

Supporting Information

Benign catalysis with zinc: atom-economical and divergent synthesis of nitrogen heterocycles by formal [3+2] annulation of isoxazoles with ynol ethers

Xin-Qi Zhu, Han Yuan, Qing Sun, Bo Zhou, Xiao-Qin Han, Zhi-Xin Zhang, Xin Lu* and Long-Wu Ye*

*i*ChEM, State Key Laboratory of Physical Chemistry of Solid Surfaces and Key Laboratory for Chemical Biology of Fujian Province, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

E-mail: longwuye@xmu.edu.cn; xinlu@xmu.edu.cn

Content	Page Number
General	2
More Reaction Condition Study	3
Preparation of Starting Materials	3
General Procedure: Zinc Catalysis	11
Crystal Data	33
Computational Studies	34
¹H and ¹³C NMR Spectra	96

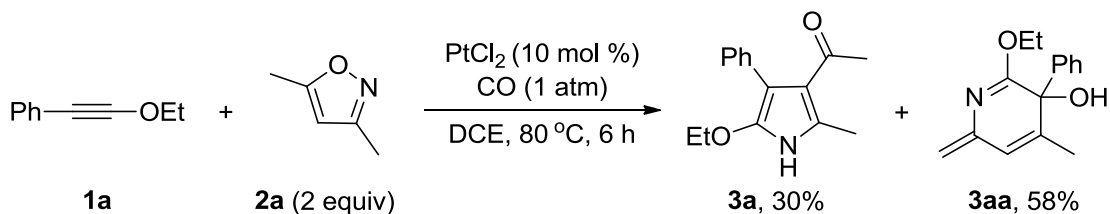
General Information. Ethyl acetate (ACS grade), hexanes (ACS grade) and anhydrous 1,2-dichloroethane (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. 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.

^1H 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).

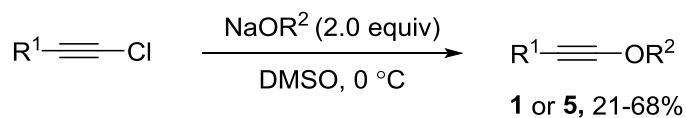
^{13}C NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform- d_3 . Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard.

More Reaction Condition Study

1. Of note, the reaction of ynol ether **1a** with isoxazole **2a** under platinum catalysis gave 2,5-dihydropyridines **3aa** as the major product.

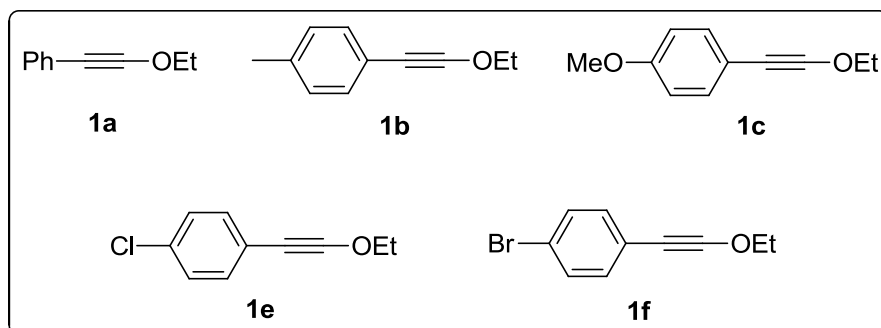


Representative synthetic procedures for the preparation of alkynyl ethers 1 or 5:

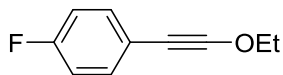


A dry reaction tube was charged with sodium alkoxide (20 mmol). The tube was sealed, evacuated, and backfilled with nitrogen. Then, a solution of chlorinated alkyne (10 mmol) in dry DMSO (5 mL) was added dropwise at 0 °C and the progress of the reaction was monitored by TLC. Upon completion, water was added at 0 °C to quench the reaction. The mixture was then extracted with ether (3 × 25 mL) and the combined organic layer was dried over MgSO₄, filtered and concentrated in vacuum. The residue was purified by flash chromatography on silica gel to afford the alkynyl ether **1** or **5**.

The data of alkynyl ethers **1a-1c**, **1e** and **1f** were reported in our previous work.¹



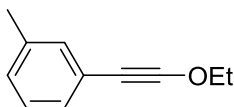
1-(ethoxyethynyl)-4-fluorobenzene (1d)



1d

This compound is known and the spectroscopic data match those reported.² ¹H NMR (400 MHz, CDCl₃) δ 7.34 – 7.26 (m, 2H), 6.98 – 6.89 (m, 2H), 4.19 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 161.5 (d, *J* = 245.0 Hz), 133.1 (d, *J* = 8.0 Hz), 120.0 (d, *J* = 3.0 Hz), 115.2 (d, *J* = 22.0 Hz), 98.0, 74.9, 38.8, 14.4.

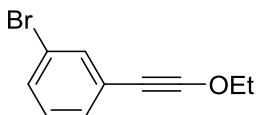
1-(ethoxyethynyl)-3-methylbenzene (1g)



1g

This compound is known and the spectroscopic data match those reported.³ ¹H NMR (400 MHz, CDCl₃) δ 7.28 – 7.18 (m, 3H), 7.06 – 6.98 (m, 1H), 4.18 (q, *J* = 7.2 Hz, 2H), 2.29 (s, 3H), 1.43 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 137.7, 132.1, 128.5, 128.0, 127.4, 123.8, 98.3, 74.8, 39.9, 21.2, 14.4.

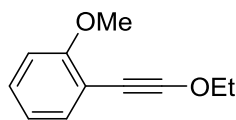
1-bromo-4-(ethoxyethynyl)benzene (1h)



1h

This compound is known and the spectroscopic data match those reported.⁴ ¹H NMR (400 MHz, CDCl₃) δ 7.52 (t, *J* = 1.6 Hz, 1H), 7.40 – 7.33 (m, 1H), 7.32 – 7.24 (m, 1H), 7.17 – 7.11 (m, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 1.47 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 134.1, 129.9, 129.6, 129.5, 126.2, 121.9, 99.6, 75.1, 38.9, 14.4.

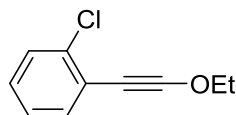
1-(ethoxyethynyl)-4-methylbenzene (1i)



1i

This compound is known and the spectroscopic data match those reported.⁵ ¹H NMR (400 MHz, CDCl₃) δ 7.37 – 7.29 (m, 1H), 7.22 – 7.15 (m, 1H), 6.91 – 6.80 (m, 2H), 4.23 (q, *J* = 7.1 Hz, 2H), 3.85 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.6, 133.3, 127.8, 120.3, 113.0, 110.4, 102.4, 55.7, 35.9, 14.5.

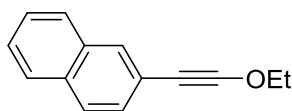
1-chloro-2-(ethoxyethynyl)benzene (1j)



1j

This compound is known and the spectroscopic data match those reported.⁴ ¹H NMR (400 MHz, CDCl₃) δ 7.40 – 7.30 (m, 2H), 7.18 – 7.07 (m, 2H), 4.26 (q, *J* = 7.1 Hz, 2H), 1.48 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 135.3, 132.8, 129.0, 127.4, 126.3, 123.9, 103.4, 75.3, 37.7, 14.4.

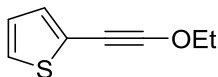
2-(ethoxyethynyl)naphthalene (1k)



1k

Pale yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 7.83 (s, 1H), 7.79 – 7.63 (m, 3H), 7.51 – 7.33 (m, 3H), 4.21 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 133.2, 132.0, 130.4, 129.1, 127.7, 127.6, 127.3, 126.2, 125.7, 121.4, 99.0, 75.0, 40.3, 14.4; IR (neat): 2975, 1749, 1695, 1635, 1520, 1473, 1457, 1339, 1026, 747; HRESIMS Calcd for [C₁₄H₁₂NNaO]⁺ (*M* + Na⁺) 219.0780, found 219.0778.

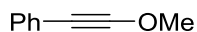
2-(ethoxyethynyl)thiophene (1l)



1l

Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.11 (d, $J = 4.9$ Hz, 1H), 7.03 (d, $J = 2.7$ Hz, 1H), 6.93 – 6.86 (m, 1H), 4.21 (q, $J = 7.1$ Hz, 2H), 1.43 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 130.4, 126.7, 125.2, 124.2, 101.7, 75.3, 33.4, 14.4; IR (neat): 2360, 2339, 2239, 1652, 1558, 1506, 1162, 1029, 785, 667; HRESIMS Calcd for $[\text{C}_8\text{H}_8\text{FNaOS}]^+$ ($\text{M} + \text{Na}^+$) 175.0188, found 175.0189.

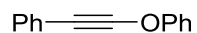
(methoxyethynyl)benzene (1m)



1m

This compound is known and the spectroscopic data match those reported.⁴ ^1H NMR (400 MHz, CDCl_3) δ 7.37 – 7.30 (m, 2H), 7.28 – 7.17 (m, 3H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 131.5, 128.2, 126.7, 123.8, 100.1, 65.9, 38.8.

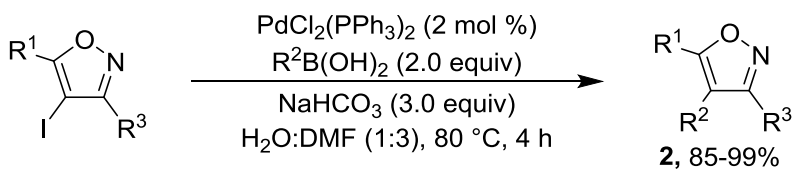
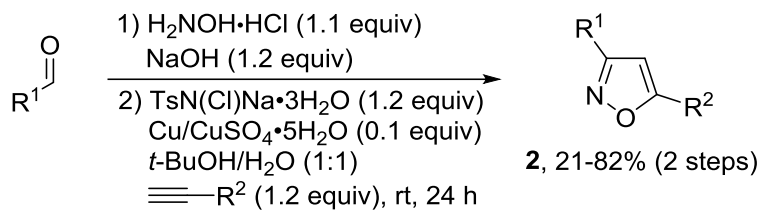
(phenoxyethynyl)benzene (1n)



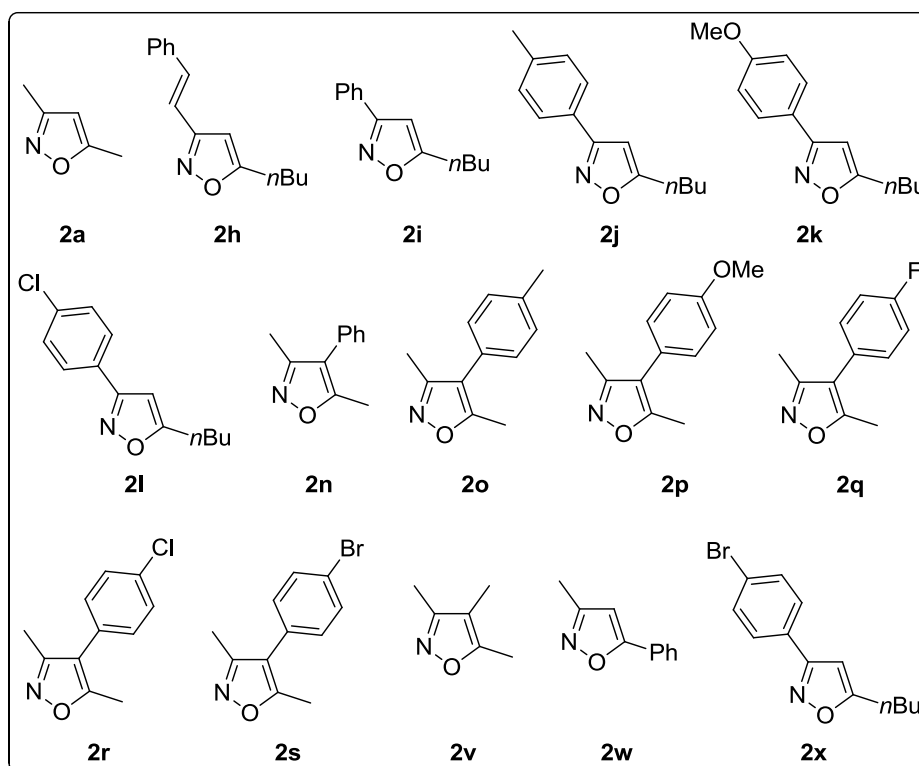
1n

This compound is known and the spectroscopic data match those reported.⁶ ^1H NMR (400 MHz, CDCl_3) δ 7.50 – 7.42 (m, 2H), 7.42 – 7.25 (m, 7H), 7.20 – 7.14 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.1, 131.7, 129.7, 128.3, 127.4, 124.5, 122.9, 115.0, 92.4, 46.3.

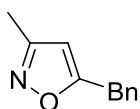
Representative synthetic procedures for the preparation of isoxazoles 2:^{1,7}



The data of isoxazoles **2h-2l**, **2n-2s** and **2x** were reported in our previous work,^{1,7} and compounds **2a**, **2v** and **2w** are commercially available.



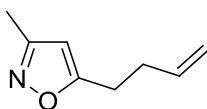
5-benzyl-3-methylisoxazole (**2b**)



2b

This compound is known and the spectroscopic data match those reported.⁸ ¹H NMR (400 MHz, CDCl₃) δ 7.36 – 7.28 (m, 2H), 7.28 – 7.20 (m, 3H), 5.73 (s, 1H), 4.01 (s, 2H), 2.22 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 171.8, 159.8, 136.1, 128.7(0), 128.6(6), 127.0, 102.5, 33.1, 11.3.

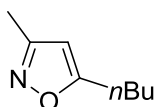
5-(but-3-en-1-yl)-3-methylisoxazole (2c)



2c

This compound is known and the spectroscopic data match those reported.⁹ ¹H NMR (400 MHz, CDCl₃) δ 5.88 – 5.76 (m, 2H), 5.13 – 4.97 (m, 2H), 2.80 (t, *J* = 7.6 Hz, 2H), 2.47 – 2.39 (m, 2H), 2.25 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 172.3, 159.5, 136.3, 115.8, 101.5, 31.2, 25.9, 11.2.

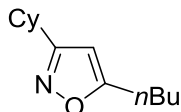
5-butyl-3-methylisoxazole (2d)



2d

This compound is known and the spectroscopic data match those reported.^{10a} ¹H NMR (400 MHz, CDCl₃) δ 5.77 (s, 1H), 2.66 (t, *J* = 7.6 Hz, 2H), 2.22 (s, 3H), 1.69 – 1.57 (m, 2H), 1.41 – 1.30 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 173.3, 159.5, 101.2, 29.4, 26.1, 22.0, 13.5, 11.2.

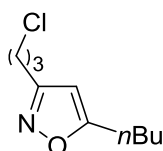
5-butyl-3-cyclohexylisoxazole (2e)



2e

Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 5.80 (s, 1H), 2.76 – 2.62 (m, 3H), 1.95 – 1.60 (m, 6H), 1.44 – 1.24 (m, 8H), 0.92 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.9, 168.2, 98.7, 35.8, 32.0, 30.9, 29.5, 26.6, 26.3, 25.9, 25.8, 22.1, 13.6; IR (neat): 2934, 2855, 1716, 1652, 1558, 1506, 1457, 815, 756, 978; HRESIMS Calcd for $[\text{C}_{13}\text{H}_{21}\text{NNaO}]^+$ ($\text{M} + \text{Na}^+$) 230.1515, found 230.1515.

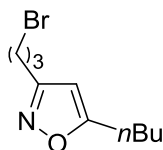
5-butyl-3-(3-chloropropyl)isoxazole (2f)



2f

Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 5.85 (s, 1H), 3.60 (t, $J = 6.4$ Hz, 2H), 2.81 (t, $J = 7.4$ Hz, 2H), 2.71 (t, $J = 7.6$ Hz, 2H), 2.20 – 2.09 (m, 2H), 1.73 – 1.60 (m, 2H), 1.45 – 1.32 (m, 2H), 0.94 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 173.7, 162.3, 100.3, 43.9, 30.8, 29.4, 26.3, 23.3, 22.1, 13.6; IR (neat): 2985, 2958, 2866, 2810, 1678, 1454, 1379, 1245, 1089, 865, 708; HRESIMS Calcd for $[\text{C}_{10}\text{H}_{16}\text{ClNNaO}]^+$ ($\text{M} + \text{Na}^+$) 224.0813, found 224.0811.

3-(3-bromopropyl)-5-butylisoxazole (2g)

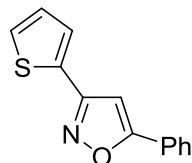


2g

Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 5.85 (s, 1H), 3.46 (t, $J = 6.6$ Hz, 2H), 2.80 (t, $J = 7.4$ Hz, 2H), 2.71 (t, $J = 7.6$ Hz, 2H), 2.29 – 2.17 (m, 2H), 1.72 – 1.61 (m, 2H), 1.46 – 1.33 (m, 2H), 0.94 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 173.7, 162.2, 100.3, 32.6, 30.9, 29.5, 26.3, 24.6, 22.1, 13.6; IR (neat): 2987, 2941, 2878, 2820,

1677, 1450, 1370, 1239, 1074, 752, 650; HRESIMS Calcd for $[C_{10}H_{16}BrNNaO]^+$ (M + Na⁺) 268.0307, found 268.0304.

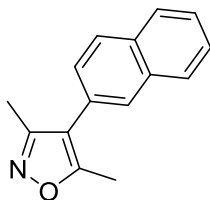
5-phenyl-3-(thiophen-2-yl)isoxazole (2m)



2m

This compound is known and the spectroscopic data match those reported.^{10b} ¹H NMR (400 MHz, CDCl₃) δ 7.83 – 7.76 (m, 2H), 7.52 – 7.36 (m, 5H), 7.14 – 7.07 (m, 1H), 6.73 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 170.3, 158.1, 130.7, 130.3, 128.9, 127.6, 127.5, 127.3, 127.1, 125.8, 97.4.

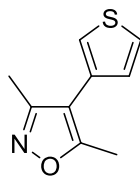
3,5-dimethyl-4-(naphthalen-2-yl)isoxazole (2t)



2t

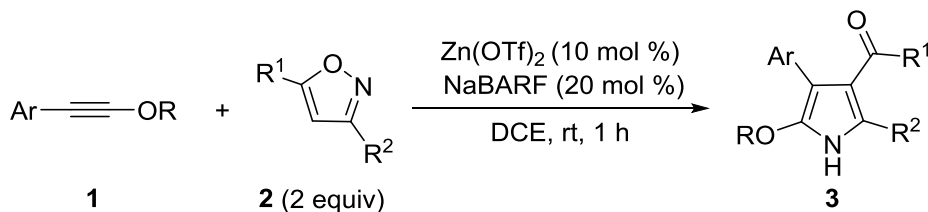
Pale yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 7.97 – 7.87 (m, 3H), 7.75 (s, 1H), 7.61 – 7.51 (m, 2H), 7.43 – 7.39 (m, 1H), 2.49 (s, 3H), 2.37 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 165.3, 158.7, 133.3, 132.4, 128.4, 128.0, 127.8, 127.7, 127.6, 126.8, 126.4, 126.2, 116.6, 11.5, 10.8; IR (neat): 2937, 1705, 1677, 1542, 1500, 1423, 1321, 1245, 1032, 722, 620; HRESIMS Calcd for $[C_{15}H_{13}NNaO]^+$ (M + Na⁺) 246.0889, found 246.0888.

3,5-dimethyl-4-(thiophen-3-yl)isoxazole (2u)



2u

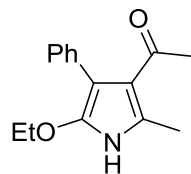
Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.44 – 7.39 (m, 1H), 7.20 – 7.17 (m, 1H), 7.11 – 7.07 (m, 1H), 2.43 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 165.0, 158.5, 130.2, 127.4, 126.0, 122.6, 111.9, 11.6, 10.9; IR (neat): 2912, 1710, 1632, 1550, 1370, 1251, 1074, 886, 758; HRESIMS Calcd for $[\text{C}_9\text{H}_9\text{NNaOS}]^+$ ($\text{M} + \text{Na}^+$) 202.0297, found 202.0294.



General procedure for the synthesis of 2-alkoxypyrroles 3:

NaBARF (0.06 mmol, 53.2 mg) and Zn(OTf)_2 (0.03 mmol, 10.9 mg) were added successively to a solution of the ynol ether **1** (0.30 mmol) and the isoxazole **2** (0.60 mmol) in dry DCE (6.0 mL), the reaction mixture was then stirred at room temperature and the progress of the reaction was monitored by TLC. The reaction typically took 1 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 2-alkoxypyrrole **3**.

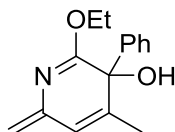
1-(5-ethoxy-2-methyl-4-phenyl-1H-pyrrol-3-yl)ethan-1-one (3a)



3a

Compound **3a** was prepared in 88% yield (64.2 mg) according to the general procedure (Table 2, entry 1). Yellow solid (mp 128-130 °C). ^1H NMR (400 MHz, CDCl_3) δ 8.53 (s, 1H), 7.39 – 7.32 (m, 4H), 7.28 – 7.27 (m, 1H), 3.78 (q, $J = 7.0$ Hz, 2H), 2.45 (s, 3H), 1.94 (s, 3H), 1.11 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 197.2, 140.8, 134.8, 130.4, 128.1, 127.3, 126.5, 119.9, 107.5, 70.3, 30.6, 15.1, 13.7; IR (neat): 3320 (br), 1733, 1716 (s), 1683, 1558, 1507, 1457, 1338, 1259, 1046, 760; HRESIMS Calcd for $[\text{C}_{15}\text{H}_{17}\text{NNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 266.1151, found 266.1153.

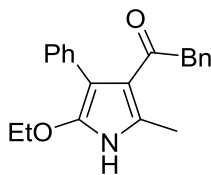
2-ethoxy-4-methyl-6-methylene-3-phenyl-3,6-dihydropyridin-3-ol (3aa)



3aa

Pale Yellow oil. ^1H NMR (500 MHz, CDCl_3) δ 7.37 – 7.28 (m, 4H), 7.28 – 7.21 (m, 1H), 6.18 (d, $J = 1.0$ Hz, 1H), 5.14 (s, 1H), 4.83 (s, 1H), 4.34 – 4.16 (m, 2H), 3.08 (s, 1H), 1.67 (s, 3H), 1.18 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 164.4, 144.5, 142.2, 138.1, 128.2, 127.5, 124.7, 121.9, 110.2, 72.4, 62.1, 15.8, 14.0; IR (neat): 3440 (br), 2965, 1678, 1526, 1507, 1478, 1315, 1158, 1046, 724; HRESIMS Calcd for $[\text{C}_{15}\text{H}_{17}\text{NNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 266.1151, found 266.1153.

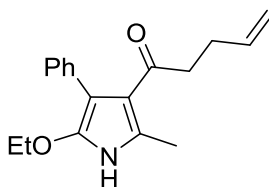
1-(5-ethoxy-2-methyl-4-phenyl-1H-pyrrol-3-yl)-2-phenylethan-1-one (3b)



3b

Compound **3b** was prepared in 85% yield (81.7 mg) according to the general procedure (Table 2, entry 2). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.52 (s, 1H), 7.42 – 7.32 (m, 4H), 7.32 – 7.25 (m, 1H), 7.21 – 7.08 (m, 3H), 7.00 – 6.90 (m, 2H), 3.74 (q, $J = 7.0$ Hz, 2H), 3.55 (s, 2H), 2.32 (s, 3H), 1.09 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 197.2, 140.8, 135.7, 134.7, 130.3, 129.4, 128.2, 128.0, 127.8, 126.5, 126.2, 119.2, 107.2, 70.2, 48.6, 15.1, 13.5; IR (neat): 3254 (br), 1699 (s), 1652, 1558, 1506, 1457, 1339, 1089, 1034, 669; HRESIMS Calcd for $[\text{C}_{21}\text{H}_{21}\text{NNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 342.1465, found 342.1465.

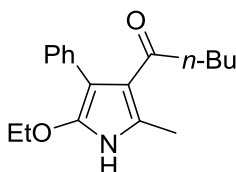
1-(5-ethoxy-2-methyl-4-phenyl-1H-pyrrol-3-yl)pent-4-en-1-one (3c)



3c

Compound **3c** was prepared in 81% yield (68.5 mg) according to the general procedure (Table 2, entry 3). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.90 (s, 1H), 7.39 – 7.31 (m, 4H), 7.29 – 7.22 (m, 1H), 5.67 – 5.54 (m, 1H), 4.83 – 4.70 (m, 2H), 3.78 (q, $J = 7.0$ Hz, 2H), 2.42 (s, 3H), 2.36 – 2.28 (m, 2H), 2.27 – 2.16 (m, 2H), 1.10 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 199.4, 140.9, 137.6, 134.8, 130.2, 128.0, 127.3, 126.4, 119.4, 114.3, 107.1, 70.2, 41.2, 28.7, 15.0, 13.6; IR (neat): 3274 (br), 3078, 2932, 1698(s), 1653, 1558, 1339, 912, 760, 701; HRESIMS Calcd for $[\text{C}_{18}\text{H}_{21}\text{NNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 306.1465, found 306.1462.

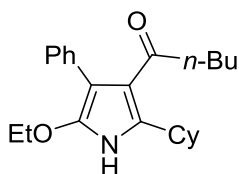
1-(5-ethoxy-2-methyl-4-phenyl-1H-pyrrol-3-yl)pentan-1-one (3d)



3d

Compound **3d** was prepared in 87% yield (73.9 mg) according to the general procedure (Table 2, entry 4). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.82 (s, 1H), 7.38 – 7.30 (m, 4H), 7.28 – 7.23 (m, 1H), 3.78 (q, $J = 7.0$ Hz, 2H), 2.43 (s, 3H), 2.25 – 2.18 (m, 2H), 1.49 – 1.38 (m, 2H), 1.14 – 1.00 (m, 5H), 0.70 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 200.8, 140.8, 134.9, 130.2, 128.0, 126.9, 126.3, 119.6, 107.2, 70.2, 42.0, 27.0, 22.2, 15.1, 13.6, 13.5; IR (neat): 3274 (br), 2957, 2932, 2872, 1716 (s), 1652, 1558, 1457, 1339, 1028, 760, 701; HRESIMS Calcd for $[\text{C}_{18}\text{H}_{23}\text{NNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 308.1621, found 308.1622.

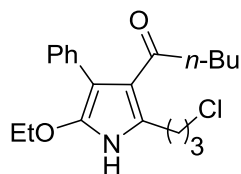
1-(2-cyclohexyl-5-ethoxy-4-phenyl-1H-pyrrol-3-yl)pentan-1-one (3e)



3e

Compound **3e** was prepared in 63% yield (66.5 mg) according to the general procedure (Table 2, entry 5). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.18 (s, 1H), 7.38 – 7.32 (m, 4H), 7.28 – 7.23 (m, 1H), 3.78 (q, $J = 7.0$ Hz, 2H), 3.35 – 3.24 (m, 1H), 2.23 – 2.14 (m, 2H), 2.04 – 1.95 (m, 2H), 1.85 – 1.78 (m, 2H), 1.50 – 1.41 (m, 4H), 1.38 – 1.27 (m, 4H), 1.13 (t, $J = 7.0$ Hz, 3H), 1.09 – 1.00 (m, 2H), 0.70 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 200.8, 140.7, 135.4, 134.9, 130.1, 128.0, 126.3, 118.6, 106.9, 70.3, 42.4, 35.5, 32.9, 29.7, 26.9, 26.5, 26.1, 22.2, 15.2, 13.7; IR (neat): 3113 (br), 2965, 2933, 2853, 1716 (s), 1684, 1558, 1457, 1013, 780, 697; HRESIMS Calcd for $[\text{C}_{23}\text{H}_{31}\text{NNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 376.2247, found 376.2249.

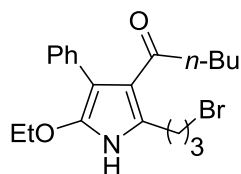
1-(2-(3-chloropropyl)-5-ethoxy-4-phenyl-1H-pyrrol-3-yl)pentan-1-one (3f)



3f

Compound **3f** was prepared in 74% yield (77.0 mg) according to the general procedure (Table 2, entry 5). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.57 (s, 1H), 7.41 – 7.32 (m, 4H), 7.31 – 7.24 (m, 1H), 3.80 (q, $J = 6.9$ Hz, 2H), 3.58 (t, $J = 6.1$ Hz, 2H), 2.98 (t, $J = 7.0$ Hz, 2H), 2.23 – 2.11 (m, 4H), 1.47 – 1.37 (m, 2H), 1.13 (t, $J = 6.9$ Hz, 3H), 1.09 – 0.99 (m, 2H), 0.70 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 200.6, 140.9, 134.7, 130.2, 129.0, 128.1, 126.5, 119.8, 107.3, 70.2, 44.8, 42.0, 32.1, 26.9, 24.6, 22.2, 15.1, 13.6; IR (neat): 3275 (br), 2968, 2930, 2867, 1717 (s), 1653, 1507, 1457, 1339, 1027, 760, 702; HRESIMS Calcd for $[\text{C}_{20}\text{H}_{26}\text{ClNNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 370.1544, found 370.1546.

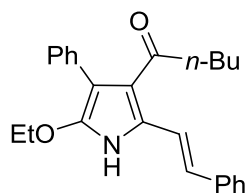
1-(2-(3-bromopropyl)-5-ethoxy-4-phenyl-1H-pyrrol-3-yl)pentan-1-one (3g)



3g

Compound **3g** was prepared in 68% yield (79.7 mg) according to the general procedure (Table 2, entry 7). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.56 (s, 1H), 7.45 – 7.32 (m, 4H), 7.32 – 7.25 (m, 1H), 3.80 (q, $J = 6.8$ Hz, 2H), 3.46 (t, $J = 6.1$ Hz, 2H), 2.98 (t, $J = 6.8$ Hz, 2H), 2.36 – 2.12 (m, 4H), 1.52 – 1.30 (m, 2H), 1.18 – 0.98 (m, 5H), 0.70 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 200.5, 140.9, 134.7, 130.2, 128.9, 128.1, 126.5, 119.9, 107.3, 70.2, 42.1, 33.9, 32.3, 26.9, 25.9, 22.2, 15.1, 13.6; IR (neat): 3195 (br), 2980, 2958, 2865, 1733 (s), 1652, 1558, 1456, 1318, 705, 588; HRESIMS Calcd for $[\text{C}_{20}\text{H}_{26}\text{BrNNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 414.1039, found 414.1040.

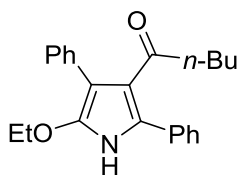
(E)-1-(5-ethoxy-4-phenyl-2-styryl-1H-pyrrol-3-yl)pentan-1-one (3h)



3h

Compound **3h** was prepared in 70% yield (77.3 mg) according to the general procedure (Table 2, entry 8). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 9.16 (s, 1H), 7.60 (d, $J = 16.8$ Hz, 1H), 7.45 – 7.39 (m, 2H), 7.39 – 7.33 (m, 4H), 7.28 – 7.23 (m, 3H), 7.21 – 7.14 (m, 1H), 6.78 (d, $J = 16.7$ Hz, 1H), 3.87 (q, $J = 7.0$ Hz, 2H), 2.25 (t, $J = 7.5$ Hz, 2H), 1.51 – 1.42 (m, 2H), 1.14 (t, $J = 7.0$ Hz, 3H), 1.11 – 1.02 (m, 2H), 0.69 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 201.5, 143.5, 137.1, 134.2, 130.0, 128.5, 128.2, 127.3, 126.5, 126.3, 125.8, 122.3, 117.9, 108.4, 70.1, 42.5, 26.8, 22.2, 15.1, 13.6; IR (neat): 3263 (br), 2965, 2825, 1698 (s), 1646, 1558, 1456, 1339, 1025, 589; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{27}\text{NNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 396.1934, found 396.1931.

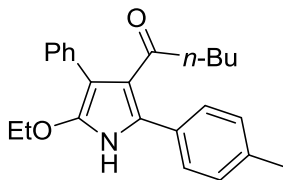
1-(5-ethoxy-2,4-diphenyl-1H-pyrrol-3-yl)pentan-1-one (**3i**)



3i

Compound **3i** was prepared in 95% yield (99.1 mg) according to the general procedure (Table 2, entry 9). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.56 (s, 1H), 7.51 – 7.45 (m, 2H), 7.44 – 7.34 (m, 6H), 7.34 – 7.24 (m, 2H), 3.88 (q, $J = 7.0$ Hz, 2H), 2.30 (t, 2H), 1.49 – 1.39 (m, 2H), 1.19 (t, $J = 7.0$ Hz, 3H), 1.13 – 1.02 (m, 2H), 0.71 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 202.2, 142.9, 133.9, 132.1, 129.5, 128.4, 128.3, 128.0, 127.6, 126.1, 126.0, 121.1, 108.0, 70.1, 43.2, 26.8, 22.1, 15.1, 13.6; IR (neat): 3246 (br), 2986, 2934, 1684 (s), 1507, 1457, 1318, 1024, 700; HRESIMS Calcd for $[\text{C}_{23}\text{H}_{25}\text{NNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 370.1778, found 370.1784.

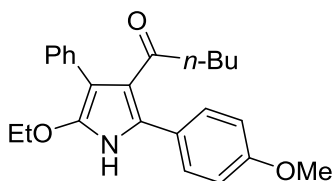
1-(5-ethoxy-4-phenyl-2-(*p*-tolyl)-1*H*-pyrrol-3-yl)pentan-1-one (3j)



3j

Compound **3j** was prepared in 88% yield (94.7 mg) according to the general procedure (Table 2, entry 10). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.38 (s, 1H), 7.40 – 7.30 (m, 6H), 7.24 – 7.20 (m, $J = 7.1$ Hz, 1H), 7.15 (d, $J = 7.9$ Hz, 2H), 3.83 (q, $J = 7.0$ Hz, 2H), 2.34 (s, 3H), 2.26 (t, $J = 7.5$ Hz, 2H), 1.45 – 1.35 (m, 2H), 1.15 (t, $J = 7.0$ Hz, 3H), 1.10 – 0.97 (m, 2H), 0.67 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 202.0, 142.6, 137.6, 134.0, 129.6, 129.3, 129.1, 128.2, 128.0, 126.2, 126.1, 120.8, 107.9, 70.1, 43.1, 26.8, 22.1, 21.2, 15.1, 13.6; IR (neat): 3268 (br), 2957, 2832, 1698 (s), 1507, 1457, 1339, 1002, 752, 699; HRESIMS Calcd for $[\text{C}_{24}\text{H}_{27}\text{NNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 384.1934, found 384.1933.

1-(5-ethoxy-2-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pentan-1-one (3k)

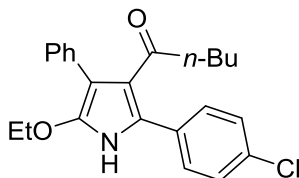


3k

Compound **3k** was prepared in 70% yield (79.1 mg) according to the general procedure except at -10 °C in 12 h (Table 2, entry 11). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.21 (s, 1H), 7.46 – 7.31 (m, 6H), 7.26 – 7.21 (m, 1H), 6.95 – 6.86 (m, 2H), 3.91 – 3.77 (m, 5H), 2.25 (t, $J = 6.8$ Hz, 2H), 1.46 – 1.36 (m, 2H), 1.17 (t, $J = 7.0$ Hz, 3H), 1.11 – 0.99 (m, 2H), 0.68 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 201.7, 159.4, 142.5, 134.1, 129.8, 129.7, 128.1, 126.2, 124.8, 120.7, 113.9, 107.9, 70.2, 55.3, 43.0, 26.8, 22.2, 15.2, 13.7; IR (neat): 3301 (br), 2912, 2896, 1716 (s), 1653, 1558, 1457, 1338, 1170,

1039, 838, 705; HRESIMS Calcd for $[C_{24}H_{27}NNaO_3]^+$ ($M + Na^+$) 400.1883, found 400.1886.

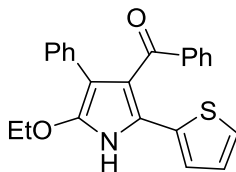
1-(2-(4-chlorophenyl)-5-ethoxy-4-phenyl-1H-pyrrol-3-yl)pentan-1-one (3l)



3l

Compound **3l** was prepared in 66% yield (75.8 mg) according to the general procedure (Table 2, entry 12). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 7.44 – 7.33 (m, 6H), 7.28 – 7.24 (m, 2H), 3.84 (q, $J = 7.0$ Hz, 2H), 2.24 (t, $J = 7.5$ Hz, 2H), 1.43 – 1.33 (m, 2H), 1.15 (t, $J = 7.0$ Hz, 3H), 1.09 – 0.97 (m, 2H), 0.67 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.4, 143.1, 133.8, 133.4, 130.5, 129.5(4), 129.4(9), 128.5, 128.1, 126.3, 124.6, 121.4, 108.1, 70.1, 43.2, 26.7, 22.1, 15.1, 13.6; IR (neat): 3268 (br), 2958, 2872, 1717 (s), 1652, 1540, 1469, 1338, 1092, 724, 590; HRESIMS Calcd for $[C_{23}H_{24}ClNNaO_2]^+$ ($M + Na^+$) 404.1388, found 404.1389.

(5-ethoxy-4-phenyl-2-(thiophen-2-yl)-1H-pyrrol-3-yl)(phenyl)methanone (3m)

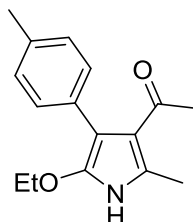


3m

Compound **3m** was prepared in 76% yield (83.3 mg) according to the general procedure (Table 2, entry 13). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 7.77 – 7.67 (m, 2H), 7.27 – 7.23 (m, 3H), 7.18 – 7.07 (m, 6H), 7.03 – 6.96 (m, 1H), 6.92 – 6.86 (m, 1H), 3.92 (q, $J = 7.0$ Hz, 2H), 1.21 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.8, 142.7, 138.3, 133.1(2), 133.0(6), 132.2, 129.9, 128.9, 127.8, 127.7, 127.3, 125.7, 125.6, 125.0, 120.4, 119.4, 109.2, 70.3, 15.2; IR (neat): 3212 (br), 1710 (s), 1652, 1620,

1585, 1540, 1458, 1258, 1012, 708; HRESIMS Calcd for $[C_{23}H_{19}NNaO_2S]^+$ ($M + Na^+$) 396.1029, found 396.1032.

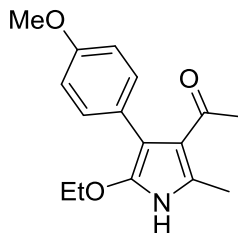
1-(5-ethoxy-2-methyl-4-(*p*-tolyl)-1*H*-pyrrol-3-yl)ethan-1-one (3n)



3n

Compound **3n** was prepared in 91% yield (74.2 mg) according to the general procedure (Table 3, entry 1). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 8.91 (s, 1H), 7.24 – 7.20 (m, 2H), 7.18 – 7.13 (m, 2H), 3.79 (q, $J = 7.1$ Hz, 2H), 3.79 (q, $J = 7.1$ Hz, 2H), 2.45 (s, 3H), 2.37 (s, 3H), 1.96 (s, 3H), 1.11 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 140.8, 136.0, 131.7, 130.2, 128.8, 127.5, 119.7, 107.4, 70.1, 30.6, 21.2, 15.1, 13.8; IR (neat): 3254 (br), 1726 (s), 1630, 1512, 1413, 1382, 1224, 1032, 668; HRESIMS Calcd for $[C_{16}H_{19}NNaO_2]^+$ ($M + Na^+$) 280.1308, found 280.1311.

1-(5-ethoxy-4-(4-methoxyphenyl)-2-methyl-1*H*-pyrrol-3-yl)ethan-1-one (3o)

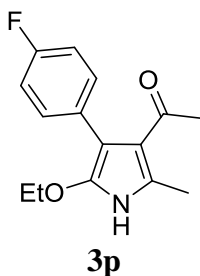


3o

Compound **3o** was prepared in 77% yield (63.0 mg) according to the general procedure (Table 3, entry 2). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 8.89 (s, 1H), 7.26 (d, $J = 8.6$ Hz, 2H), 6.92 (d, $J = 8.6$ Hz, 2H), 3.85 (s, 3H), 3.80 (q, $J = 7.0$ Hz, 2H), 2.47 (s, 3H), 1.97 (s, 3H), 1.12 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.2, 158.3, 140.8, 131.4, 127.4, 127.0, 119.7, 113.5, 107.0, 70.1, 55.1, 30.6, 15.1, 13.8; IR (neat):

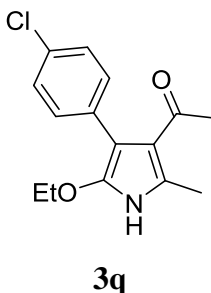
3210 (br), 1699 (s), 1558, 1457, 1339, 1252, 1175, 1033, 836, 568; HRESIMS Calcd for $[C_{16}H_{19}NNaO_3]^+$ ($M + Na^+$) 296.1257, found 296.1255.

1-(5-ethoxy-4-(4-fluorophenyl)-2-methyl-1H-pyrrol-3-yl)ethan-1-one (3p)



Compound **3p** was prepared in 96% yield (78.4 mg) according to the general procedure (Table 3, entry 3). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 9.42 (s, 1H), 7.34 – 7.25 (m, 2H), 7.10 – 7.00 (m, 2H), 3.79 (q, $J = 7.0$ Hz, 2H), 2.45 (s, 3H), 2.00 (s, 3H), 1.11 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.1, 161.6 (d, $J = 244.0$ Hz), 141.2, 131.8 (d, $J = 8.0$ Hz), 130.7 (d, $J = 3.0$ Hz), 128.2, 119.2, 114.9 (d, $J = 21.0$ Hz), 106.4, 70.2, 30.6, 15.0, 13.8; IR (neat): 3298 (br), 1716 (s), 1653, 1507, 1457, 1338, 1318, 1258, 1099, 842; HRESIMS Calcd for $[C_{15}H_{16}FNNaO_2]^+$ ($M + Na^+$) 284.1057, found 284.1061.

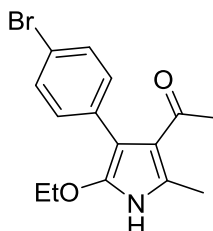
1-(4-(4-chlorophenyl)-5-ethoxy-2-methyl-1H-pyrrol-3-yl)ethan-1-one (3q)



Compound **3q** was prepared in 85% yield (71.3 mg) according to the general procedure (Table 3, entry 4). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 8.62 (s, 1H), 7.36 – 7.30 (m, 2H), 7.29 – 7.25 (m, 2H), 3.78 (q, $J = 7.1$ Hz, 2H), 2.44 (s, 3H), 2.00 (s, 3H), 1.12 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 141.1, 133.3, 132.1, 131.5, 128.2, 128.0, 119.4, 106.3, 70.2, 30.7, 15.1, 13.8; IR (neat): 3278 (br), 1725 (s), 1631,

1599, 1462, 1352, 1258, 1159, 1057, 835, 725, 668; HRESIMS Calcd for $[\text{C}_{15}\text{H}_{16}\text{ClNNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 300.0762, found 300.0761.

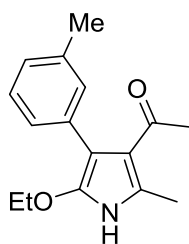
1-(4-(4-bromophenyl)-5-ethoxy-2-methyl-1H-pyrrol-3-yl)ethan-1-one (3r)



3r

Compound **3r** was prepared in 89% yield (86.9 mg) according to the general procedure (Table 3, entry 5). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 9.20 (s, 1H), 7.47 (d, $J = 8.3$ Hz, 2H), 7.21 (d, $J = 8.3$ Hz, 2H), 3.79 (q, $J = 7.0$ Hz, 2H), 2.44 (s, 3H), 2.03 (s, 3H), 1.12 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 196.9, 141.2, 133.8, 131.8, 131.1, 128.1, 120.3, 119.4, 106.3, 70.2, 30.7, 15.1, 13.8; IR (neat): 3189 (br), 1717 (s), 1653, 1558, 1457, 1312, 1258, 1010, 823, 619, 588; HRESIMS Calcd for $[\text{C}_{15}\text{H}_{16}\text{BrNNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 344.0257, found 344.0257.

1-(5-ethoxy-2-methyl-4-(*m*-tolyl)-1H-pyrrol-3-yl)ethan-1-one (3s)

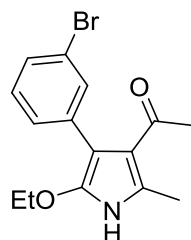


3s

Compound **3s** was prepared in 85% yield (65.6 mg) according to the general procedure (Table 3, entry 6). Pale yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 9.15 (s, 1H), 7.23 (d, $J = 7.5$ Hz, 1H), 7.18 – 7.04 (m, 3H), 3.80 (q, $J = 6.8$ Hz, 2H), 2.45 (s, 3H), 2.36 (s, 3H), 1.97 (s, 3H), 1.11 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 197.5, 140.9, 137.5, 134.7, 131.0, 127.9, 127.7, 127.4, 127.1, 119.6, 107.6, 70.2, 30.6, 21.4, 15.1, 13.7; IR

(neat): 3241 (br), 1726 (s), 1630, 1587, 1442, 1346, 1211, 1087, 668; HRESIMS Calcd for $[C_{16}H_{19}NNaO_2]^+$ ($M + Na^+$) 280.1308, found 280.1308.

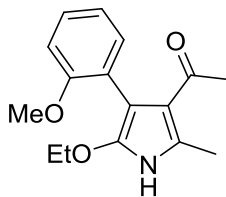
1-(4-(3-bromophenyl)-5-ethoxy-2-methyl-1H-pyrrol-3-yl)ethan-1-one (3t)



3t

Compound **3t** was prepared in 64% yield (60.8 mg) according to the general procedure (Table 3, entry 7). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 9.05 (s, 1H), 7.51 (d, 1H), 7.39 (d, $J = 7.7$ Hz, 1H), 7.28 – 7.19 (m, 2H), 3.81 (q, $J = 7.0$ Hz, 2H), 2.44 (s, 3H), 2.03 (s, 3H), 1.14 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 141.3, 137.0, 133.0, 129.4, 129.3, 128.9, 127.9, 122.0, 119.5, 106.1, 70.4, 30.7, 15.1, 13.8; IR (neat): 3287 (br), 1711 (s), 1666, 1588, 1483, 1383, 1278, 1198, 1049, 798, 668; HRESIMS Calcd for $[C_{15}H_{16}BrNNaO_2]^+$ ($M + Na^+$) 344.0257, found 344.0255.

1-(5-ethoxy-4-(2-methoxyphenyl)-2-methyl-1H-pyrrol-3-yl)ethan-1-one (3u)

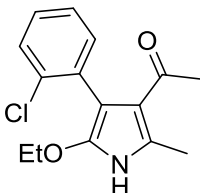


3u

Compound **3u** was prepared in 73% yield (60.2 mg) according to the general procedure (Table 3, entry 8). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 8.83 (s, 1H), 7.34 – 7.28 (m, 2H), 7.03 – 6.97 (m, 1H), 6.93 (d, $J = 8.0$ Hz, 1H), 3.84 – 3.77 (m, 5H), 2.47 (s, 3H), 1.92 (s, 3H), 1.12 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 157.4, 140.9, 132.2, 128.4, 127.3, 123.8, 120.5, 119.9, 110.5, 102.6, 69.9, 55.2, 29.2, 15.0, 13.8;

IR (neat): 3211 (br), 1684 (s), 1540, 1489, 1339, 1252, 1154, 1087, 754, 567; HRESIMS Calcd for $[C_{16}H_{19}NNaO_3]^+$ ($M + Na^+$) 296.1257, found 296.1256.

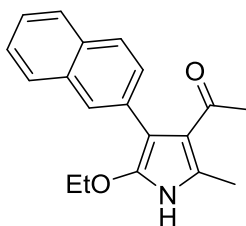
1-(4-(2-chlorophenyl)-5-ethoxy-2-methyl-1H-pyrrol-3-yl)ethan-1-one (3v)



3v

Compound **3v** was prepared in 90% yield (78.3 mg) according to the general procedure (Table 3, entry 9). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 8.80 (s, 1H), 7.47 – 7.42 (m, 1H), 7.38 – 7.32 (m, 1H), 7.28 – 7.24 (m, 2H), 3.86 – 3.70 (m, 2H), 2.49 (s, 3H), 1.90 (s, 3H), 1.10 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.1, 140.9, 135.4, 134.3, 133.0, 129.3, 128.6, 128.0, 126.6, 119.4, 104.0, 69.9, 29.6, 15.1, 14.1; IR (neat): 3173 (br), 1717 (s), 1653, 1558, 1473, 1362, 1203, 1111, 1034, 924, 759, 651; HRESIMS Calcd for $[C_{15}H_{16}ClNNaO_2]^+$ ($M + Na^+$) 300.0762, found 300.0762.

1-(5-ethoxy-2-methyl-4-(naphthalen-2-yl)-1H-pyrrol-3-yl)ethan-1-one (3w)

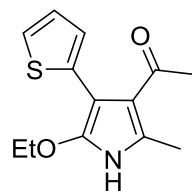


3w

Compound **3w** was prepared in 91% yield (80.1 mg) according to the general procedure (Table 3, entry 10). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 9.04 (s, 1H), 7.87 – 7.78 (m, 4H), 7.52 – 7.42 (m, 3H), 3.76 (q, $J = 7.0$ Hz, 2H), 2.47 (s, 3H), 1.98 (s, 3H), 1.06 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 141.3, 133.4, 132.4, 132.1, 128.9, 128.6, 127.8, 127.7, 127.6, 127.5, 126.0, 125.6, 119.8, 107.4, 70.3, 30.7, 15.1, 13.8;

IR (neat): 3215 (br), 1698 (s), 1558, 1506, 1457, 1419, 1338, 1158, 821, 748; HRESIMS Calcd for $[C_{19}H_{19}NNaO_2]^+$ ($M + Na^+$) 316.1308, found: 316.1311.

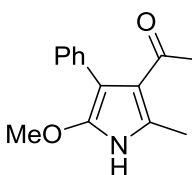
1-(5-ethoxy-2-methyl-4-(thiophen-2-yl)-1H-pyrrol-3-yl)ethan-1-one (3x)



3x

Compound **3x** was prepared in 62% yield (46.3 mg) according to the general procedure (Table 3, entry 11). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 8.74 (s, 1H), 7.31 (d, $J = 4.9$ Hz, 1H), 7.08 – 7.01 (m, 1H), 6.96 (d, $J = 6.0$ Hz, 1H), 3.90 (q, $J = 6.8$ Hz, 2H), 2.45 (s, 3H), 2.05 (s, 3H), 1.18 (t, $J = 6.9$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 142.1, 135.5, 128.1, 127.8, 126.9, 125.6, 120.2, 98.8, 70.3, 30.0, 15.2, 13.9; IR (neat): 3199 (br), 1726 (s), 1592, 1442, 1383, 1327, 1244, 1040, 850, 720, 668; HRESIMS Calcd for $[C_{13}H_{16}NO_2S]^+$ ($M + H^+$) 250.0896, found: 250.0897.

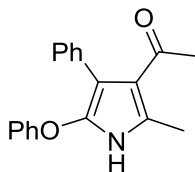
1-(5-methoxy-2-methyl-4-phenyl-1H-pyrrol-3-yl)ethan-1-one (3y)



3y

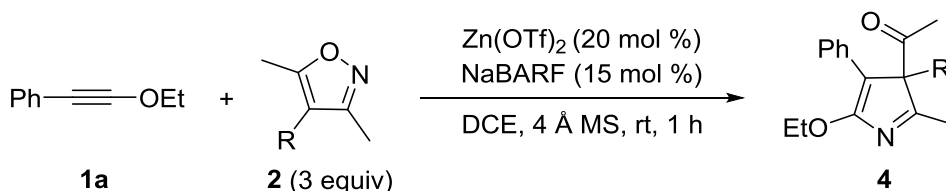
Compound **3y** was prepared in 75% yield (53.7 mg) according to the general procedure (Table 3, entry 12). Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 9.10 (s, 1H), 7.40 – 7.32 (m, 4H), 7.30 – 7.24 (m, 1H), 3.59 (s, 3H), 2.46 (s, 3H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 142.1, 134.6, 130.4, 128.1, 127.7, 126.5, 119.6, 106.6, 61.6, 30.6, 13.8; IR (neat): 3223 (br), 1710 (s), 1641, 1589, 1441, 1357, 1152, 966, 831; HRESIMS Calcd for $[C_{14}H_{15}NNaO_2]^+$ ($M + Na^+$) 252.0995, found 252.0998.

1-(2-methyl-5-phenoxy-4-phenyl-1*H*-pyrrol-3-yl)ethan-1-one (**3z**)



3z

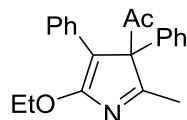
Compound **3z** was prepared in 78% yield (69.0 mg) according to the procedure (Table 3, entry 13). Pale yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 9.24 (s, 1H), 7.30 – 7.15 (m, 7H), 6.99 – 6.91 (m, 1H), 6.82 (d, *J* = 7.9 Hz, 2H), 2.42 (s, 3H), 1.91 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 197.4, 158.4, 135.6, 133.6, 129.9, 129.6, 129.5, 128.0, 126.6, 122.6, 119.5, 115.4, 110.9, 30.5, 13.8; IR (neat): 3186 (br), 1726 (s), 1658, 1620, 1572, 1535, 1441, 1118, 1005, 823, 668; HRESIMS Calcd for [C₁₉H₁₇NNaO₂]⁺ (*M* + Na⁺) 314.1151, found 314.1152.



General procedure for the synthesis of 3*H*-pyrroles **4**:

NaBARF (0.045 mmol, 39.9 mg) and Zn(OTf)₂ (0.06 mmol, 21.8 mg) was added to a mixture of the ynol ether **1a** (0.30 mmol), isoxazole **2** (0.90 mmol) and the 4 Å MS (200 mg) in dry DCE (6.0 mL), the reaction mixture was then stirred at room temperature and the progress of the reaction was monitored by TLC. The reaction typically took 1 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 3*H*-pyrrole **4**.

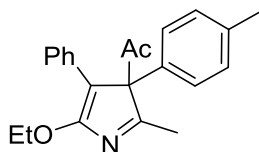
1-(5-ethoxy-2-methyl-3,4-diphenyl-3*H*-pyrrol-3-yl)ethanone (**4a**)



4a

Compound **4a** was prepared in 80% yield (76.6 mg) according to the general procedure (Table 4, entry 1). Yellow oil. This compound is known and the spectroscopic data match those reported.¹ ¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.29 (m, 5H), 7.26 – 7.20 (m, 3H), 7.06 – 6.94 (m, 2H), 4.54 – 4.42 (m, 2H), 2.02 (s, 3H), 1.46 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 204.1, 173.1, 161.0, 133.2, 132.9, 131.3, 129.4, 128.5, 128.4, 128.3, 128.2, 128.1, 84.0, 64.5, 23.0, 18.6, 14.4.

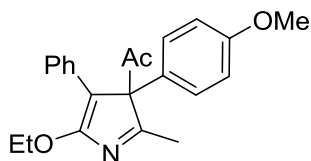
1-(5-ethoxy-2-methyl-4-phenyl-3-(p-tolyl)-3H-pyrrol-3-yl)ethan-1-one (4b)



4b

Compound **4b** was prepared in 82% yield (82.0 mg) according to the general procedure (Table 4, entry 2). Yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.27 (m, 5H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.90 (d, *J* = 8.2 Hz, 2H), 4.54 – 4.40 (m, 2H), 2.28 (s, 3H), 2.01 (s, 3H), 1.46 (s, 3H), 1.41 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 204.2, 173.2, 161.1, 138.4, 132.6, 131.5, 129.8, 129.4, 129.2, 128.3, 128.1, 128.0, 83.8, 64.4, 22.8, 21.1, 18.7, 14.7; IR (neat): 2921, 2813, 1706 (s), 1645, 1523, 1345, 1421, 1264, 1155, 1042, 855, 721; HRESIMS Calcd for [C₂₂H₂₃NNaO₂]⁺ (*M* + Na⁺) 356.1621, found 356.1621.

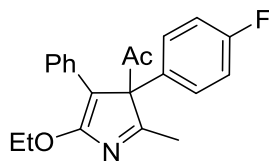
1-(5-ethoxy-3-(4-methoxyphenyl)-2-methyl-4-phenyl-3H-pyrrol-3-yl)ethan-1-one (4c)



4c

Compound **4c** was prepared in 84% yield (83.8 mg) according to the general procedure (Table 4, entry 3). Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.37 – 7.27 (m, 5H), 6.97 (d, $J = 8.8$ Hz, 2H), 6.75 (d, $J = 8.8$ Hz, 2H), 4.55 – 4.42 (m, 2H), 3.76 (s, 3H), 2.01 (s, 3H), 1.47 (s, 3H), 1.41 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.4, 173.3, 160.6, 159.7, 131.9, 131.7, 129.7, 129.5, 128.4, 128.0, 125.0, 114.0, 83.6, 64.6, 55.1, 22.9, 18.9, 14.4; IR (neat): 2931, 2845, 1713 (s), 1623, 1513, 1345, 1419, 1253, 1180, 1030, 835, 738; HRESIMS Calcd for $[\text{C}_{22}\text{H}_{23}\text{NNaO}_3]^+$ ($\text{M} + \text{Na}^+$) 372.1570, found 372.1574.

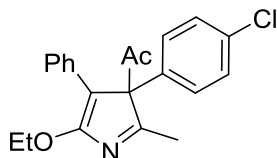
1-(5-ethoxy-3-(4-fluorophenyl)-2-methyl-4-phenyl-3H-pyrrol-3-yl)ethan-1-one (4d)



4d

Compound **4d** was prepared in 73% yield (74.1 mg) according to the general procedure (Table 4, entry 4). Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.37 – 7.28 (m, 5H), 7.02 – 6.96 (m, 2H), 6.96 – 6.89 (m, 2H), 4.54 – 4.44 (m, 2H), 2.02 (s, 3H), 1.46 (s, 3H), 1.42 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.3, 173.0, 162.5 (d, $J = 248.0$ Hz), 159.7, 133.3, 131.0, 130.1 (d, $J = 8.0$ Hz), 129.4, 128.9 (d, $J = 4.0$ Hz), 128.4, 128.2, 115.7 (d, $J = 21.0$ Hz), 83.9, 64.7, 23.0, 18.7, 14.3; IR (neat): 2927, 1715 (s), 1602, 1508, 1404, 1344, 1226, 1159, 1029, 782, 698; HRESIMS Calcd for $[\text{C}_{21}\text{H}_{20}\text{FNNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 360.1370, found 360.1372.

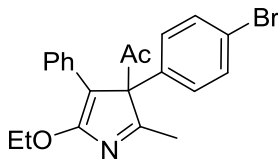
1-(3-(4-chlorophenyl)-5-ethoxy-2-methyl-4-phenyl-3H-pyrrol-3-yl)ethan-1-one (4e)



4e

Compound **4e** was prepared in 77% yield (81.5 mg) according to the general procedure (Table 4, entry 5). Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.39 – 7.29 (m, 5H), 7.21 (d, $J = 8.4$ Hz, 2H), 6.94 (d, $J = 8.4$ Hz, 2H), 4.56 – 4.41 (m, 2H), 2.02 (s, 3H), 1.48 – 1.38 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.2, 173.0, 159.5, 134.6, 133.7, 131.3, 130.9, 129.6, 129.4, 128.9, 128.4(3), 128.3(6), 83.9, 64.8, 23.1, 18.7, 14.7; IR (neat): 2923, 1714 (s), 1631, 1567, 1402, 1344, 1092, 932, 833, 698; HRESIMS Calcd for $[\text{C}_{21}\text{H}_{20}\text{ClNNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 376.1075, found 376.1078.

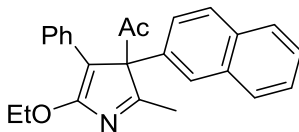
1-(3-(4-bromophenyl)-5-ethoxy-2-methyl-4-phenyl-3H-pyrrol-3-yl)ethan-1-one (**4f**)



4f

Compound **4f** was prepared in 76% yield (91.7 mg) according to the general procedure (Table 4, entry 6). Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.43 – 7.30 (m, 7H), 6.88 (d, $J = 8.4$ Hz, 2H), 4.53 – 4.44 (m, 2H), 2.01 (s, 3H), 1.48 – 1.38 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.1, 173.0, 159.5, 133.8, 131.8, 131.7, 130.9, 129.8, 129.4, 128.5, 128.4, 122.9, 83.9, 64.8, 23.1, 18.7, 14.4; IR (neat): 2927, 1714 (s), 1631, 1565, 1484, 1376, 1344, 1008, 758, 678; HRESIMS Calcd for $[\text{C}_{21}\text{H}_{20}\text{BrNNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 420.0570, found 420.0572.

1-(5-ethoxy-2-methyl-3-(naphthalen-2-yl)-4-phenyl-3H-pyrrol-3-yl)ethan-1-one (**4g**)

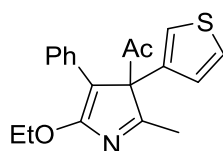


4g

Compound **4g** was prepared in 68% yield (75.3 mg) according to the general procedure (Table 4, entry 7). Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.80 – 7.73 (m, 2H), 7.67 (d, $J = 8.6$ Hz, 1H), 7.56 (s, 1H), 7.52 – 7.44 (m, 2H), 7.44 – 7.38 (m, 2H), 7.38 – 7.30 (m,

3H), 7.12 – 7.07 (m, 1H), 4.61 – 4.50 (m, 2H), 2.13 (s, 3H), 1.57 (s, 3H), 1.48 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.2, 173.2, 160.8, 133.5, 133.1, 132.8, 131.3, 130.3, 129.6, 128.4, 128.3, 128.2, 128.1, 127.5(4), 127.4(9), 126.8, 126.4, 126.0, 84.0, 64.7, 23.0, 18.8, 14.4; IR (neat): 2923, 1713 (s), 1626, 1556, 1444, 1375, 1342, 1238, 1029, 782, 694; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{23}\text{NNaO}_2]^+$ ($\text{M} + \text{Na}^+$) 392.1621, found 392.1625.

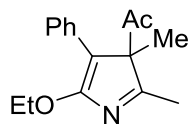
1-(5-ethoxy-2-methyl-4-phenyl-3-(thiophen-3-yl)-3H-pyrrol-3-yl)ethan-1-one (4h)



4h

Compound **4h** was prepared in 72% yield (70.2 mg) according to the general procedure (Table 4, entry 8). Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.49 – 7.36 (m, 5H), 7.24 (d, $J = 1.4$ Hz, 1H), 7.17 – 7.12 (m, 1H), 6.75 (d, $J = 5.0$ Hz, 1H), 4.48 (q, $J = 7.0$ Hz, 2H), 1.99 (s, 3H), 1.59 (s, 3H), 1.40 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 205.0, 173.2, 155.1, 132.8, 131.9, 131.8, 129.4, 128.5, 128.4, 127.0, 125.6, 125.5, 83.2, 64.8, 22.9, 19.8, 14.4; IR (neat): 2928, 1713 (s), 1630, 1563, 1404, 1340, 1207, 1029, 776, 702; HRESIMS Calcd for $[\text{C}_{19}\text{H}_{19}\text{NNaO}_2\text{S}]^+$ ($\text{M} + \text{Na}^+$) 348.1029, found 348.1027.

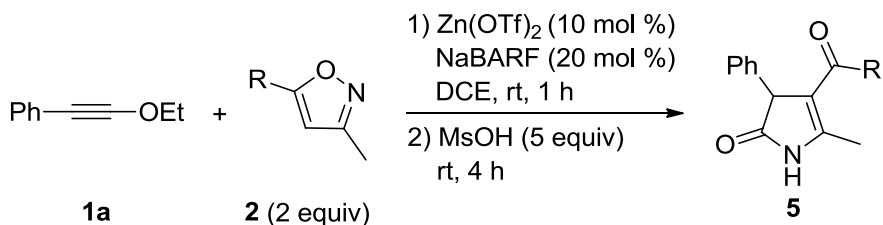
1-(5-ethoxy-2,3-dimethyl-4-phenyl-3H-pyrrol-3-yl)ethan-1-one (4i)



4i

Compound **4i** was prepared in 33% yield (25.4 mg) according to the general procedure (Table 4, entry 9). Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.51 – 7.30 (m, 5H), 4.53 – 4.37 (m, 2H), 1.96 (s, 3H), 1.91 (s, 3H), 1.47 (s, 3H), 1.41 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 206.2, 173.2, 159.1, 131.9, 131.3, 129.0, 128.2, 127.8, 84.3, 64.3,

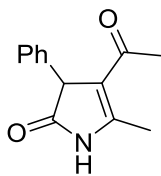
23.8, 18.9, 14.4, 11.8; IR (neat): 2939, 1710 (s), 1678, 1597, 1454, 1378, 1108, 894, 754; HRESIMS Calcd for $[C_{16}H_{19}NNaO_2]^+$ ($M + Na^+$) 280.1308, found 280.1305.



General procedure for the one-pot synthesis of γ -lactams **5**:

NaBARF (0.04 mmol, 35.4 mg) and $Zn(OTf)_2$ (0.02 mmol, 7.3 mg) was added successively to a solution of the ynol ether **1a** (0.20 mmol) and the isoxazole **2** (0.40 mmol) in dry DCE (4.0 mL), the reaction mixture was then stirred at room temperature and the progress of the reaction was monitored by TLC. The reaction typically took 1 h. Upon completion, MsOH (5 equiv) was added, the reaction mixture was then stirred at room temperature for another 4 h. Upon completion, saturated $NaHCO_3$ (aq.) was added to quench the reaction. The mixture was then extracted with DCM (3×10 mL) and the combined organic layer was dried over $MgSO_4$, filtered and concentrated in vacuum. The residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired γ -lactam **5**.

4-acetyl-5-methyl-3-phenyl-1,3-dihydro-2H-pyrrol-2-one (**5a**)

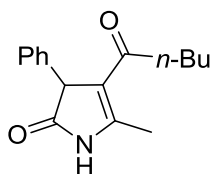


5a

Compound **5a** was prepared in 87% yield (37.5 mg) according to the general procedure. Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 9.29 (s, 1H), 7.38 – 7.28 (m, 3H), 7.24 – 7.17 (m, 2H), 4.41 (d, $J = 2.1$ Hz, 1H), 2.39 (d, $J = 2.2$ Hz, 3H), 1.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.7, 178.5, 152.4, 135.5, 129.2, 127.9(2), 127.8(7), 117.5, 54.3,

29.5, 14.2; IR (neat): 3214 (br), 1730 (s), 1660 (s), 1545, 1455, 1394, 1185, 1025, 725; HRESIMS Calcd for $[C_{13}H_{13}NNaO_2]^+$ ($M + Na^+$) 238.0838, found 238.0841.

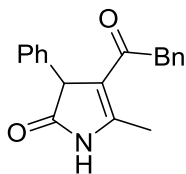
5-methyl-4-pentanoyl-3-phenyl-1,3-dihydro-2H-pyrrol-2-one (5b)



5b

Compound **5b** was prepared in 69% yield (37.2 mg) according to the general procedure. Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 7.40 – 7.27 (m, 3H), 7.25 – 7.15 (m, 2H), 4.42 (d, $J = 2.1$ Hz, 1H), 2.44 (d, $J = 2.1$ Hz, 3H), 2.31 – 1.99 (m, 2H), 1.47 – 1.31 (m, 2H), 1.19 – 1.03 (m, 2H), 0.74 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 178.6, 152.0, 135.7, 129.1, 127.9, 117.5, 54.1, 40.9, 25.8, 22.2, 14.2, 13.7; IR (neat): 3220 (br), 2957, 2855, 1725 (s), 1670 (s), 1540, 1457, 1374, 1289, 1173, 705; HRESIMS Calcd for $[C_{16}H_{19}NNaO_2]^+$ ($M + Na^+$) 280.1308, found 280.1309.

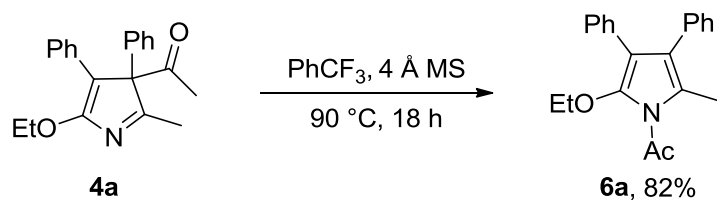
5-methyl-3-phenyl-4-(2-phenylacetyl)-1,3-dihydro-2H-pyrrol-2-one (5c)



5c

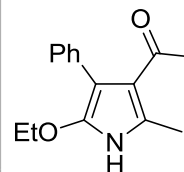
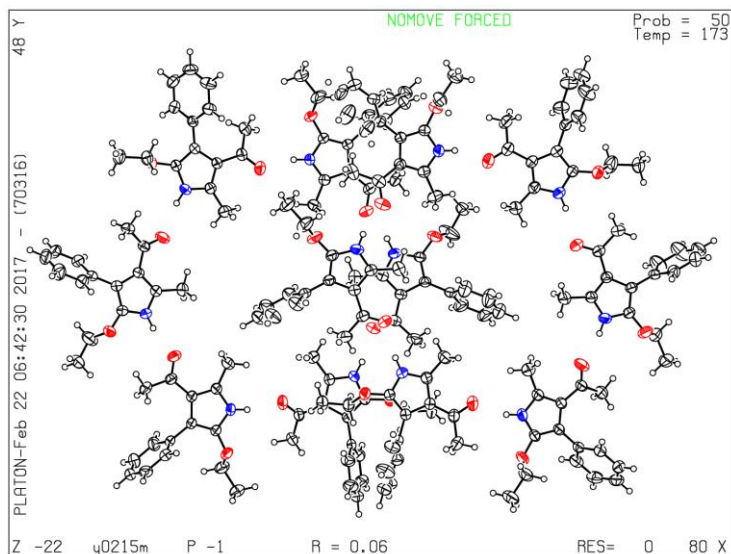
Compound **5c** was prepared in 66% yield (57.8 mg) according to the general procedure. Pale yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 8.82 (s, 1H), 7.40 – 7.30 (m, 3H), 7.26 – 7.18 (m, 5H), 6.98 – 6.90 (m, 2H), 4.34 (d, $J = 2.1$ Hz, 1H), 3.42 (q, $J = 15.5$ Hz, 2H), 2.41 (d, $J = 2.1$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.6, 178.5, 154.1, 135.3, 134.3, 129.3, 129.2, 128.5, 128.1, 128.0, 126.6, 116.4, 53.7, 48.0, 14.3; IR (neat): 3244 (br), 1734 (s), 1653 (s), 1521, 1507, 1419, 1396, 1319, 1187, 751, 704; HRESIMS Calcd for $[C_{19}H_{17}NNaO_2]^+$ ($M + Na^+$) 314.1151, found 314.1151.

1-(2-ethoxy-5-methyl-3,4-diphenyl-1H-pyrrol-1-yl)ethan-1-one (6a)



4a (0.2 mmol, 63.8 mg) was added to the suspension of 4 Å MS (150 mg) in dry PhCF₃ (2.0 mL) at room temperature. Then, the reaction mixture was stirred at 90 °C and the progress of the reaction was monitored by TLC. The reaction took 18 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 *N*-acyl pyrrole **6a** (52.3 mg, 82% yield, yellow oil). ¹H NMR (400 MHz, CDCl₃) δ 7.30 – 7.13 (m, 8H), 7.10 – 7.03 (m, 2H), 3.72 (q, *J* = 7.1 Hz, 2H), 2.69 (s, 3H), 2.34 (s, 3H), 1.16 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.9, 141.9, 134.3, 132.9, 130.5, 129.5, 127.9, 126.3, 126.0, 123.3, 121.8, 110.8, 71.3, 26.7, 15.2, 13.7; IR (neat): 2968, 1653 (s), 1558, 1507, 1457, 1362, 1318, 1076, 751, 669; HRESIMS Calcd for [C₂₁H₂₁NNaO₂]⁺ (M + Na⁺) 342.1465, found 342.1469.

Compound 3a (CCDC Number = 1819545)



Bond precision: C-C = 0.0036 Å

Wavelength=0.71073

Cell: a=19.911(3) b=20.945(3) c=23.811(4)
 alpha=106.471(3) beta=107.031(3) gamma=108.096(3)
 Temperature: 173 K

	Calculated	Reported
Volume	8223(2)	8223(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	5(C15 H17 N O2), C15 H16 N O2	5(C15 H17 N O2), C15 H16 N O2
Sum formula	C90 H101 N6 O12	C90 H101 N6 O12
Mr	1458.77	1458.76
Dx, g cm ⁻³	1.178	1.178
Z	4	4
Mu (mm ⁻¹)	0.078	0.078
F000	3116.0	3116.0
F000'	3117.38	
h,k,lmax	25,27,30	25,27,30
Nref	37692	36450
Tmin,Tmax	0.940,0.954	
Tmin'	0.940	

Correction method= Not given

Data completeness= 0.967

Theta(max)= 27.484

R(reflections)= 0.0635(22745)

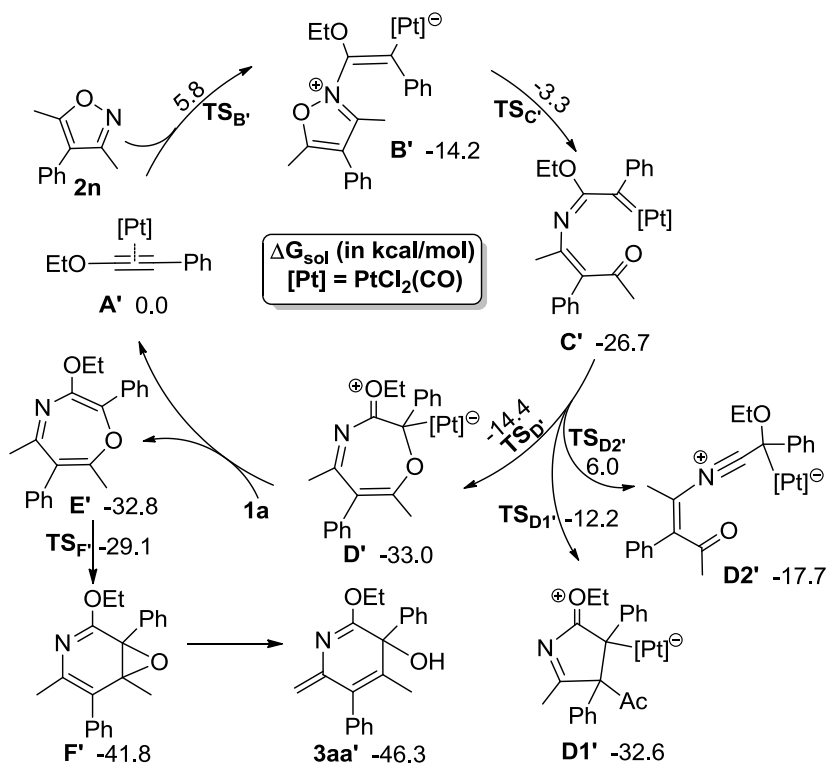
wR2(reflections)= 0.1816(36450)

S = 1.024

Npar= 1981

Computational Details

All calculations were carried out with the Gaussian 09 programs.¹¹ The geometries of all the species were fully optimized by using the density functional theory (DFT) method with the M06¹² functional. The 6-31G (d, p)¹³ basis set was used for C, H, N, O, F, S and Cl as well as the LanL (Los Alamos National Laboratory) basis sets, also known as LanL2DZ (LanL-2-double zeta),¹⁴ for Zn and Pt. 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)¹⁵ calculations. The solvent effects of DCE ($\epsilon = 10.125$) for Zn(II) catalysis and toluene ($\epsilon = 2.3741$) for Pt(II) catalysis were taken in account by using the SMD-flavor¹⁶ of self-consistent reaction field (SCRF) theory.



Scheme S1. Plausible mechanism for Pt(II)-catalyzed reaction of isoxazoles with ynol ethers. Relative free energies (ΔG_{sol}) of key intermediates and transition states were computed at the SMD-M06/6-31G(d,p)/LanL2DZ level of theory in toluene solvent at 298K.

Scheme S1 clearly shows that, in the case of the Pt(II)-catalyzed reaction of isoxazoles with ynol ethers, the platinum(II) carbene **C'**¹ favors kinetically 1,7-cyclization (via **TS_D**), but not 1,5-cyclization (via **TS_{D1}**), to give eventually the formal [4+2] annulation product, that is, 2,5-dihydropyridines **3aa'**, via 6 π electrocyclization and epoxide-opening. Such the regioselectivity of intramolecular cyclization within the key platinum(II) carbene intermediate **C'** is dominated by steric effects (i.e., in favor of the less sterically hindered carbonyl oxygen atom).¹

Reference:

1. W.-B. Shen, X.-Y. Xiao, Q. Sun, B. Zhou, X.-Q. Zhu, J.-Z. Yan, X. Lu, L.-W. Ye, *Angew. Chem. Int. Ed.* **2017**, *56*, 605.
2. Y. Jing, Y. Bai, M. Mao, G. Zhu, *J. Org. Chem.* **2014**, *79*, 9179.
3. H. Zhu, W. Jin, J. He, Y. Zhang, G. Zhu, *Adv. Synth. Catal.* **2016**, *358*, 3730.
4. H. Cai, Z. Yuan, W. Zhu, G. Zhu, *Chem. Commun.* **2011**, *47*, 8682.
5. Y. Bai, J. Yin, Z. Liu, G. Zhu, *J. Org. Chem.* **2015**, *80*, 10226.
6. J. R. Sosa, A. A. Tudjarian, T. G. Minehan, *Org. Lett.* **2008**, *10*, 5091.
7. A.-H. Zhou, Q. He, C. Shu, Y.-F. Yu, S. Liu, T. Zhao, W. Zhang, X. Lu, L.-W. Ye, *Chem. Sci.* **2015**, *6*, 1265.
8. T. J. Nitz, D. L. Volkots, D. J. Aldous, R. C. Oglesby, *J. Org. Chem.* **1994**, *59*, 5828.
9. D. J. Brunelle, *Tetrahedron Lett.* **1981**, *22*, 3699.
10. a) R. L. Sahani, R. S. Liu, *Angew. Chem. Int. Ed.* **2017**, *56*, 1026; b) S. Pusch, D. Kowalczyk, T. Opatz, *J. Org. Chem.* **2016**, *81*, 4170.
11. Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,

- O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.
12. Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215.
13. a) R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.* **1971**, *54*, 724; b) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.* **1972**, *56*, 2257; c) P. C. Hariharan, J. A. Pople, *Theo. Chim. Acta.* **1973**, *28*, 213; d) P. C. Hariharan, J. A. Pople, *Mol. Phys.* **1974**, *27*, 209; e) M. S. Gordon, *Chem. Phys. Lett.* **1980**, *76*, 163.
14. P. J. Hay, W. R. Wadt, *J. Chem. Phys.* **1985**, *82*, 270.
15. C. Gonzalez, H. B. Schlegel, *J. Phys. Chem.* **1990**, *94*, 5523.
16. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B.* **2009**, *113*, 6378.

Molecular Geometries and Energies

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

1a

Number of imaginary frequencies: 0

C	-3.40196500	2.92763300	2.71733400
C	-2.03788200	2.82982900	2.47430900
C	-1.41425600	3.69949300	1.56510200
C	-2.19377100	4.66470000	0.90716400
C	-3.55776700	4.75325300	1.15412300
C	-4.16764200	3.88752900	2.05925300
H	-3.87063900	2.24762500	3.42551700
H	-1.43943400	2.07875800	2.98585000
H	-1.71607700	5.34129000	0.20159800
H	-4.14865900	5.50576200	0.63628400
H	-5.23574100	3.96058700	2.25099200
C	-0.01284200	3.60470800	1.31339100
C	1.17705500	3.53572200	1.08827600
C	3.22886300	2.65690900	1.72984000
H	4.19241900	2.54709600	1.22572100
H	2.75180500	1.67152900	1.80085200
C	3.35886500	3.32275300	3.07080800
H	3.97684000	2.70482700	3.73072900
H	3.83174100	4.30587600	2.97460900
H	2.37815100	3.44868700	3.54420900
O	2.43947800	3.47311500	0.81398100

Energy (0K) = -461.8996579

Energy (0K) + ZPE = -461.728706

Enthalpy (298K) = -461.717362

Free Energy (298K) = -461.766355

A

Number of imaginary frequencies: 0

C	-2.95803100	4.18758900	0.68972000
C	-1.74012800	3.55772300	0.47750000
C	-1.69851000	2.28334400	-0.10743600
C	-2.89528900	1.65736700	-0.47462000
C	-4.11163400	2.29643300	-0.26373600
C	-4.14607700	3.55915600	0.32055200
H	-2.98025700	5.17430500	1.14636700
H	-0.80907000	4.04126300	0.76775900
H	-2.87139800	0.67289900	-0.94194800
H	-5.03517600	1.80191600	-0.55420800
H	-5.09903200	4.05484600	0.48984700
C	-0.41290300	1.62923000	-0.30661900
C	0.81928900	1.85827400	-0.30506900
C	2.96674900	1.84683300	0.76353200
H	3.80356100	2.48468100	0.47503000
H	3.27979700	0.79976100	0.76609700
C	2.29934500	2.27601700	2.02965500
H	3.04184800	2.22026600	2.83283200
H	1.94534400	3.31123300	1.96829400
H	1.46675800	1.61917000	2.30222500
S	2.06938700	-1.75564900	-0.10540100
O	1.45212700	-0.87641800	0.92097200
O	3.46461200	-1.51933200	-0.43634000
S	-2.36737400	-2.45623800	-0.51844800
O	-1.92978700	-1.67204900	-1.71257600
O	-1.48440000	-2.02013700	0.61076800
C	-1.82654100	-4.17328000	-0.87904000
O	-3.79076100	-2.53661500	-0.25250300
F	-1.95818500	-4.90732900	0.21277700
F	-0.56522300	-4.17251300	-1.26533900

F	-2.58238100	-4.67055000	-1.84322900
C	2.01311700	-3.44851300	0.60601100
O	1.11706000	-1.83135400	-1.26299200
F	2.88775400	-3.53009400	1.59573100
F	0.80438900	-3.71041800	1.06730600
F	2.32826400	-4.32074100	-0.33670100
Zn	-0.42064400	-0.52409200	-0.53375200
O	2.05766100	1.96383100	-0.42965400

Energy (0K) = -2449.8907198

Energy (0K) + ZPE = -2449.656008

Enthalpy (298K) = -2449.627345

Free Energy (298K) = -2449.714975

2a

Number of imaginary frequencies: 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 frequencies: 1

C	-3.67255400	2.53552000	-0.10574800
C	-2.51414200	1.76941100	-0.14956000
C	-1.47559600	2.09148900	-1.03455800
C	-1.64705600	3.17214900	-1.91176600
C	-2.80945100	3.93303600	-1.86863600
C	-3.82055400	3.62459100	-0.96096300
H	-4.46187100	2.27912900	0.59693600
H	-2.39424900	0.92322200	0.52904600
H	-0.86457900	3.40580600	-2.63104900
H	-2.92711600	4.77120000	-2.55207500
H	-4.72731600	4.22426500	-0.93013400
C	-0.24183800	1.30877500	-1.00995700
C	0.99663800	1.65917000	-1.05675300
C	3.23195400	1.64786000	-0.24094800
H	3.58324100	0.66641200	0.09108000
H	2.73716300	2.15749500	0.59122300
C	4.31269000	2.46370500	-0.88261000
H	5.10898600	2.63759200	-0.15134500
H	4.74628600	1.93390400	-1.73711600
H	3.93441700	3.43320400	-1.22217800
S	1.95849400	-1.74597900	0.74012300
O	1.41688900	-0.49876100	1.31478700
O	3.38154900	-1.79071700	0.43704400
S	-2.44052600	-2.44888300	0.15109200
O	-1.94486400	-2.17442100	-1.22901700
O	-1.59049300	-1.64893400	1.08914700

C	-1.96436000	-4.19046000	0.49380100
O	-3.87581600	-2.40284200	0.36543900
F	-2.25719300	-4.47401100	1.75299300
F	-0.67306800	-4.37144400	0.29108900
F	-2.65021300	-4.98909100	-0.30909700
C	1.70981200	-3.03306300	2.02583900
O	1.05185800	-2.19882900	-0.37204400
F	2.49750300	-2.76466300	3.05700000
F	0.45324100	-3.04953700	2.43316400
F	2.02763300	-4.21867000	1.52827100
Zn	-0.39670200	-0.69462800	-0.46352500
C	1.20756400	5.73742200	-1.73690100
C	0.64895000	5.86769000	-0.50222700
C	0.63265500	4.55502300	0.02850100
H	0.29946500	6.77401600	-0.02738000
C	0.12335700	4.08659000	1.33898100
H	0.63342300	4.60988300	2.15470100
H	-0.94695400	4.30735500	1.42733600
H	0.27311300	3.00911800	1.46116200
C	1.53035600	6.68717300	-2.81729800
H	2.60374200	6.67506200	-3.03676900
H	0.99952100	6.42213100	-3.73844300
H	1.24275200	7.69894400	-2.52292700
N	1.15765600	3.71616300	-0.84019300
O	1.51595900	4.44388500	-1.95752800
O	2.20896400	1.35662400	-1.26971300

Energy (0K) = -2774.3679509

Energy (0K) + ZPE = -2774.018958

Enthalpy (298K) = -2773.982846

Free Energy (298K) = -2774.086020

B

Number of imaginary frequencies: 0

C	-3.68713600	2.45080400	-0.00706900
C	-2.48864100	1.75536500	-0.11305500
C	-1.50173200	2.14863500	-1.03186000
C	-1.78451000	3.23029000	-1.88252500
C	-2.99041500	3.91588100	-1.78492400
C	-3.94127700	3.53803600	-0.83952000
H	-4.42939500	2.13437300	0.72248200
H	-2.29597900	0.89906600	0.53461100
H	-1.05935000	3.52279200	-2.64114300
H	-3.19186600	4.74743200	-2.45702200
H	-4.88291700	4.07703000	-0.76416600
C	-0.23116100	1.41222000	-1.07047900
C	0.95636100	2.02206200	-1.15414000
C	3.20001500	1.67003000	-0.41592500
H	3.69247100	0.70087700	-0.27821800
H	2.75693700	1.94773300	0.55008700
C	4.17730800	2.70288700	-0.91790700
H	5.06285600	2.71080000	-0.27287900
H	4.50290100	2.45906300	-1.93531200
H	3.76206800	3.71748000	-0.92001000
S	2.04678600	-1.45831600	1.07338300
O	1.57859300	-0.25977100	1.77022100
O	3.48103200	-1.58150500	0.83128300
S	-2.28662200	-2.48080500	-0.14765100
O	-1.57089200	-2.18488200	-1.43744200
O	-1.74634200	-1.59478500	0.90278500
C	-1.68123000	-4.16488100	0.27166200
O	-3.73061300	-2.61597500	-0.24931100
F	-2.04142300	-4.46314100	1.51076500

F	-0.36552500	-4.22487200	0.17122900
F	-2.21915300	-5.04264400	-0.56298100
C	1.64553500	-2.85112200	2.19618400
O	1.21416200	-1.81713200	-0.12797800
F	2.33636200	-2.71839500	3.32309100
F	0.35318500	-2.86097400	2.48434100
F	1.97316500	-4.00237900	1.62672500
Zn	-0.26794700	-0.61528900	-0.85837700
C	1.48604600	5.44247800	-1.83177800
C	0.99890700	5.60709200	-0.56470100
C	0.74058400	4.31710200	-0.07656900
H	0.85005800	6.53841400	-0.03690600
C	0.17641900	3.88911500	1.21626700
H	0.47363600	4.58847800	2.00108300
H	-0.92014200	3.89669900	1.14577300
H	0.48916200	2.87289600	1.47672000
C	1.95557800	6.37557400	-2.86546700
H	3.00402400	6.17368300	-3.11153300
H	1.36769300	6.25894400	-3.78245900
H	1.86223400	7.40217600	-2.50663200
N	1.06854100	3.45312600	-1.03588100
O	1.53382800	4.13477400	-2.14157900
O	2.14160500	1.41655500	-1.37168500

Energy (0K) = -2774.3980825

Energy (0K) + ZPE = -2774.047430

Enthalpy (298K) = -2774.011197

Free Energy (298K) = -2774.115392

TS_c

Number of imaginary frequencies: 1

C	-3.87497500	2.63890100	0.71658600
---	-------------	------------	------------

C	-2.69966500	1.90587700	0.75427400
C	-1.53166100	2.37155900	0.11647000
C	-1.60650500	3.57879700	-0.61216600
C	-2.79301500	4.29329900	-0.67283000
C	-3.92479500	3.83449200	0.00066900
H	-4.75919200	2.27282800	1.23232800
H	-2.65892900	0.96448500	1.30317100
H	-0.73443300	3.92601000	-1.16192300
H	-2.84023100	5.21149400	-1.25352100
H	-4.85139600	4.40183100	-0.04560100
C	-0.32970400	1.57845700	0.20546500
C	0.93485300	2.13045000	0.19458200
C	3.30819000	1.71781700	0.37467600
H	3.75919900	0.77188800	0.69116700
H	3.21457500	2.35359000	1.26374300
C	4.11658000	2.38089500	-0.70957900
H	5.13664300	2.56223900	-0.35301800
H	4.17606100	1.73587600	-1.59325000
H	3.67829800	3.33900900	-1.00789700
S	1.87048700	-0.89321400	2.46162100
O	1.26572600	0.36641700	2.90119700
O	3.32263300	-0.94762700	2.33757000
S	-2.31000300	-2.43257500	1.23885200
O	-1.56370800	-2.19903300	-0.04399000
O	-1.89859700	-1.38736900	2.20289100
C	-1.58118000	-3.98936300	1.88577400
O	-3.72949800	-2.71327800	1.10525100
F	-2.03253600	-4.19789700	3.11304900
F	-0.26339500	-3.91385300	1.91168900
F	-1.94445900	-4.99735900	1.10706500
C	1.48915800	-2.09095000	3.79944700

O	1.14356100	-1.49426700	1.28977500
F	2.07973700	-1.68609500	4.91841800
F	0.18407500	-2.16526500	4.00612800
F	1.94985900	-3.29216800	3.48130200
Zn	-0.43538800	-0.44903300	0.49742400
C	1.37422600	5.70095700	-0.01561400
C	0.86001700	5.55524200	1.26997200
C	0.74416200	4.20396300	1.55831000
H	0.64017100	6.35816800	1.96047200
C	0.26344600	3.61143100	2.83246700
H	0.35118900	4.34232400	3.63952800
H	-0.79450100	3.33902300	2.72364600
H	0.81874300	2.69969100	3.07522600
C	1.71985300	6.97655900	-0.69065800
H	2.79578100	7.00311900	-0.89559000
H	1.20103900	7.04395700	-1.65255400
H	1.44813100	7.83112500	-0.06689400
N	1.14615200	3.40537600	0.57158800
O	1.58548400	4.60160200	-0.65043500
O	1.99866600	1.36164900	-0.11335500

Energy (0K) = -2774.3779034

Energy (0K) + ZPE = -2774.029488

Enthalpy (298K) = -2773.993312

Free Energy (298K) = -2774.096930

C

Number of imaginary frequencies: 0

C	-2.95762600	1.26279000	-3.16632300
C	-2.00078400	0.97529300	-2.21851500
C	-0.78606100	1.72258900	-2.16737000
C	-0.58015100	2.77018000	-3.12010200

C	-1.54059800	3.04417300	-4.06480500
C	-2.72376500	2.29198800	-4.08411700
H	-3.88459000	0.69903600	-3.20427400
H	-2.15681400	0.18683000	-1.48479700
H	0.34604200	3.34173700	-3.09575600
H	-1.38897900	3.83312100	-4.79531200
H	-3.47907900	2.51375400	-4.83457200
C	0.15700200	1.40749500	-1.19554000
C	1.35800100	2.22087200	-1.00505400
C	3.73326400	2.04764800	-0.93478200
H	4.34902200	1.14421000	-0.92533300
H	3.61009800	2.40148400	0.09536000
C	4.29795800	3.10529400	-1.84443700
H	4.36624700	2.73533500	-2.87312300
H	3.68371300	4.01171500	-1.83498200
H	5.30705200	3.37221700	-1.51245600
S	2.17532200	-1.91525300	-0.30414700
O	2.18396400	-0.85067300	0.74879000
O	3.36134700	-2.02397600	-1.13611400
S	-2.39490200	-0.86650200	1.70712600
O	-2.81346200	0.39133400	1.08067900
O	-0.89943200	-1.05996800	1.67316500
C	-2.92346600	-2.16751200	0.52757300
O	-2.98916100	-1.23062100	2.98325000
F	-2.59600200	-3.36363000	0.98664400
F	-2.31336000	-1.97814600	-0.64383700
F	-4.23343500	-2.11301300	0.34225200
C	2.11929200	-3.47597700	0.65657300
O	0.85337500	-1.85572800	-0.98179000
F	3.22095800	-3.58817700	1.38230900
F	1.06597300	-3.48030000	1.45518700

F	2.03746900	-4.50002600	-0.17910700
Zn	0.22478100	-0.04831800	0.33913900
C	-0.11713000	2.42854300	2.06973000
C	-0.31035900	3.64363100	1.32967400
C	0.35367900	4.02967800	0.19336900
H	-1.01346300	4.35981100	1.75039300
C	0.08289800	5.36034500	-0.42581600
H	1.01186400	5.93866000	-0.49396900
H	-0.27747400	5.22074900	-1.45443700
H	-0.65985300	5.93134200	0.13652100
C	-0.89887400	2.27062200	3.33546700
H	-0.52547900	1.42034500	3.91167300
H	-0.87530200	3.18155900	3.94343400
H	-1.95083200	2.08618500	3.07477800
N	1.37696500	3.34571000	-0.40359300
O	0.64498500	1.50654500	1.70131000
O	2.44419900	1.58281400	-1.40888500

Energy (0K) = -2774.420908

Energy (0K) + ZPE = -2774.071942

Enthalpy (298K) = -2774.034553

Free Energy (298K) = -2774.141739

TS_D

Number of imaginary frequencies: 1

C	-2.89265300	1.65151600	-3.07865900
C	-2.02150400	1.48221100	-2.01871300
C	-0.80883500	2.20718900	-1.96341700
C	-0.49258600	3.09629900	-3.02012000
C	-1.35996900	3.24489600	-4.08635300
C	-2.55970200	2.52953200	-4.11191400
H	-3.82615200	1.09673900	-3.11317400

H	-2.25913500	0.80410300	-1.19856400
H	0.44929300	3.64328500	-3.00402600
H	-1.10790400	3.91207700	-4.90605900
H	-3.23928500	2.65162900	-4.95200700
C	0.05971600	1.98728500	-0.85598900
C	1.38342300	2.64633300	-0.79386800
C	3.71418300	2.15978800	-0.82453400
H	4.18417800	1.17849800	-0.71485900
H	3.70076100	2.66200900	0.14928000
C	4.35235000	2.98542000	-1.90600900
H	4.30734100	2.46533800	-2.86863000
H	3.86393500	3.96021900	-2.00475500
H	5.40600900	3.15282700	-1.65899900
S	2.19728100	-1.48815000	-0.36010700
O	2.16517000	-0.54756600	0.79920300
O	3.39952200	-1.48638700	-1.17614600
S	-2.29484300	-0.71038400	1.81535900
O	-2.84605400	0.47897400	1.16031600
O	-0.78383000	-0.74204000	1.75758400
C	-2.70739100	-2.08308400	0.67328900
O	-2.81976300	-1.09619400	3.11437400
F	-2.19470200	-3.22062200	1.11125100
F	-2.20215500	-1.81431400	-0.52858300
F	-4.02185300	-2.20462700	0.57081400
C	2.12992300	-3.15078600	0.41678900
O	0.88582900	-1.36568800	-1.06224300
F	3.20361300	-3.32767800	1.17076900
F	1.04590800	-3.25214600	1.16706800
F	2.09870300	-4.07683900	-0.52894700
Zn	0.19731300	0.27167800	0.33095100
C	-0.04271400	2.64570700	1.88788800

C	-0.47104100	3.58073400	0.83072800
C	0.39883900	4.37290000	0.07541400
H	-1.46350600	4.00367300	0.99595400
C	0.04860900	5.75356100	-0.32577600
H	0.94662200	6.37986000	-0.33778300
H	-0.32554100	5.72181900	-1.36124100
H	-0.72029100	6.19837800	0.30911000
C	-0.95291900	2.58147700	3.07182400
H	-0.59418700	1.83626700	3.78597200
H	-1.02899100	3.56278400	3.55532200
H	-1.96331600	2.31524100	2.73157600
N	1.57000000	3.87053900	-0.39566500
O	0.96845000	1.93691400	1.81958000
O	2.33560400	1.83649600	-1.17092600

Energy (0K) = -2774.4061692

Energy (0K) + ZPE = -2774.057253

Enthalpy (298K) = -2774.021132

Free Energy (298K) = -2774.124789

D

Number of imaginary frequencies: 0

C	-3.20244200	1.51626300	-2.42307900
C	-2.26276700	1.93282300	-1.48855100
C	-0.88964800	1.72768900	-1.69947200
C	-0.49444600	1.04869600	-2.86578300
C	-1.43981400	0.64331100	-3.80020300
C	-2.79629800	0.87751500	-3.59016600
H	-4.25885300	1.69077800	-2.23114100
H	-2.60903600	2.41402100	-0.57539700
H	0.55397700	0.82653800	-3.03503700
H	-1.10870000	0.12907700	-4.69980900

H	-3.53096200	0.55101000	-4.32232200
C	0.07894000	2.19111300	-0.67417900
C	1.45533800	2.38274100	-0.85996800
C	3.60036000	2.09384800	-1.87813300
H	4.00241900	1.20268200	-2.36531400
H	4.00952700	2.15569800	-0.86614900
C	3.82889100	3.34735200	-2.67532200
H	3.36423800	3.27247600	-3.66418400
H	3.42313100	4.22394800	-2.15829100
H	4.90443600	3.49988700	-2.81329700
S	2.35005900	-1.04750300	-0.01405800
O	1.99572700	-0.15059000	1.13544500
O	3.65081200	-0.84640600	-0.62700800
S	-2.55537600	-1.34042900	1.15148200
O	-3.14709300	-0.03274200	0.87332000
O	-1.04733700	-1.28177900	1.27283100
C	-2.71406900	-2.25047300	-0.43097900
O	-3.16735500	-2.18700500	2.16293500
F	-2.17702600	-3.45715700	-0.32878200
F	-2.08227800	-1.57375300	-1.38498200
F	-3.99186700	-2.36993000	-0.76092100
C	2.41454900	-2.72415600	0.73068300
O	1.15610100	-1.09055600	-0.90700800
F	3.36783300	-2.76103500	1.64785900
F	1.25197400	-3.00763300	1.28794900
F	2.67905600	-3.60826900	-0.21716900
Zn	-0.02615100	0.23264900	0.45678200
C	-0.89900100	2.67025200	1.67160500
C	-0.27301700	3.20796200	0.39398600
C	1.09931600	3.75496000	0.76428500
H	-0.88688100	4.03634800	0.00564600

C	1.34314000	4.70973300	1.86130000
H	2.38239800	5.04494000	1.84261200
H	0.66971600	5.57163200	1.79185200
H	1.15158500	4.23027800	2.83234700
C	-1.78628000	3.54923100	2.46313600
H	-1.84676300	3.21114300	3.49973800
H	-1.49515600	4.60207000	2.39876500
H	-2.78749200	3.46615700	2.01302300
N	2.04856000	3.25913100	0.04167400
O	-0.64361800	1.52184800	2.03427500
O	2.17078900	1.81322700	-1.78551000

Energy (0K) = -2774.4923819

Energy (0K) + ZPE = -2774.140335

Enthalpy (298K) = -2774.104538

Free Energy (298K) = -2774.208494

E

Number of imaginary frequencies: 0

C	-3.24814600	1.47716100	-2.26260000
C	-2.27586900	2.07543800	-1.47118900
C	-0.90527200	1.90300900	-1.73849100
C	-0.55538900	1.09784000	-2.83940600
C	-1.53123500	0.50208600	-3.62724200
C	-2.88407700	0.68534000	-3.34814500
H	-4.29945200	1.63265900	-2.02781100
H	-2.59045800	2.69467500	-0.63156800
H	0.49395900	0.94202300	-3.07163100
H	-1.22988800	-0.11497900	-4.47182800
H	-3.64439500	0.21583900	-3.96819600
C	0.08955000	2.54486300	-0.89876800
C	1.45167100	2.53343100	-0.97727200

C	3.59942900	2.09504800	-1.92033000
H	3.98593600	1.24150600	-2.48593700
H	4.00197000	2.04358100	-0.90290000
C	3.94722200	3.39865600	-2.59205200
H	3.51239900	3.44621400	-3.59663200
H	3.57964200	4.25171100	-2.01100400
H	5.03480900	3.49334200	-2.68470200
C	-0.90803100	2.63161800	1.45881600
C	-0.22336500	3.38274700	0.30397100
C	1.16044200	3.78601700	0.76137800
H	-0.80767000	4.28716200	0.07107100
C	1.42796100	4.63461500	1.94479800
H	2.49685300	4.85047700	2.02203200
H	0.87045500	5.57780100	1.89095200
H	1.10861500	4.12732900	2.86592200
C	-1.91419000	3.41543900	2.24205600
H	-2.24967100	2.84977000	3.11444900
H	-1.49716900	4.38192900	2.55227300
H	-2.77367500	3.64413900	1.59742400
N	2.09145000	3.28462000	0.02168300
O	-0.61736400	1.48210200	1.71081400
O	2.17853800	1.88116800	-1.88699900

Energy (0K) = -786.4877423

Energy (0K) + ZPE = -786.200048

Enthalpy (298K) = -786.181499

Free Energy (298K) = -786.246520

3a

Number of imaginary frequencies: 0

O	17.34503500	-5.48537700	-5.46445100
N	15.58966100	-6.18399200	-6.88144200

H	16.00905900	-5.81434800	-7.72710100
O	12.08238500	-8.15294500	-5.81677500
C	15.28995200	-6.63286200	-4.70862000
C	16.13905500	-6.06141000	-5.62506700
C	14.15406100	-7.11311900	-5.46563500
C	15.63135400	-6.78236500	-3.28502900
C	14.38471400	-6.81133100	-6.80899900
C	12.87781600	-7.66639700	-5.01545300
C	16.02907800	-5.67232200	-2.52890900
H	16.03282800	-4.68790200	-2.99359500
C	18.43877600	-6.41661600	-5.38372600
H	18.56754500	-6.90309000	-6.36307500
H	18.19215100	-7.19806200	-4.64937800
C	12.51354700	-7.59798600	-3.55492800
H	11.42601600	-7.67184300	-3.46457300
H	12.86911200	-6.68146900	-3.07247500
H	12.95581700	-8.44306500	-3.01346800
C	16.40602200	-5.81574500	-1.19698500
H	16.70705700	-4.94038000	-0.62496400
C	19.66251700	-5.64751600	-4.97362200
H	19.88561400	-4.85518400	-5.69662600
H	20.52873400	-6.31436900	-4.91425000
H	19.51048300	-5.18768700	-3.99021800
C	16.38993500	-7.07109700	-0.59534700
H	16.68081100	-7.18291800	0.44689900
C	13.55130000	-7.00736500	-8.02065800
H	14.01377100	-6.51983100	-8.88624200
H	12.54546500	-6.59608800	-7.88192400
H	13.41885900	-8.07016300	-8.25033300
C	15.63403500	-8.04266800	-2.67103900
H	15.35467200	-8.91831200	-3.25626600

C	16.00295900	-8.18448400	-1.33808100
H	15.99810400	-9.17125300	-0.87944200

Energy (0K) = -786.5063082

Energy (0K) + ZPE = -786.217423

Enthalpy (298K) = -786.198965

Free Energy (298K) = -786.263925

TS_{D1}

Number of imaginary frequencies: 1

C	-1.80281800	0.71066200	-4.15701900
C	-0.98605200	0.89310700	-3.04702800
C	-0.59347900	2.17902000	-2.66619700
C	-1.02865900	3.28402200	-3.41017300
C	-1.84481000	3.09949700	-4.51730200
C	-2.23037900	1.81266400	-4.89122500
H	-2.10755500	-0.29222700	-4.44505500
H	-0.65652400	0.03797200	-2.45820700
H	-0.72418700	4.28859600	-3.11824700
H	-2.18209600	3.95933700	-5.09107900
H	-2.87173200	1.67068800	-5.75801500
C	0.31551200	2.34180200	-1.51247000
C	0.52995300	3.53824200	-0.83766100
C	2.87208300	2.41554400	-1.36394100
H	2.95590000	1.39888200	-1.76996600
H	2.74105700	2.35793700	-0.27462800
C	4.02149300	3.30281300	-1.74168800
H	4.11791400	3.38252000	-2.82920400
H	3.88728400	4.30630100	-1.32251700
H	4.95113100	2.88400000	-1.34296200
S	1.83847900	-1.70634700	-0.13937300
O	2.08194700	-0.43204700	0.61285400

O	2.99050000	-2.28982300	-0.80613000
S	-2.45621100	-0.20844700	0.87421600
O	-2.68341900	0.05193800	-0.54559300
O	-1.01914200	0.01770800	1.26768100
C	-2.60842600	-2.02616100	1.04916700
O	-3.40284700	0.33901800	1.83851700
F	-2.34998300	-2.39066900	2.29693000
F	-1.76358700	-2.63595300	0.23361400
F	-3.84716700	-2.39347600	0.74200600
C	1.38999000	-2.90412200	1.18072700
O	0.59706900	-1.53483700	-0.93191400
F	2.45055800	-3.13566600	1.94080800
F	0.41601800	-2.42170600	1.93253400
F	0.99600700	-4.03870100	0.62280200
Zn	0.37331700	0.69910600	-0.06520700
C	0.24564100	2.82353200	2.32763600
C	-0.08227300	4.23011000	2.15739800
C	0.10986500	4.98129100	1.04542800
H	-0.51678300	4.73987300	3.01491400
C	-0.22396900	6.42522600	0.96030900
H	0.67669800	7.00218700	0.71768800
H	-0.94216700	6.59920500	0.14962600
H	-0.64764900	6.78777600	1.89930800
C	-0.18543600	2.18567500	3.60374300
H	0.19214000	1.16339600	3.66654900
H	0.15219300	2.77650200	4.46342400
H	-1.28275400	2.16963000	3.64330400
N	0.71057900	4.47921100	-0.10451300
O	0.85529000	2.17299900	1.46396900
O	1.66688000	2.99309300	-1.94776200

Energy (0K) = -2774.3767927

Energy (0K) + ZPE = -2774.028172

Enthalpy (298K) = -2773.992542

Free Energy (298K) = -2774.092800

D1

Number of imaginary frequencies: 0

C	-0.65994900	0.19531100	-4.49042600
C	0.20476200	0.64154100	-3.49957000
C	-0.12212300	1.76709600	-2.73635300
C	-1.31770000	2.44322300	-2.98711500
C	-2.18850300	1.98303600	-3.96930300
C	-1.86288400	0.85996000	-4.72299900
H	-0.39682800	-0.68034600	-5.07933000
H	1.14388600	0.12254200	-3.31148300
H	-1.57203400	3.33620100	-2.41664700
H	-3.11931800	2.51460500	-4.15384600
H	-2.54235600	0.50414200	-5.49395500
C	0.84048700	2.20656900	-1.67986000
C	0.40496000	3.15822100	-0.76520000
C	3.20440600	2.07347100	-1.27519200
H	3.09207000	1.03115800	-0.92077300
H	3.16704000	2.72908700	-0.39031800
C	4.49063800	2.25511600	-2.03153700
H	4.52025100	1.59821500	-2.90754700
H	4.59822200	3.29095000	-2.37124300
H	5.34250600	2.01223900	-1.38855600
S	1.64731700	-2.09605900	-0.22228300
O	2.08719200	-0.90204700	0.57394200
O	2.69751100	-2.83373000	-0.90424500
S	-2.27315300	0.13013200	0.93116300
O	-2.51242100	0.62545500	-0.42441900

O	-0.80400300	-0.02956500	1.23093900
C	-2.81711800	-1.62216500	0.91724000
O	-3.01179100	0.74713700	2.02661000
F	-2.66067400	-2.15393300	2.12147100
F	-2.11111200	-2.32030000	0.04245500
F	-4.10053700	-1.67852400	0.58356400
C	0.98514800	-3.26312300	1.03044000
O	0.45642500	-1.69497700	-1.00980100
F	1.97146200	-3.67264500	1.81407800
F	0.05473100	-2.68365100	1.76705400
F	0.46022200	-4.30482900	0.40360000
Zn	0.61634700	0.51172200	-0.13914000
C	0.65129600	2.33578900	2.49227100
C	-0.07914100	3.60800600	2.42749200
C	-0.34731600	4.34046300	1.32677600
H	-0.44607500	4.00735500	3.37137300
C	-1.07826700	5.63166900	1.34129500
H	-0.45192600	6.42073900	0.90754100
H	-1.98168100	5.56304100	0.72341100
H	-1.35852700	5.90933100	2.35942700
C	0.65741000	1.64406400	3.80716300
H	1.24258100	0.72350000	3.75486300
H	1.04982700	2.30714600	4.58788700
H	-0.37932700	1.40944700	4.08522100
N	0.03727500	3.93315300	0.04856200
O	1.22380000	1.86094200	1.50822100
O	2.13267600	2.37941500	-2.16519000

Energy (0K) = -2774.4132608

Energy (0K) + ZPE = -2774.063898

Enthalpy (298K) = -2774.027428

Free Energy (298K) = -2774.129510

TS_{D2}

Number of imaginary frequencies: 1

C	-3.68813800	2.54343700	-1.13962600
C	-2.51868400	1.98085700	-0.66738400
C	-1.26095900	2.54075700	-1.00246200
C	-1.22346000	3.67532500	-1.85134100
C	-2.39586600	4.21470900	-2.34499900
C	-3.62347500	3.65656500	-1.98096500
H	-4.64968800	2.11207200	-0.87638900
H	-2.54295300	1.08841100	-0.03980500
H	-0.26476500	4.09879200	-2.14415300
H	-2.36535800	5.07055200	-3.01343600
H	-4.54342200	4.08808000	-2.36869100
C	-0.08765100	1.89682700	-0.52635400
C	1.24352500	2.45023100	-0.82490400
C	3.33019100	1.91819600	-1.85804400
H	3.81722900	0.94612800	-1.97564200
H	3.79045800	2.44250100	-1.01396000
C	3.36005100	2.73029500	-3.12599100
H	4.39954600	2.90882400	-3.42098600
H	2.86212500	2.19502500	-3.94162000
H	2.87261900	3.70268700	-2.99222900
S	2.32718000	-1.21452400	0.32566500
O	2.07167700	-0.03598200	1.19897200
O	3.51058500	-1.18770600	-0.51828800
S	-2.05544200	-1.60881400	1.66812500
O	-2.24065600	-1.37646200	0.22432700
O	-0.85245400	-0.82911500	2.14283800
C	-1.48102100	-3.34699900	1.81455000
O	-3.21526500	-1.52000900	2.53988100

F	-1.10688200	-3.58220300	3.06246900
F	-0.46340200	-3.57077000	1.00153800
F	-2.47831900	-4.15896800	1.49552500
C	2.61731900	-2.59667600	1.50223300
O	1.03194500	-1.56576400	-0.33689500
F	3.80097500	-2.43637600	2.07477700
F	1.68233000	-2.60929400	2.43749900
F	2.59944500	-3.74652600	0.84648700
Zn	-0.07080700	0.12027600	0.51663100
C	0.02960000	3.39276400	2.05823900
C	0.39943500	4.57321500	1.34943400
C	1.10803800	4.62937500	0.17426600
H	0.14261800	5.52102700	1.81761800
C	1.41384700	5.95545800	-0.44325600
H	0.90287800	6.77654000	0.06539900
H	2.49564400	6.13436300	-0.42019800
H	1.12291200	5.94933900	-1.50218200
C	-0.56515500	3.53501800	3.42012600
H	-1.63052500	3.77898900	3.30718100
H	-0.48711900	2.59453200	3.97106200
H	-0.09828400	4.34930100	3.98216100
N	1.70256400	3.60028900	-0.49650200
O	0.15778700	2.23849200	1.57756700
O	1.97015100	1.57182100	-1.49774100

Energy (0K) = -2774.4152595

Energy (0K) + ZPE = -2774.066500

Enthalpy (298K) = -2774.030135

Free Energy (298K) = -2774.134265

D2

Number of imaginary frequencies: 0

C	-3.79047300	2.75781200	-0.92670700
C	-2.60456600	2.30729700	-0.36368400
C	-1.39299100	2.42480900	-1.06103300
C	-1.40914100	2.97646700	-2.34683400
C	-2.60609700	3.40490400	-2.91678800
C	-3.79781500	3.30821500	-2.20802400
H	-4.71823300	2.66774300	-0.36608600
H	-2.61359900	1.85477500	0.62851200
H	-0.48518300	3.07228700	-2.91800200
H	-2.59900500	3.82730500	-3.91915600
H	-4.72919800	3.65360300	-2.65021500
C	-0.14533400	1.86480700	-0.45837600
C	1.13241300	2.36484400	-1.05967200
C	3.16631500	1.73583600	-2.17060400
H	3.72855900	0.80566100	-2.04576300
H	3.63408400	2.52160400	-1.57033800
C	3.00515600	2.12370900	-3.61532300
H	3.99304600	2.26862700	-4.06488600
H	2.48992300	1.33509500	-4.17395500
H	2.44334800	3.05844600	-3.71740200
S	2.35267800	-1.36335900	0.18586200
O	2.03701600	-0.27506800	1.11625500
O	3.64671600	-1.35063100	-0.48401400
S	-2.22946500	-1.85816400	0.44298300
O	-1.96871500	-1.50317100	-0.98647400
O	-1.22530800	-1.11579600	1.26244600
C	-1.71385800	-3.61814000	0.56731000
O	-3.60799100	-1.82920800	0.89608300
F	-1.63968600	-3.95896000	1.84383800
F	-0.53809900	-3.79338400	-0.00643100
F	-2.61298600	-4.37591500	-0.04050700

C	2.36396800	-2.87882000	1.21909300
O	1.19040600	-1.63101300	-0.73875600
F	3.38366100	-2.81750800	2.06536700
F	1.23795800	-2.97223900	1.90961100
F	2.49812700	-3.95255400	0.45464200
Zn	-0.25077500	-0.21001200	-0.48055200
C	-0.07013700	3.38100200	1.46680500
C	0.21257400	4.53831800	0.75678900
C	0.86957700	4.61721200	-0.47196400
H	-0.02172900	5.47429100	1.25804300
C	1.01738000	5.93460600	-1.14242400
H	0.49608300	6.73445400	-0.61281800
H	2.07921700	6.18768300	-1.24265700
H	0.61869200	5.85259100	-2.16254400
C	-0.45979900	3.41057500	2.89256500
H	-1.52801200	3.16861200	2.97496900
H	0.08357200	2.63141600	3.43834700
H	-0.27394400	4.38565200	3.34572400
N	1.50161300	3.60488300	-1.09528300
O	-0.04623100	2.16168700	0.97877700
O	1.86791900	1.42236400	-1.59222200

Energy (0K) = -2774.4409608

Energy (0K) + ZPE = -2774.090793

Enthalpy (298K) = -2774.054376

Free Energy (298K) = -2774.159045

F

Number of imaginary frequencies: 0

C	-3.74646500	1.52349900	-0.64931200
C	-2.52051900	1.97546200	-0.17749700
C	-1.39986100	2.06507600	-1.02395900

C	-1.56555400	1.67794700	-2.36767100
C	-2.79456700	1.22816800	-2.83138100
C	-3.89450400	1.14663300	-1.98035400
H	-4.59198300	1.46406600	0.03316200
H	-2.41666100	2.26119600	0.86543200
H	-0.72152200	1.72373800	-3.04606700
H	-2.89202400	0.93771300	-3.87567100
H	-4.85347800	0.79173800	-2.35123400
C	-0.14247000	2.56565000	-0.46706300
C	1.10919300	2.58606000	-1.00915600
C	2.12129900	2.72350000	-3.14526800
H	2.26087500	2.03625800	-3.98579900
H	3.10454400	2.91918600	-2.69925400
C	1.44947900	4.00192000	-3.58368200
H	2.06617400	4.51899500	-4.32692500
H	0.46993700	3.79728000	-4.03169800
H	1.30095100	4.68405600	-2.73677300
C	-0.11142900	4.36958500	0.91309700
C	1.09776100	4.92384500	0.70855000
C	2.25969700	4.13515100	0.34145300
H	1.22527100	5.99298400	0.87087100
C	3.58130200	4.62176000	0.84015500
H	3.74592300	5.66287300	0.53344700
H	3.60708900	4.61252700	1.93725000
H	4.39373100	3.99942400	0.45609900
C	-1.35560200	5.07927300	1.28507800
H	-2.12462300	4.90800700	0.51937500
H	-1.75173200	4.68017500	2.22768100
H	-1.19184700	6.15521600	1.38910300
N	2.24704600	3.07857400	-0.41466500
O	-0.22641700	2.99602700	0.86527000

O 1.30896900 1.99562900 -2.21482400

Energy (0K) = -786.4529669

Energy (0K) + ZPE = -786.165104

Enthalpy (298K) = -786.147130

Free Energy (298K) = -786.210203

TS_G

Number of imaginary frequencies: 1

C	-3.65954300	1.23286100	-0.52725300
C	-2.43632800	1.67684800	-0.03763800
C	-1.47190000	2.22166300	-0.89919000
C	-1.78446600	2.33268300	-2.26396100
C	-3.00694100	1.88795100	-2.74770400
C	-3.94961400	1.33175100	-1.88446300
H	-4.38915400	0.80723500	0.15853600
H	-2.21483100	1.60511000	1.02444100
H	-1.06054200	2.77091300	-2.94489900
H	-3.22914900	1.98252800	-3.80859100
H	-4.90603600	0.98356600	-2.26818500
C	-0.20309000	2.70616100	-0.34725300
C	1.05445500	2.71288200	-0.98076100
C	2.21462300	2.35827800	-3.04309000
H	2.18266500	1.55302000	-3.78403600
H	3.15856500	2.28274700	-2.49283500
C	2.06419000	3.70811500	-3.70032400
H	2.86870100	3.86203800	-4.42813500
H	1.10806100	3.78008600	-4.23209100
H	2.11565900	4.51796100	-2.96389800
C	-0.22871300	4.19877800	0.88418800
C	0.96339900	4.90444100	0.82185900
C	2.13814500	4.32294000	0.32875900

H	0.95983200	5.96263100	1.07868900
C	3.46328900	4.95713200	0.61189900
H	3.34825500	5.97561000	0.99710800
H	4.00400800	4.37893300	1.37276700
H	4.08965400	4.97411300	-0.28684900
C	-1.55698100	4.80606000	1.15875000
H	-2.31894400	4.42549300	0.46758800
H	-1.88649000	4.54496500	2.17277900
H	-1.51563800	5.89477100	1.06495400
N	2.15651000	3.28394900	-0.51390900
O	-0.14270100	2.82749600	1.04637300
O	1.11903300	2.06747600	-2.16585300

Energy (0K) = -786.4456981

Energy (0K) + ZPE = -786.158863

Enthalpy (298K) = -786.141279

Free Energy (298K) = -786.203165

G

Number of imaginary frequencies: 0

C	-3.26893600	-2.05701300	-0.08678300
C	-2.10538700	-1.63954400	0.55415900
C	-1.31108000	-0.64656000	-0.01536900
C	-1.69371400	-0.06898300	-1.22870900
C	-2.85502400	-0.48609800	-1.86702100
C	-3.64578600	-1.48290600	-1.29704100
H	-3.88325800	-2.83416300	0.36288400
H	-1.80515000	-2.07393000	1.50543500
H	-1.07214600	0.70916300	-1.67268400
H	-3.14738800	-0.03048900	-2.81064300
H	-4.55555800	-1.80879300	-1.79645500
C	-0.07712700	-0.16676900	0.66913200

C	1.20804600	-0.18292000	-0.09215500
C	2.30764700	-1.04758800	-2.01815600
H	2.28919800	-2.04276800	-2.47225300
H	3.24118700	-0.93129900	-1.45839700
C	2.12874100	0.03641100	-3.05024100
H	2.93854500	-0.00843800	-3.78640400
H	1.17733800	-0.08821000	-3.57973400
H	2.14533100	1.02807200	-2.58491400
C	-0.13310600	0.87342200	1.75476500
C	1.04448500	1.73728100	1.89384600
C	2.15858800	1.51259700	1.16822200
H	0.99624400	2.57281600	2.59032000
C	3.40235500	2.32222700	1.31728100
H	3.28648000	3.10831000	2.06968800
H	4.24379600	1.68110700	1.60997100
H	3.67825700	2.78306100	0.36024900
C	-1.44503200	1.41676500	2.23190800
H	-2.25083100	0.68601700	2.12264400
H	-1.37000700	1.69300900	3.29029200
H	-1.70946500	2.31873500	1.66735800
N	2.23817300	0.53699900	0.17204500
O	0.09121400	-0.51893800	2.03074600
O	1.19880800	-1.05407100	-1.10034000

Energy (0K) = -786.4661981

Energy (0K) + ZPE = -786.177670

Enthalpy (298K) = -786.159968

Free Energy (298K) = -786.221910

3aa

Number of imaginary frequencies: 0

C	0.39734300	1.14691100	0.23769900
---	------------	------------	------------

C	-0.65220000	0.22868900	-0.37154900
C	-0.53104300	-1.15884600	0.26349100
C	-1.66686100	-1.85192500	0.67765900
C	0.72190800	-1.76291600	0.39225900
C	-1.55101600	-3.12706700	1.22641000
H	-2.64514800	-1.39072800	0.56381600
C	0.83729400	-3.03286400	0.94518600
H	1.61552100	-1.23403700	0.06027900
C	-0.30027700	-3.71954100	1.36499600
H	-2.44518100	-3.65876600	1.54516000
H	1.81964500	-3.48903700	1.04780700
H	-0.20947700	-4.71387100	1.79666500
C	1.65271900	1.37414500	-1.67659600
C	0.64485200	0.63722800	-2.42911700
C	-0.45541000	0.12020900	-1.86568500
O	-1.93203700	0.79319800	-0.15646300
N	1.43474700	1.64357000	-0.31435800
C	-1.50868200	-0.60600500	-2.63021200
C	2.77751200	1.82989000	-2.25376200
H	-2.48448700	-0.11843700	-2.51480600
H	-1.26262400	-0.64296000	-3.69605300
H	-1.62725600	-1.63589500	-2.26677100
H	2.97916900	1.64957500	-3.30651600
H	3.50821400	2.38825600	-1.67447500
O	0.09650100	1.38746200	1.51590100
C	0.97438500	2.25027600	2.25730300
C	0.40649100	2.37988800	3.64301900
H	1.04053400	3.21670400	1.74187900
H	1.97937800	1.80960300	2.25934000
H	1.05112000	3.02246200	4.25129300
H	-0.59415300	2.82502200	3.61689200

H	0.33809800	1.40170300	4.13132600
H	0.80916800	0.52556100	-3.50123900
H	-2.03104200	0.92522200	0.79804100

Energy (0K) = -786.473045

Energy (0K) + ZPE = -786.184213

Enthalpy (298K) = -786.166183

Free Energy (298K) = -786.229656

M06 (SMD, toluene) for Pt catalysis, Cartesian Coordinates and Energies in Hartree

1a

Number of imaginary frequencies: 0

C	-3.39628500	2.92599600	2.71767300
C	-2.03333000	2.82636000	2.47271400
C	-1.40864200	3.69613400	1.56551700
C	-2.18713100	4.66383600	0.91134700
C	-3.54996900	4.75449900	1.15974800
C	-4.16050000	3.88839200	2.06312900
H	-3.86567300	2.24521000	3.42464300
H	-1.43515400	2.07286900	2.98074300
H	-1.70734200	5.34007300	0.20720700
H	-4.14007300	5.50920400	0.64423000
H	-5.22825200	3.96306200	2.25605600
C	-0.00853400	3.59975400	1.31136900
C	1.17924900	3.53280900	1.07947100
C	3.22263000	2.65862500	1.72687000
H	4.19152100	2.54461900	1.23272400
H	2.74801200	1.67134200	1.80076300
C	3.34382400	3.32730500	3.06856800
H	3.95455900	2.71267900	3.73840900
H	3.81743700	4.31002700	2.97329900
H	2.35869700	3.45839900	3.53068500

O 2.44349800 3.46648500 0.80477700

Energy (0K) = -461.8979995

Energy (0K) + ZPE = -461.726766

Enthalpy (298K) = -461.715455

Free Energy (298K) = -461.764317

A'

Number of imaginary frequencies: 0

C	-2.87440000	4.18221900	3.28327300
C	-1.58299300	4.17749700	2.77934800
C	-1.34338000	3.74397700	1.46736300
C	-2.41225800	3.31133800	0.67683300
C	-3.70346500	3.31762600	1.18917400
C	-3.93701300	3.75463800	2.48894800
H	-3.05460700	4.52087700	4.30065800
H	-0.74736800	4.50892100	3.39476000
H	-2.21961900	2.96022300	-0.33583700
H	-4.52958800	2.97802700	0.56967300
H	-4.94870000	3.76025200	2.88735200
C	0.01286700	3.74099600	0.95008600
C	1.19632700	3.99566700	1.31329400
C	3.16722400	2.99223600	2.09402600
H	4.17472300	3.39321600	2.21493800
H	3.13492800	2.27652100	1.26516800
C	2.56765700	2.46424400	3.35965600
H	3.15626800	1.60466300	3.69643400
H	2.57700900	3.21888100	4.15307100
H	1.54069400	2.11493100	3.19847000
O	2.39462300	4.19144300	1.62206600
Pt	0.56249700	3.13571000	-1.01524900
Cl	1.08877200	1.00581700	-0.13992100

Cl	0.91081100	2.37308600	-3.24379700
C	0.15317200	4.82210400	-1.74076500
O	-0.09213000	5.83891300	-2.20031900

Energy (0K) = -1614.7430298

Energy (0K) + ZPE = -1614.559590

Enthalpy (298K) = -1614.540572

Free Energy (298K) = -1614.609401

2n

Number of imaginary frequencies: 0

C	0.10501900	1.31112800	0.18072900
C	1.45896400	1.20187900	0.01568500
C	1.85617900	2.53801800	-0.31102900
C	3.21774000	3.06847000	-0.58320000
H	3.94129800	2.68589000	0.14501600
H	3.57165400	2.78158000	-1.58039600
H	3.20584800	4.16099700	-0.53280900
C	-0.96490500	0.34242700	0.50032900
H	-1.25893900	0.40143200	1.55573600
H	-1.85639700	0.54772800	-0.10141600
H	-0.62794400	-0.67875700	0.29891900
N	0.83114300	3.35624300	-0.32715500
O	-0.27708400	2.57951700	-0.02411600
C	2.29591200	0.00766000	0.16455300
C	2.05929700	-0.90409800	1.20180000
C	3.34767600	-0.25232100	-0.72313600
C	2.84234100	-2.04395600	1.34028100
H	1.26530100	-0.70079900	1.91875400
C	4.13555700	-1.38769100	-0.57848100
H	3.53457300	0.43153200	-1.54881900
C	3.88486900	-2.28929900	0.45179200

H	2.64375000	-2.73861800	2.15354400
H	4.94527200	-1.57310200	-1.28088100
H	4.50104500	-3.17854900	0.56245600

Energy (0K) = -555.3497021

Energy (0K) + ZPE = -555.155433

Enthalpy (298K) = -555.143177

Free Energy (298K) = -555.192825

TS_B'

Number of imaginary frequencies: 1

C	-2.79392800	5.20769000	3.02565100
C	-1.55424000	5.03199500	2.42256100
C	-1.33157600	3.94355600	1.56954200
C	-2.37994400	3.05205600	1.30941100
C	-3.61622600	3.23024300	1.91846600
C	-3.82643000	4.30485000	2.77979300
H	-2.95628400	6.05540100	3.68805200
H	-0.74656400	5.73891400	2.60527600
H	-2.20629500	2.21023800	0.64086900
H	-4.42008200	2.52637700	1.71656700
H	-4.79743100	4.44604000	3.24922300
C	-0.02304900	3.73414300	0.95313400
C	1.17647400	3.79337500	1.42366500
C	3.22930600	2.68175800	1.68406700
H	3.43134900	2.17627500	0.73441900
H	2.60199500	2.03866300	2.30951100
C	4.45618200	3.17027200	2.39009800
H	5.08492900	2.31572400	2.65988200
H	5.04250000	3.83758800	1.75046600
H	4.18384100	3.70624600	3.30584800
O	2.42848300	3.87478300	1.32827200

Pt	0.15590000	3.13931300	-1.04408800
Cl	0.55448000	0.93690800	-0.25442300
Cl	0.23349300	2.40541900	-3.33389500
C	-0.14587000	4.87764300	-1.66083800
O	-0.32940600	5.94041200	-2.04556000
C	0.96129300	5.23686000	5.29038200
C	0.10599700	4.20898700	5.58637500
C	0.20204600	3.34883500	4.45337500
C	-0.49191700	2.06574900	4.18787100
H	-0.46351400	1.42023200	5.07211600
H	-1.54470100	2.24023800	3.93416600
H	-0.02863400	1.54323500	3.34449500
C	1.34436000	6.47496800	5.99687900
H	2.32599300	6.37249200	6.47532500
H	1.40347900	7.31394200	5.29602400
H	0.60932100	6.70757900	6.77233100
N	1.05603800	3.83637900	3.58020500
O	1.52924700	5.02979100	4.09019900
C	-0.72527900	4.03403300	6.78273700
C	-2.06886200	3.65824300	6.66267500
C	-0.19461000	4.24774500	8.06017100
C	-2.85934800	3.49985200	7.79439900
H	-2.50047600	3.51195400	5.67272200
C	-0.98971400	4.09456300	9.19024800
H	0.85574300	4.51608100	8.16620000
C	-2.32298400	3.71831500	9.06014300
H	-3.90208200	3.21014900	7.68692500
H	-0.56241500	4.26000600	10.17664600
H	-2.94355400	3.59438900	9.94442700

Energy (0K) = -2170.1078028

Energy (0K) + ZPE = -2169.728538

Enthalpy (298K) = -2169.697440

Free Energy (298K) = -2169.792967

B'

Number of imaginary frequencies: 0

C	-3.07571200	1.89946000	1.00264000
C	-1.74555500	1.70932100	0.64906200
C	-1.34393600	0.55444000	-0.04220700
C	-2.32455800	-0.38103700	-0.40576800
C	-3.65300800	-0.18992000	-0.04581700
C	-4.03305300	0.94533000	0.66550500
H	-3.36883700	2.80324200	1.53273000
H	-1.00537500	2.47092500	0.89344000
H	-2.02544300	-1.27268700	-0.95484900
H	-4.39656900	-0.93169900	-0.32787300
H	-5.07481200	1.09653000	0.93898400
C	0.06813500	0.31243300	-0.36543100
C	1.06486100	0.53590200	0.50792600
C	3.16036400	-0.52108400	0.78218200
H	2.56580600	-1.44546600	0.75030400
H	3.39524500	-0.28019300	1.83181000
C	4.40187600	-0.65590600	-0.05355300
H	5.05572300	-1.43114400	0.35934400
H	4.13515500	-0.93786000	-1.07866600
H	4.95852100	0.28717100	-0.08354800
O	2.37760200	0.55185000	0.22046900
Pt	0.60406000	-0.52034000	-2.15071600
Cl	0.70443200	-2.59557200	-0.96406000
Cl	1.26674200	-1.60645100	-4.23306100
C	0.51035000	1.10287700	-3.05518400
O	0.45558300	2.09863200	-3.62165500

C	0.84068400	1.90541300	3.74185300
C	0.07392200	0.79449400	4.00083700
C	0.07950800	0.05295500	2.79554600
C	-0.53975700	-1.25149700	2.49893600
H	-0.50452800	-1.88512600	3.39037200
H	-1.59516500	-1.11168500	2.22798500
H	-0.05079200	-1.74903300	1.65238400
C	1.25255000	3.05934600	4.55873100
H	2.26643500	2.91814100	4.95213800
H	1.25189000	3.97447700	3.95900500
H	0.56923900	3.17979100	5.40334800
N	0.78464500	0.73637900	1.89819600
O	1.27850600	1.89082200	2.47379000
C	-0.60148800	0.43090000	5.25281200
C	-1.94916600	0.05576100	5.23364200
C	0.08645700	0.46022200	6.47021100
C	-2.59606700	-0.28557900	6.41444400
H	-2.49518900	0.05494100	4.29074100
C	-0.56589900	0.12202100	7.64981000
H	1.14124700	0.73135400	6.48579700
C	-1.90583200	-0.25259100	7.62293600
H	-3.64424800	-0.57295000	6.39194600
H	-0.02328300	0.14287600	8.59171200
H	-2.41429900	-0.52020200	8.54607400

Energy (0K) = -2170.1433525

Energy (0K) + ZPE = -2169.761342

Enthalpy (298K) = -2169.730656

Free Energy (298K) = -2169.824784

TS_c

Number of imaginary frequencies: 1

C	-2.84536400	5.30102500	2.73467100
C	-1.58131200	5.00839100	2.24391100
C	-1.37709500	3.88997700	1.41301400
C	-2.48781600	3.09831300	1.06618200
C	-3.74500800	3.38422900	1.57694300
C	-3.92713000	4.48419700	2.41301500
H	-2.99149700	6.17650000	3.36343400
H	-0.74144200	5.65975400	2.47656600
H	-2.33973700	2.23938800	0.41289800
H	-4.58953300	2.75169700	1.31540200
H	-4.91621500	4.71245500	2.80316200
C	-0.05785100	3.54244700	0.91069800
C	1.08938600	3.70405900	1.66837800
C	3.36485200	2.96817800	1.68343000
H	3.80050000	2.37823700	0.86923700
H	2.95326900	2.26048700	2.41510000
C	4.37445200	3.89427000	2.30917800
H	5.22359200	3.32188700	2.69868300
H	4.75519400	4.60561900	1.56850000
H	3.93079900	4.46387800	3.13343300
O	2.29773700	3.72443700	1.08399000
Pt	0.16958800	2.64473100	-0.88701700
Cl	0.73893400	0.66342700	0.31387700
Cl	0.44151100	1.51715800	-3.02931700
C	-0.32502400	4.17364200	-1.84338100
O	-0.63688500	5.09718800	-2.44478700
C	0.93758100	5.15187200	4.92952200
C	0.27966300	3.93881400	5.16420200
C	0.36798400	3.17720800	3.99475900
C	-0.20937400	1.82604400	3.77875100
H	-0.19212200	1.24505300	4.70372500

H	-1.26083500	1.94632400	3.48053800
H	0.30193100	1.28840400	2.97325800
C	1.18031900	6.23726900	5.91421800
H	2.17394700	6.66757800	5.75986400
H	0.44745100	7.03989200	5.76786400
H	1.08568800	5.86725100	6.93838700
N	1.03369300	3.77853700	3.01149800
O	1.39946700	5.30703600	3.73903800
C	-0.35827000	3.53390300	6.42913800
C	0.09625600	2.42390800	7.14987600
C	-1.42790300	4.27978200	6.93585500
C	-0.51463100	2.06250600	8.34482300
H	0.94539000	1.85306100	6.77673700
C	-2.03050800	3.92437700	8.13690400
H	-1.79141500	5.13706800	6.37009200
C	-1.57723100	2.81276600	8.84077100
H	-0.15394300	1.19717500	8.89574700
H	-2.86162600	4.51178800	8.51983200
H	-2.05205800	2.53096000	9.77761200

Energy (0K) = -2170.1234045

Energy (0K) + ZPE = -2169.744058

Enthalpy (298K) = -2169.713339

Free Energy (298K) = -2169.807536

C'

Number of imaginary frequencies: 0

C	-2.41603700	-0.07012100	-4.23144000
C	-1.82990200	-0.35007500	-3.01276900
C	-0.70720400	0.39487800	-2.56814900
C	-0.21135000	1.44120600	-3.39358500
C	-0.82026200	1.72964200	-4.59555600

C	-1.91797300	0.97125000	-5.01498600
H	-3.26723800	-0.65213200	-4.57206300
H	-2.20570700	-1.15311300	-2.38484100
H	0.63962800	2.03398700	-3.06316100
H	-0.44892100	2.53943600	-5.21691400
H	-2.39085800	1.19711300	-5.96813300
C	-0.08000100	0.09017300	-1.33667400
C	1.22078500	0.73642200	-1.03995100
C	3.55257200	0.57109400	-1.43328500
H	4.15409600	-0.28645700	-1.74854000
H	3.62079200	0.67613100	-0.34480800
C	3.95206000	1.83160500	-2.15509700
H	3.82434700	1.71830100	-3.23762000
H	3.35876400	2.68693100	-1.81441700
H	5.00678000	2.05348300	-1.95951800
C	1.27569800	0.61521300	2.50661300
C	0.42876100	1.72706300	2.01797300
C	0.48518400	2.15125700	0.72249800
C	-0.37148600	3.23939100	0.16136400
H	0.22847100	3.91846300	-0.45596000
H	-1.13191600	2.78436400	-0.49188400
H	-0.89210800	3.80999500	0.93275000
C	1.26276100	0.33834700	3.98482300
H	2.08296900	-0.34104800	4.22810400
H	1.32968000	1.25254100	4.58456800
H	0.31520700	-0.14796400	4.25378000
N	1.40667200	1.64193500	-0.17844000
O	1.96114800	-0.08583100	1.76458100
O	2.19621400	0.19349200	-1.76870700
C	-0.49697400	2.38813800	2.98071800
C	-0.15213400	3.60302900	3.58243000

C	-1.71547400	1.79051400	3.31630200
C	-1.00585500	4.20862700	4.49869300
H	0.79722500	4.07160300	3.32300100
C	-2.56878100	2.39529800	4.23403100
H	-1.99148000	0.84671200	2.84520800
C	-2.21592600	3.60377600	4.82721900
H	-0.72477500	5.15369400	4.95900300
H	-3.51486100	1.91954000	4.48270700
H	-2.88428300	4.07487000	5.54477300
Pt	-0.73373300	-1.11633600	0.08001700
Cl	-1.47073700	-2.58611300	1.85194900
Cl	-2.81421900	0.01430500	0.10541500
C	0.91210200	-2.06853400	0.17523700
O	1.86450300	-2.69193100	0.23366500

Energy (0K) = -2170.1611564

Energy (0K) + ZPE = -2169.780971

Enthalpy (298K) = -2169.749597

Free Energy (298K) = -2169.844761

TS_D'

Number of imaginary frequencies: 1

C	-3.76479300	3.17743800	-0.94287200
C	-2.74401800	2.40607800	-0.41692900
C	-1.40476900	2.59145000	-0.84105800
C	-1.15728000	3.55296000	-1.85778700
C	-2.18878000	4.29059400	-2.40415600
C	-3.49178900	4.11779000	-1.93480000
H	-4.78176800	3.03718700	-0.58726600
H	-2.95176200	1.67266900	0.35724100
H	-0.15269300	3.67913700	-2.25179300
H	-1.98321100	5.00296500	-3.19862700

H	-4.30026700	4.71062000	-2.35636700
C	-0.34225200	1.76951700	-0.33628600
C	1.05461100	2.27449800	-0.56924600
C	3.21483100	1.66302400	-1.37783600
H	3.73883300	0.70394800	-1.33173100
H	3.60887800	2.32002500	-0.59605400
C	3.30702000	2.28352500	-2.74797400
H	4.35714100	2.45657300	-3.00583400
H	2.87602200	1.61938000	-3.50485500
H	2.78723400	3.24720300	-2.78332600
C	0.24173100	3.43560000	2.29962900
C	0.27284500	4.59883400	1.41026200
C	0.84475200	4.54916800	0.16657300
C	0.96541000	5.78903800	-0.67401500
H	0.02404500	6.34874000	-0.69278800
H	1.73043900	6.46225900	-0.26678300
H	1.26101800	5.53800300	-1.69758800
C	-0.12195300	3.64371100	3.74051000
H	-1.20096600	3.83875700	3.80837500
H	0.09880000	2.73253000	4.30112800
H	0.38842600	4.50505500	4.18400500
N	1.47928800	3.46341200	-0.39162200
O	0.50081800	2.29471400	1.90782100
O	1.84763600	1.32685800	-1.05710700
Pt	-0.64816500	-0.10802200	0.28187300
Cl	-0.99687900	-2.45689300	0.79574700
Cl	-1.99153000	0.45183000	2.16100100
C	0.38208400	-0.84624300	-1.12589100
O	0.95811000	-1.39211800	-1.94764200
C	-0.26911600	5.89418500	1.90851300
C	0.55582700	6.85836500	2.49502700

C	-1.63633700	6.16080300	1.78978900
C	0.02598900	8.06068200	2.95260900
H	1.62231200	6.65488700	2.59322400
C	-2.16813700	7.36294300	2.24542300
H	-2.28231600	5.40941600	1.33373200
C	-1.33678200	8.31519400	2.82787300
H	0.67976600	8.80105900	3.40858300
H	-3.23421700	7.55605500	2.14722600
H	-1.75063800	9.25488400	3.18681900

Energy (0K) = -2170.1418722

Energy (0K) + ZPE = -2169.762548

Enthalpy (298K) = -2169.731919

Free Energy (298K) = -2169.825117

D'

Number of imaginary frequencies: 0

C	-3.55558100	3.47258500	-0.55823800
C	-2.49690200	2.87027400	0.10799700
C	-1.28440800	2.64274300	-0.55277200
C	-1.17343900	2.99514700	-1.90130700
C	-2.24082700	3.58833000	-2.56797900
C	-3.43151700	3.84067400	-1.89651200
H	-4.49204400	3.64136300	-0.03126200
H	-2.61193300	2.54191500	1.14044000
H	-0.24687800	2.79869000	-2.44434600
H	-2.13675400	3.85355700	-3.61748400
H	-4.26403000	4.30962700	-2.41519000
C	-0.15298200	1.94075500	0.14507000
C	1.21274600	2.38296300	-0.34987100
C	3.41101900	1.82756700	-1.06715100
H	4.02524400	0.96377000	-0.80145100

H	3.73422800	2.69229800	-0.47870100
C	3.41751500	2.09763300	-2.54779200
H	4.44038400	2.30642800	-2.87797800
H	3.05236100	1.22777100	-3.10346900
H	2.79679400	2.96519800	-2.79626600
C	-0.06465500	3.53733500	2.01836400
C	0.15179800	4.69688600	1.26981100
C	0.78829300	4.67145300	0.01530800
C	0.82641900	5.89112300	-0.83848900
H	-0.13331200	6.41677800	-0.80709800
H	1.59322000	6.59280400	-0.48559500
H	1.07488300	5.61528300	-1.86740400
C	-0.40933500	3.54644000	3.45982200
H	-1.50417600	3.53757200	3.56293200
H	-0.04803600	2.62348500	3.92343000
H	-0.02176300	4.42597100	3.97763400
N	1.50255500	3.63478600	-0.44975000
O	-0.03335000	2.31144500	1.54966400
O	2.07540500	1.44701600	-0.63832500
Pt	-0.60346400	-0.11258400	0.05922200
Cl	-1.19871200	-2.46735700	-0.13632600
Cl	-1.73166500	0.00157600	2.15314600
C	0.22901300	-0.33440800	-1.59607000
O	0.70568900	-0.51907300	-2.62372000
C	-0.27764500	5.99943900	1.85319000
C	0.66106200	6.91558700	2.33550300
C	-1.63770000	6.31303600	1.92683600
C	0.24650900	8.12491300	2.88251500
H	1.72173100	6.67008400	2.28948600
C	-2.05114900	7.52424200	2.47102800
H	-2.36932400	5.60056400	1.54478600

C	-1.10991900	8.43044900	2.95000300
H	0.98374000	8.82921300	3.26097100
H	-3.11141400	7.76062700	2.52063700
H	-1.43424500	9.37631400	3.37750300

Energy (0K) = -2170.1755333

Energy (0K) + ZPE = -2169.793190

Enthalpy (298K) = -2169.763002

Free Energy (298K) = -2169.854768

E'

Number of imaginary frequencies: 0

C	-3.81981700	-2.95425200	-0.26527700
C	-2.61836000	-2.41973200	0.18093600
C	-1.55882200	-2.16815300	-0.70874900
C	-1.75490800	-2.47810000	-2.06763500
C	-2.95977000	-3.00900200	-2.50507100
C	-4.00080100	-3.25097900	-1.61189500
H	-4.61913100	-3.14187900	0.44881100
H	-2.48070300	-2.19690000	1.23531600
H	-0.95158500	-2.30603600	-2.77555400
H	-3.08684700	-3.23652400	-3.56167100
H	-4.94200900	-3.66748300	-1.96364700
C	-0.32877600	-1.58240700	-0.18173300
C	0.89581400	-1.43706600	-0.76828800
C	1.85336300	-1.08680400	-2.89351500
H	2.06408000	-1.70869500	-3.76970200
H	2.81085500	-0.83185400	-2.42120900
C	1.07280000	0.15043000	-3.26809800
H	1.65513500	0.78538400	-3.94490600
H	0.13259900	-0.11308500	-3.76644100
H	0.82359300	0.74271000	-2.37775900

C	-0.36691800	0.16583900	1.23018200
C	0.82171000	0.80374200	1.11005300
C	2.00717000	0.03299100	0.71066200
C	3.33214500	0.43264500	1.28380800
H	3.27536600	0.51990200	2.37591300
H	4.08701200	-0.31019100	1.01436800
H	3.65623300	1.41183400	0.91066700
C	-1.70496900	0.75283400	1.48922400
H	-2.41466900	0.37311400	0.74152100
H	-2.08188900	0.42871300	2.46872700
H	-1.70343900	1.84425600	1.45261200
N	2.01006300	-0.94008400	-0.14703700
O	-0.36744600	-1.21506100	1.16728100
O	1.09794800	-1.92701500	-2.01722600
C	0.96720000	2.25926500	1.35837100
C	0.56635300	2.82582600	2.57356500
C	1.53402200	3.09527900	0.38842400
C	0.71201600	4.18926800	2.80632900
H	0.14621700	2.18205500	3.34515000
C	1.68476300	4.45674800	0.62148000
H	1.85702100	2.66884000	-0.56132900
C	1.27162100	5.00870800	1.83120300
H	0.39411400	4.61087900	3.75746300
H	2.12269300	5.09120200	-0.14597700
H	1.38912300	6.07444400	2.01396100

Energy (0K) = -1017.3281597

Energy (0K) + ZPE = -1016.958841

Enthalpy (298K) = -1016.936340

Free Energy (298K) = -1017.009466

TS_F'

Number of imaginary frequencies: 1

C	-3.61490000	1.11176700	-0.35748700
C	-2.39321600	1.62122800	0.06425400
C	-1.49157400	2.18135200	-0.85353000
C	-1.86538700	2.23562800	-2.20611900
C	-3.08699200	1.72607300	-2.62126700
C	-3.96706500	1.15861700	-1.70231100
H	-4.29539500	0.67540600	0.37064600
H	-2.11915800	1.58935400	1.11573700
H	-1.18570200	2.67583400	-2.92938800
H	-3.35773200	1.77662500	-3.67378500
H	-4.92344400	0.76063100	-2.03409800
C	-0.22308900	2.72980000	-0.36555900
C	1.00060200	2.78976000	-1.05653300
C	2.12868800	2.52798500	-3.14252300
H	2.07277300	1.76529500	-3.92636800
H	3.07073400	2.39872700	-2.59873000
C	2.01563600	3.91527900	-3.72710500
H	2.80753600	4.07845200	-4.46670800
H	1.04975700	4.05032100	-4.22799300
H	2.11563400	4.68397100	-2.95203600
C	-0.21706600	4.22290700	0.85950800
C	0.96870700	4.96135000	0.79992100
C	2.13310800	4.33833000	0.28971400
C	3.50428600	4.87089700	0.58407100
H	3.51093900	5.59538300	1.40239300
H	4.15886000	4.03297100	0.84978600
H	3.94539800	5.34149500	-0.30448700
C	-1.57368800	4.77516600	1.13212900
H	-2.33096800	4.24394200	0.54383100
H	-1.83843600	4.62928400	2.18815600

H	-1.63315900	5.84136800	0.90103100
N	2.11133100	3.33685200	-0.59011400
O	-0.09446300	2.85408900	1.02015600
O	1.02813300	2.22072800	-2.28054800
C	0.98491400	6.40233900	1.15082800
C	0.54207500	6.84383500	2.40373900
C	1.45556800	7.35592900	0.23955700
C	0.56275700	8.19411400	2.73320000
H	0.18951100	6.11193800	3.12929500
C	1.48195700	8.70610800	0.56854100
H	1.79404900	7.02725300	-0.74285900
C	1.03324200	9.12966100	1.81617500
H	0.21612500	8.51687500	3.71267400
H	1.84914800	9.43152800	-0.15440500
H	1.05098400	10.18630500	2.07371300

Energy (0K) = -1017.3221916

Energy (0K) + ZPE = -1016.953637

Enthalpy (298K) = -1016.931578

Free Energy (298K) = -1017.003464

F'

Number of imaginary frequencies: 0

C	-3.55209100	-2.99417500	-0.36093600
C	-2.37744000	-2.46832000	0.16947800
C	-1.57594200	-1.62952300	-0.60121700
C	-1.96141600	-1.31822500	-1.90695300
C	-3.13405700	-1.84287600	-2.43488300
C	-3.93264900	-2.68286500	-1.66182800
H	-4.17294400	-3.64847000	0.24731800
H	-2.07651400	-2.69591200	1.18956500
H	-1.33398000	-0.66194200	-2.51070900

H	-3.42850300	-1.59345200	-3.45200500
H	-4.85251900	-3.09159700	-2.07433000
C	-0.33220300	-1.02998900	-0.03751600
C	0.94347400	-1.23233900	-0.78020300
C	2.05050600	-2.52295100	-2.43690100
H	2.00132800	-3.58954900	-2.67701000
H	2.97197200	-2.32712700	-1.87819800
C	1.96020300	-1.67140200	-3.67810700
H	2.79098300	-1.90145700	-4.35406900
H	1.02264300	-1.86279600	-4.21251500
H	2.01273200	-0.60714600	-3.42546400
C	-0.36872800	0.22489100	0.79338600
C	0.83672600	1.09191700	0.76375100
C	1.94174800	0.67100900	0.09659900
C	3.24692400	1.40046000	0.08274600
H	3.28791100	2.21823700	0.80582500
H	4.05741500	0.69417500	0.29910900
H	3.44994000	1.80749600	-0.91689600
C	-1.69481600	0.85817400	1.10067800
H	-2.50698000	0.13301900	1.00617200
H	-1.71097900	1.26130700	2.11854900
H	-1.88559400	1.68948900	0.41154900
N	1.97992000	-0.48649700	-0.67928400
O	-0.17235000	-1.07437100	1.36820500
O	0.91900900	-2.29911600	-1.58027100
C	0.79246400	2.37806000	1.49979300
C	0.62638100	2.38880300	2.89043600
C	0.90453500	3.60241000	0.83270900
C	0.58338800	3.58684000	3.59366100
H	0.54331900	1.43911500	3.41919700
C	0.86233500	4.80267500	1.53492900

H	1.02504700	3.60472900	-0.25006200
C	0.70097800	4.79820700	2.91687600
H	0.46198000	3.57534500	4.67474500
H	0.95213500	5.74571700	0.99964900
H	0.66716100	5.73640600	3.46637200

Energy (0K) = -1017.341956

Energy (0K) + ZPE = -1016.972395

Enthalpy (298K) = -1016.949908

Free Energy (298K) = -1017.023679

3aa'

Number of imaginary frequencies: 0

C	-3.36946700	-1.09991500	-0.71208200
C	-2.25644000	-1.24013800	0.11293300
C	-1.17263600	-0.37448200	-0.01686900
C	-1.22054500	0.64135600	-0.97432900
C	-2.32982800	0.77685000	-1.80032800
C	-3.40827200	-0.09507500	-1.67211900
H	-4.20984500	-1.78211500	-0.60195000
H	-2.22402000	-2.02213700	0.86792200
H	-0.38439500	1.33335900	-1.07540800
H	-2.35311600	1.56801800	-2.54661100
H	-4.27649000	0.01083100	-2.31865700
C	0.04634200	-0.50605700	0.90430100
C	1.29873000	-0.42392000	0.05782900
C	2.47739700	-1.58337000	-1.65248900
H	2.62584900	-2.65038900	-1.84619600
H	3.39245000	-1.17267900	-1.21160200
C	2.07616800	-0.84043600	-2.90152500
H	2.84494700	-0.95798100	-3.67311900
H	1.13025700	-1.22869000	-3.29554800

H	1.95764700	0.22882900	-2.69724700
C	0.02043200	0.60366200	1.93084900
C	0.88988400	1.63192800	1.84551500
C	1.94051000	1.65612500	0.81129600
C	2.74622900	2.71199600	0.60459700
H	2.66577200	3.62534300	1.18433700
H	3.50318500	2.65665200	-0.17268700
C	-1.05129000	0.47630800	2.96271800
H	-1.05105200	-0.53513300	3.38388600
H	-0.92361100	1.19534600	3.77511600
H	-2.04623400	0.63562000	2.52326100
N	2.12786800	0.53650300	-0.01515600
O	0.04225500	-1.73879400	1.59913700
O	1.42366400	-1.53790000	-0.67567100
C	0.80321100	2.79511900	2.76629600
C	1.79943200	3.04396000	3.71565900
C	-0.28287600	3.67145000	2.68509800
C	1.70728000	4.13958900	4.56706200
H	2.65154200	2.36873100	3.77973900
C	-0.37380300	4.76985600	3.53366300
H	-1.05910700	3.48317200	1.94360500
C	0.62108700	5.00604700	4.47729300
H	2.48690800	4.31666600	5.30501100
H	-1.22436800	5.44387500	3.45681600
H	0.55172200	5.86454300	5.14175900
H	0.21834500	-2.42626400	0.94213700

Energy (0K) = -1017.3475604

Energy (0K) + ZPE = -1016.977981

Enthalpy (298K) = -1016.955143

Free Energy (298K) = -1017.030989

TS_{D1}'

Number of imaginary frequencies: 1

C	-3.16399300	1.85634100	-3.31060800
C	-2.45966100	1.48748800	-2.17580700
C	-1.19652100	2.04826600	-1.88653900
C	-0.66139700	2.96684900	-2.81964600
C	-1.36823700	3.32405200	-3.95714600
C	-2.62521600	2.77839400	-4.20377100
H	-4.13848000	1.41367800	-3.49986700
H	-2.89670500	0.77820700	-1.47829900
H	0.32777200	3.39333300	-2.67047900
H	-0.92861900	4.02423100	-4.66307900
H	-3.17681000	3.05971500	-5.09769500
C	-0.45606700	1.62364100	-0.69170400
C	0.92433600	2.19392700	-0.57803300
C	3.26214600	1.80190100	-0.57198000
H	3.78171000	0.87818000	-0.30134100
H	3.24191000	2.47084100	0.29412800
C	3.84549500	2.44394100	-1.80046800
H	3.79307200	1.76602700	-2.65866100
H	3.32345400	3.37405600	-2.04707800
H	4.89913200	2.68171700	-1.62005000
C	-0.14853700	2.34771900	1.99332000
C	-0.82024700	3.24349500	0.95695800
C	0.02793200	4.04081300	0.13600600
C	-0.26022400	5.45017700	-0.22534300
H	0.63777000	5.91815400	-0.63728000
H	-1.03322300	5.44978800	-1.00978000
H	-0.65631900	6.03610800	0.60909000
C	-0.89411500	1.99708000	3.24791800
H	-0.64689900	0.96118100	3.49938200

H	-0.52094800	2.63014800	4.06376800
H	-1.97484300	2.10925000	3.17477400
N	1.11331600	3.48162600	-0.40835700
O	0.99066700	1.93359900	1.84441200
O	1.89552700	1.36831600	-0.82326000
Pt	-0.79652200	-0.25281200	0.03565500
Cl	-1.17813500	-2.52992600	0.79779100
Cl	-2.83803600	0.42283500	1.03599500
C	0.78400700	-0.99714600	-0.66910500
O	1.70186100	-1.55875500	-1.05730300
C	-2.12709800	3.87861400	1.30332700
C	-2.23826100	4.66160600	2.46030200
C	-3.21572600	3.82307200	0.43084900
C	-3.41393200	5.34471800	2.74885300
H	-1.38879400	4.74906700	3.13707600
C	-4.39423300	4.50094000	0.72232500
H	-3.14712300	3.22893800	-0.47647700
C	-4.49891700	5.26115100	1.88221100
H	-3.47866700	5.94573900	3.65300800
H	-5.23570300	4.43149200	0.03687800
H	-5.42139000	5.79086000	2.10863200

Energy (0K) = -2170.1405394

Energy (0K) + ZPE = -2169.760547

Enthalpy (298K) = -2169.730393

Free Energy (298K) = -2169.821590

D1'

Number of imaginary frequencies: 0

C	-0.97799200	-0.03451000	-3.71139200
C	-0.58850000	-0.24723600	-2.39432500
C	-0.29493900	0.82987300	-1.55202900

C	-0.36290700	2.12332200	-2.08507500
C	-0.76110900	2.33720000	-3.39991600
C	-1.06931600	1.25728900	-4.21935000
H	-1.21745000	-0.88931100	-4.33929000
H	-0.52361700	-1.26179500	-2.00826100
H	-0.11997900	2.99096100	-1.47267100
H	-0.82319700	3.35308500	-3.78286300
H	-1.37771800	1.42132900	-5.24916900
C	0.29018500	0.58997600	-0.14235500
C	1.71479700	0.79836500	-0.47986900
C	3.67677500	0.32343800	-1.74079800
H	4.15517500	-0.63912500	-1.93247900
H	4.24202700	0.87018800	-0.98167100
C	3.44225500	1.11994200	-2.99364400
H	2.79826500	0.57334700	-3.69096800
H	2.97705800	2.08561700	-2.76713700
H	4.40040000	1.31013700	-3.48797500
C	0.44675100	1.06518500	2.31636900
C	0.11619000	1.74631500	0.91367700
C	1.35562200	2.58371600	0.62807400
C	1.66324800	3.91713800	1.16958200
H	2.59933000	4.28295600	0.74295100
H	0.85005000	4.62485300	0.97350600
H	1.77715700	3.85249700	2.26011900
C	-0.69795200	0.59521800	3.16163000
H	-0.37762500	-0.30303500	3.69881900
H	-0.92497700	1.36923100	3.90632600
H	-1.60748600	0.39038200	2.59083800
N	2.25375300	1.98604500	-0.11387200
O	1.60261900	0.96725200	2.66899700
O	2.38099900	-0.05510000	-1.16605200

Pt	-0.07544300	-1.38049700	0.65399700
Cl	-0.49813600	-3.57447900	1.59819800
Cl	-2.40552400	-1.11423500	0.30122600
C	1.71804000	-1.74086100	1.02716000
O	2.80099300	-2.01056300	1.28929300
C	-1.18691500	2.52347700	1.05141000
C	-1.26516100	3.52057100	2.03529700
C	-2.34171800	2.23941600	0.31956700
C	-2.43537900	4.23732000	2.25000100
H	-0.40986700	3.73186400	2.67491500
C	-3.51607800	2.95482000	0.53713100
H	-2.35115300	1.43105600	-0.40192100
C	-3.56813200	3.96206400	1.49147800
H	-2.46221300	5.00272200	3.02206400
H	-4.39976900	2.70503100	-0.04511100
H	-4.48894300	4.51610700	1.65773500

Energy (0K) = -2170.1760622

Energy (0K) + ZPE = -2169.793963

Enthalpy (298K) = -2169.763870

Free Energy (298K) = -2169.854122

TS_{D2'}

Number of imaginary frequencies: 1

C	-1.01731300	1.38924100	-4.99931800
C	-0.24789400	1.38365900	-3.84516900
C	-0.60757600	2.19259100	-2.76490800
C	-1.74580500	2.99504900	-2.83838800
C	-2.52337500	2.98095200	-3.99143400
C	-2.15904400	2.18515500	-5.07201300
H	-0.73142600	0.76548400	-5.84262000
H	0.64198300	0.75821300	-3.77680600

H	-2.03113800	3.61132800	-1.98712700
H	-3.41588300	3.59947500	-4.04451500
H	-2.76702500	2.18126100	-5.97346900
C	0.22412600	2.15894600	-1.53691700
C	0.55958300	3.35357000	-0.85634200
C	2.83529400	2.15446300	-1.24252300
H	3.08780400	1.25768500	-1.82158900
H	2.58626400	1.88162800	-0.21023700
C	3.91117200	3.20035600	-1.30013000
H	4.10016800	3.52281500	-2.32913300
H	3.63697900	4.07091400	-0.69548100
H	4.83862600	2.78306600	-0.89447800
C	0.88934100	3.12779800	2.49982500
C	0.18632400	4.41595900	2.20597000
C	0.14447600	4.91055300	0.94914500
C	-0.54316000	6.15374700	0.50048400
H	0.11500100	6.73579500	-0.15471300
H	-1.43853500	5.89678800	-0.08331900
H	-0.84753600	6.77083800	1.34804900
C	0.43173300	2.36001700	3.70295900
H	0.90332600	1.37468200	3.69776200
H	0.68898500	2.88656200	4.63001600
H	-0.65934000	2.24781600	3.69132900
N	0.80223700	4.26204100	-0.10759100
O	1.78095100	2.70458100	1.77868200
O	1.64561000	2.71263700	-1.89194900
C	-0.53011700	5.10593400	3.30895900
C	0.18996500	5.66636800	4.36943100
C	-1.92633600	5.18062600	3.32599800
C	-0.47009300	6.29730400	5.41745600
H	1.27810100	5.60764000	4.36383700

C	-2.58648100	5.81307700	4.37440000
H	-2.49306800	4.72845900	2.51259500
C	-1.86018300	6.37326000	5.42071300
H	0.10223800	6.73356800	6.23305100
H	-3.67292700	5.86268600	4.37595400
H	-2.37710700	6.86656800	6.24071500
Pt	-0.04450500	0.51356400	-0.31543300
Cl	-0.52422500	-1.33253400	1.16196200
Cl	-1.76794400	1.83390700	0.66319400
C	1.22521400	-0.60589100	-1.11093800
O	1.96484800	-1.33986000	-1.58791100

Energy (0K) = -2170.1072126

Energy (0K) + ZPE = -2169.729170

Enthalpy (298K) = -2169.697975

Free Energy (298K) = -2169.792741

D2'

Number of imaginary frequencies: 0

C	-0.57287200	-0.61571300	-5.37886100
C	0.21819300	-0.51773100	-4.24021100
C	-0.31549600	0.00857900	-3.06238600
C	-1.64784700	0.43001900	-3.03907600
C	-2.43120100	0.33021800	-4.18121500
C	-1.89765500	-0.19208200	-5.35596900
H	-0.14764300	-1.02752800	-6.29134000
H	1.25357400	-0.84663200	-4.26089400
H	-2.08335600	0.81221200	-2.11629400
H	-3.46740000	0.65835400	-4.14936200
H	-2.51342300	-0.26999400	-6.24872100
C	0.55237100	0.06092500	-1.83203800
C	0.22252400	1.14809100	-0.93586700

C	2.88780900	0.09814400	-1.15178200
H	3.55860500	-0.73602900	-1.39917200
H	2.41976800	-0.12512300	-0.18330200
C	3.64908500	1.39775300	-1.09985800
H	4.09261800	1.62994700	-2.07417300
H	3.00459000	2.23418300	-0.80510900
H	4.45585500	1.32521300	-0.36240100
C	0.72931200	1.08971200	2.38491900
C	0.02067900	2.40940600	2.15773900
C	-0.21008000	2.84743600	0.89910400
C	-0.79038300	4.14666300	0.45098900
H	-0.16932600	4.57519700	-0.34388300
H	-1.79892800	4.01130700	0.04120000
H	-0.84151500	4.85669000	1.27874800
C	0.12231600	0.16321400	3.38736800
H	0.56602700	-0.83008000	3.28139400
H	0.30205200	0.53642800	4.40358800
H	-0.96285600	0.10128100	3.24779100
N	0.10382400	1.99319600	-0.14931900
O	1.75133600	0.84284700	1.77411500
O	1.89599300	0.14611900	-2.19249900
C	-0.37761700	3.17607200	3.35128800
C	0.55575600	3.39517300	4.37356700
C	-1.68479200	3.65160400	3.50733000
C	0.19498100	4.10209500	5.51260800
H	1.57366100	3.02235700	4.26252900
C	-2.04430000	4.34905800	4.65417700
H	-2.42757100	3.44667000	2.73873200
C	-1.10508200	4.58052900	5.65439300
H	0.93043200	4.27701800	6.29399800
H	-3.06454900	4.70663400	4.76956400

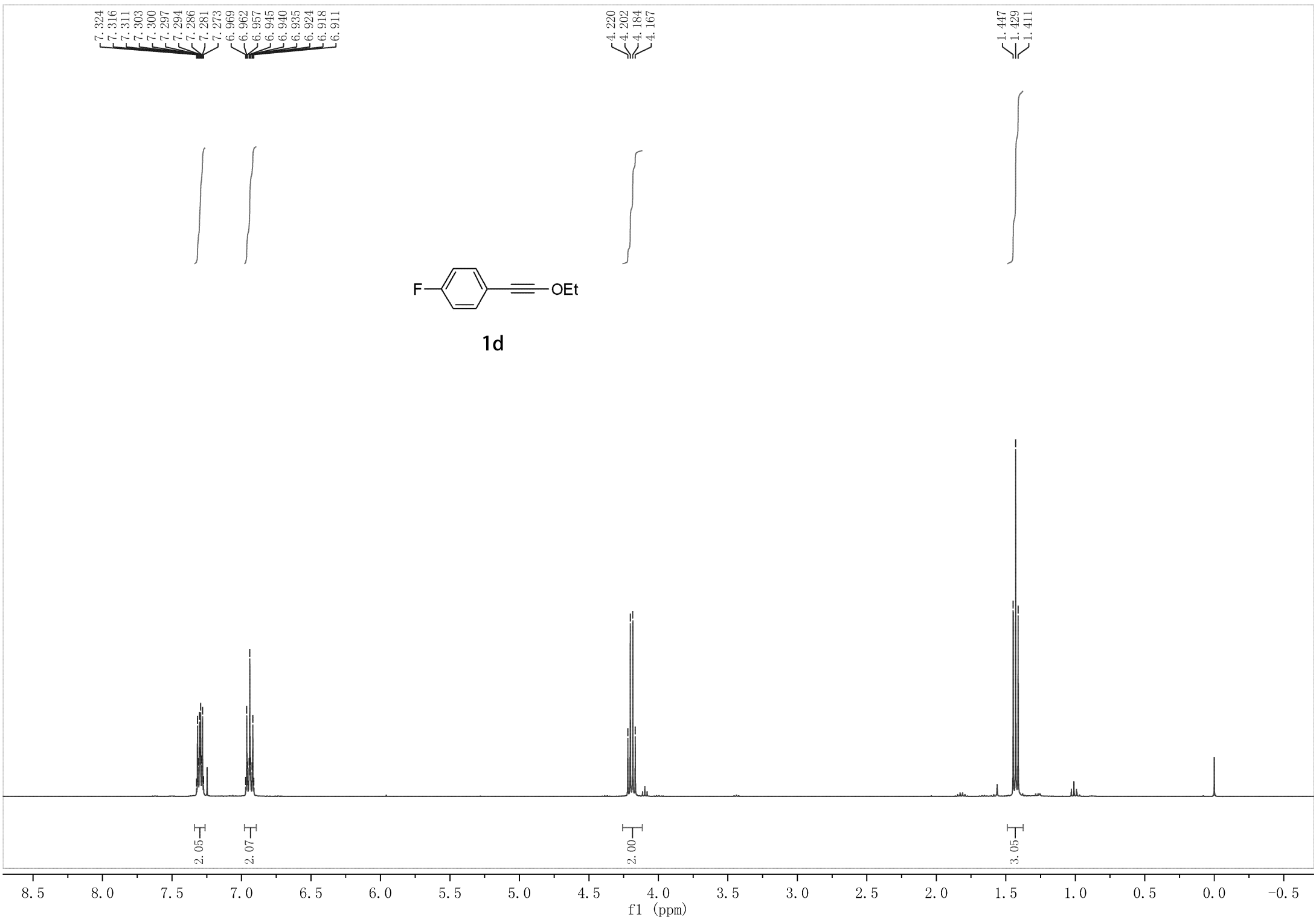
H	-1.38787500	5.12839400	6.55008900
Pt	0.02908000	-1.68170500	-0.66624500
Cl	-0.51553800	-3.72839700	0.53114000
Cl	-1.73930200	-0.52432000	0.45134100
C	1.35425500	-2.65883500	-1.54991100
O	2.14297300	-3.28174900	-2.09943500

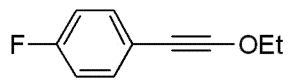
Energy (0K) = -2170.1462624

Energy (0K) + ZPE = -2169.766893

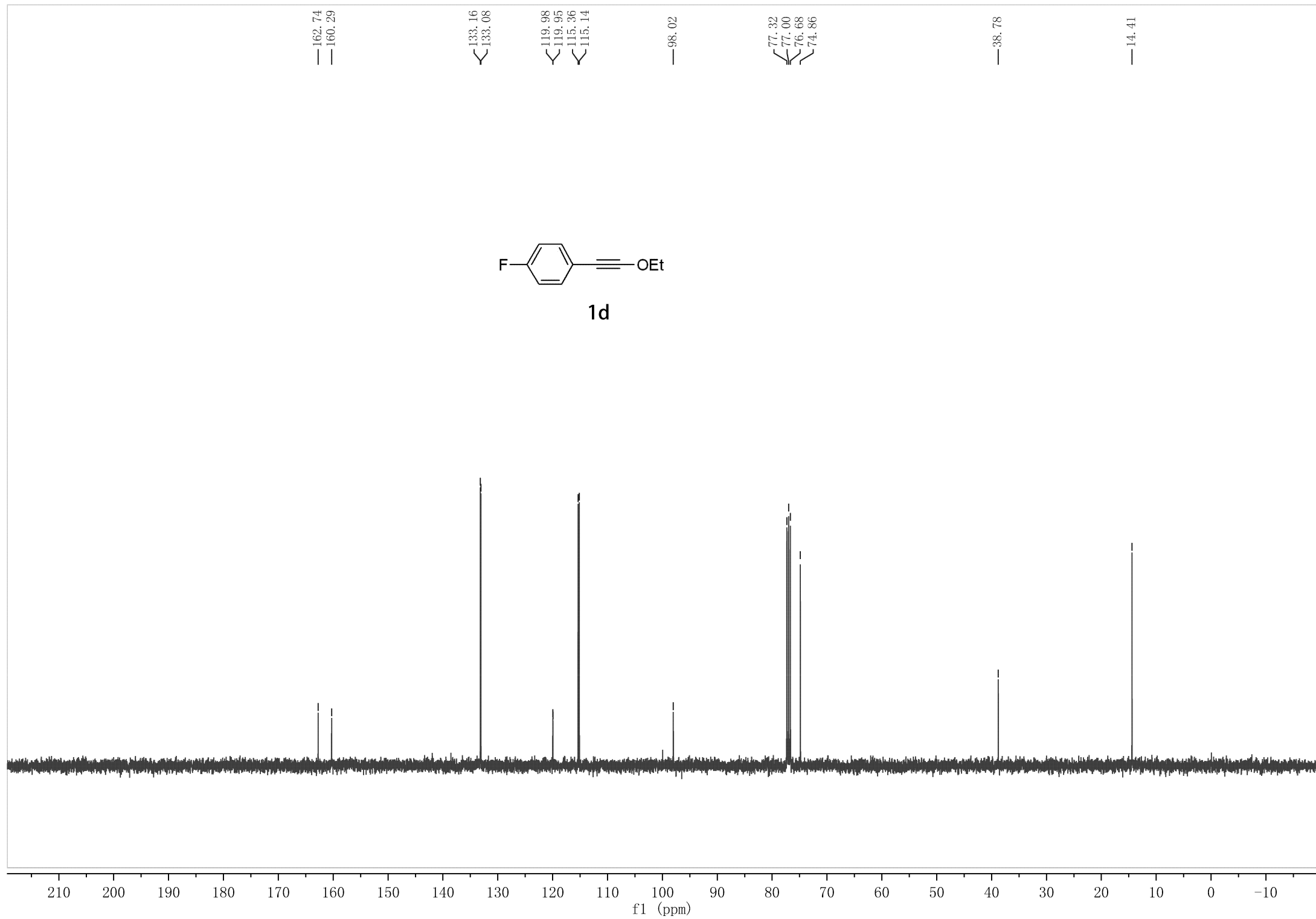
Enthalpy (298K) = -2169.735211

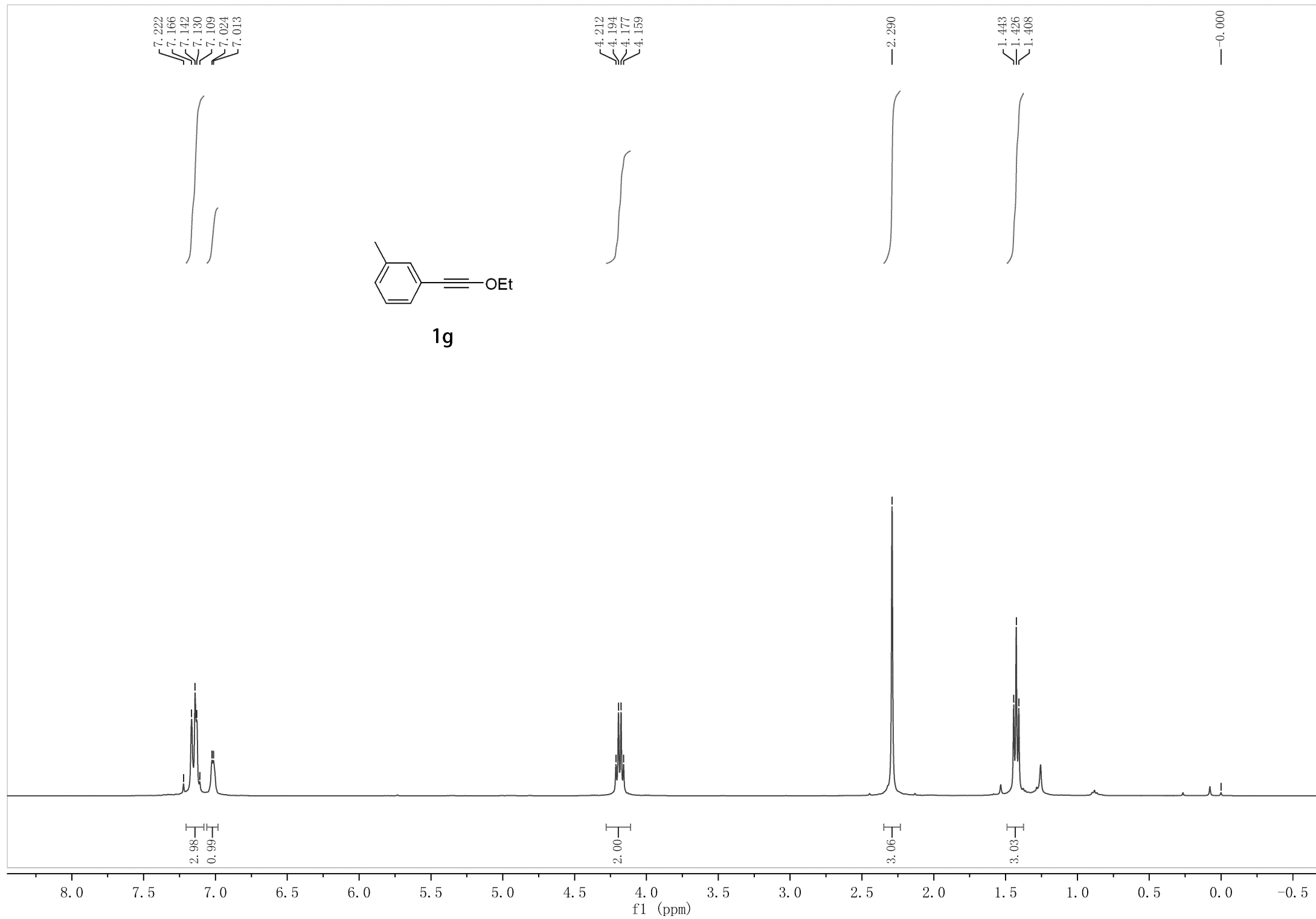
Free Energy (298K) = -2169.830453

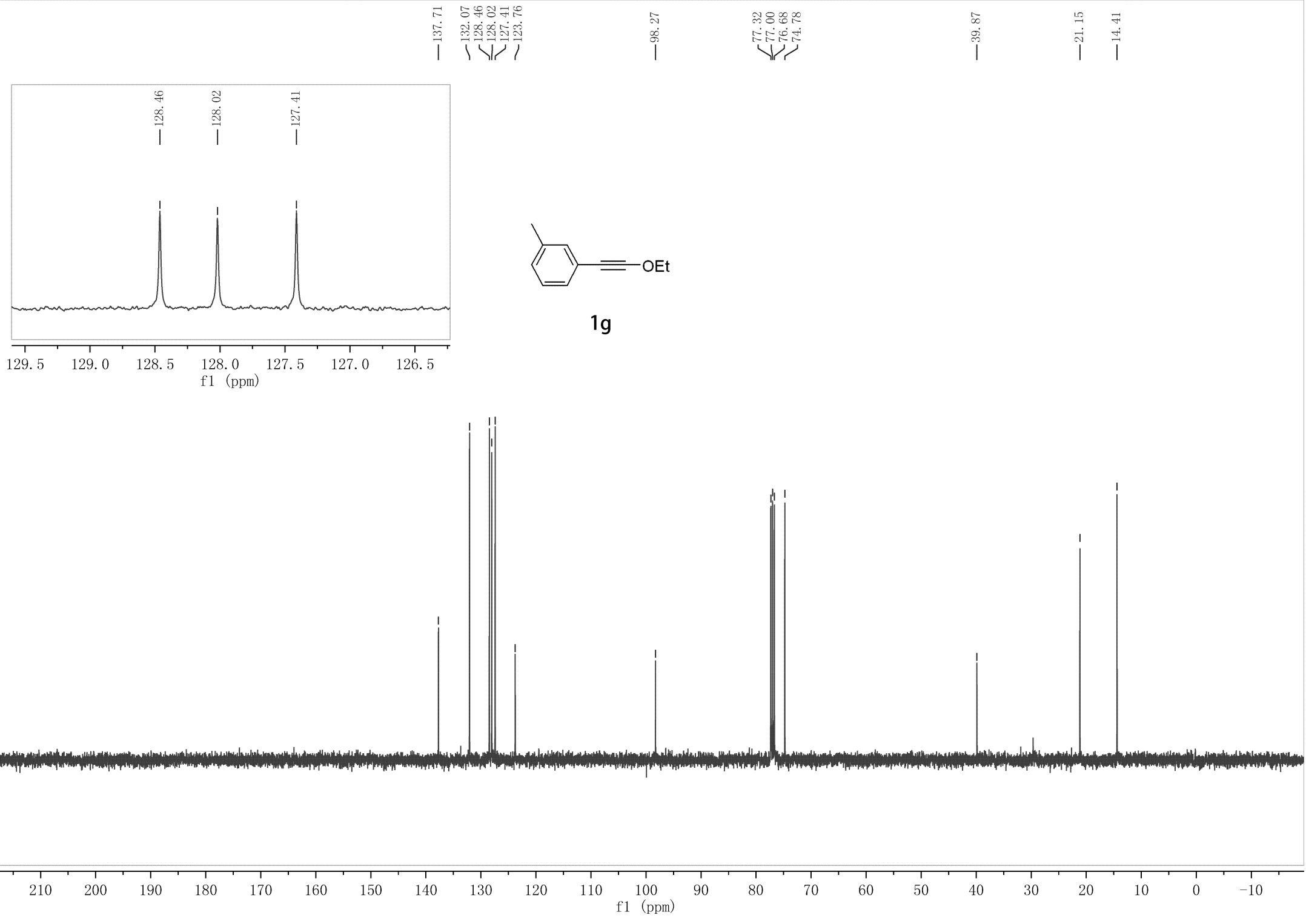


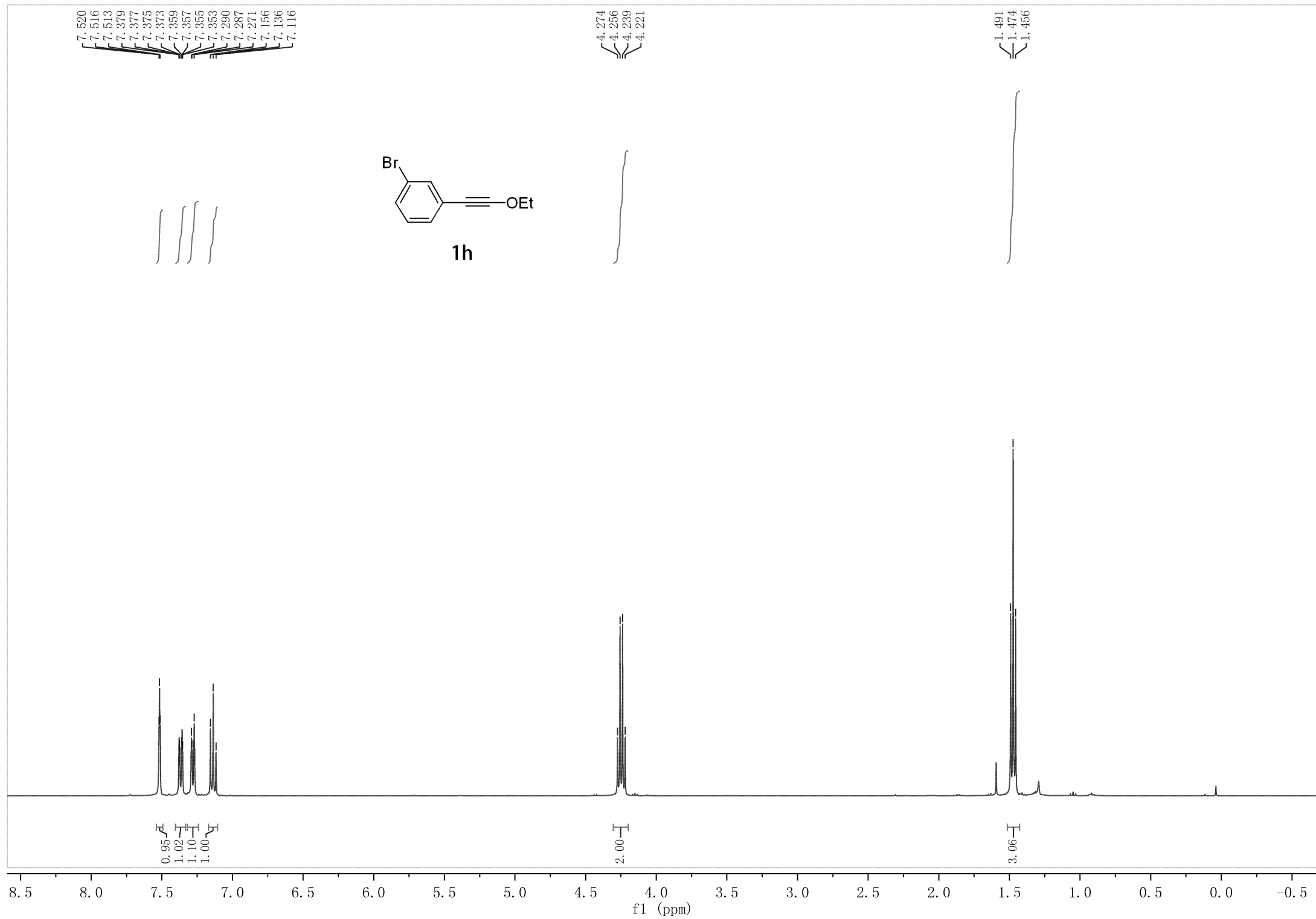


1d









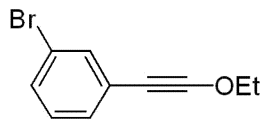
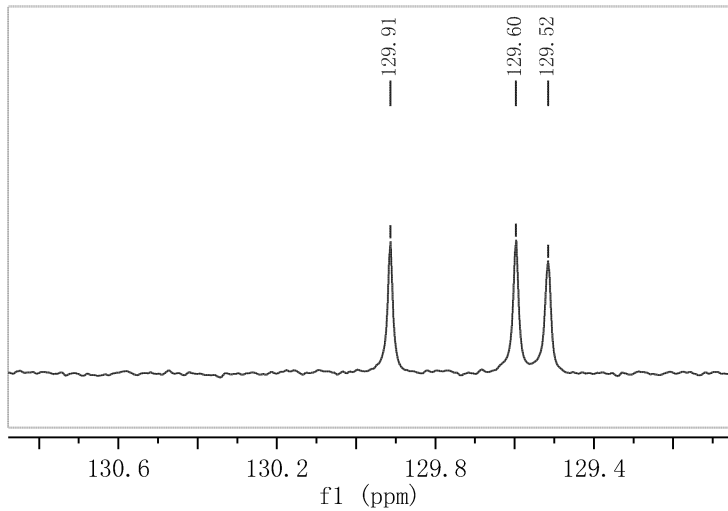
134.12
129.91
129.60
129.52
126.22
121.92

99.65

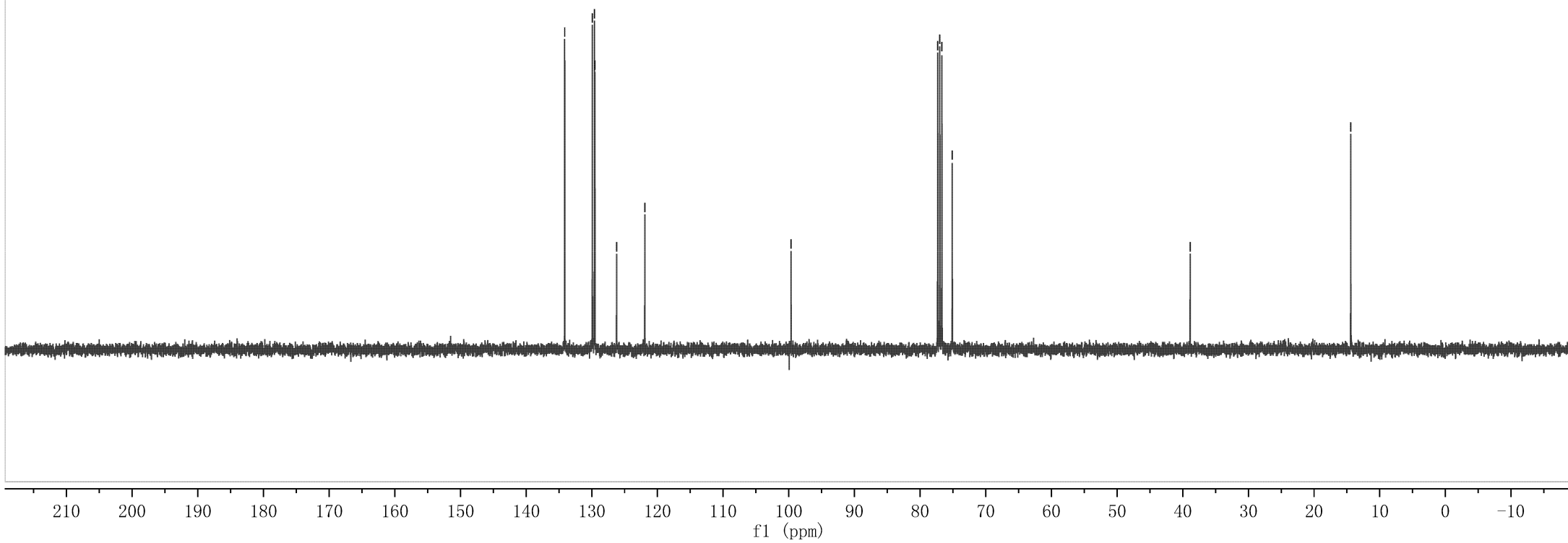
77.32
77.00
76.68
75.10

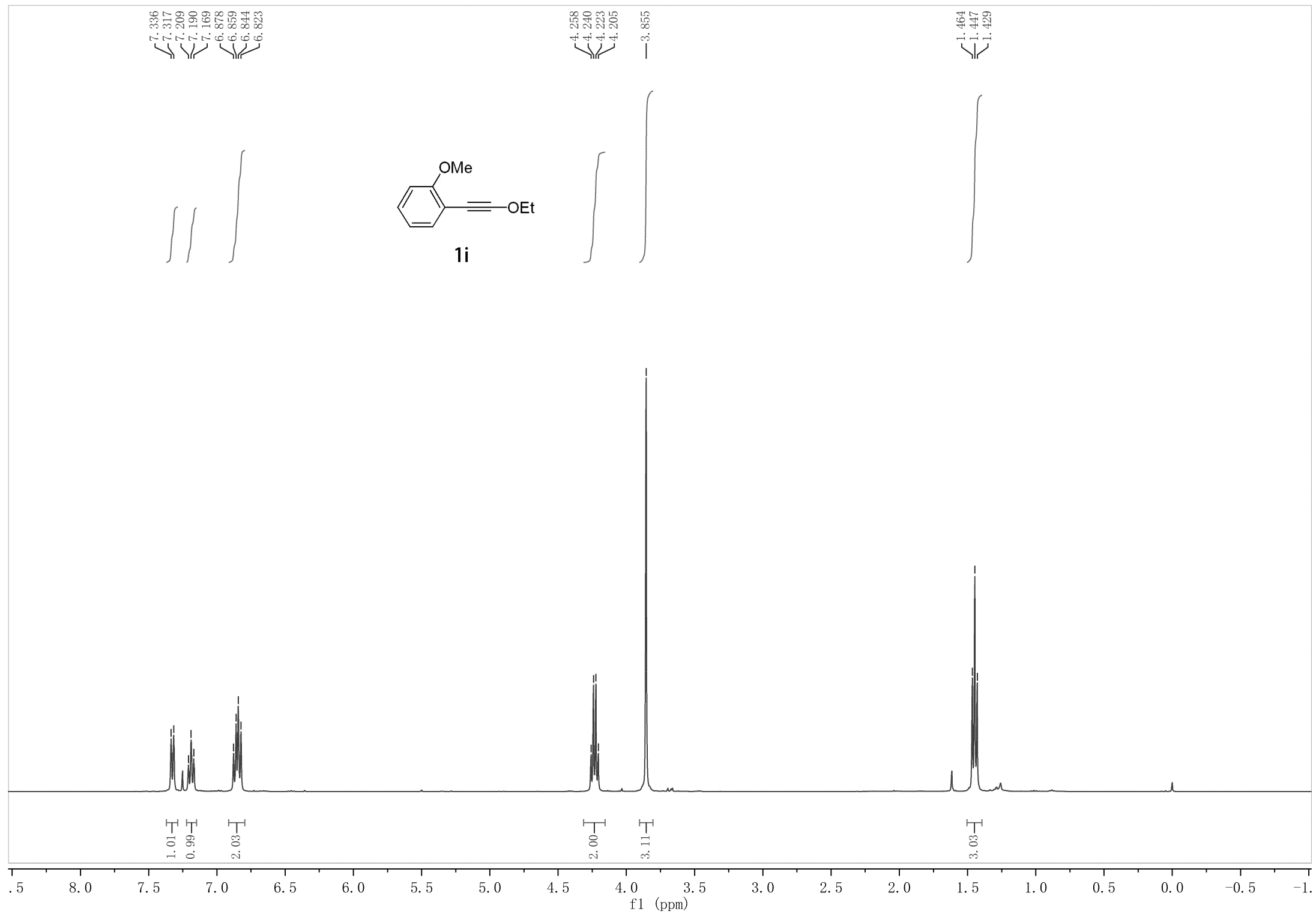
38.87

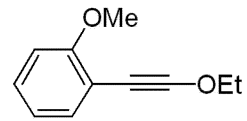
14.42



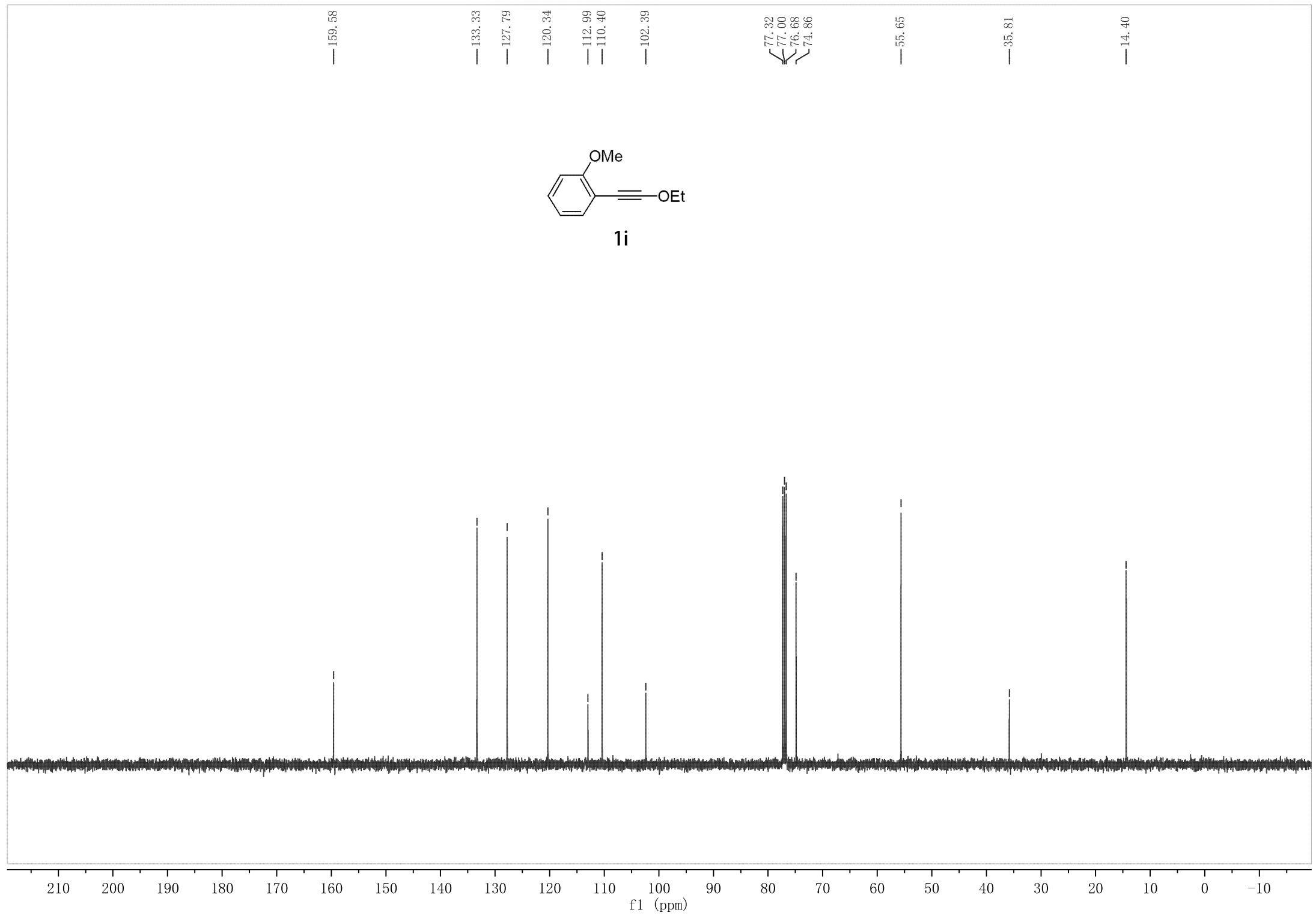
1h

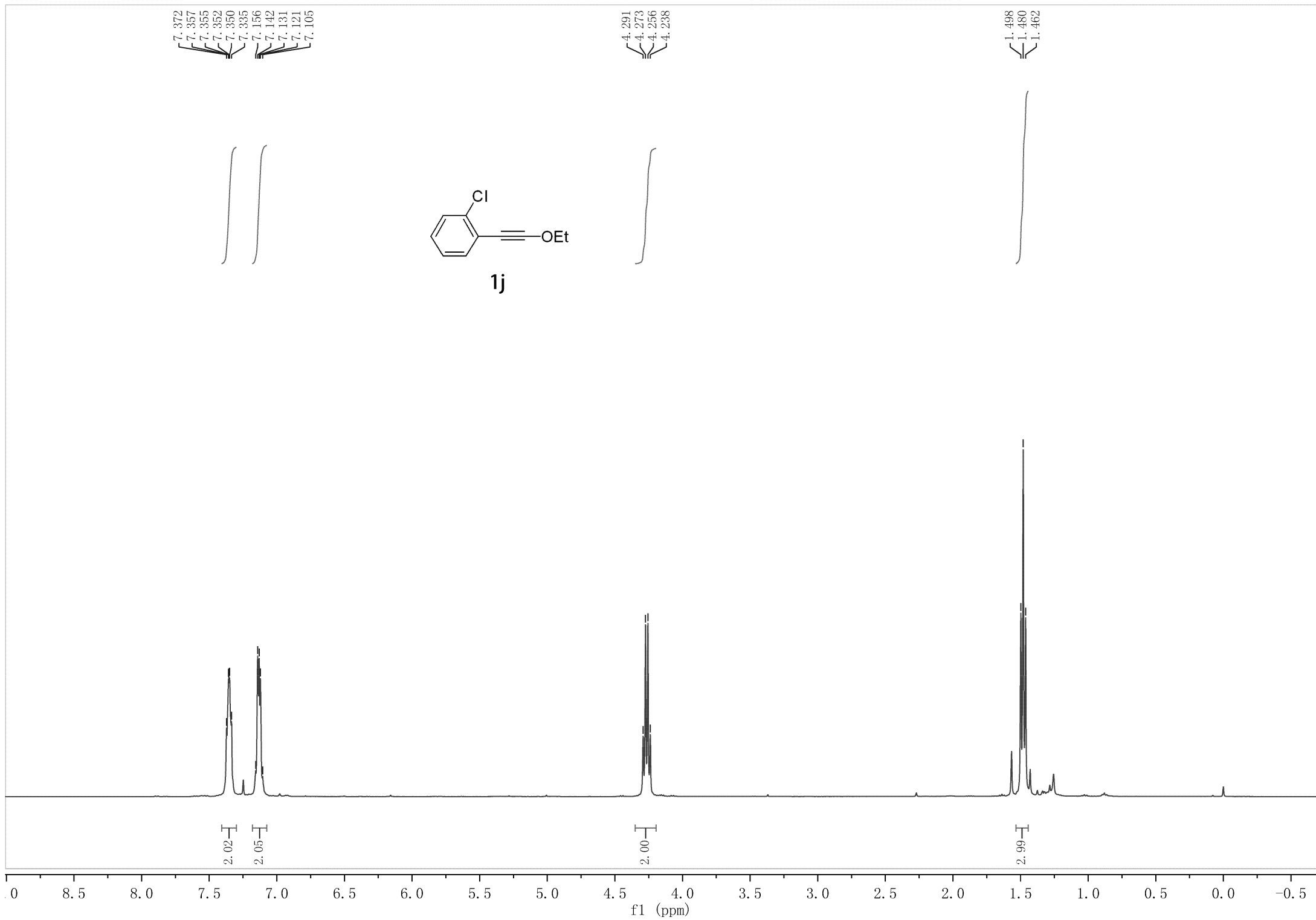


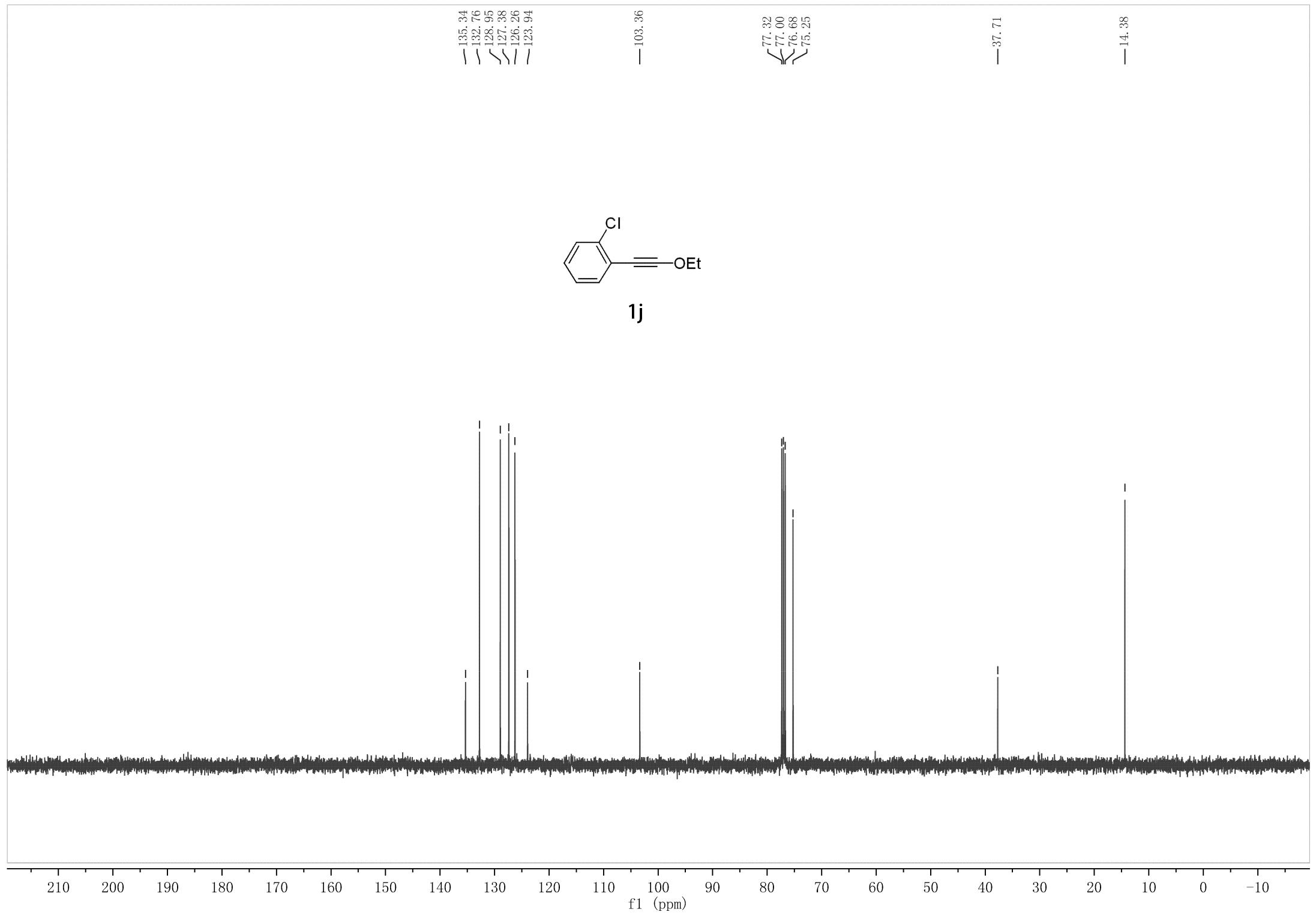
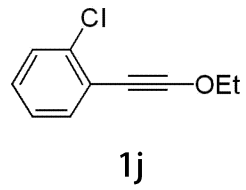




1i



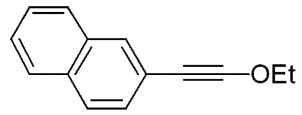




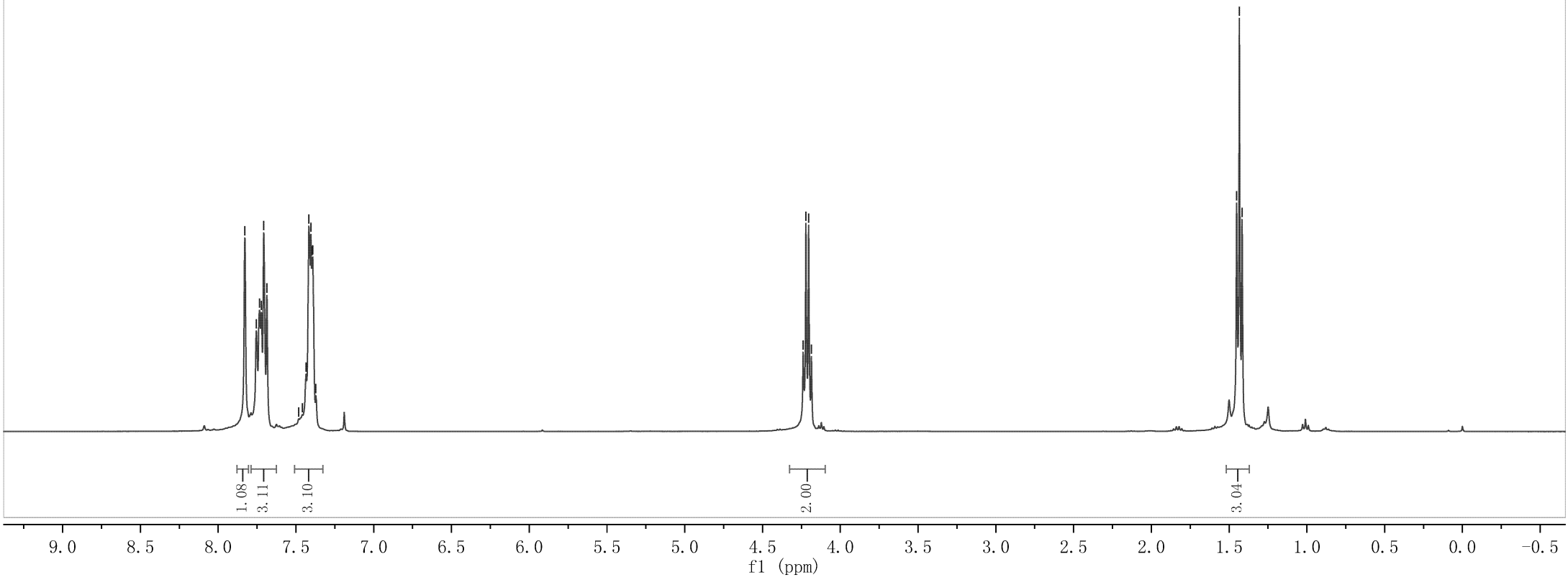
7.828
7.755
7.734
7.722
7.707
7.687
7.483
7.459
7.435
7.417
7.404
7.397
7.392
7.372

4.239
4.221
4.204
4.186

1.452
1.434
1.417



1k



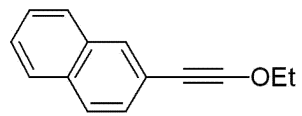
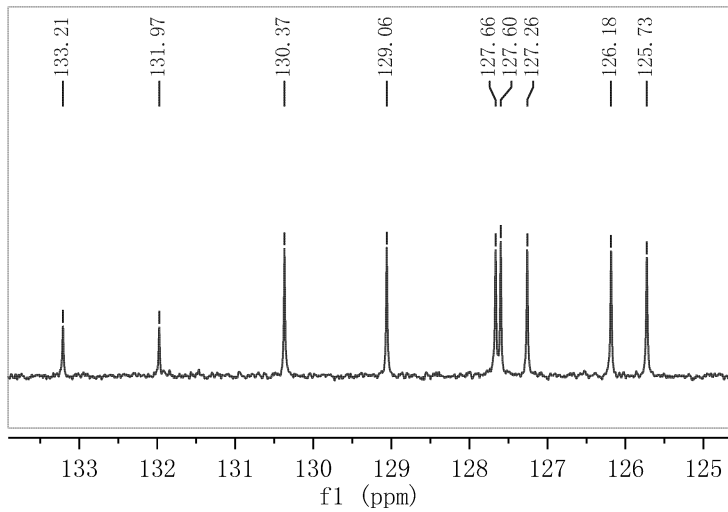
133.21
131.97
130.37
129.06
127.66
127.60
127.26
126.18
125.73
121.41

98.97

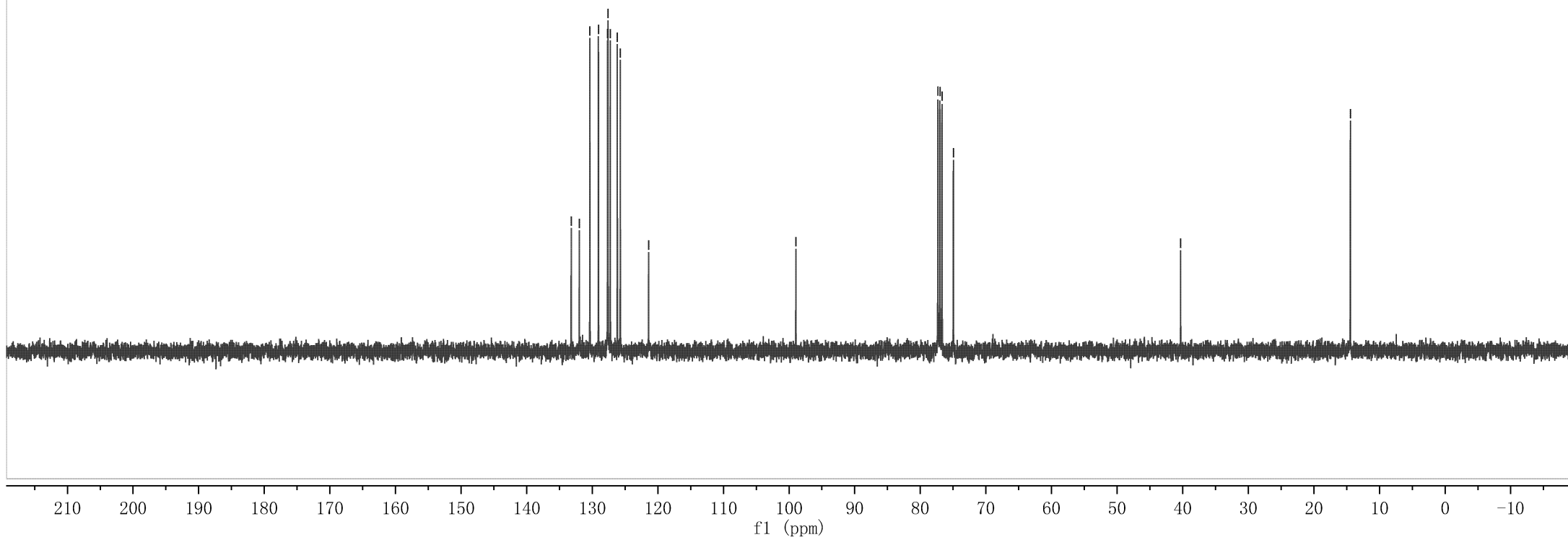
77.32
77.00
76.68
74.96

40.31

14.44



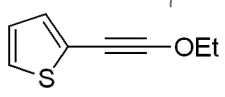
1k



7.113
7.100
7.038
7.031
6.915
6.906
6.903
6.894

4.234
4.217
4.199
4.181

1.444
1.426
1.408



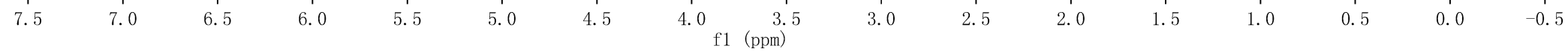
11



1.00
0.97
0.95

1.98

3.09



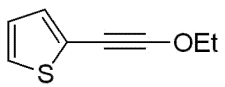
130.43
126.69
125.15
124.20

101.70

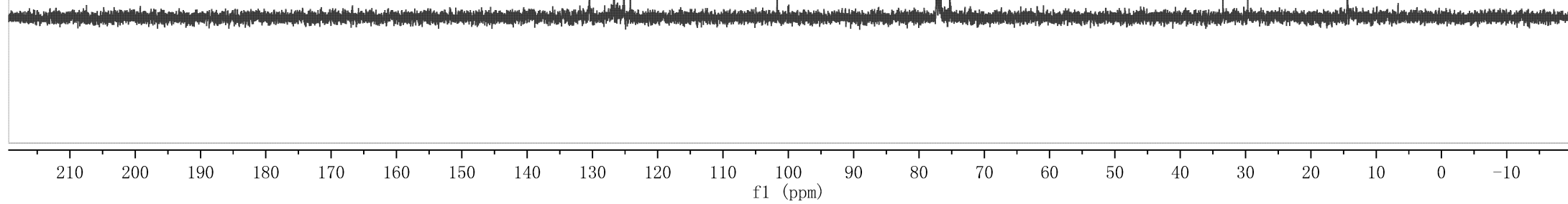
77.32
77.00
76.68
75.26

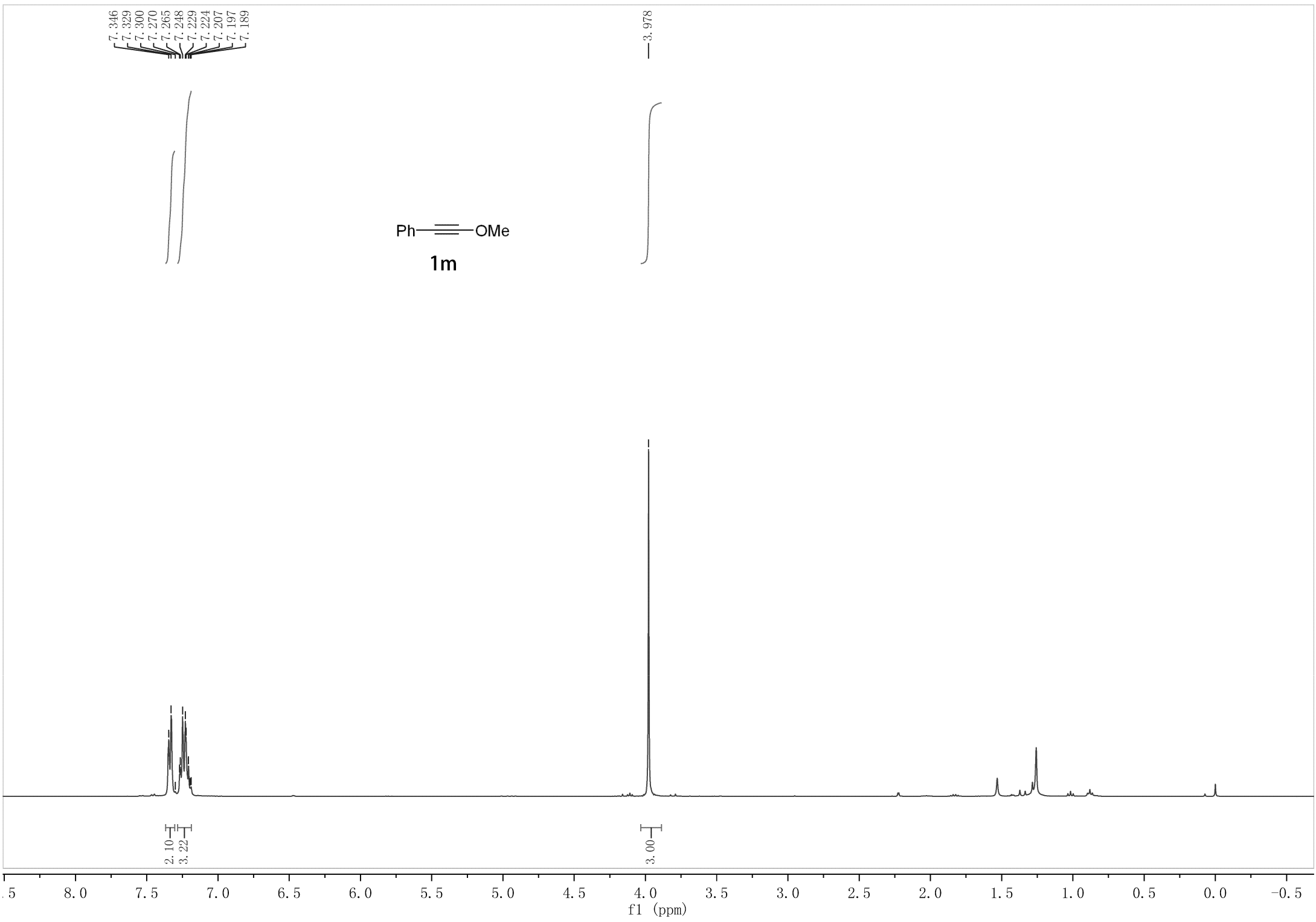
33.48

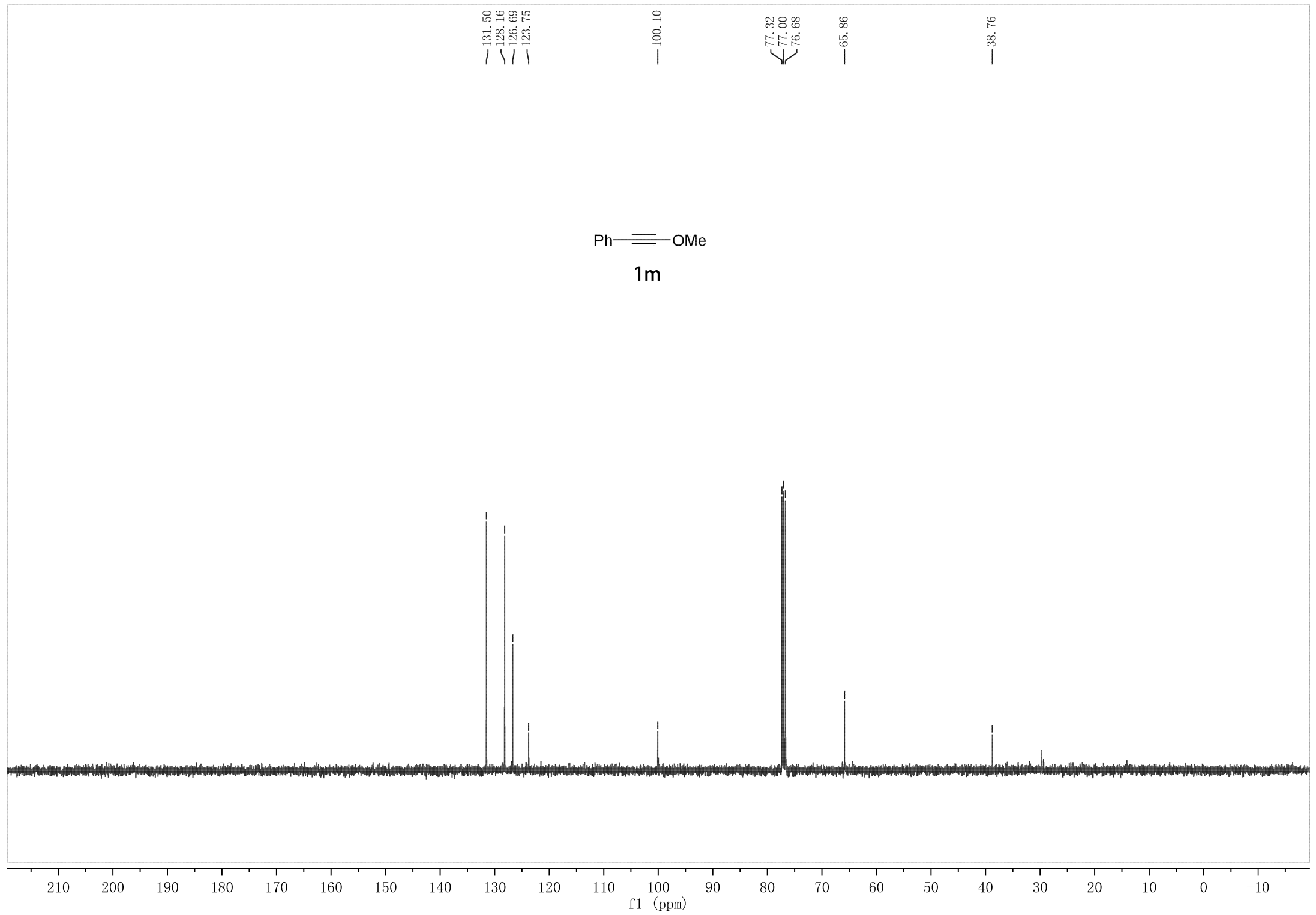
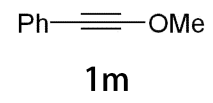
14.43

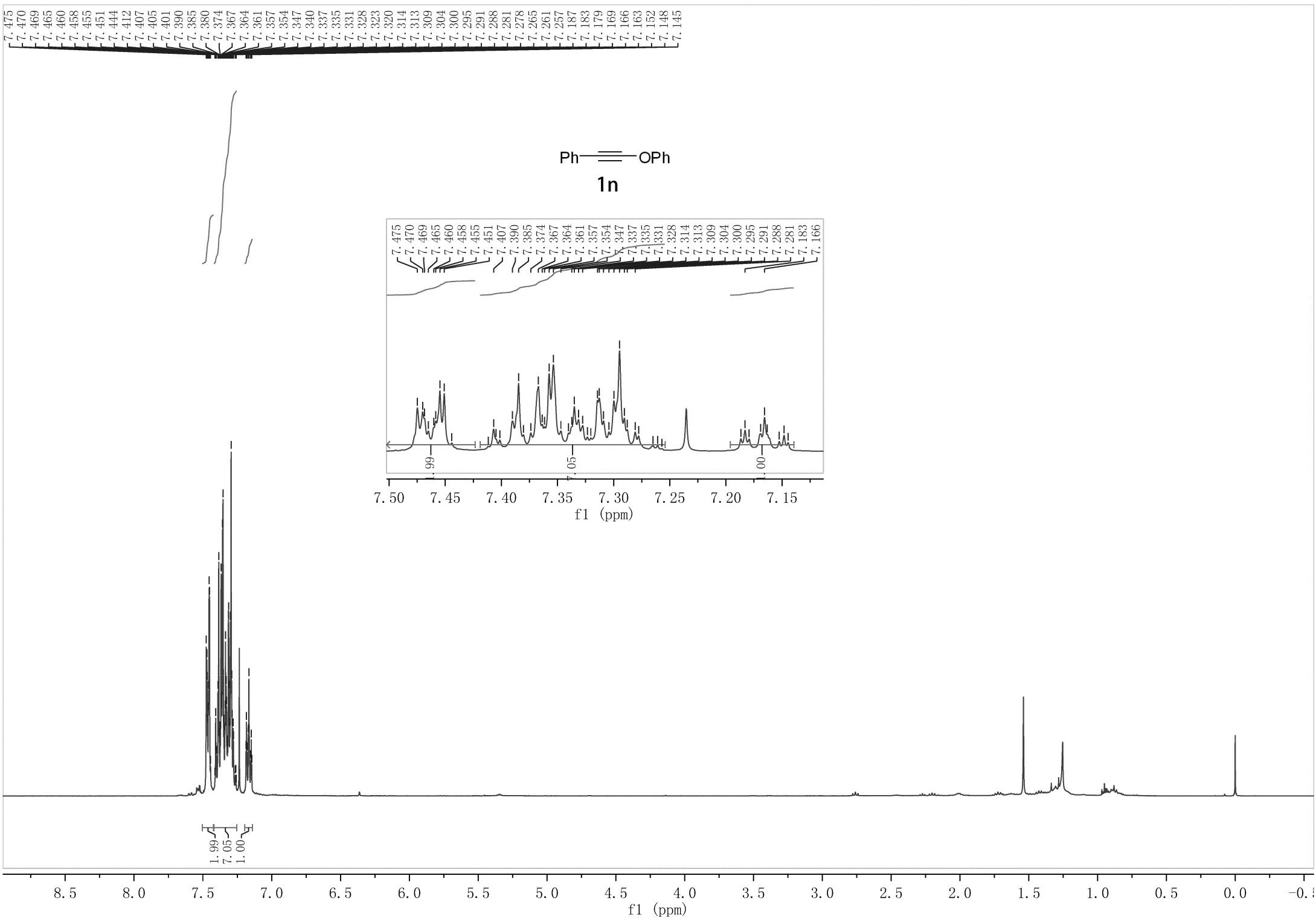


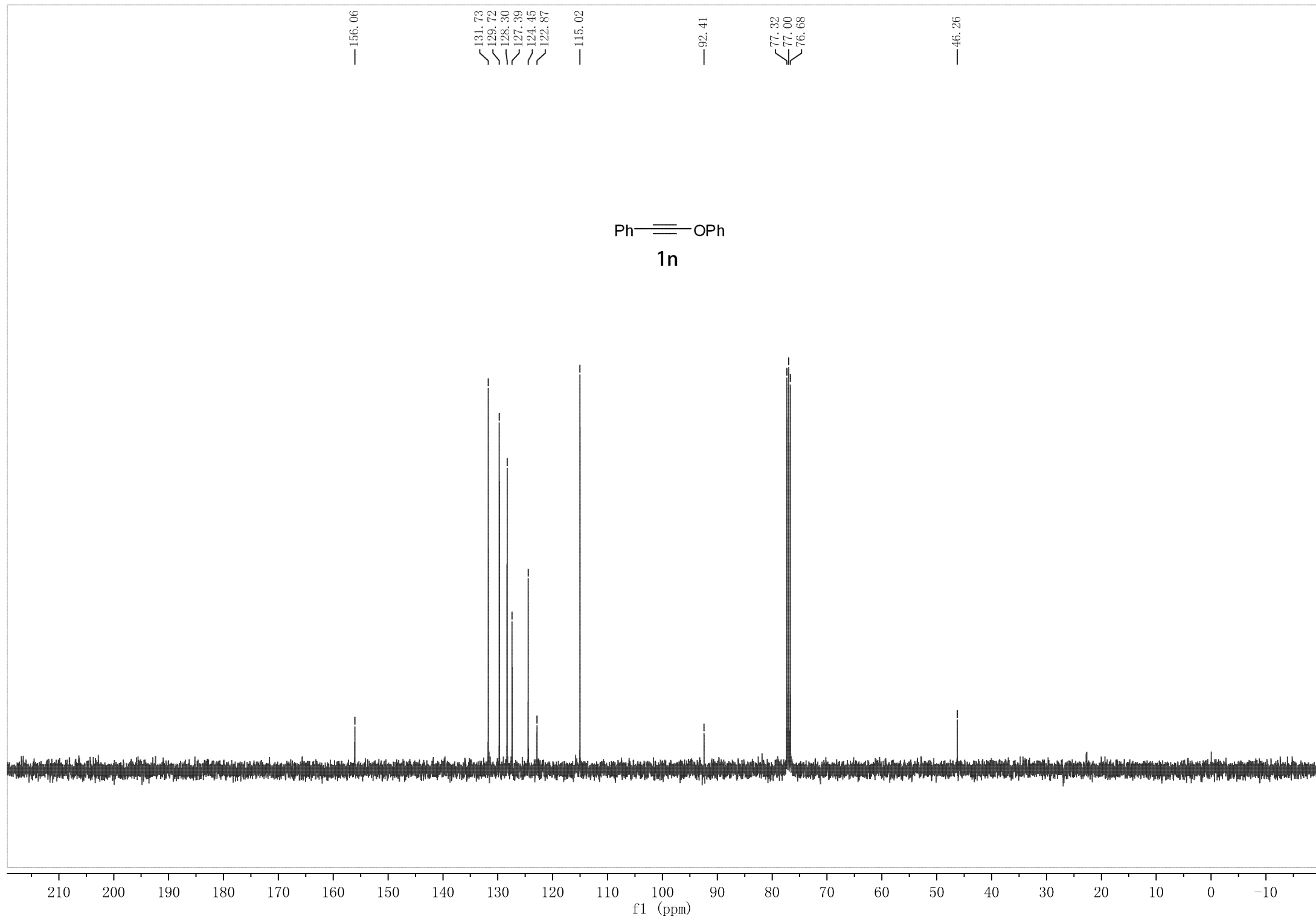
11

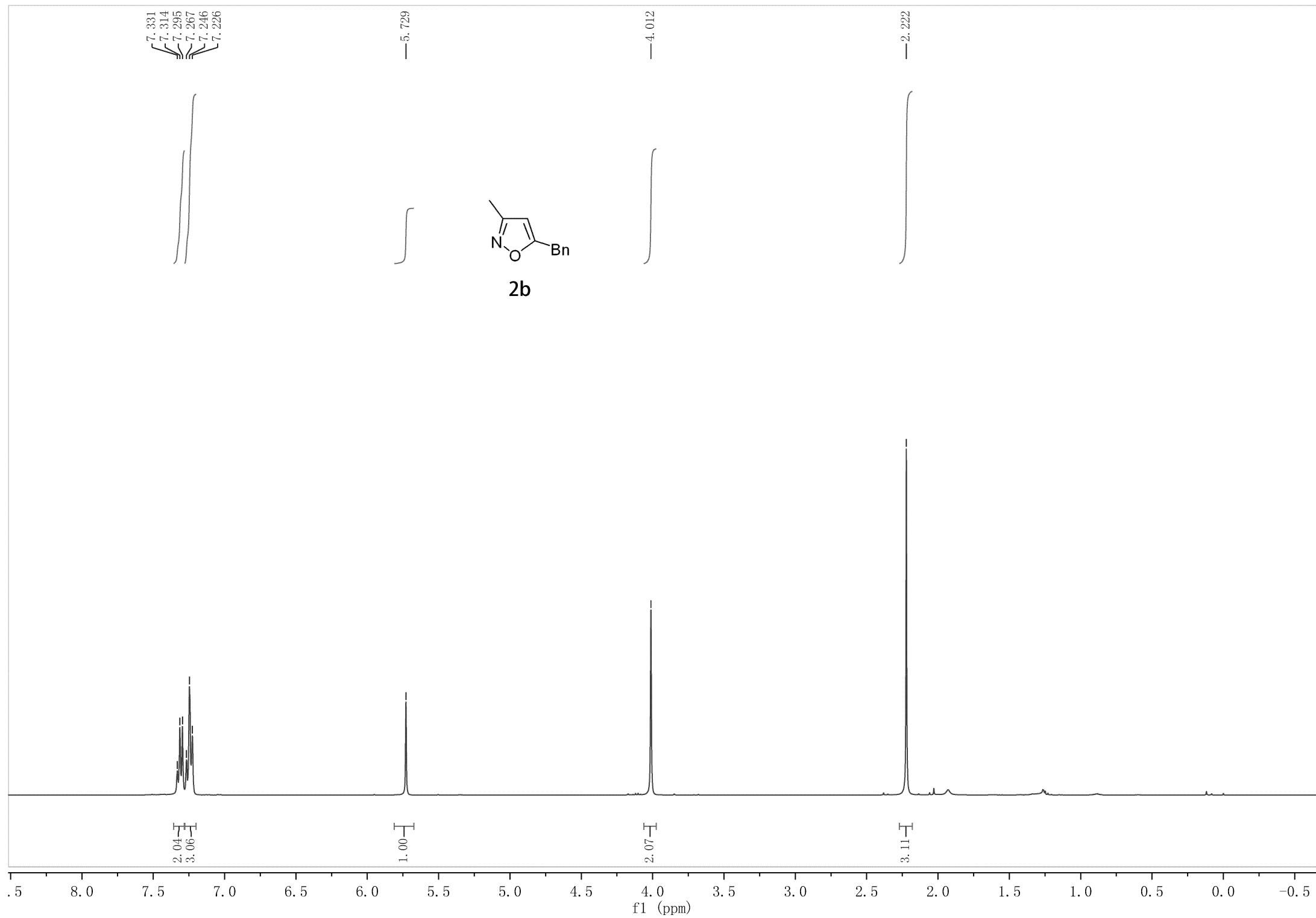


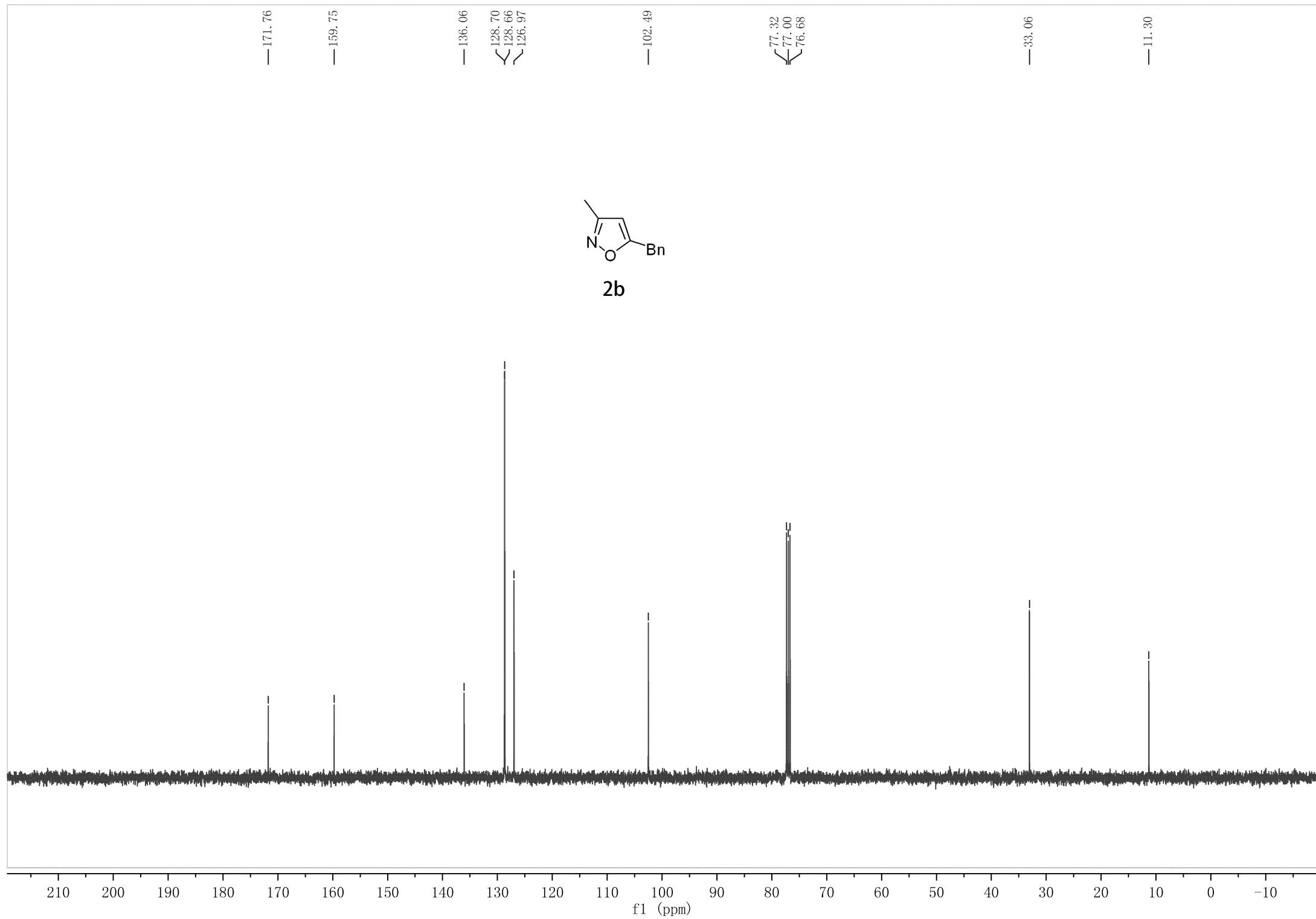


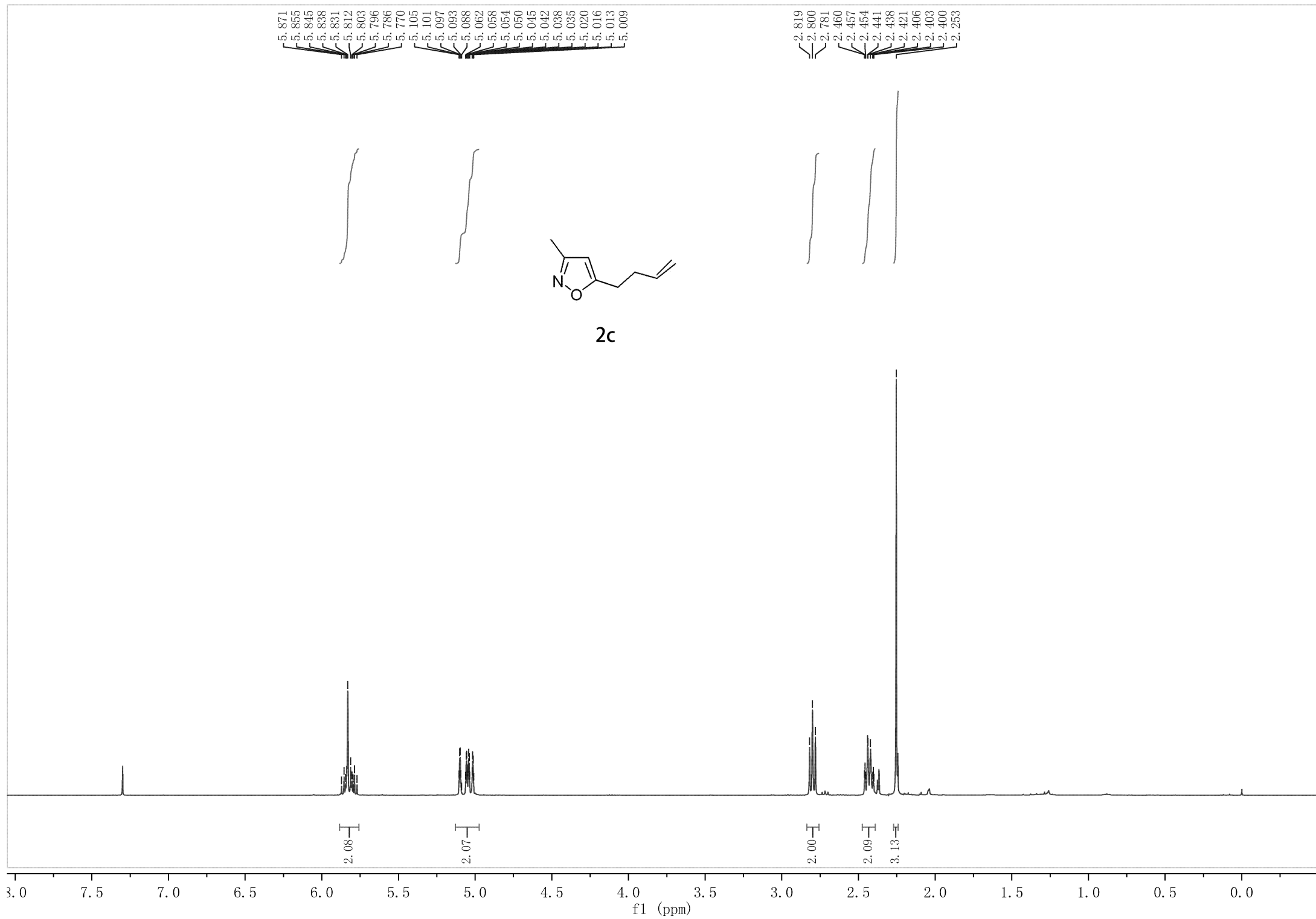


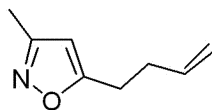












2c

— 172.30

— 159.53

— 136.32

— 115.83

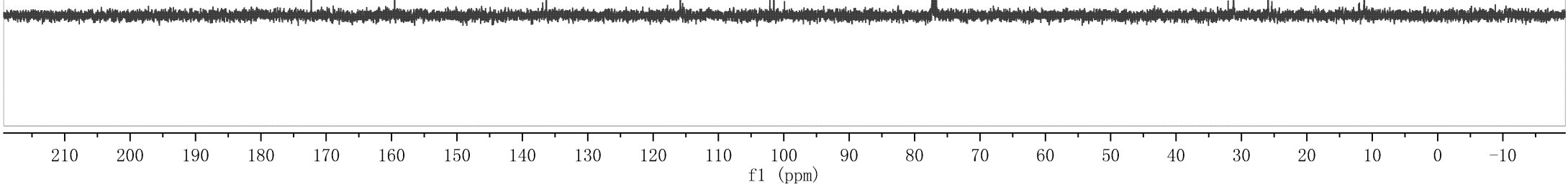
— 101.54

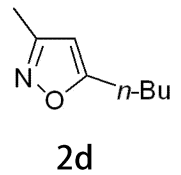
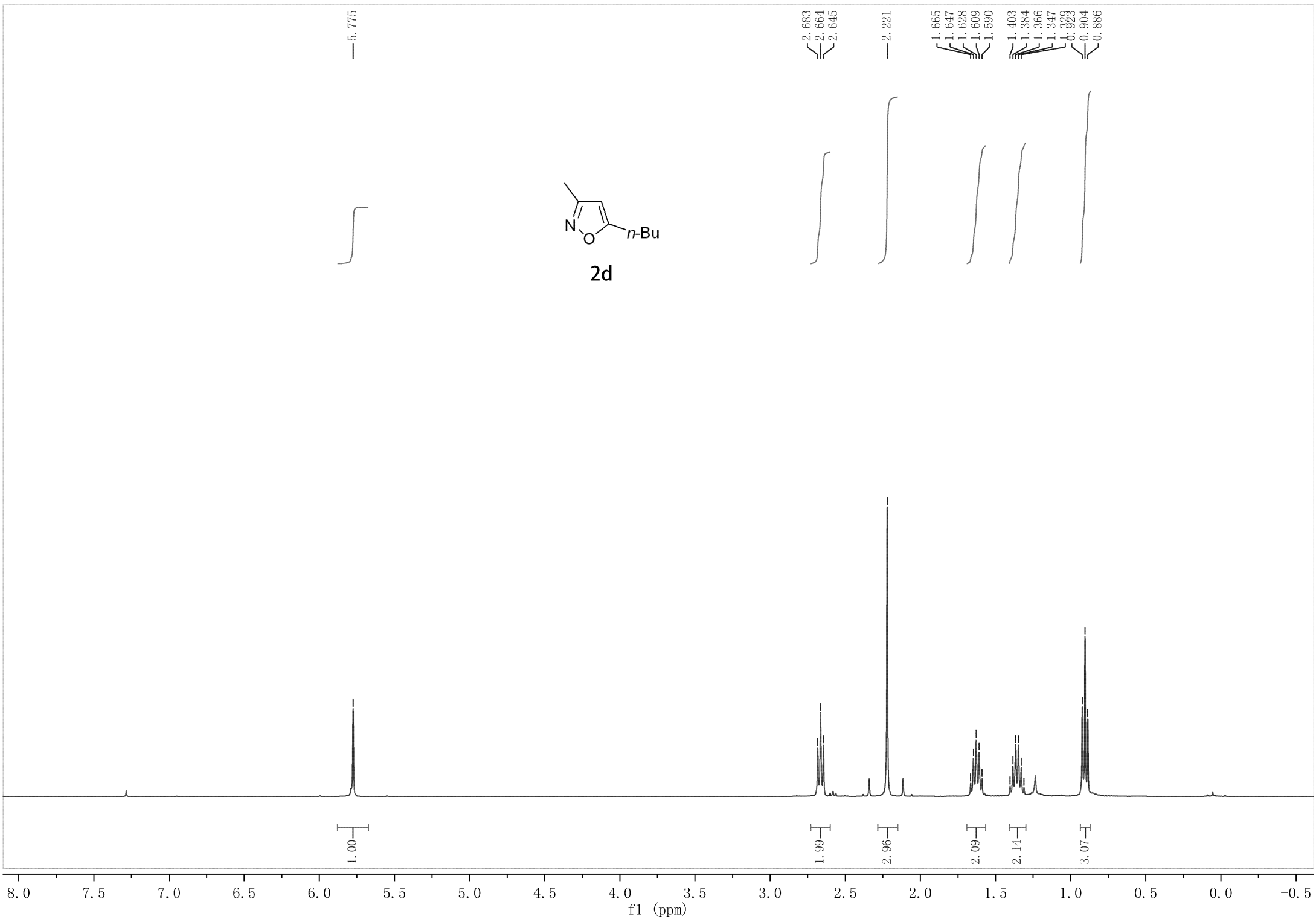
77.32
77.00
76.68

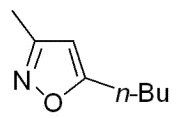
— 31.22

— 25.94

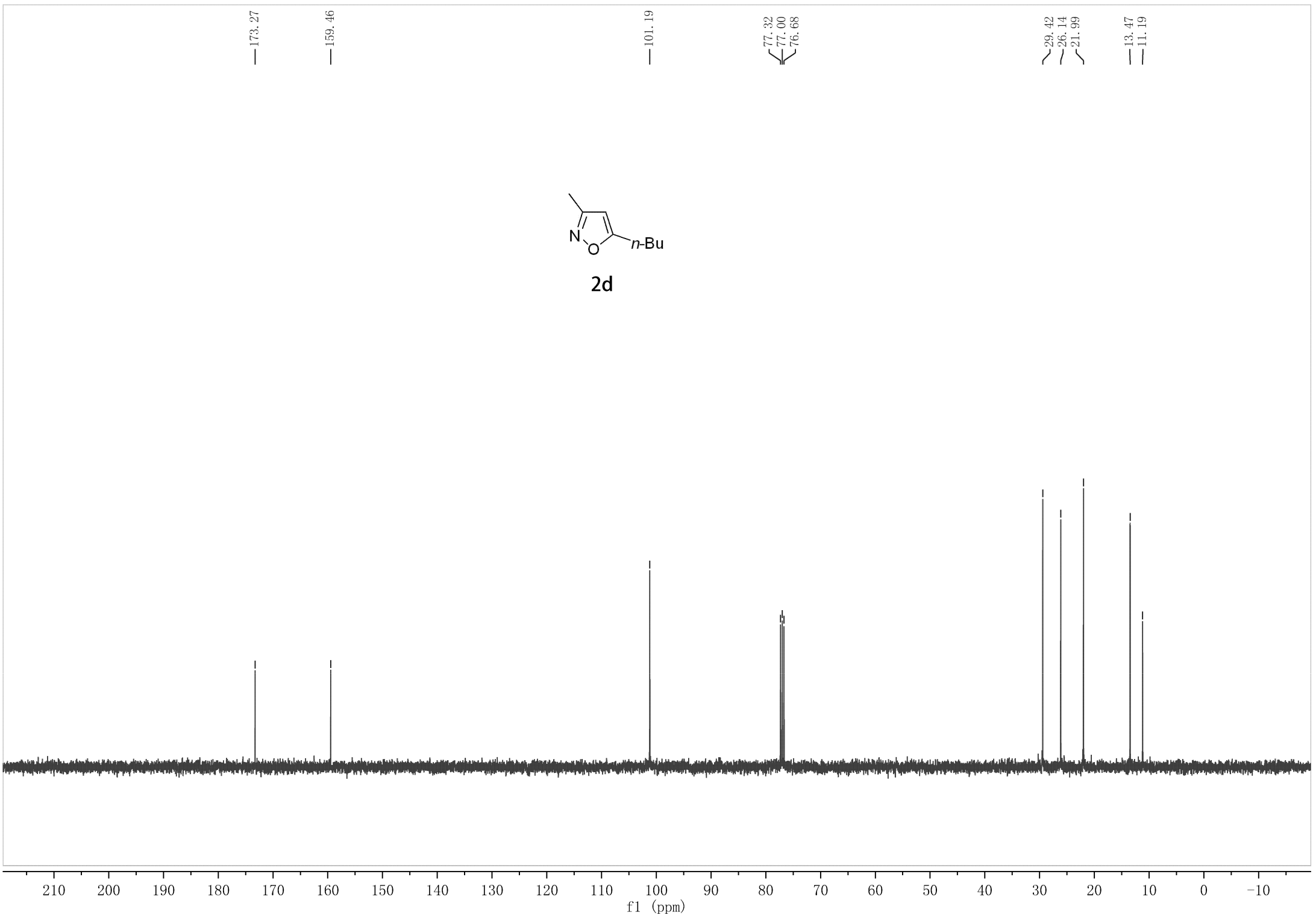
— 11.25

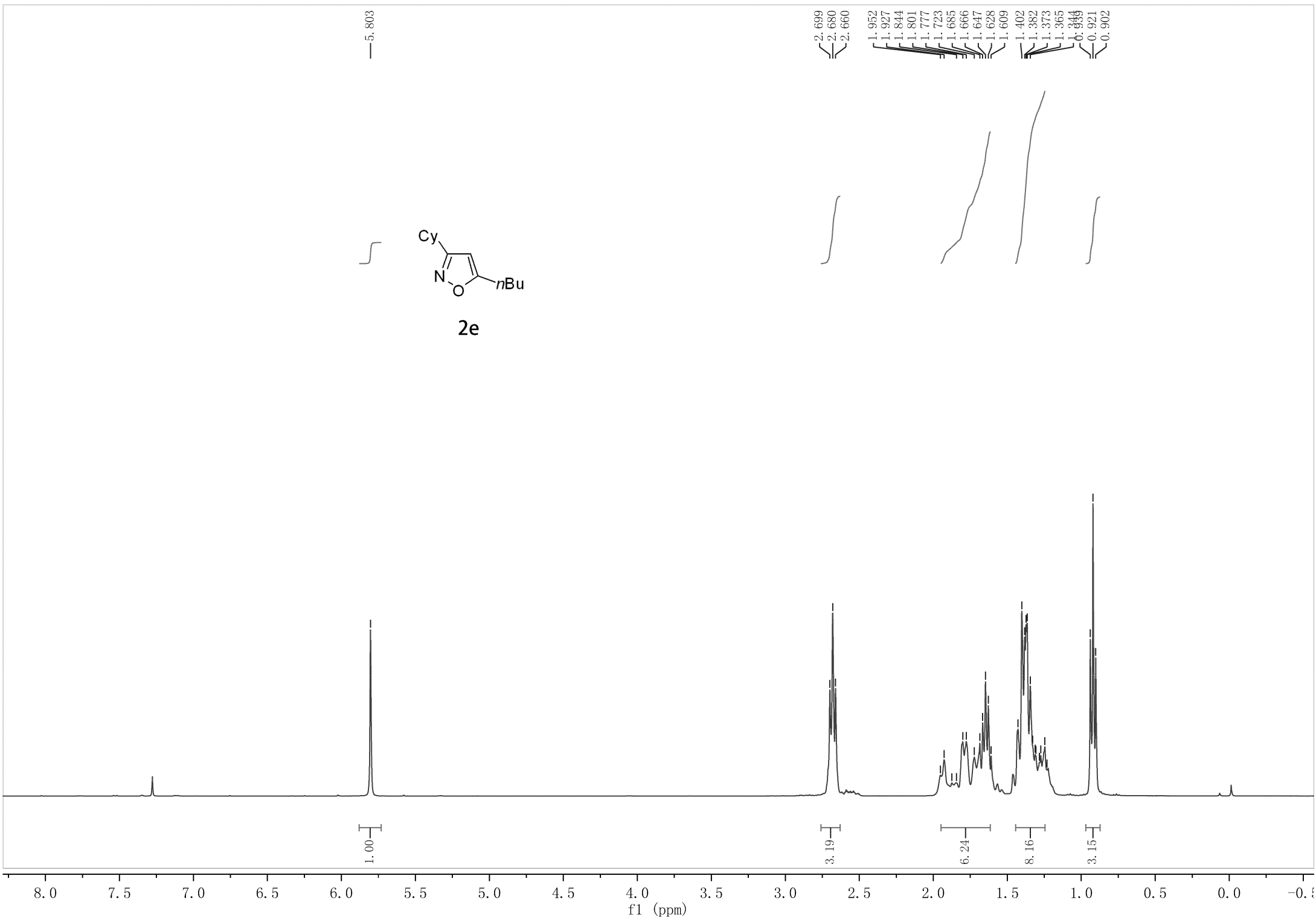






2d





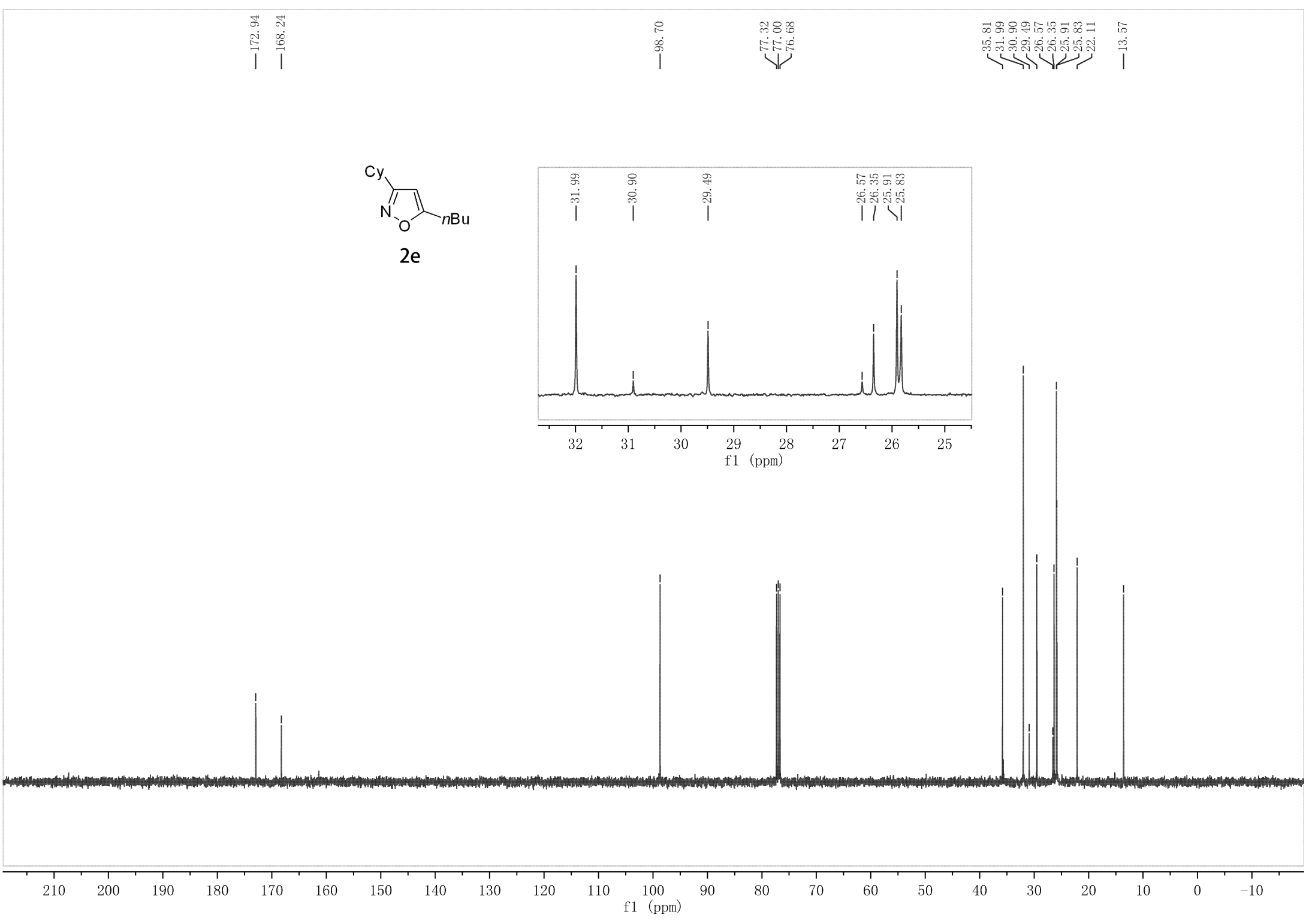
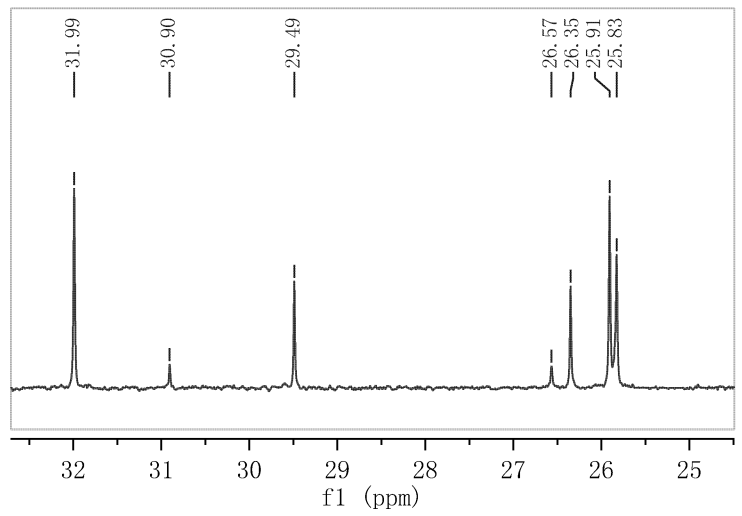
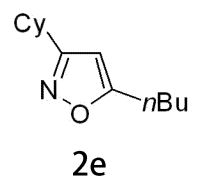
— 172.94
— 168.24

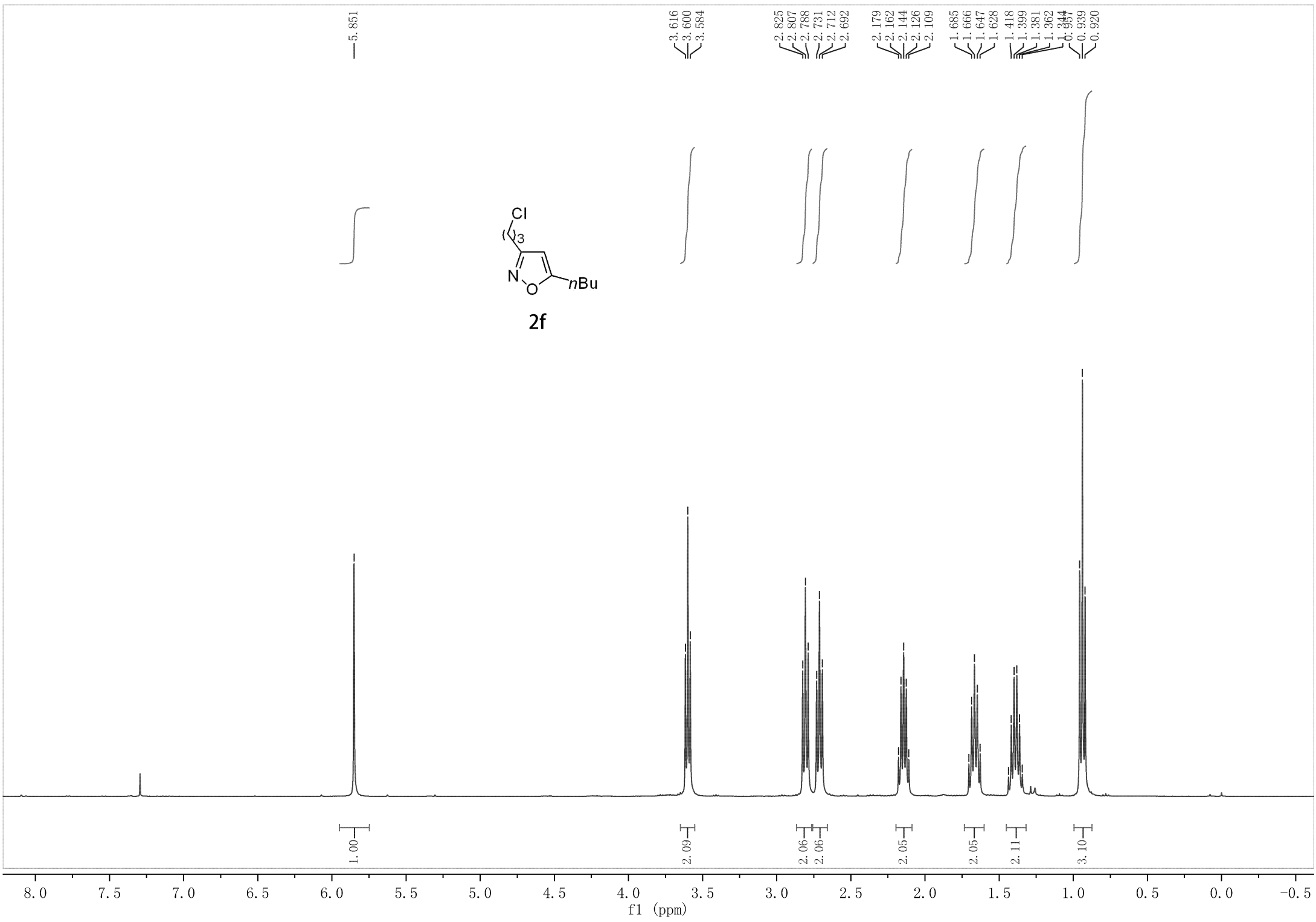
— 98.70

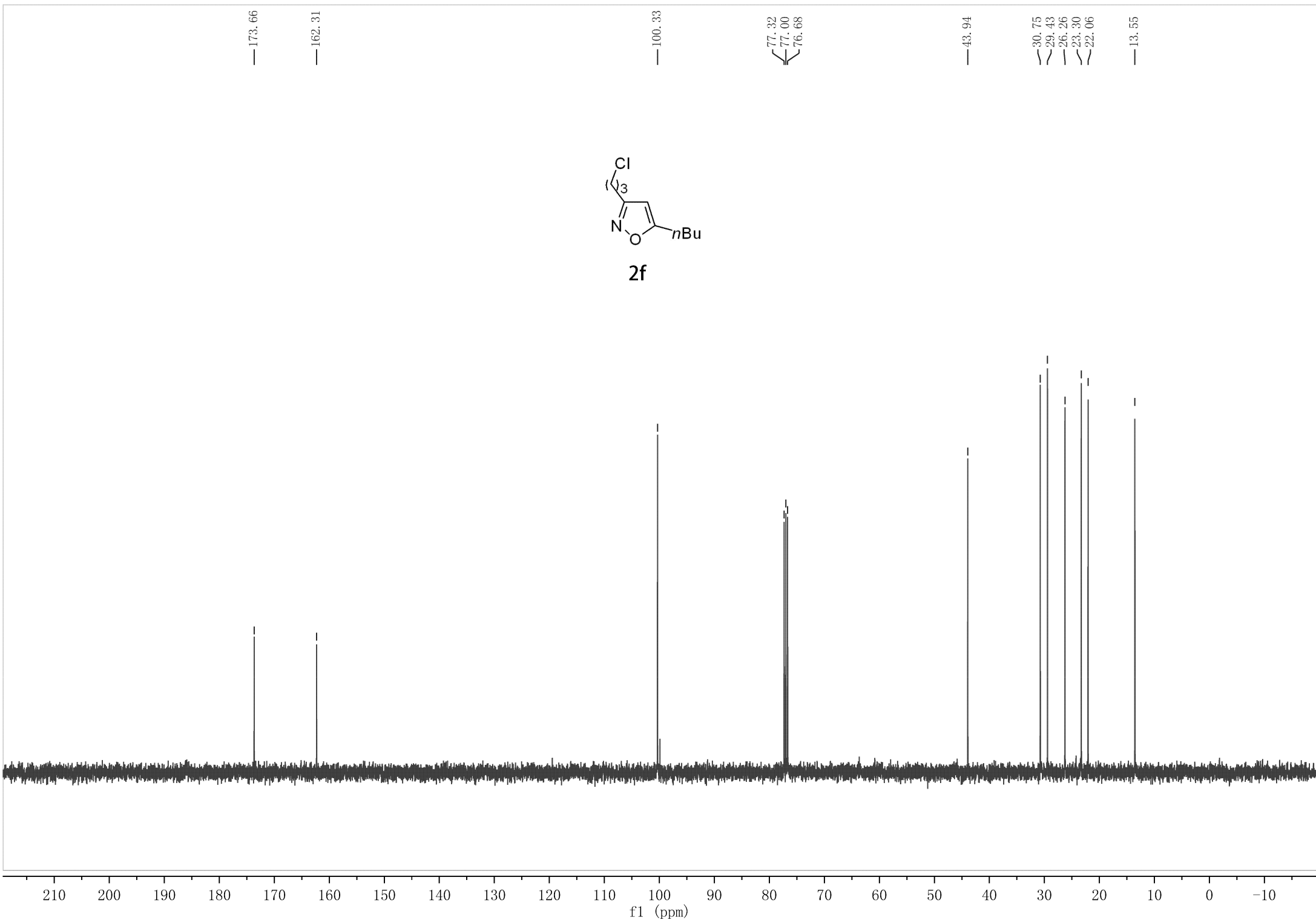
77.32
77.00
76.68

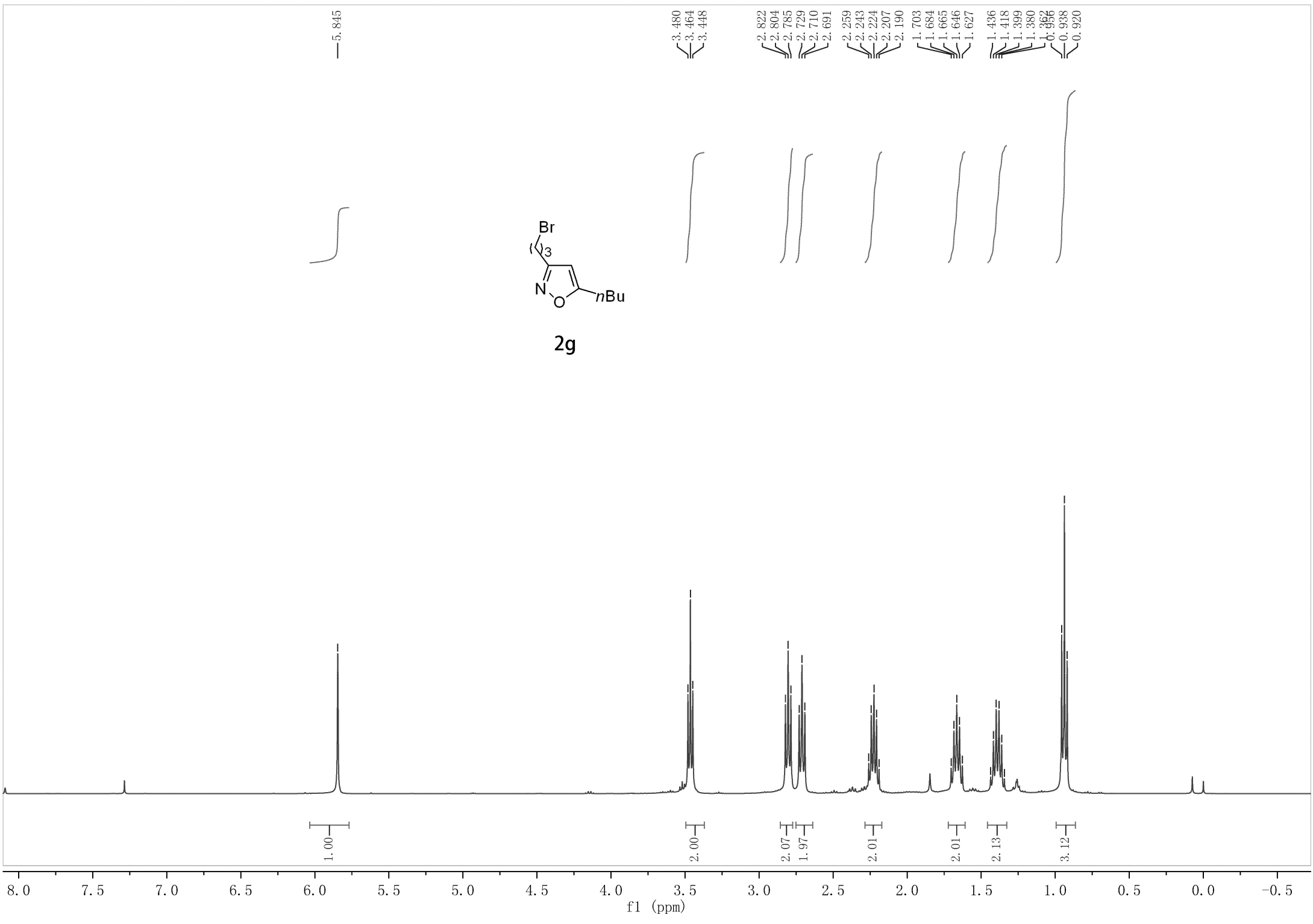
35.81
31.99
30.90
29.49
26.57
26.35
25.91
25.83
22.11

— 13.57









— 5.845

3.480
3.464
3.448

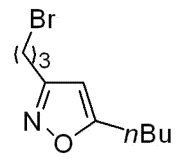
2.822
2.804
2.785
2.729
2.710
2.691

2.259
2.243
2.224
2.207
2.190

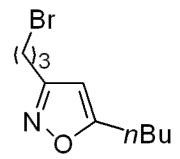
1.703
1.684
1.665
1.646
1.627

1.436
1.418
1.399
1.380
1.366

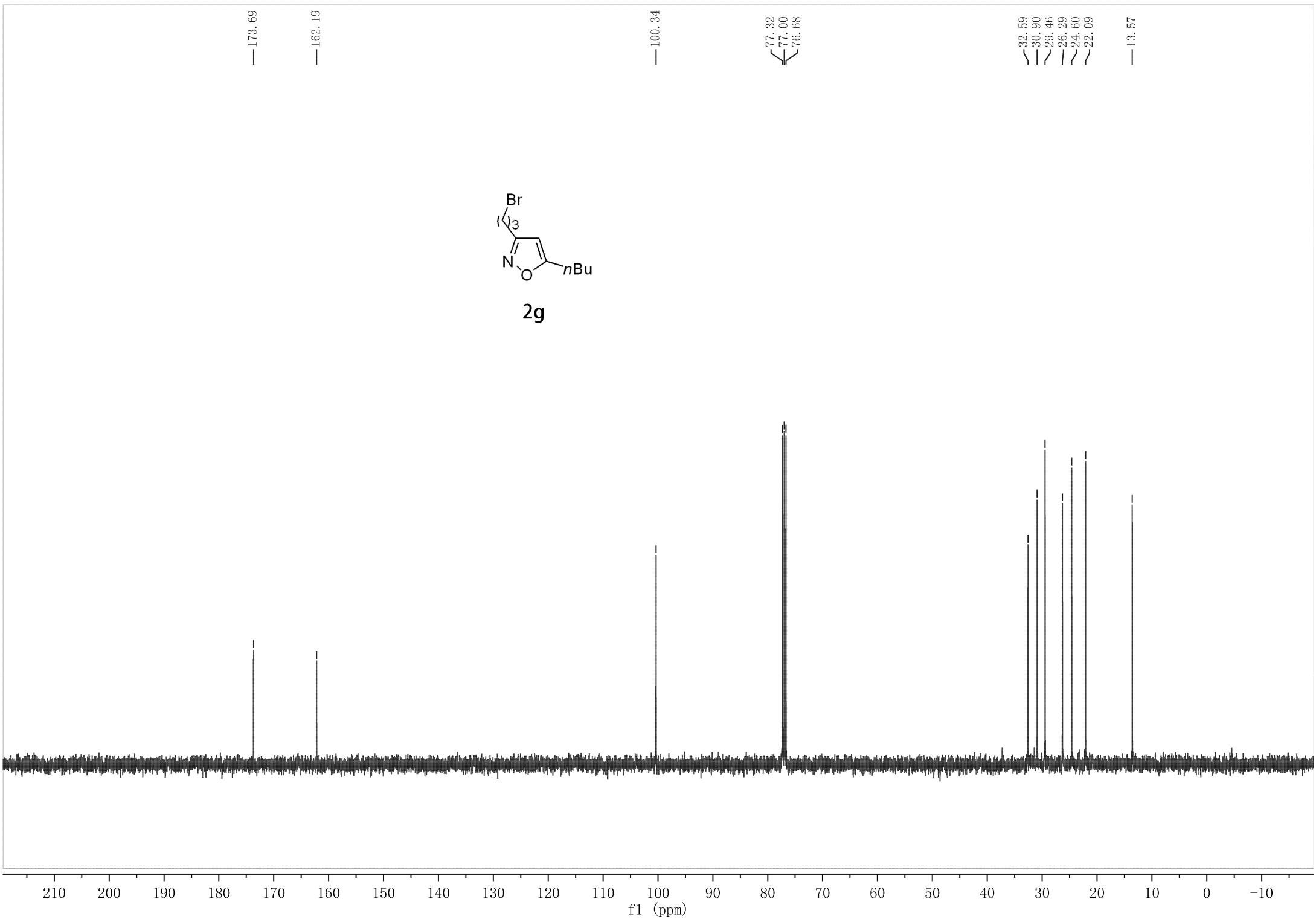
0.938
0.920

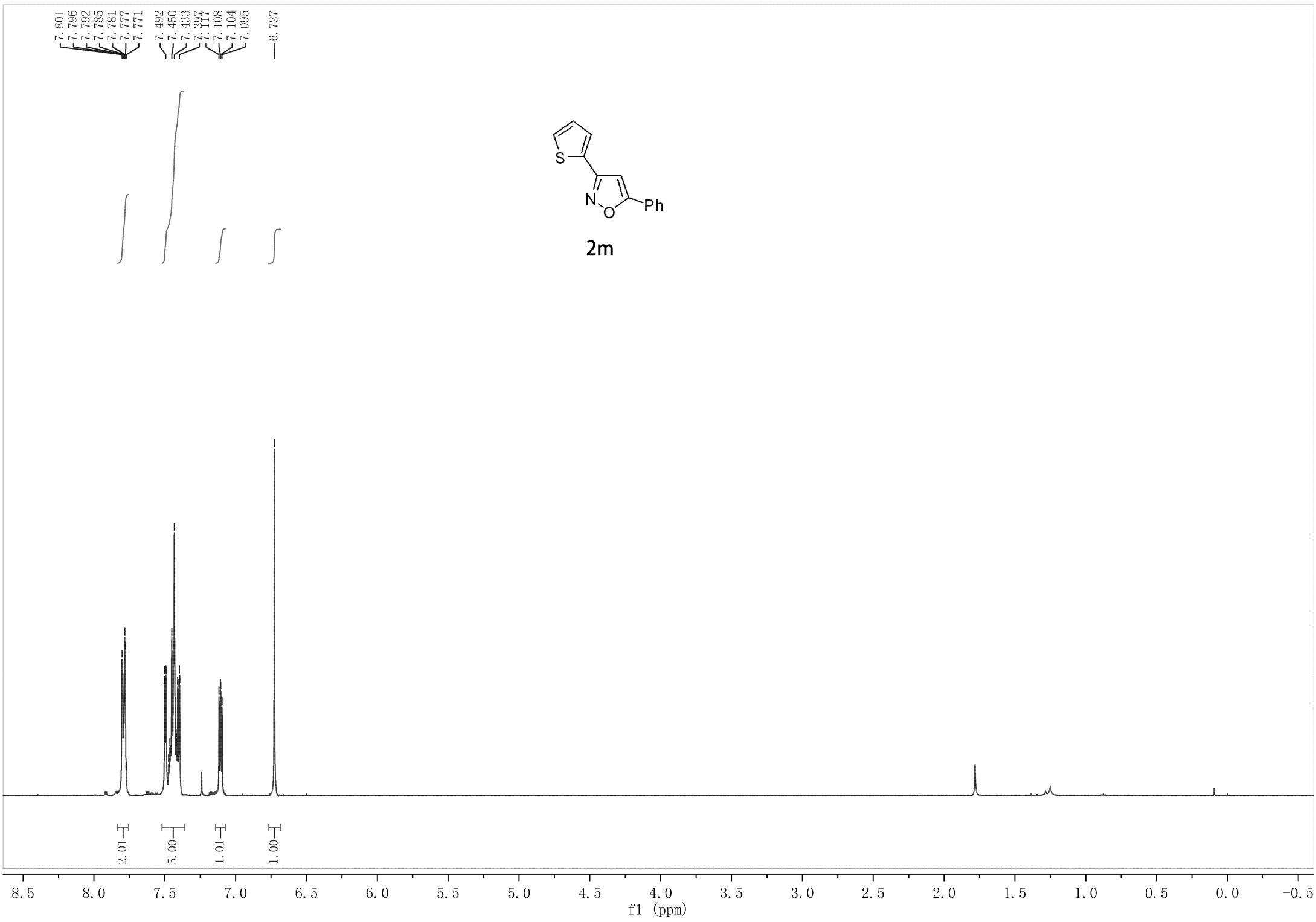


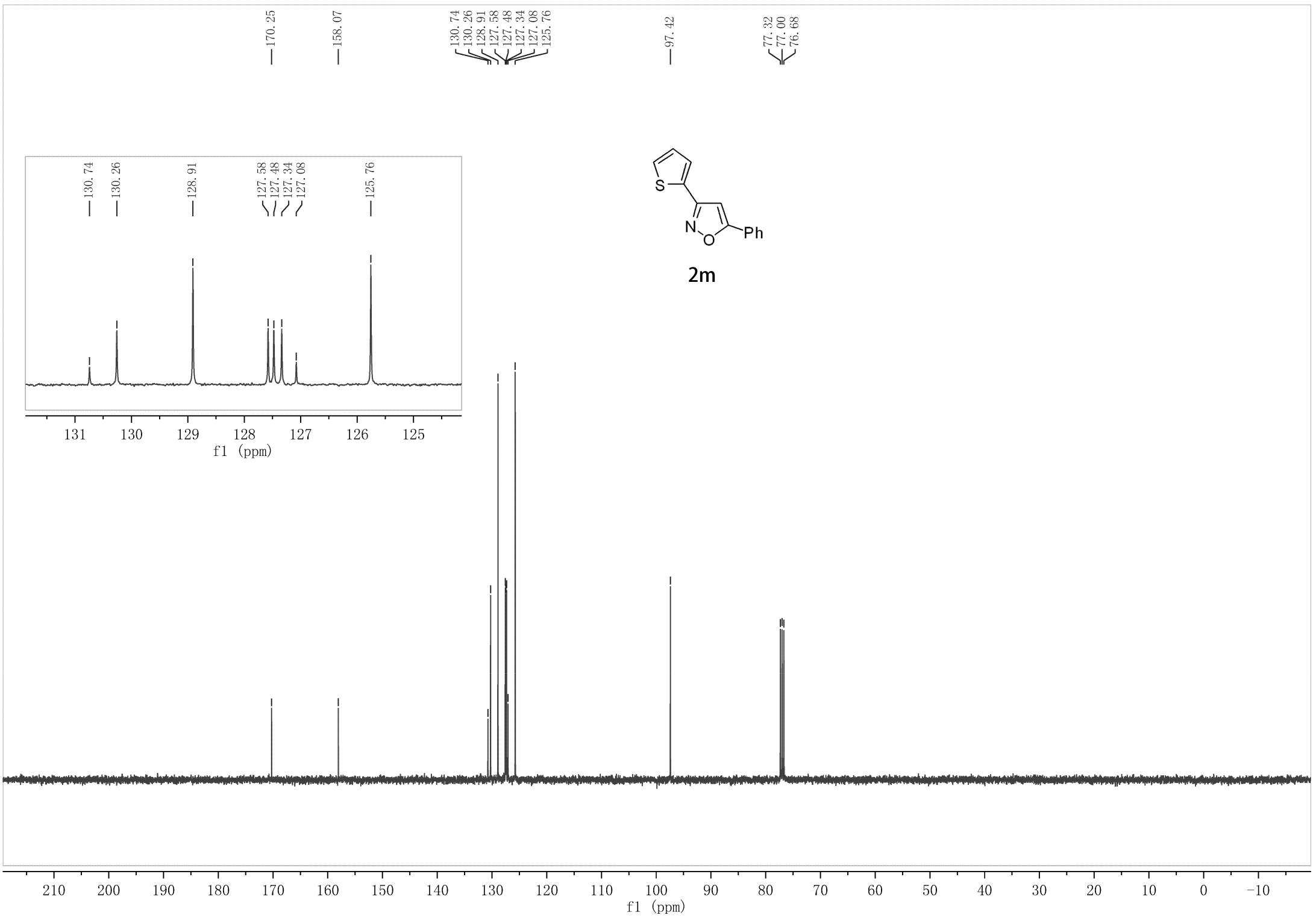
2g

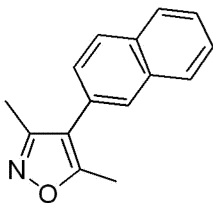


2g

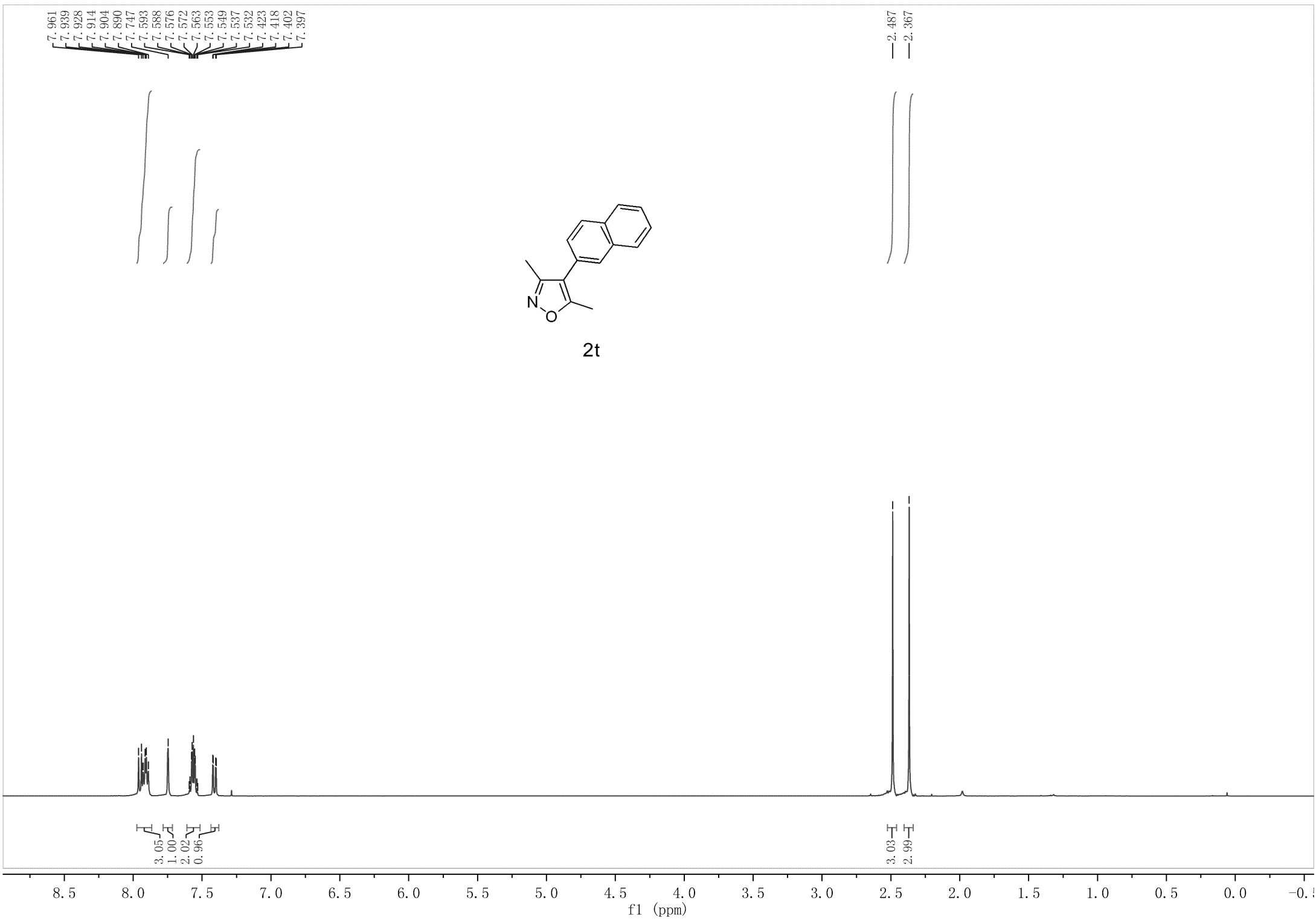


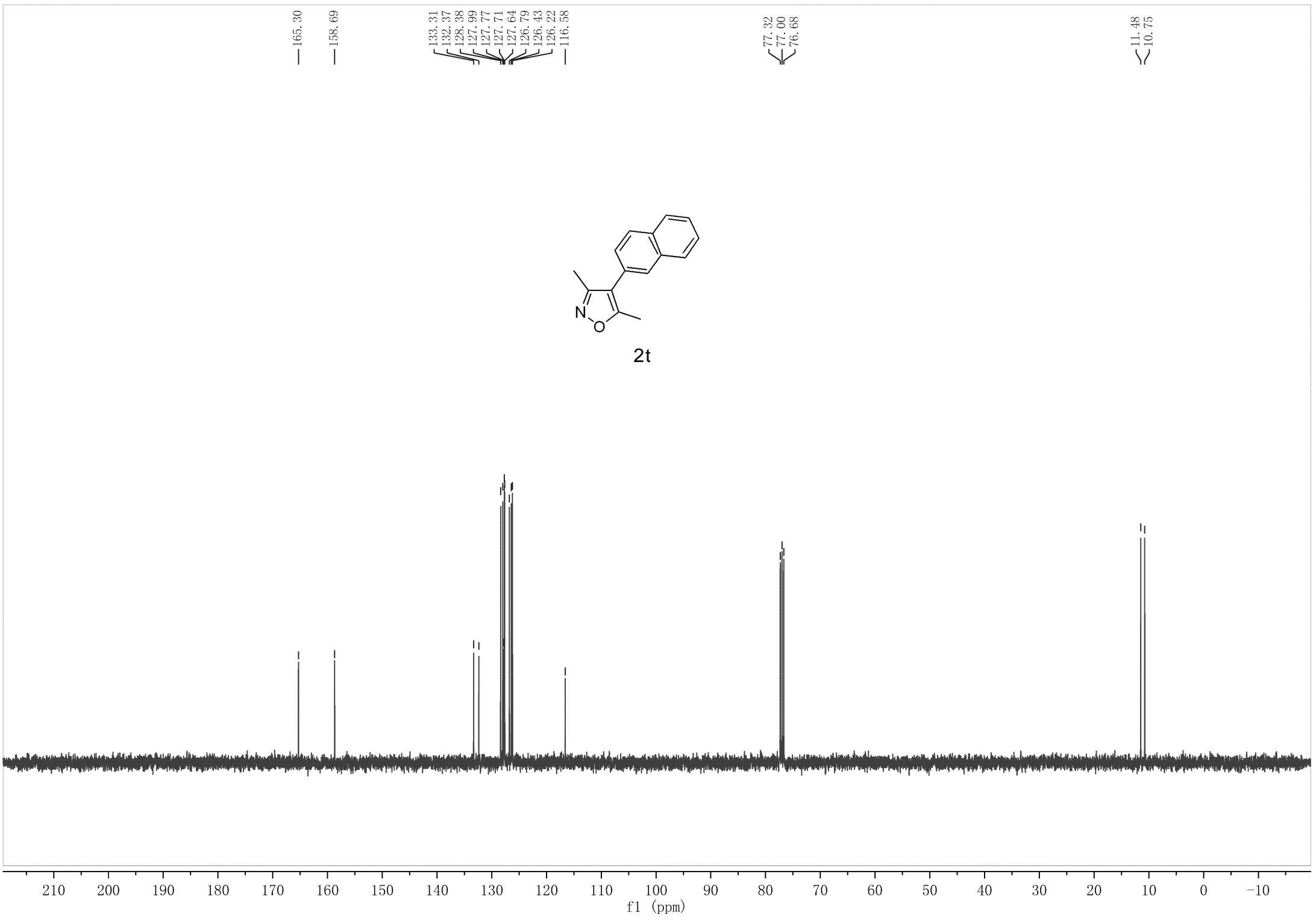






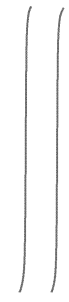
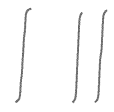
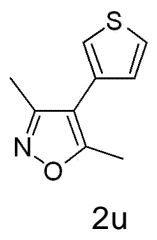
2t





7.423
7.416
7.411
7.403
7.192
7.189
7.184
7.182
7.098
7.095
7.086
7.083

2.427
2.297



0.99

0.95

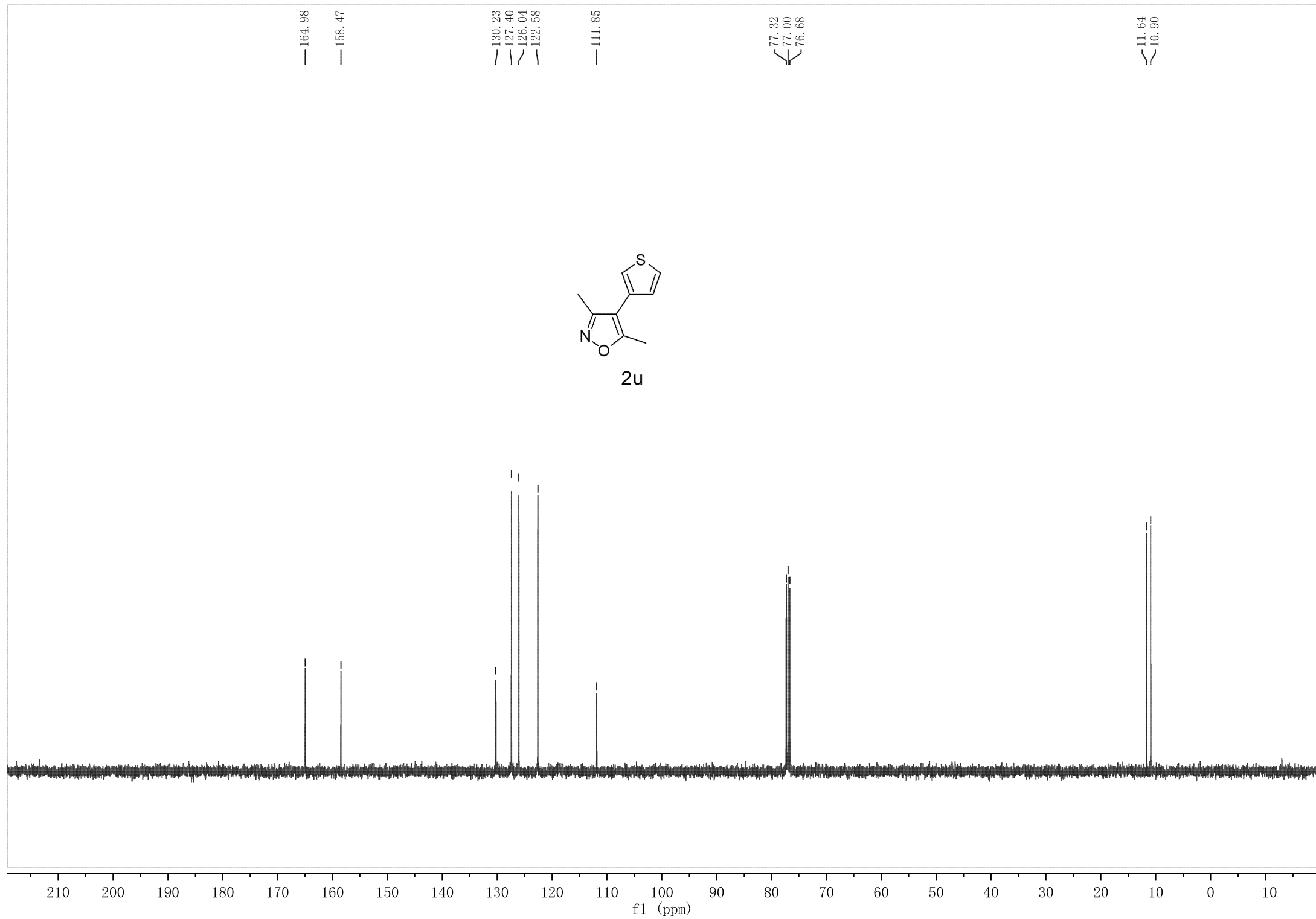
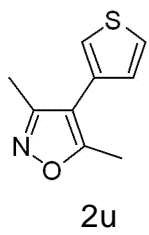
0.97

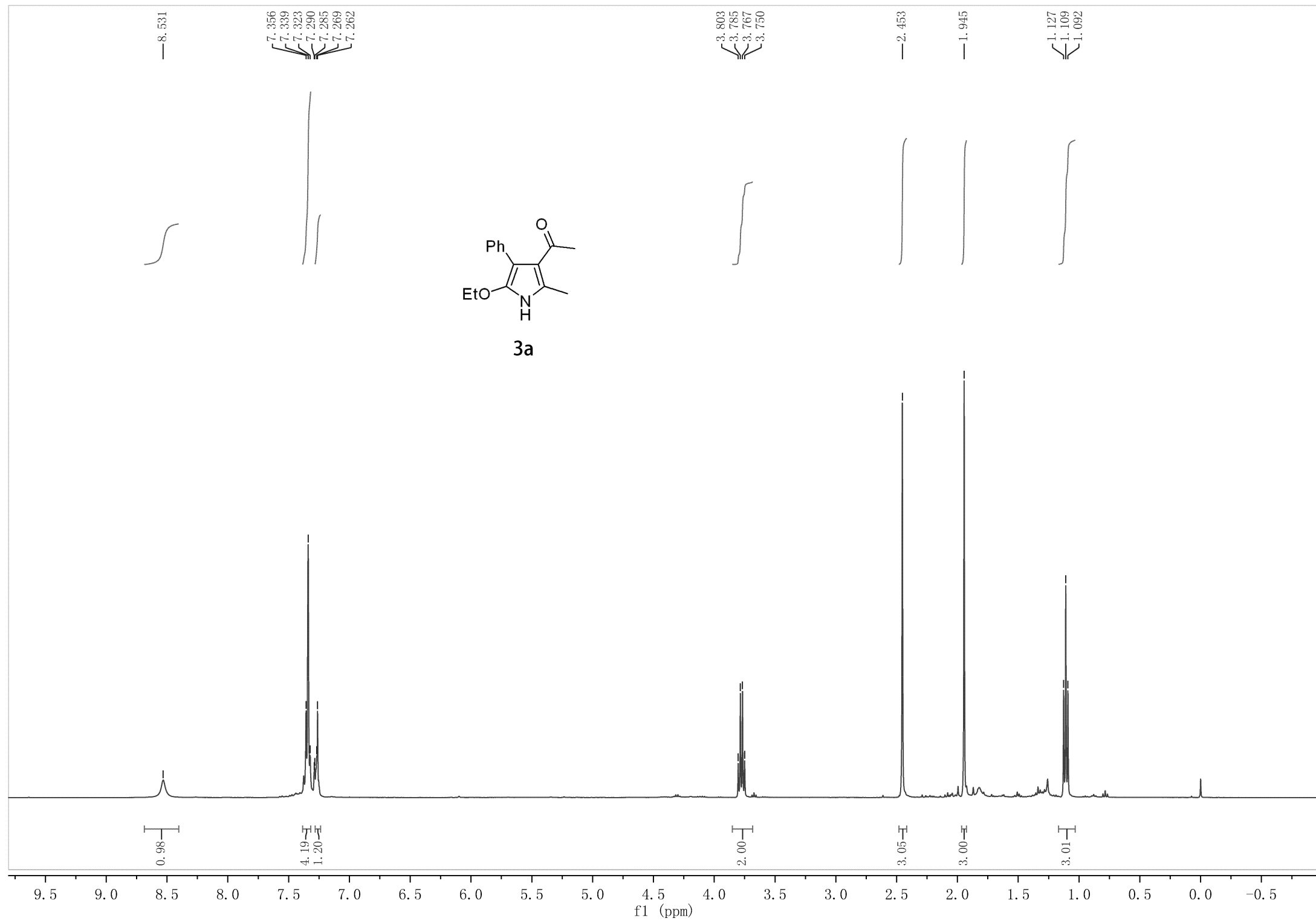
3.01

3.00

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)





— 197.16

— 140.83

— 134.81

— 130.39

— 128.07

— 127.25

— 126.46

— 119.86

— 107.53

— 77.32

— 77.00

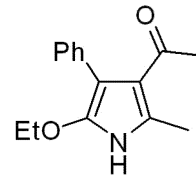
— 76.68

— 70.28

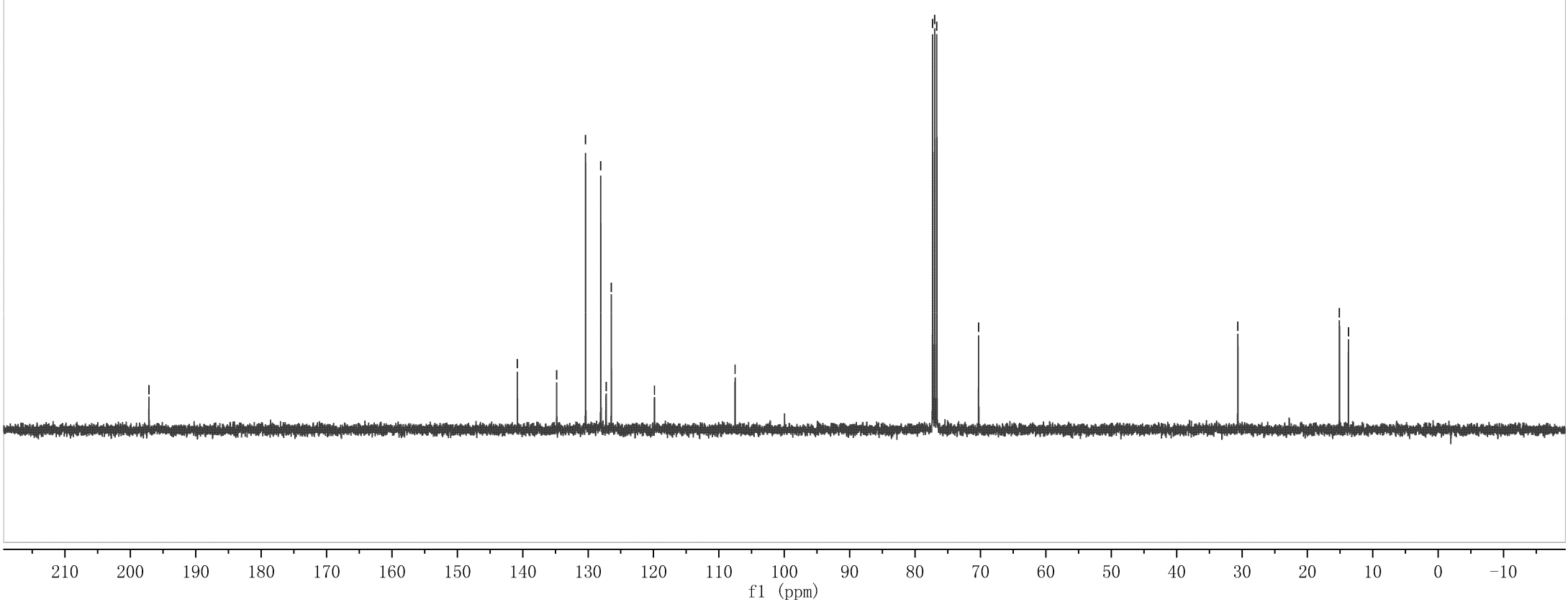
— 30.64

— 15.11

— 13.72



3a



7.370
7.363
7.335
7.324
7.319
7.312
7.295
7.279
7.274
7.268
7.263
7.254
7.251
7.244
7.239
7.234

6.177
6.175

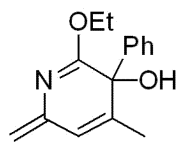
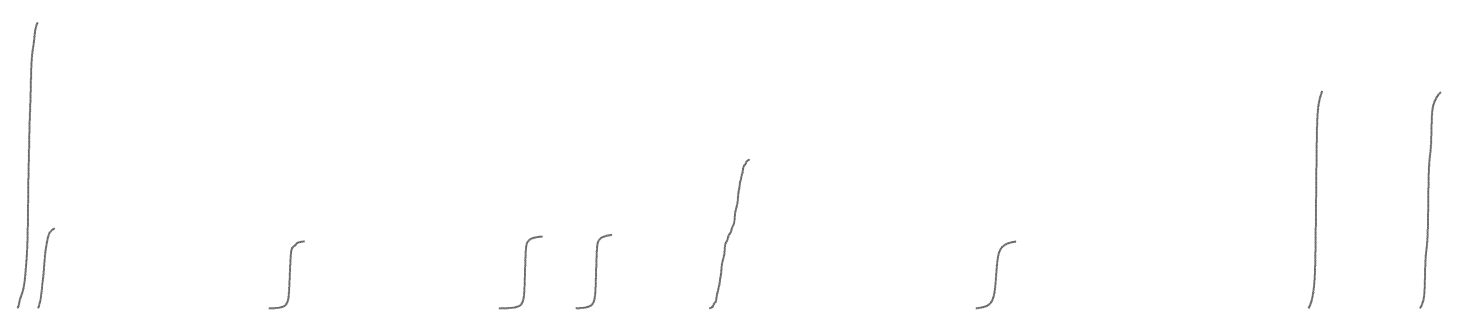
5.144

4.833
4.319
4.304
4.297
4.290
4.283
4.276
4.269
4.255
4.239
4.225
4.217
4.210
4.203
4.196
4.189
4.175

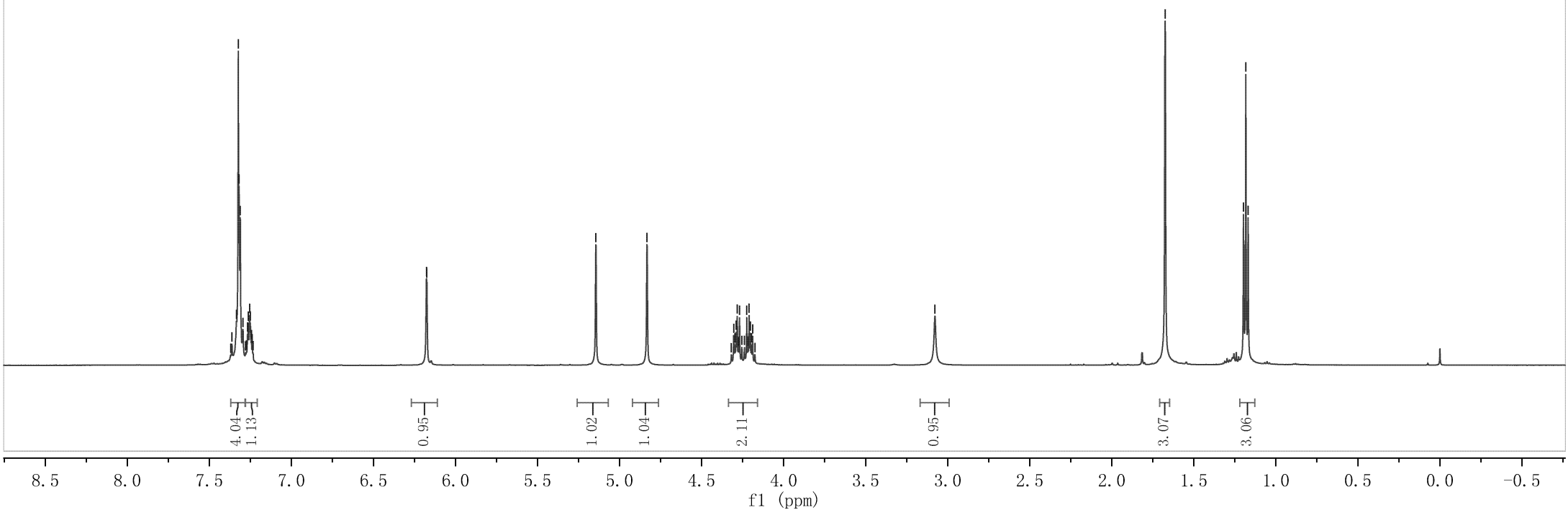
3.078

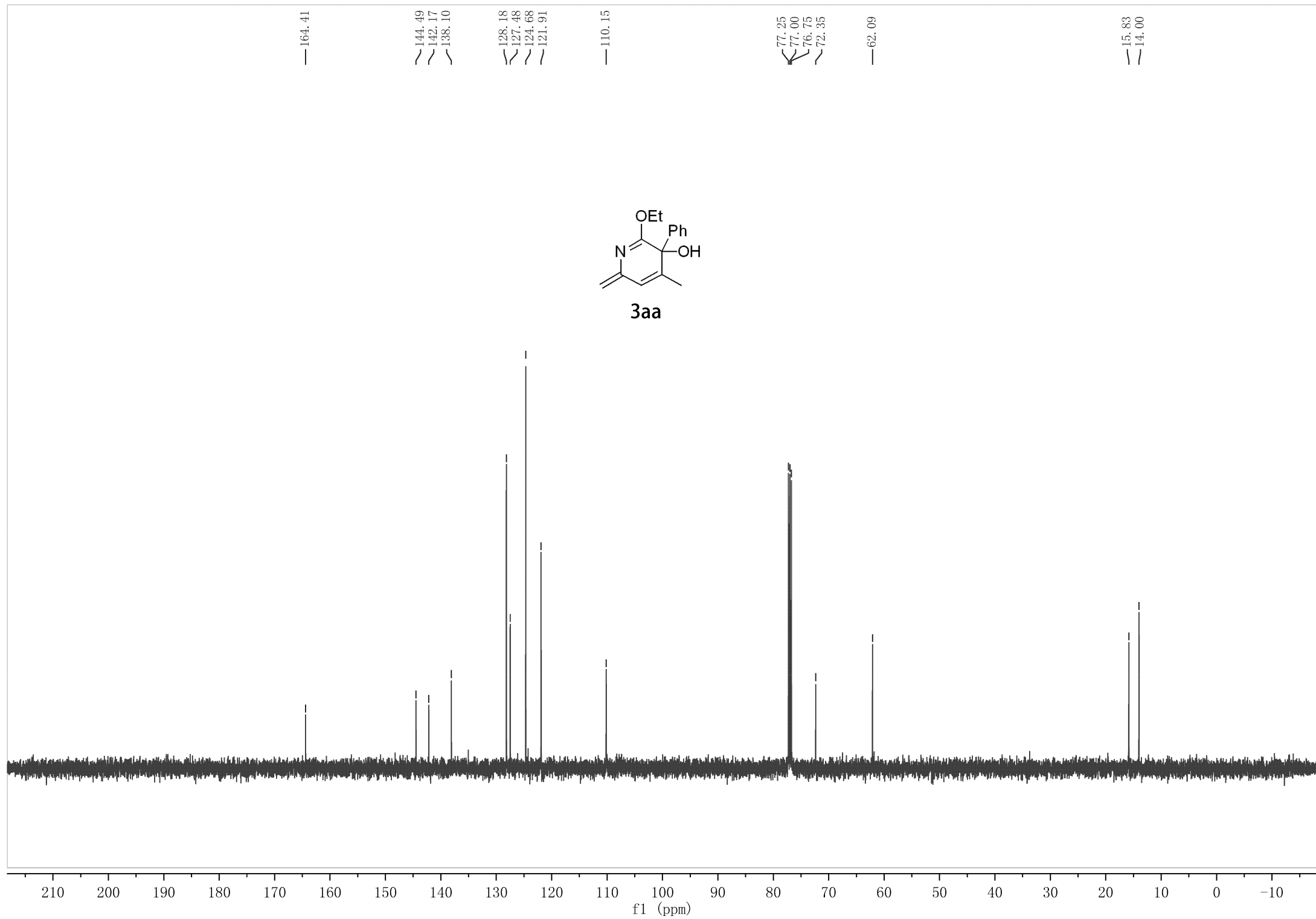
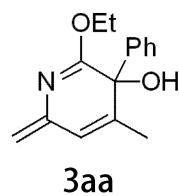
1.675

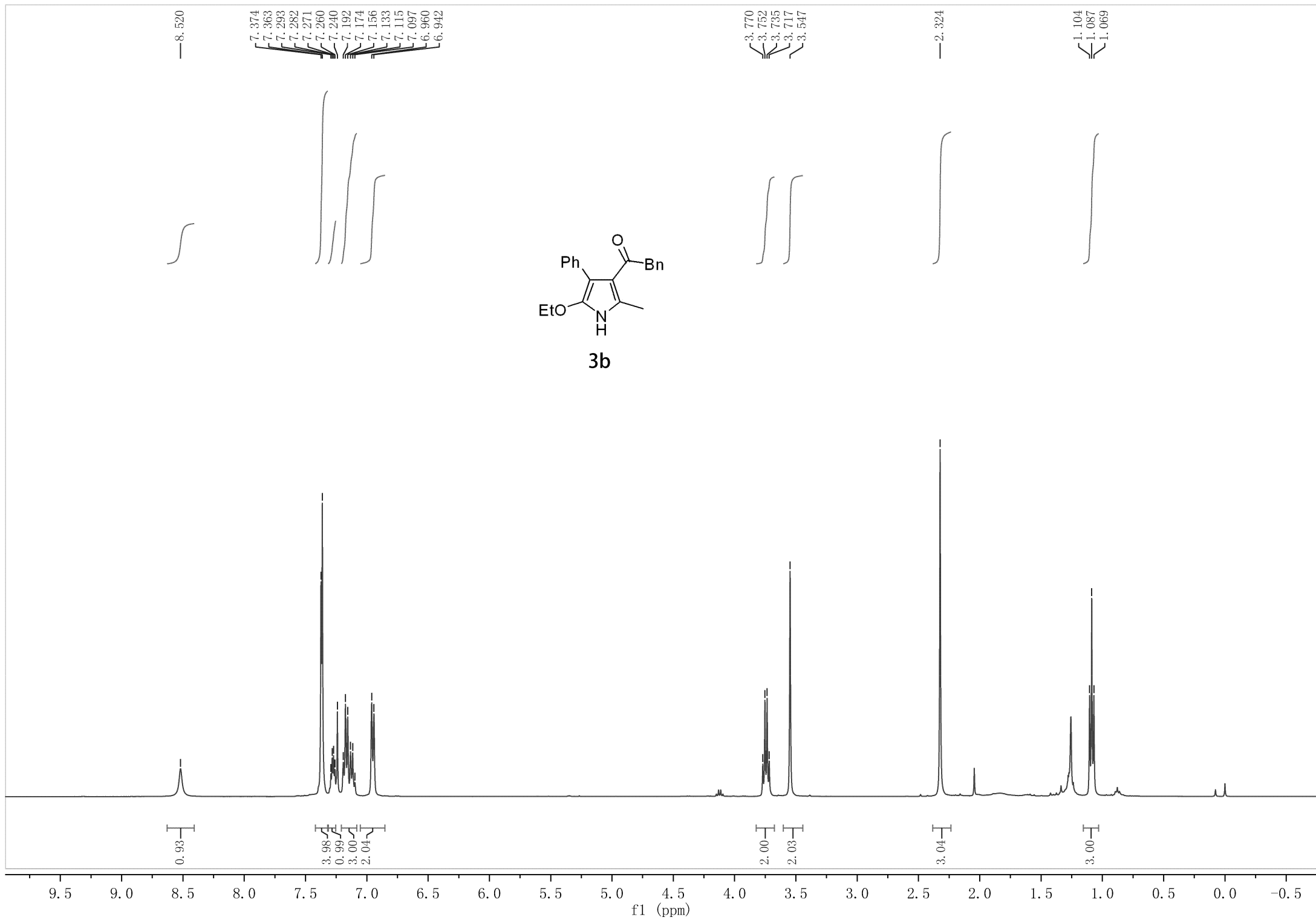
1.197
1.183
1.169

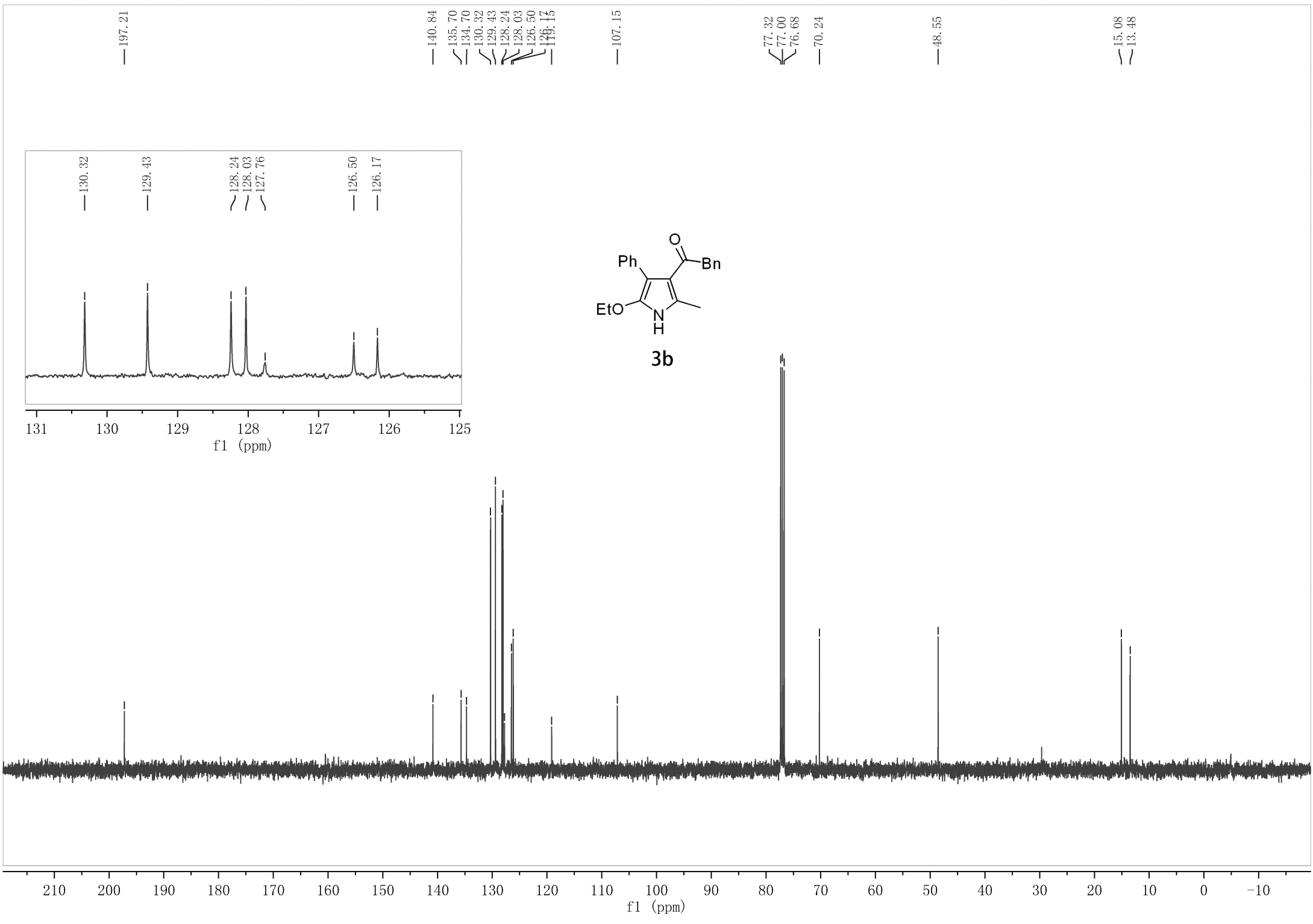


3aa









8.898

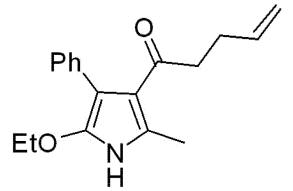
7.367
7.348
7.333
7.319
7.294
7.279
7.273
7.260
7.250
7.243
7.237

5.654
5.639
5.628
5.623
5.612
5.596
5.586
5.581
5.570
5.555
4.806
4.791
4.787
4.784
4.749
4.745

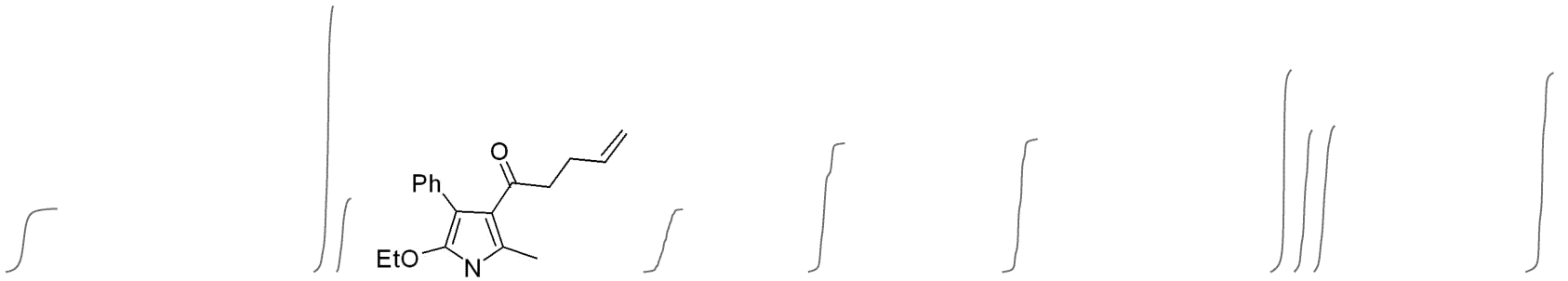
3.808
3.790
3.773
3.755

2.425
2.338
2.322
2.303
2.239
2.222
2.205
2.189

1.116
1.098
1.080



3c



0.95

4.00
1.11

0.94

1.94

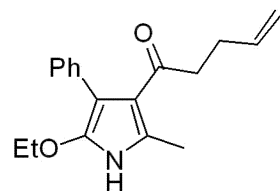
2.00

3.04
2.13
2.20

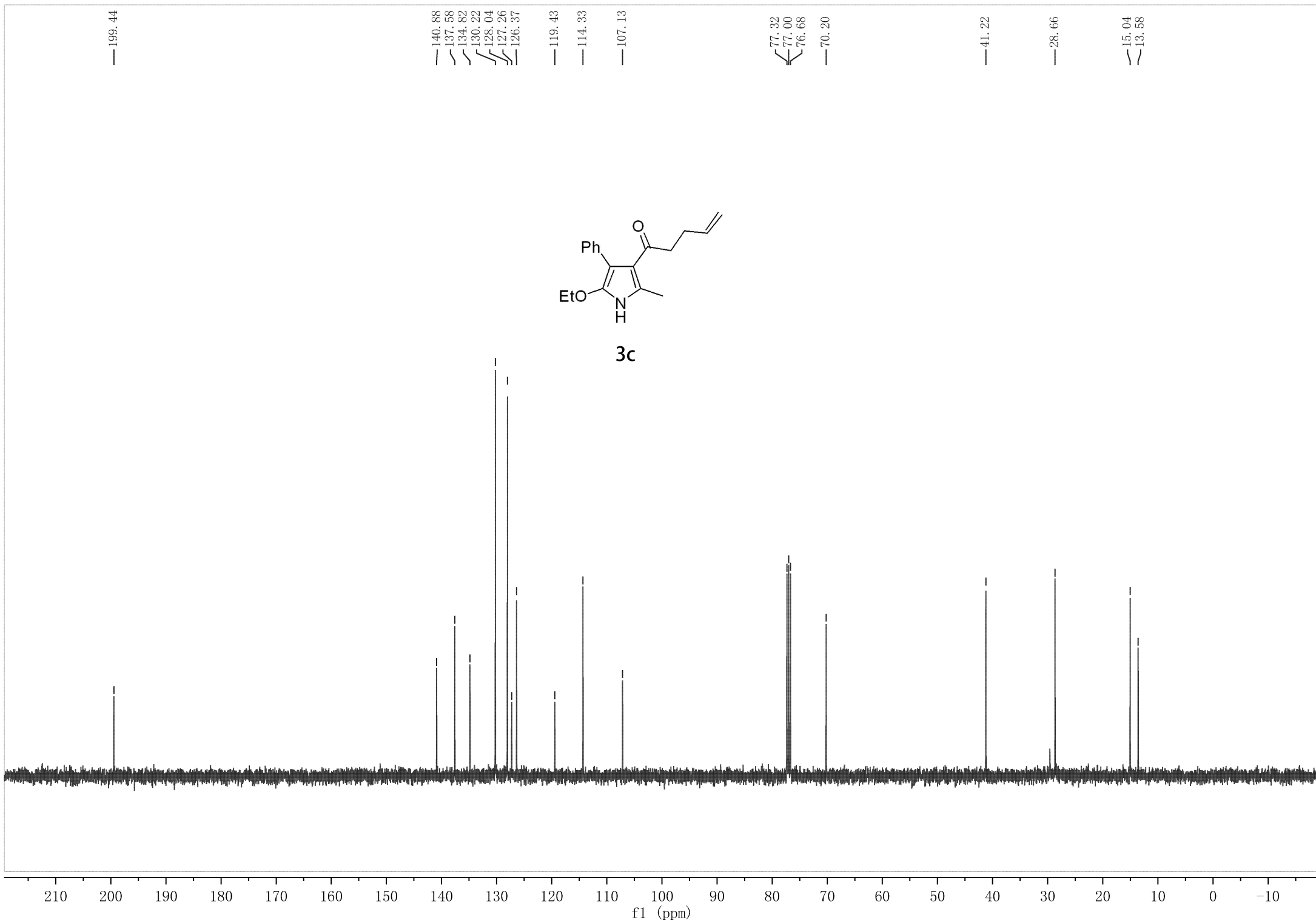
3.00

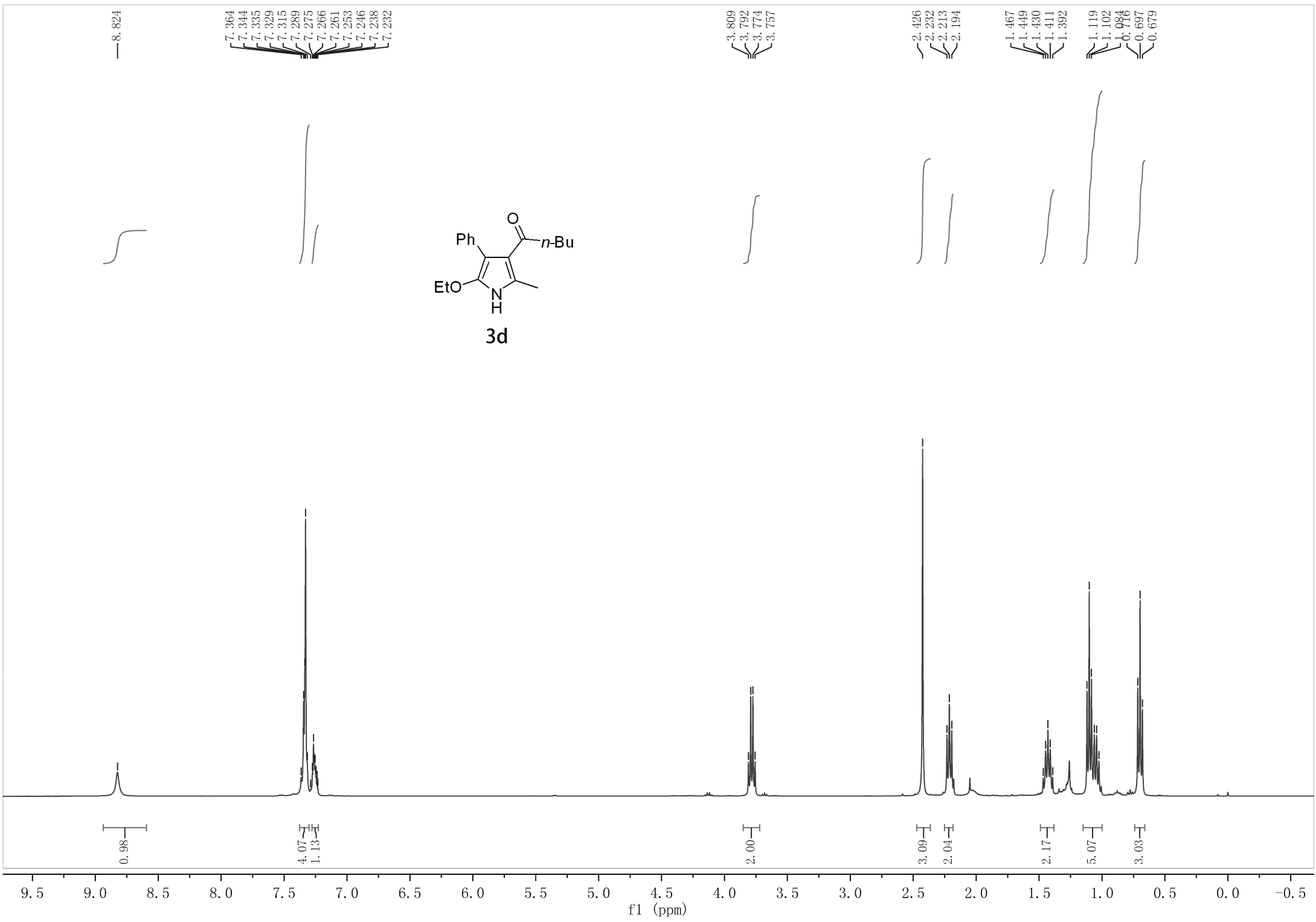
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

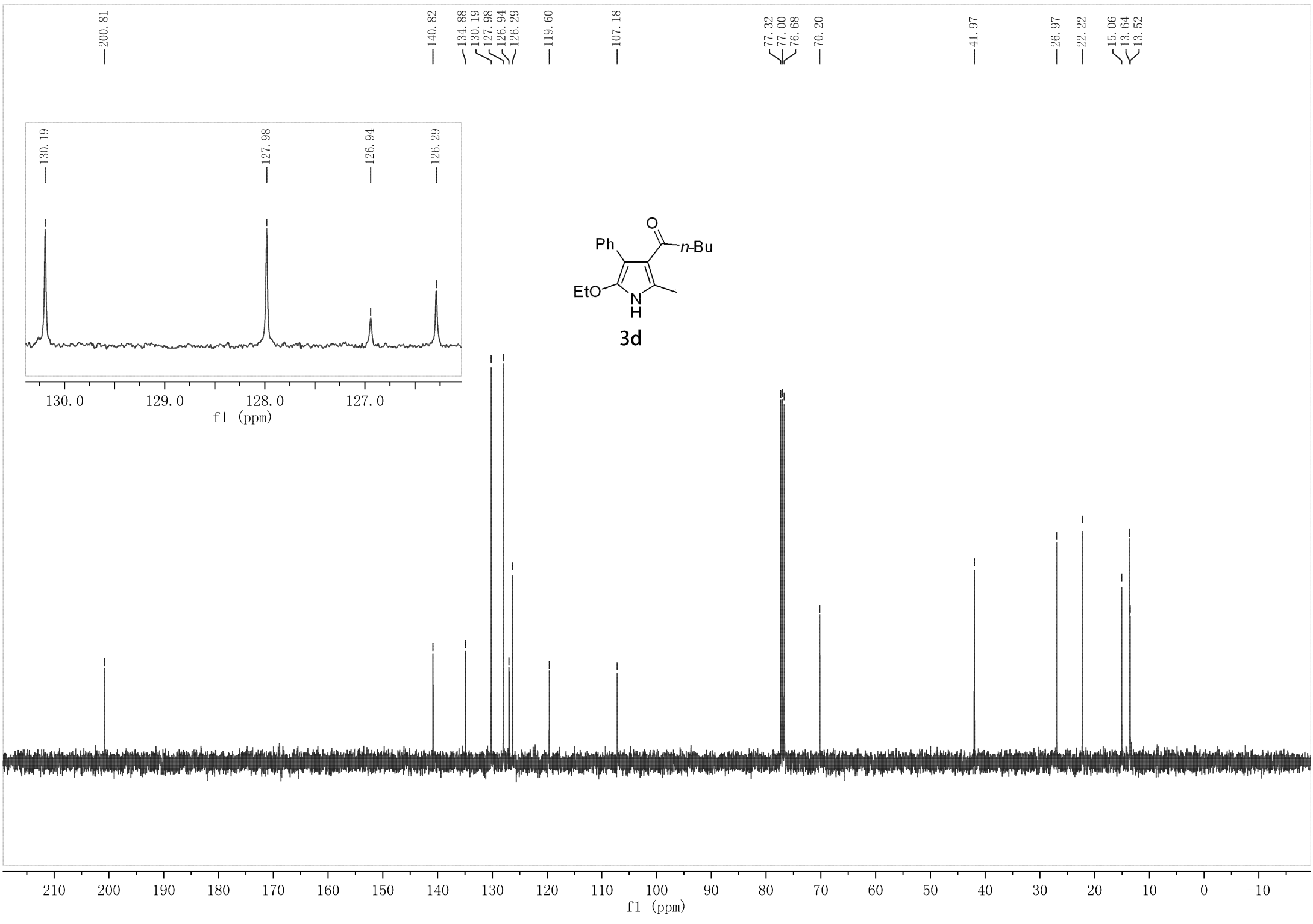
f1 (ppm)

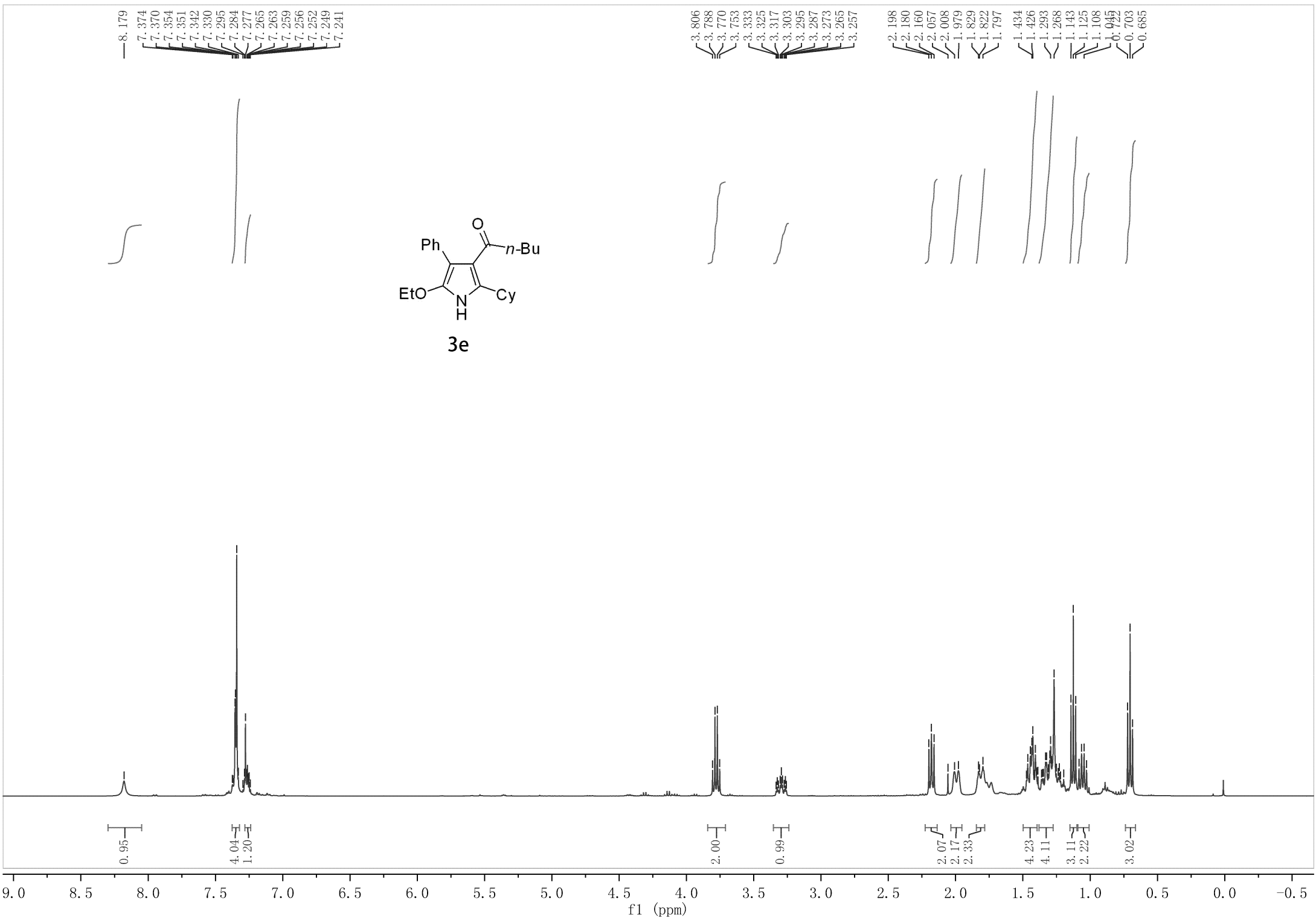


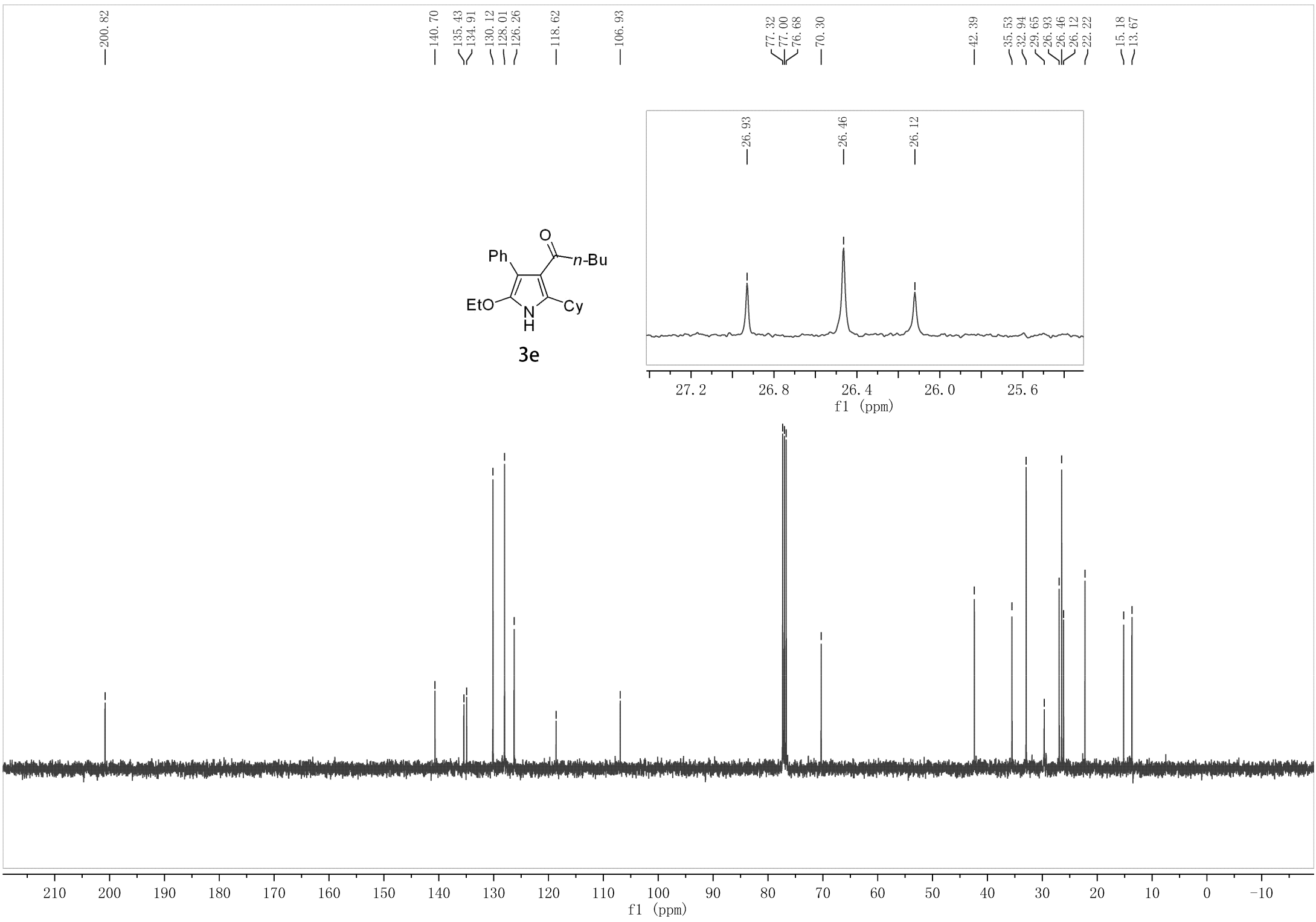
3c

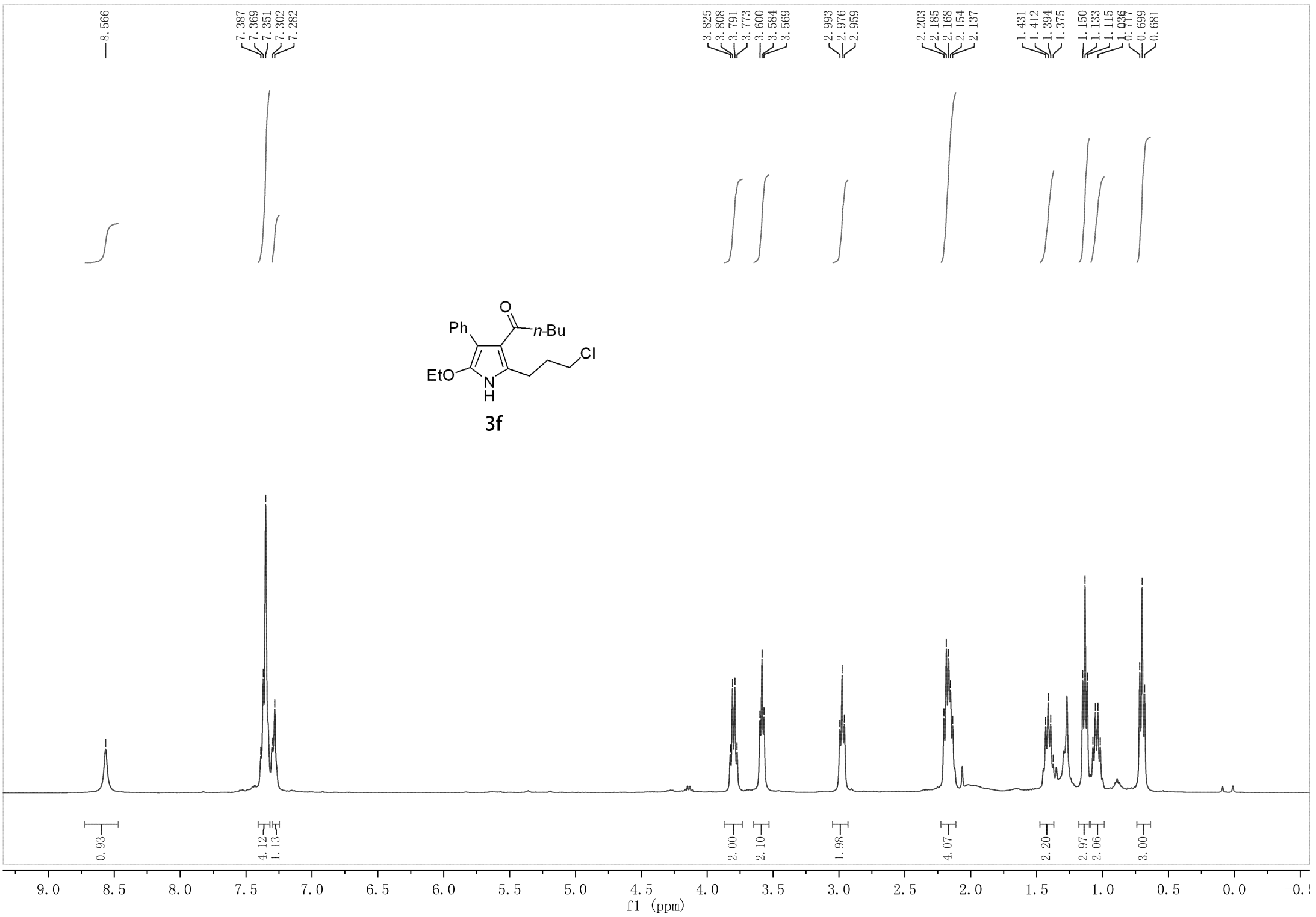












— 200.56

— 140.86

— 134.68

— 130.23

— 129.04

— 128.06

— 126.47

— 119.83

— 107.33

— 77.32

— 77.00

— 76.68

— 70.23

— 44.77

— 42.04

— 32.13

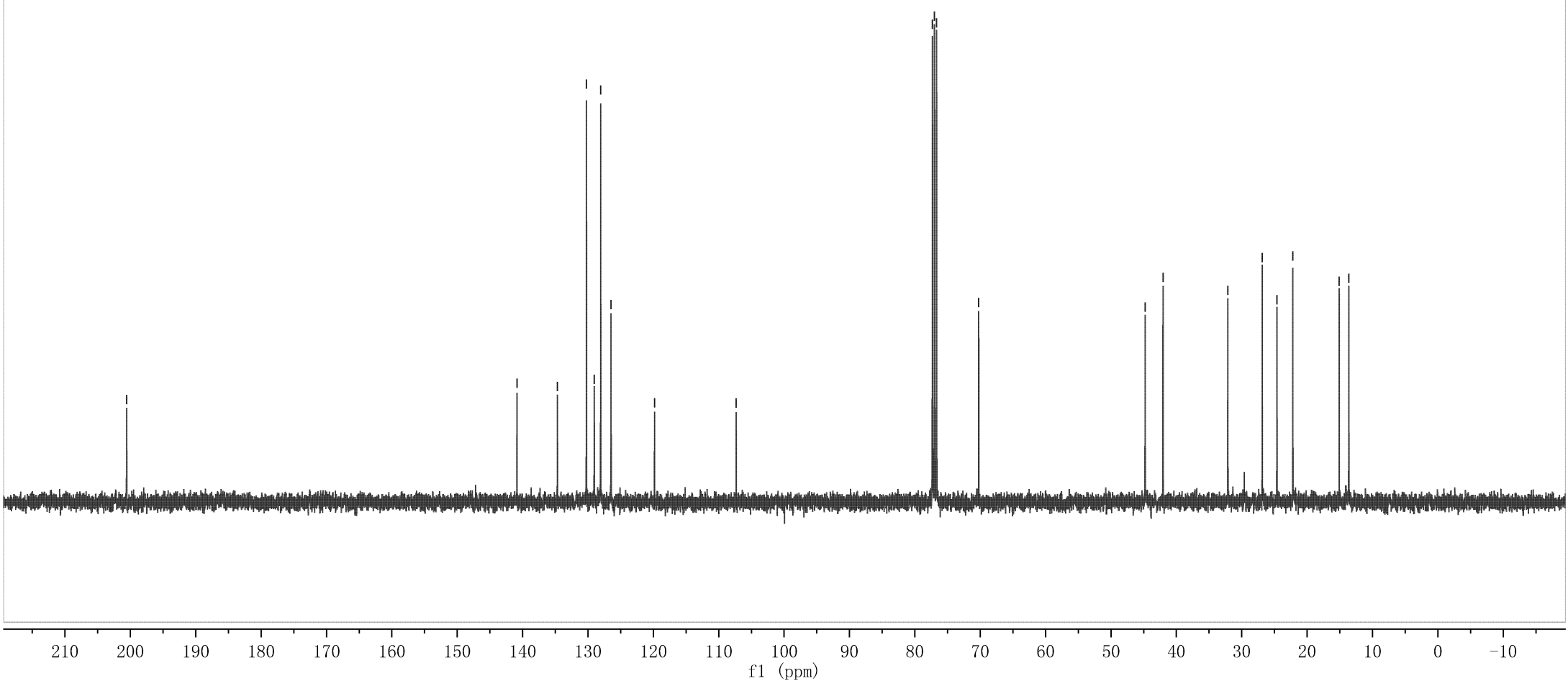
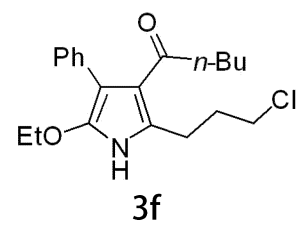
— 26.87

— 24.62

— 22.19

— 15.09

— 13.63



8.556

7.492
7.454
7.436
7.372
7.353
7.305
7.287

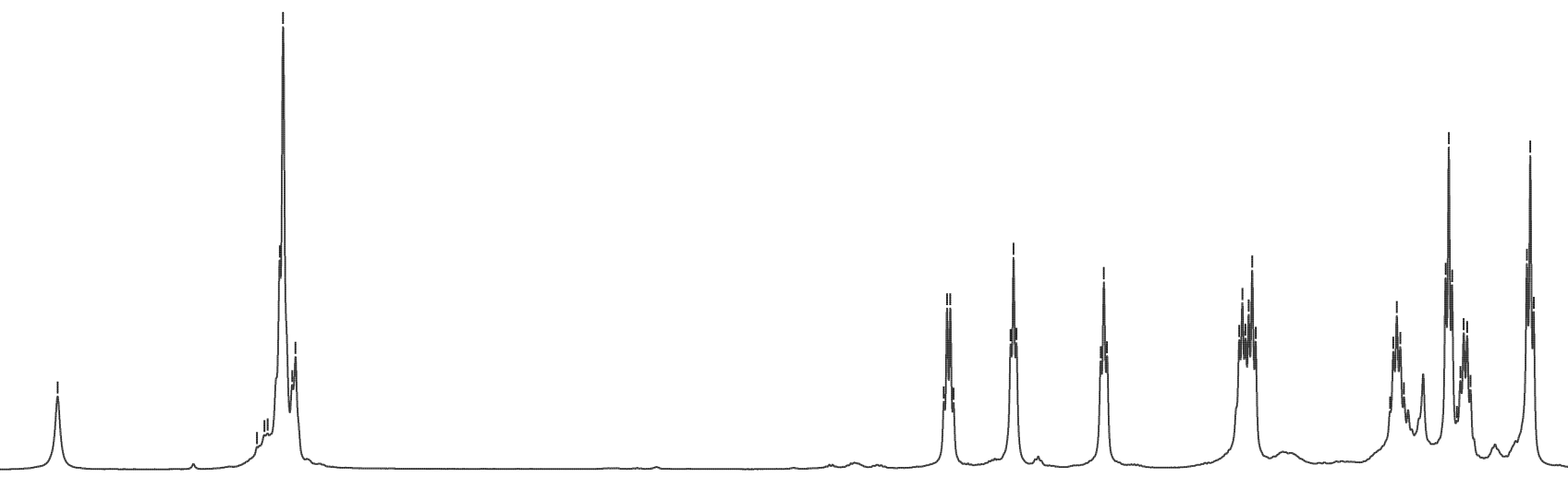
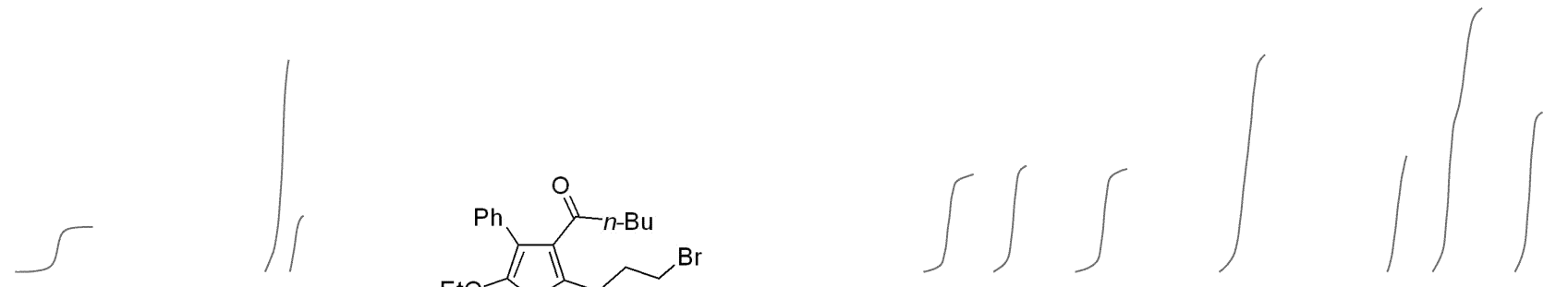
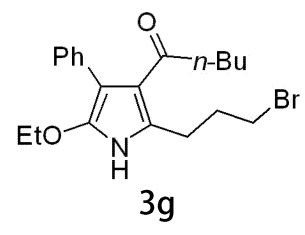
3.830
3.813
3.796
3.779
3.474
3.459
3.444

2.994
2.977
2.960

2.255
2.239
2.222
2.205
2.186
2.168

1.451
1.434
1.415
1.397
1.377

1.155
1.138
1.122
1.104
0.704
0.686



0.85

4.00
1.06

1.84

2.00

1.94

4.09

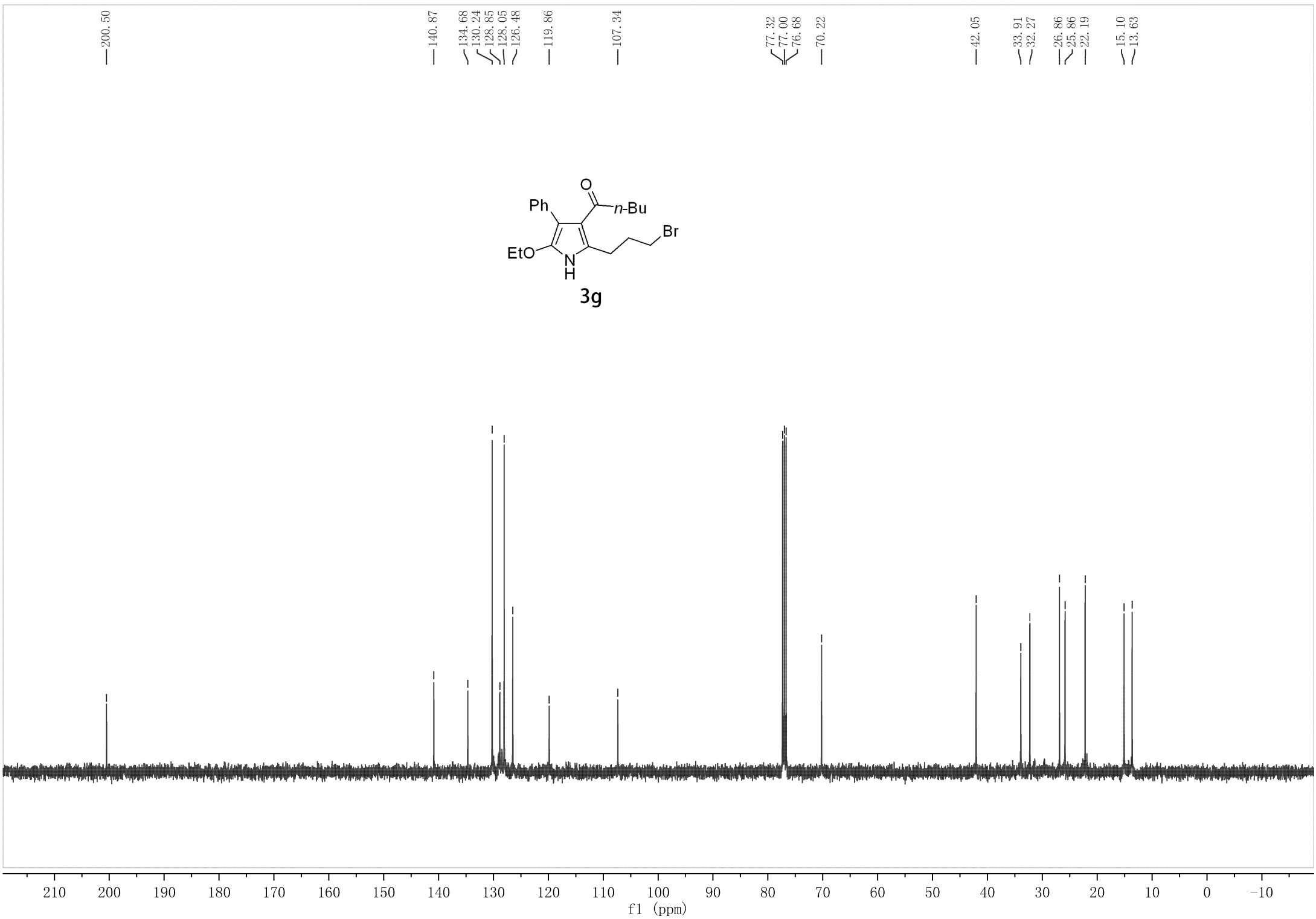
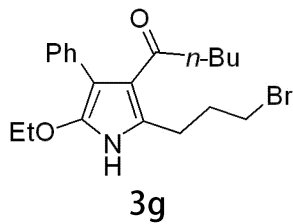
2.19

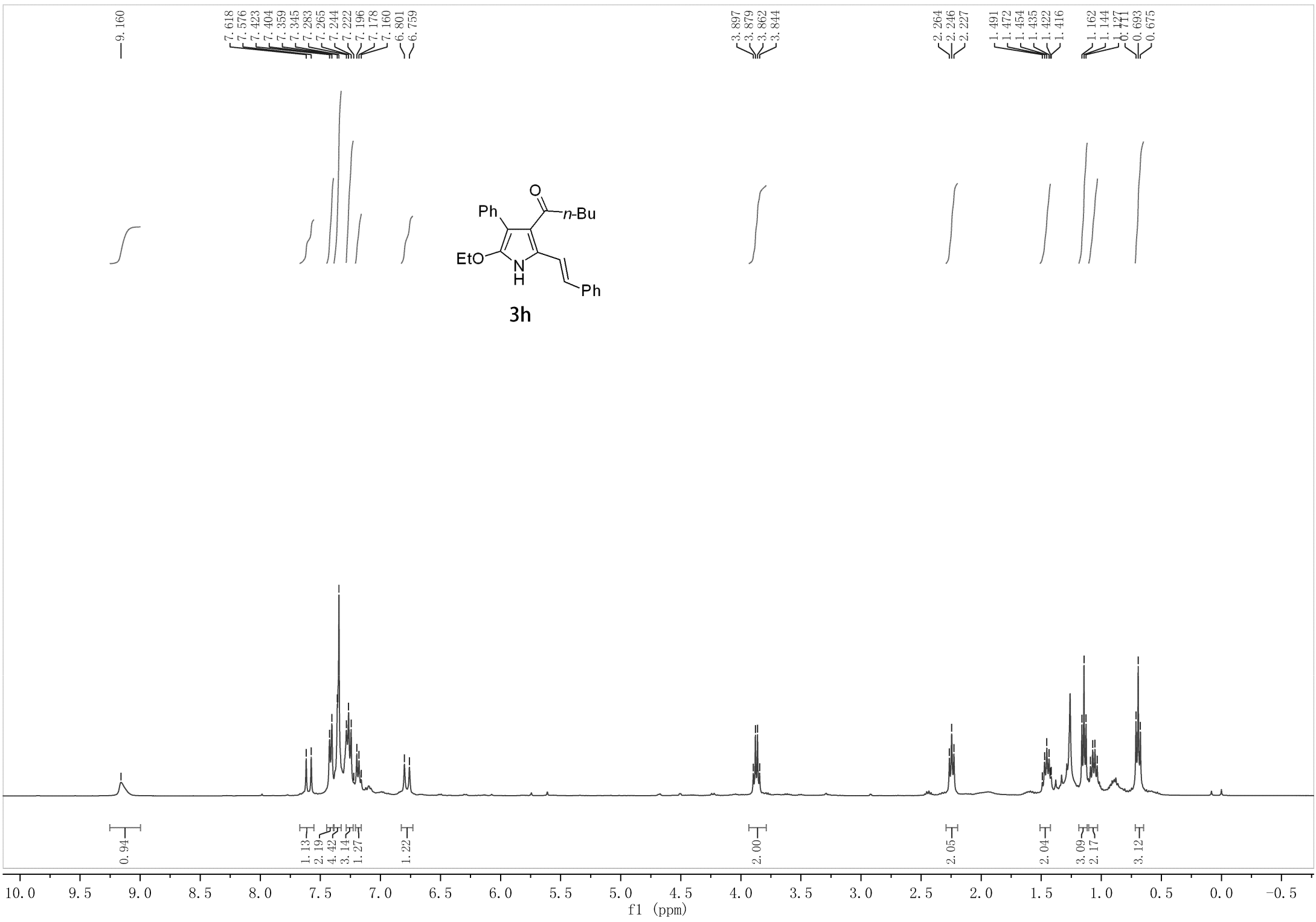
4.97

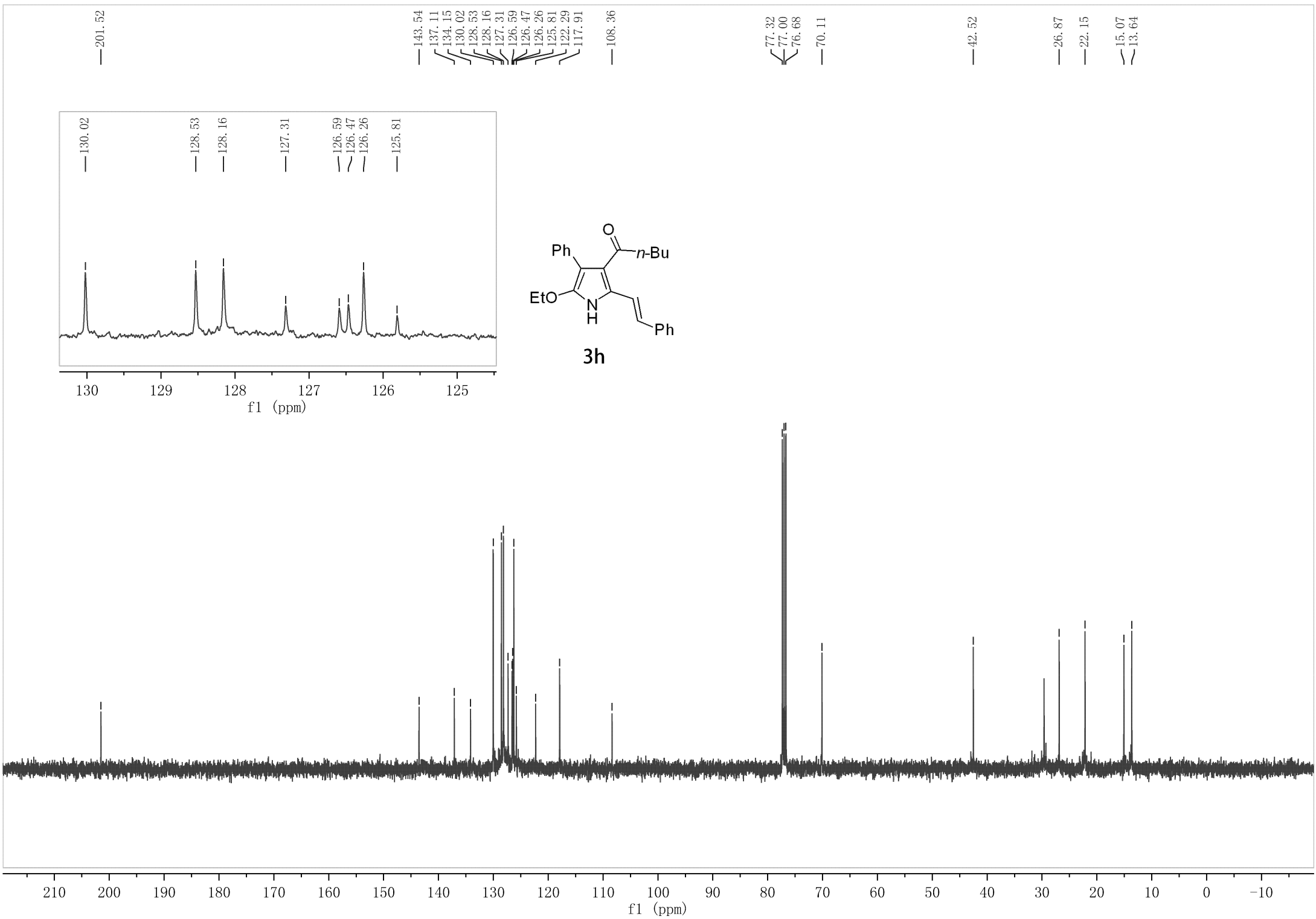
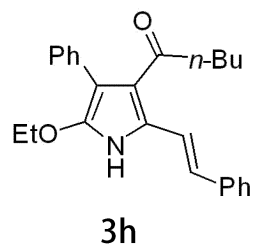
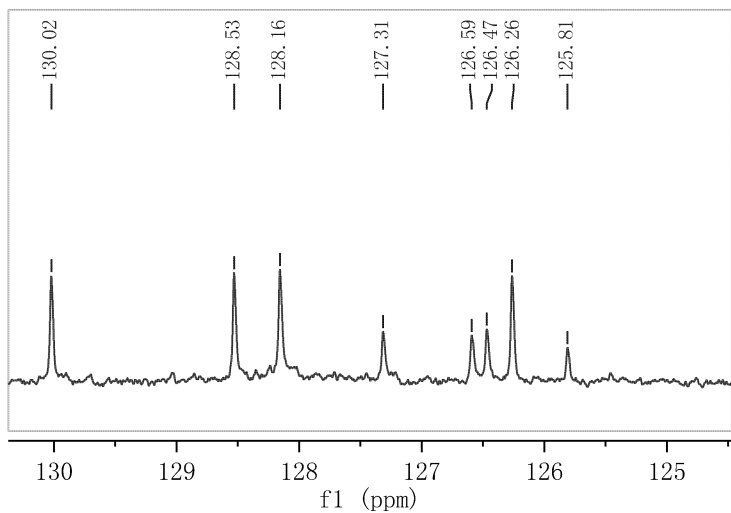
3.01

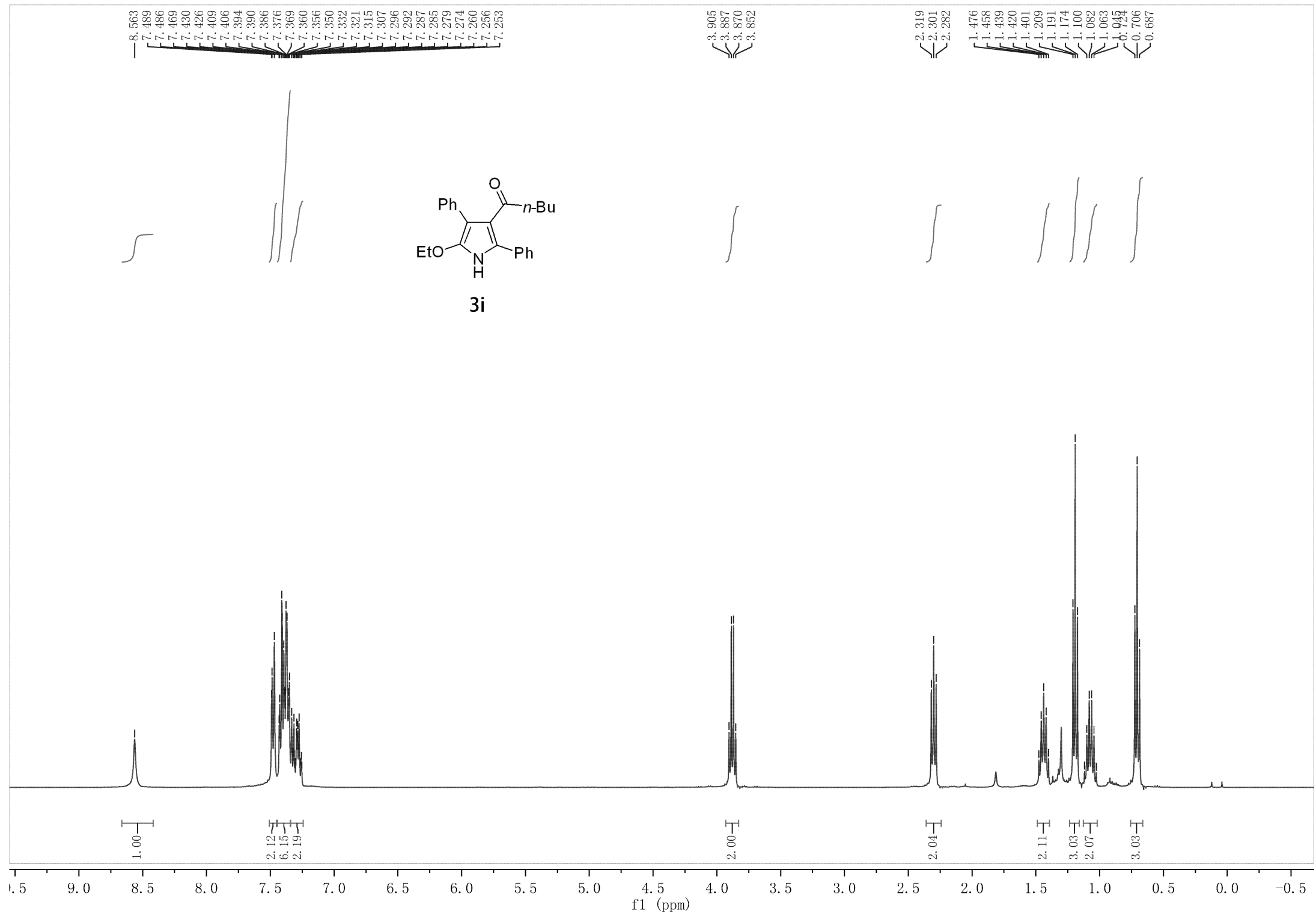
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

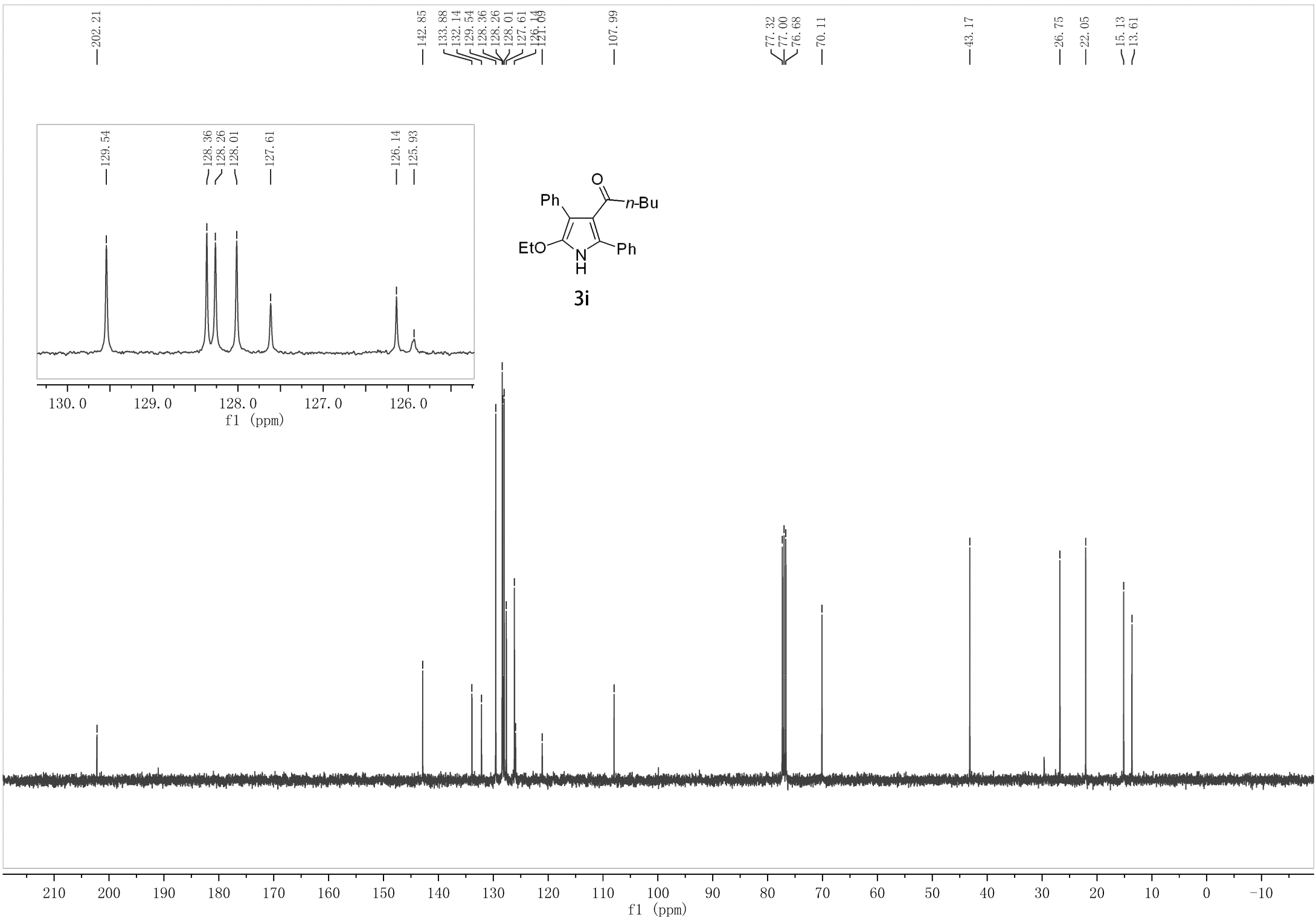
f1 (nm)

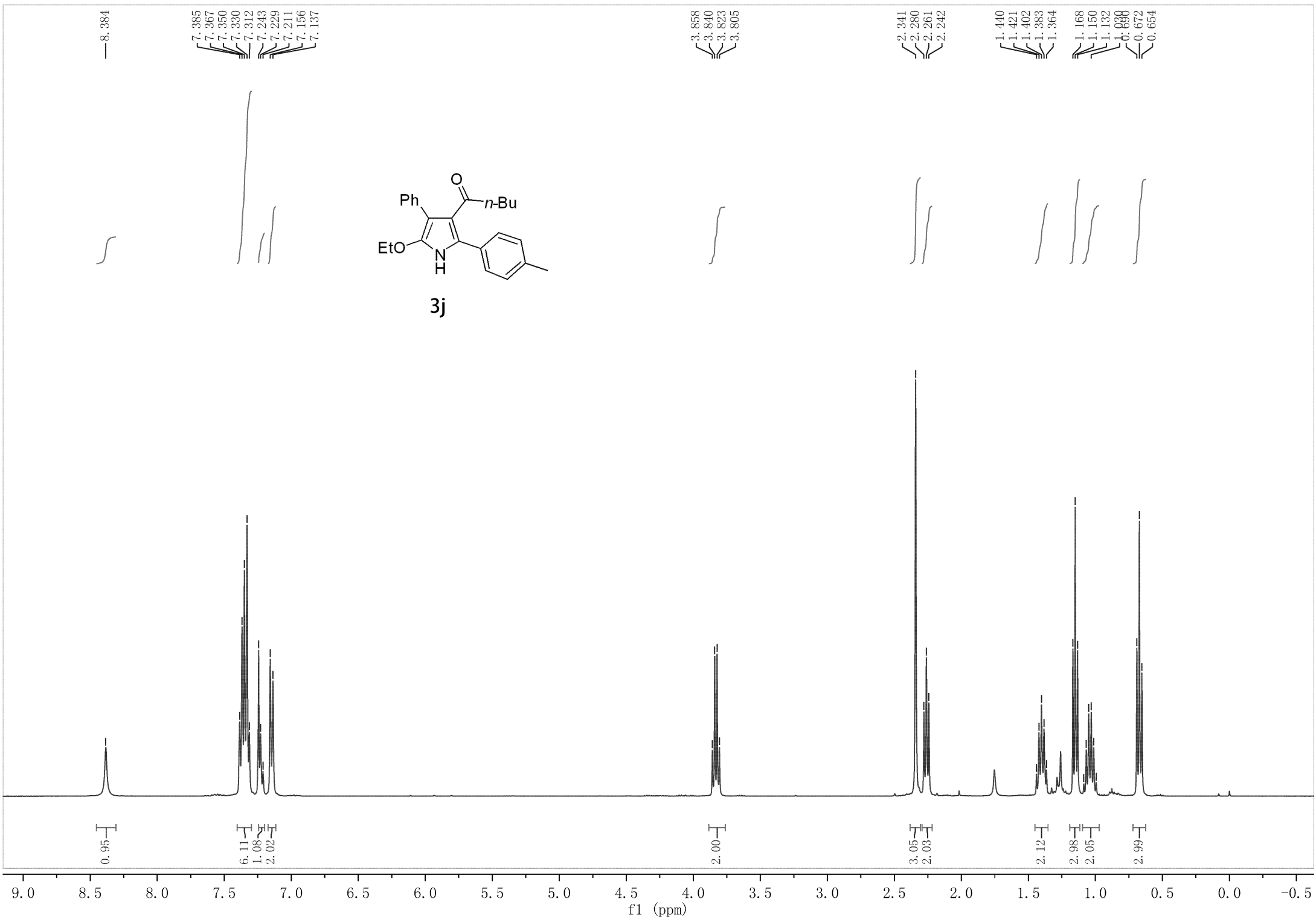


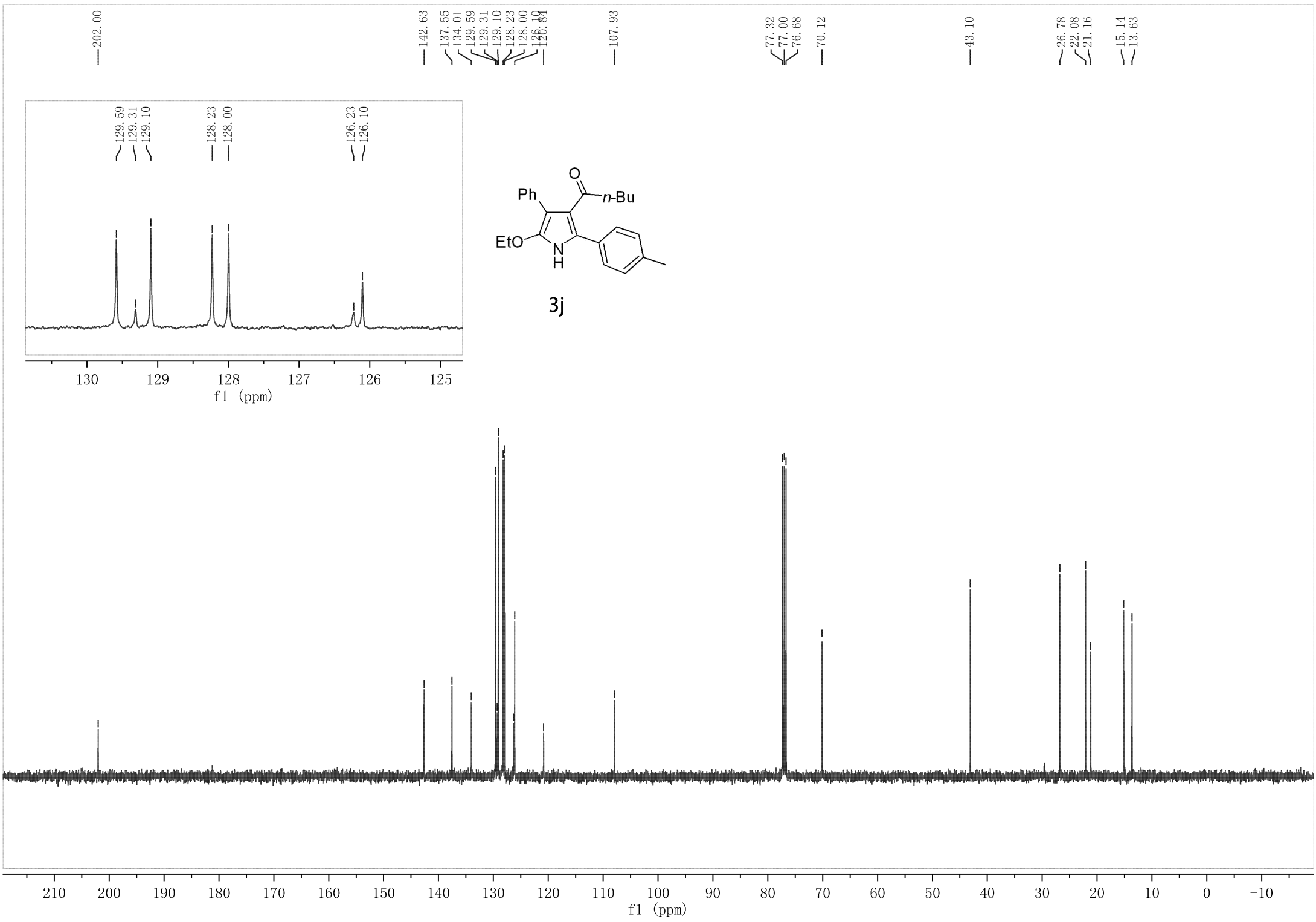


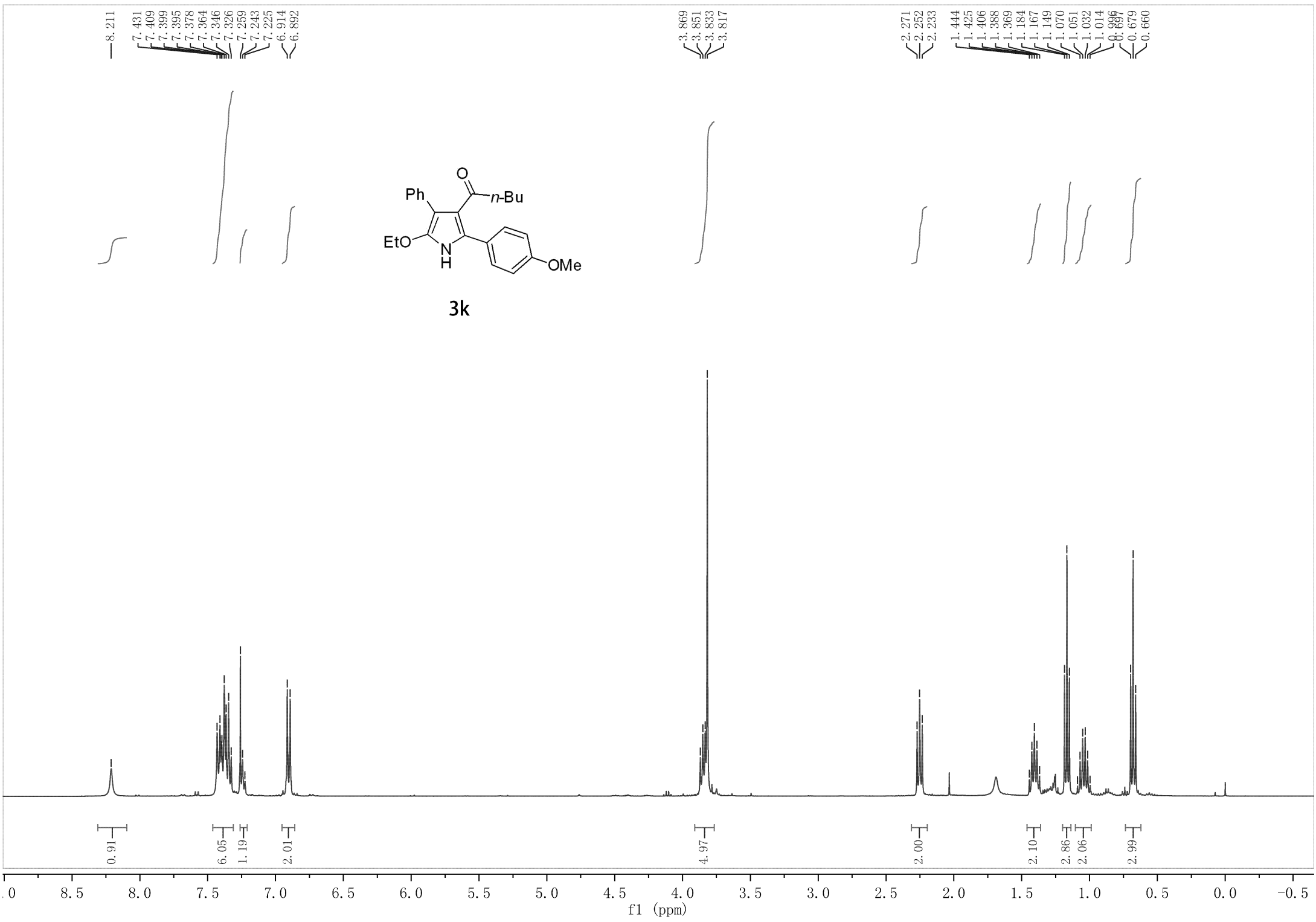


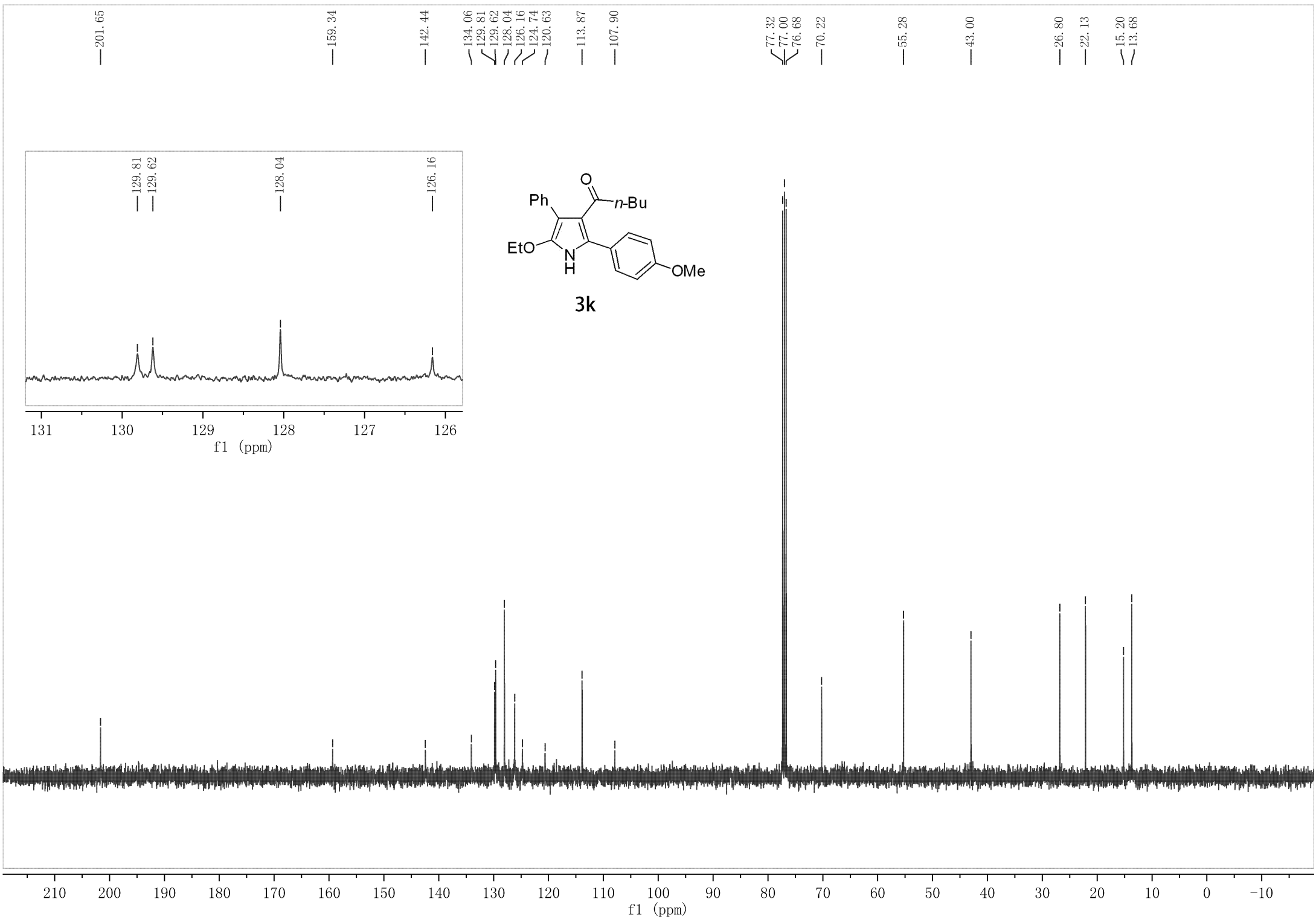










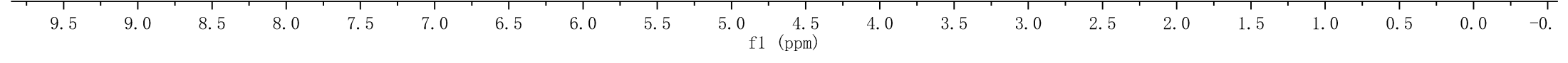
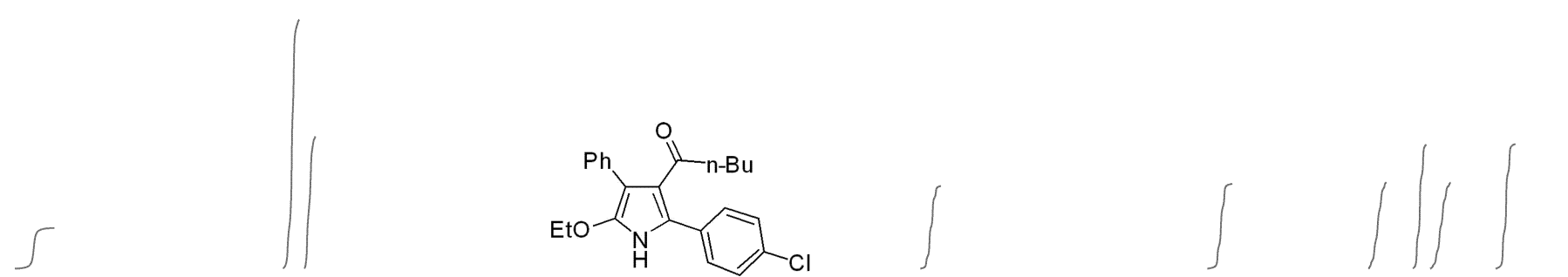
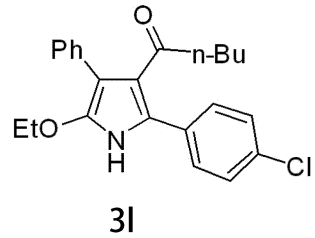


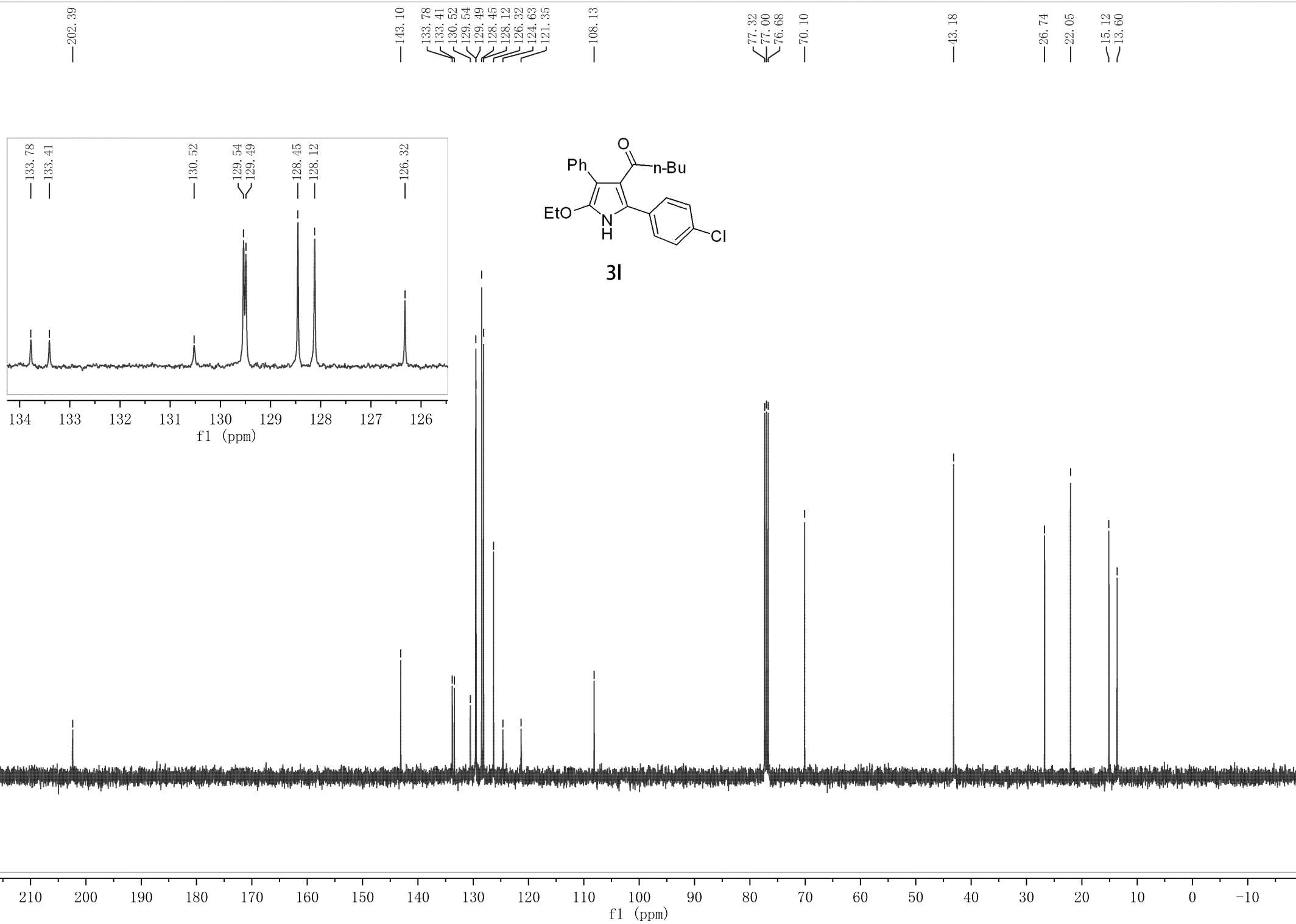
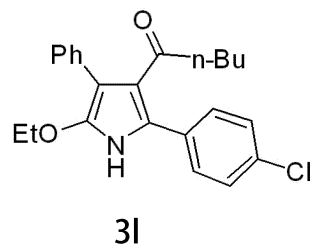
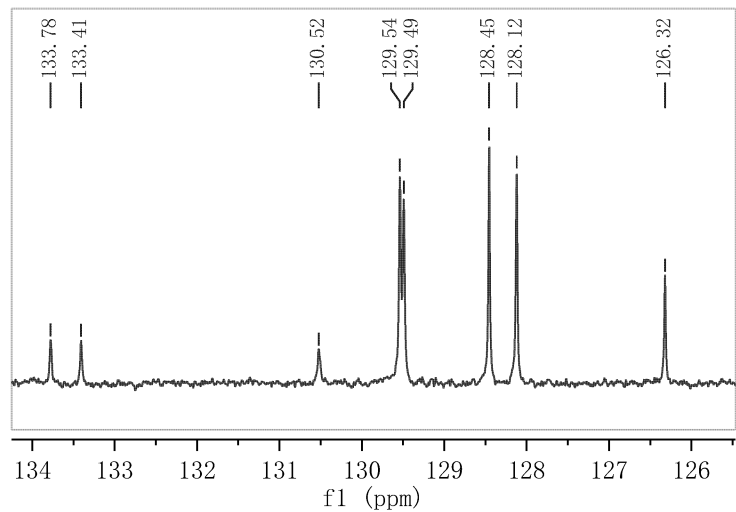
8.773

7.376
7.371
7.353
7.342
7.322
7.320
7.303
7.269
7.264
7.258
7.251
7.247
7.237
7.225

3.860
3.843
3.825
3.807

1.413
1.394
1.375
1.357
1.338
1.161
1.143
1.126
1.073
1.055
1.036
1.017
0.999
0.981
0.687
0.669
0.650





129.54
129.49
128.46
128.12
126.32

70.10

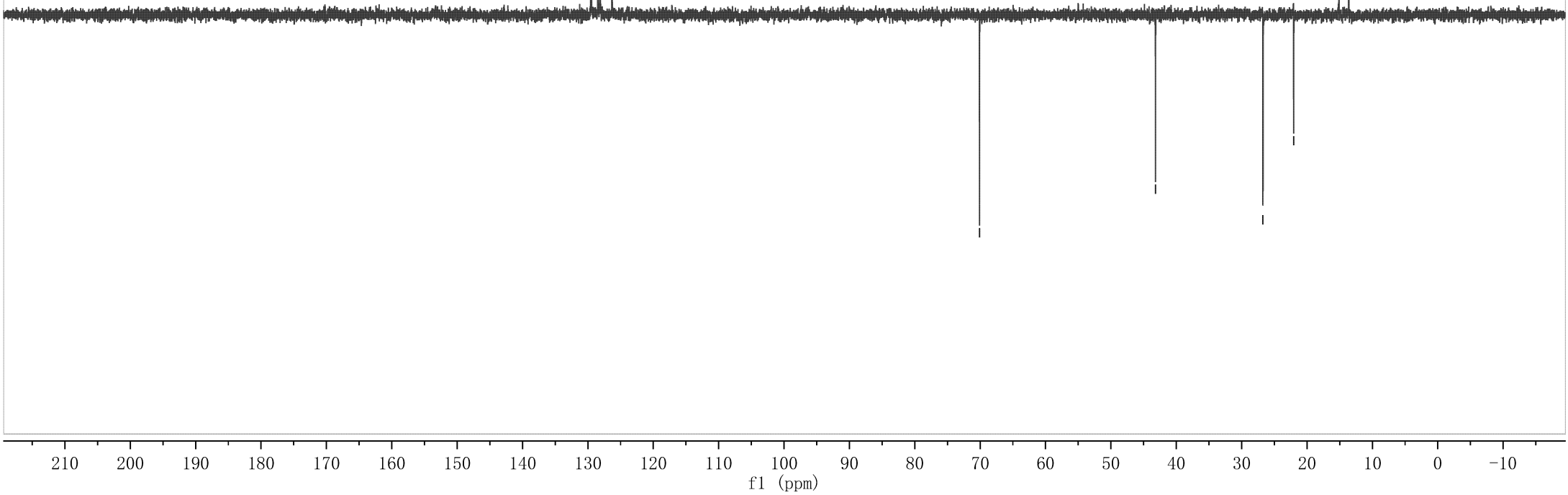
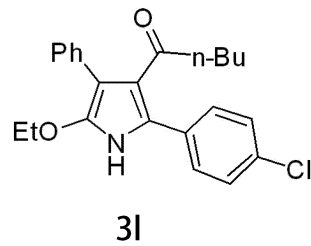
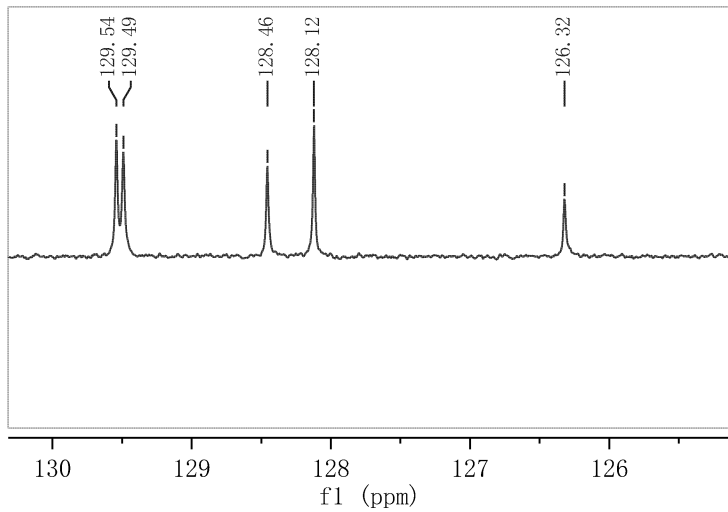
43.18

26.74

22.05

15.12

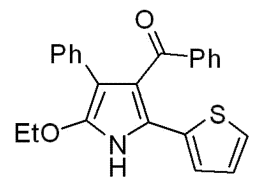
13.61



8.561
7.733
7.715
7.712
7.279
7.276
7.261
7.258
7.245
7.242
7.240
7.166
7.163
7.156
7.154
7.151
7.144
7.141
7.131
7.120
7.112
7.101
7.082
7.014
6.995
6.980
6.977
6.903
6.894
6.890
6.881

3.945
3.928
3.910
3.892

1.223
1.205
1.188

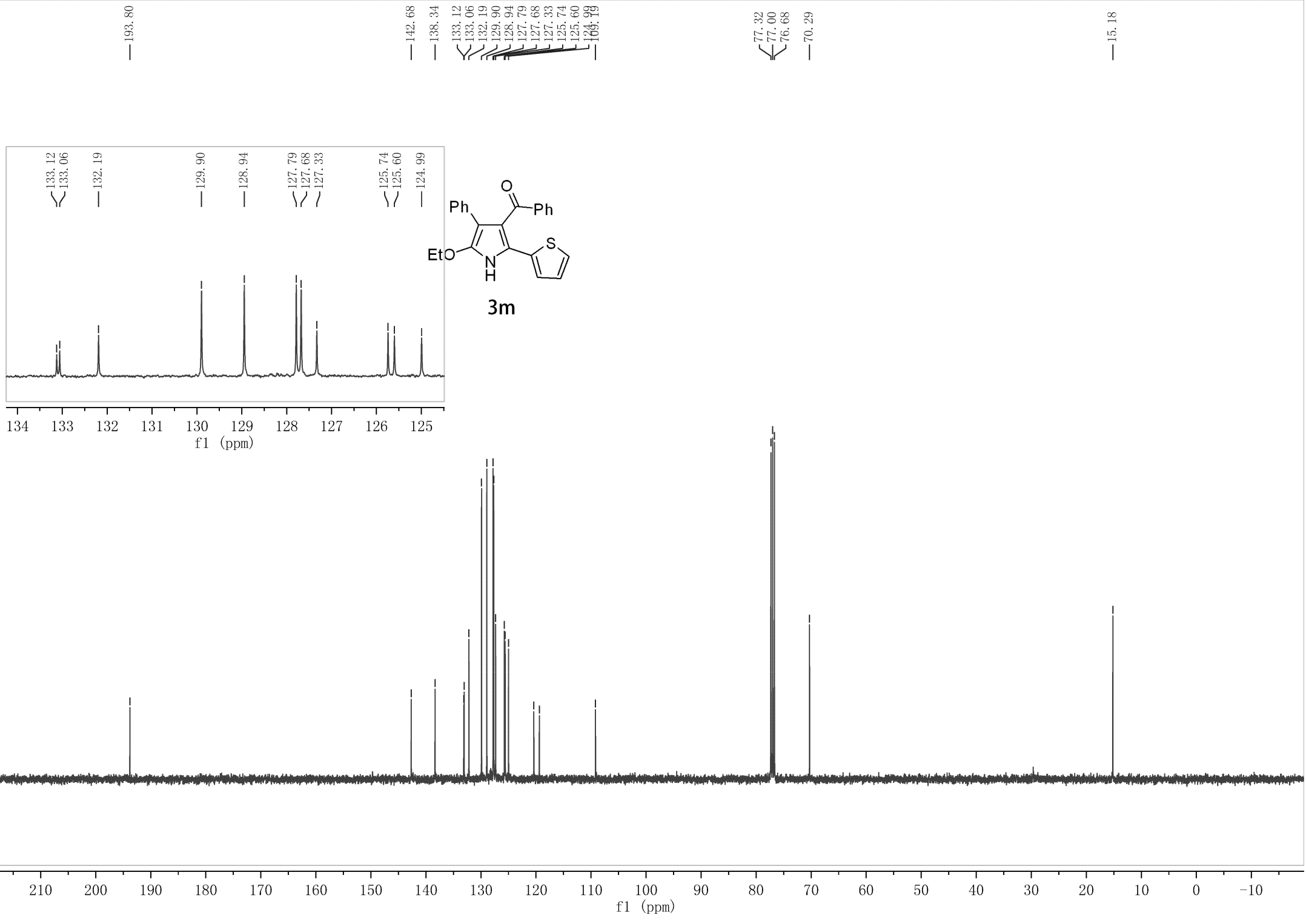


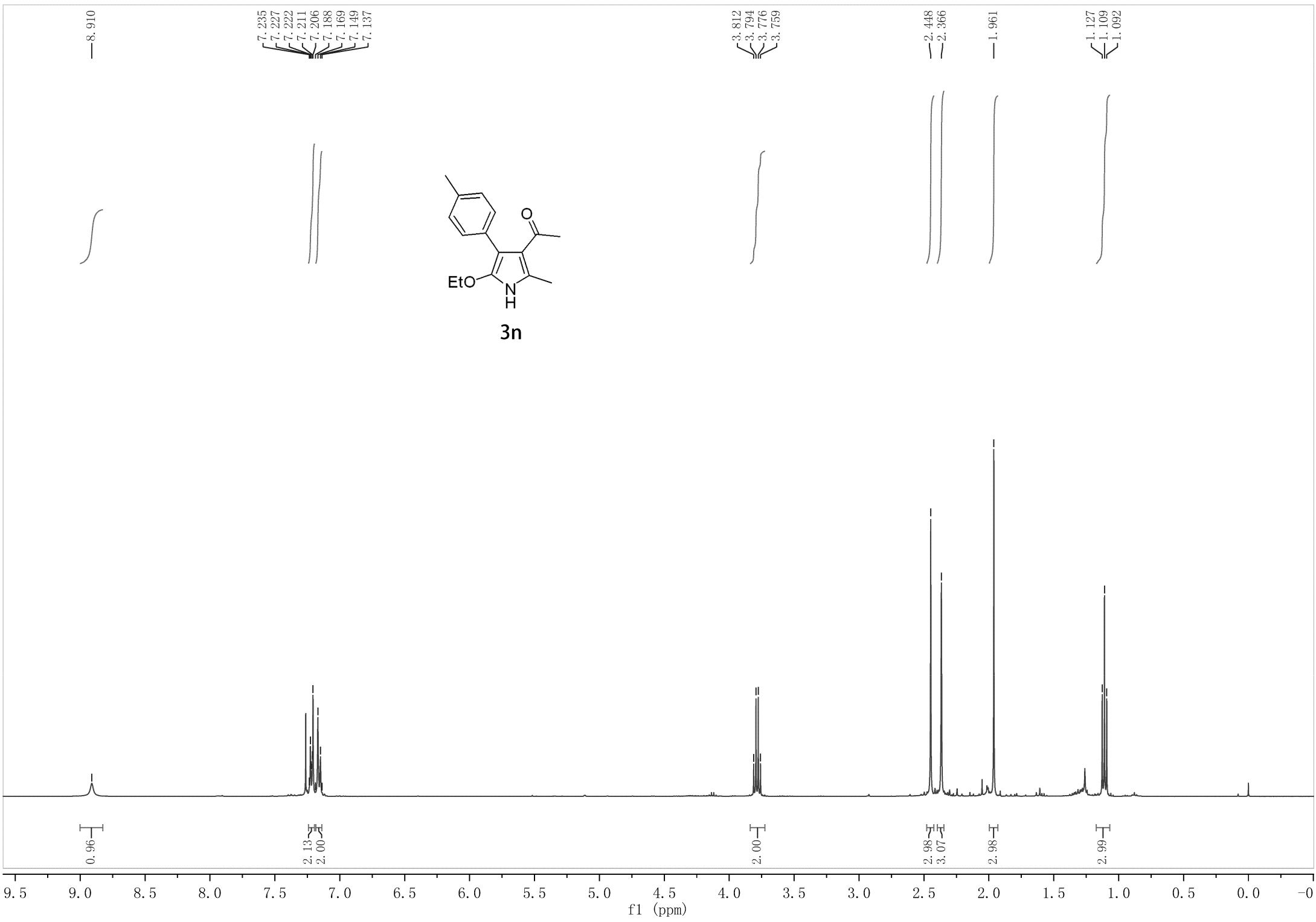
3m



0.99
1.96
3.09
6.02
1.04
1.00
2.00
3.06

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)





— 197.40

— 140.78
— 135.96
— 131.70
— 130.19
— 128.77
— 127.50

— 119.67

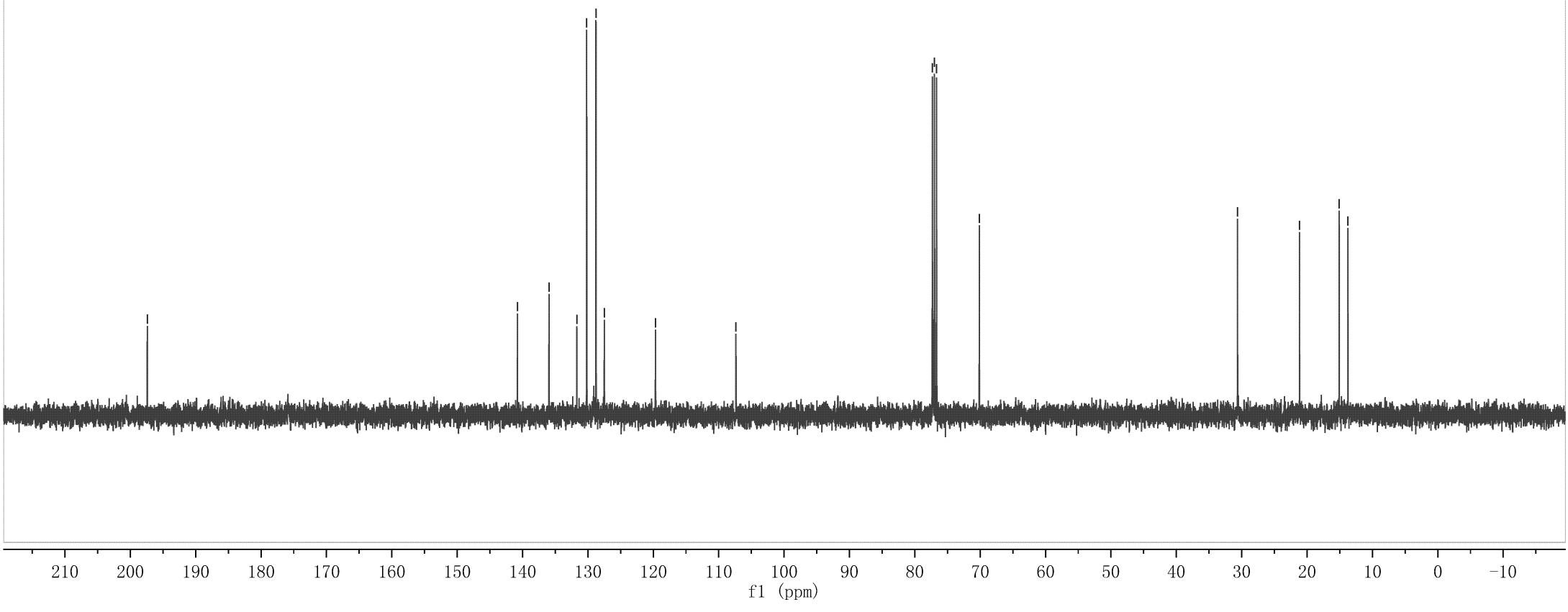
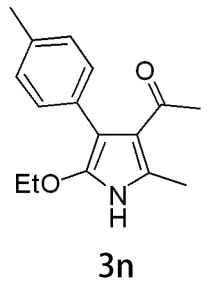
— 107.36

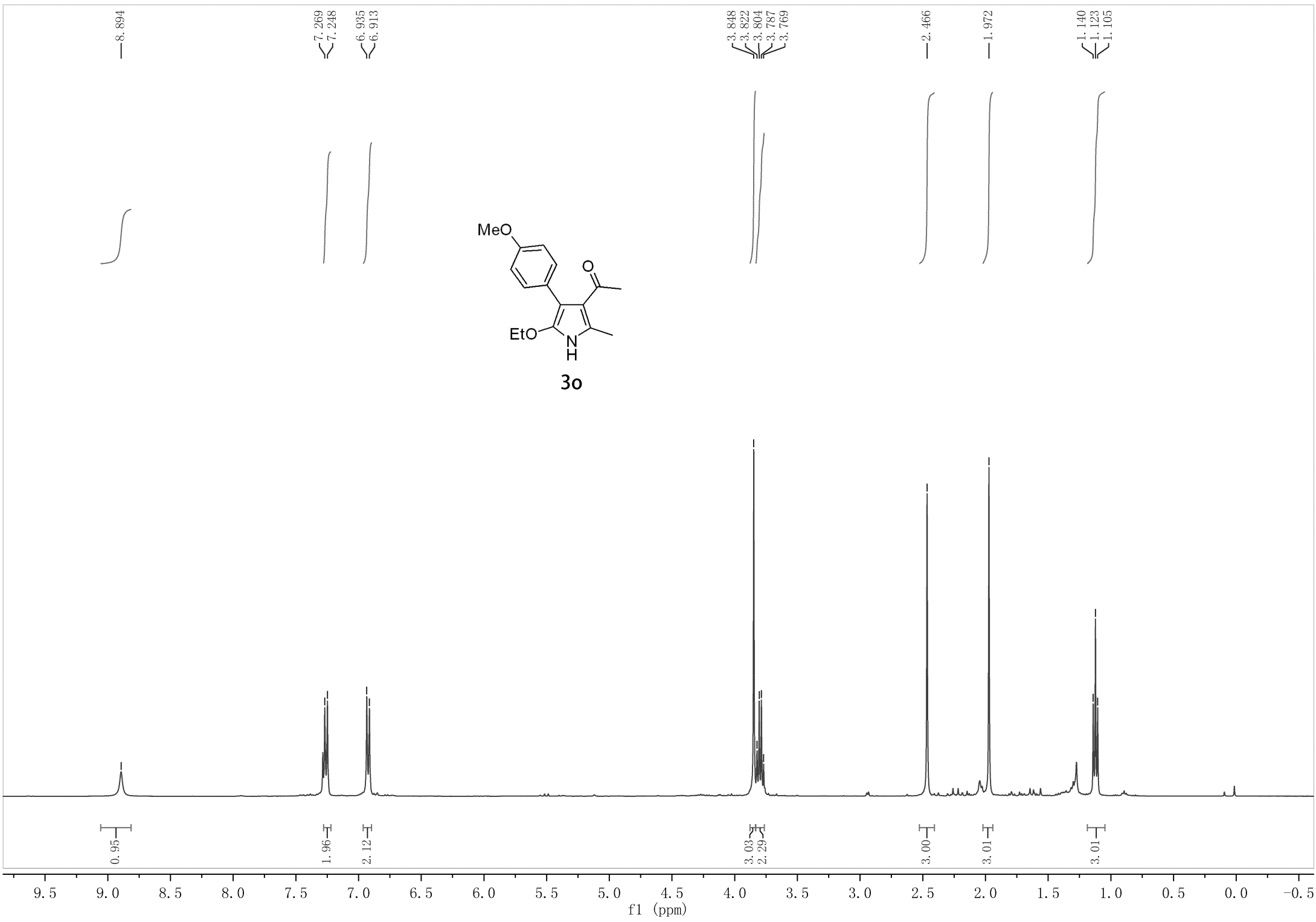
— 77.32
— 77.00
— 76.68
— 70.13

— 30.63

— 21.15

— 15.09
— 13.75





— 197.23

— 158.25

— 140.80

— 131.43

— 127.43

— 127.04

— 119.69

— 113.53

— 106.96

77.32

77.00

76.68

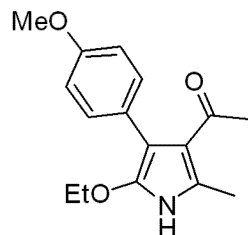
— 70.12

— 55.14

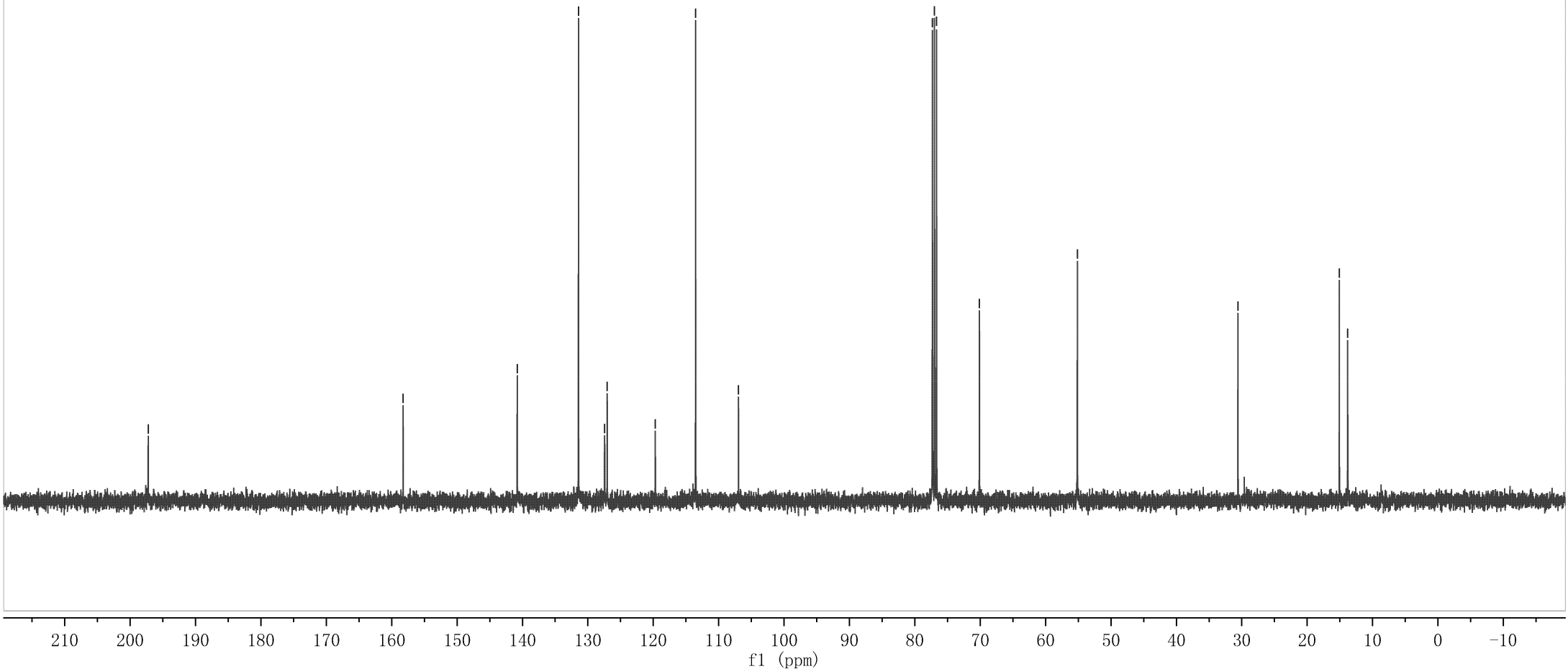
— 30.59

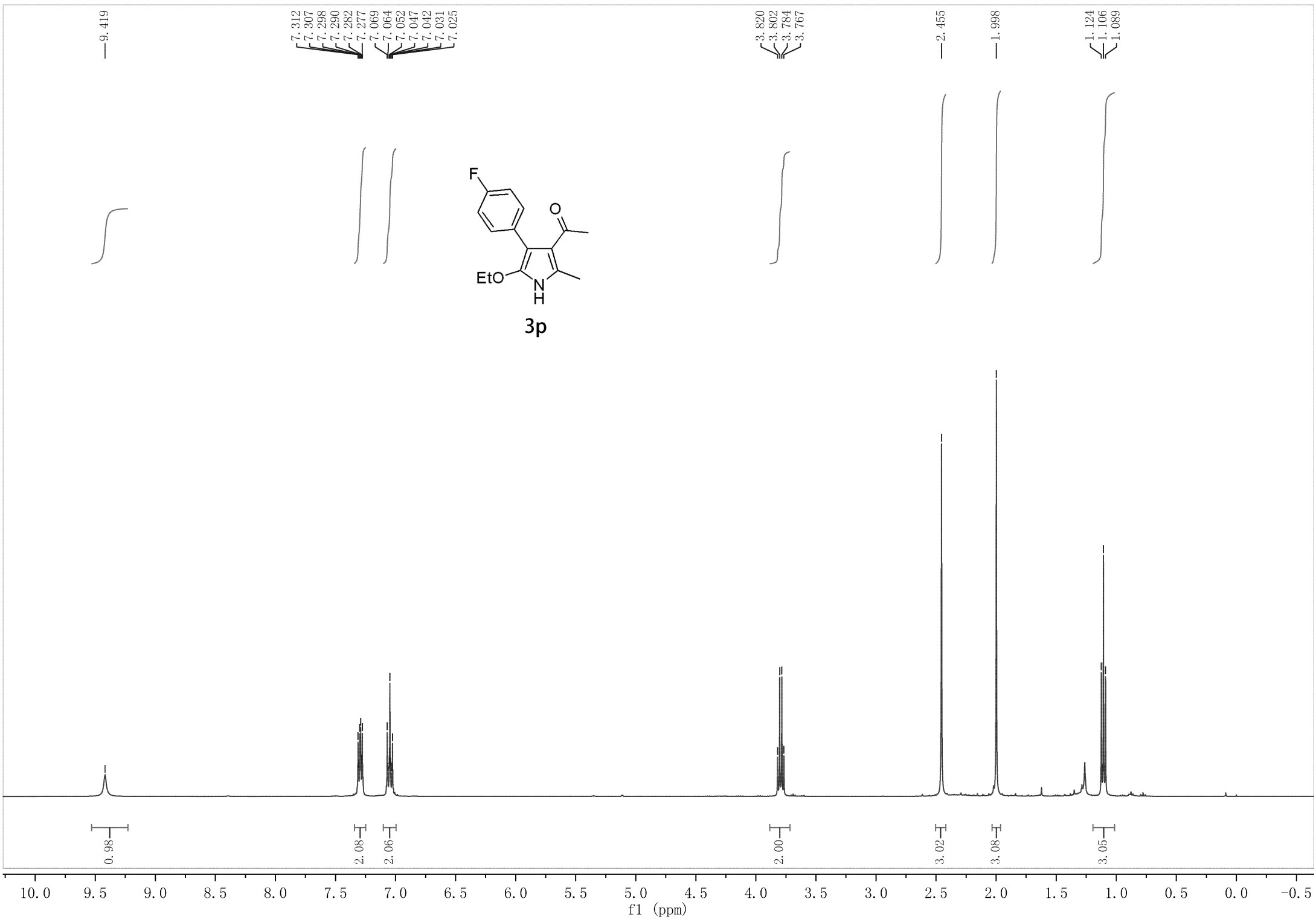
— 15.09

— 13.81



3o





— 197.05

— 162.83
— 160.39

— 141.16
— 131.83
— 131.75
— 130.75
— 130.72
— 128.18

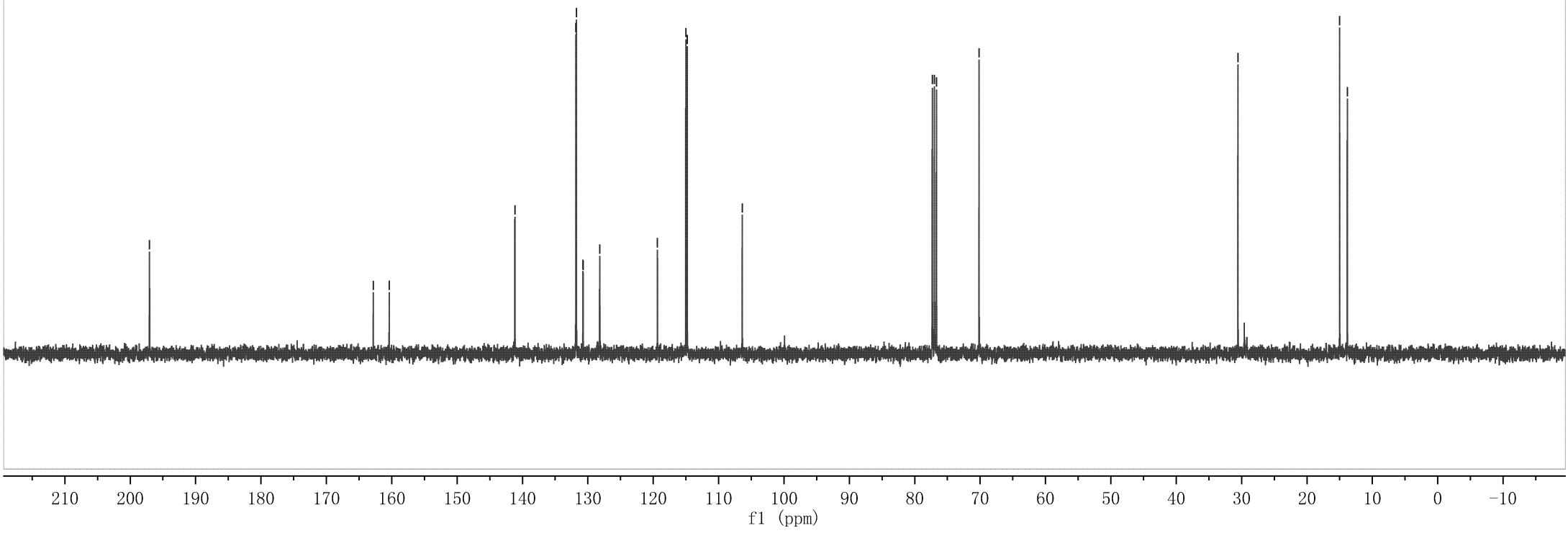
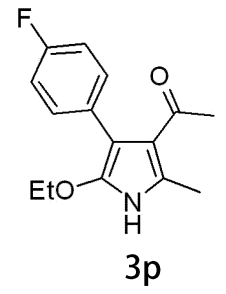
— 119.36
— 115.02
— 114.81

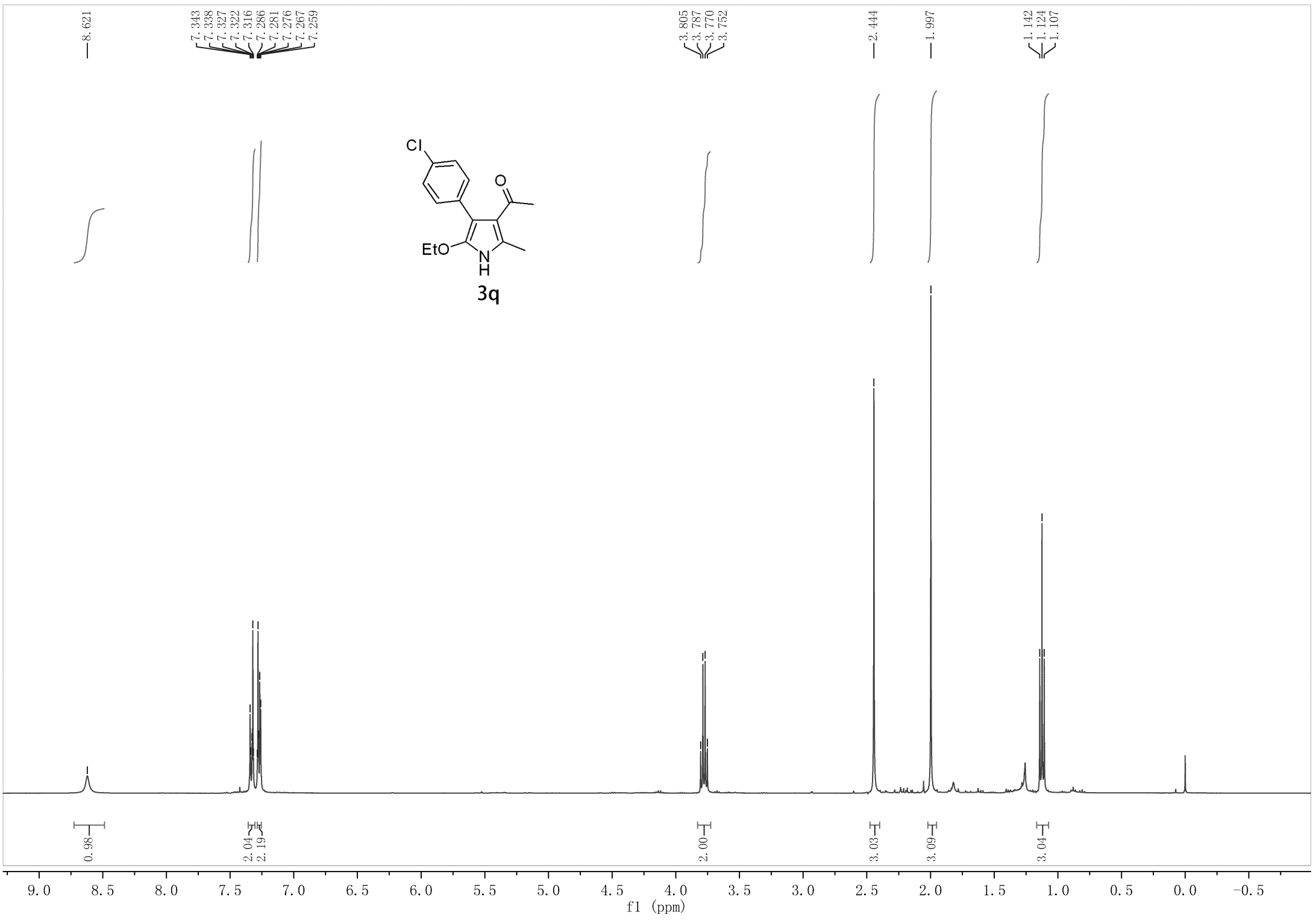
— 106.39

— 77.32
— 77.00
— 76.68
— 70.16

— 30.57

— 15.01
— 13.83





— 196.91

— 141.14

133.26

132.11

131.46

128.18

128.02

— 119.36

— 106.25

77.32

77.00

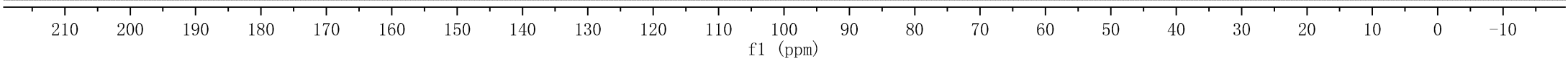
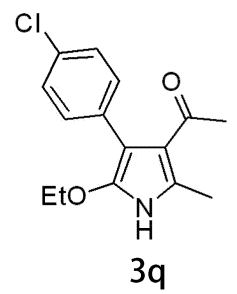
76.68

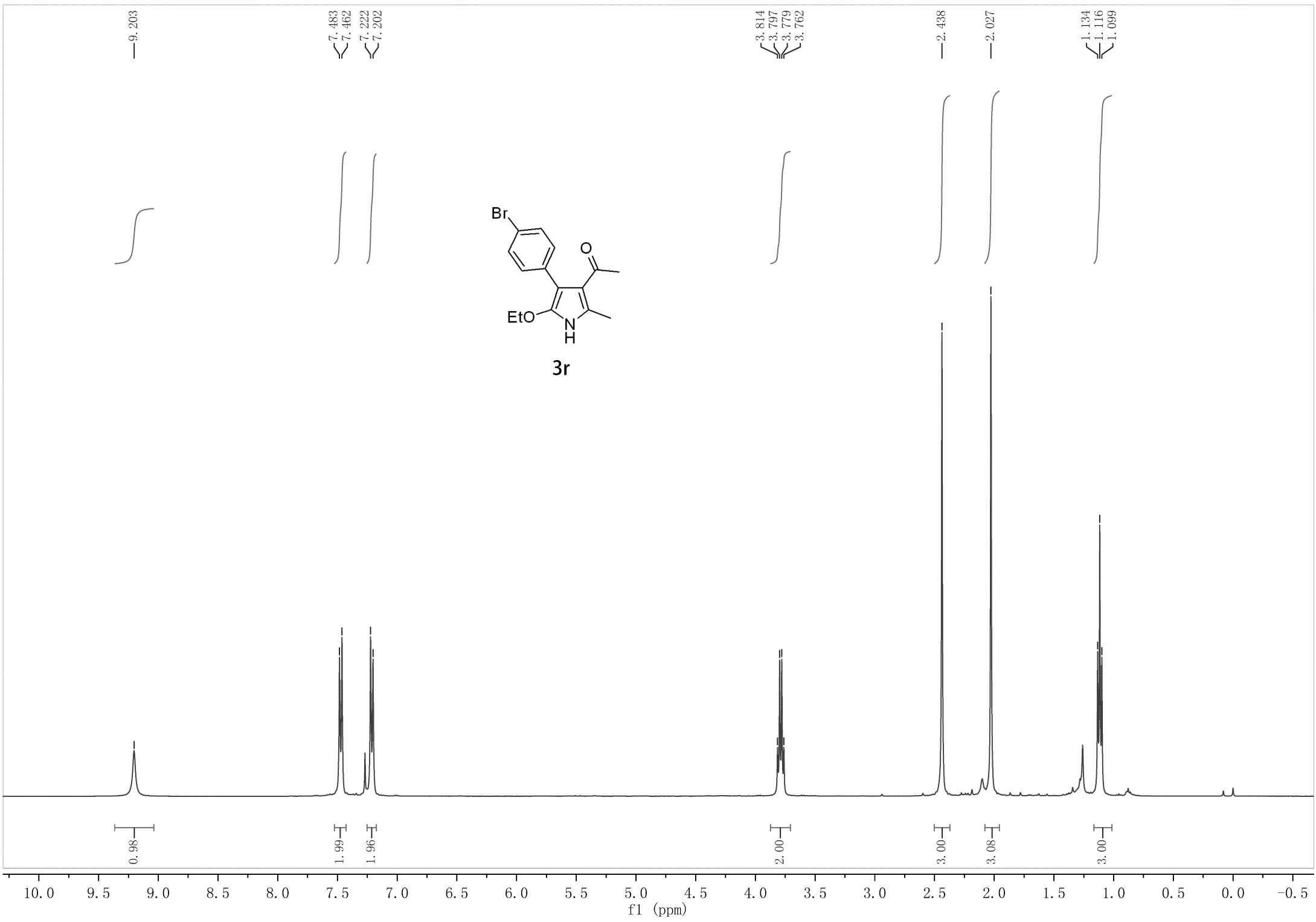
— 70.23

— 30.68

15.05

13.79





— 196.93

— 141.16

133.75

131.83

131.13

128.06

120.26

119.35

— 106.25

77.32

77.00

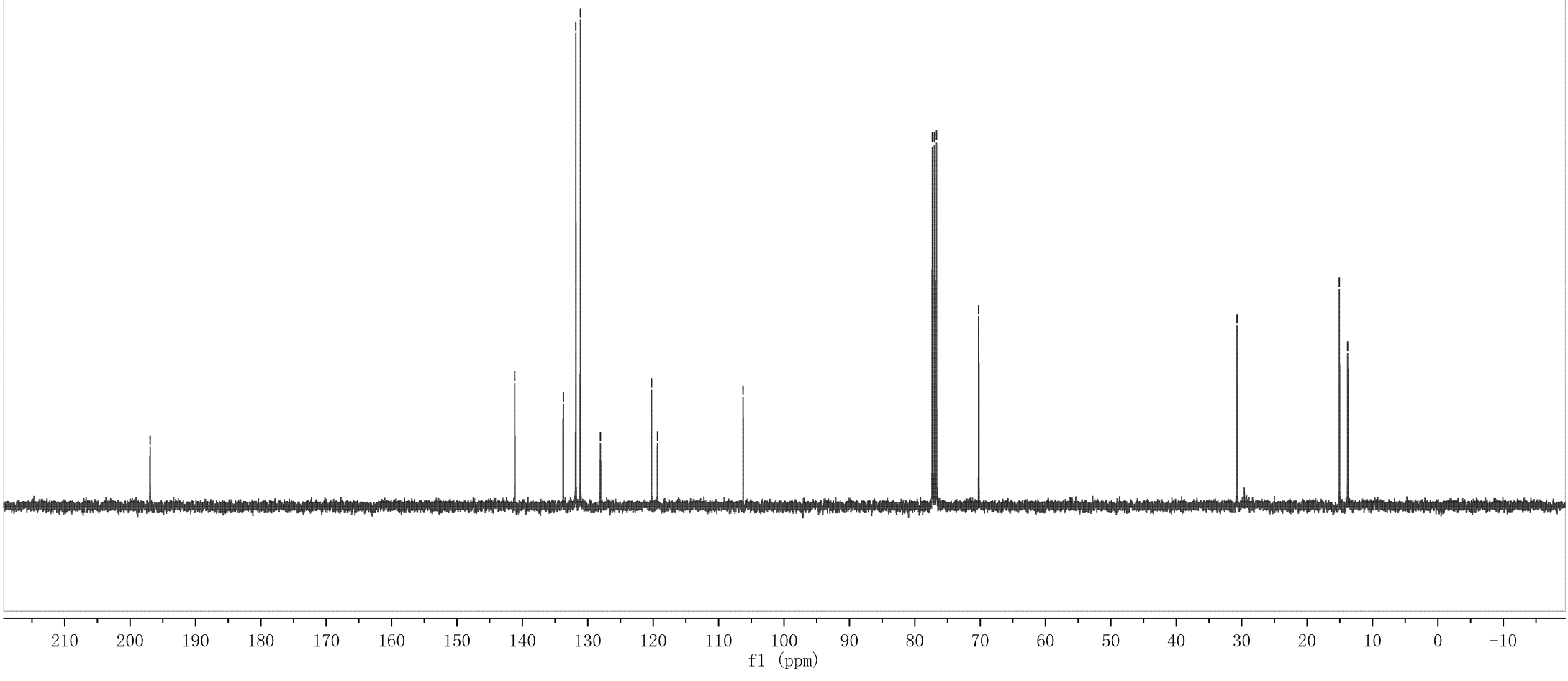
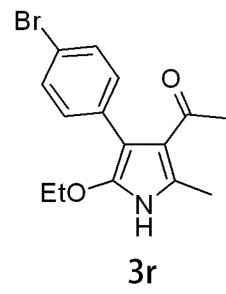
76.68

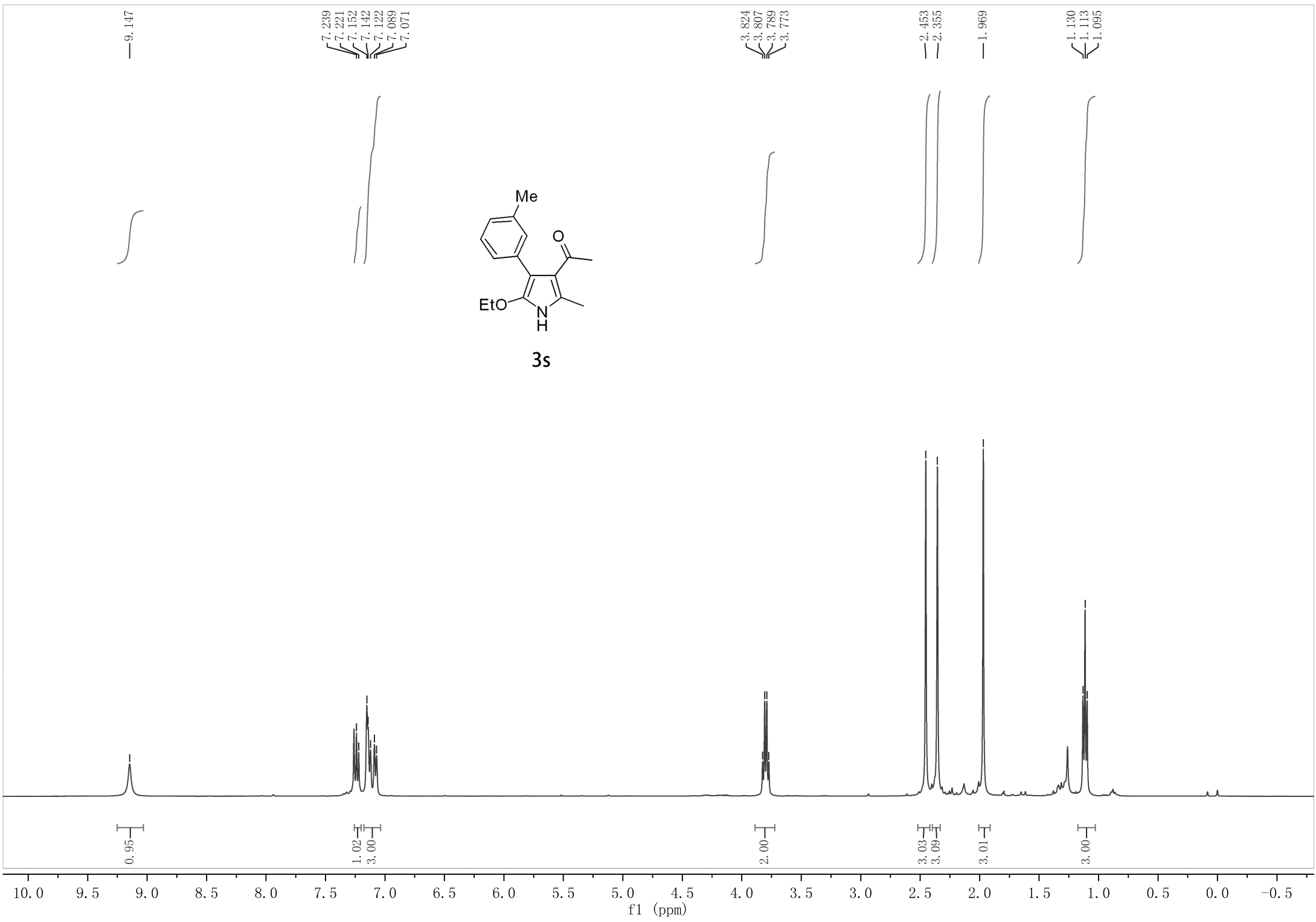
— 70.22

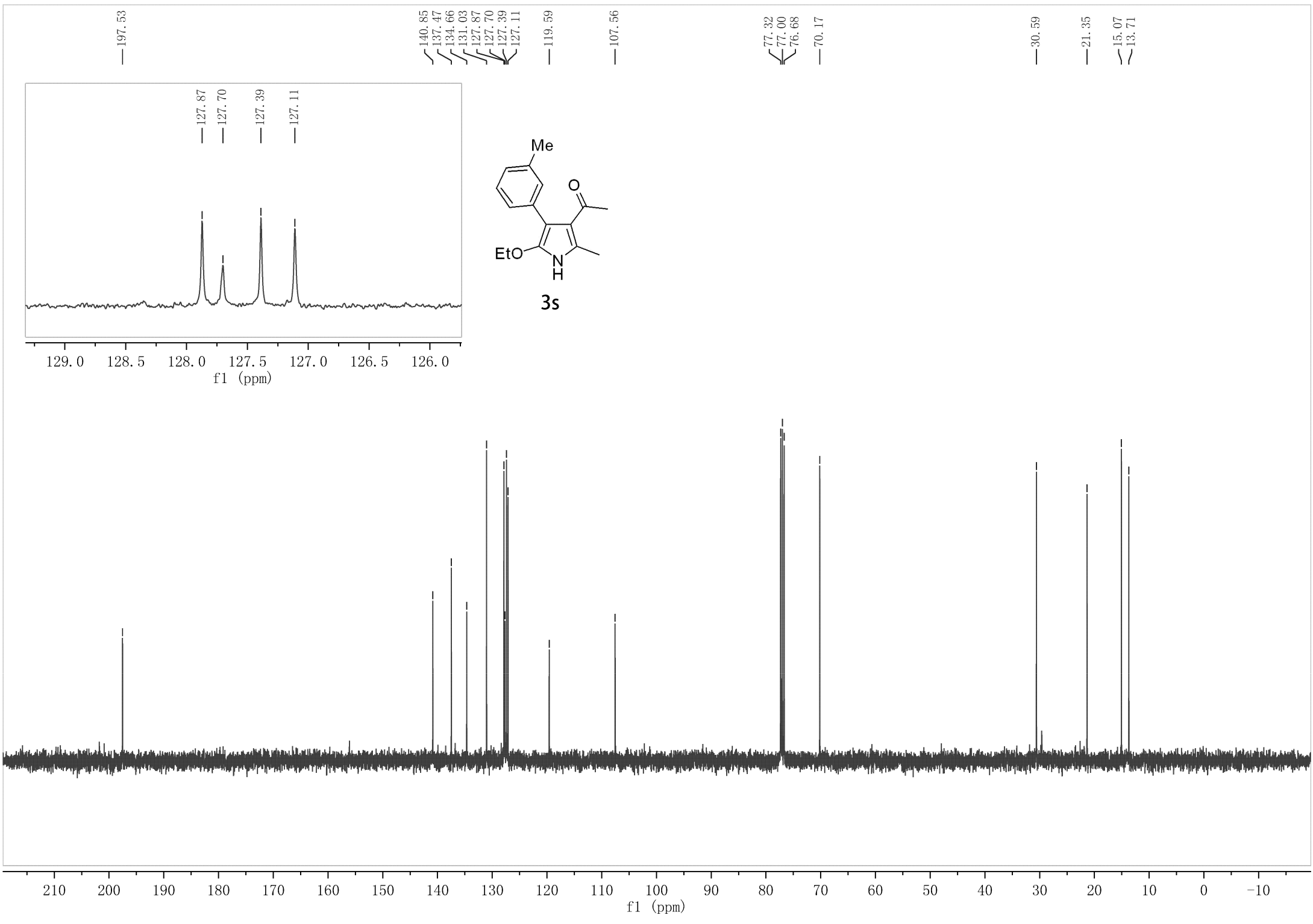
— 30.69

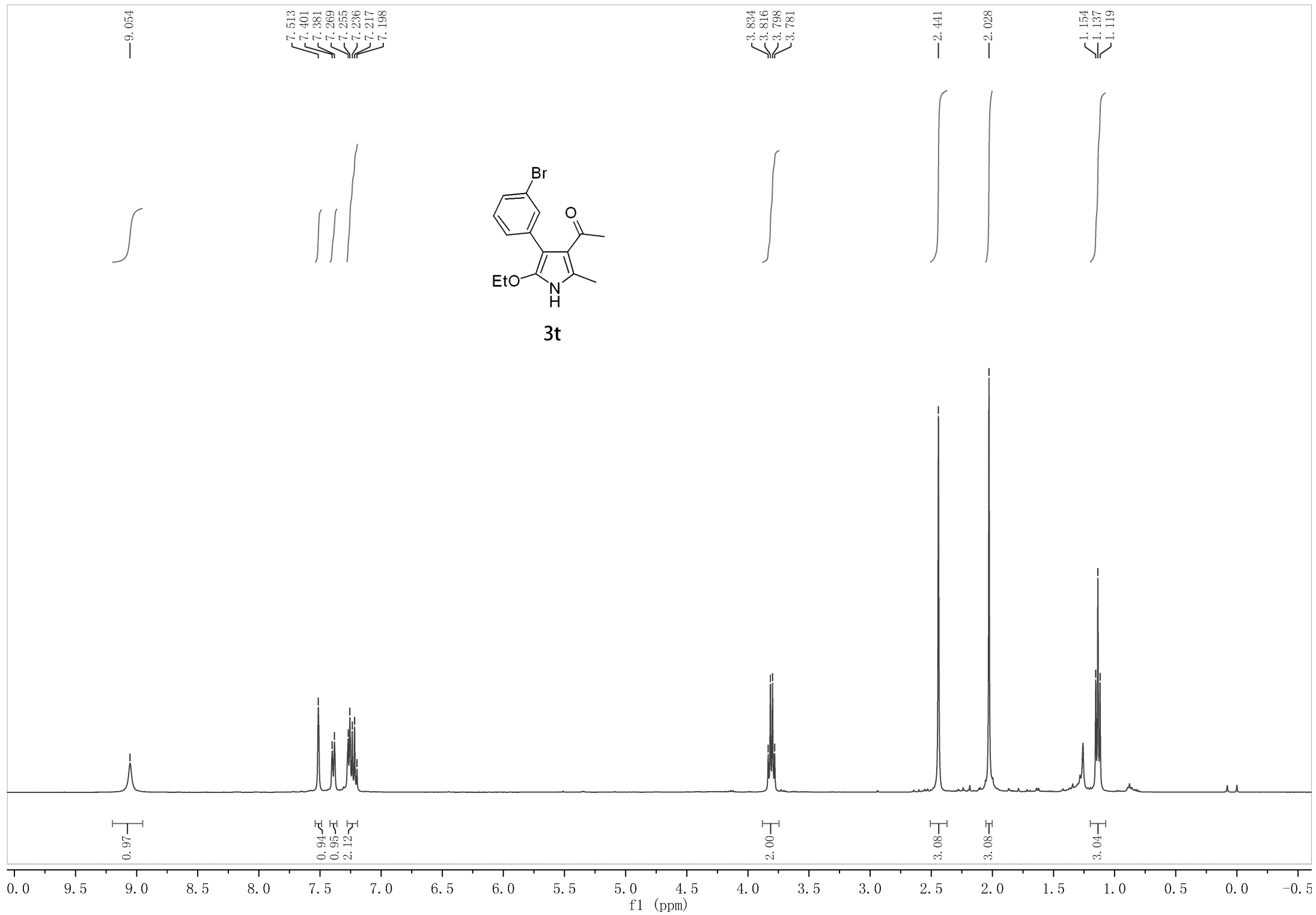
15.06

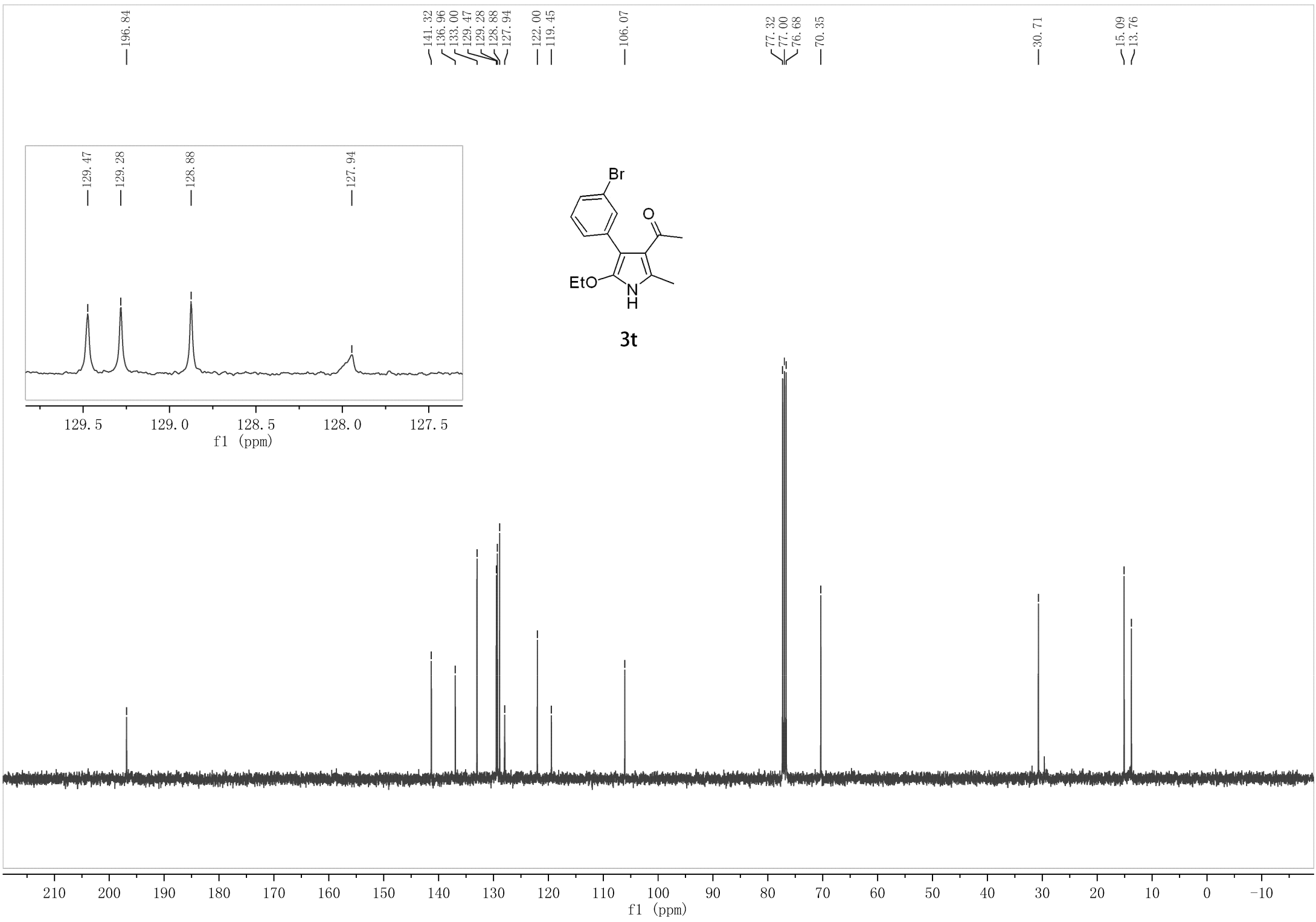
13.79

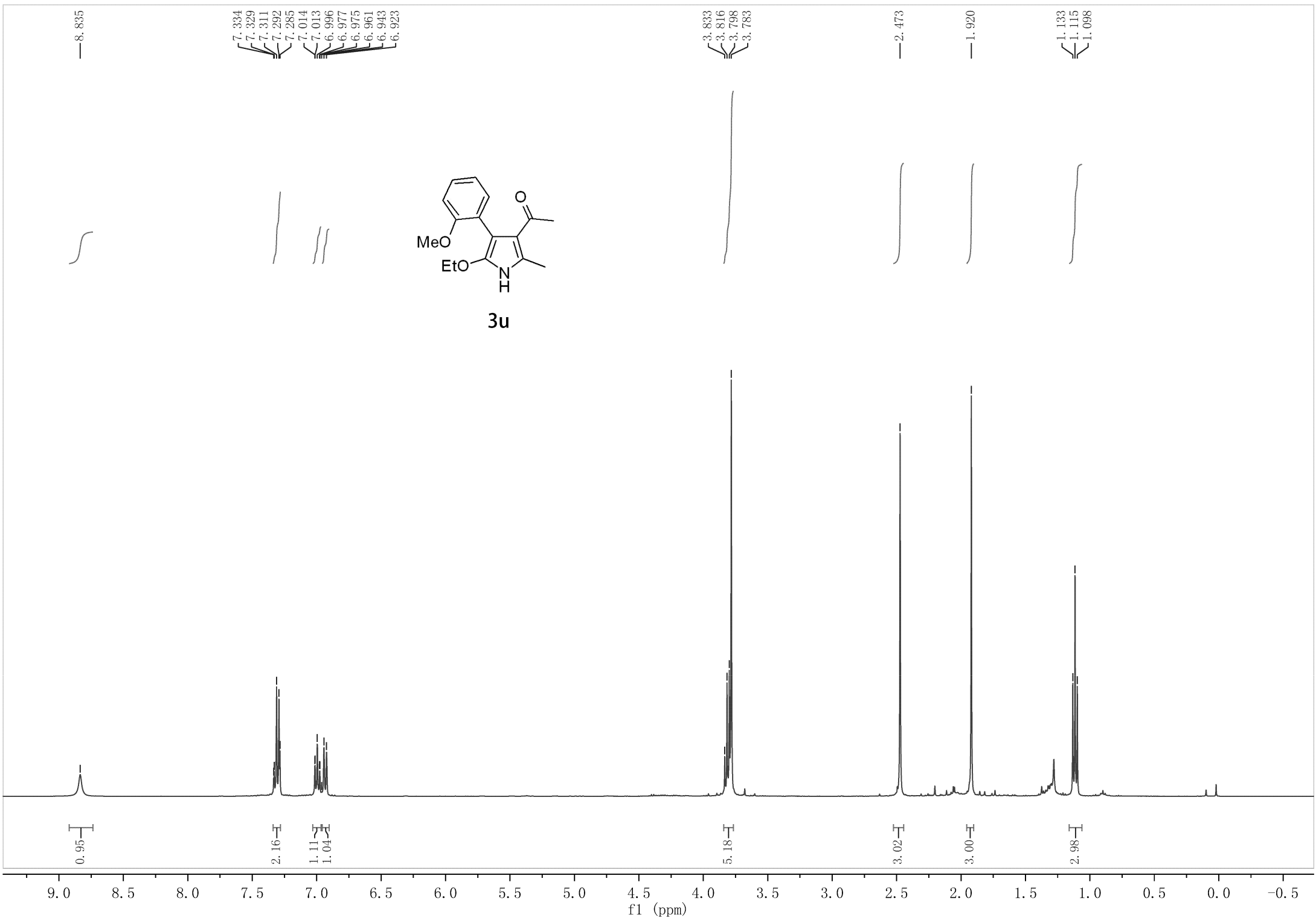












— 197.01

— 157.39

— 140.93

— 132.24

— 128.36

— 127.30

— 123.80

— 120.45

— 119.86

— 110.45

— 102.61

— 77.32

— 77.00

— 76.68

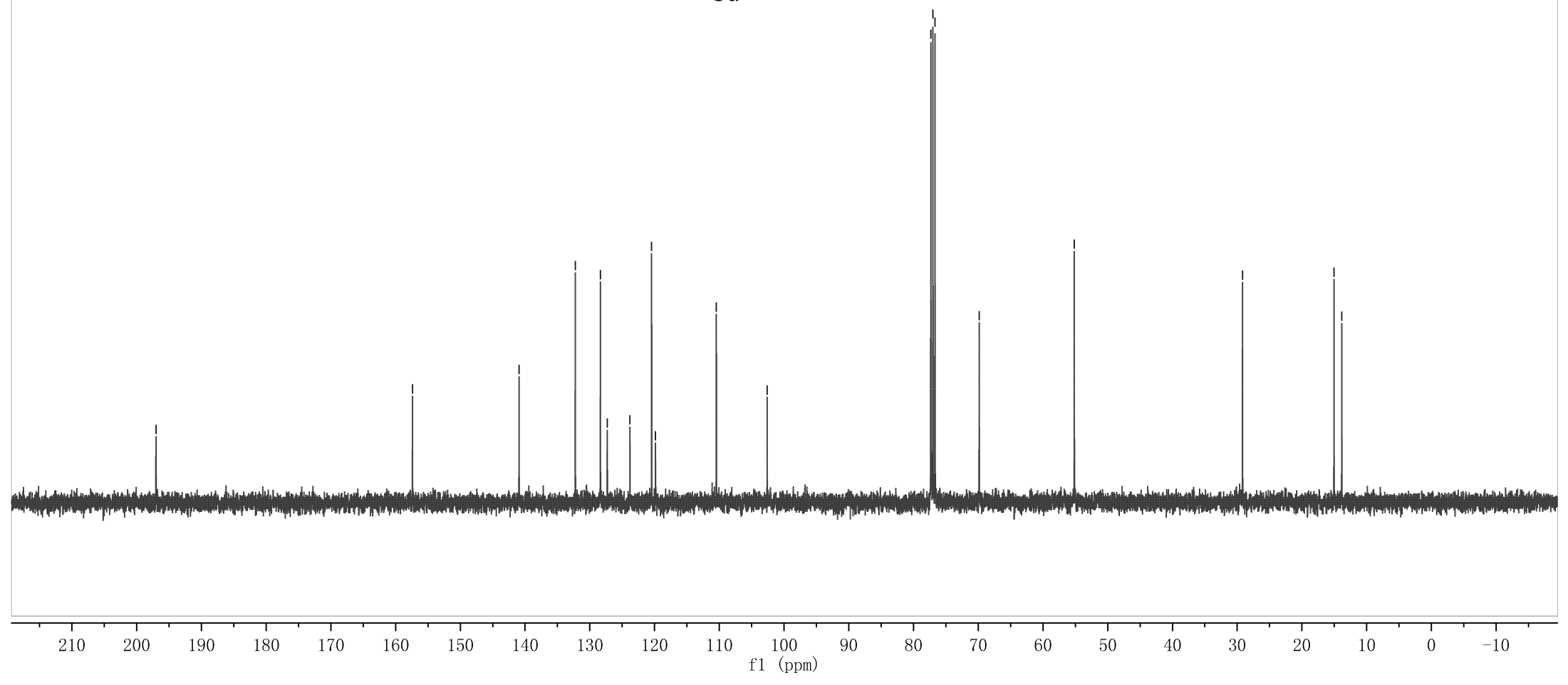
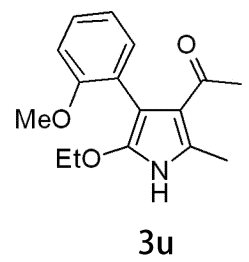
— 69.85

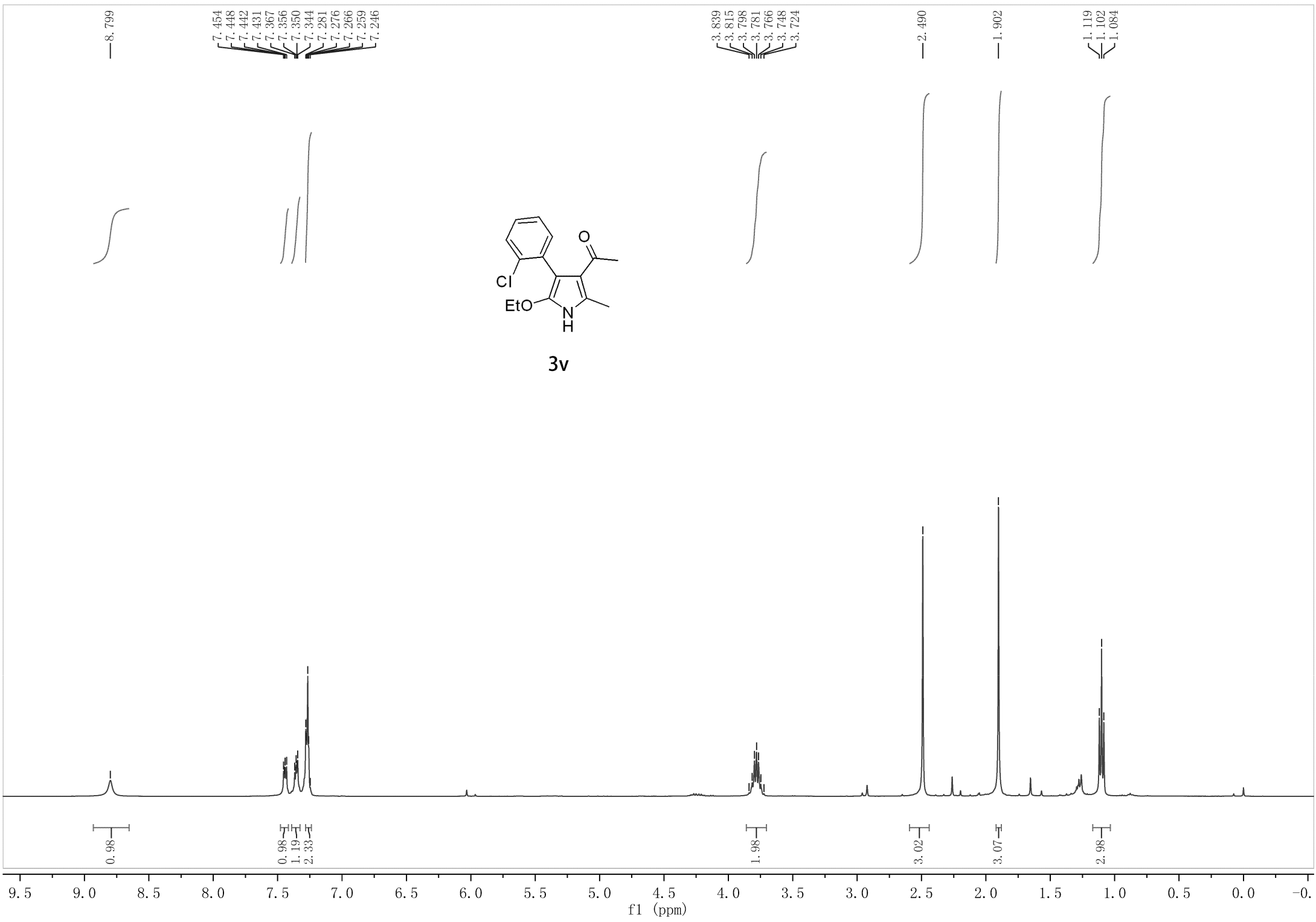
— 55.16

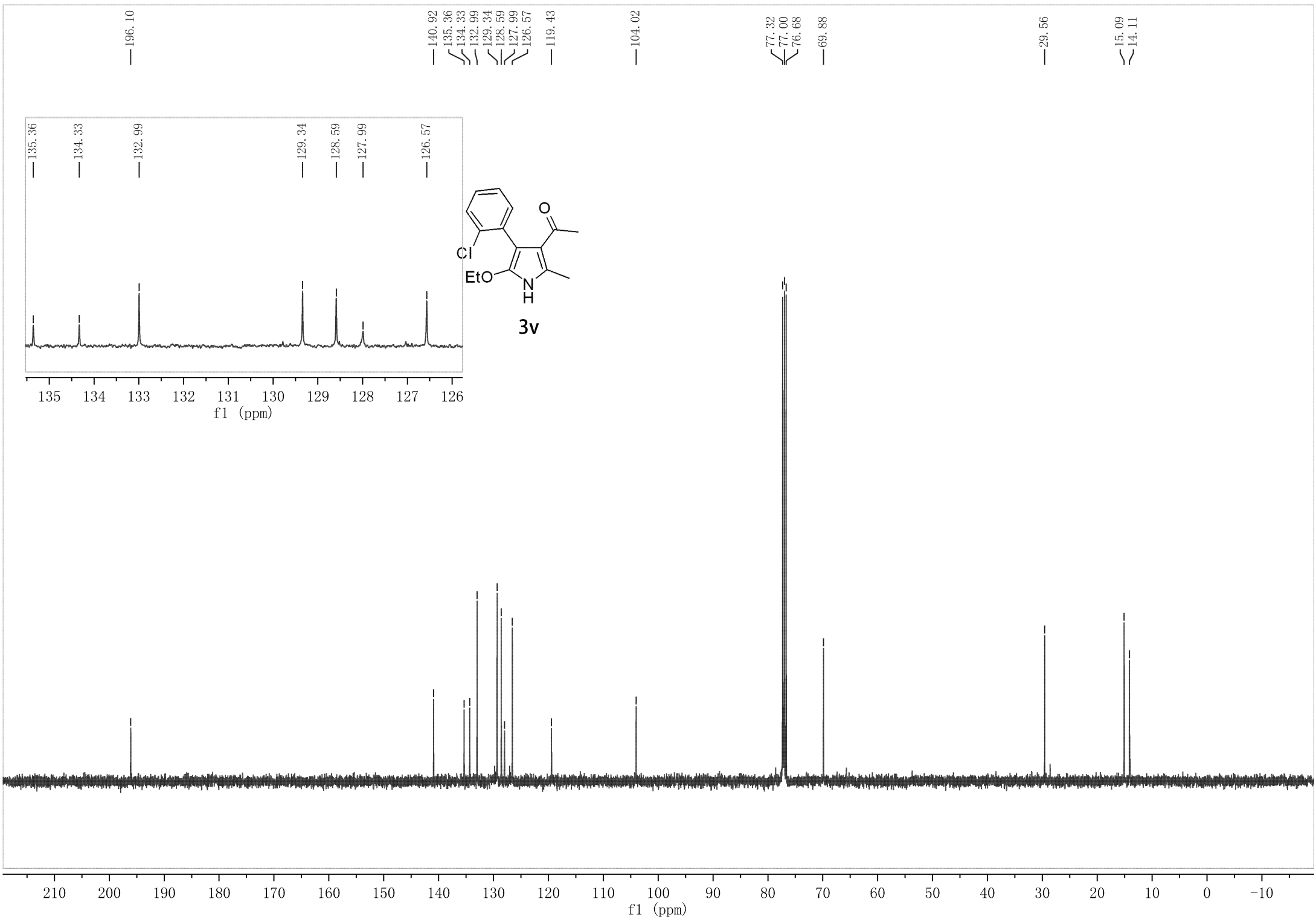
— 29.18

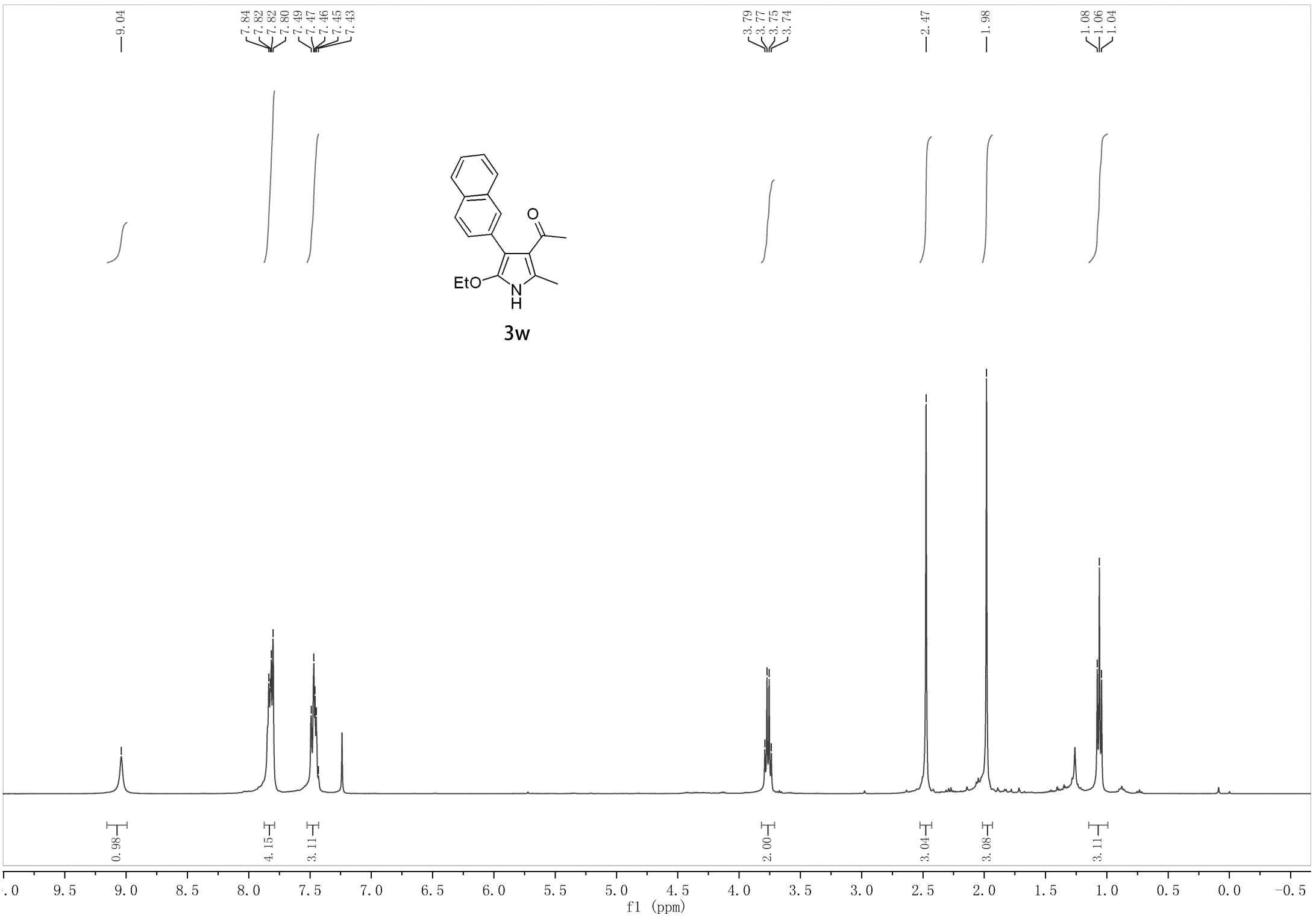
— 15.04

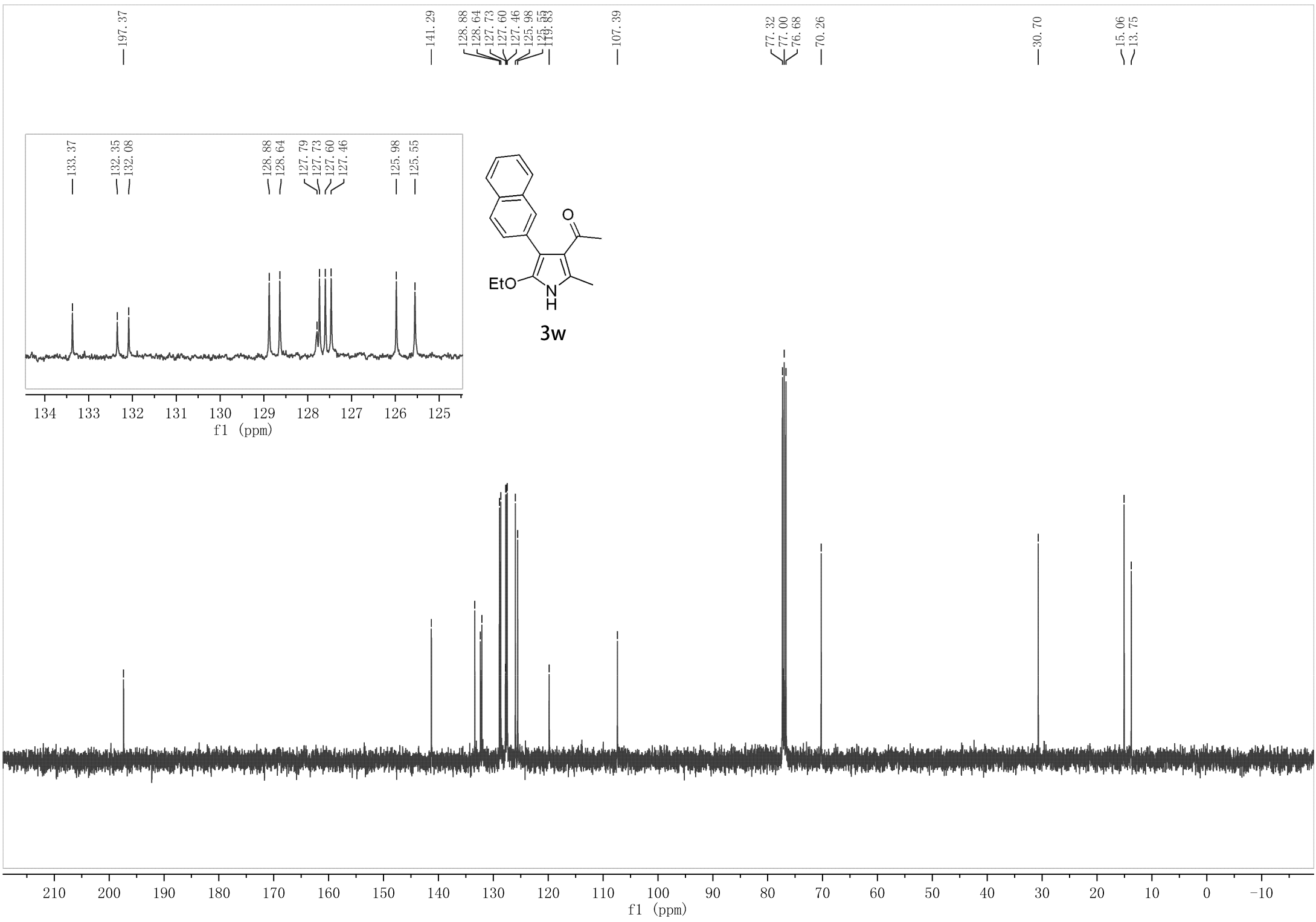
— 13.84

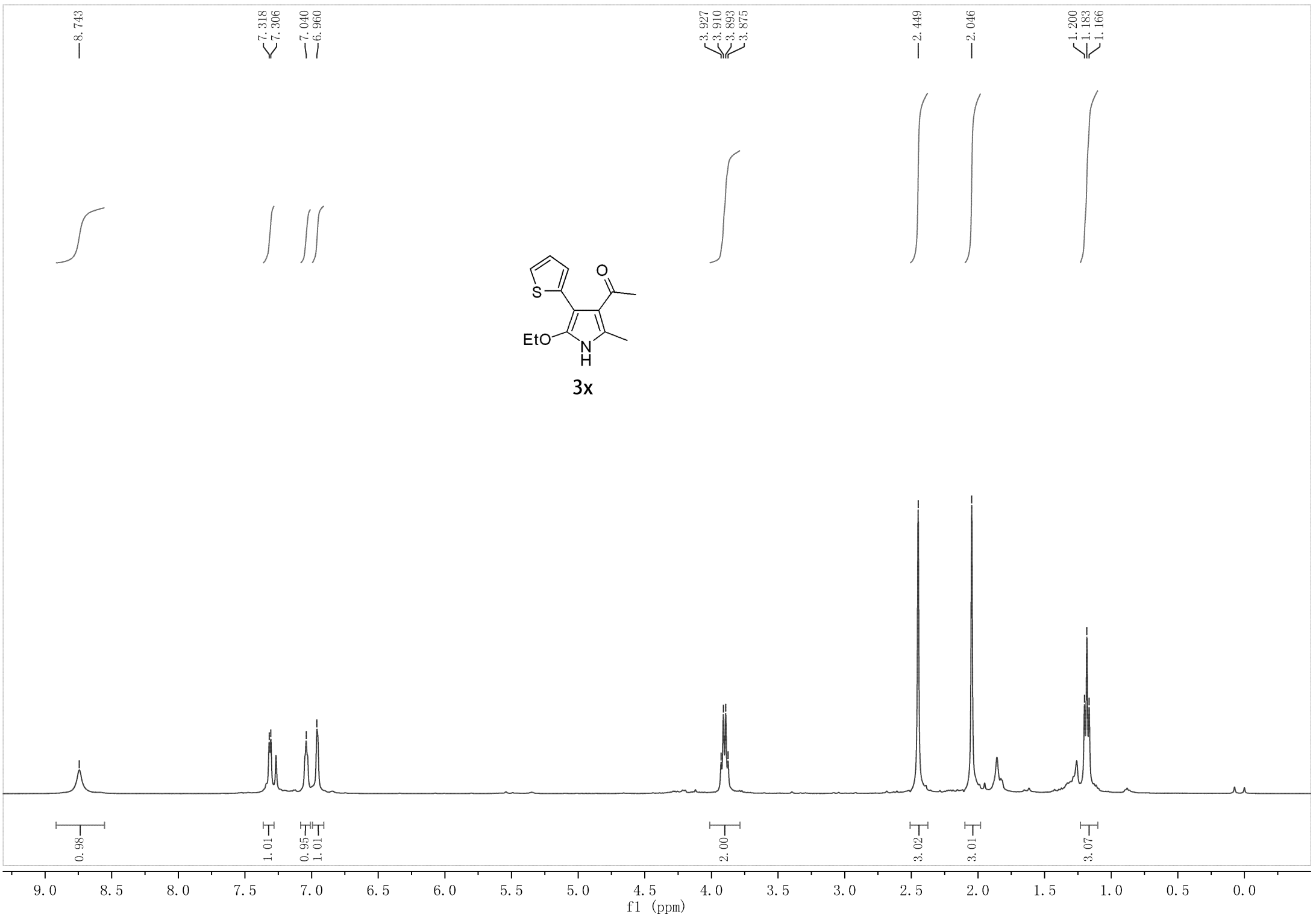












— 196.81

— 142.12

— 135.47

128.12

127.82

126.86

125.64

— 120.16

— 98.77

77.32

77.00

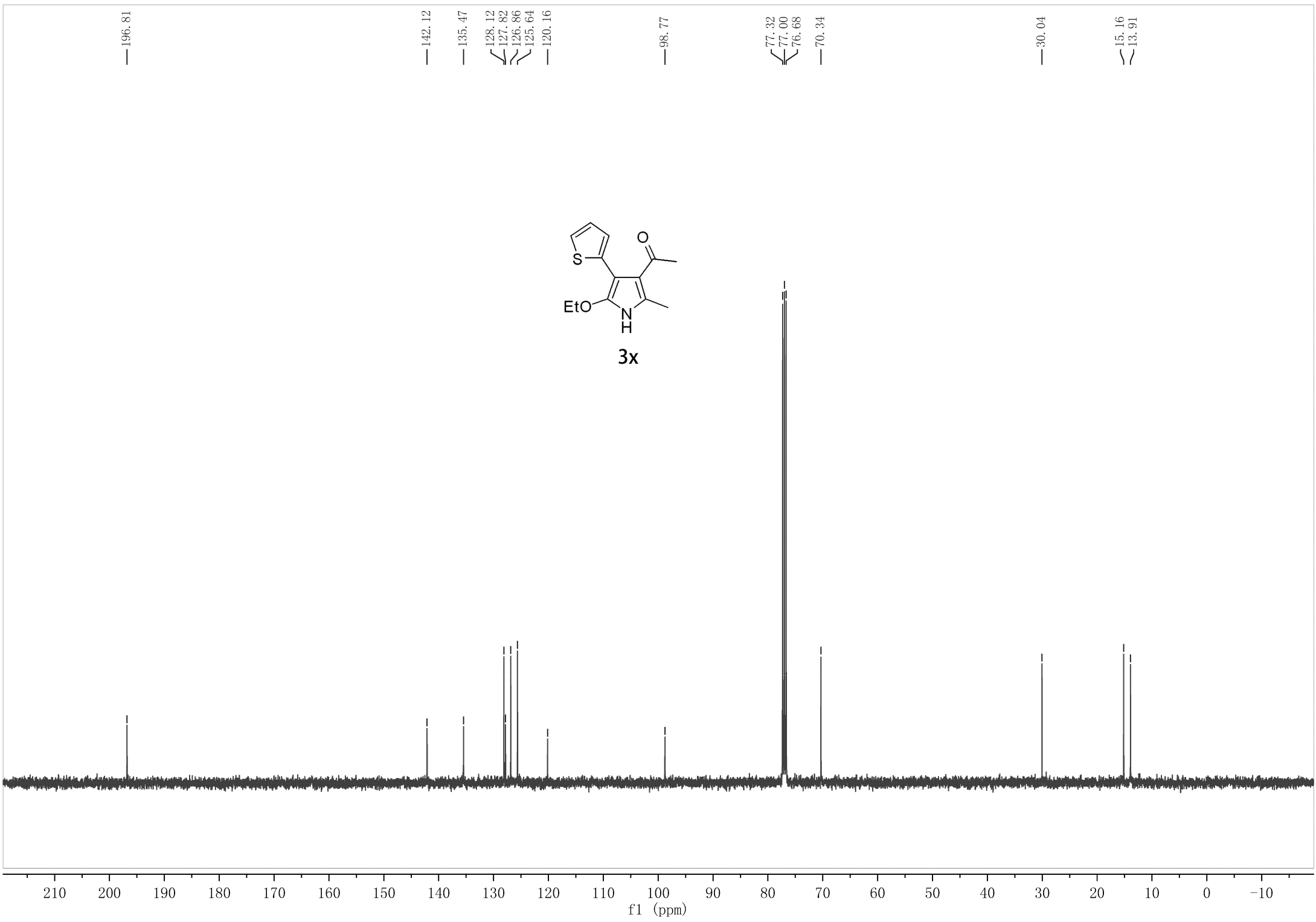
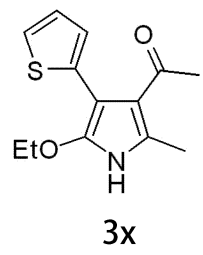
76.68

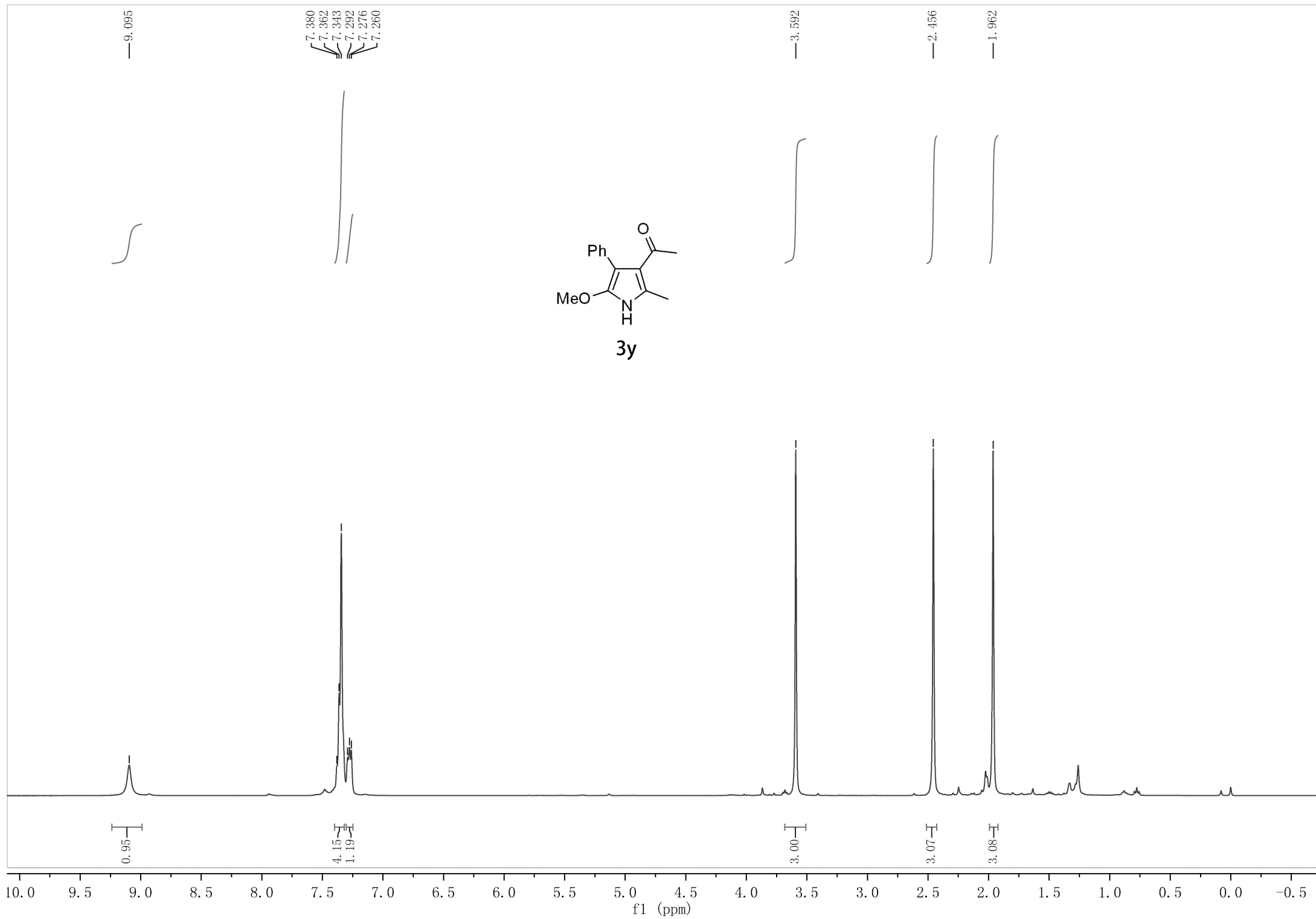
— 70.34

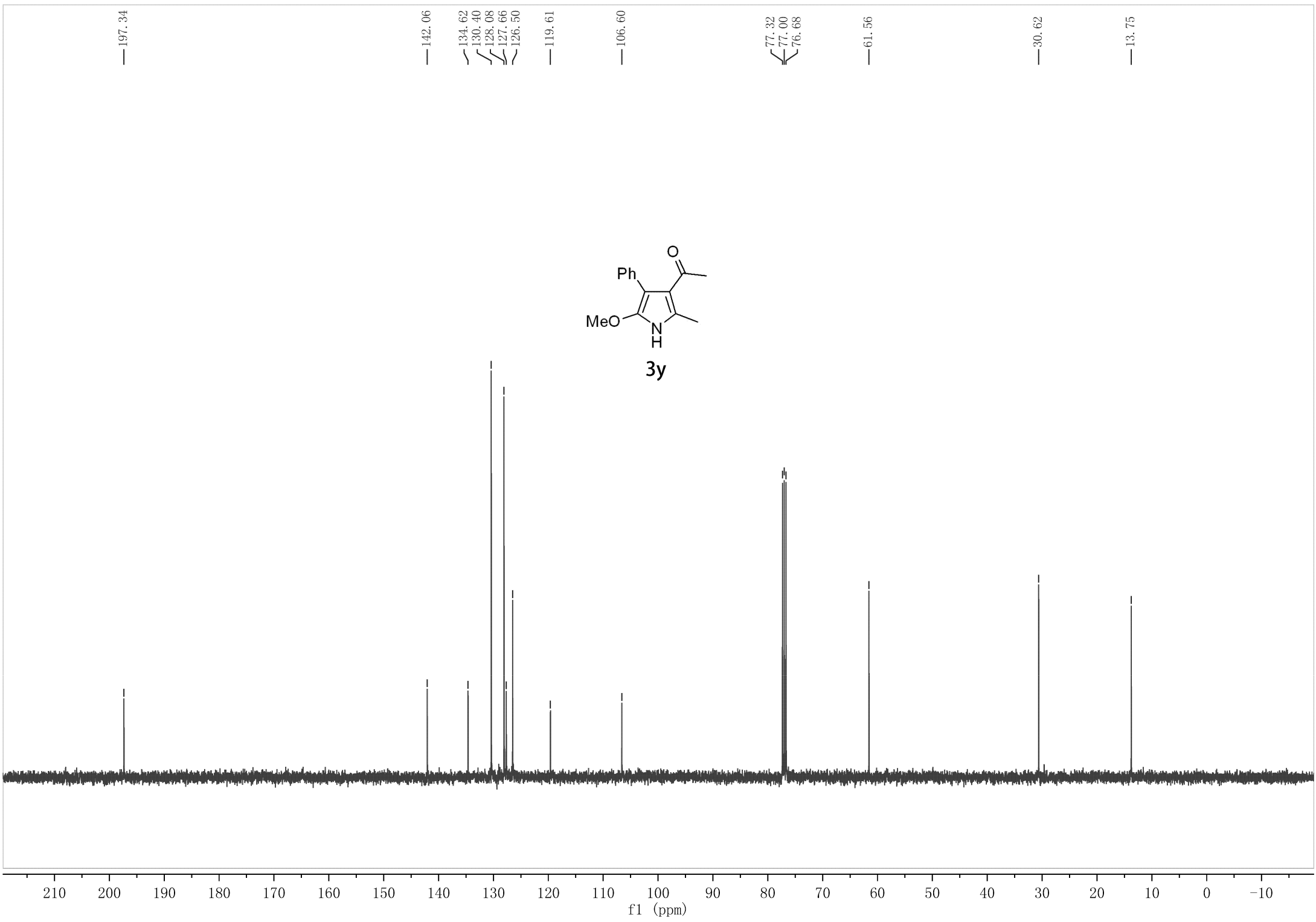
— 30.04

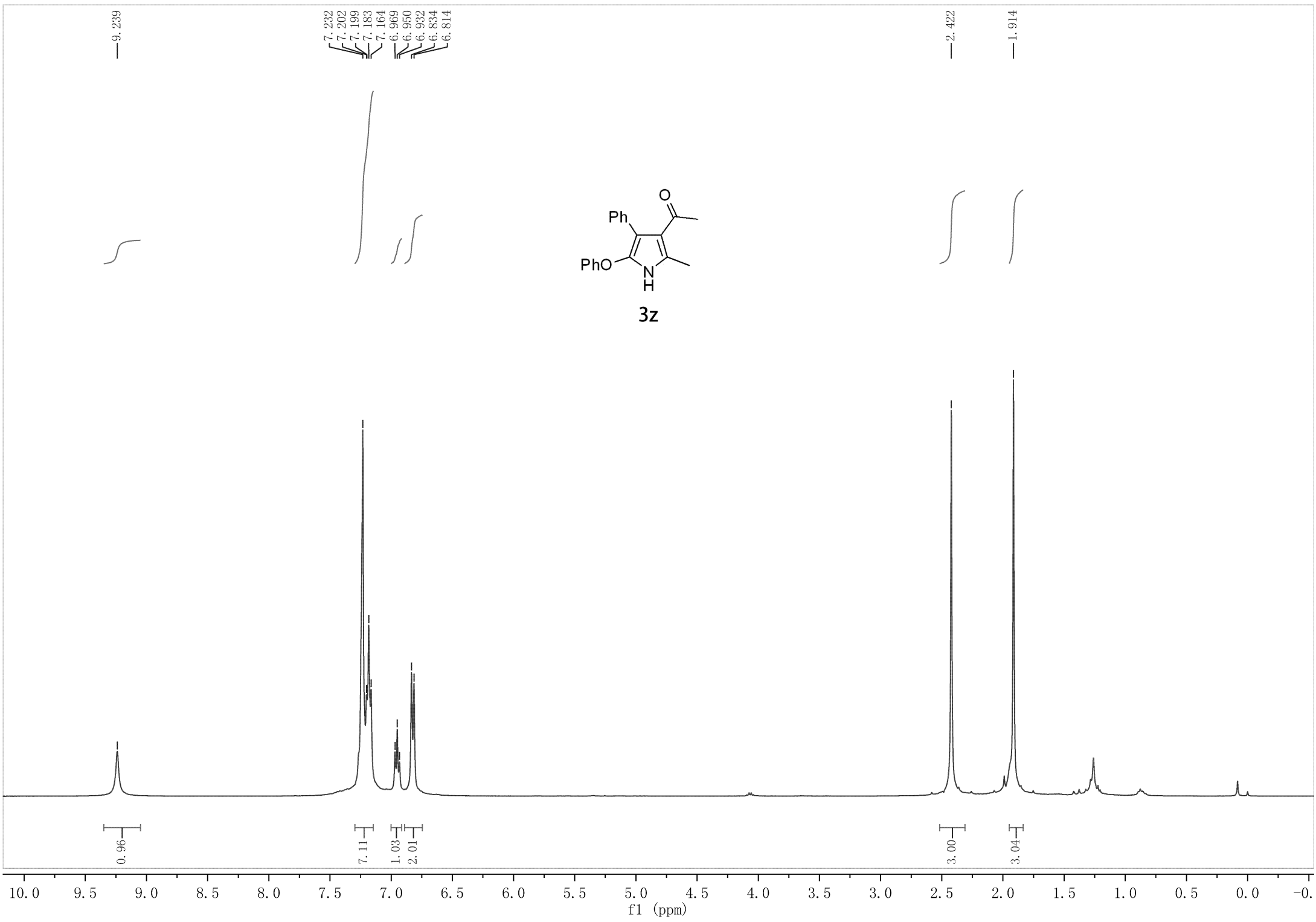
15.16

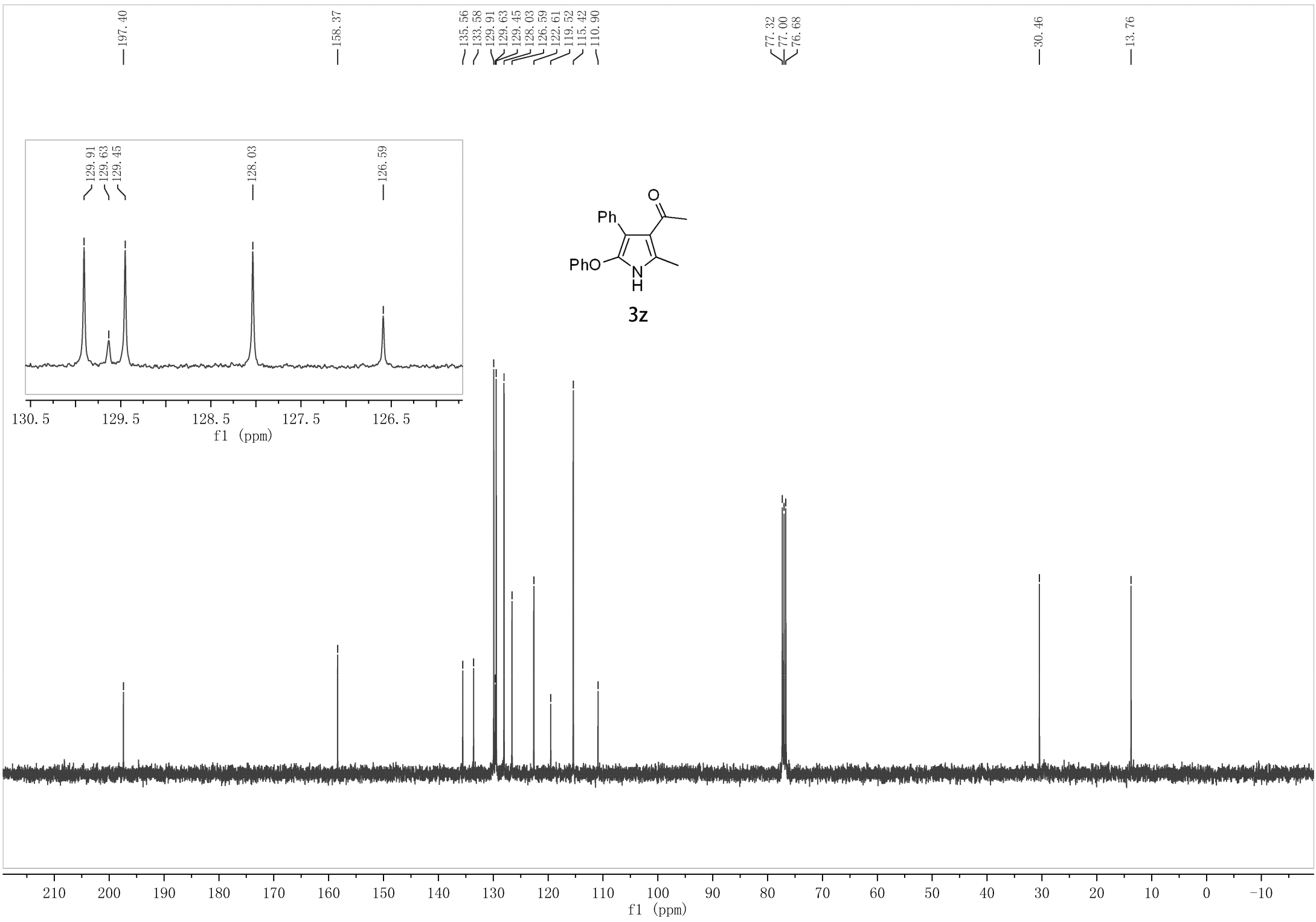
13.91

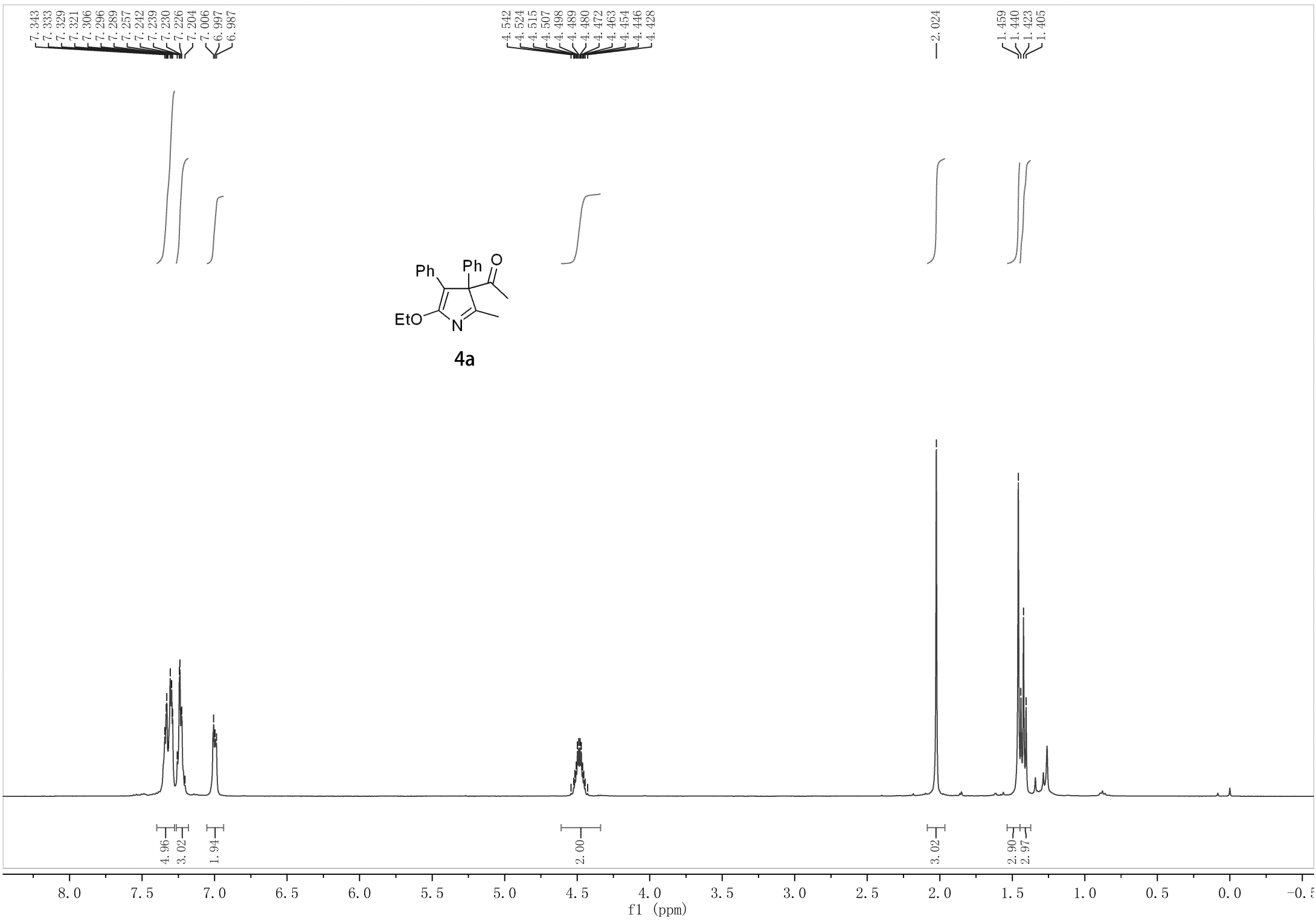


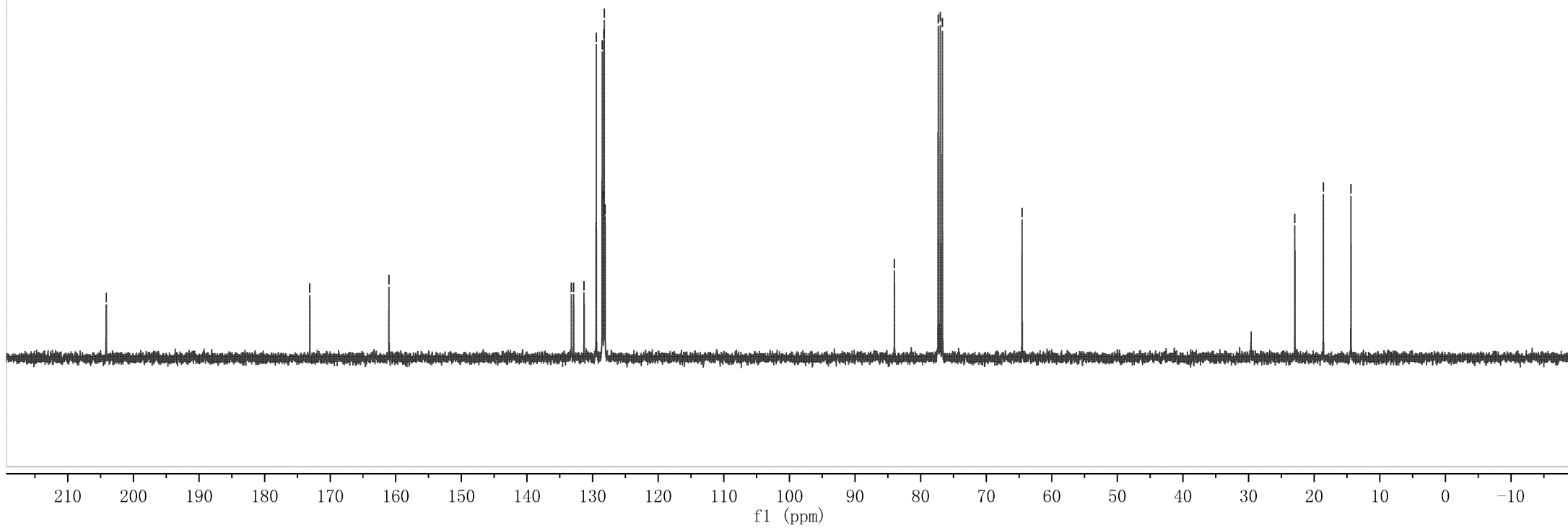
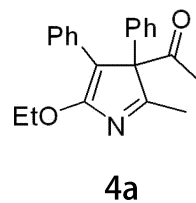
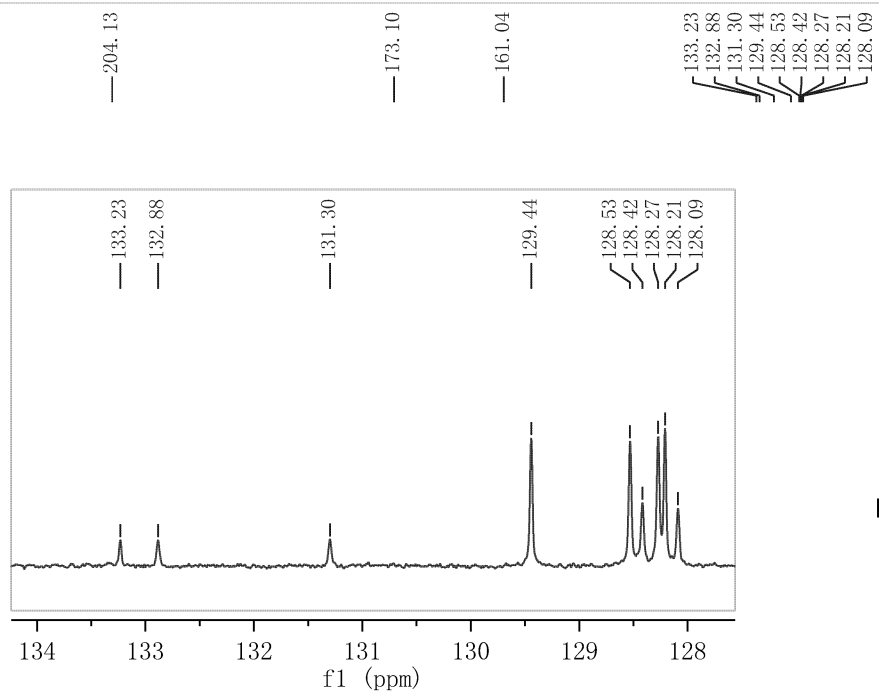


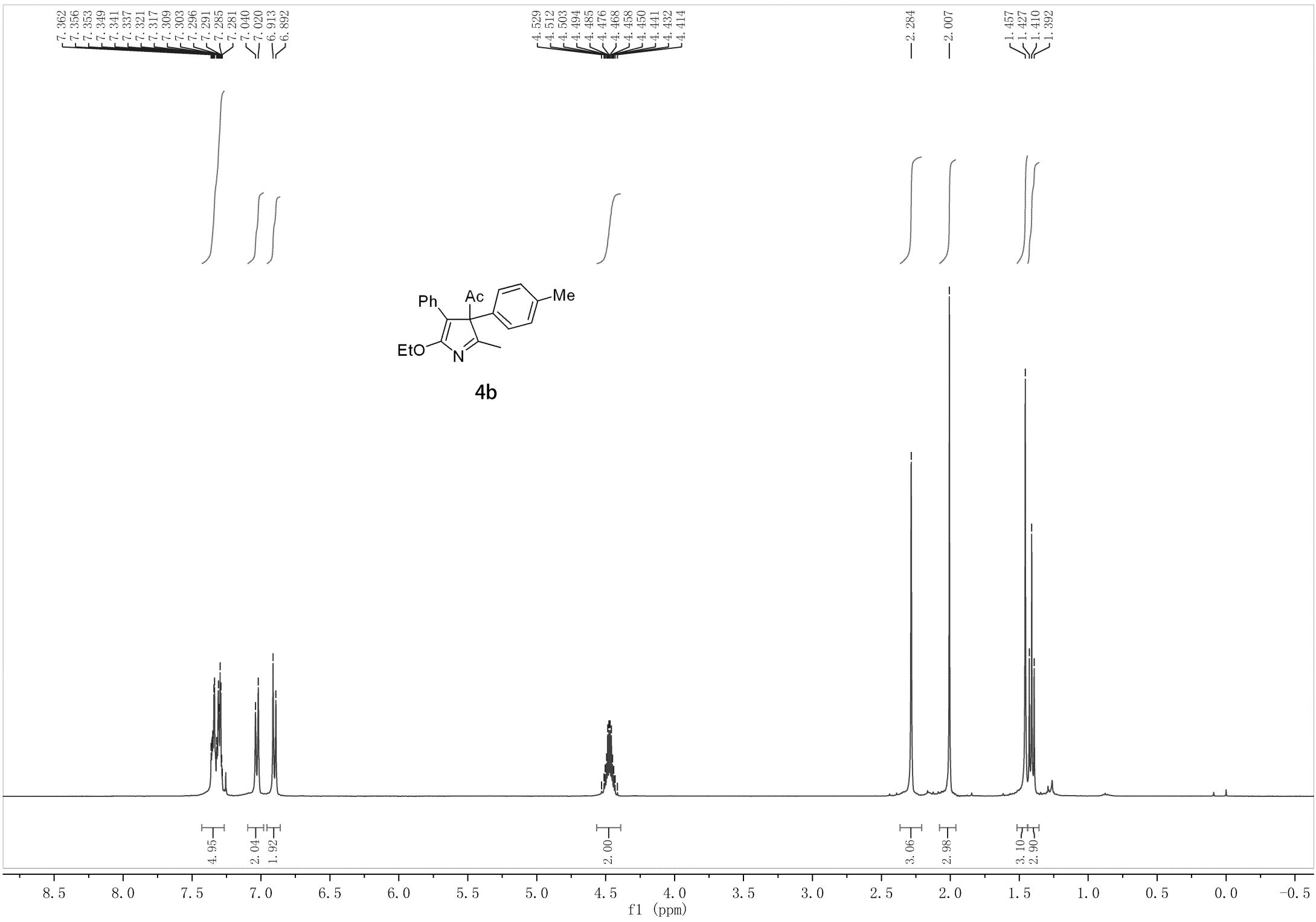


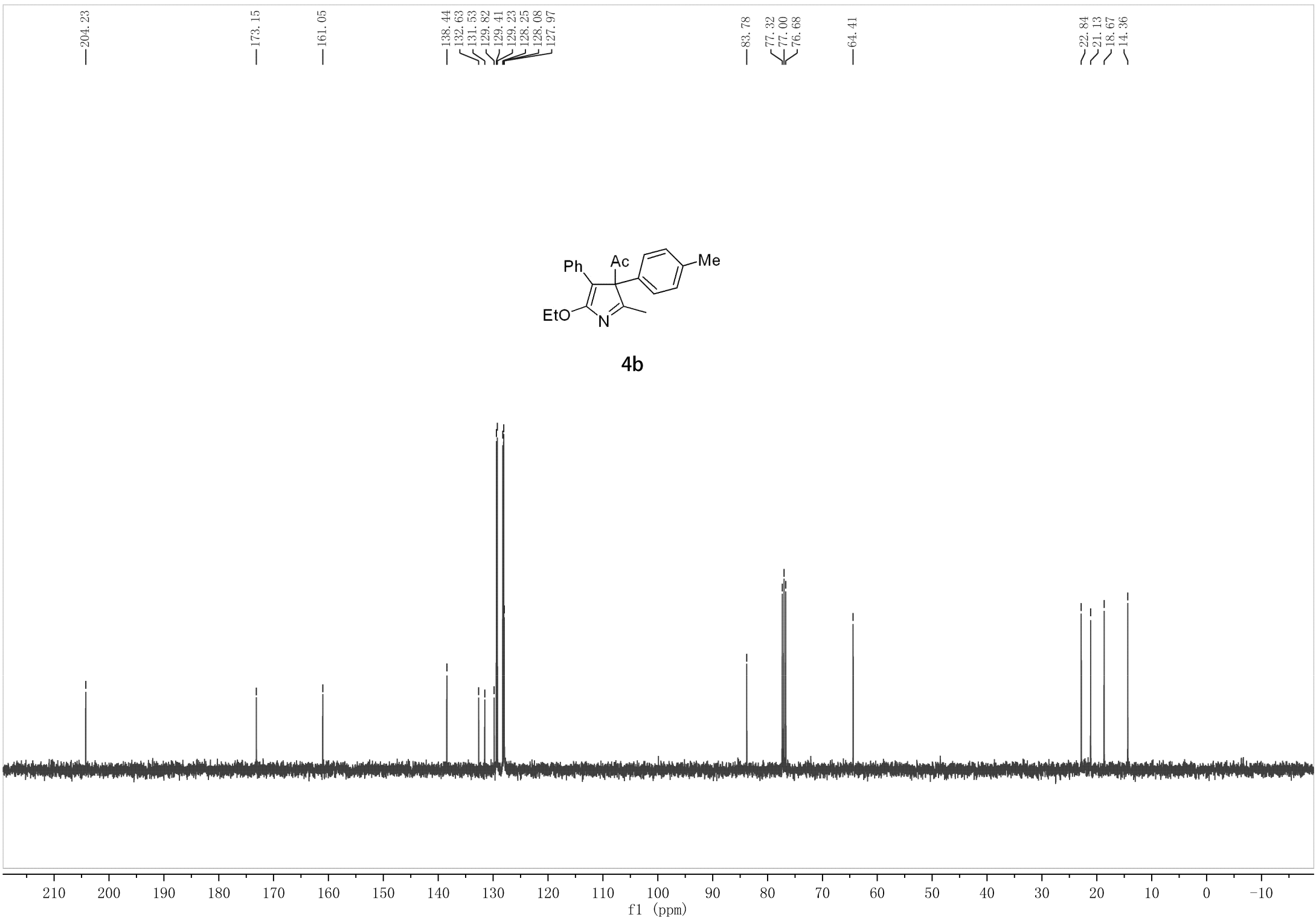


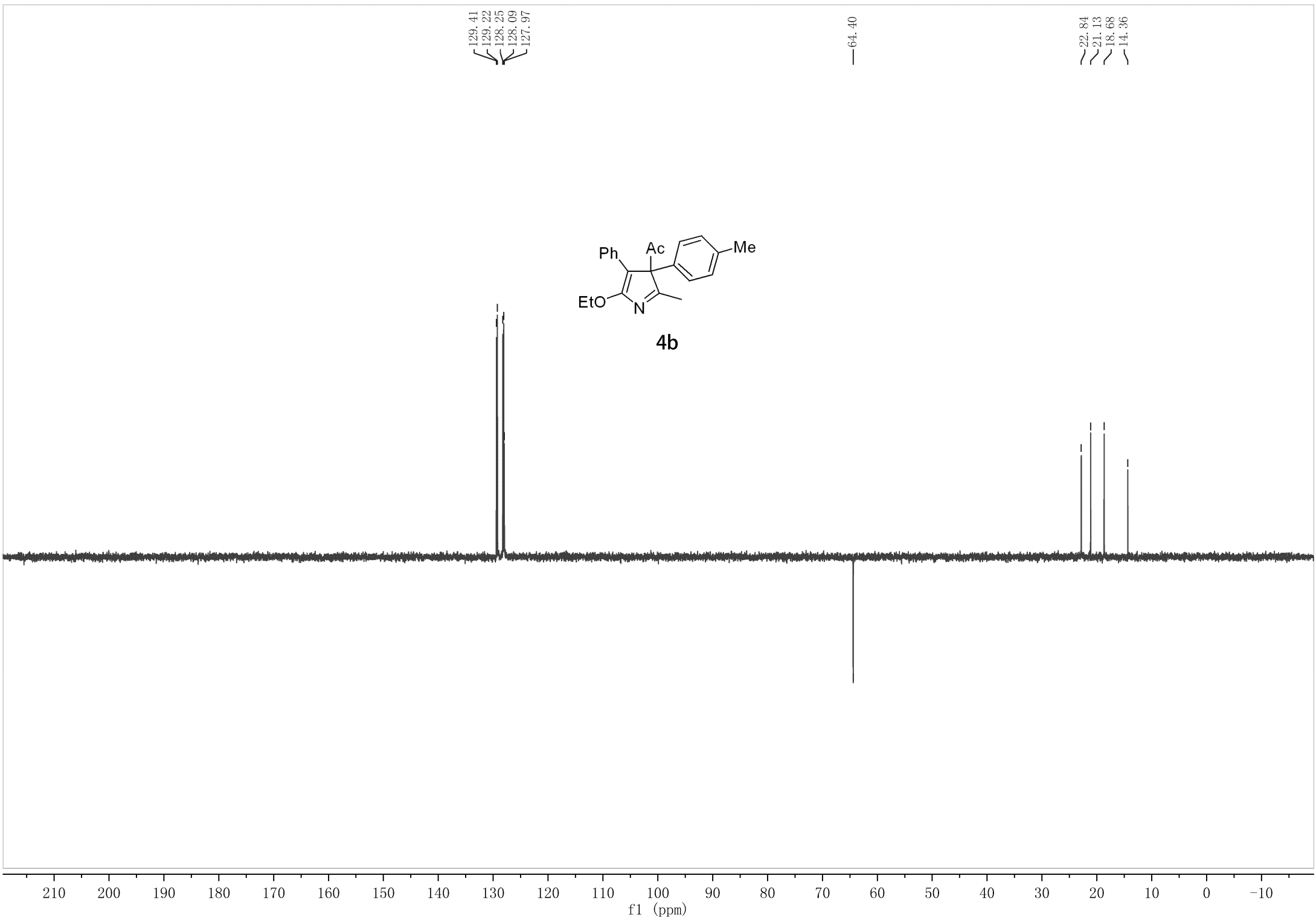


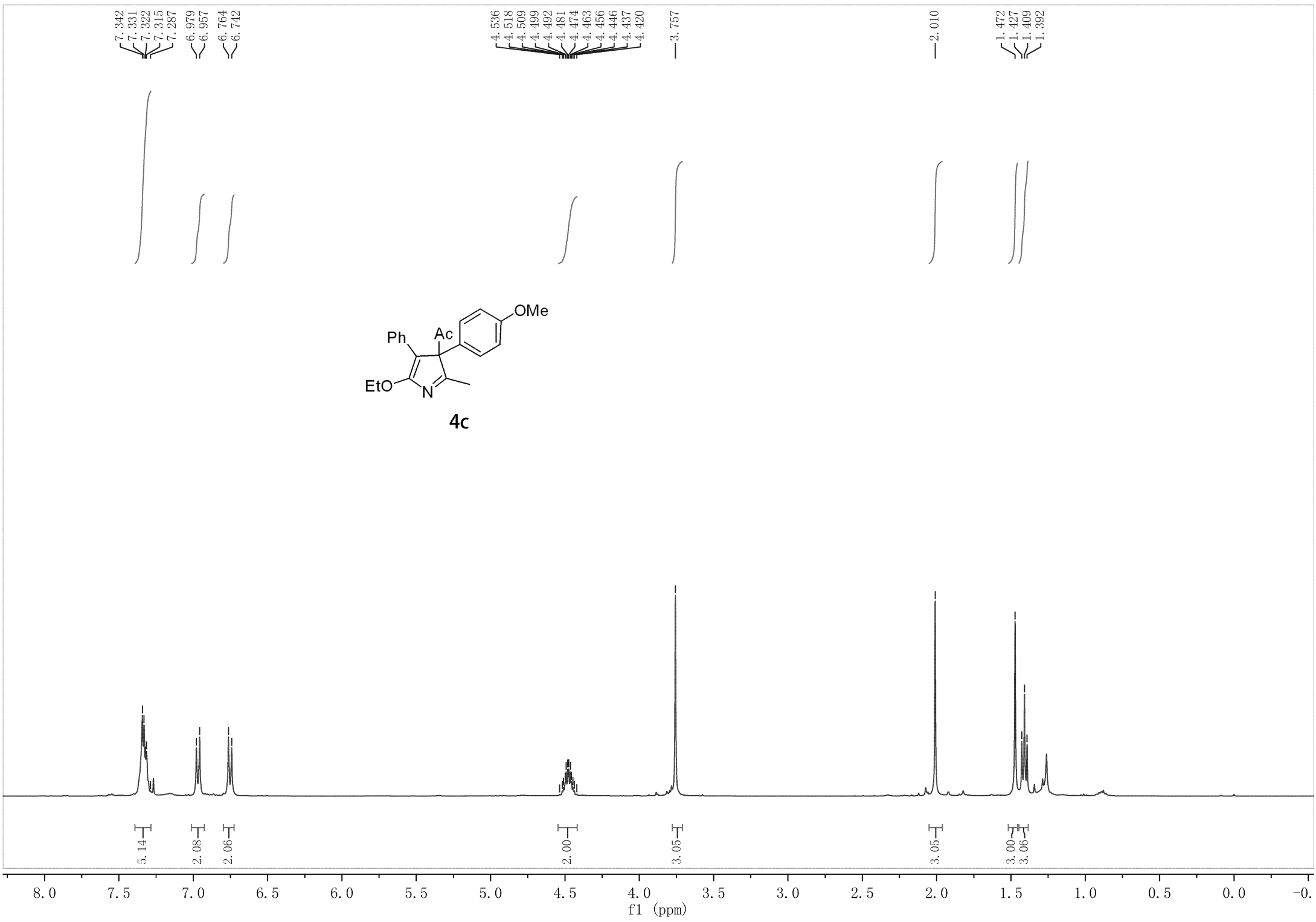


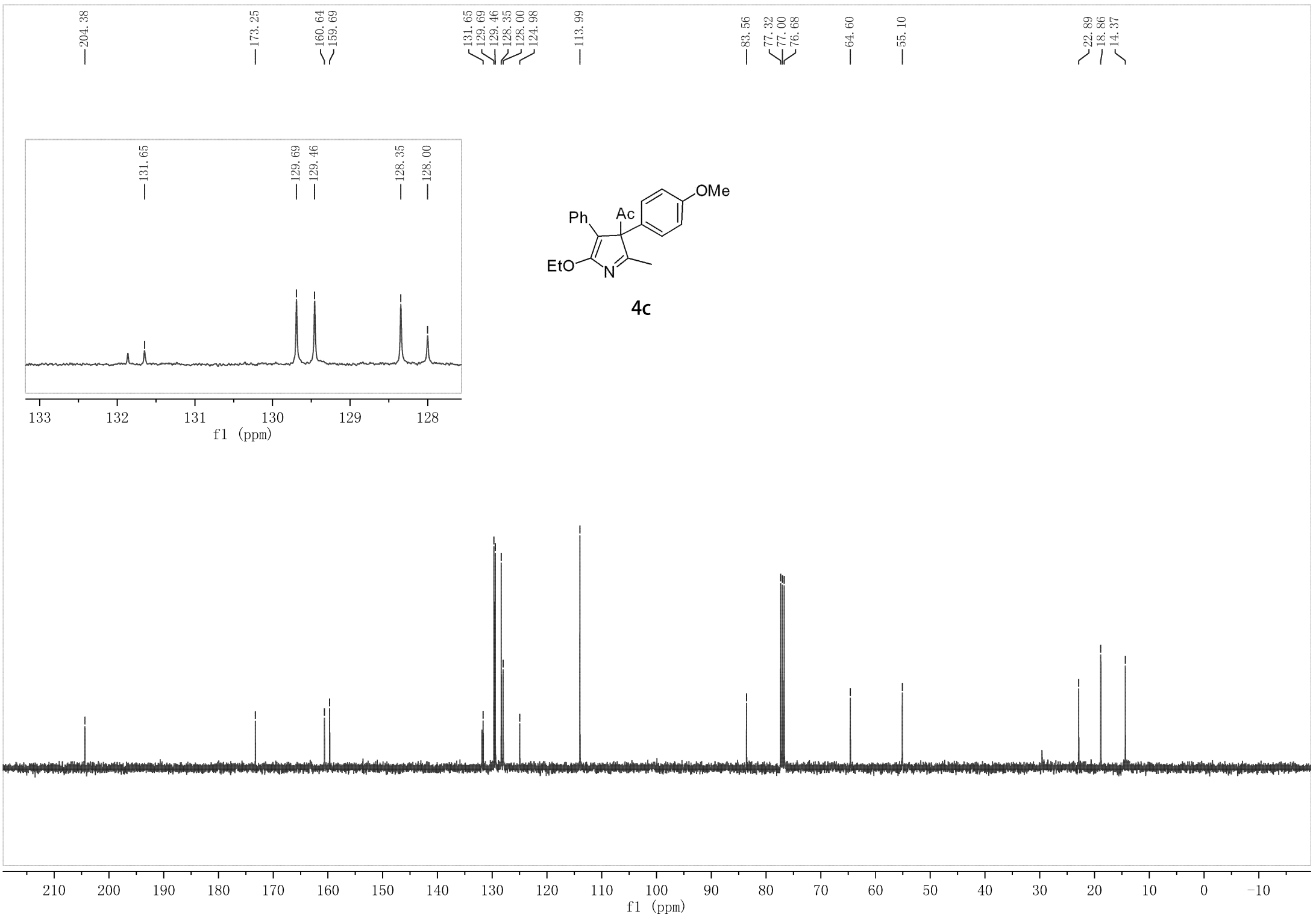










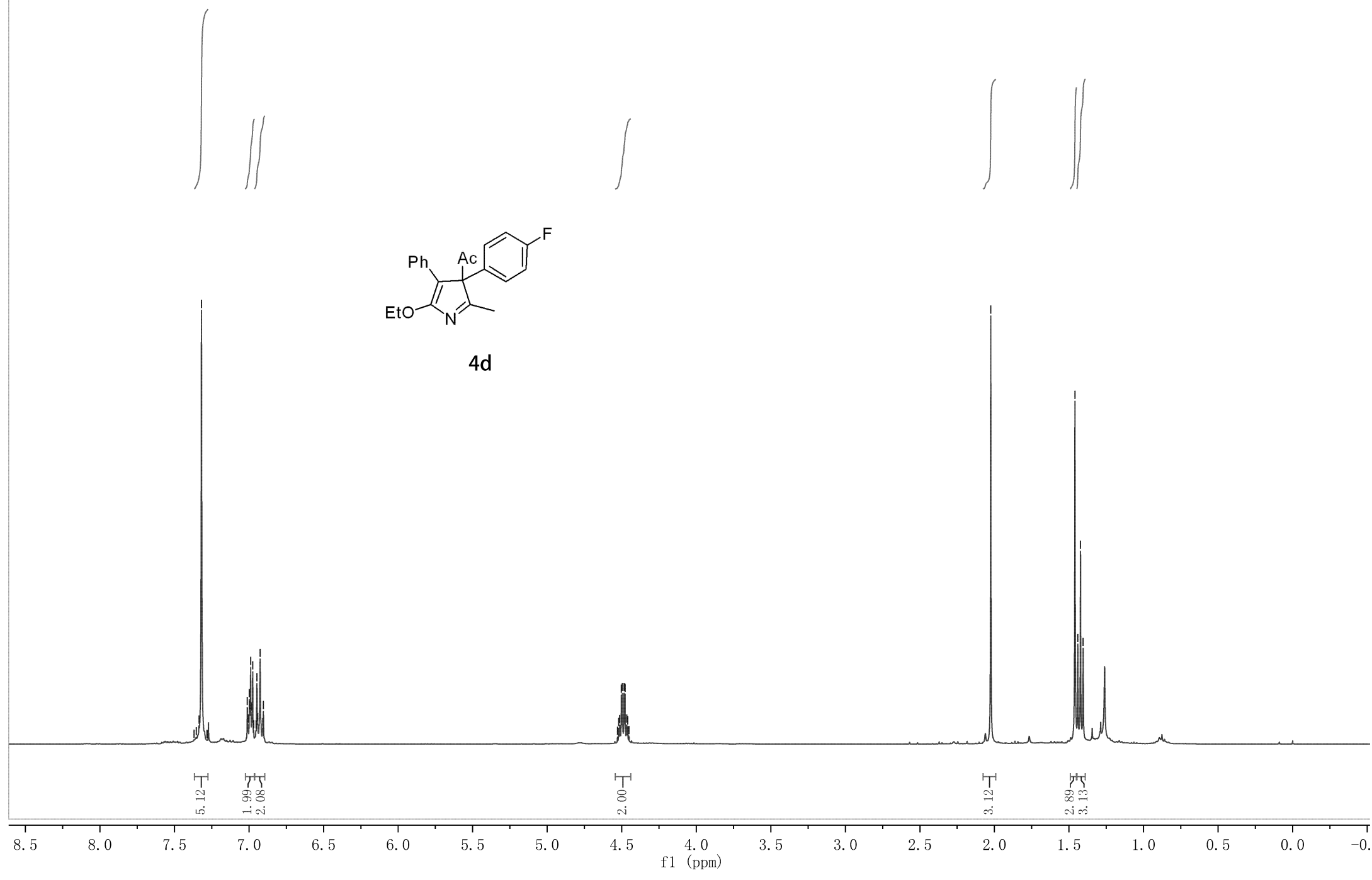
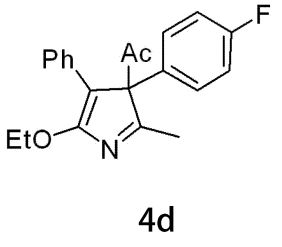


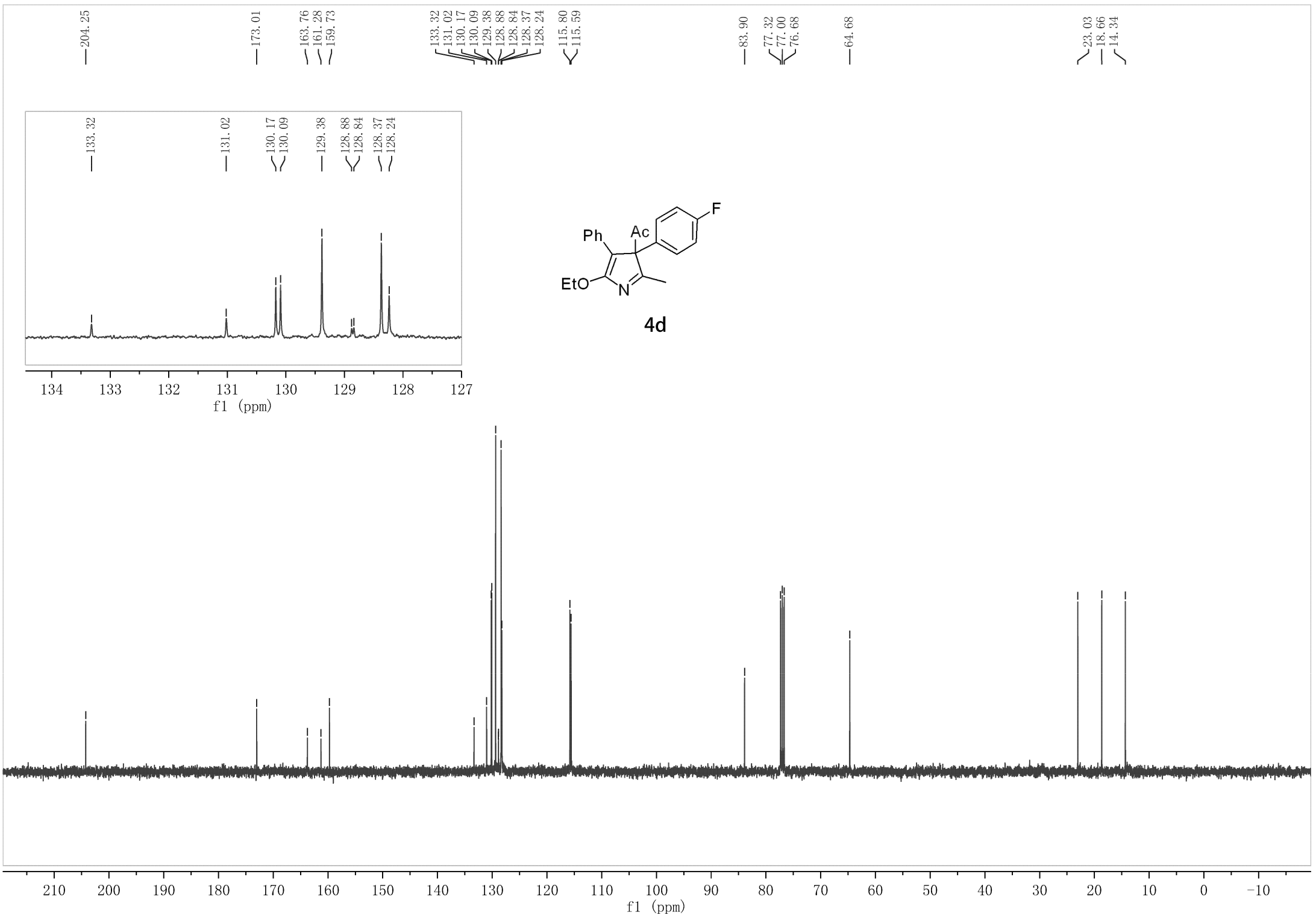
7.369
7.354
7.335
7.319
7.283
7.279
7.011
7.006
6.998
6.995
6.989
6.982
6.975
6.969
6.953
6.947
6.942
6.925
6.908
6.904

4.528
4.520
4.513
4.502
4.495
4.484
4.478
4.467
4.460
4.451

2.025

1.460
1.441
1.423
1.405



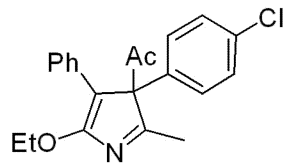


7.391
7.360
7.360
7.320
7.283
7.219
7.198
6.952
6.931

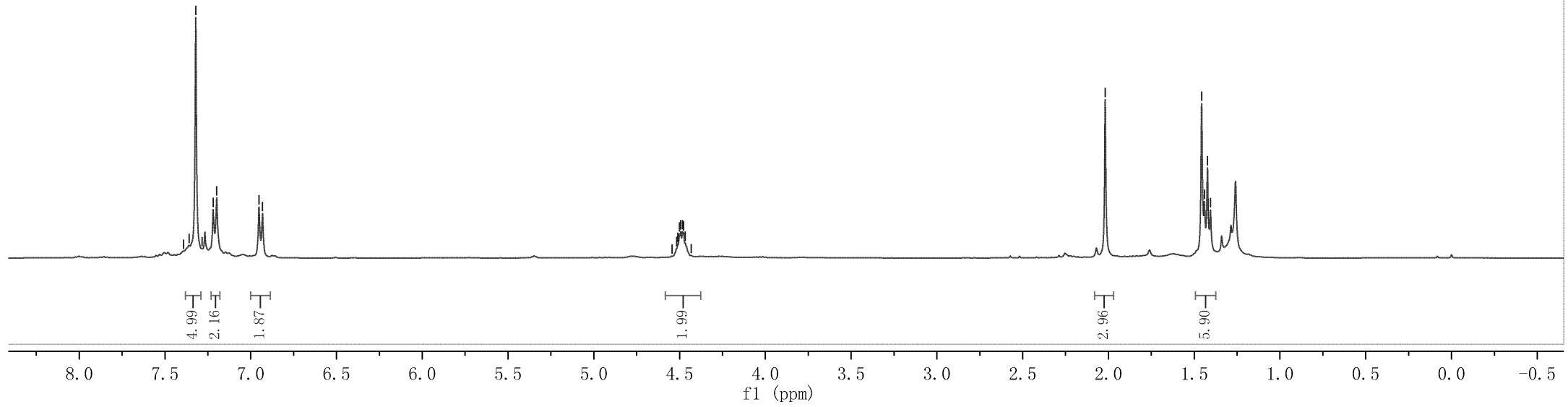
4.545
4.517
4.510
4.501
4.493
4.483
4.476
4.467
4.432

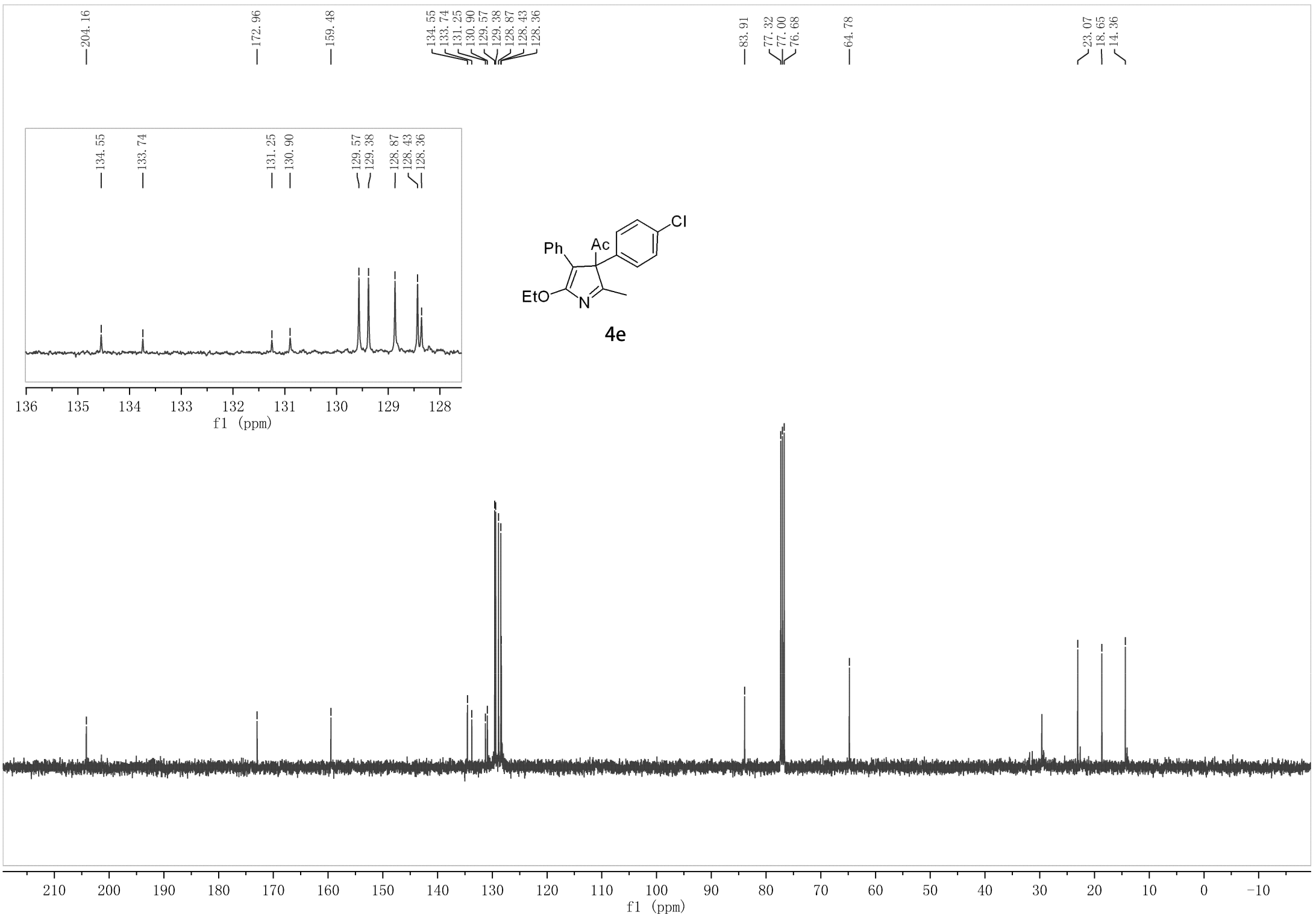
2.019

1.456
1.440
1.423
1.405



4e





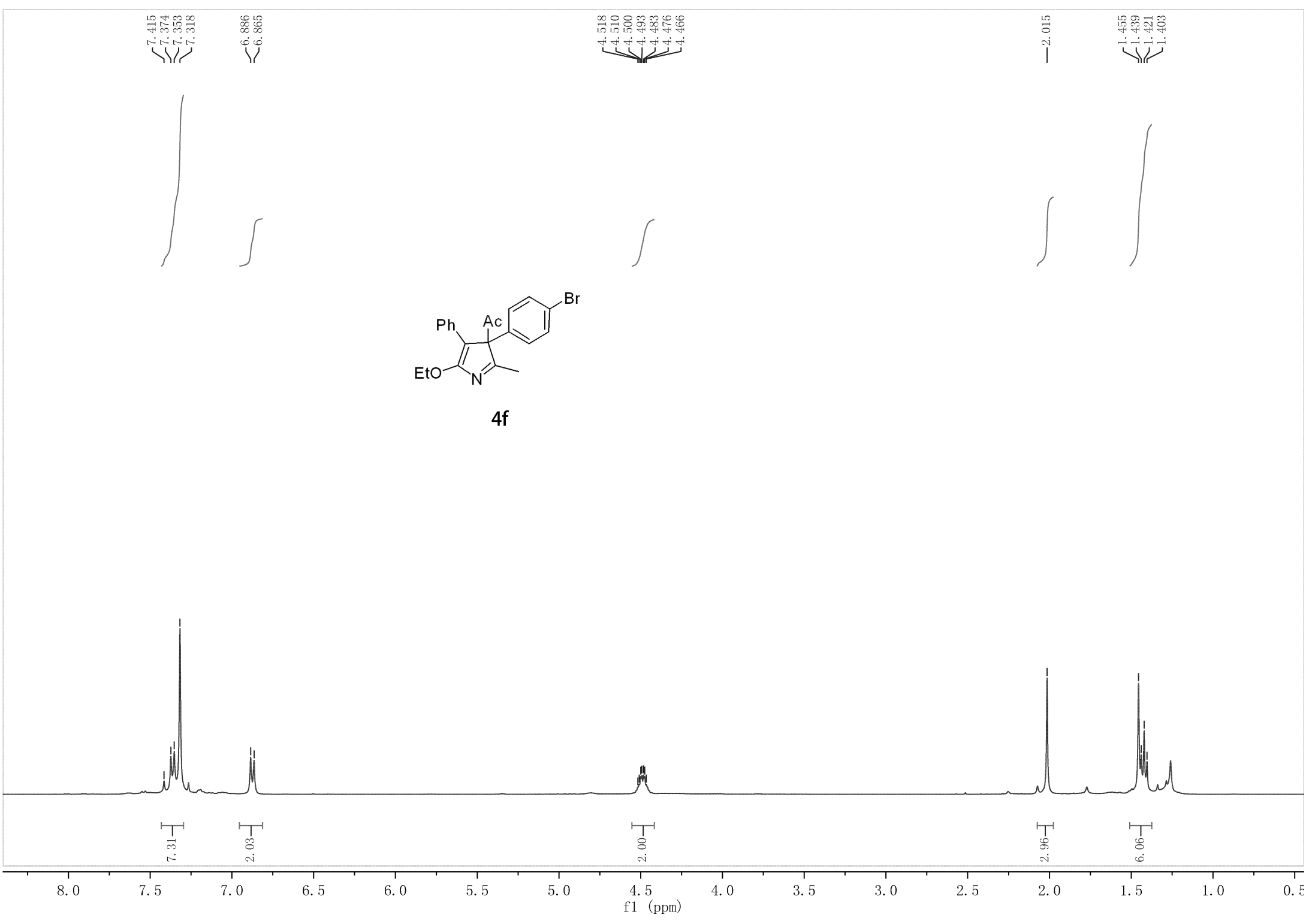
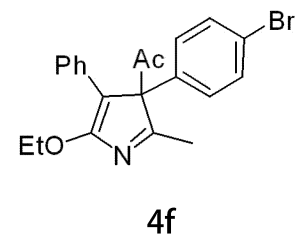
7.415
7.374
7.353
7.318

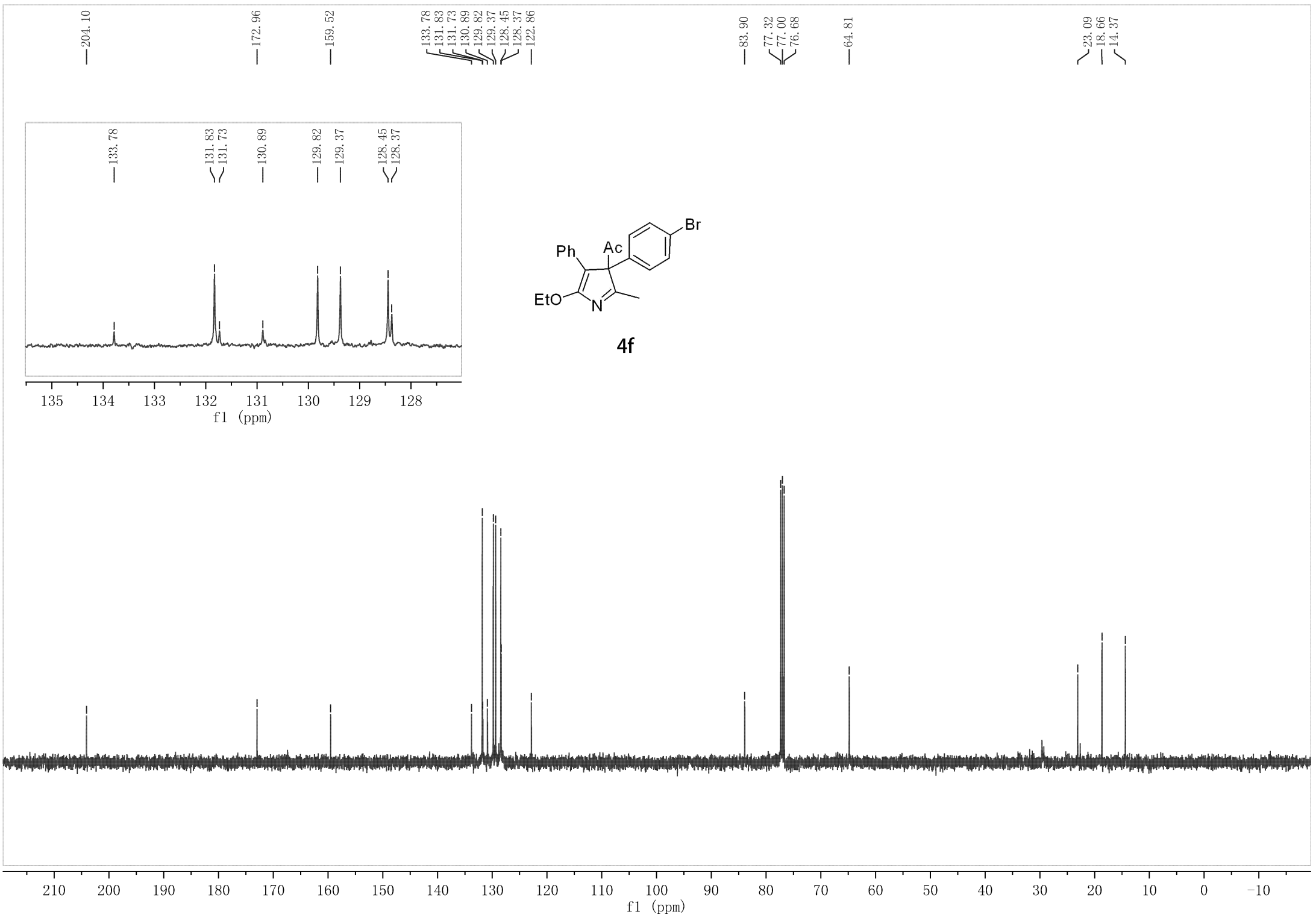
6.886
6.865

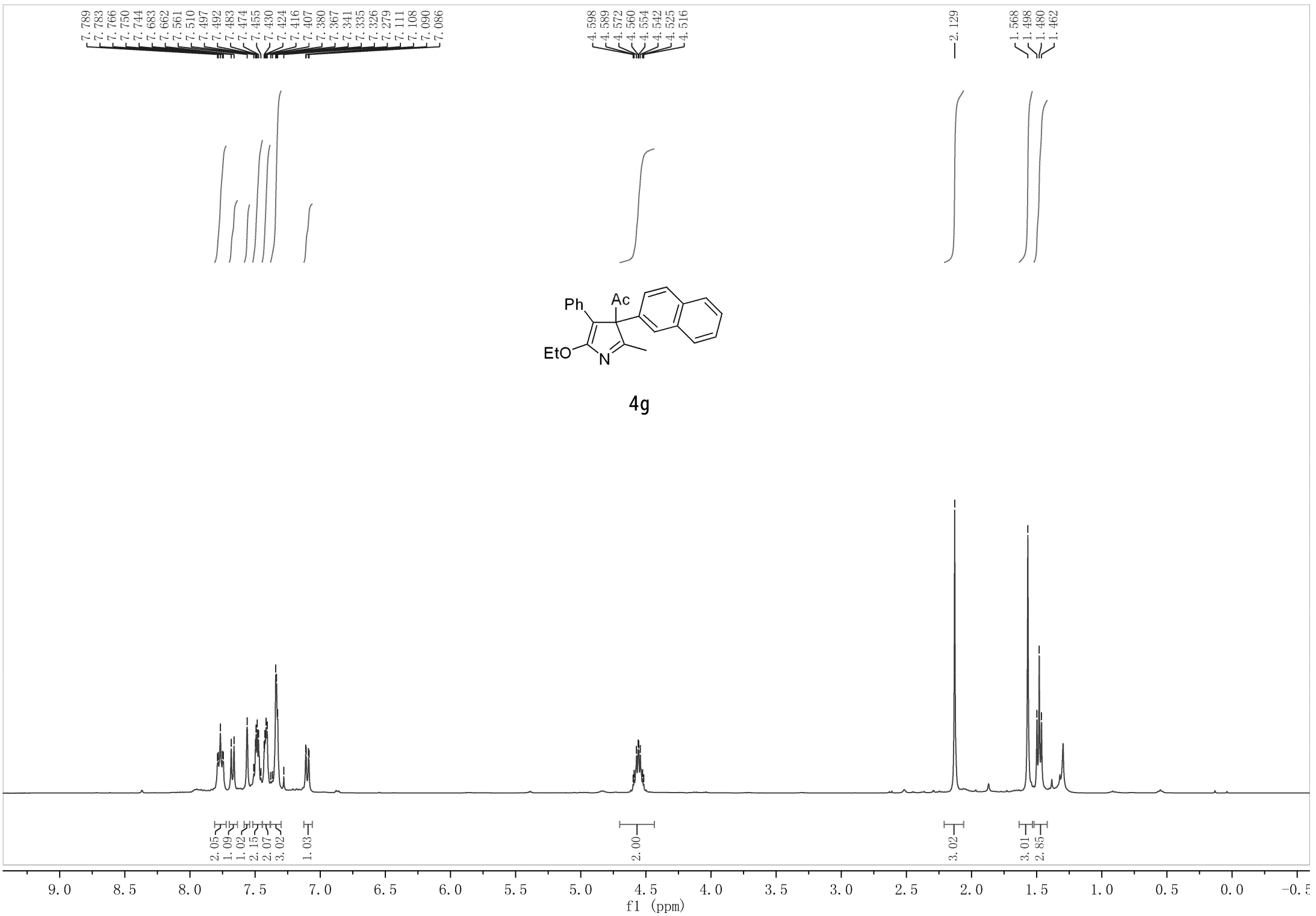
4.518
4.510
4.500
4.493
4.483
4.476
4.466

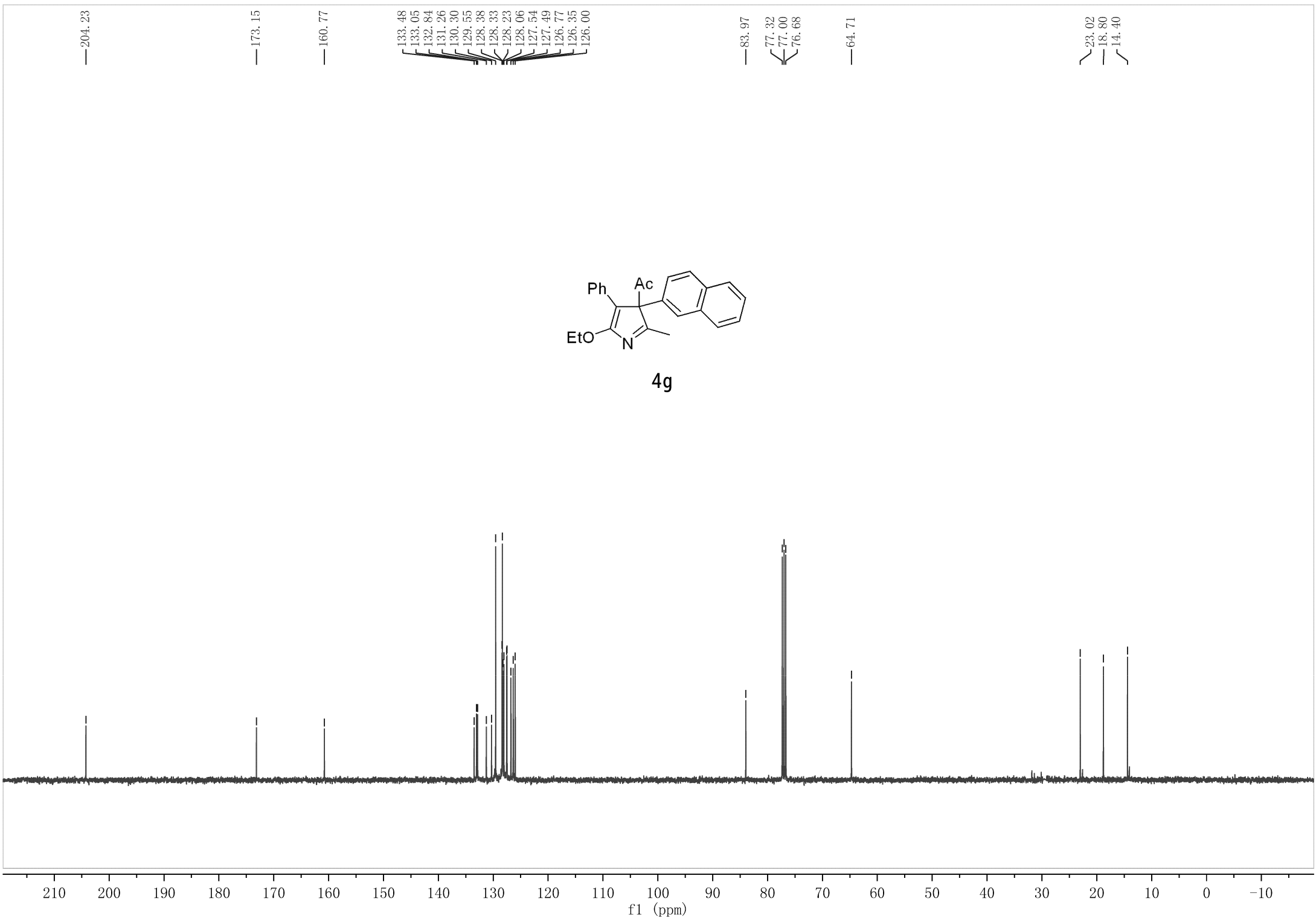
2.015

1.455
1.439
1.421
1.403







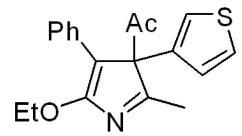
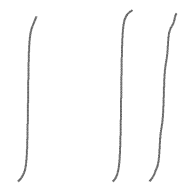
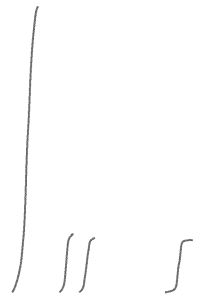


7.493
7.448
7.439
7.426
7.423
7.409
7.393
7.386
7.373

4.507
4.489
4.472
4.454

1.987

1.586
1.420
1.403
1.385



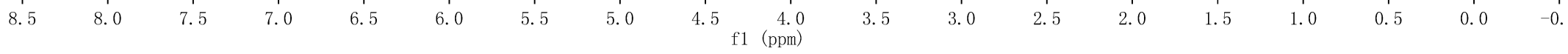
4h

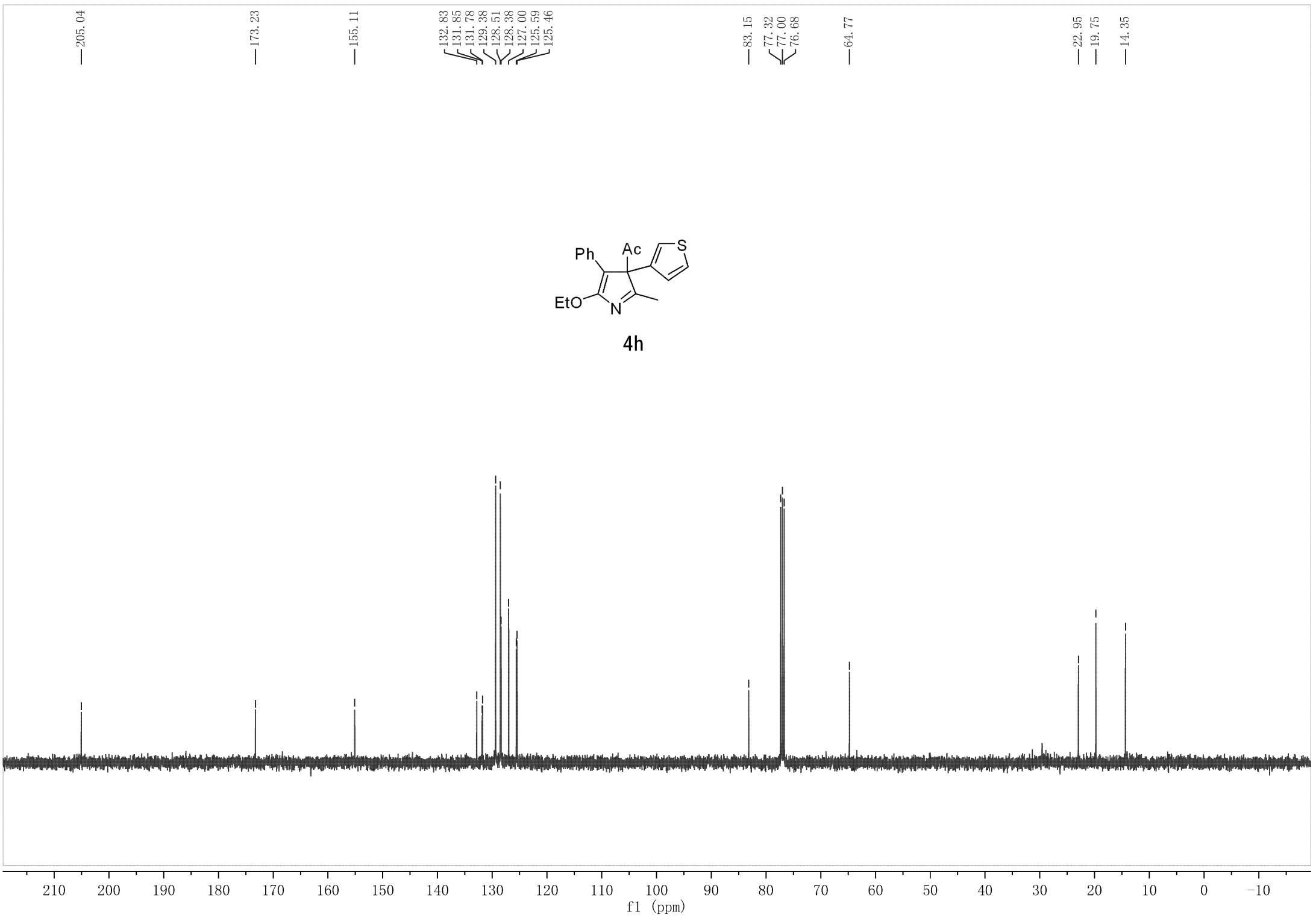
5.33
1.10
1.02
0.98

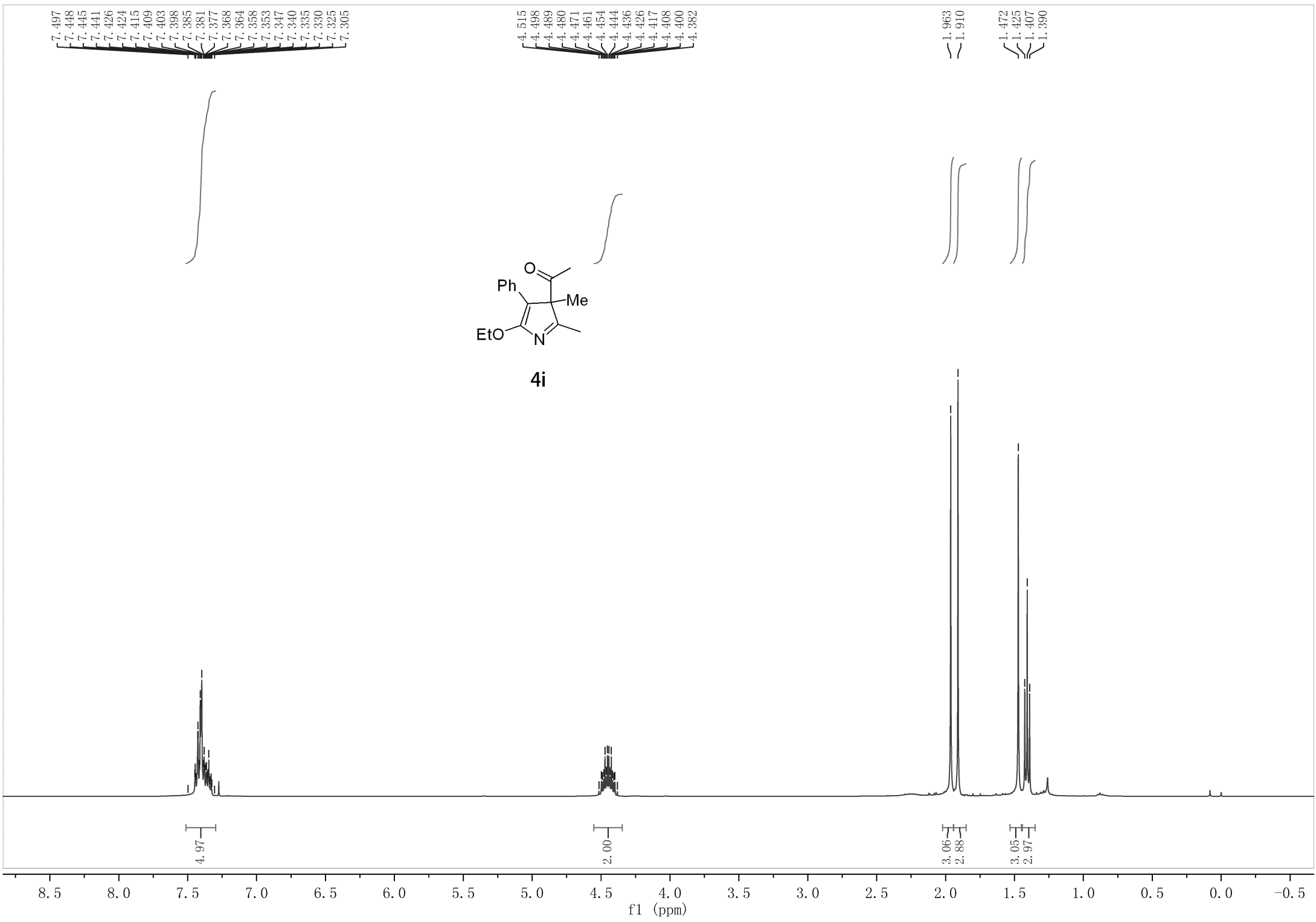
2.09

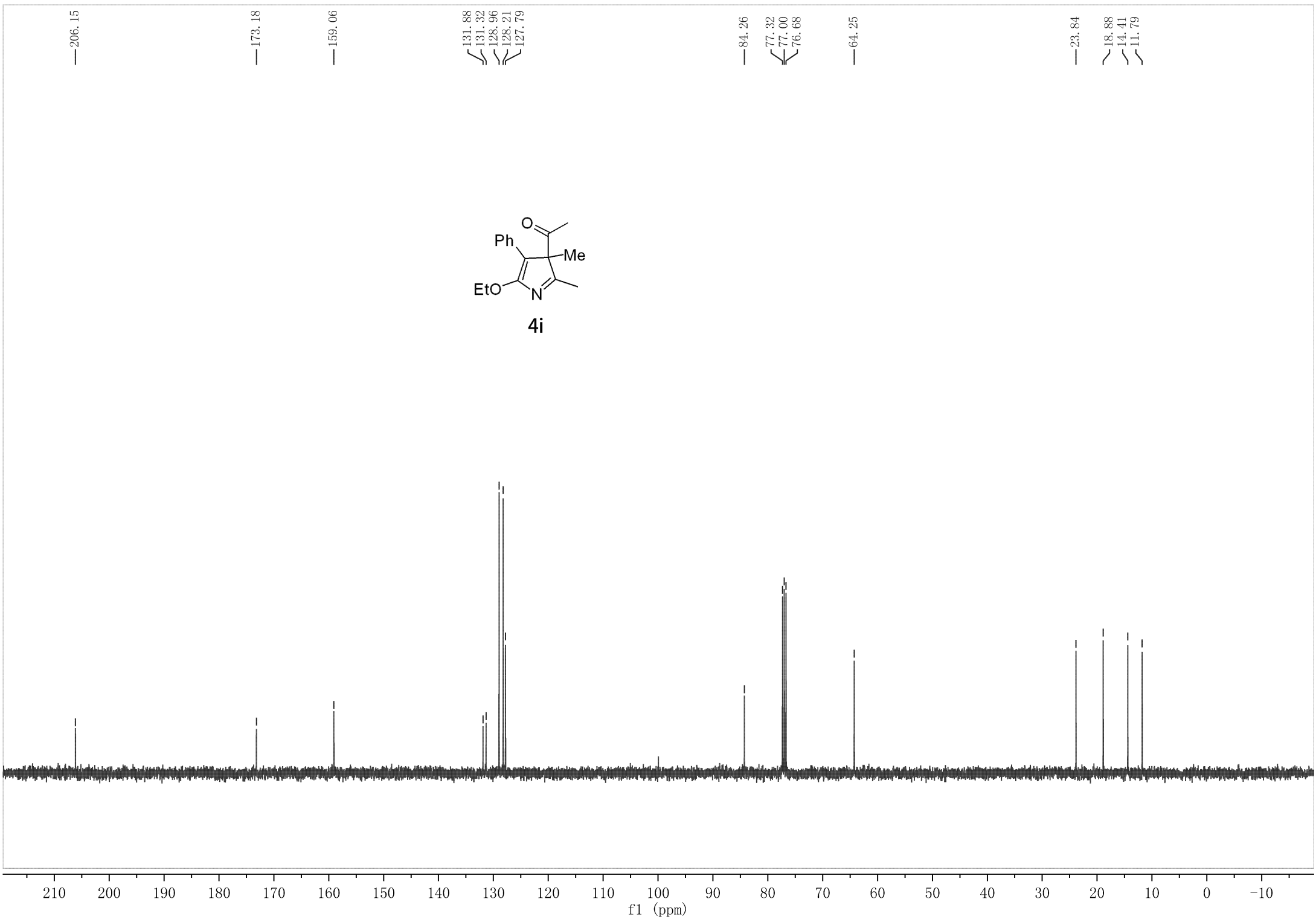
3.08

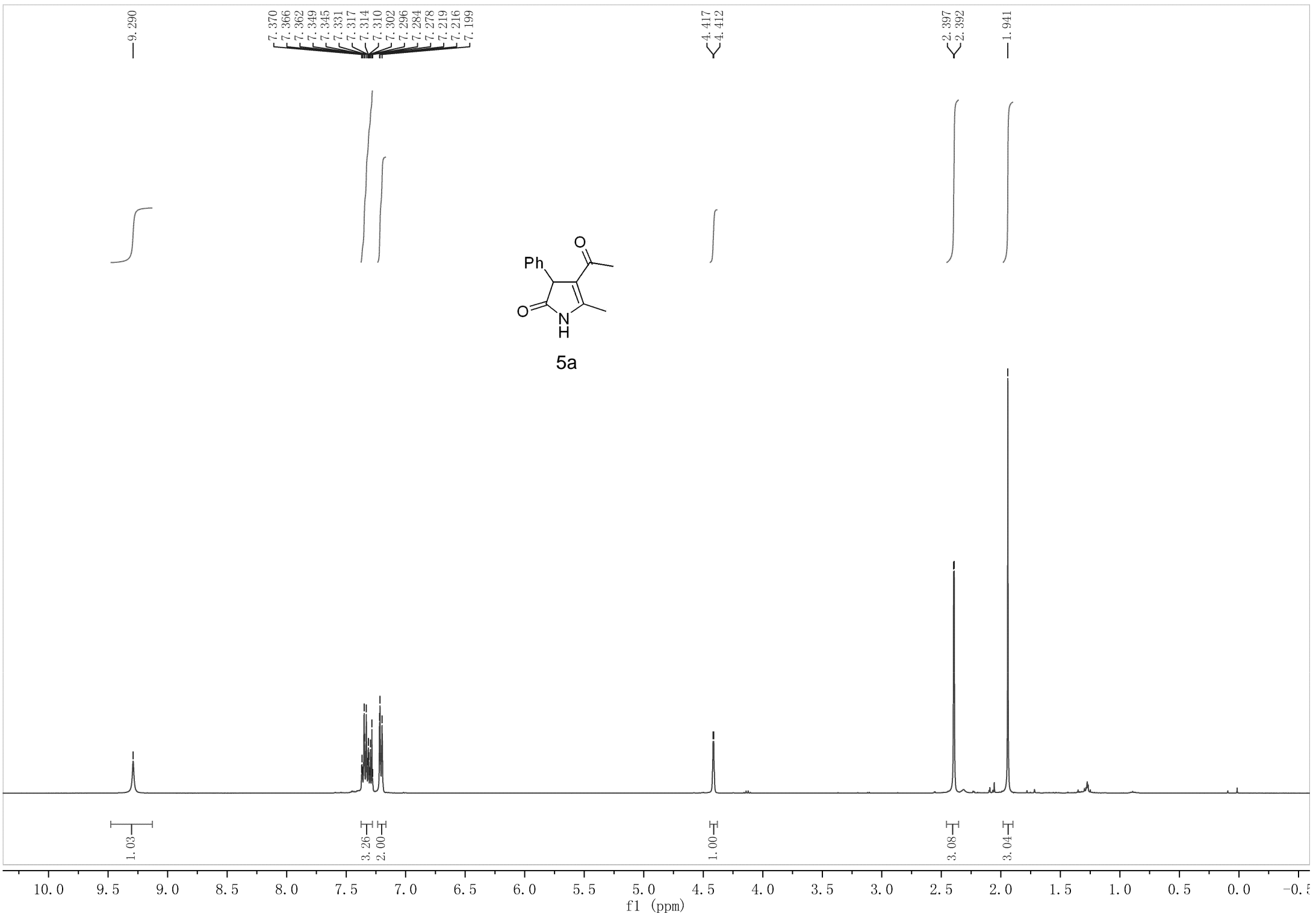
3.19
3.14

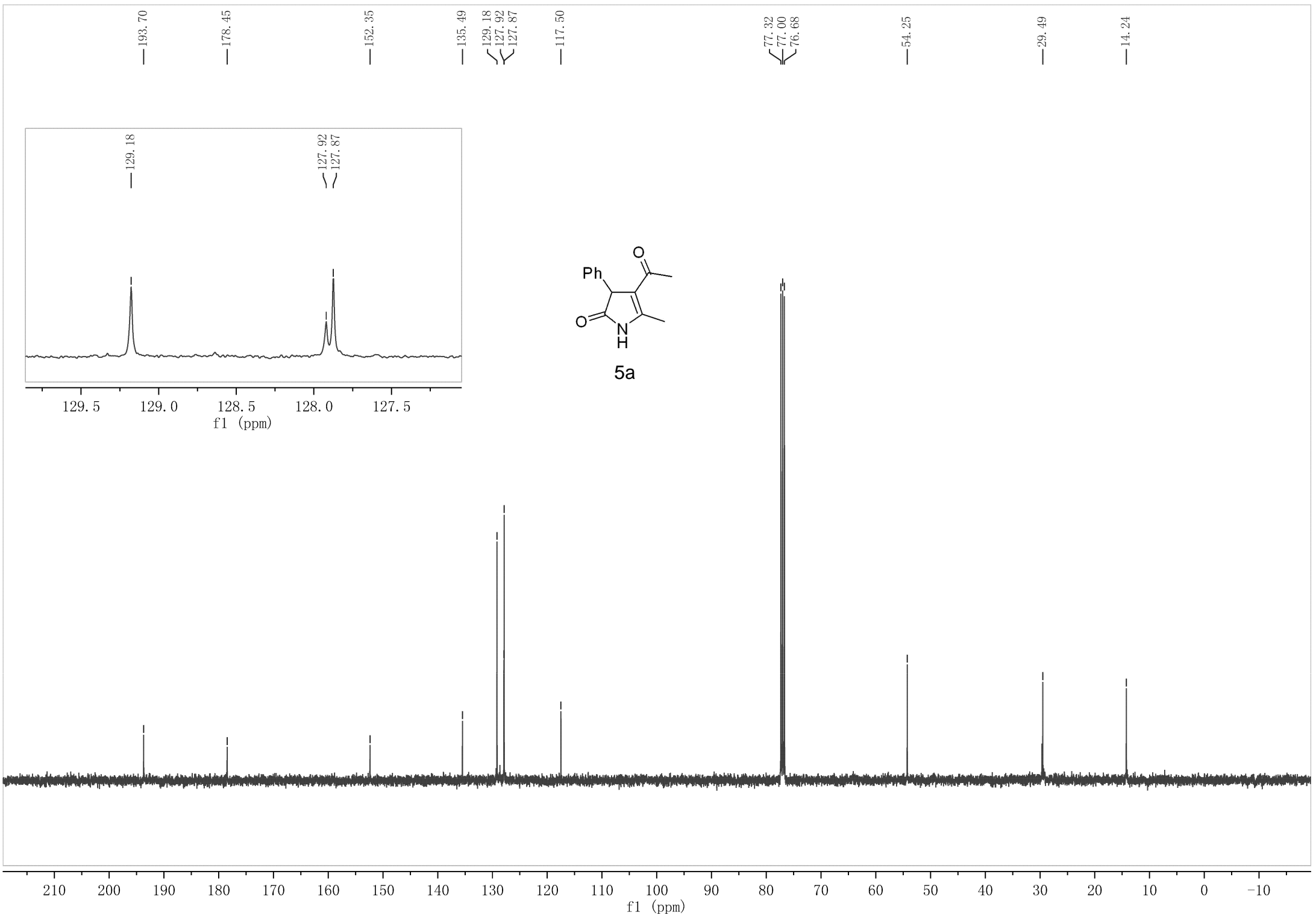








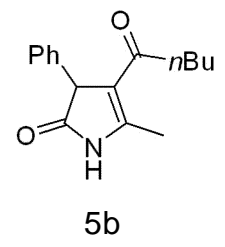




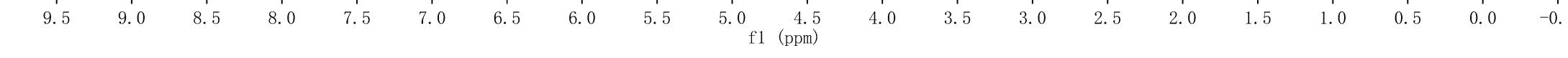
8.710
7.363
7.360
7.343
7.324
7.307
7.295
7.289
7.281
7.213
7.209
7.192

4.423
4.417

2.286
2.271
2.265
2.249
2.245
2.230
2.224
2.208
2.170
2.079
2.063
2.058
2.043
2.039
2.022
2.017
2.001
1.432
1.413
1.363
1.343
1.147
1.128
1.109
0.991
0.762
0.744
0.726



0.89
3.02
1.91
1.00
2.82
2.16
2.27
2.07
3.00



— 196.47 — 178.57 — 151.98 — 135.66 — 129.14 — 127.86 — 117.46 — 77.32 — 77.00 — 76.68 — 54.06 — 40.88 — 25.82 — 22.18 — 14.23 — 13.70

