Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Informations

$PhI(OAc)_2$-mediated C−N bond cleavage of acylhydrazines with amines for the synthesis of amides

Shun Yang,[a#] Haiying Tian,[b#] Ling Li,[a] Ying Wang,[a] Cong Xie,[a*] Xiuling Chen[a*]

[a]School of Nuclear Technology and Chemistry & Biology, Hubei University of Science and Technology, Xianning 437100, China
[b]Department of Pharmacy, Changzhi Medical College, 046000 Changzhi (P. R. China)
E-mail: cxl828800@163.com; Fax: (+) 86-715-8338007

Contents

1. General remarks

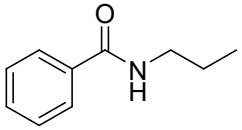
All non-aqueous reactions and manipulations were performed in oxygen atmosphere. The reactions were monitored by GC and GC-MS. The ^{1}H NMR and ^{13}C NMR spectra were recorded on a Brucker ADVANCE III spectrometer at 400 MHz and 100 MHz, respectively, and chemical shifts were reported in parts per million (ppm). Flash column chromatography was performed using silica gel 300-400 μm. GC-MS results were recorded on GC-MS QP2010, and GC analysis was performed on GC 7820A. Hydrazines were purchased from Energy Chemical, Alfa Aesar, Aladdin or Maya Reagent; amines were purchased from Aladdin, dried by standard methods before using.

2. General experimental procedure for the synthesis of amides

A 25 ml Schlenk-type tube equipped with a magnetic stir bar was charged with substrate **1** (**1a**-**1k**) (0.2 mmol), $PhI(OAc)_2$ (0.4 mmol), *n*-butyl ammonium iodide (0.4 mmol). The reaction tube was evacuated and back-filled with N_2. Amine **2** (**2a**-**2m**) (0.24 mmol) and CCl_4 (2 mL) were added at room temperature under N_2 atmosphere, then the reaction mixture was stirred at 130 ºC for 12 h. The reaction was monitored by GC or GC-MS. After completion of the reaction, the resulting solution was cooled to room temperature, and neutralized with saturated solution of NaCl. The product was extracted with EtOAc, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to give analytically pure product.

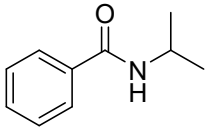
3. ^{1}H NMR and ^{13}C NMR data of products

N-propylbenzamide (**3a**)[1]



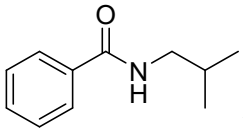
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, 2H, *J* = 6.8 Hz), 7.49 (t, 1H, *J* = 7.4 Hz), 7.42 (t, 2H, *J* = 7.6 Hz), 6.29 (s, br, 1H), 3.43 (q, 2H, *J* = 6.8 Hz), 1.59-1.69 (m, 2H), 0.98 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 134.9, 131.3, 128.5, 126.9, 41.8, 22.9, 11.4. GC-MS: m/z = 163.09.

N-isopropylbenzamide (**3b**)[1]



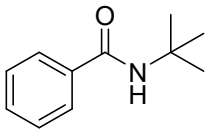
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, 2H, *J* = 7.2 Hz), 7.47 (d, 1H, *J* = 7.2 Hz), 7.41 (d, 2H, *J* = 7.2 Hz), 6.06 (s, br, 1H), 4.24-4.33 (m, 1H), 1.25 (d, 6H, *J* = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 134.9, 131.3, 128.5, 126.9, 41.8, 22.9, 11.4. GC-MS: m/z = 163.09.

N-isobutylbenzamide (**3c**)[1]



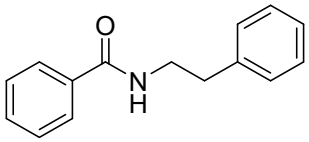
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, 2H, *J* = 6.8 Hz), 7.49 (d, 1H, *J* = 7.4 Hz), 7.42 (d, 2H, *J* = 7.2 Hz), 6.32 (s, br, 1H), 3.28 (d, 2H, *J* = 6.4 Hz), 1.86-1.94 (m, 1H), 0.97 (d, 6H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 134.9, 131.3, 128.6, 126.9, 47.4, 28.6, 20.2. GC-MS: m/z = 177.11.

N-(*tert*-butyl)benzamide (**3d**)[3]



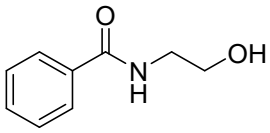
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, 2H, *J* = 6.8 Hz), 7.47 (d, 1H, *J* = 7.2 Hz), 7.41 (d, 2H, *J* = 7.4 Hz), 5.94 (s, br, 1H), 1.47 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 134.9, 131.3, 128.6, 126.9, 47.4, 28.6, 20.2. GC-MS: m/z = 177.11.

N-phenethylbenzamide (**3e**)[1]



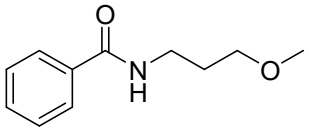
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, 2H, *J* = 8.0 Hz), 7.47 (t, 1H, *J* = 7.4 Hz), 7.39 (t, 2H, *J* = 7.4 Hz), 7.32 (t, 2H, *J* = 7.4 Hz), 7.24 (t, 3H, *J* = 6.2 Hz), 6.22 (s, br, 1H), 3.37 (q, 2H, *J* = 6.6 Hz), 2.93 (t, 2H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.5, 138.9, 134.7, 131.4, 128.8, 128.7, 128.6, 126.8, 126.6, 41.2, 35.7. GC-MS: m/z = 225.11.

N-(2-hydroxyethyl)benzamide (**3f**)



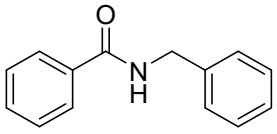
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, 2H, *J* = 8.4 Hz), 7.53 (t, 1H, *J* = 6.8 Hz), 7.45 (t, 2H, *J* = 7.4 Hz), 6.58 (s, br, 1H), 3.81 (t, 2H, *J* = 5.8 Hz), 3.75 (t, 2H, *J* = 5.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 134.1, 131.7, 128.7, 126.9, 44.2, 41.7. HRMS (EI): calcd for C9H11NO2: 165.0790; found: 165.0754.

N-(3-methoxypropyl)benzamide (**3g**)



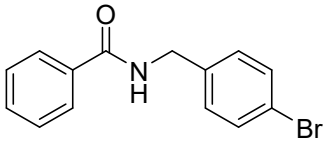
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, 2H, *J* = 6.8 Hz), 7.48 (t, 1H, *J* = 7.2 Hz), 7.45 (t, 2H, *J* = 7.2 Hz), 6.99 (s, br, 1H), 3.54-3.59 (m, 4H), 3.38 (s, 3H), 1.86-1.92 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.3, 134.8, 131.2, 128.5, 126.8, 72.2, 58.9, 38.9, 28.9. HRMS (EI): calcd for C11H15NO2: 193.1103; found: 193.1122.

N-benzylbenzamide (**3h**)[2]



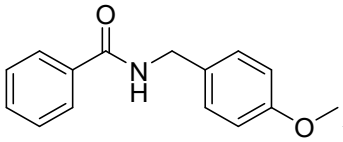
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, 2H, *J* = 7.2 Hz), 7.48 (t, 1H, *J* = 7.2 Hz), 7.40 (t, 2H, *J* = 7.2 Hz), 7.29-7.34 (m, 5H), 6.60 (s, br, 1H), 4.61 (d, 2H, *J* = 5.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.4, 138.2, 134.4, 131.6, 128.8, 128.6, 127.9, 127.6, 126.9, 44.2. GC-MS: m/z = 211.09.

N-(4-bromobenzyl)benzamide (**3i**)[2]



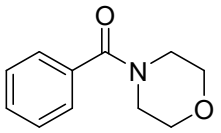
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, 2H, *J* = 7.2 Hz), 7.41-7.52 (m, 5H), 7.23 (d, 2H, *J* = 8.4 Hz), 6.53 (s, br, 1H), 4.58 (d, 2H, *J* = 6.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.4, 137.3, 134.2, 131.8, 131.7, 129.6, 128.7, 126.9, 121.5, 43.3. GC-MS: m/z = 289.01.

N-(4-methoxybenzyl)benzamide (**3j**)[2]



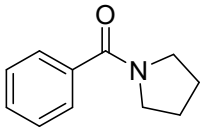
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, 2H, *J* = 7.2 Hz), 7.49 (t, 1H, *J* = 7.4 Hz), 7.42 (t, 2H, *J* = 7.4 Hz), 7.28 (d, 3H, *J* = 8.4 Hz), 6.88 (d, 2H, *J* = 8.8 Hz), 6.33 (s, br, 1H), 4.57 (d, 2H, *J* = 5.2 Hz), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.4, 137.3, 134.2, 131.8, 131.7, 129.6, 128.7, 126.9, 121.5, 43.3. GC-MS: m/z = 241.11.

morpholino(phenyl)methanone (**3k**)[3]



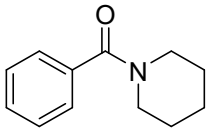
Eluent: petroleum ether/ethyl acetate (5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39-7.43 (m, 5H), 3.75 (s, br, 4H), 3.46 (s, br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.5, 135.3, 129.9, 128.6, 127.1, 66.9, 51.9, 46.5. GC-MS: m/z = 191.09.

phenyl(pyrrolidin-1-yl)methanone (**3l**)[3]



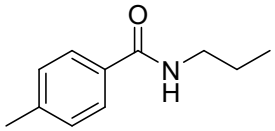
Eluent: petroleum ether/ethyl acetate (5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50-7.53 (m, 2H), 7.39-7.40 (m, 3H), 3.65 (t, 2H, *J* = 7.0 Hz), 3.42 (t, 2H, *J* = 6.6 Hz), 1.93-1.99 (m, 2H),1.86-1.90 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.7, 137.3, 129.8, 128.2, 127.1, 49.6, 46.2, 26.4, 24.5. GC-MS: m/z = 175.09.

phenyl(piperidin-1-yl)methanone (**3m**)[3]



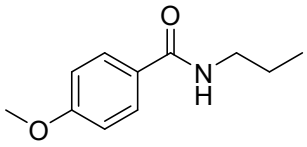
Eluent: petroleum ether/ethyl acetate (5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 (s, 5H), 3.71 (s, br, 2H), 1.68 (s, br, 4H), 1.56 (s, br, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.3, 136.5, 129.4, 128.4, 126.8, 47.9, 25.8, 24.6.GC-MS: m/z = 189.11.

4-methyl-*N*-propylbenzamide (**3n**)[1]



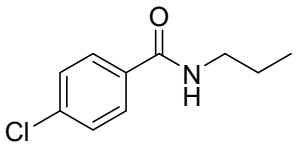
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, 2H, *J* = 8.0 Hz), 7.21 (d, 2H, *J* = 8.0 Hz), 6.10 (s, br, 1H), 3.43 (q, 2H, *J* = 7.0 Hz), 2.39 (s, 3H), 1.59-1.68 (m, 2H), 0.98 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.5, 141.7, 132.1, 129.2, 126.8, 41.7, 22.9, 21.4, 11.4. GC-MS: m/z = 177.11.

4-methoxy-*N*-propylbenzamide (**3o**)[1]



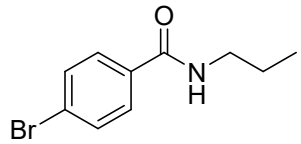
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, 2H, *J* = 8.8 Hz), 6.89 (d, 2H, *J* = 8.8 Hz), 6.17 (s, br, 1H), 3.84 (s, 3H), 3.43 (q, 2H, *J* = 6.8 Hz), 1.58-1.67 (m, 2H), 0.98 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 162.0, 128.6, 127.2, 113.7, 55.4, 41.7, 22.9, 11.4. GC-MS: m/z = 193.11.

4-chloro-*N*-propylbenzamide (**3p**)[1]



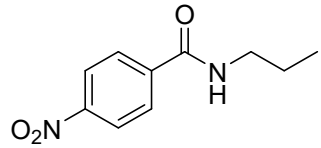
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, 2H, *J* = 6.8 Hz), 7.39 (d, 2H, *J* = 8.4 Hz), 6.12 (s, br, 1H), 3.43 (q, 2H, *J* = 6.4 Hz), 1.59-1.69 (m, 2H), 0.98 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.5, 137.6, 133.2, 128.8, 128.3, 41.9, 22.9, 11.4. GC-MS: m/z = 197.06.

4-bromo-*N*-propylbenzamide (**3q**)[1]



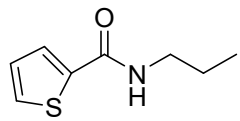
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, 2H, *J* = 8.8 Hz), 7.55 (d, 2H, *J* = 8.4 Hz), 6.16 (s, br, 1H), 3.42 (q, 2H, *J* = 6.4 Hz), 1.59-1.68 (m, 2H), 0.98 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.6, 133.7, 131.8, 128.5, 125.9, 41.8, 22.9, 11.4. GC-MS: m/z = 241.01.

4-nitro-*N*-propylbenzamide (**3r**)[1]



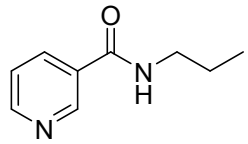
Eluent: petroleum ether/ethyl acetate (2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.27 (d, 2H, *J* = 8.8 Hz), 7.92 (d, 2H, *J* = 8.8 Hz), 6.25 (s, br, H), 3.44 (q, 2H, *J* = 6.4 Hz), 1.63-1.72 (m, 2H), 1.00 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.5, 149.6, 140.4, 128.1, 123.8, 42.1, 22.8, 11.4. GC-MS: m/z = 208.08.

N-propylthiophene-2-carboxamide (**3s**)[4]



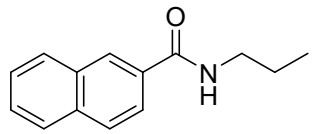
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 (dd, 1H, *J* = 1.2 Hz, *J* = 1.2 Hz), 7.44 (dd, 1H, *J* = 1.2 Hz, *J* = 1.2 Hz), 7.06 (dd, 1H, *J* = 3.6 Hz, *J* = 3.6 Hz), 6.06 (s, br, 1H), 3.44 (q, 2H, *J* = 7.2 Hz), 1.59-1.69 (m, 2H), 0.98 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.9, 139.2, 129.6, 127.8, 127.6, 41.7, 22.9, 11.4. GC-MS: m/z = 169.05.

N-propylnicotinamide (**3t**)[4]



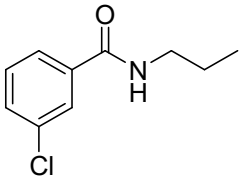
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.53 (d, 1H, *J* = 4.8 Hz), 8.19 (d, 1H, *J* = 6.8 Hz), 8.12 (s, br, 1H), 7.83 (t, 1H, *J* = 7.6 Hz), 7.40 (t, 1H, *J* = 6.4 Hz), 3.44 (q, 2H, *J* = 7.0 Hz), 1.62-1.71 (m, 2H), 0.98 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.2, 150.1, 147.9, 137.2, 125.9, 122.1, 41.1, 22.9, 11.4. GC-MS: m/z = 164.09.

N-propyl-2-naphthamide (**3u**)[1]



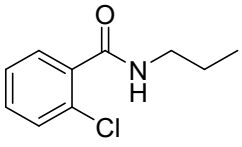
Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, 3H, *J* = 8.0 Hz), 7.96 (s, 1H), 7.51-7.54 (m, 2H), 7.46 (t, 1H, *J* =8.4 Hz), 6.17 (s, br, 1H), 3.42 (q, 2H, *J* = 7.2 Hz), 1.59-1.69 (m, 2H), 0.99 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.6, 136.9, 136.8, 134.8, 132.2, 129.5, 129.2, 128.7, 128.4, 127.9, 127.5, 122.4, 41.9, 22.9, 11.5. GC-MS: m/z = 231.11

3-chloro-*N*-propylbenzamide (**3v**)[5]



Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (s, 1H), 7.93 (dd, 1H, *J* = 2.0 Hz, *J* = 8.0 Hz), 7.53 (d, 1H, *J* = 9.2 Hz), 7.38 (d, 1H, *J* = 8.0 Hz), 6.05 (s, br, 1H), 3.75 (q, 2H, *J* = 7.4 Hz), 1.76-1.85 (m, 2H), 1.06 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.7, 135.6, 134.4, 133.6, 130.5, 129.4, 128.9, 47.0, 21.2, 11.5. GC-MS: m/z = 197.06.

2-chloro-*N*-propylbenzamide (**3w**)[5]

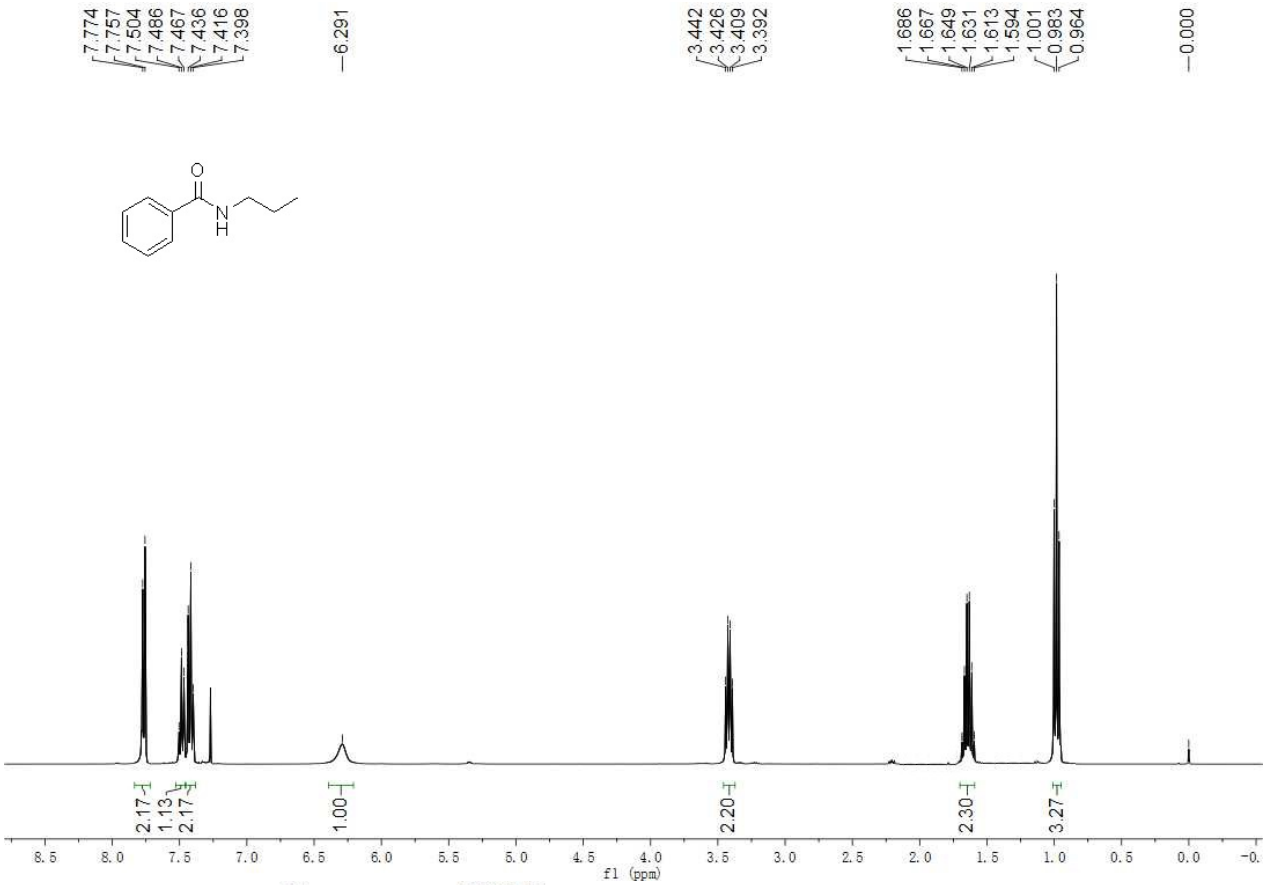


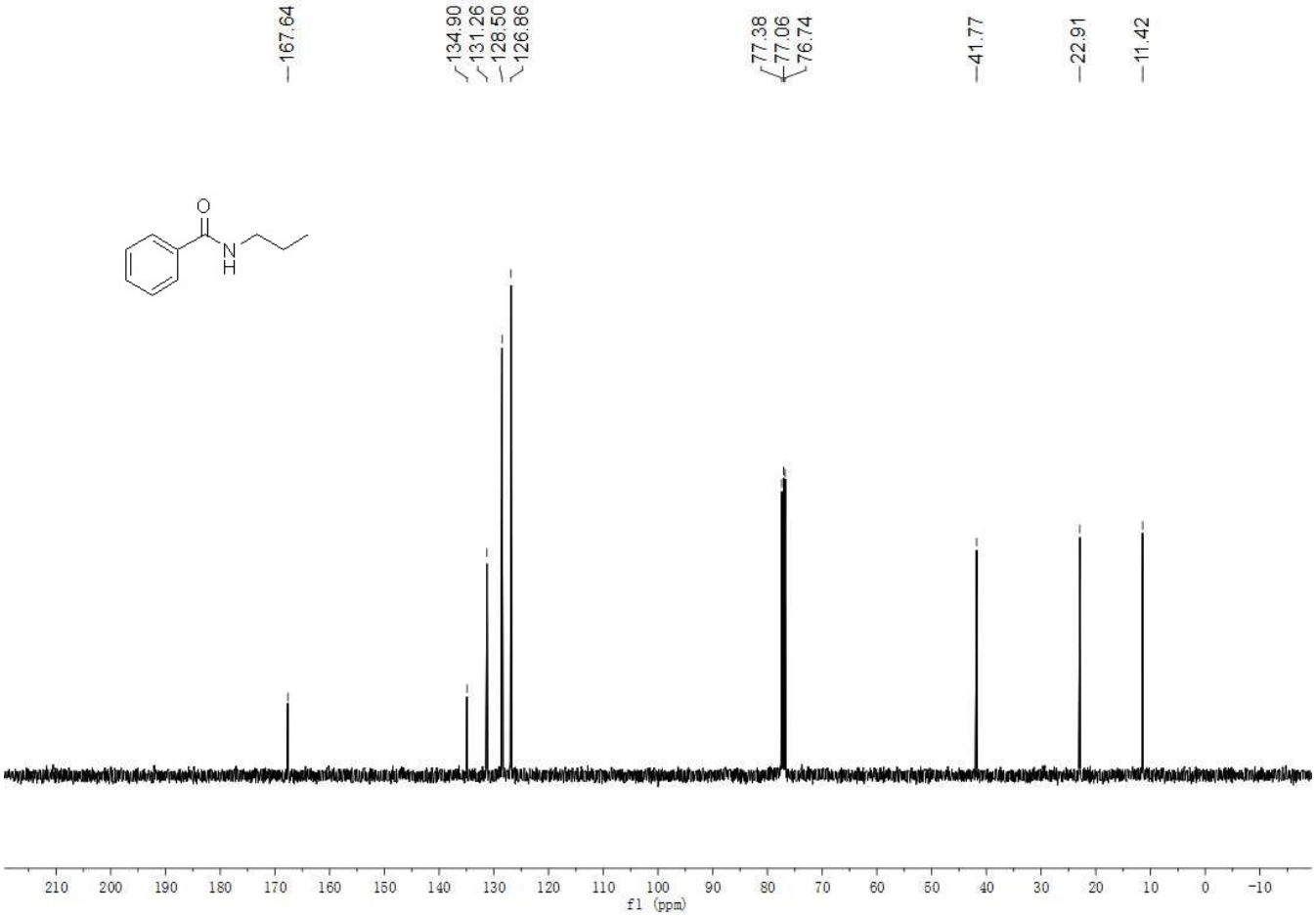
(Colourless viscous liquid) Eluent: petroleum ether/ethyl acetate (10:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 (d, 1H, *J* = 8.0 Hz), 7.19 (t, 1H, *J* = 8.4 Hz), 6.67 (t, 2H, *J* = 8.0 Hz), 6.04 (s, br, 1H), 3.39 (q, 2H, *J* = 6.6 Hz), 1.59-1.66 (m, 2H), 0.99 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.6, 137.3, 133.7, 131.6, 131.4, 131.3, 128.3, 45.1, 22.9, 11.1. GC-MS: m/z = 197.06.

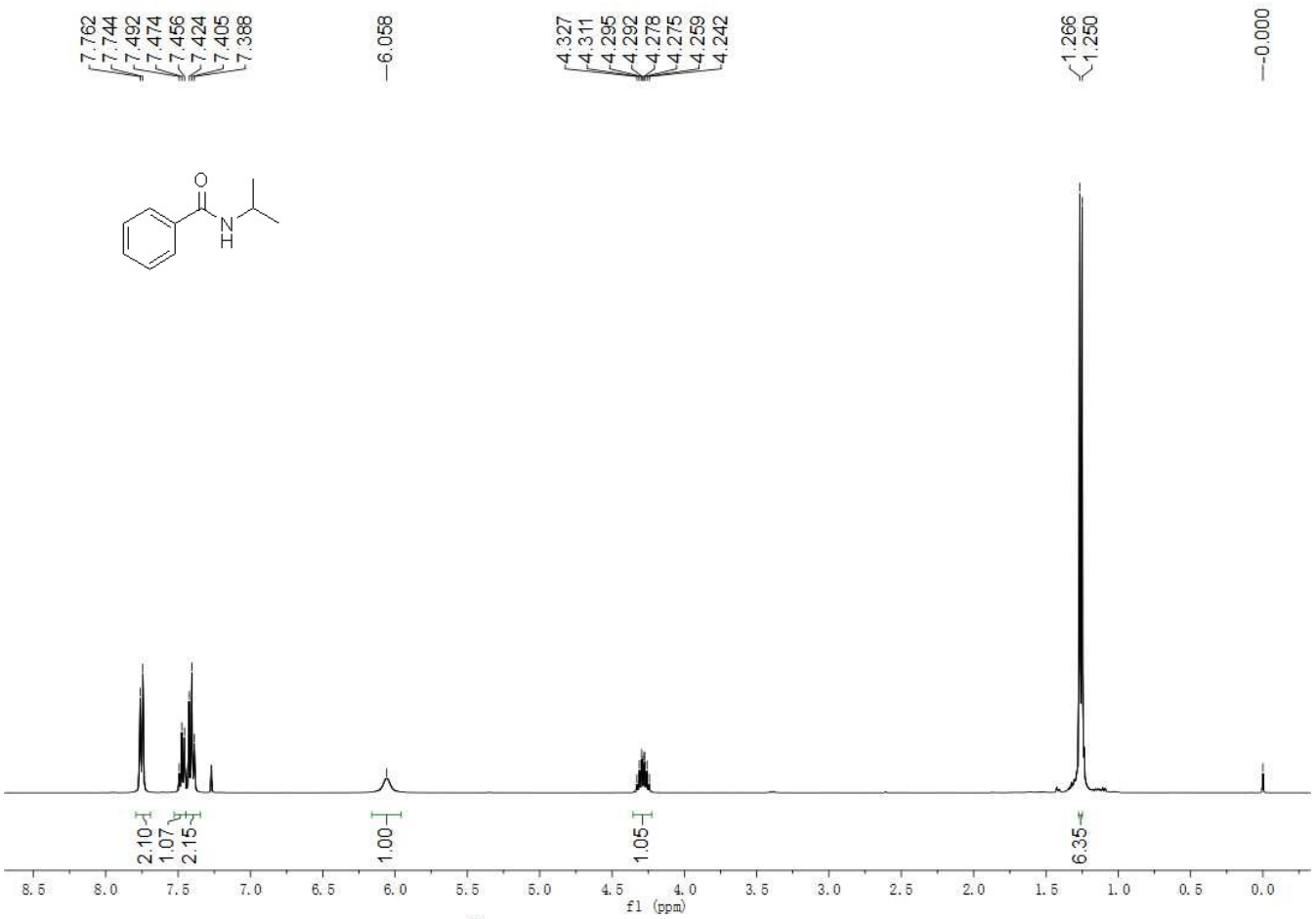
4. References

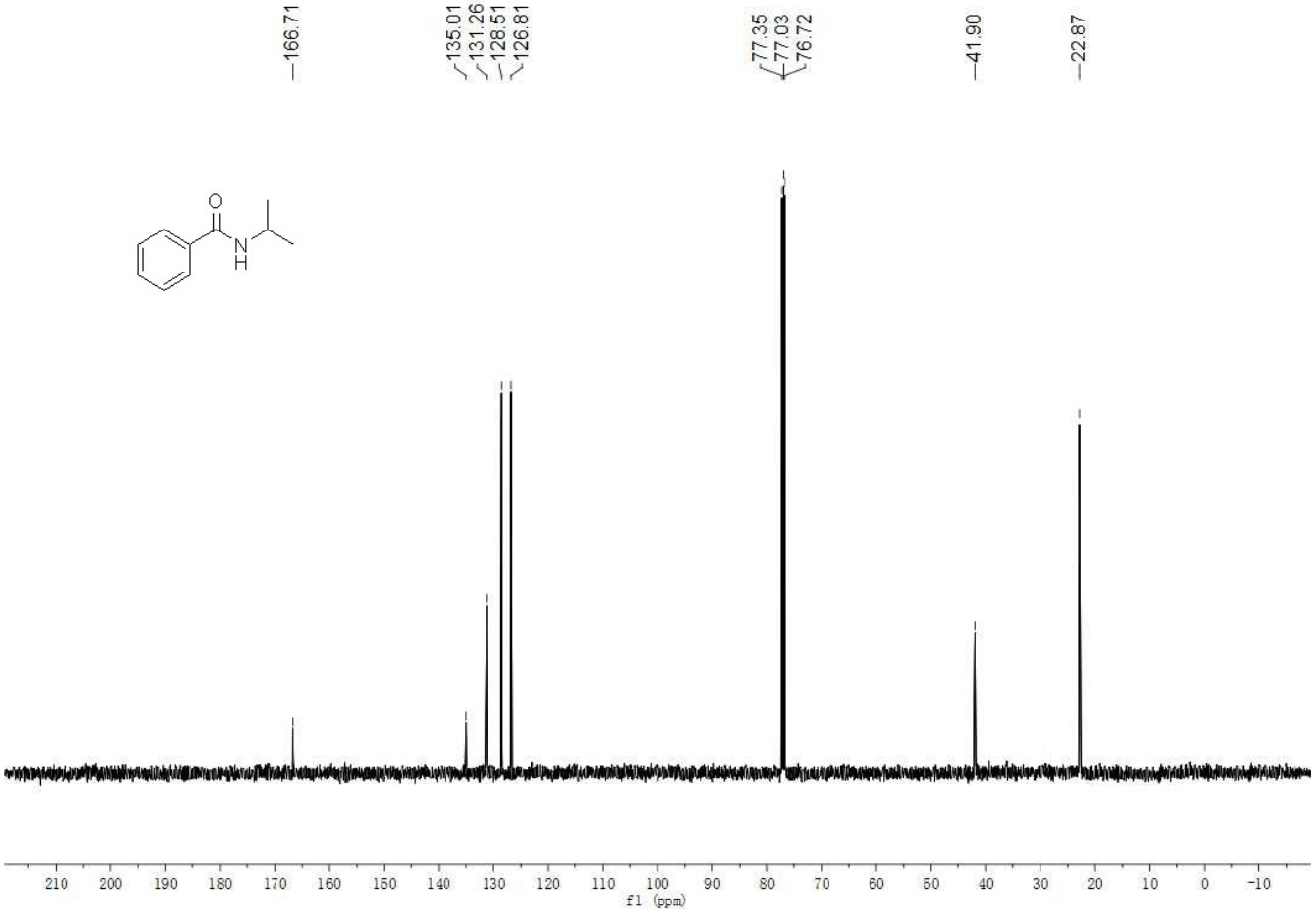
[1] H. Yang, W. Hu, S. Deng, T. Wu, H. Cen, Y. Chen, D. Zhang, B. Wang, *New J. Chem*., **2015**, *39*, 5912-5915
[2] Y. Wang, G. Zhang, A. Shoberu, J. Zou, *Tetrahedron Lett*., **2021**, *80*, 153316.
[3] X. Cui, Z. Qiao, X. Huang, X. Yang, X. Chen, S. Sun, *Studies in Synthetic Chemistry*, **2018**, *6*, 8-14.
[4] J. W. Bean, D. J.Nelson, G. E. Wright, *Biochemical Pharmacology*, **1986**, *6*, 1011-1017.
[5] M. Y. Bhat, S. Ahmed, Q. N. Ahmed, *J. Org. Chem*., **2022**, *87*, 11608-11624.

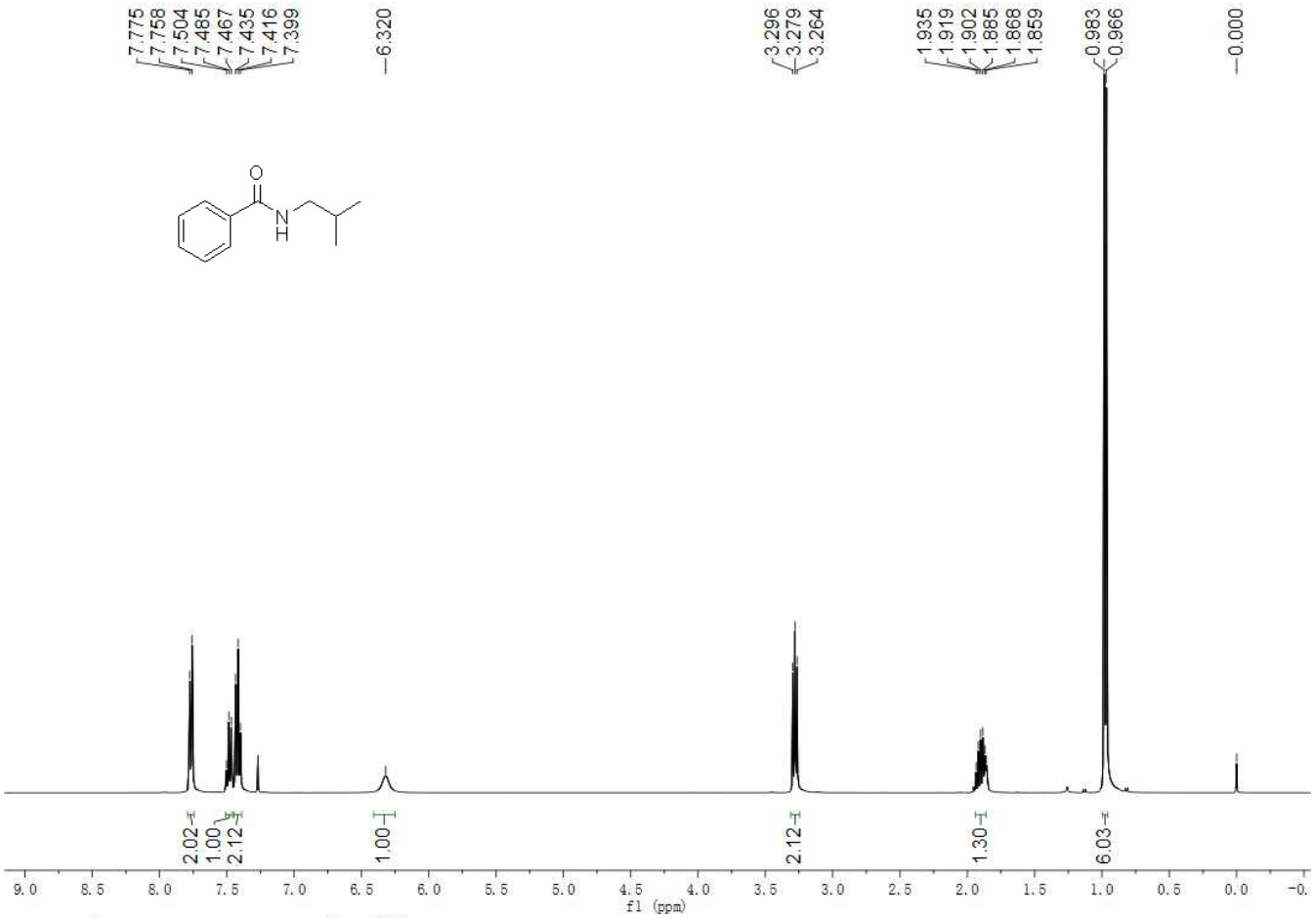
5. Copies of ^{1}H and ^{13}C NMR spectra

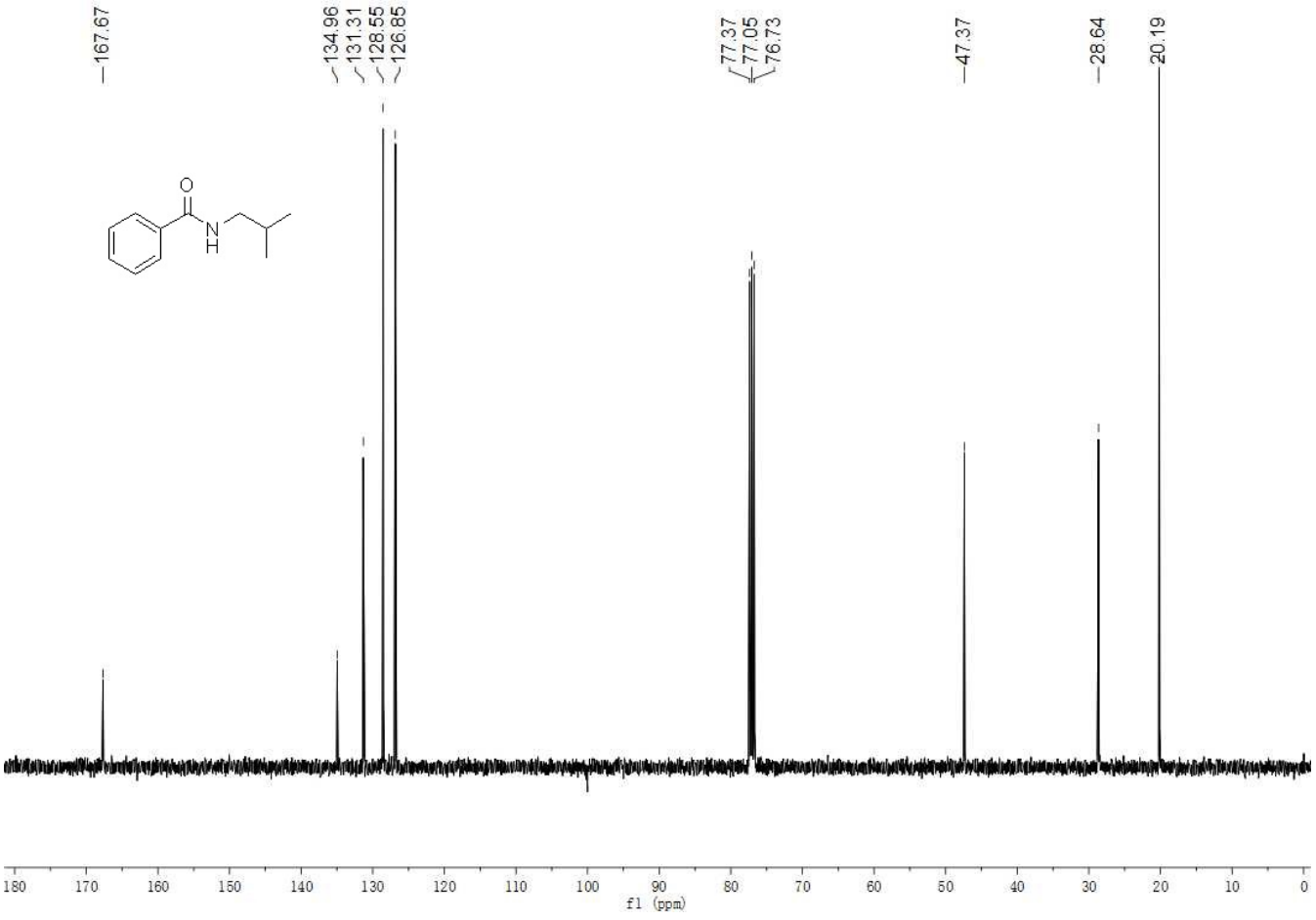


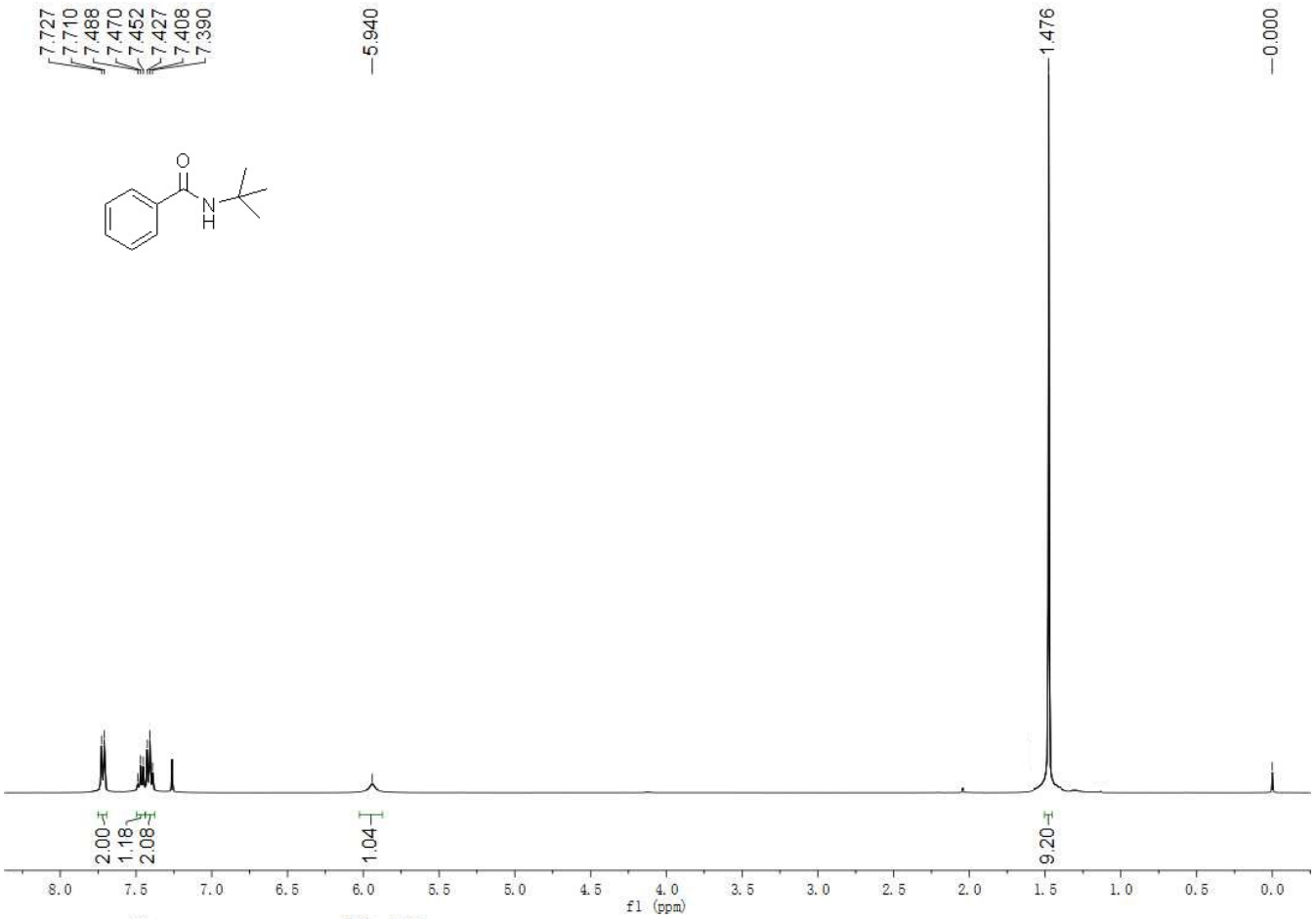


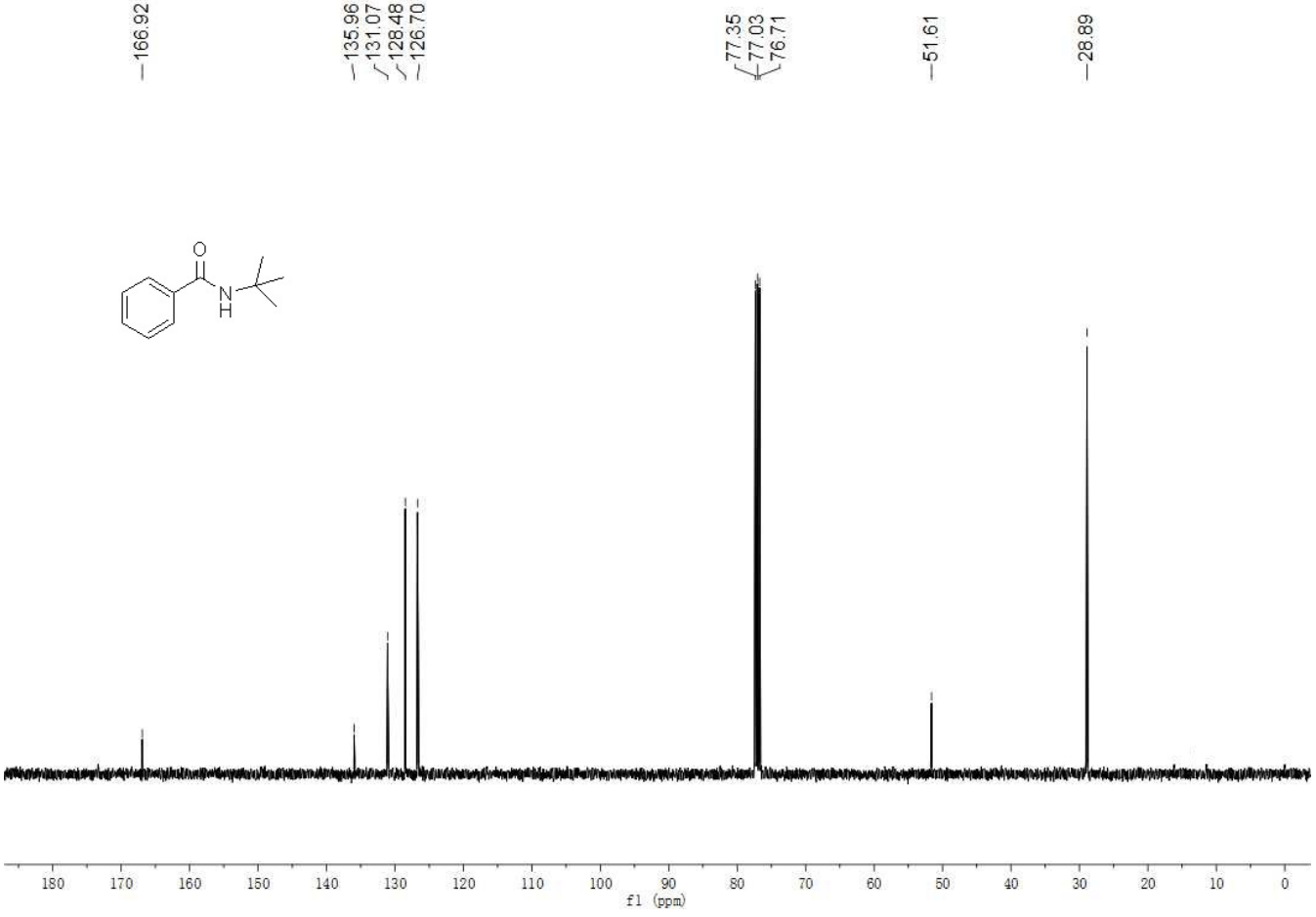

7.762
7.744
7.492
7.474
7.456
7.424
7.405
7.388
6.058
4.327
4.311
4.295
4.292
4.278
4.275
4.259
4.242
1.266
1.250
0.000
2.10
1.07
2.15
1.00
1.05
6.35
f1 (ppm)

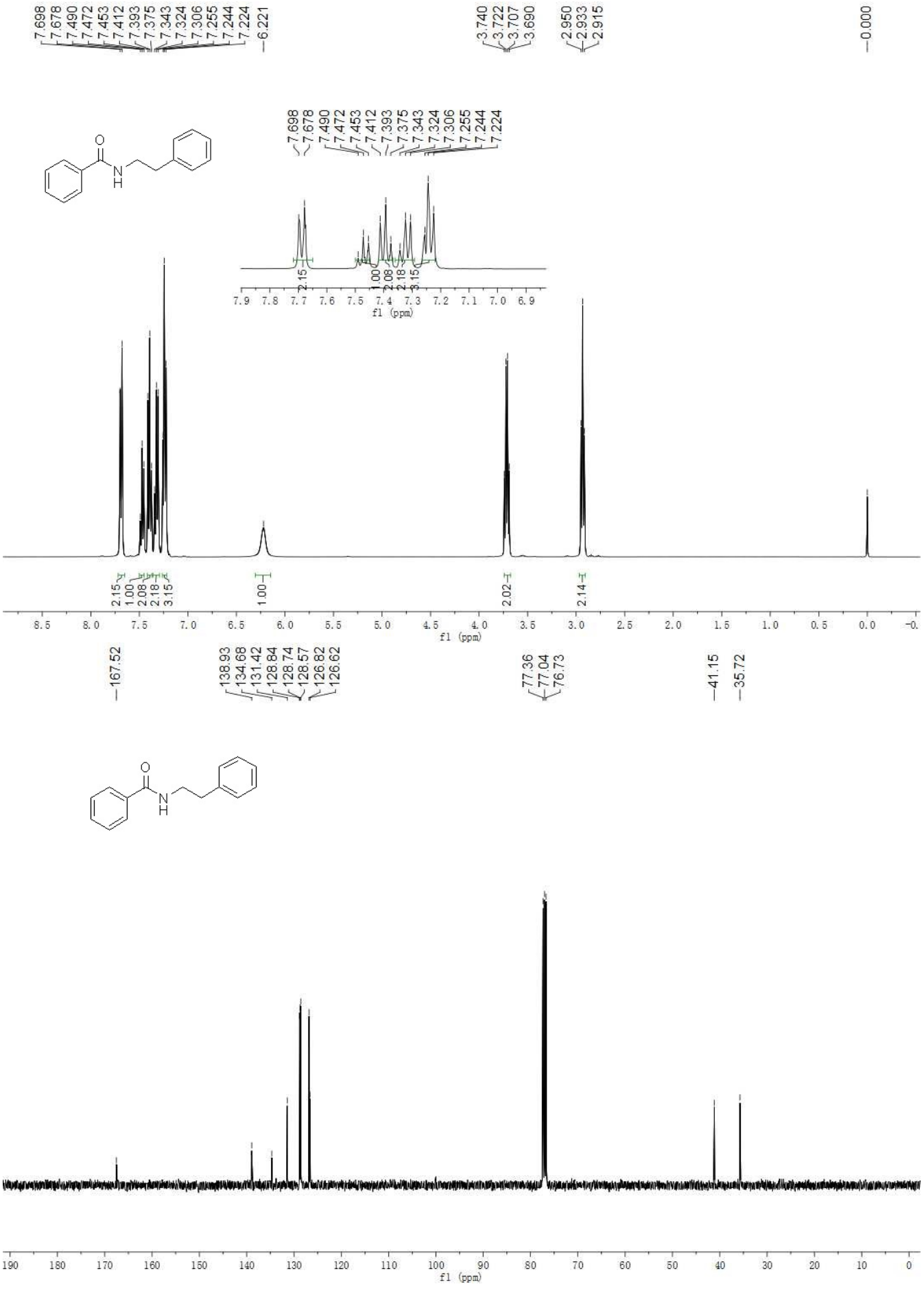

166.71
135.01
131.26
128.51
126.81
77.35
77.03
76.72
41.90
22.87
f1 (ppm)

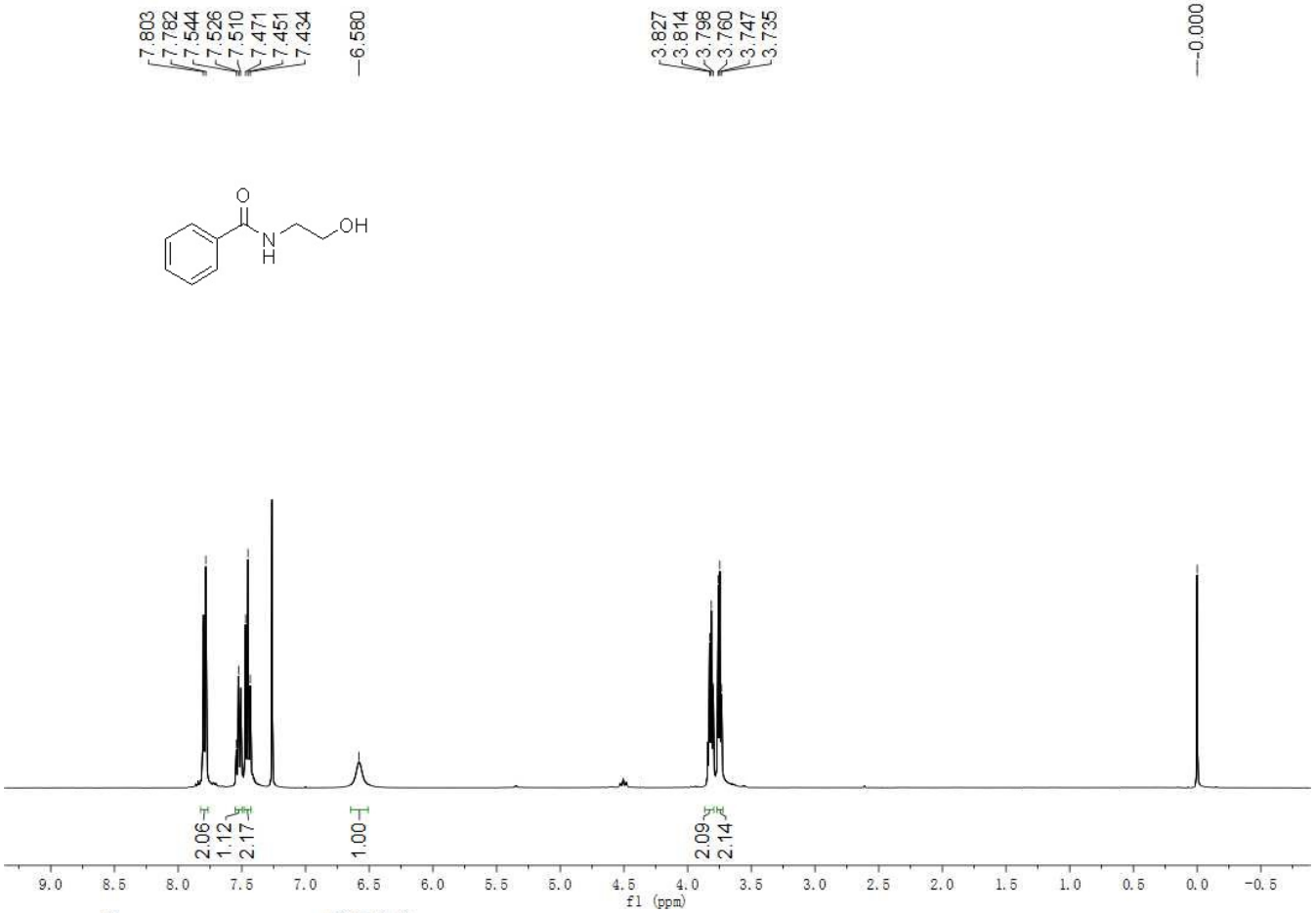

7.775
7.758
7.504
7.485
7.467
7.435
7.416
7.399
6.320
3.296
3.279
3.264
1.935
1.919
1.902
1.885
1.868
1.859
0.983
0.966
0.000
2.02
1.00
2.12
1.00
2.12
1.30
6.03
f1 (ppm)

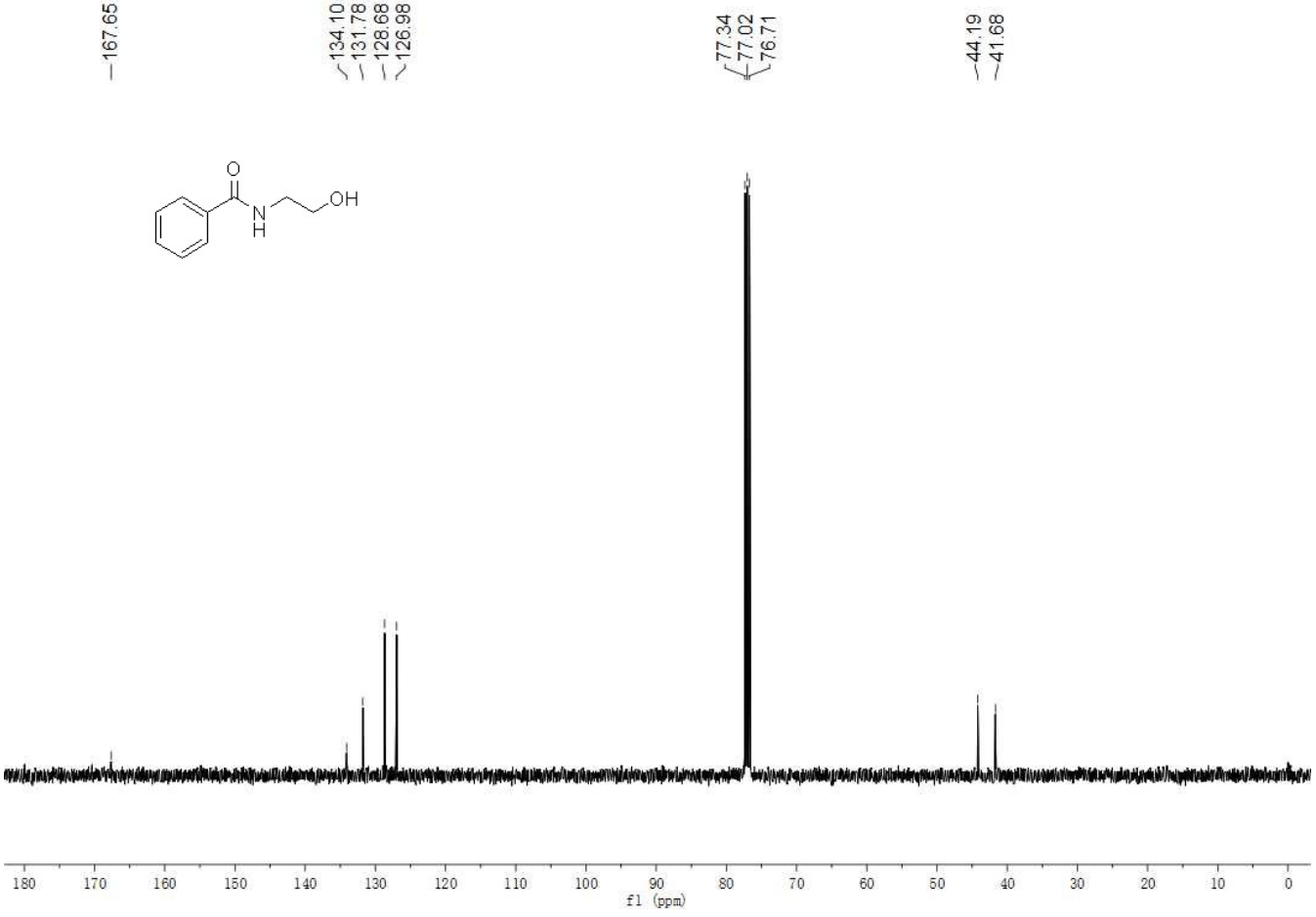

167.67
134.96
131.31
128.55
126.85
77.37
77.05
76.73
47.37
28.64
20.19
f1 (ppm)

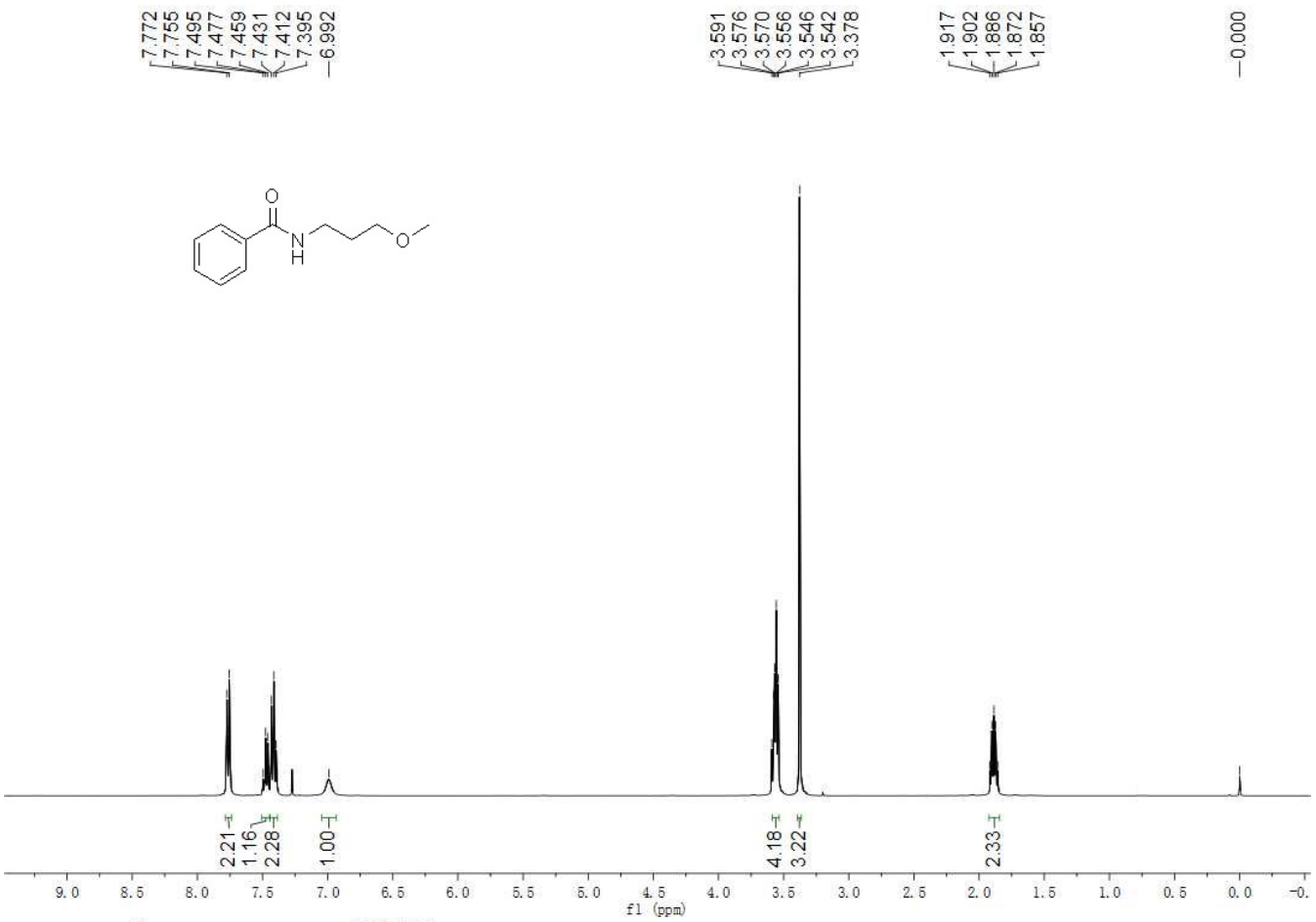

7.727
7.710
7.488
7.470
7.452
7.427
7.408
7.390
5.940
1.476
0.000
2.00
1.18
2.08
1.04
9.20
f1 (ppm)

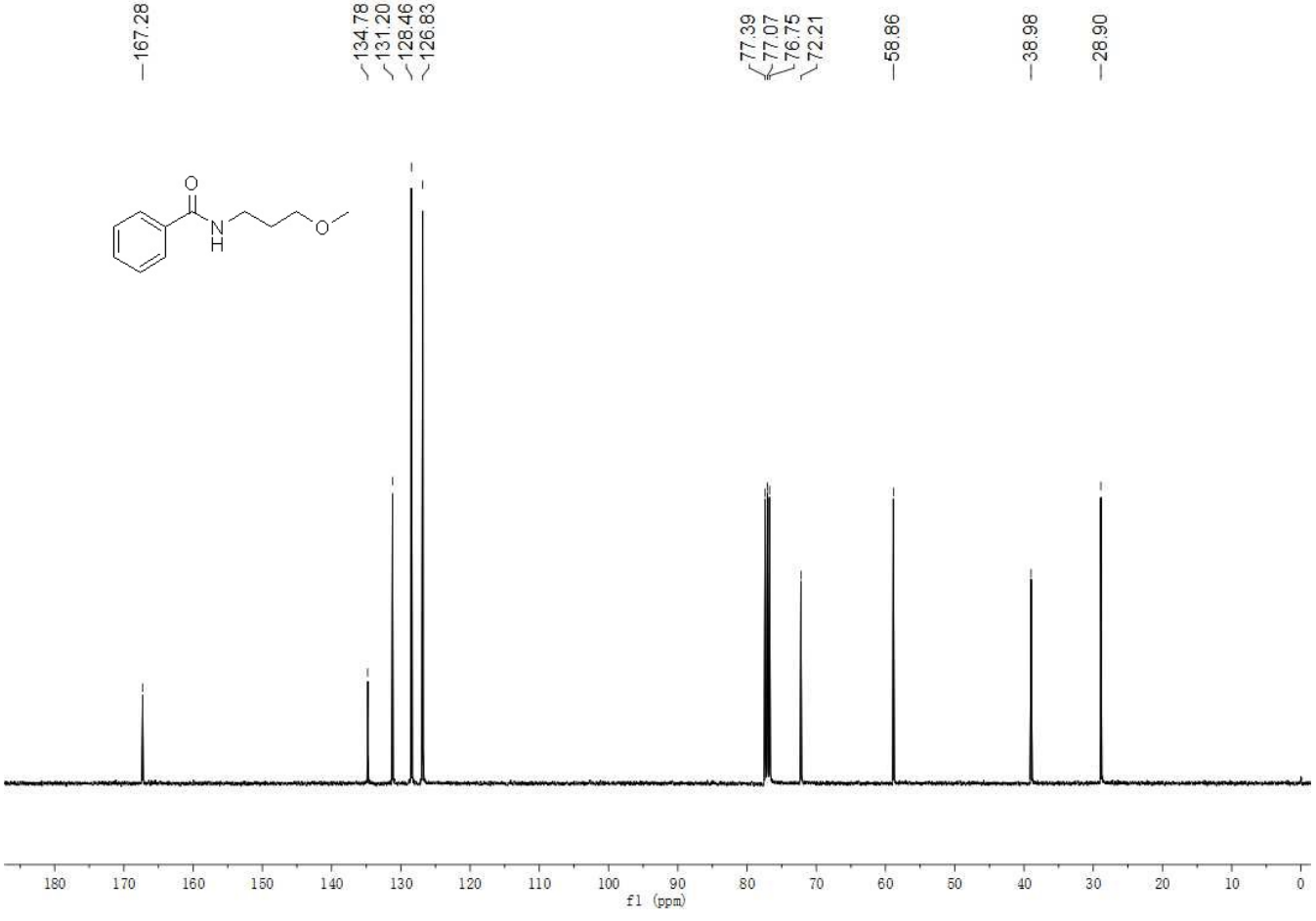

166.92
135.96
131.07
128.48
126.70
77.35
77.03
76.71
51.61
28.89
f1 (ppm)

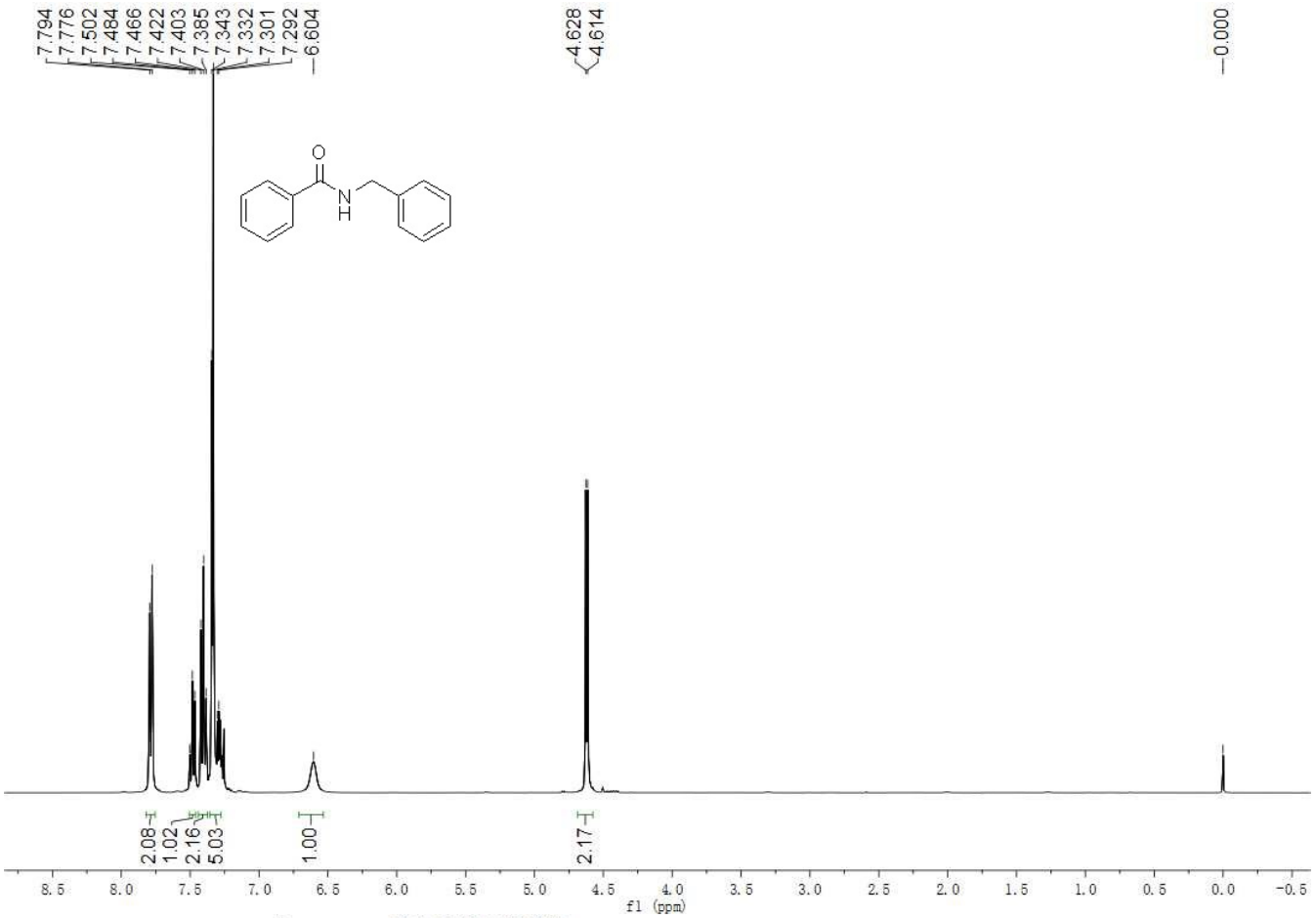

7.698
7.678
7.490
7.472
7.453
7.412
7.393
7.375
7.343
7.324
7.306
7.255
7.244
7.224
6.221
3.740
3.722
3.707
3.690
2.950
2.933
2.915
0.000
2.15
1.00
2.08
2.18
3.15
1.00
2.02
2.14
f1 (ppm)
167.52
138.93
134.68
131.42
128.84
128.74
128.57
126.82
126.62
77.36
77.04
76.73
41.15
35.72
f1 (ppm)

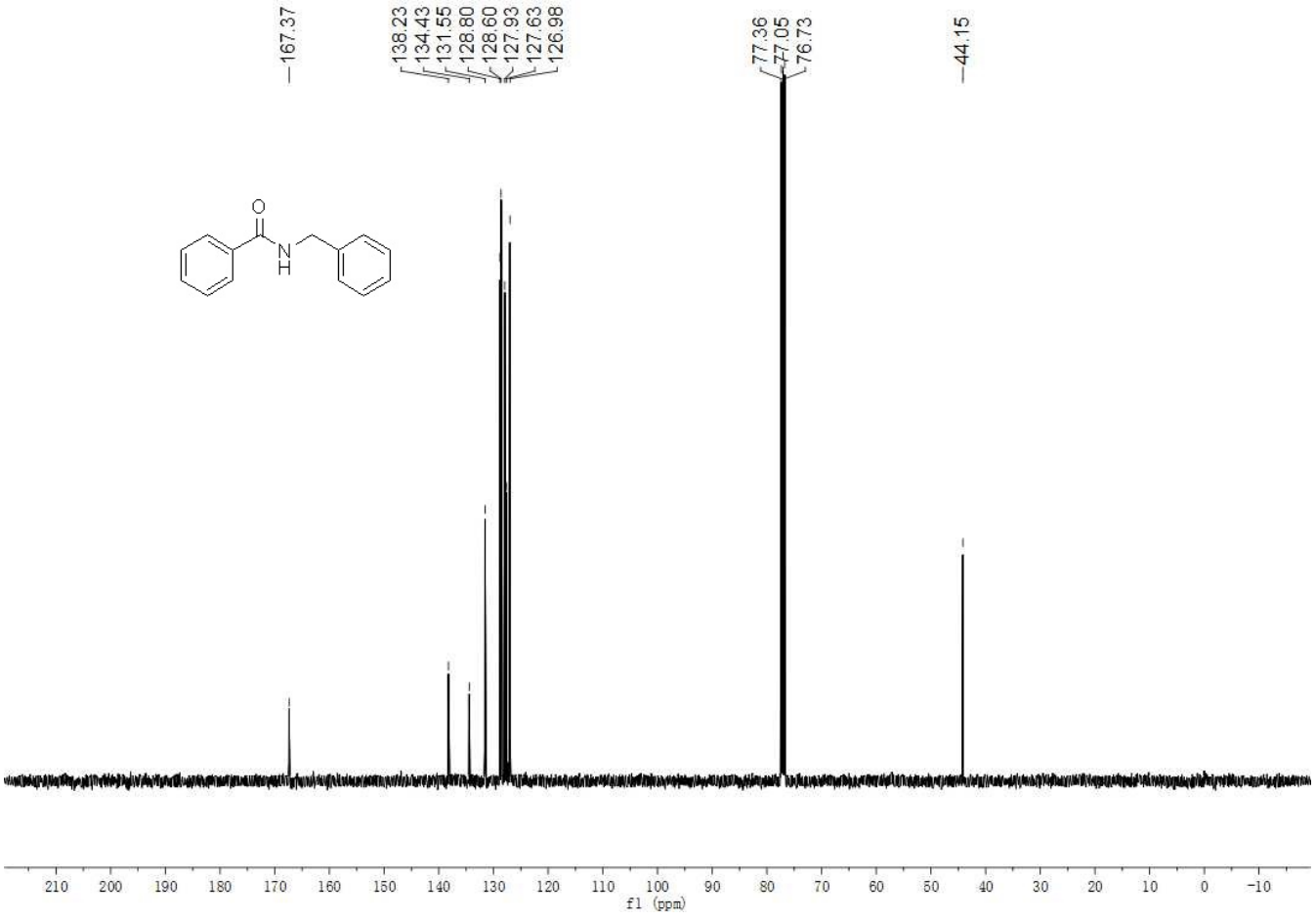

7.803
7.782
7.544
7.526
7.510
7.471
7.451
7.434
6.580
3.827
3.814
3.798
3.760
3.747
3.735
0.000
O
N
H
OH
2.06
1.12
2.17
1.00
2.09
2.14
f1 (ppm)

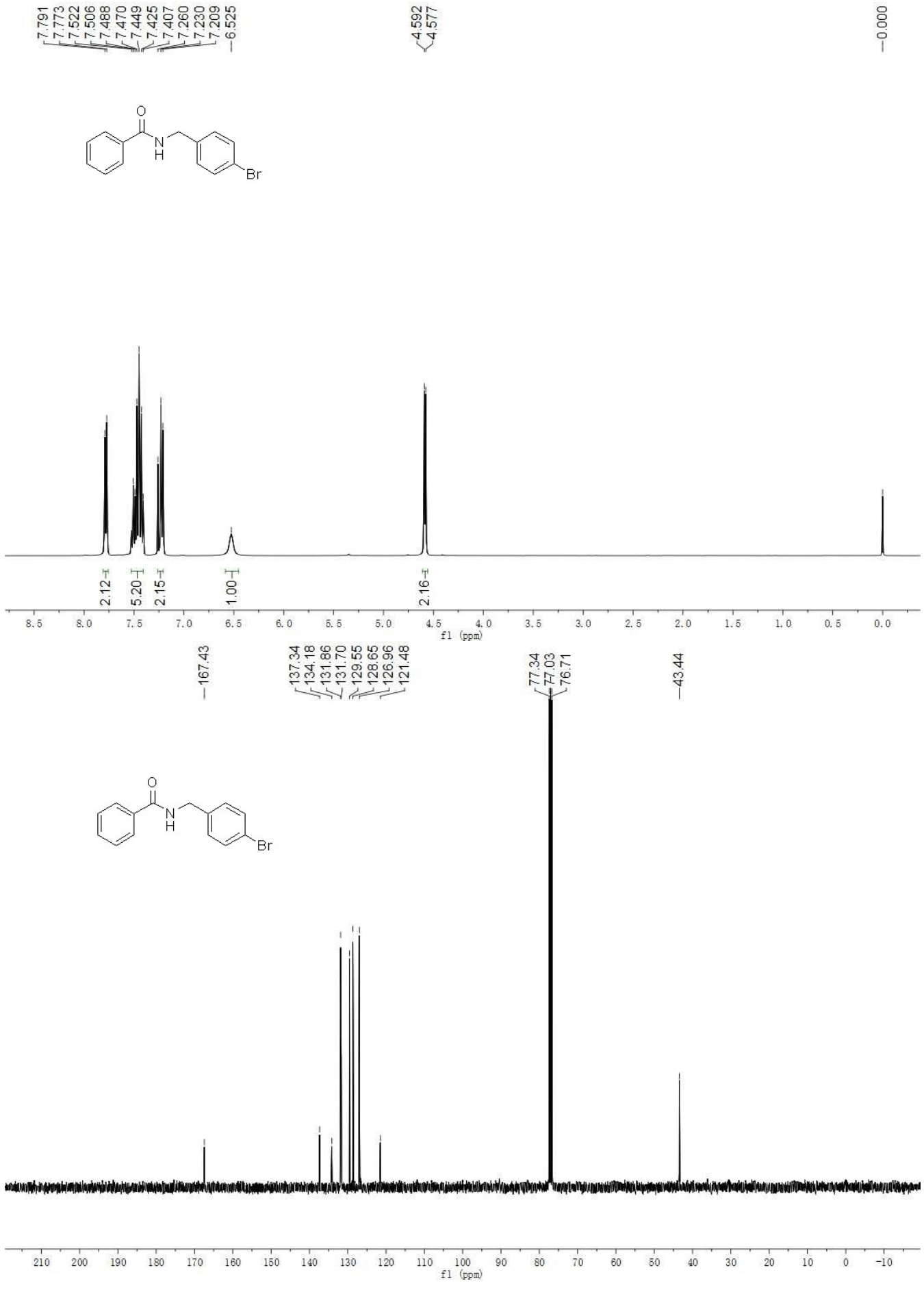

167.65
134.10
131.78
128.68
126.98
77.34
77.02
76.71
44.19
41.68
O
N
H
OH
f1 (ppm)

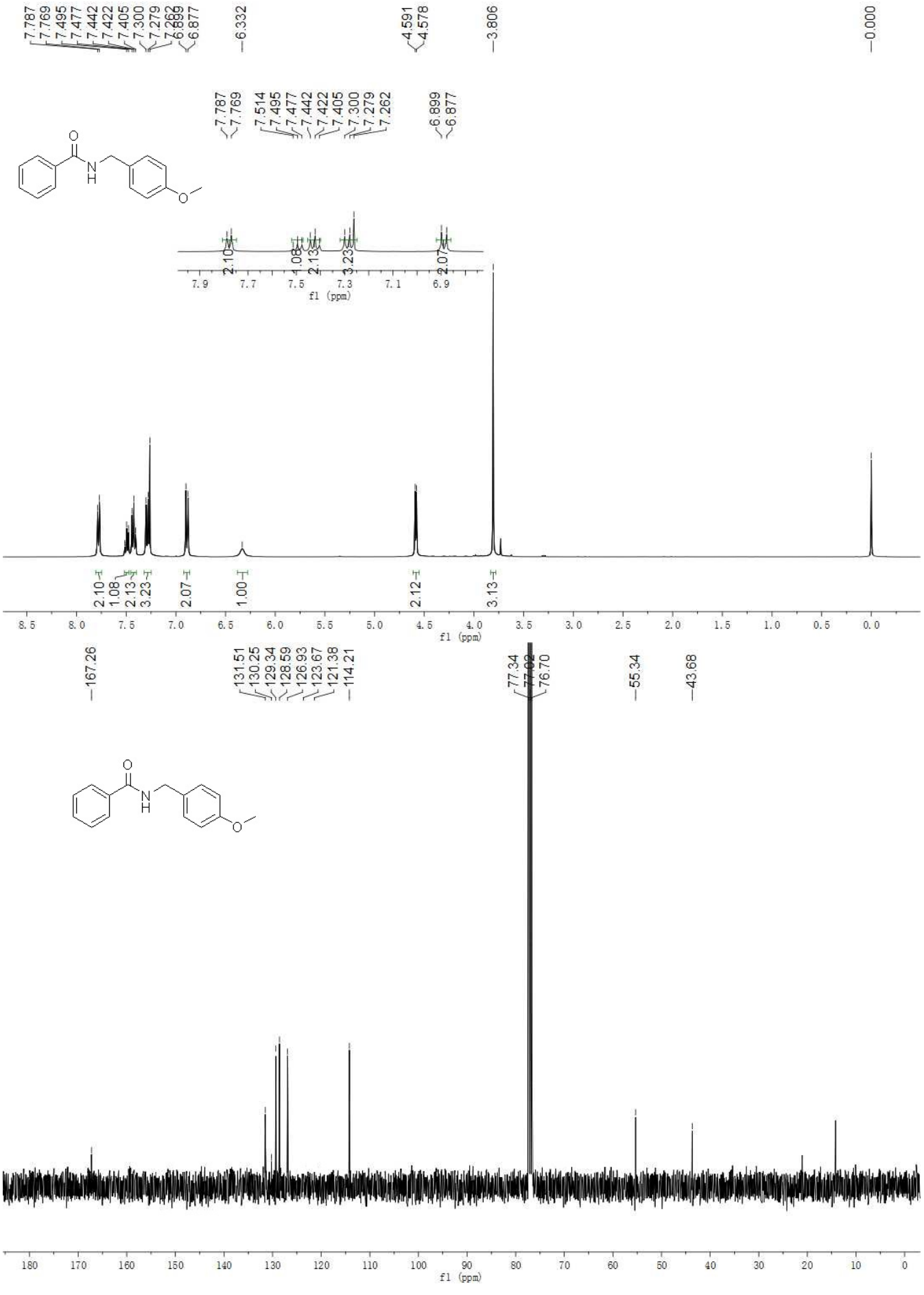

7.772
7.755
7.495
7.477
7.459
7.431
7.412
7.395
6.992
3.591
3.576
3.570
3.556
3.546
3.542
3.378
1.917
1.902
1.886
1.872
1.857
0.000
2.21
1.16
2.28
1.00
4.18
3.22
2.33
f1 (ppm)

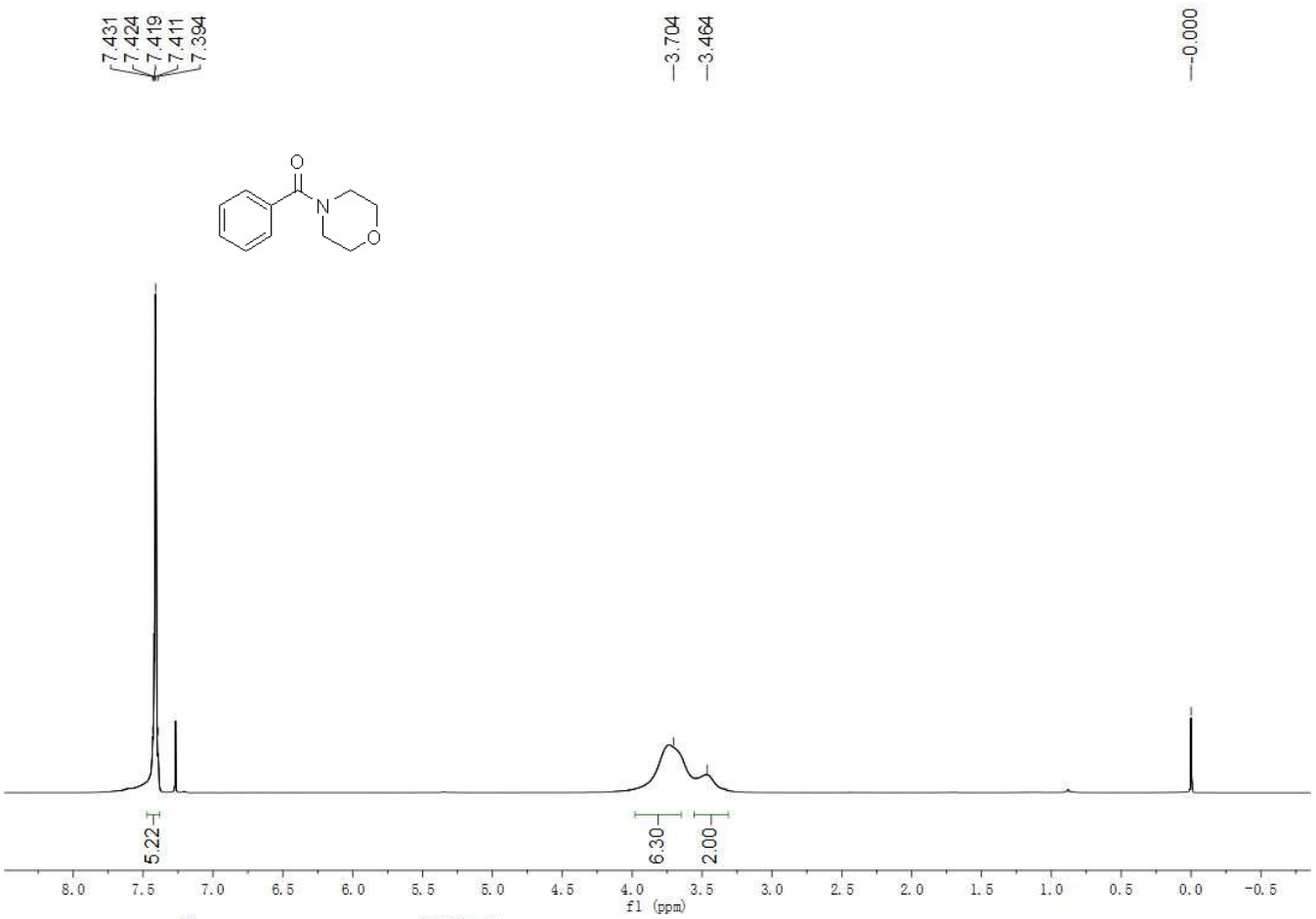

167.28
134.78
131.20
128.46
126.83
77.39
77.07
76.75
72.21
58.86
38.98
28.90
f1 (ppm)

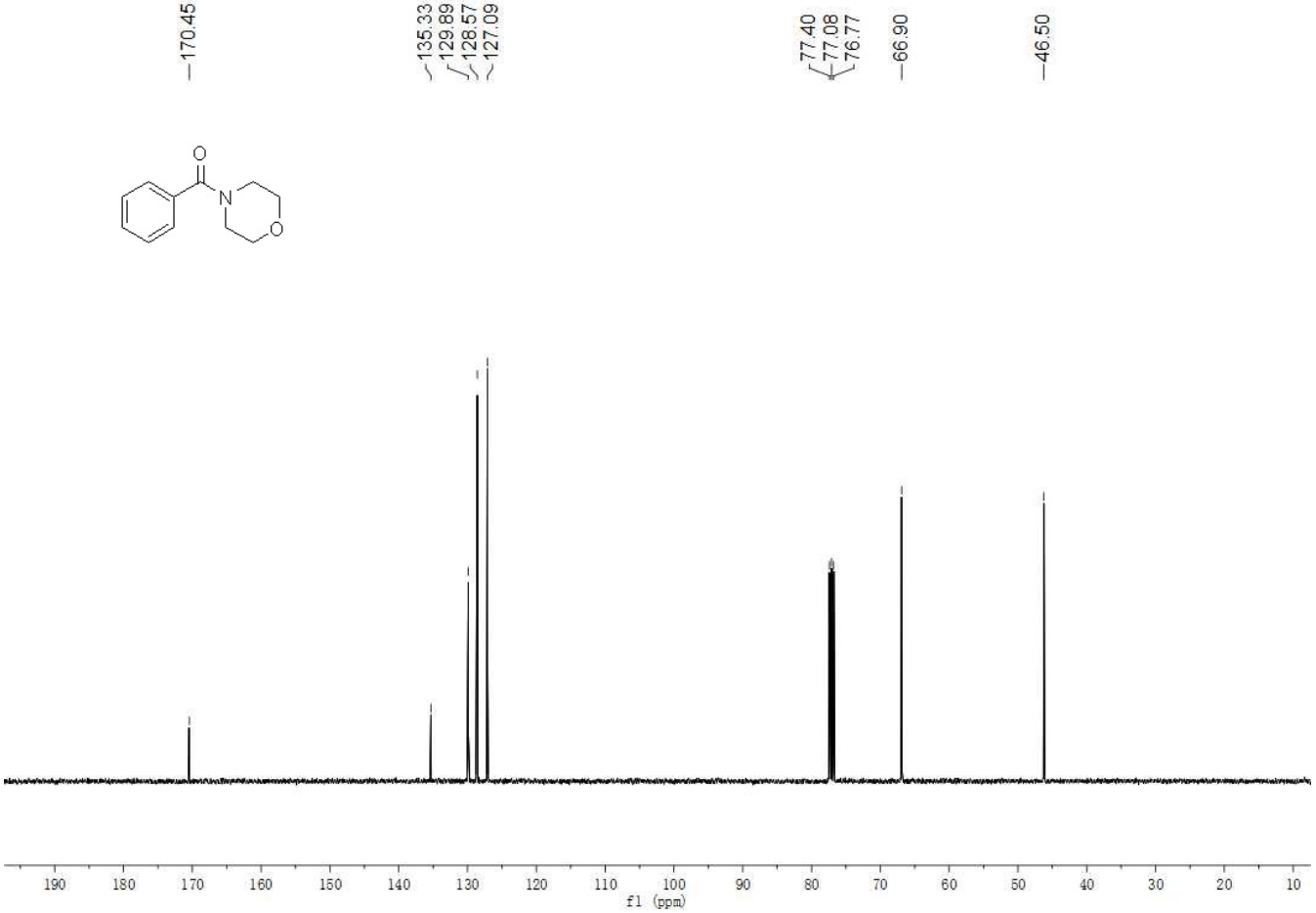

7.794
7.776
7.502
7.484
7.466
7.422
7.403
7.385
7.343
7.332
7.301
7.292
6.604
4.628
4.614
0.000
2.08
1.02
2.16
5.03
1.00
2.17
f1 (ppm)

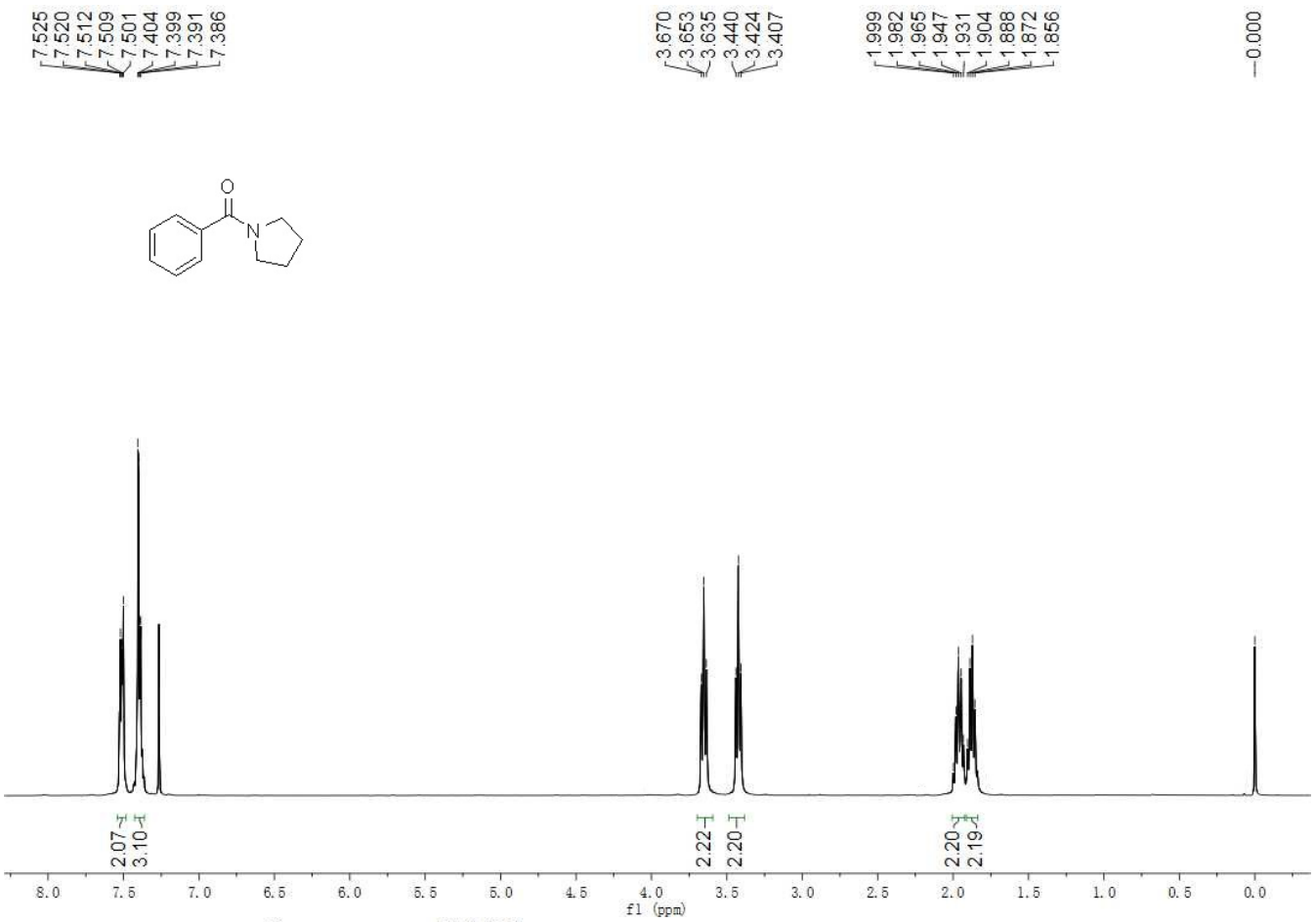

167.37
138.23
134.43
131.55
128.80
128.60
127.93
127.63
126.98
77.36
77.05
76.73
44.15
f1 (ppm)

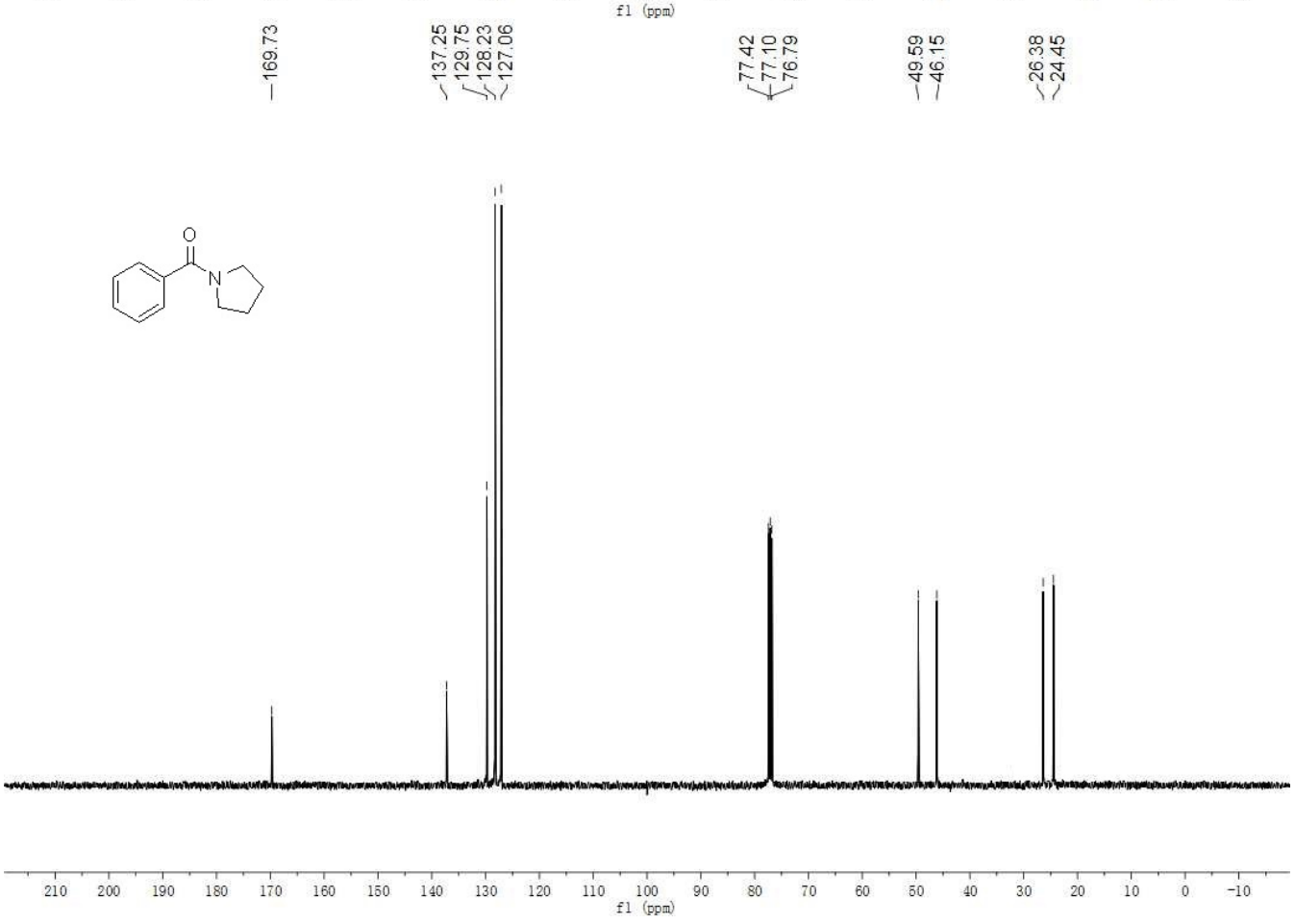

7.791
7.773
7.522
7.506
7.488
7.470
7.449
7.425
7.407
7.260
7.230
7.209
6.525
4.592
4.577
0.000
Br
2.12
5.20
2.15
1.00
2.16
f1 (ppm)
167.43
137.34
134.18
131.86
131.70
129.55
128.65
126.96
121.48
77.34
77.03
76.71
43.44
Br
f1 (ppm)

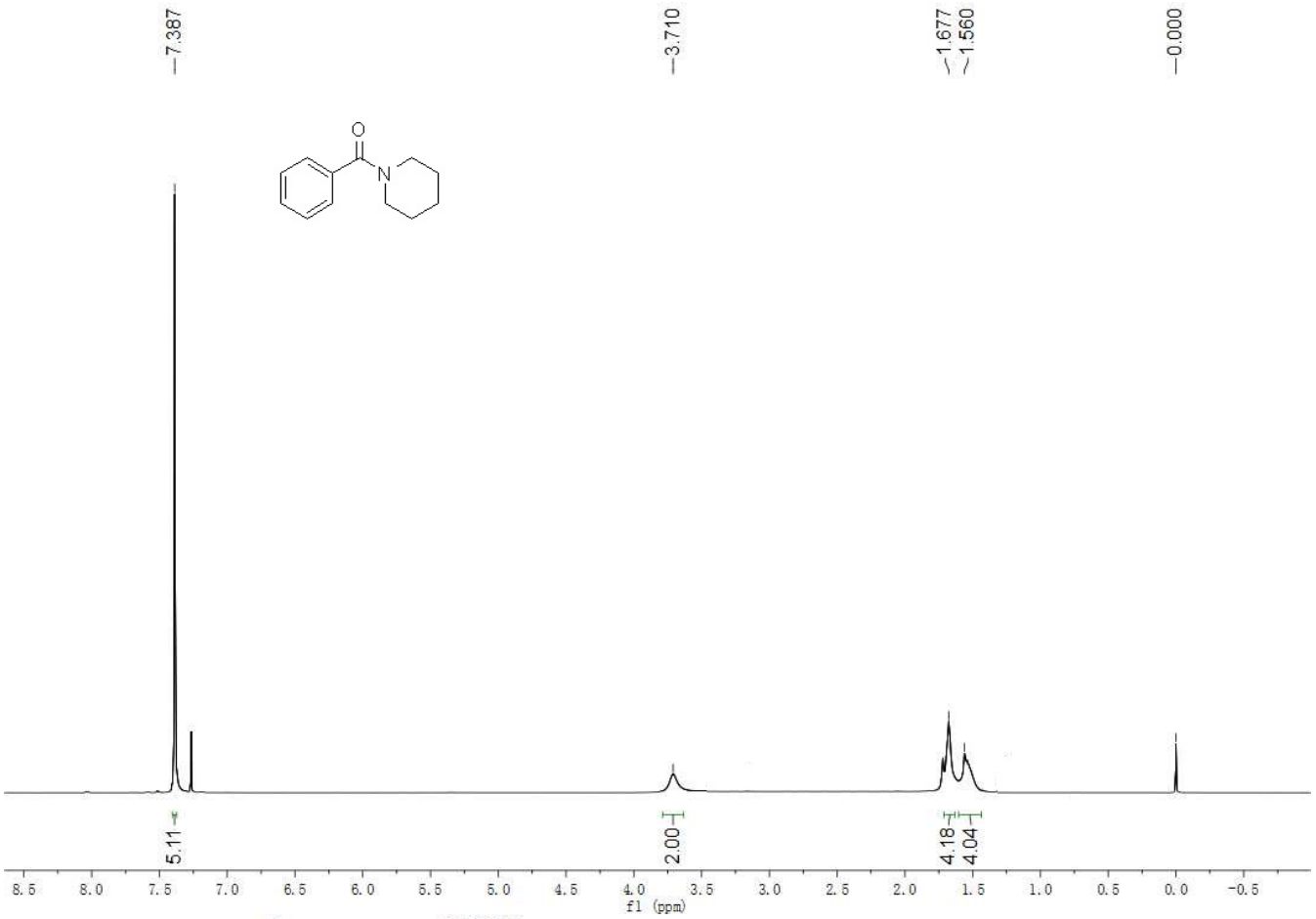

7.787
7.769
7.495
7.477
7.442
7.422
7.405
7.300
7.279
6.899
6.877
6.332
4.591
4.578
3.806
0.000
2.10
1.08
2.13
3.23
2.07
1.00
2.12
3.13
f1 (ppm)
167.26
131.51
130.25
129.34
128.59
126.93
123.67
121.38
114.21
77.34
77.02
76.70
55.34
43.68
f1 (ppm)

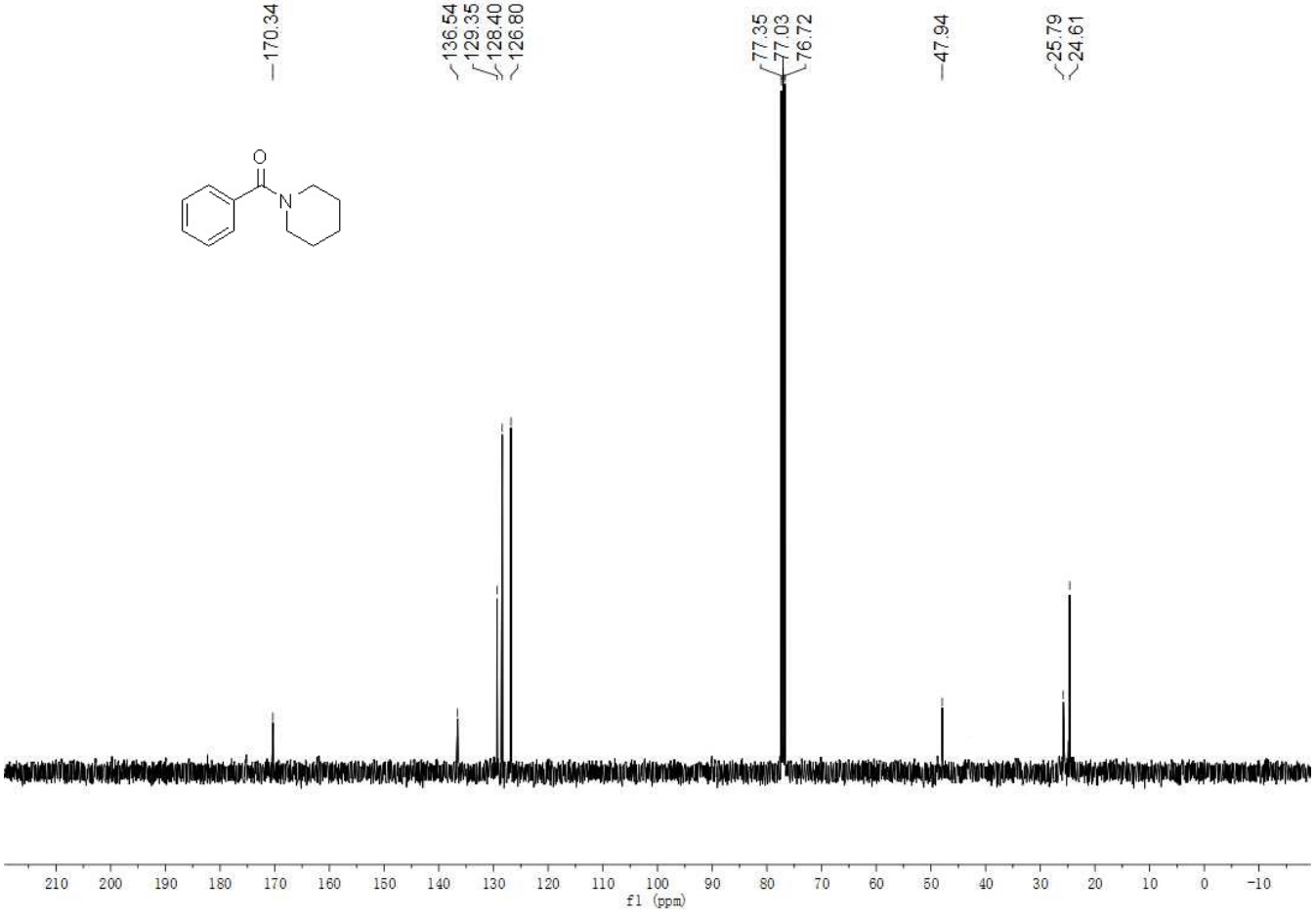

7.431
7.424
7.419
7.411
7.394
3.704
3.464
0.000
5.22
6.30
2.00
f1 (ppm)

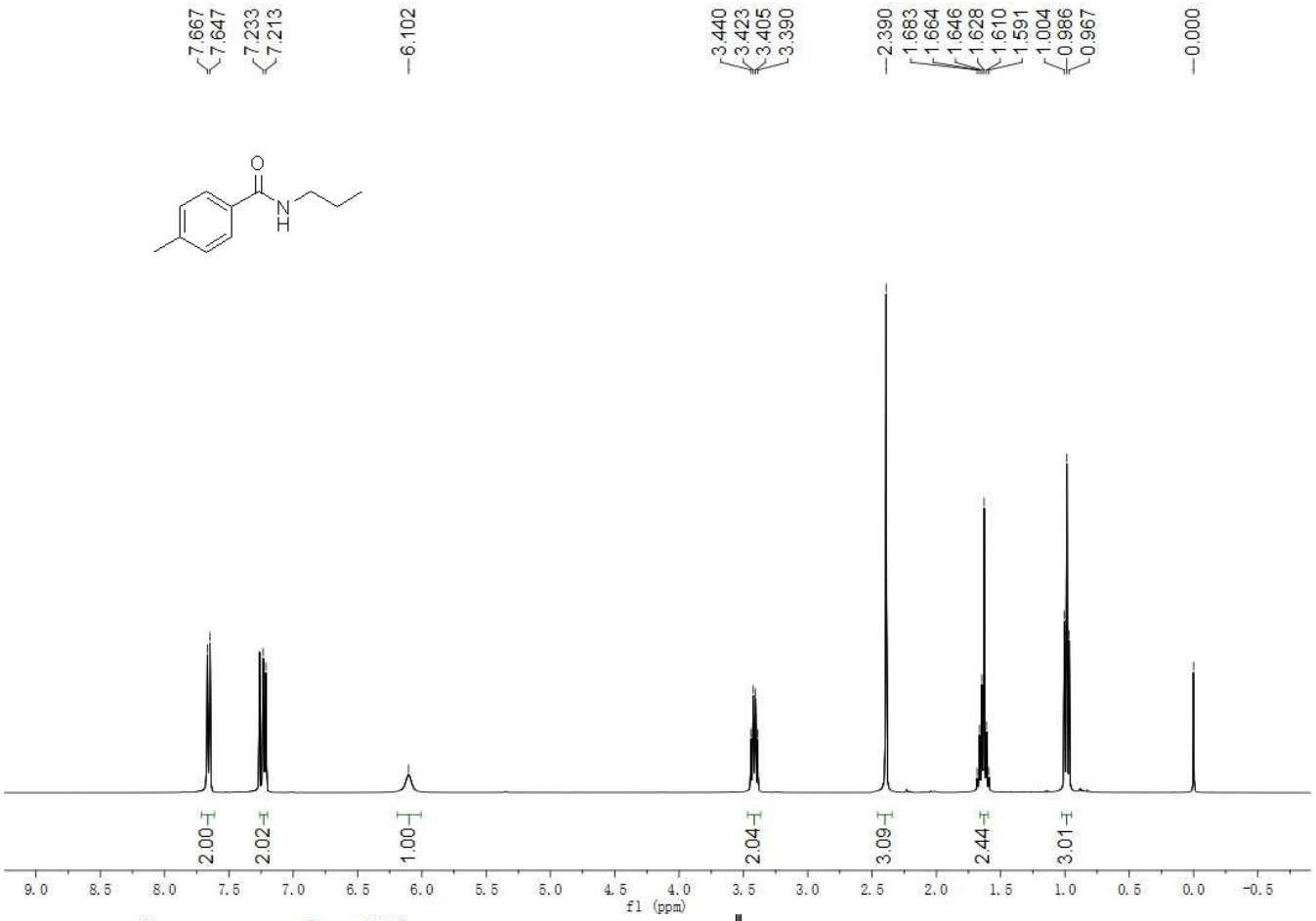

170.45
135.33
129.89
128.57
127.09
77.40
77.08
76.77
66.90
46.50
f1 (ppm)

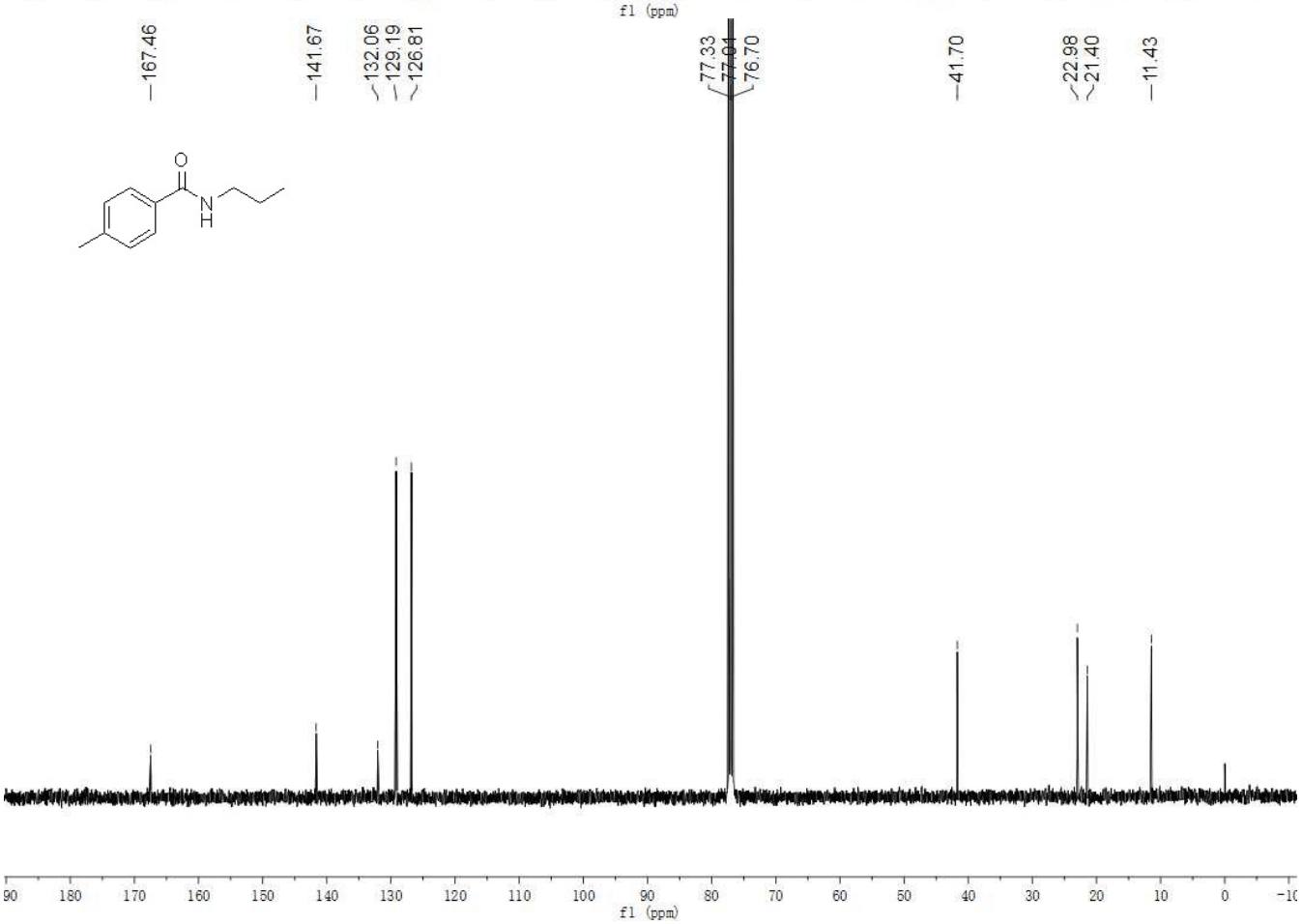

7.525
7.520
7.512
7.509
7.501
7.404
7.399
7.391
7.386
3.670
3.653
3.635
3.440
3.424
3.407
1.999
1.982
1.965
1.947
1.931
1.904
1.888
1.872
1.856
0.000
2.07
3.10
2.22
2.20
2.20
2.19
f1 (ppm)

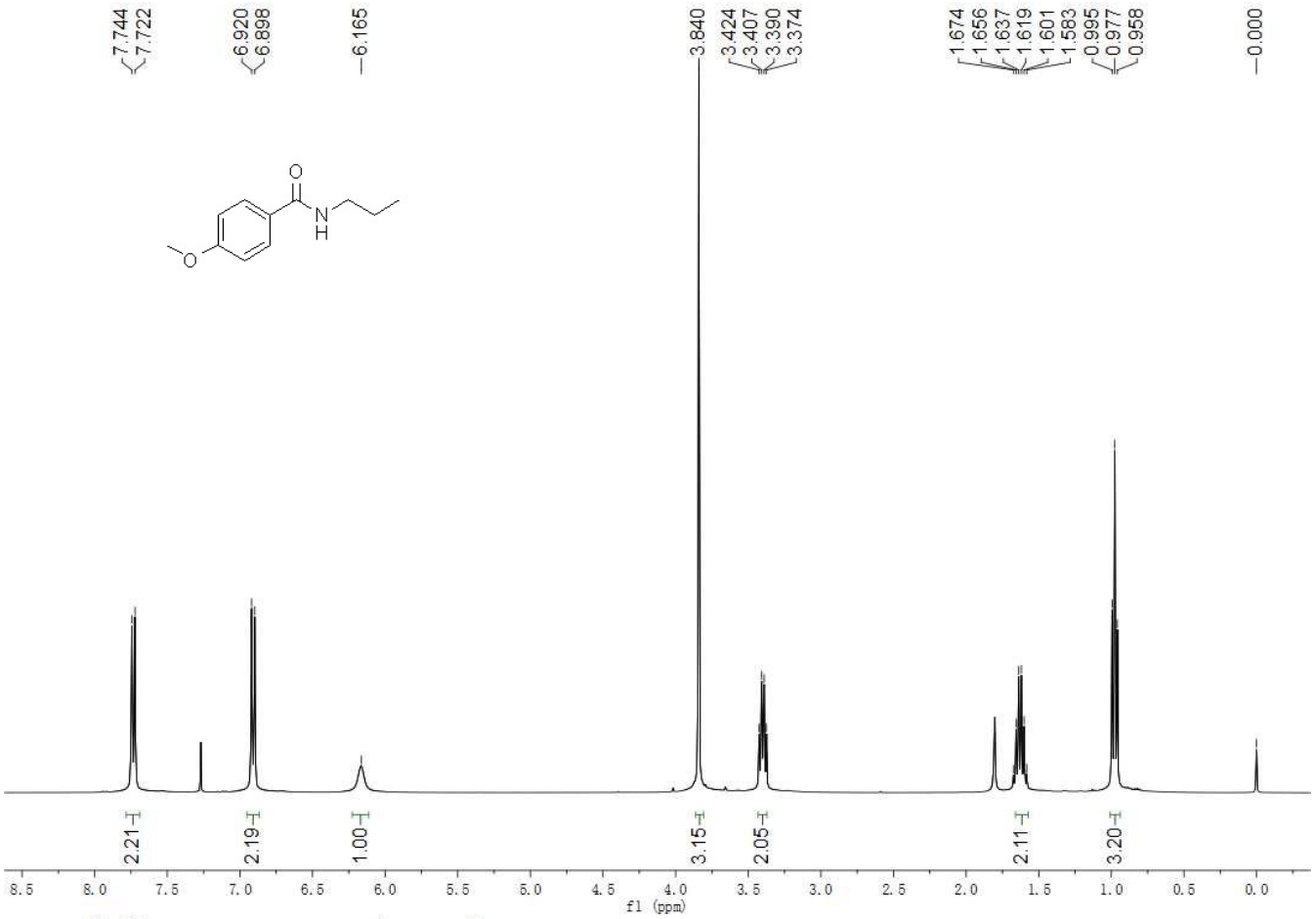

169.73
137.25
129.75
128.23
127.06
77.42
77.10
76.79
49.59
46.15
26.38
24.45
f1 (ppm)

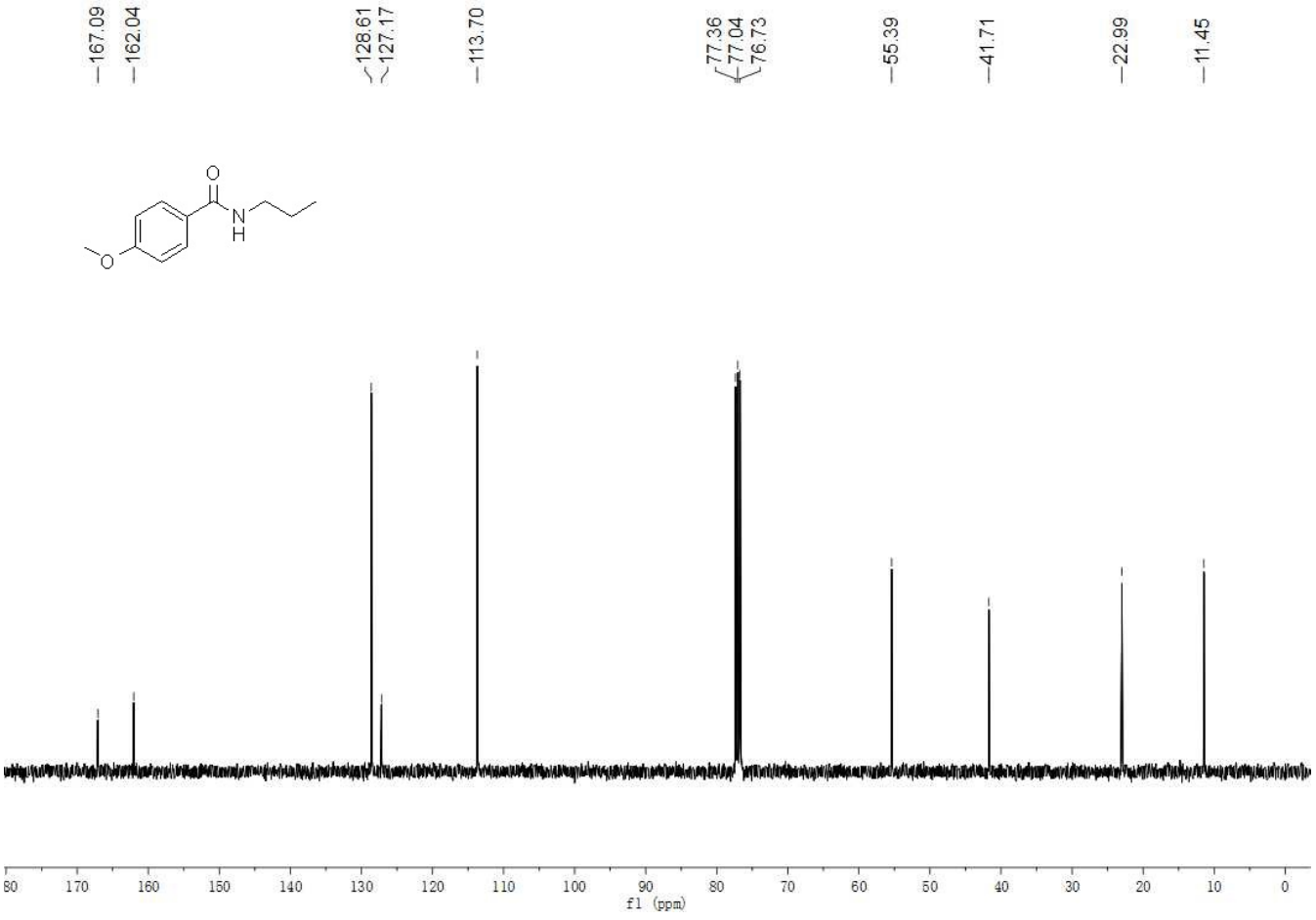

7.387
3.710
1.677
1.560
0.000
5.11
2.00
4.18
4.04
f1 (ppm)

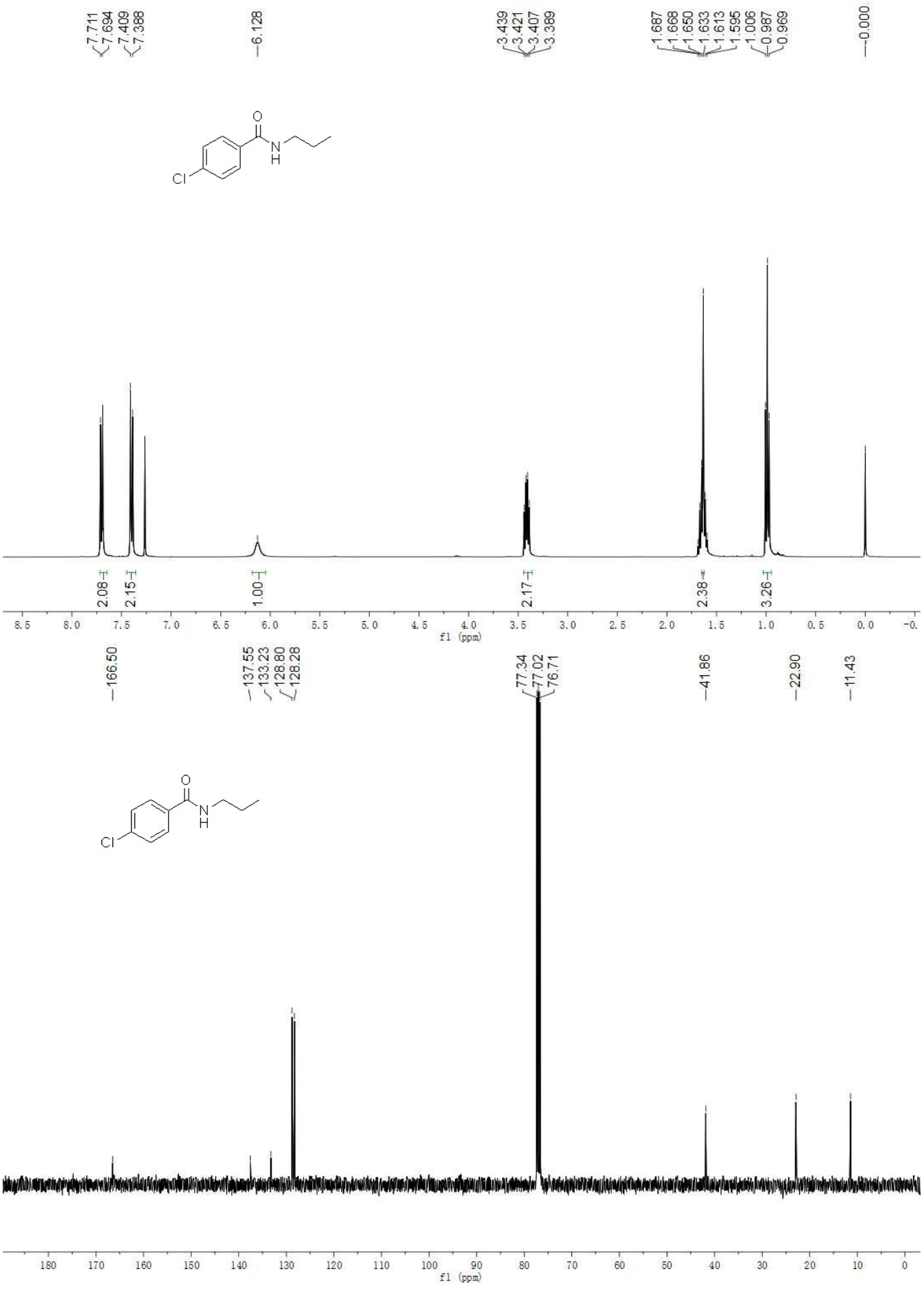

170.34
136.54
129.35
128.40
126.80
77.35
77.03
76.72
47.94
25.79
24.61
f1 (ppm)

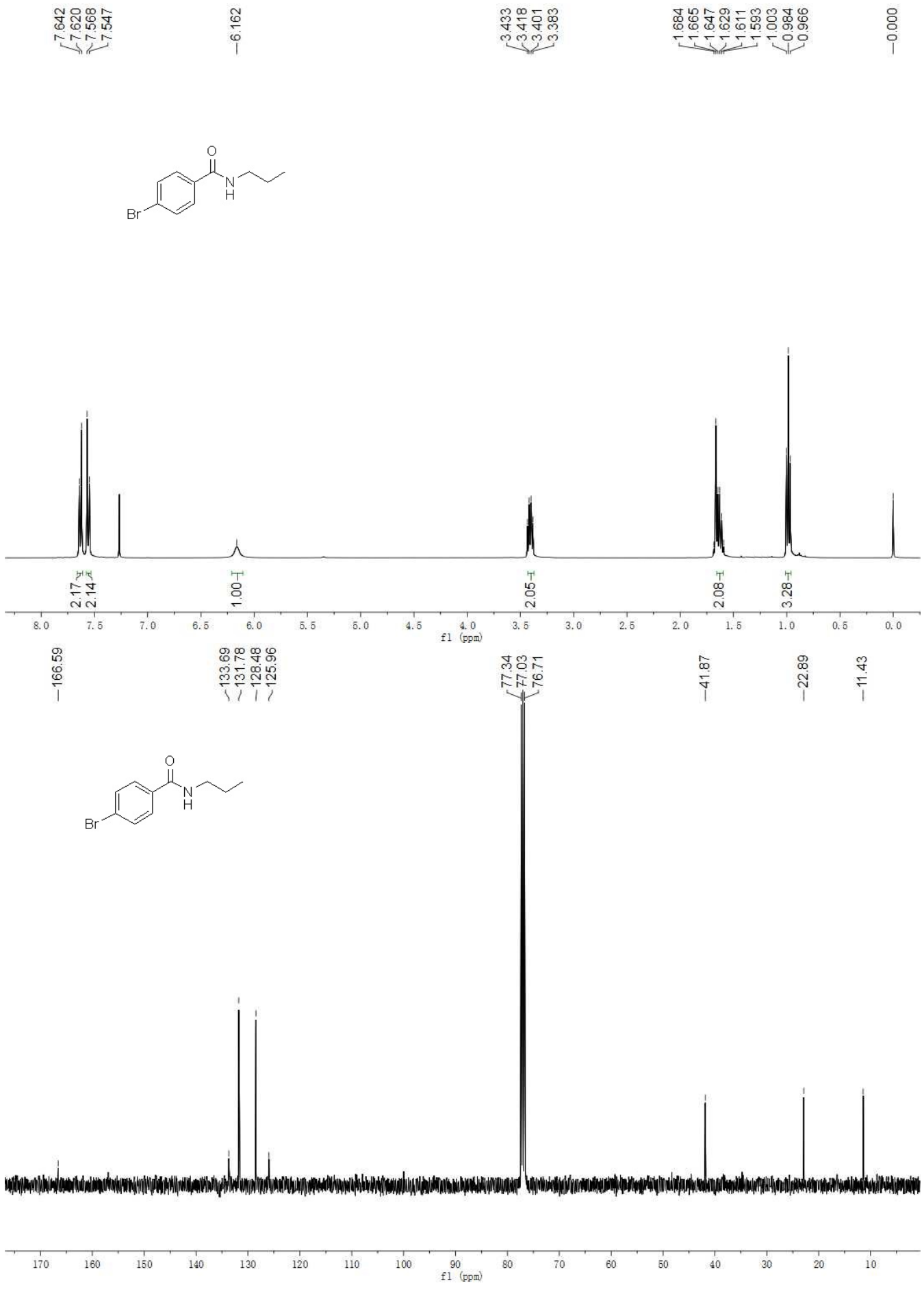

7.667
7.647
7.233
7.213
6.102
3.440
3.423
3.405
3.390
2.390
1.683
1.664
1.646
1.628
1.610
1.591
1.004
0.986
0.967
0.000
2.00
2.02
1.00
2.04
3.09
2.44
3.01
f1 (ppm)

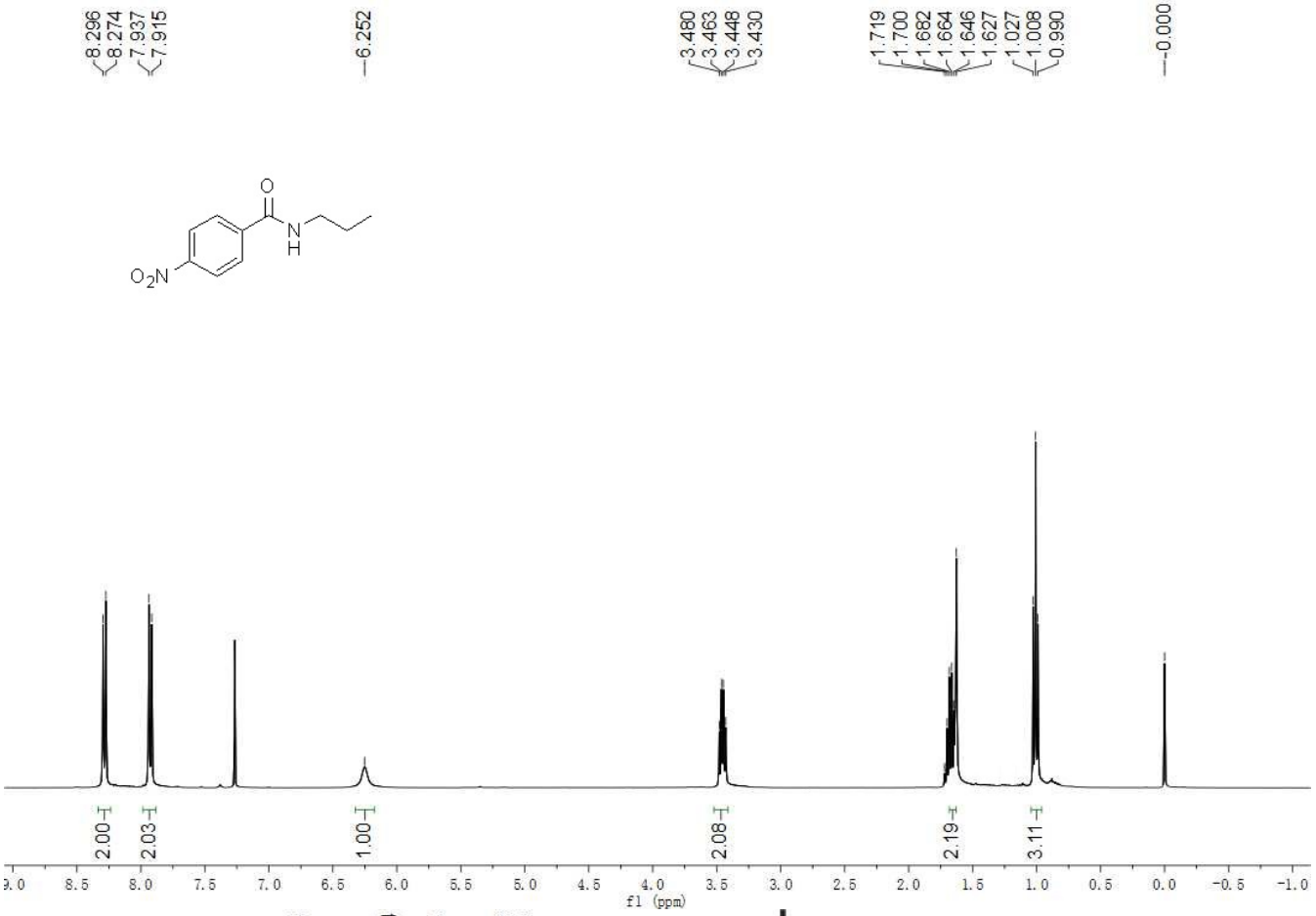

167.46
141.67
132.06
129.19
126.81
77.33
77.04
76.70
41.70
22.98
21.40
11.43
f1 (ppm)

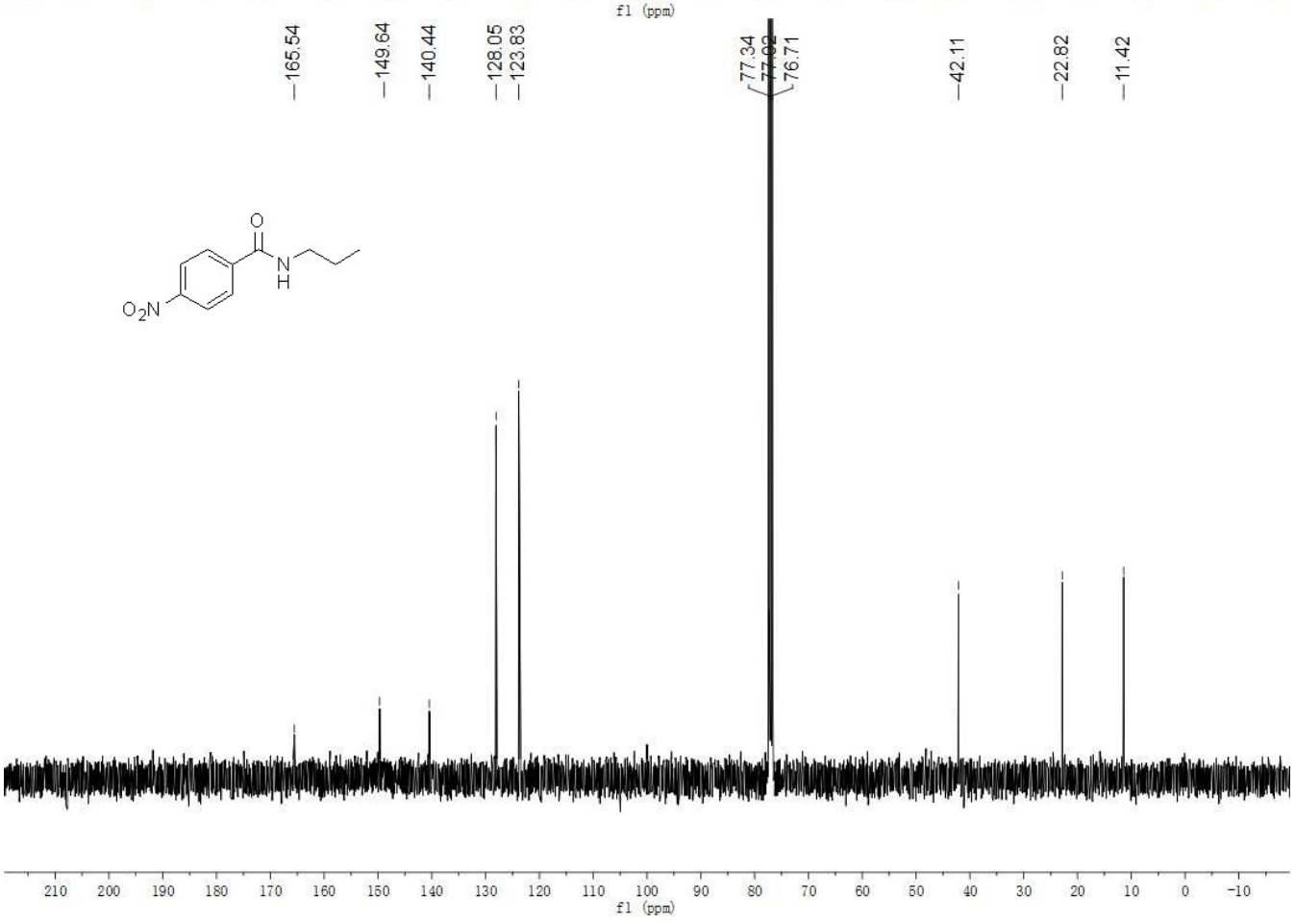

7.744
7.722
6.920
6.898
6.165
3.840
3.424
3.407
3.390
3.374
1.674
1.656
1.637
1.619
1.601
1.583
0.995
0.977
0.958
0.000
2.21
2.19
1.00
3.15
2.05
2.11
3.20
f1 (ppm)

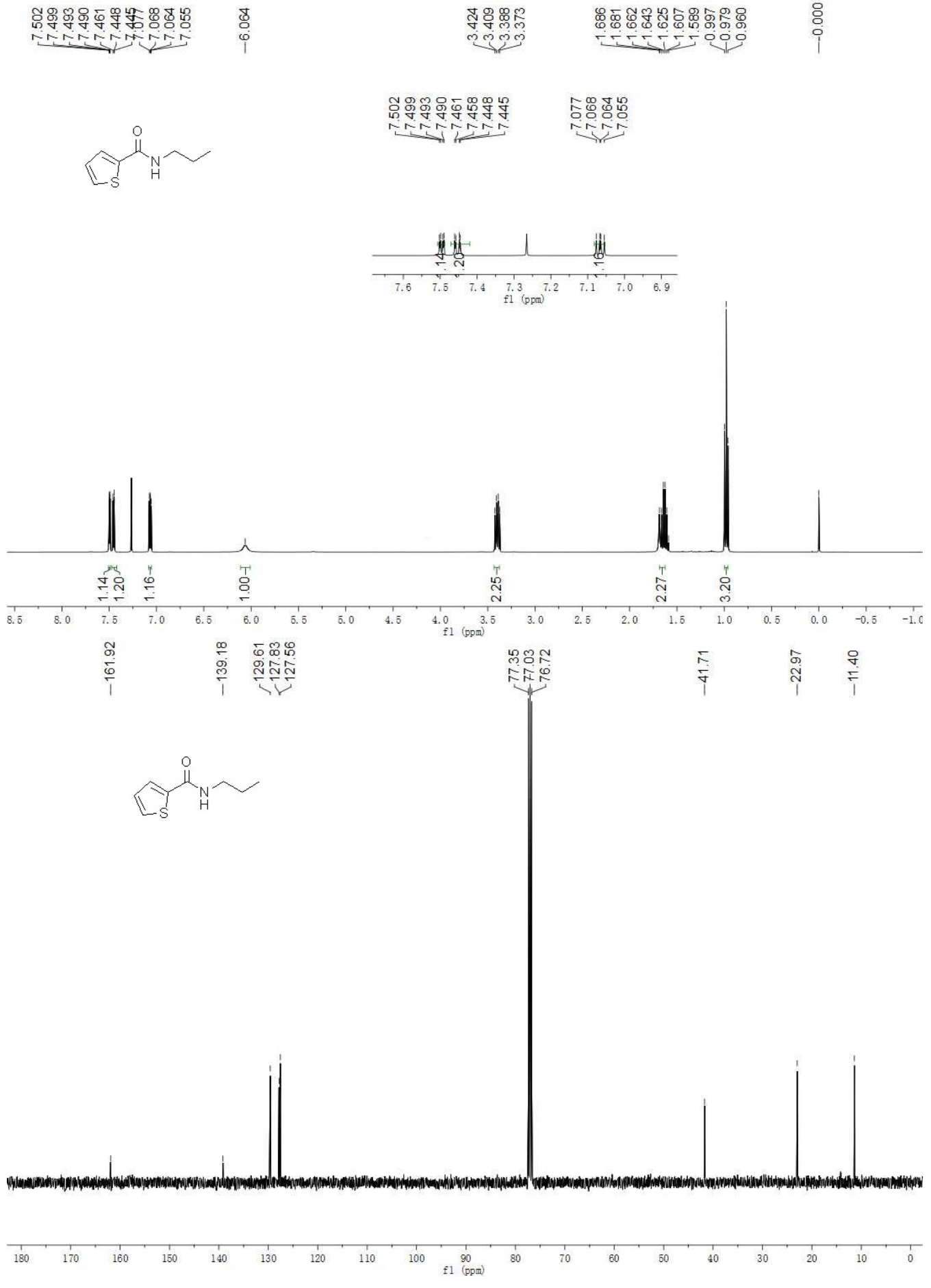

167.09
162.04
128.61
127.17
113.70
77.36
77.04
76.73
55.39
41.71
22.99
11.45
f1 (ppm)

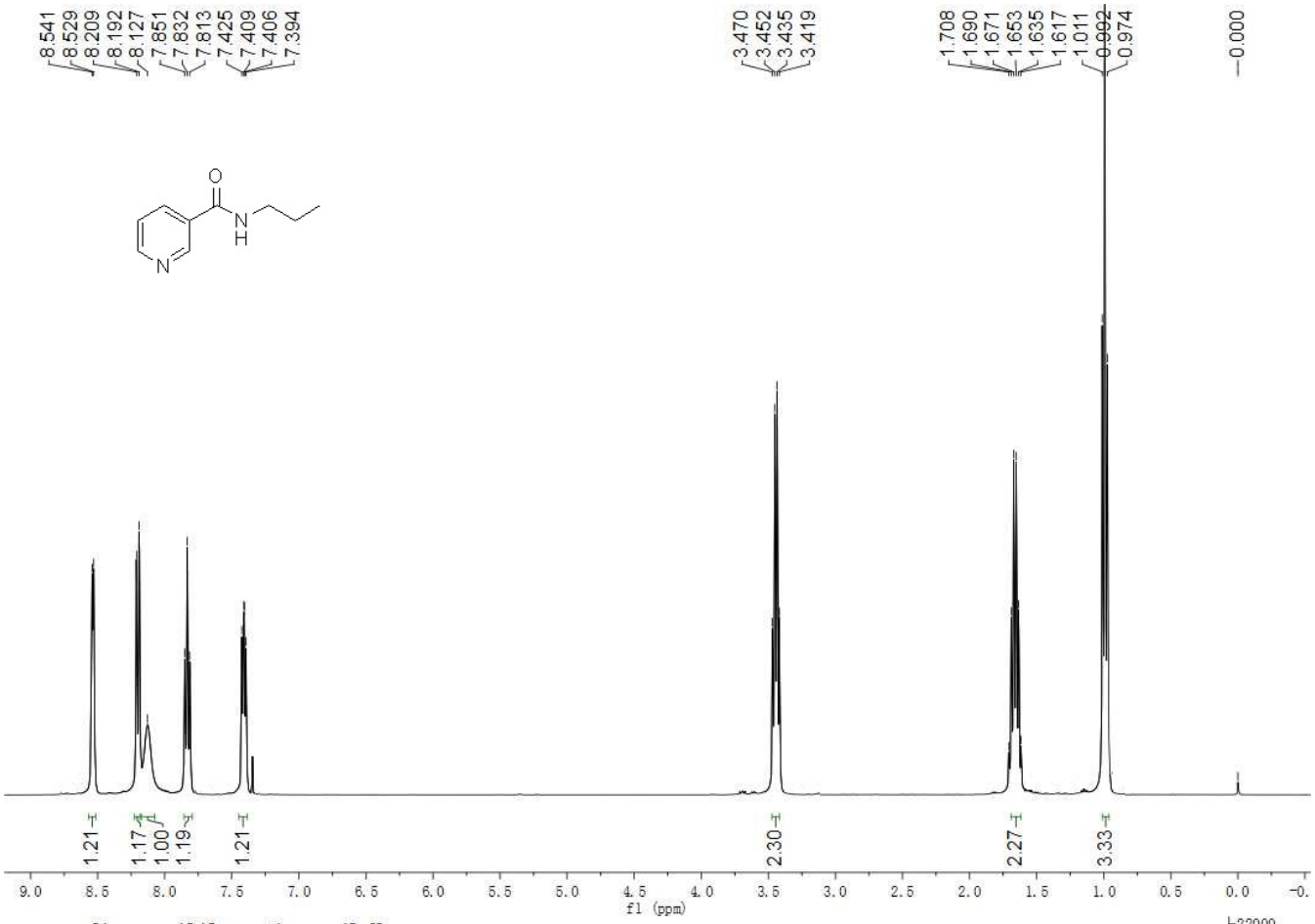

7.711
7.694
7.409
7.388
6.128
3.439
3.421
3.407
3.389
1.687
1.668
1.650
1.633
1.613
1.595
1.006
0.987
0.969
0.000
O
N
H
Cl
2.08
2.15
1.00
2.17
2.38
3.26
f1 (ppm)
166.50
137.55
133.23
128.80
128.28
77.34
77.02
76.71
41.86
22.90
11.43
O
N
H
Cl
f1 (ppm)

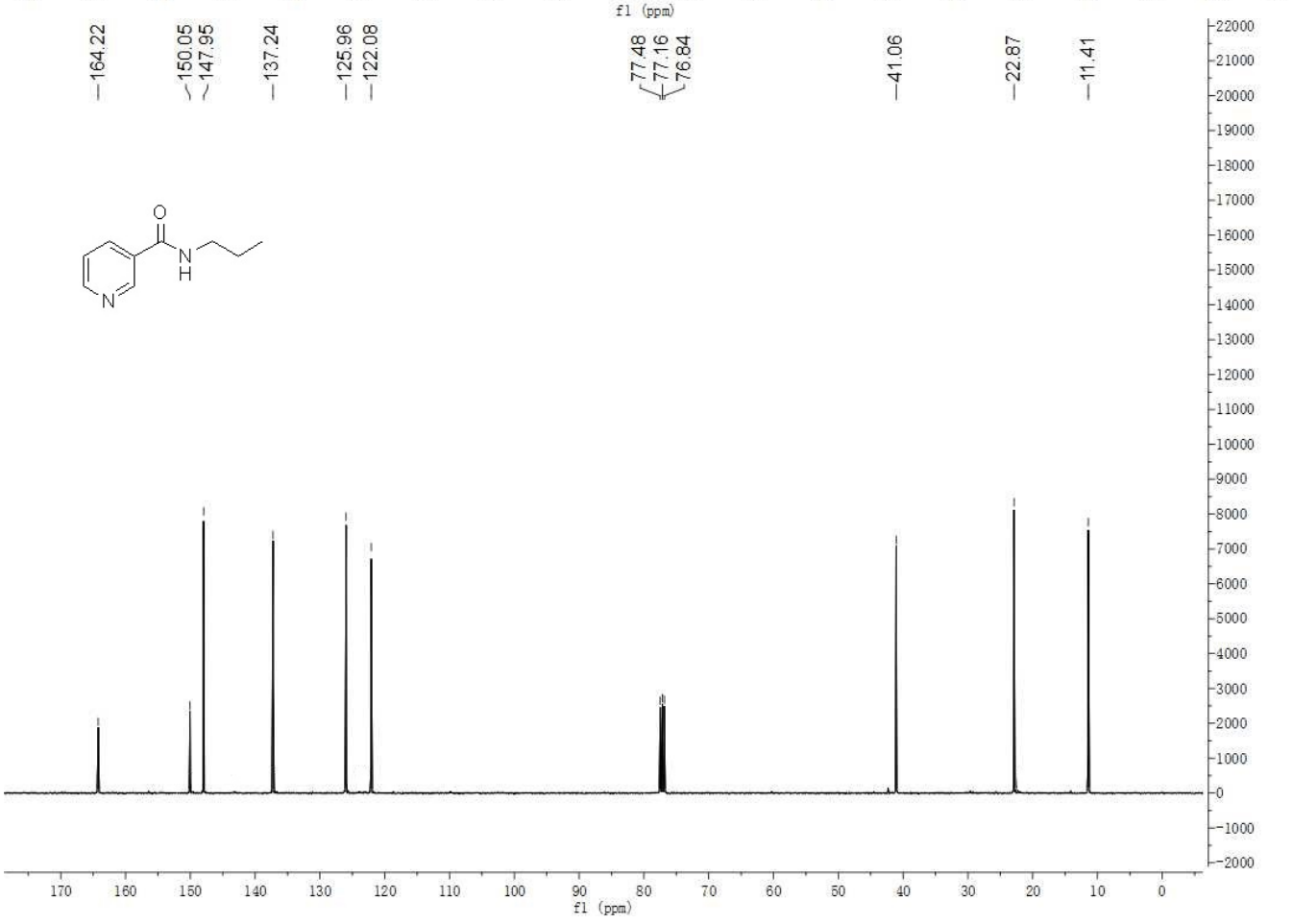

7.642
7.620
7.568
7.547
6.162
3.433
3.418
3.401
3.383
1.684
1.665
1.647
1.629
1.611
1.593
1.003
0.984
0.966
0.000
Br
2.17
2.14
1.00
2.05
2.08
3.28
f1 (ppm)
166.59
133.69
131.78
128.48
125.96
77.34
77.03
76.71
41.87
22.89
11.43
Br
f1 (ppm)

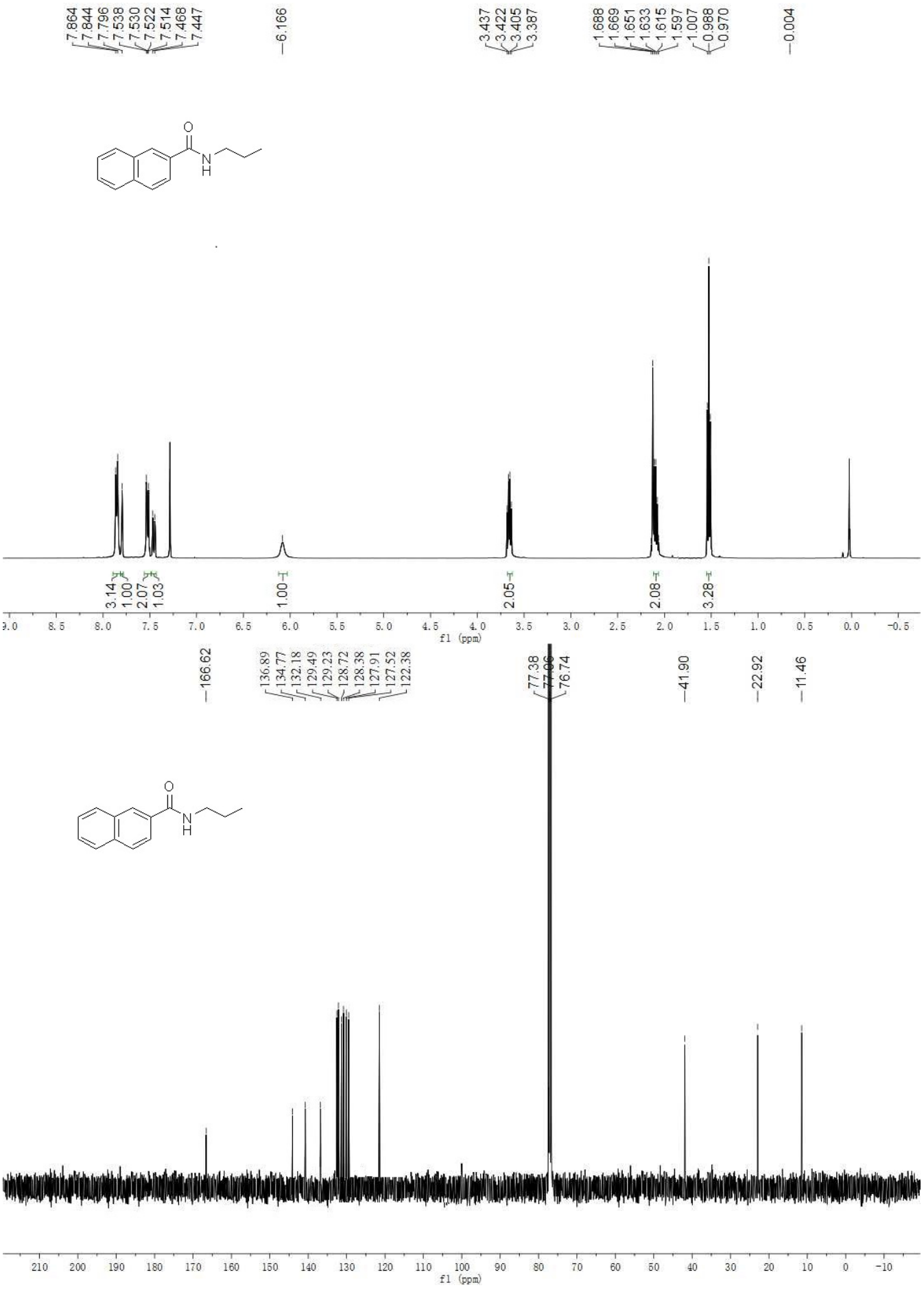

8.296
8.274
7.937
7.915
6.252
3.480
3.463
3.448
3.430
1.719
1.700
1.682
1.664
1.646
1.627
1.027
1.008
0.990
0.000
2.00
2.03
1.00
2.08
2.19
3.11
f1 (ppm)

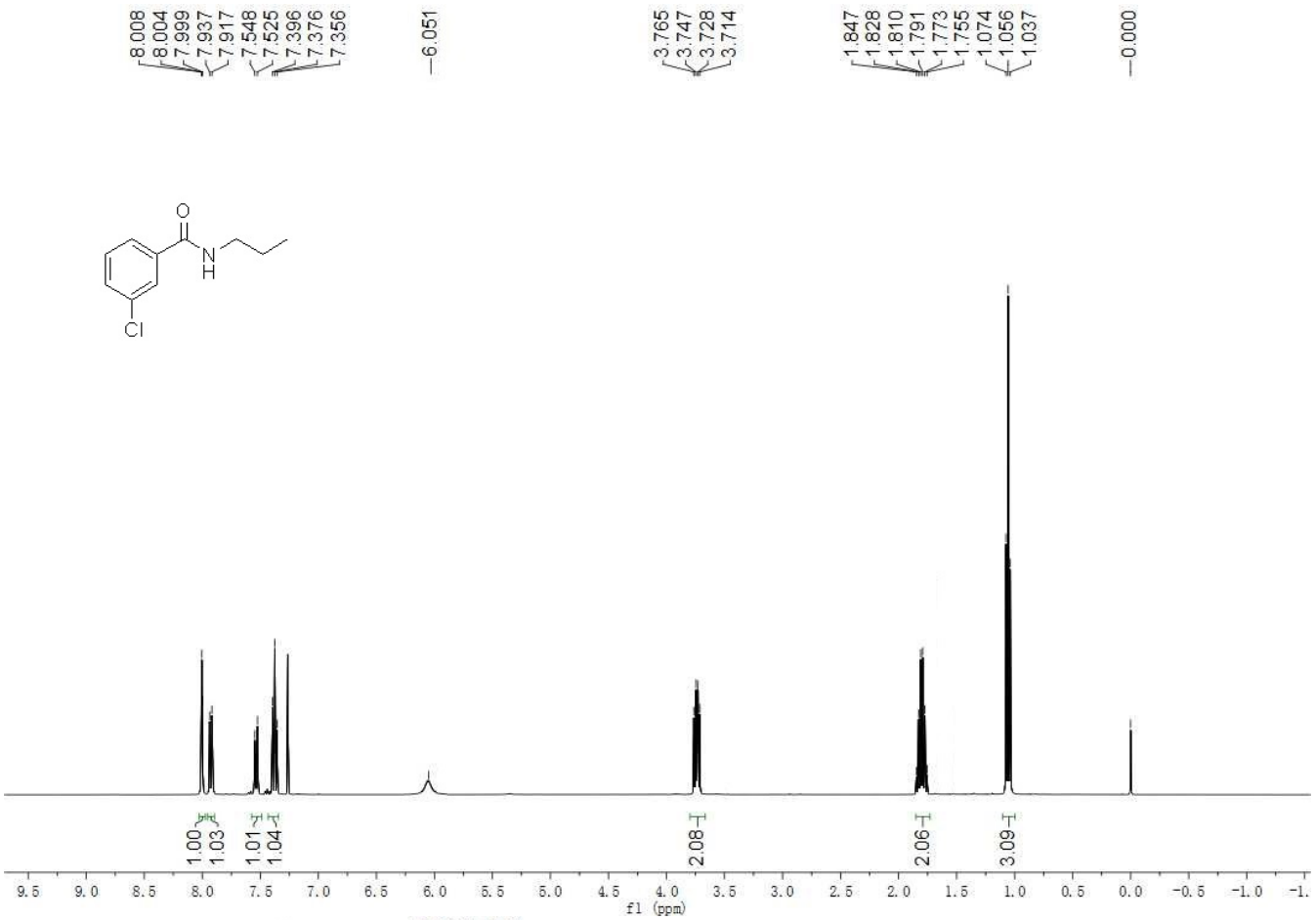

165.54
149.64
140.44
128.05
123.83
77.34
77.02
76.71
42.11
22.82
11.42
f1 (ppm)

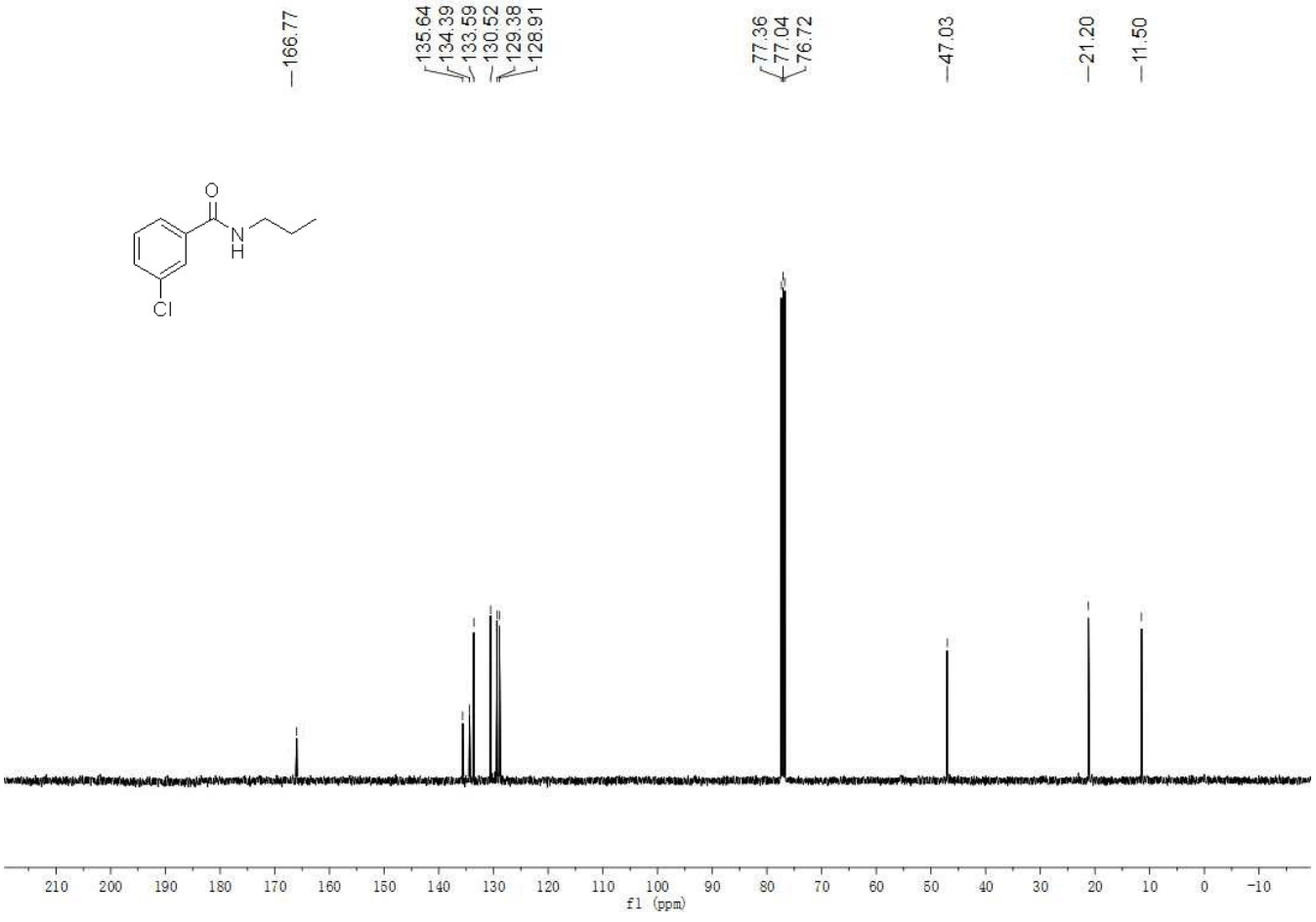

7.502
7.499
7.493
7.490
7.461
7.448
7.445
7.077
7.068
7.064
7.055
6.064
3.424
3.409
3.388
3.373
1.686
1.681
1.662
1.643
1.625
1.607
1.589
0.997
0.979
0.960
0.000
1.14
1.20
1.16
1.00
2.25
2.27
3.20
f1 (ppm)
161.92
139.18
129.61
127.83
127.56
77.35
77.03
76.72
41.71
22.97
11.40
f1 (ppm)

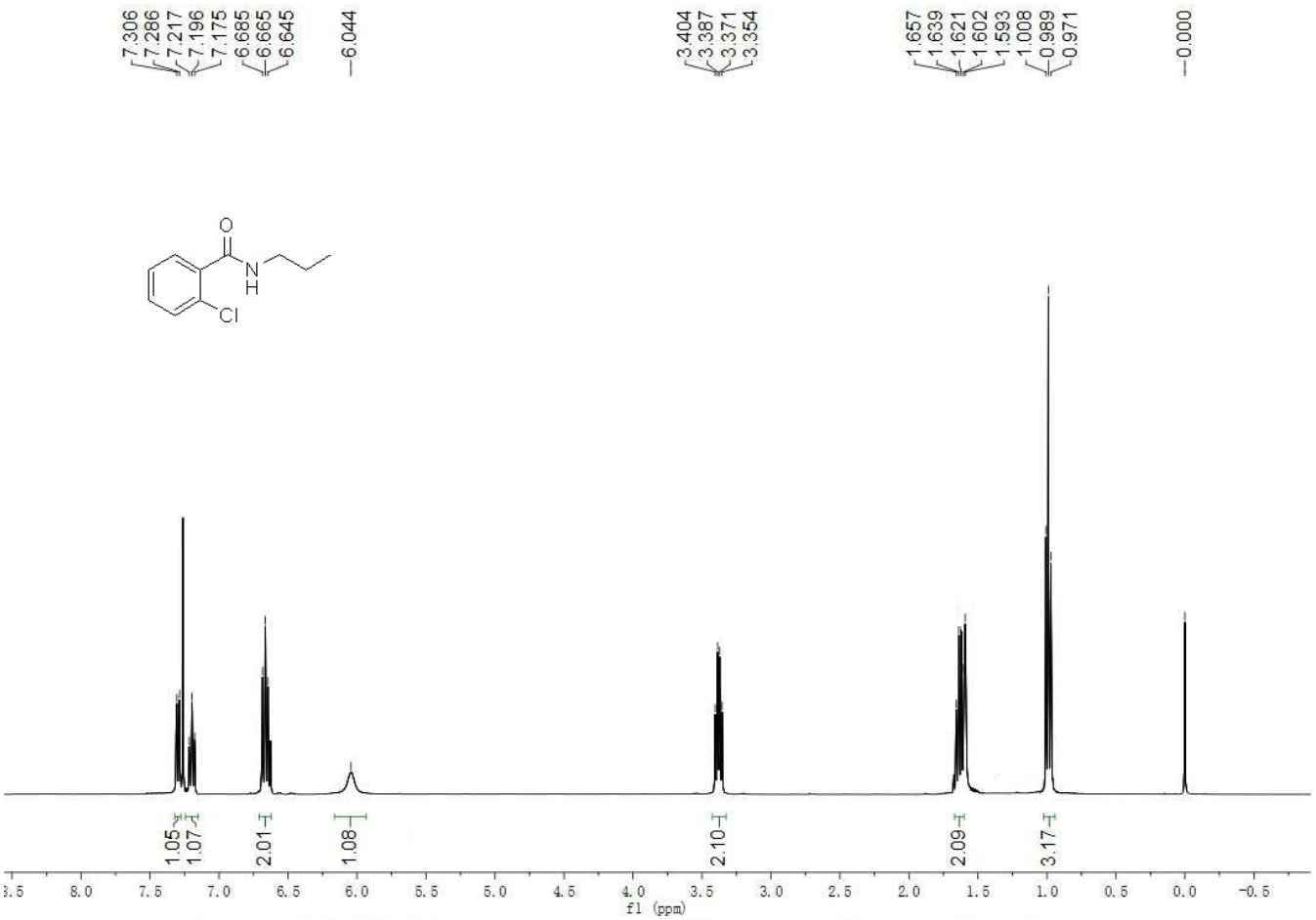

8.541
8.529
8.209
8.192
8.127
7.851
7.832
7.813
7.425
7.409
7.406
7.394
3.470
3.452
3.435
3.419
1.708
1.690
1.671
1.653
1.635
1.617
1.011
0.992
0.974
0.000
1.21
1.17
1.00
1.19
1.21
2.30
2.27
3.33
f1 (ppm)

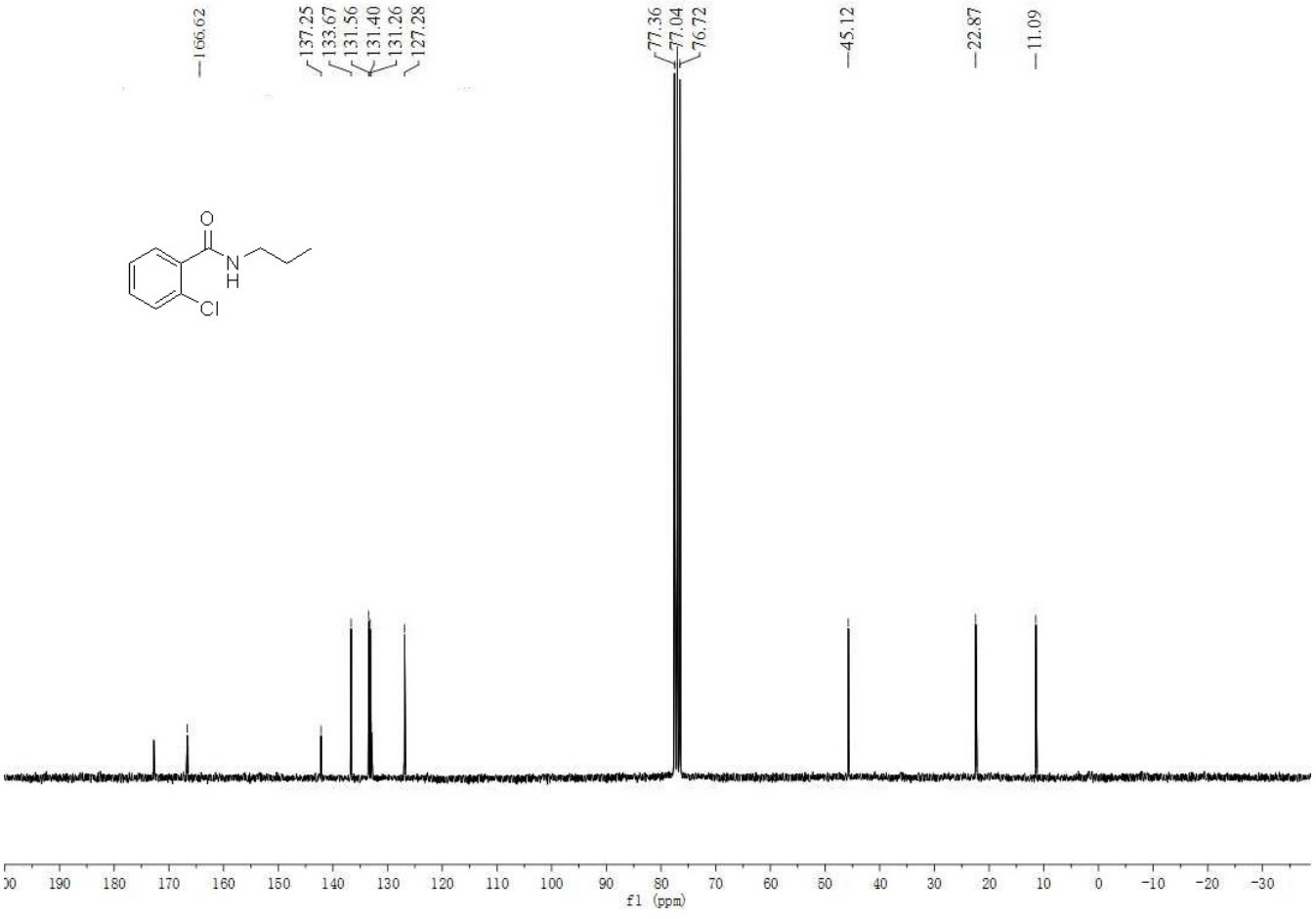

164.22
150.05
147.95
137.24
125.96
122.08
77.48
77.16
76.84
41.06
22.87
11.41
f1 (ppm)


7.864
7.844
7.796
7.538
7.530
7.522
7.514
7.468
7.447
6.166
3.437
3.422
3.405
3.387
1.688
1.669
1.651
1.633
1.615
1.597
1.007
0.988
0.970
0.004
3.14
1.00
2.07
1.03
1.00
2.05
2.08
3.28
f1 (ppm)
166.62
136.89
134.77
132.18
129.49
129.23
128.72
128.38
127.91
127.52
122.38
77.38
77.06
76.74
41.90
22.92
11.46
f1 (ppm)


8.008
8.004
7.999
7.937
7.917
7.548
7.525
7.396
7.376
7.356
6.051
3.765
3.747
3.728
3.714
1.847
1.828
1.810
1.791
1.773
1.755
1.074
1.056
1.037
0.000
1.00
1.03
1.01
1.04
2.08
2.06
3.09
f1 (ppm)


166.77
135.64
134.39
133.59
130.52
129.38
128.91
77.36
77.04
76.72
47.03
21.20
11.50
f1 (ppm)


7.306
7.286
7.217
7.196
7.175
6.685
6.665
6.645
6.044
3.404
3.387
3.371
3.354
1.657
1.639
1.621
1.602
1.593
1.008
0.989
0.971
0.000
O
N
H
Cl
1.05
1.07
2.01
1.08
2.10
2.09
3.17
f1 (ppm)


166.62
137.25
133.67
131.56
131.40
131.26
127.28
77.36
77.04
76.72
45.12
22.87
11.09
O
N
H
Cl
f1 (ppm)