Supplementary Information

Cu-Catalyzed alkylation–cyanation type difunctionalization of styrenes with aliphatic aldehydes and TMSCN via decarbonylation

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Table of Contens

I. General information

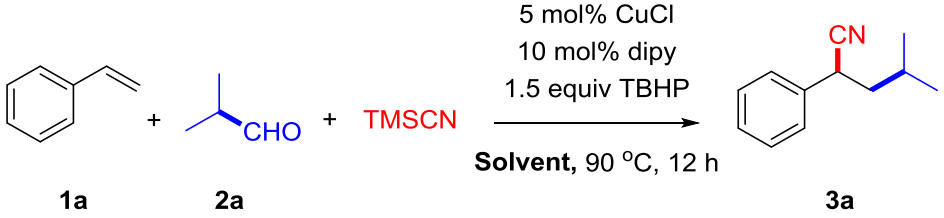
Unless otherwise noted, all commercially available compounds were used as purchased. Thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F254 precoated plates (0.25 mm). The developed chromatography was analyzed by UV lamp (254 nm). High-resolution mass spectra (HRMS) were obtained from a JEOL JMS-700 instrument (ESI). Melting points are uncorrected. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance 400 spectrometer at ambient temperature. Chemical shifts for ^{1}H NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 7.26 ppm, DMSO: δ 2.50 ppm). Chemical shifts for ^{13}C NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent as the internal standard ($CDCl_3$: δ 77.16 ppm, DMSO: δ 39.52 ppm). Data are reported as following: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, t = triplet, q = quartet, m = multiplet, br = broad signal), coupling constant (Hz) and integration.

II. General experimental procedures

A general experimental procedure is described as following:
An oven-dried microwave reaction vessel was charged with $Cu(CH_3CN)_4PF_6$ (5 mol%, 3.7 mg), 2,2'-dipy (10 mol%, 3.1 mg), styrene (**1a**, 0.2 mmol, 20.8 mg), TMSCN (0.8 mmol, 79.4 mg), isobutyraldehyde (**2a**, 1.0 mmol, 72.0 mg), TBHP (0.3 mmol, 38.6 mg, 70% in water) and trifluoromethylbenzene (1.0 mL) under air atmosphere. The vessel was sealed and stirred at 100 ℃ (oil bath temperature) for 12 h. Afterwards the resulting mixture was cooled to room temperature, concentrated in vacuo and purified by column chromatography on silica gel with a mixture of ethyl dichloromethane/petroleum ether as the eluent to give the product **3a** 22.4 mg in 65% yield.

III. Conditions optimization

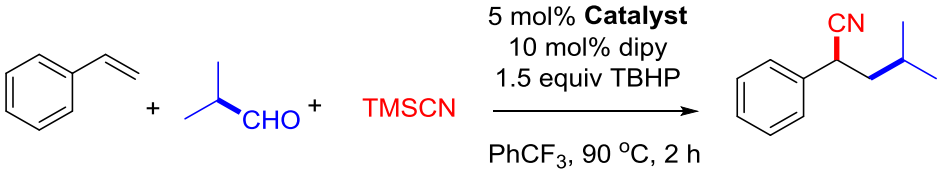
Table S1. Optimization of the solvent[a]



entry	Solvent	Yield[%][b]
1	MTBE	14
2	PhF	22
3	CH_3CN	trace
4	CH_2Cl_2	7
5	$PhCH_3$	9
6	PhCl	18
7	$PhCF_3$	30
8	EA	18

[a]Reaction conditions: styrene **1a** (1.0 equiv, 0.2 mmol), isobutyraldehyde **2a** (3.0 equiv, 0.6 mmol), TMSCN (2.0 equiv, 0.4 mmol), TBHP (1.5 equiv, 0.3 mmol, 70% in water), CuCl (5 mol%, 0.01 mmol), dipy (10 mol%, 0.02 mmol), **Solvent** (1.0 mL) were reacted at 90 °C (oil bath temperature) for 12 h under air atmosphere. [b]GC yield.

Table S2. Optimization of the catalyst[a]

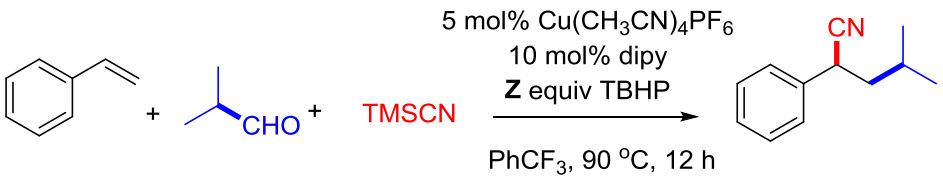


1a **2a** **3a**

entry	Catalyst(mol%)	Yield[%][b]
1	CuCl	30
2	CuBr	28
3	CuI	17
4	$Cu(acac)_2$	18
5	$CuBr_2$	7
6	$Cu(OAc)_2$	24
7	$Cu(CH_3CN)_4PF_6$	33

[a]Reaction conditions: styrene **1a** (1.0 equiv, 0.2 mmol), isobutyraldehyde **2a** (3.0 equiv, 0.6 mmol), TMSCN (2.0 equiv, 0.4 mmol), TBHP (1.5 equiv, 0.3 mmol, 70% in water), **Catalyst** (5 mol%, 0.01 mmol), dipy (10 mol%, 0.02 mmol), $PhCF_3$ (1.0 mL) were reacted at 90 °C (oil bath temperature) for 12 h under air atmosphere. [b]GC yield.

Table S3. Optimization of the the reactants ratio[a]



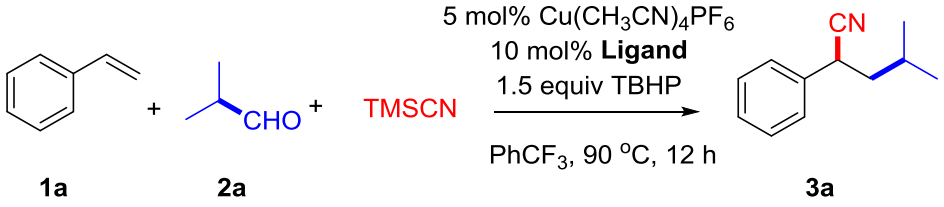
1a **2a X** equiv **Y** equiv **3a**

Entry	Ratio (X:Y:Z)	Yield[%][b]

1	**3.0:2.0:1.5**	**33**
2	**5.0:2.0:1.5**	**41**
3	**4.0:3.0:1.5**	**46**
4	**5.0:3.0:1.5**	**57**
5	**5.0:4.0:1.5**	**62**
6	**5.0:5.0:1.5**	**62**
7	**5.0:4.0:2.0**	**55**
8	**5.0:4.0:1.2**	**56**

[a]Reaction conditions: styrene **1a** (1.0 equiv, 0.2 mmol), isobutyraldehyde **2a** (**X** equiv), TMSCN (**Y** equiv), TBHP (**Z** equiv, 70% in water), $Cu(CH_3CN)_4PF_6$ (5 mol%, 0.01 mmol), dipy (10 mol%, 0.02 mmol), $PhCF_3$ (1.0 mL) were reacted at 90 ^oC (oil bath temperature) for 12 h under air atmosphere. [b]GC yield.

Table S4. Optimization of the Ligand[a]

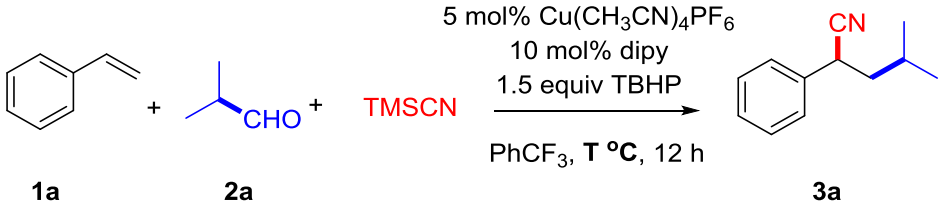


1a **2a** **3a**

Entry	Ligand	Yield[%][b]
1	**dipy**	**62**
2	**4,4'-dimethyl-2,2'-dipyridyl**	**32**
3	**4,4'-dimethoxy- 2,2'-dipyridyl**	**48**
4	**4,4'-dibromo- 2,2'-dipyridyl**	**57**
5	**4,4'-Bis-(methoxycarbonly)-2,2'-bipyridine**	**32**
6	**------**	**trace**

[a]Reaction conditions: styrene **1a** (1.0 equiv, 0.2 mmol), isobutyraldehyde **2a** (5.0 equiv, 1.0 mmol), TMSCN (4.0 equiv, 0.8 mmol), TBHP (1.5 equiv, 0.3 mmol, 70% in water), $Cu(CH_3CN)_4PF_6$ (5 mol%, 0.01 mmol), **Ligand** (10 mol%, 0.02 mmol), $PhCF_3$ (1.0 mL) were reacted at 90 ^oC (oil bath temperature) for 12 h under air atmosphere. [b]GC yield.

Table S5. Optimization of the temperature[a]



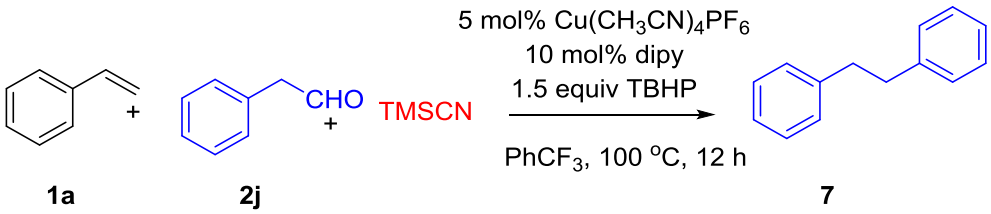
1a **2a** **3a**

Entry	T (^oC)	Yield[%][b]
1	**80**	**44**
2	**90**	**62**

3	**100**	**66**
4	**110**	**64**

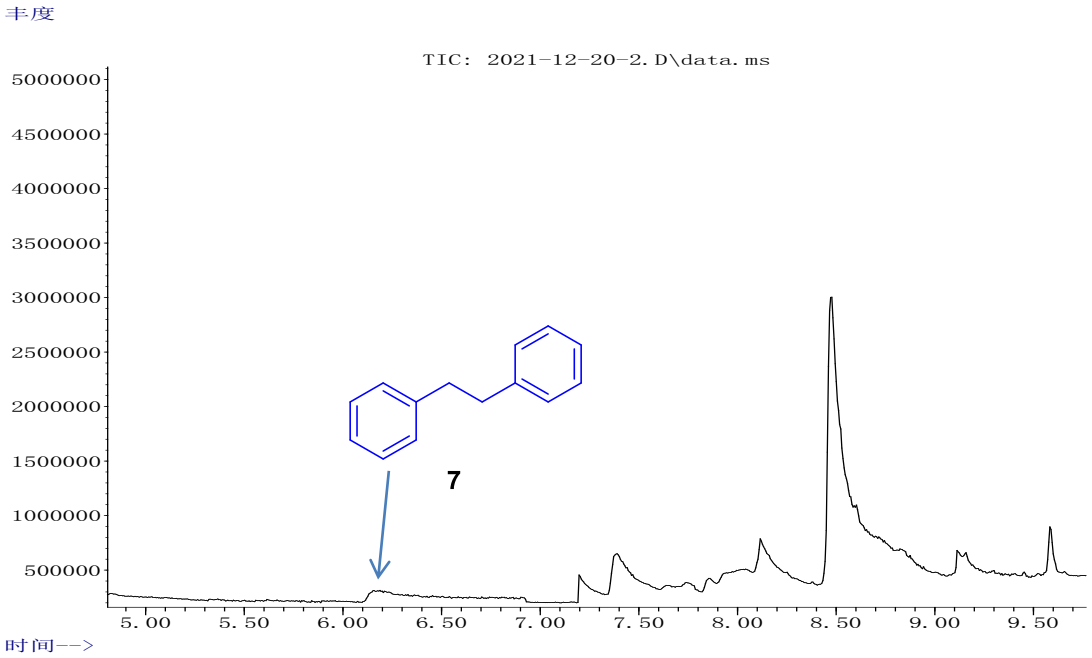
[a]Reaction conditions: styrene **1a** (1.0 equiv, 0.2 mmol), isobutyraldehyde **2a** (5.0 equiv, 1.0 mmol), TMSCN (4.0 equiv, 0.8 mmol), TBHP (1.5 equiv, 0.3 mmol, 70% in water), $Cu(CH_3CN)_4PF_6$ (5 mol%, 0.01 mmol), dipy (10 mol%, 0.02 mmol), $PhCF_3$ (1.0 mL) were reacted at **T** ^oC (oil bath temperature) for 12 h under air atmosphere. [b]GC yield.

IV. Detection of homo-coupling by-product



An oven-dried microwave reaction vessel was charged with $Cu(CH_3CN)_4PF_6$ (5 mol%, 3.7 mg), 2,2'-dipy (10 mol%, 3.1 mg), styrene (**1a**, 0.2 mmol, 20.8 mg), TMSCN (0.8 mmol, 79.4 mg), phenylacetaldehyde (**2j**, 1.0 mmol,120.0 mg), TBHP (0.3 mmol, 38.6 mg, 70% in water) and trifluoromethylbenzene (1.0 mL) under air atmosphere. The vessel was sealed and stirred at 100 ℃ (oil bath temperature) for 12 h. Then, the reaction mixture was cooled, adding 10 mL saturated NaCl solution and extracted with EA. Only a trace amount (<1%) of 1,2-diphenylethane was detected by GC-MS (as the following copied spectrum).

The oxidative decarbonylation of phenylacetaldehyde (**2j**) would produce a benzyl radical, which indeed could undergo radical-radical coupling to afford the by-product 1,2-diphenylethane **7**. However, due to the "***persistent radical effect***", the benzyl radical is so reactive that it could only exist in a very low concentration, thus suppressing it's homo-coupling.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2000000
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1000000
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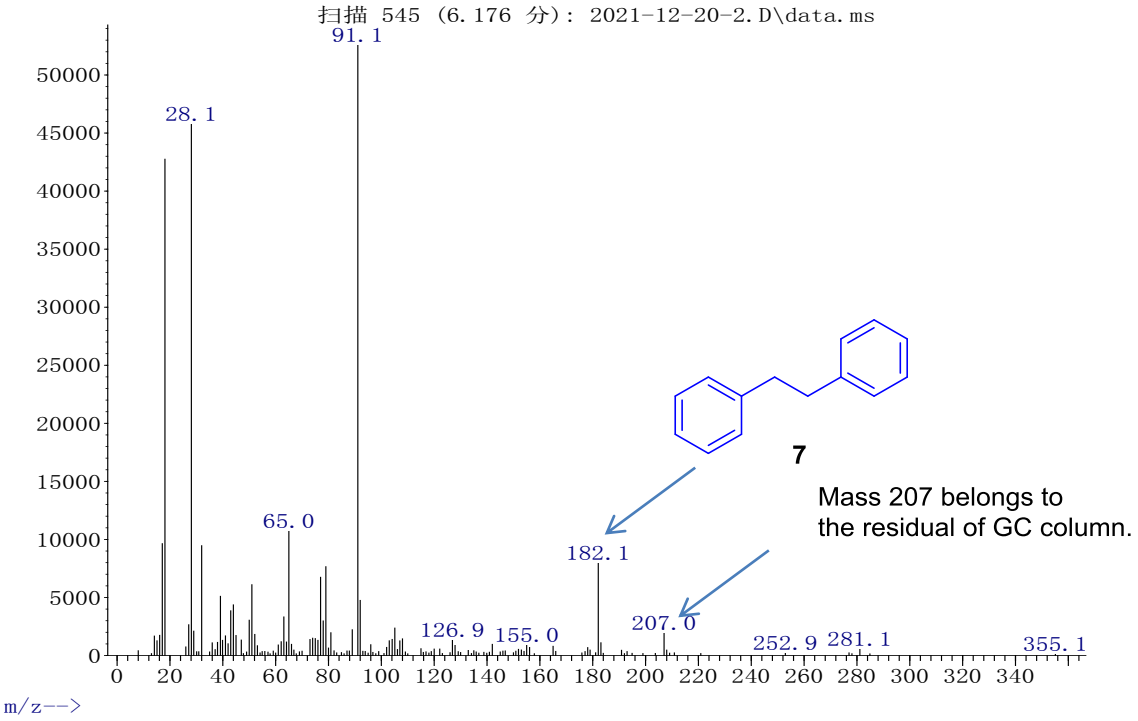
时间-->
丰度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355.1
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45000
40000
35000
30000
25000
20000
15000
10000
5000
0
0
20
40
60
80
100
120
140
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180
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260
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300
320
340
m/z-->
7
Mass 207 belongs to
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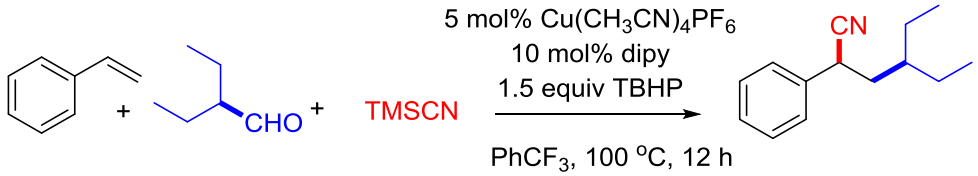
V. Scale-up experiments



1a **2d** **4d**

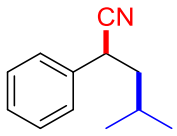
Entry	1a(mmol)	Yield[%][b]
1	**0.2**	**62**
2	**1**	**53**
3	**5**	**56**
4	**10**	**53**

[a]Reaction conditions: styrene **1a** (1.0 equiv), isobutyraldehyde **2a** (5.0 equiv), TMSCN (4.0 equiv), TBHP (1.5 equiv, 70% in water), $Cu(CH_3CN)_4PF_6$ (5 mol%), dipy (10 mol%), $PhCF_3$ were reacted at **100**°C (oil bath temperature) for 12 h under air atmosphere. [b]GC yield and isolated yield in parentheses.

Experimental Procedures:
An oven-dried microwave reaction vessel was charged with $Cu(CH_3CN)_4PF_6$ (5 mol%, 186.4 mg), 2, 2'-dipy (10 mol%, 156.2 mg), styrene (**1a**, 10 mmol, 1.04 g), TMSCN (40 mmol, 3.97 g), 2-ethylbutanal (**2d**, 50 mmol, 5.0 g), TBHP (15 mmol, 1.93 g, 70% in water) and trifluoromethylbenzene (50 mL) under air atmosphere. The vessel was sealed and stirred at 100 ℃ (oil bath temperature) for 12 h. Afterwards the resulting mixture was cooled to room temperature, concentrated in vacuo and purified by column chromatography on silica gel with a mixture of ethyl dichloromethane/petroleum ether as the eluent to give the product **4d** 1.07g in 53% yield.

VI. Spectra data of products

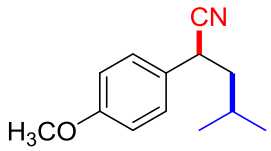
(3a) 4-Methyl-2-phenylpentanenitrile[1]



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (22.4mg, 65%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 - 7.32 (m, 5H), 3.80 (dd, *J* = 6.4 Hz, 9.6 Hz, 1H), 1.90 - 1.78 (m, 2H), 1.67 - 1.60 (m, 1H), 0.99 (d, *J* = 5.2 Hz, 3H), 0.98 (d, *J* = 5.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.49, 129.21, 128.10, 127.33, 121.12, 45.13,

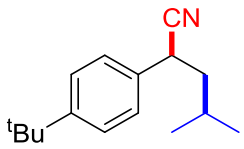
35.65, 26.18, 22.67, 21.74. IR (cm^{-1}): 2959, 2871, 2239, 1460, 699.

(3b) 4-Methyl-2-(4-methoxyphenyl)pentanenitrile[1]



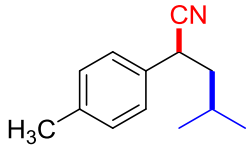
The title compound was prepared according to the general procedure described above by the reaction between 4-methoxystyrene (**1b**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (20.3 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (dt, *J* = 3.2 Hz, 10.0 Hz, 2H), 6.90 (dt, *J* = 2.8 Hz, 9.6 Hz, 2H), 3.81 (s, 3H), 3.75 (dd, *J* = 6.4 Hz, 9.2 Hz, 1H), 1.91 - 1.75 (m, 2H), 1.61 (m, 1H), 0.98 (d, *J* = 3.6 Hz, 3H), 0.97 (d, *J* = 3.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.41, 128.47, 128.47, 121.43, 114.59, 55.48, 45.16, 34.82, 26.10, 22.64, 21.82. IR (cm^{-1}): 2959, 2872, 2238, 1253, 832.

(3c) 2-(4-Tert-butylphenyl)-4-methylpentanenitrile



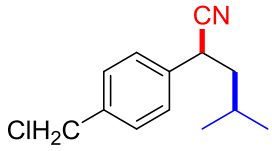
The title compound was prepared according to the general procedure described above by the reaction between 4-tert-butylstyrene (**1c**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (27.4 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 - 7.37 (m, 2H), 7.26 - 7.24 (m, 2H), 3.78 (dd, *J* = 6.0 Hz, 9.2 Hz, 1H), 1.93 - 1.79 (m, 2H) 1.65 - 1.58 (m, 1H), 1.31 (s, 9H), 0.99 (d, *J* = 4.8 Hz, 3H), 0.97 (d, *J* = 4.8 Hz, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.11, 133.38, 126.99, 126.11, 121.32, 45.08, 35.14, 34.66, 31.39, 26.15, 22.70, 21.73. IR (cm^{-1}): 2961, 2871, 2239, 1466, 835. HRMS: calcd. for $C_{16}H_{23}N\ Na^{+}$ $[M + Na]^{+}$: 252.1723; Found: 252.1728.

(3d) 4-Methyl-2-(4-methylphenyl)pentanenitrile



The title compound was prepared according to the general procedure described above by the reaction between 4-methylphenylene (**1d**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (22.0 mg, 59%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 - 7.16 (m, 4H), 3.77 (dd, *J* = 6.4 Hz, 9.2 Hz, 1H), 2.35 (s, 3H), 1.92 - 1.76 (m, 2H), 1.64 - 1.57 (m, 1H). 0.98 (d, *J* = 4.8 Hz, 3H), 0.97 (d, *J* = 4.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.91, 133.43, 129.86, 127.21, 121.35, 45.16, 35.22, 26.12, 22.66, 21.77, 21.19; IR (cm^{-1}): 2922, 2852, 2362, 1464, 809. HRMS: calcd. for $C_{13}H_{17}N\ Na^{+}$ $[M + Na]^{+}$: 210.1253; Found: 210.1255.

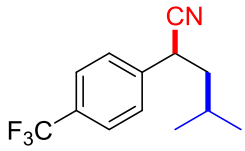
(3e) 2-(4-(chloromethyl)phenyl)-4-methylpentanenitrile



The title compound was prepared according to the general procedure described above by the reaction between 1-(chloromethyl)-4-ethenyl-benzene (**1e**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (24.3 mg, 55%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 4.57 (s, 2H), 3.81 (dd, *J* = 6.0 Hz, 9.2 Hz, 1H), 1.93 - 1.77 (m, 2H), 1.65 - 1.58 (m, 1H), 0.99 (d, *J* = 4.8 Hz, 3H), 0.98 (d, *J* = 4.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.47, 136.67, 129.39, 127.71, 120.81, 45.62, 44.98, 35.32, 26.15, 22.62, 21.68. IR (cm^{-1}): 2957, 2870, 2362, 1240, 753. HRMS: calcd. for $C_{13}H_{16}ClN\ Na^{+}$ $[M + Na]^{+}$: 244.0863; Found: 244.0876.

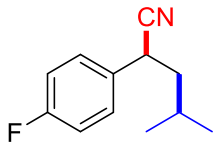
(3f) 4-methyl-2-(4-(trifluoromethyl)phenyl)pentanenitrile



The title compound was prepared according to the general procedure described above by the reaction between 4-vinylbenzotrifluoride (**1f**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (25.8 mg, 53%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.0 Hz, 2H), 7.47 (d, *J* = 8.0 Hz, 2H), 3.88 (dd, *J* = 6.0 Hz, 9.6 Hz, 1H), 1.96 - 1.88 (m, 2H), 1.67 - 1.61 (m, 1H), 1.00 (t, *J* = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.46, 130.64 (q, *J* = 32.6 Hz), 127.83, 126.55 (q, *J* = 3.7 Hz), 123.96 (d, *J* = 270.5 Hz), 120.29, 45.01, 35.60, 26.28, 22.68, 21.68; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.71 (s, 1F). IR (cm^{-1}): 2962, 2874, 2243, 1127, 740.07. HRMS: calcd. for $C_{13}H_{14}F_3N\ Na^{+}$ $[M + Na]^{+}$: 264.0971; Found: 264.0982.

(3g) 2-(4-fluorophenyl)-4-methylpentanenitrile

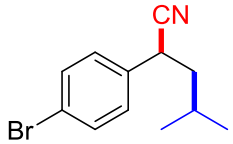


The title compound was prepared according to the general procedure described above by the reaction between 4-fluorostyrene (**1g**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (21.7 mg, 57%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 - 7.28 (m, 2H), 7.10 - 7.04 (m, 2H), 3.79 (dd, *J* = 6.4 Hz, 9.6 Hz, 1H), 1.93 - 1.78 (m, 2H), 1.64 - 1.57 (m, 1H), 0.99 (d, *J* = 4.4 Hz, 3H),

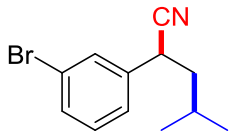
0.98 (d, J = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.44 (d, J = 245.6 Hz), 132.23 (d, J = 3.2 Hz), 129.03 (d, J = 8.2 Hz), 120.96, 116.20 (d, J = 21.6 Hz), 45.13, 34.94, 26.13, 22.65, 21.73; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.96 (s, 1F). IR (cm^{-1}): 2925, 2240, 2853, 1231, 837. HRMS: calcd. for $C_{12}H_{14}FN\ Na^+$ $[M + Na]^+$: 214.1002; Found: 214.1002.

(3h) 2-(4-bromophenyl)-4-methylpentanenitrile



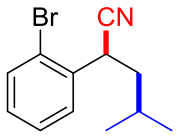
The title compound was prepared according to the general procedure described above by the reaction between 4-bromostyrene (**1h**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (39.8 mg, 60%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 - 2.28 (m, 2H), 7.09 - 7.05 (m, 2H), 3.79 (dd, J = 6.4 Hz, 9.6 Hz, 1H), 1.93 - 1.78 (m, 2H), 1.64 - 1.60 (m, 1H), 1.00 (d, J = 3.6 Hz, 3H), 0.98 (d, J = 3.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.48, 132.37, 129.03, 122.13, 120.57, 44.93, 35.16, 26.15, 22.62, 21.70. IR (cm^{-1}): 2959, 2872, 2240, 1488, 828. HRMS: calcd. for $C_{12}H_{14}BrN\ Na^+$ $[M + Na]^+$: 274.0202; Found: 274.0200.

(3i) 2-(3-bromophenyl)-4-methylpentanenitrile



The title compound was prepared according to the general procedure described above by the reaction between 3-bromostyrene (**1i**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (41.8 mg, 63%)
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 - 7.44 (m, 2H), 7.29 - 7.33 (m, 2H), 3.78 (dd, J = 6.0 Hz, 9.6 Hz, 1H), 1.93 - 1.80 (m, 2H), 1.64 - 1.57 (m, 1H), 1.00 (d, J = 4.0 Hz, 3H), 0.99 (d, J = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.64, 131.36, 130.77, 130.45, 126.01, 123.17, 120.42, 44.96, 35.30, 26.22, 22.69, 21.65. IR (cm^{-1}): 2959, 2872, 2241, 1471, 693. HRMS: calcd. for $C_{12}H_{14}BrN\ Na^+$ $[M + Na]^+$: 274.0202; Found: 274.0204.

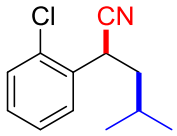
(3j) 2-(2-bromophenyl)-4-methylpentanenitrile



The title compound was prepared according to the general procedure described above by the reaction between 2-bromostyrene (**1j**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (41.8 mg, 63%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 - 7.56 (m, 2H), 7.39 - 7.35 (m, 1H), 7.21 - 7.17

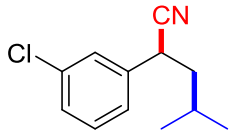
(m, 1H), 4.33 (dd, *J* = 6.8 Hz, 23.2 Hz, 1H), 2.01 - 1.91 (m, 1H), 1.82 - 1.76 (m, 1H), 1.67 - 1.60 (m, 1H), 1.07 (d, *J* = 6.8 Hz, 3H), 1.01 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.15, 133.44, 129.73, 128.93, 128.50, 122.87, 120.57, 43.78, 35.67, 26.71, 23.18, 21.20. IR (cm^{-1}): 2959, 2872, 2241, 1469, 755. HRMS: calcd. for $C_{12}H_{14}BrN\ Na^+$ $[M + Na]^+$: 274.0202; Found: 274.0212.

(3k) 2-(2-chlorophenyl)-4-methylpentanenitrile



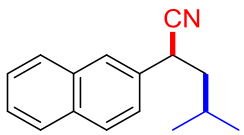
The title compound was prepared according to the general procedure described above by the reaction between 2-chlorostyrene (**1k**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (24.1mg, 58%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 - 7.29 (m, 3H), 7.24 - 7.21 (m, 1H), 3.79 (dd, *J* = 6.0 Hz, 9.2 Hz, 1H), 1.93 - 1.79 (m, 2H), 1.65 - 1.58 (m, 1H), 1.00 (d, *J* = 4.0 Hz, 3H), 0.99 (d, *J* = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.37, 135.07, 130.50, 128.41, 127.55, 125.54, 120.44, 44.91, 35.33, 26.19, 22.66, 21.65. IR (cm^{-1}): 2960, 2872, 2241, 1473, 784. HRMS: calcd. for $C_{12}H_{14}ClN\ Na^+$ $[M + Na]^+$: 230.0707; Found: 230.0706.

(3l) 2-(3-chlorophenyl)-4-methylpentanenitrile



The title compound was prepared according to the general procedure described above by the reaction between 3-chlorostyrene (**1l**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (24.1 mg, 58%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 - 7.30 (m, 3H), 7.24 - 7.21 (m, 1H), 3.79 (dd, *J* = 6.0 Hz, 9.2 Hz, 1H), 1.94 - 1.79 (m, 2H), 1.65 - 1.58 (m, 1H), 1.00 (d, *J* = 4.0 Hz, 3H), 0.99 (d, *J* = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.40, 135.13, 130.53, 128.45, 127.60, 125.56, 120.46, 44.96, 35.38, 26.23, 22.70, 21.69. IR (cm^{-1}): 2959, 2931, 2241, 1473, 784. HRMS: calcd. for $C_{12}H_{14}ClN\ Na^+$ $[M + Na]^+$: 230.0707; Found: 230.0704 .

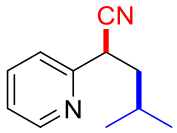
(3m) 4-methyl-2-(naphthalen-2-yl)pentanenitrile



The title compound was prepared according to the general procedure described above by the reaction between 2-vinylnaphthalene (**1m**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (25.4 mg, 57%).

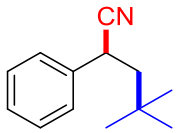
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 - 7.81(m, 4H), 7.54 - 7.48 (m, 2H), 7.42 - 7.40 (m, 1H), 3.97 (dd, *J* = 6.0 Hz, 9.6 Hz, 1H), 2.02 - 1.95 (m, 1H), 1.90 - 1.82 (m, 1H), 1.76 - 1.69 (m, 1H), 1.01 (t, *J* = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.71, 133.42, 132.87, 129.17, 127.91, 127.82, 126.79, 126.53, 126.31, 124.90, 121.13, 44.97, 35.77, 26.22, 22.68, 21.77. IR (cm^{-1}): 2959, 2871.2, 2239, 1465, 749. HRMS: calcd. for $C_{16}H_{17}N\ Na^+$ $[M + Na]^+$: 246.1253; Found: 246.1266.

(3n) 4-methyl-2-(pyridin-3-yl)pentanenitrile[2]



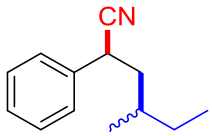
The title compound was prepared according to the general procedure described above by the reaction between 2-vinylpyridine (**1n**) with TMSCN and isobutyraldehyde (**2a**), and purified by flash column chromatography as colorless oil (15.0 mg, 43%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (dd, *J* = 0.8 Hz, 4.8 Hz, 1H), 7.72 (td, *J* = 1.6 Hz, 7.6Hz, 1H), 7.43 (d, *J* = 7.6 Hz, 1H), 7.24 (ddd, *J* = 0.8 Hz, 4.8 Hz, 7.6 Hz, 1H), 4.0 (dd, *J* = 6.0 Hz, 10.0 Hz, 1H), 1.98 - 1.86 (m, 2H), 1.84 - 1.75 (m, 1H), 0.99 (t, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.87, 149.98, 137.47, 123.01, 121.74, 120.35, 43.25, 38.24, 26.33, 22.82, 21.57. IR (cm^{-1}): 2960, 2873, 2242, 1470, 770.

(4b) 4,4-dimethyl-2-phenylpentanenitrile[3]



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with TMSCN and pivalaldehyde (**2b**), and purified by flash column chromatography as colorless oil (28.1 mg, 75%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 - 7.30 (m, 5H), 3.75 (dd, *J* = 3.6 Hz, 10.4 Hz, 1H), 2.04 (dd, *J* = 10.4 Hz, 14.0 Hz, 1H), 1.66 (dd, *J* = 3.6 Hz, 14.0 Hz, 1H), 1.05 (s, 9H); ^{13}C NMR (100 MHz, CDCl3) δ 137.94, 129.25, 127.96, 127.25, 122.24, 50.04, 33.38, 31.28, 29.48. IR (cm^{-1}): 2957, 2870, 2239, 1473, 699.

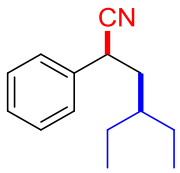
(4c) 4-methyl-2-phenylhexanenitrile[4]



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with TMSCN and 2-methylbutanal (**2c**), and purified by flash column chromatography as colorless oil (19.8 mg, 53%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 - 7.29 (m, 5H), 3.86 - 3.78 (m, 1H), 1.99 (ddd, *J* = 4.0 Hz, 10.8 Hz, 13.6 Hz, 0.52×1H), 1.84 - 1.77 (m, 0.99×1H), 1.73 - 1.64 (m,

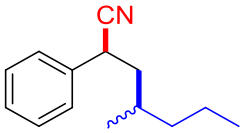
0.52×1H), 1.57 - 1.34 (m, 2H), 1.29 - 1.16 (m, 1H), 1.00 - 0.86 (m, 6H); ^{13}C NMR δ (100 MHz, $CDCl_3$) 136.69, 136.42, 129.20, 128.11, 128.05, 127.39, 127.26, 121.38, 120.98, 43.32, 42.96, 35.66, 35.31, 32.63, 32.05, 29.67, 28.44, 19.00, 18.55, 11.19, 10.86. IR (cm^{-1}): 2962, 2876, 2239, 1458, 699.

(4d) 4-ethyl-2-phenylhexanenitrile[5]



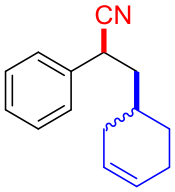
The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with TMSCN and 2-ethylbutanal (**2d**), and purified by flash column chromatography as colorless oil (24.5 mg, 61%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 - 7.32 (m, 5H), 3.81 (dd, *J* = 6.0 Hz, 9.6 Hz, 1H), 1.96 - 1.88 (m, 1H), 1.73 - 1.64 (m, 1H), 1.53 - 1.28 (m, 5H), 0.90 - 0.85 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.71, 129.23, 128.11, 127.34, 121.25, 39.98, 38.09, 35.58, 25.30, 24.52, 10.73, 10.18. IR (cm^{-1}): 2963, 2875, 2239, 1458, 699.

(4e) 4-methyl-2-phenylheptanenitrile



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with TMSCN and 2-methylpentanal (**2e**) and purified by flash column chromatography as colorless oil (22.1 mg, 55%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 - 7.30 (m, 5H), 3.86 - 3.79 (m, 1H), 1.97 (m, 0.45×1H), 1.88 - 1.82 (m, 0.56×1H), 1.80-1.75 (m, 1H), 1.65 - 1.62 (m, 0.49×1H), 1.57 - 1.50 (m, 0.51×1H), 1.42 - 1.11 (m, 4H), 1.00 - 0.86 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.68, 136.40, 129.22, 128.13, 128.07, 127.41, 127.28, 121.43, 121.01, 43.70, 43.42, 39.34, 38.26, 35.64, 35.30, 30.81, 30.42, 19.94, 19.78, 19.57, 19.02, 14.35. IR (cm^{-1}): 2959, 2871, 2239, 1458, 699. HRMS: calcd. for $C_{14}H_{19}N\,Na^+$ $[M + Na]^+$: 224.1410; Found: 224.1422.

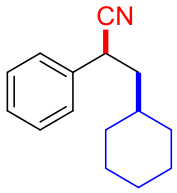
(4f) 3-(cyclohex-3-en-1-yl)-2-phenylpropanenitrile



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with TMSCN and 1-cyclohexene-3-carboxaldehyde (**2f**), and purified by flash column chromatography

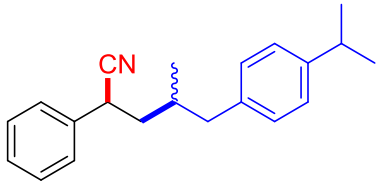
as colorless oil (20.3 mg, 48%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 - 7.32 (m, 5H), 5.66 - 5.64 (m, 2H), 3.89 - 3.83 (m, 1H), 2.20 (t, *J* = 18.4 Hz, 1H), 2.07 (s, 2H), 2.01 - 1.93 (m, 1H), 1.84 - 1.71 (m, 4H), 1.36 - 1.27 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.46, 136.37, 129.27, 128.18, 128.17, 127.39, 127.33, 127.13, 125.74, 125.48, 121.19, 121.08, 43.02, 42.59, 35.14, 35.06, 31.67, 31.44, 31.33, 31.10, 28.85, 27.92, 24.87, 24.70. IR (cm^{-1}): 2918, 2844, 2239, 1451, 698. HRMS: calcd. for $C_{15}H_{17}N\ Na^+$ $[M + Na]^+$: 234.1253; Found: 234.1260.

(4g) 3-cyclohexyl-2-phenylpropanenitrile[6]



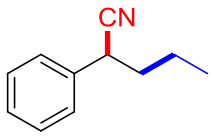
The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with TMSCN and cyclohexanecarbaldehyde (**4g**), and purified by flash column chromatography as colorless oil (16.2 mg, 38%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 - 7.29 (m, 5H), 3.84 (dd, *J* = 6.4 Hz, 10.0 Hz, 1H), 1.90 - 1.80 (m, 2H), 1.75 - 1.60 (m, 6H), 1.57 - 1.47 (m, 1H), 1,32 - 1.09 (m, 2H), 1.01 - 0.88 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.61, 129.21, 128.07, 127.33, 121.27, 45.83, 35.41, 34.92, 33.39, 32.46, 26.45, 26.07, 25.98. IR (cm^{-1}): 2925, 2862, 2239, 2449, 699.

(4h) 5-(4-isopropylphenyl)-4-methyl-2-phenylpentanenitrile



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with TMSCN and 3-(4-isopropylphenyl)-2-methylpropanal (**2h**), and purified by flash column chromatography as colorless oil (36.1 mg, 62%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 - 7.33 (m, 4H), 7.24 - 7.22 (m, 1H), 7.15 - 7.13 (m, 2H), 7.06 - 7.02 (m, 2H), 3.86 (dd, *J* = 6.0 Hz, 10.4 Hz, 0.50×1H), 3.71 (t, *J* = 8.0 Hz, 0.48×1H)，2.92 - 2.85 (m, 1H), 2.66 - 2.59 (m, 1H), 2.50 - 2.41 (m, 1H), 2.09 - 1.99 (m, 1H), 1.87 - 1.86 (m, 1H), 1.63-1.62 (m, 0.60×1H), 1.58 - 1.56 (m, 0.41×1H), 1.24 (d, *J* = 6.8 Hz, 6H), 0.97 (dd, *J* = 6.4 Hz, 17.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.88, 146.79, 137.29, 137.21, 136.40, 136.10, 129.24, 129.22, 129.17, 128.19, 128.14, 127.44, 127.35, 126.51, 121.40, 120.83, 43.20, 43.01, 42.70, 42.51, 35.58, 35.45, 33.82, 32.90, 32.74, 24.18, 19.89, 19.02. IR (cm^{-1}): 2969, 2871, 2239, 1457, 698. HRMS: calcd. for $C_{21}H_{25}N\ Na^+$ $[M + Na]^+$: 314.1879; Found: 314.1895.

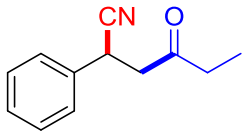
(4i) 2-phenylpentanenitrile[7]



An oven-dried microwave reaction vessel was charged with $Cu(CH_3CN)_4PF_6$ (0.01 mmol, 5 mol %), dipy (0.02 mmol,10 mol%), styrene (**1a**, 0.2 mmol, 1.0 equiv), TMSCN (0.8 mmol, 4.0 equiv), propionaldehyde (**4i**, 1.0 mmol, 5.0 equiv) , TBHP (0.24 mmol 1.5 equiv, 70% in water) and trifluorotoluene (1.0 mL) under air atmosphere. The vessel was sealed and heated was stirred at 150 ℃ (oil bath temperature) for 12 h. Afterwards the resulting mixture was cooled to room temperature, and purified by flash column chromatography as colorless oil (9.5 mg, 30%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.4 - 7.37 (m, 2H), 7.34 - 7.30 (m, 3H), 3.79 (dd, *J* = 6.4 Hz, 8.8 Hz, 1H), 1.97 -1.79 (m, 2H), 1.59 - 1.43 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.14, 129.17, 128.11, 127.37, 121.07, 38.02, 37.30, 20.44, 13.56. IR (cm^{-1}): 2961, 2874, 2239, 1455, 699.

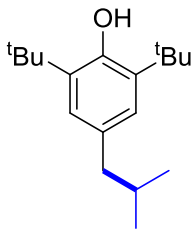
(5) 4-oxo-2-phenylhexanenitrile[8]



The title compound was prepared according to the general procedure described above by the reaction between styrene (**1a**) with TMSCN and propionaldehyde (**4i**), and purified by flash column chromatography as colorless oil (10.8 mg, 29%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 - 7.31 (m, 5H), 4.37 (dd, *J* = 6.4 Hz, 7.6 Hz, 1H), 3.15 (dd, *J* = 8.0 Hz, 18.0 Hz, 1H), 2.93 (dd, *J* = 6.4 Hz, 18.0 Hz, 1H), 2.53 -2.33 (m, 2H), 1.06 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.12, 135.19, 129.36, 128.47, 127.48, 120.61, 47.65, 36.27, 31.76, 7.57. IR (cm^{-1}): 2979, 2243, 1717, 1114, 700.

(6) 4-isobutyl-2,6-di-tert-butyl-4-methylphenol[9]



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (s, 2H), 5.01 (s, 1H), 2.38 (d, *J* = 7.2 Hz, 2H), 1.79 (m, *J* = 6.8 Hz, 1H), 1.44 (s, 18H), 0.91 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.80, 135.50, 132.38, 125.68, 45.57, 34.37, 30.54, 30.54, 22.63. IR (cm^{-1}): 3647, 2924, 2360, 1435, 1159.

VII. References

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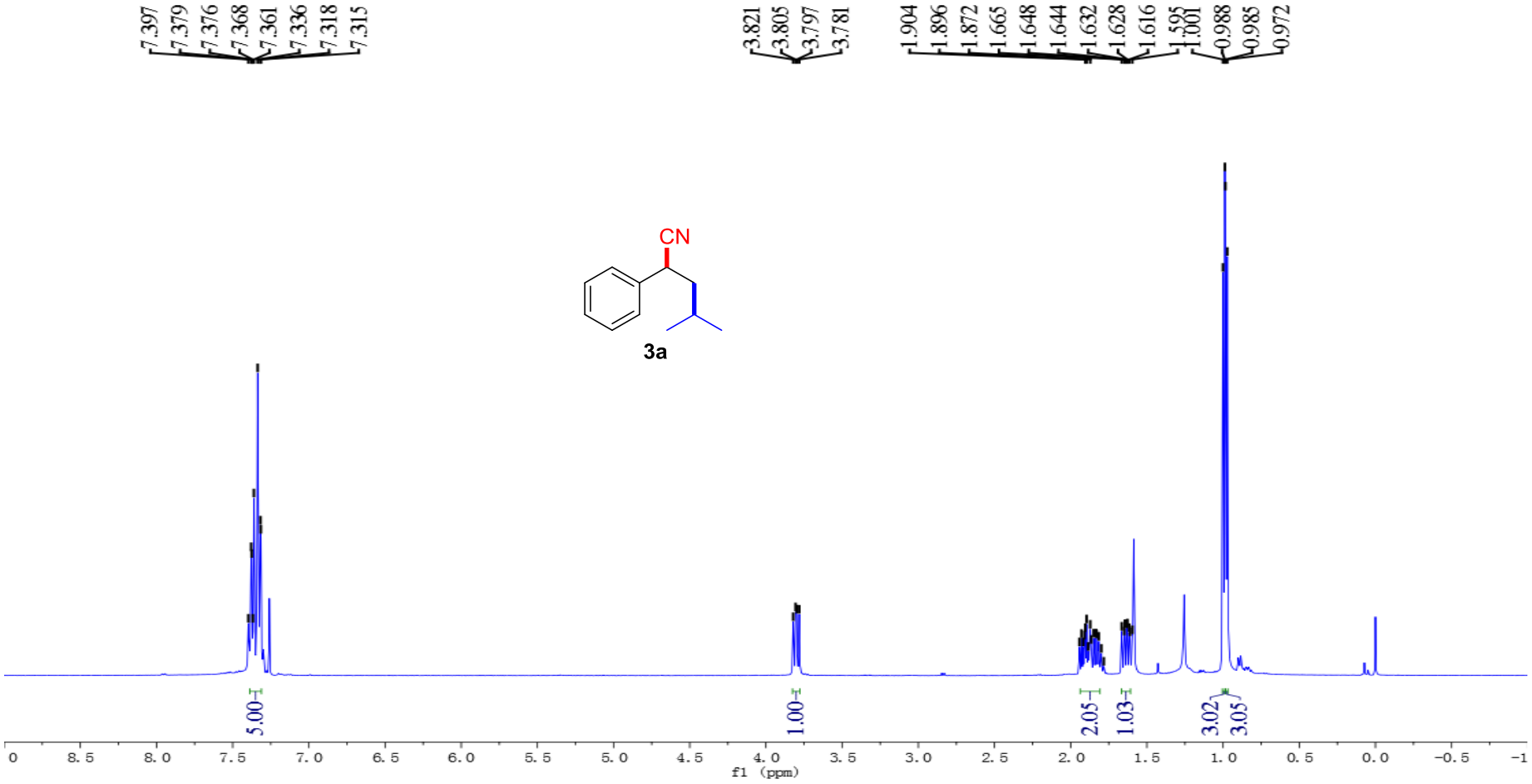
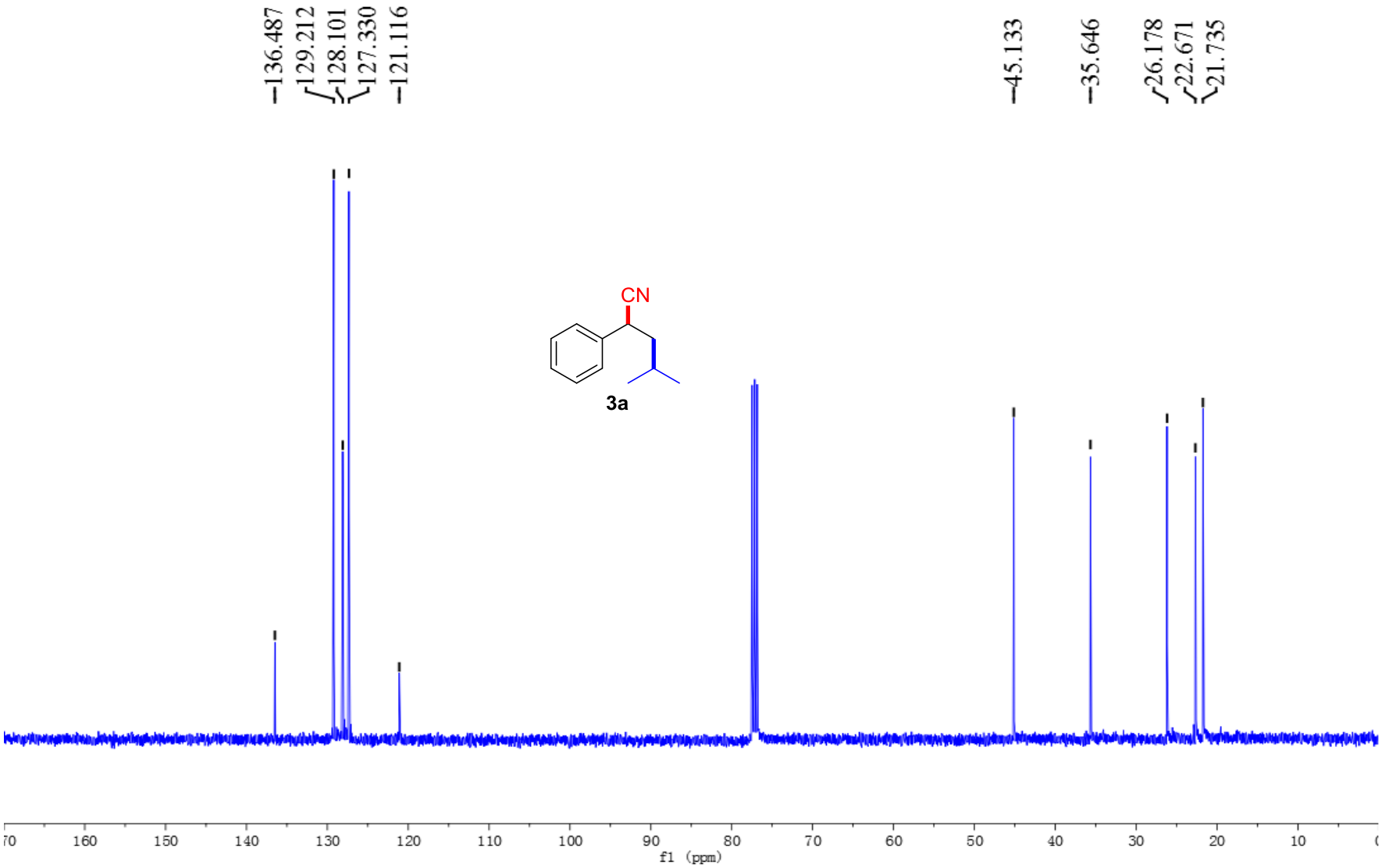
(9)J. P. Phillips, J. G. Gillmore, P. Schwartz, L. E. Brammer, D. J. Berger and J. M. Tanko, *J. Am. Chem. Soc*. 1998, **120**, 195-202.

VIII. Copies of ^{1}H, ^{19}F and ^{13}C NMR spectra of products

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21.735
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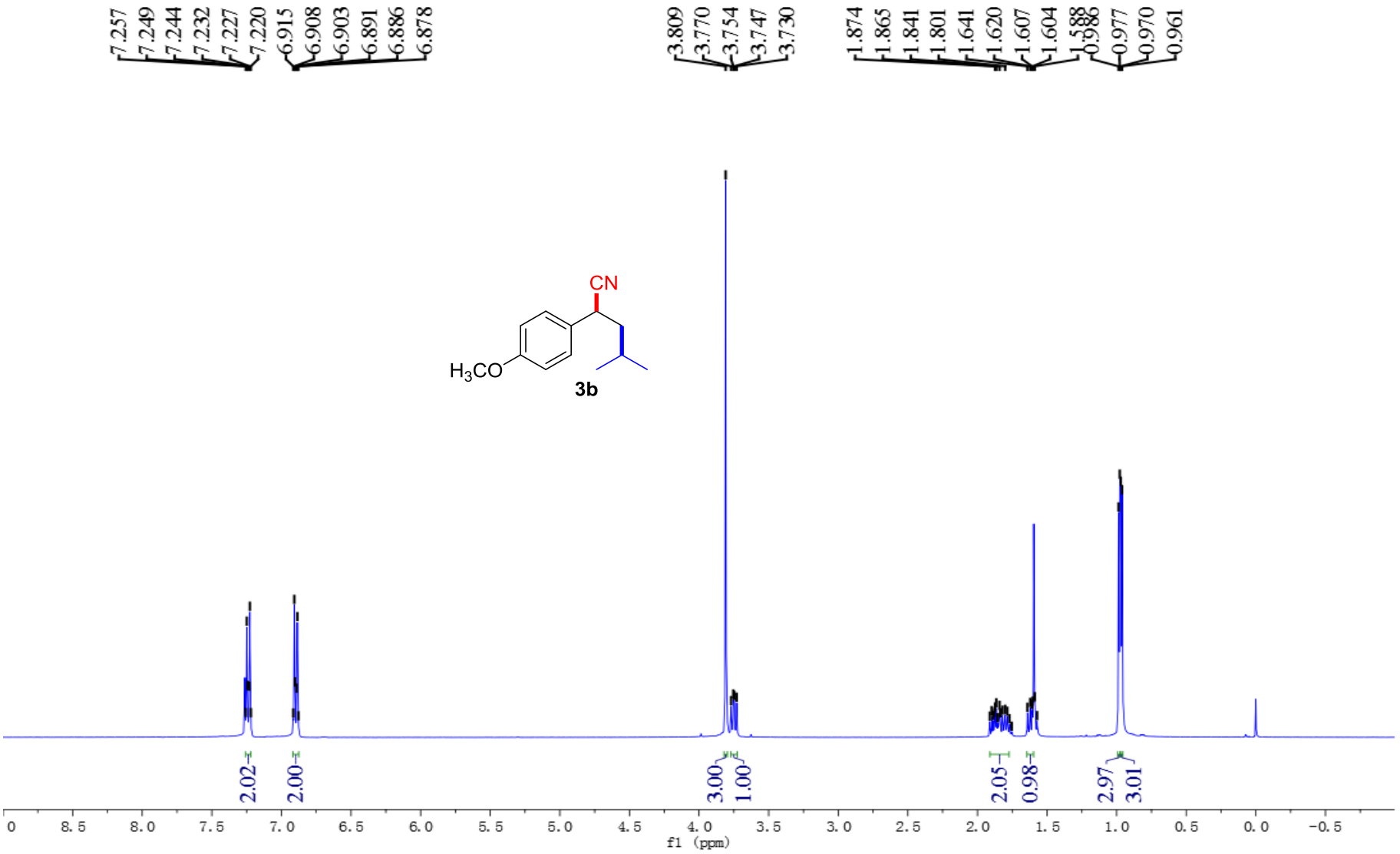
f1 (ppm)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3.754
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3.730
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1.641
1.620
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1.604
1.588
0.986
0.977
0.970
0.961
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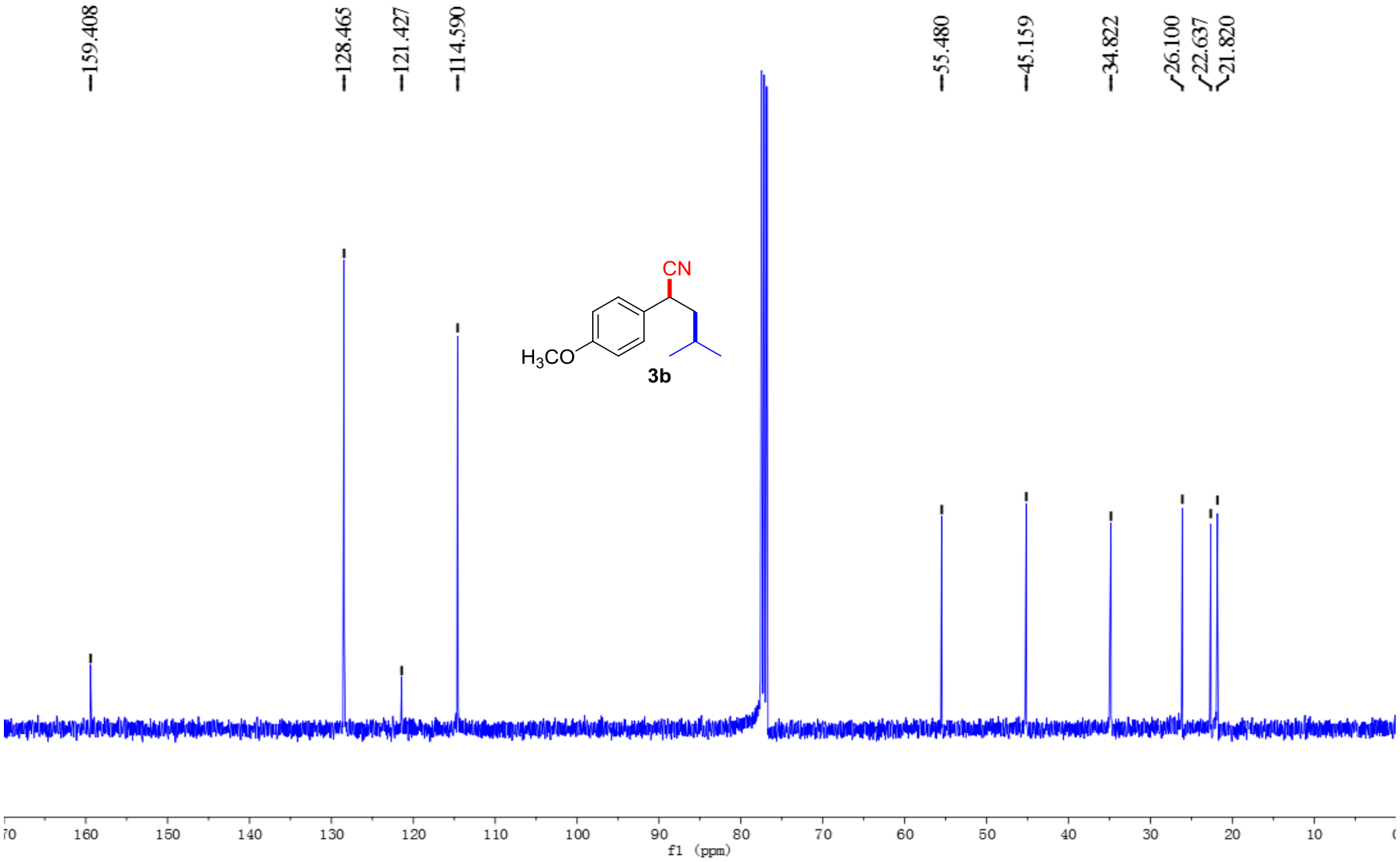
f1 (ppm)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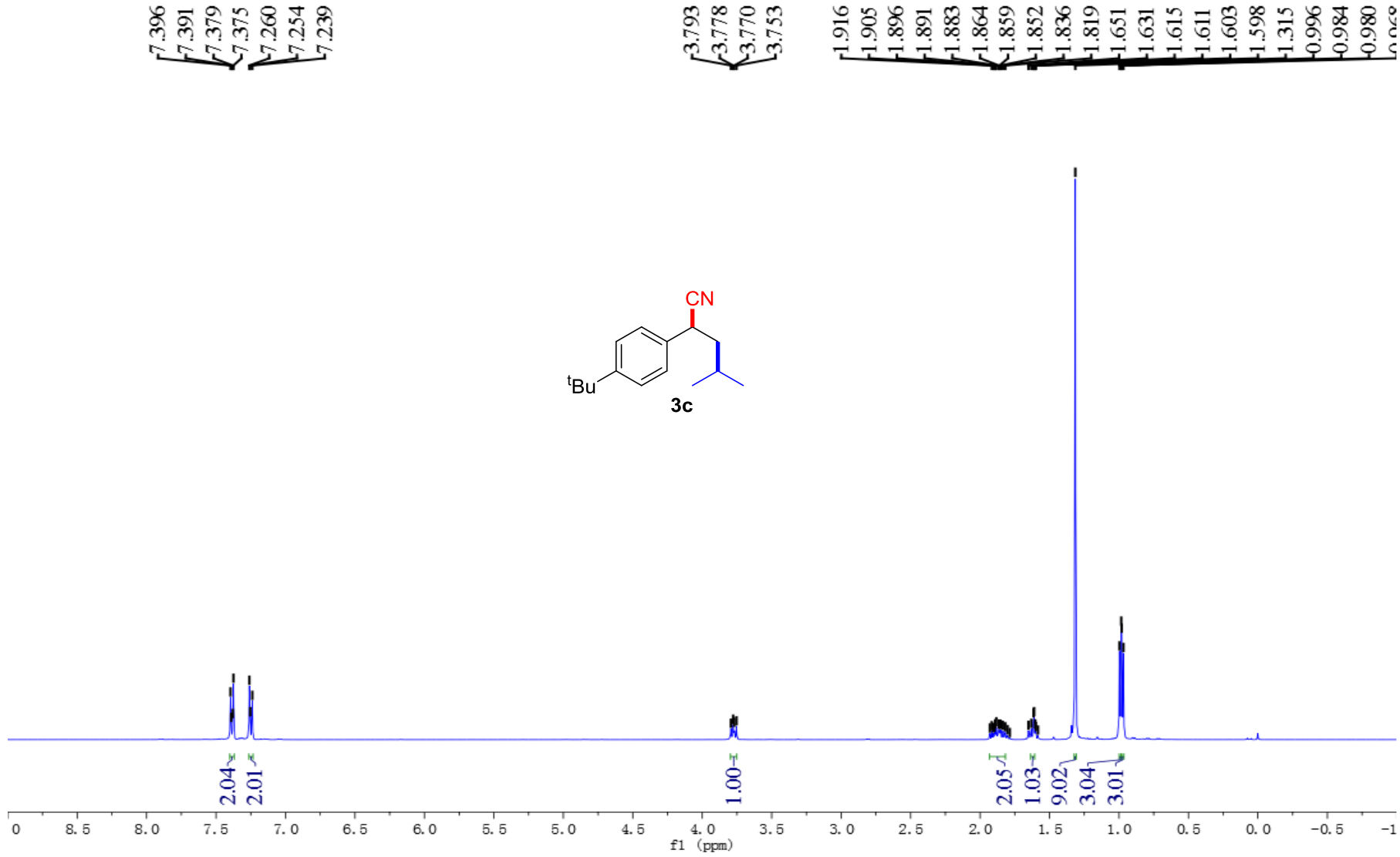
f1 (ppm)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1.896
1.891
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1.859
1.852
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1.631
1.615
1.611
1.603
1.598
1.315
0.996
0.984
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2.05
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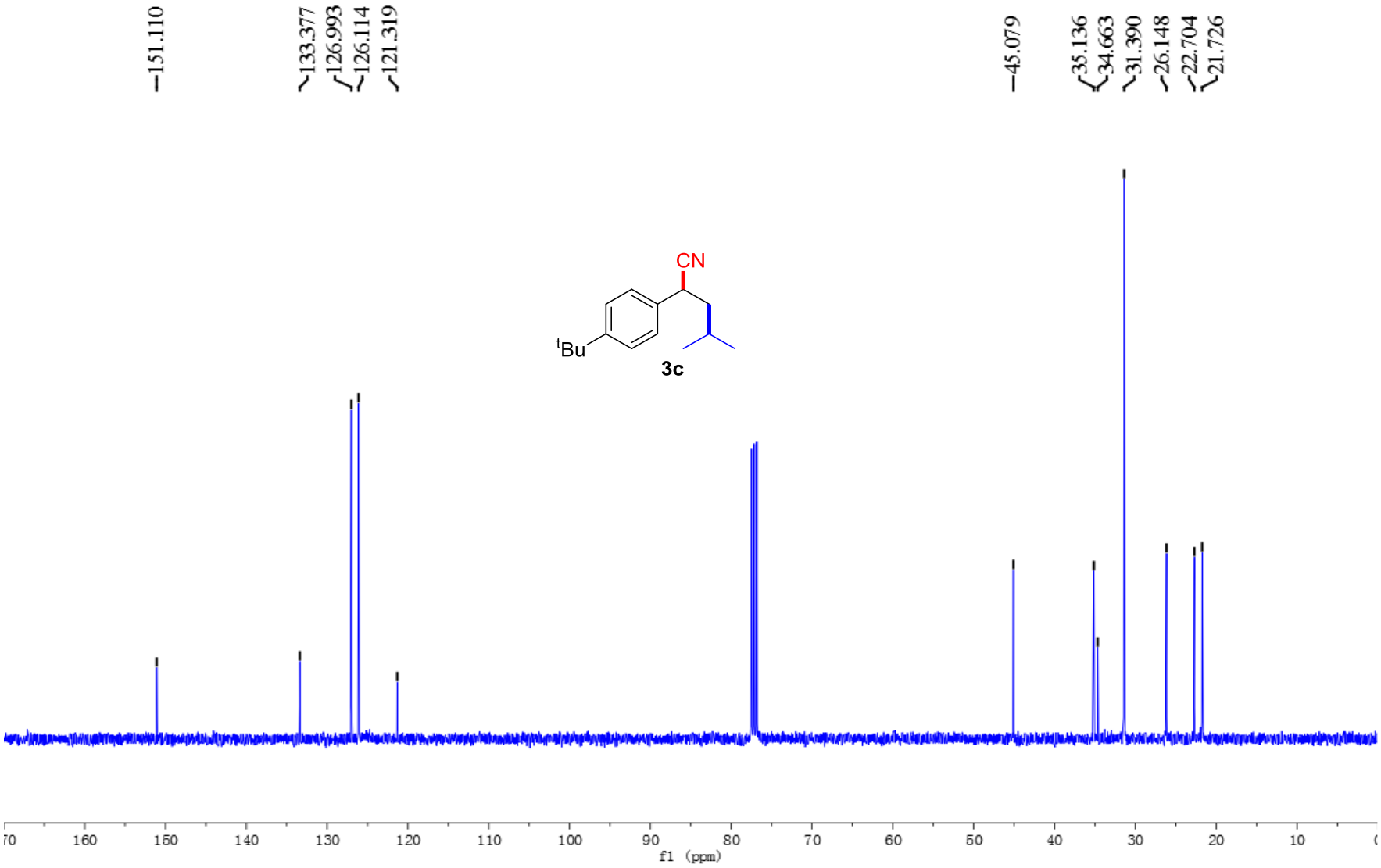
3.01
f1 (ppm)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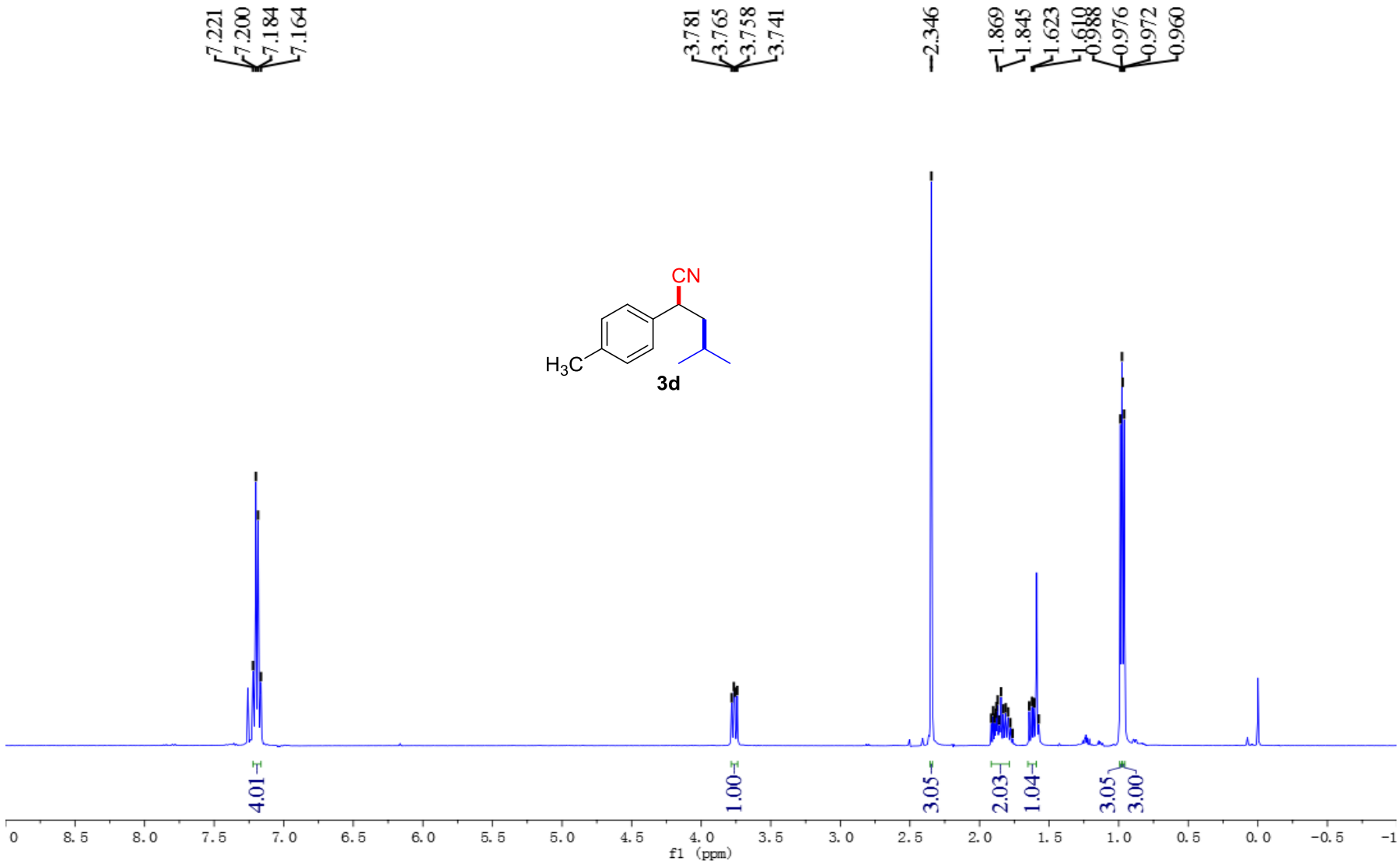
tBu
3c
f1 (ppm)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0.988
0.976
0.972
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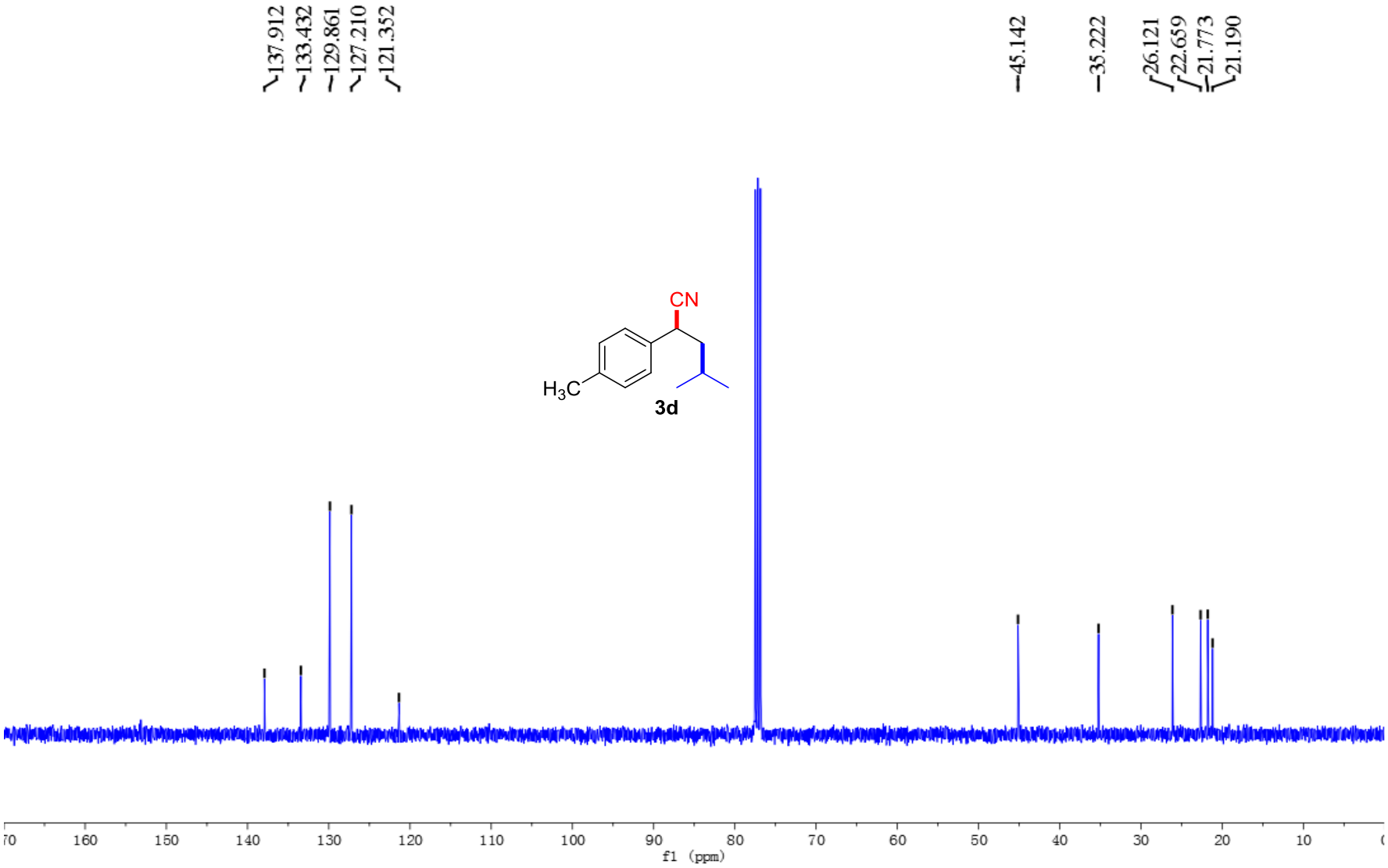
1.04
3.05
3.00
f1 (ppm)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H3C
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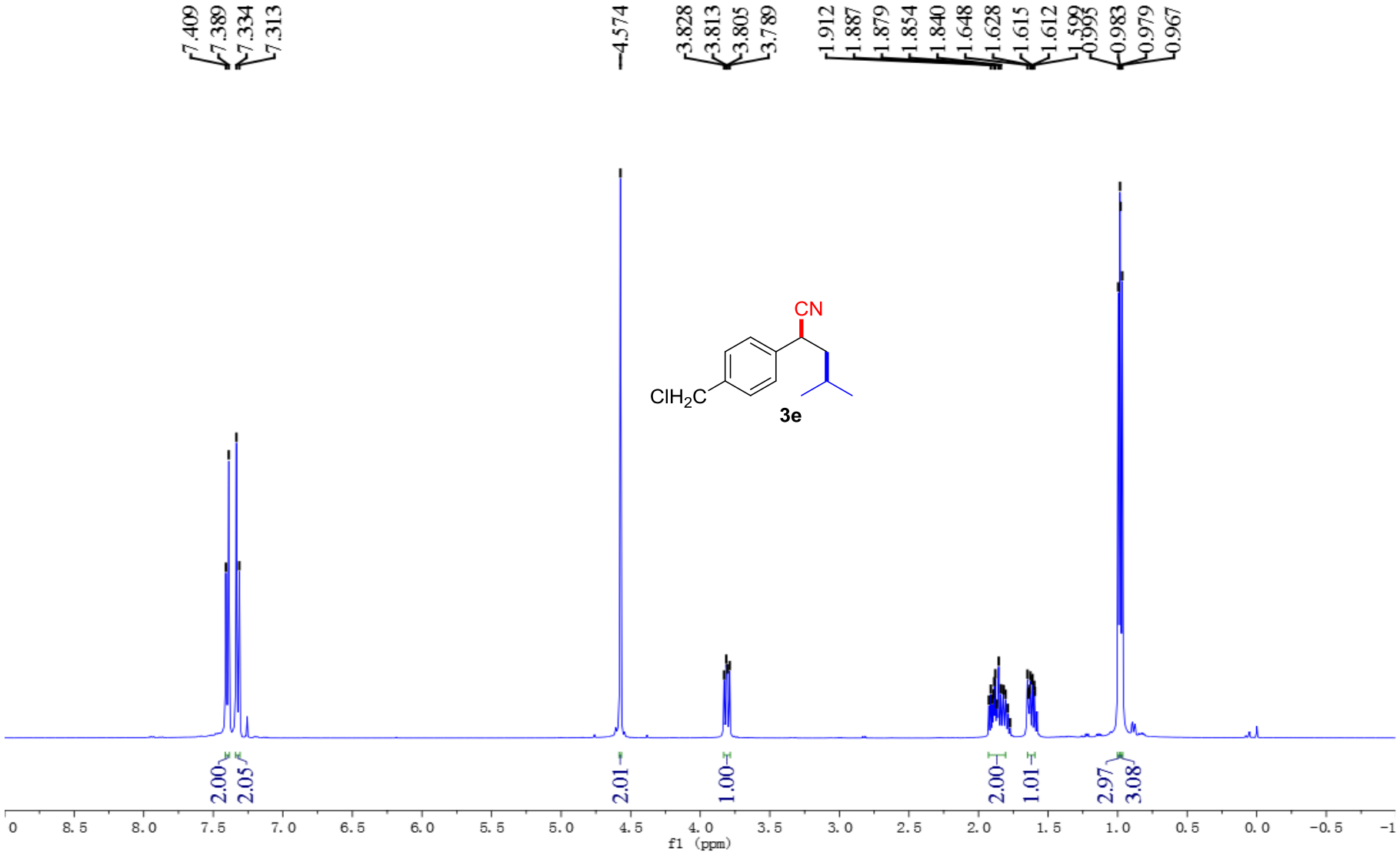
f1 (ppm)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1.840
1.648
1.628
1.615
1.612
1.599
0.995
0.983
0.979
0.967
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ClH2C
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2.00
1.01
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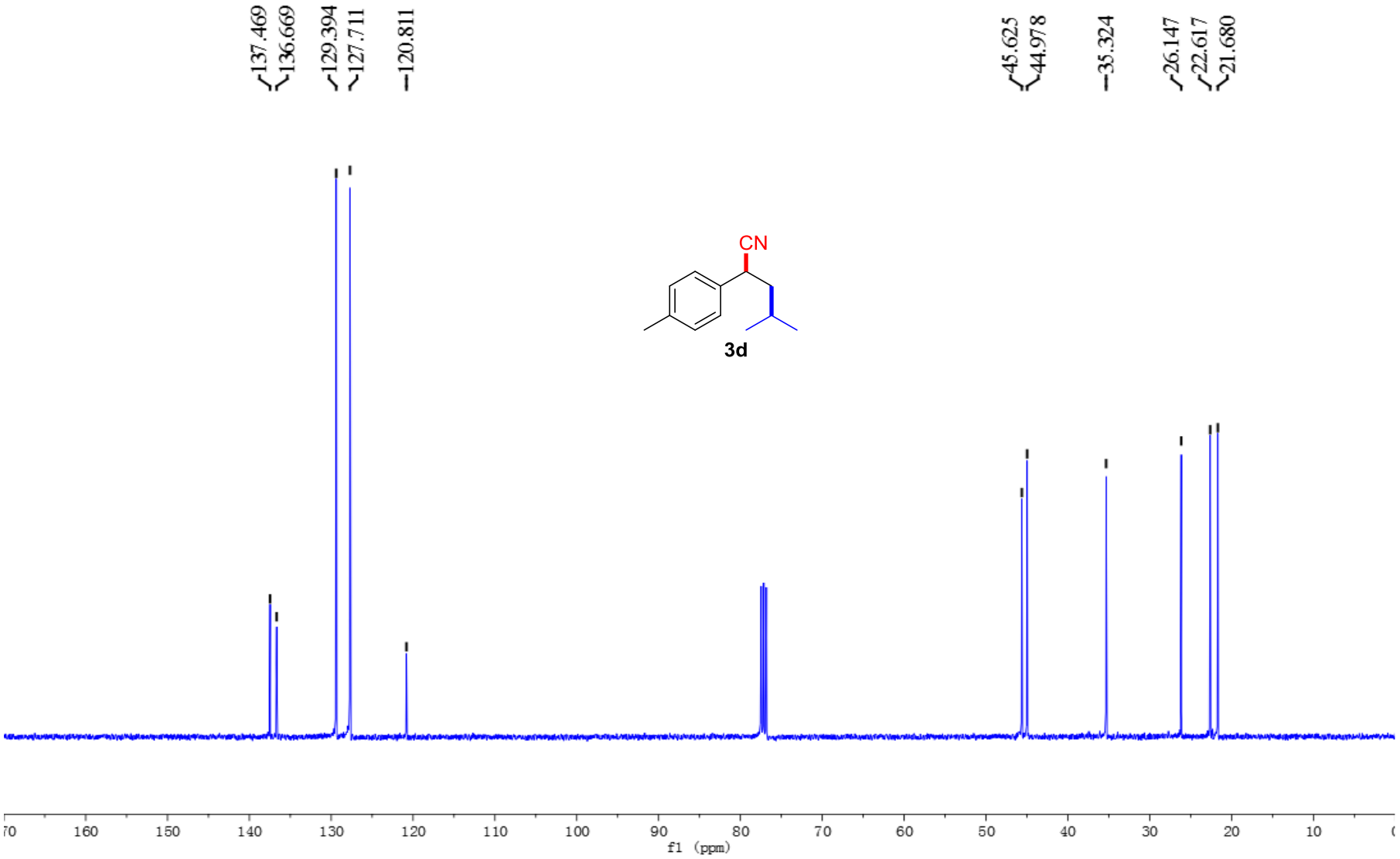
f1 (ppm)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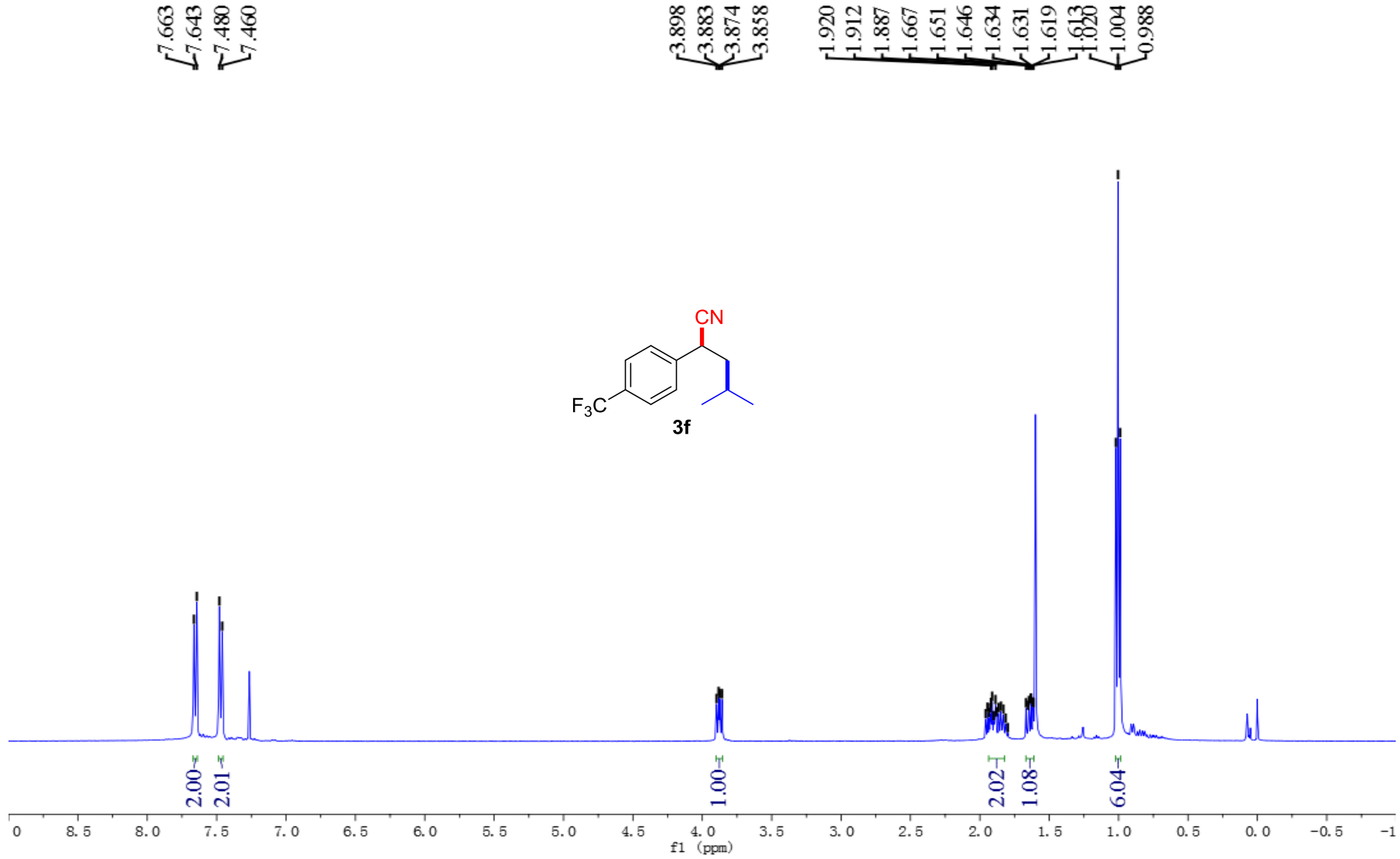
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1.646
1.634
1.631
1.619
1.613
1.020
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CN
F3C
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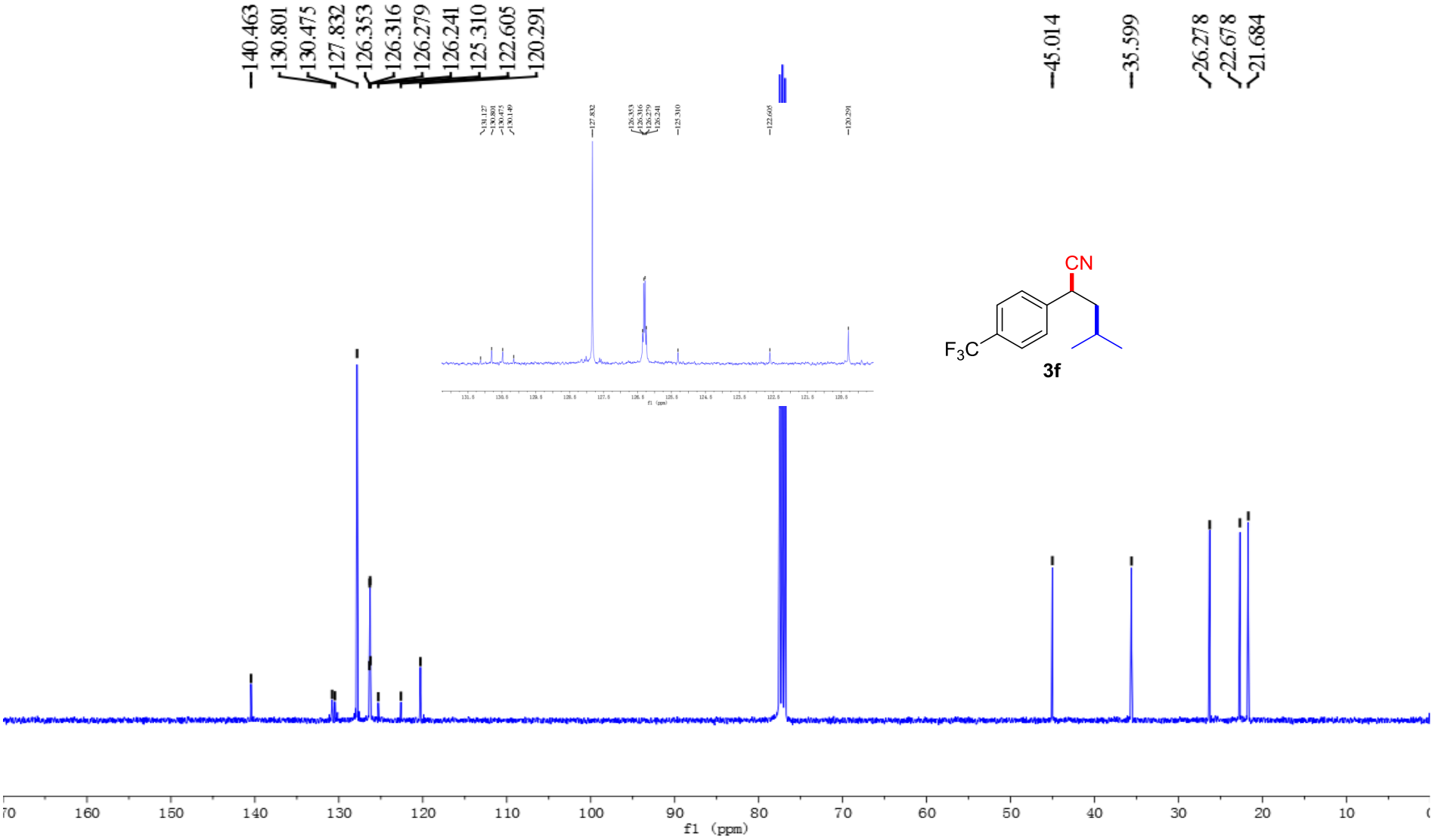
2.01
1.00
2.02
1.08
6.04
f1 (ppm)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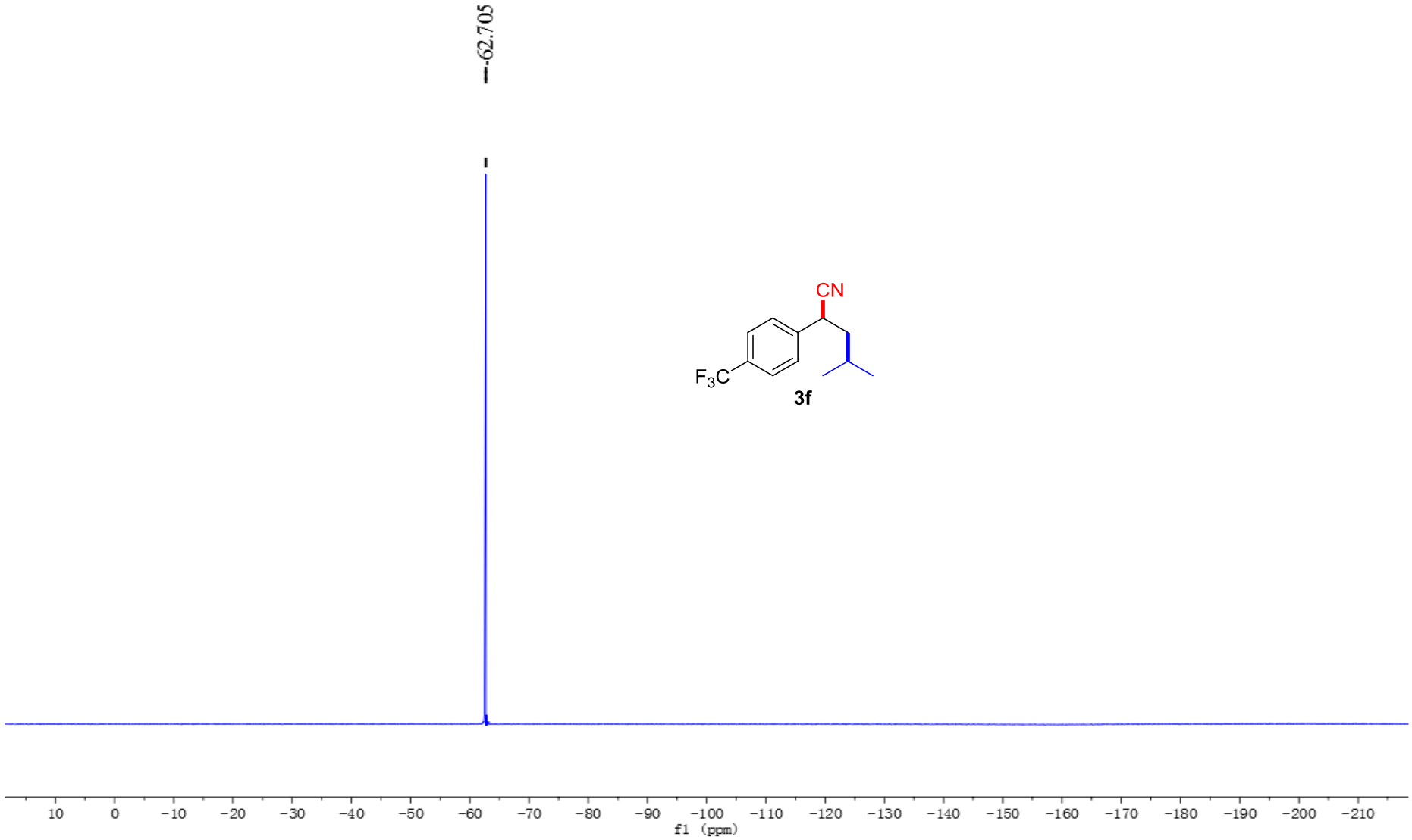
CN
F3C
3f
f1 (ppm)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-200
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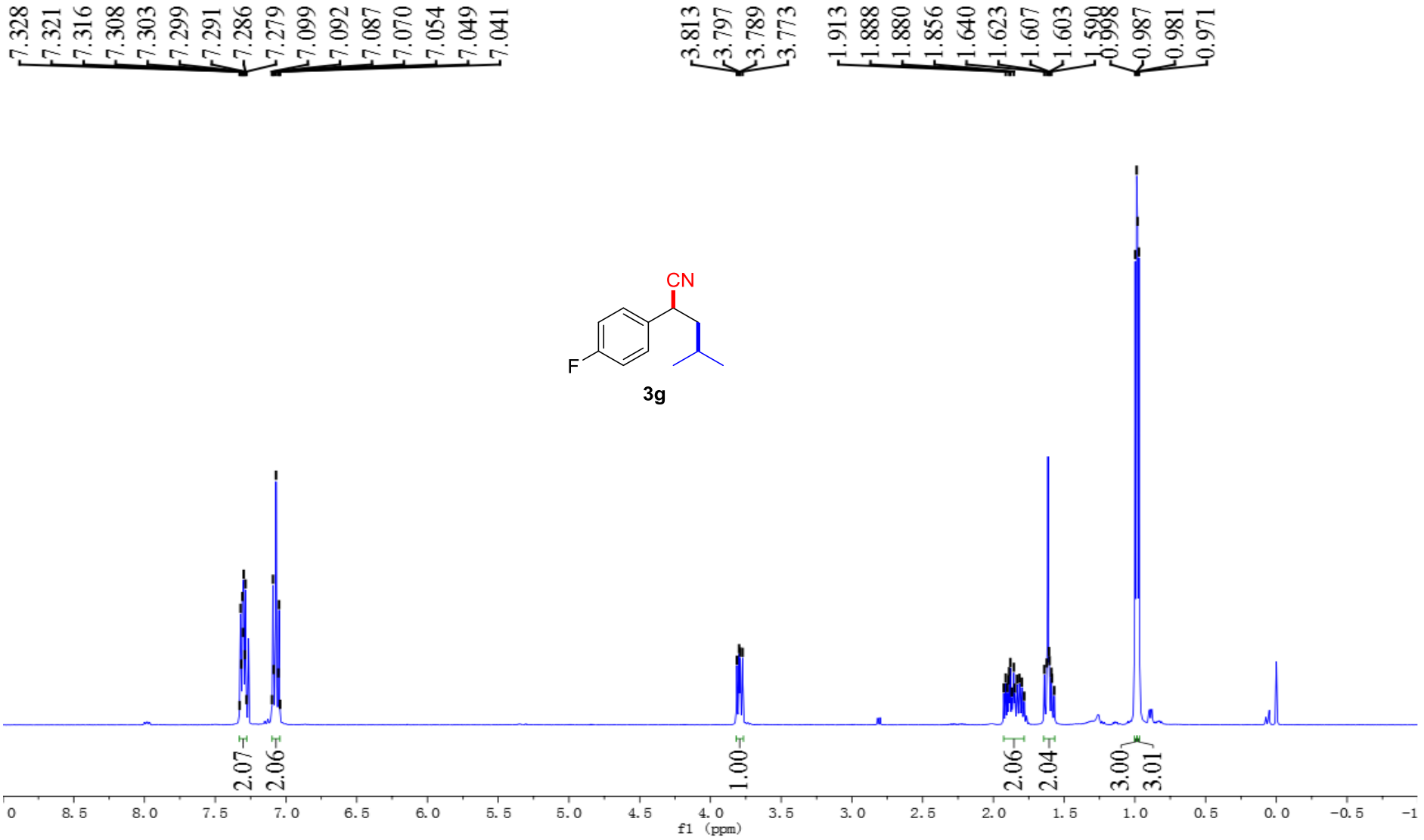
f1 (ppm)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7.087
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7.054
7.049
7.041
3.813
3.797
3.789
3.773
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1.880
1.856
1.640
1.623
1.607
1.603
1.590
0.988
0.987
0.981
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F
3g
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2.06
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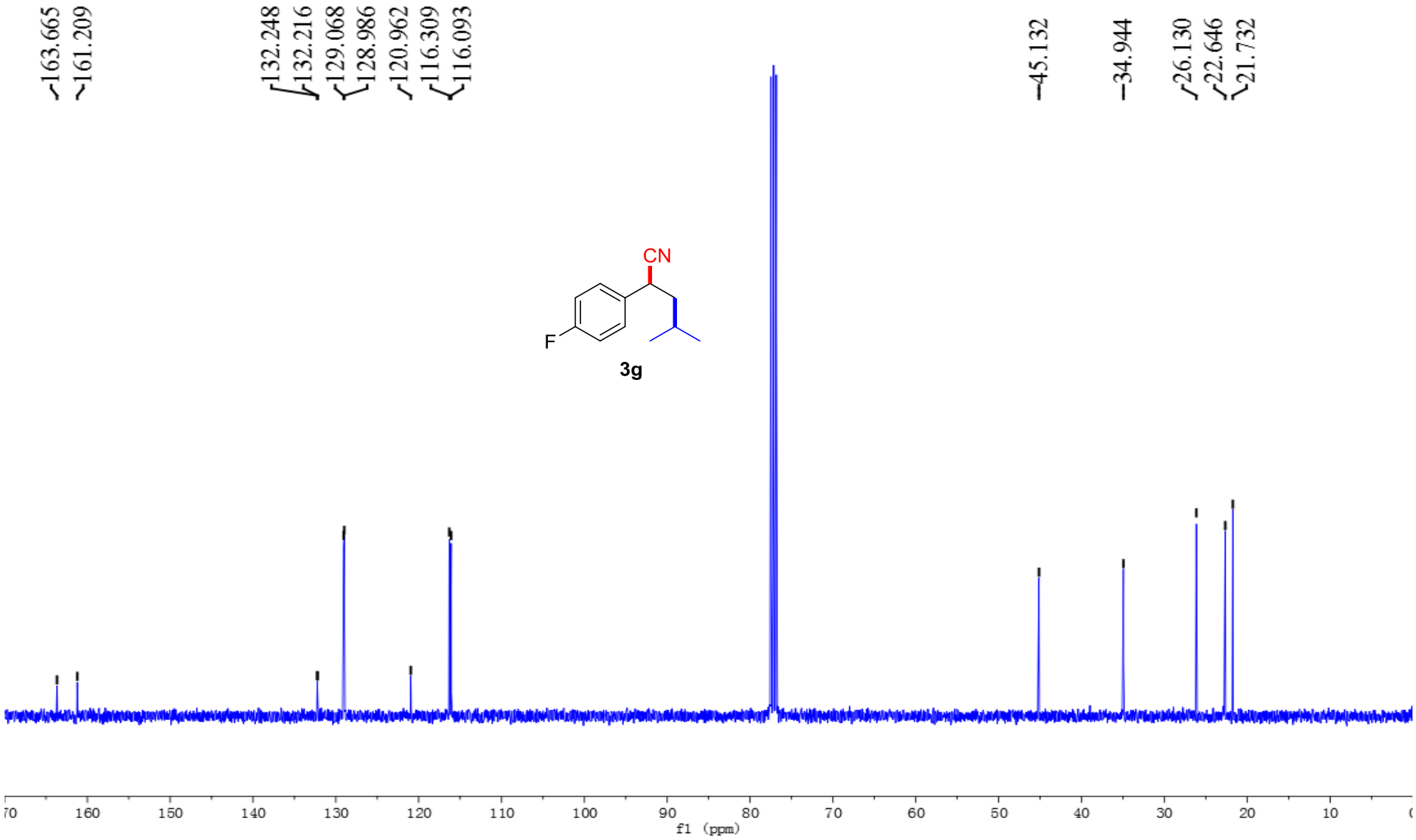
2.04
3.00
3.01
f1 (ppm)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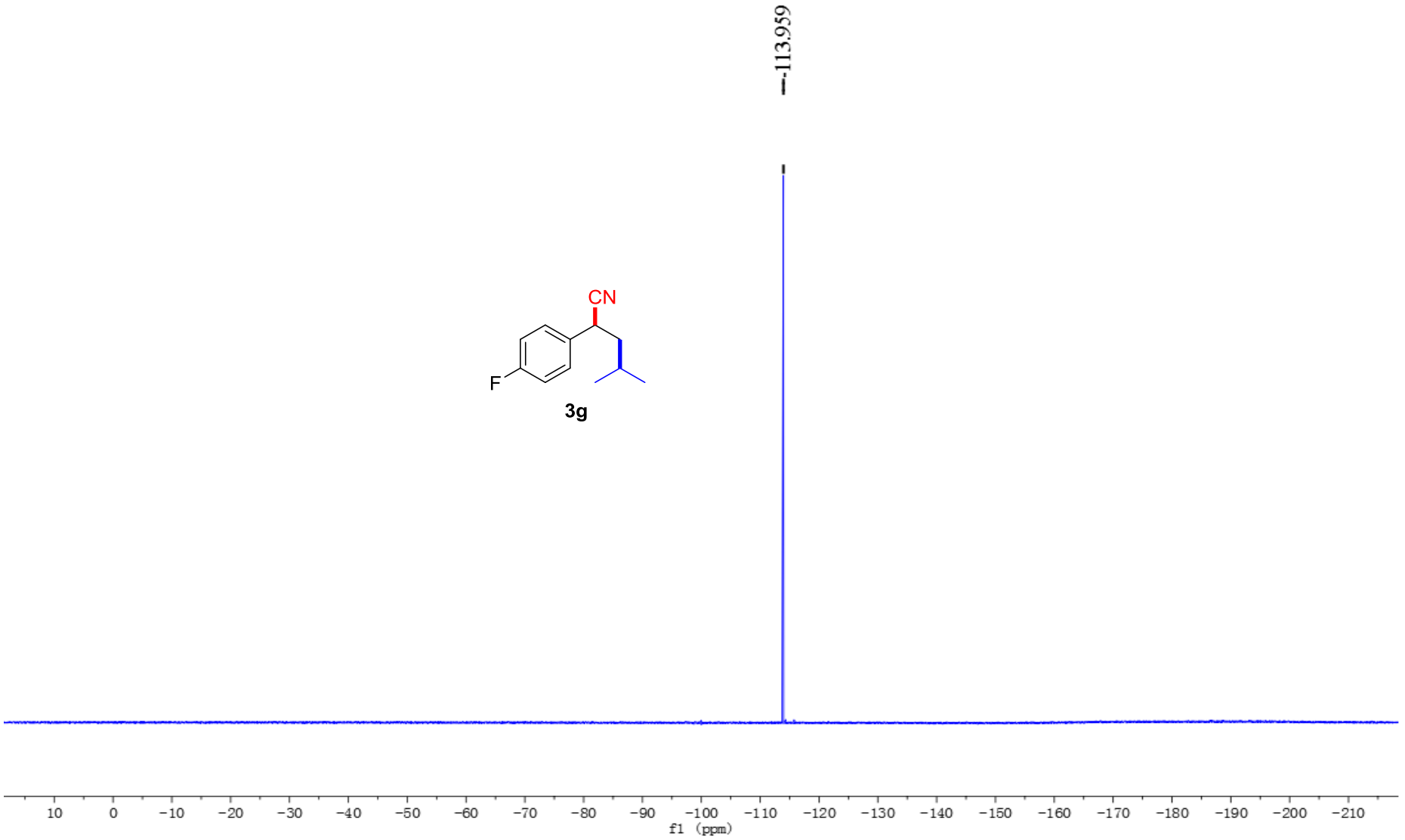
F
3g
f1 (ppm)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-70
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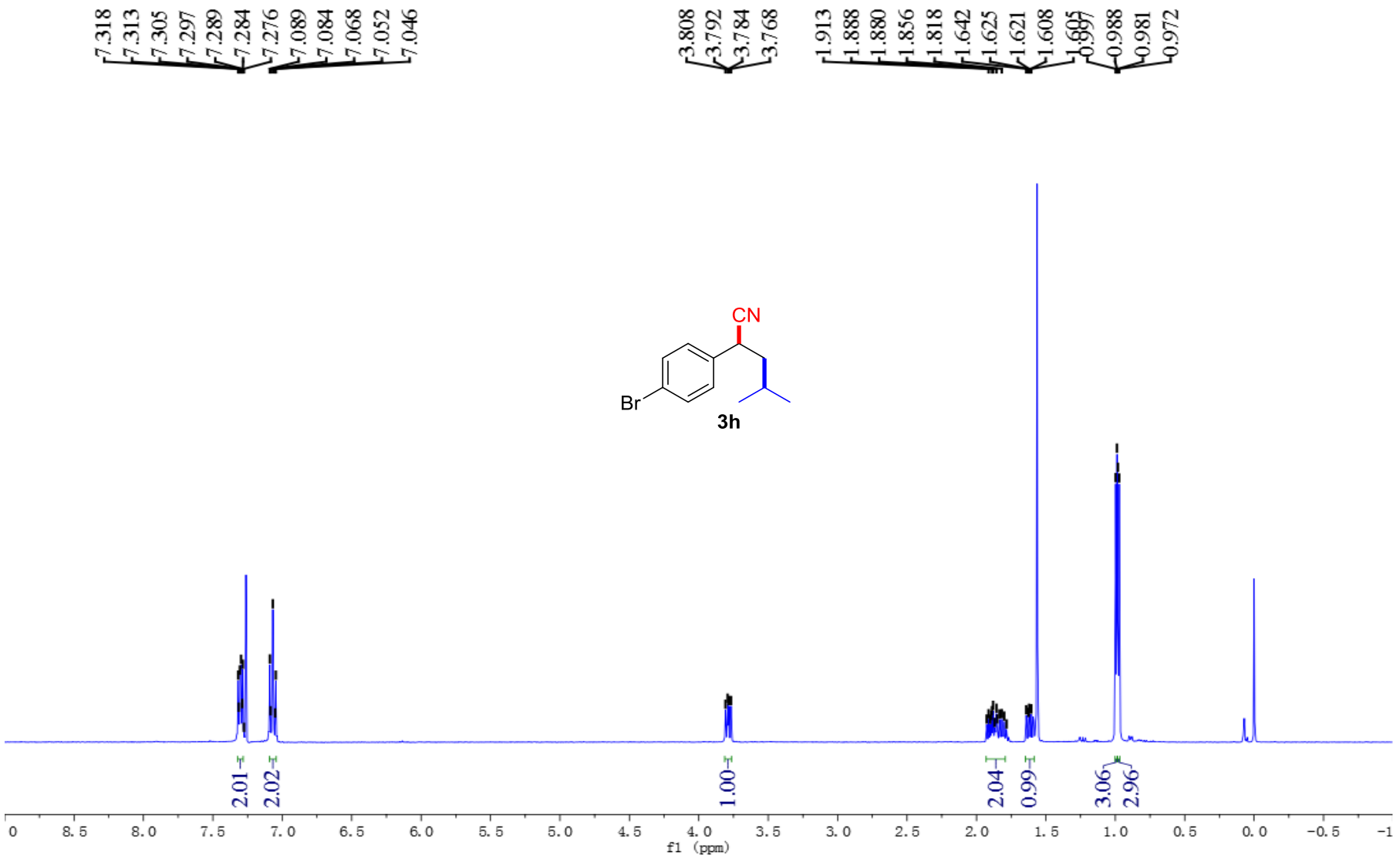
-170
-180
-190
-200
-210
f1 (ppm)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1.888
1.880
1.856
1.818
1.642
1.625
1.621
1.608
1.605
0.997
0.988
0.981
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Br
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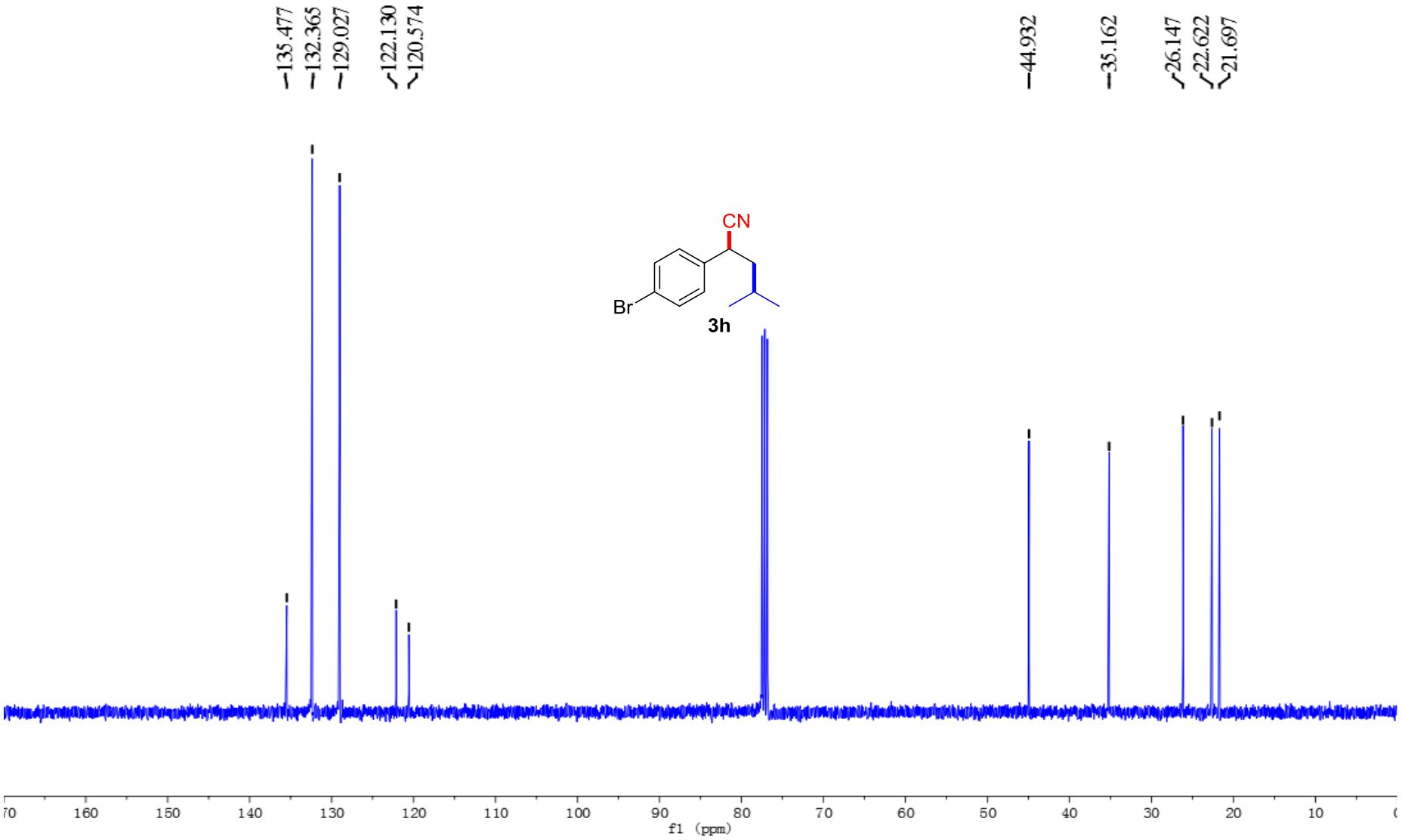
f1 (ppm)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Br
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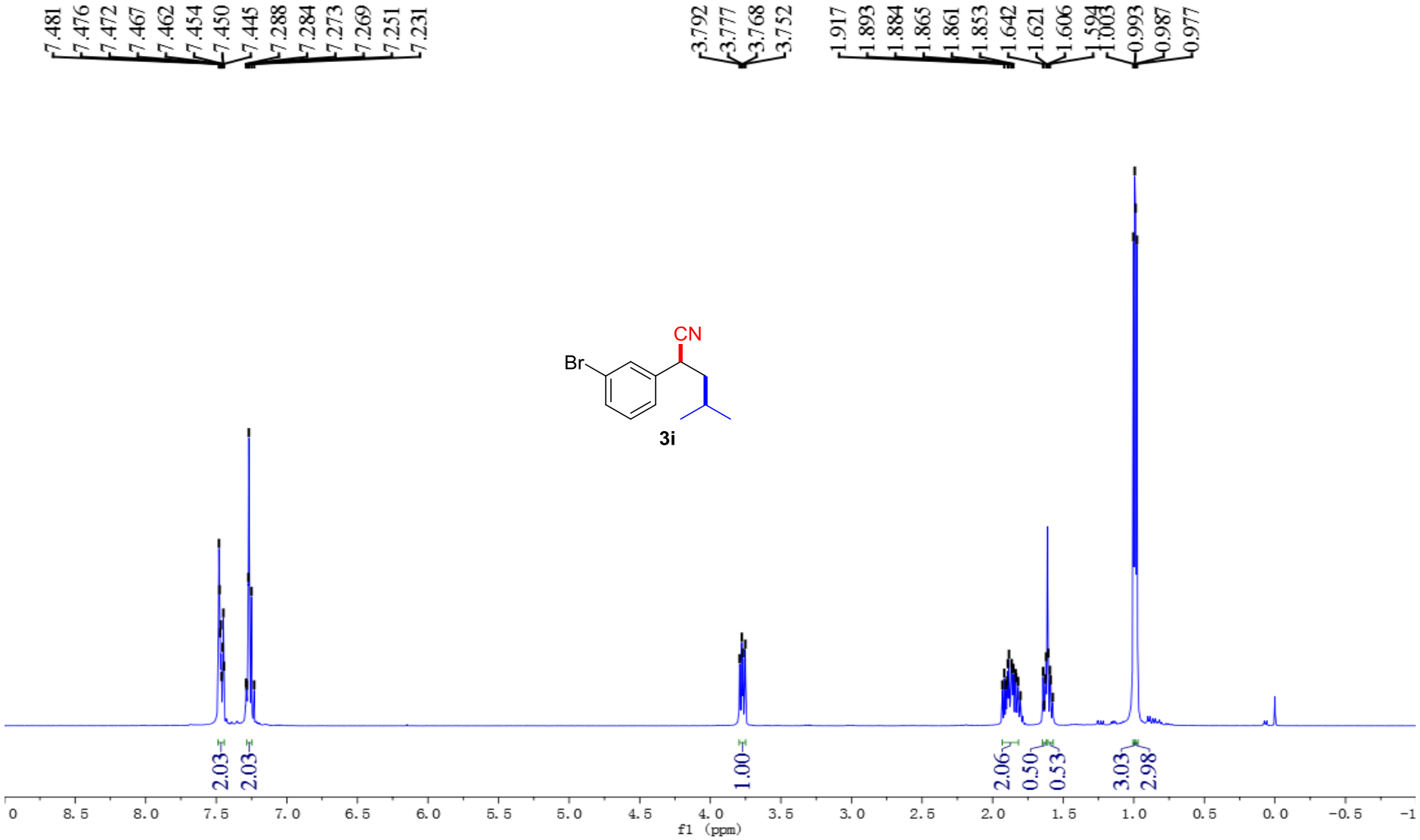
f1 (ppm)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3.768
3.752
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1.884
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1.642
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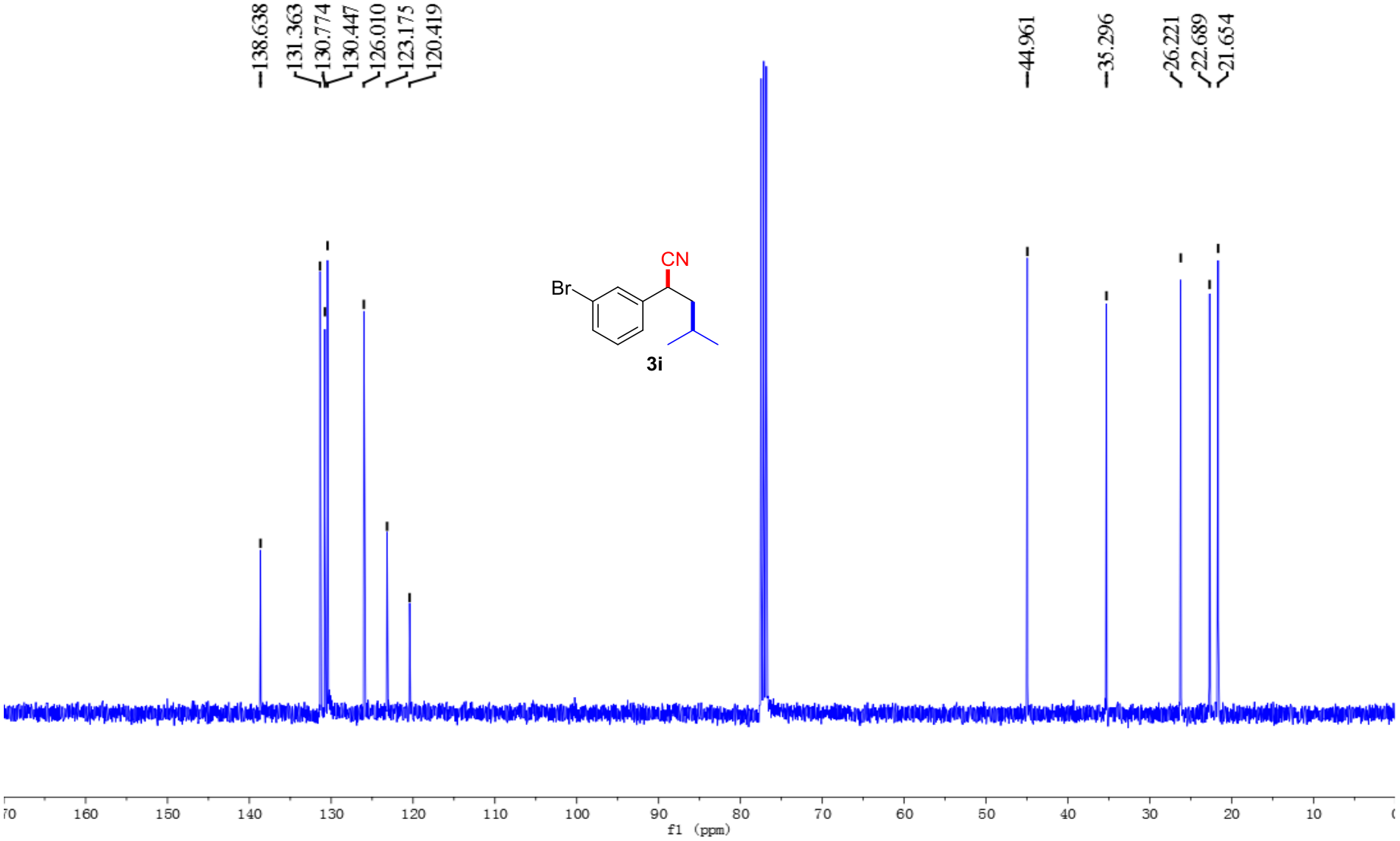
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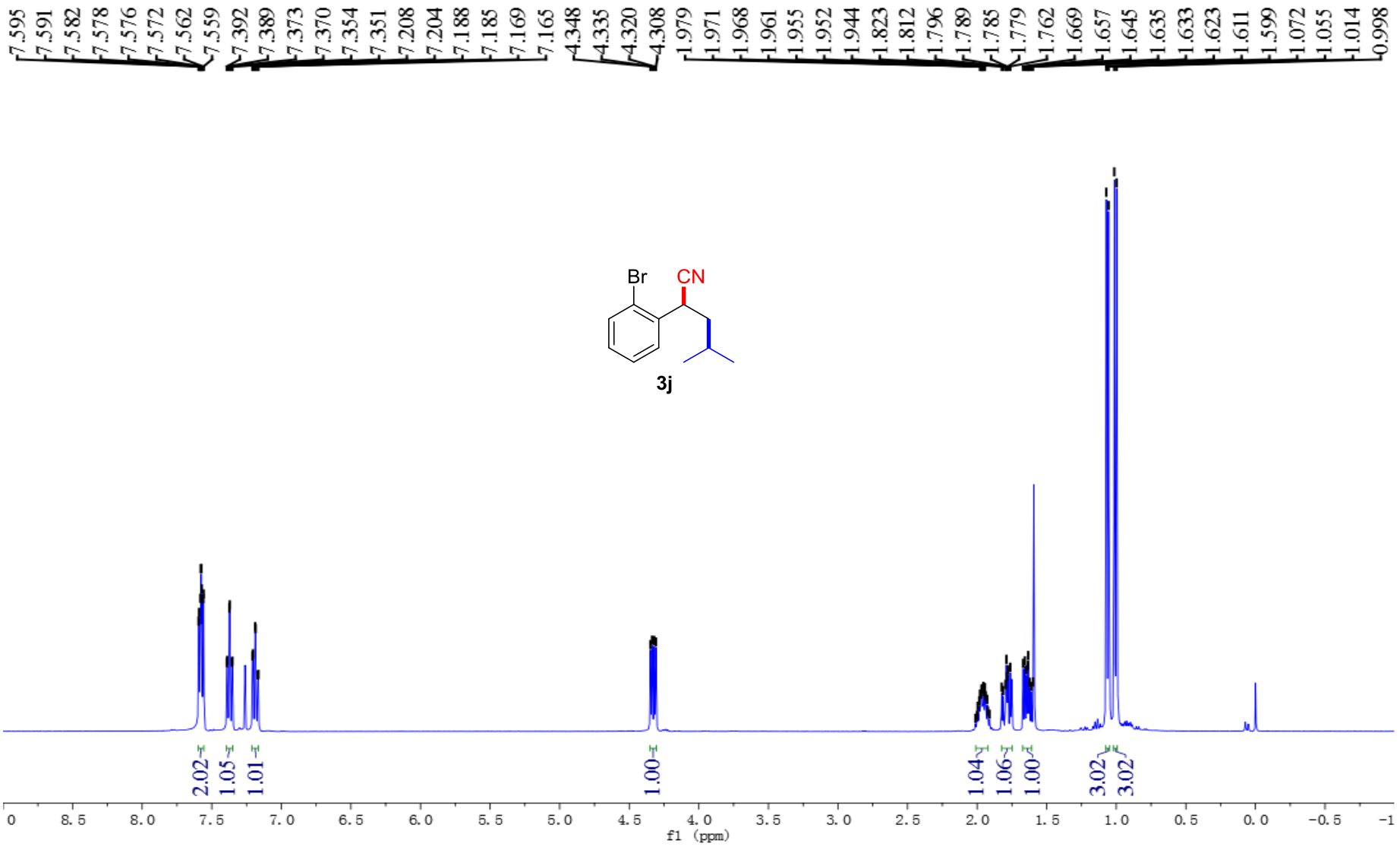
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1.00
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3.02
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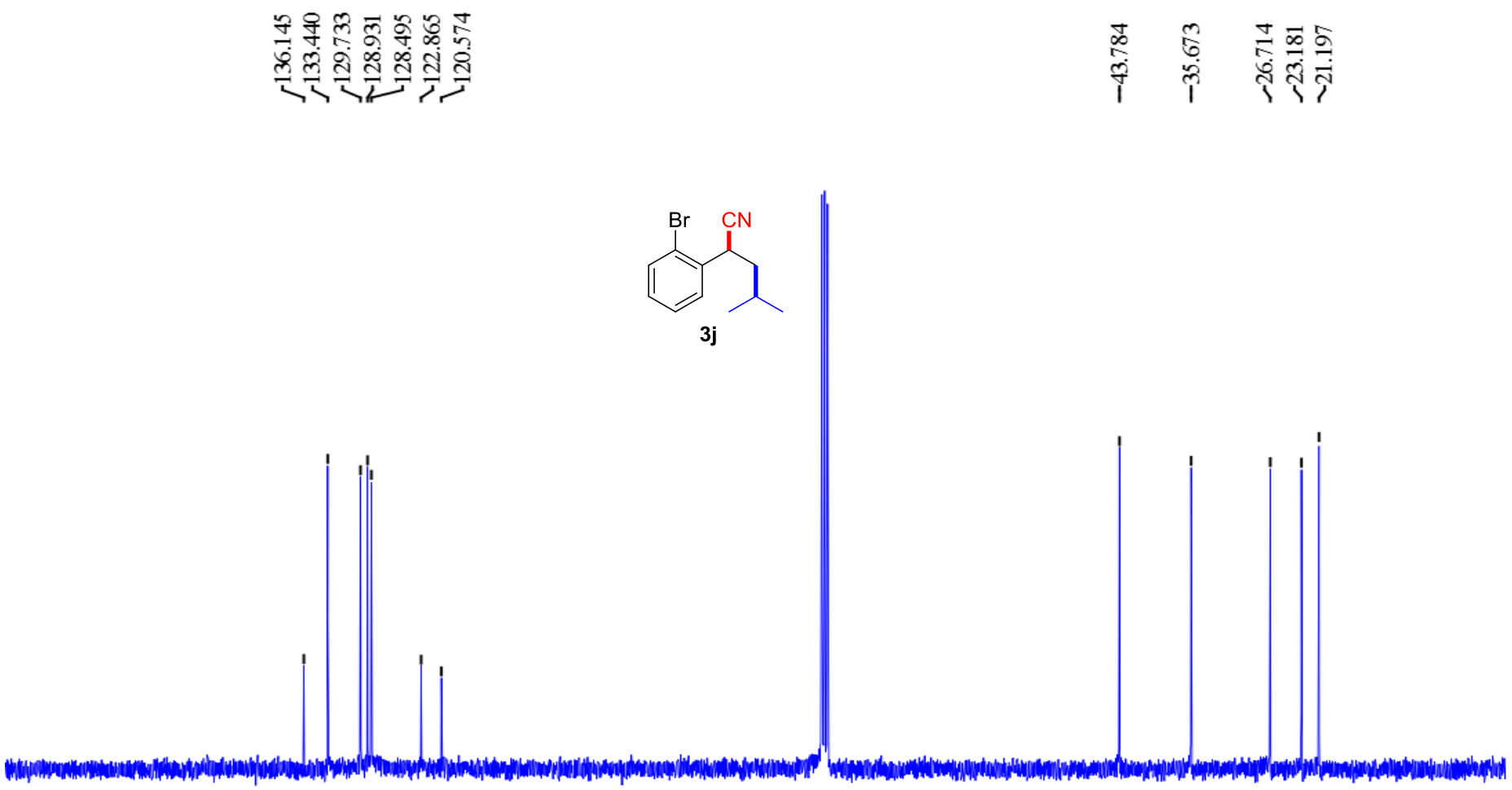
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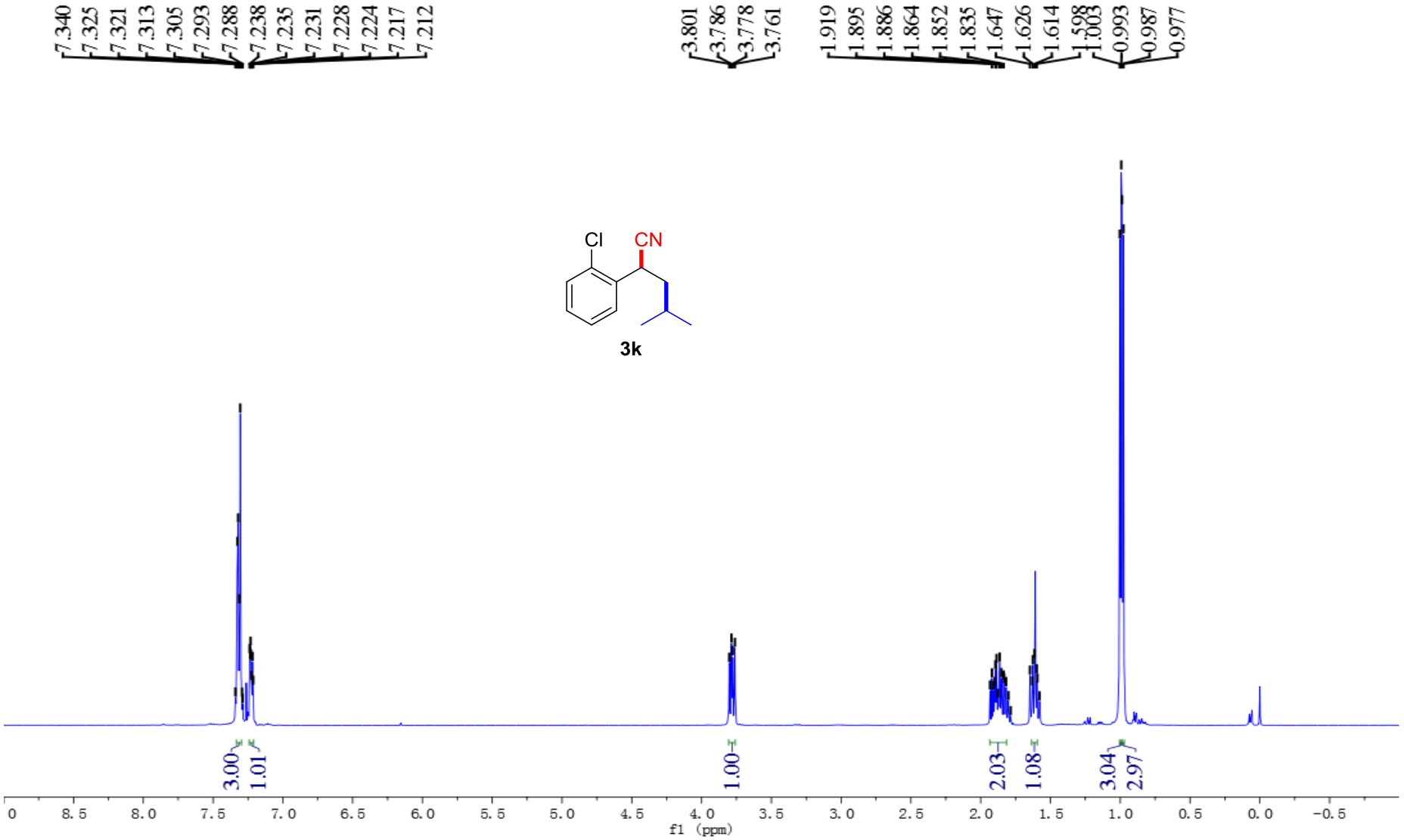
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1.864
1.852
1.835
1.647
1.626
1.614
1.598
1.003
0.993
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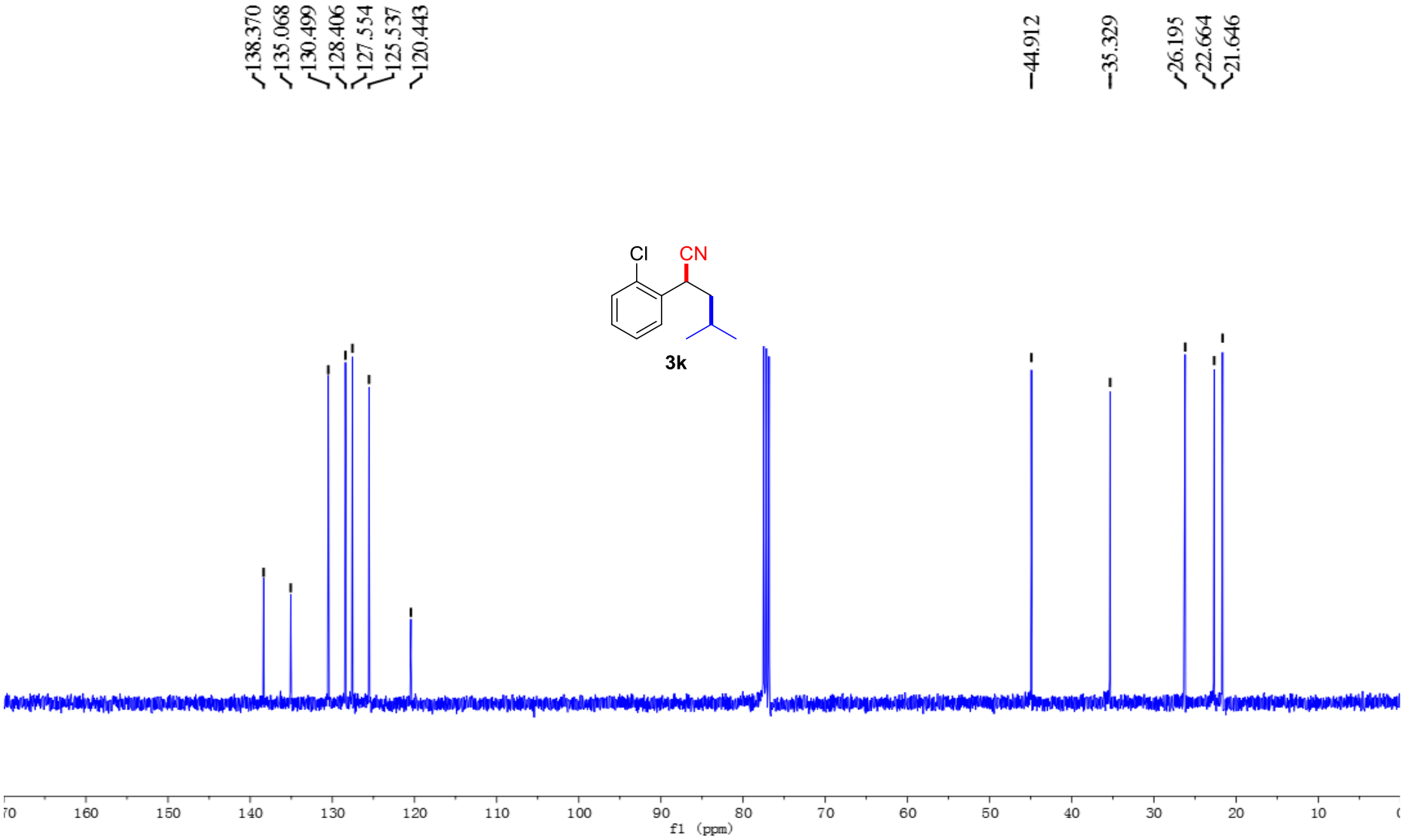
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60
50
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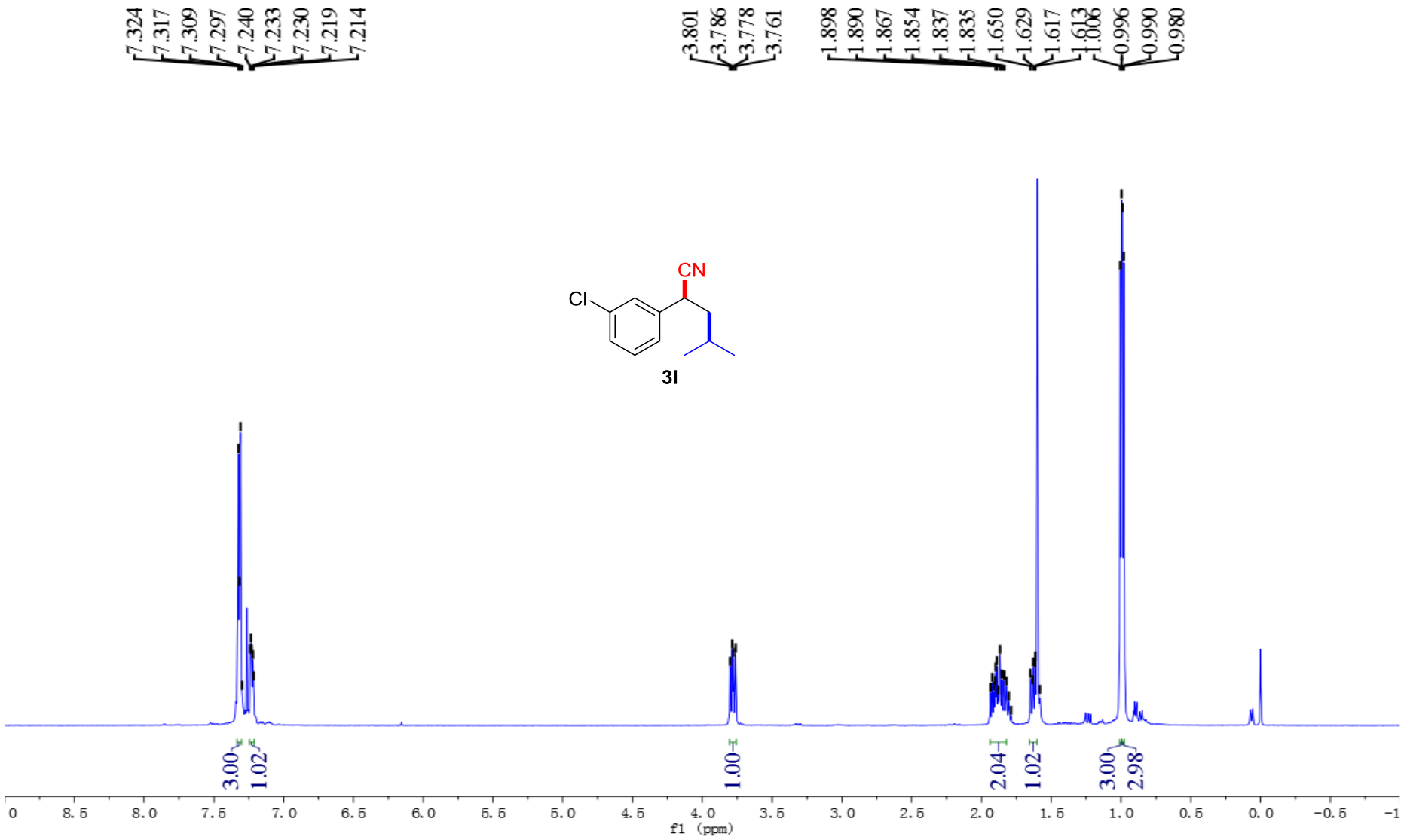
20
10
f1 (ppm)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1.890
1.867
1.854
1.837
1.835
1.650
1.629
1.617
1.613
1.008
0.996
0.990
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Cl
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1.00
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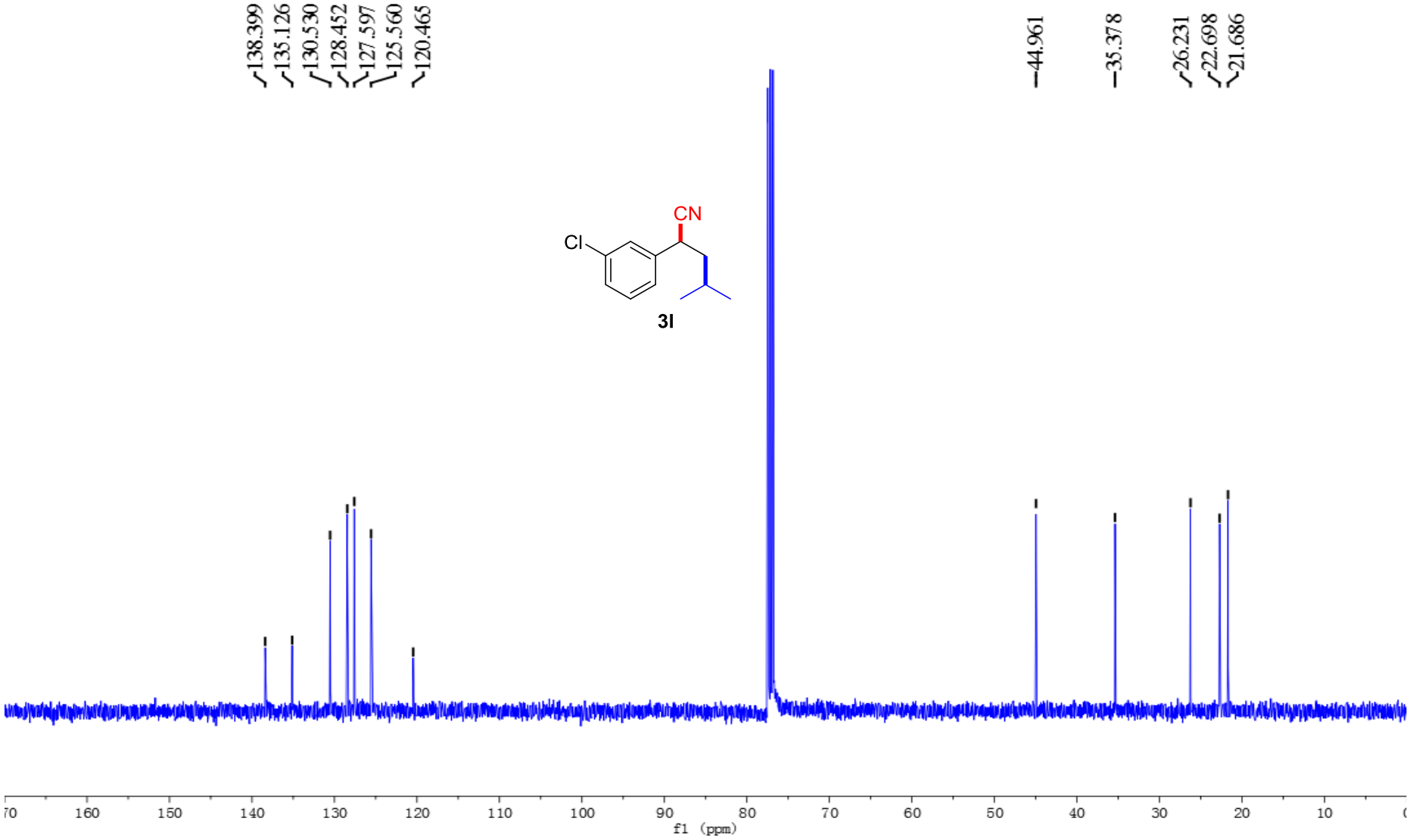
1.02
3.00
2.98
f1 (ppm)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Cl
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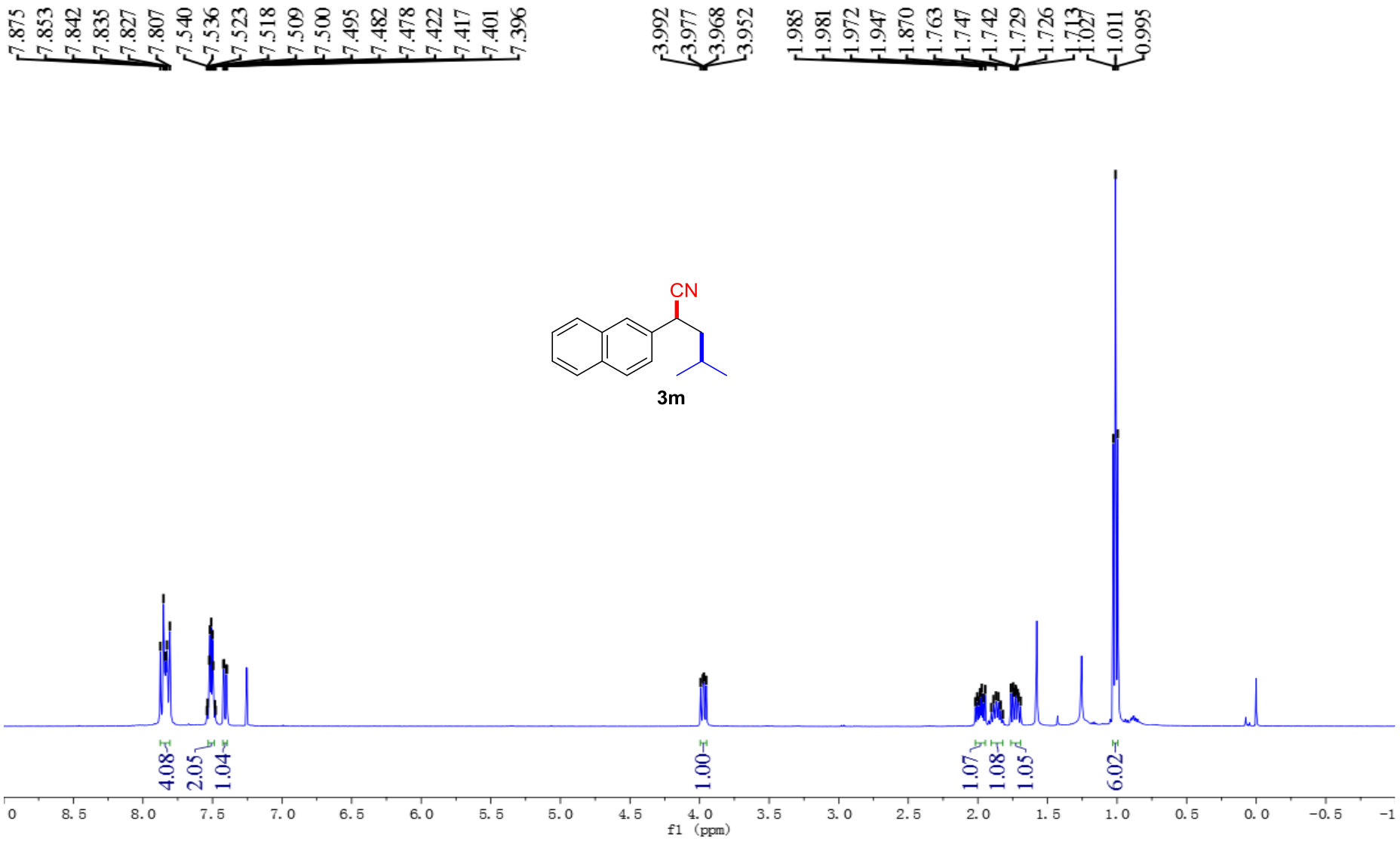
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7.417
7.401
7.396
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3.977
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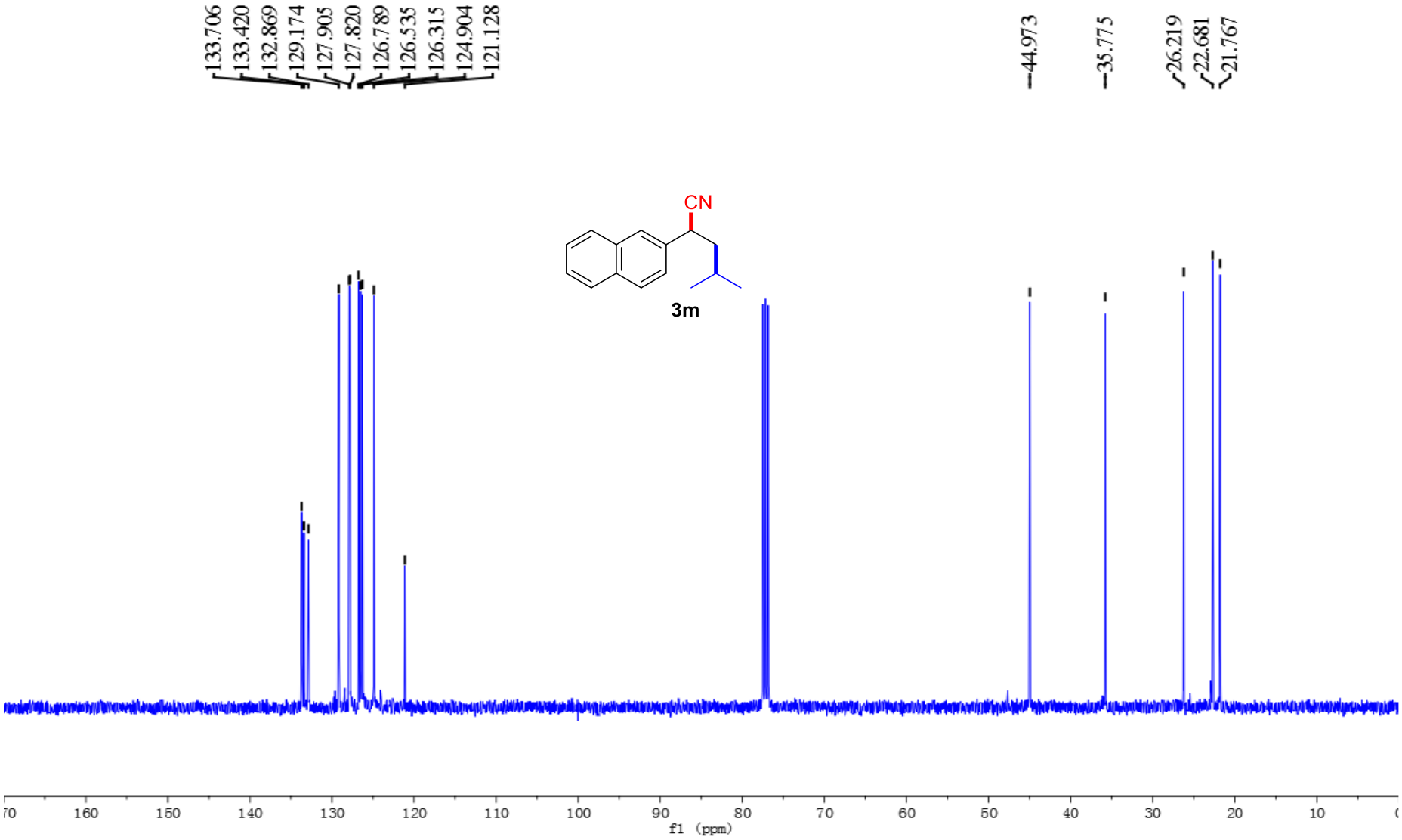
f1 (ppm)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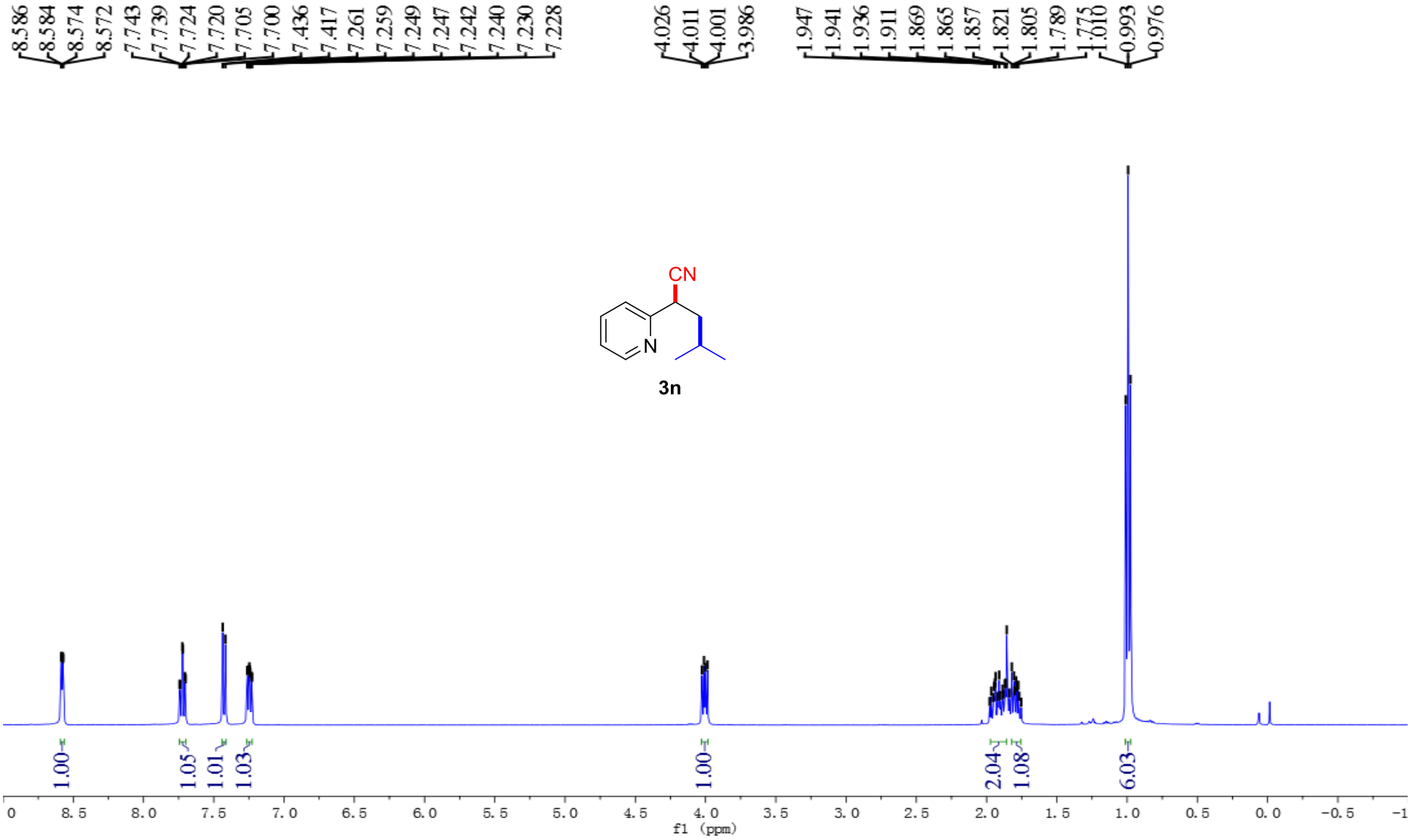
f1 (ppm)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7.228
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4.011
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1.947
1.941
1.936
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1.865
1.857
1.821
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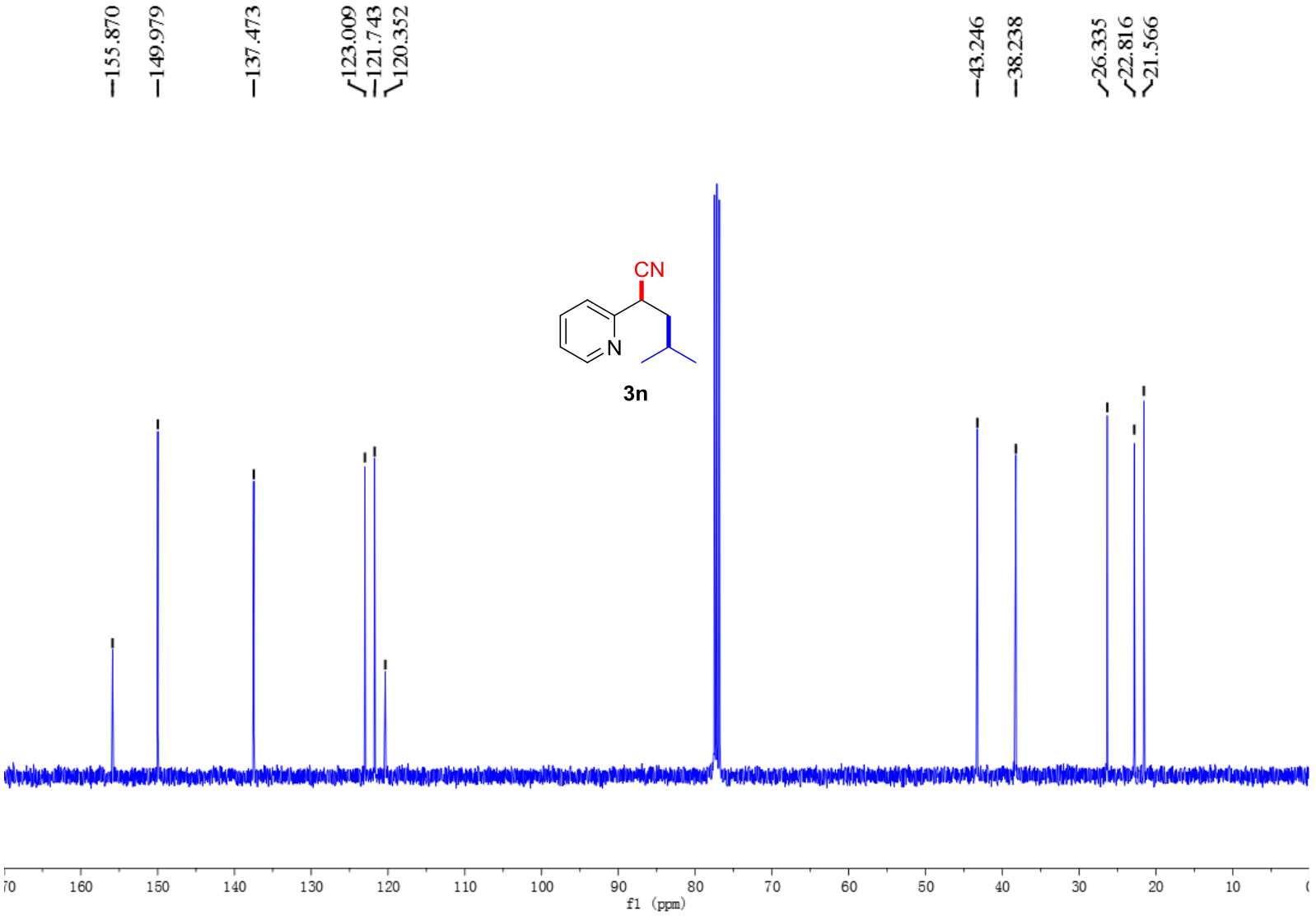
1.789
1.775
1.010
0.993
0.976
CN
N
3n
1.00
1.05
1.01
1.03
1.00
2.04
1.08
6.03
f1 (ppm)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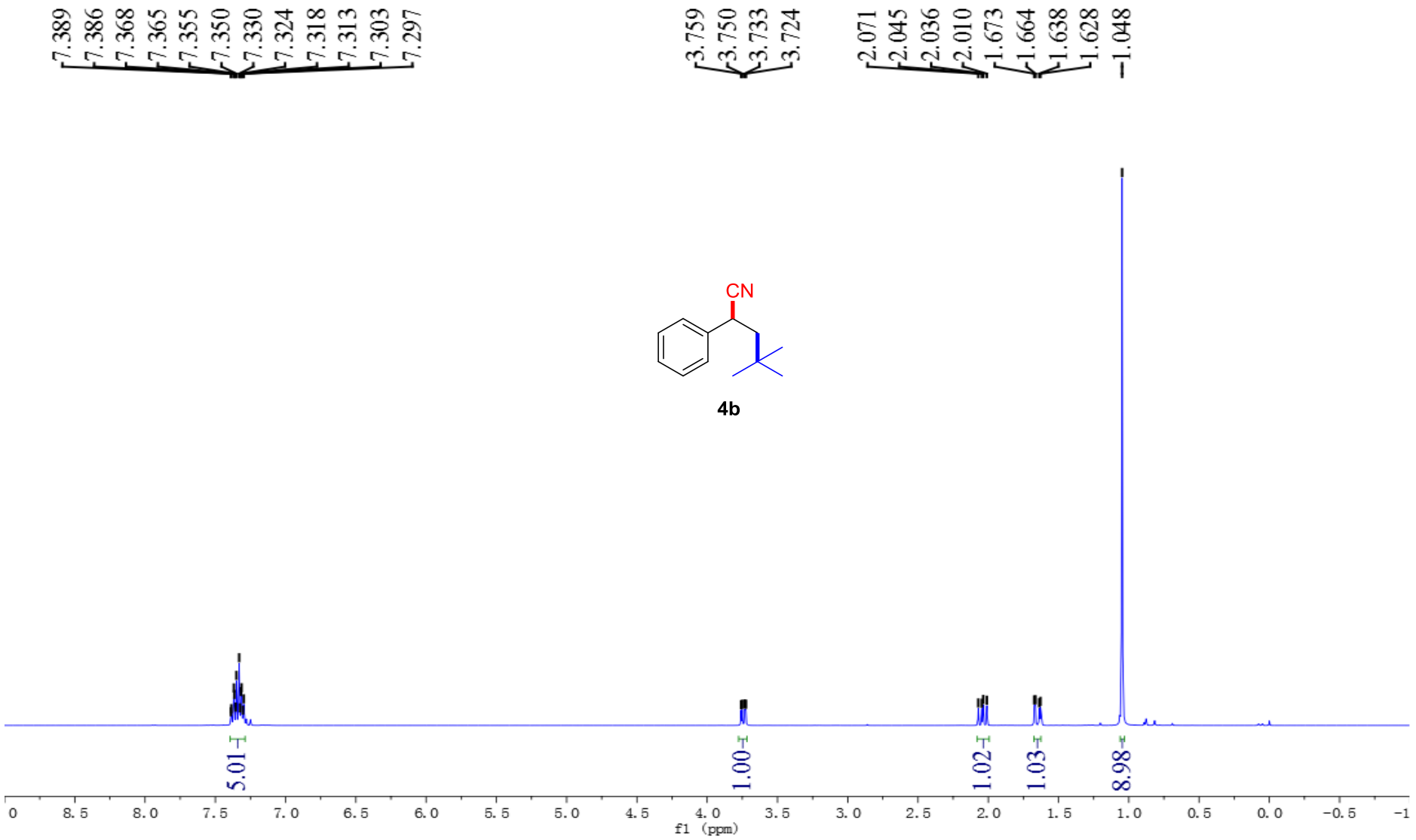
149.979
137.473
123.009
121.743
120.352
43.246
38.238
26.335
22.816
21.566
CN
N
3n
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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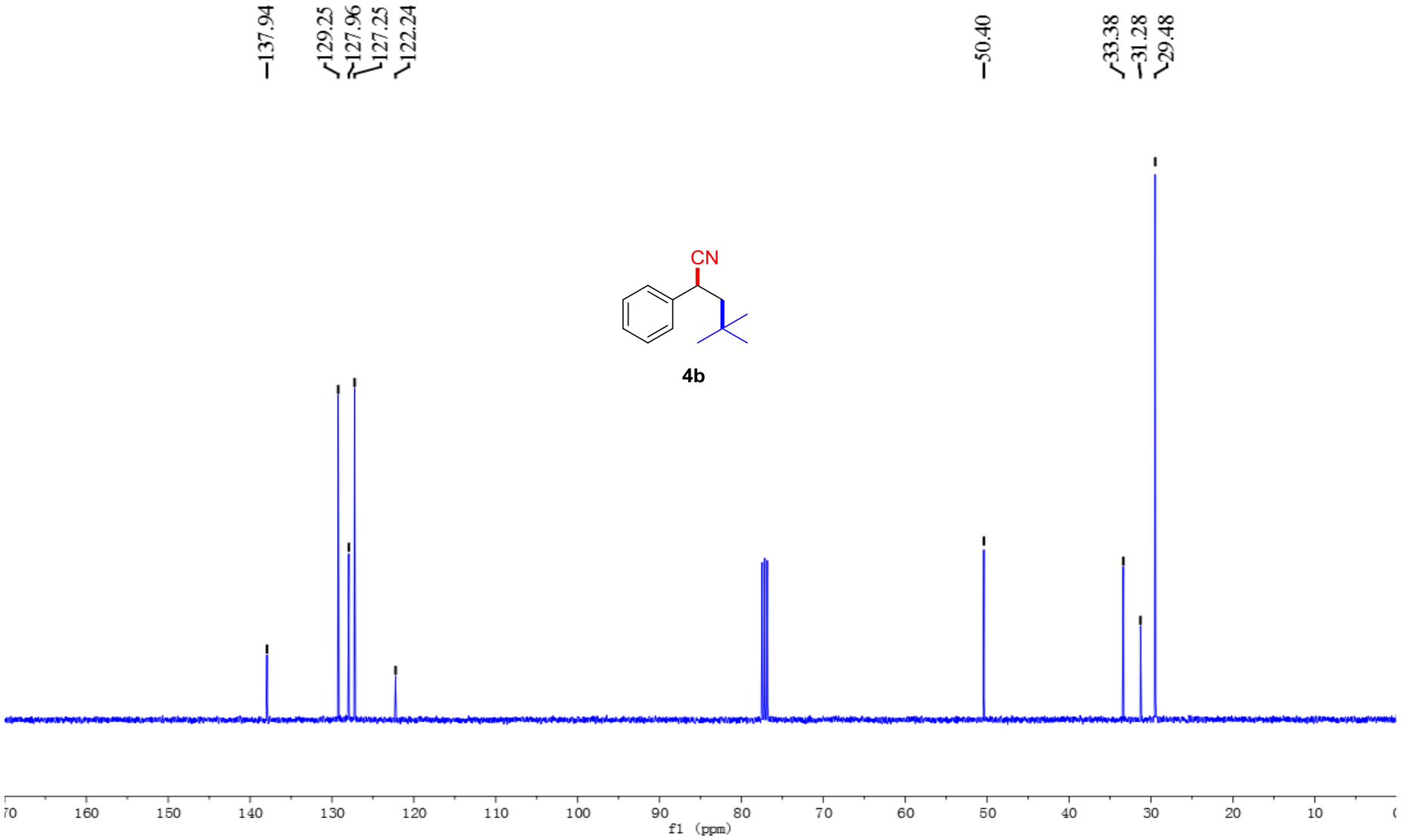
7.386
7.368
7.365
7.355
7.350
7.330
7.324
7.318
7.313
7.303
7.297
3.759
3.750
3.733
3.724
2.071
2.045
2.036
2.010
1.673
1.664
1.638
1.628
1.048
CN
5.01
1.00
1.02
1.03
8.98
f1 (ppm)

4b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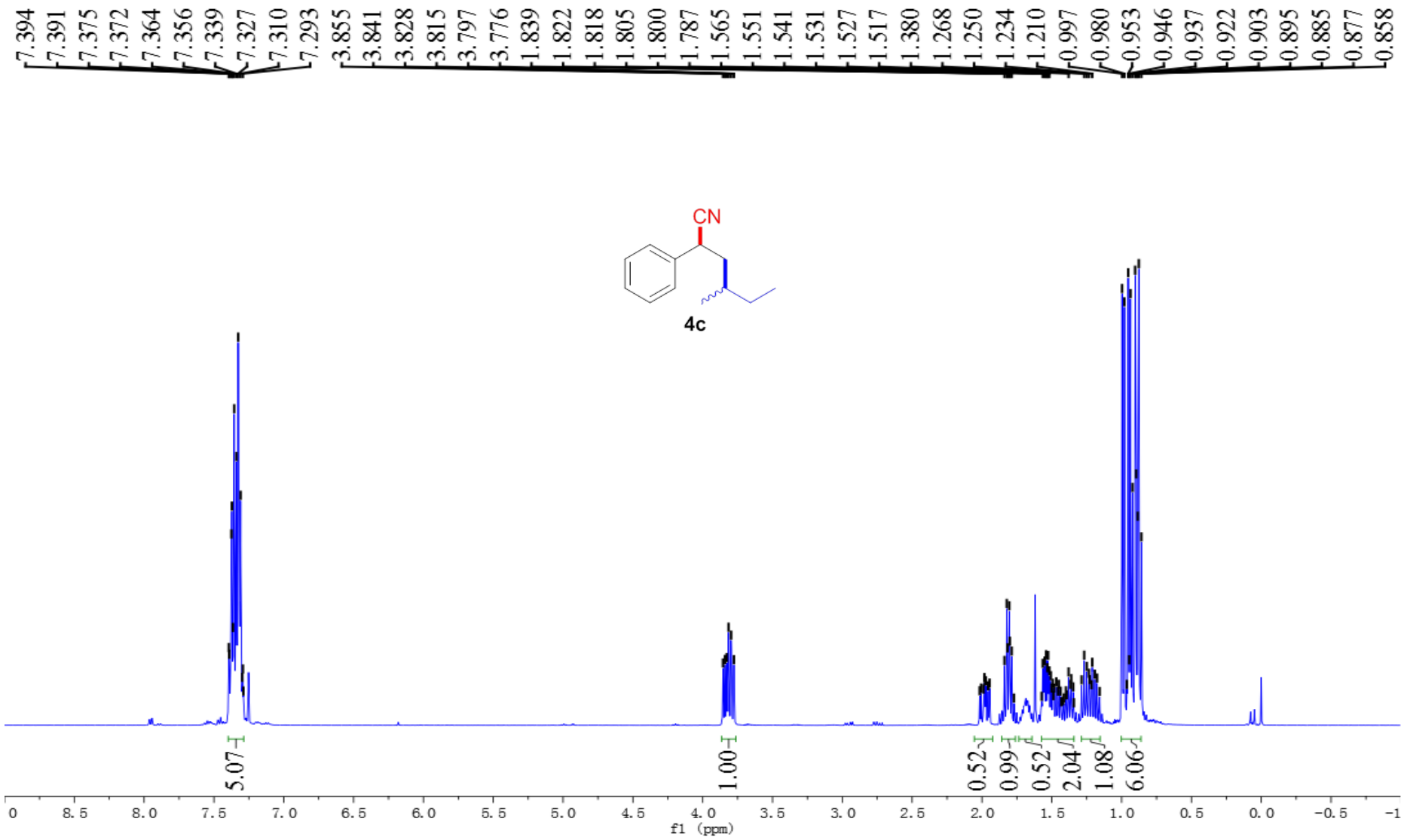
129.25
127.96
127.25
122.24
50.40
33.38
31.28
29.48
CN
4b
f1 (ppm)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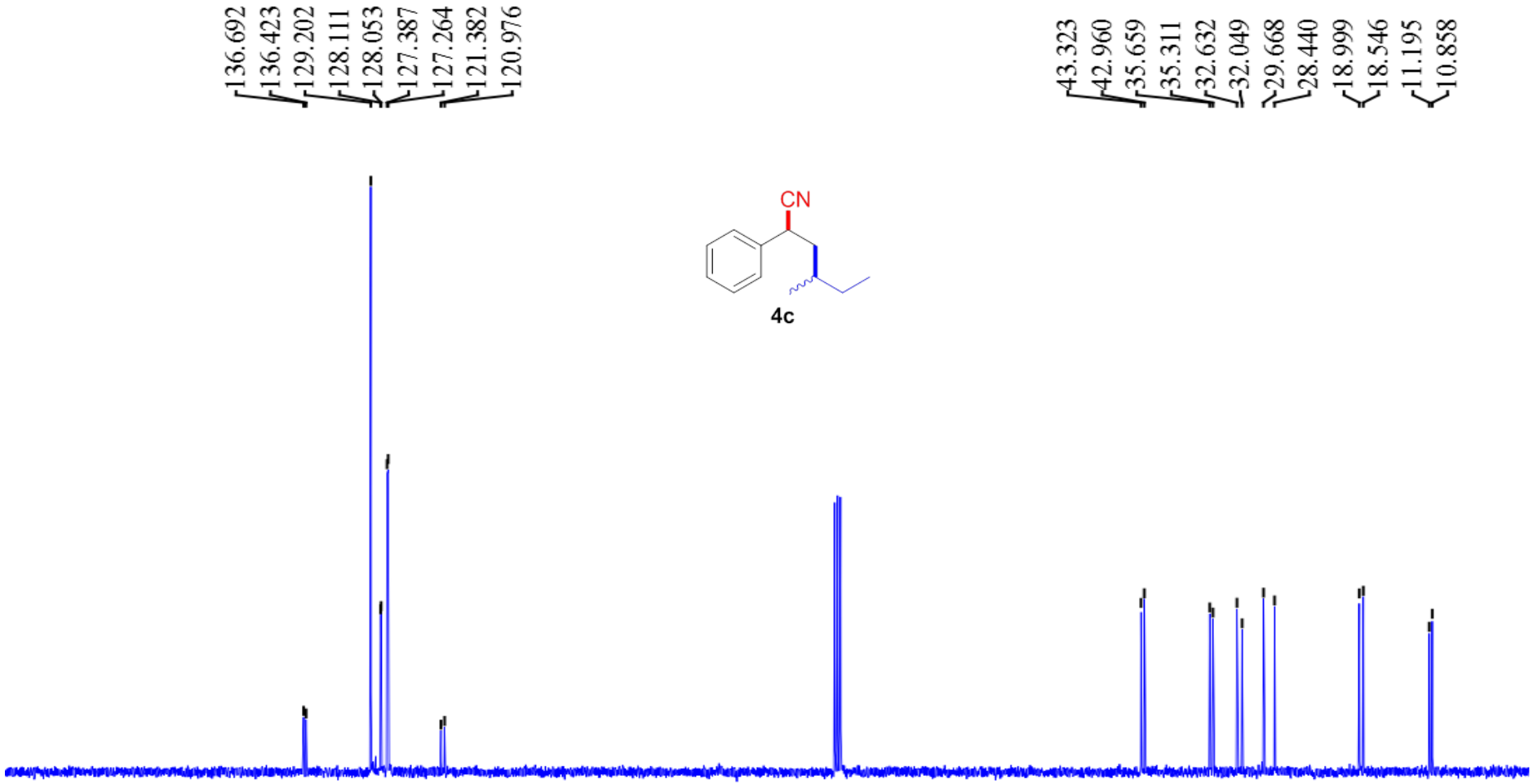
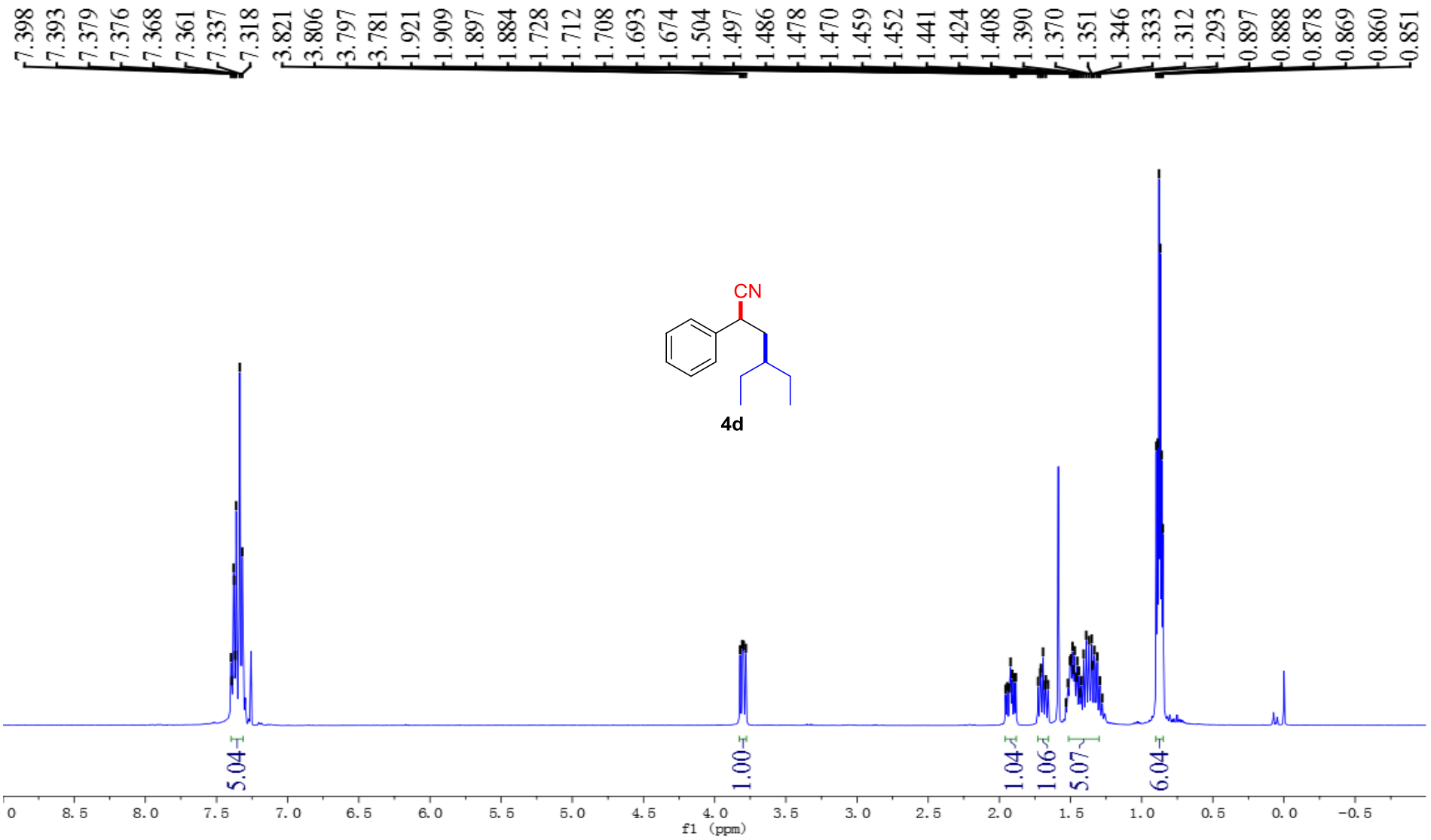
7.391
7.375
7.372
7.364
7.356
7.339
7.327
7.310
7.293
3.855
3.841
3.828
3.815
3.797
3.776
1.839
1.822
1.818
1.805
1.800
1.787
1.565
1.551
1.541
1.531
1.527
1.517
1.380
1.268
1.250
1.234
1.210
0.997
0.980
0.953
0.946
0.937
0.922
0.903
0.895
0.885
0.877
0.858
CN
4c
5.07
1.00
0.52
0.99
0.52
2.04
1.08
6.06
f1 (ppm)


136.692
136.423
129.202
128.111
128.053
127.387
127.264
121.382
120.976
43.323
42.960
35.659
35.311
32.632
32.049
29.668
28.440
18.999
18.546
11.195
10.858
CN
4c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7.393
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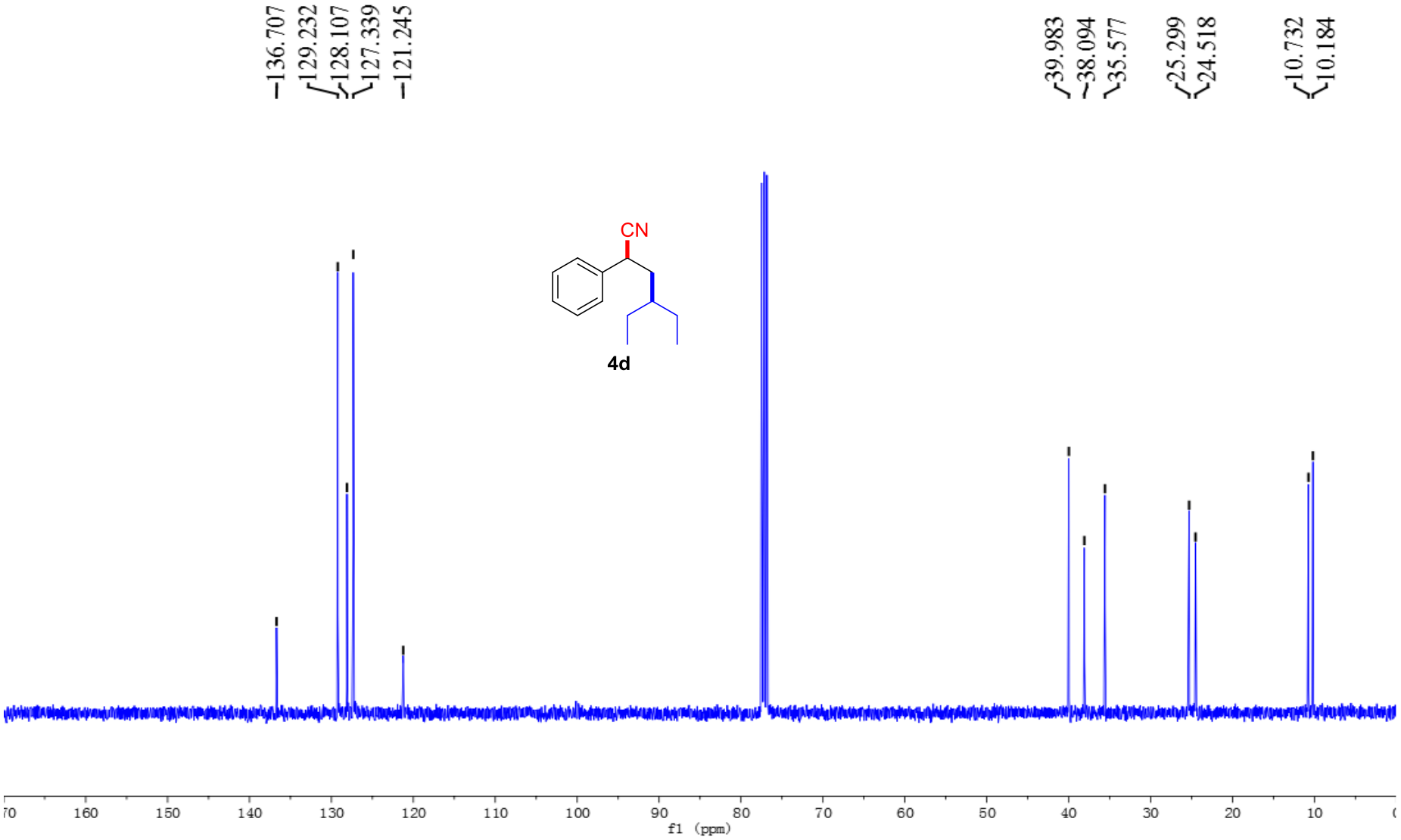
7.376
7.368
7.361
7.337
7.318
3.821
3.806
3.797
3.781
1.921
1.909
1.897
1.884
1.728
1.712
1.708
1.693
1.674
1.504
1.497
1.486
1.478
1.470
1.459
1.452
1.441
1.424
1.408
1.390
1.370
1.351
1.346
1.333
1.312
1.293
0.897
0.888
0.878
0.869
0.860
0.851
CN
4d
5.04
1.00
1.04
1.06
5.07
6.04
f1 (ppm)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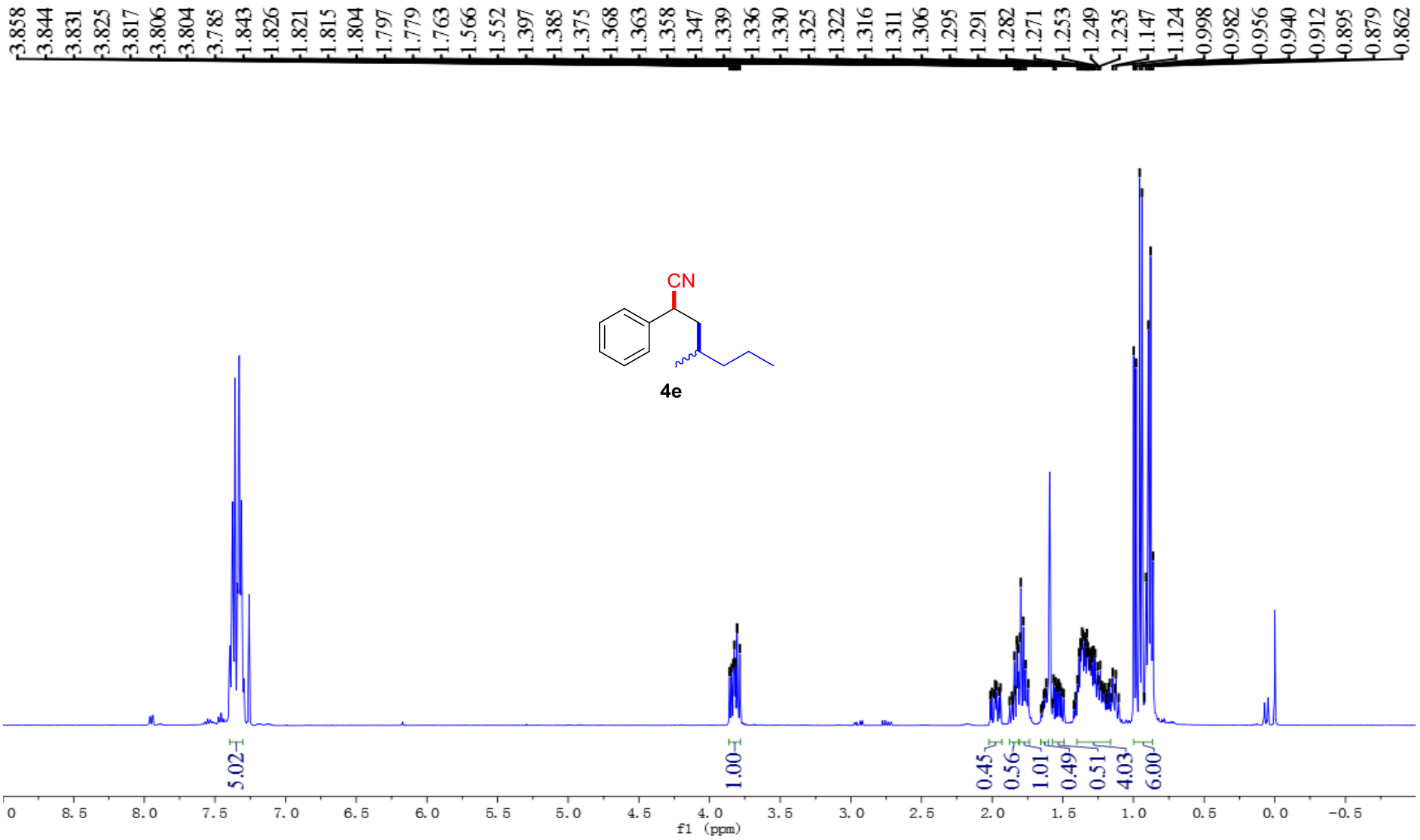
129.232
128.107
127.339
121.245
39.983
38.094
35.577
25.299
24.518
10.732
10.184
CN
4d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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3.831
3.825
3.817
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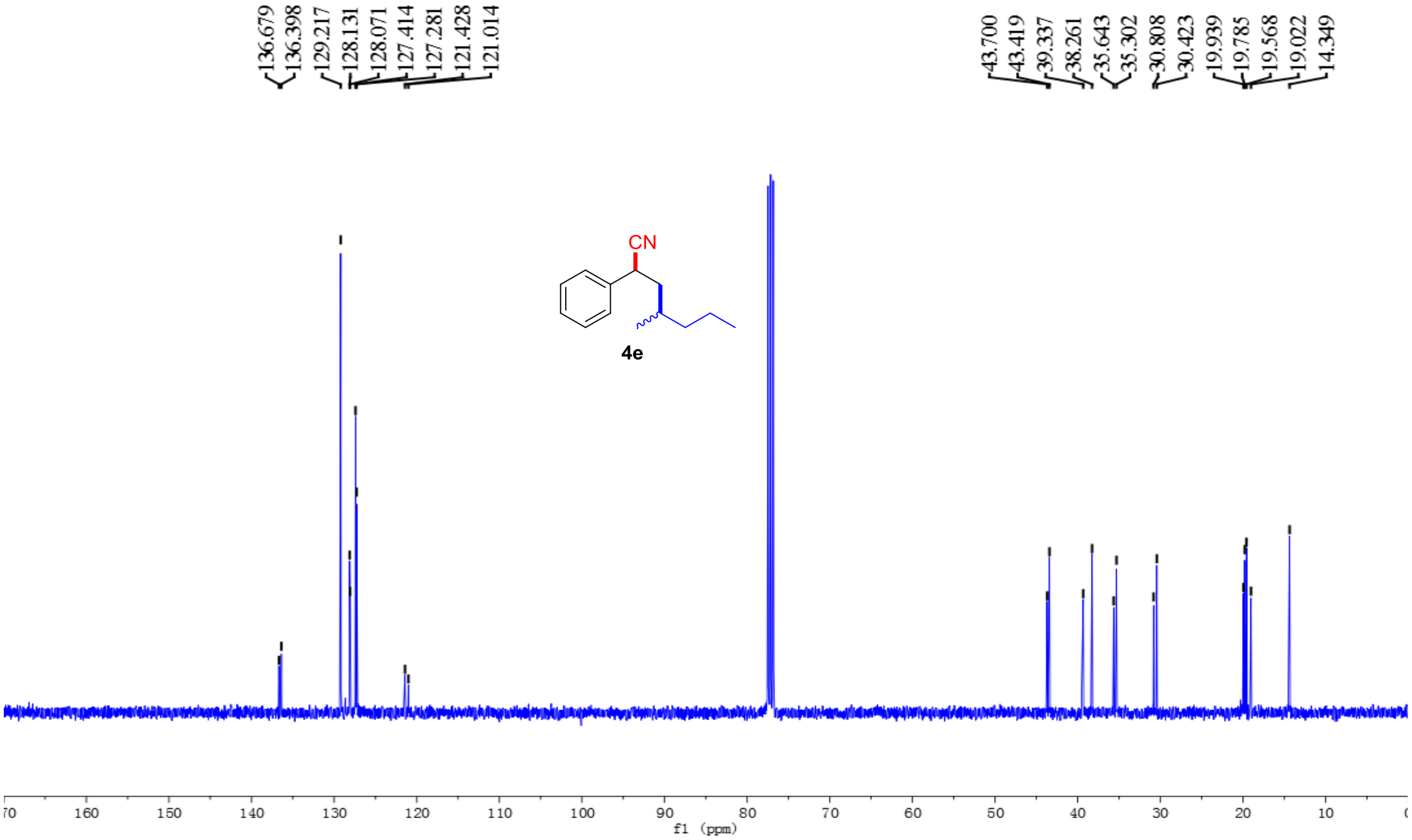
3.804
3.785
1.843
1.826
1.821
1.815
1.804
1.797
1.779
1.763
1.566
1.552
1.397
1.385
1.375
1.368
1.363
1.358
1.347
1.339
1.336
1.330
1.325
1.322
1.316
1.311
1.306
1.295
1.291
1.282
1.271
1.253
1.249
1.235
1.147
1.124
0.998
0.982
0.956
0.940
0.912
0.895
0.879
0.862
CN
4e
5.02
1.00
0.45
0.56
1.01
0.49
0.51
4.03
6.00
f1 (ppm)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129.217
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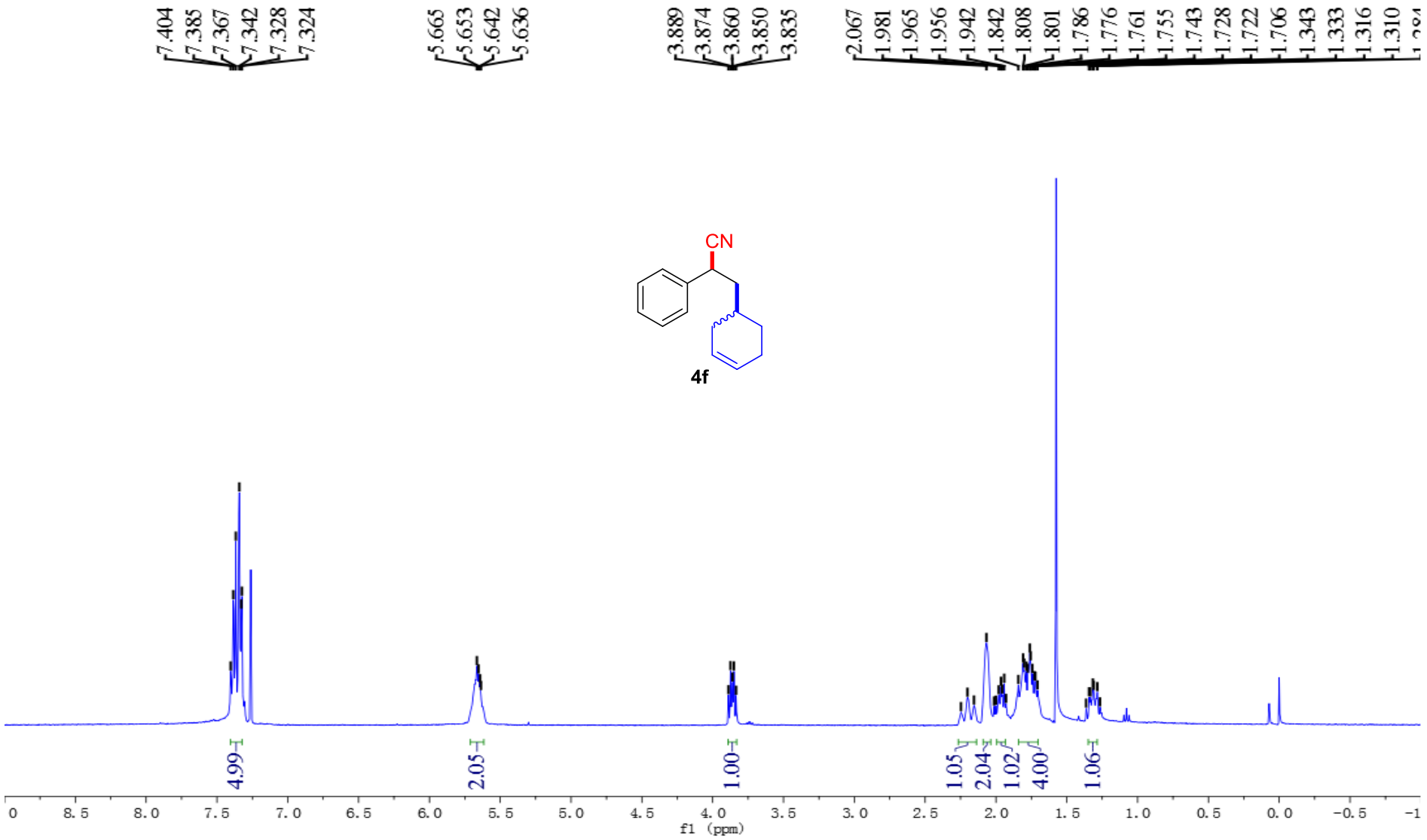
128.071
127.414
127.281
121.428
121.014
43.700
43.419
39.337
38.261
35.643
35.302
30.808
30.423
19.939
19.785
19.568
19.022
14.349
CN
4e
f1 (ppm)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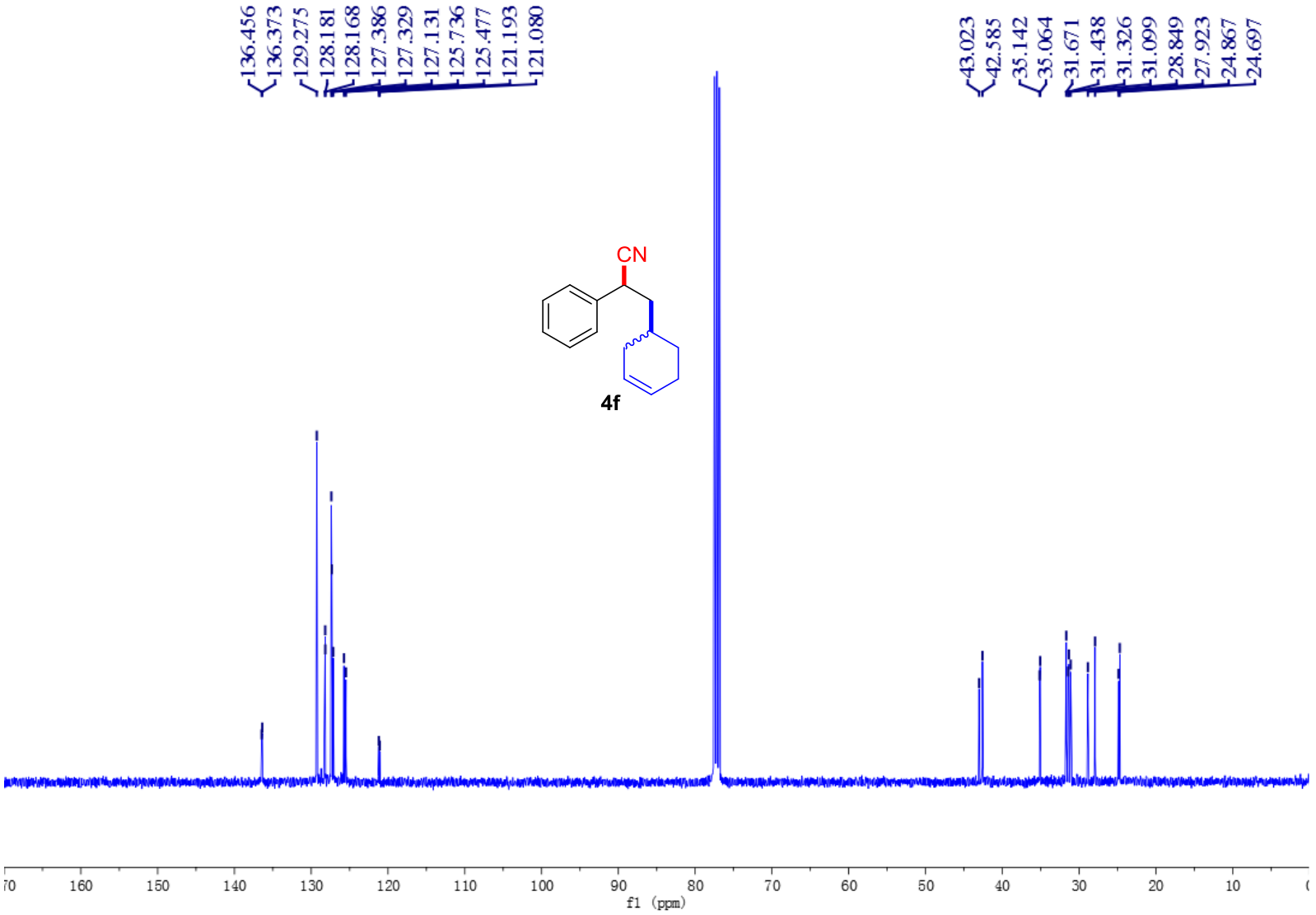
7.385
7.367
7.342
7.328
7.324
5.665
5.653
5.642
5.636
3.889
3.874
3.860
3.850
3.835
2.067
1.981
1.965
1.956
1.942
1.842
1.808
1.801
1.786
1.776
1.761
1.755
1.743
1.728
1.722
1.706
1.343
1.333
1.316
1.310
CN
4f
4.99
2.05
1.00
1.05
2.04
1.02
4.00
1.06
f1 (ppm)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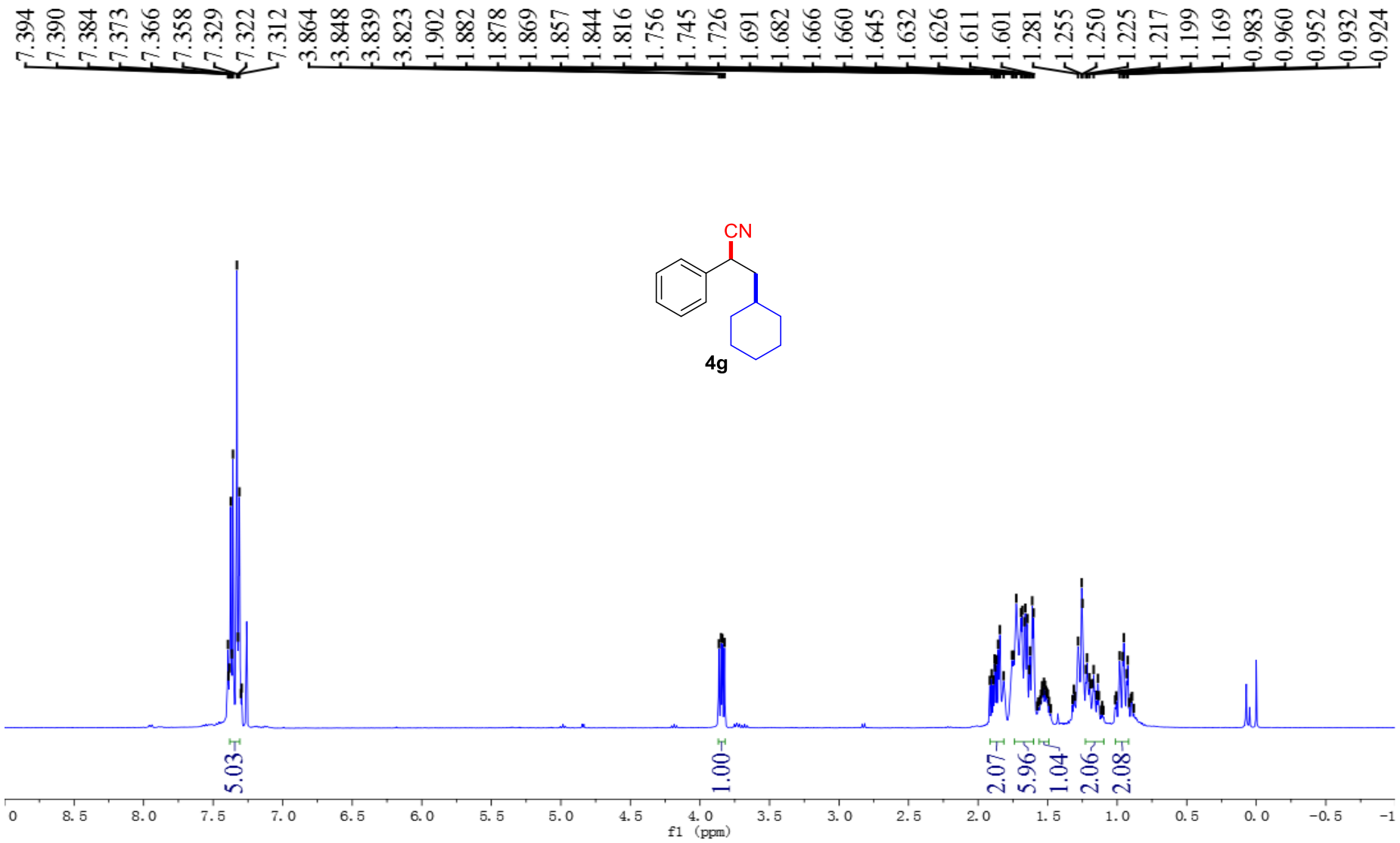
128.168
127.386
127.329
127.131
125.736
125.477
121.193
121.080
43.023
42.585
35.142
35.064
31.671
31.438
31.326
31.099
28.849
27.923
24.867
24.697
CN
4f
f1 (ppm)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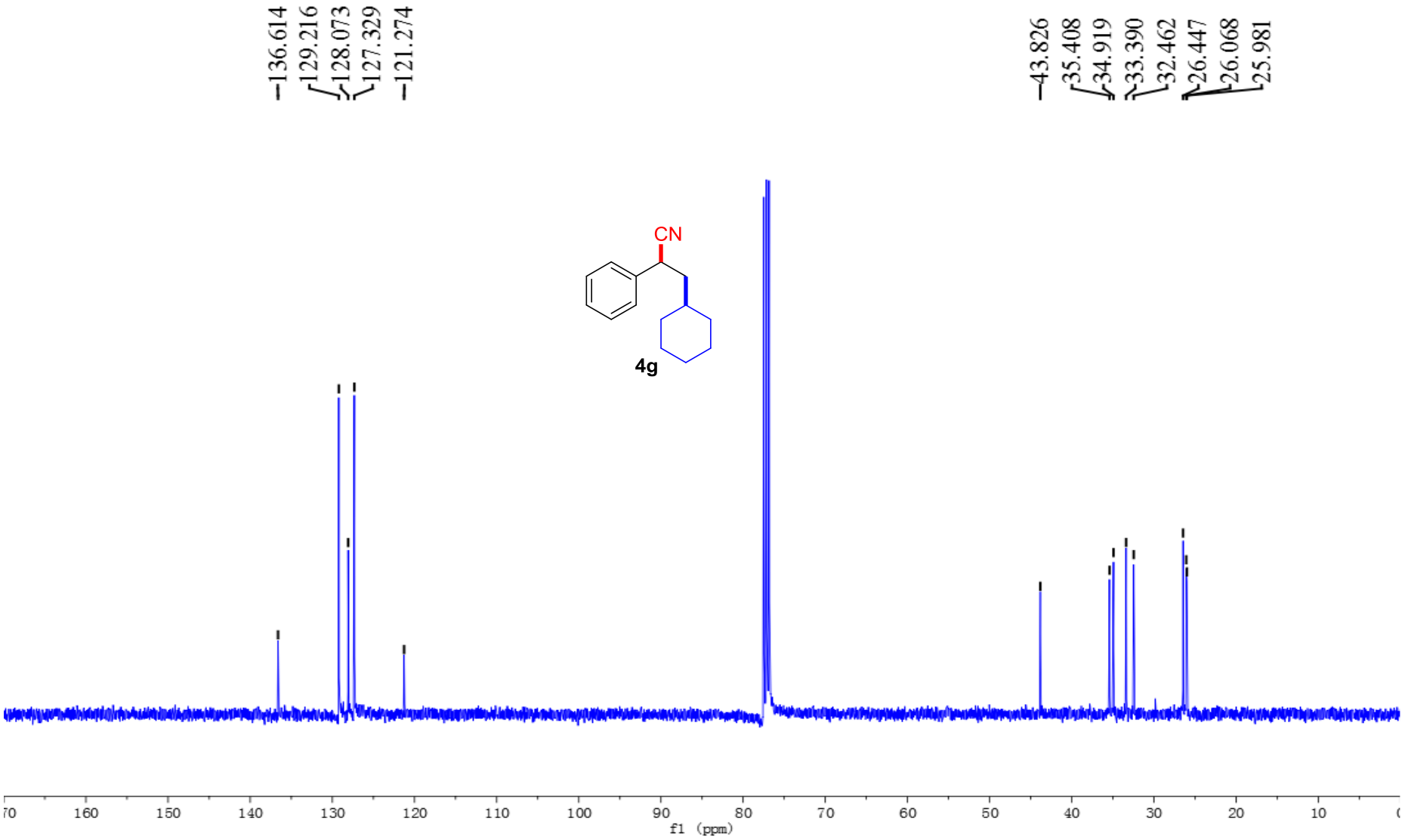
7.390
7.384
7.373
7.366
7.358
7.329
7.322
7.312
3.864
3.848
3.839
3.823
1.902
1.882
1.878
1.869
1.857
1.844
1.816
1.756
1.745
1.726
1.691
1.682
1.666
1.660
1.645
1.632
1.626
1.611
1.601
1.281
1.255
1.250
1.225
1.217
1.199
1.169
0.983
0.960
0.952
0.932
0.924
CN
4g
5.03
1.00
2.07
5.96
1.04
2.06
2.08
f1 (ppm)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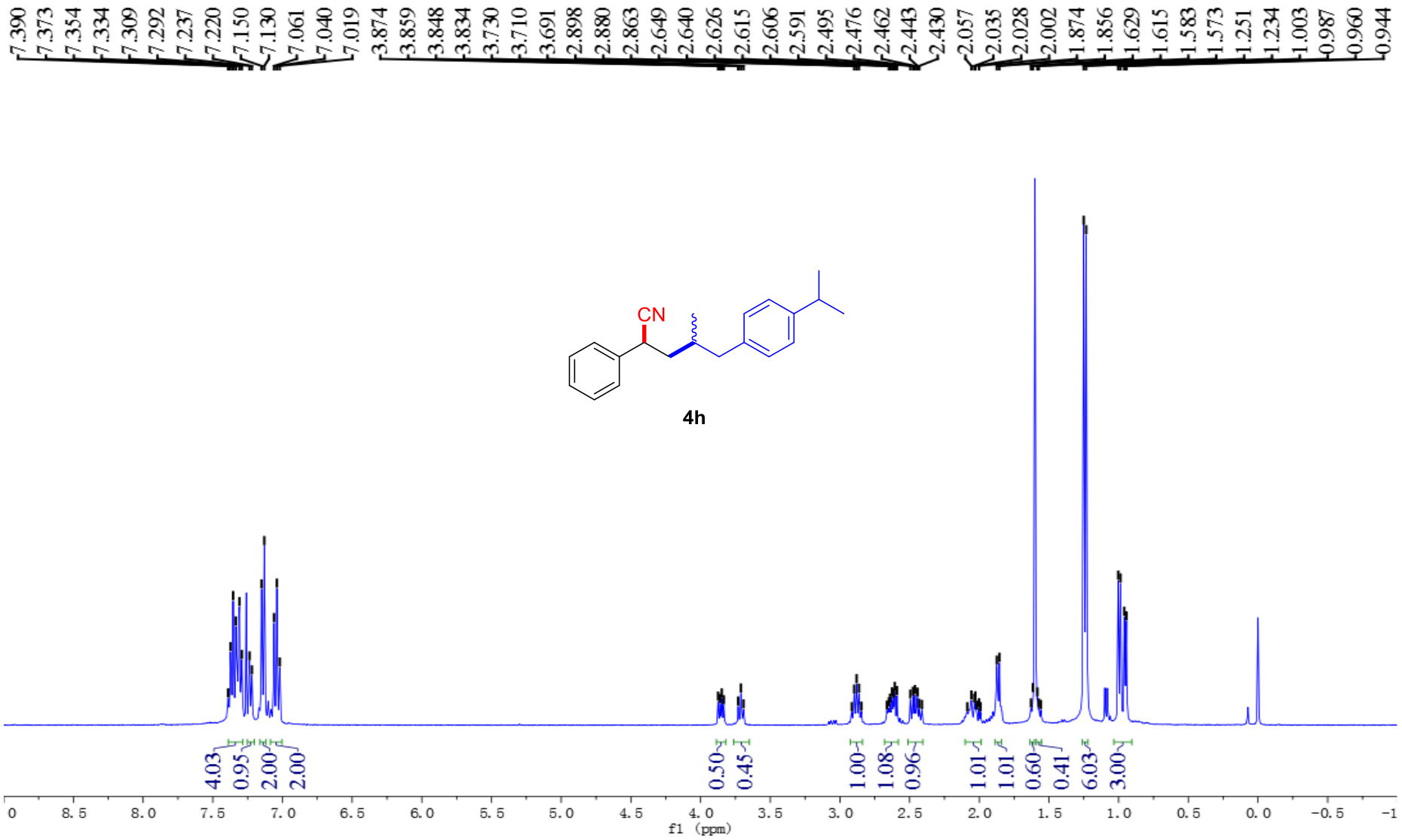
129.216
128.073
127.329
121.274
43.826
35.408
34.919
33.390
32.462
26.447
26.068
25.981
CN
4g
f1 (ppm)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7.373
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7.334
7.309
7.292
7.237
7.220
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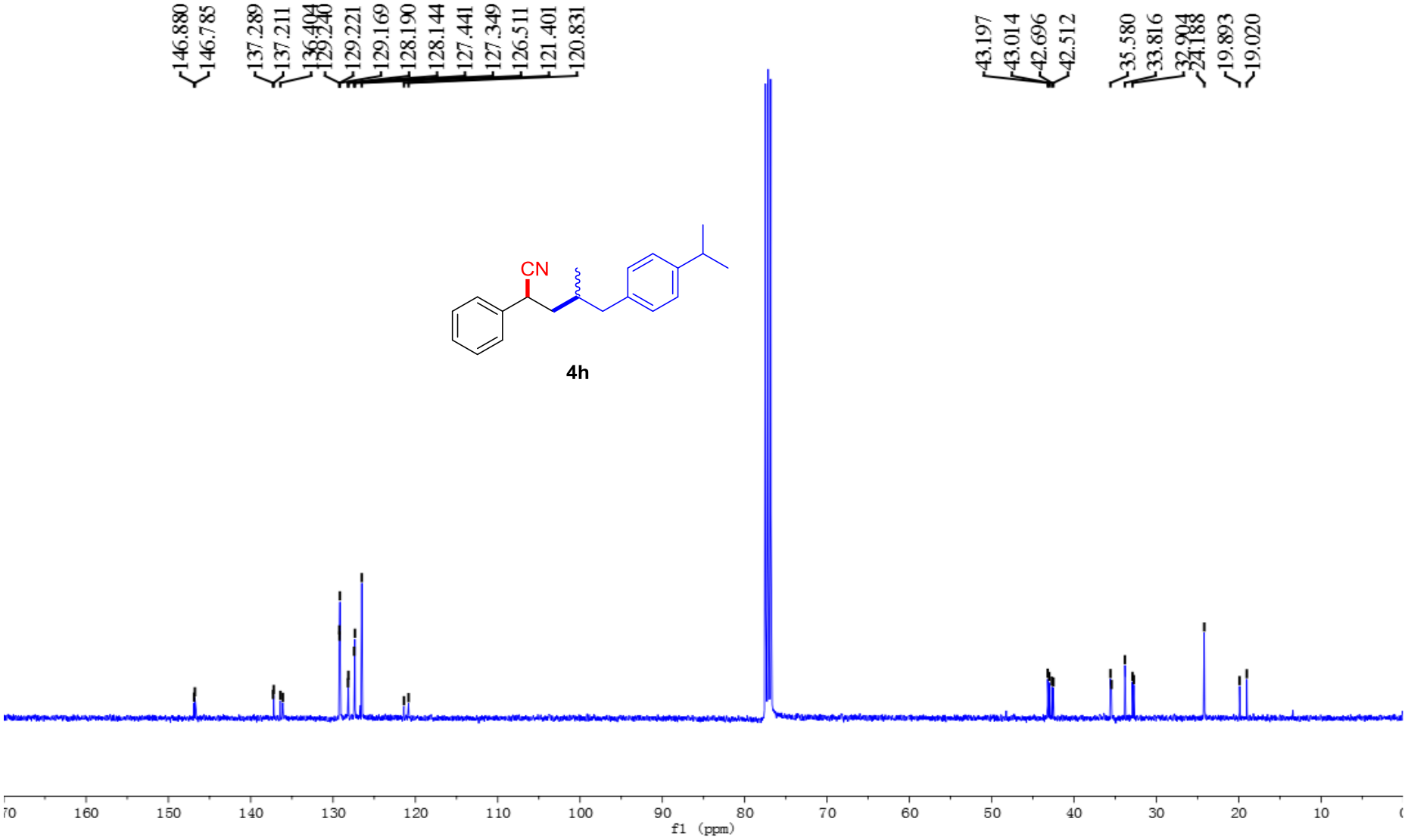
7.130
7.061
7.040
7.019
3.874
3.859
3.848
3.834
3.730
3.710
3.691
2.898
2.880
2.863
2.649
2.640
2.626
2.615
2.606
2.591
2.495
2.476
2.462
2.443
2.430
2.057
2.035
2.028
2.002
1.874
1.856
1.629
1.615
1.583
1.573
1.251
1.234
1.003
0.987
0.960
0.944
CN
4h
4.03
0.95
2.00
2.00
0.50
0.45
1.00
1.08
0.96
1.01
1.01
0.60
0.41
6.03
3.00
f1 (ppm)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127.441
127.349
126.511
121.401
120.831
43.197
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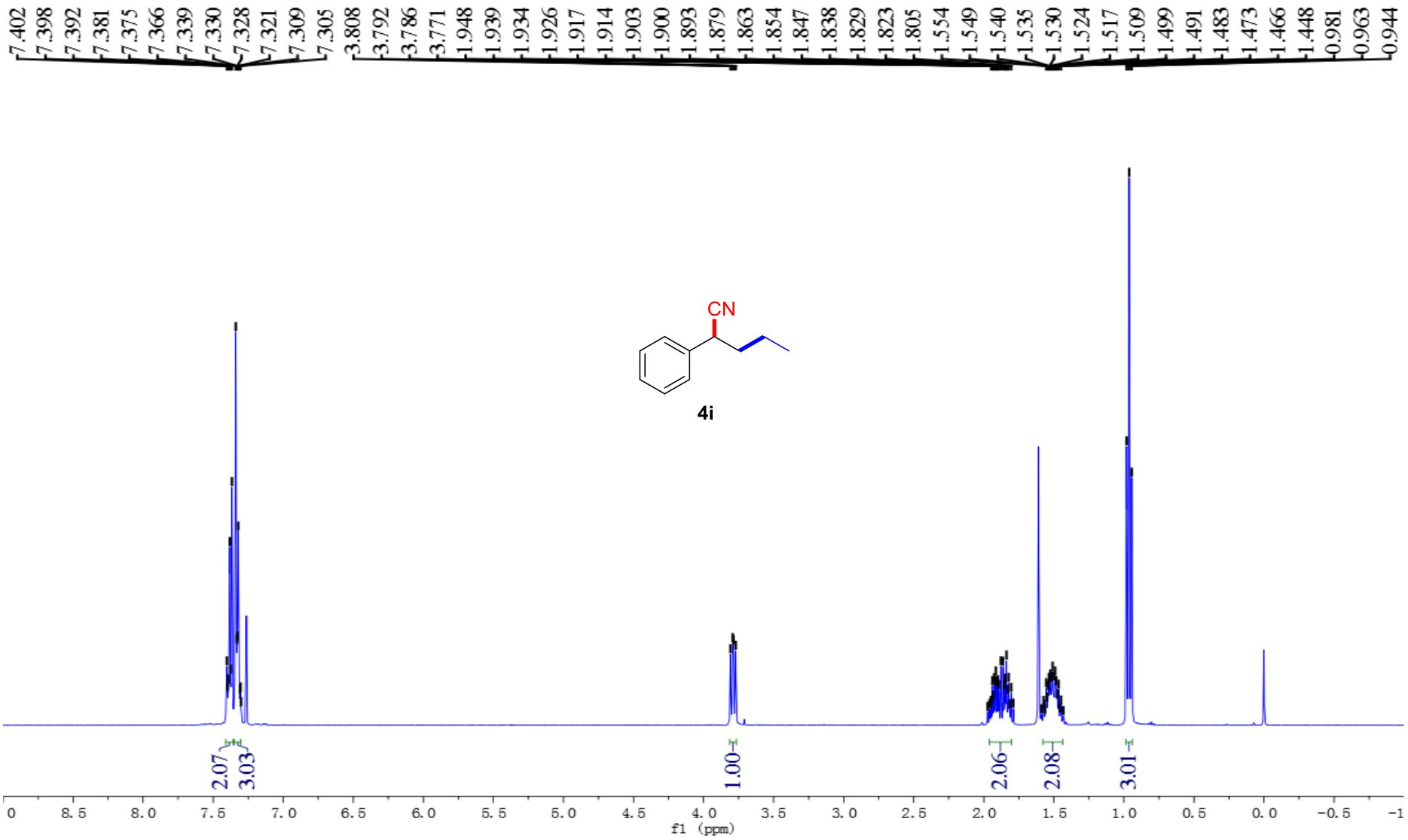
42.512
35.580
33.816
32.904
24.188
19.893
19.020
CN
4h
f1 (ppm)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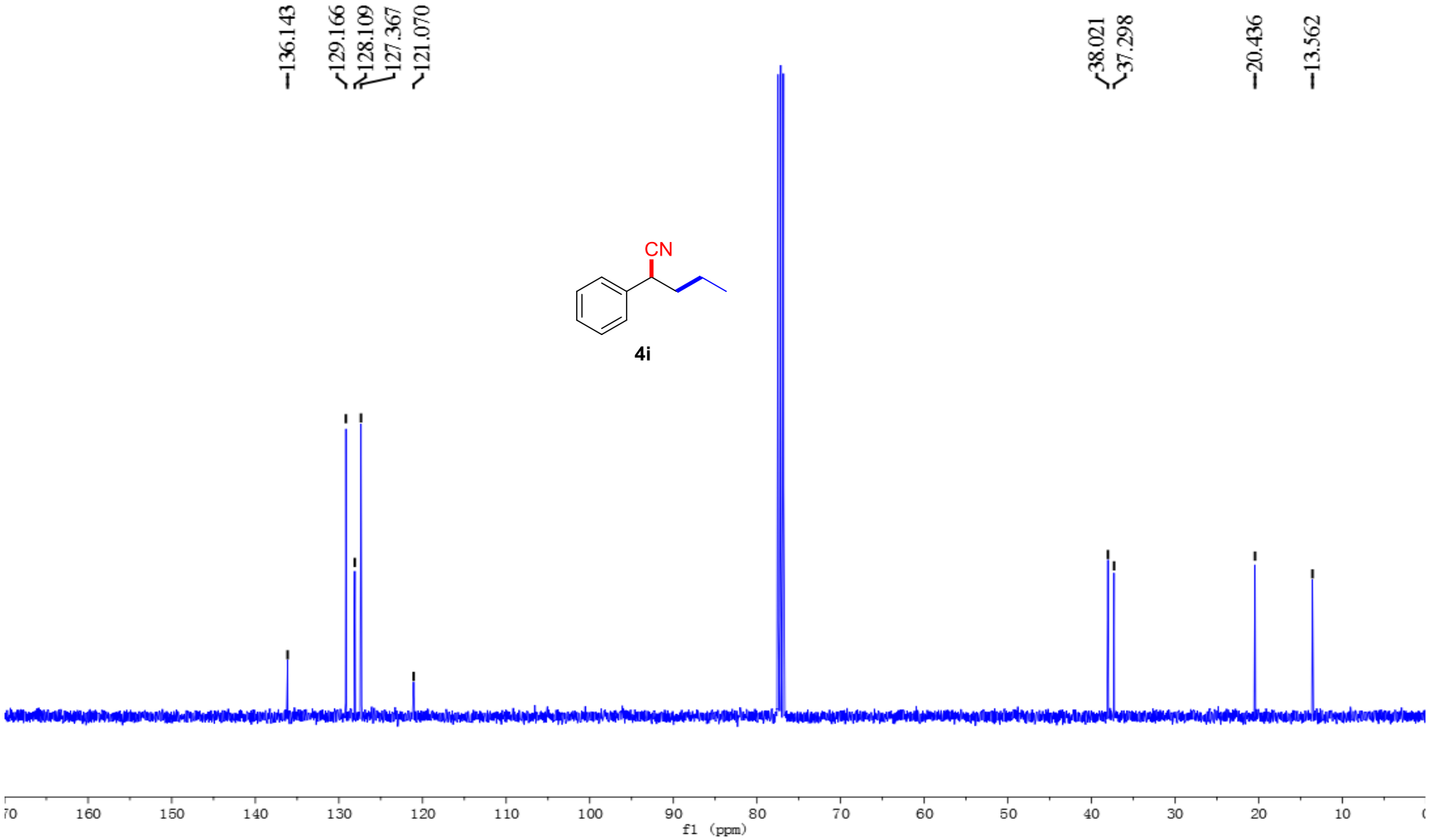
7.321
7.309
7.305
3.808
3.792
3.786
3.771
1.948
1.939
1.934
1.926
1.917
1.914
1.903
1.900
1.893
1.879
1.863
1.854
1.847
1.838
1.829
1.823
1.805
1.554
1.549
1.540
1.535
1.530
1.524
1.517
1.509
1.499
1.491
1.483
1.473
1.466
1.448
0.981
0.963
0.944
CN
4i
2.07
3.03
1.00
2.06
2.08
3.01
f1 (ppm)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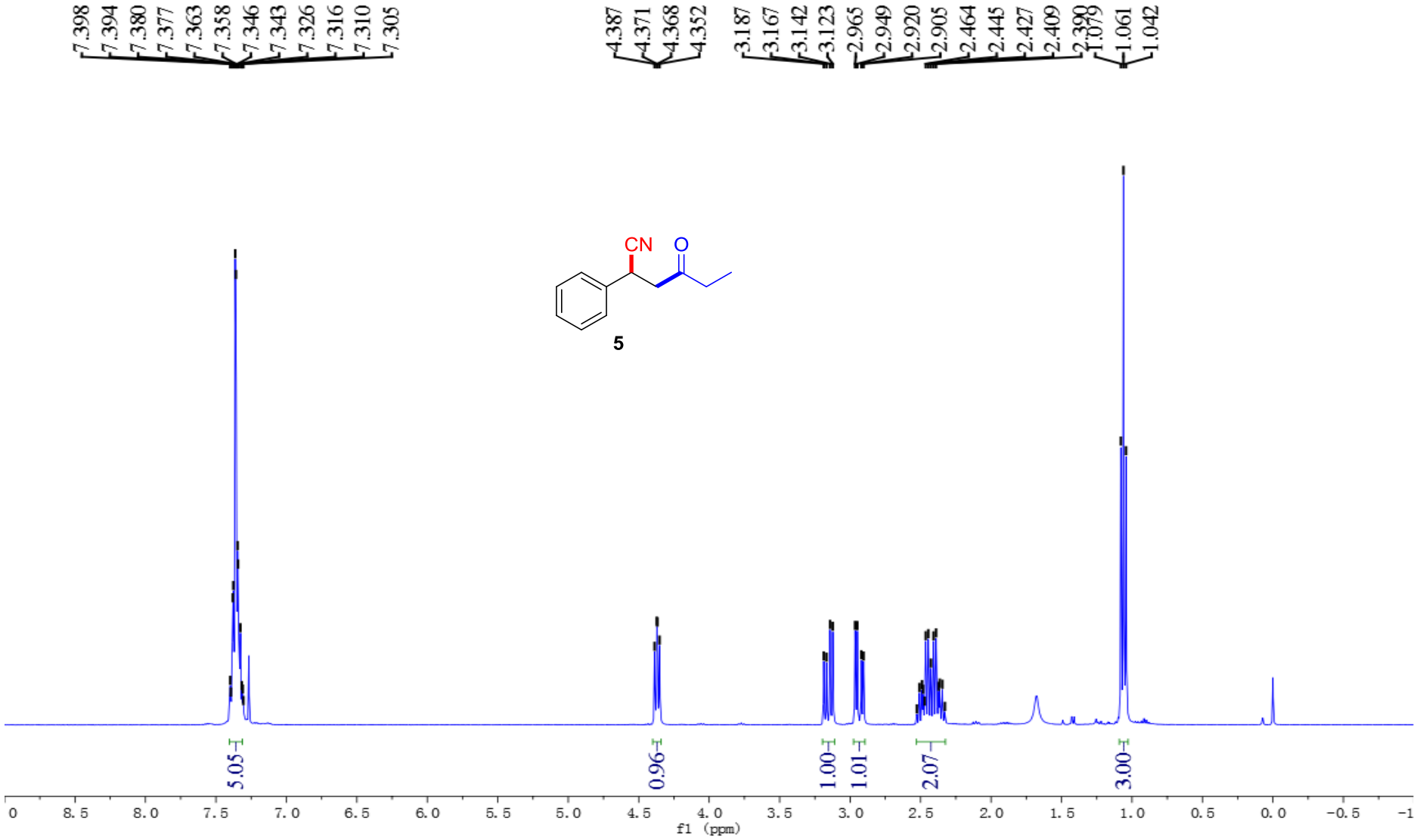
38.021
37.298
20.436
13.562
CN
4i
f1 (ppm)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7.394
7.380
7.377
7.363
7.358
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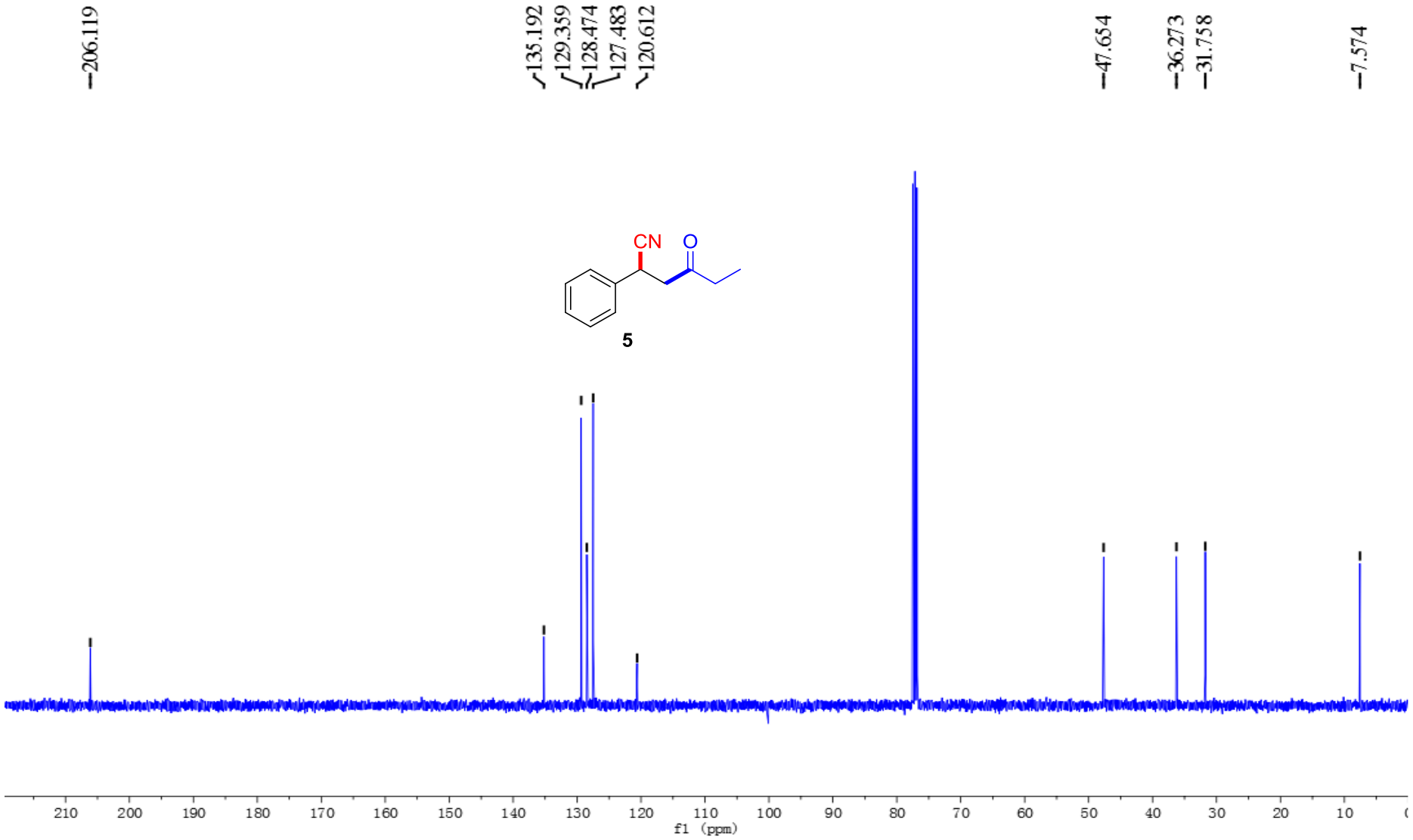
7.343
7.326
7.316
7.310
7.305
4.387
4.371
4.368
4.352
3.187
3.167
3.142
3.123
2.965
2.949
2.920
2.905
2.464
2.445
2.427
2.409
2.390
1.079
1.061
1.042
CN
O
5
5.05
0.96
1.00
1.01
2.07
3.00
f1 (ppm)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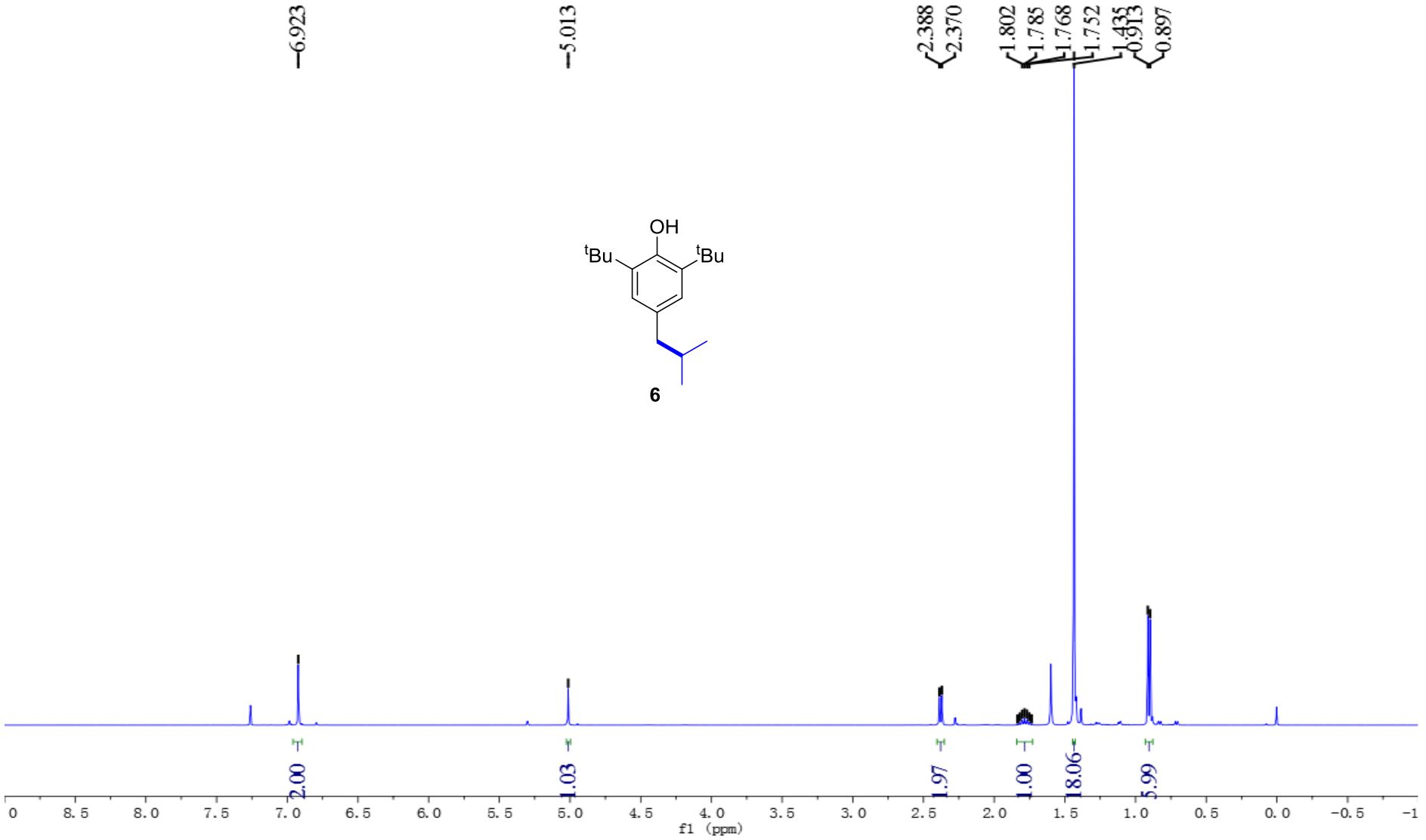
128.474
127.483
120.612
47.654
36.273
31.758
7.574
CN
O
5
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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2.388
2.370
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1.785
1.768
1.752
1.435
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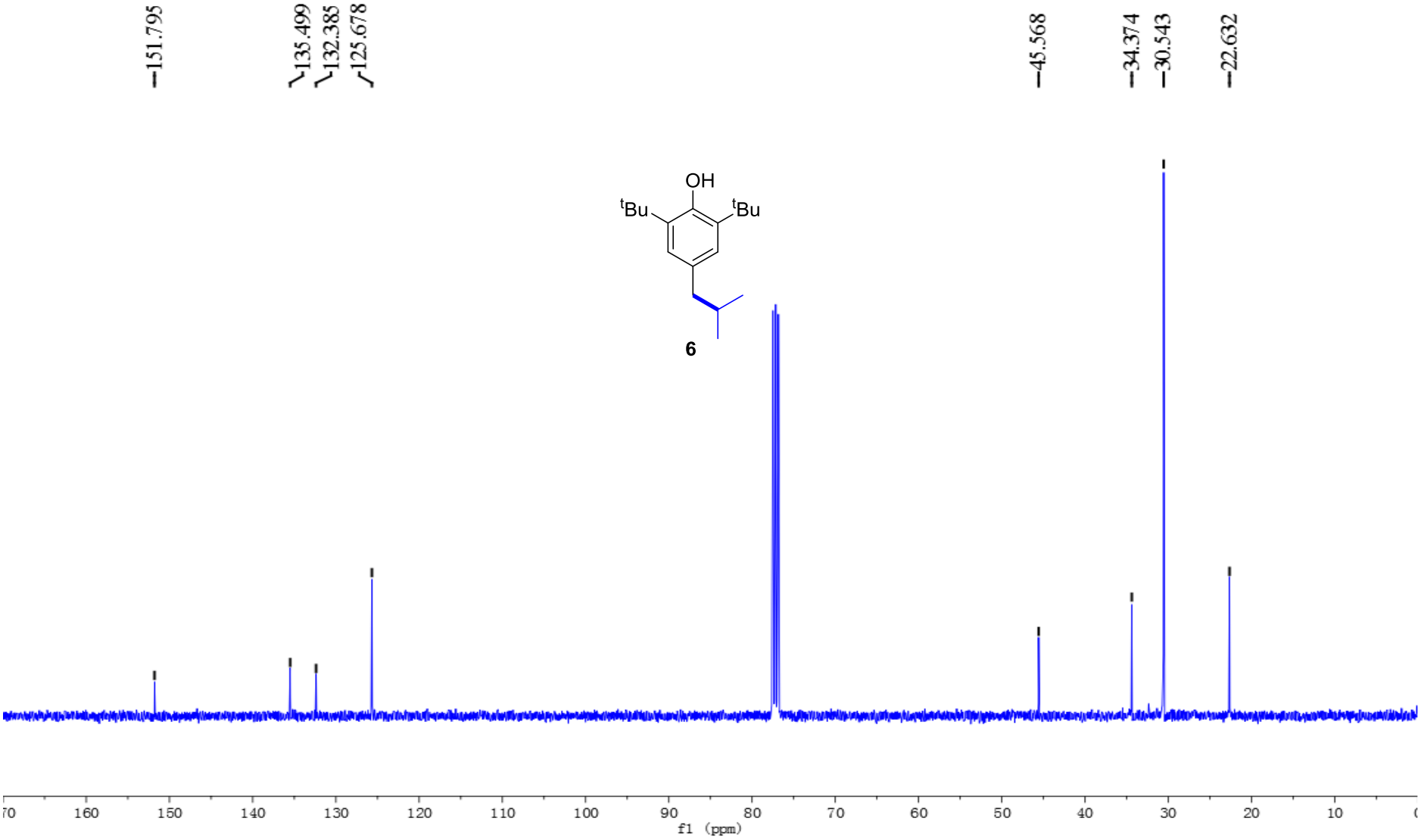
0.897
OH
tBu
tBu
6
2.00
1.03
1.97
1.00
18.06
5.99
f1 (ppm)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34.374
30.543
22.632
OH
tBu
tBu
6
f1 (ppm)