Supporting Information

Zinc-catalyzed reaction of isoxazoles with thioynol ethers involving an unprecedented 1,2-sulfur migration

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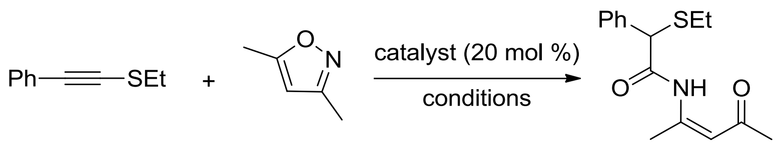
General Information. Ethyl acetate (ACS grade), hexanes (ACS grade) and anhydrous 1,2-dichloroethane (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed over silica gel (300-400 mesh). Infrared spectra were recorded on a Nicolet AVATER FTIR330 spectrometer as thin film and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Micromass QTOF2 Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

^{1}H NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform-d_3. Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. The data is being reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, brs = broad singlet, coupling constant(s) in Hz, integration).

^{13}C NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform-d_3. Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard.

More Reaction Condition and Mechanism Studies

1. Other reaction condition studies on the reaction of thioynol ether **1a** with isoxazole **2a**.[a]

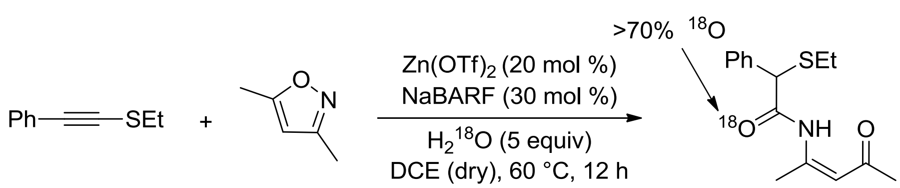


1a **2a** (3 equiv) **3a**

Entry	Catalyst	Reaction conditions	Yield[b] (%) 3a	1a
1	Cy-JohnPhosAuNTf_2 (10 mol %)	DCE, 60 °C, 24 h	<1	>90
2[c]	(**Ar**O)$_3$PAuNTf_2 (10 mol %)	DCE, 60 °C, 24 h	<1	>90
3	CF_3CO_2H	DCE, 60 °C, 24 h	<1	>90
4	MsOH	DCE, 60 °C, 24 h	<1	>90
5	$Zn(OTf)_2$	DCE, 60 °C, 24 h	38	30
6	$Cu(OTf)_2$	DCE, 60 °C, 24 h	<1	<2
7	$Sc(OTf)_3$	DCE, 60 °C, 24 h	18	52
8	$In(OTf)_3$	DCE, 60 °C, 24 h	11	63
9	NaBARF	DCE, 60 °C, 24 h	21	25
10	$Zn(OTf)_2$/NaBARF (20 mol %)	DCE, 60 °C, 18 h	58	<2
11	$ZnCl_2$/NaBARF (20 mol %)	DCE, 60 °C, 18 h	55	<2
12	$Zn(OTf)_2$/$AgNTf_2$ (20 mol %)	DCE, 60 °C, 24 h	29	30
13	$Zn(OTf)_2$/$AgPF_6$ (20 mol %)	DCE, 60 °C, 24 h	23	34

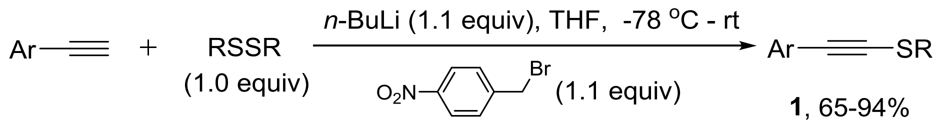
[a] Reaction conditions: [**1a**] = 0.05 M, in vials. [b] Measured by ^1H NMR using diethyl phthalate as the internal standard. [c] **Ar** = 2,4-di-*tert*-butylphenyl

2. The control experiment with $H_2{}^{18}O$ isotopic labeling proved that the oxygen atom in the amide group of **3a** originates from water.

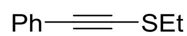


1a **2a** (3 equiv) **3a**, 56%

Representative synthetic procedures for the preparation of thioynol ethers 1:[1]



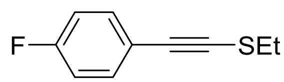
ethyl(phenylethynyl)sulfane (1a)



1a

This compound is known and the spectroscopic data match those reported.[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.36 (m, 2H), 7.32 – 7.22 (m, 3H), 2.80 (q, J = 7.3 Hz, 2H), 1.44 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.3, 128.2, 127.9, 123.5, 93.4, 29.9, 14.4.

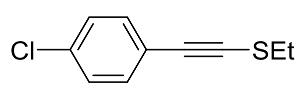
ethyl((4-fluorophenyl)ethynyl)sulfane (1b)



1b

This compound is known and the spectroscopic data match those reported.[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.36 (m, 2H), 7.08 – 6.94 (m, 2H), 2.84 (q, J = 7.3 Hz, 2H), 1.47 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 Hz, $CDCl_3$) δ 162.3 (d, J = 248.0 Hz), 133.4 (d, J = 9.0 Hz), 119.6 (d, J = 4.0 Hz), 115.5 (d, J = 21.0 Hz), 92.3, 78.9, 29.9, 14.7.

((4-chlorophenyl)ethynyl)(ethyl)sulfane (1c)

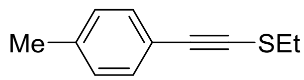


1c

This compound is known and the spectroscopic data match those reported.[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.30 (m, 2H), 7.29 – 7.24 (m, 2H), 2.82 (q, J = 7.3 Hz, 2H), 1.45

(t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.9, 132.5, 128.6, 122.0, 92.3, 80.6, 29.9, 14.7.

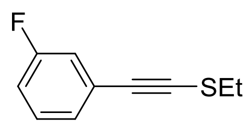
ethyl(*p*-tolylethynyl)sulfane (1d)



1d

This compound is known and the spectroscopic data match those reported.[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, J = 7.9 Hz, 2H), 7.08 (d, J = 8.0 Hz, 2H), 2.78 (q, J = 7.3 Hz, 2H), 2.32 (s, 3H), 1.43 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 131.4, 128.9, 120.4, 93.5, 78.1, 29.9, 21.4, 14.6.

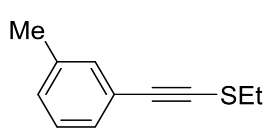
ethyl((3-fluorophenyl)ethynyl)sulfane (1e)



1e

Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 – 7.19 (m, 1H), 7.16 – 7.14 (m, 1H), 7.09 – 7.06 (m, 1H), 6.97 – 6.93 (m, 1H), 2.79 (q, J = 7.3 Hz, 2H), 1.43 (t, J = 7.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.2 (d, J = 245.0 Hz), 129.7 (d, J = 8.8 Hz), 126.9 (d, J = 2.5 Hz), 125.3 (d, J = 10.0 Hz), 117.8 (d, J = 22.5 Hz), 115.0 (d, J = 21.3 Hz), 92.3 (d, J = 2.5 Hz), 80.9, 29.8, 14.6; IR (neat): 2958, 2899, 1654, 1580, 1450, 1325, 1189, 1075, 856, 652; HRESIMS Calcd for $[C_{10}H_9FNaS]^+$ (M + Na^+) 203.0301, found 203.0305.

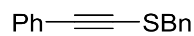
ethyl(m-tolylethynyl)sulfane (1f)



1f

Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 – 7.18 (m, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 7.09 – 7.00 (m, 1H), 2.76 (q, *J* = 7.3 Hz, 2H), 2.28 (s, 3H), 1.42 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.9, 132.0, 128.9, 128.5, 128.1, 123.3, 93.6, 78.7, 30.0, 21.2, 14.7; IR (neat): 2989, 2875, 1650, 1582, 1420, 1314, 1154, 1014, 706; HRESIMS Calcd for $[C_{11}H_{12}NaS]^+$ (M + Na^+) 199.0552, found 199.0553.

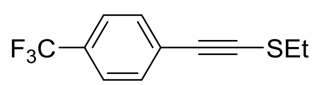
benzyl(phenylethynyl)sulfane (1g)



1g

This compound is known and the spectroscopic data match those reported.[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.29 (m, 7H), 7.29 – 7.24 (m, 3H), 4.01 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.5, 131.2, 129.0, 128.5, 128.2, 128.0, 127.7, 123.3, 94.6, 79.2, 40.3.

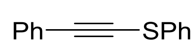
ethyl((4-(trifluoromethyl)phenyl)ethynyl)sulfane (1h)



1h

Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.2 Hz, 2H), 2.84 (q, *J* = 7.3 Hz, 2H), 1.46 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.2, 129.4 (q, *J* = 32 Hz), 127.4, 123.9 (q, *J* = 270 Hz), 125.2 (q, *J* = 4 Hz), 92.5, 82.9, 30.0, 14.7; IR (neat): 2934, 2887, 1658, 1584, 1440, 1333, 1257, 1153, 856, 652; HRESIMS Calcd for $[C_{11}H_9F_3NaS]^+$ (M + Na^+) 253.0269, found 253.0265.

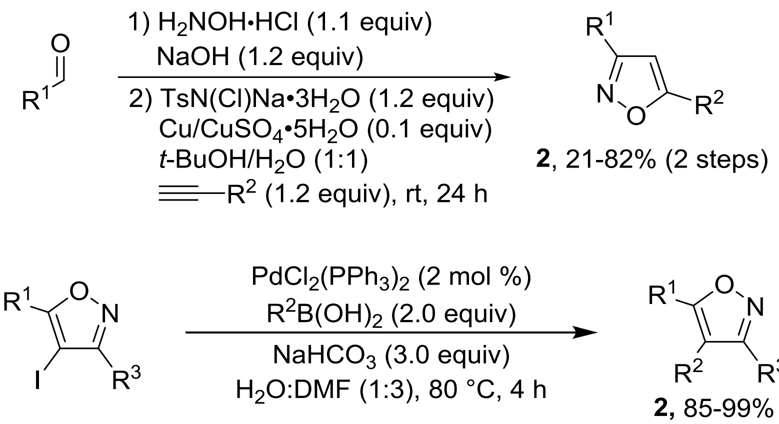
phenyl(phenylethynyl)sulfane (1i)



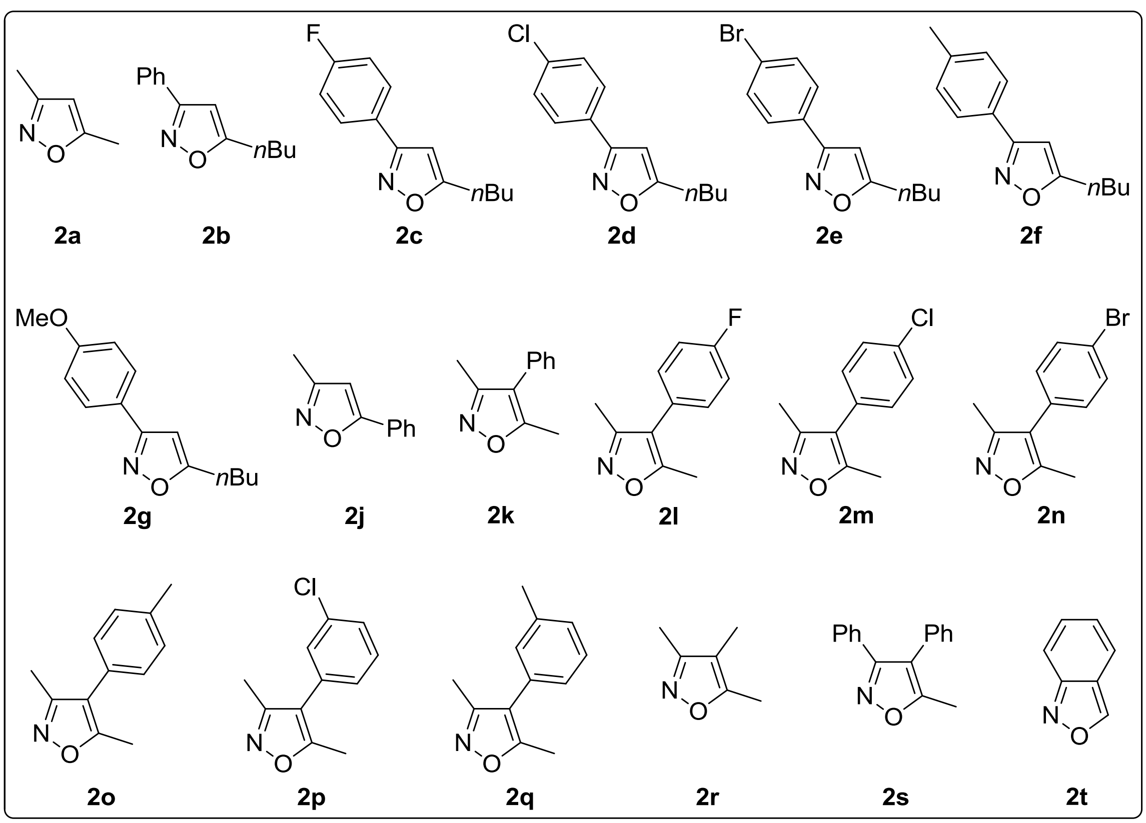
1i

This compound is known and the spectroscopic data match those reported.[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.44 (m, 4H), 7.37 – 7.16 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.9, 131.7, 129.2, 128.6, 128.3, 126.5, 126.2, 122.9, 97.9, 75.5.

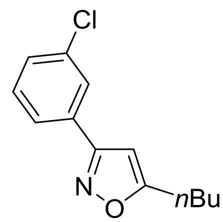
Representative synthetic procedures for the preparation of isoxazoles 2:[3,4]



The data of isoxazoles **2b**-**2g** and **2j**-**2s** were reported in our previous work,[4,5] and compounds **2a** and **2t** are commercially available.



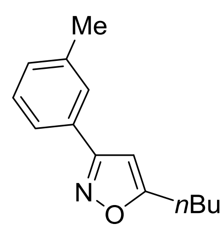
5-butyl-3-(3-chlorophenyl)isoxazole (2h)



2h

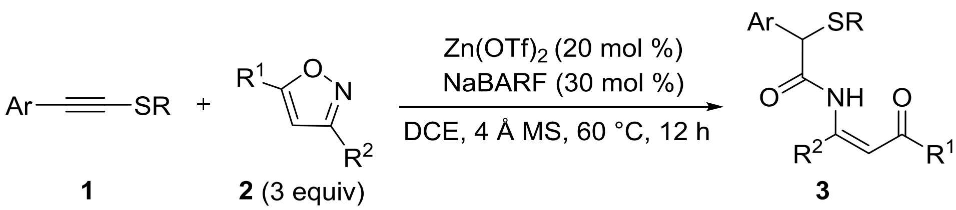
Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.67 (d, *J* = 7.0 Hz, 1H), 7.41 – 7.35 (m, 2H), 6.27 (s, 1H), 2.79 (t, *J* = 7.6 Hz, 2H), 1.76 – 1.70 (m, 2H), 1.46 – 1.39 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.7, 161.2, 134.8, 131.2, 130.1, 129.7, 126.8, 124.8, 98.7, 29.5, 26.4, 22.1, 13.6; IR (neat): 2960, 2934, 2875, 1596, 1457, 1415, 1079, 964, 783, 680; HRESIMS Calcd for $[C_{13}H_{14}ClNNaO]^+$ (M + Na^+) 258.0656, found 258.0655.

5-butyl-3-(*m*-tolyl)isoxazole (2i)



2i

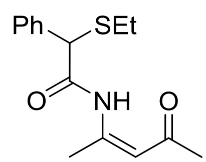
Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (s, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 7.6 Hz, 1H), 6.26 (s, 1H), 2.76 (t, *J* = 7.6 Hz, 2H), 2.38 (s, 3H), 1.75 – 1.67 (m, 2H), 1.46 – 1.37 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.1, 162.4, 138.5, 130.5, 129.3, 128.7, 127.3, 123.9, 98.8, 29.6, 26.5, 22.2, 21.4, 13.7; IR (neat): 2936, 2878, 2800, 1654, 1560, 1458, 1363, 834, 781, 669; HRESIMS Calcd for $[C_{14}H_{17}NNaO]^+$ (M + Na^+) 238.1202, found 238.1205.



General procedure for the synthesis of β-keto enamides 3:

NaBARF (0.09 mmol, 79.7 mg) and $Zn(OTf)_2$ (0.06 mmol, 21.8 mg) was added to a mixture of the thioynol ether **1** (0.30 mmol), isoxazole **2** (0.90 mol) and the 4 Å MS (200 mg) in DCE (6.0 mL) at room temperature. Then, the reaction mixture was stirred at 60 ℃ and the progress of the reaction was monitored by TLC. The reaction typically took 12 h. Upon completion, the mixture was concentrated and the residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired β-keto enamide **3**.

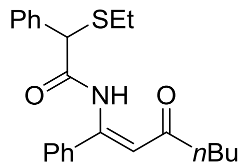
(*Z*)-2-(ethylthio)-*N*-(4-oxopent-2-en-2-yl)-2-phenylacetamide (3a)



3a

Compound **3a** was prepared in 72% yield (59.8 mg) according to the general procedure (Table 2, entry 1). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.84 (s, 1H), 7.50 (d, *J* = 7.4 Hz, 2H), 7.41 – 7.26 (m, 3H), 5.36 (s, 1H), 4.62 (s, 1H), 2.57 (q, *J* = 7.3 Hz, 2H), 2.34 (s, 3H), 2.13 (s, 3H), 1.27 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 170.3, 154.5, 136.0, 128.8, 128.3, 128.2, 106.5, 56.1, 30.4, 26.2, 21.7, 14.1; IR (neat): 3352 (br), 1719 (s), 1679 (s), 1558, 1457, 1242, 1198, 1067, 706, 675; HRESIMS Calcd for $[C_{15}H_{19}NNaO_2S]^+$ (M + Na^+) 300.1029, found 300.1034.

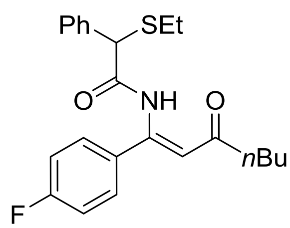
(*Z*)-2-(ethylthio)-*N*-(3-oxo-1-phenylhept-1-en-1-yl)-2-phenylacetamide (3b)



3b

Compound **3b** was prepared in 65% yield (73.6 mg) according to the general procedure (Table 2, entry 2). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.34 (s, 1H), 7.52 (d, *J* = 7.3 Hz, 2H), 7.40 – 7.27 (m, 6H), 7.24 (d, *J* = 6.8 Hz, 2H), 5.64 (s, 1H), 4.62 (s, 1H), 2.61 (q, *J* = 7.4 Hz, 2H), 2.47 (t, *J* = 7.5 Hz, 2H), 1.67 – 1.59 (m, 2H), 1.41 – 1.31 (m, 2H), 1.28 (t, *J* = 7.4 Hz, 3H), 0.92 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.6, 169.3, 153.1, 136.1, 135.7, 129.5, 128.8, 128.3, 128.2, 128.0, 127.0, 109.3, 55.6, 43.7, 26.8, 26.4, 22.4, 14.1, 13.8; IR (neat): 3355 (br), 2947, 2896, 1719 (s), 1680 (s), 1557, 1439, 1274, 1185, 1089, 704; HRESIMS Calcd for $[C_{23}H_{27}NNaO_2S]^+$ (M + Na^+) 404.1655, found 404.1658.

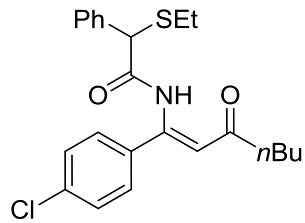
(*Z*)-2-(ethylthio)-*N*-(1-(4-fluorophenyl)-3-oxohept-1-en-1-yl)-2-phenylacetamide (3c).



3c

Compound **3c** was prepared in 64% yield (74.0 mg) according to the general procedure (Table 2, entry 3). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.34 (s, 1H), 7.51 (d, *J* = 7.3 Hz, 2H), 7.41 – 7.28 (m, 3H), 7.25 – 7.17 (m, 2H), 7.04 – 6.93 (m, 2H), 5.61 (s, 1H), 4.62 (s, 1H), 2.61 (q, *J* = 7.4 Hz, 2H), 2.48 (t, *J* = 7.5 Hz, 2H), 1.67 – 1.59 (m, 2H), 1.39 – 1.32 (m, 2H), 1.28 (t, *J* = 7.4 Hz, 3H), 0.92 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.5, 169.5, 163.5 (d, *J* = 249.0 Hz), 152.0, 136.1, 131.6 (d, *J* = 4.0 Hz), 129.0 (d, *J* = 9.0 Hz), 128.9, 128.3, 128.2, 115.1 (d, *J* = 22.0 Hz), 109.2, 55.6, 43.7, 26.8, 26.4, 22.4, 14.1, 13.8; IR (neat): 3378 (br), 2963, 2945, 1717 (s), 1683 (s), 1587, 1462, 1255, 1199, 1132, 1078, 751; HRESIMS Calcd for $[C_{23}H_{26}FNNaO_2S]^+$ (M + Na^+) 422.1560, found 422.1558.

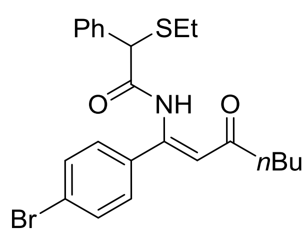
(*Z*)-*N*-(1-(4-chlorophenyl)-3-oxohept-1-en-1-yl)-2-(ethylthio)-2-phenylacetamide (3d)



3d

Compound **3d** was prepared in 62% yield (76.9 mg) according to the general procedure (Table 2, entry 4). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.31 (s, 1H), 7.51 (d, *J* = 7.5 Hz, 2H), 7.41 – 7.31 (m, 3H), 7.28 – 7.25 (m, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 5.62 (s, 1H), 4.61 (s, 1H), 2.60 (q, *J* = 7.4 Hz, 2H), 2.48 (t, *J* = 7.5 Hz, 2H), 1.67 – 1.58 (m, 2H), 1.40 – 1.31 (m, 2H), 1.28 (t, *J* = 7.4 Hz, 3H), 0.92 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.6, 169.5, 151.7, 136.0, 135.6, 134.1, 128.9, 128.2(8), 128.2(6), 128.2(3), 128.2(2), 109.4, 55.5, 43.7, 26.7, 26.4, 22.3, 14.1, 13.8; IR (neat): 3368 (br), 2952, 2929, 1716 (s), 1684 (s), 1558, 1457, 1281, 1136, 1068, 698, 669; HRESIMS Calcd for $[C_{23}H_{26}ClNNaO_2S]^+$ (M + Na^+) 438.1265, found 438.1261.

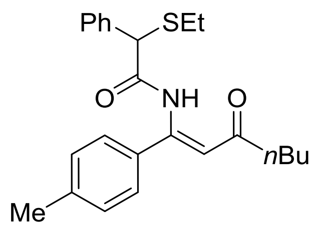
(*Z*)-*N*-(1-(4-bromophenyl)-3-oxohept-1-en-1-yl)-2-(ethylthio)-2-phenylacetamide (3e)



3e

Compound **3e** was prepared in 63% yield (72.5 mg) according to the general procedure (Table 2, entry 5). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.32 (s, 1H), 7.56 – 7.48 (m, 2H), 7.47 – 7.41 (m, 2H), 7.40 – 7.30 (m, 3H), 7.13 – 7.06 (m, 2H), 5.62 (s, 1H), 4.61 (s, 1H), 2.61 (q, J = 7.4 Hz, 2H), 2.52 – 2.44 (m, 2H), 1.67 – 1.58 (m, 2H), 1.39 – 1.33 (m, 2H), 1.28 (t, J = 7.4 Hz, 3H), 0.92 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.6, 169.5, 151.8, 136.0, 134.6, 131.2, 128.9, 128.5, 128.3, 128.2, 123.9, 109.4, 55.5, 43.7, 26.8, 26.4, 22.4, 14.1, 13.8; IR (neat): 3325 (br), 2963, 2901, 1718 (s), 1679 (s), 1554, 1448, 1268, 1068, 715, 658; HRESIMS Calcd for $[C_{23}H_{26}BrNNaO_2S]^+$ (M + Na^+) 482.0760, found 482.0758.

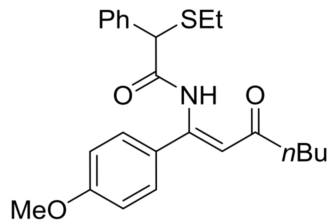
(*Z*)-2-(ethylthio)-*N*-(3-oxo-1-(*p*-tolyl)hept-1-en-1-yl)-2-phenylacetamide (3f)



3f

Compound **3f** was prepared in 71% yield (83.0 mg) according to the general procedure (Table 2, entry 6). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.34 (s, 1H), 7.56 – 7.50 (m, 2H), 7.40 – 7.33 (m, 2H), 7.33 – 7.27 (m, 1H), 7.17 – 7.07 (m, 4H), 5.64 (s, 1H), 4.62 (s, 1H), 2.61 (q, J = 7.4 Hz, 2H), 2.50 – 2.42 (m, 2H), 2.33 (s, 3H), 1.67 – 1.58 (m, 2H), 1.40 – 1.31 (m, 2H), 1.28 (t, J = 7.4 Hz, 3H), 0.92 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.5, 169.4, 153.2, 139.8, 136.2, 132.7, 128.8, 128.7, 128.3, 128.1, 126.9, 108.9, 55.6, 43.6, 26.9, 26.3, 22.3, 21.3, 14.0, 13.8; IR (neat): 3323 (br), 2988, 2899, 1716 (s), 1684 (s), 1578, 1412, 1285, 1113, 1011, 701, 656; HRESIMS Calcd for $[C_{24}H_{29}NNaO_2S]^+$ (M + Na^+) 418.1811, found 418.1812.

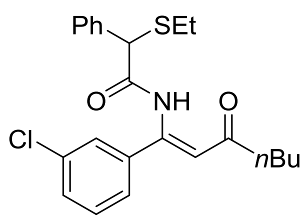
(*Z*)-2-(ethylthio)-*N*-(1-(4-methoxyphenyl)-3-oxohept-1-en-1-yl)-2-phenylacetamide (3g)



3g

Compound **3g** was prepared in 61% yield (75.0 mg) according to the general procedure (Table 2, entry 7). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.33 (s, 1H), 7.56 – 7.49 (m, 2H), 7.40 – 7.34 (m, 2H), 7.34 – 7.28 (m, 1H), 7.23 – 7.17 (m, 2H), 6.86 – 6.77 (m, 2H), 5.64 (s, 1H), 4.63 (s, 1H), 3.79 (s, 3H), 2.61 (q, *J* = 7.4 Hz, 2H), 2.47 (t, *J* = 7.2 Hz, 2H), 1.66 – 1.58 (m, 2H), 1.41 – 1.32 (m, 2H), 1.28 (t, *J* = 7.4 Hz, 3H), 0.92 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.5, 169.5, 160.9, 152.9, 136.2, 128.8, 128.6, 128.3, 128.1, 127.6, 113.5, 108.5, 55.7, 55.2, 43.6, 26.9, 26.4, 22.4, 14.1, 13.8; IR (neat): 3318 (br), 2968, 2924, 1717 (s), 1682 (s), 1589, 1487, 1221, 1165, 1078, 768, 699; HRESIMS Calcd for $[C_{24}H_{29}NNaO_3S]^+$ (M + Na^+) 434.1760, found 434.1766.

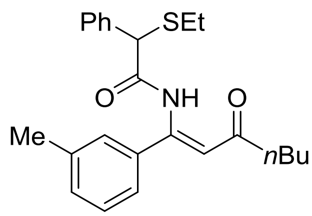
(*Z*)-*N*-(1-(3-chlorophenyl)-3-oxohept-1-en-1-yl)-2-(ethylthio)-2-phenylacetamide (3h)



3h

Compound **3h** was prepared in 66% yield (82.2 mg) according to the general procedure (Table 2, entry 8). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.27 (s, 1H), 7.51 (d, *J* = 6.8 Hz, 2H), 7.41 – 7.31 (m, 4H), 7.26 – 7.21 (m, 2H), 7.10 (d, *J* = 7.6 Hz, 1H), 5.63 (s, 1H), 4.62 (s, 1H), 2.62 (q, *J* = 7.6 Hz, 2H), 2.49 (t, *J* = 7.2 Hz, 2H), 1.63 – 1.35 (m, 2H), 1.35 – 1.30 (m, 2H), 1.29 (t, *J* = 7.4 Hz, 3H), 0.93 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.6, 169.5, 151.3, 137.6, 136.0, 134.0, 129.5, 129.2, 128.9, 128.3, 128.2, 127.0, 125.2, 109.7, 55.5, 43.8, 26.8, 26.4, 22.4, 14.1, 13.8; IR (neat): 3333 (br), 2971, 2861, 1723 (s), 1660 (s), 1547, 1470, 1298, 1153, 1099, 782; HRESIMS Calcd for $[C_{23}H_{26}ClNNaO_2S]^+$ (M + Na^+) 438.1265, found 438.1261.

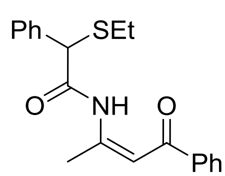
(*Z*)-2-(ethylthio)-*N*-(3-oxo-1-(*m*-tolyl)hept-1-en-1-yl)-2-phenylacetamide (3i)



3i

Compound **3i** was prepared in 69% yield (81.8 mg) according to the general procedure (Table 2, entry 9). Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.29 (s, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.39 – 7.30 (m, 3H), 7.18 – 7.15 (m, 2H), 7.05 – 7.01 (m, 2H), 5.65 (s, 1H), 4.63 (s, 1H), 2.62 (q, *J* = 7.5 Hz, 2H), 2.47 (t, *J* = 7.5 Hz, 2H), 2.29 (s, 3H), 1.66 – 1.59 (m, 2H), 1.38 – 1.32 (m, 2H), 1.29 (t, *J* = 7.4 Hz, 1H), 0.92 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.7, 169.4, 153.2, 137.7, 136.2, 135.6, 130.4, 128.8, 128.3, 128.2, 127.9, 127.5, 124.2, 109.2, 55.6, 43.7, 26.9, 26.4, 22.4, 21.3, 14.1, 13.8; IR (neat): 3315 (br), 2985, 2944, 1714 (s), 1659 (s), 1587, 1494, 1392, 1102, 993, 778; HRESIMS Calcd for $[C_{24}H_{29}NNaO_2S]^+$ (M + Na^+) 418.1811, found 418.1807.

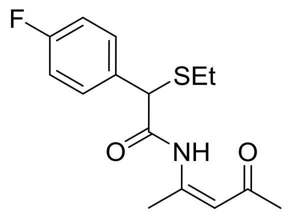
(*Z*)-2-(ethylthio)-*N*-(4-oxo-4-phenylbut-2-en-2-yl)-2-phenylacetamide (3j)



3j

Compound **3j** was prepared in 62% yield (61.9 mg) according to the general procedure (Table 2, entry 10). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.33 (s, 1H), 7.95 – 7.86 (m, 2H), 7.59 – 7.49 (m, 3H), 7.48 – 7.41 (m, 2H), 7.40 – 7.34 (m, 2H), 7.33 – 7.27 (m, 1H), 6.08 (s, 1H), 4.69 (s, 1H), 2.61 (q, *J* = 7.4 Hz, 2H), 2.49 (s, 3H), 1.29 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.3, 170.4, 156.6, 138.5, 136.1, 132.4, 128.9, 128.5, 128.3, 128.2, 127.7, 102.9, 56.1, 26.3, 22.5, 14.1; IR (neat): 3335 (br), 1716 (s), 1684 (s), 1540, 1521, 1457, 1396, 1268, 1065, 766, 699; HRESIMS Calcd for $[C_{20}H_{21}NNaO_2S]^+$ (M + Na^+) 362.1185, found 362.1181.

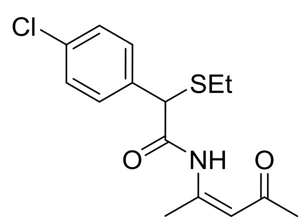
(*Z*)-2-(ethylthio)-2-(4-fluorophenyl)-*N*-(4-oxopent-2-en-2-yl)acetamide (3k)



3k

Compound **3k** was prepared in 76% yield (67.3 mg) according to the general procedure (Table 2, entry 11). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.87 (s, 1H), 7.56 – 7.42 (m, 2H), 7.11 – 6.99 (m, 2H), 5.38 (s, 1H), 4.61 (s, 1H), 2.57 (q, *J* = 7.4 Hz, 2H), 2.35 (s, 3H), 2.15 (s, 3H), 1.27 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 170.0, 162.5 (d, *J* = 246.0 Hz), 154.5, 131.9 (d, *J* = 3.0 Hz), 130.0 (d, *J* = 8.0 Hz), 115.8 (d, *J* = 22.0 Hz), 106.6, 55.2, 30.4, 26.3, 21.7, 14.0; IR (neat): 3385 (br), 1717 (s), 1684 (s), 1558, 1457, 1396, 1259, 1158, 796, 669; HRESIMS Calcd for $[C_{15}H_{18}FNNaO_2S]^+$ (M + Na^+) 318.0934, found 318.0933.

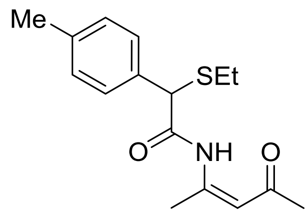
(*Z*)-2-(4-chlorophenyl)-2-(ethylthio)-*N*-(4-oxopent-2-en-2-yl)acetamide (3l)



3l

Compound **3l** was prepared in 55% yield (51.0 mg) according to the general procedure (Table 2, entry 12). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.87 (s, 1H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 5.38 (s, 1H), 4.58 (s, 1H), 2.56 (q, *J* = 7.4 Hz, 2H), 2.34 (s, 3H), 2.15 (s, 3H), 1.27 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.7, 169.8, 154.5, 134.7, 134.1, 129.6, 129.0, 106.6, 55.3, 30.4, 26.3, 21.7, 14.1; IR (neat): 3350 (br), 1716 (s), 1684 (s), 1540, 1457, 1362, 1259, 1091, 781, 702; HRESIMS Calcd for $[C_{18}H_{15}ClNNaO_2S]^+$ $(M + Na^+)$ 334.0639, found 334.0639.

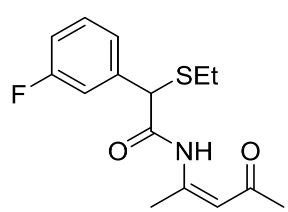
(*Z*)-2-(ethylthio)-*N*-(4-oxopent-2-en-2-yl)-2-(*p*-tolyl)acetamide (3m)



3m

Compound **3m** was prepared in 60% yield (52.4 mg) according to the general procedure (Table 2, entry 13). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.84 (s, 1H), 7.39 (d, *J* = 8.1 Hz, 2H), 7.17 (d, *J* = 7.9 Hz, 2H), 5.35 (d, *J* = 0.6 Hz, 1H), 4.60 (s, 1H), 2.56 (q, *J* = 7.4 Hz, 2H), 2.34 (d, *J* = 0.9 Hz, 3H), 2.33 (s, 3H), 2.14 (s, 3H), 1.27 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 170.5, 154.6, 138.0, 133.0, 129.5, 128.1, 106.4, 55.8, 30.4, 26.2, 21.8, 21.1, 14.1; IR (neat): 3335 (br), 1717 (s), 1698 (s), 1558, 1507, 1418, 1338, 1318, 669, 568; HRESIMS Calcd for $[C_{16}H_{21}NNaO_2S]^+$ $(M + Na^+)$ 314.1185, found 314.1186.

(*Z*)-2-(ethylthio)-2-(3-fluorophenyl)-*N*-(4-oxopent-2-en-2-yl)acetamide (3n)

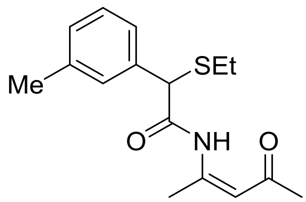


3n

Compound **3n** was prepared in 71% yield (62.8 mg) according to the general procedure (Table 2, entry 14). Pale yellow oil. ^{1}H NMR (400 MHz,) δ 12.88 (s, 1H), 7.36 – 7.23 (m, 3H), 7.01 (t, *J* = 8.0 Hz, 1H), 5.39 (s, 1H), 4.60 (s, 1H), 2.58 (q, *J* = 7.2 Hz, 2H), 2.35 (s, 3H), 2.15 (s, 3H), 1.28 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz,) δ 199.6, 169.6, 164.1 (d, *J* = 246.0 Hz), 154.4, 138.6 (d, *J* = 7.0 Hz), 130.3 (d, *J* = 8.0 Hz), 124.1 (d, *J* = 3.0

Hz), 115.4 (d, J = 22.0 Hz), 115.3 (d, J = 21.0 Hz), 106.7, 55.5, 30.4, 26.3, 21.7, 14.1; IR (neat): 3388 (br), 2930, 1713 (s), 1650 (s), 1600, 1470, 1454, 1245, 1120, 774, 683; HRESIMS Calcd for $[C_{15}H_{18}FNNaO_2S]^+$ (M + Na^+) 318.0934, found 318.0939.

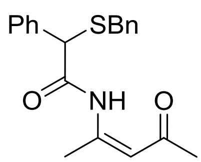
(*Z*)-2-(ethylthio)-*N*-(4-oxopent-2-en-2-yl)-2-(*m*-tolyl)acetamide (3o)



3o

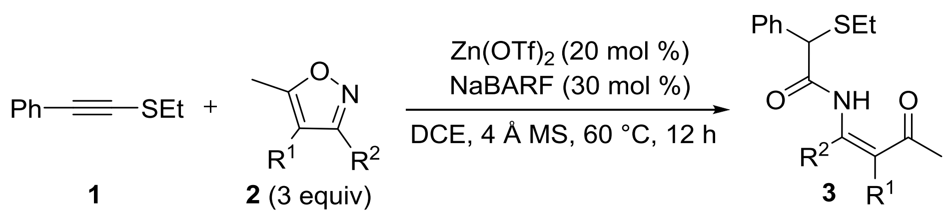
Compound **3o** was prepared in 62% yield (54.1 mg) according to the general procedure (Table 2, entry 15). Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.84 (s, 1H), 7.35 – 7.30 (m, 2H), 7.27 – 7.22 (m, 1H), 7.11 (d, J = 7.5 Hz, 1H), 5.36 (s, 1H), 4.57 (s, 1H), 2.57 (q, J = 7.5 Hz, 2H), 2.35 (s, 6H), 2.14 (s, 3H), 1.27 (t, J = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.4, 170.4, 154.6, 138.6, 136.0, 129.1, 129.0, 128.8, 125.3, 106.5, 56.1, 30.4, 26.3, 21.8, 21.4, 14.1; IR (neat): 3344 (br), 2933, 1723 (s), 1657 (s), 1558, 1466, 1245, 1118, 760, 621; HRESIMS Calcd for $[C_{16}H_{21}NNaO_2S]^+$ (M + Na^+) 314.1185, found 314.1192.

(*Z*)-2-(benzylthio)-*N*-(4-oxopent-2-en-2-yl)-2-phenylacetamide (3p)



3p

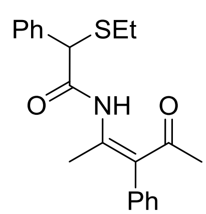
Compound **3p** was prepared in 67% yield (67.4 mg) according to the general procedure (Table 2, entry 16). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.77 (s, 1H), 7.47 (d, J = 7.3 Hz, 2H), 7.42 – 7.30 (m, 7H), 7.28 – 7.21 (m, 1H), 5.34 (s, 1H), 4.45 (s, 1H), 3.76 (dd, J = 34.8, 13.6 Hz, 2H), 2.32 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.4, 169.9, 154.4, 136.9, 135.8, 129.0, 128.9, 128.5, 128.4, 128.3, 127.3, 106.5, 55.7, 36.6, 30.4, 21.7; IR (neat): 3310 (br), 1716 (s), 1688 (s), 1521, 1507, 1489, 1457, 1396, 1339, 1259, 669; HRESIMS Calcd for $[C_{20}H_{21}NNaO_2S]^+$ (M + Na^+) 362.1185, found 362.1190.



General procedure for the synthesis of β-keto enamides 3:

NaBARF (0.09 mmol, 79.8 mg) and $Zn(OTf)_2$ (0.06 mmol, 21.8 mg) was added to a mixture of the thioynol ether **1** (0.30 mmol), isoxazole **2** (0.90 mol) and the 4 Å MS (200 mg) in DCE (6.0 mL) at room temperature. Then, the reaction mixture was stirred at 60 ℃ and the progress of the reaction was monitored by TLC. The reaction typically took 12 h. Upon completion, the mixture was concentrated and the residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired β-keto enamide **3**.

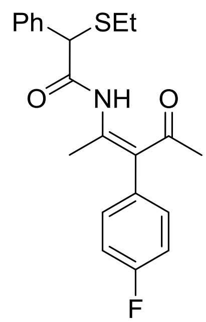
(*Z*)-2-(ethylthio)-*N*-(4-oxo-3-phenylpent-2-en-2-yl)-2-phenylacetamide (3q)



3q

Compound **3q** was prepared in 74% yield (78.4 mg) according to the general procedure (Table 3, entry 1). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.60 (s, 1H), 7.63 – 7.54 (m, 2H), 7.45 – 7.31 (m, 6H), 7.18 – 7.09 (m, 2H), 4.69 (s, 1H), 2.62 (q, *J* = 7.4 Hz, 2H), 2.12 (s, 3H), 1.92 (s, 3H), 1.31 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.3, 170.6, 152.3, 138.1, 136.3, 130.7, 128.9, 128.8, 128.3, 128.2, 127.5, 119.9, 56.4, 31.2, 26.2, 19.4, 14.1; IR (neat): 3315 (br), 1716 (s), 1683 (s), 1540, 1507, 1489, 1457, 1338, 1212, 704, 669; HRESIMS Calcd for $[C_{21}H_{23}NNaO_2S]^+$ (M + Na^+) 376.1342, found 376.1349.

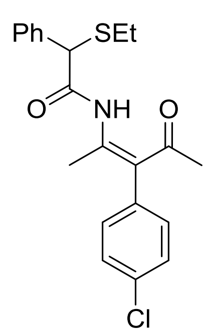
(*Z*)-2-(ethylthio)-*N*-(3-(4-fluorophenyl)-4-oxopent-2-en-2-yl)-2-phenylacetamide (3r)



3r

Compound **3r** was prepared in 64% yield (71.2 mg) according to the general procedure (Table 3, entry 2). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.58 (s, 1H), 7.60 – 7.55 (m, 2H), 7.42 – 7.38 (m, 2H), 7.36 – 7.32 (m, 1H), 7.14 – 7.07 (m, 4H), 4.68 (s, 1H), 2.61 (q, *J* = 7.4 Hz, 2H), 2.12 (s, 3H), 1.91 (s, 3H), 1.31 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.0, 170.6, 162.2 (d, *J* = 246.0 Hz), 152.8, 136.3, 134.1 (d, *J* = 4.0 Hz), 132.4 (d, *J* = 7.0 Hz), 128.9, 128.4, 128.2, 118.8, 115.9 (d, *J* = 21.0 Hz), 56.5, 31.1, 26.3, 19.3, 14.1; IR (neat): 3387 (br), 1719 (s), 1654 (s), 1541, 1507, 1425, 1328, 1203, 1115, 732, 688; HRESIMS Calcd for $[C_{21}H_{22}FNNaO_2S]^+$ (M + Na^+) 394.1247, found 394.1248.

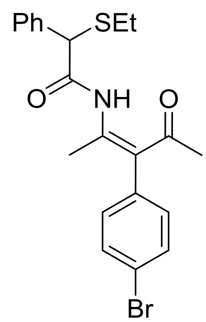
(*Z*)-*N*-(3-(4-chlorophenyl)-4-oxopent-2-en-2-yl)-2-(ethylthio)-2-phenylacetamide (3s)



3s

Compound **3s** was prepared in 61% yield (70.8 mg) according to the general procedure (Table 3, entry 3). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.55 (s, 1H), 7.55 (d, *J* = 7.2 Hz, 2H), 7.41 – 7.30 (m, 5H), 7.08 (d, *J* = 8.4 Hz, 2H), 4.66 (s, 1H), 2.60 (q, *J* = 7.4 Hz, 2H), 2.11 (s, 3H), 1.90 (s, 3H), 1.29 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.7, 170.6, 152.8, 136.7, 136.3, 133.8, 132.2, 129.2, 128.9, 128.4, 128.2, 118.7, 56.5, 31.2, 26.3, 19.4, 14.1; IR (neat): 3342 (br), 1721 (s), 1658 (s), 1538, 1329, 1207, 1113, 937, 734, 716, 691; HRESIMS Calcd for $[C_{21}H_{22}ClNNaO_2S]^+$ (M + Na^+) 410.0952, found 410.0955.

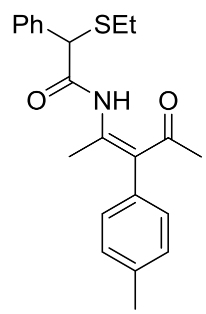
(*Z*)-*N*-(3-(4-bromophenyl)-4-oxopent-2-en-2-yl)-2-(ethylthio)-2-phenylacetamide (3t)



3t

Compound **3t** was prepared in 58% yield (75.0 mg) according to the general procedure (Table 3, entry 4). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.56 (s, 1H), 7.56 – 7.52 (m, 4H), 7.41 – 7.37 (m, 2H), 7.34 – 7.31 (m, 1H), 7.02 (d, *J* = 8.4 Hz, 2H), 4.66 (s, 1H), 2.60 (q, *J* = 7.4 Hz, 2H), 2.11 (s, 3H), 1.90 (s, 3H), 1.29 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6, 170.6, 152.8, 137.2, 136.2, 132.5, 132.2, 128.9, 128.4, 128.2, 121.9, 118.7, 56.5, 31.2, 26.3, 19.4, 14.1; IR (neat): 3358 (br), 1721 (s), 1650 (s), 1552, 1427, 1330, 1230, 1207, 1115, 687, 543; HRESIMS Calcd for $[C_{21}H_{22}BrNNaO_2S]^+$ (M + Na^+) 454.0447, found 454.0449.

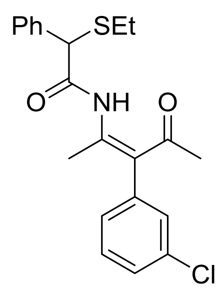
(*Z*)-2-(ethylthio)-*N*-(4-oxo-3-(*p*-tolyl)pent-2-en-2-yl)-2-phenylacetamide (3u)



3u

Compound **3u** was prepared in 66% yield (72.7 mg) according to the general procedure (Table 3, entry 5). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.56 (s, 1H), 7.56 (d, *J* = 7.1 Hz, 2H), 7.41 – 7.37 (m, 2H), 7.34 – 7.30 (m, 1H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 4.67 (s, 1H), 2.60 (q, *J* = 7.4 Hz, 2H), 2.37 (s, 3H), 2.11 (s, 3H), 1.91 (s, 3H), 1.30 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.6, 170.5, 152.2, 137.3, 136.4, 135.1, 130.6, 129.6, 128.8, 128.4, 128.2, 119.8, 56.5, 31.2, 26.3, 21.1, 19.3, 14.1; IR (neat): 3330 (br), 1714 (s), 1681 (s), 1585, 1538, 1442, 1246, 1201, 1116, 817, 690; HRESIMS Calcd for $[C_{22}H_{25}NNaO_2S]^+$ (M + Na^+) 390.1498, found 390.1497.

(*Z*)-*N*-(3-(3-chlorophenyl)-4-oxopent-2-en-2-yl)-2-(ethylthio)-2-phenylacetamide (3v)

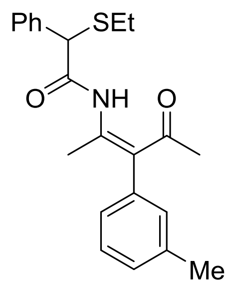


3v

Compound **3v** was prepared in 68% yield (78.9 mg) according to the general procedure (Table 3, entry 6). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.57 (s, 1H), 7.57 – 7.54 (m, 2H), 7.42 – 7.37 (m, 2H), 7.36 – 7.31 (m, 3H), 7.17 – 7.16 (m, 1H), 7.07 – 7.02 (m, 1H), 4.67 (s, 1H), 2.60 (q, *J* = 7.2 Hz, 2H), 2.12 (s, 3H), 1.91 (s, 3H), 1.30 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.5, 170.7, 153.0, 140.1, 136.2, 134.7, 130.8, 130.2, 129.1, 128.9, 128.3, 128.2, 127.9, 118.6, 56.5, 31.1, 26.3, 19.4, 14.1; IR (neat):

3358 (br), 1728 (s), 1682 (s), 1557, 1539, 1394, 1206, 1113, 783, 689; HRESIMS Calcd for $[C_{21}H_{22}ClNNaO_2S]^+$ (M + Na^+) 410.0952, found 410.0943

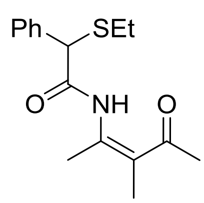
(*Z*)-2-(ethylthio)-*N*-(4-oxo-3-(*m*-tolyl)pent-2-en-2-yl)-2-phenylacetamide (3w)



3w

Compound **3w** was prepared in 70% yield (77.0 mg) according to the general procedure (Table 3, entry 7). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.56 (s, 1H), 7.56 (d, *J* = 7.2 Hz, 2H), 7.41 – 7.37 (m, 2H), 7.35 – 7.30 (m, 1H), 7.29 – 7.24 (m, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 6.95 – 6.91 (m, 2H), 4.67 (s, 1H), 2.60 (q, *J* = 7.2 Hz, 2H), 2.35 (s, 3H), 2.11 (s, 3H), 1.91 (s, 3H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.4, 170.6, 152.2, 138.6, 138.1, 136.4, 131.3, 128.9, 128.8, 128.4, 128.3, 128.2, 127.7, 120.1, 56.5, 31.1, 26.3, 21.3, 19.4, 14.2; IR (neat): 3378 (br), 2915, 1719 (s), 1683 (s), 1558, 1435, 1328, 1215, 1122, 680; HRESIMS Calcd for $[C_{22}H_{25}NNaO_2S]^+$ (M + Na^+) 390.1498, found 390.1491.

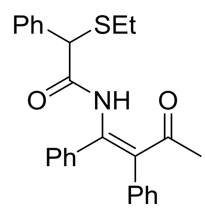
(*Z*)-2-(ethylthio)-*N*-(3-methyl-4-oxopent-2-en-2-yl)-2-phenylacetamide (3x)



3x

Compound **3x** was prepared in 58% yield (51.0 mg) according to the general procedure except at 80 ^{o}C in 24 h (Table 3, entry 8). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.35 (s, 1H), 7.54 – 7.47 (m, 2H), 7.38 – 7.26 (m, 3H), 4.60 (s, 1H), 2.56 (q, *J* = 7.4 Hz, 2H), 2.38 (s, 3H), 2.26 (s, 3H), 1.91 (s, 3H), 1.27 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.0, 170.1, 150.0, 136.5, 128.7, 128.2, 128.0, 111.6, 56.4, 30.0, 26.2, 17.3, 14.6, 14.1; IR (neat): 3315 (br), 1717 (s), 1684 (s), 1558, 1473, 1419, 1396, 1339, 1236, 750, 669; HRESIMS Calcd for $[C_{16}H_{21}NNaO_2S]^+$ (M + Na^+) 314.1185, found 314.1186.

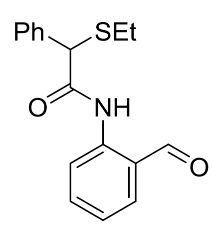
(*Z*)-2-(ethylthio)-*N*-(3-oxo-1,2-diphenylbut-1-en-1-yl)-2-phenylacetamide (3y)



3y

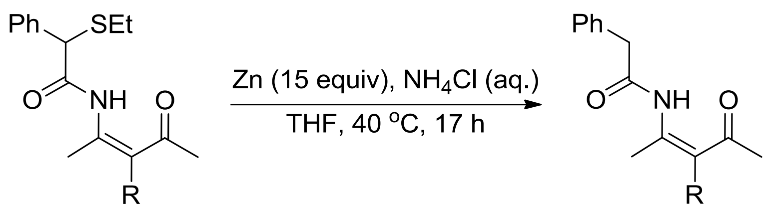
Compound **3y** was prepared in 72% yield (89.6 mg) according to the general procedure (Table 3, entry 9). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.92 (s, 1H), 7.54 – 7.51 (m, 2H), 7.41 – 7.31 (m, 3H), 7.14 – 7.01 (m, 6H), 6.98 – 6.94 (m, 2H), 6.91 – 6.86 (m, 2H), 4.62 (s, 1H), 2.63 (q, J = 7.6 Hz, 2H), 2.02 (s, 3H), 1.30 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.4, 169.2, 150.2, 137.0, 136.2, 134.9, 131.5, 128.8, 128.3, 128.2, 128.0, 127.8, 127.3, 126.9, 121.7, 55.9, 31.3, 26.3, 14.1; IR (neat): 3318 (br), 1725 (s), 1669 (s), 1558, 1502, 1412, 1305, 1247, 1178, 1008, 689; HRESIMS Calcd for $[C_{26}H_{25}NNaO_2S]^+$ (M + Na^+) 438.1498, found 438.1493.

2-(ethylthio)-*N*-(2-formylphenyl)-2-phenylacetamide (3z)



3z

Compound **3z** was prepared in 81% yield (72.7 mg) according to the general procedure except in the absent of 4 Å MS. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.86 (s, 1H), 9.91 (s, 1H), 8.73 (d, *J* = 8.4 Hz, 1H), 7.70 – 7.63 (m, 1H), 7.63 – 7.50 (m, 3H), 7.40 – 7.28 (m, 3H), 7.27 – 7.19 (m, 1H), 4.75 (s, 1H), 2.72 – 2.55 (m, 2H), 1.30 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.2, 170.1, 140.3, 136.4, 136.0, 135.9, 128.9, 128.2(0), 128.1(6), 123.3, 122.1, 119.9, 56.1, 26.5, 14.1.; IR (neat): 3377 (br), 1708 (s), 1658 (s), 1578, 1457, 1354, 1242, 1178, 1058, 747, 657; HRESIMS Calcd for $[C_{17}H_{17}NNaO_2S]^+$ ($M + Na^+$) 322.0872, found 322.0870.

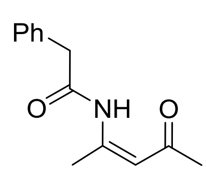


3 **4a-4b**

General procedure for the synthesis of β-keto enamides 4a–4b:

Zinc powder (3 mmol, 195 mg) was added to a solution of the compound **3** (0.2 mmol) in the mixture of saturated NH_4Cl (aq.) and THF (3 mL, v/v = 1:1) at room temperature. The reaction mixture was stirred at 40 °C and the progress of the reaction was monitored by TLC. The reaction typically took 17 h. Upon completion, the mixture was then concentrated and the residue was purified by chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford the desired β-keto enamide **4a** or **4b**.

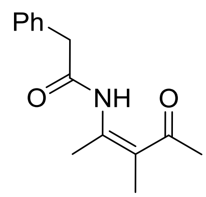
(*Z*)-*N*-(4-oxopent-2-en-2-yl)-2-phenylacetamide (4a)



4a

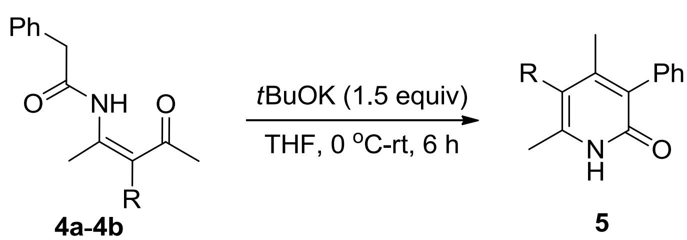
Compound **4a** was prepared in 72% yield (31.0 mg) according to the general procedure. Yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 12.35 (s, 1H), 7.42 – 7.27 (m, 5H), 5.30 (s, 1H), 3.66 (s, 2H), 2.35 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 170.7, 155.0, 133.7, 129.4, 128.8, 127.4, 105.8, 45.6, 30.4, 21.8; IR (neat): 3325 (br), 1716 (s), 1684 (s), 1540, 1457, 1419, 1362, 1260, 1120, 721; HRESIMS Calcd for $[C_{13}H_{15}NNaO_2]^+$ (M + Na$^+$) 240.0995, found 240.0999.

(*Z*)-*N*-(3-methyl-4-oxopent-2-en-2-yl)-2-phenylacetamide (4b)



4b

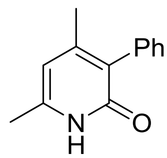
Compound **4b** was prepared in 77% yield (35.2 mg) according to the general procedure. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.93 (s, 1H), 7.39 – 7.31 (m, 4H), 7.31 – 7.24 (m, 1H), 3.63 (s, 2H), 2.38 (d, J = 0.5 Hz, 3H), 2.22 (s, 3H), 1.89 (d, J = 0.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.1, 170.6, 150.7, 134.2, 129.3, 128.7, 127.1, 110.7, 45.9, 30.1, 17.3, 14.5; IR (neat): 3333 (br), 1717 (s), 1684 (s), 1559, 1475, 1396, 1339, 1173, 750, 705; HRESIMS Calcd for $[C_{14}H_{17}NNaO_2]^+$ (M + Na$^+$) 254.1151, found 254.1153.



General procedure for the synthesis of 2-pyridones 5a-5b:

*t*BuOK (0.3 mmol, 33.6 mg) was added to a solution of the compound **4a** or **4b** (0.2 mmol) in THF (2.0 mL) at 0 °C. The reaction mixture was then allowed warm to room temperature and the progress of the reaction was monitored by TLC. The reaction typically took 6 h. Upon completion, the mixture was then concentrated and the residue was purified by chromatography on silica gel (eluent: dichloromethane/methanol) to afford the desired product 2-pyridone **5**.

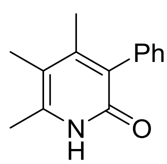
4,6-dimethyl-3-phenylpyridin-2(1*H*)-one (5a)



5a

Compound **5a** was prepared in 64% yield (25.4 mg) according to the general procedure. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.70 (s, 1H), 7.43 – 7.35 (m, 2H), 7.34 – 7.23 (m, 3H), 5.97 (s, 1H), 2.21 (s, 3H), 2.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 149.4, 143.0, 135.9, 130.3, 128.0, 127.2, 126.9, 109.0, 20.6, 18.7; IR (neat): 3265 (br), 1670 (s), 1578, 1507, 1436, 1338, 1318, 757, 704; HRESIMS Calcd for $[C_{13}H_{13}NNaO]^+$ (M + Na^+) 222.0889, found 222.0888.

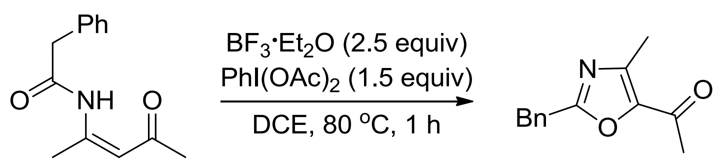
4,5,6-trimethyl-3-phenylpyridin-2(1*H*)-one (5b)



5b

Compound **5b** was prepared in 77% yield (32.6 mg) according to the general procedure. Pale Yellow oil. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.42 (s, 1H), 7.42 – 7.34 (m, 2H), 7.33 – 7.25 (m, 1H), 7.14 (d, *J* = 7.0 Hz, 2H), 2.20 (s, 3H), 1.95 (s, 3H), 1.91 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.4, 148.5, 139.8, 137.8, 130.9, 128.2, 128.1, 127.0, 111.4, 18.6, 17.2, 13.7; IR (neat): 3265 (br), 1653 (s), 1540, 1507, 1473, 1396, 1260, 751, 669; HRESIMS Calcd for $[C_{14}H_{15}NNaO]^+$ (M + Na^+) 236.1046, found 236.1050.

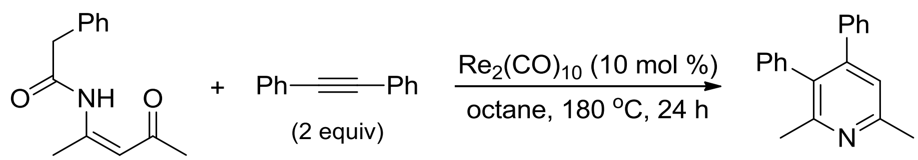
1-(2-benzyl-4-methyloxazol-5-yl)ethan-1-one (5c)



4a **5c**, 83%

Compound **5c** was prepared according to the known procedures.[6] Pale Yellow oil (62.4 mg, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.29 (m, 4H), 7.29 – 7.24 (m, 1H), 4.12 (s, 2H), 2.47 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.4, 163.5, 145.5, 145.0, 134.3, 128.7(3), 127.6(9), 127.3, 34.7, 27.4, 13.5; IR (neat): 2975; 1720 (s), 1652, 1578, 1501, 1478, 1358, 1102, 1011, 744; HRESIMS Calcd for $[C_{13}H_{13}NNaO_2]^+$ (M + Na^+) 238.0838, found 238.0841.

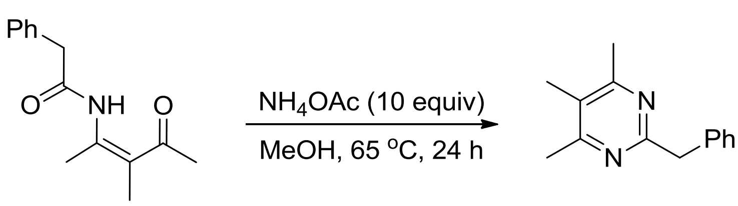
2,6-dimethyl-3,4-diphenylpyridine (5d)



4a **5d**, 70%

A mixture of $Re_2(CO)_{10}$ (19.6 mg, 0.03 mmol), **4a** (0.3 mmol, 65.1 mg), diphenylacetylene (0.6 mmol, 106.9 mg), and octane (0.5 mL) was stirred at 180 °C for 24 h under a nitrogen atmosphere. After the reaction mixture was cooled to 25 °C, the mixture was then concentrated and the residue was purified by chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford pyridine **5d** (54.7 mg, 70% yield, yellow oil). This compound is known and the spectroscopic data match those reported.[7] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.19 (m, 3H), 7.19 – 7.13 (m, 3H), 7.09 – 7.00 (m, 5H), 2.61 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.2, 156.1, 149.2, 139.5, 138.4, 132.3, 130.3, 129.2, 128.0, 127.7, 127.2, 126.8, 121.8, 24.2, 23.9.

2-benzyl-4,5,6-trimethylpyrimidine (5e)

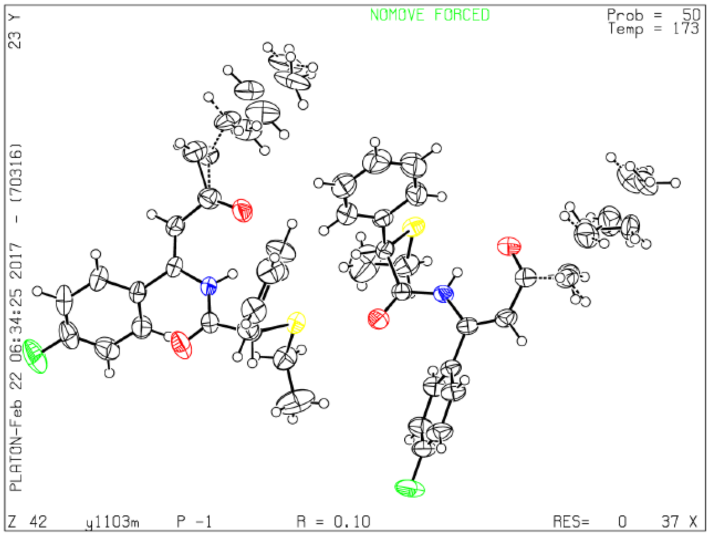


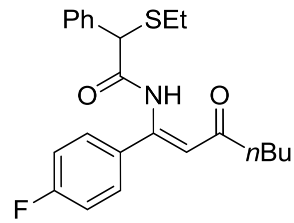
4b **5e**, 55%

NH_4OAc (231.0 mg, 3 mmol) was added to a solution of compound **4b** (0.3 mmol, 76.3 mg) in dry MeOH (3.0 mL) at room temperature. The reaction mixture was stirred at 65

^{o}C and the progress of the reaction was monitored by TLC. Upon completion, the mixture was then concentrated and the residue was purified by chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford pyrimidine **5e** (31.4 mg, 55% yield, yellow oil). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 7.5 Hz, 2H), δ 7.30 – 7.23 (m, 2H), δ 7.22 – 7.14 (m, 1H), 4.16 (s, 2H), 2.44 (s, 6H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 164.6, 139.0, 129.0, 128.2, 126.2, 124.2, 45.5, 22.4, 13.7; IR (neat): 2926, 1698, 1646, 1507, 1489, 1362, 1318, 993, 731, 669; HRESIMS Calcd for $[C_{14}H_{16}N_2Na]^+$ (M + Na^+) 235.1206, found 235.1203.

Compound 3c (CCDC Number = 1819543)





Bond precision: C-C = 0.0061 A Wavelength=0.71073

Cell:	a=8.7586(18)	b=12.203(3)	c=19.973(4)
	alpha=91.534(4)	beta=96.604(4)	gamma=90.138(4)
Temperature:	173 K		

	Calculated	Reported
Volume	2119.8(8)	2119.8(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20.45 H19.45 F N O2 S, C20 H19 F N O2 S, C2 H4, 1.55(C H2), 2(	0.5(C23 H26 F N O2 S), 0.5(C23 H25.55 F N O2 S)
Sum formula	C46 H51.55 F2 N2 O4 S2	C23 H26 F N O2 S
Mr	798.56	399.51
Dx,g cm-3	1.251	1.252
Z	2	4
Mu (mm-1)	0.179	0.179
F000	847.1	848.0
F000’	847.97	
h,k,lmax	11,15,25	11,15,25
Nref	9731	9239
Tmin,Tmax	0.914,0.931	
Tmin’	0.914	

Correction method= Not given

Data completeness= 0.949 Theta(max)= 27.484

R(reflections)= 0.0960(6760) wR2(reflections)= 0.2668(9239)

S = 1.081 Npar= 589

Computational Details

All calculations were carried out with the Gaussian 09 programs.[8] The geometries of all the species were fully optimized by using the density functional theory (DFT) method with the M06[9] functional. The 6-31G (d, p)[10] basis set was used for C, H, N, O, F and S as well as the Lanl (Los Alamos National Laboratory) basis sets, also known as LanL2DZ (Lanl-2-double zeta),[11] for Zn. Frequency calculations at the same theoretical level were performed to confirm each stationary point to be either a local minimum or a transition state (TS). The transition states were verified by intrinsic reaction coordinate (IRC)[12] calculations. The solvent effects of DCE (ε = 10.125) were taken in account by using the SMD-flavor[13] of self-consistent reaction field (SCRF) theory.

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Molecular Geometries and Energies

M06 (SMD, DCE) Cartesian Coordinates and Energies in Hartree

1a

Number of imaginary freguencies: 0

C	-3.29825700	2.88277600	2.72331000
C	-1.95158800	2.75279300	2.41134600
C	-1.34097800	3.65887100	1.52905500
C	-2.10903700	4.69082300	0.96599800
C	-3.45734600	4.80571900	1.27743600
C	-4.05553600	3.90588600	2.15702400
H	-3.76063100	2.17780600	3.41053300
H	-1.35764300	1.95184900	2.84613800
H	-1.63680000	5.39403000	0.28356500
H	-4.04448700	5.60613600	0.83287800
H	-5.11115000	4.00176300	2.40052900
C	0.04113100	3.53048400	1.20812100
C	1.22395800	3.41548700	0.93637700
S	2.84734100	3.28436800	0.48954900
C	3.53693400	2.44141700	1.98108500
H	4.58170800	2.25524800	1.70725800
H	3.03502100	1.47244600	2.07184900
C	3.41874600	3.26855800	3.23788200
H	3.85061800	2.72380700	4.08571200
H	3.94685900	4.22338300	3.13874300
H	2.36915000	3.47997100	3.47308500

Energy (0K) = -784.885886

Energy (0K) + ZPE = -784.718563

Enthalpy (298K) = -784.706557

Free Energy (298K) = -784.757208

A

Number of imaginary freguencies: 0

C	-4.07682800	1.92892600	0.77367400
C	-2.79961000	1.41183800	0.59990300
C	-1.81144000	2.18711400	-0.02042400
C	-2.11780200	3.48121400	-0.46955200
C	-3.39957900	3.98358100	-0.30352300
C	-4.37859900	3.21016400	0.31860100
H	-4.83964700	1.32730600	1.26087600
H	-2.55610400	0.41321600	0.96392100
H	-1.34370700	4.07227800	-0.95381000
H	-3.63609700	4.98364500	-0.65860400
H	-5.38163100	3.60951200	0.44799000
C	-0.48049800	1.67336300	-0.22997600
C	0.73715700	1.83556100	-0.45760100
C	3.19474600	1.79273100	0.75210600
H	4.23873700	1.62343300	0.46386400
H	2.81900000	0.88589400	1.23937100
C	3.01285100	3.04210800	1.57527300
H	3.56044100	2.93746400	2.51882400
H	3.39538900	3.92746200	1.05613100
H	1.95700900	3.20949300	1.81724800
S	1.99690800	-1.82914300	-0.01612100
O	1.35733200	-0.90776300	0.96316400
O	3.40418300	-1.62745700	-0.31008600
S	-2.44555300	-2.41221500	-0.40302200
O	-2.01451100	-1.66165300	-1.62047300
O	-1.51733400	-1.99034000	0.69674900
C	-1.95245300	-4.15204600	-0.72309200
O	-3.86223300	-2.44314000	-0.09500600
F	-2.07985100	-4.84466600	0.39606600
F	-0.69699200	-4.19004300	-1.12904200

F	-2.73630600	-4.66635600	-1.65465800
C	1.90249200	-3.50105500	0.74492200
O	1.06902800	-1.91667200	-1.19419600
F	2.76551100	-3.56411600	1.74600800
F	0.68771300	-3.73908500	1.20005500
F	2.21745900	-4.40266500	-0.17029300
Zn	-0.43215200	-0.55737900	-0.48371600
S	2.33461800	1.89224000	-0.88871700

Energy (0K) = -2772.8715957

Energy (0K) + ZPE = -2772.640850

Enthalpy (298K) = -2772.611465

Free Energy (298K) = -2772.700439

2a

Number of imaginary freguencies: 0

C	0.08003600	1.31100900	-0.03167700
C	1.43567500	1.24041900	0.03919200
C	1.85720400	2.59592700	-0.03005800
H	2.04968400	0.35432900	0.12601900
C	3.24038700	3.13506400	0.00014700
H	3.75378300	2.84121600	0.92233800
H	3.82839100	2.74611100	-0.83857800
H	3.22635700	4.22712800	-0.06007800
C	-0.99660400	0.29973400	-0.01765700
H	-1.68827200	0.47654200	0.81380800
H	-1.58021000	0.33565300	-0.94474500
H	-0.57164500	-0.70141400	0.08825800
N	0.83158700	3.41169600	-0.13346500
O	-0.29667900	2.59748800	-0.13512800

Energy (0K) = -324.469373

Energy (0K) + ZPE = -324.356301

Enthalpy (298K) = -324.348467

Free Energy (298K) = -324.387087

TS_B

Number of imaginary freguencies: 1

C	-3.71016800	2.45925900	0.01246100
C	-2.55047400	1.70127300	-0.09201400
C	-1.56265300	2.03388900	-1.03121200
C	-1.78673500	3.11426100	-1.89890400
C	-2.95718600	3.85604600	-1.80324200
C	-3.91551900	3.53911900	-0.84199000
H	-4.45828800	2.19938300	0.75738400
H	-2.38993900	0.85547400	0.57786000
H	-1.04291600	3.35830600	-2.65407800
H	-3.12364600	4.68683000	-2.48515100
H	-4.82807700	4.12610700	-0.76905300
C	-0.32681400	1.25854200	-1.08926800
C	0.91045600	1.59600300	-1.26049800
S	2.46327200	1.15401300	-1.72066000
C	3.47934700	1.58082000	-0.23020000
H	4.15811800	0.72588000	-0.12920900
H	2.79866500	1.55358500	0.62712900
C	4.22202300	2.88783700	-0.38081600
H	4.88550400	3.02682000	0.48090500
H	4.84321400	2.89628800	-1.28342900
H	3.54094200	3.74491700	-0.42297100
S	1.97298500	-1.64661900	0.79059700
O	1.45355100	-0.41172200	1.39410700
O	3.39249800	-1.71302300	0.47265900
S	-2.46247600	-2.49027700	0.15264200
O	-1.92948800	-2.25416300	-1.22712700

O	-1.65292800	-1.64428300	1.07901500
C	-1.93999200	-4.20798400	0.53453900
O	-3.90411900	-2.47007000	0.31609900
F	-2.22373200	-4.47841700	1.79787000
F	-0.64219600	-4.33601200	0.33282700
F	-2.59338900	-5.04611600	-0.25407200
C	1.71622300	-2.95007700	2.05614300
O	1.06619000	-2.10331400	-0.32562300
F	2.49571100	-2.69530100	3.09808900
F	0.45537000	-2.96835500	2.45441100
F	2.03579500	-4.13369800	1.55313100
Zn	-0.46793100	-0.76554100	-0.58566500
C	1.46664800	5.69898800	-1.79921600
C	1.02313300	5.83565200	-0.51952500
C	0.75856200	4.51298400	-0.08349500
H	0.90304700	6.75122400	0.04318800
C	0.23470600	4.04538800	1.22221100
H	0.74668600	4.55637200	2.04342100
H	-0.83421100	4.27917700	1.30412400
H	0.36423600	2.96453400	1.33970300
C	1.91507600	6.65067000	-2.83248200
H	2.94312800	6.43221800	-3.14176800
H	1.27894400	6.58728000	-3.72241000
H	1.87301600	7.67031600	-2.44307200
N	1.03572000	3.66630400	-1.05181400
O	1.47942700	4.39272400	-2.13276900

Energy (0K) = -3097.3400039

Energy (0K) + ZPE = -3096.994813

Enthalpy (298K) = -3096.957895

Free Energy (298K) = -3097.066561

B

Number of imaginary freguencies: 0

C	-3.71882700	2.47250500	0.08250100
C	-2.52465500	1.77119500	-0.03255500
C	-1.55053100	2.15126000	-0.97030500
C	-1.84058100	3.22291000	-1.83174200
C	-3.04509800	3.90852100	-1.72999700
C	-3.98221400	3.54587100	-0.76450800
H	-4.45126300	2.16980700	0.82729500
H	-2.32480700	0.92474700	0.62661400
H	-1.12601000	3.50315800	-2.60468800
H	-3.25622400	4.72892100	-2.41250900
H	-4.92227900	4.08694500	-0.68526700
C	-0.28651000	1.40330900	-1.02448900
C	0.91171500	2.00299700	-1.17322500
S	2.42819200	1.15795400	-1.51813000
C	3.50803200	1.68992400	-0.12322200
H	4.17092400	0.82963500	0.02924100
H	2.87580300	1.75135200	0.76974300
C	4.28729000	2.95966900	-0.38516400
H	4.98732400	3.14526900	0.43864900
H	4.86963300	2.88586100	-1.31046600
H	3.63591000	3.83824000	-0.46579500
S	1.96259300	-1.52718000	0.88870700
O	1.39408800	-0.35632200	1.56478400
O	3.39697100	-1.54241000	0.62755300
S	-2.40466800	-2.37185300	0.06297100
O	-1.81958900	-2.07776200	-1.28775200
O	-1.65494300	-1.57800200	1.06593800
C	-1.90159700	-4.10894300	0.37476800
O	-3.85572100	-2.37220400	0.14445500

F	-2.21664200	-4.43533500	1.61927900
F	-0.60037100	-4.24363700	0.19875200
F	-2.54063300	-4.91167900	-0.46383300
C	1.69492600	-2.91901800	2.05348400
O	1.11959600	-1.95095100	-0.28634900
F	2.44191700	-2.72993500	3.13507100
F	0.42494900	-2.98618900	2.41777300
F	2.04806600	-4.06281300	1.48231900
Zn	-0.37415800	-0.60543000	-0.69654000
C	1.43805000	5.42391100	-1.86568200
C	0.98325300	5.58574000	-0.58762600
C	0.73131600	4.29332900	-0.09846900
H	0.85353200	6.51508600	-0.05142500
C	0.22013500	3.87259500	1.21899600
H	0.70372600	4.46134900	2.00357200
H	-0.85784900	4.07379600	1.26826300
H	0.38089300	2.80603100	1.39981800
C	1.88651800	6.35618900	-2.90978900
H	2.92812500	6.15201200	-3.18109700
H	1.27680100	6.24259500	-3.81277400
H	1.80471200	7.38276800	-2.54801900
N	1.02676900	3.43209300	-1.07072400
O	1.47272600	4.11563200	-2.17962100

Energy (0K) = -3097.372088

Energy (0K) + ZPE = -3097.024913

Enthalpy (298K) = -3096.987984

Free Energy (298K) = -3097.094028

TS$_C$

Number of imaginary freguencies: 1

C	-3.85986200	2.56073900	0.72377100

C	-2.67194200	1.85233800	0.77968700
C	-1.52127200	2.30780400	0.09741700
C	-1.62737200	3.48060100	-0.68642500
C	-2.82775400	4.16589600	-0.76591100
C	-3.94044400	3.71627000	-0.05359400
H	-4.72930900	2.20853400	1.27246900
H	-2.60823300	0.94894600	1.38682500
H	-0.76718200	3.81933800	-1.25925900
H	-2.90282400	5.05437600	-1.38775000
H	-4.87895900	4.26210600	-0.11535300
C	-0.30836500	1.54018600	0.19025200
C	0.95868000	2.10791900	0.04891100
S	2.34068200	1.13041800	-0.47956300
C	3.67275900	1.71724300	0.64353800
H	4.33214500	0.84724200	0.73629500
H	3.21115400	1.86695700	1.62701000
C	4.41794300	2.93505900	0.14453800
H	5.22951400	3.18416400	0.83912800
H	4.86307700	2.74992800	-0.83964900
H	3.76091600	3.80772700	0.05829500
S	1.98060400	-1.24577400	2.23843300
O	1.45368700	0.02095800	2.76636600
O	3.40680900	-1.33366400	1.95773200
S	-2.43204200	-2.19911700	1.48694100
O	-1.82545700	-2.00467500	0.13096400
O	-1.70830400	-1.29750700	2.42615300
C	-1.89887700	-3.88411100	1.97773500
O	-3.88258300	-2.21089800	1.55801600
F	-2.23309900	-4.09384400	3.24116500
F	-0.59180600	-3.99951900	1.84164500
F	-2.50271900	-4.77615800	1.20840200

C	1.70059500	-2.48278900	3.56562800
O	1.09343000	-1.77344400	1.14122700
F	2.44129800	-2.16328300	4.61941700
F	0.42761500	-2.50444800	3.92503900
F	2.05204600	-3.68787000	3.13809000
Zn	-0.42625200	-0.44817800	0.74015400
C	1.35864800	5.69773600	-0.26470900
C	0.99409600	5.55358500	1.07563100
C	0.90666400	4.20615900	1.39363600
H	0.86364200	6.35963900	1.78557300
C	0.57852700	3.64576800	2.73358400
H	0.77815300	4.38967000	3.50825100
H	-0.48800300	3.38913800	2.76760800
H	1.14847900	2.73239100	2.93087500
C	1.63561200	6.98738400	-0.95143700
H	2.69285200	7.02845000	-1.23657300
H	1.04539000	7.05526300	-1.87095000
H	1.40326100	7.83411900	-0.30140000
N	1.17932400	3.37884200	0.39114700
O	1.49429000	4.61208800	-0.92893600

Energy (0K) = -3097.3475014

Energy (0K) + ZPE = -3097.002700

Enthalpy (298K) = -3096.965908

Free Energy (298K) = -3097.070223

C

Number of imaginary freguencies: 0

C	-2.78218800	1.46859900	-3.42728400
C	-1.83500900	1.16563300	-2.47289600
C	-0.64377200	1.94239200	-2.36671000
C	-0.44305200	3.03237000	-3.27217900

C	-1.39223100	3.31991400	-4.22275500
C	-2.55713800	2.53982000	-4.29610900
H	-3.69310900	0.88305300	-3.50545200
H	-1.98602400	0.34011000	-1.77432700
H	0.47003700	3.62214800	-3.20858100
H	-1.24687300	4.13994200	-4.91950200
H	-3.30229600	2.77456200	-5.05277800
C	0.28241800	1.59862100	-1.38488900
C	1.48617200	2.39491700	-1.19299800
S	2.90019000	1.69726400	-1.99535200
C	4.15795200	2.97315100	-1.59868000
H	5.10938400	2.44468900	-1.72182300
H	4.04302500	3.21628000	-0.53752300
C	4.06603200	4.19171700	-2.48893500
H	4.19175000	3.92548600	-3.54394900
H	3.10247400	4.70102300	-2.37132200
H	4.85700000	4.90293200	-2.22295000
S	1.51739100	-2.40727000	-0.11542400
O	1.84422900	-1.08787900	0.52340000
O	2.59705500	-3.03988600	-0.85533700
S	-2.68914500	-1.05136700	1.02247500
O	-2.94558700	-1.01801100	-0.41959800
O	-1.27288000	-0.68230600	1.37654900
C	-2.73930500	-2.83170000	1.46218600
O	-3.67199800	-0.42904400	1.90105700
F	-2.37013500	-3.00008100	2.72402200
F	-1.94019700	-3.53128800	0.67517700
F	-3.98187800	-3.27784800	1.31417500
C	1.23436200	-3.49650300	1.33617700
O	0.19764800	-2.28392900	-0.77003300
F	2.36376700	-3.61652900	2.01927300

F	0.30446000	-2.98302900	2.12506300
F	0.84833700	-4.69380600	0.92171700
Zn	0.11823400	0.03797700	0.06876700
C	0.11856300	2.41418000	1.99277900
C	-0.04147600	3.69130200	1.35050200
C	0.57196800	4.11825400	0.20394100
H	-0.67962200	4.41247700	1.85841000
C	0.32438500	5.49189400	-0.32827600
H	1.26183800	6.06110100	-0.34390600
H	-0.02362400	5.42768900	-1.36820300
H	-0.41717200	6.03329400	0.26415500
C	-0.56096400	2.23351400	3.31342500
H	-0.26767800	1.28487000	3.76805100
H	-0.33457200	3.06600100	3.98929400
H	-1.64889700	2.23495400	3.16231100
N	1.55262700	3.45659500	-0.48959600
O	0.77149700	1.47190000	1.49648300

Energy (0K) = -3097.3851992

Energy (0K) + ZPE = -3097.040218

Enthalpy (298K) = -3097.002666

Free Energy (298K) = -3097.109619

TS_D

Number of imaginary freguencies: 1

C	0.32727900	0.38795100	4.50337400
C	-0.23256000	0.77515600	3.29862800
C	-0.05435700	2.09260800	2.82201300
C	0.69707500	3.00940400	3.59690600
C	1.26913900	2.60811400	4.78855600
C	1.08120000	1.29985600	5.24215700
H	0.18318400	-0.62441300	4.87018000

H	-0.82141000	0.07481400	2.71003100
H	0.83560400	4.02989100	3.24087200
H	1.85739900	3.30838100	5.37516400
H	1.52667100	0.98986000	6.18453200
C	-0.60894000	2.47339300	1.55830900
C	-0.66871200	3.84113900	1.16844500
C	-3.31947900	4.09950600	0.31514800
H	-2.75523000	3.55574700	-0.45191700
H	-4.23512100	3.54134500	0.53629600
C	-3.58158400	5.52855100	-0.10021500
H	-2.64549300	6.05663500	-0.31280400
H	-4.12696600	6.08218000	0.67139100
H	-4.18954700	5.53049600	-1.01247100
S	0.48927000	-1.00567300	-0.05715500
O	0.70344900	0.30080400	-0.74692700
O	1.61177400	-1.56023700	0.67897200
S	-3.96673000	0.08024500	-0.60491400
O	-3.86024200	0.13734800	0.85436400
O	-2.68910100	0.54423700	-1.26388500
C	-3.98405700	-1.70408600	-1.04344000
O	-5.16507200	0.62110500	-1.23088500
F	-3.88595800	-1.83968900	-2.35843900
F	-2.98525500	-2.34858200	-0.46520000
F	-5.12991600	-2.23572600	-0.63696400
C	0.16217000	-2.17737400	-1.42968800
O	-0.81918800	-0.91951500	0.64982700
F	1.23940800	-2.27457900	-2.19394600
F	-0.85239900	-1.73844200	-2.15627000
F	-0.13328400	-3.36788100	-0.93392500
Zn	-1.23816700	1.18860600	-0.03416600
C	0.38641700	2.91706600	-1.90214100

C	1.35786000	3.75962000	-1.24921500
C	1.16107500	4.52904300	-0.14057200
H	2.33495900	3.83226800	-1.72307500
C	2.23766100	5.39572400	0.41463400
H	2.40919500	5.14568600	1.46967200
H	1.92385500	6.44592100	0.38614100
H	3.17369400	5.28009500	-0.13628300
C	0.79652000	2.28668700	-3.19246900
H	0.09796700	1.49009900	-3.46142800
H	1.81570200	1.89054700	-3.12772900
H	0.79689500	3.04920200	-3.98283900
N	-0.05228900	4.70533500	0.49786700
O	-0.75913000	2.71027200	-1.44890800
S	-2.32540800	4.03341700	1.87754500

Energy (0K) = -3097.3829364

Energy (0K) + ZPE = -3097.038654

Enthalpy (298K) = -3097.001535

Free Energy (298K) = -3097.106928

D

Number of imaginary freguencies: 0

C	-0.07332500	0.13987300	4.54318200
C	-0.32838900	1.05307600	3.52668400
C	0.71600200	1.53117100	2.72916000
C	2.01836600	1.07847200	2.96866000
C	2.26546600	0.16214500	3.98484100
C	1.22282300	-0.31230500	4.77506200
H	-0.89645300	-0.22125500	5.15545700
H	-1.34400600	1.40698300	3.35616600
H	2.84629900	1.43553200	2.35681700
H	3.28259300	-0.18318500	4.15525500

H	1.41873200	-1.03111600	5.56688200
C	0.41035400	2.45261000	1.58812300
C	1.42172000	3.01126400	0.86119800
C	-2.29186300	2.81632500	0.78243900
H	-2.00068600	2.76556400	-0.27535800
H	-2.39713600	1.79555100	1.17340000
C	-3.57737200	3.59622800	0.95002900
H	-3.48228900	4.61842400	0.56586100
H	-3.87967900	3.64833300	2.00212600
H	-4.37874600	3.09950100	0.39209400
S	1.87504100	-1.31071600	0.34587000
O	2.05350900	0.07177100	-0.22617200
O	2.96821700	-1.81897800	1.15266800
S	-2.55652900	-0.65279500	-0.88414800
O	-2.75215800	-0.67384900	0.56479200
O	-1.20972100	-0.09112200	-1.28956900
C	-2.34499700	-2.40549800	-1.37889900
O	-3.64434400	-0.15177400	-1.71335600
F	-2.12322500	-2.47986400	-2.68404600
F	-1.32628100	-2.94893500	-0.73467600
F	-3.45143300	-3.07645700	-1.08785500
C	1.84575300	-2.36021800	-1.15904200
O	0.49436800	-1.38556200	0.87788300
F	3.03883500	-2.33663200	-1.73560300
F	0.94315400	-1.89840200	-2.01018900
F	1.54118900	-3.60287800	-0.82458100
Zn	0.05134800	0.77166300	-0.00318400
C	1.64526200	2.10542200	-2.23738700
C	2.78542500	2.99639400	-2.03479400
C	3.07843600	3.65479600	-0.89178600
H	3.49011500	3.10341600	-2.85687000

C	4.26242500	4.53123500	-0.72053400
H	4.90169800	4.15165000	0.08584800
H	3.94054800	5.53745400	-0.42500700
H	4.84241100	4.59218600	-1.64368200
C	1.72610100	1.12048200	-3.34549200
H	0.79394300	0.55466300	-3.42589000
H	2.56153800	0.43511000	-3.14624300
H	1.95163400	1.62645800	-4.29185200
N	2.29963500	3.54088800	0.26060700
O	0.65902400	2.16270400	-1.48906200
S	-0.94847000	3.65416000	1.71549700

Energy (0K) = -3097.4073228

Energy (0K) + ZPE = -3097.060883

Enthalpy (298K) = -3097.023613

Free Energy (298K) = -3097.128645

TS_{D1}

Number of imaginary freguencies: 1

C	-3.00026500	1.95763900	-3.09194000
C	-2.08852900	1.67534900	-2.08926900
C	-0.85464300	2.35859400	-2.03095800
C	-0.55925500	3.32431100	-3.02437600
C	-1.46910600	3.59057500	-4.02946200
C	-2.69144000	2.91296000	-4.05991200
H	-3.94951800	1.43015400	-3.12870000
H	-2.31095900	0.92329200	-1.33096800
H	0.39353000	3.85333600	-3.00427900
H	-1.23558300	4.32453900	-4.79600000
H	-3.40484300	3.12767400	-4.85202100
C	0.05313000	2.05023200	-0.96539200
C	1.40990900	2.62379500	-0.99217900

S	2.55686000	1.62118500	-1.82107300
C	4.12846100	2.53562400	-1.55192400
H	4.89545100	1.75879900	-1.63901800
H	4.11604800	2.89001200	-0.51714900
C	4.32383700	3.64757100	-2.55685700
H	4.32431800	3.26392000	-3.58259600
H	3.53907200	4.40641000	-2.46752200
H	5.29001800	4.13392800	-2.37871000
S	1.81813100	-1.90648300	-0.08178300
O	1.94915800	-0.65154900	0.72963300
O	2.98290600	-2.29855500	-0.85741600
S	-2.50389900	-1.01106900	1.33400700
O	-2.89251000	-0.74629300	-0.05382400
O	-1.08124400	-0.59855300	1.62335000
C	-2.39540300	-2.84065300	1.45153700
O	-3.42995000	-0.62189700	2.38844500
F	-1.99485800	-3.19572500	2.66343000
F	-1.54982200	-3.32055900	0.55445800
F	-3.59932000	-3.35297500	1.22721000
C	1.62895700	-3.21257600	1.19228900
O	0.50769600	-1.85943400	-0.77119700
F	2.77969600	-3.37760400	1.82777700
F	0.69810800	-2.86521300	2.06374900
F	1.28273500	-4.35008100	0.60936100
Zn	0.10581300	0.29372900	0.25980000
C	-0.16795500	2.59041500	1.72814100
C	-0.36432800	3.62728000	0.70867400
C	0.65836500	4.37106100	0.09905200
H	-1.30370700	4.17032900	0.82942700
C	0.58258800	5.84264600	-0.03945100
H	1.51248200	6.28086200	0.34439800

H	0.53930000	6.10679200	-1.10537700
H	-0.27197900	6.27350300	0.48466100
C	-1.27185500	2.47650300	2.72970900
H	-1.12030300	1.60132700	3.36484200
H	-1.32514800	3.38593900	3.34095000
H	-2.23340800	2.39360100	2.20431300
N	1.73283700	3.78013600	-0.47692400
O	0.80096500	1.81928800	1.75282500

Energy (0K) = -3097.3639353

Energy (0K) + ZPE = -3097.019250

Enthalpy (298K) = -3096.982700

Free Energy (298K) = -3097.086244

D1

Number of imaginary freguencies: 0

C	-3.44483000	1.62697800	-2.83107000
C	-2.45837700	1.67194800	-1.85181900
C	-1.25035000	2.34226200	-2.07250900
C	-1.06924000	2.99294100	-3.30106900
C	-2.05326600	2.95042900	-4.28151600
C	-3.24307800	2.26434300	-4.05100800
H	-4.36791900	1.08557000	-2.63822500
H	-2.63627700	1.16077000	-0.90380500
H	-0.14797700	3.54332000	-3.48506900
H	-1.89062900	3.45849300	-5.22943200
H	-4.01042700	2.22603400	-4.82058400
C	-0.18669600	2.43115600	-1.03081100
C	1.18063600	2.30770300	-1.29670900
S	1.88277700	1.50898100	-2.66030600
C	3.68585400	1.61560700	-2.31237500
H	4.09502400	0.81082400	-2.93373400

H	3.84052100	1.33142900	-1.26704100
C	4.28501800	2.95646300	-2.66711500
H	4.11493200	3.20687300	-3.72008300
H	3.86303700	3.75397600	-2.04670500
H	5.36769000	2.93063000	-2.49592400
S	2.01964000	-0.76780600	0.52333300
O	1.41376400	0.31353400	1.36607800
O	3.39437000	-0.57372400	0.09564000
S	-2.47704400	-1.93225200	0.54226300
O	-2.50087900	-1.79623300	-0.91251900
O	-1.47289600	-1.01385600	1.19755800
C	-1.72531100	-3.57628300	0.85275900
O	-3.74969900	-1.97381100	1.25033500
F	-1.54061100	-3.75876500	2.15230200
F	-0.56210500	-3.69042300	0.22970600
F	-2.54781700	-4.51320200	0.39713300
C	2.05858400	-2.22034600	1.64588900
O	1.01887400	-1.11278800	-0.52763000
F	2.95123300	-2.00218900	2.59895500
F	0.87098400	-2.40018200	2.19263900
F	2.40306100	-3.29512400	0.95781100
Zn	-0.42859100	0.42248900	0.23673500
C	-1.08048400	3.07924700	1.30598900
C	-0.24501800	3.44512200	0.09718500
C	1.22409800	3.56954600	0.46339700
H	-0.57808700	4.42574100	-0.28450500
C	1.72487300	4.29024800	1.64780300
H	2.81541200	4.34461000	1.62455500
H	1.29876300	5.29802200	1.71302100
H	1.42171300	3.75116100	2.55786600
C	-1.70982000	4.16670600	2.08644200

H	-2.05315000	3.80734100	3.05829900
H	-1.03966700	5.02655000	2.19329200
H	-2.57471400	4.51975800	1.50603900
N	1.99941300	2.92974100	-0.35061800
O	-1.22040000	1.89646400	1.61578200

Energy (0K) = -3097.4527992

Energy (0K) + ZPE = -3097.103859

Enthalpy (298K) = -3097.067684

Free Energy (298K) = -3097.169333

TS_{D2}

Number of imaginary freguencies: 1

C	-3.31580300	1.75705300	-2.42605700
C	-2.28104700	1.21625800	-1.68625200
C	-1.04438200	1.89056500	-1.56780100
C	-0.87265800	3.11351300	-2.25664700
C	-1.90149800	3.63769500	-3.01900800
C	-3.12404700	2.96858200	-3.09180600
H	-4.26527700	1.23463000	-2.50116500
H	-2.40634000	0.25358900	-1.18669700
H	0.08392300	3.62995300	-2.21146200
H	-1.75856100	4.57055400	-3.55761900
H	-3.93251600	3.39015900	-3.68446700
C	-0.00427500	1.28760100	-0.78137200
C	1.28676200	1.97113600	-0.64604300
S	2.57832000	1.00965100	-1.35509800
C	3.91647200	2.24955800	-1.51771500
H	4.80490200	1.63951700	-1.71456000
H	4.04126200	2.71948600	-0.53735300
C	3.67232400	3.25895900	-2.61731500
H	3.54565700	2.76974600	-3.58895900

H	2.78209900	3.86501900	-2.41293600
H	4.52936200	3.93871600	-2.68803200
S	1.77844800	-2.29961500	0.79566700
O	1.47050300	-0.93515300	1.32407800
O	3.16241400	-2.58627200	0.46324300
S	-2.85375700	-2.11661900	0.76751300
O	-2.73298200	-2.27972200	-0.68333300
O	-1.67005800	-1.37622100	1.33982300
C	-2.62665100	-3.80019000	1.46178900
O	-4.12937400	-1.66541400	1.30733900
F	-2.52424900	-3.73754000	2.78115400
F	-1.53947300	-4.36874300	0.96760400
F	-3.68101400	-4.53968100	1.14236800
C	1.38102000	-3.40767800	2.20605400
O	0.74682500	-2.61727000	-0.23408200
F	2.29394300	-3.24719500	3.15201400
F	0.19052600	-3.11242900	2.69786800
F	1.38924500	-4.66604600	1.79641000
Zn	-0.28370600	-0.60166000	0.08001900
C	-0.78927600	2.55582100	1.76448100
C	-0.32578300	3.82475200	1.31936200
C	0.68471300	4.04662200	0.41552200
H	-0.76355200	4.69676200	1.80094400
C	1.04845900	5.44591800	0.04137600
H	2.10007000	5.63699600	0.28466000
H	0.94964500	5.57464800	-1.04509100
H	0.41681700	6.18399700	0.54164700
C	-1.69845900	2.49850800	2.94486200
H	-1.94153400	1.46367100	3.19561100
H	-1.23654800	2.99628400	3.80496200
H	-2.62197200	3.04550000	2.71577400

N	1.52797900	3.12782300	-0.14478300
O	-0.46364500	1.47495700	1.20607700

Energy (0K) = -3097.378941

Energy (0K) + ZPE = -3097.033781

Enthalpy (298K) = -3096.996748

Free Energy (298K) = -3097.102780

D2

Number of imaginary freguencies: 0

C	-3.25222300	2.49756500	-2.00572200
C	-2.23437000	2.07705200	-1.16085800
C	-0.89118000	2.33891500	-1.47203900
C	-0.59960000	3.01752100	-2.66092900
C	-1.62382800	3.41929400	-3.51547700
C	-2.95169800	3.16952200	-3.18993700
H	-4.28662500	2.28812600	-1.74277400
H	-2.48106700	1.53187100	-0.24857600
H	0.43315900	3.23688600	-2.93234800
H	-1.37552100	3.94281200	-4.43613800
H	-3.74939000	3.49241400	-3.85446800
C	0.18759000	1.81041700	-0.57882700
C	1.52018700	2.47649400	-0.75233200
S	2.80944400	1.44488700	-1.26135300
C	4.19993400	2.61534900	-1.49160300
H	5.08646500	1.97237900	-1.47795700
H	4.23236100	3.24922800	-0.59984100
C	4.10191500	3.41499600	-2.77203700
H	4.07591500	2.76166900	-3.65054000
H	3.20919300	4.05020000	-2.78095400
H	4.97831000	4.06719500	-2.86132200
S	2.12785100	-1.84352600	0.52866800

O	1.75548500	-0.58542600	1.20570700
O	3.53255800	-2.10234700	0.26189400
S	-2.55627900	-1.71724600	0.00778900
O	-2.30968300	-1.93608700	-1.41904000
O	-1.41809000	-0.96599000	0.65152900
C	-2.40505400	-3.38561700	0.75515400
O	-3.86707200	-1.23682000	0.42247000
F	-2.36569200	-3.30026500	2.07611600
F	-1.30679600	-3.98530800	0.32181400
F	-3.45705700	-4.11125700	0.39879800
C	1.61547600	-3.16737700	1.69490000
O	1.20918000	-2.03283800	-0.65274700
F	2.47204500	-3.19939700	2.70541600
F	0.40458600	-2.92364800	2.16582500
F	1.62532200	-4.33662600	1.07560600
Zn	0.06223500	-0.27862000	-0.56995500
C	-0.46379900	3.13299800	1.40320300
C	-0.13368500	4.38012300	0.89616500
C	0.81827700	4.63396600	-0.09154400
H	-0.60398300	5.23616700	1.37380900
C	1.00332300	6.01531700	-0.60733400
H	1.96476900	6.41405900	-0.26077400
H	1.05291900	5.98620600	-1.70347100
H	0.20055200	6.68516200	-0.29214900
C	-1.25167800	2.96741500	2.64290500
H	-0.82295100	2.16102000	3.24767000
H	-1.29919800	3.89023800	3.22345800
H	-2.27057500	2.65443800	2.37609600
N	1.70861700	3.74246100	-0.56604300
O	-0.14414600	1.98310700	0.85305800

Energy (0K) = -3097.3991631

Energy (0K) + ZPE = -3097.053093

Enthalpy (298K) = -3097.016037

Free Energy (298K) = -3097.121946

H_2O

Number of imaginary freguencies: 0

O	1.60711900	1.40696800	0.00000000
H	2.56870600	1.45719400	0.00000000
H	1.33332500	2.33034200	0.00000000

Energy (0K) = -76.3915317

Energy (0K) + ZPE = -76.370017

Enthalpy (298K) = -76.366237

Free Energy (298K) = -76.388322

3a

Number of imaginary freguencies: 0

C	-1.64937300	1.51222600	-4.41510400
C	-0.78800100	0.99857900	-3.45454300
C	0.27245500	1.76761600	-2.96564900
C	0.44644700	3.06646300	-3.44871300
C	-0.41636400	3.58070900	-4.41370500
C	-1.46300900	2.80569100	-4.90146900
H	-2.47124700	0.90286900	-4.78465100
H	-0.92576800	-0.01488800	-3.07861000
H	1.26224400	3.68496500	-3.07602900
H	-0.26786900	4.59280100	-4.78364100
H	-2.13765900	3.20822200	-5.65369500
C	1.21863600	1.15971200	-1.95767300
C	1.86261100	2.23842100	-1.08905900
S	2.45425000	0.01989400	-2.70180800
C	3.19269700	1.03686700	-4.04056500

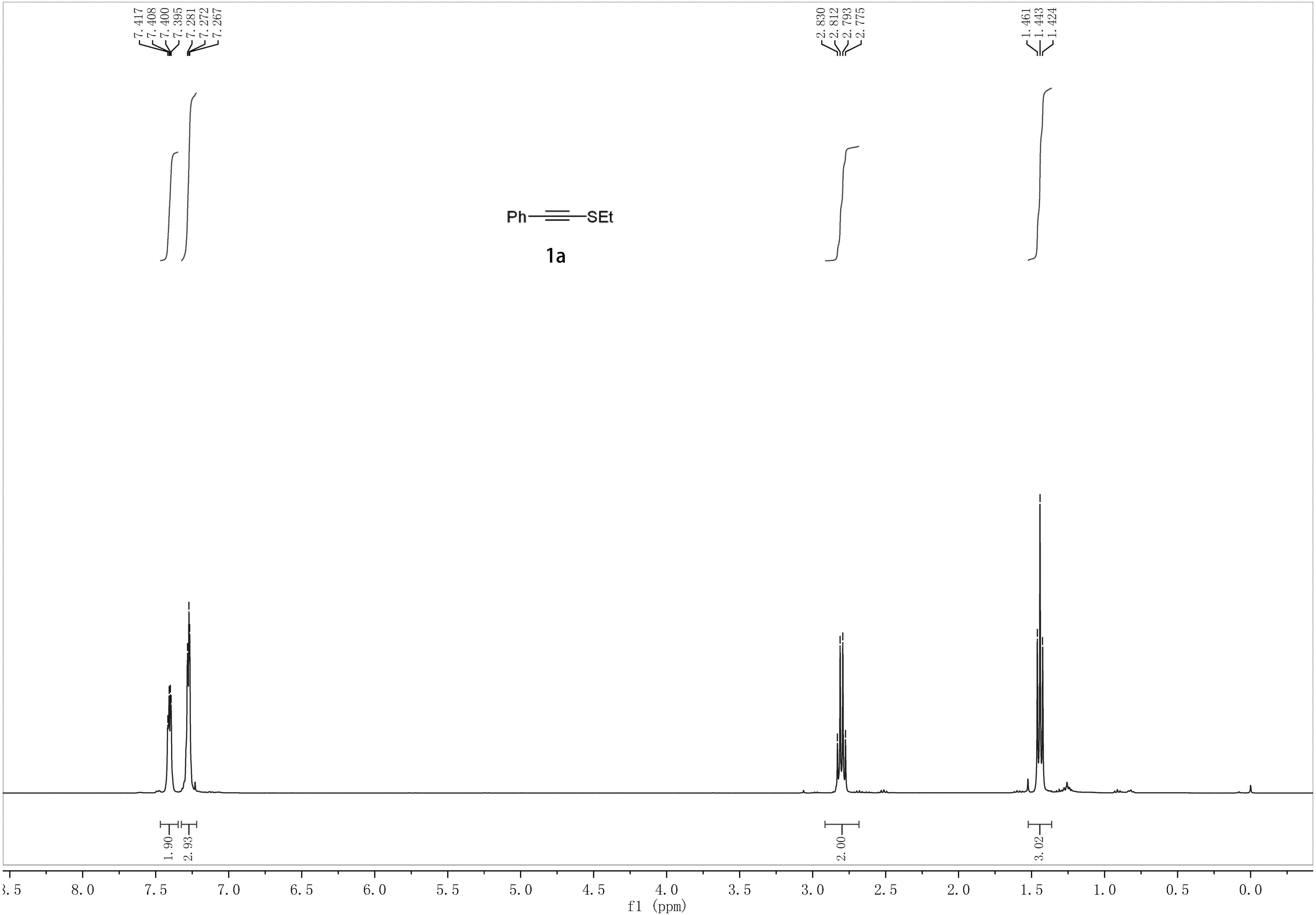
H	4.24045300	0.71667500	-4.08174100
H	3.20109100	2.07637300	-3.69665200
C	2.52507900	0.86388900	-5.38898000
H	3.05218900	1.45327500	-6.15019700
H	2.54396900	-0.18560700	-5.70509100
H	1.47919000	1.19161600	-5.37267500
C	-1.06677000	3.23449200	1.81506400
C	0.18383700	3.96291400	1.70862300
C	1.17155800	3.70256500	0.80304300
H	0.34427100	4.78323300	2.40446100
C	2.41664100	4.51878200	0.77386900
H	2.35791400	5.30427100	1.53172800
H	3.30031200	3.90078400	0.96298300
H	2.56595300	4.97674900	-0.20970300
C	-2.00968100	3.69853700	2.88763500
H	-2.27495600	4.75108200	2.72875100
H	-2.91577500	3.08797300	2.88748300
H	-1.52587800	3.63955700	3.87040600
N	1.00284900	2.67231200	-0.10099800
O	-1.37224900	2.28463900	1.08124200
O	2.97525400	2.68979700	-1.28315800
H	0.64228300	0.48766500	-1.30600300
H	0.09352200	2.20470700	0.00283800

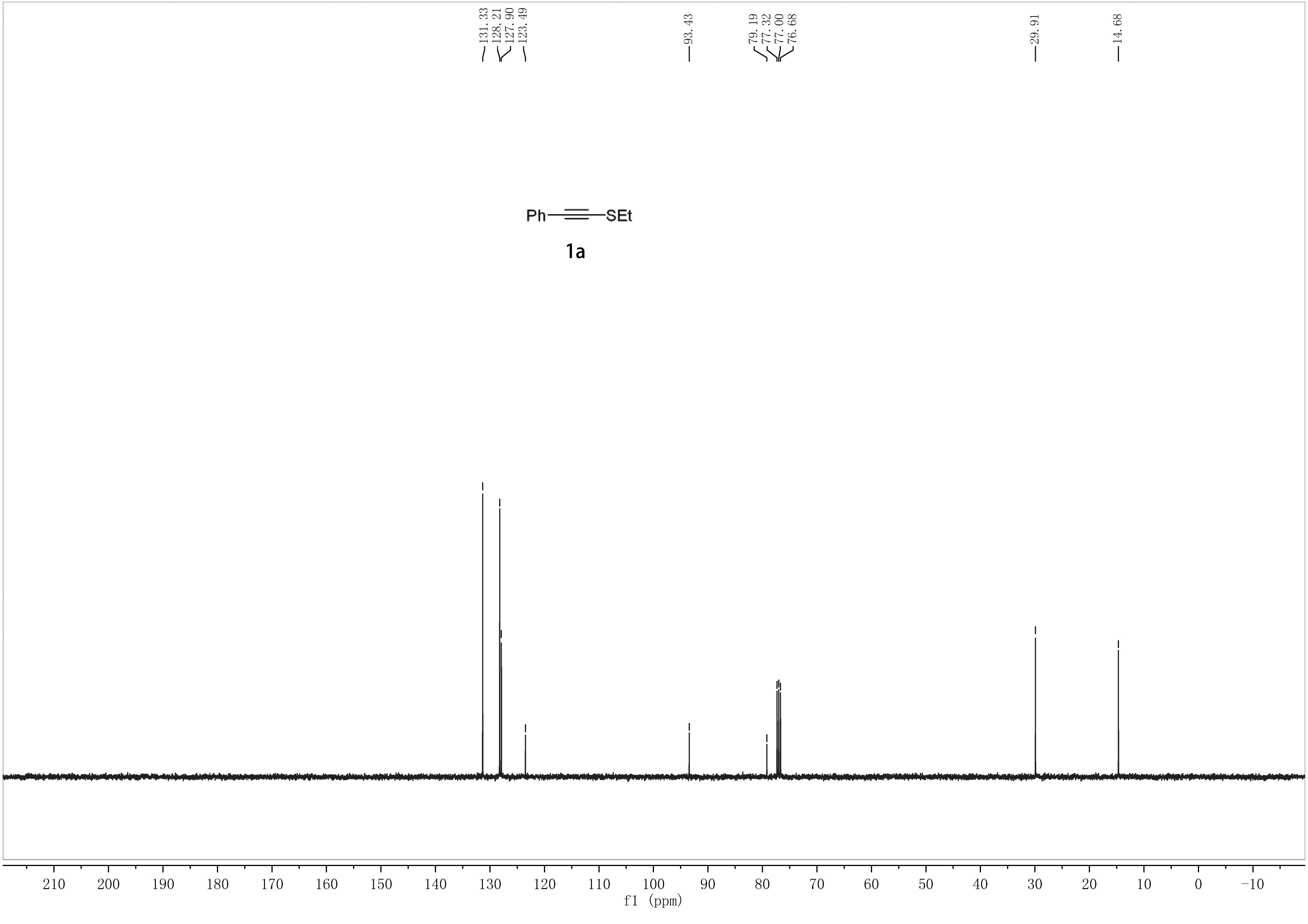
Energy (0K) = -1185.890419

Energy (0K) + ZPE = -1185.578773

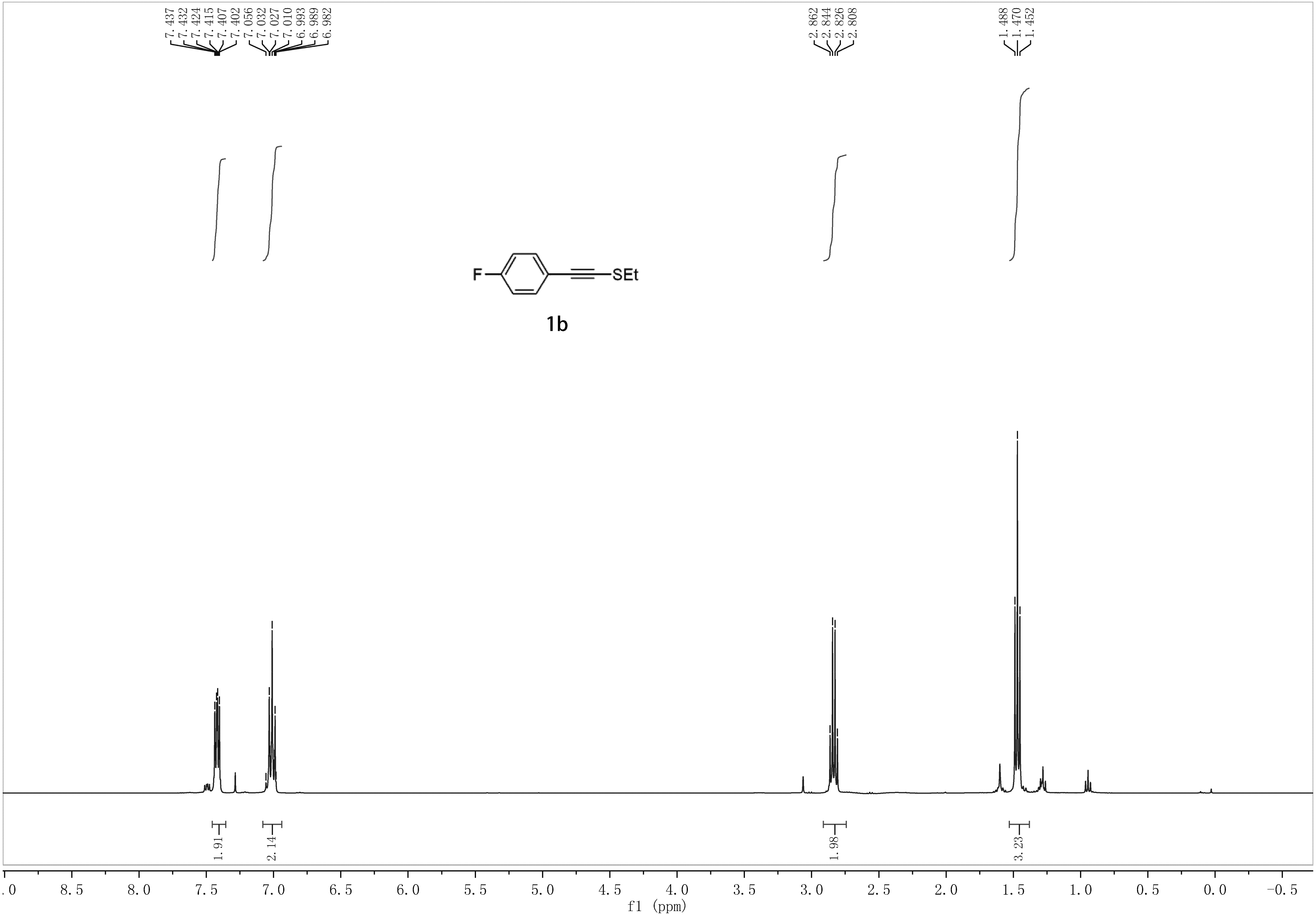
Enthalpy (298K) = -1185.557584

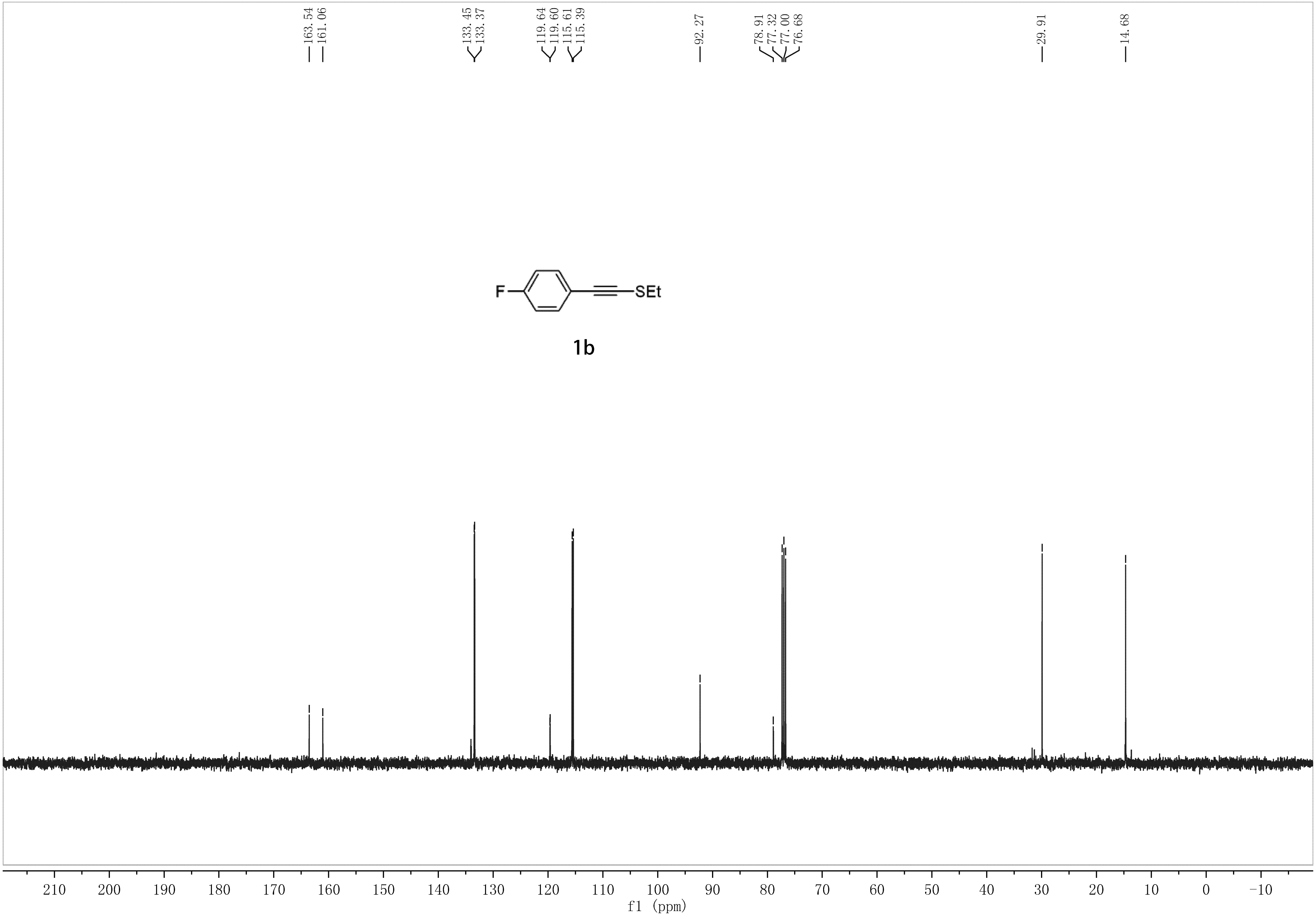
Free Energy (298K) = -1185.630909

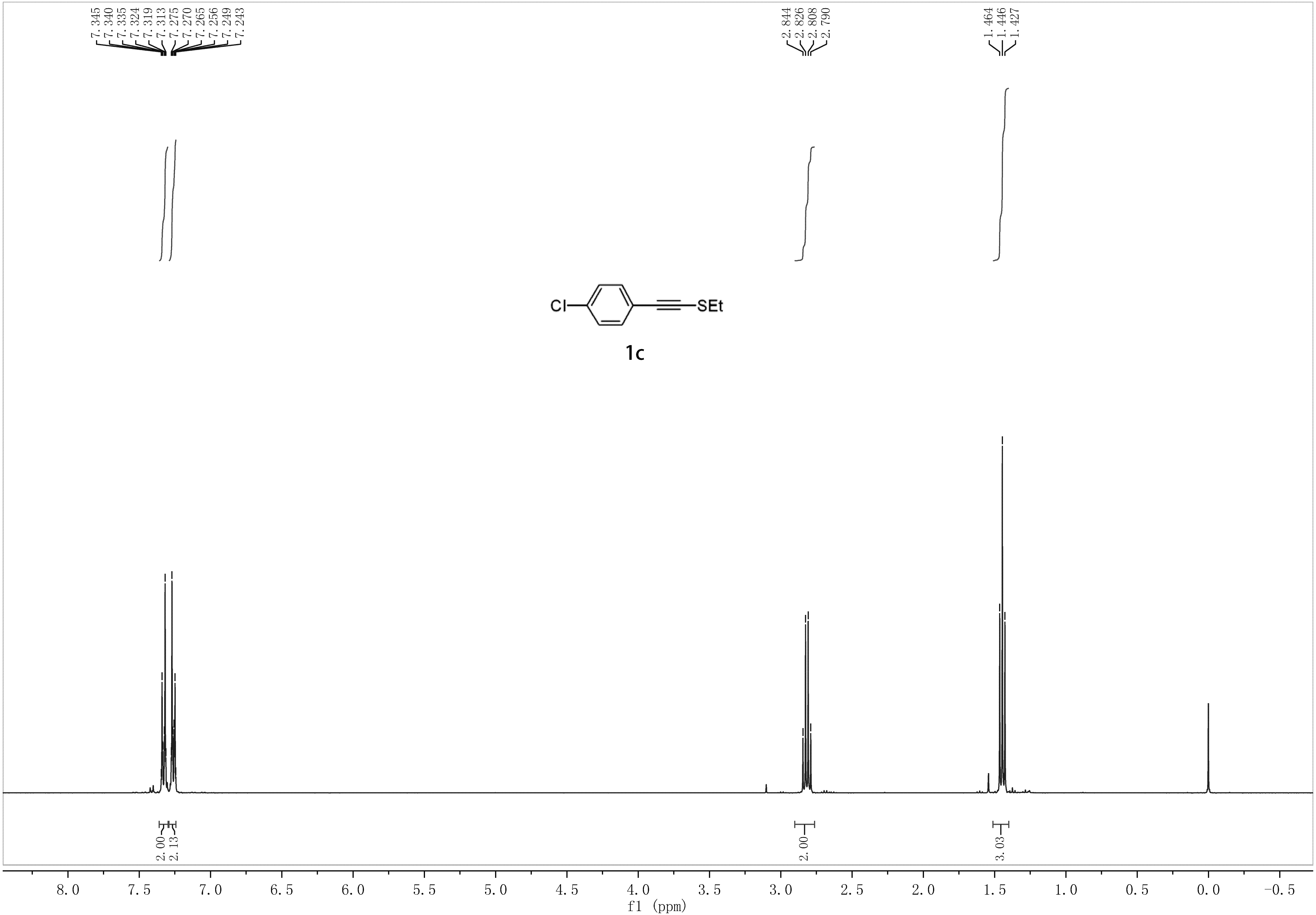

7.417
7.408
7.400
7.395
7.281
7.272
7.267
2.830
2.812
2.793
2.775
1.461
1.443
1.424
Ph—≡—SEt
1a
1.90
2.93
2.00
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

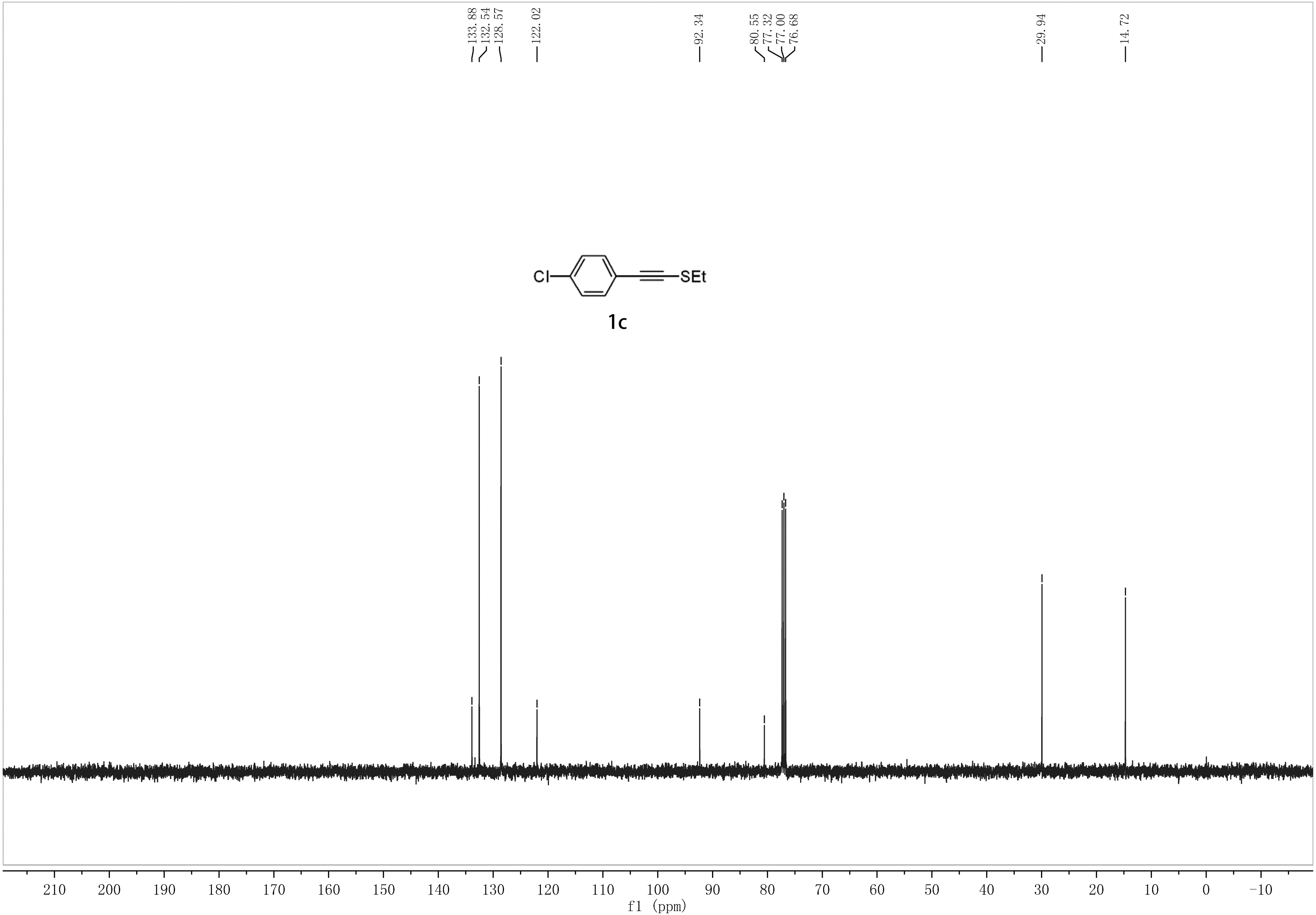


131.33
128.21
127.90
123.49
93.43
79.19
77.32
77.00
76.68
29.91
14.68
Ph—≡—SEt
1a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

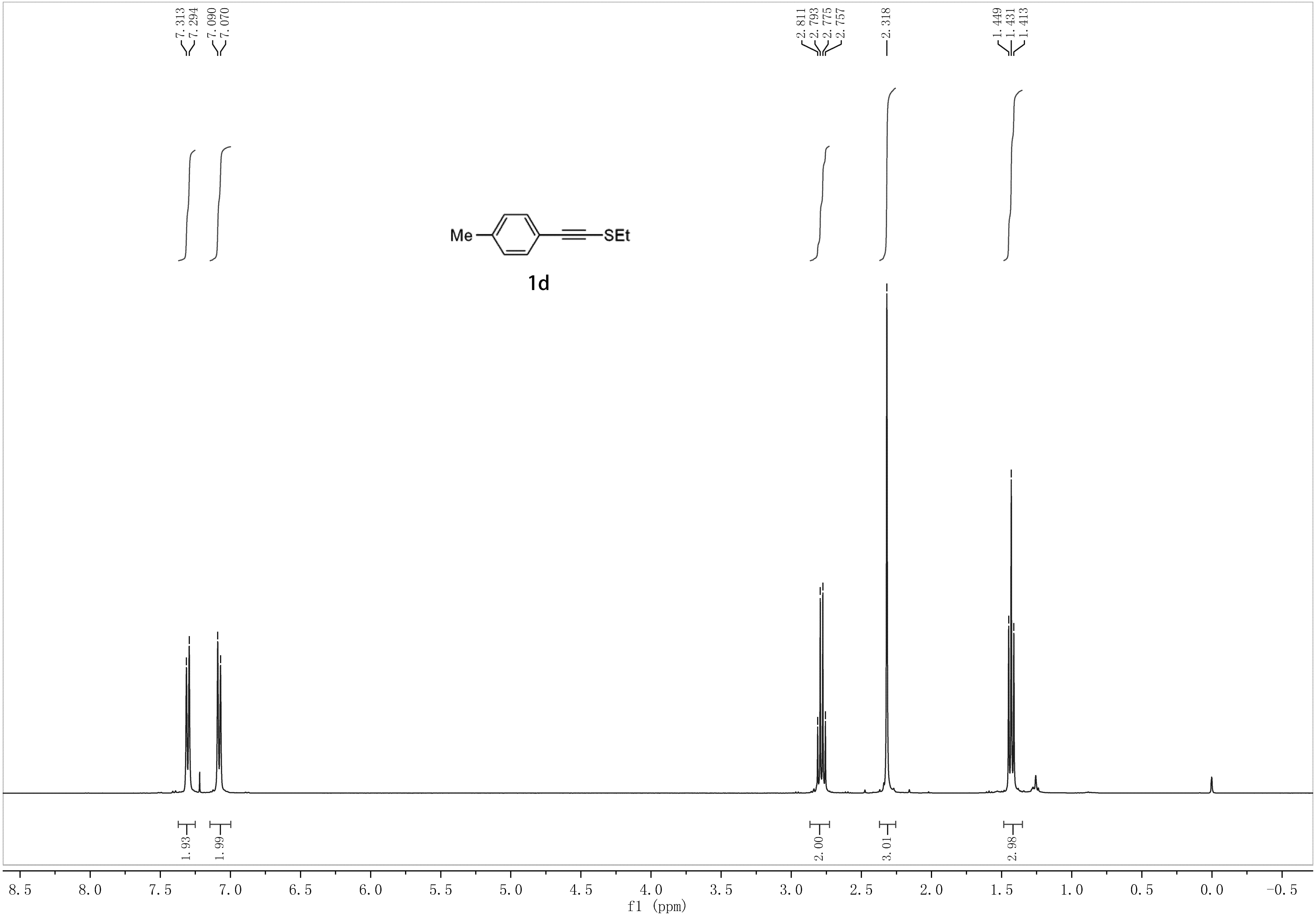

7.437
7.432
7.424
7.415
7.407
7.402
7.056
7.032
7.027
7.010
6.993
6.989
6.982
2.862
2.844
2.826
2.808
1.488
1.470
1.452
F
SEt
1b
1.91
2.14
1.98
3.23
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

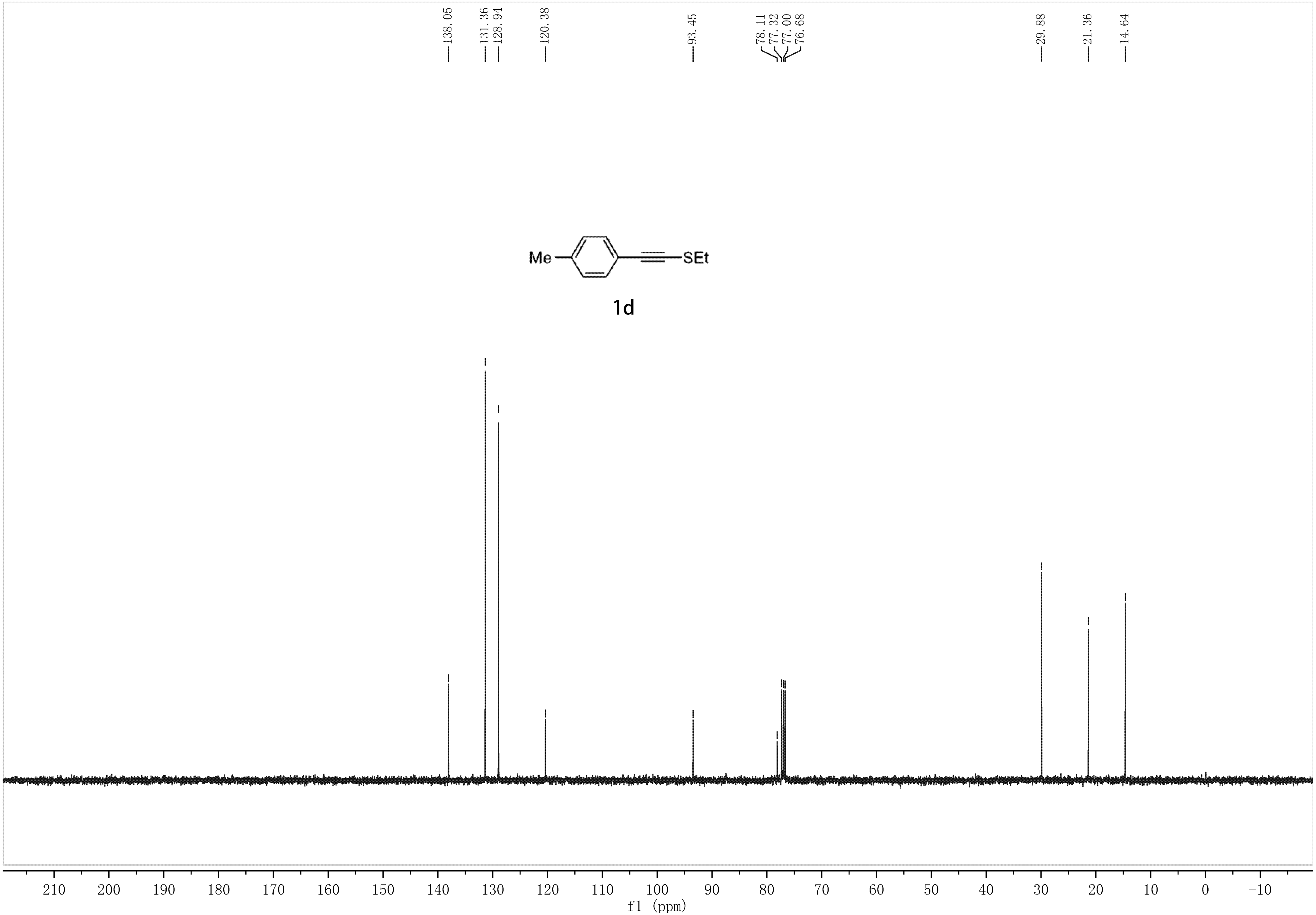

163.54
161.06
133.45
133.37
119.64
119.60
115.61
115.39
92.27
78.91
77.32
77.00
76.68
29.91
14.68
F
SEt
1b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

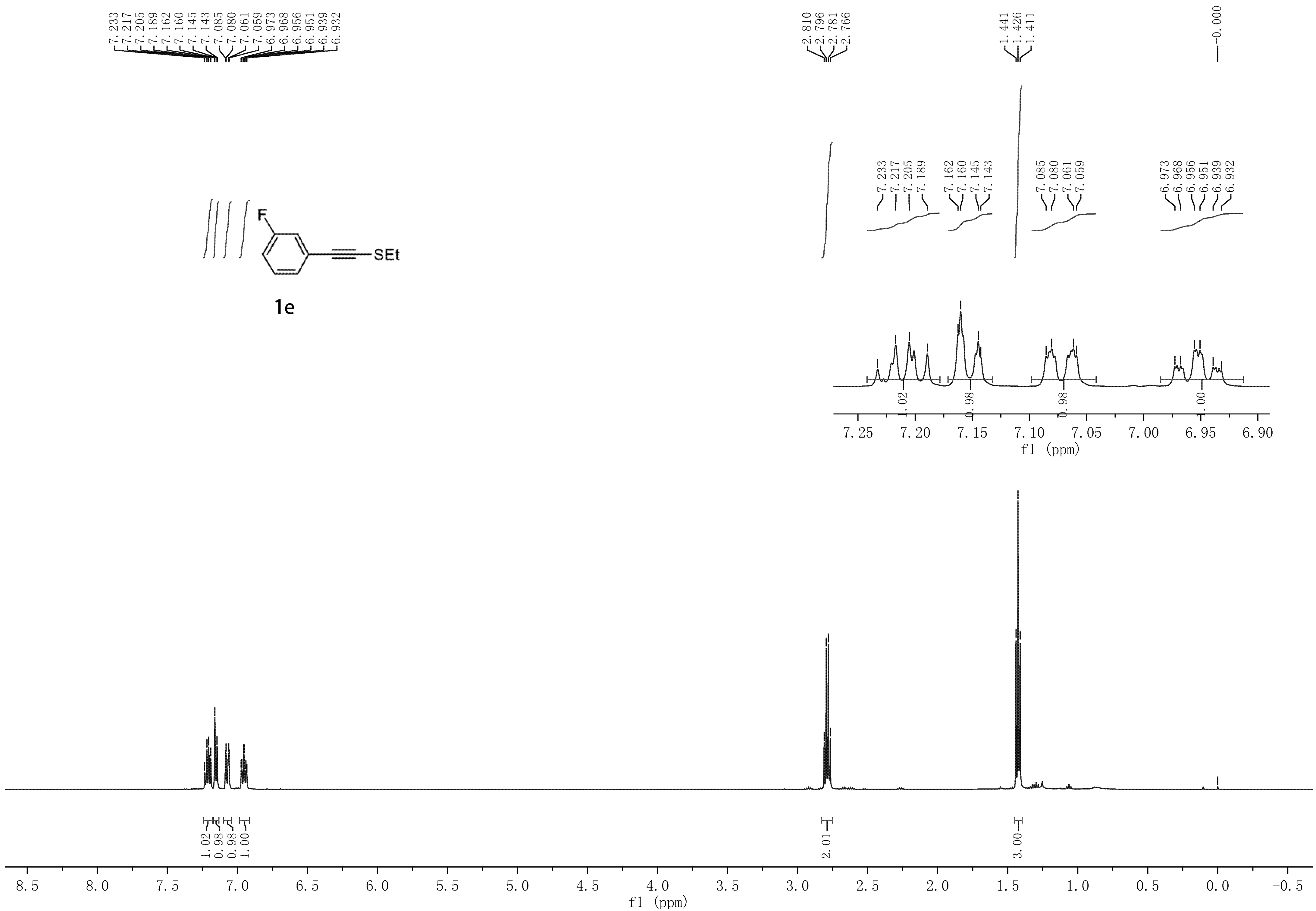

7.345
7.340
7.335
7.324
7.319
7.313
7.275
7.270
7.265
7.256
7.249
7.243
2.844
2.826
2.808
2.790
1.464
1.446
1.427
Cl
SEt
1c
2.00
2.13
2.00
3.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)



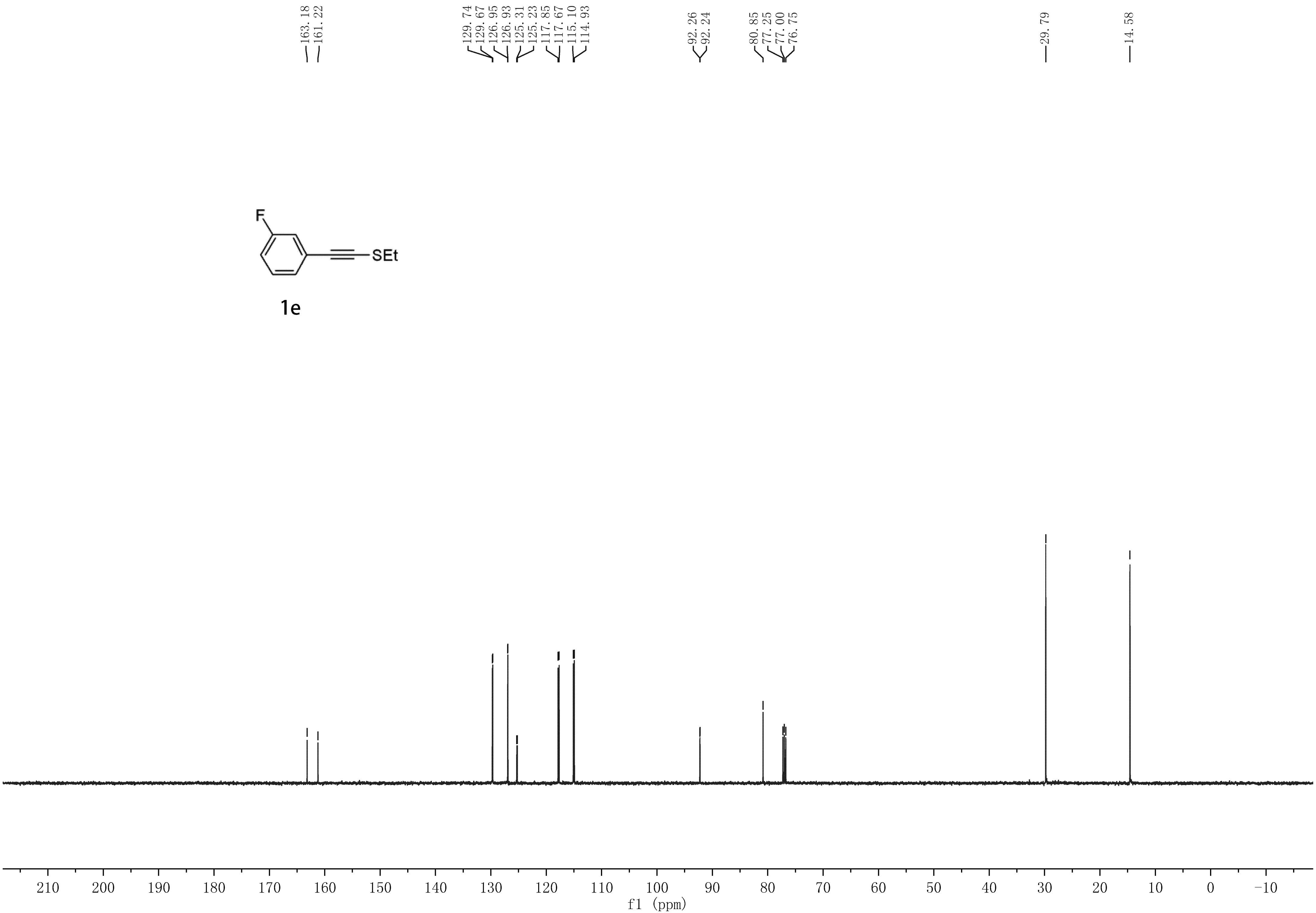
133.88
132.54
128.57
122.02
92.34
80.55
77.32
77.00
76.68
29.94
14.72
Cl
SEt
1c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

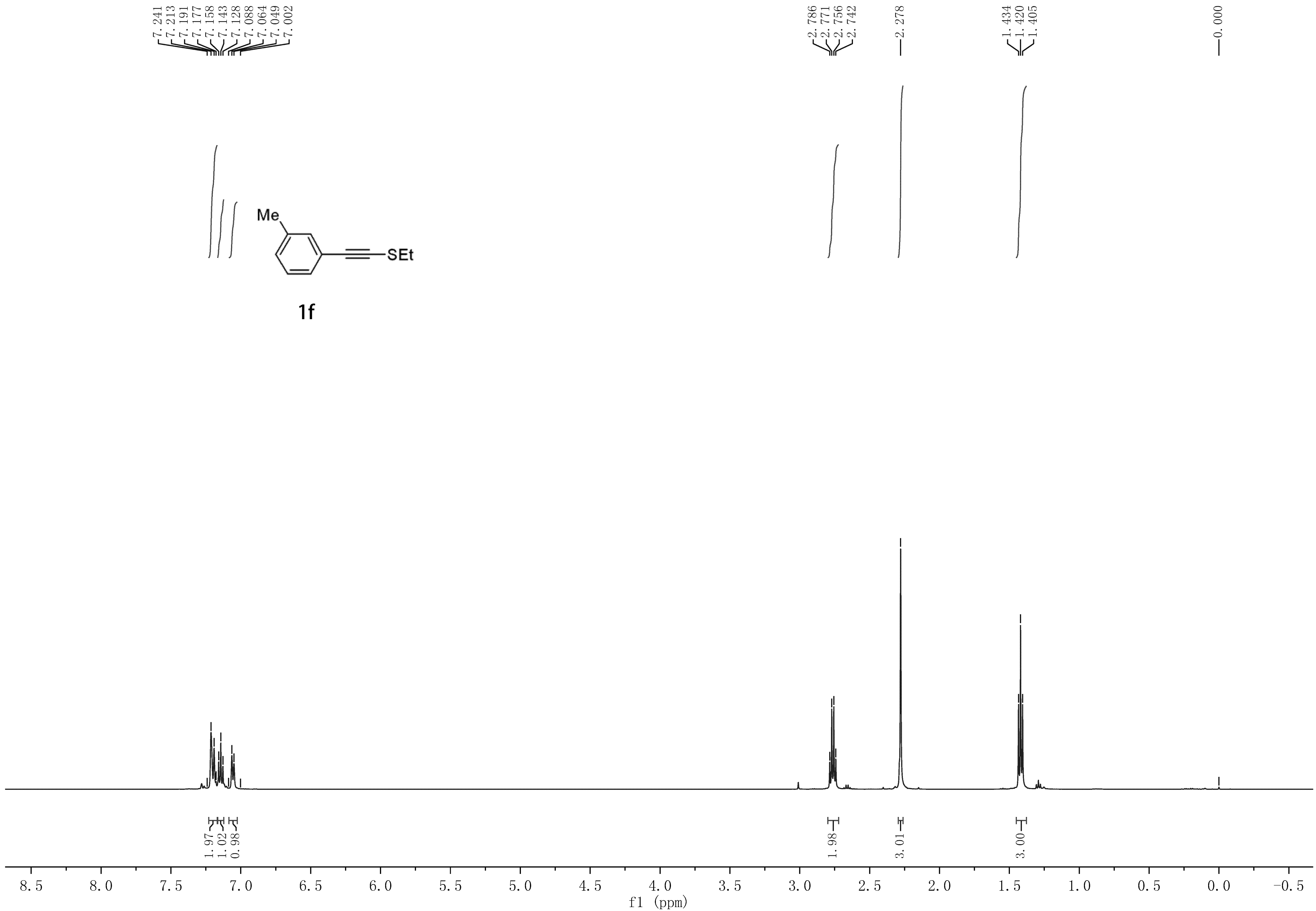

7.313
7.294
7.090
7.070
2.811
2.793
2.775
2.757
2.318
1.449
1.431
1.413
Me
SEt
1d
1.93
1.99
2.00
3.01
2.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

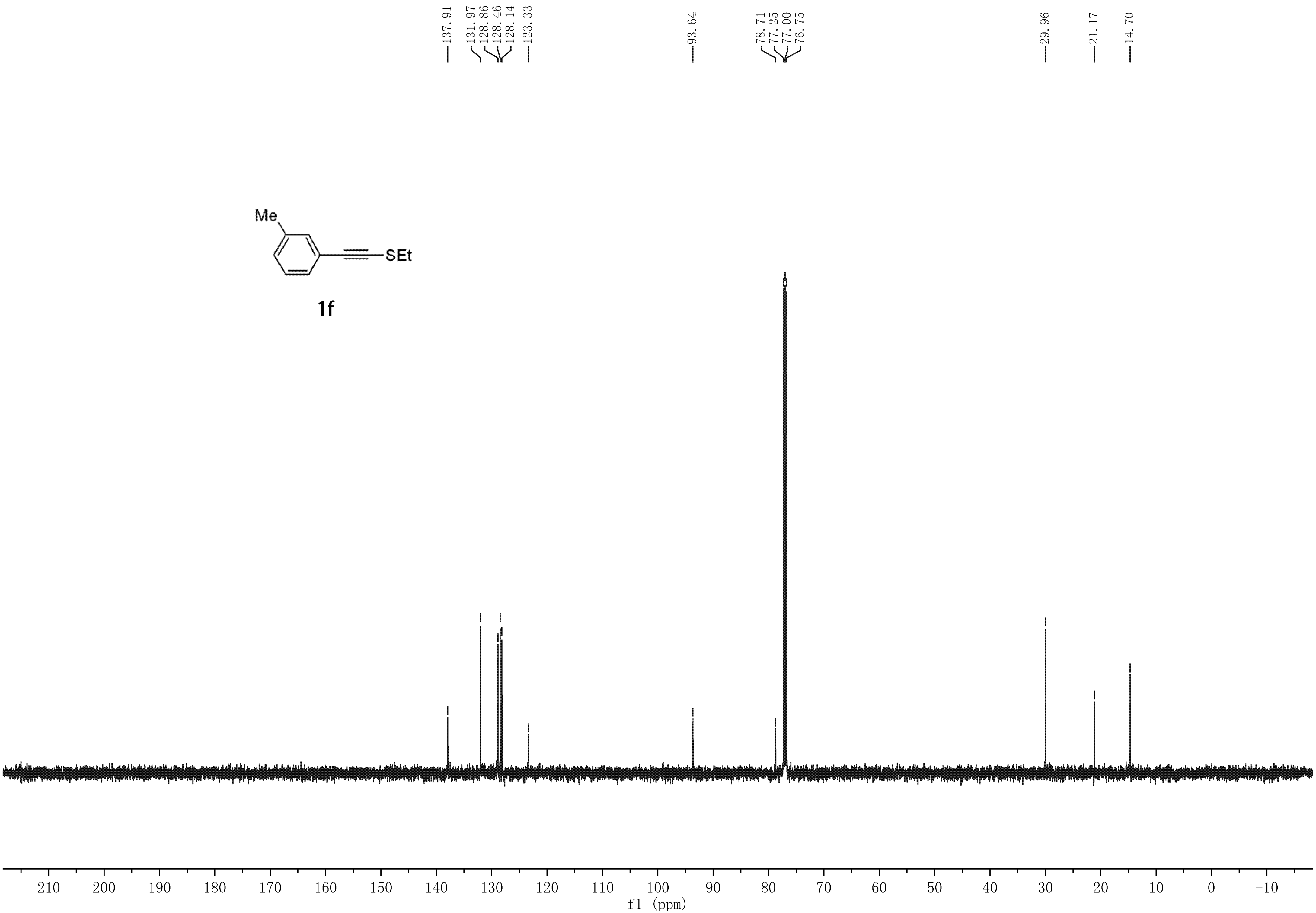

138.05
131.36
128.94
120.38
93.45
78.11
77.32
77.00
76.68
29.88
21.36
14.64
Me
SEt
1d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

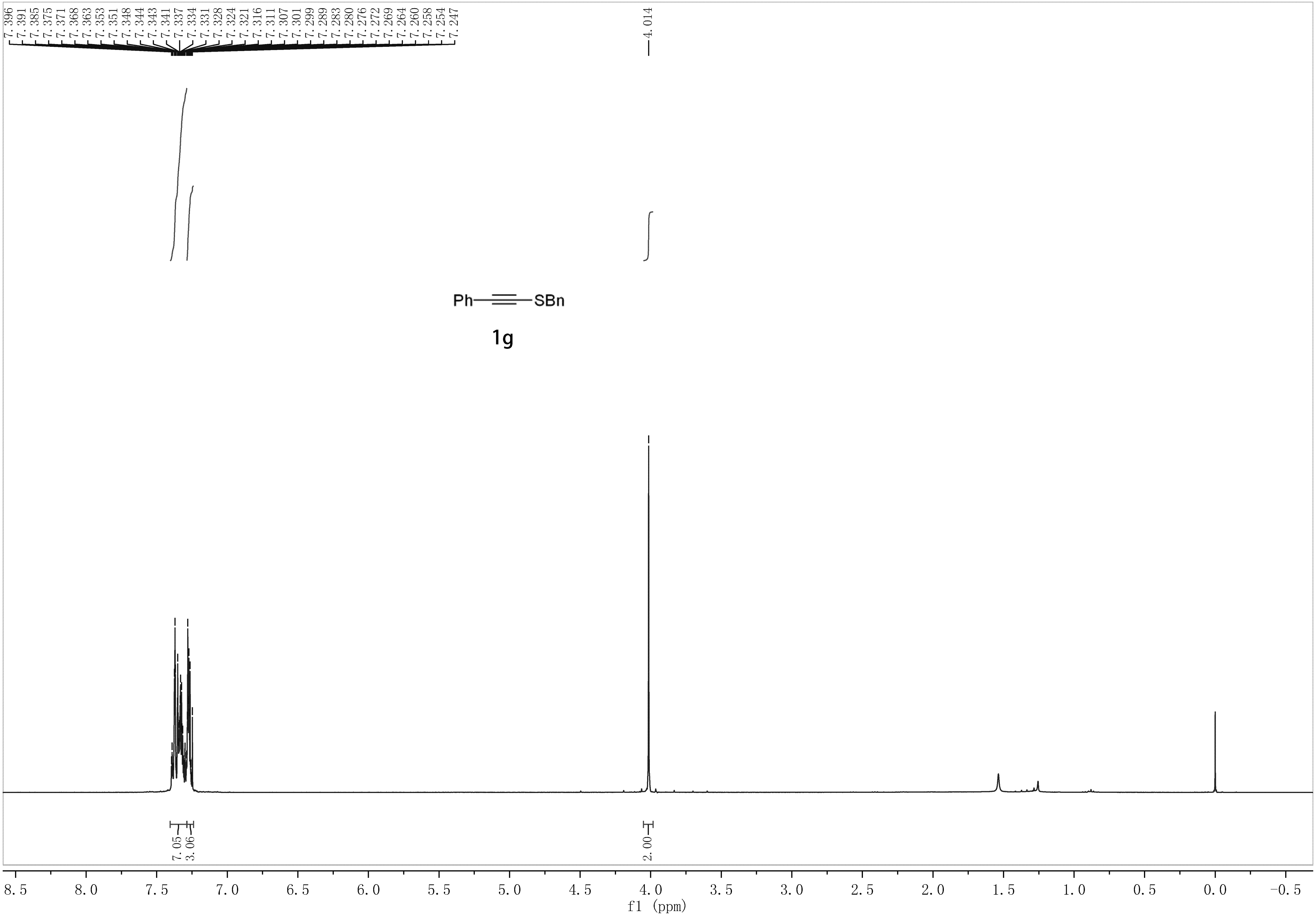


7.233
7.217
7.205
7.189
7.162
7.160
7.145
7.143
7.085
7.080
7.061
7.059
6.973
6.968
6.956
6.951
6.939
6.932
2.810
2.796
2.781
2.766
1.441
1.426
1.411
0.000
F
SEt
1e
1.02
0.98
0.98
1.00
2.01
3.00
7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

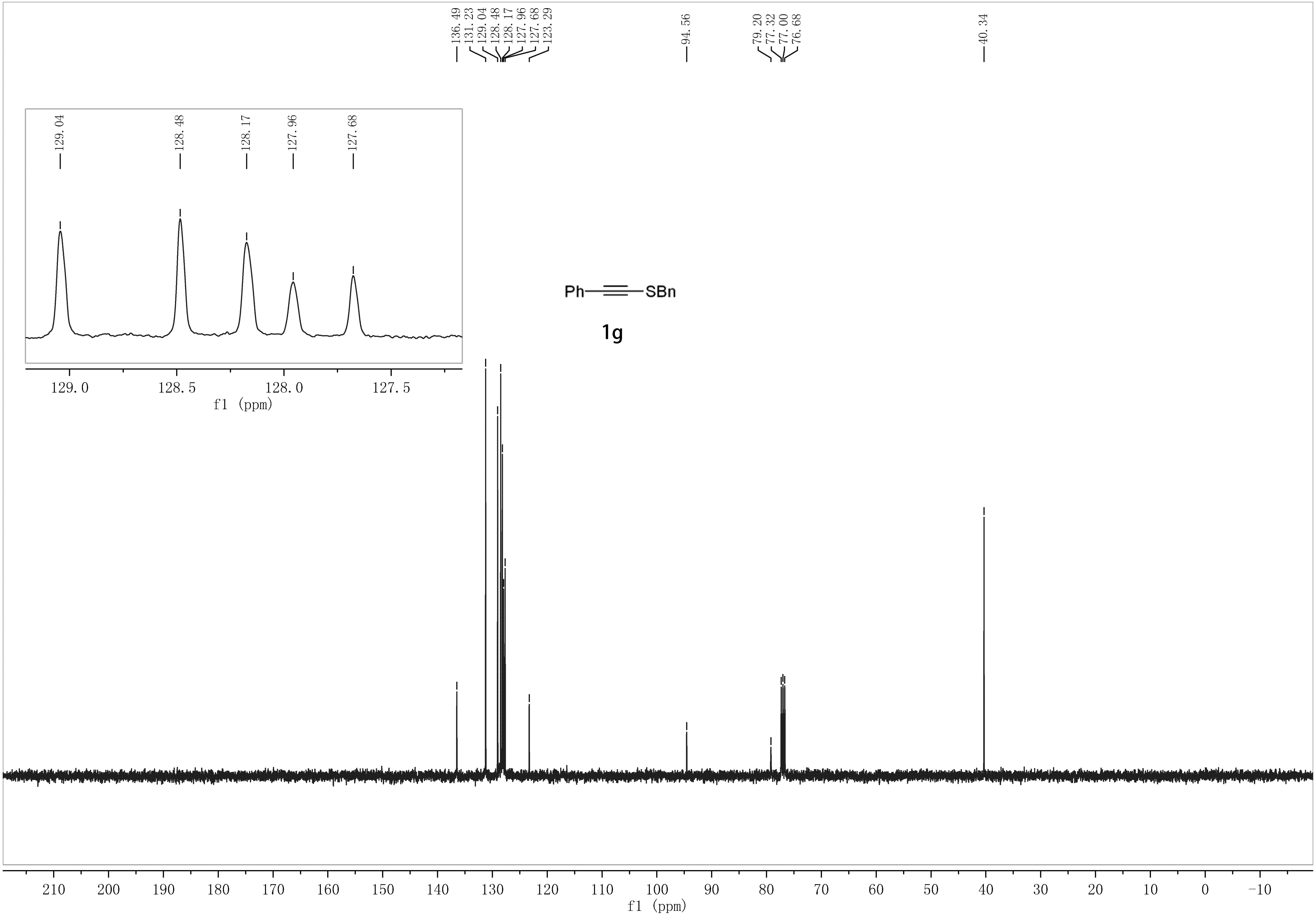

163.18
161.22
129.74
129.67
126.95
126.93
125.31
125.23
117.85
117.67
115.10
114.93
92.26
92.24
80.85
77.25
77.00
76.75
29.79
14.58
F
SEt
1e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

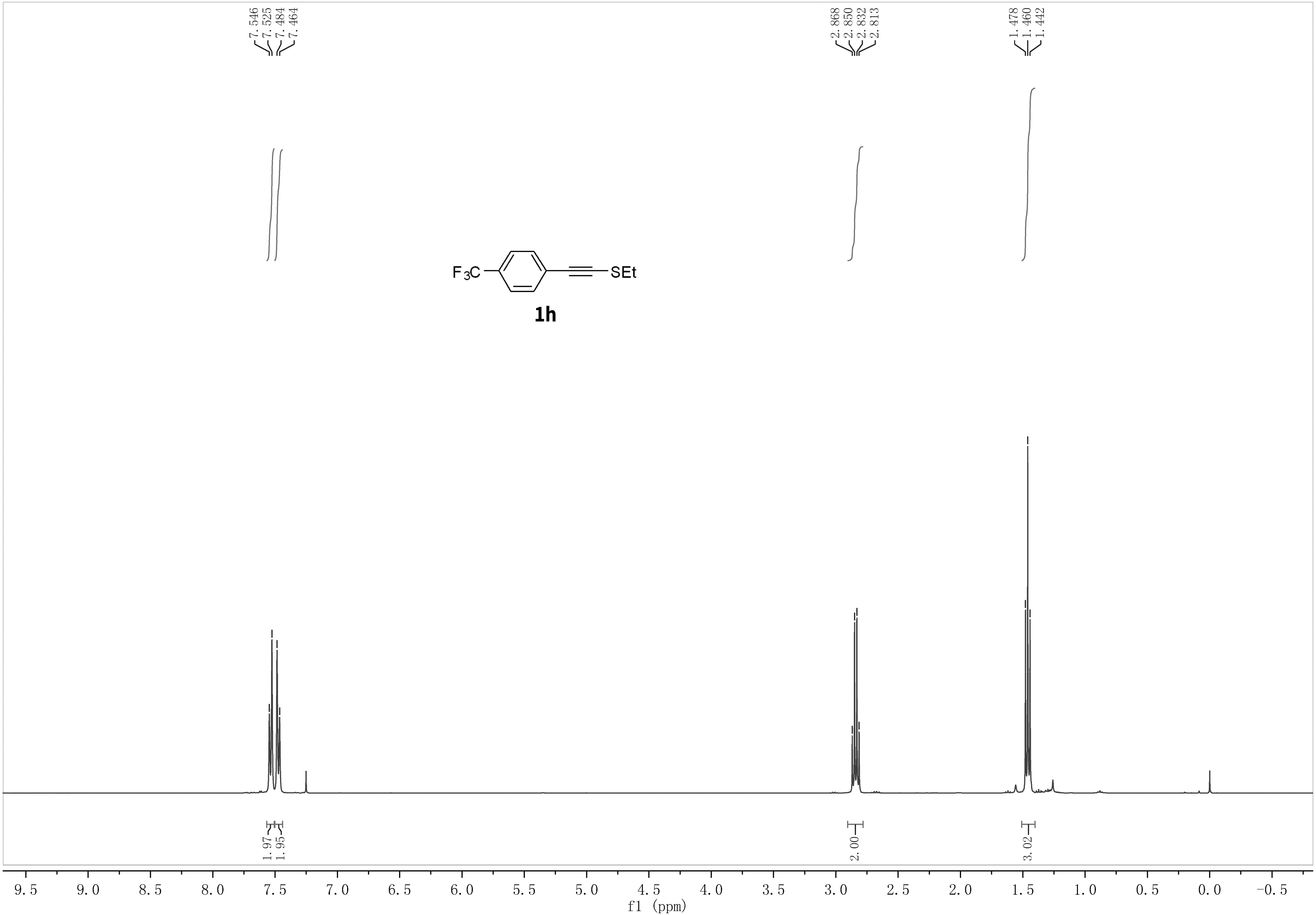

7.241
7.213
7.191
7.177
7.158
7.143
7.128
7.088
7.064
7.049
7.002
2.786
2.771
2.756
2.742
2.278
1.434
1.420
1.405
0.000
Me
SEt
1f
1.97
1.02
0.98
1.98
3.01
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

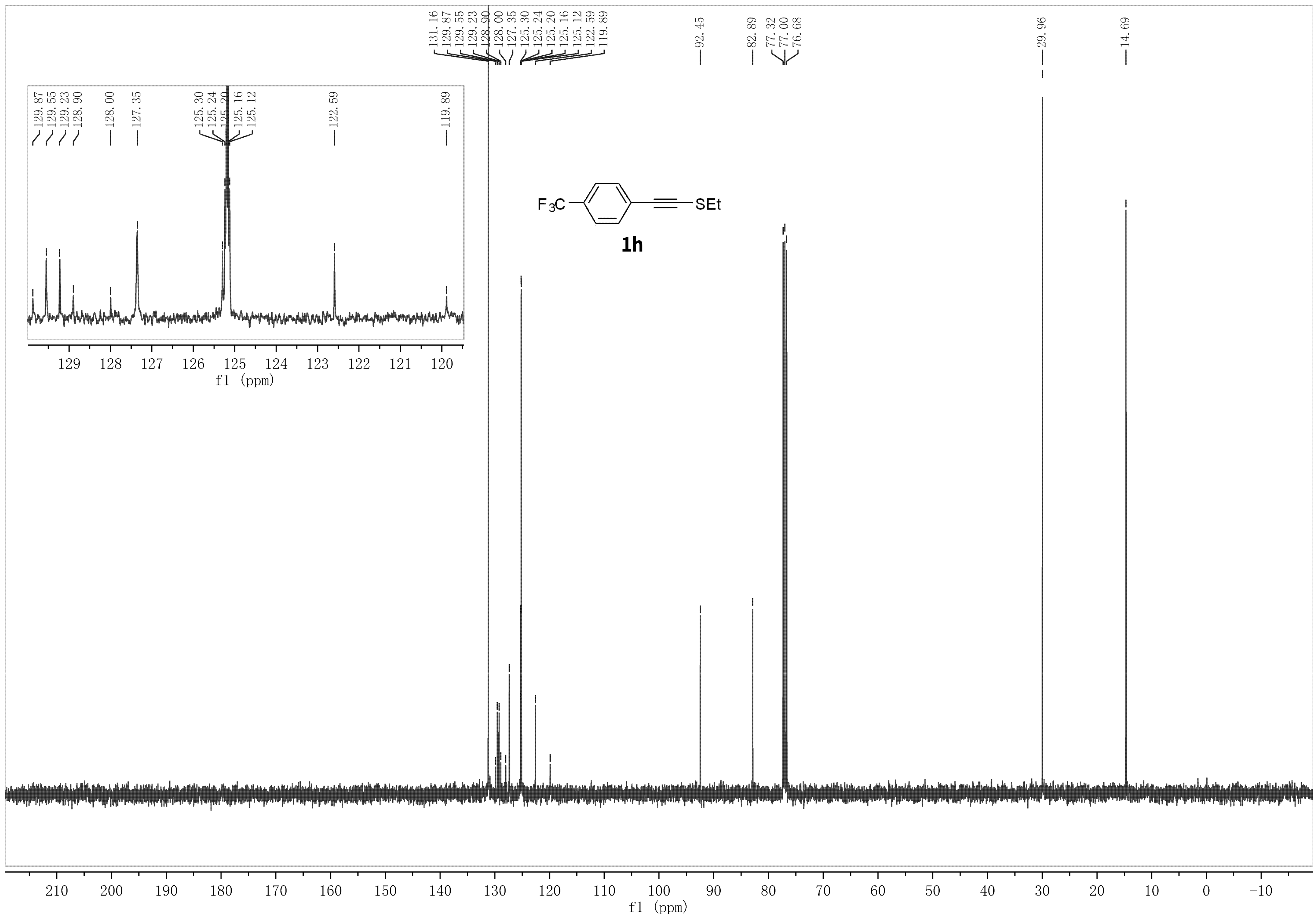

137.91
131.97
128.86
128.46
128.14
123.33
93.64
78.71
77.25
77.00
76.75
29.96
21.17
14.70
Me
SEt
1f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

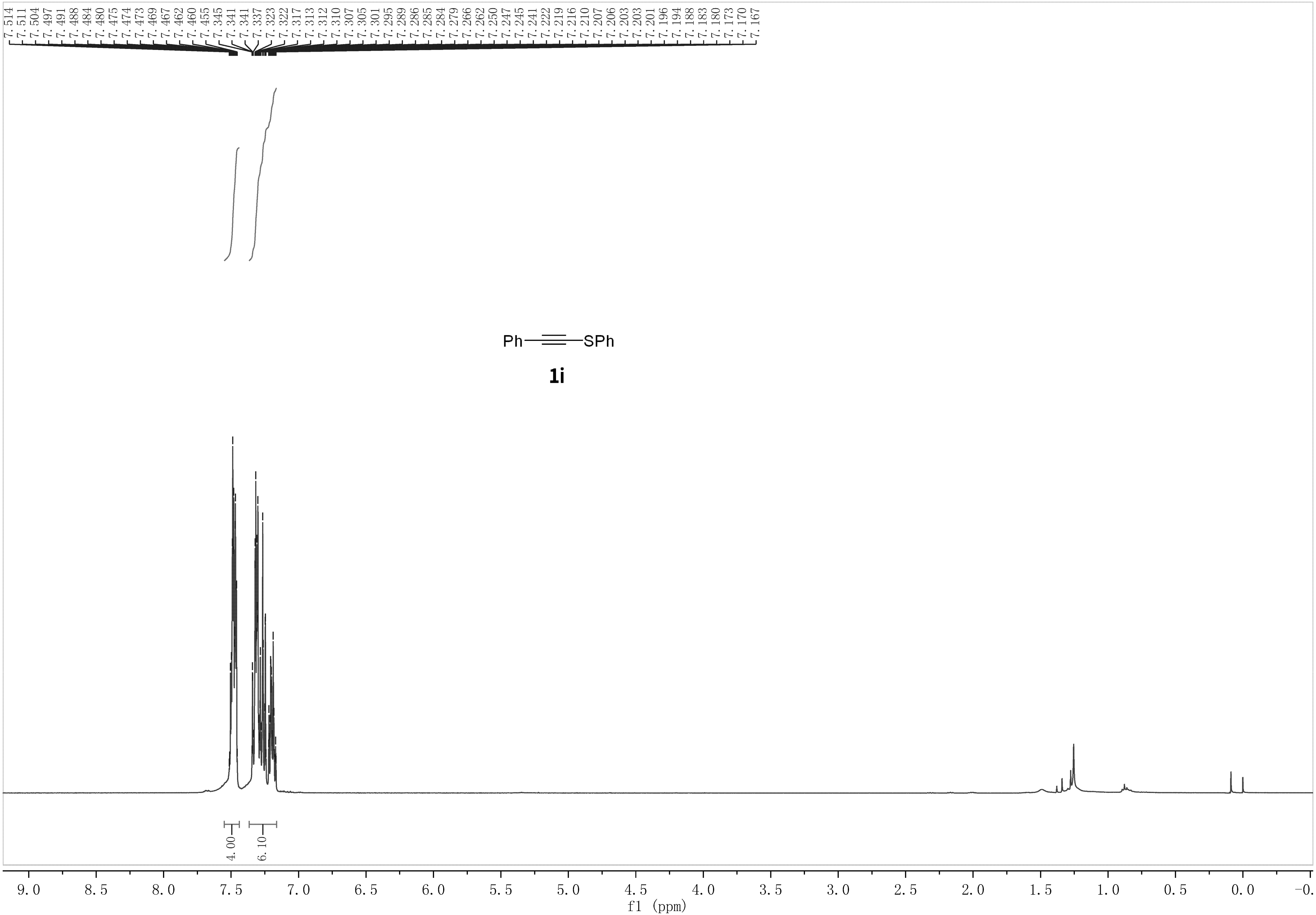


7.396
7.391
7.385
7.375
7.371
7.368
7.363
7.353
7.351
7.348
7.344
7.343
7.341
7.337
7.334
7.331
7.328
7.324
7.321
7.316
7.311
7.307
7.301
7.299
7.289
7.283
7.280
7.276
7.272
7.269
7.264
7.260
7.258
7.254
7.247
4.014
Ph SBn
1g
7.05
3.06
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

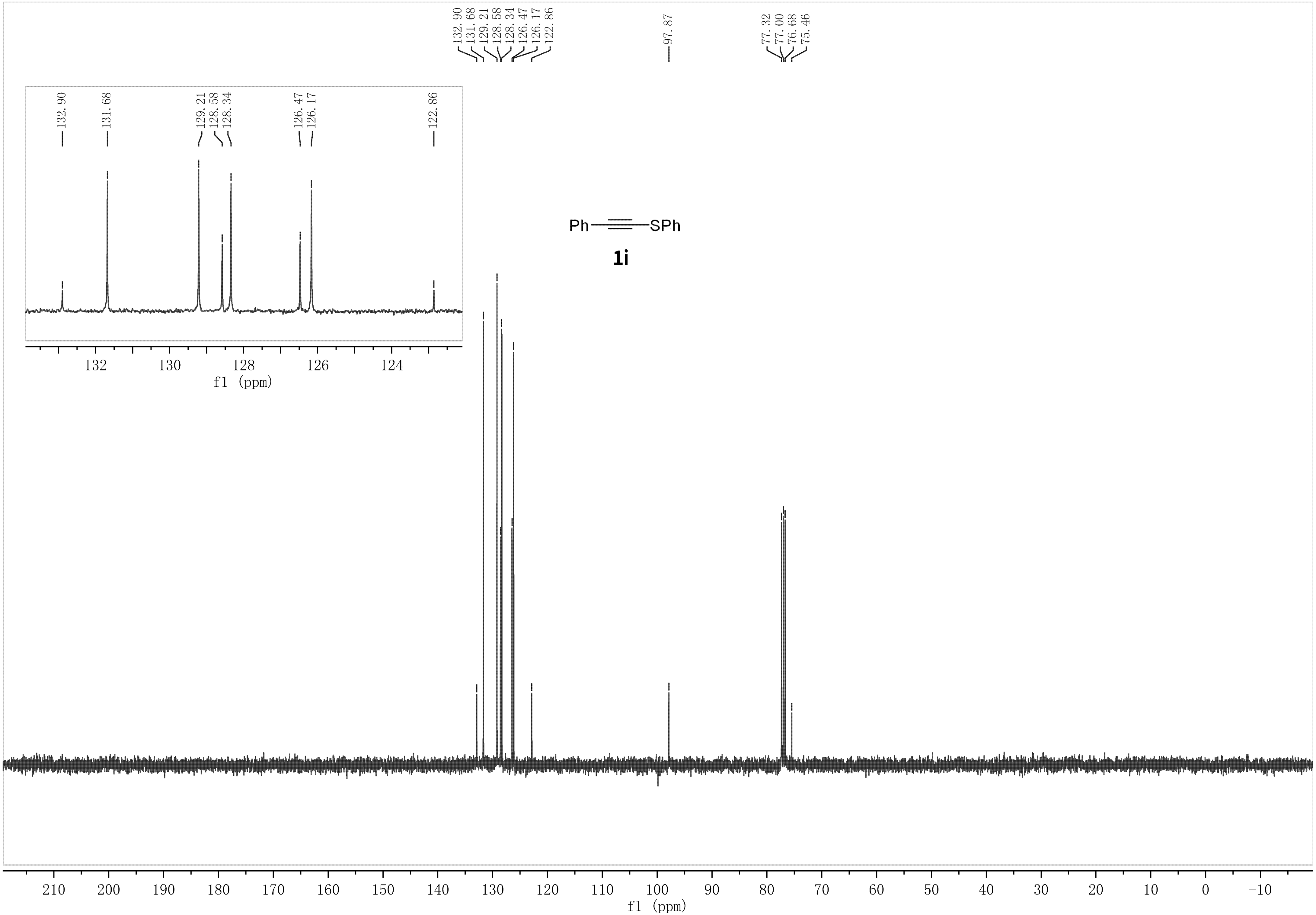

136.49
131.23
129.04
128.48
128.17
127.96
127.68
123.29
94.56
79.20
77.32
77.00
76.68
40.34
129.04
128.48
128.17
127.96
127.68
129.0
128.5
128.0
127.5
f1 (ppm)
Ph—≡—SBn
1g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

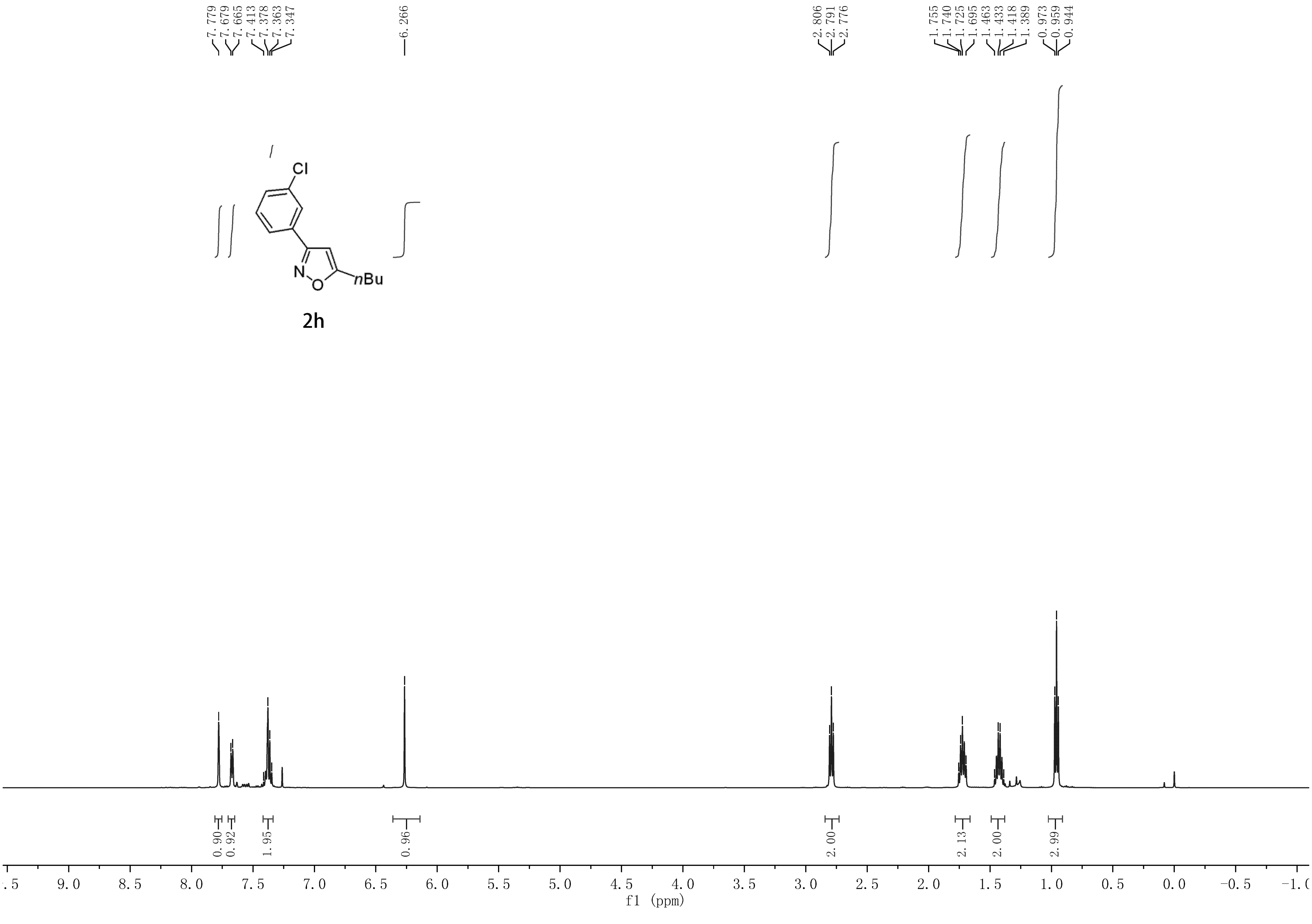

7.546
7.525
7.484
7.464
2.868
2.850
2.832
2.813
1.478
1.460
1.442
F3C
SEt
1h
1.97
1.95
2.00
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


131.16
129.87
129.55
129.23
128.90
128.00
127.35
125.30
125.24
125.20
125.16
125.12
122.59
119.89
92.45
82.89
77.32
77.00
76.68
29.96
14.69
F3C
SEt
1h
f1 (ppm)

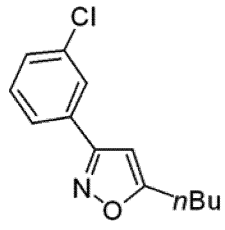


7.514 7.511 7.504 7.497 7.491 7.488 7.484 7.480 7.475 7.474 7.473 7.469 7.467 7.462 7.460 7.455 7.345 7.341 7.341 7.337 7.323 7.322 7.317 7.313 7.312 7.310 7.307 7.305 7.301 7.295 7.289 7.286 7.285 7.284 7.279 7.266 7.262 7.250 7.247 7.245 7.241 7.222 7.219 7.216 7.210 7.207 7.206 7.203 7.203 7.201 7.196 7.194 7.188 7.183 7.180 7.173 7.170 7.167
Ph—≡—SPh
1i
4.00
6.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


132.90
131.68
129.21
128.58
128.34
126.47
126.17
122.86
97.87
77.32
77.00
76.68
75.46
Ph—≡—SPh
1i
132
130
128
126
124
f1 (ppm)
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)

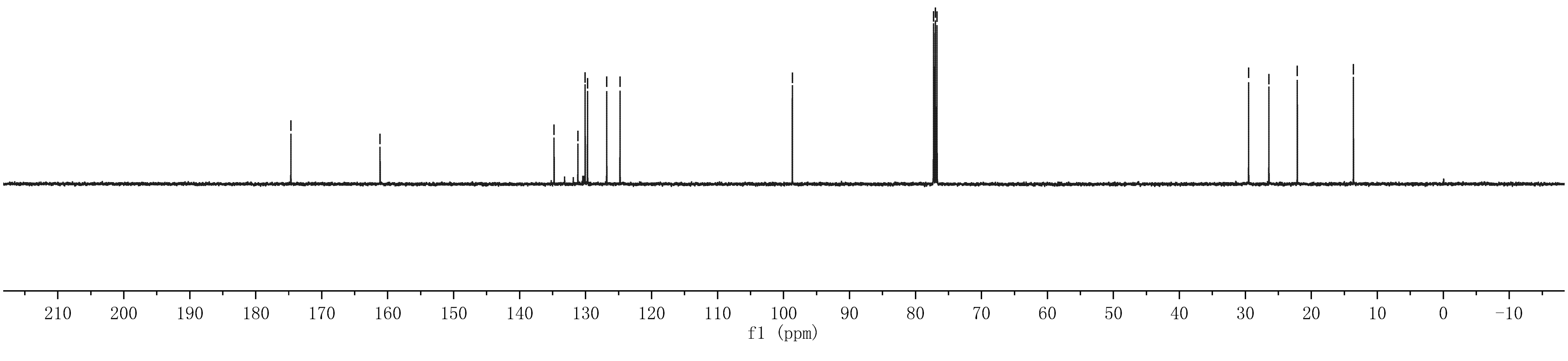


7.779
7.679
7.665
7.413
7.378
7.363
7.347
6.266
2.806
2.791
2.776
1.755
1.740
1.725
1.695
1.463
1.433
1.418
1.389
0.973
0.959
0.944
Cl
N
O
nBu
2h
0.90
0.92
1.95
0.96
2.00
2.13
2.00
2.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

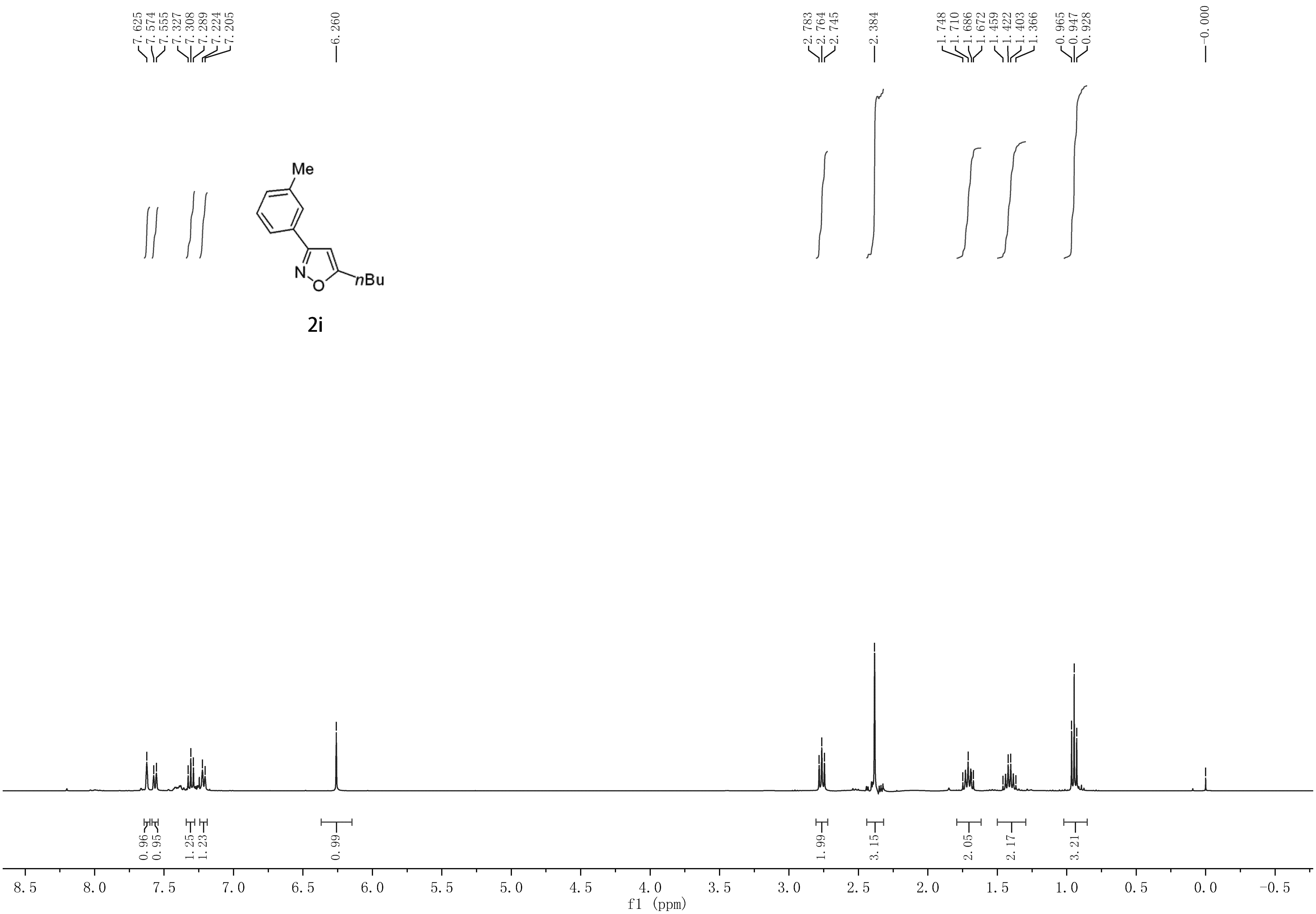


Cl
N
O
nBu

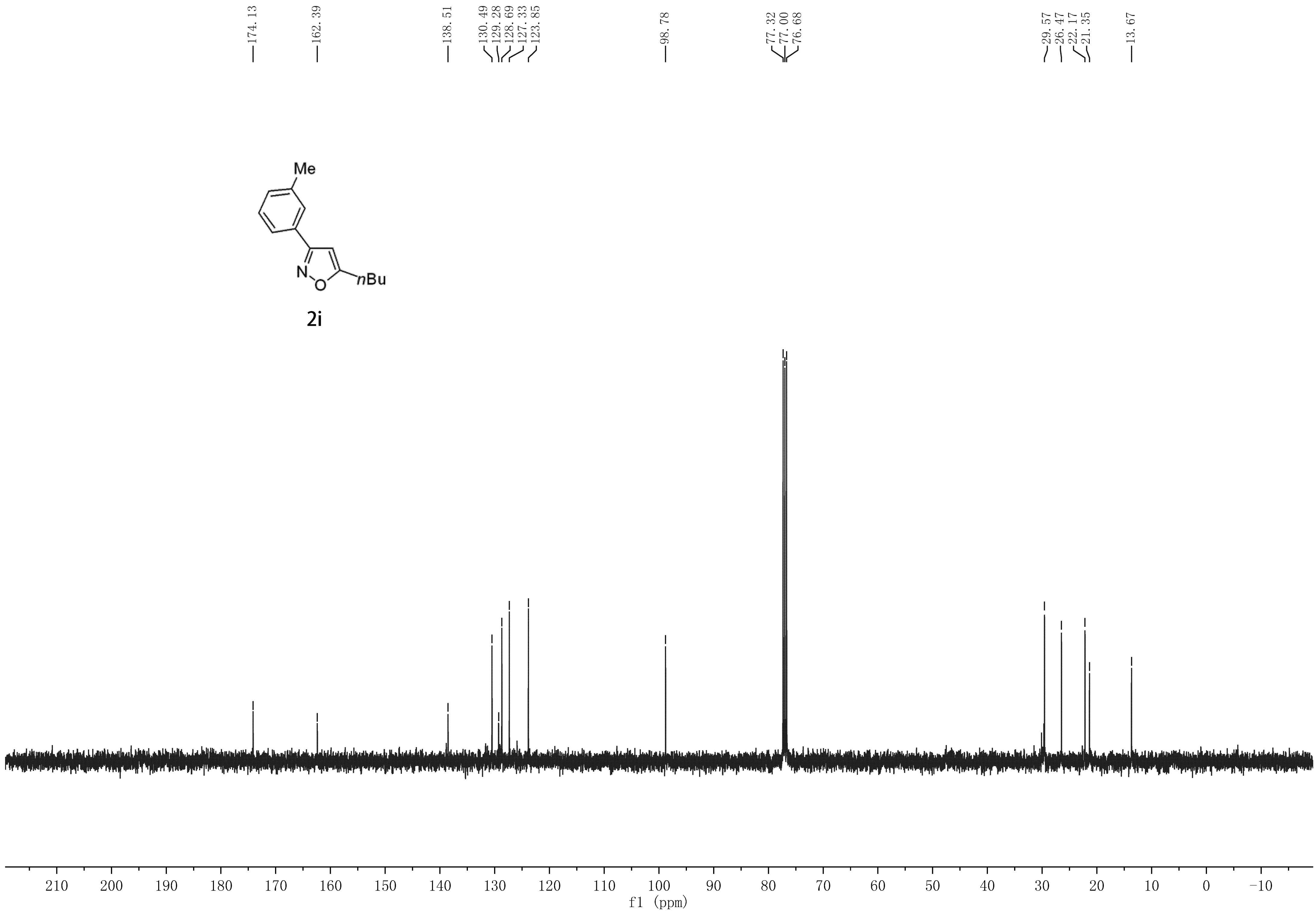
2h

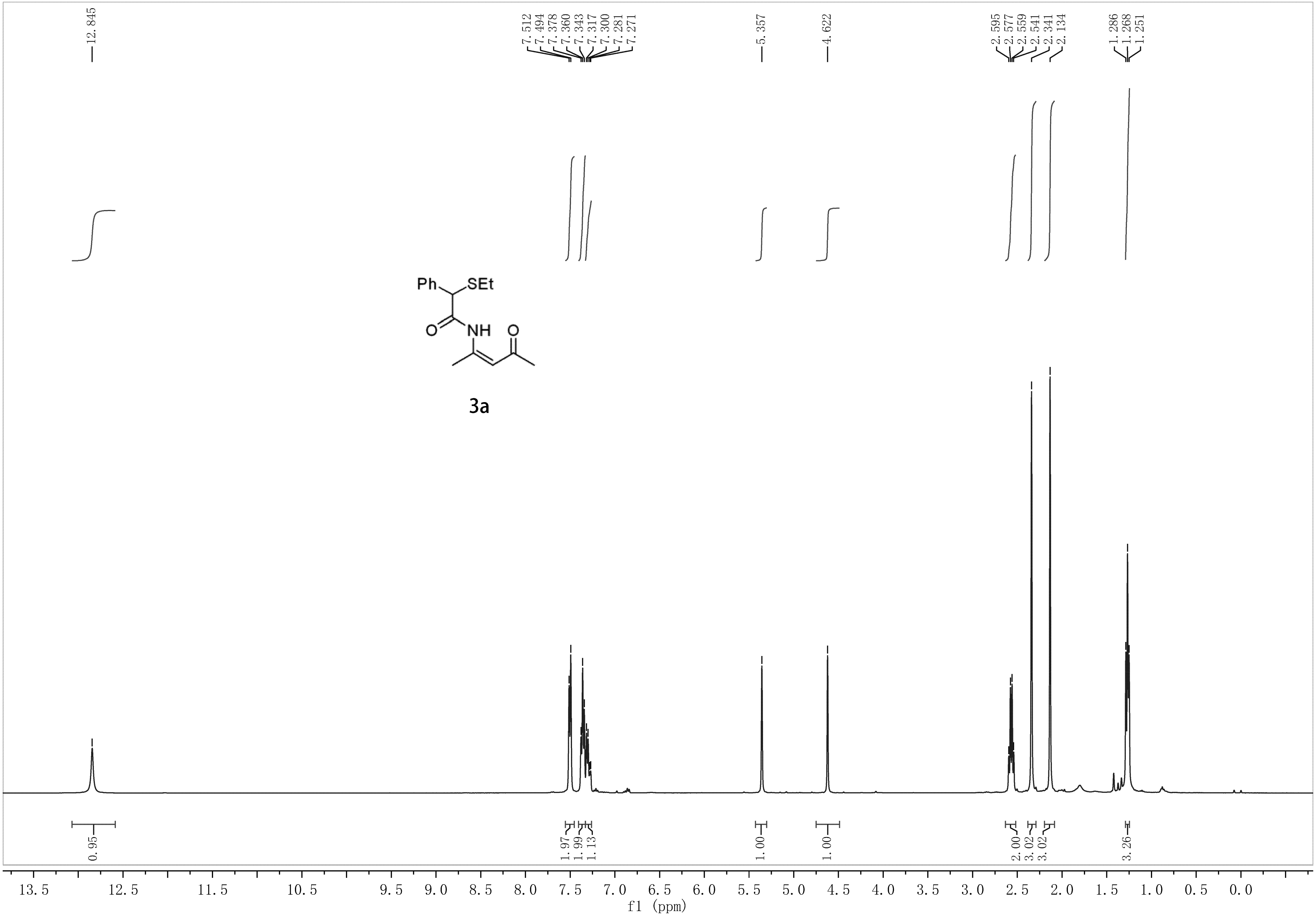


174.67
161.15
134.78
131.17
130.07
129.71
126.80
124.79
98.67
77.25
77.00
76.75
29.51
26.43
22.13
13.62
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

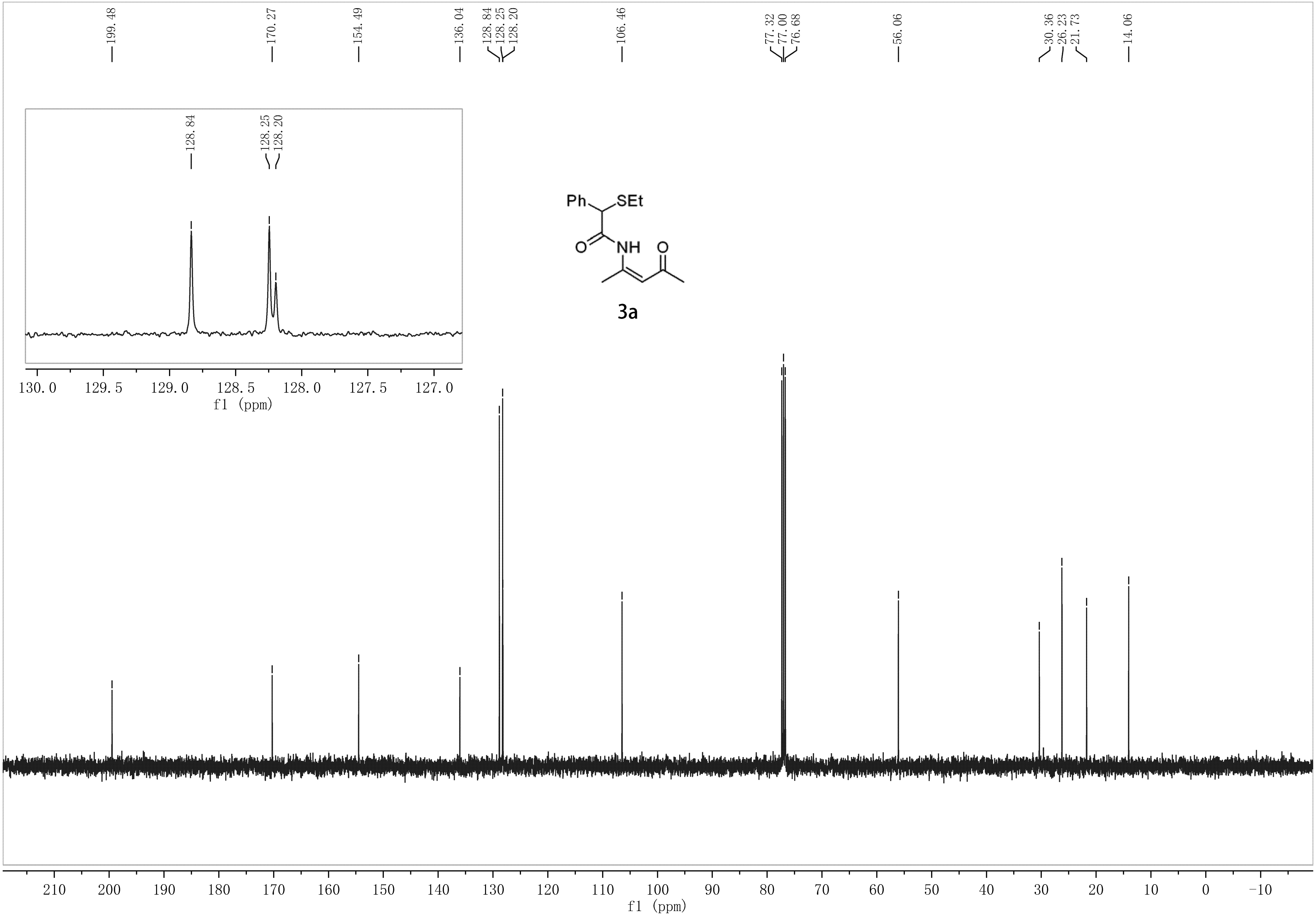


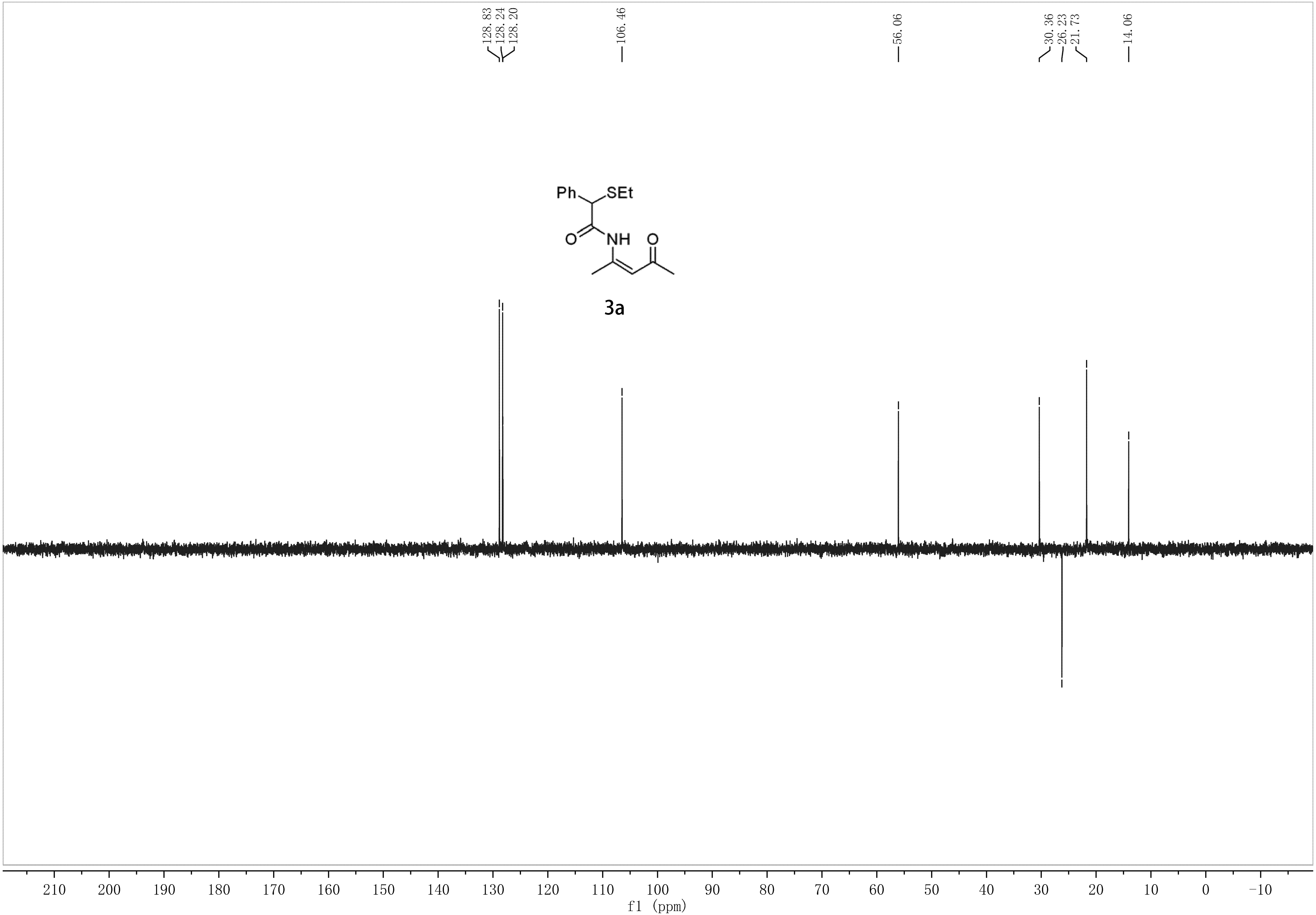
7.625
7.574
7.555
7.327
7.308
7.289
7.224
7.205
6.260
2.783
2.764
2.745
2.384
1.748
1.710
1.686
1.672
1.459
1.422
1.403
1.366
0.965
0.947
0.928
-0.000
Me
N
O
nBu
2i
0.96
0.95
1.25
1.23
0.99
1.99
3.15
2.05
2.17
3.21
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


174.13
162.39
138.51
130.49
129.28
128.69
127.33
123.85
98.78
77.32
77.00
76.68
29.57
26.47
22.17
21.35
13.67
Me
N
O
nBu
2i
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)



12.845
7.512
7.494
7.378
7.360
7.343
7.317
7.300
7.281
7.271
5.357
4.622
2.595
2.577
2.559
2.541
2.341
2.134
1.286
1.268
1.251
Ph
SEt
O
NH
O
3a
0.95
1.97
1.99
1.13
1.00
1.00
2.00
3.02
3.02
3.26
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


199.48
170.27
154.49
136.04
128.84
128.25
128.20
106.46
77.32
77.00
76.68
56.06
30.36
26.23
21.73
14.06
Ph
SEt
O
NH
O
3a
130.0 129.5 129.0 128.5 128.0 127.5 127.0
f1 (ppm)
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)


128.83
128.24
128.20
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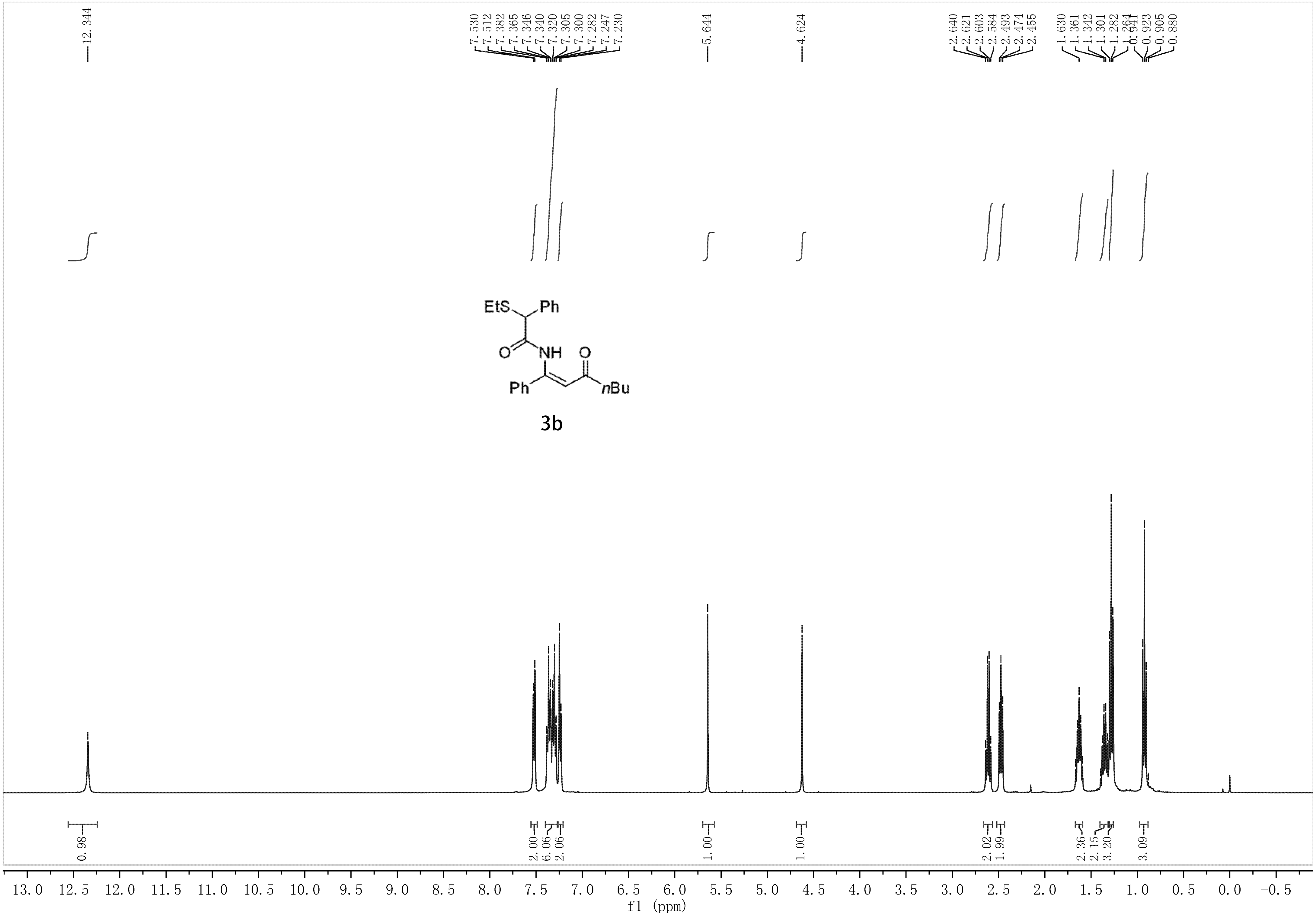
56.06
30.36
26.23
21.73
14.06
Ph
SEt
O
NH
O
3a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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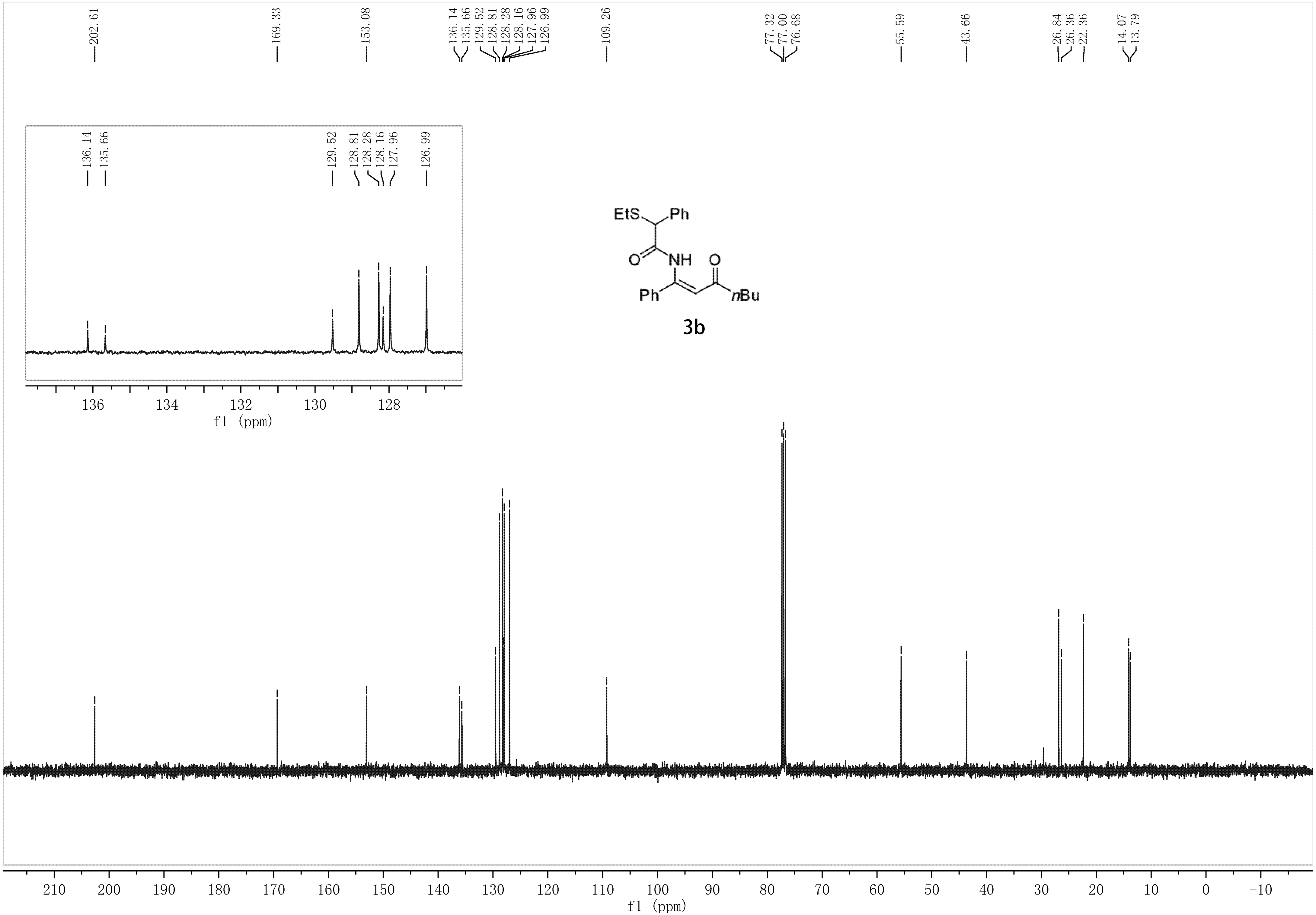
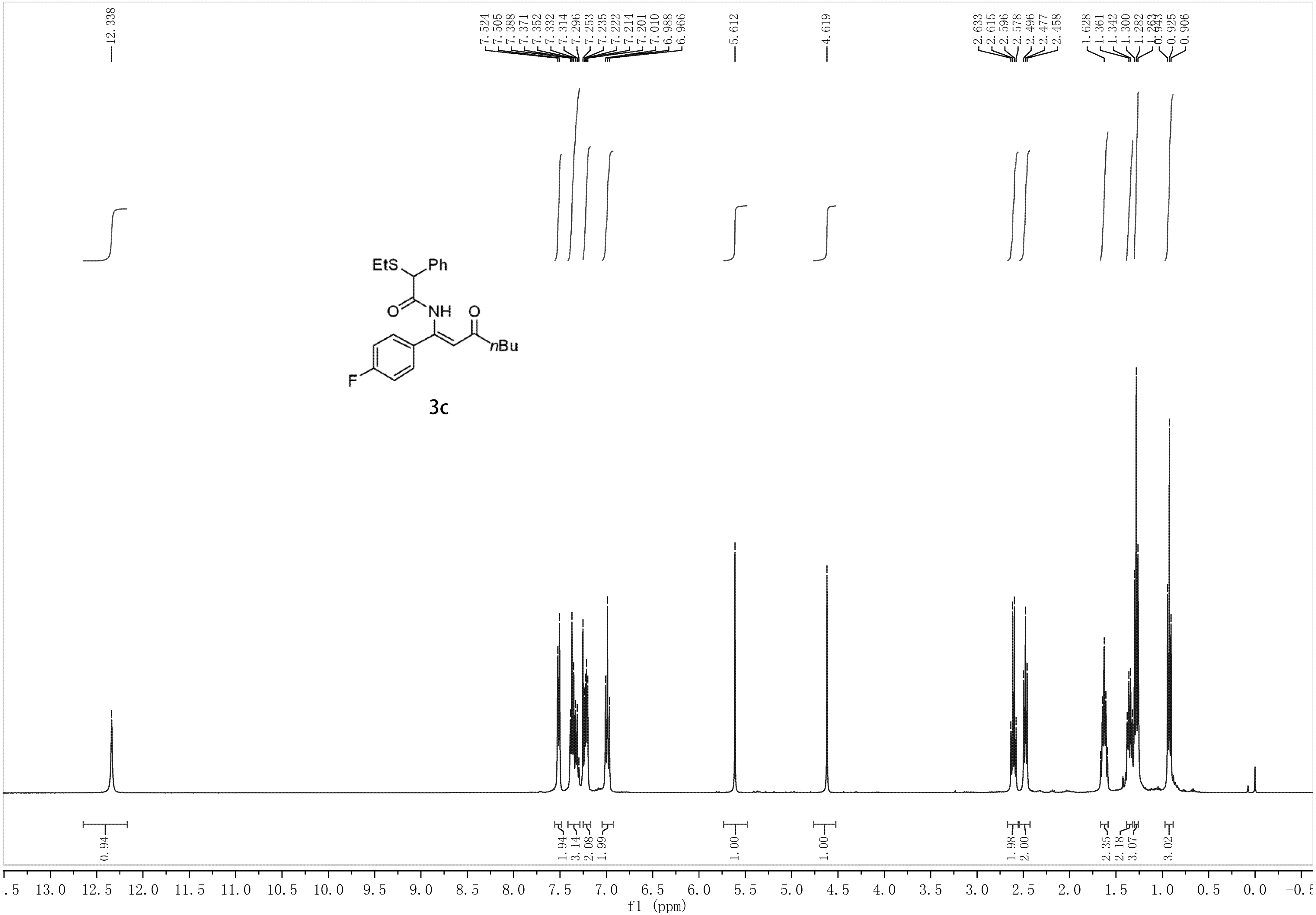
7.530
7.512
7.382
7.365
7.346
7.340
7.320
7.305
7.300
7.282
7.247
7.230
5.644
4.624
2.640
2.621
2.603
2.584
2.493
2.474
2.455
1.630
1.361
1.342
1.301
1.282
1.264
0.941
0.923
0.905
0.880
EtS
Ph
O
NH
O
Ph
nBu
3b
0.98
2.00
6.06
2.06
1.00
1.00
2.02
1.99
2.36
2.15
3.20
3.09
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



202.61
169.33
153.08
136.14
135.66
129.52
128.81
128.28
128.16
127.96
126.99
109.26
77.32
77.00
76.68
55.59
43.66
26.84
26.36
22.36
14.07
13.79
EtS
Ph
O
NH
O
Ph
nBu
3b
136
134
132
130
128
f1 (ppm)
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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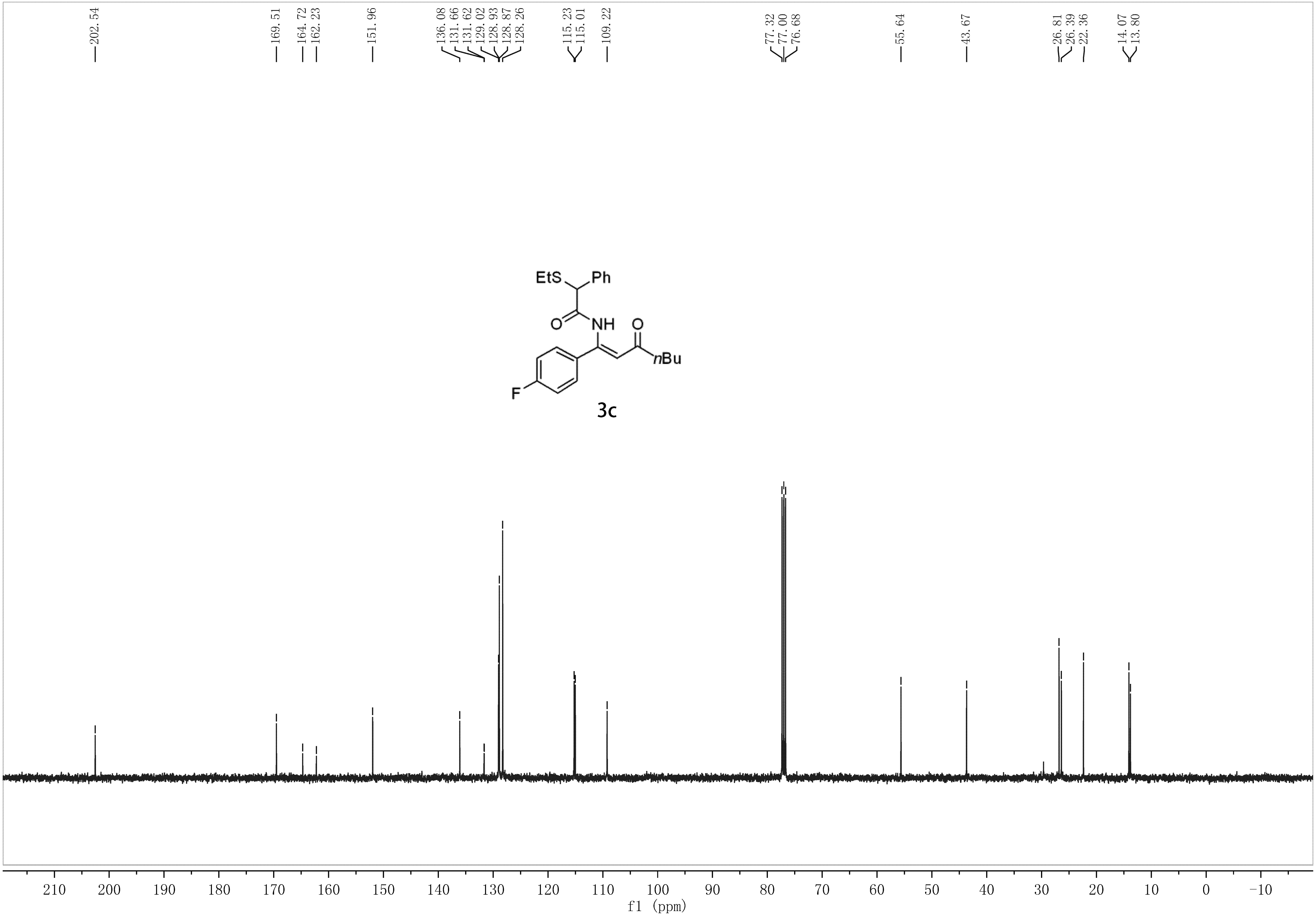
5.612
4.619
2.633 2.615 2.596 2.578 2.496 2.477 2.458
1.628 1.361 1.342 1.300 1.282 1.263 0.943 0.925 0.906
EtS
Ph
O
NH
O
nBu
F
3c
0.94
1.94 3.14 2.08 1.99
1.00
1.00
1.98 2.00
2.35 2.18 3.07
3.02
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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164.72
162.23
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136.08
131.66
131.62
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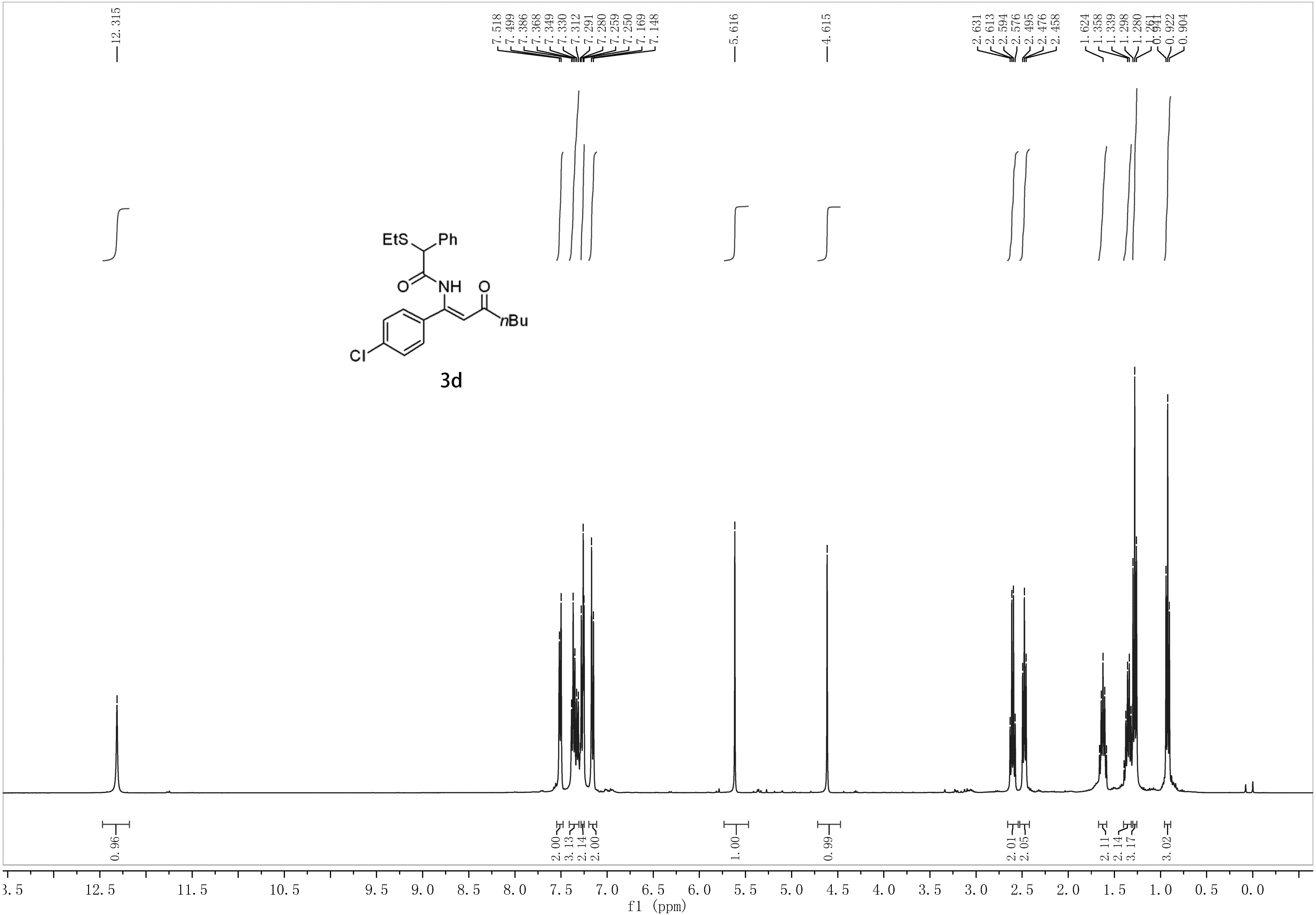
128.93
128.87
128.26
115.23
115.01
109.22
77.32
77.00
76.68
55.64
43.67
26.81
26.39
22.36
14.07
13.80
EtS
Ph
O
NH
O
nBu
F
3c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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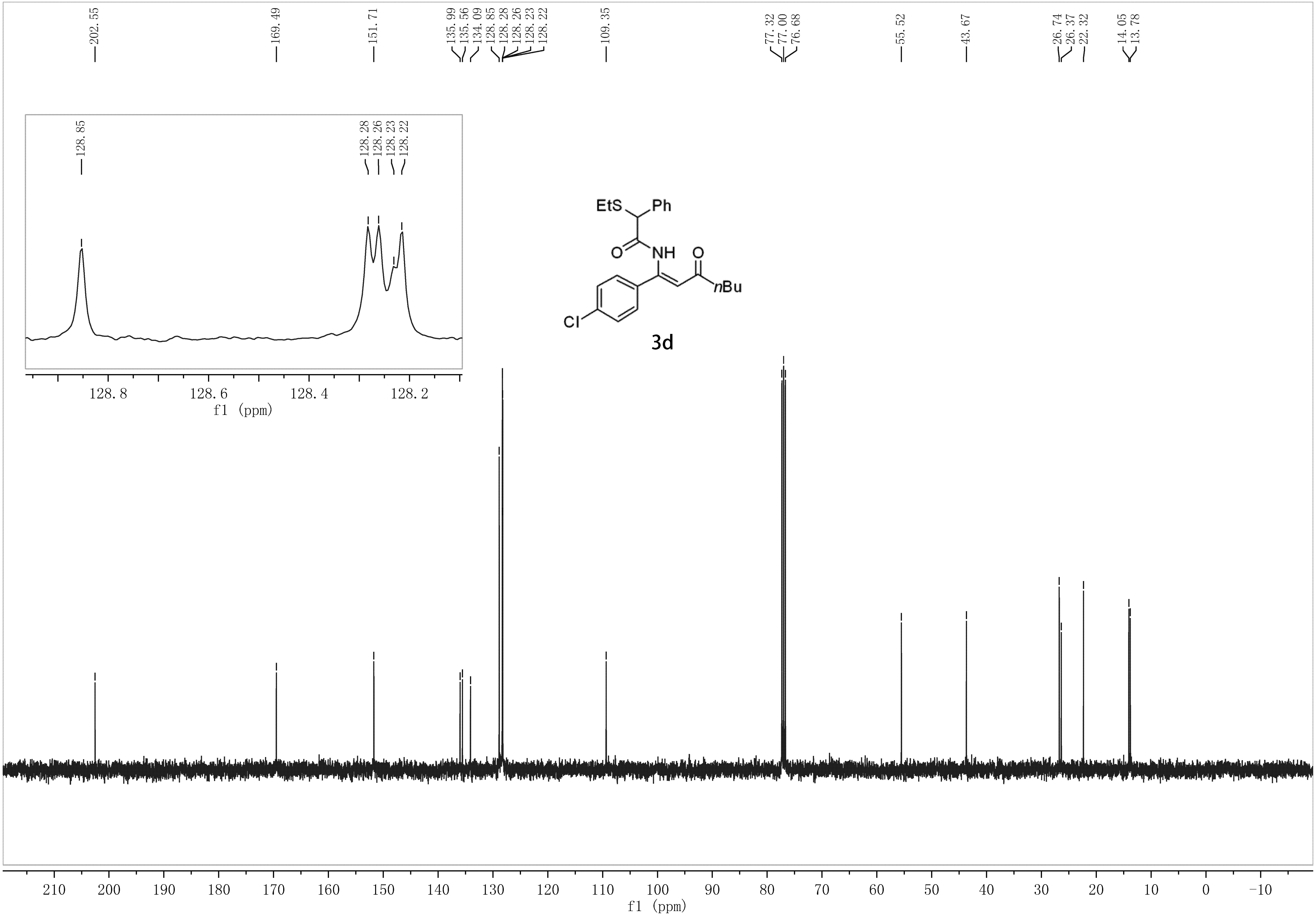
7.499
7.386
7.368
7.349
7.330
7.312
7.291
7.280
7.259
7.250
7.169
7.148
5.616
4.615
2.631
2.613
2.594
2.576
2.495
2.476
2.458
1.624
1.358
1.339
1.298
1.280
1.261
0.941
0.922
0.904
EtS
Ph
O
NH
O
nBu
Cl
3d
0.96
2.00
3.13
2.14
2.00
1.00
0.99
2.01
2.05
2.11
2.14
3.17
3.02
3.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



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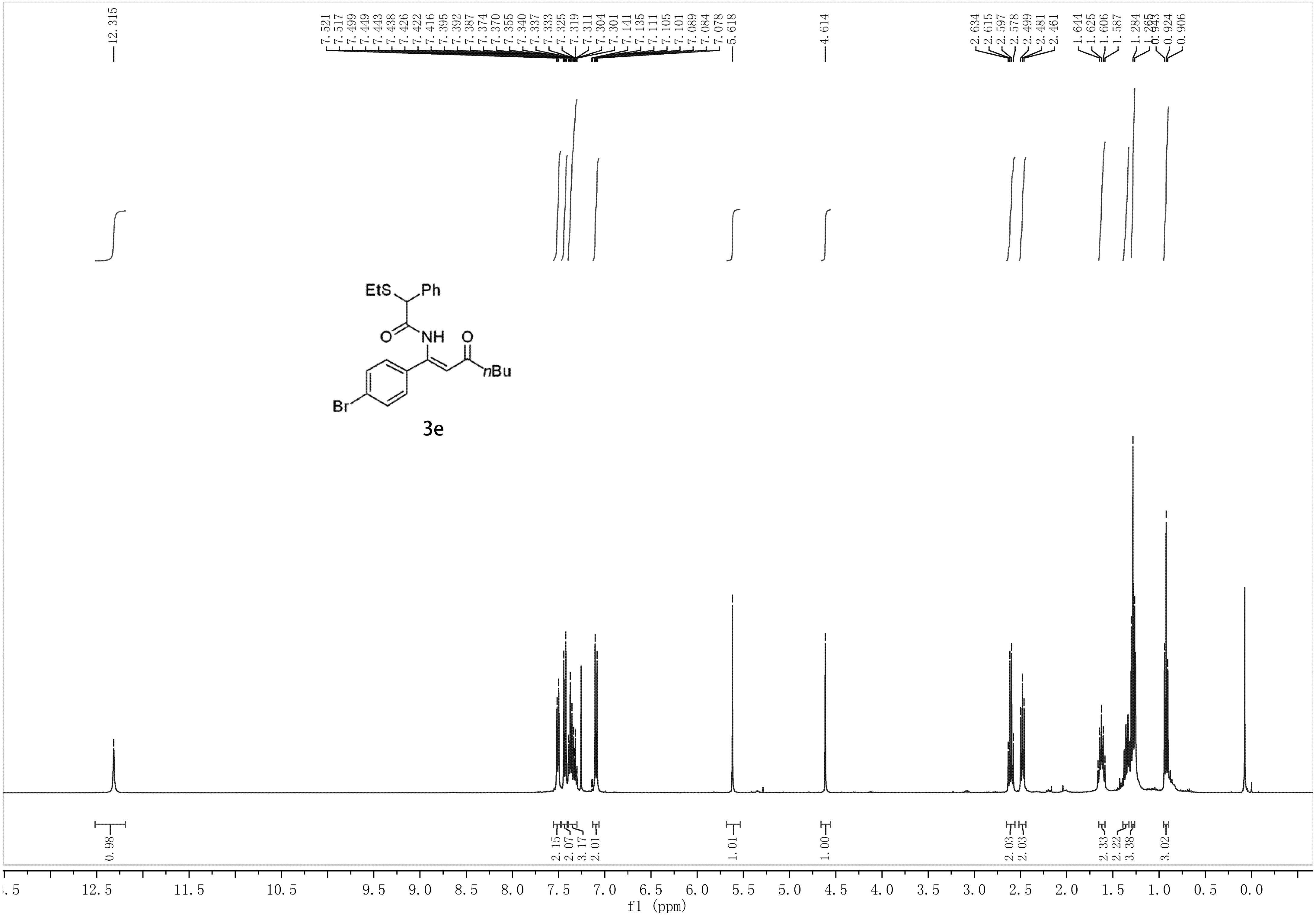
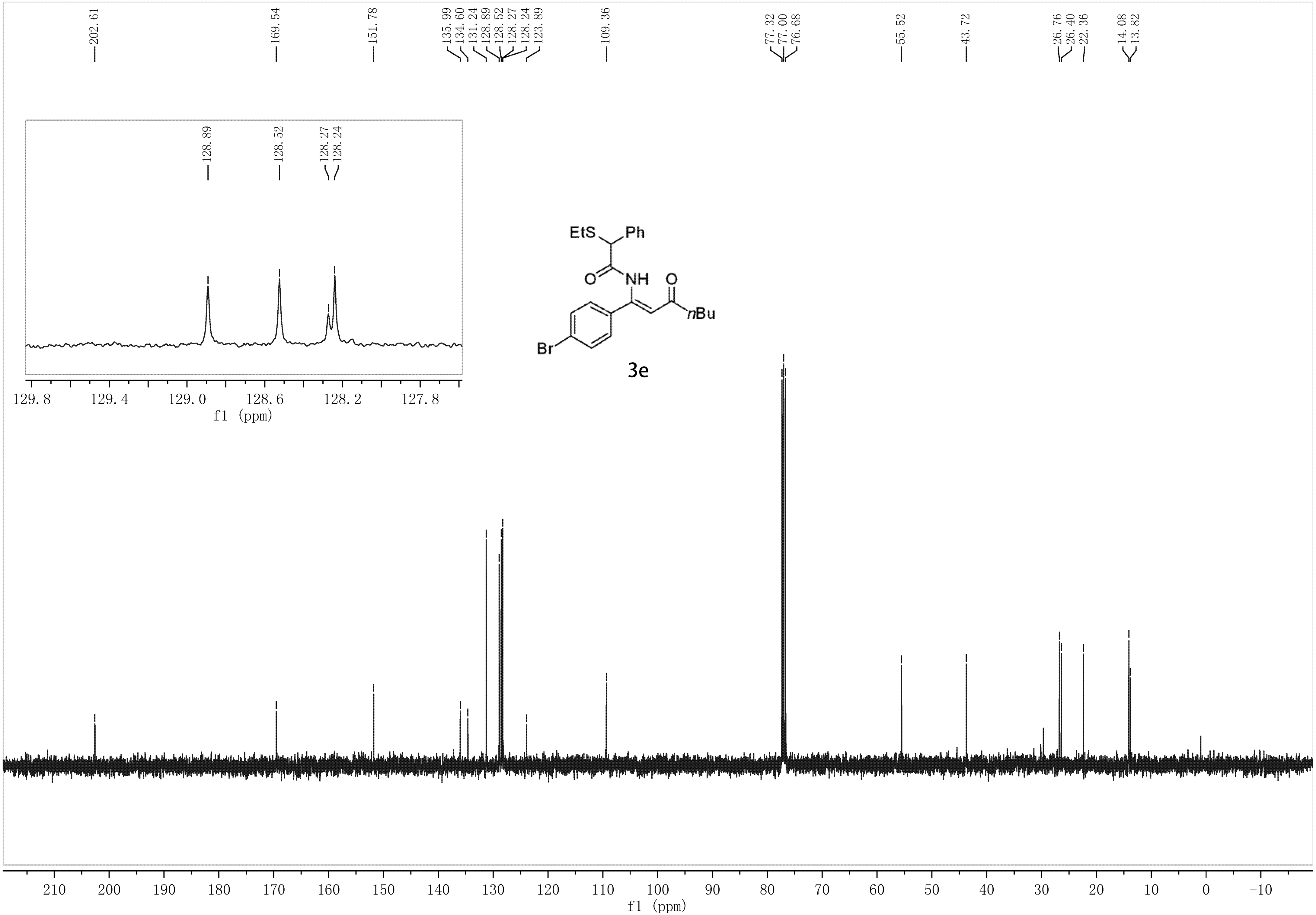
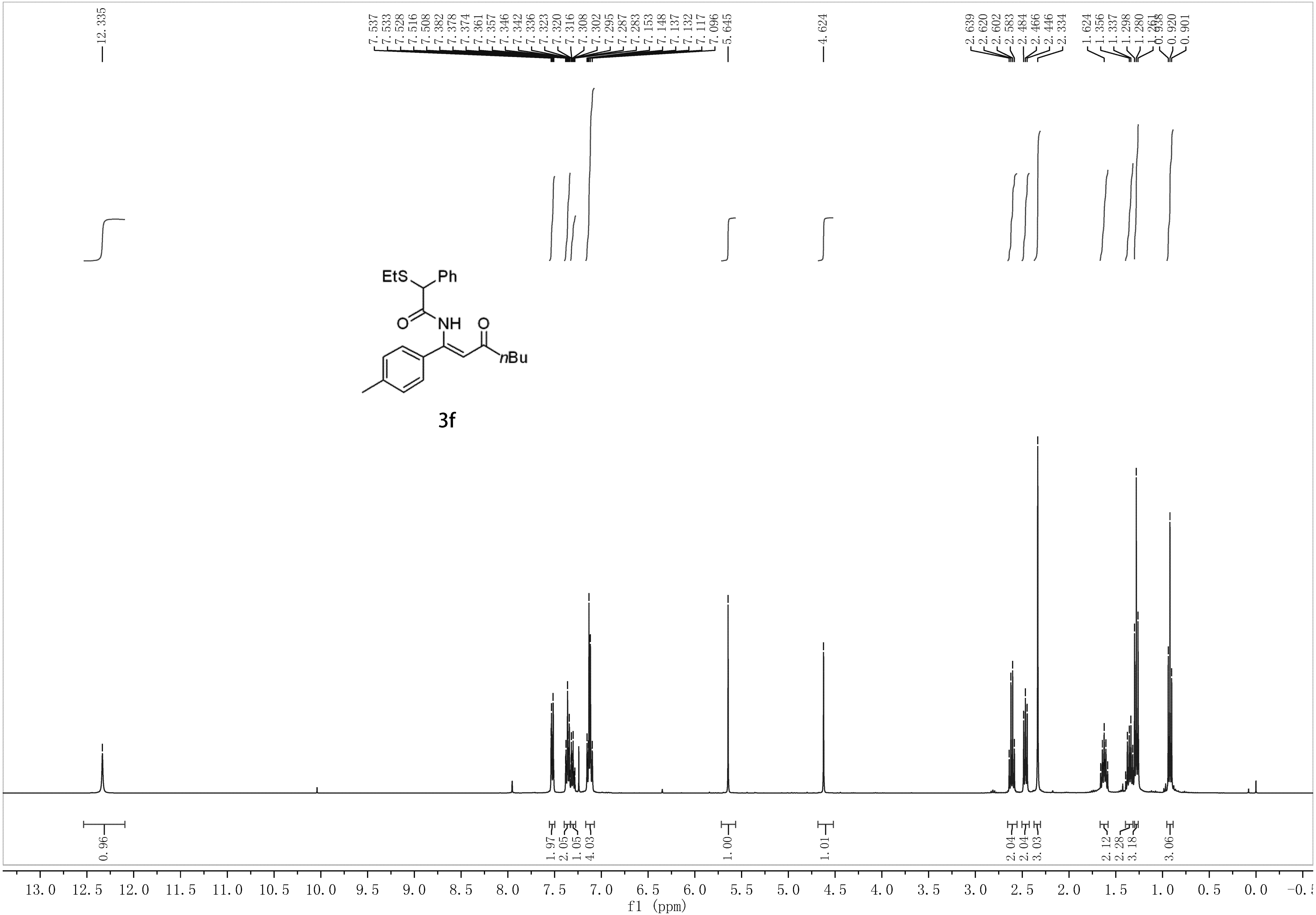
169.49
151.71
135.99
135.56
134.09
128.85
128.28
128.26
128.23
128.22
109.35
77.32
77.00
76.68
55.52
43.67
26.74
26.37
22.32
14.05
13.78
EtS
Ph
O
NH
O
nBu
Cl
3d
f1 (ppm)


12.315
7.521 7.517 7.499 7.449 7.443 7.438 7.426 7.422 7.416 7.395 7.392 7.387 7.374 7.370 7.355 7.340 7.337 7.333 7.325 7.319 7.311 7.304 7.301 7.141 7.135 7.111 7.105 7.101 7.089 7.084 7.078 5.618
4.614
2.634 2.615 2.597 2.578 2.499 2.481 2.461
1.644 1.625 1.606 1.587 1.284 1.265 0.943 0.924 0.906
EtS Ph
O NH O
nBu
Br
3e
0.98
2.15 2.07 3.17 2.01
1.01
1.00
2.03 2.03
2.33 2.22 3.38
3.02
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


202.61
169.54
151.78
135.99
134.60
131.24
128.89
128.52
128.27
128.24
123.89
109.36
77.32
77.00
76.68
55.52
43.72
26.76
26.40
22.36
14.08
13.82
EtS
Ph
O
NH
O
nBu
Br
3e
129.8 129.4 129.0 128.6 128.2 127.8
f1 (ppm)
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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7.528
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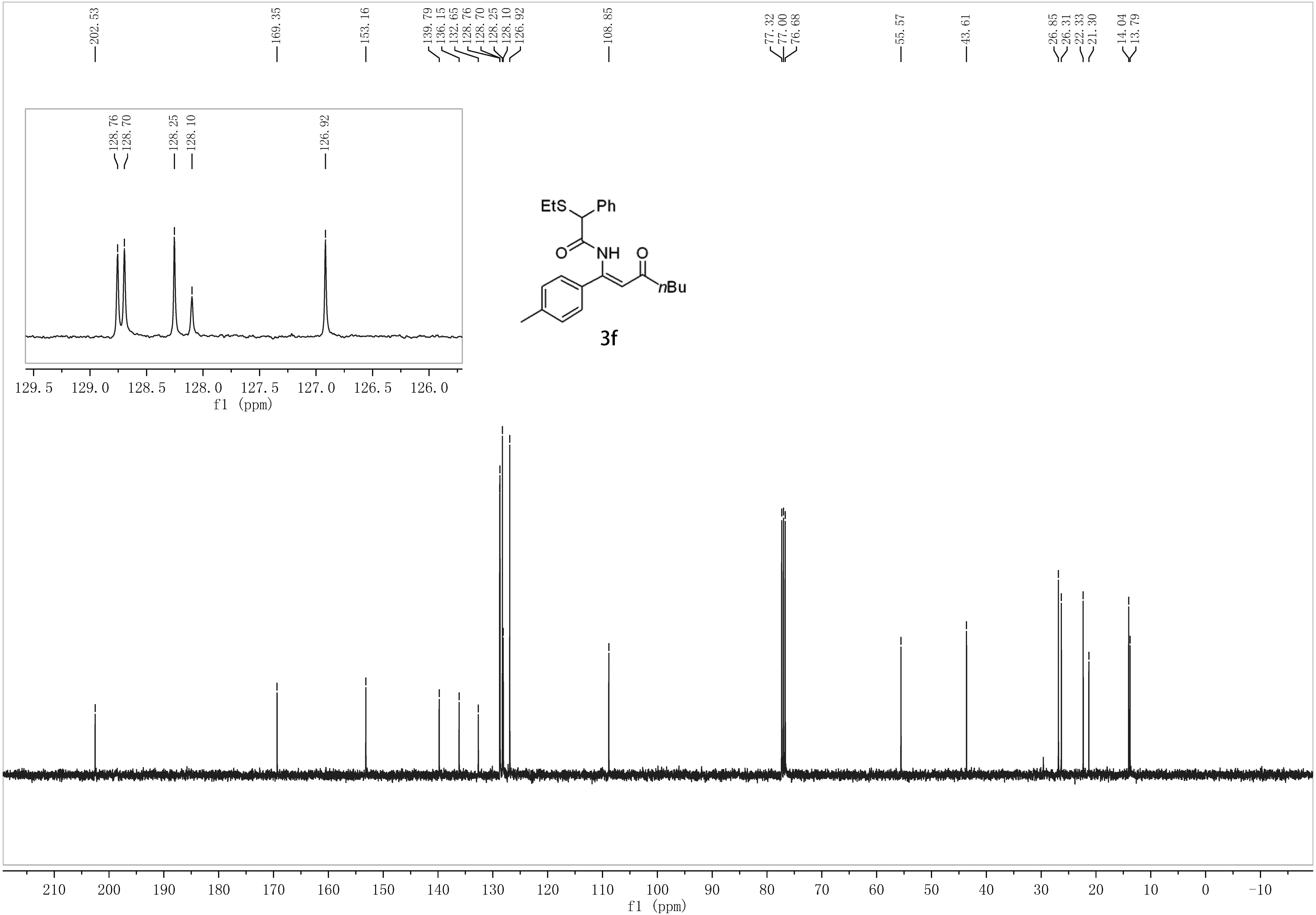
7.508
7.382
7.378
7.374
7.361
7.357
7.346
7.342
7.336
7.323
7.320
7.316
7.308
7.302
7.295
7.287
7.283
7.153
7.148
7.137
7.132
7.117
7.096
5.645
4.624
2.639
2.620
2.602
2.583
2.484
2.466
2.446
2.334
1.624
1.356
1.337
1.298
1.280
1.261
0.938
0.920
0.901
EtS
Ph
O
NH
O
nBu
3f
0.96
1.97
2.05
1.05
4.03
1.00
1.01
2.04
2.04
3.03
2.12
2.28
3.18
3.06
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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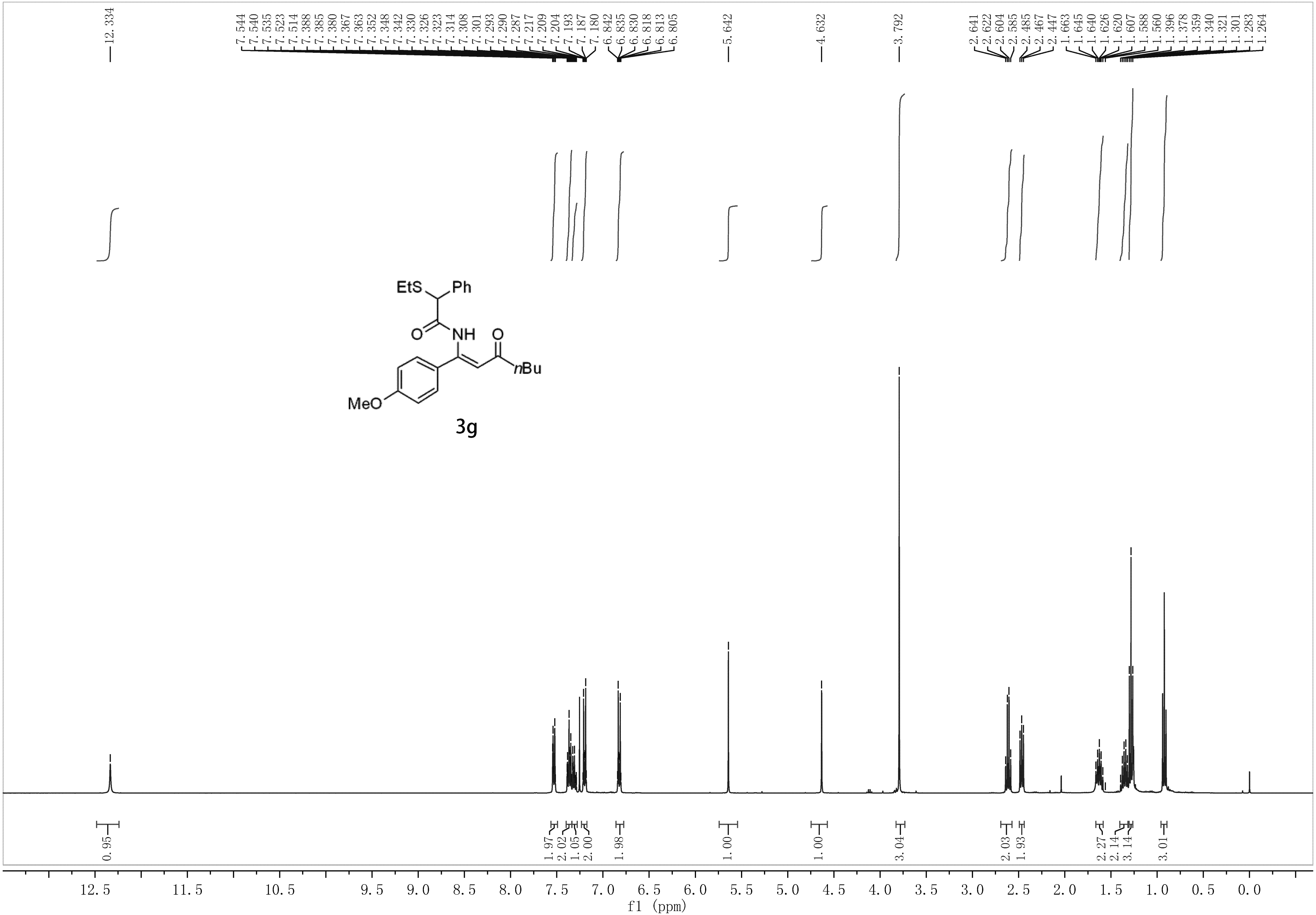
169.35
153.16
139.79
136.15
132.65
128.76
128.70
128.25
128.10
126.92
108.85
77.32
77.00
76.68
55.57
43.61
26.85
26.31
22.33
21.30
14.04
13.79
EtS
Ph
O
NH
O
nBu
3f
129.5 129.0 128.5 128.0 127.5 127.0 126.5 126.0
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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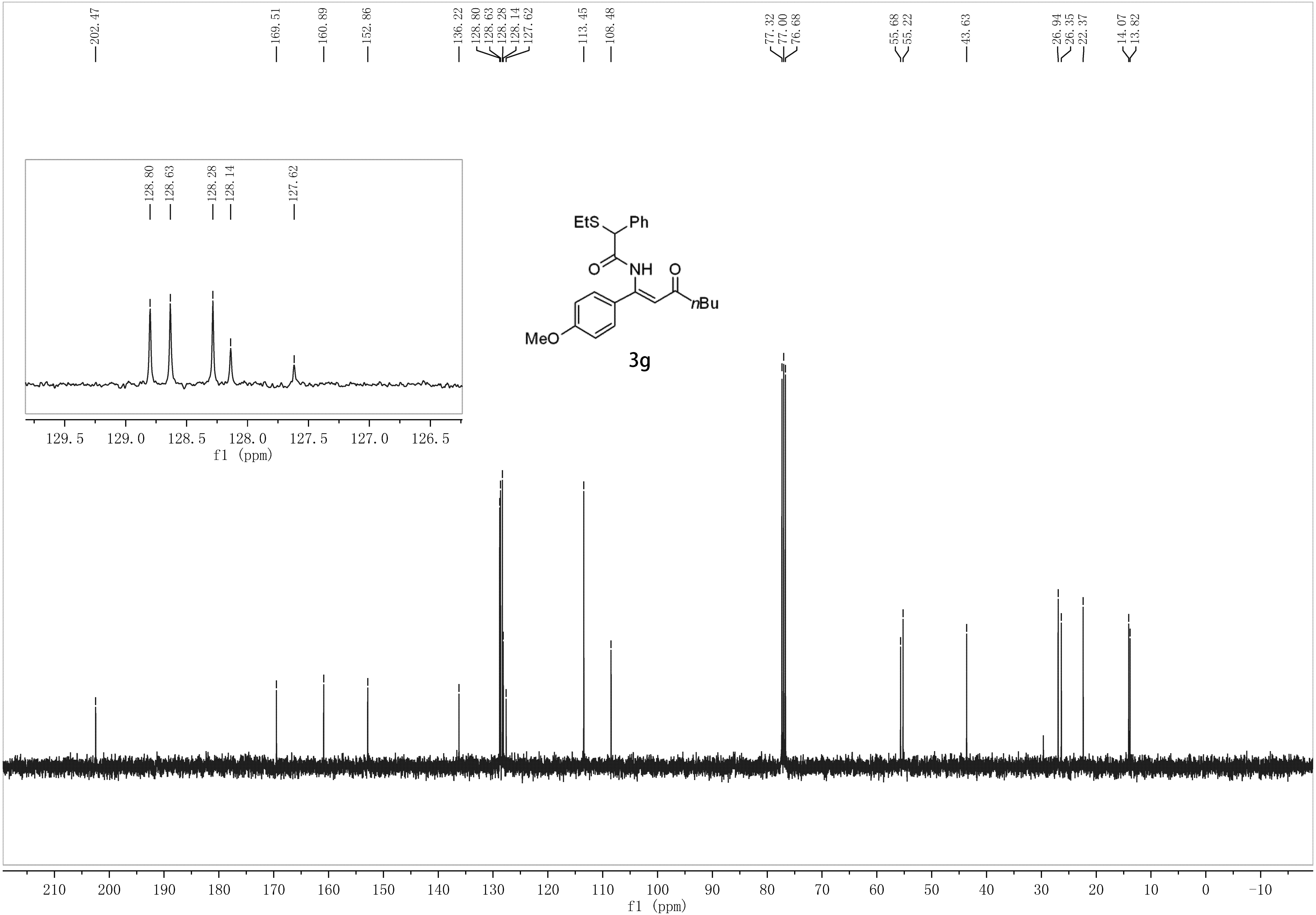
7.540
7.535
7.523
7.514
7.388
7.385
7.380
7.367
7.363
7.352
7.348
7.342
7.330
7.326
7.323
7.314
7.308
7.301
7.293
7.290
7.287
7.217
7.209
7.204
7.193
7.187
7.180
6.842
6.835
6.830
6.818
6.813
6.805
5.642
4.632
3.792
2.641
2.622
2.604
2.585
2.485
2.467
2.447
1.663
1.645
1.640
1.626
1.620
1.607
1.588
1.560
1.396
1.378
1.359
1.340
1.321
1.301
1.283
1.264
EtS
Ph
O
NH
O
nBu
MeO
3g
0.95
1.97
2.02
1.05
2.00
1.98
1.00
1.00
3.04
2.03
1.93
2.27
2.14
3.14
3.01
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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127.62
113.45
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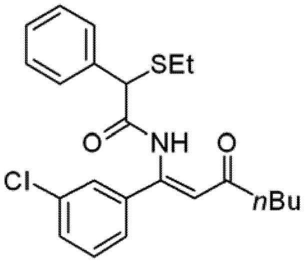
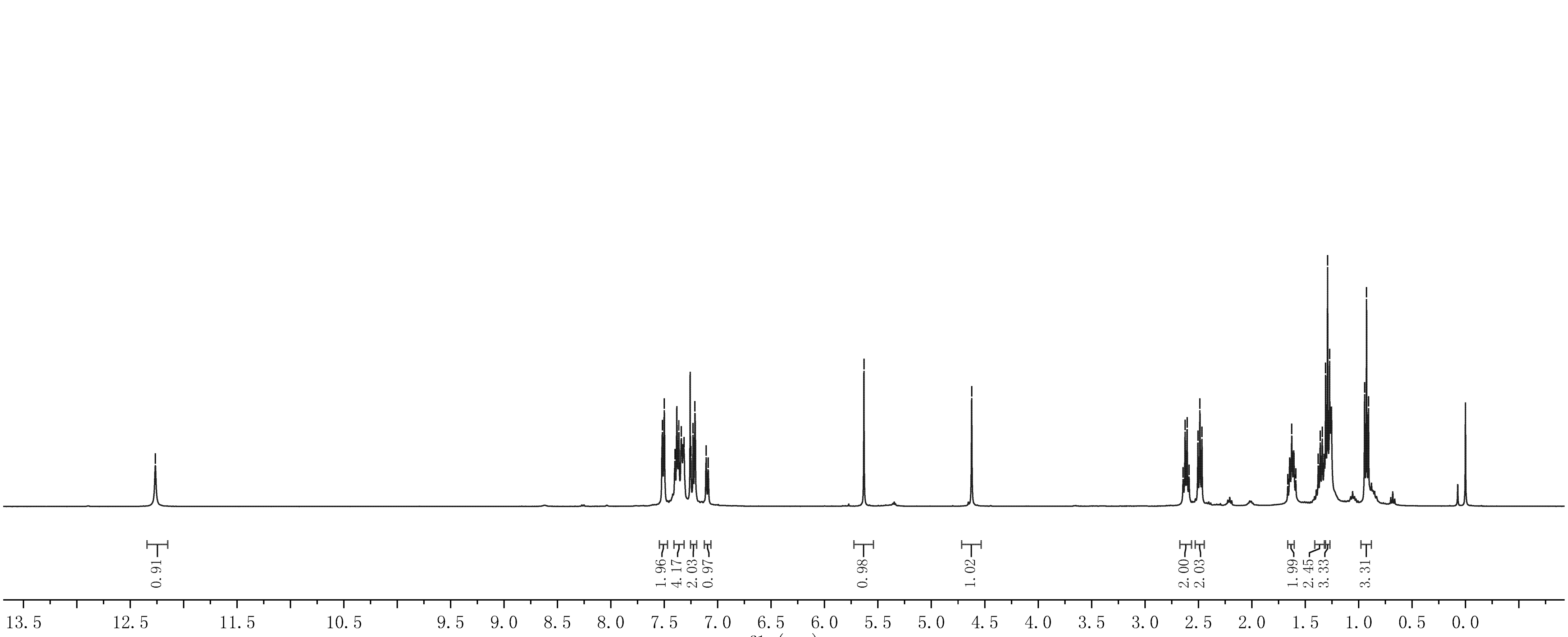
77.00
76.68
55.68
55.22
43.63
26.94
26.35
22.37
14.07
13.82
EtS
Ph
O
NH
O
nBu
MeO
3g
f1 (ppm)


SEt
O
NH
O
Cl
nBu

3h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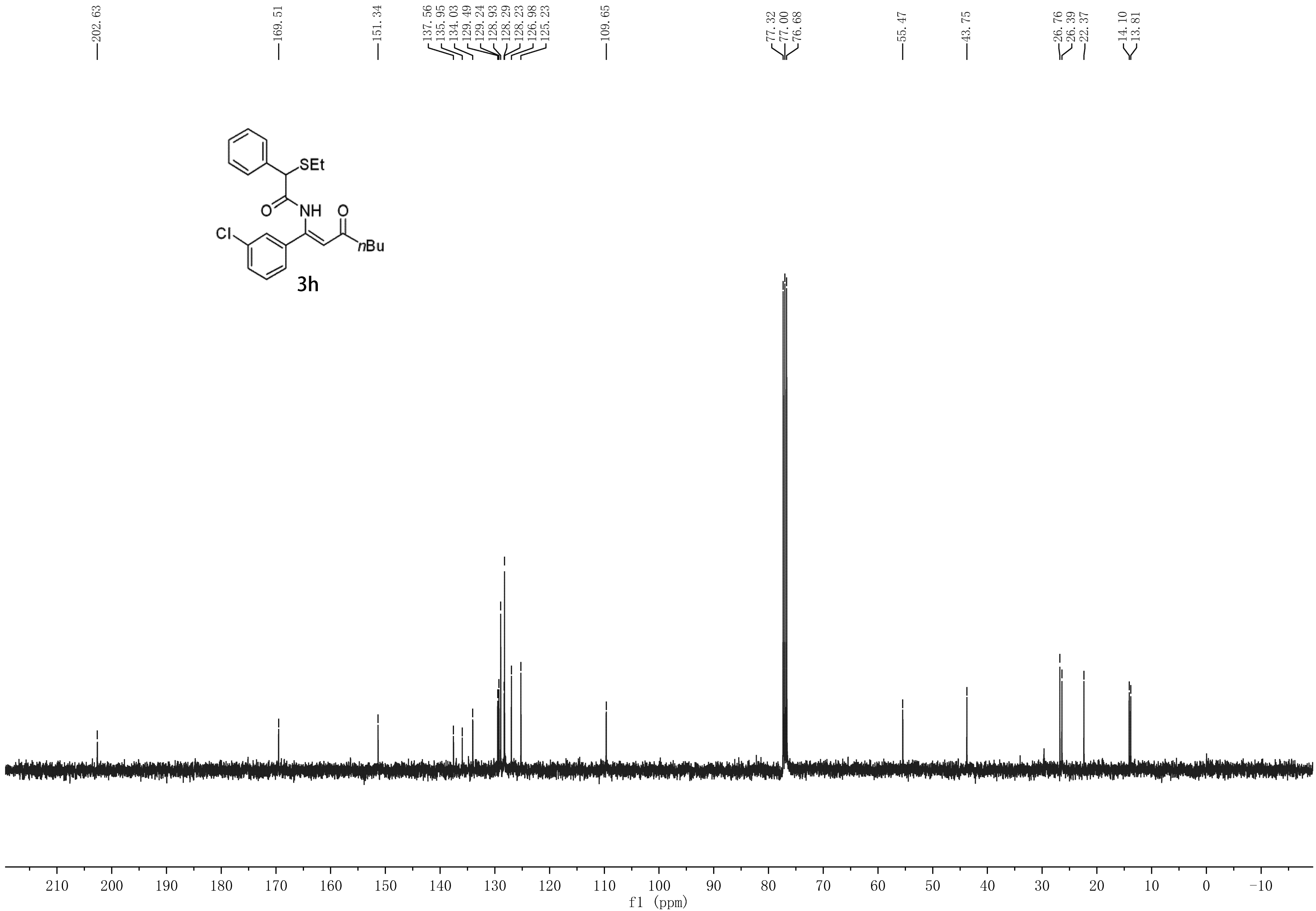
7.250
7.231
7.213
7.108
7.089
5.631
4.622
2.643
2.624
2.606
2.587
2.504
2.486
2.467
1.626
1.359
1.340
1.309
1.290
1.272
0.944
0.925
0.907
0.91
1.96
4.17
2.03
0.97
0.98
1.02
2.00
2.03
1.99
2.45
3.33
3.31
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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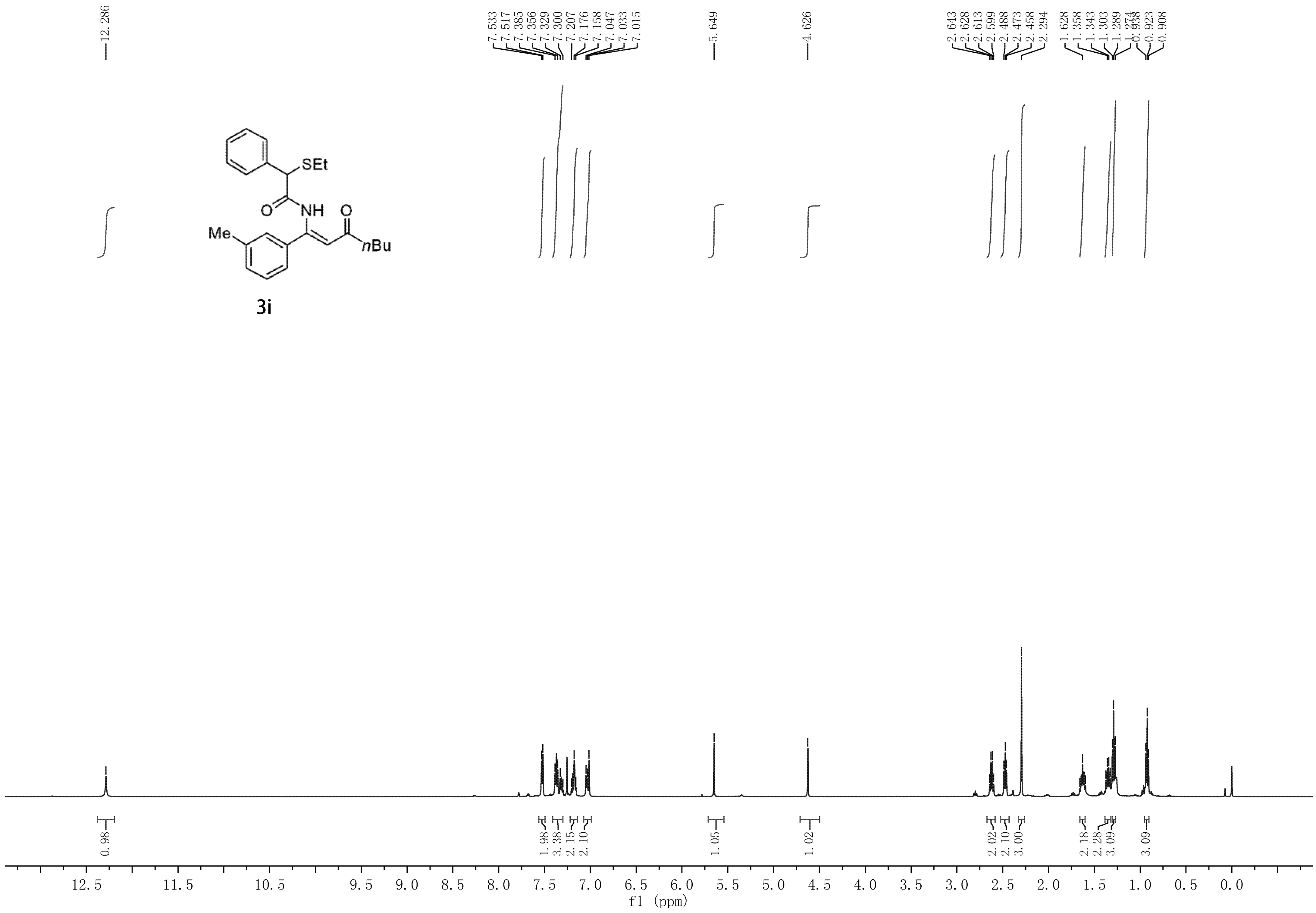
134.03
129.49
129.24
128.93
128.29
128.23
126.98
125.23
109.65
77.32
77.00
76.68
55.47
43.75
26.76
26.39
22.37
14.10
13.81
SEt
O
NH
O
Cl
nBu
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


SEt
O
NH
O
Me
nBu
3i
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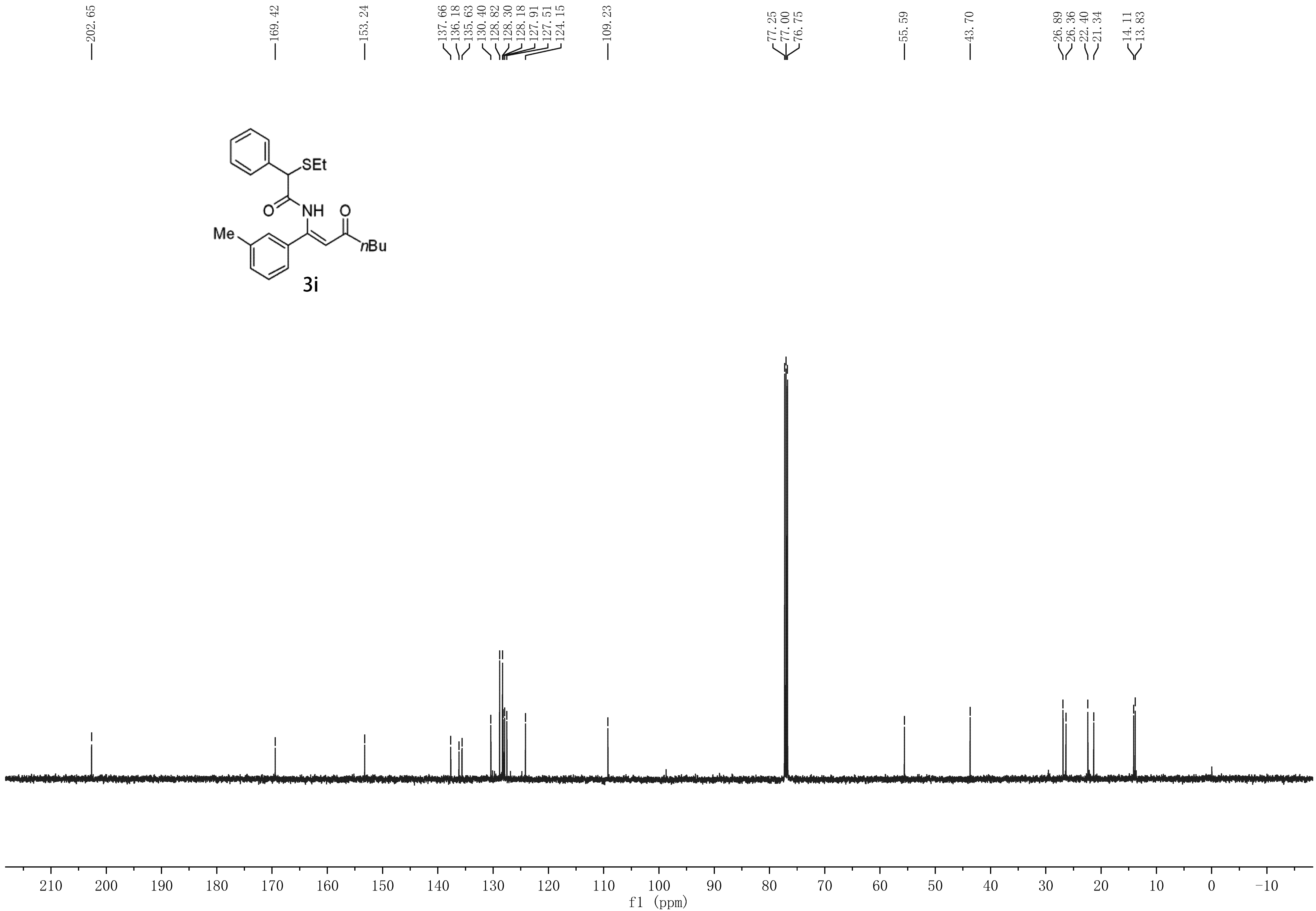
7.517
7.385
7.356
7.329
7.300
7.207
7.176
7.158
7.047
7.033
7.015
5.649
4.626
2.643
2.628
2.613
2.599
2.488
2.473
2.458
2.294
1.628
1.358
1.343
1.303
1.289
1.274
0.938
0.923
0.908
0.98
1.98
3.38
2.15
2.10
1.05
1.02
2.02
2.10
3.00
2.18
2.28
3.09
3.09
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



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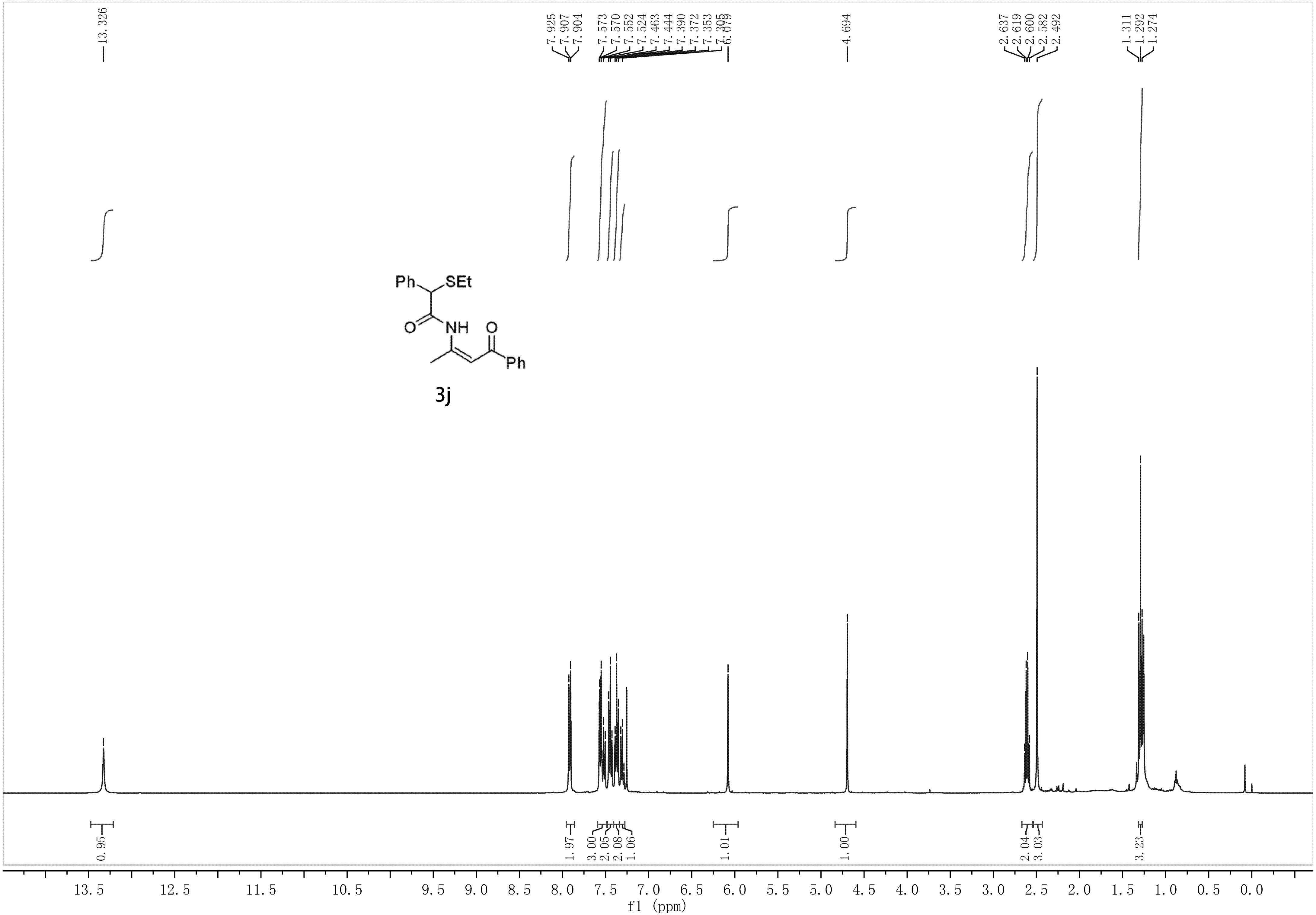
169.42
153.24
137.66
136.18
135.63
130.40
128.82
128.30
128.18
127.91
127.51
124.15
109.23
77.25
77.00
76.75
55.59
43.70
26.89
26.36
22.40
21.34
14.11
13.83
SEt
O
NH
O
Me
nBu
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



13.326
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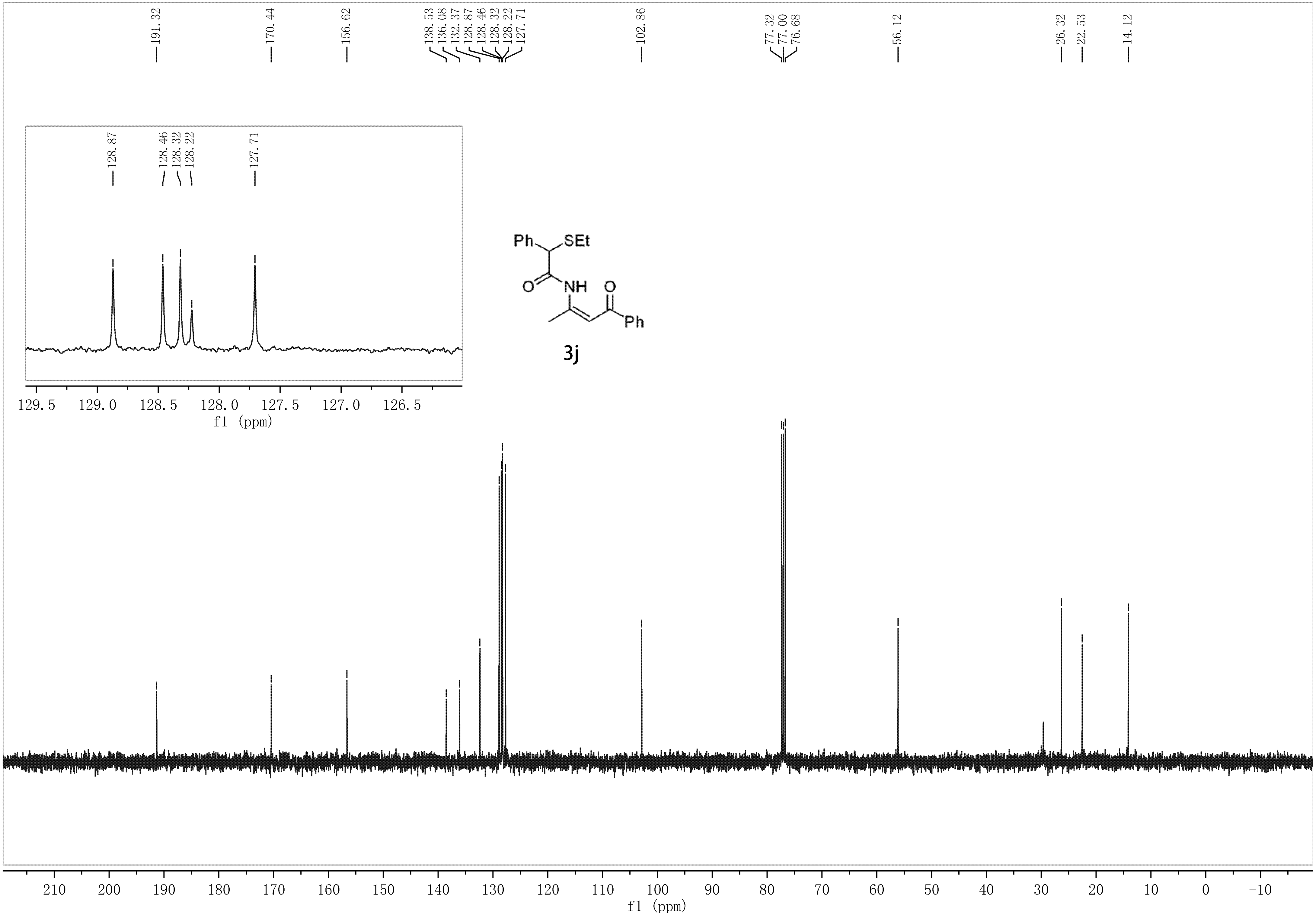
7.904
7.573
7.570
7.552
7.524
7.463
7.444
7.390
7.372
7.353
7.305
6.079
4.694
2.637
2.619
2.600
2.582
2.492
1.311
1.292
1.274
Ph
SEt
O
NH
O
Ph
3j
0.95
1.97
3.00
2.05
2.08
1.06
1.01
1.00
2.04
3.03
3.23
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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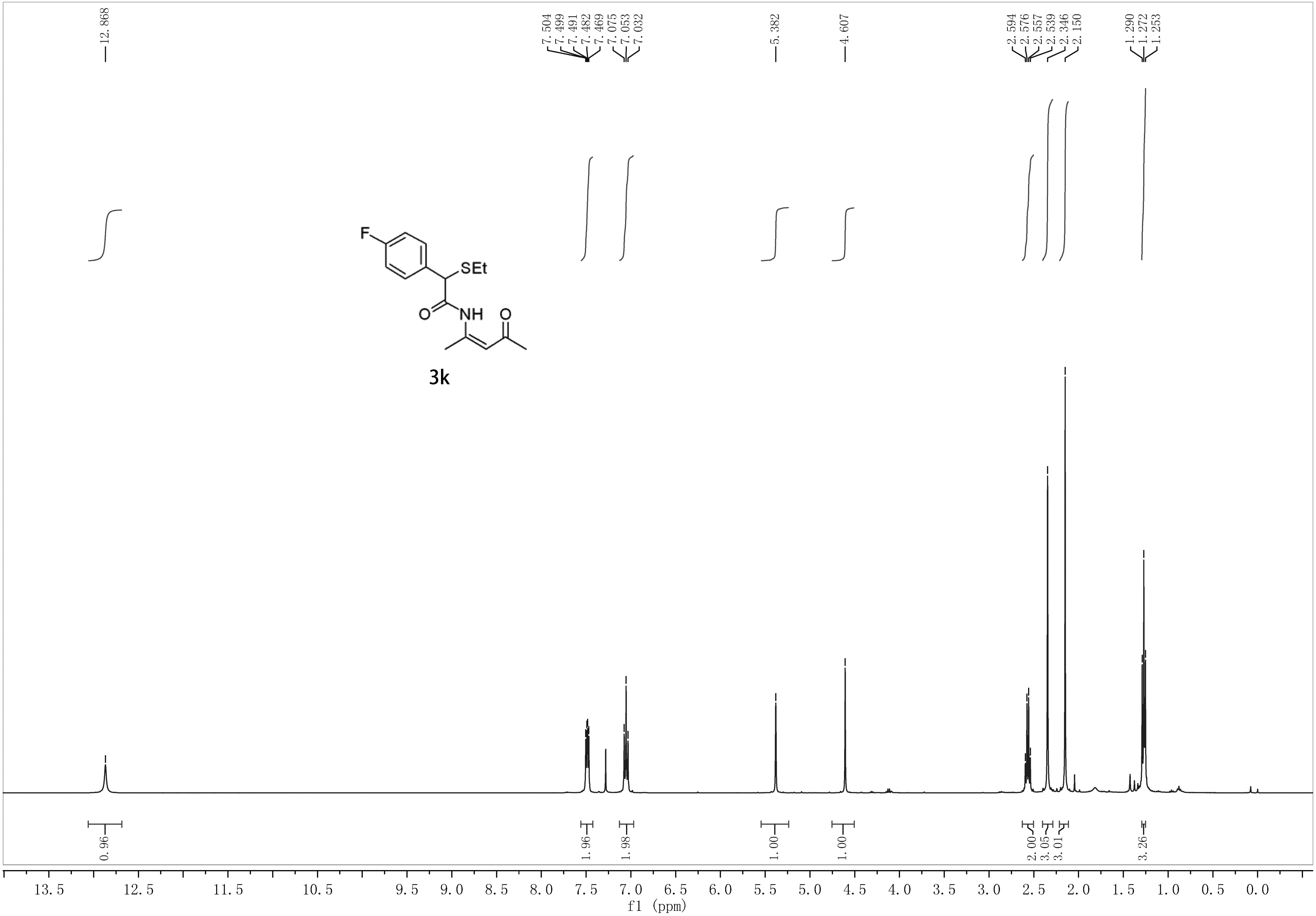
138.53
136.08
132.37
128.87
128.46
128.32
128.22
127.71
102.86
77.32
77.00
76.68
56.12
26.32
22.53
14.12
Ph
SEt
O
NH
O
Ph
3j
129.5 129.0 128.5 128.0 127.5 127.0 126.5
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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7.053
7.032
5.382
4.607
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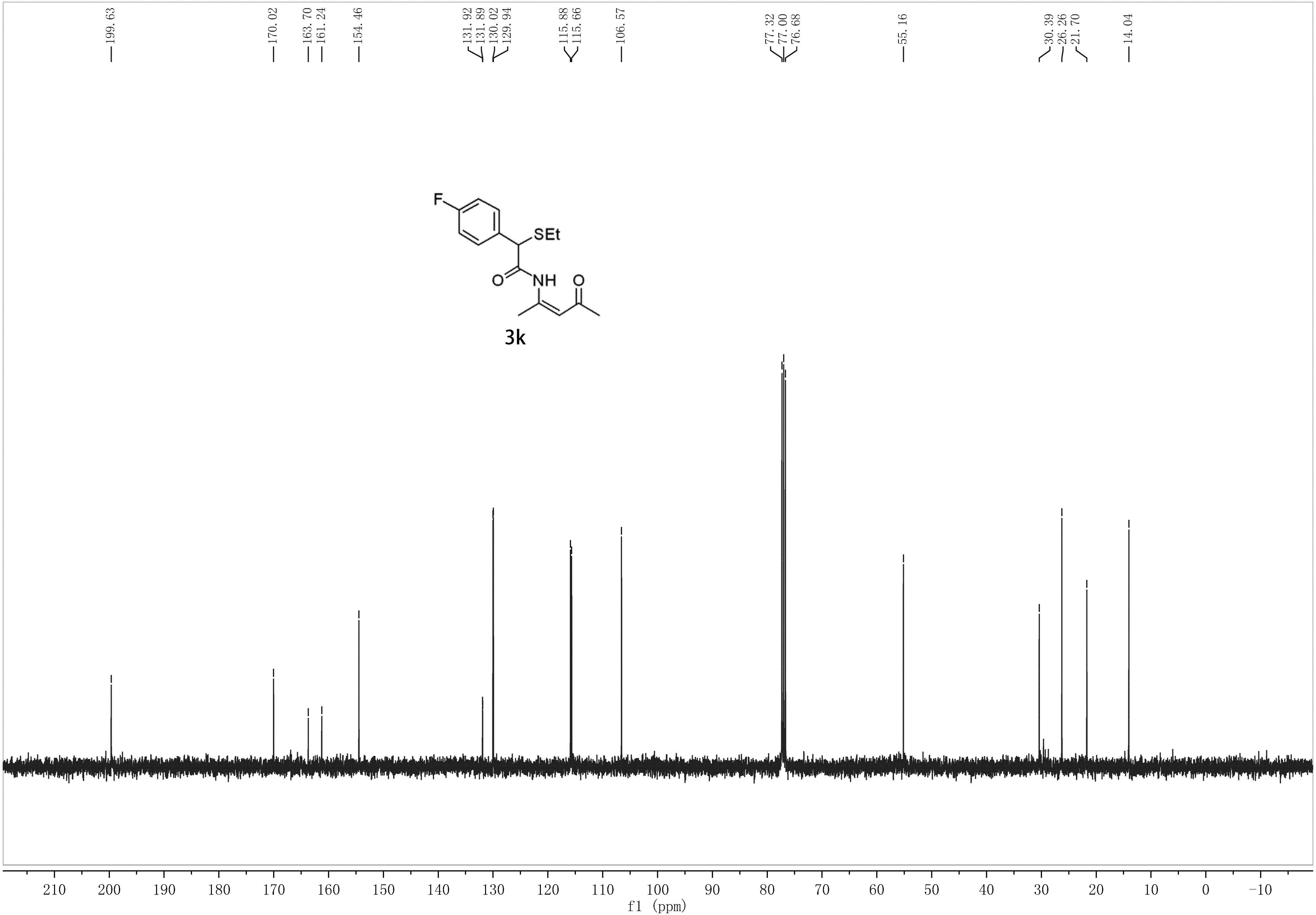
2.576
2.557
2.539
2.346
2.150
1.290
1.272
1.253
F
SEt
O
NH
O
3k
0.96
1.96
1.98
1.00
1.00
2.00
3.05
3.01
3.26
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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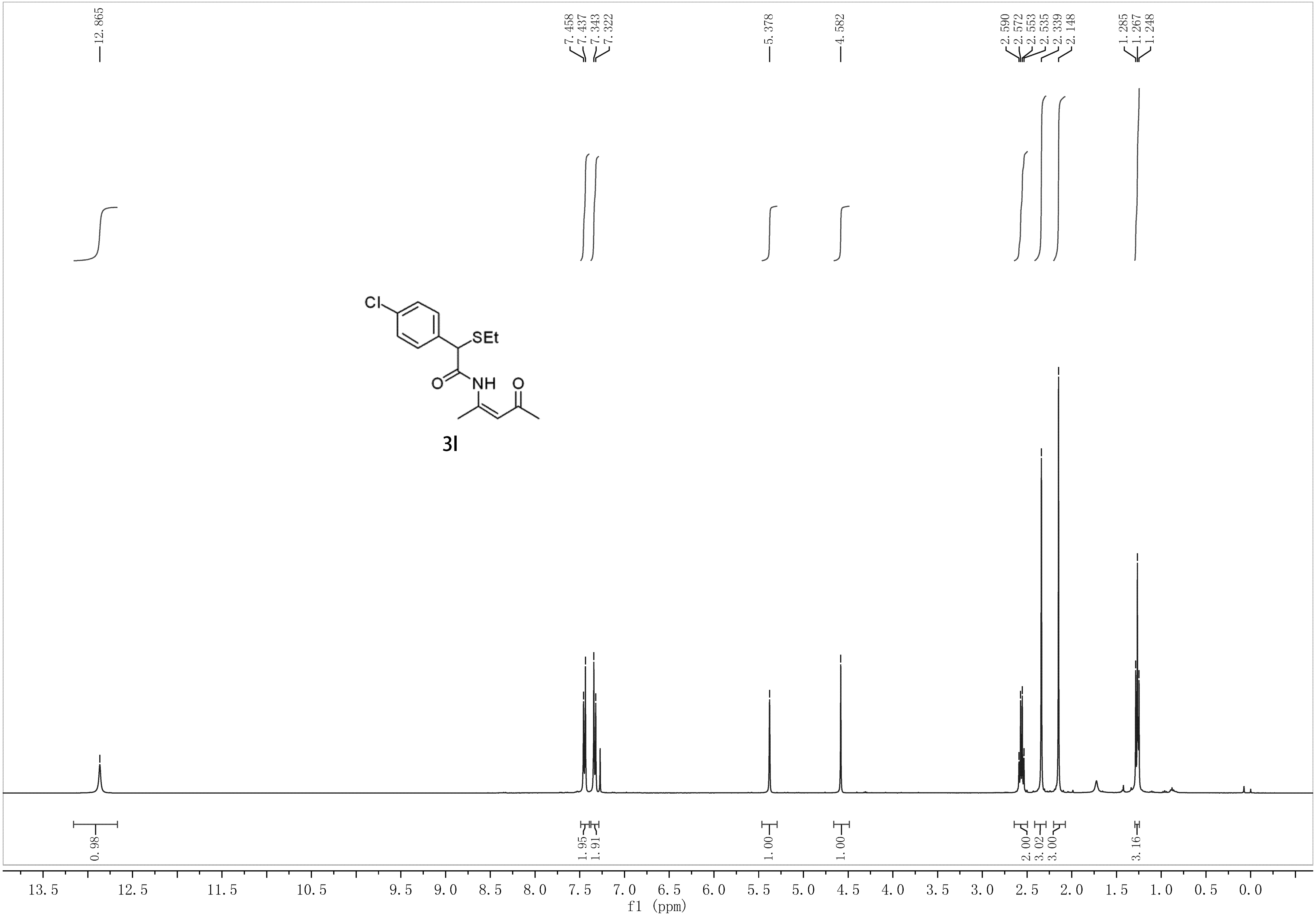
163.70
161.24
154.46
131.92
131.89
130.02
129.94
115.88
115.66
106.57
77.32
77.00
76.68
55.16
30.39
26.26
21.70
14.04
F
SEt
O
NH
O
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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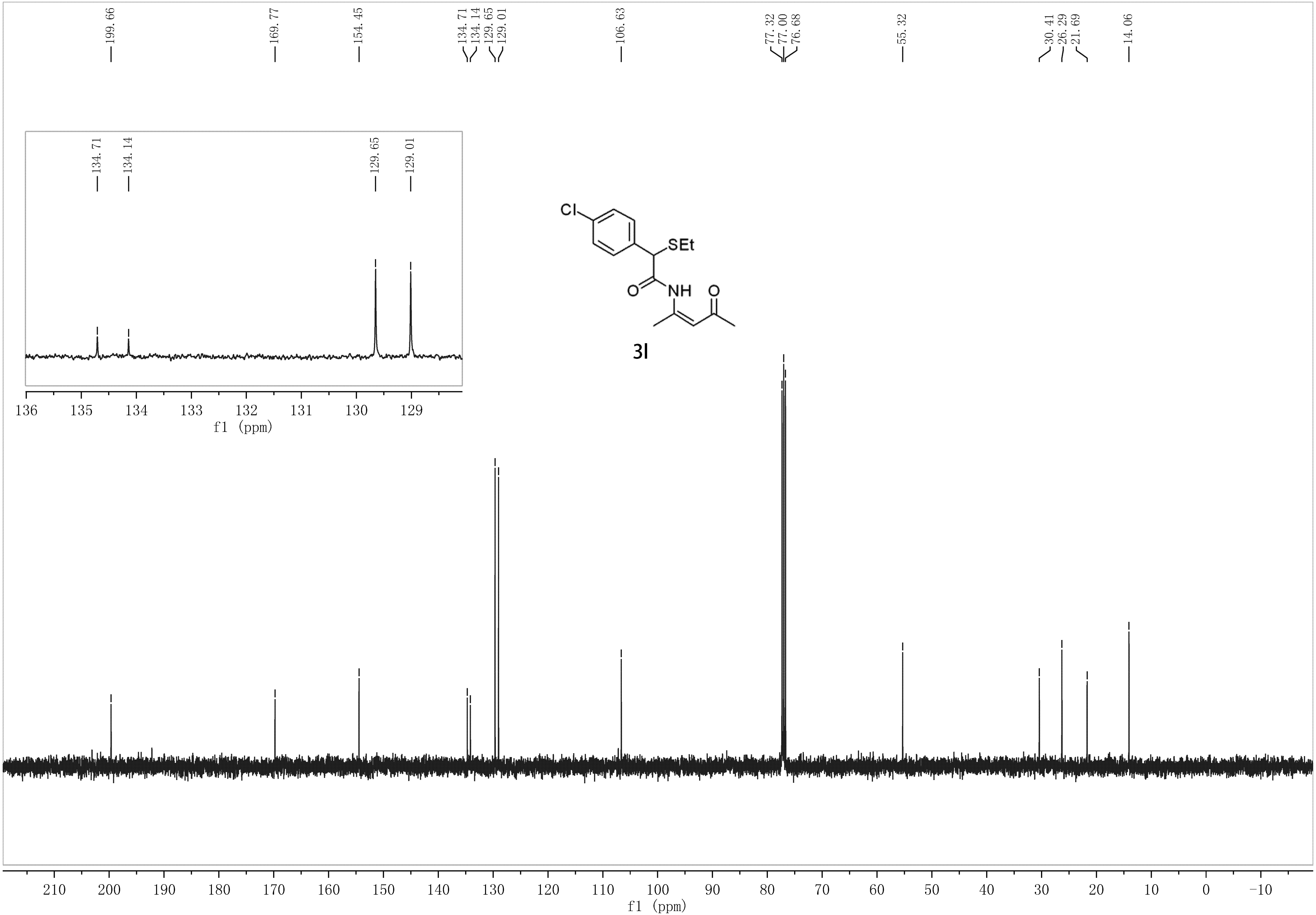
4.582
2.590
2.572
2.553
2.535
2.339
2.148
1.285
1.267
1.248
Cl
SEt
O
NH
O
3l
0.98
1.95
1.91
1.00
1.00
2.00
3.02
3.00
3.16
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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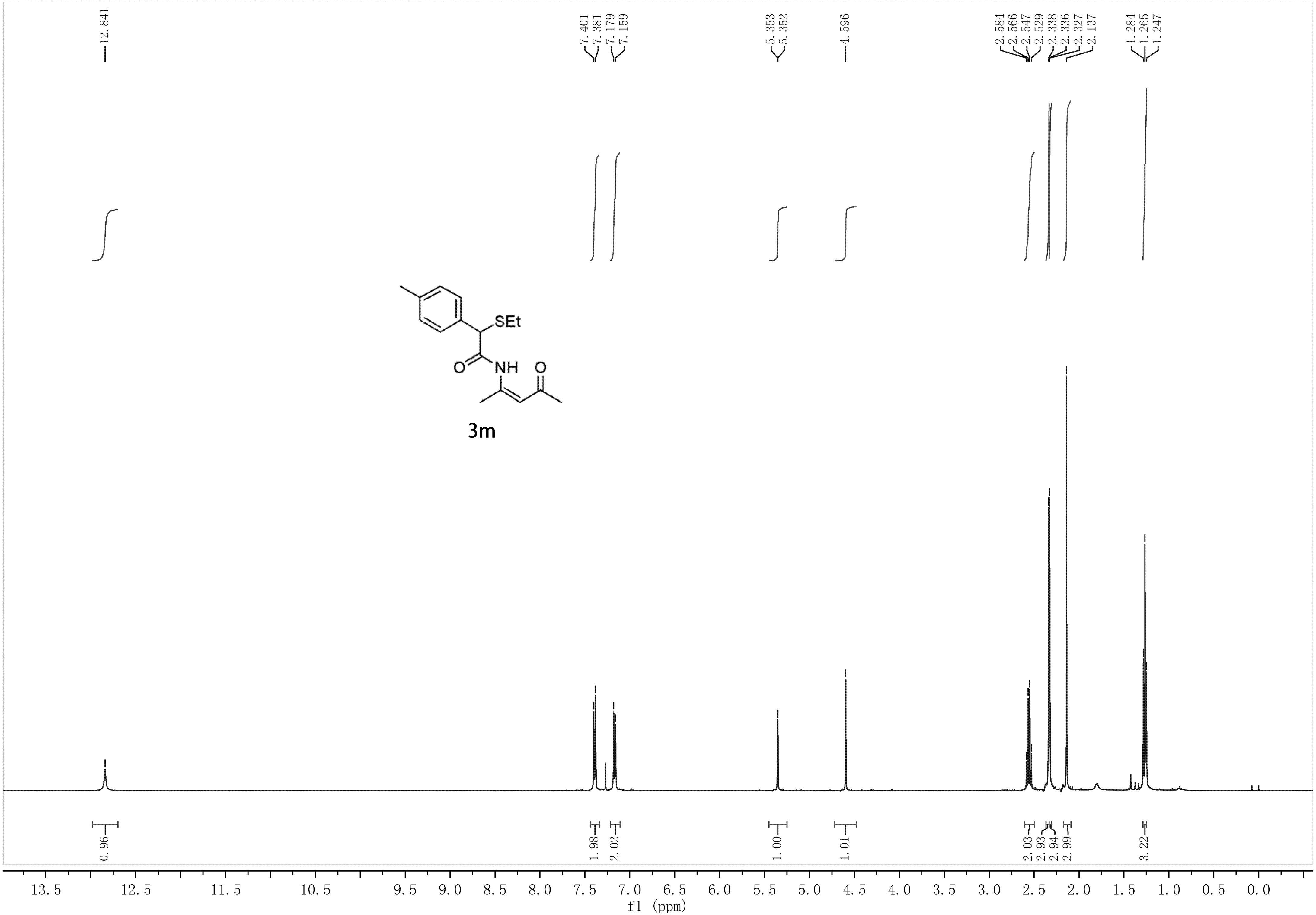
169.77
154.45
134.71
134.14
129.65
129.01
106.63
77.32
77.00
76.68
55.32
30.41
26.29
21.69
14.06
Cl
SEt
O
NH
O
3l
f1 (ppm)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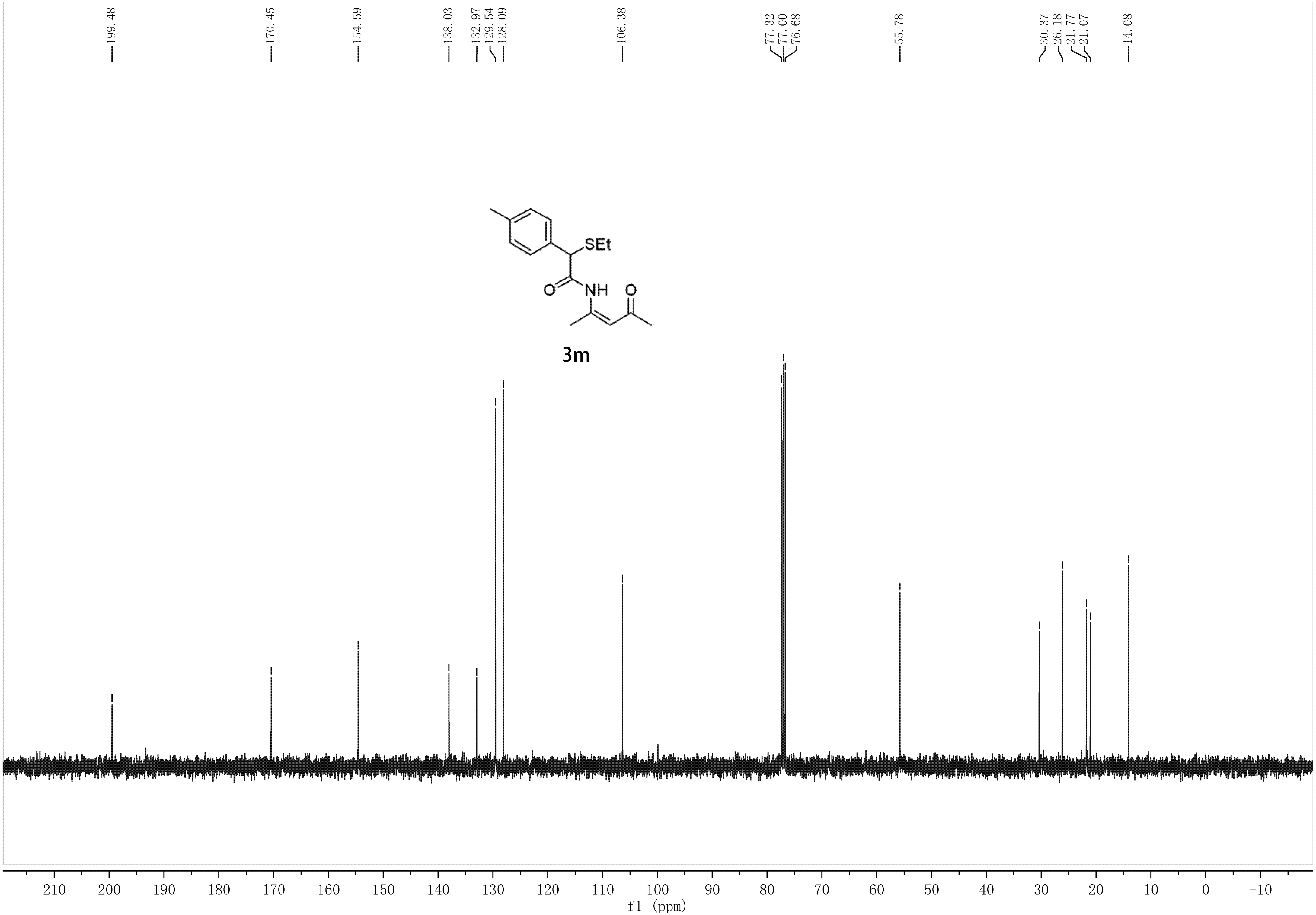
7.381
7.179
7.159
5.353
5.352
4.596
2.584
2.566
2.547
2.529
2.338
2.336
2.327
2.137
1.284
1.265
1.247
SEt
O
NH
O
3m
0.96
1.98
2.02
1.00
1.01
2.03
2.93
2.94
2.99
3.22
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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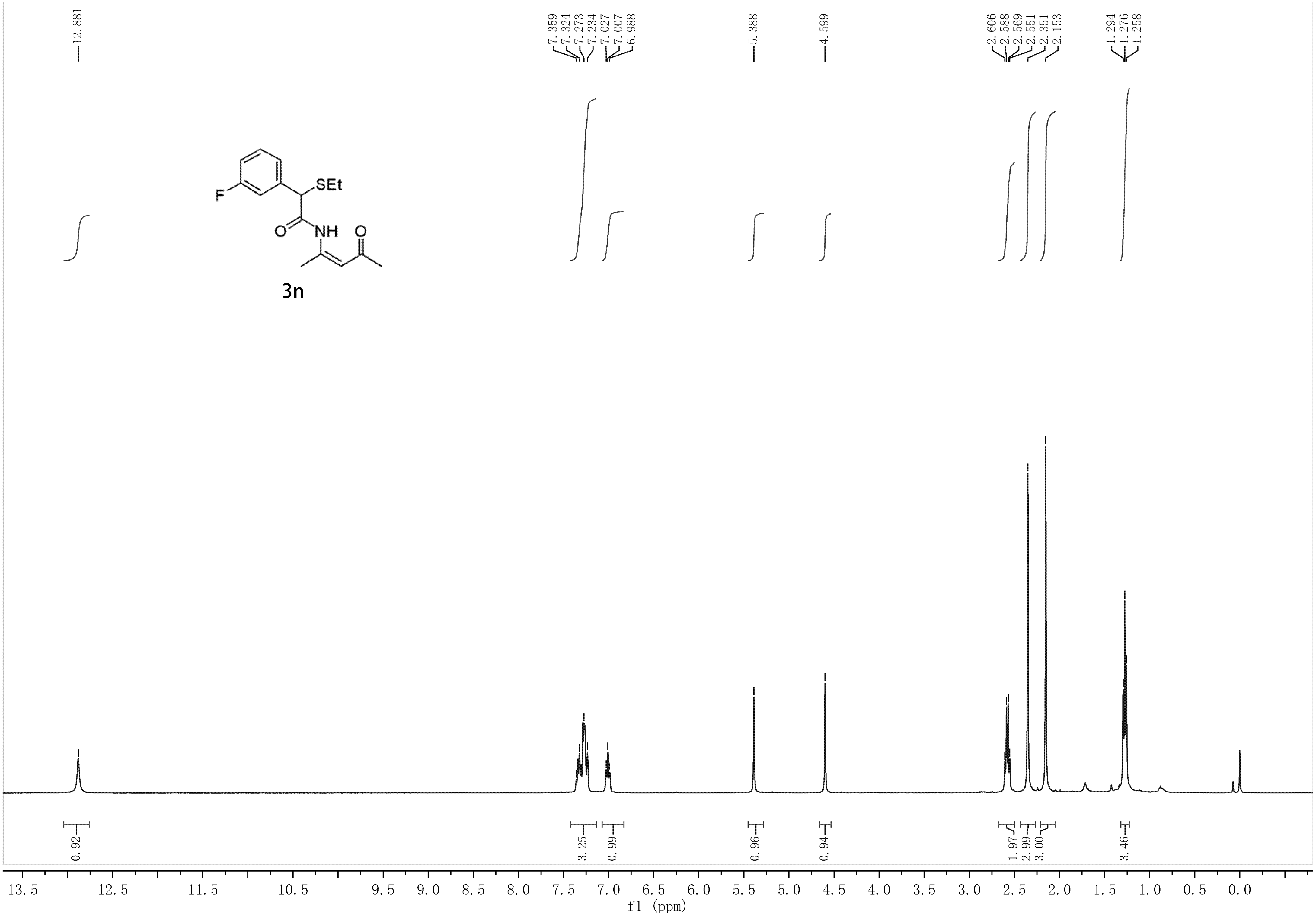
170.45
154.59
138.03
132.97
129.54
128.09
106.38
77.32
77.00
76.68
55.78
30.37
26.18
21.77
21.07
14.08
SEt
NH
O
O
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



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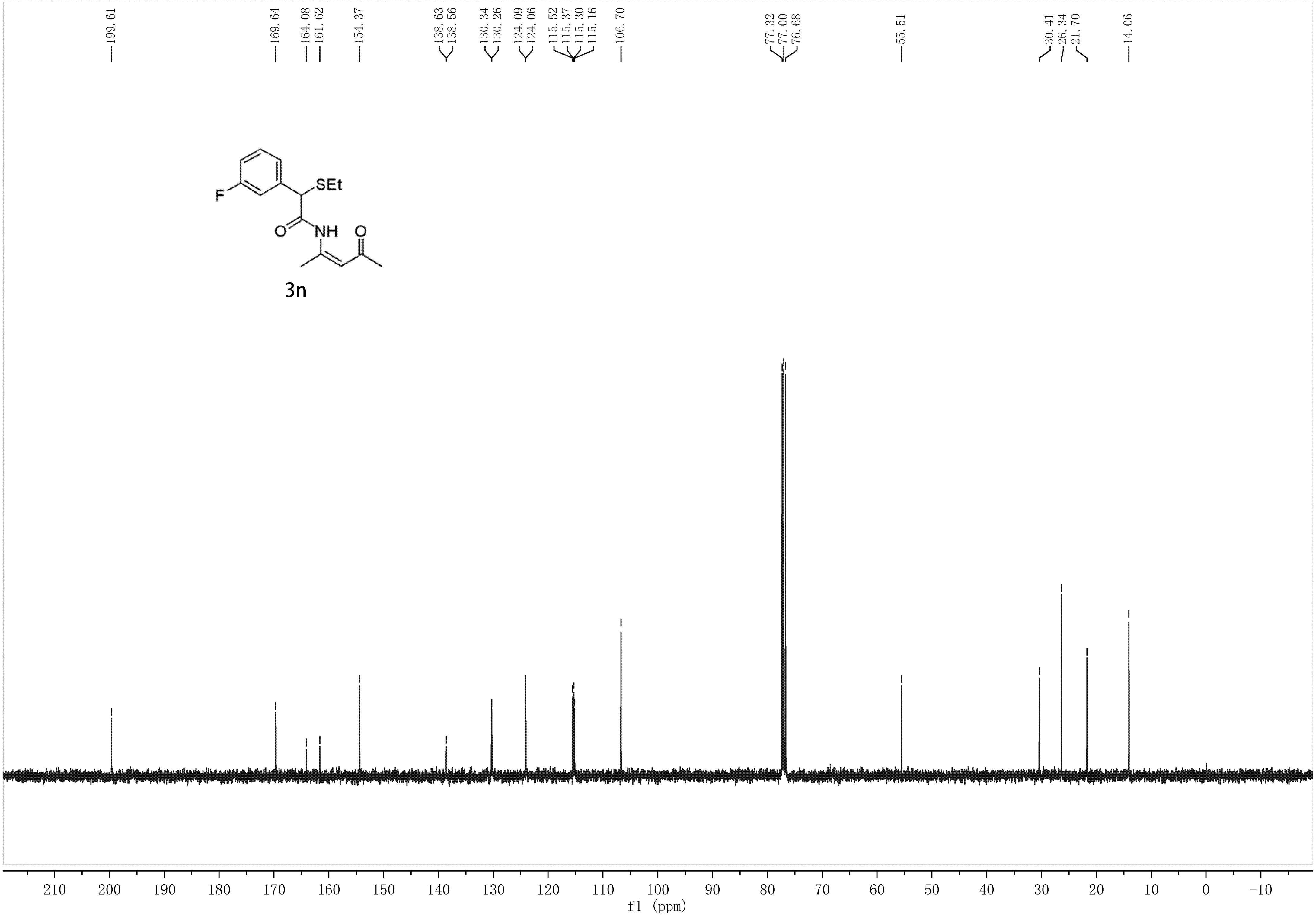
7.359
7.324
7.273
7.234
7.027
7.007
6.988
5.388
4.599
2.606
2.588
2.569
2.551
2.351
2.153
1.294
1.276
1.258
F
SEt
O
NH
O
3n
0.92
3.25
0.99
0.96
0.94
1.97
2.99
3.00
3.46
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



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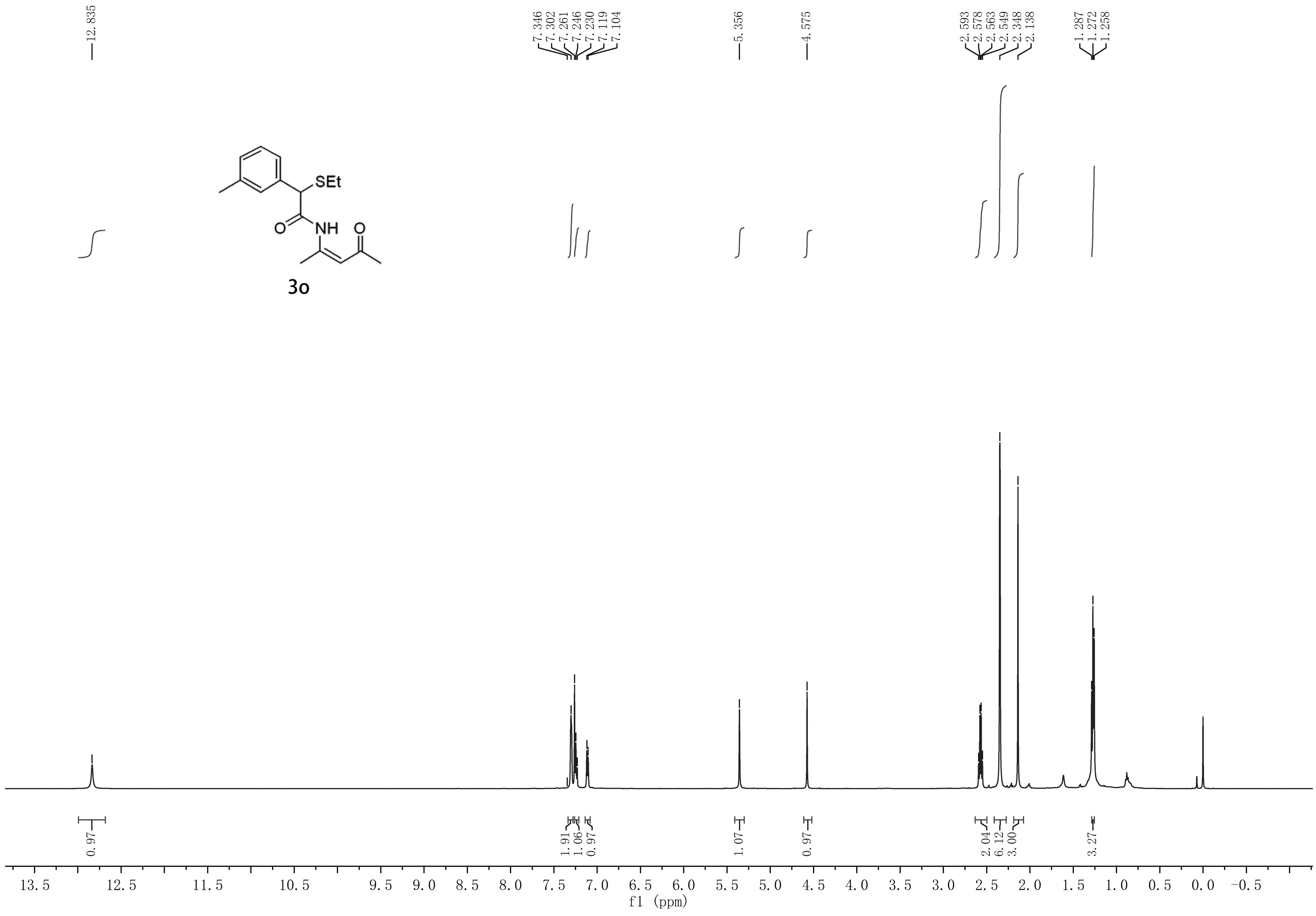
169.64
164.08
161.62
154.37
138.63
138.56
130.34
130.26
124.09
124.06
115.52
115.37
115.30
115.16
106.70
77.32
77.00
76.68
55.51
30.41
26.34
21.70
14.06
F
SEt
O
NH
O
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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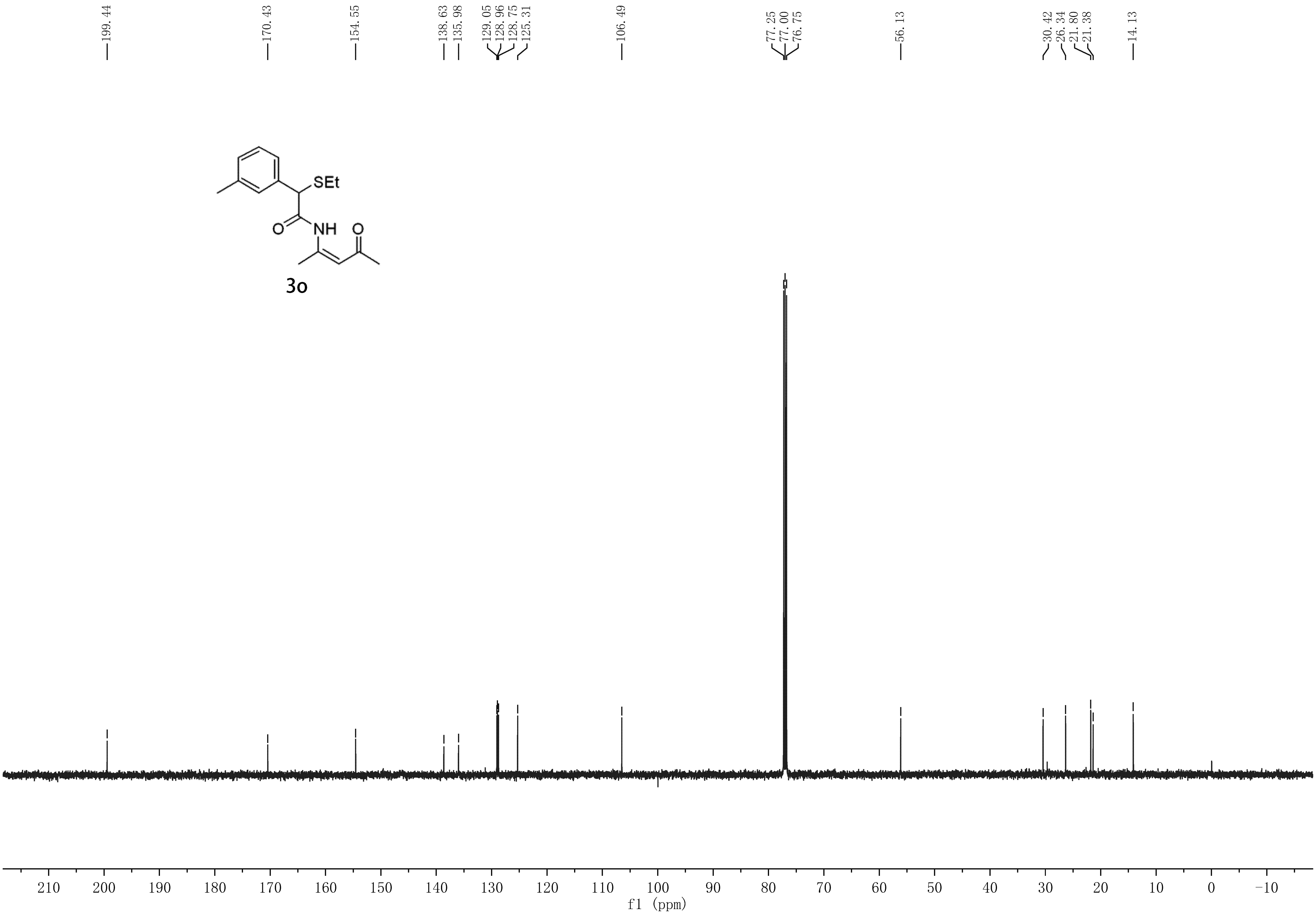
7.302
7.261
7.246
7.230
7.119
7.104
5.356
4.575
2.593
2.578
2.563
2.549
2.348
2.138
1.287
1.272
1.258
SEt
O
NH
O
3o
0.97
1.91
1.06
0.97
1.07
0.97
2.04
6.12
3.00
3.27
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)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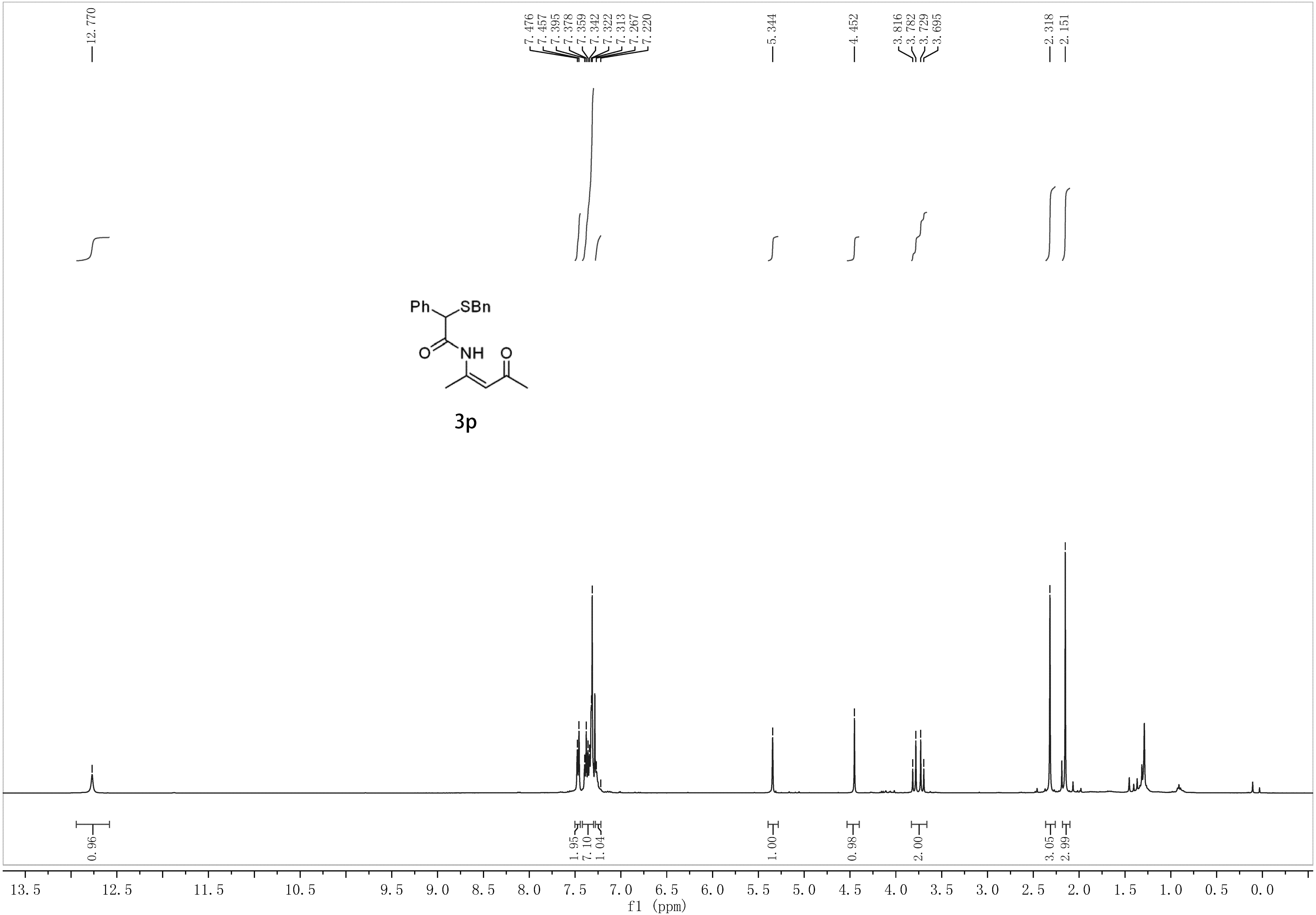
129.05
128.96
128.75
125.31
106.49
77.25
77.00
76.75
56.13
30.42
26.34
21.80
21.38
14.13
SEt
O
NH
O
3o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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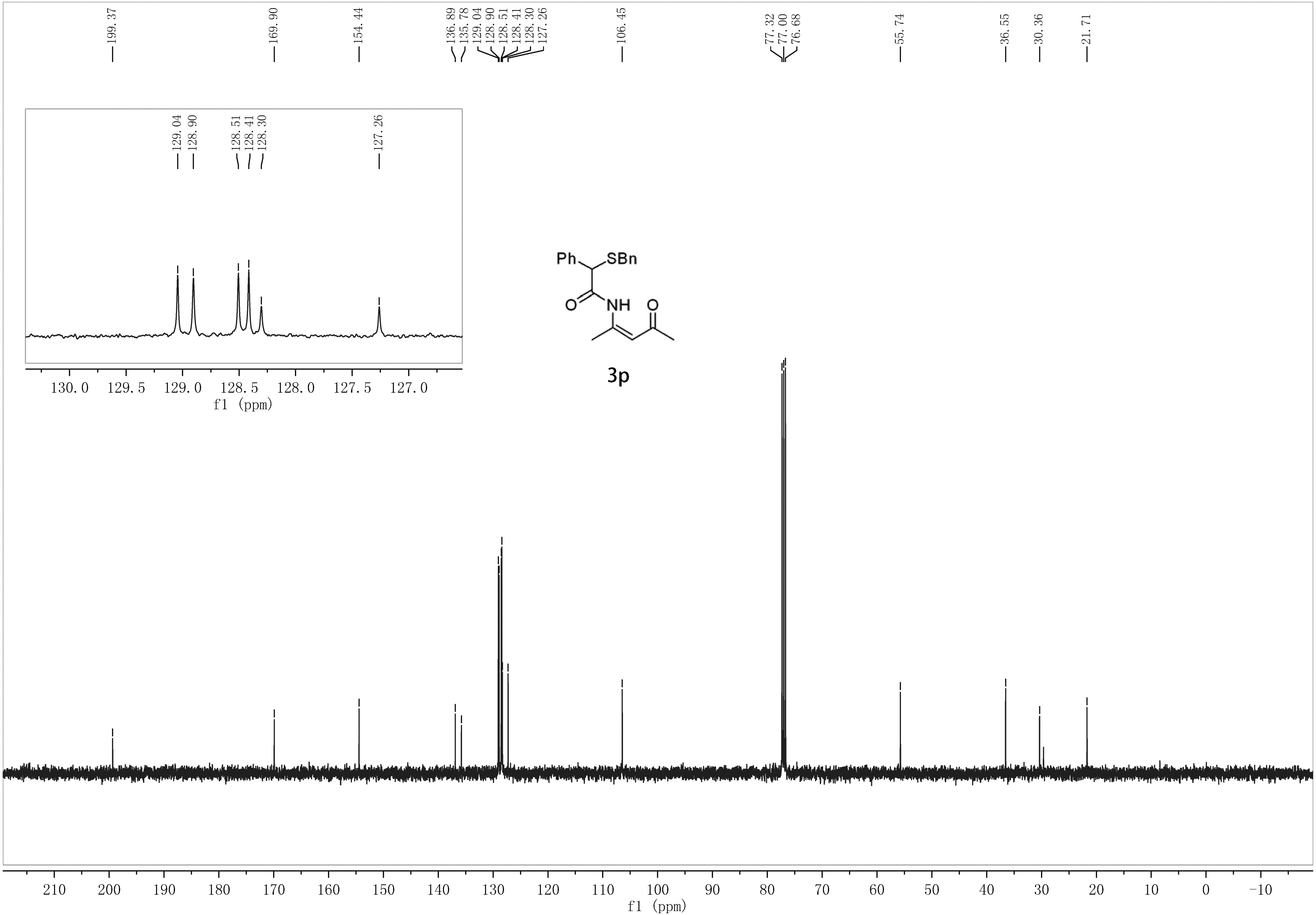
7.457
7.395
7.378
7.359
7.342
7.322
7.313
7.267
7.220
5.344
4.452
3.816
3.782
3.729
3.695
2.318
2.151
Ph
SBn
O
NH
O
3p
0.96
1.95
7.10
1.04
1.00
0.98
2.00
3.05
2.99
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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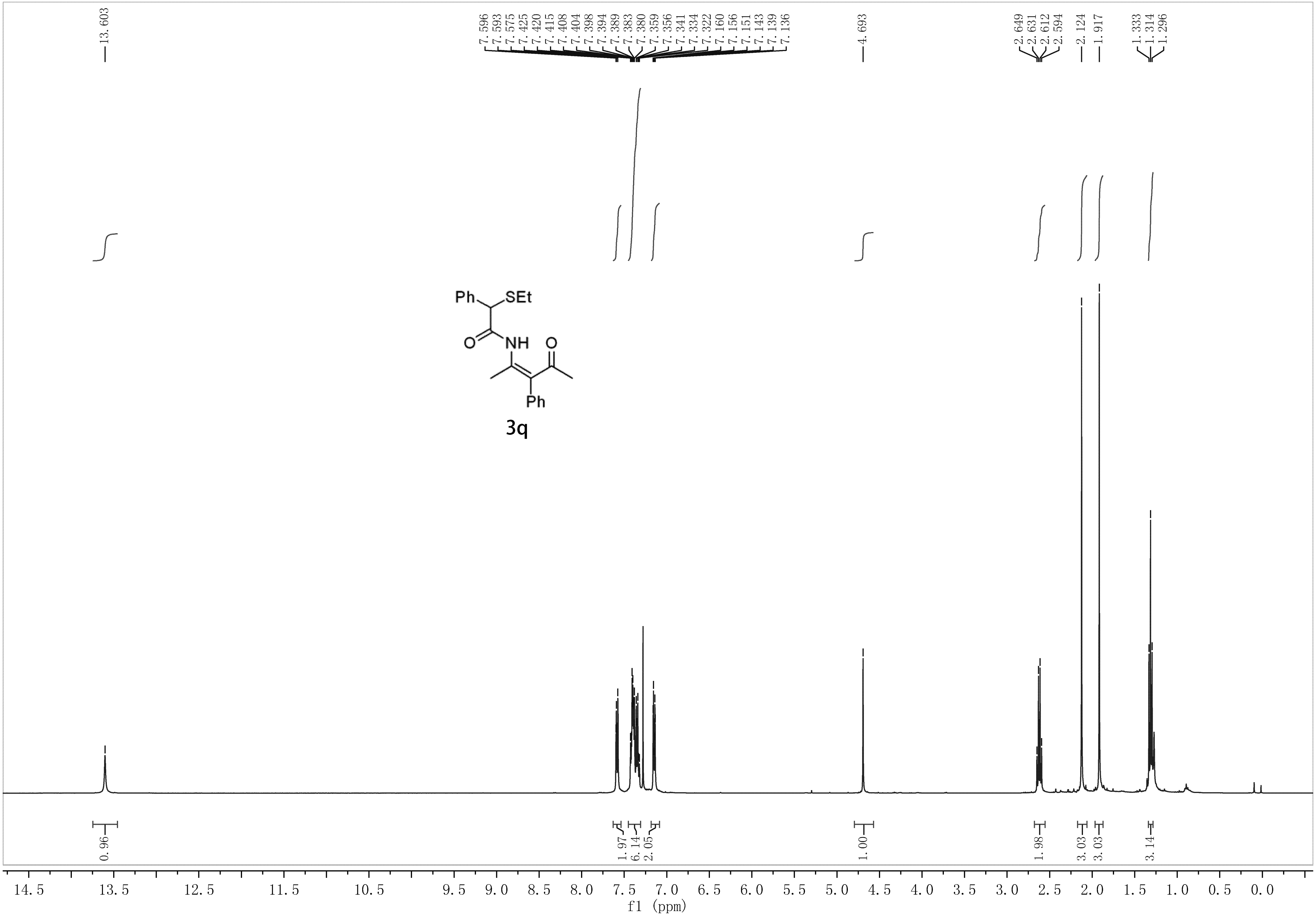
169.90
154.44
136.89
135.78
129.04
128.90
128.51
128.41
128.30
127.26
106.45
77.32
77.00
76.68
55.74
36.55
30.36
21.71
130.0
129.5
129.0
128.5
128.0
127.5
127.0
f1 (ppm)
Ph
SBn
O
NH
O
3p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)



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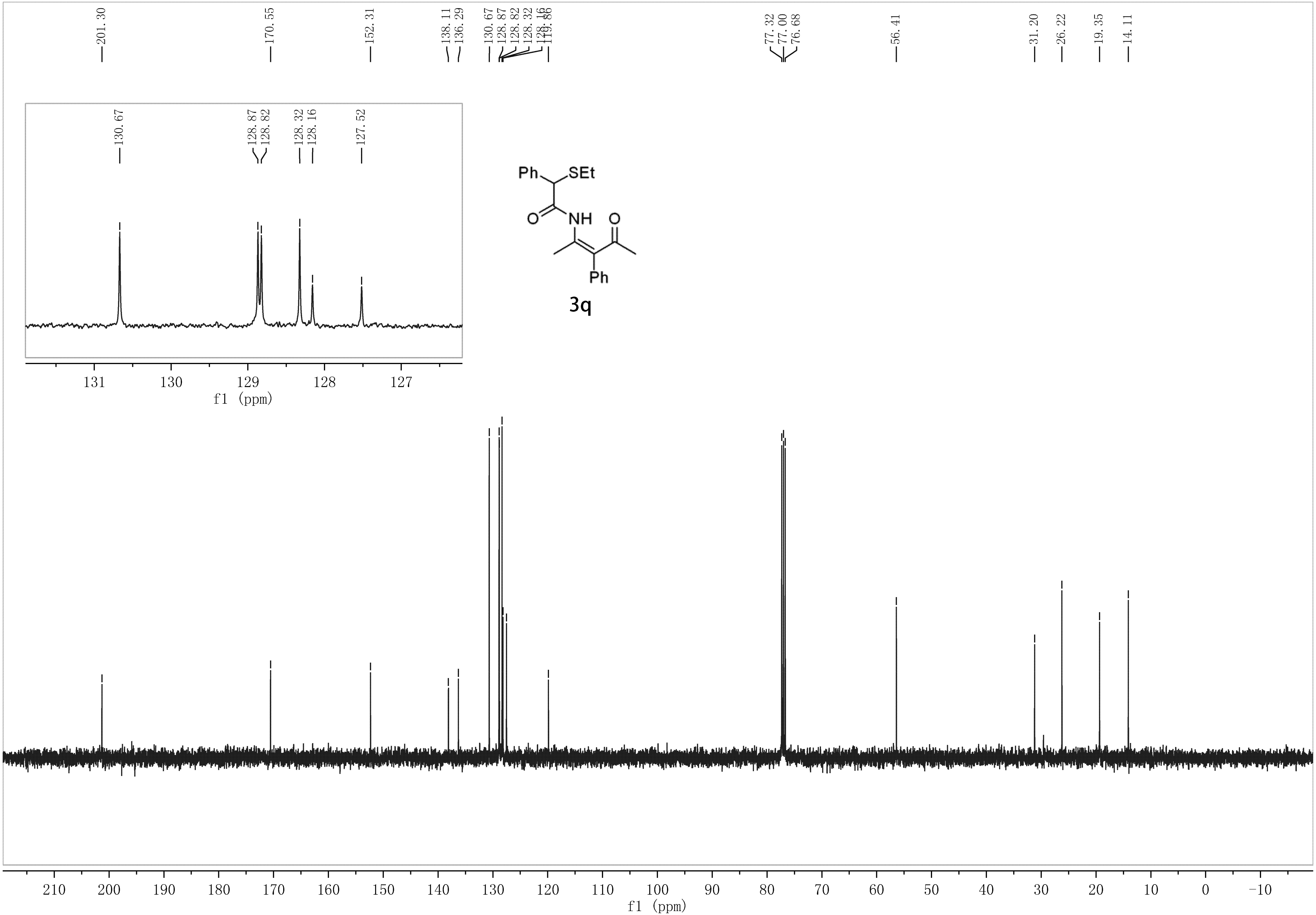
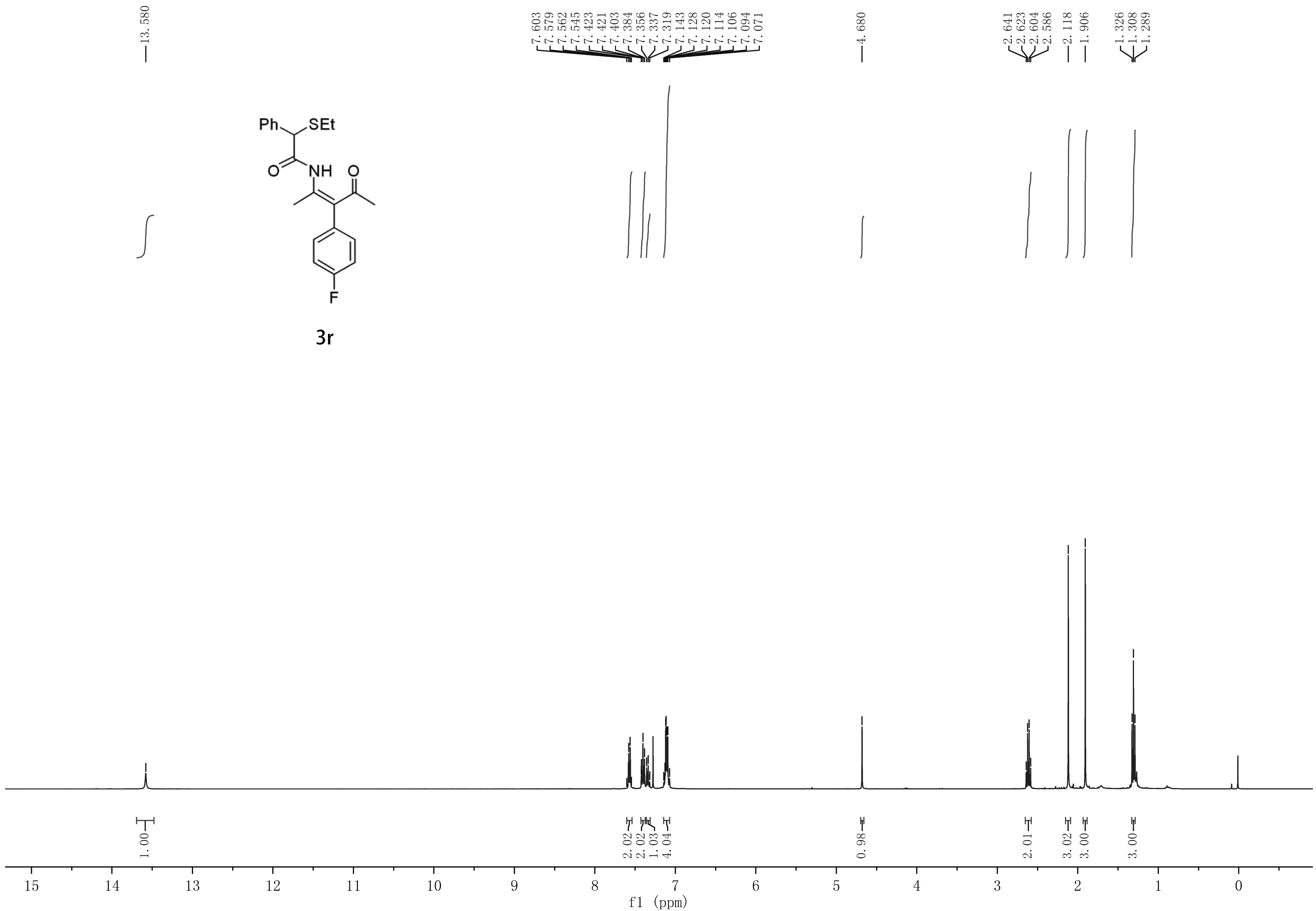
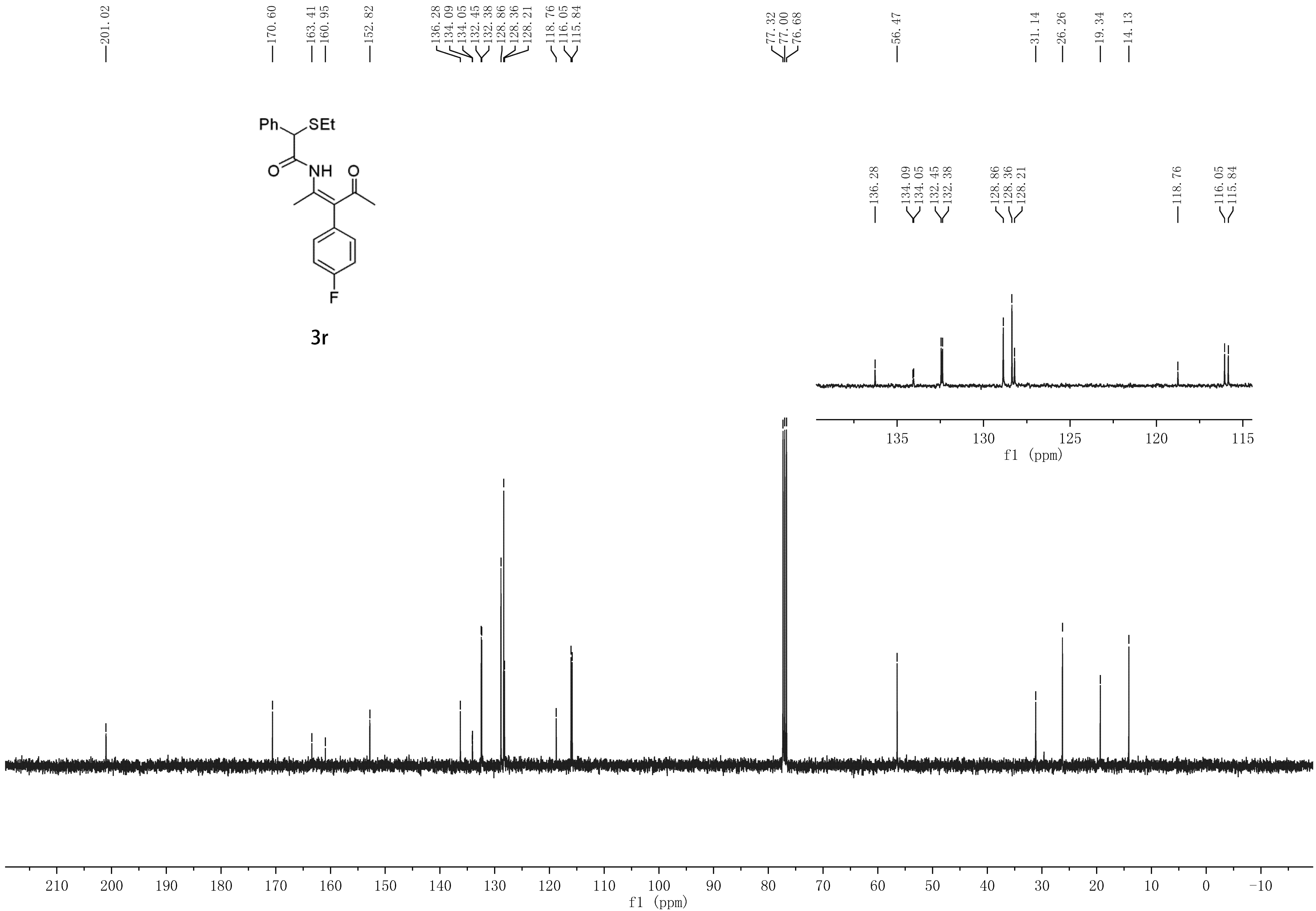
7.596
7.593
7.575
7.425
7.420
7.415
7.408
7.404
7.398
7.394
7.389
7.383
7.380
7.359
7.356
7.341
7.334
7.322
7.160
7.156
7.151
7.143
7.139
7.136
4.693
2.649
2.631
2.612
2.594
2.124
1.917
1.333
1.314
1.296
Ph
SEt
O
NH
O
Ph
3q
0.96
1.97
6.14
2.05
1.00
1.98
3.03
3.03
3.14
14.5 13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


201.30
170.55
152.31
138.11
136.29
130.67
128.87
128.82
128.32
128.16
119.86
77.32
77.00
76.68
56.41
31.20
26.22
19.35
14.11
130.67
128.87
128.82
128.32
128.16
127.52
131
130
129
128
127
f1 (ppm)
Ph
SEt
O
NH
O
Ph
3q
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)



13.580
7.603
7.579
7.562
7.545
7.423
7.421
7.403
7.384
7.356
7.337
7.319
7.143
7.128
7.120
7.114
7.106
7.094
7.071
4.680
2.641
2.623
2.604
2.586
2.118
1.906
1.326
1.308
1.289
Ph
SEt
O
NH
O
F
3r
1.00
2.02
2.02
1.03
4.04
0.98
2.01
3.02
3.00
3.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)



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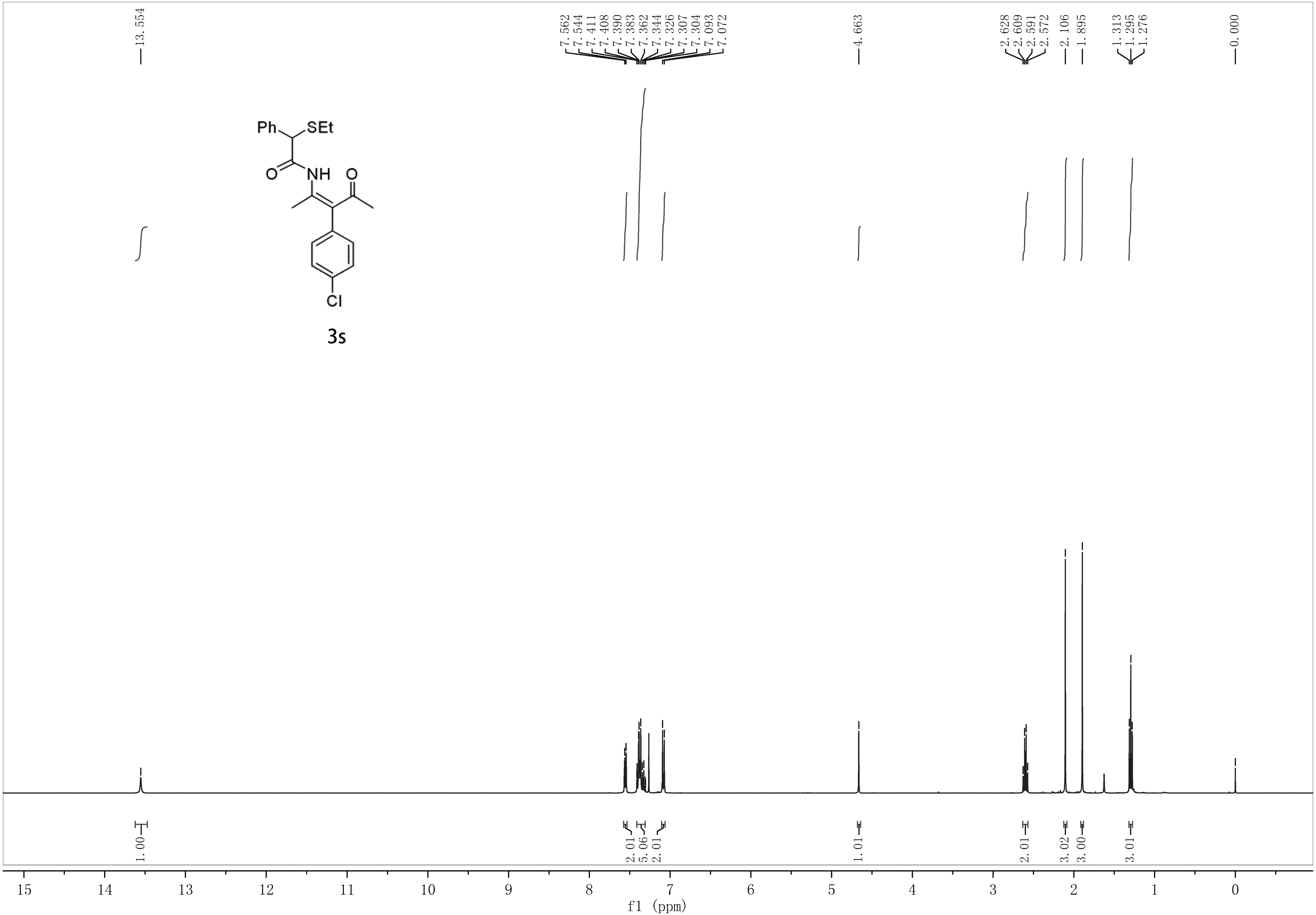
170.60
163.41
160.95
152.82
136.28
134.09
134.05
132.45
132.38
128.86
128.36
128.21
118.76
116.05
115.84
77.32
77.00
76.68
56.47
31.14
26.26
19.34
14.13
Ph
SEt
O
NH
O
F
3r
f1 (ppm)



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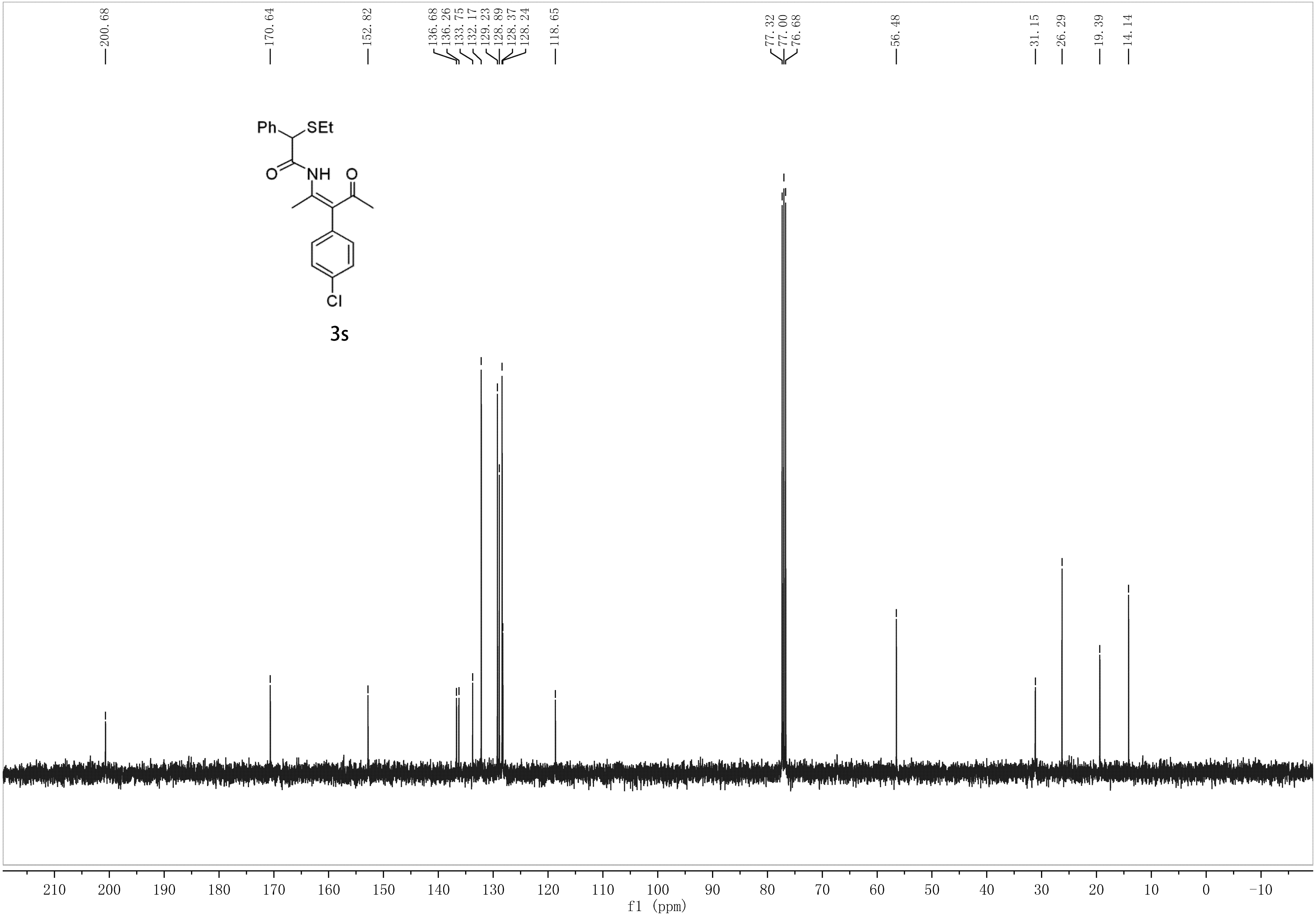
7.562
7.544
7.411
7.408
7.390
7.383
7.362
7.344
7.326
7.307
7.304
7.093
7.072
4.663
2.628
2.609
2.591
2.572
2.106
1.895
1.313
1.295
1.276
0.000
Ph
SEt
O
NH
O
Cl
3s
1.00
2.01
5.06
2.01
1.01
2.01
3.02
3.00
3.01
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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136.26
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129.23
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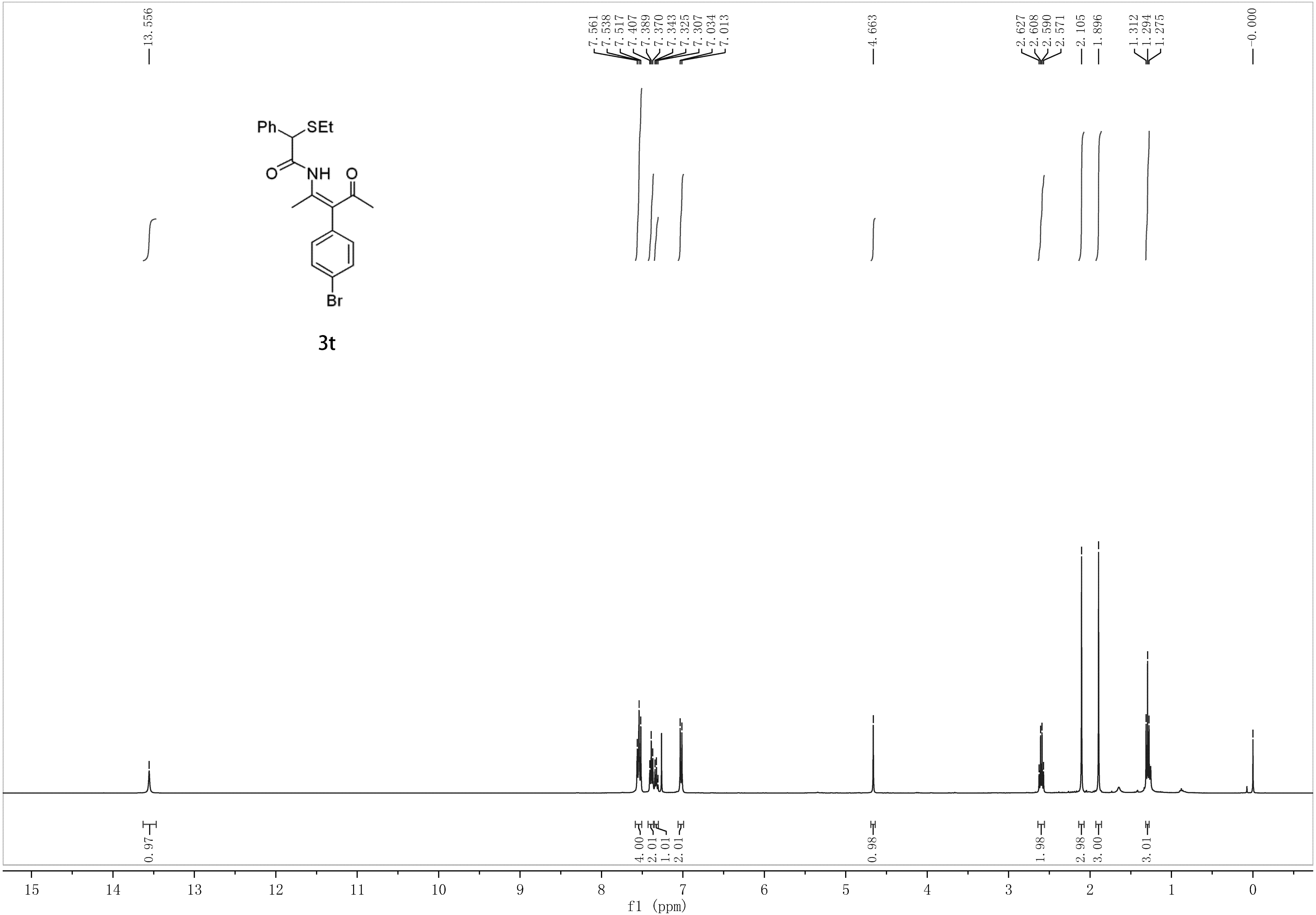
128.37
128.24
118.65
77.32
77.00
76.68
56.48
31.15
26.29
19.39
14.14
Ph
SEt
O
NH
O
Cl
3s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.517
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7.343
7.325
7.307
7.034
7.013
4.663
2.627
2.608
2.590
2.571
2.105
1.896
1.312
1.294
1.275
-0.000
Ph
SEt
O
NH
O
Br
3t
0.97
4.00
2.01
1.01
2.01
0.98
1.98
2.98
3.00
3.01
15
14
13
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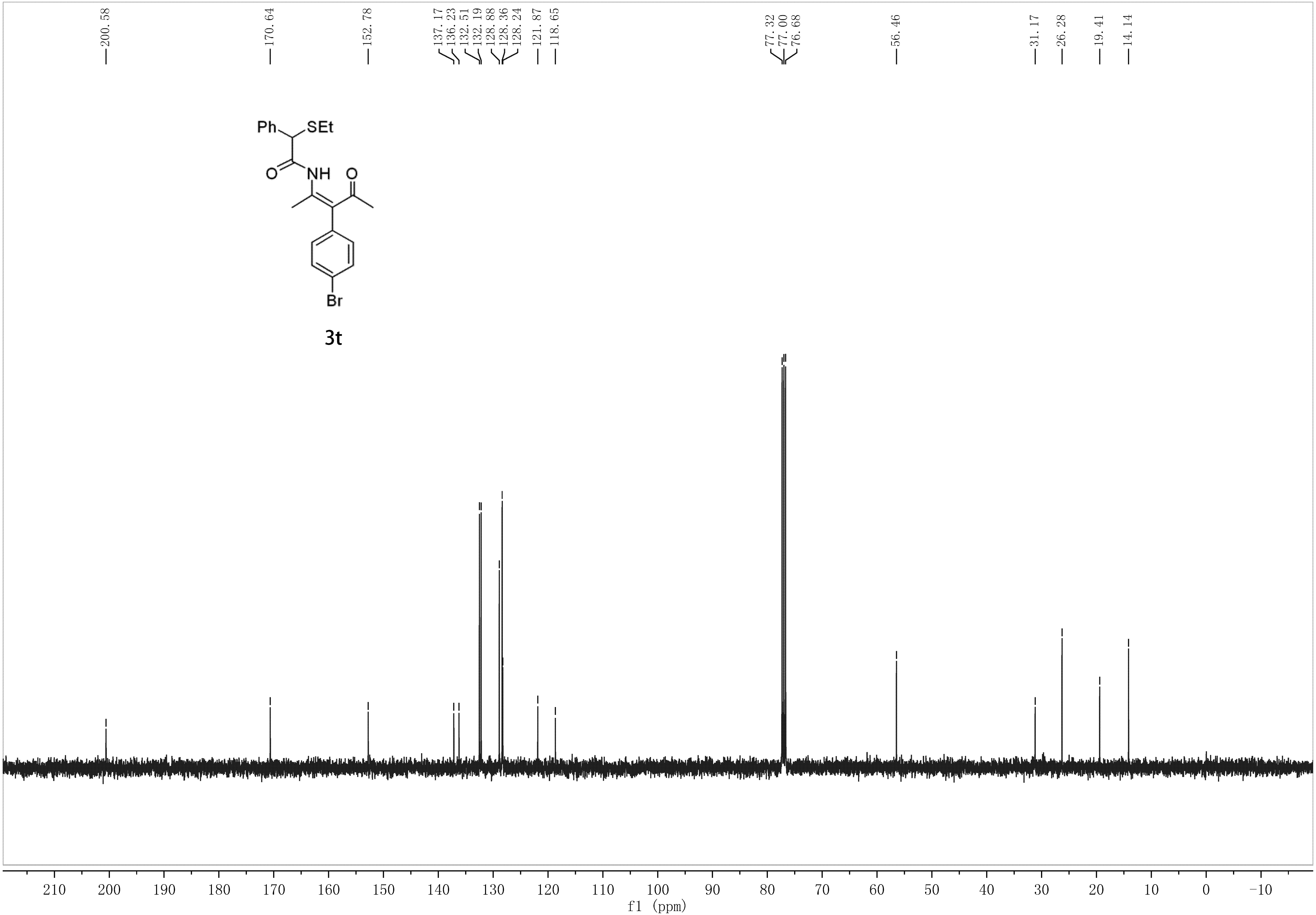
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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132.19
128.88
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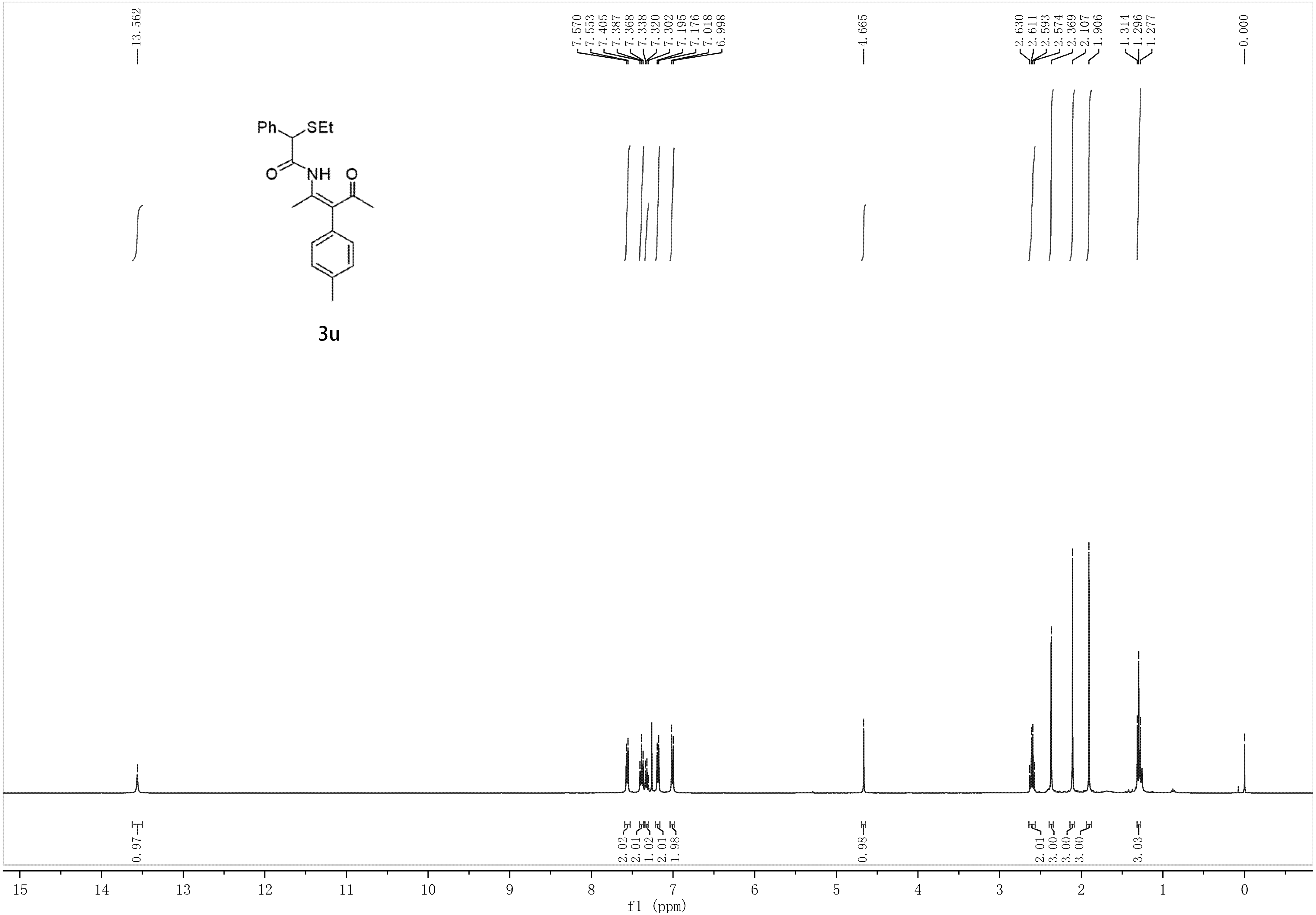
128.24
121.87
118.65
77.32
77.00
76.68
56.46
31.17
26.28
19.41
14.14
Ph
SEt
O
NH
O
Br
3t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)



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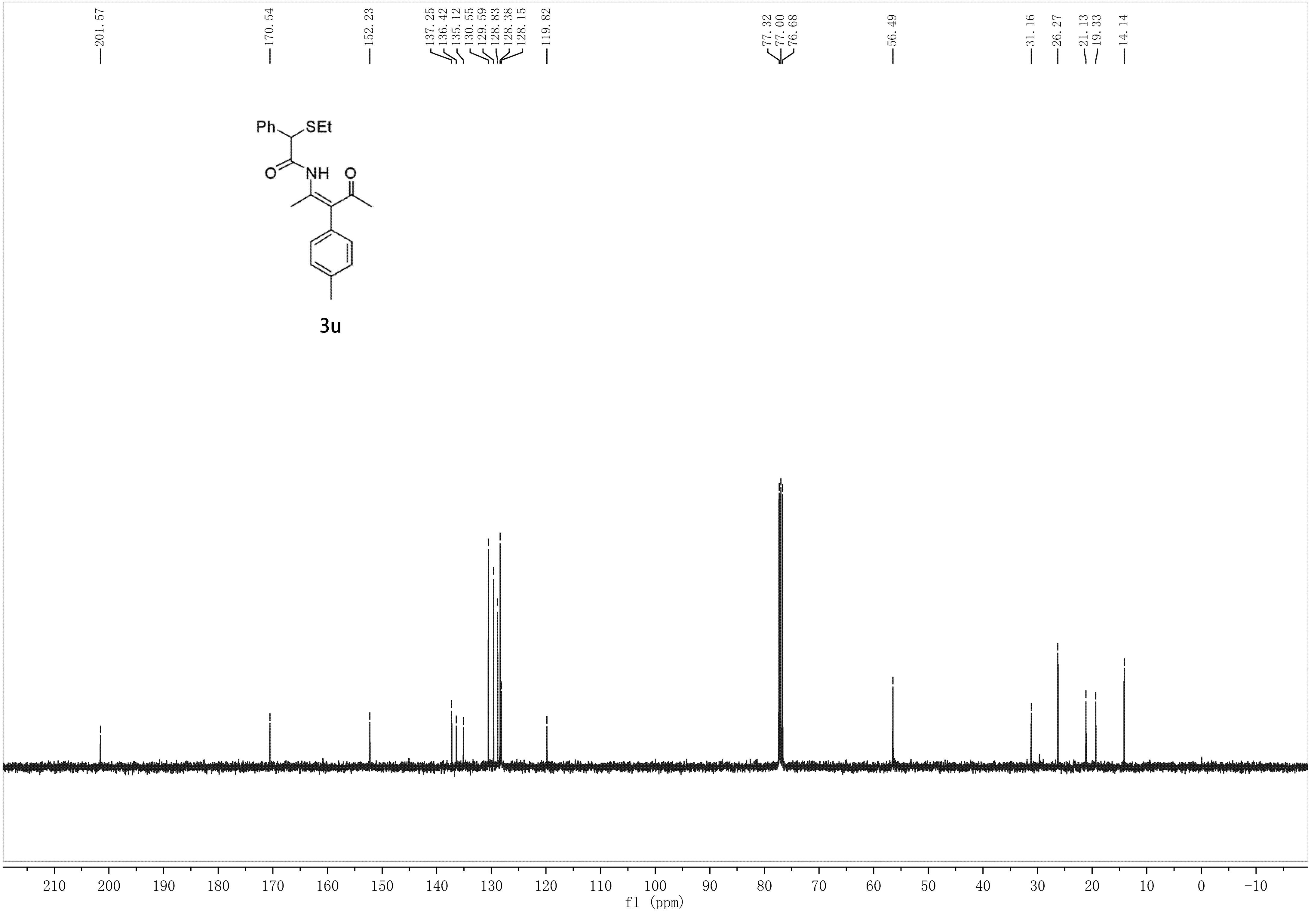
7.570
7.553
7.405
7.387
7.368
7.338
7.320
7.302
7.195
7.176
7.018
6.998
4.665
2.630
2.611
2.593
2.574
2.369
2.107
1.906
1.314
1.296
1.277
0.000
Ph
SEt
O
NH
O
3u
0.97
2.02
2.01
1.02
2.01
1.98
0.98
2.01
3.00
3.00
3.00
3.03
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)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136.42
135.12
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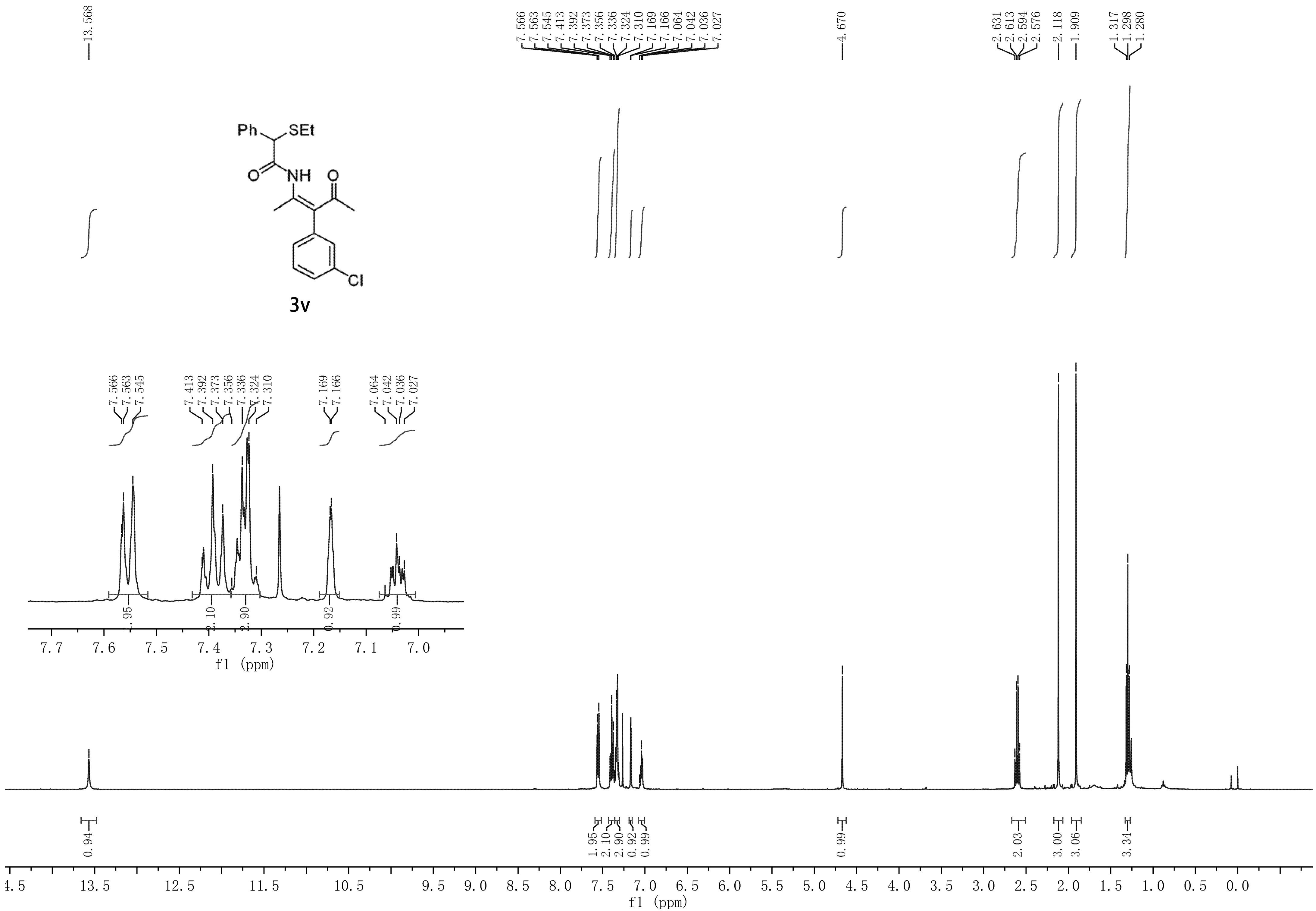
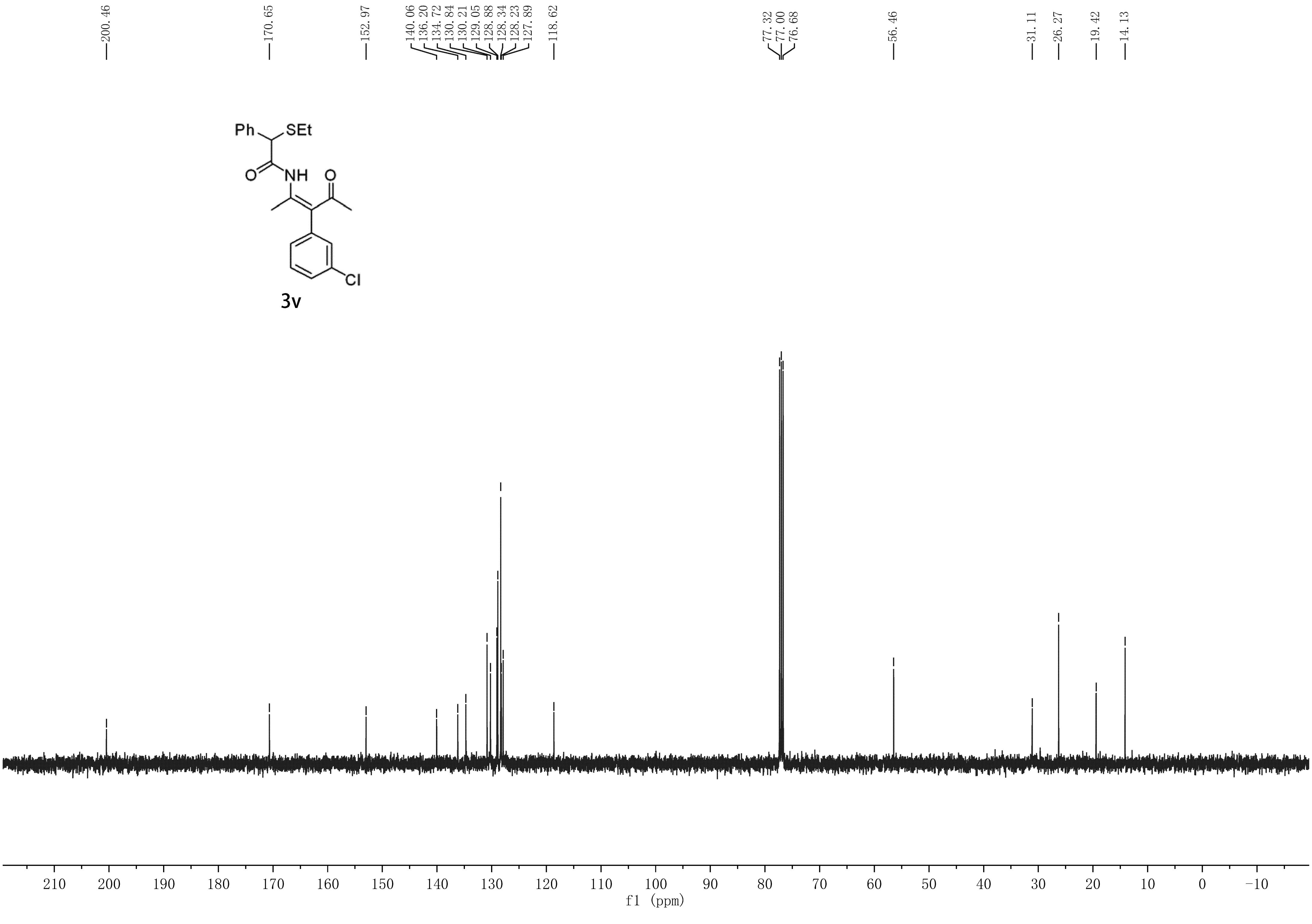
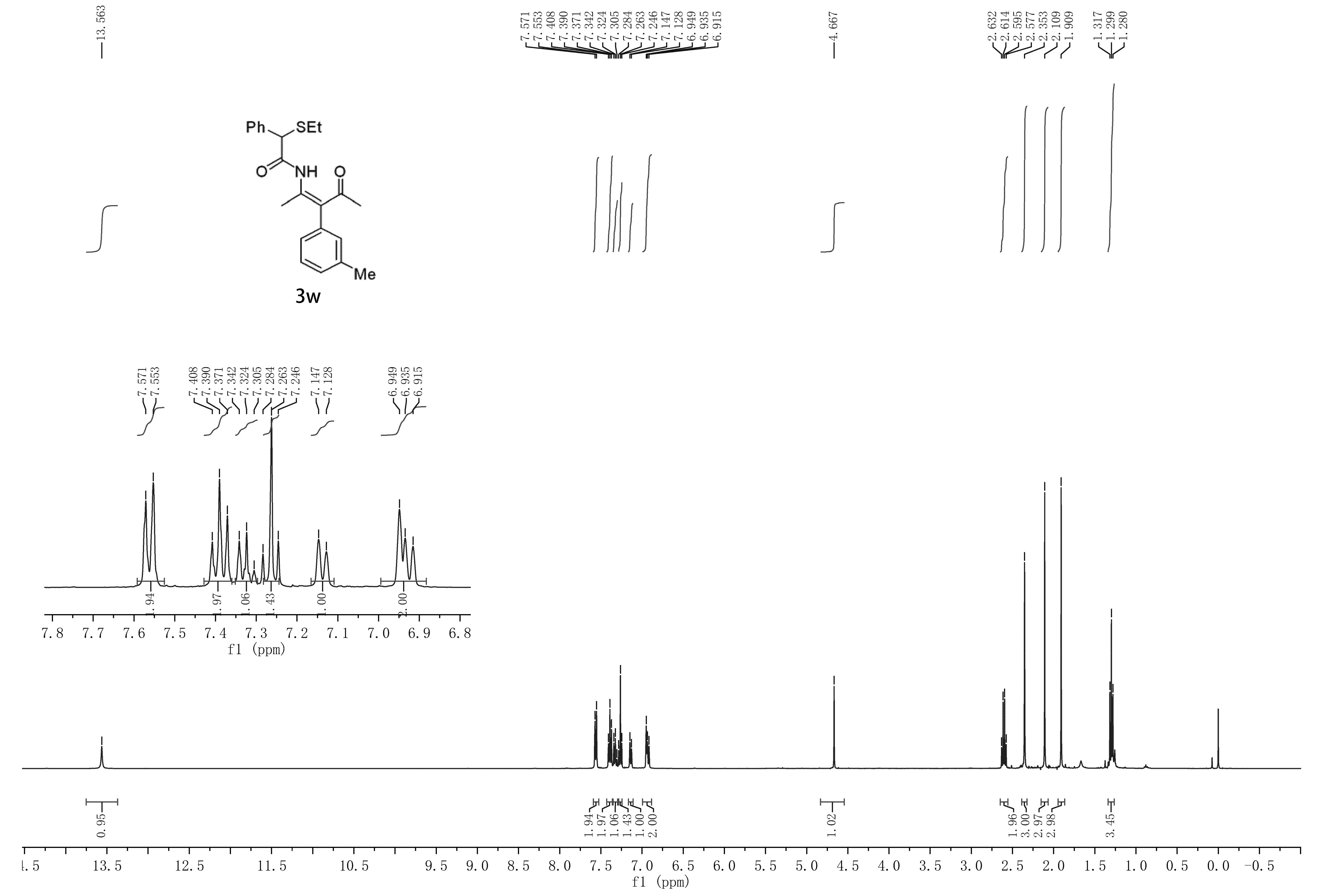
129.59
128.83
128.38
128.15
119.82
77.32
77.00
76.68
56.49
31.16
26.27
21.13
19.33
14.14
Ph
SEt
O
NH
O
3u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

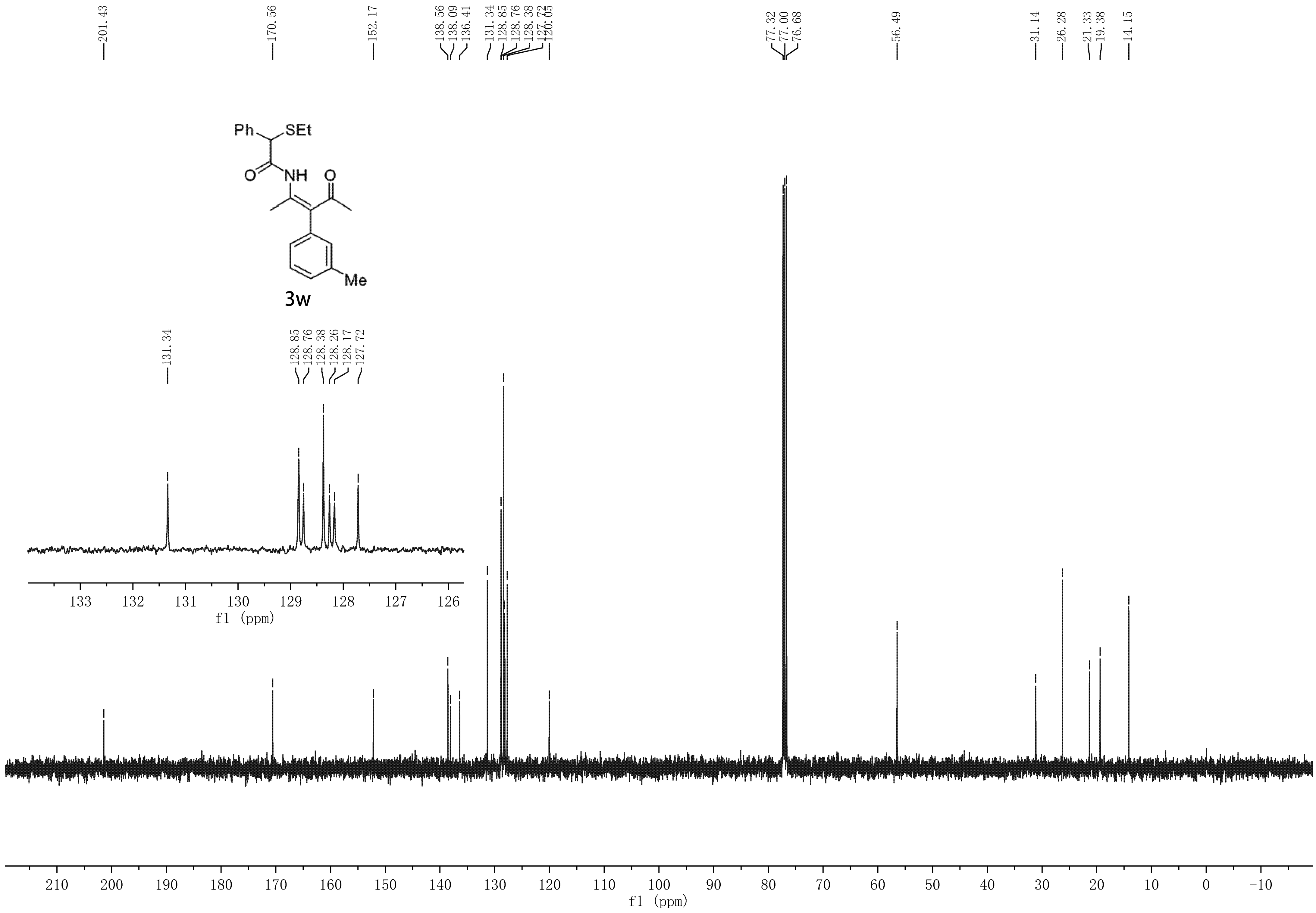

13.568
7.566 7.563 7.545 7.413 7.392 7.373 7.356 7.336 7.324 7.310 7.169 7.166 7.064 7.042 7.036 7.027
4.670
2.631 2.613 2.594 2.576
2.118
1.909
1.317 1.298 1.280
Ph
SEt
O
NH
O
Cl
3v
1.95
2.10
2.90
0.92
0.99
f1 (ppm)
0.94
1.95 2.10 2.90 0.92 0.99
0.99
2.03
3.00
3.06
3.34
f1 (ppm)



200.46
170.65
152.97
140.06
136.20
134.72
130.84
130.21
129.05
128.88
128.34
128.23
127.89
118.62
77.32
77.00
76.68
56.46
31.11
26.27
19.42
14.13
Ph
SEt
O
NH
O
Cl
3v
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)



13.563
7.571 7.553 7.408 7.390 7.371 7.342 7.324 7.305 7.284 7.263 7.246 7.147 7.128 6.949 6.935 6.915
4.667
2.632 2.614 2.595 2.577 2.353 2.109 1.909
1.317 1.299 1.280
Ph
SEt
O
NH
O
Me
3w
0.95
1.94 1.97 1.06 1.43 1.00 2.00
1.02
1.96 3.00 2.97 2.98
3.45
f1 (ppm)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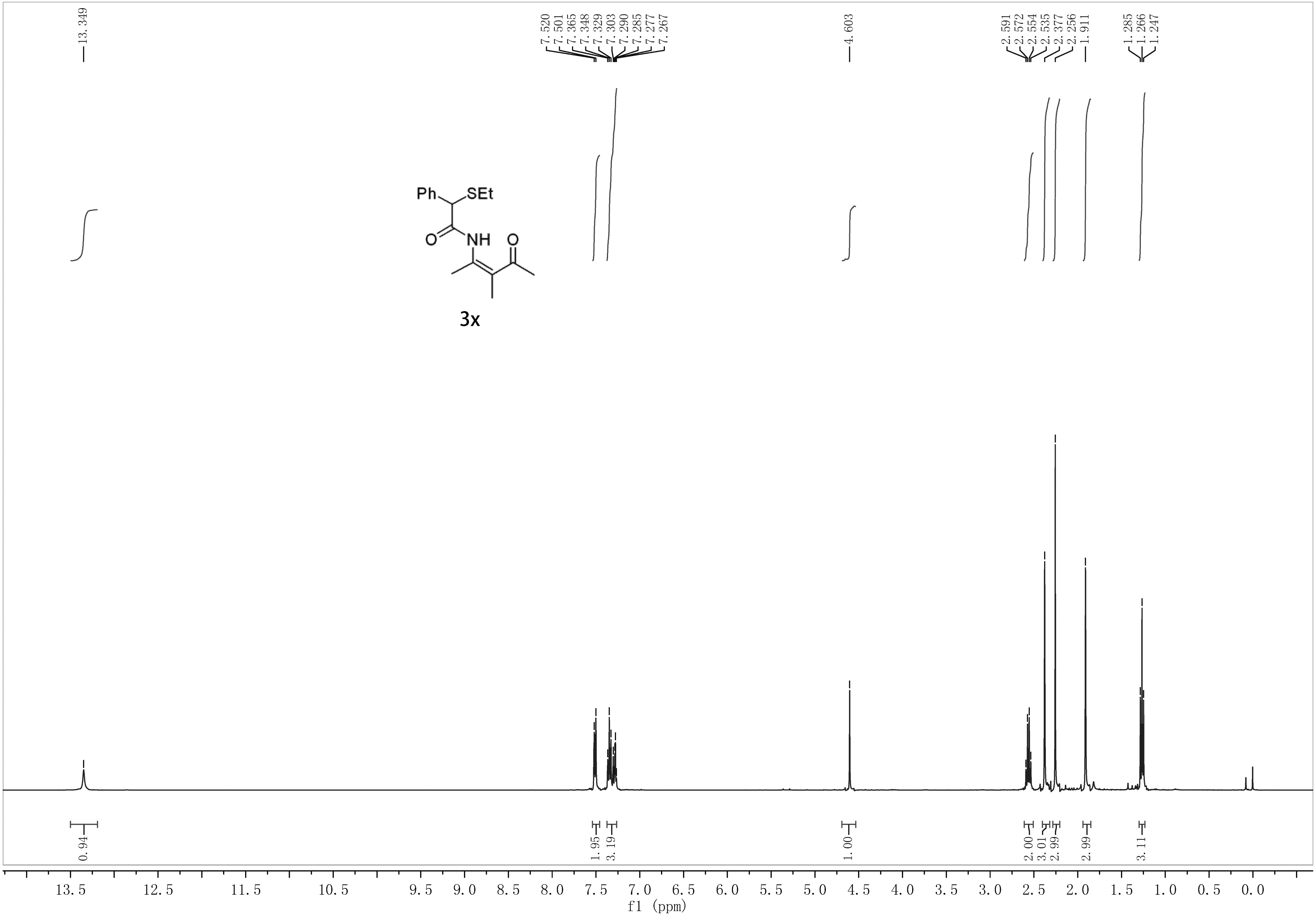
136.41
131.34
128.85
128.76
128.38
127.72
120.05
77.32
77.00
76.68
56.49
31.14
26.28
21.33
19.38
14.15
Ph
SEt
O
NH
O
Me
3w
131.34
128.85
128.76
128.38
128.26
128.17
127.72
133 132 131 130 129 128 127 126
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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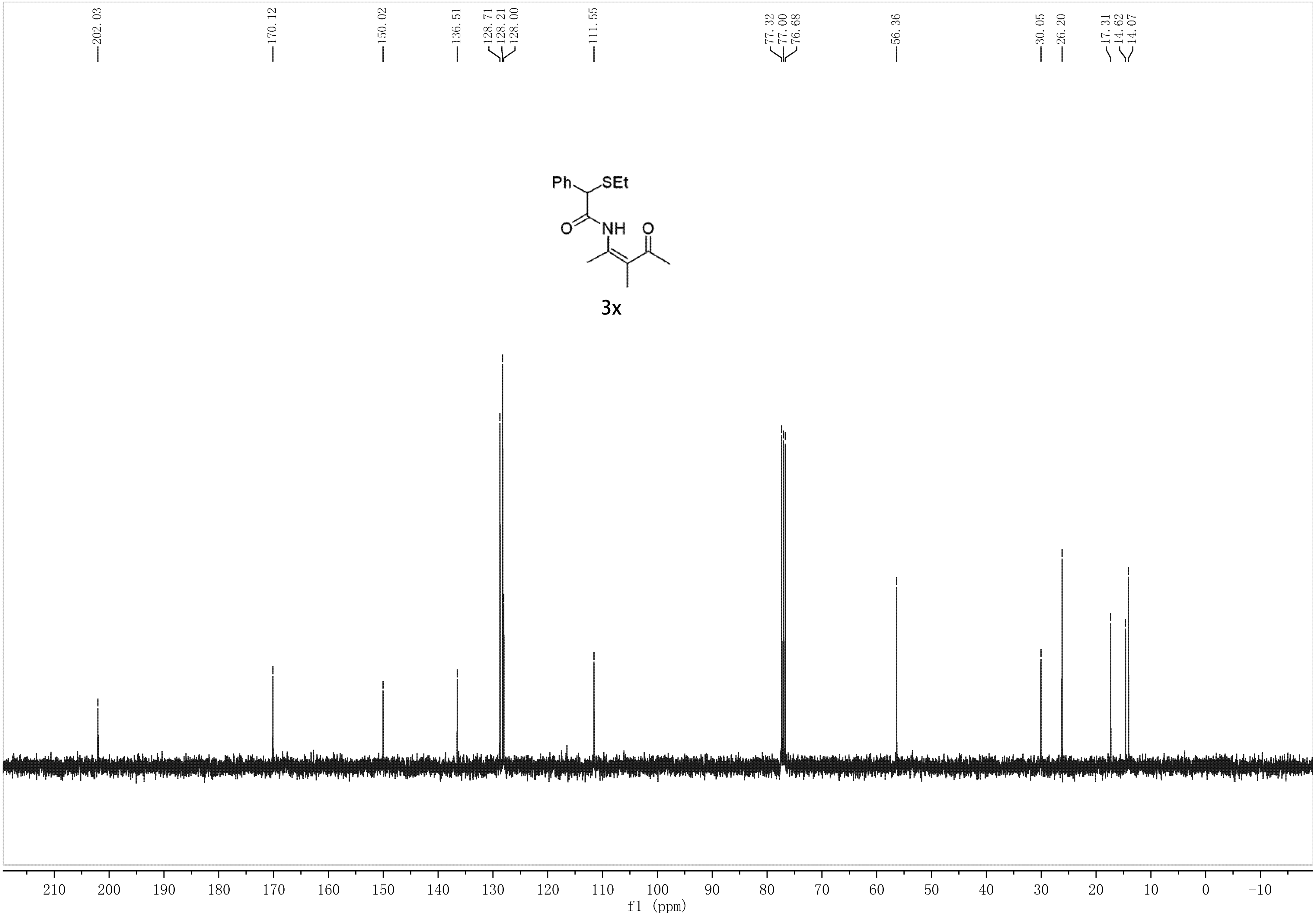
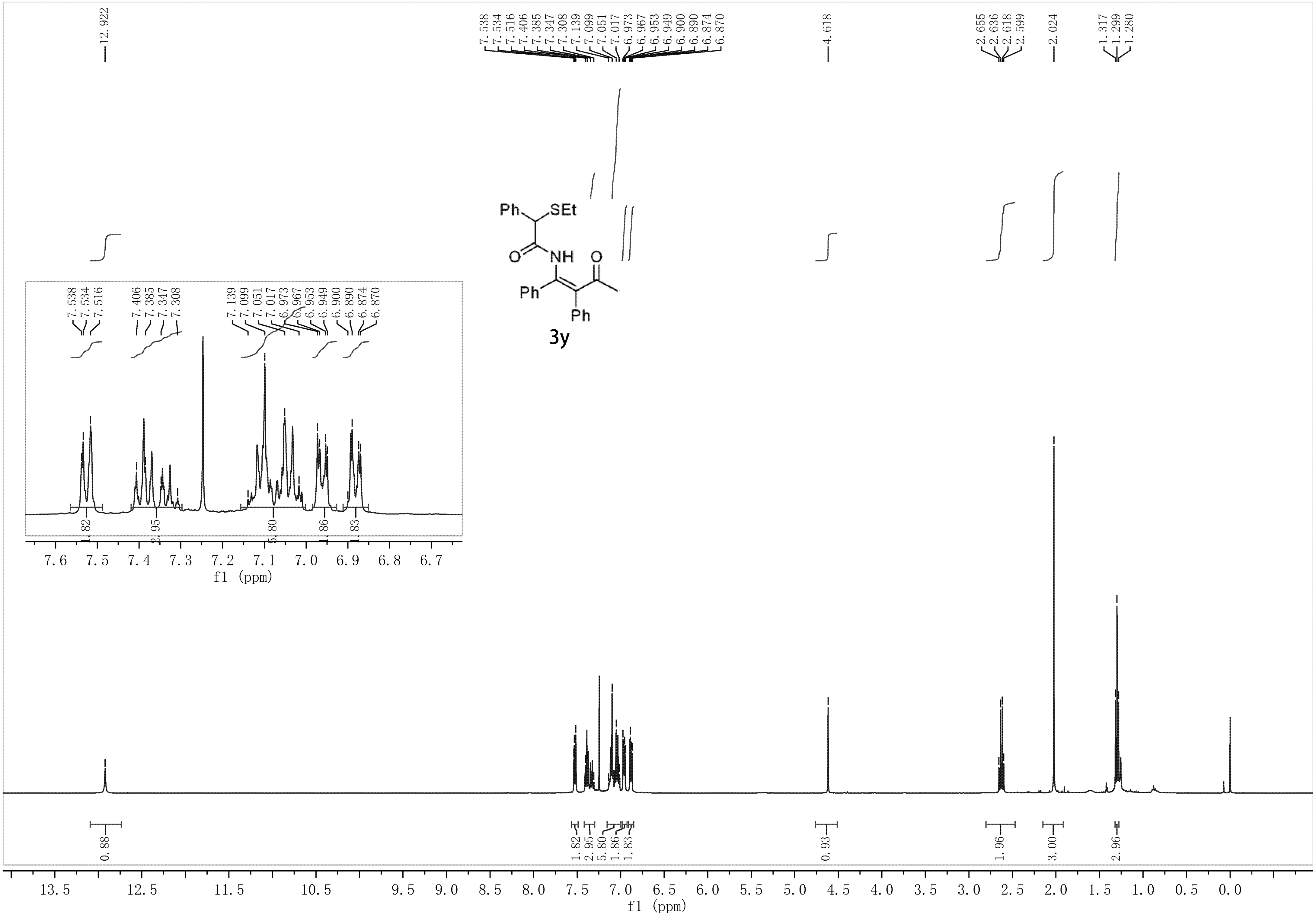
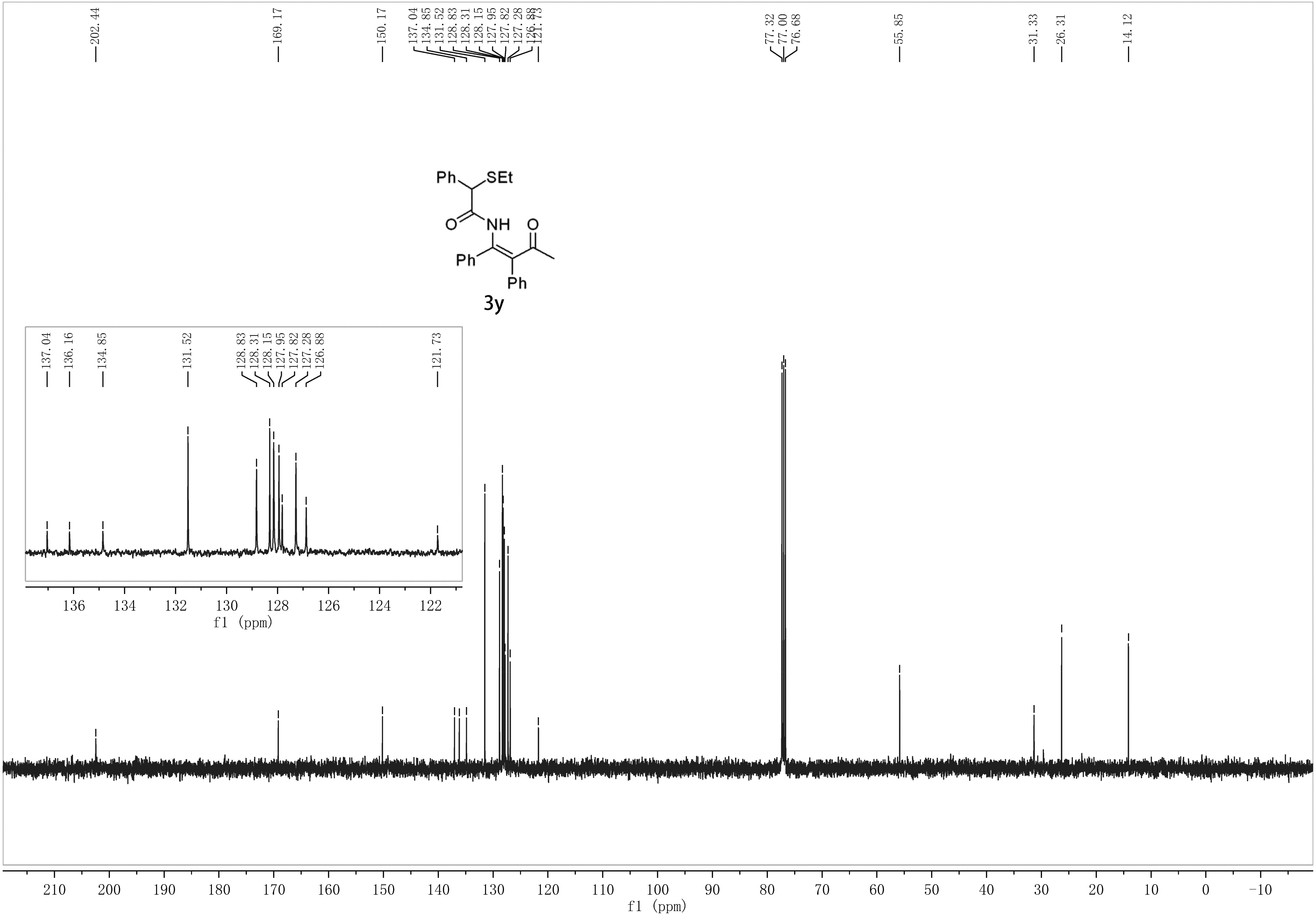
7.365
7.348
7.329
7.303
7.290
7.285
7.277
7.267
4.603
2.591
2.572
2.554
2.535
2.377
2.256
1.911
1.285
1.266
1.247
Ph
SEt
O
NH
O
3x
0.94
1.95
3.19
1.00
2.00
3.01
2.99
2.99
3.11
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

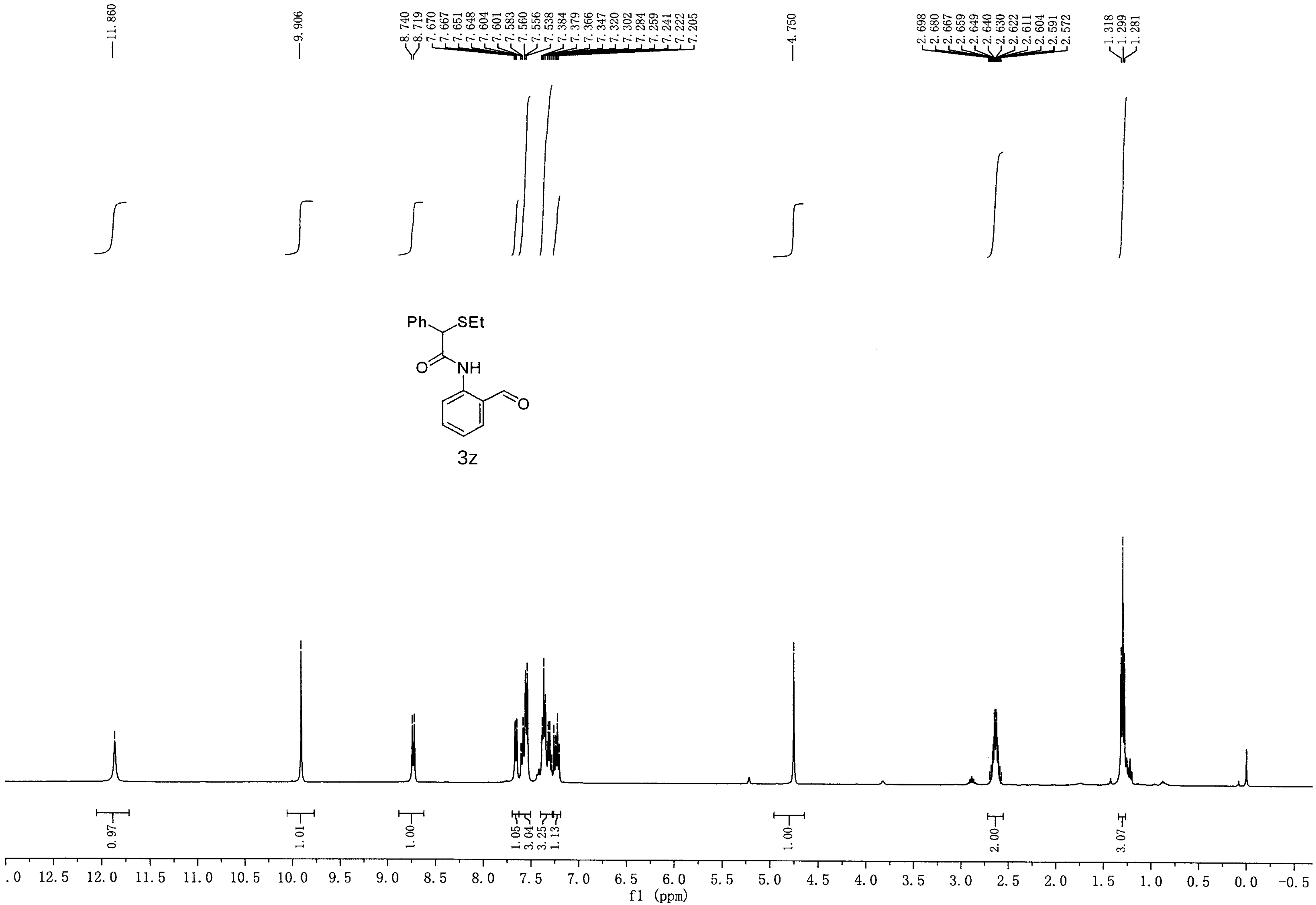


202.03
170.12
150.02
136.51
128.71
128.21
128.00
111.55
77.32
77.00
76.68
56.36
30.05
26.20
17.31
14.62
14.07
Ph
SEt
O
NH
O
3x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



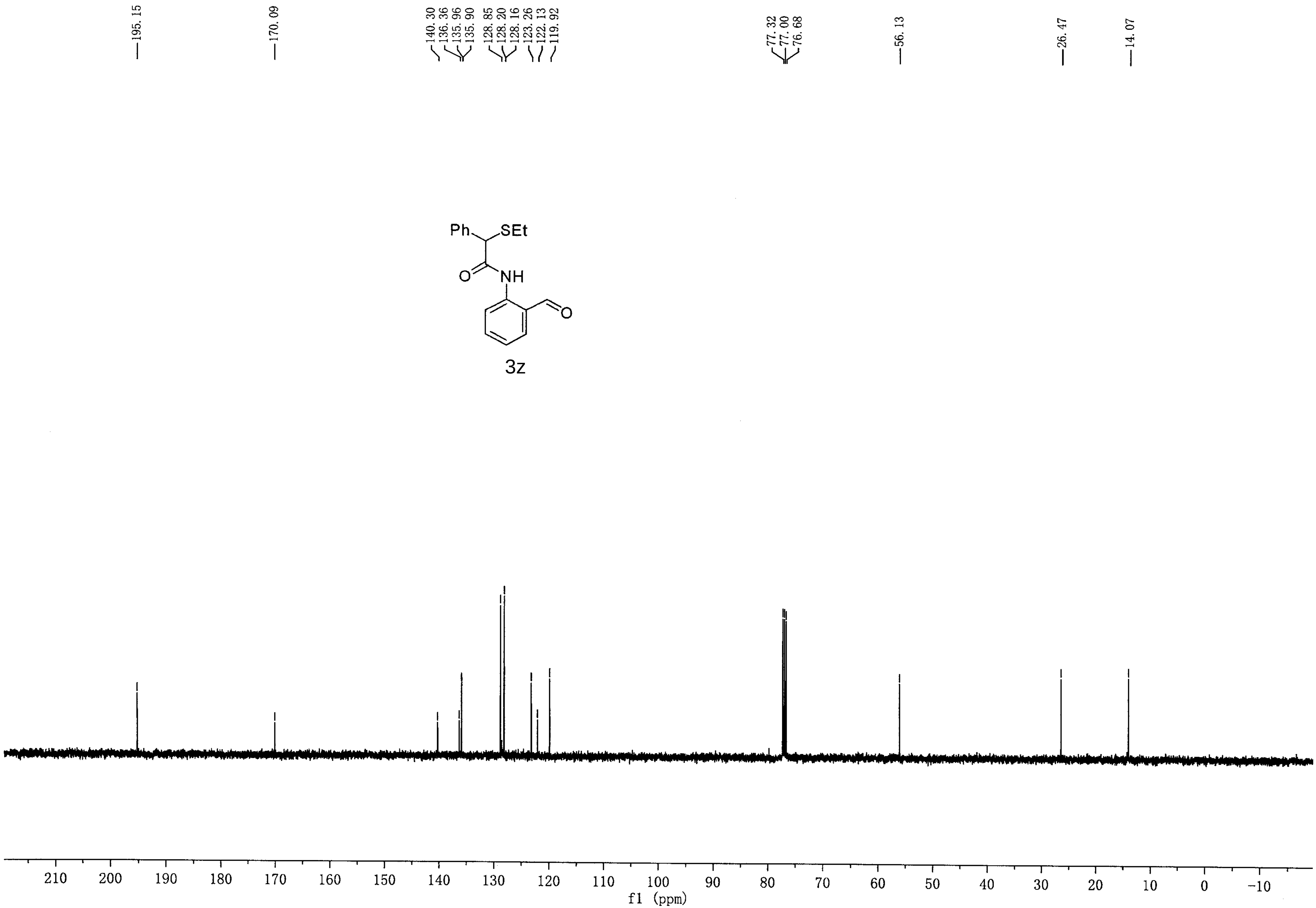
12.922
7.538 7.534 7.516 7.406 7.385 7.347 7.308 7.139 7.099 7.051 7.017 6.973 6.967 6.953 6.949 6.900 6.890 6.874 6.870
4.618
2.655 2.636 2.618 2.599
2.024
1.317 1.299 1.280
Ph
SEt
O
NH
O
Ph
Ph
3y
0.88
1.82
2.95
5.80
1.86
1.83
0.93
1.96
3.00
2.96
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

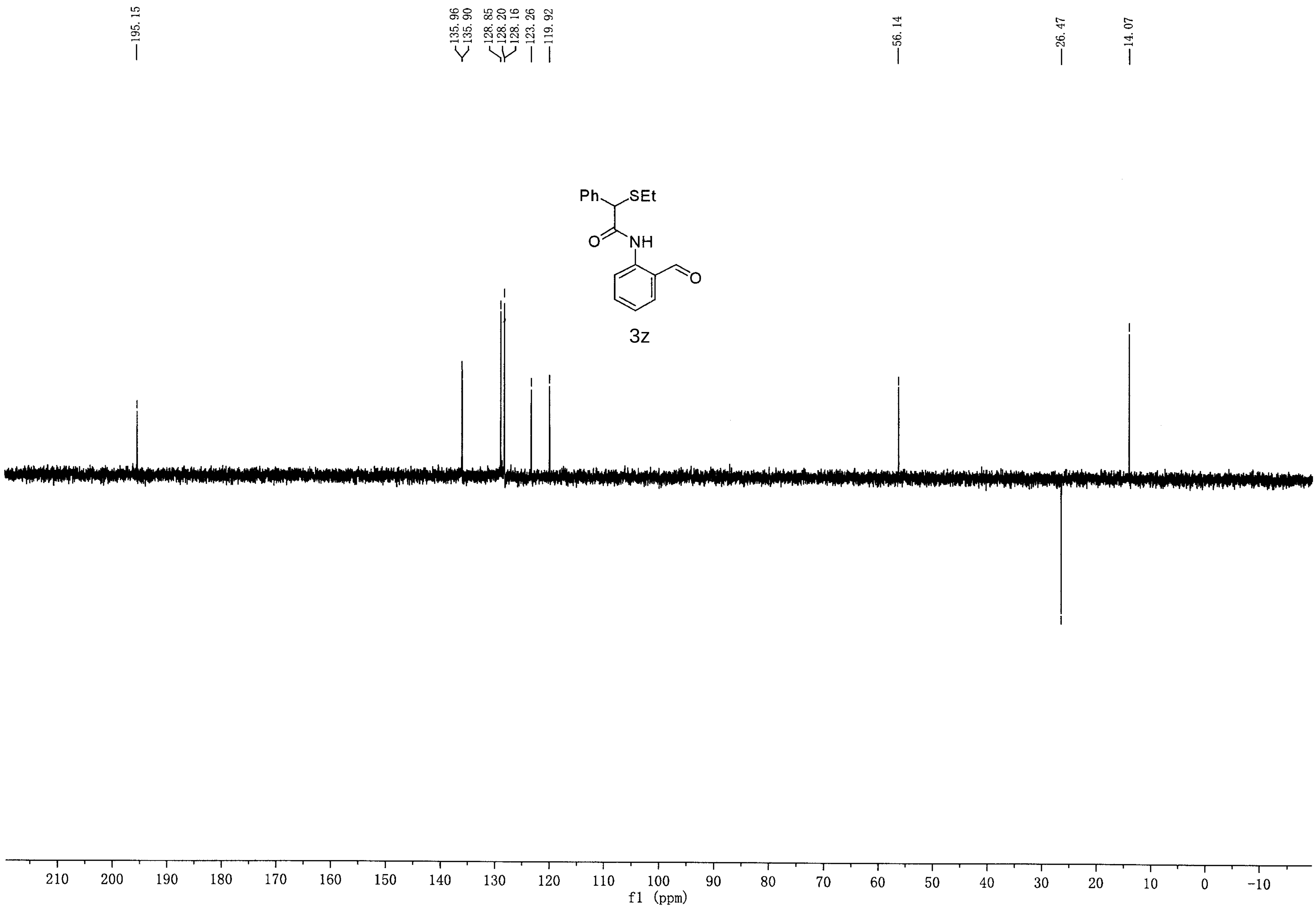

202.44
169.17
150.17
137.04
134.85
131.52
128.83
128.31
128.15
127.95
127.82
127.28
126.88
121.73
77.32
77.00
76.68
55.85
31.33
26.31
14.12
Ph
SEt
O
NH
O
Ph
Ph
3y
137.04
136.16
134.85
131.52
128.83
128.31
128.15
127.95
127.82
127.28
126.88
121.73
136
134
132
130
128
126
124
122
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

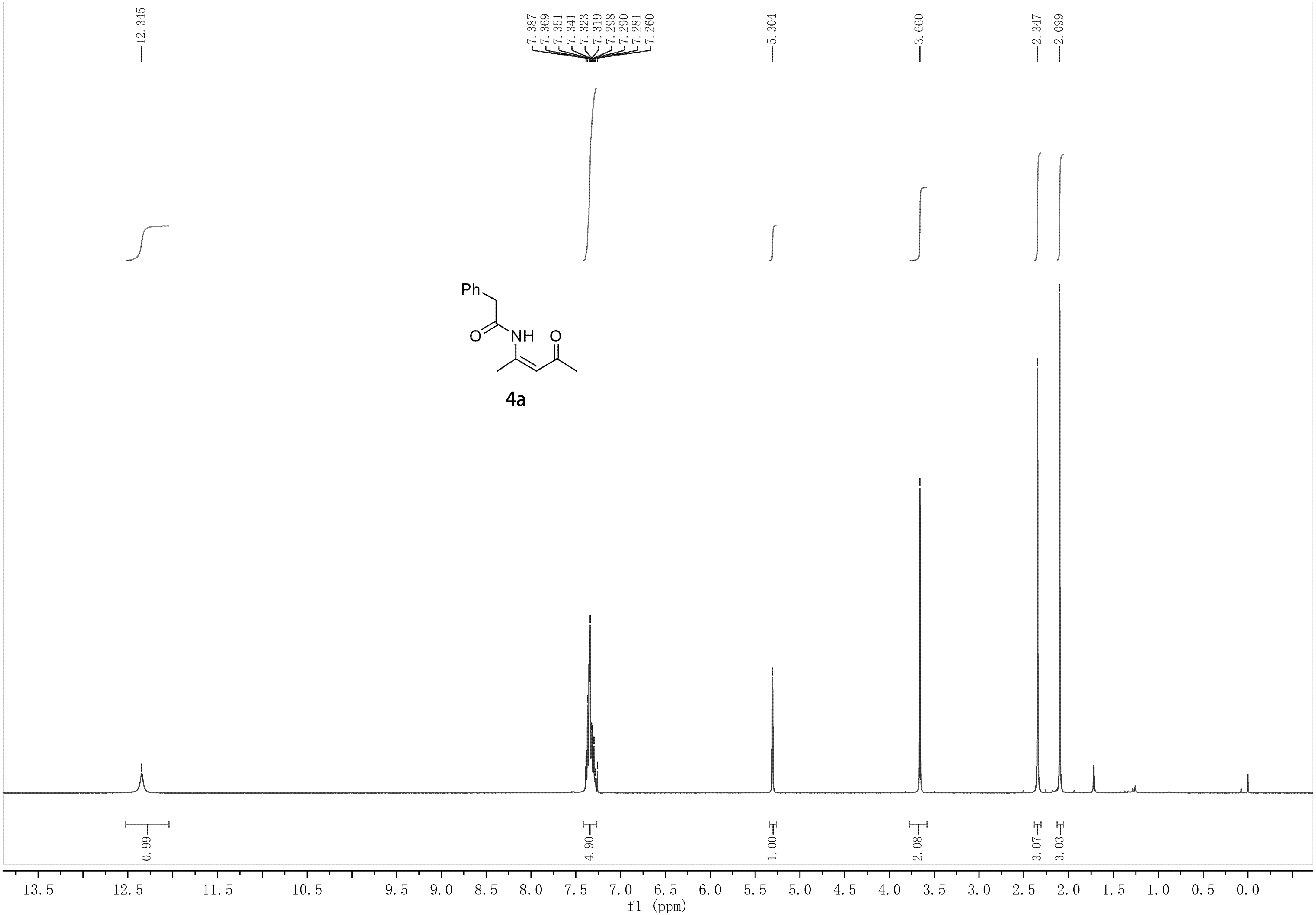


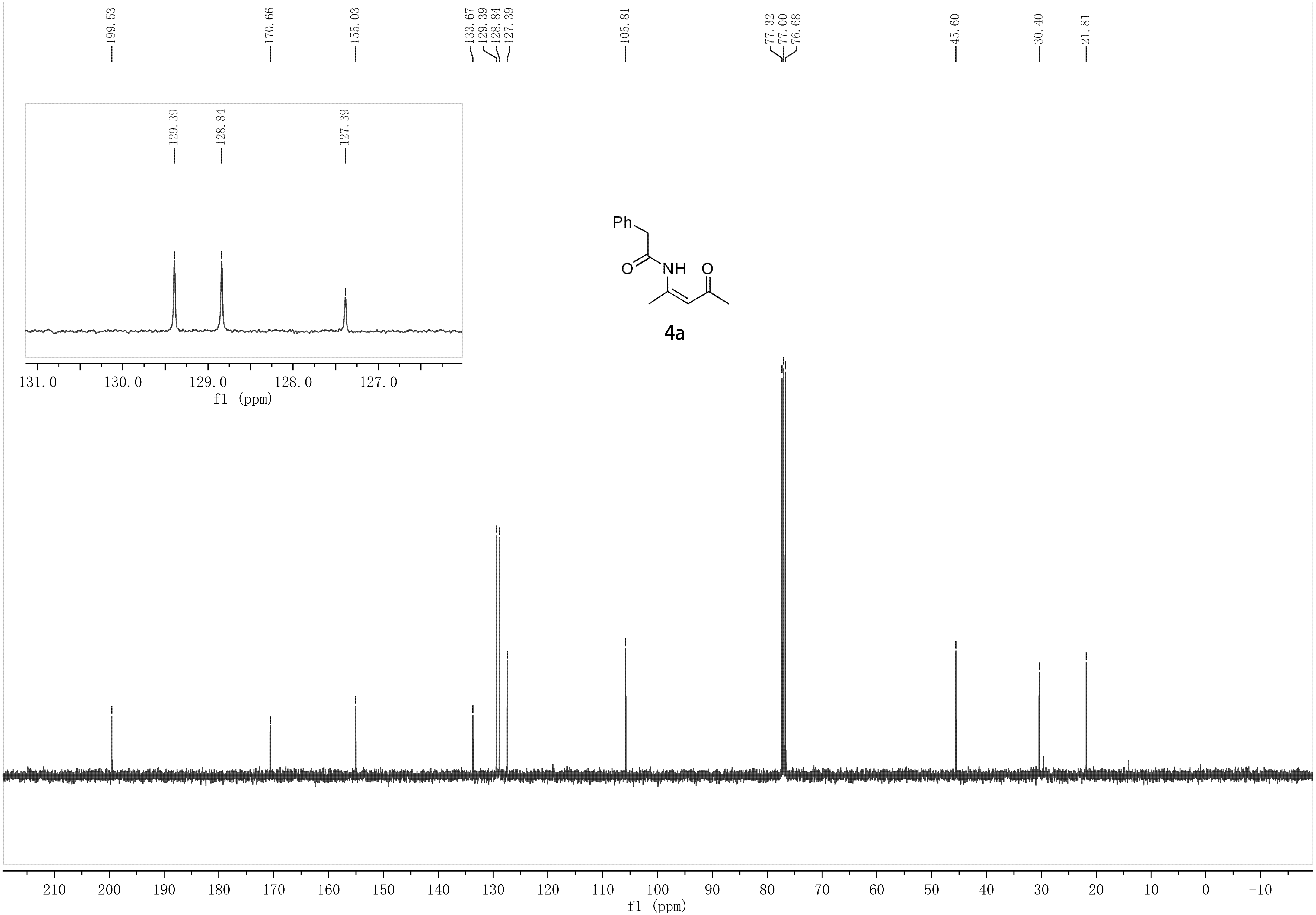
11.860
9.906
8.740
8.719
7.670
7.667
7.651
7.648
7.604
7.601
7.583
7.560
7.556
7.538
7.384
7.379
7.366
7.347
7.320
7.302
7.284
7.259
7.241
7.222
7.205
4.750
2.698
2.680
2.667
2.659
2.649
2.640
2.630
2.622
2.611
2.604
2.591
2.572
1.318
1.299
1.281
Ph
SEt
O
NH
O
0.97
1.01
1.00
1.05
3.04
3.25
1.13
1.00
2.00
3.07
f1 (ppm)

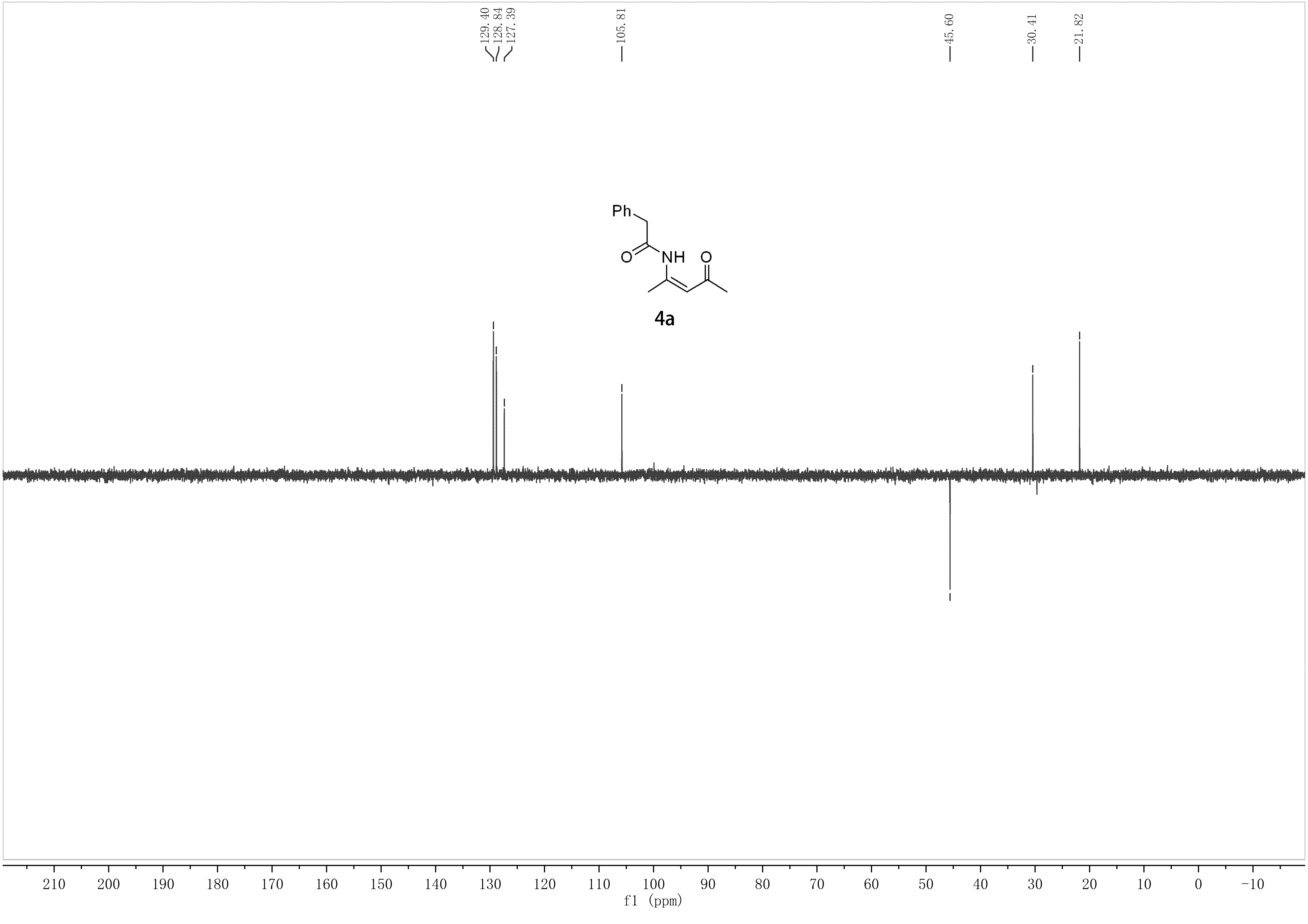
3z


195.15
170.09
140.30
136.36
135.96
135.90
128.85
128.20
128.16
123.26
122.13
119.92
77.32
77.00
76.68
56.13
26.47
14.07
Ph
SEt
O
NH
O
3z
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)

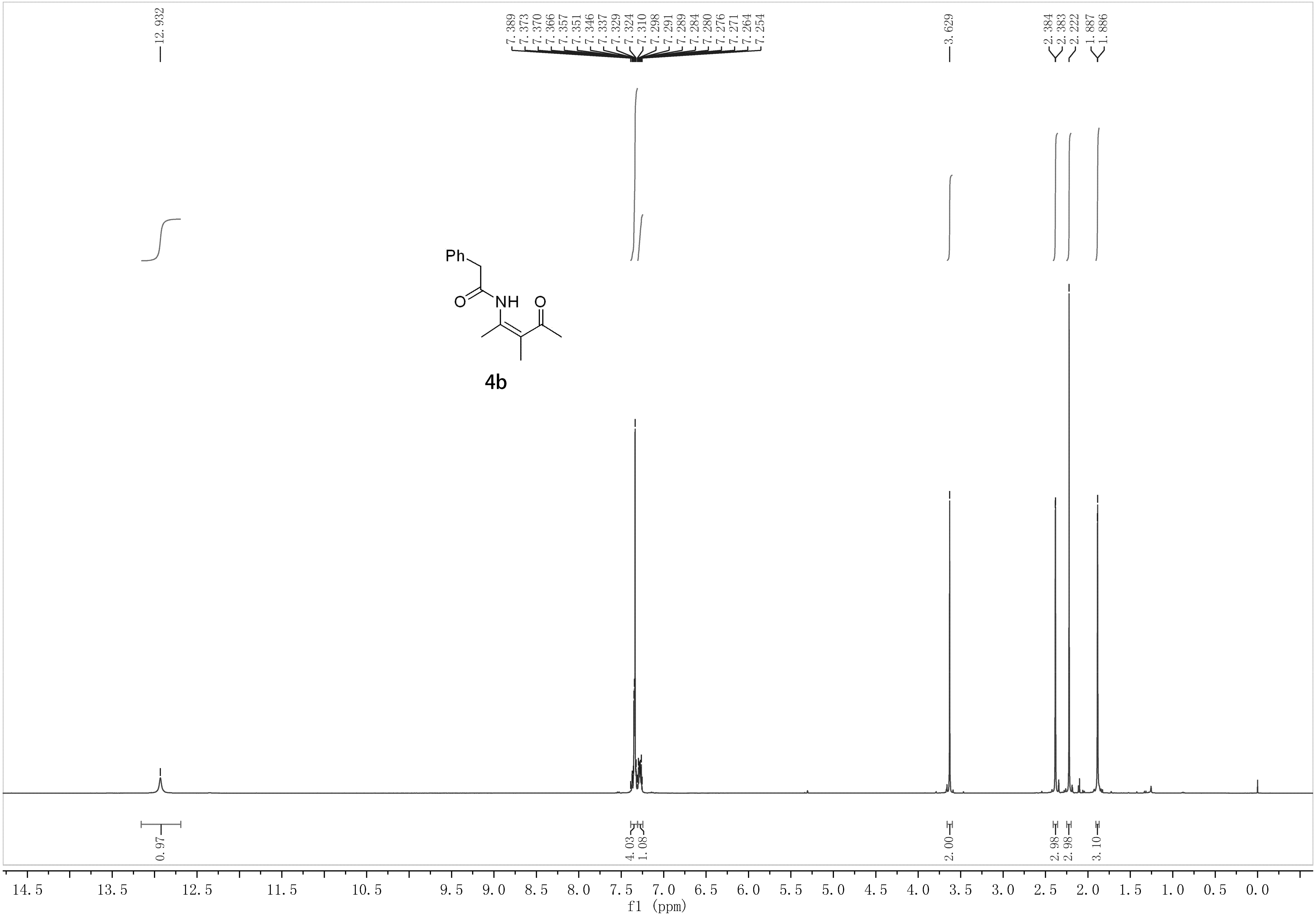

195.15
135.96
135.90
128.85
128.20
128.16
123.26
119.92
56.14
26.47
14.07
Ph
SEt
O
NH
O
3z
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

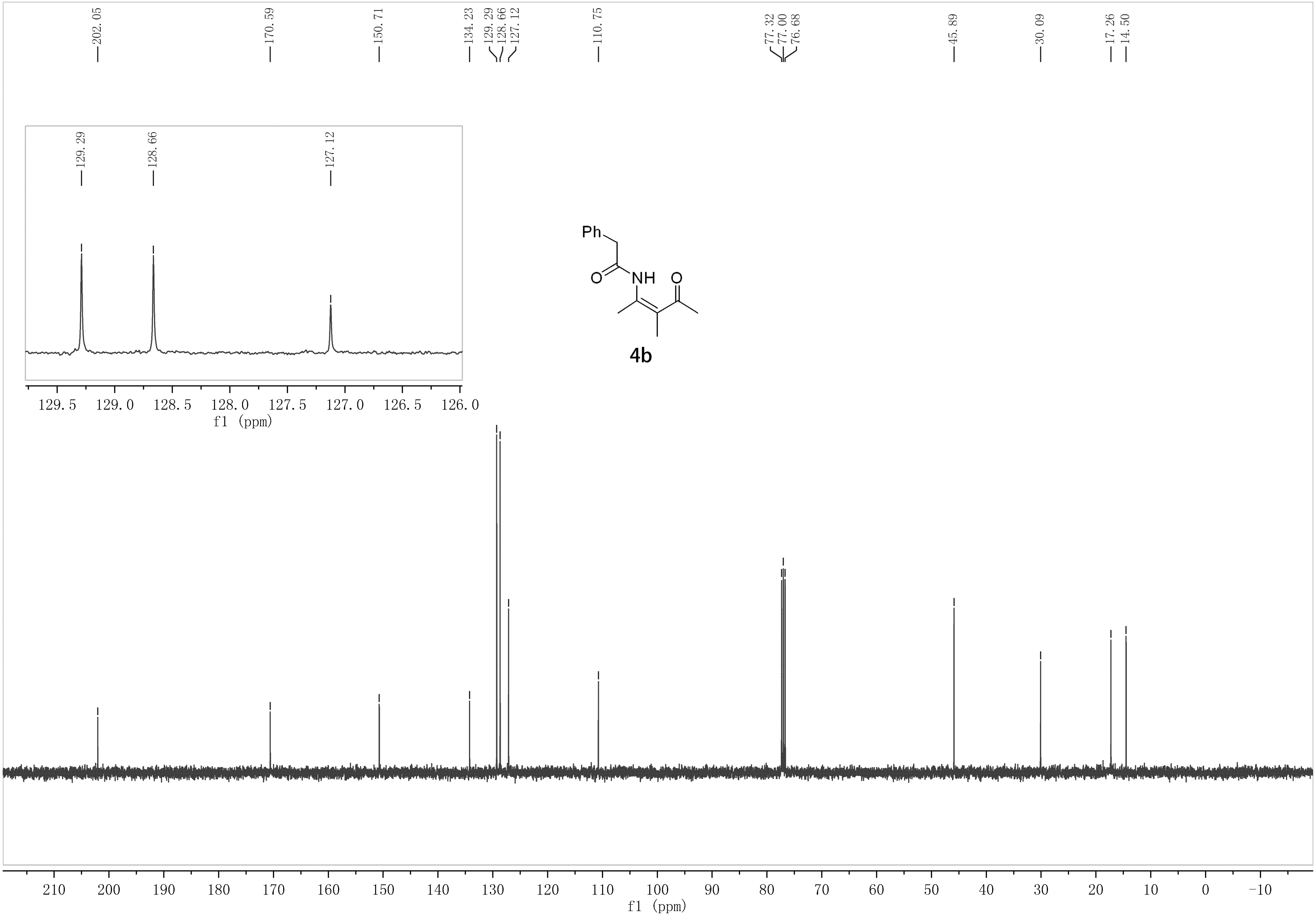

12.345
7.387 7.369 7.351 7.341 7.323 7.319 7.298 7.290 7.281 7.260
5.304
3.660
2.347
2.099
Ph
O
NH
O
4a
0.99
4.90
1.00
2.08
3.07
3.03
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

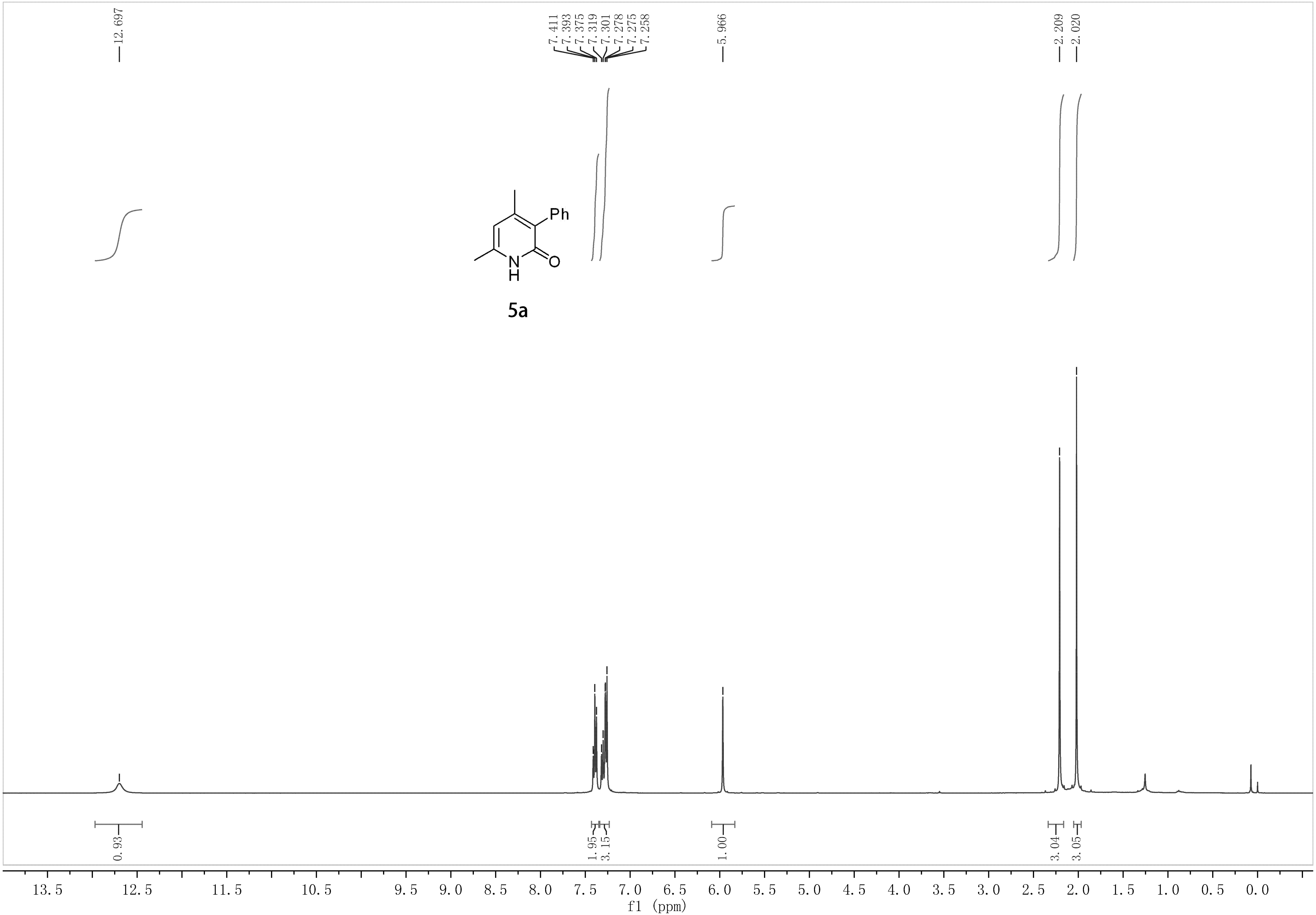

199.53
170.66
155.03
133.67
129.39
128.84
127.39
105.81
77.32
77.00
76.68
45.60
30.40
21.81
Ph
O
NH
O
4a
131.0
130.0
129.0
128.0
127.0
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)



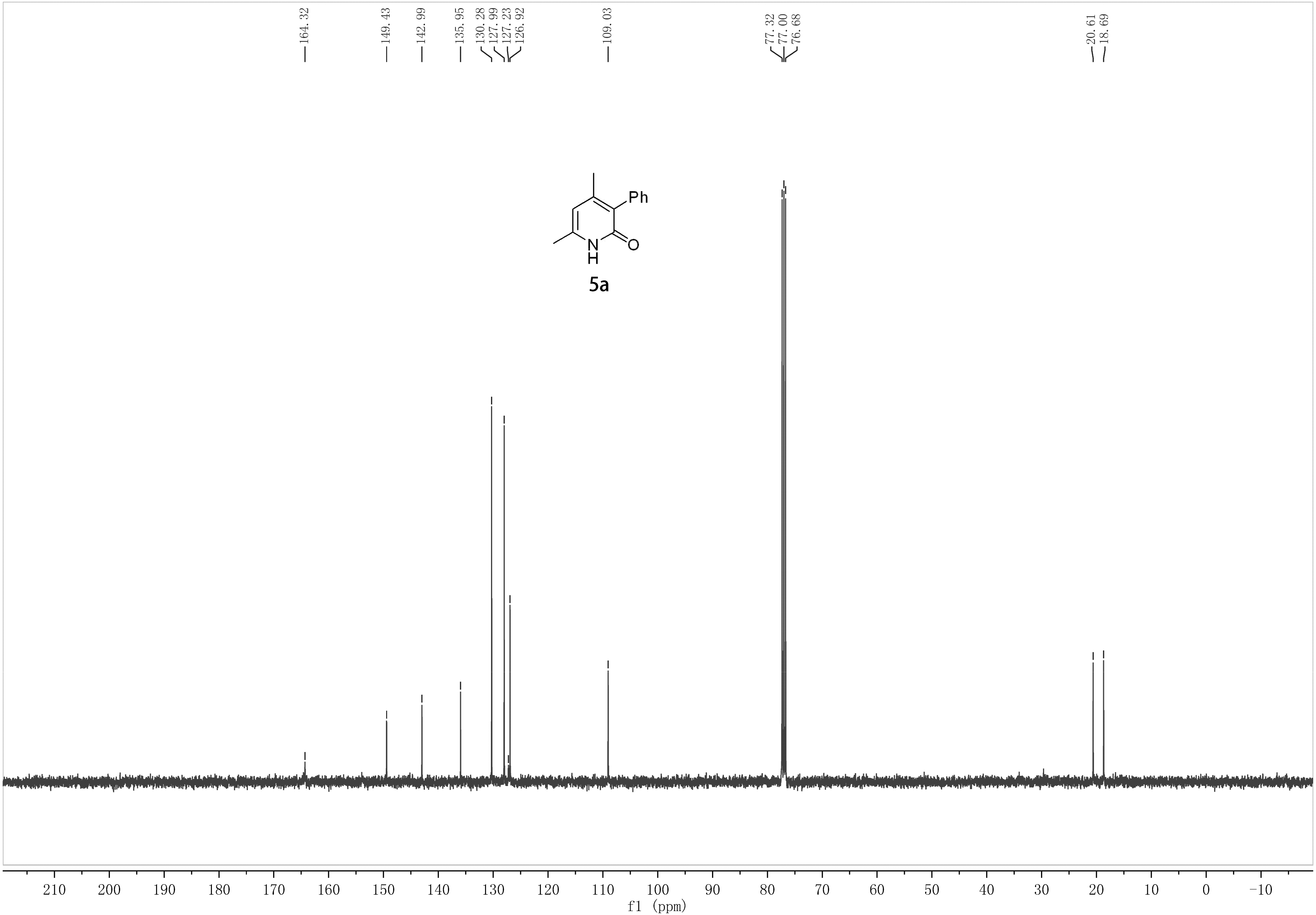
129.40
128.84
127.39
105.81
45.60
30.41
21.82
Ph
NH
O
O
4a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


12.932
7.389
7.373
7.370
7.366
7.357
7.351
7.346
7.337
7.329
7.324
7.310
7.298
7.291
7.289
7.284
7.280
7.276
7.271
7.264
7.254
3.629
2.384
2.383
2.222
1.887
1.886
Ph
O
NH
O
4b
0.97
4.03
1.08
2.00
2.98
2.98
3.10
14.5 13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

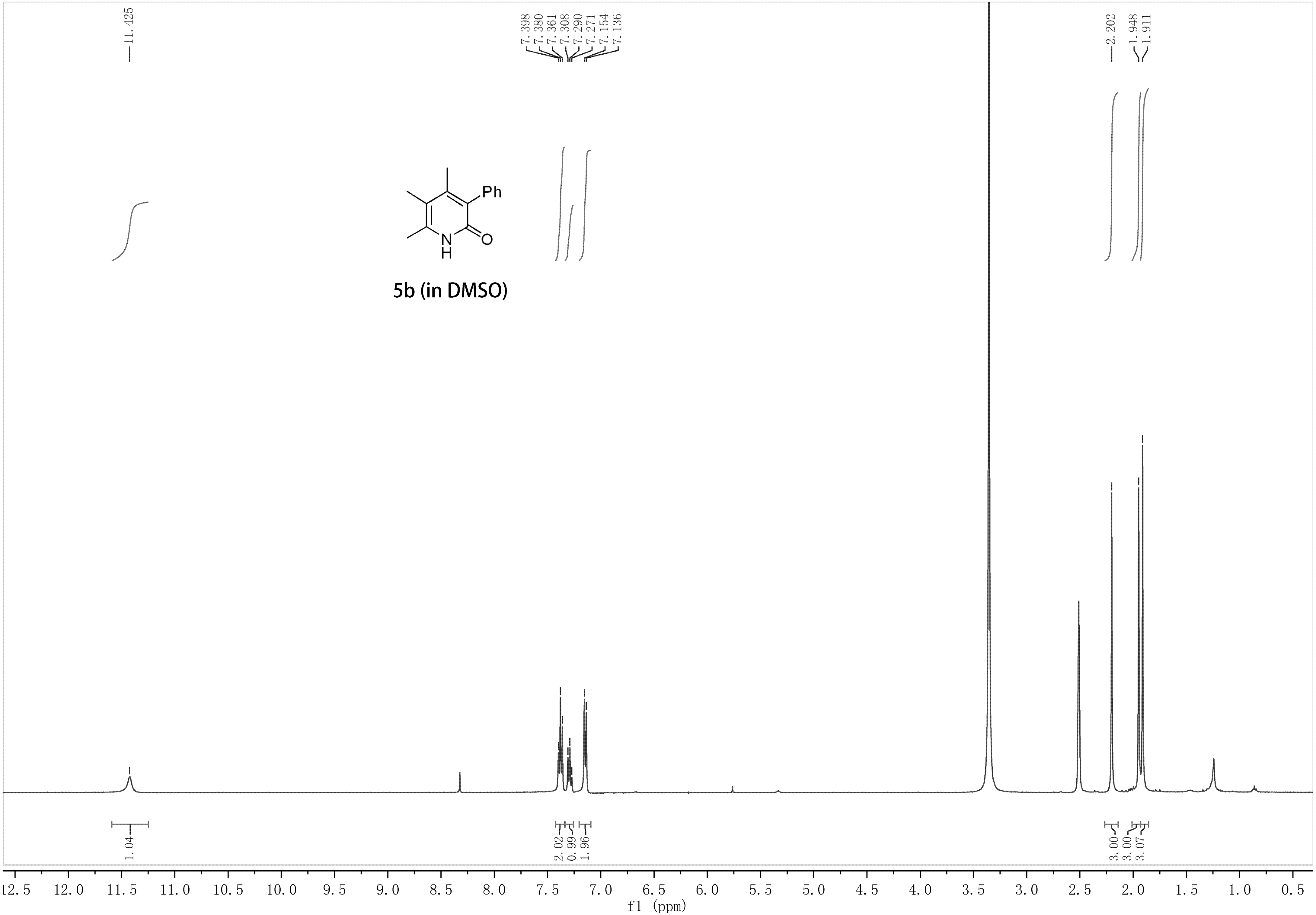

202.05
170.59
150.71
134.23
129.29
128.66
127.12
110.75
77.32
77.00
76.68
45.89
30.09
17.26
14.50
129.29
128.66
127.12
129.5 129.0 128.5 128.0 127.5 127.0 126.5 126.0
f1 (ppm)
Ph
O
NH
O
4b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

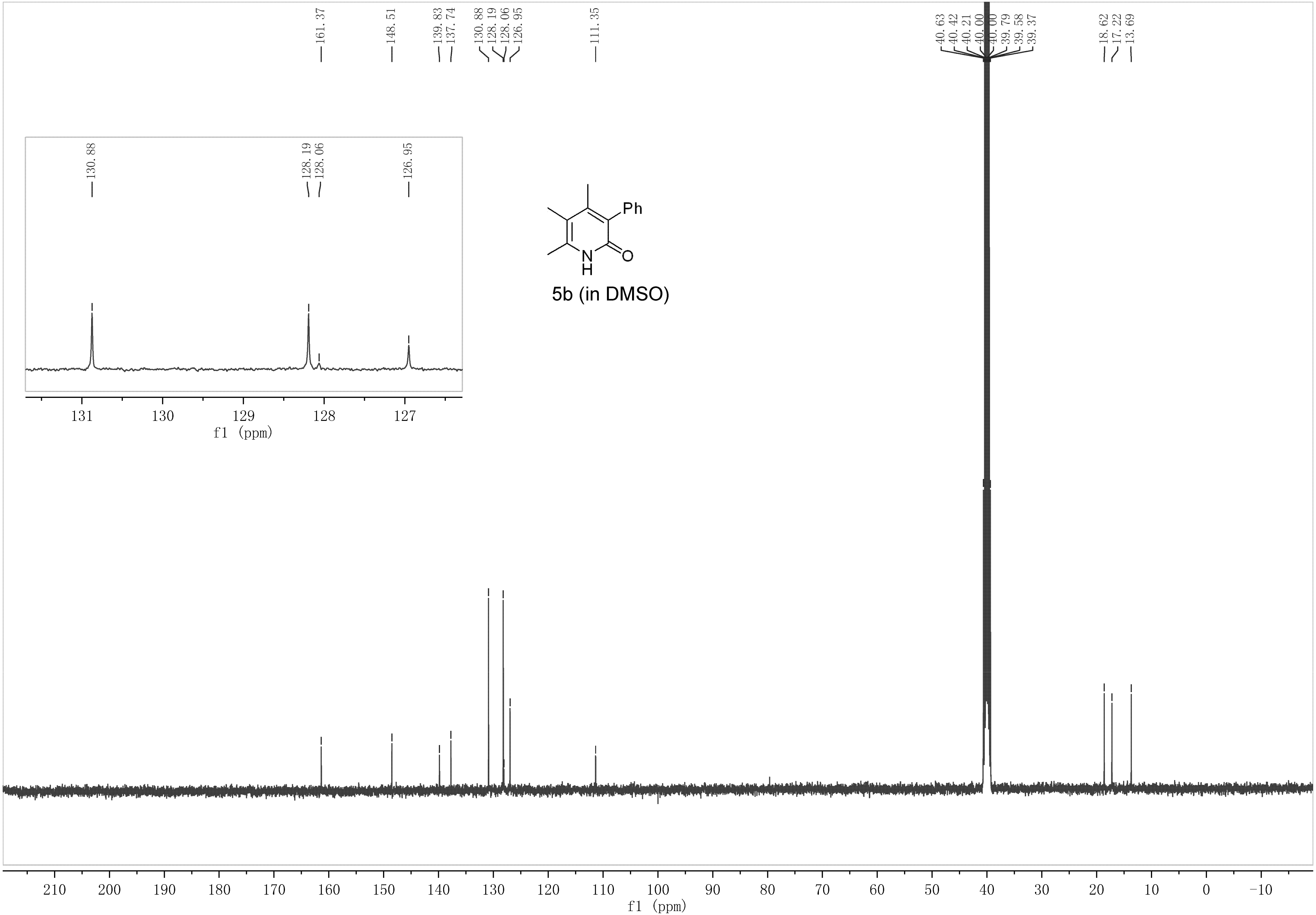


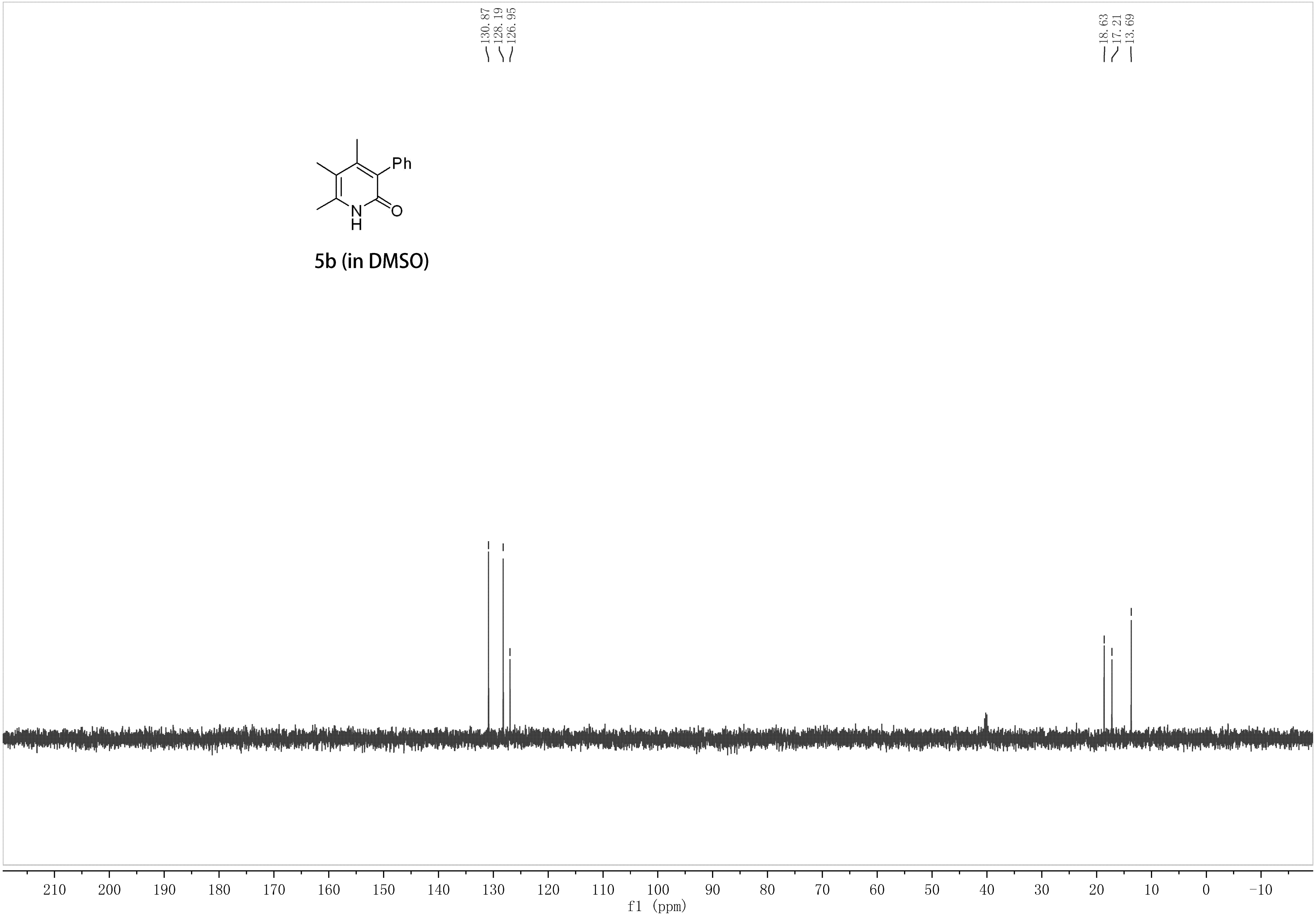
12.697
7.411
7.393
7.375
7.319
7.301
7.278
7.275
7.258
5.966
2.209
2.020
Ph
N
H
O
5a
0.93
1.95
3.15
1.00
3.04
3.05
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



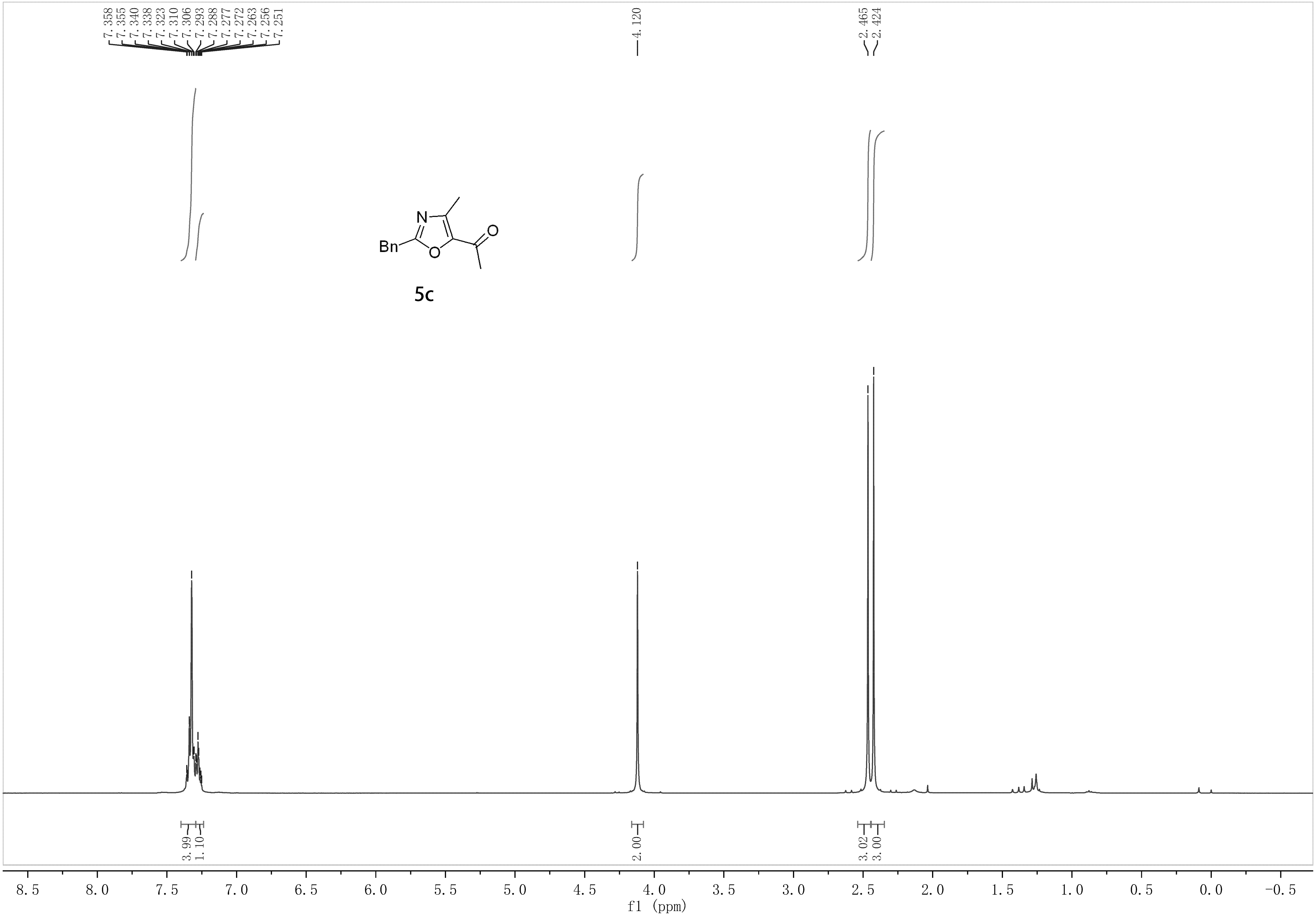
164.32
149.43
142.99
135.95
130.28
127.99
127.23
126.92
109.03
77.32
77.00
76.68
20.61
18.69
Ph
N
H
O
5a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

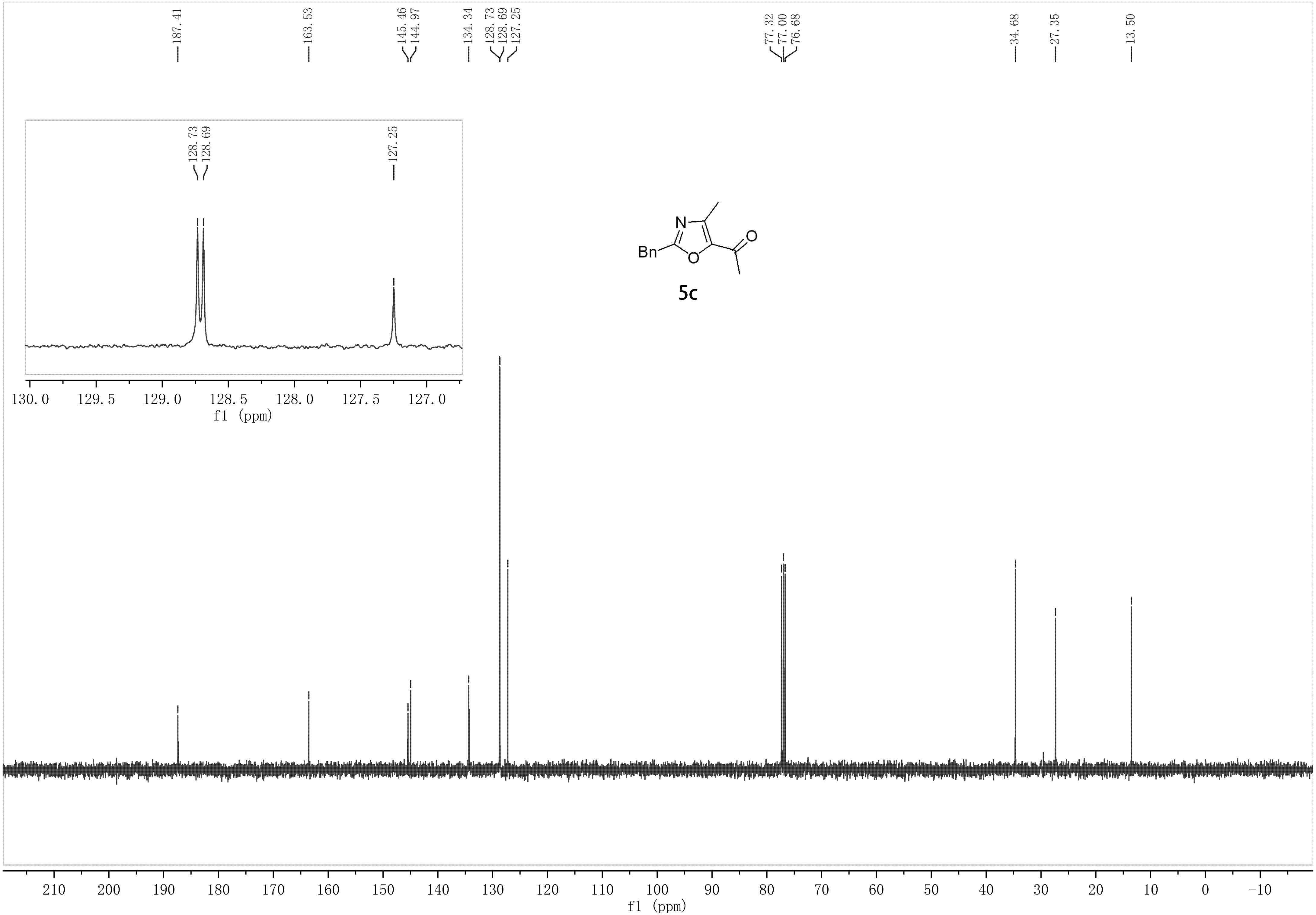

11.425
7.398
7.380
7.361
7.308
7.290
7.271
7.154
7.136
2.202
1.948
1.911
Ph
N
H
O
5b (in DMSO)
1.04
2.02
0.99
1.96
3.00
3.00
3.07
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


161.37
148.51
139.83
137.74
130.88
128.19
128.06
126.95
111.35
40.63
40.42
40.21
40.00
40.00
39.79
39.58
39.37
18.62
17.22
13.69
Ph
N
H
O
5b (in DMSO)
131
130
129
128
127
f1 (ppm)
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)

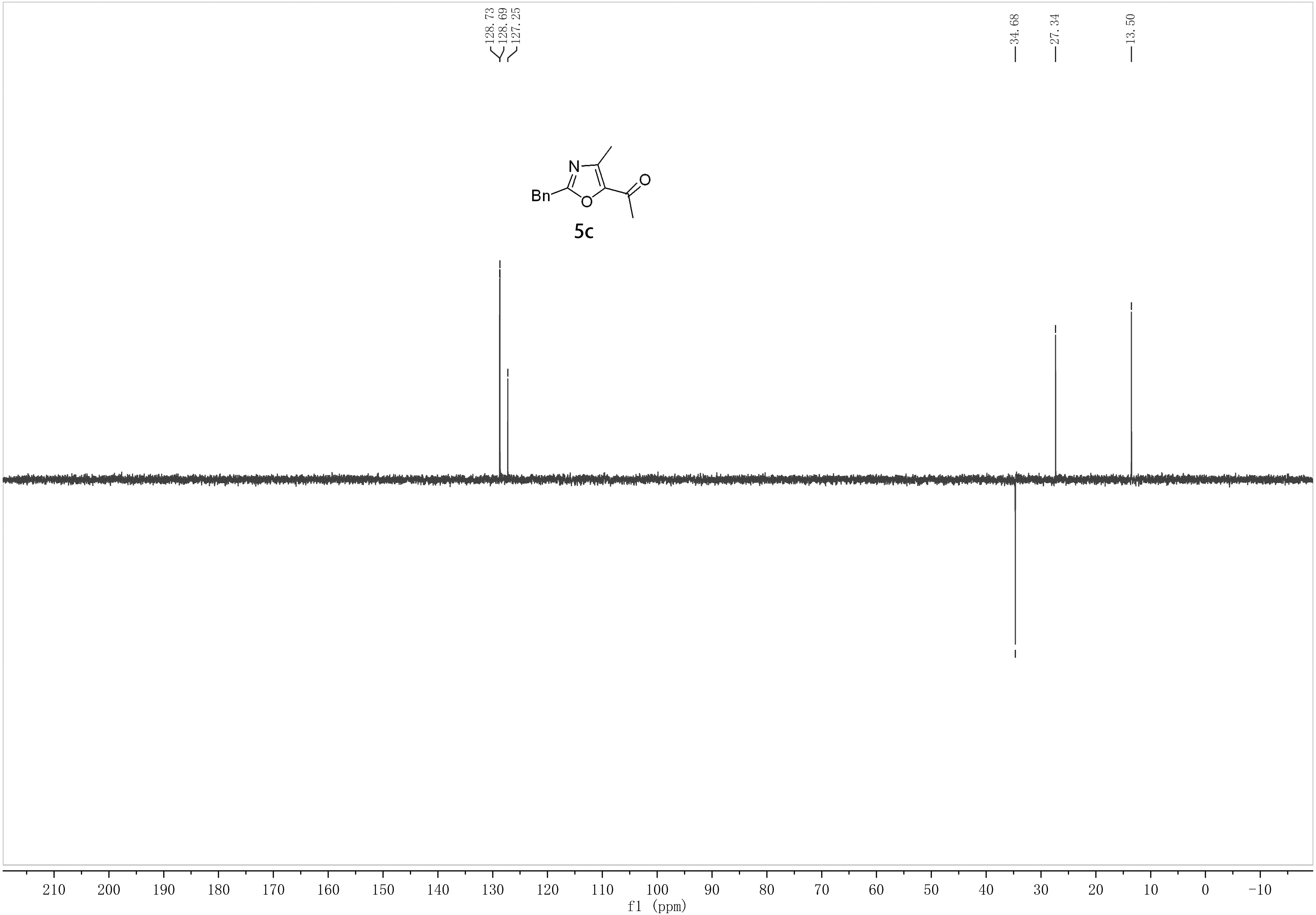


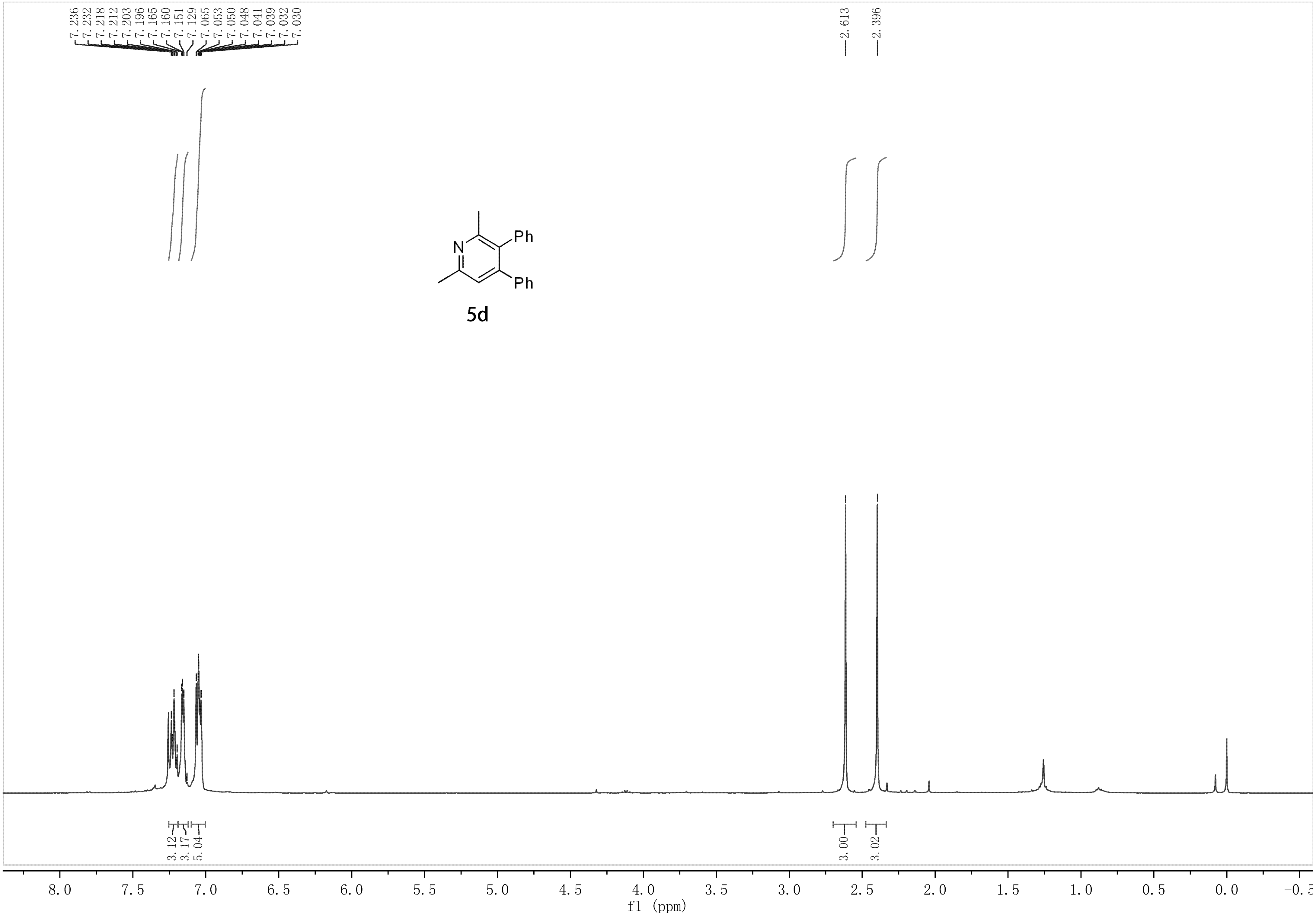
130.87
128.19
126.95
18.63
17.21
13.69
Ph
N
H
O
5b (in DMSO)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


7.358
7.355
7.340
7.338
7.323
7.310
7.306
7.293
7.288
7.277
7.272
7.263
7.256
7.251
4.120
2.465
2.424
Bn
N
O
O
5c
3.99
1.10
2.00
3.02
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

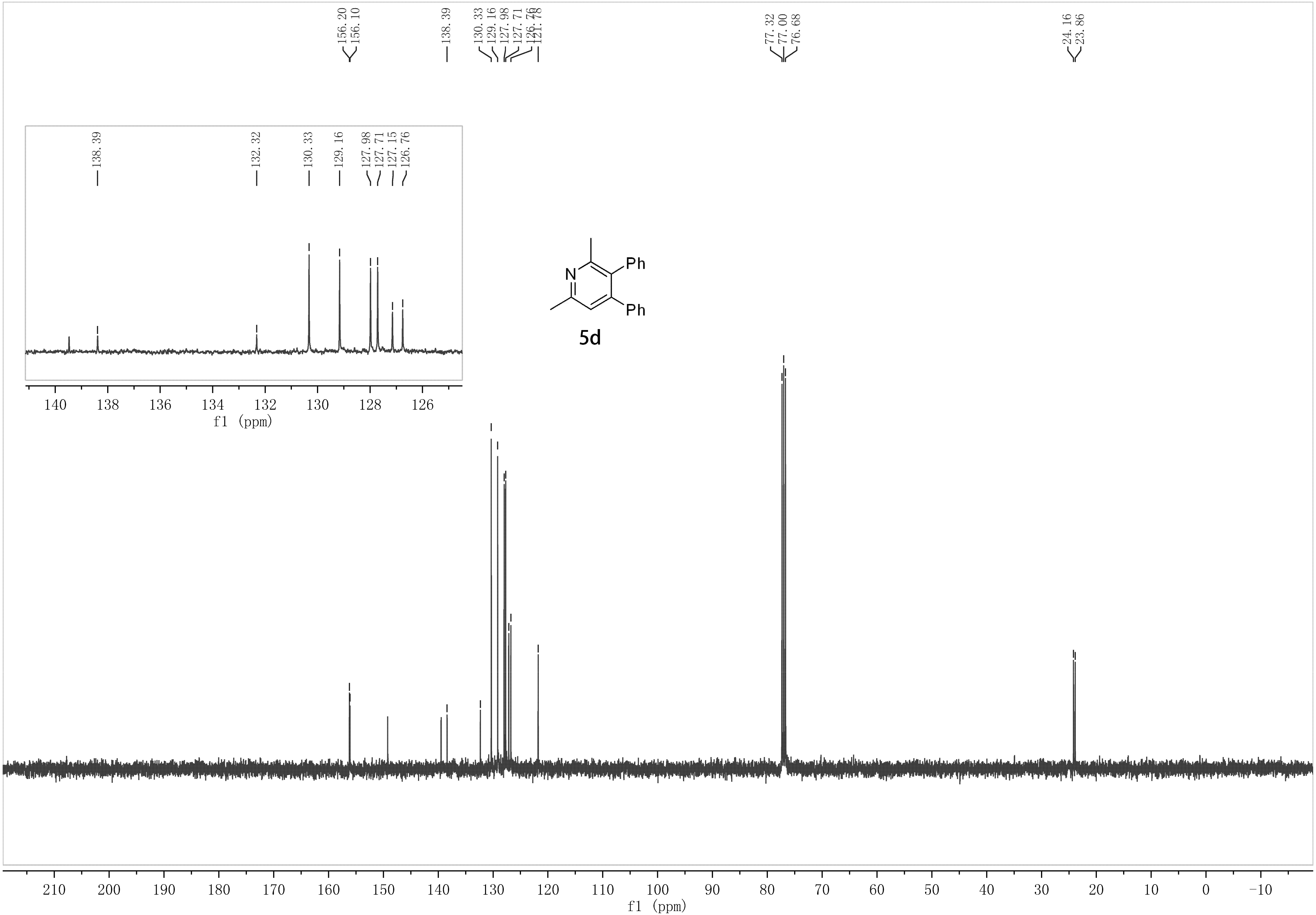


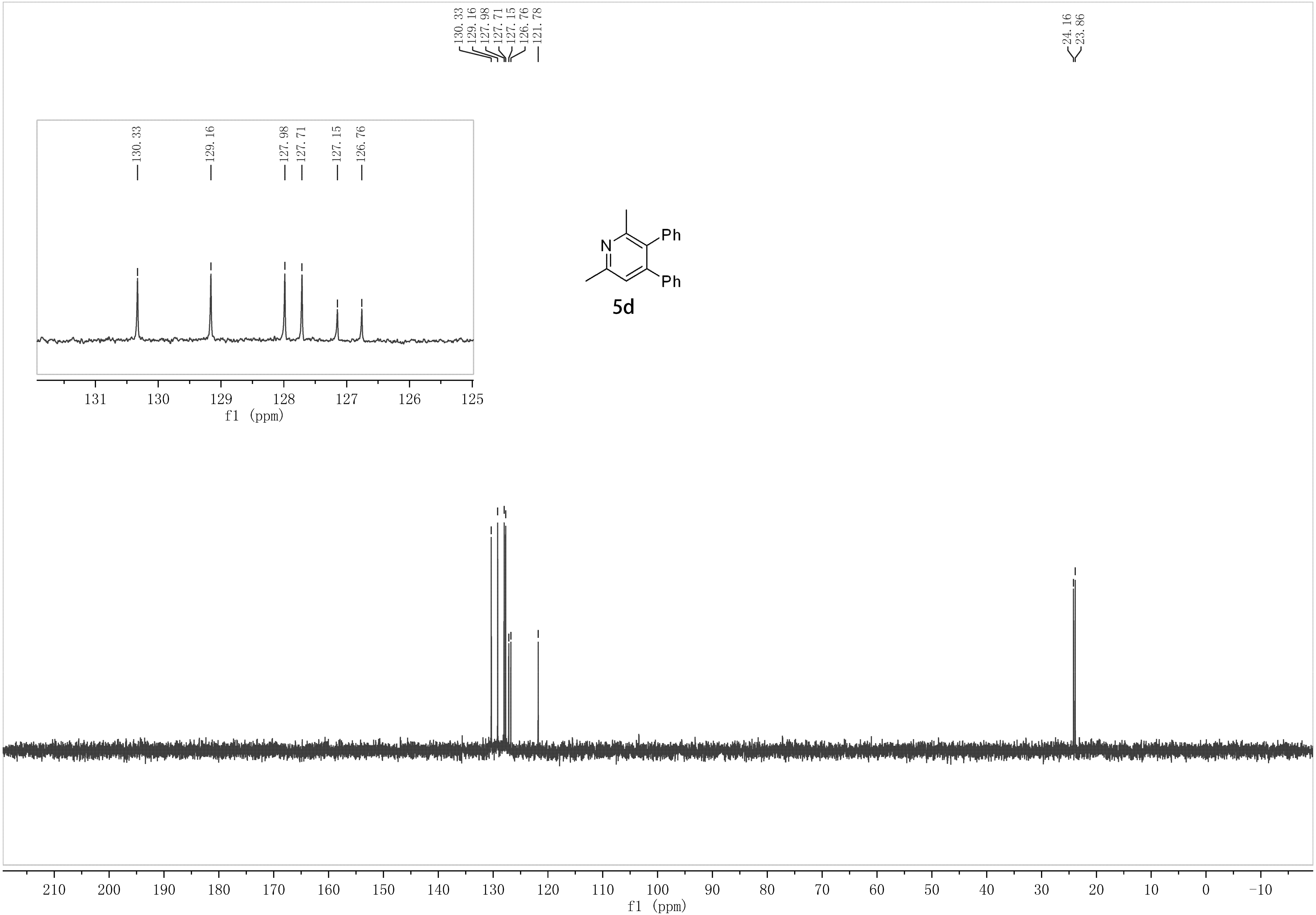
187.41
163.53
145.46
144.97
134.34
128.73
128.69
127.25
77.32
77.00
76.68
34.68
27.35
13.50
Bn
N
O
O
5c
130.0 129.5 129.0 128.5 128.0 127.5 127.0
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


128.73
128.69
127.25
34.68
27.34
13.50
N
O
Bn
5c
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)

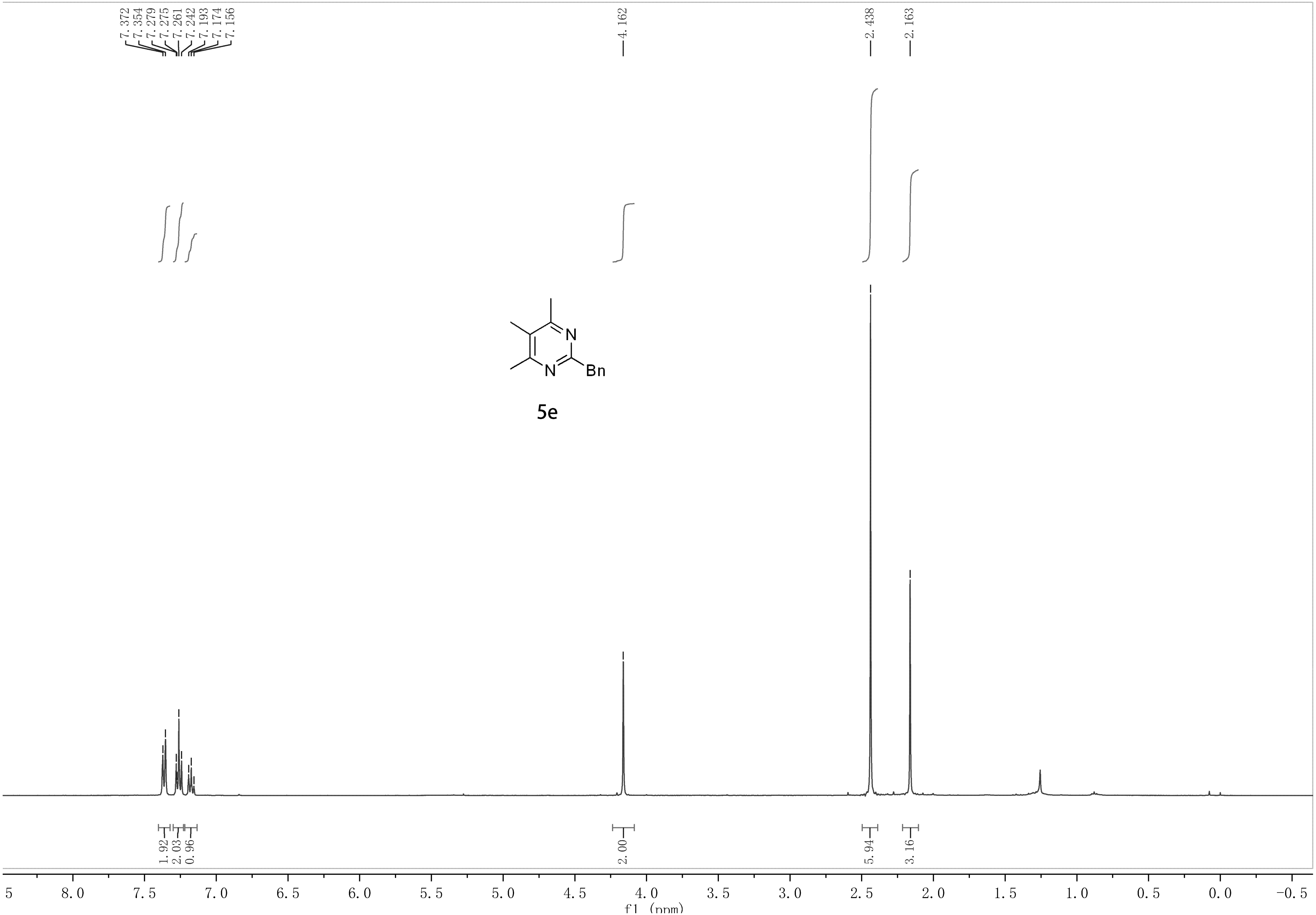

7.236
7.232
7.218
7.212
7.203
7.196
7.165
7.160
7.151
7.129
7.065
7.053
7.050
7.048
7.041
7.039
7.032
7.030
2.613
2.396
3.12
3.17
5.04
3.00
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
N
Ph
Ph

5d

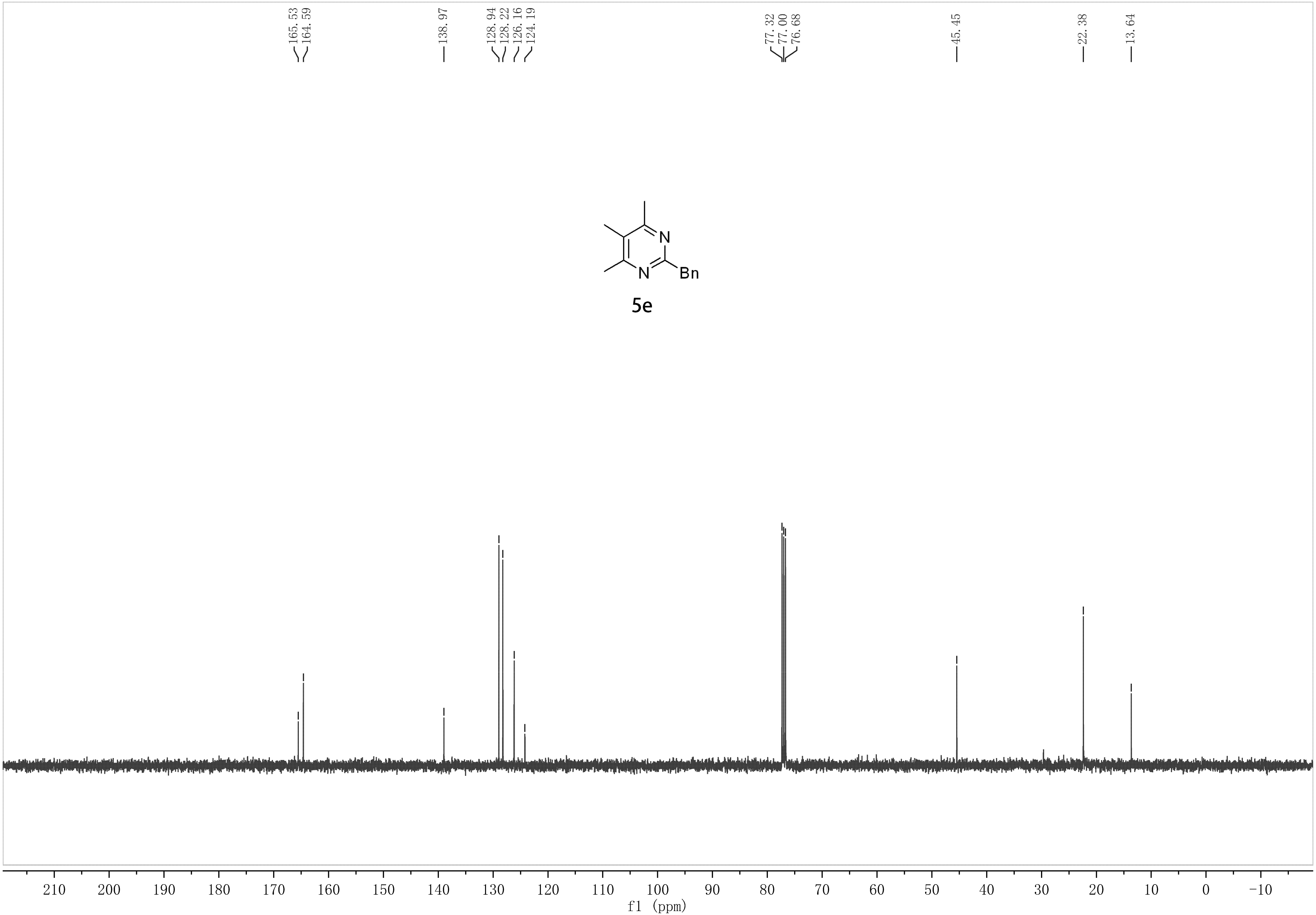

156.20
156.10
138.39
130.33
129.16
127.98
127.71
126.76
121.78
77.32
77.00
76.68
24.16
23.86
138.39
132.32
130.33
129.16
127.98
127.71
127.15
126.76
140 138 136 134 132 130 128 126
f1 (ppm)
N
Ph
Ph
5d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

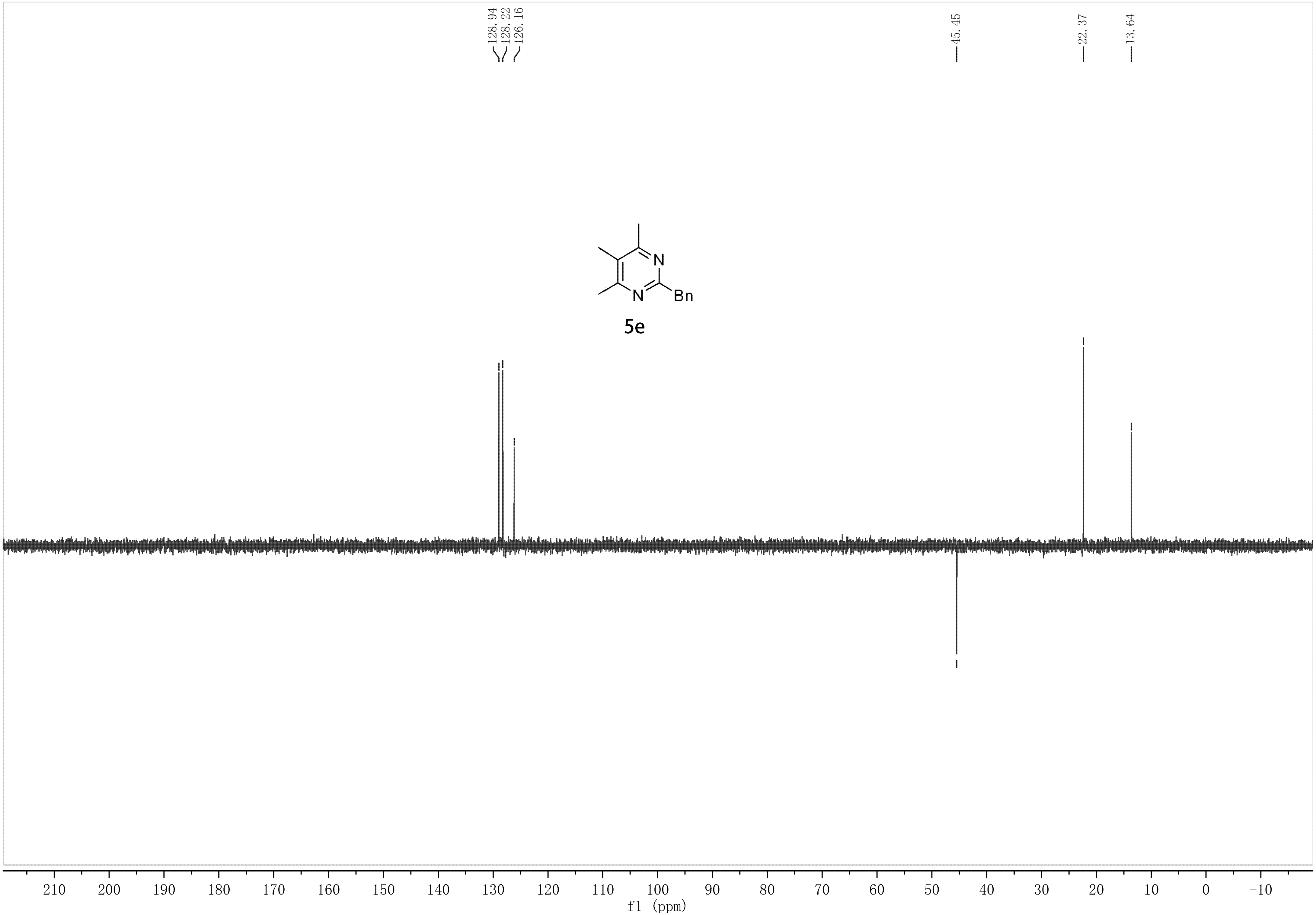


130.33
129.16
127.98
127.71
127.15
126.76
121.78
24.16
23.86
N
Ph
Ph
5d
131 130 129 128 127 126 125
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



7.372
7.354
7.279
7.275
7.261
7.242
7.193
7.174
7.156
4.162
2.438
2.163
N
N
Bn
5e
1.92
2.03
0.96
2.00
5.94
3.16
5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


165.53
164.59
138.97
128.94
128.22
126.16
124.19
77.32
77.00
76.68
45.45
22.38
13.64
N
N
Bn
5e
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)


128.94
128.22
126.16
45.45
22.37
13.64
N
N
Bn
5e
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)