Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Copper-Mediated Oxidative *N*-Cyanation Reaction Using CuCN

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1. General Considerations

All chemicals were used as received without further purification unless stated otherwise. ^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature on a 300, 400 or 500 MHz spectrometer (75, 100 or 125 MHz for ^{13}C). NMR experiments are reported in δ units, parts per million (ppm), and were referenced to $CDCl_3$ (δ 7.26 or 77.0 ppm) as the internal standard. The coupling constants *J* are given in Hz. Column chromatography was performed using EM Silica gel 60 (300-400 meshes) or neutral aluminum oxide (200-300 meshes).

2. Experimental Procedures

(a) General Procedure for 0.3 mmol Scale

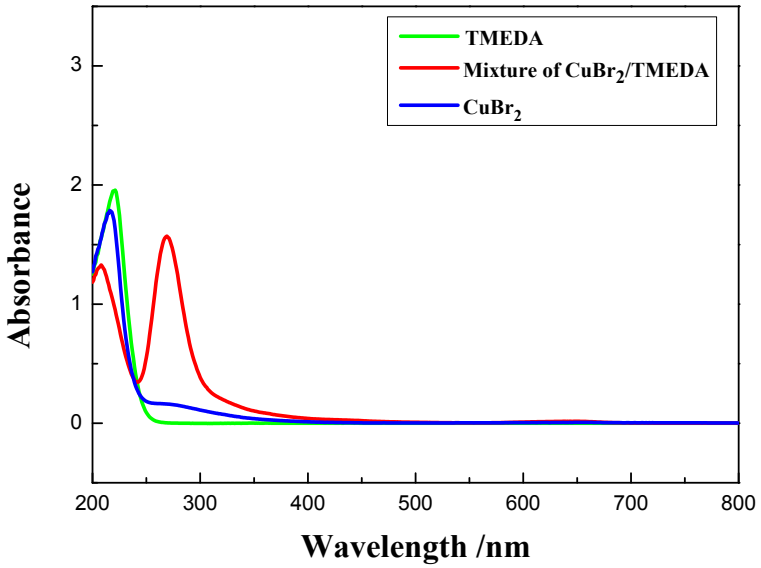
Under O_2, a 20 mL of Schlenk tube equipped with a stir bar was charged with *sec*-amine (0.3 mmol), CuCN (0.6 mmol, 53.7 mg), $CuBr_2$ (0.05 mol, 11.2 mg), TMEDA (0.6 mmol， 89 μL), Na_2SO_4 (0.6 mmol， 85.2 mg) and CH_3CN (3 mL). The tube was sealed with a Teflon lined cap. The reaction mixture was stirred at 50 °C for 12 h in oil bath. After the completion of the reaction (monitored by TLC), the solvent was concentrated in vacuum and the residue was purified by flash column chromatography on silica gel or Al_2O_3 with petroleum ether-ethyl acetate as the eluent to give the desired product.

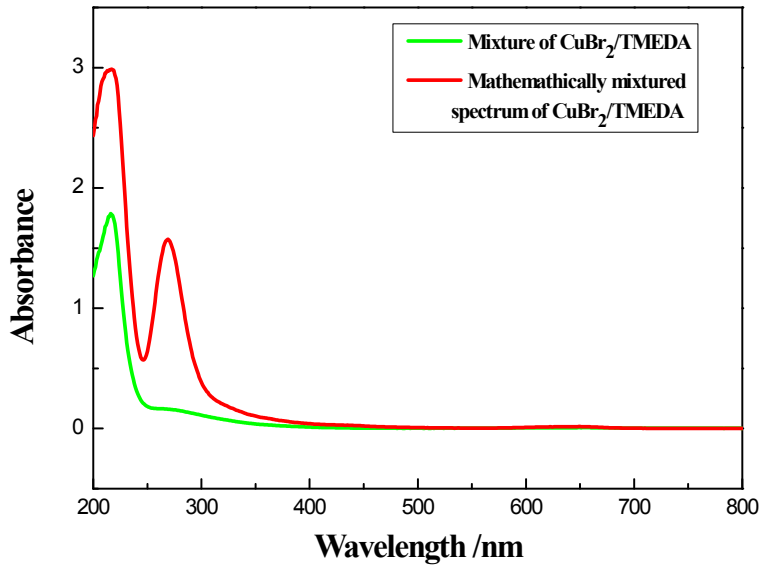
(b) Procedure for 20 mmol Scale

A 250 mL round-bottom flask equipped with a stir-bar was charged with *N*-methylbenzylamine (20 mmol, 2.42 g), CuCN (40 mmol, 3.50 g), $CuBr_2$ (1 mmol, 223 mg), TMEDA (40 mmol, 2.33 g), Na_2SO_4 (40 mmol, 2.84 g) and CH_3CN (125 mL). A balloon filled with oxygen gas was connected to the reaction flask. The reaction mixture was stirred at 50 °C for 12 h in oil bath. After the completion of the reaction (monitored by TLC), the solvent was concentrated in vacuum and the residue was purified by flash column chromatography on silica gel with petroleum ether-ethyl acetate as the eluent to give the desired product.

3. Research of Mechanism

(a) Test of UV





UV-Vis Analysis:

All absorbance measurements were carried out on an UVmini-1240 spectrophotometer equipped with a quartz cell. The concentration of $CuBr_2$ and TMEDA were 0.0015 mg/mL and 0.015 mg/mL, respectively.

The above UV-Vis results imply that TMEDA acts as a ligand.

(b) Consumption of O_2

Consumption of O_2 in Blank Experiment:

Under O_2, a Schlenk tube equipped with a stir bar was charged with CuCN (0.4 mmol), $CuBr_2$ (0.03 mol), TMEDA (0.4 mmol), Na_2SO_4 (0.4 mmol) and CH_3CN (3 mL). The reaction mixture was stirred at 50 °C for 12 h in oil bath. Then, consumption of O_2 was tested, and the amount of O_2 was 2.3 mL.

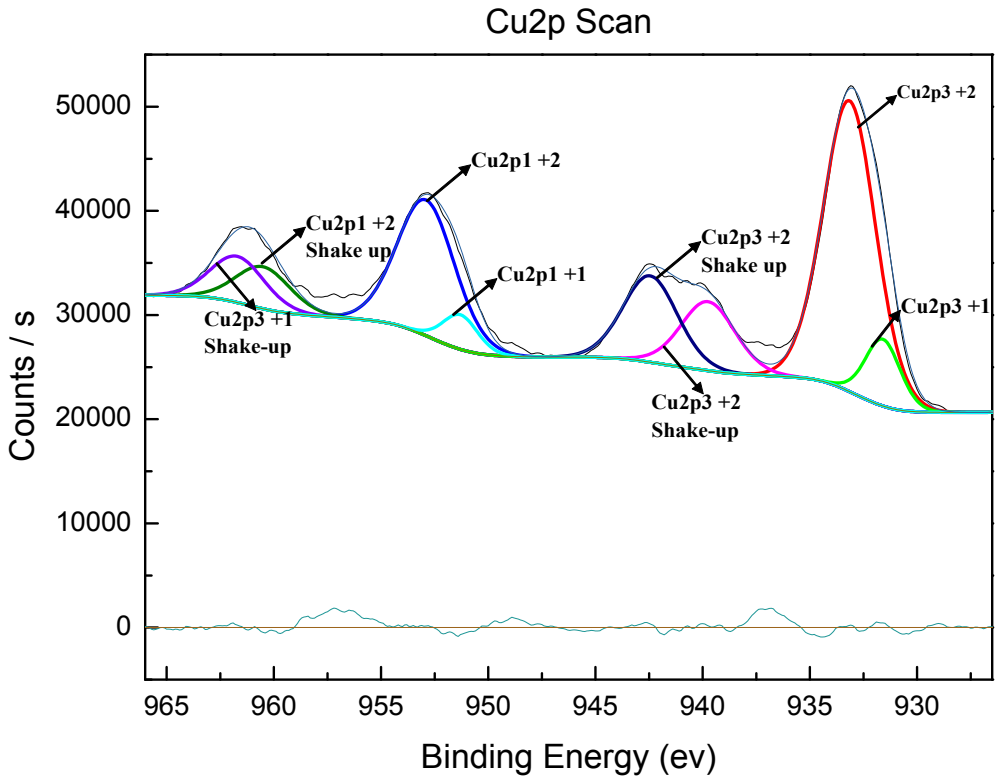
Consumption of O_2 in Cyanation Reaction:

Under O_2, a Schlenk tube equipped with a stir bar was charged with *N*-methylbenzylamine (0.2 mmol), CuCN (0.4 mmol), $CuBr_2$ (0.03 mol), TMEDA (0.4 mmol), Na_2SO_4 (0.4 mmol) and CH_3CN (3 mL). The reaction mixture was stirred at 50 °C for 12 h in oil bath. Then, consumption of O_2 was tested and found to be 4.1 mL. The test temperature is 8 ^oC.

The consumed O_2 for the oxidative coupling is 1.8 mL. After calculation, the consumed O_2 was 0.078 mmol and the *N*-cyanation product was 0.166 mmol. Thus, the ratio of the consumed O_2 and the *N*-cyanation product was found to be nearly 1:2.

(c) XPS Study

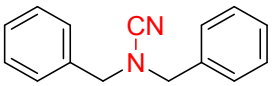
X-ray photoelectron spectroscopy (XPS) was carried for the determination of Cu oxidation state.



The above XPS results indicated that almost Cu (Ⅰ) was converted to Cu (Ⅱ).

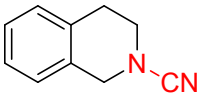
4. Characterization Data for the Products

_N,N_-Dibenzylcyanamide (3a): [1]



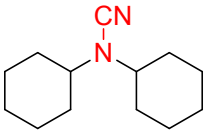
White solid; m.p.: 51-53 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 4.12 (s, 4H), 7.30-7.34 (m, 4H), 7.36-7.43 (m, 6H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 54.1, 118.3, 128.6, 128.6, 128.8, 134.2. IR(prism): 3049, 3041, 3018, 2930, 2881, 2210, 1616, 1586, 1500, 1460, 1080, 733, 689.

3,4-Dihydro-2(1H)-isoquinolinecarbonitrile (3b):



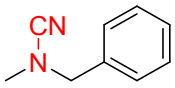
White solid; m.p.: 68-70 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.96 (t, J = 5.8 Hz, 2H), 3.48 (t, J = 5.9 Hz, 2H), 4.41 (s, 2H), 7.03-7.06 (m, 1H), 7.12-7.22 (m, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 27.4, 46.5, 49.8, 117.8, 125.8, 126.5, 127.0, 129.0, 130.6, 132.4. MS (EI): 158 (M^+); HRMS (ESI) m/z calcd for $C_{10}H_{11}N_2$ $(M+H)^+$ 159.0917, found 159.0913. IR(prism): 3092, 3041, 2941, 2902, 2861, 2215, 1610, 1592, 1502.

Dicyclohexylcyanamide (3c):



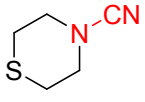
Yellowish liquid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.08-1.29 (m, 6H), 1.37-1.48 (m, 4H), 1.58-1.61 (m, 2H), 1.77-1.90 (m, 8H), 2.70-2.78 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 25.0, 25.1, 31.7, 58.0, 115.4. MS (EI): 206 (M^+); HRMS (ESI) m/z calcd for $C_{12}H_{23}N_2$ $(M+H)^+$ 207.1856, found 207.1858. IR(neat): 2951, 2856, 2192, 1460.

Benzylmethylcyanamide (3d):



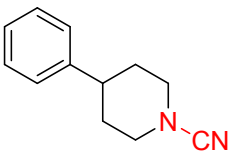
Colorless liquid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.68 (s, 3H), 4.06 (s, 2H), 7.23-7.31 (m, 5H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 37.6, 56.9, 118.6, 128.2, 128.4, 128.7, 134.2. MS (EI): 146 (M^+); HRMS (ESI) m/z calcd for $C_9H_{11}N_2$ $(M+H)^+$ 147.0917, found 147.0908. IR(neat): 3041, 3016, 2948, 2908, 2223, 1610, 1460.

Thiomorpholine-4-carbonitrile (3e):



White solid; m.p.: 41-43 °C. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 2.70 (t, J = 5.1 Hz, 4H), 3.46 (t, J = 5.1 Hz, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 26.1, 50.8, 117.4. MS (EI): 128 (M^+); HRMS (ESI) m/z calcd for $C_5H_9N_2S$ $(M+H)^+$ 129.0481, found 129.0478. IR(prism): 2958, 2921, 2849, 2209, 1460.

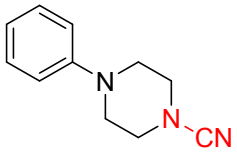
4-Phenylpiperidine-1-carbonitrile (3f):



White solid; m.p.: 69-71 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.74-

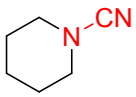
1.76 (m, 4H), 2.48-2.53 (m, 1H), 3.04-3.06 (m, 2H), 3.40-3.44 (m, 2H), 7.09-7.26 (m, 5H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 31.7, 40.9, 49.8, 118.1, 126.4, 126.5, 128.4, 144.4. MS (EI): 186 (M^+); HRMS (ESI) *m/z* calcd for $C_{12}H_{15}N_2$ $(M+H)^+$ 187.1230, found 187.1222. IR(prism): 3058, 3041, 2947, 2932, 2853, 2209, 1605, 1483, 1455.

4-Phenylpiperazine-1-carbonitrile (3g):



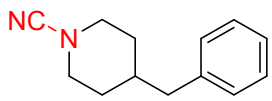
Yellowish liquid. ^{1}H NMR ($CDCl_3$, 400MHz) δ 3.23 (t, *J* = 4.5 Hz, 4H), 3.39 (t, *J* = 4.5 Hz, 4H), 6.90-6.94 (m, 3H), 7.27-7.31 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 48.7, 49.0, 117.0, 117.4, 121.1, 129.2, 150.6. MS (EI): 187 (M^+); HRMS (ESI) *m/z* calcd for $C_{11}H_{14}N_3$ $(M+H)^+$ 188.1182, found 188.1183. IR(neat): 3073 3042, 2966, 2907, 2825, 2209, 1597, 1586, 1498, 1452.

Piperidine-1-carbonitrile (3h):



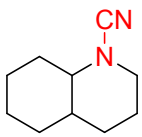
Colorless liquid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.56-1.58 (m, 2H), 1.61-1.66 (m, 4H), 3.15-3.18 (m, 4H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 23.0, 24.5, 50.1, 118.6. MS (EI): 110 (M^+); HRMS (ESI) *m/z* calcd for $C_6H_{11}N_2$ $(M+H)^+$ 111.0917, found 111.0914. IR(neat): 2917, 2848, 2209, 1453.

4-Benzylpiperidine-1-carbonitrile (3i):



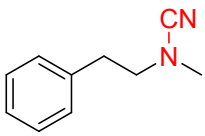
Colorless liquid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.20-1.37 (m, 2H), 1.49-1.62 (m, 3H), 2.48-2.51 (m, 2H), 2.84-2.93 (m, 2H), 3.30-3.36 (m, 2H), 7.05-7.08 (m, 2H), 7.12-7.26 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 30.8, 36.8, 42.8, 49.7, 118.5, 126.2, 128.4, 129.0, 139.3. MS (EI): 200 (M^+); HRMS (ESI) *m/z* calcd for $C_{13}H_{17}N_2$ $(M+H)^+$ 201.1386, found 201.1382. IR(neat): 3088, 3058, 3031, 2947, 2914, 2848, 2217, 1602, 1503, 1458.

Octahydroquinoline-1(2H)-carbonitrile (3j):



Colorless liquid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.87-1.06 (m, 2H), 1.15-1.40 (m, 4H), 1.56-1.66 (m, 5H), 1.78-1.81 (m, 1H), 1.98-2.01 (m, 1H), 2.38-2.39 (m, 1H) , 2.96-2.99 (m, 1H) , 3.36-3.39 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 24.5, 24.8, 25.2, 29.9, 30.8, 31.8, 40.7, 51.0, 62.1, 116.5. MS (EI): 164 (M^+); HRMS (ESI) *m/z* calcd for $C_{10}H_{17}N_2$ $(M+H)^+$ 165.1386, found 165.1380. IR(neat): 2941, 2862, 2213, 1460, 1122.

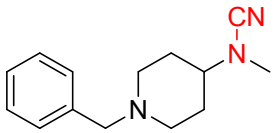
***N*-methyl-*N*-phenethylcyanamide (3k):**



Colorless liquid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.82 (s, 3H), 2.93-2.98 (m, 2H), 3.20-3.25 (m, 2H), 7.22-7.36 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 33.8, 39.1, 54.3, 118.2, 126.8, 128.6, 128.6,

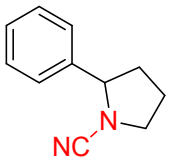
137.4. MS (EI): 160 (M^+); HRMS (ESI) *m/z* calcd for $C_{10}H_{13}N_2$ $(M+H)^+$ 161.1073, found 161.1063. IR(neat): 3088, 3068, 3036, 2932, 2858, 2209, 1593, 1503, 1456.

***N*-(1-Benzylpiperidin-4-yl)-*N*-methylcyanamide (3l):**



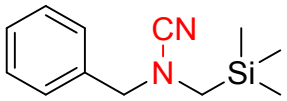
Colorless liquid. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 1.68-1.76 (m, 2H), 1.88-1.90 (m, 2H), 1.99-2.04 (m, 2H), 2.74-2.75 (m, 1H), 2.84 (s, 3H), 2.89-2.92 (m, 2H), 3.49 (s, 2H), 7.23-7.26 (m, 1H), 7.28-7.32 (m, 4H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 29.5, 36.6, 51.8, 58.2, 62.5, 117.3, 127.0, 128.2, 128.8, 138.1. MS (EI): 229 (M^+); HRMS (ESI) *m/z* calcd for $C_{14}H_{20}N_3$ $(M+H)^+$ 230.1652, found 230.1656. IR(neat): 3090, 3068, 3036, 2932, 2863, 2210, 1062.

2-Phenylpyrrolidine-1-carbonitrile (3m):



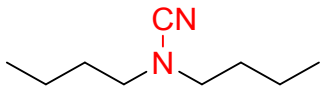
Colorless liquid. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 1.82-1.89 (m, 1H), 1.94-2.07 (m, 2H), 2.29-2.36 (m, 1H), 3.56-3.60 (m, 1H), 3.68-3.72 (m, 1H), 4.64-4.67 (m, 1H), 7.28-7.32 (m, 3H), 7.35-7.38 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 24.7, 35.5, 51.4, 65.8, 116.9, 126.2, 128.1, 128.7, 139.6. MS (EI): 172 (M^+); HRMS (ESI) *m/z* calcd for $C_{11}H_{12}N_2Na$ $(M+Na)^+$ 195.0893, found 195.0879. IR(neat): 3058, 3045, 2982, 2961, 2883, 2218, 1608, 1496, 1453.

***N*-Benzyl-*N*-((trimethylsilyl)methyl)cyanamide (3n):**



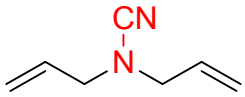
Colorless liquid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.15 (s, 9H), 2.36 (s, 2H), 4.16 (s, 2H), 7.30-7.42 (m, 5H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ -2.3, 40.9, 59.4, 119.4, 128.4, 128.4, 128.8, 134.8. MS (EI): 218 (M^+); HRMS (ESI) *m/z* calcd for $C_{12}H_{19}N_2Si$ $(M+H)^+$ 219.1312, found 219.1294. IR(neat): 3089, 3067, 3042, 2956, 2903, 2209, 1697, 1613, 1502, 1458, 1370, 1253.

***N,N*-Dibutylcyanamide (3o):**



Colorless liquid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.91-0.96 (m, 6H), 1.32-1.44 (m, 4H), 1.56-1.66 (m, 4H), 2.94-2.99 (m, 4H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 13.6, 19.6, 29.6, 51.2, 117.9. MS (EI): 154 (M^+); HRMS (ESI) *m/z* calcd for $C_9H1_9N_2$ $(M+H)^+$ 155.1543, found 155.1532. IR(neat): 2958, 2932, 2869, 2209, 1360.

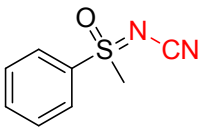
***N,N*-Diallylcyanamide (3p):**



Colorless liquid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 3.59-3.61 (m, 4H), 5.27-5.33 (m, 4H), 5.76-5.87 (m, 2H); ^{13}C NMR ($CDCl_3$,

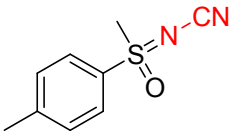
125 MHz) δ 53.3, 117.5, 120.5, 130.8. MS (EI): 122 (M^+); HRMS (ESI) *m/z* calcd for $C_7H_{11}N_2$ $(M+H)^+$ 123.0917, found 123.0907. IR(neat): 3012, 2923, 2851, 2216, 1451.

_N_-(Cyano) methyl phenyl sulfoximine (4a): [2]



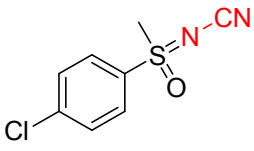
White solid; m.p.: 69-72 °C. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 3.34 (s, 3H), 7.66-7.69 (m, 2H), 7.77-7.78 (m, 1H), 7.80-7.99 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 44.7, 111.8, 127.8, 130.2, 135.4, 135.9. IR(prism): 3193, 3012, 2919, 2853, 2197, 1625, 1470, 1378, 1253, 1188, 1143.

_N_-(Cyano) methyl 4-methylphenyl sulfoximine (4b):



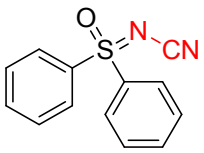
White solid; m.p.: 84-86 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.48 (s, 3H), 3.31 (s, 3H), 7.44-7.47 (m, 2H), 7.83-7.86 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 21.6, 44.8, 112.0, 127.8, 130.8, 132.7, 146.9. MS (EI): 194 (M^+); HRMS (ESI) *m/z* calcd for $C_9H_{11}N_2OS$ $(M+H)^+$ 195.0587, found 195.0579. IR(prism): 3022, 2993, 2923, 2173, 1583, 1492, 1376.

_N_-(Cyano) methyl 4-chlorophenyl sulfoximine (4c):



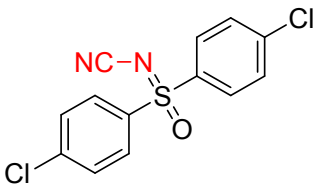
White solid; m.p.: 108-110 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 3.35 (s, 3H), 7.63-7.68 (m, 2H), 7.91-7.96 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 44.8, 111.4, 129.4, 130.6, 134.3, 142.6. MS (EI): 214 (M^+); HRMS (ESI) *m/z* calcd for $C_8H_8ClN_2OS$ $(M+H)^+$ 215.0040, found 215.0035. IR(prism): 3096, 3022, 2923, 2197, 1572, 1480, 1390, 1250, 1197, 820, 780.

_N_-(Cyano) diphenyl sulfoximine (4d): [2]



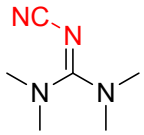
White solid; m.p.: 108-110 °C. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.56-7.59 (m, 4H), 7.65-7.68 (m, 2H), 7.97-7.98 (m, 4H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 111.9, 127.7, 129.9, 134.7, 137.0. IR(prism): 3084, 3060, 3026, 3005, 2197, 1578, 1477, 1245.

_N_-(Cyano)-4,4'-Dichlorodiphenyl sulfoximine (4e):



White solid; m.p.: 137-139 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.56-7.59 (m, 4H), 7.90-7.93 (m, 4H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 111.2, 129.3, 130.5, 135.2, 142.1. MS (EI): 310 (M^+); HRMS (ESI) *m/z* calcd for $C_{13}H_8Cl_2N_2OSNa$ $(M+Na)^+$ 332.9627, found 332.9613. IR(prism): 3086, 3067, 3047, 3026, 2203, 1578, 1472, 1258, 1196, 1082, 824, 761.

2-Cyano-1,1,3,3-tetramethylguanidine (4f):



Yellowish liquid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.93 (s, 12H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 39.9, 117.6, 166.0. MS (EI): 140 (M^+); HRMS (ESI) *m*/*z* calcd for $C_6H_{13}N_4$ $(M+H)^+$ 141.1135, found 141.1136. IR(neat): 3087, 3042, 2963, 2891, 2186, 1450, 1259.

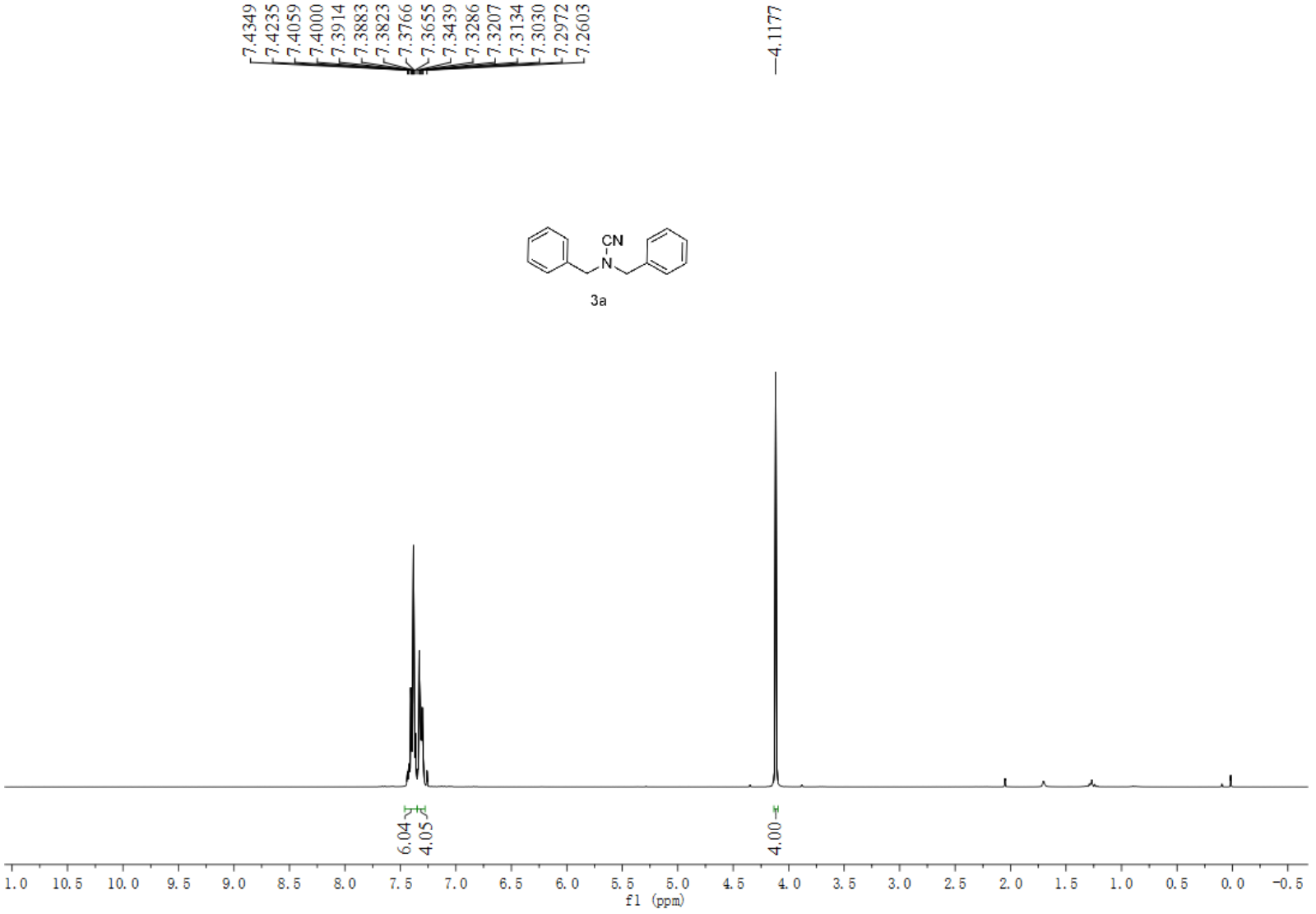
5. References

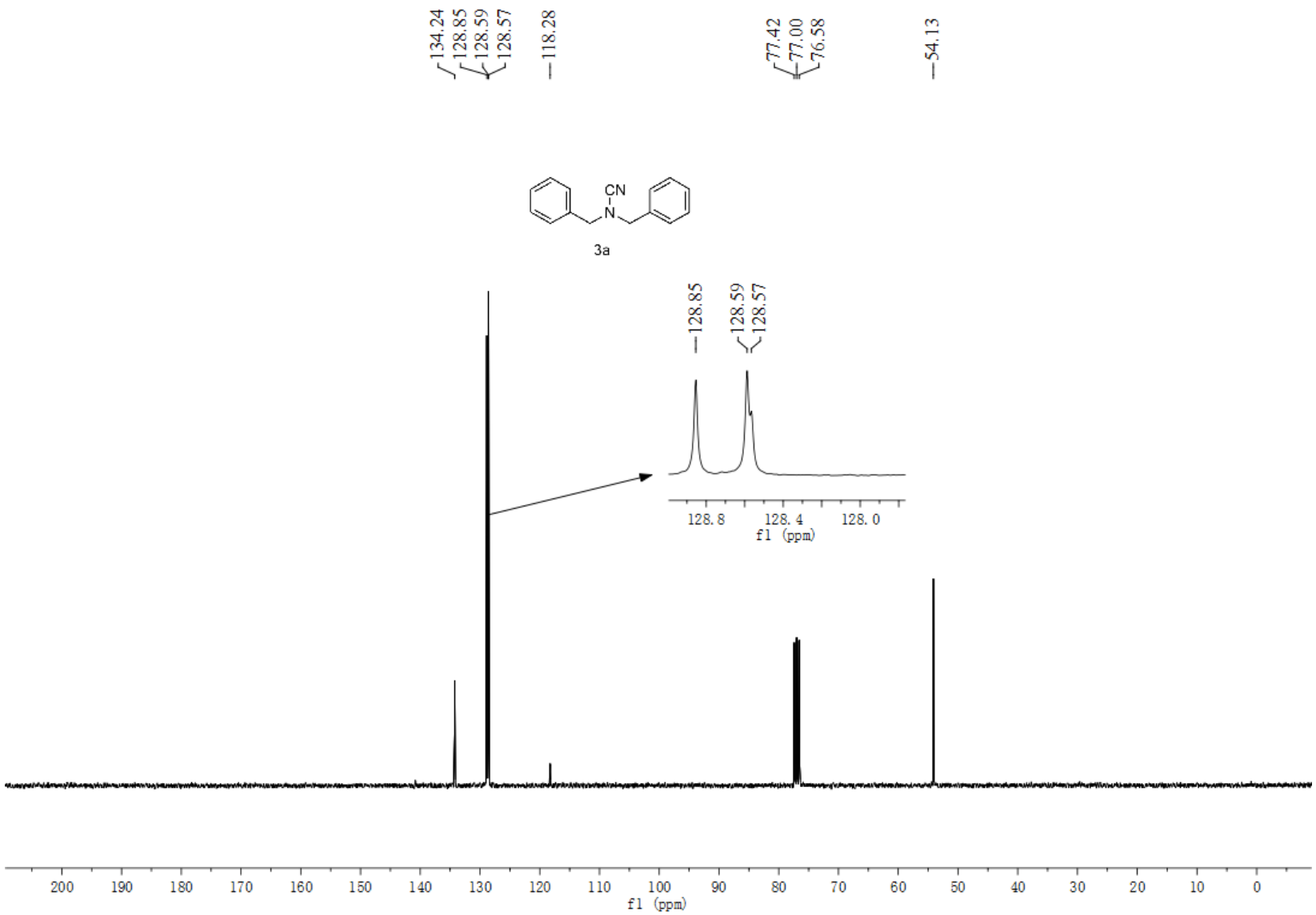
1 C. Zhu, J.-B. Xia and C. Chen, *Org. Lett.*, 2014, **16**, 247.

2 O. G. Mancheño, O. Bistri, and C. Bolm, *Org. Lett.,* 2007, **9**, 3809.

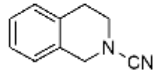
6. Copies of the ^{1}H NMR and ^{13}C NMR spectra

***N*,*N*-Dibenzylcyanamide (3a)**

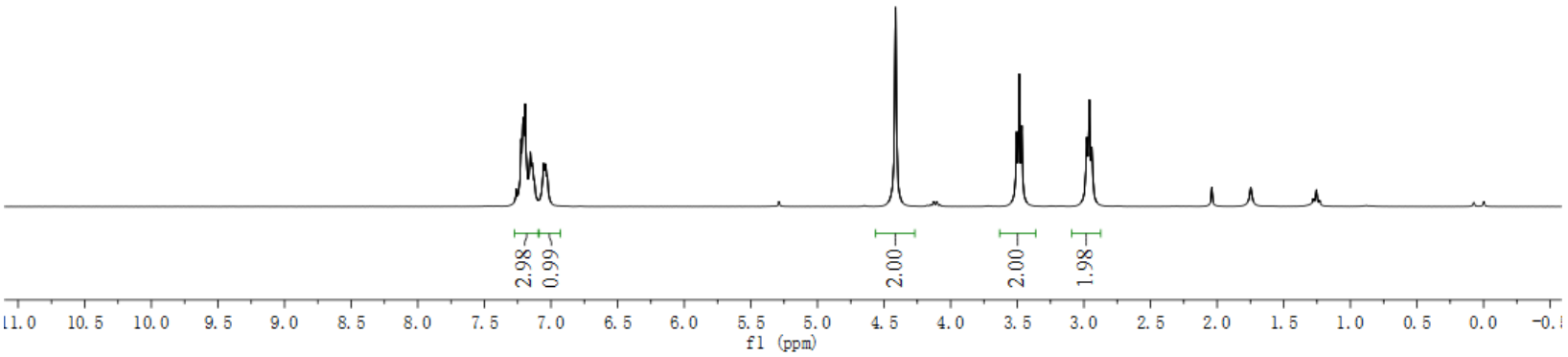


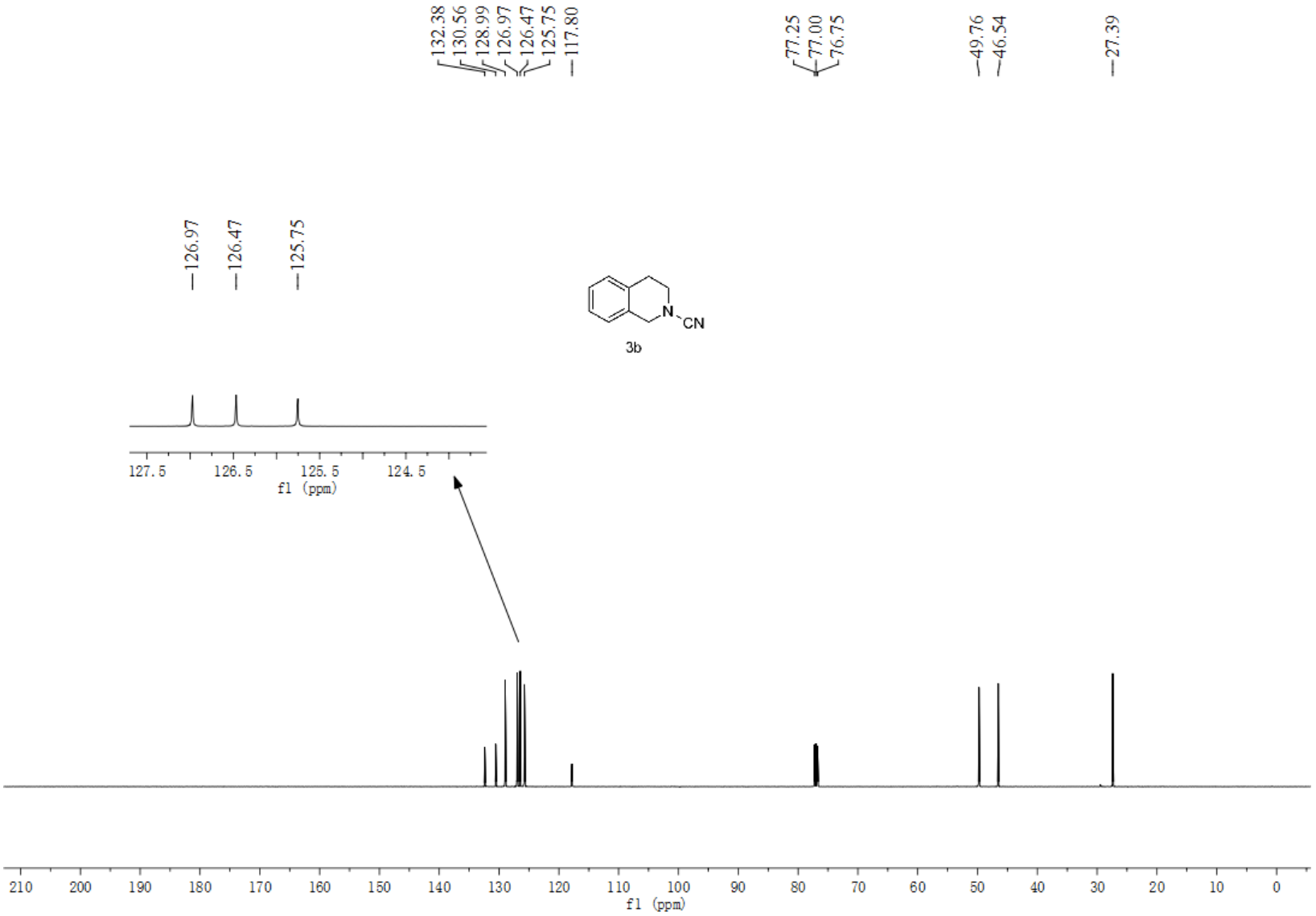

134.24
128.85
128.59
128.57
118.28
77.42
77.00
76.58
54.13
CN
N
3a
128.85
128.59
128.57
128.8
128.4
128.0
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3,4-Dihydro-2(1H)-isoquinolinecarbonitrile (3b)

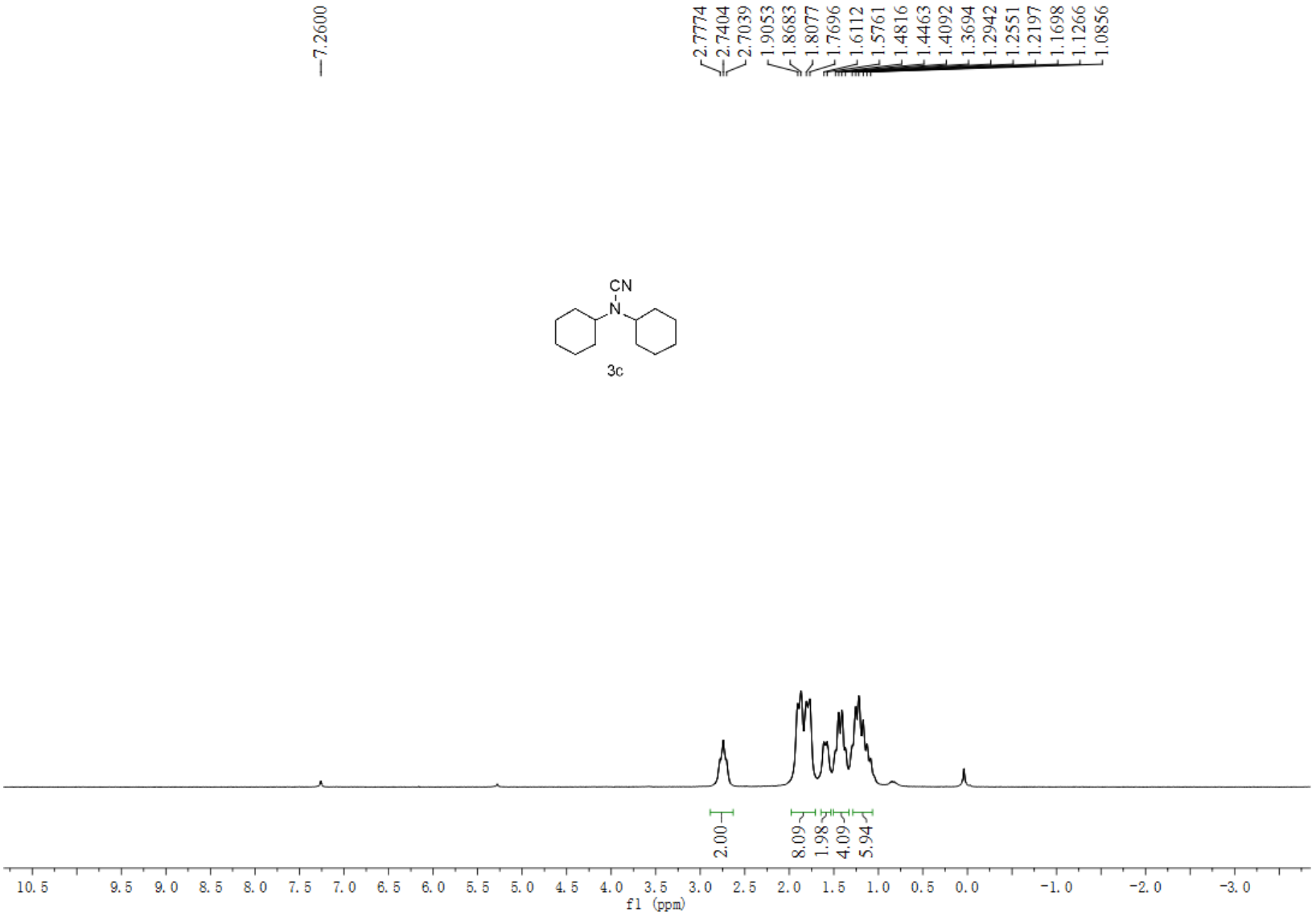


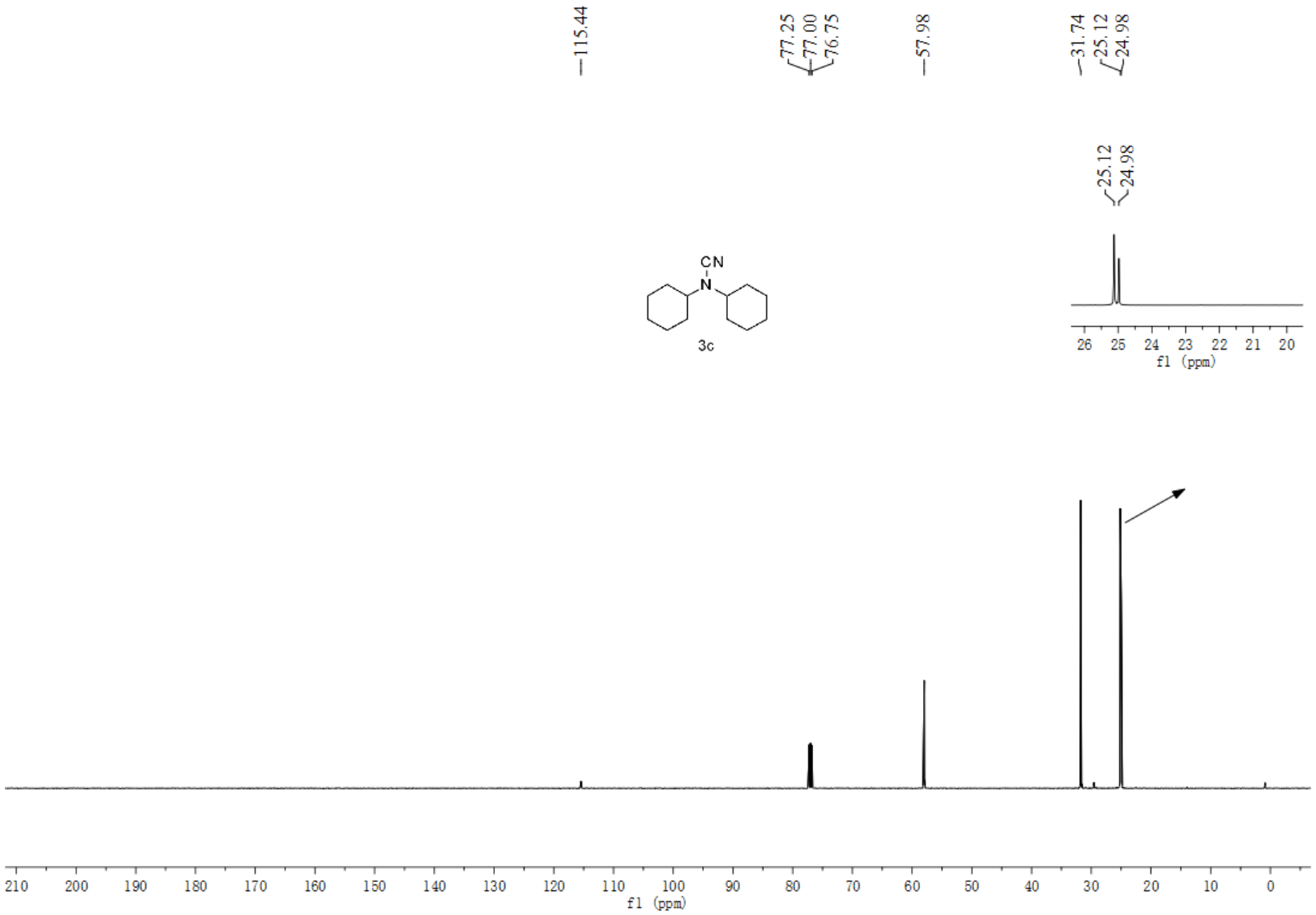
3b



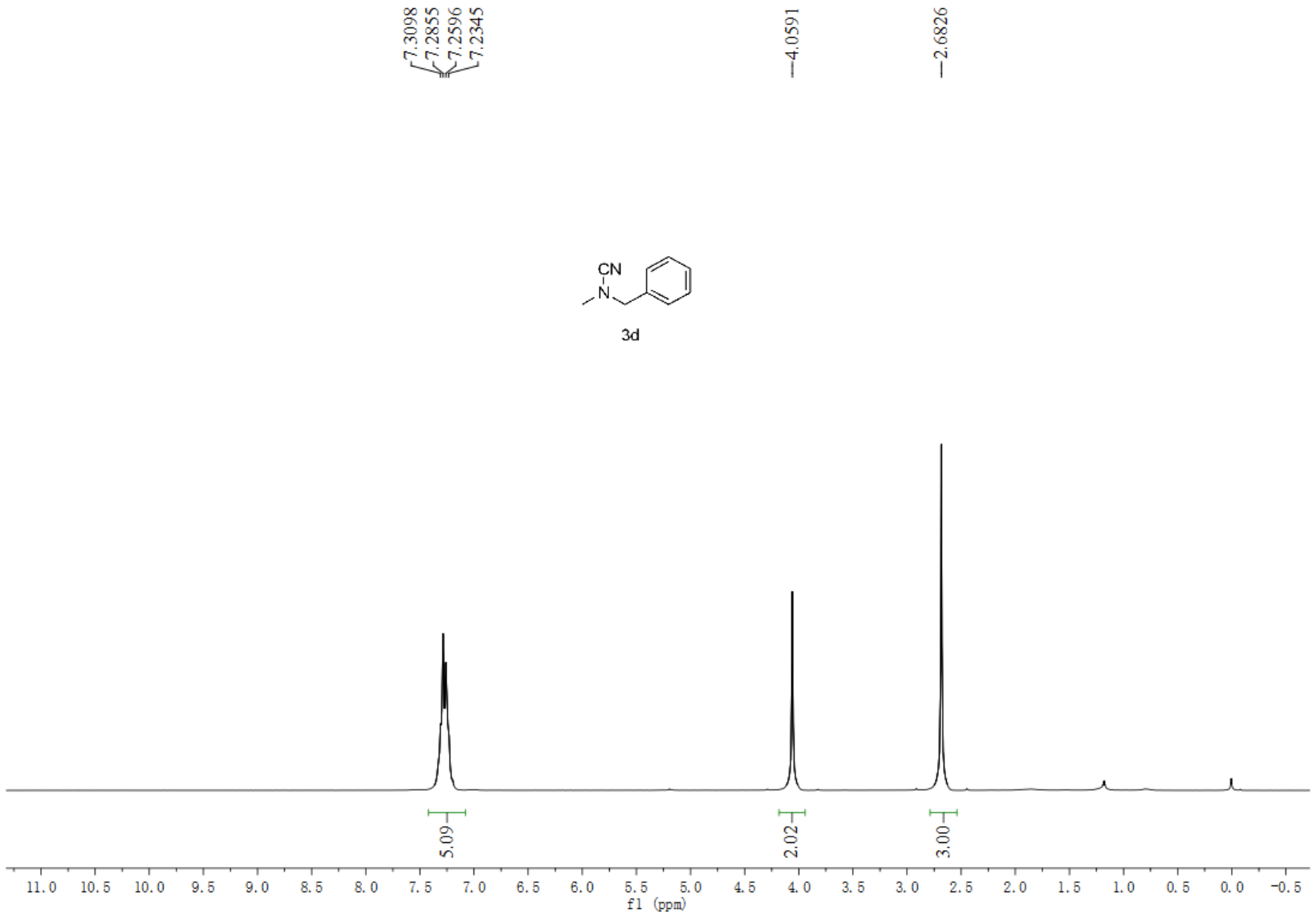

132.38
130.56
128.99
126.97
126.47
125.75
117.80
77.25
77.00
76.75
49.76
46.54
27.39
126.97
126.47
125.75
N
CN
3b
127.5
126.5
125.5
124.5
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

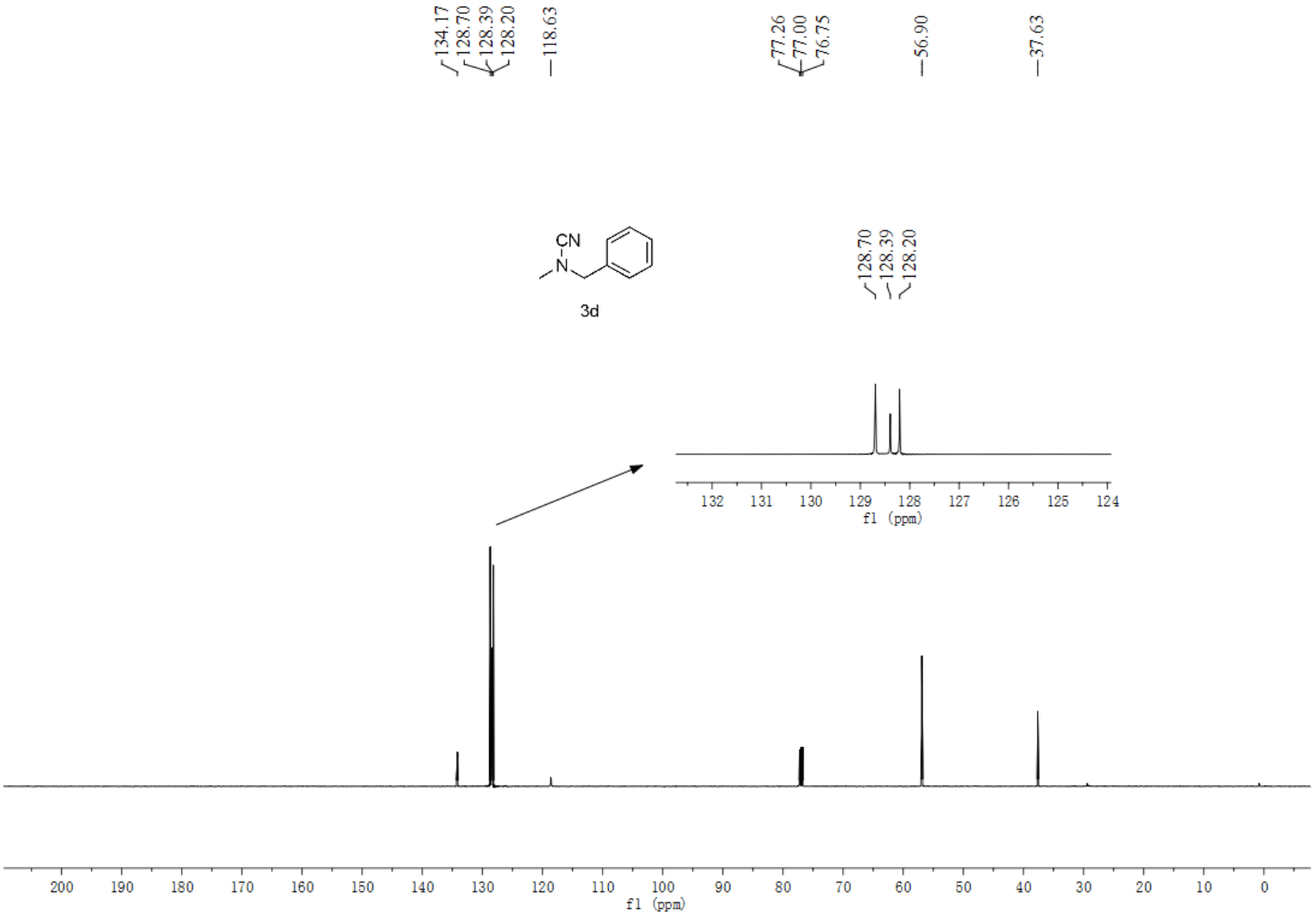
Dicyclohexylcyanamide (3c)



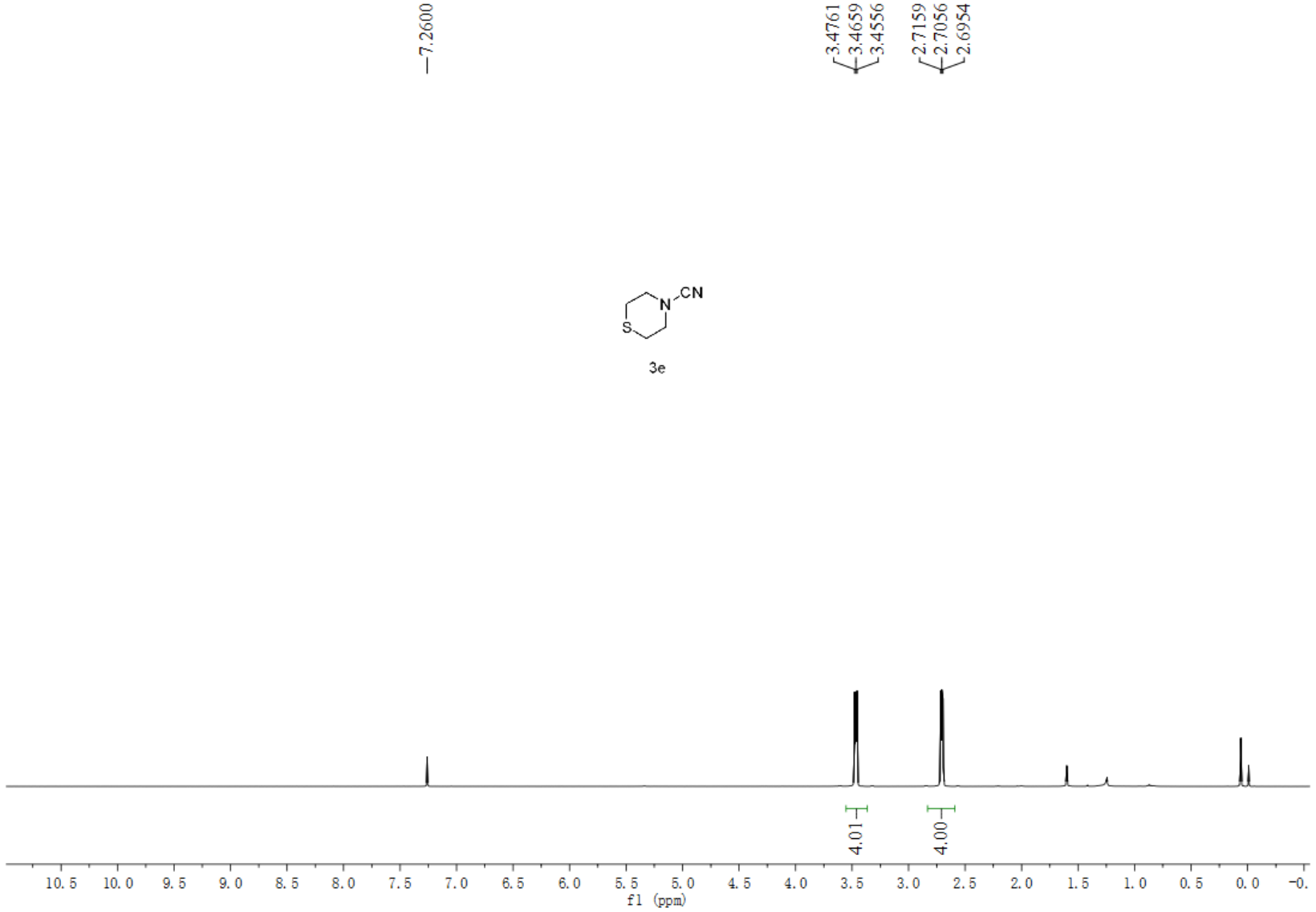

115.44
77.25
77.00
76.75
57.98
31.74
25.12
24.98
CN
N
3c
25.12
24.98
26 25 24 23 22 21 20
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

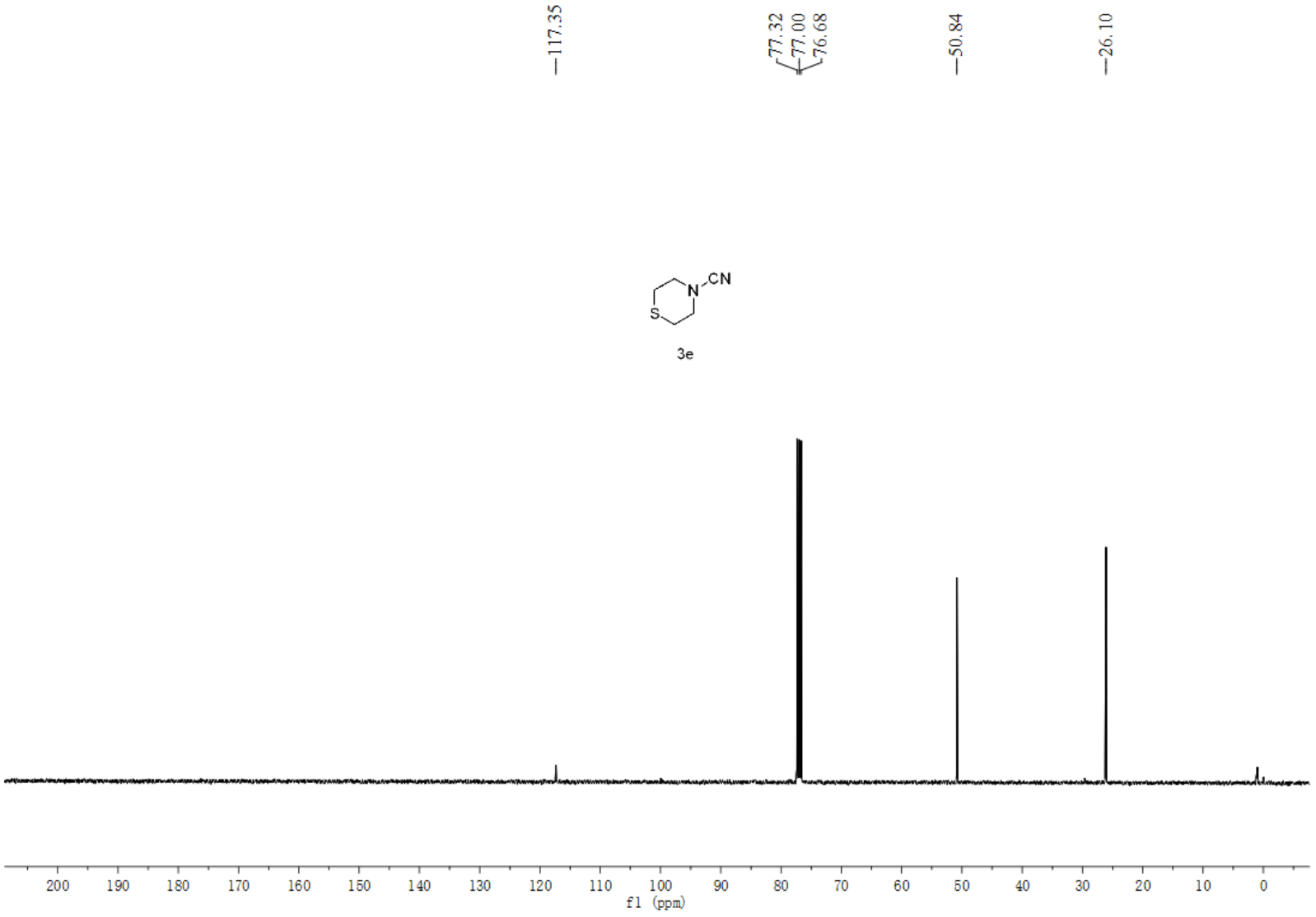
Benzylmethylcyanamide (3d)



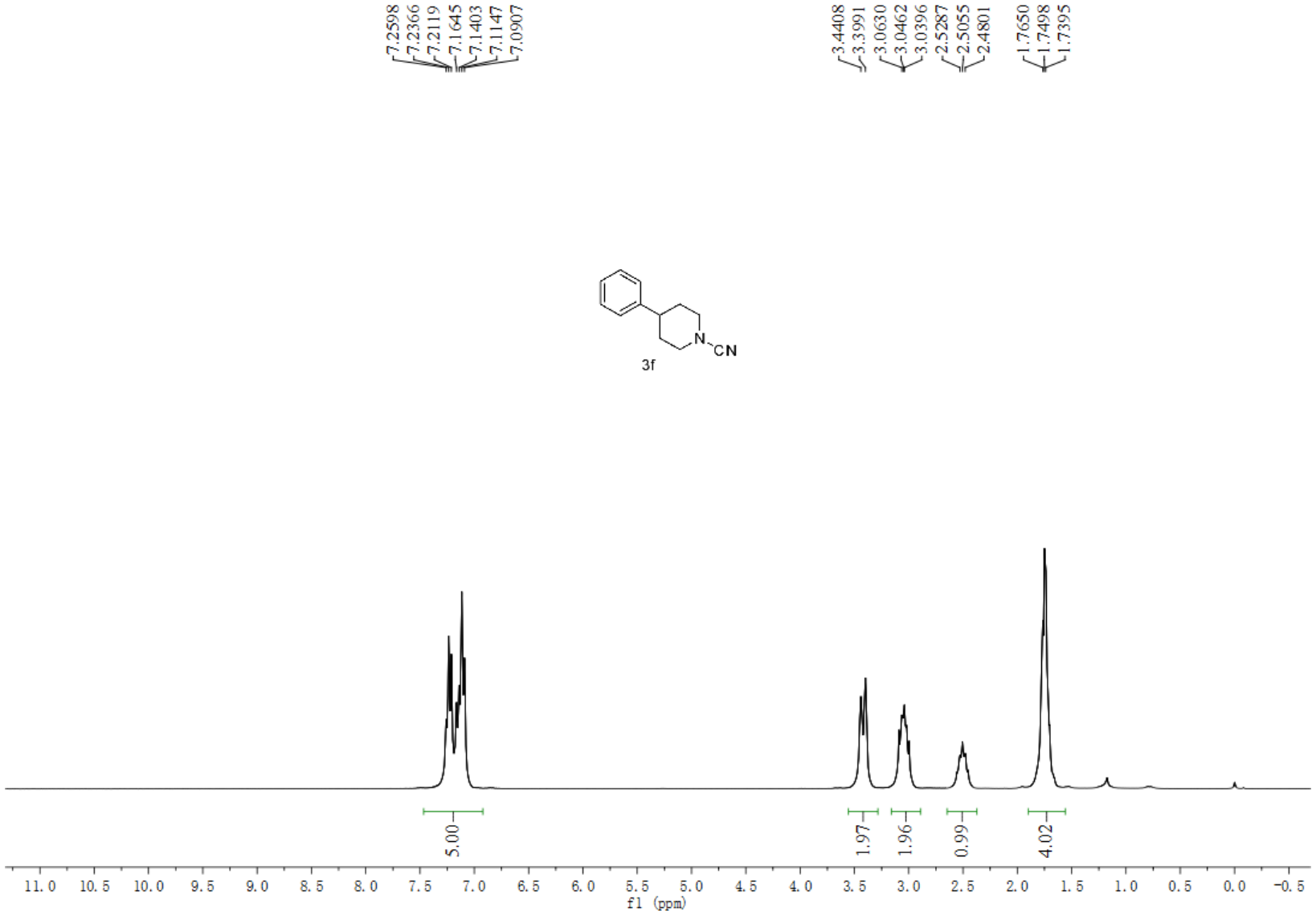

134.17
128.70
128.39
128.20
118.63
77.26
77.00
76.75
56.90
37.63
CN
N
3d
128.70
128.39
128.20
132 131 130 129 128 127 126 125 124
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

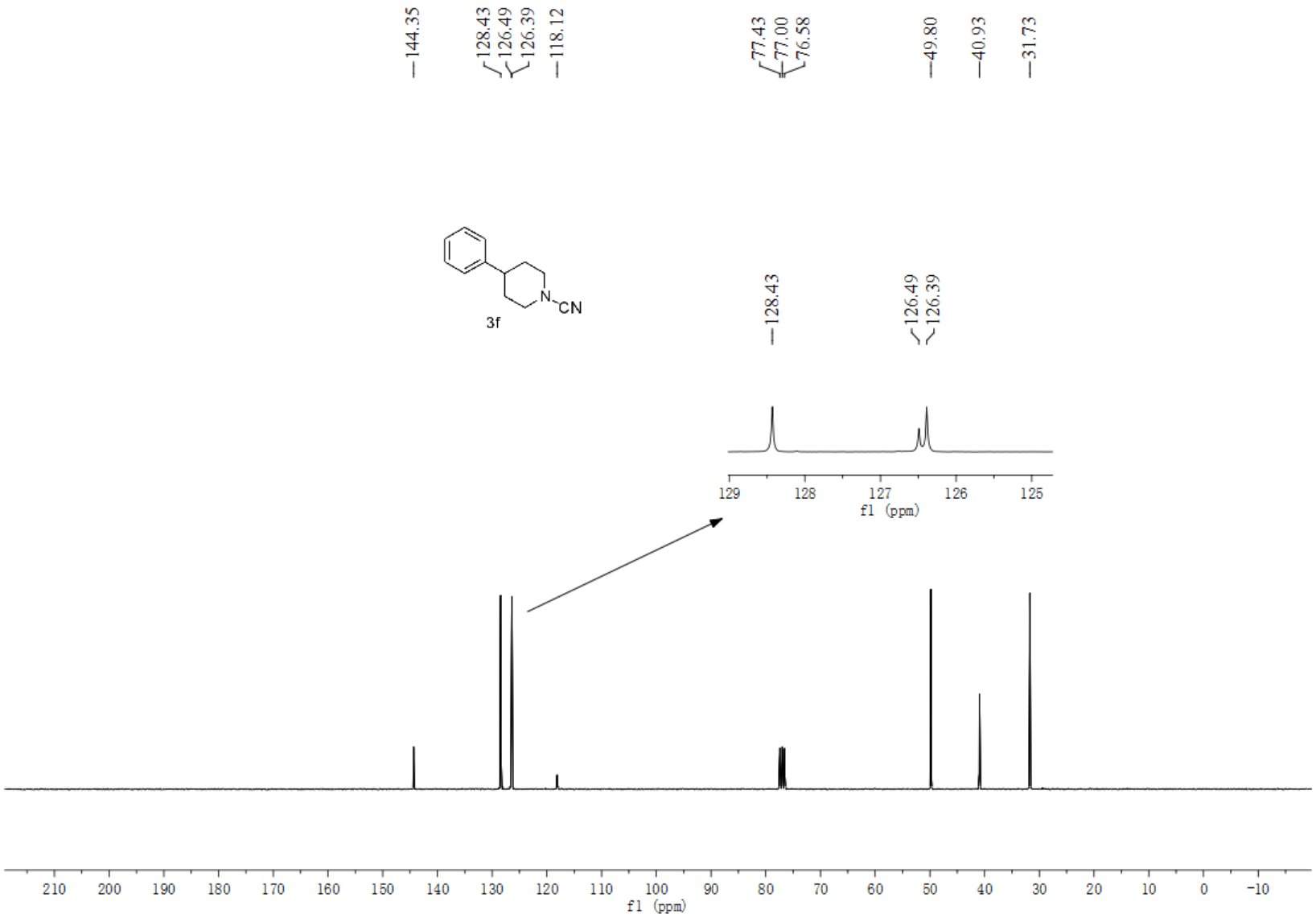
Thiomorpholine-4-carbonitrile (3e)



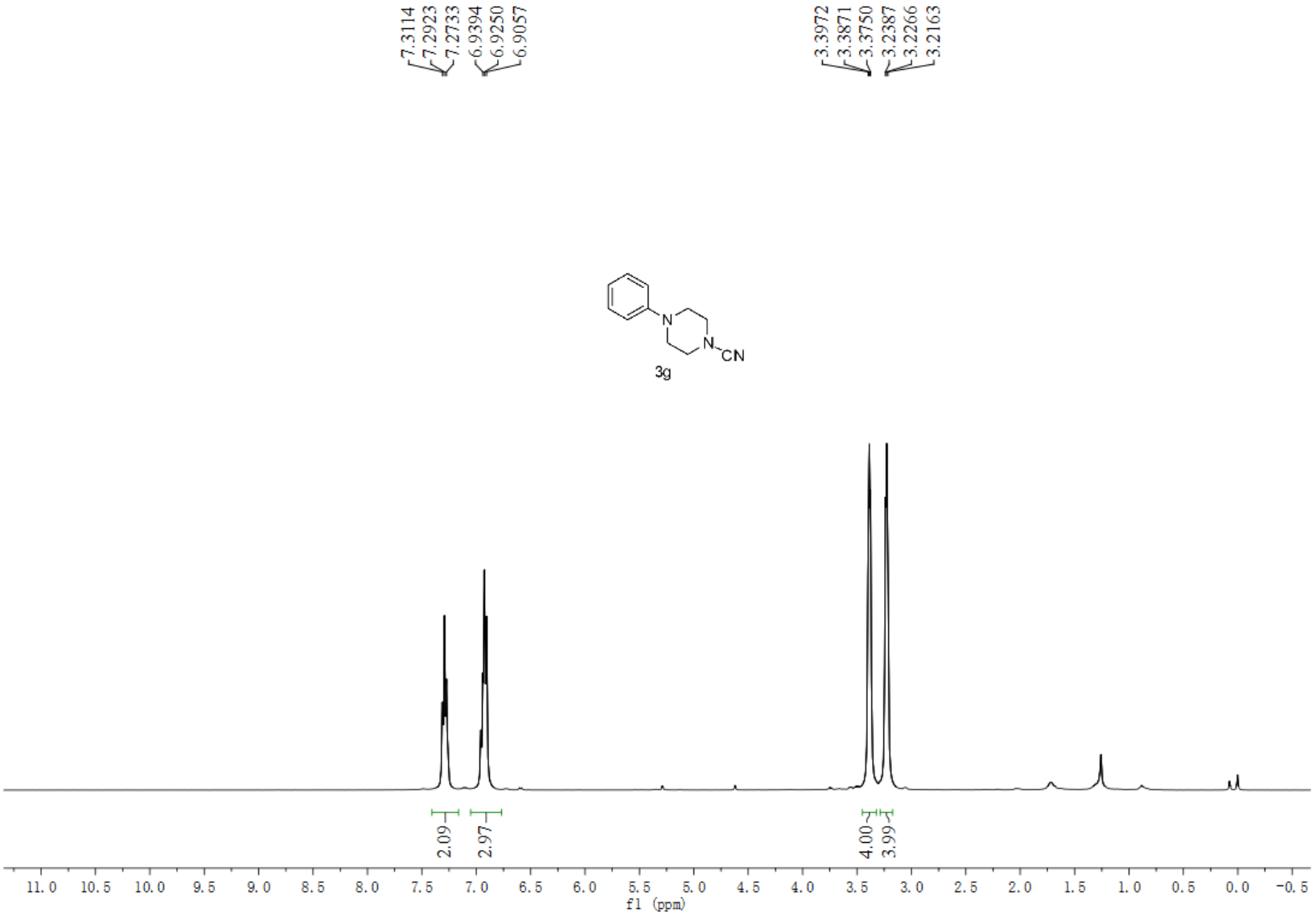

117.35
77.32
77.00
76.68
50.84
26.10
N
CN
S
3e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

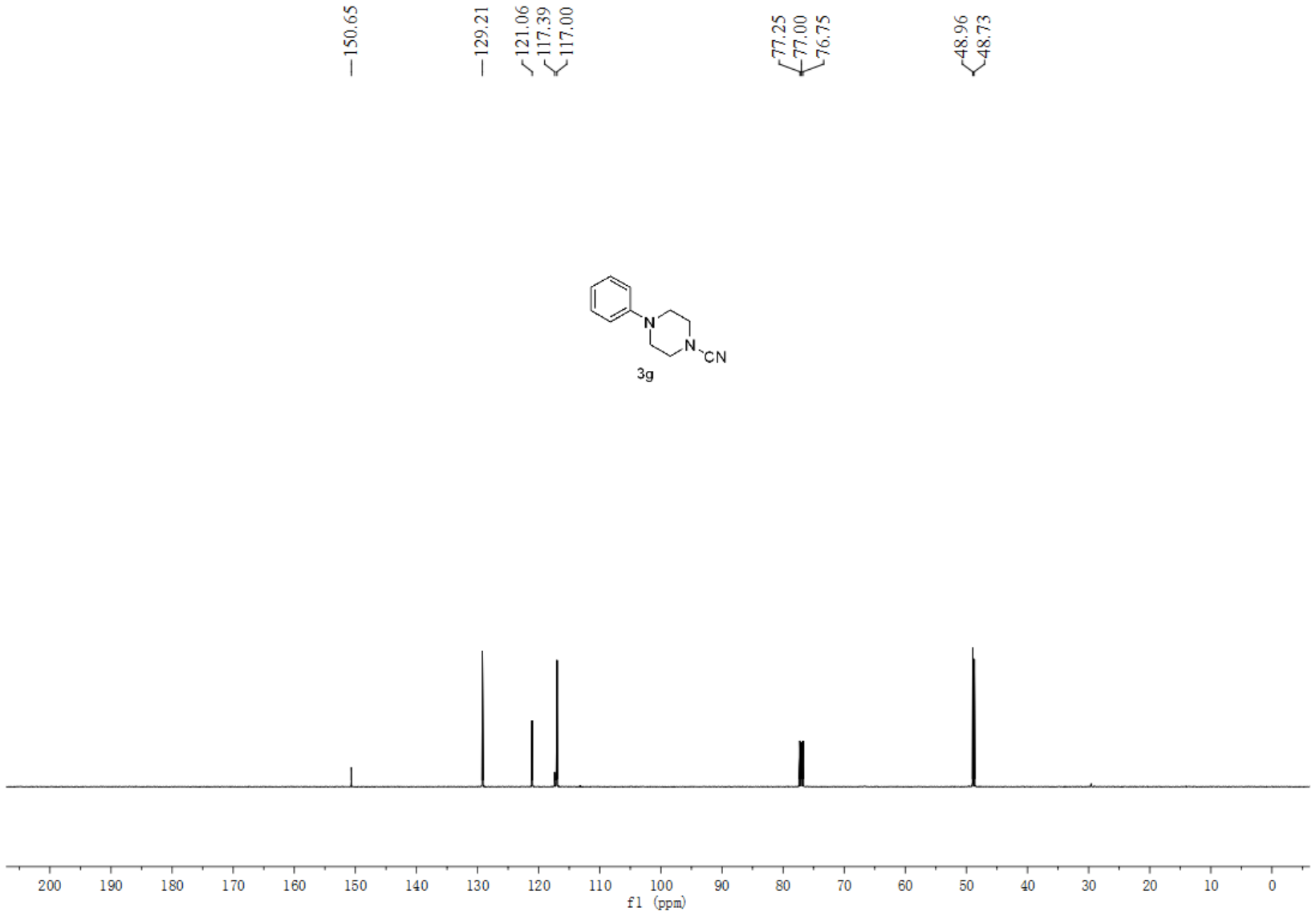
4-Phenylpiperidine-1-carbonitrile (3f)



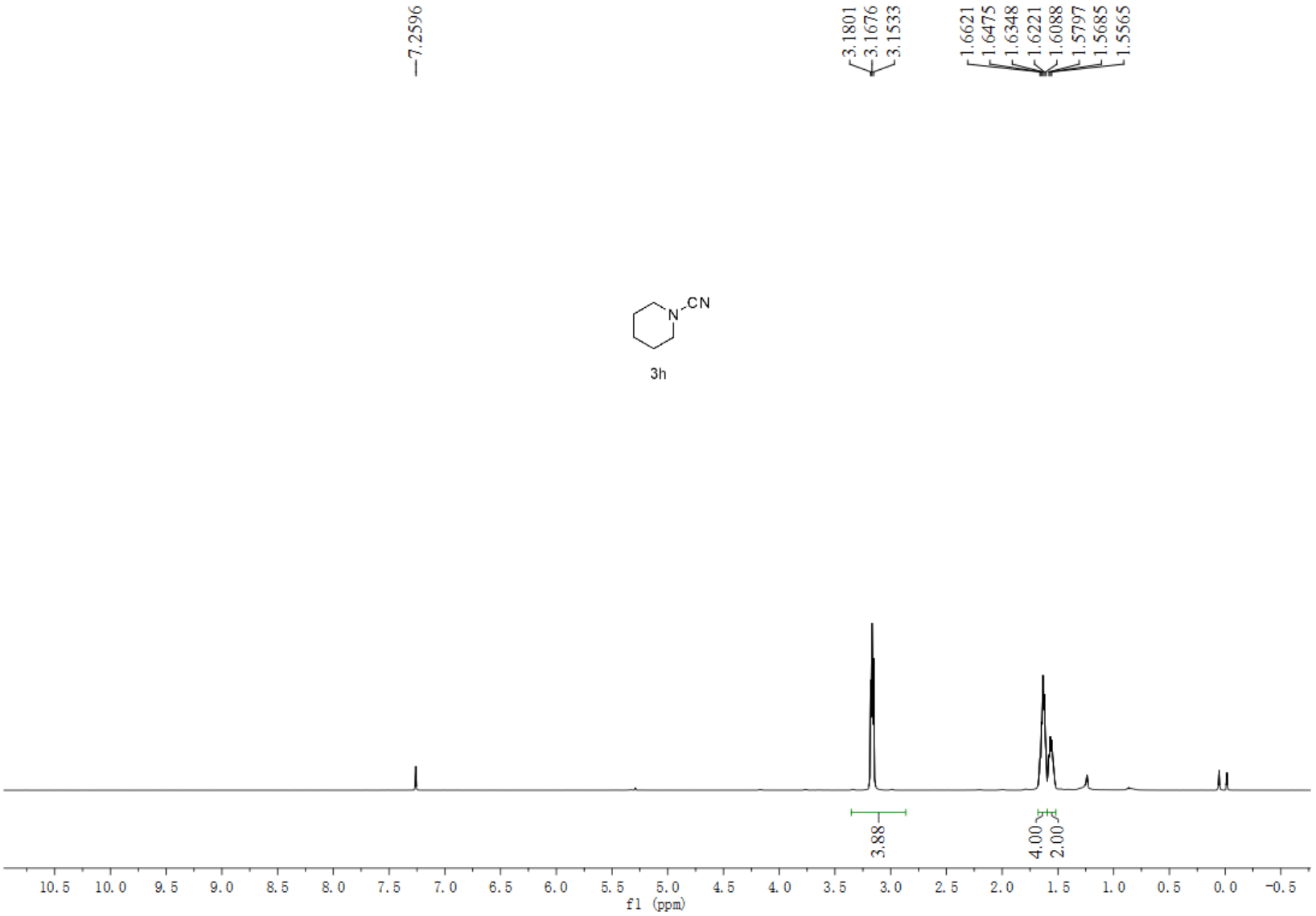

144.35
128.43
126.49
126.39
118.12
77.43
77.00
76.58
49.80
40.93
31.73
N
CN
3f
128.43
126.49
126.39
129
128
127
126
125
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

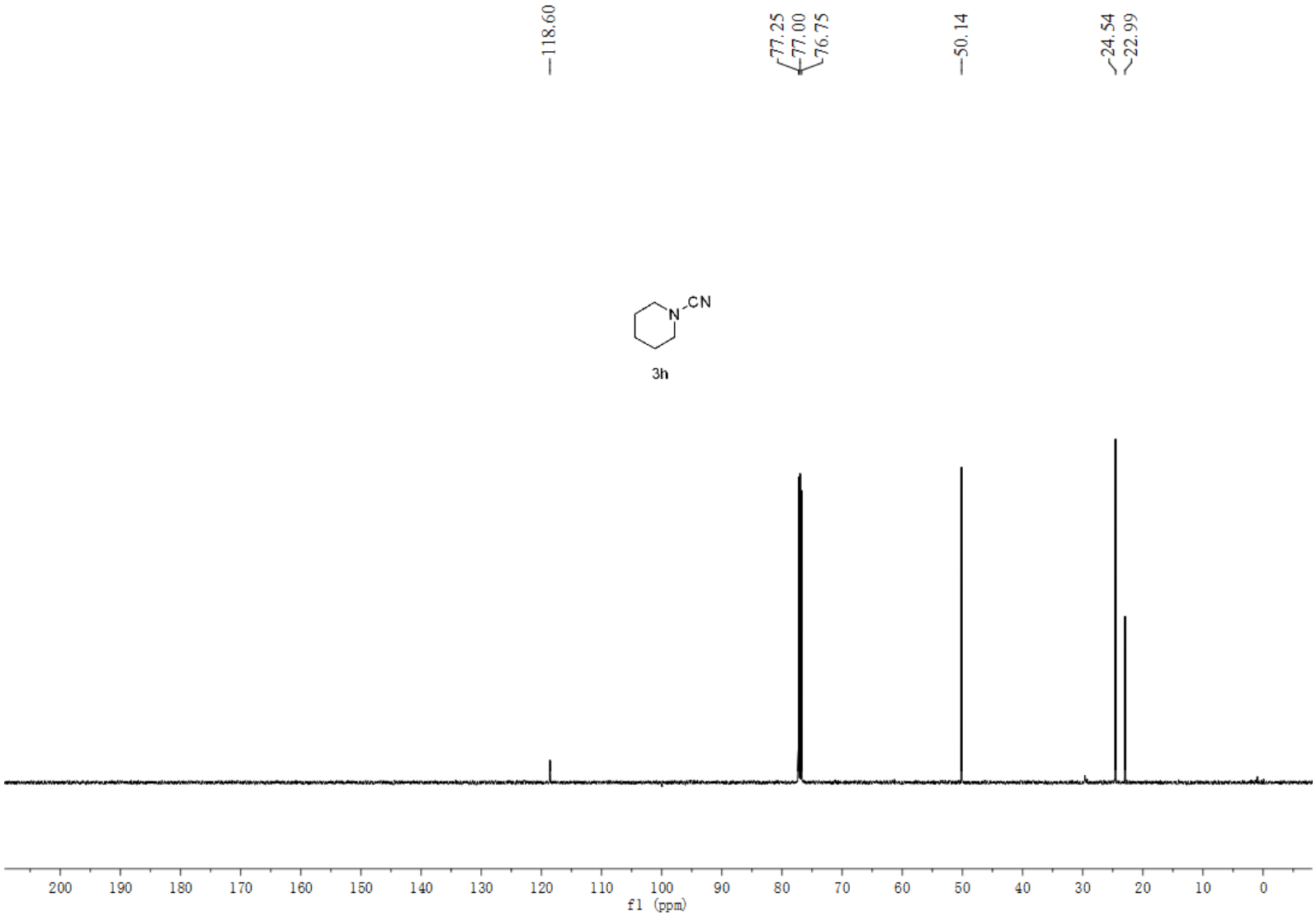
4-Phenylpiperazine-1-carbonitrile (3g)



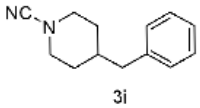

150.65
129.21
121.06
117.39
117.00
77.25
77.00
76.75
48.96
48.73
N
N
CN
3g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Piperidine-1-carbonitrile (3h)

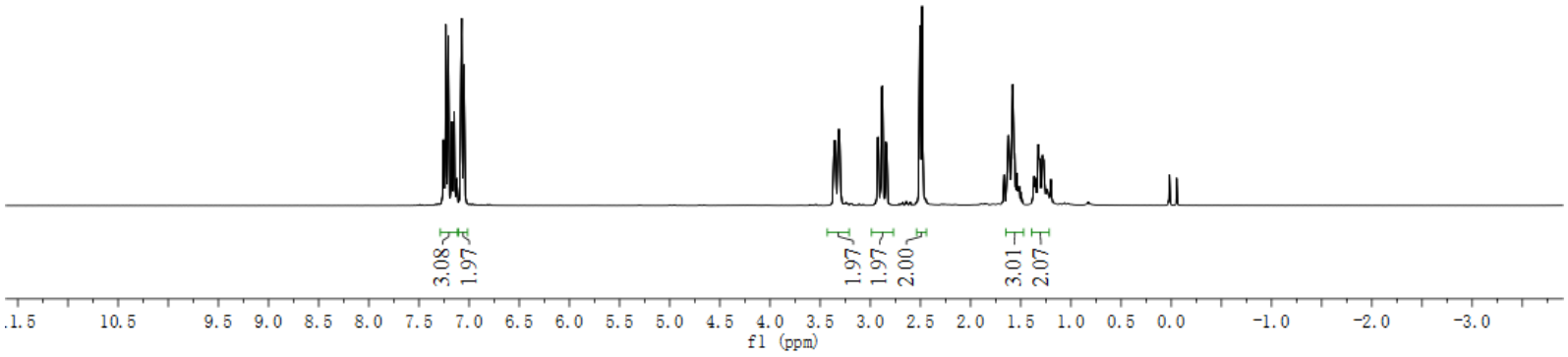


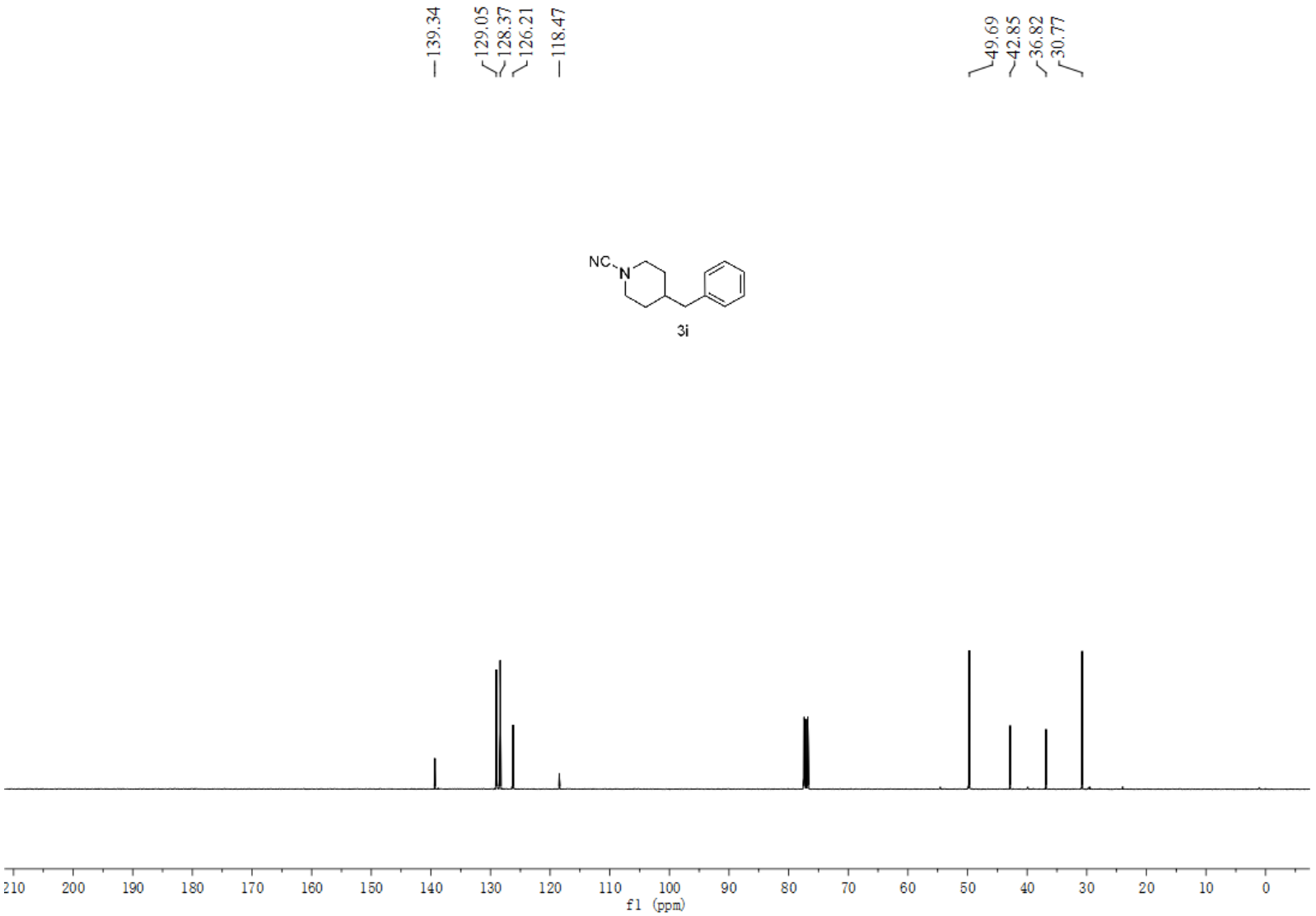

118.60
77.25
77.00
76.75
50.14
24.54
22.99
N
CN
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4-Benzylpiperidine-1-carbonitrile (3i)

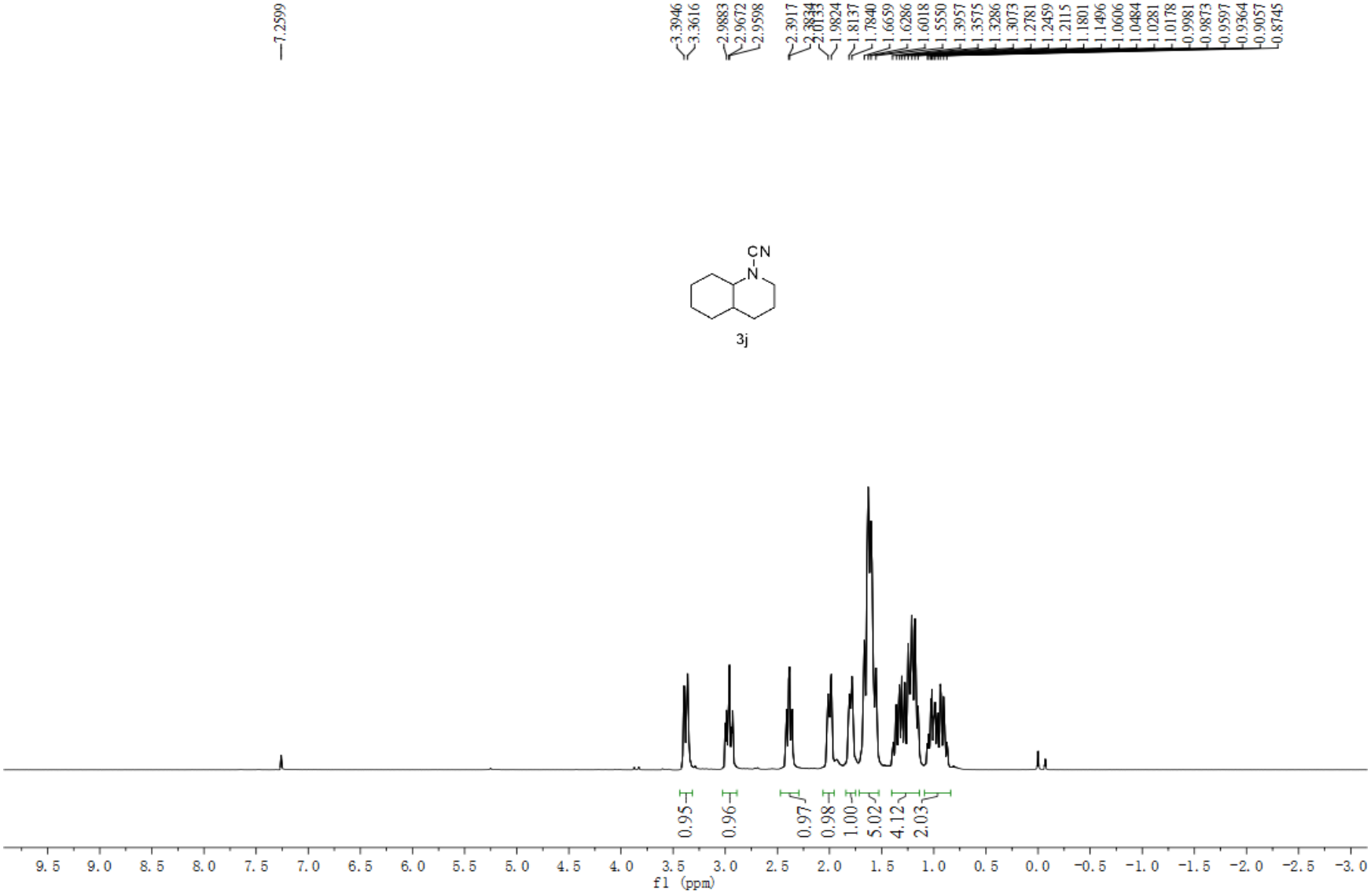


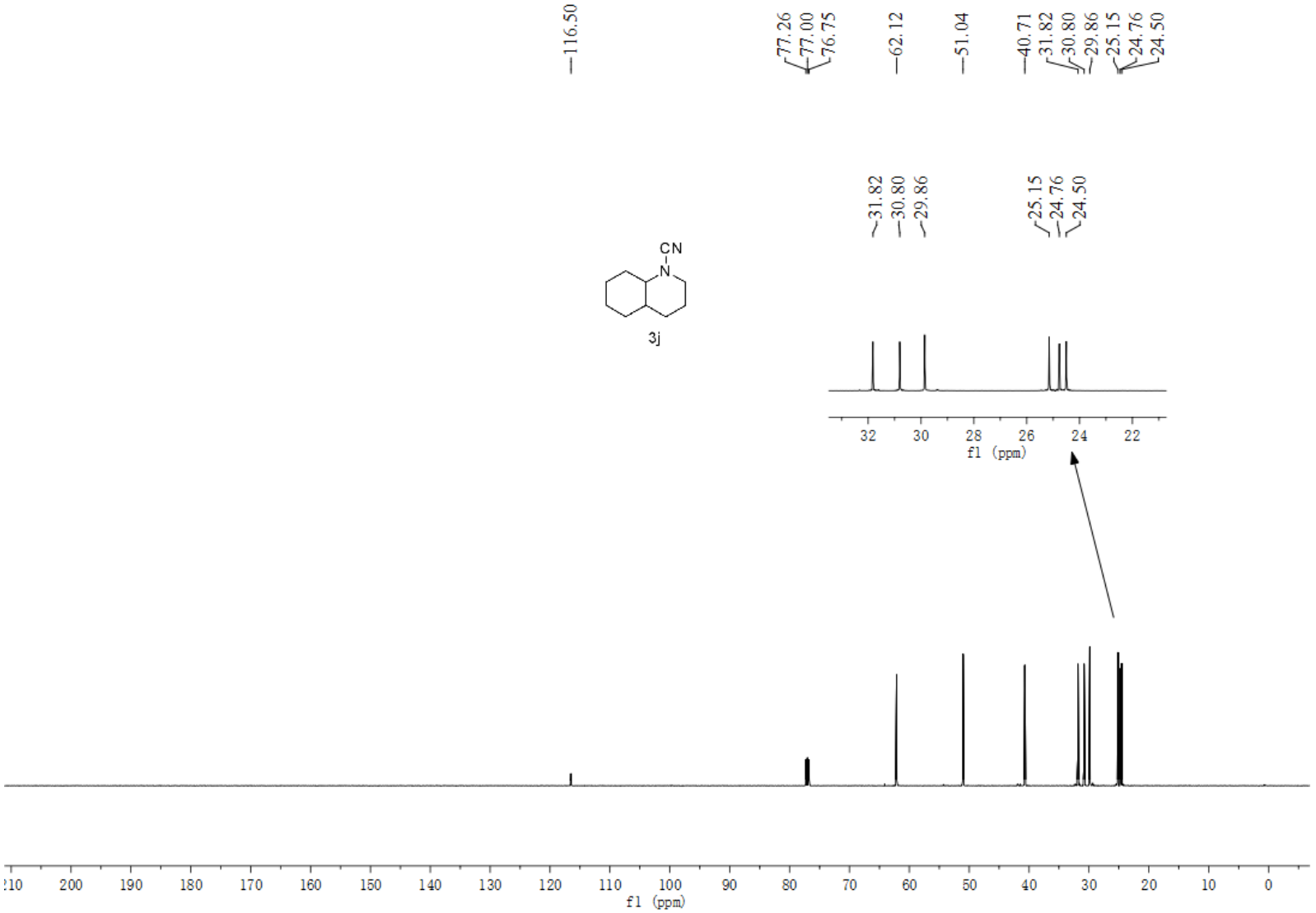
3i



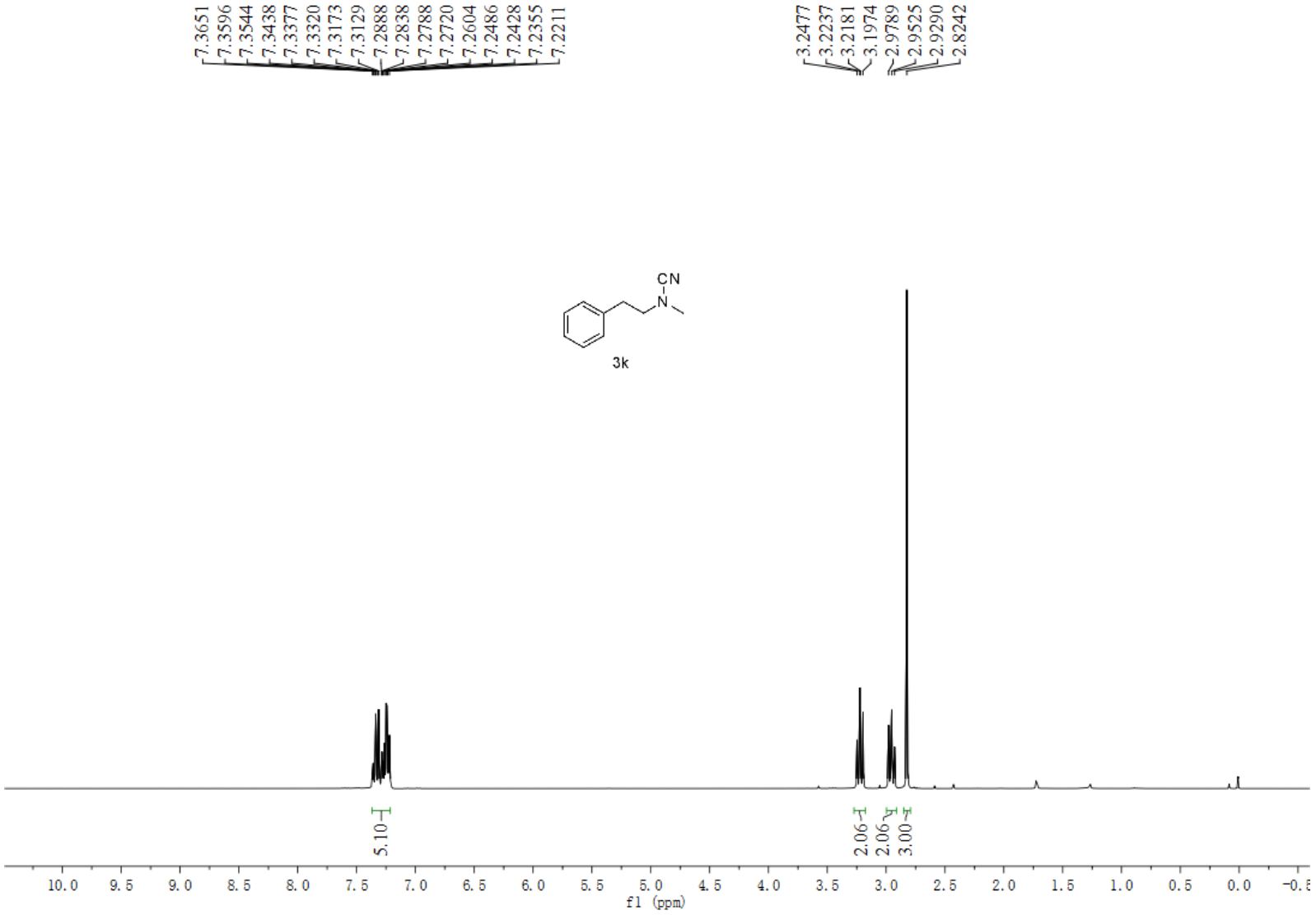

139.34
129.05
128.37
126.21
118.47
49.69
42.85
36.82
30.77
NC
N
3i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

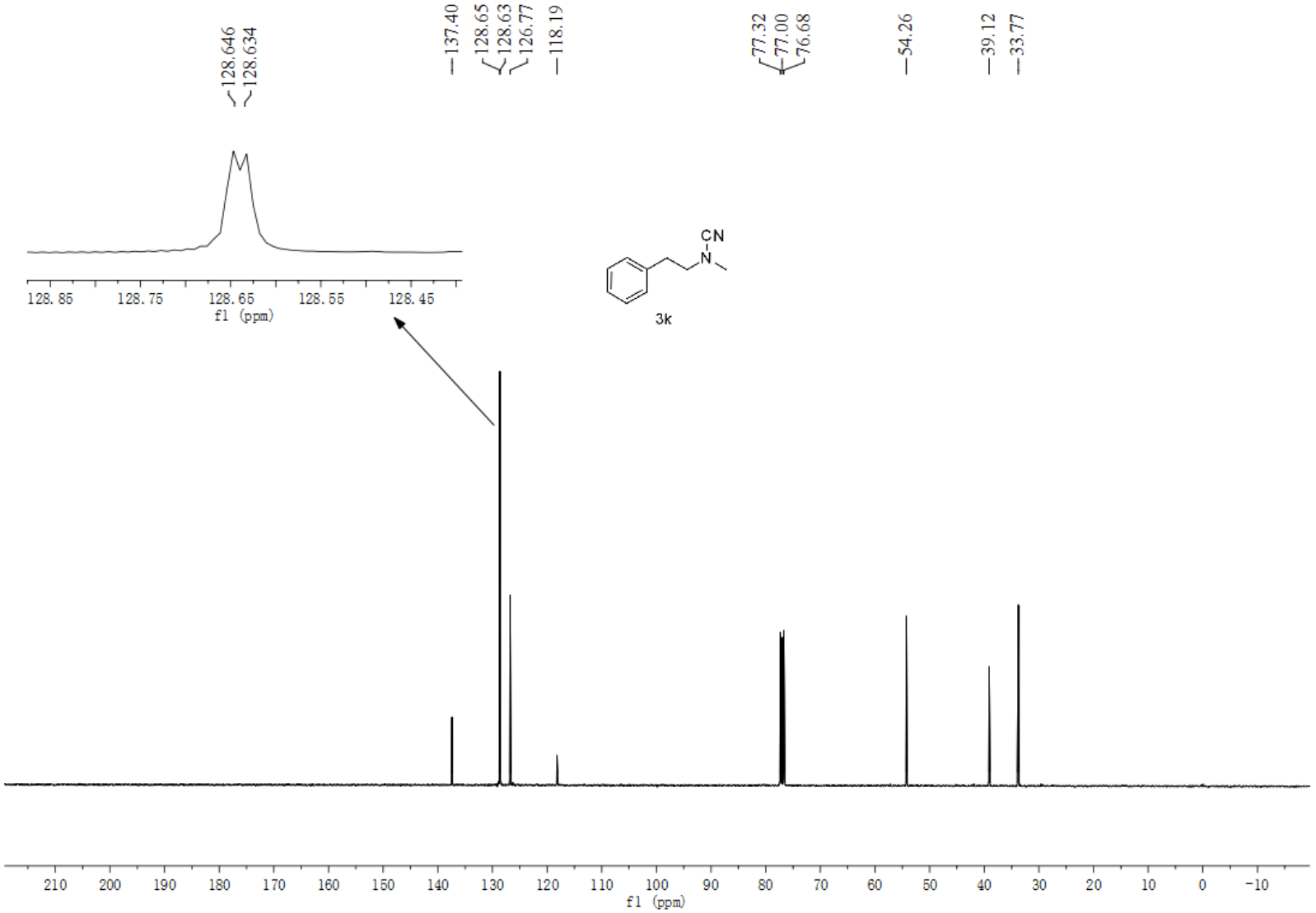
Octahydroquinoline-1(2H)-carbonitrile (3j)



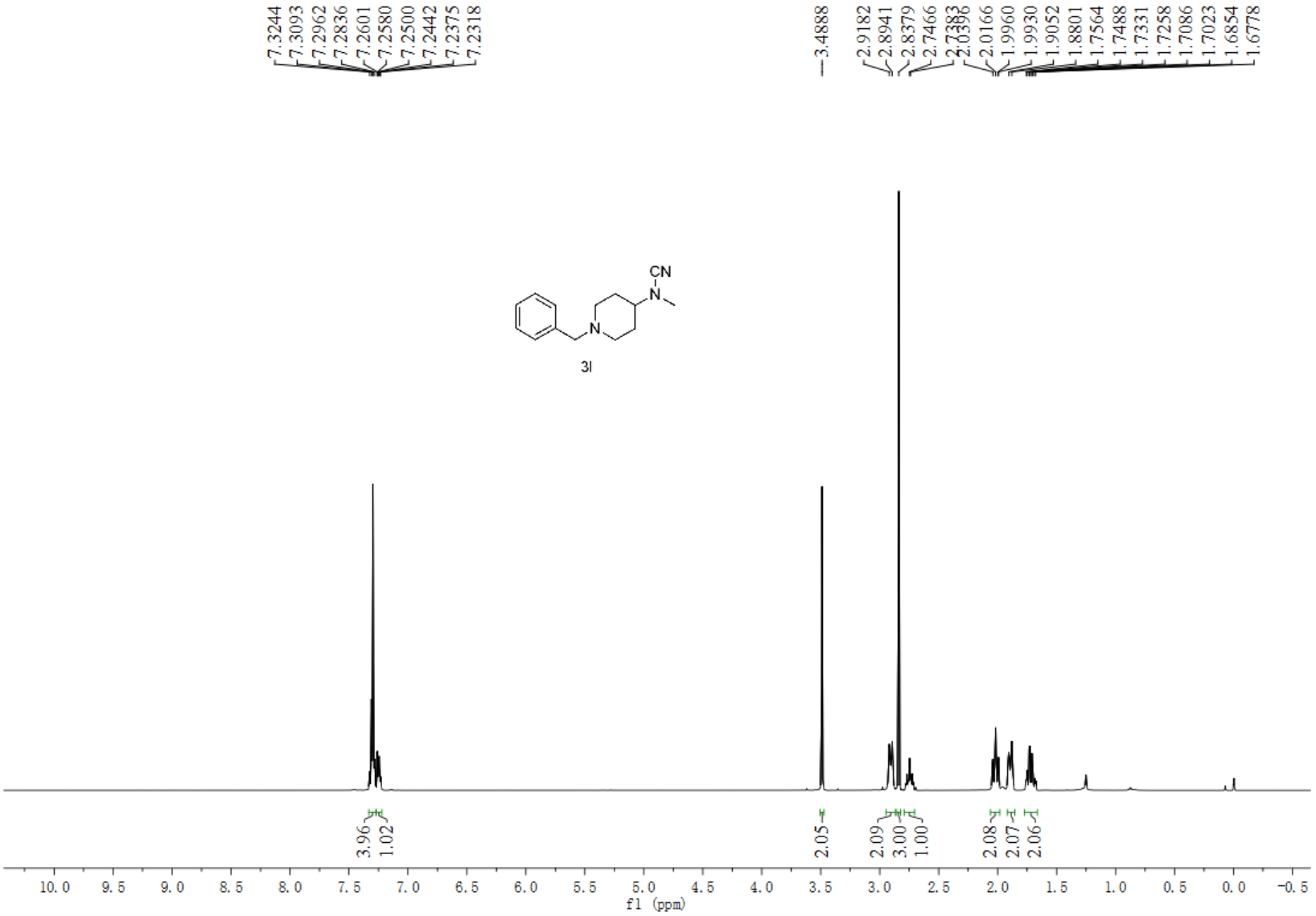

116.50
77.26
77.00
76.75
62.12
51.04
40.71
31.82
30.80
29.86
25.15
24.76
24.50
CN
N
3j
f1 (ppm)
f1 (ppm)

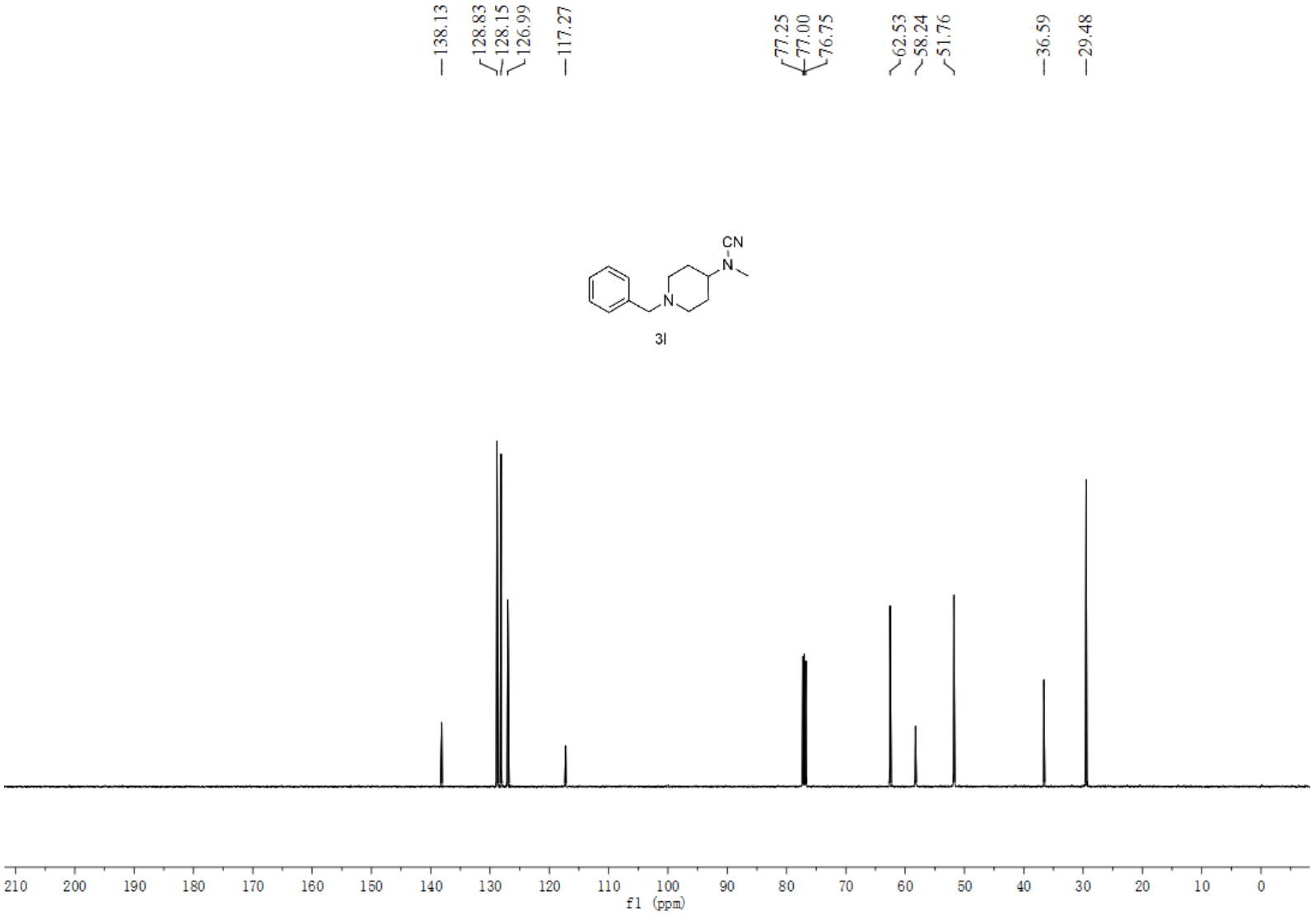
N-Methyl-*N*-phenethylcyanamide (3k)



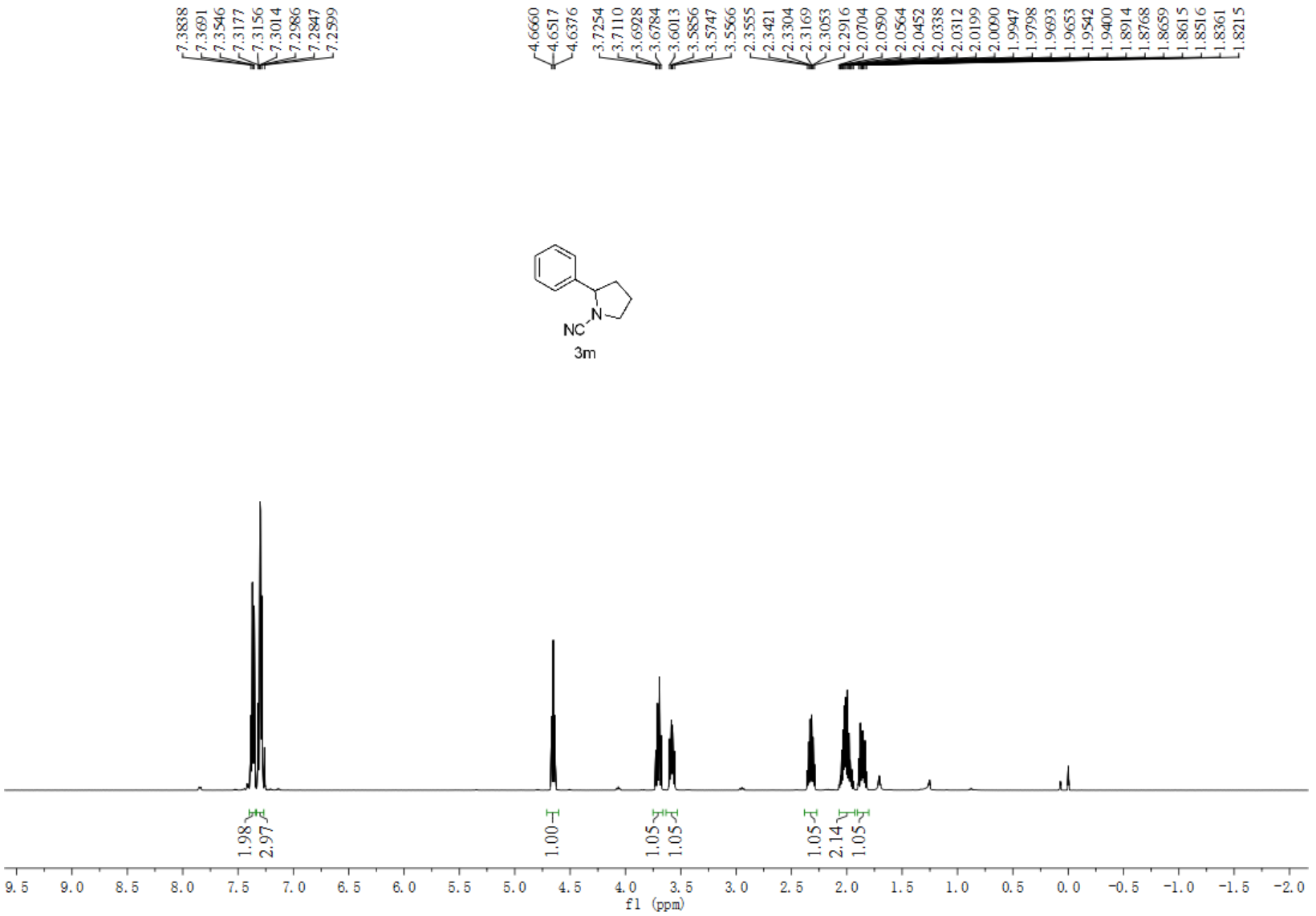

128.646
128.634
137.40
128.65
128.63
126.77
118.19
77.32
77.00
76.68
54.26
39.12
33.77
128.85
128.75
128.65
128.55
128.45
f1 (ppm)
CN
N
3k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

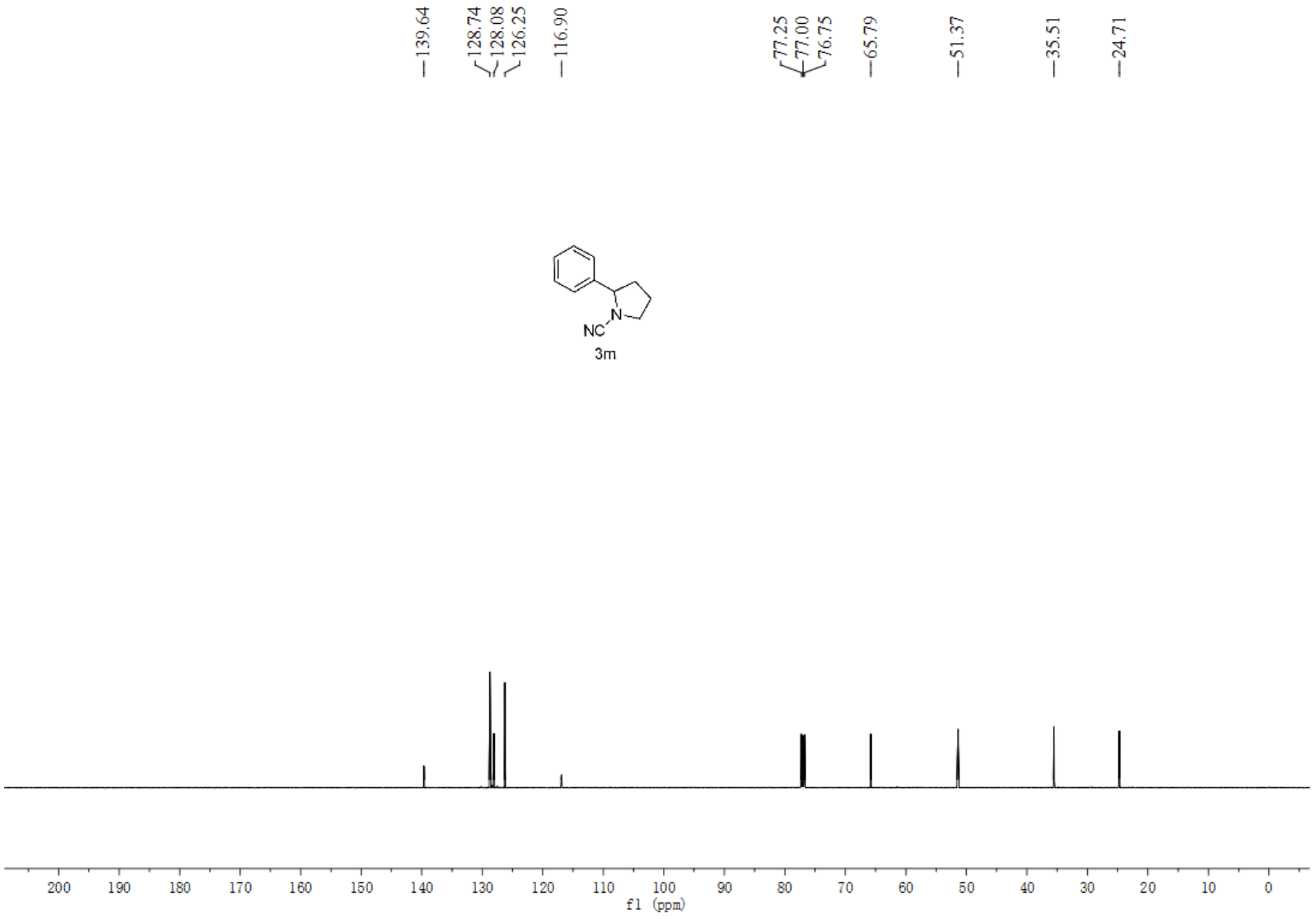
_N_-(1-Benzylpiperidin-4-yl)-N-methylcyanamide (3l)



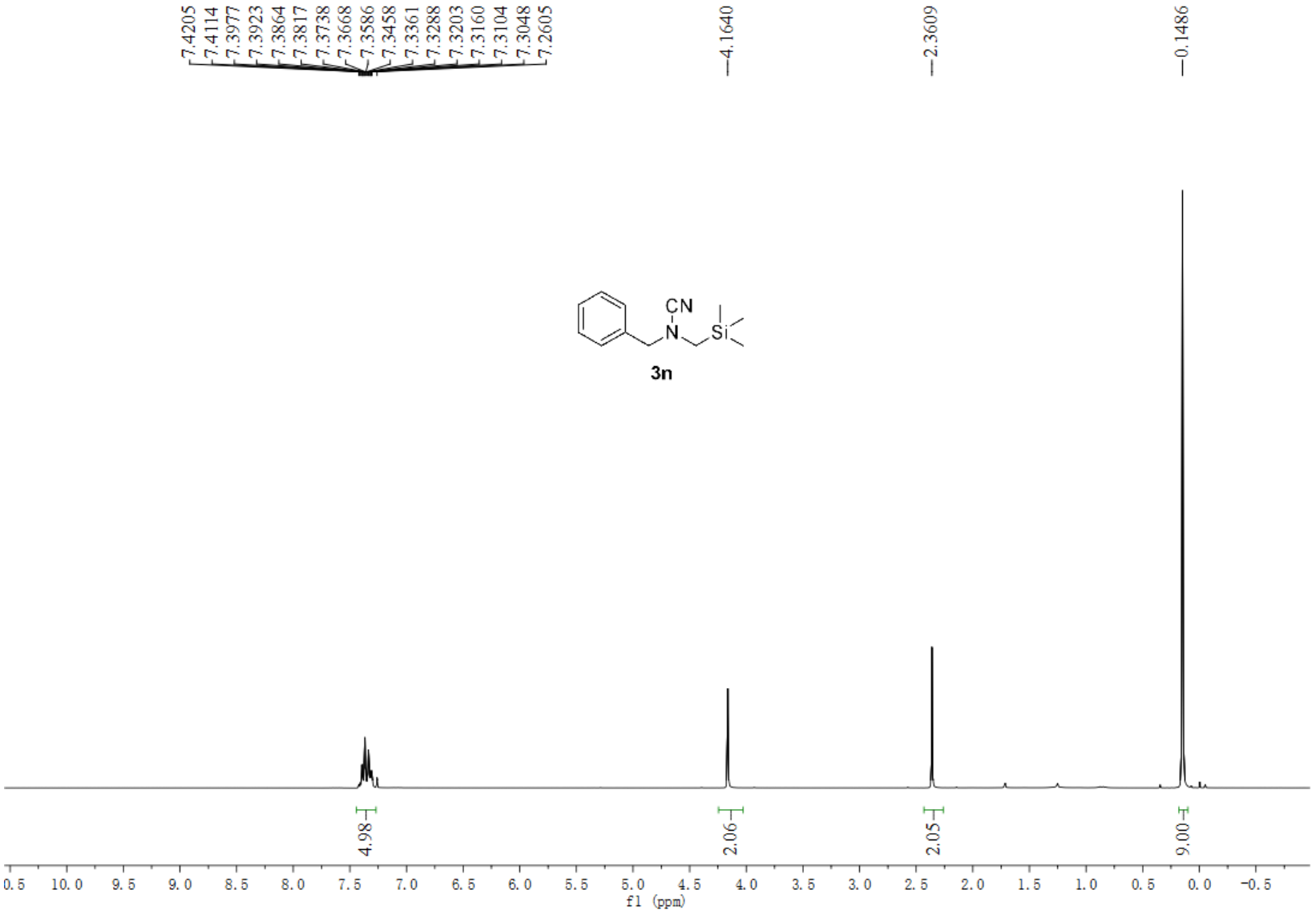

138.13
128.83
128.15
126.99
117.27
77.25
77.00
76.75
62.53
58.24
51.76
36.59
29.48
CN
N
N
3l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

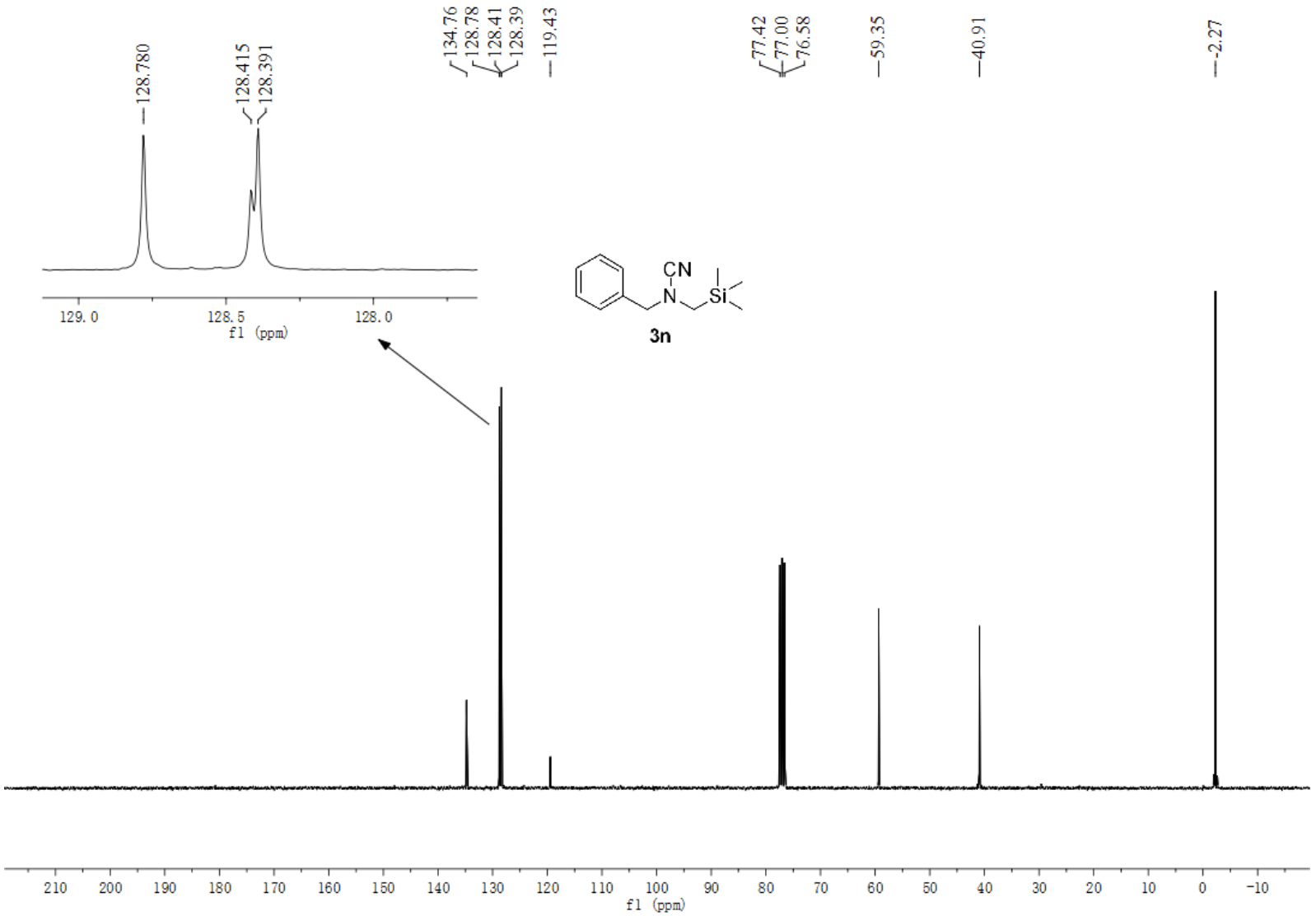
2-Phenylpyrrolidine-1-carbonitrile (3m)



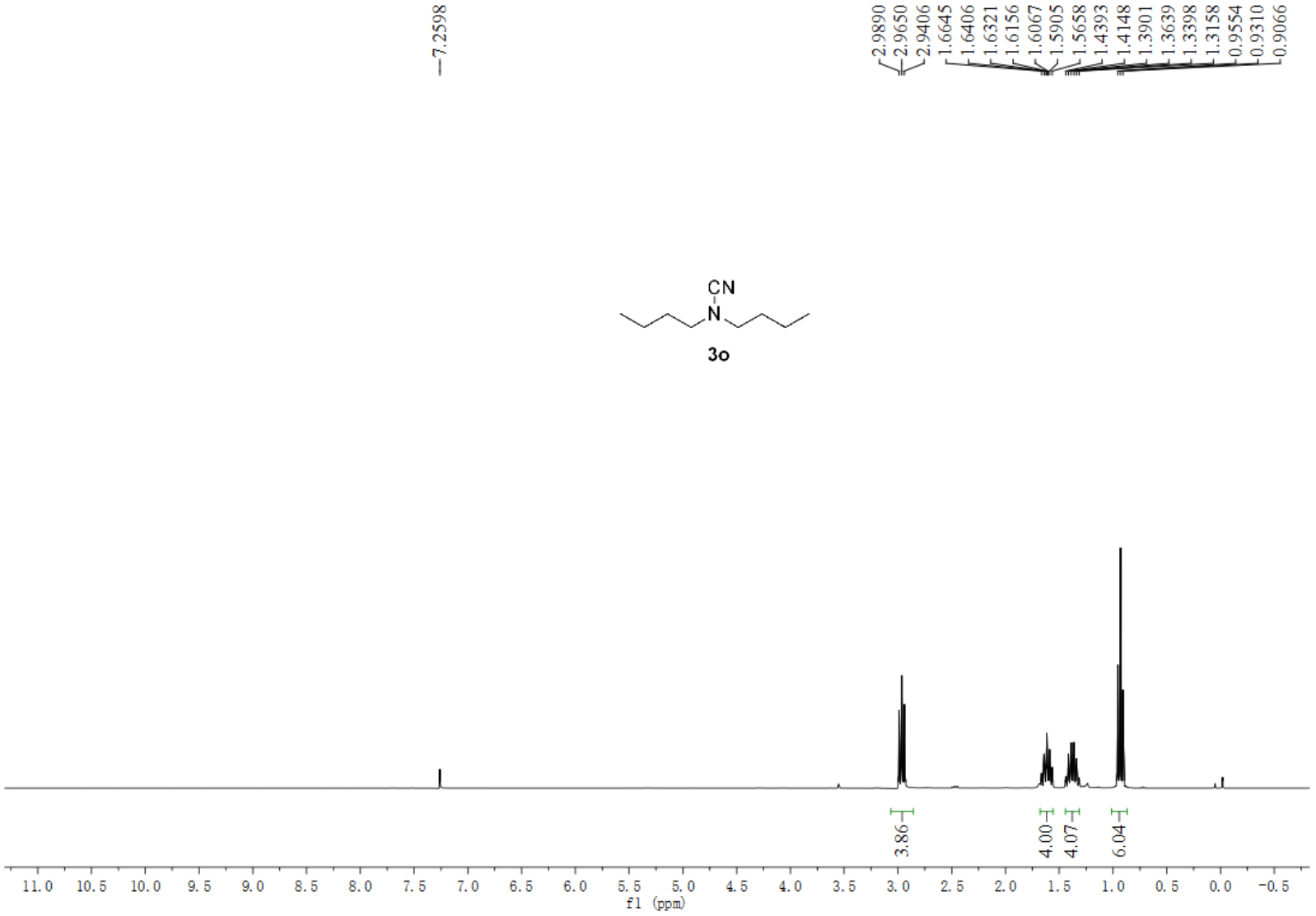

139.64
128.74
128.08
126.25
116.90
77.25
77.00
76.75
65.79
51.37
35.51
24.71
NC
N
3m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

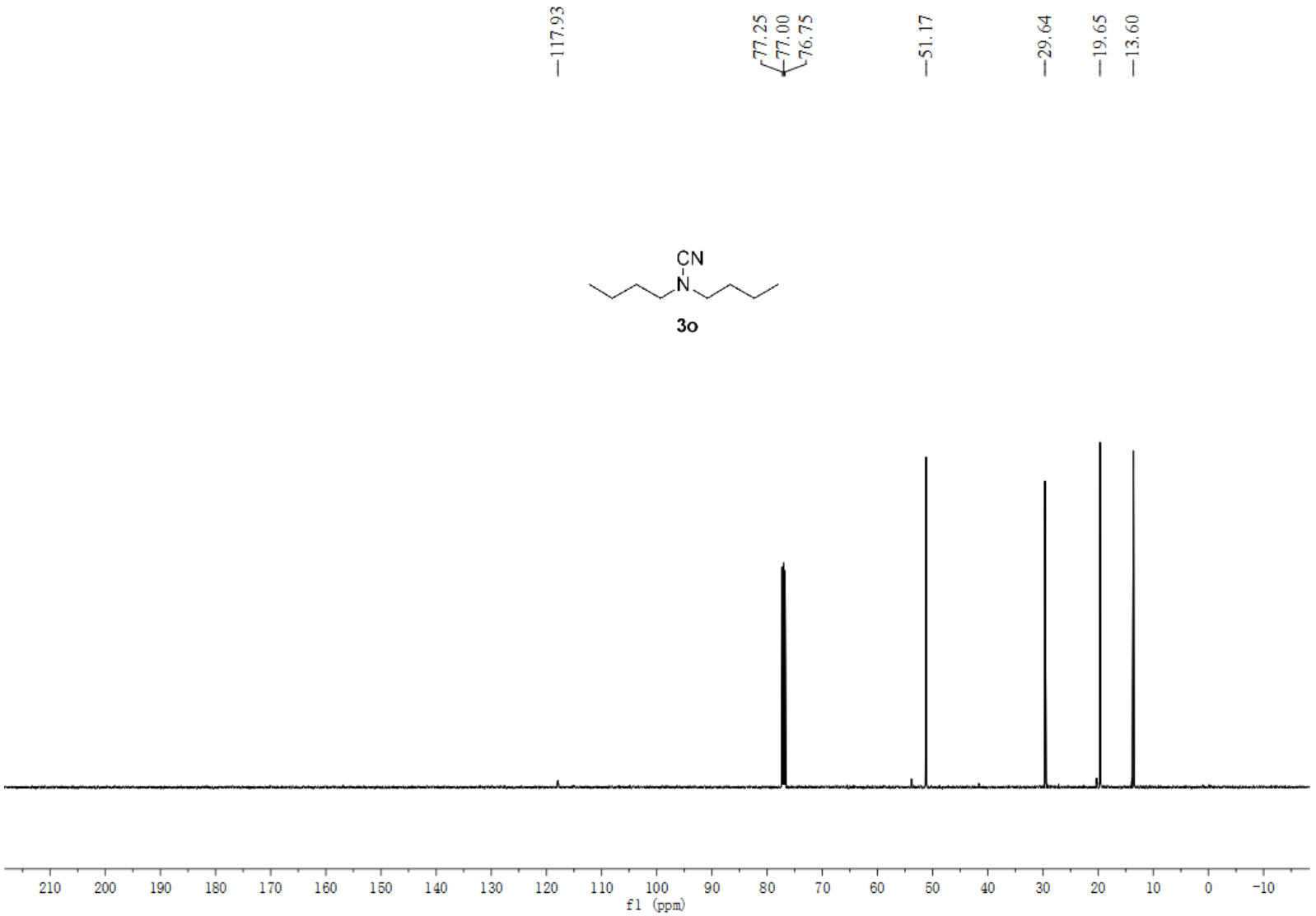
N-Benzyl-*N*-((trimethylsilyl)methyl)cyanamide (3n)



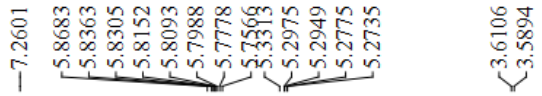

128.780
128.415
128.391
134.76
128.78
128.41
128.39
119.43
77.42
77.00
76.58
59.35
40.91
2.27
129.0
128.5
128.0
f1 (ppm)
CN
N
Si
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

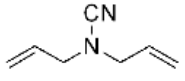
N,N-Dibutylcyanamide (3o)



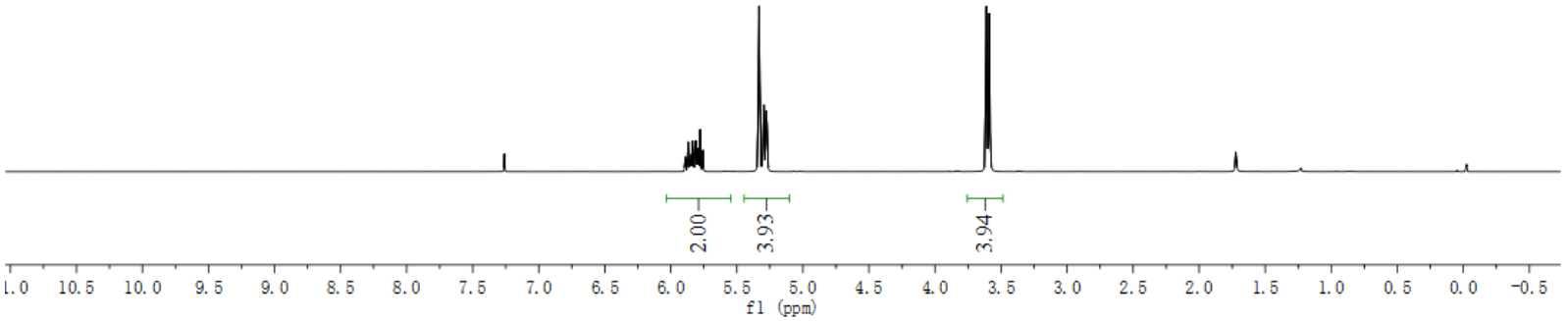

117.93
77.25
77.00
76.75
51.17
29.64
19.65
13.60
CN
N
3o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

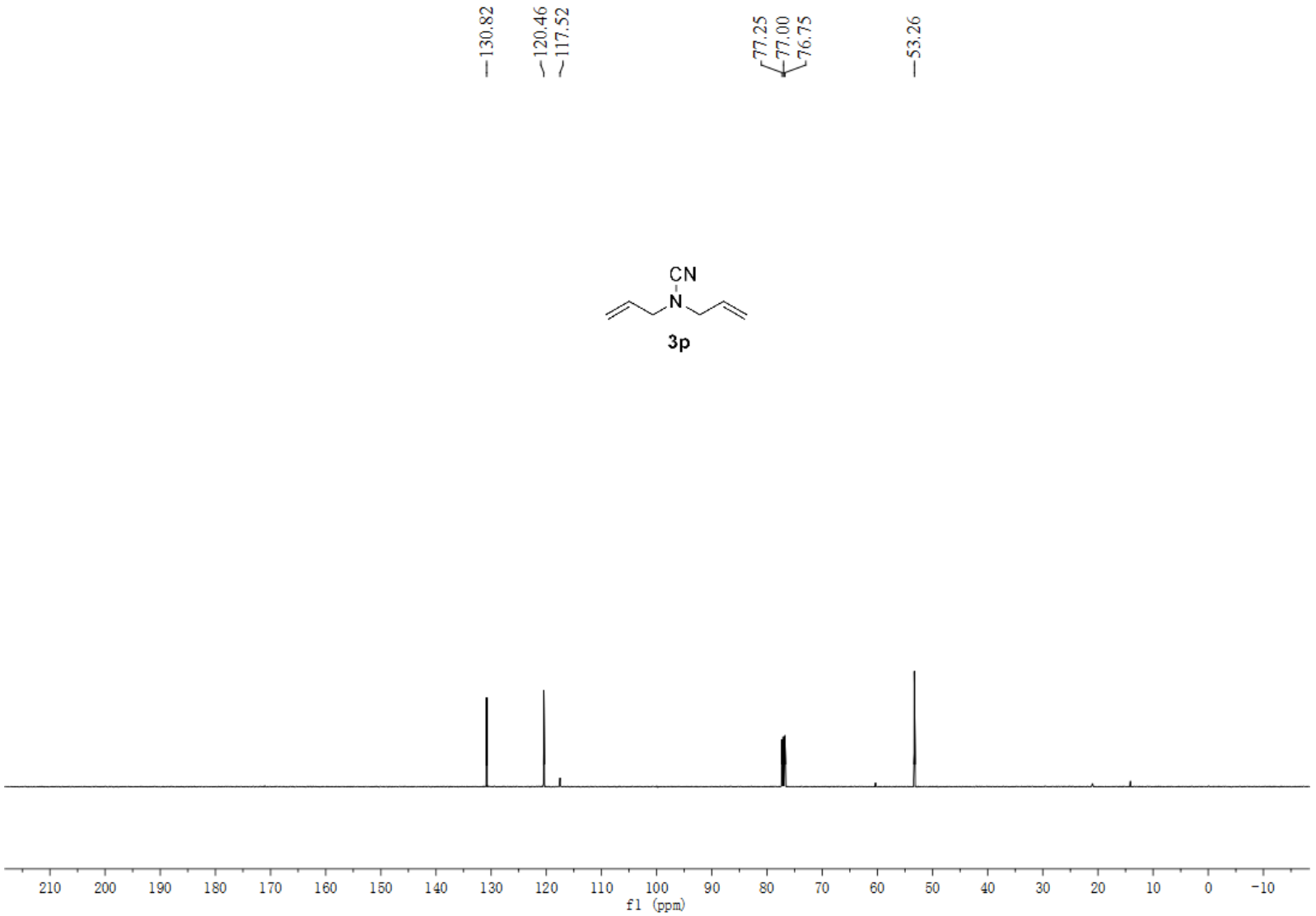
N,N-Diallylcyanamide (3o)



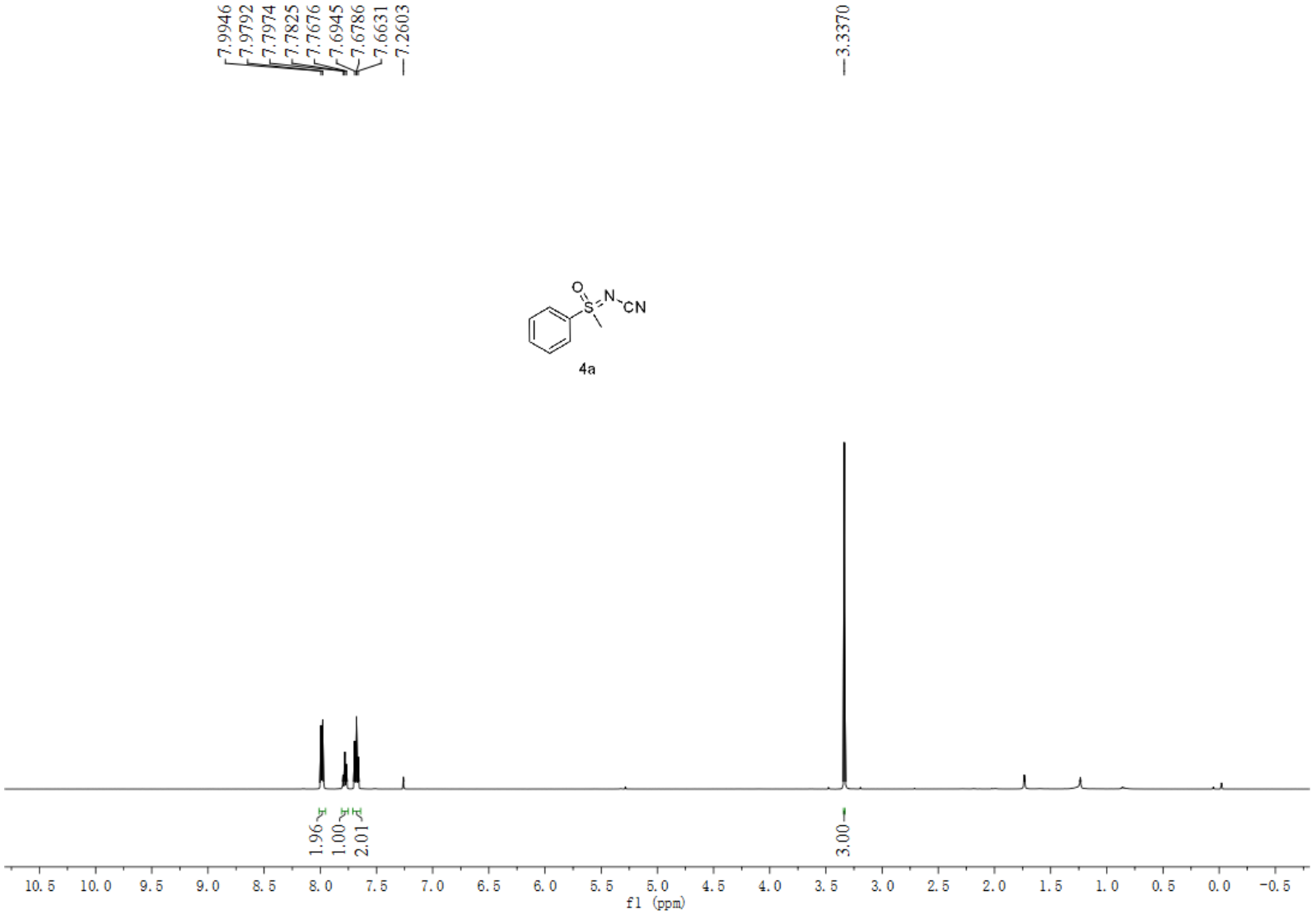


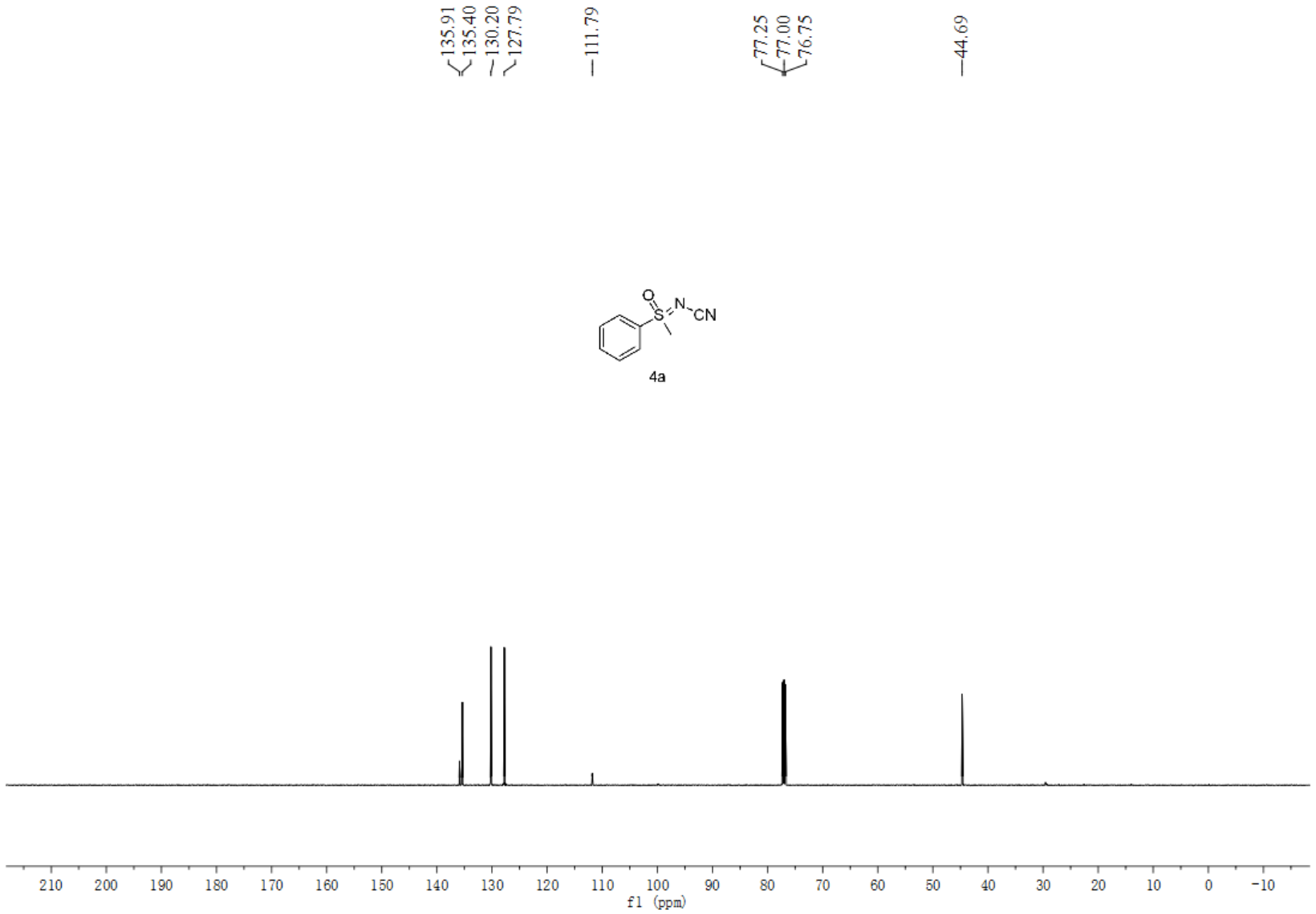
3p



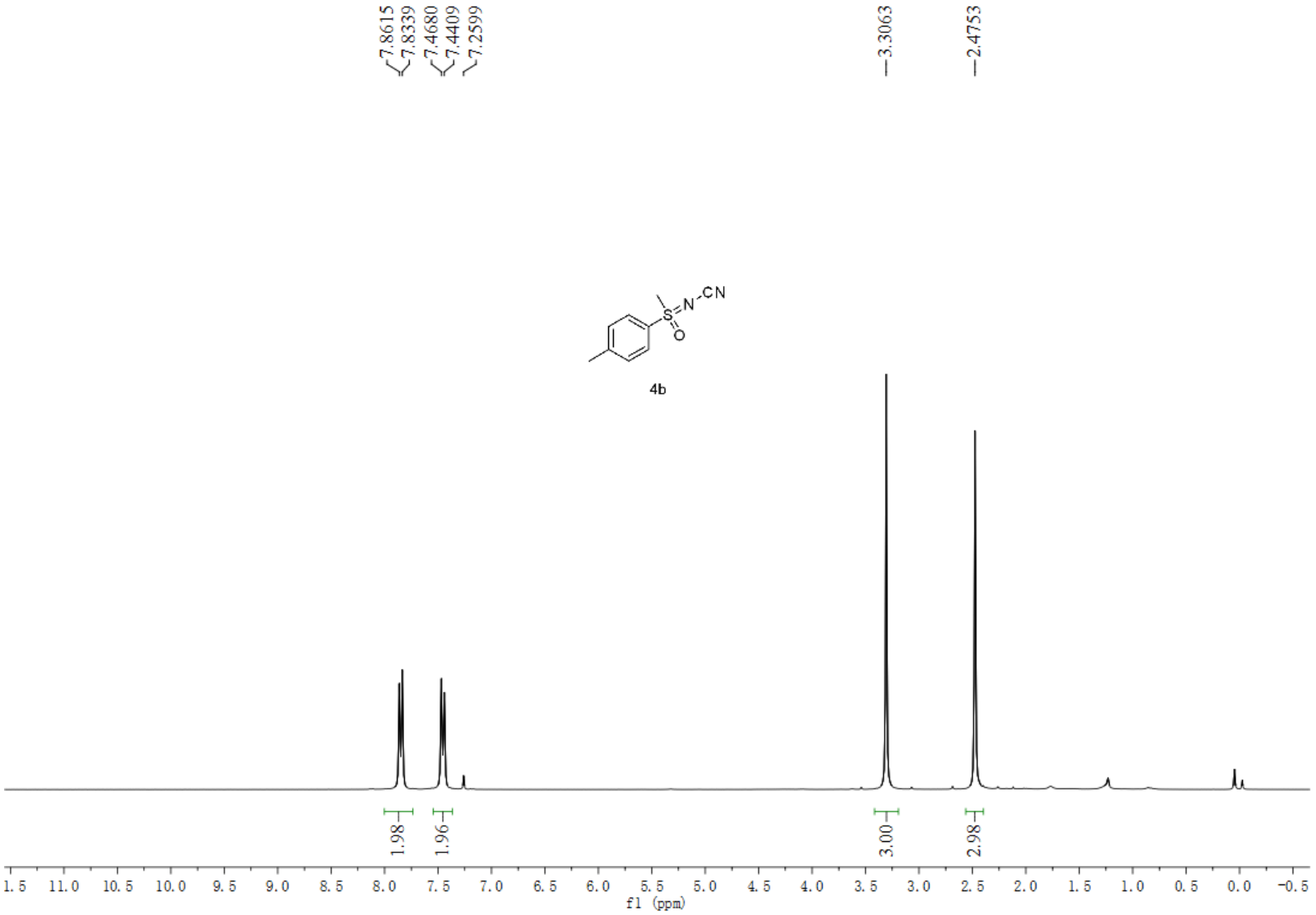

130.82
120.46
117.52
77.25
77.00
76.75
53.26
CN
N
3p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

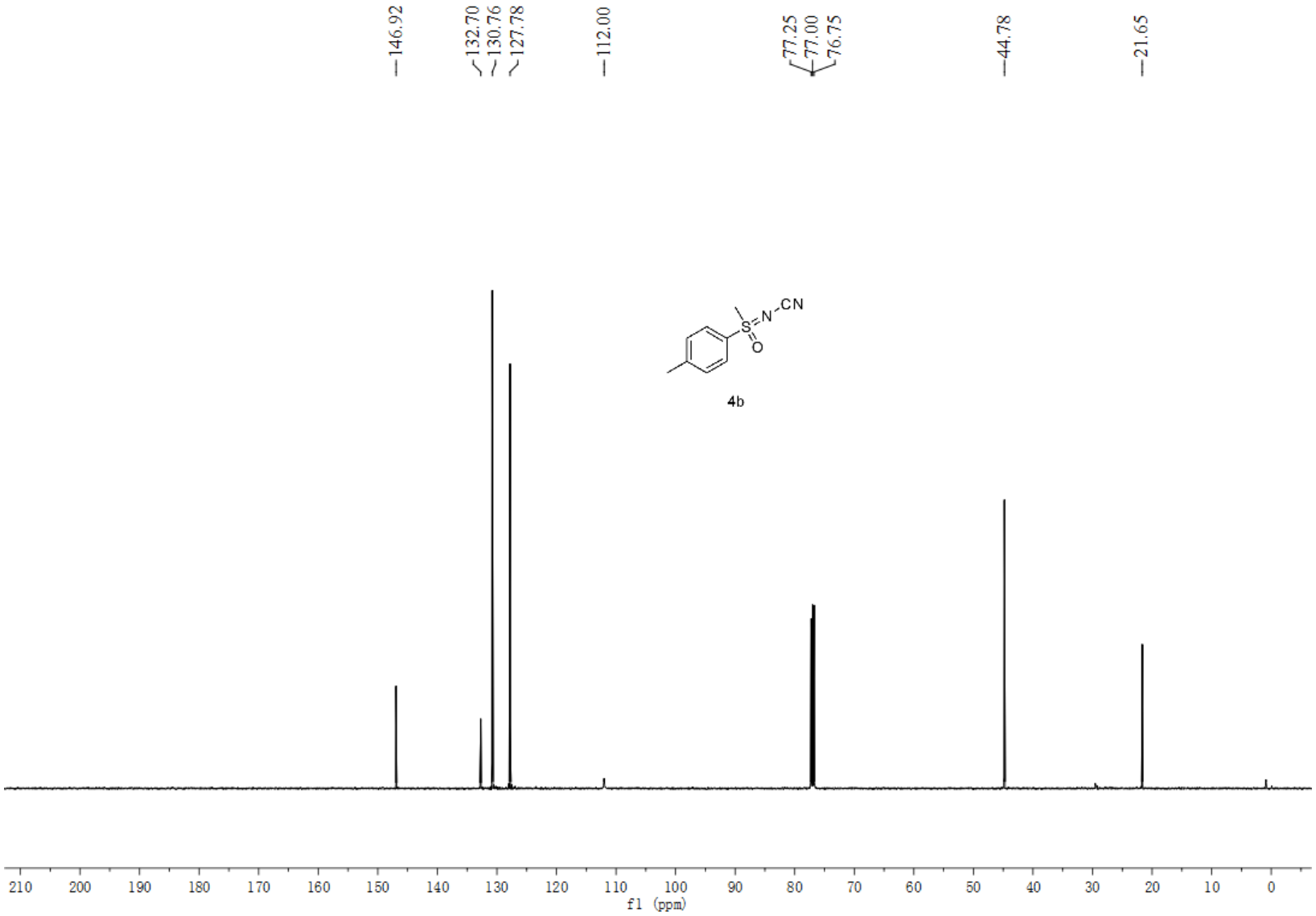
N-(Cyano) methyl phenyl sulfoximine (4a)



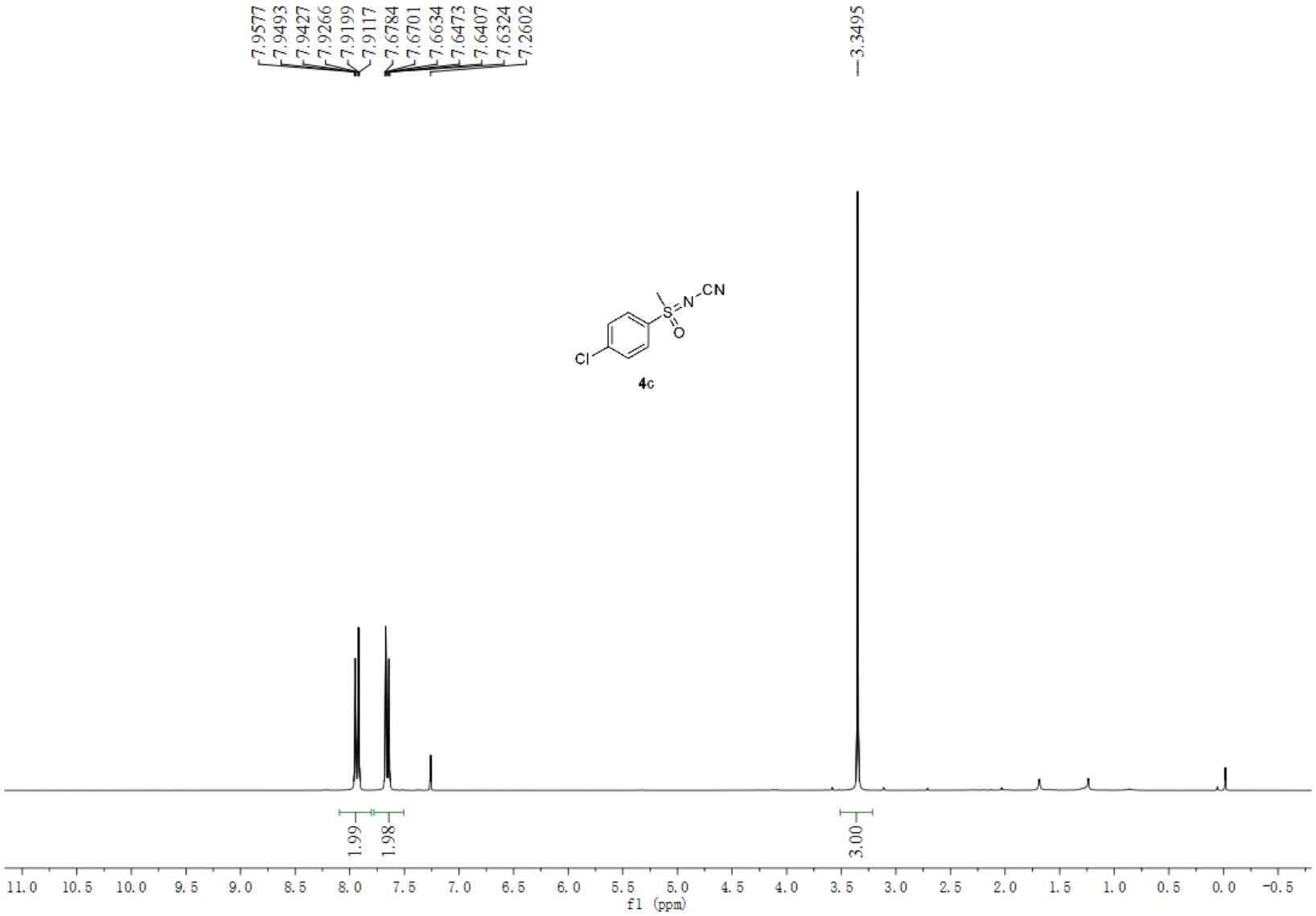

135.91
135.40
130.20
127.79
111.79
77.25
77.00
76.75
44.69
O
S
N
CN
4a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

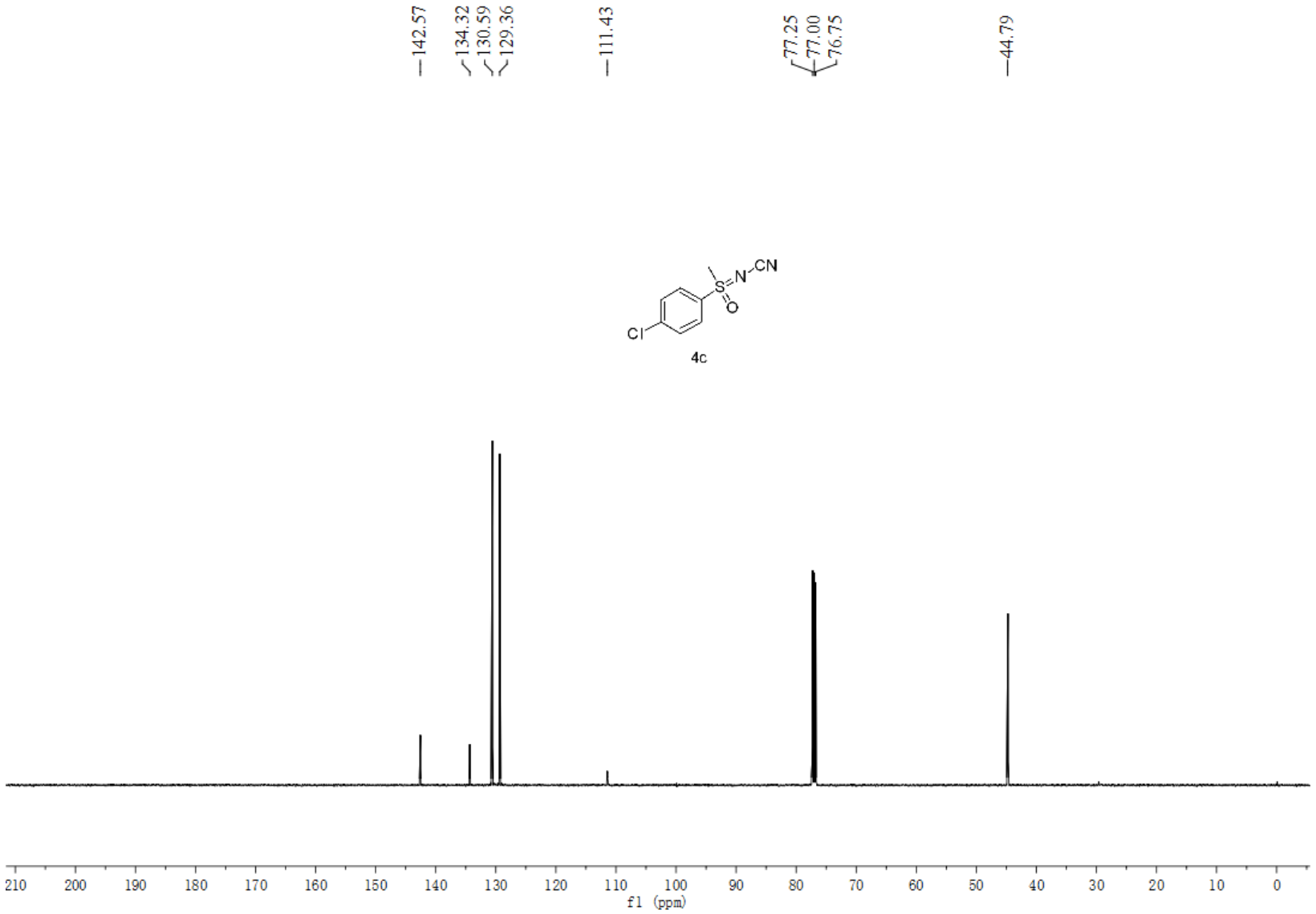
_N_-(Cyano) methyl 4-methylphenyl sulfoximine (4b)



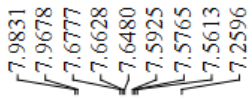

146.92
132.70
130.76
127.78
112.00
77.25
77.00
76.75
44.78
21.65
CN
S
N
O
4b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

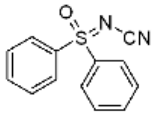
_N_-(Cyano) methyl 4-chlorophenyl sulfoximine (4c)



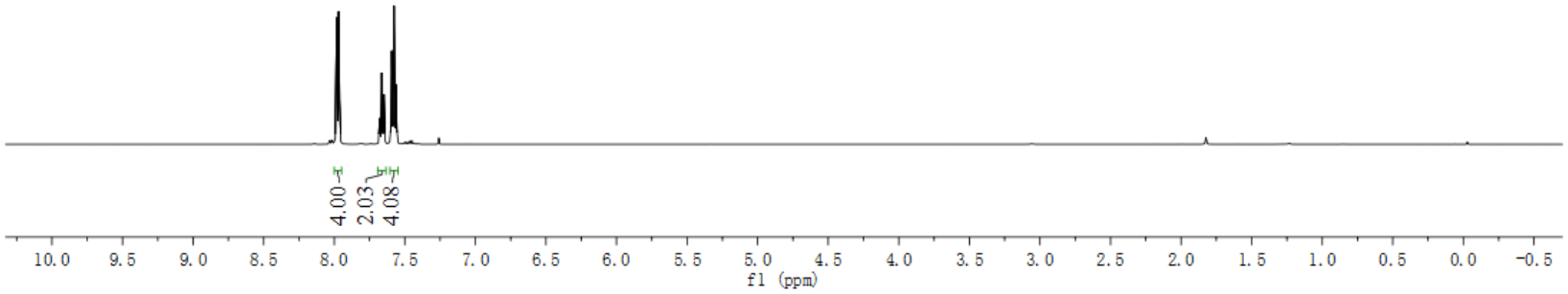

142.57
134.32
130.59
129.36
111.43
77.25
77.00
76.75
44.79
Cl
S
N
CN
O
4c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

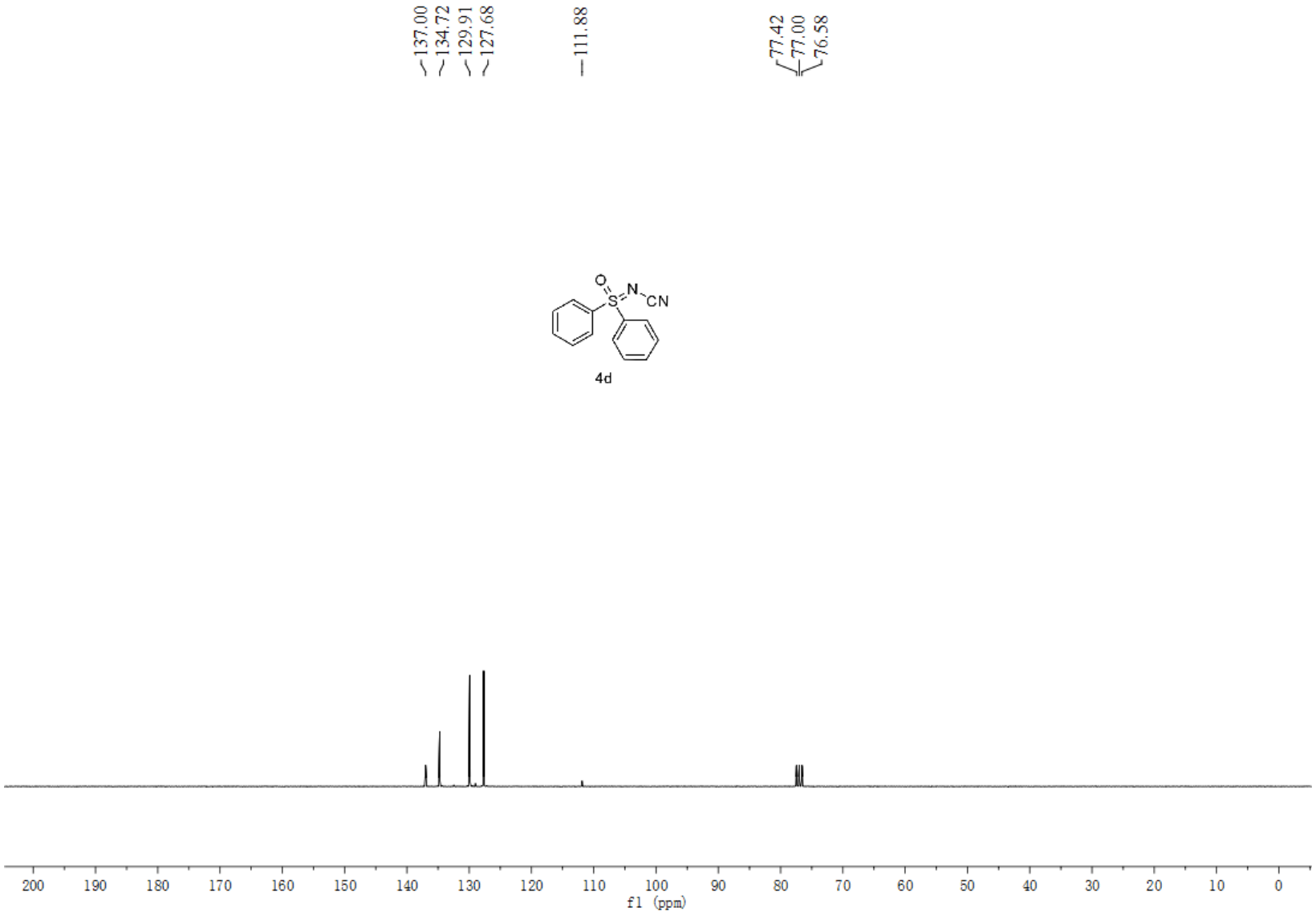
N-(Cyano) diphenyl sulfoximine (4d)



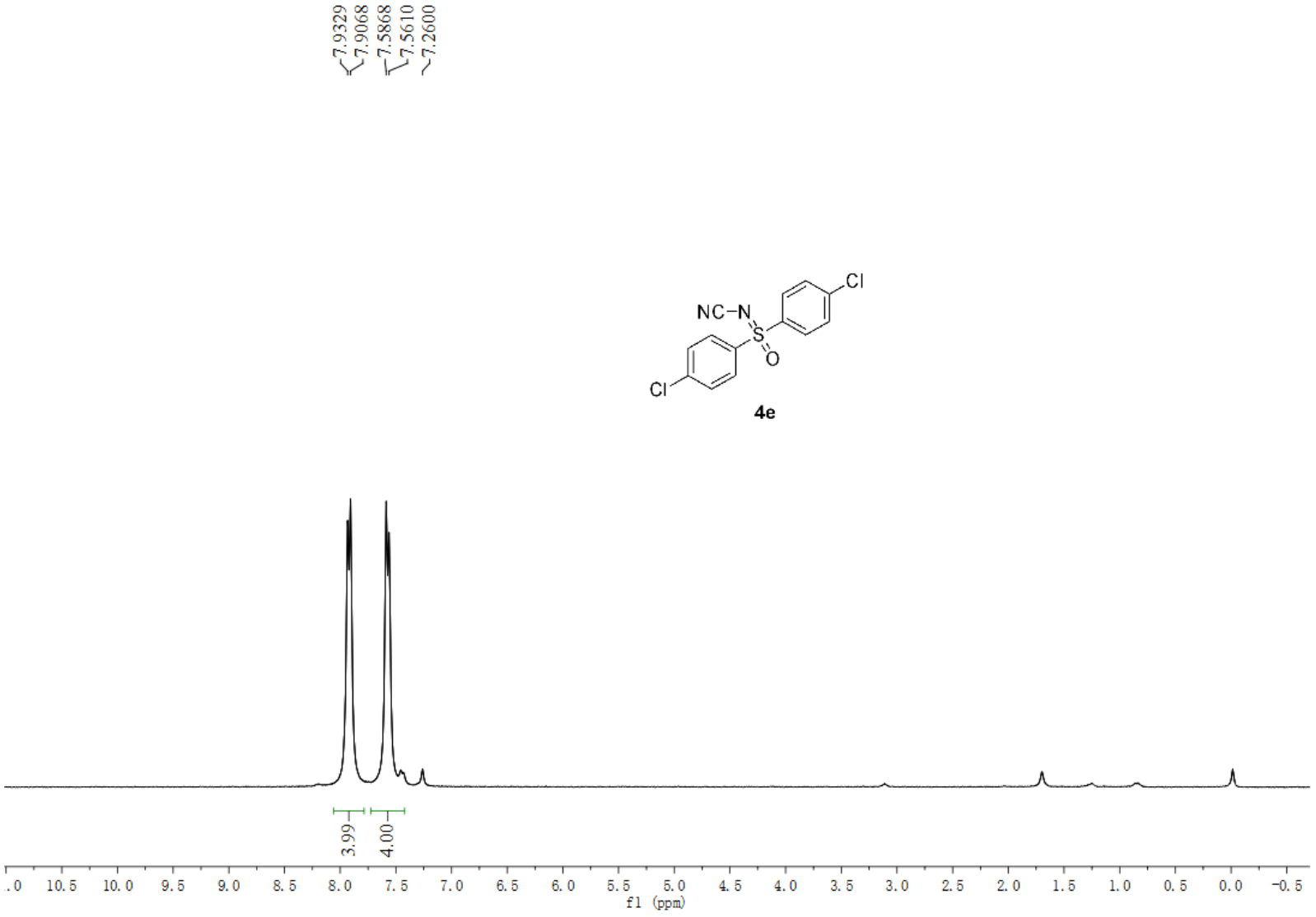


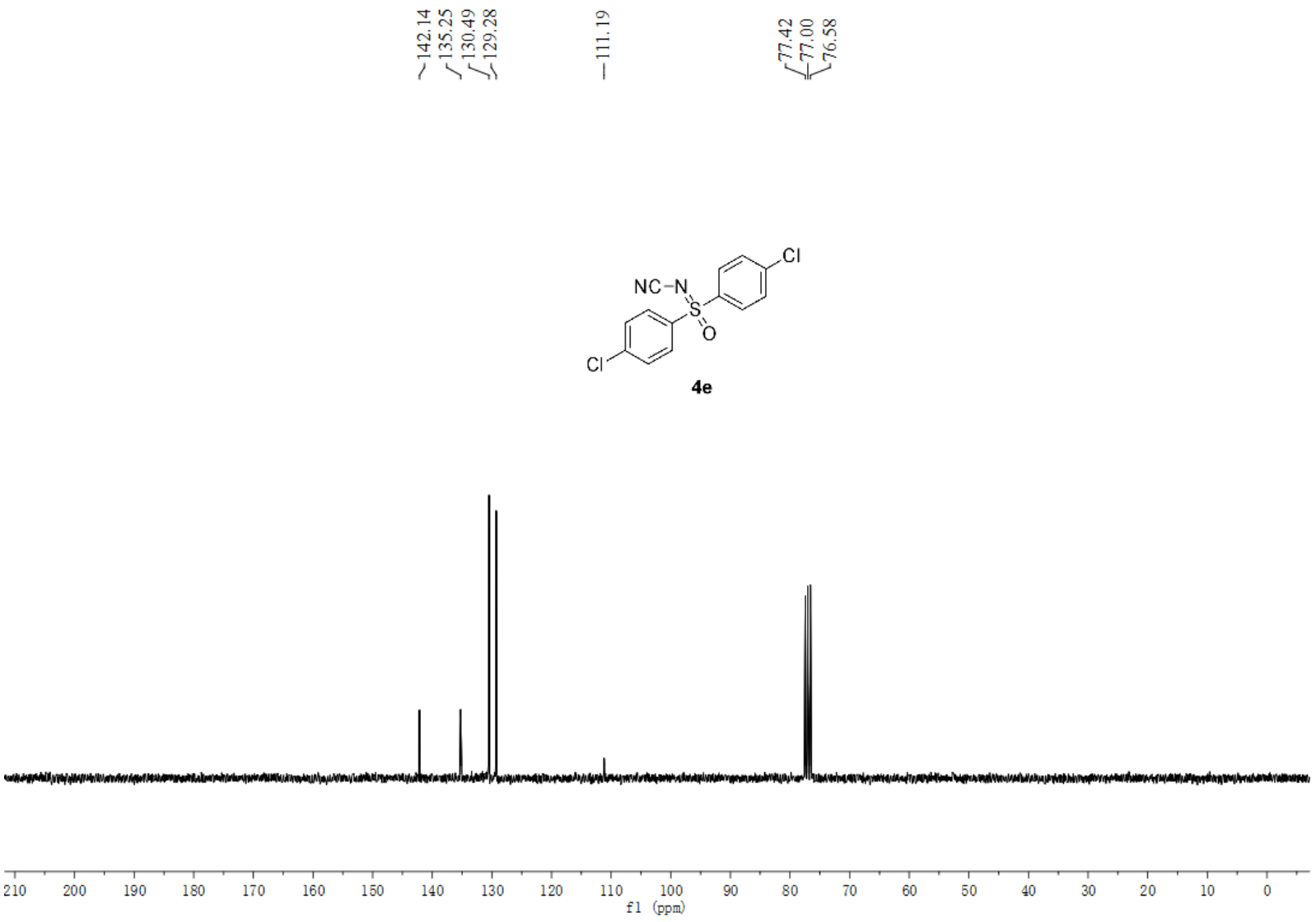
4d



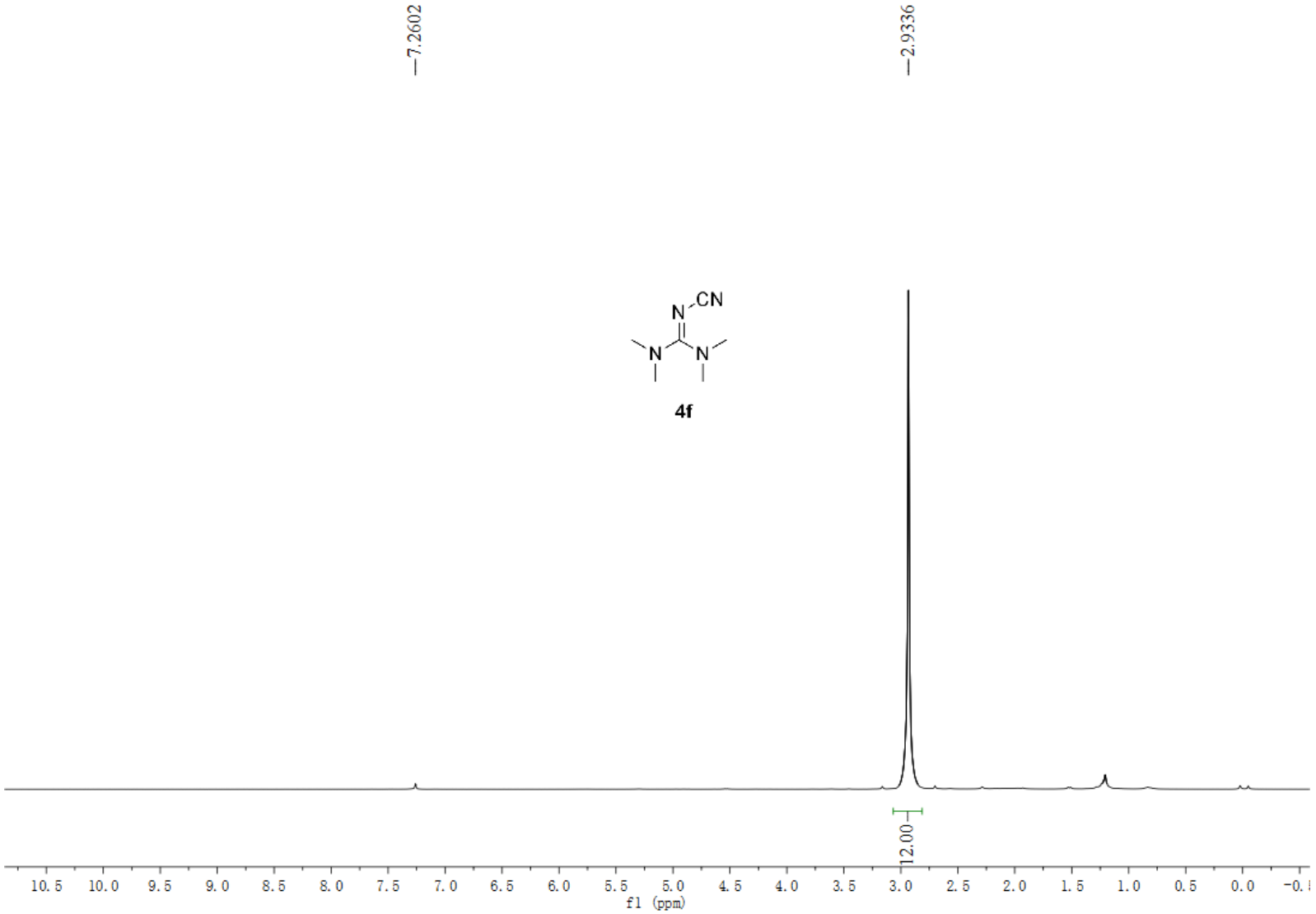

137.00
134.72
129.91
127.68
111.88
77.42
77.00
76.58
O
S
N
CN
4d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

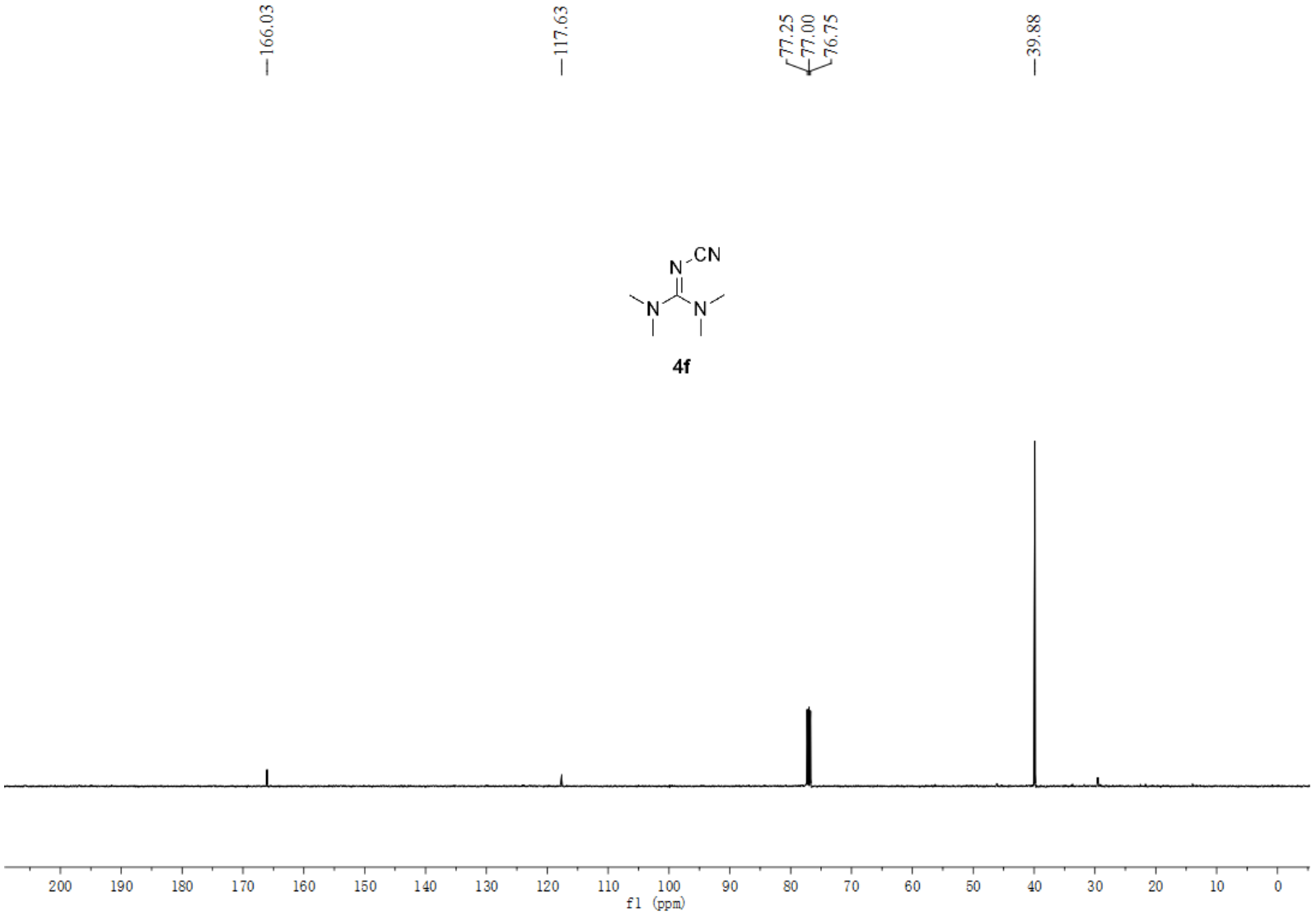
N-(Cyano)-4,4’-Dichlorodiphenyl sulfoximine (4e)




142.14
135.25
130.49
129.28
111.19
77.42
77.00
76.58
NC–N
S
O
Cl
Cl
4e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2-Cyano-1,1,3,3-tetramethylguanidine (4f)




166.03
117.63
77.25
77.00
76.75
39.88
N
CN
N
N
4f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)