Supporting Information

Cyanation and Cyanomethylation of Aryltrimethylammonium Salts via Electrochemical Cleavage of C–N Bonds

Xianqiang Kong, [†‡] Yuchang Wang,[†] Yiyi Chen,[†] Xiaohui Chen,[†] Long Lin,[‡] and Zhong-Yan Cao[§]*

[†] School of Chemical Engineering and Materials, Changzhou Institute of Technology, No. 666 Liaohe Road, Changzhou 213032, China.

[‡] College of Chemistry, Chemical Engineering and Biotechnology, Donghua University, 2999 North Renmin Lu, Shanghai 201620, China.

[§] College of Chemistry and Chemical Engineering, Henan University, Kaifeng 475004, China.

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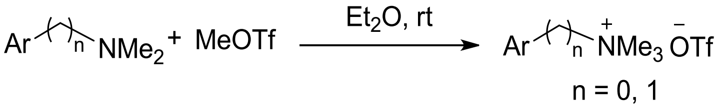
1. General

Commercial reagents and solvents were obtained from the commercial providers and used without further purification. The products were purified using a commercial flash chromatography system or a regular glass column. TLC was developed on silica gel 60 F254 glassplates.^{1}H NMR (500 MHz) ,^{13}C NMR (126 MHz) and ^{19}F NMR (471 MHz) spectra were recorded on a Bruker NMR apparatus. The chemical shifts are reported in δ (ppm) values (^{1}H and ^{13}C NMR relative to $CHCl_3$, δ 7.26 ppm for ^{1}H NMR and δ 77.0 ppm for ^{13}C NMR). Or alternatively, ^{1}H NMR chemical shifts were referenced to tetramethylsilane signal (0 ppm). Multiplicities are recorded by s (singlet), d (doublet), t (triplet), q (quartet), p (pentet), h (hextet), m (multiplet) and br (broad). Coupling constants (*J*), are reported in Hertz (Hz). Commercial reagents were used without any further purification.

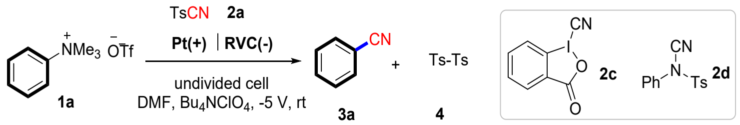
2. General Procedure for Preparation of Ammonium Triflates 1

Ammonium Triflates **1** were prepared according to reported synthetic procedures.[1]



Dimethylamine (5 mmol, 1.0 equiv) was dissolved in Et_2O (10 mL). MeOTf (6.5 mmol, 1.3 equiv) was added dropwise at 0 °C. After complete addition, the reaction mixture was stirred for an additional 15−60 min at 0 °C. The solution was concentrated and washed with Et_2O (2 × 20 mL). The resulting compounds were dried under vacuum to give a salt.

3. Optimization of Reaction Conditions



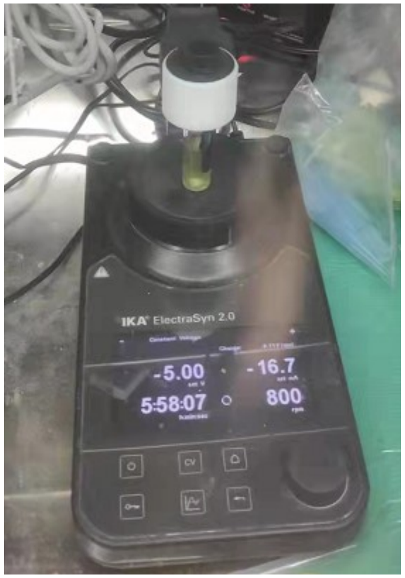
Entry	Variation from standard conditions[a]	Yield of **2a** (%)[b]
1	none	78/71
2	I instead of OTf	Trace/Trace
3	Cl instead of OTf	12/8
4	Br instead of OTf	Trace/Trace
5	Et_3N as additive	63/58
6	Acetone instead of DMF	12/8
7	DCE instead of DMF	NR
8	1:1 DMF/MeOH instead of DMF	15/12
9	CH_3CN instead of DMF	NR
10	DMSO instead of DMF	23/18
11	$I = 10$ mA/cm^2 (constant current)	43/36
12	−4.5 V instead of −5 V	69/62
13	−5.3 V instead of −5 V	52/47
14	No n-Bu_4NClO_4	9/ Trace
15	n-Bu_4NPF_6 instead of n-Bu_4NClO_4	NR
16	Et_4NOTs instead of n-Bu_4NClO_4	NR
17	$LiClO_4$ instead of n-Bu_4NClO_4	NR
18	Pt (+)|C (−) instead of Pt (+)|RVC (−)	58/52
19	Pt (+)|Pt (−) instead of Pt (+)|RVC (−)	NR
20	C (+)|Pt (−) instead of Pt (+)|RVC (−)	NR
21	RVC (+)|RVC (−) instead of Pt (+)|RVC (−)	61/59
22	RVC (+)|Pt (−) instead of Pt (+)|RVC (−)	NR
23	**2c** instead of **2a**	15/0
24	**2d** instead of **2a**	27/0
25	No electric current	NR

[a] Standard conditions: reticulated vitreous carbon (RVC) cathode (100 PPI, 1 cm × 0.5 cm), Pt anode (1 cm × 0.2 cm), $V = -5.0$ V, **1a** (0.50 mmol, 1 equiv), **2** (0.60 mmol, 1.2 equiv), DMF (4 mL), n-Bu_4NClO_4 (0.1 mol/L), 25 °C. [b] Isolated yields are reported. NR = no reaction.

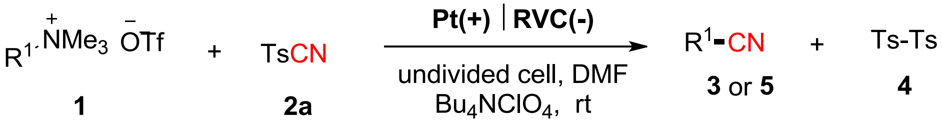
Discussion: we chose aryltrimethylammonium triflate **1a** as a model substrate and TsCN (**2a**) as the cyanation agent, and we carried out reactions in an undivided cell under various conditions (Table 1). Encouragingly, when the reaction was performed in DMF containing *n*-Bu_4NClO_4 at a constant voltage of −5 V using a Pt plate as the anode and reticulated vitreous carbon (RVC) as the cathode, desired nitrile **3a** was obtained in 78% isolated yield (entry 1). We also obtained a 71% yield of 4,4-dimethyldiphenyl disulfone (**4**) in the reaction. Evaluation of several different substrate anions (entries 2–4) showed that the triflate ion gave the highest yield. Anodic Me_3N oxidation was appreciable under these conditions. Because we regarded the Me_3N generated in situ as a sacrificial agent that was oxidized at the anode, we added an external sacrificial agent (Et_3N) to the reaction mixture. However, this additive failed to improve the yield (entry 5). Replacing DMF with acetone, DCE, 1:1 DMF/MeOH, CH_3CN, or DMSO resulted in low yields (entries 6–10). When we carried out the reaction under constant-current conditions or at a higher or lower voltage, the yield decreased dramatically (entries 11–13). In the absence of *n*-Bu_4NClO_4 electrolyte, the yield was dropped to 9% (entry 14). When *n*-Bu_4NPF_6, *n*-Bu_4NOTs, or $LiClO_4$ was used instead, no reaction occurred (entries 15–17). Variation of the electrode materials has a dramatic effect on the yield (entries 18–22). Moreover, although the desired product **3a** was detected when **2c** or **2d** was used as the cyanation agent, the yield was very low (entries 23 and 24). Finally, in the absence of an electric current, no **3a** was obtained (entry 25).

4. General Procedure for the Cyanation and Cyanomethylation

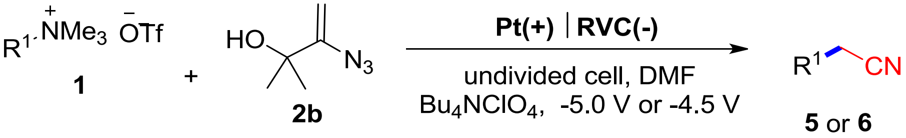
Reticulated Vitreous Carbon (RVC, Right) and Pt(Left)



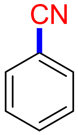
Current controlled electrolysis (ElectraSyn 2.0 apparatus, IKA)



General Procedure for the Cyanation of 1 with TsCN. An undivided cell was equipped with a reticulated vitreous carbon (RVC) anode (100 PPI, 1 cm × 0.5 cm) and Pt cathode (1 cm × 0.2 cm) and connected to a DC regulated power supply. To the cell was added aryl- or benzyltrimethylammonium salts **1** (0.50 mmol), TsCN **2a** (0.6 mmol, 109 mg), *n*-Bu_4NClO_4 (137 mg) and DMF (4 mL). The mixture was electrolyzed using V = -5.0 V at room temperature under magnetic stirring for 6-8 hours. TLC analysis indicated that the electrolysis was complete (witnessed by the disappearance of the **1**). The reaction mixture was poured into diethyl ether (30 mL), washed with water two times (20 mL × 2), dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel using a mixture of petroleum ether/EtOAc (v : v = 50 : 1) as eluent to afford the desired pure product **3** or **5** and **4** (white solid).

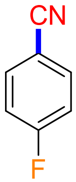


General Procedure for the Cyanomethylation with 3-Azido-2-methylbut-3-en-2-ol. An undivided cell was equipped with a reticulated vitreous carbon (RVC) anode (100 PPI, 1 cm × 0.5 cm) and Pt cathode (1 cm × 0.2 cm) and connected to a DC regulated power supply. To the cell was added aryl- or benzyltrimethylammonium salts **1**, 3-azido-2-methylbut-3-en-2-ol **2b** (0.55 mmol, 70 mg), *n*-Bu_4NClO_4 (137 mg) and DMF (4 mL). The mixture was electrolyzed using V = -5.0 V at 30 °C under magnetic stirring. When TLC analysis indicated that the electrolysis was complete (witnessed by the disappearance of the **1**). The reaction mixture was poured into diethyl ether (30 mL), washed with water two times (20 mL × 2), dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel using a mixture of petroleum ether/EtOAc (v : v = 50 : 1) as eluent to afford the desired pure product **5** or **6**.



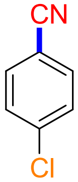
3a

Benzonitrile (**3a**),[2] 40.2 mg, 78% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.68 – 7.64 (m, 2H), 7.64 – 7.59 (m, 1H), 7.48 (t, *J* = 7.9 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 132.8, 132.1, 129.2, 118.9, 112.4. (Ts-Ts **4** was isolated with 71% yield.)



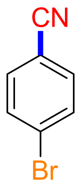
3b

4-Fluorobenzonitrile (**3b**),[2] 48.4 mg, 80% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.75 – 7.67 (m, 2H), 7.23 – 7.16 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.1 (d, *J* = 257.0 Hz), 134.7 (d, *J* = 8.8 Hz), 118.0, 116.9 (d, *J* = 22.7 Hz), 108.6 (d, *J* = 3.8 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -102.4. (Ts-Ts **4** was isolated with 75% yield.)



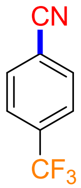
3c

4-Chlorobenzonitrile (**3c**),[2] 54.8 mg, 80% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.63-7.60 (m, 2H), 7.49-7.47 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.5, 133.4, 129.7, 118.0, 110.8. (Ts-Ts **4** was isolated with 73% yield.)



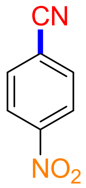
3d

4-Bromobenzonitrile (**3d**),[2] 63.9 mg, 71% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.68 – 7.62 (m, 2H), 7.60 – 7.51 (m, 2H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 133.4, 132.7, 128.0, 118.1, 111.3. (Ts-Ts **4** was isolated with 65% yield.)



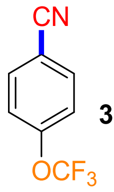
3e

4-(Trifluoromethyl)benzonitrile (**3e**),[2] 67.5 mg, 79% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.78 (d, *J* = 8.3 Hz, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 134.5 (q, *J* = 26.9 Hz), 132.7, 126.2 (q, *J* = 9.1 Hz), 123.1 (q, *J* = 219.0 Hz), 117.4, 116.1. ^{19}F NMR (471 MHz, CDCl$_3$) δ -63.6. (Ts-Ts **4** was isolated with 71% yield.)



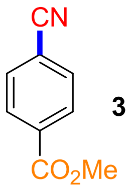
3f

4-Nitrobenzonitrile (**3f**),[2] 17.0 mg, 23% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.38 (d, *J* = 8.4 Hz, 2H), 7.92 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 150.1, 133.5, 124.3, 118.3, 116.8. (Ts-Ts **4** was isolated with 15% yield.)



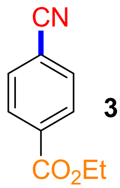
3g

4-(Trifluoromethoxy)benzonitrile (**3g**),[2] 64.5 mg, 69% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.78 – 7.70 (m, 2H), 7.41 – 7.31 (m, 2H). ^{13}C NMR (101 MHz, CDCl$_3$): δ 152.2 (q, *J* = 1.0 Hz), 134.2, 121.2, 120.2 (q, *J* = 208.4 Hz), 117.6, 110.8. ^{19}F NMR (471 MHz, CDCl$_3$) δ -57.8. (Ts-Ts **4** was isolated with 65% yield.)



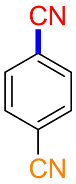
3h

Methyl 4-cyanobenzoate (**3h**),[2] 60.0 mg, 72% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.18 – 8.11 (m, 2H), 7.83 – 7.70 (m, 2H), 3.96 (s, 3H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 165.4, 133.9, 132.2, 130.1, 118.0, 116.4, 52.7. (Ts-Ts **4** was isolated with 69% yield.)



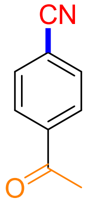
3i

Ethyl 4-cyanobenzoate (**3i**),[2] 63.9 mg, 73% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.28 – 8.10 (m, 2H), 7.95 – 7.60 (m, 2H), 4.44 (d, J = 7.2, 1.1 Hz, 2H), 1.43 (td, J = 7.1, 1.0 Hz, 3H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 165.0, 134.3, 132.2, 130.1, 118.0, 116.3, 61.8, 14.2. (Ts-Ts **4** was isolated with 69% yield.)



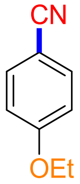
3j

Terephthalonitrile (**3j**),[2] 48.6 mg, 76% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.82 (d, J = 1.2 Hz, 4H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 132.8, 117.0, 116.7. (Ts-Ts **4** was isolated with 71% yield.)



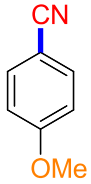
3k

4-Acetylbenzonitrile (**3k**),[2] 55.1 mg, 76% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.13 – 8.02 (m, 2H), 7.87 – 7.72 (m, 2H), 2.67 (s, 3H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 196.5, 139.9, 132.5, 128.7, 117.9, 116.4, 26.8. (Ts-Ts **4** was isolated with 72% yield.)



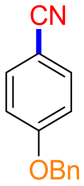
3l

4-Ethoxybenzonitrile (**3l**),[2] 60.3 mg, 82% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.57 (dd, J = 9.1, 2.4 Hz, 2H), 7.11 – 6.84 (m, 2H), 4.08 (q, J = 7.0 Hz, 2H), 1.44 (t, J = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 162.3, 134.0, 119.3, 115.2, 103.7, 63.9, 14.6. (Ts-Ts **4** was isolated with 76% yield.)



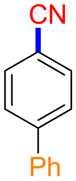
3m

4-Methoxybenzonitrile (**3m**),[2] 53.9 mg, 81% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.57 (dd, J = 8.8, 1.6 Hz, 2H), 6.95 (dd, J = 8.8, 1.6 Hz, 2H), 3.85 (s, 3H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 162.9, 134.0, 119.2, 114.8, 103.9, 55.6. (Ts-Ts **4** was isolated with 76% yield.)



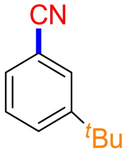
3n

4-(Benzyloxy)benzonitrile (**3n**),[2] 85.7 mg, 82% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.63 – 7.59 (m, 2H), 7.47 – 7.33 (m, 4H), 7.42 – 7.36 (m, 1H), 7.06 – 7.03 (m, 2H), 5.14 (s, 2H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 162.0, 135.7, 134.0, 128.8, 128.5, 127.5, 119.2, 115.6, 104.3, 70.3. (Ts-Ts **4** was isolated with 76% yield.)



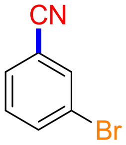
3o

[1,1'-Biphenyl]-4-carbonitrile (**3o**),[2] 67.1 mg, 75% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.79 – 7.74 (m, 2H), 7.74 – 7.68 (m, 2H), 7.66 – 7.59 (m, 2H), 7.55 – 7.48 (m, 2H), 7.49 – 7.43 (m, 1H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 145.7, 139.2, 132.6, 129.1, 128.7, 127.8, 127.3, 119.0, 110.9. (Ts-Ts **4** was isolated with 70% yield.)



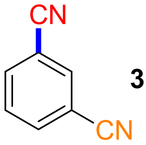
3p

3-(*Tert*-butyl)benzonitrile (**3p**),[2] 61.2 mg, 77% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.68 (t, J = 1.8 Hz, 1H), 7.64 (dq, J = 7.9, 1.5 Hz, 1H), 7.48 (dq, J = 7.5, 1.3 Hz, 1H), 7.41 (td, J = 7.7, 1.2 Hz, 1H), 1.35 (s, 9H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 152.5, 130.1, 129.2, 129.2, 128.9, 119.4, 112.1, 34.9, 31.0. (Ts-Ts **4** was isolated with 71% yield.)



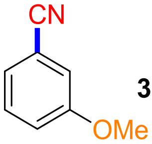
3q

3-Bromobenzonitrile (**3q**),[2] 72.0 mg, 80% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.80 (t, J = 1.8 Hz, 1H), 7.76 (dt, J = 8.2, 1.5 Hz, 1H), 7.62 (dt, J = 7.7, 1.3 Hz, 1H), 7.38 (t, J = 7.9 Hz, 1H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 136.2, 134.8, 130.7, 130.7, 122.9, 117.3, 114.2. (Ts-Ts **4** was isolated with 76% yield.)



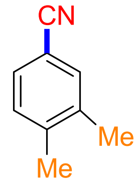
3r

Isophthalonitrile (**3r**),[2] 58.7 mg, 76% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.98 (s, 1H), 7.93 (d, J = 7.9 Hz, 2H), 7.68 (t, J = 7.9 Hz, 1H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 136.0, 135.4, 130.4, 116.6, 114.2. (Ts-Ts **4** was isolated with 71% yield.)



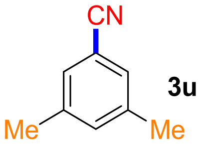
3s

3-Methoxybenzonitrile (**3s**),[2] 52.5 mg, 79% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.37 – 7.32 (m, 1H), 7.20 (dt, J = 7.6, 1.2 Hz, 1H), 7.12 – 7.10 (m, 2H), 3.80 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.6, 130.4, 124.4, 119.2, 118.7, 116.9, 113.1, 55.5. (Ts-Ts **4** was isolated with 70% yield.)



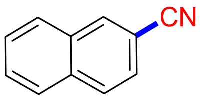
3t

3,4-Dimethylbenzonitrile (**3t**),[2] 53.1 mg, 81% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.45 – 7.36 (m, 2H), 7.23 (d, *J* = 7.7 Hz, 1H), 2.34 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.5, 137.9, 132.8, 130.3, 129.6, 119.3, 109.5, 20.1, 19.6. (Ts-Ts **4** was isolated with 72% yield.)



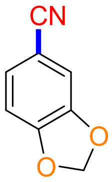
3u

3,5-Dimethylbenzonitrile (**3u**),[2] 50.4 mg, 77% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.27 (s, 2H), 7.23 (s, 1H), 2.36 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.0, 134.6, 129.7, 119.2, 112.0, 21.0. (Ts-Ts **4** was isolated with 70% yield.)



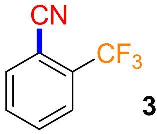
3v

2-Naphthonitrile (**3v**),[2] 63.5 mg, 83% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.23 (d, *J* = 1.8 Hz, 1H), 7.97 – 7.85 (m, 3H), 7.71 – 7.55 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 134.7, 134.2, 132.3, 129.2, 129.1, 128.4, 128.1, 127.7, 126.3, 119.3, 109.4. (Ts-Ts **4** was isolated with 75% yield.)



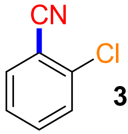
3w

Benzo[d][1,3]dioxole-5-carbonitrile (**3w**),[2] 58.8 mg, 80% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.22 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.04 (d, *J* = 1.7 Hz, 1H), 6.87 (d, *J* = 8.0 Hz, 1H), 6.08 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.6, 148.1, 128.2, 118.9, 111.4, 109.1, 104.9, 102.3. (Ts-Ts **4** was isolated with 75% yield.)



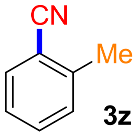
3x

2-(Trifluoromethyl)benzonitrile (**3x**),[2] 59.8 mg, 70% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.63 (dd, J = 7.7, 1.5 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.53 (s, 1H), 7.49 (d, J = 8.4 Hz, 1H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 149.2 (q, *J* = 1.3 Hz), 131.0, 130.6, 125.6, 124.4, 120.2 (q, *J* = 259.6 Hz), 117.2, 114.1. ^{19}F NMR (471 MHz, CDCl$_3$) δ -58.2. (Ts-Ts **4** was isolated with 68% yield.)



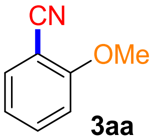
3y

2-Chlorobenzonitrile (**3y**),[2] 43.2 mg, 63% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.70 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.60 – 7.50 (m, 2H), 7.40 (td, *J* = 7.5, 1.5 Hz, 1H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 136.9, 134.0, 133.9, 130.1, 127.2, 116.0, 113.4. (Ts-Ts **4** was isolated with 57% yield.)



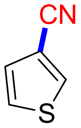
3z

2-Methylbenzonitrile (**3z**),[2] 35.1 mg, 60% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.59 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.49 (td, *J* = 7.7, 1.4 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 2.55 (s, 3H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 141.9, 132.7, 132.5, 130.3, 126.2, 118.1, 112.8, 20.4. (Ts-Ts **4** was isolated with 52% yield.)



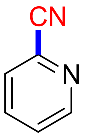
3aa

2-Methoxybenzonitrile (**3aa**),[2] 36.6 mg, 55% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.56 (ddd, *J* = 9.7, 5.7, 2.7 Hz, 2H), 7.11 – 6.94 (m, 2H), 3.94 (s, 3H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 161.3, 134.4, 133.8, 120.8, 116.5, 111.3, 101.8, 56.0. (Ts-Ts **4** was isolated with 48% yield.)



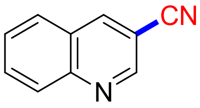
3ab

Thiophene-3-carbonitrile (**3ab**),[2] 38.9 mg, 72% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.96 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.45 (dd, *J* = 5.1, 3.0 Hz, 1H), 7.32 (dd, *J* = 5.1, 1.2 Hz, 1H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 135.4, 128.7, 127.4, 115.2, 110.7. (Ts-Ts **4** was isolated with 67% yield.)



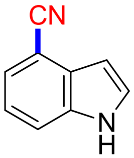
3ac

Picolinonitrile (**3ac**),[2] 32.8 mg, 63% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.72 (dt, *J* = 6.5, 2.0 Hz, 1H), 7.87 (td, *J* = 7.8, 1.7 Hz, 1H), 7.71 (dt, *J* = 7.7, 1.2 Hz, 1H), 7.55 (ddd, *J* = 7.8, 4.8, 1.3 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.2, 137.1, 133.9, 128.6, 127.0, 117.2. (Ts-Ts **4** was isolated with 58% yield.)



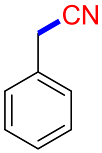
3ad

Quinoline-3-carbonitrile (**3ad**),[2] 52.4 mg, 68% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 9.04 (d, *J* = 2.1 Hz, 1H), 8.55 (d, *J* = 2.1 Hz, 1H), 8.25 – 8.15 (m, 1H), 7.99 – 7.89 (m, 2H), 7.77 – 7.67 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.7, 148.8, 141.5, 132.8, 129.9, 128.5, 128.3, 126.2, 117.1, 106.6. (Ts-Ts **4** was isolated with 61% yield.)



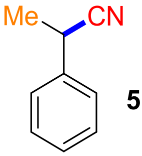
3ae

4-(4-Methylphenylsulfonimidoyl)morpholine (**3ae**),[2] 44.0 mg, 62% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 9.01 – 8.73 (s, br, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.57 – 7.49 (m, 1H), 7.44 (t, *J* = 2.9 Hz, 1H), 7.26 (q, *J* = 7.8, 7.2 Hz, 1H), 6.84 – 6.66 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.6, 129.3, 127.2, 125.4, 121.6, 119.1, 116.2, 102.7, 101.5. (Ts-Ts **4** was isolated with 55% yield.)



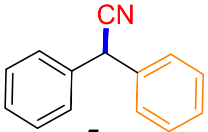
5a

2-Phenylacetonitrile (**5a**),[2] For cyanation reaction, 7.0 mg **5a** was isolated, 12% yield; Ts-Ts **4** was isolated with trace yield; for cyanomethylation reaction, 36.9 mg **5a** was isolated, 63% yield; ^{1}H NMR (500 MHz, Chloroform-d) δ 7.50 – 7.33 (m, 5H), 3.75 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 130.1, 129.2, 128.1, 128.0, 118.0, 23.6.



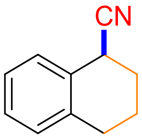
5b

2-Phenylpropanenitrile (**5b**),[2] 32.1 mg, 49% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.31 – 7.13 (m, 5H), 3.75 (q, *J* = 7.3 Hz, 1H), 1.49 (d, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.1, 129.2, 128.1, 126.7, 121.7, 31.3, 21.5. (Ts-Ts **4** was isolated with 41% yield.)



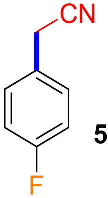
5c

2,2-Diphenylacetonitrile (**5c**),[2] 40.5 mg, 42% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.48 – 7.31 (m, 10H), 5.18 (s, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 136.0, 129.2, 128.3, 127.8, 119.8, 42.6. (Ts-Ts **4** was isolated with 36% yield.)



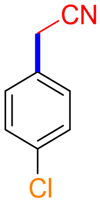
5d

1,2,3,4-Tetrahydronaphthalene-1-carbonitrile (**5d**),[2] 36.9 mg, 47% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.40 (dd, *J* = 6.6, 2.3 Hz, 1H), 7.25 (tt, *J* = 7.4, 5.4 Hz, 2H), 7.16 (dd, *J* = 6.5, 2.4 Hz, 1H), 4.01 (t, *J* = 6.4 Hz, 1H), 2.96 – 2.73 (m, 2H), 2.24-2.13 (m, 2H), 2.11-2.02 (m, 1H), 1.92-1.83 (m, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 136.5, 129.9, 129.8, 128.9, 128.0, 126.6, 121.9, 30.8, 28.4, 27.4, 20.8. (Ts-Ts **4** was isolated with 41% yield.)



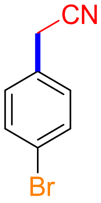
5e

2-(4-Fluorophenyl)acetonitrile (**5e**),[2] 45.2 mg, 67% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.32 (dd, *J* = 8.5, 5.2 Hz, 2H), 7.08 (td, *J* = 8.7, 2.3 Hz, 2H), 3.74 (s, 2H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 162.4 (d, *J* = 248.2 Hz), 129.7 (d, *J* = 8.8 Hz), 125.7 (d, *J* = 3.8 Hz), 116.1 (d, *J* = 22.7 Hz), 117.8, 22.9. ^{19}F NMR (471 MHz, CDCl$_3$) δ -113.9.



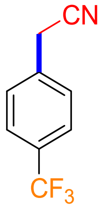
5f

2-(4-Chlorophenyl)acetonitrile (**5f**),[2] 48.3 mg, 64% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.40 – 7.34 (m, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 3.74 (s, 2H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 134.1, 129.3, 129.3, 128.5, 117.5, 23.1.



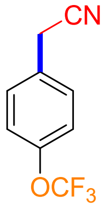
5g

2-(4-Bromophenyl)acetonitrile (**5g**),[2] 62.1 mg, 64% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.53 (dt, *J* = 8.4, 1.6 Hz, 2H), 7.27 – 7.16 (m, 2H), 3.73 (s, 2H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 132.3, 129.6, 129.0, 122.2, 117.4, 23.2.



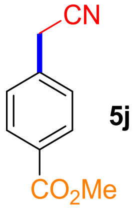
5h

2-(4-(Trifluoromethyl)phenyl)acetonitri (**5h**),[2] 50.9 mg, 55% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.66 (d, *J* = 8.1 Hz, 2H), 7.49 (d, *J* = 7.9 Hz, 2H), 3.84 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 134.0, 130.5 (q, *J* = 32.8 Hz), 128.4, 126.1 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 273.4 Hz), 117.1. ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.8.



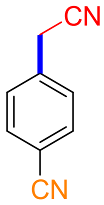
5i

2-(4-(Trifluoromethoxy)phenyl)acetonitrile (**5i**),[2] 59.3 mg, 59% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.40 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.3 Hz, 2H), 3.79 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.0, 129.5, 128.6, 121.7, 120.4 (q, *J* = 258.3 Hz), 117.4, 23.1. ^{19}F NMR (471 MHz, $CDCl_3$) δ -58.0.



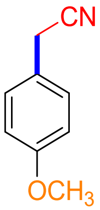
5j

Methyl 4-(cyanomethyl)benzoate (**5j**),[2] 42.9 mg, 49% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 8.07 (d, *J* = 8.2 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 2H), 3.94 (s, 3H), 3.84 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.4, 134.8, 130.4, 130.1, 128.0, 117.2, 52.3, 23.7.



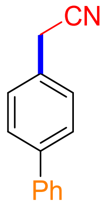
5k

4-(Cyanomethyl)benzonitrile (**5k**),[2] 36.2 mg, 51% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.81 – 7.65 (m, 2H), 7.49 (d, *J* = 8.2 Hz, 2H), 3.86 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.3, 132.9, 128.8, 118.2, 116.7, 112.3, 23.8.



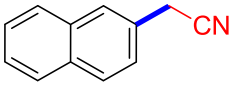
5l

2-(4-Methoxyphenyl)acetonitrile (**5l**),2 49.98 mg, 68% yield. 1H NMR (500 MHz, Chloroform-d) δ 7.28 – 7.21 (m, 2H), 6.98 – 6.89 (m, 2H), 3.83 (s, 3H), 3.70 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.4, 129.1, 121.8, 118.3, 114.5, 55.4, 22.8.



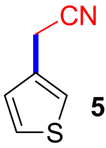
5m

2-([1,1'-Biphenyl]-4-yl)acetonitrile (**5m**),[2] 59.8 mg, 62% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.74 – 7.58 (m, 4H), 7.52 – 7.46 (m, 2H), 7.46 – 7.38 (m, 3H), 3.82 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.1, 140.2, 128.9, 128.9, 128.4, 127.9, 127.7, 127.1, 117.8, 23.4.



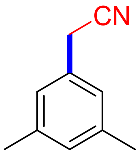
5n

2-(Naphthalen-2-yl)acetonitrile (**5n**),[2] 50.9 mg, 61% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 (dt, *J* = 9.5, 5.6 Hz, 4H), 7.55 (qd, *J* = 6.9, 3.5 Hz, 2H), 7.41 (dd, *J* = 8.4, 2.0 Hz, 1H), 3.93 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 133.4, 132.7, 129.1, 127.8, 127.7, 127.2, 126.9, 126.8, 126.5, 125.5, 117.9, 23.9.



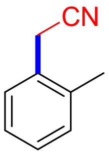
5o

2-(Thiophen-3-yl)acetonitrile (**5o**),[2] 32.0 mg, 52% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.37 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.26 (dd, *J* = 2.9, 1.4 Hz, 1H), 7.04 (dd, *J* = 5.1, 1.4 Hz, 1H), 3.74 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 129.6, 127.3, 127.1, 123.2, 117.8, 18.8.



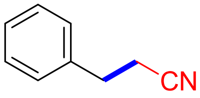
5p

2-(3,5-Dimethylphenyl)acetonitrile (**5p**),[2] 40.6 mg, 56% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 6.98 (d, *J* = 7.3 Hz, 3H), 3.69 (s, 2H), 2.35 (d, *J* = 1.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.9, 129.7, 129.6, 125.7, 118.2, 23.4, 21.2.



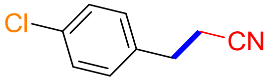
5q

2-(3,5-Dimethylphenyl)acetonitrile (**5q**),[2] 38.6 mg, 59% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.41 – 7.36 (m, 1H), 7.33 – 7.22 (m, 3H), 3.69 (s, 2H), 2.37 (s, 3H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 136.1, 130.7, 128.6, 128.4, 126.8, 117.6, 21.9, 19.3.



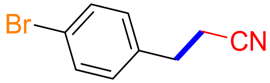
6a

3-Phenylpropanenitrile (**6a**),[2] 32.1 mg, 49% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.41 – 7.35 (m, 2H), 7.34 – 7.30 (m, 1H), 7.29 – 7.25 (m, 2H), 2.98 (t, J = 7.4 Hz, 2H), 2.63 (t, J = 7.4 Hz, 2H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 138.2, 128.9, 128.3, 127.3, 119.3, 31.6, 19.3.



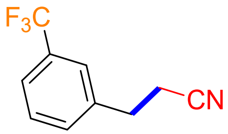
6b

3-(4-Chlorophenyl)propanenitrile (**6b**),[2] 26.4 mg, 32% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.41 – 7.30 (m, 2H), 7.20 (d, J = 8.0 Hz, 2H), 2.95 (t, J = 7.3 Hz, 2H), 2.63 (td, J = 7.3, 1.2 Hz, 2H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 136.5, 133.2, 129.7, 129.1, 118.8, 30.9, 19.3.



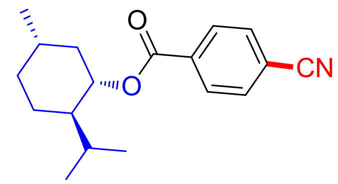
6c

3-(4-Bromophenyl)propanenitrile (**6c**),[2] 35.4 mg, 34% yield. ^{1}H NMR (500 MHz, Chloroform-d) δ 7.52 – 7.42 (m, 2H), 7.21 – 6.99 (m, 2H), 2.92 (t, J = 7.3 Hz, 2H), 2.62 (t, J = 7.3 Hz, 2H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 137.0, 132.0, 130.1, 121.2, 118.9, 31.0, 19.2.

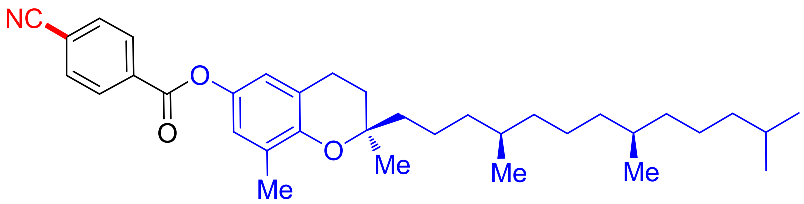


6d

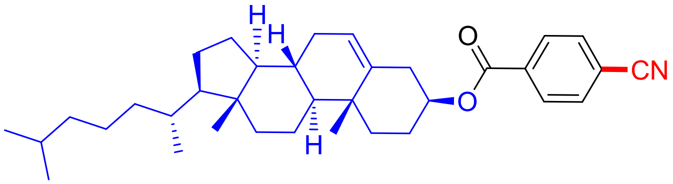
3-(3-(Trifluoromethyl)phenyl)propanenitrile (**6d**),[2] 29.9 mg, 30% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.60 – 7.56 (m, 1H), 7.54 – 7.44 (m, 3H), 3.05 (t, J = 7.3 Hz, 2H), 2.68 (t, J = 7.3 Hz, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 138.9, 131.8, 131.2 (q, J = 32.3 Hz), 129.4, 125.1 (q, J = 3.0 Hz), 124.2 (q, J = 3.7 Hz), 124.0 (q, J = 273.4 Hz), 118.6, 31.3, 19.2. ^{19}F NMR (376 MHz, CDCl$_3$) δ -62.7.



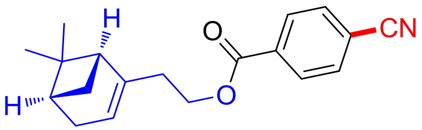
(1*S*,2*R*,5*S*)-2-Isopropyl-5-methylcyclohexyl 4-cyanobenzoate,[3] 43.3 mg, 76% yield. ^{1}H NMR (400 MHz, CDCl3) δ 8.15 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 8.5 Hz, 2H), 4.97 (td, *J* = 10.9, 4.4 Hz, 1H), 2.12 (dtd, *J* = 12.0, 4.1, 1.7 Hz, 1H), 1.97 – 1.86 (m, 1H), 1.71 (s, 2H), 1.57 (ddt, *J* = 12.4, 10.8, 3.3 Hz, 2H), 1.13 (tdd, *J* = 12.1, 10.3, 7.8 Hz, 2H), 0.93 (dd, *J* = 6.9, 4.9 Hz, 6H), 0.91 – 0.85 (m, 1H), 0.80 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.4, 134.6, 132.2, 130.1, 118.0, 116.2, 75.9, 47.2, 40.8, 34.2, 31.4, 26.5, 23.6, 22.0, 20.7, 16.5.



(*R*)-2,8-Dimethyl-2-((4*R*,8*R*)-4,8,12-trimethyltridecyl)chroman-6-yl 4-cyanobenzoate,[3] 76.5 mg, 72% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 – 8.05 (m, 2H), 7.79 – 7.69 (m, 2H), 5.48 – 5.34 (m, 1H), 4.88 (tdd, *J* = 9.6, 7.5, 4.5 Hz, 1H), 2.49 – 2.44 (m, 2H), 2.06 – 0.84 (m, 41H), 0.69 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 139.3, 134.7, 132.2, 130.1 123.2, 118.1, 116.2, 75.6, 56.7, 56.1, 50.0, 42.3, 39.7, 39.5, 38.1, 37.0, 36.6, 36.2, 35.8, 31.9, 31.9, 28.2, 28.0, 27.8, 24.3, 23.9, 22.9, 22.6, 21.1, 19.4, 18.7, 11.9.



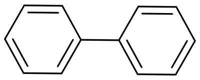
(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-cyanobenzoate,[4] 71.1 mg, 69% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 – 8.26 (m, 2H), 7.88 – 7.75 (m, 2H), 2.62 (t, *J* = 6.7 Hz, 2H), 2.12 (s, 3H), 2.02 (d, *J* = 15.9 Hz, 6H), 1.82 (td, *J* = 12.0, 10.6, 5.7 Hz, 2H), 1.67 – 1.49 (m, 4H), 1.44 – 1.03 (m, 24H), 0.86 (t, *J* = 6.7 Hz, 14H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.6, 149.8, 140.4, 133.5, 132.5, 130.6, 126.6, 124.9, 123.4, 118.0, 117.7, 116.9, 75.2, 39.4, 37.4, 37.3, 32.8, 32.8, 32.7, 28.0, 24.8, 24.5, 22.8, 22.7, 22.7, 21.1, 20.7, 19.8, 19.7, 19.6, 13.1, 12.2, 11.9.



2-((1*R*,5*S*)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethyl 4-cyanobenzoate, 36.6 mg, 62% yield. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.22 – 8.05 (m, 2H), 7.87 – 7.66 (m, 2H), 5.37 (tt, *J* = 3.0, 1.5 Hz, 1H), 4.46 – 4.28 (m, 2H), 2.44 (tt, *J* = 7.0, 1.4 Hz, 2H), 2.38 (dt, *J* = 8.5, 5.6 Hz, 1H), 2.24 (ddt, *J* = 11.1, 2.7, 1.4 Hz, 2H), 2.11 (dt, *J* = 6.5, 2.4 Hz, 2H), 1.28 (s, 3H), 1.16 (d, *J* = 8.5 Hz, 1H), 0.83 (s, 4H). ^{13}C NMR (100 MHz, CDCl$_3$) δ 164.8, 143.9, 134.2, 132.2, 130.0, 119.2, 118.0, 116.3, 64.0, 45.7, 40.7, 38.0, 35.9, 31.7, 31.4, 26.2, 21.1. HRMS m/z (ESI) calcd. for $C_{19}H_{21}NNaO_2$ $(M + Na)^+$ 318.1470, found 318.1470.

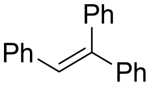
Ts-Ts
4

4,4'-Dimethyldiphenyl disulfone (**4**), ^{1}H NMR (400 MHz, Chloroform-d) δ 7.84 (d, *J* = 8.4 Hz, 4H), 7.43 (d, *J* = 8.1 Hz, 4H), 2.51 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 148.1, 131.5, 130.4, 128.0, 22.0.



7

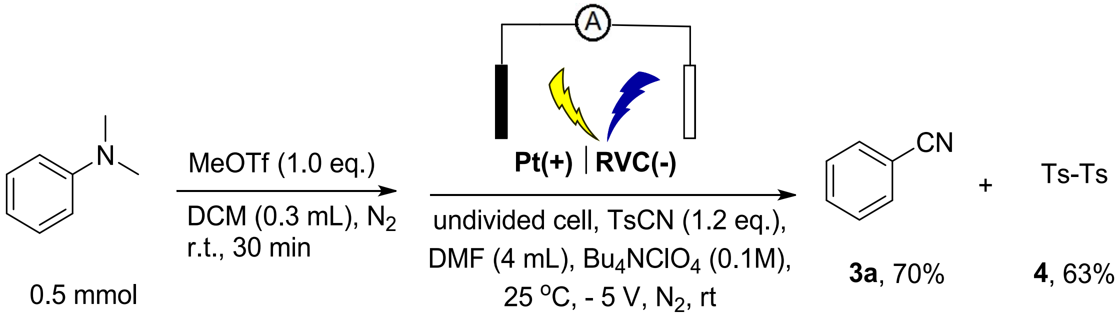
1,1'-Biphenyl (**7**), 20% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 7.6 Hz, 4H), 7.44 (t, *J* = 7.5 Hz, 4H), 7.34 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 141.3, 128.9, 127.4, 127.3.



11

Ethene-1,1,2-triyltribenzene (**11**), 27% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.31 (q, *J* = 8.0, 5.9 Hz, 8H), 7.20 (dd, *J* = 7.0, 2.8 Hz, 2H), 7.12 (d, *J* = 7.3 Hz, 3H), 7.03 (d, *J* = 7.2 Hz, 2H), 6.97 (s, 1H). ^{13}C NMR (126 MHz, CDCl$_3$) δ 143.5, 142.6, 140.4, 137.4, 130.5, 129.6, 128.7, 128.3, 128.2, 128.0, 127.7, 127.6, 127.5, 126.8.

5. One-pot-two-step Reaction



Methyl triflate (56.6 µL, 0.50 mmol) was added dropwise into the DCM solution of *N*,*N*-dimethylaniline (63.4 µL, 0.05 mmol) in a Schlenk tube with a strong stirring at room temperature. After 30 minutes, the solution of the TsCN **2a** (0.6 mmol, 109 mg), *n*-Bu_4NClO_4 (137mg) in 4 mL DMF were added by syringe respectively. The mixture was electrolyzed using V = -4.5 V at 30 °C under magnetic stirring. When TLC analysis indicated that the electrolysis was complete. The reaction mixture was poured into diethyl ether (30 mL), washed with water two times (20 mL × 2), dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel using a mixture of petroleum ether/EtOAc (v : v = 50 : 1) as eluent to afford the desired pure product **3a** (36.1 mg, 70%).

6. Cyclic Voltammetry

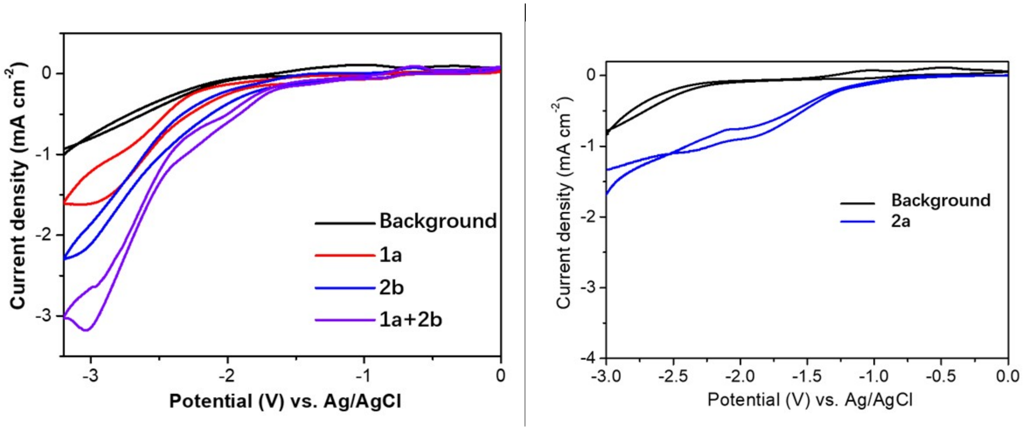
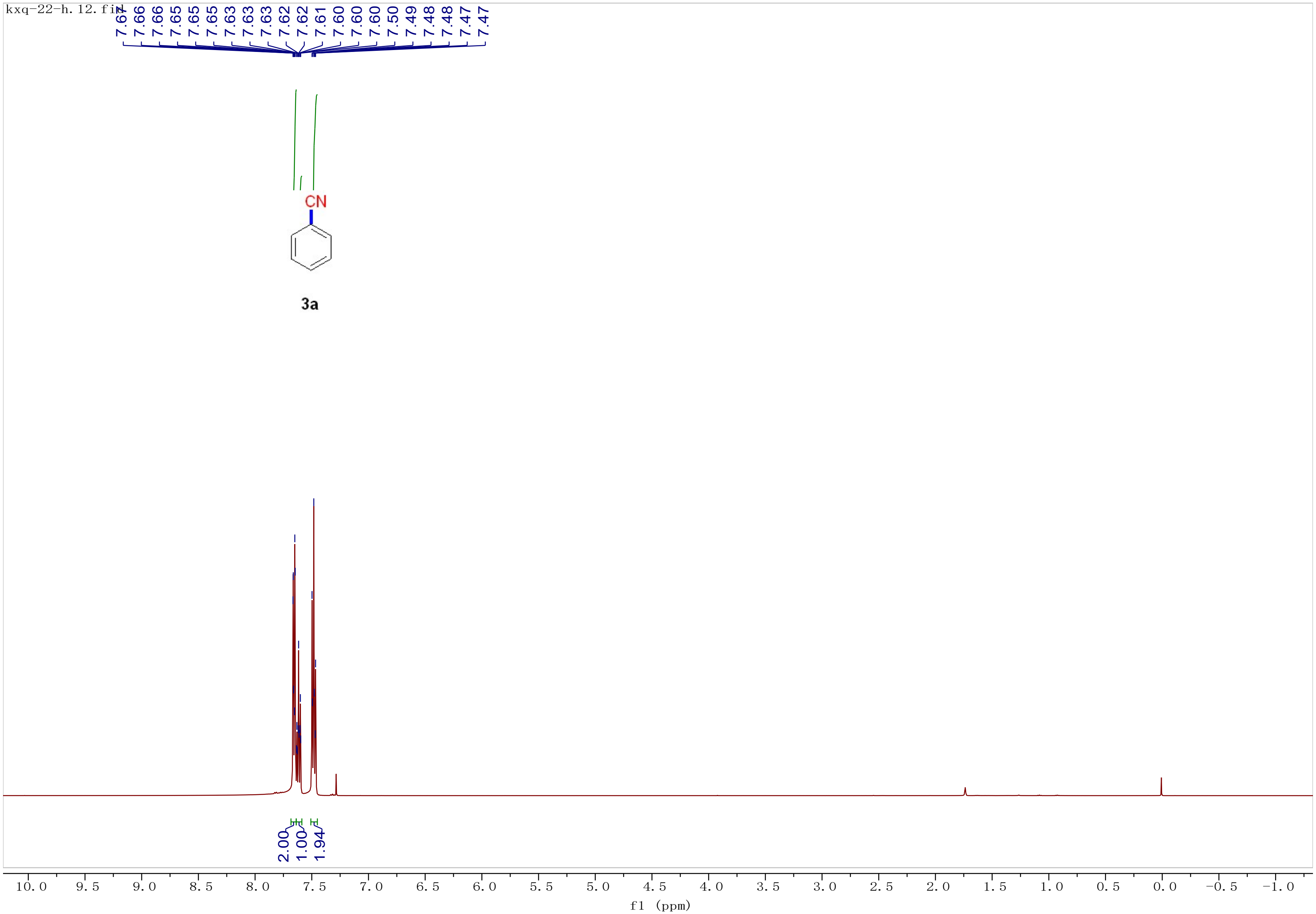
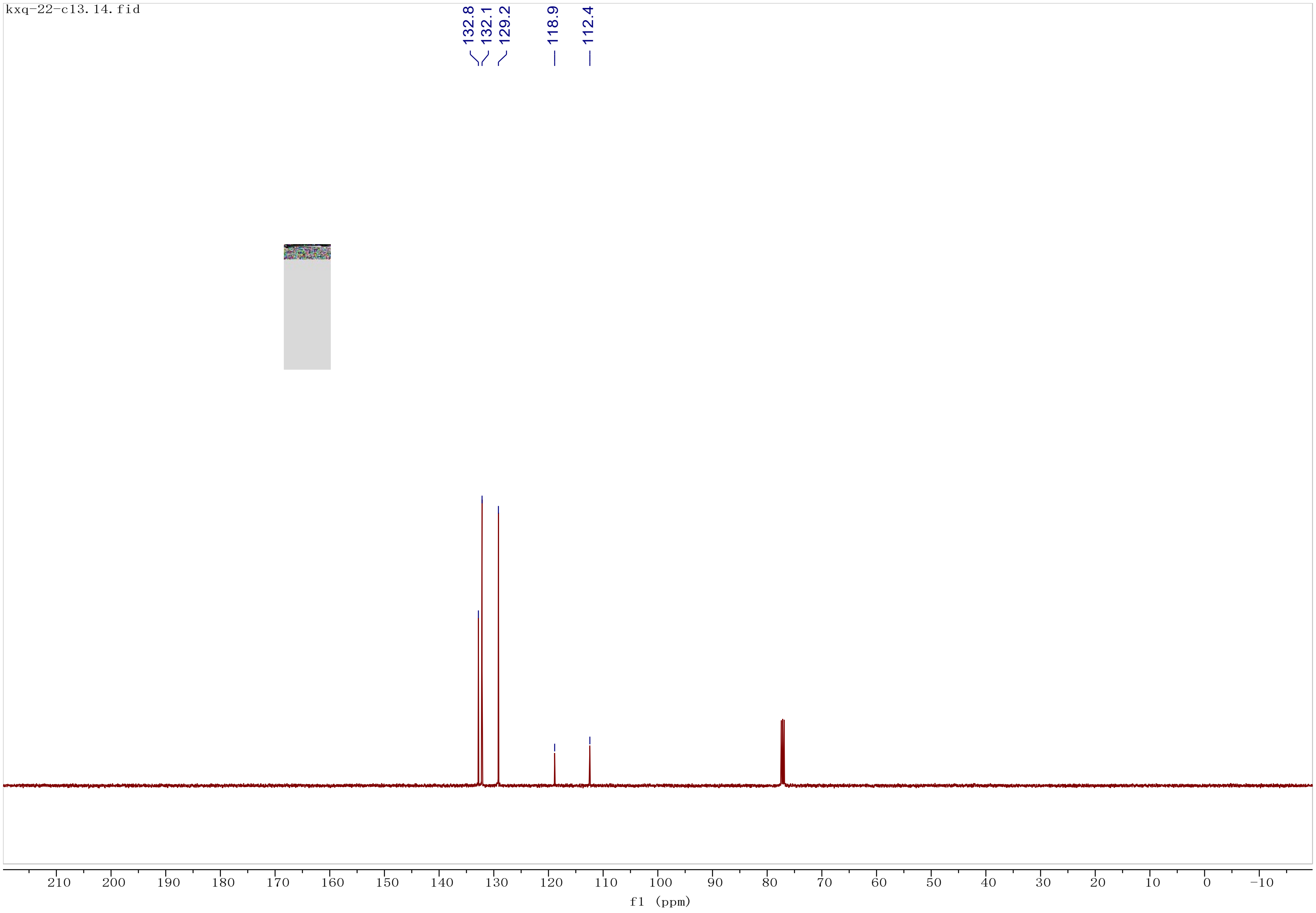


Fig. S1 Cyclic voltammograms of related compounds in DMF with 0.10 M n-Bu$_4$NClO$_4$ under N$_2$ atmosphere. 2 mm diameter Pt electrode, carbon rod, and Ag/AgCl were used as the working, counter, and the reference electrode. Voltammograms were recorded at 100 mV s^{-1}. Left: (1) background; (2) **2b** (0.05 M); (3) **1a** (0.05 M); (4) 2d (0.05 M). Right: (1) background; (2) **2a** (0.05 M).

7. Copies of NMR spectra

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180
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90
80
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40
30
20
10
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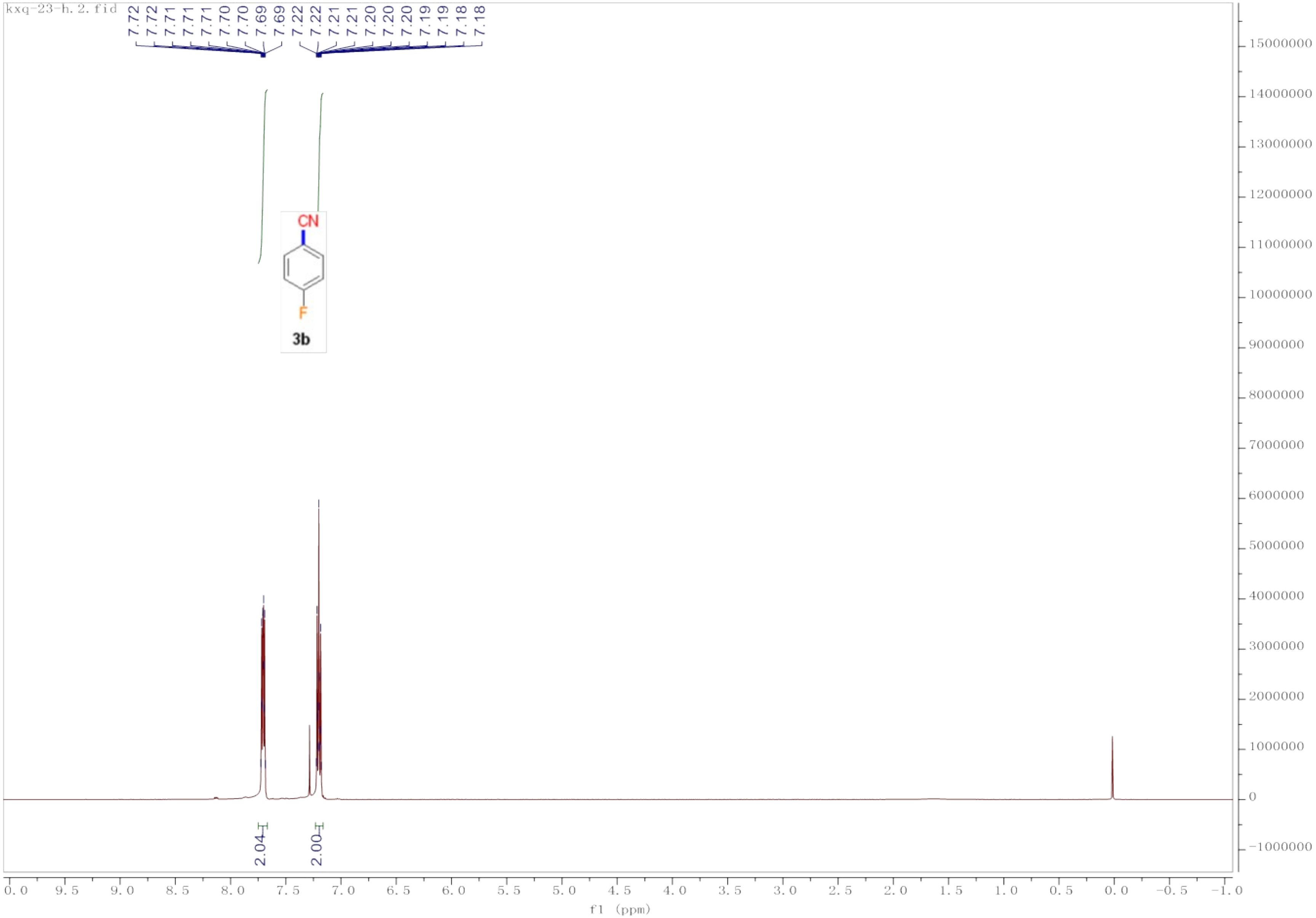
f1 (ppm)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7.22
7.21
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7.20
7.20
7.20
7.19
7.19
7.18
7.18
CN
F
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2.00
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14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
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8.5
8.0
7.5
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6.5
6.0
5.5
5.0
4.5
4.0
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1.5
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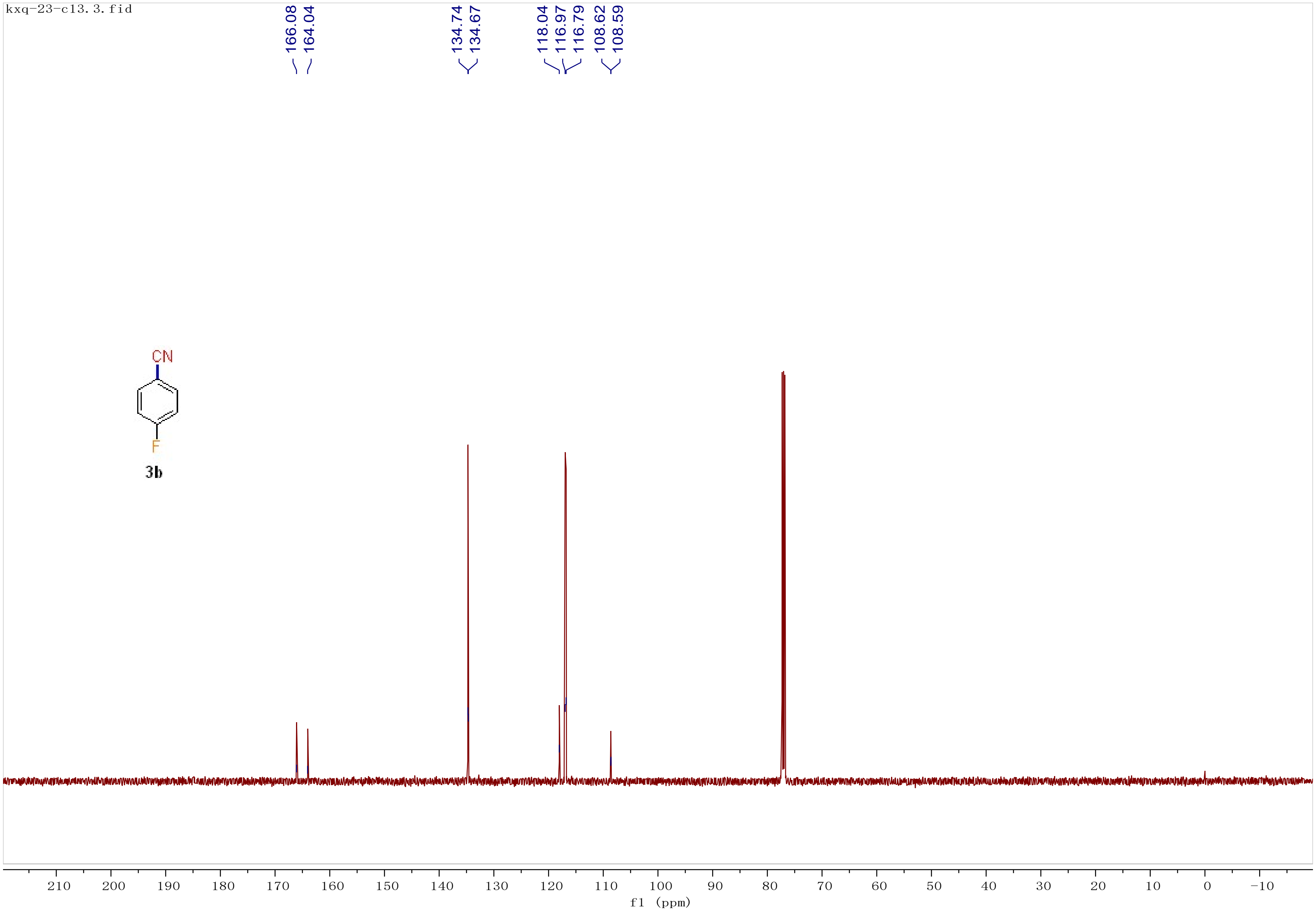
f1 (ppm)

3b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116.79
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190
180
170
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30
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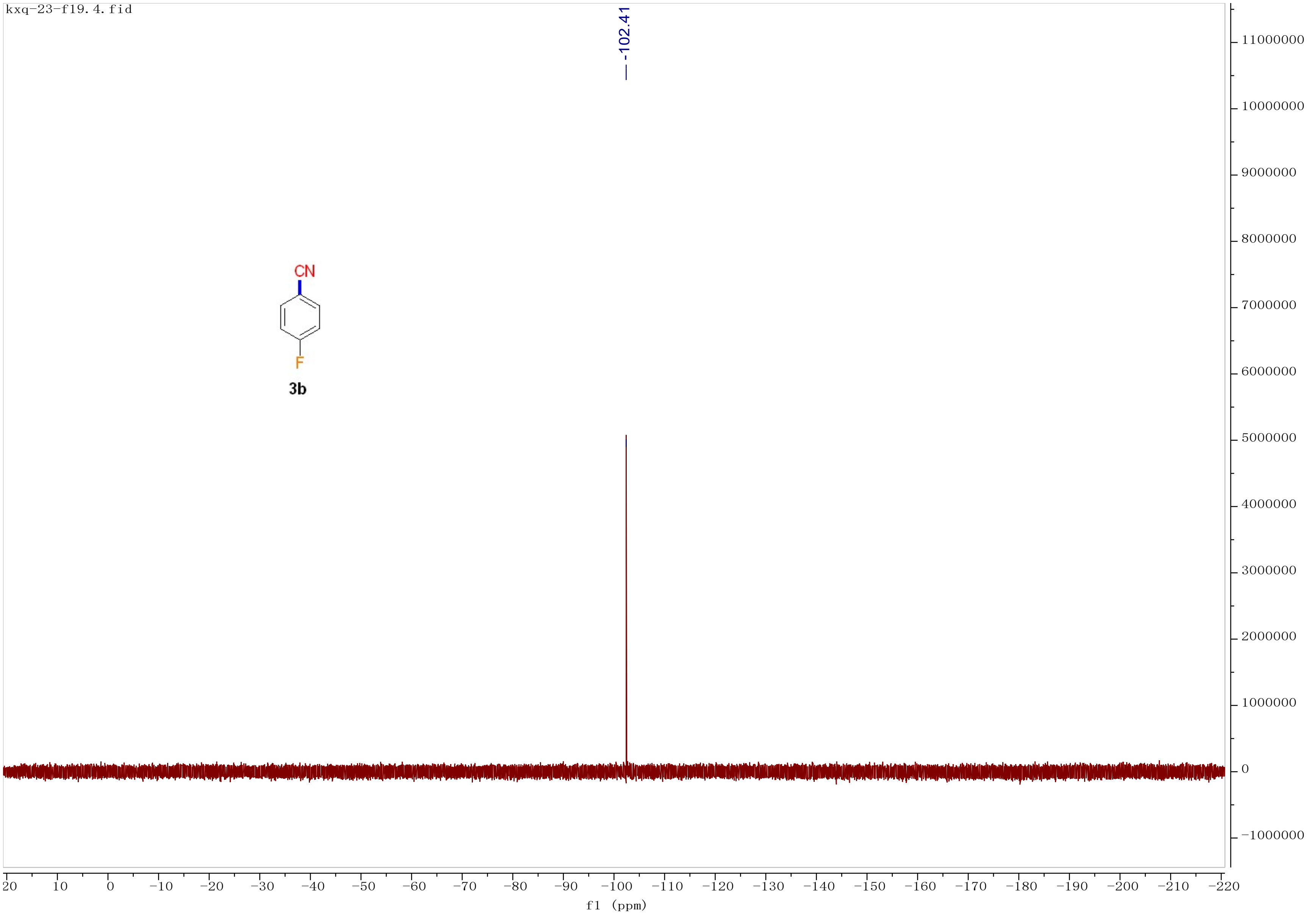
f1 (ppm)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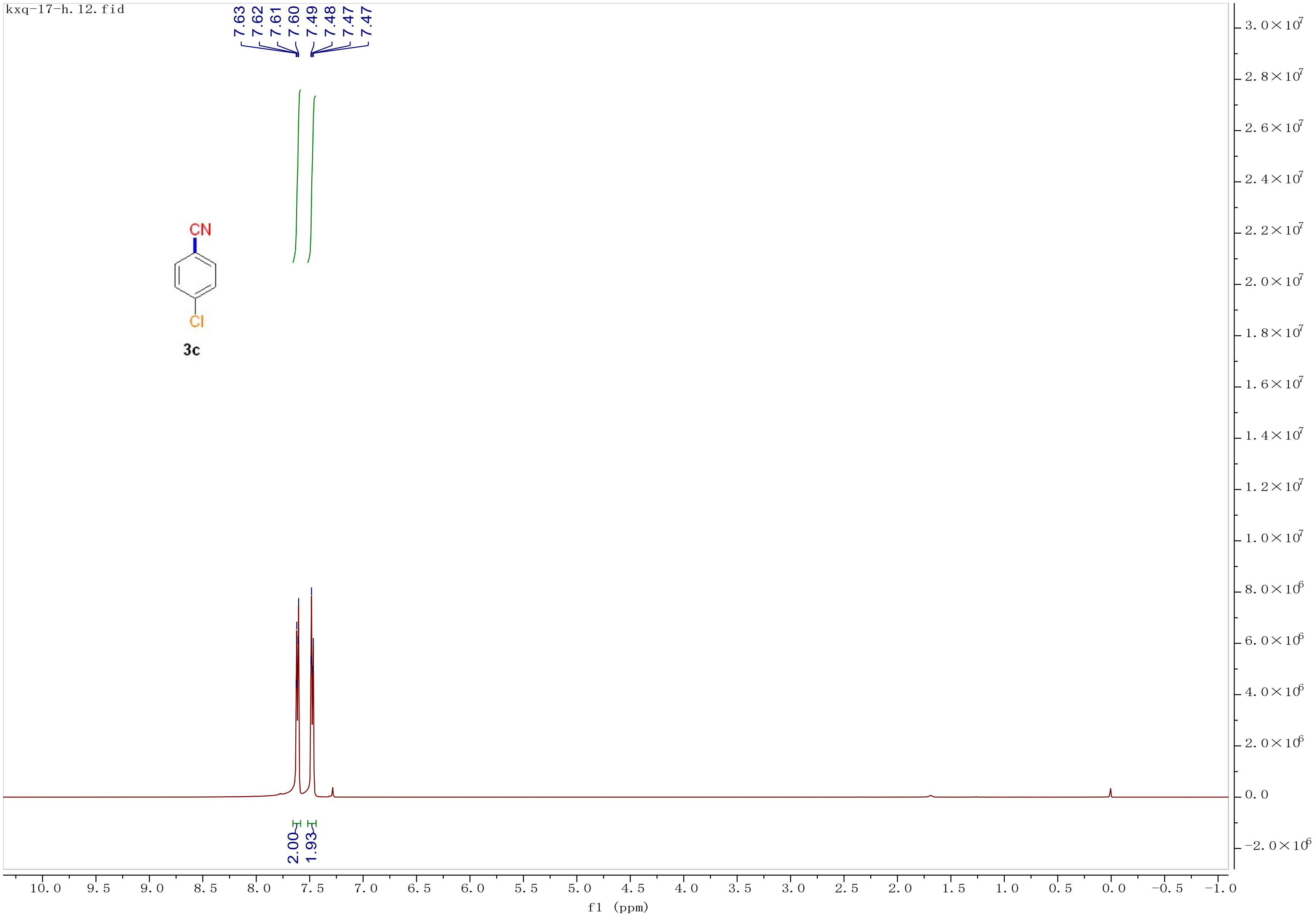
f1 (ppm)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2.4×10^7
2.2×10^7
2.0×10^7
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1.2×10^7
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6.0×10^6
4.0×10^6
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9.0
8.5
8.0
7.5
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6.0
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5.0
4.5
4.0
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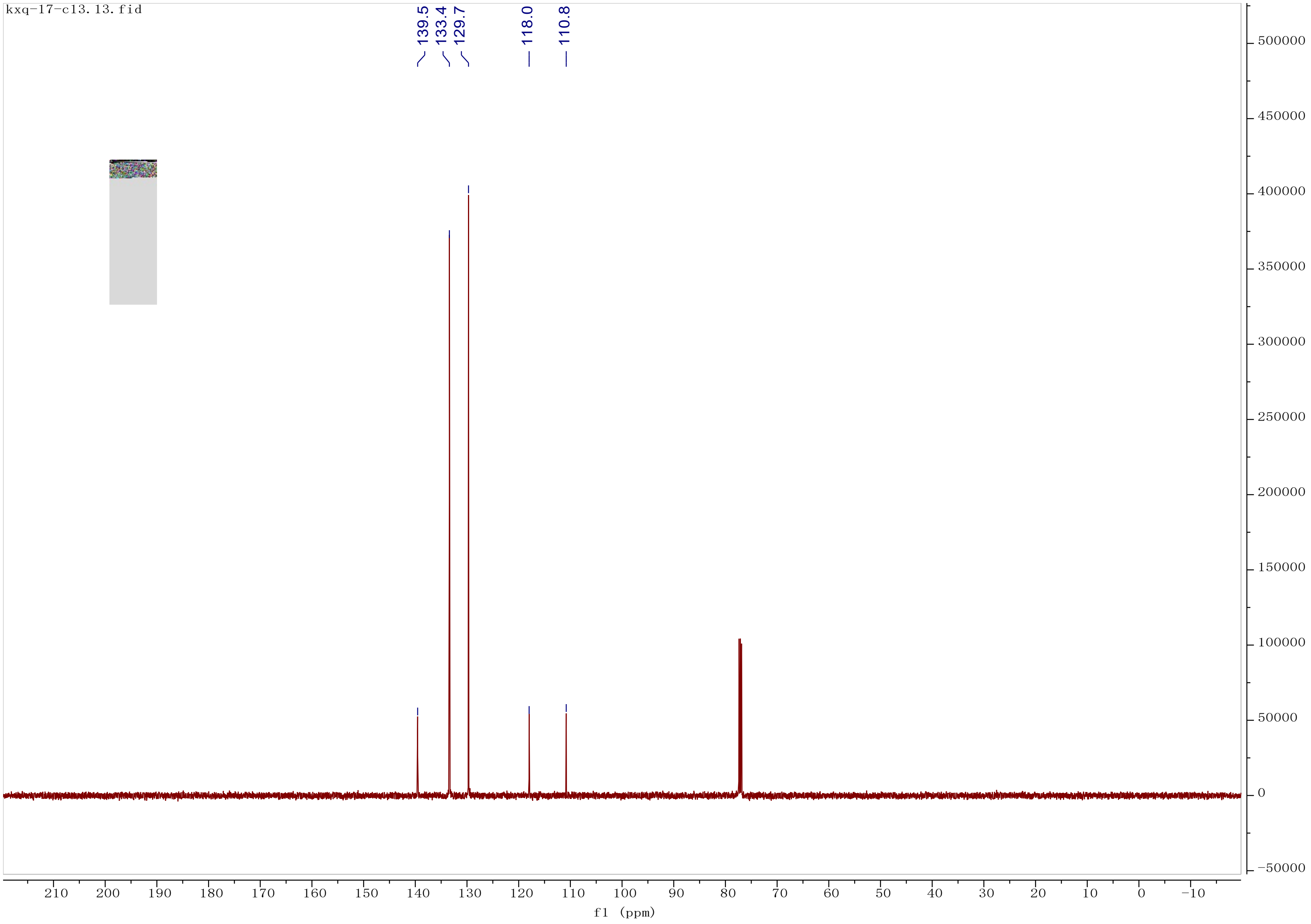
f1 (ppm)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80
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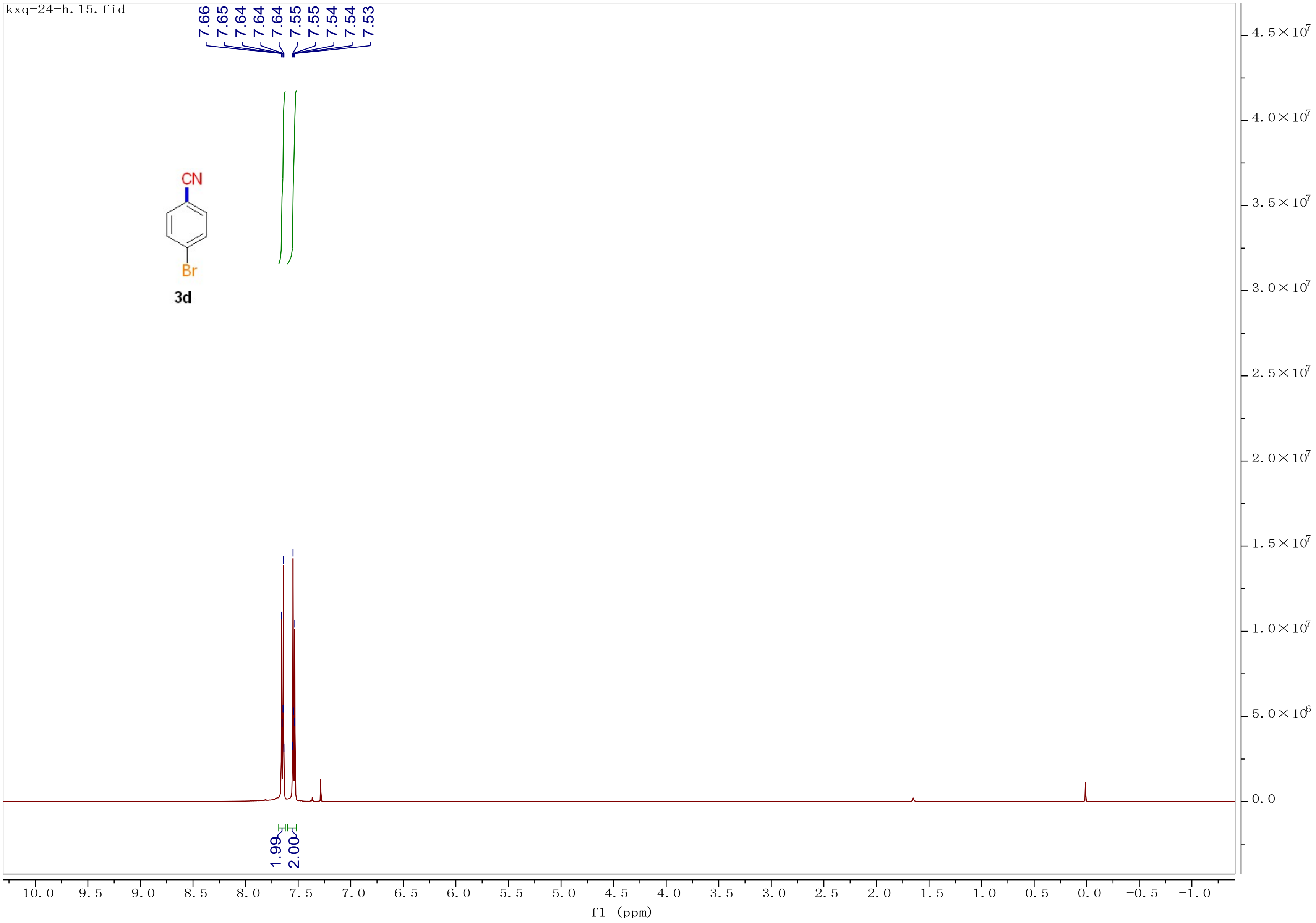
f1 (ppm)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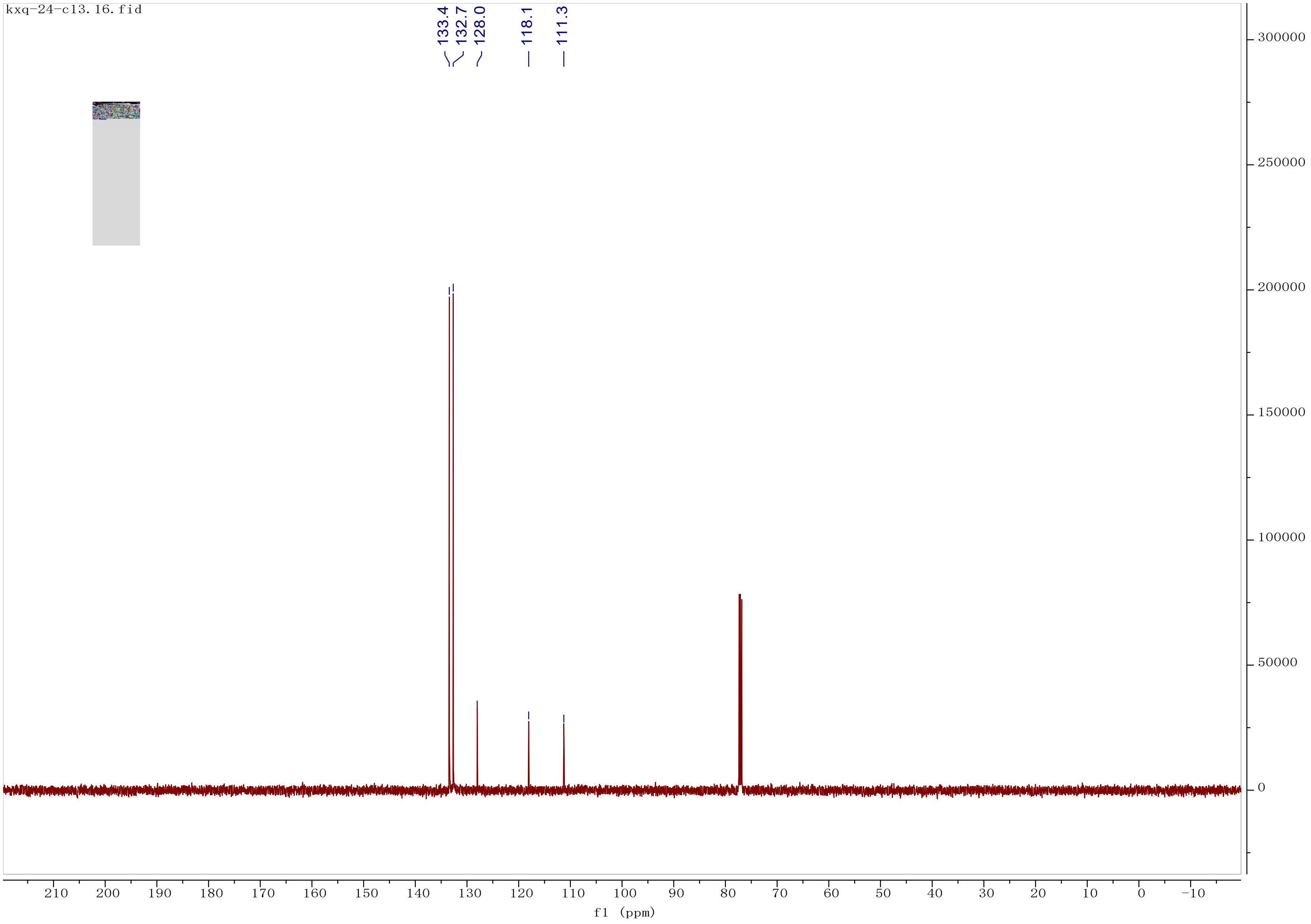
3d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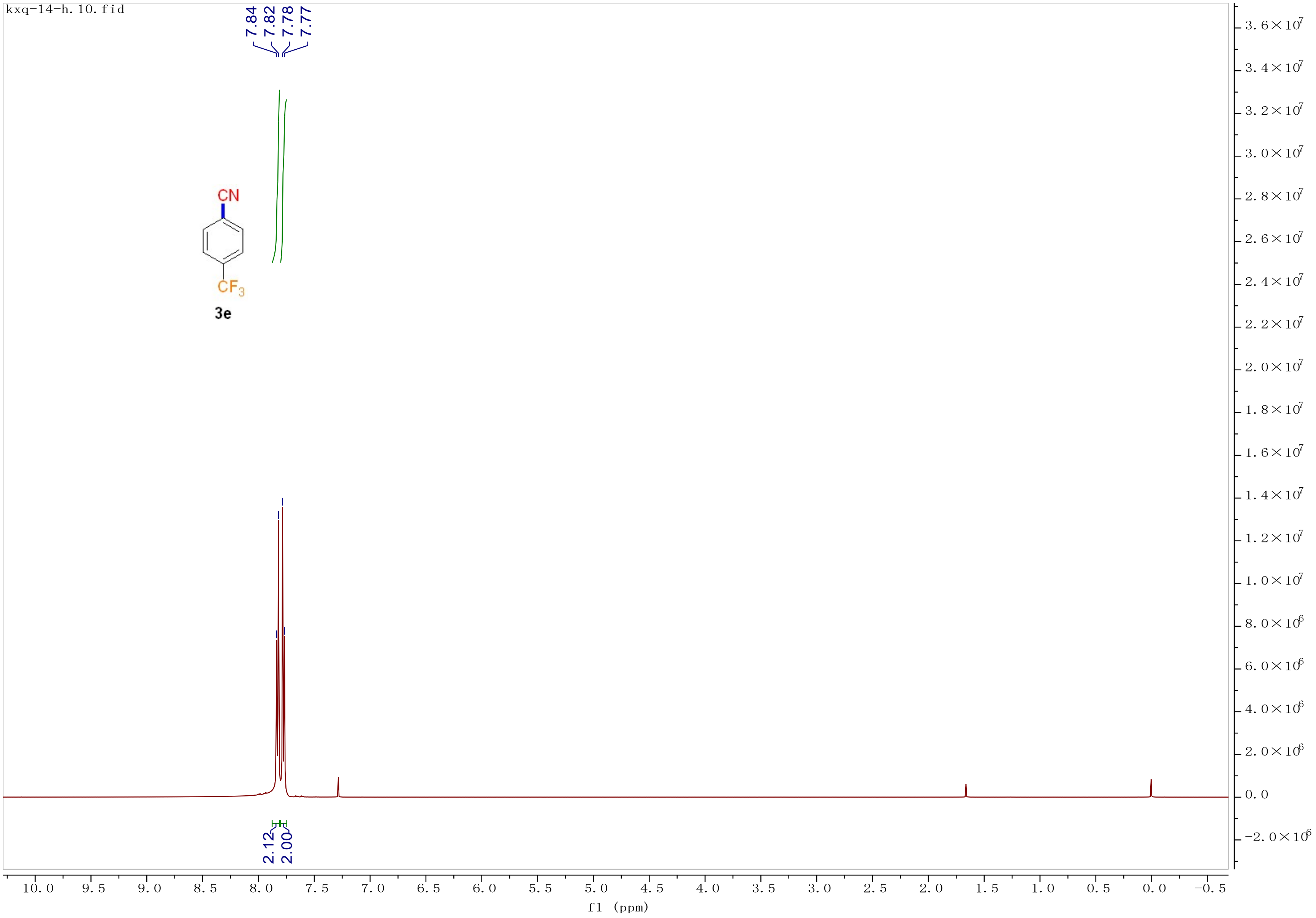
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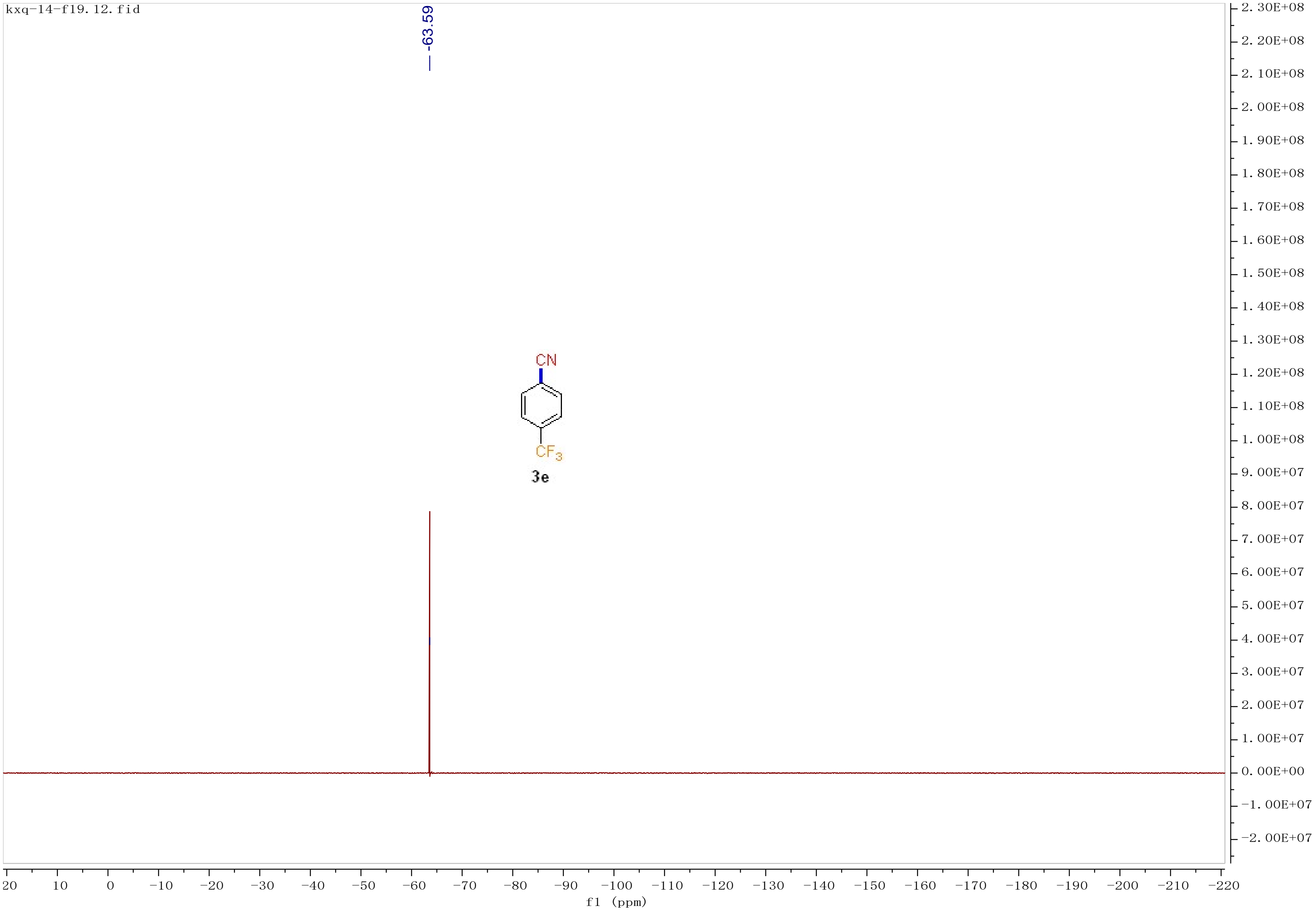
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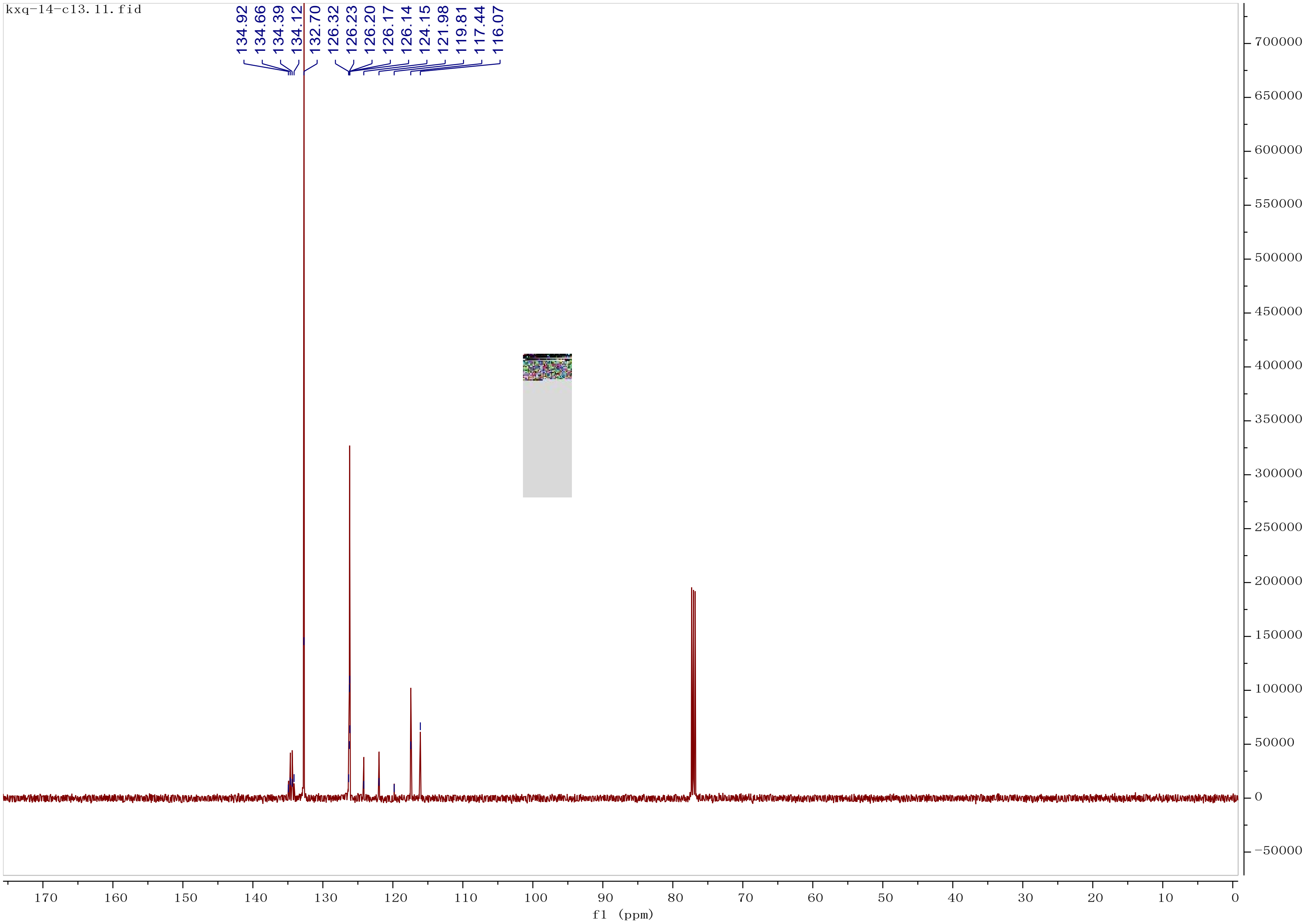
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450000
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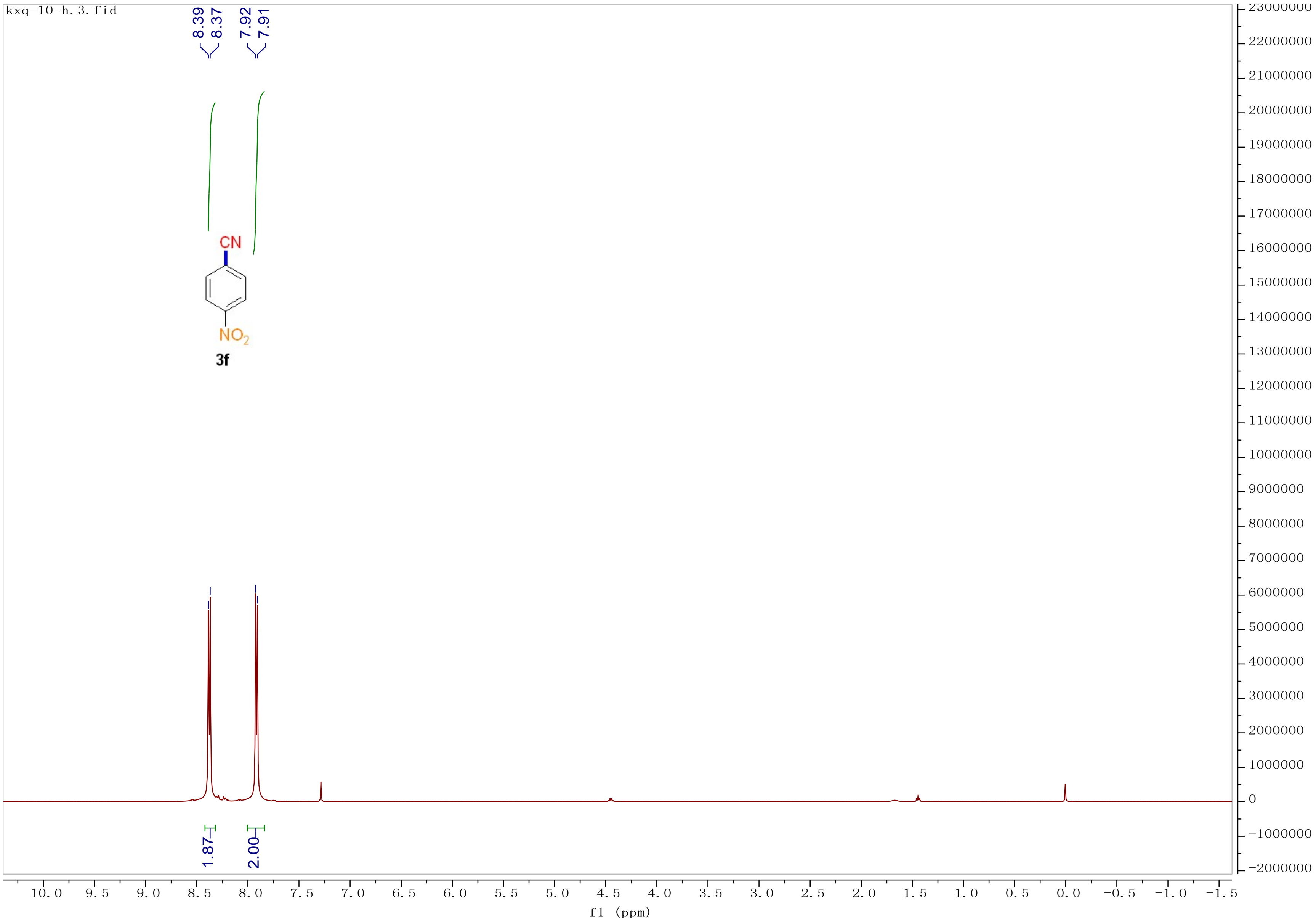
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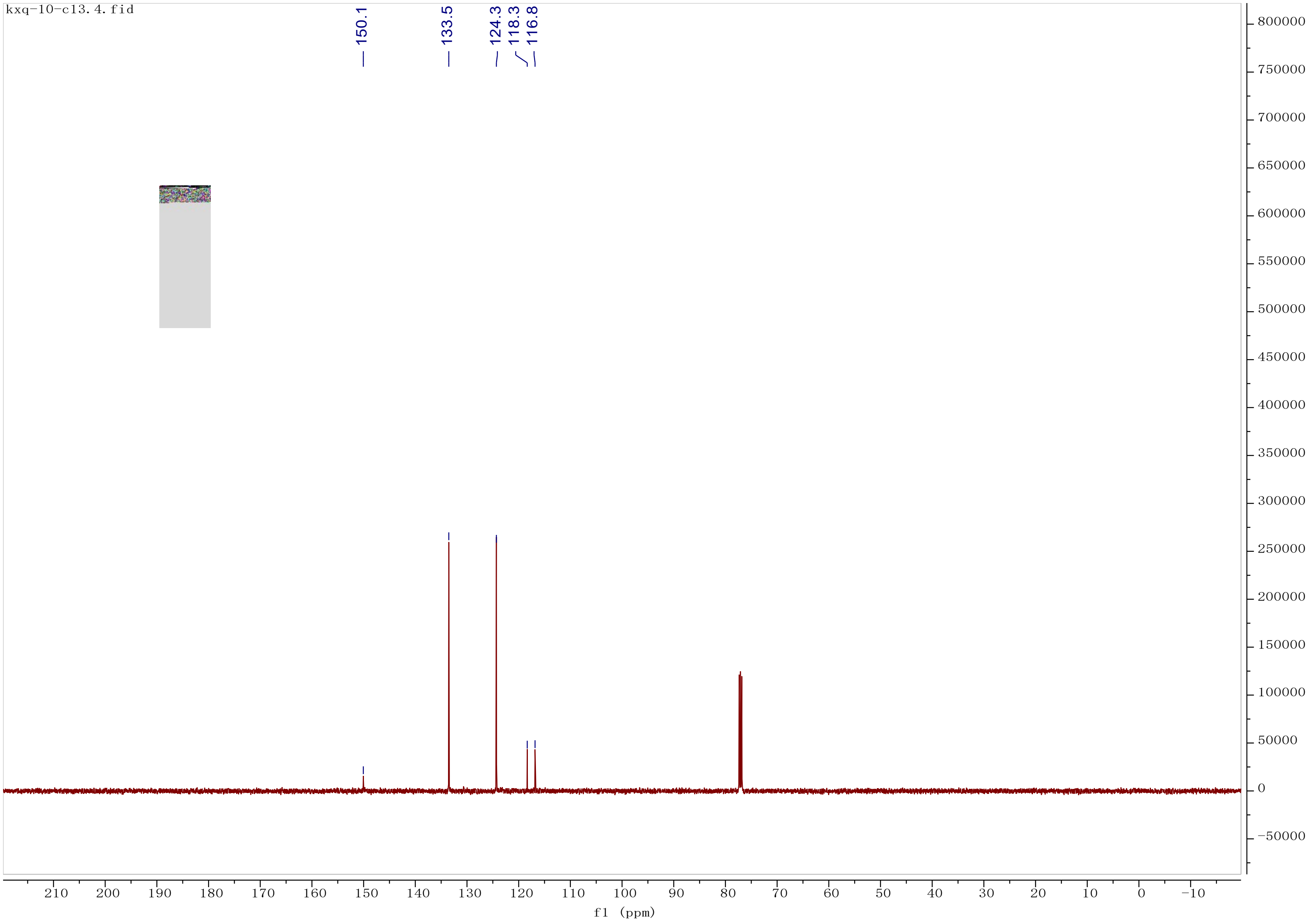
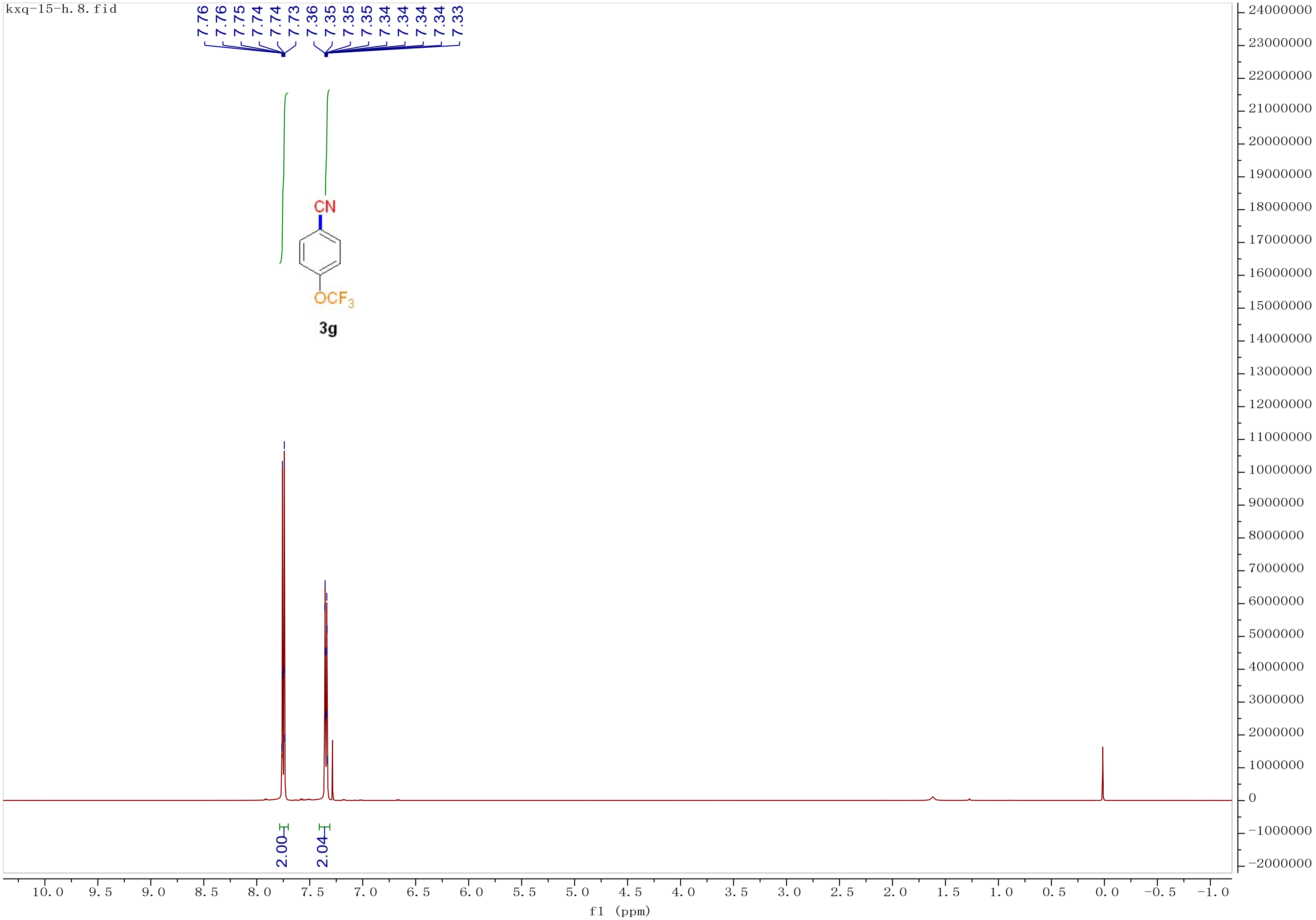
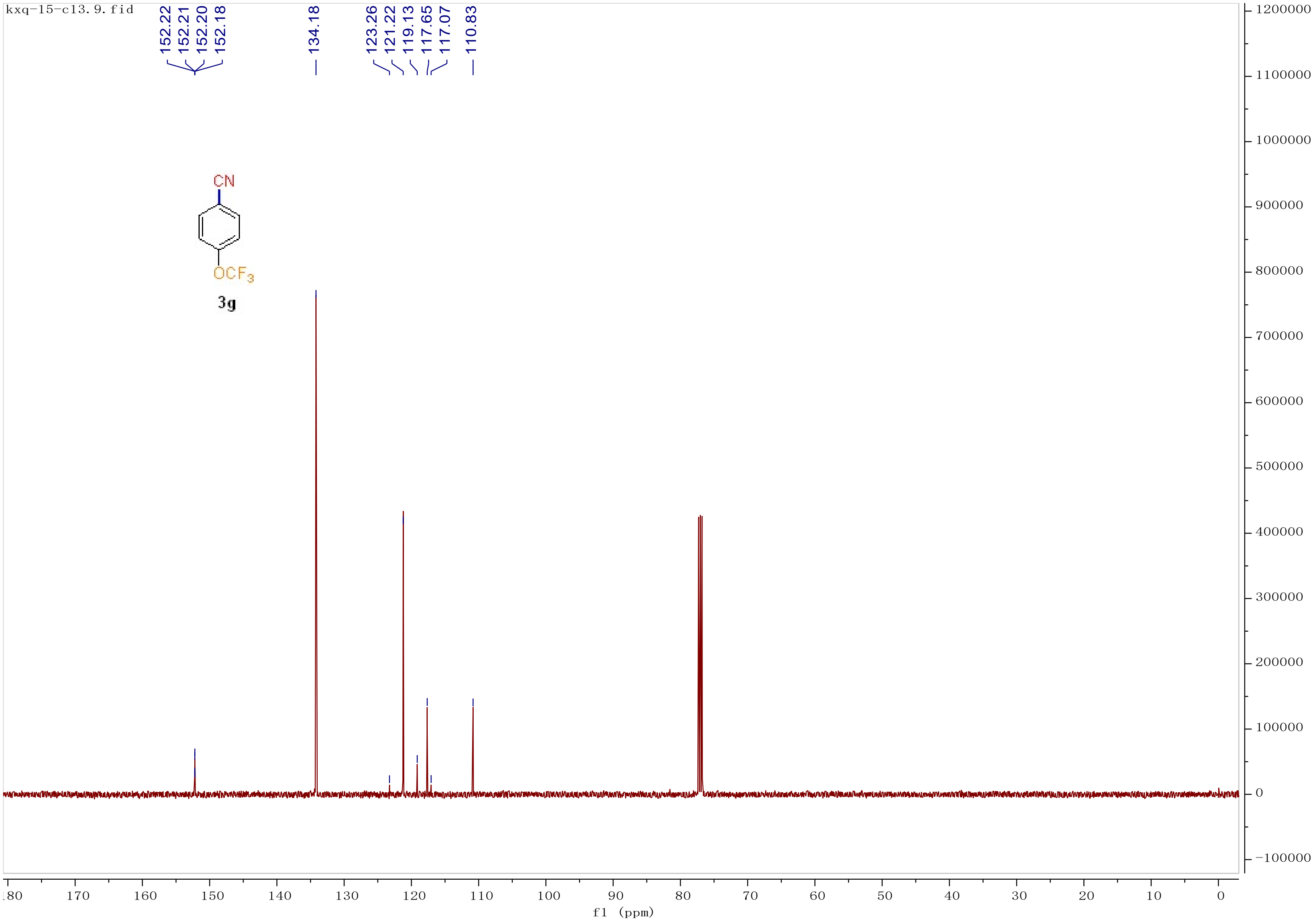
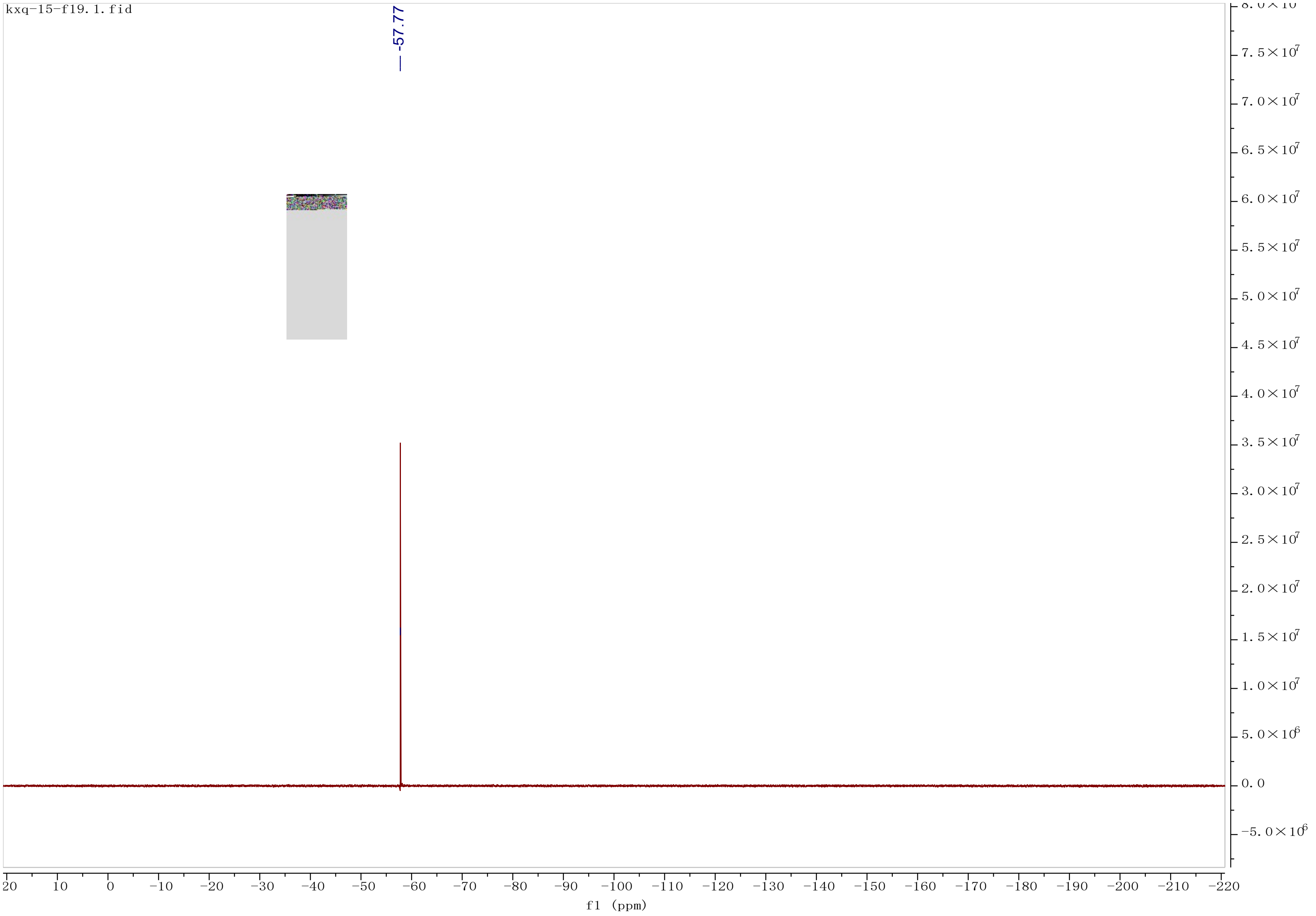
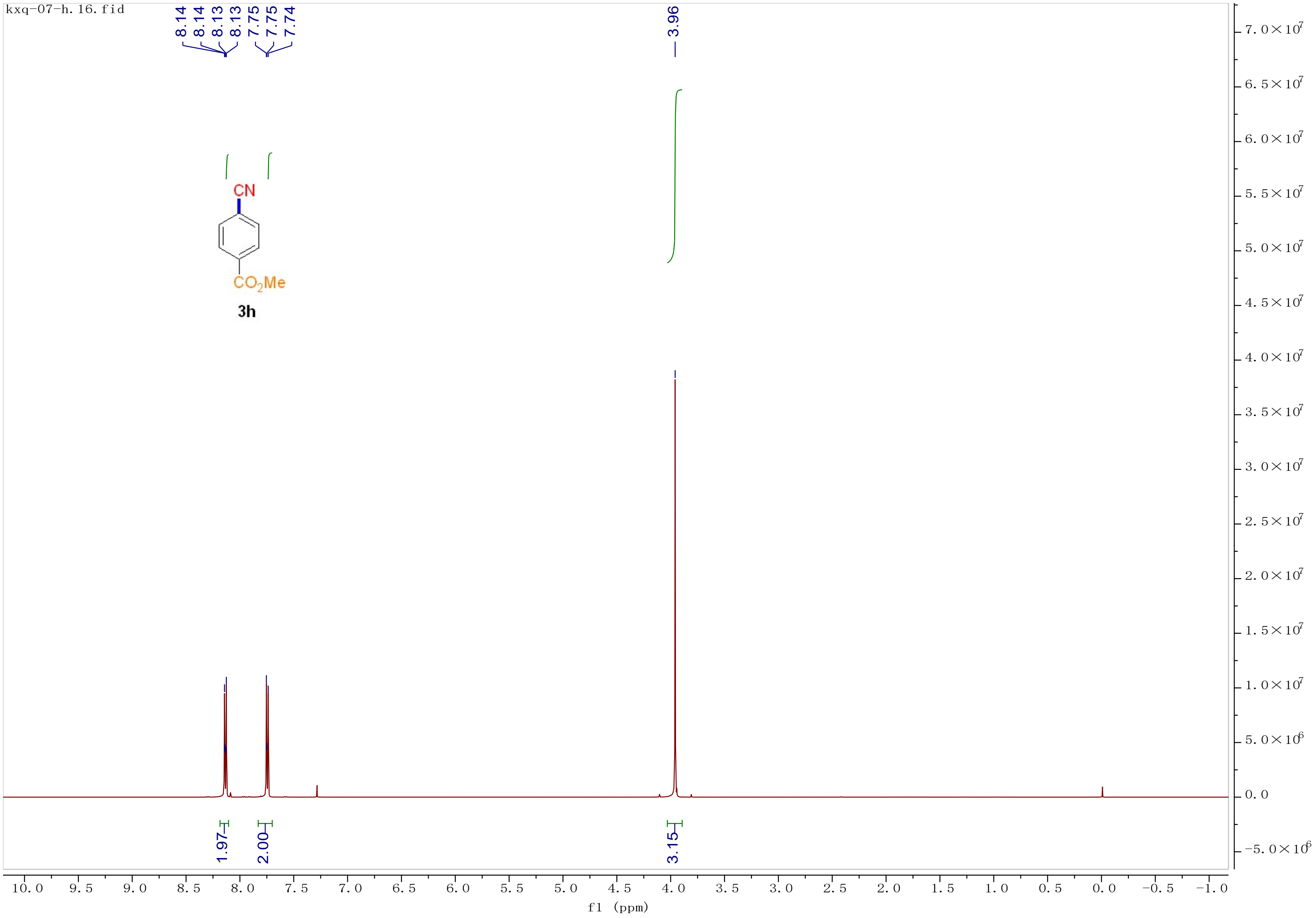
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
f1 (ppm)

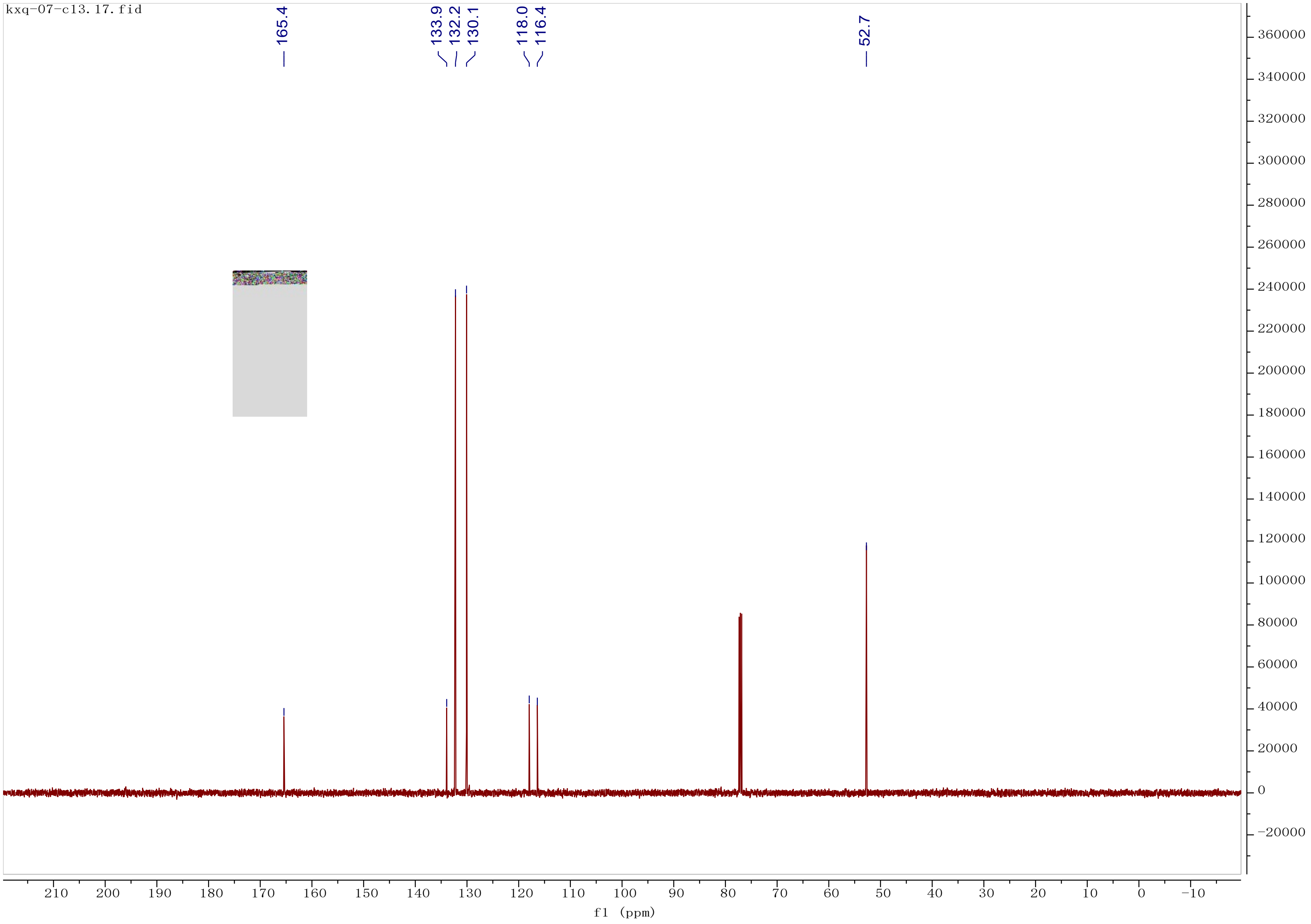

kxq-10-c13.4.fid
150.1
133.5
124.3
118.3
116.8
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

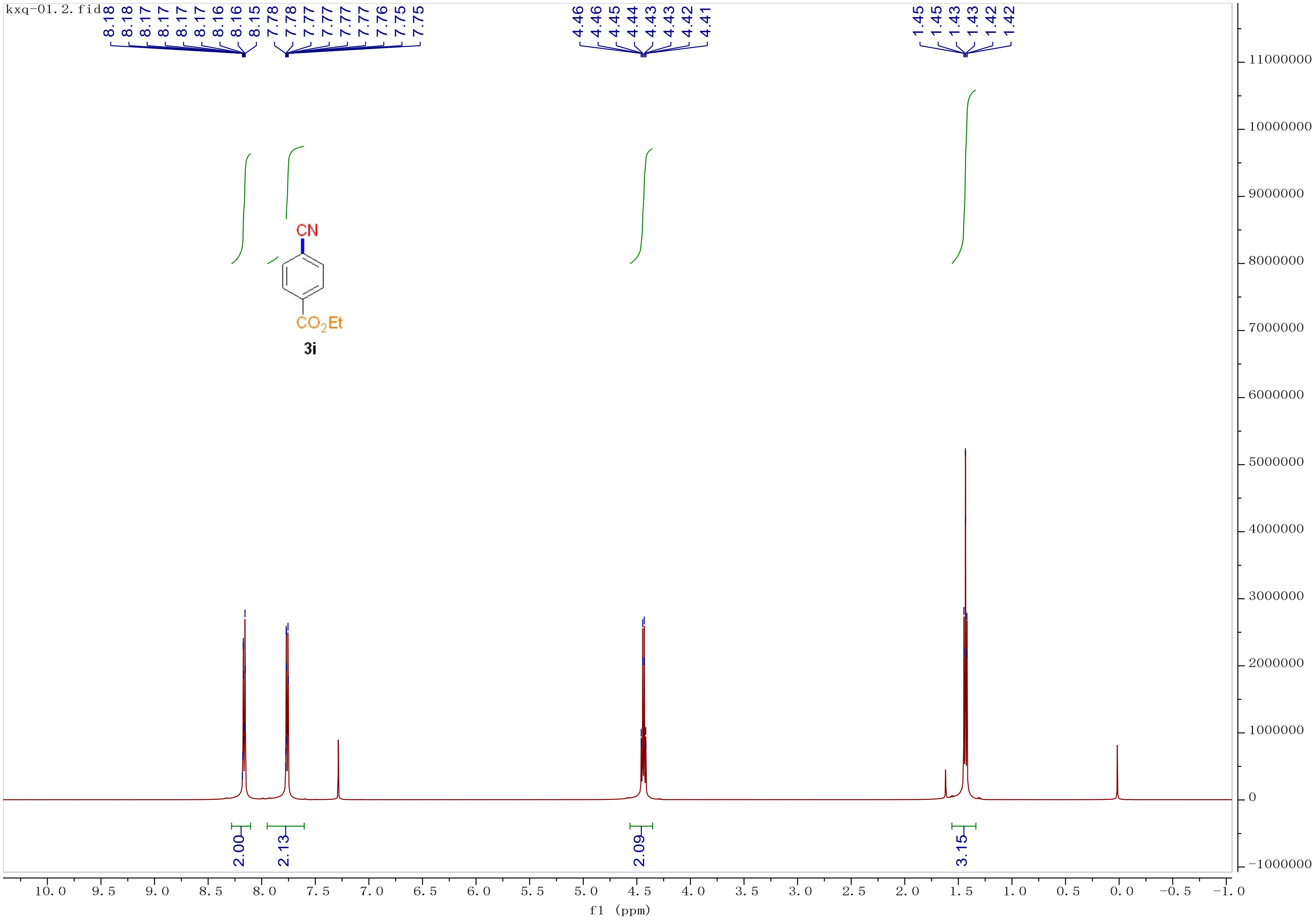

kxq-15-h.8.fid
7.76
7.76
7.75
7.74
7.74
7.73
7.36
7.35
7.35
7.35
7.34
7.34
7.34
7.34
7.33
CN
OCF3
3g
2.00
2.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
24000000
23000000
22000000
21000000
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
-2000000

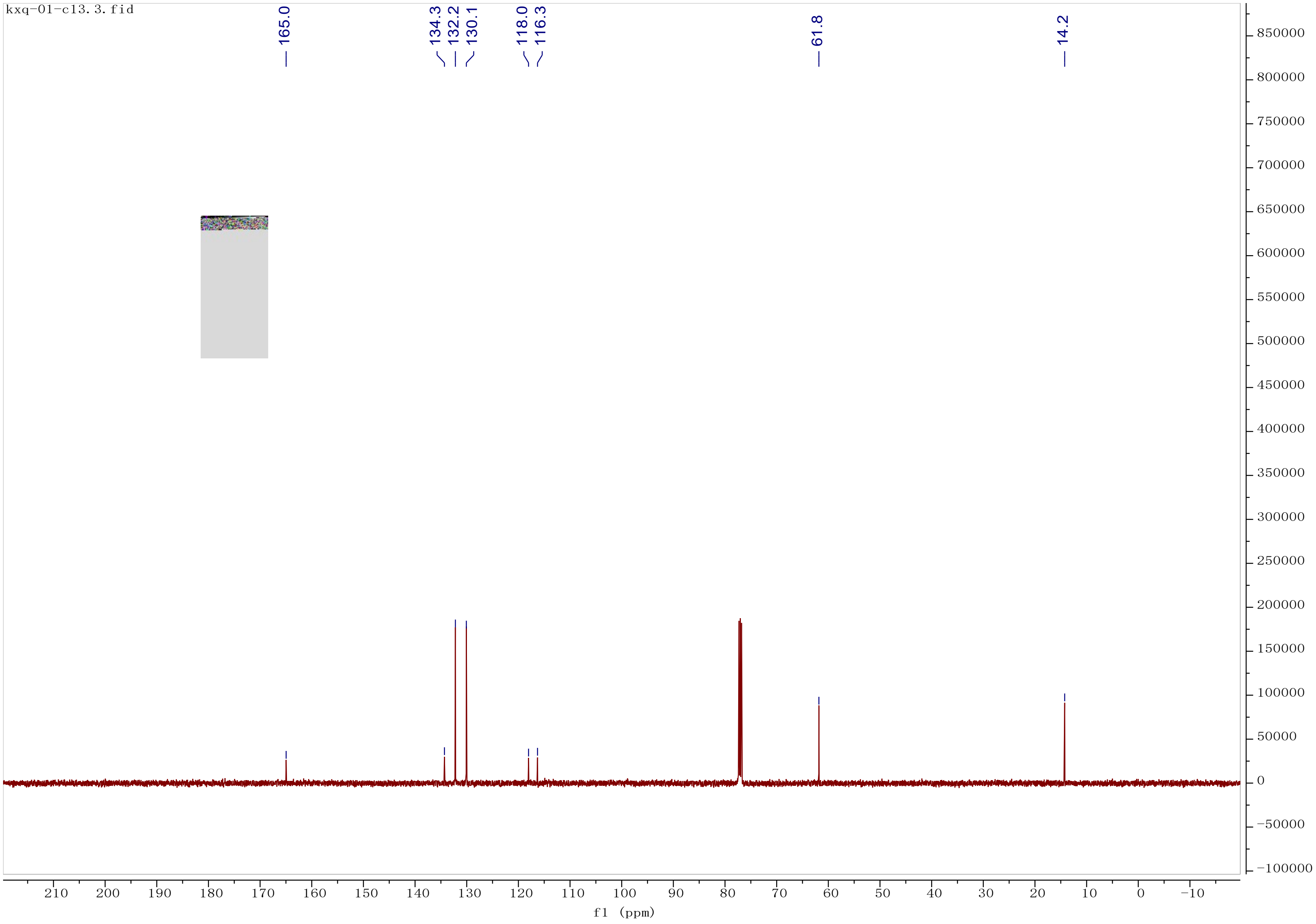

kxq-15-c13.9.fid
152.22
152.21
152.20
152.18
134.18
123.26
121.22
119.13
117.65
117.07
110.83
CN
OCF3
3g
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

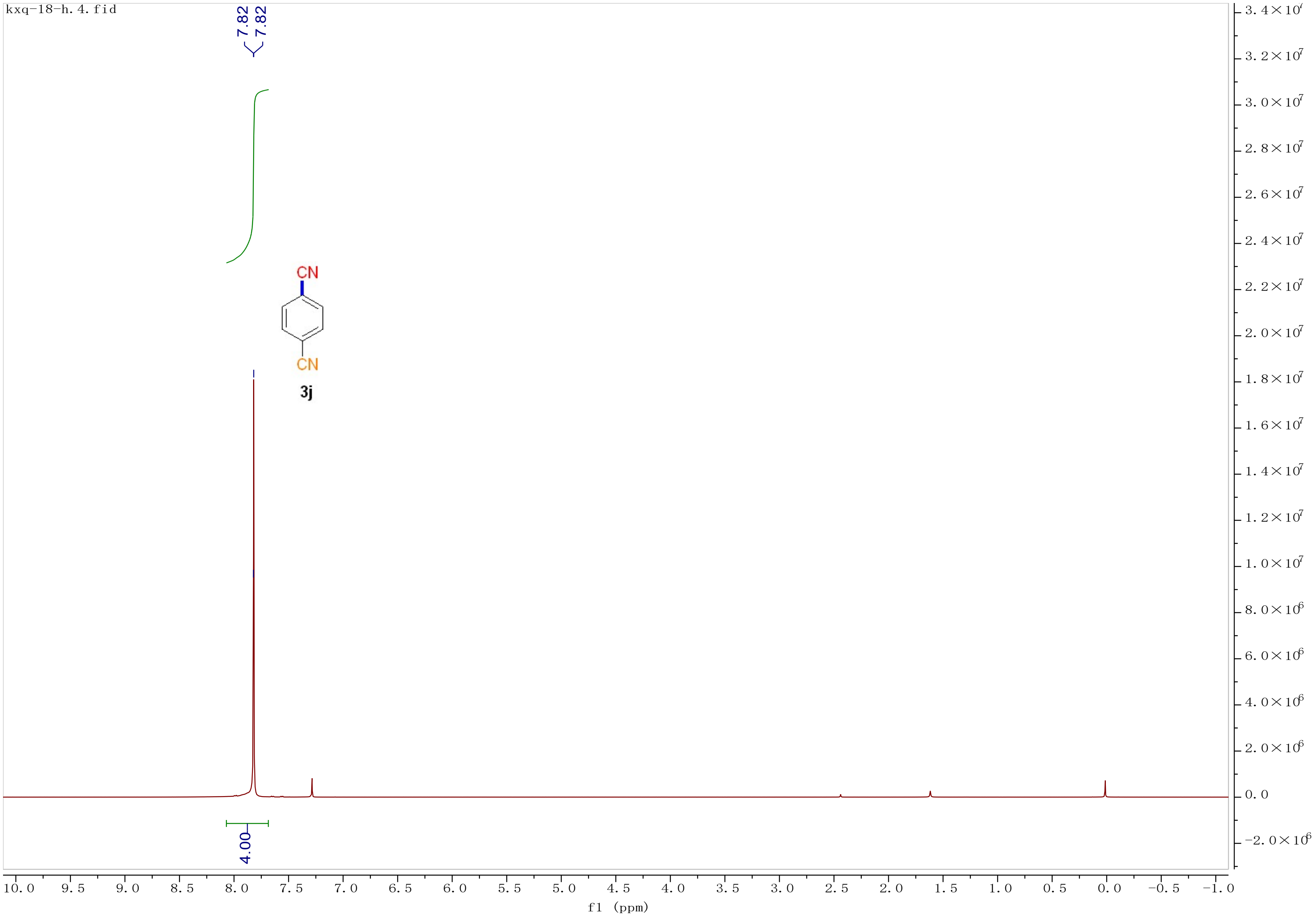

kxq-15-f19.1.fid
-57.77
8.0×10⁷
7.5×10⁷
7.0×10⁷
6.5×10⁷
6.0×10⁷
5.5×10⁷
5.0×10⁷
4.5×10⁷
4.0×10⁷
3.5×10⁷
3.0×10⁷
2.5×10⁷
2.0×10⁷
1.5×10⁷
1.0×10⁷
5.0×10⁶
0.0
−5.0×10⁶
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 −220
f1 (ppm)


kxq-07-h.16.fid
8.14
8.14
8.13
8.13
7.75
7.75
7.74
3.96
CN
CO2Me
3h
1.97
2.00
3.15
7.0×10^7
6.5×10^7
6.0×10^7
5.5×10^7
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
-5.0×10^6
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

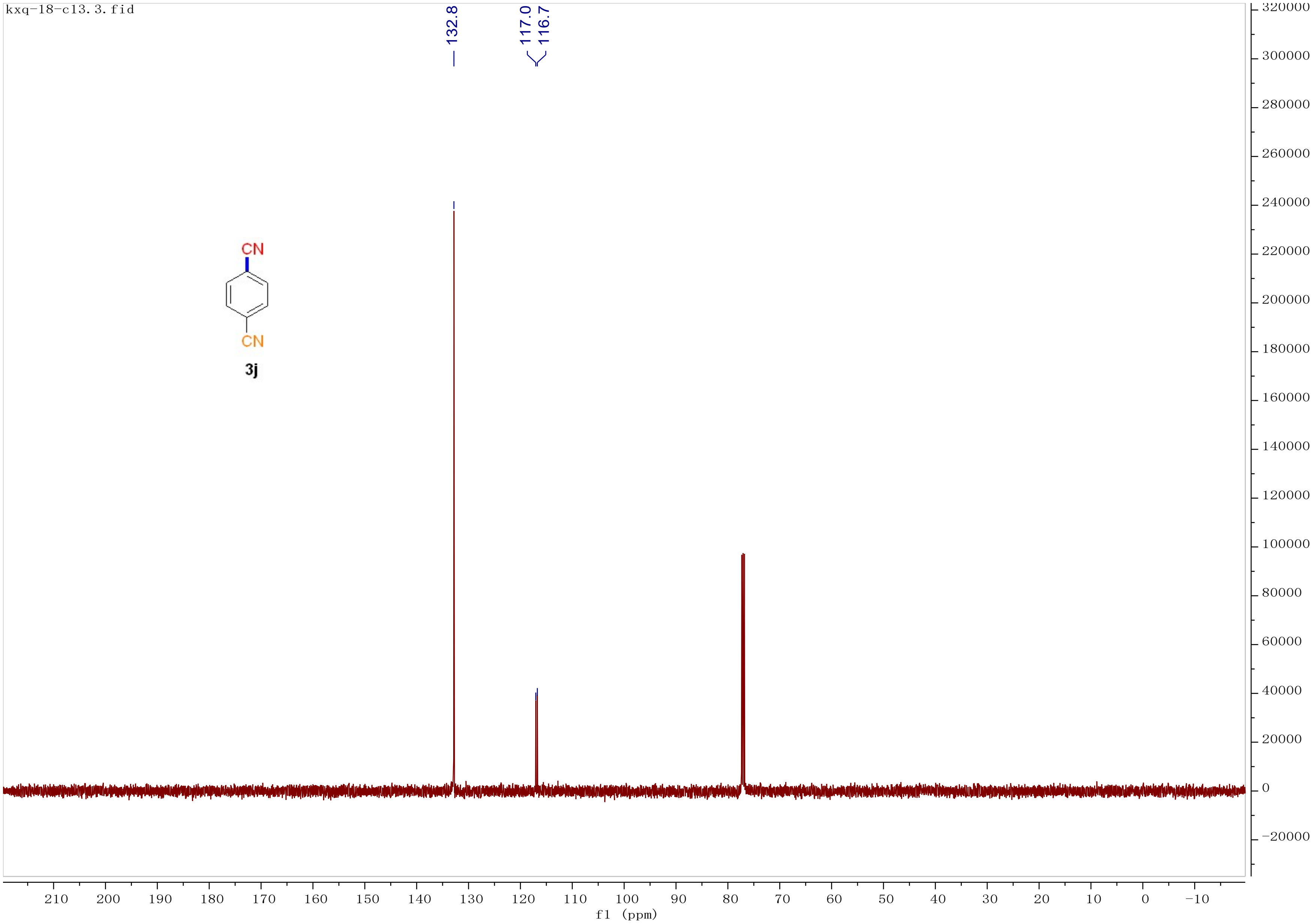

kxq-07-c13.17.fid
165.4
133.9
132.2
130.1
118.0
116.4
52.7
360000
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

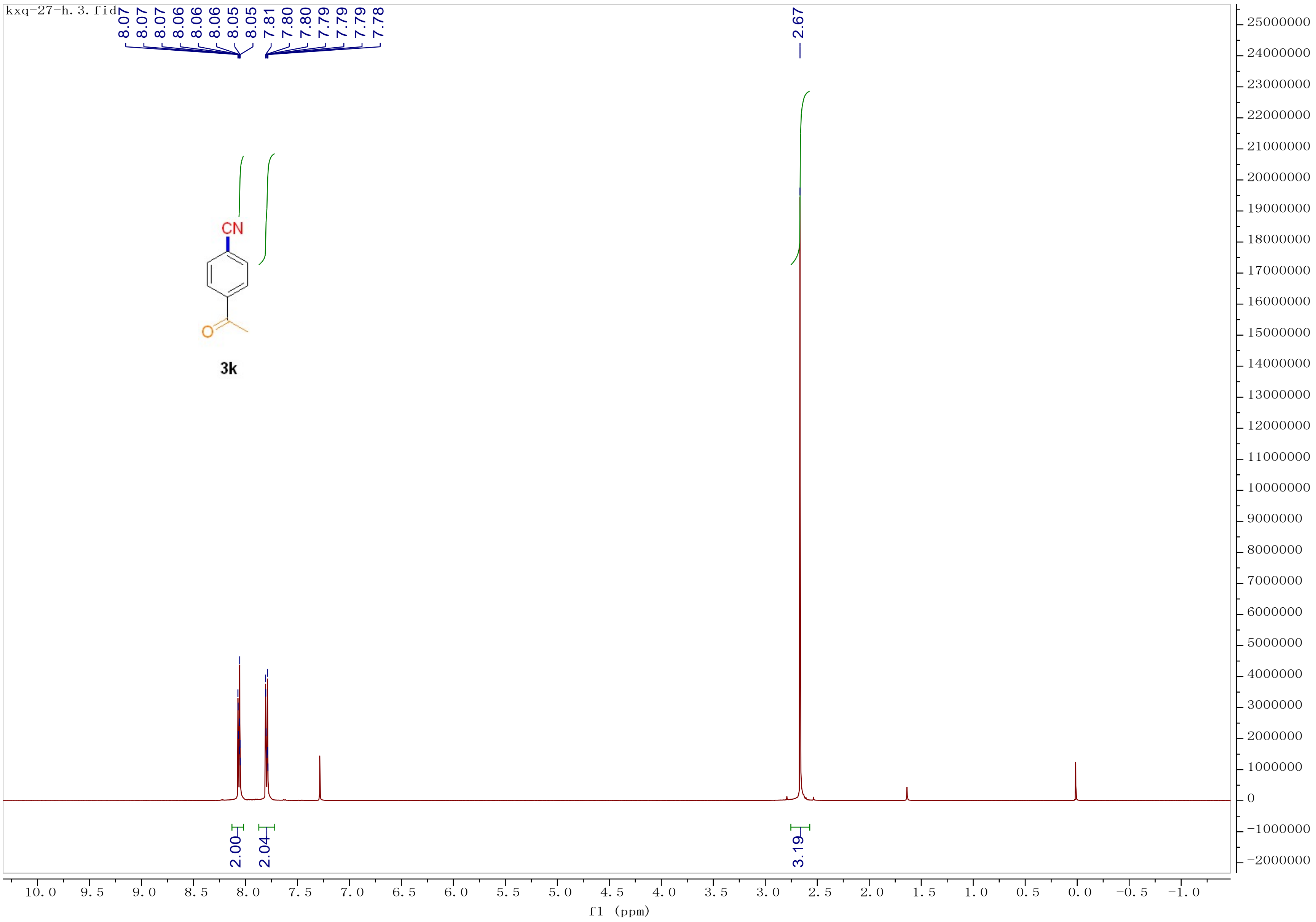

kxq-01.2.fid
8.18
8.18
8.17
8.17
8.17
8.17
8.16
8.16
8.15
7.78
7.78
7.77
7.77
7.77
7.77
7.76
7.75
7.75
4.46
4.46
4.45
4.44
4.43
4.43
4.42
4.41
1.45
1.45
1.43
1.43
1.42
1.42
CN
CO2Et
3i
2.00
2.13
2.09
3.15
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

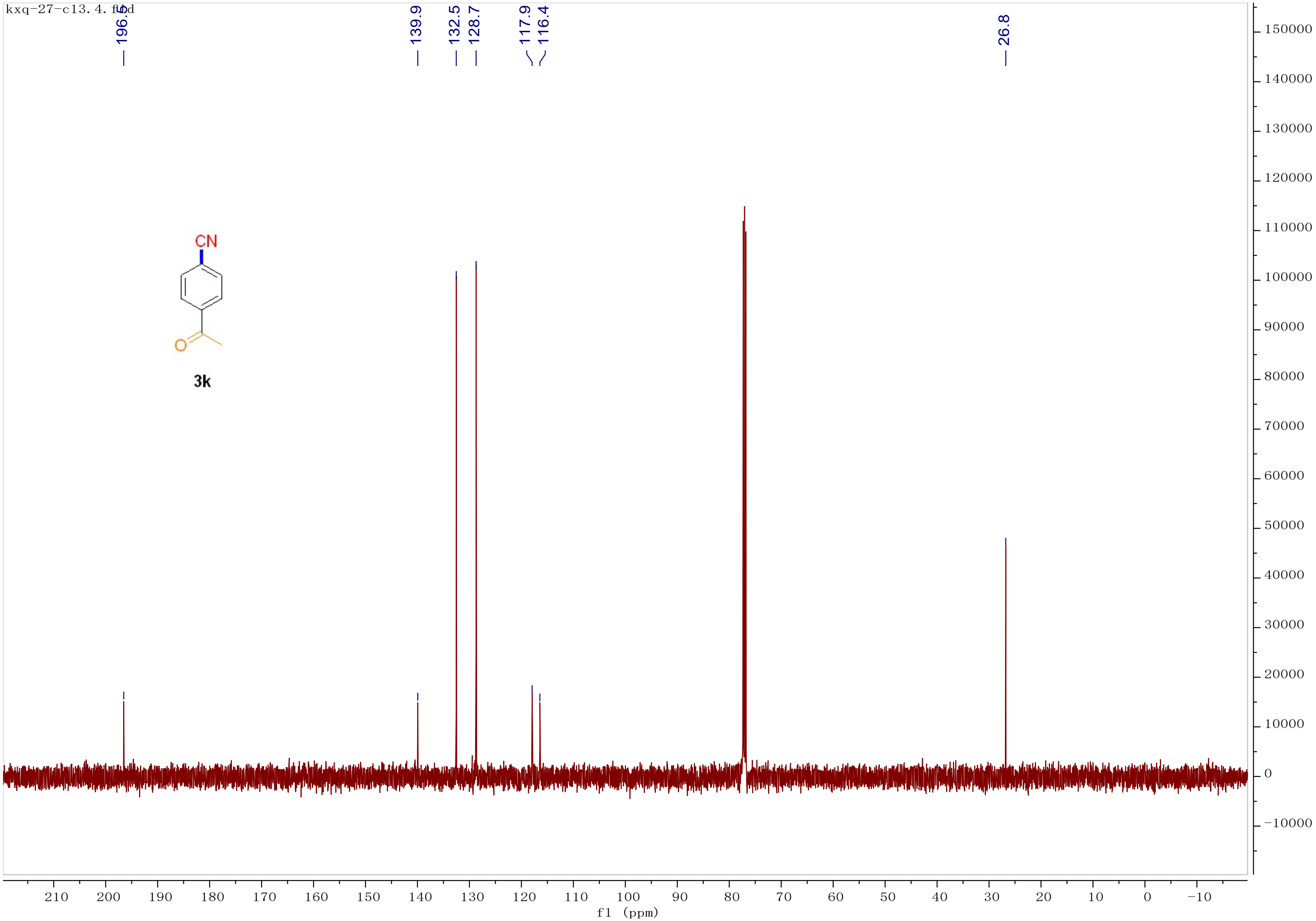

kxq-01-c13.3.fid
165.0
134.3
132.2
130.1
118.0
116.3
61.8
14.2
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
−50000
−100000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


kxq-18-h.4.fid
7.82
7.82
CN
CN
4.00
3.4×10⁷
3.2×10⁷
3.0×10⁷
2.8×10⁷
2.6×10⁷
2.4×10⁷
2.2×10⁷
2.0×10⁷
1.8×10⁷
1.6×10⁷
1.4×10⁷
1.2×10⁷
1.0×10⁷
8.0×10⁶
6.0×10⁶
4.0×10⁶
2.0×10⁶
0.0
−2.0×10⁶
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
f1 (ppm)

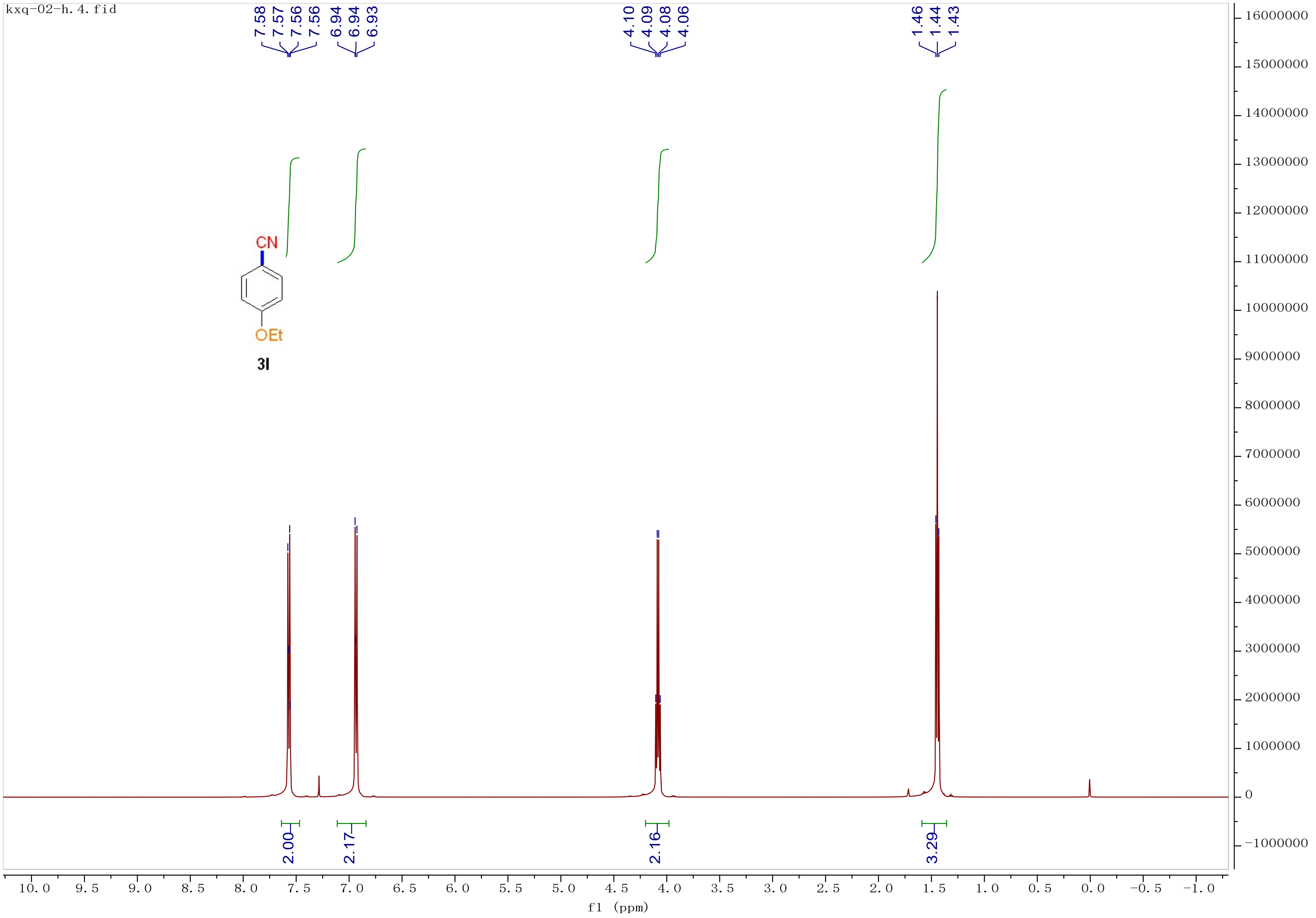
3j

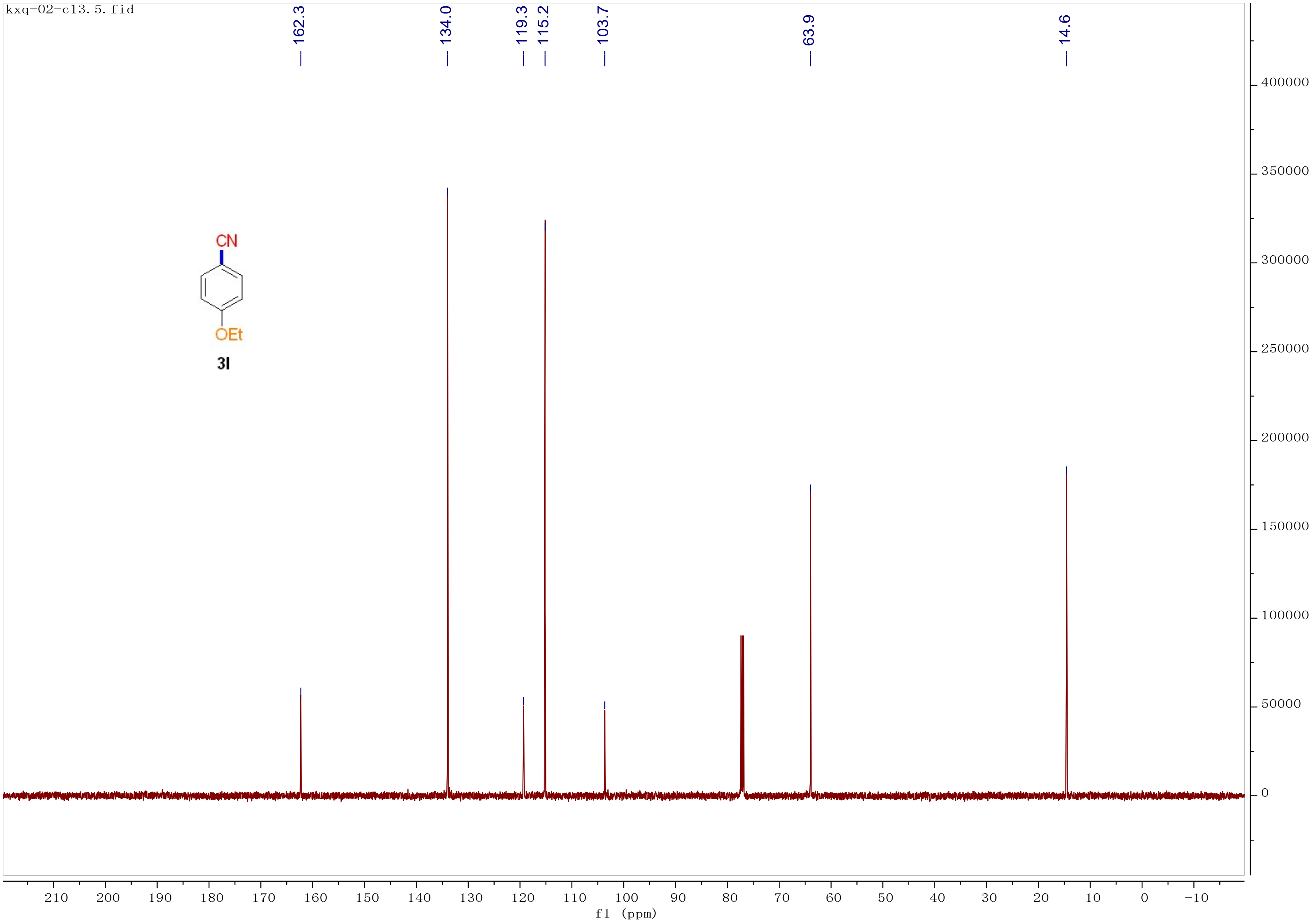

kxq-18-c13.3.fid
132.8
117.0
116.7
CN
CN
3j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000

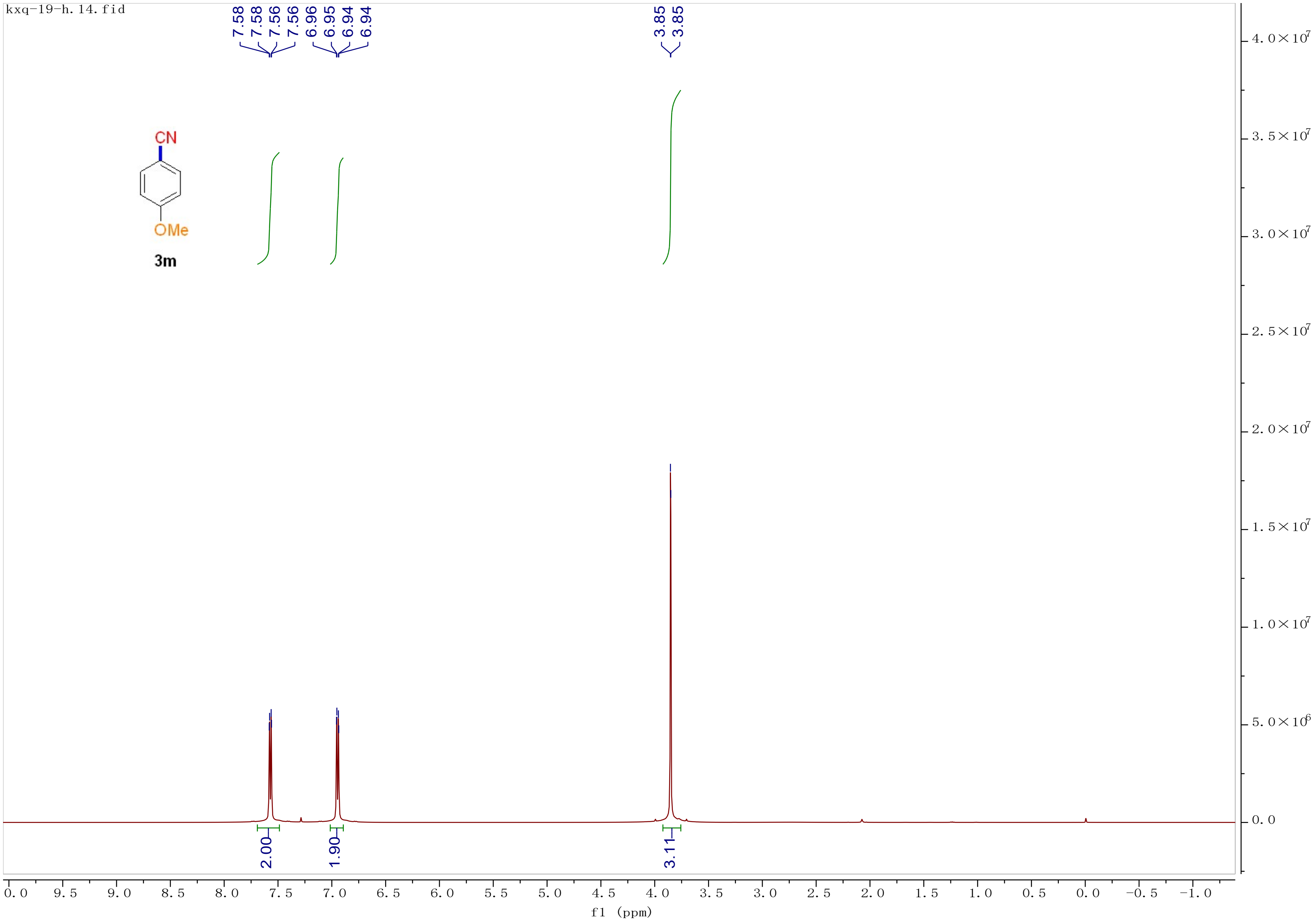

kxq-27-h.3.fid
8.07
8.07
8.07
8.06
8.06
8.06
8.05
8.05
7.81
7.80
7.80
7.79
7.79
7.79
7.78
2.67
CN
O
3k
2.00
2.04
3.19
25000000
24000000
23000000
22000000
21000000
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
-2000000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

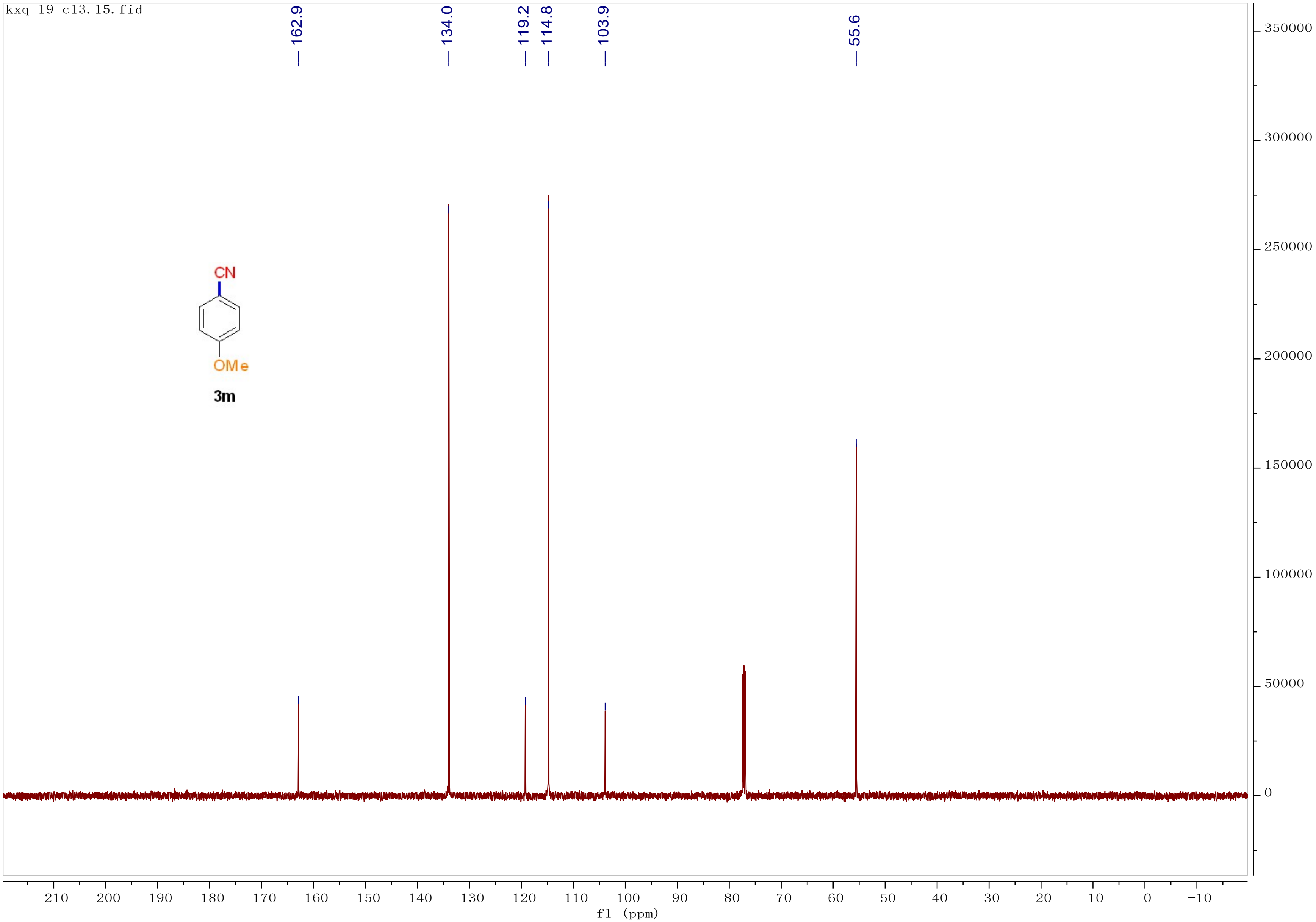

kxq-27-c13.4.fid
196.5
139.9
132.5
128.7
117.9
116.4
26.8
CN
O
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

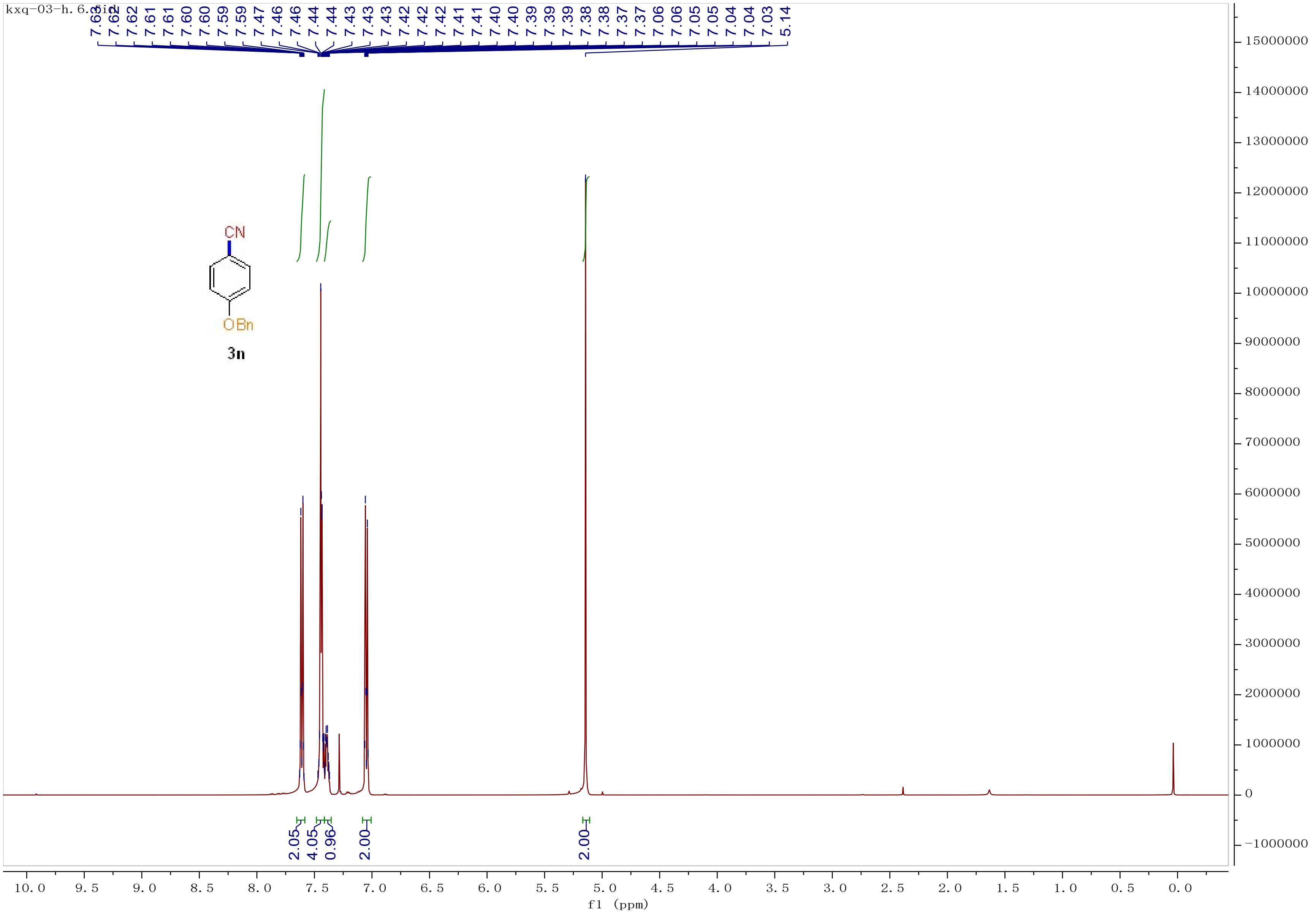
3k


kxq-02-h.4.fid
7.58
7.57
7.56
7.56
6.94
6.94
6.93
4.10
4.09
4.08
4.06
1.46
1.44
1.43
CN
OEt
3l
2.00
2.17
2.16
3.29
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

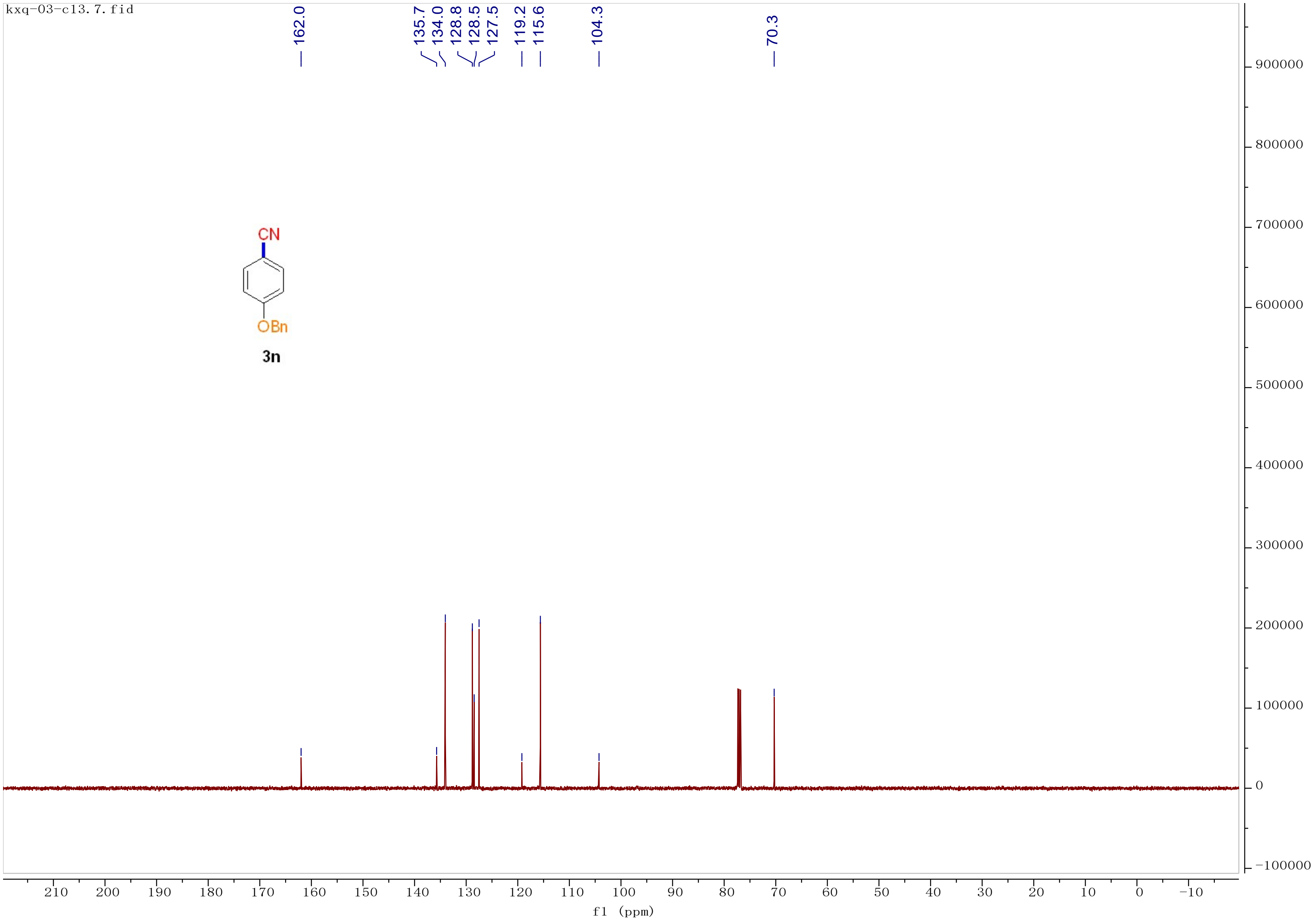

kxq-02-c13.5.fid
162.3
134.0
119.3
115.2
103.7
63.9
14.6
CN
OEt
3l
400000
350000
300000
250000
200000
150000
100000
50000
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

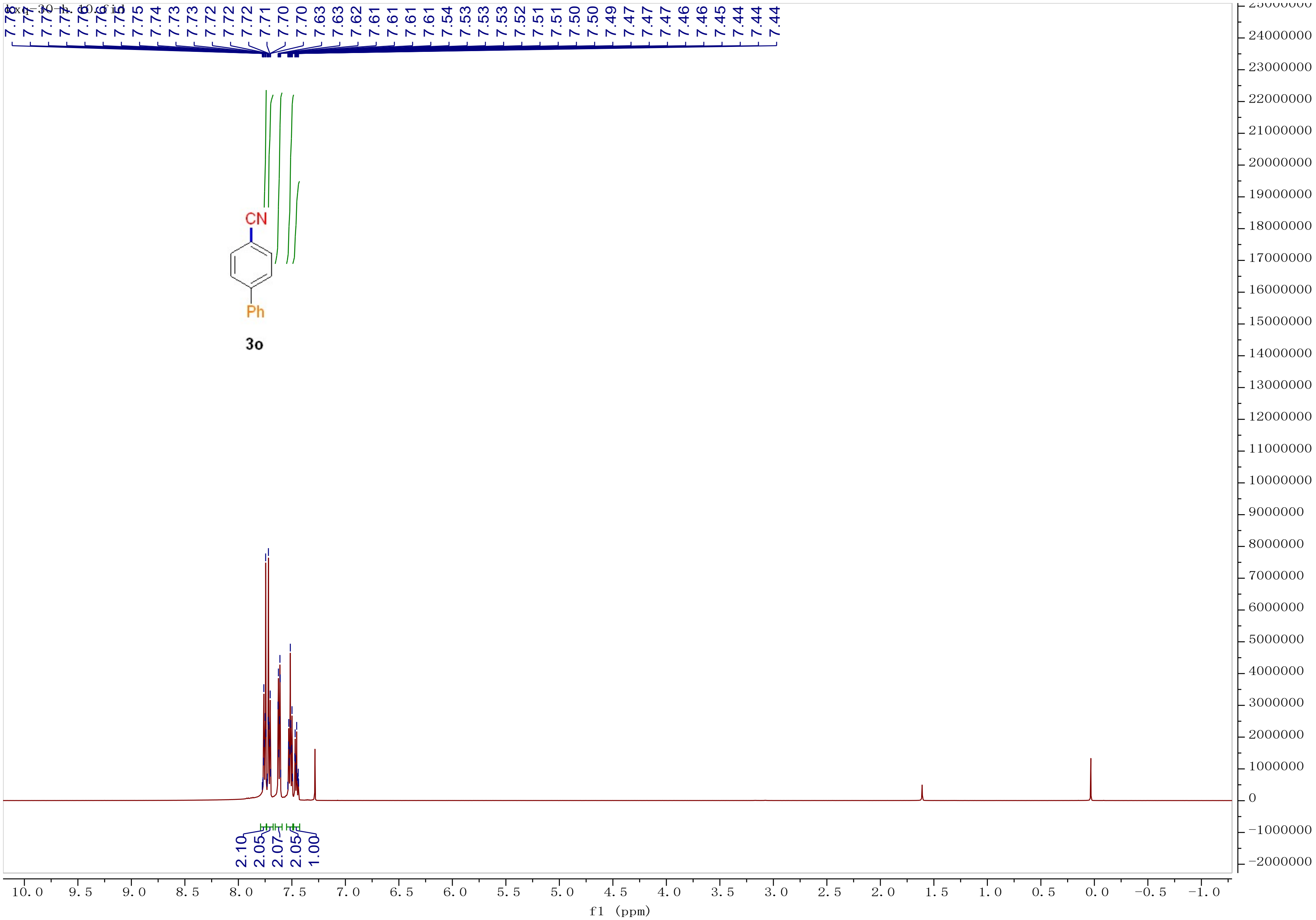

kxq-19-h.14.fid
7.58
7.58
7.56
7.56
6.96
6.95
6.94
6.94
3.85
3.85
CN
OMe
3m
2.00
1.90
3.11
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

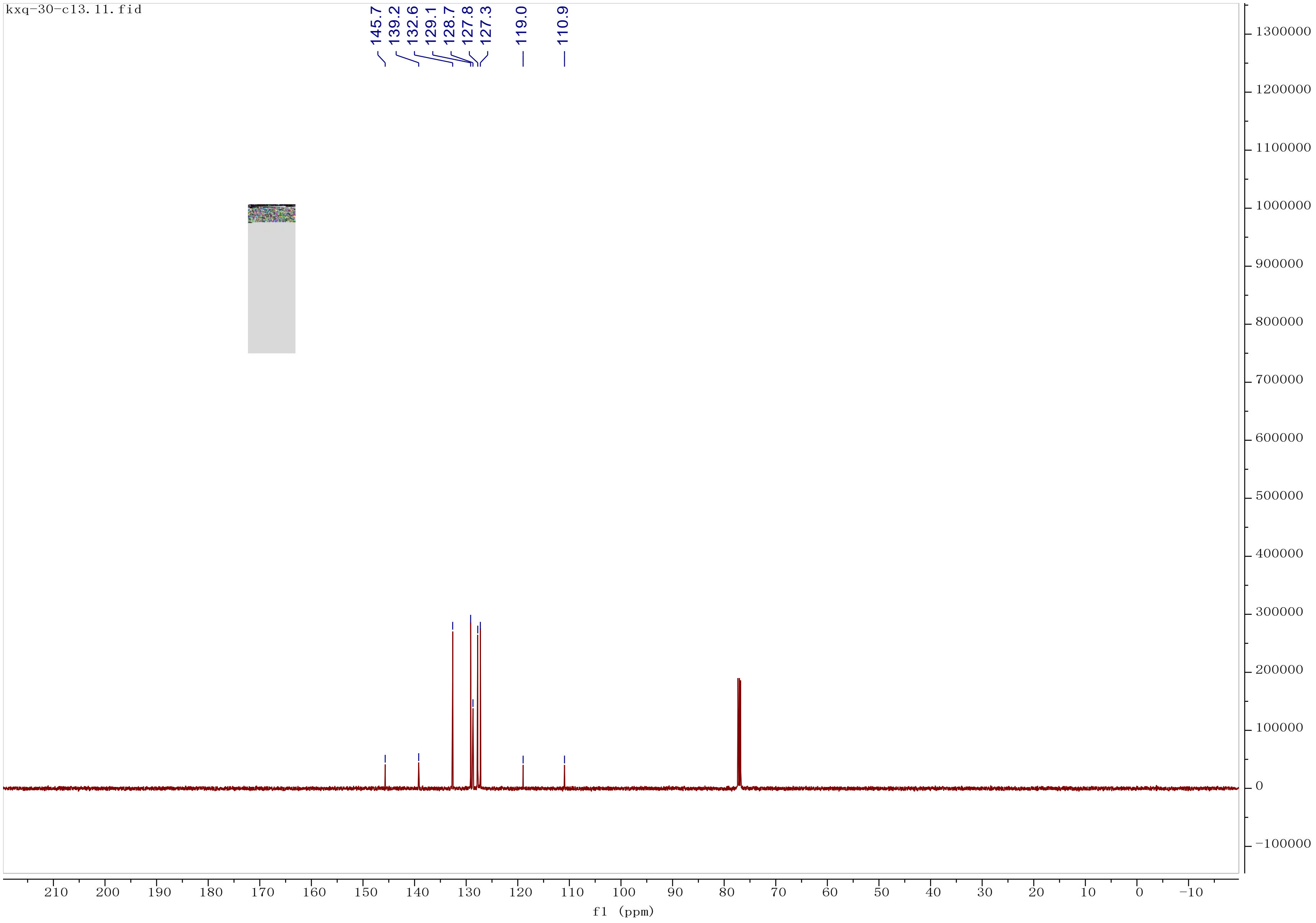

kxq-19-c13.15.fid
162.9
134.0
119.2
114.8
103.9
55.6
CN
OMe
3m
350000
300000
250000
200000
150000
100000
50000
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

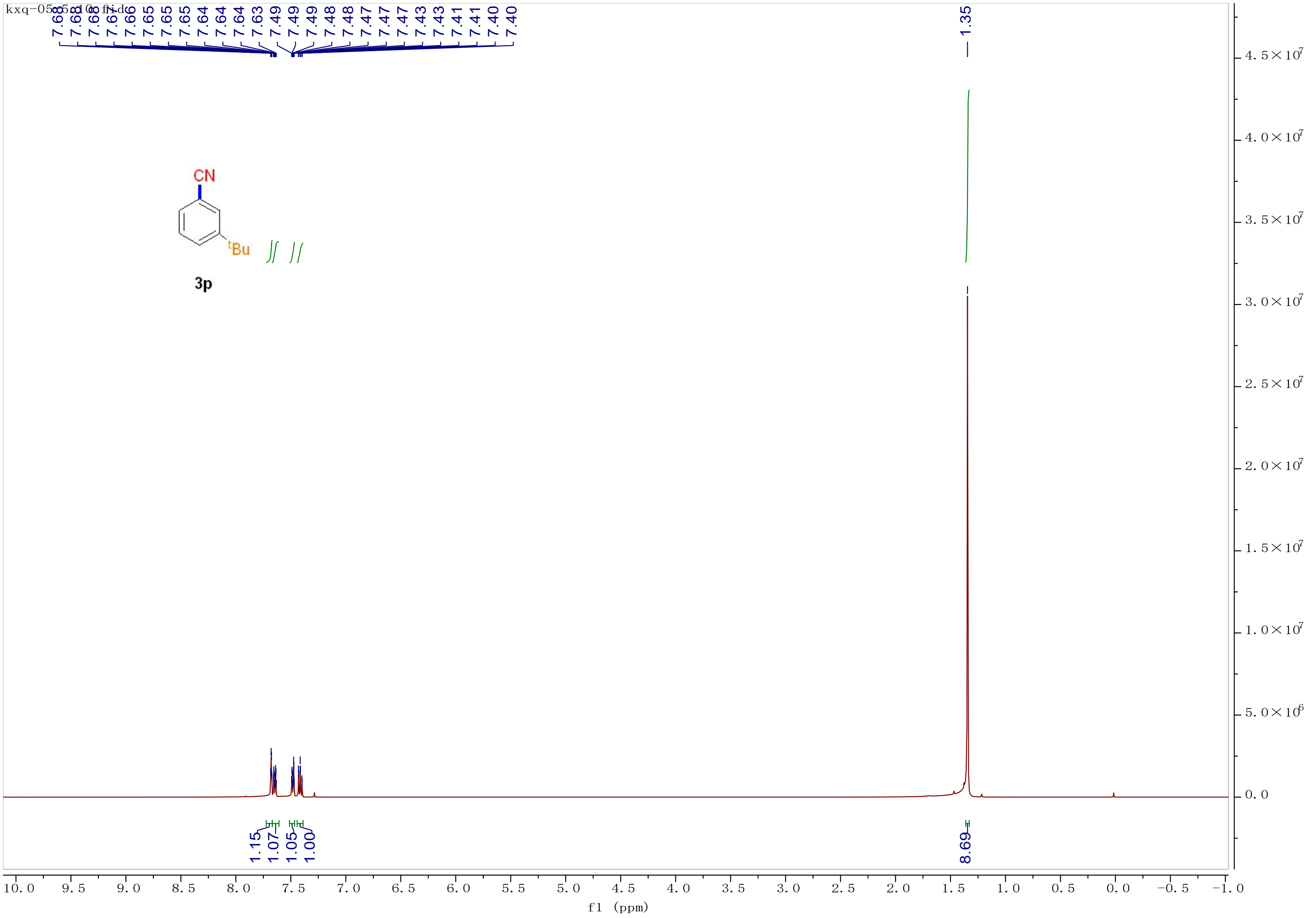

kxq-03-h.6.fid
7.63
7.62
7.62
7.61
7.61
7.60
7.60
7.59
7.59
7.47
7.46
7.46
7.44
7.44
7.44
7.43
7.43
7.43
7.42
7.42
7.42
7.41
7.41
7.40
7.40
7.39
7.39
7.39
7.38
7.38
7.37
7.37
7.06
7.06
7.05
7.05
7.04
7.04
7.03
5.14
CN
OBn
2.05
4.05
0.96
2.00
2.00
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
−1000000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

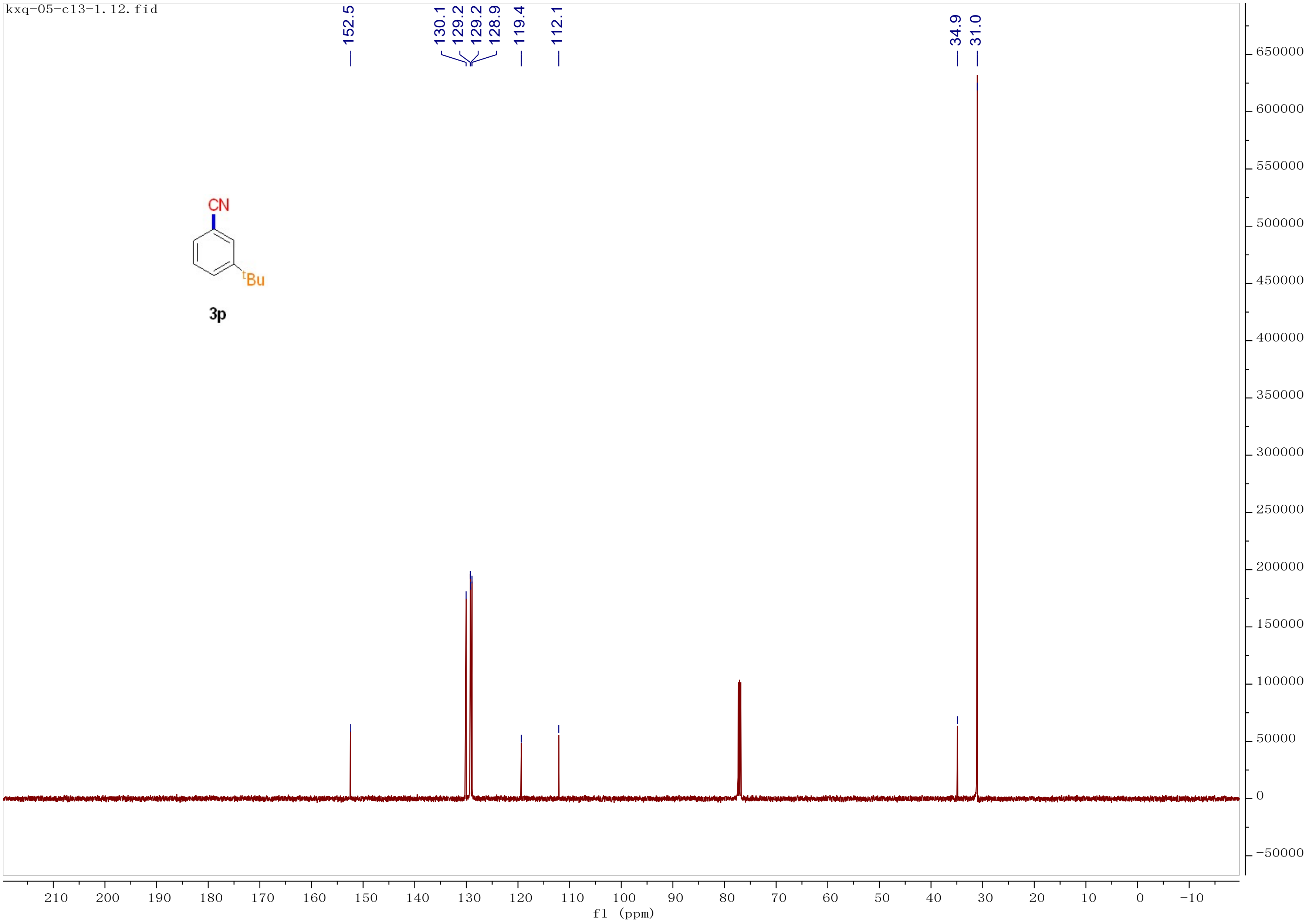
3n

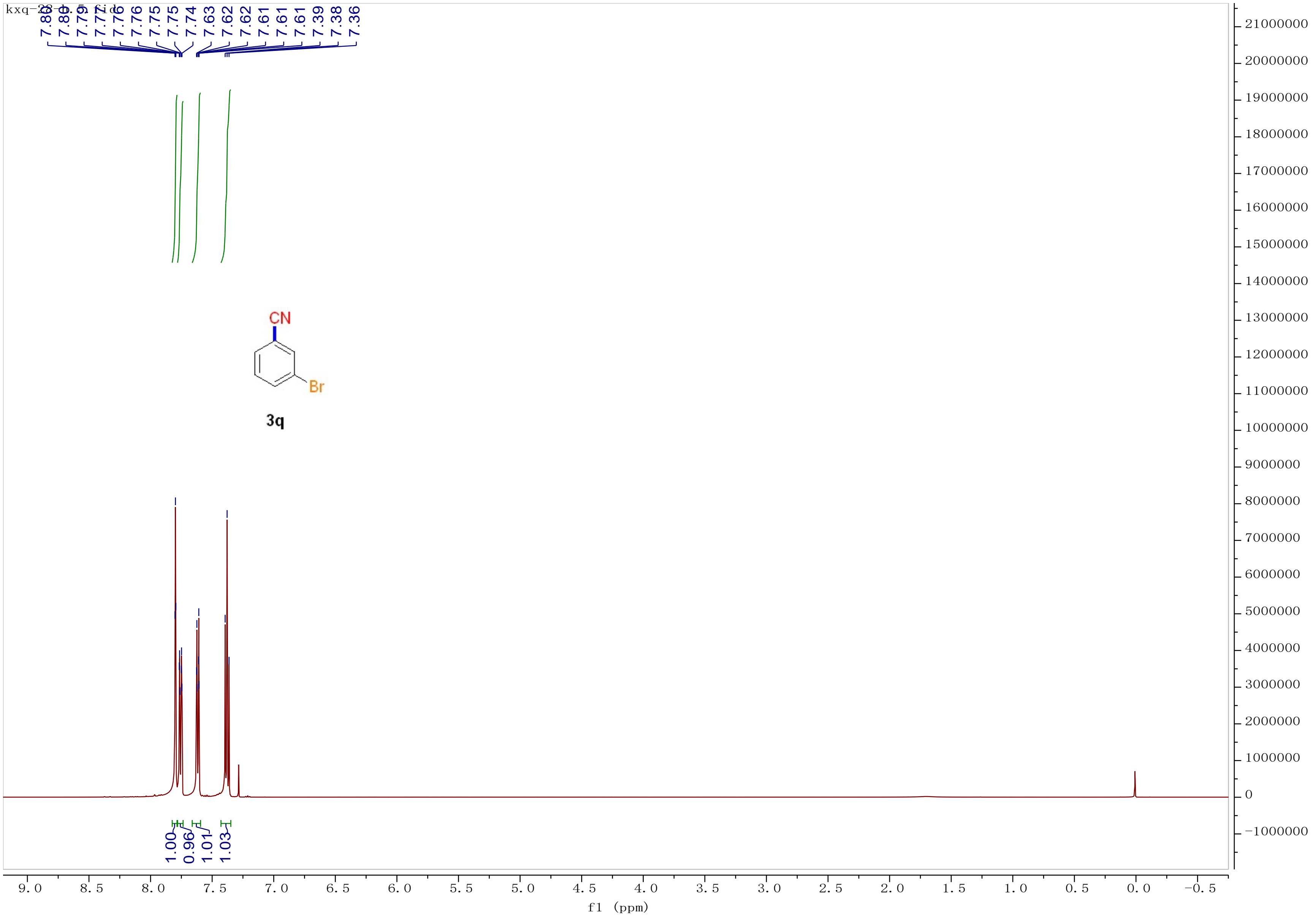

kxq-03-c13.7.fid
162.0
135.7
134.0
128.8
128.5
127.5
119.2
115.6
104.3
70.3
CN
OBn
3n
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


dxq-30-h.10.fid
7.75
7.74
7.73
7.73
7.72
7.72
7.72
7.71
7.70
7.70
7.63
7.63
7.62
7.61
7.61
7.61
7.61
7.54
7.53
7.53
7.53
7.52
7.51
7.51
7.50
7.50
7.49
7.47
7.47
7.47
7.46
7.46
7.45
7.44
7.44
7.44
CN
Ph
3o
2.10
2.05
2.07
2.05
1.00
25000000
24000000
23000000
22000000
21000000
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
-2000000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

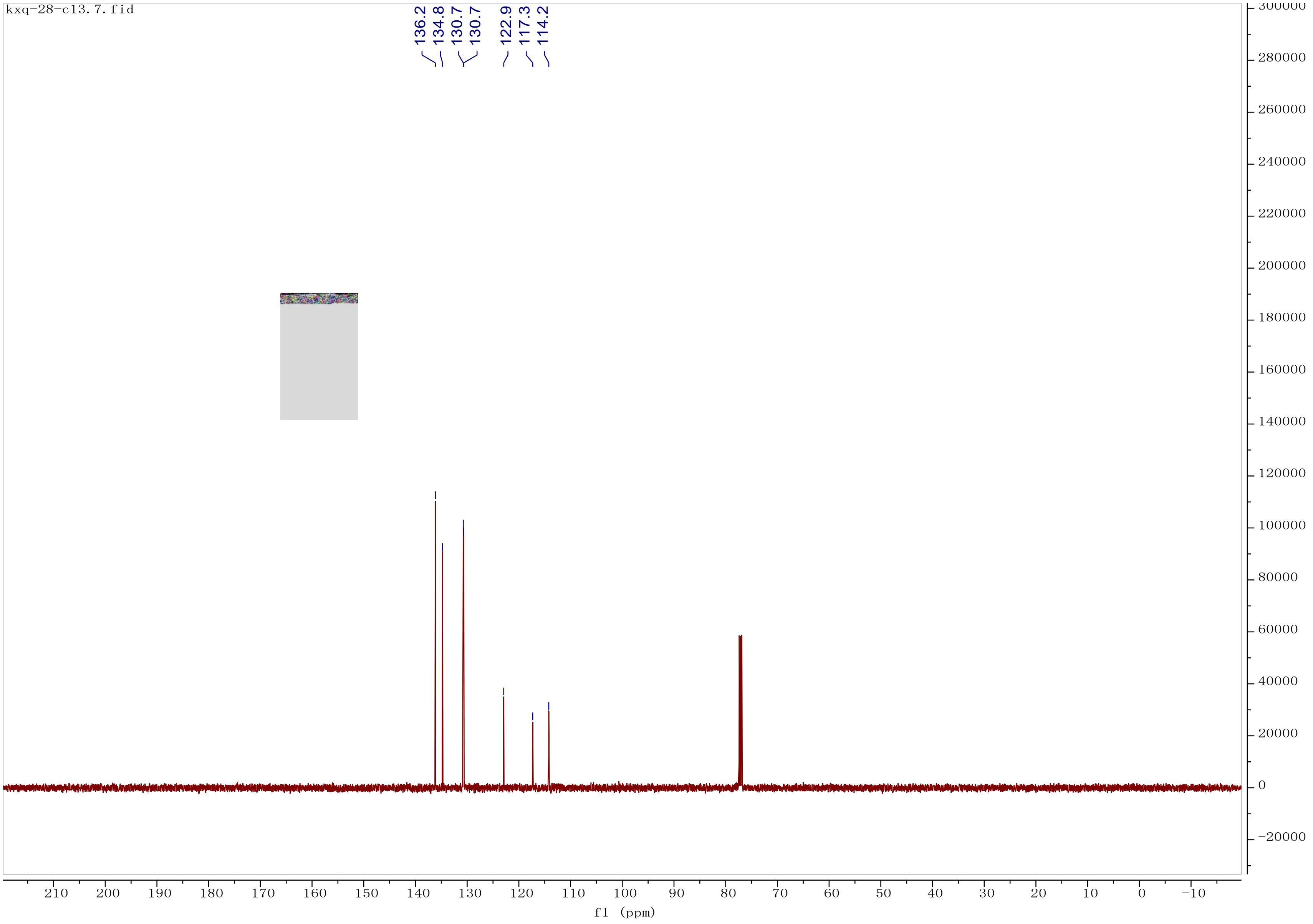

kxq-30-c13.11.fid
145.7
139.2
132.6
129.1
128.7
127.8
127.3
119.0
110.9
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

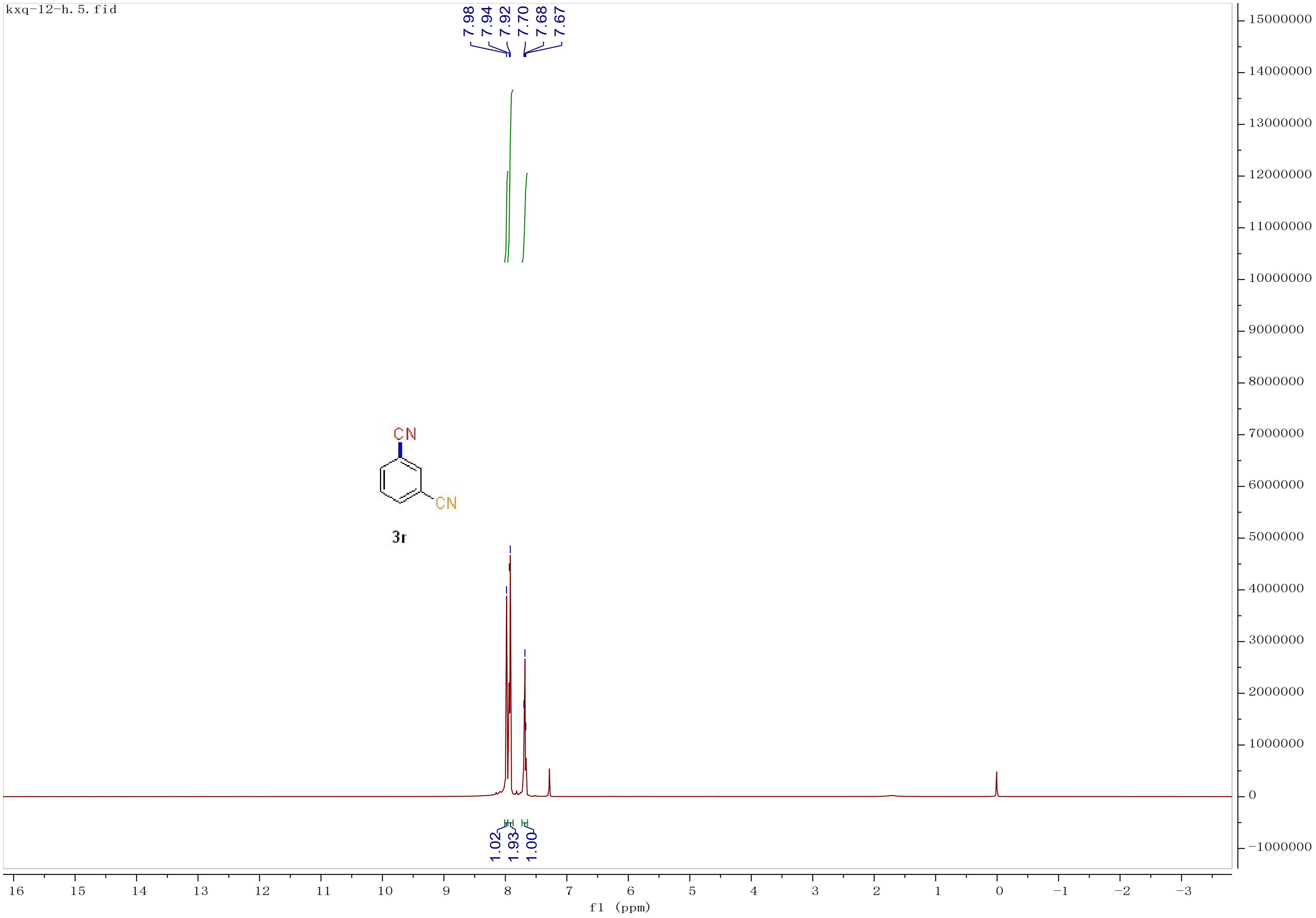

kxq-05-5-10.fid
7.68
7.68
7.68
7.67
7.66
7.65
7.65
7.65
7.64
7.64
7.64
7.63
7.49
7.49
7.49
7.48
7.48
7.47
7.47
7.47
7.43
7.43
7.41
7.41
7.40
7.40
1.35
CN
tBu
3p
1.15
1.07
1.05
1.00
8.69
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


kxq-05-c13-1.12.fid
152.5
130.1
129.2
129.2
128.9
119.4
112.1
34.9
31.0
CN
tBu
3p
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
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)

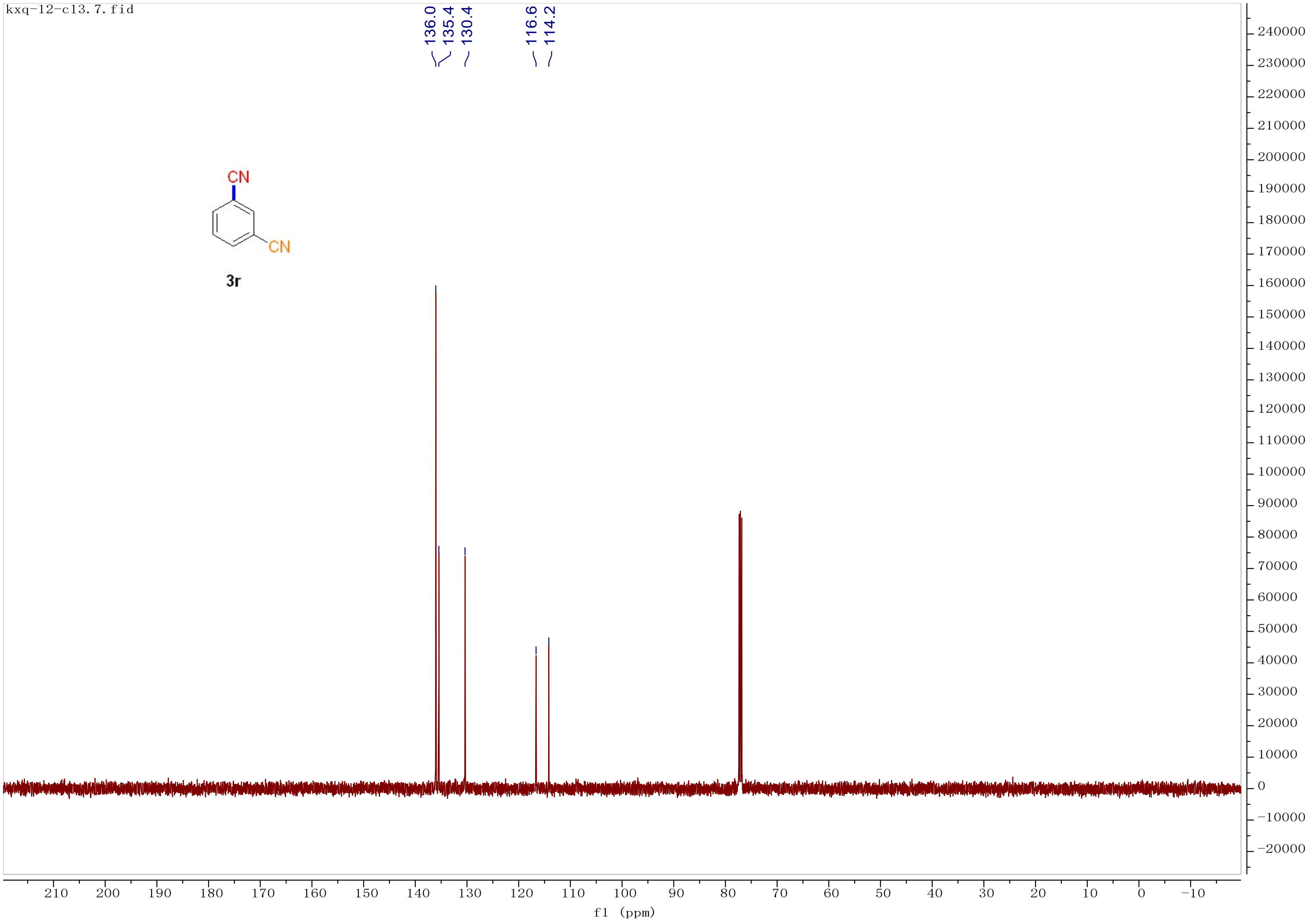

kxq-23-1.5.fid
7.80
7.80
7.79
7.77
7.76
7.76
7.75
7.75
7.74
7.63
7.62
7.62
7.61
7.61
7.61
7.39
7.38
7.36
CN
Br
1.00
0.96
1.01
1.03
21000000
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
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)

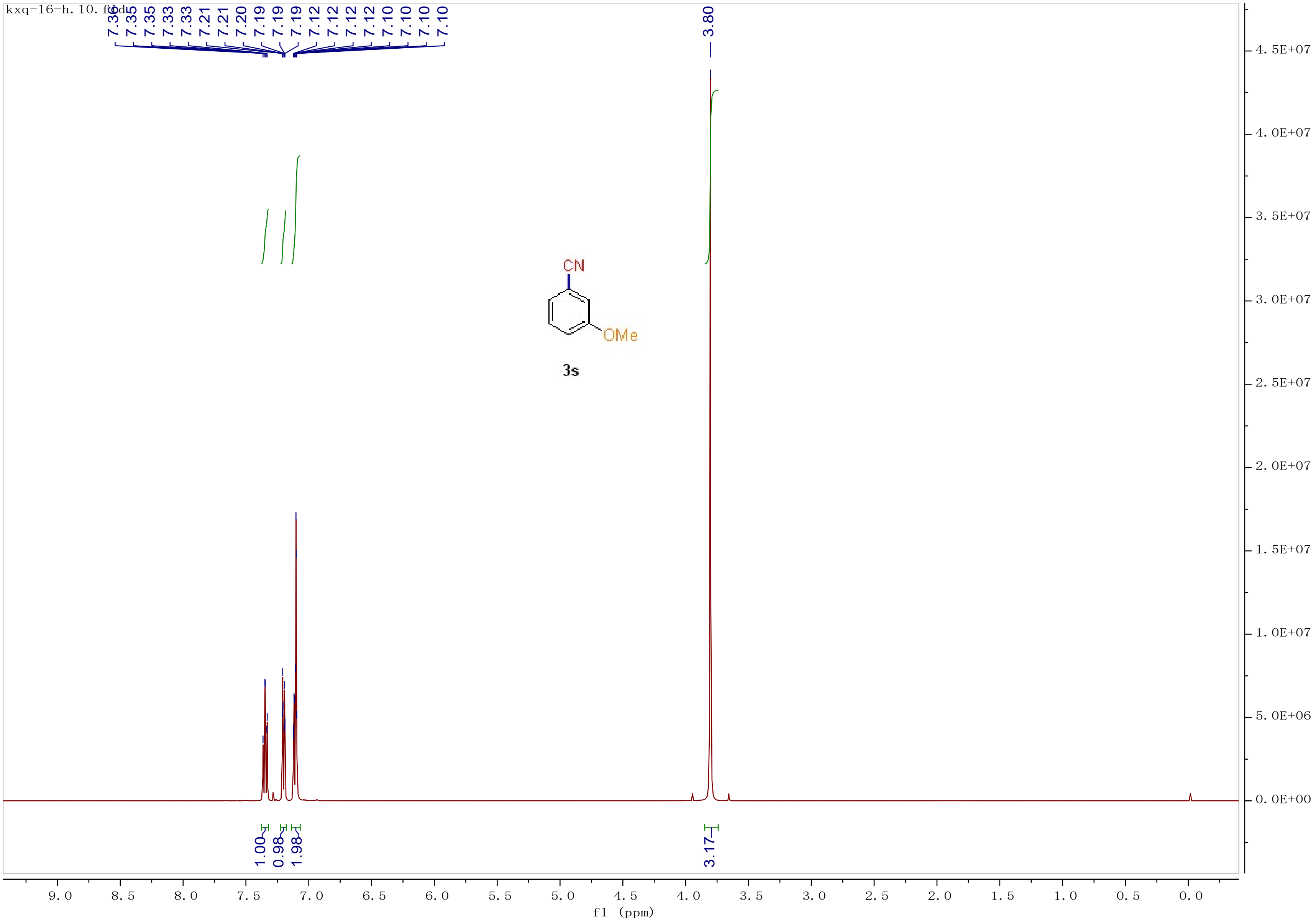
3q

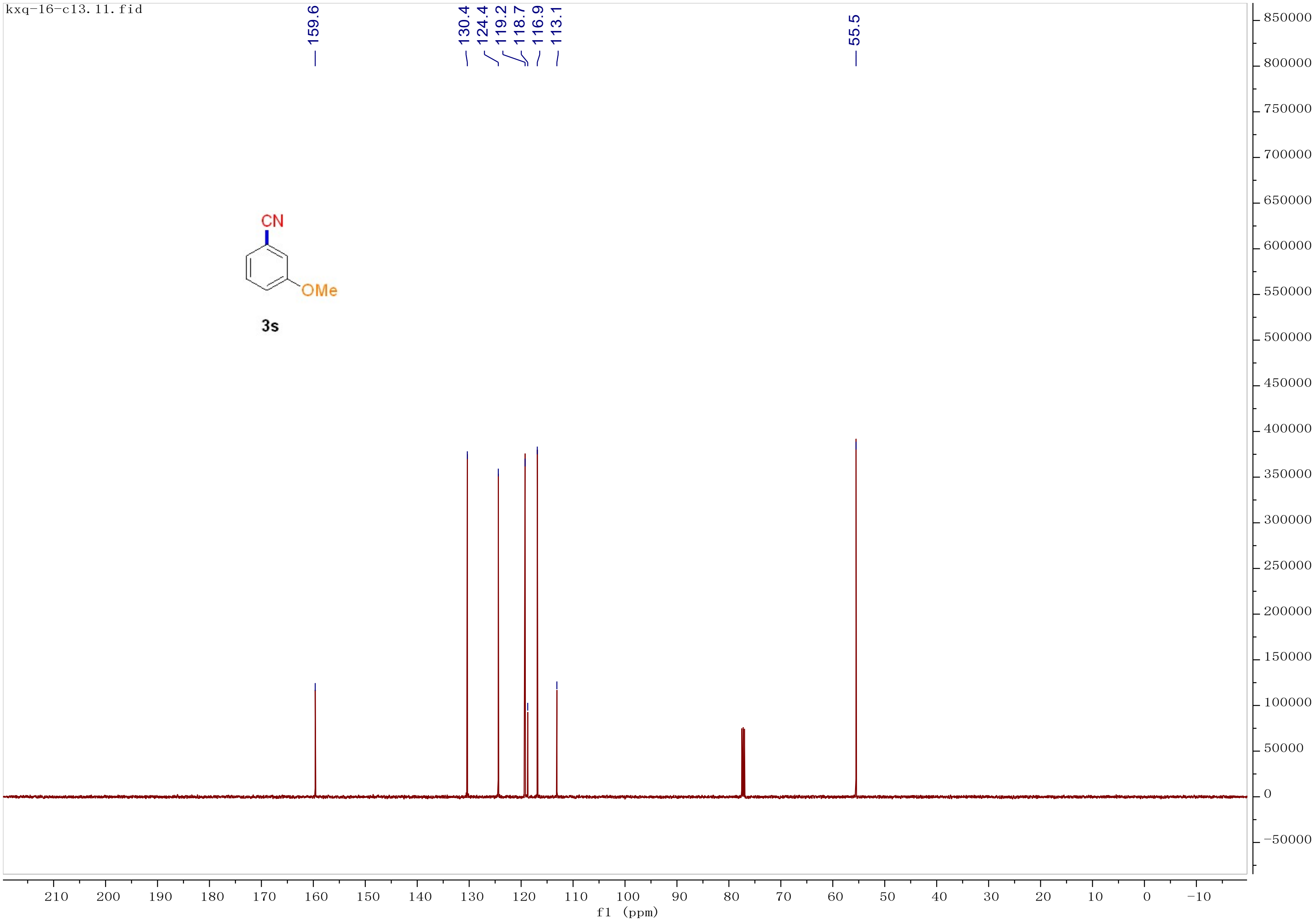

kxq-28-c13.7.fid
136.2
134.8
130.7
130.7
122.9
117.3
114.2
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

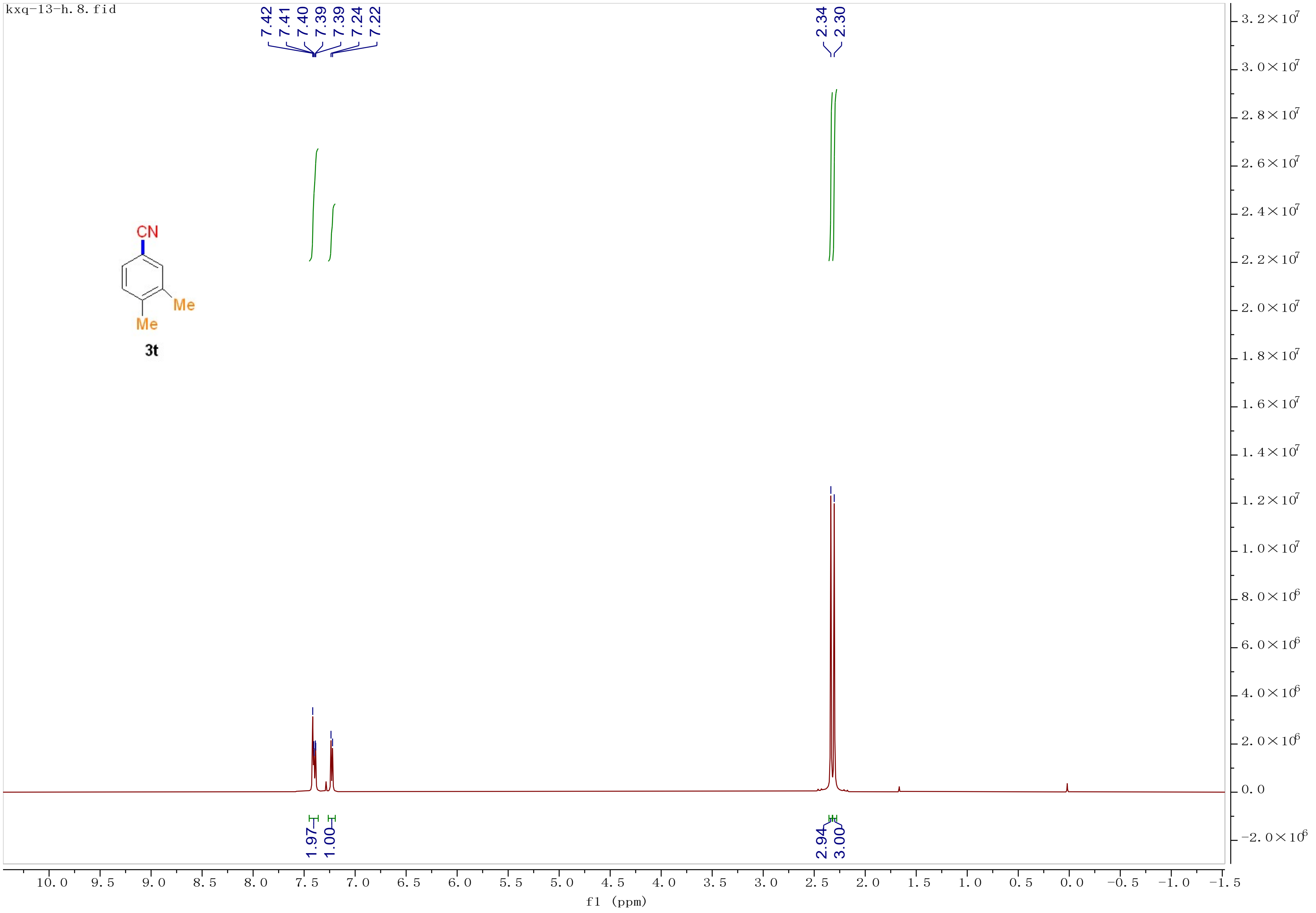

kxq-12-h.5.fid
7.98
7.94
7.92
7.70
7.68
7.67
CN
CN
1.02
1.93
1.00
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

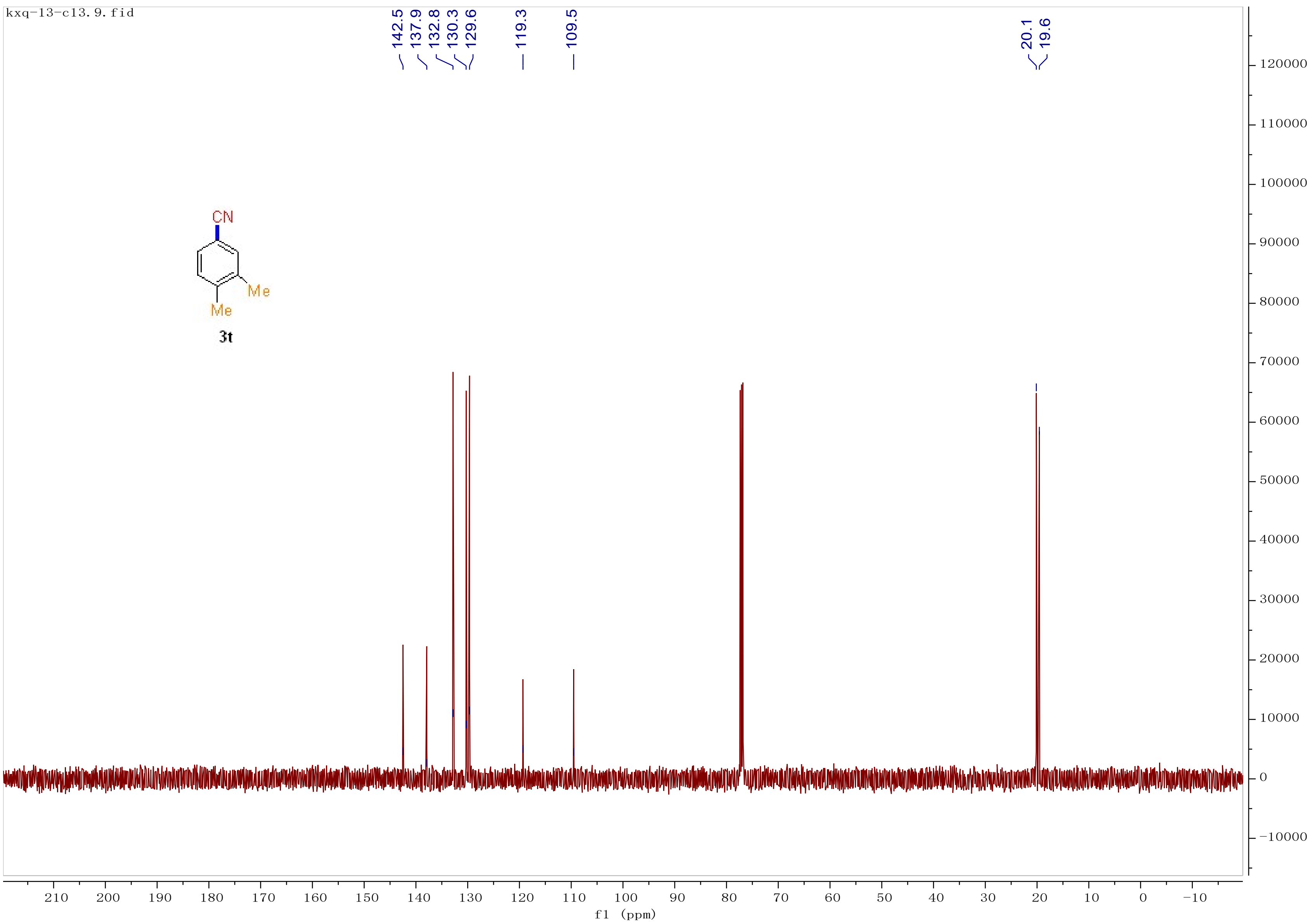
3r

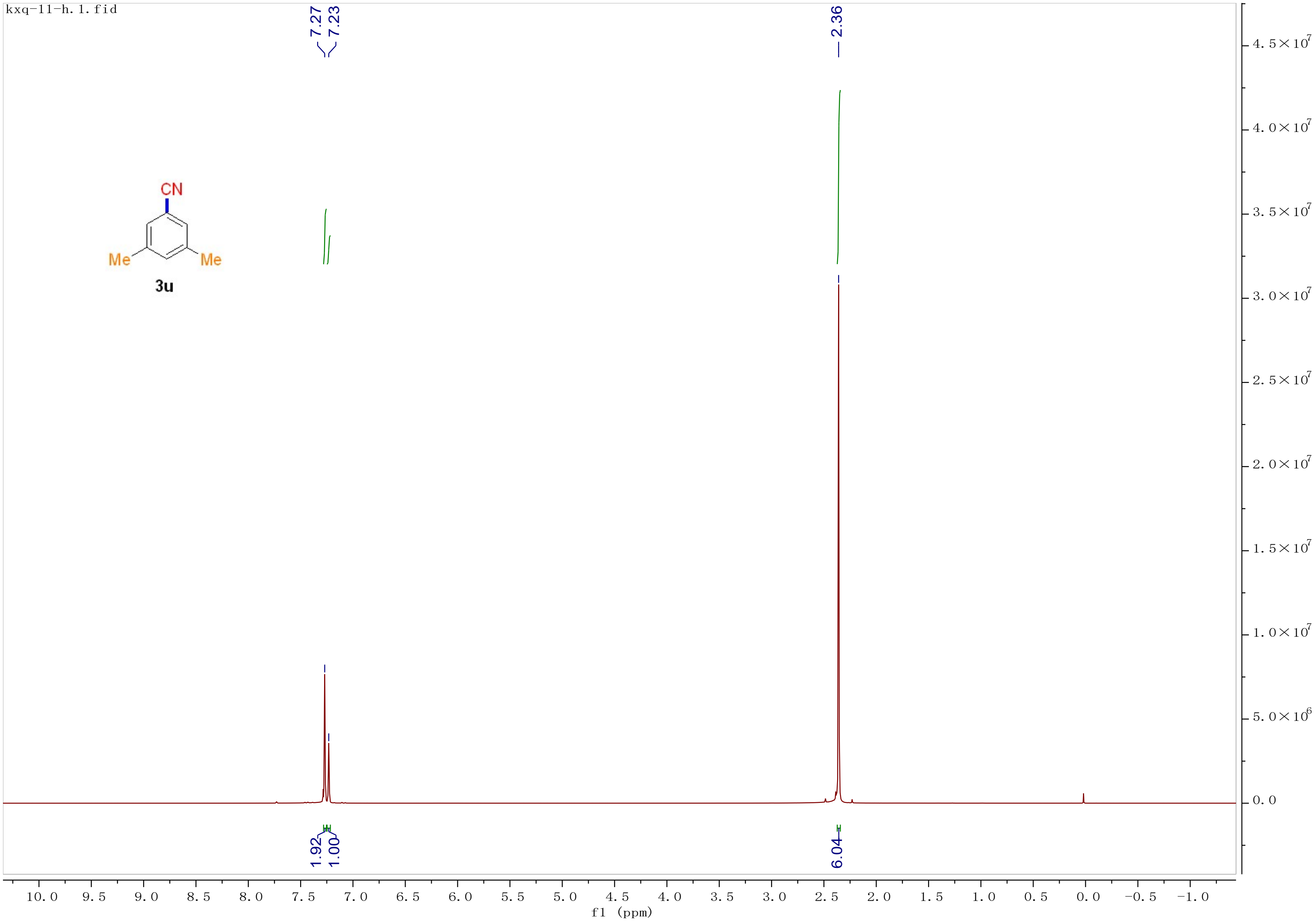

kxq-12-c13.7.fid
136.0
135.4
130.4
116.6
114.2
CN
CN
3r
240000
230000
220000
210000
200000
190000
180000
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
−20000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

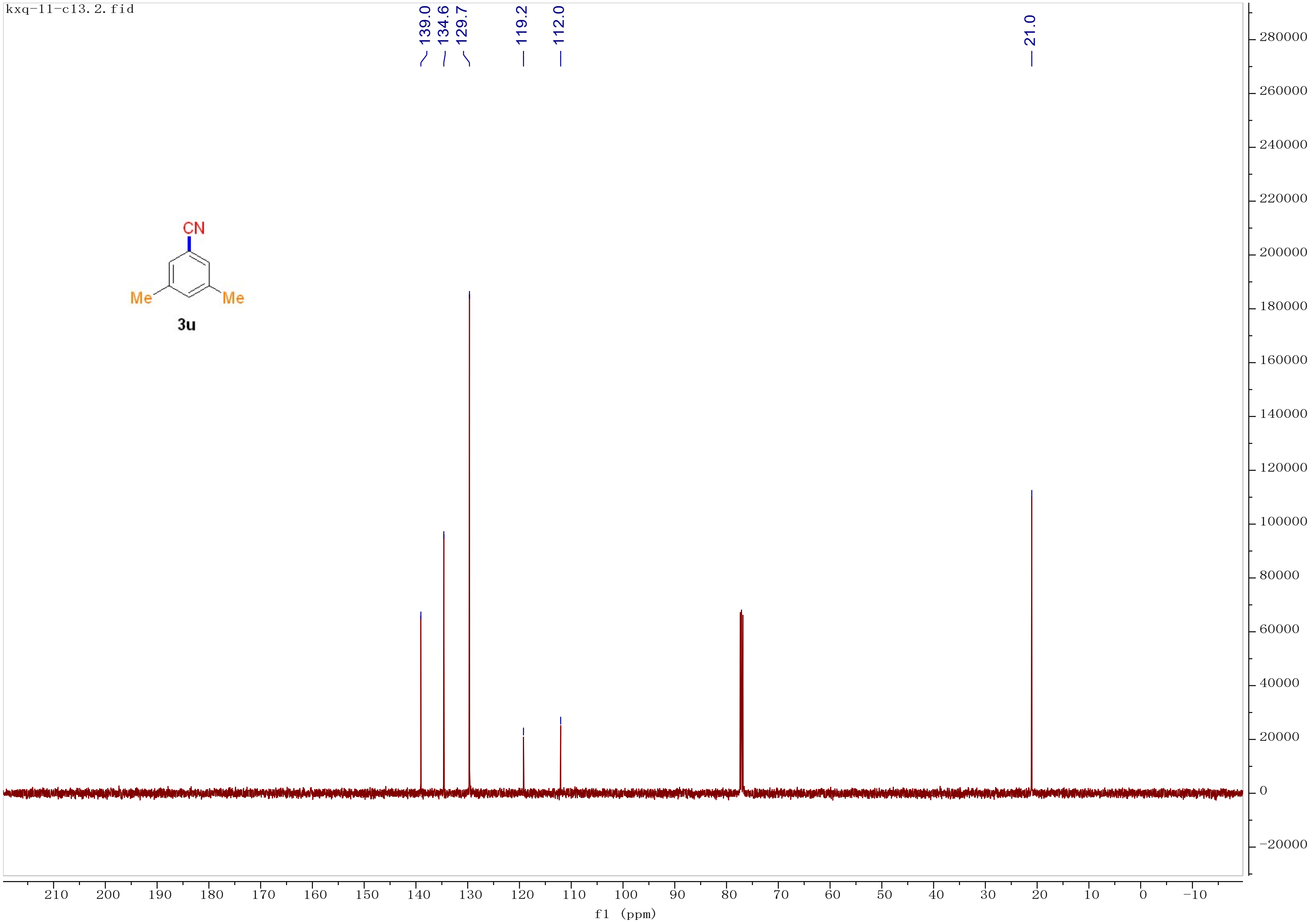

kxq-16-h.10.fid
7.36
7.35
7.35
7.33
7.33
7.21
7.21
7.20
7.19
7.19
7.19
7.12
7.12
7.12
7.12
7.10
7.10
7.10
7.10
3.80
CN
OMe
3s
1.00
0.98
1.98
3.17
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

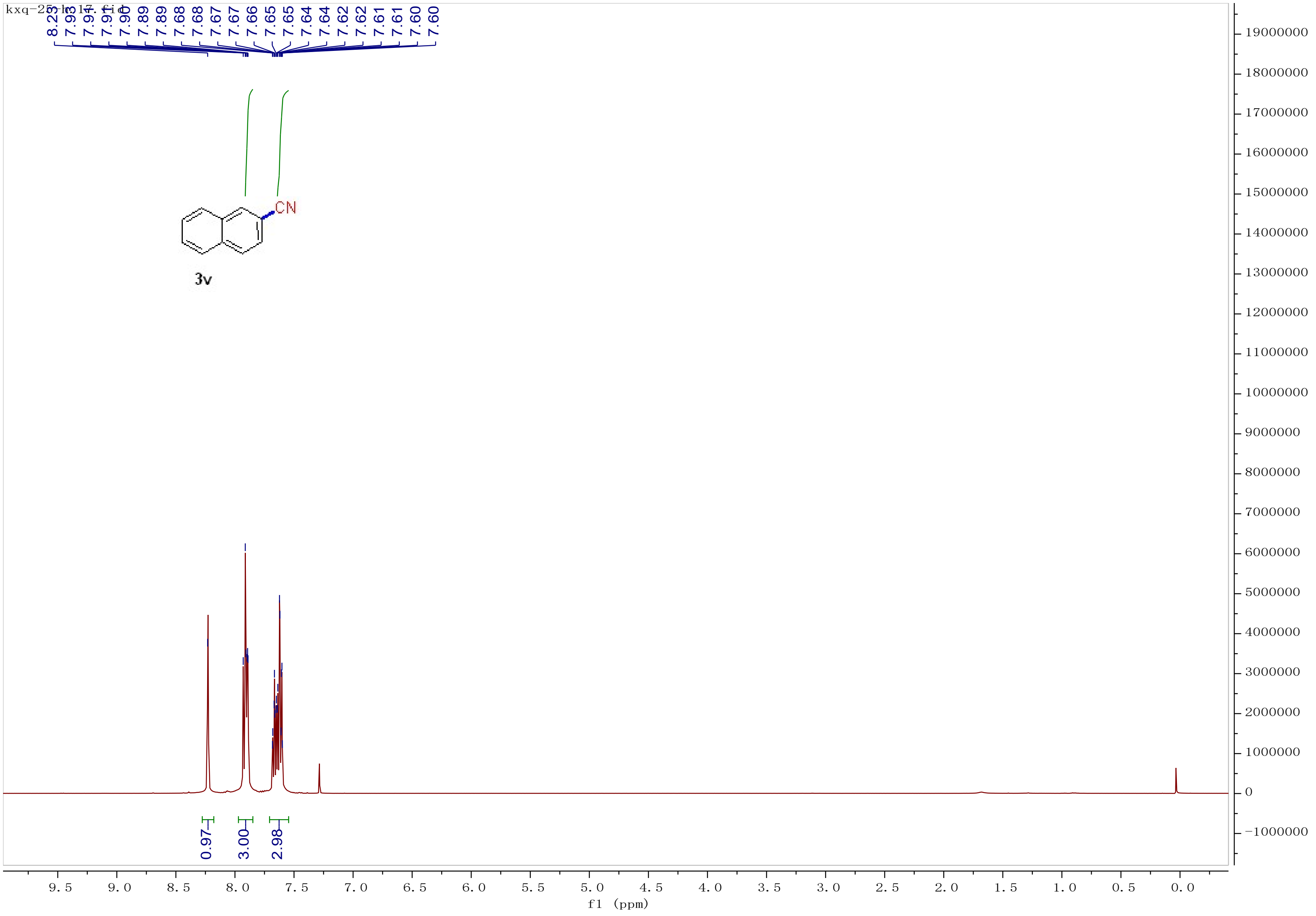

kxq-16-c13.11.fid
159.6
130.4
124.4
119.2
118.7
116.9
113.1
55.5
CN
OMe
3s
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

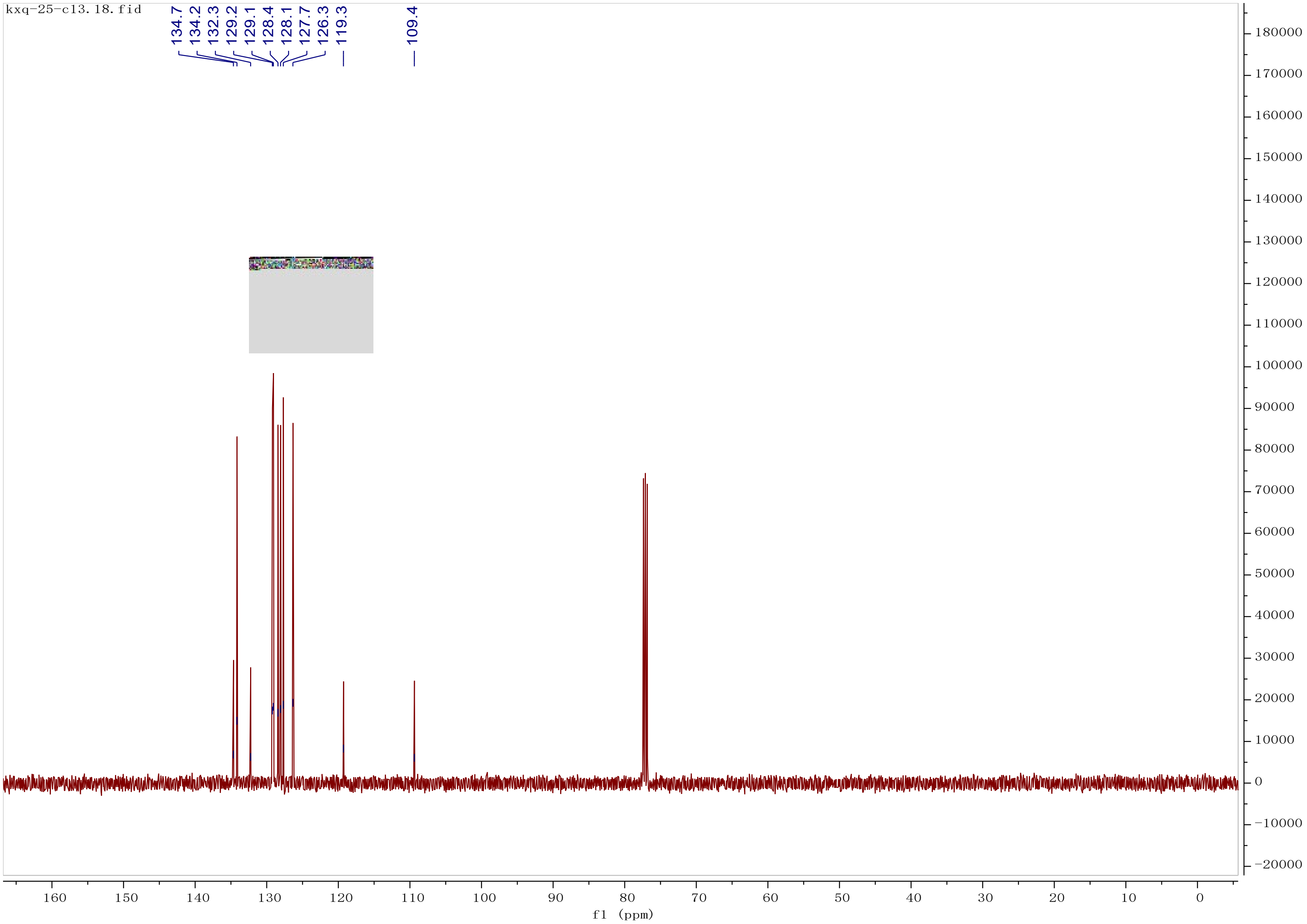

kxq-13-h.8.fid
7.42
7.41
7.40
7.39
7.39
7.24
7.22
2.34
2.30
CN
Me
Me
3t
1.97
1.00
2.94
3.00
3.2×10^7
3.0×10^7
2.8×10^7
2.6×10^7
2.4×10^7
2.2×10^7
2.0×10^7
1.8×10^7
1.6×10^7
1.4×10^7
1.2×10^7
1.0×10^7
8.0×10^6
6.0×10^6
4.0×10^6
2.0×10^6
0.0
-2.0×10^6
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

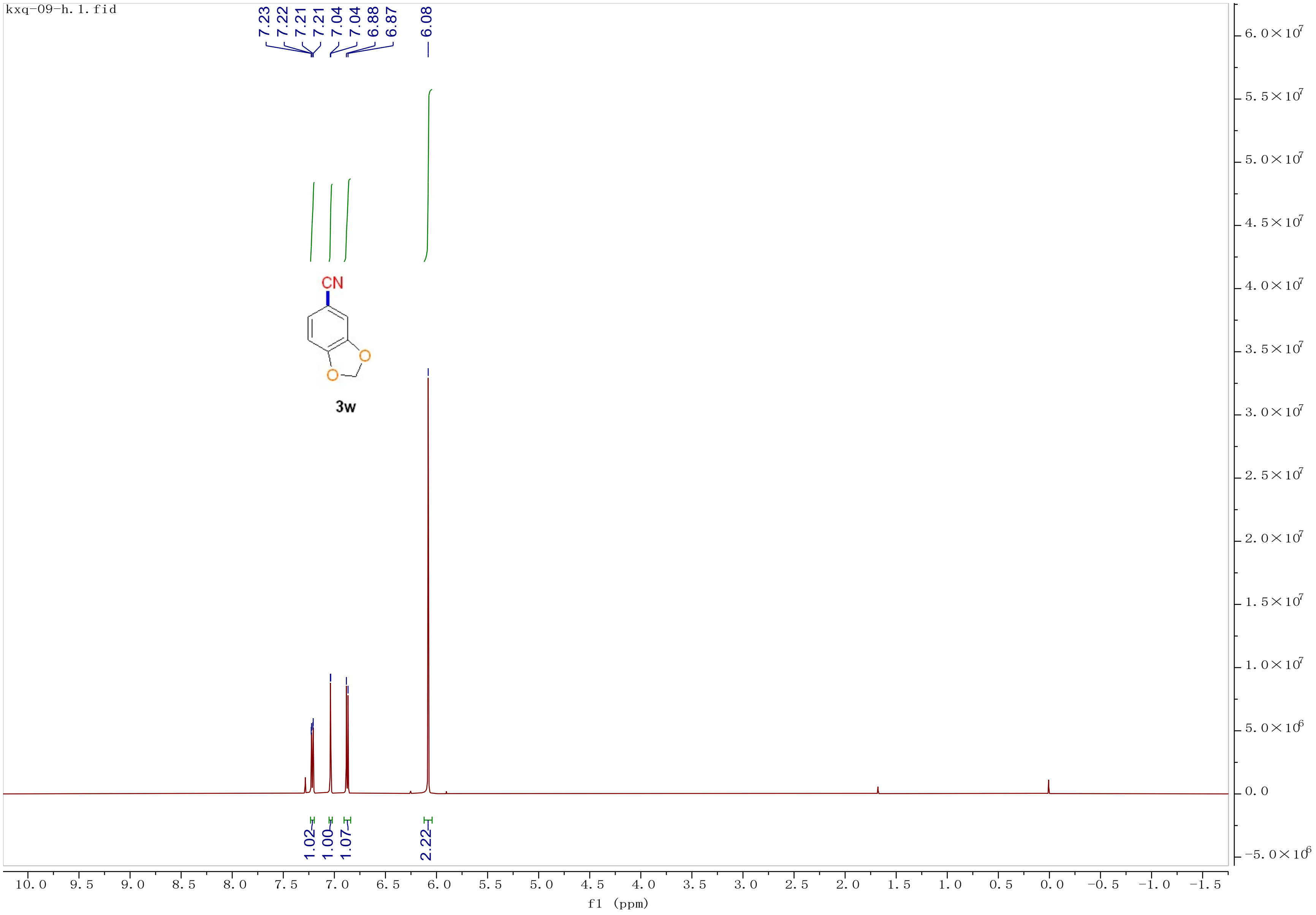

kxq-13-c13.9.fid
142.5
137.9
132.8
130.3
129.6
119.3
109.5
20.1
19.6
CN
Me
Me
3t
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

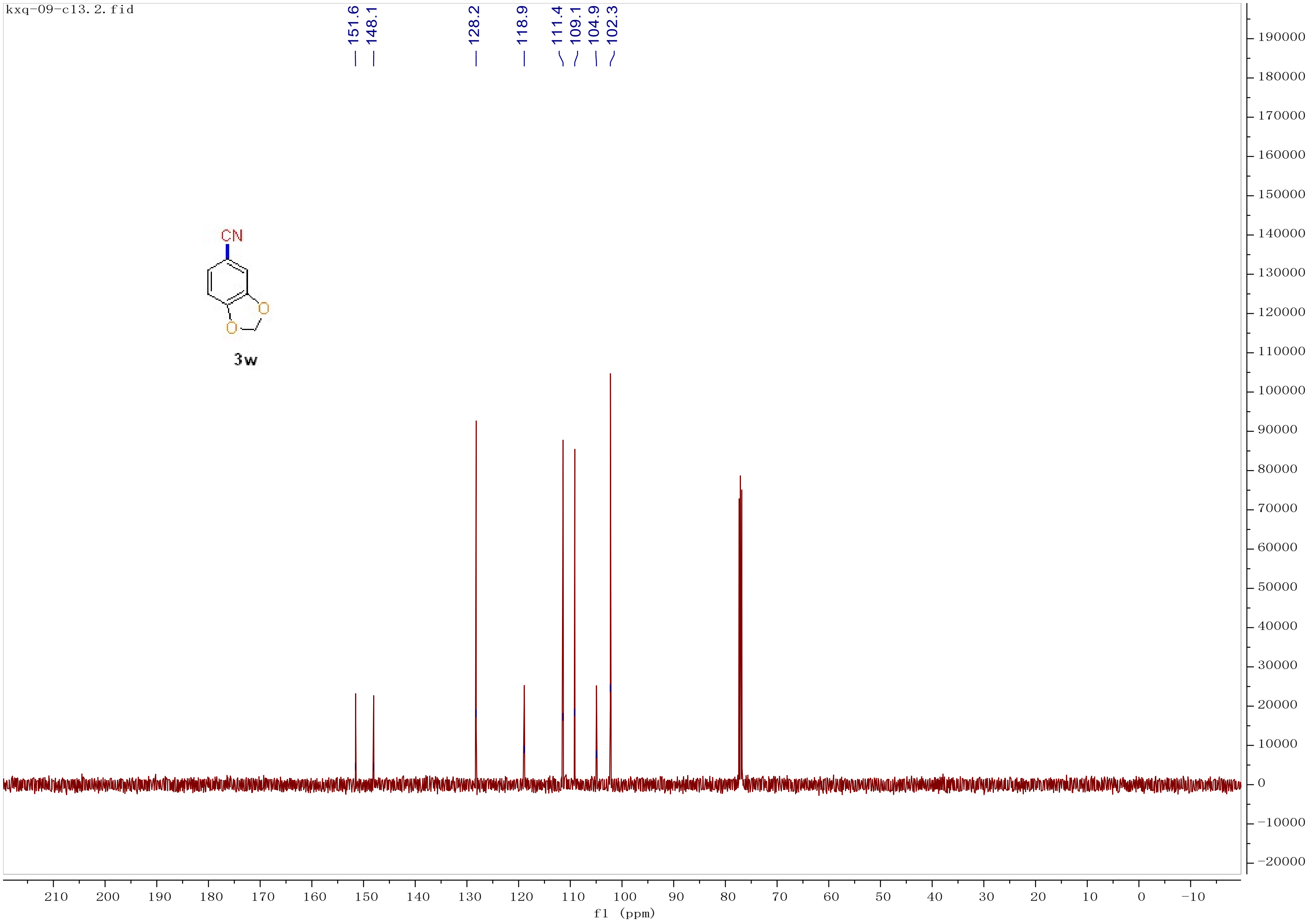

kxq-11-h.1.fid
7.27
7.23
2.36
CN
Me
Me
3u
1.92
1.00
6.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0

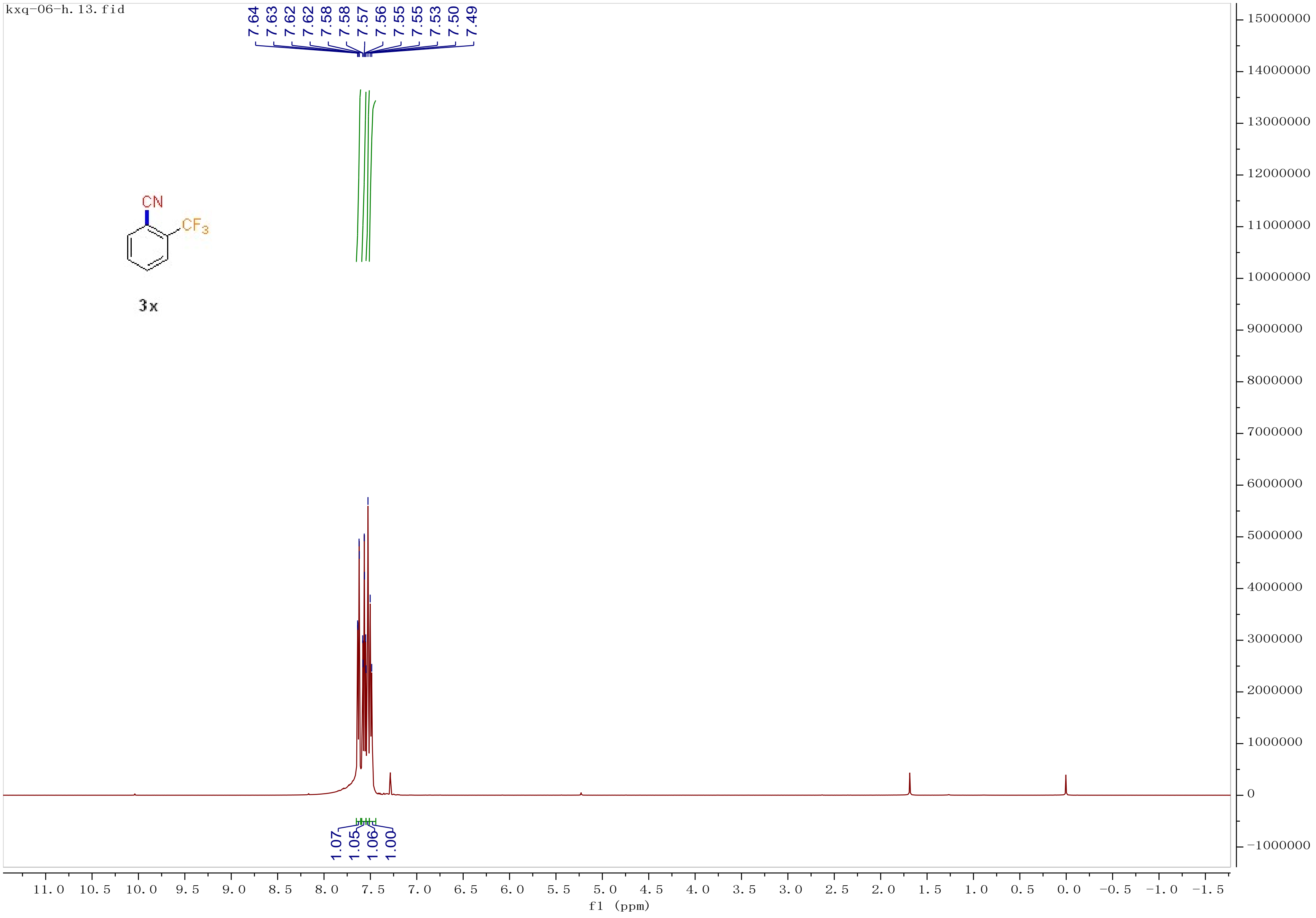

kxq-11-c13.2.fid
139.0
134.6
129.7
119.2
112.0
21.0
CN
Me
Me
3u
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


kxq-25-h.17.fid
8.23
7.93
7.91
7.91
7.90
7.89
7.89
7.68
7.68
7.67
7.67
7.66
7.65
7.65
7.64
7.64
7.62
7.62
7.61
7.61
7.60
7.60
CN
3v
0.97
3.00
2.98
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)
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000

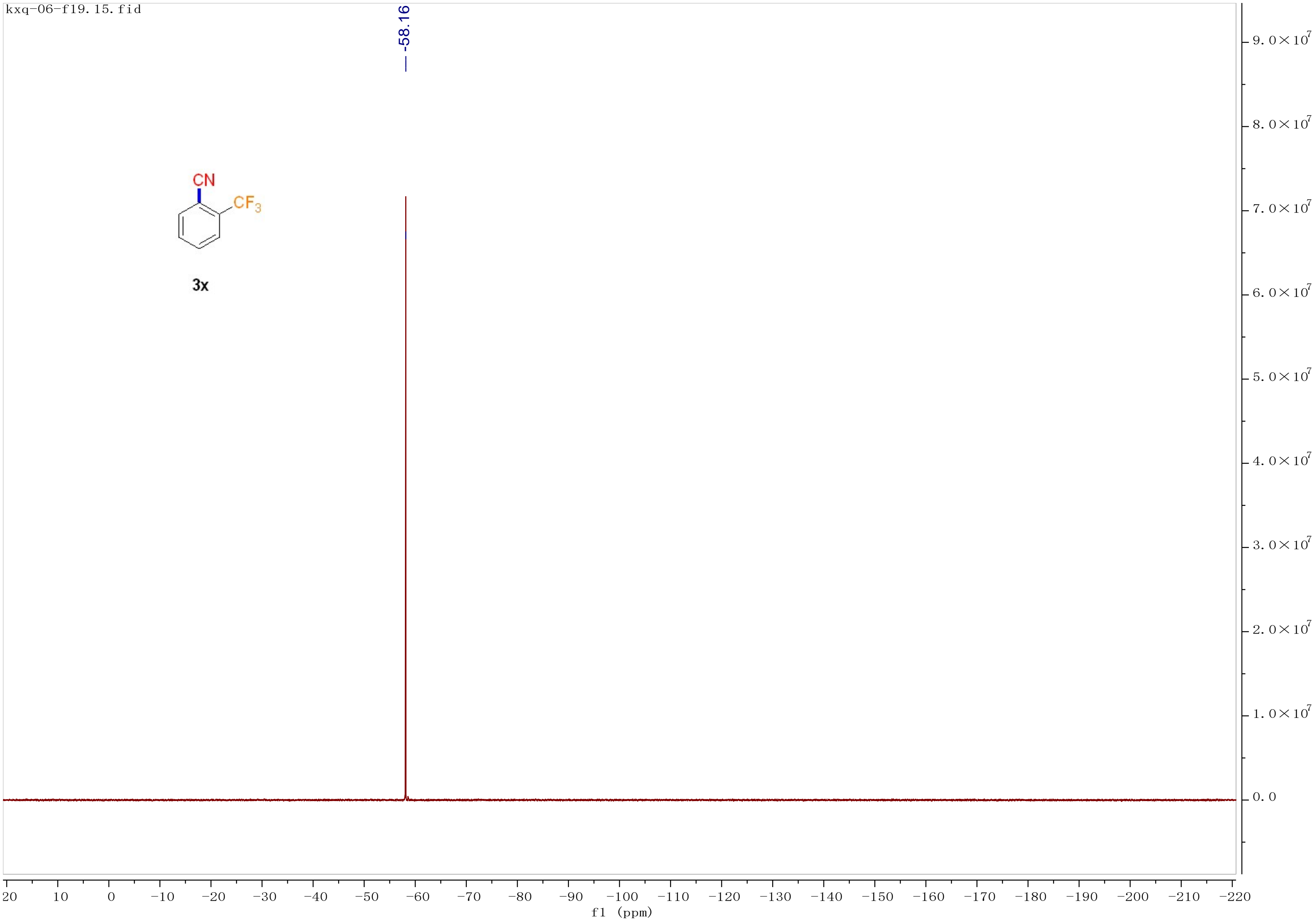

kxq-25-c13.18.fid
134.7
134.2
132.3
129.2
129.1
128.4
128.1
127.7
126.3
119.3
109.4
180000
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
-20000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

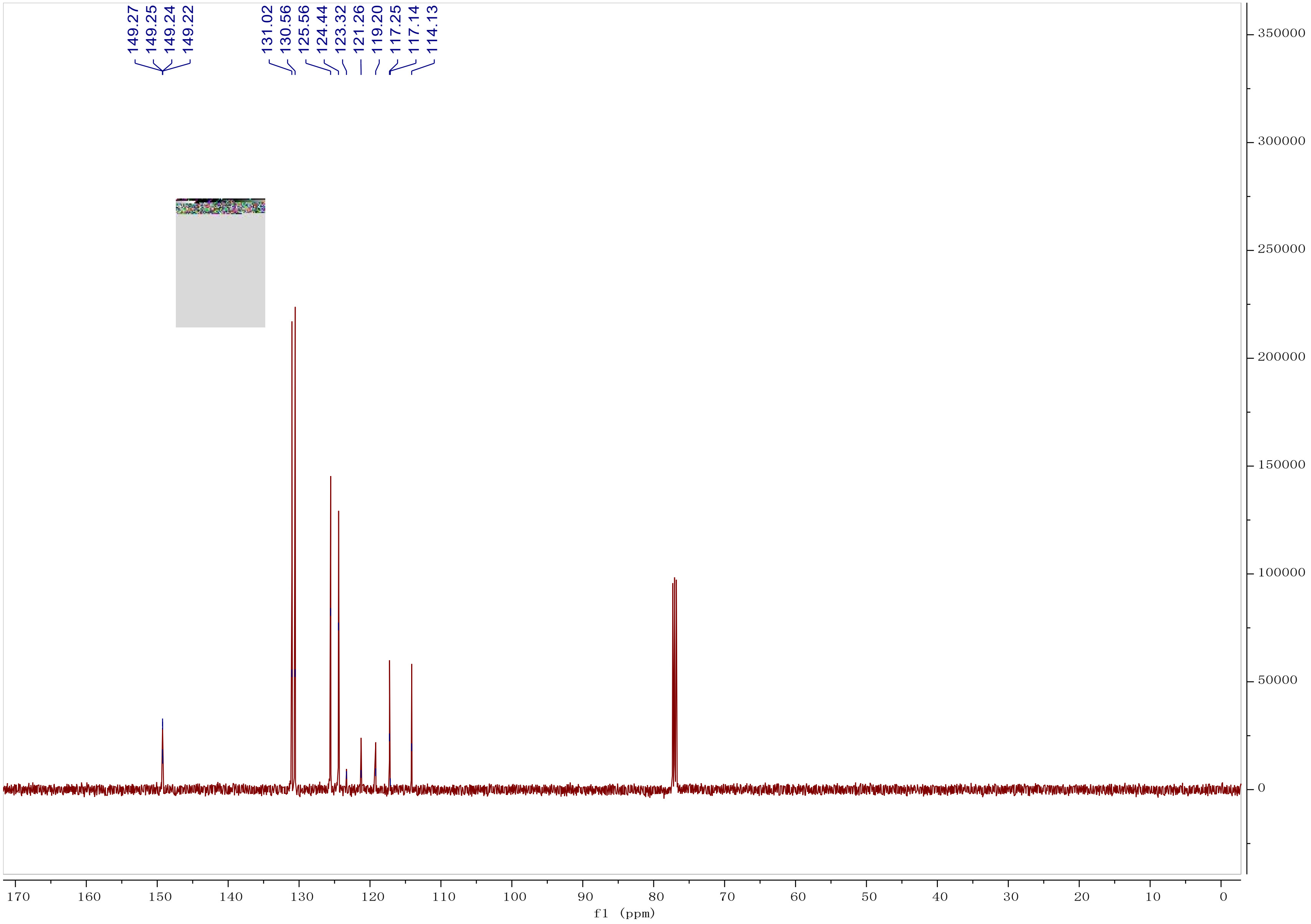

kxq-09-h.1.fid
7.23
7.22
7.21
7.21
7.04
7.04
6.88
6.87
6.08
CN
O
O
3w
1.02
1.00
1.07
2.22
6.0×10^7
5.5×10^7
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
-5.0×10^6
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

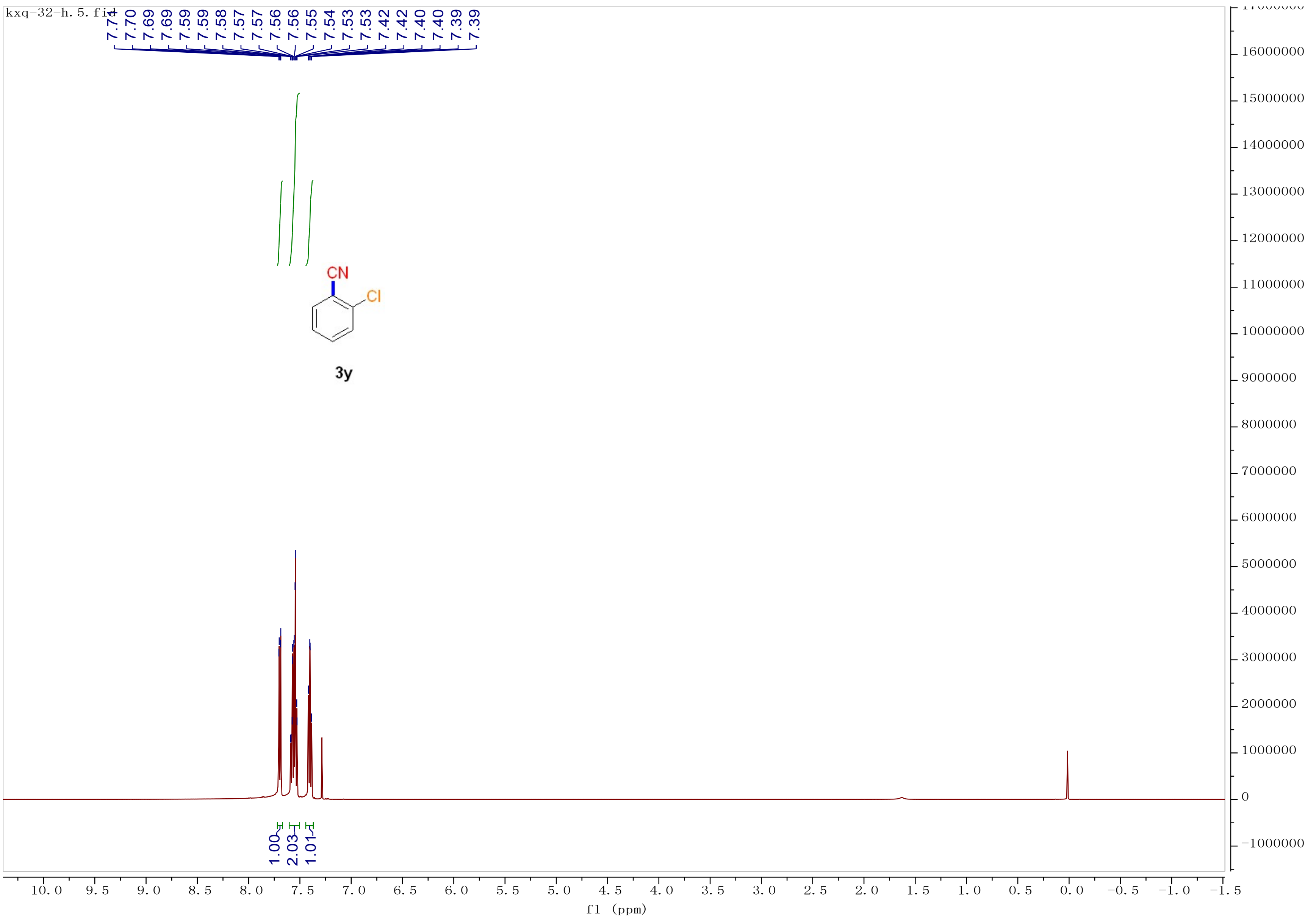

kxq-09-c13.2.fid
151.6
148.1
128.2
118.9
111.4
109.1
104.9
102.3
CN
O
O
3w
190000
180000
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
−20000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

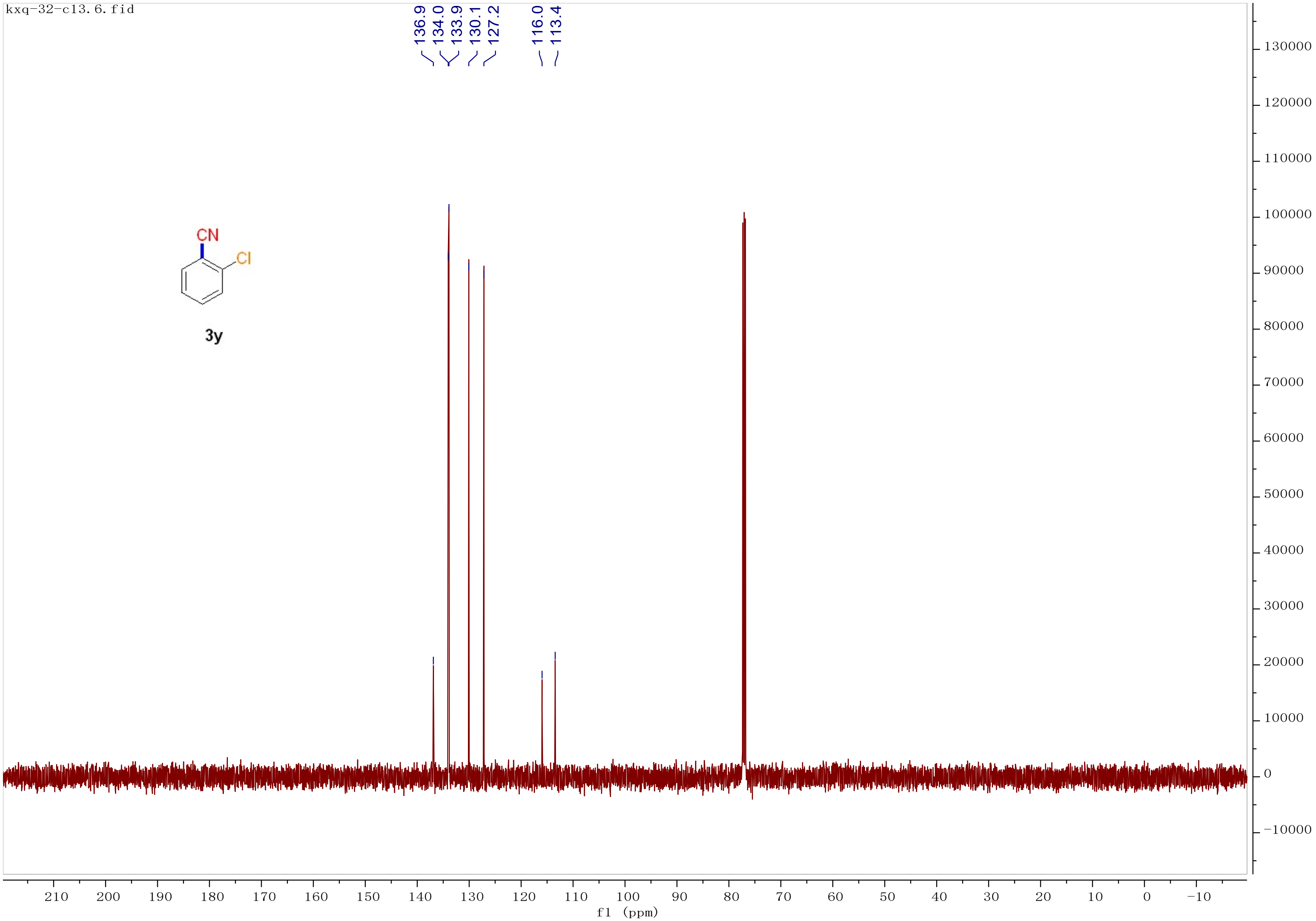

kxq-06-h.13.fid
7.64
7.63
7.62
7.62
7.58
7.58
7.57
7.56
7.55
7.55
7.53
7.50
7.49
CN
CF3
1.07
1.05
1.06
1.00
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

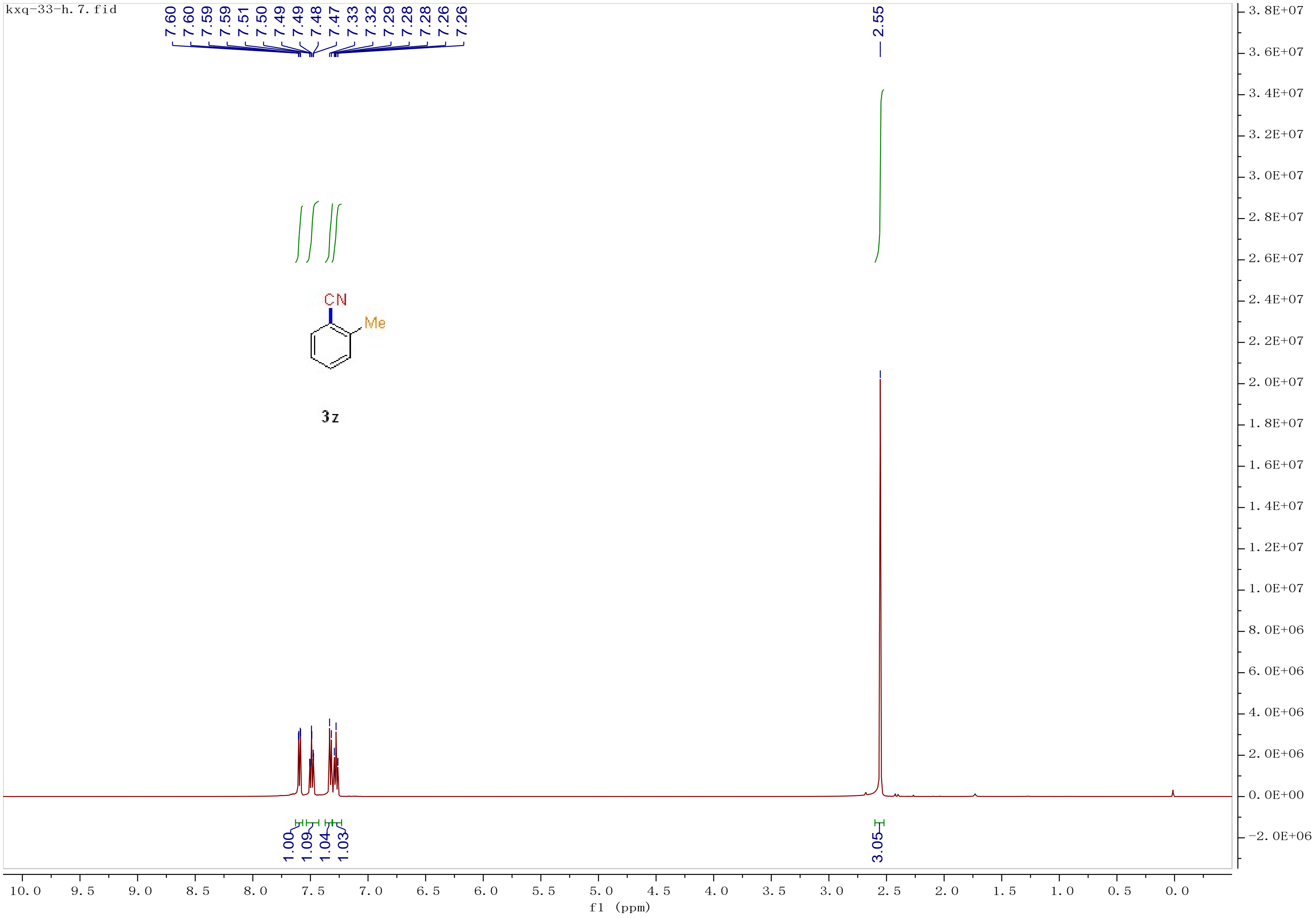
3x

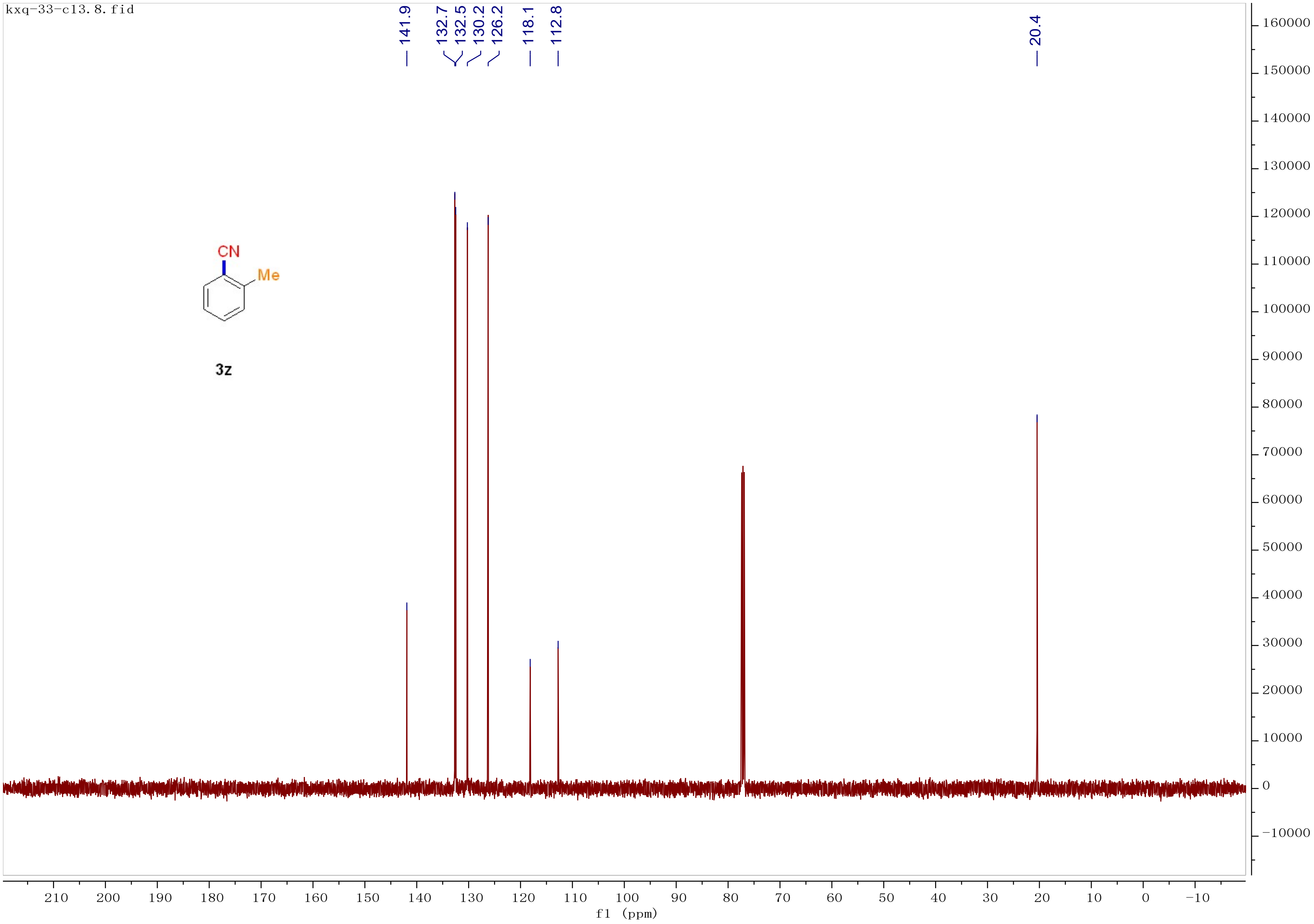

kxq-06-f19.15.fid
-58.16
CN
CF3
3x
9.0×10^7
8.0×10^7
7.0×10^7
6.0×10^7
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 −220
f1 (ppm)


149.27
149.25
149.24
149.22
131.02
130.56
125.56
124.44
123.32
121.26
119.20
117.25
117.14
114.13
350000
300000
250000
200000
150000
100000
50000
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

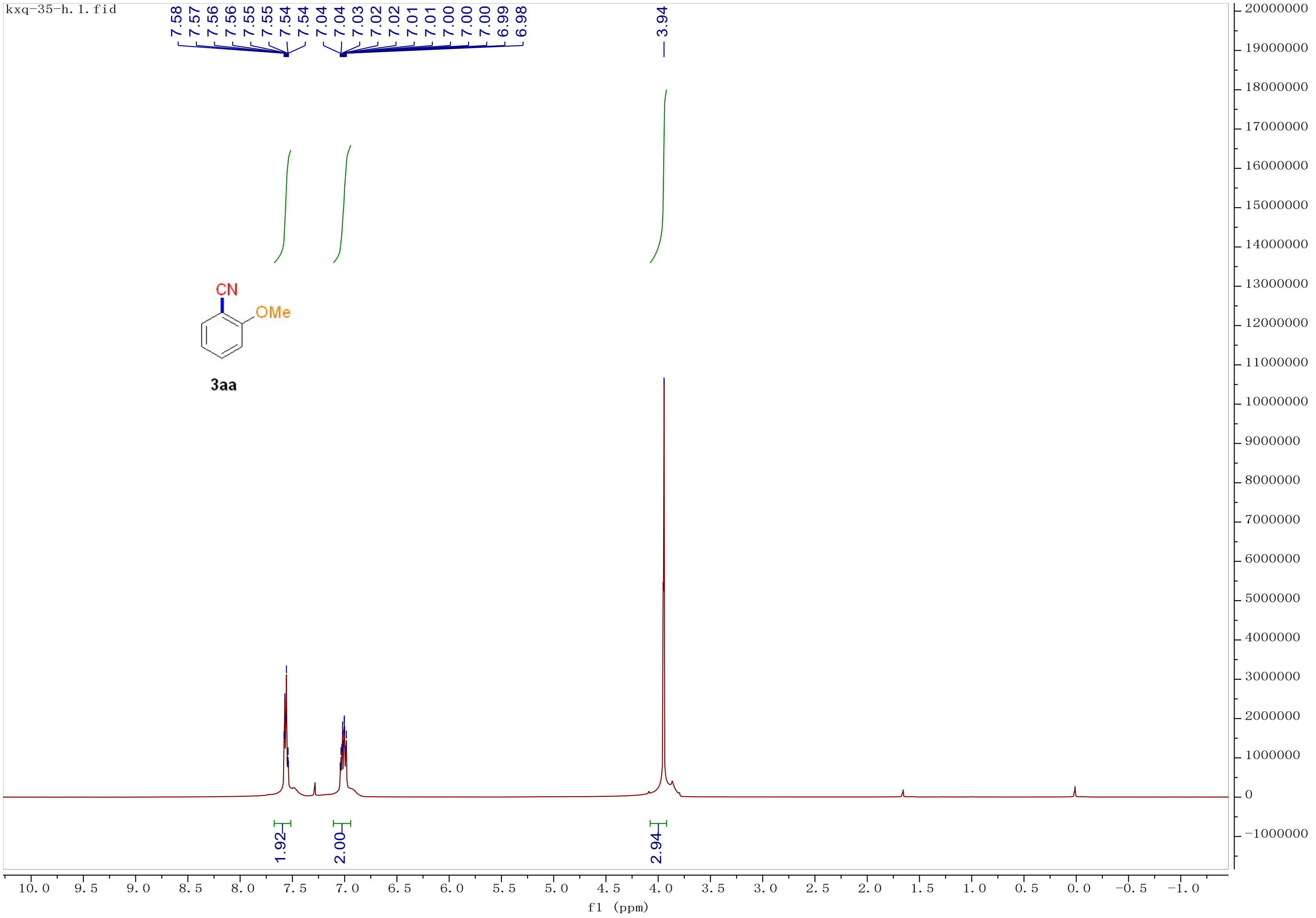

kxq-32-h.5.fid
7.71
7.70
7.69
7.69
7.59
7.59
7.58
7.57
7.57
7.56
7.56
7.55
7.54
7.53
7.53
7.42
7.42
7.40
7.40
7.39
7.39
CN
Cl
3y
1.00
2.03
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000

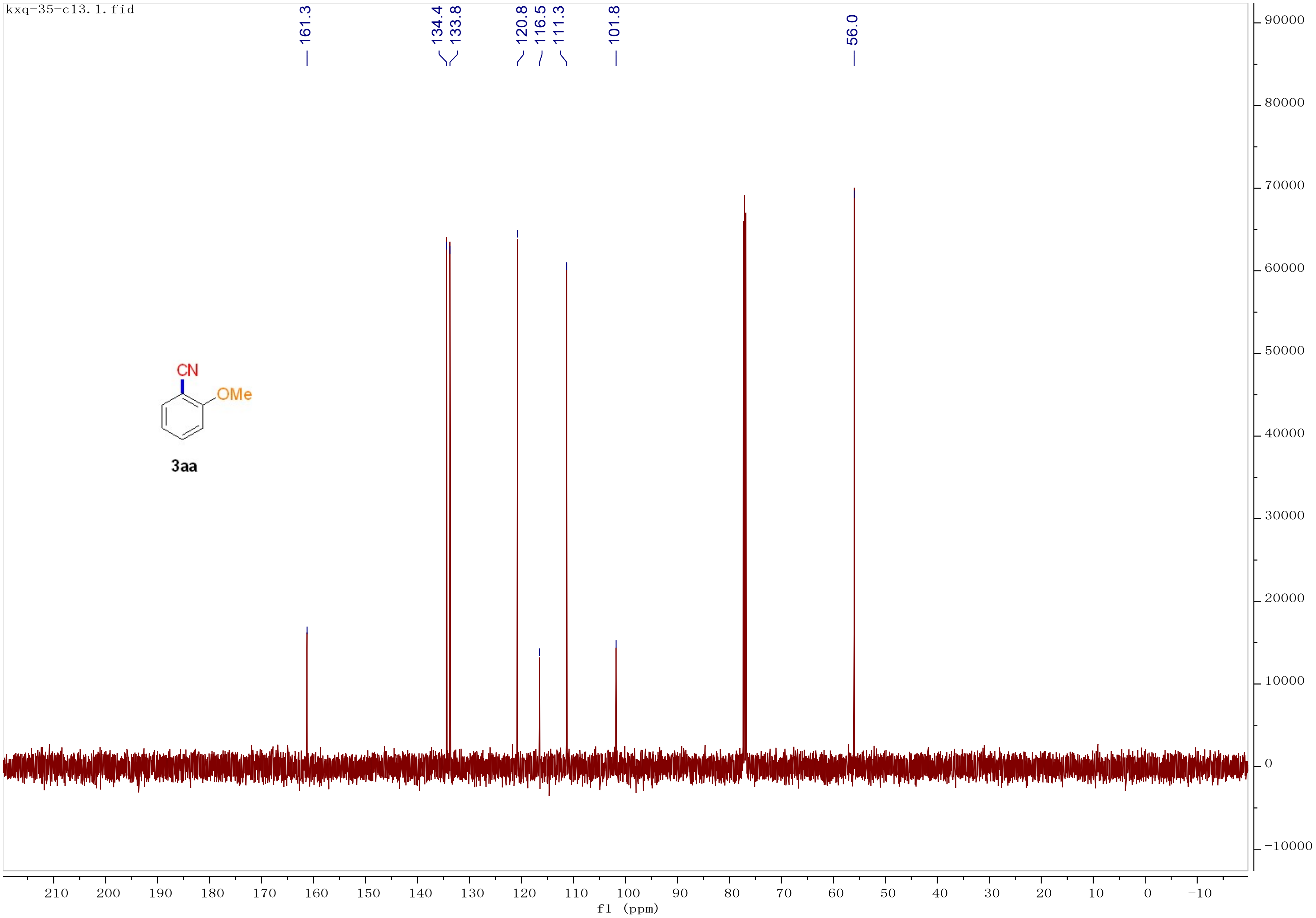

kxq-32-c13.6.fid
136.9
134.0
133.9
130.1
127.2
116.0
113.4
CN
Cl
3y
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

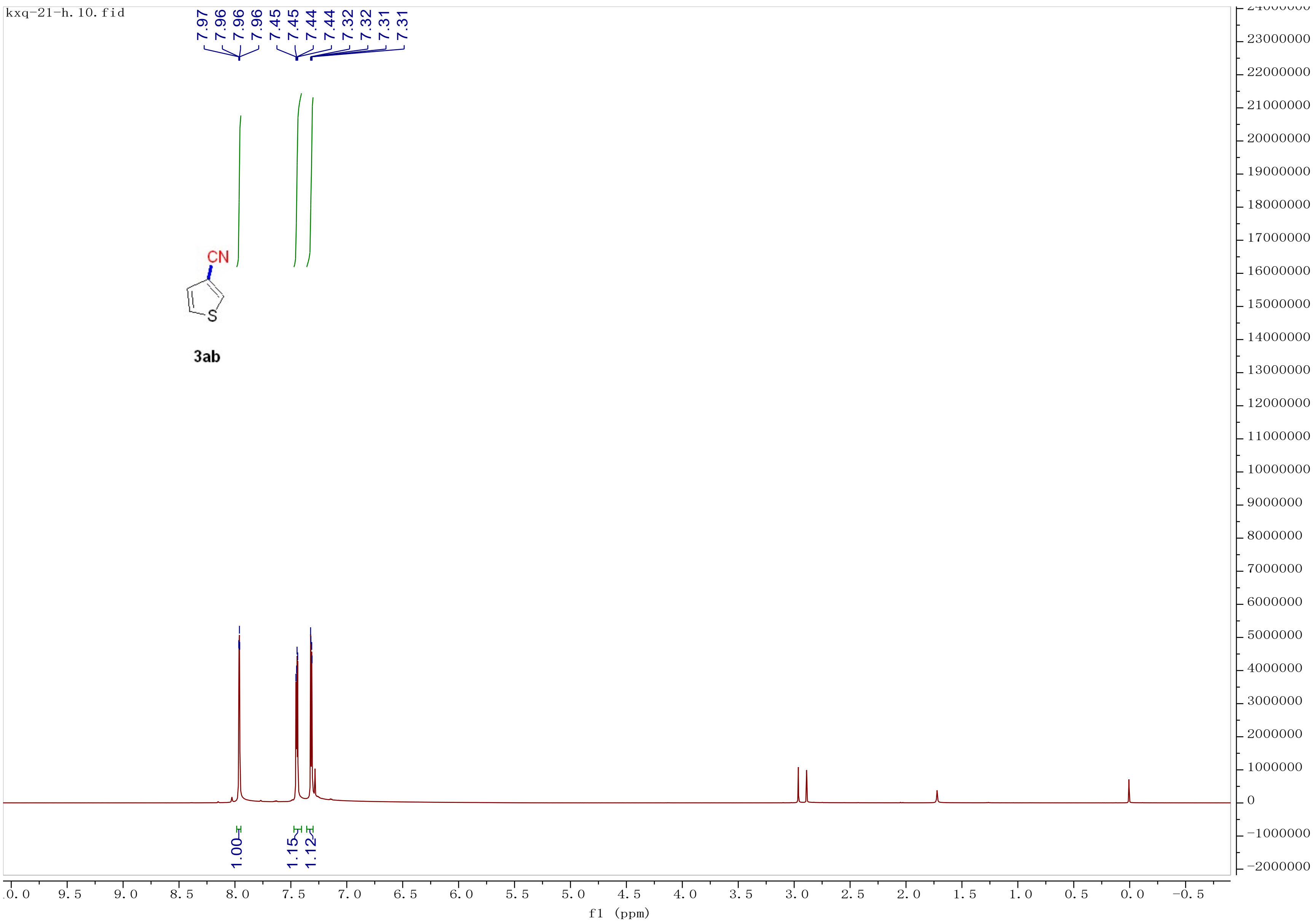

kxq-33-h.7.fid
7.60
7.60
7.59
7.59
7.51
7.50
7.49
7.49
7.48
7.47
7.33
7.32
7.29
7.28
7.28
7.26
7.26
2.55
CN
Me
3z
1.00
1.09
1.04
1.03
3.05
3.8E+07
3.6E+07
3.4E+07
3.2E+07
3.0E+07
2.8E+07
2.6E+07
2.4E+07
2.2E+07
2.0E+07
1.8E+07
1.6E+07
1.4E+07
1.2E+07
1.0E+07
8.0E+06
6.0E+06
4.0E+06
2.0E+06
0.0E+00
-2.0E+06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

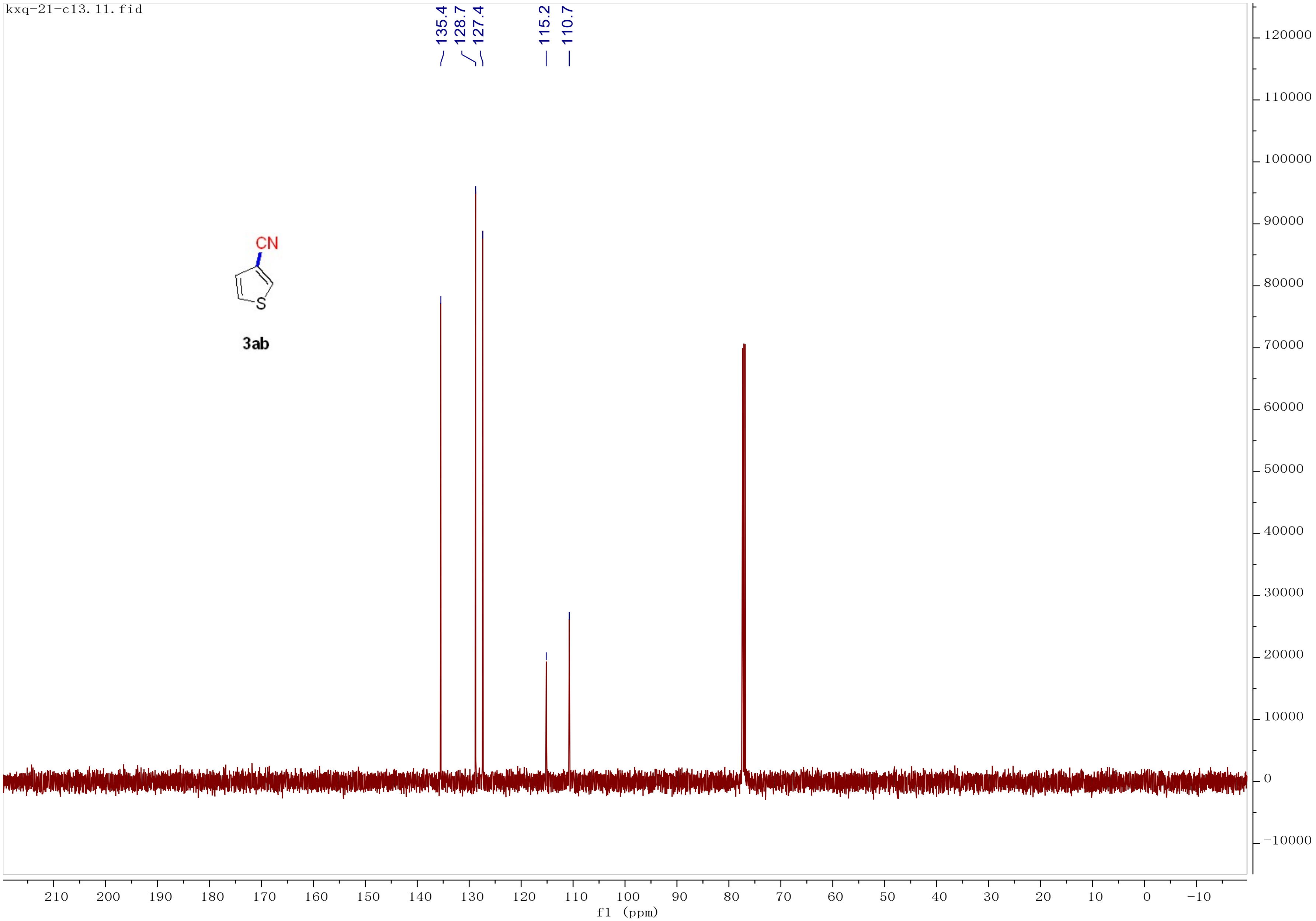

kxq-33-c13.8.fid
141.9
132.7
132.5
130.2
126.2
118.1
112.8
20.4
CN
Me
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

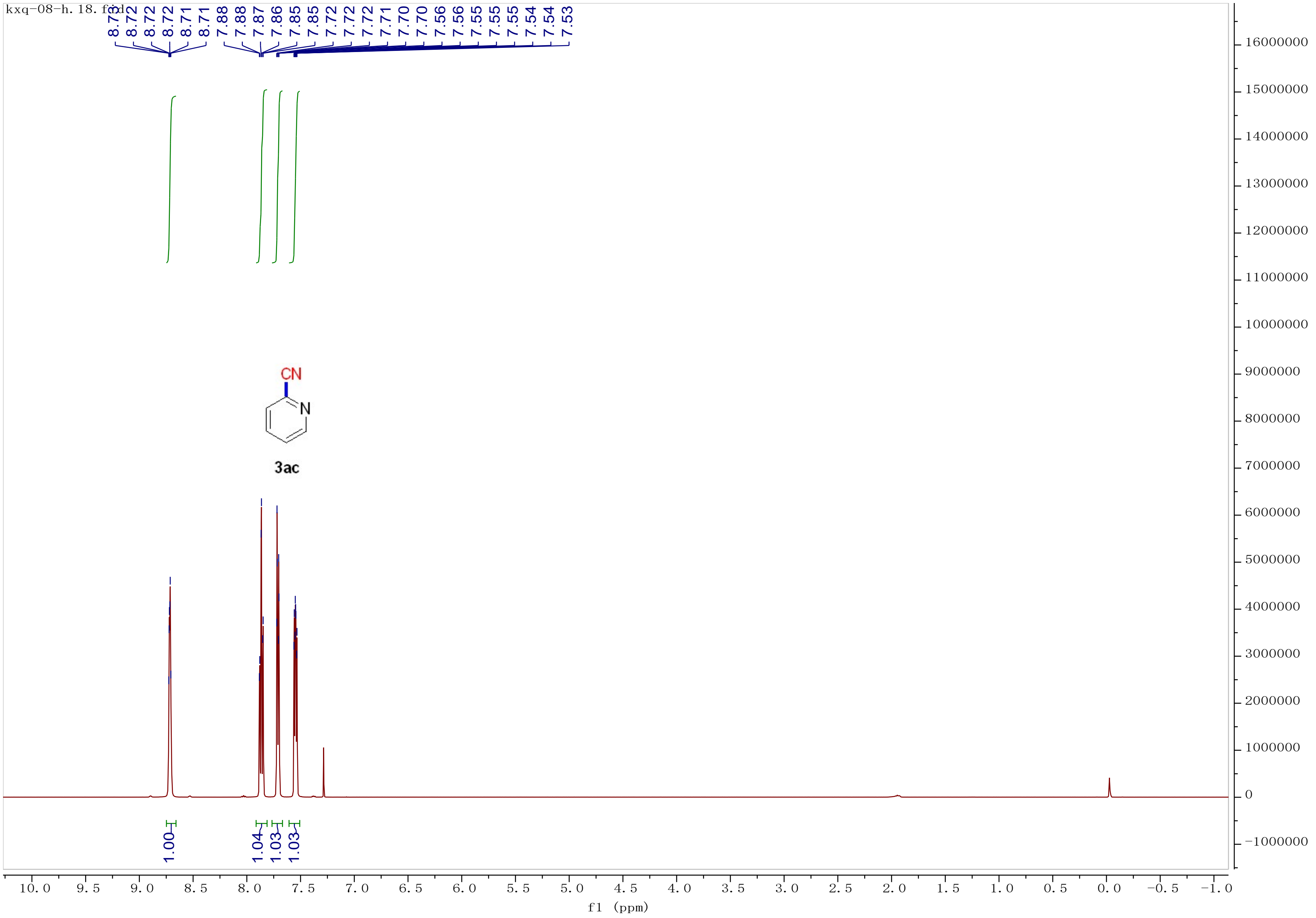
3z

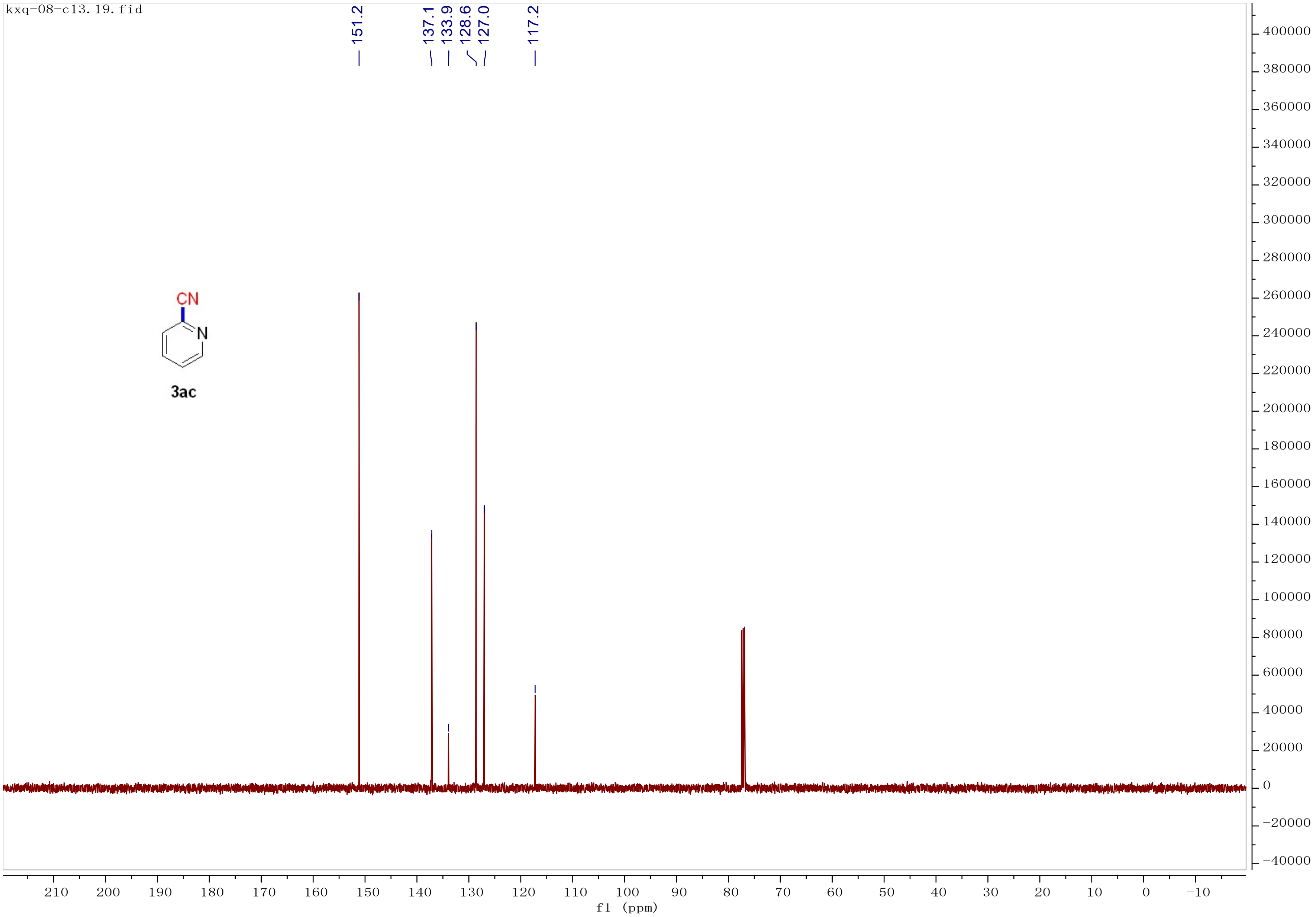

kxq-35-h.1.fid
7.58
7.57
7.56
7.56
7.55
7.55
7.54
7.54
7.04
7.04
7.03
7.02
7.02
7.01
7.01
7.00
7.00
7.00
6.99
6.98
3.94
CN
OMe
3aa
1.92
2.00
2.94
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000

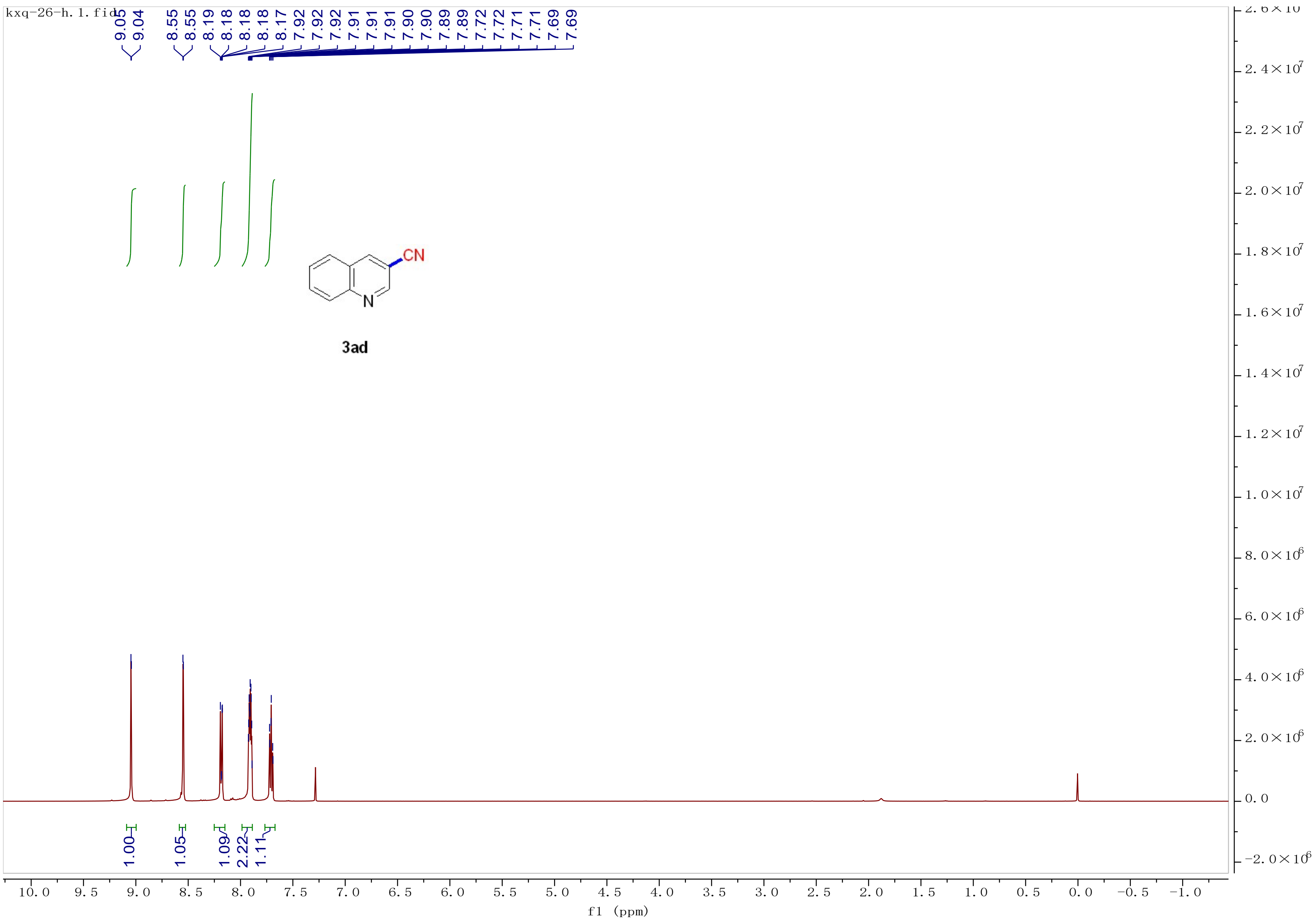

kxq-35-c13.1.fid
161.3
134.4
133.8
120.8
116.5
111.3
101.8
56.0
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
CN
OMe
3aa


kxq-21-h.10.fid
7.97
7.96
7.96
7.96
7.45
7.45
7.44
7.44
7.32
7.32
7.31
7.31
CN
S
3ab
1.00
1.15
1.12
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
24000000
23000000
22000000
21000000
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
-2000000

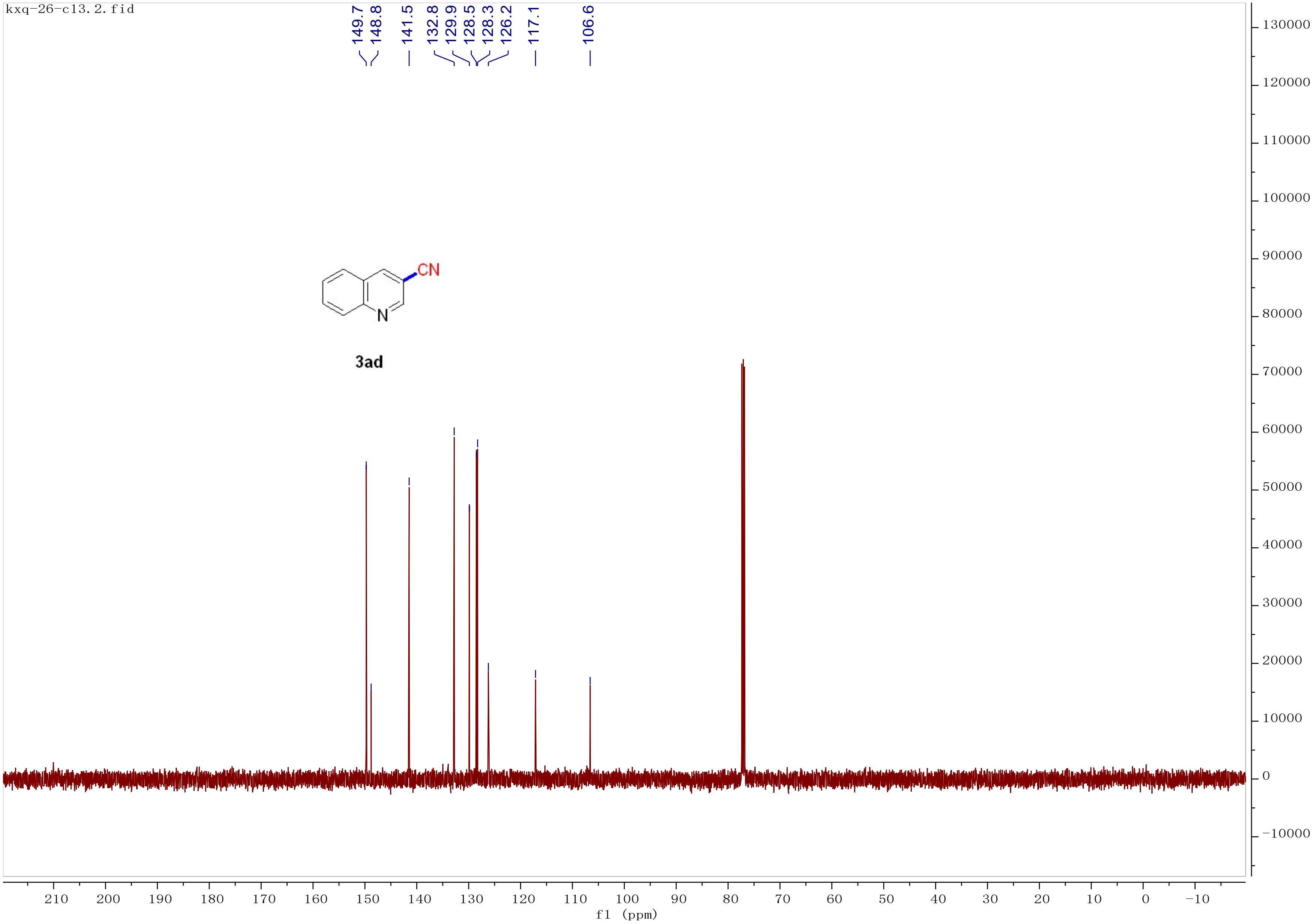

kxq-21-c13.11.fid
135.4
128.7
127.4
115.2
110.7
CN
S
3ab
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

kxq-08-h.18.fid
8.73
8.72
8.72
8.72
8.71
8.71
7.88
7.88
7.87
7.86
7.85
7.85
7.72
7.72
7.72
7.71
7.70
7.70
7.56
7.56
7.55
7.55
7.55
7.54
7.54
7.53
CN
N
3ac
1.00
1.04
1.03
1.03
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

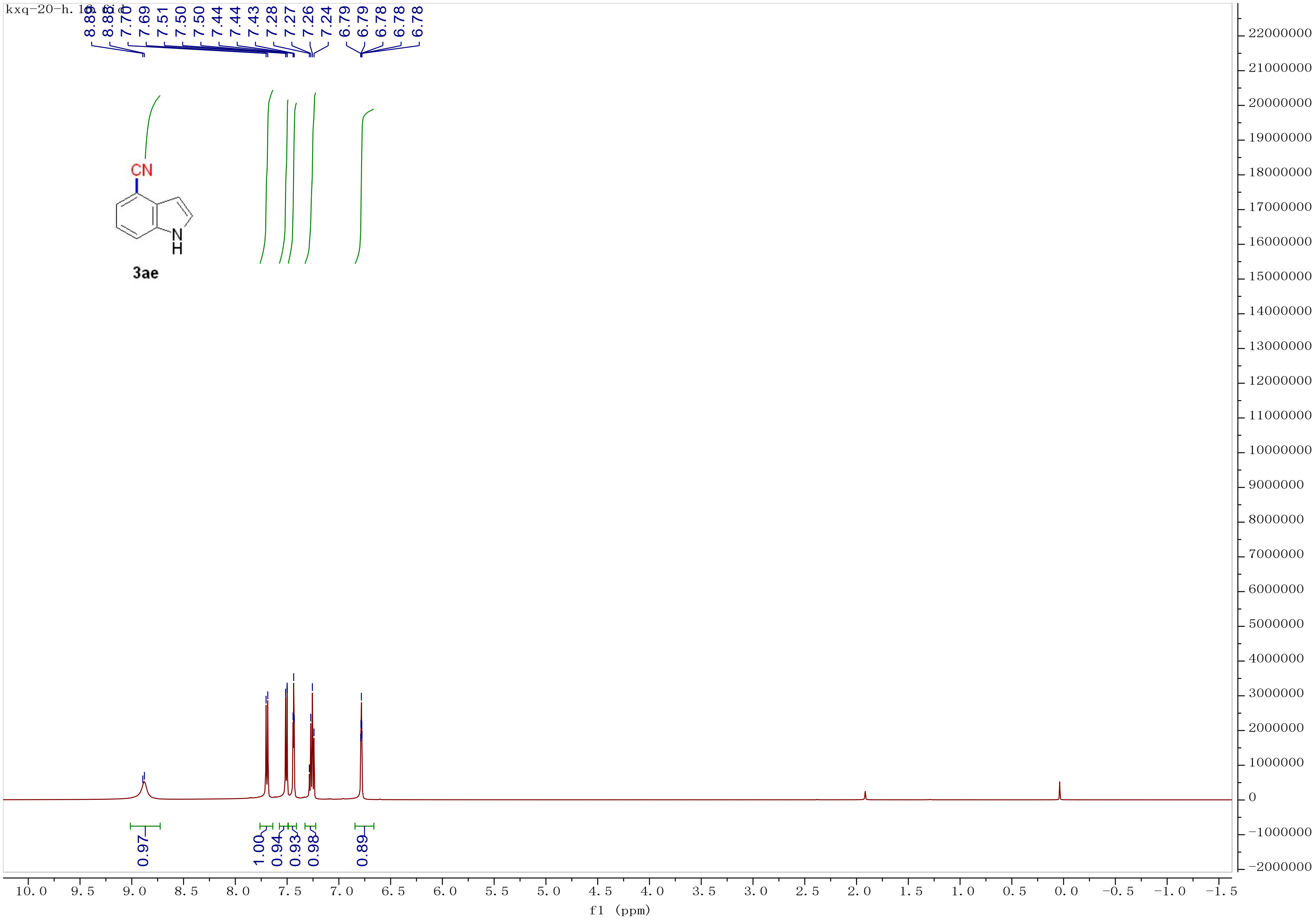

kxq-08-c13.19.fid
151.2
137.1
133.9
128.6
127.0
117.2
CN
N
3ac
400000
380000
360000
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
-40000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

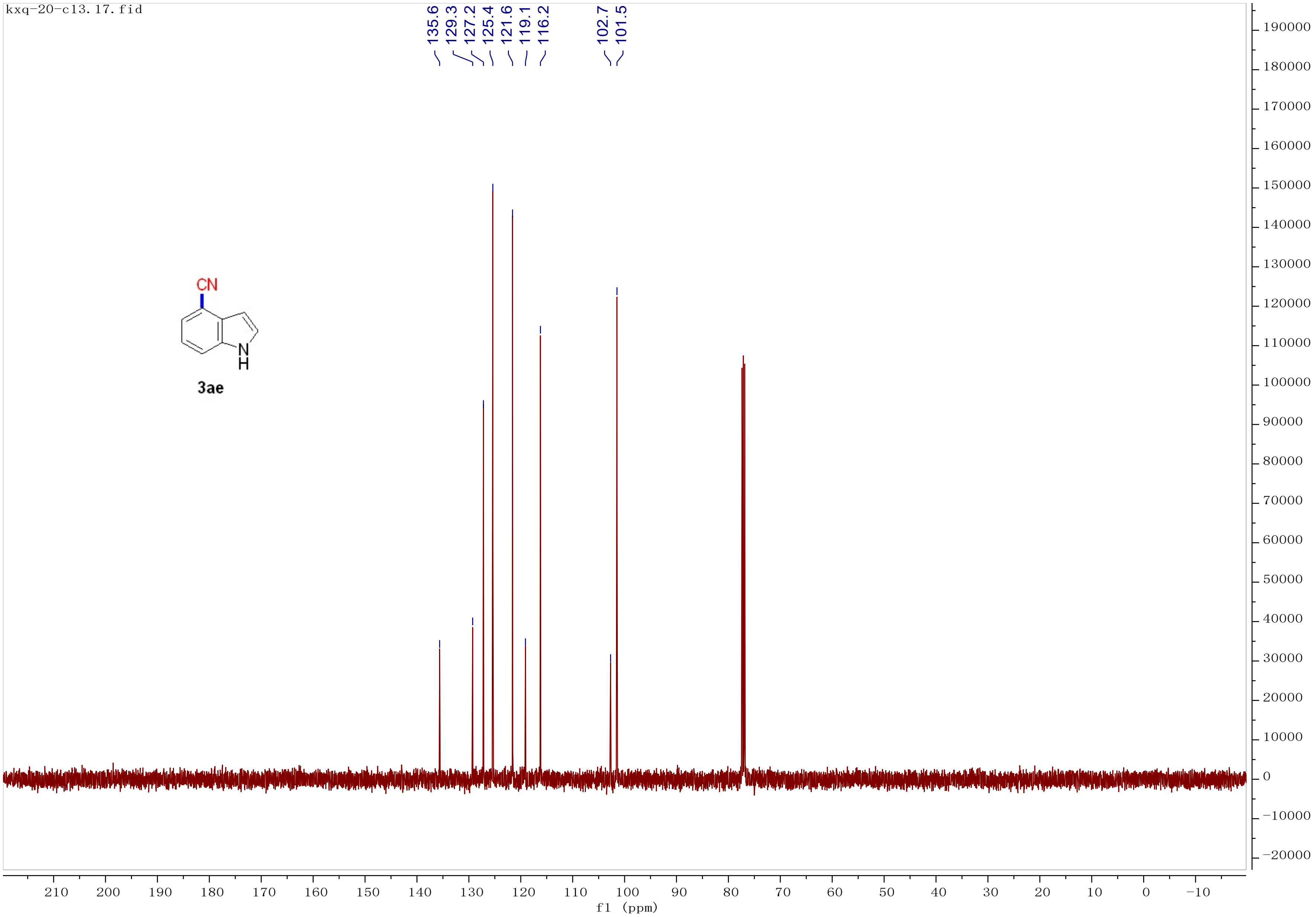

kxq-26-h.1.fid
9.05
9.04
8.55
8.55
8.19
8.18
8.18
8.18
8.17
7.92
7.92
7.92
7.91
7.91
7.91
7.90
7.90
7.89
7.89
7.72
7.72
7.71
7.71
7.69
7.69
CN
N
1.00
1.05
1.09
2.22
1.11
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
f1 (ppm)
2.6×10^7
2.4×10^7
2.2×10^7
2.0×10^7
1.8×10^7
1.6×10^7
1.4×10^7
1.2×10^7
1.0×10^7
8.0×10^6
6.0×10^6
4.0×10^6
2.0×10^6
0.0
−2.0×10^6

3ad


kxq-26-c13.2.fid
149.7
148.8
141.5
132.8
129.9
128.5
128.3
126.2
117.1
106.6
CN
N
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
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)

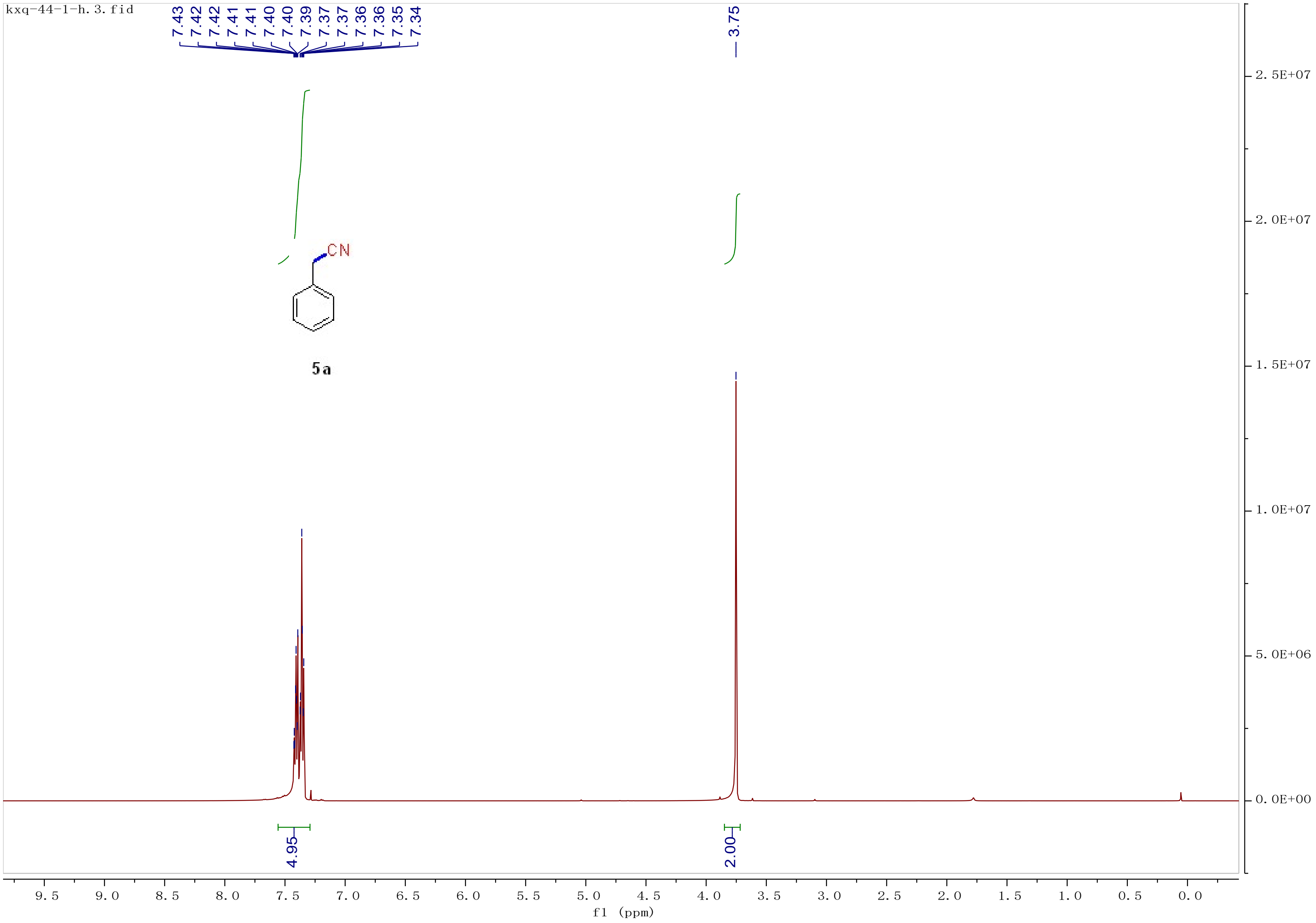
3ad

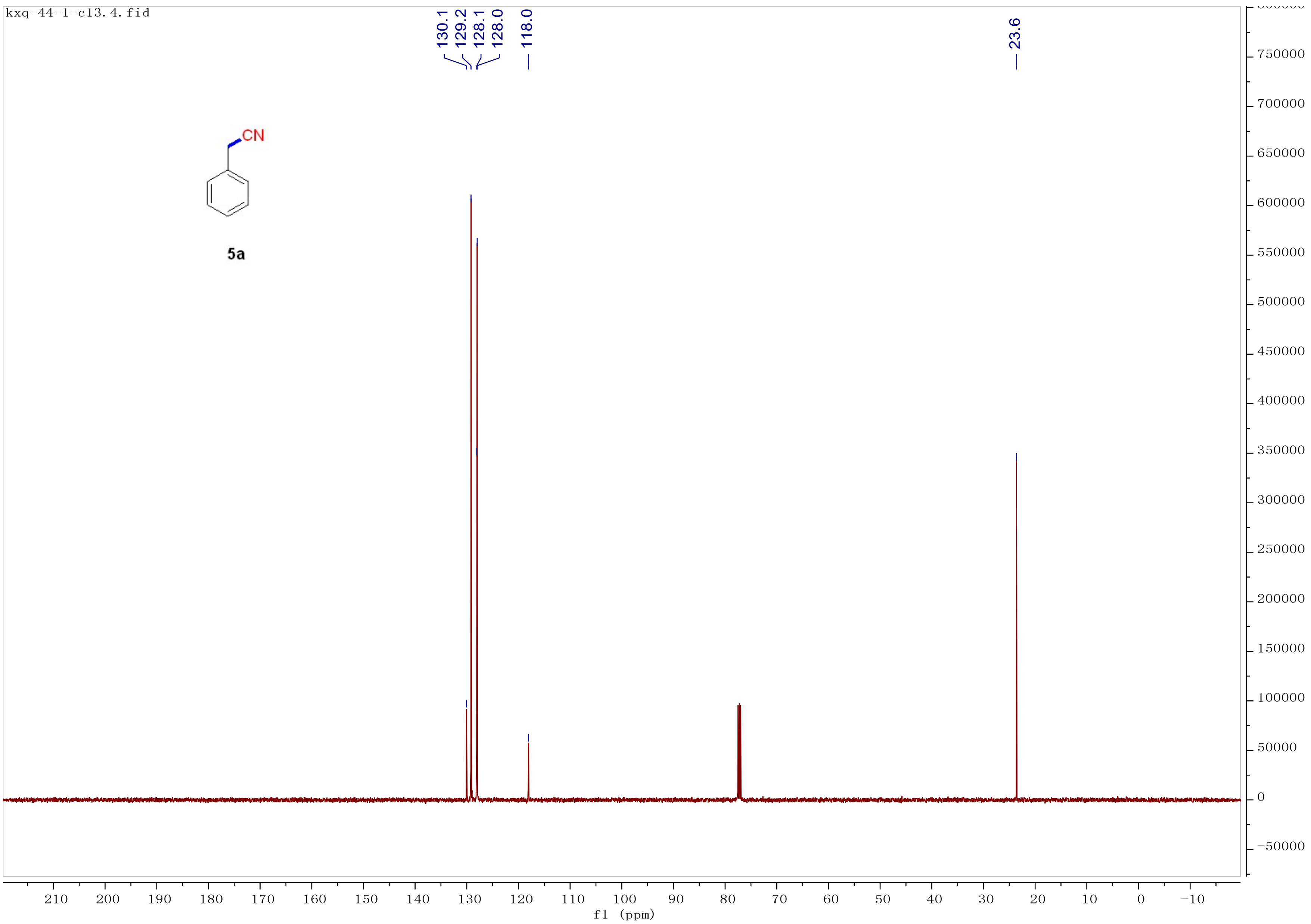

kxq-20-h.10.fid
8.89
8.88
7.70
7.69
7.51
7.50
7.44
7.44
7.43
7.28
7.27
7.26
7.24
6.79
6.79
6.78
6.78
6.78
CN
N
H
3ae
0.97
1.00
0.94
0.93
0.98
0.89
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)
22000000
21000000
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
-2000000

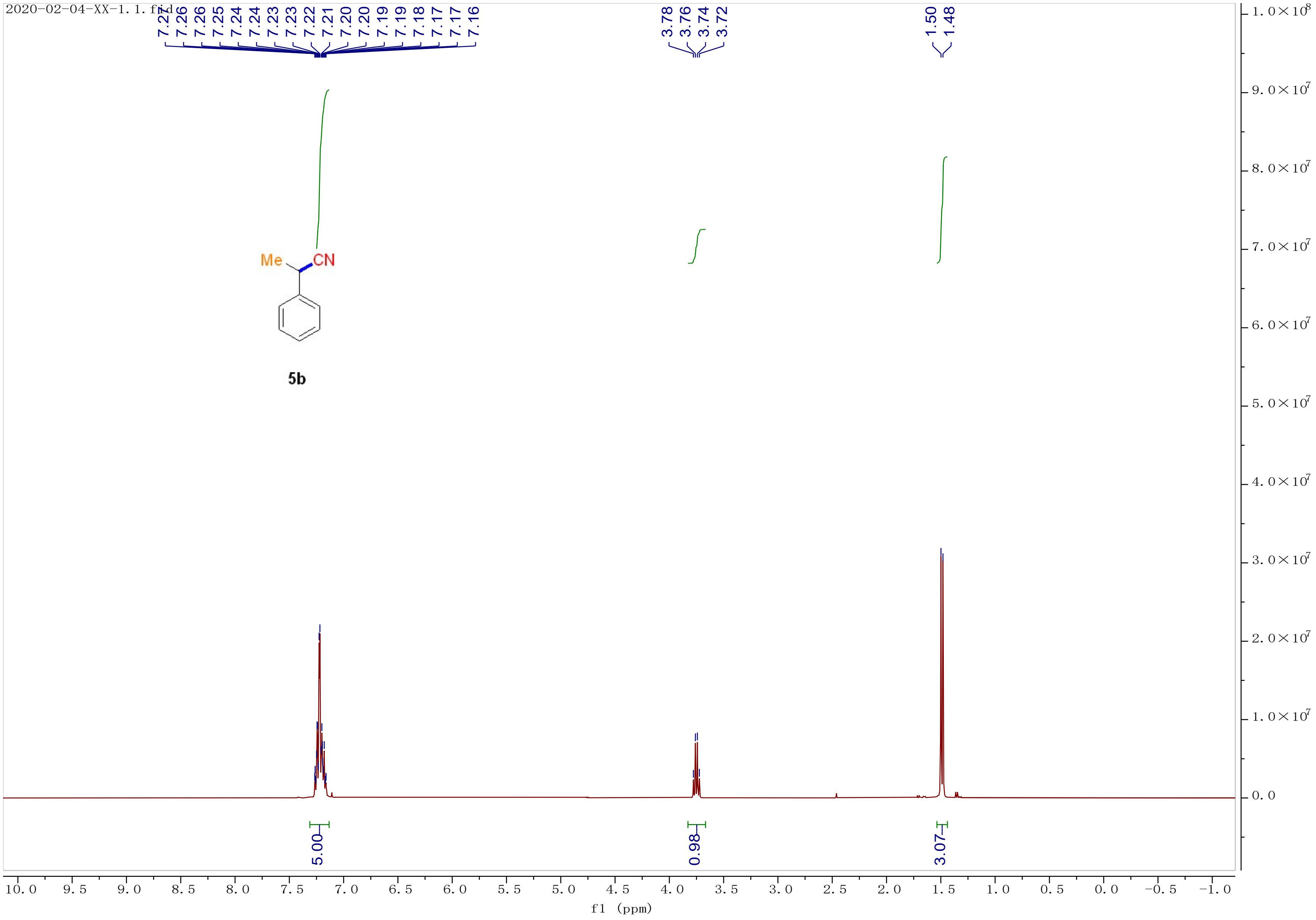


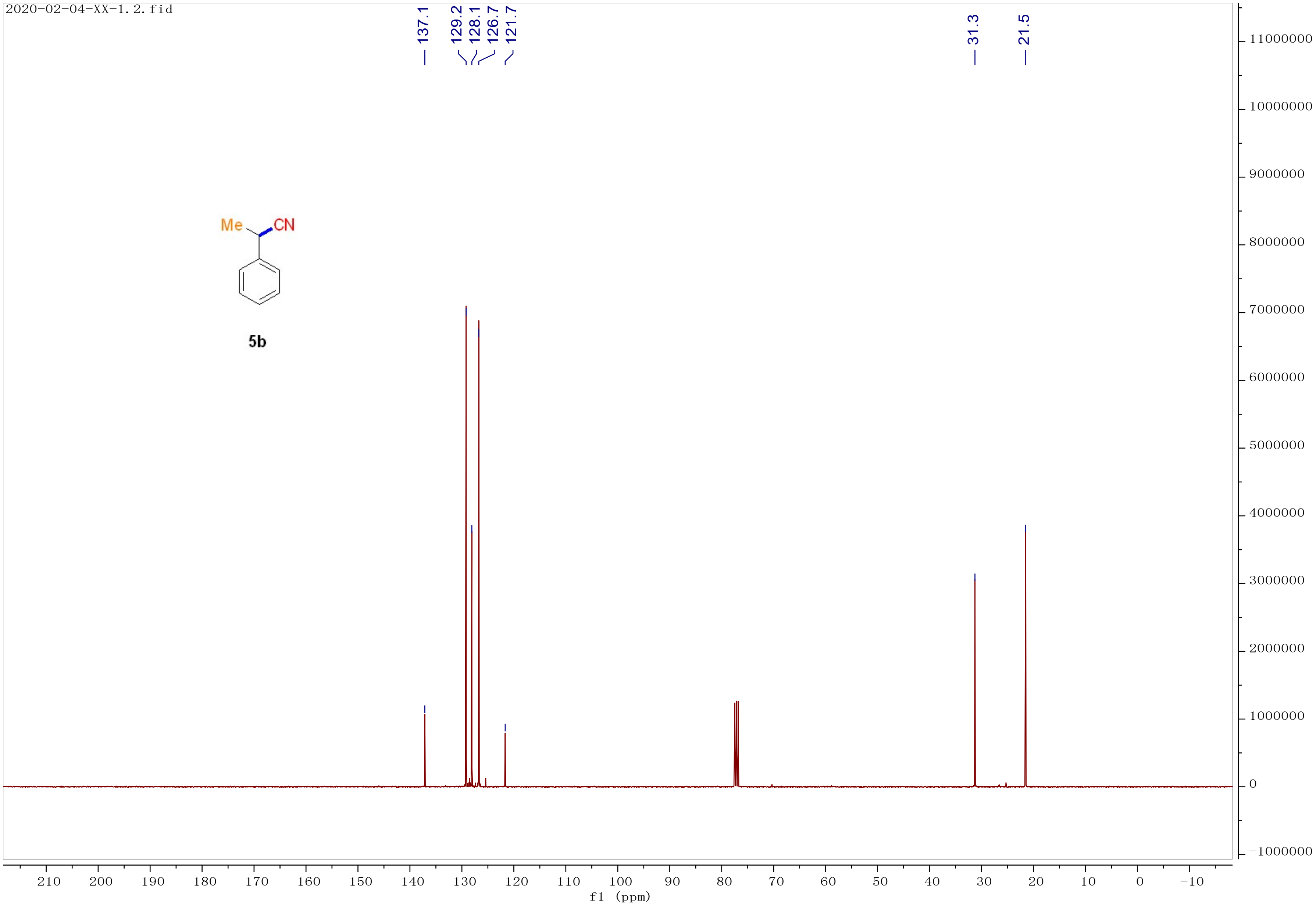
3ae

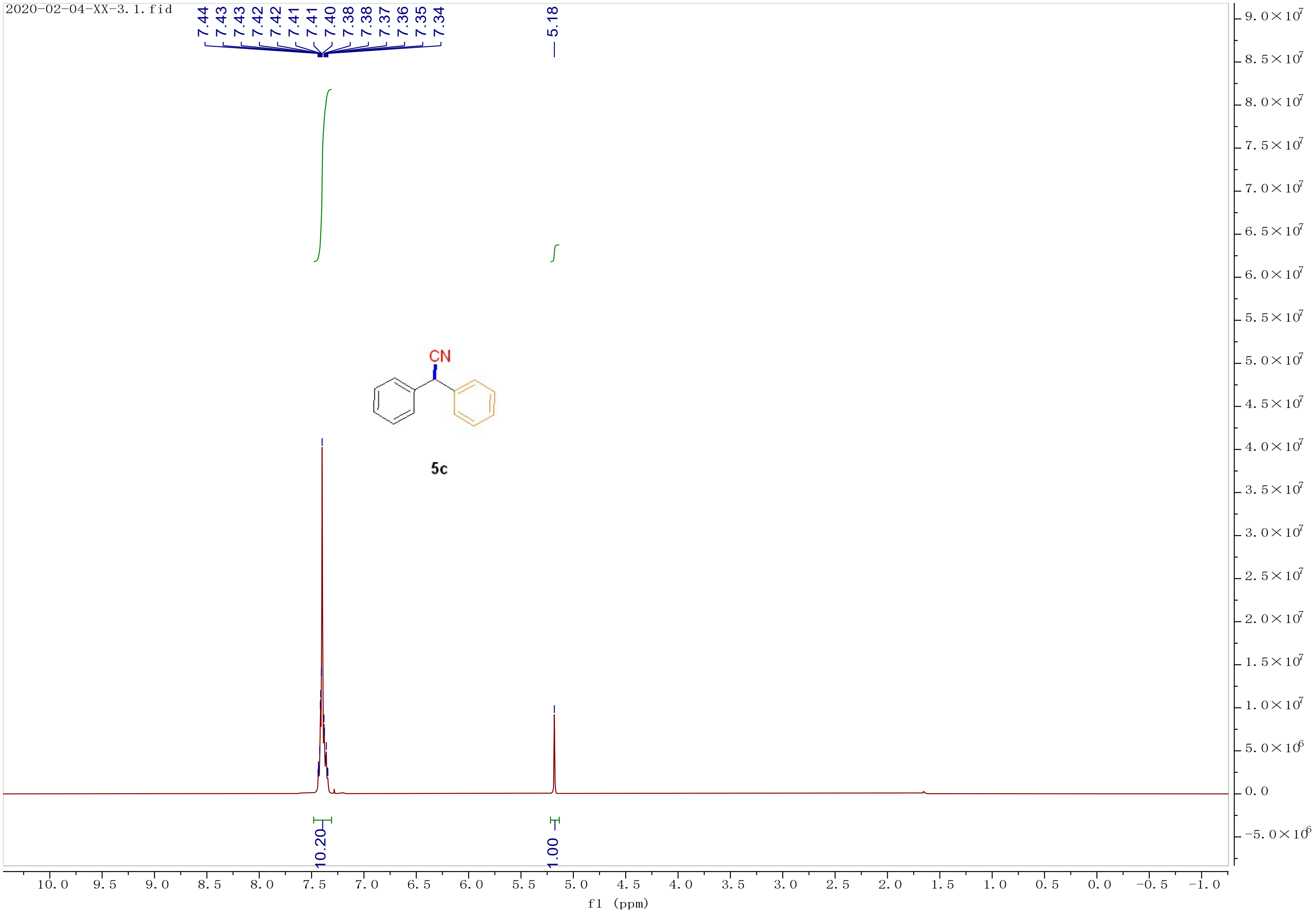
kxq-20-c13.17.fid
135.6
129.3
127.2
125.4
121.6
119.1
116.2
102.7
101.5
CN
N
H
190000
180000
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
−20000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


kxq-44-1-h.3.fid
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.39
7.37
7.37
7.36
7.36
7.35
7.34
3.75
CN
5a
4.95
2.00
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+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)

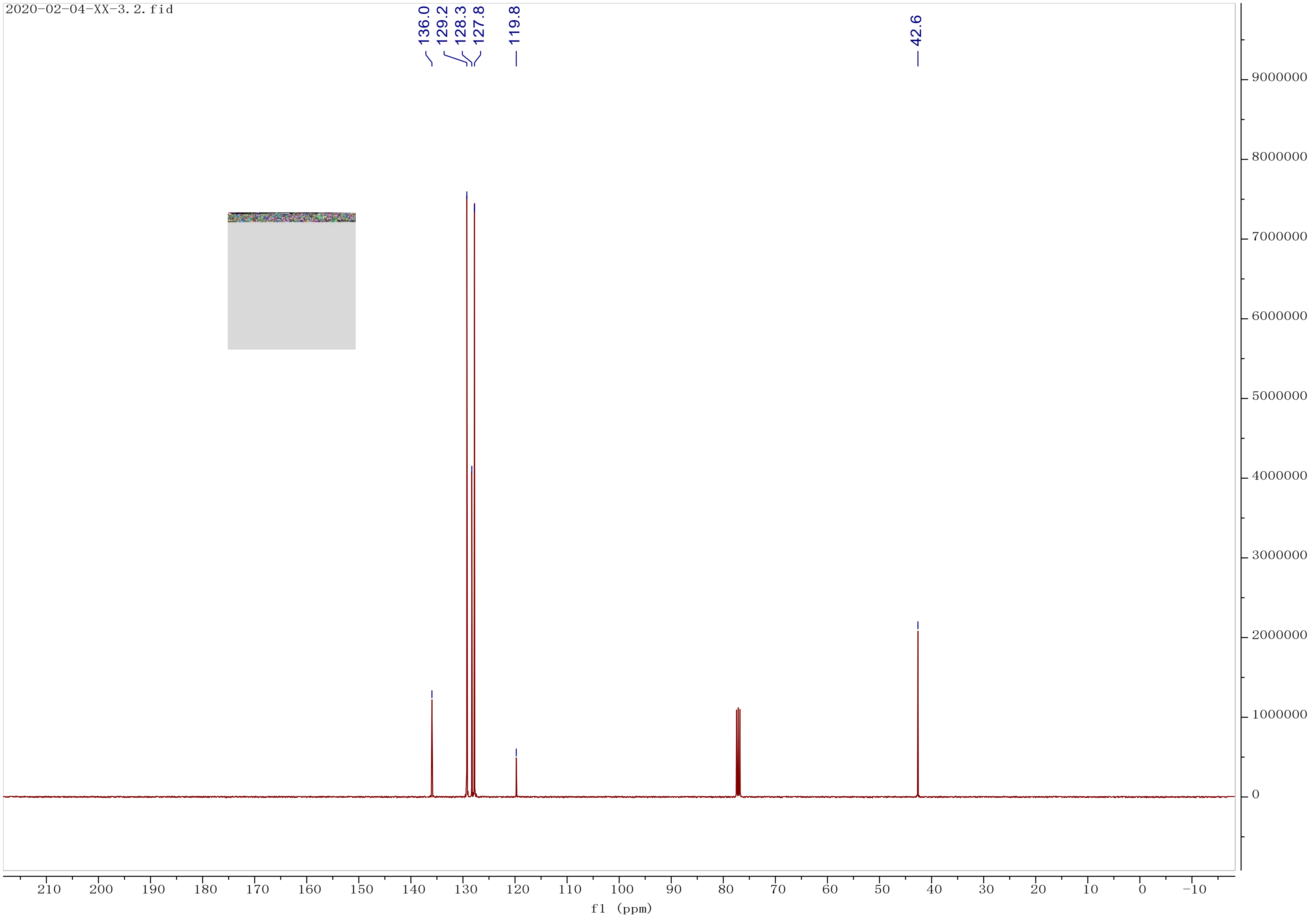

kxq-44-1-c13.4.fid
130.1
129.2
128.1
128.0
118.0
23.6
CN
5a
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
−50000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

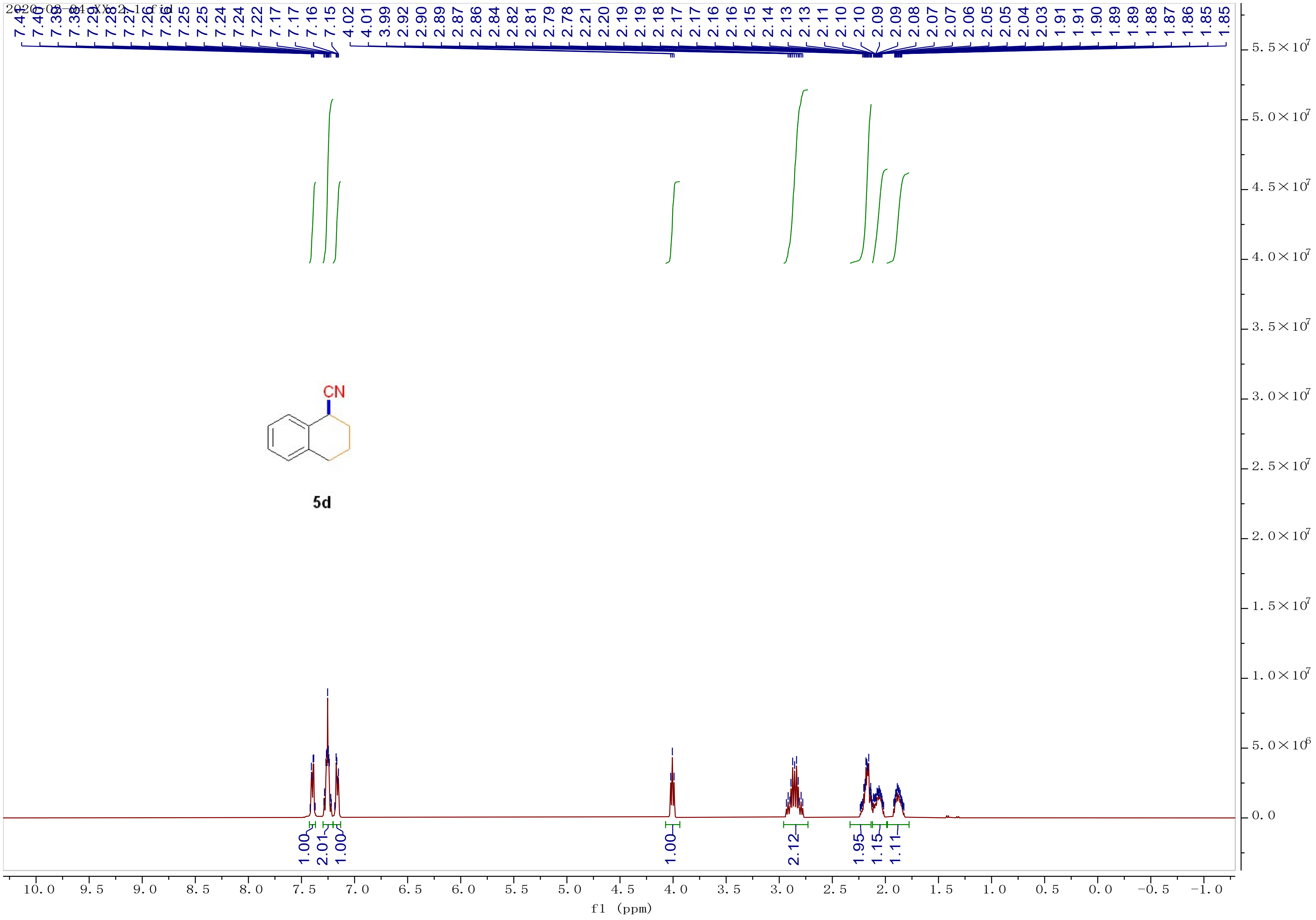

2020-02-04-XX-1.1.fid
7.27
7.26
7.26
7.25
7.24
7.24
7.23
7.23
7.22
7.21
7.20
7.20
7.19
7.19
7.18
7.17
7.17
7.16
3.78
3.76
3.74
3.72
1.50
1.48
Me
CN
5b
5.00
0.98
3.07
1.0×10^8
9.0×10^7
8.0×10^7
7.0×10^7
6.0×10^7
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

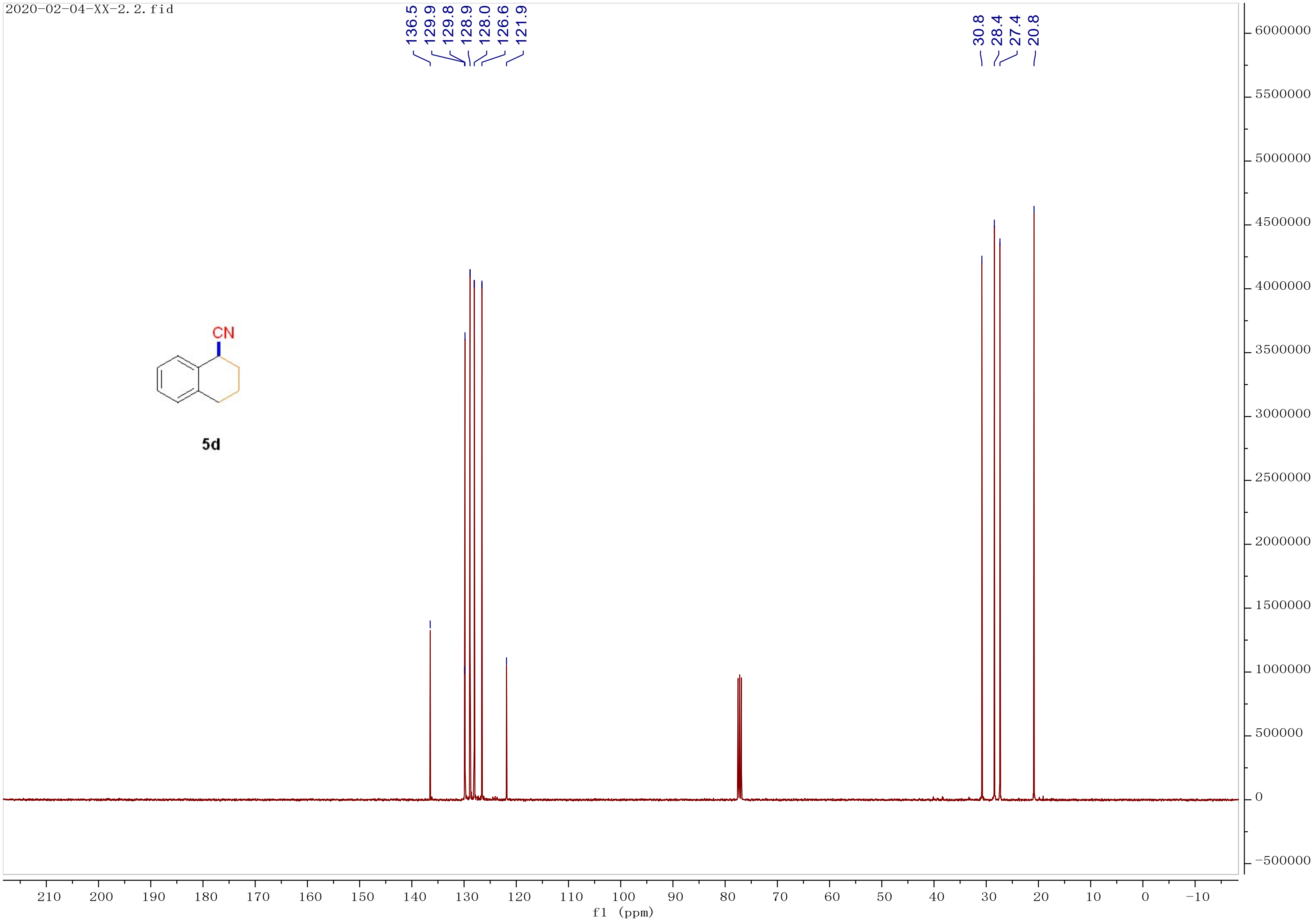

2020-02-04-XX-1.2.fid
137.1
129.2
128.1
126.7
121.7
31.3
21.5
Me
CN
5b
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
−1000000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


2020-02-04-XX-3.1.fid
7.44
7.43
7.43
7.42
7.42
7.41
7.41
7.40
7.38
7.38
7.37
7.36
7.35
7.34
5.18
CN
10.20
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
9.0×10^7
8.5×10^7
8.0×10^7
7.5×10^7
7.0×10^7
6.5×10^7
6.0×10^7
5.5×10^7
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
-5.0×10^6

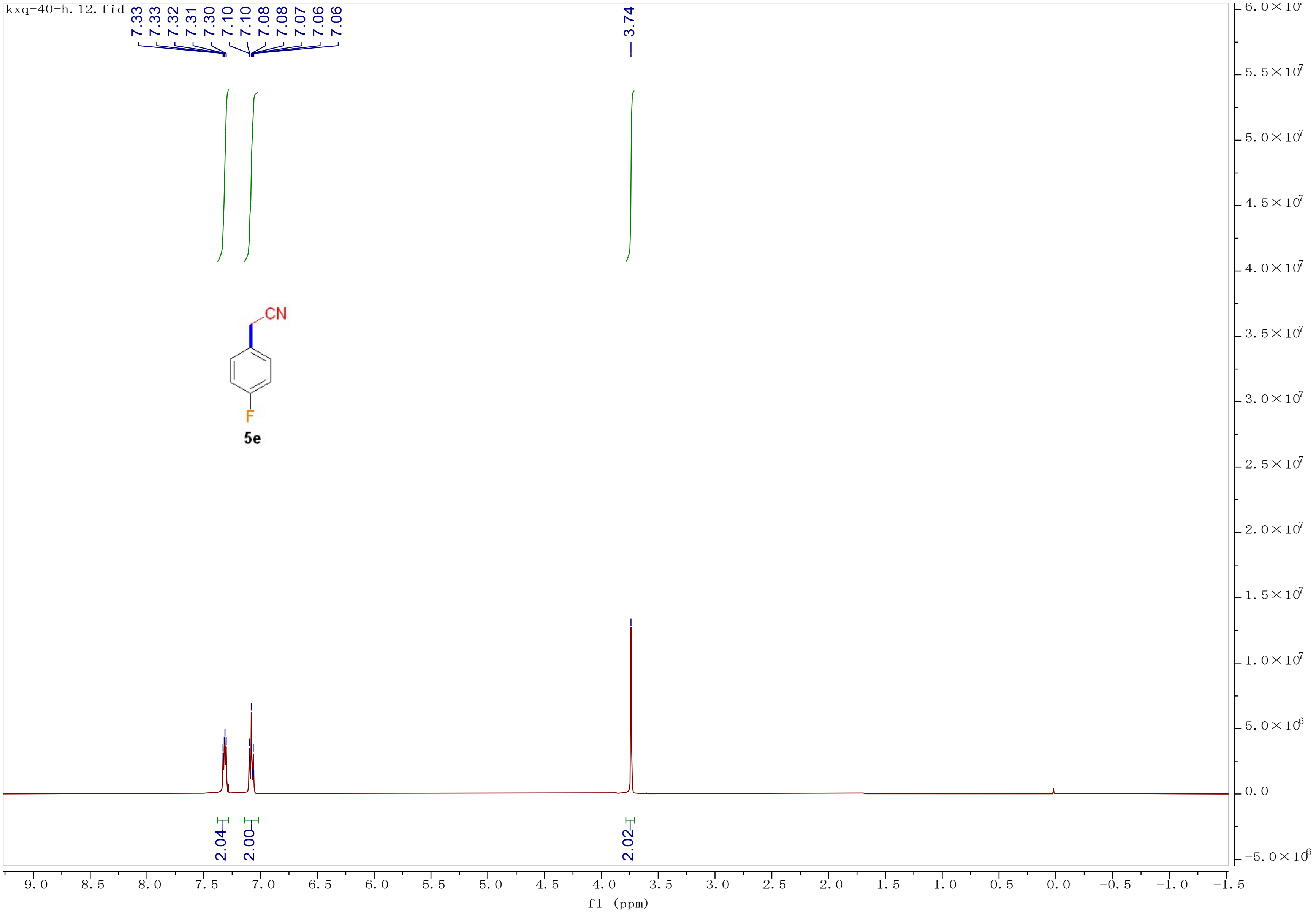
5c

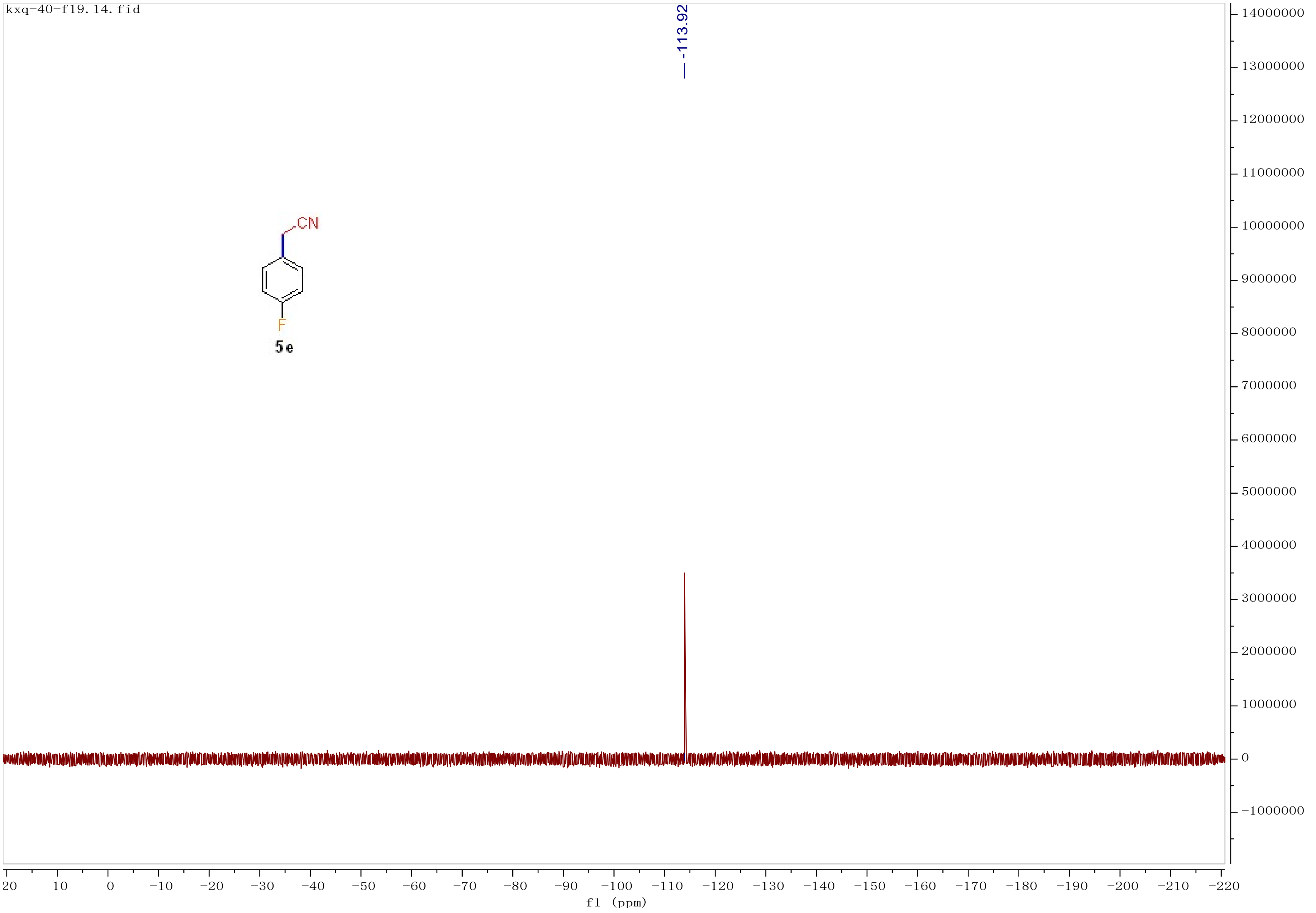

2020-02-04-XX-3.2.fid
136.0
129.2
128.3
127.8
119.8
42.6
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

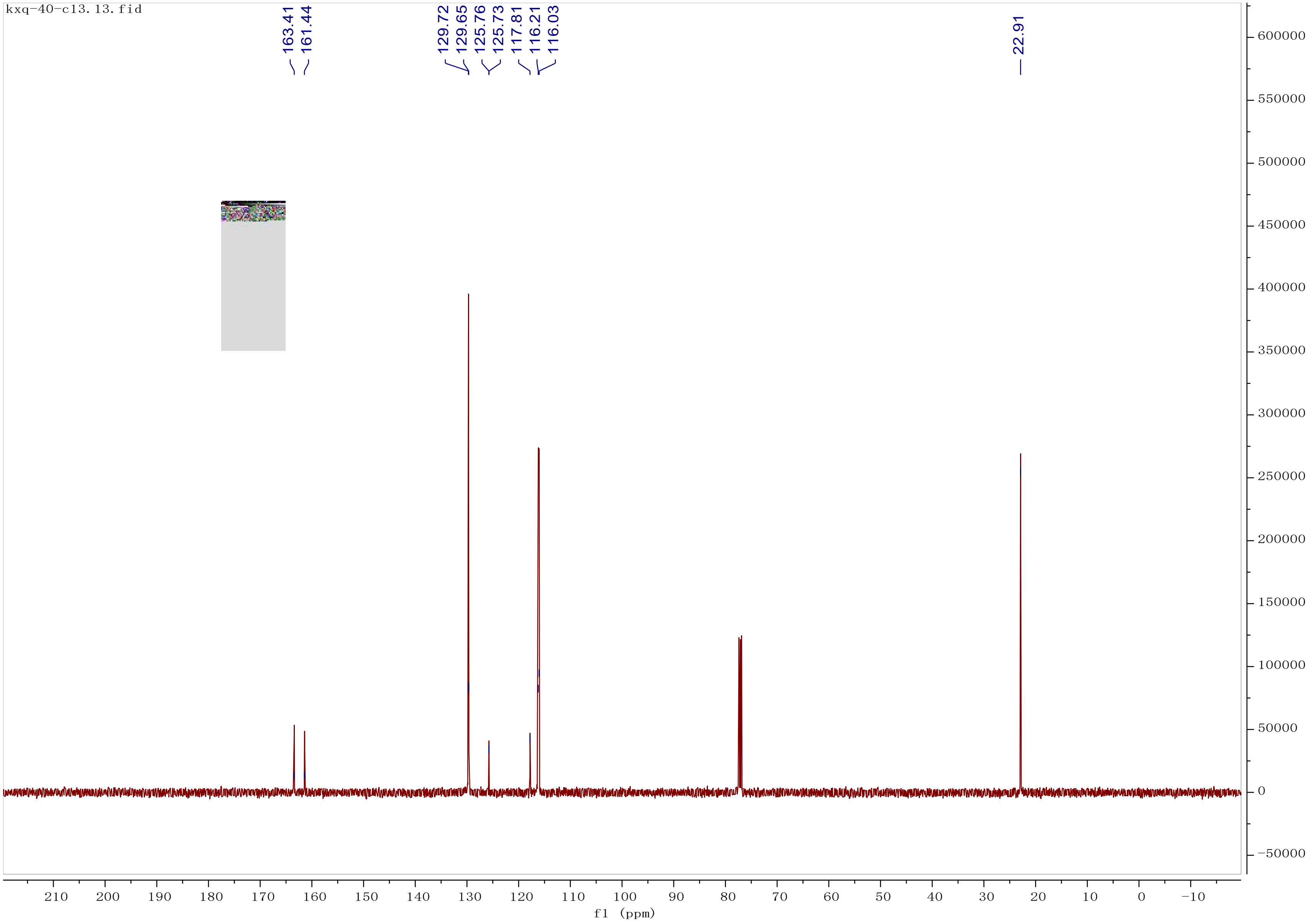

2020-08-04-XX-2.1c.fid
7.41
7.40
7.39
7.38
7.29
7.28
7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.22
7.17
7.17
7.16
7.15
4.02
4.01
3.99
2.92
2.90
2.89
2.87
2.86
2.84
2.82
2.81
2.79
2.78
2.21
2.20
2.19
2.19
2.18
2.17
2.17
2.16
2.15
2.14
2.13
2.13
2.11
2.10
2.09
2.09
2.08
2.07
2.07
2.06
2.05
2.05
2.04
2.03
1.91
1.91
1.90
1.89
1.89
1.88
1.87
1.86
1.85
1.85
CN
5d
1.00
2.01
1.00
1.00
2.12
1.95
1.15
1.11
5.5×10^7
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

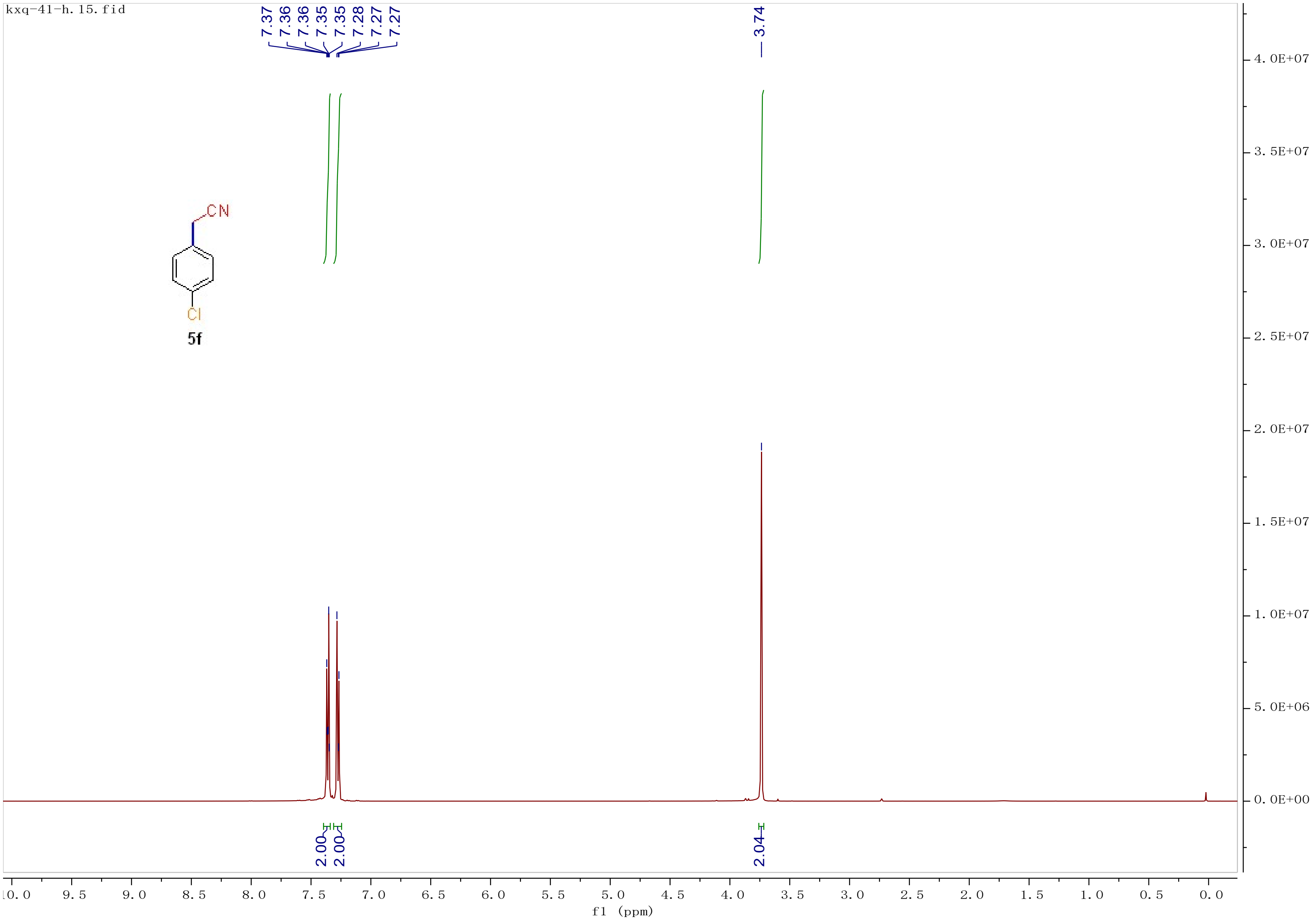

2020-02-04-XX-2.2.fid
136.5
129.9
129.8
128.9
128.0
126.6
121.9
30.8
28.4
27.4
20.8
CN
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
-500000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

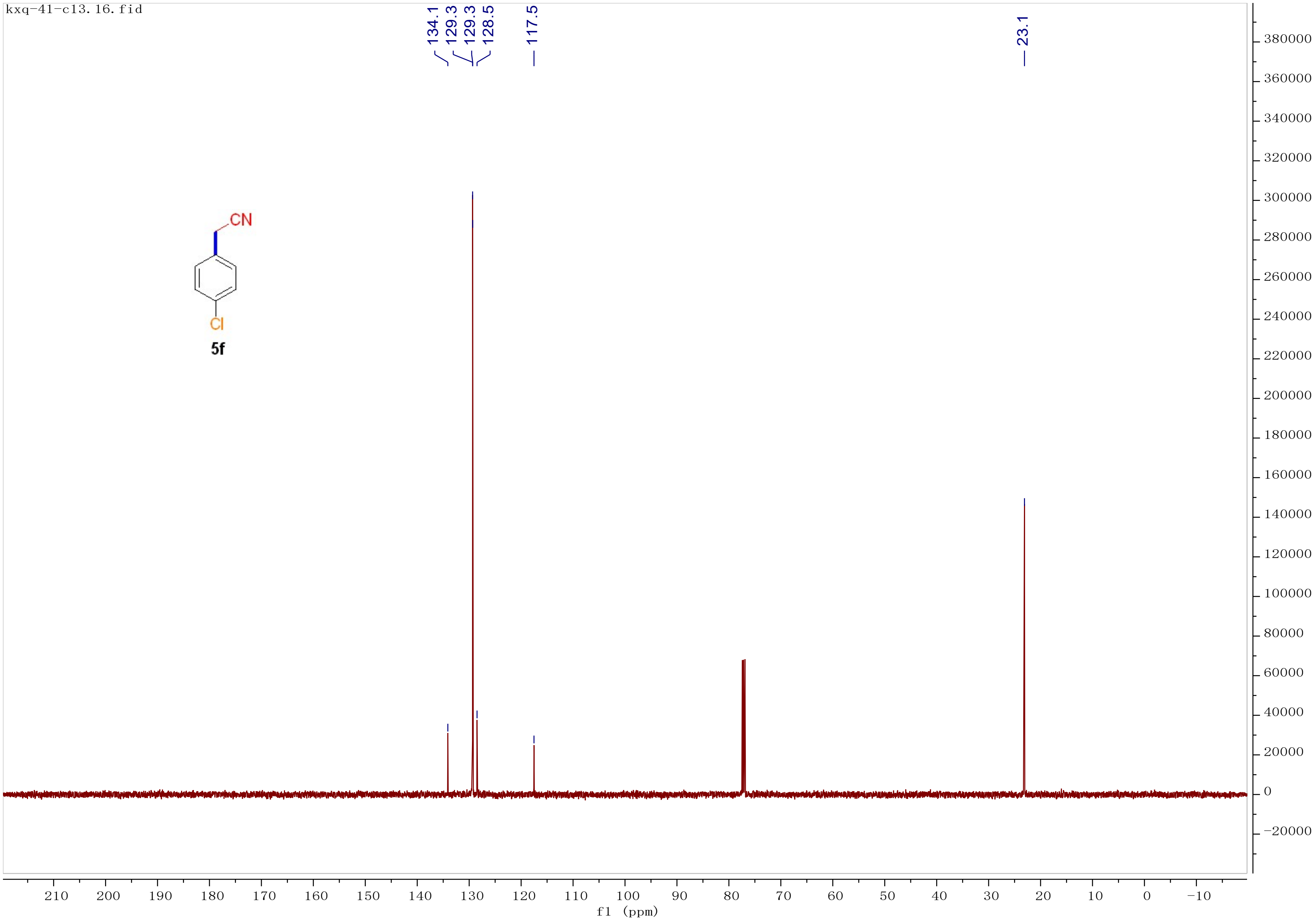
5d

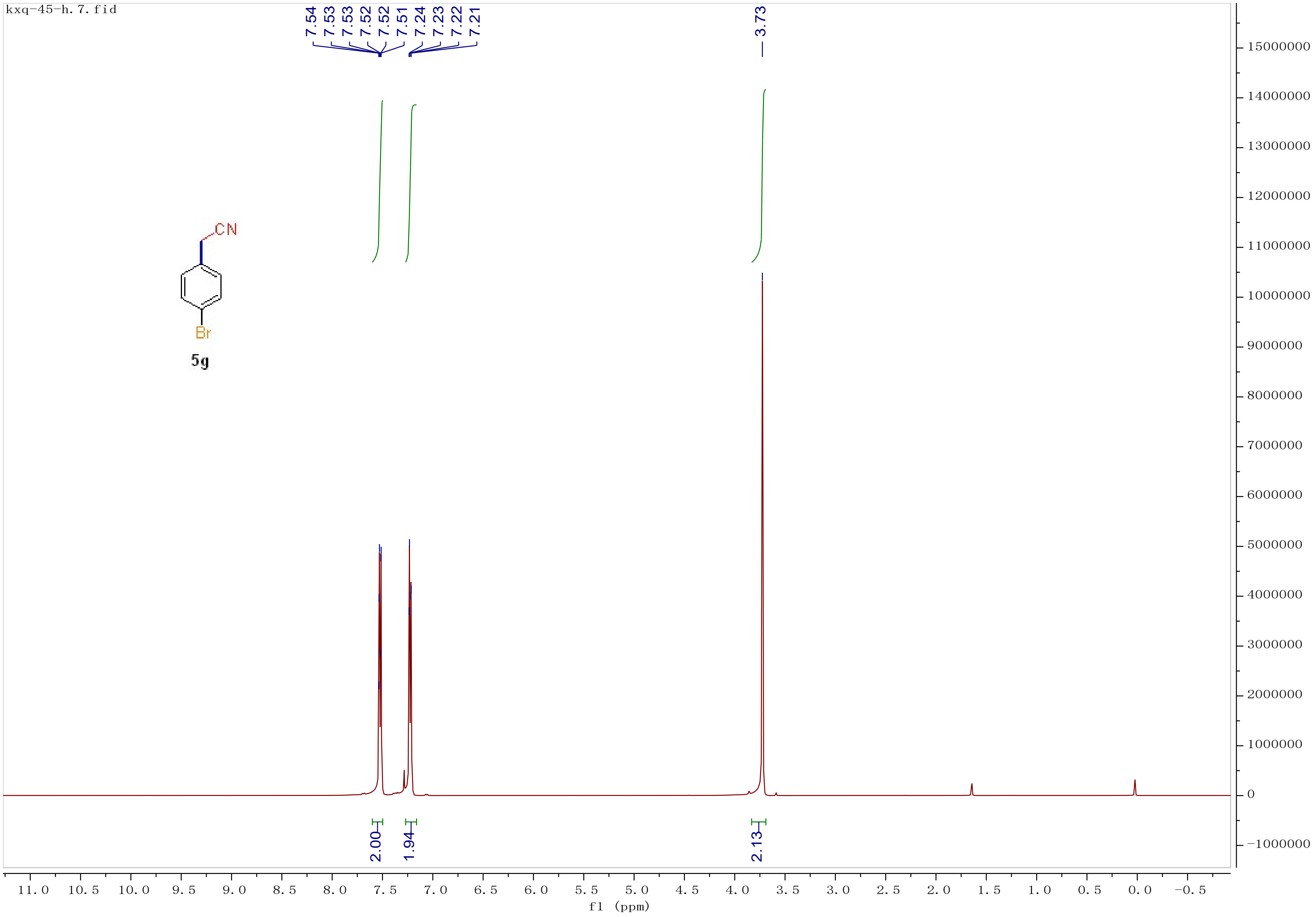

kxq-40-h.12.fid
7.33
7.33
7.32
7.31
7.30
7.10
7.10
7.08
7.08
7.07
7.06
7.06
3.74
CN
F
5e
2.04
2.00
2.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)
6.0×10^7
5.5×10^7
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
-5.0×10^6

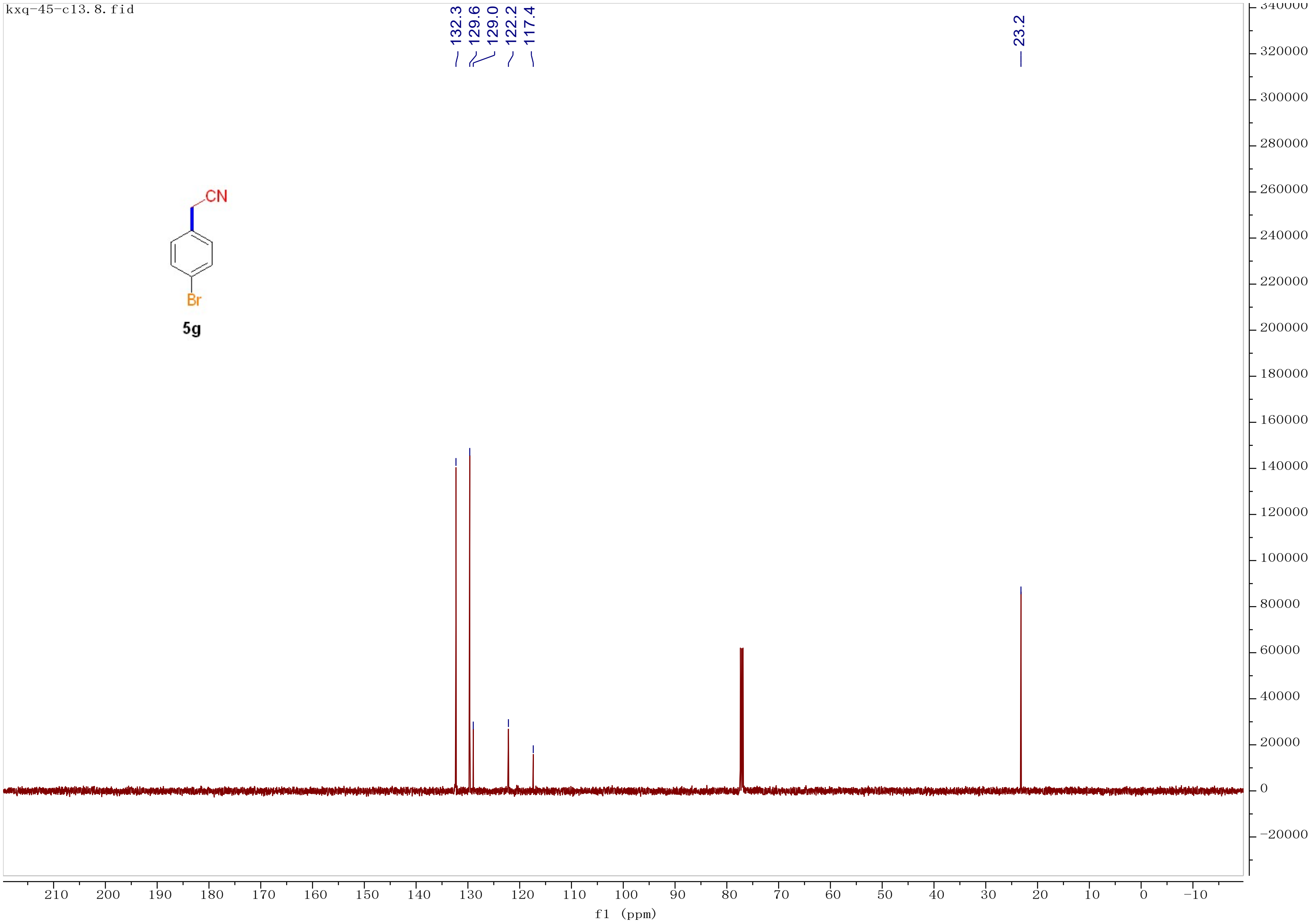

kxq-40-f19.14.fid
-113.92
CN
F
5e
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
−1000000
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
−220
f1 (ppm)


kxq-40-c13.13.fid
163.41
161.44
129.72
129.65
125.76
125.73
117.81
116.21
116.03
22.91
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
−50000
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)

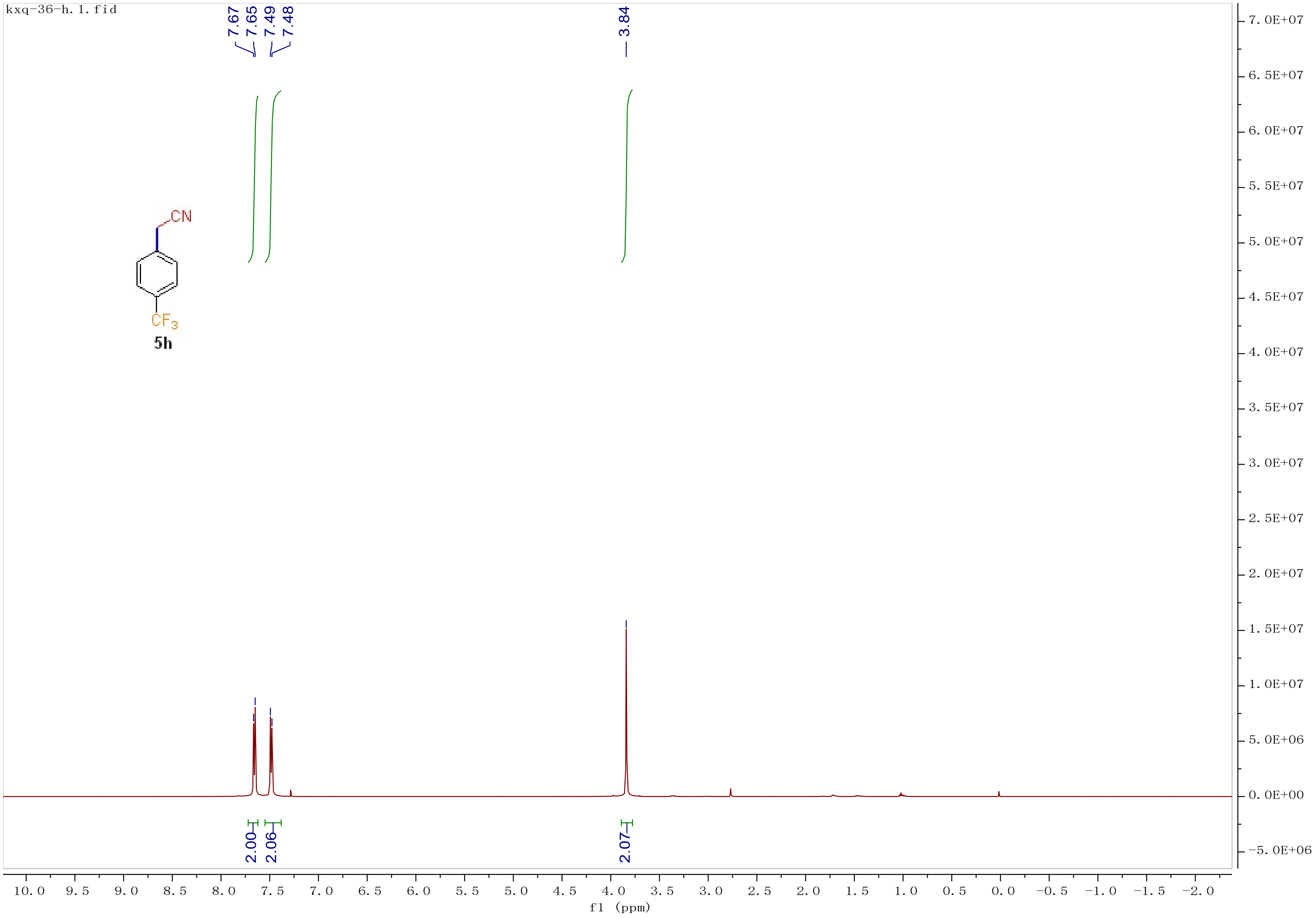

kxq-41-h.15.fid
7.37
7.36
7.36
7.35
7.35
7.28
7.27
7.27
3.74
CN
Cl
5f
2.00
2.00
2.04
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

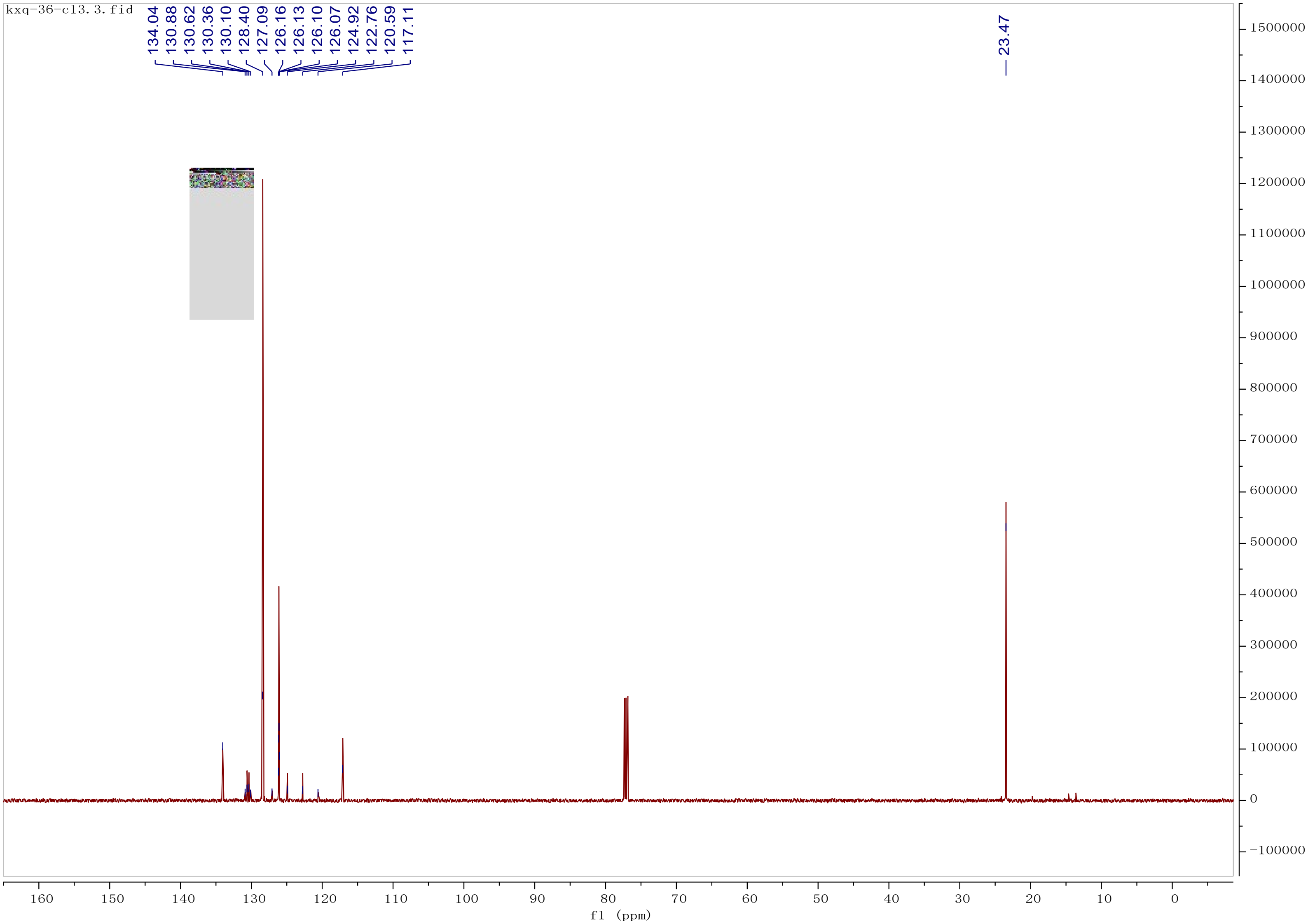

kxq-41-c13.16.fid
134.1
129.3
129.3
128.5
117.5
23.1
CN
Cl
5f
380000
360000
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

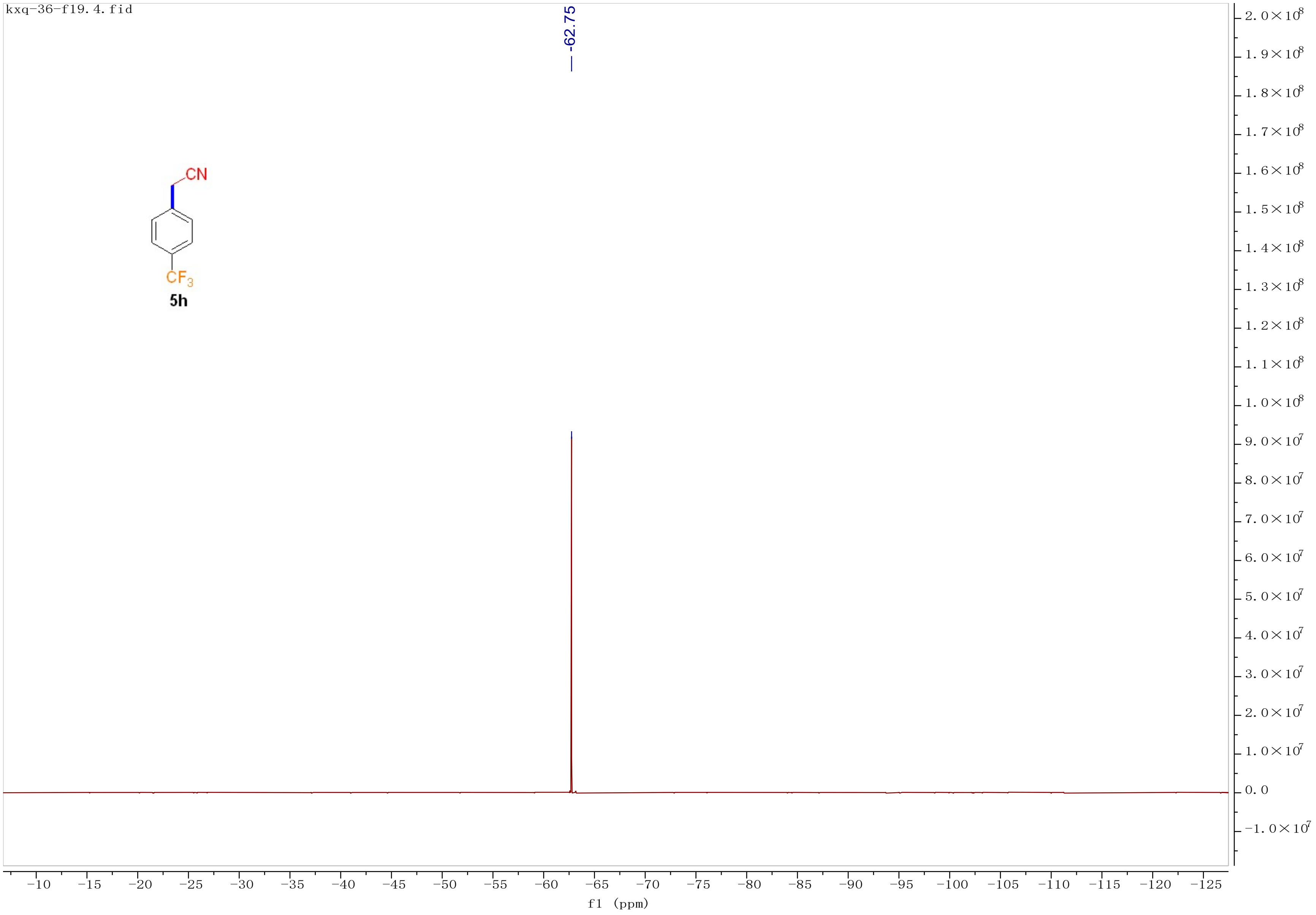

kxq-45-h.7.fid
7.54
7.53
7.53
7.52
7.52
7.51
7.24
7.23
7.22
7.21
3.73
CN
Br
5g
2.00
1.94
2.13
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
−1000000
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

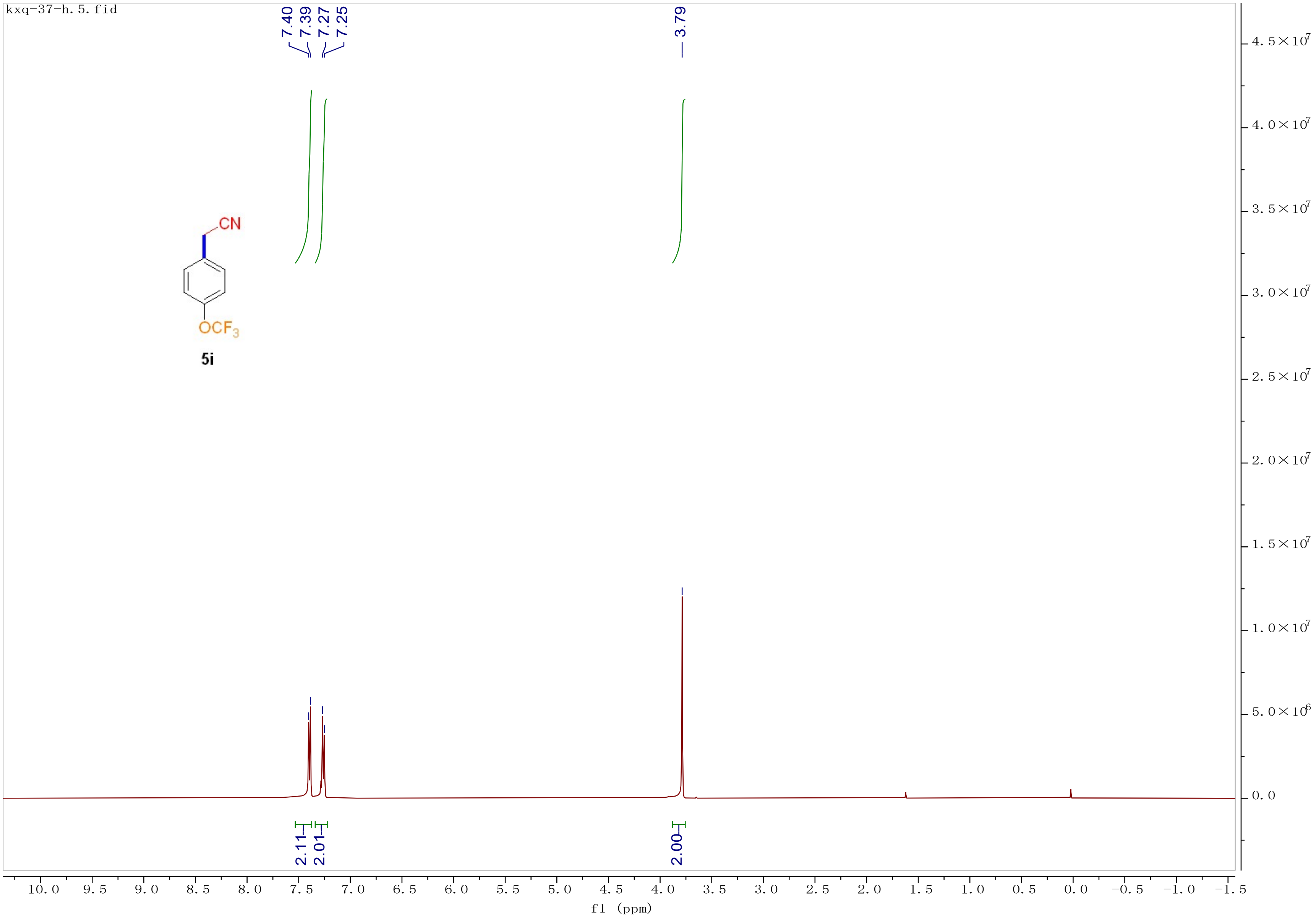

kxq-45-c13.8.fid
132.3
129.6
129.0
122.2
117.4
23.2
CN
Br
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
−20000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

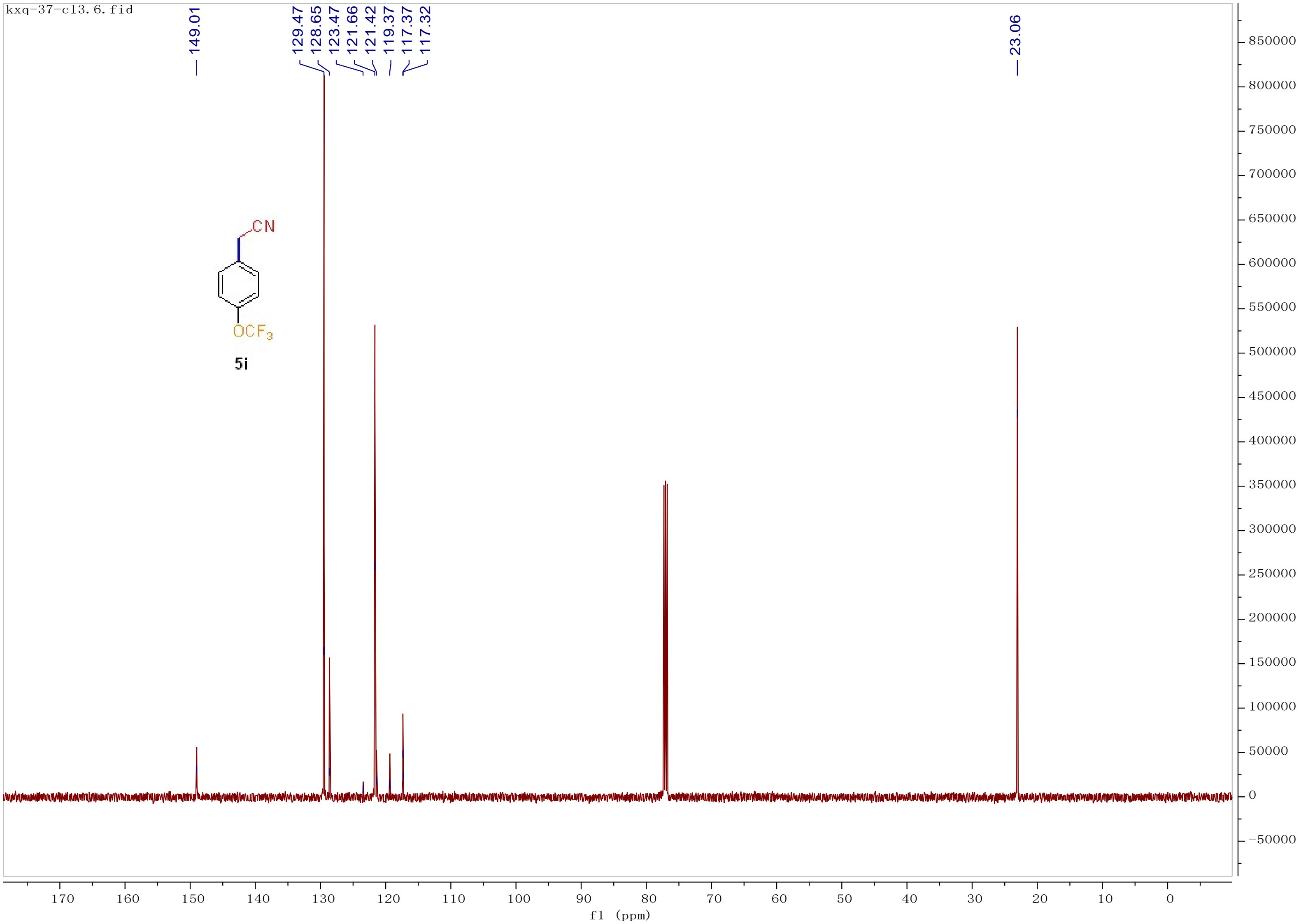
5g

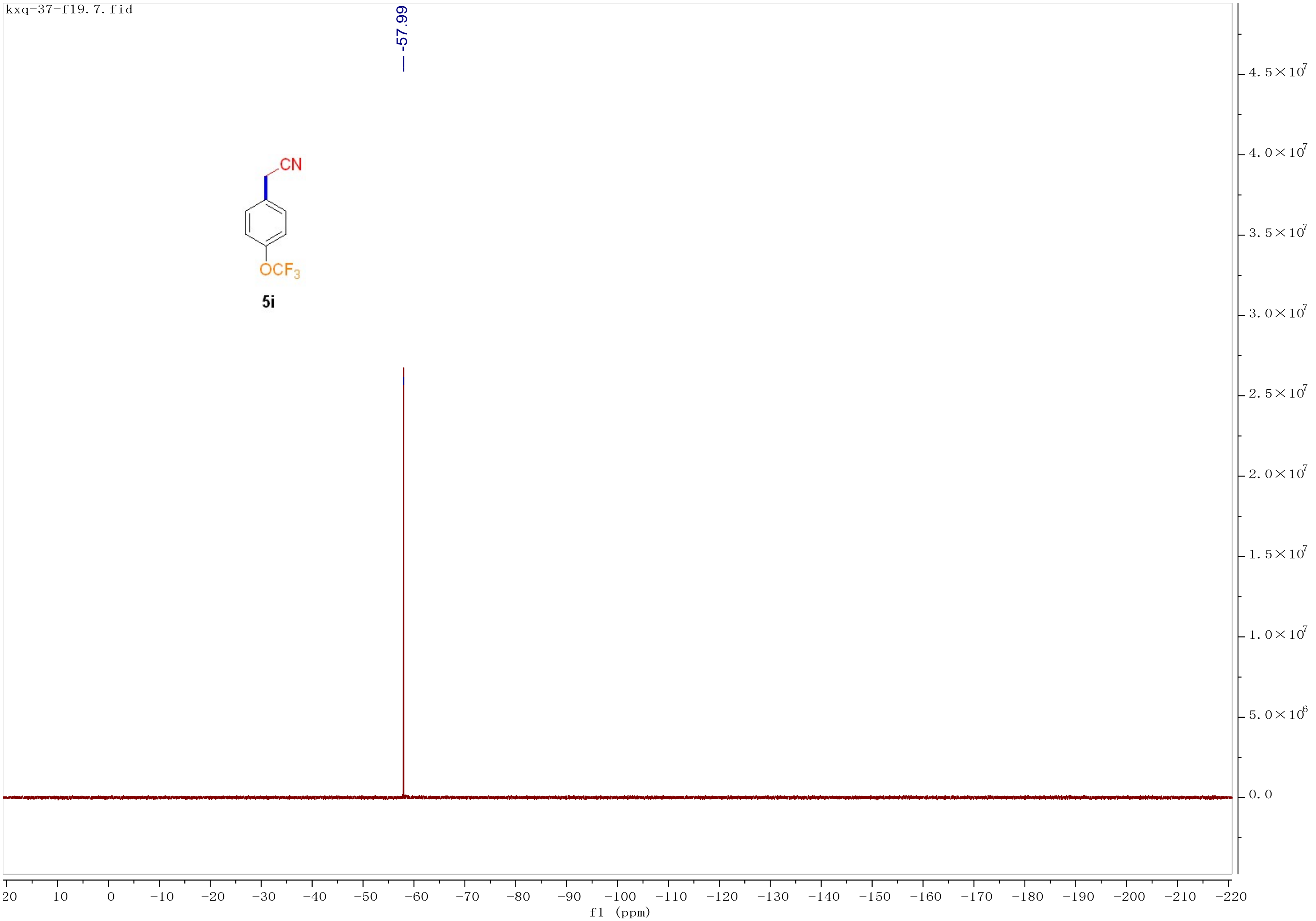

kxq-36-h.1.fid
7.67
7.65
7.49
7.48
3.84
CN
CF3
5h
2.00
2.06
2.07
7.0E+07
6.5E+07
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
-5.0E+06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
f1 (ppm)


kxq-36-c13.3.fid
134.04
130.88
130.62
130.36
130.10
128.40
127.09
126.16
126.13
126.10
126.07
124.92
122.76
120.59
117.11
23.47
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
−100000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

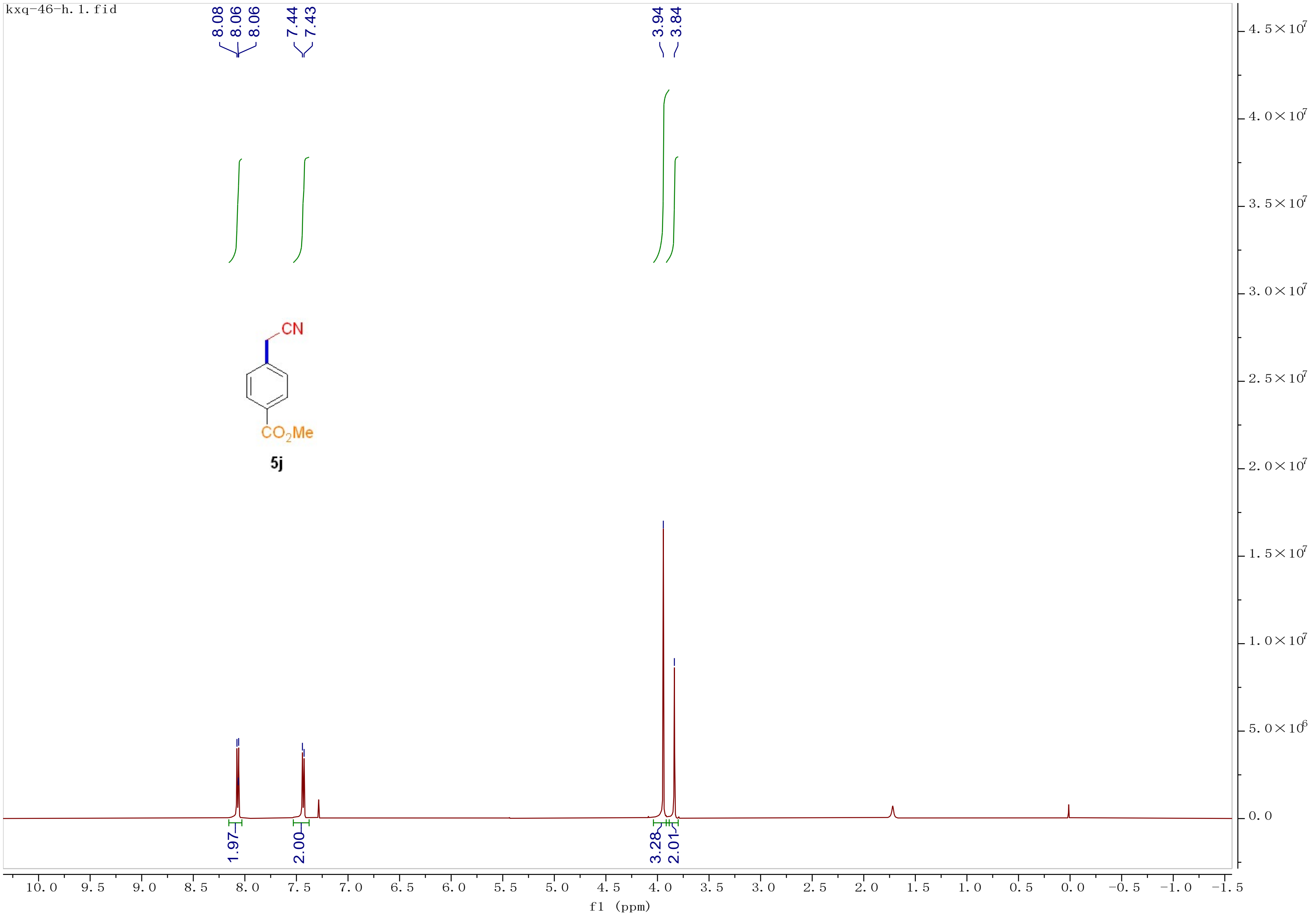

kxq-36-f19.4.fid
-62.75
CN
CF_3
5h
2.0×10^8
1.9×10^8
1.8×10^8
1.7×10^8
1.6×10^8
1.5×10^8
1.4×10^8
1.3×10^8
1.2×10^8
1.1×10^8
1.0×10^8
9.0×10^7
8.0×10^7
7.0×10^7
6.0×10^7
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
−1.0×10^7
−10 −15 −20 −25 −30 −35 −40 −45 −50 −55 −60 −65 −70 −75 −80 −85 −90 −95 −100 −105 −110 −115 −120 −125
f1 (ppm)

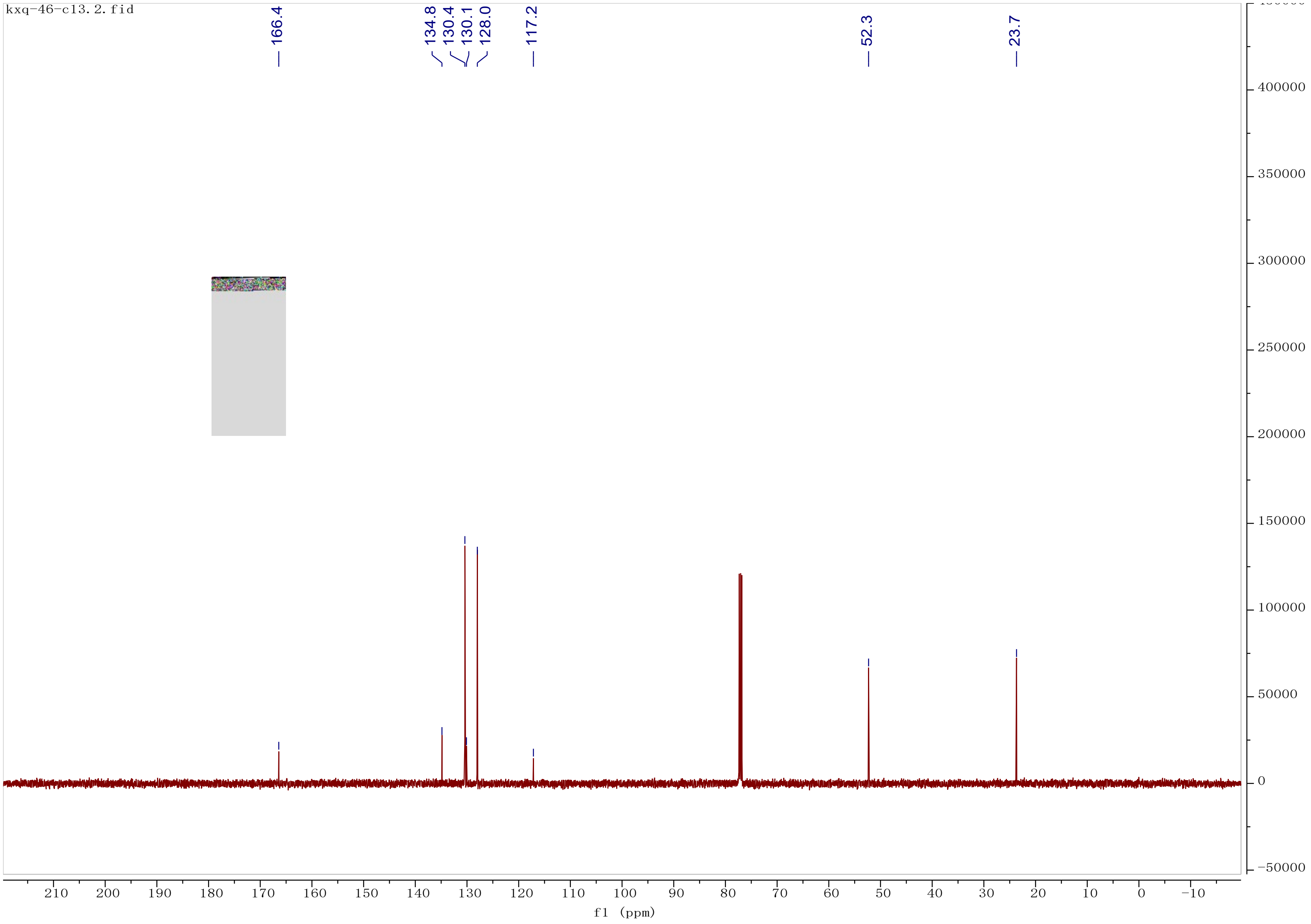

kxq-37-h.5.fid
7.40
7.39
7.27
7.25
3.79
CN
OCF$_3$
5i
2.11
2.01
2.00
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
f1 (ppm)

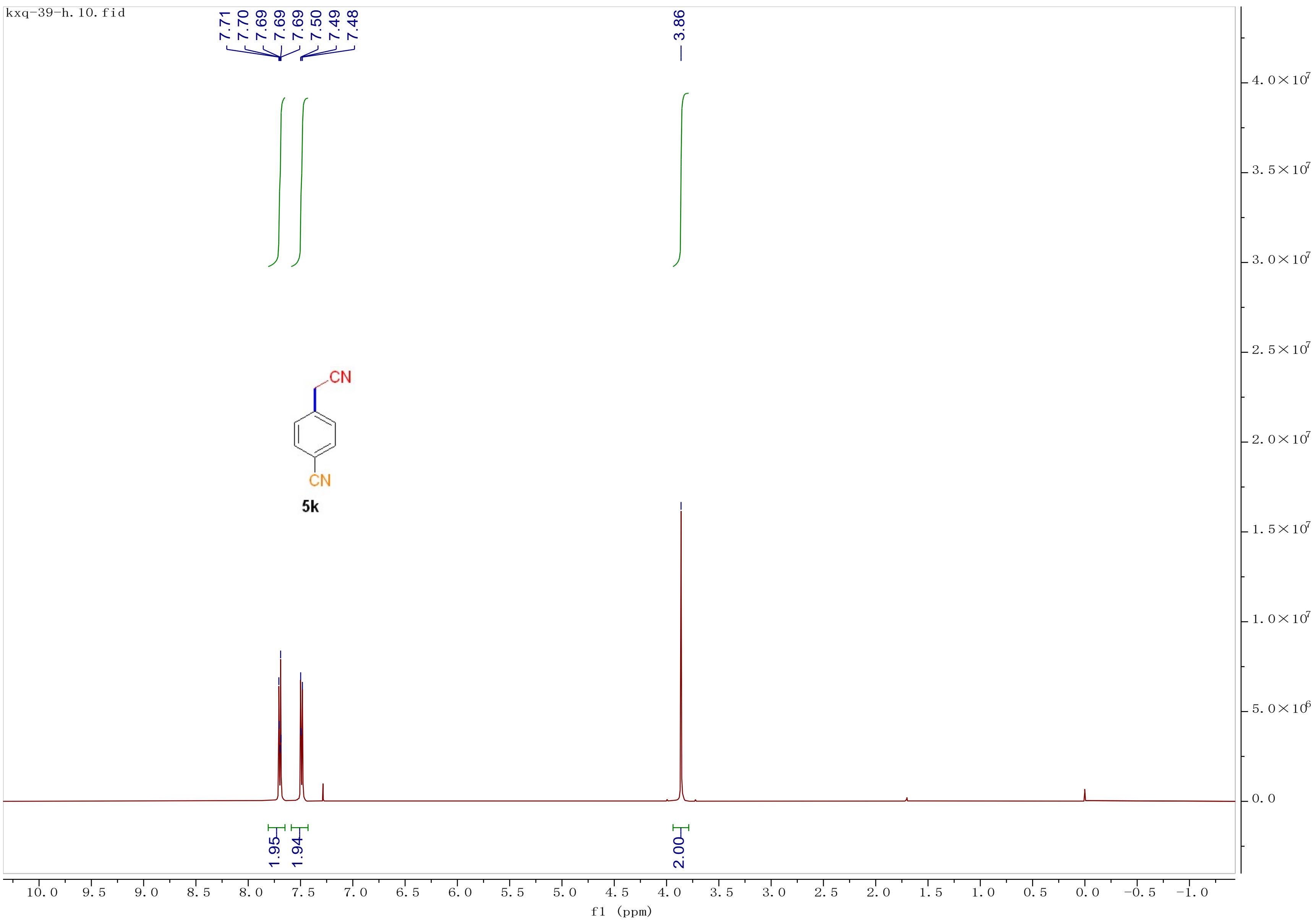

kxq-37-c13.6.fid
149.01
129.47
128.65
123.47
121.66
121.42
119.37
117.37
117.32
23.06
CN
OCF3
5i
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
−50000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

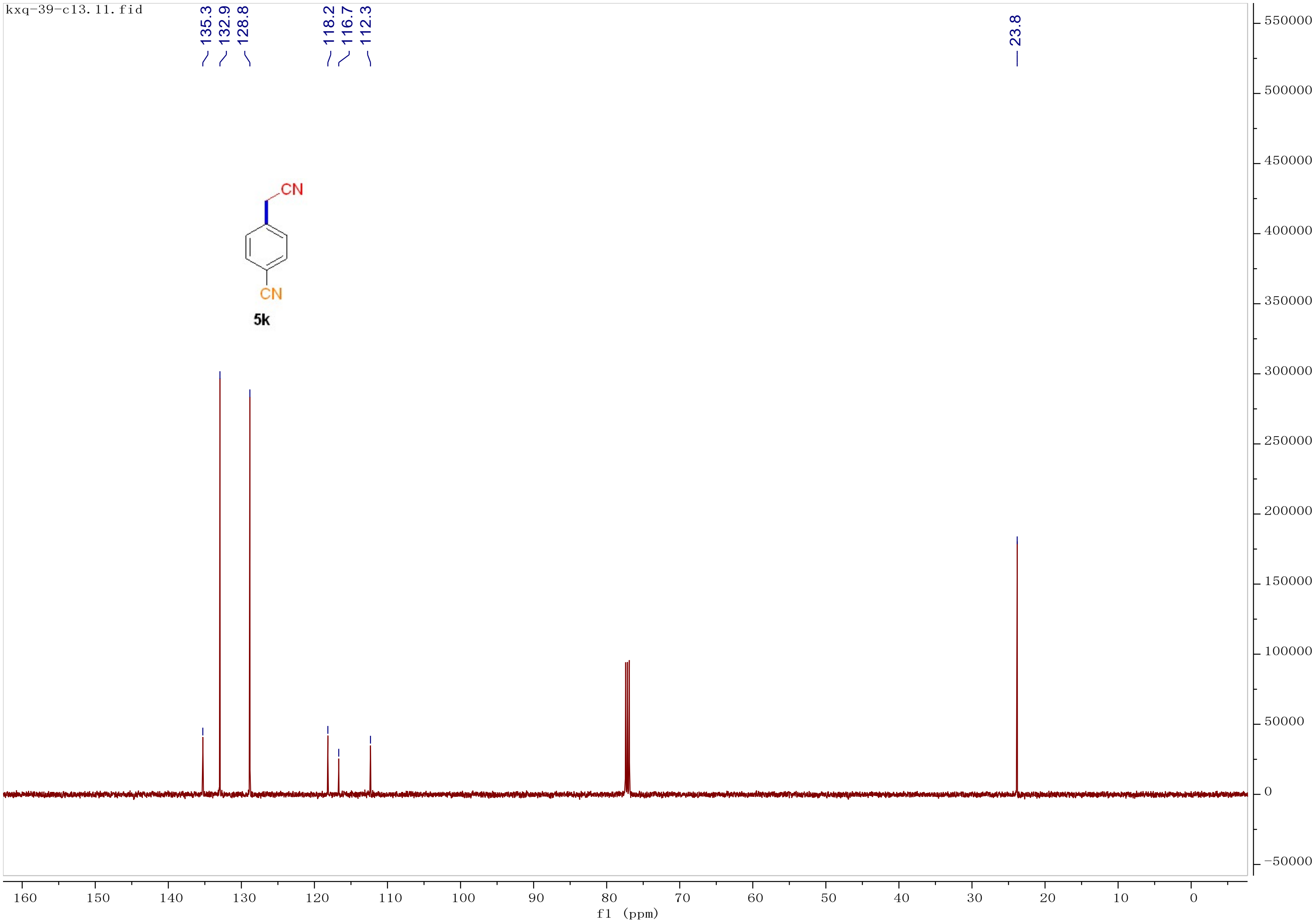

kxq-37-f19.7.fid
-57.99
CN
OCF3
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 −220
f1 (ppm)

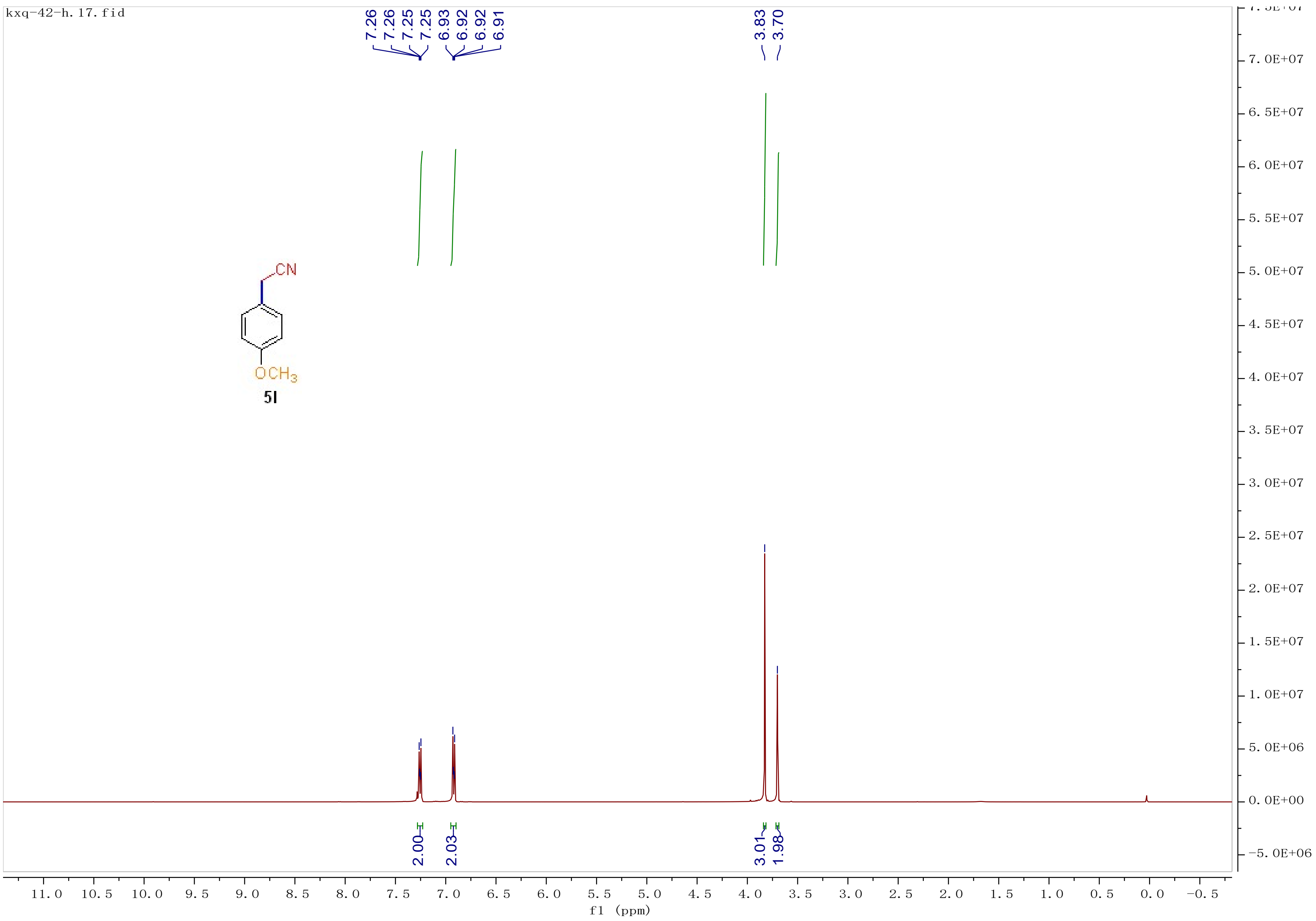
5i

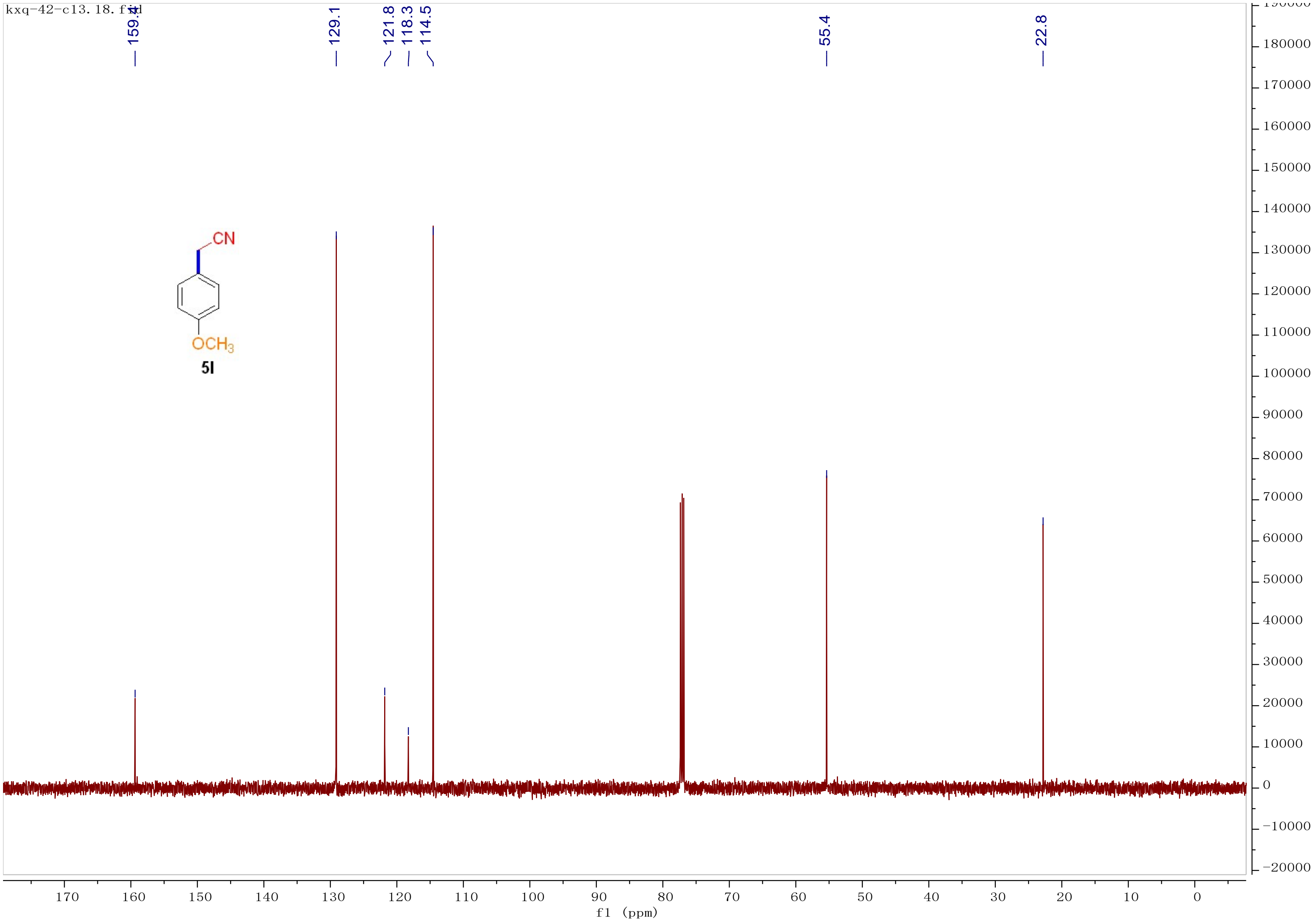

kxq-46-h.1.fid
8.08
8.06
8.06
7.44
7.43
3.94
3.84
CN
CO2Me
5j
1.97
2.00
3.28
2.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
f1 (ppm)
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0

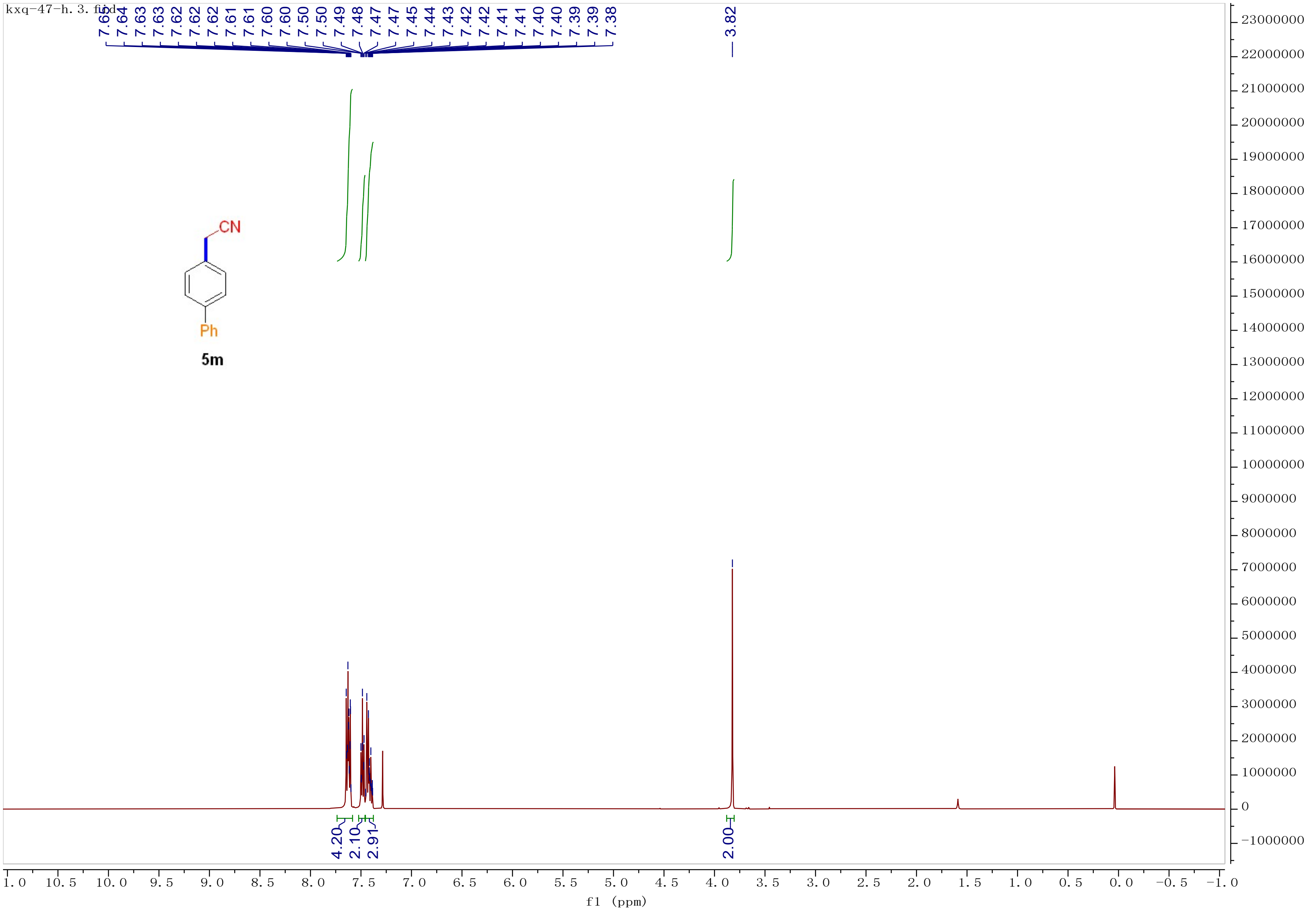

kxq-46-c13.2.fid
166.4
134.8
130.4
130.1
128.0
117.2
52.3
23.7
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

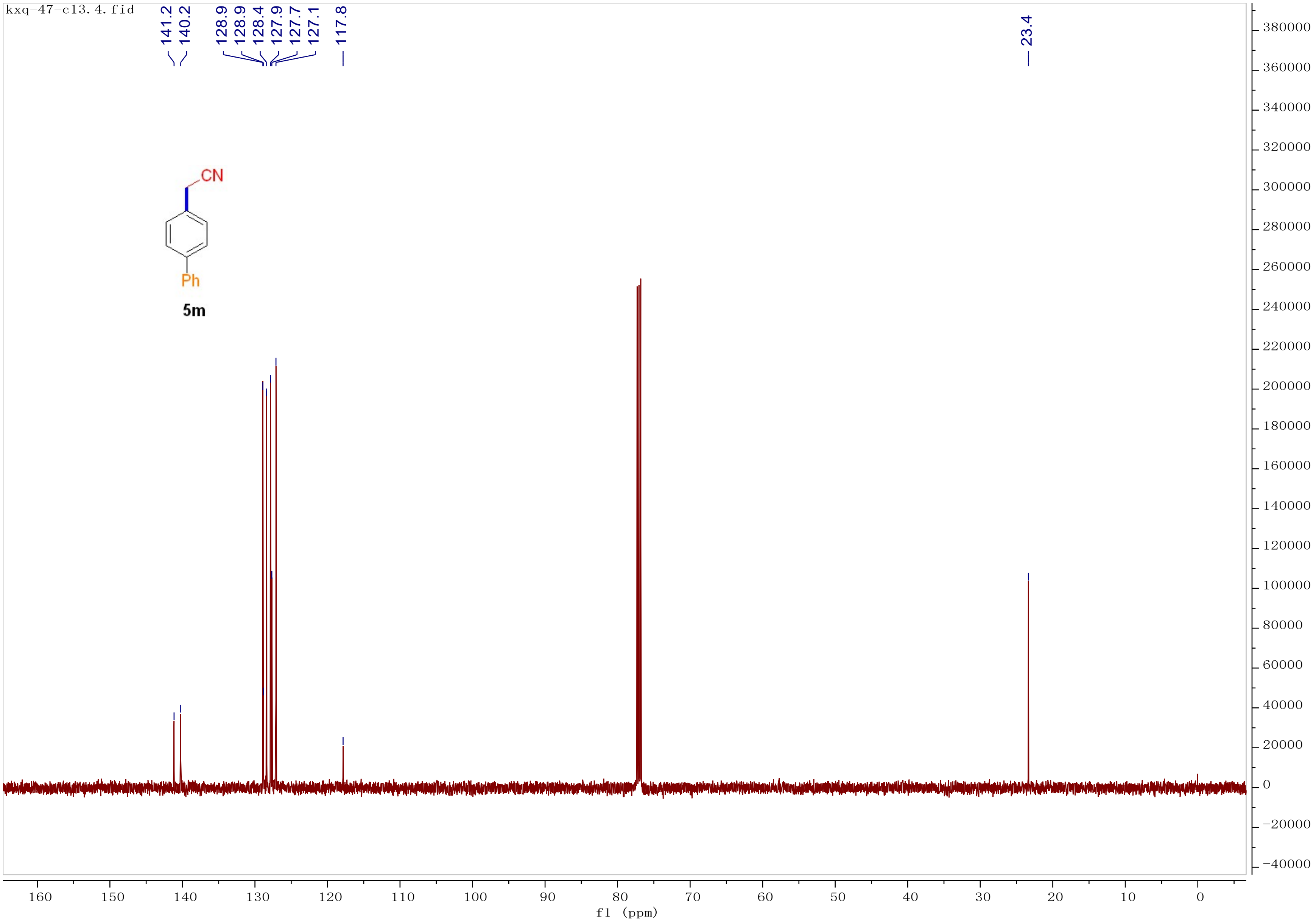

kxq-39-h.10.fid
7.71
7.70
7.69
7.69
7.69
7.50
7.49
7.48
3.86
CN
CN
5k
1.95
1.94
2.00
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


kxq-39-c13.11.fid
135.3
132.9
128.8
118.2
116.7
112.3
23.8
CN
CN
5k
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

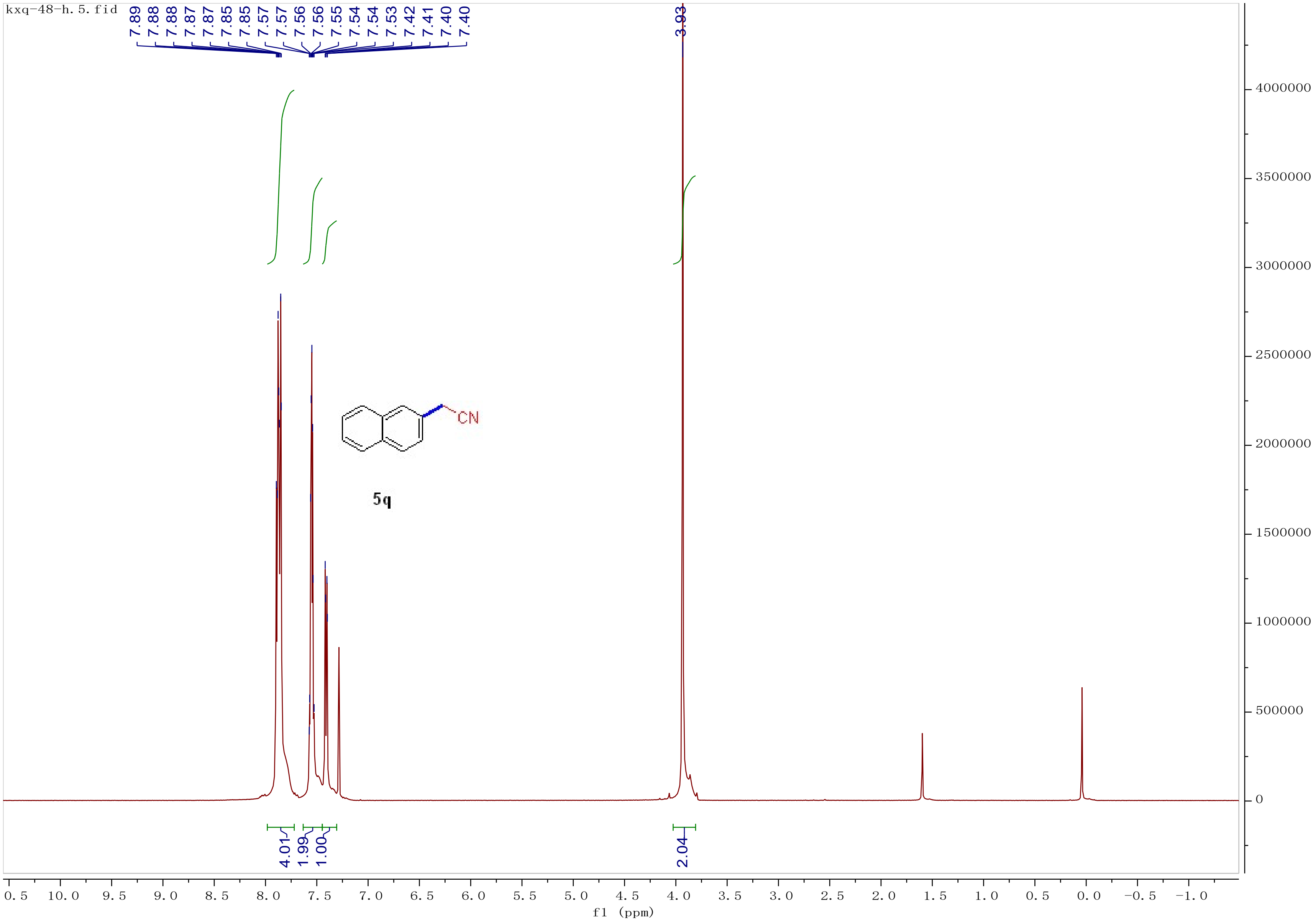

kxq-42-h.17.fid
7.26
7.26
7.25
7.25
6.93
6.92
6.92
6.91
3.83
3.70
CN
OCH3
5l
2.00
2.03
3.01
1.98
7.5E+07
7.0E+07
6.5E+07
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
-5.0E+06
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

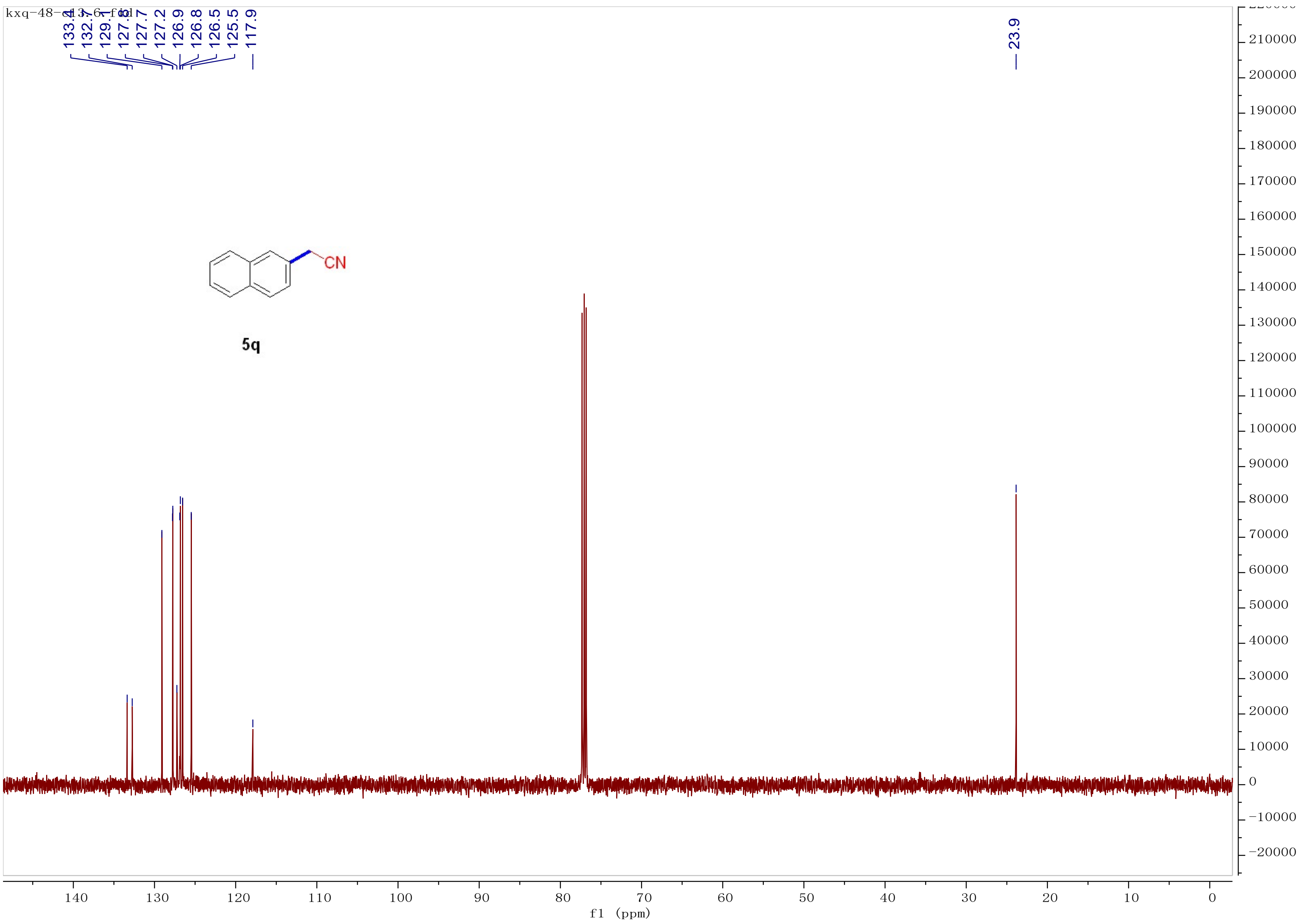

kxq-42-c13.18.fid
159.4
129.1
121.8
118.3
114.5
55.4
22.8
CN
OCH$_3$
5l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
190000
180000
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
−20000


kxq-47-h.3.fid
7.65
7.64
7.63
7.63
7.62
7.62
7.62
7.61
7.61
7.60
7.60
7.50
7.50
7.49
7.48
7.47
7.47
7.45
7.44
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.39
7.39
7.38
3.82
CN
Ph
5m
4.20
2.10
2.91
2.00
23000000
22000000
21000000
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
1.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

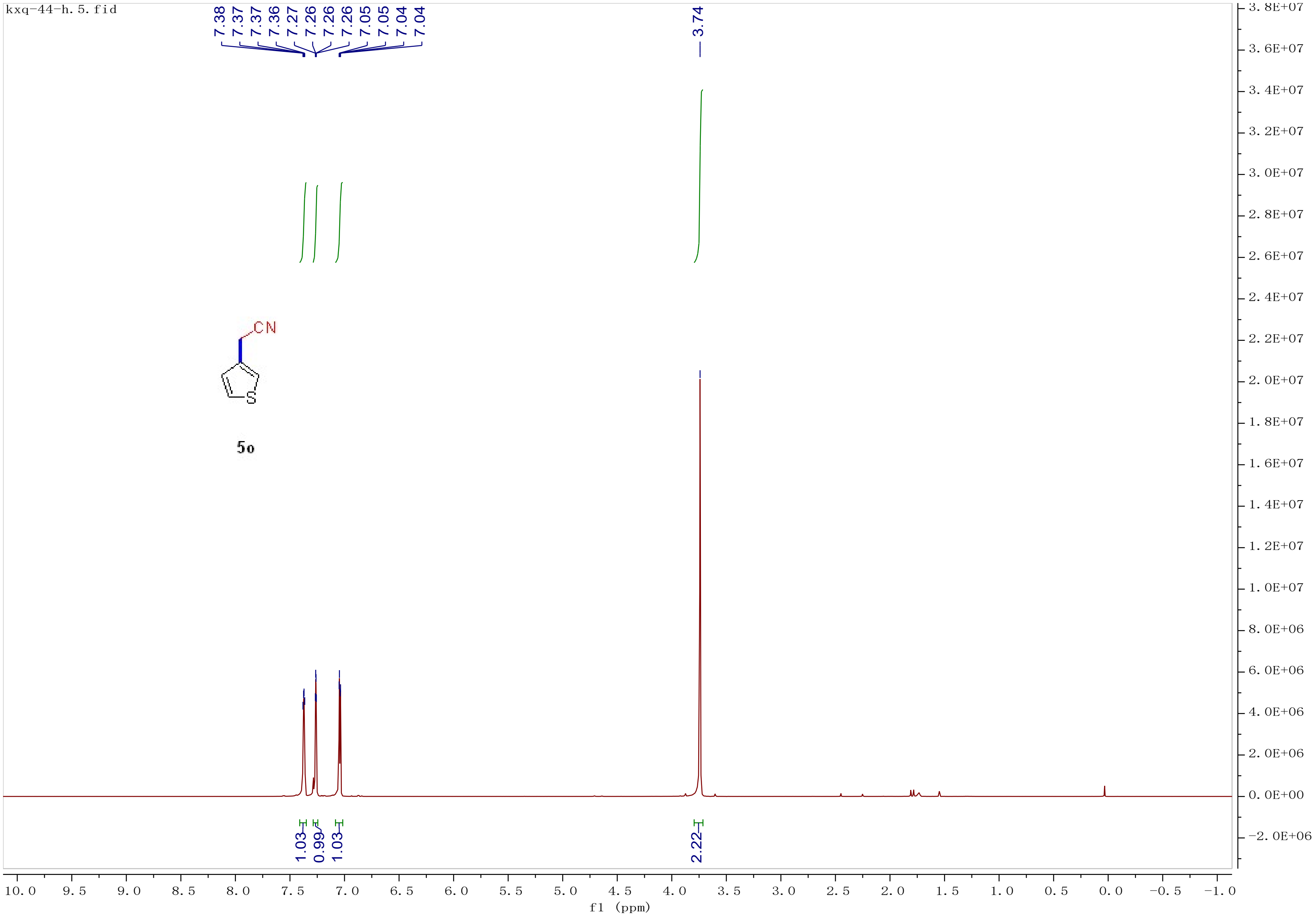

kxq-47-c13.4.fid
141.2
140.2
128.9
128.9
128.4
127.9
127.7
127.1
117.8
23.4
CN
Ph
380000
360000
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
−20000
−40000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

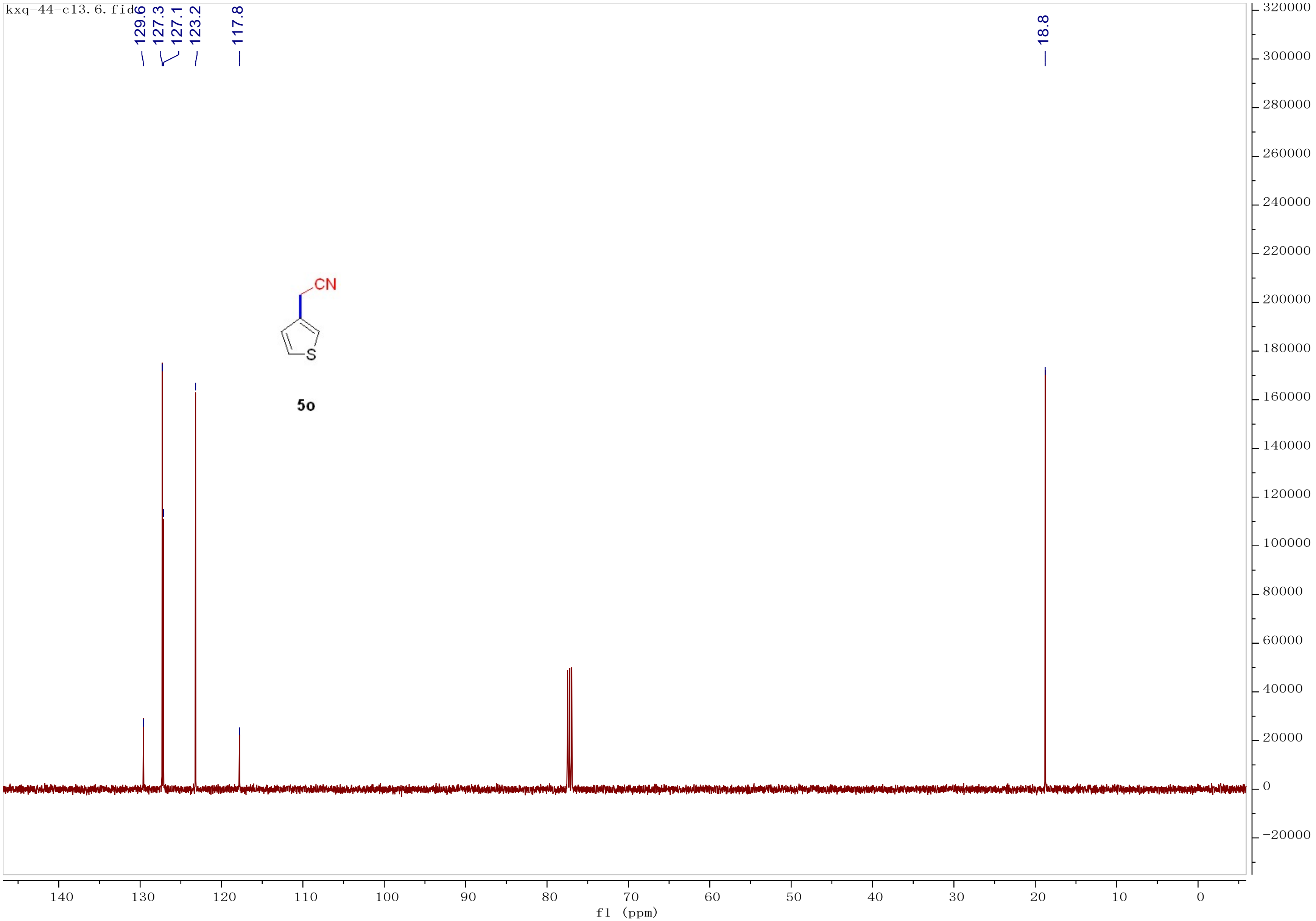
5m

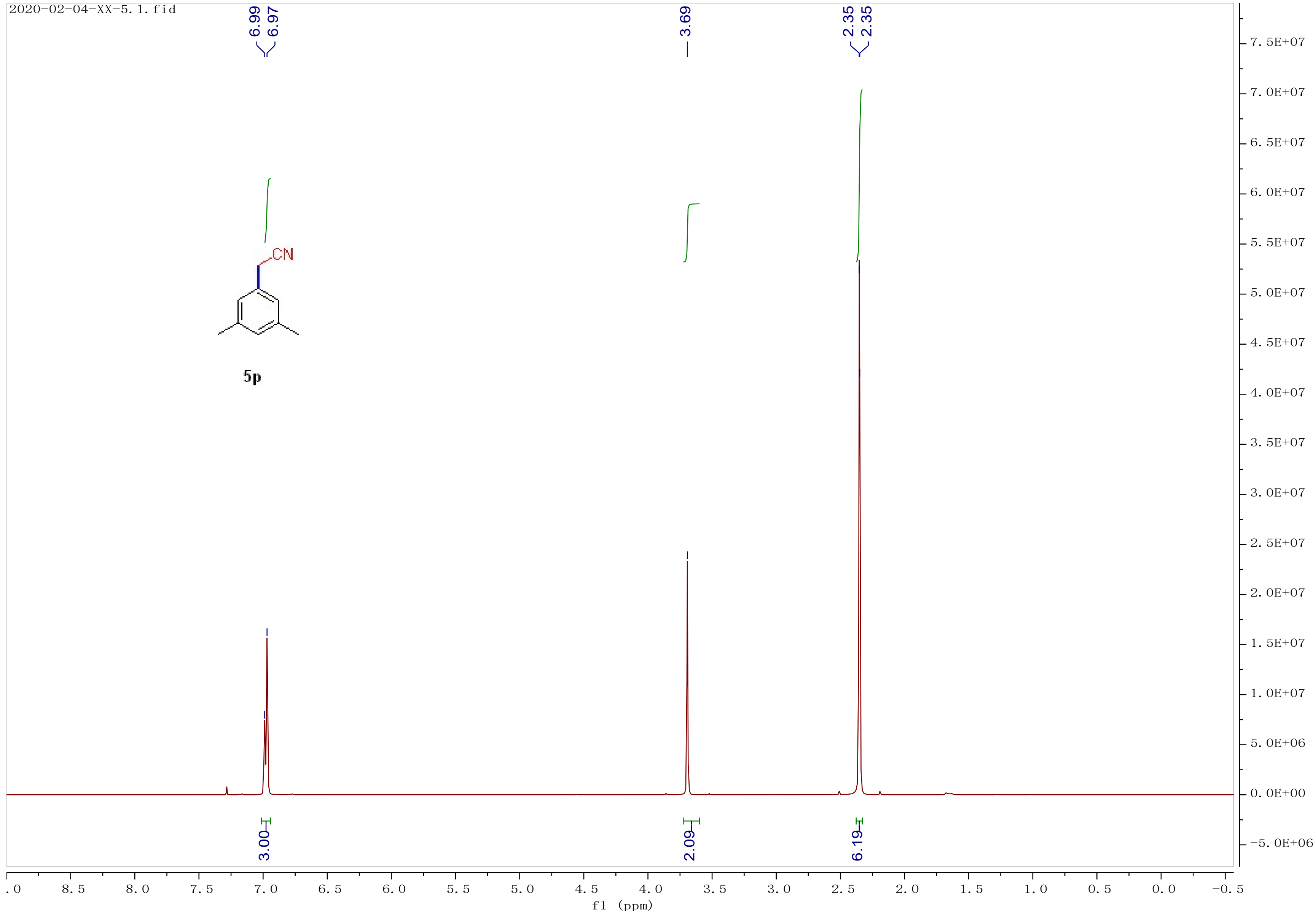

kxq-48-h.5.fid
7.89
7.88
7.88
7.87
7.87
7.85
7.85
7.57
7.57
7.56
7.56
7.55
7.54
7.54
7.53
7.42
7.41
7.40
7.40
3.93
CN
5q
4.01
1.99
1.00
2.04
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

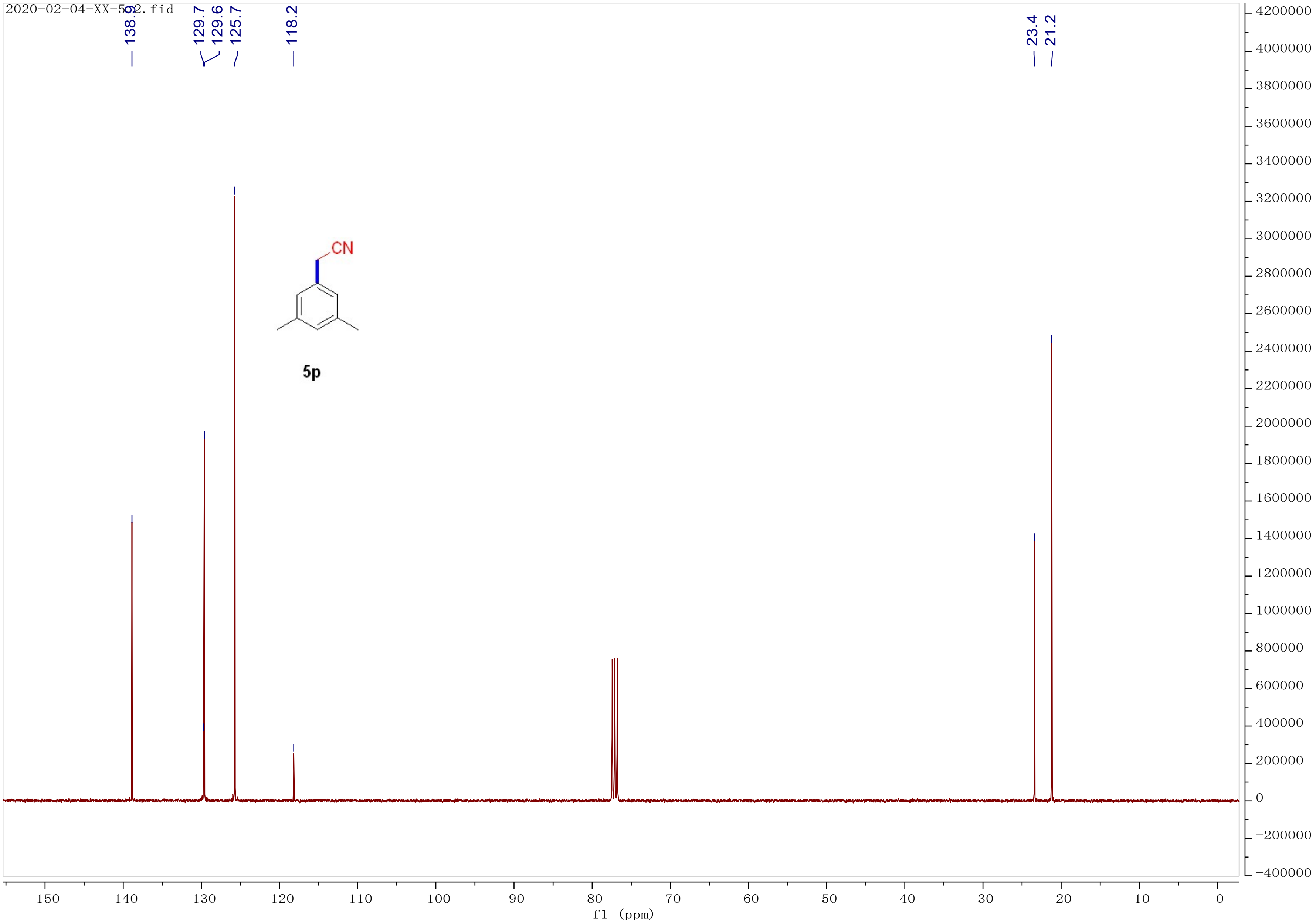

kxq-48-c13.6.fid
133.4
132.7
129.1
127.8
127.7
127.2
126.9
126.8
126.5
125.5
117.9
23.9
CN
210000
200000
190000
180000
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
−20000
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

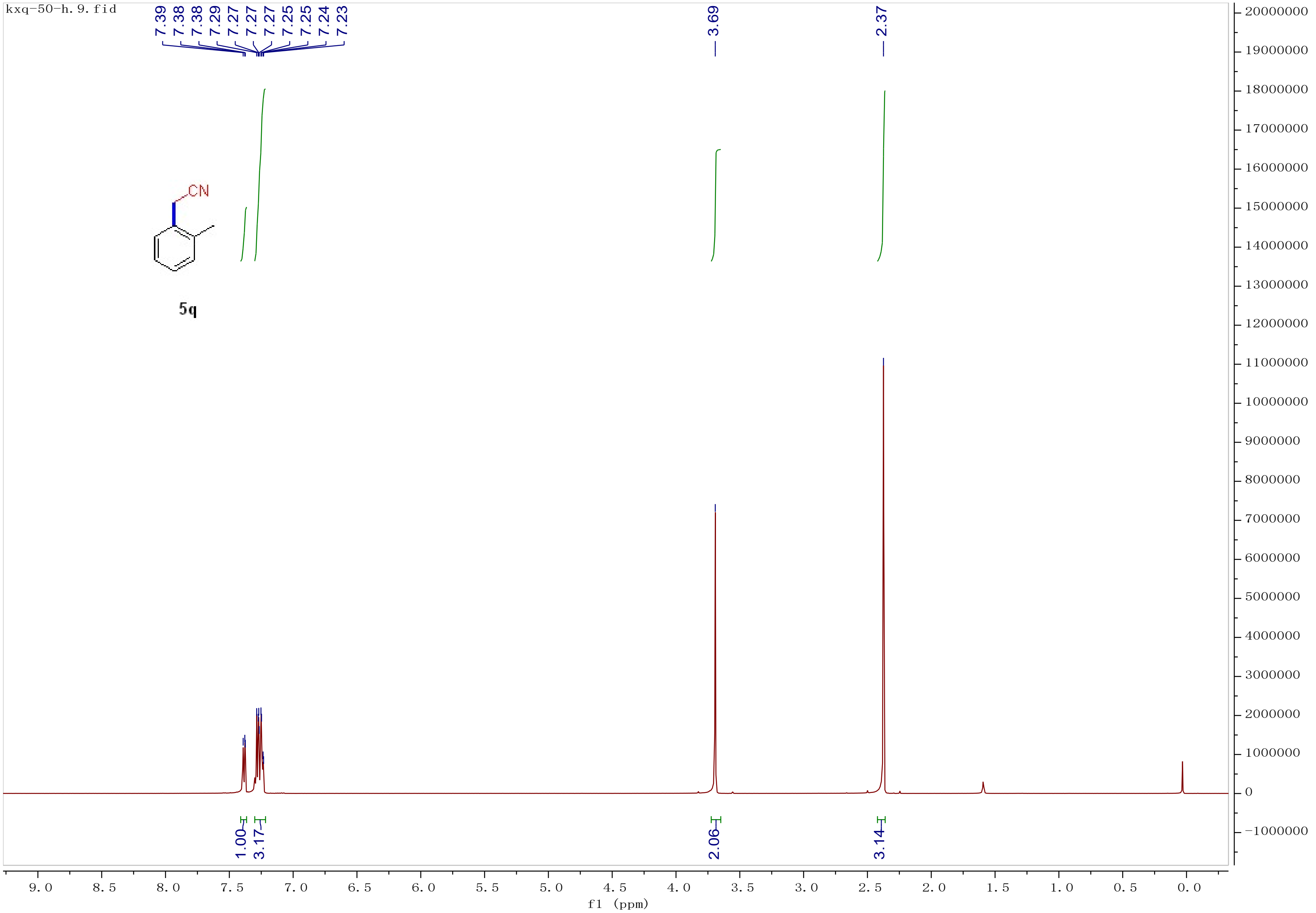
5q

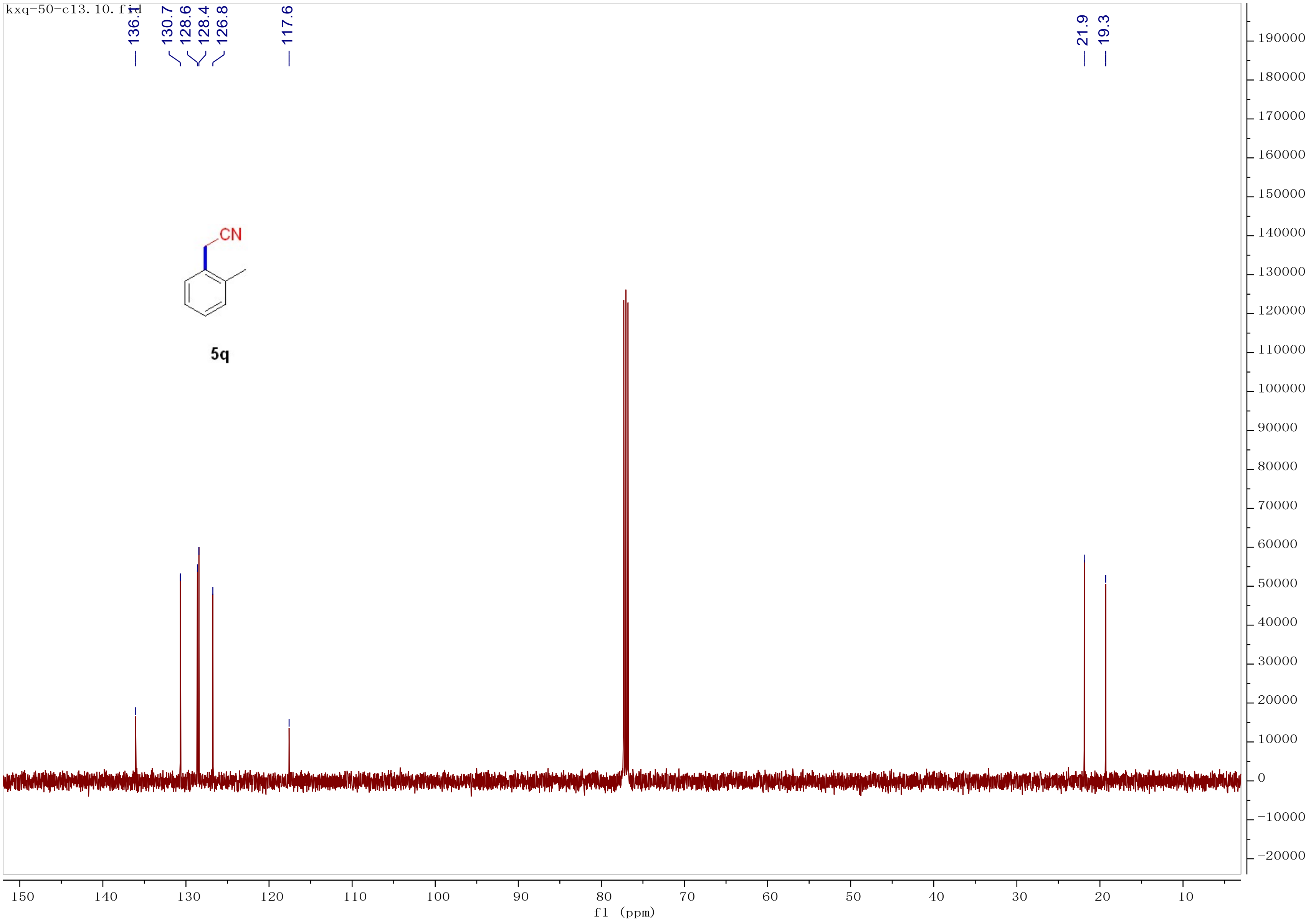

kxq-44-h.5.fid
7.38
7.37
7.37
7.36
7.27
7.26
7.26
7.26
7.05
7.05
7.04
7.04
3.74
CN
S
5o
1.03
0.99
1.03
2.22
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
3.8E+07
3.6E+07
3.4E+07
3.2E+07
3.0E+07
2.8E+07
2.6E+07
2.4E+07
2.2E+07
2.0E+07
1.8E+07
1.6E+07
1.4E+07
1.2E+07
1.0E+07
8.0E+06
6.0E+06
4.0E+06
2.0E+06
0.0E+00
-2.0E+06

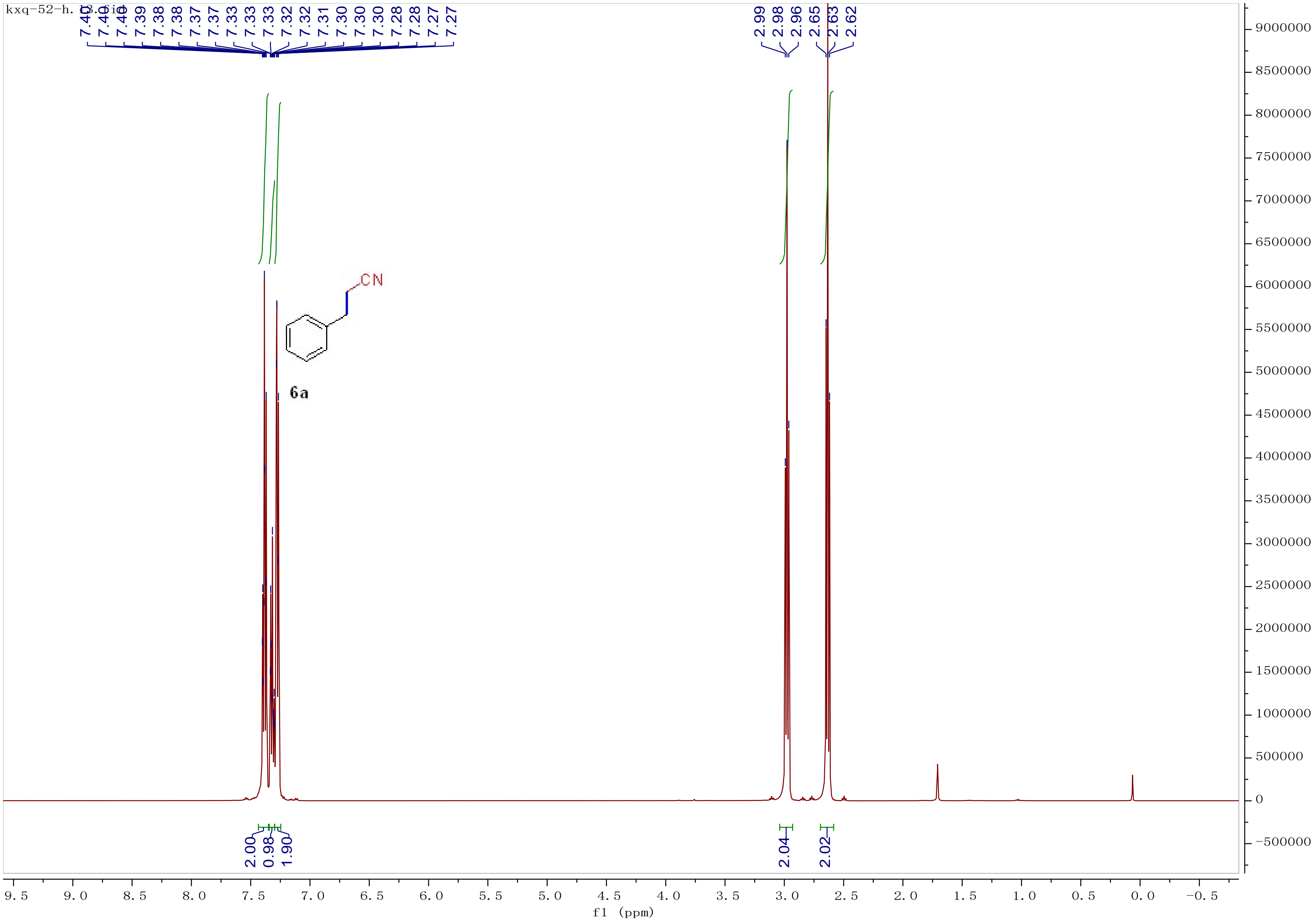

kxq-44-c13.6.fid
129.6
127.3
127.1
123.2
117.8
18.8
CN
S
5o
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

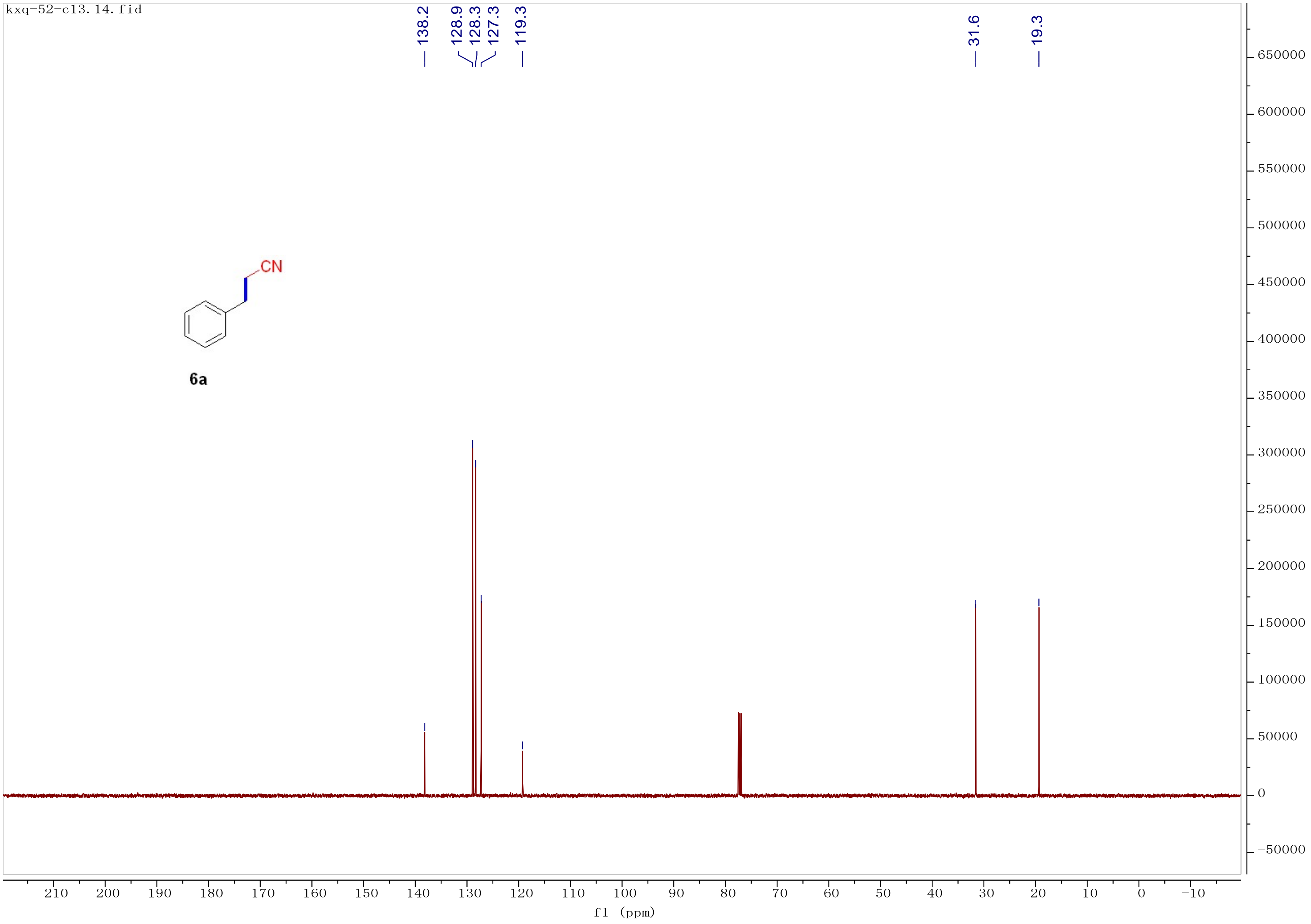

2020-02-04-XX-5.1.fid
6.99
6.97
3.69
2.35
2.35
CN
5p
3.00
2.09
6.19
7.5E+07
7.0E+07
6.5E+07
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
-5.0E+06
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

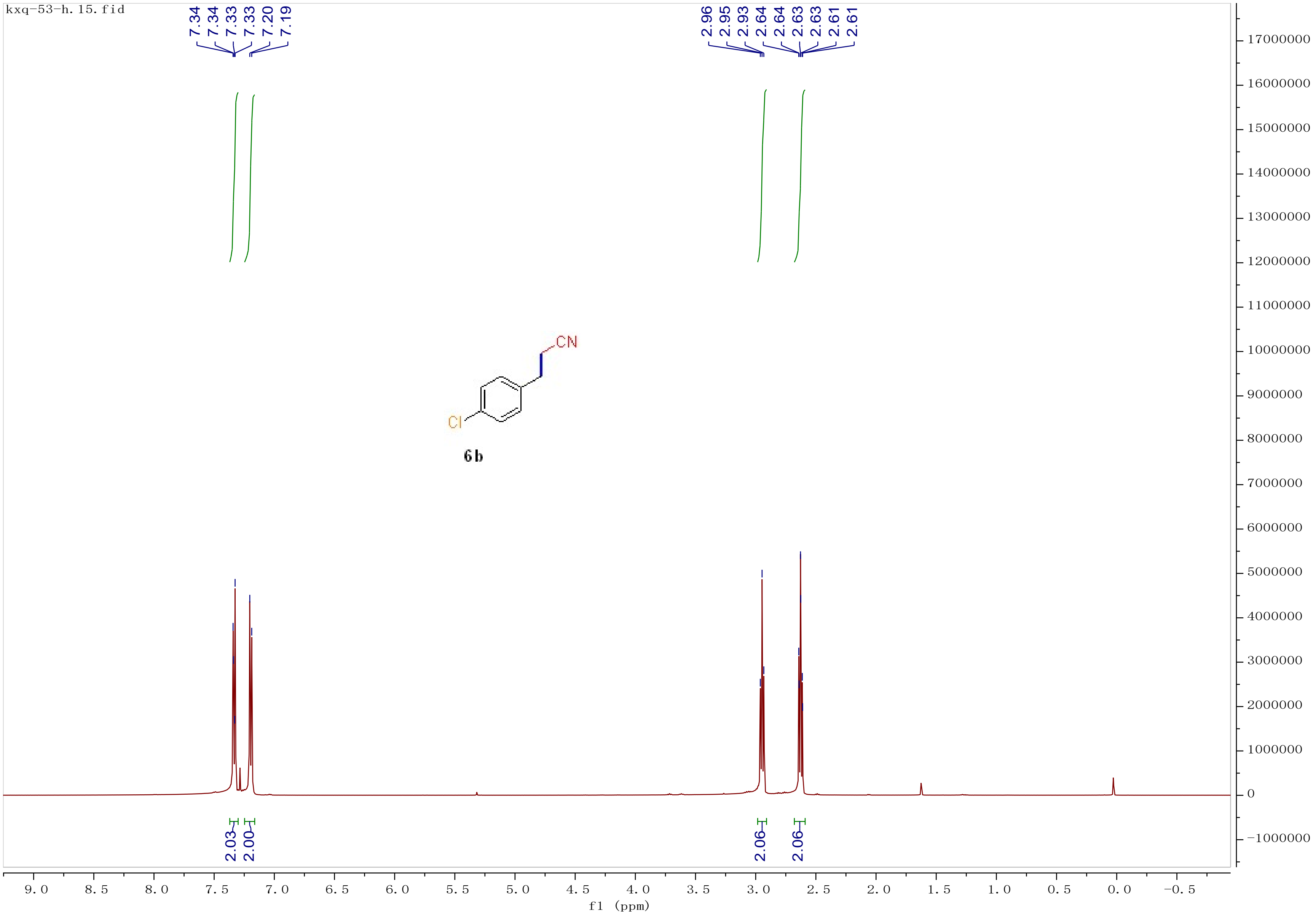

2020-02-04-XX-5[illegible]2.fid
138.9
129.7
129.6
125.7
118.2
23.4
21.2
CN
5p
4200000
4000000
3800000
3600000
3400000
3200000
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
−200000
−400000
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

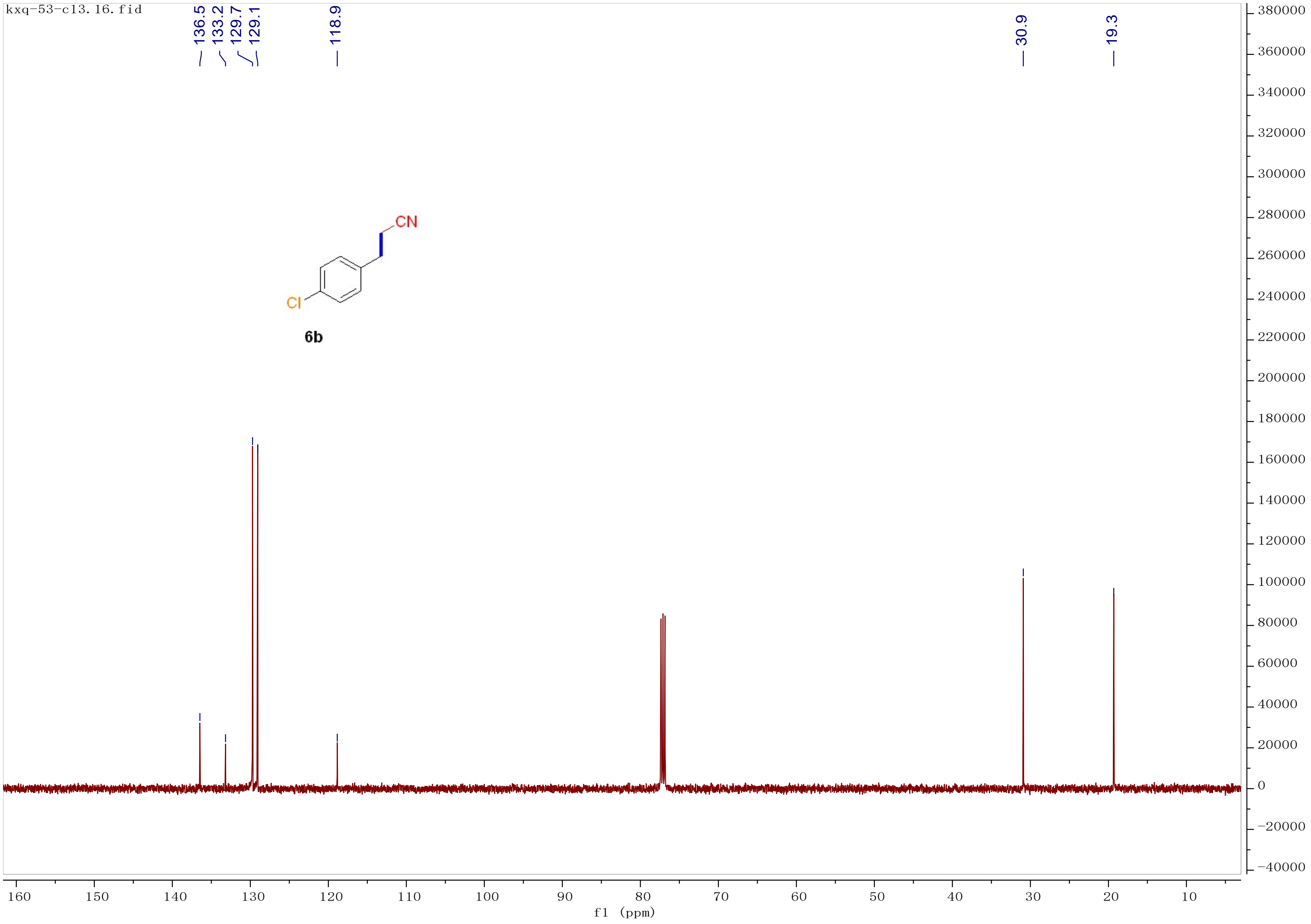

kxq-50-h.9.fid
7.39
7.38
7.38
7.29
7.27
7.27
7.27
7.25
7.25
7.24
7.23
3.69
2.37
CN
5q
1.00
3.17
2.06
3.14
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
9.0
8.5
8.0
7.5
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)

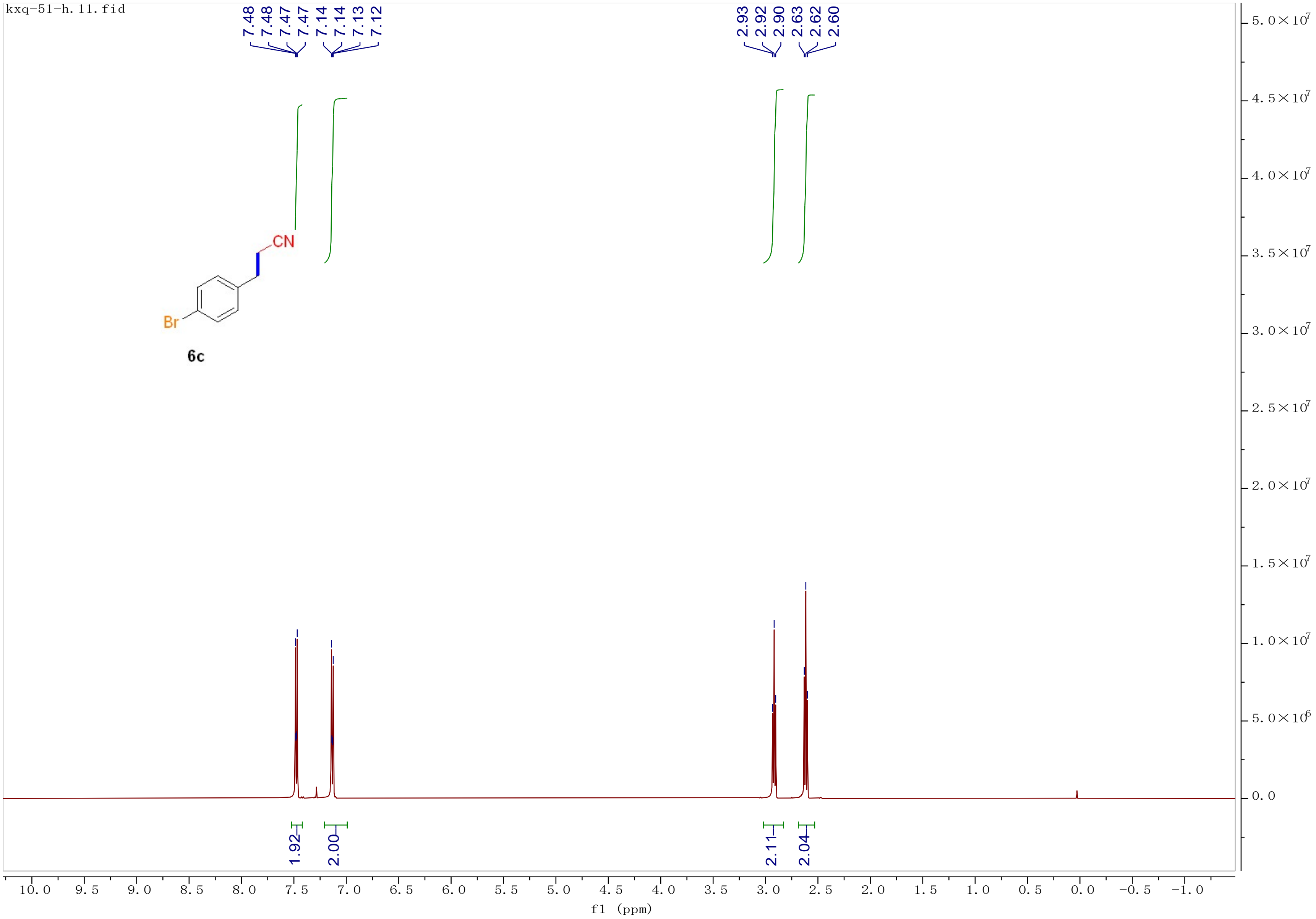

kxq-50-c13.10.fid
136.1
130.7
128.6
128.4
126.8
117.6
21.9
19.3
CN
5q
190000
180000
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
-20000
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


kxq-52-h.10.fid
7.40
7.40
7.40
7.39
7.38
7.38
7.37
7.37
7.33
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.30
7.28
7.28
7.27
7.27
2.99
2.98
2.96
2.65
2.63
2.62
CN
6a
2.00
0.98
1.90
2.04
2.02
9000000
8500000
8000000
7500000
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
-500000
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)

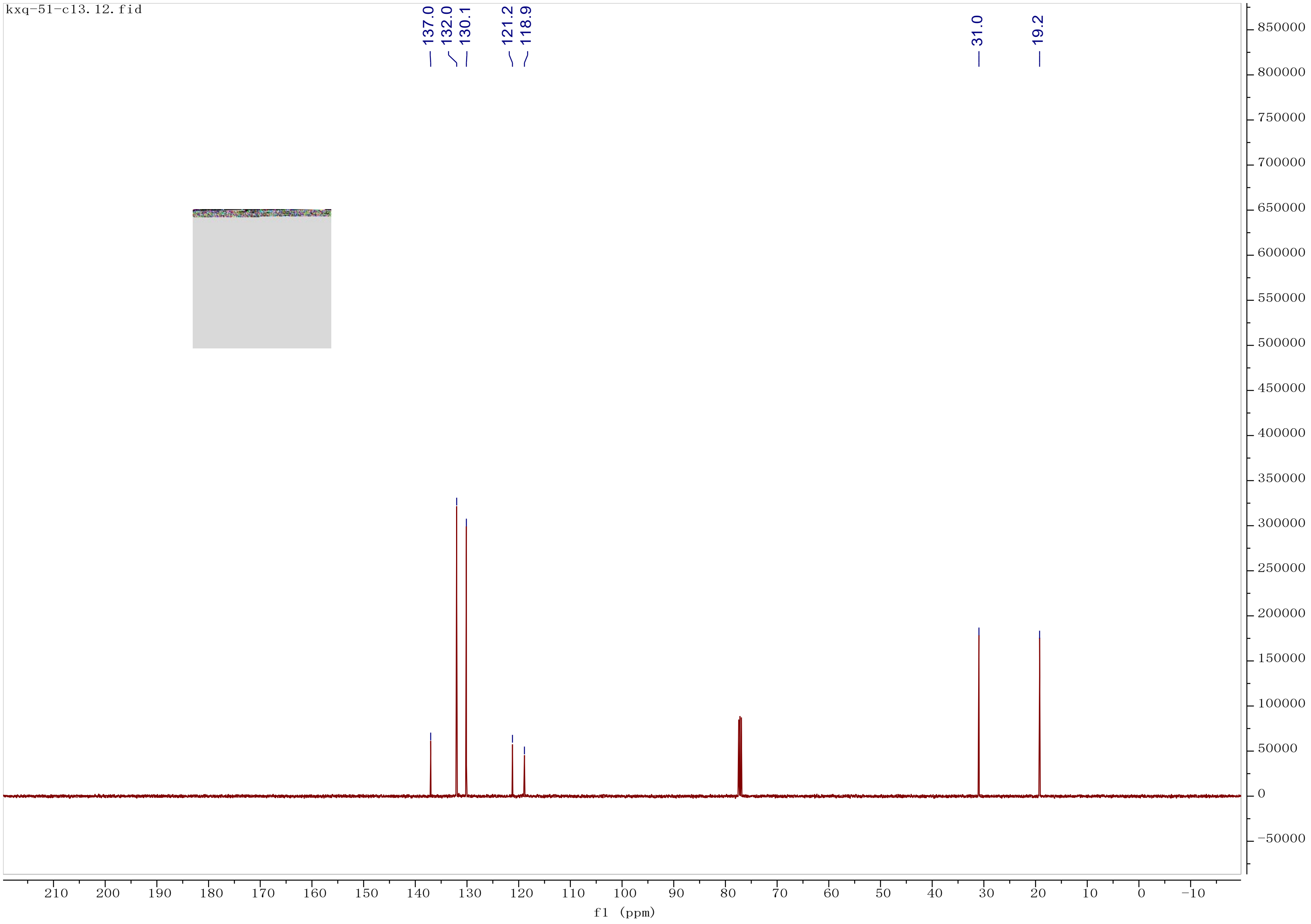

kxq-52-c13.14.fid
138.2
128.9
128.3
127.3
119.3
31.6
19.3
CN
6a
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
−50000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

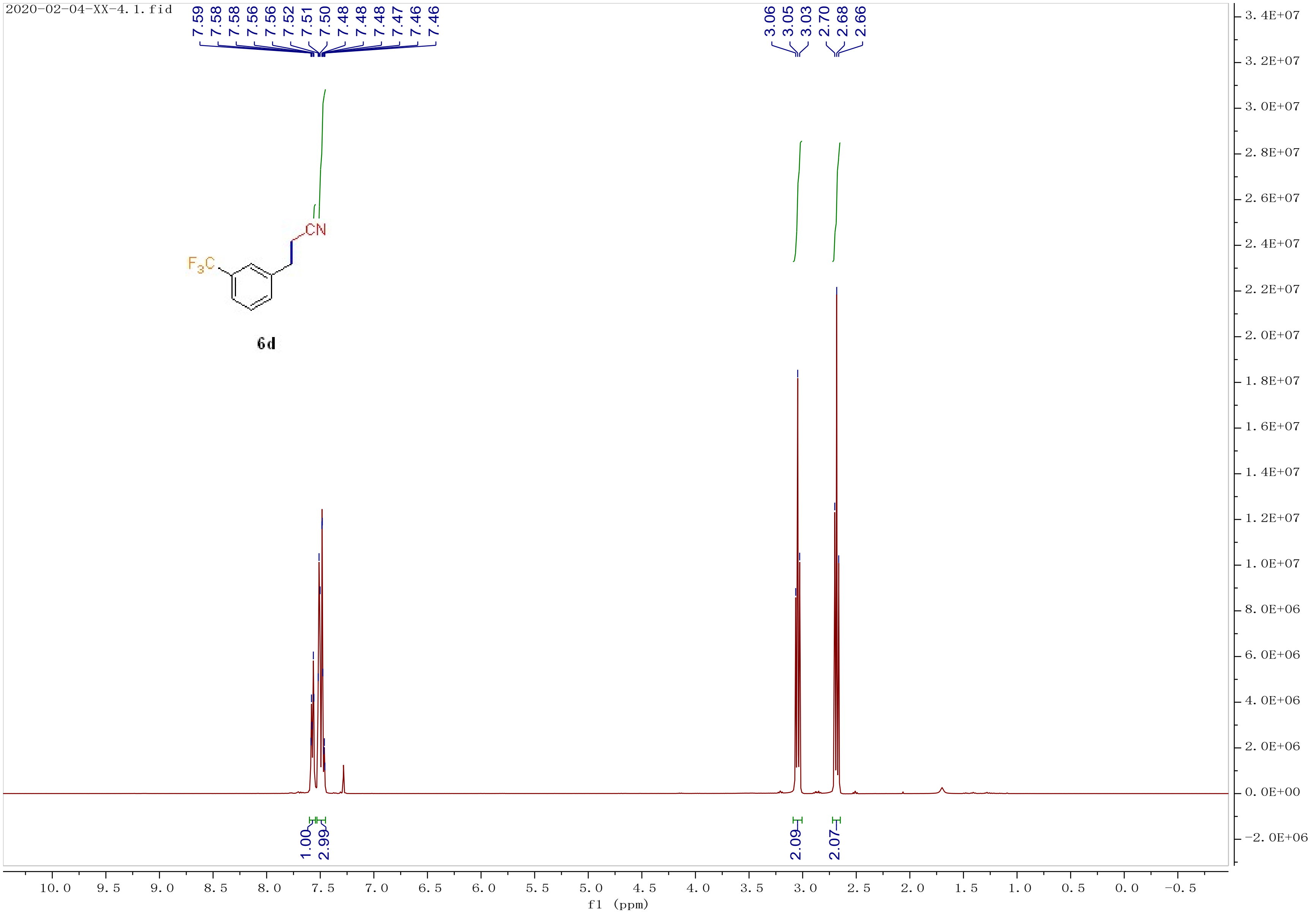

kxq-53-h.15.fid
7.34
7.34
7.33
7.33
7.20
7.19
2.96
2.95
2.93
2.64
2.64
2.63
2.63
2.61
2.61
CN
Cl
6b
2.03
2.00
2.06
2.06
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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)


kxq-53-c13.16.fid
136.5
133.2
129.7
129.1
118.9
30.9
19.3
CN
Cl
6b
380000
360000
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
-40000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

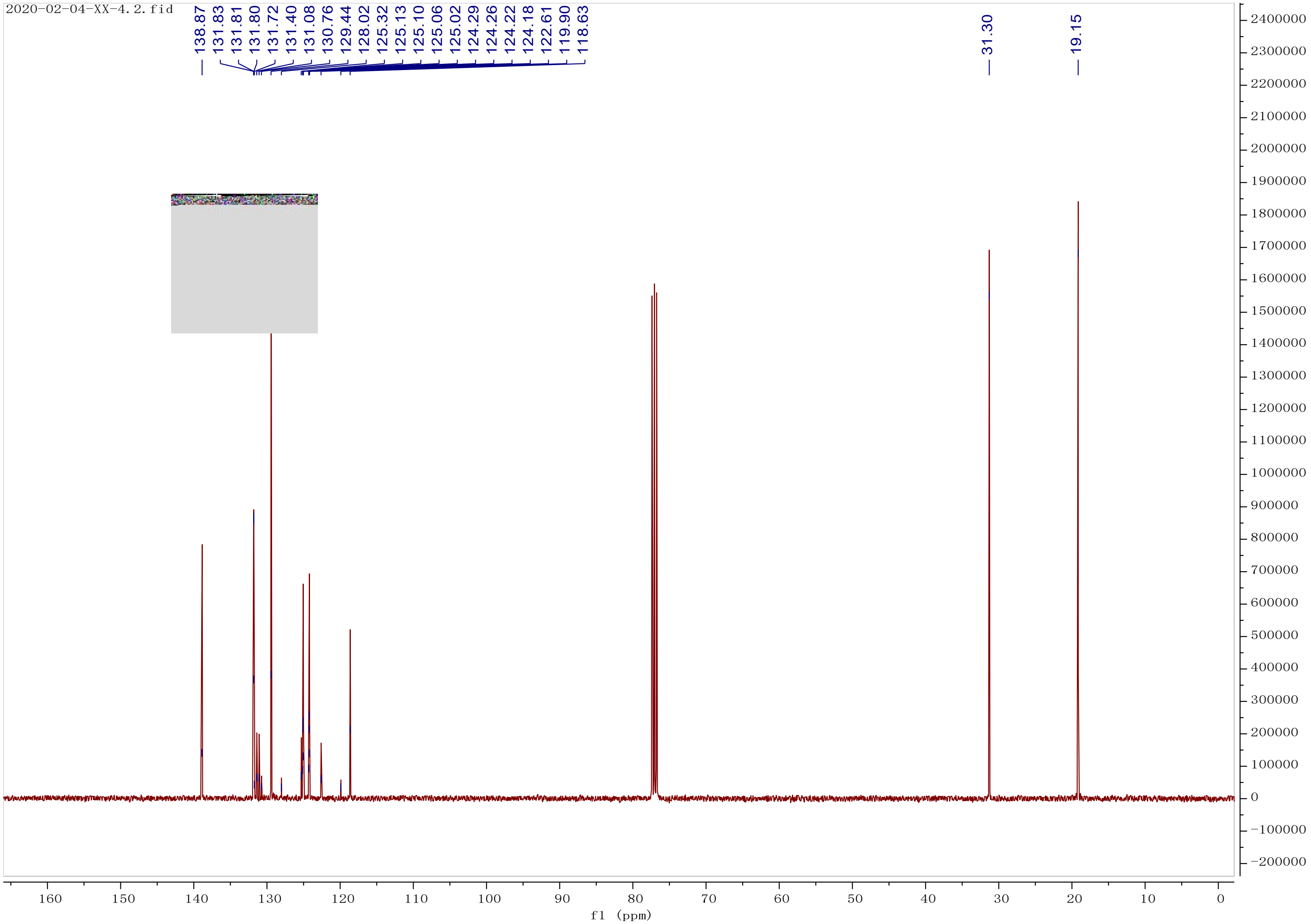

kxq-51-h.11.fid
7.48
7.48
7.47
7.47
7.14
7.14
7.13
7.12
2.93
2.92
2.90
2.63
2.62
2.60
CN
Br
1.92
2.00
2.11
2.04
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

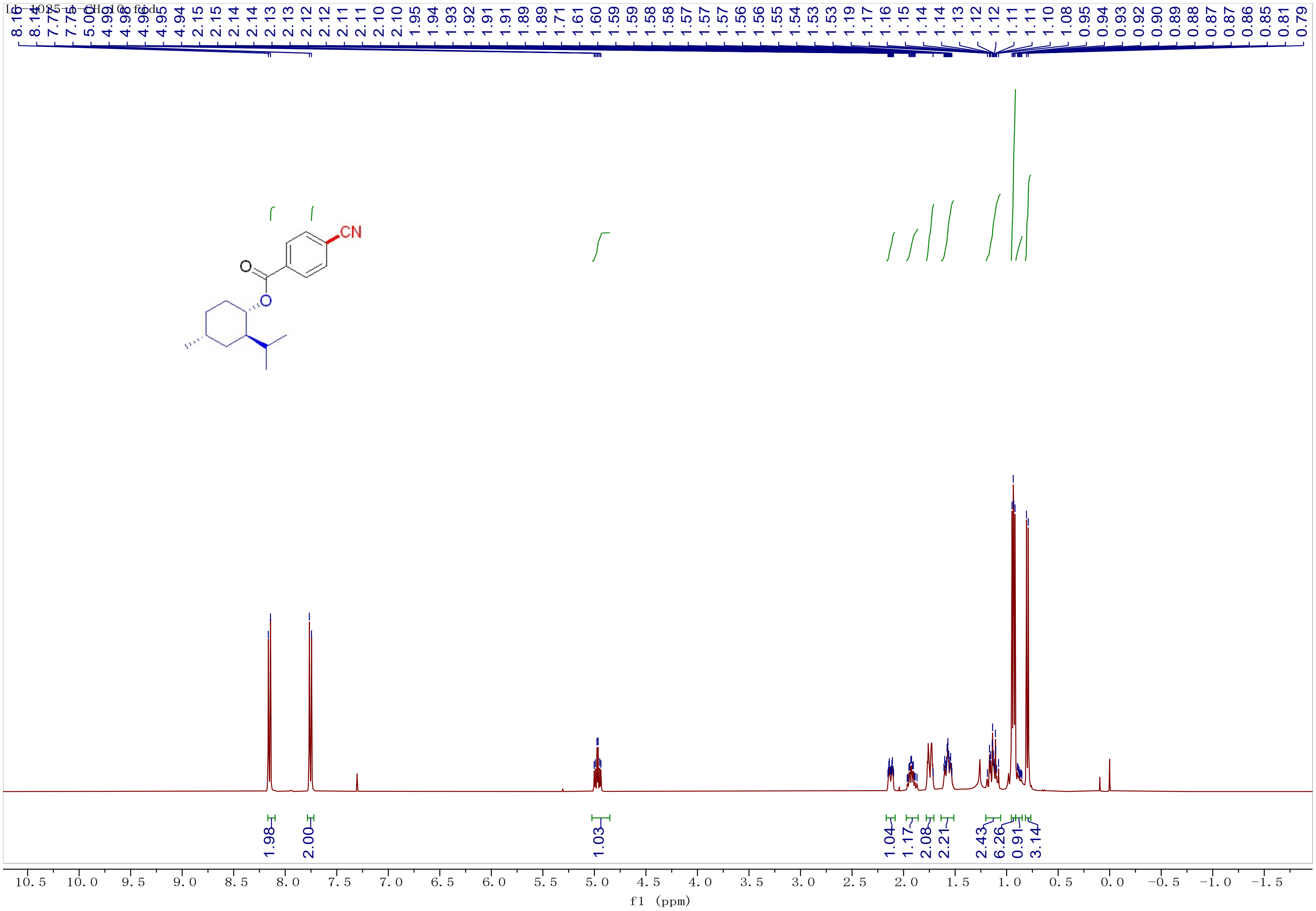
6c

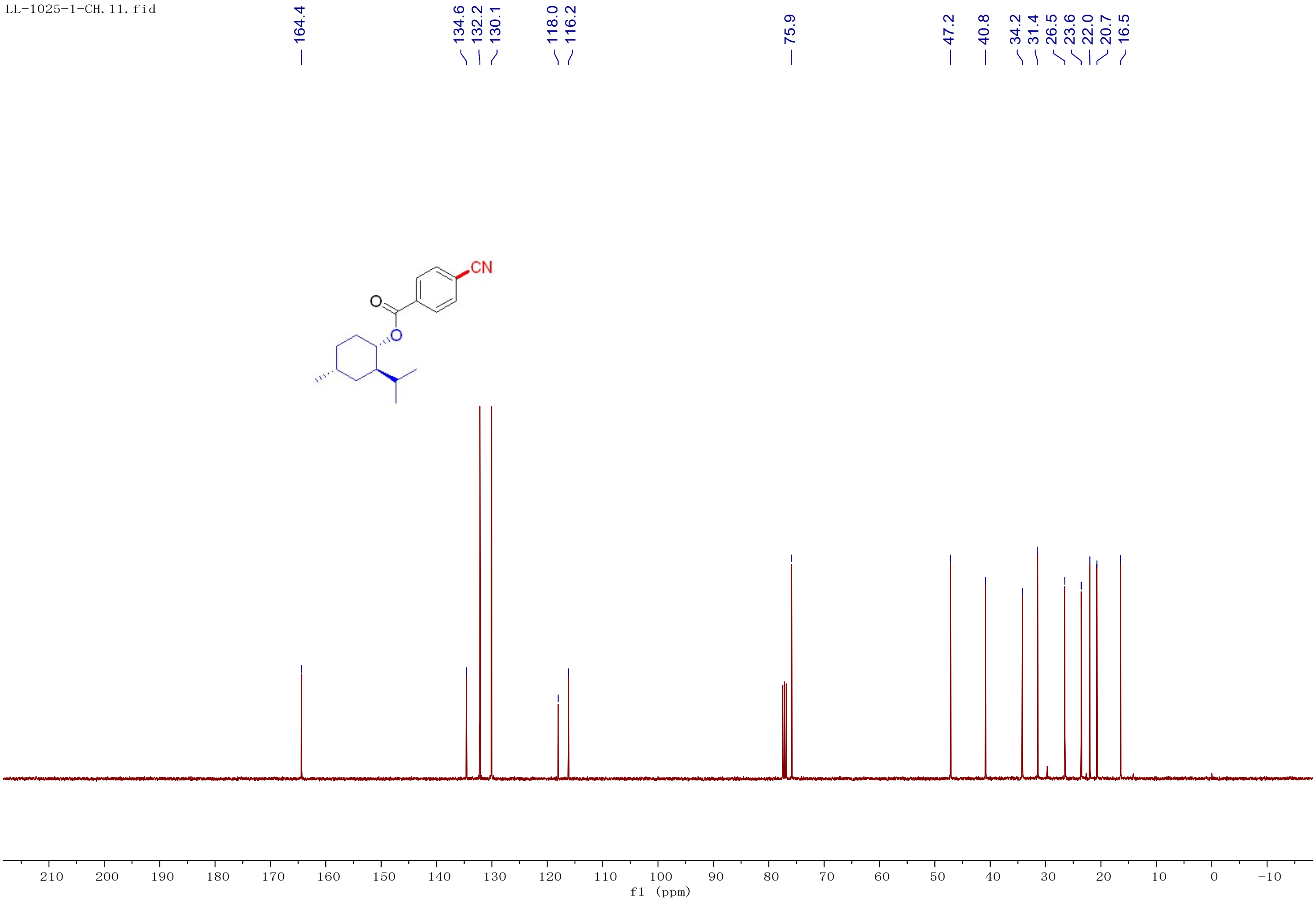

kxq-51-c13.12.fid
137.0
132.0
130.1
121.2
118.9
31.0
19.2
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

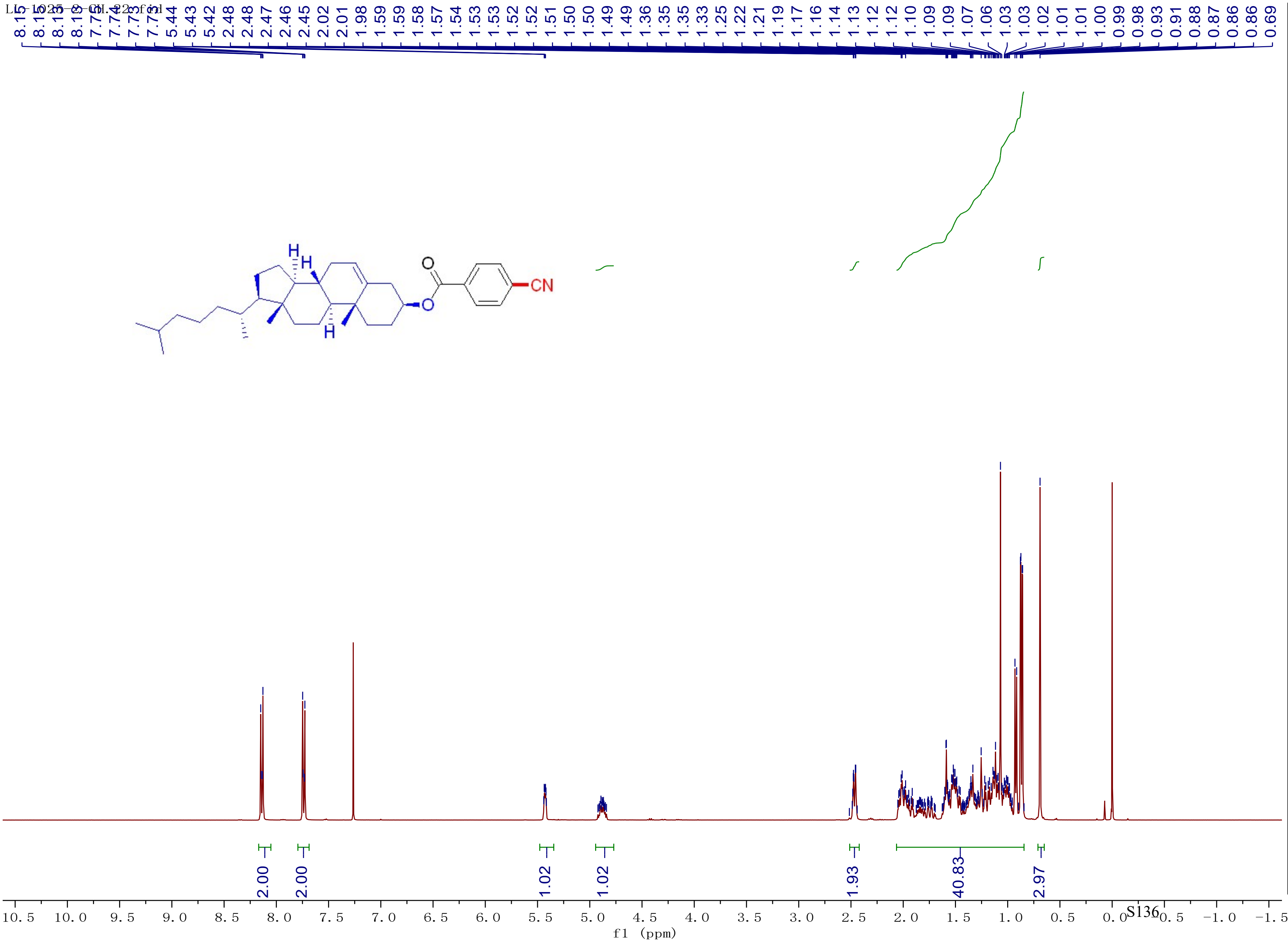

2020-02-04-XX-4.1.fid
7.59
7.58
7.58
7.56
7.56
7.52
7.51
7.50
7.48
7.48
7.48
7.47
7.46
7.46
3.06
3.05
3.03
2.70
2.68
2.66
F_3C
CN
1.00
2.99
2.09
2.07
3.4E+07
3.2E+07
3.0E+07
2.8E+07
2.6E+07
2.4E+07
2.2E+07
2.0E+07
1.8E+07
1.6E+07
1.4E+07
1.2E+07
1.0E+07
8.0E+06
6.0E+06
4.0E+06
2.0E+06
0.0E+00
-2.0E+06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

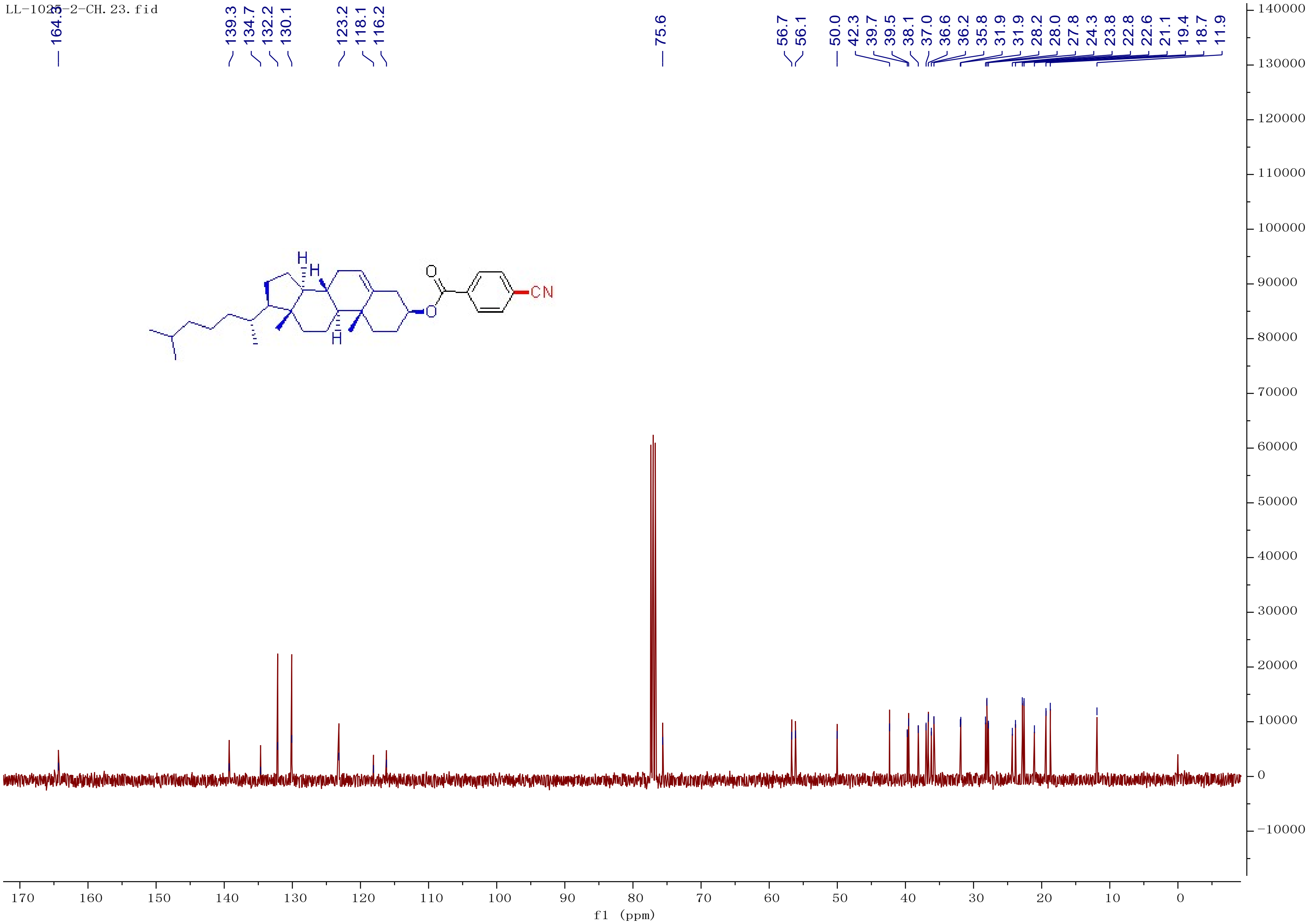
6d


2020-02-04-XX-4.2.fid
138.87
131.83
131.81
131.80
131.72
131.40
131.08
130.76
129.44
128.02
125.32
125.13
125.10
125.06
125.02
124.29
124.26
124.22
124.18
122.61
119.90
118.63
31.30
19.15
2400000
2300000
2200000
2100000
2000000
1900000
1800000
1700000
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
-200000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

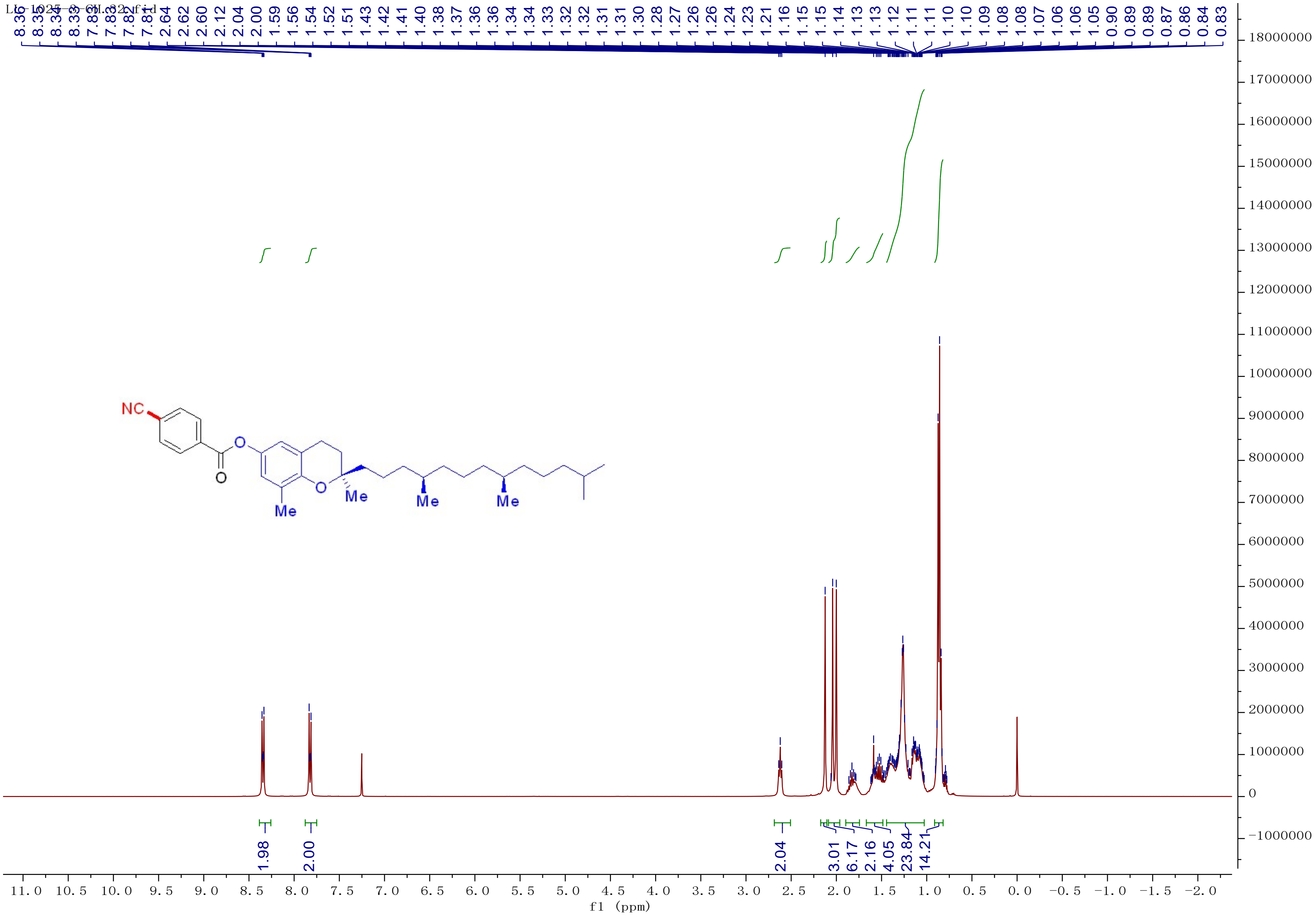

Lb-1025-1-CH.10.fid
8.16
8.14
7.75
7.75
5.00
4.99
4.98
4.96
4.95
4.94
2.15
2.15
2.14
2.14
2.13
2.13
2.12
2.12
2.11
2.11
2.10
2.10
1.95
1.94
1.93
1.92
1.91
1.91
1.89
1.89
1.71
1.61
1.60
1.59
1.59
1.58
1.58
1.57
1.57
1.57
1.56
1.56
1.55
1.54
1.53
1.53
1.19
1.17
1.16
1.15
1.14
1.14
1.13
1.12
1.12
1.11
1.11
1.10
1.08
0.95
0.94
0.93
0.92
0.90
0.89
0.88
0.87
0.87
0.86
0.85
0.81
0.79
CN
O
O
1.98
2.00
1.03
1.04
1.17
2.08
2.21
2.43
6.26
0.91
3.14
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

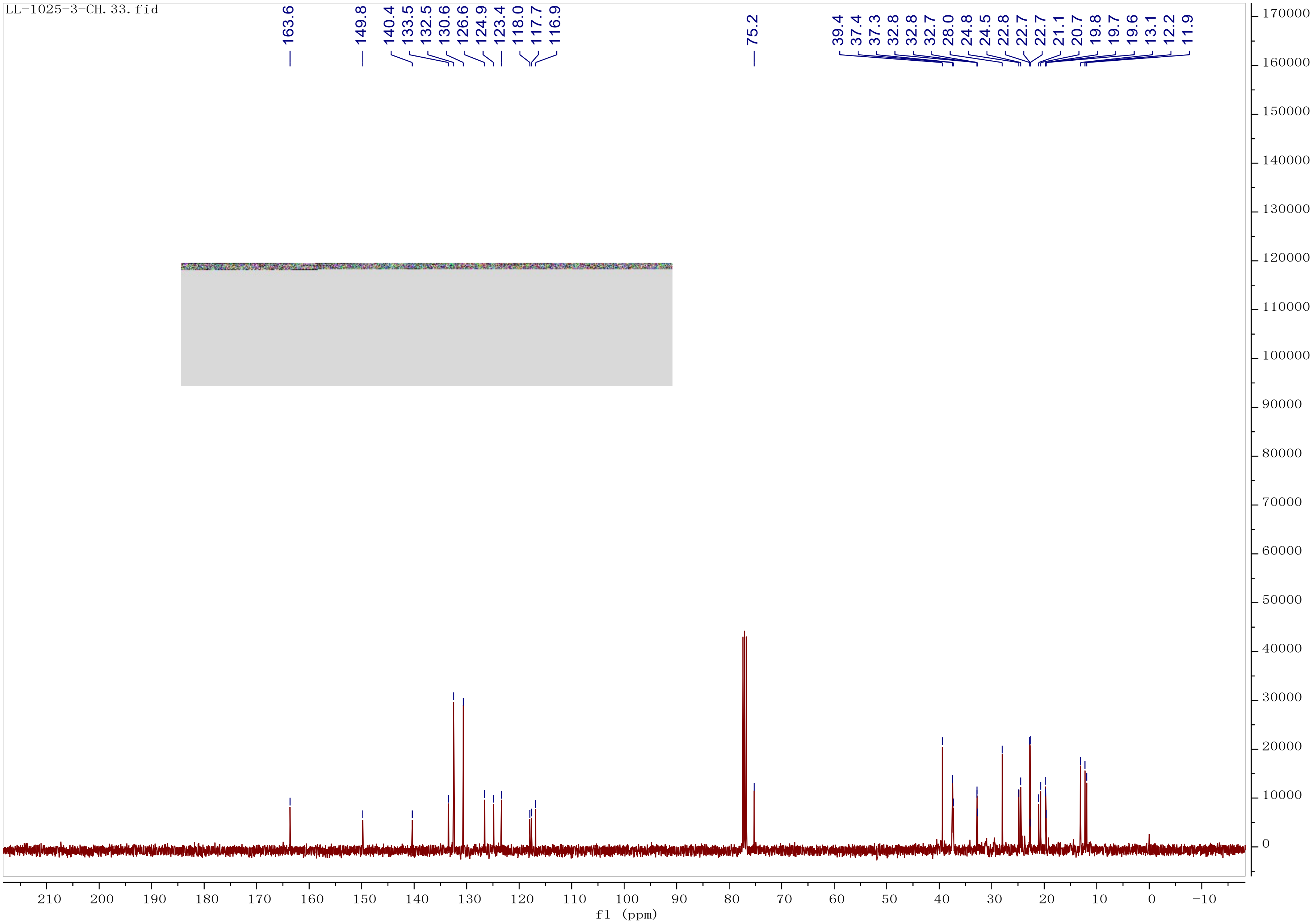

LL-1025-1-CH.11.fid
164.4
134.6
132.2
130.1
118.0
116.2
75.9
47.2
40.8
34.2
31.4
26.5
23.6
22.0
20.7
16.5
O
O
CN
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

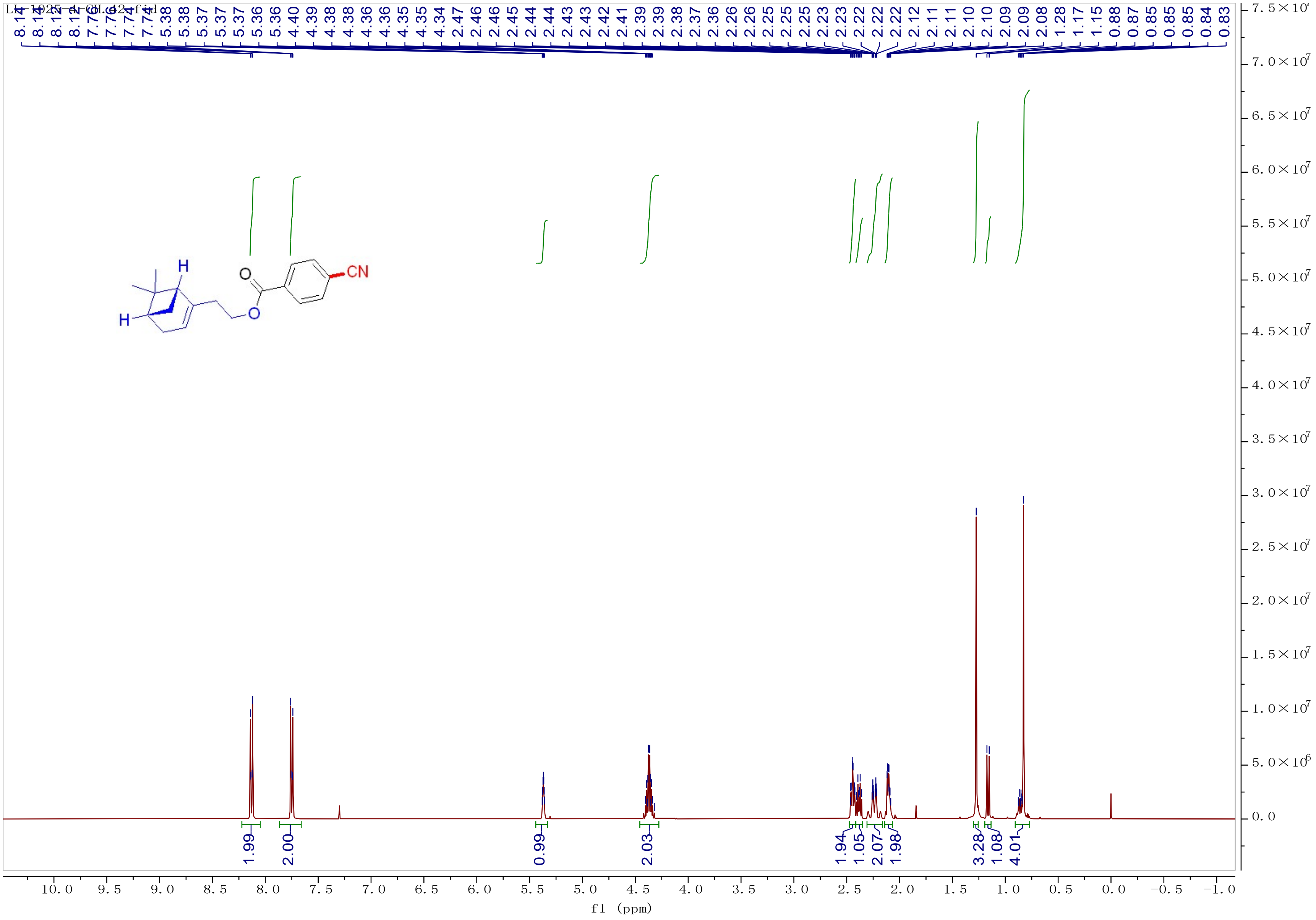

LL-1025-2-CH.22.fid
8.15
8.15
8.13
8.13
7.75
7.74
7.73
7.73
5.44
5.43
5.42
2.48
2.48
2.47
2.46
2.45
2.02
2.01
1.98
1.59
1.59
1.58
1.57
1.54
1.53
1.53
1.52
1.52
1.51
1.50
1.50
1.49
1.49
1.36
1.35
1.35
1.33
1.25
1.22
1.21
1.19
1.17
1.16
1.14
1.13
1.12
1.12
1.10
1.09
1.09
1.07
1.06
1.03
1.03
1.02
1.01
1.01
1.00
0.99
0.98
0.93
0.91
0.88
0.87
0.86
0.86
0.69
H
H
H
O
O
CN
2.00
2.00
1.02
1.02
1.93
40.83
2.97
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

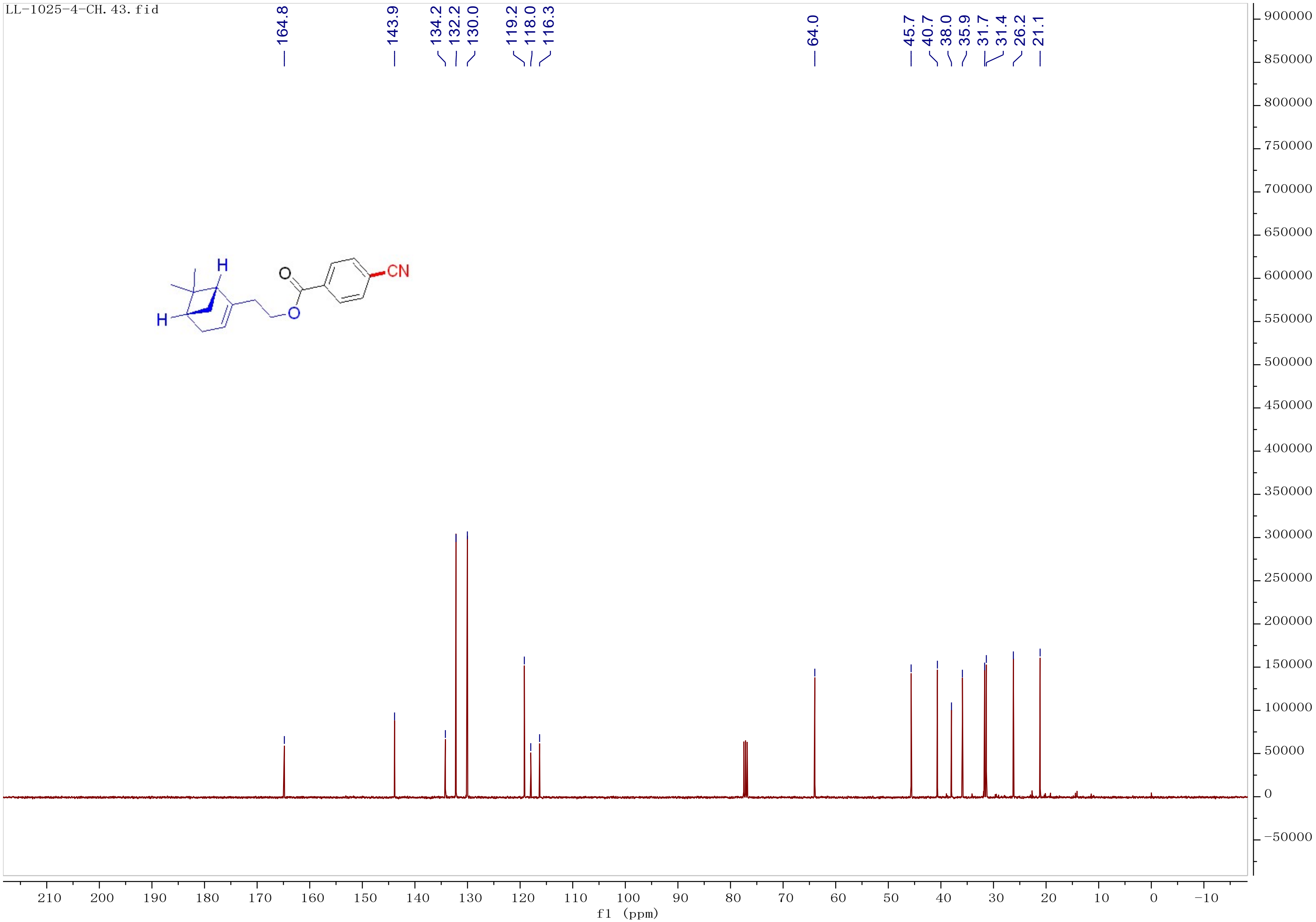


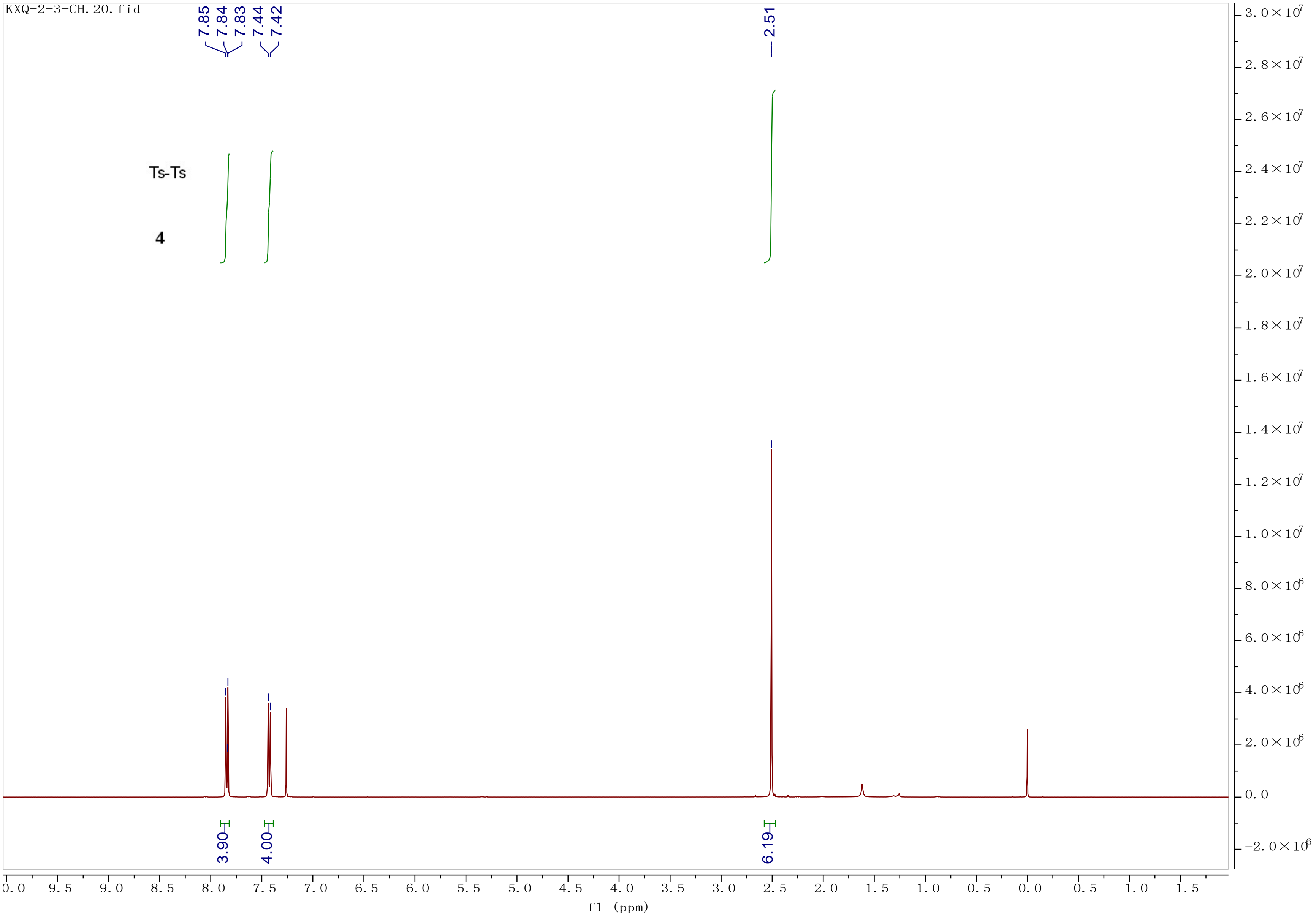
LL-1025-2-CH.23.fid
164.5
139.3
134.7
132.2
130.1
123.2
118.1
116.2
75.6
56.7
56.1
50.0
42.3
39.7
39.5
38.1
37.0
36.6
36.2
35.8
31.9
31.9
28.2
28.0
27.8
24.3
23.8
22.8
22.6
21.1
19.4
18.7
11.9
H
H
H
O
O
CN
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

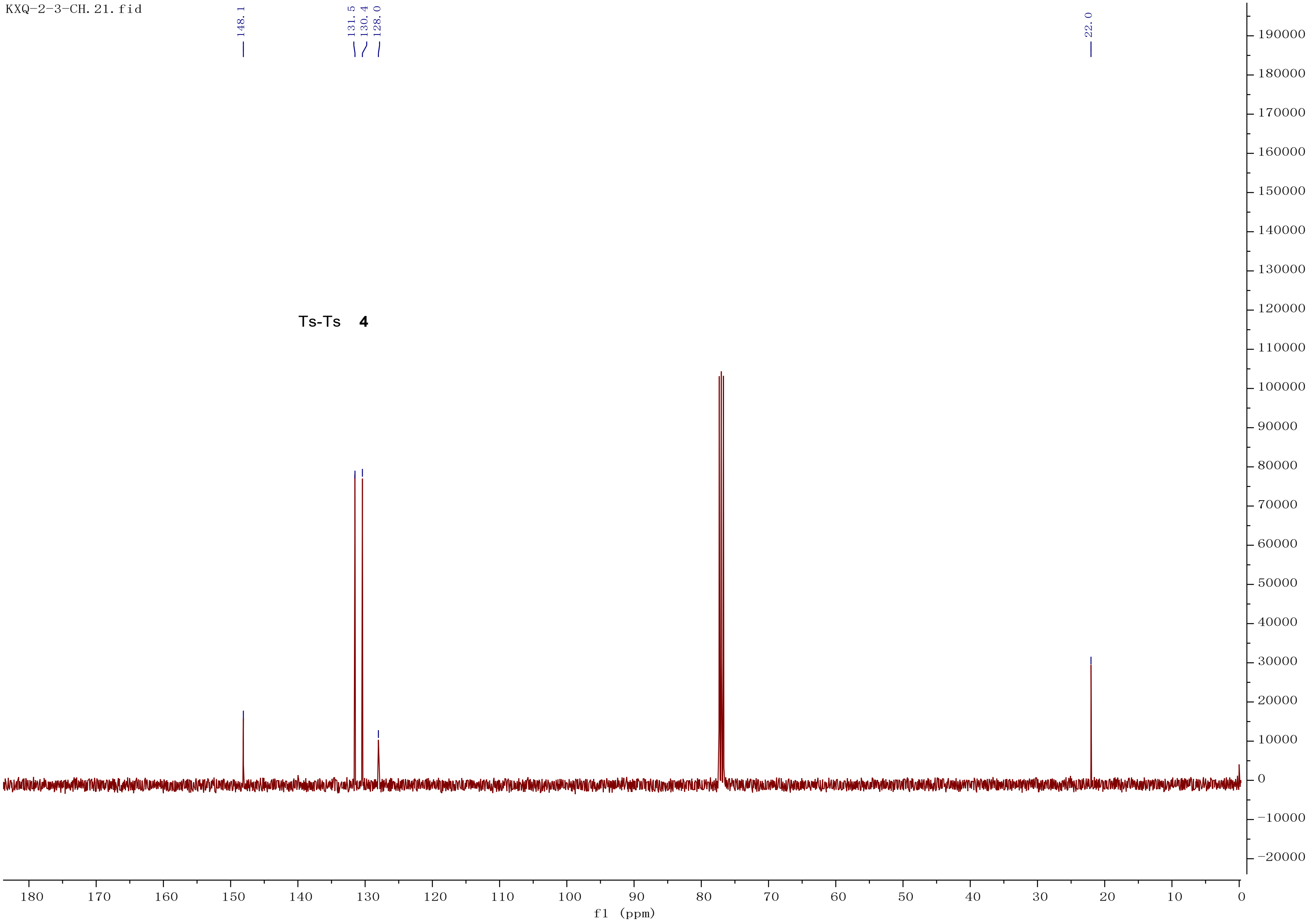

LLC-1025-3-CH.32.fid
8.36 8.35 8.34 8.33 7.83 7.83 7.82 7.81 2.64 2.62 2.60 2.12 2.04 2.00 1.59 1.56 1.54 1.52 1.51 1.43 1.42 1.41 1.40 1.38 1.37 1.36 1.36 1.34 1.34 1.33 1.32 1.32 1.31 1.31 1.30 1.28 1.27 1.26 1.26 1.24 1.23 1.21 1.16 1.15 1.15 1.14 1.13 1.13 1.12 1.11 1.11 1.10 1.10 1.09 1.08 1.08 1.07 1.06 1.06 1.05 0.90 0.89 0.89 0.87 0.86 0.84 0.83
NC
O
O
O
Me
Me
Me
Me
1.98
2.00
2.04
3.01
6.17
2.16
4.05
23.84
14.21
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5 −2.0
f1 (ppm)
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
−1000000

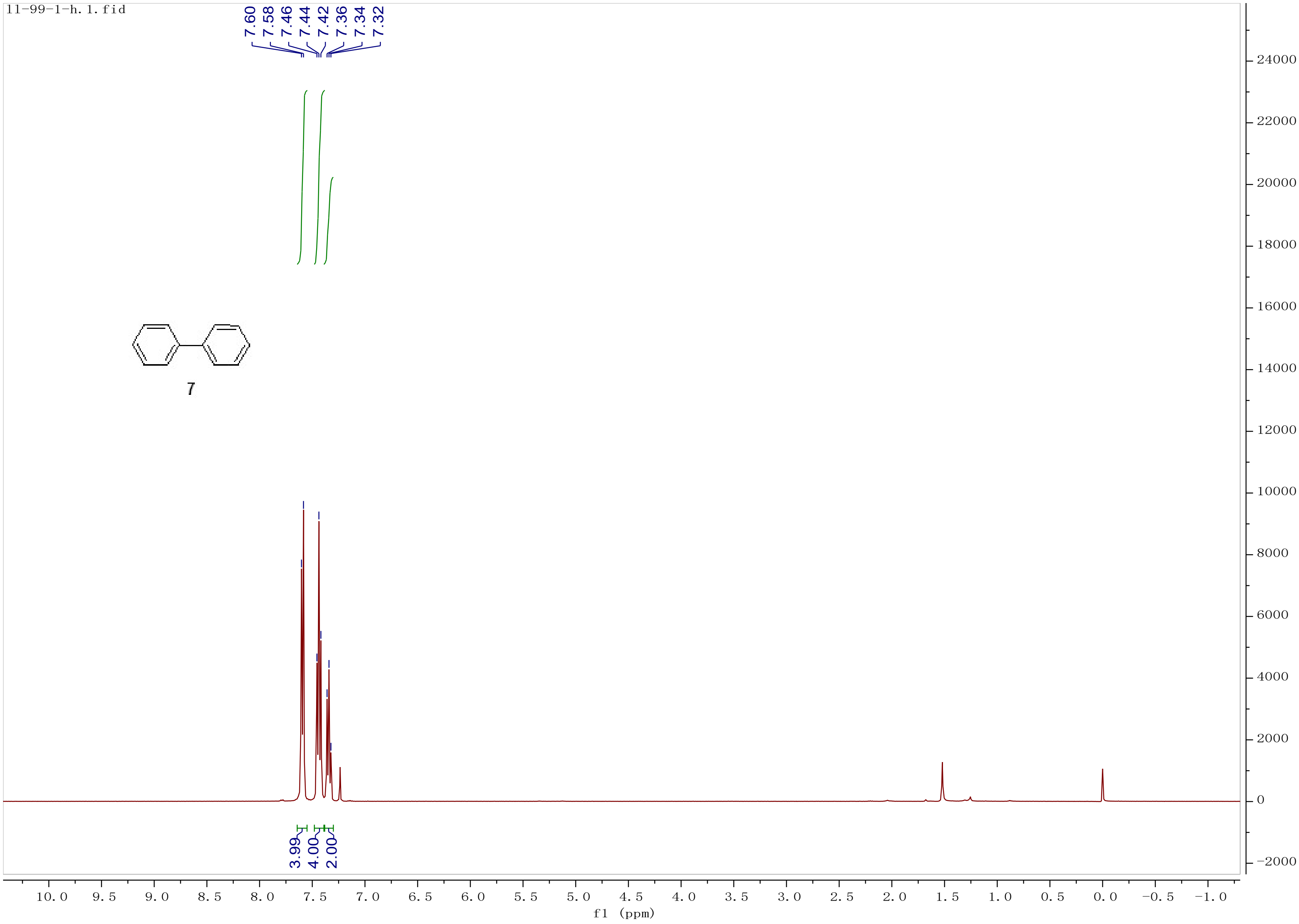

LL-1025-3-CH.33.fid
163.6
149.8
140.4
133.5
132.5
130.6
126.6
124.9
123.4
118.0
117.7
116.9
75.2
39.4
37.4
37.3
32.8
32.8
32.7
28.0
24.8
24.5
22.8
22.7
22.7
21.1
20.7
19.8
19.7
19.6
13.1
12.2
11.9
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
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)

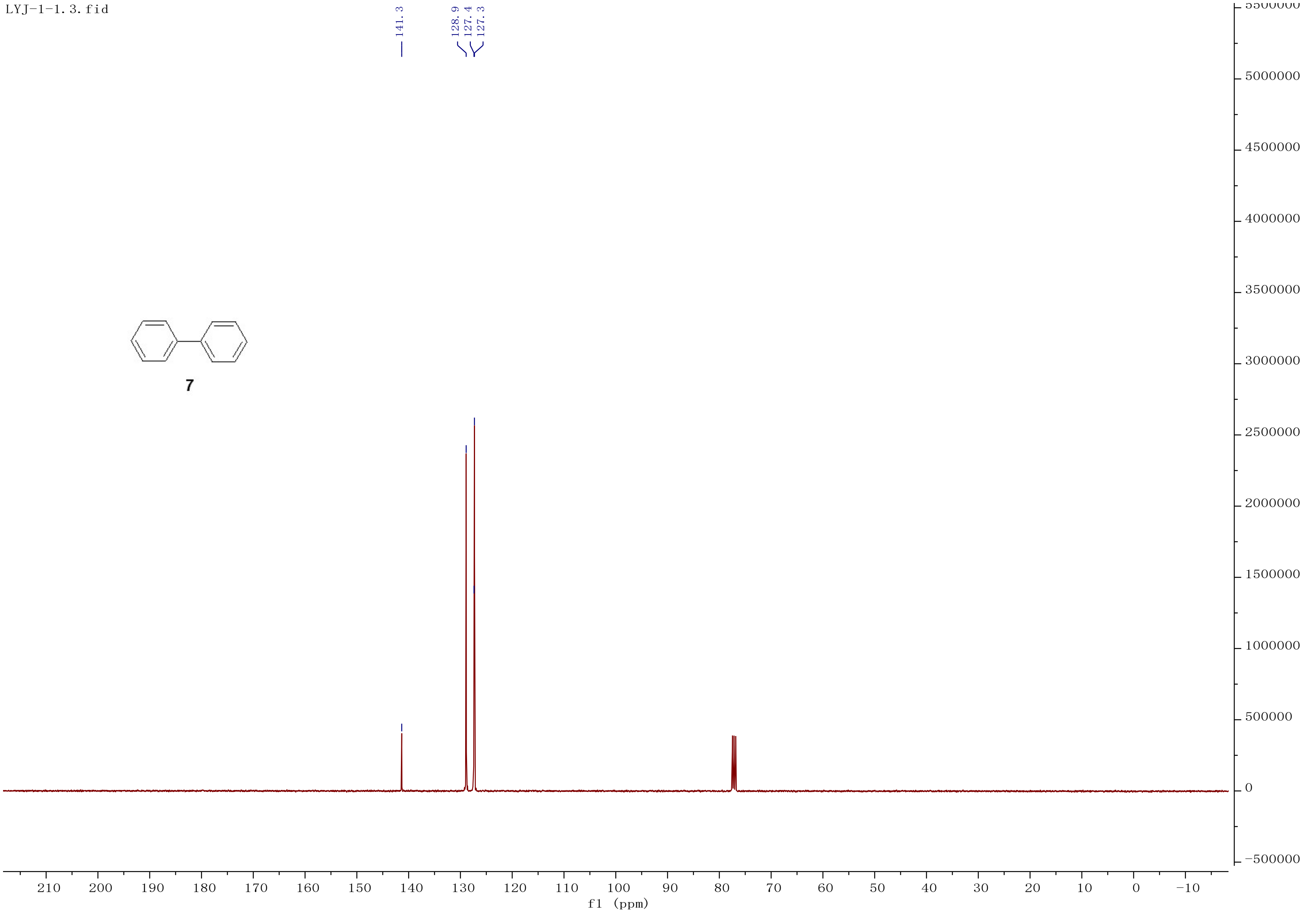

LL-1025-4-CH.42.fid
8.14
8.14
8.12
8.12
7.76
7.76
7.74
7.74
5.38
5.38
5.37
5.37
5.37
5.36
5.36
4.40
4.39
4.38
4.38
4.36
4.36
4.35
4.35
4.34
2.47
2.46
2.46
2.45
2.44
2.44
2.43
2.43
2.42
2.41
2.39
2.39
2.38
2.37
2.36
2.26
2.26
2.25
2.25
2.23
2.23
2.22
2.22
2.22
2.12
2.11
2.11
2.10
2.10
2.09
2.09
2.08
1.28
1.17
1.15
0.88
0.87
0.85
0.85
0.85
0.84
0.83
H
H
O
O
CN
1.99
2.00
0.99
2.03
1.94
1.05
2.07
1.98
3.28
1.08
4.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
7.5×10⁷
7.0×10⁷
6.5×10⁷
6.0×10⁷
5.5×10⁷
5.0×10⁷
4.5×10⁷
4.0×10⁷
3.5×10⁷
3.0×10⁷
2.5×10⁷
2.0×10⁷
1.5×10⁷
1.0×10⁷
5.0×10⁶
0.0

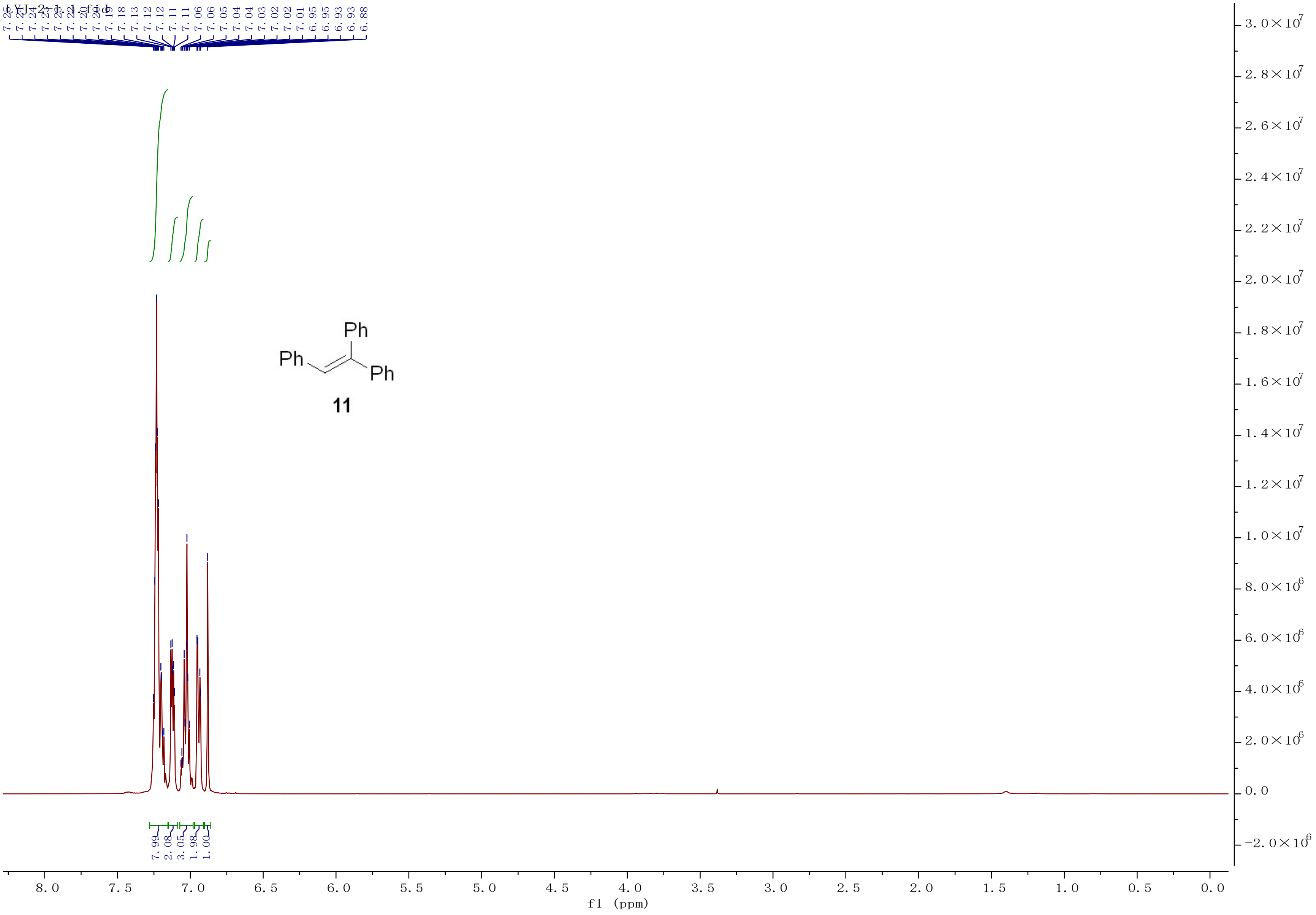

LL-1025-4-CH.43.fid
164.8
143.9
134.2
132.2
130.0
119.2
118.0
116.3
64.0
45.7
40.7
38.0
35.9
31.7
31.4
26.2
21.1
H
H
O
O
CN
900000
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


KXQ-2-3-CH.20.fid
7.85
7.84
7.83
7.44
7.42
2.51
Ts-Ts
4
3.90
4.00
6.19
3.0×10^7
2.8×10^7
2.6×10^7
2.4×10^7
2.2×10^7
2.0×10^7
1.8×10^7
1.6×10^7
1.4×10^7
1.2×10^7
1.0×10^7
8.0×10^6
6.0×10^6
4.0×10^6
2.0×10^6
0.0
−2.0×10^6
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
f1 (ppm)

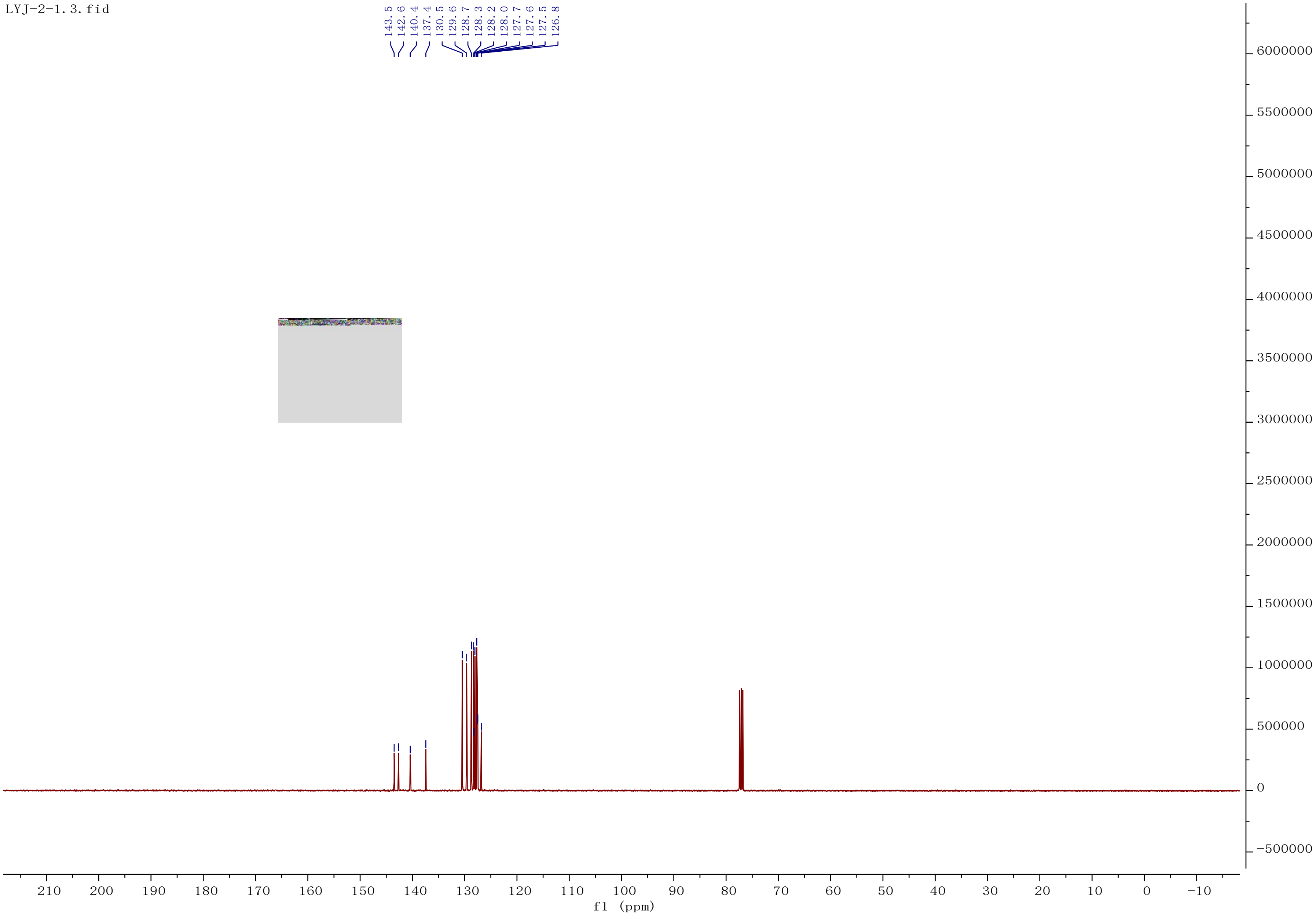

KXQ-2-3-CH.21.fid
148.1
131.5
130.4
128.0
22.0
Ts-Ts **4**
190000
180000
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
−10000
−20000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


ll-99-1-h.1.fid
7.60
7.58
7.46
7.44
7.42
7.36
7.34
7.32
7
3.99
4.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000


LYJ-1-1.3.fid
141.3
128.9
127.4
127.3
7
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
−500000
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)


LYJ-2-1.1.fid
7.25
7.24
7.24
7.23
7.23
7.22
7.20
7.20
7.19
7.18
7.13
7.12
7.12
7.11
7.11
7.06
7.06
7.05
7.04
7.04
7.03
7.02
7.02
7.01
6.95
6.95
6.93
6.93
6.88
Ph
Ph
Ph
7.99
2.08
3.05
1.98
1.00
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
f1 (ppm)
3.0×10^7
2.8×10^7
2.6×10^7
2.4×10^7
2.2×10^7
2.0×10^7
1.8×10^7
1.6×10^7
1.4×10^7
1.2×10^7
1.0×10^7
8.0×10^6
6.0×10^6
4.0×10^6
2.0×10^6
0.0
-2.0×10^6

11


LYJ-2-1.3.fid
143.5
142.6
140.4
137.4
130.5
129.6
128.7
128.3
128.2
128.0
127.7
127.6
127.5
126.8
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
−500000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

8. References

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