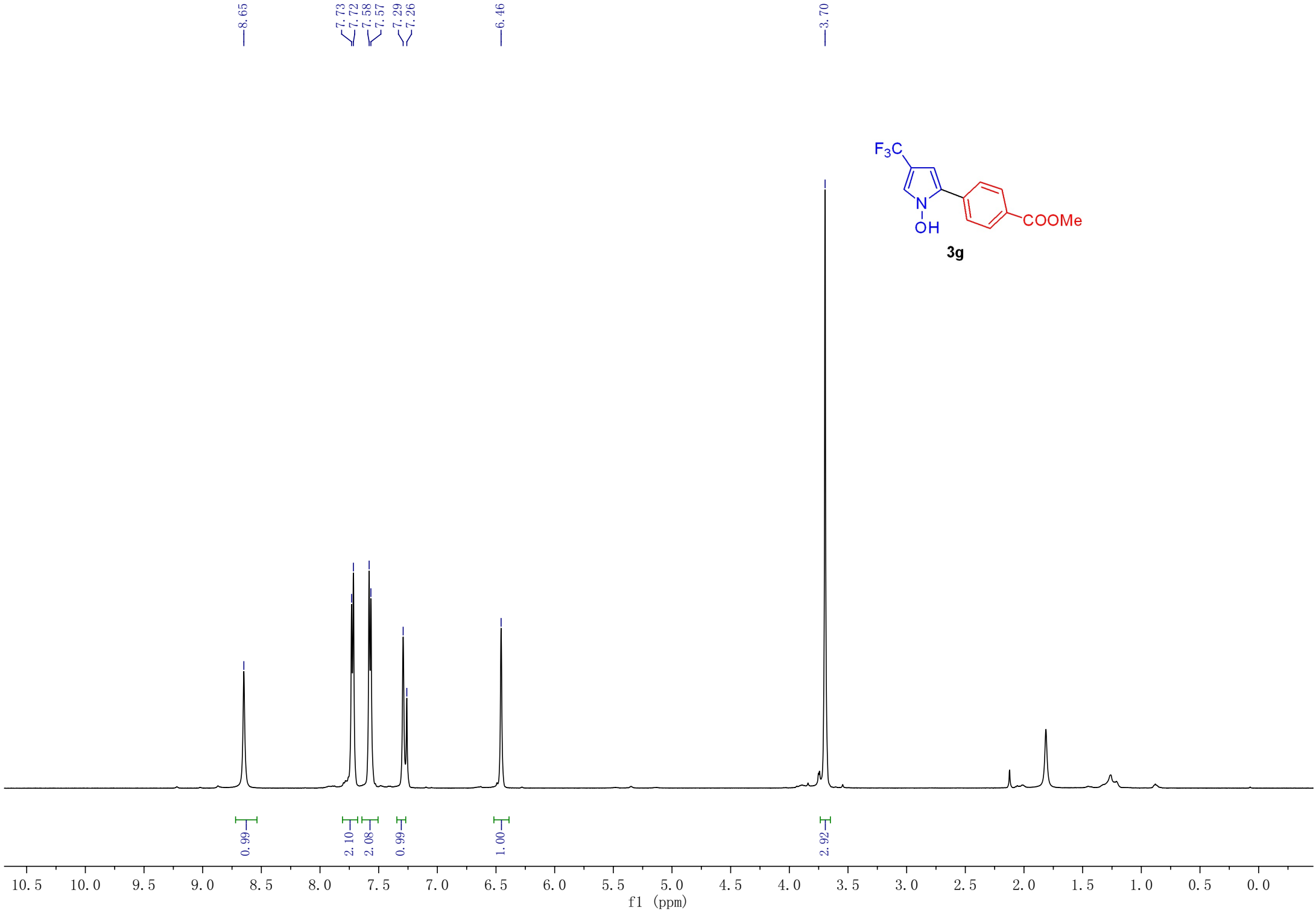

-57.53
F3C
N
OH
Br
3e
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
f1 (ppm)

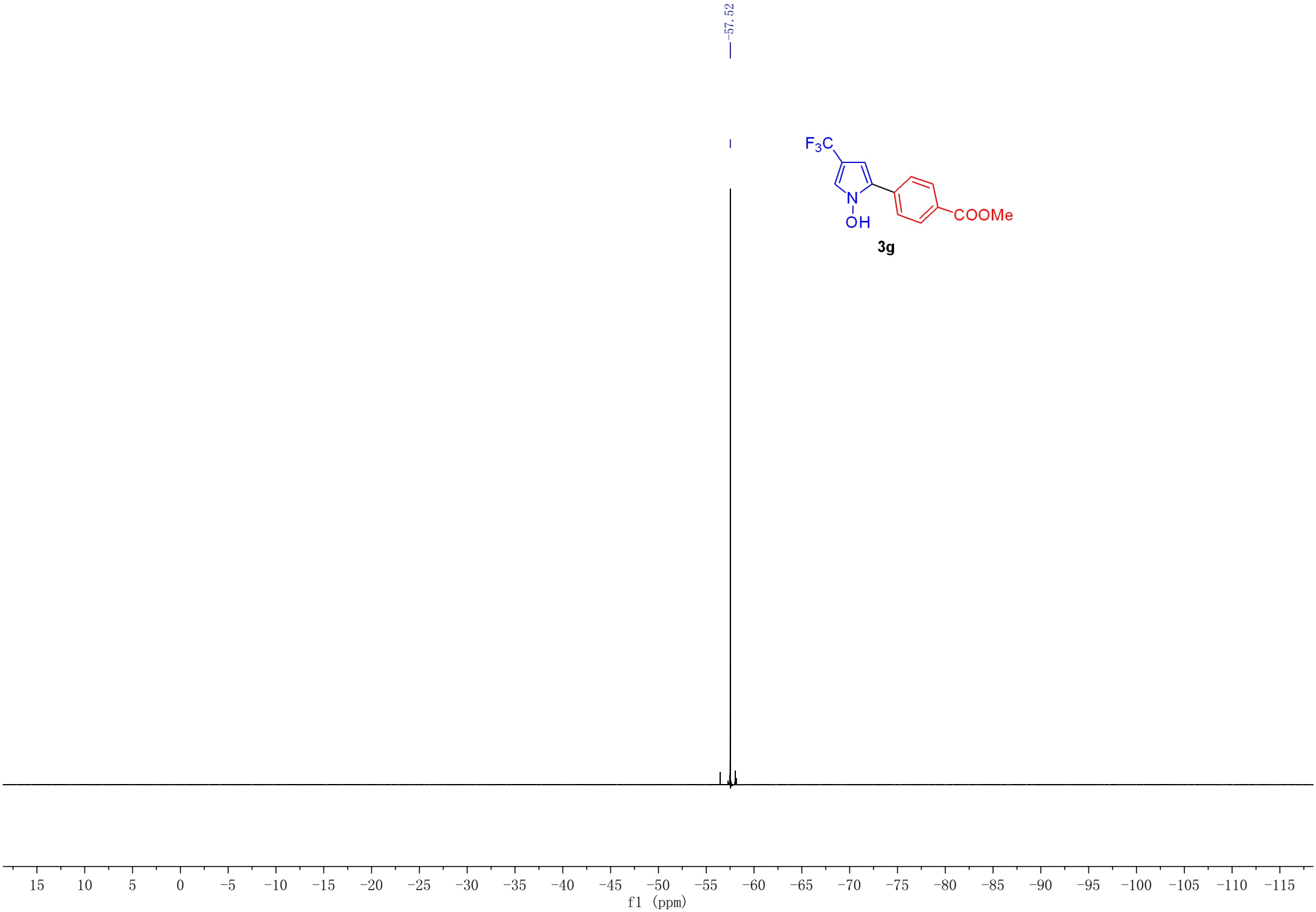

131.79
129.41
128.92
128.66
127.31
124.67
122.02
121.74
119.38
117.99
117.95
117.90
117.85
110.55
110.18
101.71
101.68
101.65
77.32
77.00
76.68
F3C
N
OH
Br
3e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

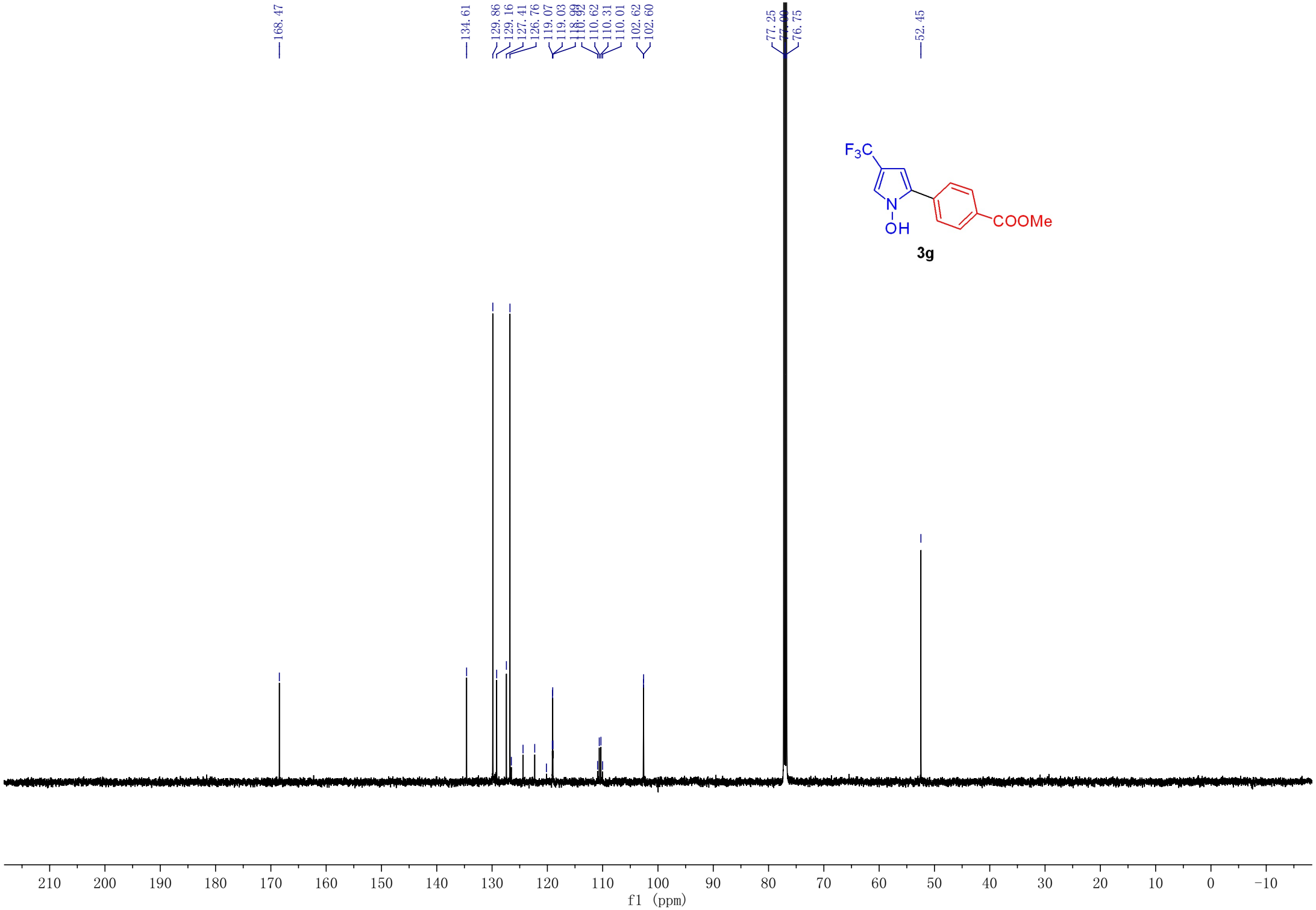

7.77
7.75
7.67
7.65
7.28
7.26
7.24
7.24
7.24
7.24
6.48
6.48
F3C
N
OH
CF3
3f
2.07
2.13
0.90
1.00
1.03
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

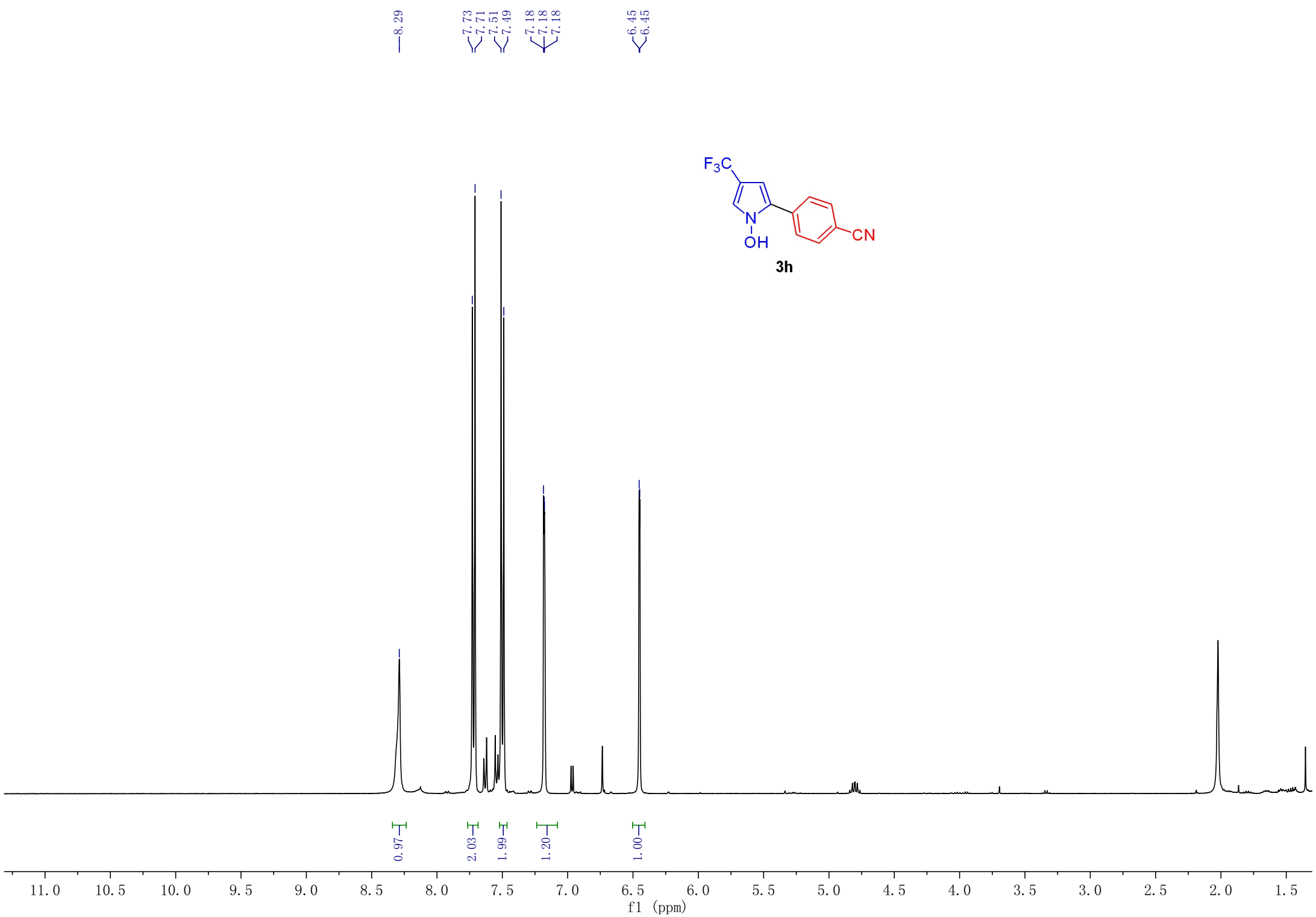

-57.69
-62.68
F3C
N
OH
CF3
3f
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
f1 (ppm)

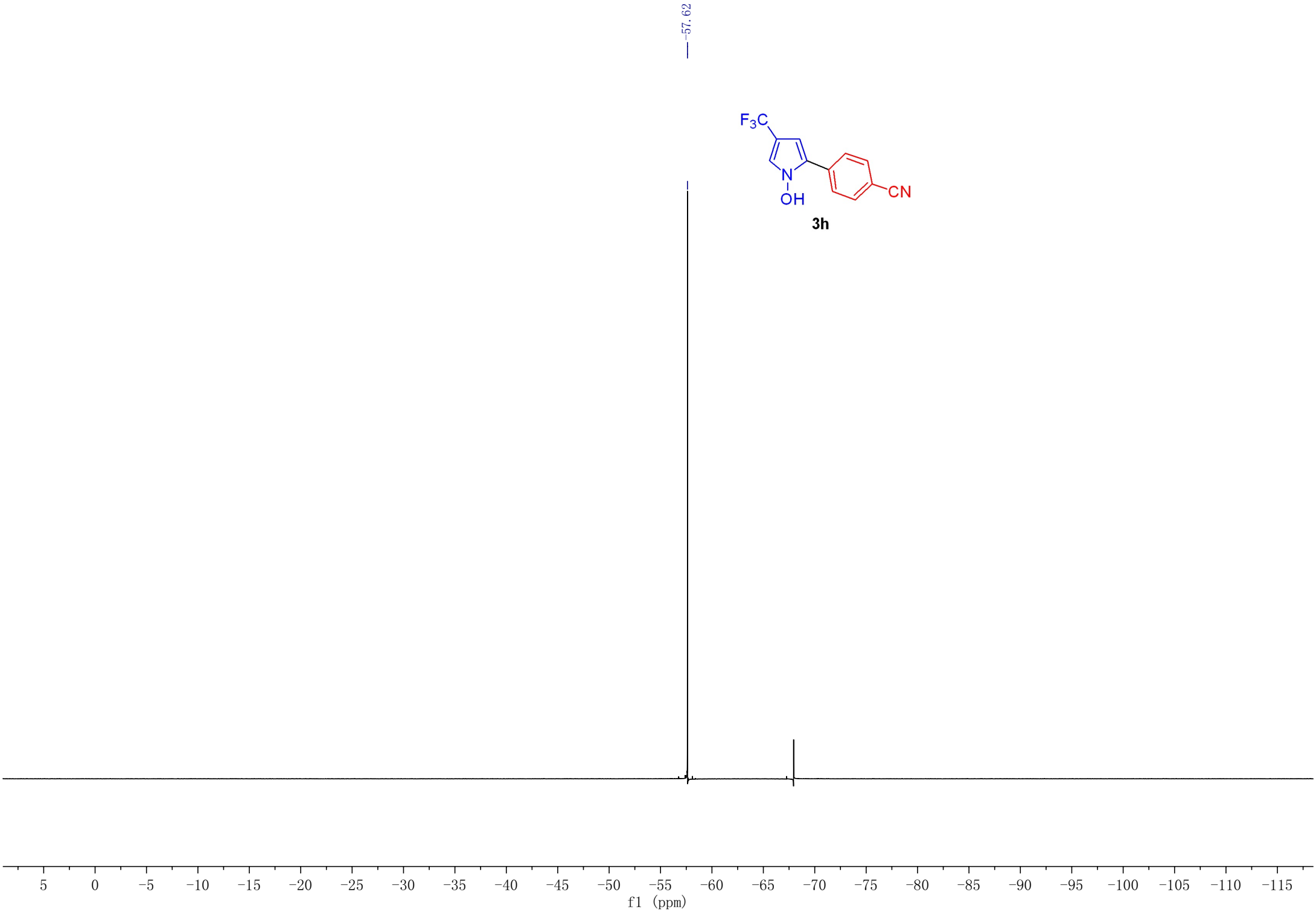

133.19
129.99
129.66
129.33
129.10
129.01
127.46
125.85
125.67
125.64
125.60
125.56
125.40
124.57
122.70
121.93
120.90
118.59
118.55
118.50
118.45
111.31
110.93
110.55
110.17
102.70
102.67
102.64
102.62
77.31
77.00
76.68
F3C
N
OH
CF3
3f
f1 (ppm)


8.65
7.73
7.72
7.58
7.57
7.29
7.26
6.46
3.70
F3C
N
OH
COOMe
3g
0.99
2.10
2.08
0.99
1.00
2.92
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)


-57.52
F3C
N
OH
COOMe
3g
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
f1 (ppm)


168.47
134.61
129.86
129.16
127.41
126.76
119.07
119.03
110.62
110.31
110.01
102.62
102.60
77.25
76.75
52.45
F3C
N
OH
COOMe
3g
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)


8.29
7.73
7.71
7.51
7.49
7.18
7.18
7.18
6.45
6.45
F3C
N
OH
CN
3h
0.97
2.03
1.99
1.20
1.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)


-57.62
F3C
N
OH
CN
3h
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
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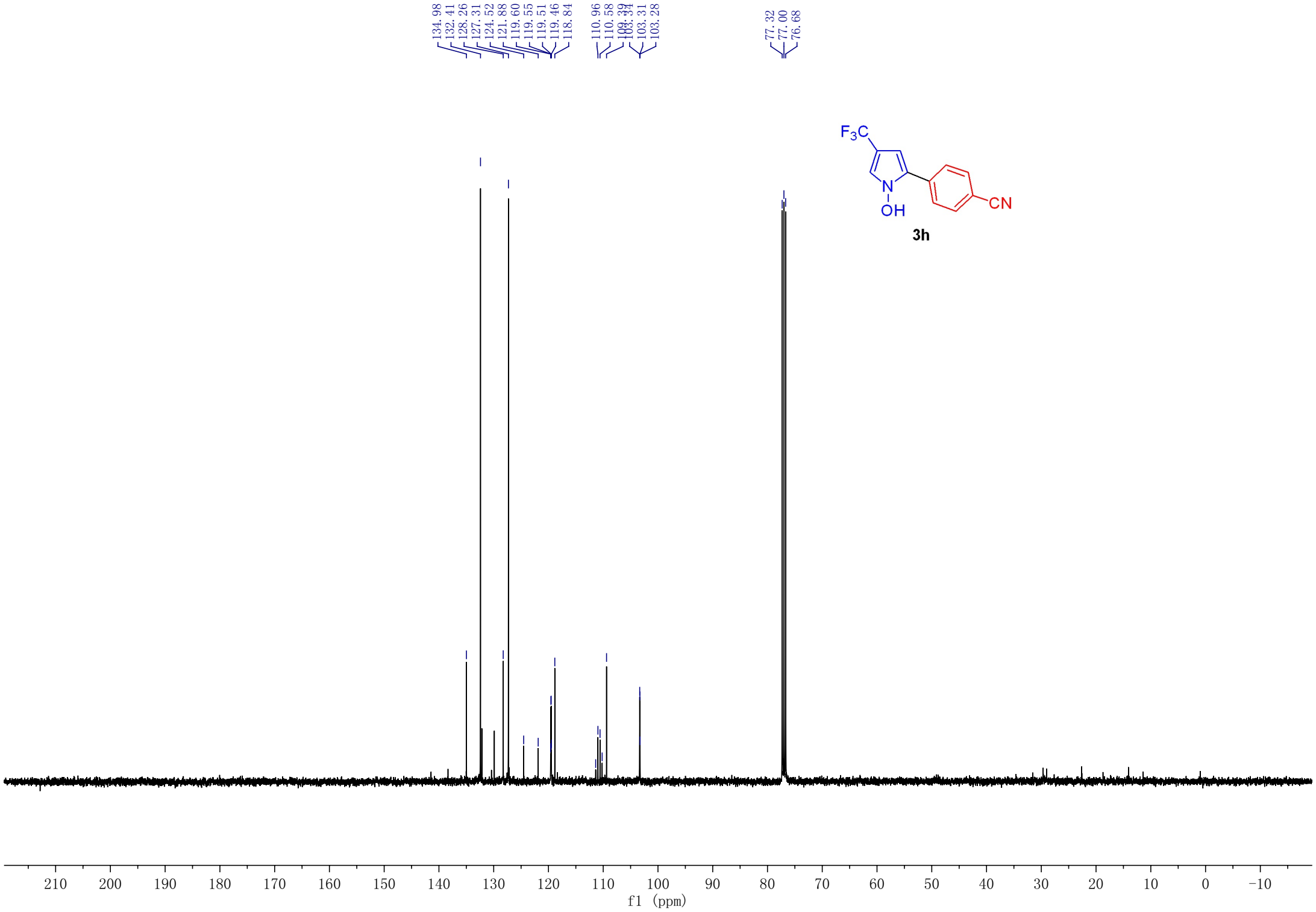
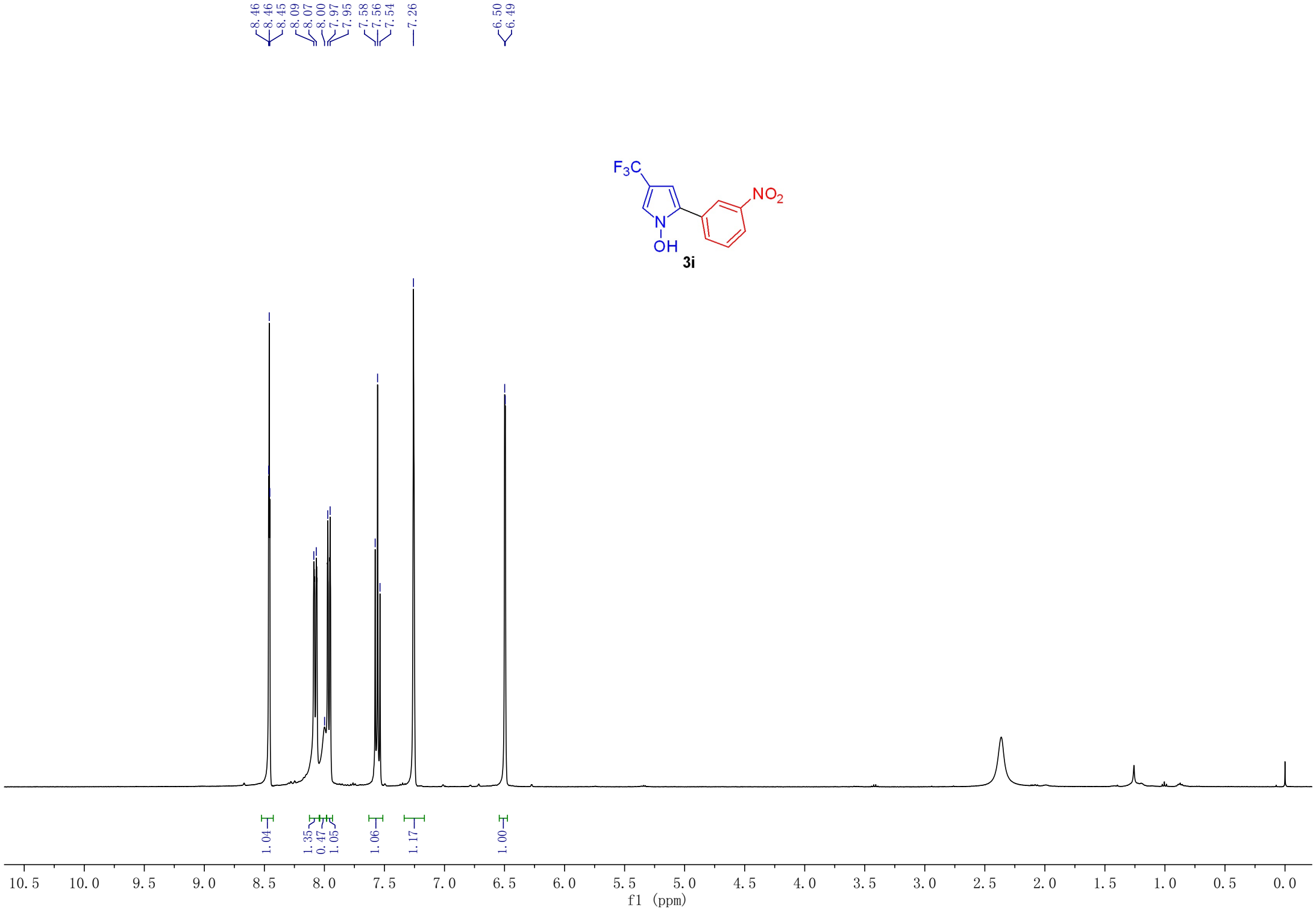
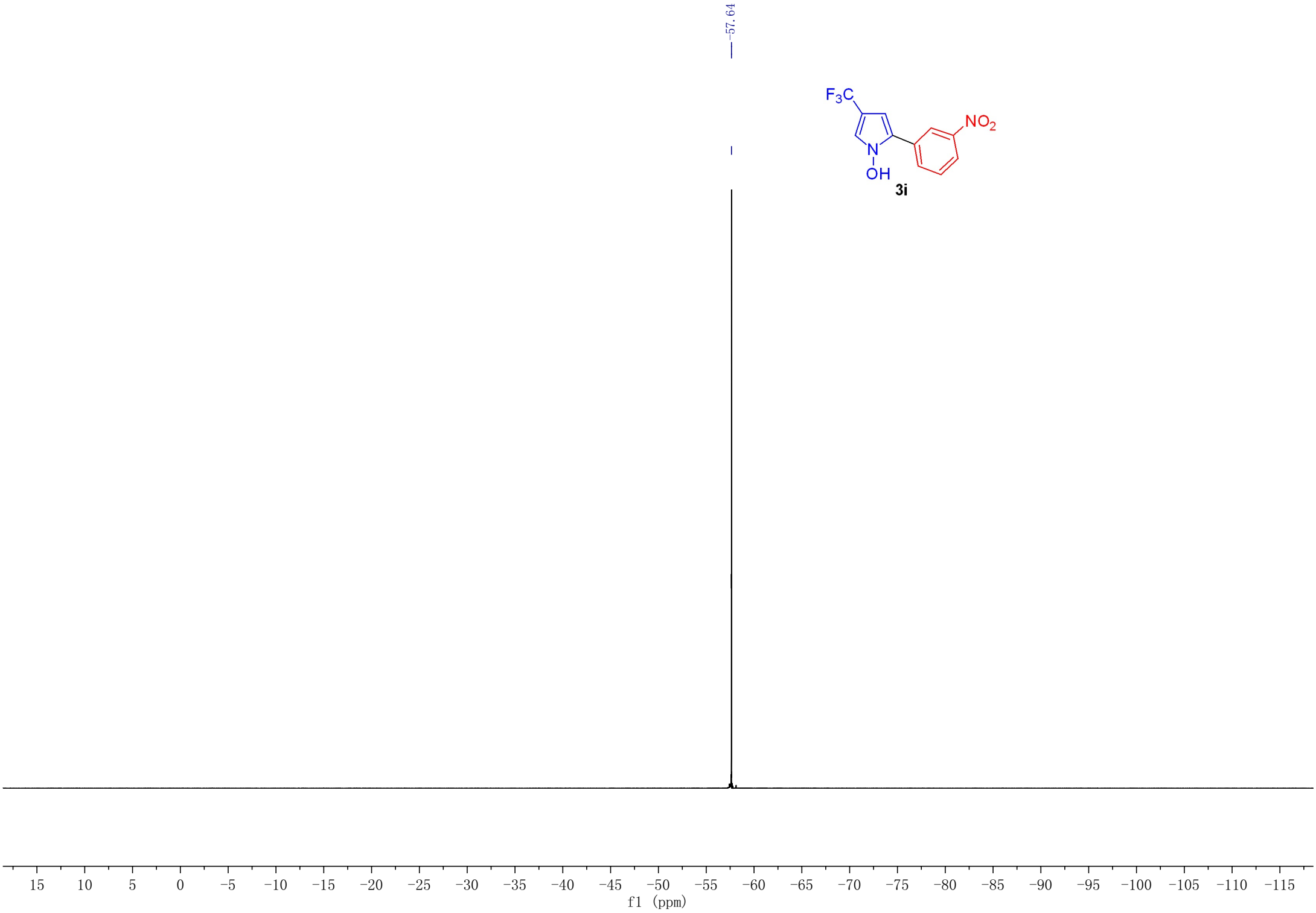
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
f1 (ppm)


134.98
132.41
128.26
127.31
124.52
121.88
119.60
119.55
119.51
119.46
118.84
110.96
110.58
103.31
103.28
77.32
77.00
76.68
F3C
N
OH
CN
3h
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)


8.46
8.46
8.45
8.09
8.07
8.00
7.97
7.95
7.58
7.56
7.54
7.26
6.50
6.49
F3C
NO2
N
OH
3i
1.04
1.35
0.47
1.05
1.06
1.17
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-57.64
F3C
NO2
N
OH
3i
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
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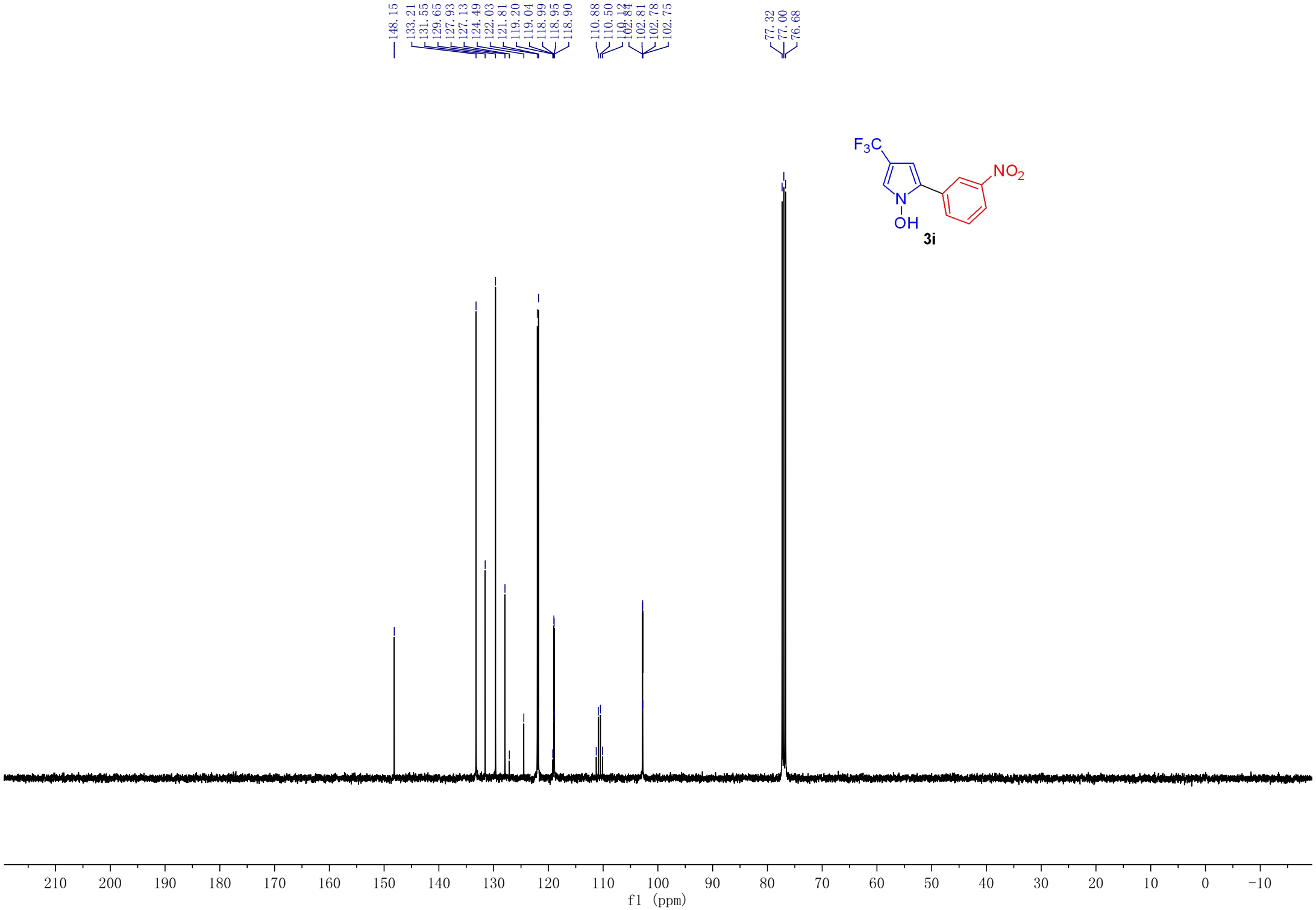
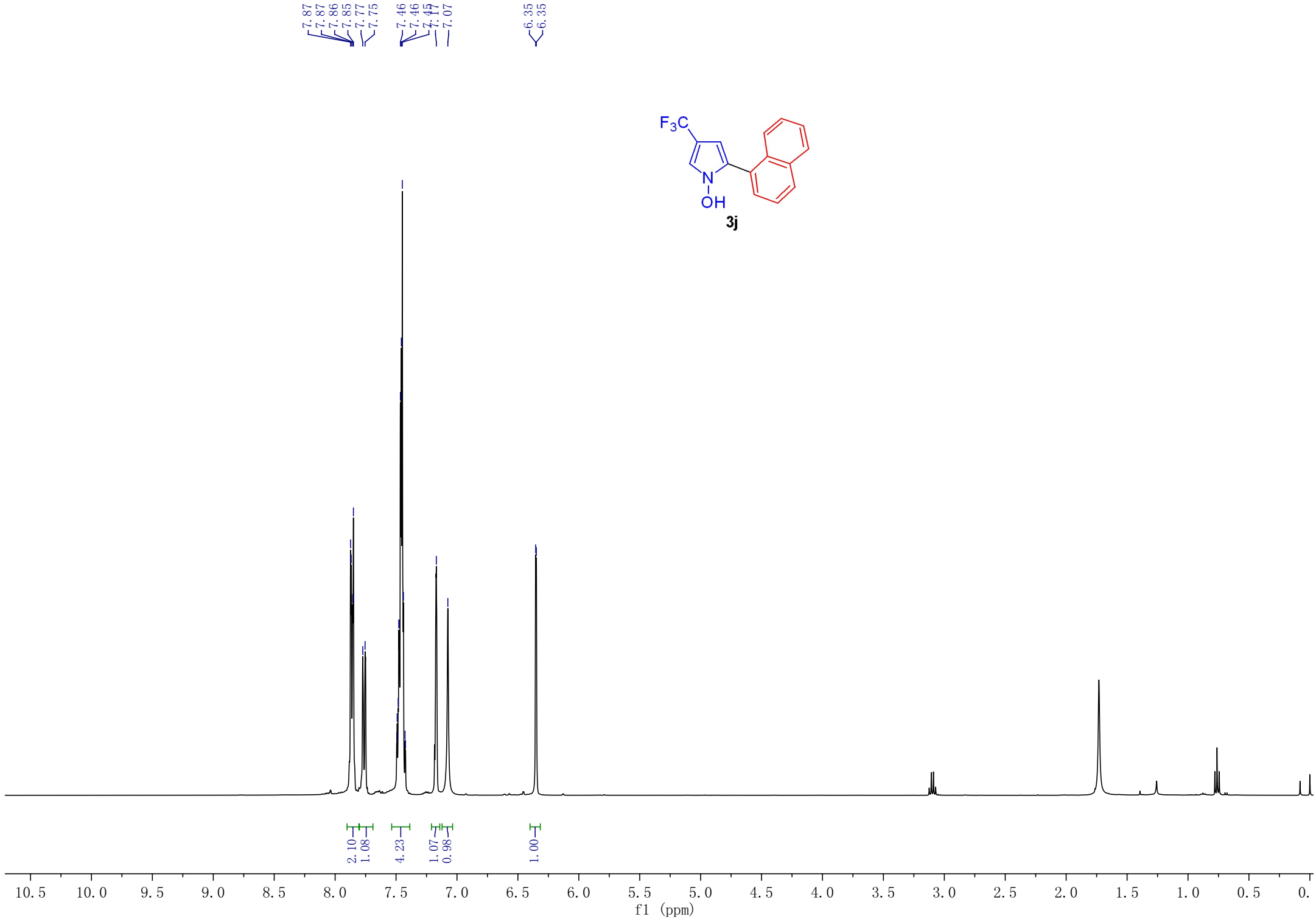
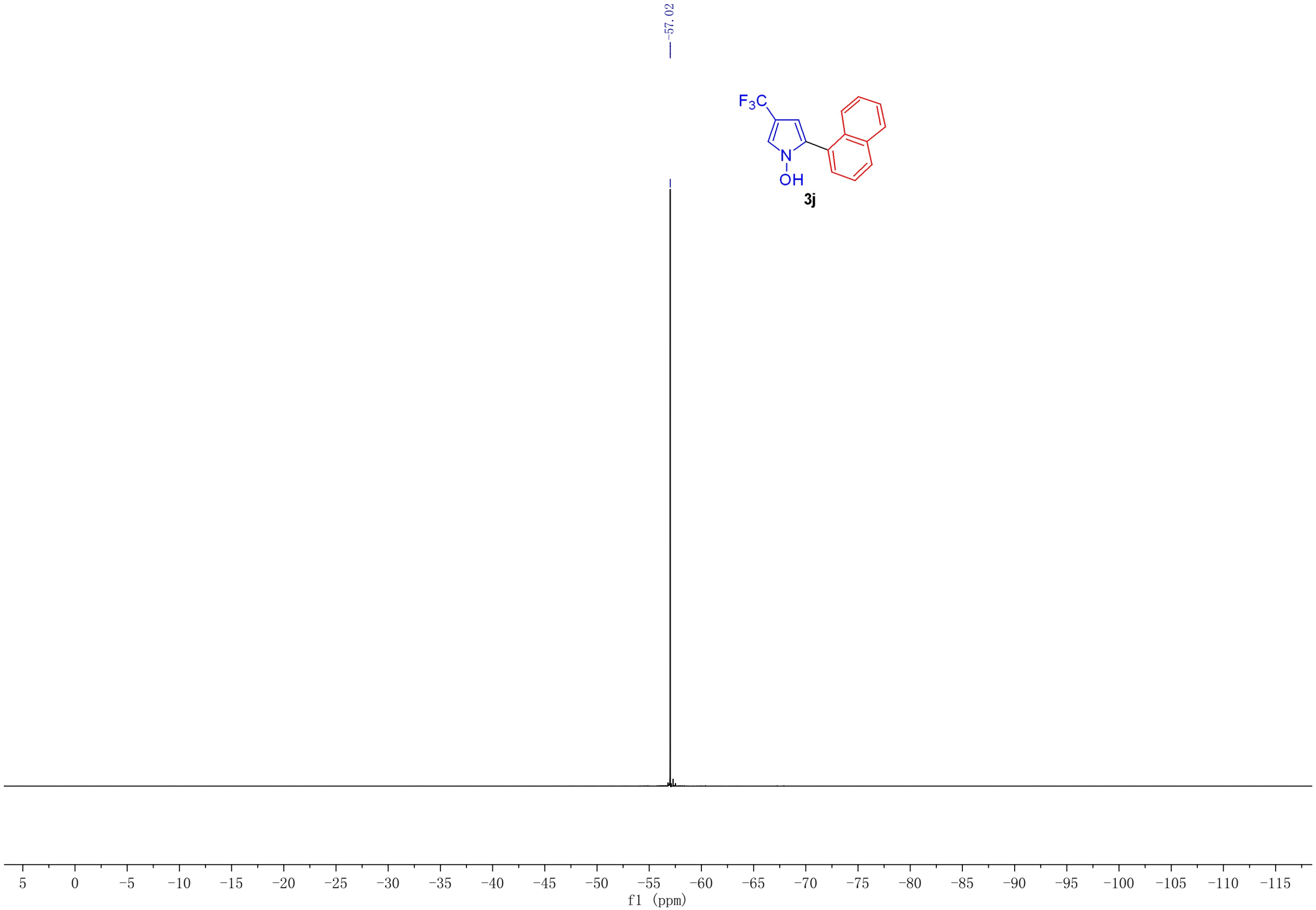
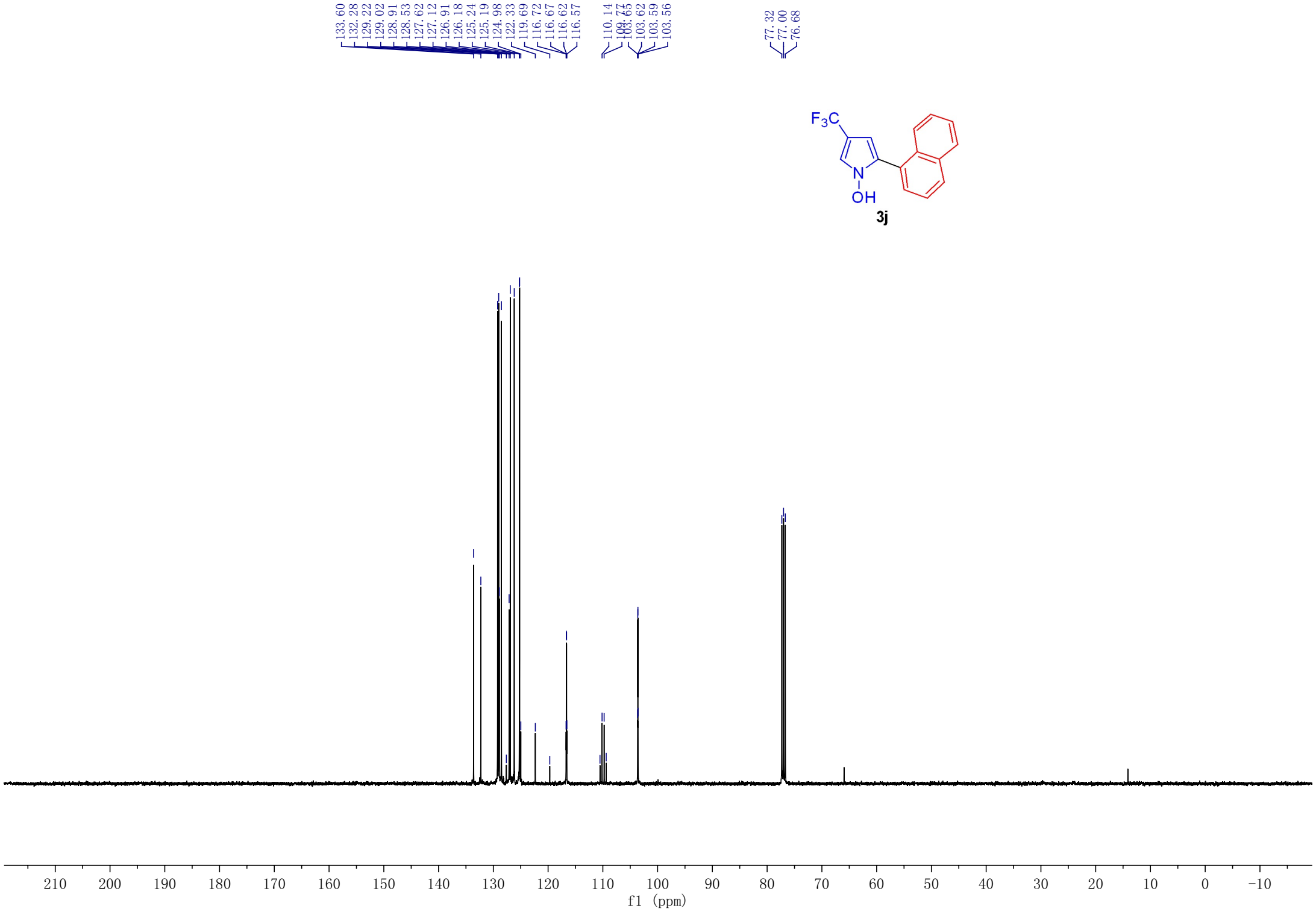
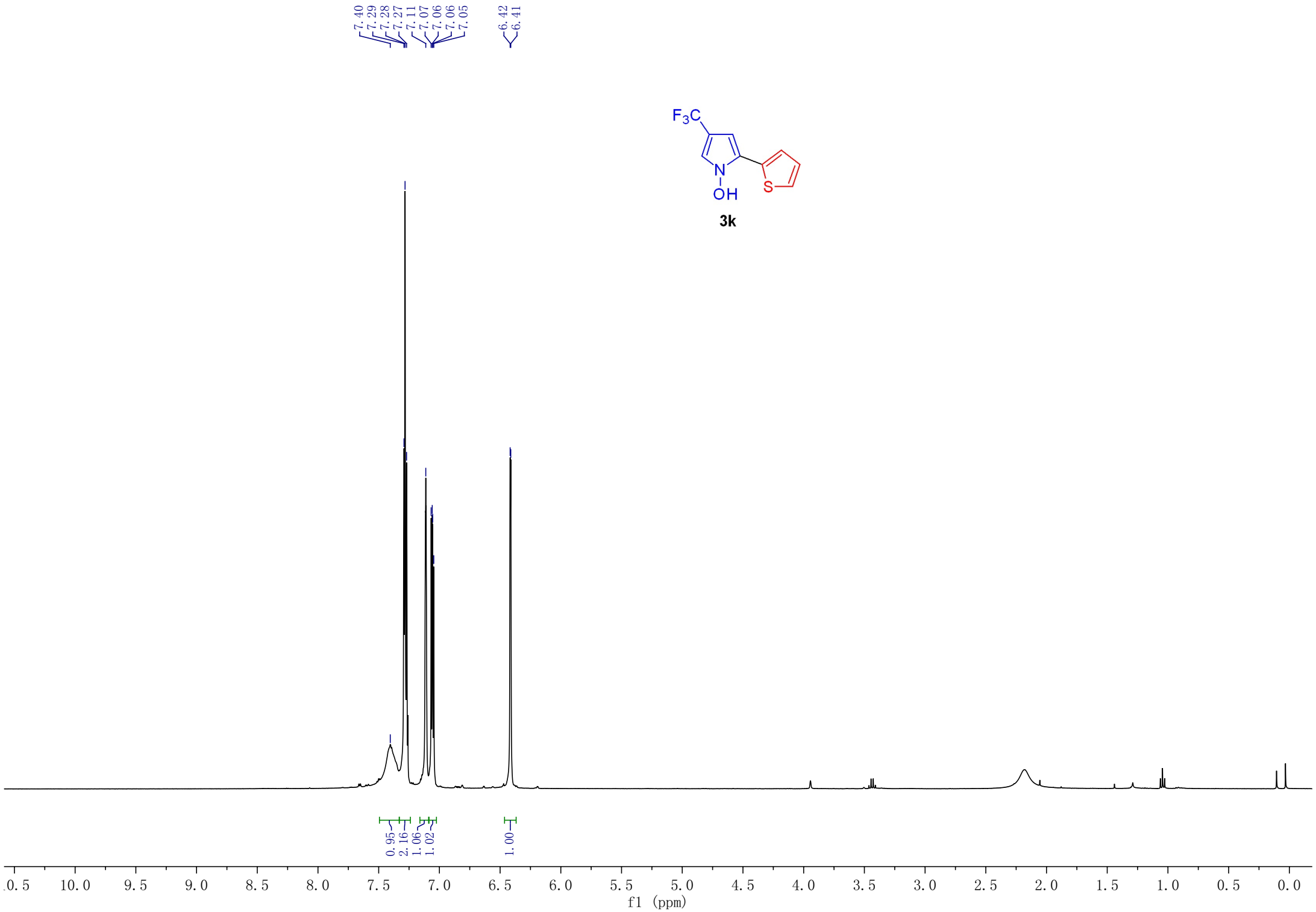
-90
-95
-100
-105
-110
-115
f1 (ppm)

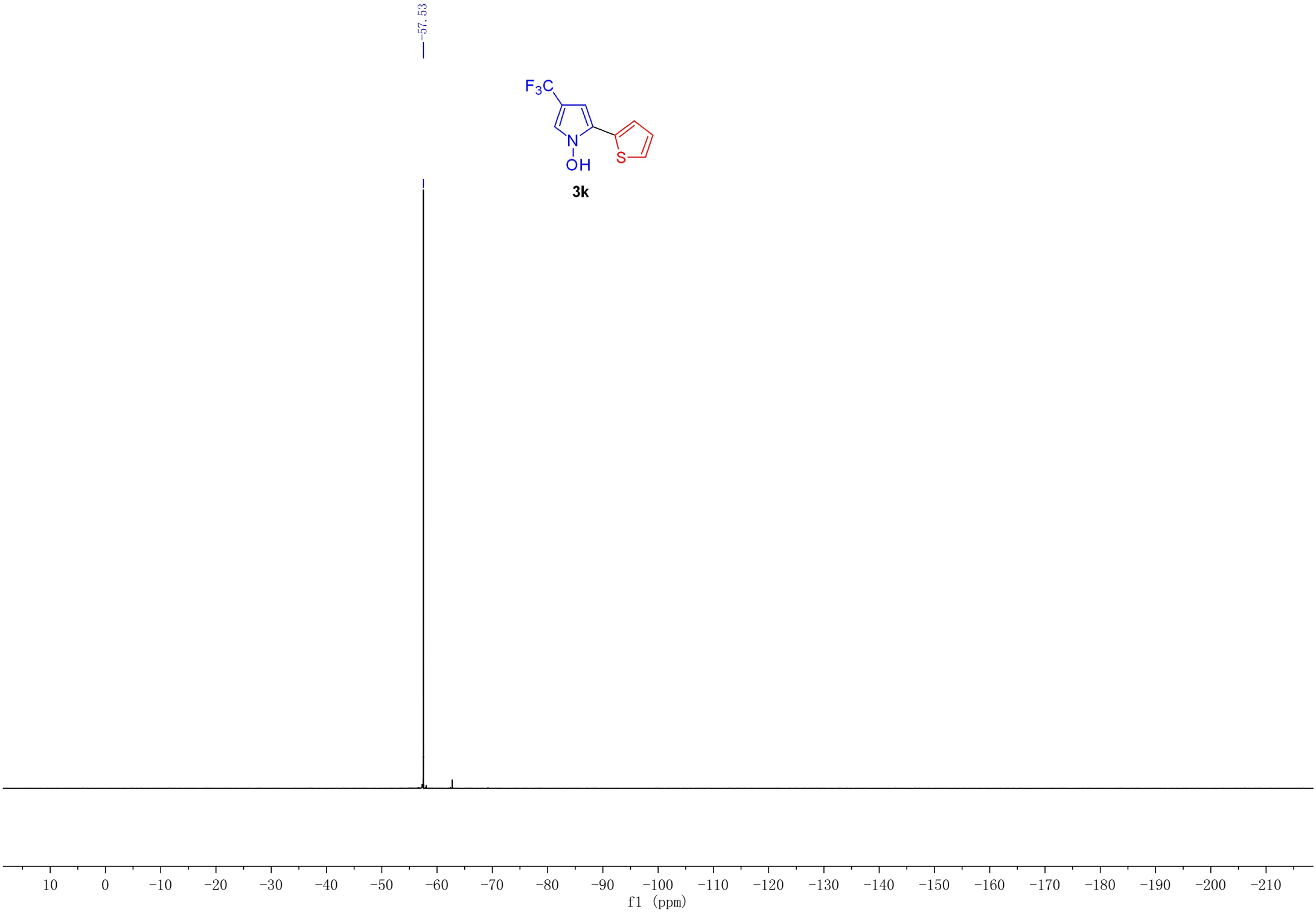

148.15
133.21
131.55
129.65
127.93
127.13
124.49
122.03
121.81
119.20
119.04
118.99
118.95
118.90
110.88
110.50
102.81
102.78
102.75
77.32
77.00
76.68
F3C
NO2
N
OH
3i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

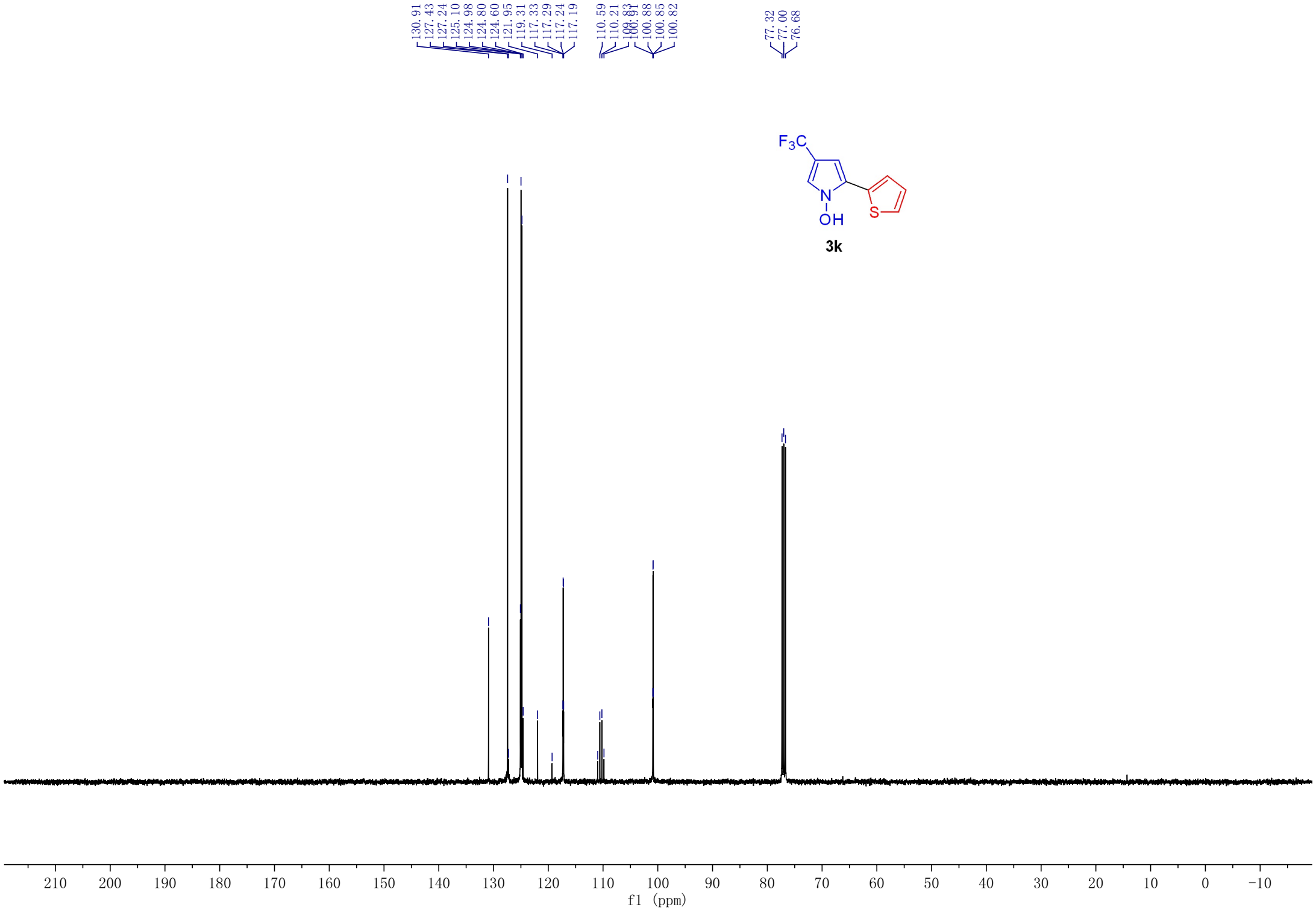

7.87
7.87
7.86
7.85
7.77
7.75
7.46
7.46
7.45
7.07
6.35
6.35
F3C
N
OH
3j
2.10
1.08
4.23
1.07
0.98
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

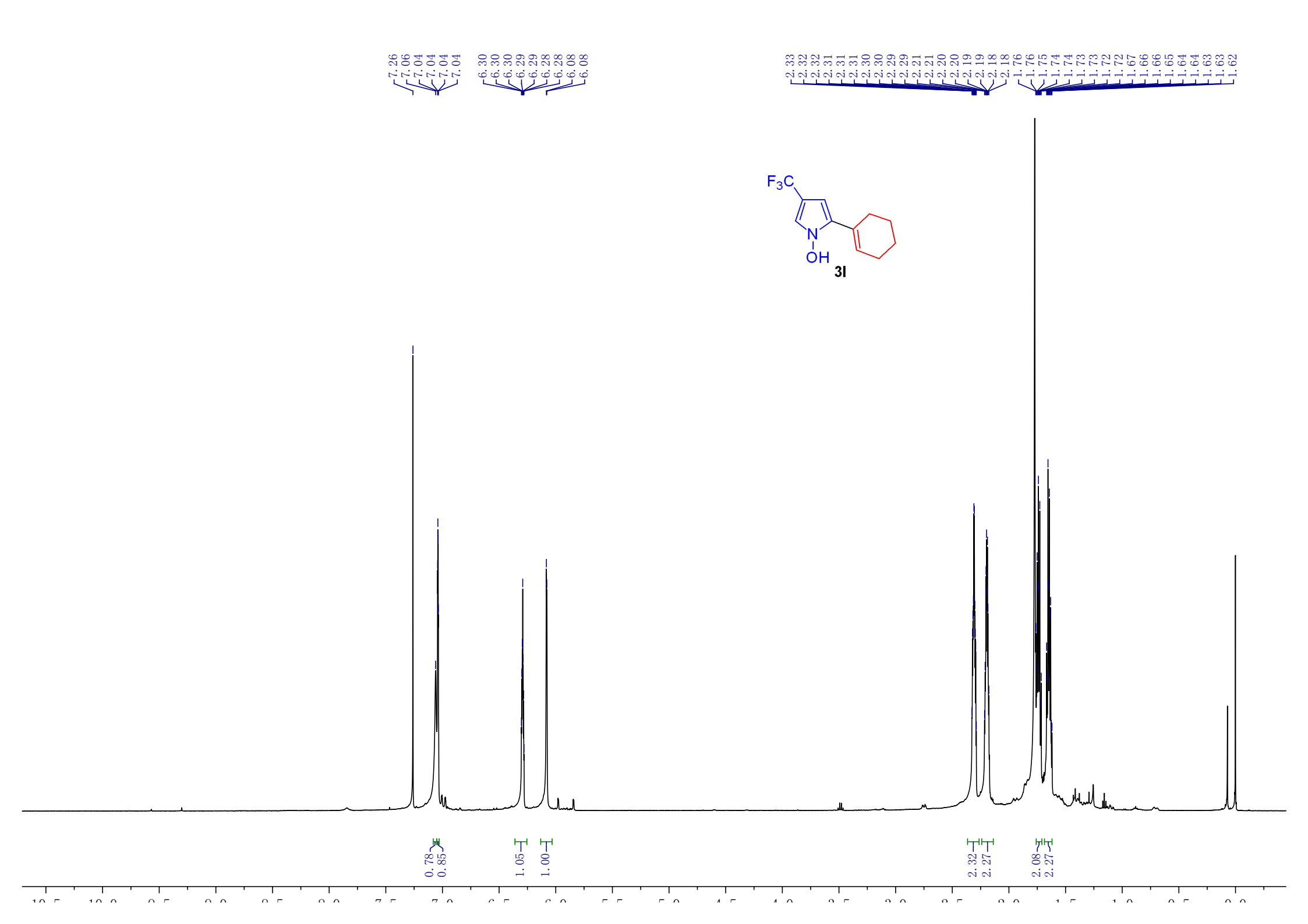

-57.02
F3C
N
OH
3j
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
f1 (ppm)

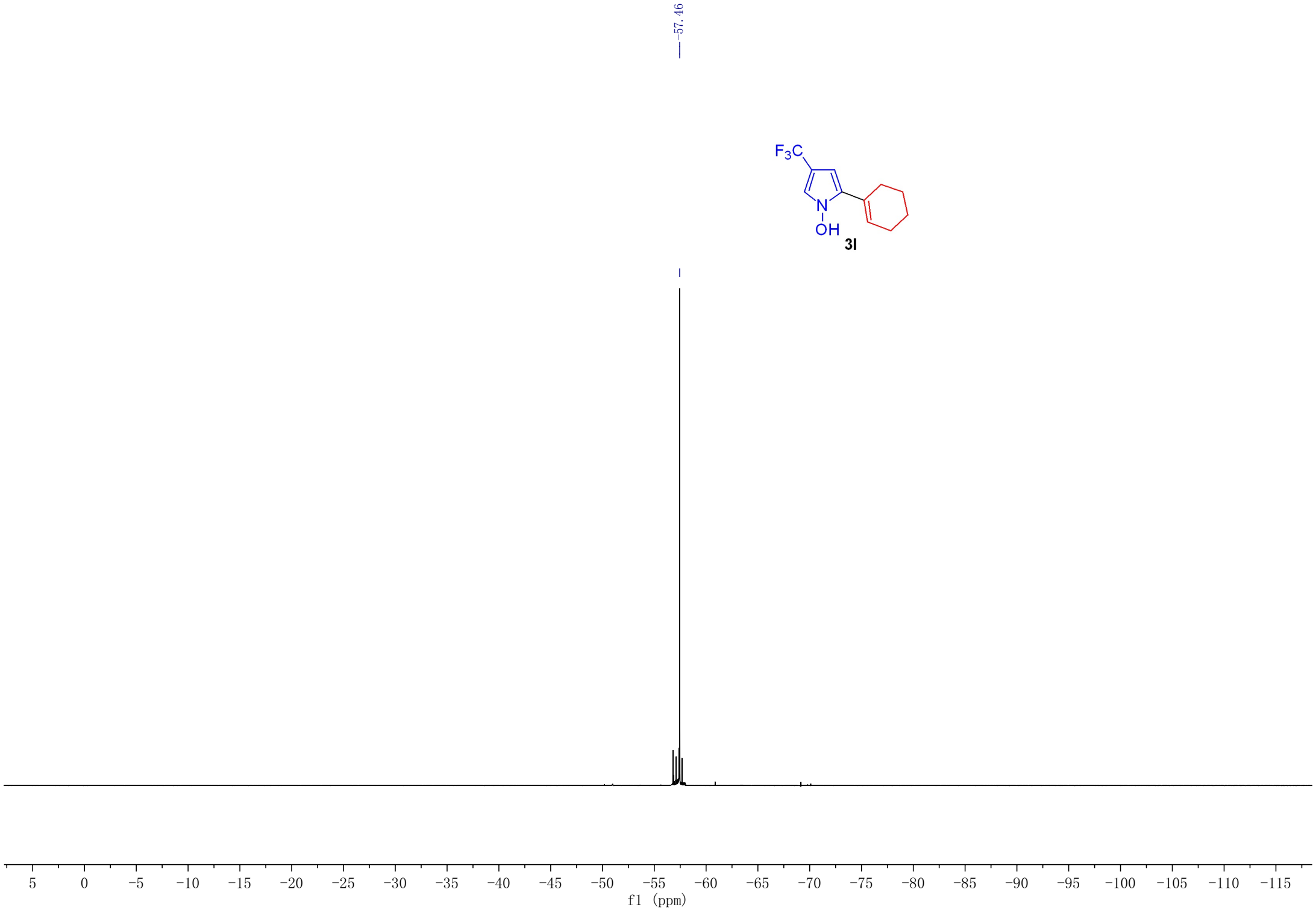

133.60
132.28
129.22
129.02
128.91
128.53
127.62
127.12
126.91
126.18
125.24
125.19
124.98
122.33
119.69
116.72
116.67
116.62
116.57
110.14
103.62
103.59
103.56
77.32
77.00
76.68
F3C
N
OH
3j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.40
7.29
7.28
7.27
7.11
7.07
7.06
7.06
7.05
6.42
6.41
F3C
N
OH
S
3k
0.95
2.16
1.06
1.02
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-57.53
F3C
N
OH
S
3k
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


130.91
127.43
127.24
125.10
124.98
124.80
124.60
121.95
119.31
117.33
117.29
117.24
117.19
110.59
110.21
100.88
100.85
100.82
77.32
77.00
76.68
F3C
N
OH
S
3k
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)


7.26
7.06
7.04
7.04
7.04
7.04
6.30
6.30
6.30
6.29
6.29
6.28
6.28
6.08
6.08
2.33
2.32
2.32
2.31
2.31
2.31
2.30
2.30
2.29
2.29
2.21
2.20
2.20
2.19
2.19
2.18
2.18
1.76
1.76
1.75
1.74
1.74
1.73
1.73
1.72
1.72
1.67
1.66
1.66
1.65
1.64
1.64
1.63
1.63
1.62
F3C
N
OH
3l
0.78
0.85
1.05
1.00
2.32
2.27
2.08
2.27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F3C
N
OH
3l
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
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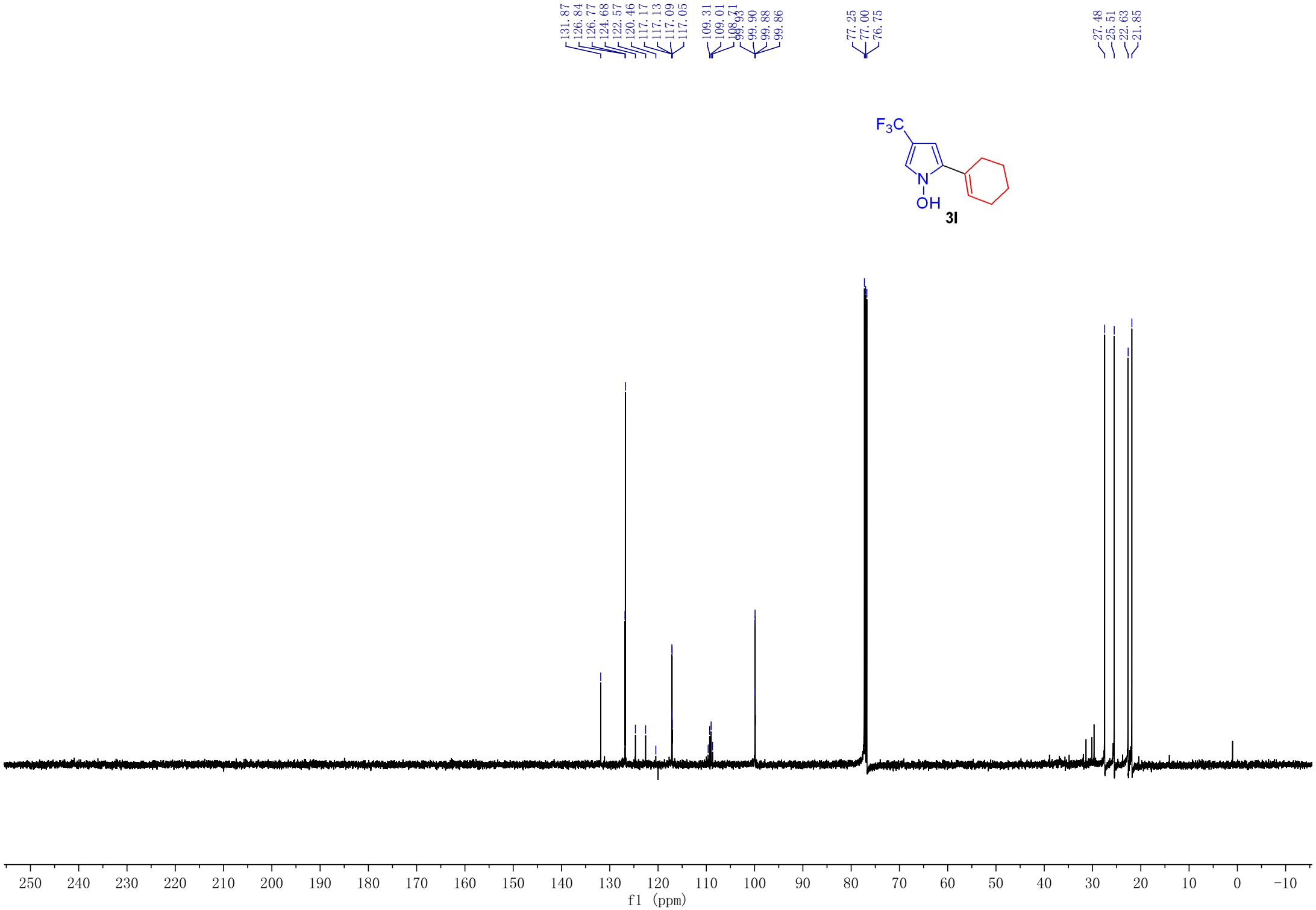
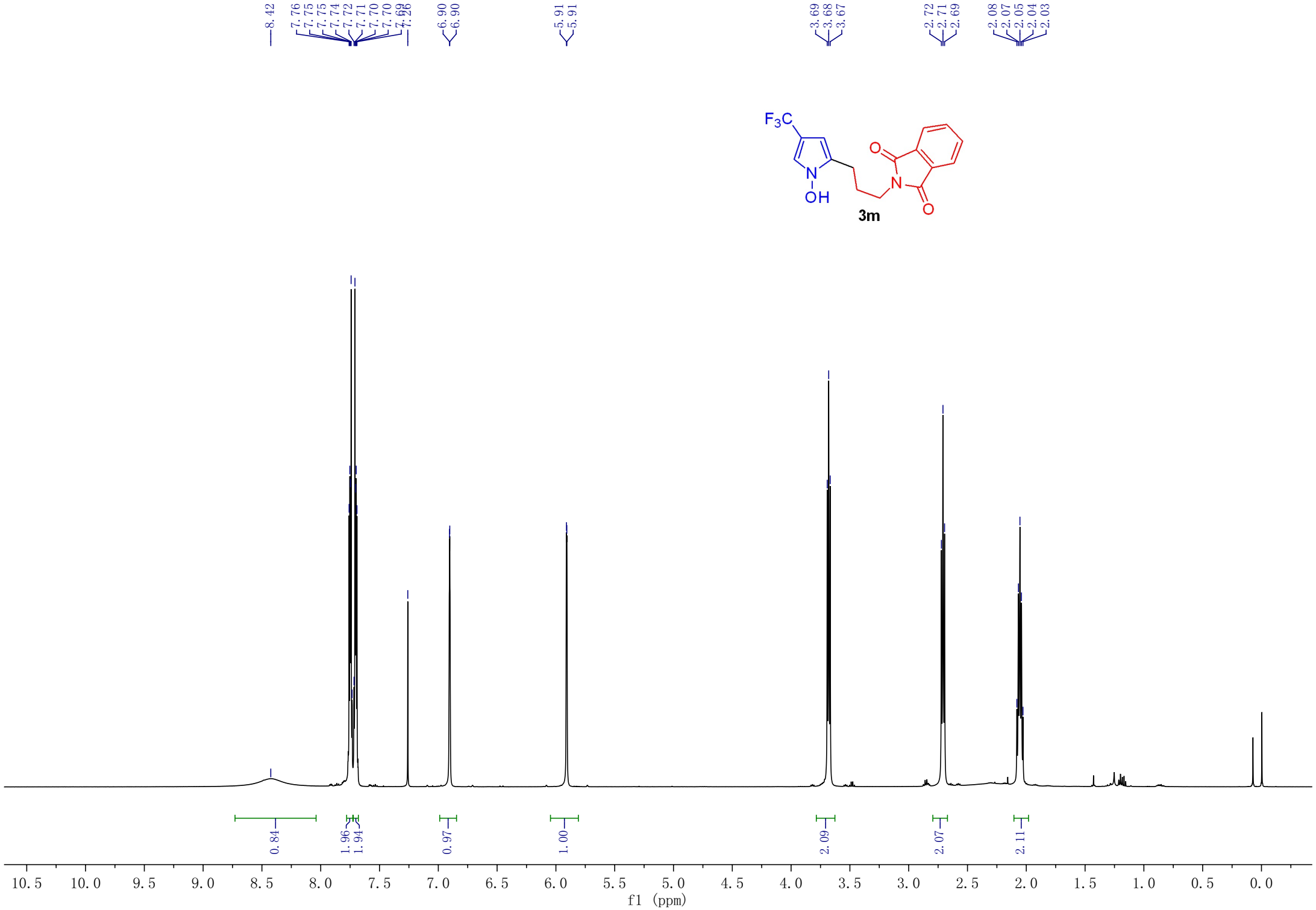
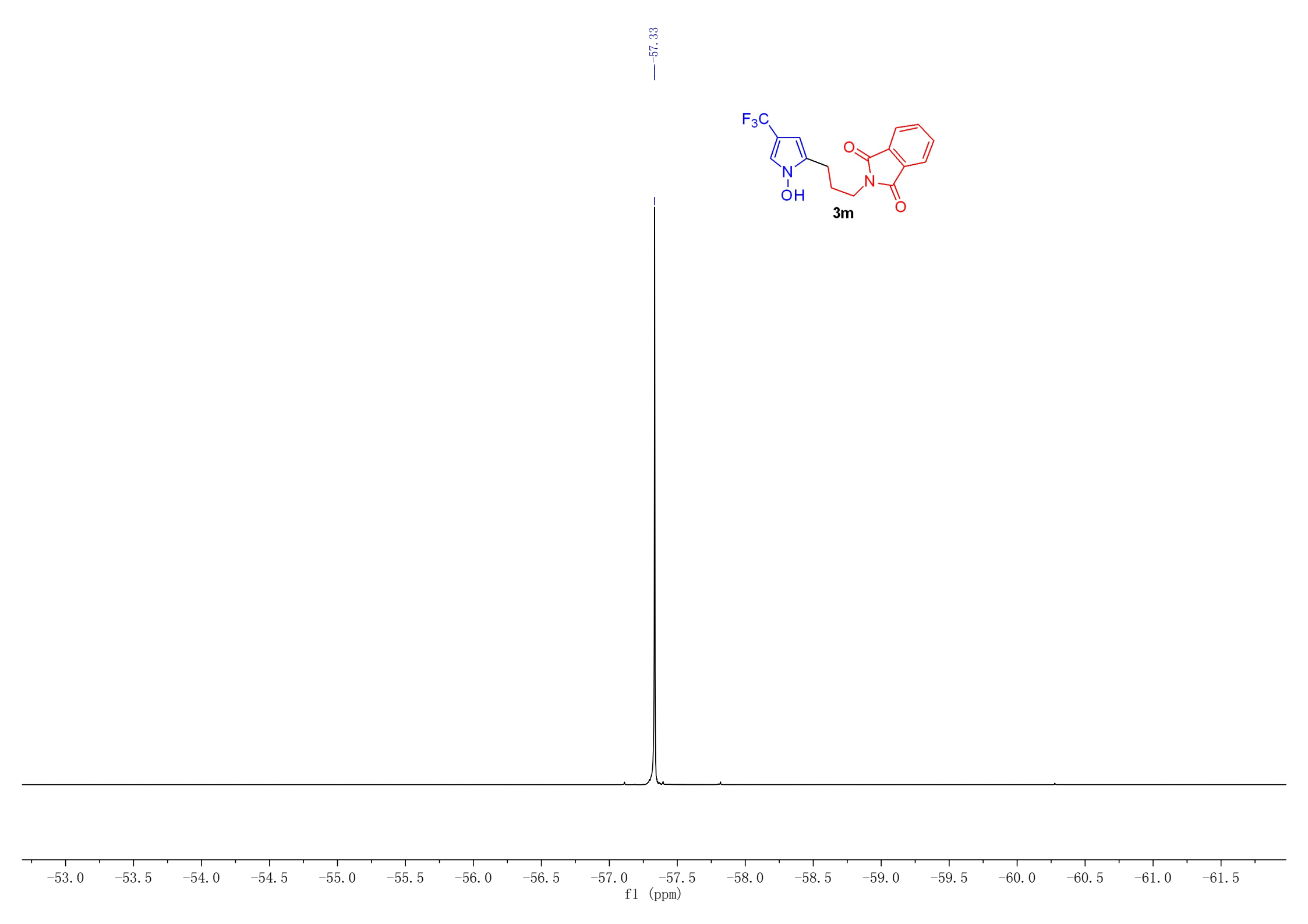
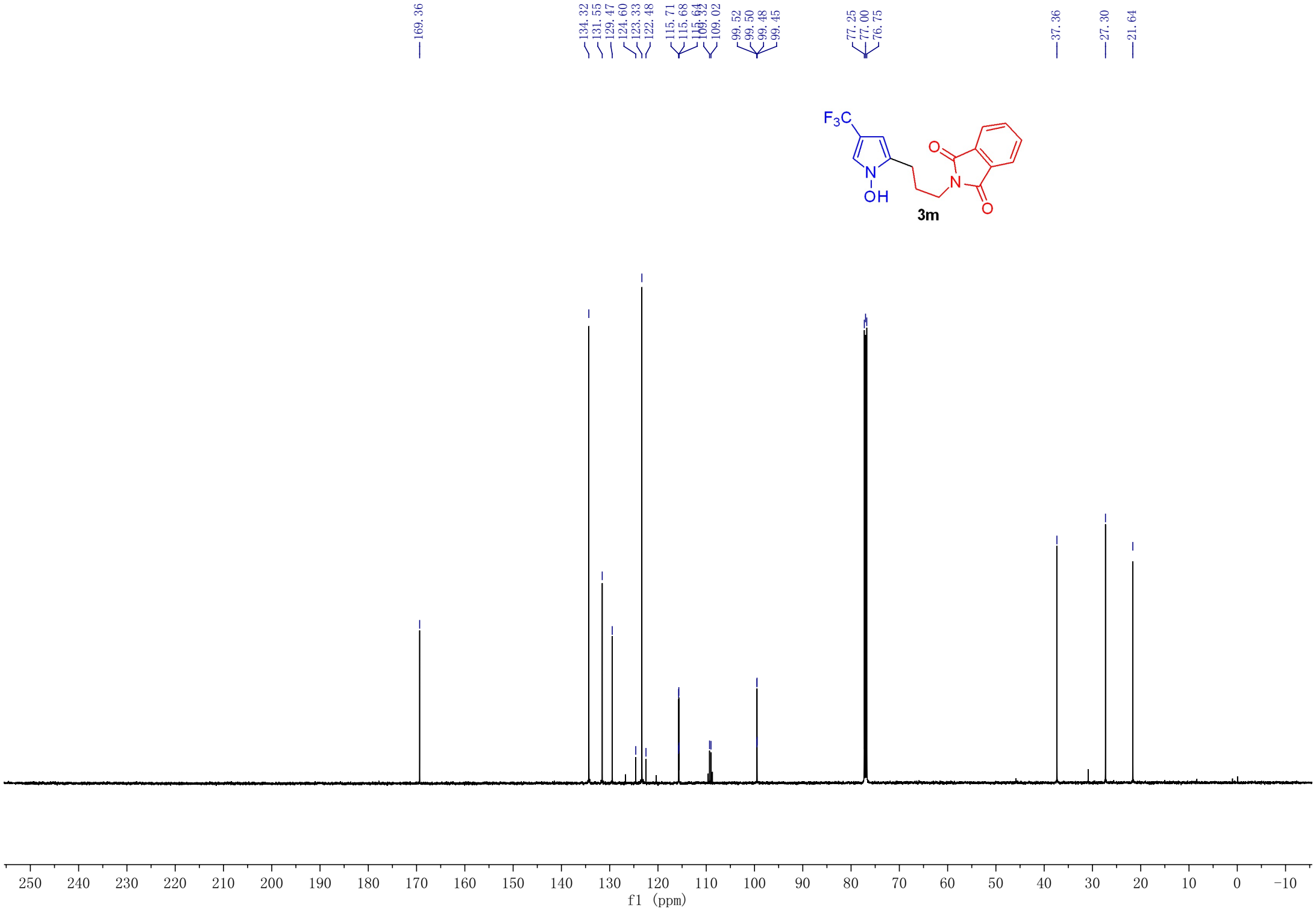
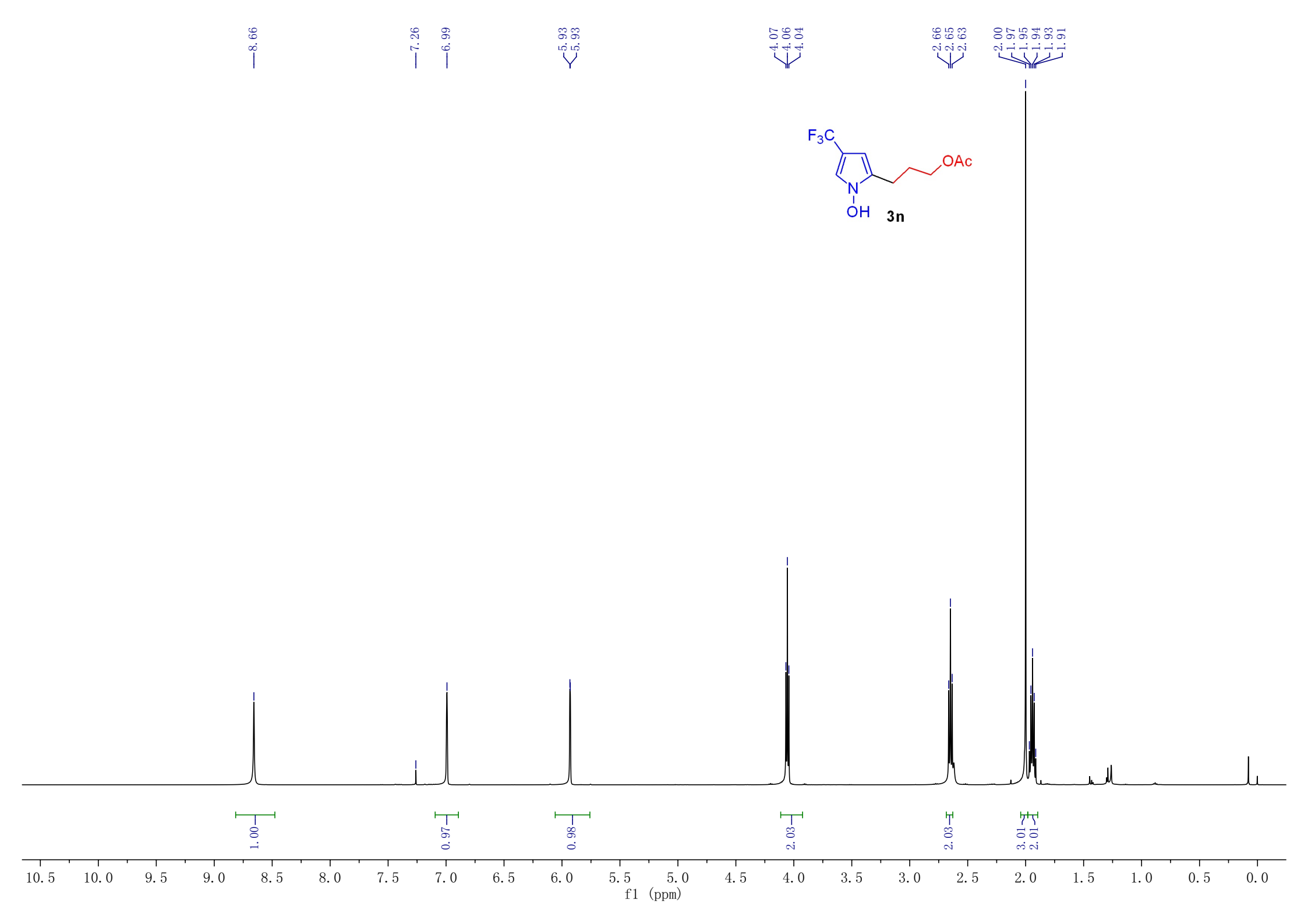
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
f1 (ppm)

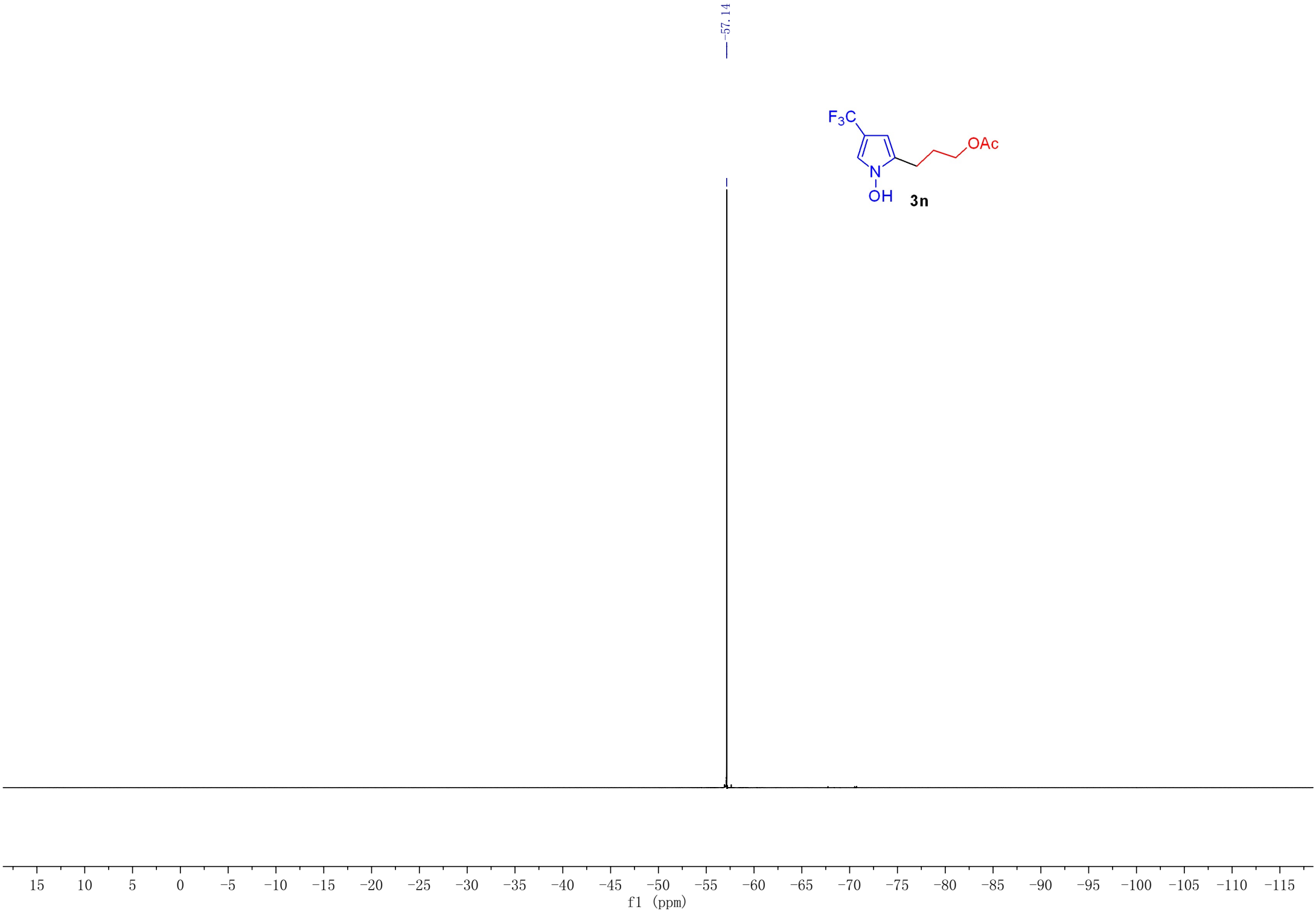

131.87
126.84
126.77
124.68
122.57
120.46
117.17
117.13
117.09
117.05
109.31
109.01
108.71
99.93
99.90
99.88
99.86
77.25
77.00
76.75
27.48
25.51
22.63
21.85
F3C
N
OH
3l
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

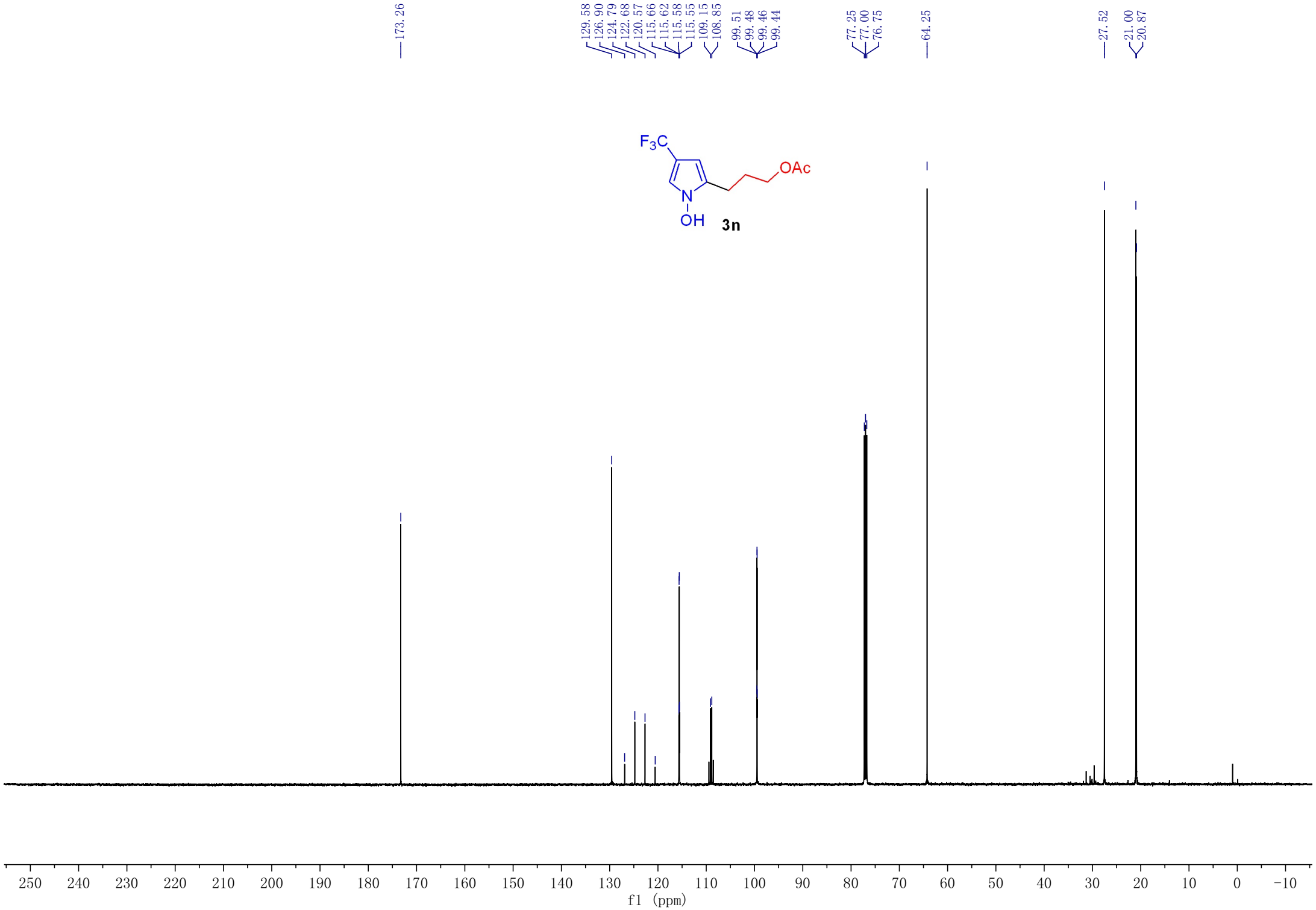

8.42
7.76
7.75
7.75
7.74
7.72
7.71
7.70
7.70
6.90
6.90
5.91
5.91
3.69
3.68
3.67
2.72
2.71
2.69
2.08
2.07
2.05
2.04
2.03
F3C
N
OH
O
N
O
3m
0.84
1.96
1.94
0.97
1.00
2.09
2.07
2.11
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

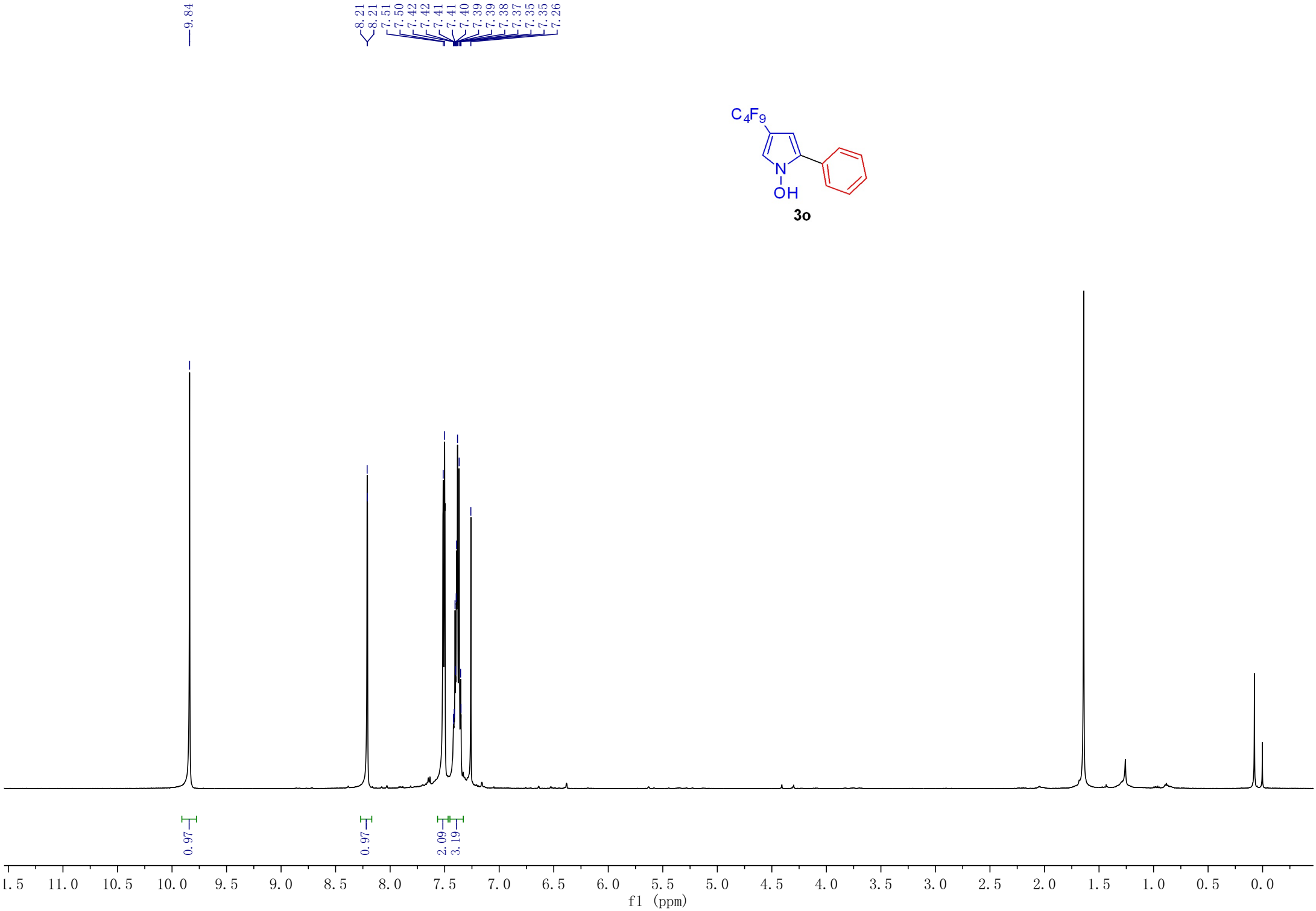

-57.33
F3C
N
OH
O
N
O
3m
-53.0
-53.5
-54.0
-54.5
-55.0
-55.5
-56.0
-56.5
-57.0
-57.5
-58.0
-58.5
-59.0
-59.5
-60.0
-60.5
-61.0
-61.5
f1 (ppm)

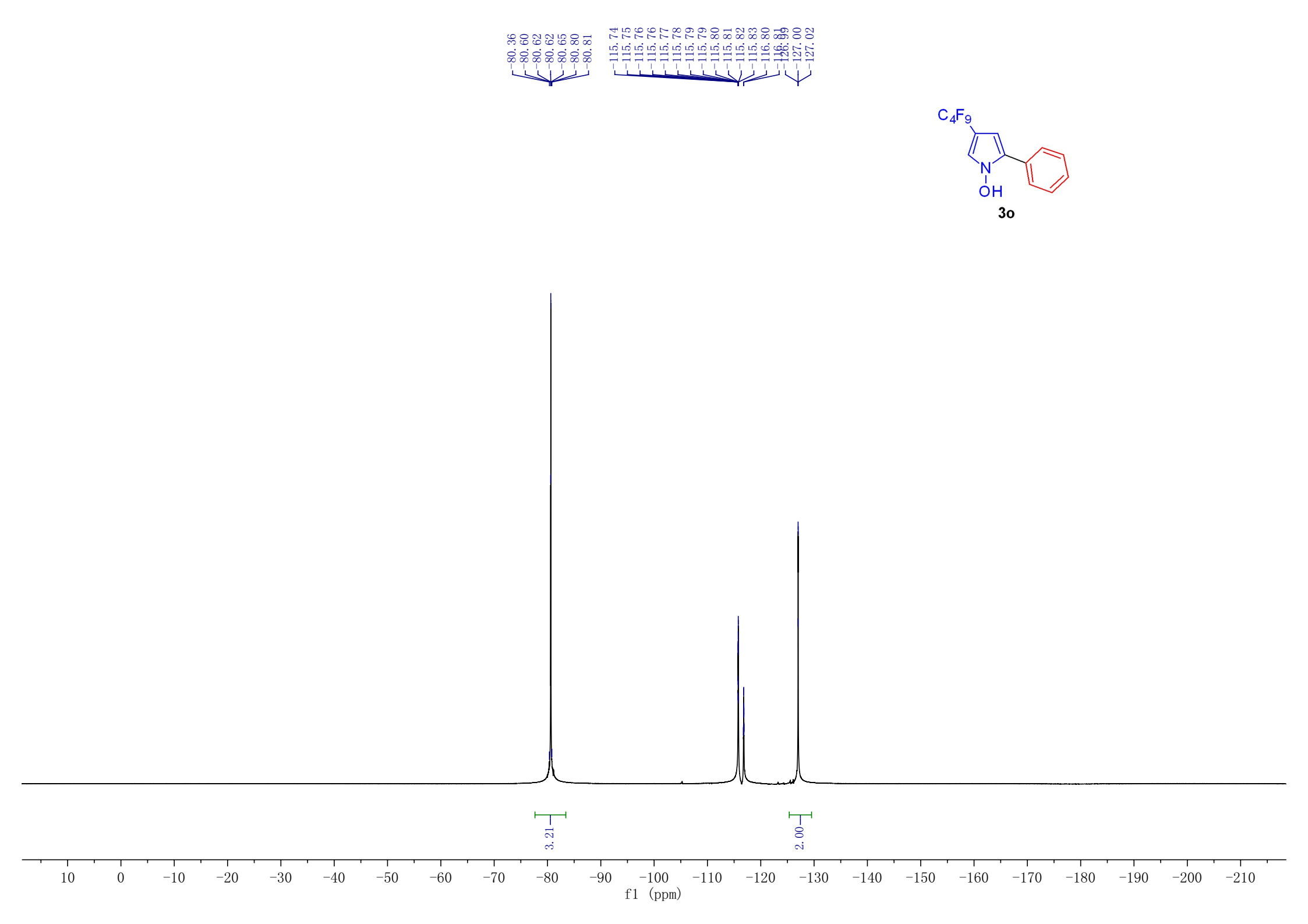

169.36
134.32
131.55
129.47
124.60
123.33
122.48
115.71
115.68
109.02
99.52
99.50
99.48
99.45
77.25
77.00
76.75
37.36
27.30
21.64
F3C
N
OH
O
N
O
3m
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

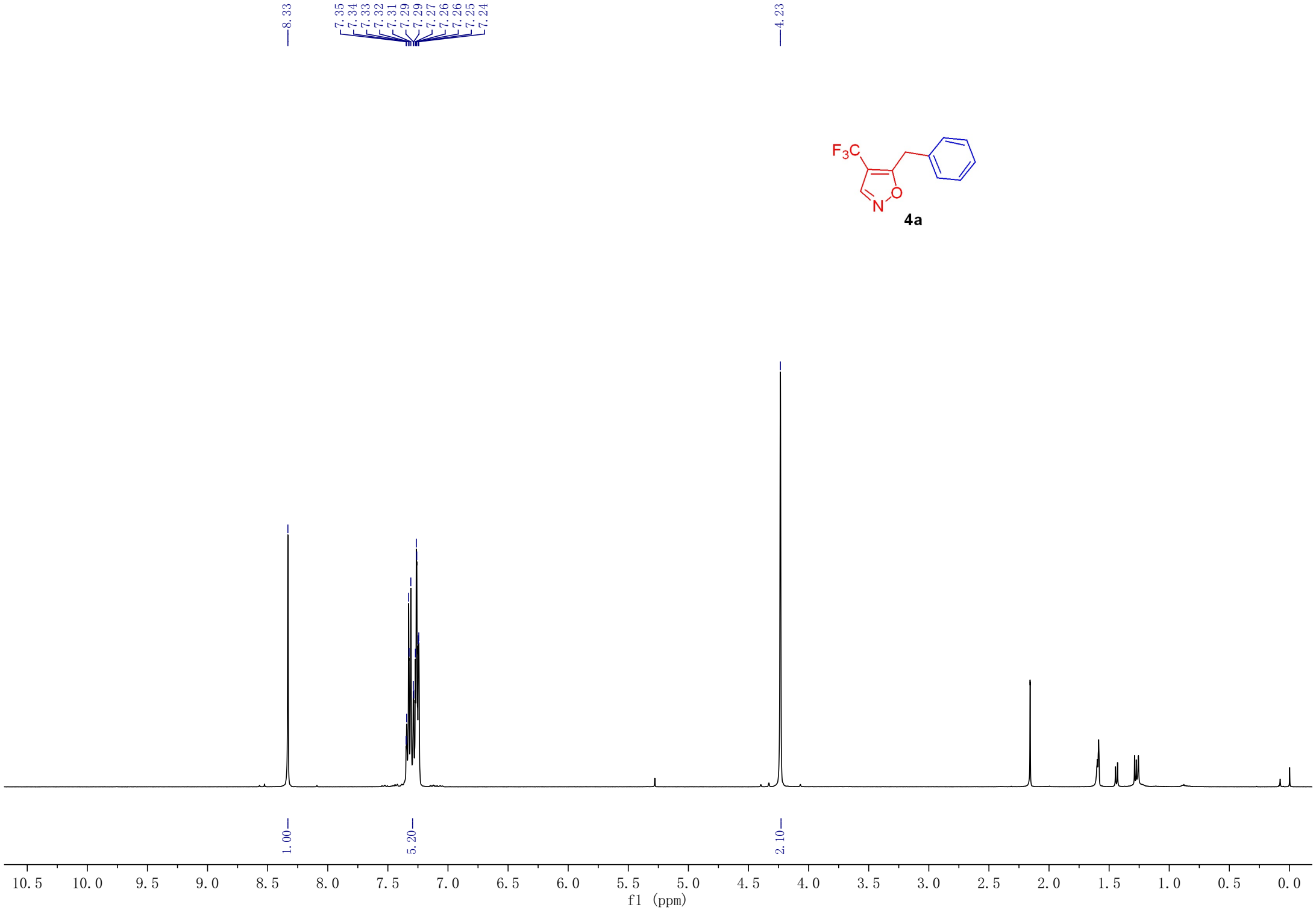

8.66
7.26
6.99
5.93
5.93
4.07
4.06
4.04
2.66
2.65
2.63
2.00
1.97
1.95
1.94
1.93
1.91
F3C
OAc
N
OH
3n
1.00
0.97
0.98
2.03
2.03
3.01
2.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

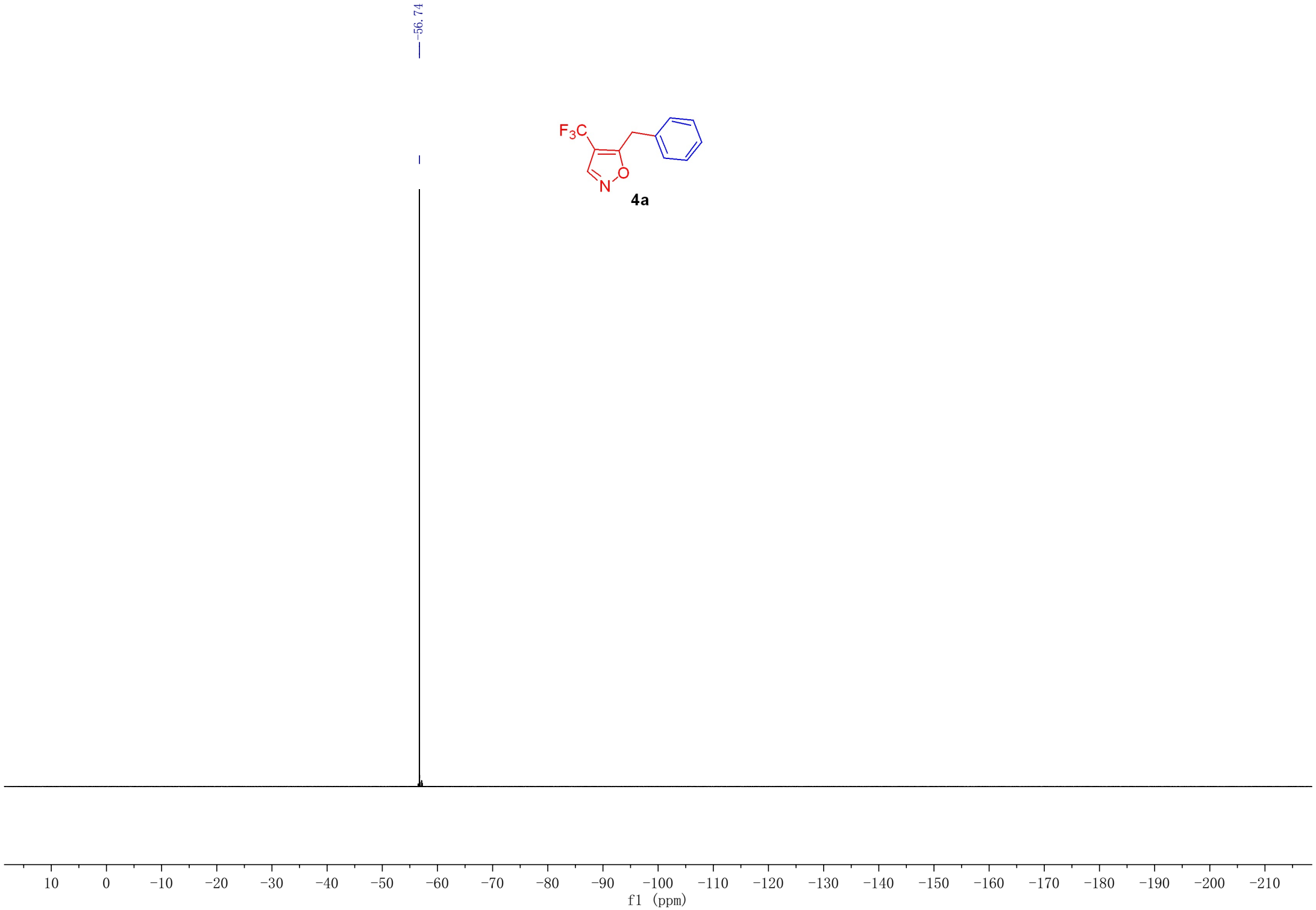

-57.14
F3C
OAc
N
OH
3n
15
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
f1 (ppm)


173.26
129.58
126.90
124.79
122.68
120.57
115.66
115.62
115.58
115.55
109.15
108.85
99.51
99.48
99.46
99.44
77.25
77.00
76.75
64.25
27.52
21.00
20.87
F3C
OAc
N
OH
3n
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


9.84
8.21
8.21
7.51
7.50
7.42
7.42
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.35
7.35
7.26
C4F9
N
OH
3o
0.97
0.97
2.09
3.19
f1 (ppm)


80.36
80.60
80.62
80.62
80.65
80.80
80.81
115.74
115.75
115.76
115.76
115.77
115.78
115.79
115.79
115.80
115.81
115.82
115.83
116.80
126.99
127.00
127.02
C4F9
N
OH
3o
3.21
2.00
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)


8.33
7.35
7.34
7.33
7.32
7.31
7.29
7.29
7.27
7.26
7.26
7.25
7.24
4.23
F3C
O
N
4a
1.00
5.20
2.10
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)


-56.74
F3C
O
N
4a
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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-100
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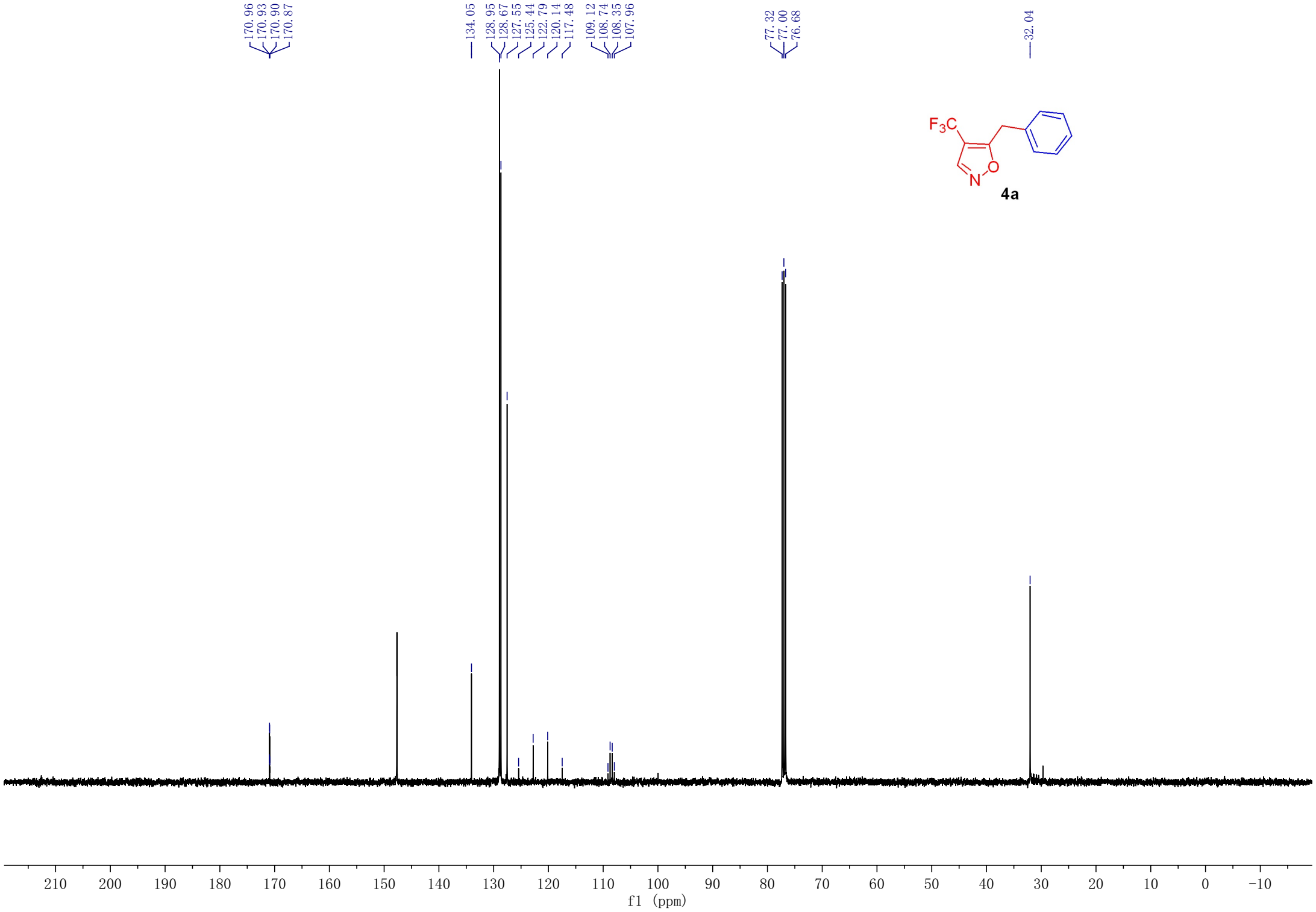
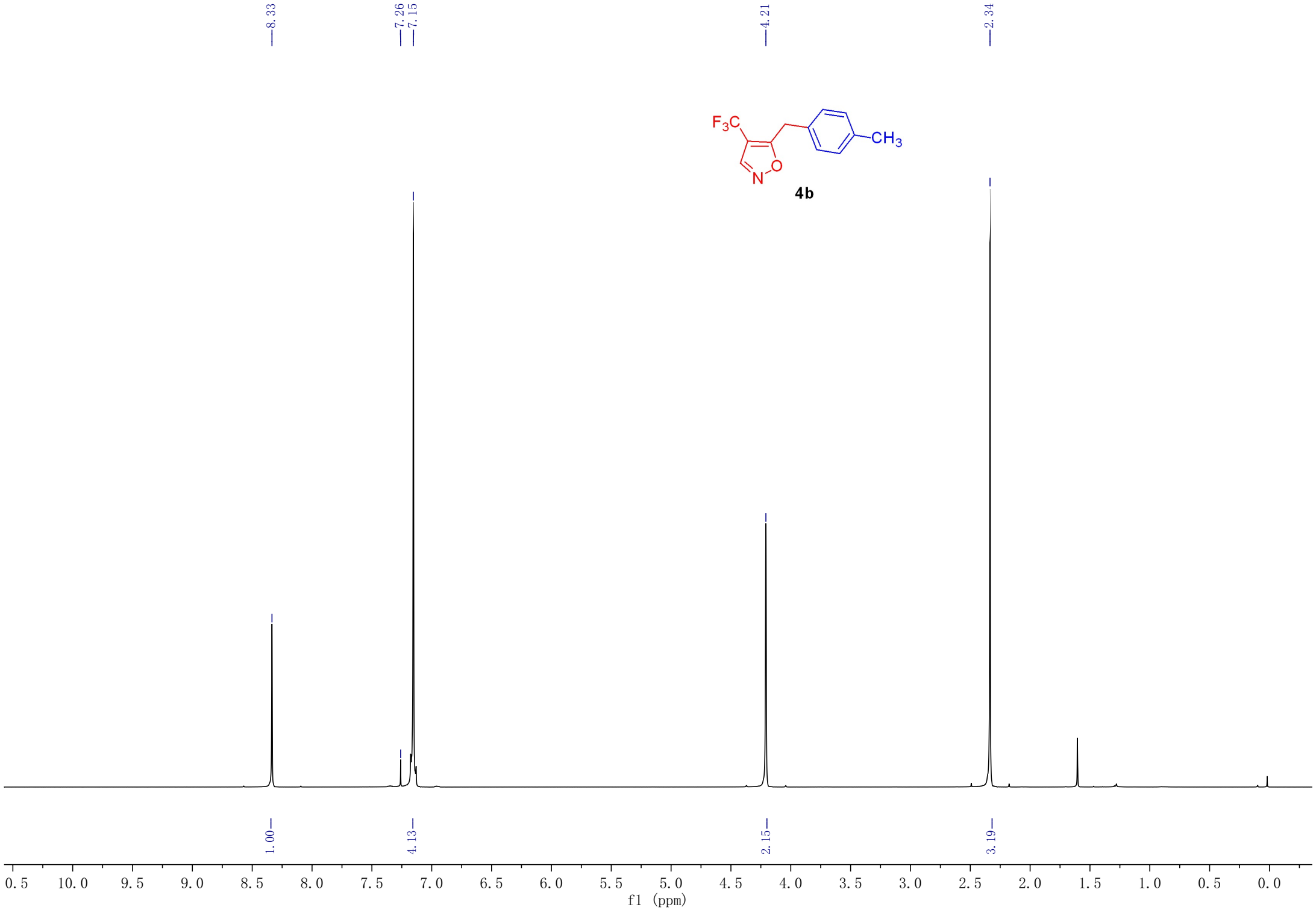
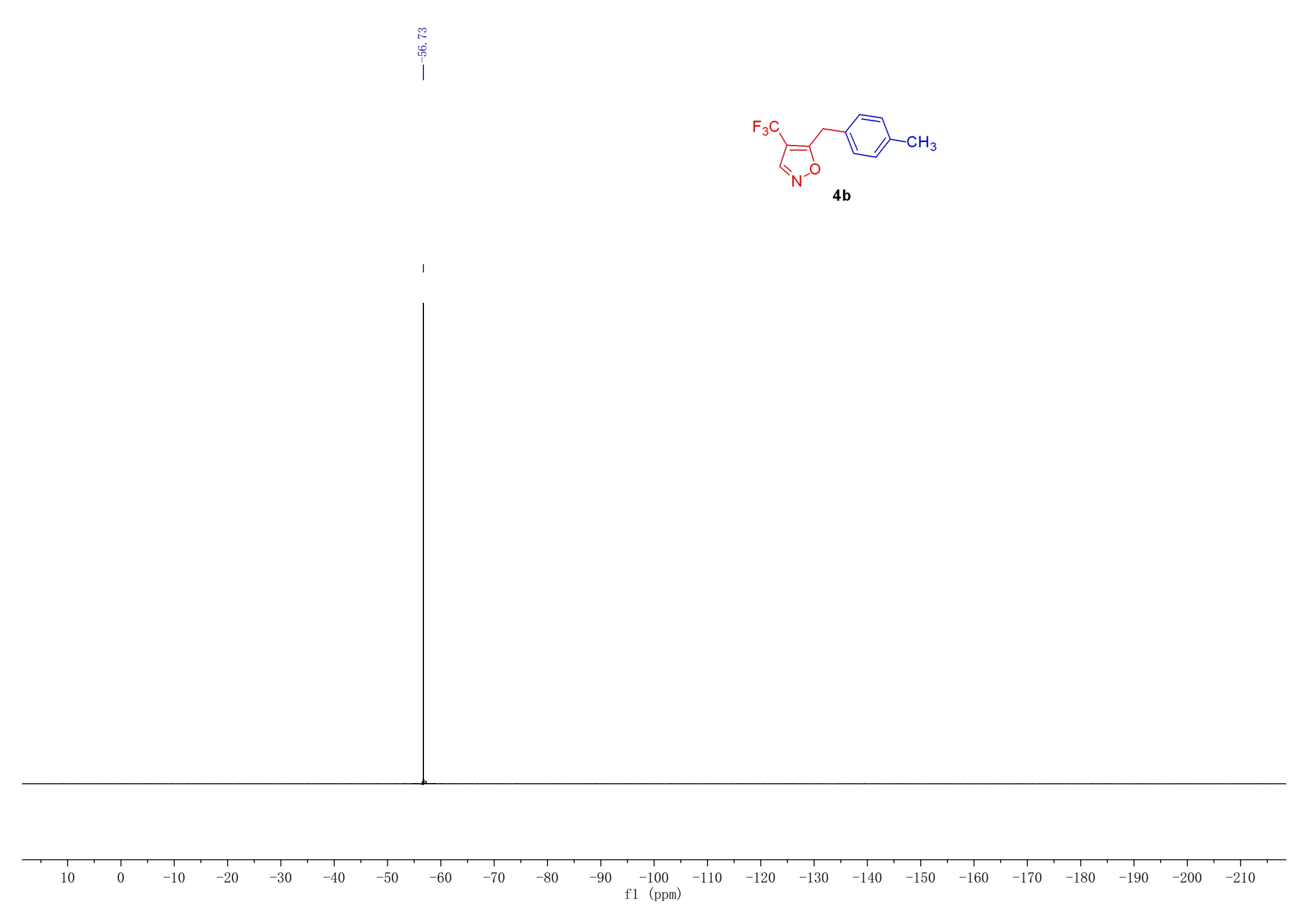
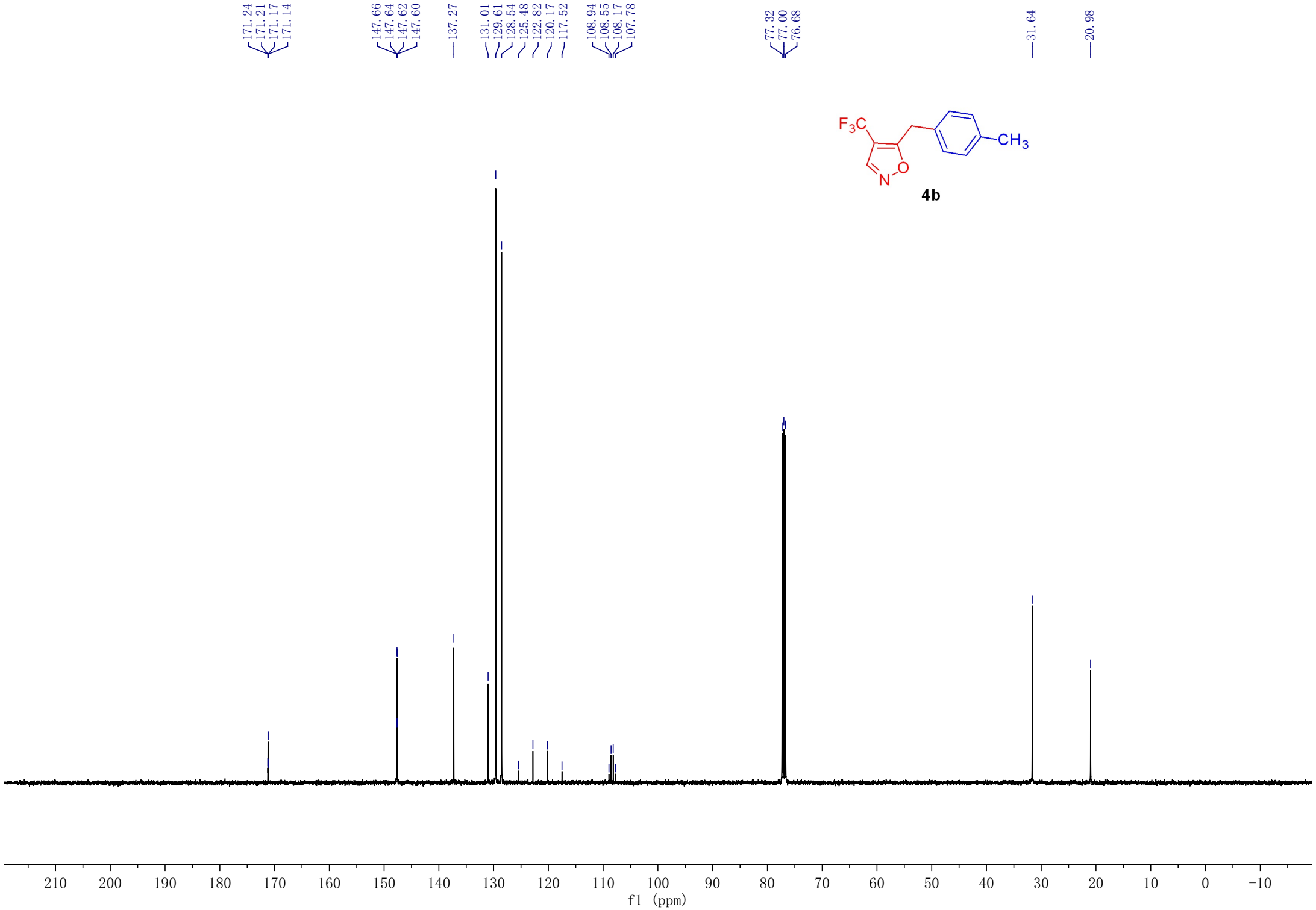
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


170.96
170.93
170.90
170.87
134.05
128.95
128.67
127.55
125.44
122.79
120.14
117.48
109.12
108.74
108.35
107.96
77.32
77.00
76.68
32.04
F3C
O
N
4a
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)


8.33
7.26
7.15
4.21
2.34
F3C
CH3
N
O
4b
1.00
4.13
2.15
3.19
0.5
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)


-56.73
F3C
CH3
N
O
4b
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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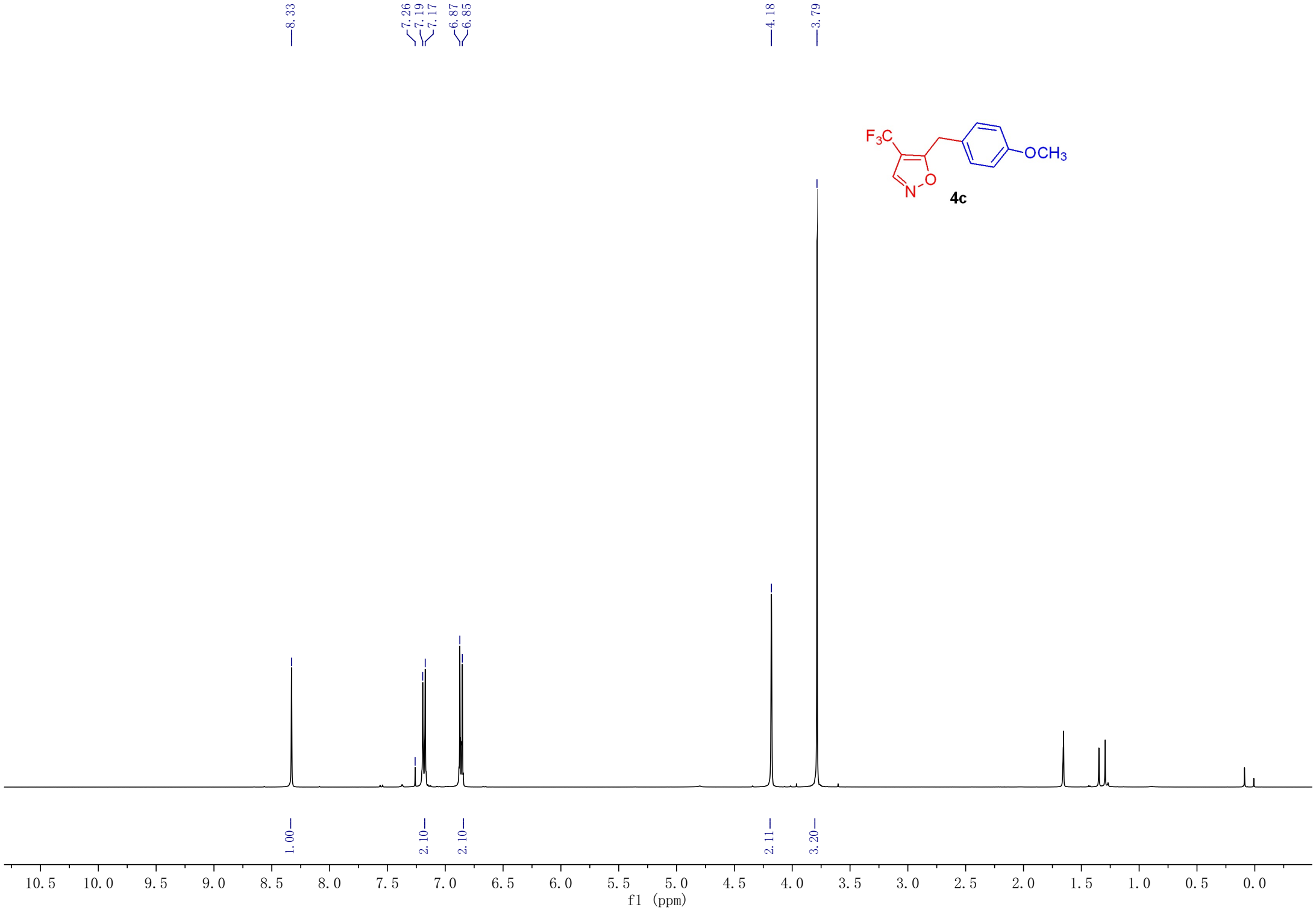
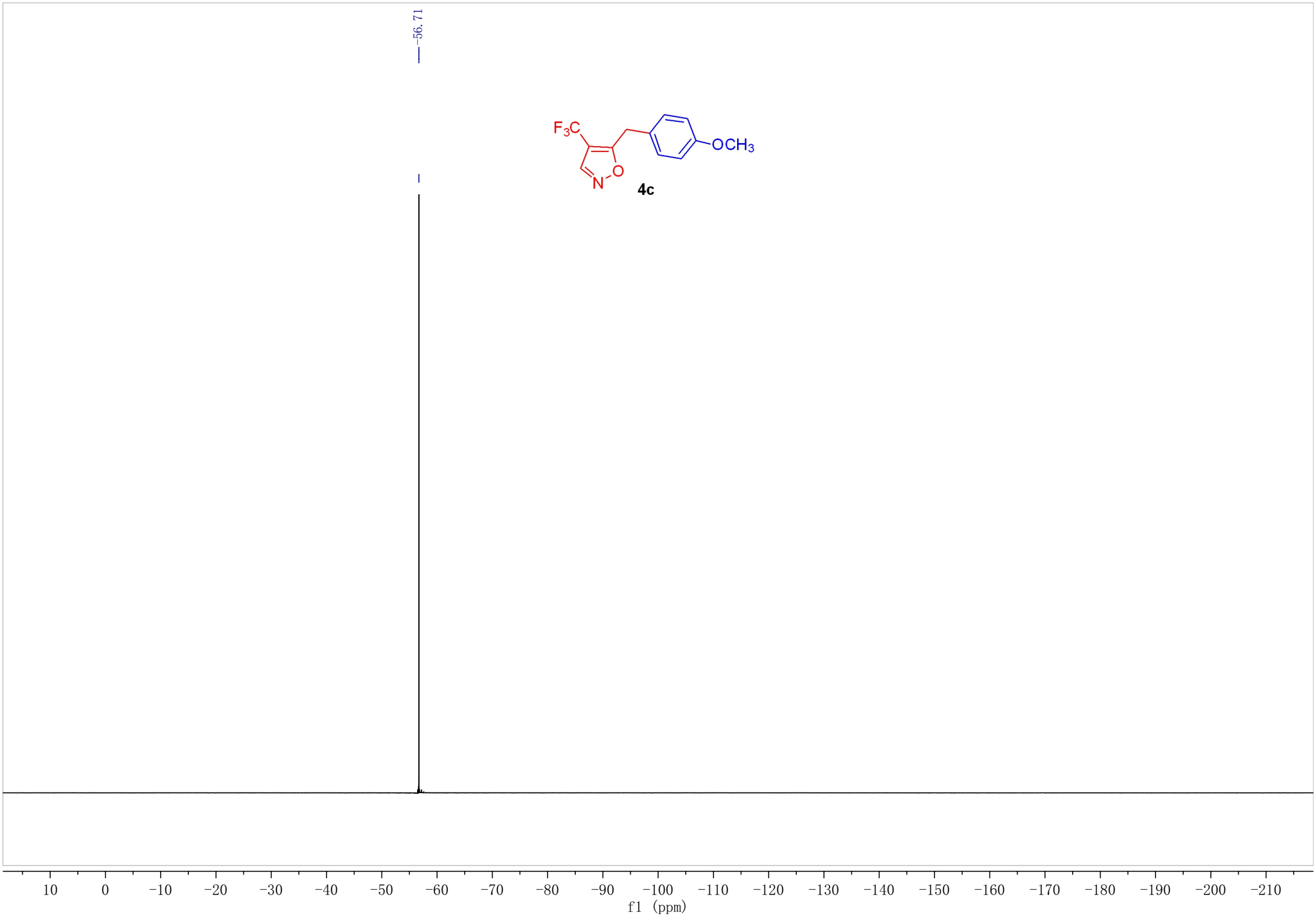
171.21
171.17
171.14
147.66
147.64
147.62
147.60
137.27
131.01
129.61
128.54
125.48
122.82
120.17
117.52
108.94
108.55
108.17
107.78
77.32
77.00
76.68
31.64
20.98
F3C
CH3
N
O
4b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.33
7.26
7.19
7.17
6.87
6.85
4.18
3.79
F3C
OCH3
N
O
4c
1.00
2.10
2.10
2.11
3.20
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)


-56.71
F3C
OCH3
N
O
4c
10
0
-10
-20
-30
-40
-50
-60
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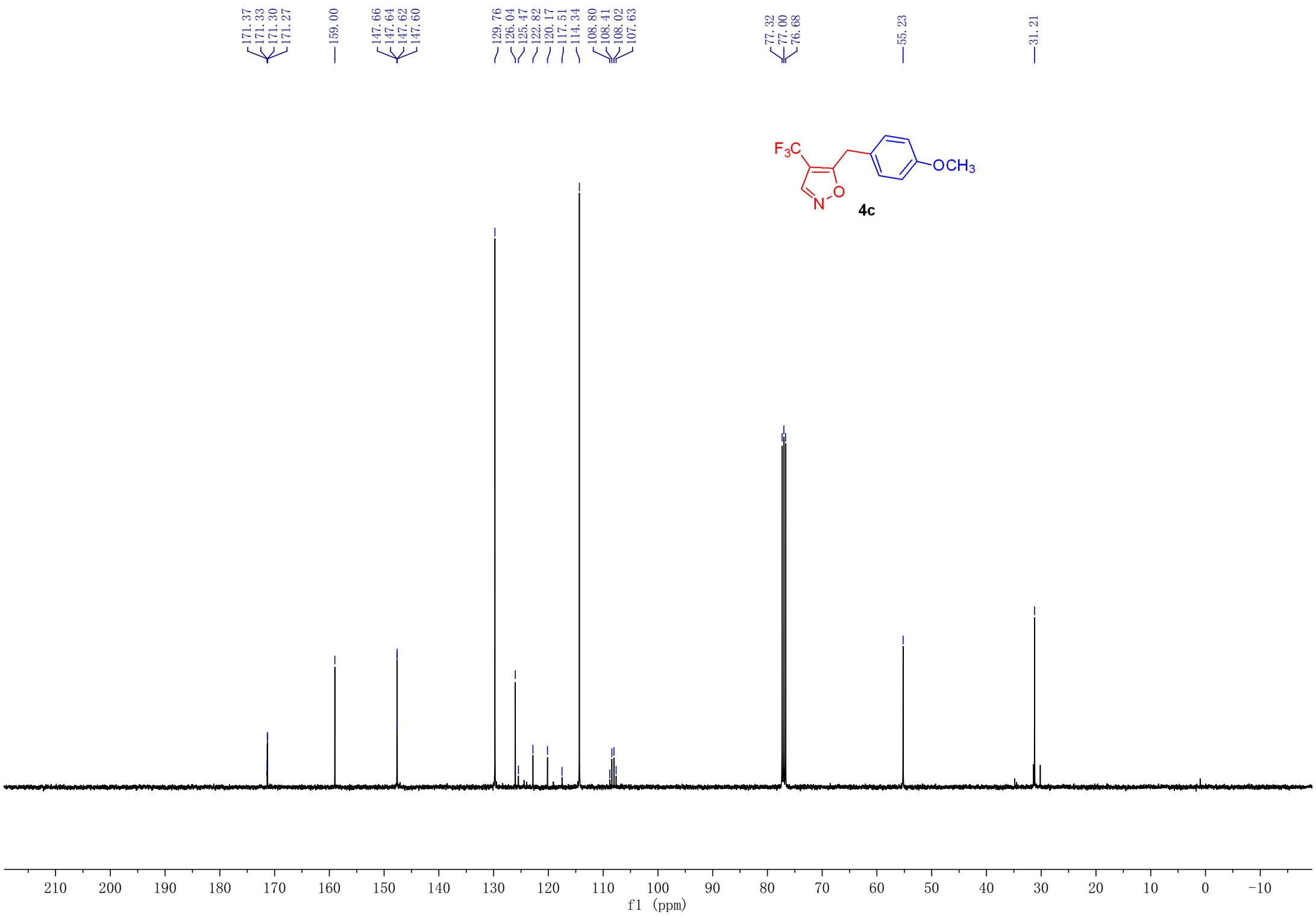
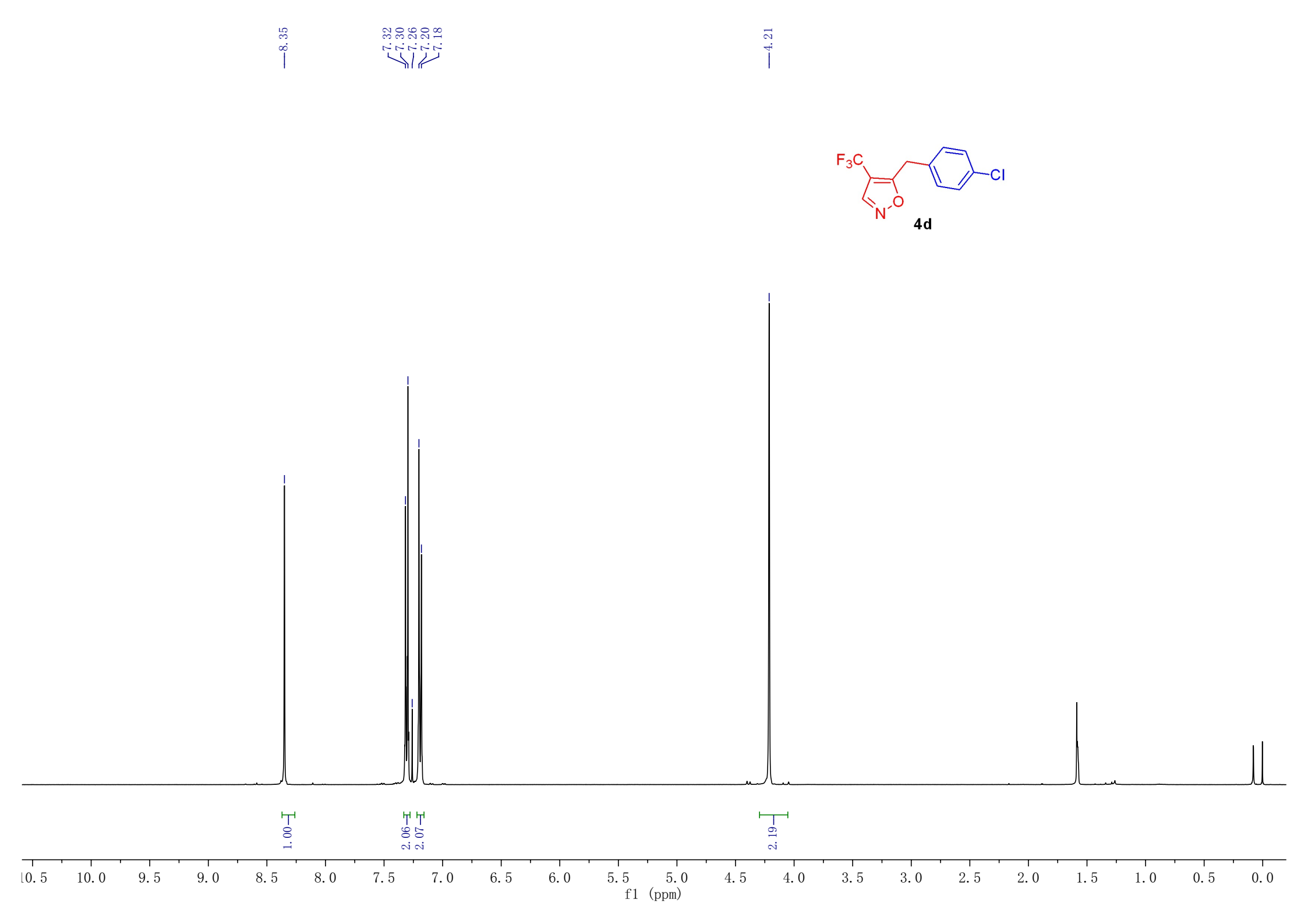
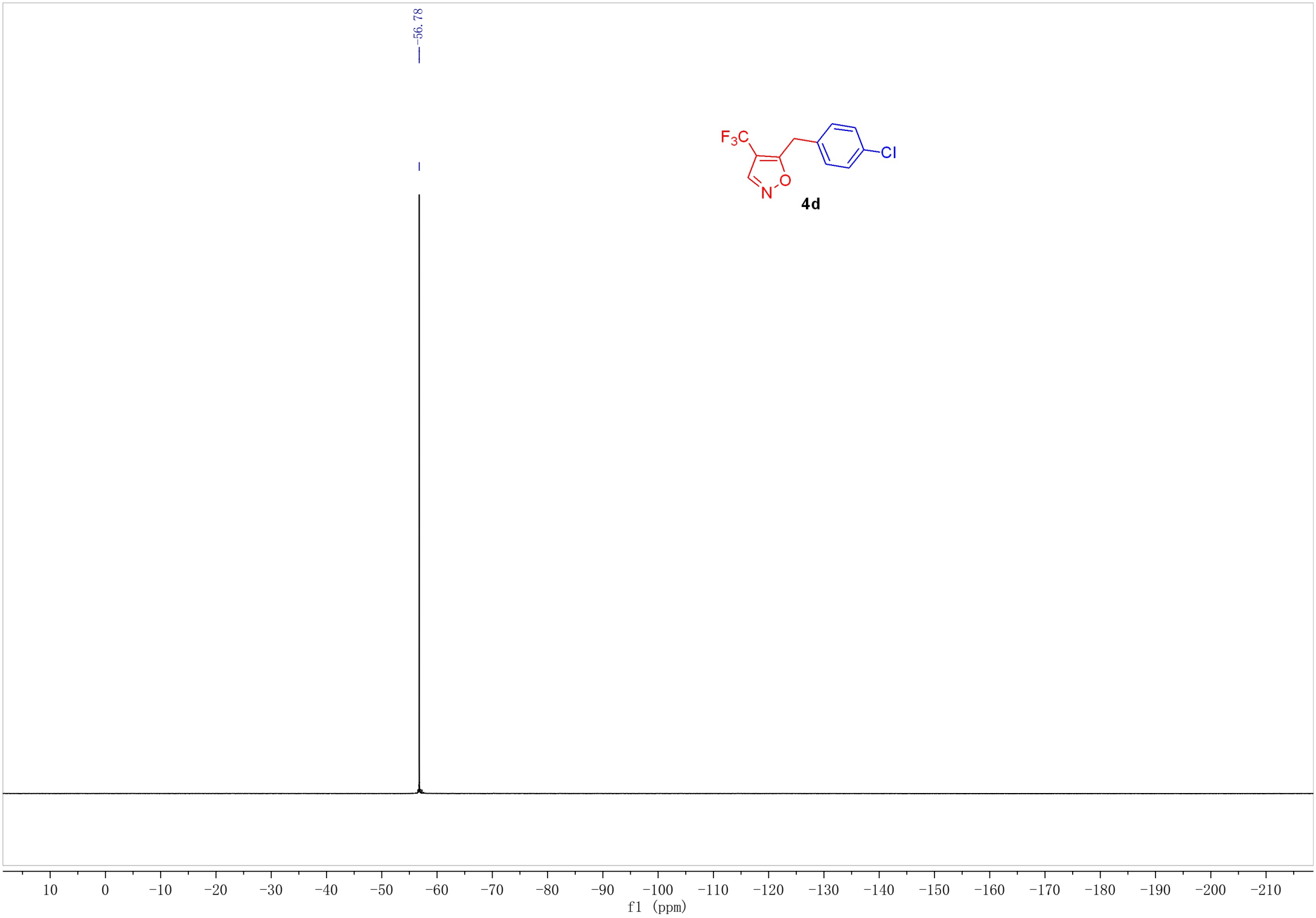
-170
-180
-190
-200
-210
f1 (ppm)


171.37
171.33
171.30
171.27
159.00
147.66
147.64
147.62
147.60
129.76
126.04
125.47
122.82
120.17
117.51
114.34
108.80
108.41
108.02
107.63
77.32
77.00
76.68
55.23
31.21
F3C
OCH3
N
O
4c
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)


8.35
7.32
7.30
7.26
7.20
7.18
4.21
F3C
Cl
N
O
4d
1.00
2.06
2.07
2.19
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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F3C
Cl
N
O
4d
10
0
-10
-20
-30
-40
-50
-60
-70
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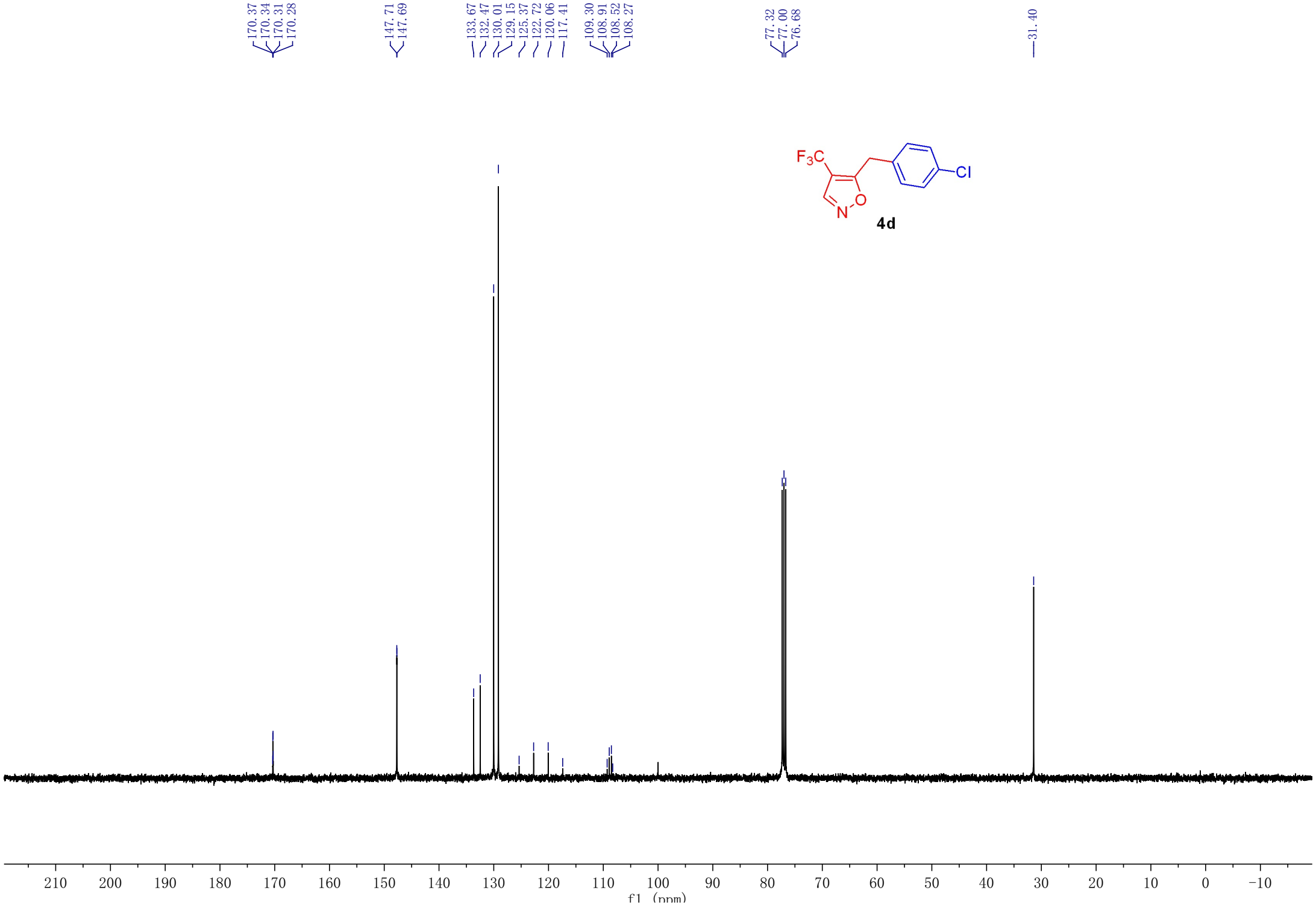
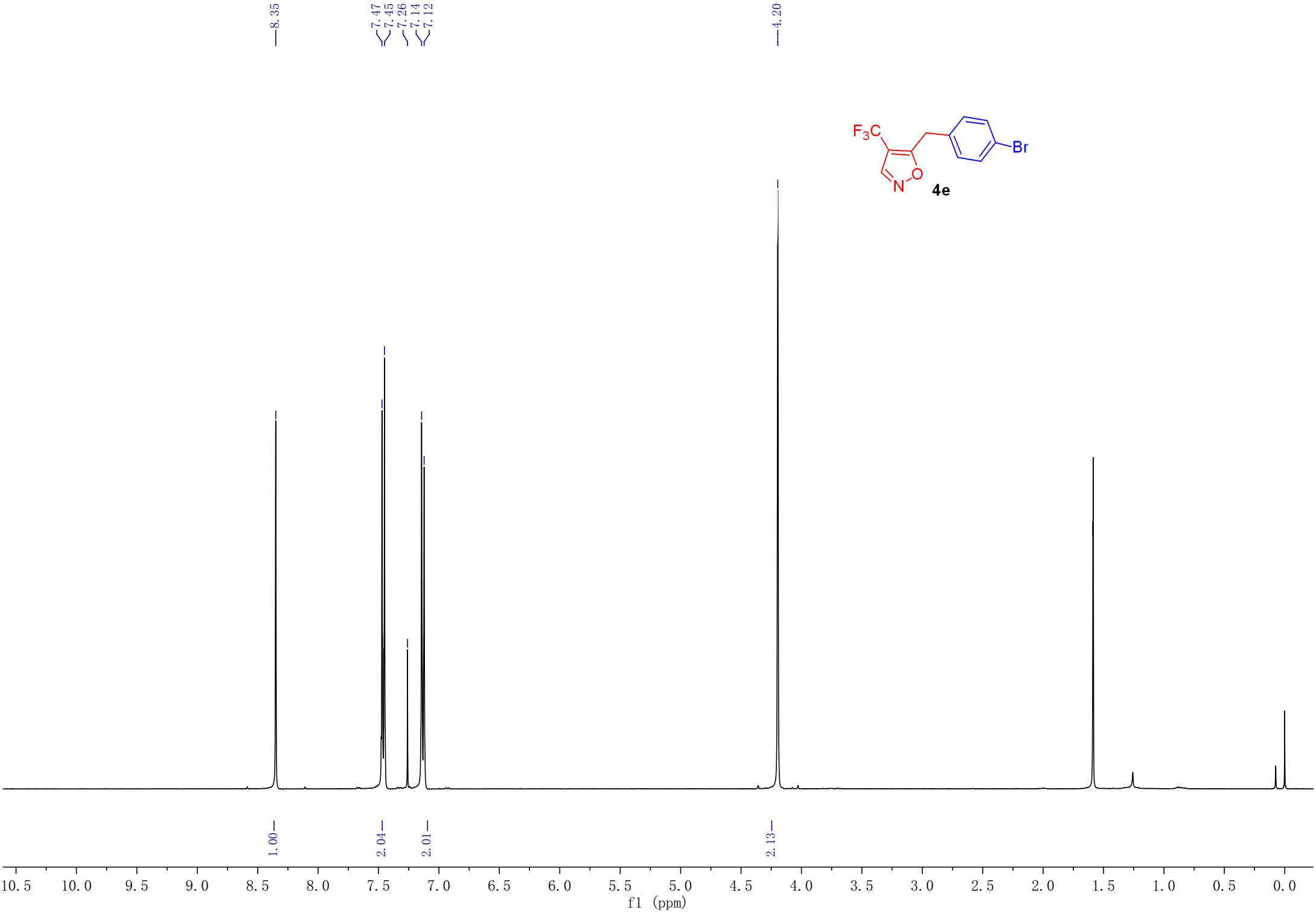
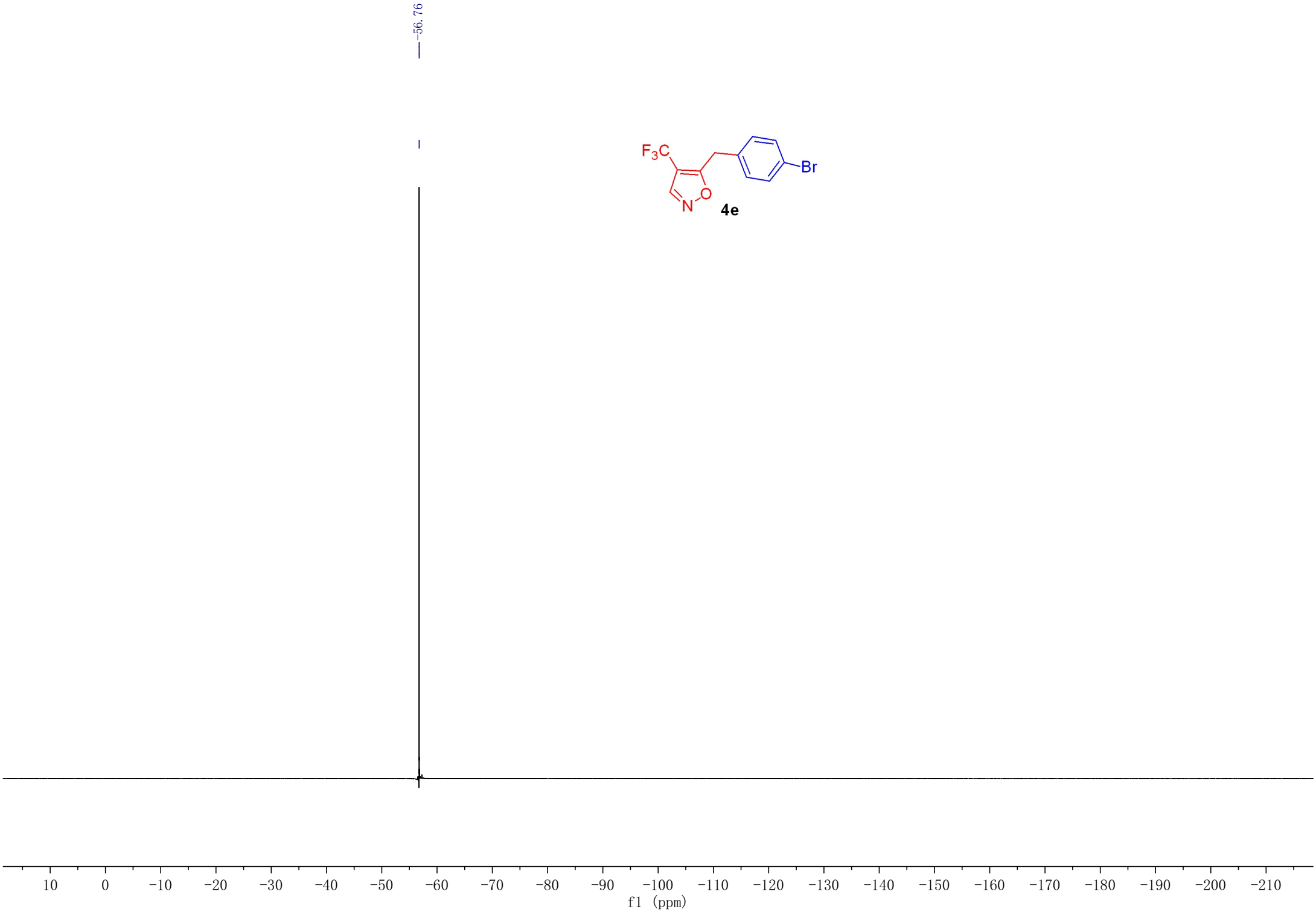
-160
-170
-180
-190
-200
-210
f1 (ppm)


170.37
170.34
170.31
170.28
147.71
147.69
133.67
132.47
130.01
129.15
125.37
122.72
120.06
117.41
109.30
108.91
108.52
108.27
77.32
77.00
76.68
31.40
F3C
Cl
N
O
4d
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)


8.35
7.47
7.45
7.26
7.14
7.12
4.20
F3C
Br
N
O
4e
1.00
2.04
2.01
2.13
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)


-56.76
F3C
Br
N
O
4e
10
0
-10
-20
-30
-40
-50
-60
-70
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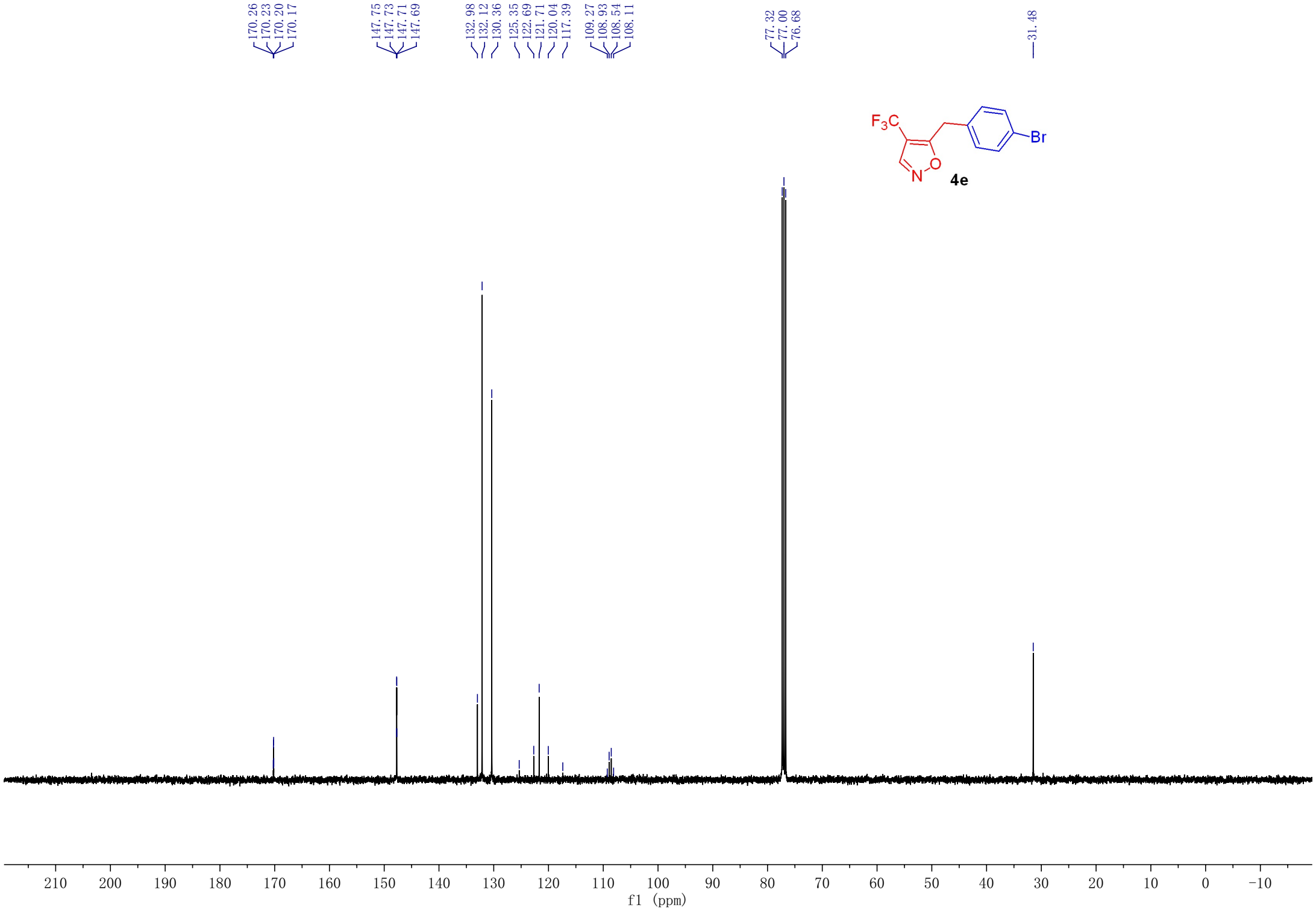
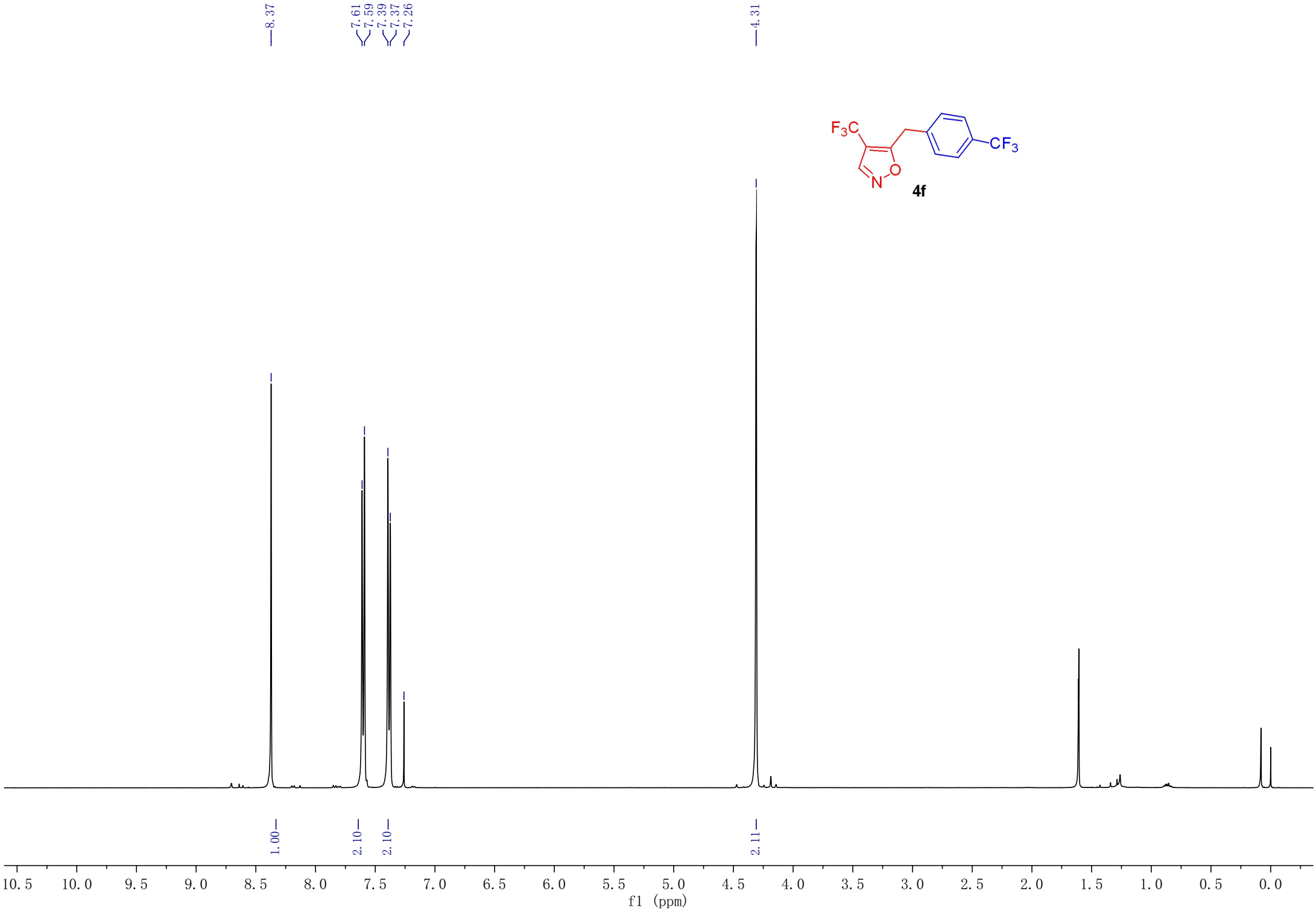
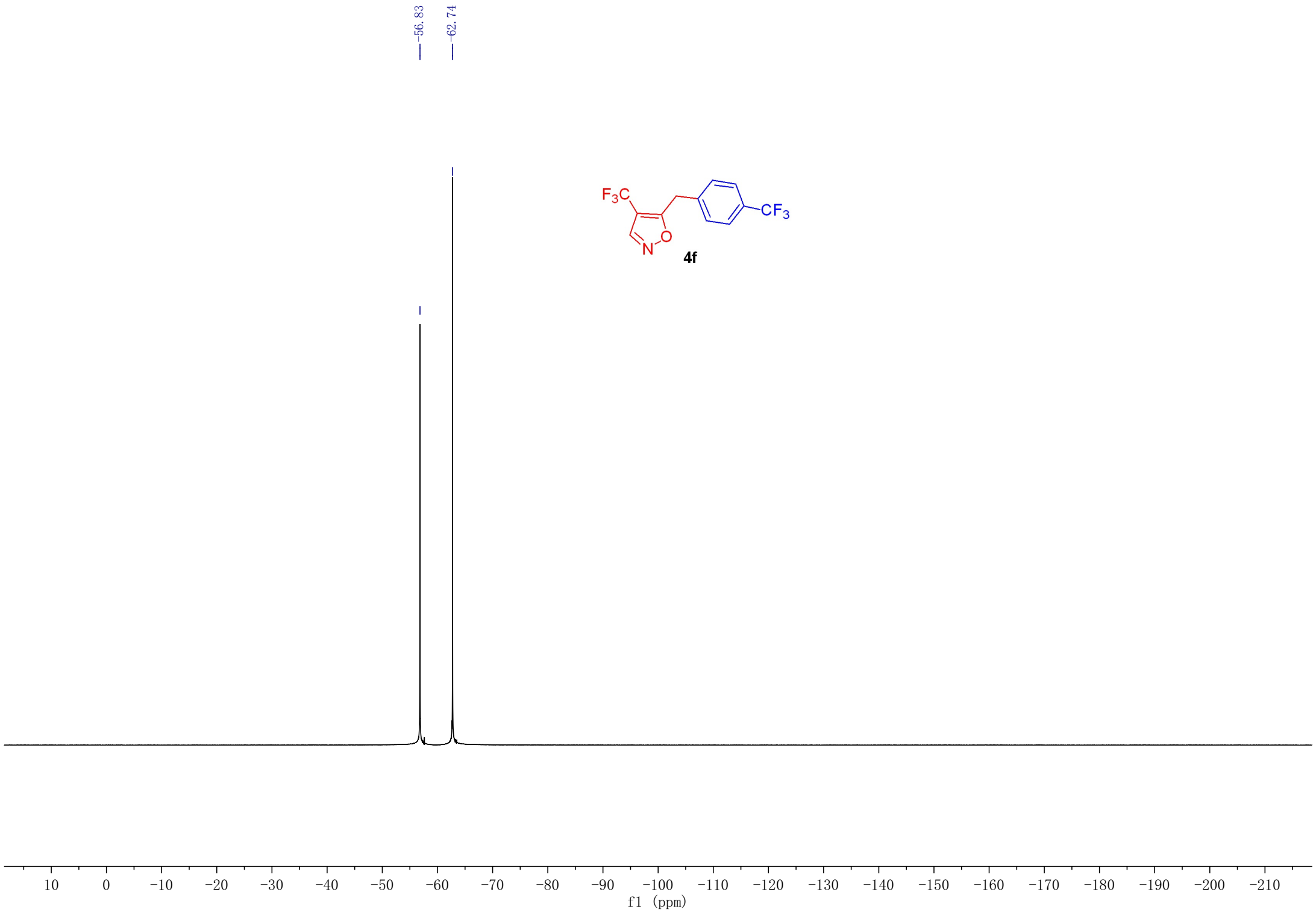
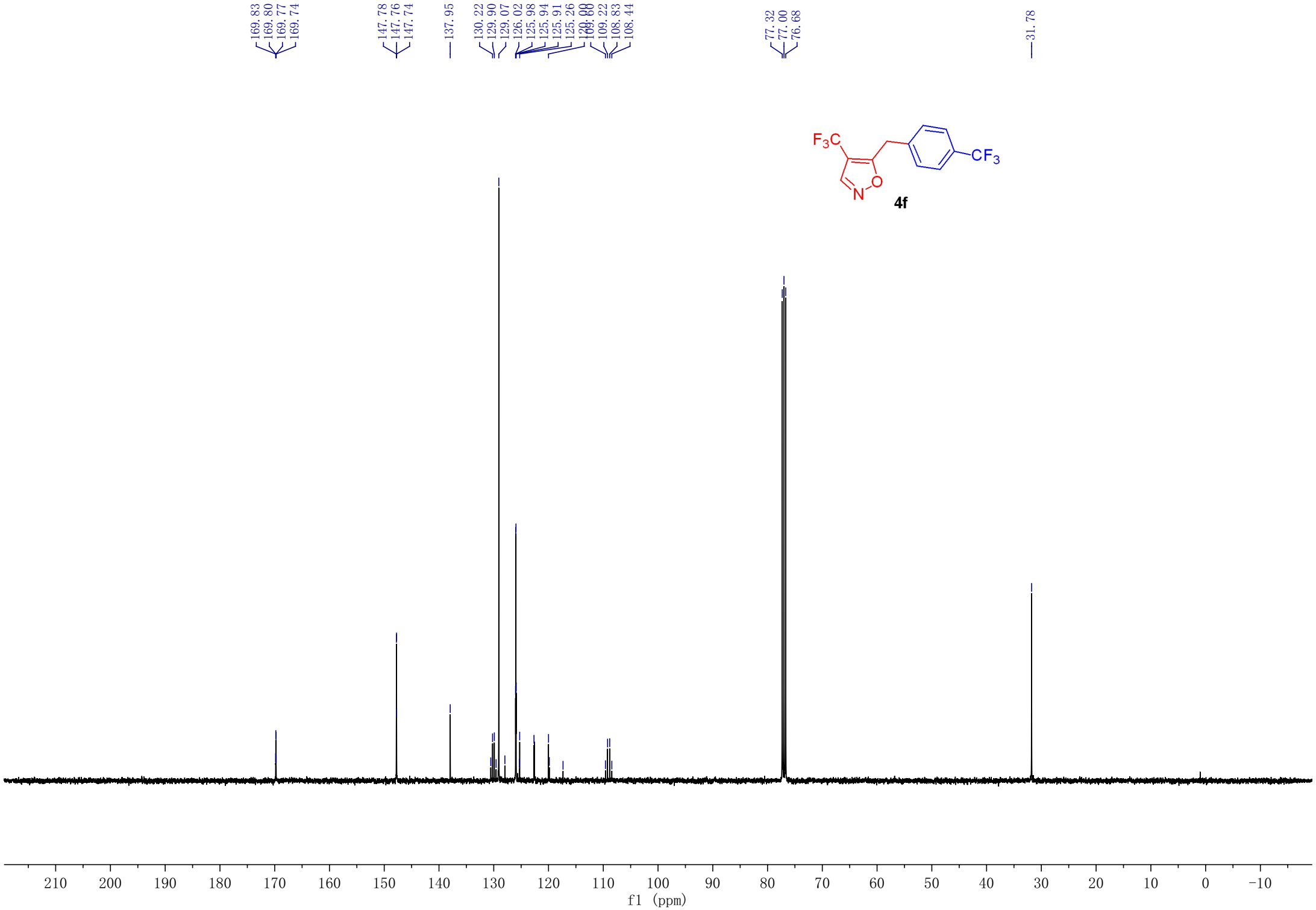
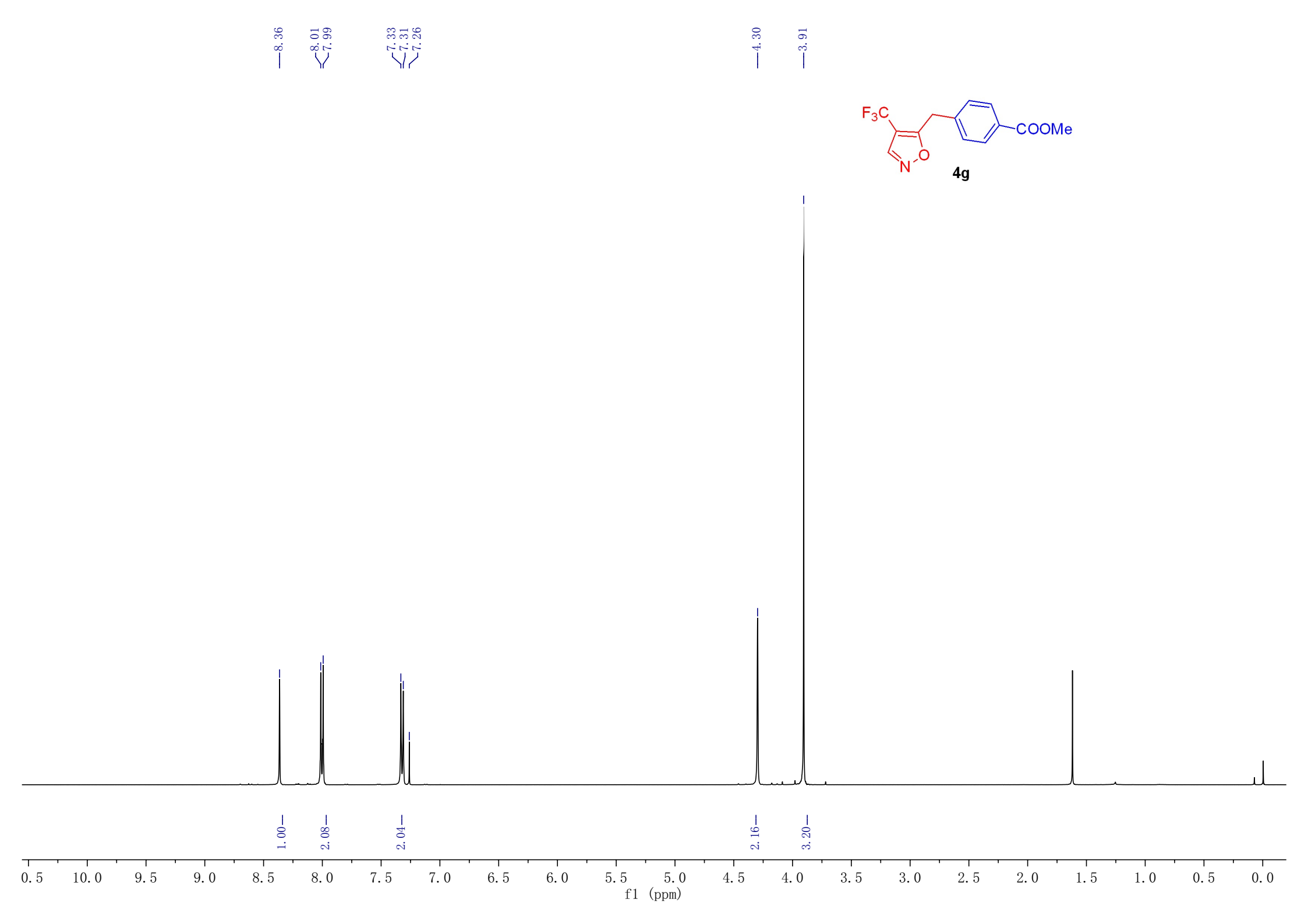
-170
-180
-190
-200
-210
f1 (ppm)

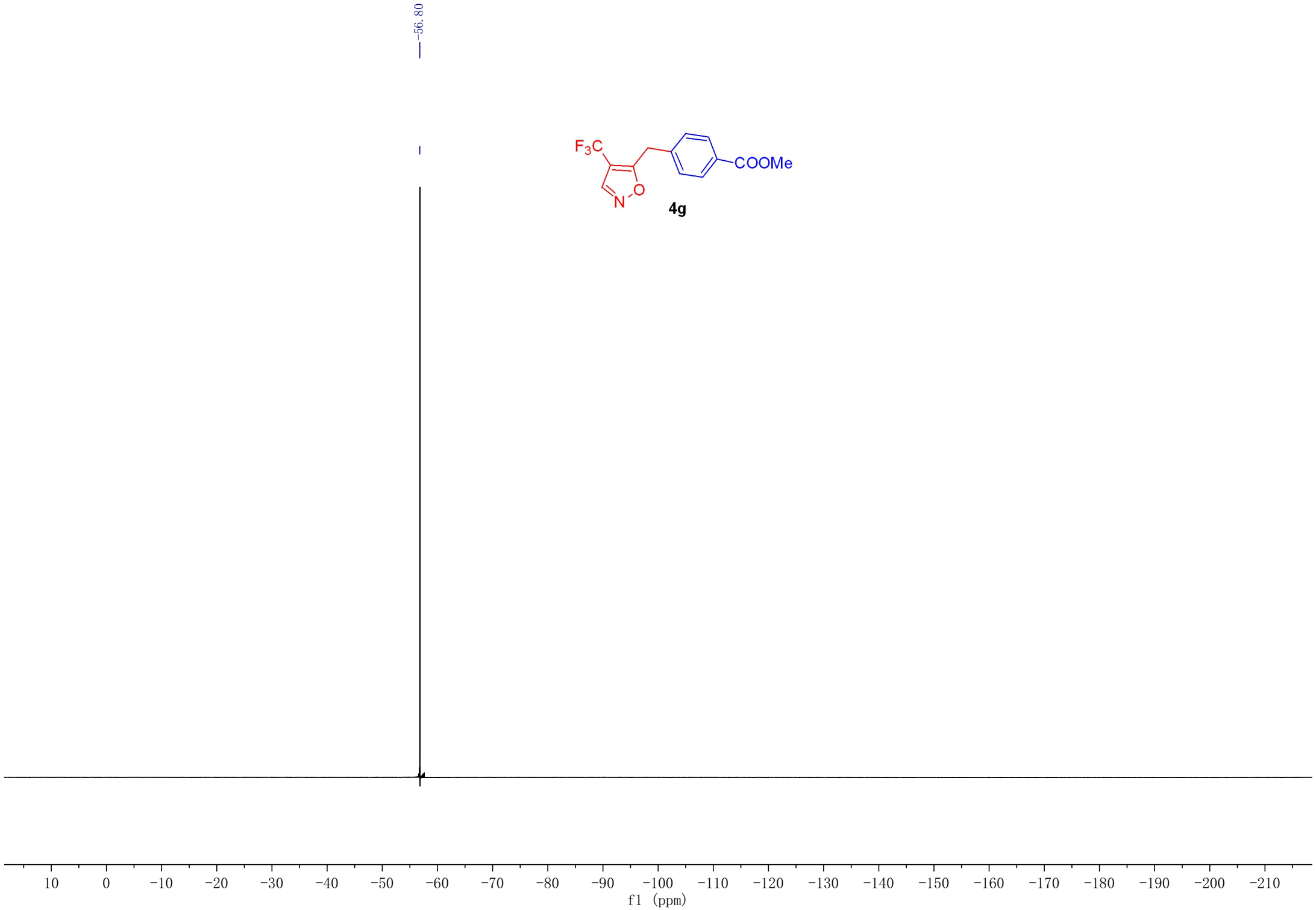

170.26
170.23
170.20
170.17
147.75
147.73
147.71
147.69
132.98
132.12
130.36
125.35
122.69
121.71
120.04
117.39
109.27
108.93
108.54
108.11
77.32
77.00
76.68
31.48
F3C
Br
O
N
4e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

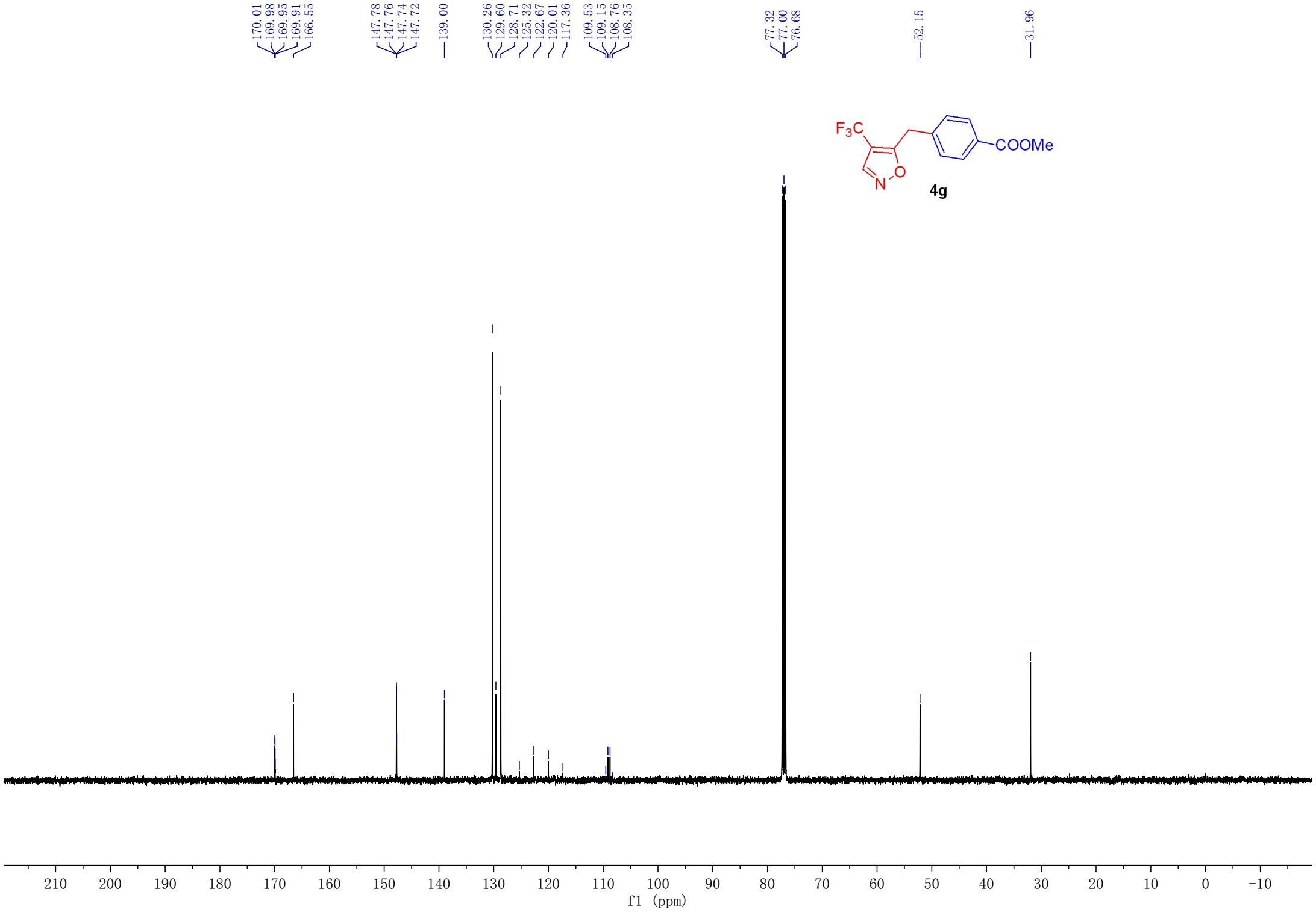

8.37
7.61
7.59
7.39
7.37
7.26
4.31
F3C
CF3
O
N
4f
1.00
2.10
2.10
2.11
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-56.83
-62.74
F3C
CF3
N
O
4f
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)


169.83
169.80
169.77
169.74
147.78
147.76
147.74
137.95
130.22
129.90
129.07
126.02
125.98
125.94
125.91
125.26
109.22
108.83
108.44
77.32
77.00
76.68
31.78
F3C
CF3
N
O
4f
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)


8.36
8.01
7.99
7.33
7.31
7.26
4.30
3.91
F3C
COOMe
N
O
4g
1.00
2.08
2.04
2.16
3.20
0.5
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)


-56.80
F3C
COOMe
N
O
4g
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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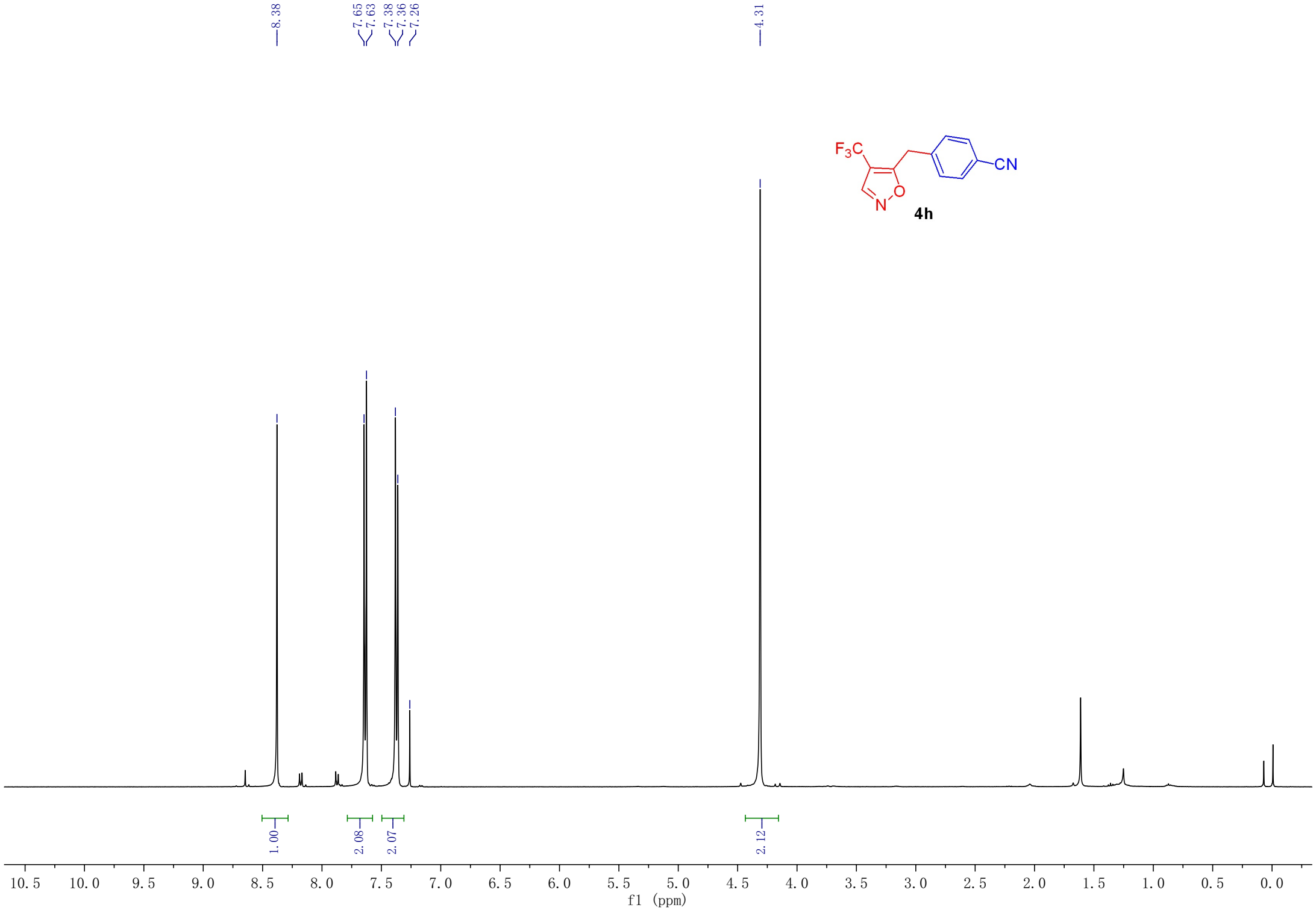
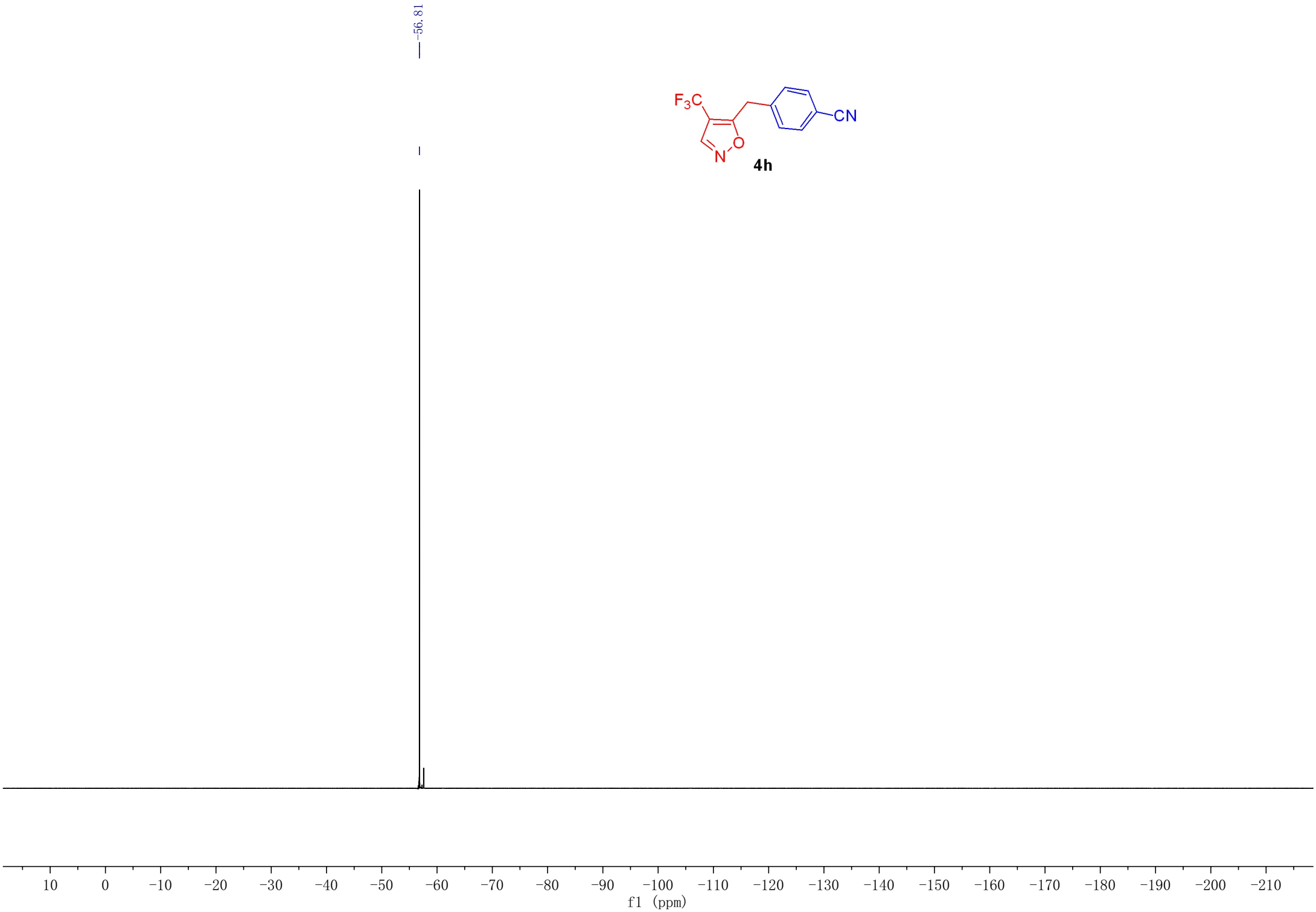
169.98
169.95
169.91
166.55
147.78
147.76
147.74
147.72
139.00
130.26
129.60
128.71
125.32
122.67
120.01
117.36
109.53
109.15
108.76
108.35
77.32
77.00
76.68
52.15
31.96
F3C
COOMe
N
O
4g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.38
7.65
7.63
7.38
7.36
7.26
4.31
F3C
CN
N
O
4h
1.00
2.08
2.07
2.12
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)


-56.81
F3C
CN
N
O
4h
10
0
-10
-20
-30
-40
-50
-60
-70
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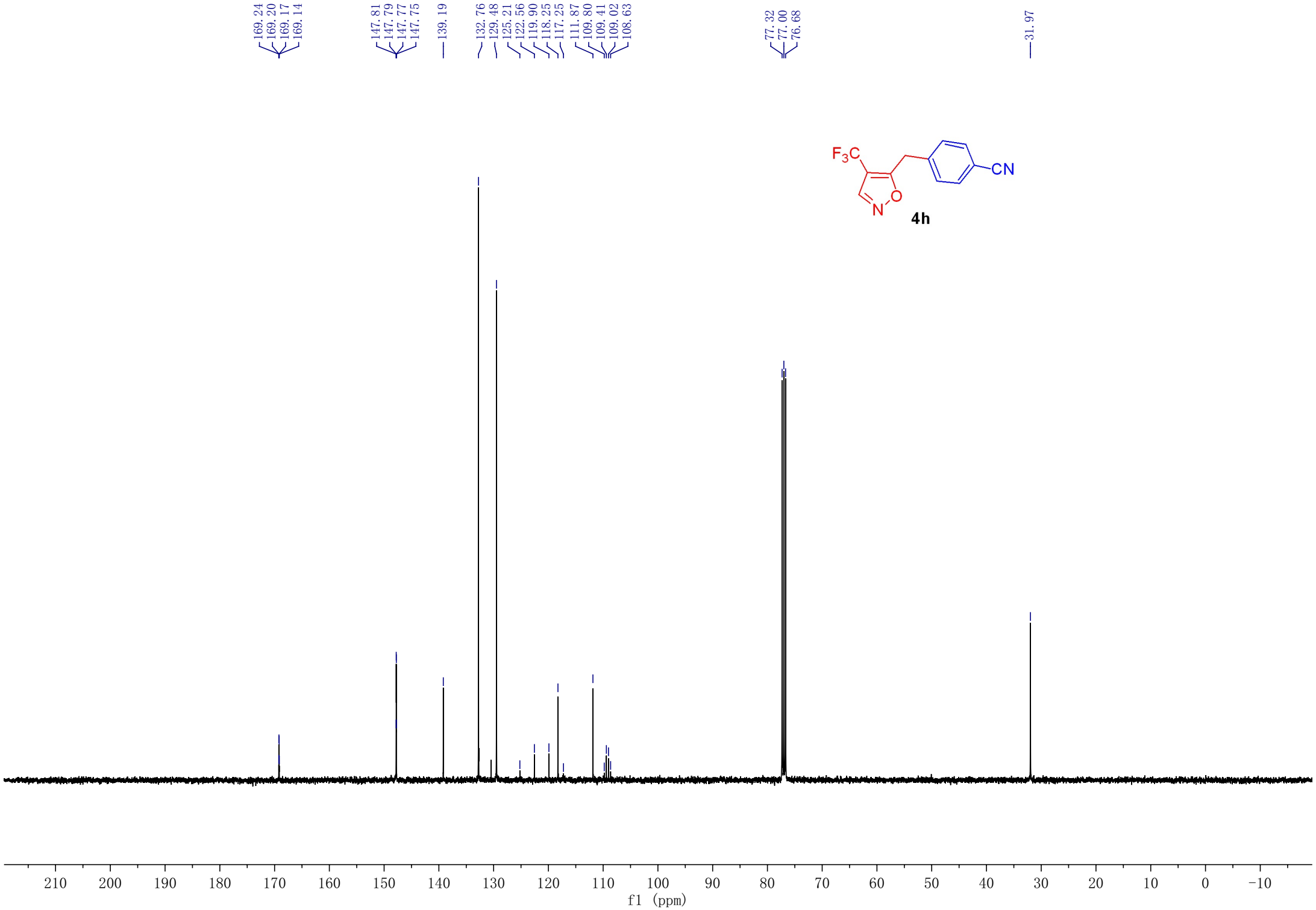
-170
-180
-190
-200
-210
f1 (ppm)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169.20
169.17
169.14
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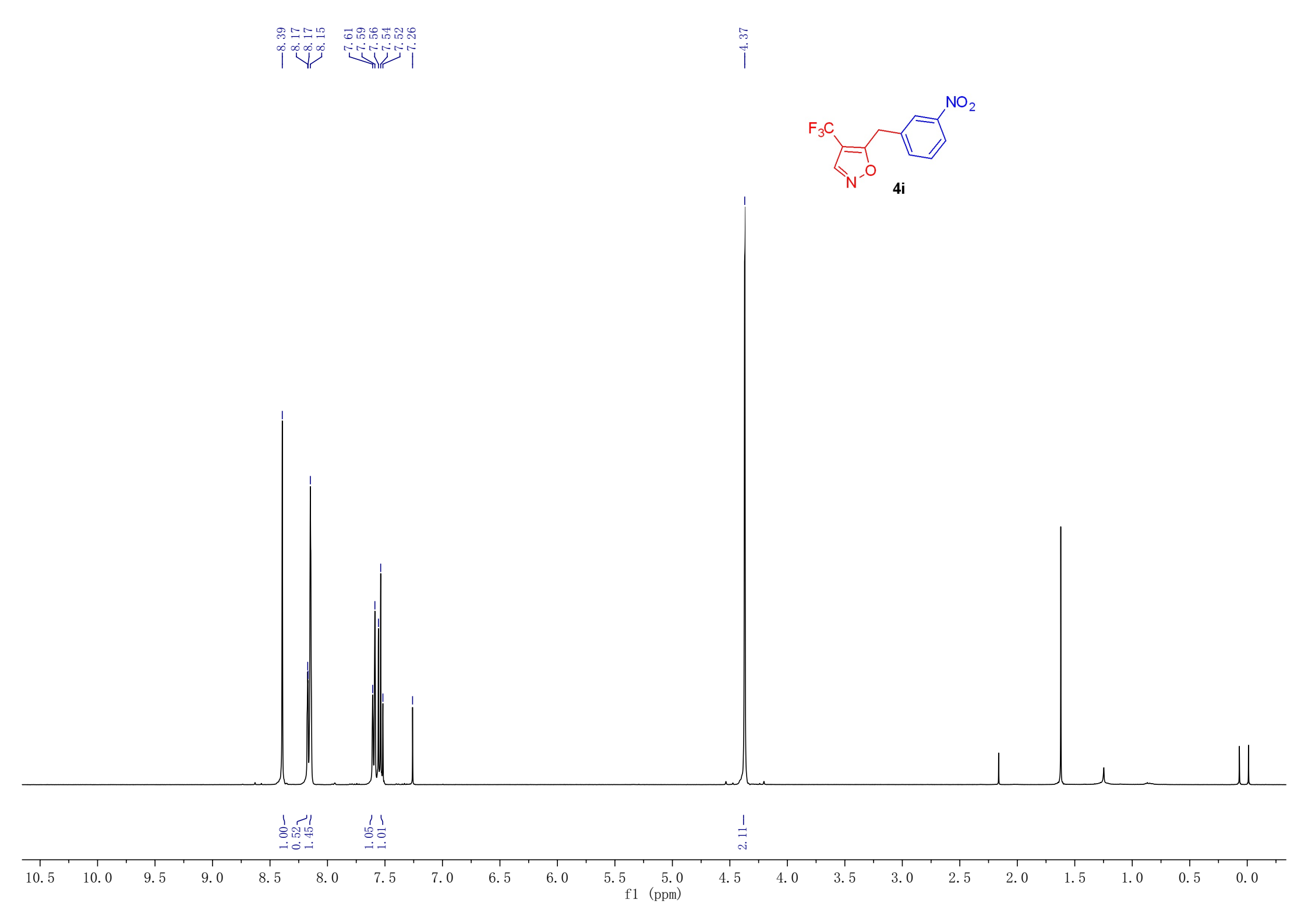
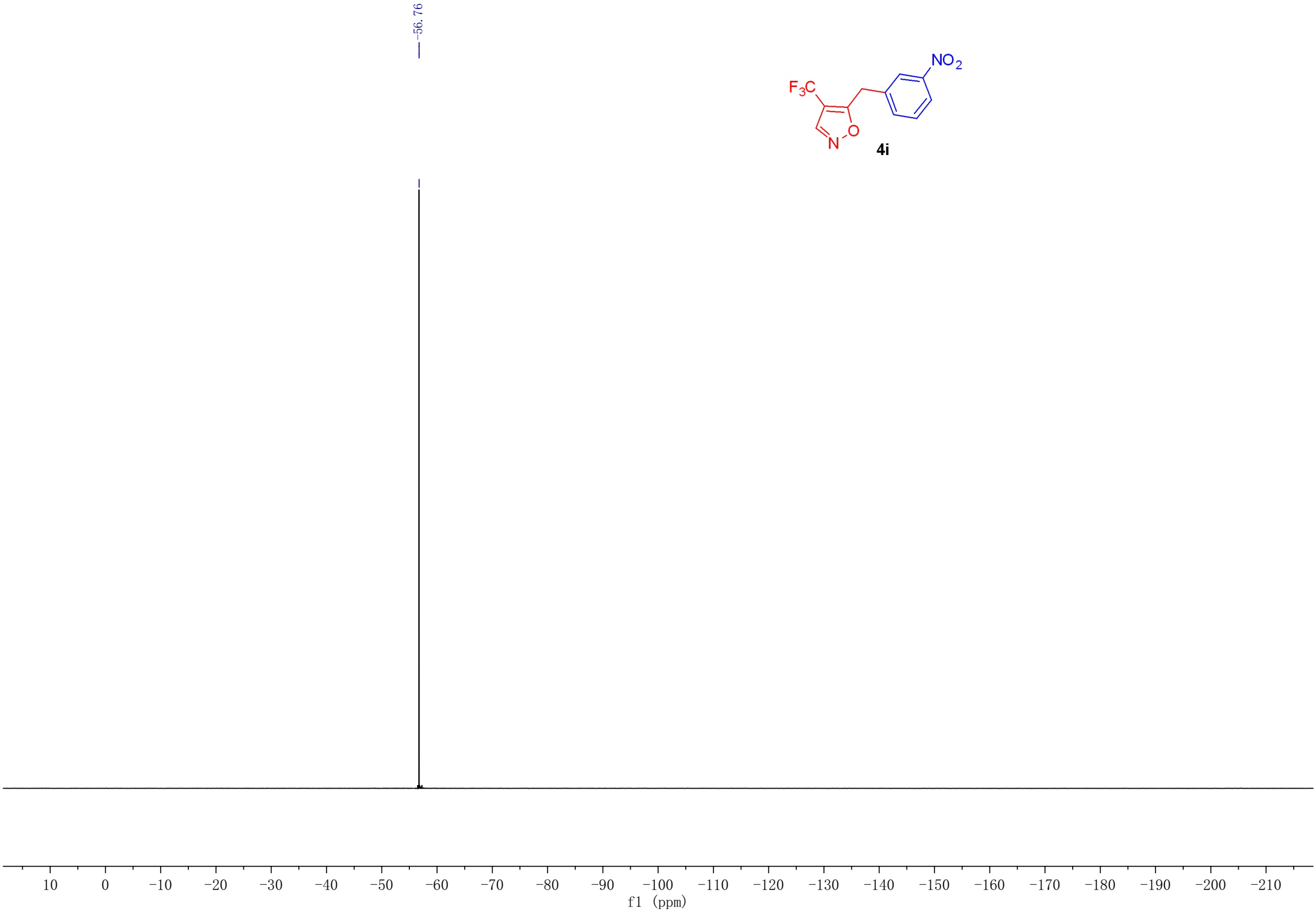
147.79
147.77
147.75
139.19
132.76
129.48
125.21
122.56
119.90
118.25
117.25
111.87
109.80
109.41
109.02
108.63
77.32
77.00
76.68
31.97
F3C
CN
N
O
4h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.39
8.17
8.17
8.15
7.61
7.59
7.56
7.54
7.52
7.26
4.37
NO2
F3C
O
N
4i
1.00
0.52
1.45
1.05
1.01
2.11
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)


-56.76
NO2
F3C
O
N
4i
10
0
-10
-20
-30
-40
-50
-60
-70
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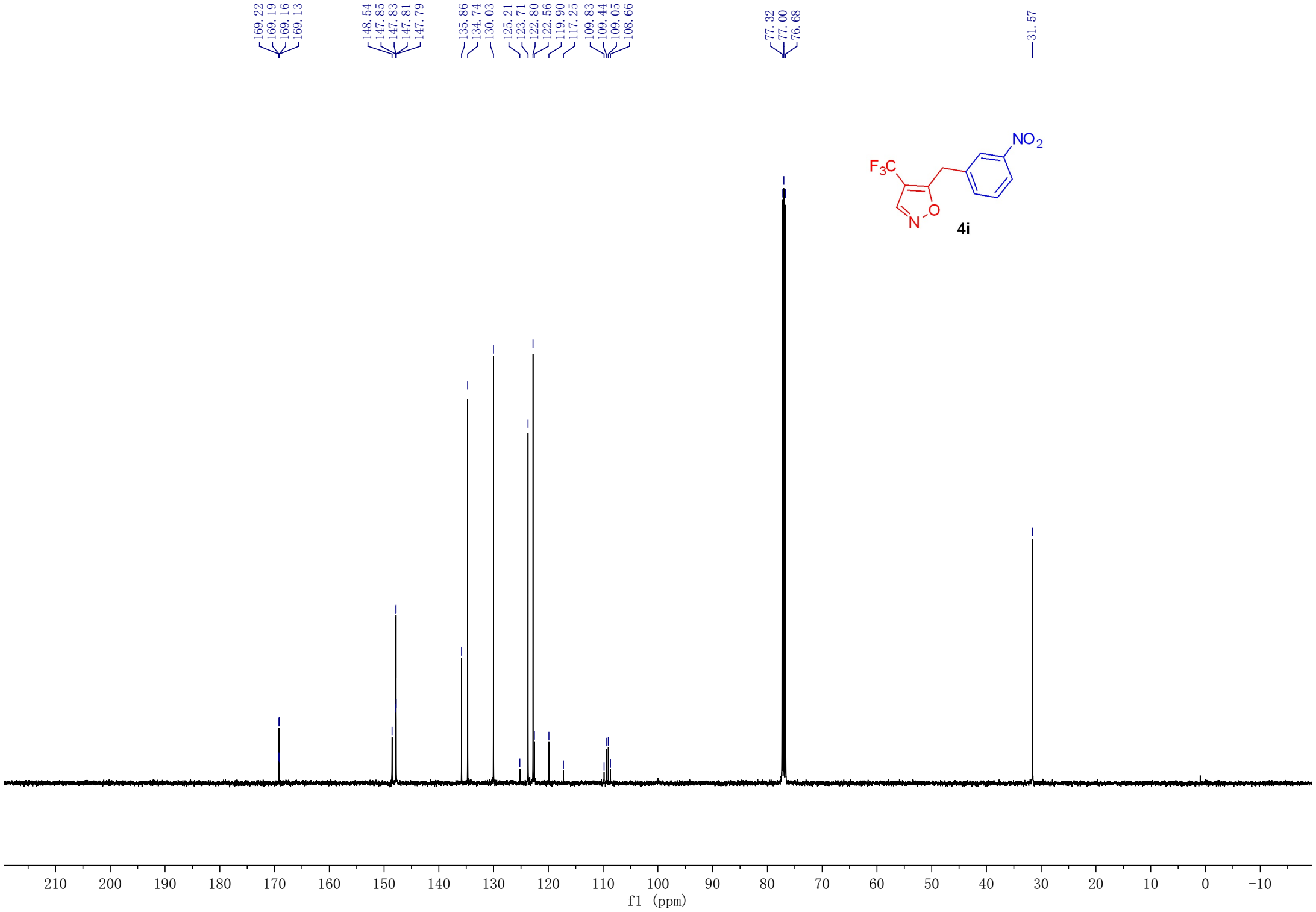
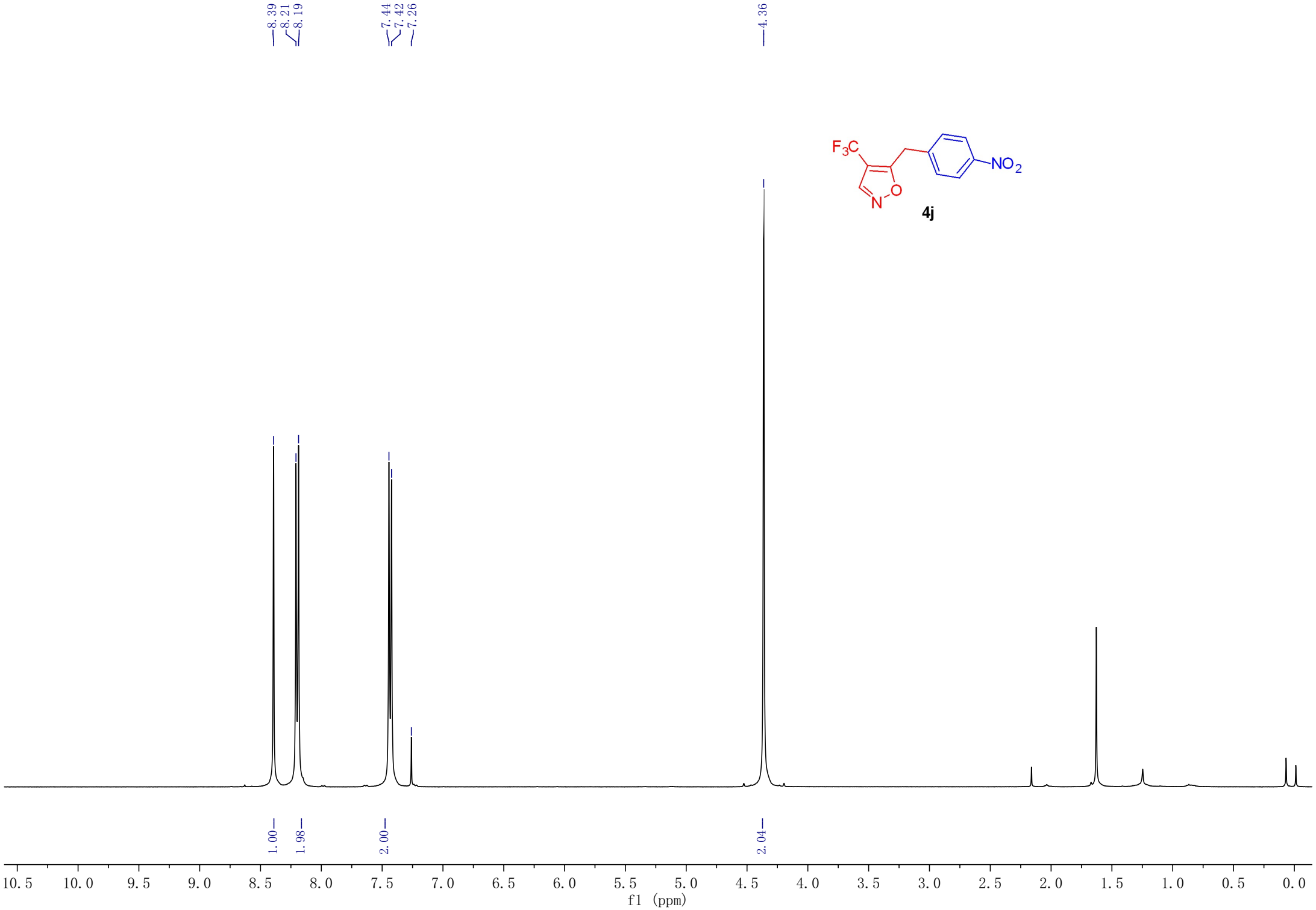
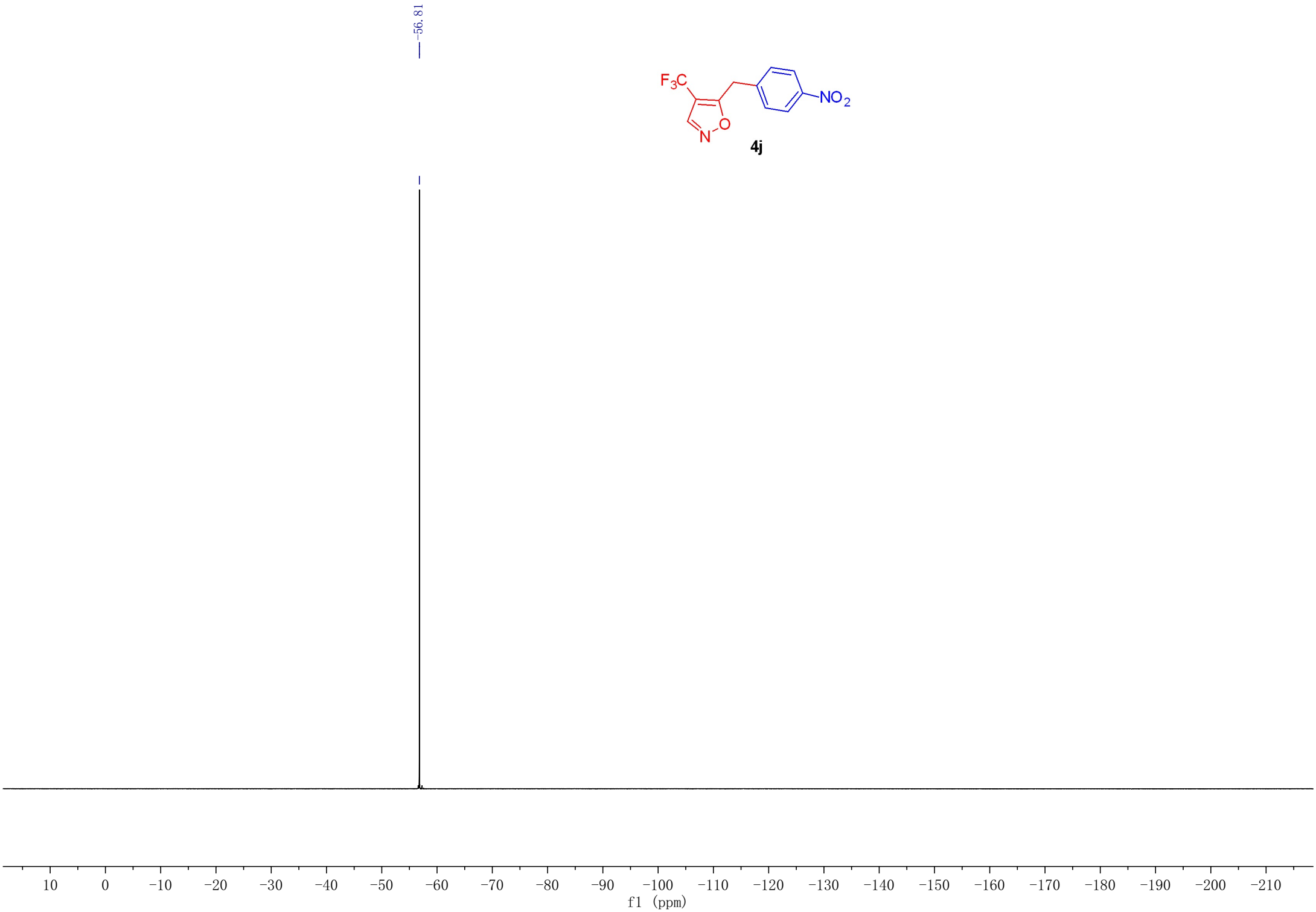
-170
-180
-190
-200
-210
f1 (ppm)


169.22
169.19
169.16
169.13
148.54
147.85
147.83
147.81
147.79
135.86
134.74
130.03
125.21
123.71
122.80
122.56
119.90
117.25
109.83
109.44
109.05
108.66
77.32
77.00
76.68
31.57
NO2
F3C
O
N
4i
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)


8.39
8.21
8.19
7.44
7.42
7.26
4.36
F3C
NO2
N
O
4j
1.00
1.98
2.00
2.04
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)


-56.81
F3C
NO2
N
O
4j
10
0
-10
-20
-30
-40
-50
-60
-70
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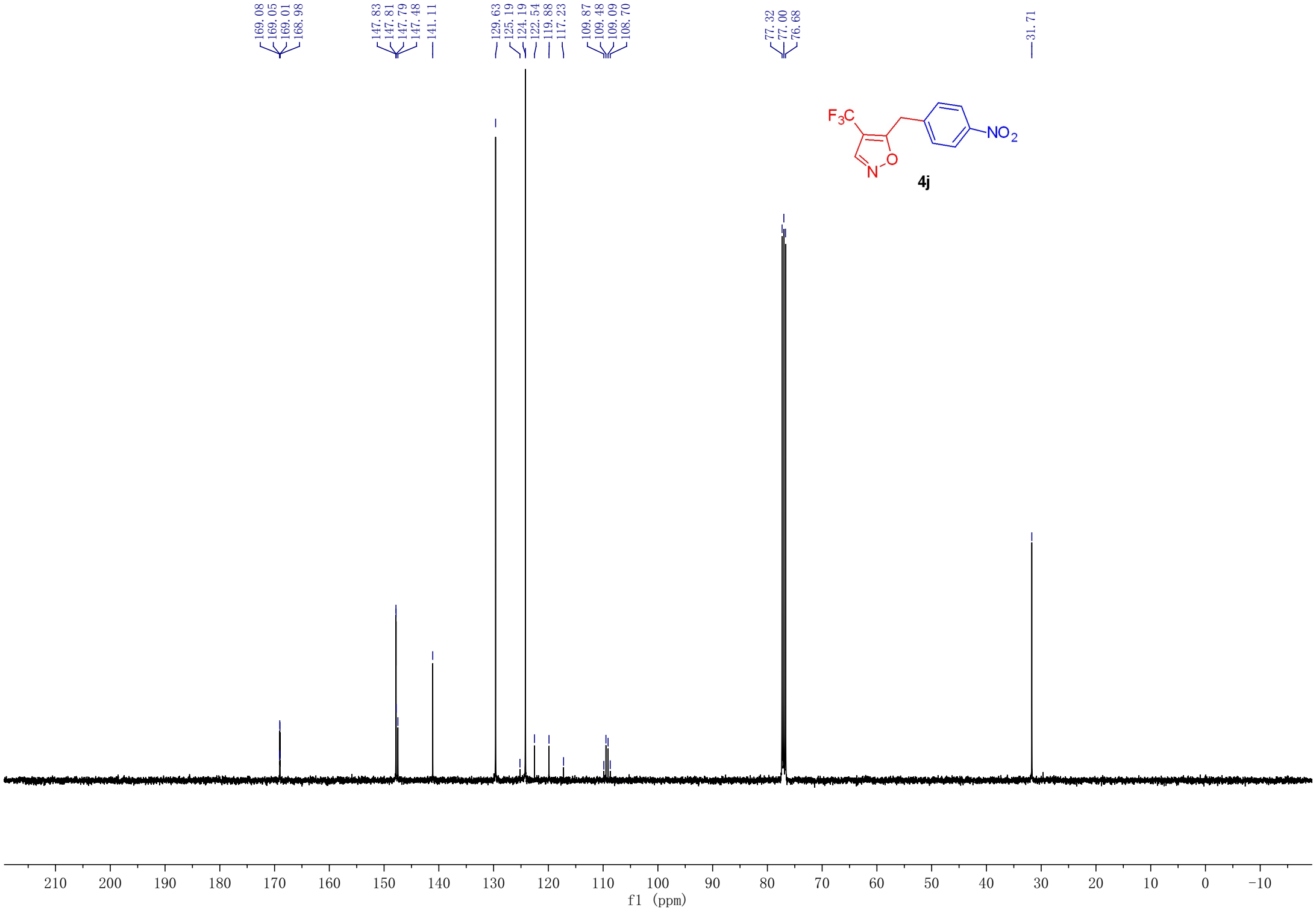
-160
-170
-180
-190
-200
-210
f1 (ppm)


169.08
169.05
169.01
168.98
147.83
147.81
147.79
147.48
141.11
129.63
125.19
124.19
122.54
119.88
117.23
109.87
109.48
109.09
108.70
77.32
77.00
76.68
31.71
F3C
NO2
N
O
4j
210
200
190
180
170
160
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140
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120
110
100
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80
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30
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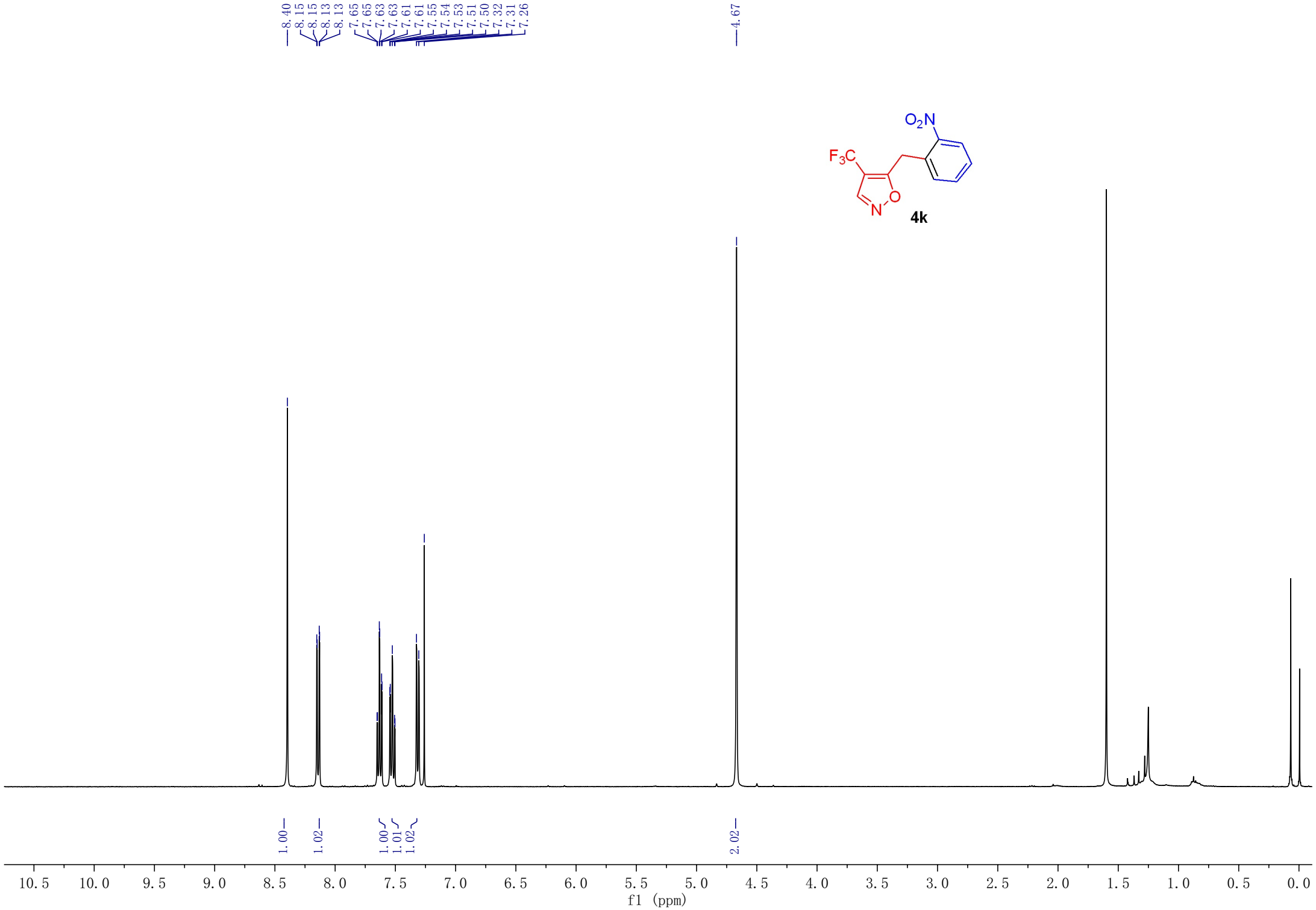
f1 (ppm)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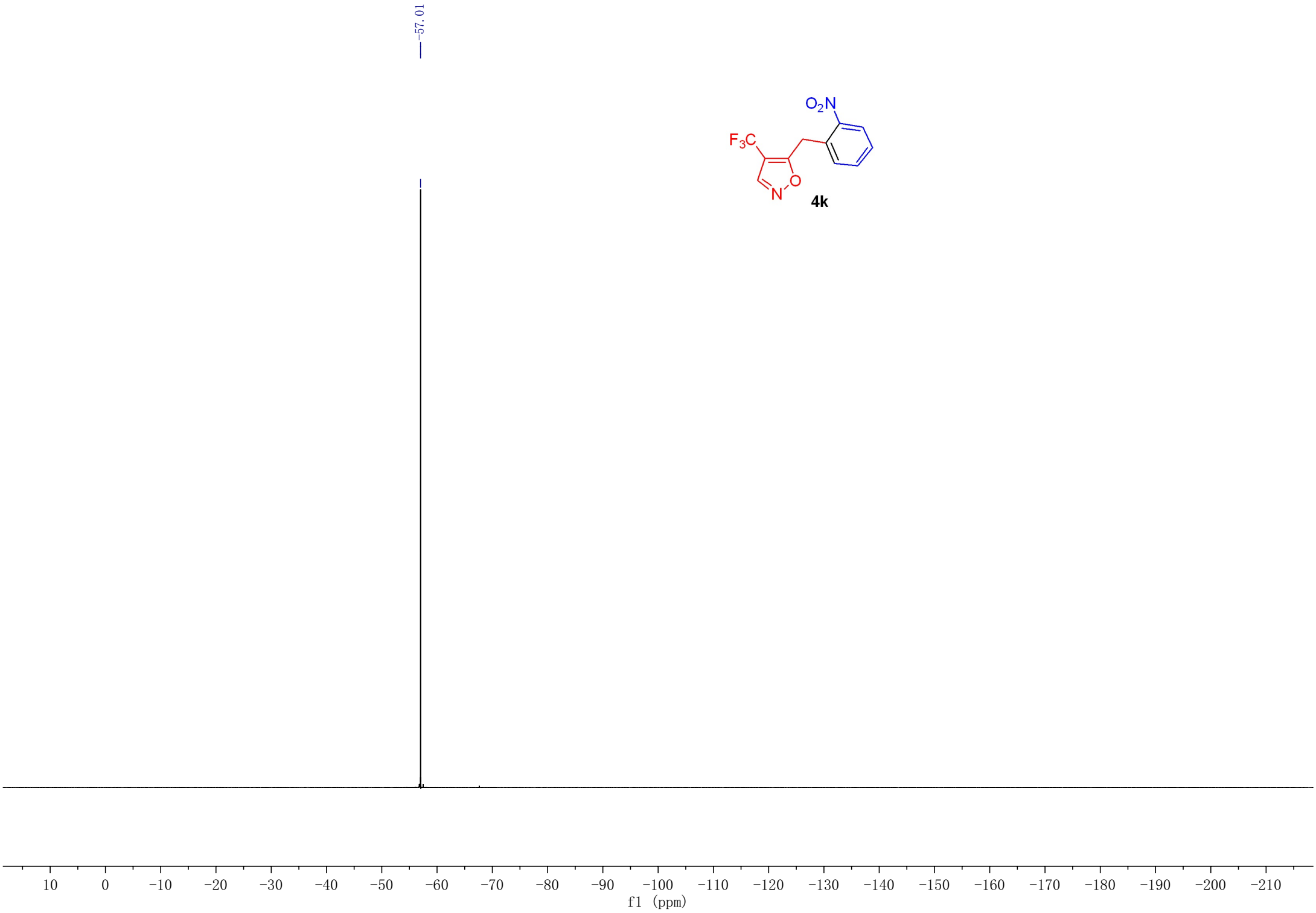
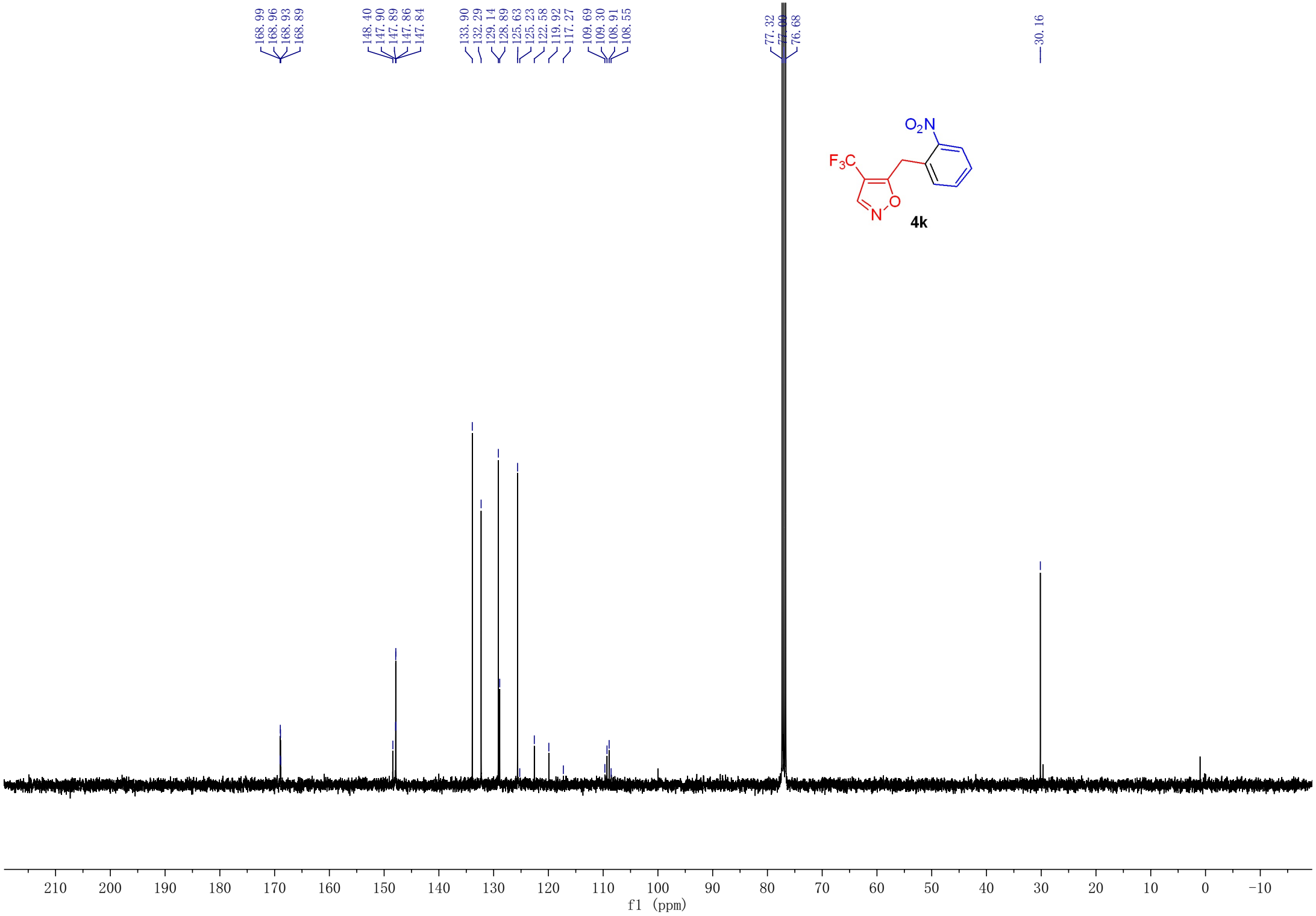
8.15
8.15
8.13
8.13
7.65
7.65
7.63
7.63
7.61
7.61
7.55
7.54
7.53
7.51
7.50
7.32
7.31
7.26
4.67
O2N
F3C
O
N
4k
1.00
1.02
1.00
1.01
1.02
2.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-57.01
O_2N
F_3C
O
N
4k
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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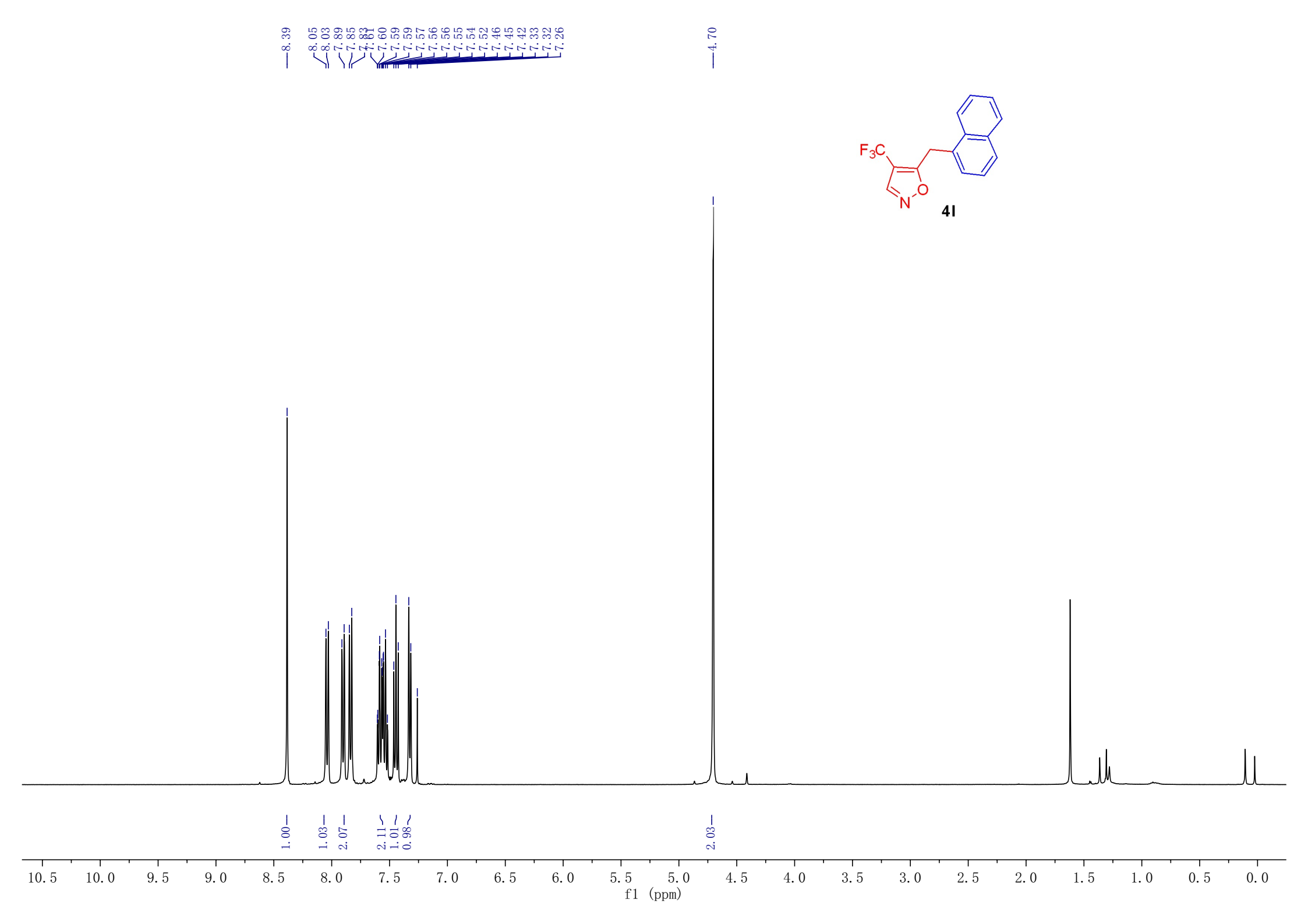
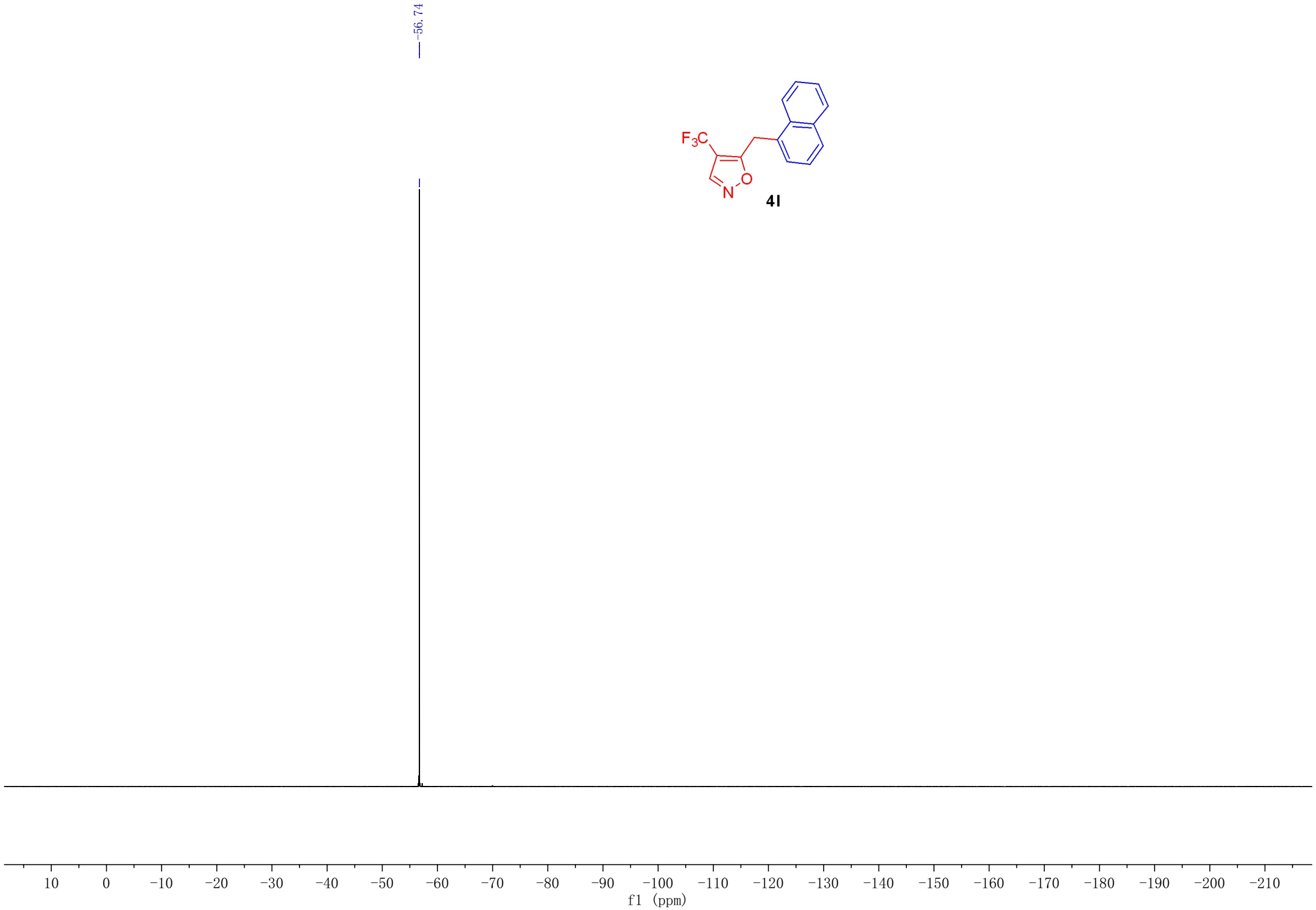
168.96
168.93
168.89
148.40
147.90
147.89
147.86
147.84
133.90
132.29
129.14
128.89
125.63
125.23
122.58
119.92
117.27
109.69
109.30
108.91
108.55
77.32
77.00
76.68
30.16
O2N
F3C
O
N
4k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.39
8.05
8.03
7.89
7.85
7.83
7.61
7.60
7.59
7.59
7.57
7.56
7.56
7.55
7.54
7.52
7.46
7.45
7.42
7.33
7.32
7.26
4.70
F3C
N
O
4l
1.00
1.03
2.07
2.11
1.01
0.98
2.03
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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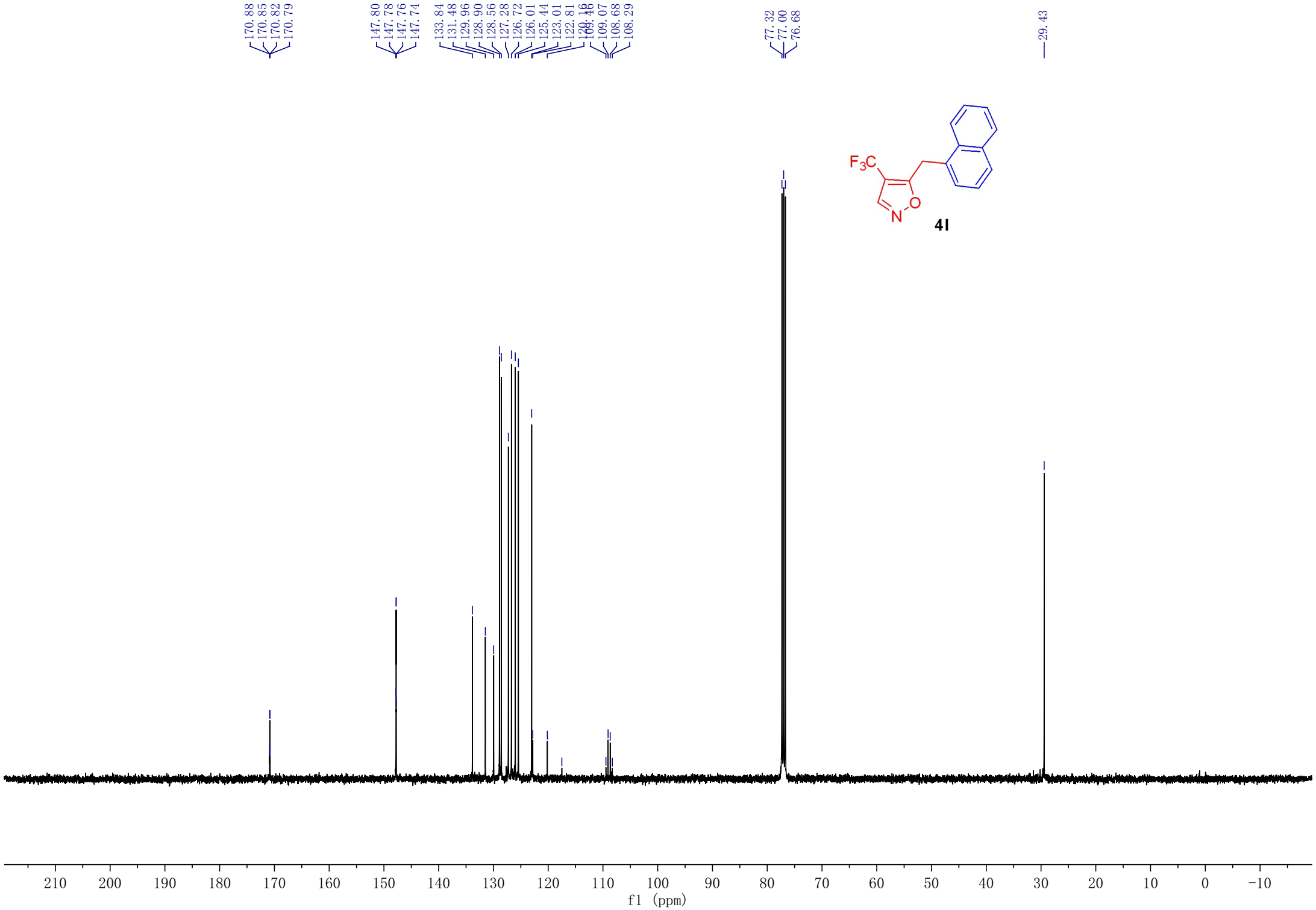
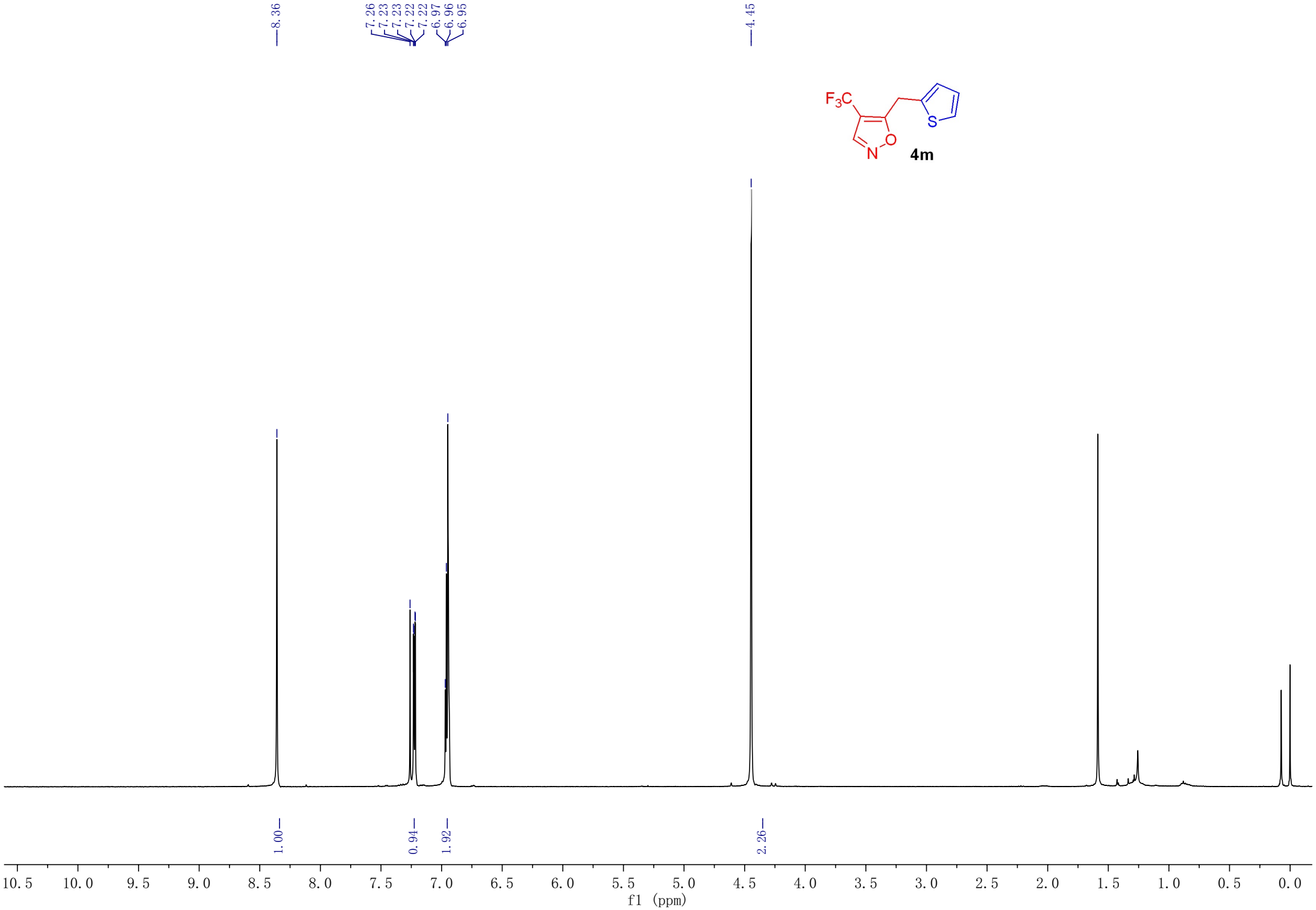
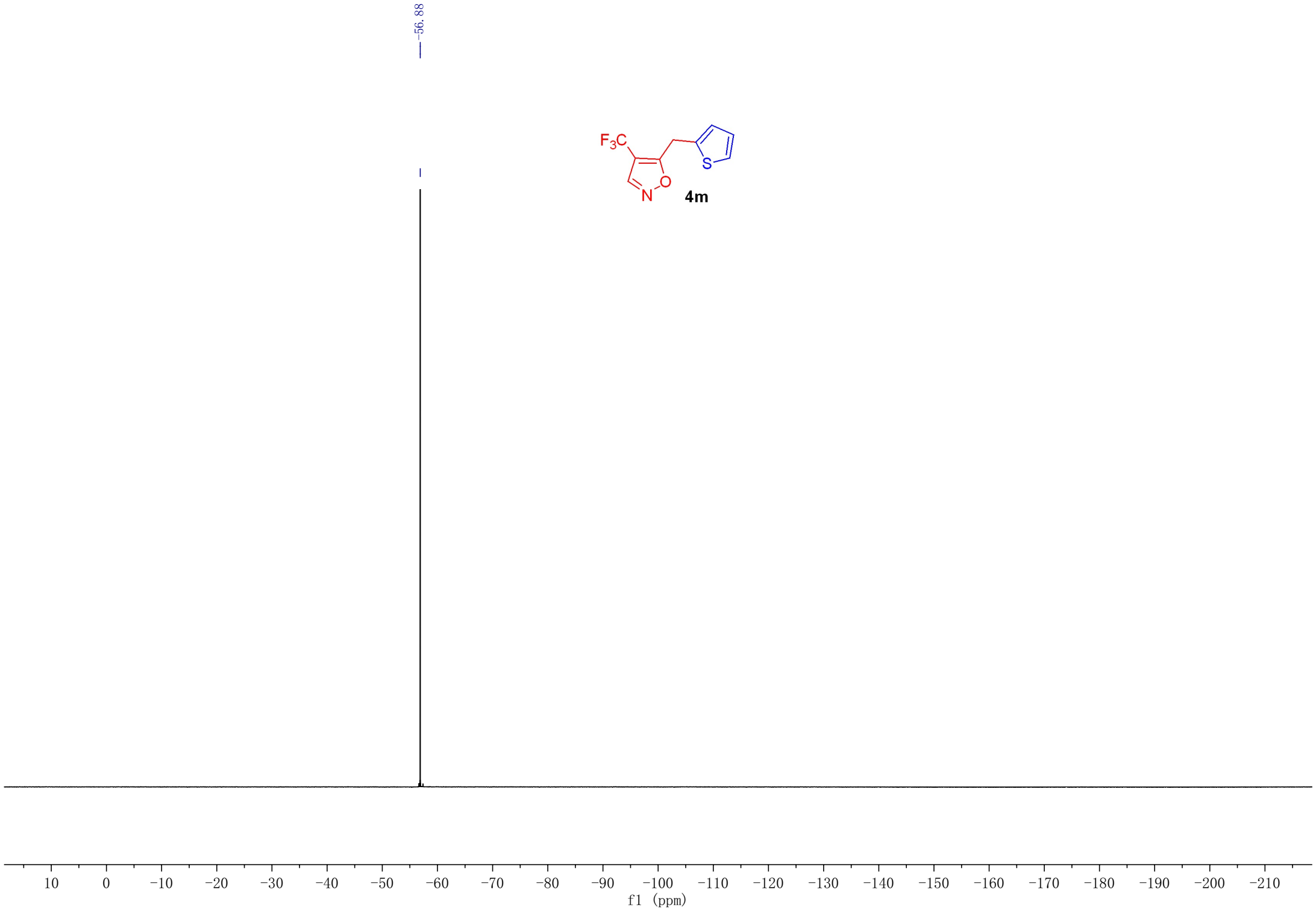
F3C
O
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

4l


170.88
170.85
170.82
170.79
147.80
147.78
147.76
147.74
133.84
131.48
129.96
128.90
128.56
127.28
126.72
126.01
125.44
123.01
122.81
109.07
108.68
108.29
77.32
77.00
76.68
29.43
F3C
N
O
4l
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)


8.36
7.26
7.23
7.23
7.22
7.22
6.97
6.96
6.95
4.45
F3C
S
O
N
4m
1.00
0.94
1.92
2.26
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-56.88
F3C
S
O
N
4m
10
0
-10
-20
-30
-40
-50
-60
-70
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-120
-130
-140
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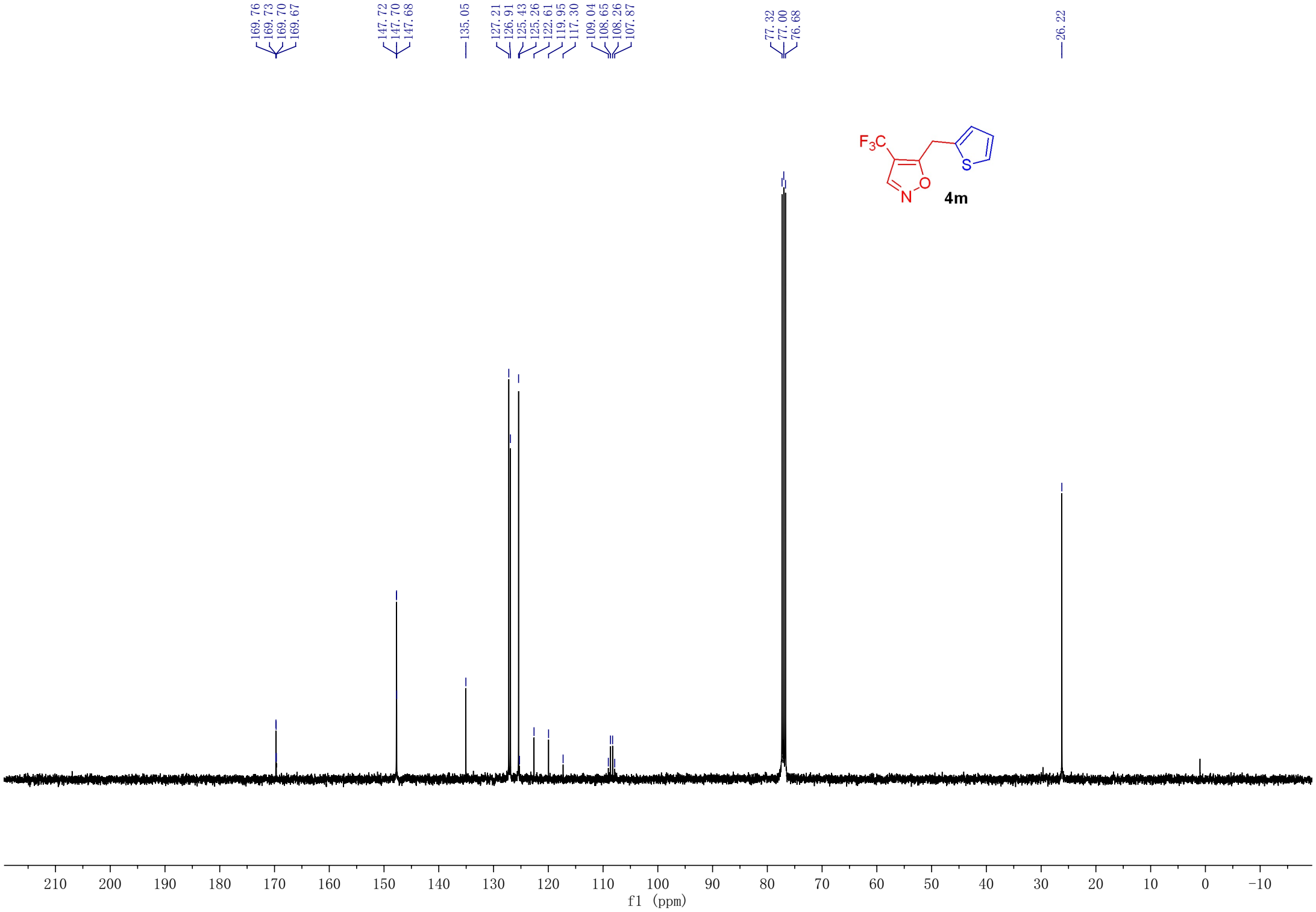
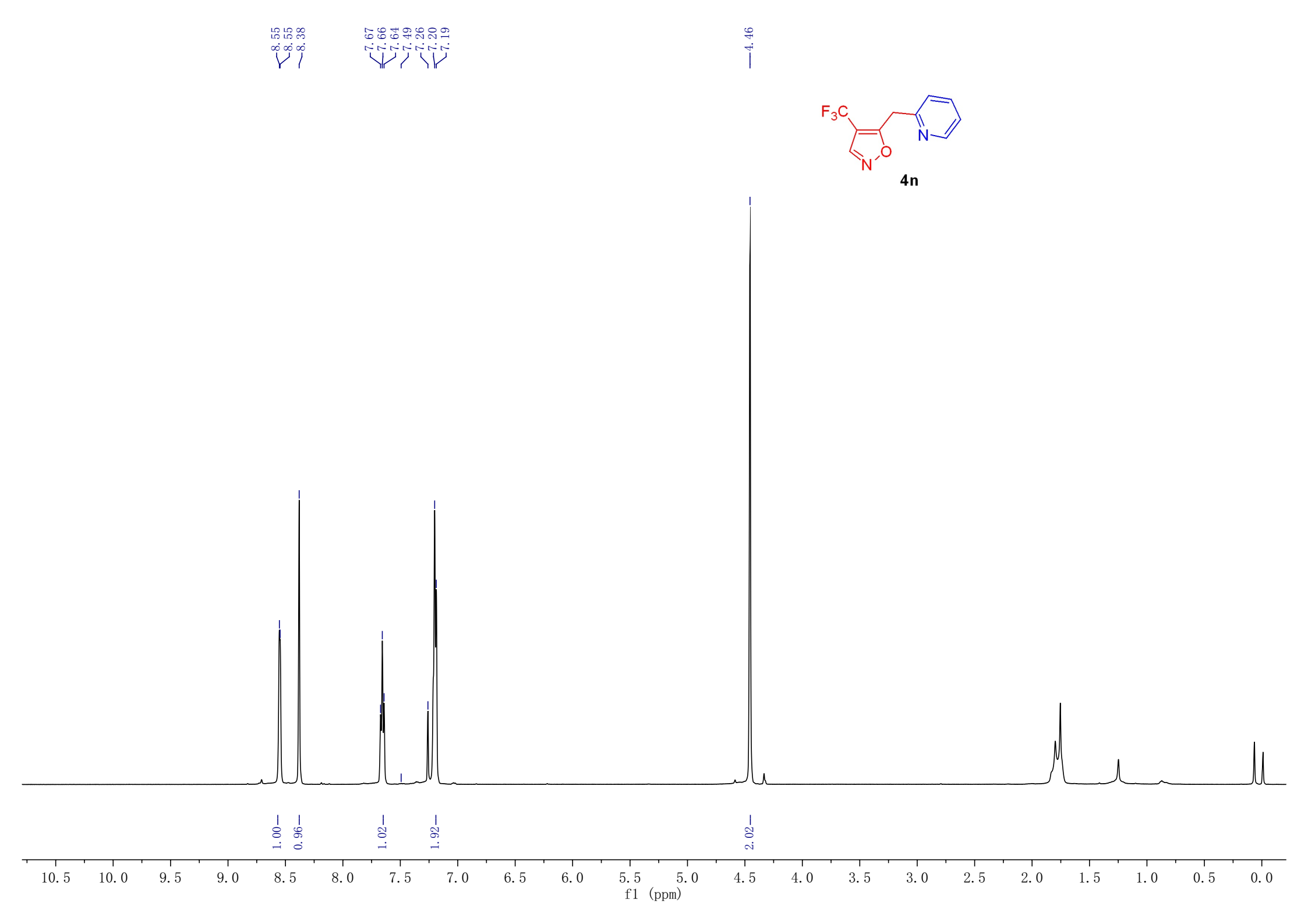
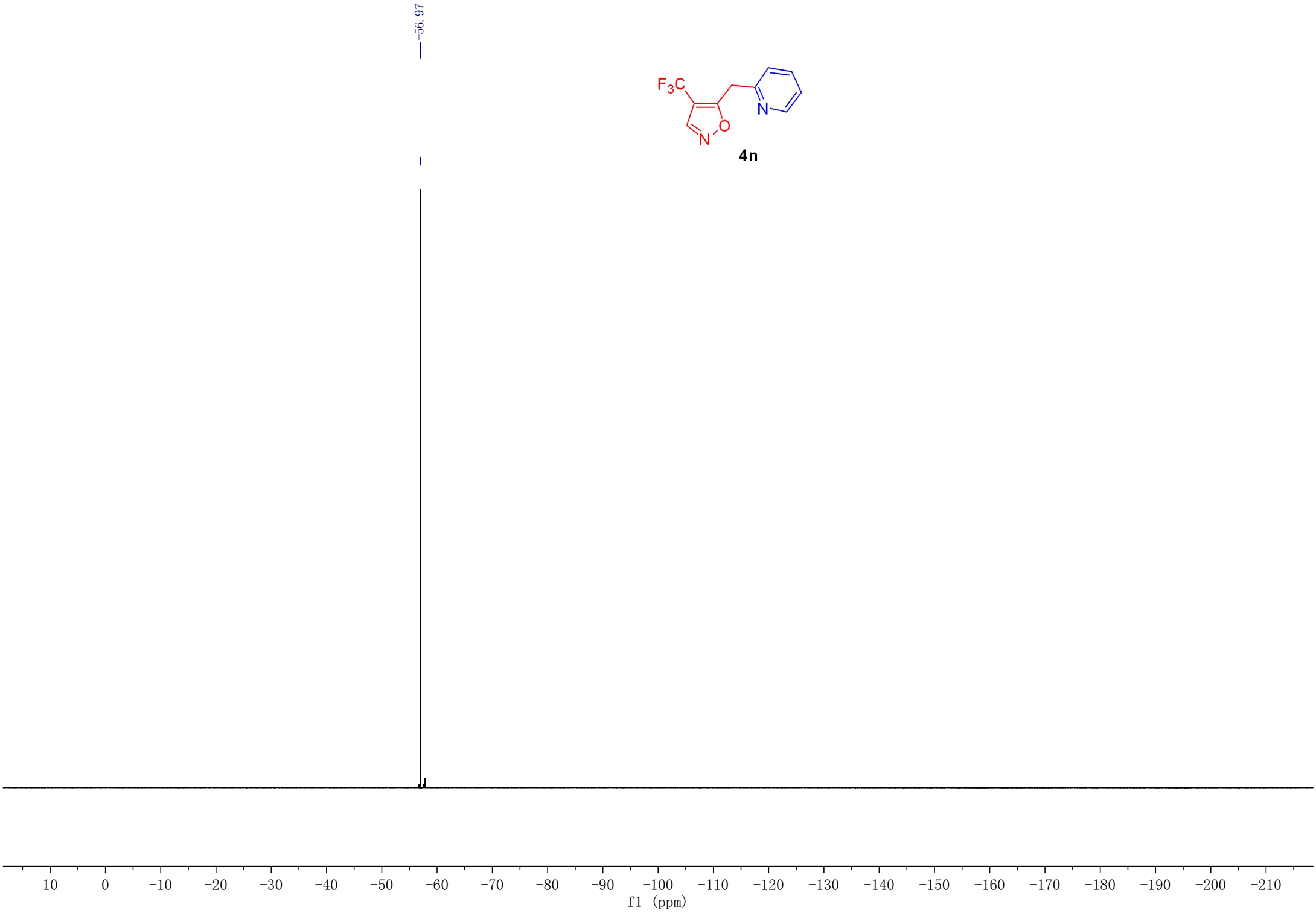
-160
-170
-180
-190
-200
-210
f1 (ppm)


169.76
169.73
169.70
169.67
147.72
147.70
147.68
135.05
127.21
126.91
125.43
125.26
122.61
119.95
117.30
109.04
108.65
108.26
107.87
77.32
77.00
76.68
26.22
F3C
S
O
N
4m
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)


8.55
8.55
8.38
7.67
7.66
7.64
7.49
7.26
7.20
7.19
4.46
F3C
N
O
N
4n
1.00
0.96
1.02
1.92
2.02
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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F3C
N
O
N
4n
10
0
-10
-20
-30
-40
-50
-60
-70
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-130
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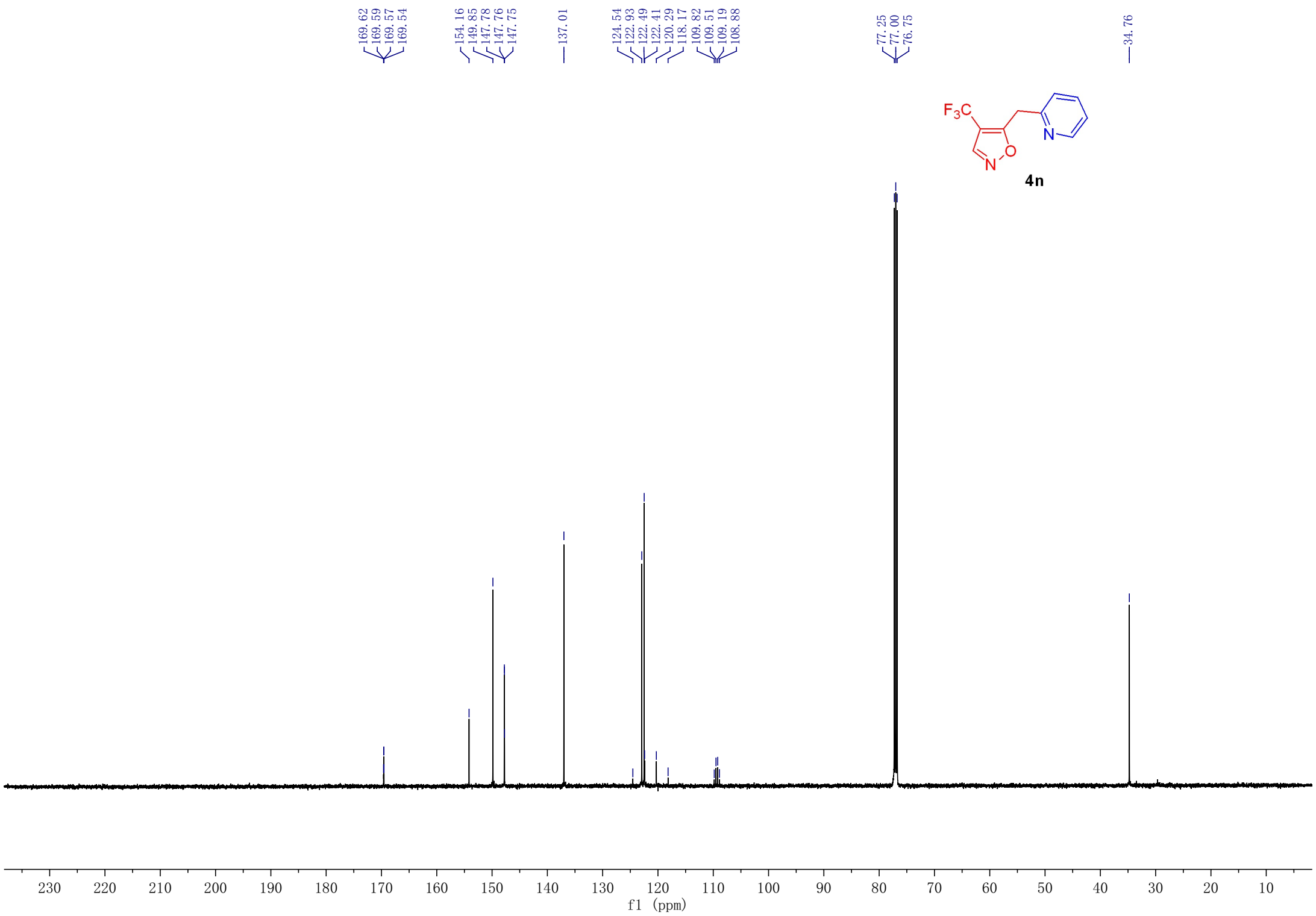
-160
-170
-180
-190
-200
-210
f1 (ppm)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169.54
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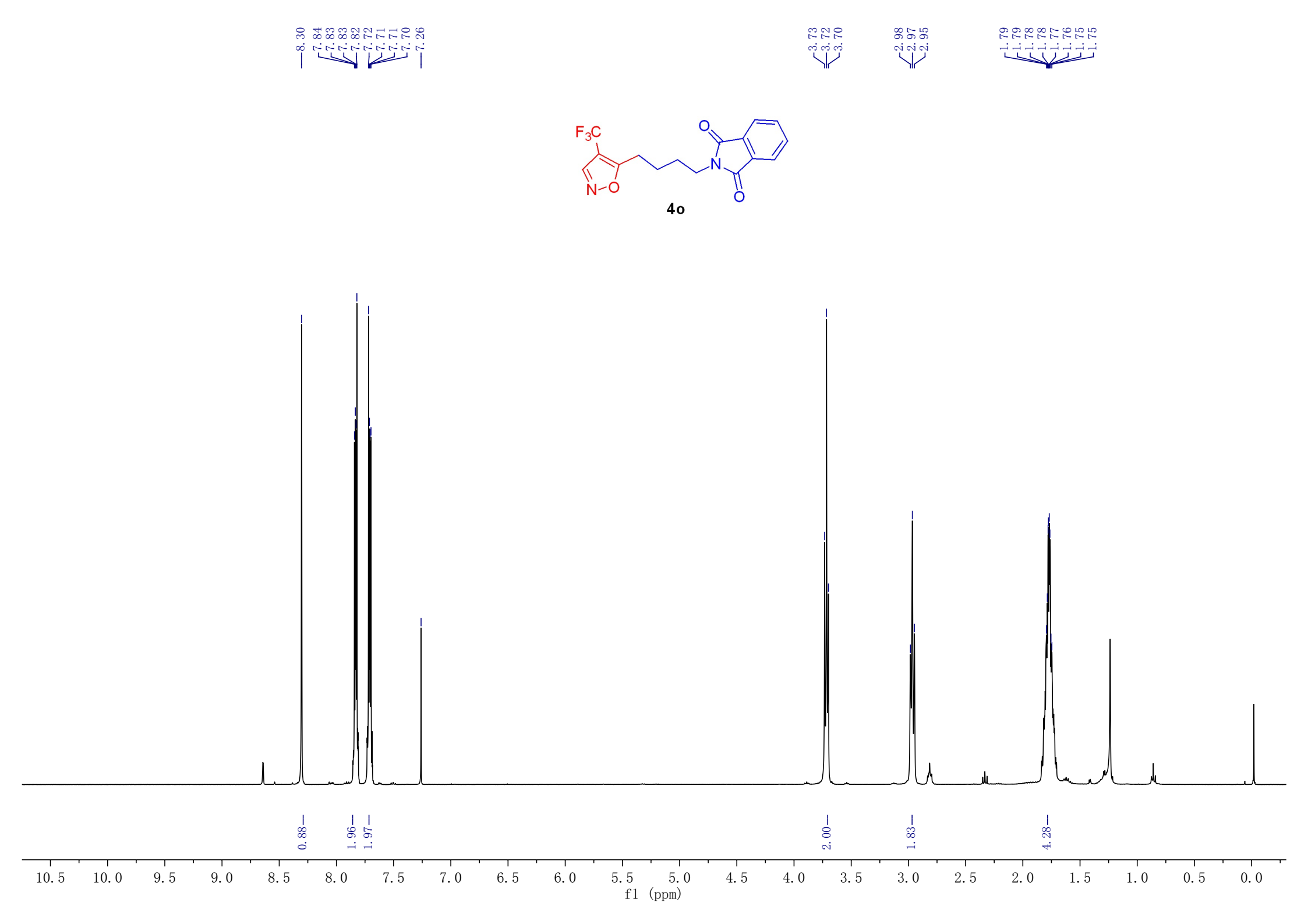
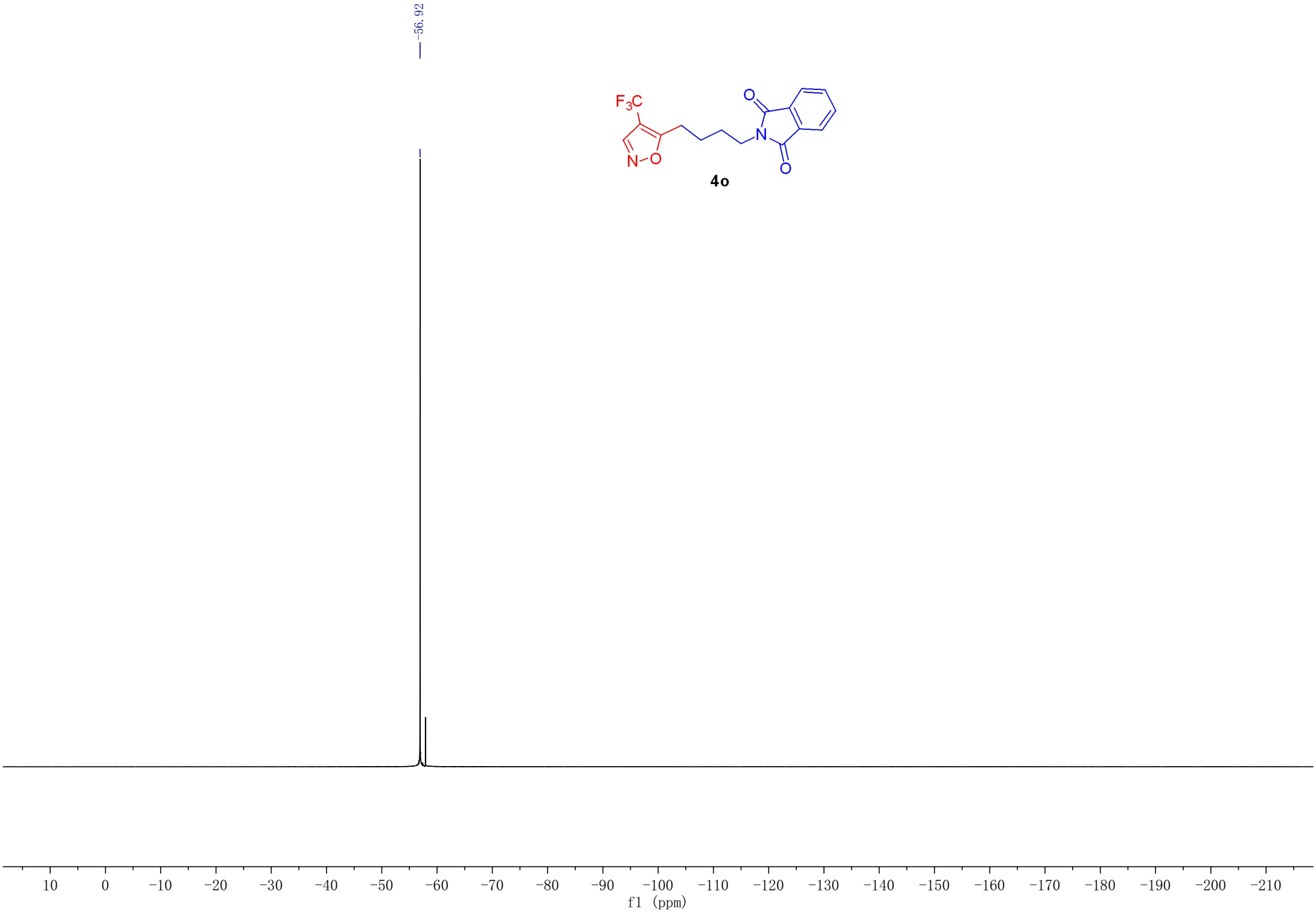
149.85
147.78
147.76
147.75
137.01
124.54
122.93
122.49
122.41
120.29
118.17
109.82
109.51
109.19
108.88
77.25
77.00
76.75
34.76
F3C
N
O
N
4n
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.30
7.84
7.83
7.83
7.82
7.72
7.71
7.71
7.70
7.26
3.73
3.72
3.70
2.98
2.97
2.95
1.79
1.79
1.78
1.78
1.77
1.76
1.75
1.75
F3C
O
N
O
N
O
O
4o
0.88
1.96
1.97
2.00
1.83
4.28
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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O
O
N
O
O
4o
10
0
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-20
-30
-40
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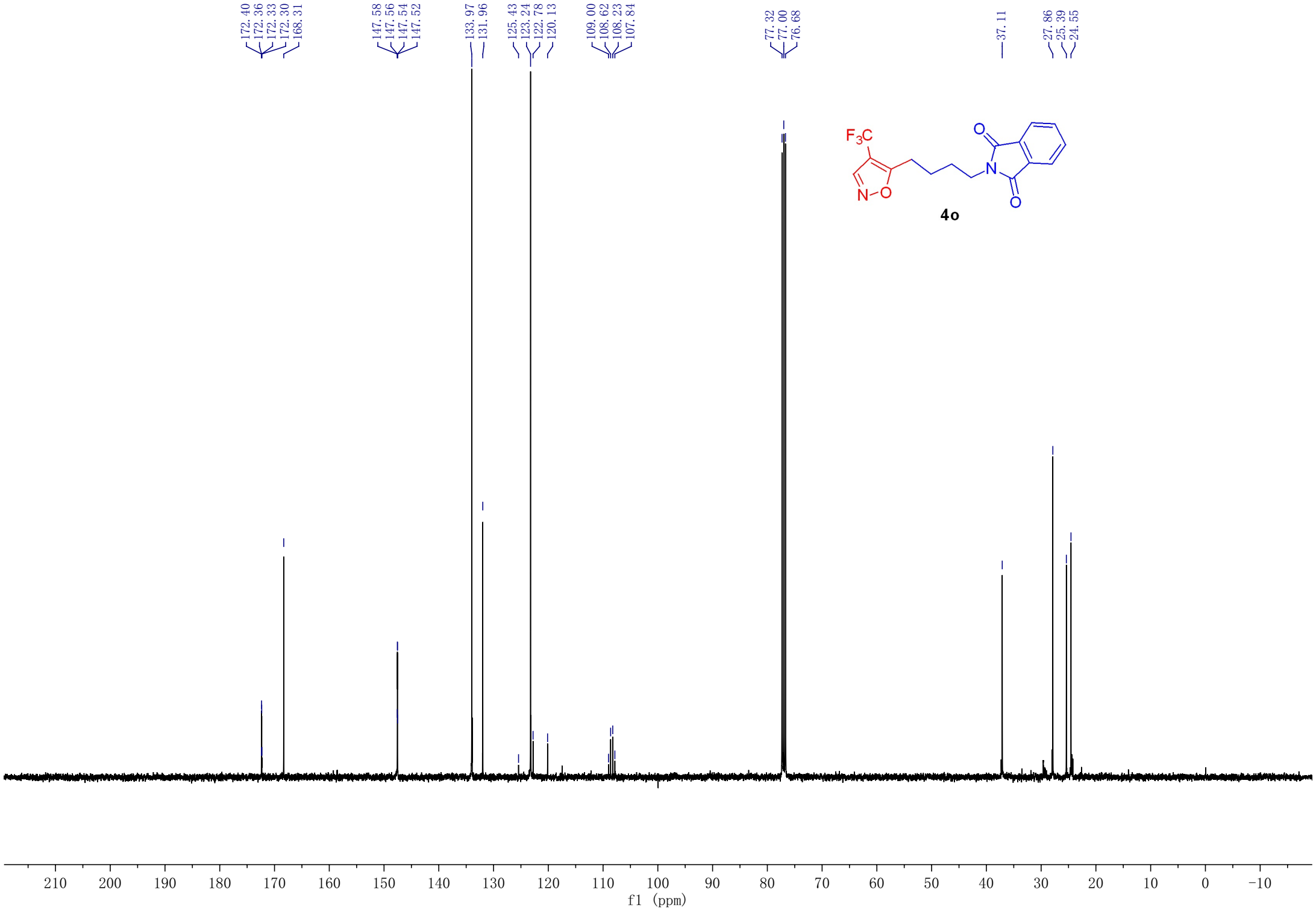
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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172.30
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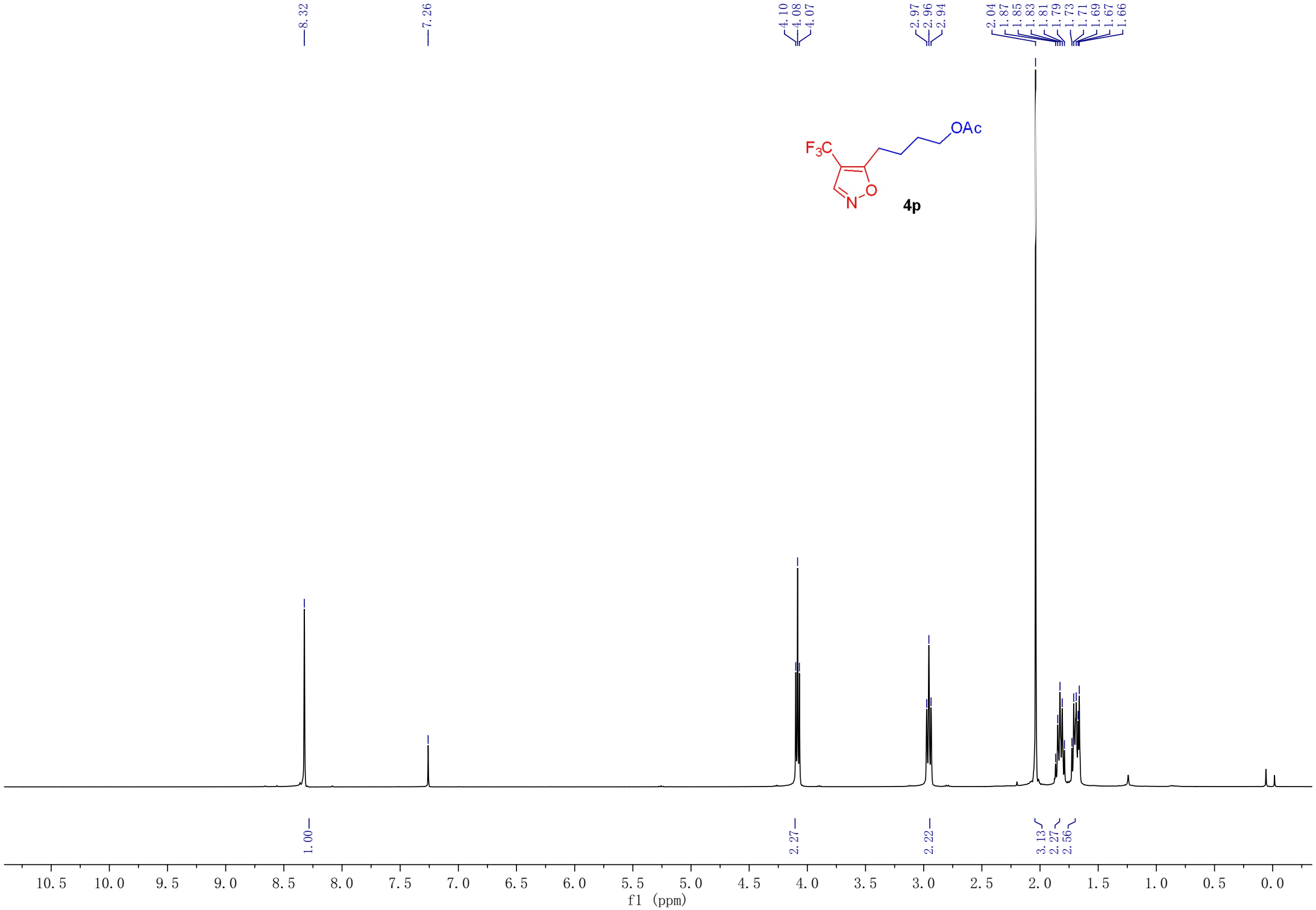
147.54
147.52
133.97
131.96
125.43
123.24
122.78
120.13
109.00
108.62
108.23
107.84
77.32
77.00
76.68
37.11
27.86
25.39
24.55
F3C
O
N
N-O
O
O
4o
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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4.07
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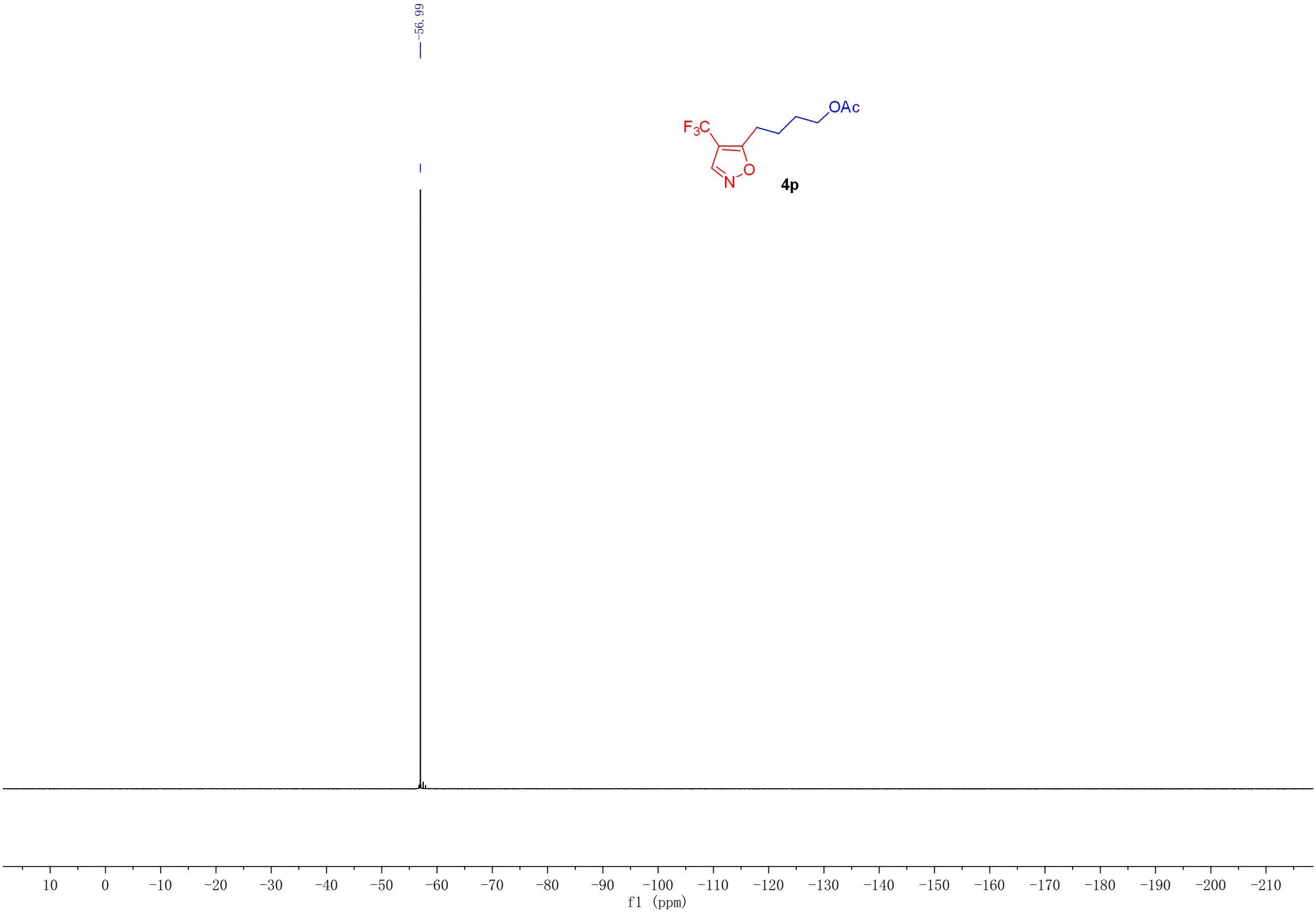
2.96
2.94
2.04
1.87
1.85
1.83
1.81
1.79
1.73
1.71
1.69
1.67
1.66
F3C
OAc
N
O
4p
1.00
2.27
2.22
3.13
2.27
2.56
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-56.99
OAc
F3C
N
O
4p
10
0
-10
-20
-30
-40
-50
-60
-70
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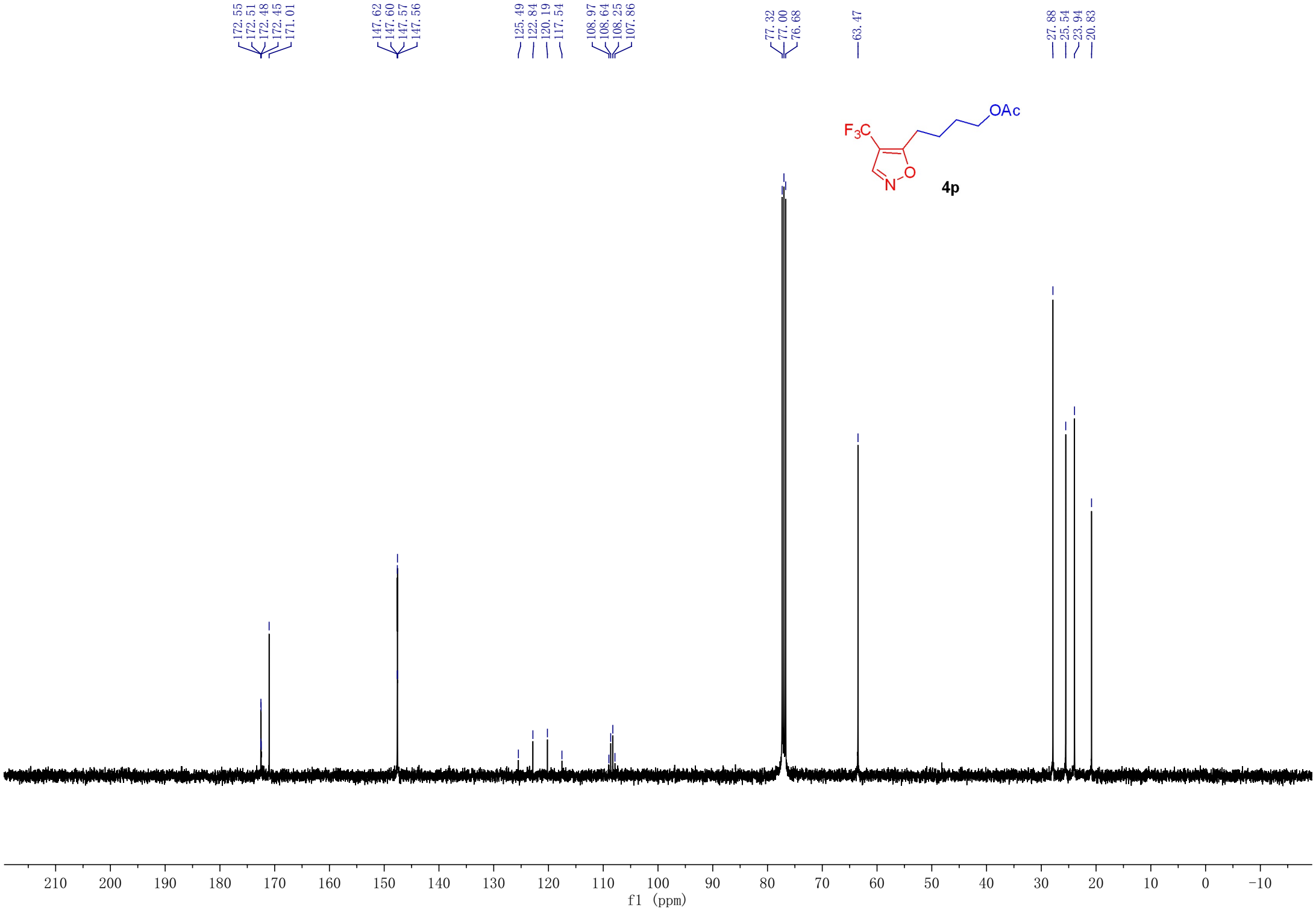
-160
-170
-180
-190
-200
-210
f1 (ppm)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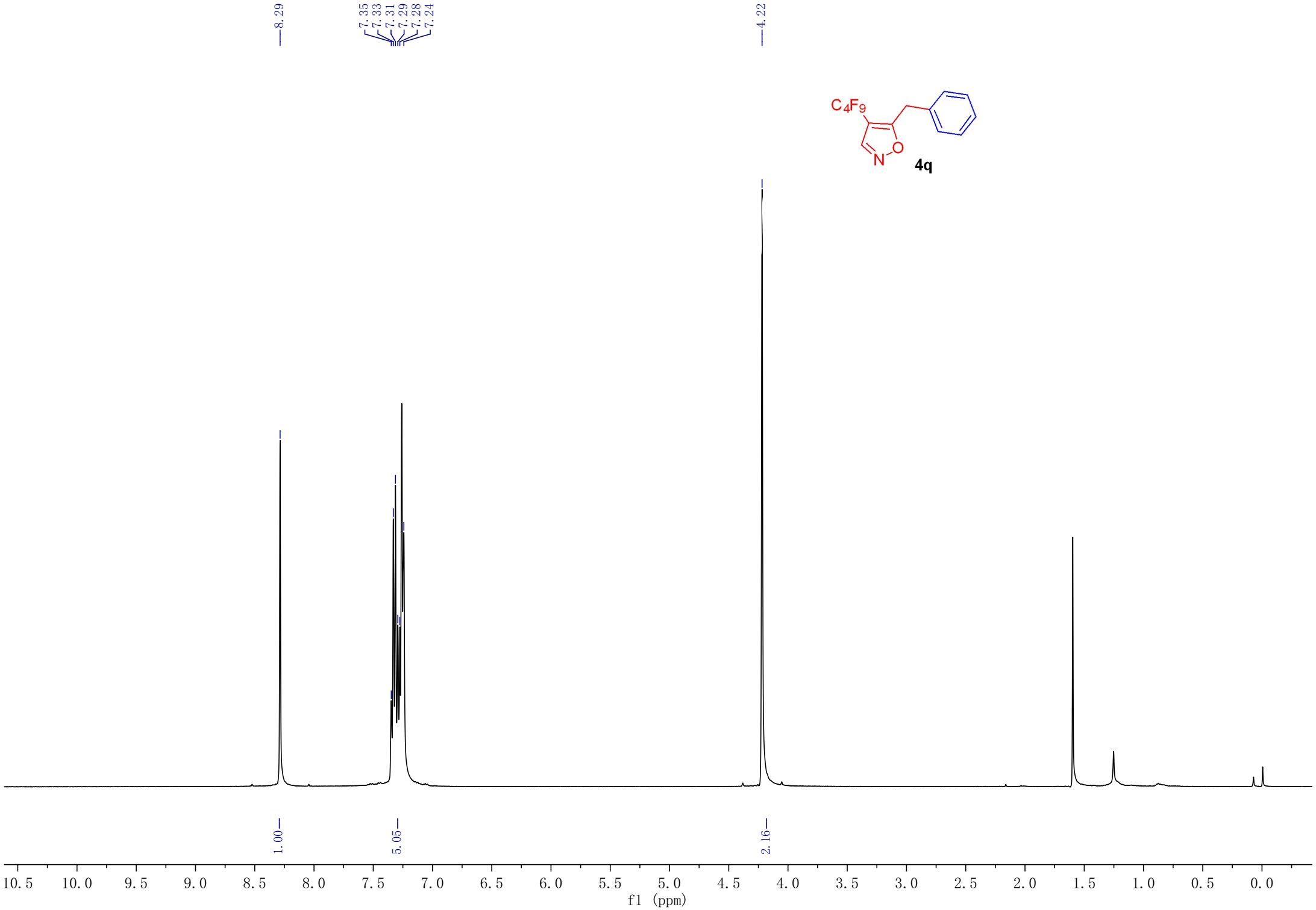
147.57
147.56
125.49
122.84
120.19
117.54
108.97
108.64
108.25
107.86
77.32
77.00
76.68
63.47
27.88
25.54
23.94
20.83
OAc
F3C
O
N
4p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.29
7.35
7.33
7.31
7.29
7.28
7.24
4.22
C4F9
O
N
4q
1.00
5.05
2.16
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
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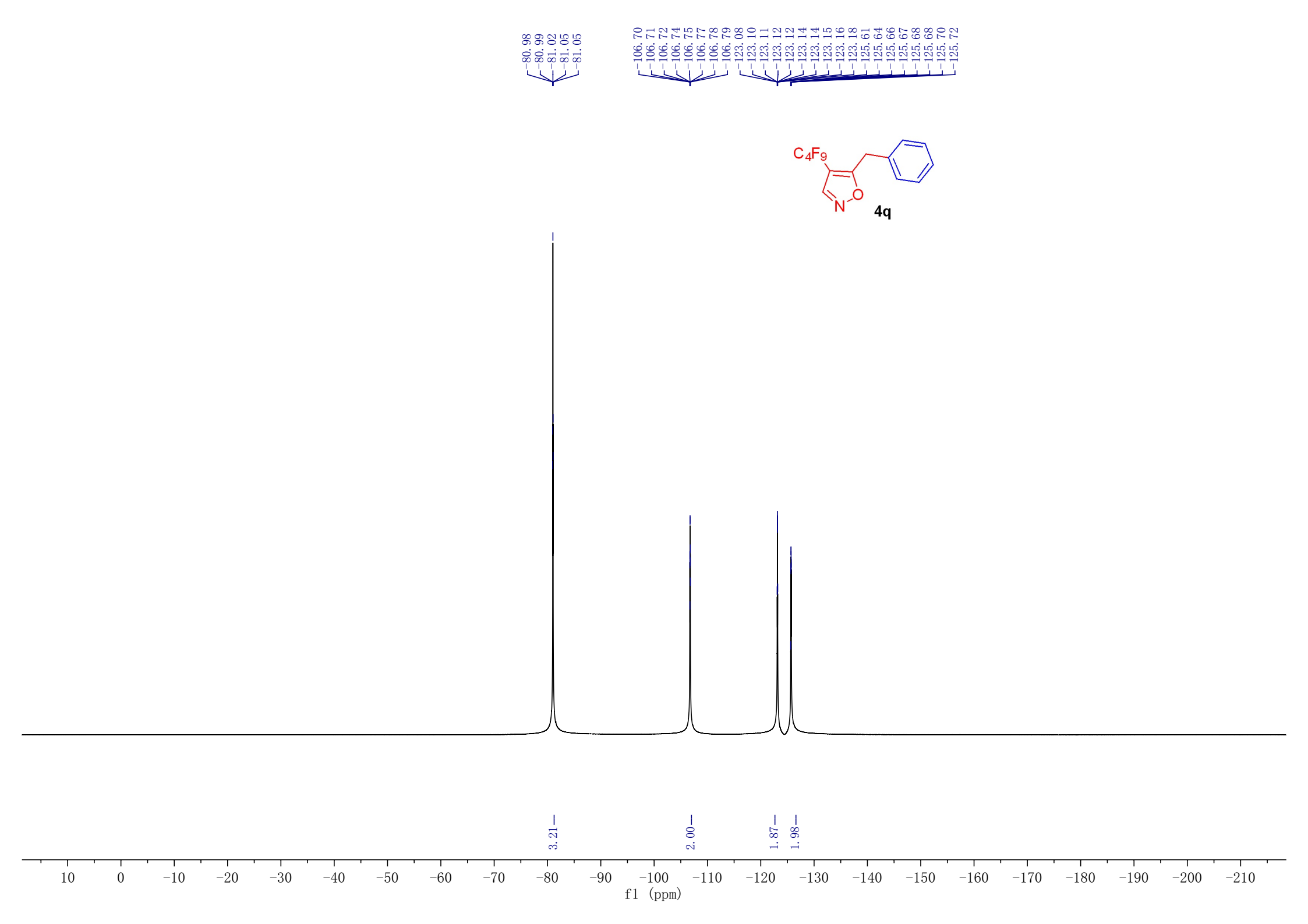
0.0
f1 (ppm)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80.99
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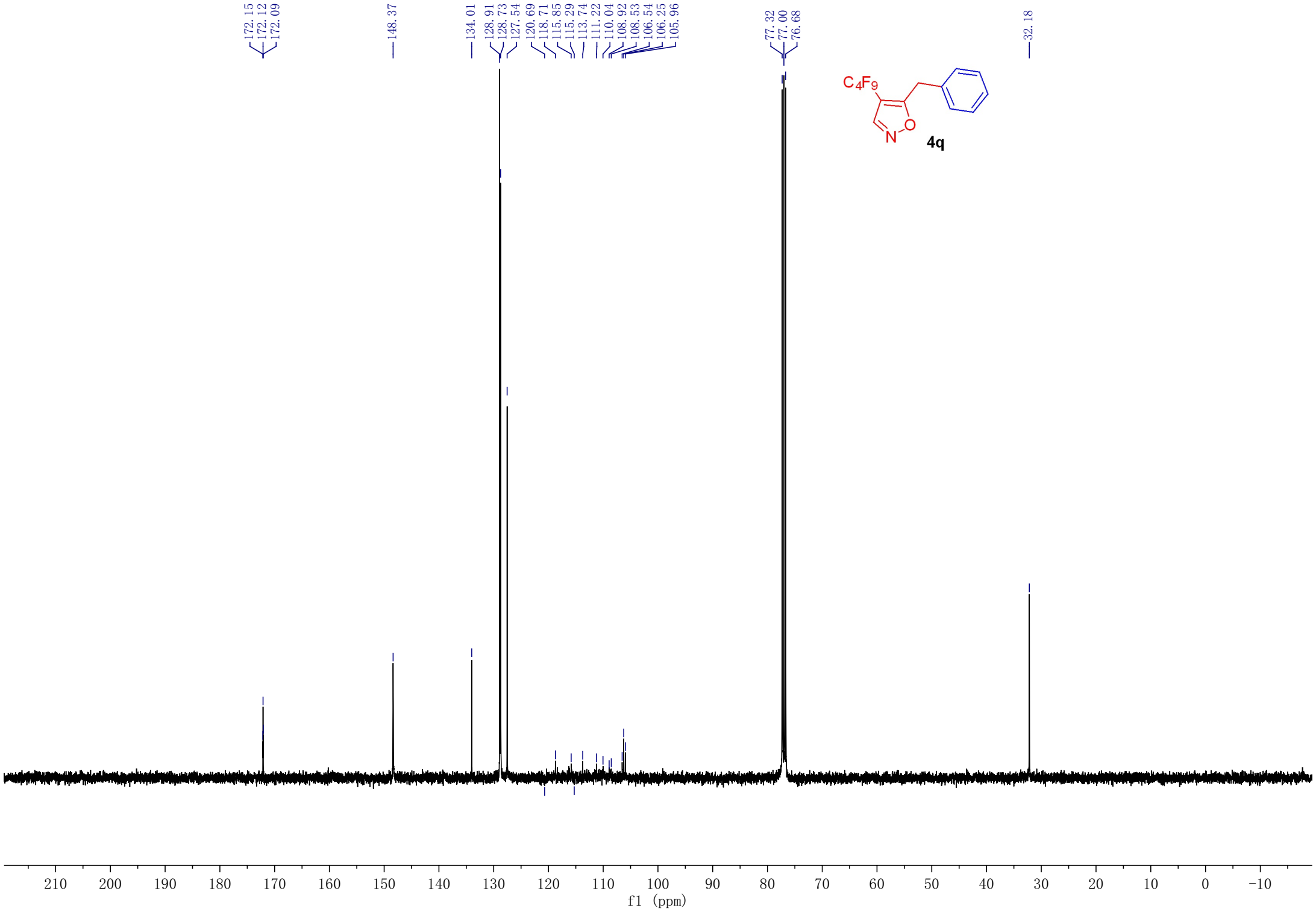
81.05
81.05
106.70
106.71
106.72
106.74
106.75
106.77
106.78
106.79
123.08
123.10
123.11
123.12
123.12
123.14
123.14
123.15
123.16
123.18
125.61
125.64
125.66
125.67
125.68
125.68
125.70
125.72
C4F9
O
N
4q
3.21
2.00
1.87
1.98
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


172.15
172.12
172.09
148.37
134.01
128.91
128.73
127.54
120.69
118.71
115.85
115.29
113.74
111.22
110.04
108.92
108.53
106.54
106.25
105.96
77.32
77.00
76.68
32.18
C4F9
N
O
4q
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)