Supporting Information

The Synthesis of Cyanoformamides *via* a CsF-Promoted Decyanation/Oxidation Cascade of 2-Dialkylamino-Malononitriles

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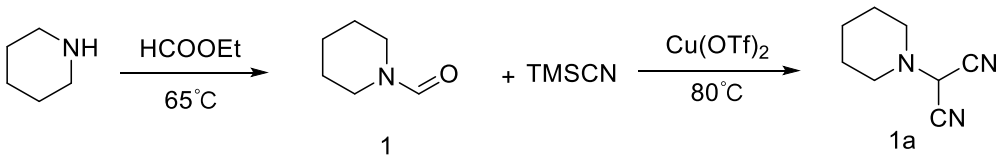
content

1. General Information

All reactions under standard conditions were carried out using anhydrous solvent under argon, dry atmosphere and monitored by thin-layer chromatography (TLC) on gel F254 plates. All products were purified through silica gel chromatography (200~300 mesh). Column chromatography was carried out with light petroleum ether (bp. 60~90 ^{o}C), ethyl acetate and dichloromethane as eluent. ^{1}H and ^{13}C spectra were recorded in $CDCl_3$ on 400 (300) MHz instruments and spectral data were reported in ppm. High-resolution mass spectral analysis (HRMS) data were measured on the Apex II by means of the ESI technique.

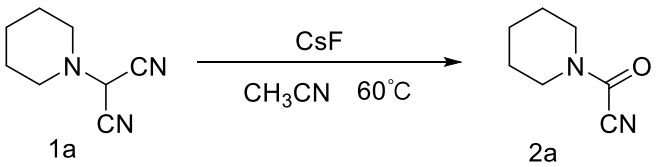
2. General experimental procedure

2.1 General experimental procedure A for products 1a-1ab



To a stirred solution of HCOOEt (1.8 mL, 22.5 mmol) was added Piperidine (1 g, 11.75 mmol) under argon atmosphere. The mixture was stirred in 65 ℃ for 12 h. After the reaction was complete which is monitored by TLC, The magnet was removed and the solvent in the reaction flask was evaporated to dryness and purified by column chromatography to give N-formylpiperidine. To a stirred solution of 3 N-formylpiperidine (0.5g, 4.419 mmol) in n-heptane (20 mL) were successively added trimethylsilanecarbonitrile (0.964 mL, 9.722 mmol) and andbis(((trifluoromethyl)sulfonyl)oxy)copper (0.16 g, 0.442 mmol) at 80 ℃ under argonatmosphere. The reaction mixture was continued stirring for 8h. Upon completion of the reaction (monitored by TLC), the reaction mixture was quenched by slow addition of water. The aqueous layer was extracted three times with EtOAc and the combined organic layerswere washed with brine, dried over sodium sulfate, and evaporated to dryness and purified by column chromatography to afford pure desired product as a light white solid.

2.2 General experimental procedure B for products 2a-2ab

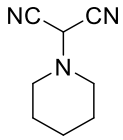


To a stirred solution of 2-(piperidin-1-yl)malononitrile (50 mg, 0.335 mmol) in solvent CH_3CN (2 mL) was added CsF (200 mg, 0.730 mmol). Then the mixture was

heated to 80 ℃ and stirred at last for 12 hours. Upon completion of the reaction (monitored by TLC), the reaction mixture was quenched by slow addition of water. The aqueous layer was extracted three times with EtOAc and the combined organic layers were washed with brine, dried over sodium sulfate, and evaporated to dryness and purified by column chromatography to afford desired product 2 as a yellow liquic(39 mg, 86%). The reaction provides the hydrazone derivatives **2a-2aa** in about 70−85% yields.

3. Characterization of new products

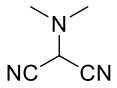
3.1 Characterization of substrates 1a–1ab



1a

2-(piperidin-1-yl)malononitrile(1a)

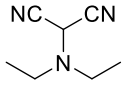
1a was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.62 (s, 1H), 2.63(d, *J* = 5.2 Hz, 4H), 1.71–1.65 (m, 4H), 1.51–1.46 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 109.89, 51.18, 48.89, 25.13, 22.88.



1b

2-(dimethylamino)malononitrile(1b)

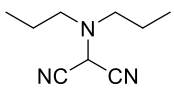
1b was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.64 (s, 1H), 2.44 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 109.73, 48.98, 41.86.



1c

2-(diethylamino)malononitrile(1c)

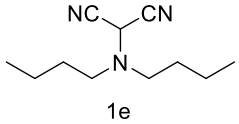
1c was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.78 (s, 1H), 2.70 (dd, *J* = 7.2 , 14.4 Hz, 4H), 1.16 (t, *J* = 7.2 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 110.76, 46.12, 44.92, 12.59.



1d

2-(dipropylamino)malononitrile(1d)

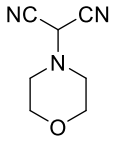
1d was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.73 (s, 1H), 2.61–2.58 (m, 4H), 1.58–1.49 (m, 4H), 0.95 (t, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 110.82, 54.08, 45.60, 20.54, 11.33.



1e

2-(dibutylamino)malononitrile (1e)

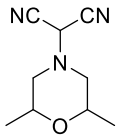
1e was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.75 (s, 1H), 2.61–2.59 (t, *J* = 7.2 Hz, 4H), 1.51–1.44 (m, 4H), 1.40–1.31 (m, 4H), 0.93 (t, *J* = 7.3 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 110.79, 52.40, 45.55, 29.23, 20.05, 13.72.



1f

2-morpholinomalononitrile(1f)

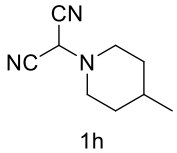
1f was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.64 (s, 1H), 3.80–3.78 (m, 4H), 2.72 (t, *J* = 4.4 Hz, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 109.35, 65.93, 49.92, 48.27.



1g

2-(2,6-dimethylmorpholino)malononitrile (1g)

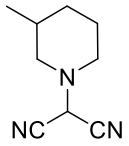
1g was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.66 (s, 1H), 3.72–3.66 (m, 2H), 2.76–2.73 (m, 2H), 2.13 (t, *J* = 10.4 Hz, 2H), 1.19 (s, 3H), 1.17 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 109.43,70.93, 55.14, 47.85, 18.66.



1h

2-(4-methylpiperidin-1-yl)malononitrile(1h)

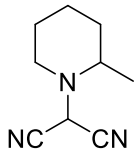
1h was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.64 (s, 1H), 2.94–2.90 (m, 2H), 2.43–2.36 (m, 2H), 1.77–1.72 (m, 2H), 1.49–1.38 (m, 1H), 1.36–1.25 (m, 2H), 0.95 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 109.89, 50.67, 48.66, 33.34, 29.52, 21.33.



1i

2-(3-methylpiperidin-1-yl)malononitrile (1i)

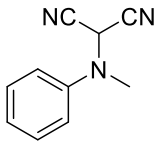
1i was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.63 (s, 1H), 2.89–2.82 (m, 2H), 2.31 (td, *J* = 14.0, 11.2 Hz, 1H), 2.01 (t, *J* = 10.2 Hz, 1H), 1.81–1.77 (m, 1H), 1.78–1.76(m, 1H), 1.74 (s, 1H), 1.74–1.70 (m, 1H), 1.68–1.58 (m, 1H), 0.93 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 109.91, 58.04, 50.71, 48.72, 31.41, 30.73, 24.59, 19.13.



1j

2-(2-methylpiperidin-1-yl)malononitrile (1j)

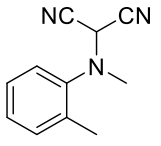
1j was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.00(s, 1H), 3.19–3.14(m, 1H), 2.45–2.37(m, 2H), 1.78–1.56(m, 2H), 1.38–1.24(m, 2H), 1.13(s, 3H), 1.11(s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 111.38, 108.98, 55.13, 50.76, 45.01, 34.15, 25.36, 23.71, 19.54.



1k

2-(methyl(phenyl)amino)malononitrile (1k)

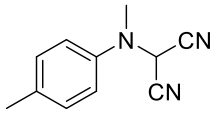
1k was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41–7.36 (m, 2H), 7.15–7.1 (m, 1H), 7.06–7.03 (m, 2H), 5.43 (s, 1H), 3.09 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.28, 129.78, 123.98, 118.59, 110.27, 46.75, 37.34.



1l

2-(methyl(o-tolyl)amino)malononitrile (1l)

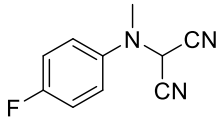
1l was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33–7.18 (m 4H), 4.91 (s, 1H), 2.96 (s, 3H), 2.36 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.66, 133.37, 131.29, 126.85, 126.44, 121.40, 110.34, 47.27, 37.92, 17.08.



1m

2-(methyl(p-tolyl)amino)malononitrile (1m)

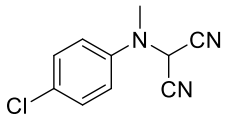
1m was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.11–7.06 (m, 2H), 6.92–6.88 (m, 2H), 5.20 (s, 1H), 3.80 (s, 3H), 2.99 (s, 3H); **^{13}C NMR**(100 MHz, $CDCl_3$) δ 157.05, 139.91, 122.21, 114.85, 110.36, 55.45, 48.42, 38.37.



1n

2-((4-fluorophenyl)(methyl)amino)malononitrile (1n)

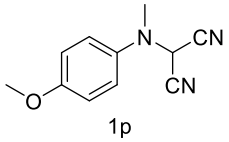
1n was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.07–7.05 (m, 4H), 5.26 (s, 1H), 3.01 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.65 (d, *J* = 243.4 Hz), 142.61, 121.79 (d, *J* = 8.1 Hz), 116.49 (d, *J* = 22.7 Hz), 110.14, 47.80, 38.13.



1o

2-((4-chlorophenyl)(methyl)amino)malononitrile (1o)

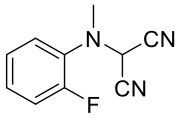
1o was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35–7.31 (m, 2H), 7.00–6.16 (m, 2H), 5.35 (s, 1H), 3.05 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.84, 129.83, 129.59, 120.20, 109.98, 46.81, 37.63.



1p

2-((4-methoxyphenyl)(methyl)amino)malononitrile (1p)

1p was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.09–7.05 (m, 2H), 6.91–6.84 (m, 2H), 5.24 (s, 1H), 3.77 (s, 3H), 2.97 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.68 139.68, 121.81, 114.62, 110.40, 55.24, 48.13, 38.11.

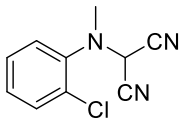


1q

2-((2-fluorophenyl)(methyl)amino)malononitrile (1q)

1q was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.19–7.10 (m, 4H), 5.39 (s, 1H), 3.06 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 155.50 (d, *J* = 245.2 Hz), 134.10 (d, *J* = 9.3 Hz), 126.37 (d, *J* = 8.2 Hz), 125.07 (d, *J* = 3.7 Hz), 121.66, 116.67 (d, *J* = 20.1 Hz),

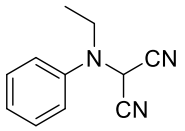
110.05, 46.44, 36.88.



1r

2-((2-chlorophenyl)(methyl)amino)malononitrile (1r)

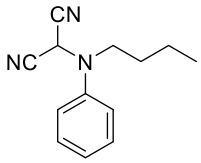
1r was obtained through the general procedure A . **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46–7.44 (m, 1H), 7.33–7.28 (m, 2H), 7.22–7.18 (m, 1H), 5.36 (s, 1H), 3.06 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.25, 130.84, 129.00, 128.12, 127.18, 122.85, 109.99, 46.66, 37.10.



1s

2-(ethyl(phenyl)amino)malononitrile (1s)

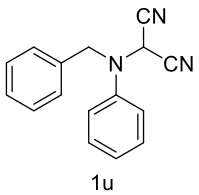
1s was obtained through the general procedure A. **^{1}H NMR**(400 MHz, $CDCl_3$) δ 7.43–7.37 (m, 2H), 7.20–7.12 (m, 2H), 7.13–7.10 (m, 1H), 5.30 (s, 1H), 3.45 (dd, *J* = 14.4, 7.2 Hz, 2H), 1.22 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.37, 129.63, 124.59, 120.75, 110.93, 45.80, 45.66, 12.64.



1t

2-(butyl(phenyl)amino)malononitrile (1t)

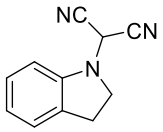
1t was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41–7.36 (m, 2H), 7.20–7.12 (m, 3H), 5.28 (s, 1H), 3.36 (t, *J* = 7.2 Hz, 2H), 1.6 –1.52 (m, 2H), 1.44–1.35 (m, 2H), 0.94 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.73, 129.63, 124.74, 121.05, 110.89, 50.76, 46.48, 29.09, 19.80, 13.52.



1u

2-(benzyl(phenyl)amino)malononitrile (1u)

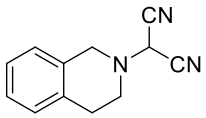
1u was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32–7.28 (m, 6H), 7.27–7.23 (m, 1H), 7.17 (d, *J* = 7.6 Hz, 2H), 7.10 (t, *J* = 7.6 Hz, 1H), 5.12 (s, 1H), 4.39 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.09, 134.96, 129.47, 128.80, 128.25, 128.03, 124.83, 120.90, 111.54, 54.07, 44.29



1v

2-(indolin-1-yl)malononitrile (1v)

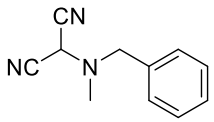
1v was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24–7.19 (m, 2H), 7.00–6.96 (m, 1H), 6.70 (d, *J* = 6.8 Hz, 1H), 5.42 (s, 1H), 3.57 (t, *J* = 8.0 Hz, 2H), 3.10 (t, *J* = 8.0 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.91, 130.69, 127.64, 125.45, 122.30, 109.86, 108.88, 52.00, 41.28, 28.11.



1w

2-(3,4-dihydroisoquinolin-2(1H)-yl)malononitrile(1w)

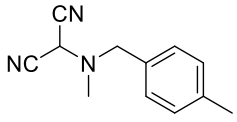
1w was obtained through the general procedure A**. ^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24–7.14 (m, 3H), 7.09–7.07 (m, 1H), 4.85 (s, 1H), 3.93 (s, 2H), 3.04–2.98 (m, 4H); **^{13}C NMR** (100 MHz, CDCl3) δ 132.35, 131.49, 128.71, 126.98, 126.45, 126.26, 109.66, 52.19, 48.15, 48.10, 28.70.



1x

2-(benzyl(methyl)amino)malononitrile (1x)

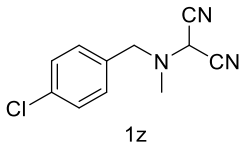
1x was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43–7.35 (m, 5H), 4.62 (s, 1H), 3.70 (s, 2H), 2.56 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 134.79, 128.77, 128.36, 109.84, 58.71, 46.09, 39.25.



1y

2-(methyl(4-methylbenzyl)amino)malononitrile (1y)

1y was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24–7.21 (m, 4H), 4.64 (s, 1H), 3.67 (s, 2H), 2.57 (s, 3H), 2.40 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.23, 131.68, 129.47, 128.78, 109.87, 58.51, 45.85, 39.25, 20.92.

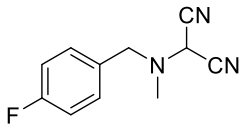


1z

2-((4-chlorobenzyl)(methyl)amino)malononitrile（1z）

1z was obtained through the general procedure A . **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 –7.25 (m,

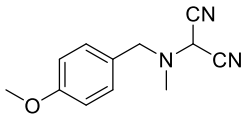
4H), 4.66 (s, 1H), 3.64 (s, 2H), 2.48 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 133.92, 133.43, 130.04, 128.79, 109.74, 57.85, 46.38, 39.02.



1aa

2-((4-fluorobenzyl)(methyl)amino)malononitrile（1aa）

1aa was obtained through the general procedure A. **^{1}H NMR** (400 MHz,$CDCl_3$) δ 7.33–7.29 (m, 2H), 7.09–7.03 (m, 2H), 4.64 (s, 1H), 3.66 (s, 2H), 2.52 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.51 (d, *J* = 245.8 Hz), 130.70 (d, *J* = 2.5 Hz), 130.54 (d, *J* = 8.1 Hz), 115.79, 115.57, 109.82, 57.94, 46.23, 39.13.

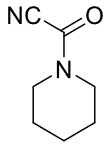


1ab

2-((4-methoxybenzyl)(methyl)amino)malononitrile(1ab)

1ab was obtained through the general procedure A. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.25–7.21 (m, 2H), 6.91–6.87 (m, 2H), 4.59 (s, 1H), 3.80 (s, 3H), 3.61 (s, 2H), 2.55 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.77, 130.25, 126.67, 114.31, 109.93, 58.36, 55.21, 45.72, 39.40.

3.2 Characterization of substrates 2a–2aa

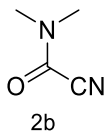


2a

piperidine-1-carbonyl cyanide (2a)

2a(43mg) was obtained through the general procedure B in 86% yield as a yellow liquid.

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.71 (t, *J* = 6.3 Hz, 2H), 3.58 (t, *J* = 5.7 Hz, 2H), 1.77–1.54 (m, 6H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 142.71, 110.25, 47.83, 42.71, 25.92, 24.64, 23.63; **HRMS** (ESI) calcd for $C_7H_{10}N_2O$ $[M+Na]^+$: 161.0685 found 161.0692.

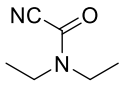


2b

N,N-dimethylcarbamoyl cyanide (2b)

2b(35mg) was obtained through the general procedure B in 77% yield as a white liquid.

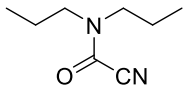
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.28(s, 3H), 3.01(s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 144.73, 110.45, 37.85, 34.31.**;HRMS** (ESI) calcd for $C_4H_6N_2O$ $[M+H]^+$: 99.0553 found 99.0542.



2c

N,N-diethylcarbamoyl cyanide (2c)

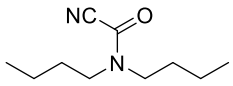
2c(27.5mg) was obtained through the general procedure B in 55% yield as a light white liquid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 3.58 (dd, *J* = 14.4, 7.2 Hz, 2H), 3.40 (dd, *J* = 14.4, 7.2 Hz, 2H), 1.29 (t, *J* = 14.4, 3H), 1.13 (t, *J* = 7.2, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 144.08, 110.63, 43.49, 39.82, 14.31, 12.17; **HRMS** (ESI) calcd for $C_6H_{10}N_2O$ $[M+Na]^+$: 149.0685 found 149.0688.



2d

N,N-dipropylcarbamoyl cyanide (2d)

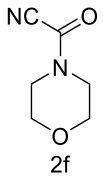
2d(39mg) was obtained through the general procedure B in 78% yield as a light white liquid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 3.51 (t, *J* = 7.2 Hz, 2H), 3.34–3.29 (m, 2H), 1.71–1.62 (m, 2H), 1.61–1.54 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H), 0.90 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 144.77, 110.79, 50.49, 46.75, 21.88, 20.21, 11.11, 10.80; **HRMS** (ESI) calcd for $C_8H_{14}N_2O$ $[M+H]^+$: 155.1179 found 155.1181.



2e

N,N-dibutylcarbamoyl cyanide (2e)

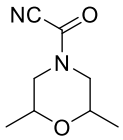
2e(44mg) was obtained through the general procedure B in 88% yield as a yellow liquid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.54 (t, *J* = 7.2 Hz, 2H), 3.36 (t, *J* = 7.6 Hz, 2H), 1.66–1.59 (m, 2H), 1.57–1.50 (m, 2H), 1.43–1.29 (m, 4H), 0.98 (t, *J* = 7.6 Hz, 3H), 0.93 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.74, 110.84, 48.84, 45.06, 30.81, 29.01, 19.99, 19.68, 13.62, 13.56; **HRMS** (ESI) calcd for $C_{10}H_{18}N_2O$ $[M+H]^+$: 183.1492 found 183.1495.



2f

morpholine-4-carbonyl cyanide (2f)

2f(43.5mg) was obtained through the general procedure B in 87% yield as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.75 (s, 4H), 3.71–3.67 (m, 2H), 3.64–3.61(m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 109.88, 66.40, 65.80, 46.93, 42.47; **HRMS** (ESI) calcd for $C_6H_8N_2O_2$ $[M+H]^+$: 141.0659 found 141.0661; **mp** 54.1–60.1 ℃.

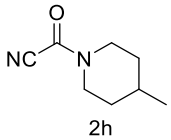


2g

2,6-dimethylmorpholine-4-carbonyl cyanide (2g)

2g(40mg) was obtained through the general procedure B in 80% yield as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.26 (dt, *J* = 13.2, 2 Hz, 1H), 4.00 (dt, *J* = 13.2, 2 Hz, 1H), 3.66–3.49 (m, 2H), 2.97 (dd, *J* = 13.2, 10.8 Hz, 1H), 2.51 (dd, *J* = 13.6, 10.8 Hz, 1H), 1.24(d, *J* = 6.4 Hz, 3H), 1.21 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.02, 110.06, 72.01, 71.34, 51.96, 47.39, 18.49, 18.38; **HRMS** (ESI) calcd for $C_8H_{12}N_2O_2$ $[M+H]^+$: 169.0972 found 169.0974; **mp** 52.4–58.9 ℃.

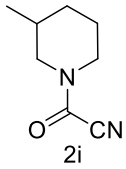


2h

4-methylpiperidine-1-carbonyl cyanide (2h)

2h(42.5mg) was obtained through the general procedure B in 85% yield as a liquid.

^{1}H NMR (300 MHz, $CDCl_3$) δ 4.41–4.33 (m, 1H), 4.20–4.12 (m, 1H), 3.20 (td, *J* = 15.9, 12.9 Hz, 1H), 2.73 (td, *J* = 15.9, 12.9 Hz, 1H), 1.84 – 1.60 (m, 3H), 1.26–1.07 (m, 2H), 0.96 (d, *J* = 6.3 Hz, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 142.93, 110.41, 47.39, 42.30, 34.10, 32.88, 30.62, 21.24; **HRMS** (ESI) calcd for $C_8H_{12}N_2O$ $[M+H]^+$: 153.1022 found 153.1025.

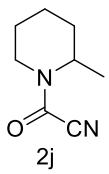


2i

3-methylpiperidine-1-carbonyl cyanide (2i)

2i(42mg) was obtained through the general procedure B in 84% yield as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.19–4.12 (m, 2H), 4.06–4.01 (m, 1H), 3.97–3.93 (m, 1H), 3.15 (ddd, *J* = 13.2, 12.8, 12 Hz, 1H), 2.87 (dd, *J* = 13.2, 10.4 Hz, 1H), 2.79 (ddd, *J* = 13.2, 11.6, 3.6 Hz, 1H), 2.41 (dd, *J* = 12.8, 10.8 Hz, 1H), 1.84–1.80 (m, 2H), 1.79–1.68 (m, 2H), 1.67–1.53 (m, 2H), 1.52–1.35 (m, 2H), 1.22–1.11 (m, 2H), 0.92 (d, *J* = 6.8 Hz, 3H), 0.88 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.78, 110.32, 53.90, 48.80, 47.45, 42.35, 32.15, 32.06, 31.59, 30.63, 30.54, 25.35, 23.79, 18.40, 18.14; **HRMS** (ESI) calcd for $C_8H_{12}N_2O$ $[M+H]^+$: 153.1022 found 153.1025; **mp** 53.2–60.4 ℃.

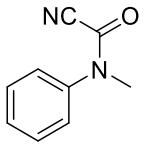


2j

2-methylpiperidine-1-carbonyl cyanide (2j)

2j (41mg) was obtained through the general procedure B in 82% yield as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.74–4.68 (m, 1H), 4.54–4.49 (m, 1H), 4.30–4.25 (m, 1H), 4.04–3.99 (m, 1H), 3.30 (td, *J* = 13.6, 3.2 Hz, 1H), 2.82 (td, *J* = 16.4, 2.8 Hz, 1H), 1.83–1.75 (m, 2H), 1.74–1.70 (m, 2H), 1.70–1.68 (m, 2H), 1.67–1.65 (m, 2H), 1.64–1.54 (m, 2H), 1.53–1.35 (m, 2H), 1.33 (d, *J* = 6.8 Hz, 3H), 1.19 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.25, 110.45, 51.13, 45.46, 42.92, 37.53, 30.45, 29.21, 25.86, 24.75, 18.42, 18.40, 17.21, 15.36; **HRMS** (ESI) calcd for $C_8H_{12}N_2O$ $[M+H]^+$: 153.1022 found 153.1025; **mp** 56.3–60.3 ℃.

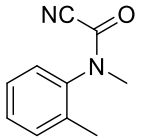


2k

N-methyl-N-phenyl-carbamoyl cyanide (2k)

2k(44.5mg) was obtained through the general procedure B in 89% yield as a white solid.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51–7.48 (m, 3H), 7.33–7.30(m, 2H), 3.60 (t, *J* = 1.6 Hz, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$) δ 144.32, 139.54, 129.94, 129.55, 128.07, 126.82, 124.77, 110.52, 36.59; **HRMS** (ESI) calcd for $C_9H_8N_2O$ $[M+Na]^+$: 183.0529 found 183.0532; **mp** 53.6–61.8 ℃.

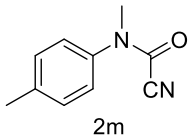


2l

N-methyl-N-(*o*-tolyl)-carbamoyl cyanide (2l)

2l(37mg) was obtained through the general procedure B in 74% yield as a white solid.

^{1}H NMR(400 MHz, $CDCl_3$) δ 7.43–7.31 (m, 3H), 7.29–7.21 (m, 1H), 3.28 (s, 3H), 2.31 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.03, 138.43, 135.95, 131.87, 130.32, 128.30, 127.82, 110.50, 35.77, 17.21; **HRMS** (ESI) calcd for $C_{10}H_{10}N_2O$ $[M+H]^+$: 175.0866 found 175.0867; **mp** 69.9–77.2 ℃.

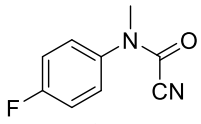


2m

N-methyl-N-(*p*-tolyl)-carbamoyl cyanide (2m)

2m(42.5mg) was obtained through the general procedure B in 85% yield as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24–7.18 (m, 2H), 6.97–6.93 (m, 2H), 3.84 (s, 3H), 3.32 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.58, 139.93, 137.10, 130.63, 130.08, 126.68, 124.62, 110.66, 36.72, 21.13; **HRMS** (ESI) calcd for $C_{10}H_{10}N_2O$ $[M+H]^+$: 175.0866 found 175.0867; **mp** 82.5–86.9 ℃.

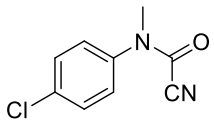


2n

N-(4-fluorophenyl)-N-methyl-carbamoyl cyanide (2n)

2n(32mg) was obtained through the general procedure B in 64% yield as a yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33–7.28 (m, 2H), 7.21-7.11(m, 2H), 3.34 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.81 (d, *J* = 249.5 Hz), 144.50, 135.73, 129.10 (d, *J* = 9.2 Hz), 127.31 (*J* = 12.9 Hz), 126.89 (d, *J* = 8.8 Hz), 117.21 (d, *J* = 23 Hz), 116.54 (d, *J* = 23 Hz), 110.41, 36.85; **HRMS** (ESI) calcd for $C_9H_7FN_2O$ $[M+H]^+$: 179.0615 found 179.0616; **mp** 61.8–64.3 ℃.

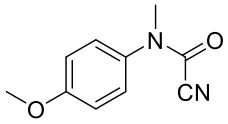


2o

N-(4-chlorophenyl)-N-methyl-carbamoyl cyanide (2o)

2o(39mg) was obtained through the general procedure B in 78% yield as a yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52–7.49 (m, 2H), 7.31–7.28 (m, 2H), 3.37 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.28, 138.17, 135.77, 130.36, 129.67, 128.33, 126.18, 110.37, 36.73; **HRMS** (ESI) calcd for $C_9H_7ClN_2O$ $[M+H]^+$: 195.0320 found 195.0320; **mp** 80.9–84.0 ℃.

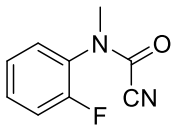


2p

N-(4-methoxyphenyl)-N-methyl-carbamoyl cyanide (2p)

2p(42mg) was obtained through the general procedure B in 84% yield as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23–7.22 (m, 2H), 7.00–6.97 (m, 2H), 3.89–3.79 (m, 3H), 3.60–3.27 (m, 3H); **^{13}C NMR** (100 MHz, CDCl3) δ 160.24, 144.74, 132.30, 128.29, 115.12, 114.67, 110.70, 55.45, 36.85; **HRMS** (ESI) calcd for $C_{10}H_{10}N_2O_2$ $[M+H]^+$: 191.0815 found 191.0811; **mp** 58.8–61.4 ℃.

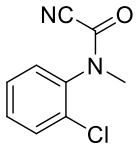


2q

N-(2-fluorophenyl)-N-methyl-carbamoyl cyanide (2q)

2q(25.5mg) was obtained through the general procedure B in 51% yield as a red solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51–7.45 (m, 2H), 7.37–7.29 (m, 1H), 7.28–7.24 (m, 1H), 3.32 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.10 (d, *J* = 250.8 Hz), 144.84, 131.91 (d, *J* = 8.0 Hz), 129.49, 127.31 (d, *J* = 12.9 Hz), 125.44 (d, *J* = 4.0 Hz), 117.27 (d, *J* = 19.5 Hz), 110.20, 36.09; **HRMS** (ESI) calcd for $C_9H_7FN_2O$ $[M+H]^+$: 179.0615 found 179.0616; **mp** 46.2–50.4 ℃.

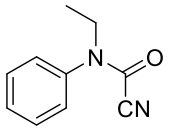


2r

N-(2-chlorophenyl)-N-methyl-carbamoyl cyanide(2r)

2r(32mg) was obtained through the general procedure B in 64% yield as a light yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59–7.56 (m, 1H), 7.49–7.36 (m, 3H), 3.30 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.87, 137.04, 133.18, 131.55, 131.00, 130.01, 128.59, 110.24, 35.57; **HRMS** (ESI) calcd for $C_9H_7ClN_2O$ $[M+H]^+$: 195.0320 found 195.0321.

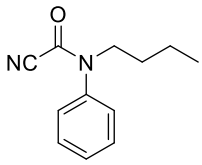


2s

N-ethyl-N-phenyl-carbamoyl cyanide (2s)

2s(42mg)was obtained through the general procedure B in 84% yield as a yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52–7.46 (m, 3H), 7.28–7.25(m, 2H), 3.81 (dd, *J* = 14.4, 7.2 Hz, 2H), 1.15 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.18, 138.07, 130.02, 129.81, 128.06, 126.41, 110.61, 44.29, 12.27; **HRMS** (ESI) calcd for $C_{10}H_{10}N_2O$ $[M+H]^+$: 175.0866 found 175.0867; **mp** 39.0–48.3 ℃.

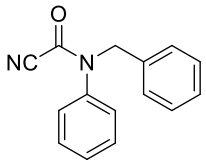


2t

N-butyl-N-phenyl-carbamoyl cyanide (2t)

2t(38mg) was obtained through the general procedure B in 78% yield as a yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53–7.44 (m, 3H), 7.39–7.20 (m, 2H), 3.79 (t, *J* = 7.6 Hz, 2H), 1.56–1.49 (m, 2H), 1.36–1.26 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.49, 138.41, 130.05, 129.80, 127.96, 110.64, 49.04, 29.02, 19.77, 13.56; **HRMS** (ESI) calcd for $C_{12}H_{14}N_2O$ $[M+H]^+$: 203.1179 found 203.1180; **mp** 31.0–38.5 ℃.



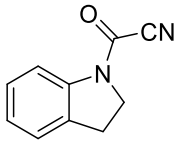
2u

N-benzyl-N-phenyl-carbamoyl cyanide(2u)

2u(36.5mg) was obtained through the general procedure B in 73% yield as a yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44–7.36 (m, 3H), 7.34–7.25 (m, 3H), 7.20–7.12 (m, 2H), 7.12–7.04 (m, 2H), 4.90 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.71, 138.09, 134.47, 129.87, 129.84, 129.44 128.92, 128.69, 128.49, 128.29, 128.21, 127.86, 126.32, 110.50, 52.95; **HRMS**

(ESI) calcd for $C_{15}H_{12}N_2O$ $[M+H]^+$: 237.1022 found 237.1023.

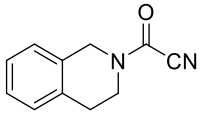


2v

indoline-1-carbonyl cyanide (2v)

2v(20mg) was obtained through the general procedure B in 40% yield as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.2 Hz, 1H), 7.33–7.15 (m, 3H), 4.35 (t, *J* = 8 Hz, 2H), 3.29 (t, *J* = 8.4 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.19, 132.54, 127.86, 126.56, 125.16, 117.59, 113.16, 110.92, 49.07, 27.45; **HRMS** (ESI) calcd for $C_{10}H_8N_2O$ $[M+H]^+$: 173.0709 found 173.0710; **mp** 100.1–101.8 ℃.

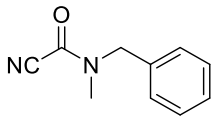


2w

3,4-dihydroisoquinoline-2(1H)-carbonyl cyanide(2w)

2w(42.5mg) was obtained through the general procedure B in 85% yield as a light white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31–7.13 (m, 4H), 4.91 (s, 1H), 4.76 (s, 1H), 4.20 (t, *J* = 8 Hz, 1H), 3.86 (t, *J* = 8.4 Hz, 1H), 3.23 (t, *J* = 7.2 Hz, 1H), 2.94 (t, *J* = 8.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.58, 143.32, 133.42, 132.74, 130.36, 130.18, 128.66, 128.54, 127.44, 127.04, 126.85, 126.72, 126.21, 125.92, 110.31, 110.26, 47.98, 44.45, 44.14, 40.33, 28.85, 27.46; **HRMS** (ESI.) calcd for $C_{11}H_{10}N_2O$ $[M+Na]^+$: 209.0685 found 209.0690, **mp** 74.3–79.6 ℃.

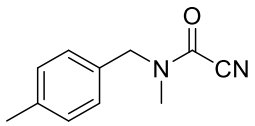


2x

N-benzyl-N-methyl-carbamoyl cyanide (2x)

2x(34.5mg) was obtained through the general procedure B in 69% yield as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42–7.30 (m, 6H), 7.29–7.22 (m, 4H), 4.75 (s, 2H), 4.58 (s, 2H), 3.15 (s, 3H), 2.90 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.98, 144.57, 134.03, 133.61, 129.06, 128.88, 128.63, 128.29, 127.46, 110.65, 110.43, 54.45, 50.20, 35.31, 32.03; **HRMS** (ESI) calcd for $C_{10}H_{10}N_2O$ $[M+K]^+$: 213.0425 found 213.0428; **mp** 55.6–64.7 ℃.

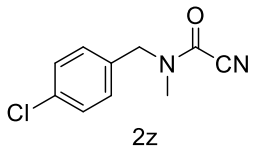


2y

N-methyl-N-(4-methylbenzyl)-carbamoyl cyanide(2y)

2y(41mg) was obtained through the general procedure B in 82% yield as a yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23–7.14 (m, 8H) , 4.72 (s, 2H), 4.55 (s, 2H), 3.16 (s, 3H), 2.90 (s, 3H), 2.37 (s, 3H), 2.35 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.95, 144.53, 138.55, 138.16, 131.05, 130.60, 129.71, 129.54, 128.34, 127.49, 110.71, 110.48, 54.26, 49.97, 35.22, 35.18, 31.88, 29.55, 25.72, 20.97; **HRMS** (ESI) calcd for $C_{11}H_{12}N_2O$ $[M+Na]^+$: 211.0842 found 211.0842.

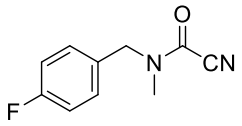


2z

N-(4-chlorobenzyl)-N-methyl-carbamoyl cyanide(2z)

2z(36.5mg) was obtained through the general procedure B in 73% yield as a white solid.

^{1}H NMR(400 MHz, $CDCl_3$) δ 7.39–7.30 (m, 4H), 7.22–7.15 (m, 4H), 4.72 (s, 2H), 4.55 (s, 2H), 3.16 (s, 3H), 2.90 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.04, 144.52, 134.59, 134.22, 132.62, 132.20, 129.70, 129.28, 129.06, 128.86, 110.53, 110.31, 53.77, 49.60, 35.36, 32.06; **HRMS** (ESI) calcd for $C_{10}H_9ClN_2O$ $[M+H]^+$: 209.0476 found 209.0477; **mp** 80.4–85.1 ℃.

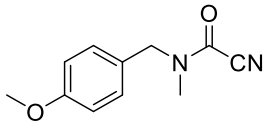


2aa

N-(4-fluorobenzyl)-N-methyl-carbamoyl cyanide(2aa)

2aa(34.5mg) was obtained through the general procedure B in 69% yield as a white solid.

^{1}H NMR (400 MHz,$CDCl_3$) δ 7.26–7.20 (m, 4H), 7.11–7.00 (m, 4H), 4.72 (s, 2H), 4.54 (s, 2H), 3.16 (s, 3H), 2.89 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.75 (d, *J* = 246.8 Hz), 162.58 (d, *J* = 246.1 Hz), 145.05, 144.52, 130.24 (d, *J* = 8.3 Hz), 131.02 (d, *J* = 3.4 Hz), 129.54 (d, *J* = 3 Hz), 129.41 (d, J = 8.4 Hz), 116.26, 116.02 (d, *J* = 4.6 Hz), 115.78, 110.62, 110.38, 53.80, 49.59, 35.30, 31.99; **HRMS** (ESI) calcd for $C_{10}H_9FN_2O$ $[M+H]^+$: 193.0772 found 193.0773; **mp** 62.3–66.6 ℃.



2ab

N-(4-methoxybenzyl)-N-methyl-carbamoyl cyanide(2ab)

2ab(43mg) was obtained through the general procedure B in 86% yield as a white liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21–7.16 (m, 4H), 6.94–6.84 (m, 4H), 4.69 (s, 2H), 4.52 (s, 2H), 3.81 (s, 3H), 3.80 (s, 3H), 3.14 (s, 3H), 2.89 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) 159.80, 159.56, 144.90, 144.41, 130.03, 129.66, 129.19, 128.83, 126.11, 125.55, 114.60, 114.40, 114.25, 114.07, 110.75, 110.49, 55.34, 55.10, 54.01, 49.68, 35.28, 34.97, 31.96, 31.62; **HRMS** (ESI) calcd for $C_{11}H_{12}N_2O_2$ $[M+Na]^+$: 227.0791 found 227.0793.

REFERENCES

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3. Alonso‐Alija, C.; Dembowsky, K.; Feurer, A.; Huetter, J.; Perzborn, E.; Stahl, E.; Stasch, J.‐P.; Straub, A. patent (WO2000006569) 2000.
4. Stansfield, F.; Coomassie, M. D. J. Chem. Soc. Perkin Trans. 1, 1979, 2708‐271

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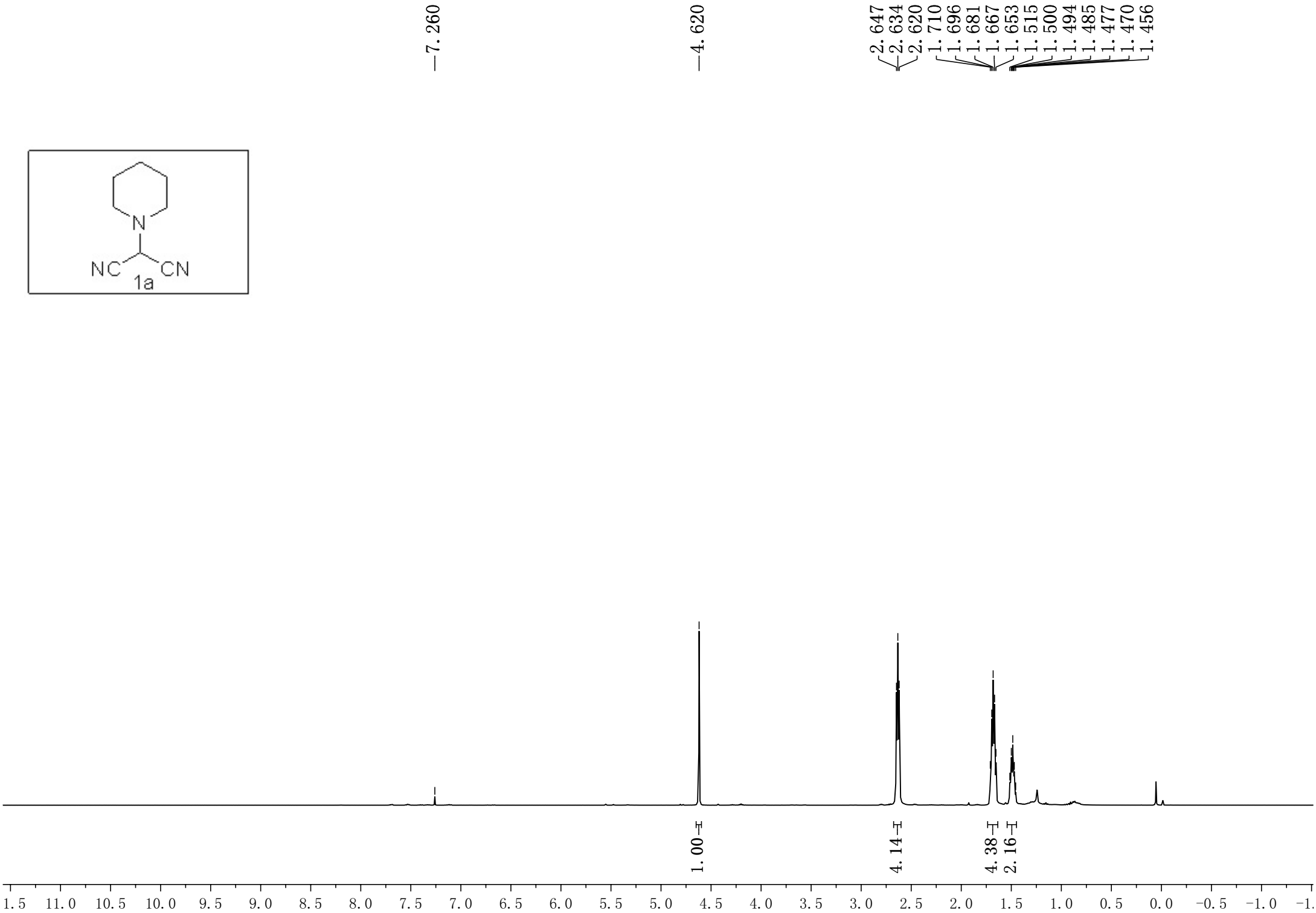
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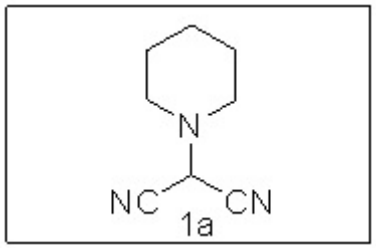

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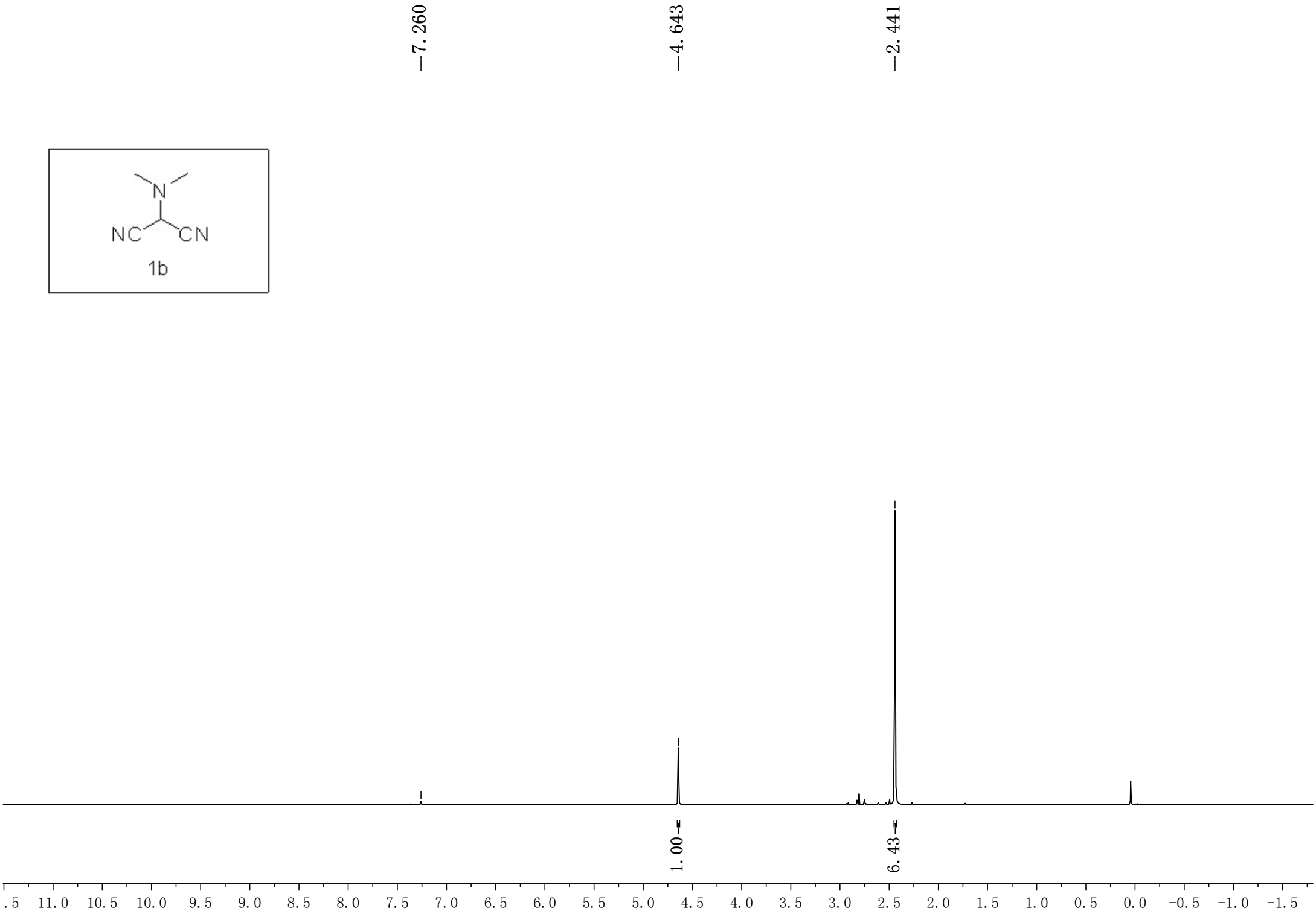
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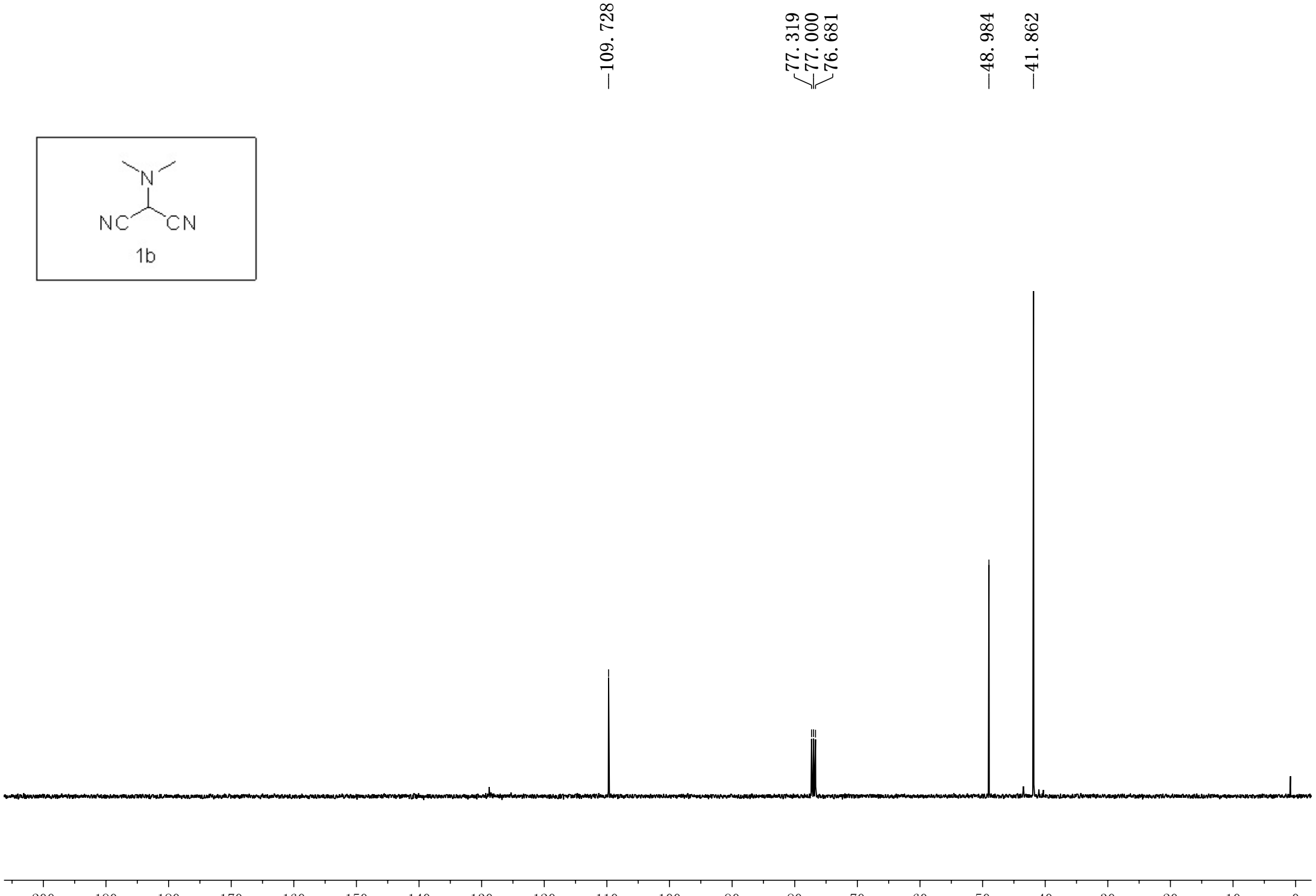
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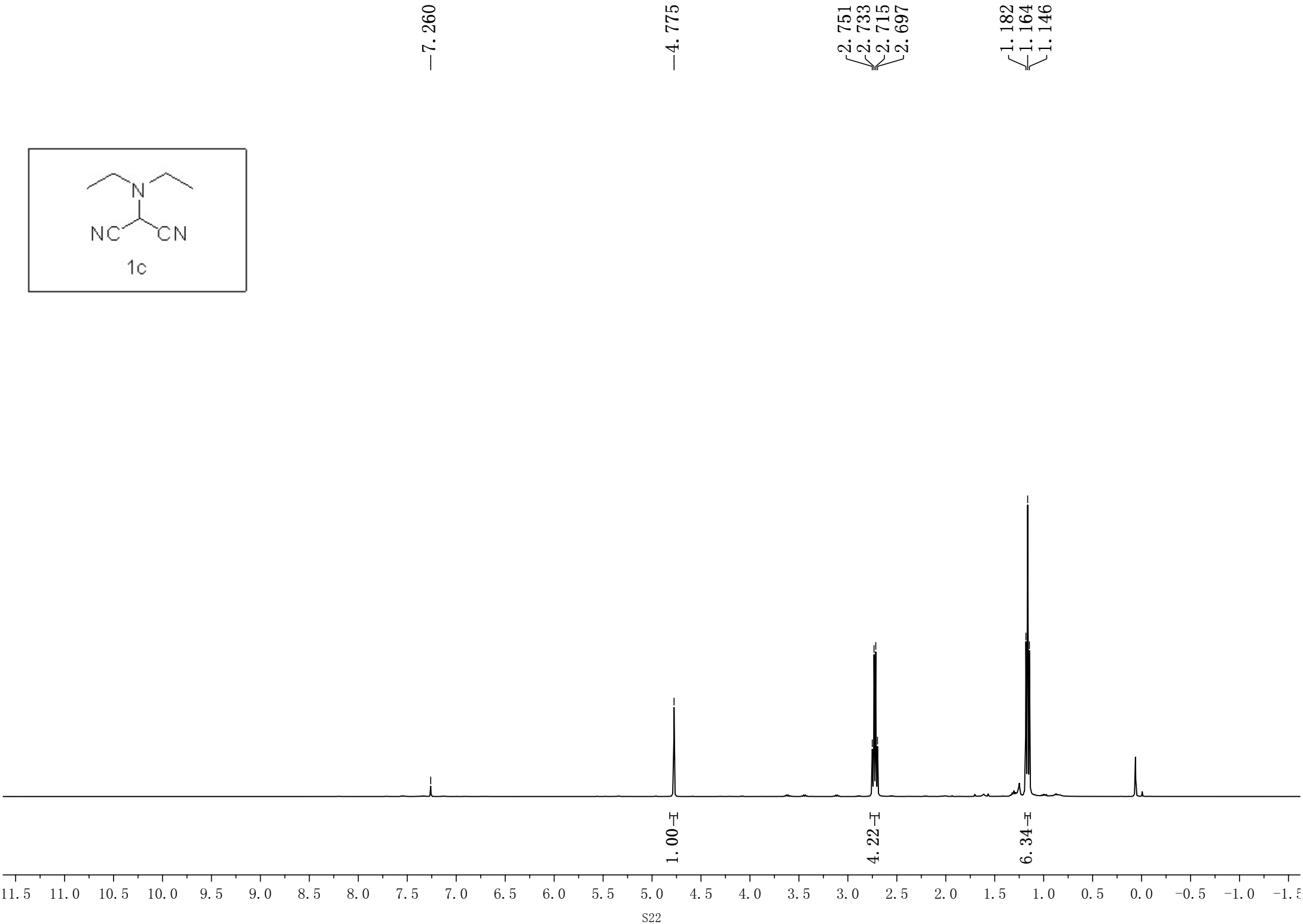
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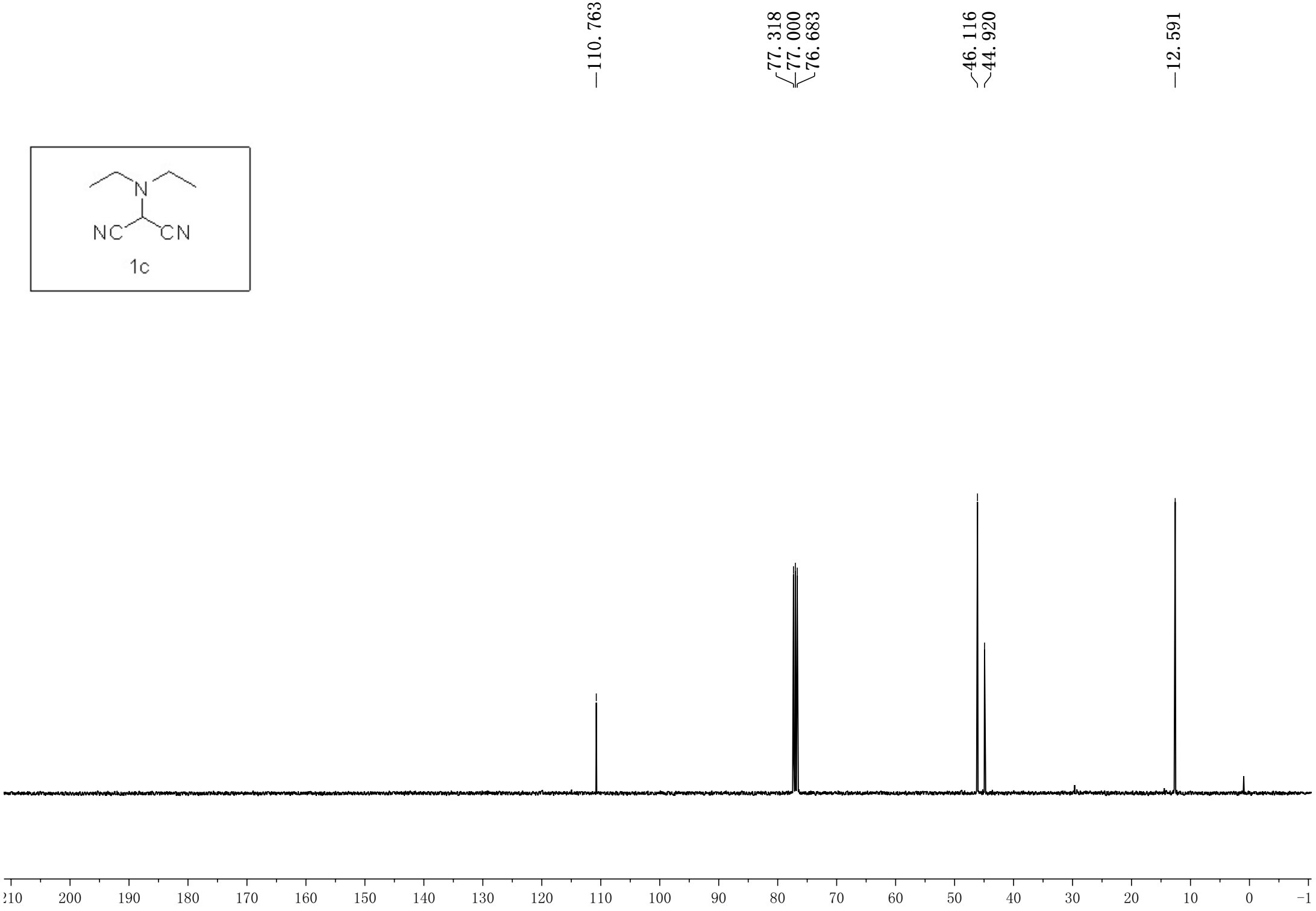
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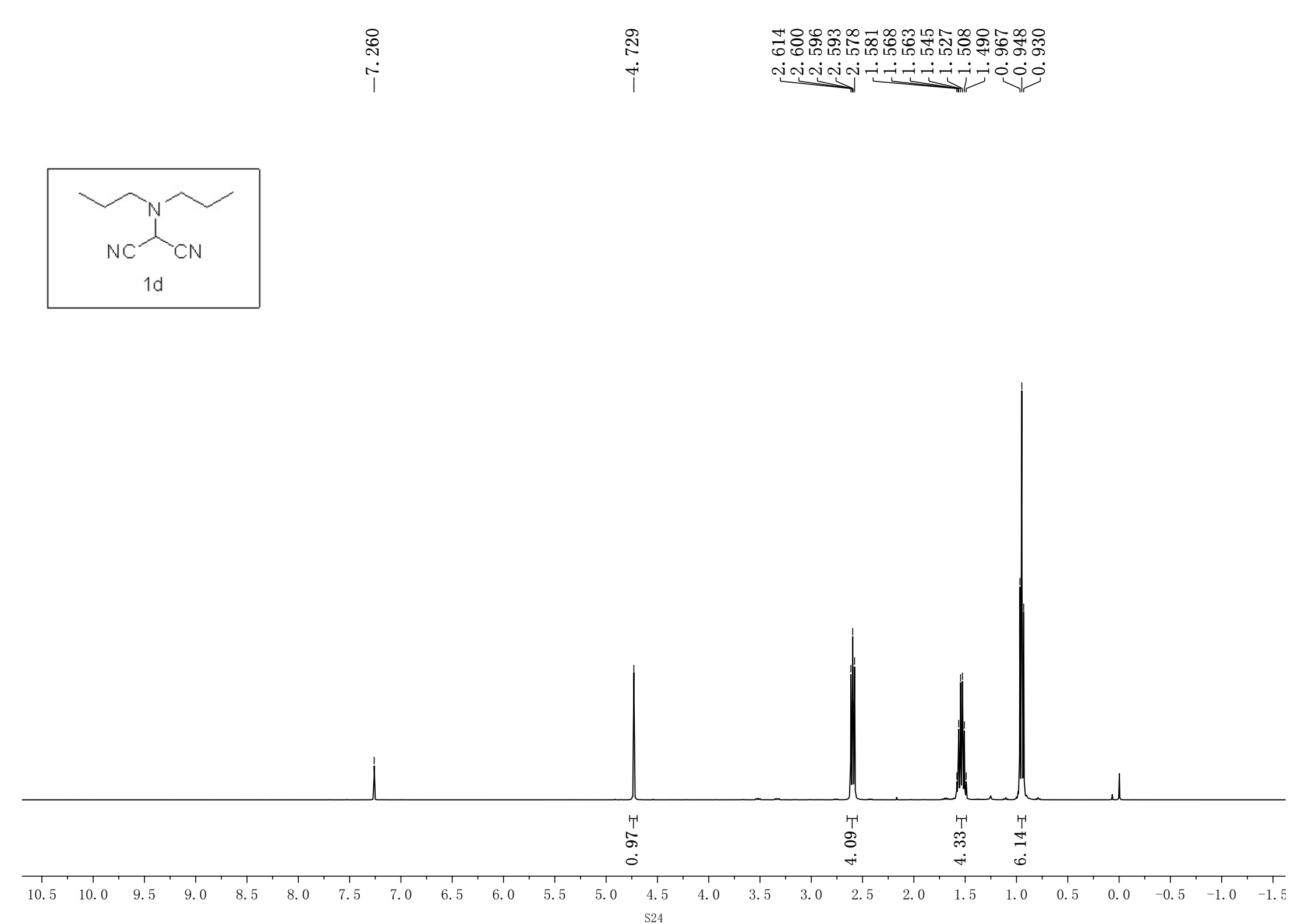
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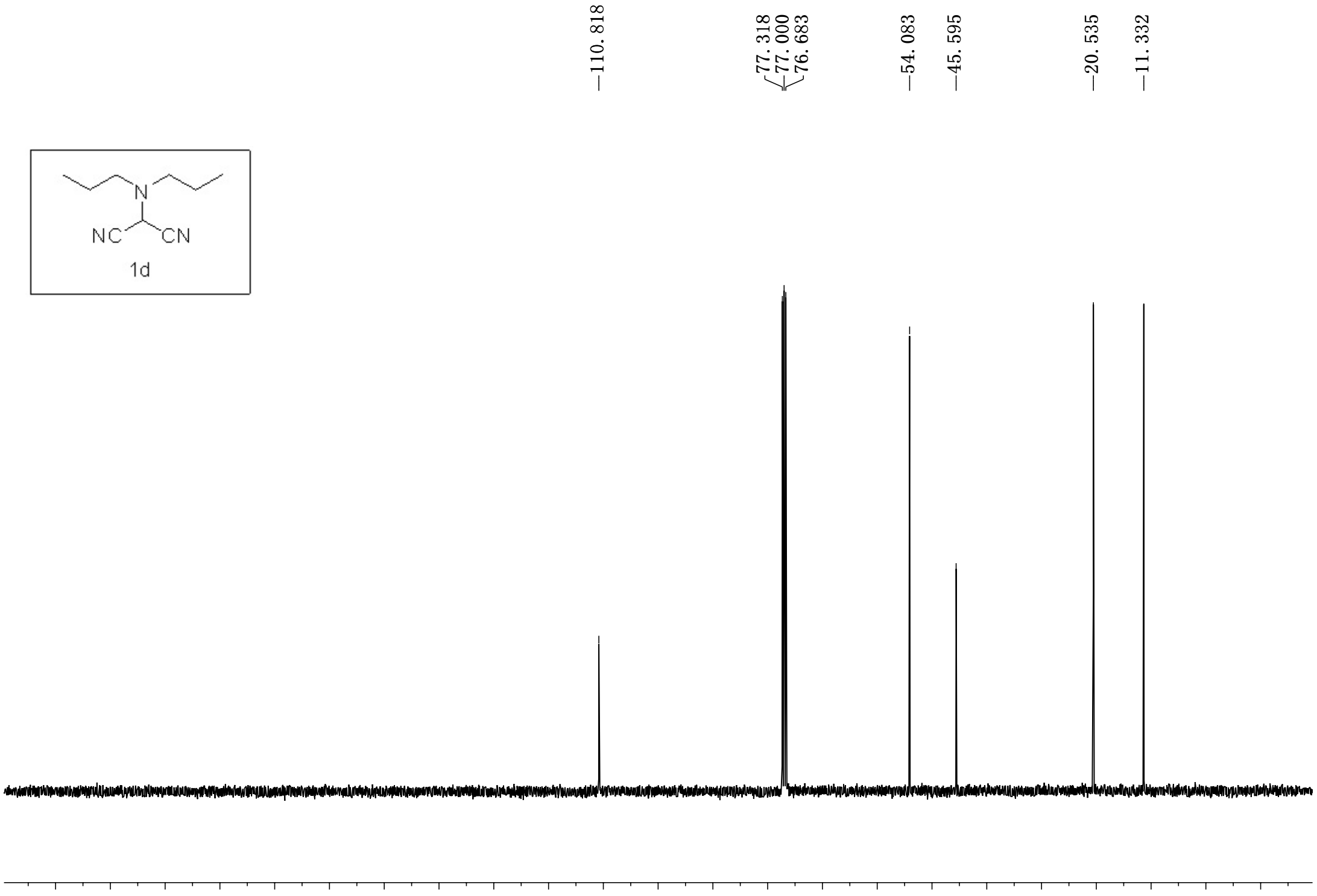
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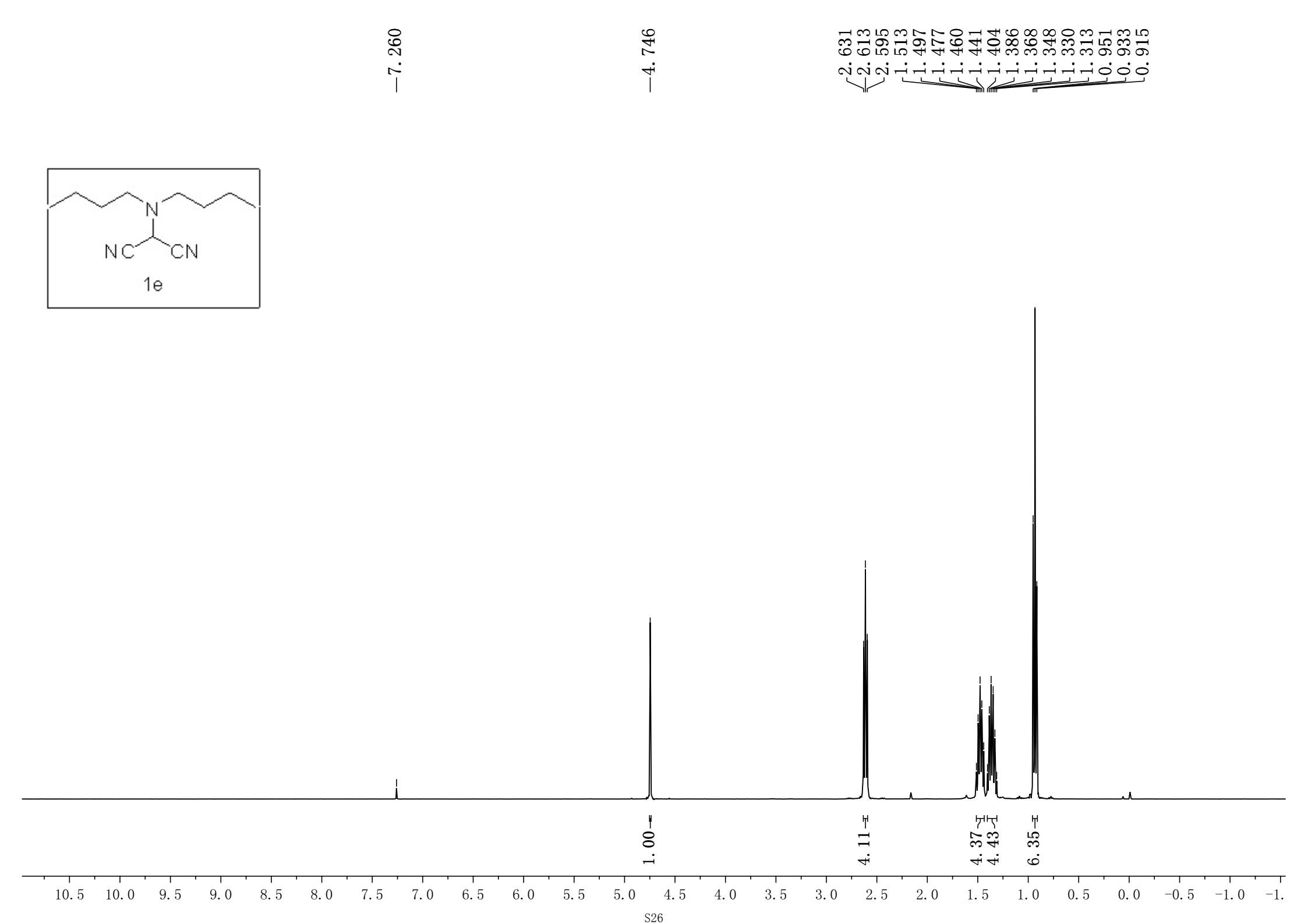
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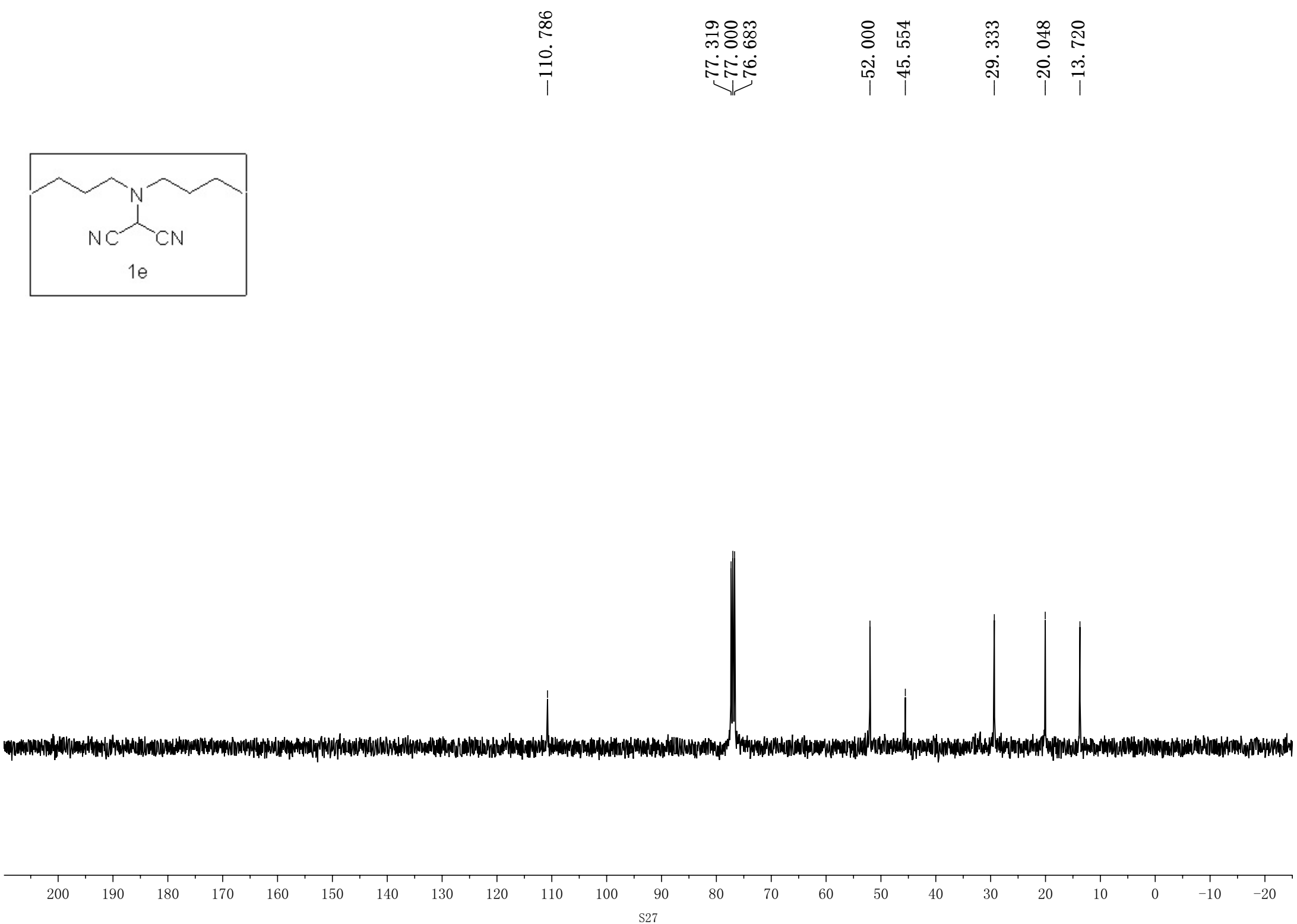
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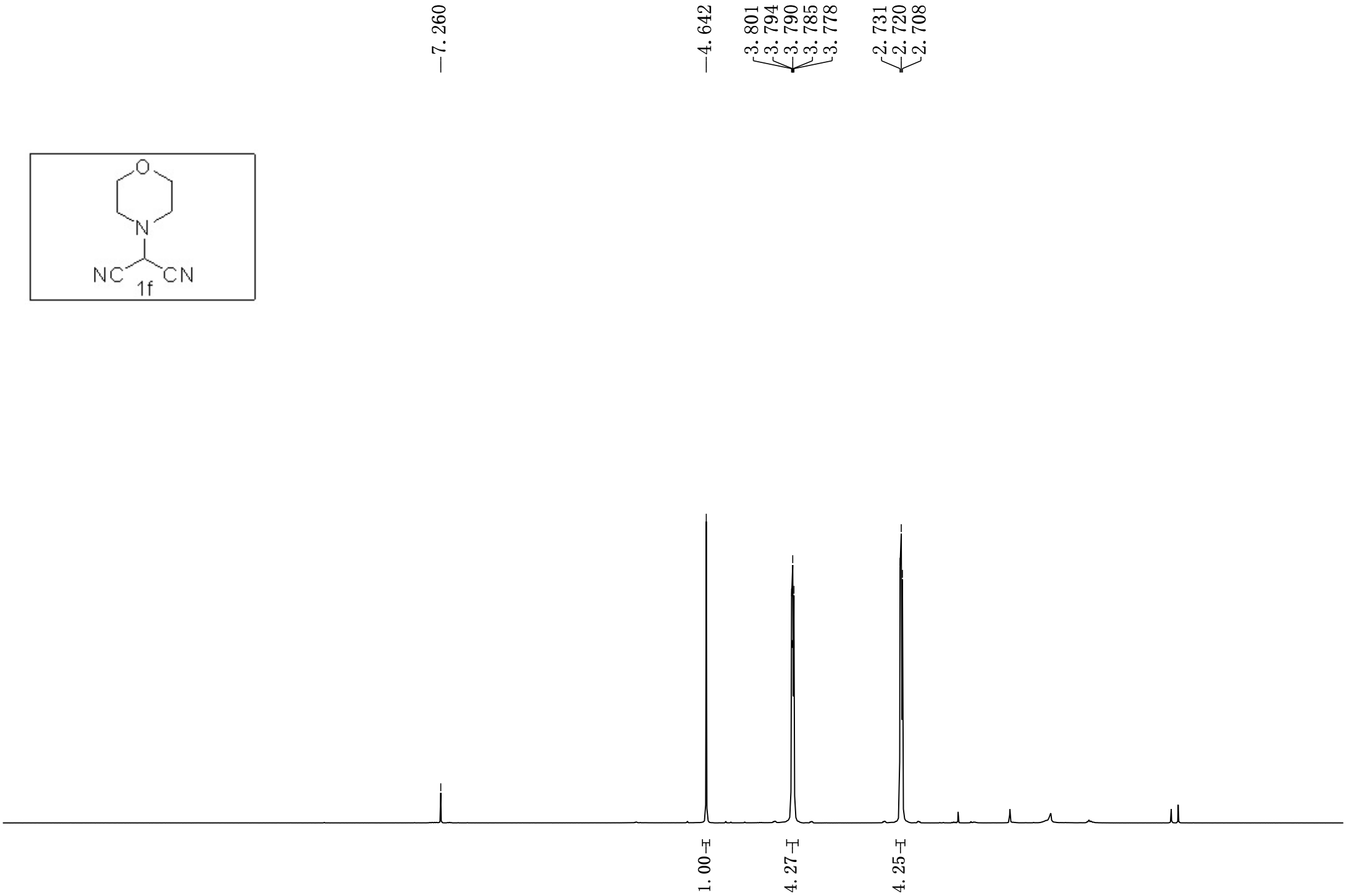
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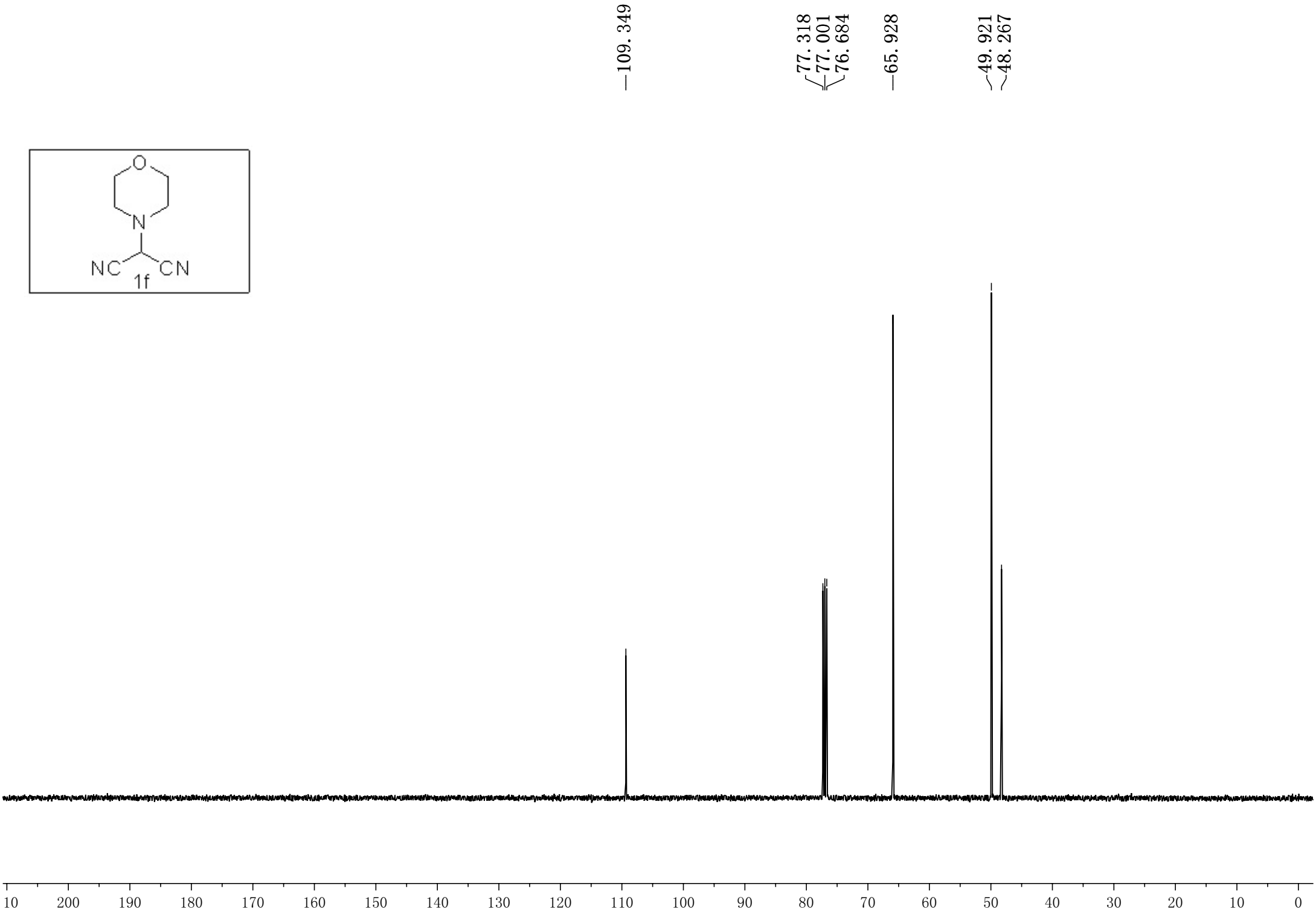
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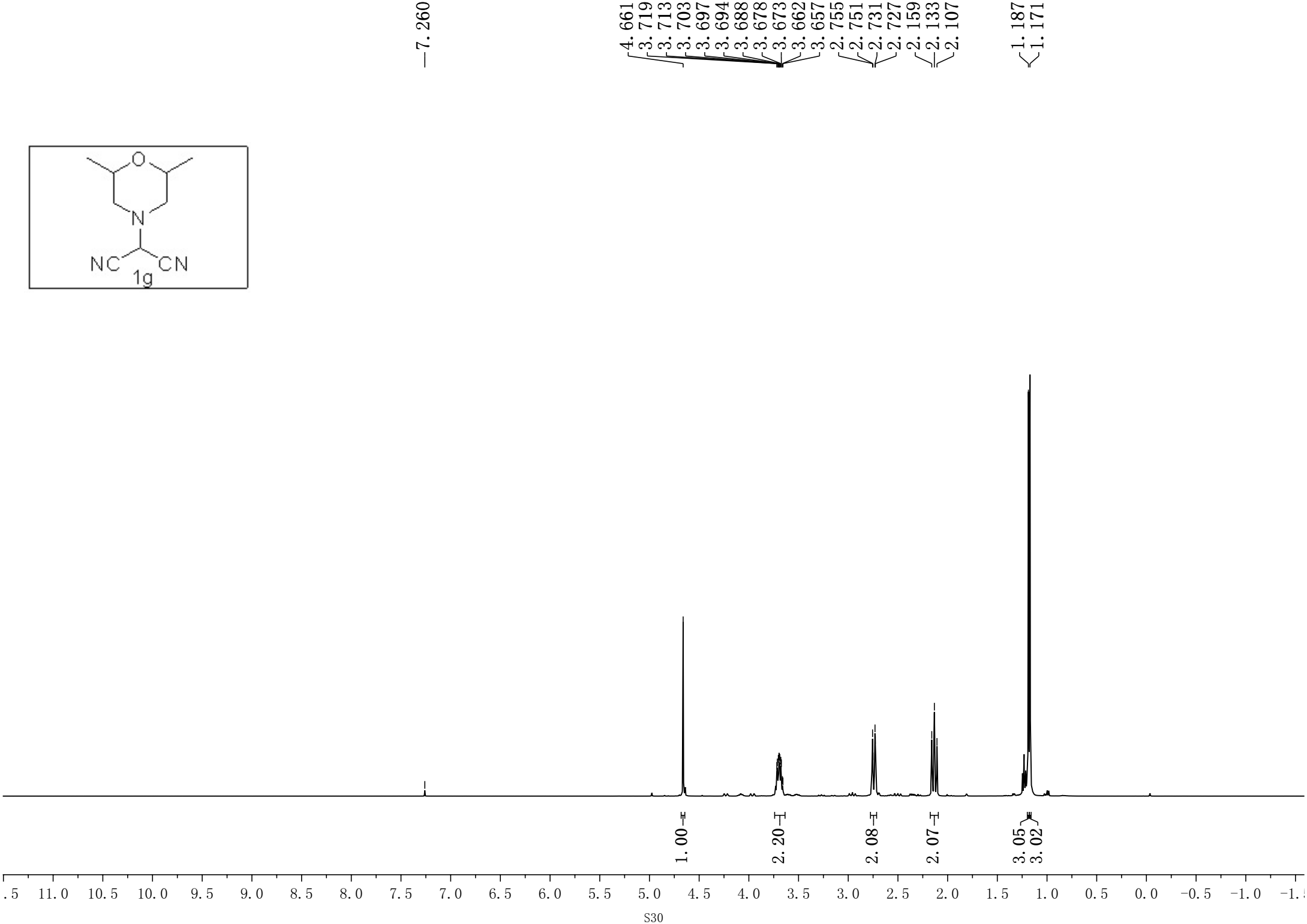
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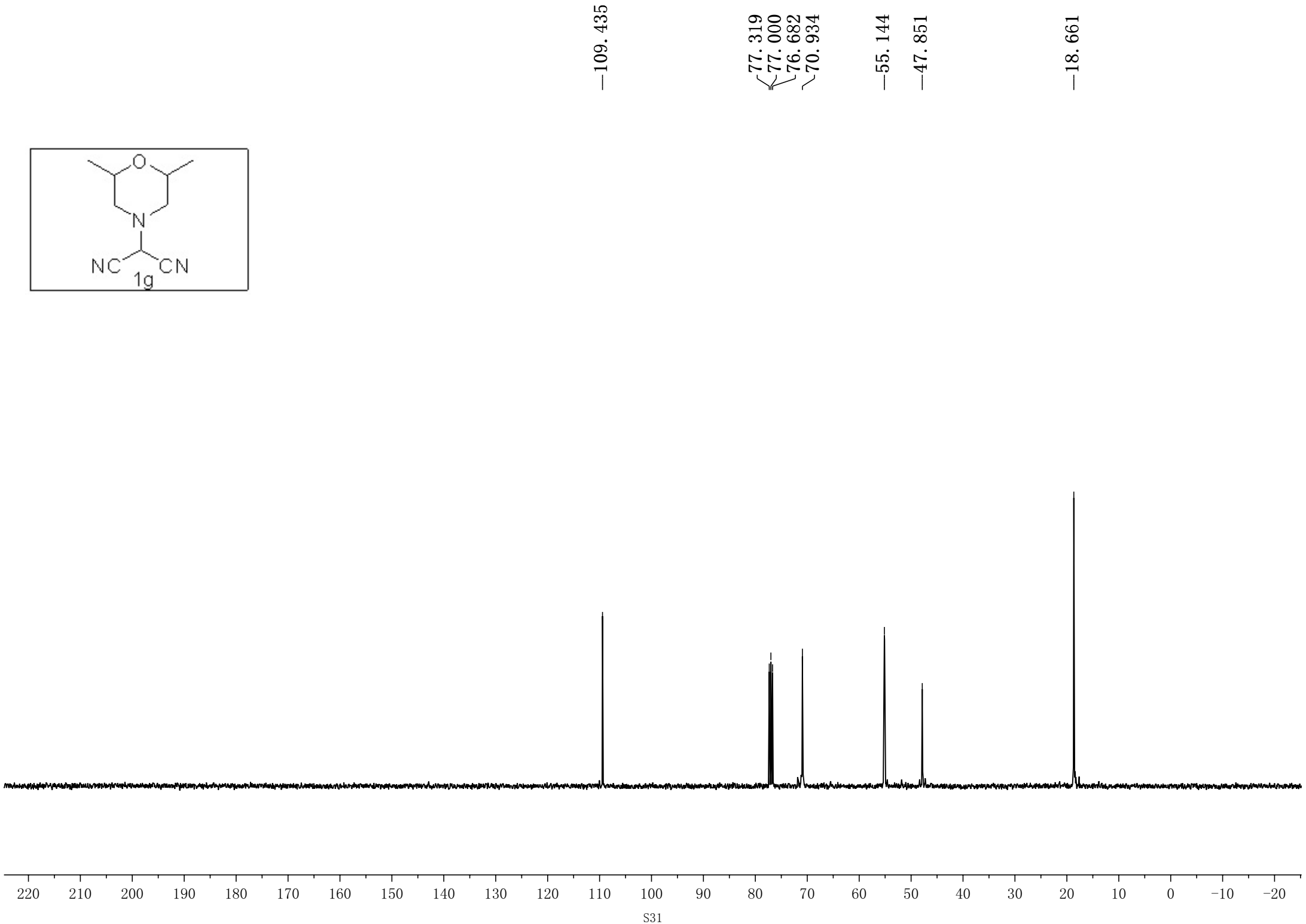
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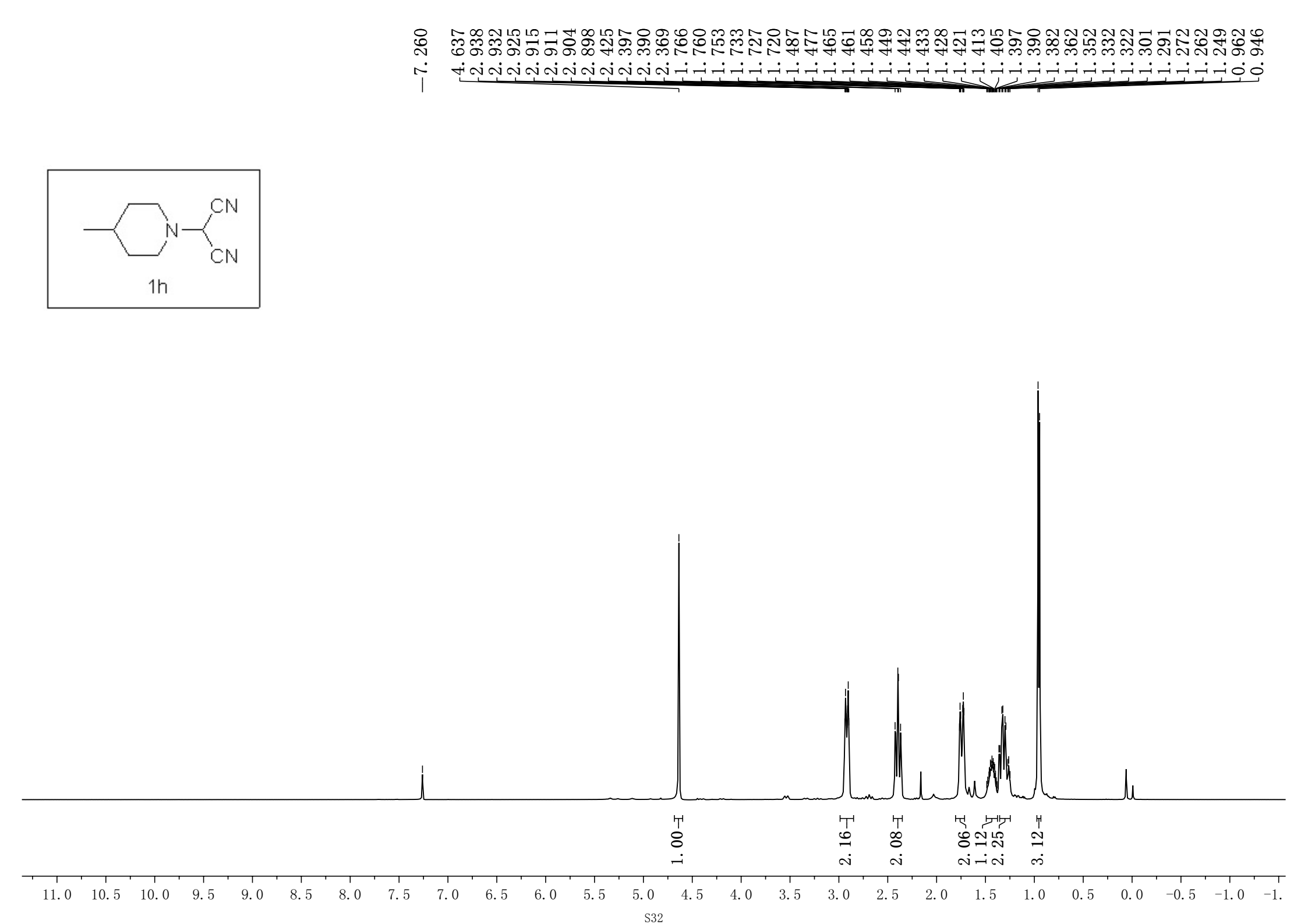
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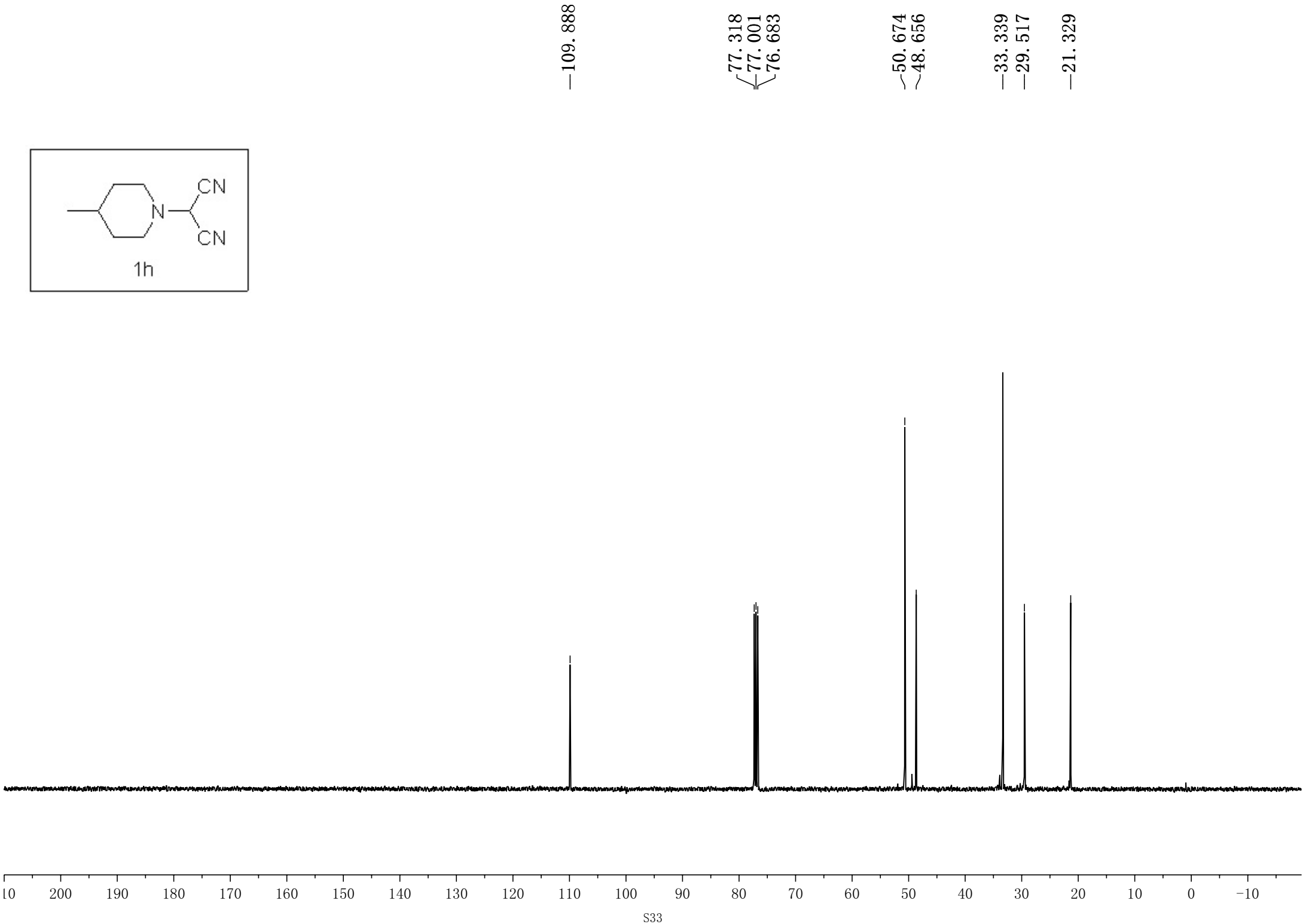
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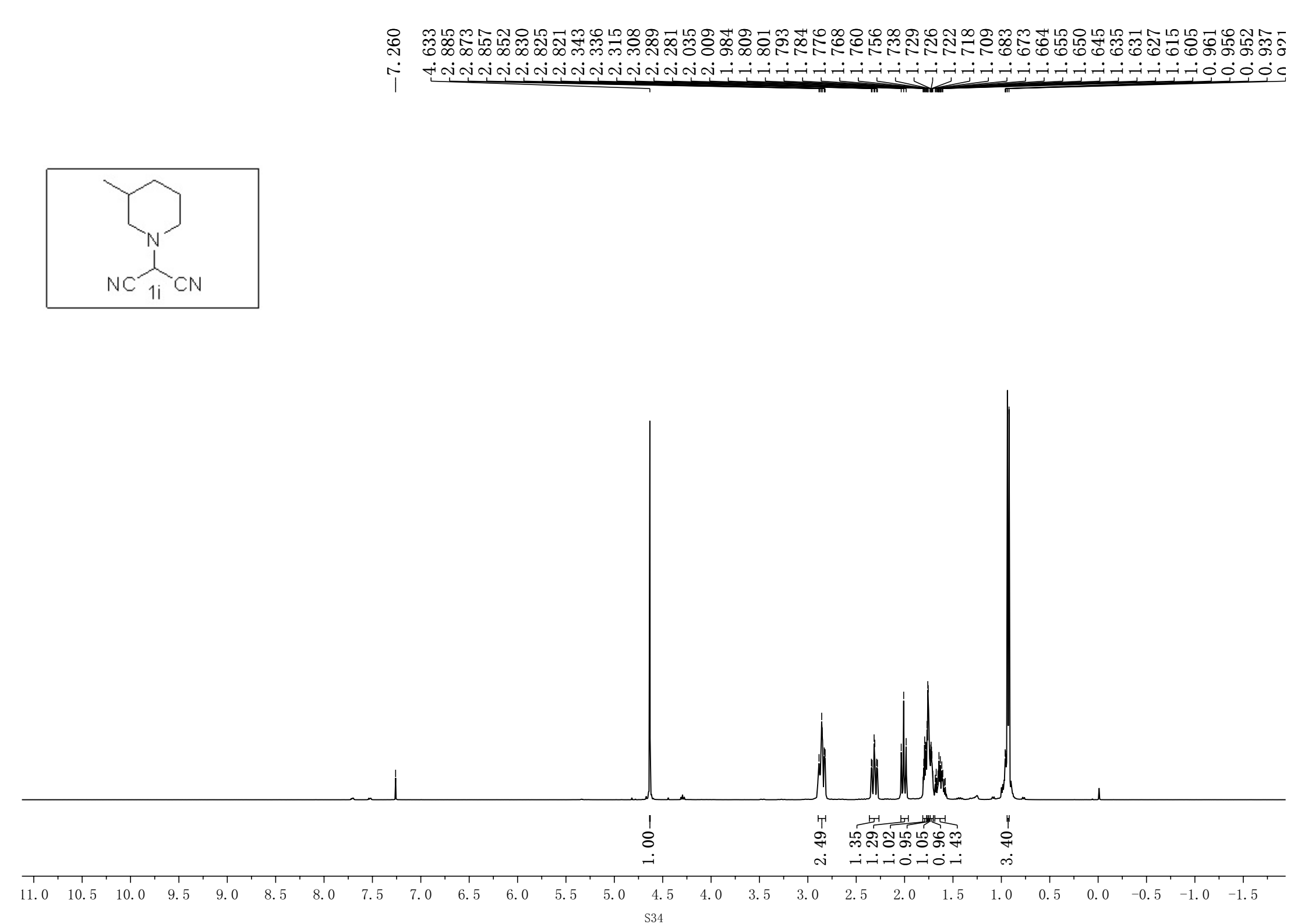
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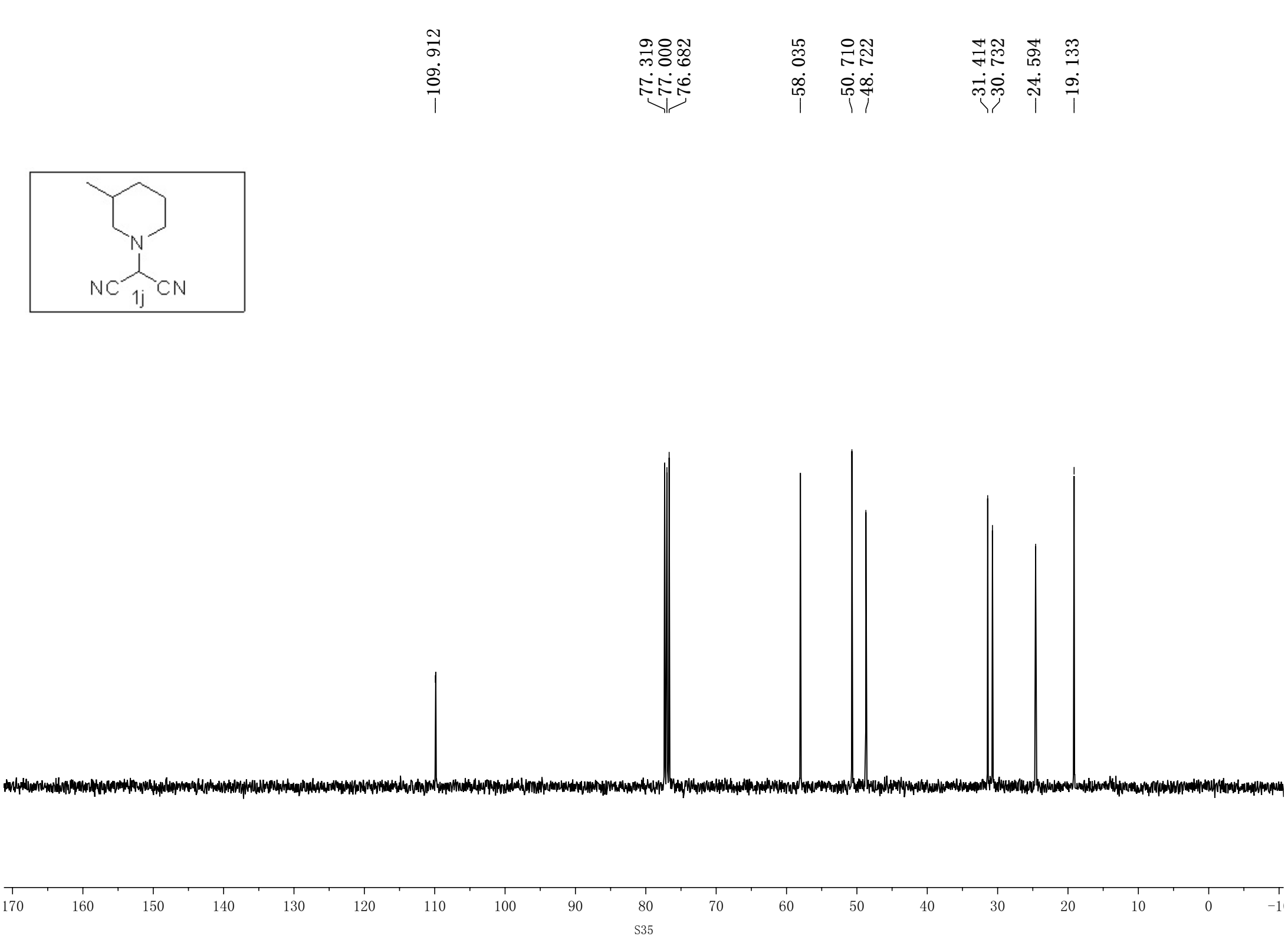
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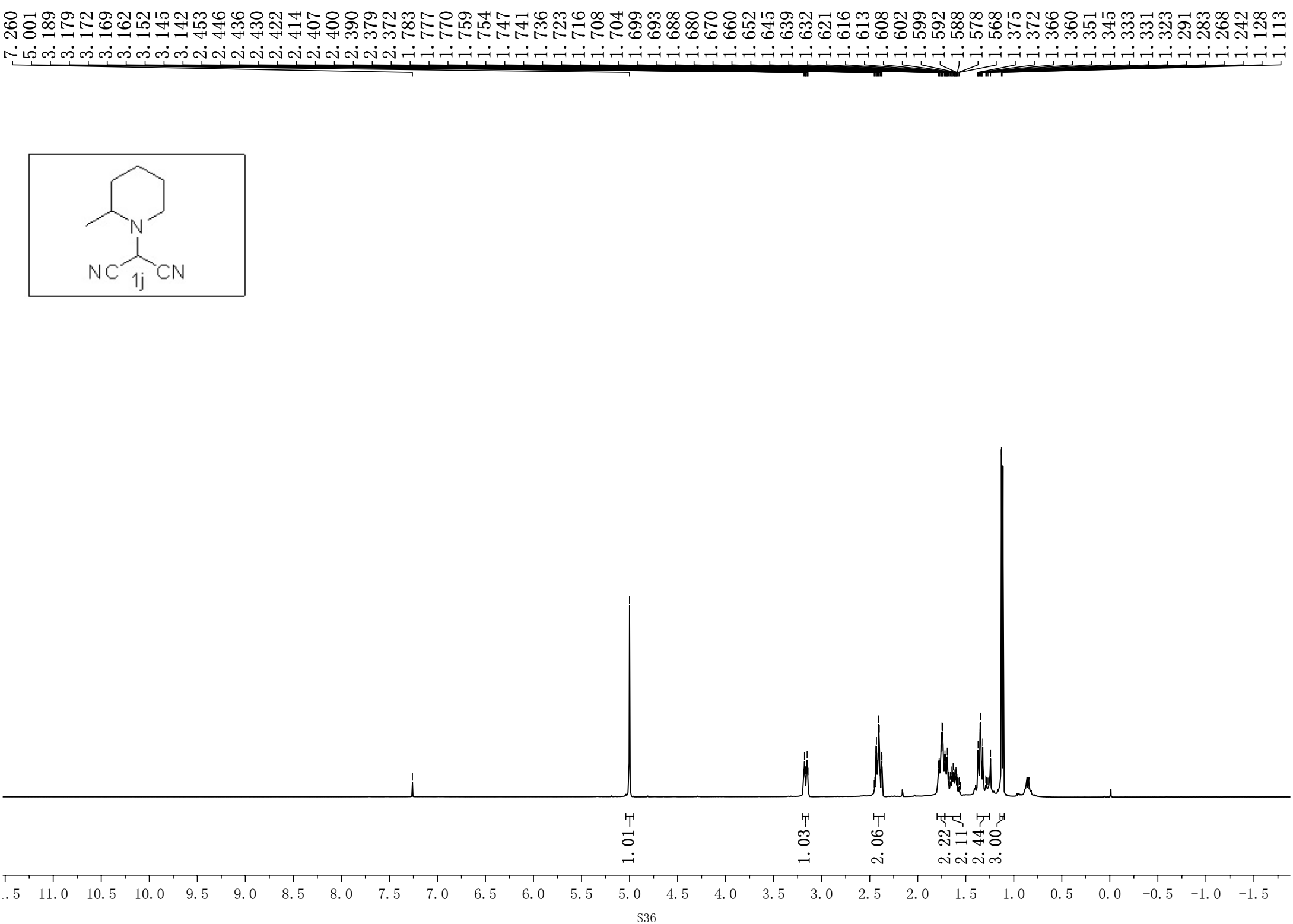
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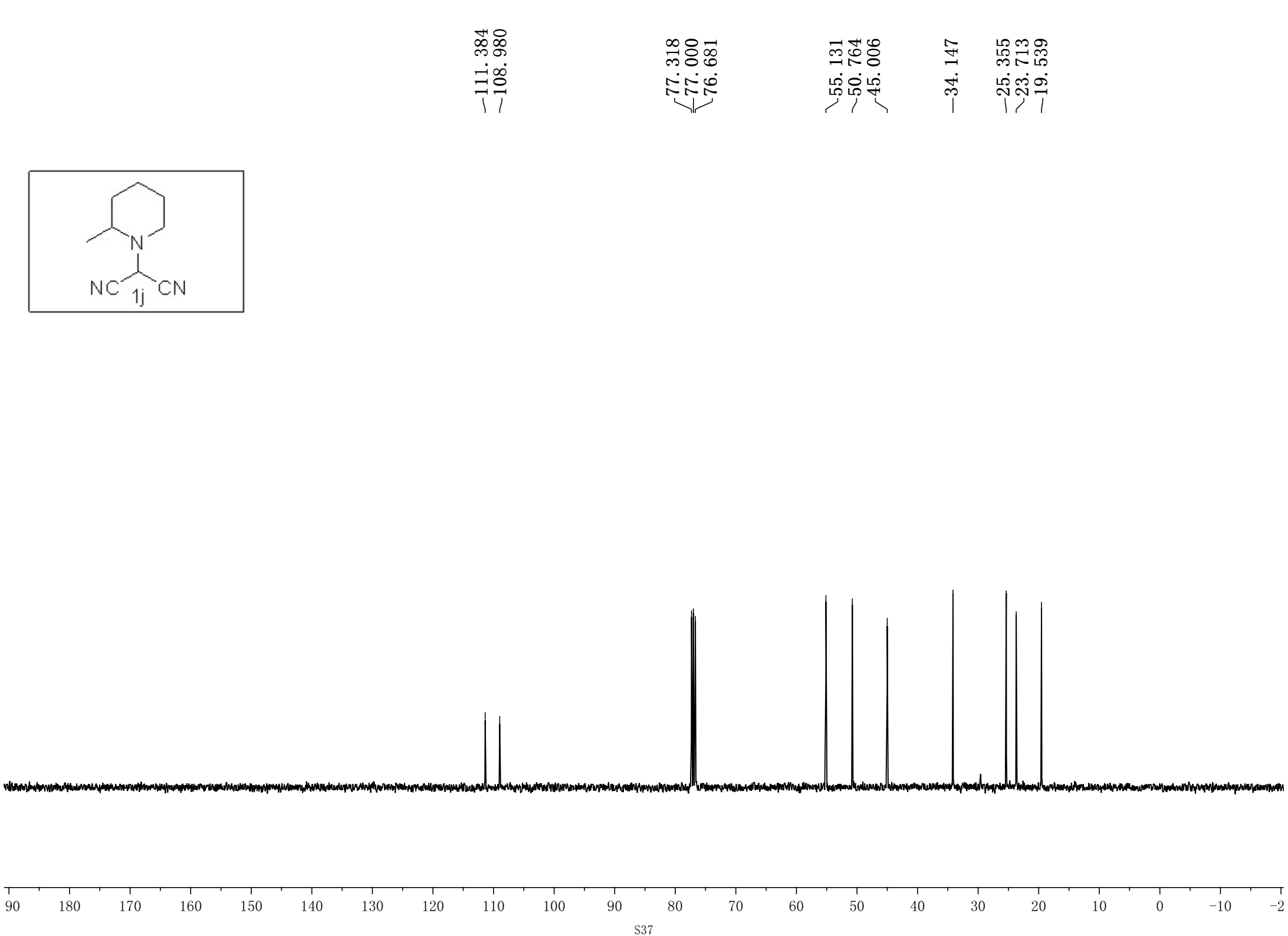
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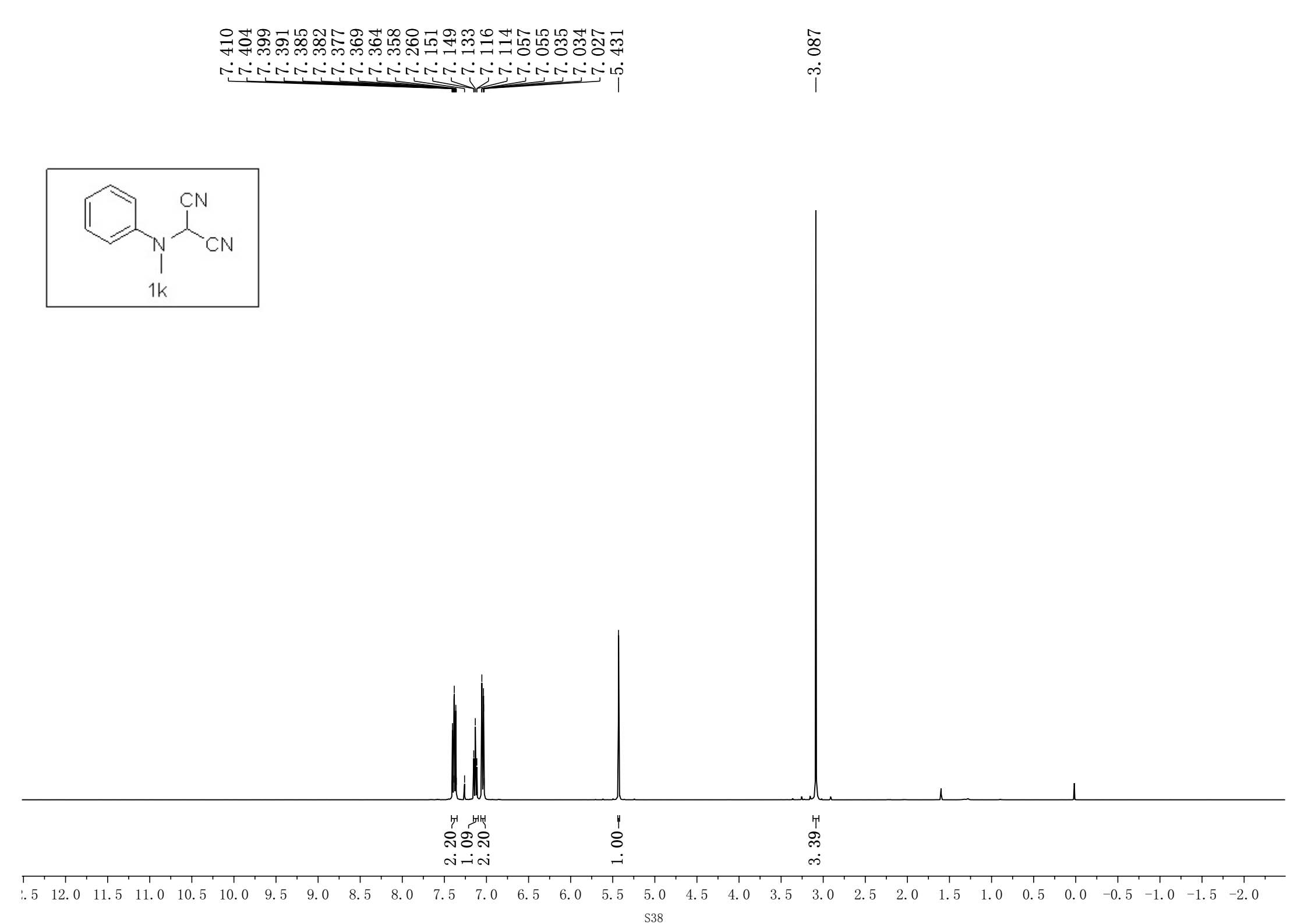
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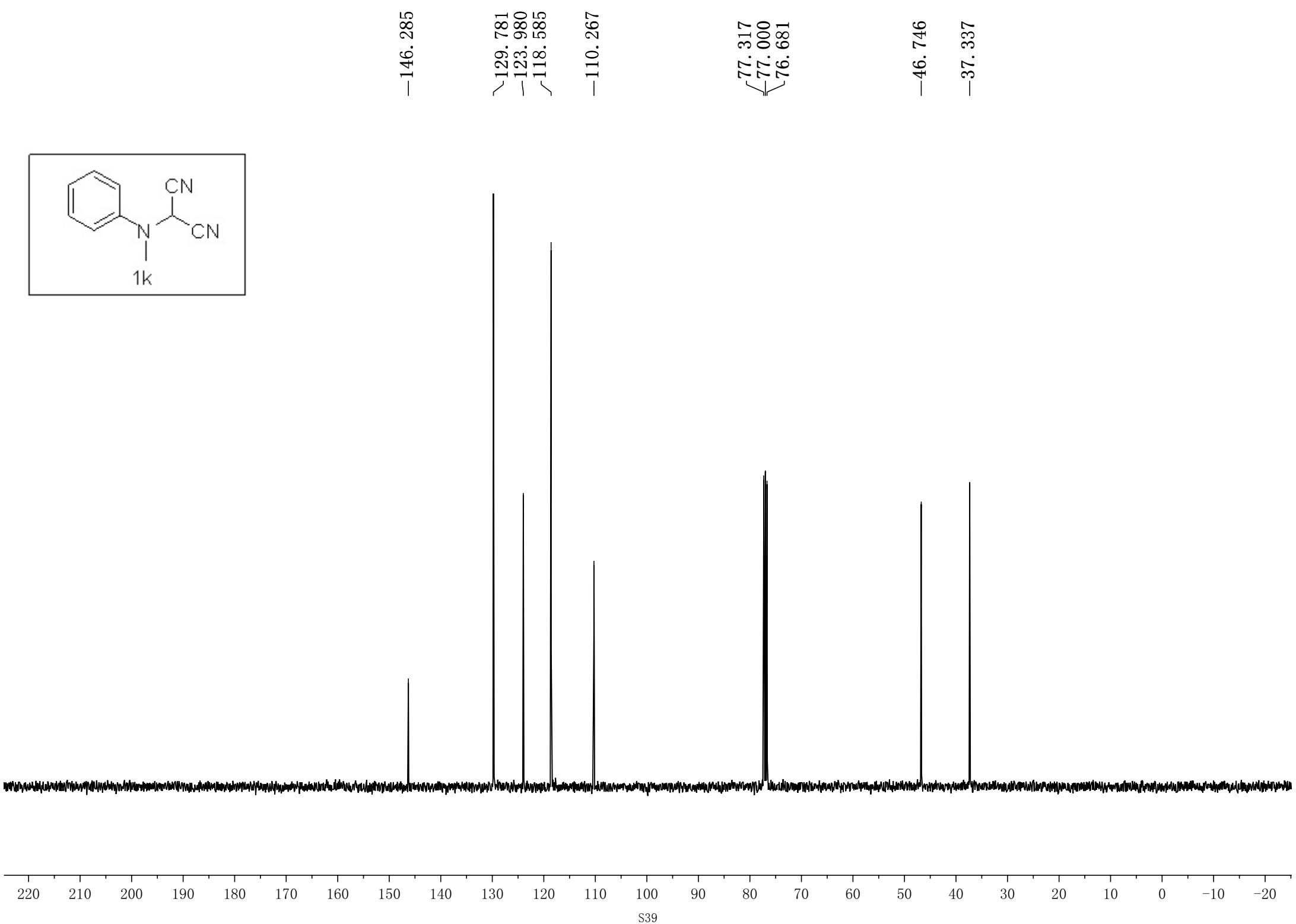
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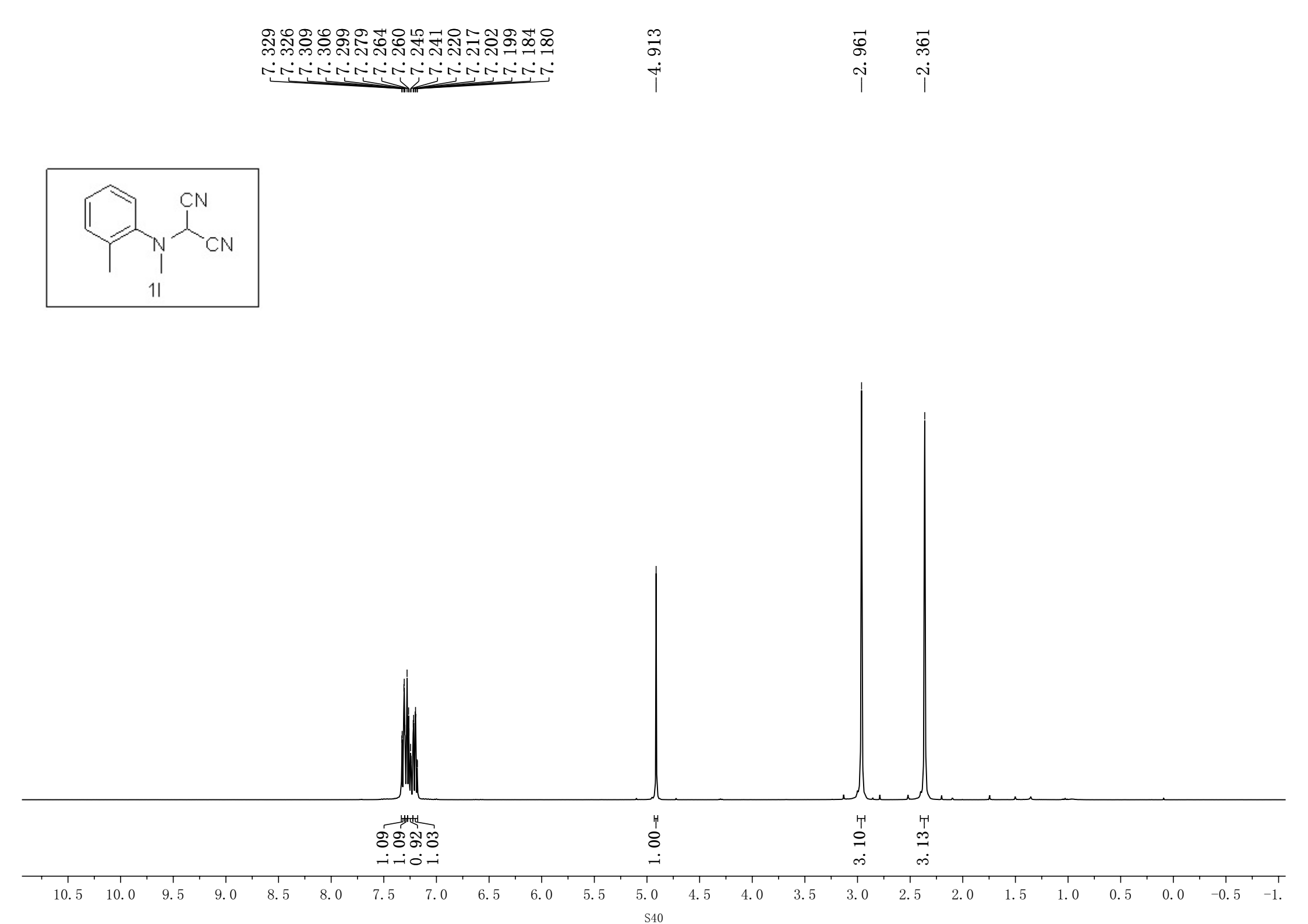
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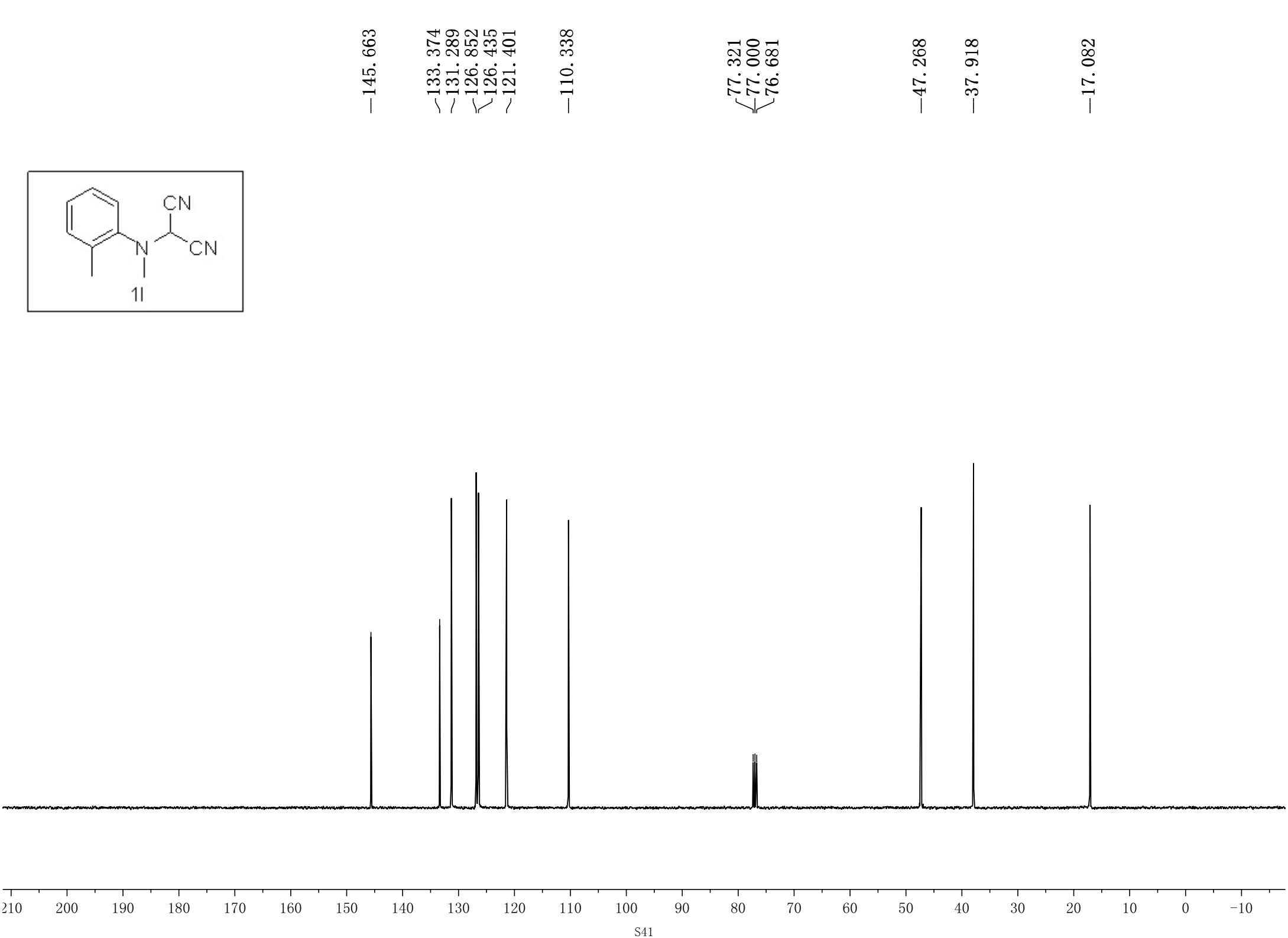
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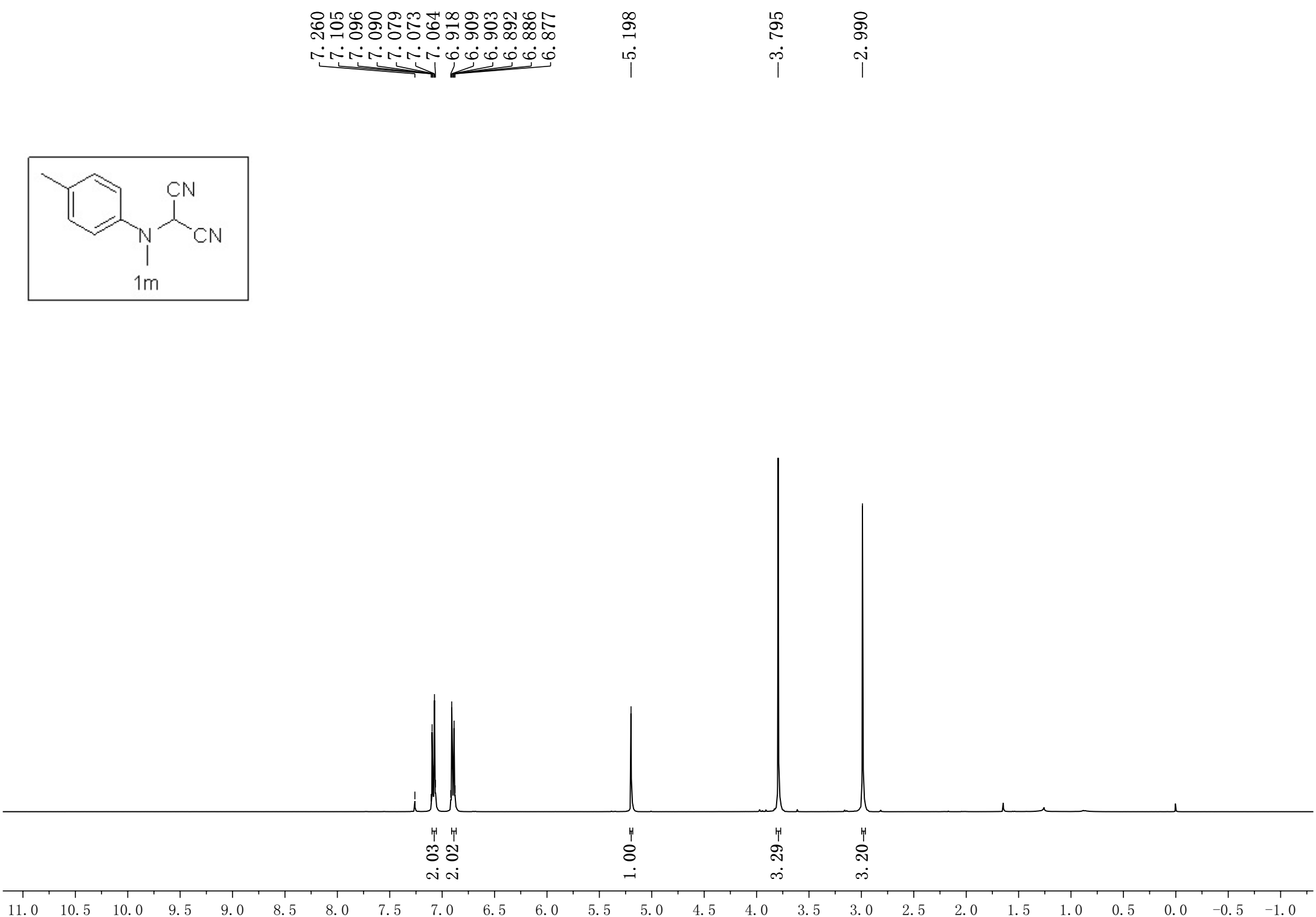
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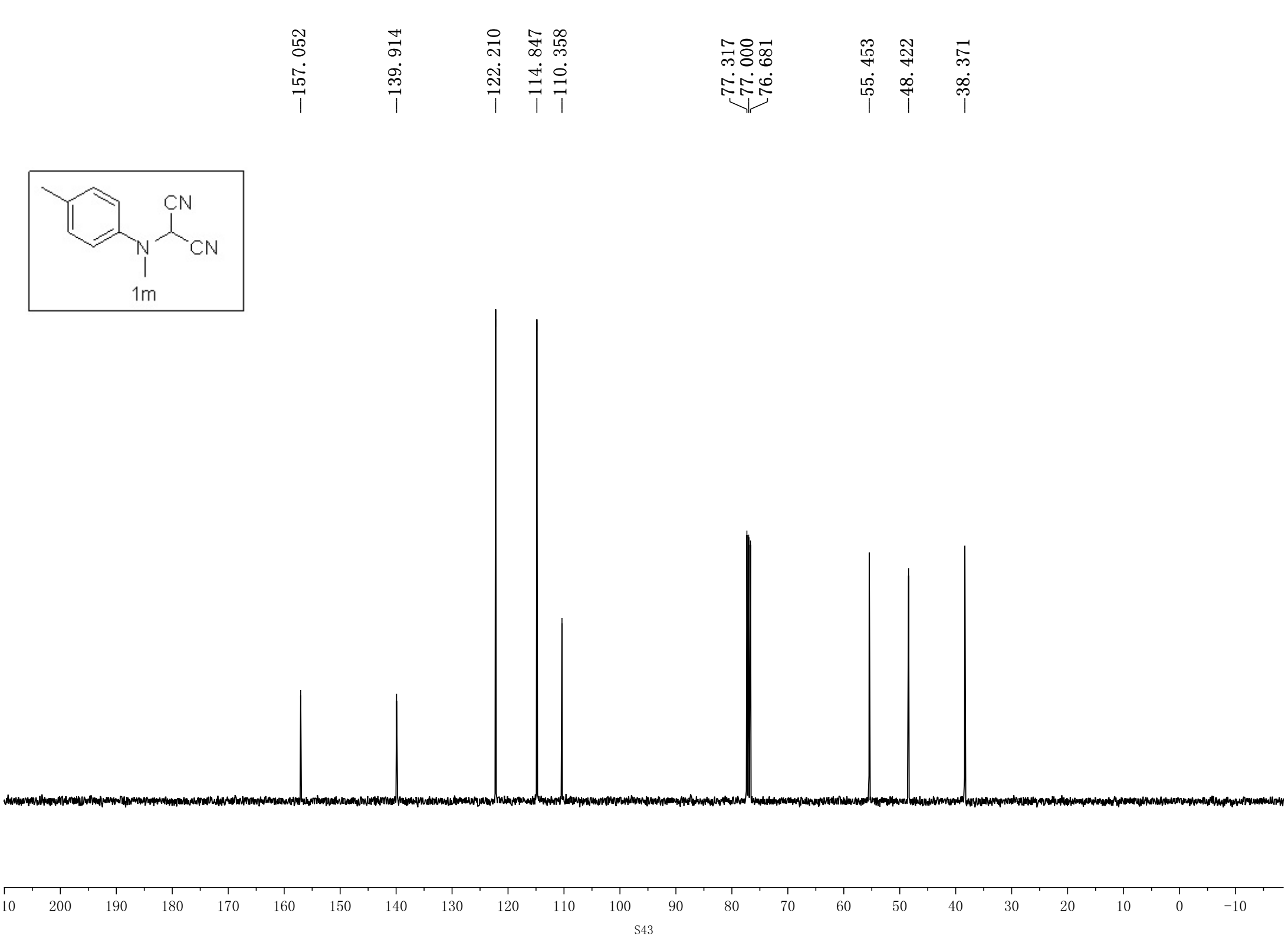
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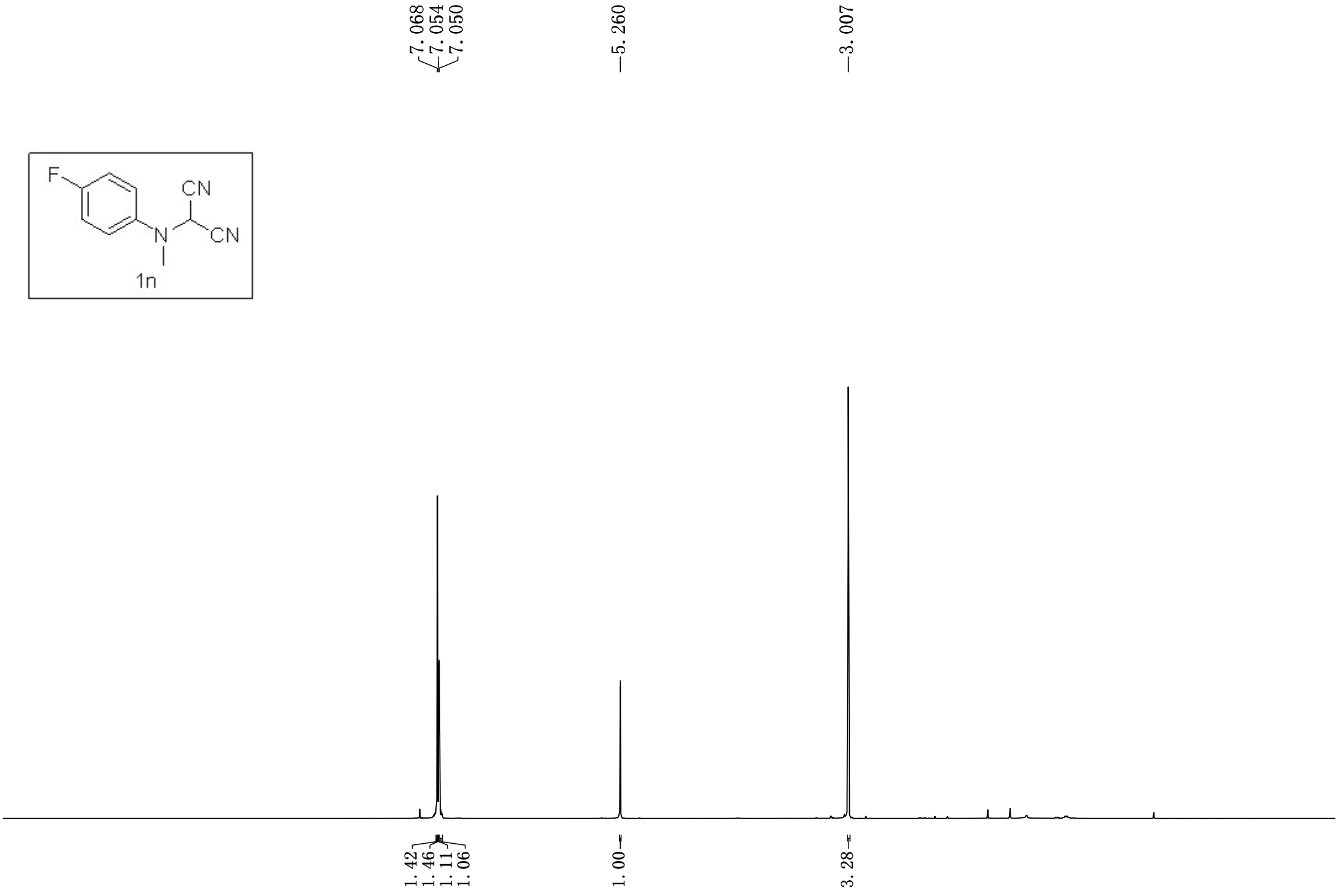
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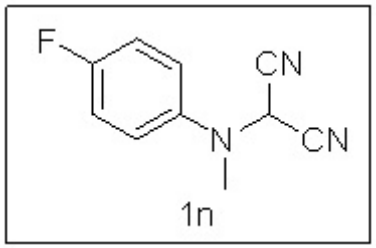

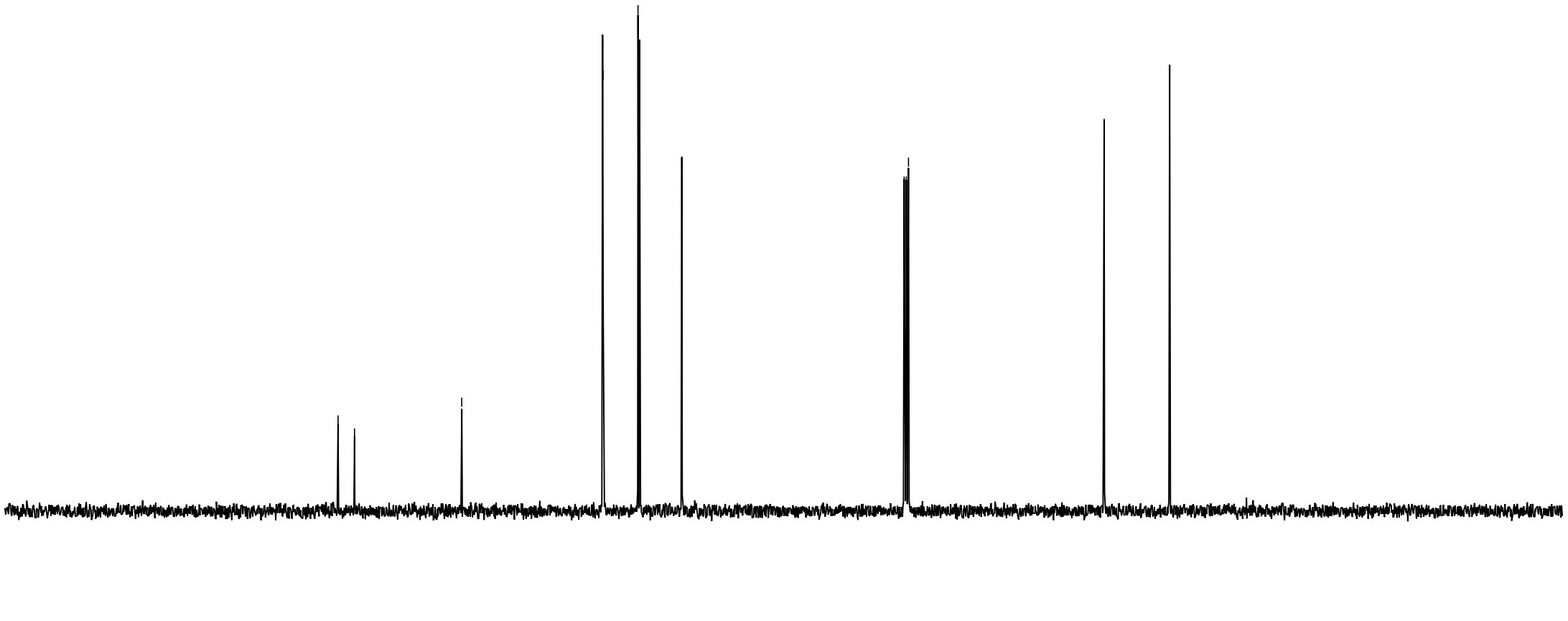

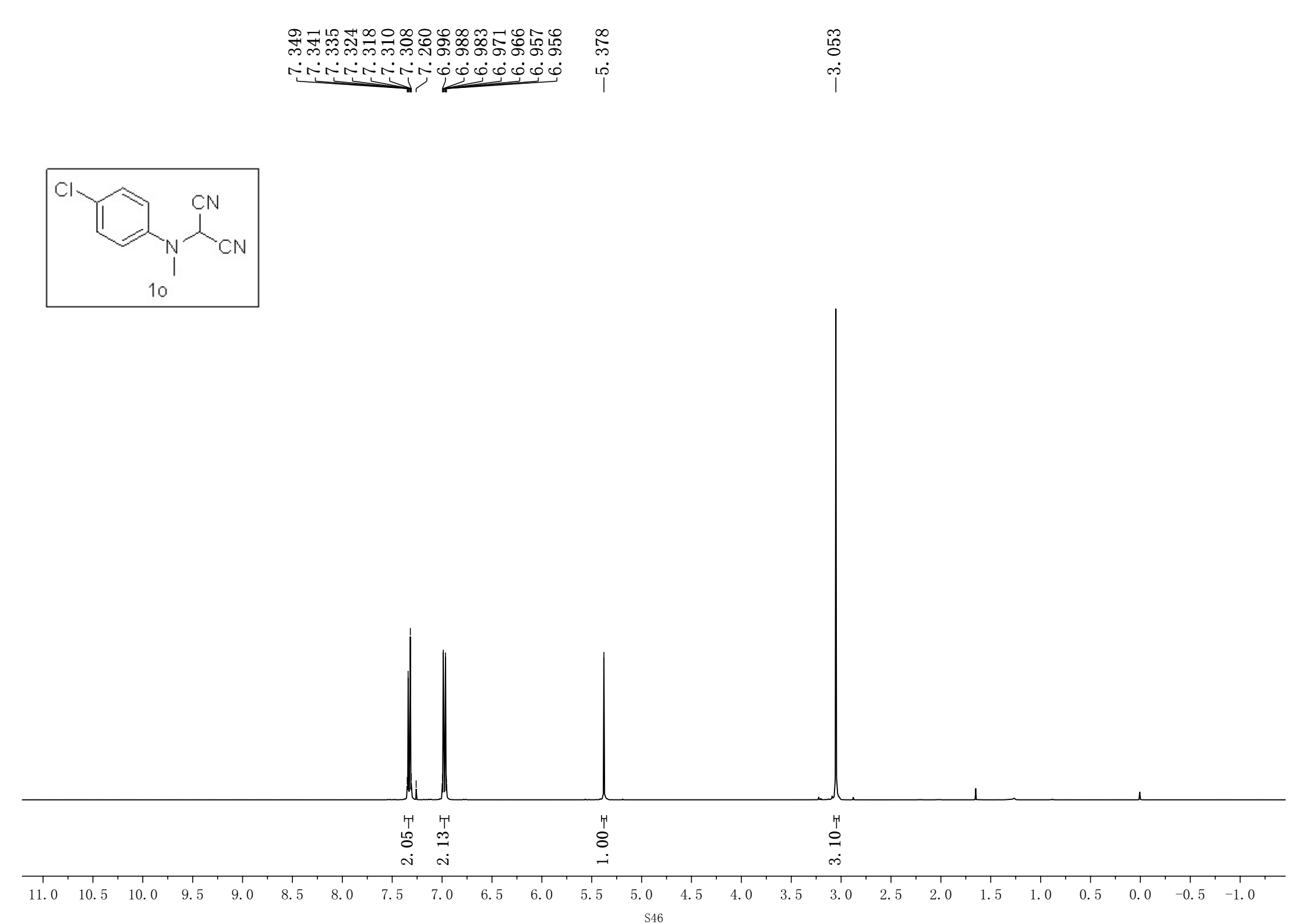
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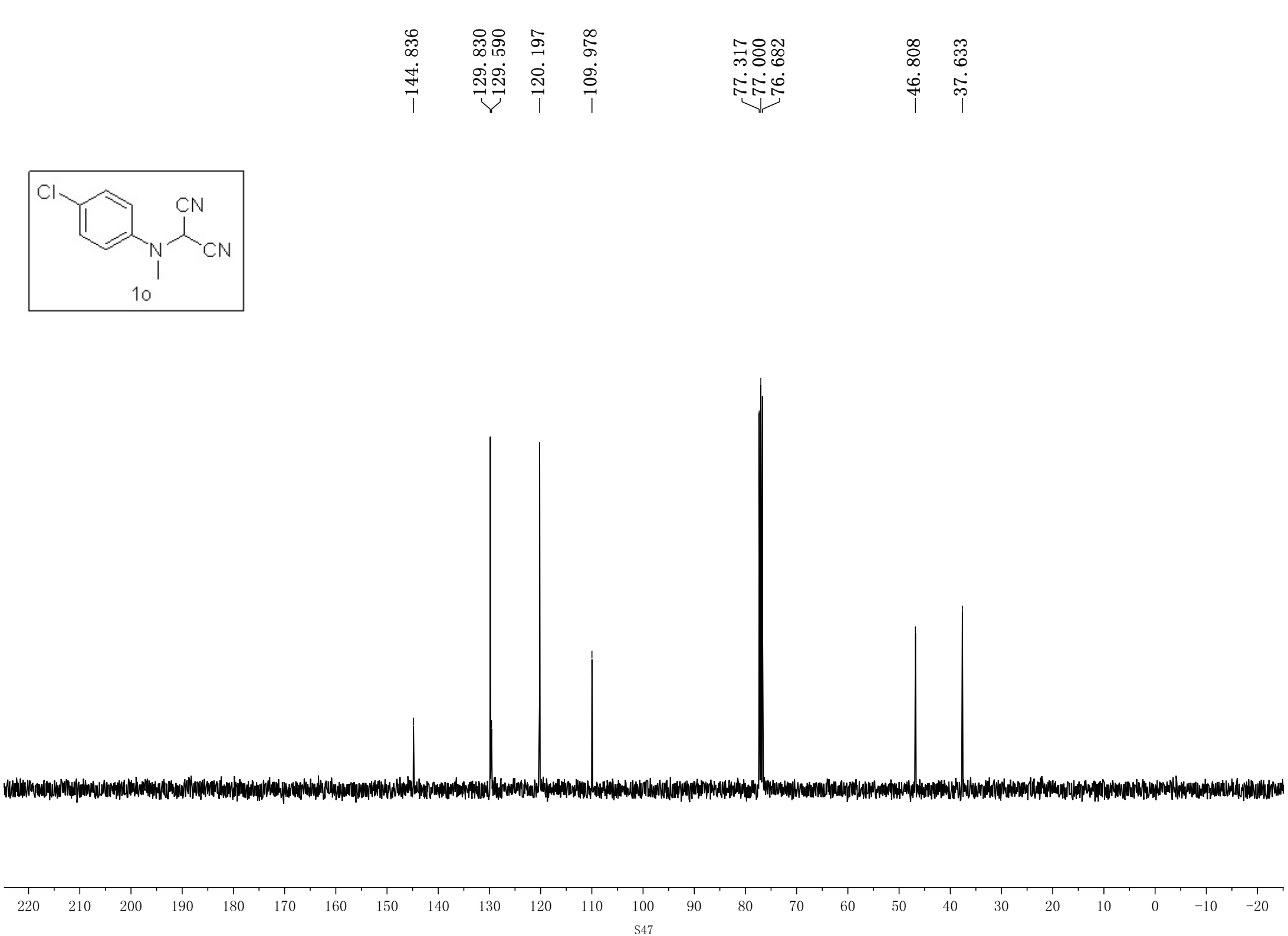
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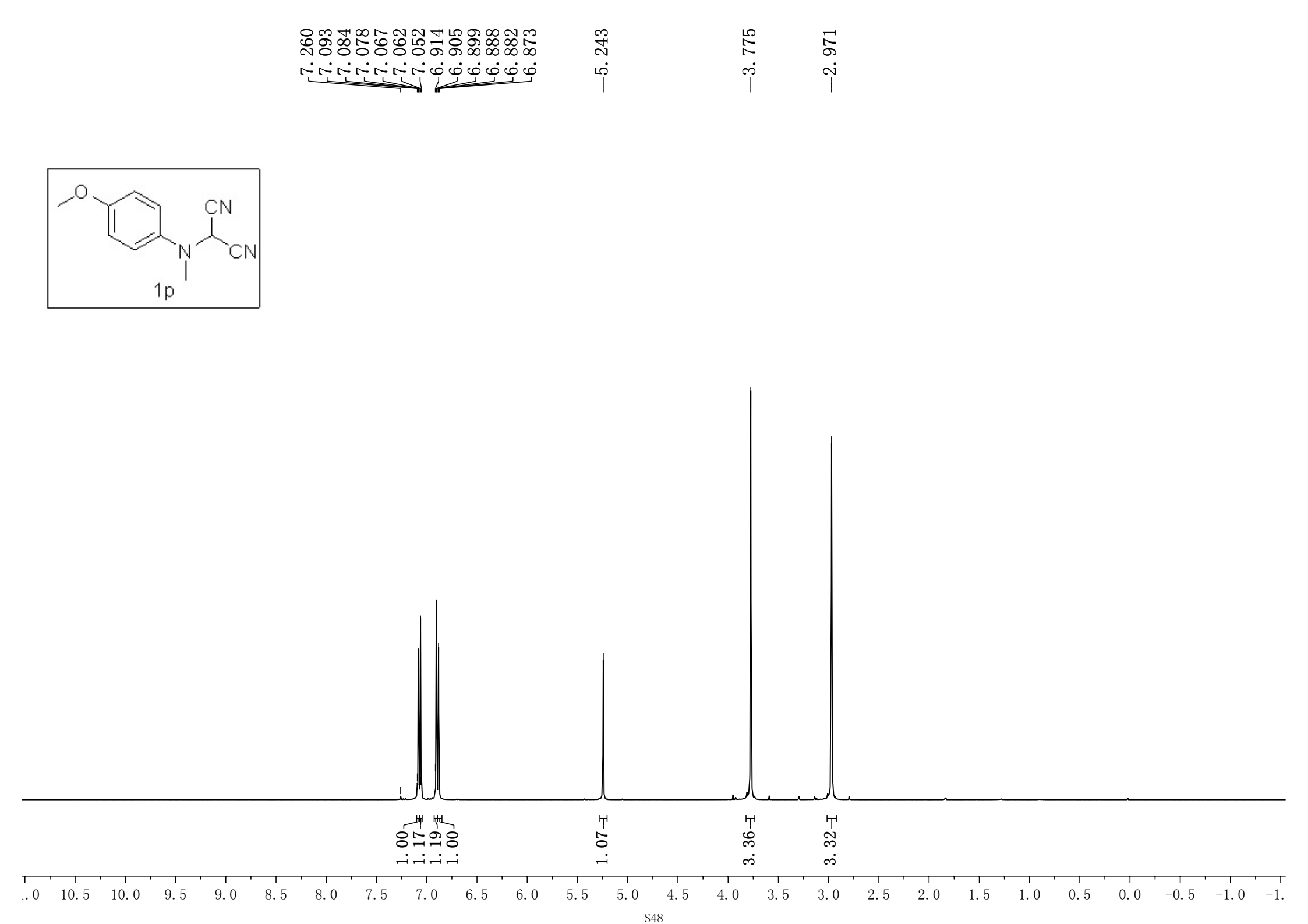
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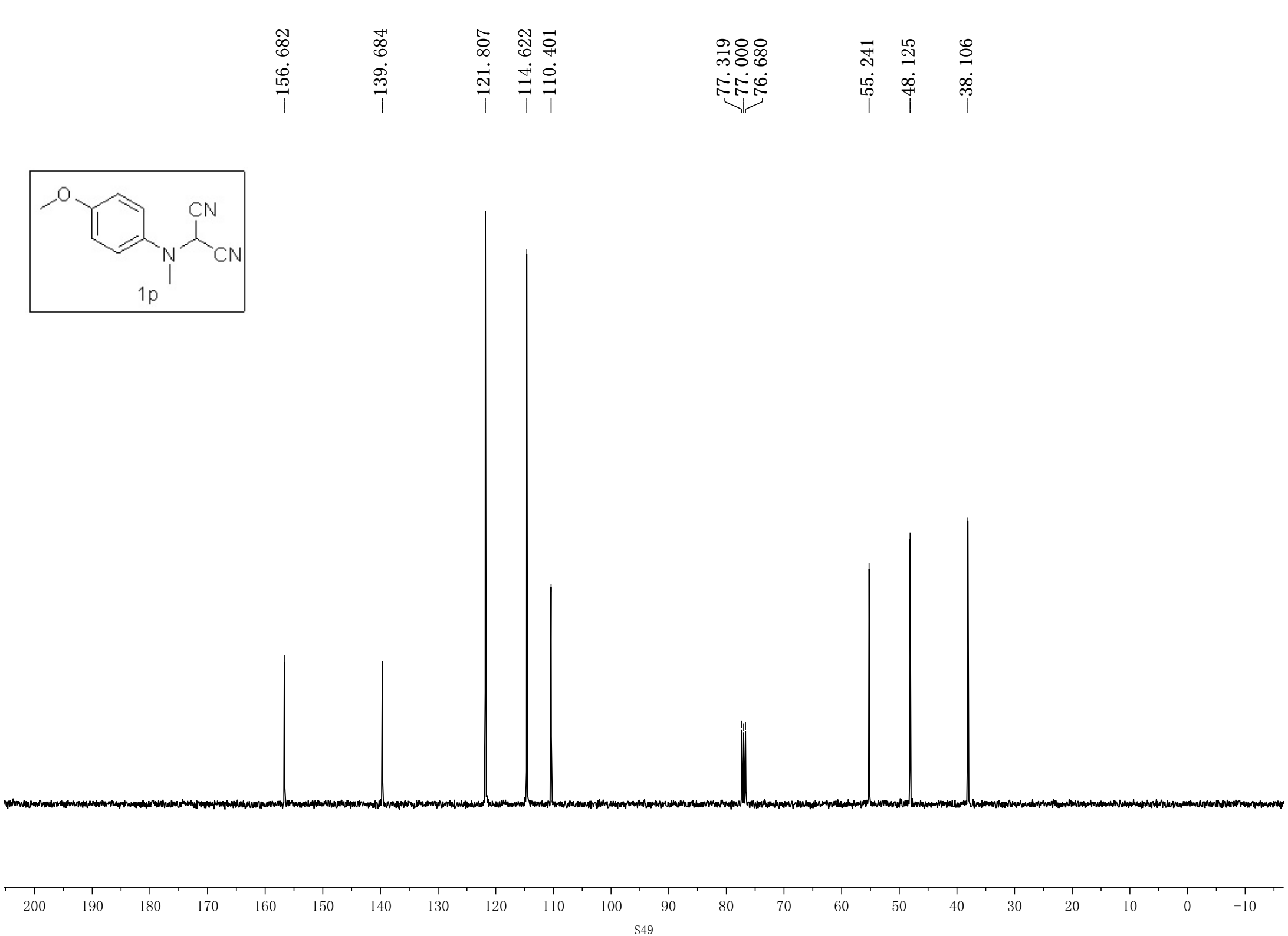
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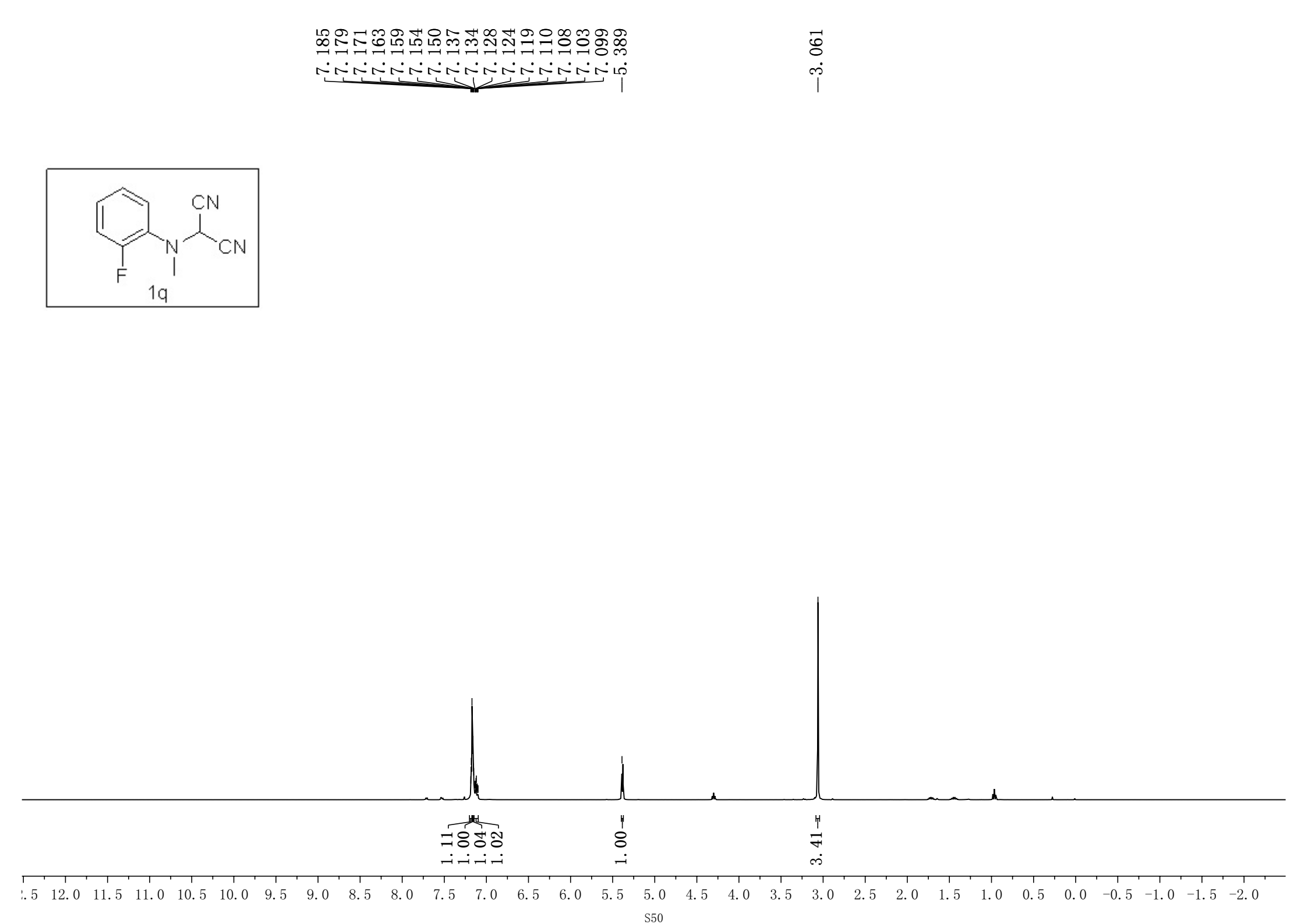
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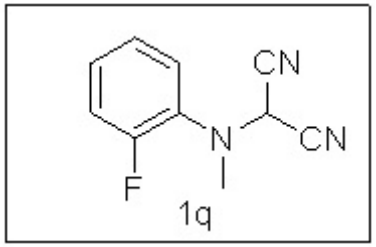

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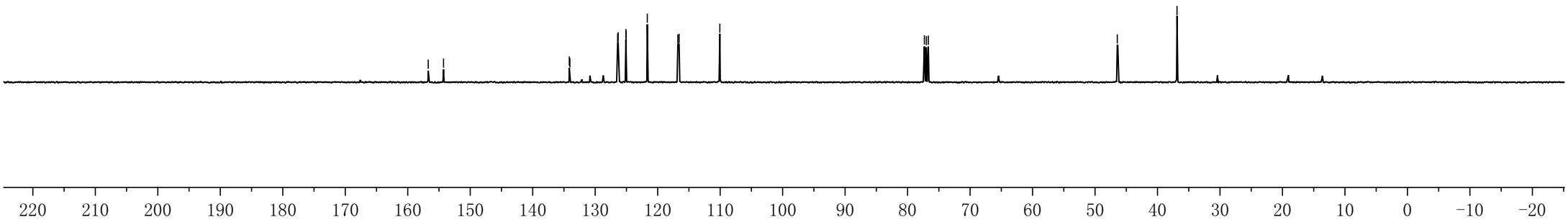

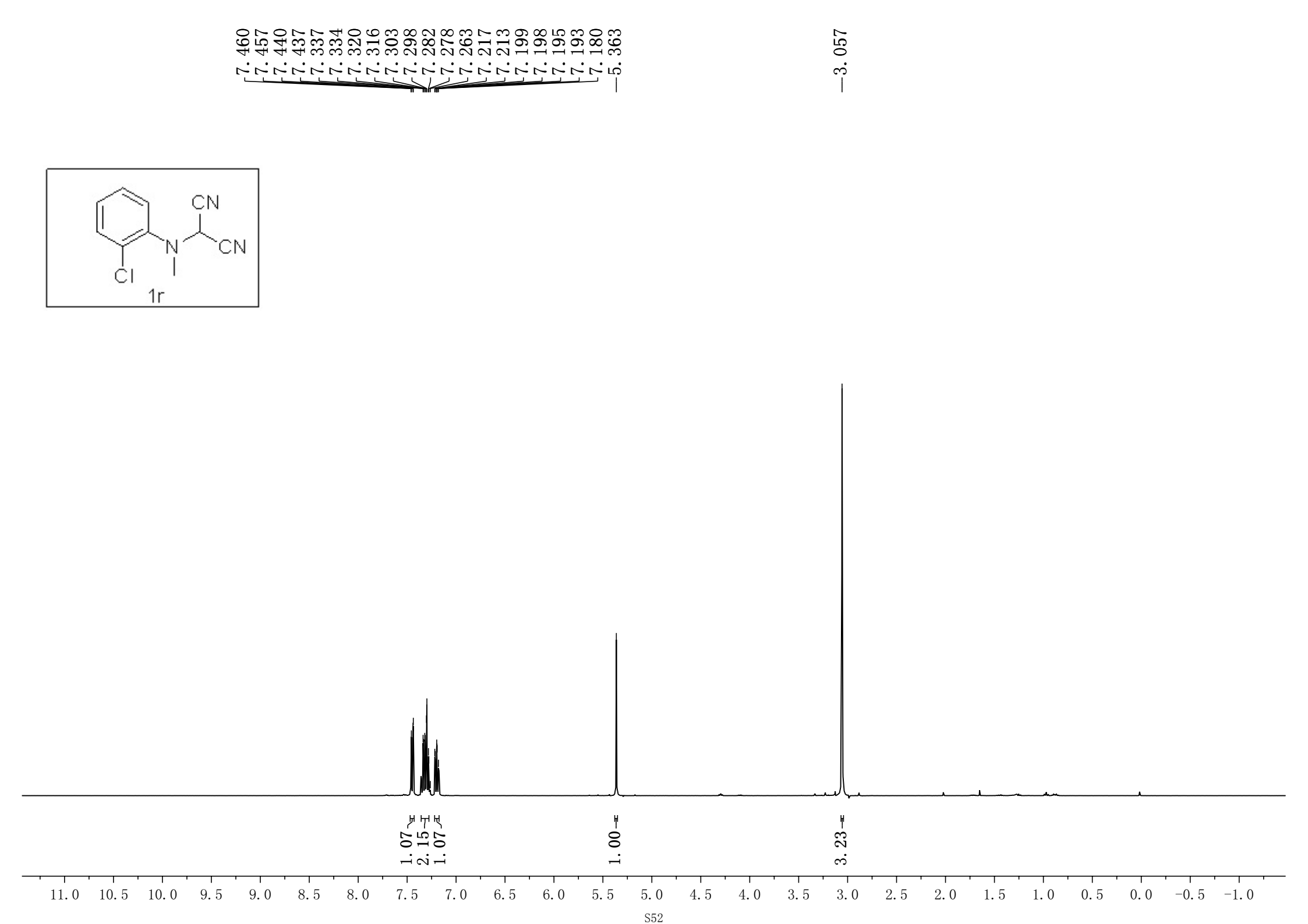
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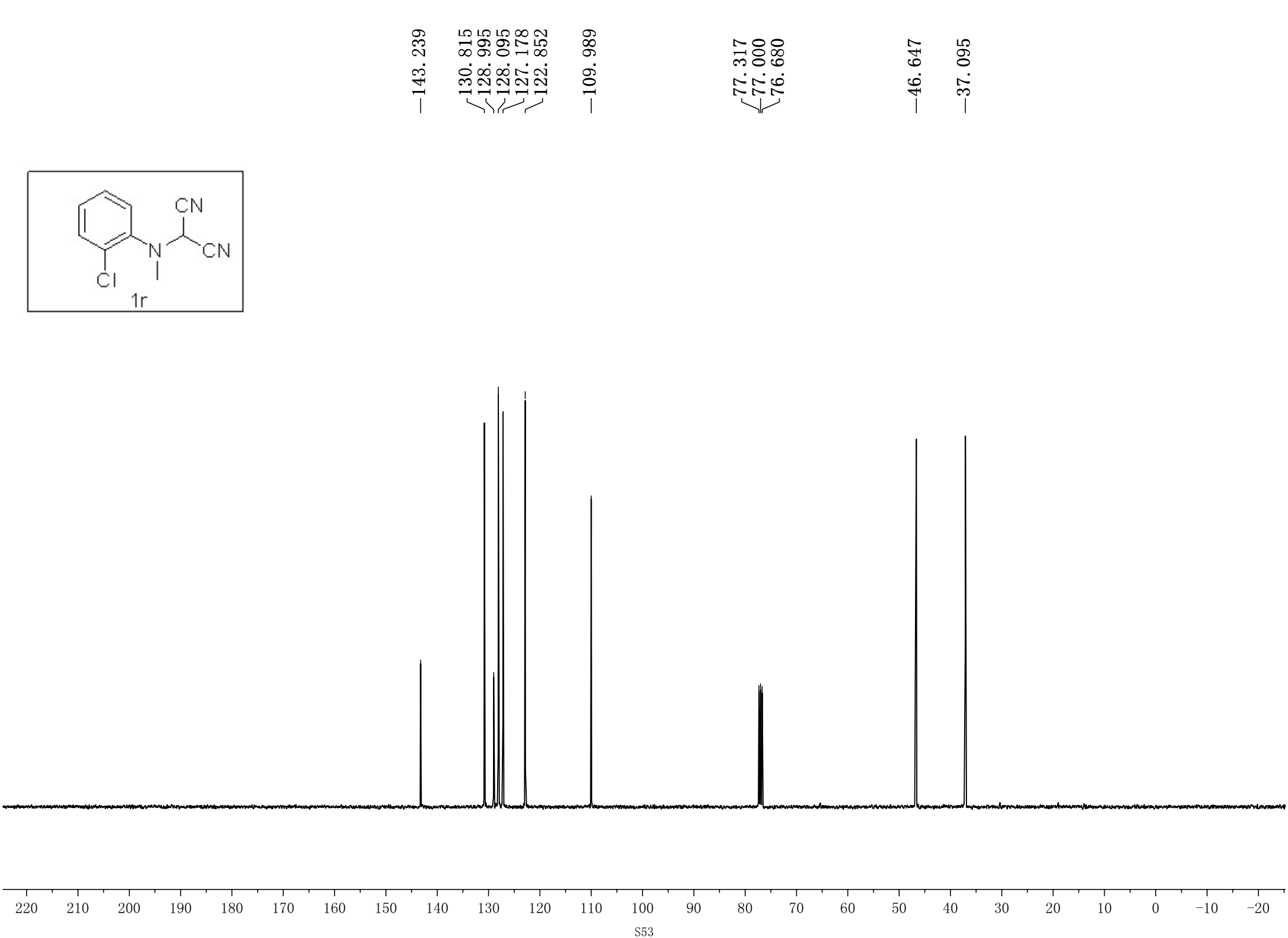
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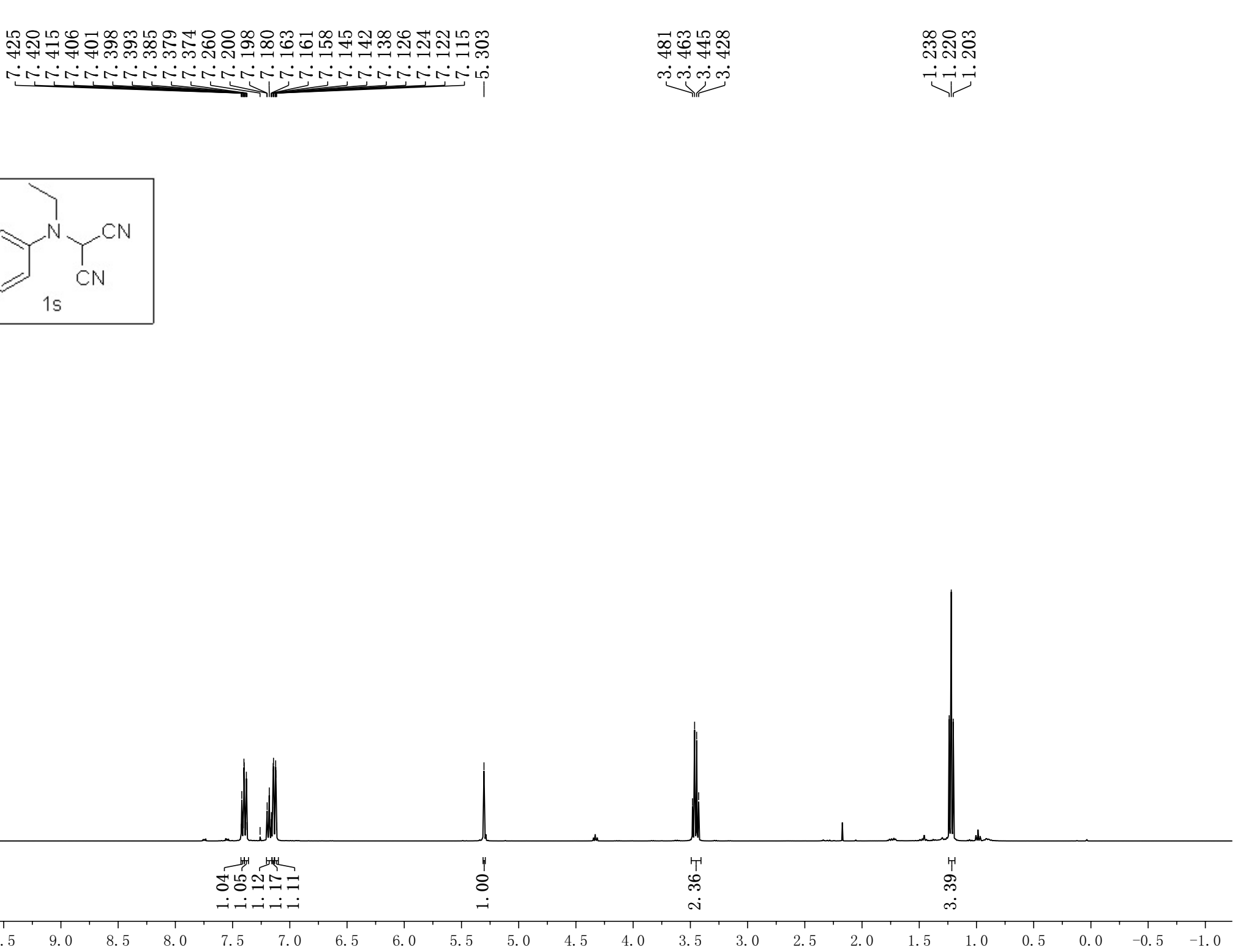
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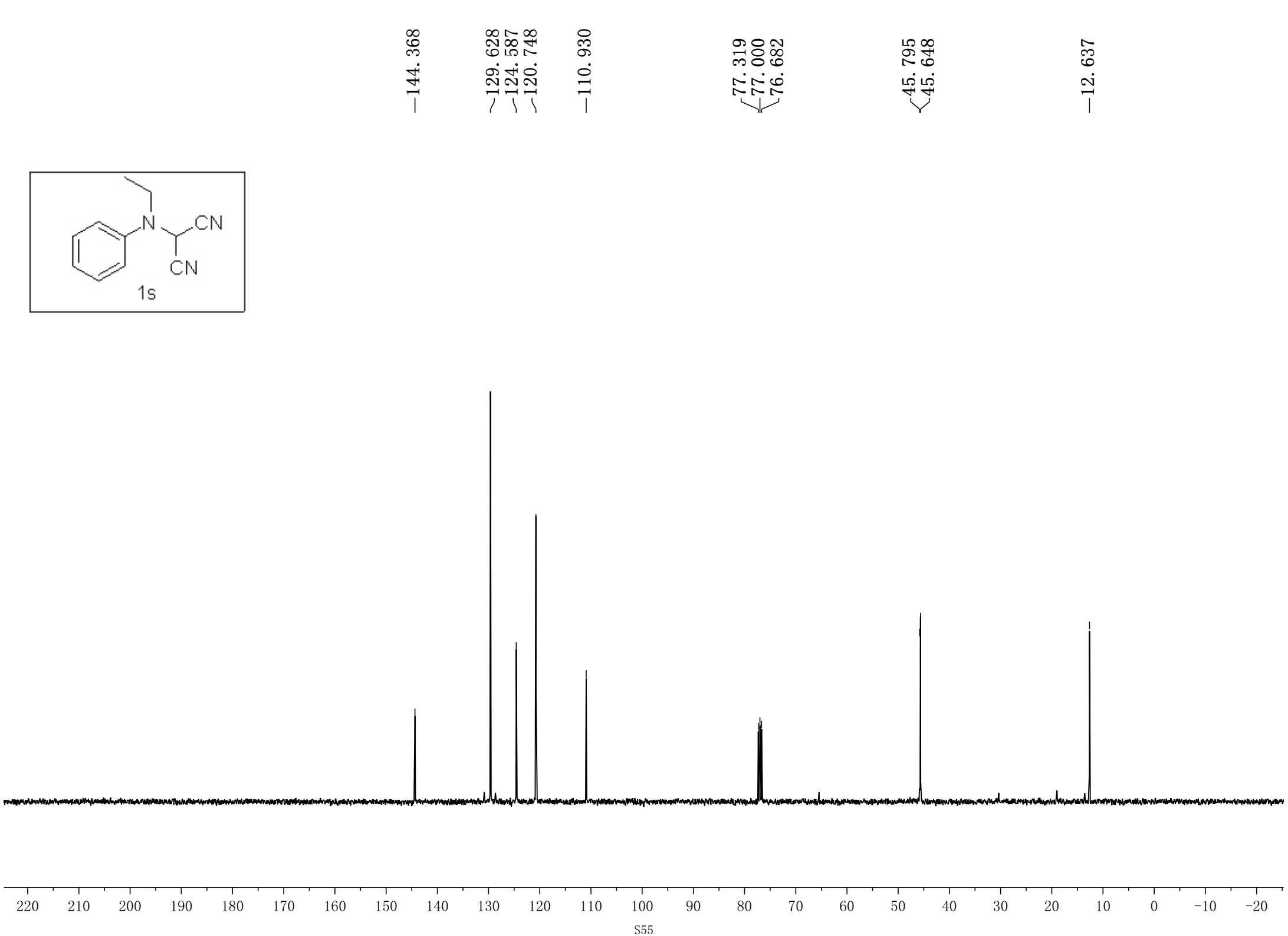
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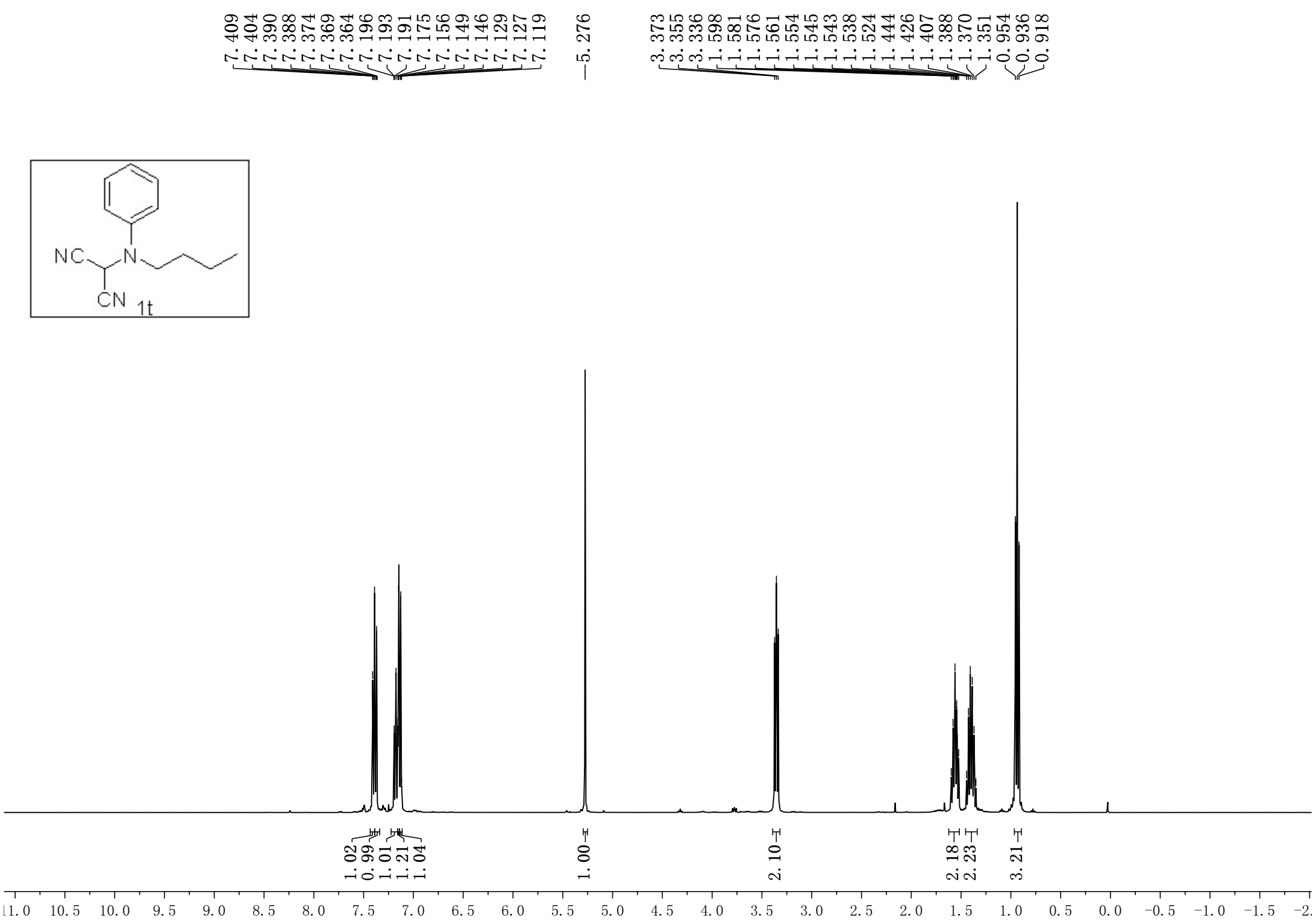
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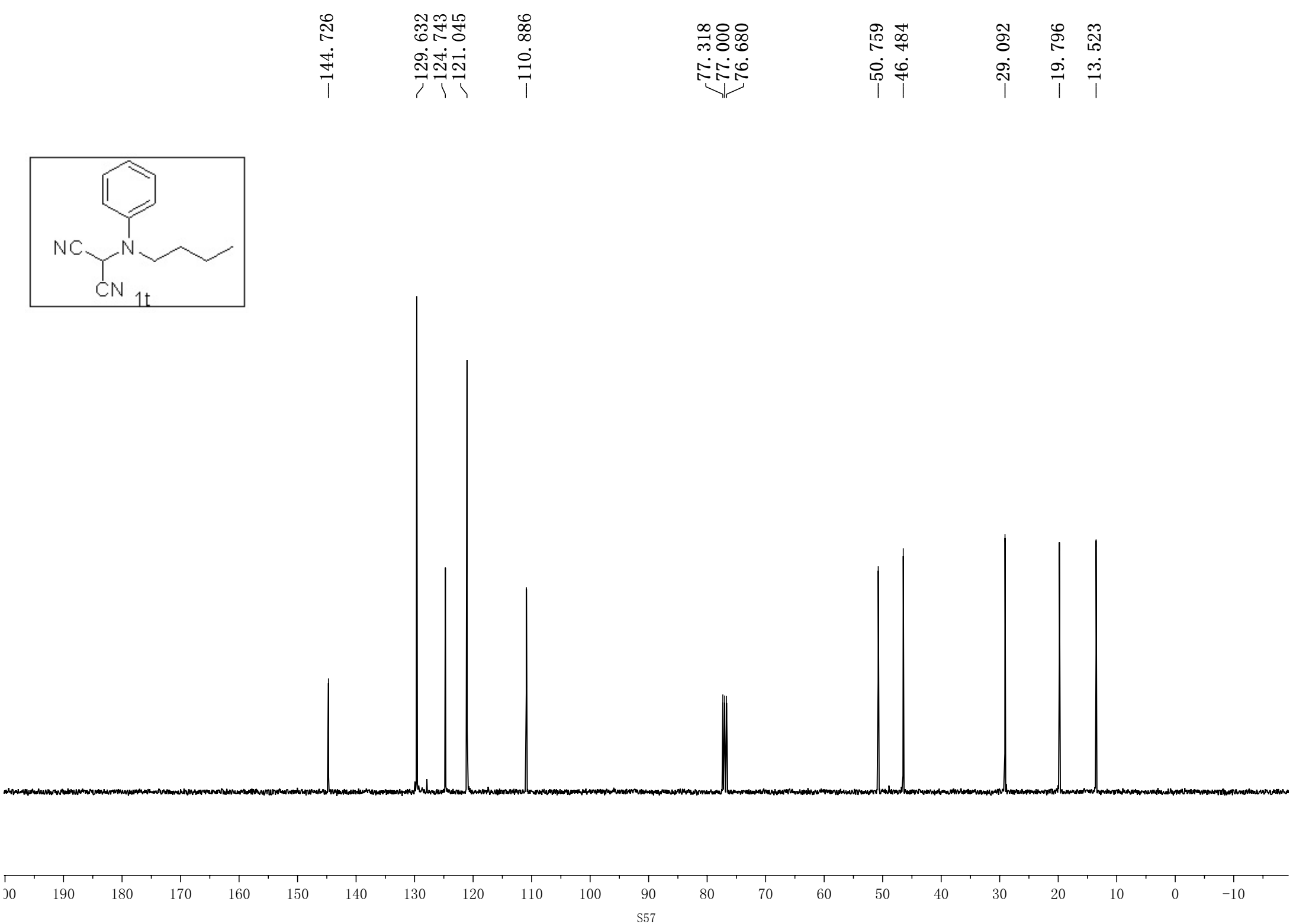
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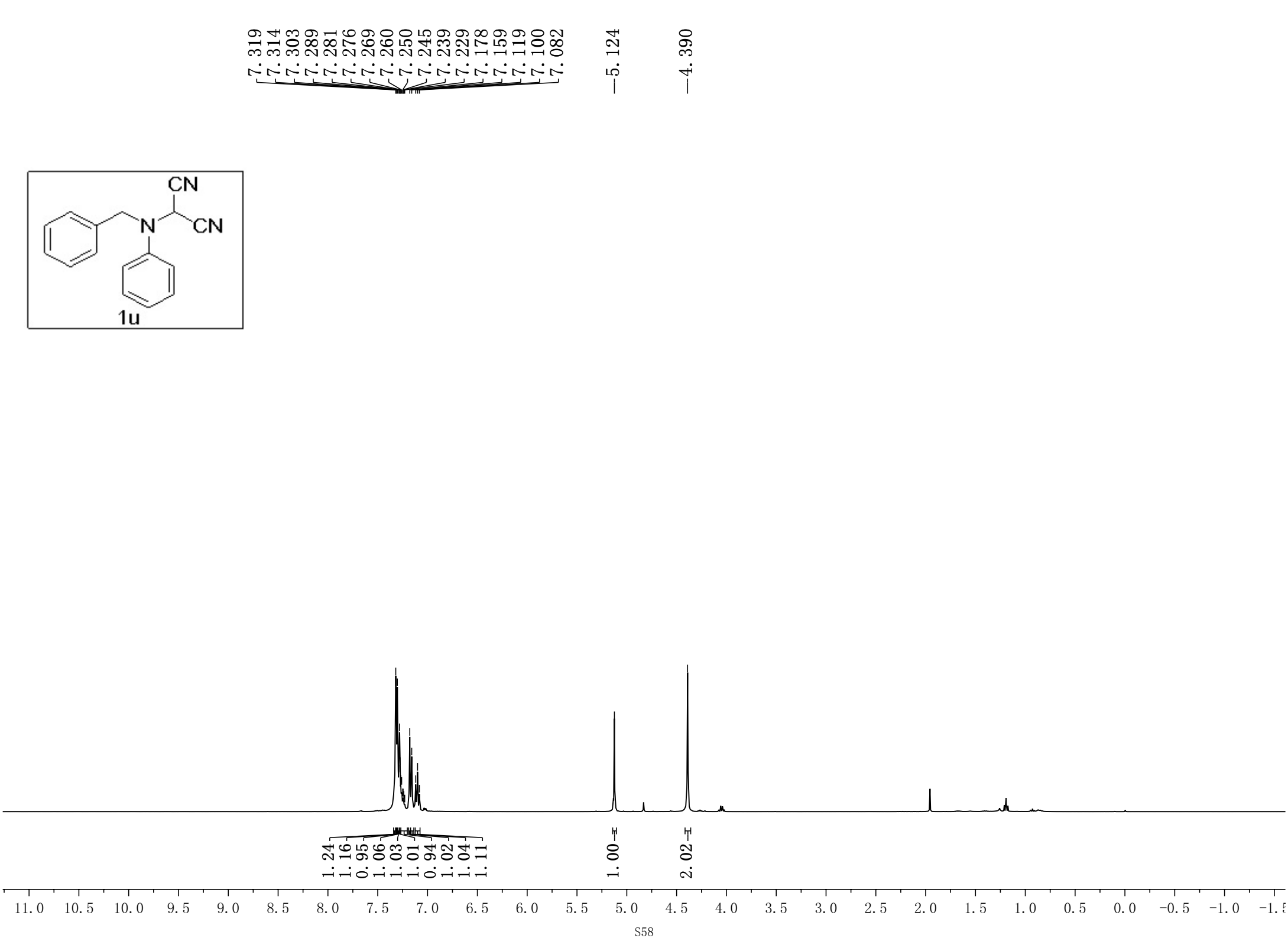
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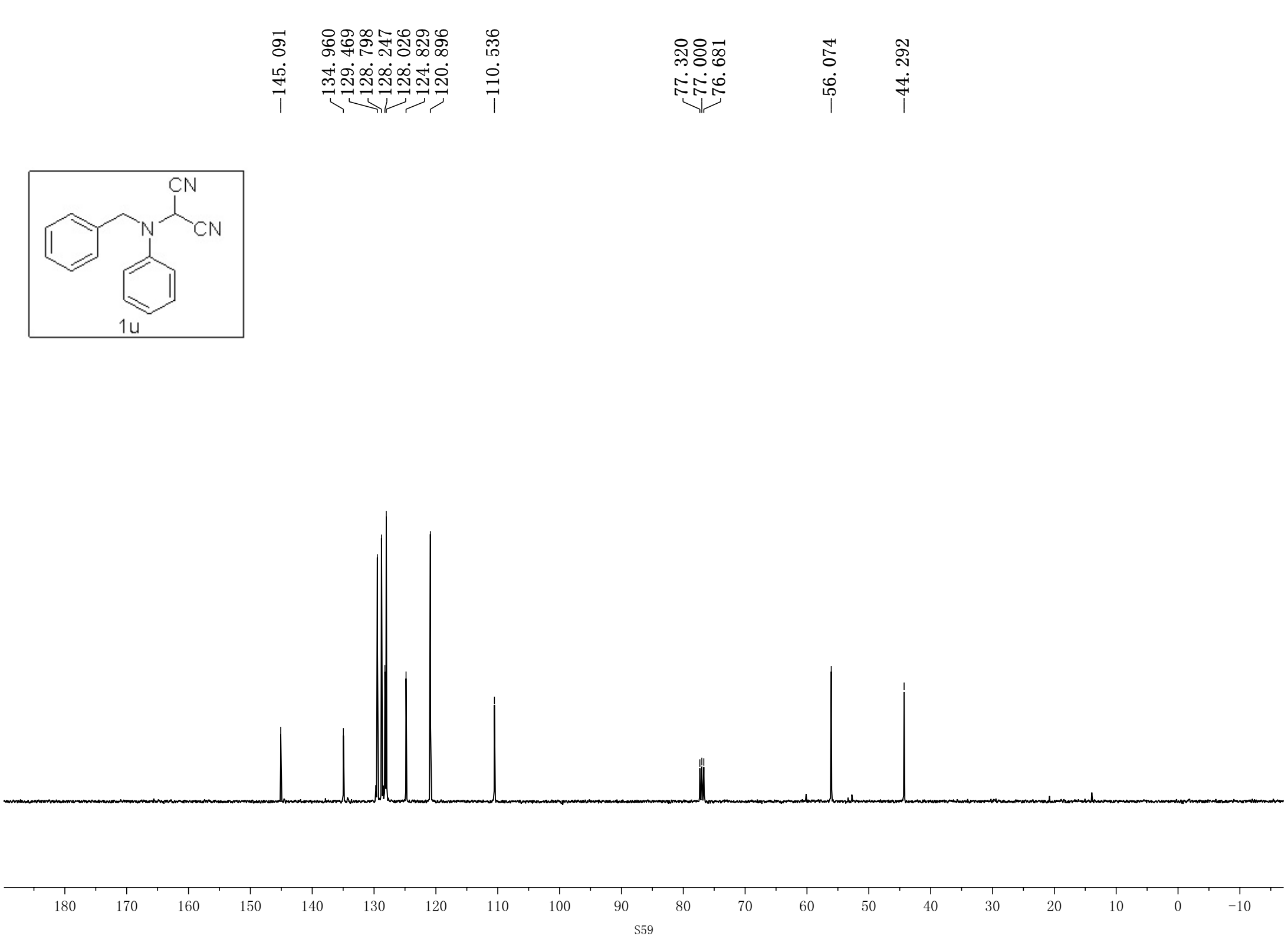
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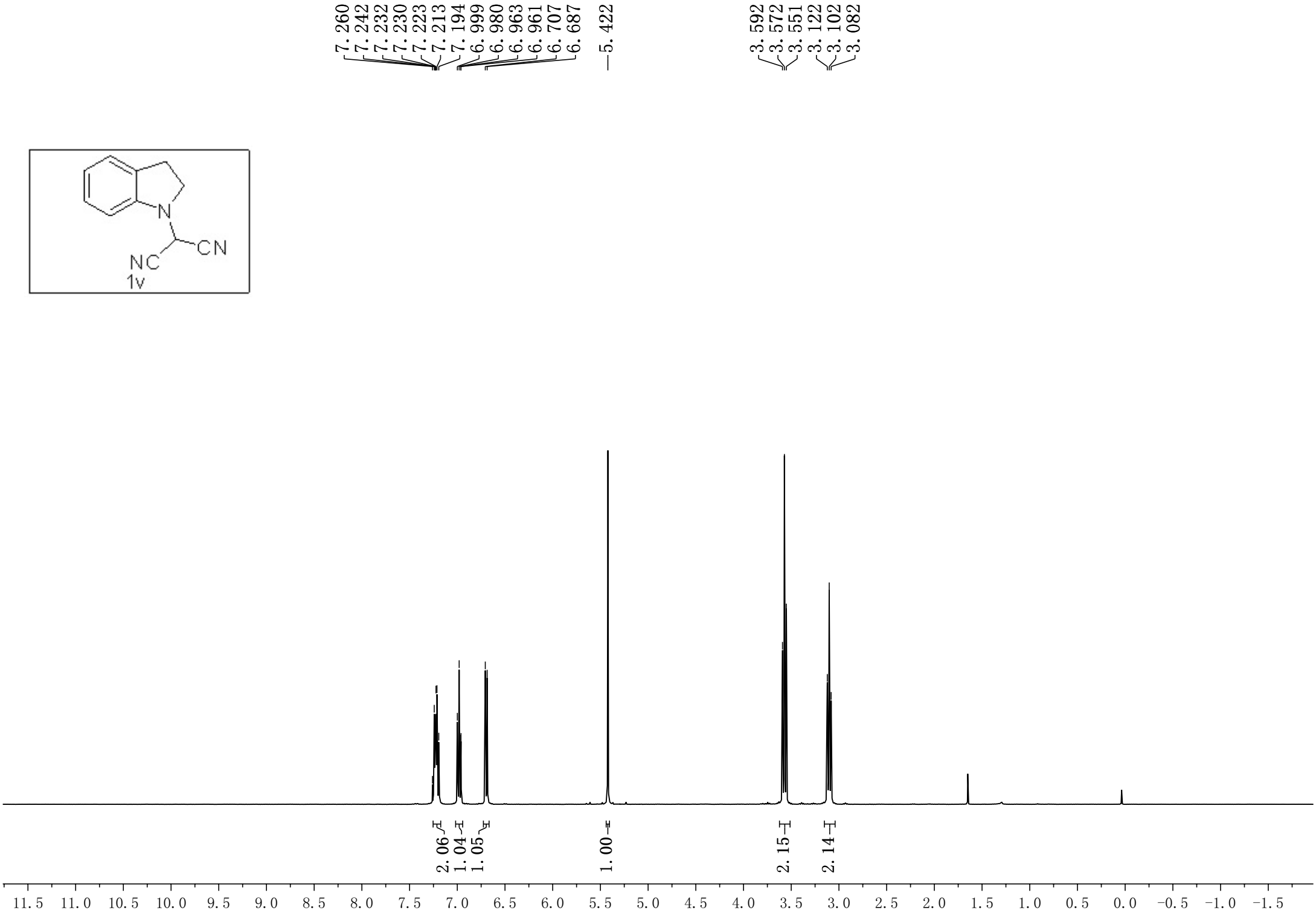
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3.572
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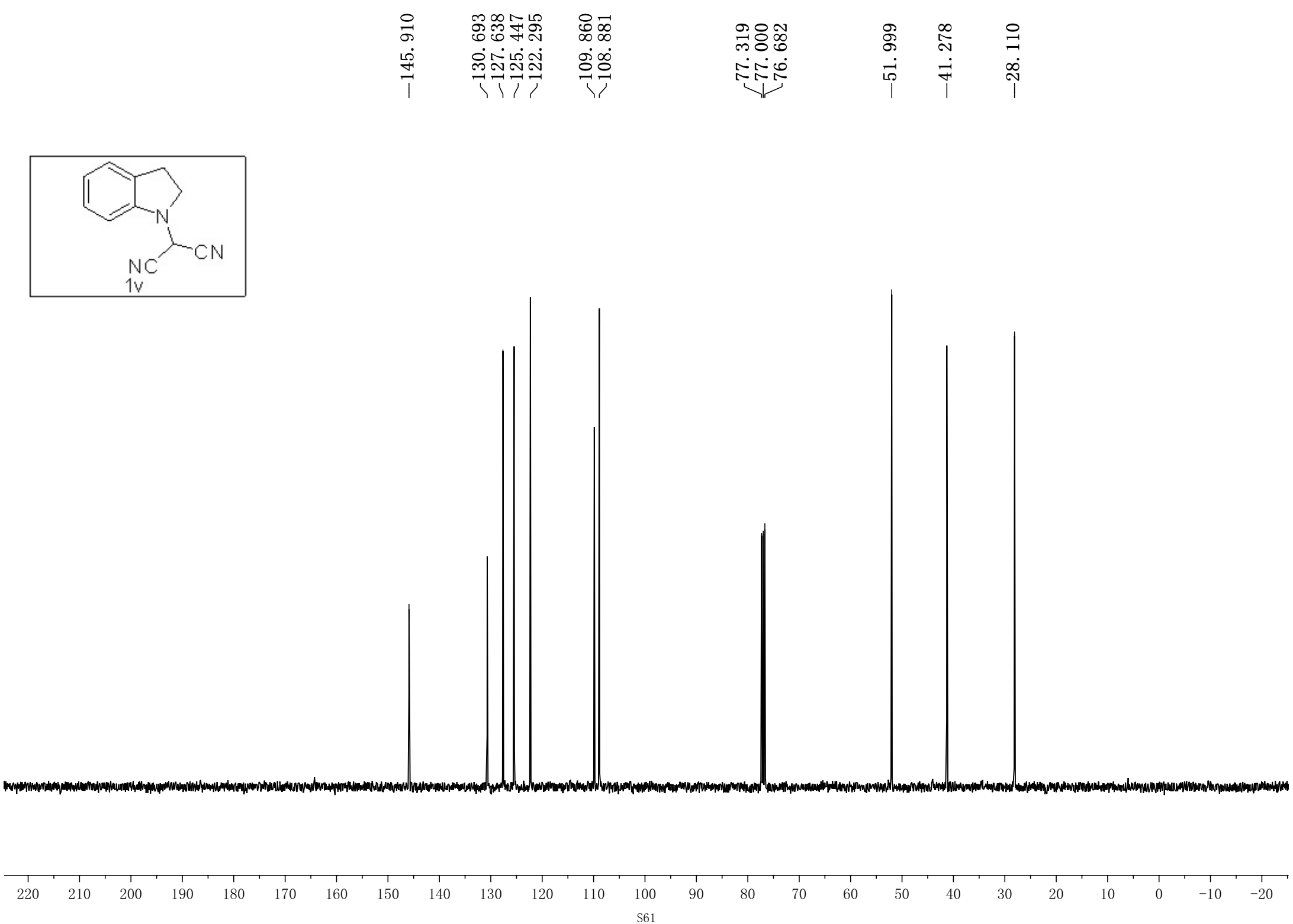
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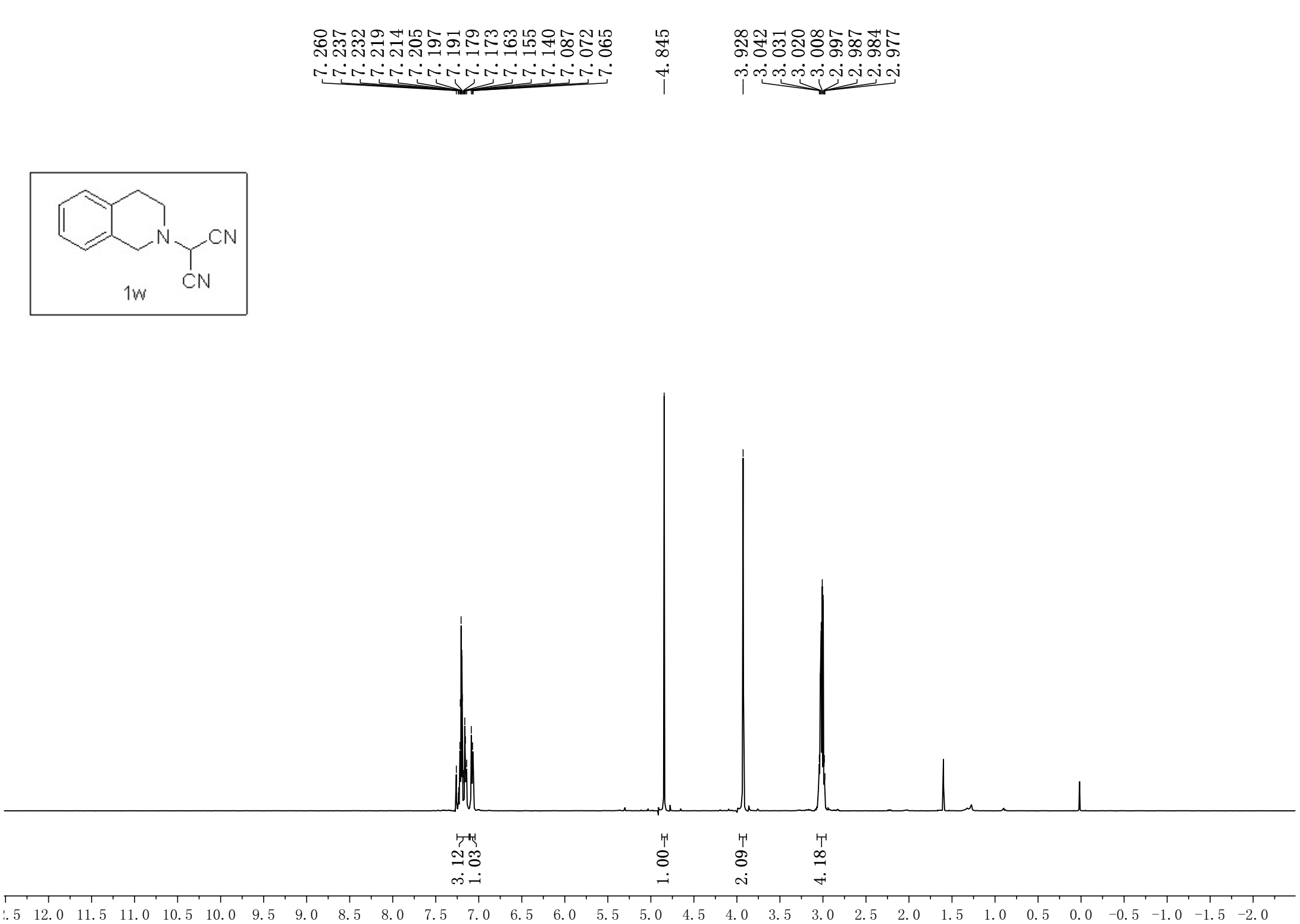
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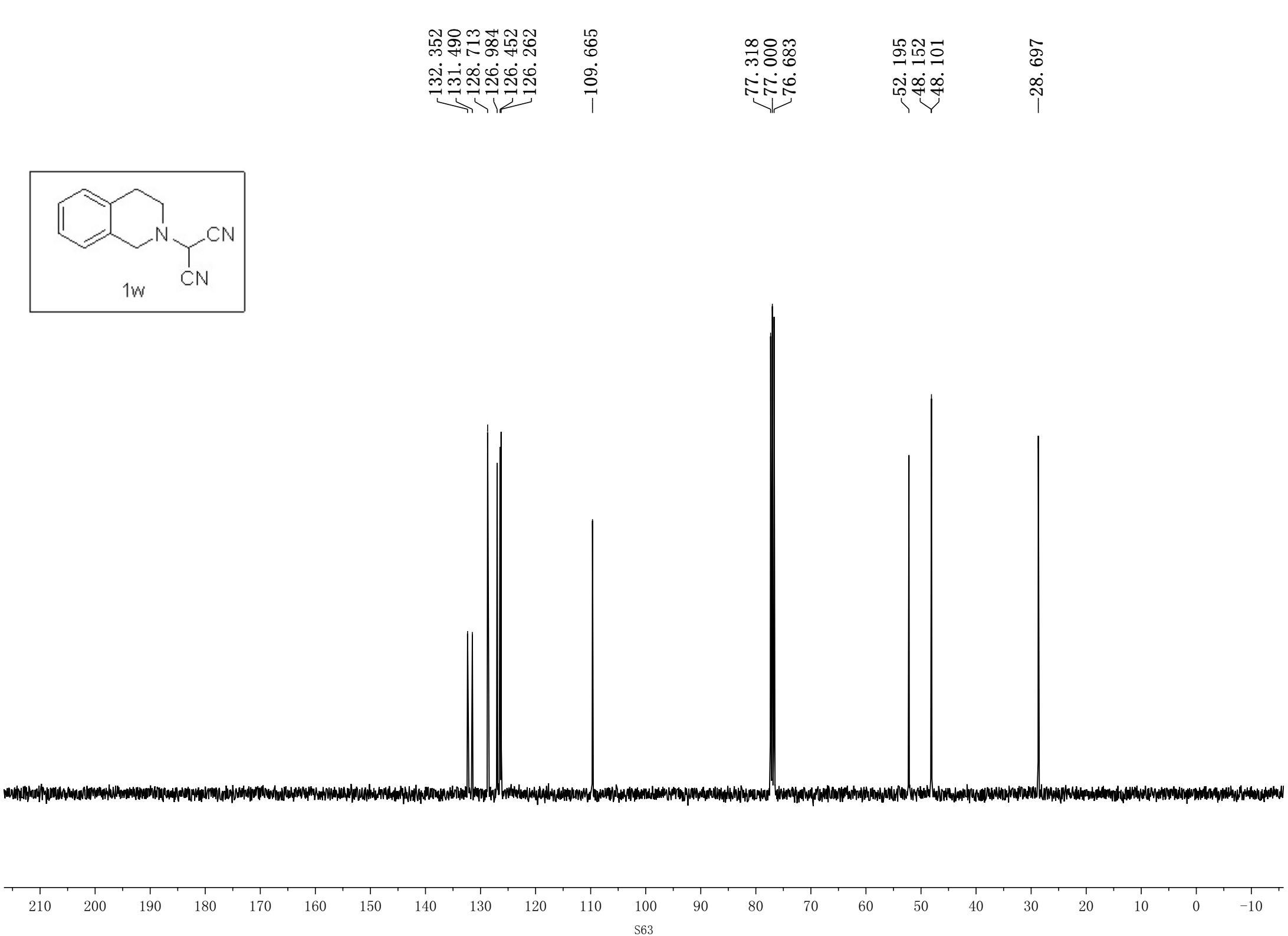
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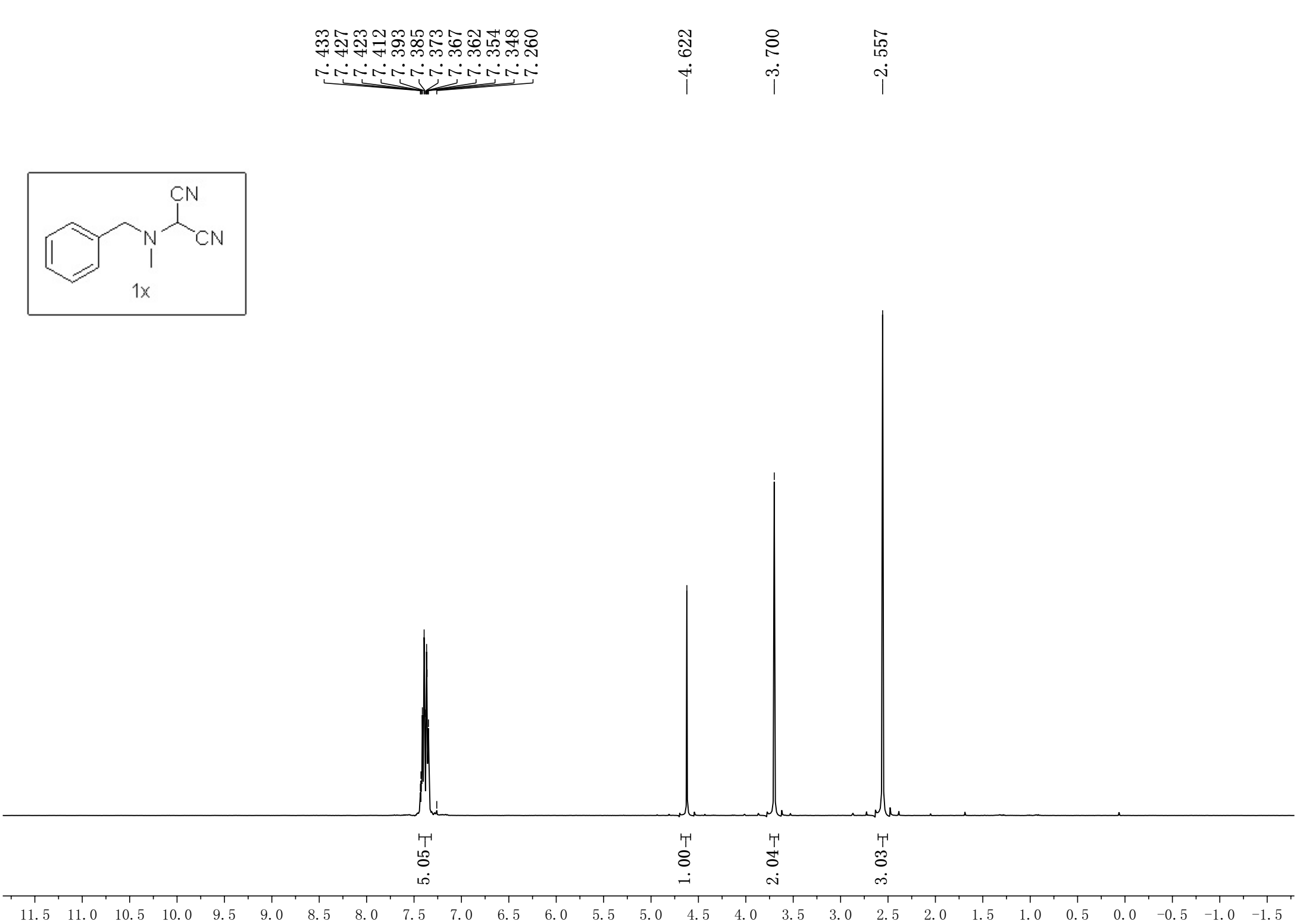
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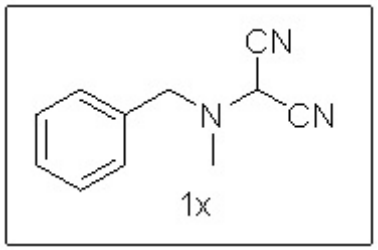

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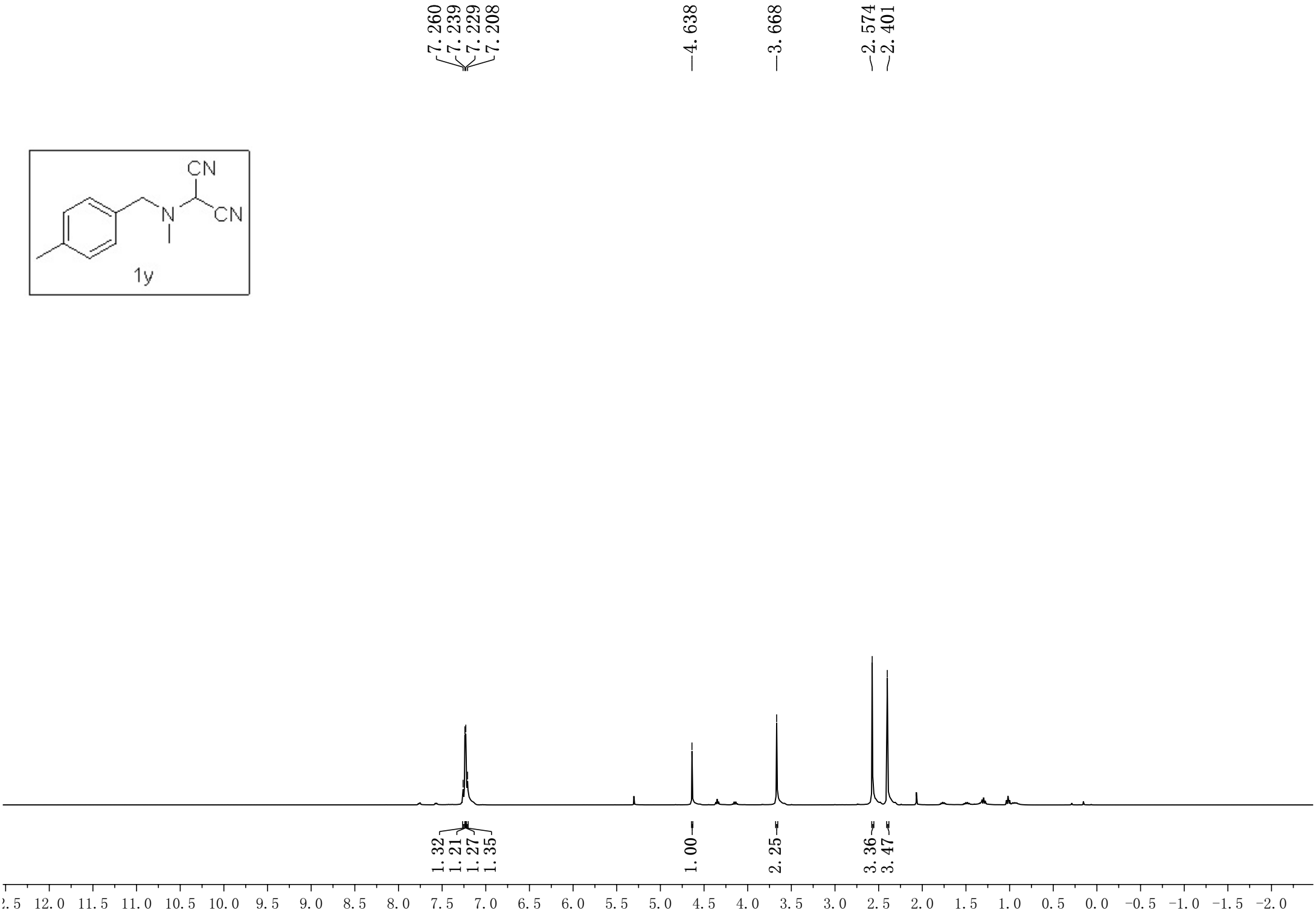
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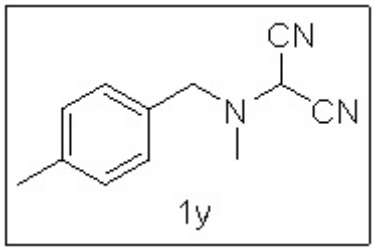

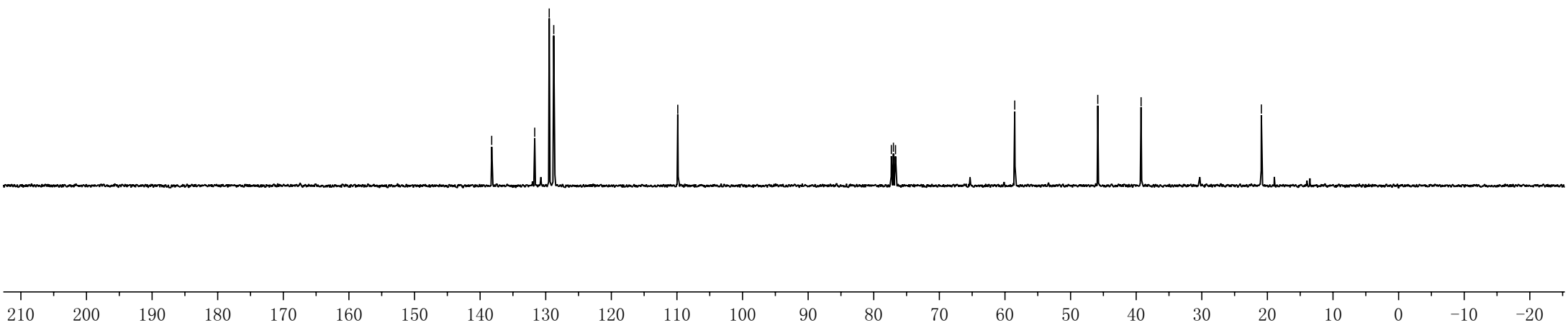

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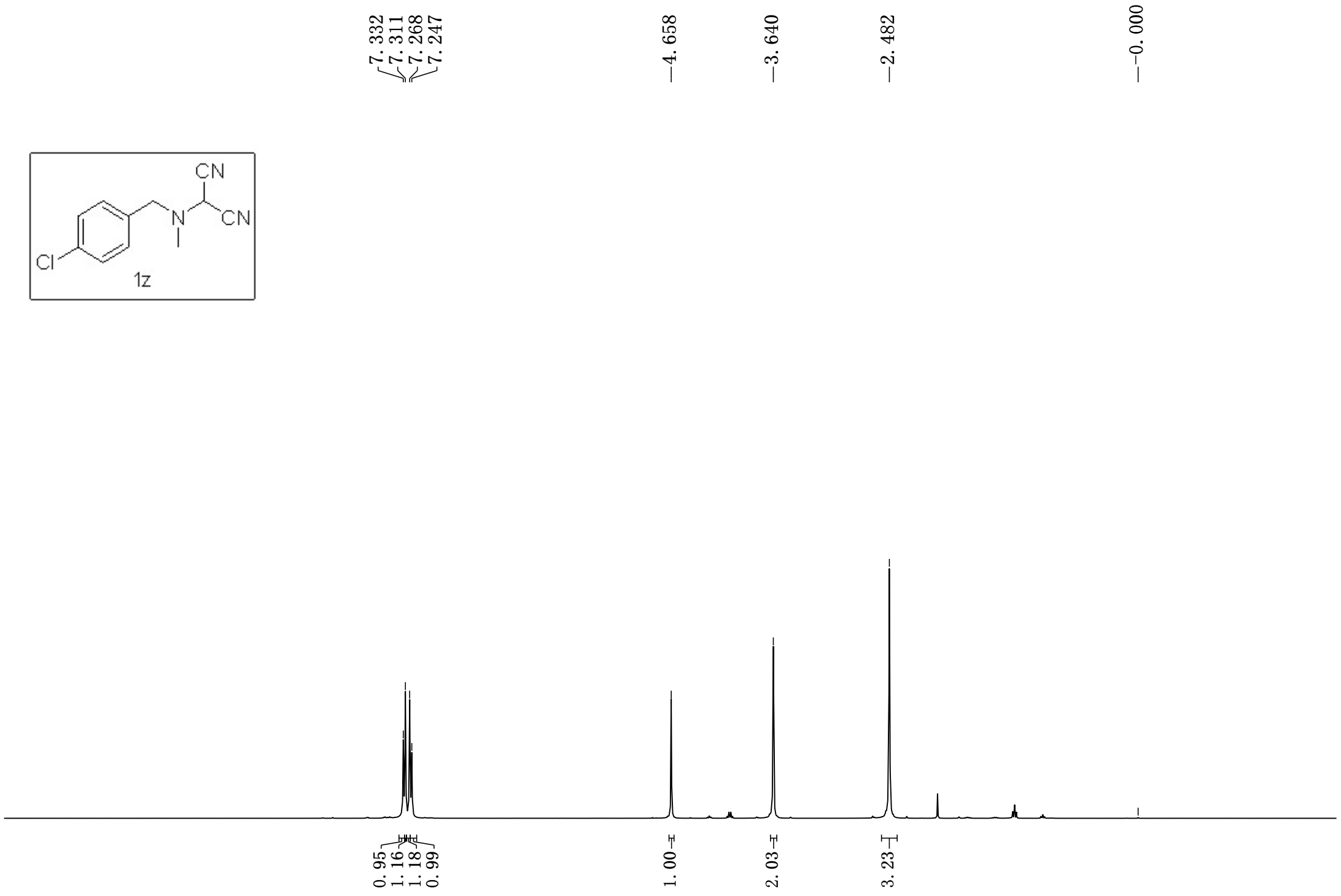
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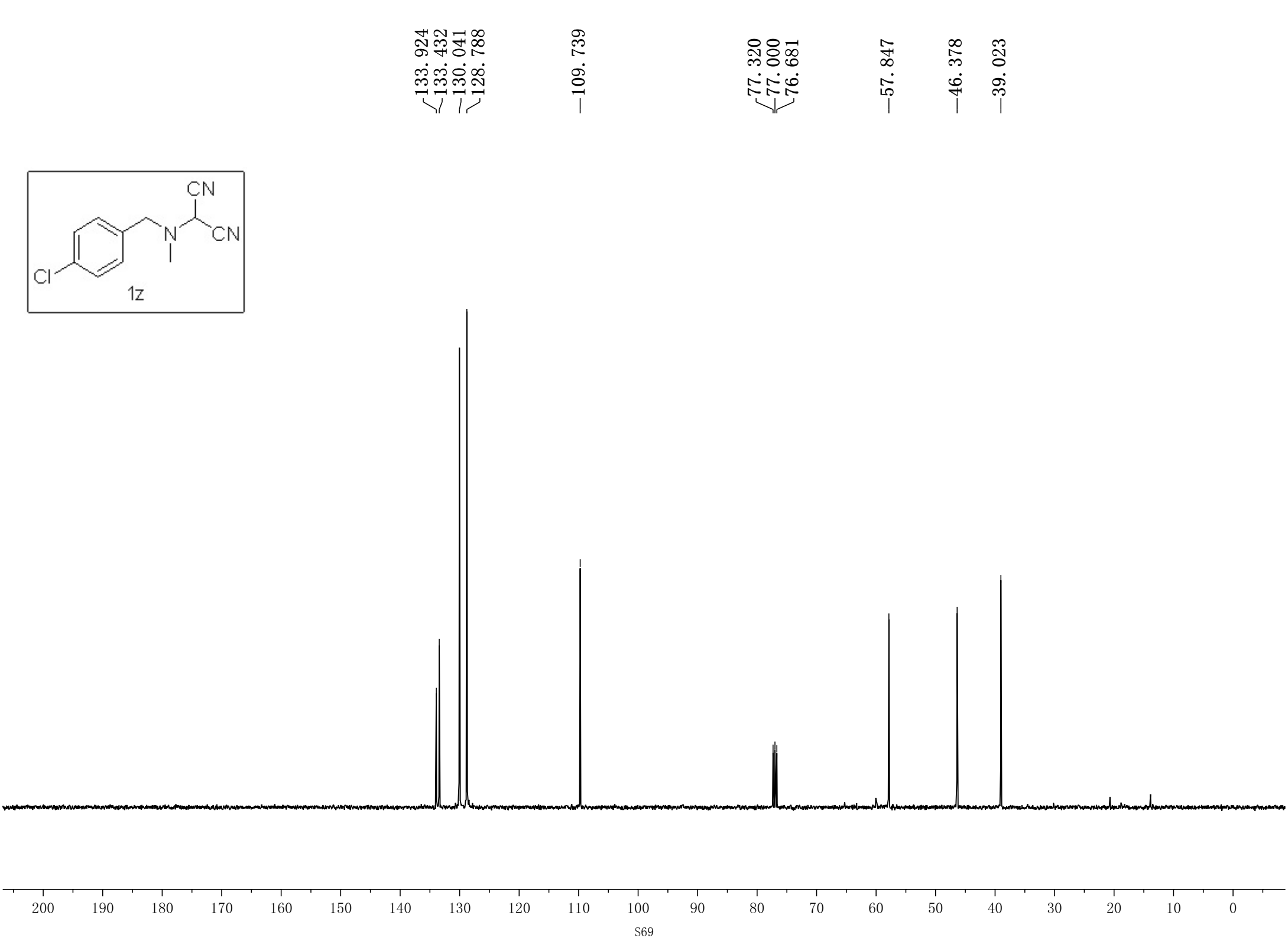
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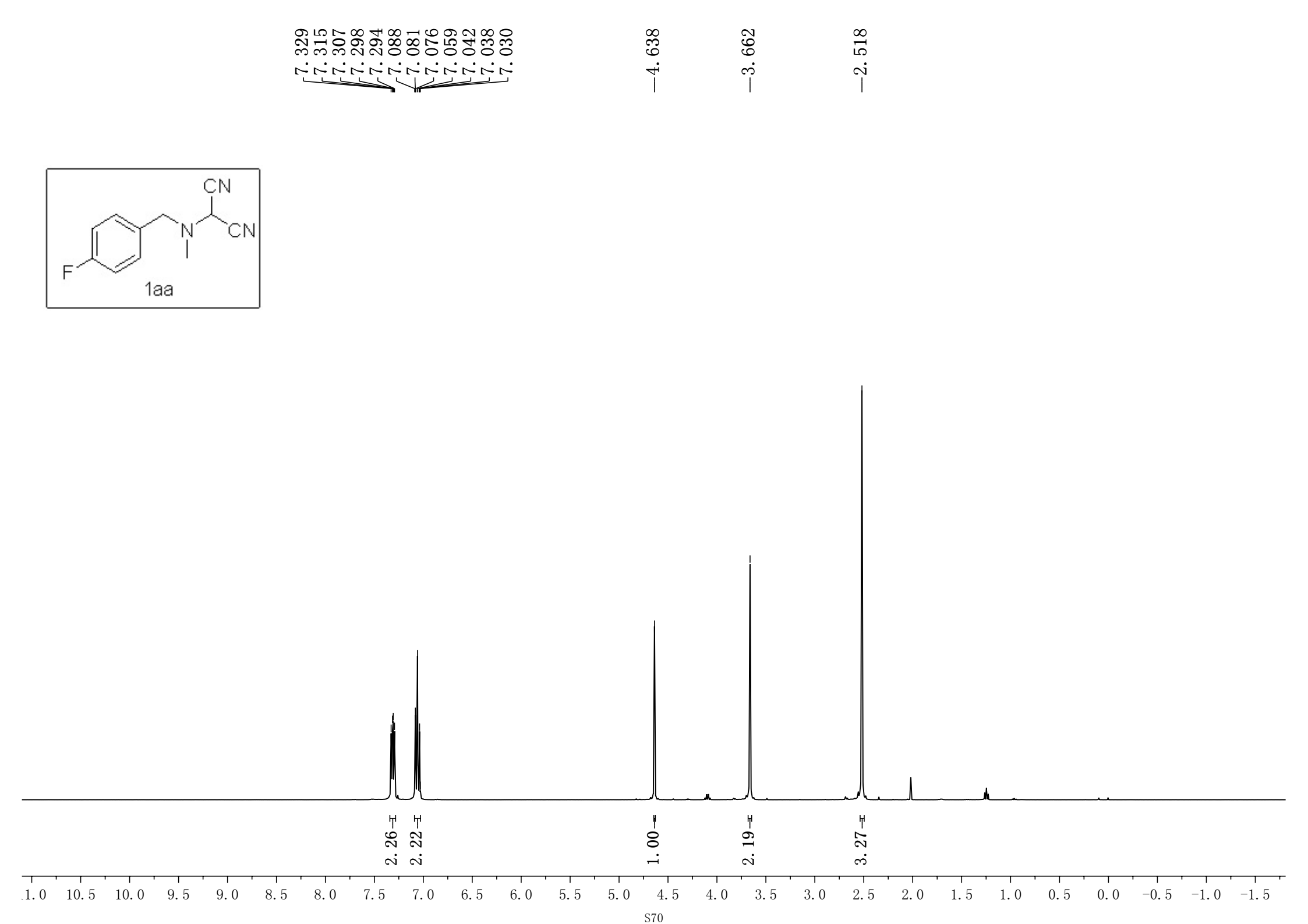
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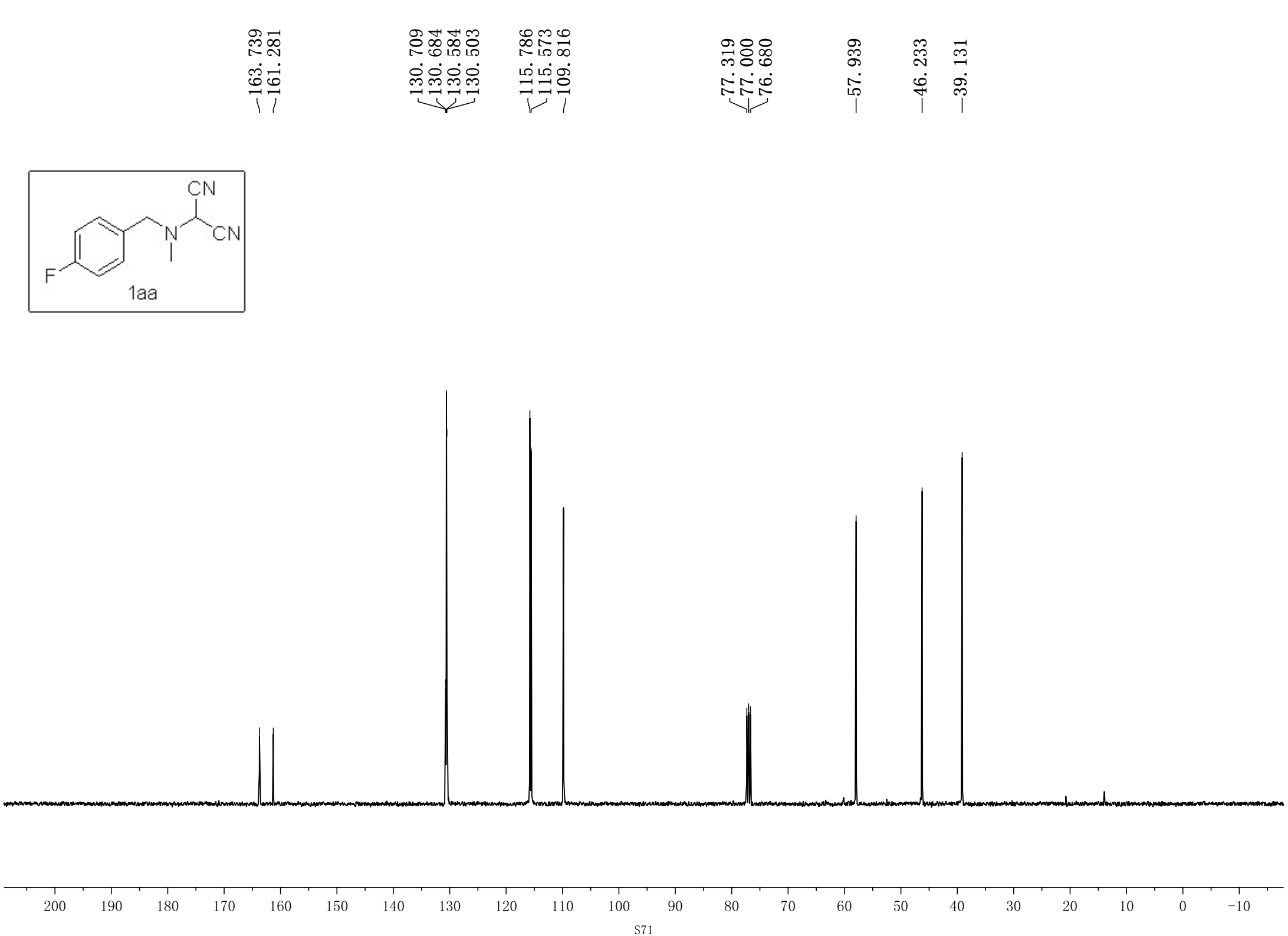
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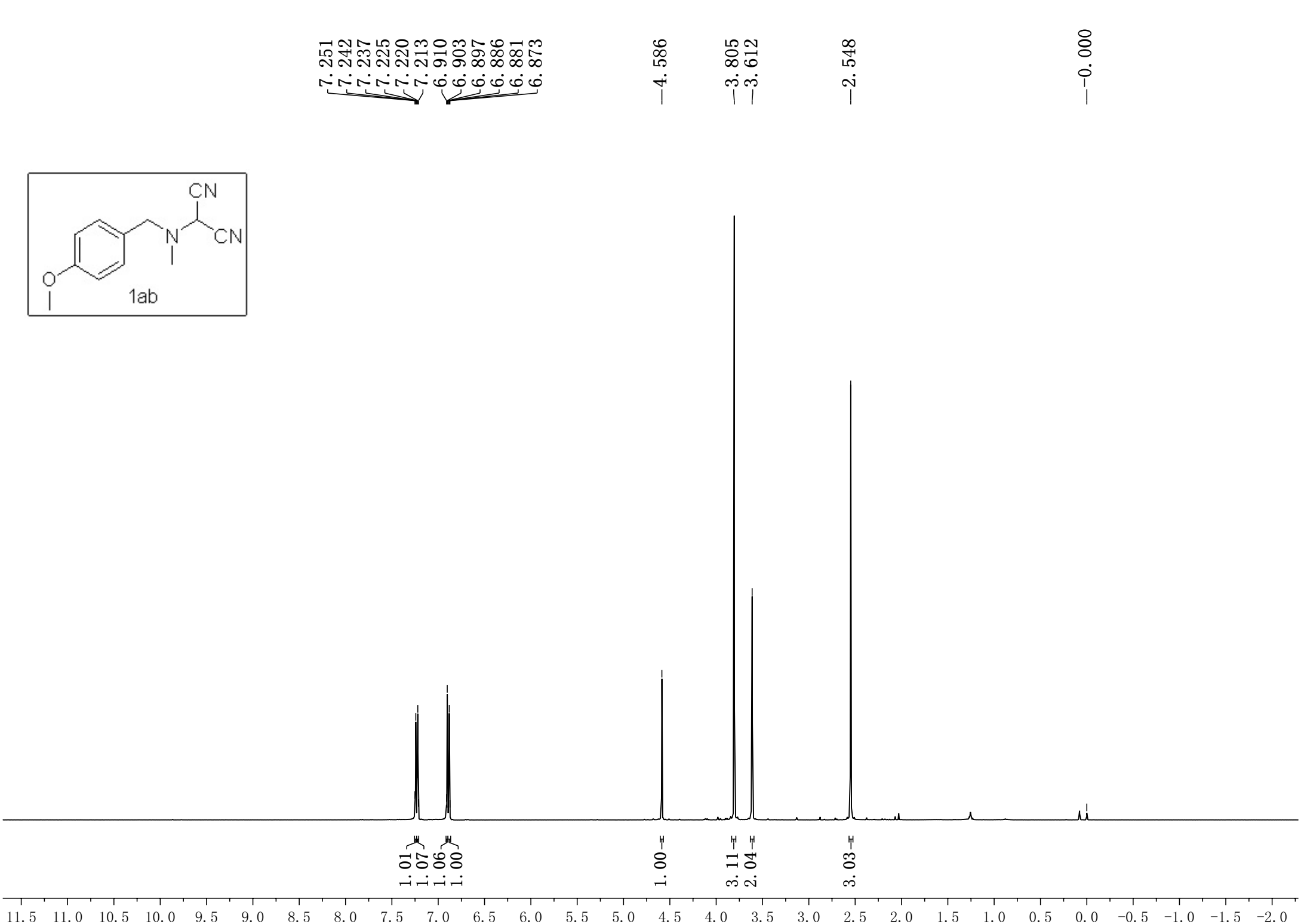
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2.04
3.03
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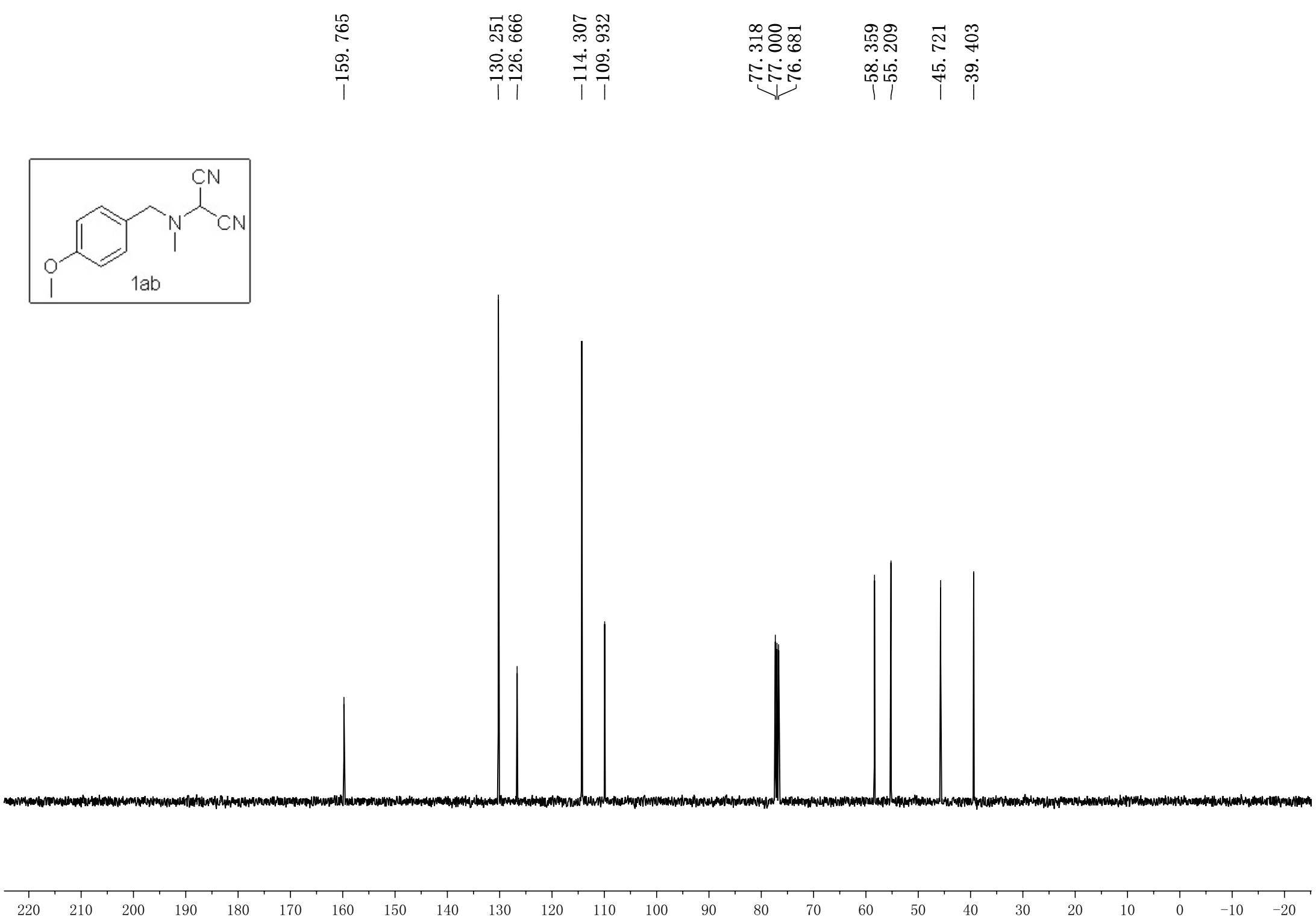
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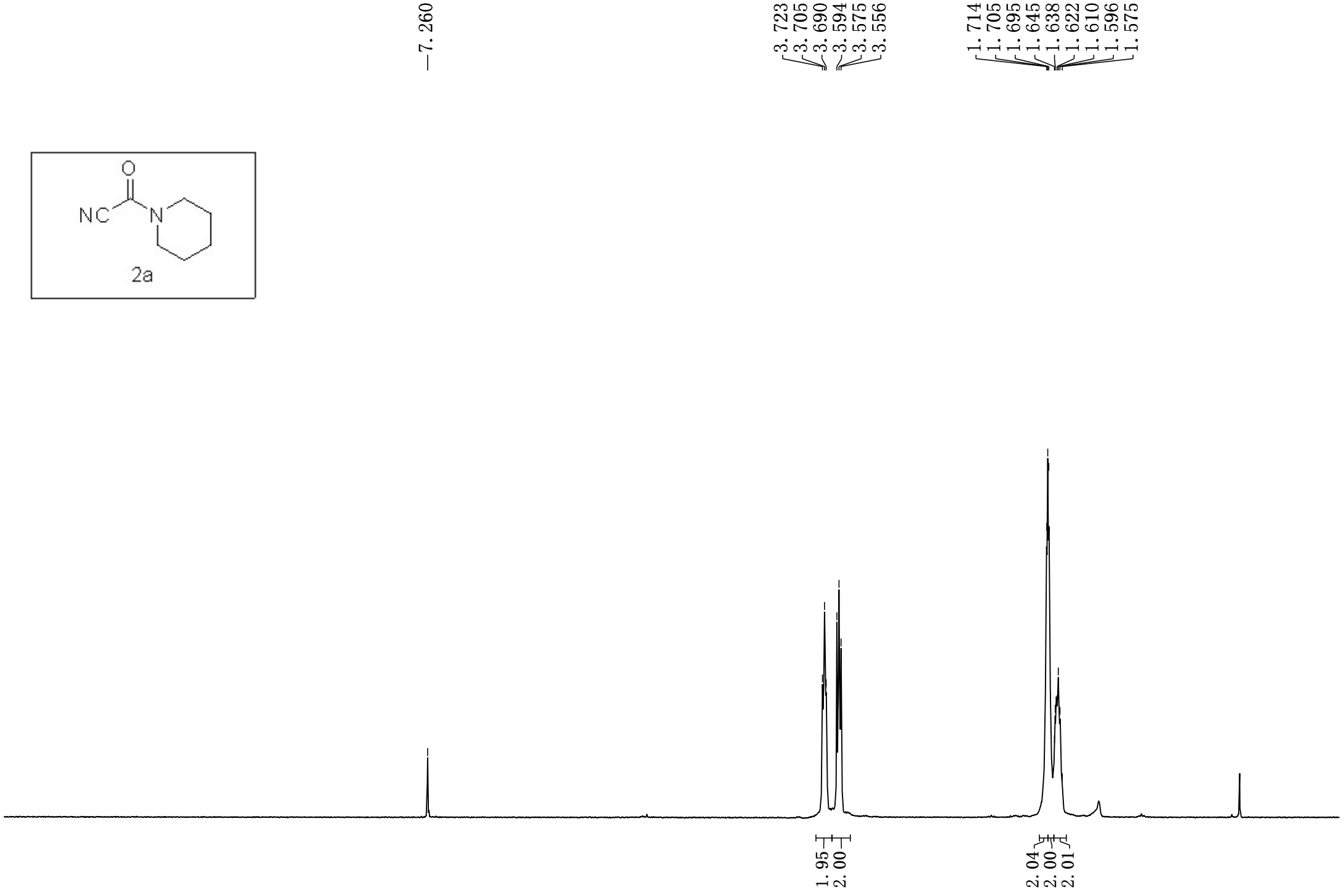
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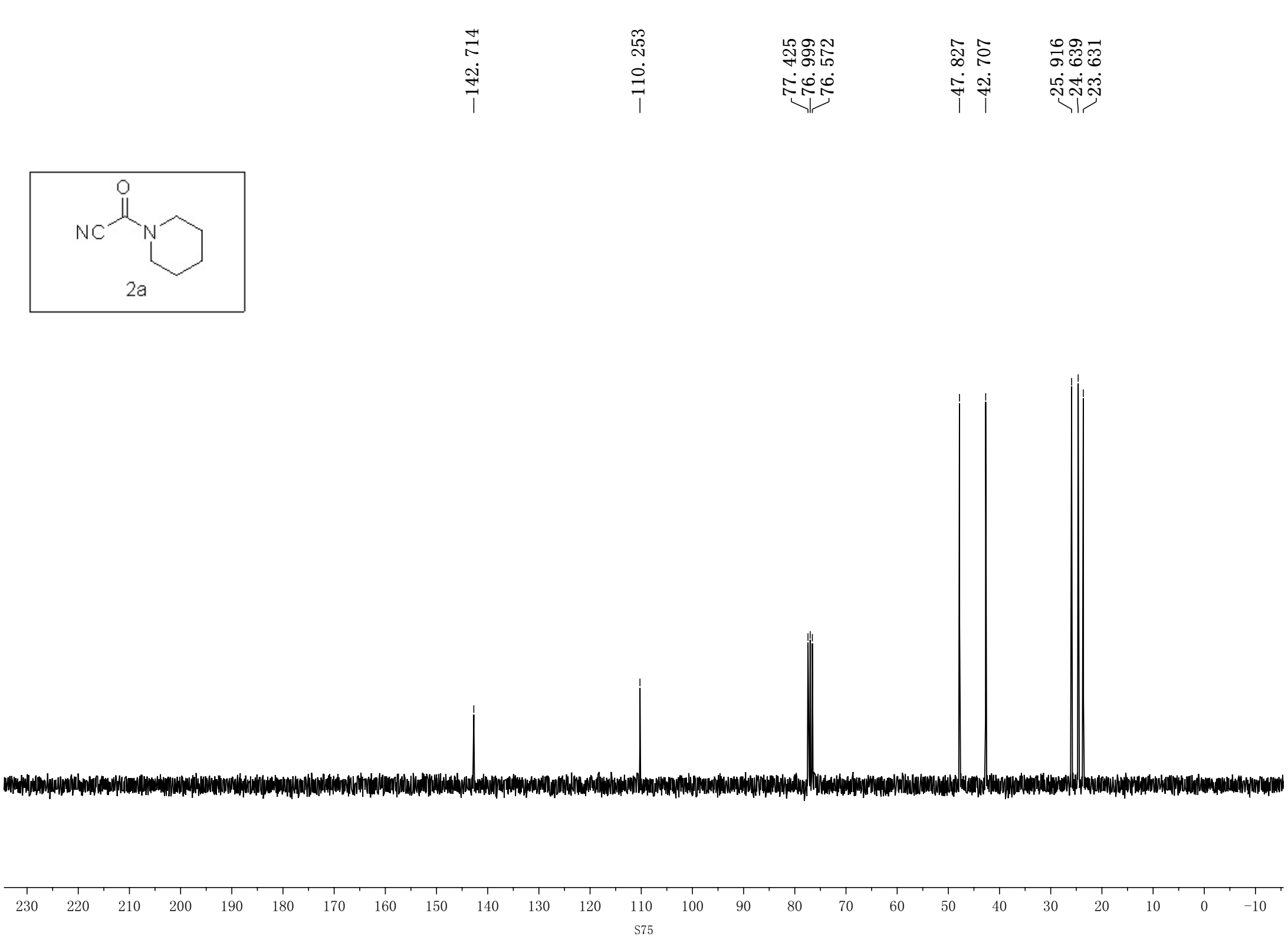
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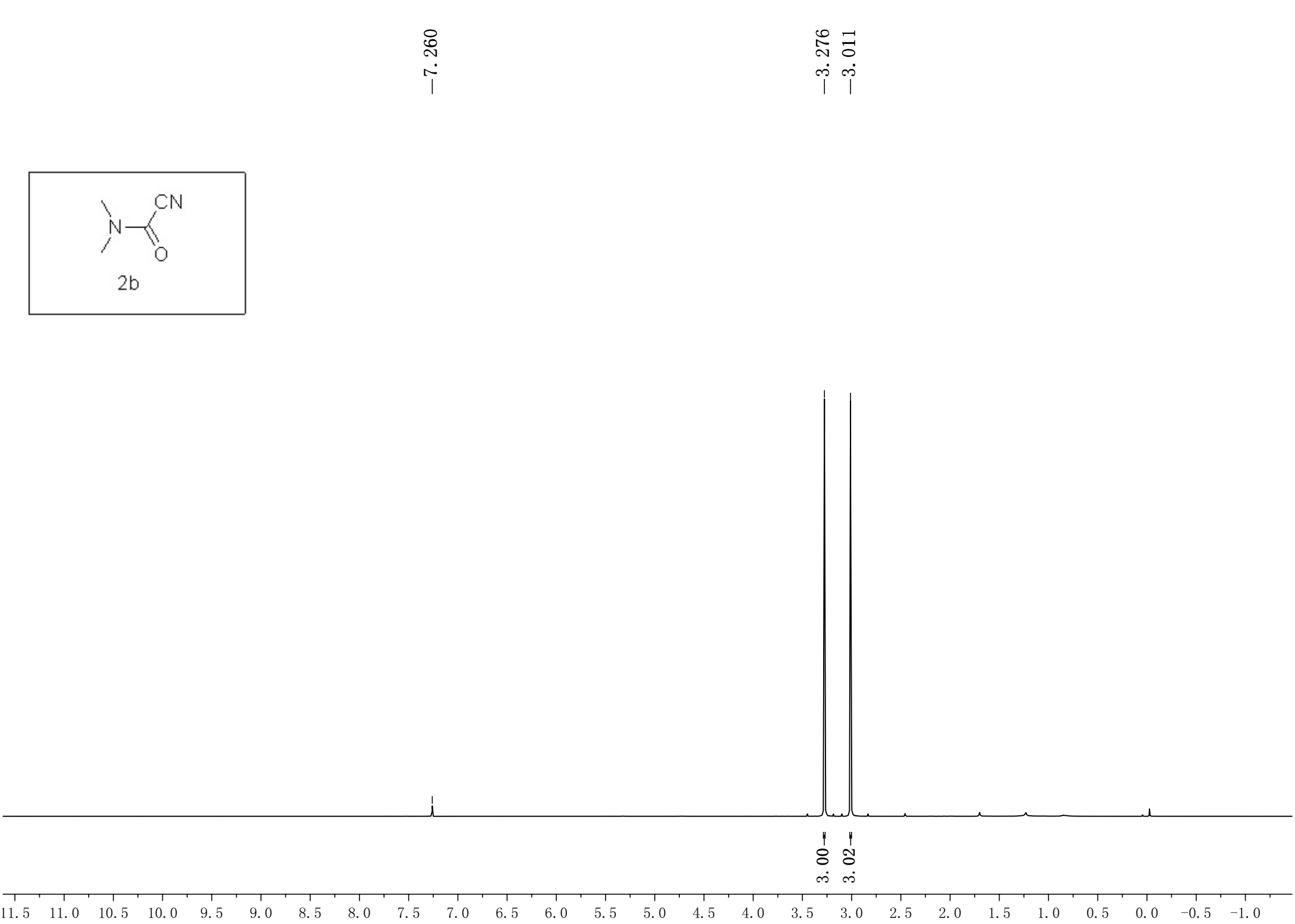
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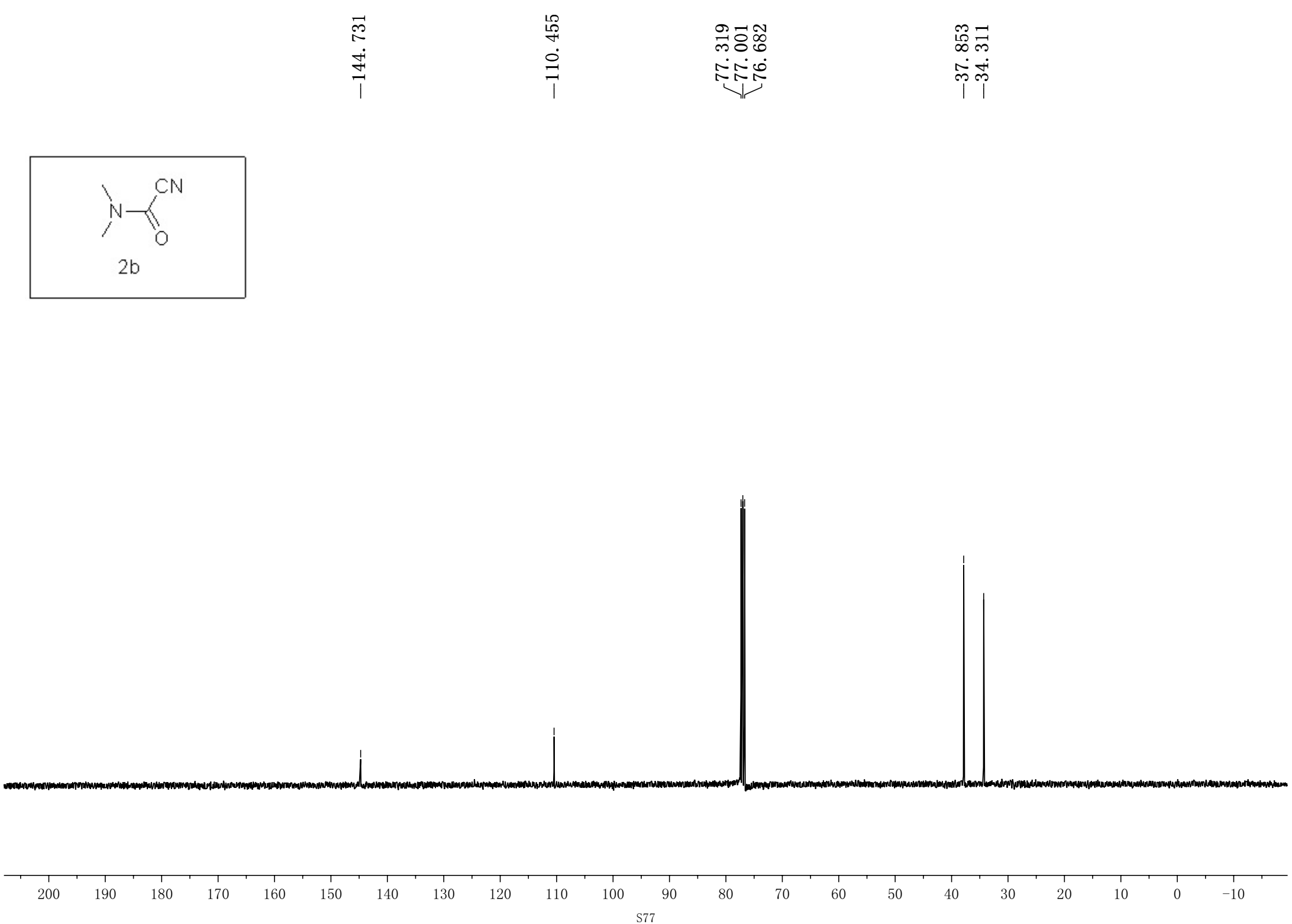
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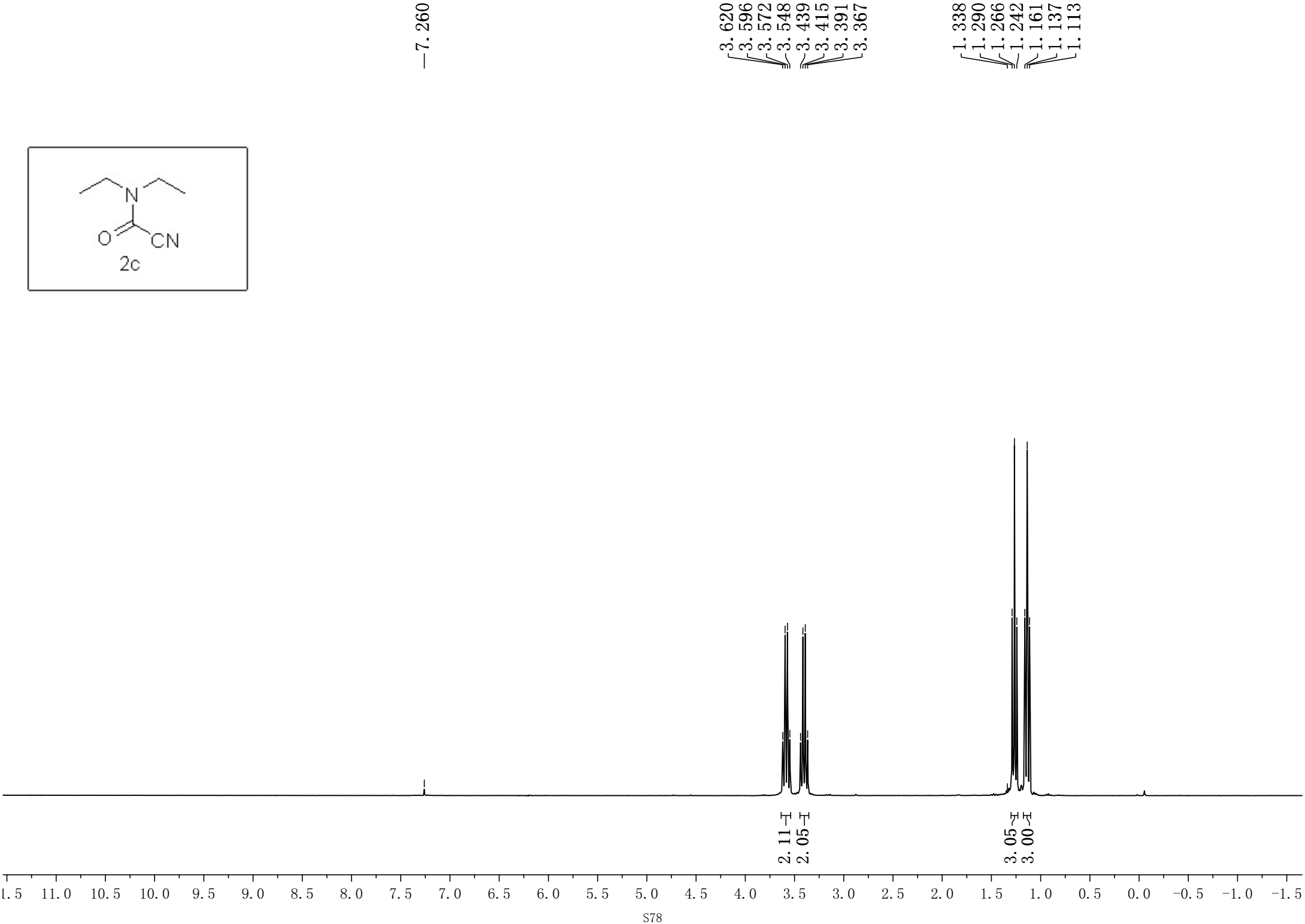
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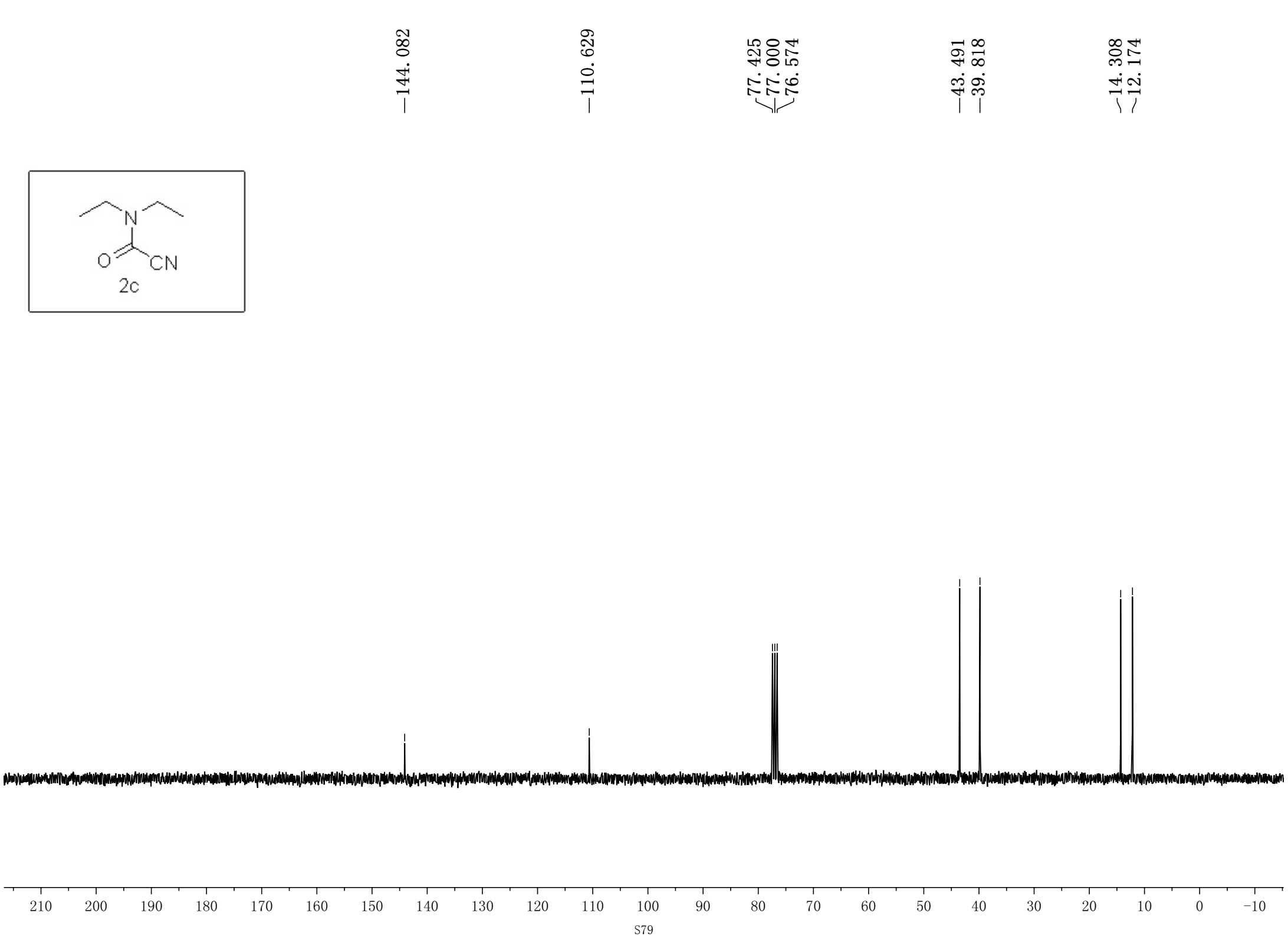
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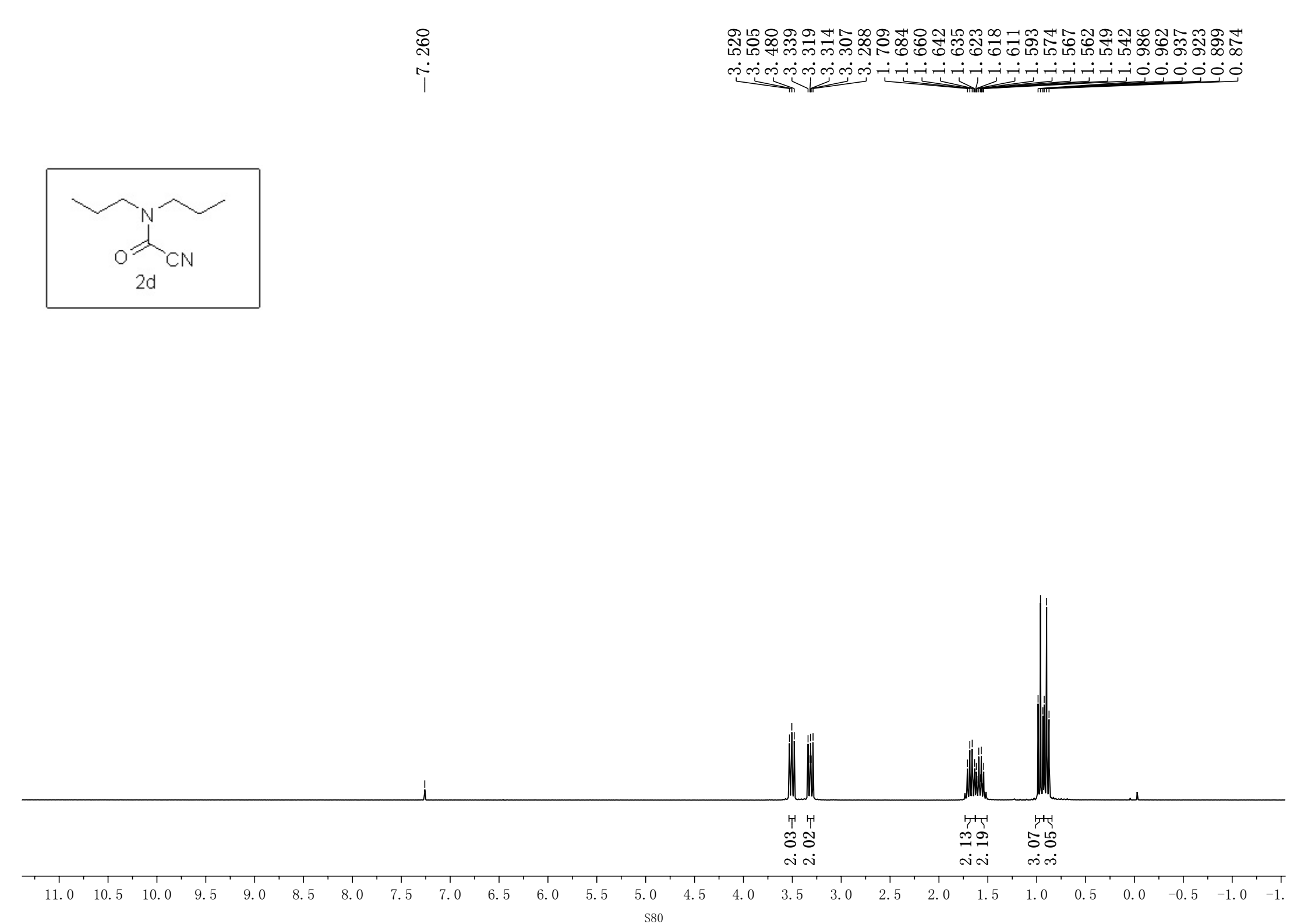
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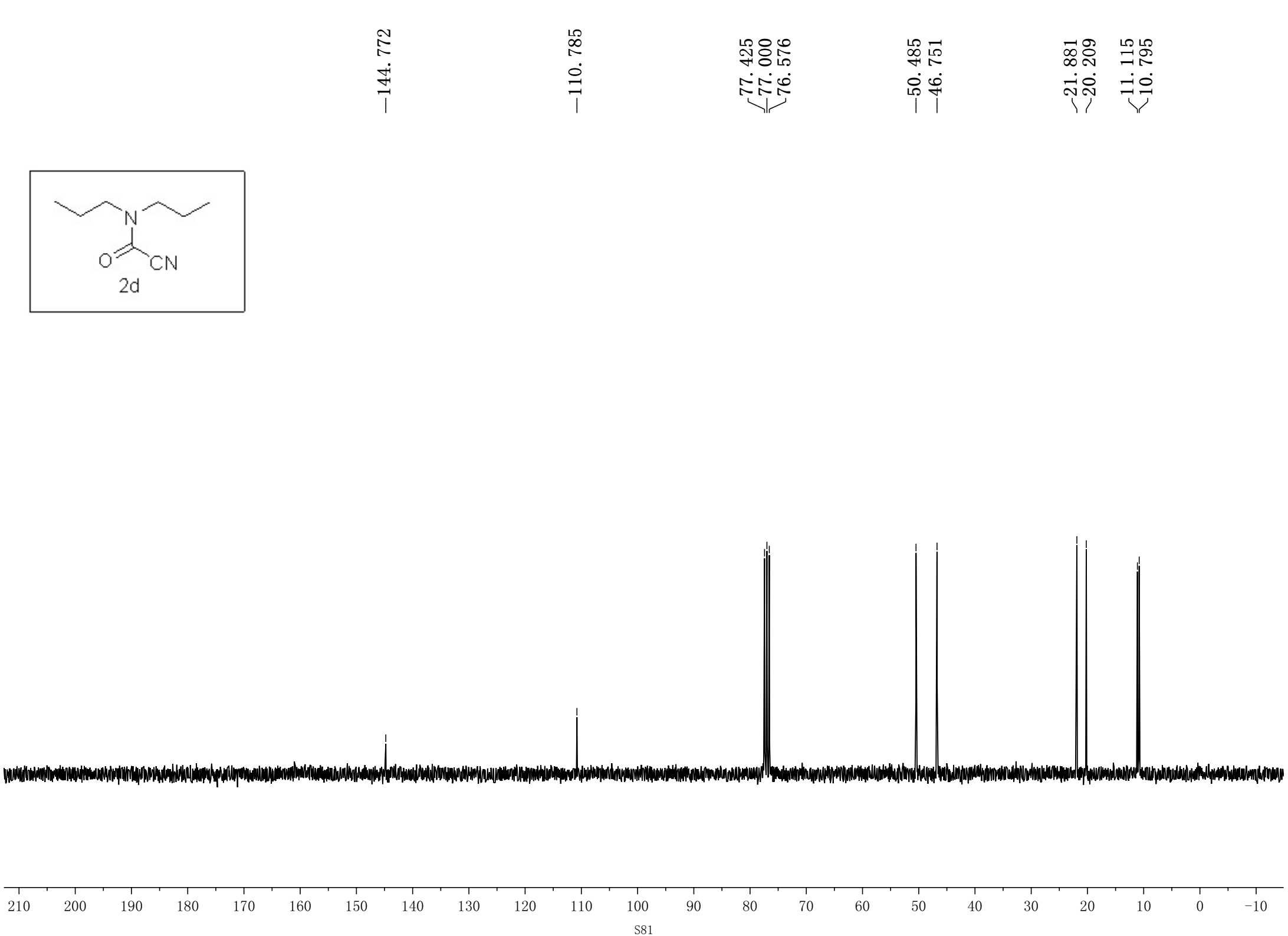
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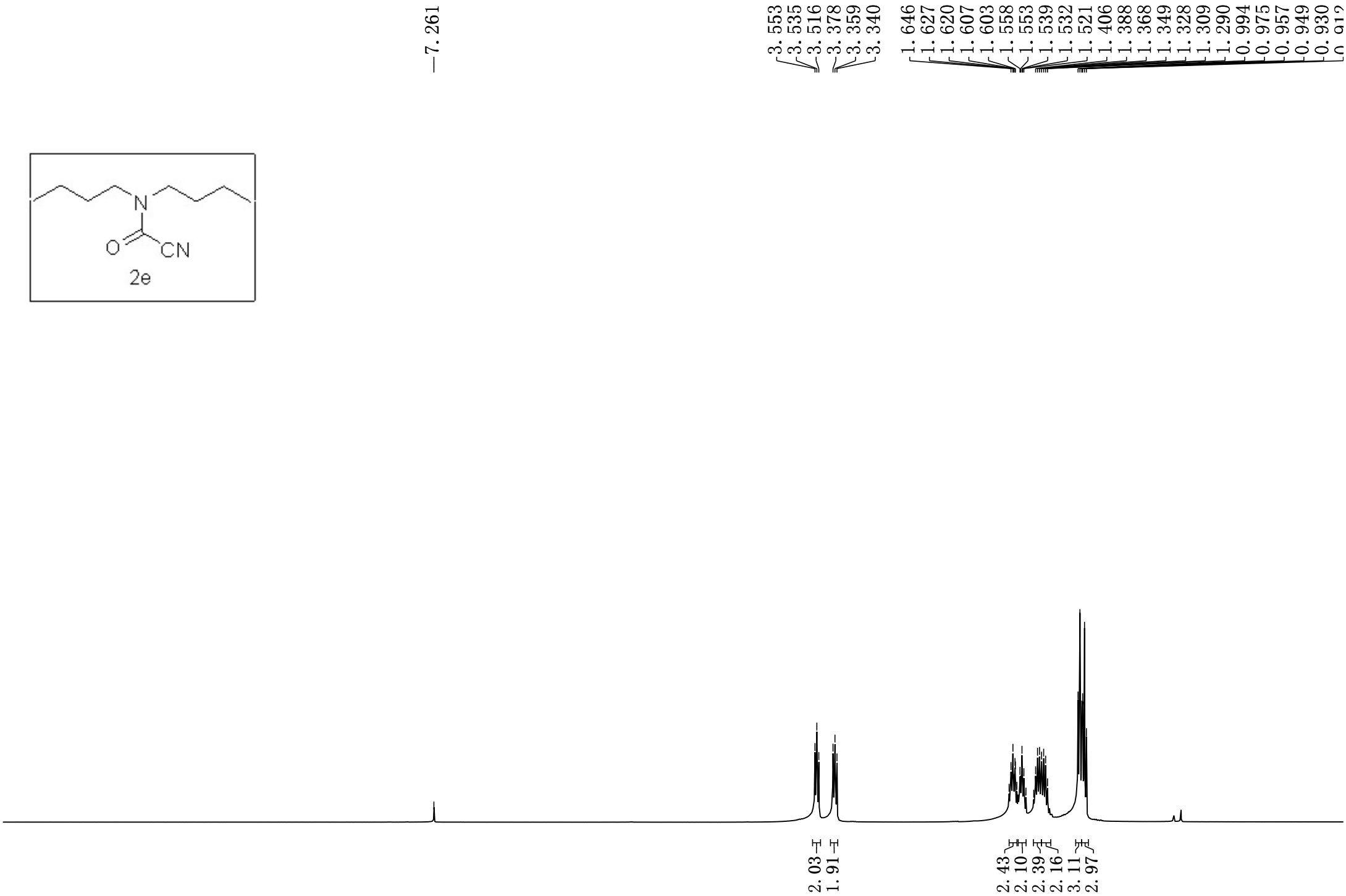
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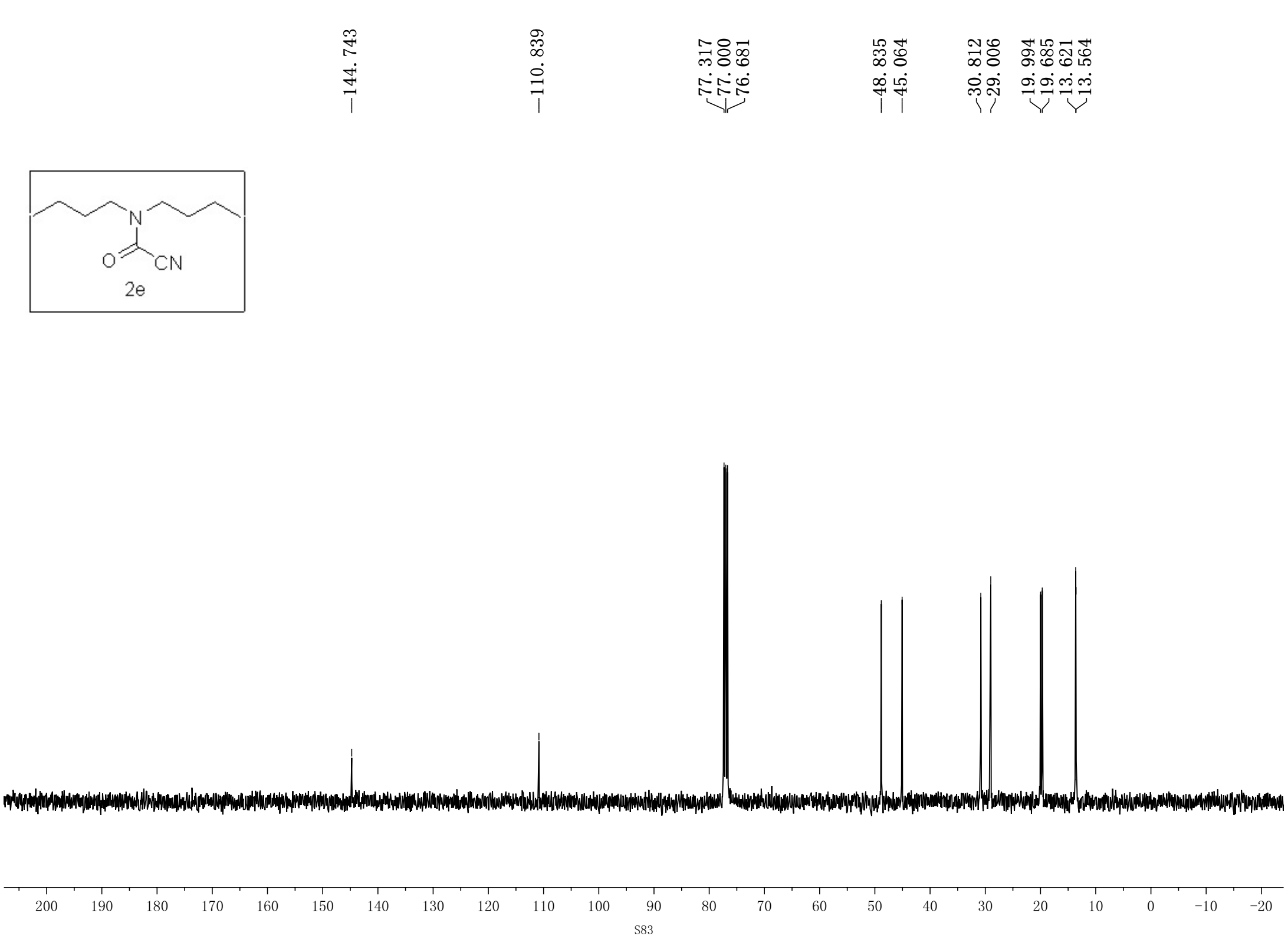
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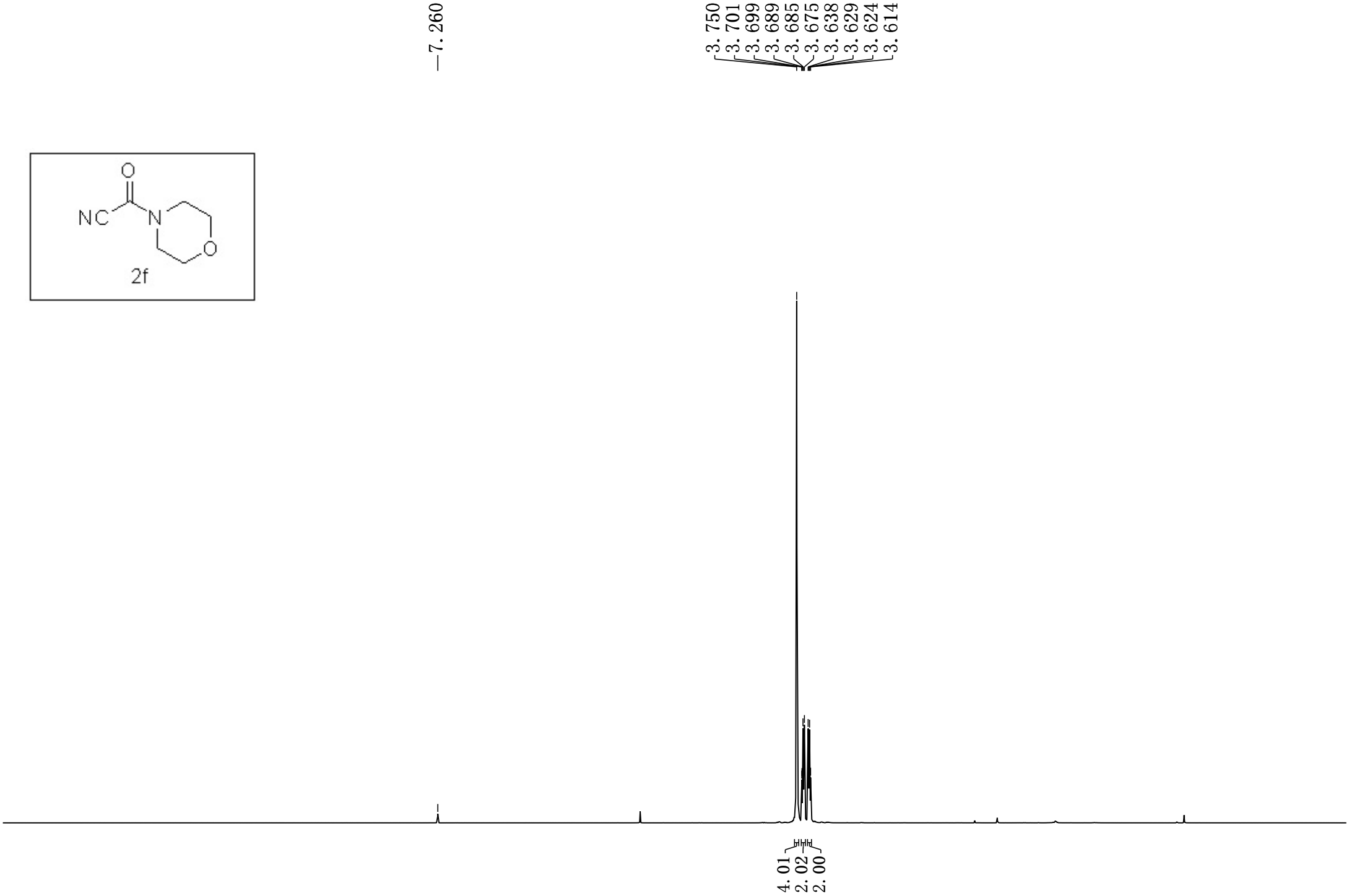
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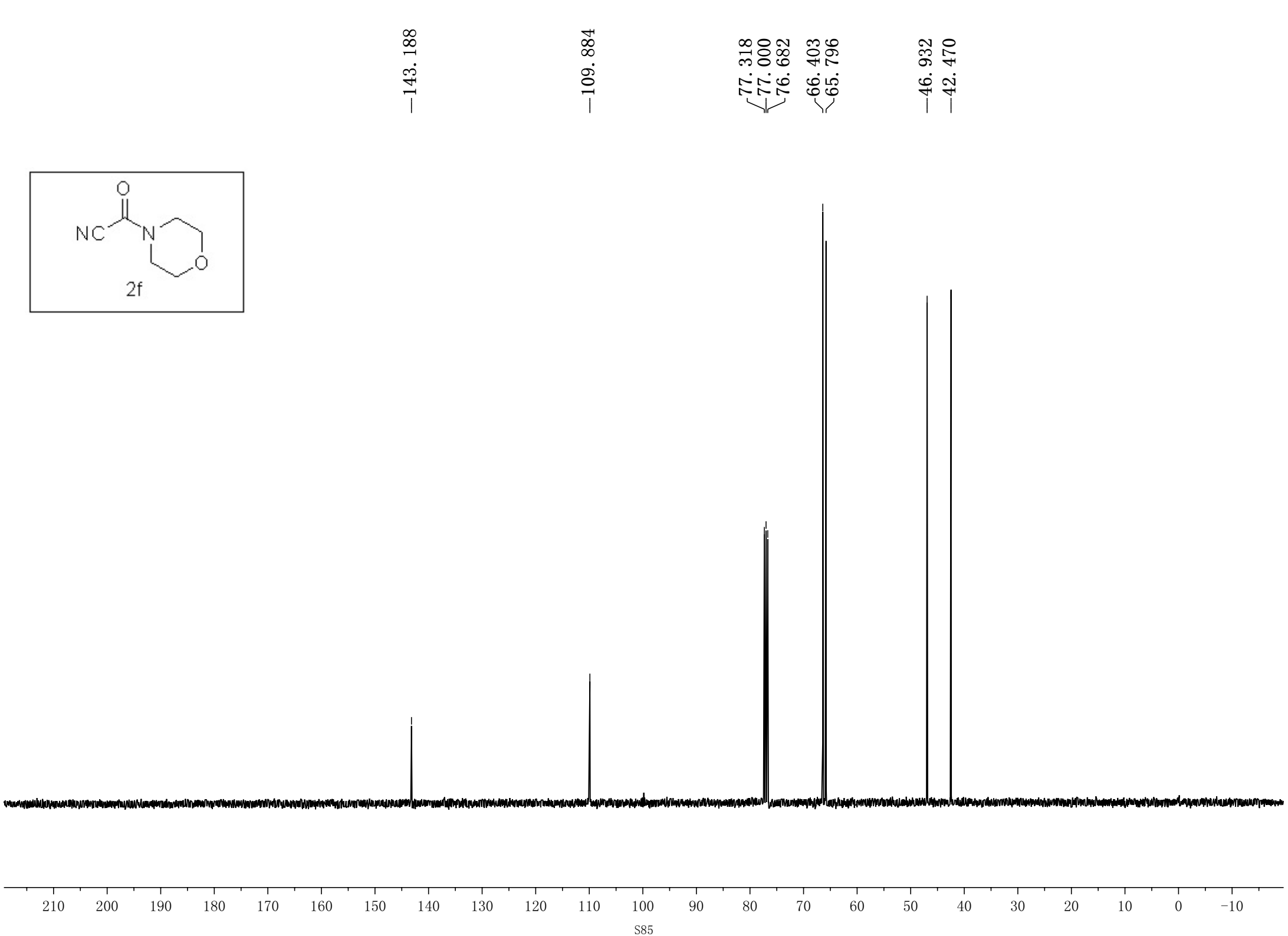
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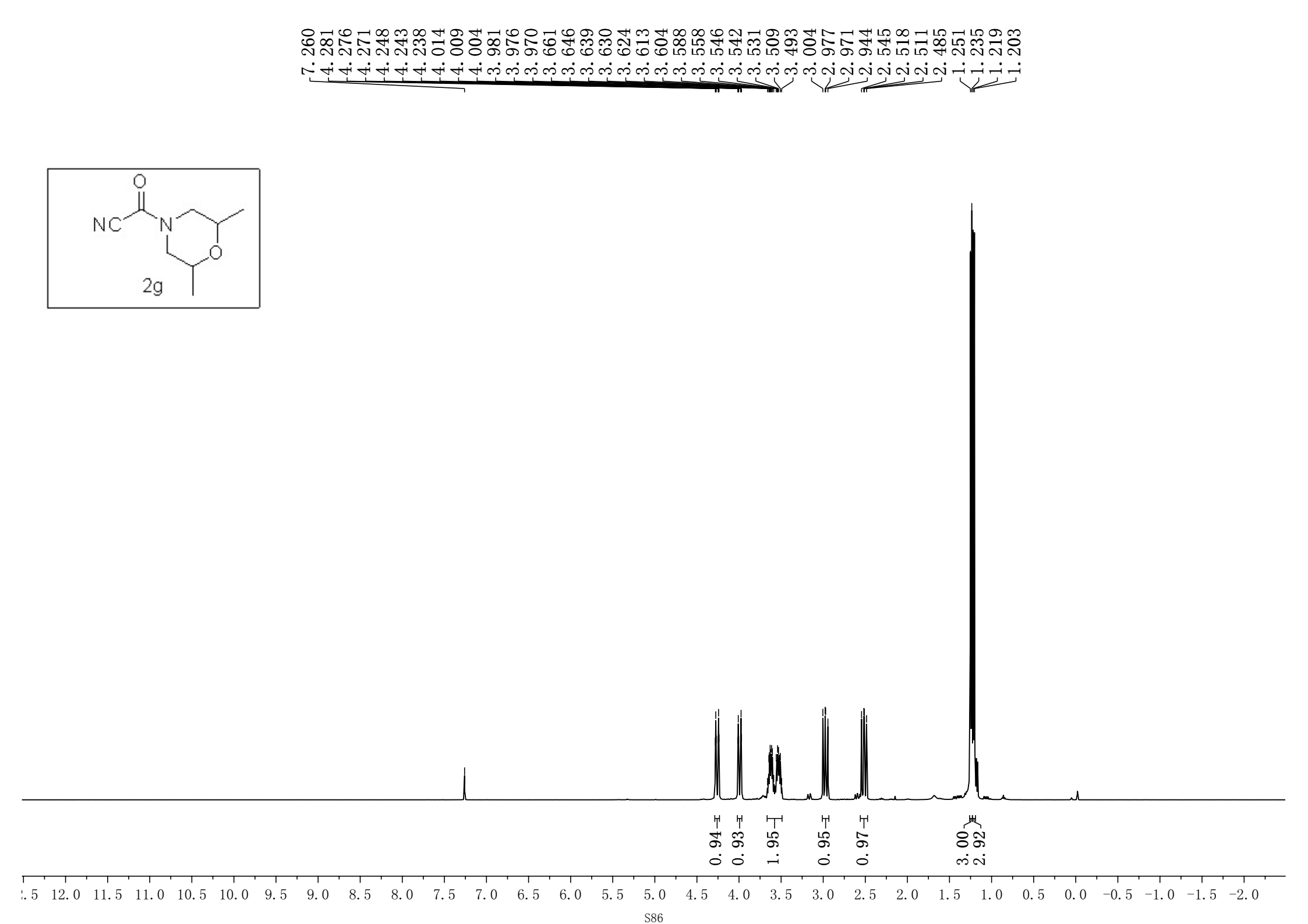
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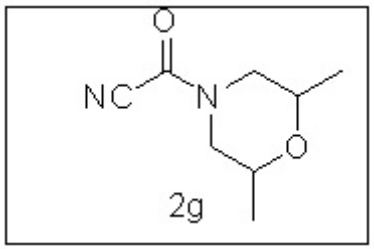

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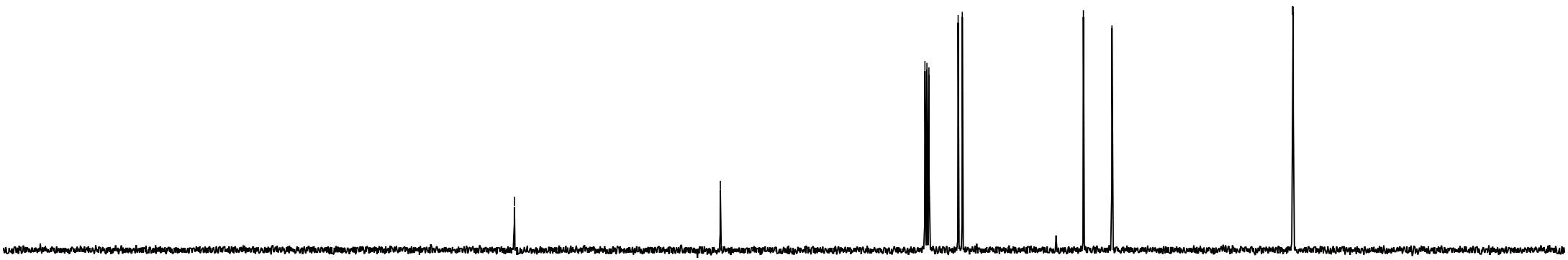

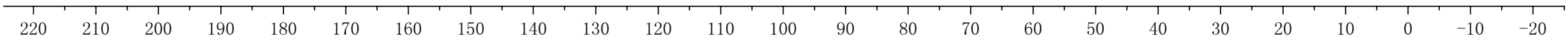

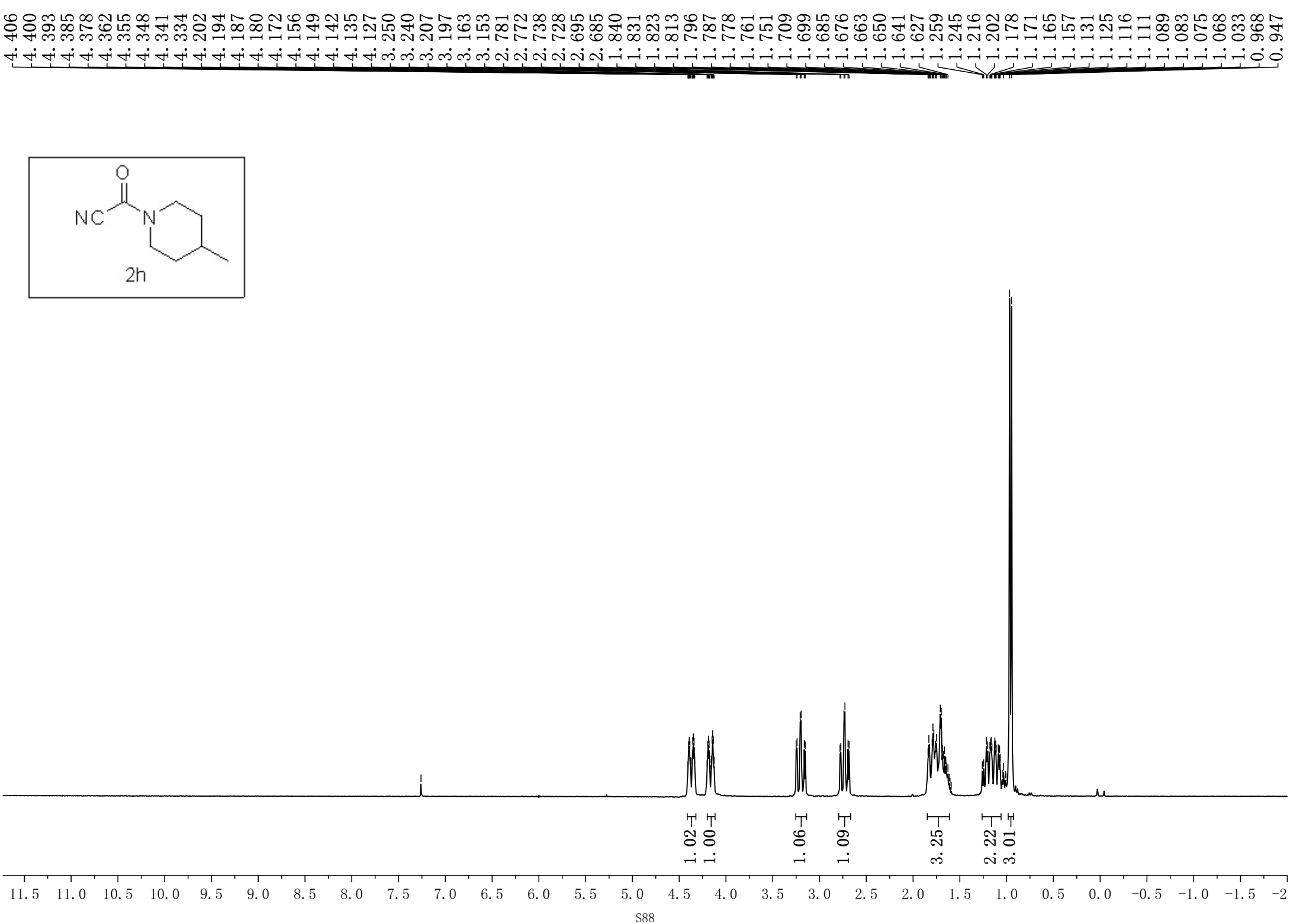
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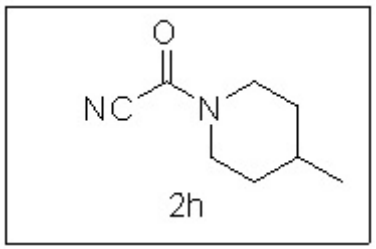

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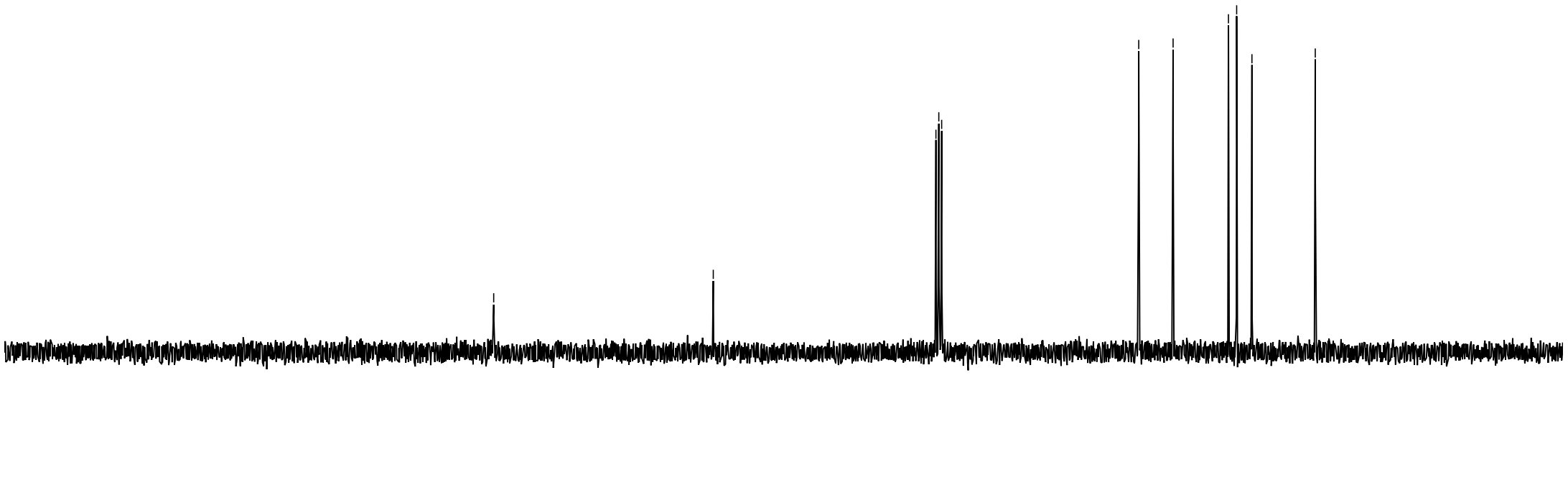

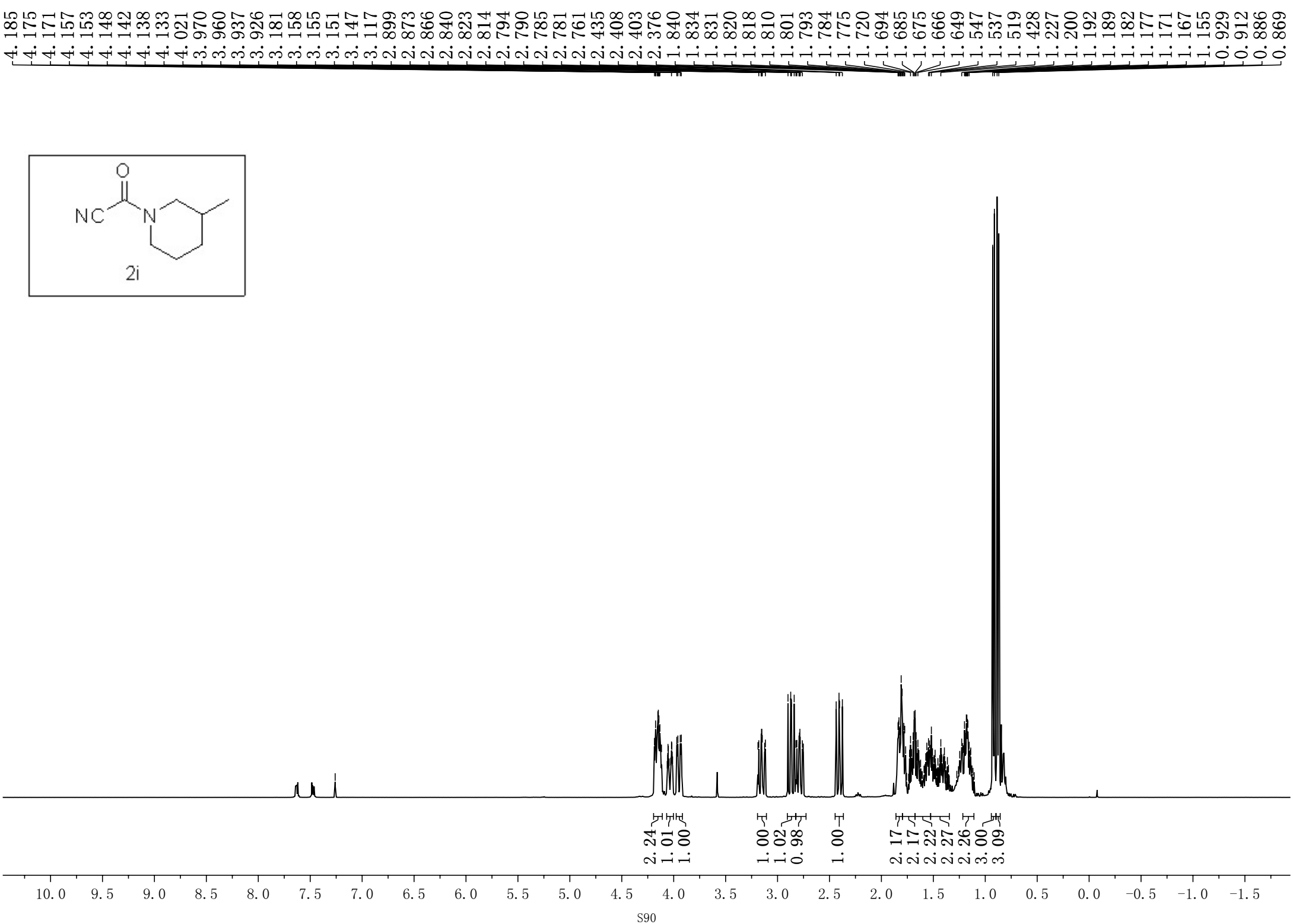
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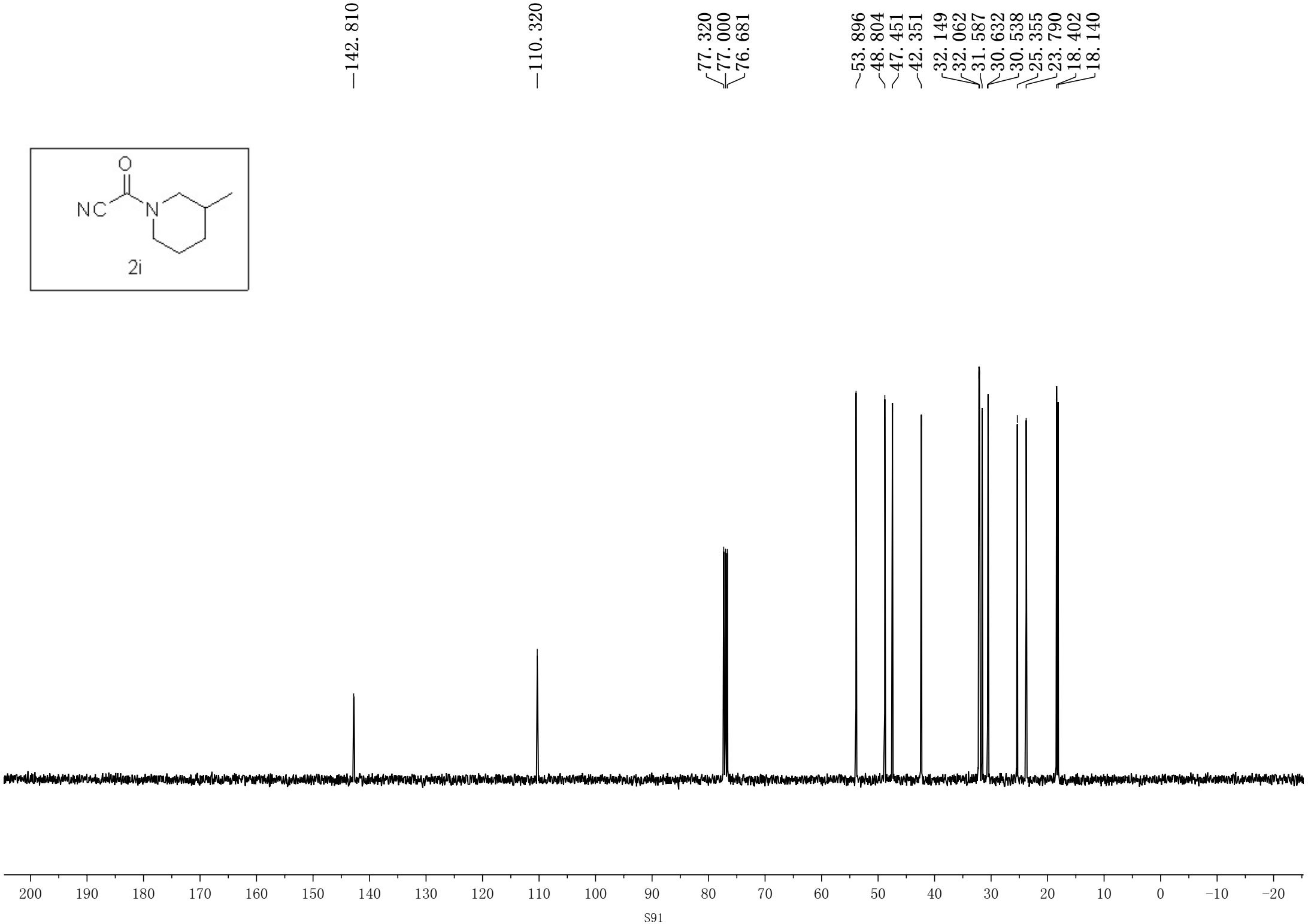
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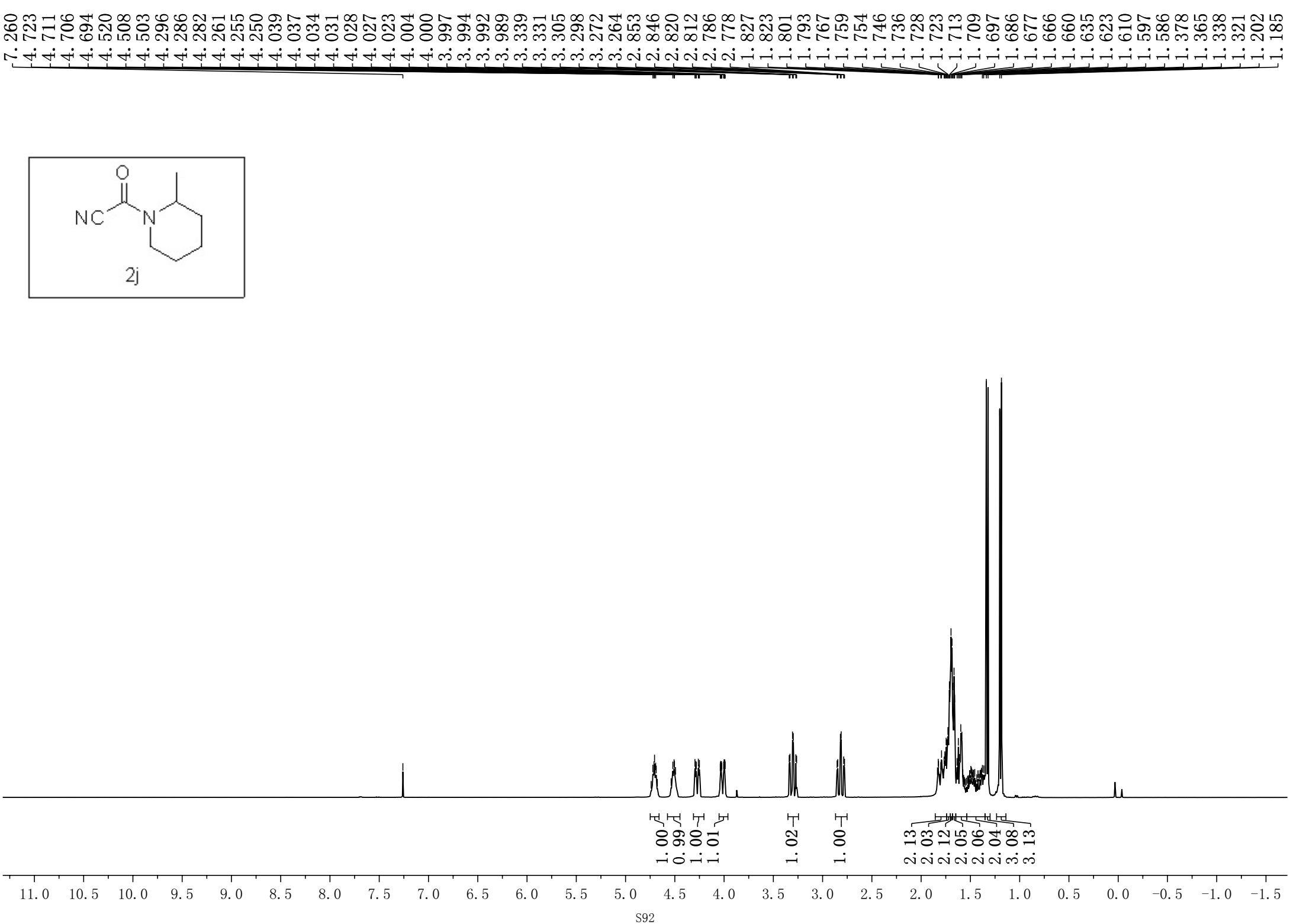
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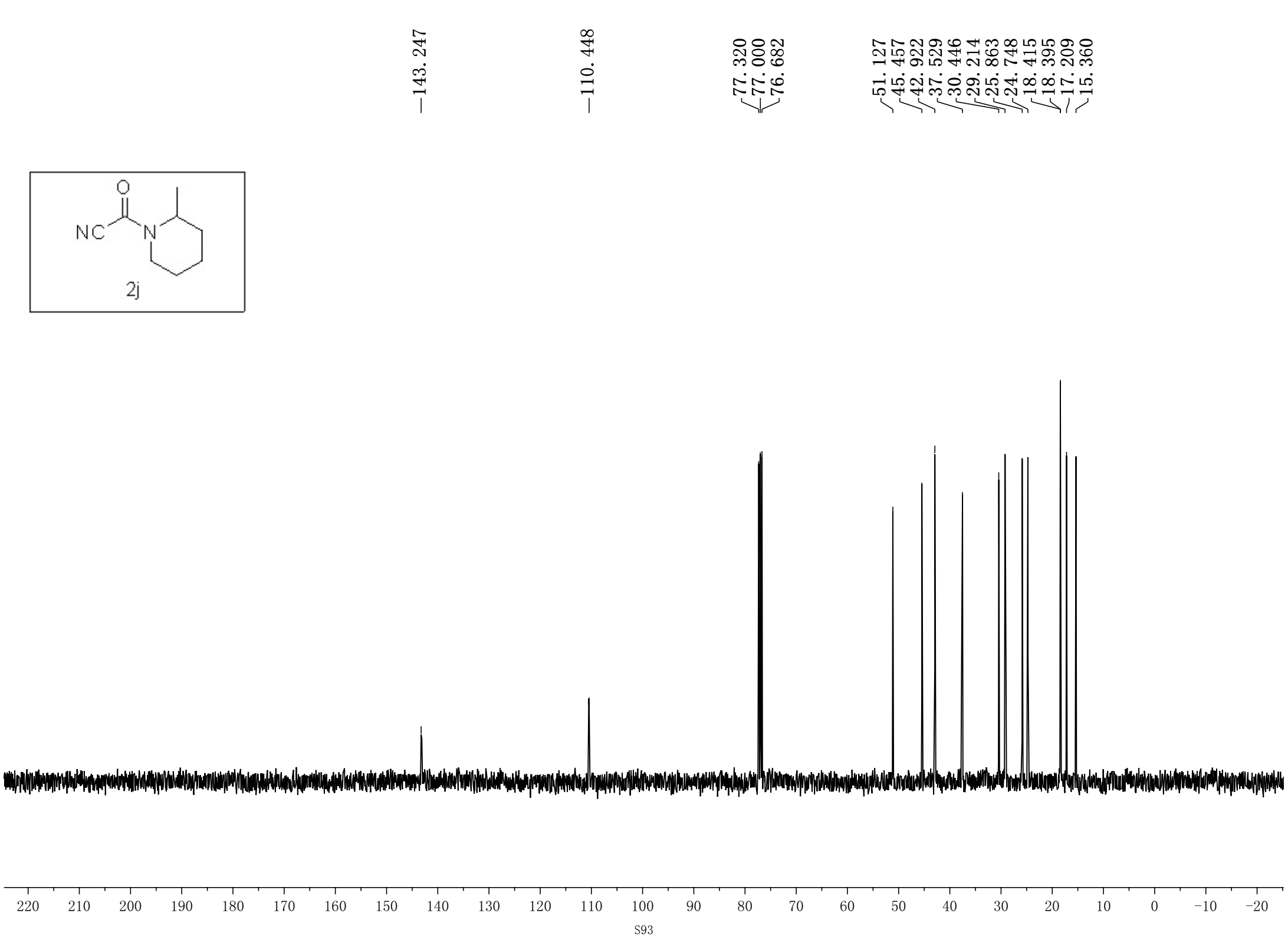
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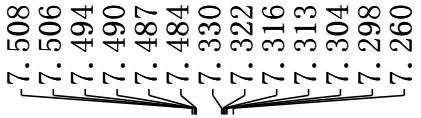
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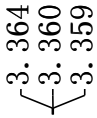
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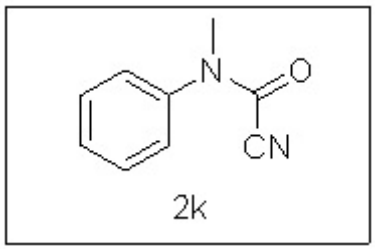
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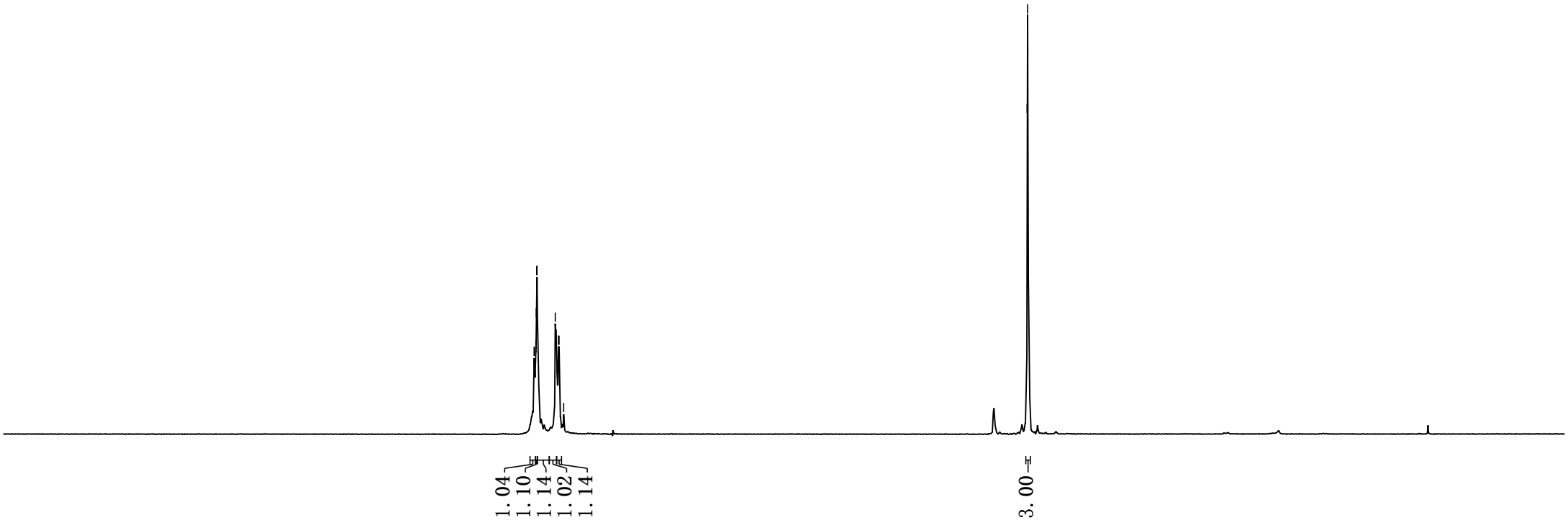
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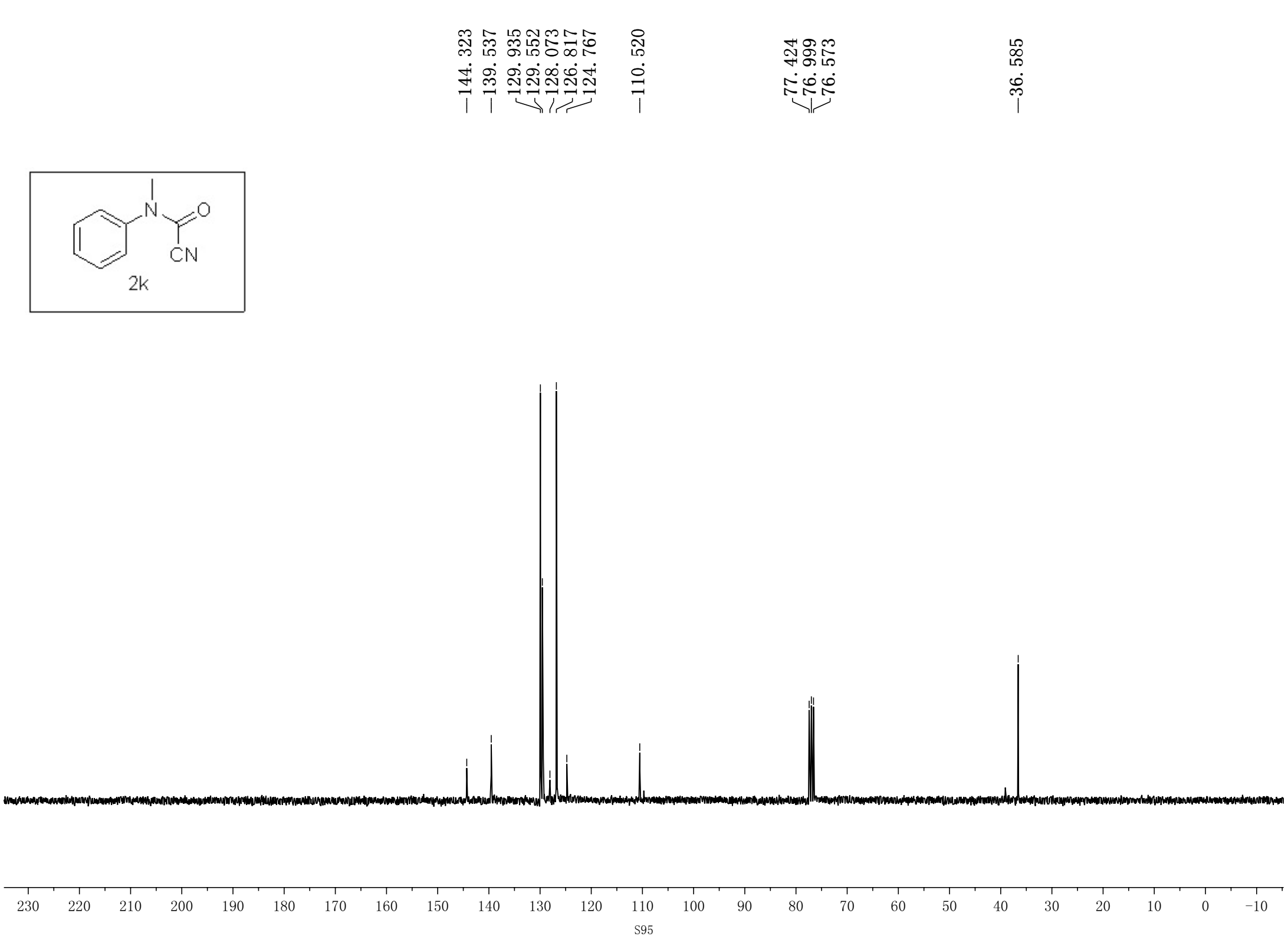
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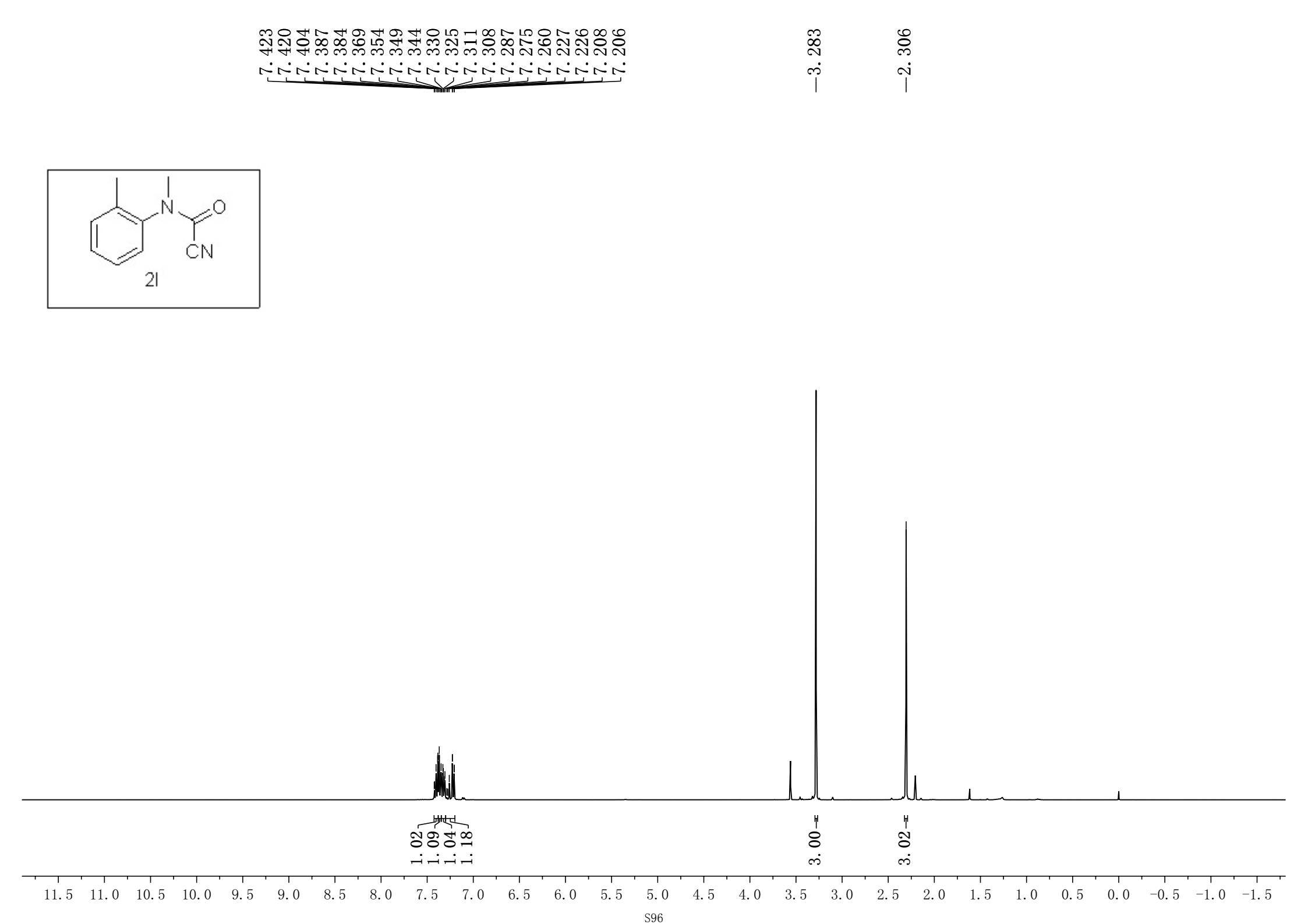
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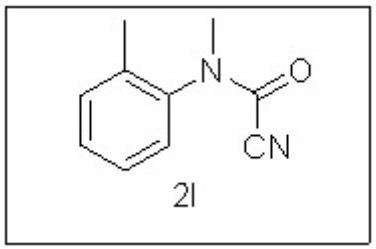

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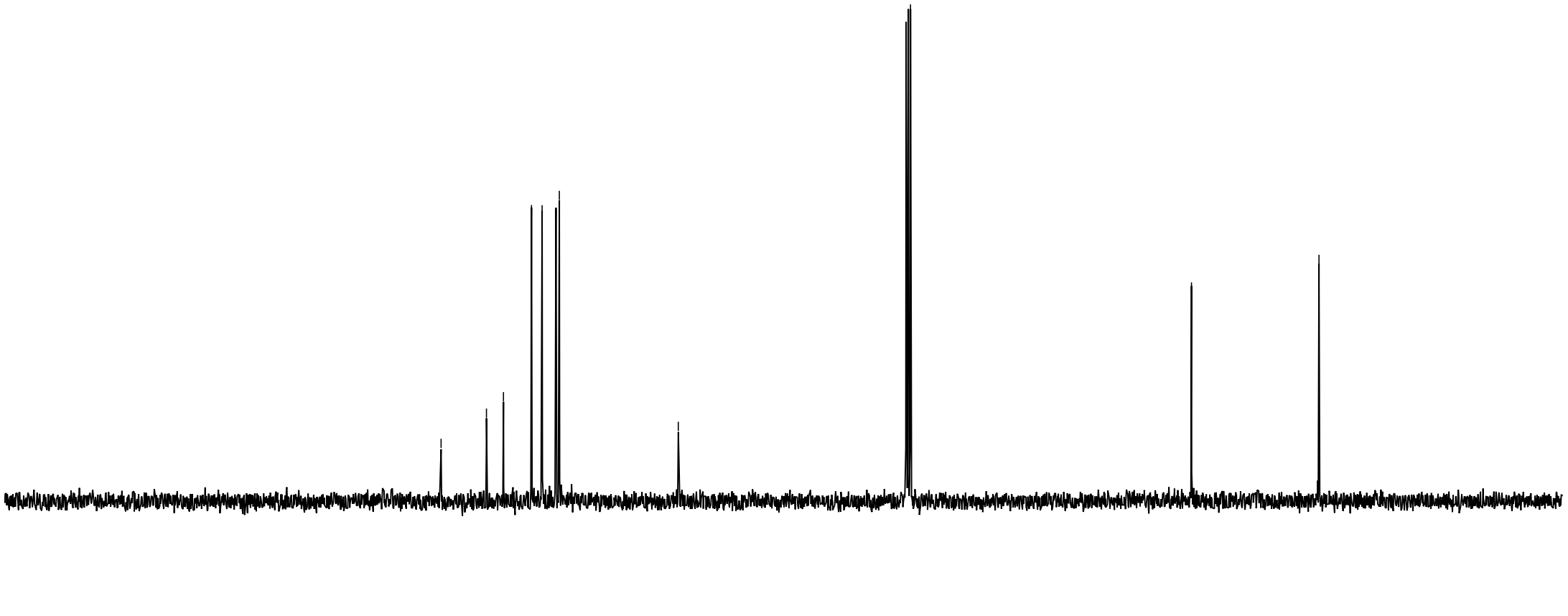

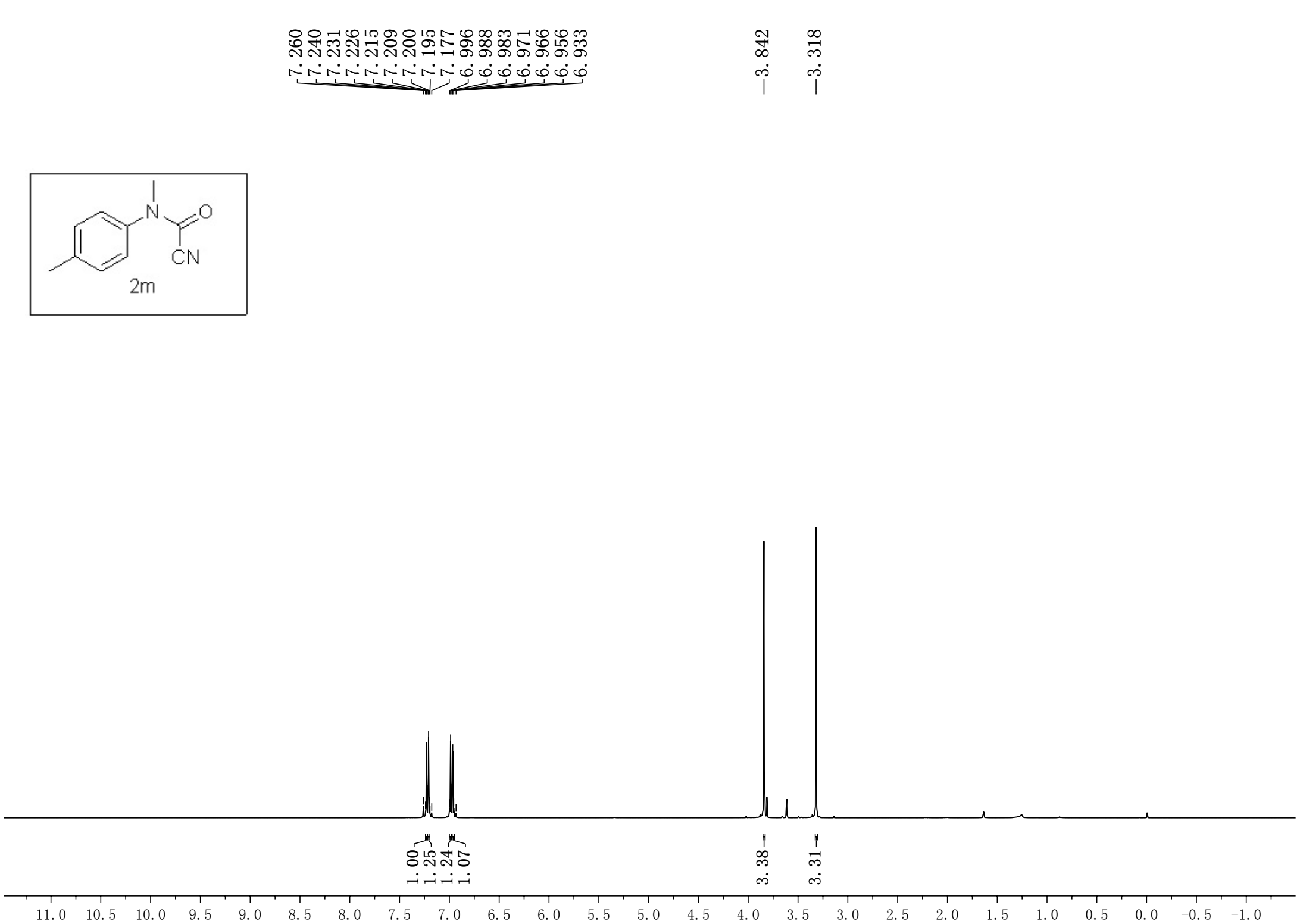
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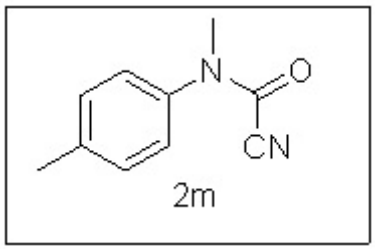

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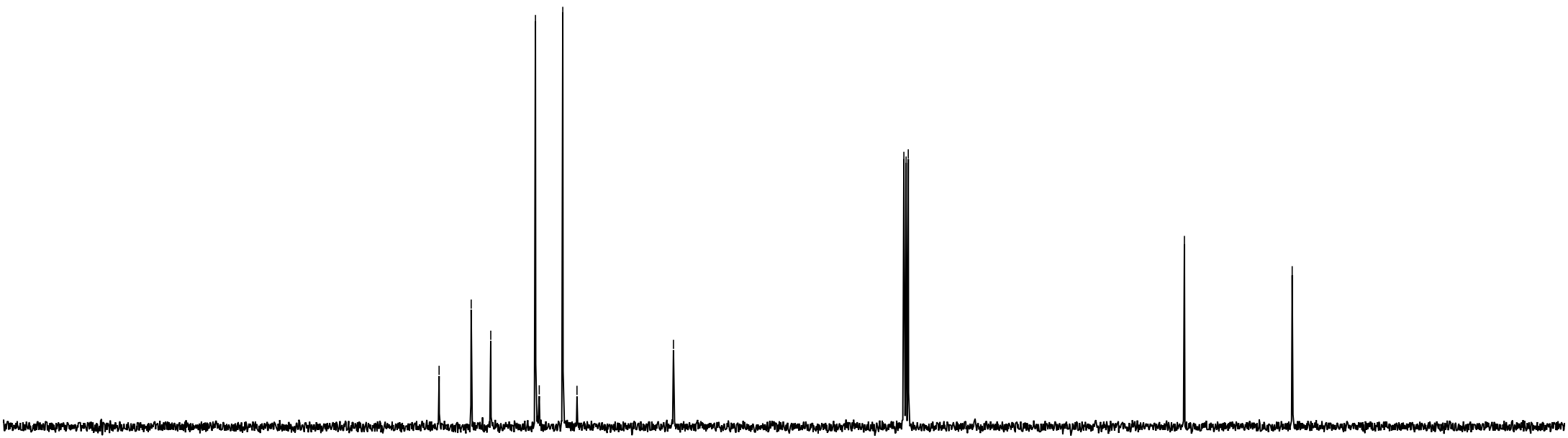

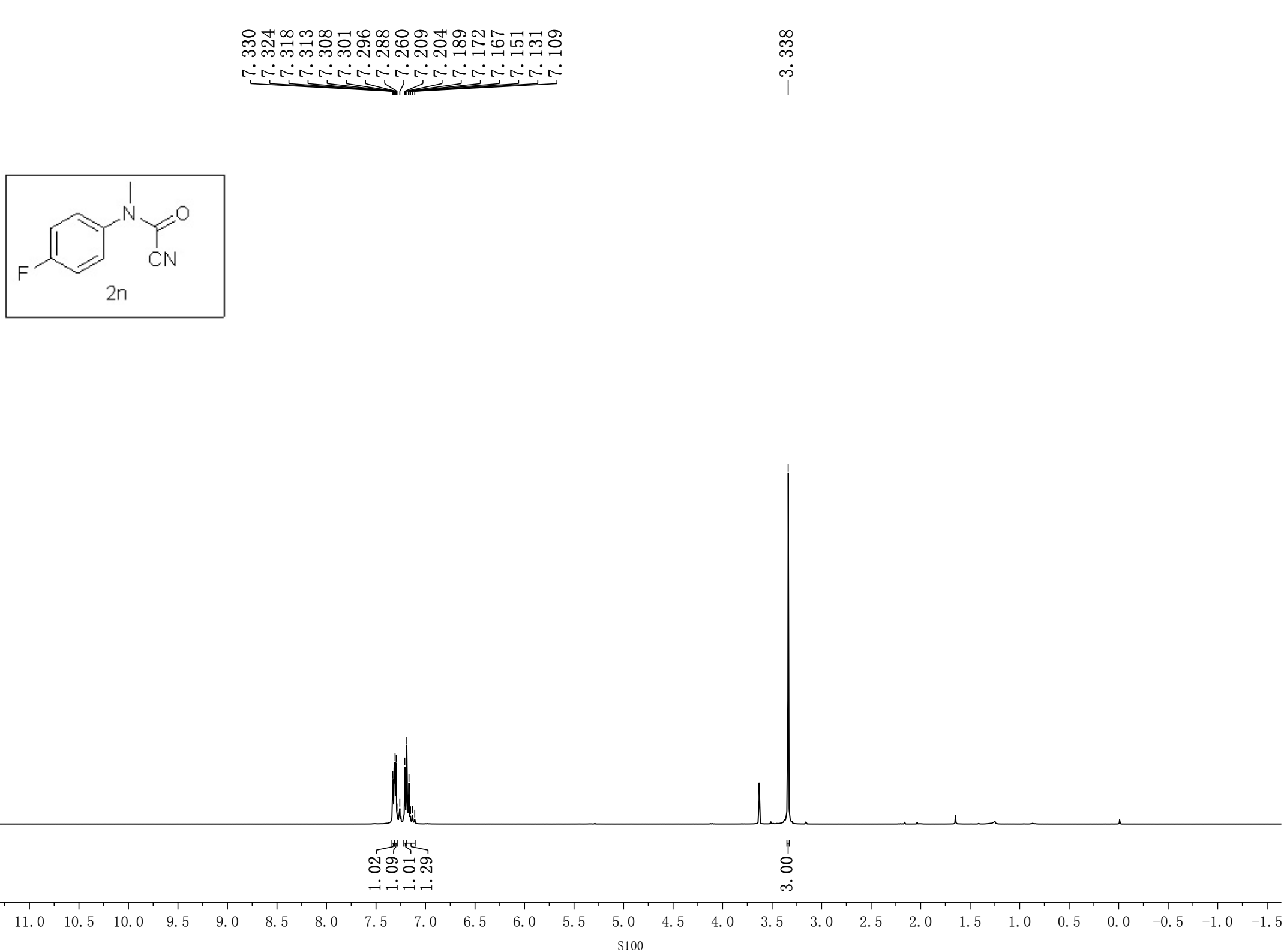
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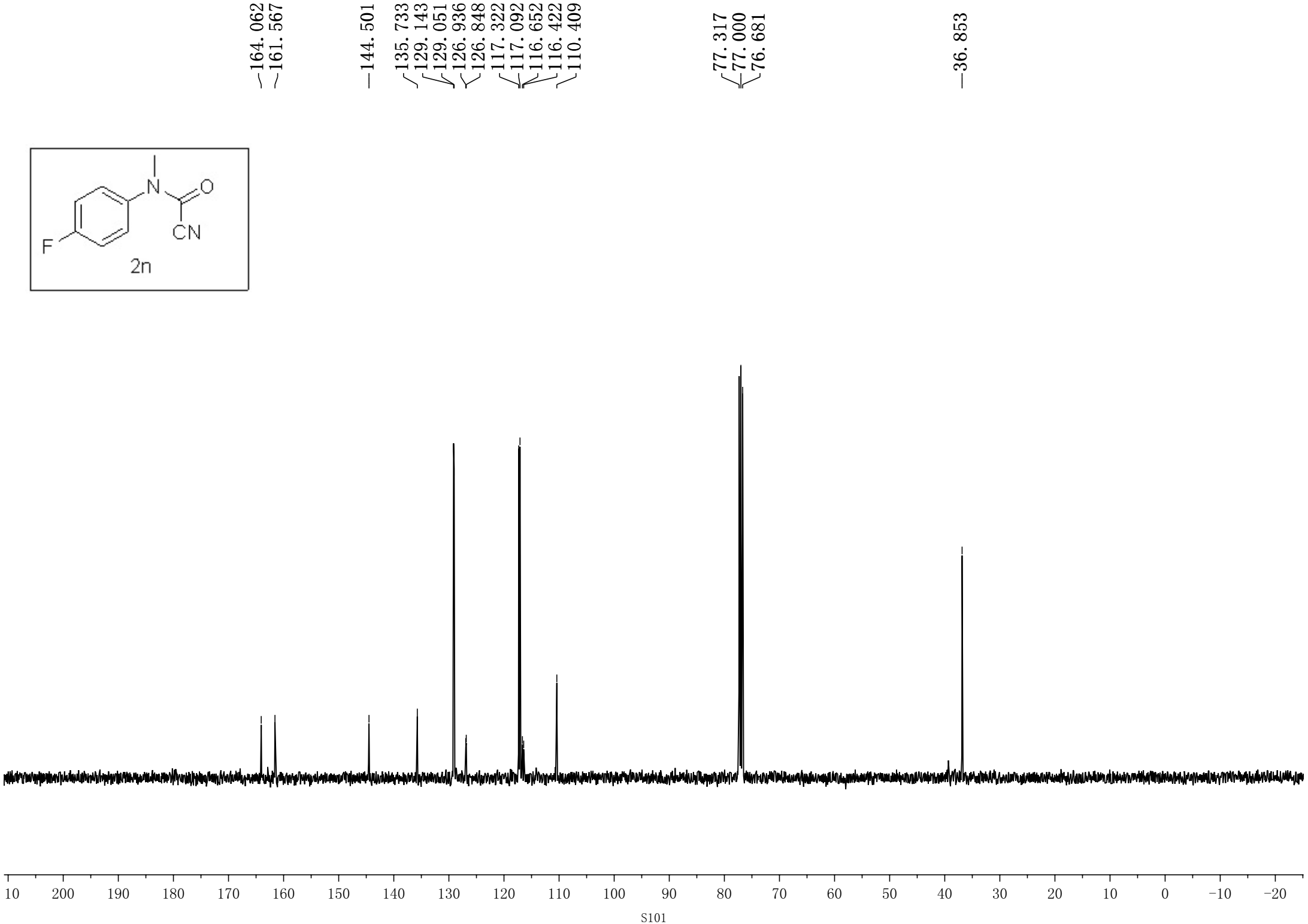
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O
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F
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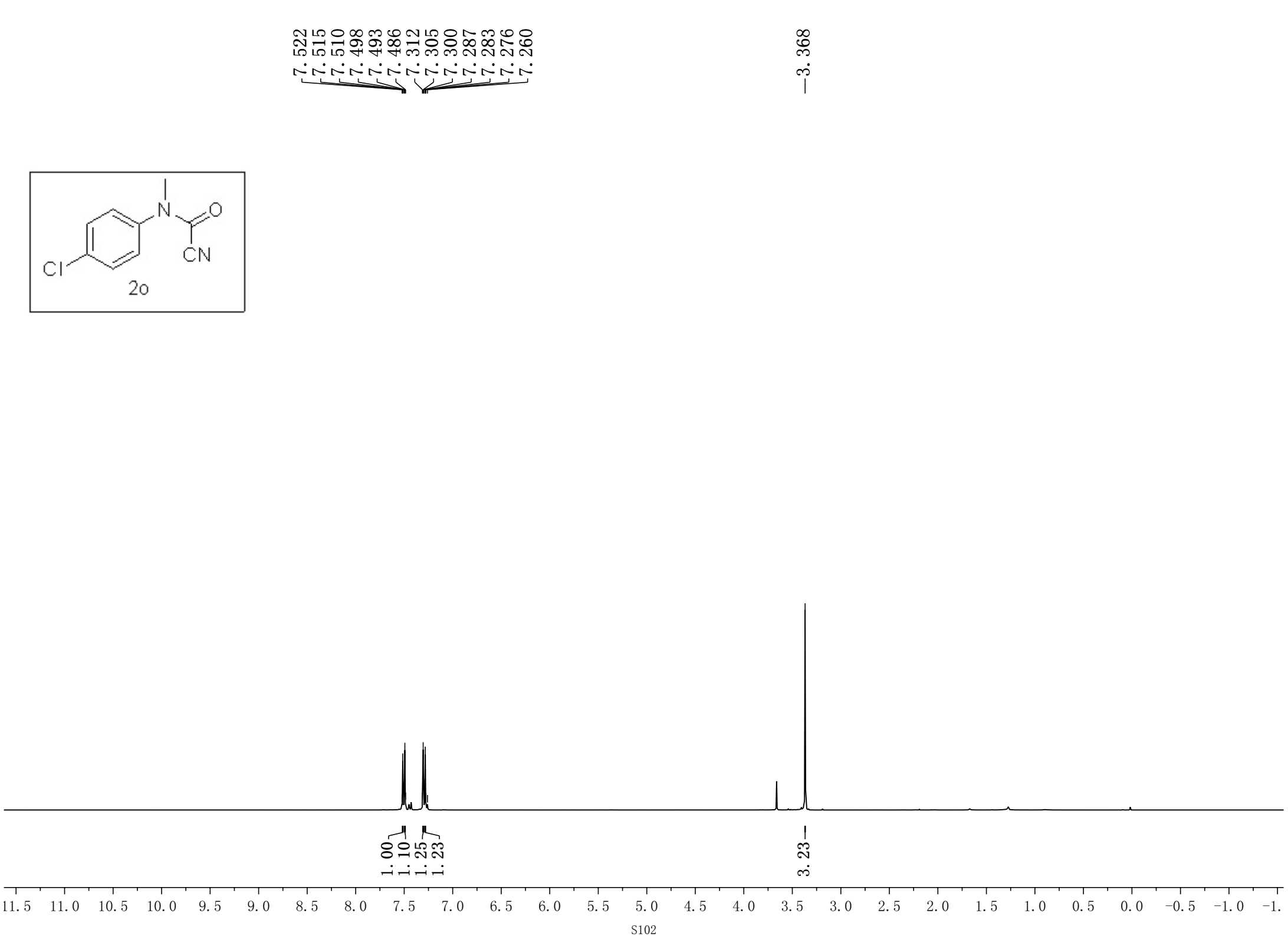
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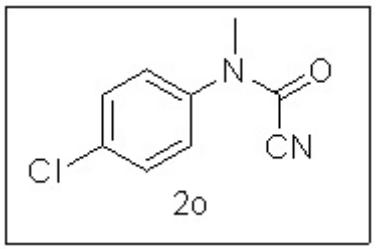

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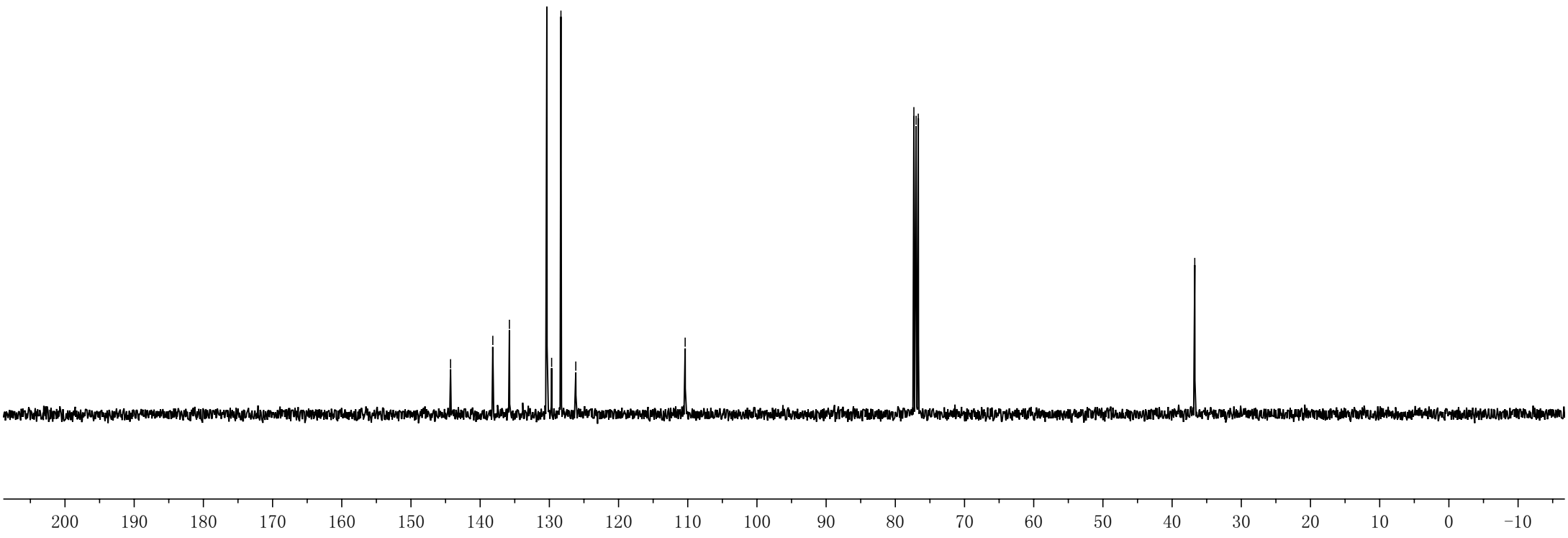

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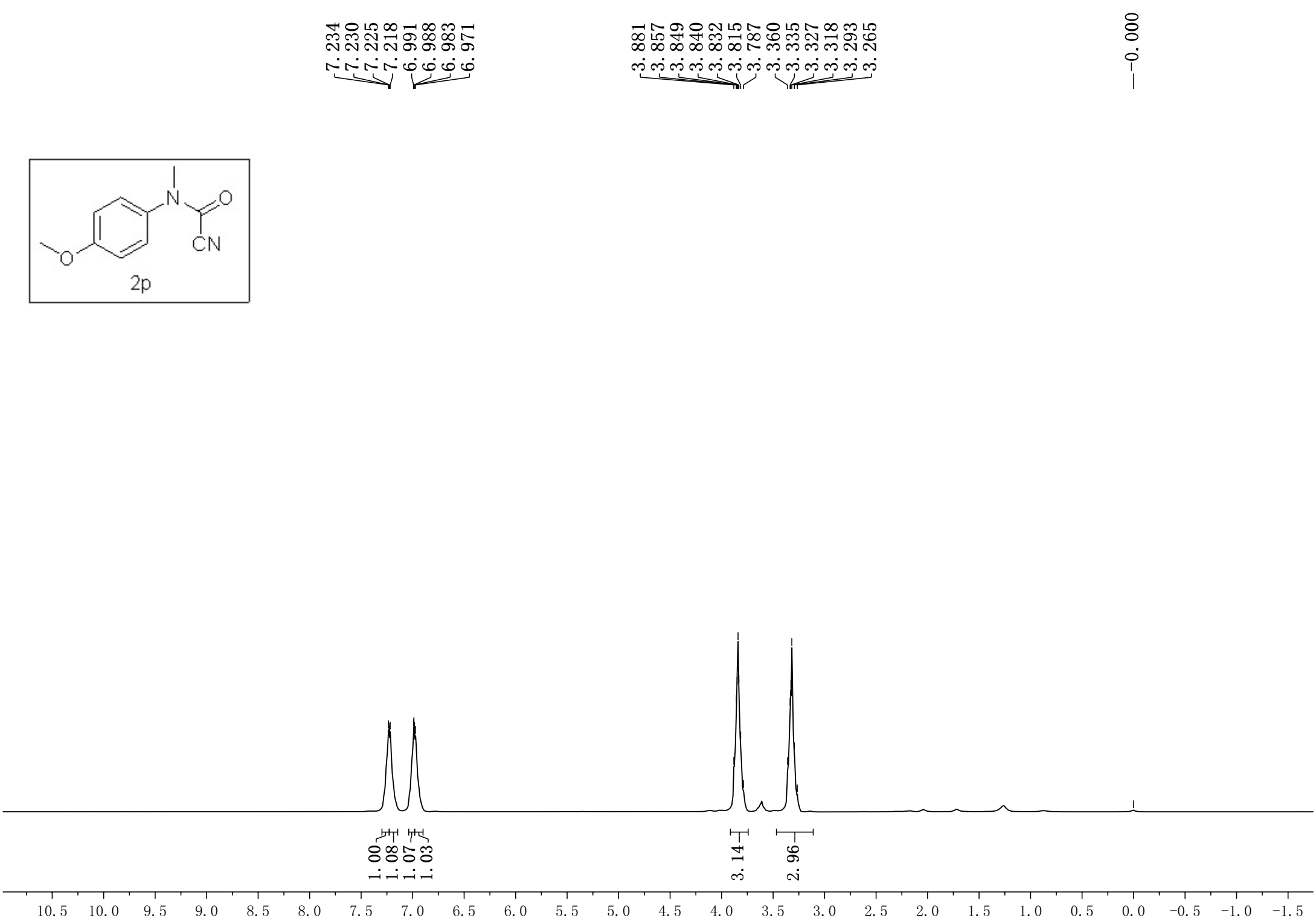
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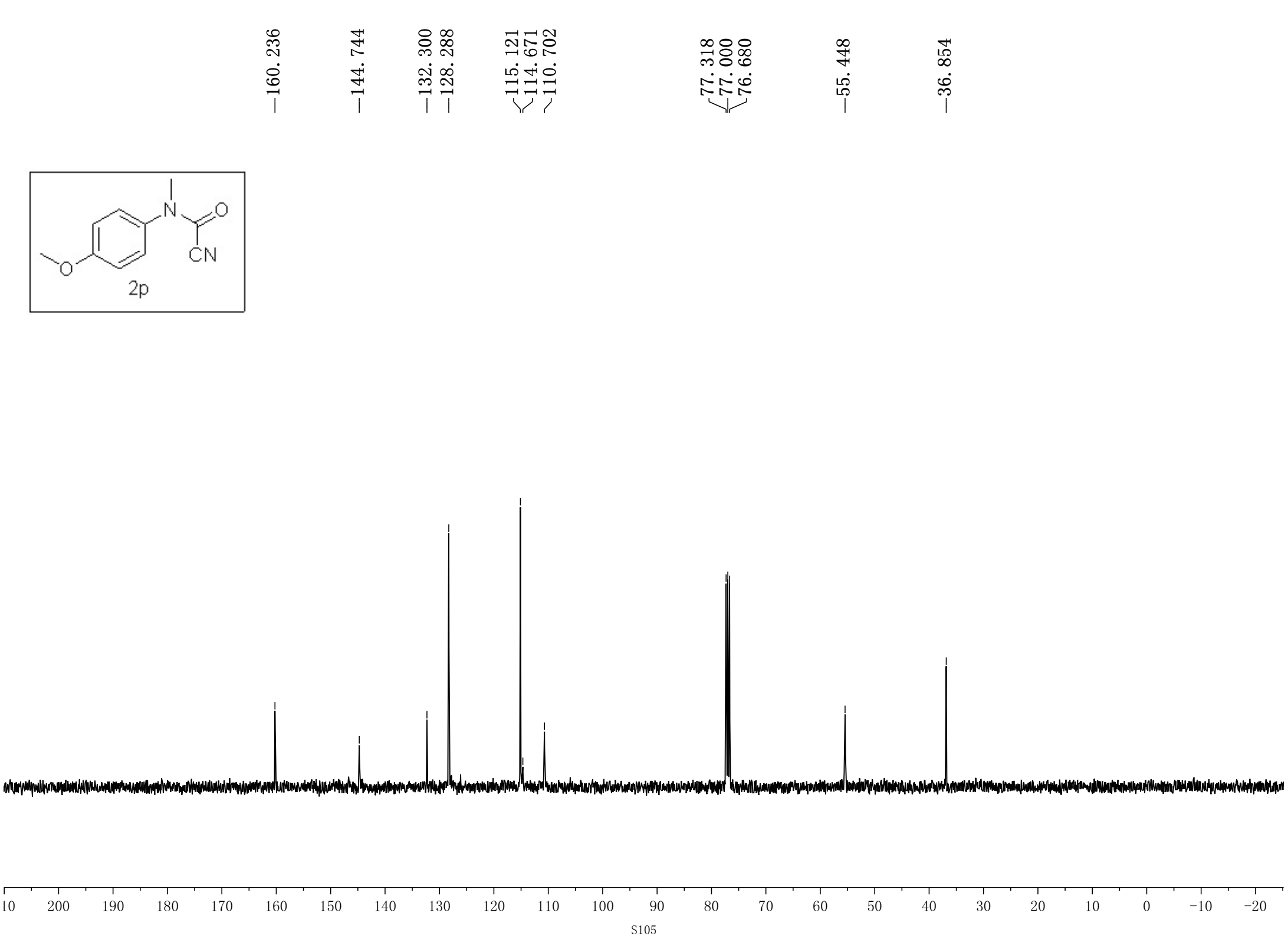
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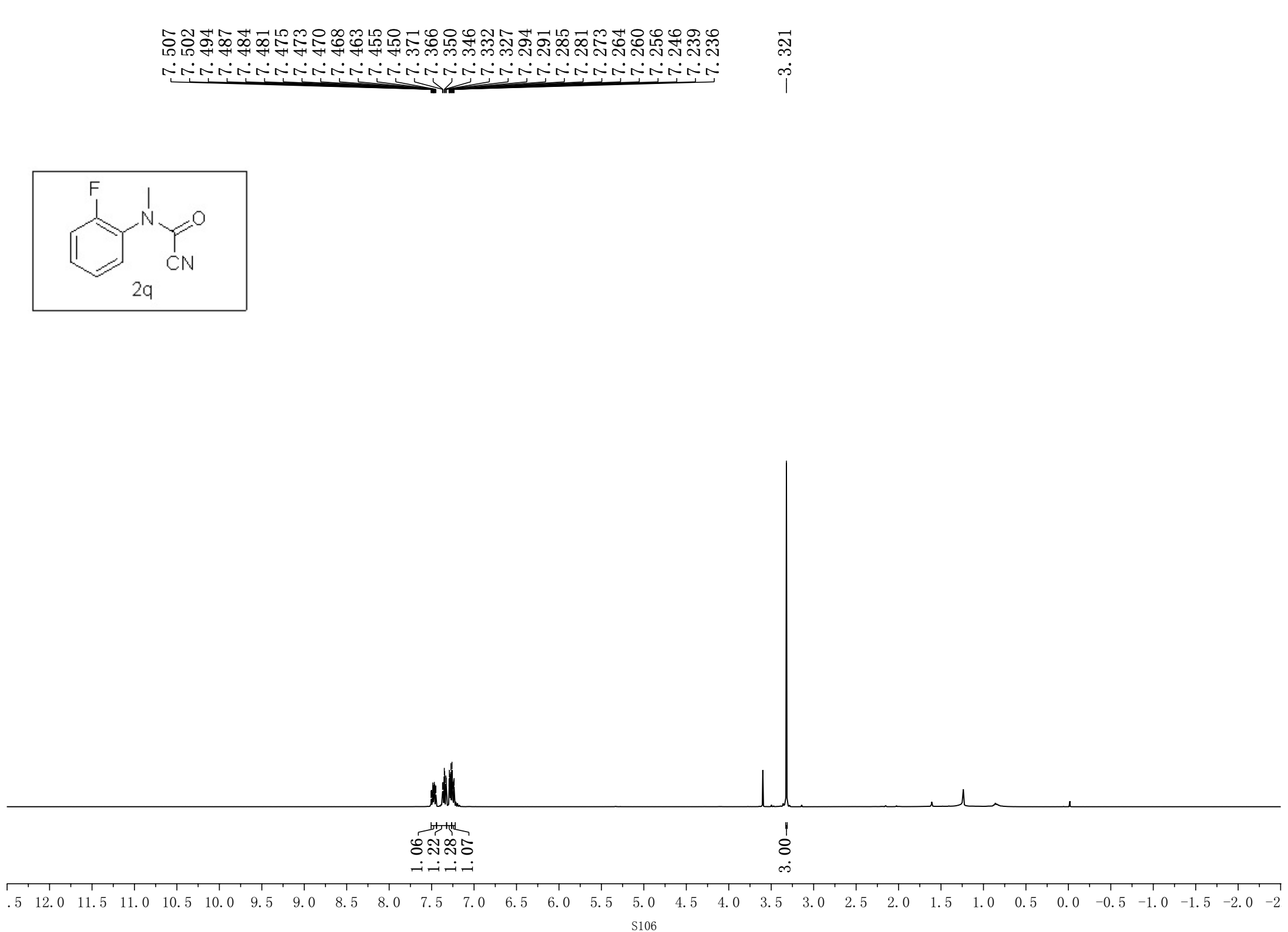
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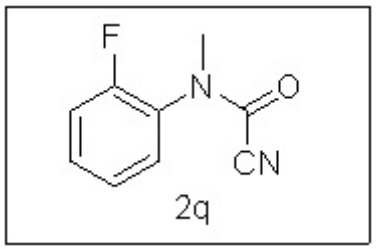

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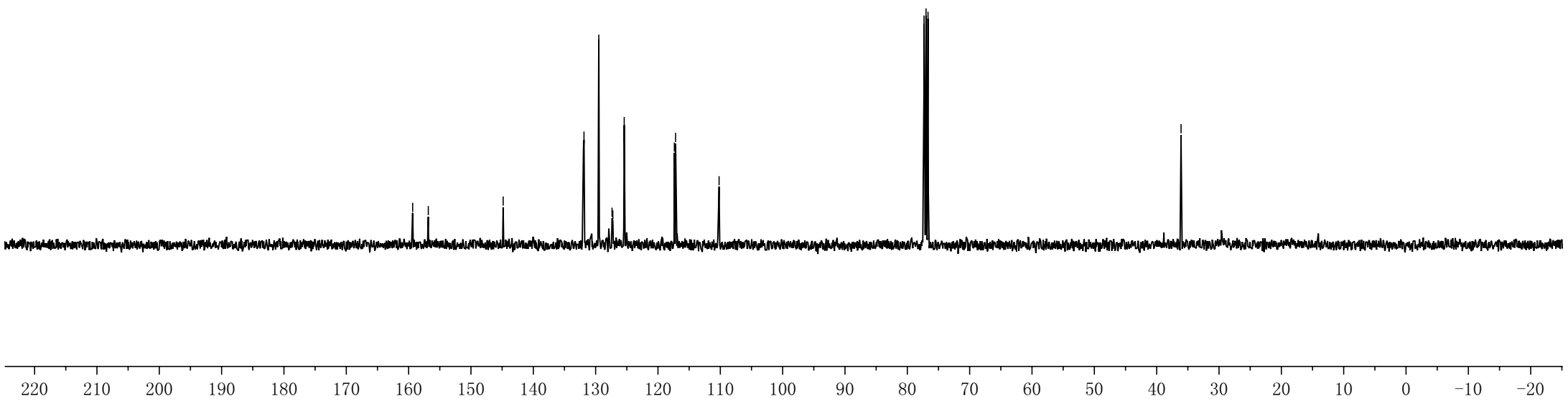

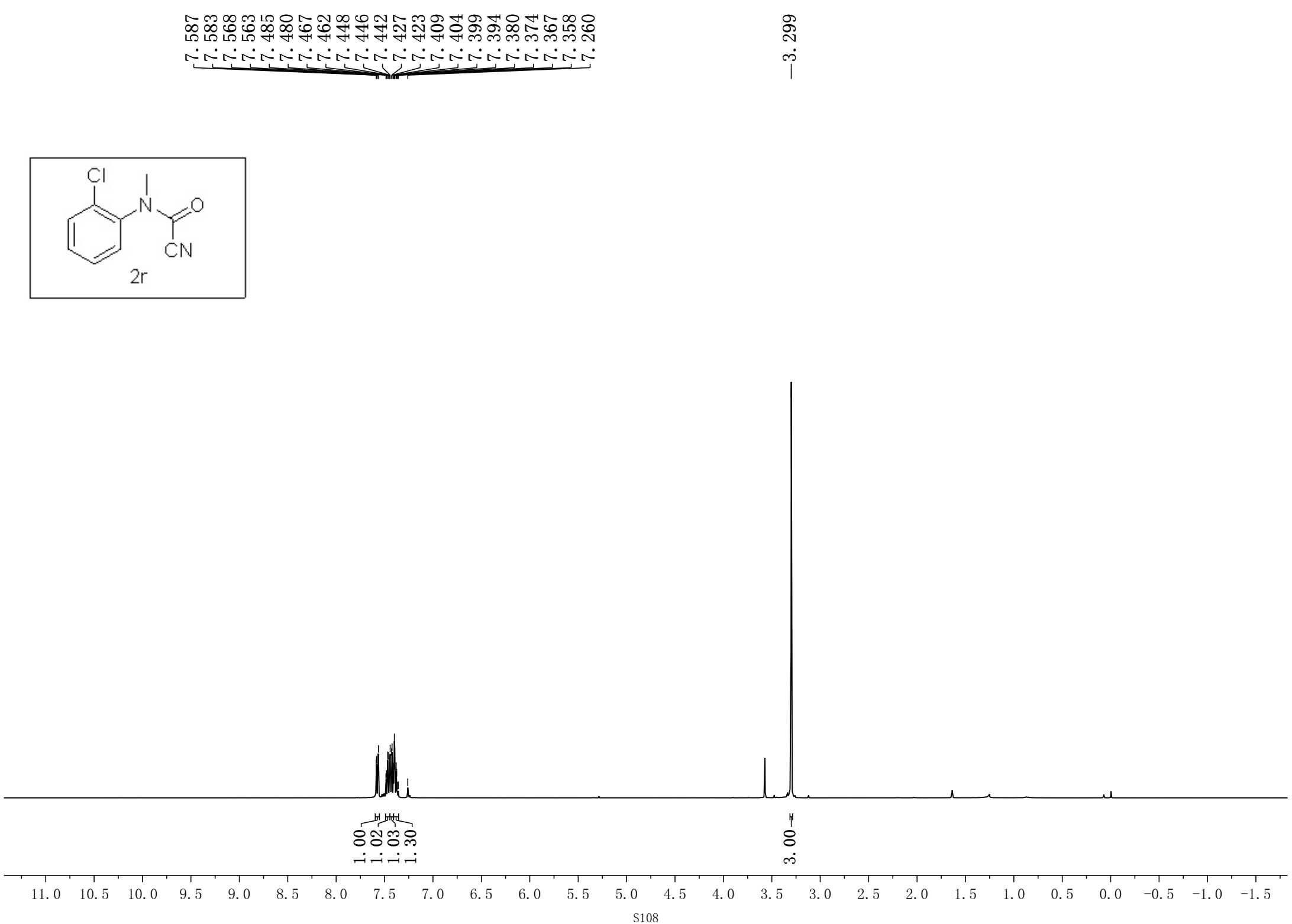
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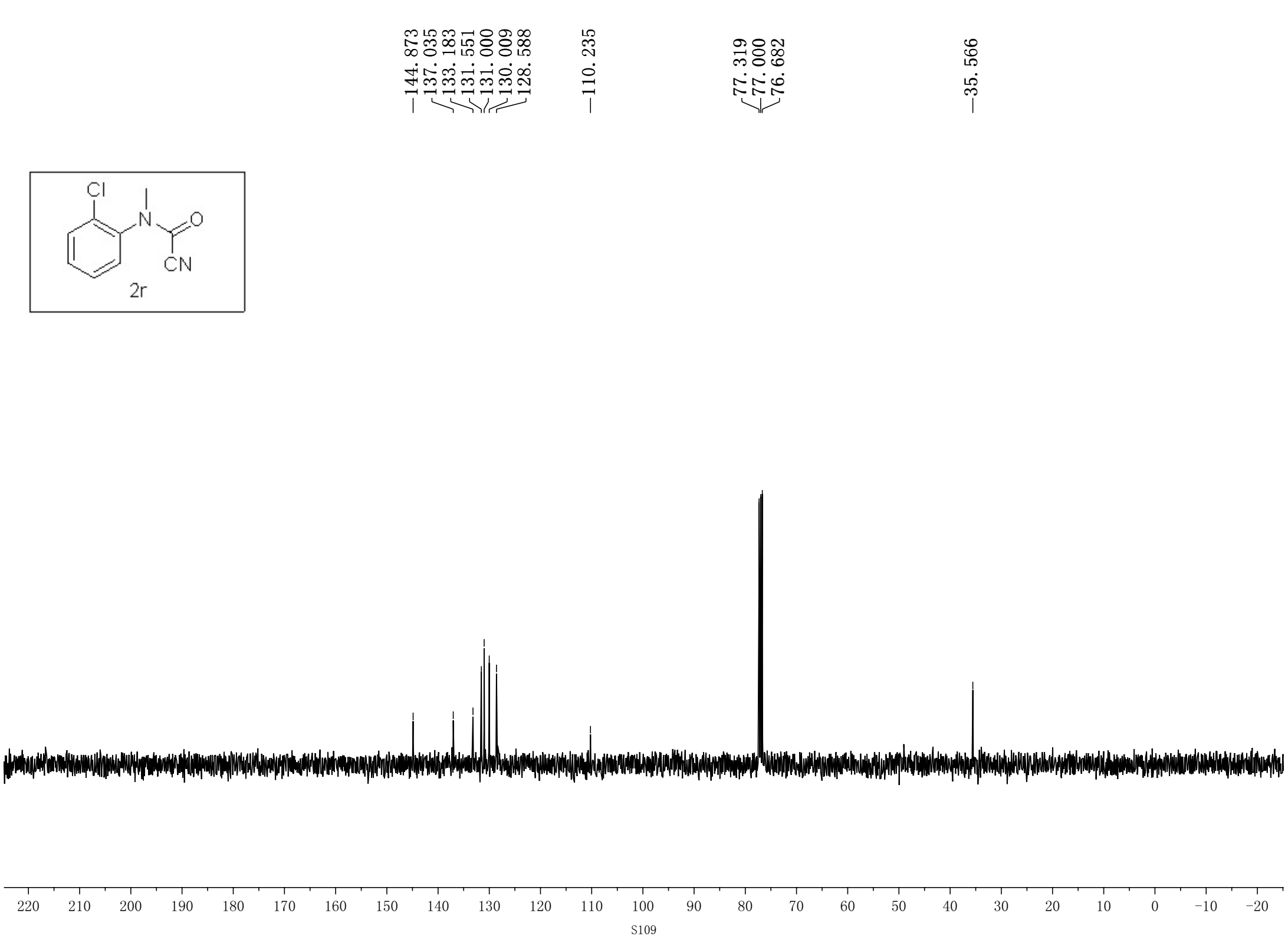
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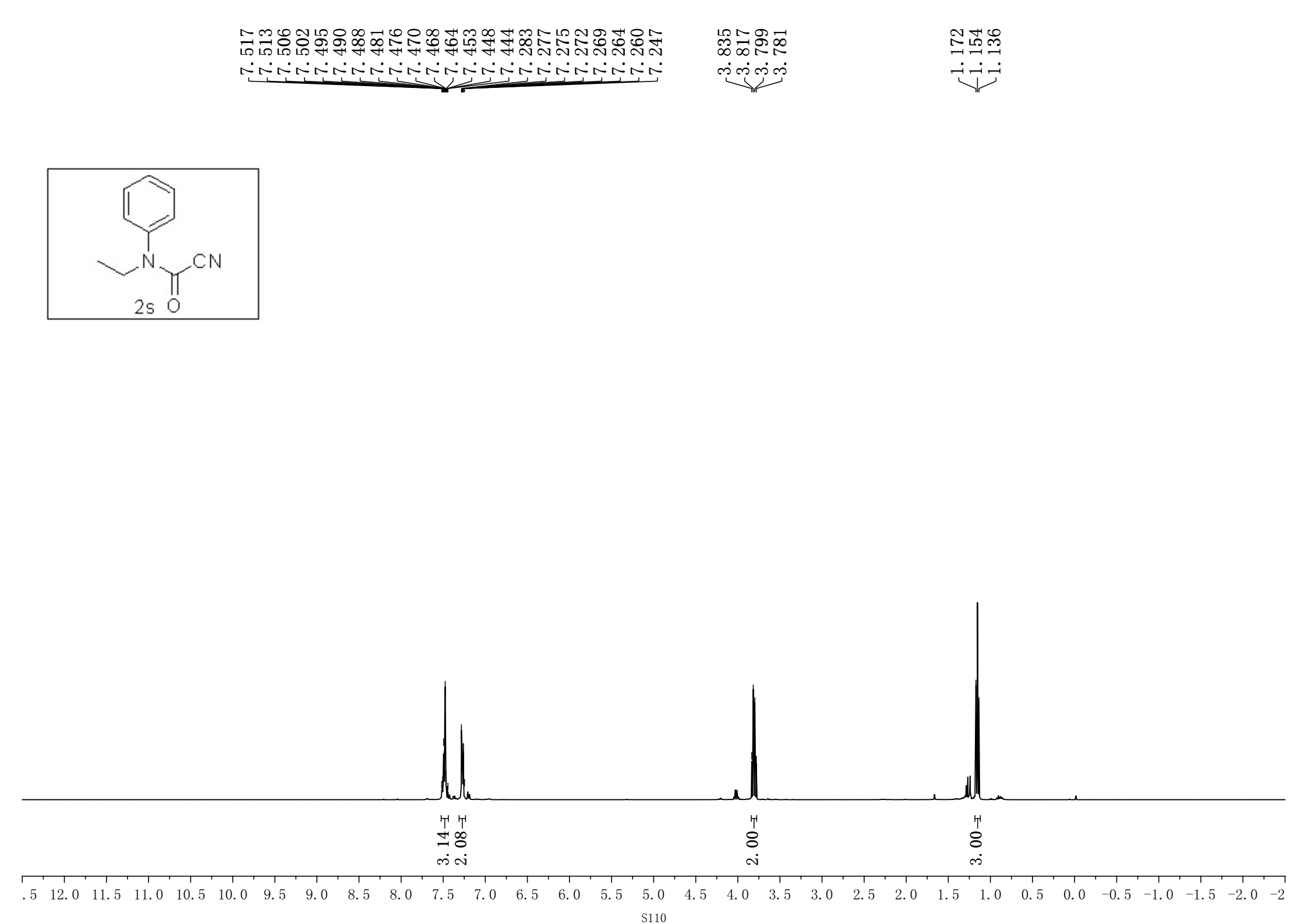
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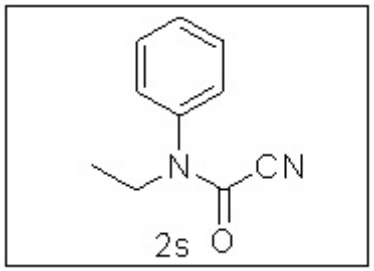

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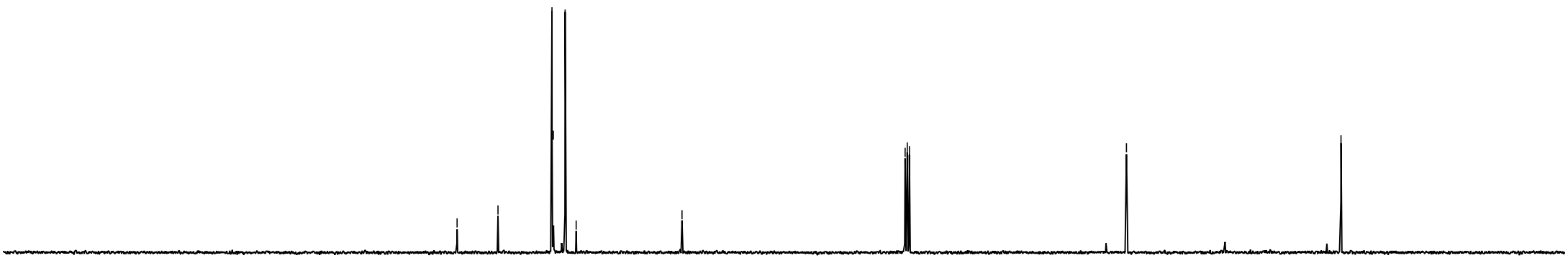

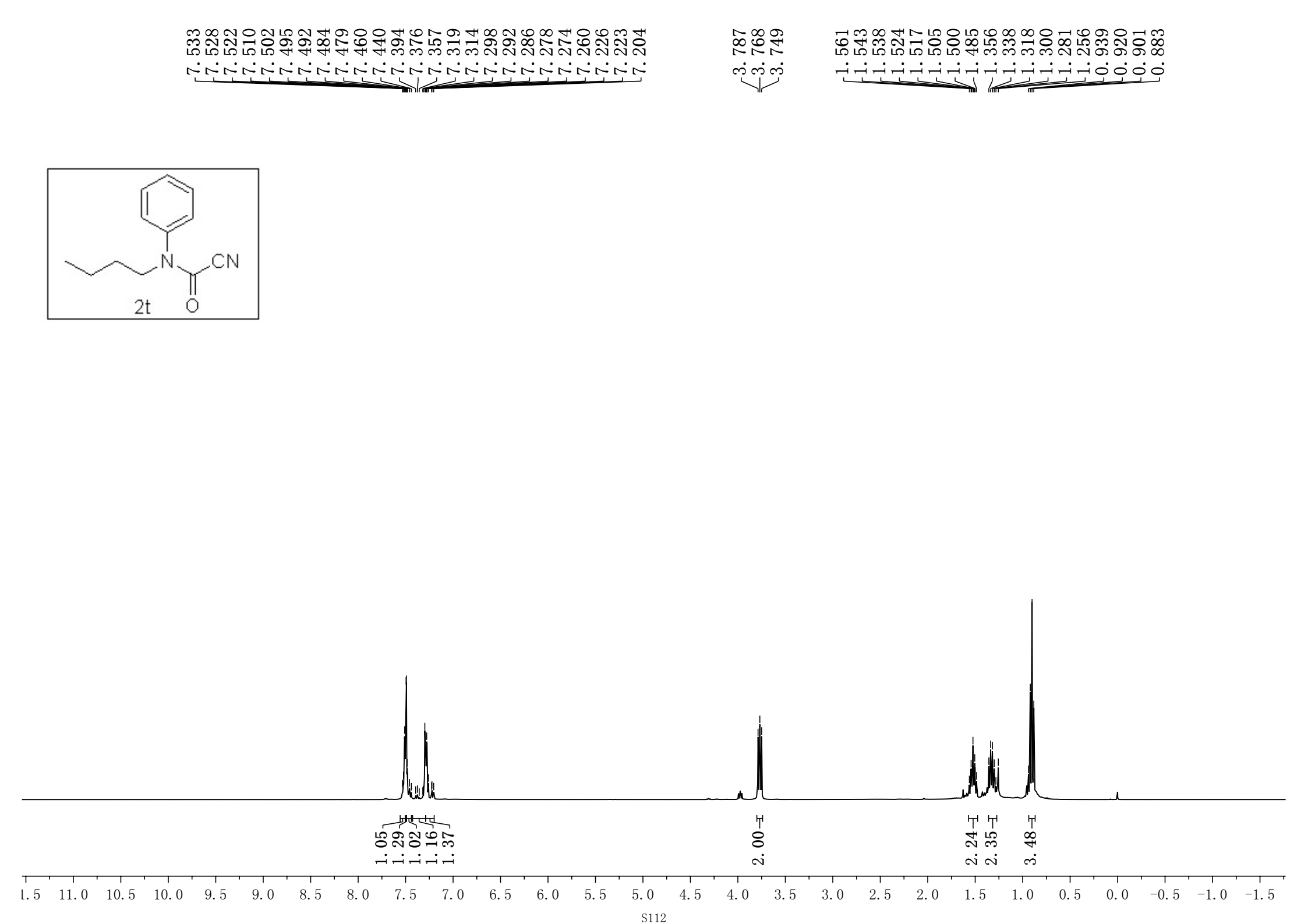
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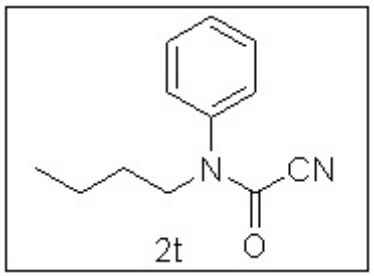

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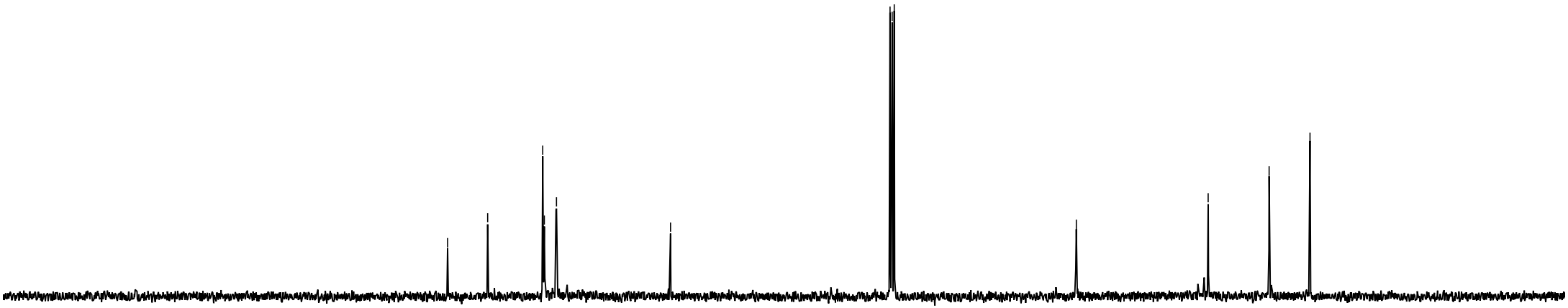

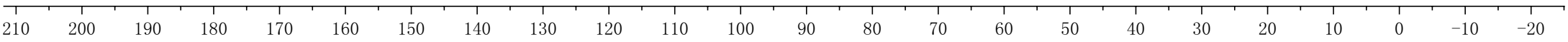

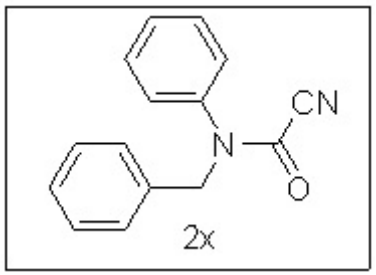
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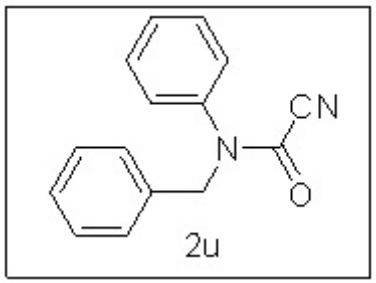

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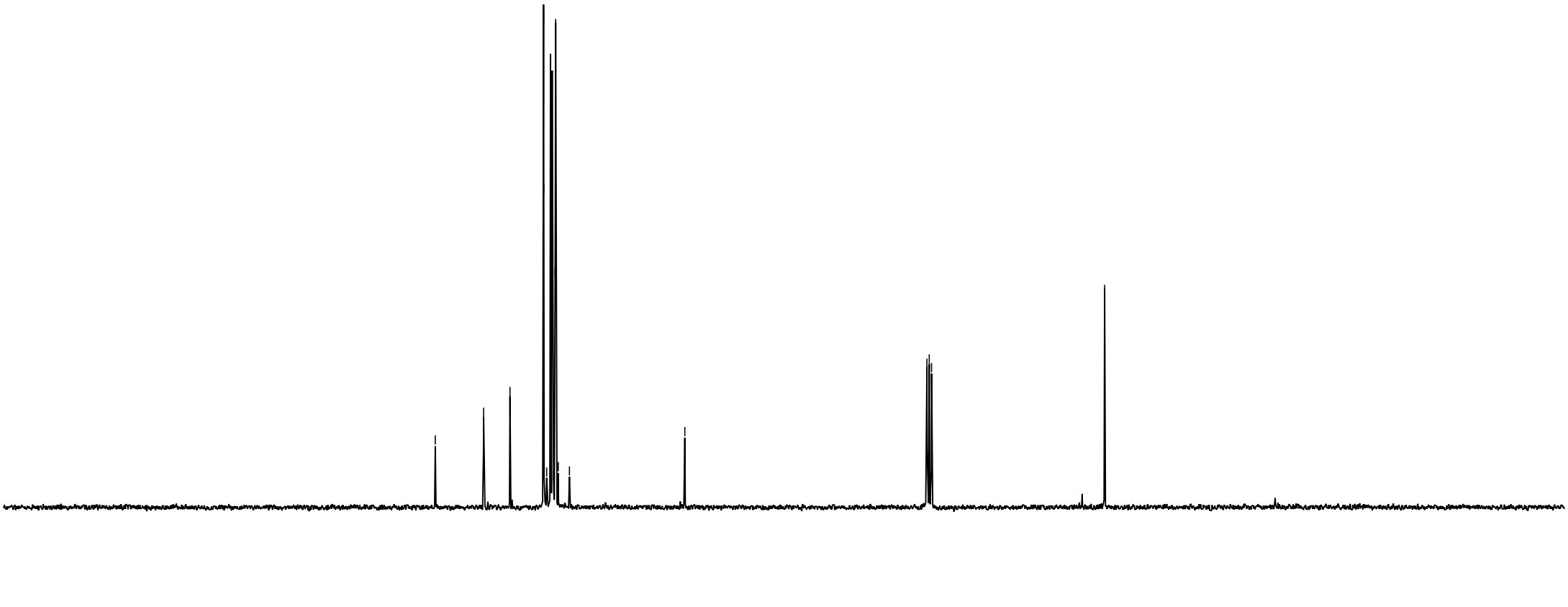

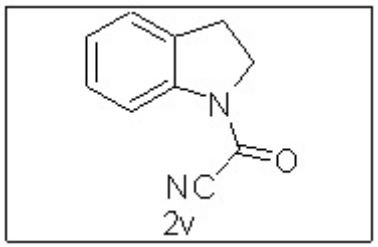

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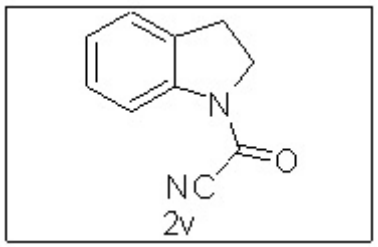
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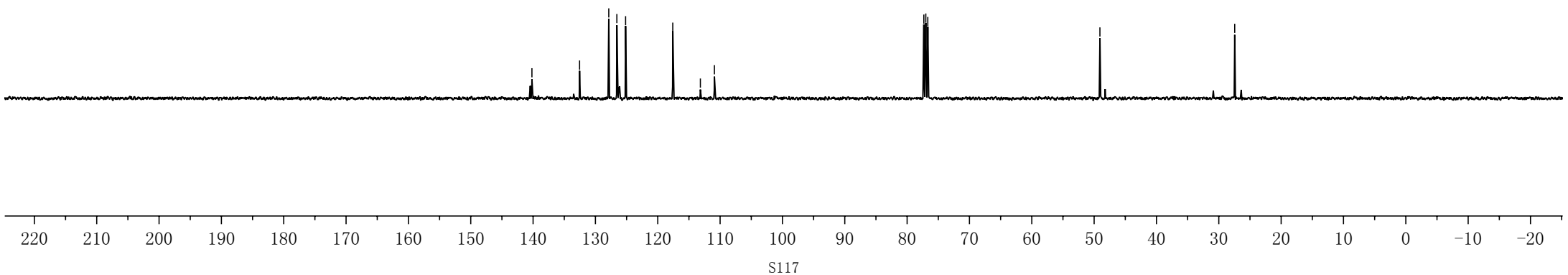
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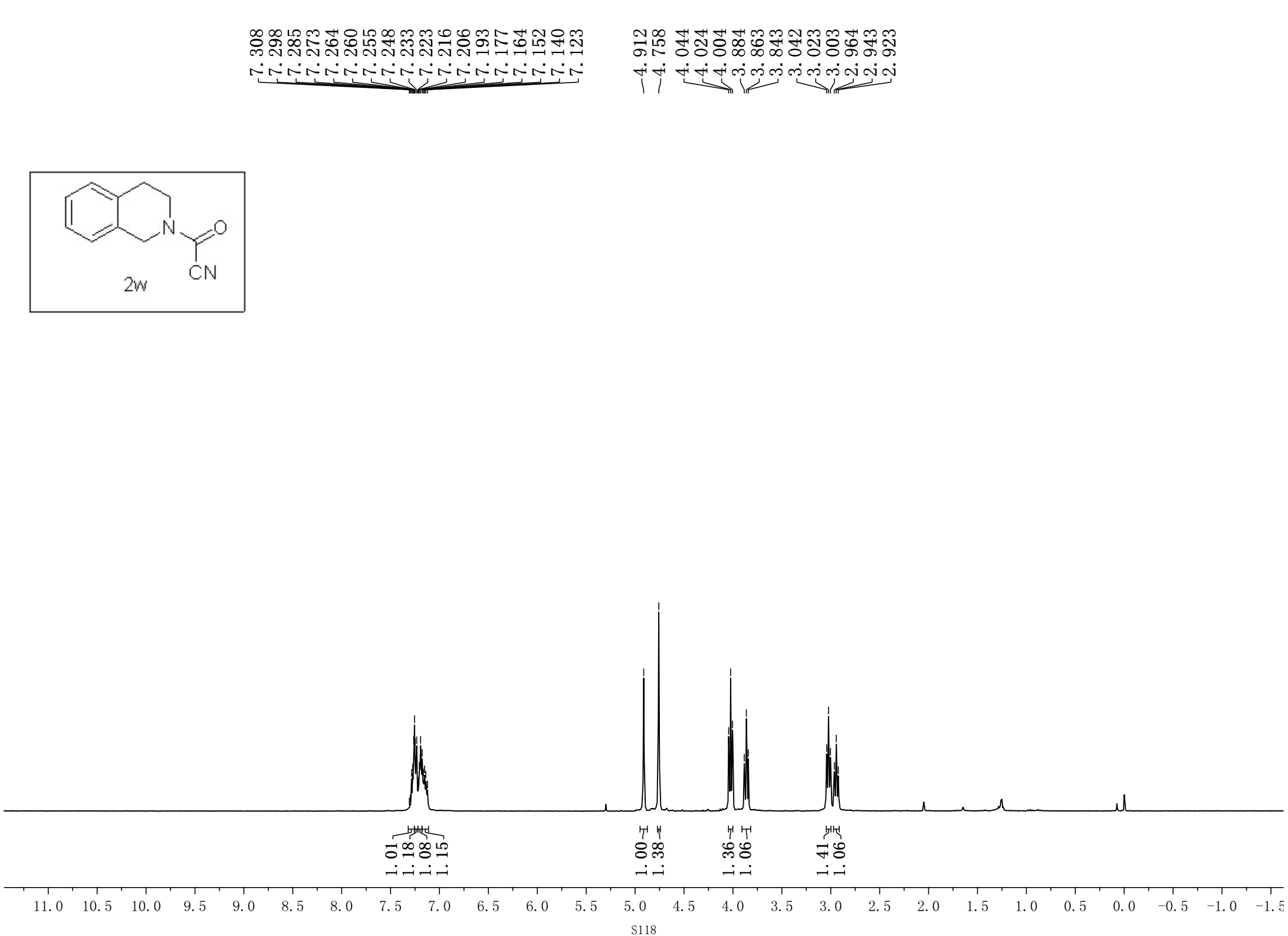
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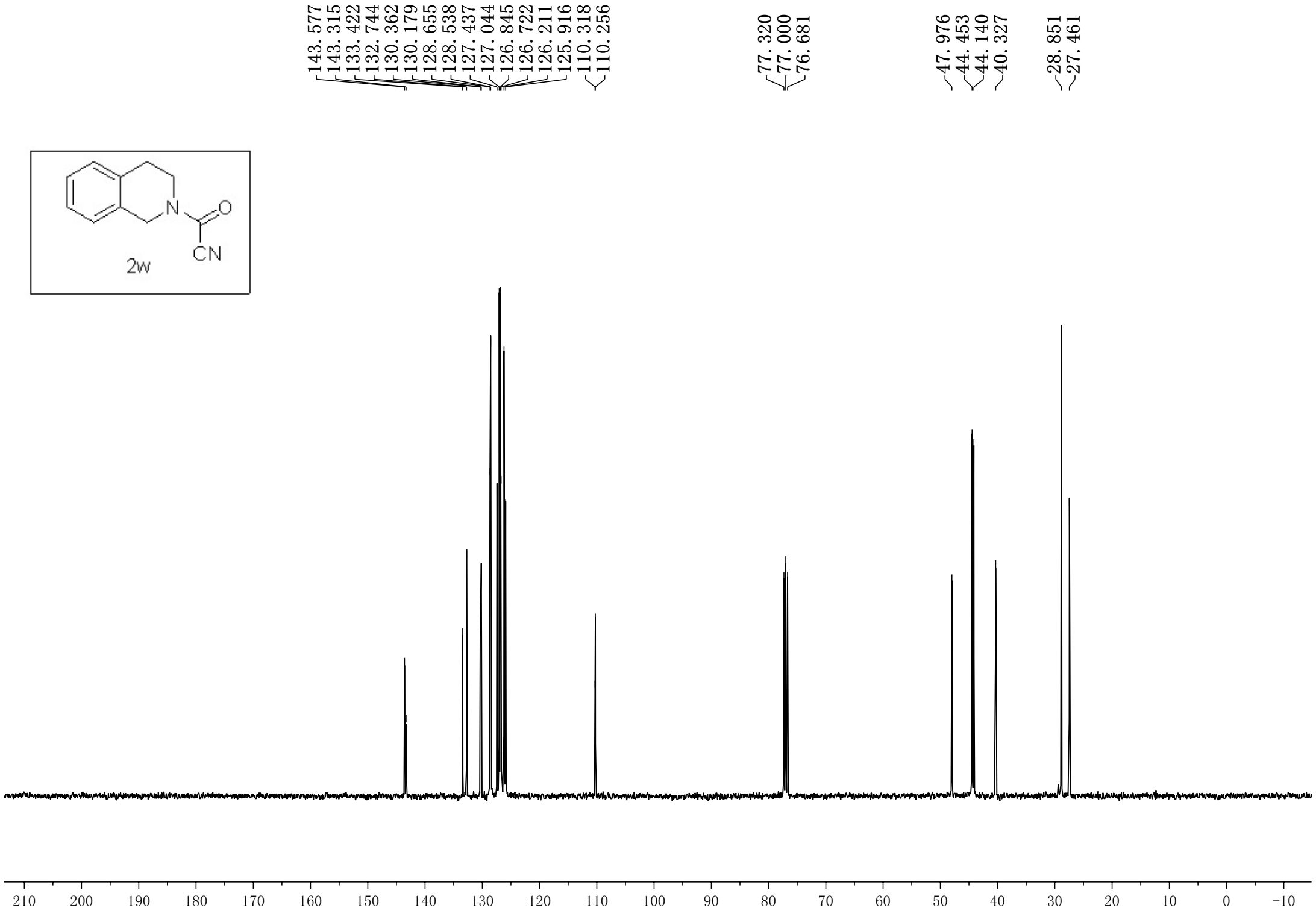
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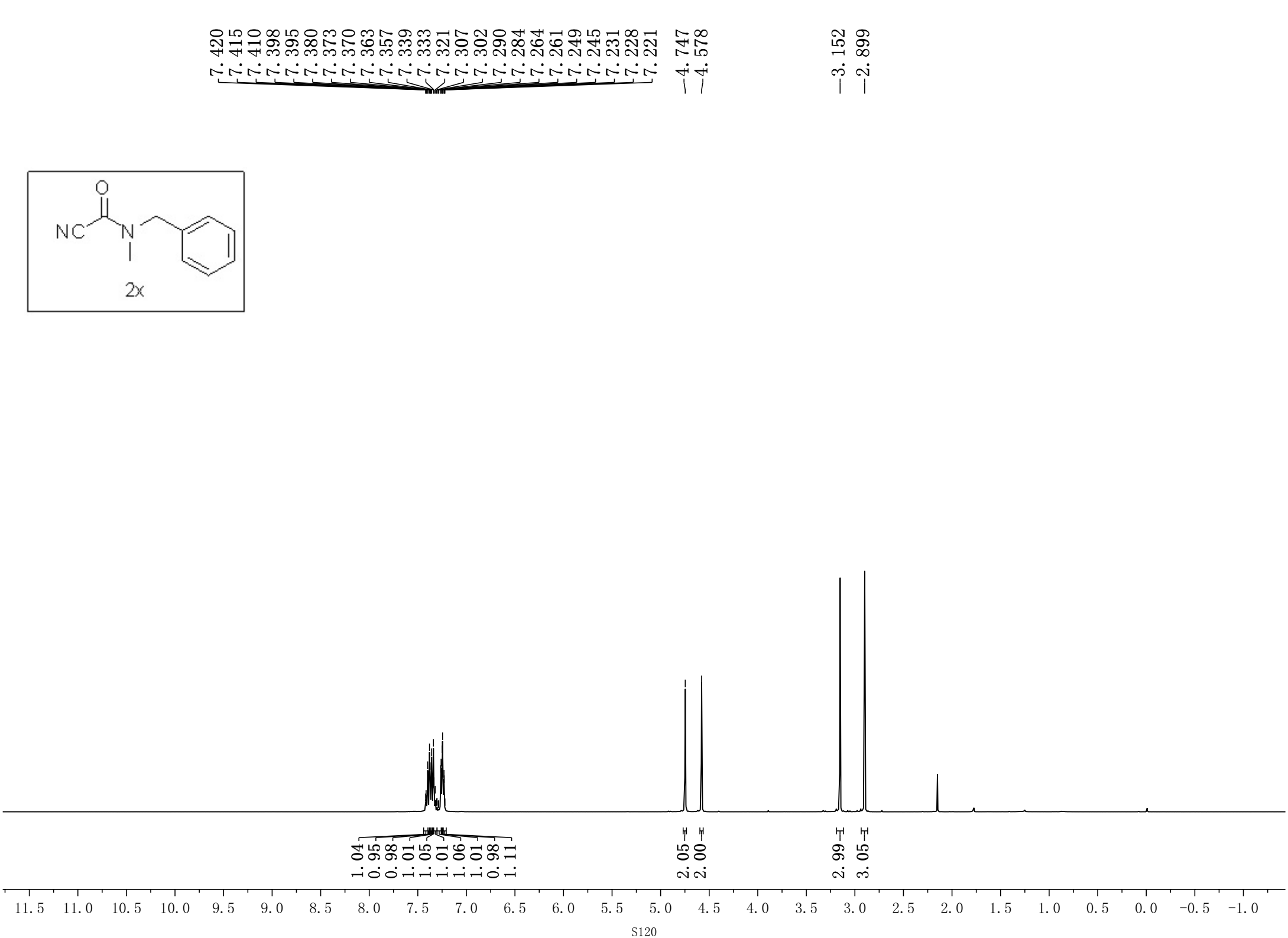
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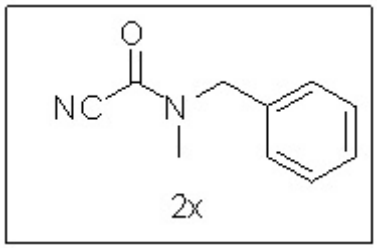

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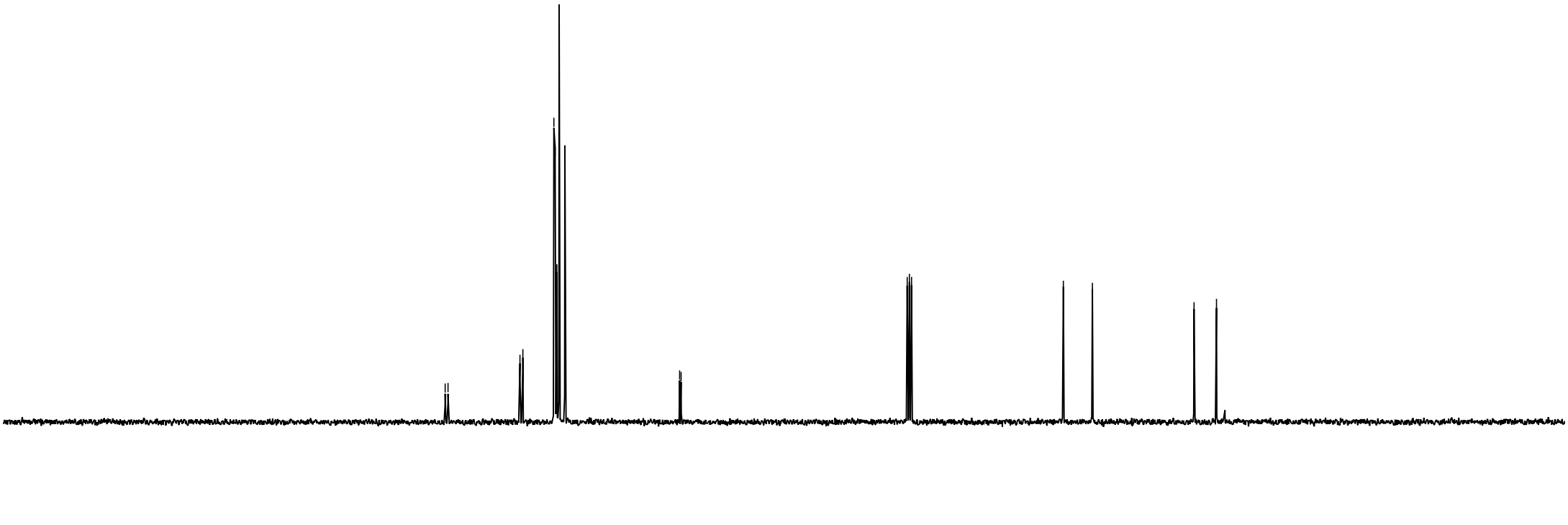

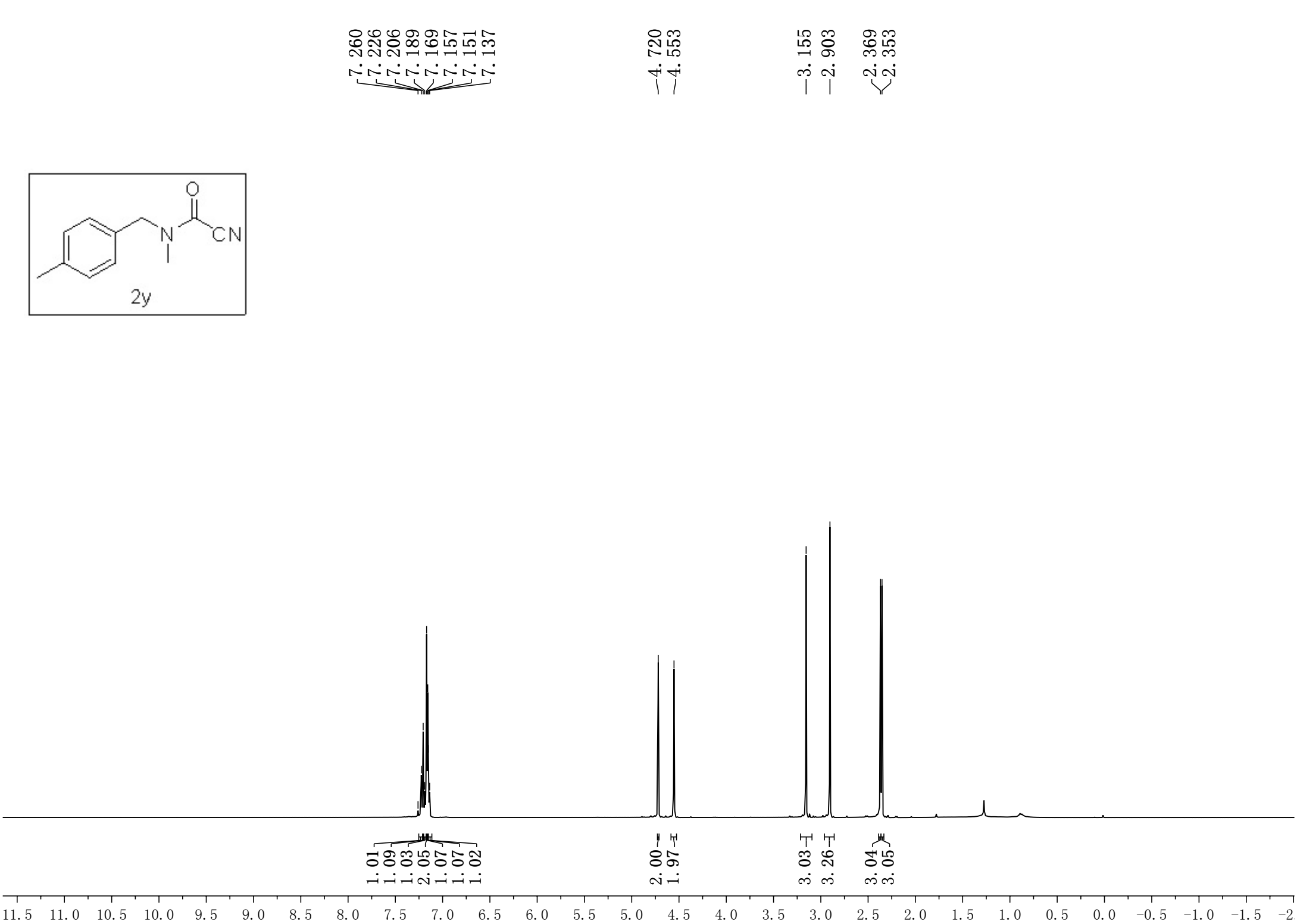
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CN
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1.09
1.03
2.05
1.07
1.07
1.02
2.00
1.97
3.03
3.26
3.04
3.05
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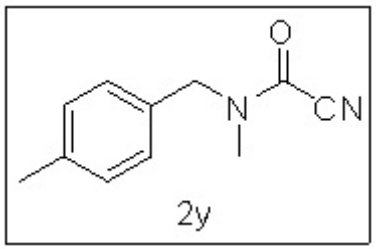

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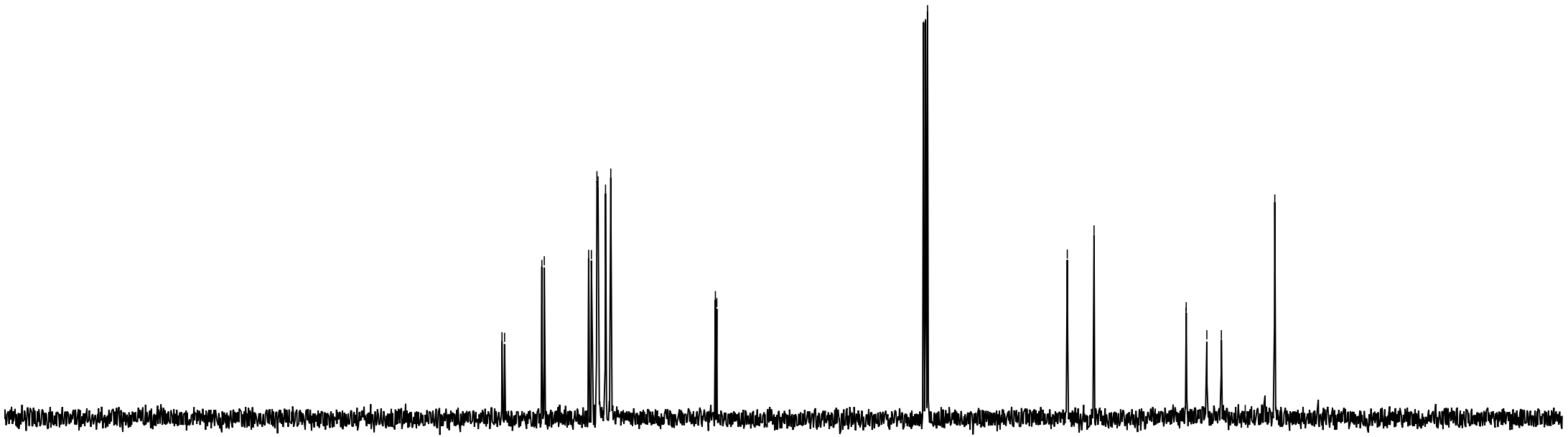

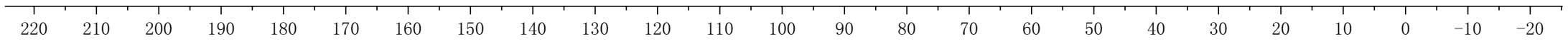

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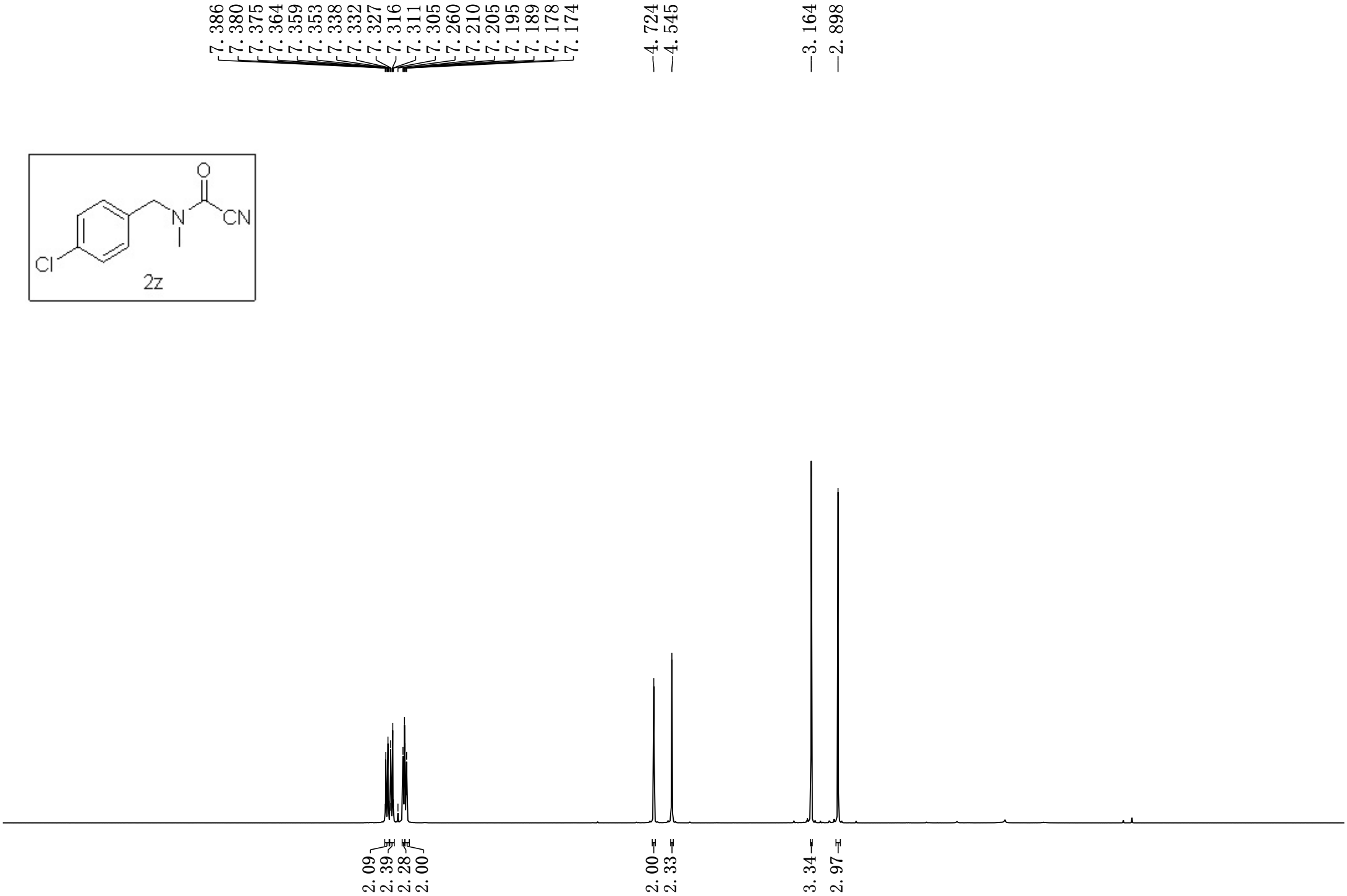
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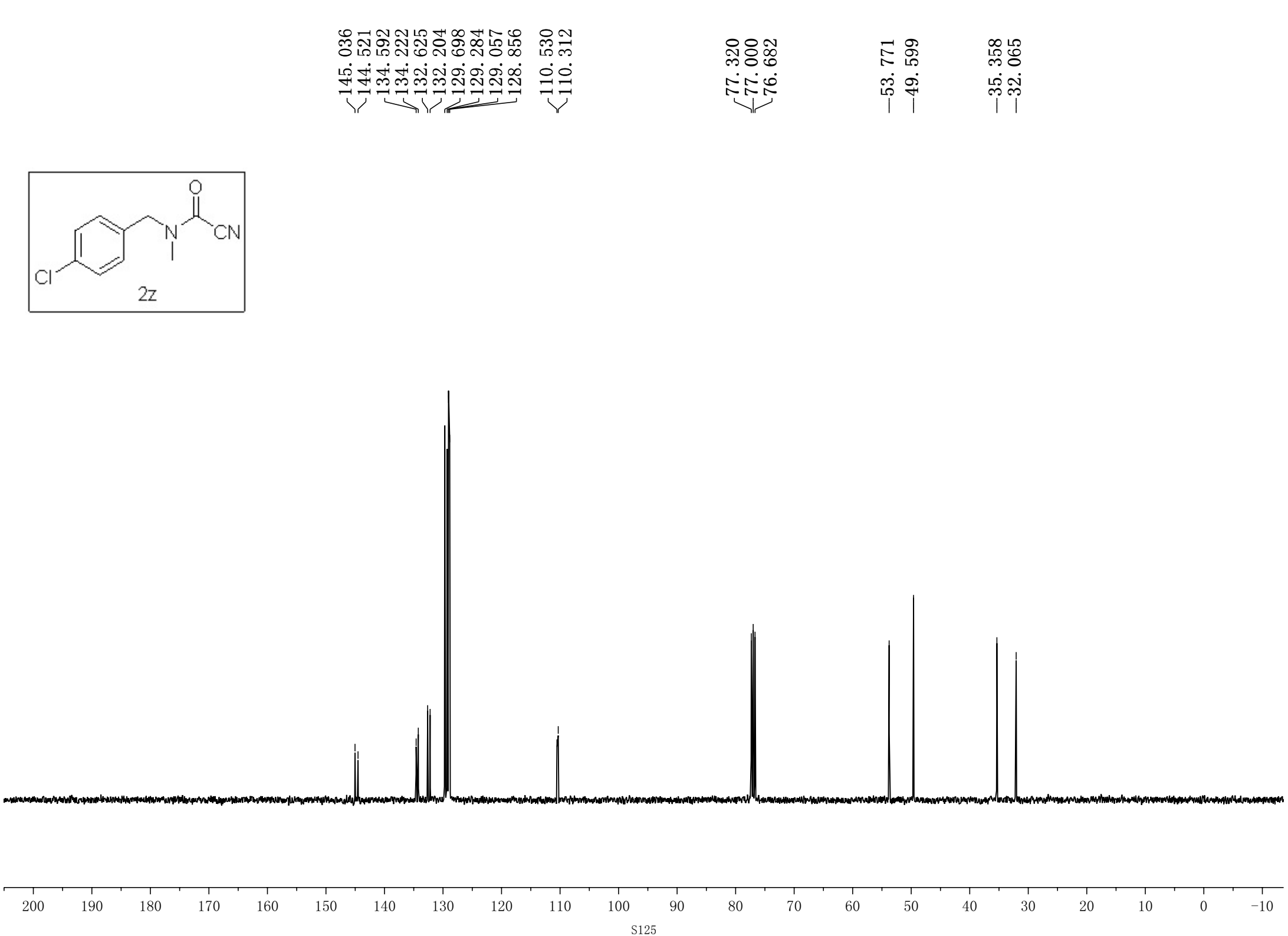
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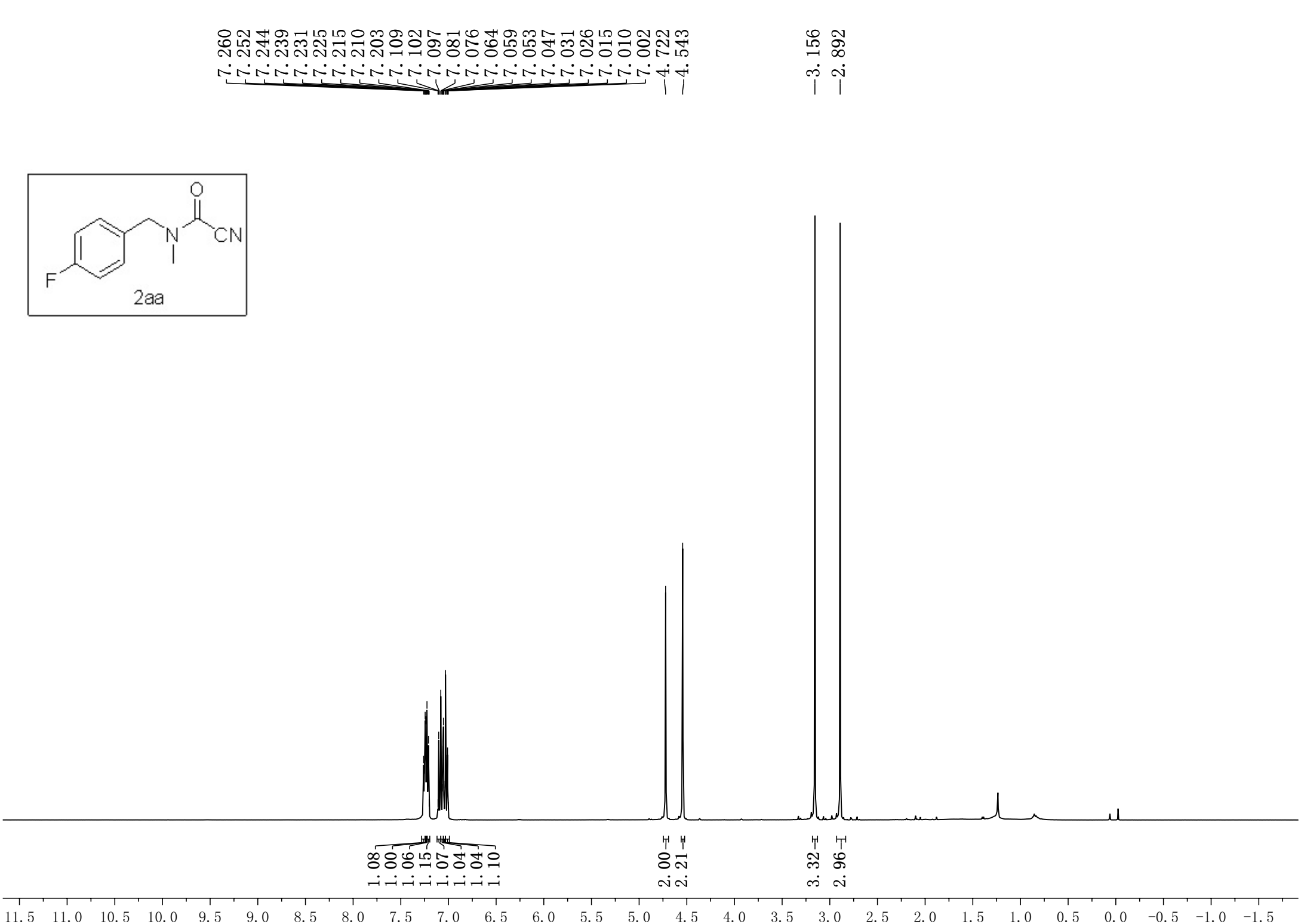
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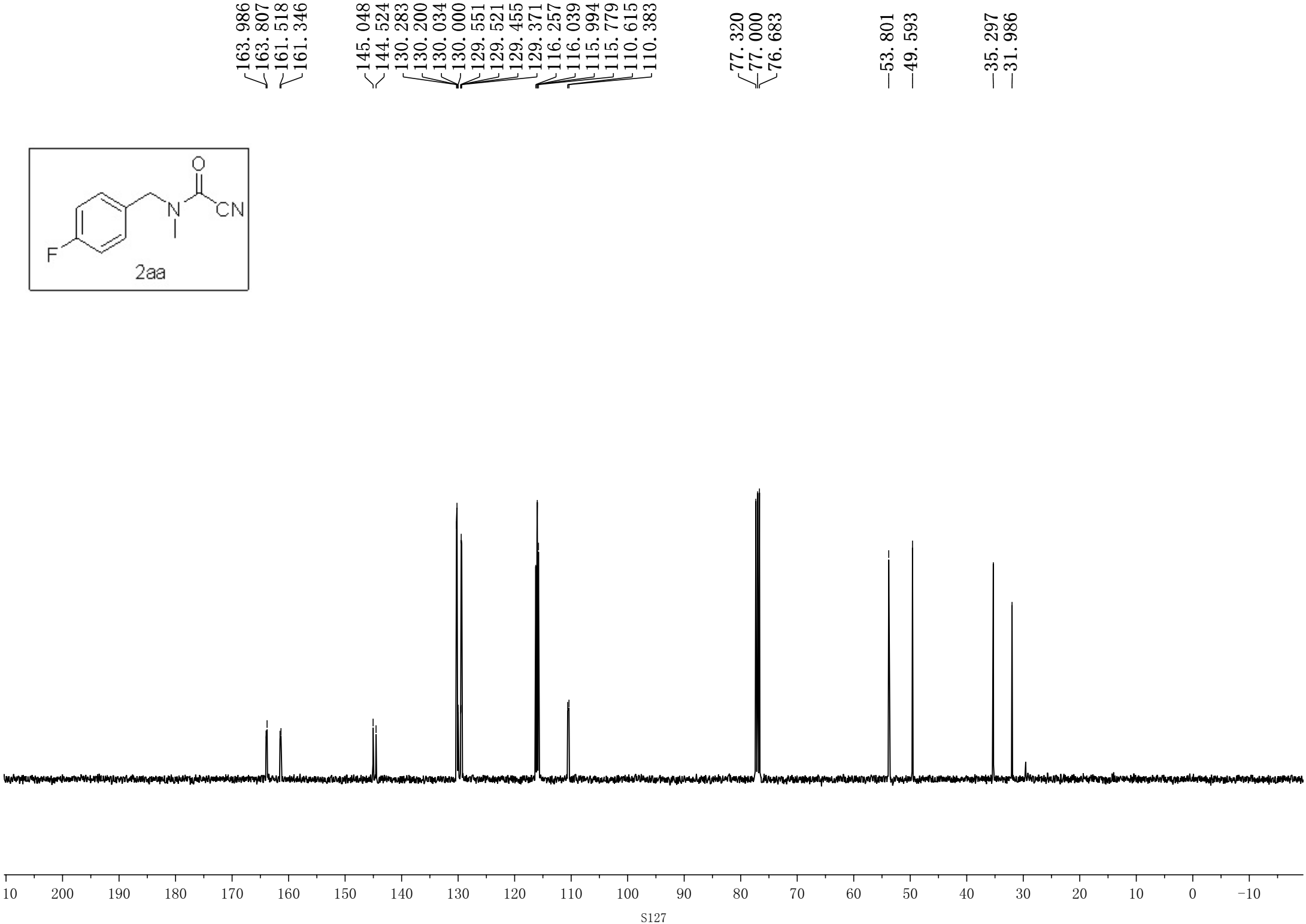
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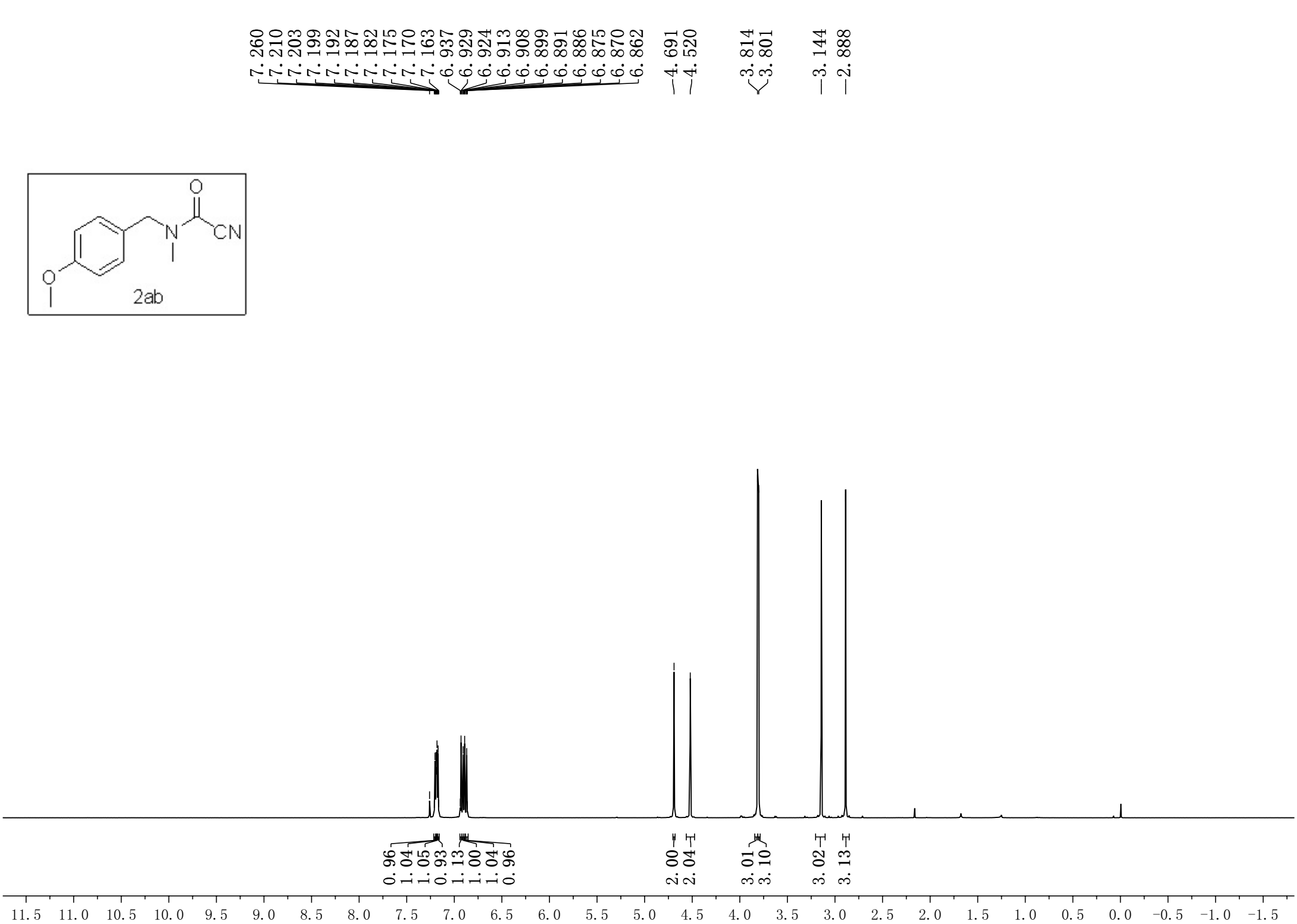
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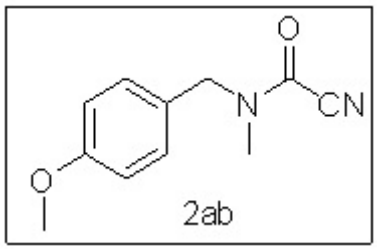

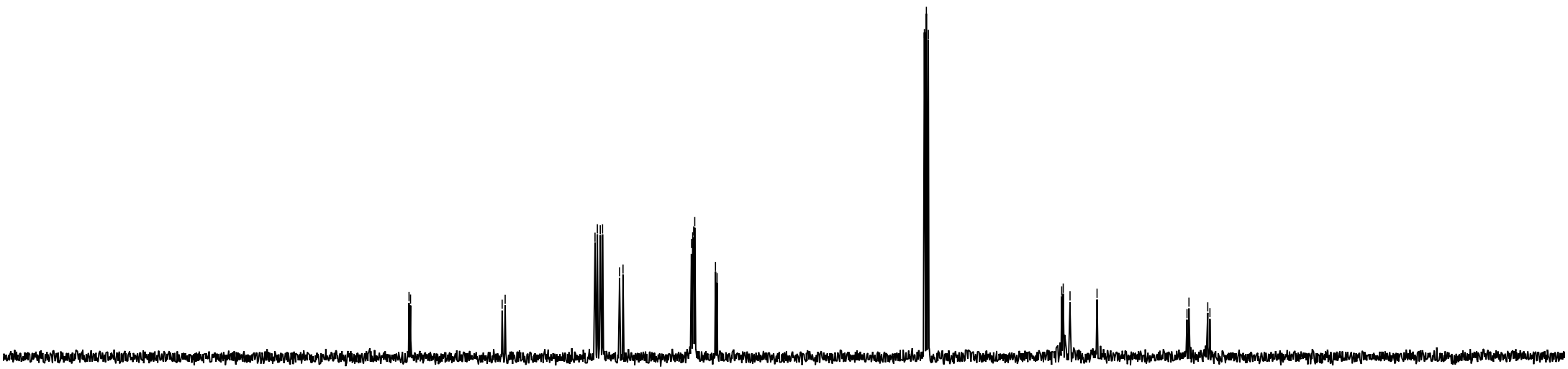

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