Intramolecular Csp^3-H/C-C Bond Amination of Alkyl Azides for the Selective Synthesis of Cyclic Imines and Tertiary Amines

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Supplementary Information

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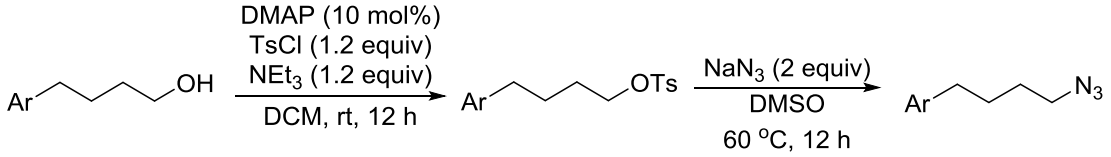
(A) General Remarks

All manipulations were conducted with schlenk tube. ^{1}H-NMR spectra were recorded on Bruker AVIII-400 spectrometers. Chemical shifts (in ppm) were calibrated with $CDCl_3$ (tetramethylsilane, δ = 0 ppm). ^{13}C-NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.0 ppm). HR-ESI-MS spectra were measured on a Fourier Transform Ion Cyclotron Resonance Mass spectrometer (APEX IV, Bruker). HR-EI-MS spectra were recorded on a GCT-MS Micromass UK spectrometer. HR-APCI-MS spectra were recorded on a Thermo Scientific EXACTIVE mass spectrometer. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification.

(B) Preparation of Starting Materials

a) Typical procedure for preparation of alkyl azides 1 and 3:

Procedure A: The starting materials **1a**, **1c**, **1f** and **1g** were prepared according to previously reported literatures.[1,2]

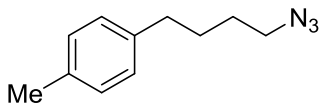


Tosyl chloride (TsCl, 2.29 g, 12 mmol) was added in batches to a mixture of 4-dimethylaminopyridine (DMAP, 123 mg, 1.0 mmol), triethylamine (1.21 g, 12 mmol) and 4-arylbutan-1-ol (10 mmol) in dichloromethane (40 mL). The resulting mixture was stirred at room temperature for 12 hours. Next, the mixture was diluted with water (40 mL) and extracted with dichloromethane for three times (30 mL×3). The combined organic phase was washed with saturated brine (30 mL) and dried over anhydrous $MgSO_4$. Then, the organic phase was evaporated in vacuo and purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford 4-arylbutyl 4-methylbenzenesulfonate.

4-Arylbutyl 4-methylbenzenesulfonate (5 mmol) was dissolved in DMSO (10 mL). NaN_3 (0.65 g, 10 mmol) was added in batches to the solution at 60 ^{o}C. The resulting mixture was stirred at 60 ^{o}C for 12 hours. Next, the mixture was diluted with water (30

mL) and extracted with ethyl acetate for three times (30 mL×3). The organic phase was washed with saturated brine for twice (30 mL×2) and dried over anhydrous $MgSO_4$. Then, the organic phase was evaporated in vacuo and purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford the product **1a**, **1c**, **1f** or **1g**.

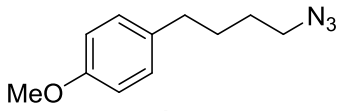
1-(4-azidobutyl)-4-methylbenzene (1a)



1a

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.11-7.05 (m, 4H), 3.26 (t, *J* = 6.6Hz, 2H), 2.60 (t, *J* = 7.4Hz, 2H), 2.32 (s, 3H), 1.70-1.60 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 138.7, 135.3, 129.0, 128.2, 51.3, 34.9, 28.5, 28.4, 20.9; **HRMS (EI)** exact mass calc'd for $C_{11}H_{15}N_3$ ($[M]^+$): 189.1266; found *m/z*: 189.1268.

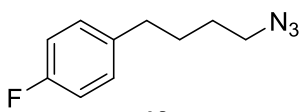
1-(4-azidobutyl)-4-methoxybenzene (1c)



1c

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.09 (d, *J* = 8.4Hz, 2H), 6.83 (d, *J* = 8.4Hz, 2H), 3.78 (s, 3H), 3.27 (t, *J* = 6.4Hz, 2H), 2.58 (t, *J* = 7.2Hz, 2H), 1.69-1.58 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.8, 133.9, 129.2, 113.8, 55.2, 51.3, 34.4, 28.6, 28.3; **HRMS (EI)** exact mass calc'd for $C_{11}H_{15}N_3O$ ($[M]^+$): 205.1215; found *m/z*: 205.1212.

1-(4-azidobutyl)-4-fluorobenzene (1f)

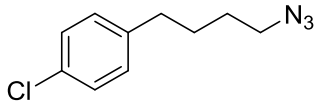


1f

Pale yellow oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.14-7.10 (m, 2H), 6.99-6.94 (m, 2H), 3.28 (t, *J* = 6.6Hz, 2H), 2.61 (t, *J* = 7.4Hz, 2H), 1.71-1.59 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 161.3 (d, $^1J_{C\text{-}F}$ = 242.4Hz), 137.4 (d, $^4J_{C\text{-}F}$ = 3.2Hz), 129.6 (d, $^3J_{C\text{-}F}$ = 8.4Hz),

115.1 (d, $^{2}J_{C\text{-}F}$ = 20.6Hz), 51.3, 34.5, 28.5, 28.3; **HRMS (EI)** exact mass calc'd for $C_{11}H_{15}N_3$ ([M]$^+$): 189.1266; found *m/z*: 189.1265

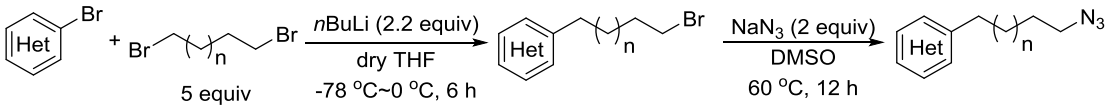
1-(4-azidobutyl)-4-chlorobenzene (1g)



1g

Pale yellow oil; **^{1}H-NMR (400MHz, CDCl$_3$)** δ 7.25 (d, *J* = 8.0Hz, 2H), 7.10 (d, *J* = 8.4Hz, 2H), 3.28 (t, *J* = 6.6Hz, 2H), 2.61 (t, *J* = 7.4Hz, 2H), 1.72-1.59 (m, 4H); **^{13}C-NMR (100MHz, CDCl$_3$)** δ 140.2, 131.6, 129.7, 128.5, 51.3, 34.7, 28.3; **HRMS (APCI)** exact mass calc'd for $C_{10}H_{13}N_{35}Cl$ ([M-N_2+H]$^+$): 182.0731; found *m/z*: 182.0729

Procedure B: The starting materials **1b**, **1d**, **1e**, **1h-k**, **3a-g** and **3i-o** were prepared according to previously reported literature.[2-4]

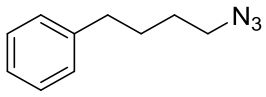


To a stirred solution of arylbromide (6 mmol) in anhydrous THF (30 mL) under an argon atmosphere, *n*-butyllithium (5.5 mL, 2.4 M in hexane) was slowly added at -78 °C. The reaction mixture was stirred at -78 °C for 1 hour, and then warmed to 0 °C. The solution of dibromoalkane (30 mmol) in anhydrous THF (10 mL) was added to the reaction mixture at once under stirring. The reaction solution was allowed to stir at 0 °C for 6 hours. The reaction was quenched with water (30 mL), and the mixture was extracted with ethyl acetate for three times (20 mL×3). The organic phase was dried over anhydrous $MgSO_4$, evaporated in vacuo and purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford aryl bromoalkane.

Aryl bromoalkane (5 mmol) was dissolved in DMSO (10 mL). NaN_3 (0.65 g, 10 mmol) was added in batches to the solution at 60 °C. The resulting mixture was stirred at 60 °C for 12 hours. Next, the mixture was diluted with water (30 mL) and extracted with ethyl acetate for three times (30 mL×3). The organic phase was washed with saturated brine for twice (30 mL×2) and dried over anhydrous $MgSO_4$. Then, the organic phase was evaporated in vacuo and purified by flash chromatography on silica

gel (eluent: petroleum ether/ethyl acetate) to afford the product **1b**, **1d**, **1e**, **1h-k**, **3a-g** or **3i-o**.

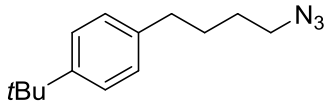
(4-azidobutyl)benzene (1b)[3]



1b

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.30-7.27 (m, 2H), 7.21-7.17 (m, 3H), 3.27 (t, *J* = 6.6Hz, 2H), 2.64 (t, *J* = 7.4Hz, 2H), 1.75-1.59 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 141.8, 128.4, 125.9, 51.3, 35.3, 28.4

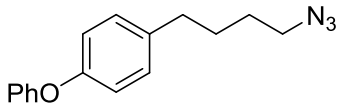
1-(4-azidobutyl)-4-(*tert*-butyl)benzene (1d)



1d

Pale yellow oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.31 (d, *J* = 8.4Hz, 2H), 7.11 (d, *J* = 8.0Hz, 2H), 3.28 (t, *J* = 6.4Hz, 2H), 2.61 (t, *J* = 7.2Hz, 2H), 1.70-1.64 (m, 4H), 1.31 (s, 9H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 148.7, 138.7, 128.0, 125.2, 51.4, 34.8, 34.3, 31.4, 28.5, 28.4; **HRMS (EI)** exact mass calc'd for $C_{14}H_{21}N_3$ ($[M]^+$): 231.1735; found *m/z*: 231.1738

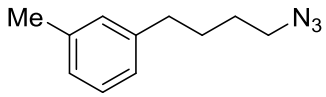
1-(4-azidobutyl)-4-phenoxybenzene (1e)



1e

Pale yellow oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.33-7.29 (m, 2H), 7.14-7.12 (m, 2H), 7.09-7.05 (m, 1H), 7.00-6.98 (m, 2H), 6.95-6.92 (m, 2H), 3.29 (t, *J* = 6.6Hz, 2H), 2.62 (t, *J* = 7.2Hz, 2H), 1.72-1.61 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.6, 155.2, 136.8, 129.7, 129.5, 122.9, 119.0, 118.5, 51.3, 34.6, 28.5, 28.4; **HRMS (EI)** exact mass calc'd for $C_{16}H_{17}N_3O$ ($[M]^+$): 267.1372; found *m/z*: 267.1375

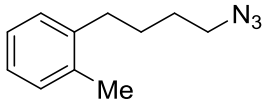
1-(4-azidobutyl)-3-methylbenzene (1h)



1h

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.19-7.15 (m, 1H), 7.01-6.96 (m, 3H), 3.27 (t, *J* = 6.8Hz, 2H), 2.60 (t, *J* = 7.2Hz, 2H), 2.33 (s, 3H), 1.72-1.60 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 141.7, 137.9, 129.2, 128.2, 126.6, 125.3, 51.3, 35.3, 28.44, 28.42, 21.4; **HRMS (APCI)** exact mass calc'd for $C_{11}H_{16}N$ ($[M-N_2+H]^+$): 162.1277; found *m/z*: 162.1276

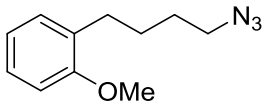
1-(4-azidobutyl)-2-methylbenzene (1i)



1i

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.15-7.11 (m, 4H), 3.30 (t, *J* = 6.4Hz, 2H), 2.65-2.61 (m, 2H), 2.30 (s, 3H), 1.69-1.65 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 140.0, 135.8, 130.2, 128.8, 126.0, 125.9, 51.3, 32.7, 28.7, 27.2, 19.2; **HRMS (APCI)** exact mass calc'd for $C_{11}H_{16}N$ ($[M-N_2+H]^+$): 162.1277; found *m/z*: 162.1276

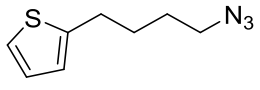
1-(4-azidobutyl)-2-methoxybenzene (1j)



1j

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.22-7.18 (m, 1H), 6.78-6.73 (m, 3H), 3.80 (s, 3H), 3.28 (t, *J* = 6.6Hz, 2H), 2.62 (t, *J* = 7.4Hz, 2H), 1.73-1.61 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 159.7, 143.4, 129.3, 120.8, 114.2, 111.1, 55.1, 51.3, 35.4, 28.4, 28.3; **HRMS (EI)** exact mass calc'd for $C_{11}H_{15}N_3O$ ($[M]^+$): 205.1215; found *m/z*: 205.1212

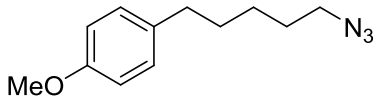
2-(4-azidobutyl)thiophene (1k)



1k

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.13-7.11 (m, 1H), 6.93-6.91 (m, 1H), 6.80-6.78 (m, 1H), 3.29 (t, *J* = 6.8Hz, 2H), 2.87 (t, *J* = 7.2Hz, 2H), 1.79-1.73 (m, 2H), 1.70-1.64 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 144.6, 126.7, 124.3, 123.1, 51.2, 29.3, 28.8, 28.2; **HRMS (APCI)** exact mass calc'd for $C_8H_{12}NS$ ($[M-N_2+H]^+$): 154.0685; found *m/z*: 154.0683

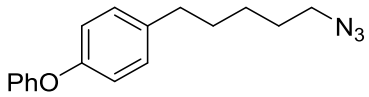
1-(5-azidopentyl)-4-methoxybenzene (3a)



3a

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.08 (d, *J* = 8.4Hz, 2H), 6.82 (d, *J* = 8.8Hz, 2H), 3.78 (s, 3H), 3.25 (t, *J* = 7.0Hz, 2H), 2.56 (t, *J* = 7.6Hz, 2H), 1.65-1.57 (m, 4H), 1.43-1.37 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.7, 134.3, 129.2, 113.7, 55.2, 51.4, 34.8, 31.2, 28.7, 26.2; **HRMS (EI)** exact mass calc'd for $C_{12}H_{17}N_3O$ ($[M]^+$): 219.1372; found *m/z*: 219.1373

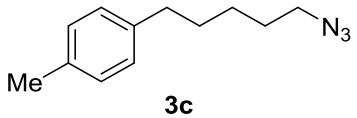
1-(5-azidopentyl)-4-phenoxybenzene (3b)



3b

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.33-7.29 (m, 2H), 7.14-7.12 (m, 2H), 7.09-7.05 (m, 1H), 7.00-6.98 (m, 2H), 6.95-6.91 (m, 2H), 3.26 (t, *J* = 7.0Hz, 2H), 2.60 (t, *J* = 7.8Hz, 2H), 1.68-1.60 (m, 4H), 1.46-1.40 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.6, 155.1, 137.3, 129.6, 129.5, 122.9, 119.0, 118.5, 51.4, 35.0, 31.1, 28.7, 26.3; **HRMS (EI)** exact mass calc'd for $C_{17}H_{19}N_3O$ ($[M]^+$): 281.1528; found *m/z*: 281.1523

1-(5-azidopentyl)-4-methylbenzene (3c)

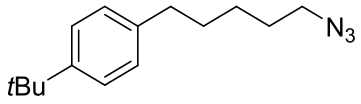


3c

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.10-7.04 (m, 4H), 3.24 (t, *J* = 7.0Hz, 2H), 2.58 (t, *J* = 7.6Hz, 2H), 2.31 (s, 3H), 1.66-1.58 (m, 4H), 1.44-1.36 (m, 2H); **^{13}C-**

NMR (100MHz, $CDCl_3$) δ 139.2, 135.2, 129.0, 128.2, 51.4, 35.3, 31.1, 28.7, 26.3, 20.9; **HRMS (EI)** exact mass calc'd for $C_{12}H_{17}N_3$ ($[M]^+$): 203.1422; found *m/z*: 203.1421

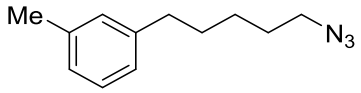
1-(5-azidopentyl)-4-(*tert*-butyl)benzene (3d)



3d

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.30 (d, *J* = 8.4Hz, 2H), 7.10 (d, *J* = 8.4Hz, 2H), 3.25 (t, *J* = 6.8Hz, 2H), 2.59 (t, *J* = 7.8Hz, 2H), 1.66-1.59 (m, 4H), 1.44-1.40 (m, 2H), 1.31 (s, 9H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 148.5, 139.2, 128.0, 125.2, 51.4, 35.2, 34.3, 31.4, 30.9, 28.7, 26.4; **HRMS (EI)** exact mass calc'd for $C_{15}H_{23}N_3$ ($[M]^+$): 245.1892; found *m/z*: 245.1888

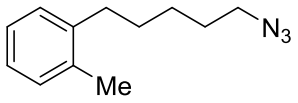
1-(5-azidopentyl)-3-methylbenzene (3e)



3e

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.19-7.15 (m, 1H), 7.00-6.96 (m, 3H), 3.25 (t, *J* = 7.0Hz, 2H), 2.58 (t, *J* = 7.8Hz, 2H), 2.33 (s, 3H), 1.67-1.59 (m, 4H), 1.45-1.39 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 142.2, 137.8, 129.2, 128.2, 126.5, 125.3, 51.4, 35.7, 31.0, 28.7, 26.4, 21.4; **HRMS (APCI)** exact mass calc'd for $C_{12}H_{18}N$ ($[M-N_2+H]^+$): 176.1434; found *m/z*: 174.1432

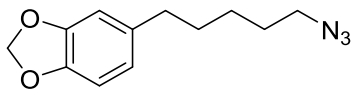
1-(5-azidopentyl)-2-methylbenzene (3f)



3f

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.14-7.09 (m, 4H), 3.26 (t, *J* = 7.0Hz, 2H), 2.60 (t, *J* = 7.8Hz, 2H), 2.30 (s, 3H), 1.68-1.56 (m, 4H), 1.49-1.43 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 140.4, 135.8, 130.1, 128.7, 125.9, 51.4, 33.1, 29.7, 28.8, 26.7, 19.2; **HRMS (APCI)** exact mass calc'd for $C_{12}H_{18}N$ ($[M-N_2+H]^+$): 176.1434; found *m/z*: 176.1431

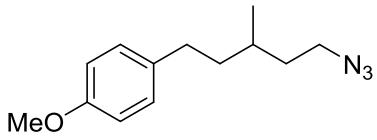
5-(5-azidopentyl)benzo[*d*][1,3]dioxole (3g)



3g

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 6.73-6.71 (m, 1H), 6.67-6.66 (m, 1H), 6.62-6.60 (m, 1H), 5.91 (s, 2H), 3.25 (t, *J* = 7.0Hz, 2H), 2.54 (t, *J* = 7.6Hz, 2H), 1.65-1.56 (m, 4H), 1.43-1.37 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 147.5, 145.5, 136.1, 121.0, 108.8, 108.1, 100.7, 51.4, 35.4, 31.2, 28.7, 26.2; **HRMS (EI)** exact mass calc'd for $C_{12}H_{15}N_3O_2$ ($[M]^+$): 233.1164; found *m/z*: 233.1165

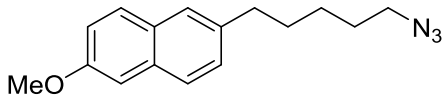
1-(5-azido-3-methylpentyl)-4-methoxybenzene (3i)



3i

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.09 (d, *J* = 8.4Hz, 2H), 6.82 (d, *J* = 8.8Hz, 2H), 3.78 (s, 3H), 3.35-3.22 (m, 2H), 2.65-2.48 (m, 2H), 1.72-1.55 (m, 3H), 1.49-1.42 (m, 2H), 0.96 (d, *J* = 6.4Hz, 3H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.7, 134.6, 129.1, 113.8, 55.2, 49.4, 38.9, 35.6, 32.3, 30.0, 19.2; **HRMS (EI)** exact mass calc'd for $C_{13}H_{19}N_3O$ ($[M]^+$): 233.1528; found *m/z*: 233.1526

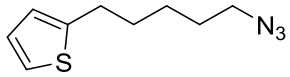
2-(5-azidopentyl)-6-methoxynaphthalene (3j)



3j

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.66 (d, *J* = 8.4Hz, 2H), 7.52 (s, 1H), 7.27 (dd, *J* = 8.2Hz, 1.8Hz, 1H), 7.13-7.10 (m, 2H), 3.89 (s, 3H), 3.24 (t, *J* = 7.0Hz, 2H), 2.74 (t, *J* = 7.6Hz, 2H), 1.73-1.67 (m, 2H), 1.66-1.59 (m, 2H), 1.46-1.40 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.1, 137.4, 132.9, 129.1, 128.9, 127.7, 126.7, 126.2, 118.7, 105.6, 55.2, 51.4, 35.7, 30.9, 28.7, 26.3; **HRMS (EI)** exact mass calc'd for $C_{16}H_{19}N_3O$ ($[M]^+$): 269.1528; found *m/z*: 269.1527

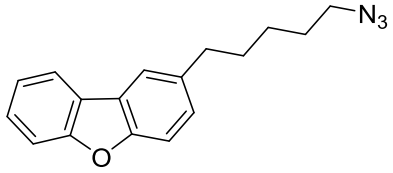
2-(5-azidopentyl)thiophene (3k)



3k

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.12-7.10 (m, 1H), 6.92-6.90 (m, 1H), 6.78-6.77 (m, 1H), 3.26 (t, *J* = 6.8Hz, 2H), 2.84 (t, *J* = 7.4Hz, 2H), 1.75-1.59 (m, 4H), 1.48-1.41 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 145.1, 126.7, 124.1, 122.9, 51.3, 31.2, 29.7, 28.6, 26.1; **HRMS (APCI)** exact mass calc'd for $C_9H_{14}NS$ ($[M-N_2+H]^+$): 168.0842; found *m/z*: 168.0839

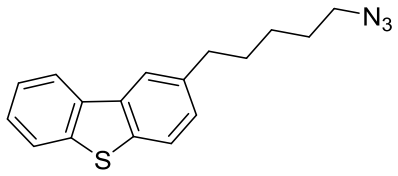
2-(5-azidopentyl)dibenzo[*b,d*]furan (3l)



3l

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.93-7.91 (m, 1H), 7.73 (s, 1H), 7.55-7.53 (m ,1H), 7.48-7.41 (m, 2H), 7.34-7.30 (m, 1H), 7.26-7.24 (m, 1H), 3.25 (t, *J* = 7.0Hz, 2H), 2.77 (t, *J* = 7.6Hz, 2H), 1.76-1.60 (m, 4H), 1.48-1.40 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 156.5, 154.7, 136.8, 127.6, 126.9, 124.21, 124.18, 122.5, 120.5, 120.0, 111.6, 111.2, 51.3, 35.6, 31.5, 28.7, 26.3; **HRMS (EI)** exact mass calc'd for $C_{17}H_{17}N_3O$ ($[M]^+$): 279.1372; found *m/z*: 279.1375

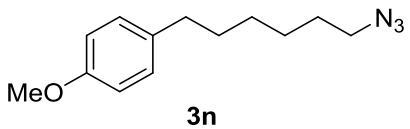
2-(5-azidopentyl)dibenzo[*b,d*]thiophene (3m)



3m

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 8.15-8.12 (m, 1H), 7.94 (s, 1H), 7.84-7.82 (m, 1H), 7.76-7.74 (m, 1H), 7.46-7.42 (m, 2H), 7.28-7.26 (m, 1H), 3.26 (t, *J* = 7.0Hz, 2H), 2.79 (t, *J* = 7.6Hz, 2H), 1.77-1.61 (m, 4H), 1.49-1.43 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 139.8, 138.7, 136.8, 135.7, 135.4, 127.5, 126.6, 124.2, 122.8, 122.5, 121.5, 121.1, 51.3, 35.8, 31.3, 28.7, 26.3; **HRMS (EI)** exact mass calc'd for $C_{17}H_{17}N_3S$ ($[M]^+$): 295.1143; found *m/z*: 295.1140

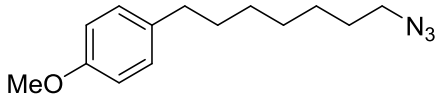
1-(6-azidohexyl)-4-methoxybenzene (3n)



3n

Colorless oil; **^{1}H-NMR (400MHz, CDCl$_3$)** δ 7.08 (d, *J* = 8.4Hz, 2H), 6.82 (d, *J* = 8.8Hz, 2H), 3.78 (s, 3H), 3.24 (t, *J* = 7.0Hz, 2H), 2.55 (t, *J* = 7.6Hz, 2H), 1.63-1.56 (m, 4H), 1.41-1.32 (m, 4H); **^{13}C-NMR (100MHz, CDCl$_3$)** δ 157.7, 134.6, 129.2, 113.7, 55.2, 51.4, 34.8, 31.5, 28.74, 28.66, 26.6; **HRMS (EI)** exact mass calc'd for $C_{13}H_{19}N_3O$ ($[M]^+$): 233.1528; found *m/z*: 233.1524

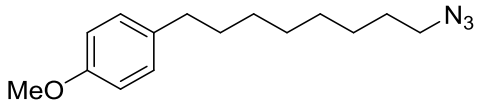
1-(7-azidoheptyl)-4-methoxybenzene (3o)



3o

Colorless oil; **^{1}H-NMR (400MHz, CDCl$_3$)** δ 7.08 (d, *J* = 8.8Hz, 2H), 6.82 (d, *J* = 8.4Hz, 2H), 3.78 (s, 3H), 3.24 (t, *J* = 7.0Hz, 2H), 2.54 (t, *J* = 7.8Hz, 2H), 1.60-1.55 (m, 4H), 1.37-1.30 (m, 6H); **^{13}C-NMR (100MHz, CDCl$_3$)** δ 157.6, 134.8, 129.2, 113.6, 55.2, 51.4, 34.9, 31.5, 28.99, 28.98, 28.8, 26.6; **HRMS (EI)** exact mass calc'd for $C_{14}H_{21}N_3O$ ($[M]^+$): 247.1685; found *m/z*: 247.1687

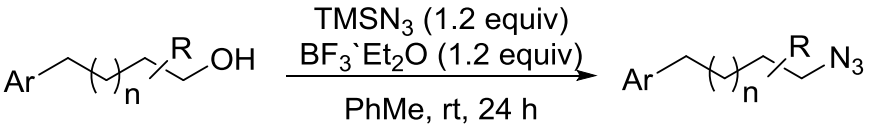
1-(8-azidooctyl)-4-methoxybenzene (3p)



3p

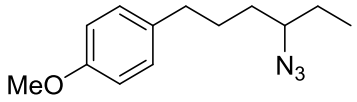
Colorless oil; **^{1}H-NMR (400MHz, CDCl$_3$)** δ 7.09-7.07 (m, 2H), 6.84-6.81 (m, 2H), 3.78 (s, 3H), 3.24 (t, *J* = 7.0Hz, 2H), 2.54 (t, *J* = 7.8Hz, 2H), 1.60-1.55 (m, 4H), 1.37-1.31 (m, 8H); **^{13}C-NMR (100MHz, CDCl$_3$)** δ 157.6, 134.9, 129.2, 113.6, 55.2, 51.4, 35.0, 31.6, 29.3, 29.1, 29.0, 28.8, 26.7; **HRMS (EI)** exact mass calc'd for $C_{15}H_{23}N_3O$ ($[M]^+$): 261.1841; found *m/z*: 261.1839

Procedure C: The starting materials **1l-o** and **3h** were prepared according to previously reported literatures.[5]



Boron trifluoride etherate (0.85 g, 6 mmol) was added dropwise at room temperature to a stirring solution of alcohol (3 mmol) and trimethylsilyl azide (0.68 g, 6 mmol) in toluene (10 mL) under Argon. The reaction mixture was stirred at room temperature for 24 hours and quenched with water (10 mL). The aqueous phase was extracted with ethyl acetate for three times (10 mL×3). The combined organic phase was washed with saturated brine (20 mL), dried over anhydrous $MgSO_4$, evaporated in vacuo and purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford alkyl azide **1l-o** or **3h**.

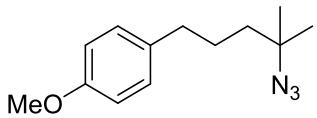
1-(4-azidohexyl)-4-methoxybenzene (1l)



1l

Pale yellow oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.09 (d, *J* = 8.8Hz, 2H), 6.83 (d, *J* = 8.4Hz, 2H), 3.79 (s, 3H), 3.21-3.18 (m, 1H), 2.58 (t, *J* = 7.4Hz, 2H), 1.78-1.49 (m, 6H), 0.96 (t, *J* = 7.4Hz, 3H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.8, 134.0, 129.2, 113.8, 64.5, 55.2, 34.7, 33.5, 28.1, 27.4, 10.5; **HRMS (EI)** exact mass calc'd for $C_{13}H_{19}N_3O$ ($[M]^+$): 233.1528; found *m/z*: 233.1530

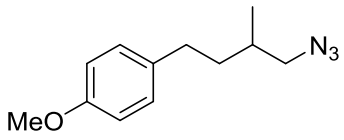
1-(4-azido-4-methylpentyl)-4-methoxybenzene (1m)



1m

Pale yellow oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.09 (d, *J* = 8.4Hz, 2H), 6.83 (d, *J* = 8.4Hz, 2H), 3.79 (s, 3H), 2.56 (t, *J* = 7.6Hz, 2H), 1.68-1.61 (m, 2H), 1.52-1.48 (m, 2H), 1.24 (s, 6H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.8, 134.1, 129.2, 113.8, 61.5, 55.2, 41.0, 35.1, 26.3, 25.9; **HRMS (EI)** exact mass calc'd for $C_{13}H_{19}N_3O$ ($[M]^+$): 233.1528; found *m/z*: 233.1532

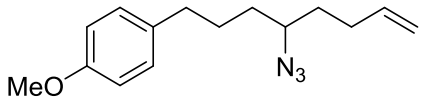
1-(4-azido-3-methylbutyl)-4-methoxybenzene (1n)



1n

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.09 (d, *J* = 8.8Hz, 2H), 6.83 (d, *J* = 8.8Hz, 2H), 3.78 (s, 3H), 3.23 (dd, *J* = 12Hz, 5.6Hz, 1H), 3.15 (dd, *J* = 11.8Hz, 6.6Hz, 1H), 2.66-2.49 (m, 2H), 1.78-1.66 (m, 2H), 1.49-1.43 (m, 1H), 1.01 (d, *J* = 6.8Hz, 3H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.8, 134.1, 129.1, 113.8, 57.7, 55.2, 36.1, 33.1, 32.2, 17.6; **HRMS (EI)** exact mass calc'd for $C_{12}H_{17}N_3O$ ($[M]^+$): 219.1372; found *m/z*: 219.1375

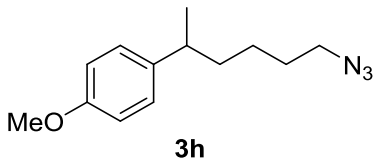
1-(4-azidooct-7-en-1-yl)-4-methoxybenzene (1o)



1o

Pale yellow oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ7.09 (d, *J* = 8.8Hz, 2H), 6.83 (d, *J* = 8.8Hz, 2H), 5.83-5.72 (m, 1H), 5.07-4.98 (m, 2H), 3.79 (s, 3H), 3.31-3.25 (m, 1H), 2.58 (t, *J* = 7.6Hz, 2H), 2.23-2.06 (m, 2H), 1.79-1.51 (m, 6H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.8, 137.4, 133.9, 129.2, 115.4, 113.8, 62.3, 55.2, 34.6, 33.9, 33.6, 30.3, 28.0; **HRMS (EI)** exact mass calc'd for $C_{15}H_{21}N_3O$ ($[M]^+$): 259.1685; found *m/z*: 259.1689

1-(6-azidohexan-2-yl)-4-methoxybenzene (3h)

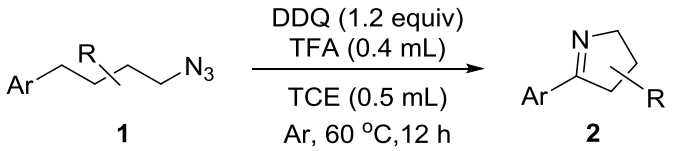


3h

Colorless oil; **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.09 (d, *J* = 8.4Hz, 2H), 6.84 (d, *J* = 8.4Hz, 2H), 3.79 (s, 3H), 3.20 (t, *J* = 7.0Hz, 2H), 2.68-2.59 (m, 1H), 1.60-1.51 (m, 4H), 1.36-1.21 (m, 5H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.8, 139.4, 127.7, 113.8, 55.2, 51.4, 39.0, 38.0, 28.9, 24.8, 22.5; **HRMS (EI)** exact mass calc'd for $C_{13}H_{19}N_3O$ ($[M+H]^+$): 233.1528; found *m/z*: 233.1532

(C) Experimental Procedure

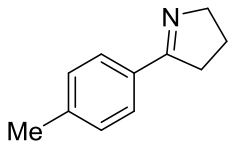
a) Typical procedure for synthesis of imines 2:



1 **2**

DDQ (81.7 mg, 0.36 mmol) was added to a 25 mL seal tube with a magnetic bar under Argon. Next, 1,1,2,2-tetrachloroethane (0.5 mL), TFA (0.4 mL) and alkyl azide (**1**, 0.3 mmol) were added in sequence. The mixture was stirred at 60 °C under argon for 12 hours as monitored by TLC. Then, the reaction mixture was diluted with ethyl acetate (6 mL) and treated with 2M NaOH aqueous solution (6 mL). The aqueous phase was extracted with ethyl acetate for three times (6 mL×3). The combined organic solvent was dried over anhydrous $MgSO_4$ and removed by rotary evaporation. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford imine **2**.

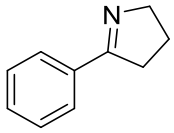
5-(p-tolyl)-3,4-dihydro-*2H*-pyrrole (2a)[6]



2a

The reaction of **1a** (56.8 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 60 °C afforded 34.9 mg (73%) of **2a** as a brown solid. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.73 (d, *J* = 8.0Hz, 2H), 7.20 (d, *J* = 8.0Hz, 2H), 4.04 (t, *J* = 7.4Hz, 2H), 2.92 (t, *J* = 8.2Hz, 2H), 2.37 (s, 3H), 2.05-1.97 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 173.1, 140.4, 131.9, 129.1, 127.5, 61.3, 34.8, 22.6, 21.3

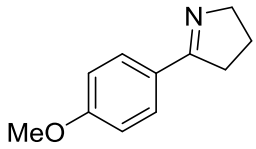
5-phenyl-3,4-dihydro-*2H*-pyrrole (2b)[6]



2b

The reaction of **1b** (52.6 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 80 ºC afforded 20.0 mg (46%) of **2b** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.85-7.83 (m, 2H), 7.41-7.37 (m, 3H), 4.06 (t, *J* = 6.8Hz, 2H), 2.95 (t, *J* = 7.6Hz, 2H), 2.07-2.00 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 173.3, 134.6, 130.3, 128.4, 127.6, 61.5, 34.9, 22.6

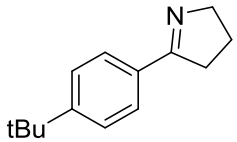
5-(4-methoxyphenyl)-3,4-dihydro-*2H*-pyrrole (2c)[6]



2c

The reaction of **1c** (61.6 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 34.7 mg (66%) of **2c** as a yellow solid. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.79 (d, *J* = 8.0Hz, 2H), 6.91 (d, *J* = 7.6Hz, 2H), 4.03 (t, *J* = 6.8Hz, 2H), 3.83 (s, 3H), 2.91 (t, *J* = 7.8Hz, 2H), 2.05-1.97 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 172.6, 161.2, 129.1, 127.4, 113.6, 61.2, 55.2, 34.8, 22.6

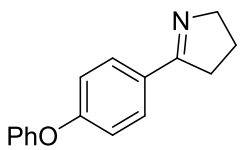
5-(4-(*tert*-butyl)phenyl)-3,4-dihydro-*2H*-pyrrole (2d)[7]



2d

The reaction of **1d** (69.4 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 60 ºC afforded 42.2 mg (70%) of **2d** as yellow oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.77 (d, *J* = 8.8Hz, 2H), 7.42 (d, *J* = 8.4Hz, 2H), 4.04 (t, *J* = 7.4Hz, 2H), 2.92 (t, *J* = 8.2Hz, 2H), 2.05-1.97 (m, 2H), 1.33 (s, 9H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 173.0, 153.5, 131.8, 127.3, 125.3, 61.4, 34.8, 34.7, 21.1, 22.6

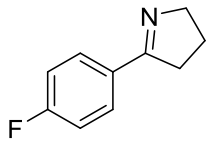
5-(4-phenoxyphenyl)-3,4-dihydro-*2H*-pyrrole (2e)



2e

The reaction of **1e** (80.2 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 49.1 mg (69%) of **2e** as a pale yellow solid. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.4Hz, 2H), 7.35 (t, *J* = 7.8Hz, 2H), 7.13 (t, *J* = 7.2Hz, 1H), 7.05-6.99 (m, 4H), 4.04 (t, *J* = 7.0Hz, 2H), 2.91 (t, *J* = 8.2Hz, 2H), 2.06-1.98 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 172.4, 159.3, 156.4, 129.8, 129.5, 129.2, 123.8, 119.4, 118.0, 61.4, 34.8, 22.7; **HRMS(ESI)** exact mass calc'd for $C_{16}H_{16}NO$ ($[M+H]^+$): 238.1232; found *m/z*: 238.1230

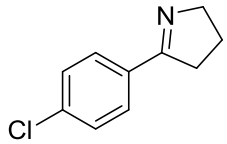
5-(4-fluorophenyl)-3,4-dihydro-*2H*-pyrrole (2f)[6]



2f

The reaction of **1f** (58.0 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 80 ºC afforded 12.7 mg (26%) of **2f** as red oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.85-7.82 (m, 2H), 7.11-7.06 (m, 2H), 4.05 (t, *J* = 7.0Hz, 2H), 2.93 (t, *J* = 8.0Hz, 2H), 2.08-2.01 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 172.1, 164.1 (d, $^1J_{C\text{-}F}$ = 248.7Hz), 130.9 (d, $^4J_{C\text{-}F}$ = 2.9Hz), 129.6 (d, $^3J_{C\text{-}F}$ = 8.3Hz), 115.4 (d, $^2J_{C\text{-}F}$ = 20.9Hz), 61.5, 34.9, 22.7

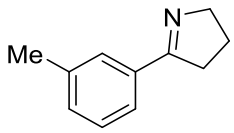
5-(4-chlorophenyl)-3,4-dihydro-*2H*-pyrrole (2g)[6]



2g

The reaction of **1g** (62.9 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 80 ºC afforded 16.7 mg (31%) of **2g** as a red solid. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.77 (d, *J* = 8.0Hz, 2H), 7.37 (d, *J* = 8.4Hz, 2H), 4.06 (t, *J* = 7.2Hz, 2H), 2.91 (t, *J* = 8.0Hz, 2H), 2.08-2.01 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 172.2, 136.3, 133.0, 128.9, 128.6, 61.6, 34.9, 22.7

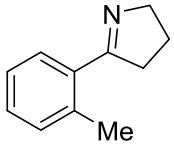
5-(*m*-tolyl)-3,4-dihydro-*2H*-pyrrole (2h)[6]



2h

The reaction of **1h** (56.8 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 60 °C afforded 29.6 mg (62%) of **2h** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.70 (s, 1H), 7.59 (d, *J* = 7.6Hz, 1H), 7.28 (t, *J* = 7.6Hz, 1H), 7.23 (d, *J* = 7.6Hz, 1H), 4.05 (t, *J* = 7.2Hz, 2H), 2.92 (t, *J* = 8.0Hz, 2H), 2.38 (s, 3H), 2.05-1.98 (m ,2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 173.4, 138.0, 134.5, 131.0, 128.2, 128.0, 124.8, 61.4, 34.9, 22.6, 21.2

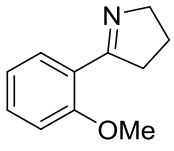
5-(*o*-tolyl)-3,4-dihydro-*2H*-pyrrole (2i)



2i

The reaction of **1i** (56.8 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 60 °C afforded 18.2 mg (38%) of **2i** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.42 (d, *J* = 7.2Hz, 1H), 7.28-7.18 (m, 3H), 4.08 (t, *J* = 7.2Hz, 2H), 2.91 (t, *J* = 8.0Hz, 2H), 2.51 (s, 3H), 2.03-1.95 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 175.1, 137.0, 135.1, 131.1, 128.9, 128.7, 125.5, 61.9, 38.3, 22.7, 21.5; **HRMS(ESI)** exact mass calc'd for $C_{11}H_{14}N$ ($[M+H]^+$): 160.1126; found *m/z*: 160.1127

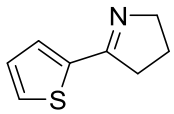
5-(2-methoxyphenyl)-3,4-dihydro-*2H*-pyrrole (2j)[6]



2j

The reaction of **1j** (61.6 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 60 °C afforded 21.6 mg (41%) of **2j** as orange oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.46-7.45 (m, 1H), 7.37-7.27 (m, 2H), 6.99-6.96 (m, 1H), 4.06 (t, *J* = 7.2Hz, 2H), 3.85 (s, 3H), 2.94 (t, *J* = 8.Hz, 2H), 2.07-1.99 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 173.3, 159.6, 135.9, 129.3, 120.4, 116.9, 111.7, 61.4, 55.3, 35.0, 22.6

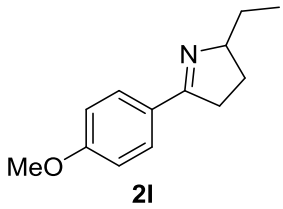
5-(thiophen-2-yl)-3,4-dihydro-*2H*-pyrrole (2k)[6]



2k

The reaction of **1k** (54.4 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 14.5 mg (32%) of **2k** as dark green oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.40-7.39 (m, 1H), 7.32-7.31 (m, 1H), 7.07-7.04 (m, 1H), 4.02 (t, *J* = 7.0Hz, 2H), 2.93 (t, *J* = 8.2Hz, 2H), 2.08-2.00 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 167.8, 139.4, 129.0, 128.9, 127.3, 61.1, 35.5, 22.9

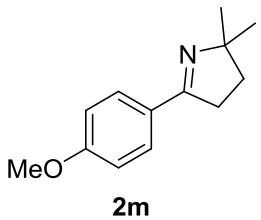
2-ethyl-5-(4-methoxyphenyl)-3,4-dihydro-*2H*-pyrrole (2l)



2l

The reaction of **1l** (70.0 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 38.4 mg (63%) of **2l** as a brown solid. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.79 (d, *J* = 8.8Hz, 2H), 6.90 (d, *J* = 8.8Hz, 2H), 4.12-4.06 (m, 1H), 3.82 (s, 3H), 3.01-2.93 (m, 1H), 2.87-2.79 (m, 1H), 2.20-2.12 (m, 1H), 1.89-1.83 (m, 1H), 1.63-1.48 (m, 2H), 1.01 (t, *J* = 7.4Hz, 3H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 171.0, 161.2, 129.1, 127.6, 113.6, 74.4, 55.2, 34.8, 29.4, 28.0, 10.8; **HRMS(ESI)** exact mass calc'd for $C_{13}H_{18}NO$ ($[M+H]^+$): 204.1388; found *m/z*: 204.1390

5-(4-methoxyphenyl)-2,2-dimethyl-3,4-dihydro-*2H*-pyrrole (2m)

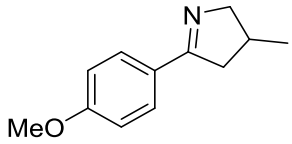


2m

The reaction of **1m** (70.0 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 43.3 mg (71%) of **2m** as an orange solid. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.77 (d, *J* = 8.8Hz, 2H), 6.89 (d, *J* = 8.8Hz, 2H), 3.82 (s, 3H), 2.97

(t, *J* = 7.8Hz, 2H), 1.83 (t, *J* = 7.8Hz, 2H), 1.32 (s, 6H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 168.9, 161.2, 129.1, 127.7, 113.6, 72.7, 55.2, 36.4, 35.0, 28.8; **HRMS(ESI)** exact mass calc'd for $C_{13}H_{18}NO$ ($[M+H]^+$): 204.1388; found *m/z*: 204.1390

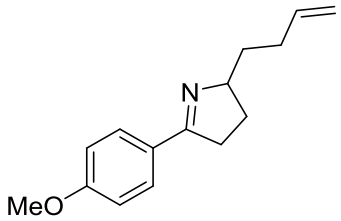
5-(4-methoxyphenyl)-3-methyl-3,4-dihydro-*2H*-pyrrole (2n)[8]



2n

The reaction of **1n** (65.8 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 41.4 mg (73%) of **2n** as a dark yellow solid. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.77 (d, *J* = 8.8Hz, 2H), 6.91 (d, *J* = 8.8Hz, 2H), 4.18-4.11 (m, 1H), 3.83 (s, 3H), 3.64-3.58 (m, 1H), 3.12-3.04 (m, 1H), 2.56-2.47 (m, 2H), 1.09 (d, *J* = 6.8Hz, 3H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 172.0, 161.2, 129.0, 127.6, 113.6, 68.7, 55.2, 43.0, 31.4, 20.3

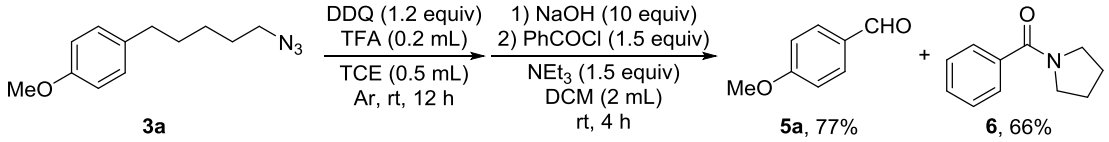
2-(but-3-en-1-yl)-5-(4-methoxyphenyl)-3,4-dihydro-*2H*-pyrrole (2o)



2o

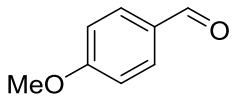
The reaction of **1o** (77.8 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 33.7 mg (49%) of **2o** as an orange solid. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.78 (d, *J* = 8.8Hz, 2H), 6.90 (d, *J* = 8.8Hz, 2H), 5.95-5.85 (m, 1H), 5.09-5.03 (m, 1H), 4.98-4.95 (m, 1H), 4.19-4.12 (m, 1H), 3.83 (s, 3H), 3.02-2.94 (m, 1H), 2.88-2.79 (m, 1H), 2.27-2.14 (m, 3H), 1.97-1.88 (m, 1H), 1.63-1.53 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 171.1, 161.2, 138.7, 129.2, 127.6, 114.4, 113.6, 72.5, 55.2, 35.9, 34.8, 30.9, 28.6; **HRMS(ESI)** exact mass calc'd for $C_{15}H_{20}NO$ ($[M+H]^+$): 230.1545; found *m/z*: 230.1542

b) Procedure for synthesis of 4-methoxybenzaldehyde 5a and phenyl(pyrrolidin-1-yl)methanone 6:



DDQ (81.7 mg, 0.36 mmol) was added to a 25 mL seal tube with a magnetic bar under Argon. Next, 1,1,2,2-tetrachloroethane (0.5 mL), TFA (0.2 mL) and 1-(5-azidopentyl)-4-methoxybenzene **3a** (65.8 mg, 0.3 mmol) were added in sequence. The mixture was stirred at room temperature under argon for 12 hours. After that, the reaction was diluted with dichloromethane (2 mL) and NaOH solid (0.12 g, 3.0 mmol) was added in batches to neutralize TFA. Then, triethylamine (45.5 mg, 0.45 mmol) and benzoyl chloride (63.3 mg, 0.45 mmol) were added in sequence. The reaction mixture was stirred at room temperature for 4 hours. Finally, the solvent was removed by rotary evaporation and the residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to afford 31.5 mg (77%) of 4-methoxybenzaldehyde **5a** as colorless oil and 34.7 mg (66%) of phenyl(pyrrolidin-1-yl)methanone **6** as pale yellow oil.

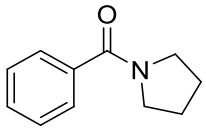
4-methoxybenzaldehyde (5a)[9]



5a

^{1}H-NMR (400MHz, $CDCl_3$) δ 9.89 (s, 1H), 7.84 (d, *J* = 8.4Hz, 2H), 7.01 (d, J = 8.8Hz, 2H), 3.89 (s, 3H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 190.8, 164.6, 131.9, 129.9, 114.3, 55.5

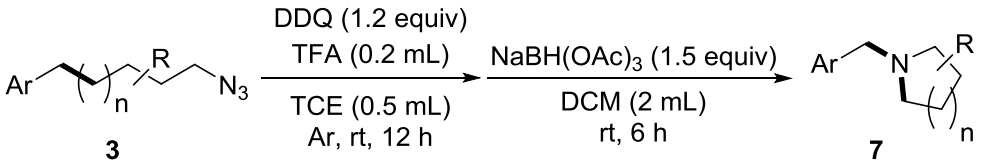
phenyl(pyrrolidin-1-yl)methanone (6)[10]



6

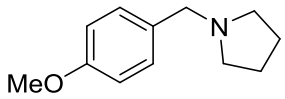
^{1}H-NMR (400MHz, $CDCl_3$) δ 7.52-7.49 (m, 2H), 7.41-7.37 (m, 3H), 3.65 (t, *J* = 7.0Hz, 2H), 3.42 (t, *J* = 6.6Hz, 2H), 1.99-1.92 (m, 2H), 1.90-1.83 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 169.6, 137.2, 129.6, 128.1, 127.0, 49.5, 46.0, 26.3, 24.3

c) Typical procedure for synthesis of tertiary amines 7:



DDQ (81.7 mg, 0.36 mmol) was added to a 25 mL seal tube with a magnetic bar under Argon. Next, 1,1,2,2-tetrachloroethane (0.5 mL), TFA (0.2 mL) and alkyl azide **3** (0.3 mmol) were added in sequence. The mixture was stirred at room temperature under argon for 12 hours. After that, the solvent was evaporated in vacuo and the reaction mixture was diluted with dichloromethane (2 mL). Then, $NaBH(OAc)_3$ (95.4 mg, 0.45 mmol) was added in batches and the mixture was stirred at room temperature for 6 hours. The reaction mixture was carefully quenched with saturated $NaHCO_3$ aqueous solution (6 mL) and extracted with ethyl acetate for three times (6 mL×3). The combined organic solvent was dried over anhydrous $MgSO_4$ and removed by rotary evaporation. The residue was purified by flash chromatography on silica gel (eluent: dichloromethane/methanol with 0.5%(V/V) triethylamine) to afford tertiary amine **7**.

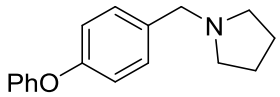
1-(4-methoxybenzyl)pyrrolidine (7a)[11]



7a

The reaction of **3a** (65.8 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 31.6 mg (55%) of **7a** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.25 (d, *J* = 8.4Hz, 2H), 6.85 (d, *J* = 8.8Hz, 2H), 3.79 (s, 3H), 3.59 (s, 2H), 2.55-2.52 (m ,4H), 1.81-1.77 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 158.7, 130.9, 130.1, 113.6, 59.9, 55.2, 53.9, 23.3

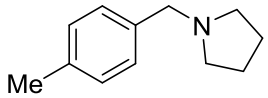
1-(4-phenoxybenzyl)pyrrolidine (7b)



7b

The reaction of **3b** (84.4 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 54.7 mg (72%) of **7b** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.33-7.29 (m, 4H), 7.09-7.05 (m, 1H), 7.00-6.93 (m, 4H), 3.61 (s, 2H), 2.56-2.52 (m, 4H), 1.82-1.77 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.3, 156.1, 133.7, 130.3, 129.6, 123.0, 118.6, 59.8, 53.9, 23.3; **HRMS(ESI)** exact mass calc'd for $C_{17}H_{20}NO$ ($[M+H]^+$): 254.1545; found *m/z*: 254.1546

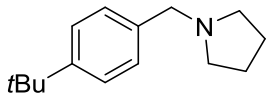
1-(4-methylbenzyl)pyrrolidine (7c)[12]



7c

The reaction of **3c** (61.0 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 60 °C afforded 20.0 mg (38%) of **7c** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.21 (d, *J* = 7.6Hz, 2H), 7.11 (d, *J* = 7.6Hz, 2H), 3.57 (s, 2H), 2.51-2.47 (m, 4H), 2.32 (s, 3H), 1.78-1.75 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 136.3, 136.2, 128.8, 60.3, 54.0, 23.4, 21.0

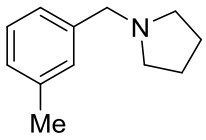
1-(4-(*tert*-butyl)benzyl)pyrrolidine (7d)[13]



7d

The reaction of **3d** (73.6 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 60 °C afforded 50.9 mg (78%) of **7d** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.33 (d, *J* = 8.0Hz, 2H), 7.25 (d, *J* = 8.4Hz, 2H), 3.59 (s, 2H), 2.53-2.50 (m, 4H), 1.79-1.76 (m, 4H), 1.31 (s, 9H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 149.7, 136.2, 128.6, 125.0, 60.3, 54.1, 34.4, 31.4, 23.4

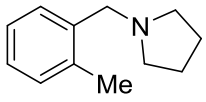
1-(3-methylbenzyl)pyrrolidine (7e)[12]



7e

The reaction of **3e** (61.0 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 60 °C afforded 24.7 mg (47%) of **7e** as pale brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.19 (t, *J* = 7.4Hz, 1H), 7.16 (s, 1H), 7.11 (d, *J* = 7.6Hz, 1H), 7.05 (d, *J* = 7.6Hz, 1H), 3.58 (s, 2H), 2.53-2.50 (m, 4H), 2.34 (s, 3H), 1.80-1.77 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 139.0, 137.8, 129.6, 128.0, 127.6, 126.0, 60.7, 54.1, 23.4, 21.3

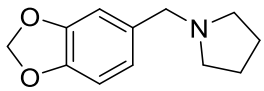
1-(2-methylbenzyl)pyrrolidine (7f)[12]



7f

The reaction of **3f** (61.0 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.4 mL) at 60 °C afforded 18.4 mg (35%) of **7f** as pale orange oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.31-7.29 (m, 1H), 7.16-7.14 (m, 3H), 3.59 (s, 2H), 2.53-2.50 (m, 4H), 2.36 (s, 3H), 1.79-1.75 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 137.8, 136.7, 130.1, 129.2, 126.7, 125.6, 58.1, 54.3, 23.5, 19.2

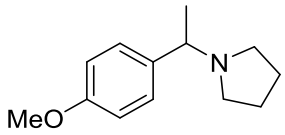
1-(benzo[*d*][1,3]dioxol-5-ylmethyl)pyrrolidine (7g)[14]



7g

The reaction of **3g** (70.0 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 30.2 mg (49%) of **7g** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 6.86 (s, 1H), 6.78-6.73 (m, 2H), 5.93 (s, 2H), 3.54 (s, 2H), 2.53-2.50 (m, 4H), 1.81-1.76 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 147.5, 146.5, 132.9, 121.9, 109.4, 107.9, 100.8, 60.3, 53.9, 23.3

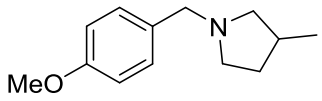
1-(1-(4-methoxyphenyl)ethyl)pyrrolidine (7h)



7h

The reaction of **3h** (70.0 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 24.0 mg (39%) of **7h** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.24 (d, *J* = 8.4Hz, 2H), 6.84 (d, *J* = 8.4Hz, 2H), 3.79 (s, 3H), 3.13 (q, *J* = 6.7Hz, 1H), 2.56-2.50 (m, 2H), 2.37-2.32 (m, 2H), 1.78-1.71 (m, 4H), 1.38 (d, *J* = 6.4Hz, 3H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 158.4, 137.9, 128.1, 113.5, 65.2, 55.1, 52.9, 23.3, 23.1; **HRMS(ESI)** exact mass calc'd for $C_{13}H_{20}NO$ ($[M+H]^+$): 206.1545; found *m/z*: 206.1542

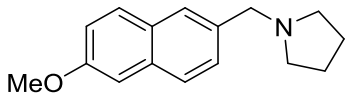
1-(4-methoxybenzyl)-3-methylpyrrolidine (7i)



7i

The reaction of **3i** (70.0 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 33.3 mg (54%) of **7i** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.32 (d, *J* = 8.4Hz, 2H), 6.87 (d, *J* = 8.4Hz, 2H), 3.80 (s, 3H), 3.70 (s, 2H), 3.00-2.96 (m, 1H), 2.90-2.84 (m, 1H), 2.69-2.63 (m, 1H), 2.39-2.30 (m, 1H), 2.19-2.02 (m, 2H), 1.47-1.39 (m, 1H), 1.04 (d, *J* = 6.8Hz, 3H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 158.5, 131.4, 130.0, 113.5, 62.0, 60.1, 55.2, 54.0, 32.5, 31.8, 20.3; **HRMS (ESI)** exact mass calc'd for $C_{16}H_{20}NO$ ($[M+H]^+$): 242.1545; found *m/z*: 242.1541

1-((6-methoxynaphthalen-2-yl)methyl)pyrrolidine (7j)

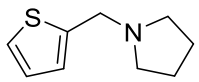


7j

The reaction of **3j** (80.8 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at 60 °C afforded 23.9 mg (33%) of **7j** as a orange solid. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.71-7.67 (m, 3H), 7.46-7.44 (m, 1H), 7.14-7.11 (m, 2H), 3.90 (s, 3H), 3.73 (s, 2H), 2.56-2.53 (m, 4H), 1.81-1.77 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 157.4,

134.6, 133.7, 129.2, 128.9, 127.9, 127.1, 126.6, 118.6, 105.6, 60.8, 55.2, 54.2, 23.4; **HRMS (ESI)** exact mass calc'd for $C_{16}H_{20}NO$ ($[M+H]^+$): 242.1545; found *m/z*: 242.1543

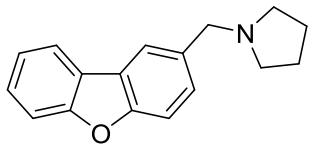
1-(thiophen-2-ylmethyl)pyrrolidine (7k)



7k

The reaction of **3k** (58.6 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 21.6 mg (43%) of **7k** as orange oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.20 (dd, *J* = 4.8Hz, 1.2Hz, 1H), 6.94-6.92 (m, 2H), 3.83 (s, 2H), 2.57-2.54 (m, 4H), 1.81-1.77 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 142.7, 126.3, 125.3, 124.5, 54.5, 53.9, 23.5; **HRMS(ESI)** exact mass calc'd for $C_9H_{14}NS$ ($[M+H]^+$): 168.0847; found *m/z*: 168.0846

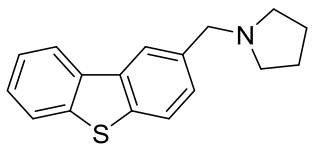
1-(dibenzo[*b,d*]furan-2-ylmethyl)pyrrolidine (7l)



7l

The reaction of **3l** (83.8 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 65.0 mg (81%) of **7l** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.94-7.92 (m, 2H), 7.54 (d, *J* = 8.0Hz, 1H), 7.49 (d, *J* = 8.4Hz, 1H), 7.44-7.39 (m, 2H), 7.33-7.29 (m, 1H), 3.75 (s, 2H), 2.56-2.53 (m, 4H), 1.82-1.78 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 156.5, 155.4, 133.9, 128.1, 127.0, 124.24, 124.17, 122.6, 120.8, 120.7, 111.6, 111.1, 60.7, 54.1, 23.4; **HRMS(ESI)** exact mass calc'd for $C_{17}H_{18}NO$ ($[M+H]^+$): 252.1388; found *m/z*: 252.1386

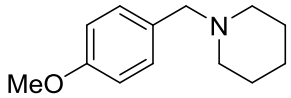
1-(dibenzo[*b,d*]thiophen-2-ylmethyl)pyrrolidine (7m)



7m

The reaction of **3m** (88.6 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 64.2 mg (80%) of **7m** as brown oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 8.17-8.13 (m, 1H), 8.11 (d, *J* = 1.2Hz, 1H), 7.83-7.79 (m, 1H), 7.76 (d, *J* = 8.0Hz, 1H), 7.44-7.39 (m, 3H), 3.76 (s, 2H), 2.56-2.53 (m, 4H), 1.81-1.77 (m, 4H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 139.7, 137.9, 135.8, 135.6, 135.5, 127.9, 126.5, 124.2, 122.7, 122.4, 121.7, 121.6, 60.7, 54.2, 23.4; **HRMS(ESI)** exact mass calc'd for $C_{17}H_{18}NS$ ($[M+H]^+$): 268.1160; found *m/z*: 268.1160

1-(4-methoxybenzyl)piperidine (7n)[11]



7n

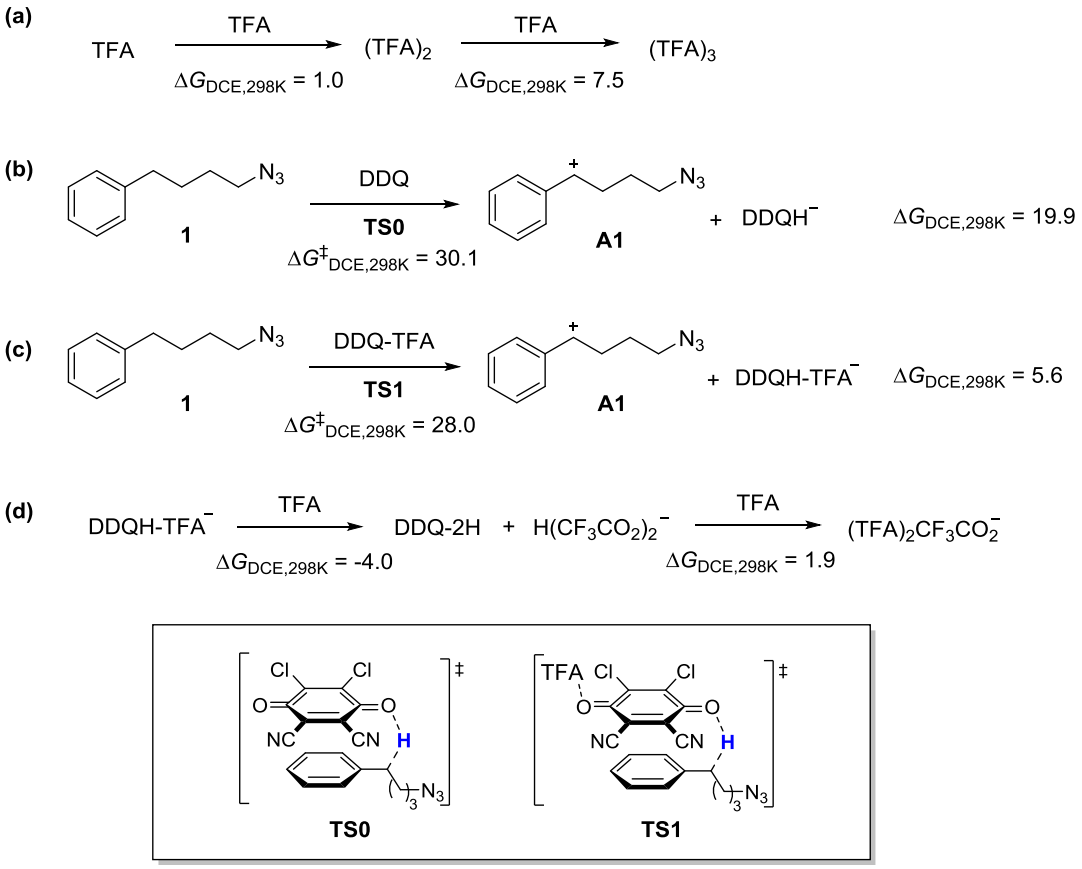
The reaction of **3n** (70.0 mg, 0.3 mmol), DDQ (81.7 mg, 0.36 mmol) and TFA (0.2 mL) at room temperature afforded 19.1 mg (31%) of **7n** as pale yellow oil. **^{1}H-NMR (400MHz, $CDCl_3$)** δ 7.22 (d, *J* = 8.4Hz, 2H), 6.84 (d, *J* = 8.4Hz, 2H), 3.79 (s, 3H), 3.41 (s, 2H), 2.35 (brs, 4H), 1.59-1.53 (m, 4H), 1.44-1.40 (m, 2H); **^{13}C-NMR (100MHz, $CDCl_3$)** δ 158.5, 130.8, 130.4, 113.4, 63.2, 55.2, 54.3, 25.9, 24.4

D) Details of Calculation and Discussion

All of the DFT calculations were performed with the Gaussian 09 program package.[15] The geometry optimization of all the minima involved were performed at the M06-2X level of theory[16] with 6-31+G(d,p) basis set[17] for all atoms (keyword 5D was used in the calculations). The structures of the reactants, intermediates, transition states, and products were fully optimized without any restriction. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum or a transition state and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. IRC calculations[18] were used to confirm that the transition states found from the optimization calculations connect the related reactants and products. Single-point calculations were performed with def2-TZVP basis set at

the optimized geometries for all the intermediates and transition states. Solvent is expected to impact both the optimized geometries and the energies of the hydride transfer transition states and the zwitterionic complexes. Solvation effects were taken into account by applying the PCM[19] solvation model with 1,2-dichloroethane (DCE) solvent in both geometry optimization and single-point energy calculations. Through the same approach full optimization, without any restriction, was carried out for the model reactions. The reported energies are Gibbs free energies in DCE solution ($\Delta G_{DCE,298K}$).

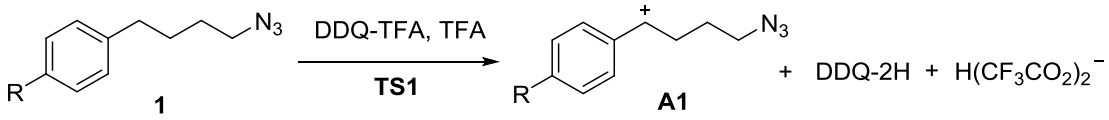
We first studied the possible structures of TFA and DDQ in the reaction system. The computed reaction energies are shown that the dimer of TFA is slightly endergonic by 1.0 kcal mol^{-1}, while the trimer of TFA is further endergonic by 7.5 kcal mol^{-1} (Scheme S1a). This reveals that TFA remains predominantly as monomer and dimer in the reaction system. Then we studied the O-attack hydride transfer pathway of the C-H cleavage step or oxidation step in the reaction between DDQ and alkyl azide **1**, which has proved to be the most thermodynamically favorable pathway in some similar cases.[20] The hydride transfer pathway through **TS0** requires Gibbs free energy barrier of 30.1 kcal mol^{-1} to form the carbocation intermediate **A1** and $DDQH^-$ with Gibbs free energy of 19.9 kcal mol^{-1} (Scheme S1b). In the presence of TFA, the hydride transfer from **1** to the complex of DDQ and TFA through **TS1** requires Gibbs free energy barrier of 28.0 kcal mol^{-1} to form the carbocation intermediate **A1** and DDQH-TFA^- with Gibbs free energy of 5.6 kcal mol^{-1} (Scheme S1c). The formed DDQH-TFA^- species can be stabilized by another TFA molecule to afford DDQ-2H and $H(CF_3CO_2)_2^-$ species, which is exergonic by 4.0 kcal mol^{-1} (Scheme S1d). One more TFA molecule added to dimer $H(CF_3CO_2)_2^-$ anion is endergonic by 1.9 kcal mol^{-1} to form trimer $(TFA)_2CF_3CO_2^-$ anion. Therefore, $H(CF_3CO_2)_2^-$ species is likely to be the stable anion in the reaction system.



Scheme S1. Additional computational data for the oxidation of alkyl azide **1** at the benzylic position by DDQ with TFA. All energies are in kcal mol^{-1}.

The substrate effects in Table 2 were also explored and the typical calculational and experimental observation was shown in Table S1. There is large effect of aryl substitution on the activation and reaction energies of hydride transfer. The electron-donor groups such as methoxyl and methyl groups result in the low activation energies of hydride transfer and afford stable carbocations. Therefore, the substrates with electron-donor groups provide good yields of amination products (entries 1-2). For the substrates with electron-neutral and week electron-withdrawing groups, the activation energies of hydride transfer were increased significantly and the corresponding carbocations becomes less stable (entries 3-5). As a result, the yields of amination products decrease even at high temperature reaction condition. The experimental observed electronic effects on the Ar group is consistent with first oxidation step with hydride transfer as the rate-determining step.

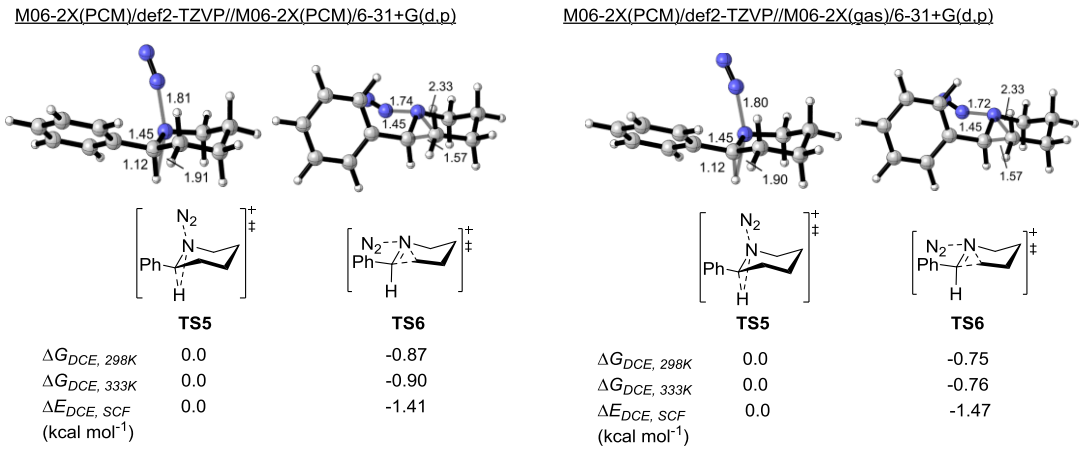
Table S1. Electronic eff ects on the activation and reaction energies of hydride transfer.[a]



Entry	R	$\Delta^{\ddagger}G_{DCE,298K}$ (**TS1**)	$\Delta G_{DCE,298K}$	T(°C)	*t* (h)	Yield(%)
1	MeO	22.1	-9.0	RT	12	66
2	Me	23.8	-3.4	60	12	73
3	H	28.0	1.6	80	12	46
4	F	27.6	0.0	80	12	26
5	Cl	27.4	1.5	80	12	31

[a]All energies are in kcal mol^{-1} with respect to the separate reactants (**1**, DDQ-TFA, and TFA).

The calculated TS-barrier difference between **TS5** and **TS6** was further explored. The geometry optimization performed at the M06-2X(PCM)/6-31+G(d,p) level and M06-2X(gas)/6-31+G(d,p) level provide similar structures. Single-point calculations performed at the M06-2X(PCM)/def2-TZVP level based on both the optimized geometries give the close results. The 1,2-alkyl shift pathway through **TS6** is favored by 1.41 or 1.47 kcal mol^{-1} than 1,2-H shift pathway through **TS5** in the activation energies ($\Delta E_{DCE,SCF}$). DFT calculations performed at 298 and 333 K show that **TS6** is favored by 0.87 kcal mol^{-1} ($\Delta G_{DCE,298K}$) or 0.90 kcal mol^{-1} ($\Delta G_{DCE,333K}$) than **TS5** in the Gibbs free energy barrier, indicating that 1,2-alkyl shift pathway is the predominant pathway.



Scheme S2. The activation energies and structures of Schmidt rearrangement through **TS5** and **TS6**.

DFT-Computed Energies of All Stationary Points

Table S2. Sum of electronic and thermal enthalpies (*H*, in Hartree), sum of electronic and thermal free energies (*G*, in Hartree), thermal correction to Gibbs free energy (*CGFE*, in Hartree), electronic energy in DCE (E_{DCE}, in Hartree), and free energies in DCE ($G_{DCE,298K}$, in Hartree). For transition state structures, one imaginary frequency (IFreq) was observed and given below. For all minimum structures, no imaginary frequency was observed.

Structure	*H*	*G*	*CGFE*	E_{DCE}	$G_{DCE,298K}$	IFreq
TFA	-526.593839	-526.632480	0.008214	-526.857640	-526.849426	
$(TFA)_2$	-1053.204191	-1053.263674	0.035766	-1053.732969	-1053.697203	
$(TFA)_3$	-1579.806261	-1579.886267	0.064288	-1580.598952	-1580.534664	
1	-552.631723	-552.687787	0.176806	-553.051977	-552.875171	
DDQ	-1484.768944	-1484.822536	0.023767	-1485.130550	-1485.106783	
TS0	-2037.381490	-2037.466210	0.220971	-2038.154943	-2037.933972	-1315.15
A1	-551.806294	-551.860412	0.167640	-552.216233	-552.048593	
$DDQH^-$	-1485.566358	-1485.619832	0.034852	-1485.936471	-1485.901619	
DDQ-TFA	-2011.370888	-2011.445350	0.051767	-2011.997157	-2011.945390	
TS1	-2563.988216	-2564.092293	0.250720	-2565.026589	-2564.775869	-1434.91
$DDQH\text{-}TFA^-$	-2012.192928	-2012.265488	0.062477	-2012.825451	-2012.762974	
DDQ-2H	-1486.007807	-1486.061039	0.048347	-1486.393371	-1486.345024	
$H(CF_3CO_2)^-$	-1052.783595	-1052.843377	0.019307	-1053.293051	-1053.273744	
$(TFA)_2CF_3CO_2^-$	-1579.397595	-1579.473700	0.052880	-1580.172953	-1580.120073	
C	-551.845448	-551.895683	0.173284	-552.255086	-552.081802	
TS2	-551.819407	-551.869552	0.168889	-552.223978	-552.055089	-396.37
2-H	-442.492038	-442.536657	0.167604	-442.846784	-442.679180	
TS3	-551.809151	-551.860787	0.167658	-552.214931	-552.047273	-426.35
E1	-442.446802	-442.493184	0.165213	-442.800860	-442.635647	
N_2	-109.481675	-109.503417	-0.012671	-109.535774	-109.548445	
3	-591.897071	-591.955663	0.204268	-592.359206	-592.154938	
TS4	-2603.254567	-2603.362514	0.276596	-2604.334582	-2604.057986	-1465.31
A3	-591.073604	-591.131595	0.193550	-591.525228	-591.331678	
D	-591.116888	-591.168517	0.201749	-591.568390	-591.366641	
TS5	-591.092536	-591.144864	0.196392	-591.538613	-591.342221	-377.50
4-H	-481.760676	-481.807367	0.196029	-482.157710	-481.961681	
TS6	-591.093237	-591.145911	0.197242	-591.540855	-591.343613	-452.91

E3	-481.742498	-481.790005	0.195162	-482.139636	-481.944474	
1-OMe	-667.079483	-667.141687	0.206286	-667.578898	-667.372612	
TS1-OMe	-2678.446868	-2678.555954	0.281074	-2679.563936	-2679.282862	-1528.31
A1-OMe	-666.270562	-666.330524	0.197823	-666.76085	-666.563027	
1-Me	-667.079483	-591.960779	0.202322	-592.362253	-592.159931	
TS1-Me	-2603.264401	-2603.372343	0.275712	-2604.343086	-2604.067374	-1497.25
A1-Me	-591.082344	-591.141183	0.19196	-591.533348	-591.341388	
1-F	-651.850667	-651.908368	0.16781	-652.306056	-652.138246	
TS1-F	-2663.206218	-2663.313082	0.240397	-2664.280063	-2664.039666	-1465.19
A1-F	-651.025987	-651.082605	0.157749	-651.472057	-651.314308	
1-Cl	-1012.206683	-1012.265604	0.165555	-1012.65647	-1012.490915	
TS1-Cl	-3023.562474	-3023.670799	0.237686	-3024.630374	-3024.392688	-1479.54
A1-Cl	-1011.378823	-1011.437399	0.154729	-1011.819254	-1011.664525	

The coordinates of all stationary points (Å)

TFA

C	-0.94300700	0.15491000	-0.00053300
O	-1.48563600	1.22390800	-0.00001000
O	-1.51238500	-1.03777300	-0.00005300
H	-2.48038400	-0.94309100	0.00026200
C	0.59344900	-0.00126200	-0.00002000
F	0.99612200	-0.67588800	-1.08223500
F	0.99538100	-0.67624200	1.08225800
F	1.18204100	1.18903300	0.00037300

$(TFA)_2$

C	-1.86862300	0.01704700	0.00002500
O	-1.23620500	1.05408800	0.00020600
O	-1.41046200	-1.19792500	-0.00008900
H	-0.40950100	-1.19857600	-0.00001000
C	-3.41165500	0.03162900	-0.00003100
F	-3.87681700	-0.59773700	1.08274000
F	-3.87679500	-0.59854800	-1.08233100
F	-3.87218100	1.27643900	-0.00050000
C	1.86861800	-0.01697900	-0.00002900
O	1.23614000	-1.05398600	-0.00018300
O	1.41056100	1.19802800	0.00031800
H	0.40962600	1.19879700	0.00040400
C	3.41165000	-0.03166900	-0.00007100
F	3.87207500	-1.27651300	-0.00153500
F	3.87679600	0.59677500	1.08325200
F	3.87688300	0.59936000	-1.08182300

$(TFA)_3$

O	0.17777300	1.12085600	-0.04498800
C	-0.17910700	2.28696100	-0.05509000
O	-1.38893400	2.73182300	-0.12461100
C	0.85698800	3.42786400	0.03396600
O	1.11254900	-1.70403500	-0.09015700
C	2.24625100	-1.30388400	-0.02645400
O	2.65239400	-0.05593600	0.03594800
C	3.45698700	-2.26088500	-0.00258500
C	-2.77126200	-0.49906400	-0.06545400
O	-3.00265300	0.68935700	-0.14842400
O	-1.62298200	-1.10480800	-0.02212300
C	-3.93044500	-1.51554100	0.03406800
H	1.86516000	0.53707000	0.02199600
H	-0.85521400	-0.48669200	-0.05815800
H	-2.03881800	1.96283400	-0.15415000
F	0.66862100	4.13314700	1.14957400
F	0.74198400	4.24662000	-1.01088900
F	2.08868100	2.92118700	0.05017100
F	4.28881900	-1.99022500	-1.01452400
F	4.13761100	-2.12062500	1.14103400
F	3.06147800	-3.52489700	-0.10699000
F	-3.96033600	-2.03847800	1.26403500
F	-3.76411800	-2.50912100	-0.84014000
F	-5.09304900	-0.92249300	-0.20622100

1

N	-4.15296800	-0.07167300	0.40456600
C	-2.84648100	0.04296700	-0.28894800
H	-2.76162800	-0.74633900	-1.04641700

H	-2.78272300	1.01398400	-0.79597100
N	-5.13003700	0.02578000	-0.33548100
N	-6.08544600	0.10397000	-0.93797400
C	-1.74011300	-0.09117500	0.74281600
H	-1.86132100	0.69220200	1.50054200
H	-1.84611800	-1.05489600	1.25528700
C	-0.35765500	0.00886800	0.10323700
H	-0.25776400	0.96711100	-0.42337200
H	-0.23861100	-0.77919800	-0.65178700
C	0.77082300	-0.11348800	1.13579000
H	0.66837100	0.68962600	1.87536400
H	0.66303400	-1.06294900	1.67357100
C	2.13402100	-0.04693900	0.49257800
C	2.78274400	-1.21321400	0.07324700
C	2.75535200	1.18444600	0.25540500
C	4.02067600	-1.15413700	-0.56646800
H	2.31287800	-2.17767900	0.25301000
C	3.99269800	1.24982400	-0.38451100
H	2.26453000	2.09978800	0.57917900
C	4.62990500	0.07941100	-0.79769900
H	4.51072500	-2.07079500	-0.88095900
H	4.46114100	2.21441800	-0.55614600
H	5.59481800	0.12881900	-1.29276500

DDQ

C	-1.39997500	0.67285700	0.00000200
C	-1.39997800	-0.67285100	0.00001700
C	-0.11563200	-1.45272000	0.00011200
C	1.15971500	-0.67373200	0.00003700
C	1.15971800	0.67373400	0.00001800
C	-0.11562700	1.45272800	0.00000500
Cl	2.58590000	-1.60617500	0.00000800
Cl	2.58590900	1.60616600	-0.00001300
C	-2.60830400	-1.44492700	-0.00002500
N	-3.58086200	-2.06929100	-0.00005100
C	-2.60830400	1.44493000	-0.00003600
N	-3.58086300	2.06928900	-0.00007600
O	-0.13865100	-2.65843000	-0.00005500
O	-0.13864400	2.65843600	0.00008000

TS0

C	-0.45418800	0.62719200	-0.69065500
C	-0.89509700	-0.65819900	-1.14299900
C	-2.22554700	-0.99977700	-1.14580100
C	-3.27457800	-0.02728600	-0.77937400
C	-2.79135200	1.31732700	-0.40006100
C	-1.46546900	1.60961600	-0.33108100
O	0.80256700	0.90607000	-0.65393900
O	-4.46132000	-0.32022900	-0.80418100
Cl	-4.00559400	2.45848700	0.00610800
Cl	-0.89000200	3.13848800	0.19583300
C	0.45167300	-0.77374100	1.73129800
C	0.26527200	-2.14928200	1.39939700
C	-0.98691600	-2.72214000	1.45465400
C	-2.10747200	-1.94189900	1.80295700
C	-1.94740100	-0.60520700	2.17431100
C	-0.68903800	-0.02414100	2.13118300
H	1.11864300	-2.75049300	1.10362900
H	-1.11742000	-3.76835700	1.19836000
H	-3.09582700	-2.39227000	1.81279800
H	-2.80933400	-0.01532400	2.47065500
H	-0.55867500	1.01760000	2.41567200
N	-3.00932200	-3.34744100	-1.90268100
C	-2.66121700	-2.29484800	-1.56869400
N	0.92358900	-2.30923700	-1.97959600
C	0.11295400	-1.57808600	-1.59725200
C	1.69047800	-0.09568800	1.54484200
H	1.30197900	0.50385300	0.31832000
H	1.79306400	0.85044700	2.08316300
C	2.97821000	-0.79335000	1.19132100
H	2.80525300	-1.54384600	0.41129800
H	3.33323100	-1.33668900	2.08032300
C	4.05662000	0.18780600	0.72792700
H	3.71242900	0.71459000	-0.17160300
H	4.23503600	0.94309900	1.50132200
C	5.36473100	-0.53596400	0.42527000
H	5.21714100	-1.29609200	-0.35188600
H	5.74089500	-1.03526700	1.31977300
N	6.44152600	0.39693600	0.02266200
N	6.29329600	0.88357700	-1.09932500
N	6.24930700	1.37894300	-2.11582000

A1

N	-3.74037500	-0.00761600	-0.72394700
C	-2.81169200	-0.09633800	0.42155200
H	-2.74462700	0.87239700	0.93106000
H	-3.16787800	-0.84440300	1.14004300
N	-4.88105200	0.34913200	-0.42396800

N	-5.95119800	0.66843400	-0.24881900
C	-1.45439300	-0.50101600	-0.13440900
H	-1.54341200	-1.46836900	-0.63810400
H	-1.12430800	0.23561200	-0.87265200
C	-0.41615100	-0.58153700	1.01663300
H	-0.78508500	-1.29679600	1.76203900
H	-0.29761300	0.39450200	1.48828200
C	0.83896600	-1.11170800	0.46704600
C	2.01296900	-0.41778900	0.20086200
C	3.10093900	-1.13771900	-0.38250700
C	2.15564600	0.97812500	0.47008500
C	4.28126400	-0.48890600	-0.67793200
H	2.98323100	-2.19774700	-0.58662500
C	3.33756000	1.61409800	0.16395400
H	1.33596500	1.53536200	0.90889300
C	4.39357500	0.88099800	-0.40447100
H	5.11244000	-1.02599300	-1.11891100
H	3.45898100	2.67289300	0.35921700
H	5.32249200	1.39231900	-0.63836500
H	0.82608800	-2.16867100	0.19738700

DDQH$^-$

C	-1.32021600	0.67860100	-0.00001000
C	-1.33714100	-0.73829200	-0.00008000
C	-0.14128300	-1.52937300	-0.00020800
C	1.07711800	-0.73288800	-0.00005600
C	1.07456300	0.64758000	-0.00004600
C	-0.12934700	1.38590200	-0.00004800
Cl	2.56247800	-1.61492700	0.00006900
Cl	2.55661400	1.55837600	0.00003700
C	-2.57735000	-1.43744100	-0.00002100
N	-3.58883200	-2.00831600	0.00006400
C	-2.54749800	1.41915000	0.00010700
N	-3.54266000	2.01233000	0.00021200
O	-0.12926500	-2.78423700	-0.00012800
O	-0.17322900	2.74249600	-0.00013200
H	0.72275800	3.10776500	0.00050000

DDQ-TFA

C	2.82037800	-0.73588900	-0.37164900
C	1.92012600	-1.33947800	0.42600200
C	0.80729300	-0.56332200	1.06107700
C	0.77265900	0.90830100	0.83946000
C	1.67091900	1.51579400	0.03971800
C	2.75872300	0.74209200	-0.63579900
Cl	-0.47204600	1.74812500	1.64846600
Cl	1.66176400	3.18890700	-0.26764700
C	1.94943400	-2.74681000	0.69794500
N	1.97629000	-3.88043700	0.92079600
C	3.88475700	-1.45116500	-1.01186000
N	4.74370000	-2.02625700	-1.52877400
O	-0.02416600	-1.14488500	1.72288000
O	3.56730900	1.26178300	-1.36269800
C	-2.61027400	-0.42490300	-0.12437800
O	-1.57803400	-0.22085600	-0.70781700
O	-2.76916000	-0.74224700	1.14358900
H	-1.89532000	-0.81250200	1.58253100
C	-3.98433300	-0.33583100	-0.82234100
F	-4.60343100	-1.52074800	-0.78350600
F	-4.76363100	0.56031000	-0.20809600
F	-3.84132800	0.02563100	-2.09254400

TS1

C	0.74580800	-0.36182100	-0.02264000
C	0.48135800	0.56617300	1.03891400
C	-0.68046200	1.29798400	1.07323300
C	-1.74461500	1.08875100	0.08476700
C	-1.47380700	0.10065400	-0.96593900
C	-0.28661700	-0.56215500	-1.02829300
O	1.85534200	-1.00185400	-0.06280100
O	-2.80570900	1.71507700	0.15826900
Cl	-2.69717200	-0.10498400	-2.14867300
Cl	0.08318200	-1.65636400	-2.29340100
C	2.60286500	1.68147800	-1.02372100
C	2.64470100	2.62853300	0.04164100
C	1.64455700	3.56576800	0.19002400
C	0.54698800	3.57305100	-0.69161500
C	0.49856900	2.68001900	-1.76521800
C	1.50657200	1.74097100	-1.92673400
H	3.47522200	2.61544000	0.73960000
H	1.68802800	4.28121800	1.00448000
H	-0.25105900	4.29611400	-0.55171300
H	-0.33503500	2.70905800	-2.46009600
H	1.47493500	1.04320200	-2.76059100
N	-1.12689400	3.02603500	2.94840400
C	-0.93506200	2.24790800	2.11329100
N	2.26531000	0.77941600	2.91035600

C	1.47358600	0.69106300	2.07191900
C	3.53940600	0.60690100	-1.13494200
H	2.71719700	-0.34423800	-0.57548800
H	3.59510600	0.14038000	-2.12272400
C	4.79184100	0.51579700	-0.29915300
H	4.57042700	0.75000300	0.74839300
H	5.49968500	1.28035300	-0.65313000
C	5.44615900	-0.86434100	-0.38268900
H	4.75106100	-1.62386800	-0.00252400
H	5.66822400	-1.11487700	-1.42578600
C	6.73875500	-0.90205700	0.42694400
H	6.54524000	-0.65075400	1.47726000
H	7.45623700	-0.18041900	0.03307200
N	7.42012900	-2.21336400	0.33756000
N	6.86859300	-3.11119200	0.97584200
N	6.44029200	-3.99803900	1.53310600
C	-4.78950100	-0.77038100	0.53304400
O	-3.68513100	-1.17084800	0.80027100
O	-5.12862400	0.41437500	0.08353700
H	-4.31113800	0.97573600	-0.01012600
C	-6.03663000	-1.66920100	0.67571900
F	-5.71558800	-2.83848400	1.22091000
F	-6.58333900	-1.90010500	-0.52527300
F	-6.96242400	-1.08352200	1.44350200

DDQH-TFA-

C	2.86416200	0.62972200	0.31331900
C	1.84426000	1.33498600	-0.36020300
C	0.73220100	0.68130600	-0.90665100
C	0.68989500	-0.72968700	-0.77890000
C	1.68310100	-1.42124200	-0.09534600
C	2.78559300	-0.75132400	0.46396400
Cl	-0.60730700	-1.57807600	-1.52544200
Cl	1.62270200	-3.14092800	0.08094300
C	1.92461700	2.75915700	-0.49229100
N	2.00921700	3.90965100	-0.59261700
C	3.99296200	1.31971700	0.86241500
N	4.90441800	1.88157500	1.30269200
O	-0.18489400	1.37918800	-1.54938500
H	-1.19713800	1.13892800	-1.29142500
O	3.77545500	-1.37504400	1.12838400
H	3.61236000	-2.32875700	1.17885500
C	-2.59318900	0.49335800	0.25313100
O	-1.69110300	0.20074400	1.03359600
O	-2.52252500	0.96577600	-0.92020500
C	-4.05741500	0.23976400	0.70072300
F	-4.15139300	-0.12232300	1.98526600
F	-4.82398400	1.33155300	0.53687200
F	-4.61184100	-0.74540100	-0.03342200

DDQ-2H

C	-1.32799000	0.70356800	-0.0000010
C	-1.32799000	-0.70356800	0.0000010
C	-0.12781200	-1.41520800	0.0000020
C	1.07892300	-0.69598400	0.0000010
C	1.07892400	0.69598400	-0.0000010
C	-0.12781200	1.41520800	-0.0000020
Cl	2.55321700	-1.58859600	0.0000030
Cl	2.55321700	1.58859600	-0.0000030
C	-2.56132100	-1.43322800	0.0000010
N	-3.55934900	-2.01843500	0.0000070
C	-2.56132100	1.43322800	-0.0000030
N	-3.55934900	2.01843500	-0.0000040
O	-0.19378700	-2.75385000	0.0000030
H	0.69025900	-3.15122400	0.0000070
O	-0.19378700	2.75385000	-0.0000050
H	0.69025900	3.15122400	-0.0000040

$H(CF_3CO_2)^-$

C	-2.01973400	0.48201200	-0.04900300
O	-1.86423400	1.64662100	-0.36030200
O	-1.14384700	-0.40565900	0.26370500
H	-0.06781000	-0.02989600	0.23942100
C	-3.45104700	-0.10842300	0.01100700
F	-3.73501700	-0.55359000	1.24588000
F	-3.57996400	-1.14806500	-0.82941500
F	-4.37647600	0.79555500	-0.31684000
C	2.01557900	-0.48323500	-0.05024200
O	1.13463900	0.38564100	0.25476500
O	1.88409800	-1.65723100	-0.36375900
C	3.44773200	0.11248600	0.01197200
F	3.57699100	1.15534900	-0.82728300
F	4.38691900	-0.78147100	-0.31336700
F	3.73058800	0.56087700	1.24801500

$(TFA)_2CF_3CO_2^-$

O	2.45332100	1.27534700	-0.03827600
C	2.74511700	0.06248300	0.00716900

O	2.02340100	-0.94739600	0.08540400
C	4.26382900	-0.25890600	0.00522200
O	-0.58218600	0.93512700	-1.36000900
C	-0.73167100	1.63419100	-0.38155500
O	0.17326900	2.11853700	0.40832300
C	-2.15331300	2.10008400	0.00760600
C	-1.27296400	-1.35534500	0.39085000
O	-1.24958100	-0.50024900	1.24655100
O	-0.28921200	-1.81778200	-0.31762100
C	-2.60174200	-2.03571100	-0.00818200
H	1.12494400	1.73080000	0.17256900
H	0.60169700	-1.33935200	-0.11966100
F	4.55503100	-1.22265800	-0.88020700
F	4.63838900	-0.70298700	1.21904900
F	5.02253900	0.80157800	-0.28594900
F	-2.28888700	2.32556700	1.31519000
F	-2.43519000	3.25054200	-0.63384700
F	-3.06792100	1.19985400	-0.36166700
F	-2.49677000	-3.37104100	0.04209600
F	-2.94188900	-1.70027500	-1.26003000
F	-3.59133400	-1.66734600	0.80374700

C

C	0.69738700	-0.60144600	-0.61244500
H	0.81187300	-0.68535600	-1.69723900
C	1.45363500	-1.72291700	0.11165800
H	1.30348900	-2.67058900	-0.40690400
H	1.06916700	-1.82016600	1.13138800
N	1.55917000	0.57376400	-0.18315400
C	2.85873800	0.21571800	0.46632900
H	3.65909200	0.81346900	0.03089000
H	2.76807800	0.40471000	1.53858800
N	1.13674000	1.75425500	-0.25416600
N	0.73623800	2.79330300	-0.32555900
C	-0.74561600	-0.39139000	-0.24408300
C	-1.72833900	-0.49560600	-1.22920300
C	-1.11139500	-0.10057200	1.07576200
C	-3.07255100	-0.32829400	-0.89617900
H	-1.44392700	-0.71305800	-2.25491500
C	-2.45138800	0.08072600	1.40325400
H	-0.35107300	-0.01047300	1.84914100
C	-3.43386100	-0.03808200	0.41749100
H	-3.83304500	-0.41921500	-1.66455800
H	-2.72982800	0.31131400	2.42620700
H	-4.47897700	0.09938400	0.67521100
C	2.91899200	-1.27393700	0.12535100
H	3.51249800	-1.81377900	0.86363500
H	3.37401000	-1.41070300	-0.85889900

TS2

C	0.73056200	-0.59692700	-0.56574700
N	1.46101300	0.65060100	-0.69610300
C	2.88047100	0.31768700	-0.57712400
H	3.18865400	0.34345500	-1.63373000
H	3.41524600	1.14005000	-0.10000300
N	1.04757100	1.48172200	0.81110600
N	0.75151500	2.32381500	1.45128800
H	0.89681500	-0.93061000	-1.61726800
C	-0.74467300	-0.40265300	-0.34522300
C	-1.43067800	0.58138300	-1.06814000
C	-1.43322000	-1.19807700	0.57317200
C	-2.79064900	0.78099700	-0.85495200
H	-0.89929300	1.18895000	-1.79583700
C	-2.79779100	-0.99681200	0.78053600
H	-0.91628900	-1.97450400	1.12782400
C	-3.47588800	-0.00791300	0.07096700
H	-3.31646700	1.54821400	-1.41340700
H	-3.32797100	-1.61455600	1.49769500
H	-4.53748000	0.14635200	0.23453700
C	1.54987400	-1.48142700	0.37369700
H	1.27345600	-1.24471400	1.40773700
H	1.36404900	-2.54222500	0.20386100
C	3.00442200	-1.07115500	0.07428100
H	3.61165700	-1.03595900	0.97845700
H	3.47234400	-1.76803100	-0.62271300

2-H

C	-0.88359500	-0.00812800	-0.03003300
N	-1.62886600	-1.05905300	-0.16958100
C	-3.07830600	-0.78878200	-0.21272700
H	-3.40940400	-0.87620800	-1.25124500
H	-3.60468800	-1.52341500	0.39613400
C	0.57206400	-0.02499900	-0.00155000
C	1.29386400	-1.22302200	0.13271400
C	1.25667500	1.19410000	-0.11619400
C	2.68112200	-1.19586200	0.14134600
H	0.78666900	-2.17479900	0.25762500
C	2.64691500	1.21294500	-0.11649400

H	0.70670900	2.12370600	-0.21864500
C	3.35741800	0.02033900	0.01234300
H	3.23708400	-2.11996300	0.25374700
H	3.17331700	2.15580500	-0.21426800
H	4.44237300	0.03597700	0.01840800
C	-1.74845100	1.21769000	0.05117700
H	-1.39727200	1.91185500	0.81597500
H	-1.68939500	1.72771700	-0.91906400
C	-3.14939700	0.64501200	0.32619300
H	-3.33780100	0.62838800	1.40154200
H	-3.93754600	1.22141600	-0.15593500
H	-1.25783700	-1.99286600	-0.31785700

TS3

C	0.70427500	-0.51498500	-0.47715700
H	0.94314800	-0.52629000	-1.54664500
C	1.41584900	-1.77950300	0.17996700
H	1.18049000	-2.61161000	-0.48507700
H	0.98950200	-1.96560000	1.16487600
N	1.55535700	0.33108400	0.28415200
C	2.96022800	0.09912700	-0.05963700
H	3.16069400	0.30277300	-1.11401100
H	3.60235100	0.68393500	0.59428600
N	1.17998500	2.07158900	-0.23234700
N	0.78971600	3.09487600	-0.15622200
C	-0.75632100	-0.36176900	-0.19654400
C	-1.66513100	-0.51350600	-1.24539400
C	-1.21538600	-0.07680400	1.09414400
C	-3.03222600	-0.38126200	-1.00599100
H	-1.30486500	-0.73249900	-2.24704600
C	-2.58027700	0.06159400	1.32740200
H	-0.50768700	0.04160200	1.91058800
C	-3.48933100	-0.09221100	0.27856000
H	-3.73699700	-0.49903700	-1.82228200
H	-2.93575500	0.28718600	2.32739100
H	-4.55320800	0.01386800	0.46455600
C	2.93089400	-1.42218700	0.23595200
H	3.34522700	-1.63704000	1.21904400
H	3.50625600	-1.95109500	-0.52257500

E1

C	-0.57761900	-0.95291500	-0.10600400
H	-0.66006400	-2.03804500	-0.16416900
C	-2.14778200	1.07502500	0.06569600
H	-1.92189800	1.65088400	-0.83411100
H	-1.71869900	1.55165800	0.94934400
N	-1.70100900	-0.33253000	-0.07412500
C	-3.08809000	-0.85924900	-0.07776100
H	-3.33932900	-1.28067800	-1.05247100
H	-3.24479000	-1.59391800	0.71251900
C	0.75556700	-0.38538800	-0.05870700
C	1.81123900	-1.30699000	0.05268400
C	1.03501700	0.99226300	-0.12255400
C	3.12548000	-0.86209300	0.11633900
H	1.59428700	-2.37042500	0.09314600
C	2.35172400	1.42774600	-0.06495800
H	0.24472800	1.72374800	-0.23316800
C	3.39445900	0.50525300	0.05784000
H	3.93564200	-1.57689300	0.20728700
H	2.56834100	2.48887700	-0.11906700
H	4.42012500	0.85678300	0.10272700
C	-3.60326300	0.57391900	0.18128300
H	-4.03240900	0.71042400	1.17202600
H	-4.27925600	0.95986700	-0.57833100

N_2

N	0.00000000	0.00000000	0.54905700
N	0.00000000	0.00000000	-0.54905700

3

N	4.66107200	-0.12251500	-0.77611800
C	3.64067300	0.02997100	0.29032400
H	3.78559400	-0.74728400	1.05104400
H	3.75707500	1.00843300	0.77304800
N	5.82210200	-0.00833300	-0.38810600
N	6.91908900	0.08200400	-0.12236300
C	2.26350900	-0.09112600	-0.33820200
H	2.15403600	0.68224100	-1.10790600
H	2.18533400	-1.06157800	-0.84285000
C	1.15214000	0.04734700	0.70013100
H	1.25394600	1.00947400	1.22053600
H	1.26229300	-0.73494100	1.46332000
C	-0.24018900	-0.04244400	0.07961400
H	-0.35917200	0.74797800	-0.67313700
H	-0.34888900	-0.99840500	-0.44962100
C	-1.35956600	0.08470100	1.12124800
H	-1.23601800	1.02825300	1.66639800
H	-1.26146600	-0.72576200	1.85371400

C	-2.72942900	0.04153400	0.49041300
C	-3.37459600	1.22107100	0.10377100
C	-3.36175000	-1.18001800	0.23183300
C	-4.61926100	1.18463500	-0.52450200
H	-2.89604000	2.17804900	0.29982700
C	-4.60577500	-1.22288700	-0.39681900
H	-2.87377600	-2.10558500	0.52983400
C	-5.23926200	-0.03925400	-0.77702000
H	-5.10602400	2.11128200	-0.81385000
H	-5.08240700	-2.18027800	-0.58549500
H	-6.20929100	-0.07115300	-1.26349300

TS4

C	0.40736200	-0.32572600	-0.13353900
C	0.13792600	0.50202500	1.00723900
C	-1.05298900	1.17385600	1.13579200
C	-2.13749500	0.99917400	0.16262100
C	-1.86274200	0.10430000	-0.96769800
C	-0.65124400	-0.49674200	-1.11861200
O	1.54165500	-0.90605000	-0.26105200
O	-3.21734500	1.57795700	0.31244200
Cl	-3.11652700	-0.06195500	-2.12512100
Cl	-0.27626400	-1.47335400	-2.47510600
C	2.12794900	1.87804000	-1.02600200
C	2.16836000	2.73384100	0.11362700
C	1.13355500	3.60870600	0.37122500
C	0.00593300	3.63782800	-0.47184500
C	-0.04290100	2.83447000	-1.61409900
C	0.99880000	1.96041500	-1.88471200
H	3.02351300	2.69770300	0.78101900
H	1.17256600	4.25540400	1.24143200
H	-0.81795900	4.30837600	-0.24584000
H	-0.90127600	2.88171200	-2.27703500
H	0.96969400	1.33323800	-2.77270500
N	-1.52091800	2.70950500	3.16678400
C	-1.31763700	2.01889300	2.26044900
N	1.97262200	0.65249600	2.83521400
C	1.15851800	0.59239700	2.01591900
C	3.10222900	0.85951600	-1.26722900
H	2.35525400	-0.16522600	-0.75419800
H	3.12310600	0.48343300	-2.29450800
C	4.40339700	0.74304600	-0.51265900
H	4.23262800	0.82857500	0.56721400
H	5.04839100	1.58717000	-0.79906400
C	5.11711500	-0.57385400	-0.82146400
H	4.47849500	-1.41342400	-0.51746700
H	5.25878200	-0.65955400	-1.90652200
C	6.47021300	-0.67863700	-0.12162300
H	6.32884200	-0.60983200	0.96494500
H	7.11237600	0.15847800	-0.41943900
C	-5.11600000	-0.97270100	0.58216800
O	-3.99007000	-1.36874700	0.74680300
O	-5.50274500	0.23399000	0.24376400
H	-4.70122300	0.81892600	0.14909600
C	-6.33818300	-1.90009100	0.75384900
F	-5.95496700	-3.12975400	1.08390300
F	-7.04153300	-1.96728300	-0.38354900
F	-7.14904300	-1.43767400	1.71331300
C	7.17186100	-1.98847500	-0.46471700
H	7.34748800	-2.05777000	-1.53955400
H	6.55820000	-2.84747700	-0.16555200
N	8.51628500	-2.09261800	0.15017900
N	8.50228100	-2.22939700	1.37366400
N	8.59292200	-2.36084000	2.49433500

A3

N	4.58537300	0.22708500	0.39812700
C	3.33940500	-0.06573200	-0.34623700
H	3.09487900	0.77373200	-1.00865200
H	3.47553900	-0.96363000	-0.96191000
N	5.56506600	0.43722200	-0.31701500
N	6.51837100	0.64341900	-0.89013700
C	2.23065300	-0.28113900	0.67162200
H	2.50421400	-1.11380300	1.32874600
H	2.13928300	0.61470700	1.29547200
C	0.90138300	-0.57709900	-0.01972400
H	0.98829500	-1.47899400	-0.63535400
H	0.62321400	0.24982700	-0.68199300
C	-0.22318800	-0.77321600	1.03907300
H	0.07607700	-1.60095700	1.69365500
H	-0.33848300	0.13144000	1.63651900
C	-1.44918000	-1.17146900	0.34020200
C	-2.59266500	-0.41441500	0.10764400
C	-2.73867700	0.92512300	0.58093100
C	-3.64993400	-1.01650100	-0.64033600
C	-3.89700900	1.61971400	0.31201300
H	-1.94129600	1.39637700	1.14429000
C	-4.80678700	-0.31105600	-0.89728000

H	-3.52888200	-2.03428000	-0.99920100
C	-4.92467400	1.00135300	-0.42090800
H	-4.02081800	2.63720300	0.66321100
H	-5.61518600	-0.76155400	-1.46061700
H	-5.83457100	1.55765500	-0.62488000
H	-1.43989300	-2.17518300	-0.08811000

D

C	0.51625000	-0.44934300	-0.54200200
H	0.67839700	-0.41523200	-1.62611900
C	1.23453500	-1.65661600	0.05728000
H	0.80284200	-2.54061300	-0.42081900
H	1.00487600	-1.71720200	1.12696400
N	1.21755500	0.78123400	0.02095300
C	2.70926700	0.91553300	-0.10425500
H	2.94102700	1.03021800	-1.16816400
H	2.99610700	1.81613200	0.43940200
N	0.55942300	1.87057800	-0.04835100
N	-0.03246500	2.81241800	-0.03797800
C	-0.95583000	-0.37535800	-0.22923200
C	-1.88623700	-0.36035800	-1.26990900
C	-1.39596500	-0.32542000	1.09887900
C	-3.25143700	-0.31388400	-0.98592800
H	-1.54511200	-0.38990100	-2.30120600
C	-2.75792600	-0.26765100	1.37926700
H	-0.67618500	-0.32503700	1.91408100
C	-3.68664400	-0.26664200	0.33672300
H	-3.97062800	-0.30916300	-1.79831800
H	-3.09512900	-0.22672700	2.40966700
H	-4.74840600	-0.22656800	0.55728400
C	2.74694200	-1.59774400	-0.15653900
H	3.21022400	-2.48572800	0.27986500
H	2.97291900	-1.60930000	-1.23008100
C	3.33304000	-0.33955200	0.48258800
H	3.17115800	-0.35187000	1.56562700
H	4.41034300	-0.27642000	0.30822400

TS5

C	0.49755600	-0.52409300	-0.55967200
H	0.65177400	-0.80442500	-1.62790900
C	1.25896500	-1.50953000	0.32246400
H	0.82431900	-2.50280500	0.18777200
H	1.09948200	-1.22051100	1.37058500
N	1.09835100	0.78883600	-0.68217200
C	2.54328100	0.85830200	-0.77681900
H	2.65396800	0.61589000	-1.85061300
H	2.83302800	1.90646400	-0.68158100
N	0.74618200	1.51602900	0.93374300
N	0.37575700	2.26338500	1.64828200
C	-0.99457700	-0.38870000	-0.33883900
C	-1.72540900	0.48207300	-1.15654900
C	-1.64991100	-1.10758600	0.66309900
C	-3.09361600	0.64109300	-0.96589400
H	-1.21943200	1.03297400	-1.94459700
C	-3.02353800	-0.94665100	0.85096900
H	-1.10555000	-1.79220000	1.30449700
C	-3.74546500	-0.07379000	0.04107700
H	-3.65287400	1.31607300	-1.60532500
H	-3.52521000	-1.50519200	1.63419600
H	-4.81370500	0.04735700	0.18901000
C	2.75267700	-1.51724000	0.00322100
H	3.27115200	-2.18104900	0.69880300
H	2.91446800	-1.91668600	-1.00477700
C	3.32541400	-0.10603000	0.10022000
H	3.28019300	0.25620500	1.13559900
H	4.37409200	-0.07693000	-0.20428800

4-H

C	0.58651700	0.04868600	-0.05085900
N	1.21415700	-1.00921700	-0.45698800
C	2.67518400	-1.21999700	-0.47796800
H	2.84537800	-2.24122700	-0.13250300
H	2.99109200	-1.15320400	-1.52351500
C	-0.88542900	0.02495800	-0.01477300
C	-1.55490400	-1.15606800	0.34223900
C	-1.62107500	1.17590500	-0.33005500
C	-2.94412100	-1.18569500	0.37084800
H	-0.99550000	-2.03743500	0.64257700
C	-3.01142100	1.13317800	-0.31437200
H	-1.11928900	2.09261900	-0.61936300
C	-3.67274700	-0.04360700	0.03620800
H	-3.45717900	-2.09542600	0.66306600
H	-3.57810200	2.01975300	-0.57664300
H	-4.75727200	-0.06939100	0.05582100
C	1.34798800	1.24812500	0.41628400
H	0.86918500	2.14048200	0.00453900
H	1.18320700	1.30061600	1.50138800
H	0.65230400	-1.77939800	-0.81460300

C	2.83645600	1.19780100	0.08146100
H	2.98597500	1.43072800	-0.97865000
H	3.35985100	1.96100600	0.66024300
C	3.38304000	-0.19315500	0.38810400
H	4.45468600	-0.25323200	0.18748800
H	3.22963600	-0.43214500	1.44637200

TS6

C	0.55142600	-0.41659900	-0.45274700
H	0.76006700	-0.44370300	-1.52933600
C	1.24153900	-1.66636300	0.21104100
H	0.73322200	-2.52678000	-0.23232800
H	1.02088900	-1.65770400	1.28312100
N	1.25367600	0.66611500	0.20089400
C	2.63069000	0.84082600	-0.21821300
H	2.74722400	0.80108000	-1.30557800
H	3.01521400	1.77211200	0.19674300
N	0.42613700	2.11095300	-0.30169500
N	-0.03106100	3.10598900	-0.21009000
C	-0.92576500	-0.37832100	-0.17361300
C	-1.81863600	-0.67119300	-1.20608500
C	-1.40850000	-0.06760100	1.10219900
C	-3.19183800	-0.64941200	-0.96662500
H	-1.44112600	-0.91330400	-2.19614000
C	-2.78087300	-0.03880200	1.33548900
H	-0.71378900	0.15698700	1.90779300
C	-3.67307200	-0.33078600	0.30238800
H	-3.88308700	-0.87484300	-1.77197600
H	-3.15397400	0.20853800	2.32392200
H	-4.74205600	-0.30996500	0.48784500
C	2.74137500	-1.67271100	-0.05018600
H	3.19839500	-2.52082300	0.46717300
H	2.93578700	-1.79867200	-1.12113400
C	3.35121300	-0.36954200	0.44363000
H	3.27175000	-0.28376600	1.53101900
H	4.40487000	-0.26752900	0.17145100

E3

C	0.23049400	-0.95036100	-0.10122700
H	0.26678500	-2.03667100	-0.17132300
C	1.68878100	1.05879200	0.12563900
H	1.03940100	1.47814200	0.89570800
H	1.50306500	1.55757700	-0.83070900
N	1.38640700	-0.38300000	-0.04313400
C	2.64817900	-1.18068600	-0.08992500
H	2.75524000	-1.68058800	0.87703700
H	2.57265700	-1.92401000	-0.88340400
C	-1.09839600	-0.36574000	-0.06419700
C	-2.14162600	-1.28857800	0.14075200
C	-1.40737100	0.99638000	-0.24215900
C	-3.46072100	-0.86060300	0.20496700
H	-1.91006400	-2.34339900	0.25629100
C	-2.73086800	1.41374600	-0.19140400
H	-0.63920000	1.72896600	-0.44729300
C	-3.75514600	0.49265400	0.04013600
H	-4.25509800	-1.57906500	0.37308900
H	-2.96532200	2.46226800	-0.33807500
H	-4.78514700	0.83171500	0.08123400
C	3.17487000	1.07406800	0.47831600
H	3.63872400	2.01987800	0.19728000
H	3.30659500	0.92761500	1.55433800
C	3.72683500	-0.12494400	-0.29686300
H	3.82325500	0.11600000	-1.35966200
H	4.69407400	-0.46580800	0.07321000

1-OMe

N	5.10591800	0.09741200	0.20405700
C	3.74418600	-0.28944200	-0.24014700
H	3.64529300	-0.11238600	-1.31850800
H	3.58537900	-1.35873500	-0.05191800
N	6.01483300	-0.52559300	-0.34122800
N	6.91429100	-1.04719900	-0.78957700
C	2.73195600	0.54112800	0.52910600
H	2.86827300	0.36485900	1.60296500
H	2.93172800	1.60419000	0.34845100
C	1.29969800	0.20304200	0.12306800
H	1.10470600	-0.86339100	0.29722900
H	1.16637800	0.37578600	-0.95307900
C	0.26364800	1.03094300	0.89450000
H	0.39572300	0.85701100	1.96918400
H	0.45325000	2.09655900	0.71722800
C	-1.15042500	0.69050300	0.49302400
C	-1.77179700	1.33730700	-0.58489900
C	-1.86360200	-0.31436100	1.14510700
C	-3.05265900	0.99192700	-0.99339400
H	-1.24220200	2.12867500	-1.11065500
C	-3.15438800	-0.67942000	0.75078900
H	-1.40744700	-0.83134500	1.98644900

C	-3.75145200	-0.02208500	-0.32638300
H	-3.53427900	1.49722300	-1.82463700
H	-3.67328900	-1.46444900	1.28786700
O	-5.00157000	-0.29217600	-0.79580300
C	-5.74260800	-1.31018700	-0.14503400
H	-5.91754200	-1.05924400	0.90706800
H	-6.69625000	-1.37063700	-0.66769900
H	-5.22779300	-2.27517900	-0.21070800

TS1-OMe

C	0.84916900	-0.73243700	0.05843700
C	0.58076000	0.15712400	1.15069800
C	-0.58690700	0.88201700	1.21743500
C	-1.64959100	0.70596900	0.22788800
C	-1.38171700	-0.24664500	-0.85350900
C	-0.19294500	-0.90542600	-0.94329300
O	1.97622200	-1.32547300	-0.03318700
O	-2.70953300	1.34019700	0.32069200
Cl	-2.60727700	-0.40873100	-2.04350900
Cl	0.17474100	-1.95058200	-2.25046400
C	2.51509400	1.49563500	-0.85536200
C	2.52092200	2.40938200	0.24941100
C	1.49821200	3.29586000	0.44142600
C	0.38599100	3.30613800	-0.44689100
C	0.36992100	2.44892200	-1.56809300
C	1.41618200	1.56809100	-1.75496200
H	3.35375600	2.40436000	0.94479100
H	1.49525800	3.99082300	1.27436200
H	-0.44573000	2.47595100	-2.28117900
H	1.40821300	0.91427000	-2.62405600
N	-1.03480000	2.56877200	3.12907400
C	-0.83964900	1.80536900	2.28094100
N	2.39771400	0.35816300	2.99076100
C	1.58826500	0.27137300	2.16895400
C	3.50817000	0.48111400	-1.02866200
H	2.81838000	-0.53728800	-0.53798500
H	3.59285500	0.10209300	-2.05166600
C	4.79335400	0.46782800	-0.22918500
H	4.57566900	0.58773800	0.83881400
H	5.40585300	1.33022200	-0.52903700
C	5.58693600	-0.82190500	-0.44052100
H	4.98097700	-1.68191200	-0.12707100
H	5.81610800	-0.95363400	-1.50397600
C	6.88988500	-0.79676900	0.35170700
H	6.68916400	-0.67361900	1.42343700
H	7.51729400	0.03551800	0.02834100
N	7.71155700	-2.00833400	0.12753200
N	7.25343500	-3.02966200	0.64181800
N	6.91821700	-4.01798400	1.07934900
C	-4.71622900	-1.13353100	0.57181200
O	-3.62683700	-1.56235000	0.85745400
O	-5.02710400	0.08251300	0.19359300
H	-4.19498400	0.63443100	0.15238400
C	-5.97330500	-2.02904800	0.58664900
F	-5.68749200	-3.23956500	1.05621200
F	-6.45664500	-2.16180700	-0.65646800
F	-6.93582500	-1.49580200	1.34730600
O	-0.56891100	4.17770500	-0.15858100
C	-1.68385500	4.31491800	-1.05021600
H	-2.22411400	3.36972200	-1.13407000
H	-2.32385600	5.06795200	-0.59684000
H	-1.33761200	4.65498700	-2.02965100

A1-OMe

N	4.68493200	-0.23467900	-0.74570100
C	3.73885500	-0.09620000	0.38205100
H	3.55743500	-1.07525500	0.84218200
H	4.15572600	0.57387500	1.14368500
N	5.79424100	-0.66367500	-0.42549500
N	6.83903200	-1.04926600	-0.22951700
C	2.44662600	0.47898100	-0.17637900
H	2.65284200	1.45173900	-0.63400700
H	2.06073800	-0.18193000	-0.95863700
C	1.39450300	0.62809600	0.94308700
H	1.81802600	1.25691200	1.73804400
H	1.15419600	-0.34533600	1.37348400
C	0.20560000	1.33319600	0.41804400
C	-1.06452300	0.84321500	0.23695800
C	-2.07344400	1.71512300	-0.30997900
C	-1.43673400	-0.50801200	0.55768400
C	-3.34548300	1.27820500	-0.51321200
H	-1.80108900	2.73669500	-0.55749100
C	-2.70900600	-0.95835800	0.35255200
H	-0.69810100	-1.18884400	0.96509800
C	-3.68168500	-0.06594100	-0.18378400
H	-4.12076900	1.91596800	-0.92089900
H	-2.97002500	-1.97986700	0.59598000
H	0.37642300	2.36753800	0.11541600

O	-4.92474400	-0.40454000	-0.40927700
C	-5.38602800	-1.73507500	-0.11711700
H	-4.83721100	-2.46051700	-0.72058600
H	-5.27226300	-1.94376600	0.94828500
H	-6.43750200	-1.73694500	-0.39078000

1-Me

N	4.66142500	0.18937200	0.22798200
C	3.31930200	-0.23148500	-0.24389500
H	3.21790100	-0.00709300	-1.31320700
H	3.20535300	-1.31437300	-0.10819300
N	5.59791300	-0.34225000	-0.36540800
N	6.52001100	-0.78054600	-0.85502400
C	2.26923800	0.51749200	0.55773000
H	2.41385000	0.30317100	1.62351200
H	2.41834300	1.59550600	0.42193200
C	0.85465400	0.12915600	0.13512000
H	0.70799800	-0.95025100	0.27316900
H	0.71593000	0.33137800	-0.93511800
C	-0.21942800	0.88496700	0.92856100
H	-0.08206000	0.68371500	1.99790600
H	-0.08022900	1.96294400	0.78362000
C	-1.61417700	0.48987400	0.51005900
C	-2.28514900	1.17485500	-0.50568700
C	-2.25300200	-0.61098600	1.09300100
C	-3.55391300	0.77330100	-0.92661100
H	-1.81084300	2.03471400	-0.97394100
C	-3.51871800	-1.01149300	0.67307900
H	-1.75081200	-1.15907400	1.88750500
C	-4.19220100	-0.32485500	-0.34496000
H	-4.05570300	1.32449300	-1.71820500
H	-3.99473800	-1.86879000	1.14382200
C	-5.56907200	-0.75616200	-0.78458900
H	-5.58628400	-1.82069600	-1.03663900
H	-6.30311700	-0.59694400	0.01183800
H	-5.89623400	-0.19271300	-1.66169600

TS1-Me

C	0.82216300	-0.60054300	-0.01376400
C	0.53952200	0.31592200	1.05230100
C	-0.63015100	1.03750000	1.08128200
C	-1.67038200	0.84441700	0.06967700
C	-1.40352600	-0.16703900	-0.95776000
C	-0.21235700	-0.82393800	-1.01246200
O	1.95672000	-1.18868000	-0.07776500
O	-2.71055200	1.51386400	0.09929600
Cl	-2.62479500	-0.39009300	-2.13959300
Cl	0.16752500	-1.92369000	-2.26998000
C	2.54191900	1.57483200	-0.99155500
C	2.52948600	2.51662900	0.08143600
C	1.48086000	3.39319300	0.24052300
C	0.36421500	3.36101700	-0.62838400
C	0.38792000	2.46924600	-1.71759900
C	1.44358100	1.59734400	-1.89713300
H	3.35954300	2.54609800	0.77963400
H	1.48978900	4.10135200	1.06406800
H	-0.44685400	2.46121400	-2.41460700
H	1.44690400	0.91422600	-2.74371400
N	-1.10666900	2.78119100	2.93442300
C	-0.89910400	1.99218300	2.11311400
N	2.33006200	0.56455300	2.91262600
C	1.53287200	0.45902300	2.08122900
C	3.53417100	0.55350200	-1.11275200
H	2.78834500	-0.44706700	-0.58359800
H	3.62706000	0.11710500	-2.11145900
C	4.78995100	0.53310100	-0.27284300
H	4.54621300	0.73062000	0.77742200
H	5.44792400	1.34914300	-0.60617800
C	5.53512800	-0.79897400	-0.37395600
H	4.88306800	-1.61169000	-0.02832500
H	5.79562100	-1.00922600	-1.41719600
C	6.80884500	-0.77357100	0.46517800
H	6.57546300	-0.56465600	1.51670200
H	7.48592600	0.00436700	0.10837700
N	7.57930600	-2.03356100	0.35915100
N	7.05805600	-2.99127100	0.93257900
N	6.66257200	-3.92691200	1.43139500
C	-4.78014600	-0.88563000	0.53856000
O	-3.69416100	-1.30894800	0.84300900
O	-5.07180200	0.28516500	0.02346300
H	-4.23478500	0.81519100	-0.08074000
C	-6.06028700	-1.73071200	0.71343600
F	-5.78051400	-2.89530500	1.29061100
F	-6.62581100	-1.97468200	-0.47594500
F	-6.95612800	-1.08696600	1.47059500
C	-0.80323400	4.27588000	-0.42626200
H	-0.65203900	4.93709500	0.42801700
H	-0.97118200	4.88209000	-1.32200800

H	-1.71891900	3.69152300	-0.25983400

A1-Me

N	4.25380200	-0.11259000	-0.75335400
C	3.31961900	-0.00126500	0.38641500
H	3.19130700	-0.97942300	0.86528800
H	3.71311400	0.70177700	1.13036800
N	5.38076600	-0.50516600	-0.44722500
N	6.43980200	-0.85686100	-0.26566400
C	1.99418500	0.50072900	-0.16648200
H	2.14695800	1.47286000	-0.64522100
H	1.62859900	-0.19521600	-0.92741500
C	0.95217300	0.62179100	0.97172100
H	1.34805800	1.31247600	1.72829300
H	0.78282300	-0.34864600	1.43991000
C	-0.27834100	1.22230300	0.42974400
C	-1.51468800	0.62664900	0.25669700
C	-2.55752900	1.39739500	-0.34976700
C	-1.78821900	-0.72767000	0.63389500
C	-3.79658900	0.84530600	-0.56822800
H	-2.35267300	2.42541400	-0.63398300
C	-3.02938700	-1.26313600	0.40731200
H	-1.01593100	-1.33005400	1.09817500
C	-4.05132900	-0.49116900	-0.19734700
H	-4.58575400	1.43094100	-1.02719200
H	-3.24217900	-2.28876500	0.69043800
H	-0.18385200	2.25439000	0.08849800
C	-5.38402500	-1.11025500	-0.45833700
H	-5.30969200	-1.74625700	-1.34920200
H	-5.68475900	-1.75332600	0.37211300
H	-6.15183900	-0.35790700	-0.64010000

1-F

N	4.62723600	0.18258800	0.26248400
C	3.29111900	-0.14249000	-0.29451200
H	3.17582800	0.33505000	-1.27560100
H	3.20173700	-1.22778000	-0.42866500
N	5.57088700	-0.21011100	-0.42113500
N	6.49912200	-0.53353300	-0.98290400
C	2.23142000	0.36215700	0.66923600
H	2.38132600	-0.11334600	1.64599700
H	2.36412100	1.44137200	0.81229700
C	0.82223600	0.07390300	0.15843400
H	0.69673200	-1.00485700	-0.00353600
H	0.67272400	0.55771100	-0.81574800
C	-0.25921100	0.56236100	1.13092800
H	-0.12396100	0.06409100	2.09810700
H	-0.12827000	1.63725300	1.30297800
C	-1.65049900	0.29849400	0.61000600
C	-2.31833500	1.25724300	-0.15900100
C	-2.28154700	-0.92940800	0.83954300
C	-3.58304700	1.00832500	-0.69042900
H	-1.84474000	2.21796300	-0.34433000
C	-3.54560600	-1.20238200	0.31917300
H	-1.77945700	-1.68606100	1.43737400
C	-4.16761700	-0.22218200	-0.43757500
H	-4.11018000	1.74736900	-1.28390200
H	-4.04389400	-2.14959400	0.49436700
F	-5.39735100	-0.47643400	-0.94703100

TS1-F

C	0.76615400	-0.52245400	0.00937500
C	0.50406500	0.39735500	1.07833400
C	-0.65706200	1.13072600	1.11997200
C	-1.72190300	0.93167400	0.13037600
C	-1.45466800	-0.05140200	-0.92646300
C	-0.26800300	-0.71513200	-0.99535600
O	1.88200500	-1.14934900	-0.04570700
O	-2.77694100	1.56743700	0.20444200
Cl	-2.67930700	-0.24608900	-2.10924500
Cl	0.10175500	-1.79531200	-2.27256100
C	2.57761500	1.57257200	-0.96851600
C	2.62128200	2.51109400	0.10615000
C	1.62995900	3.45172500	0.27161900
C	0.55085300	3.44529600	-0.62314500
C	0.46743000	2.57285100	-1.70485400
C	1.47737900	1.63971200	-1.86672800
H	3.45247000	2.49423100	0.80292400
H	1.65121000	4.17371500	1.08048400
H	-0.37501200	2.63406800	-2.38575200
H	1.44029800	0.95108200	-2.70741500
N	-1.08756000	2.86921400	2.98863600
C	-0.90423500	2.08305900	2.15910900
N	2.30335900	0.61075900	2.93495000
C	1.50290300	0.51992000	2.10510200
C	3.52447000	0.50901200	-1.10091600
H	2.73402700	-0.46698700	-0.55436300
H	3.57995800	0.06394200	-2.09848100

C	4.78934300	0.42620200	-0.28197900
H	4.57796100	0.63977600	0.77210400
H	5.48196800	1.20584000	-0.63266600
C	5.45975900	-0.94391500	-0.39743000
H	4.77648000	-1.71908800	-0.02740100
H	5.67564700	-1.17090500	-1.44720500
C	6.75940800	-0.98423900	0.40050500
H	6.57214800	-0.75883200	1.45785200
H	7.46559100	-0.24610100	0.01699000
N	7.45465700	-2.28523900	0.27599300
N	6.90840900	-3.20747800	0.88347500
N	6.48571200	-4.11532400	1.41039900
C	-4.77981400	-0.91325200	0.54855000
O	-3.68018300	-1.31398800	0.83409000
O	-5.11385700	0.27861900	0.11396000
H	-4.29625900	0.84080600	0.03715100
C	-6.02498500	-1.82155700	0.63600500
F	-5.71568500	-2.99521100	1.17862400
F	-6.52197800	-2.04110600	-0.58867000
F	-6.98411800	-1.25282400	1.37446700
F	-0.42022100	4.34041600	-0.44555900

A1-F

N	4.18747100	-0.10559500	-0.74842300
C	3.26096500	0.03850000	0.39339500
H	3.12141500	-0.92890100	0.89078100
H	3.66603600	0.75037800	1.12236000
N	5.30625400	-0.52116900	-0.44173500
N	6.35718500	-0.89588400	-0.26001600
C	1.93957000	0.54625700	-0.16487800
H	2.10230400	1.50360100	-0.66894500
H	1.55849200	-0.16461800	-0.90395400
C	0.90912900	0.71046900	0.98169700
H	1.30746000	1.43896100	1.69956700
H	0.75622800	-0.23966800	1.49438900
C	-0.33078000	1.26877000	0.42123400
C	-1.54780000	0.63055900	0.24444100
C	-2.60730700	1.35880900	-0.38698400
C	-1.77022700	-0.72688200	0.64245300
C	-3.82566300	0.76753000	-0.61641300
H	-2.43543300	2.38821400	-0.68599900
C	-2.98373800	-1.32353200	0.41418200
H	-0.97978300	-1.29158400	1.12227000
C	-3.98251600	-0.56215500	-0.21123300
H	-4.64844100	1.28595600	-1.09332600
H	-3.19231500	-2.34888000	0.69482600
H	-0.26377600	2.29708700	0.06321500
F	-5.14648300	-1.14244200	-0.43237000

1-Cl

N	5.09106400	0.23076000	0.01384400
C	3.73429600	-0.35983500	-0.09098100
H	3.58809700	-0.76845800	-1.09877300
H	3.63294200	-1.18007400	0.63059400
N	6.00765000	-0.56499000	-0.18320400
N	6.91372500	-1.22325400	-0.34921600
C	2.71353600	0.72775100	0.19475900
H	2.88910600	1.12698000	1.20097900
H	2.86539900	1.55305900	-0.51111700
C	1.28373300	0.20476400	0.08197500
H	1.13915800	-0.64180300	0.76597100
H	1.10513000	-0.17523500	-0.93242600
C	0.24590500	1.28902500	0.40127200
H	0.40275900	1.64531000	1.42619700
H	0.40402000	2.14489400	-0.26528100
C	-1.16658900	0.78304400	0.24738600
C	-1.84618600	0.92022800	-0.96671700
C	-1.81133000	0.12242900	1.29855500
C	-3.13477400	0.41715600	-1.13692600
H	-1.36372100	1.43263200	-1.79515600
C	-3.09919700	-0.38876200	1.15016700
H	-1.30311600	0.00727200	2.25279200
C	-3.74697000	-0.23431600	-0.07137200
H	-3.65643400	0.53187600	-2.08100200
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Cl	-5.36648000	-0.86864200	-0.26955300

TS1-Cl

C	0.82829100	-0.66632000	-0.00871400
C	0.55599400	0.22097300	1.08422200
C	-0.61734600	0.93254300	1.14959100
C	-1.68005900	0.74644400	0.15595700
C	-1.40892500	-0.21923400	-0.91600500
C	-0.21245500	-0.86294900	-1.00540900
O	1.96096200	-1.26109500	-0.09183800
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Cl	0.16476300	-1.91574000	-2.30325200

C	2.58807200	1.49493900	-0.96037000	C	-5.97937700	-2.01932100	0.62317000
C	2.59763400	2.41062100	0.13394600	F	-5.66995600	-3.19798800	1.15465900
C	1.56680100	3.30200700	0.32656300	F	-6.46443600	-2.22630900	-0.60861600
C	0.46833500	3.28387100	-0.55476100	F	-6.94725800	-1.46321300	1.35961100
C	0.43940200	2.43196400	-1.66325700	Cl	-0.84026500	4.37292900	-0.28830800
C	1.48460000	1.54566000	-1.85478000				
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H	1.57739700	3.99516500	1.16075200	N	4.53244100	-0.37253500	-0.75510200
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N	-1.06630300	2.62823200	3.05224900	H	4.17261200	0.93677300	0.87561400
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C	1.56264100	0.34352200	2.10319400	C	2.35433700	0.51439100	-0.21863100
C	3.56427600	0.46322900	-1.11244600	H	2.51151200	1.32395600	-0.93788500
H	2.78693300	-0.54335000	-0.57908400	H	1.90650000	-0.32850100	-0.75328400
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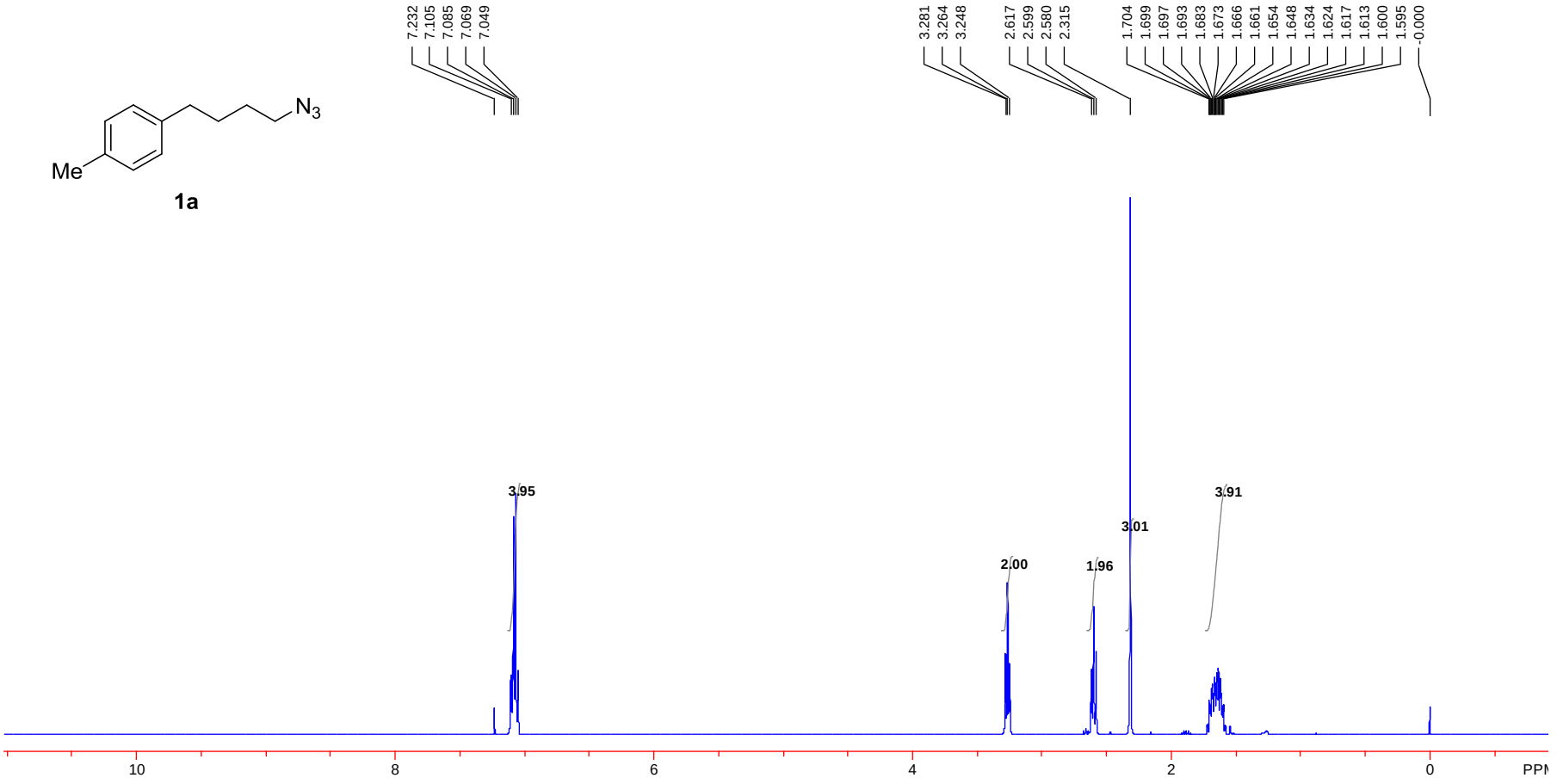
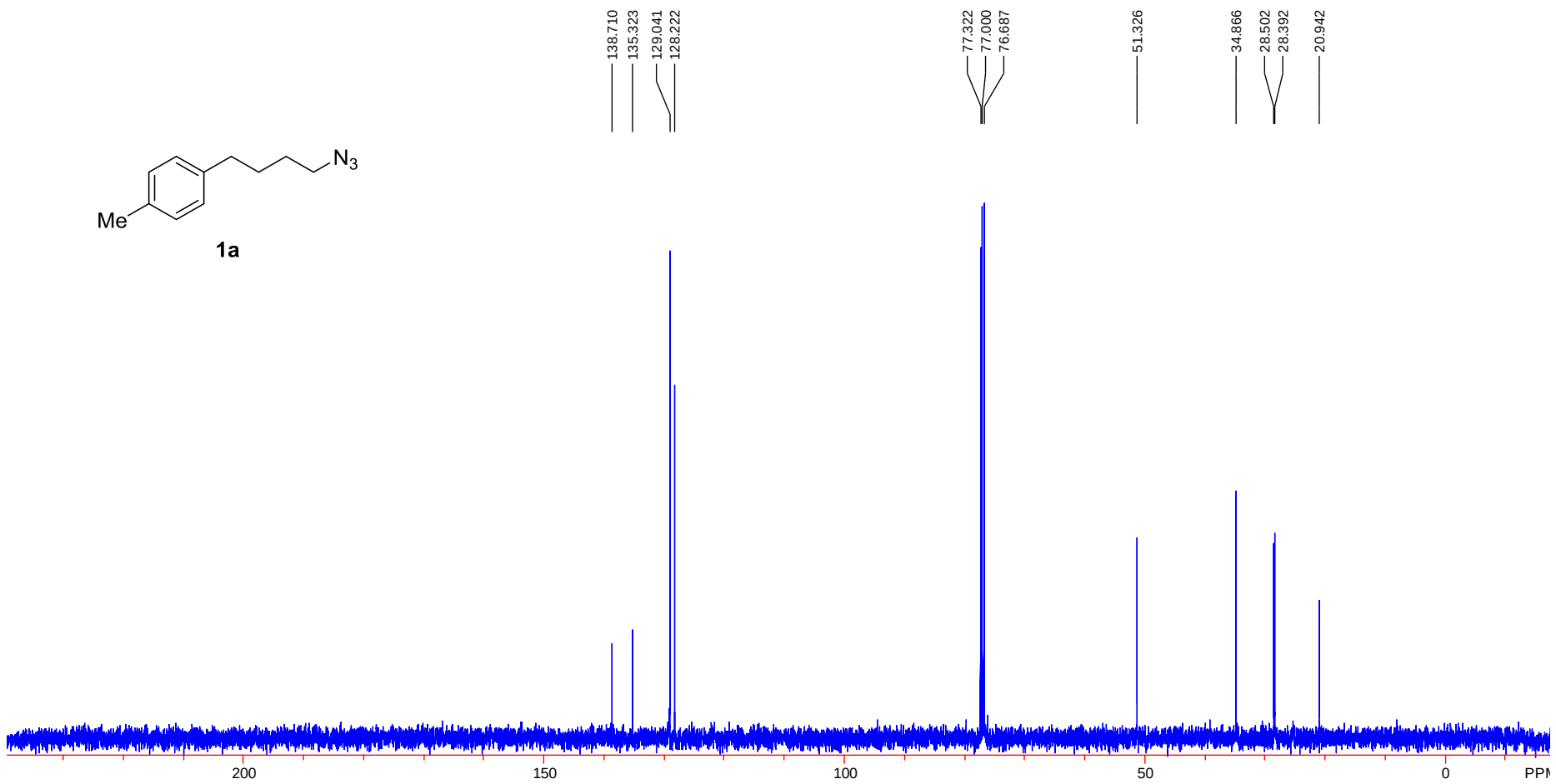
(F) NMR Spectra of Compounds

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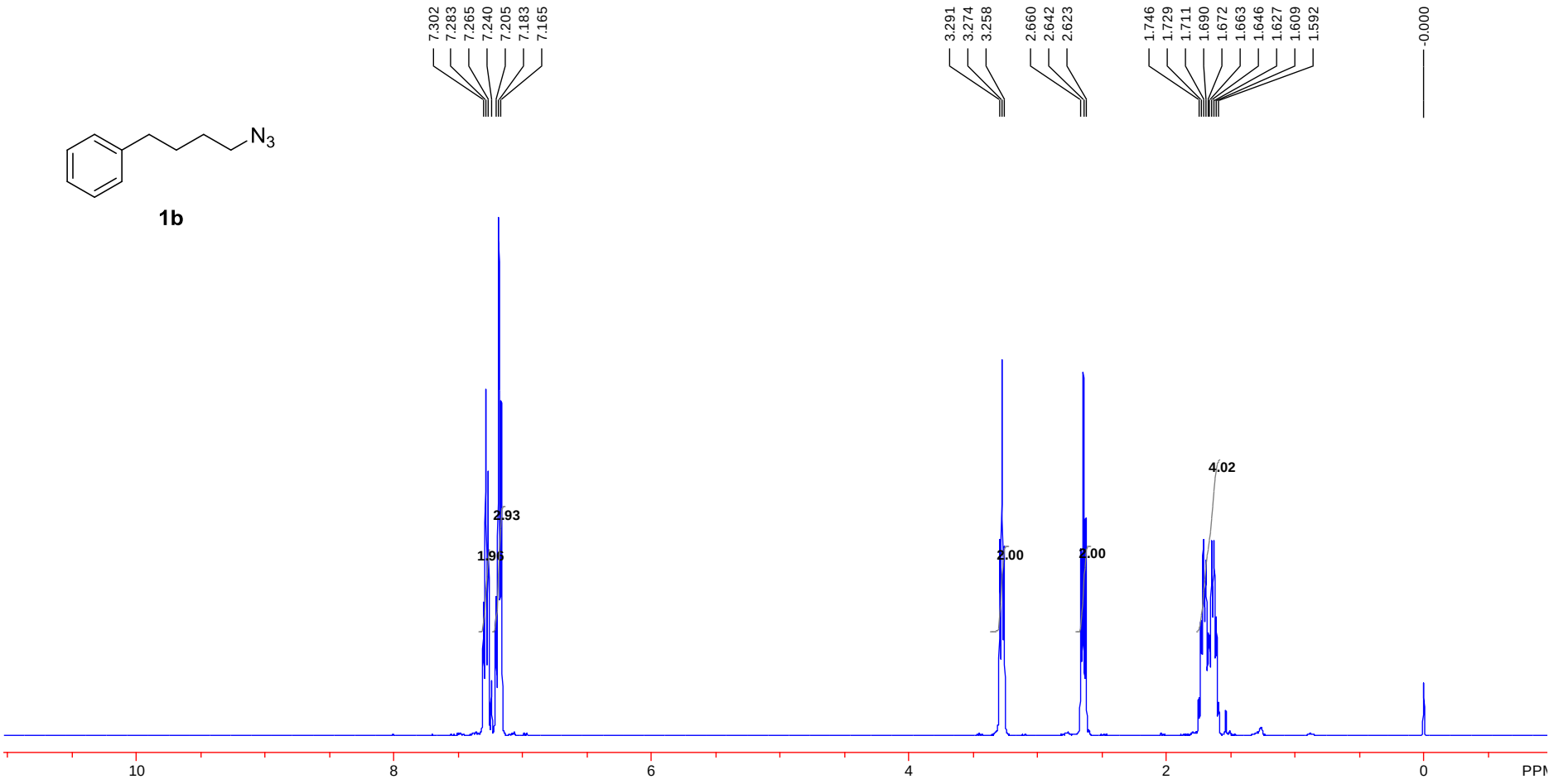
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1.592
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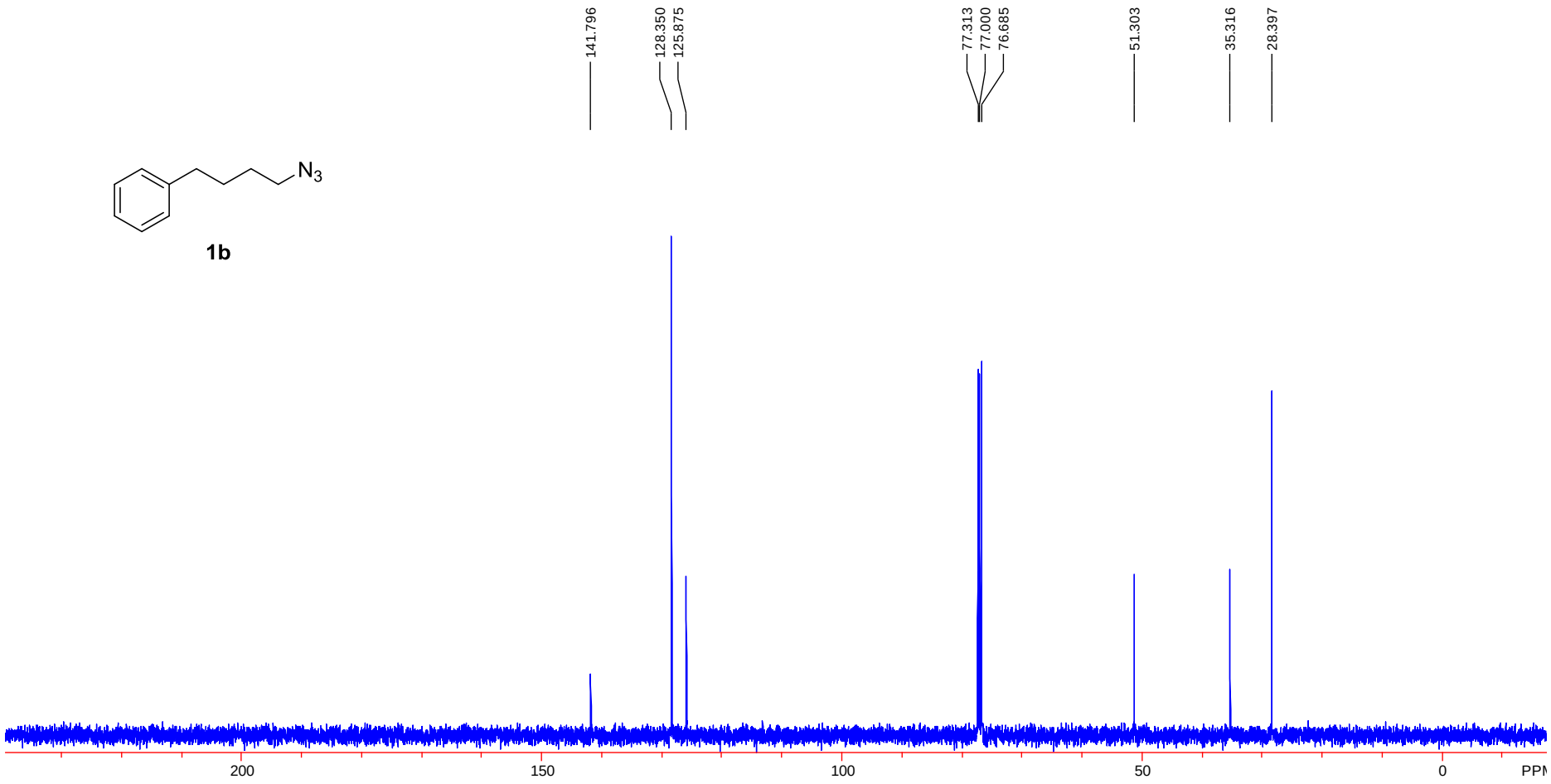
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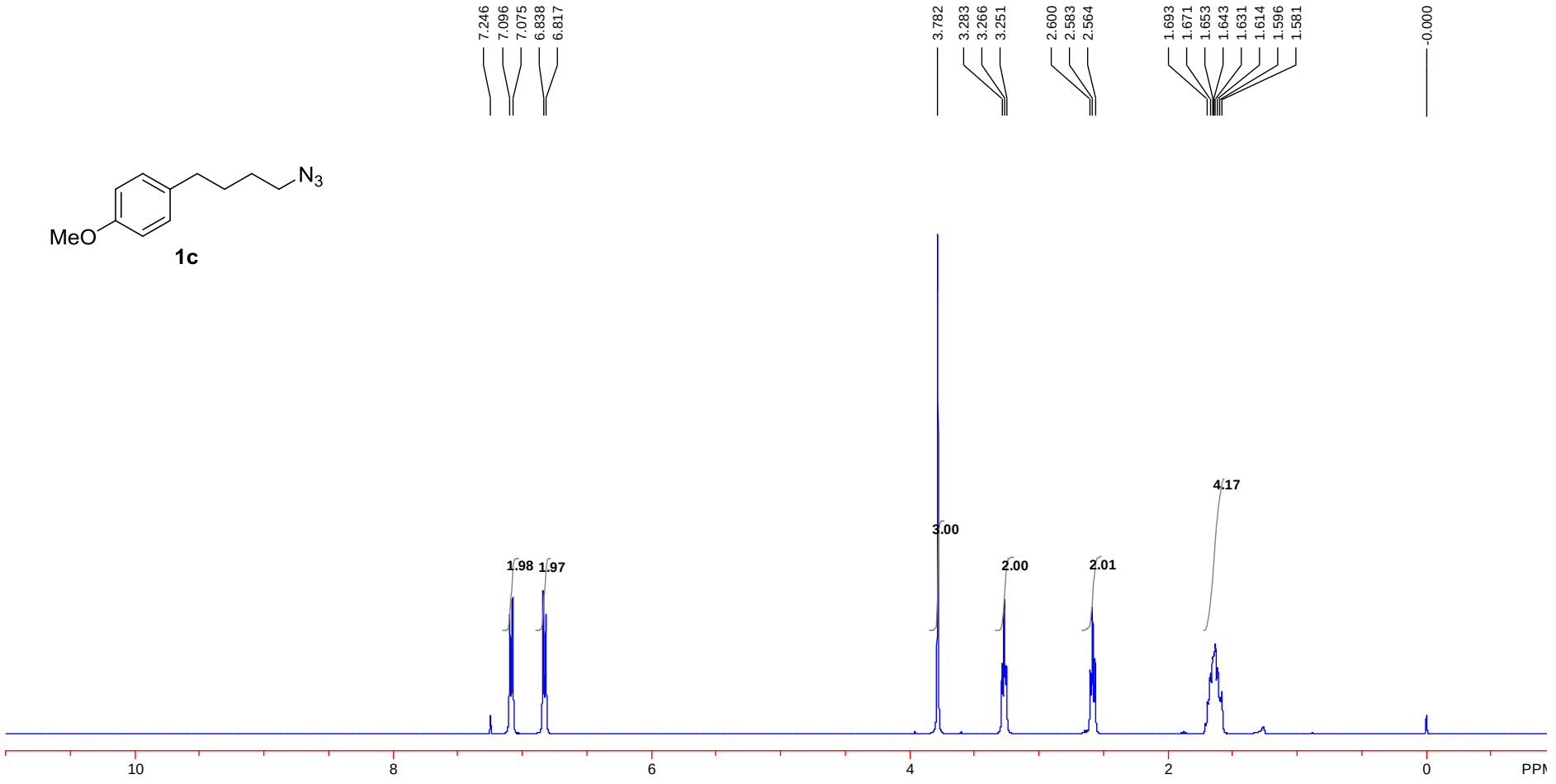
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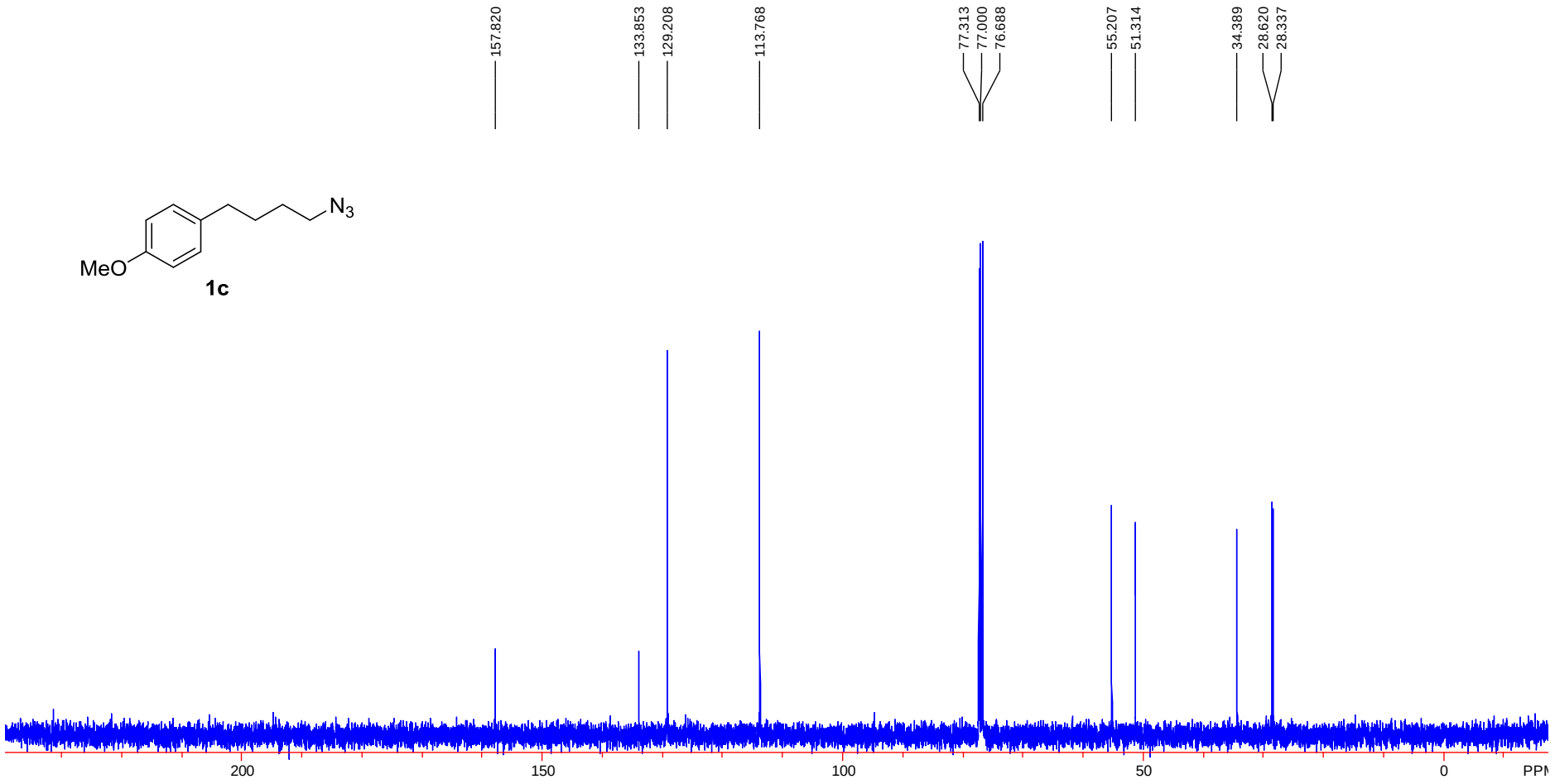
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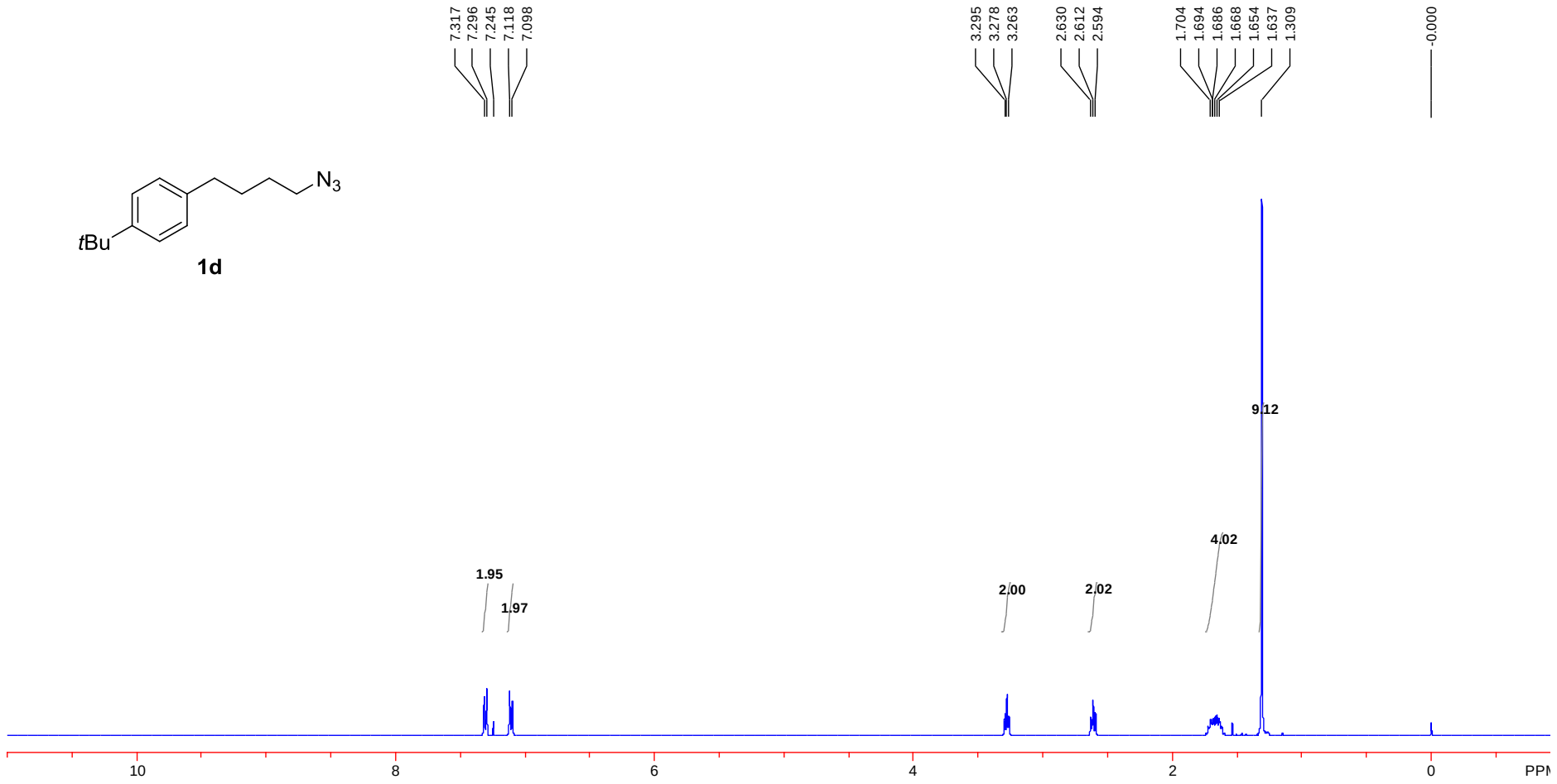
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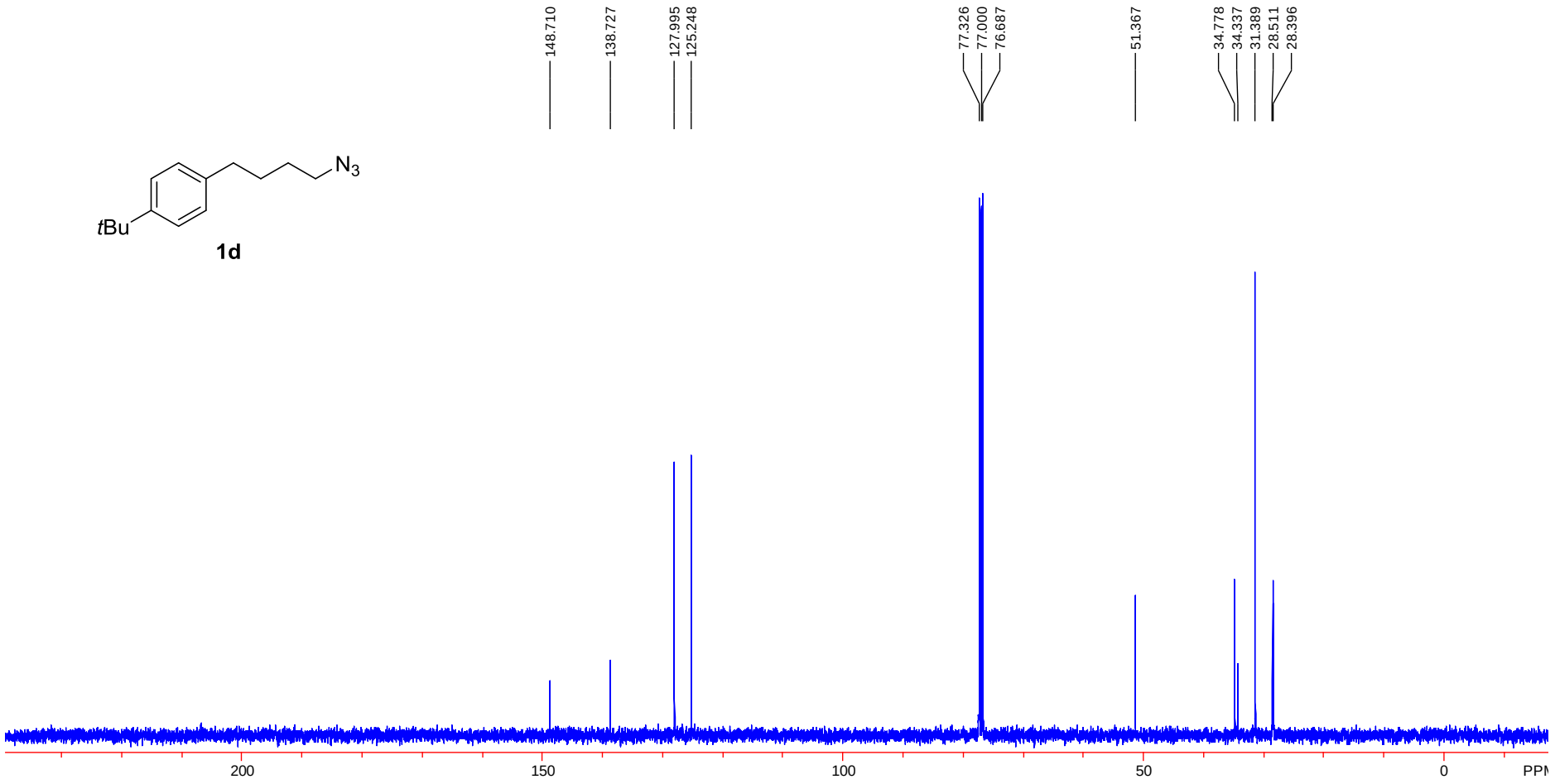
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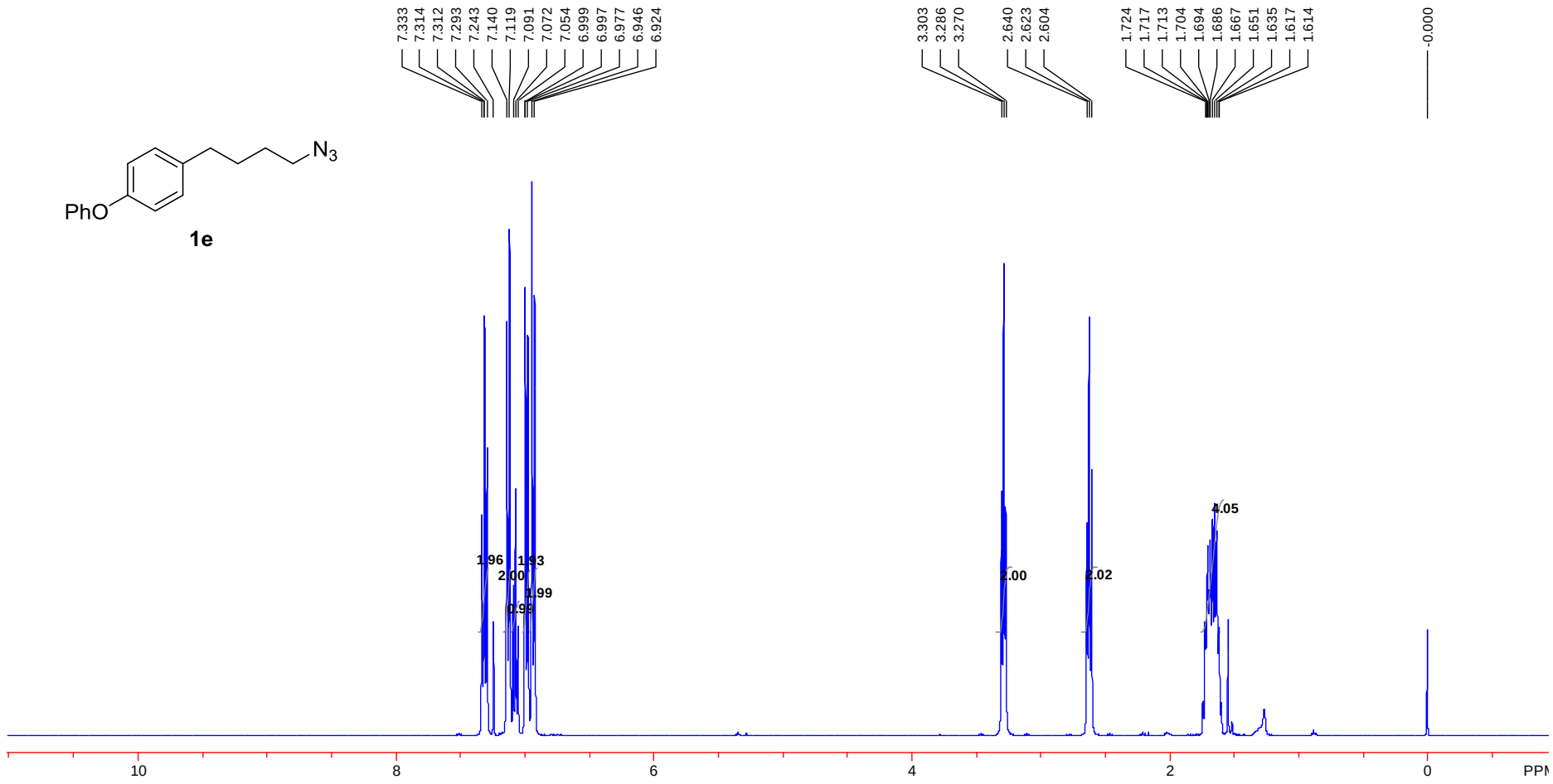
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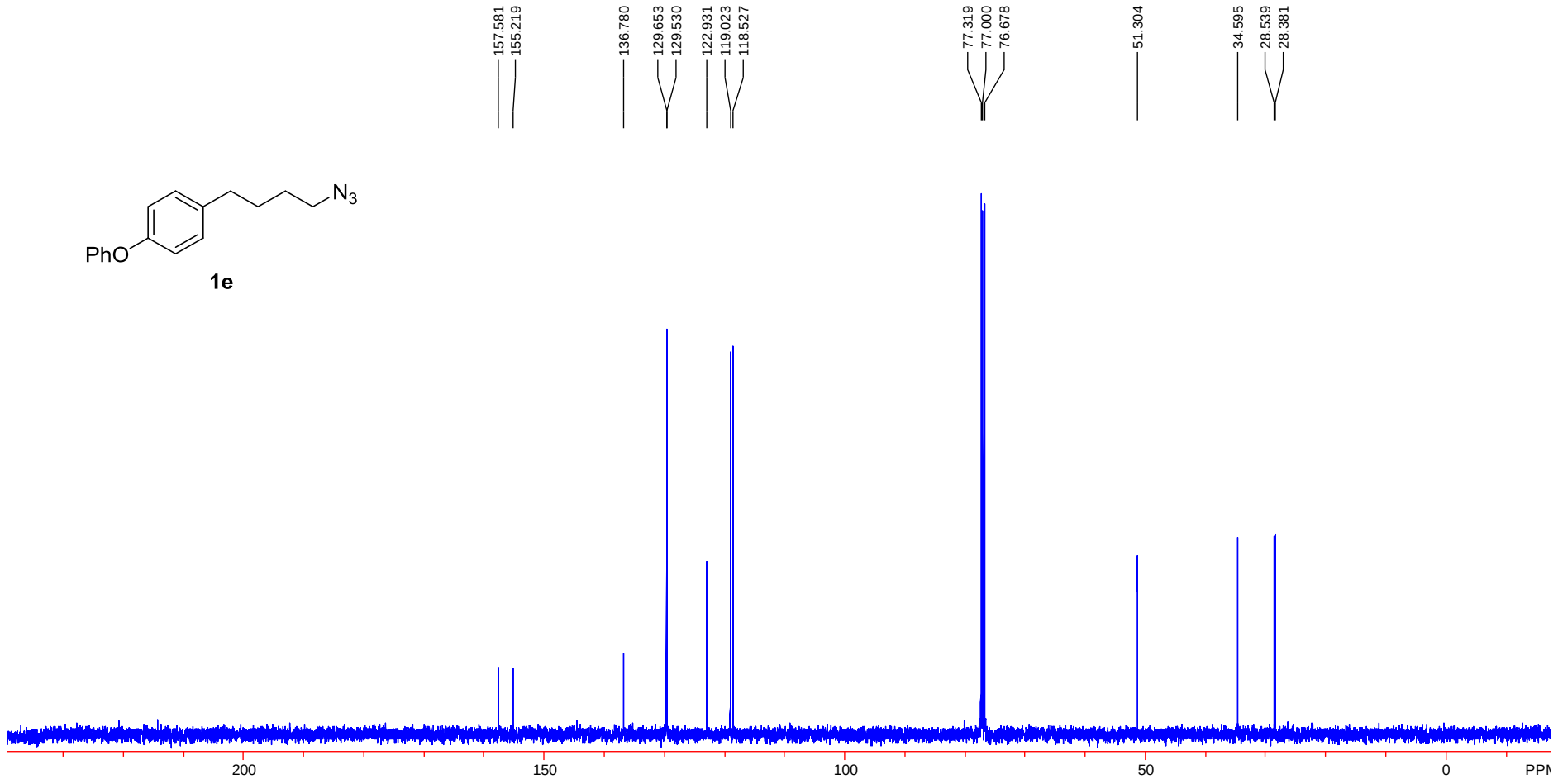
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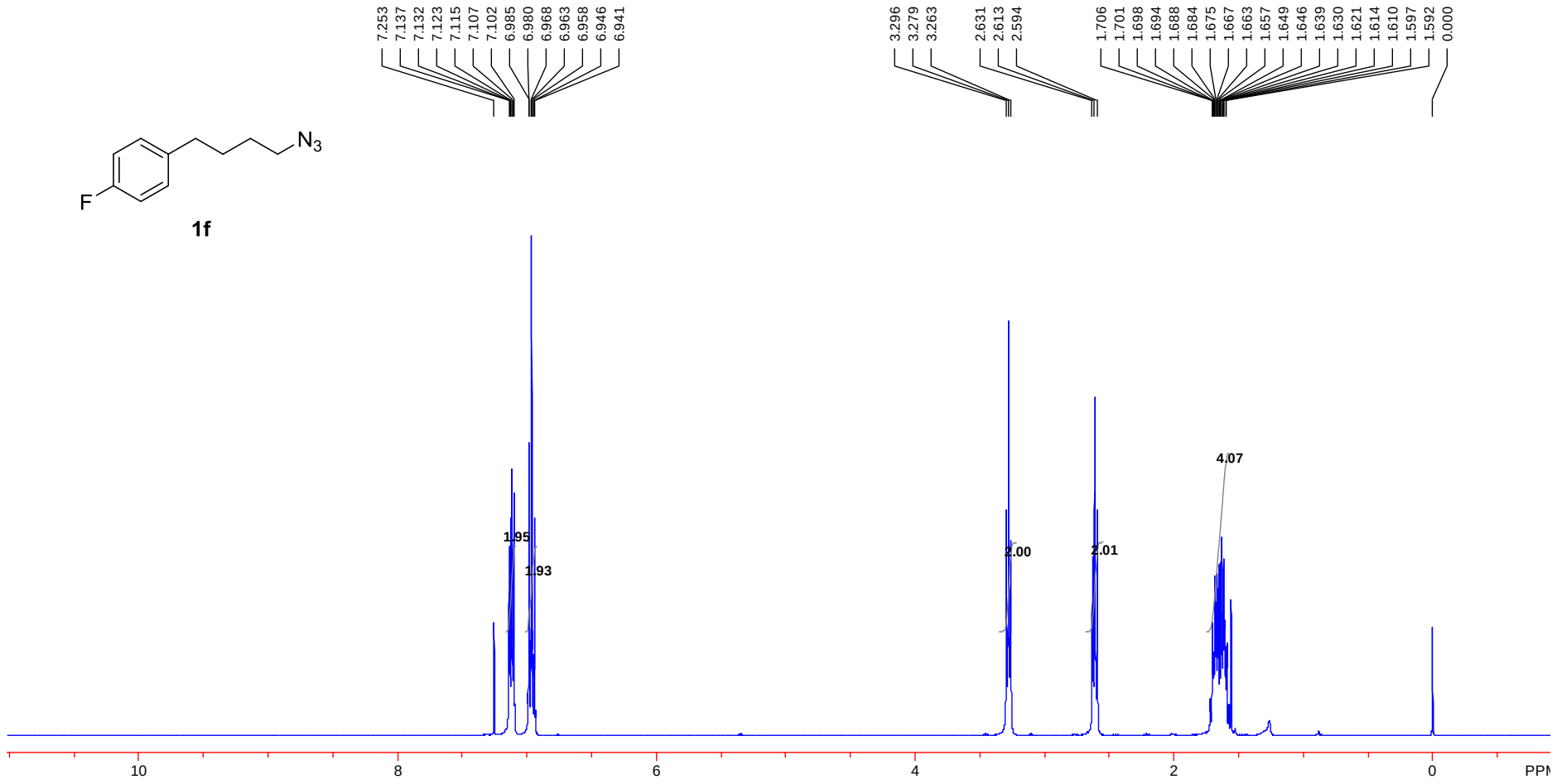
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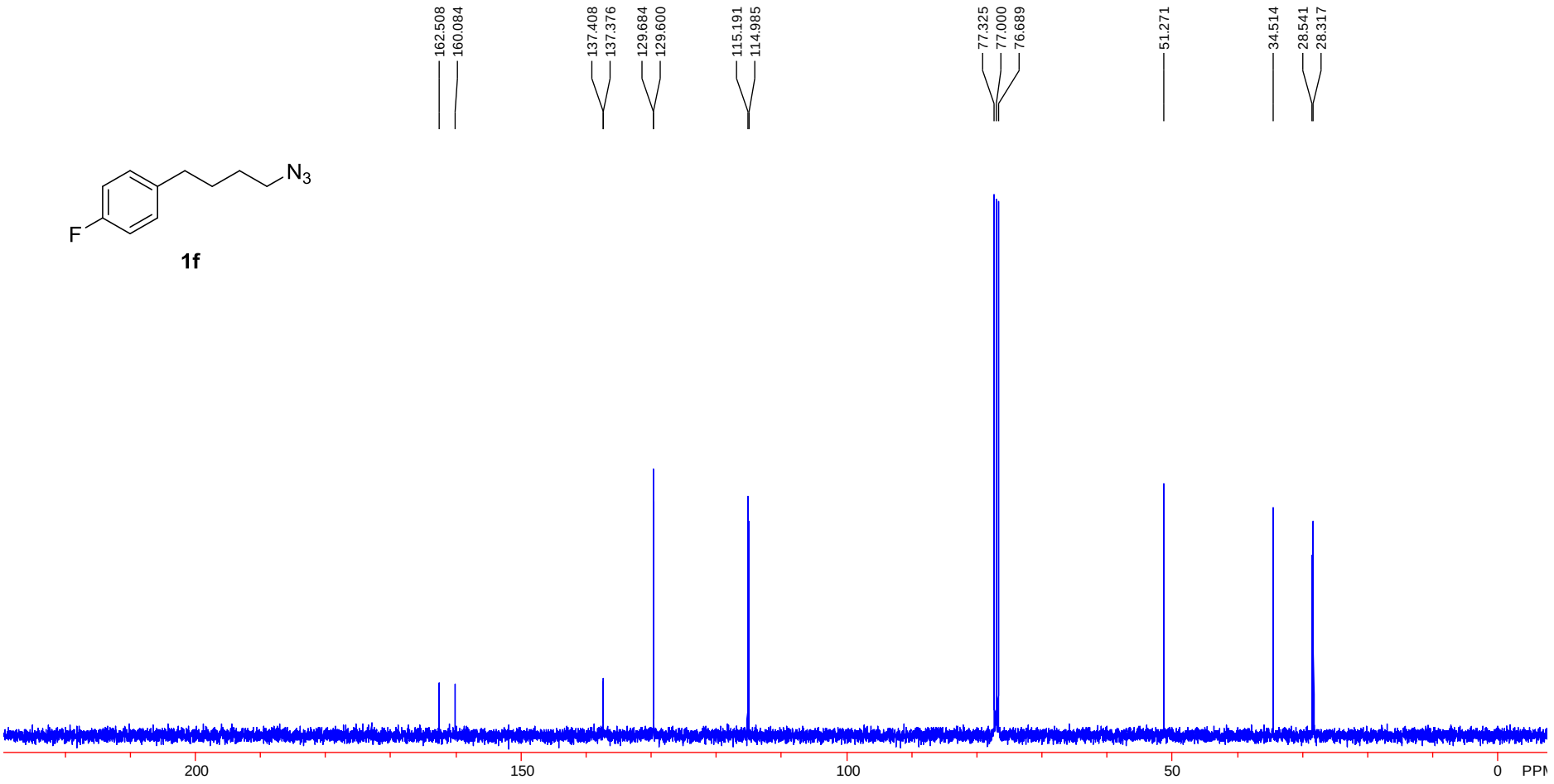
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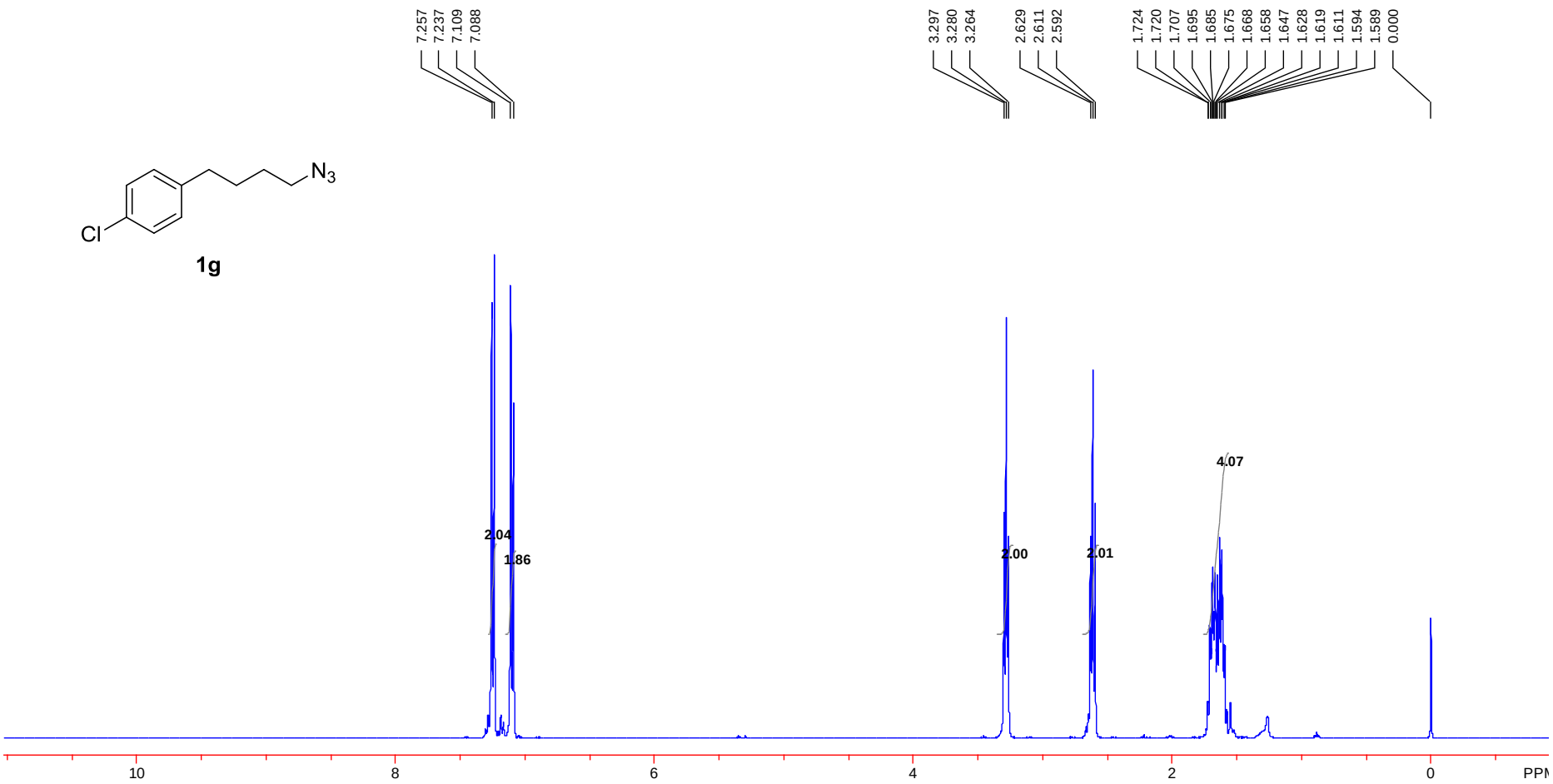
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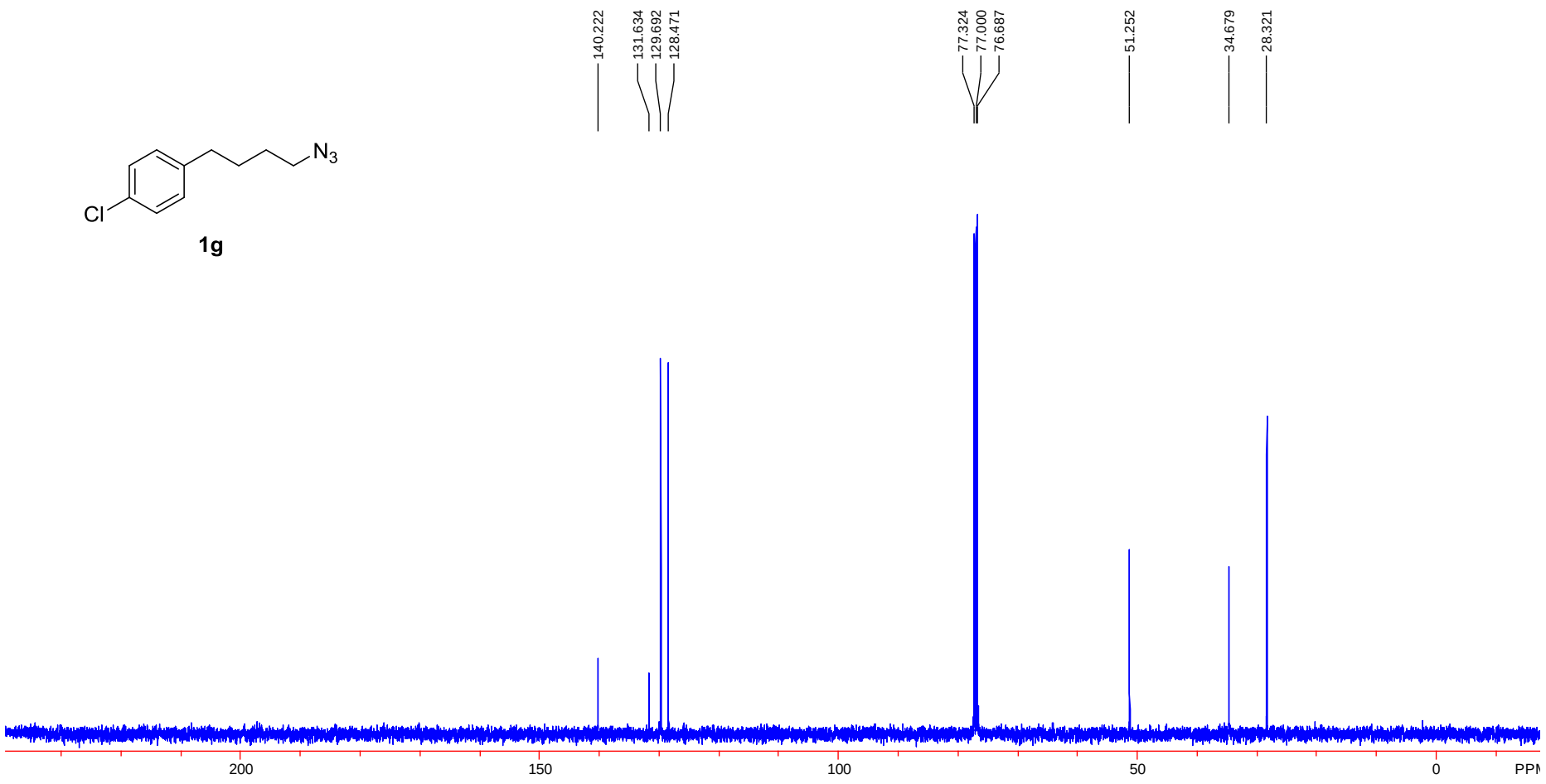
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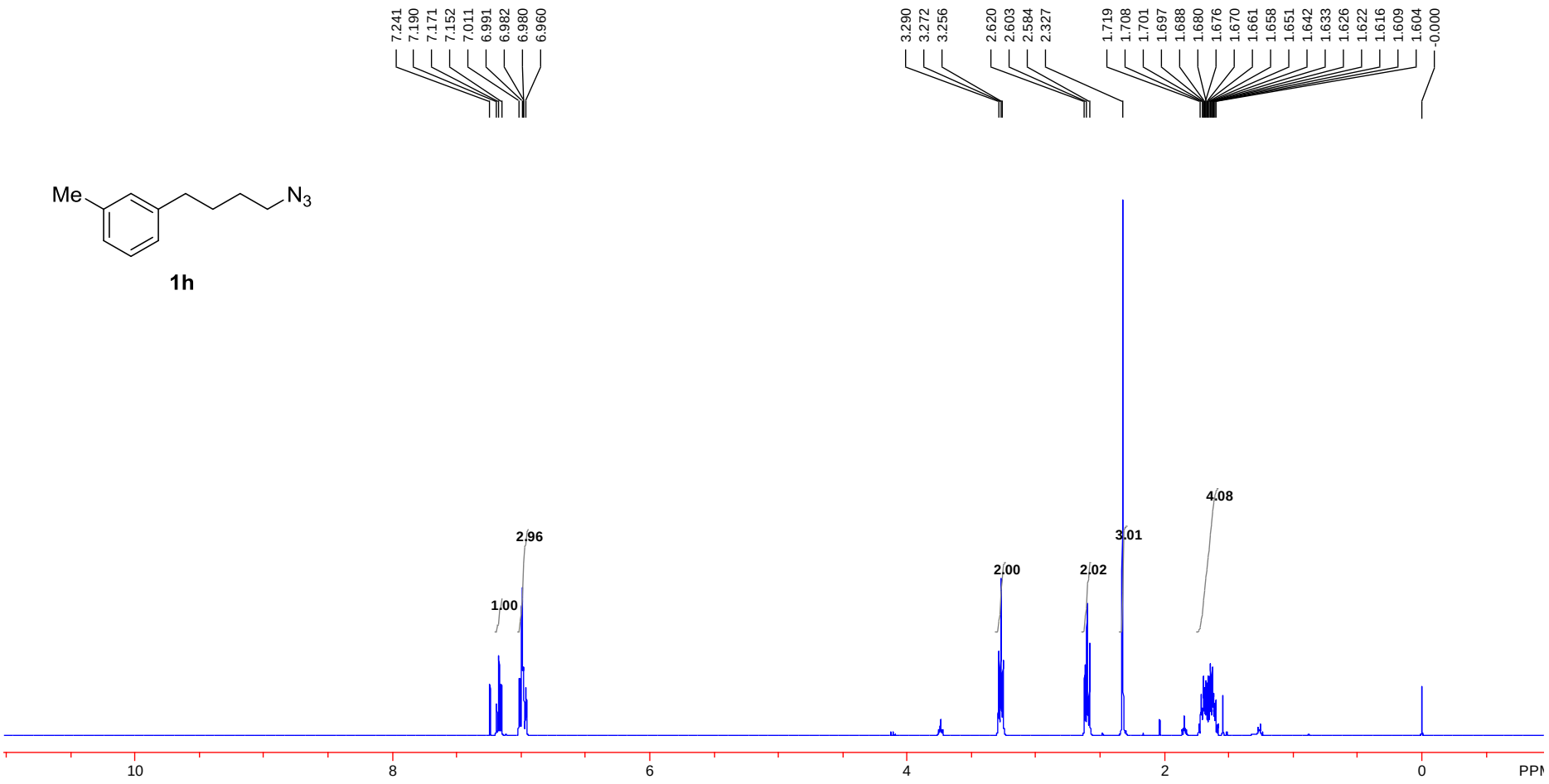
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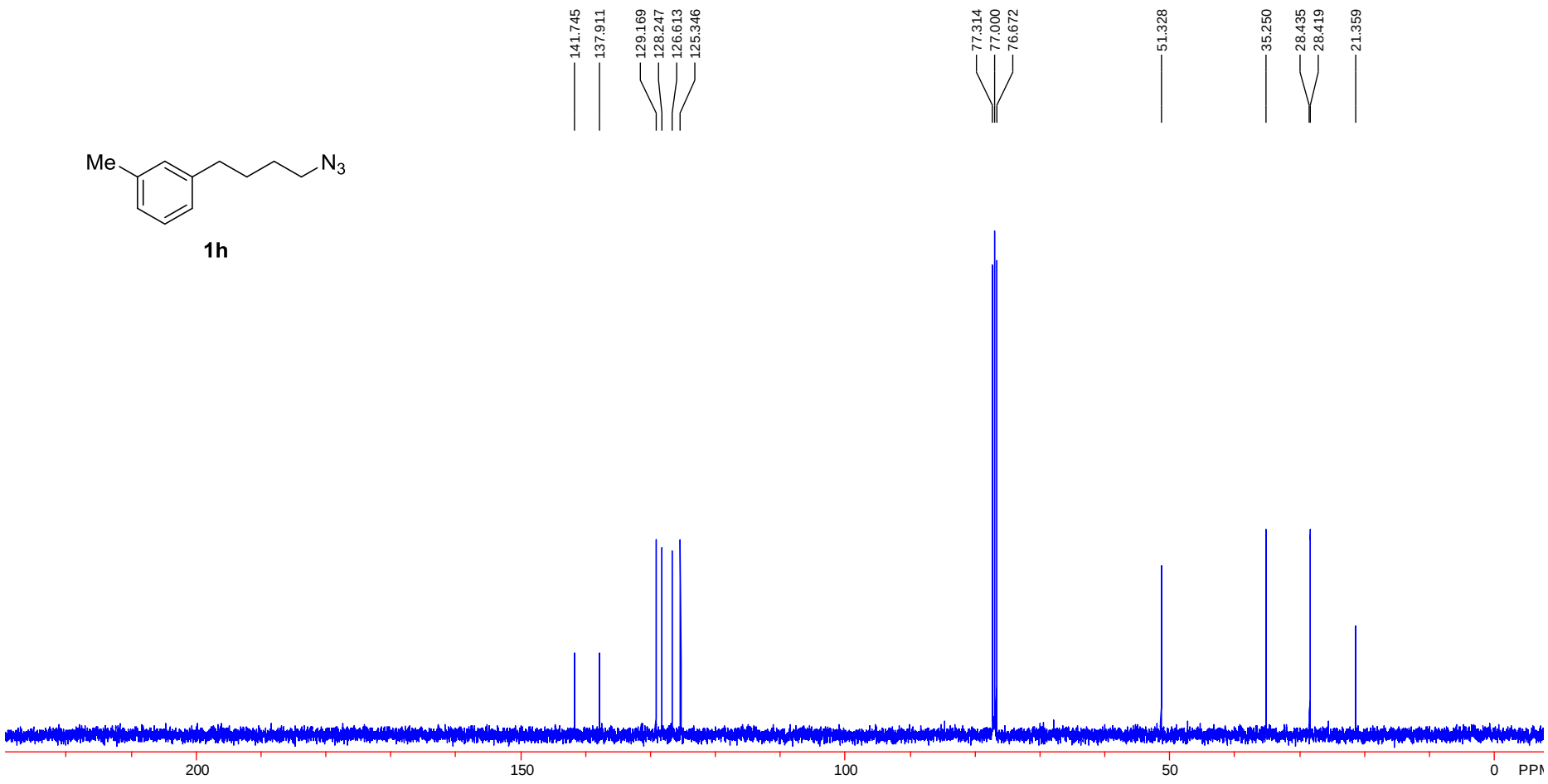
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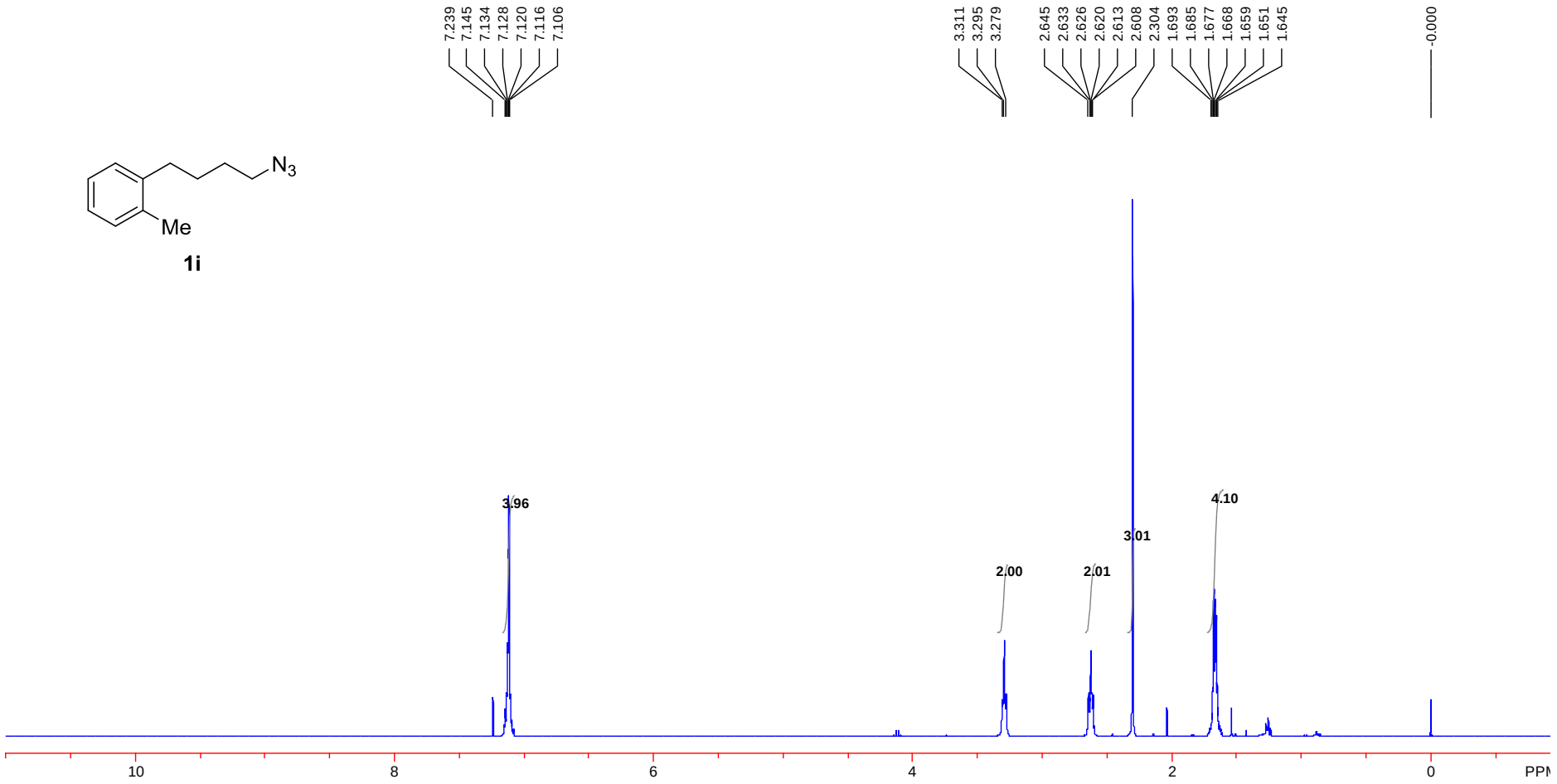
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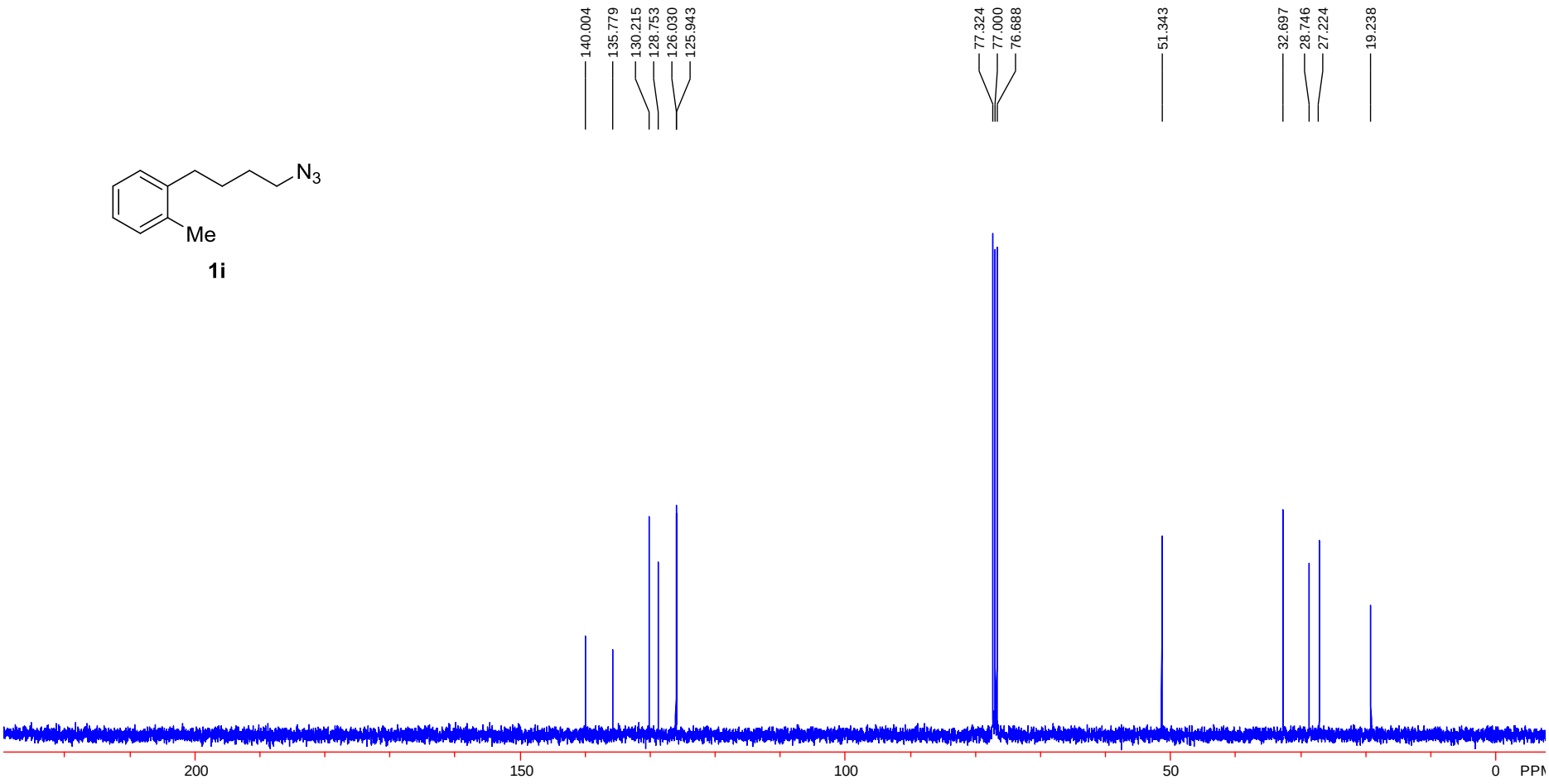
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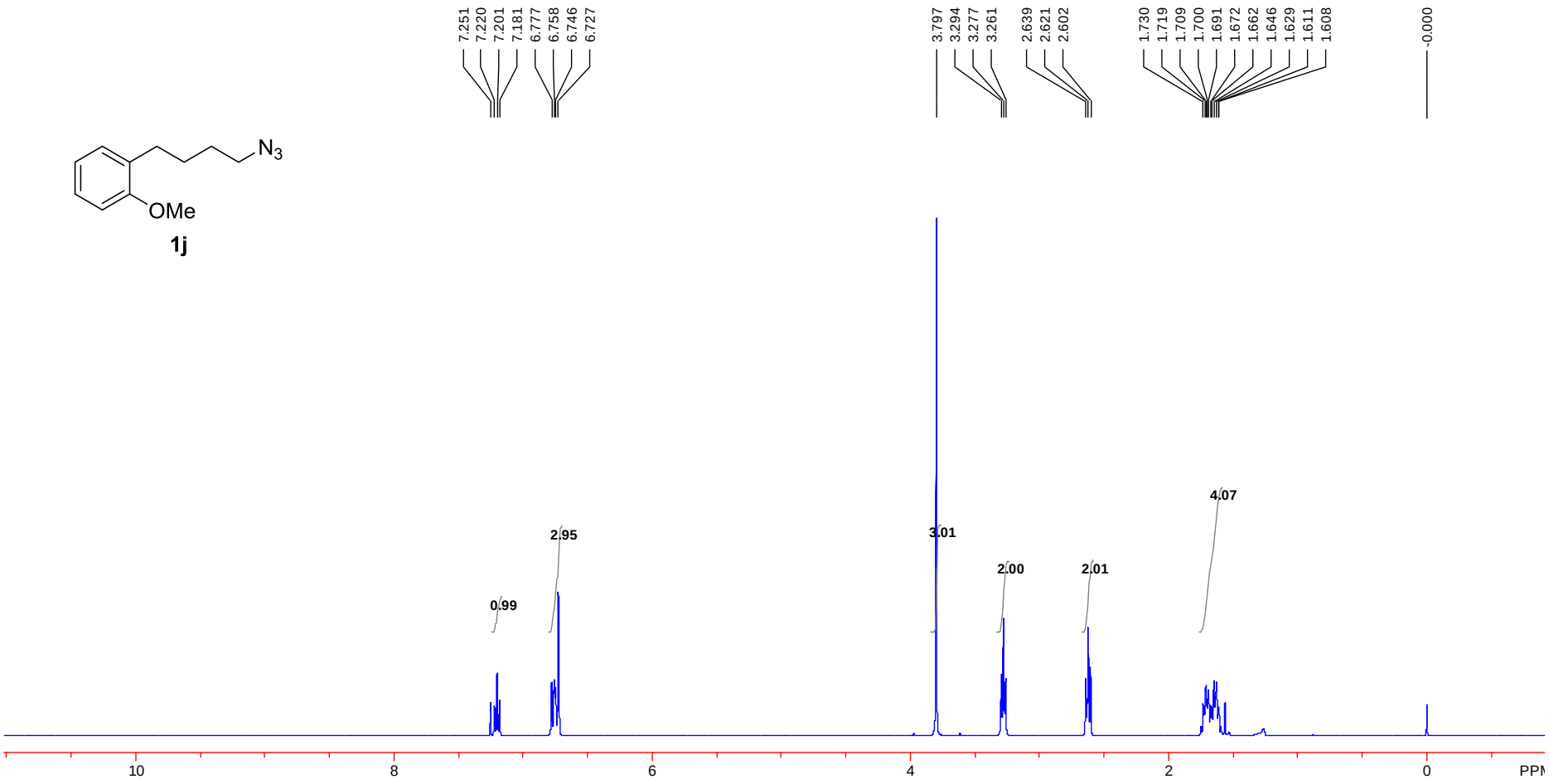
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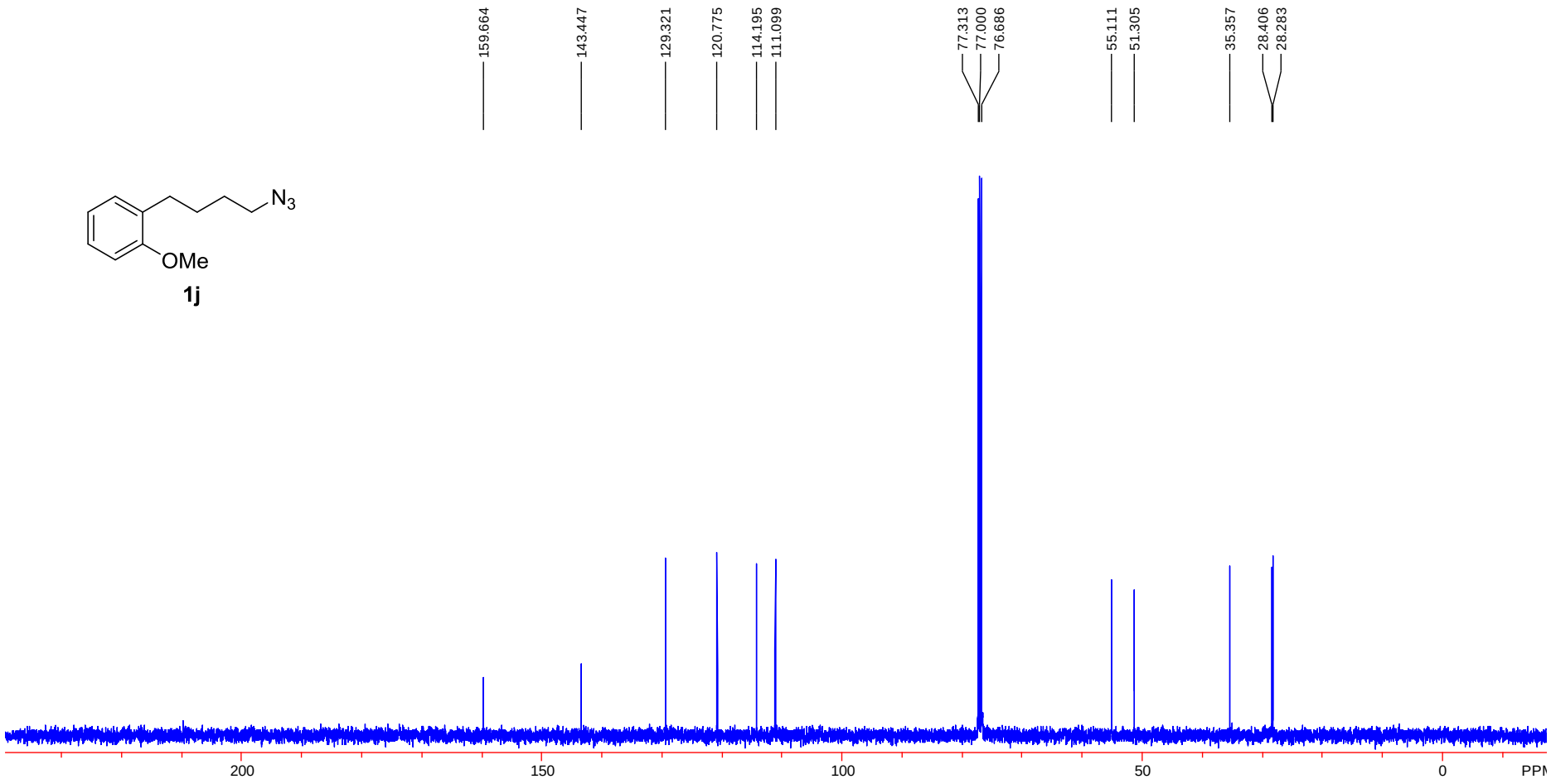
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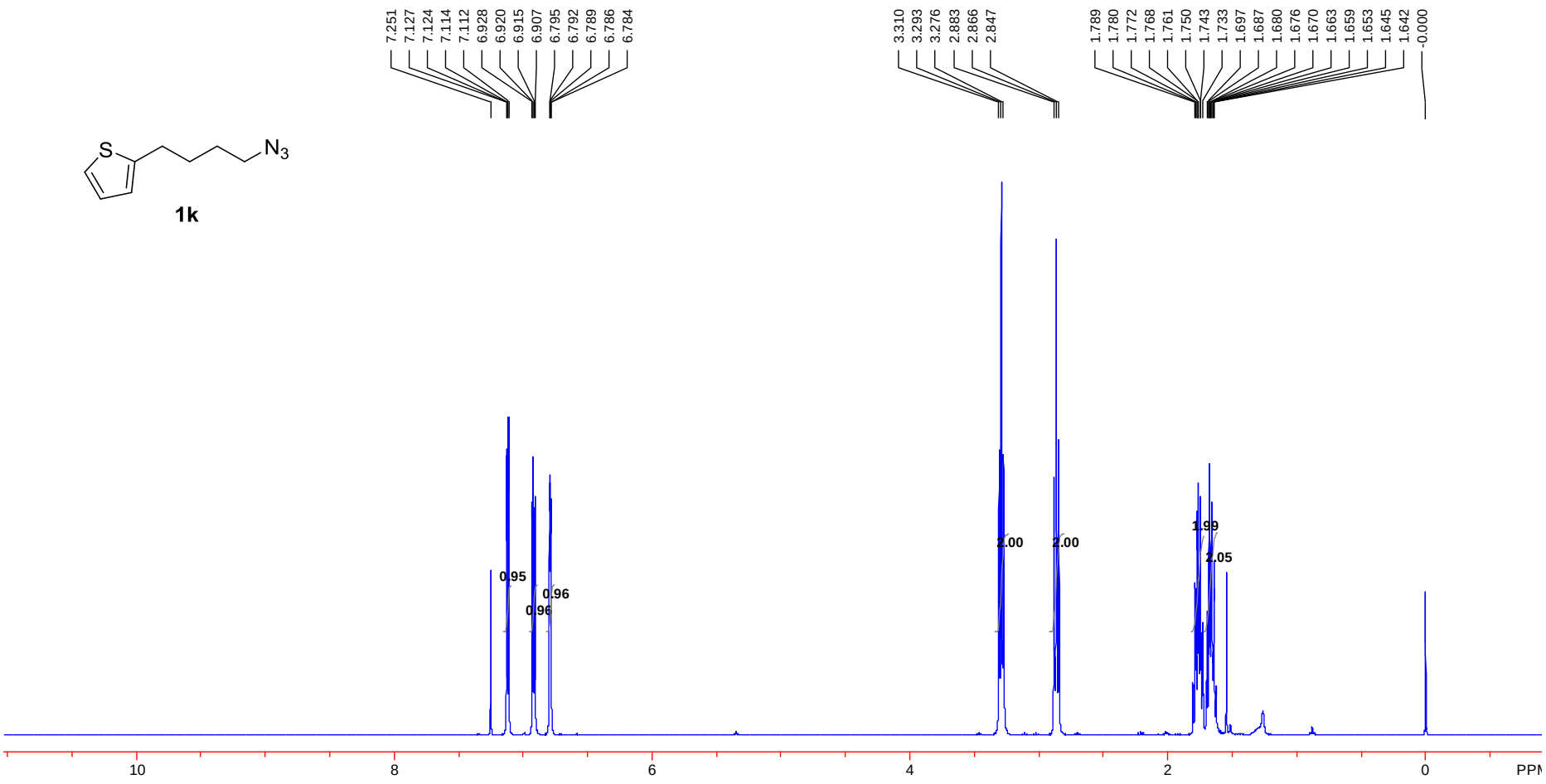
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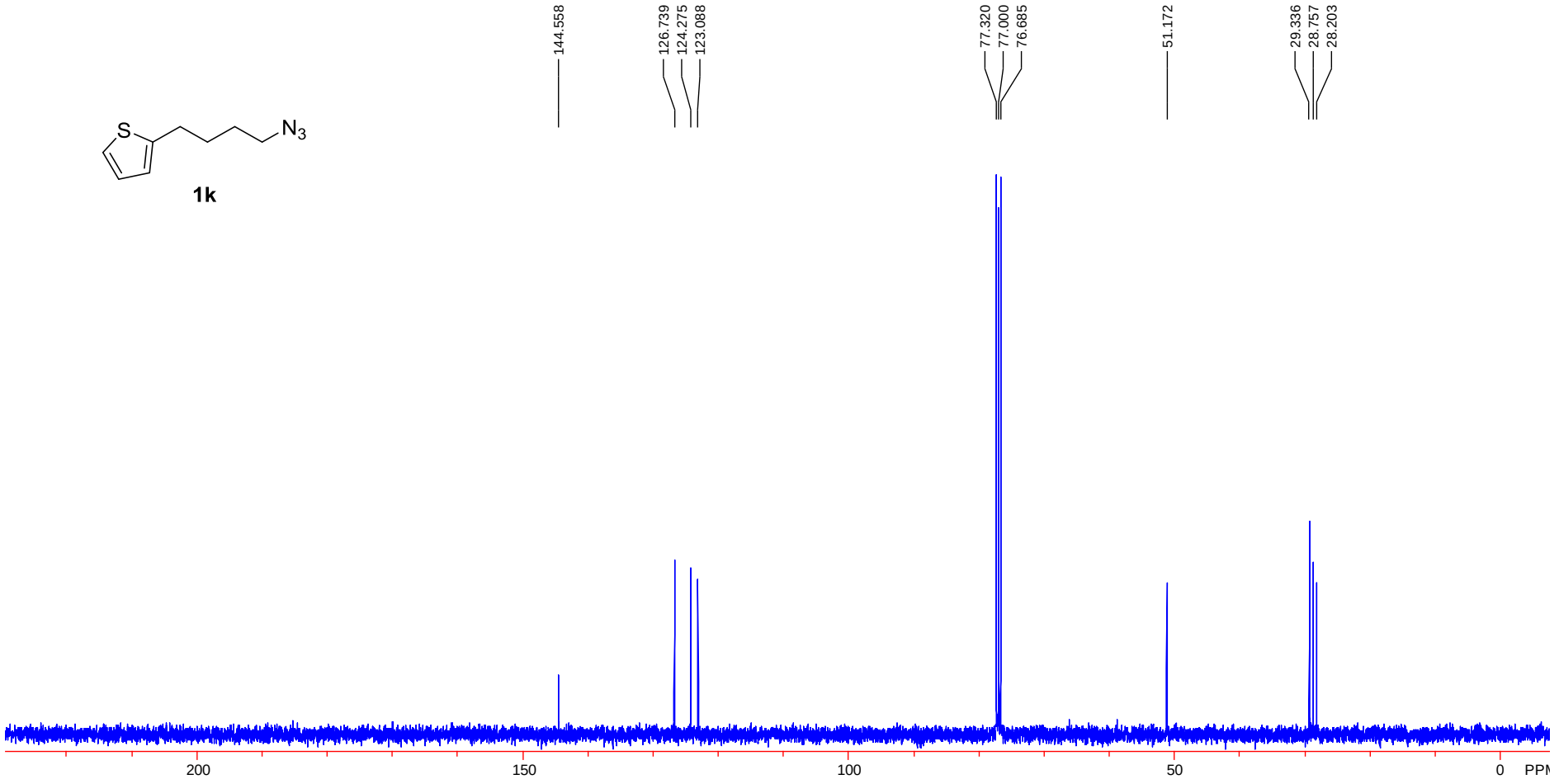
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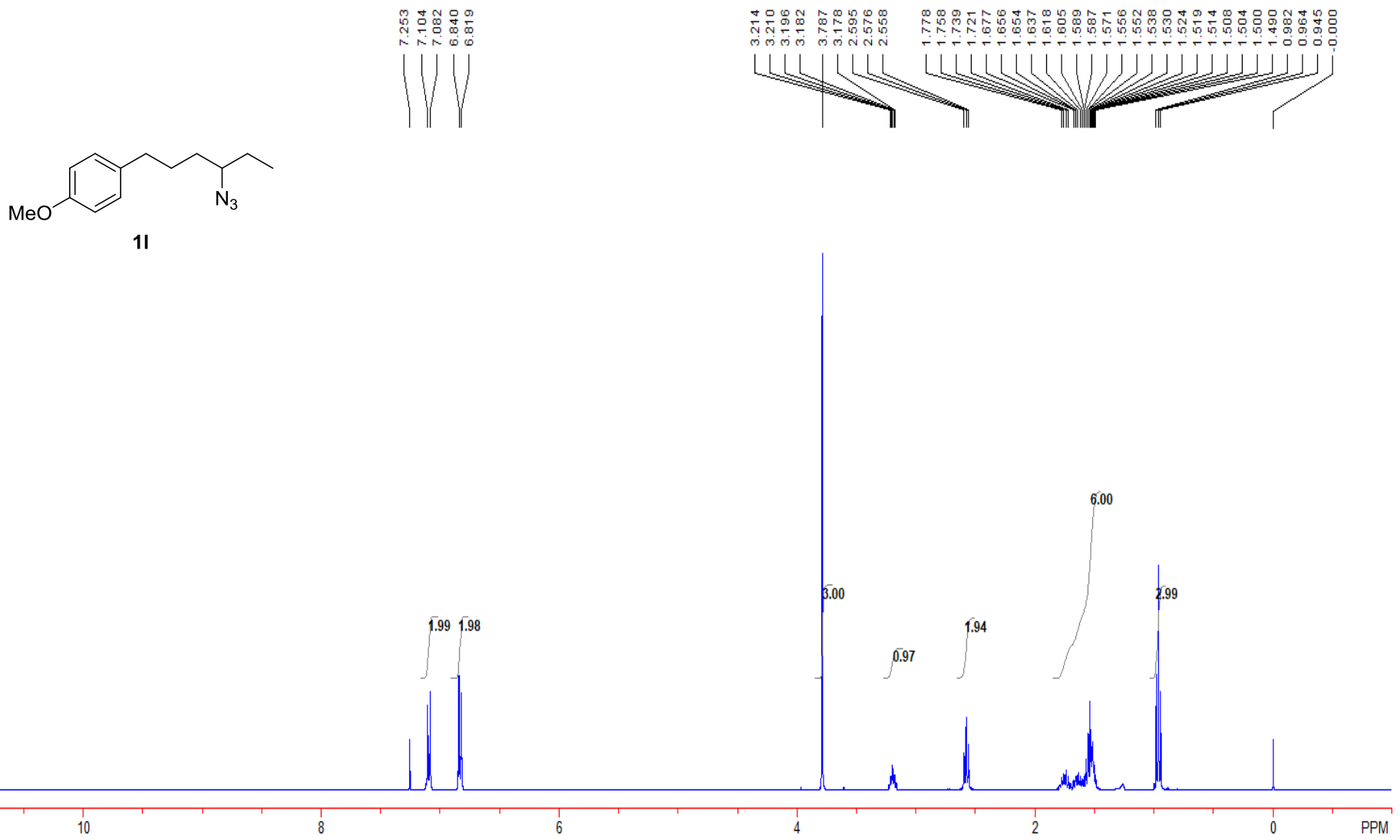
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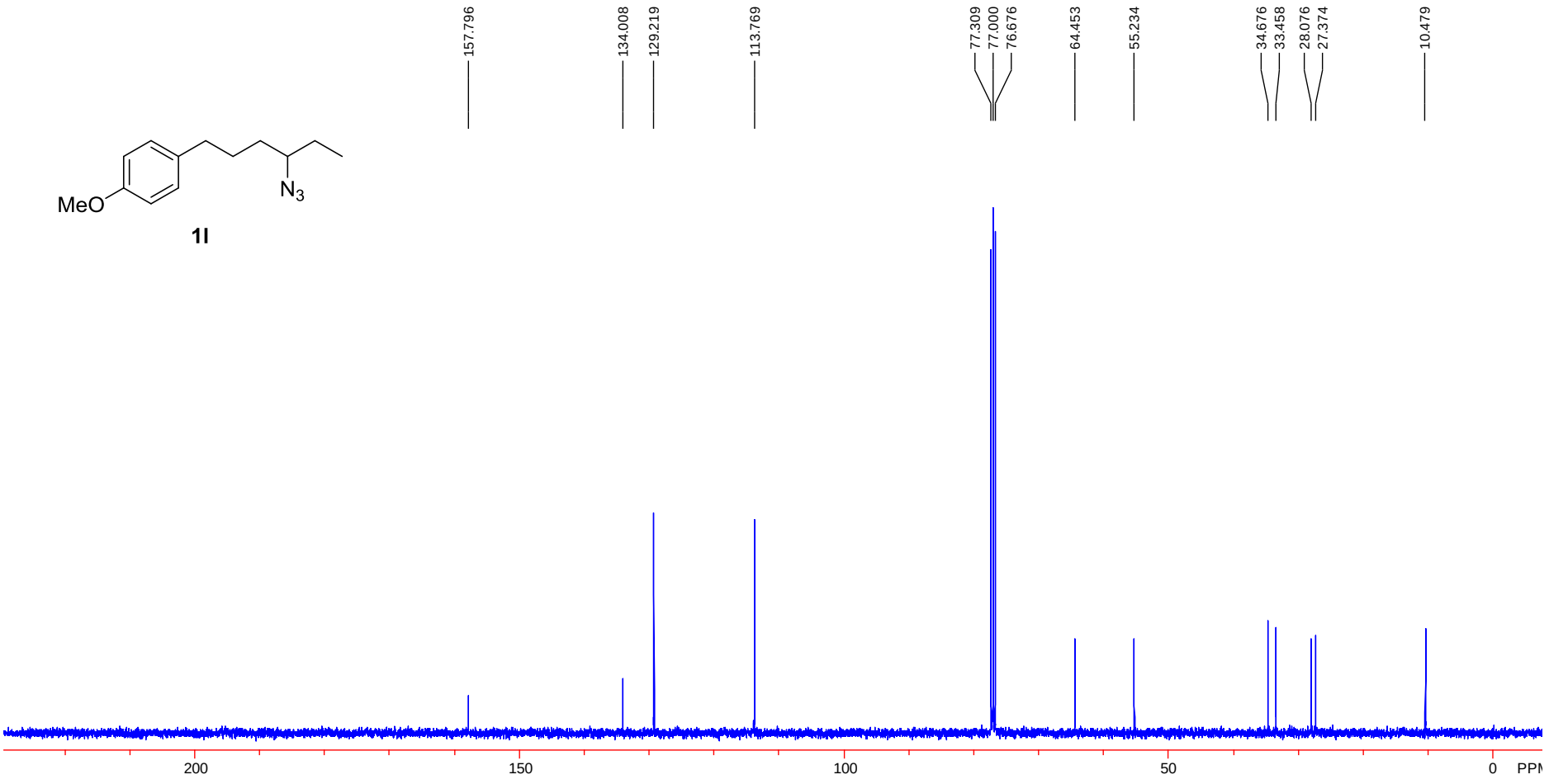
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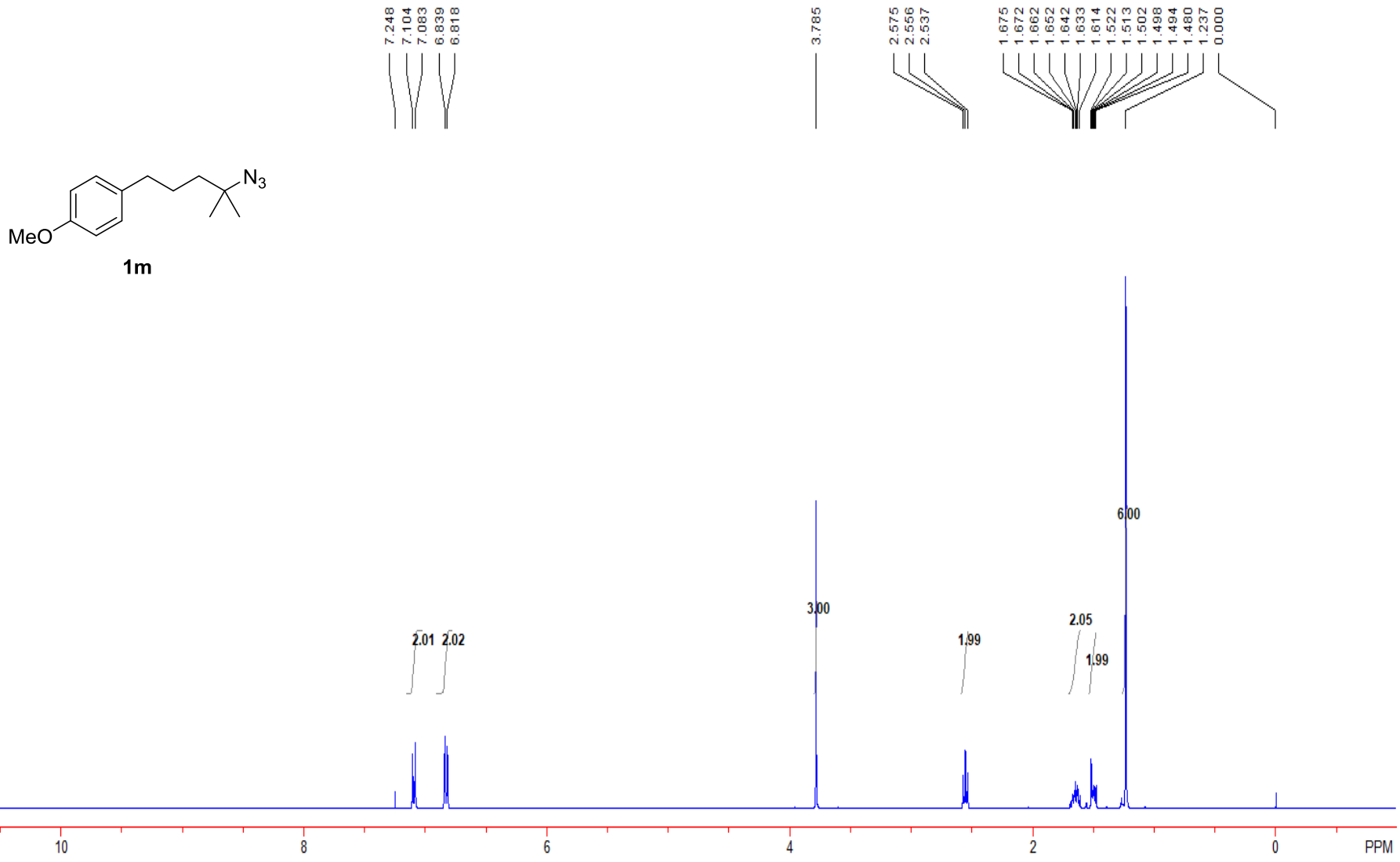
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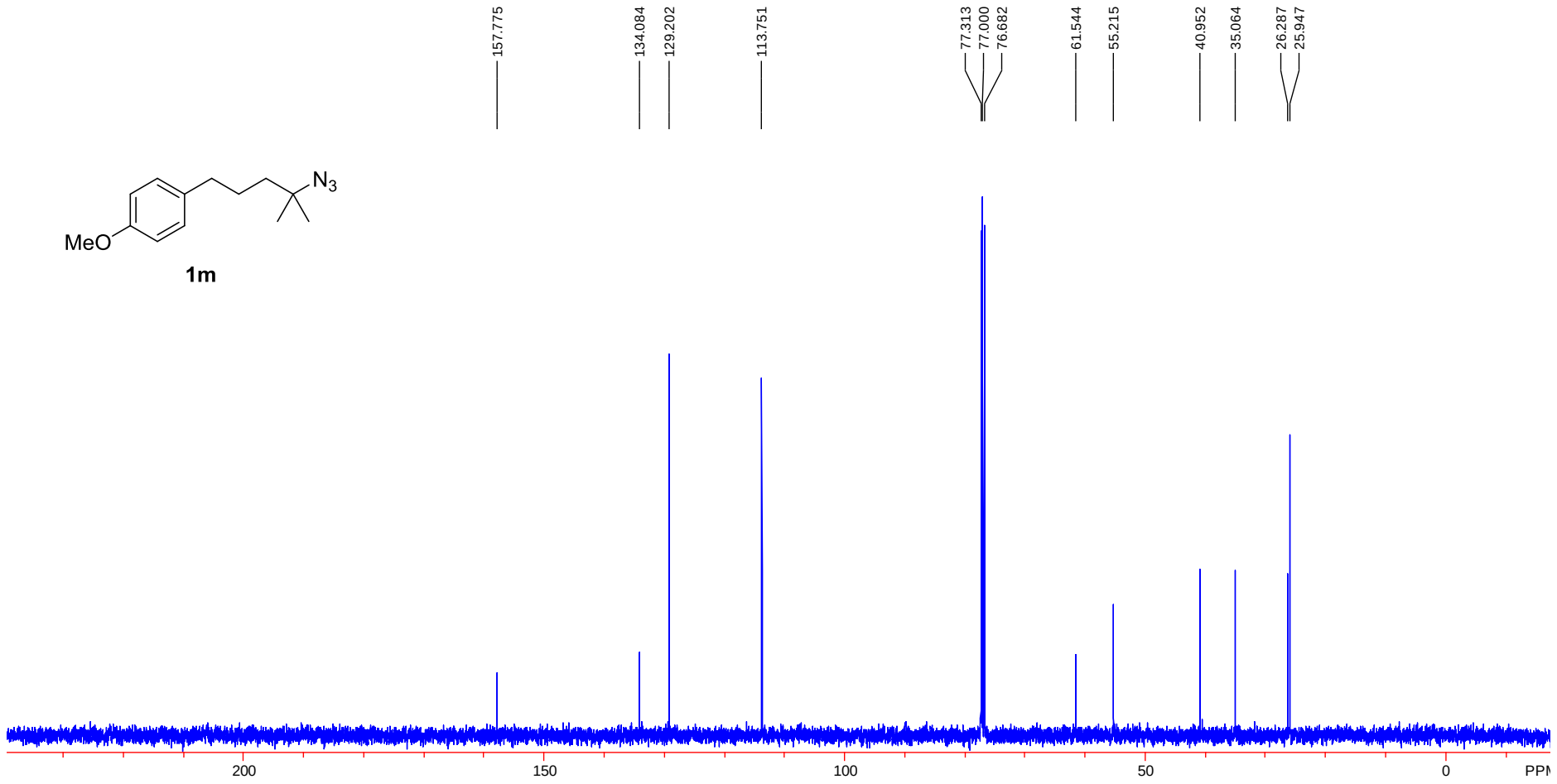
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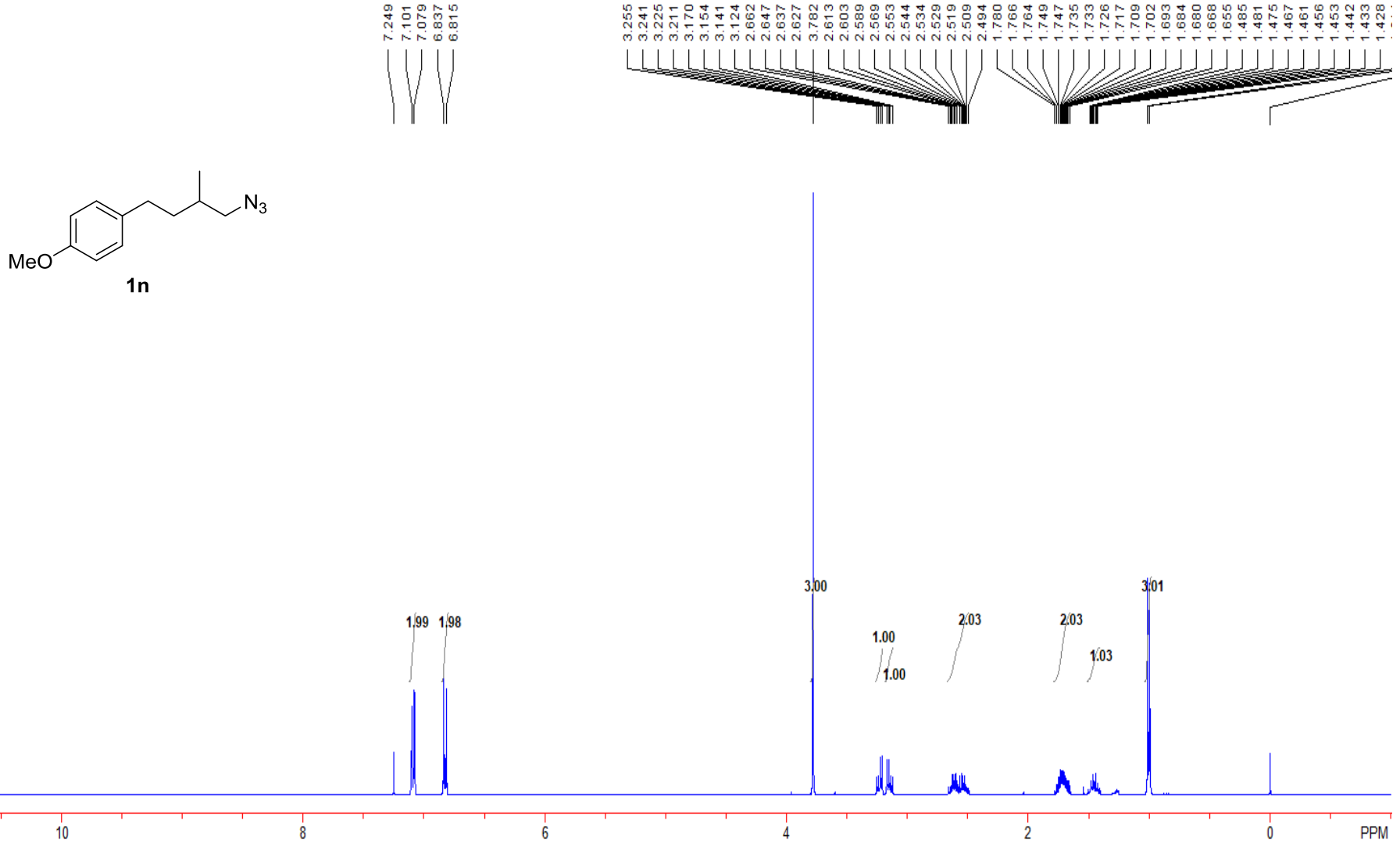
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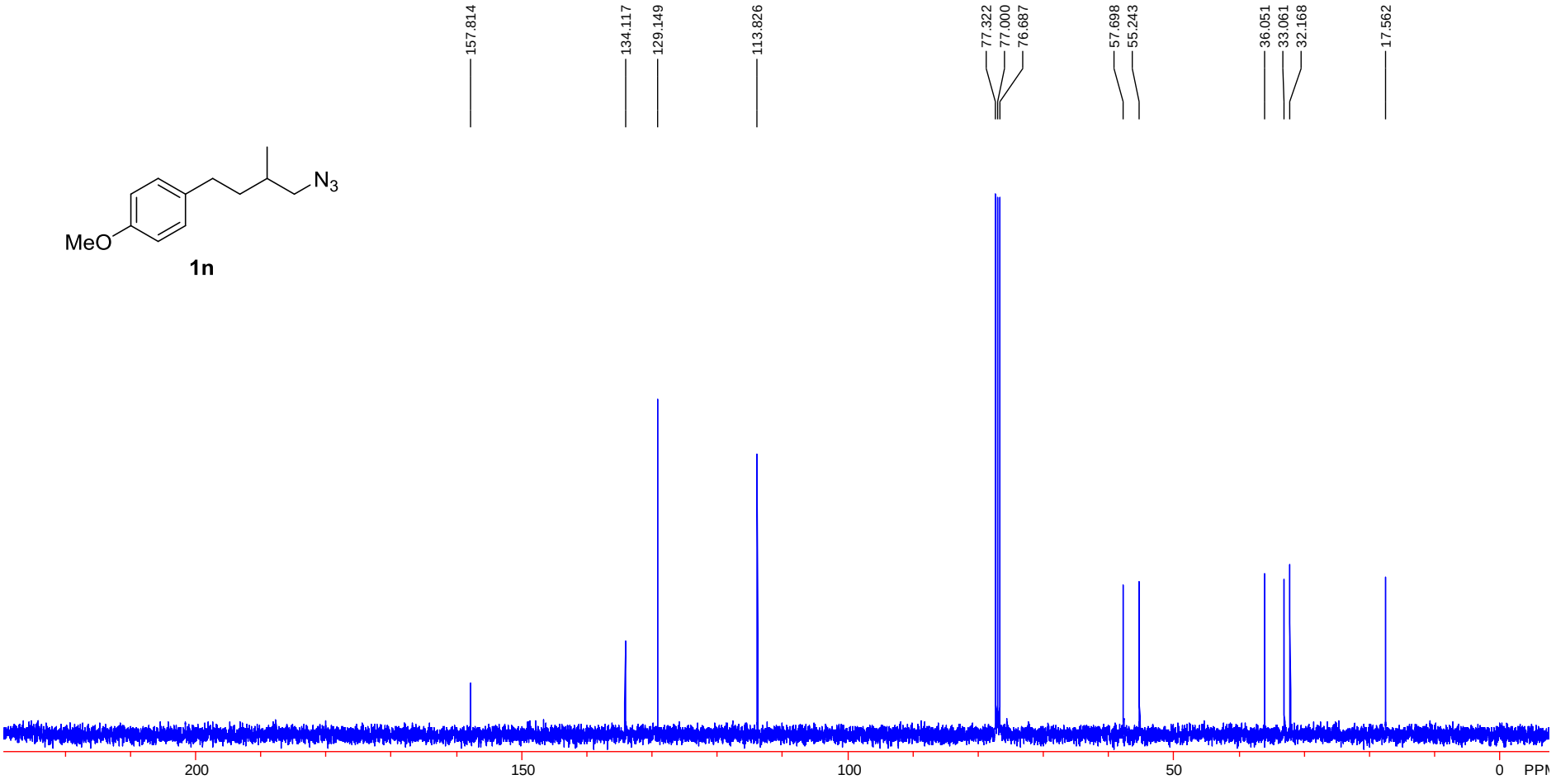
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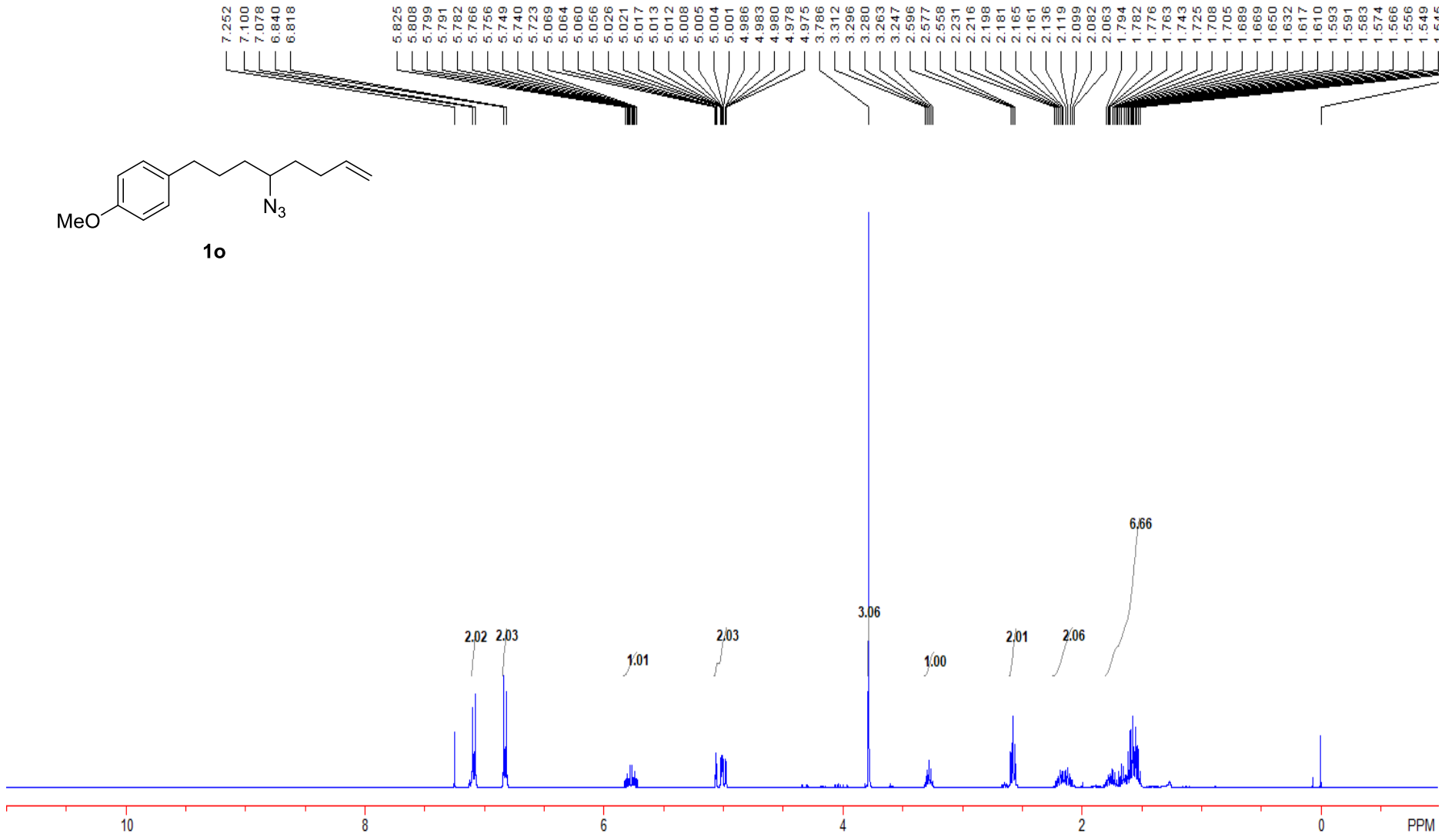
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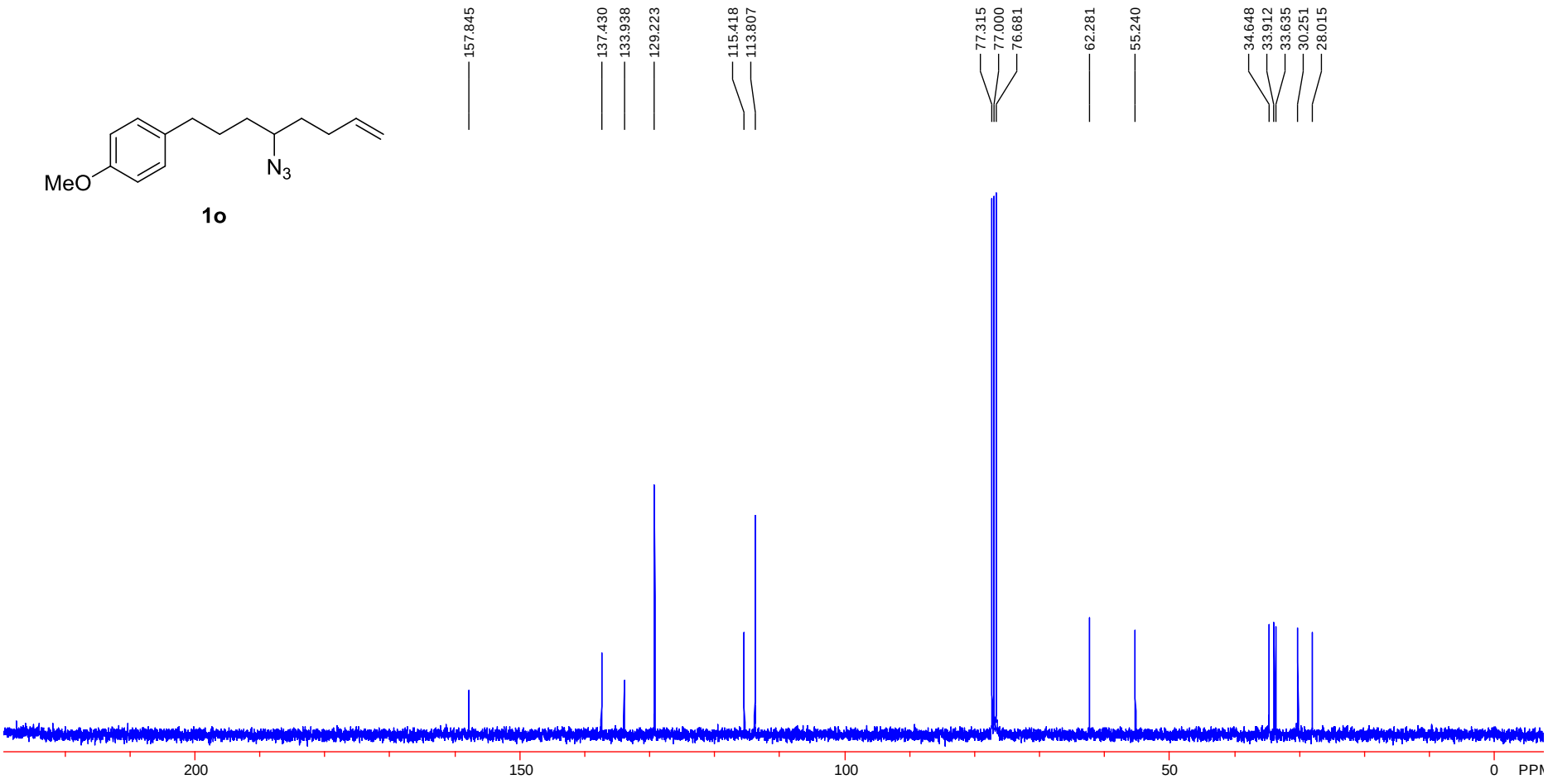
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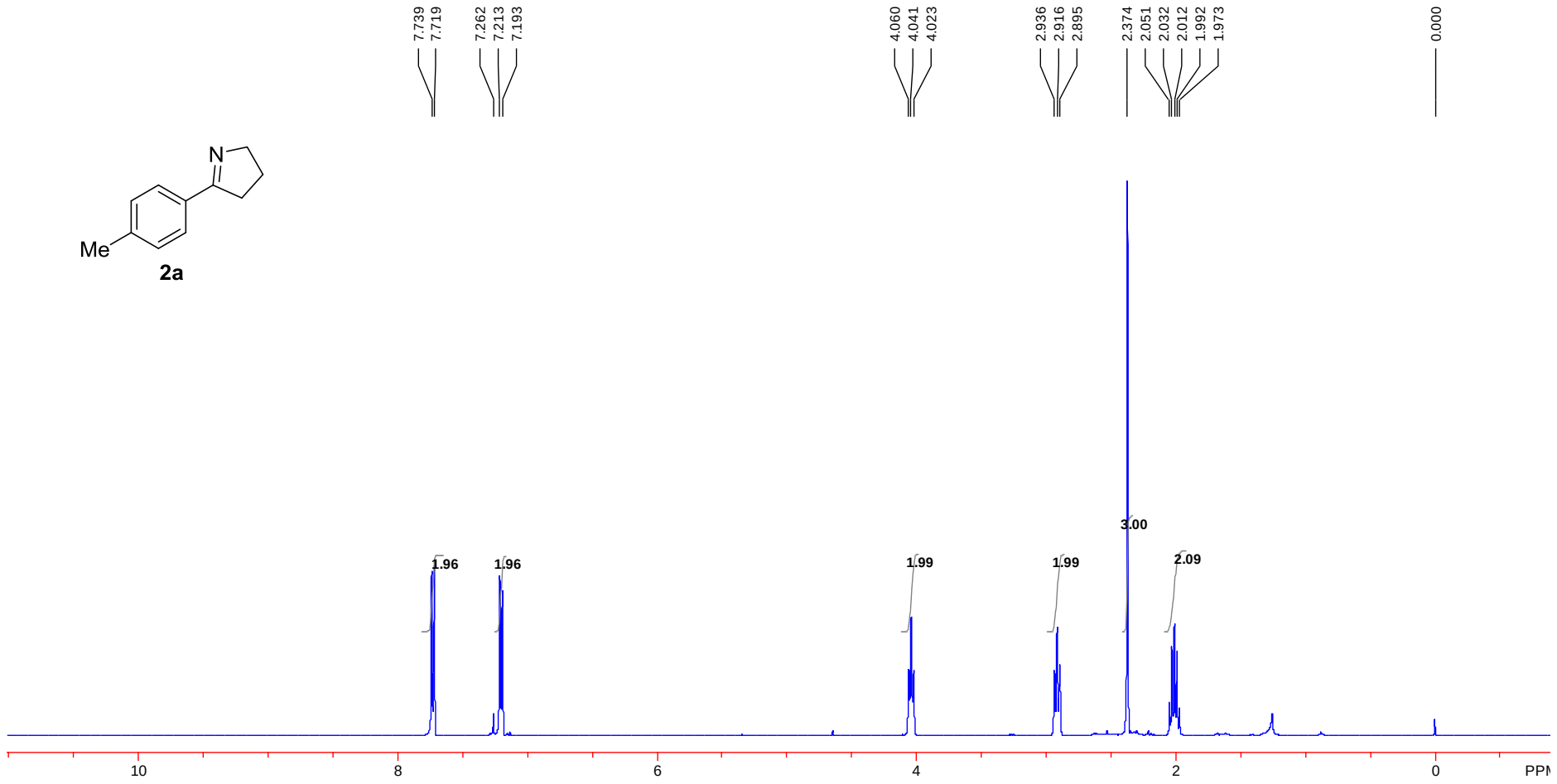
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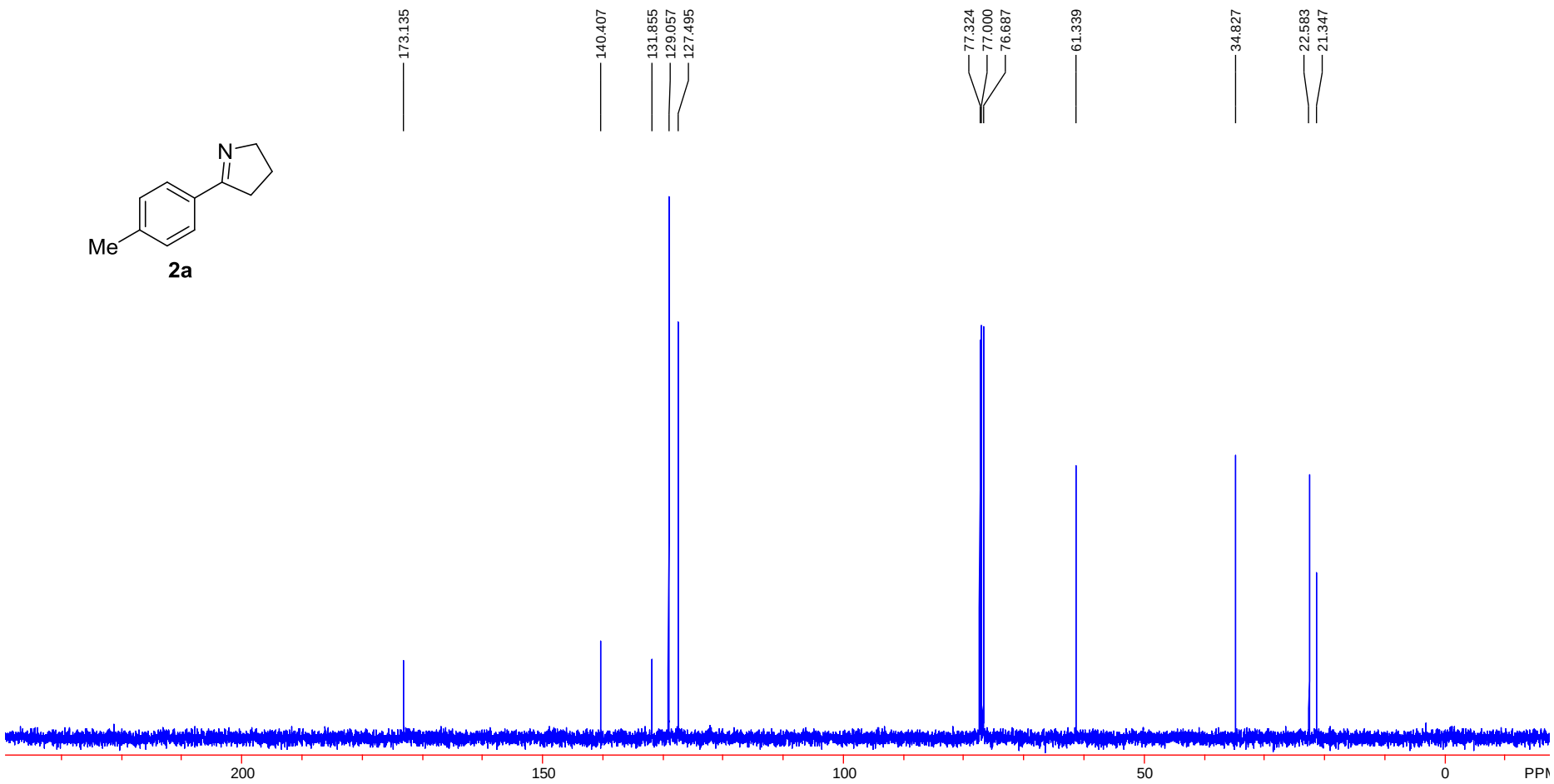
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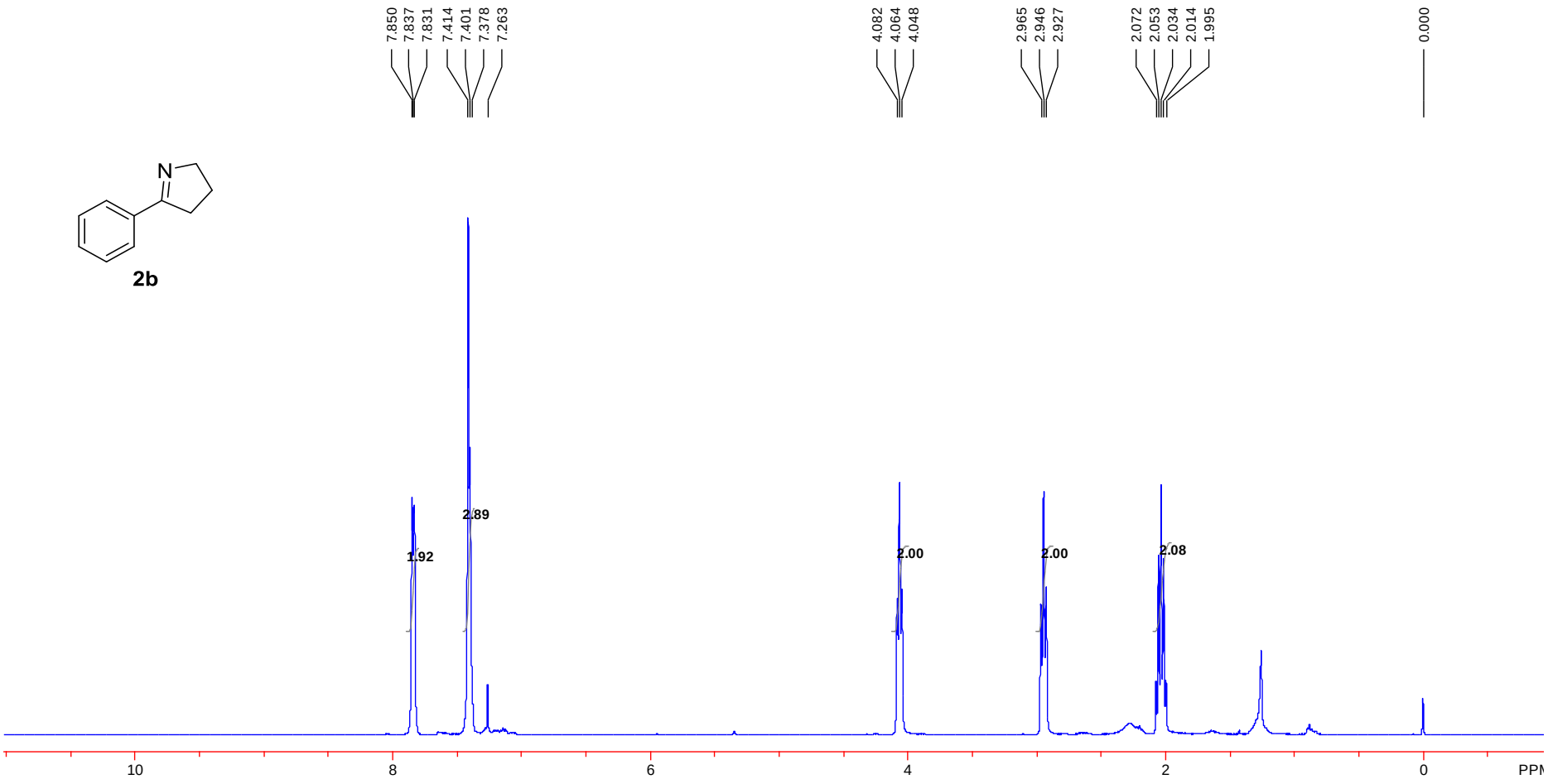
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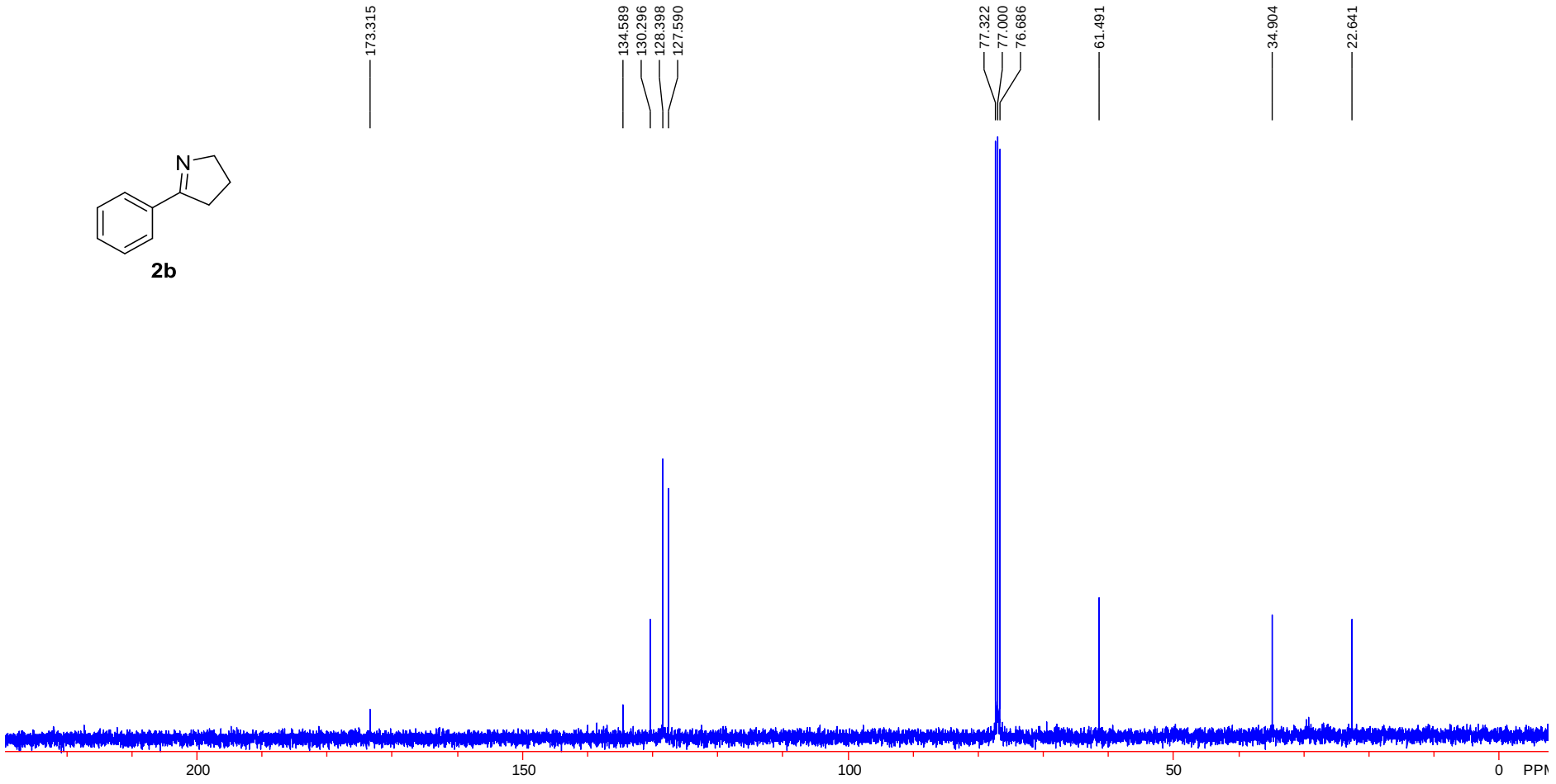
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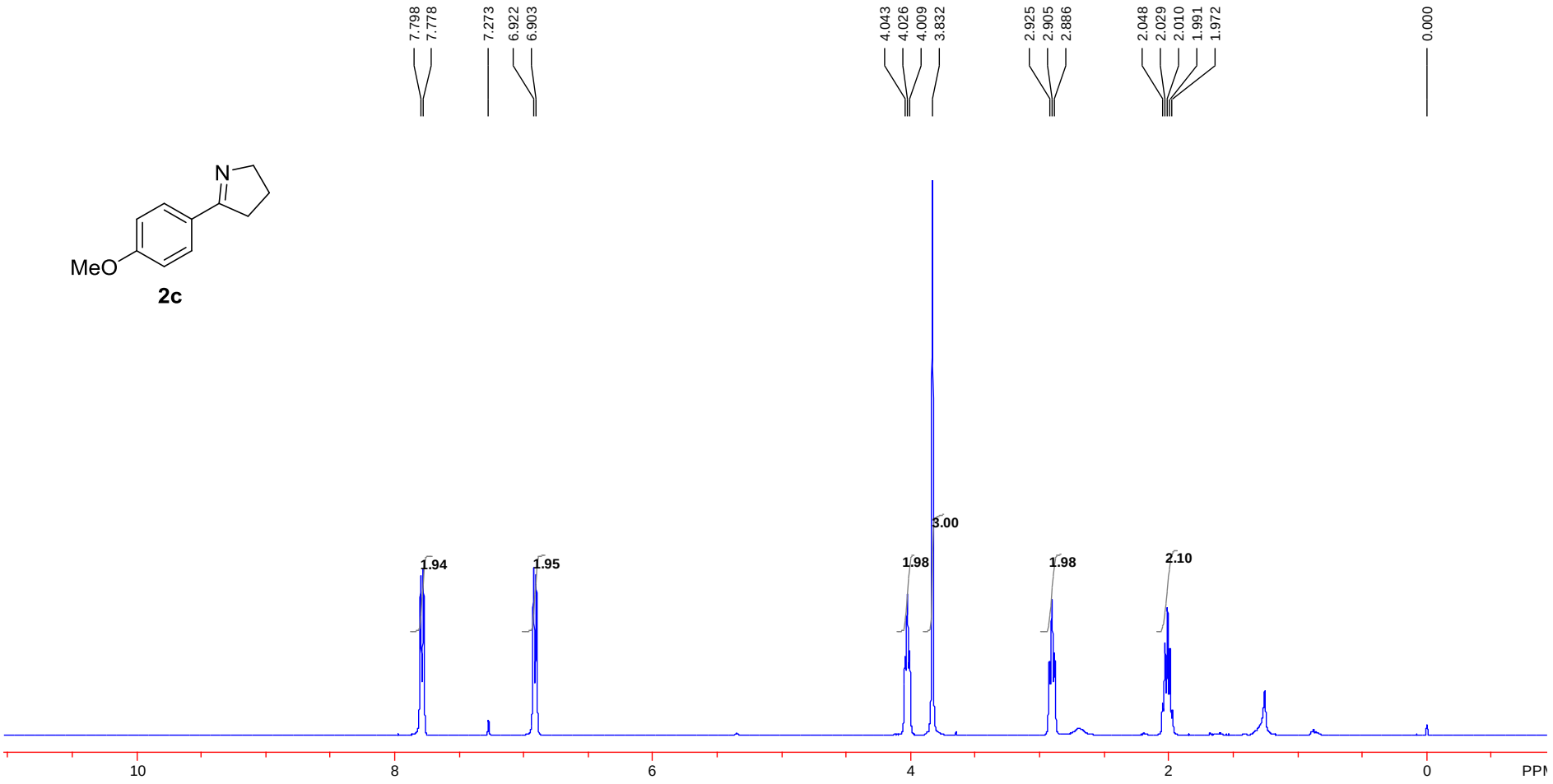
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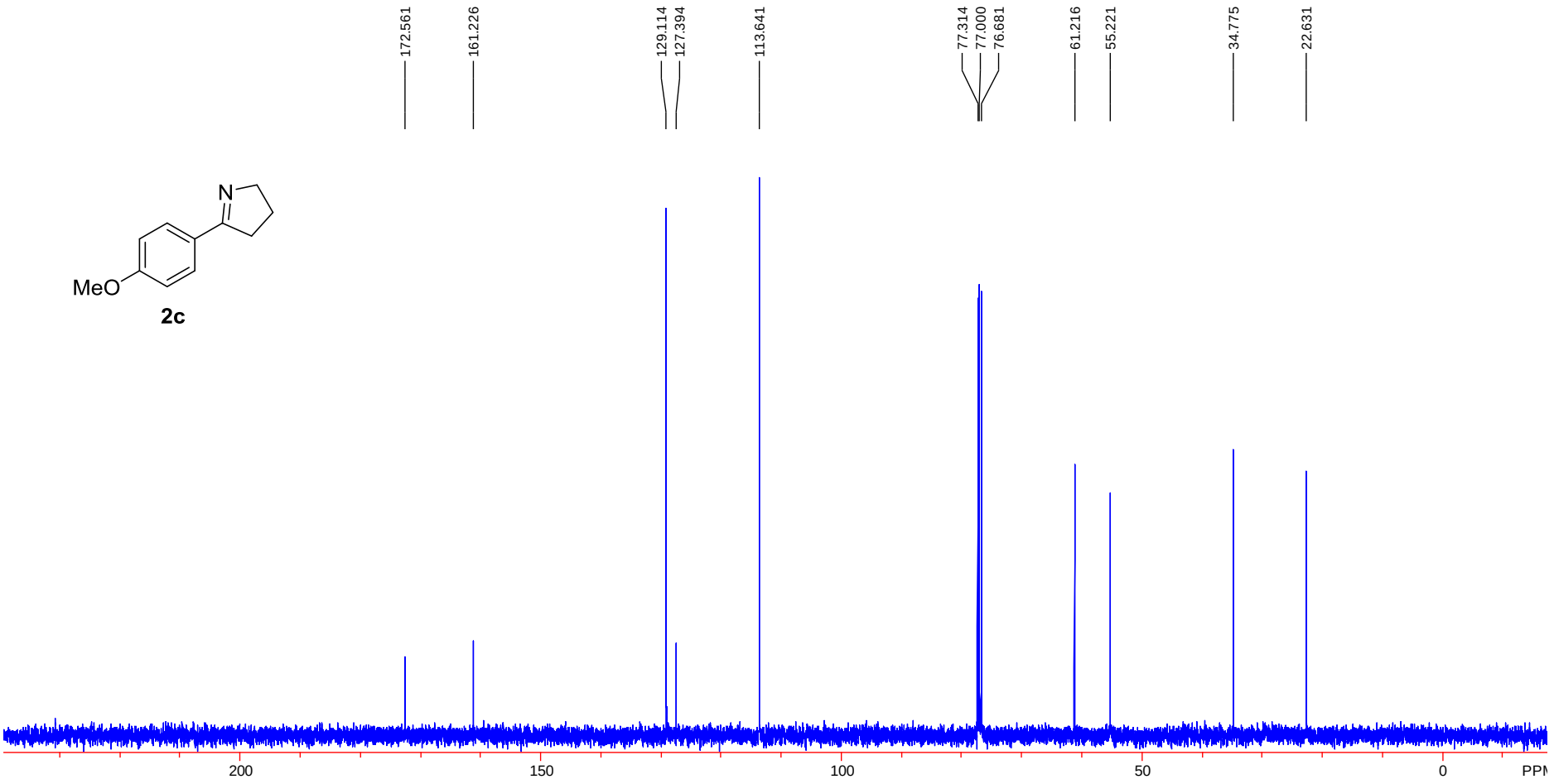
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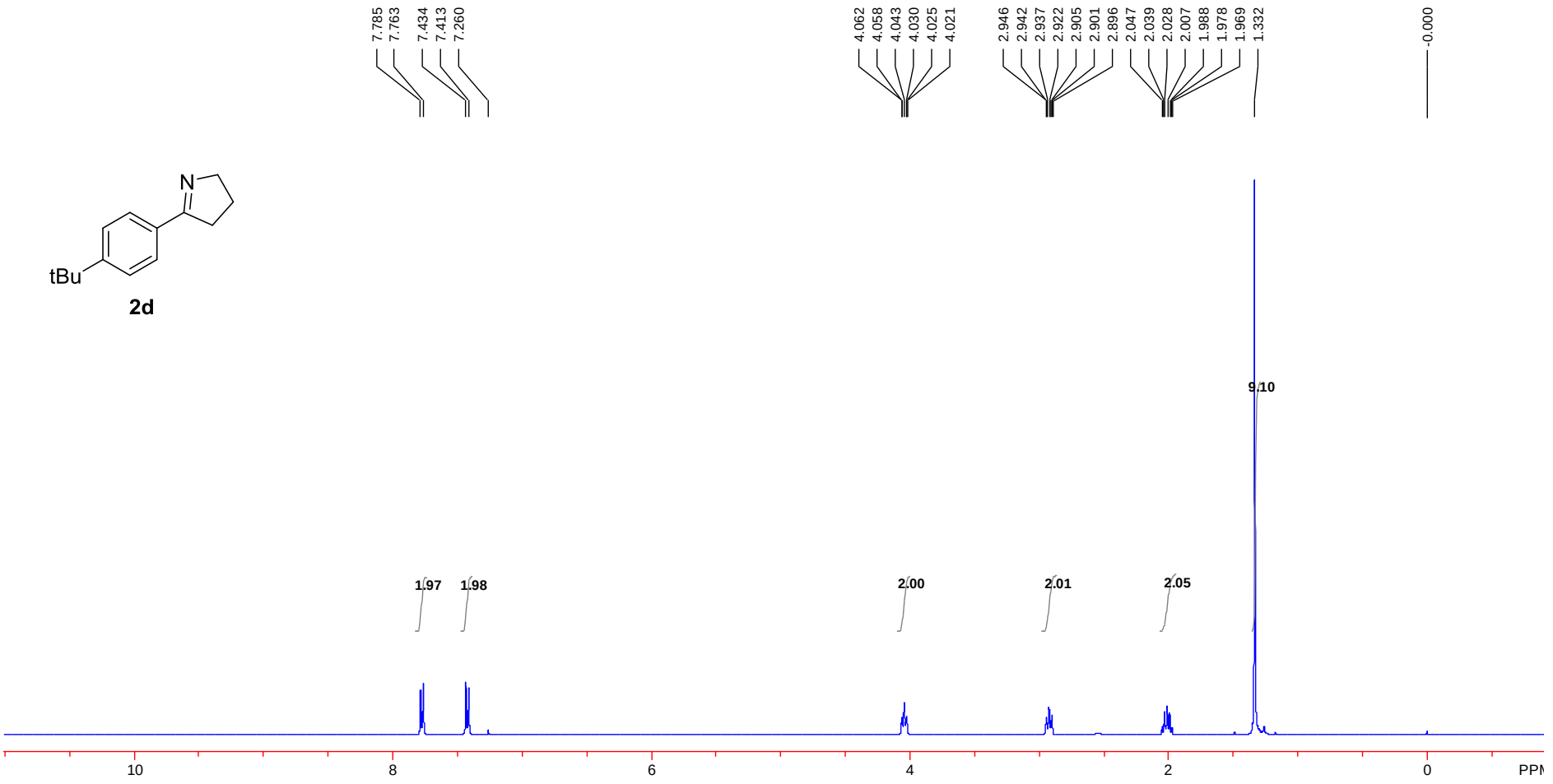
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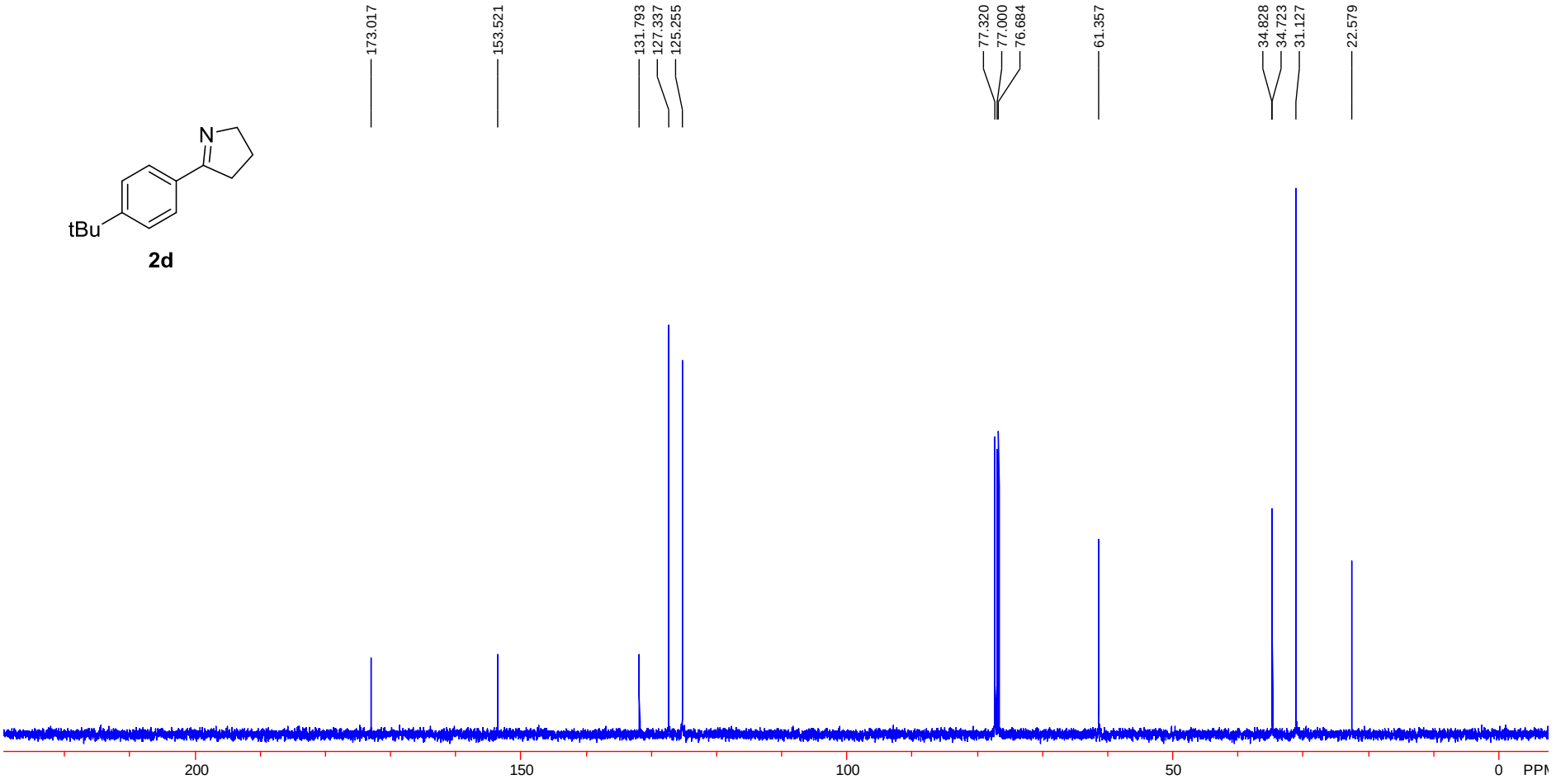
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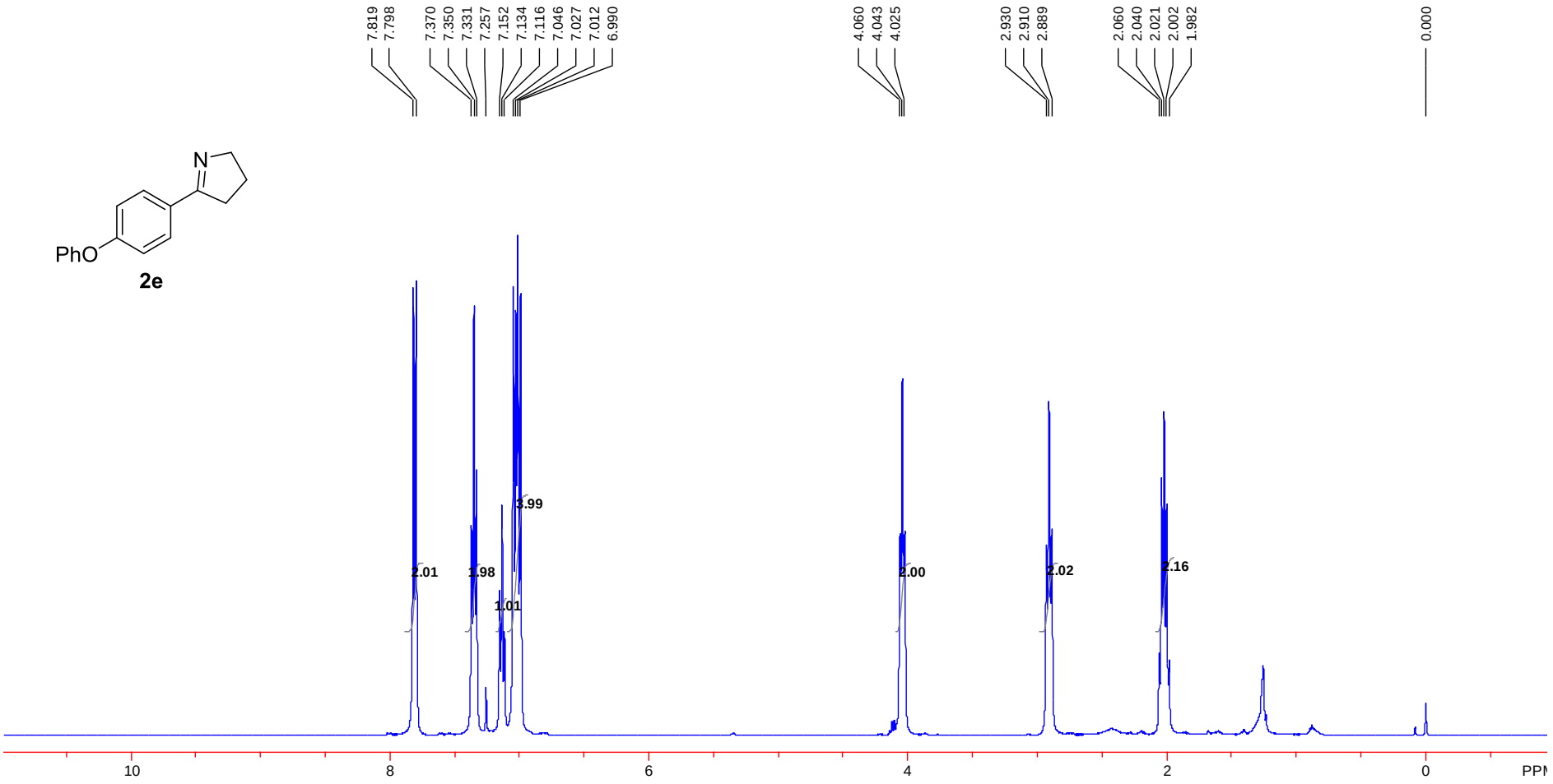
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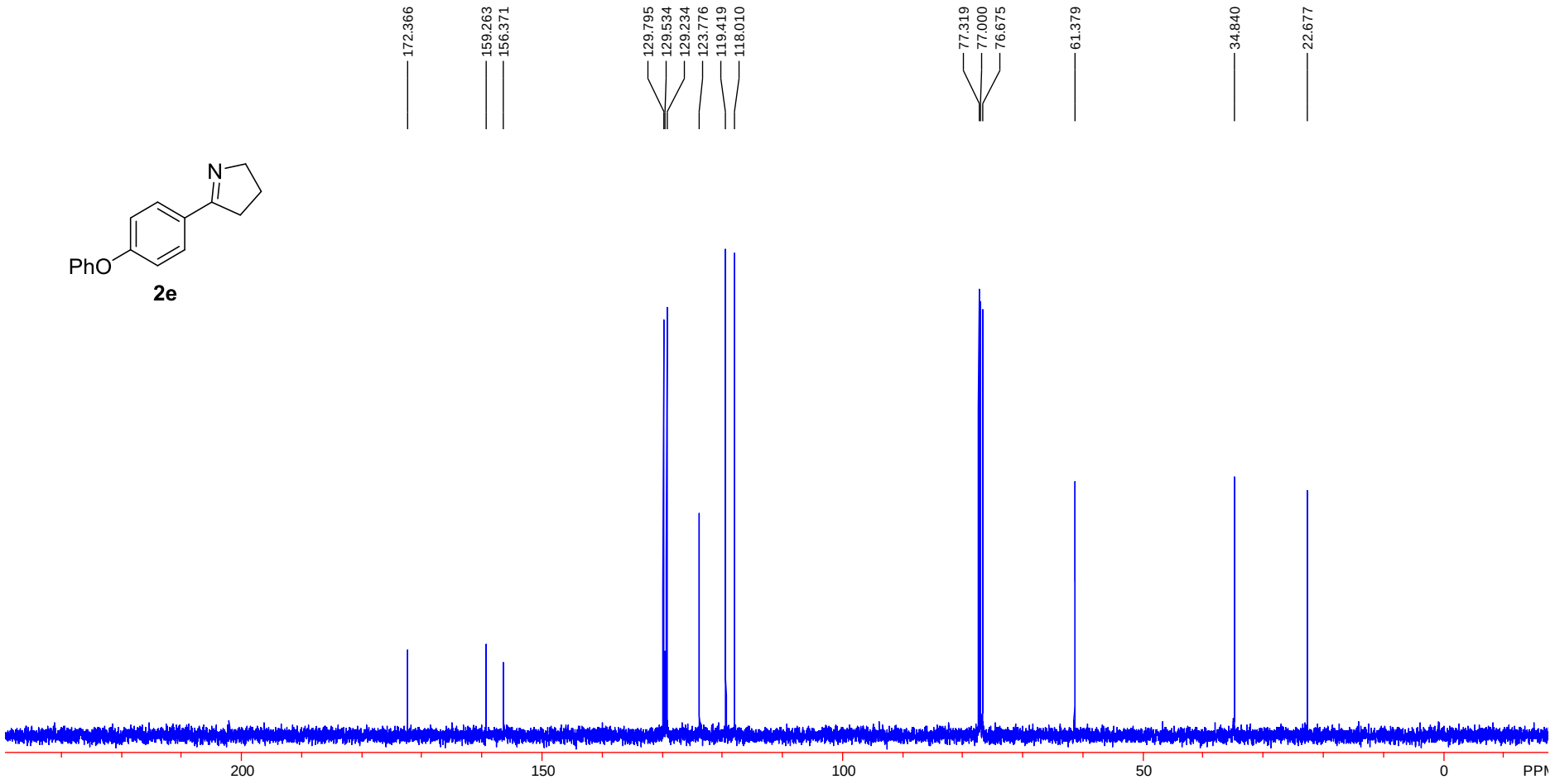
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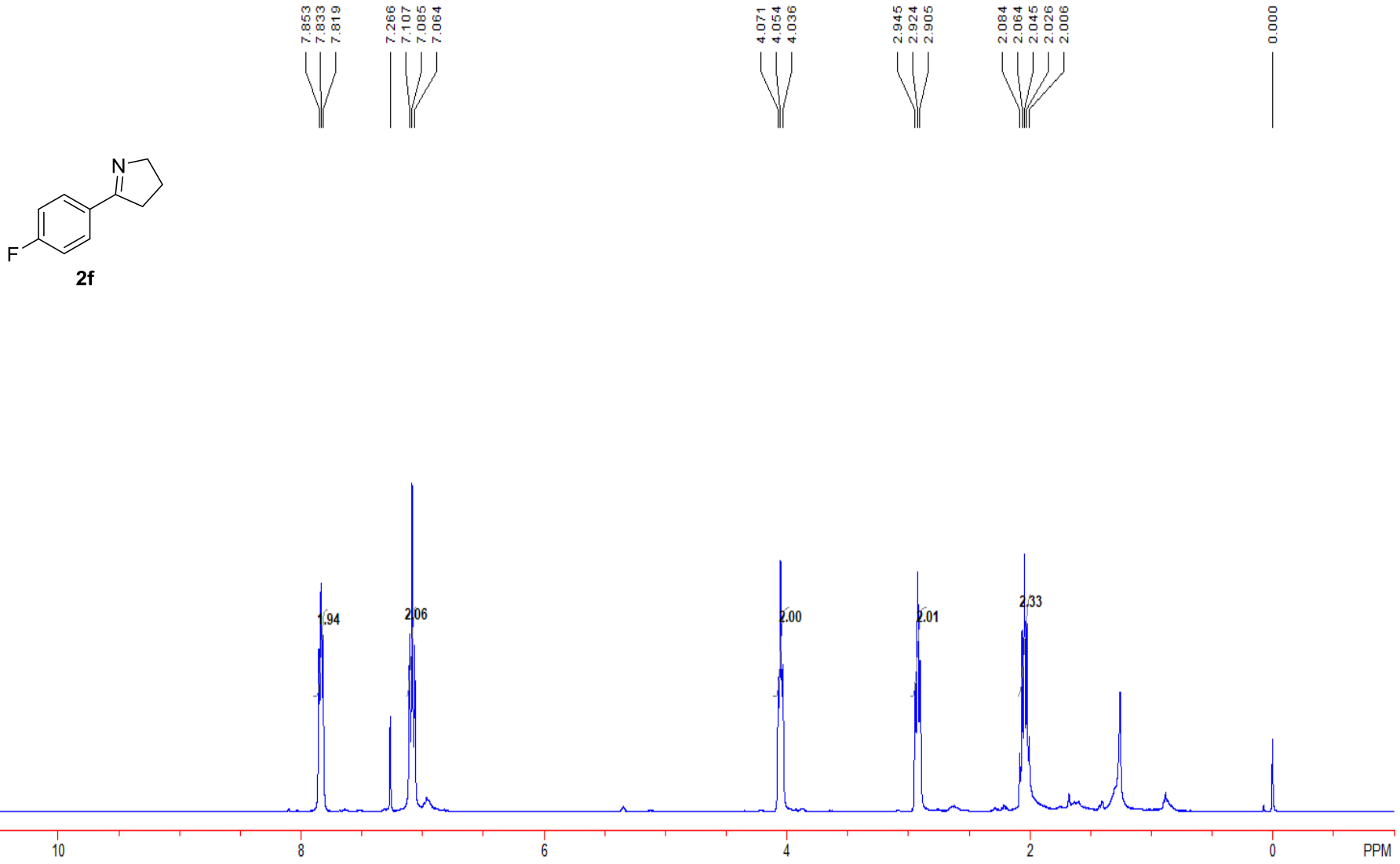
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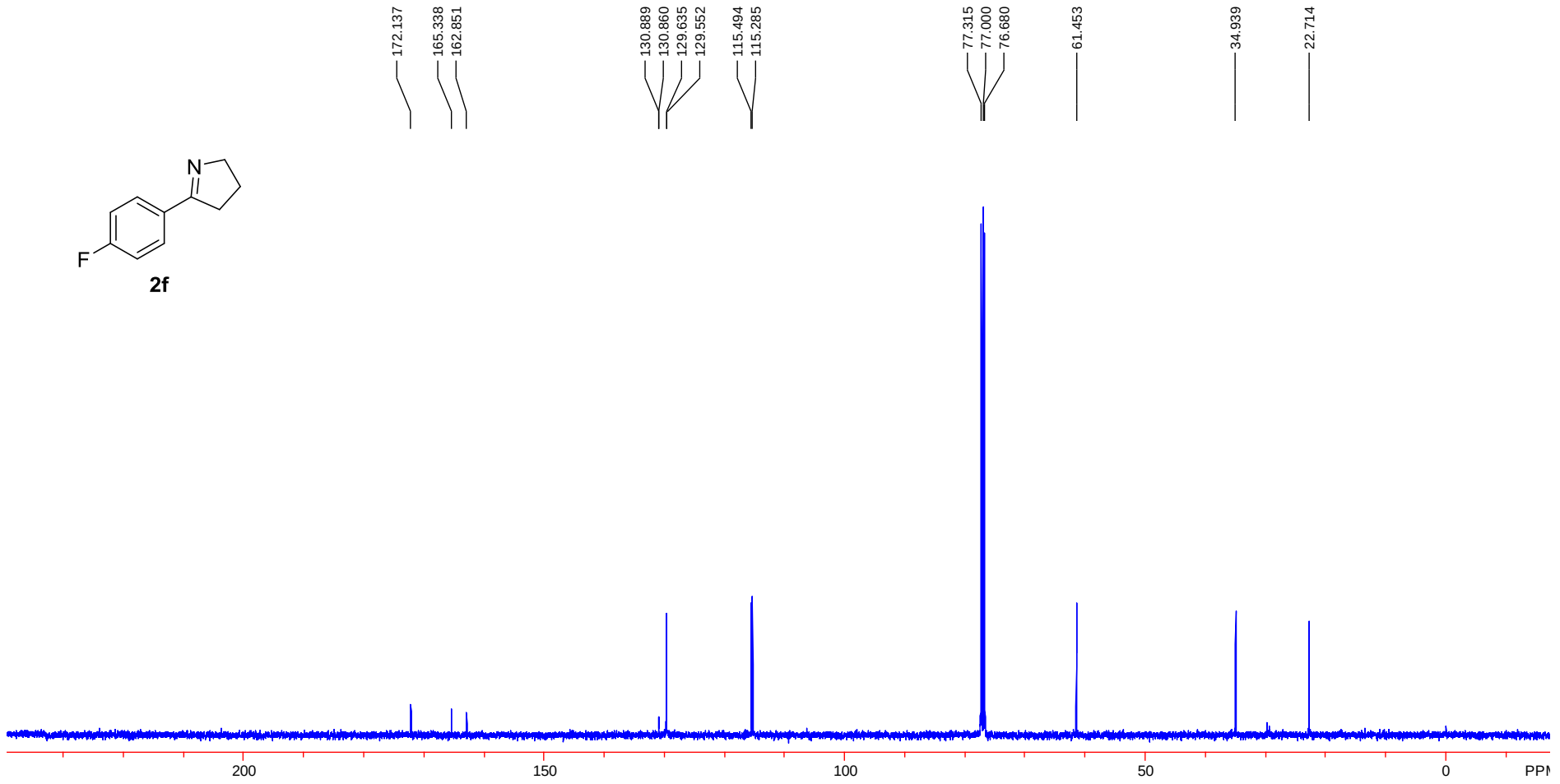
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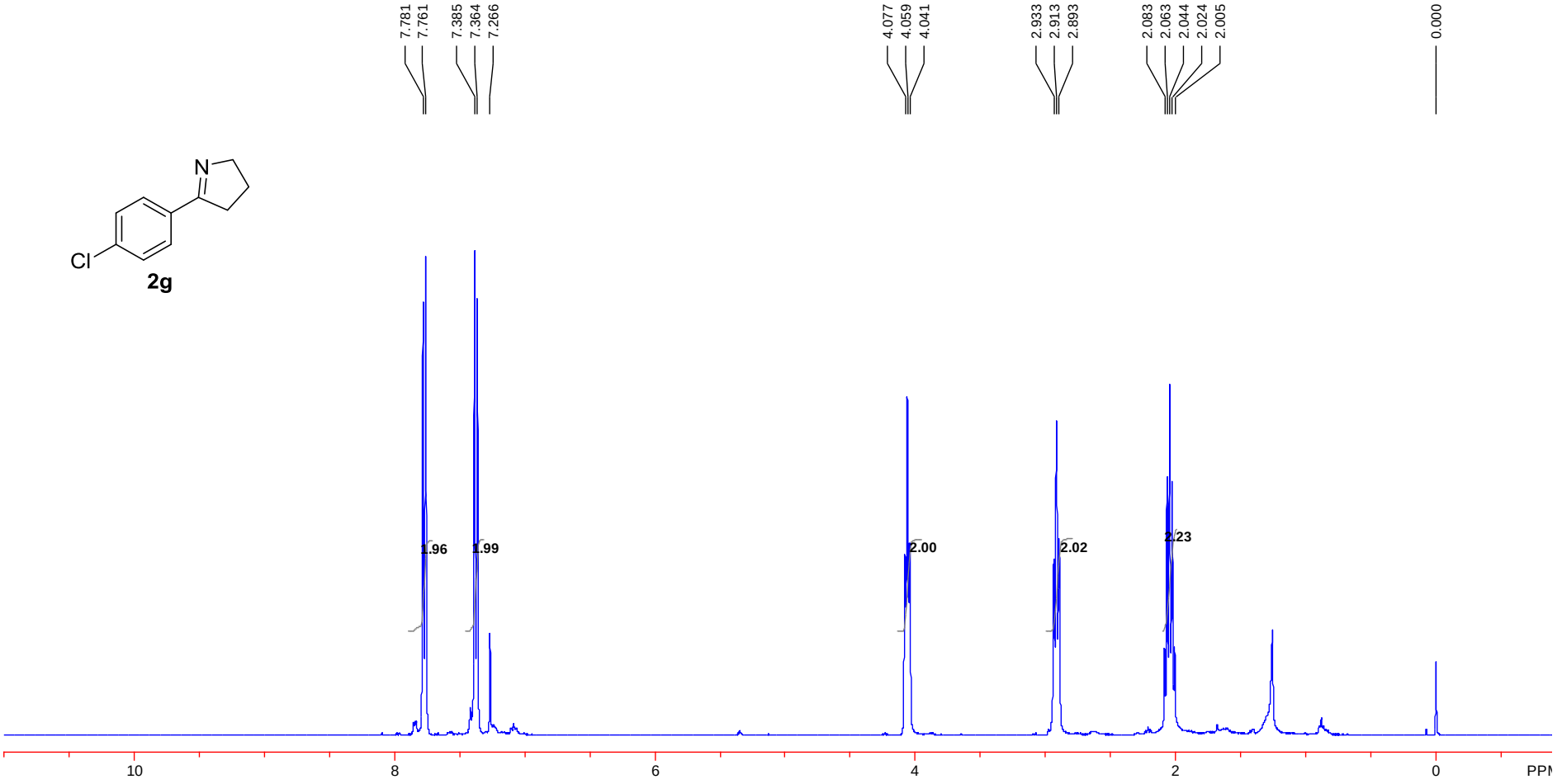
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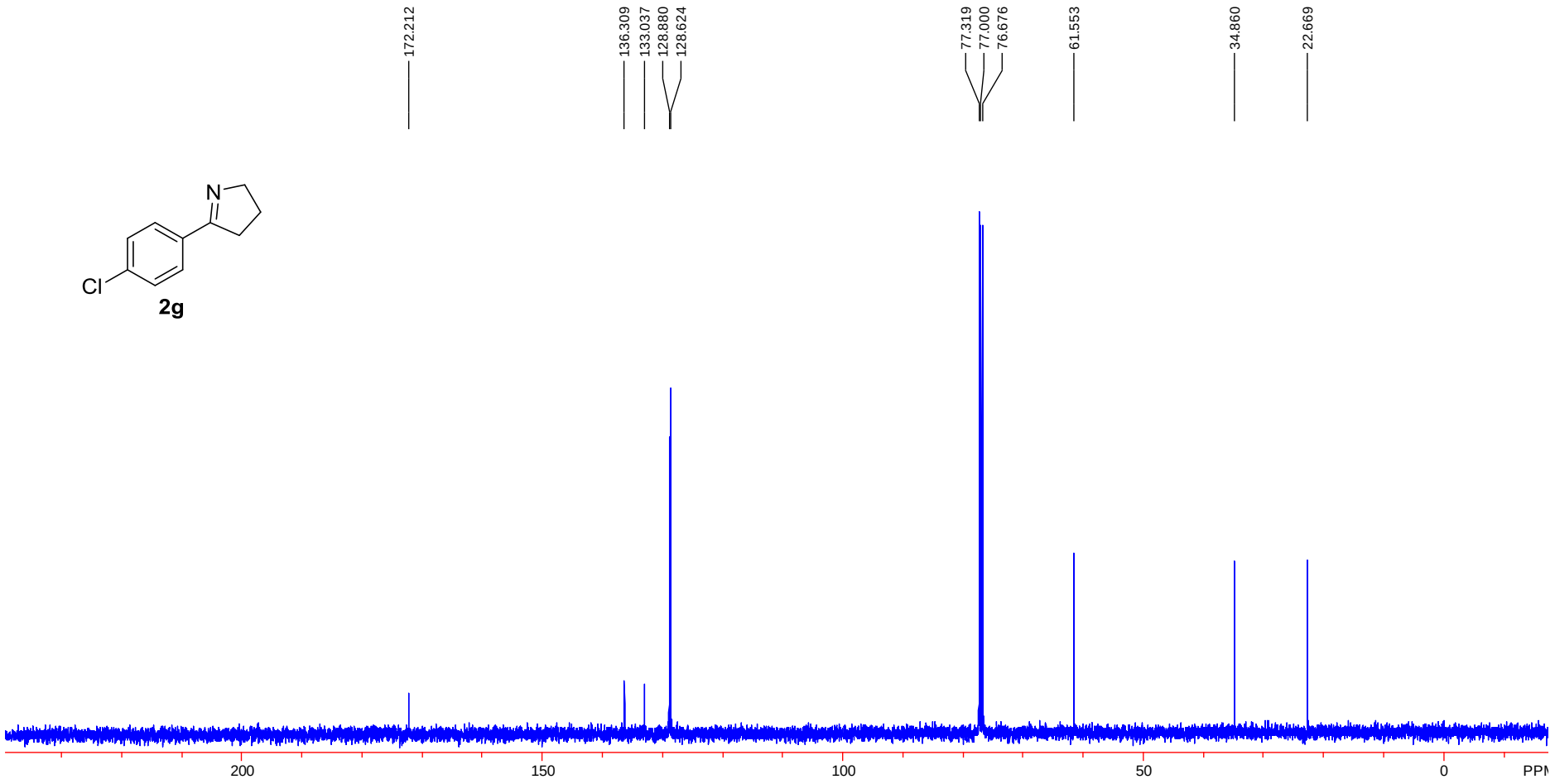
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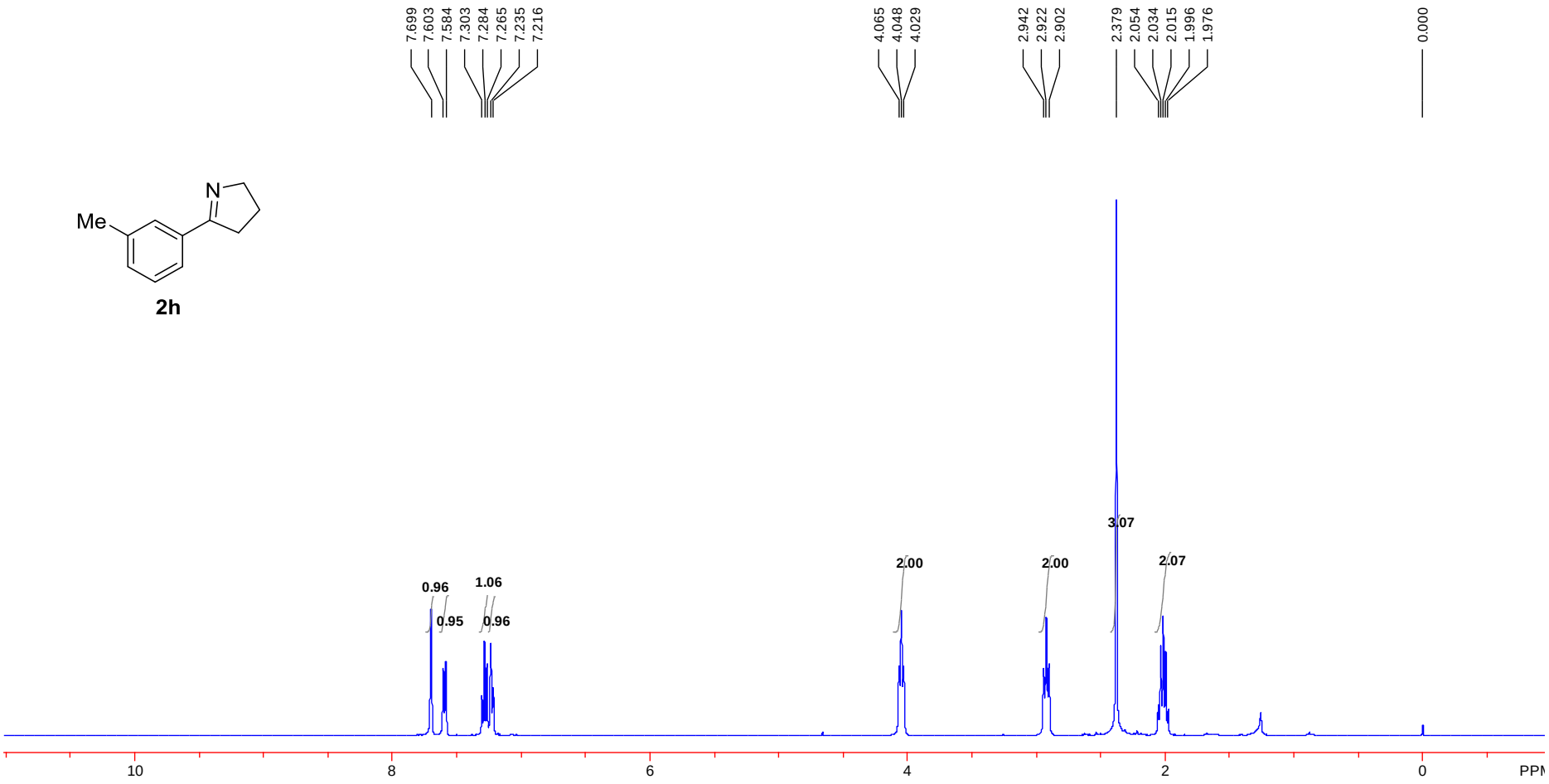
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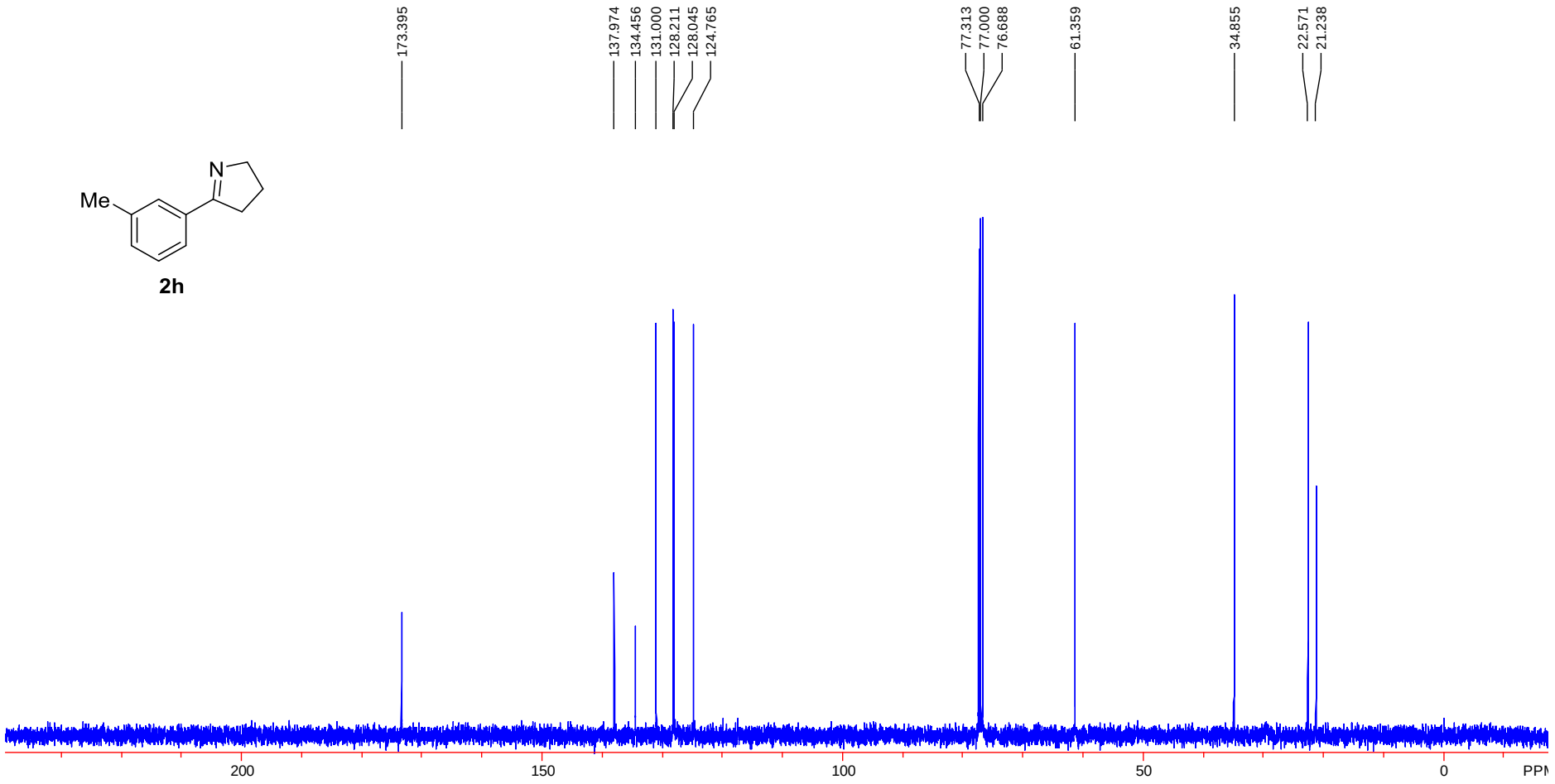
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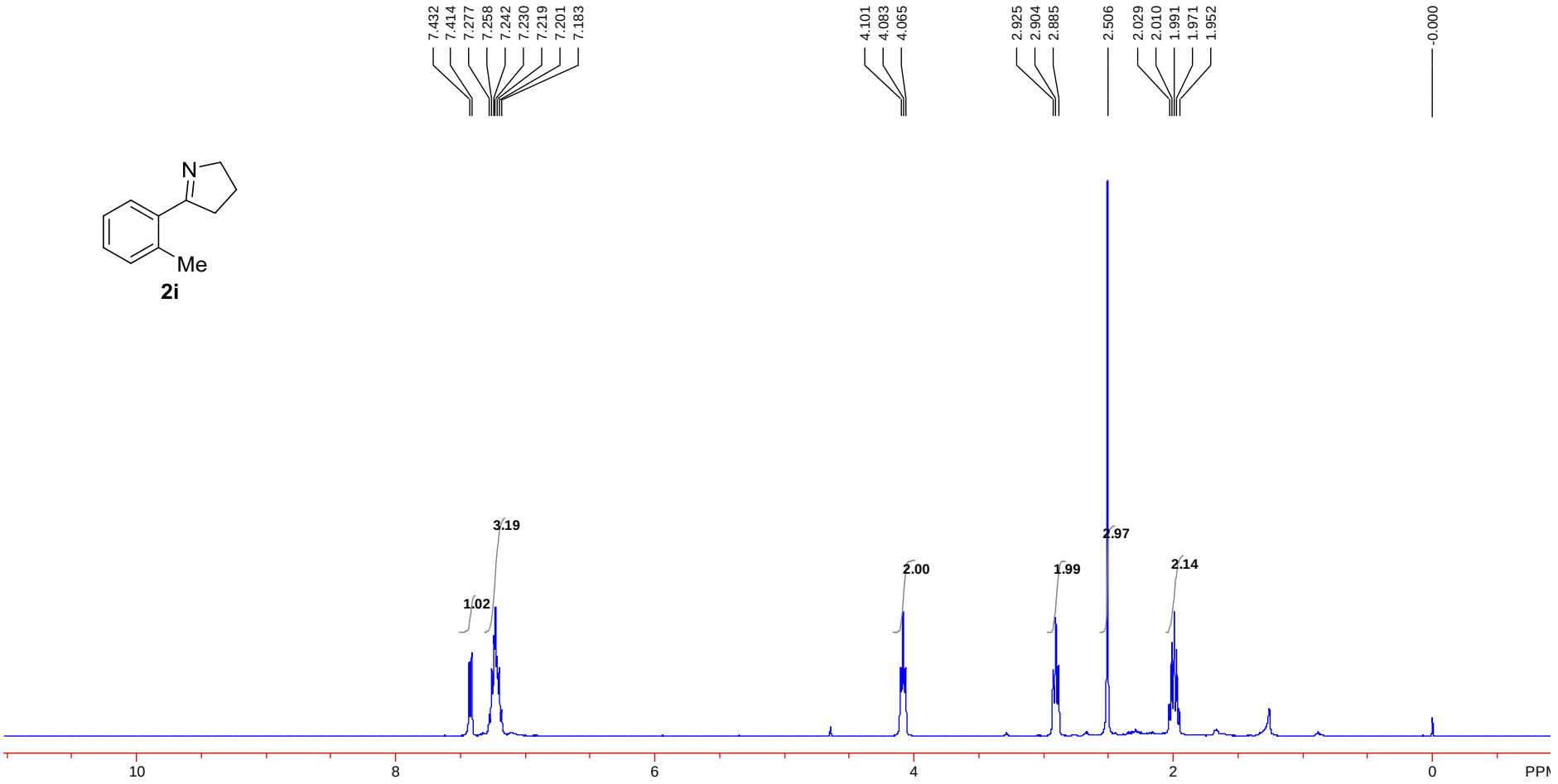
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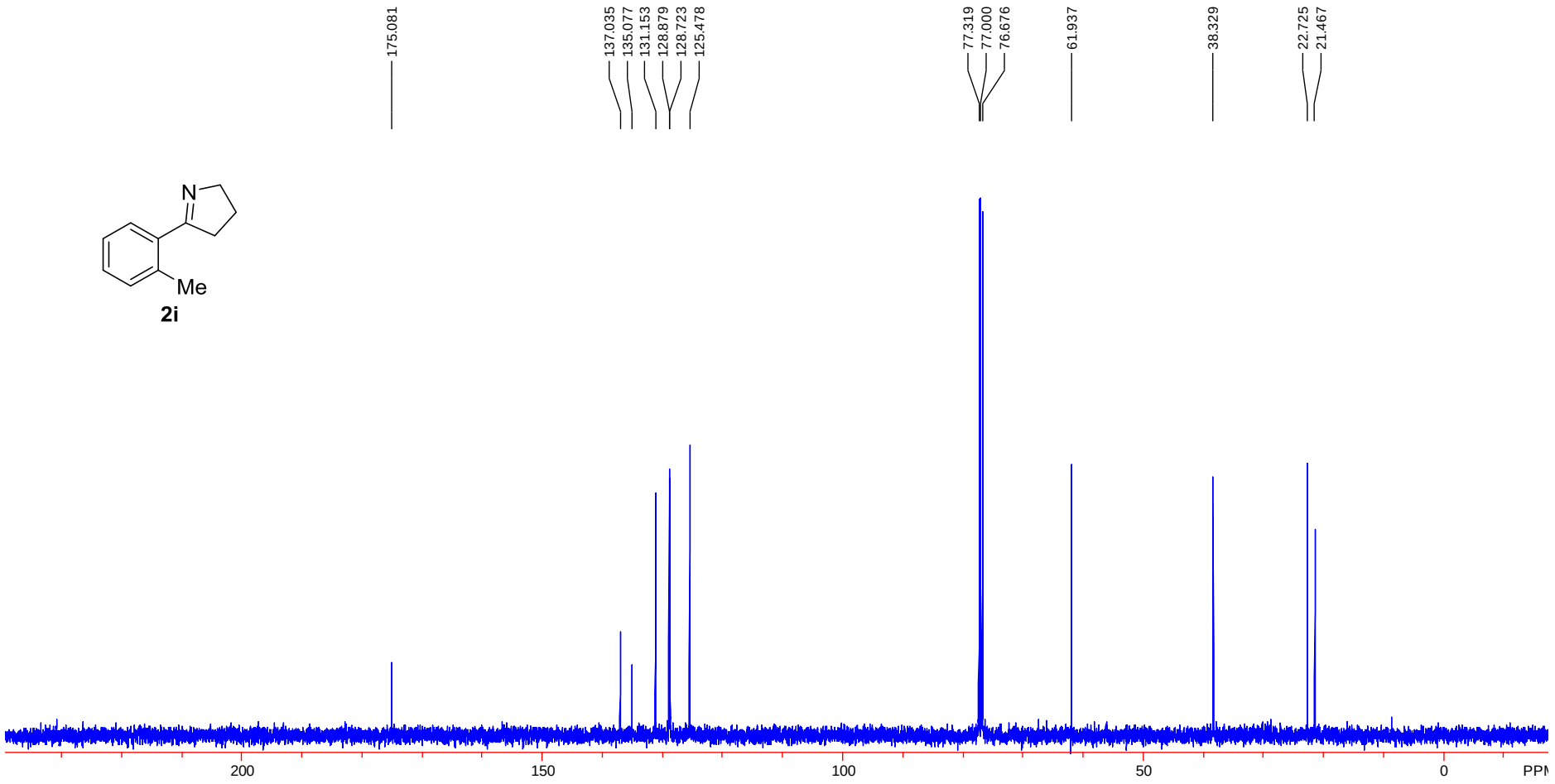
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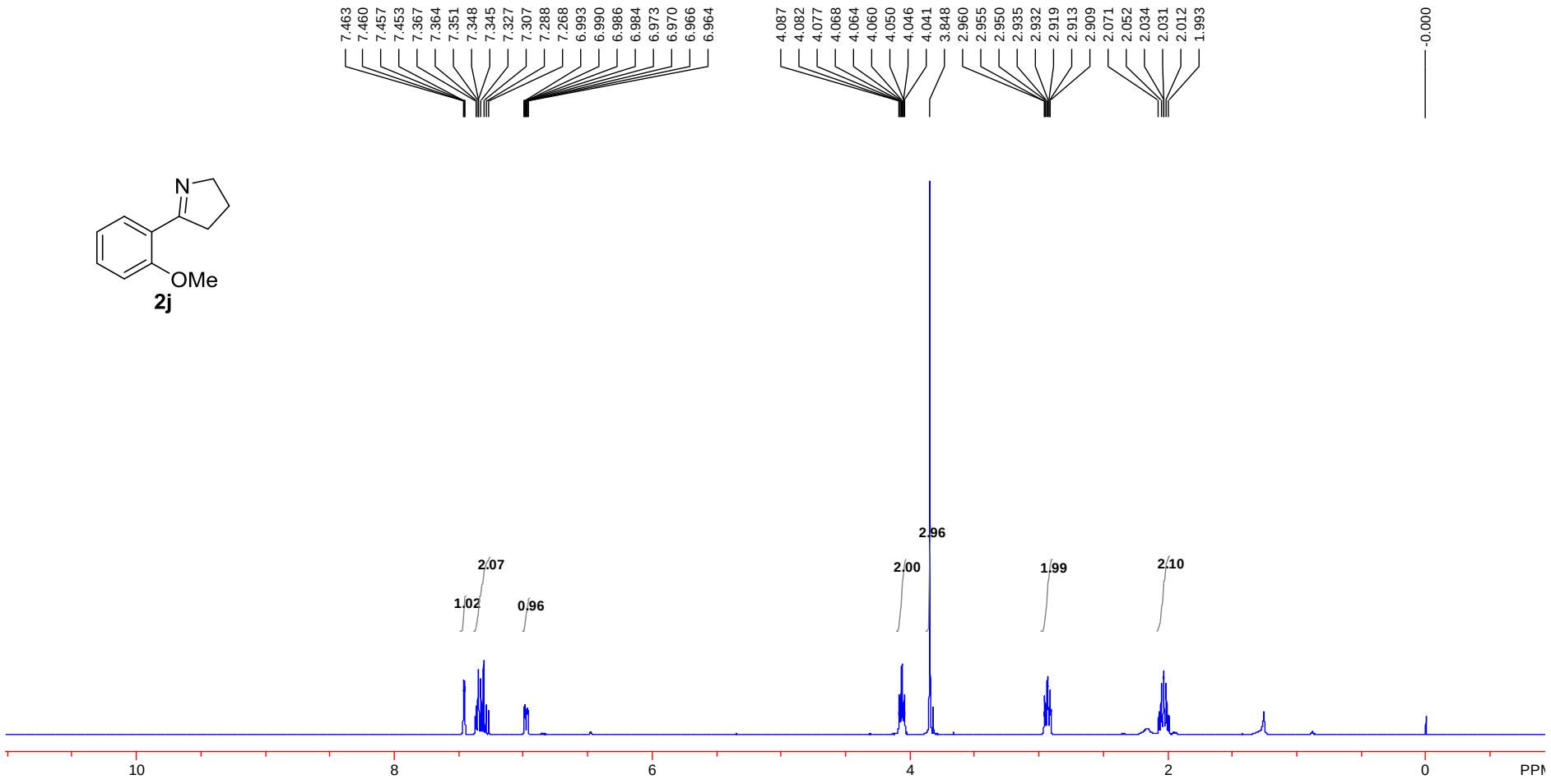
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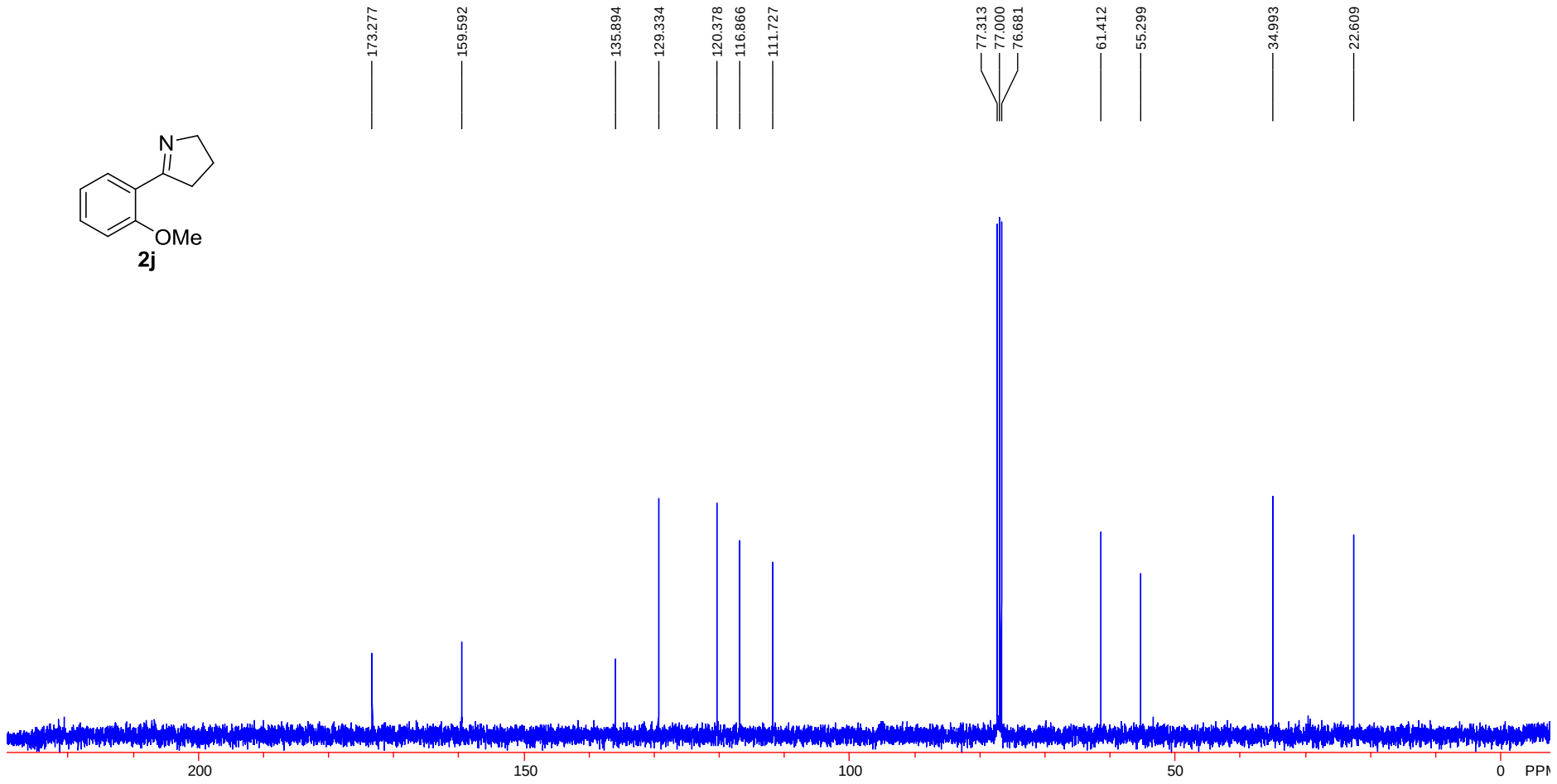
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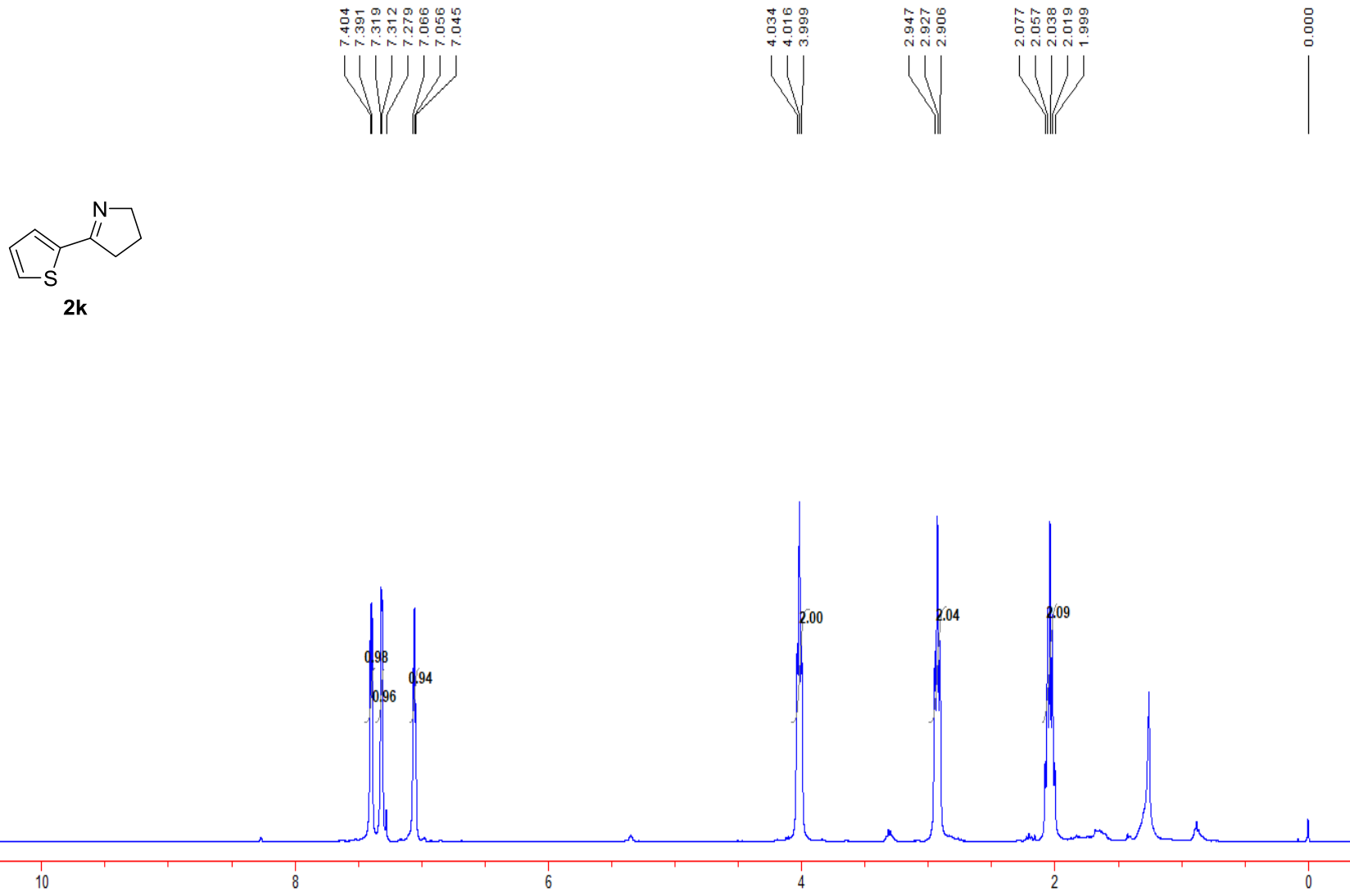
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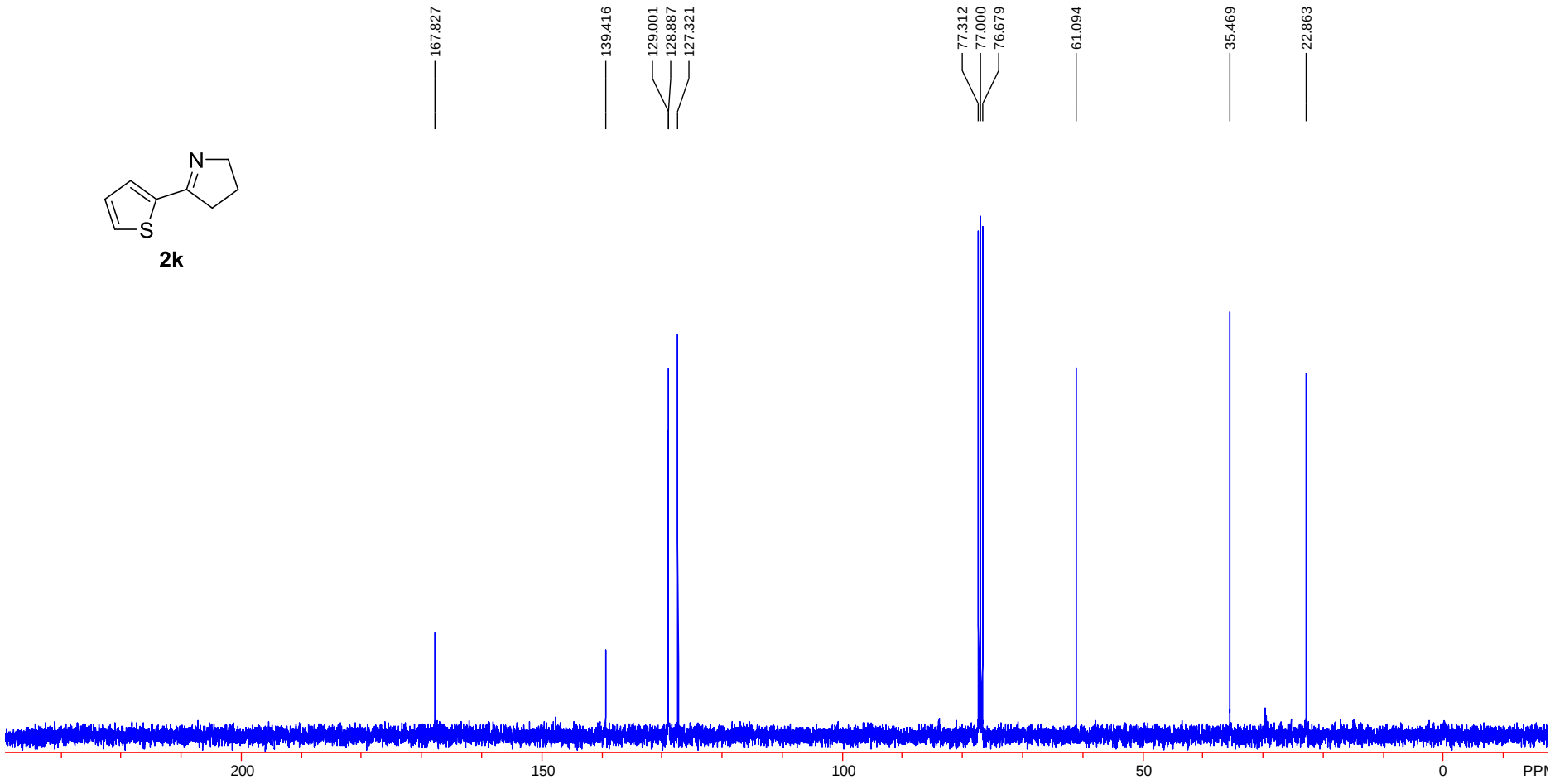
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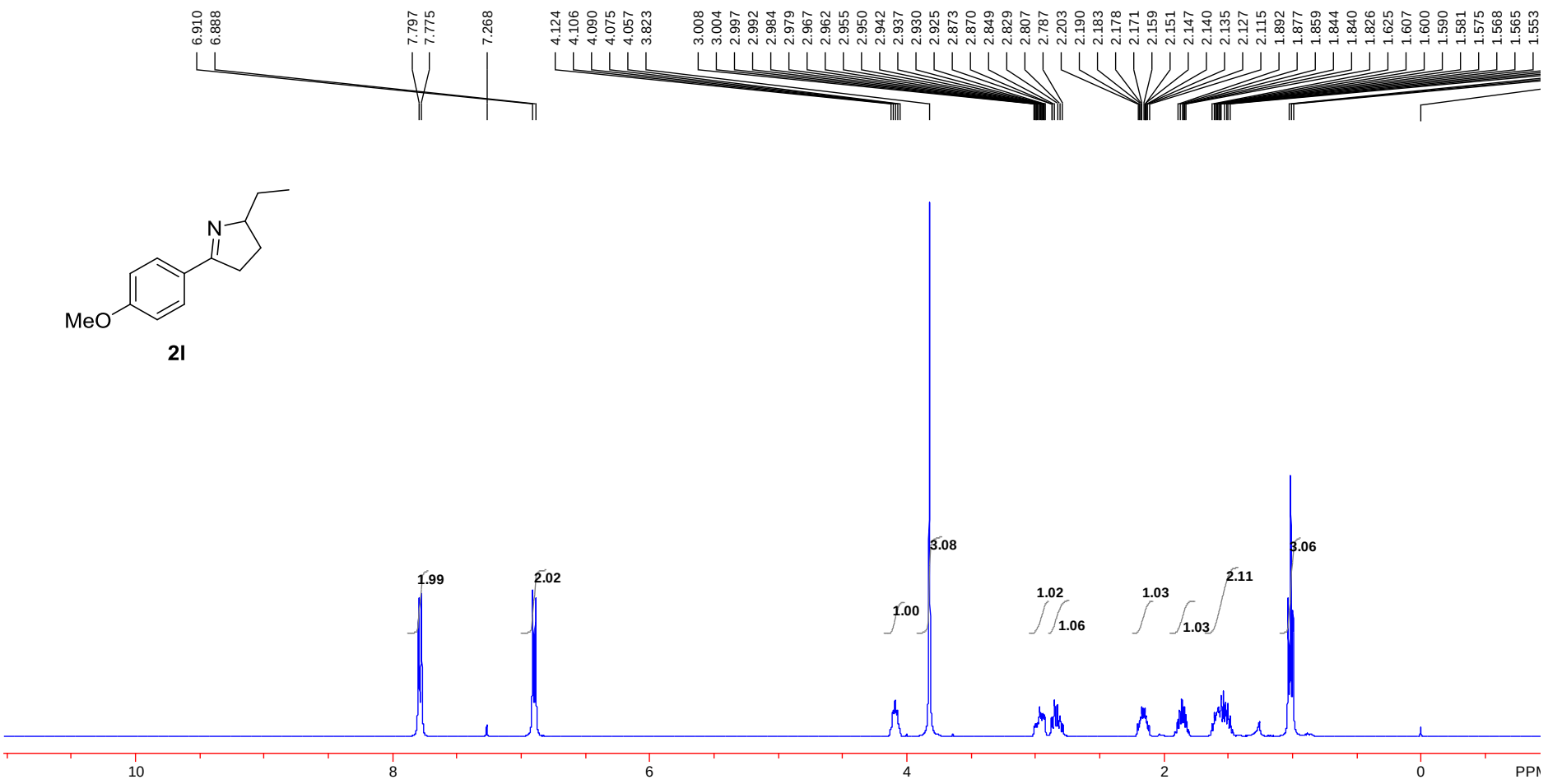
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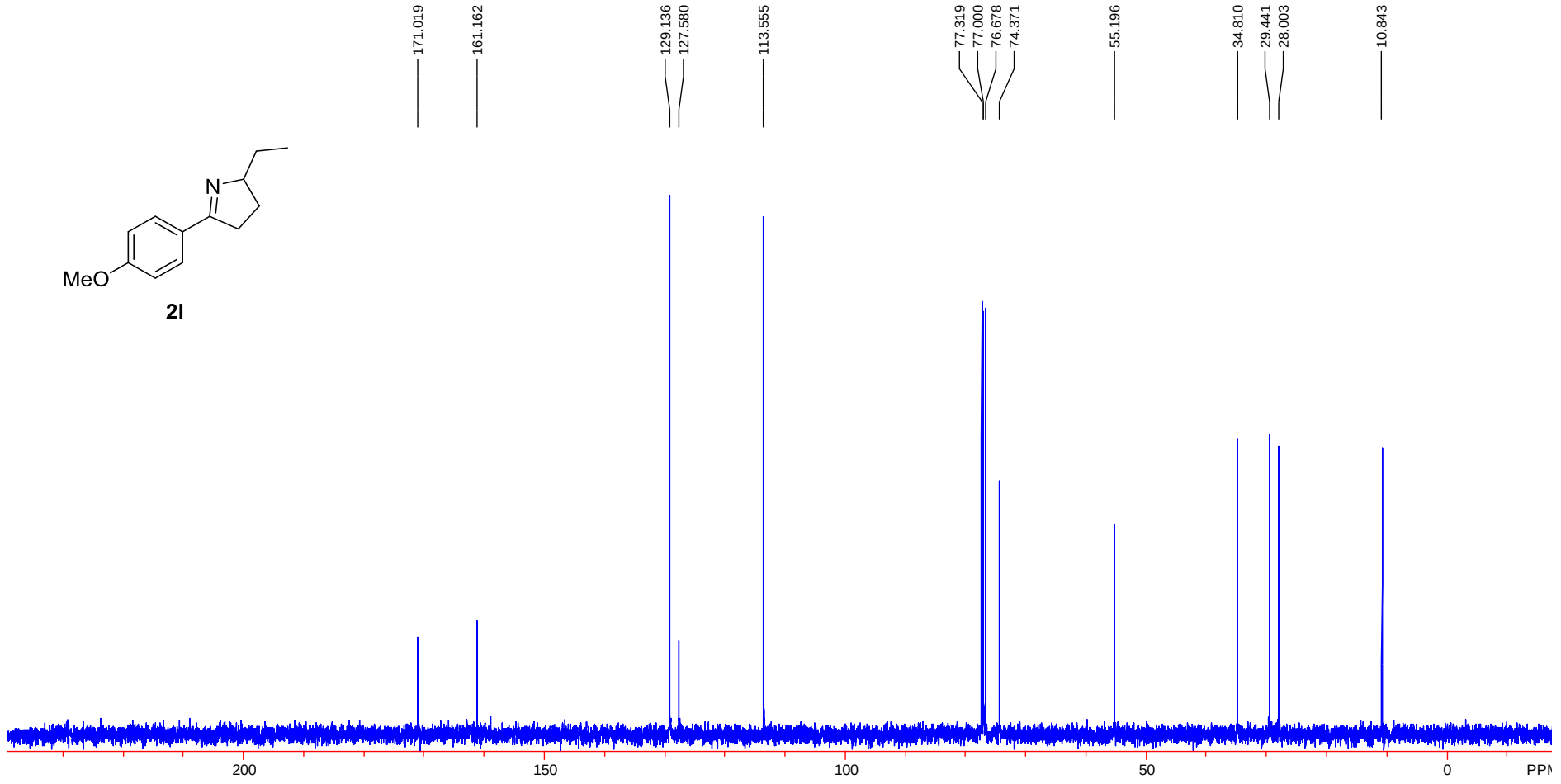
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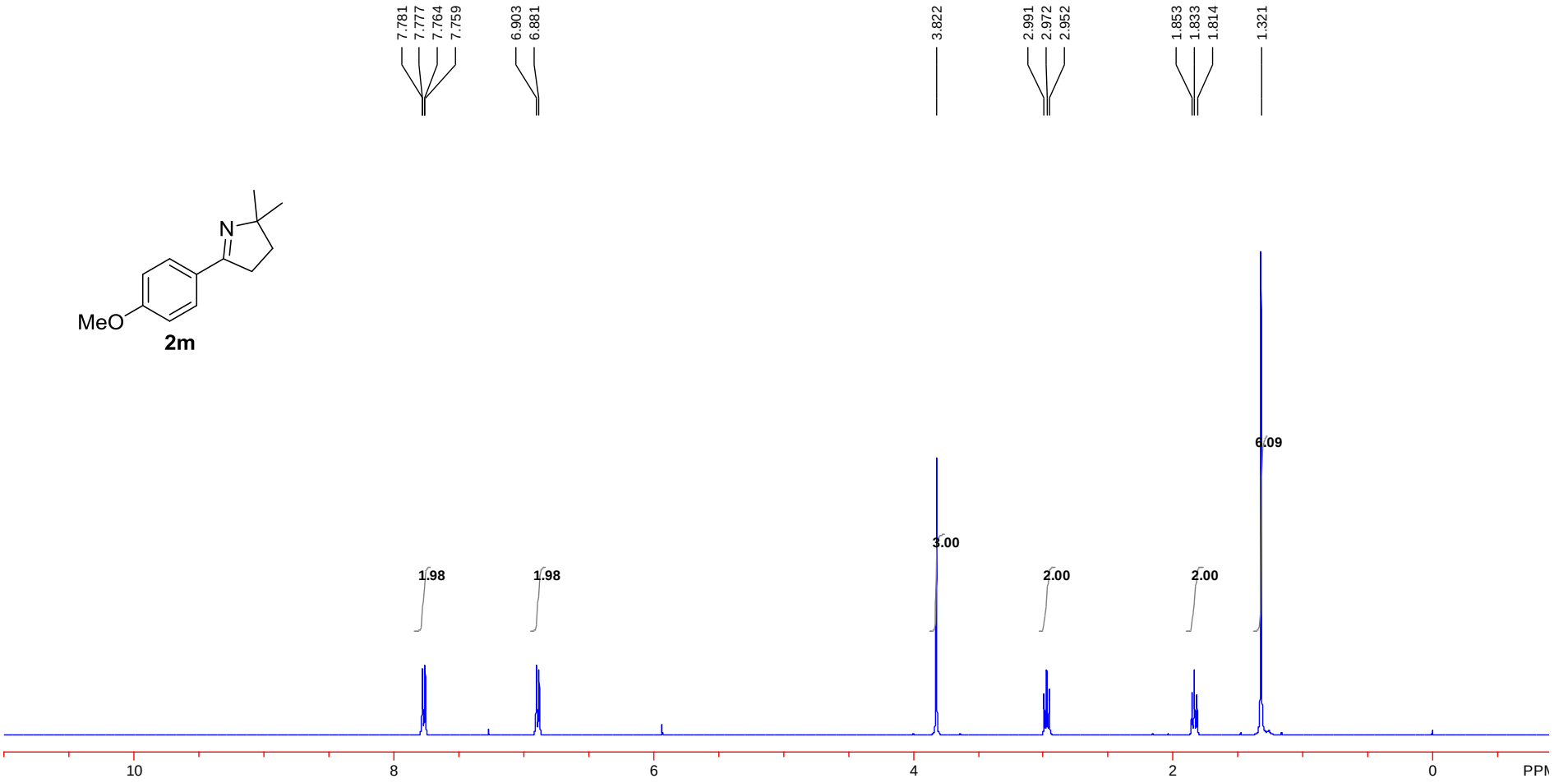
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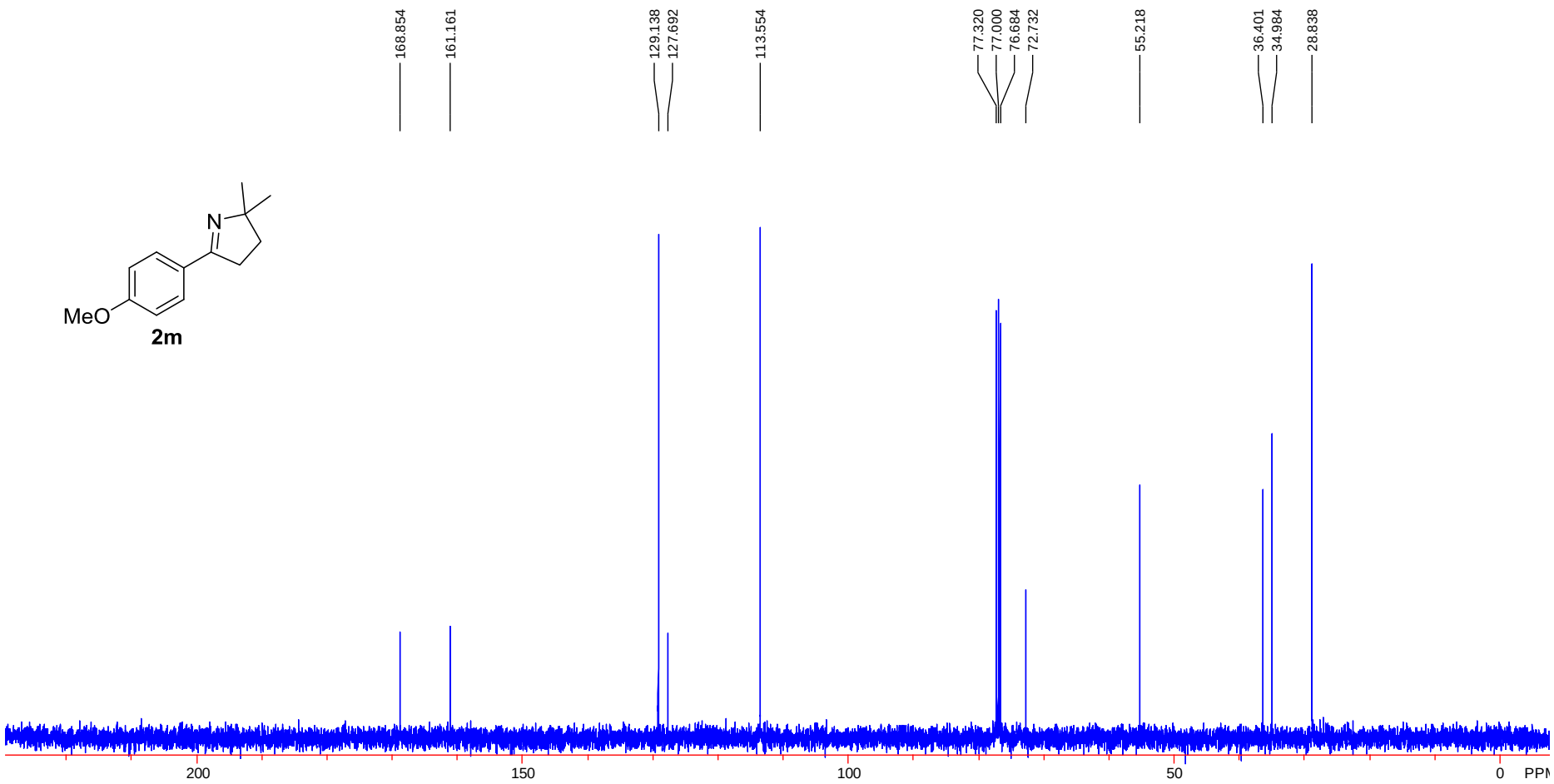
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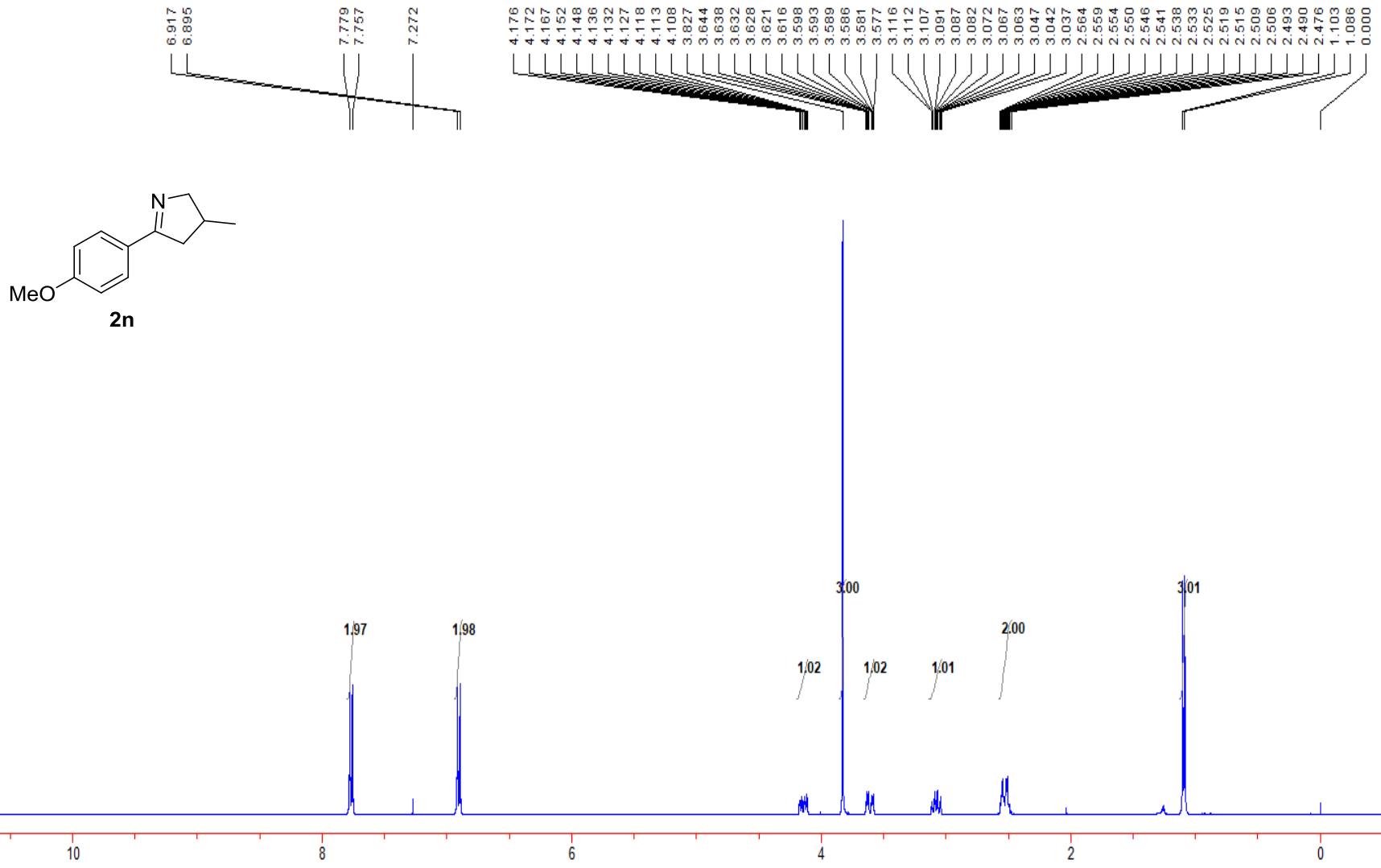
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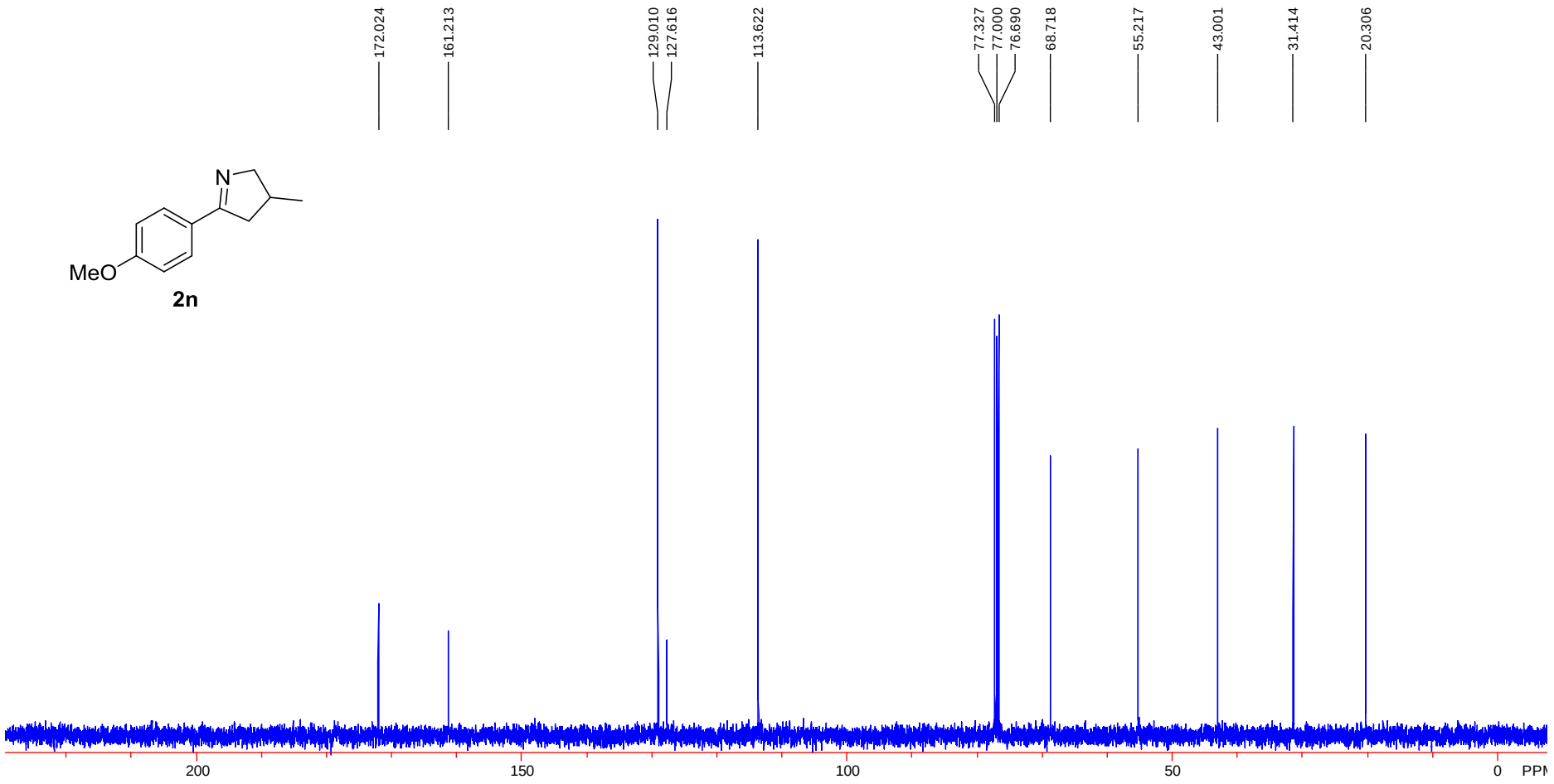
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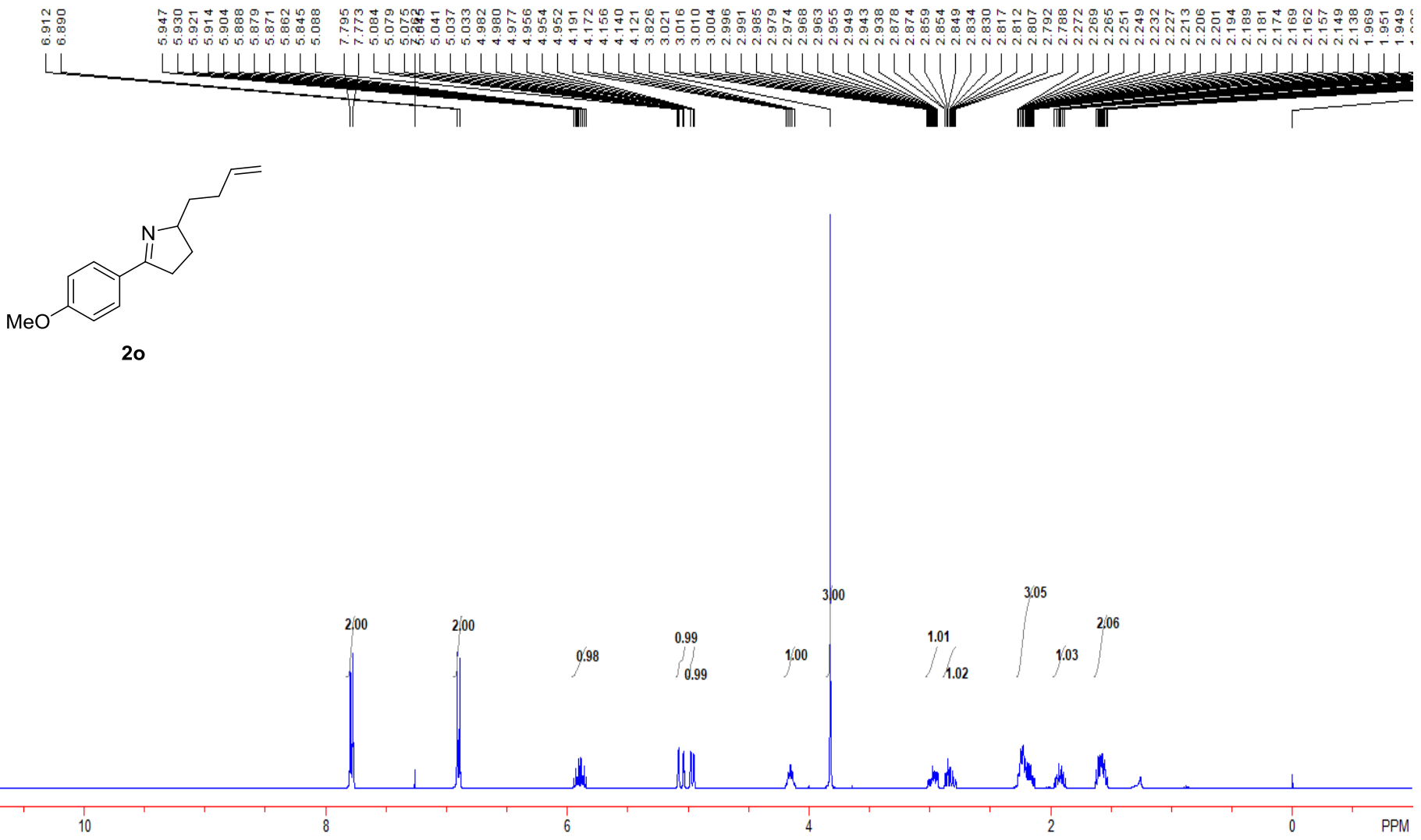
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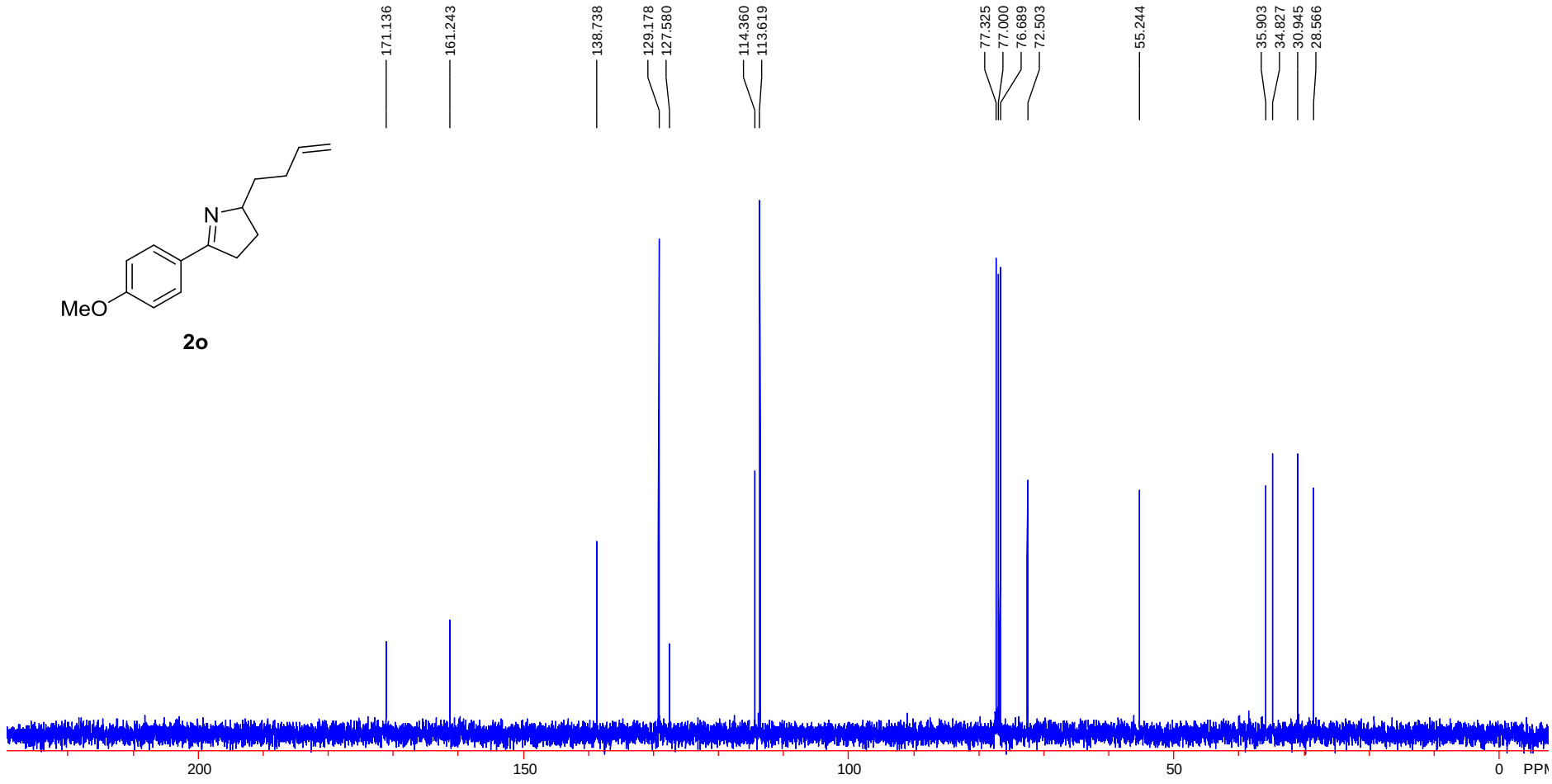
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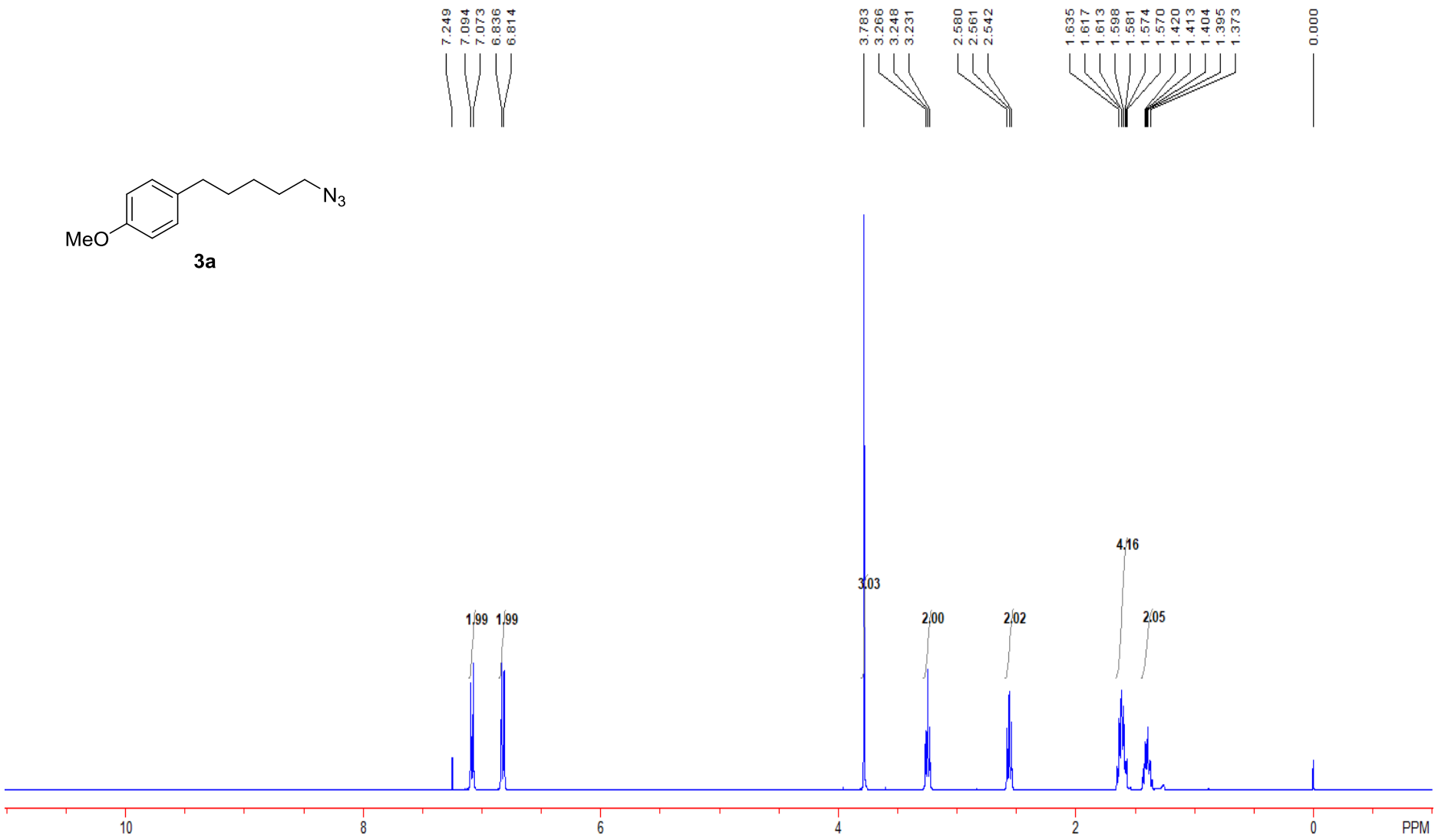
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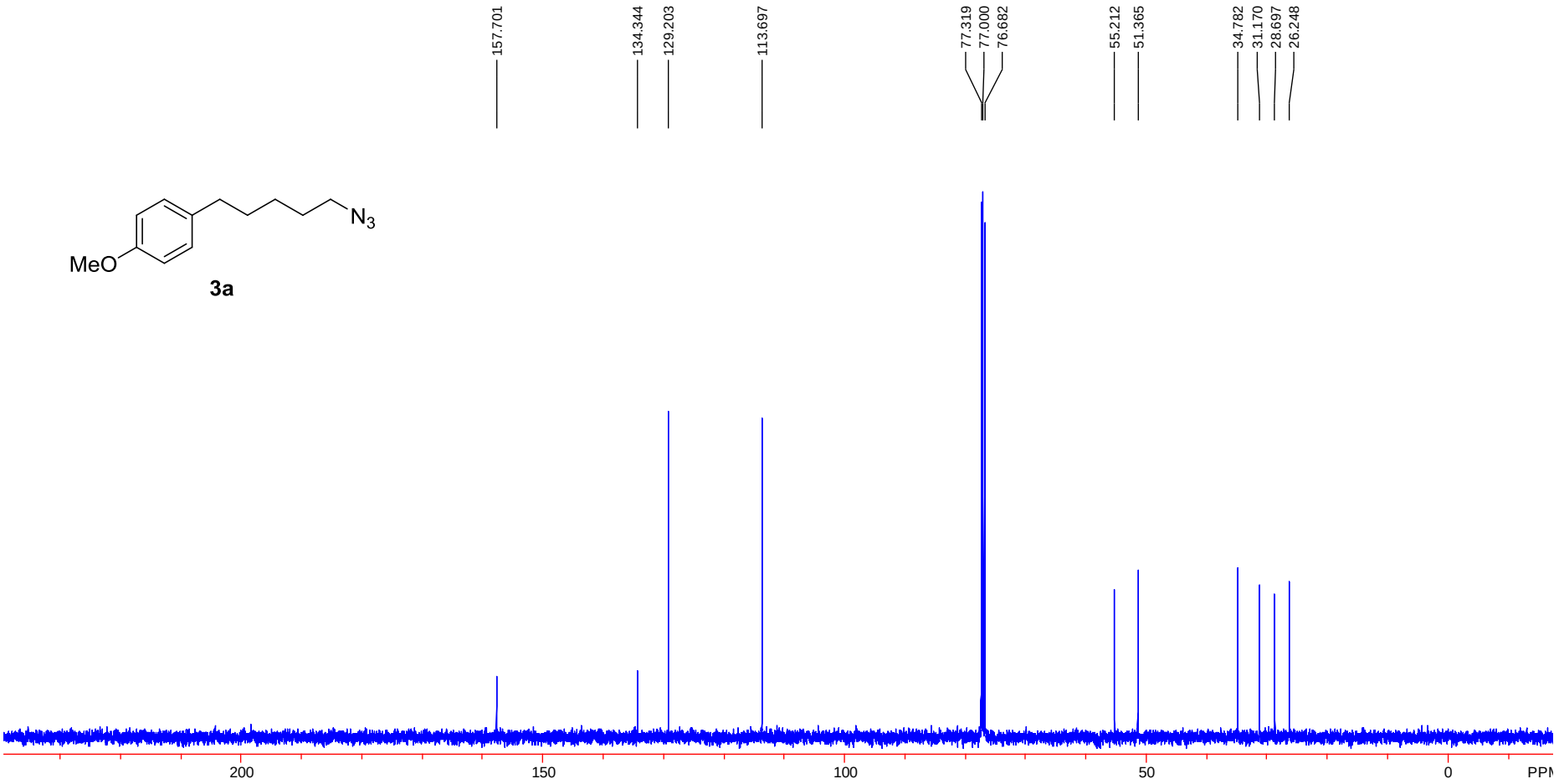
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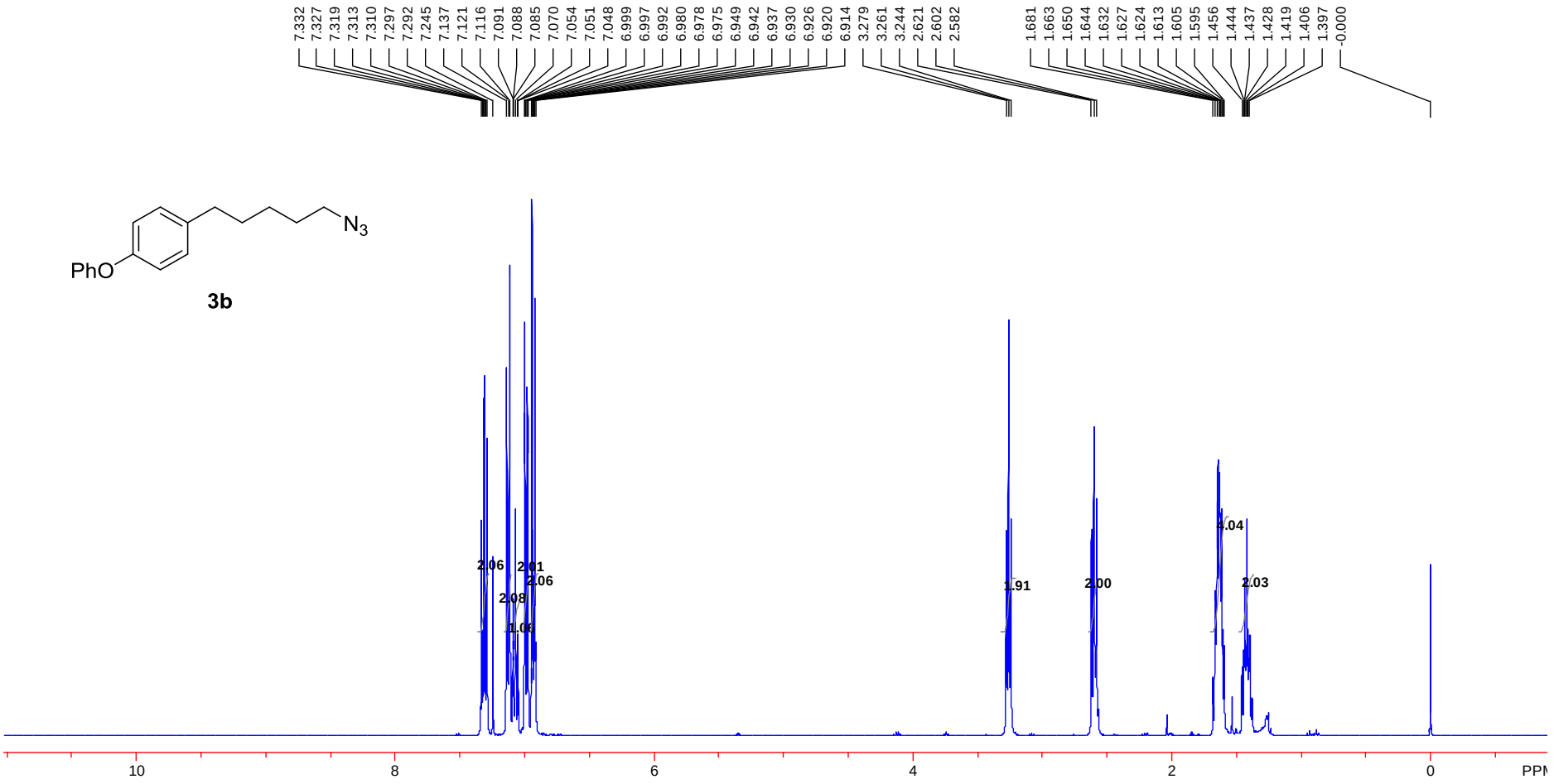
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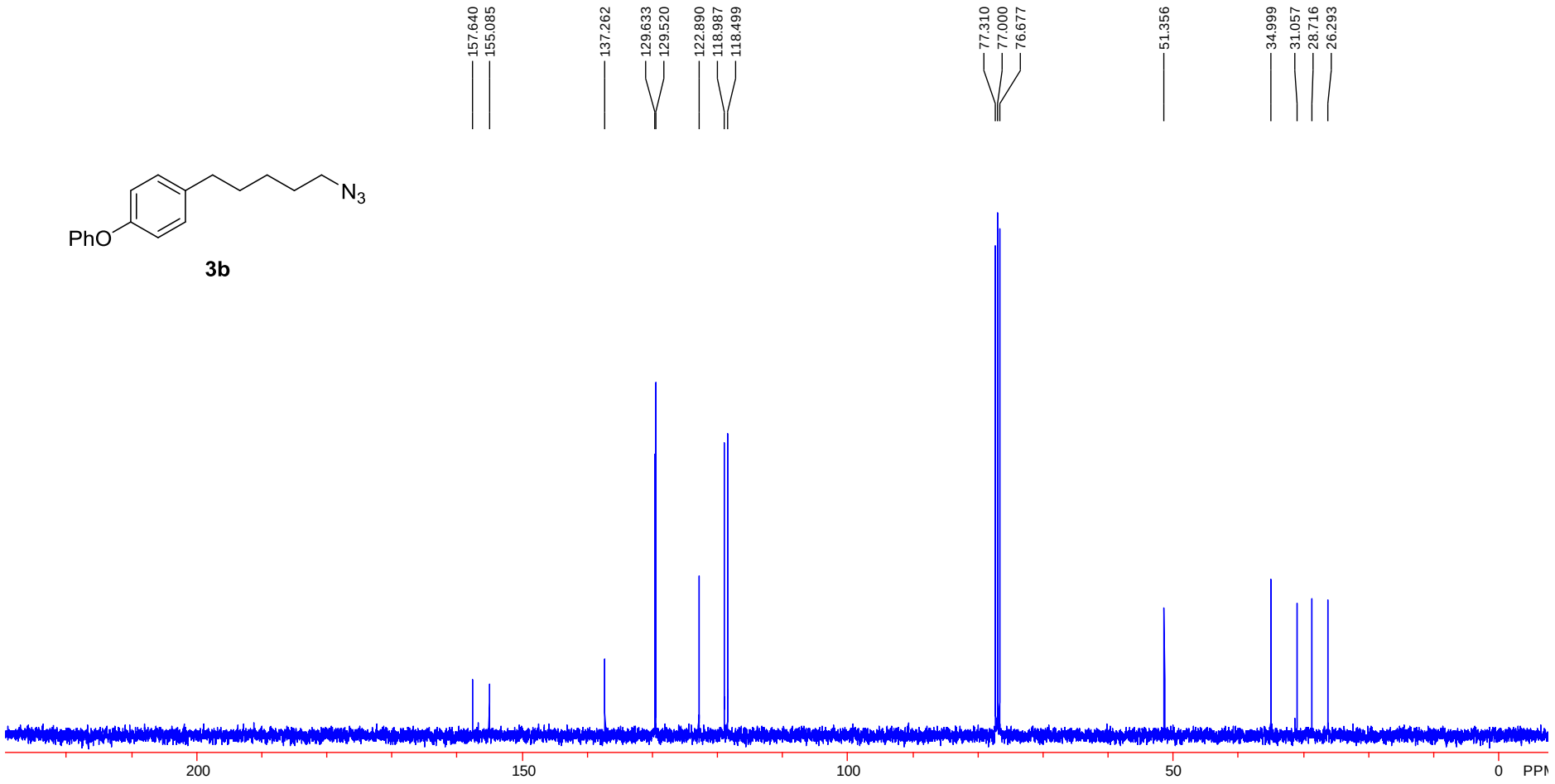
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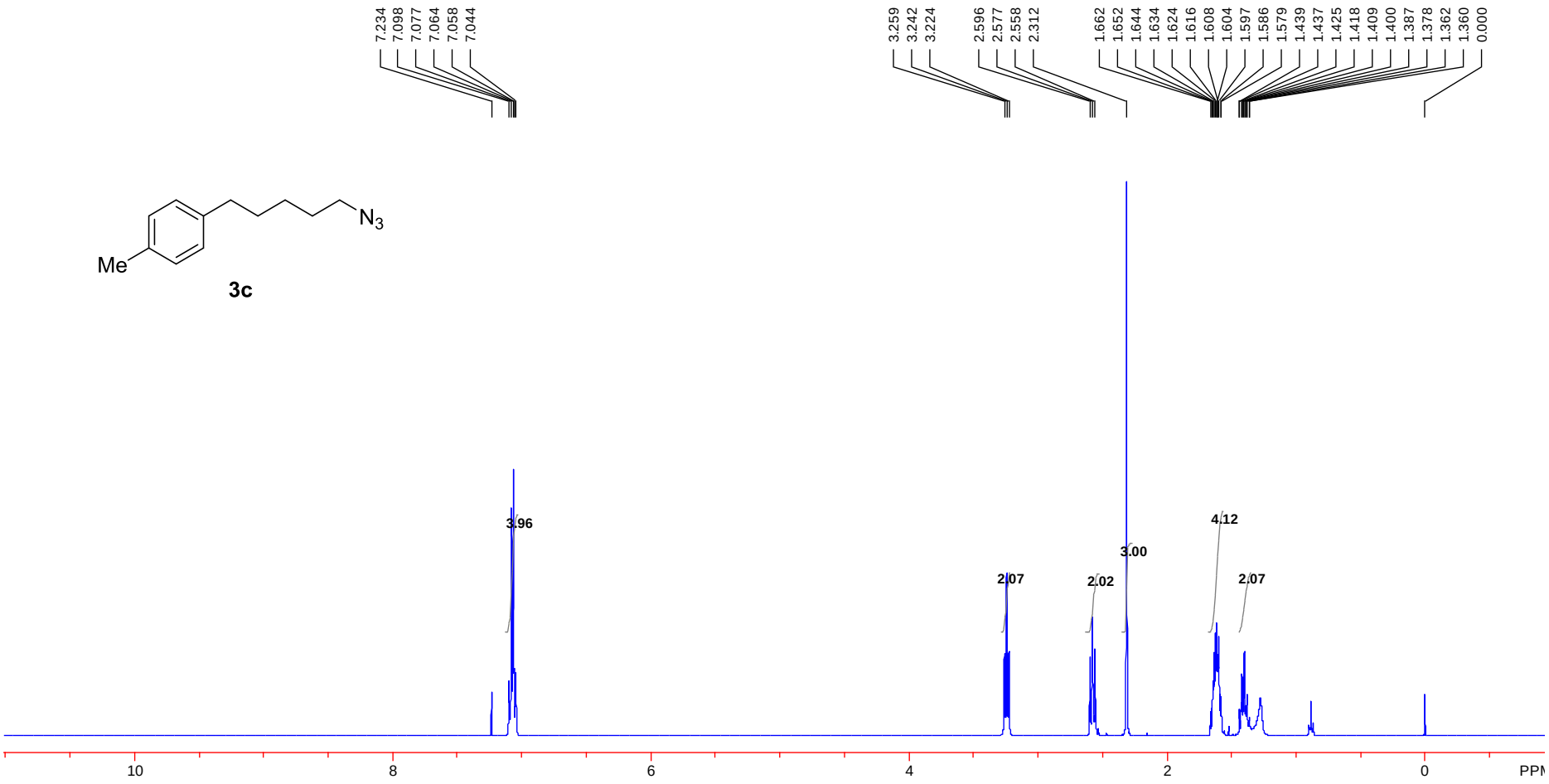
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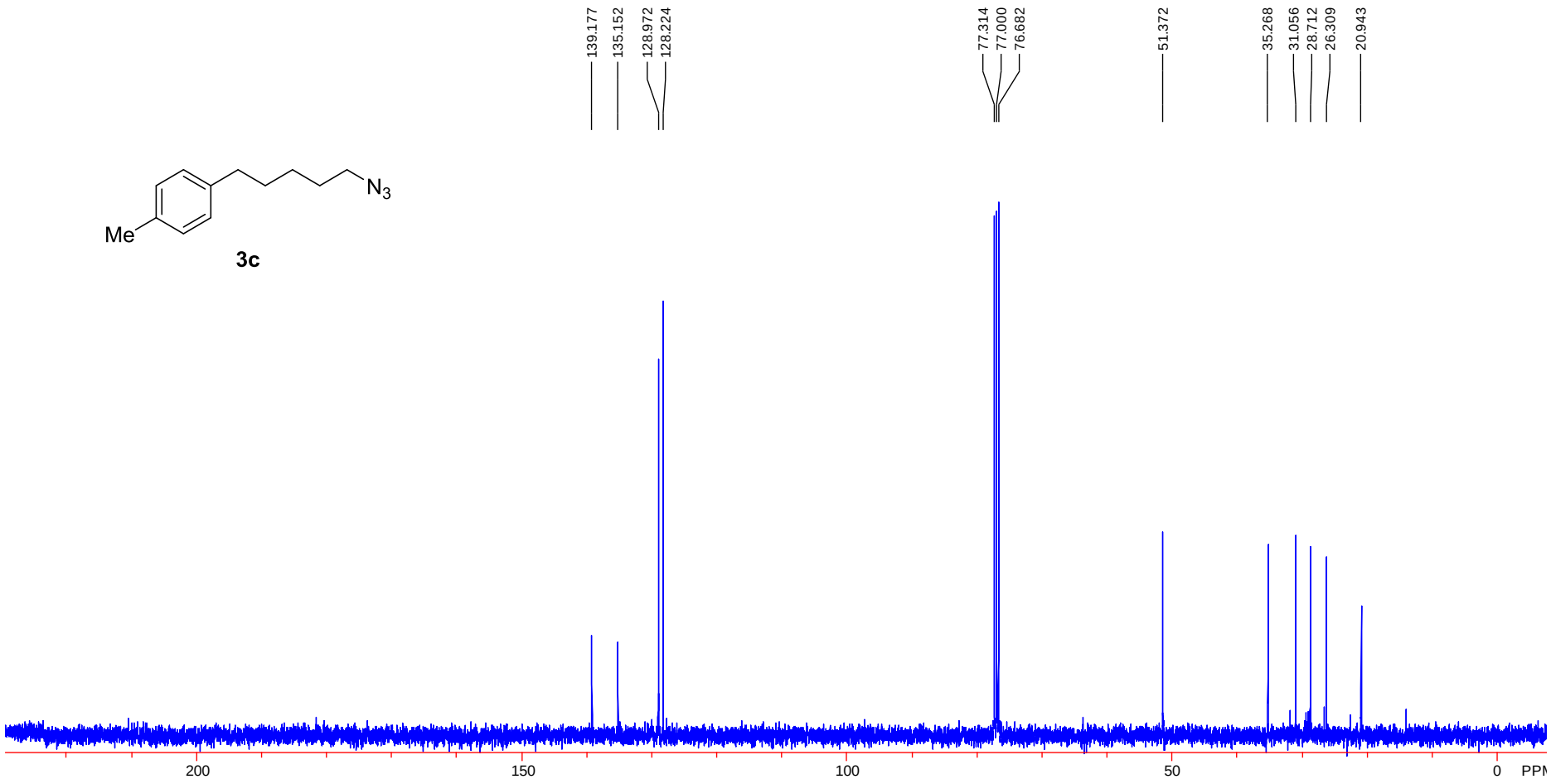
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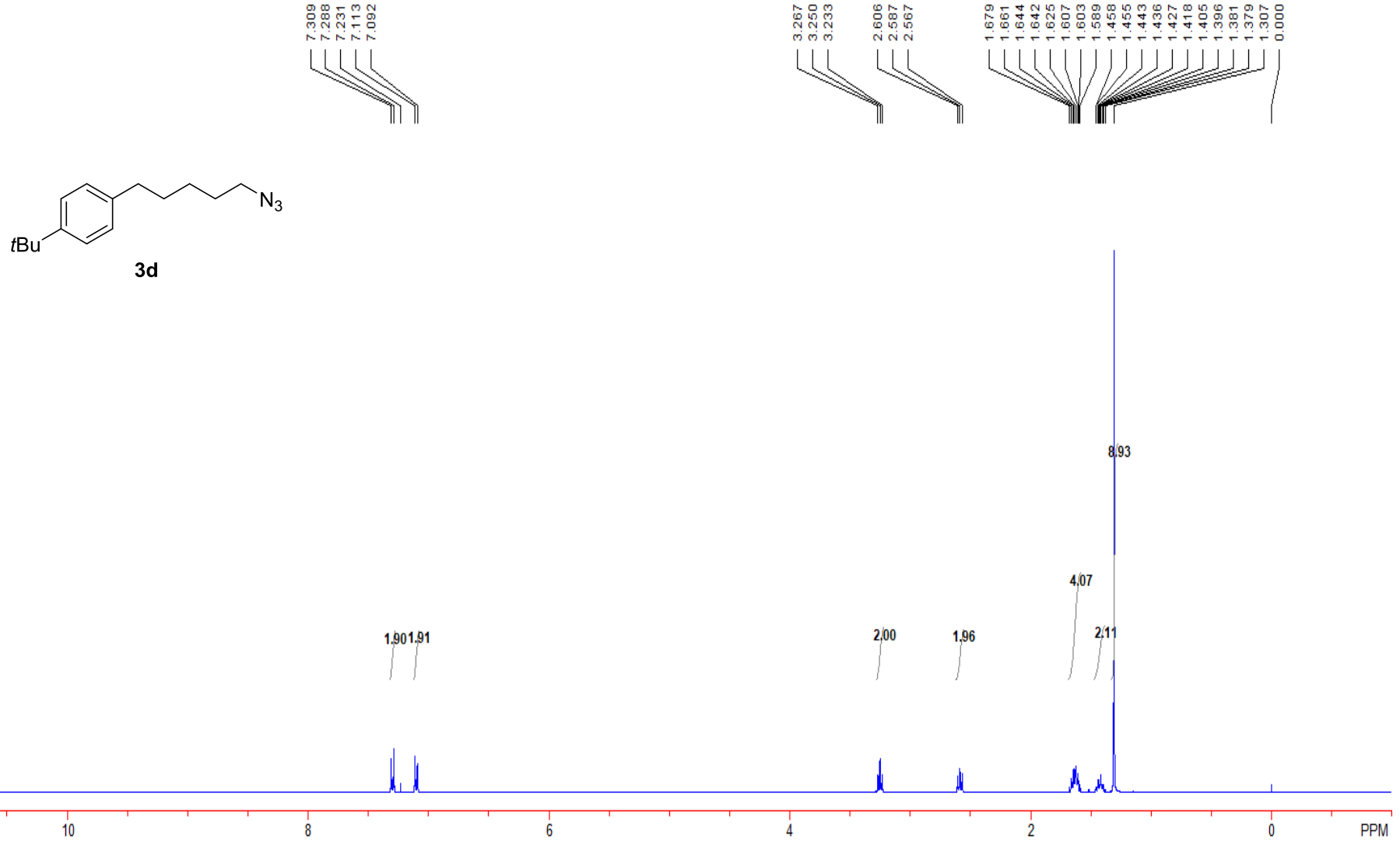
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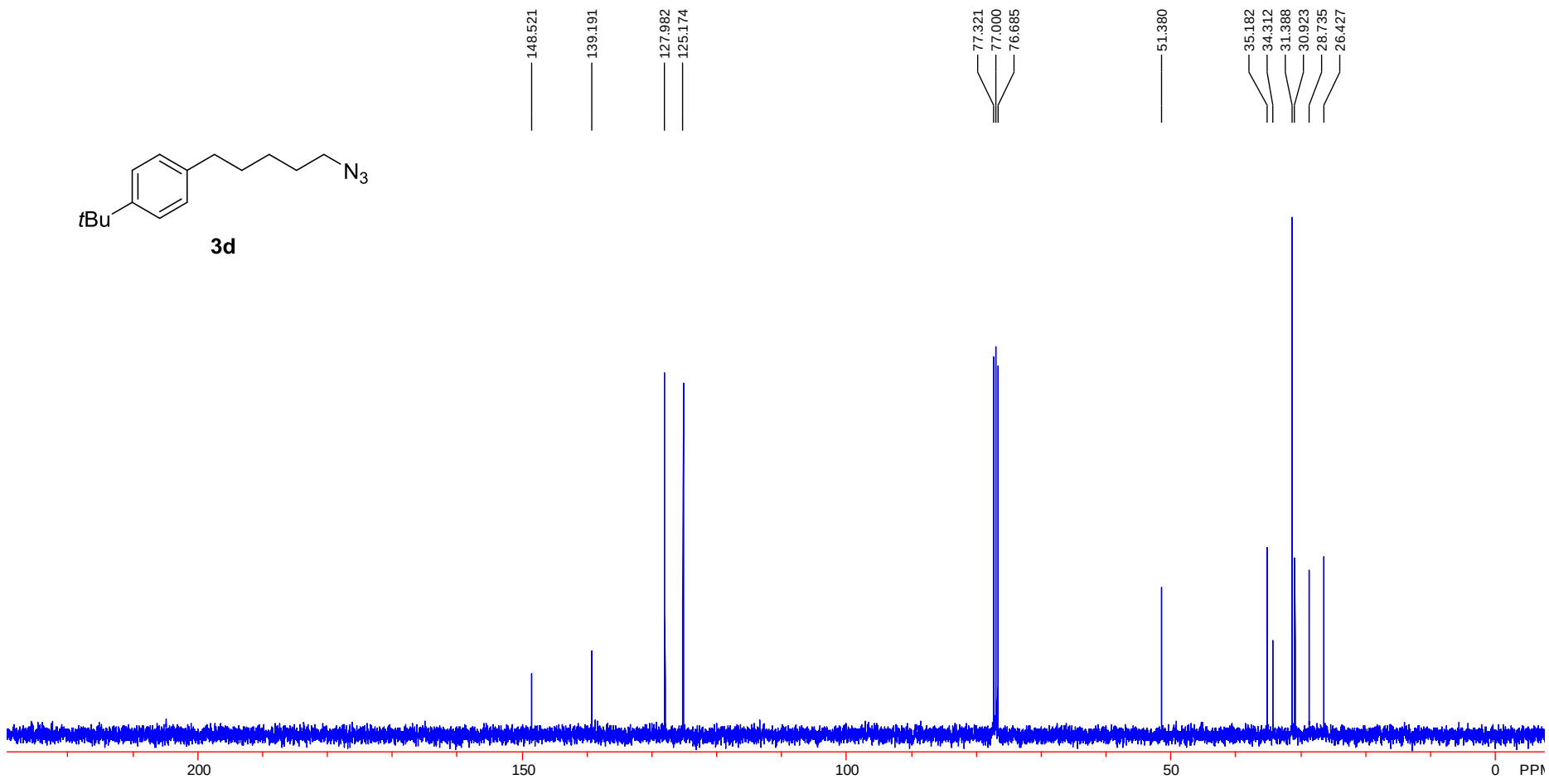
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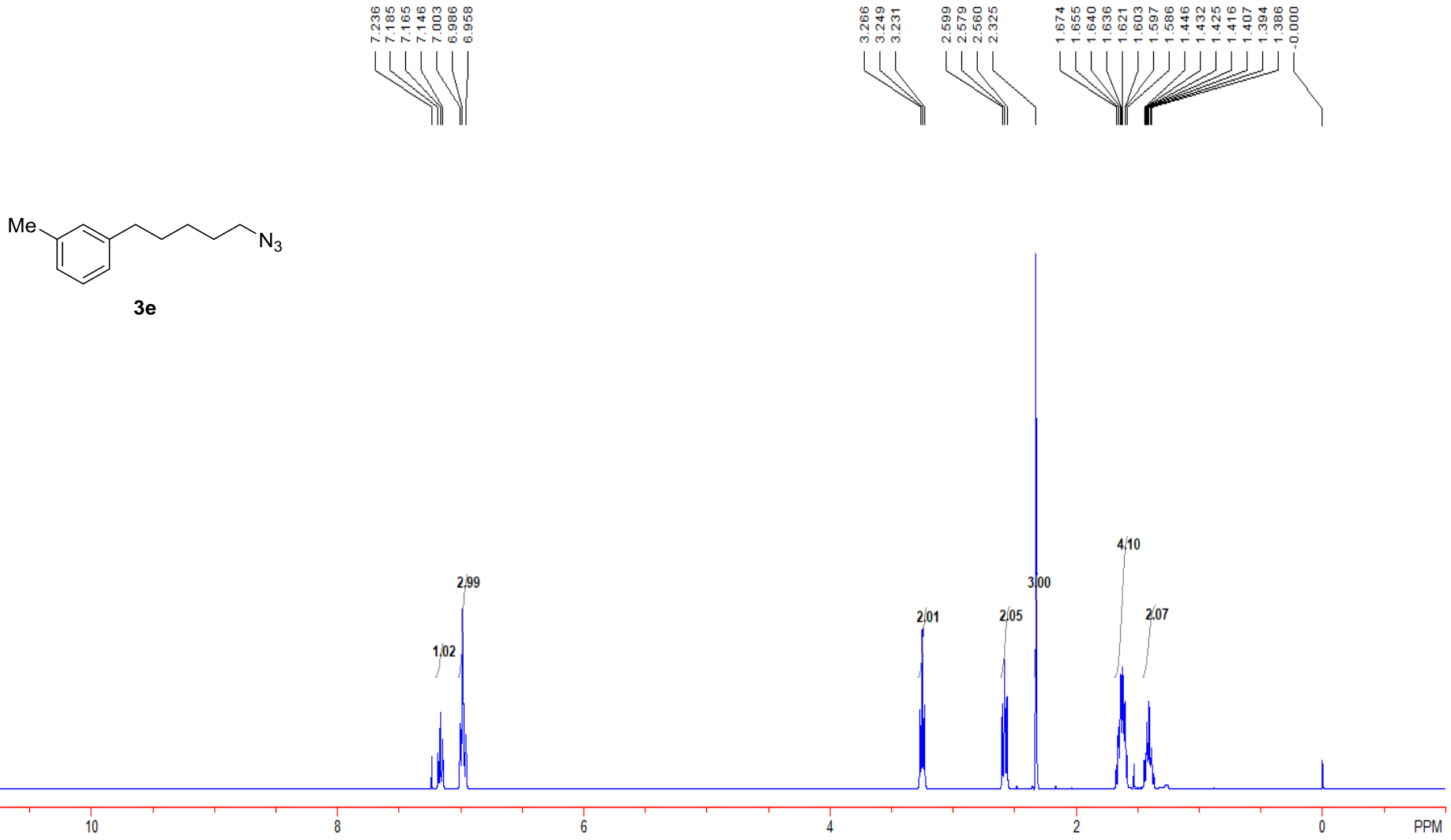
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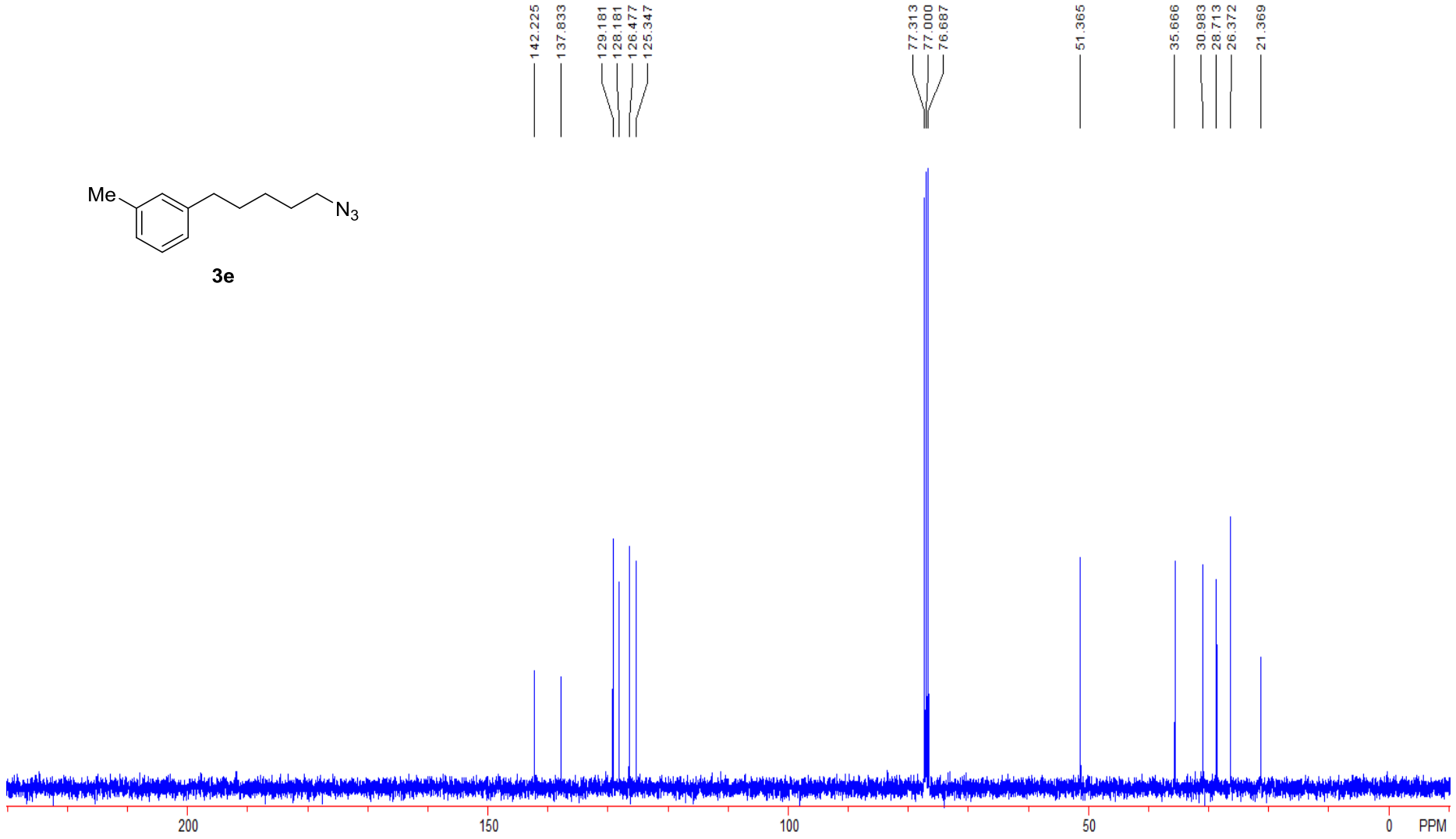
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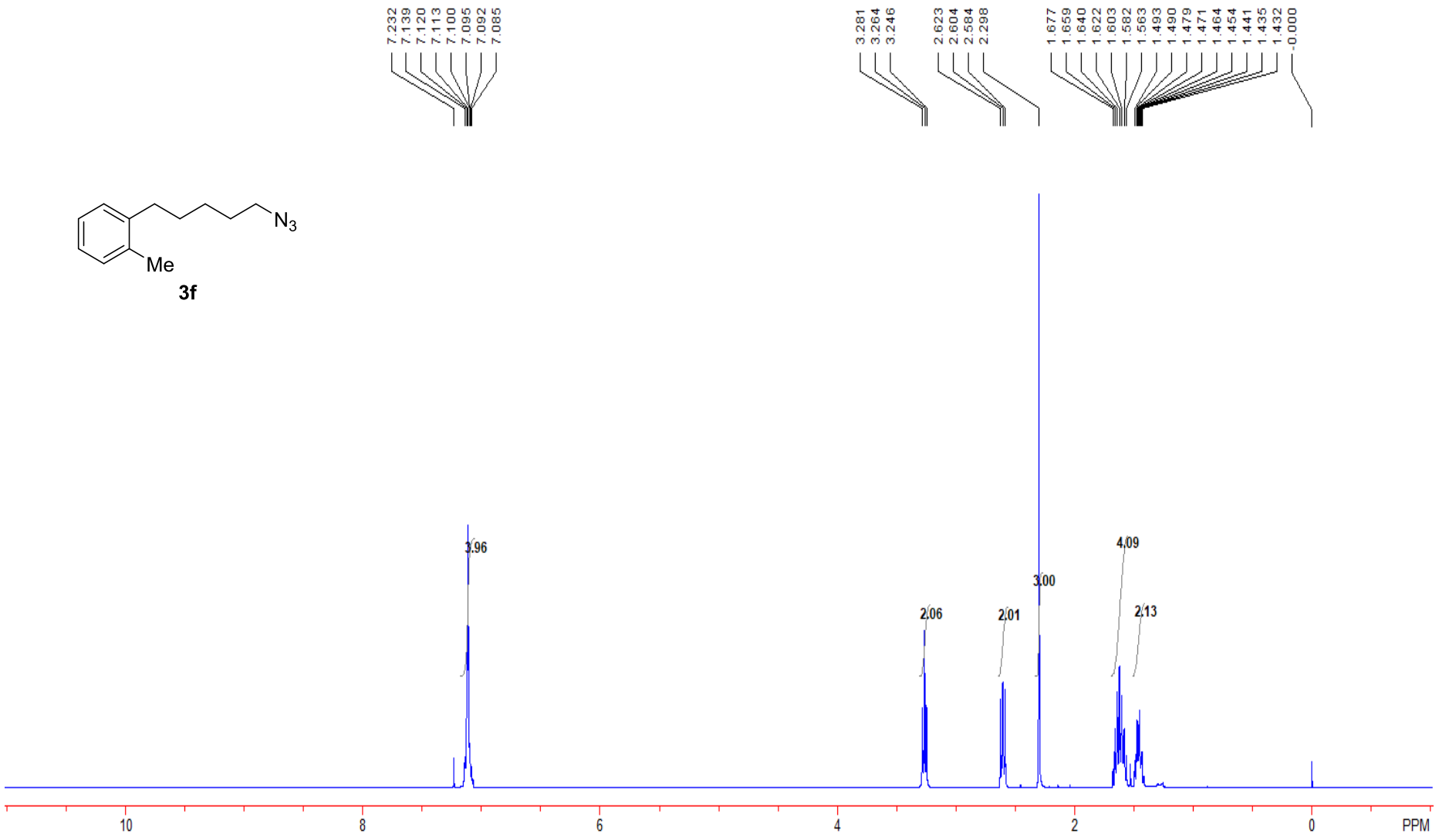
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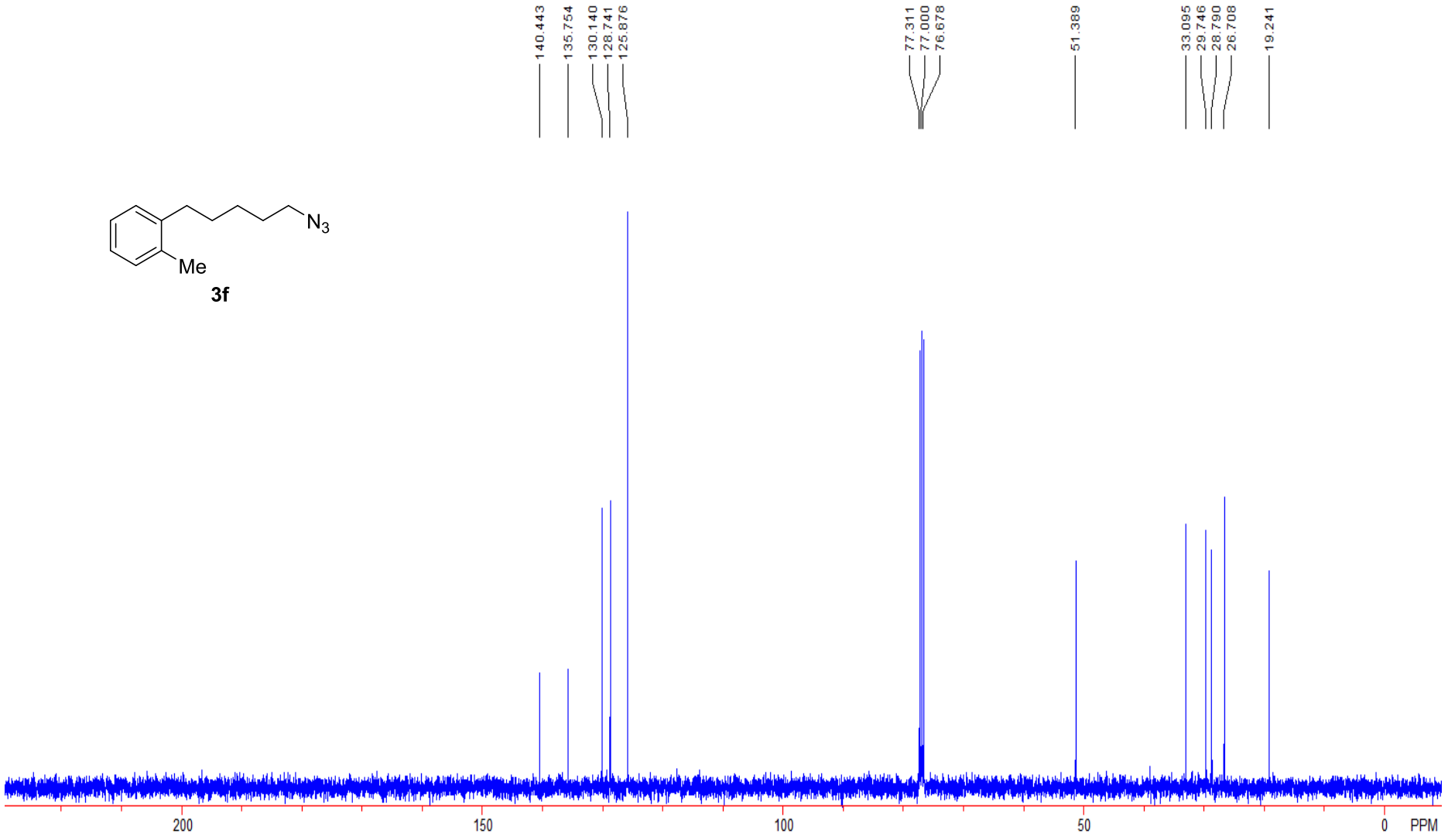
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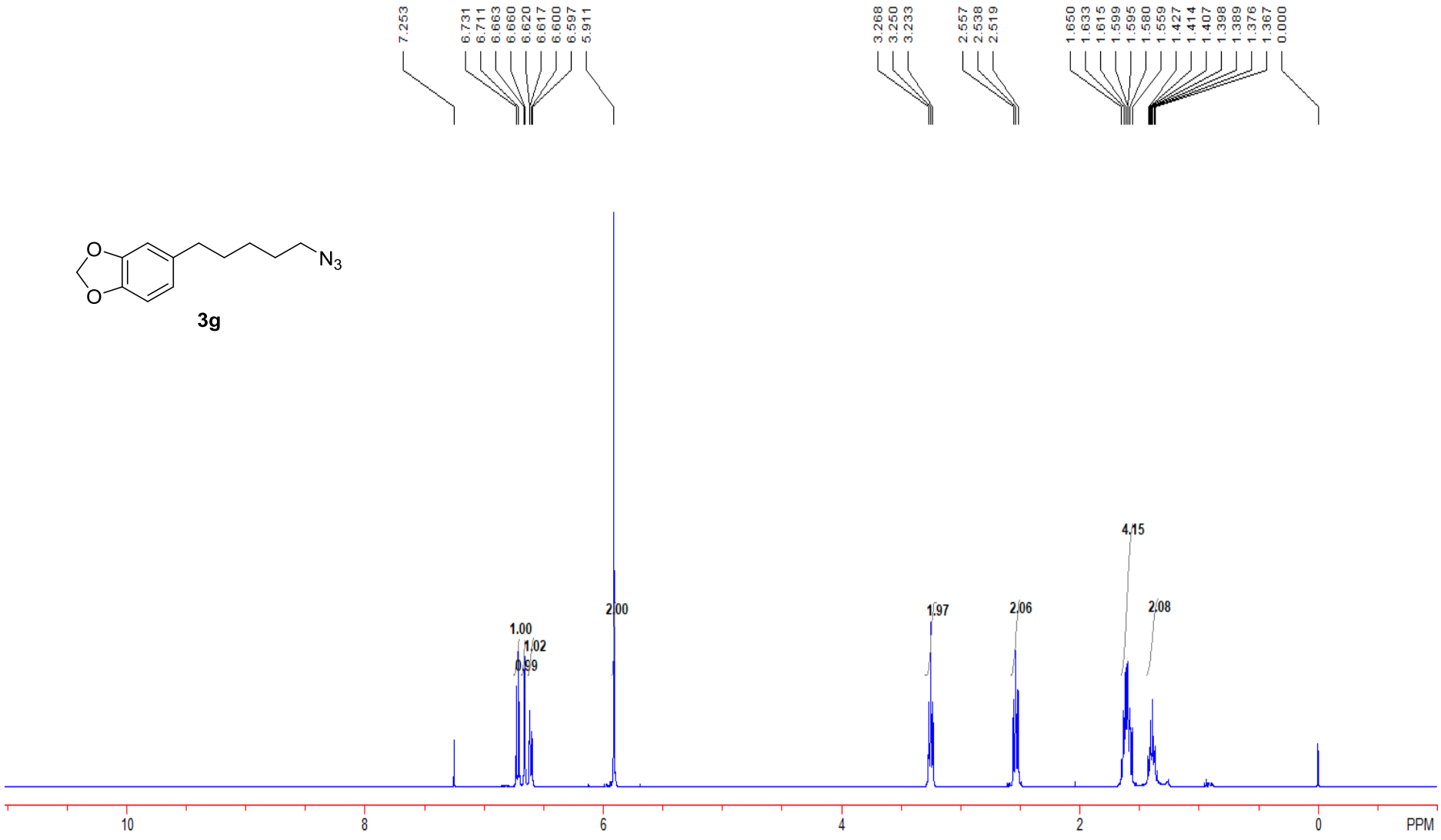
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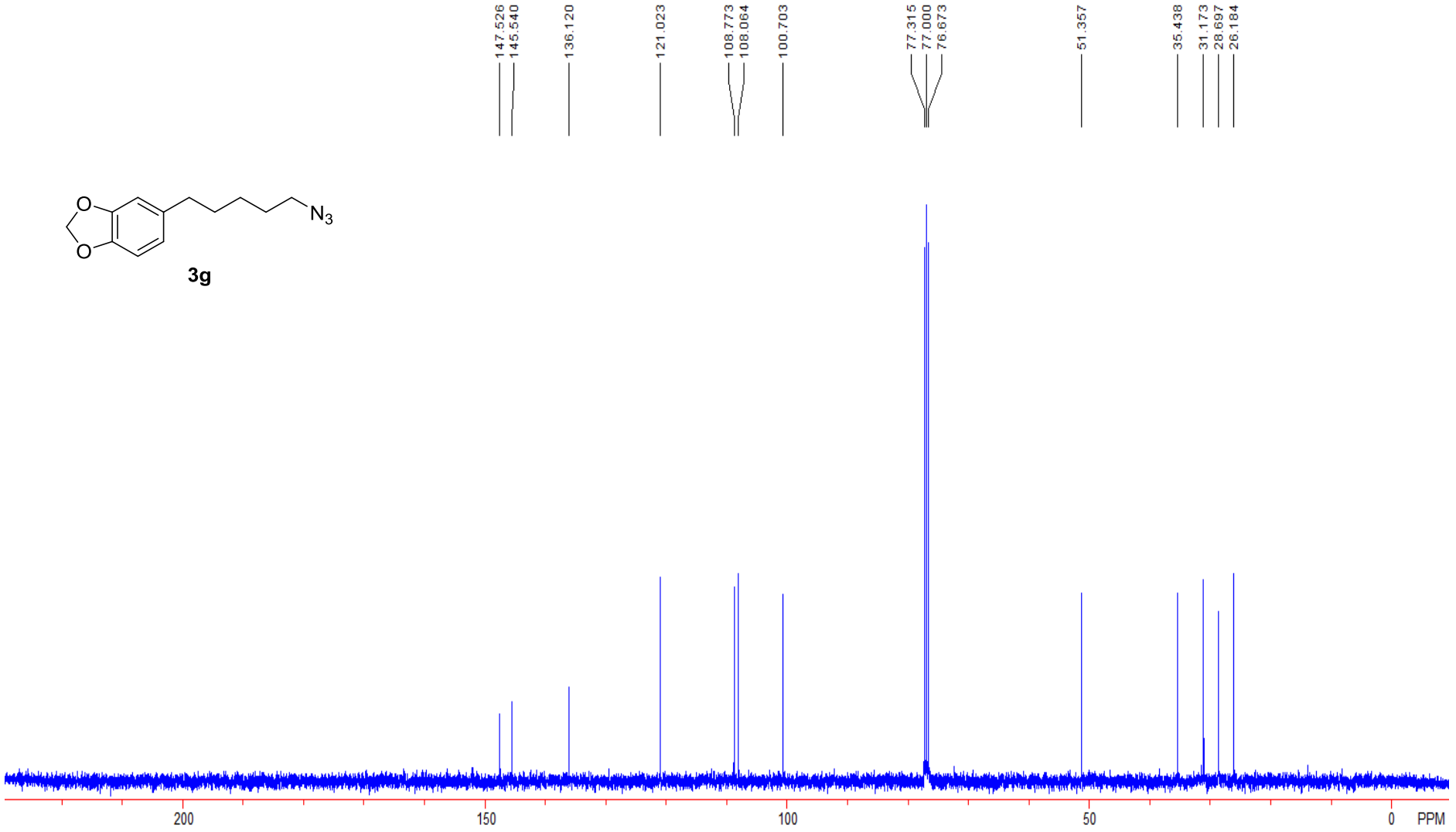
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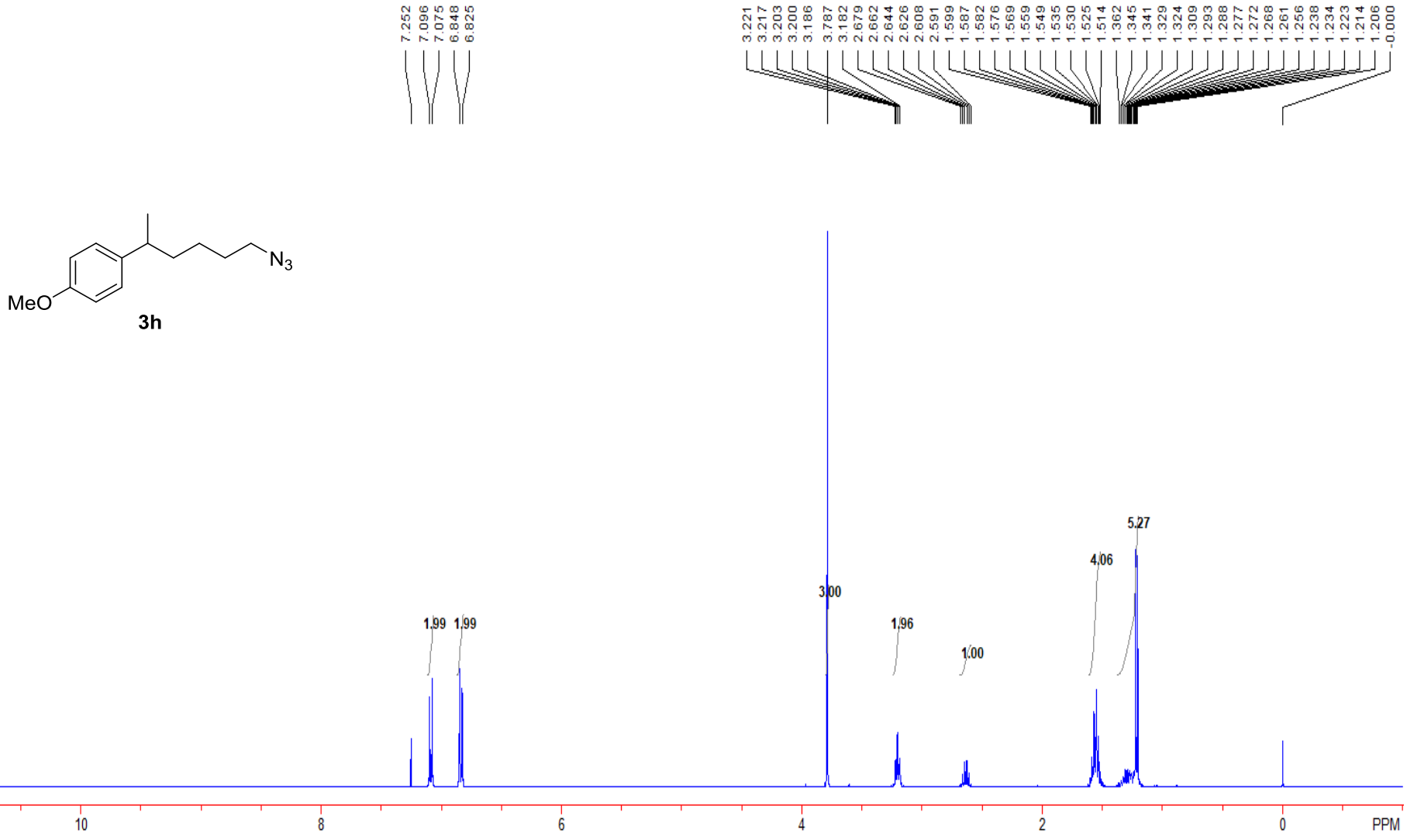
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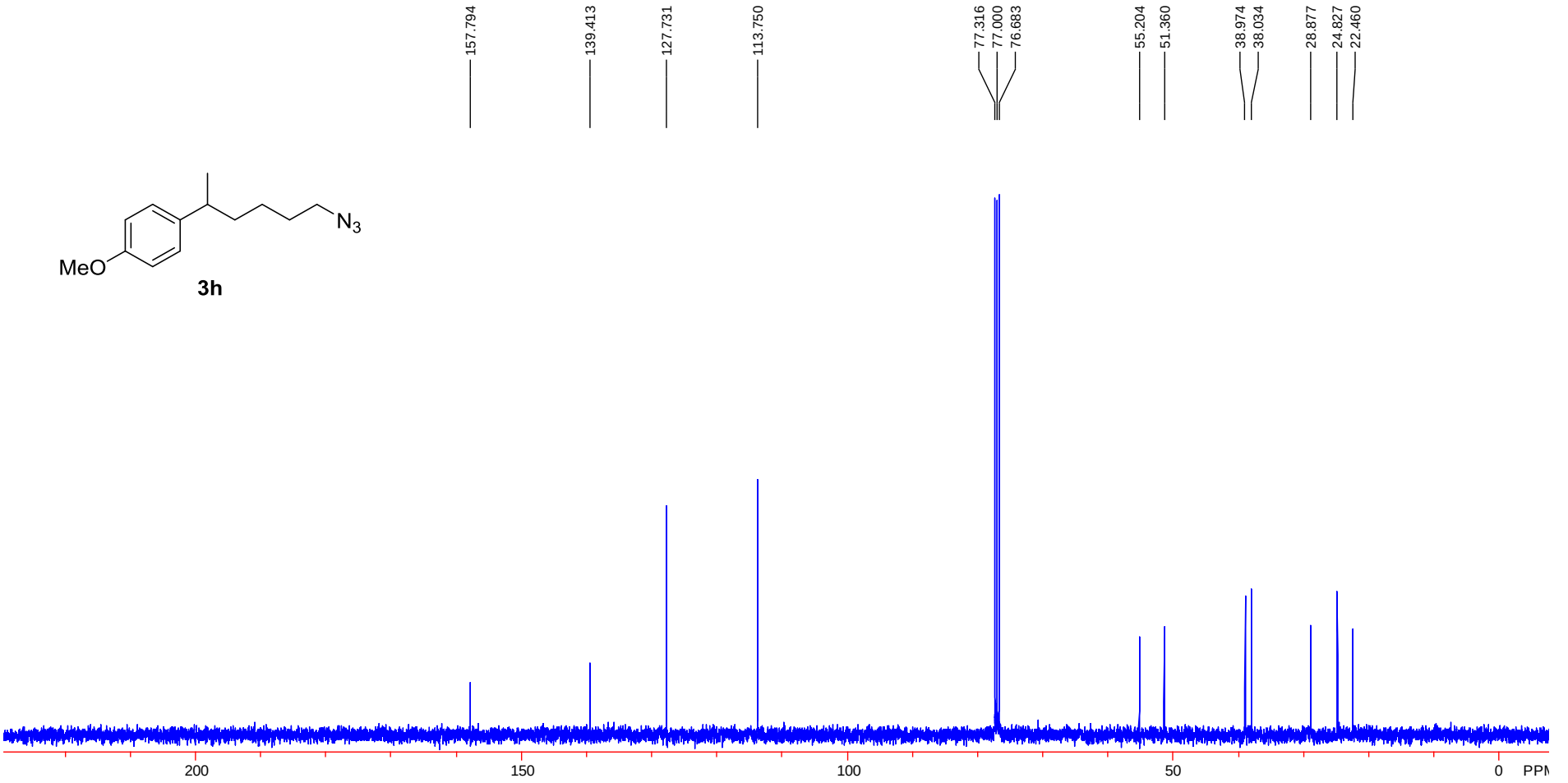
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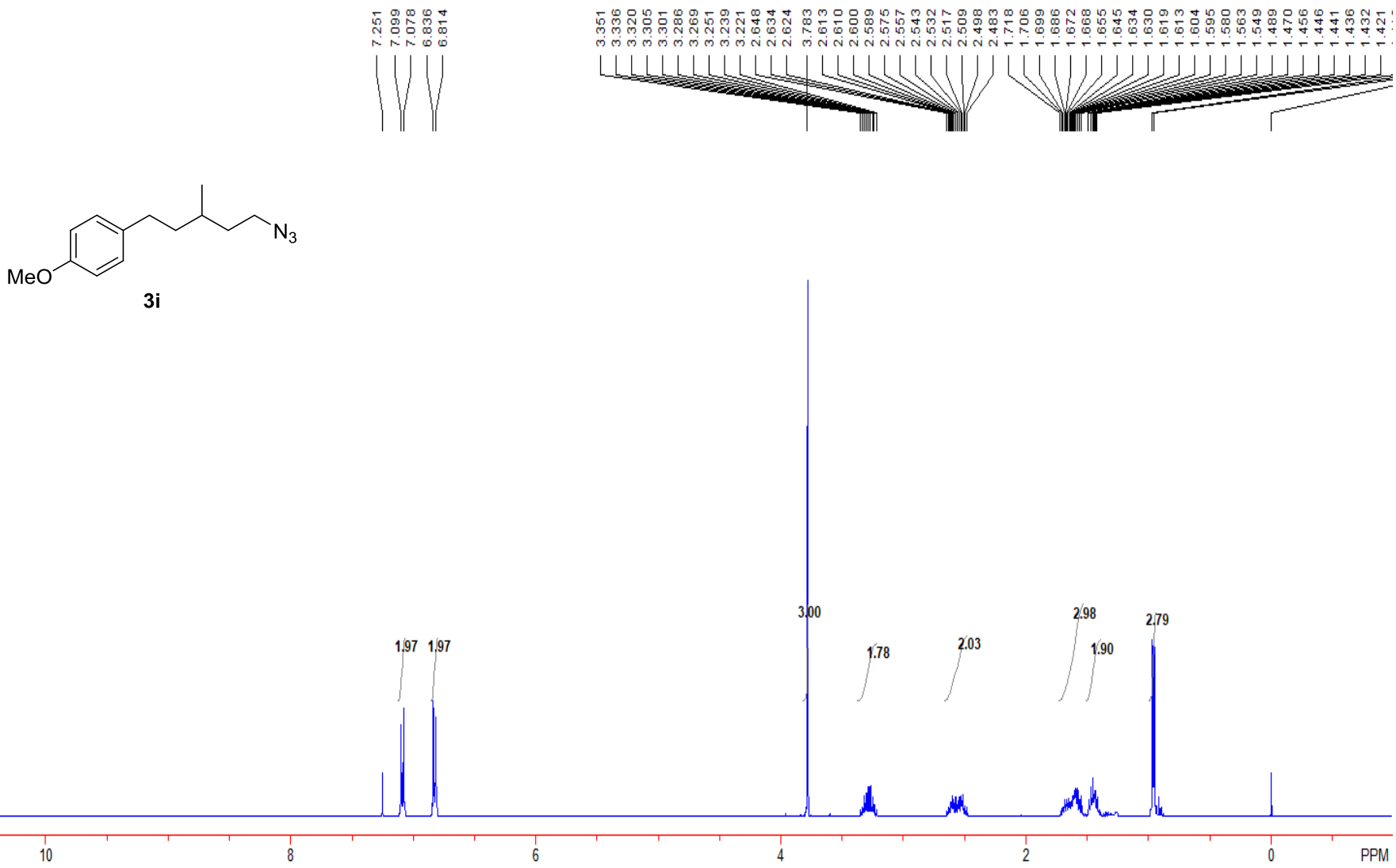
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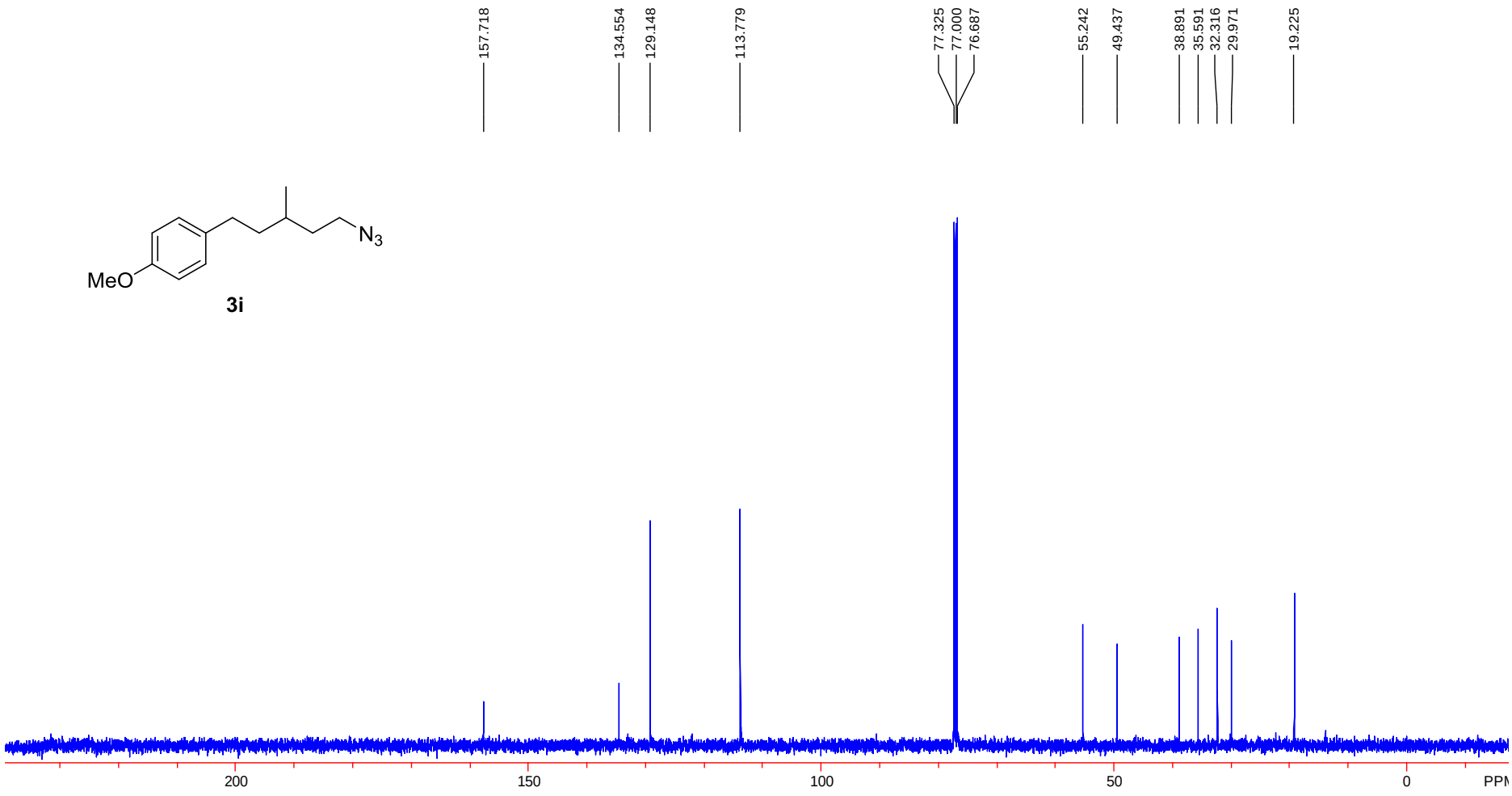
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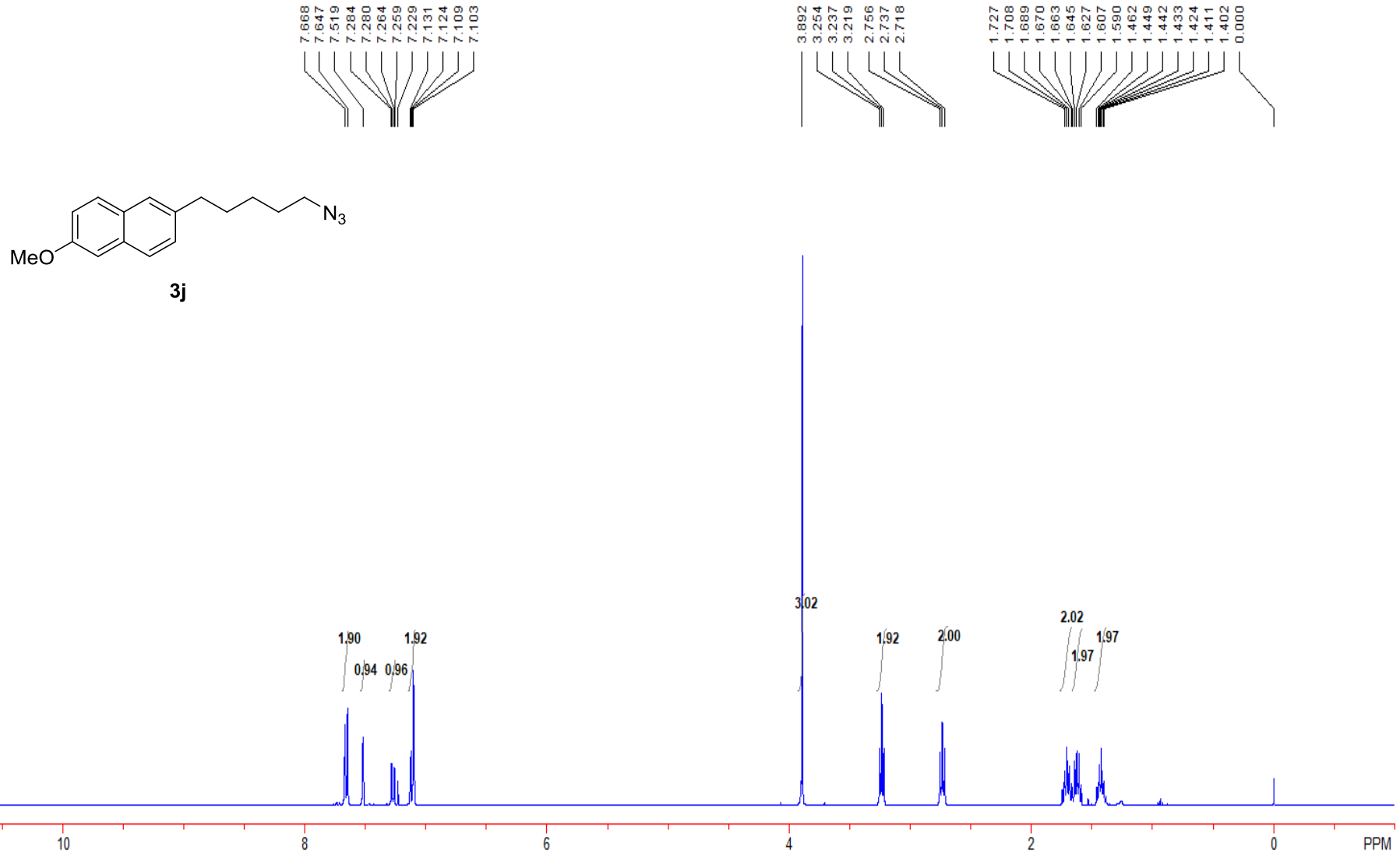
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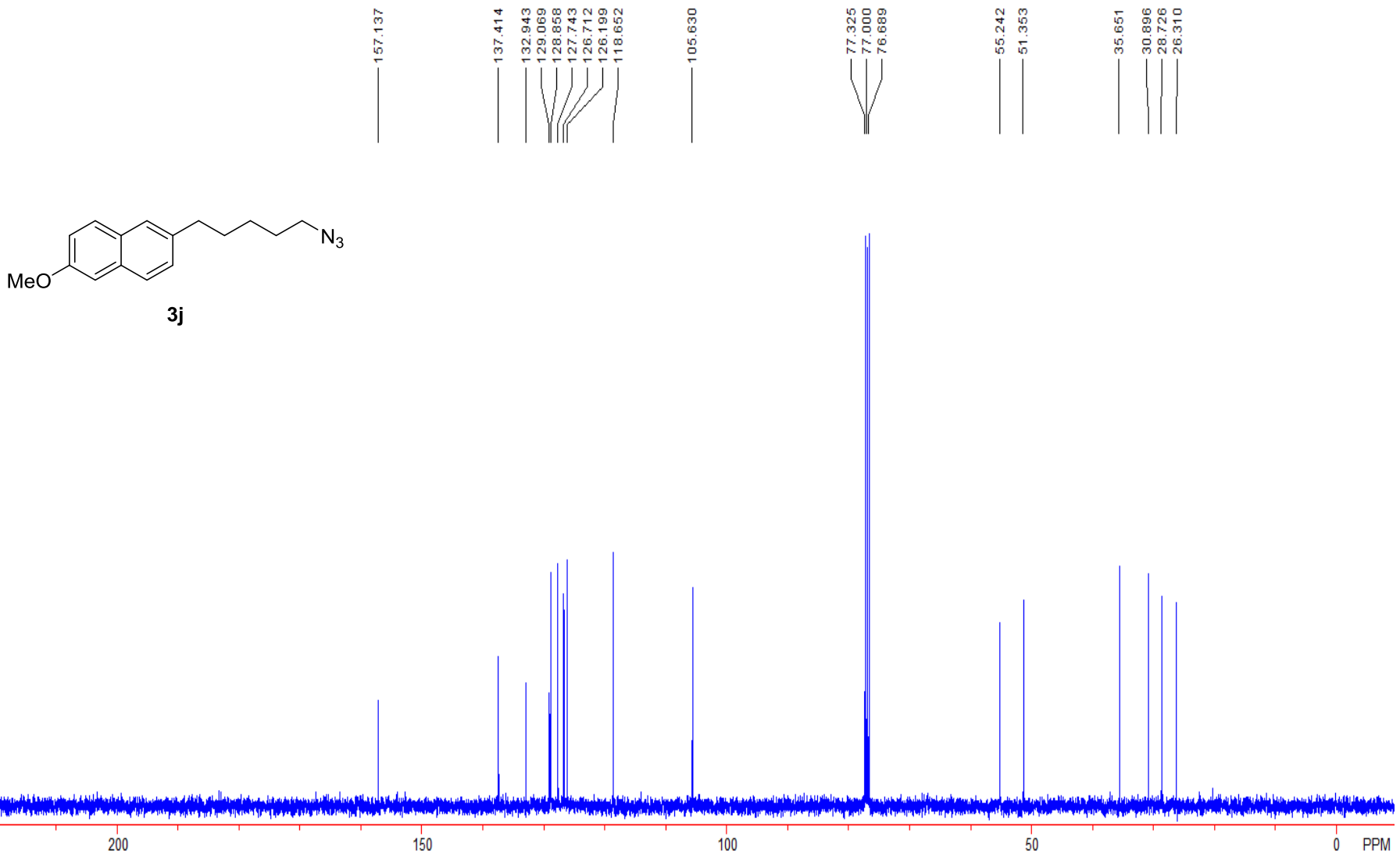
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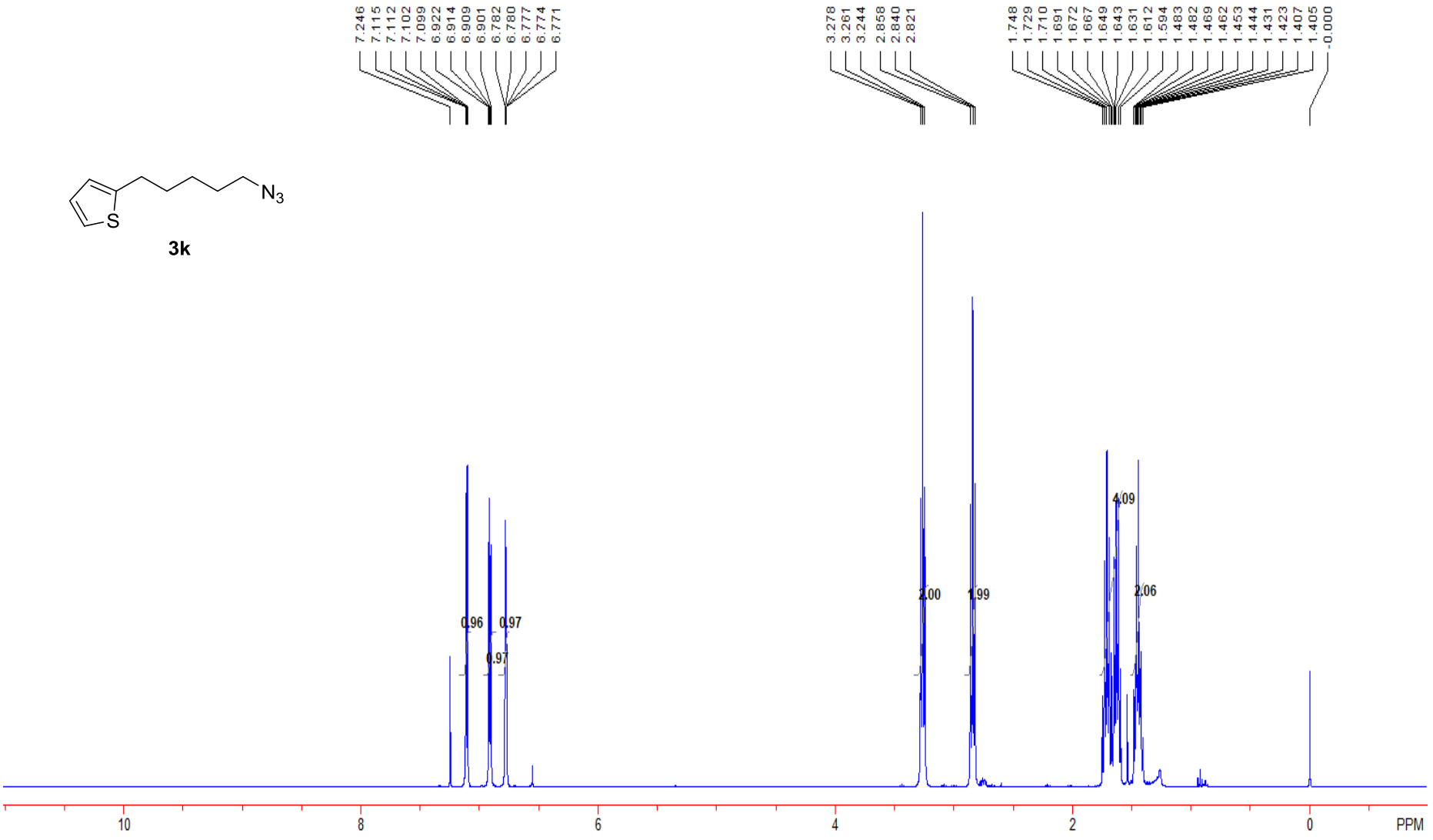
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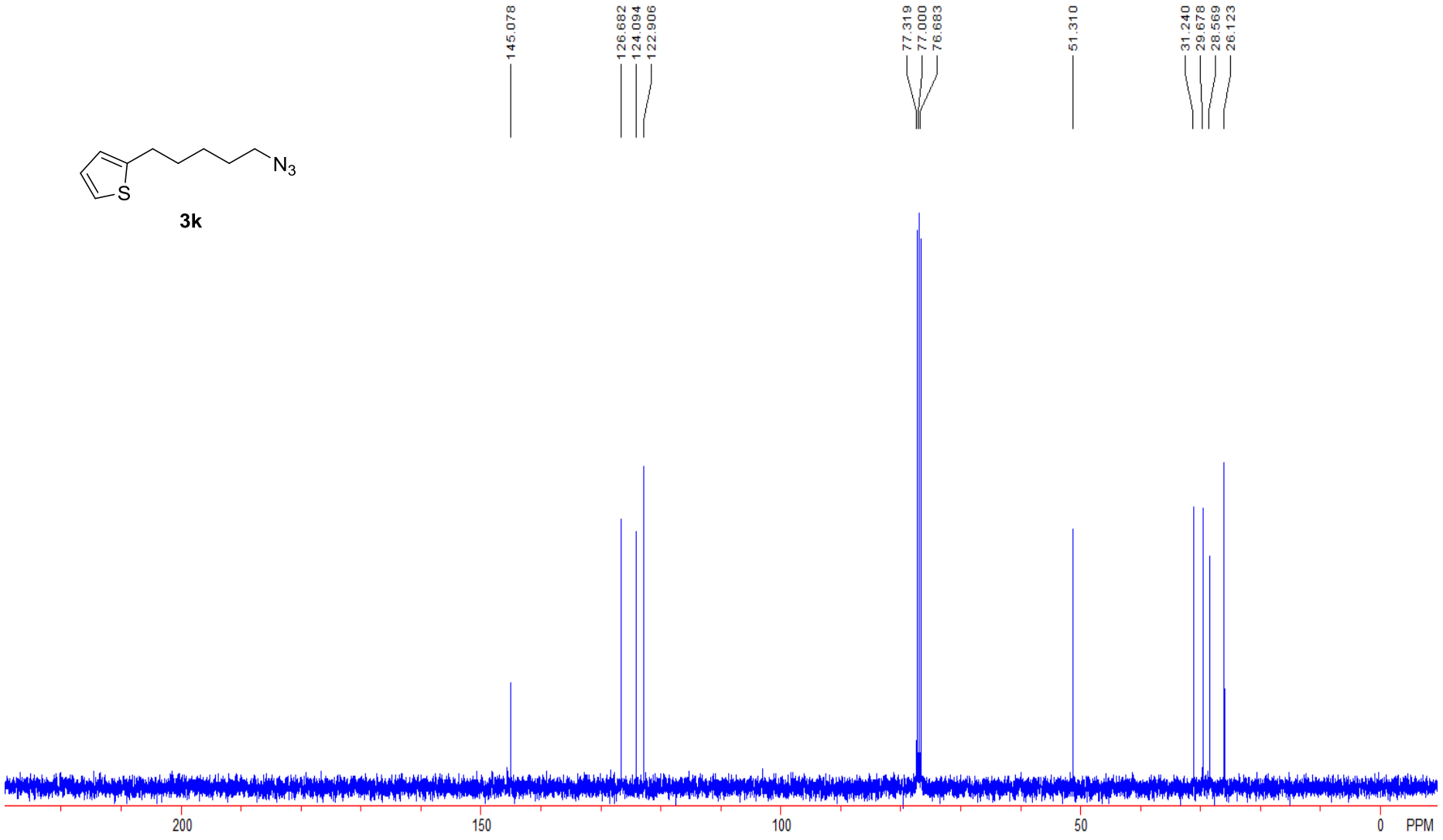
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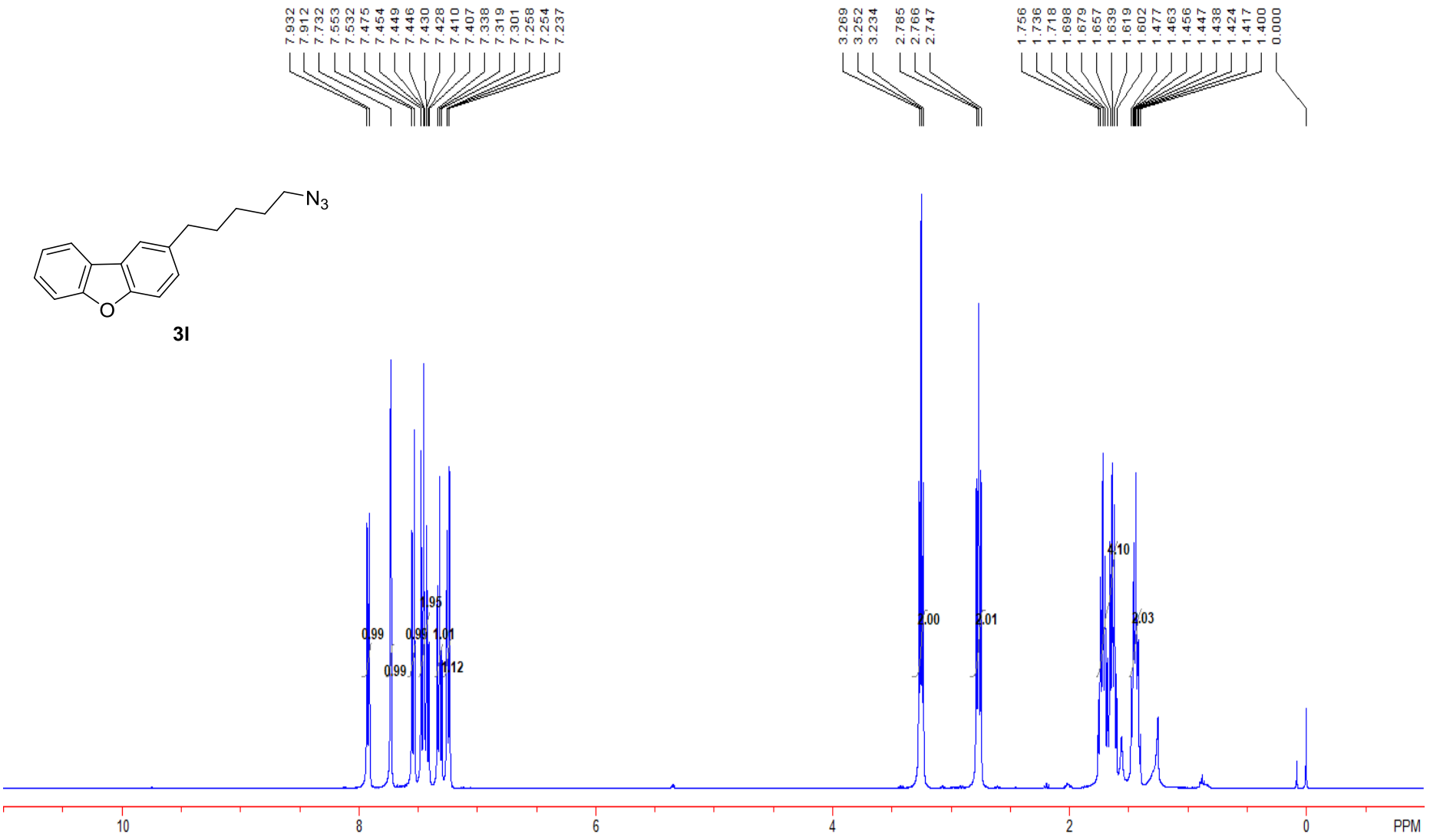
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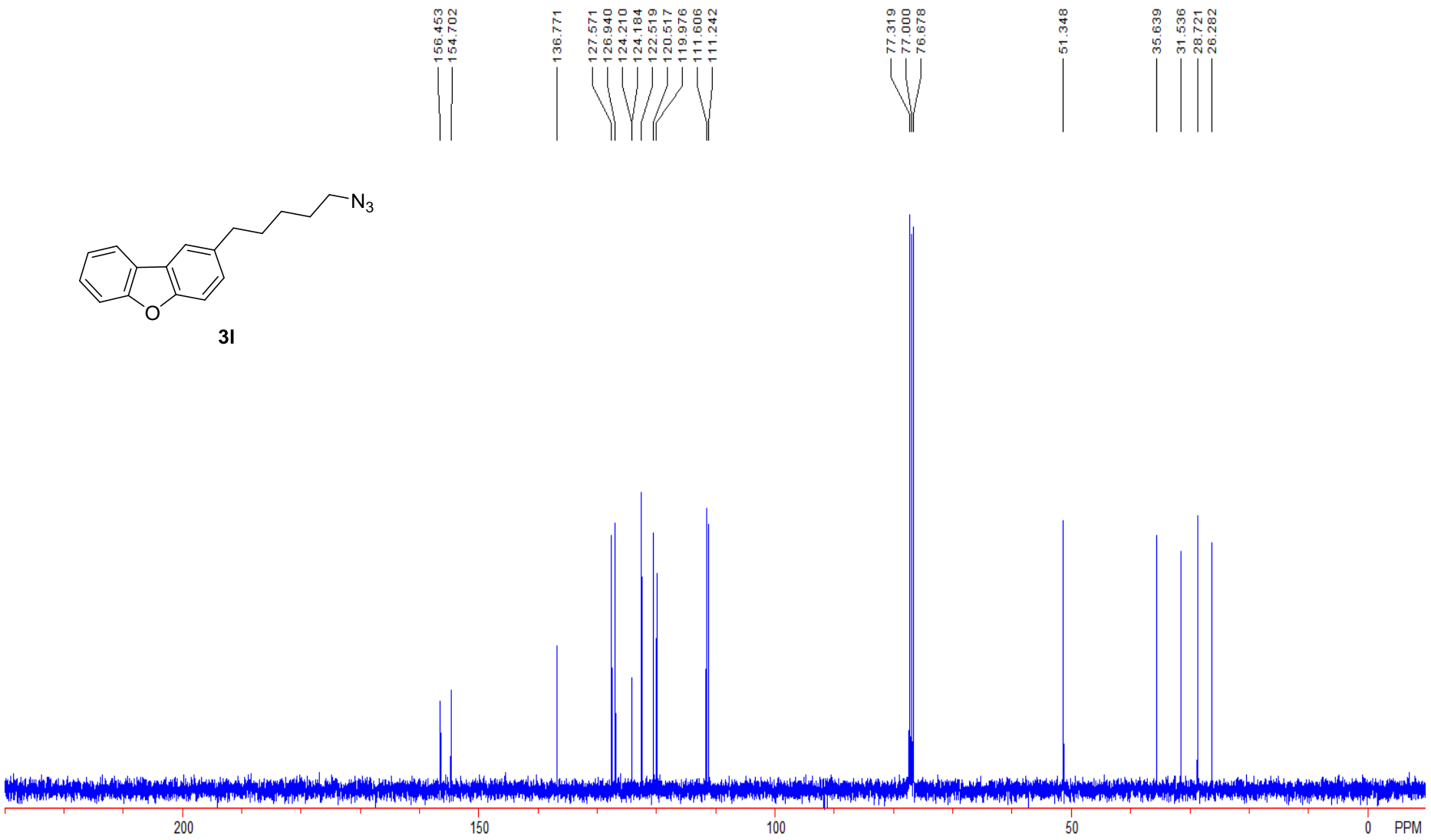
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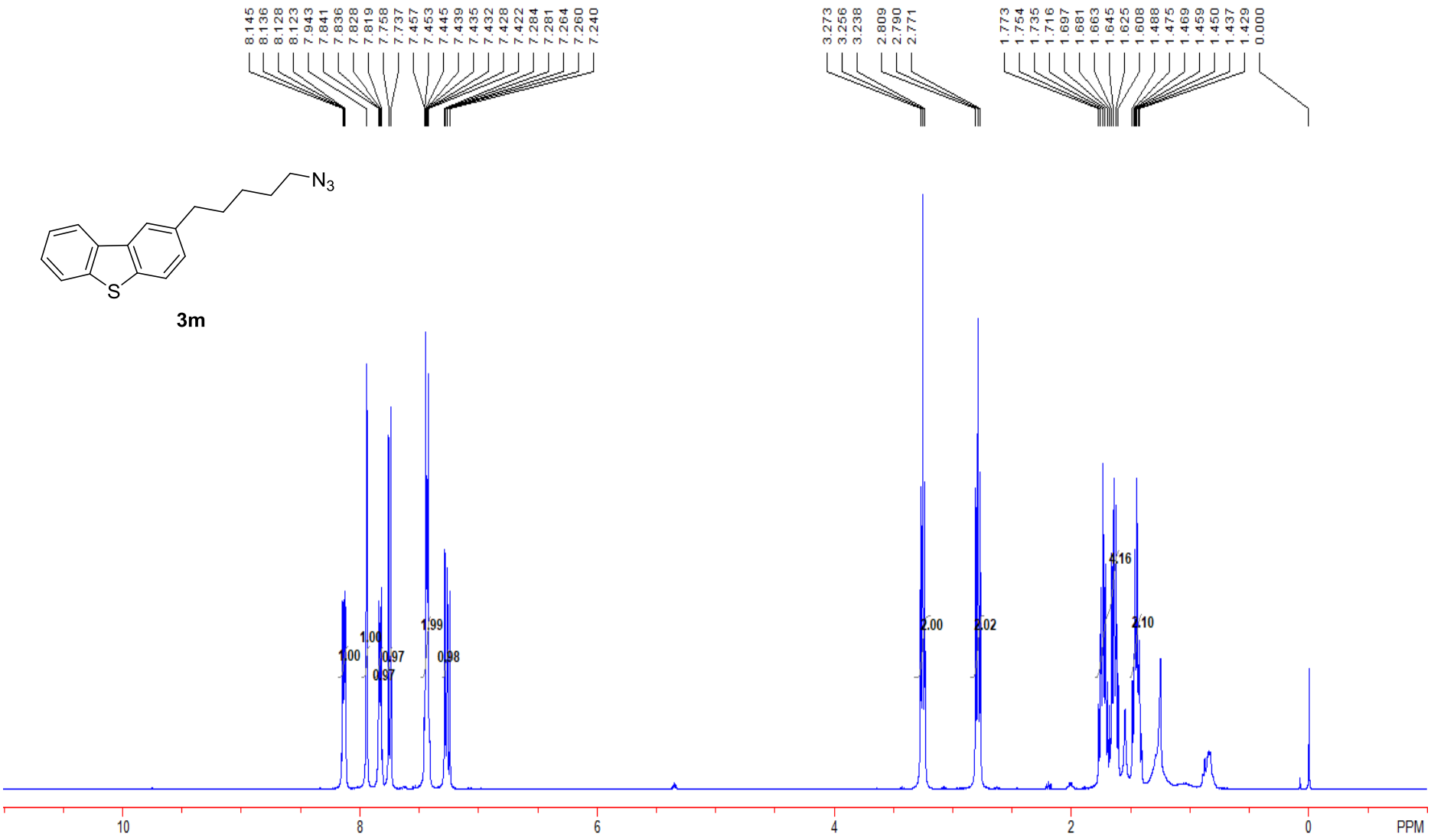
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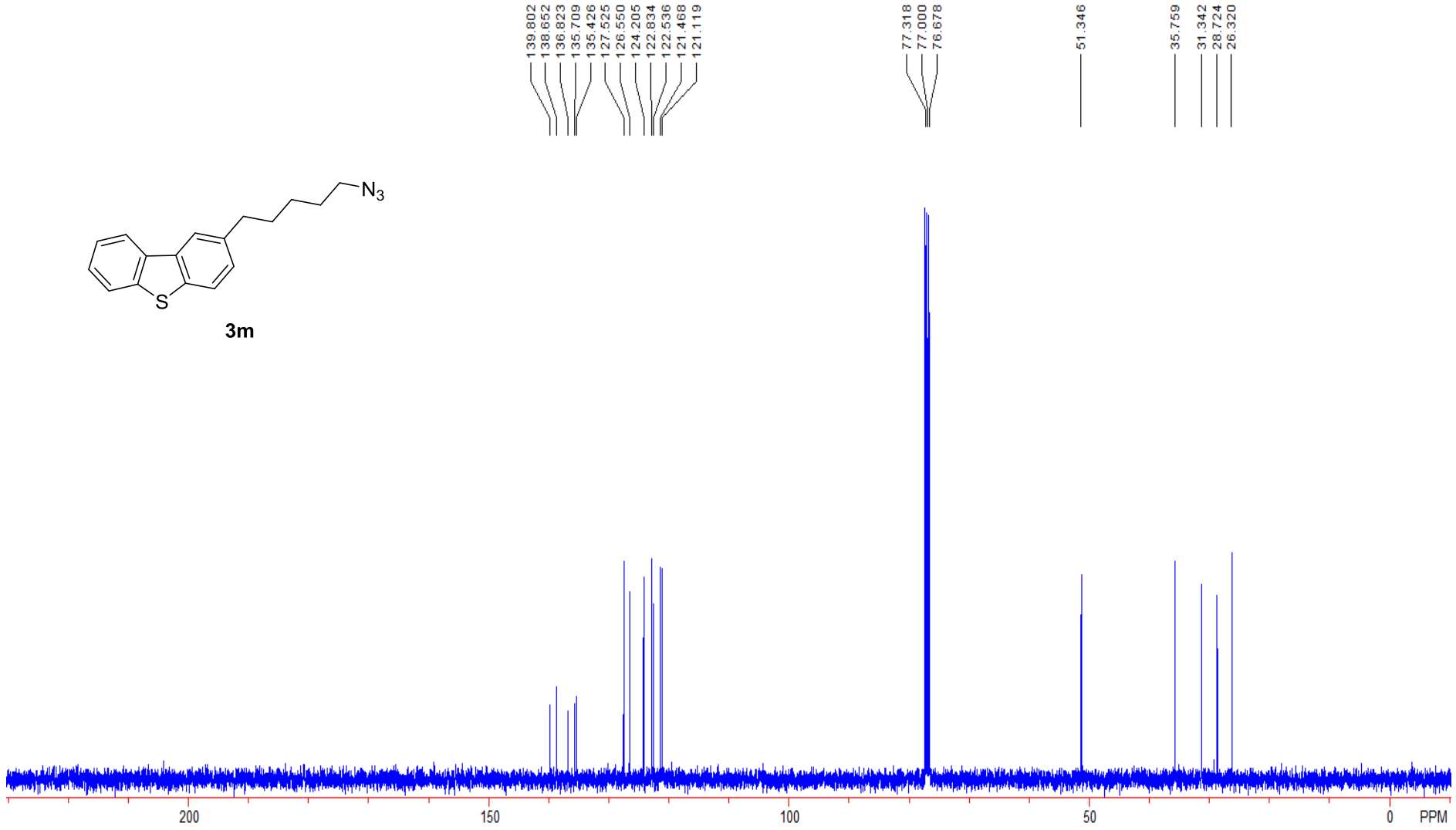
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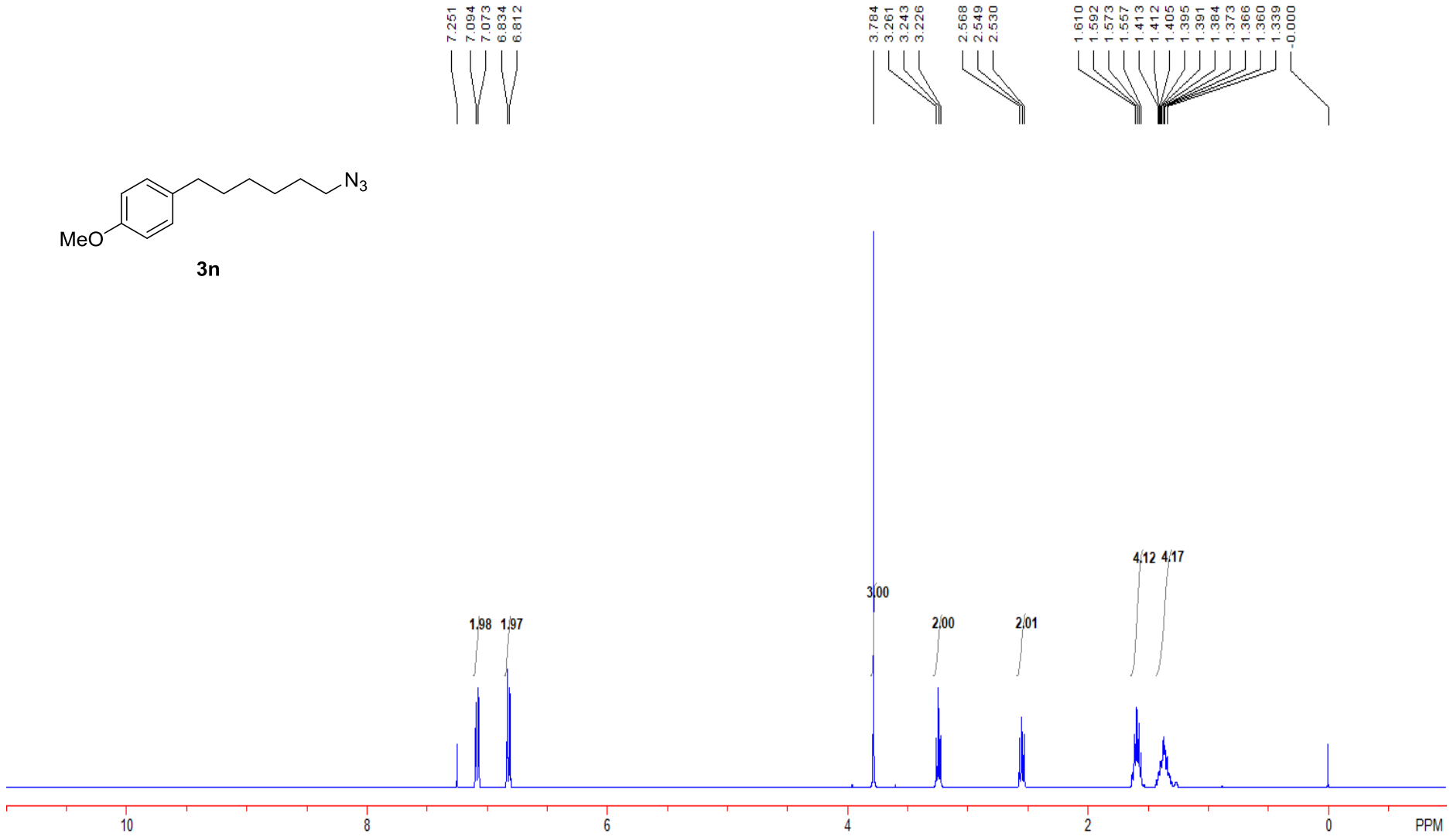
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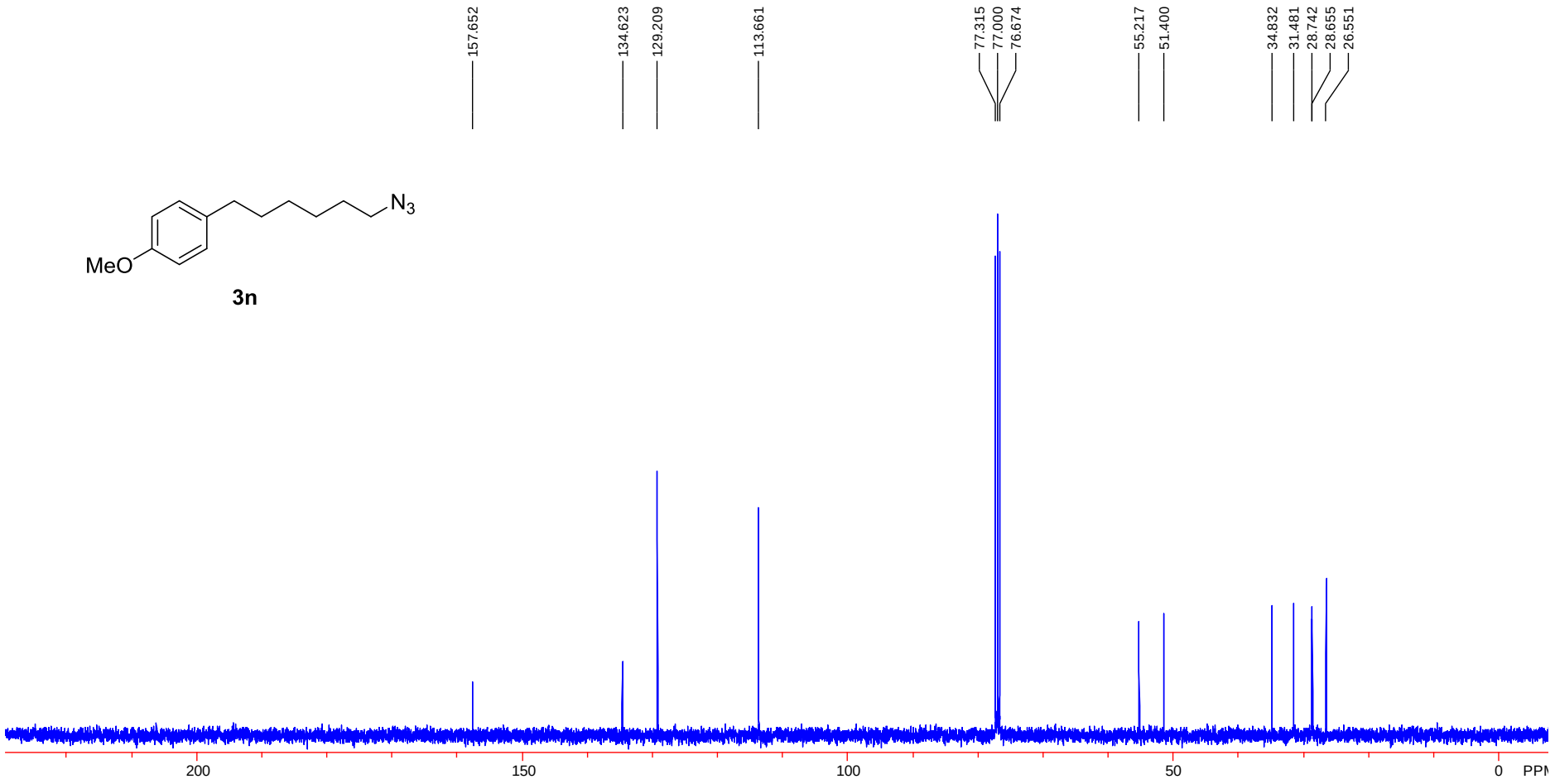
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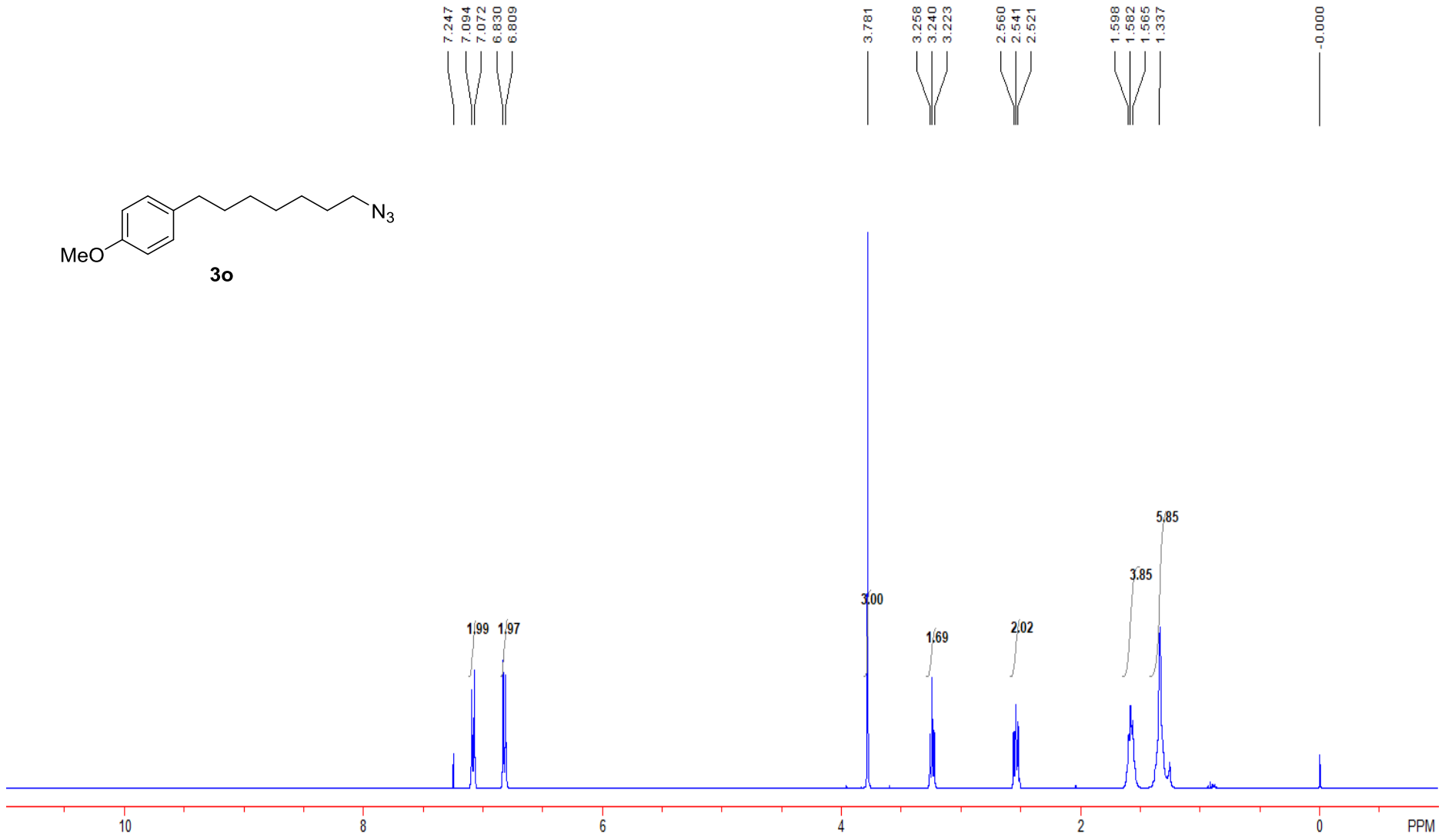
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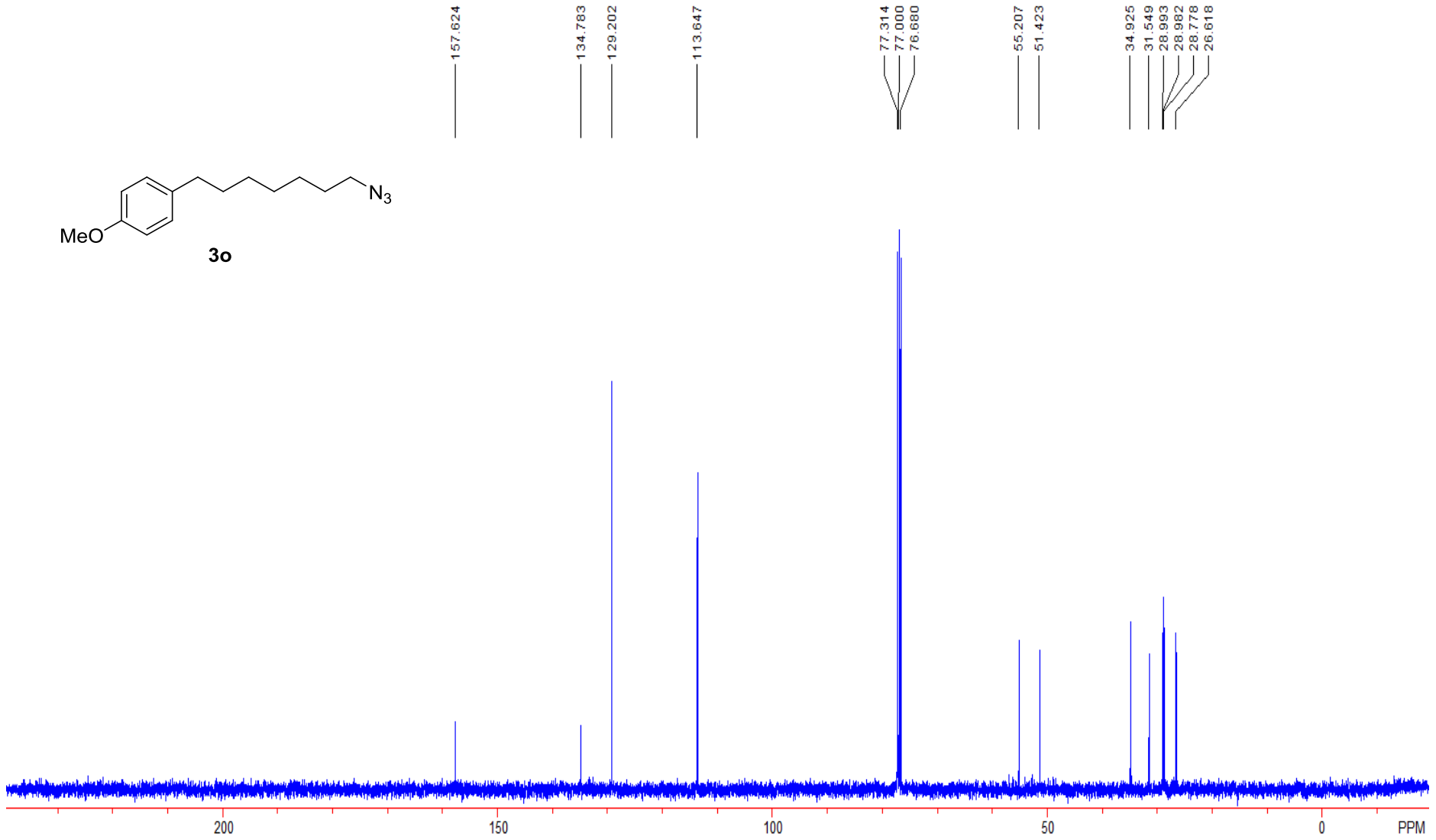
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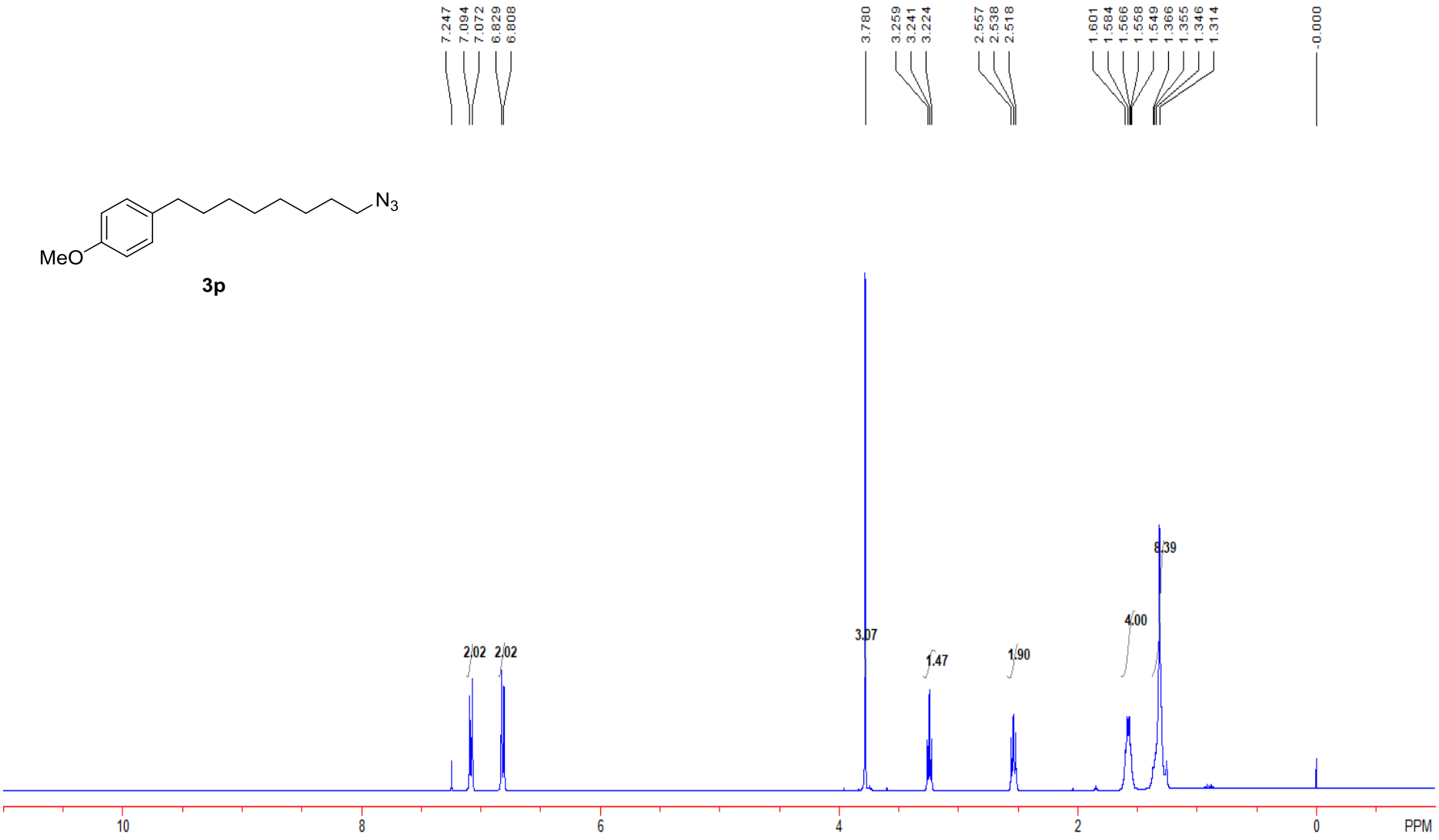
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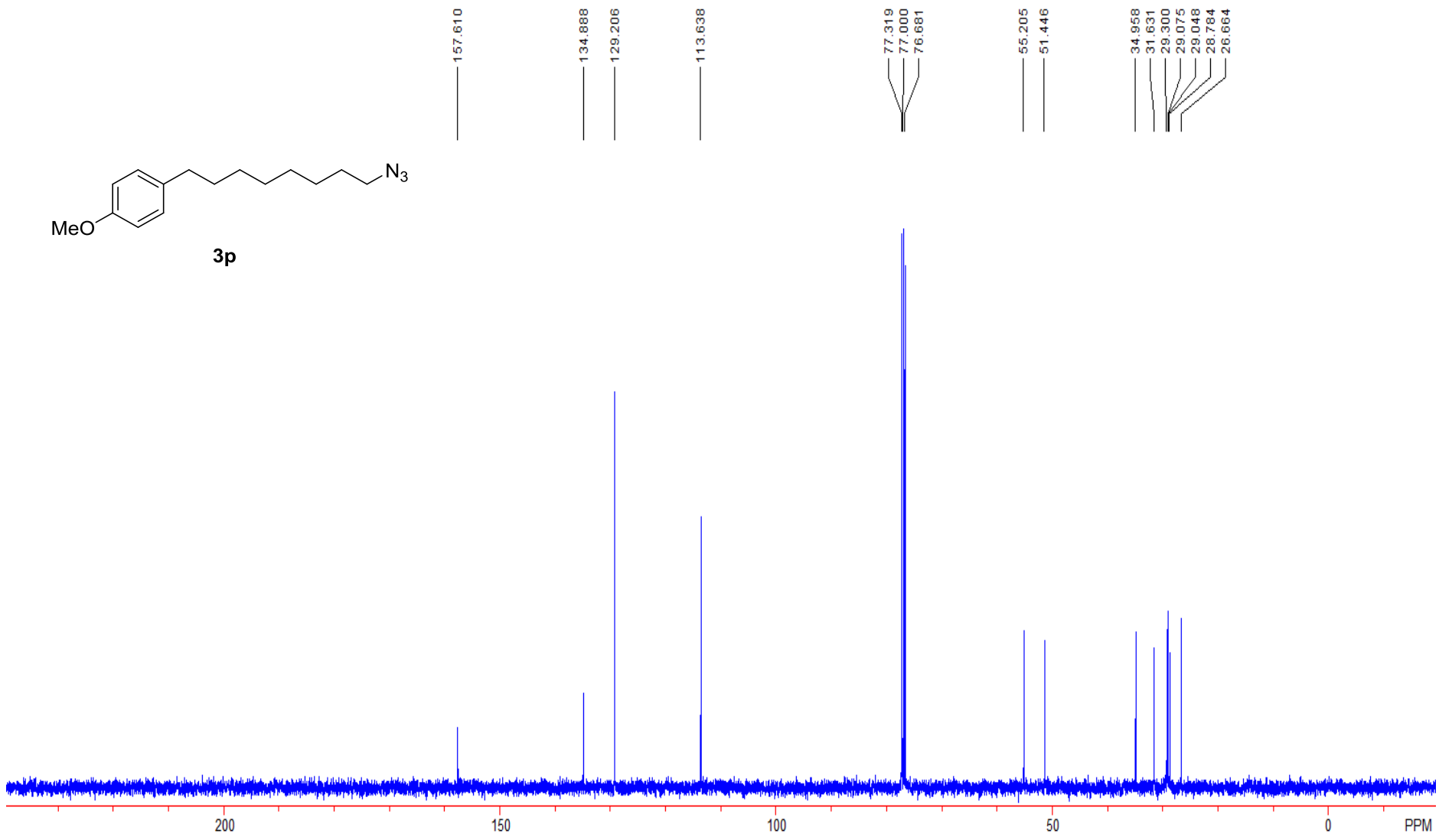
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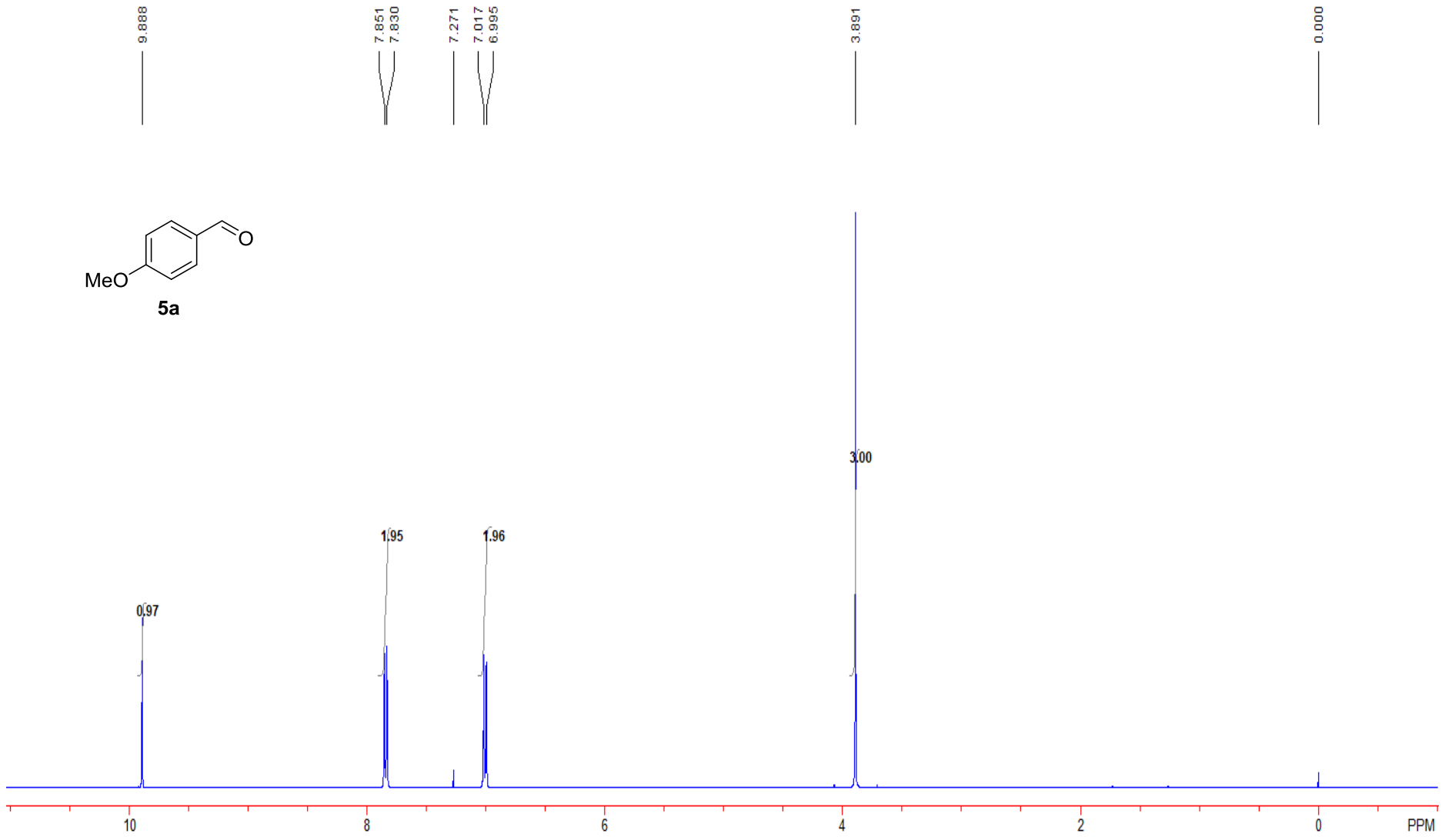
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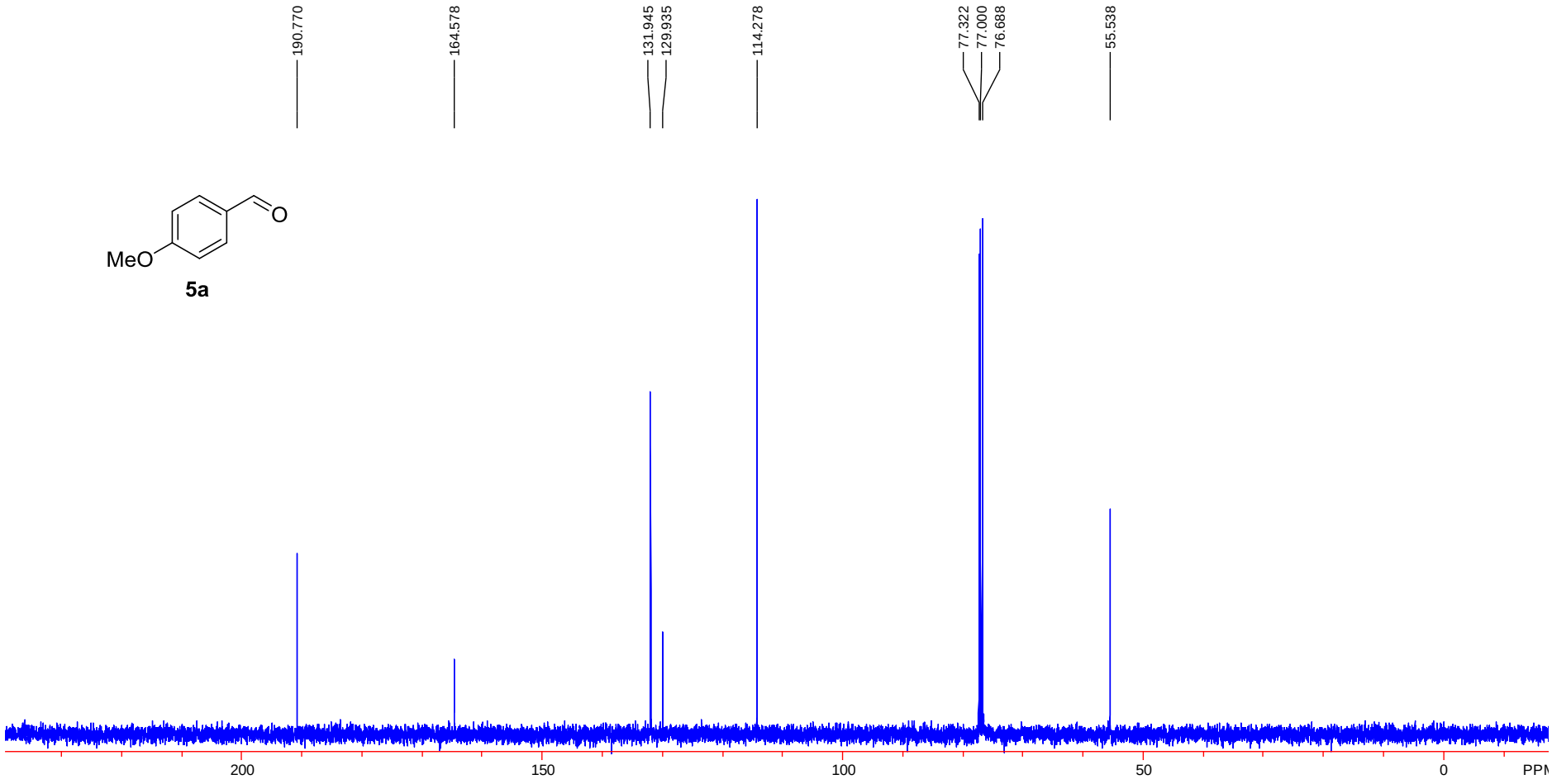
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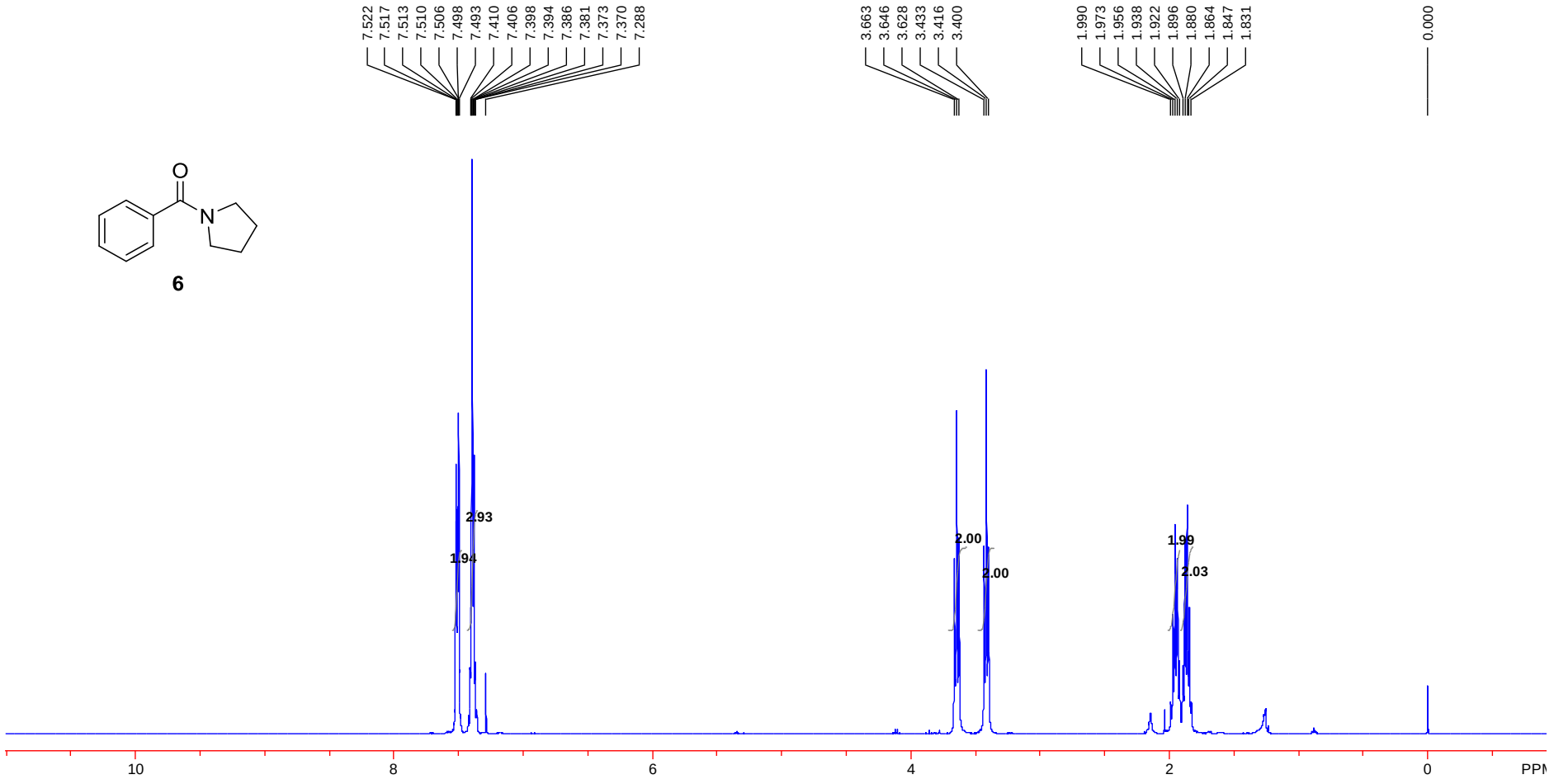
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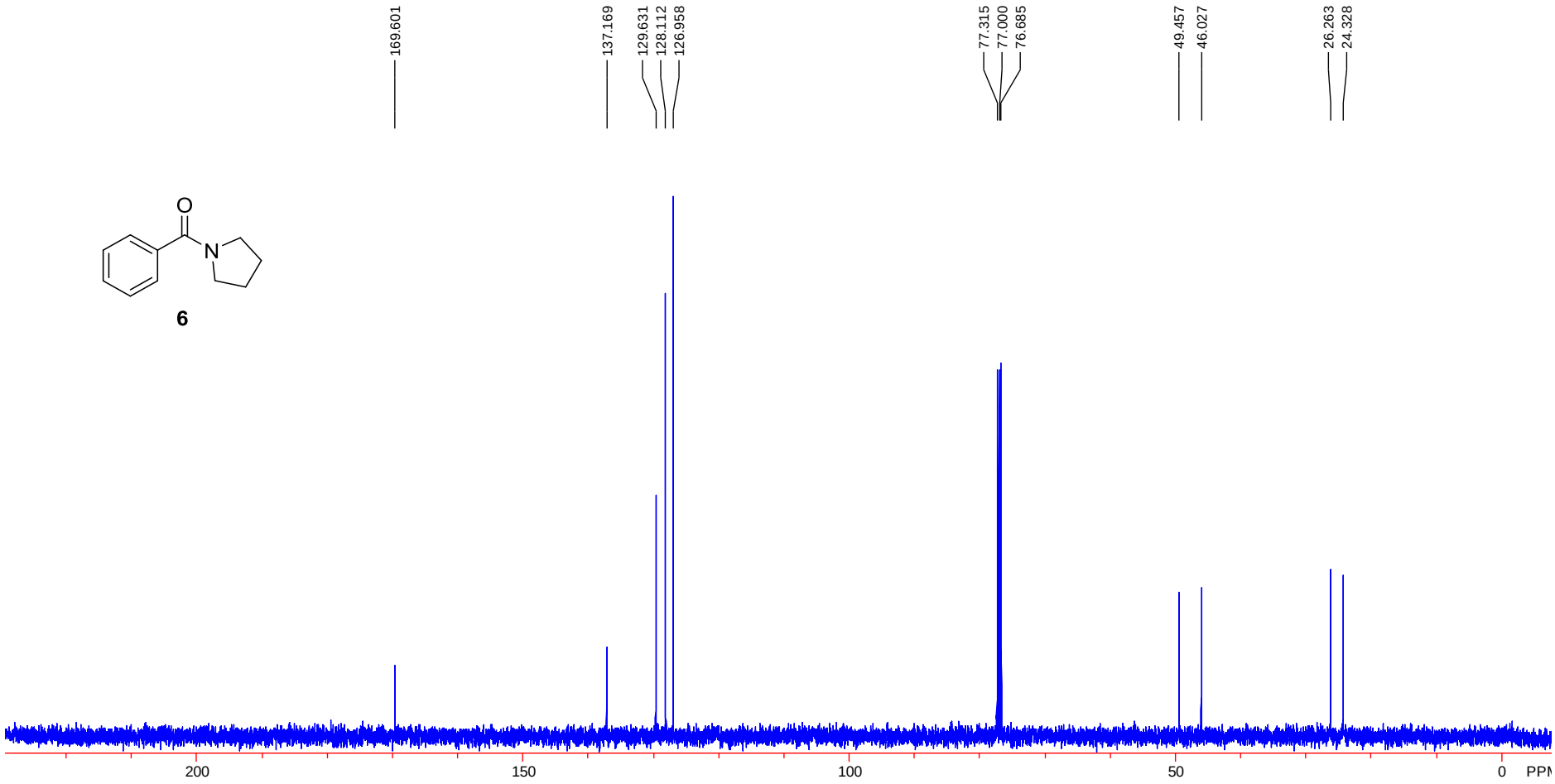
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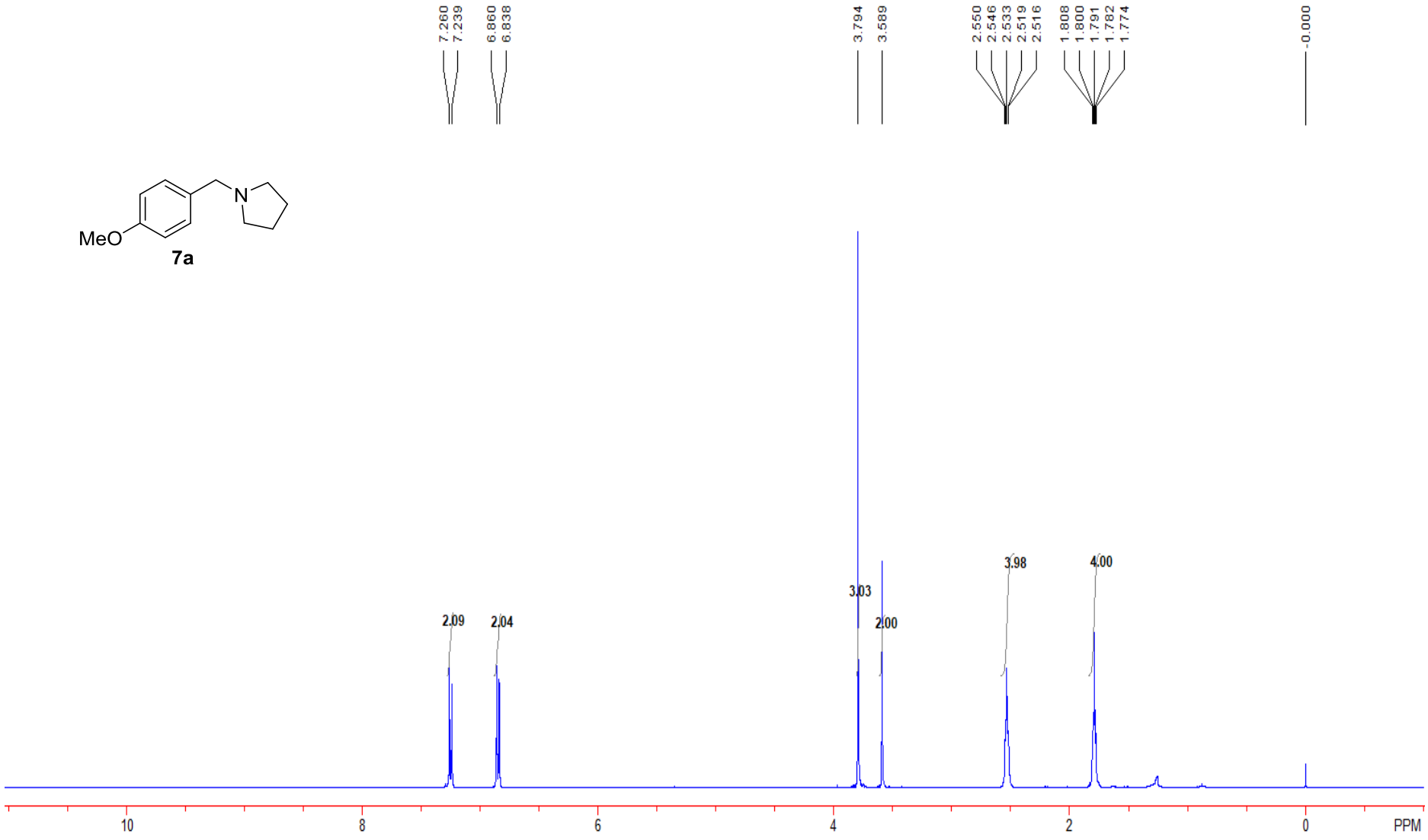
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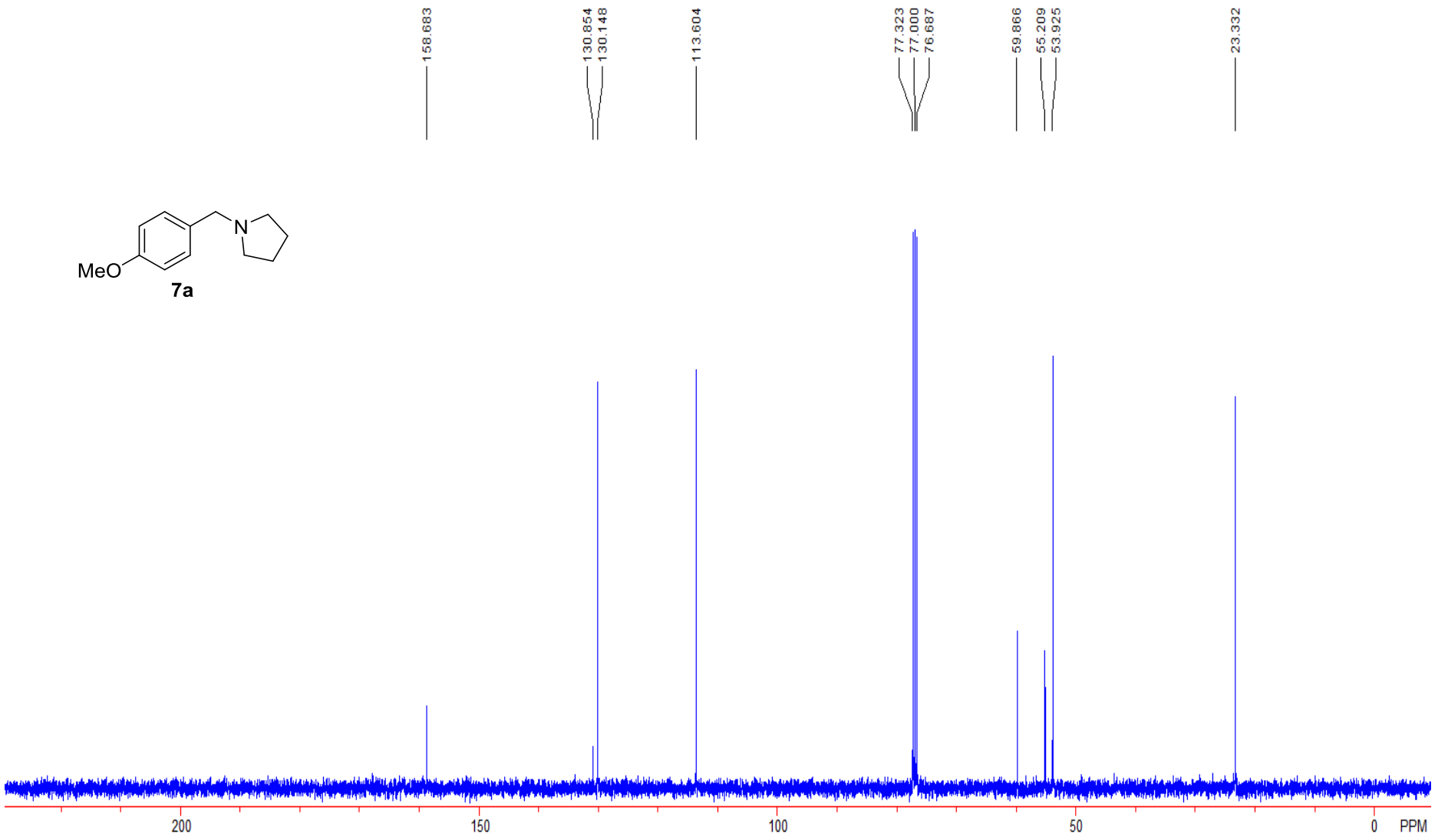
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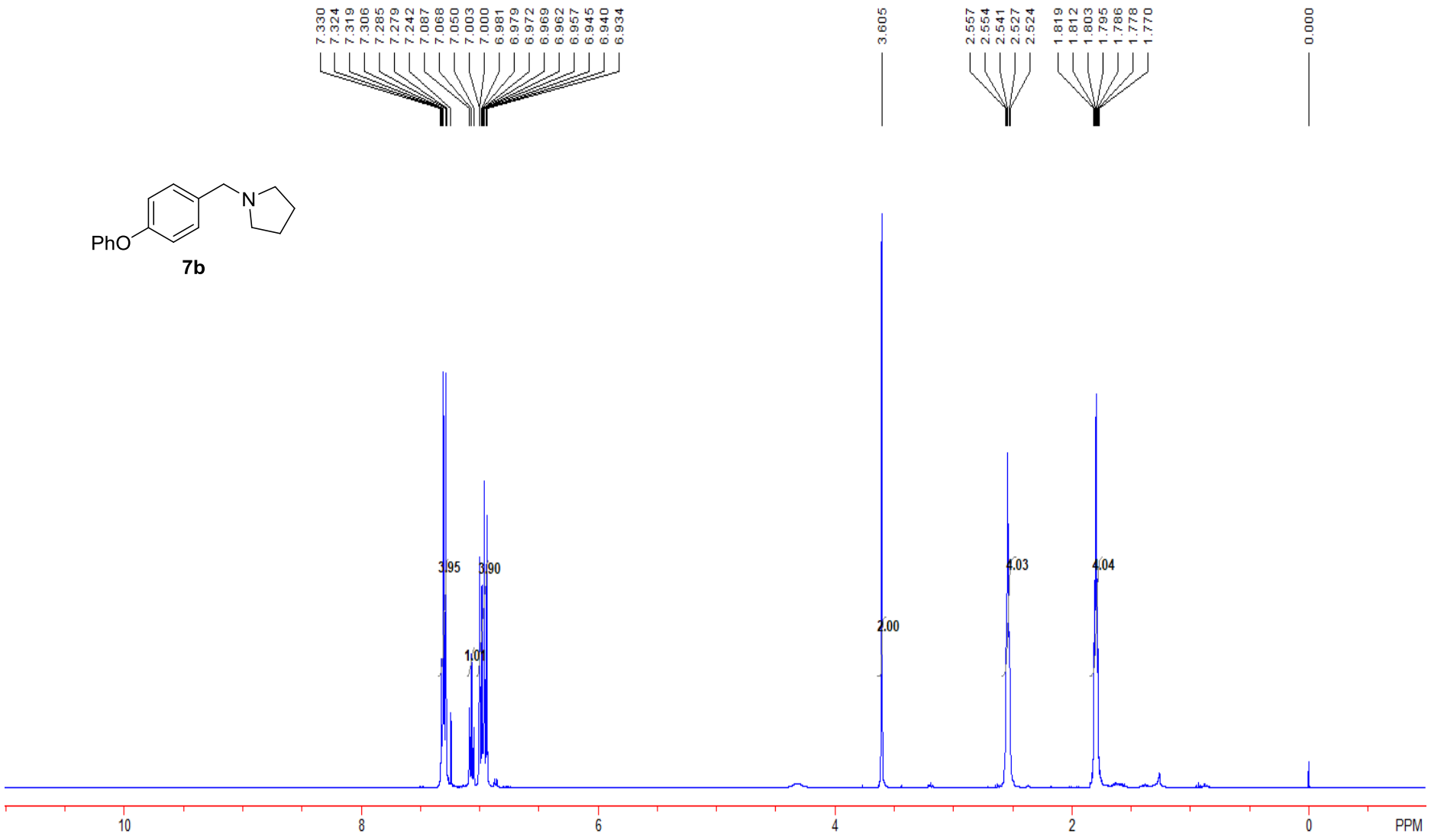
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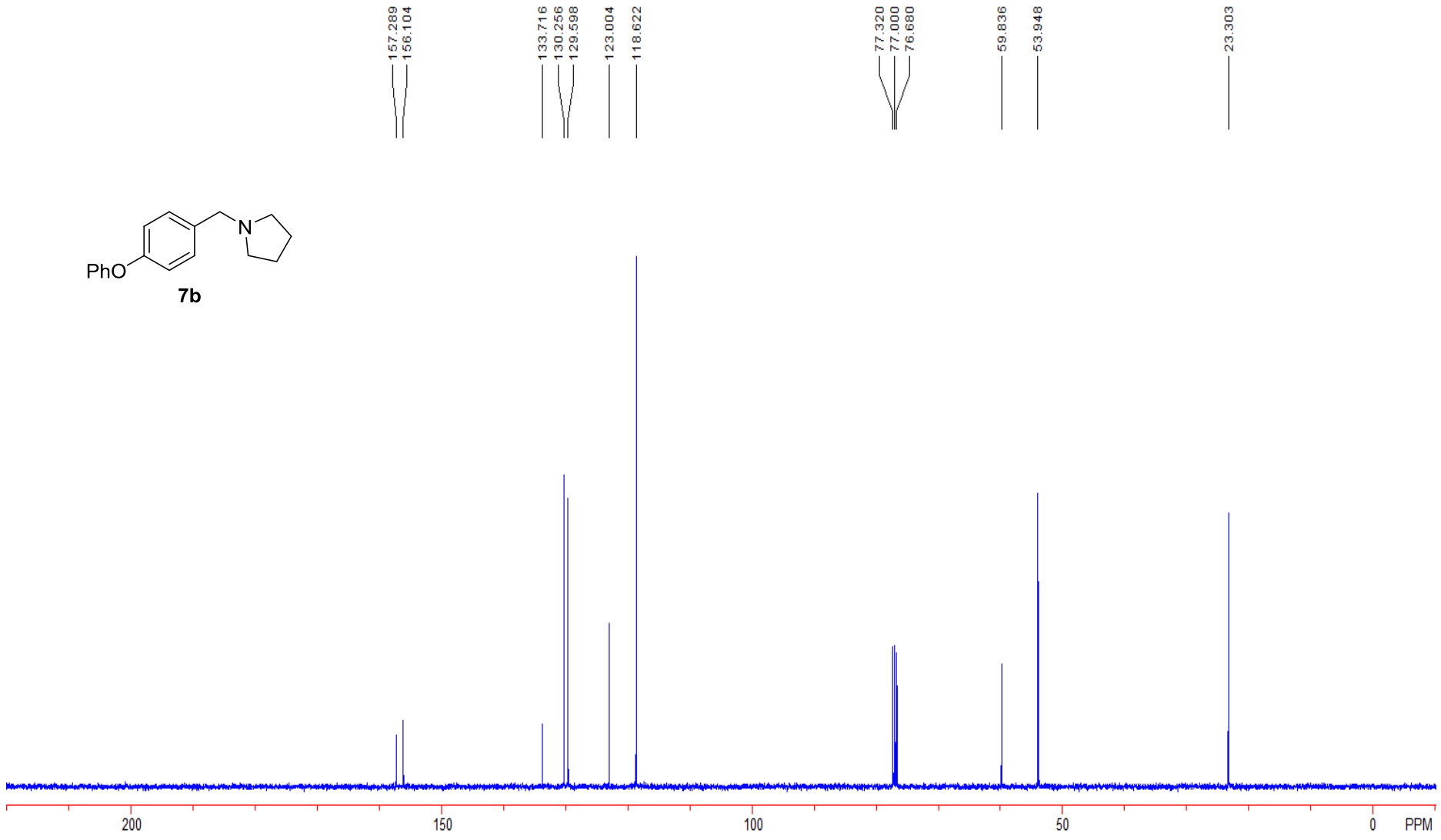
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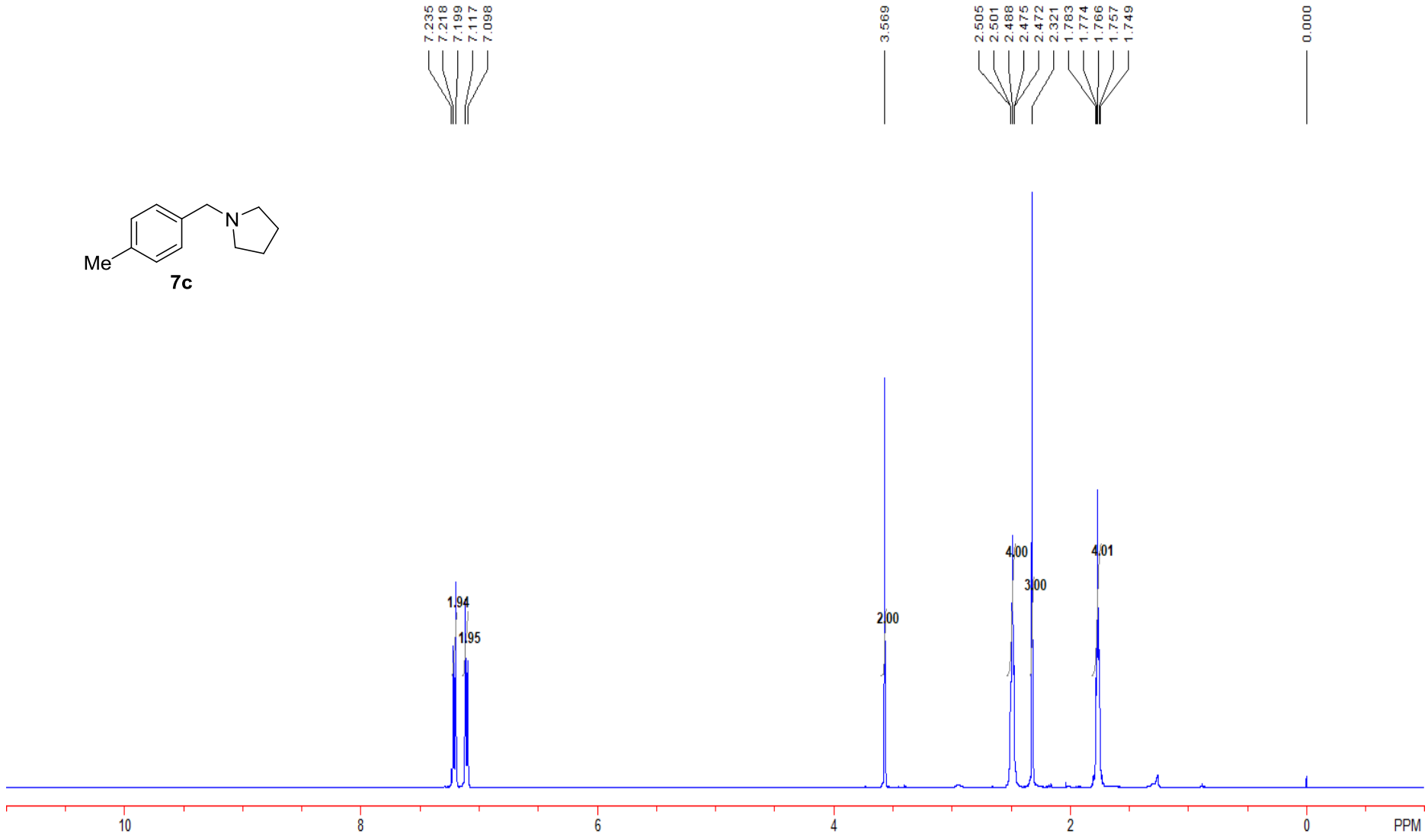
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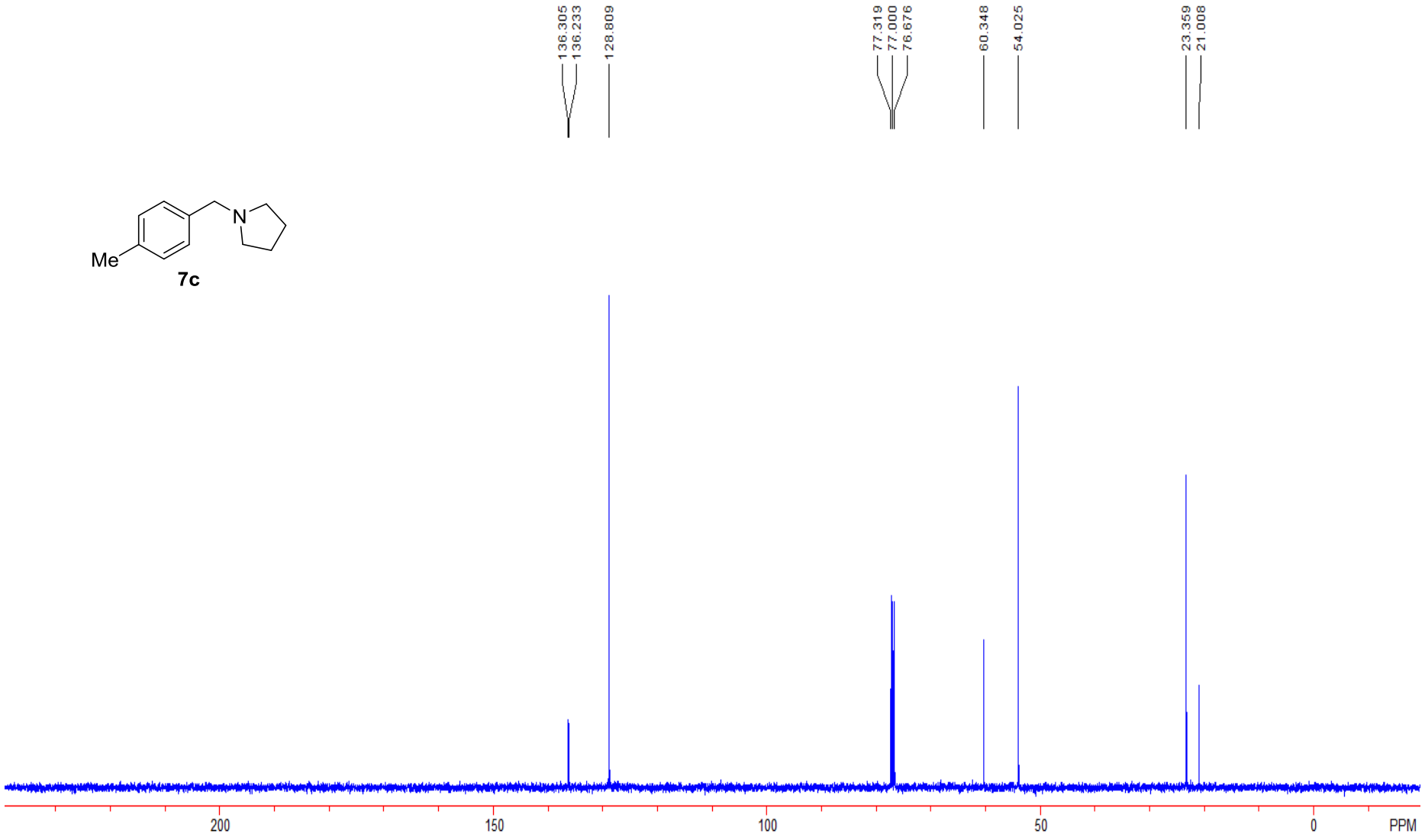
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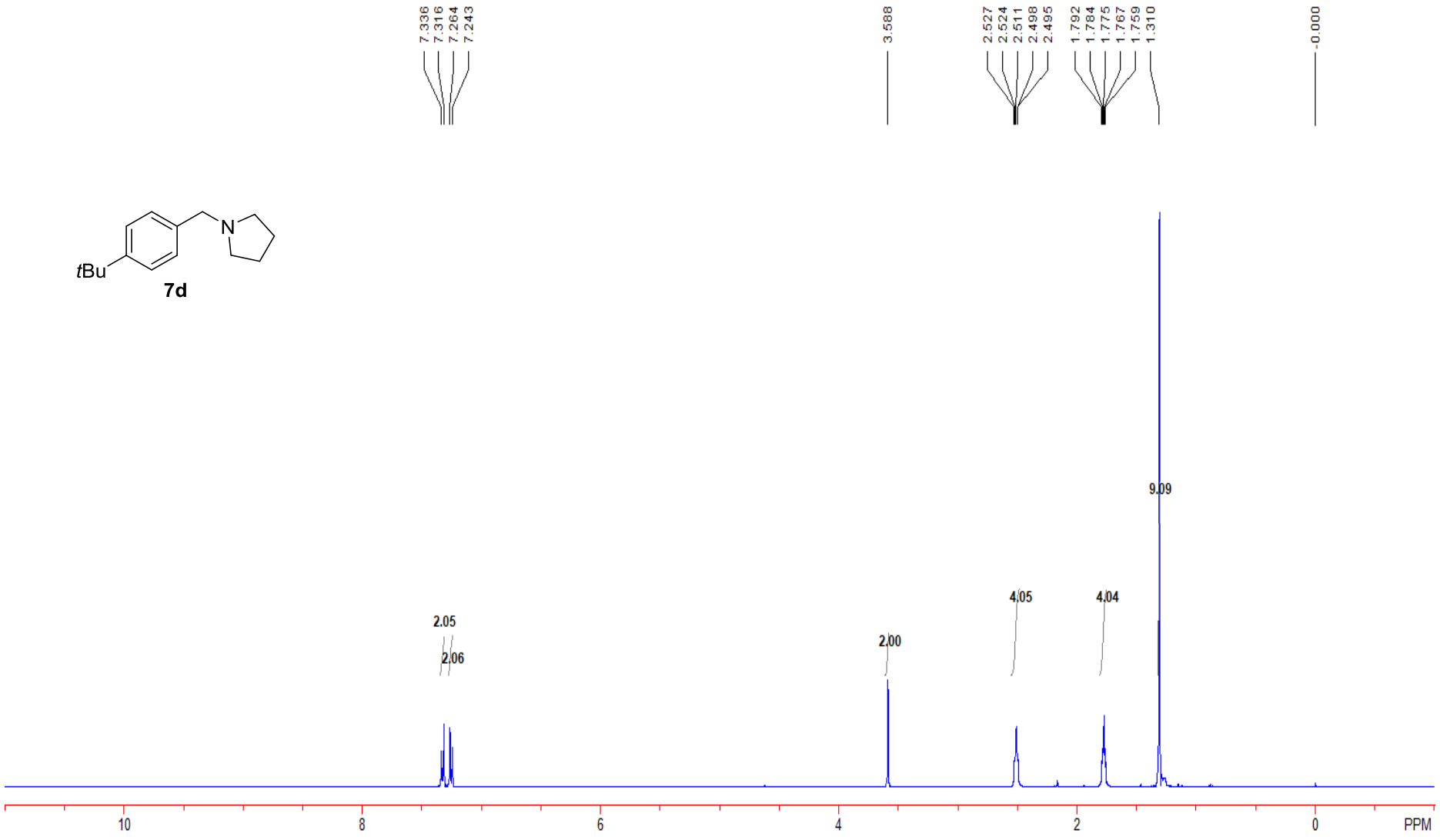
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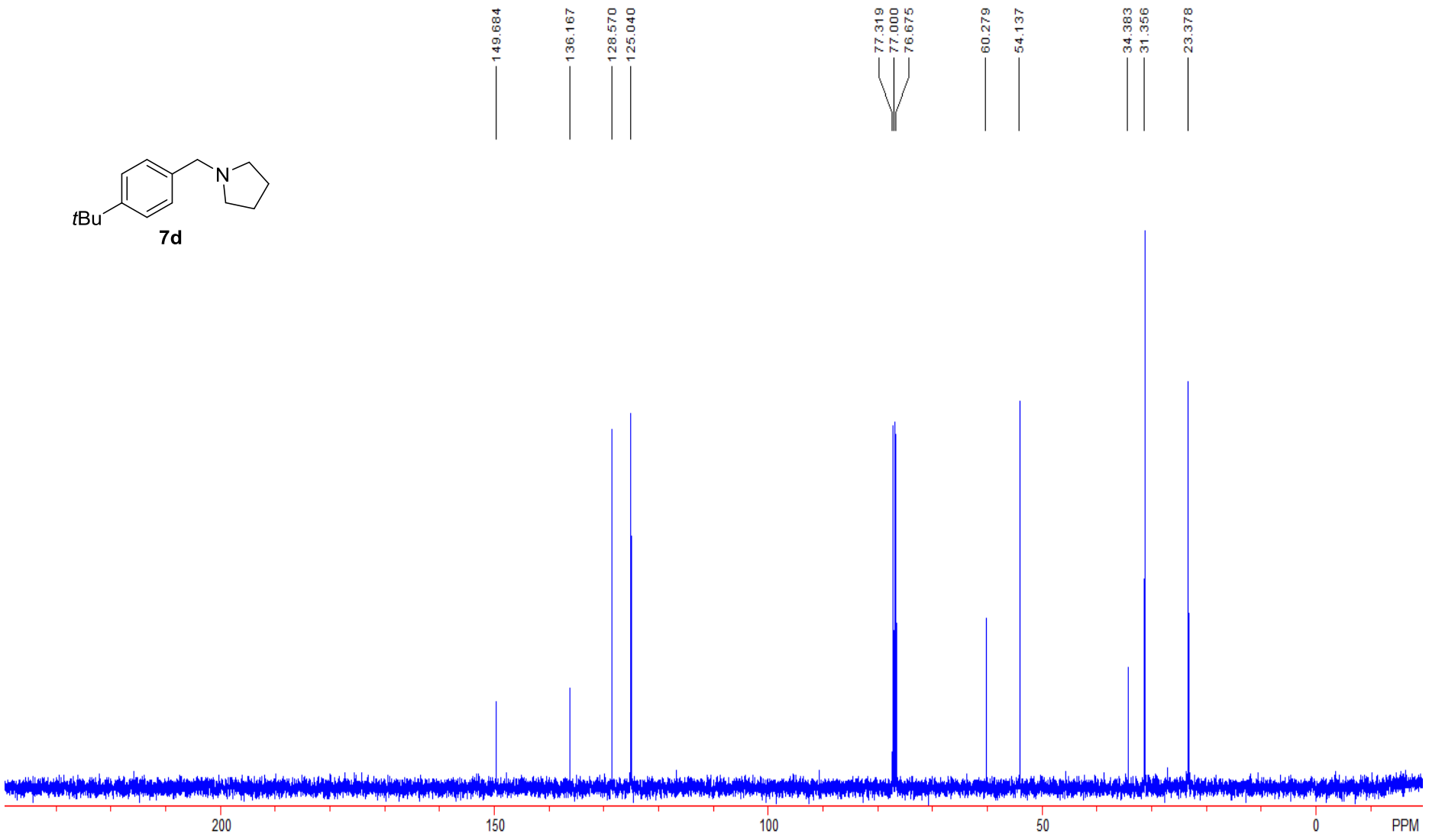
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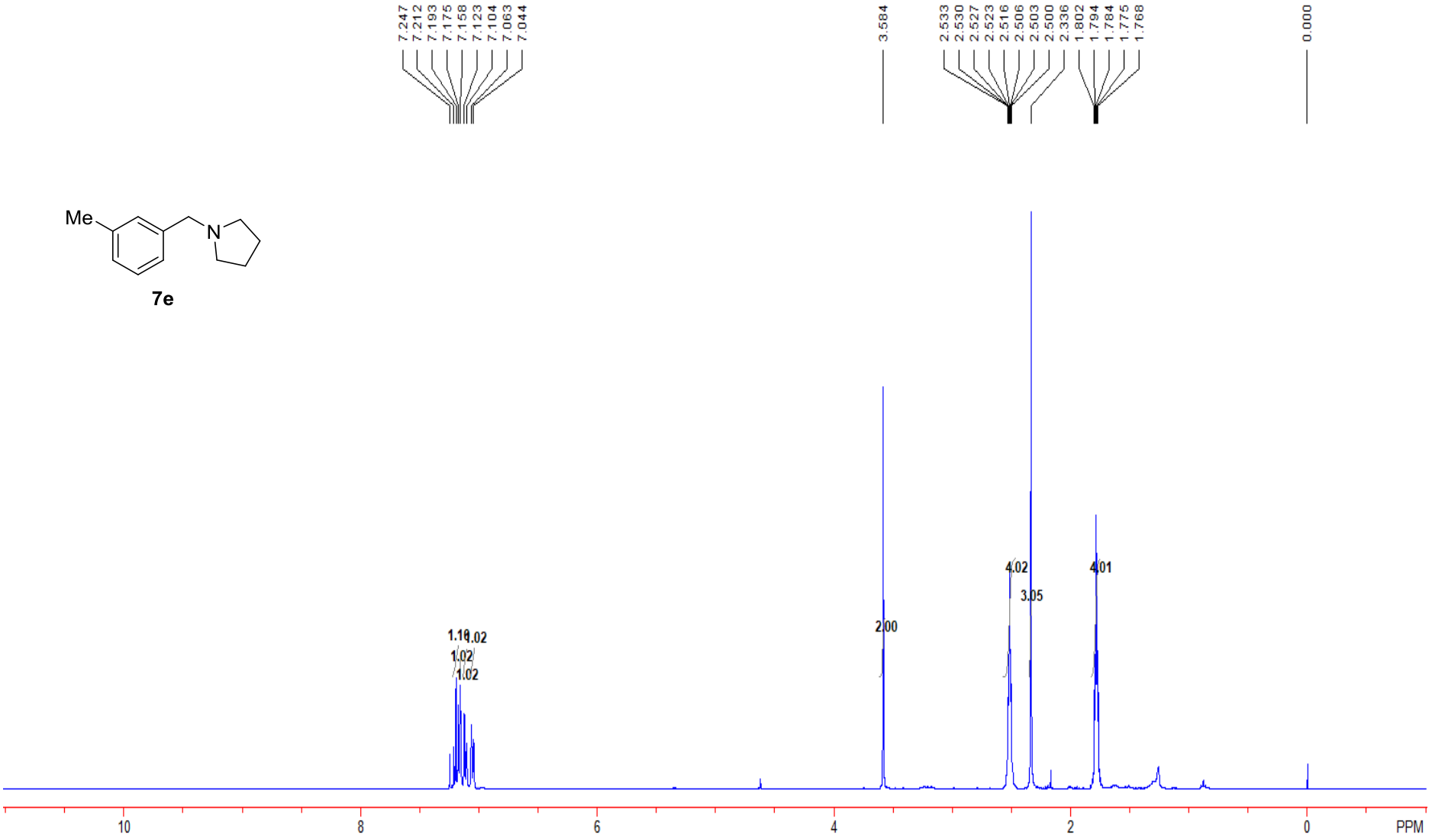
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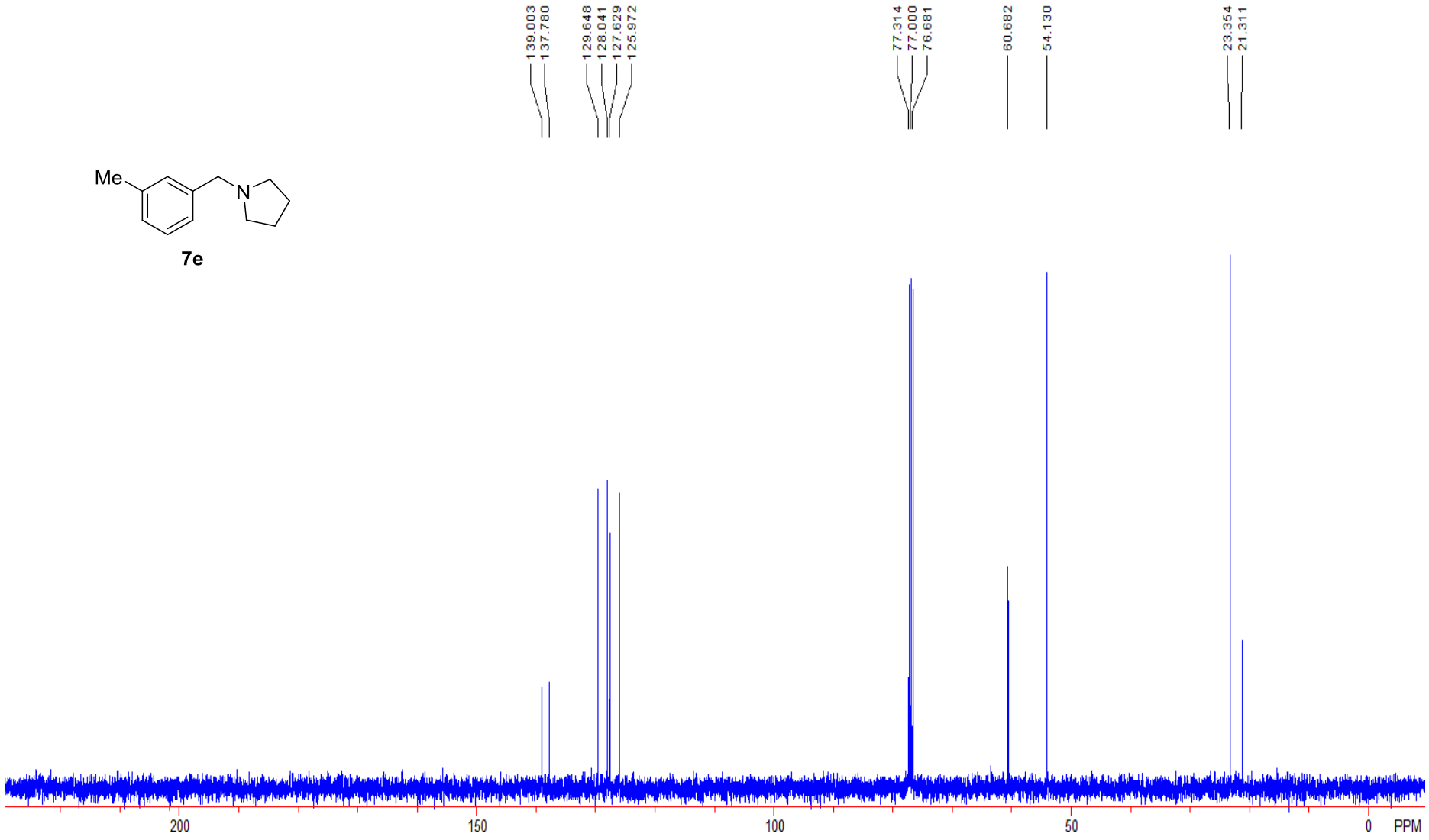
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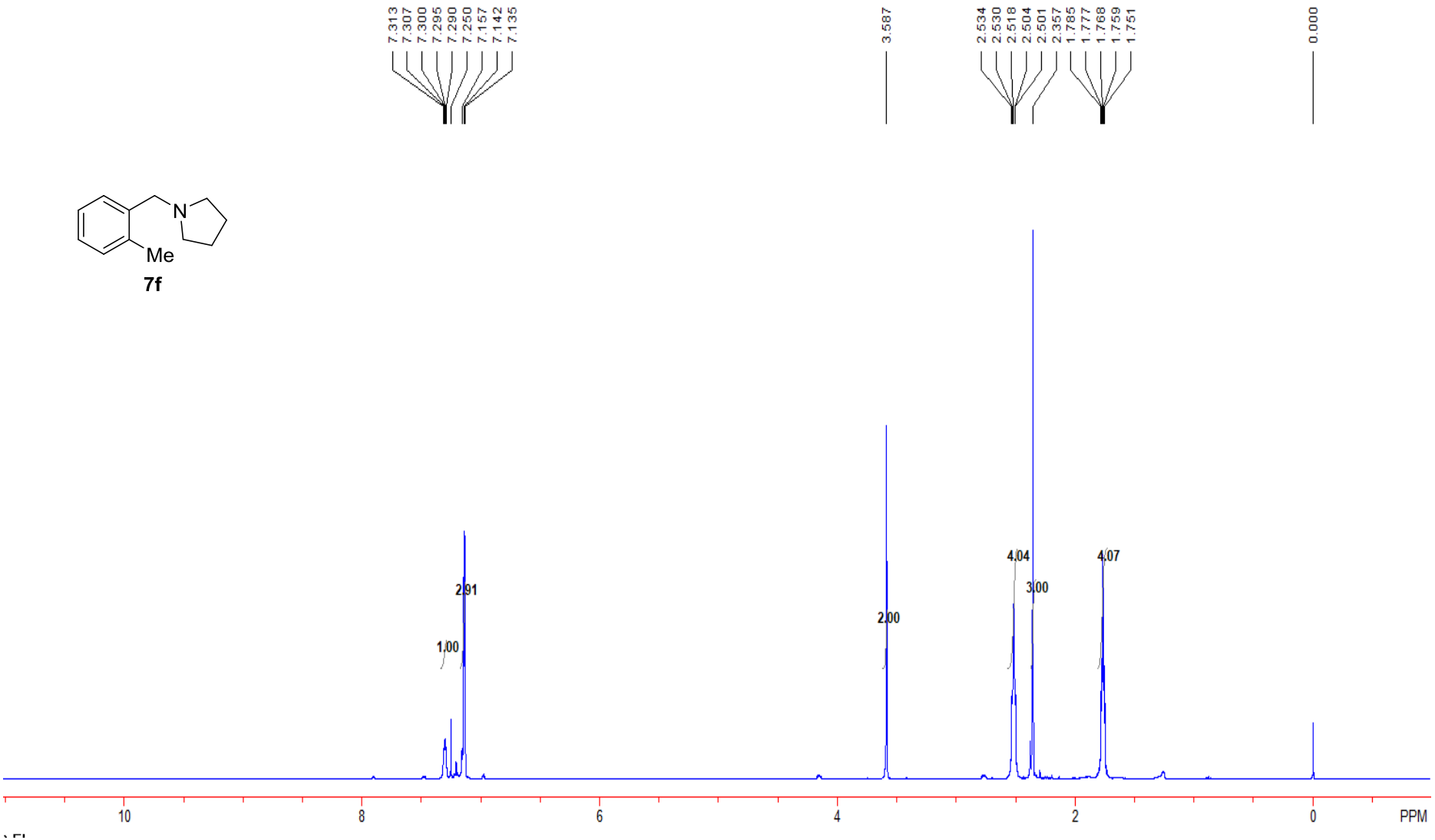
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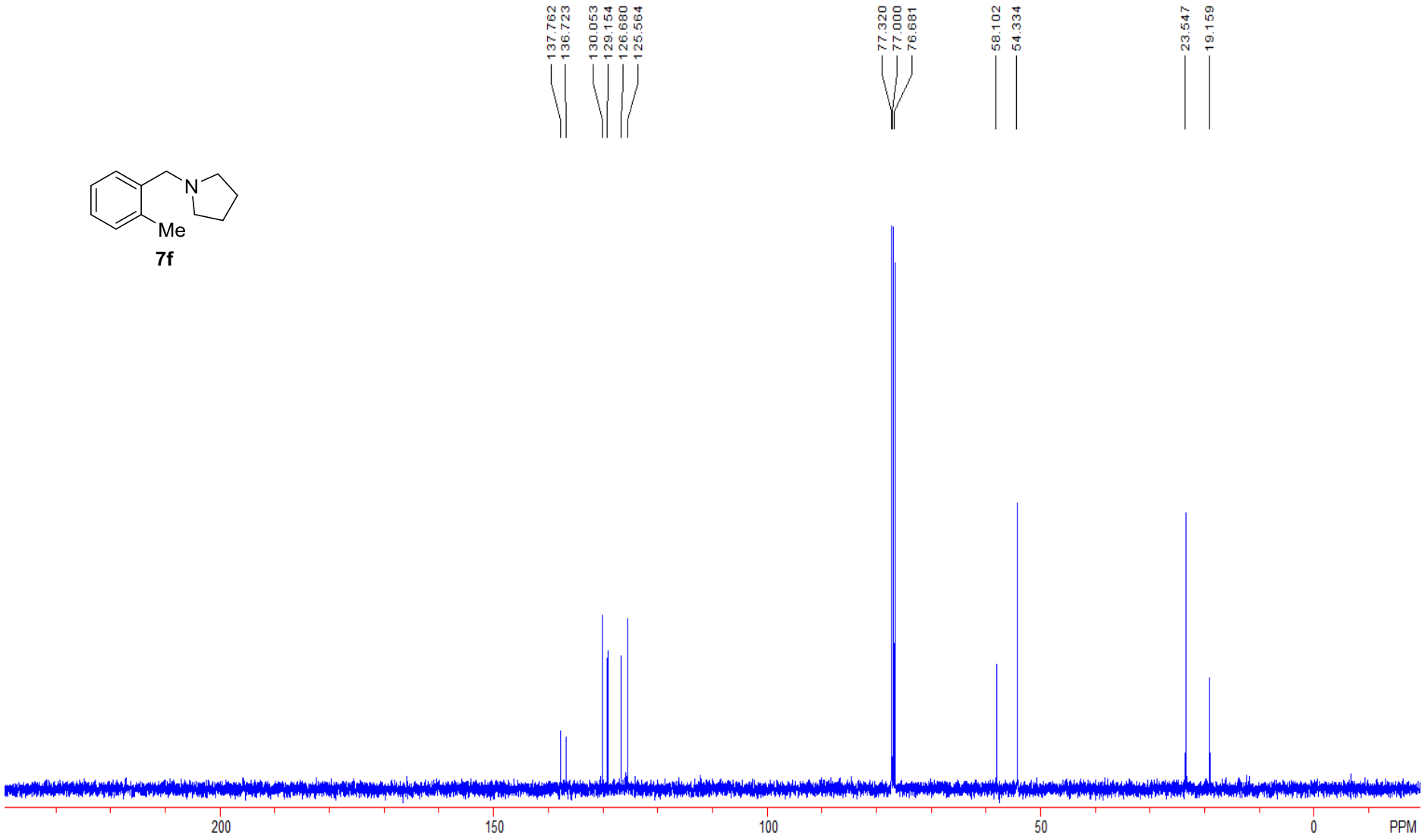
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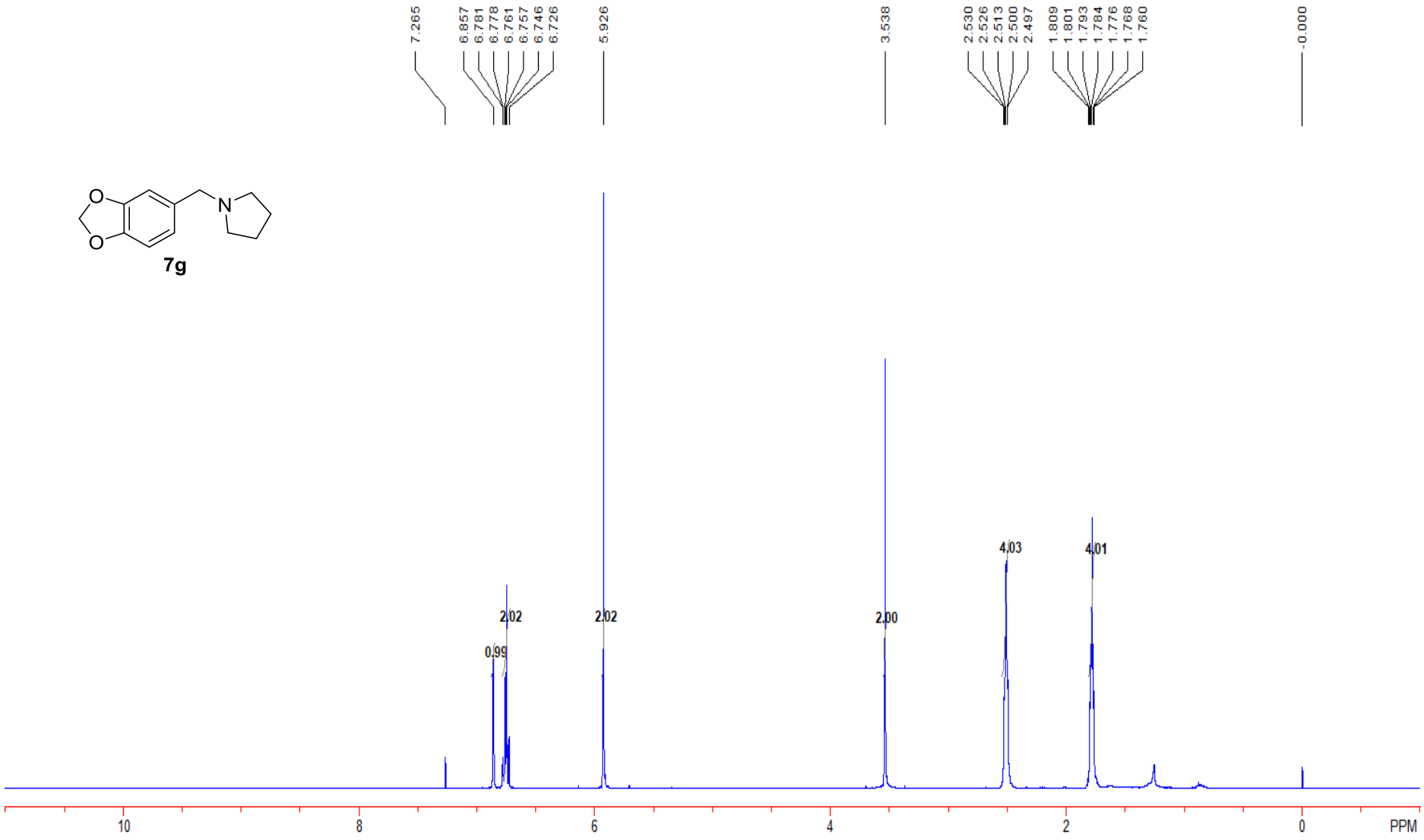
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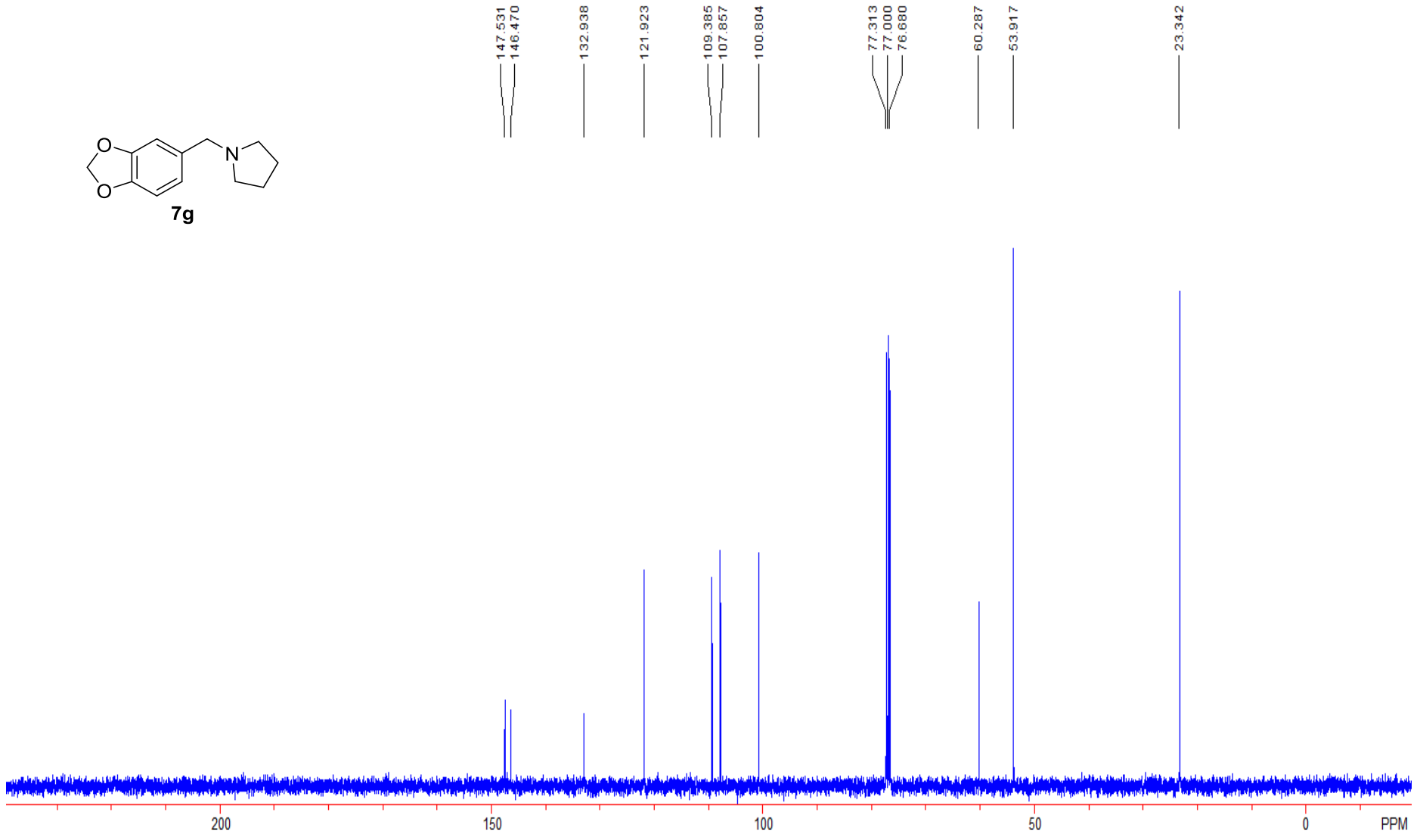
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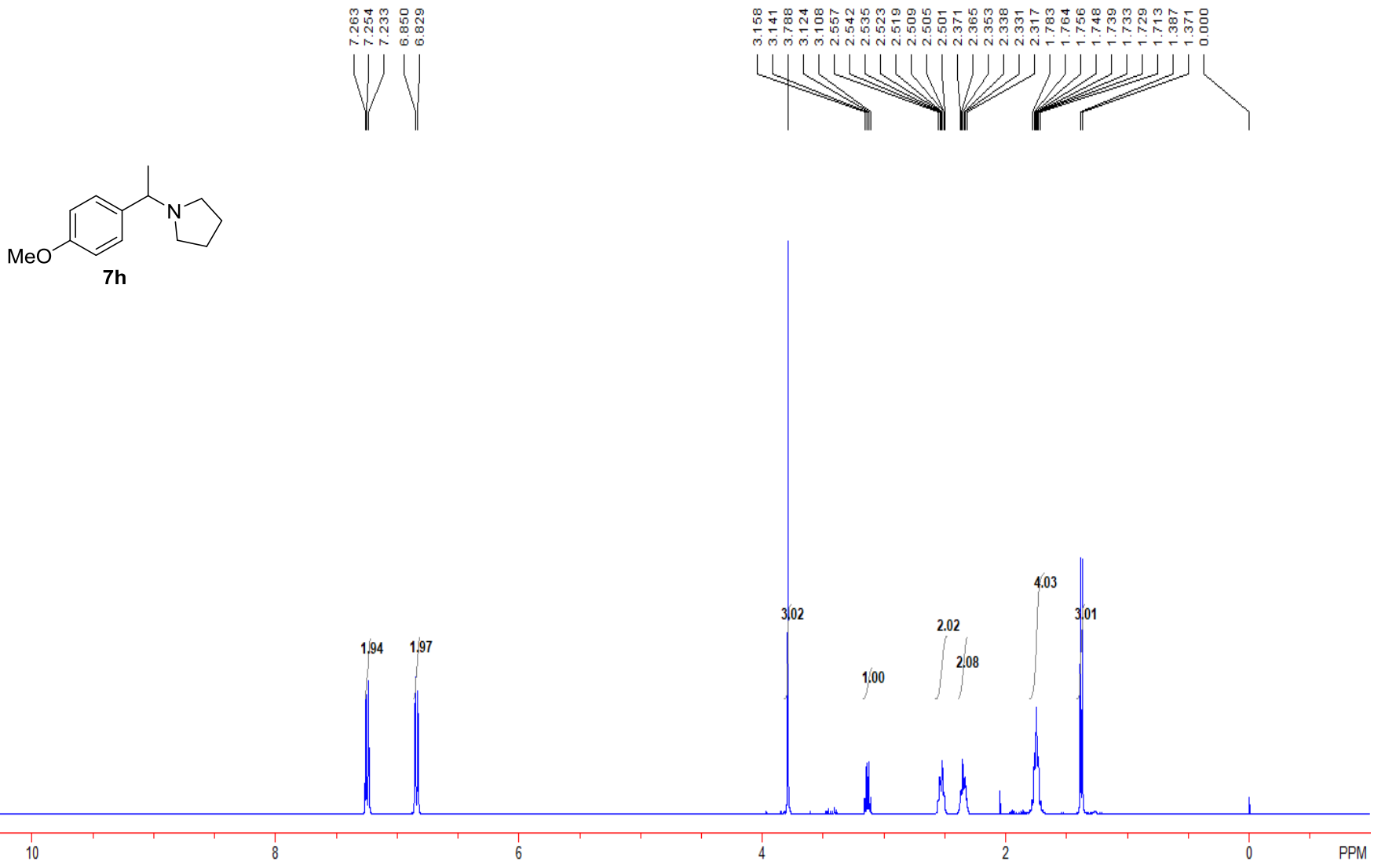
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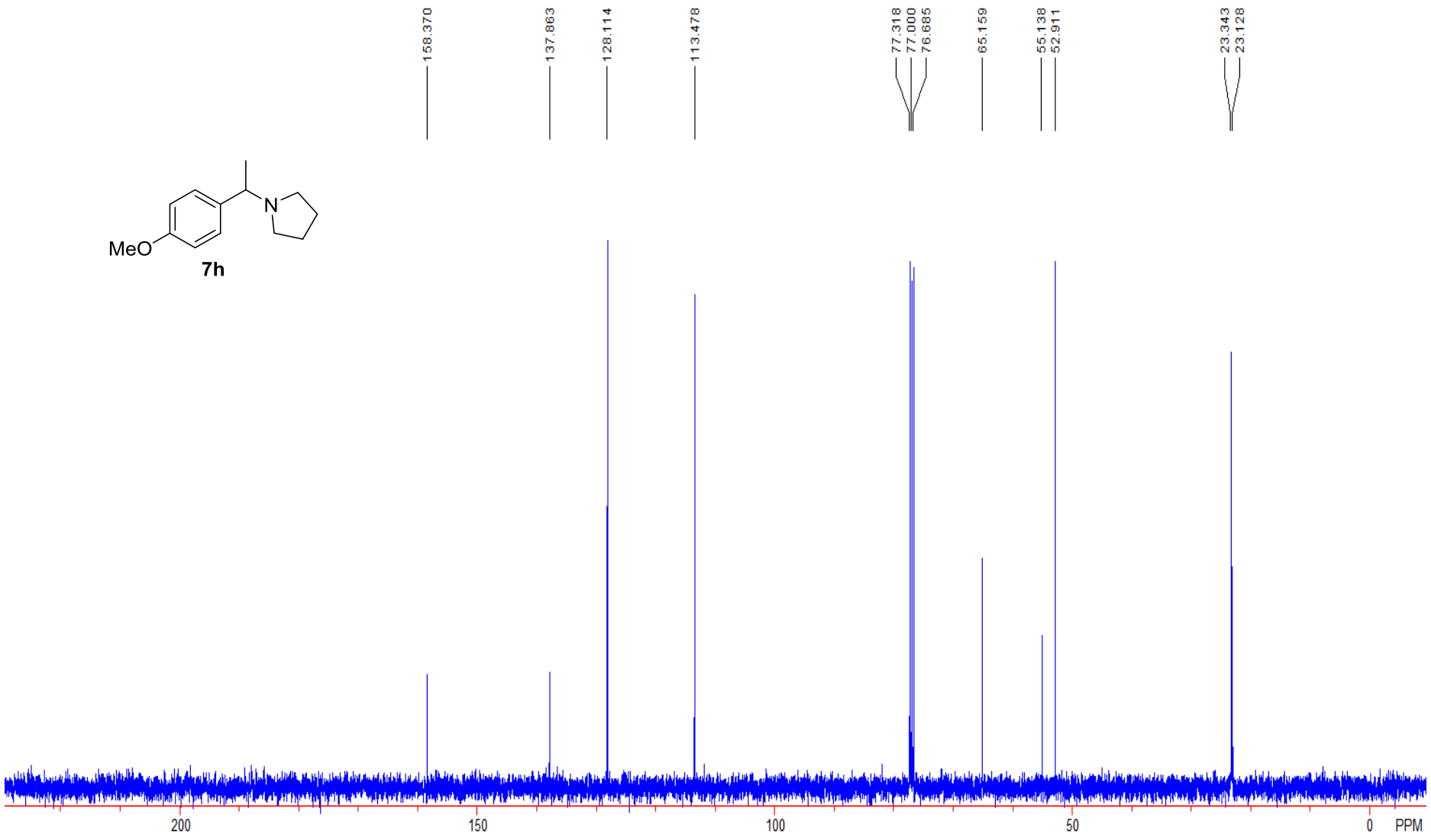
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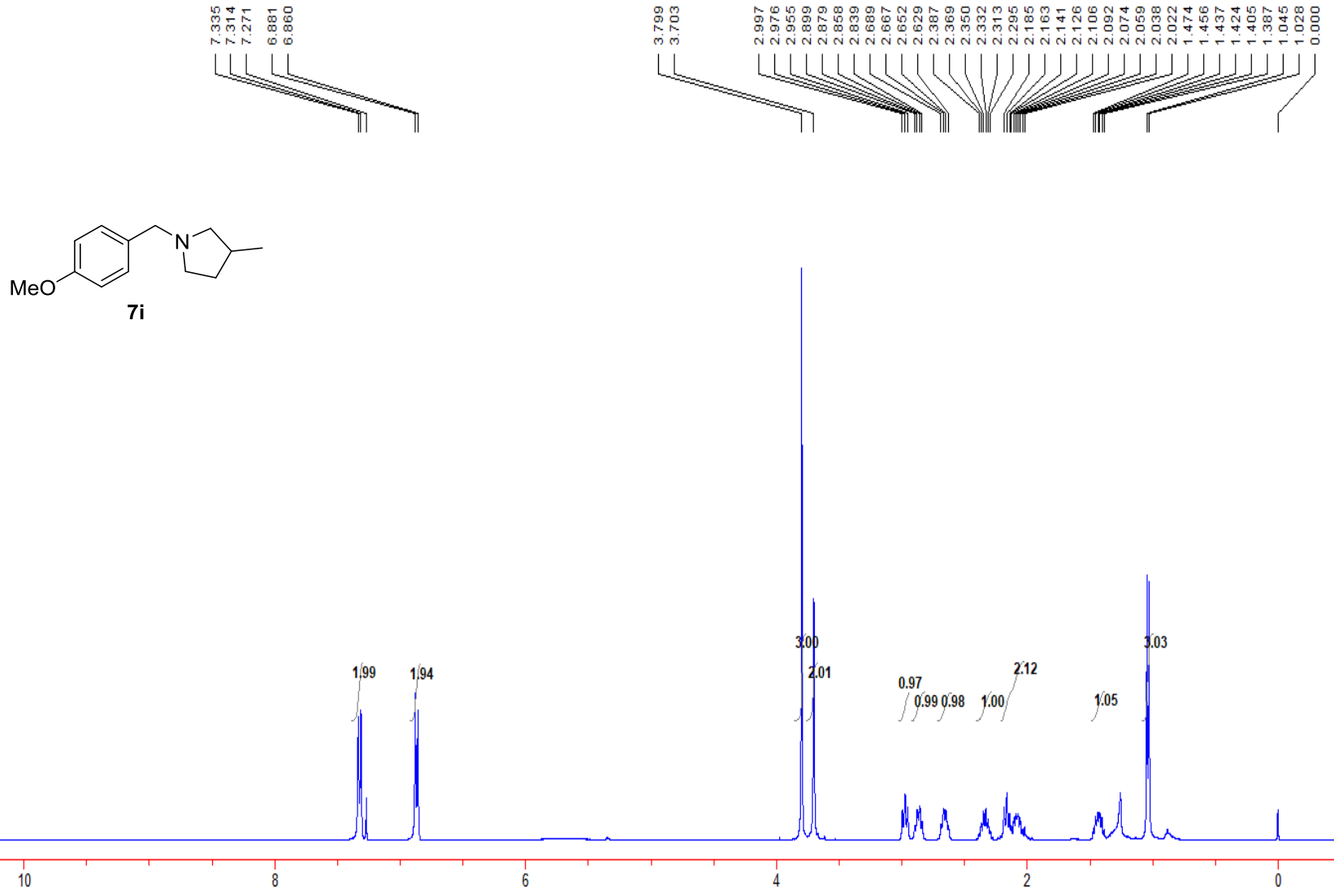
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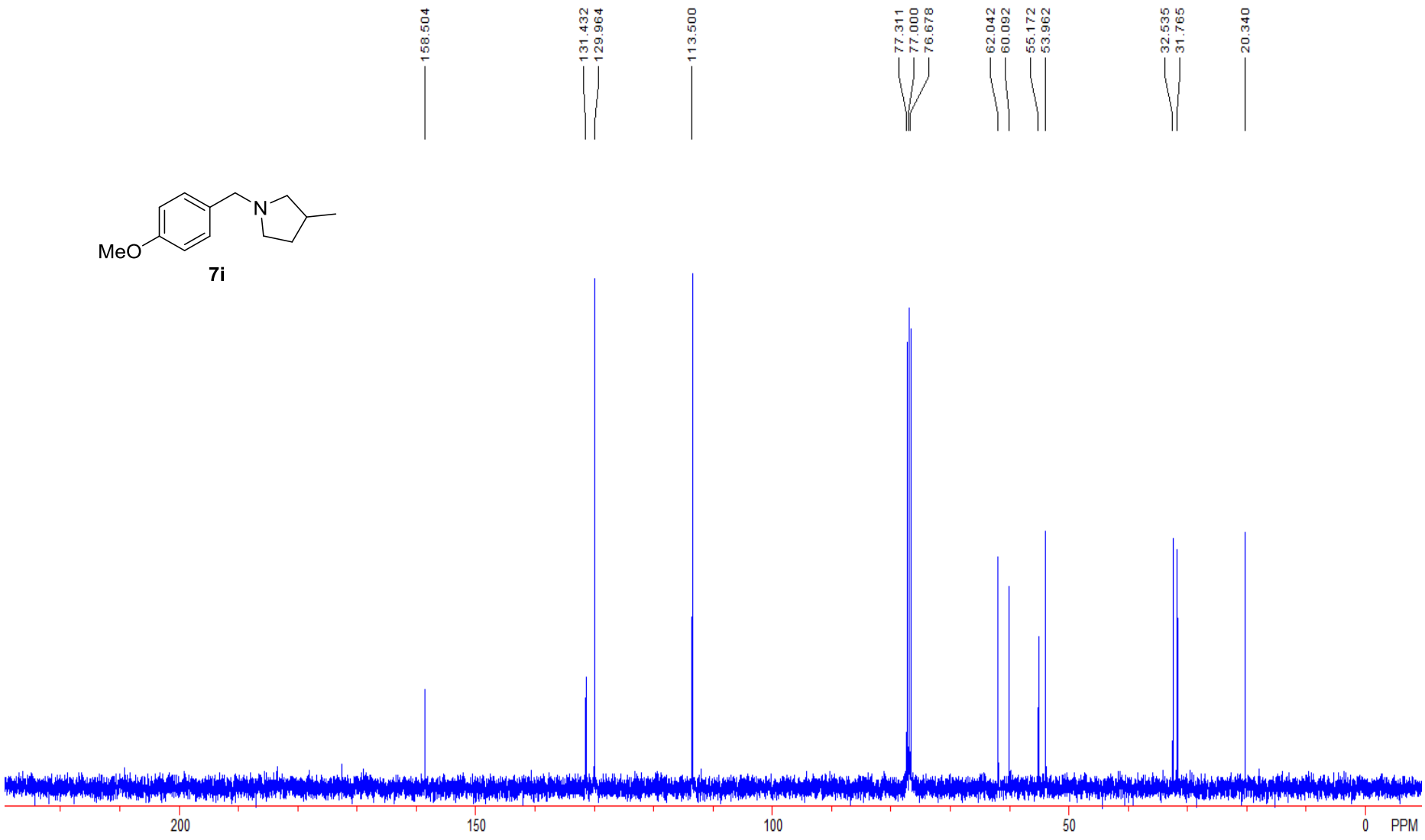
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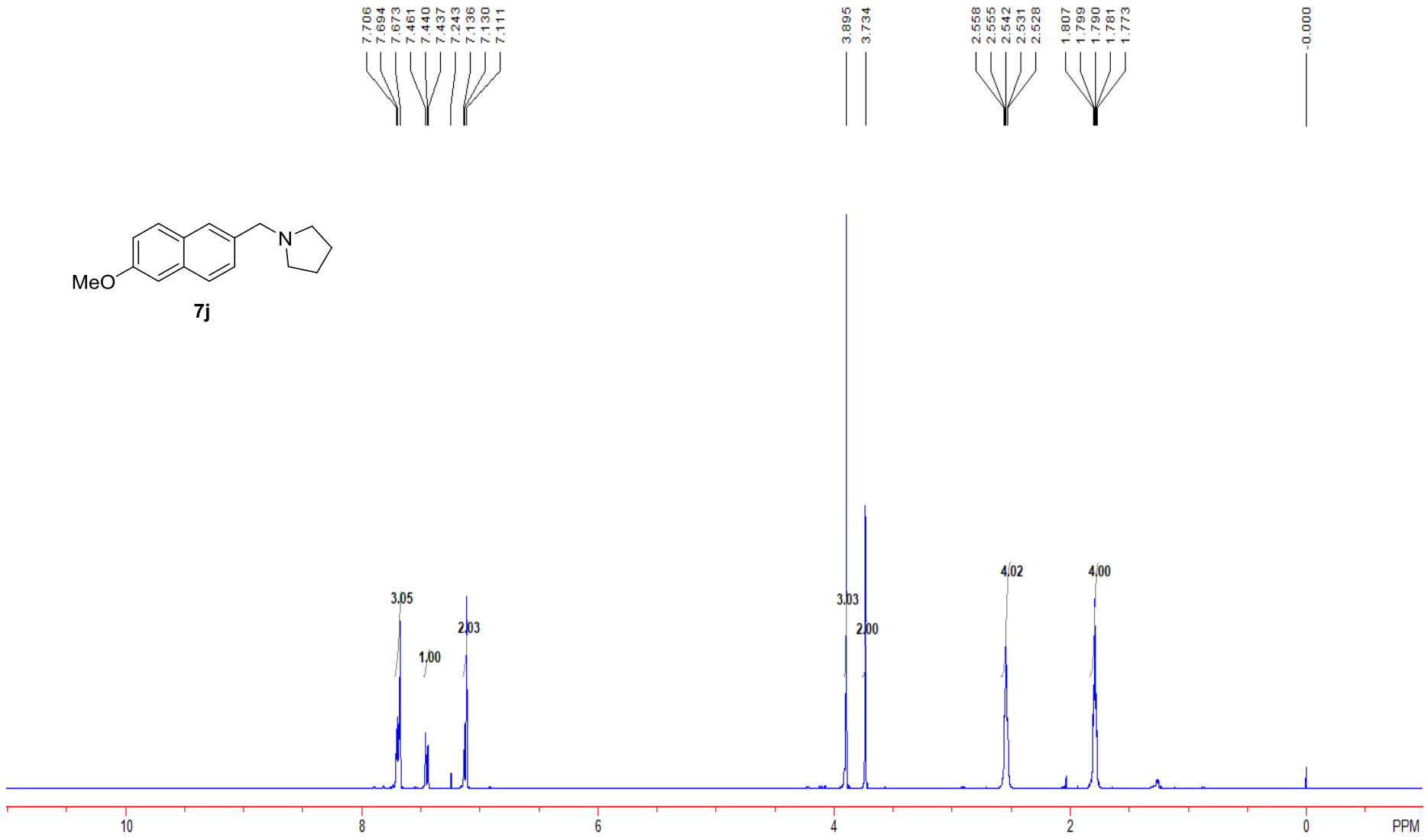
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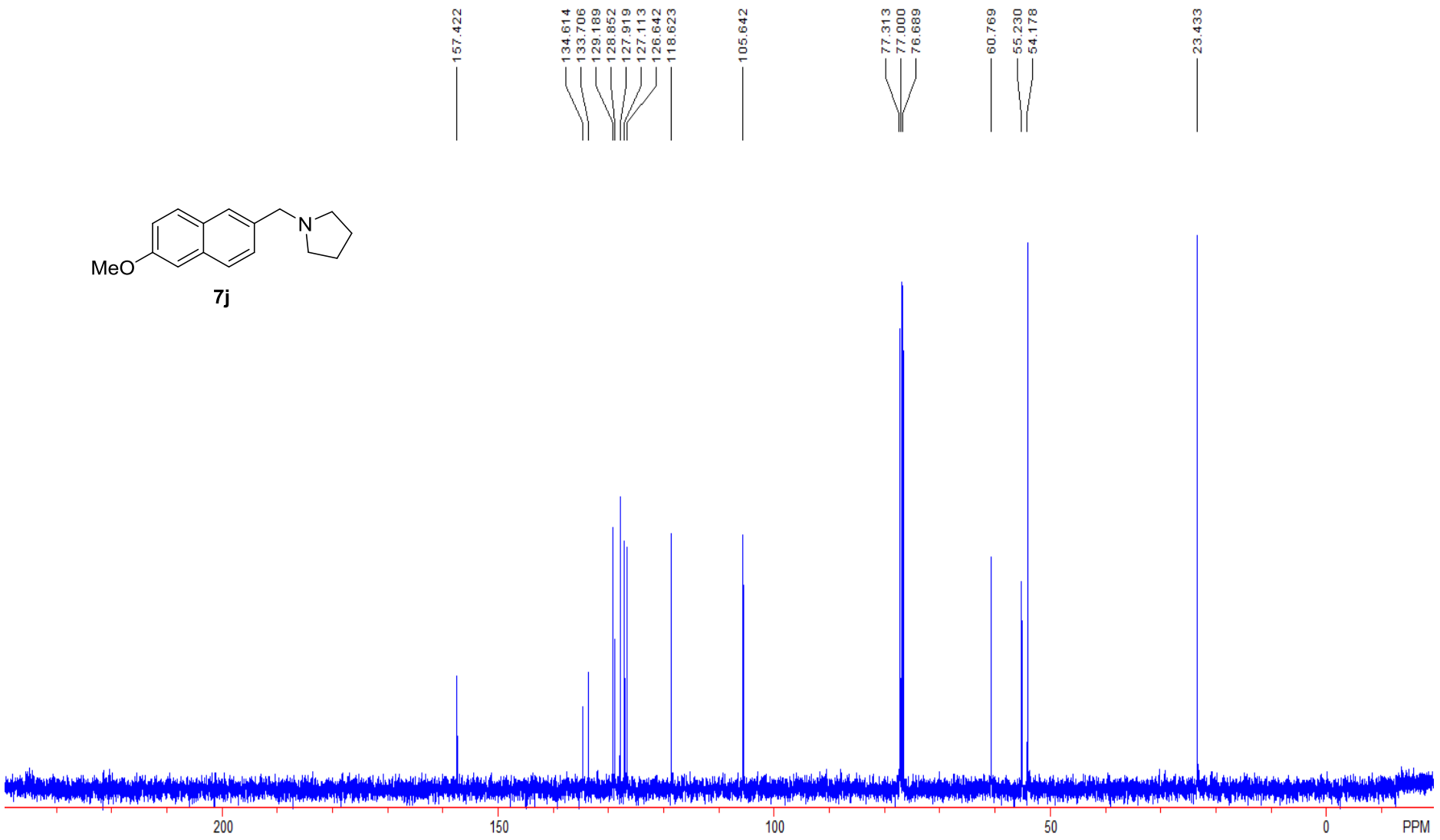
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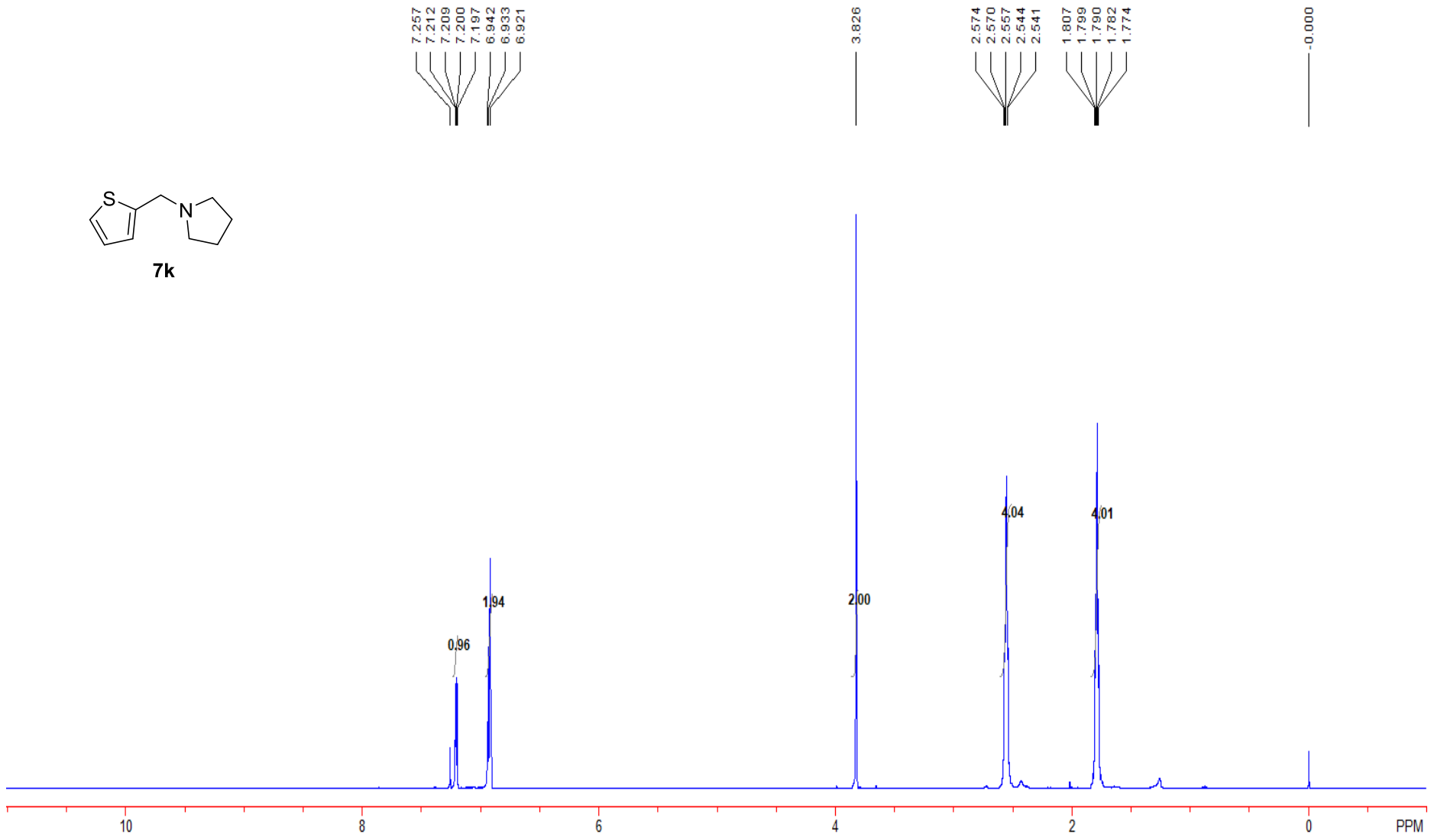
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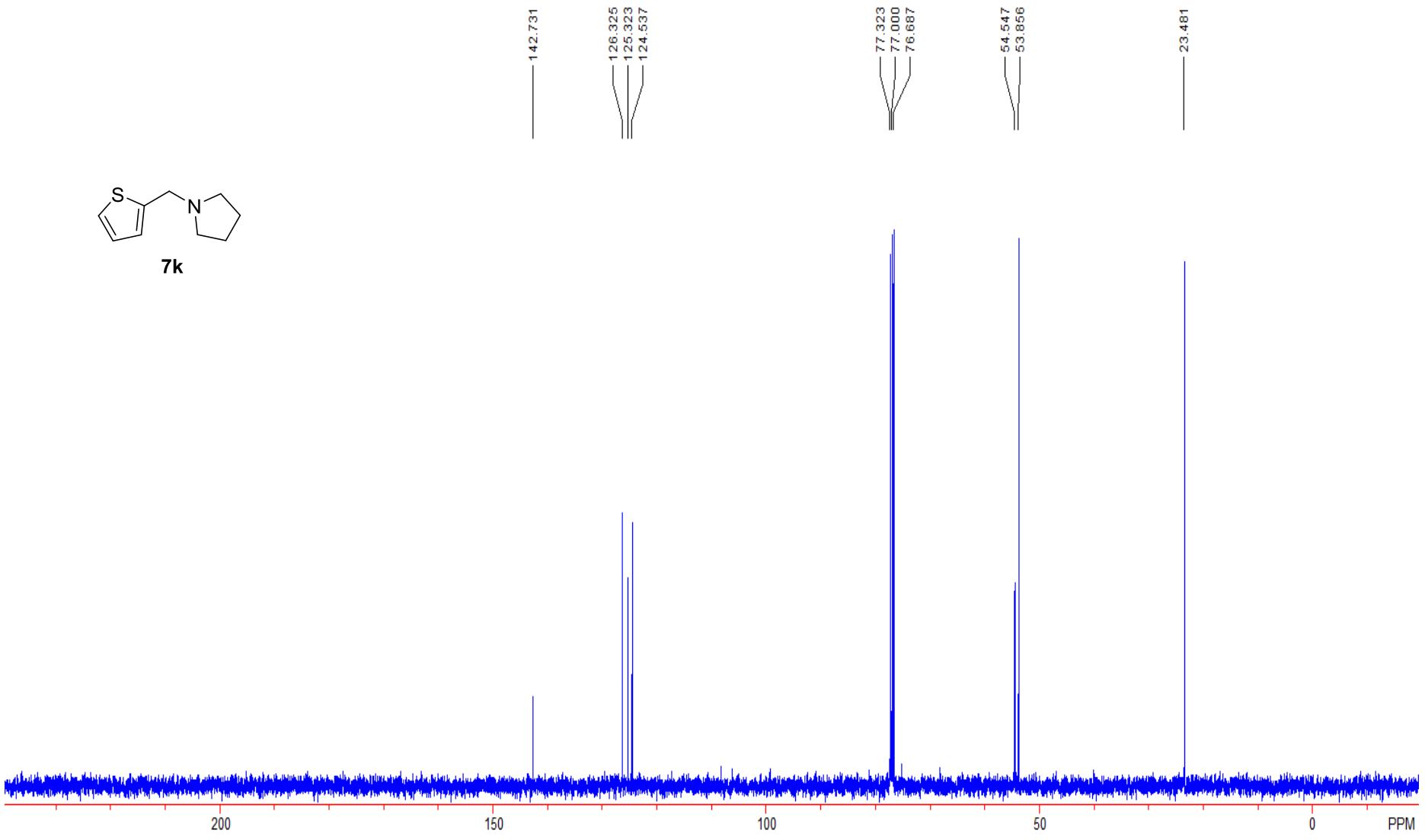
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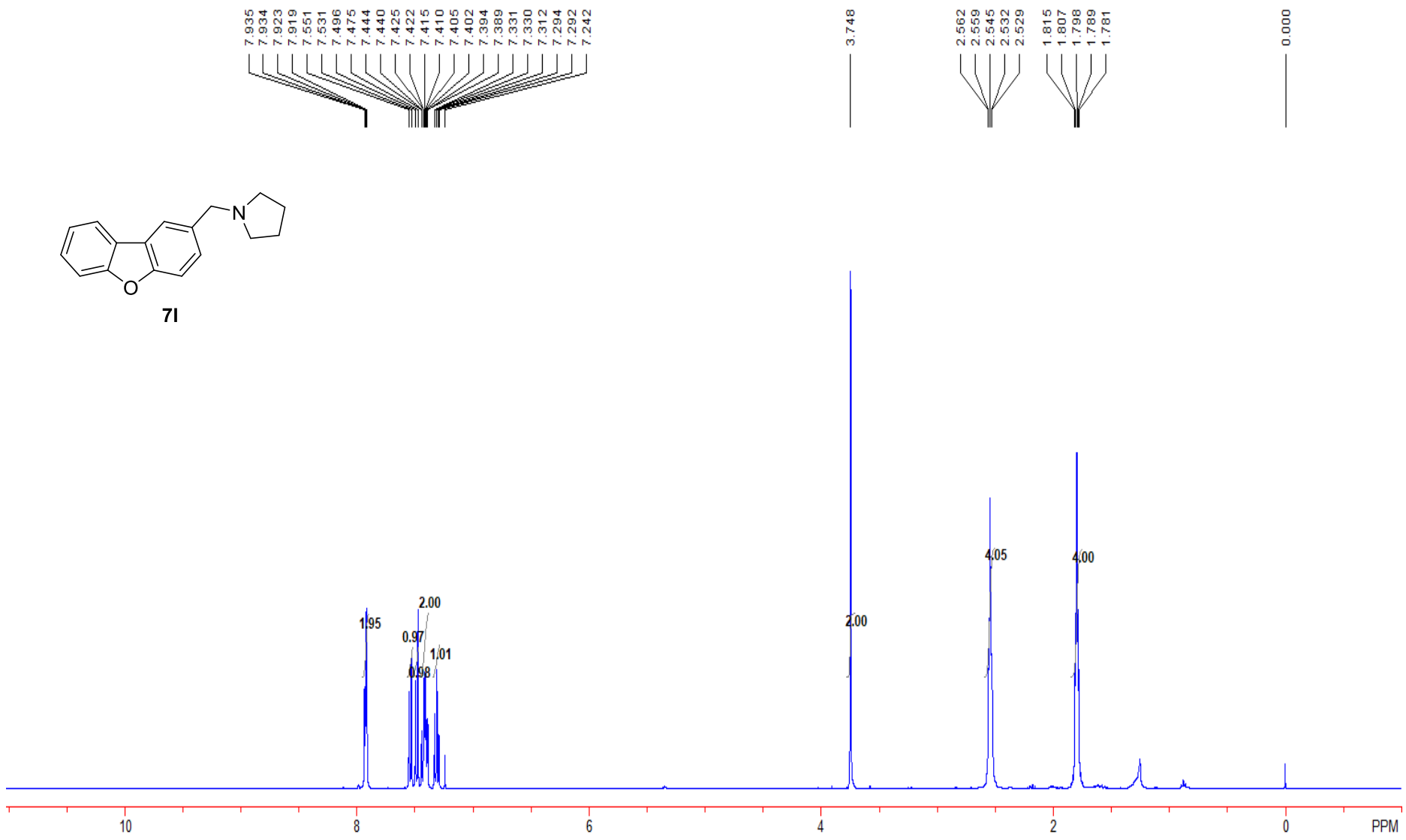
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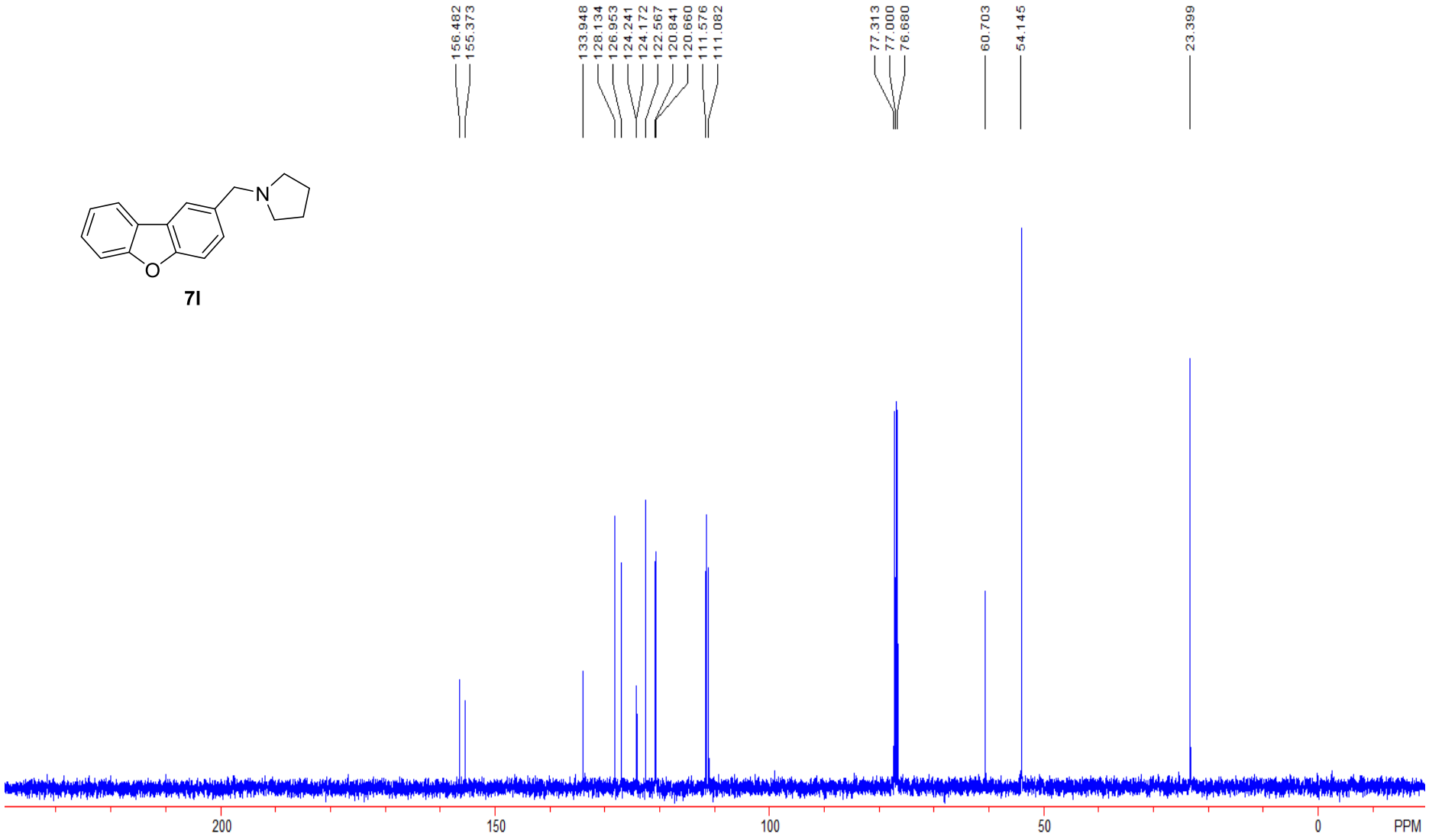
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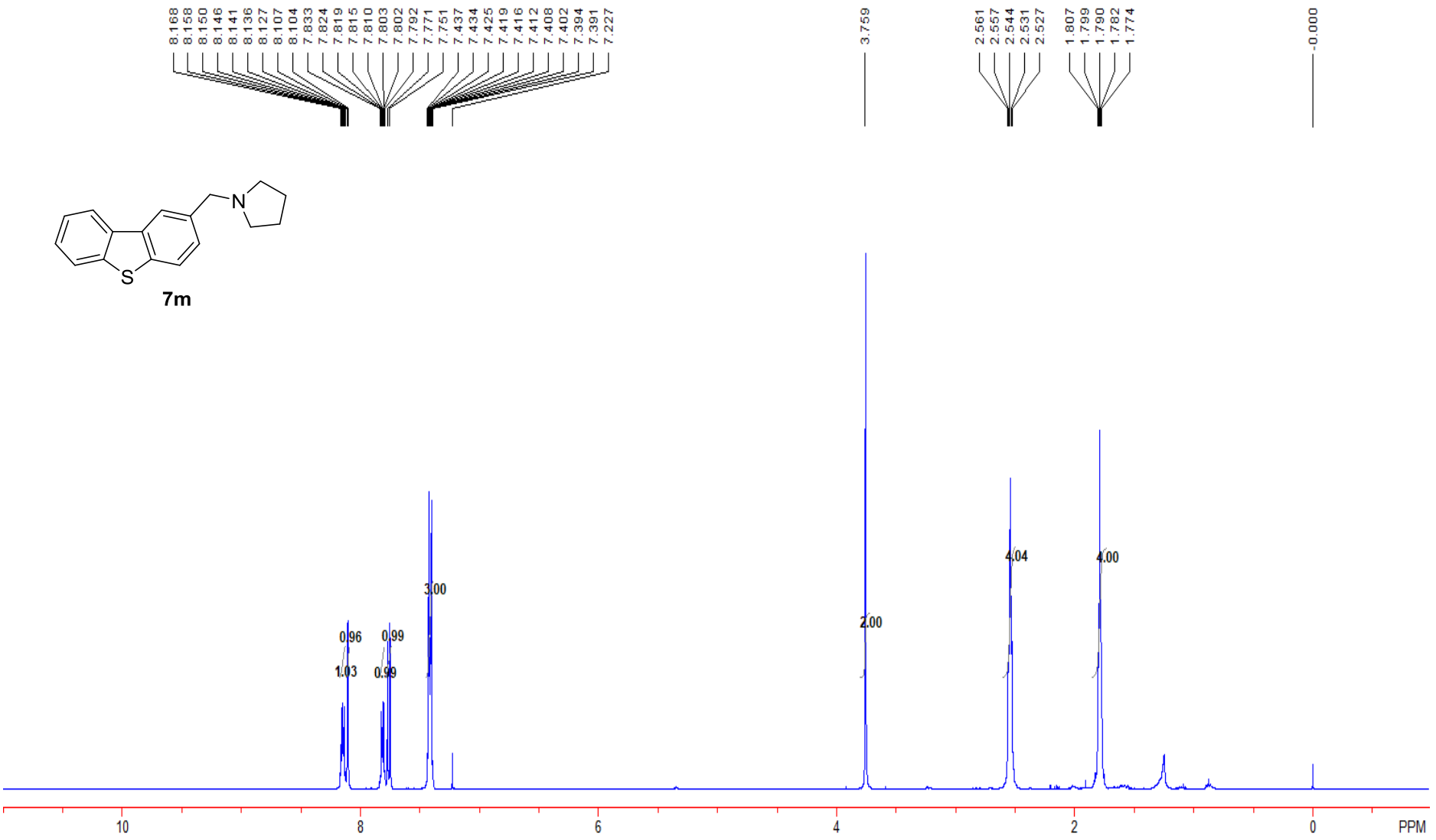
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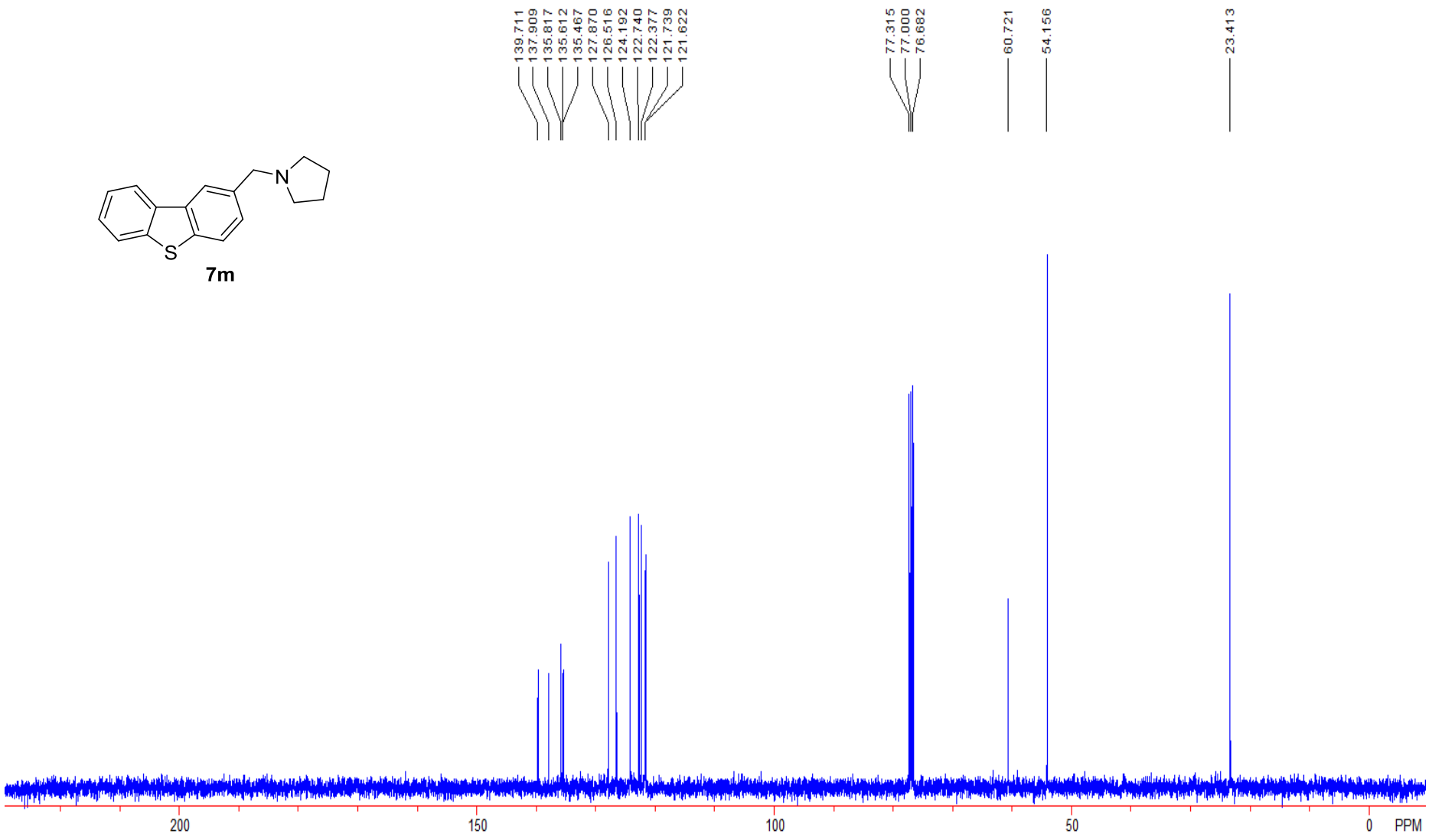
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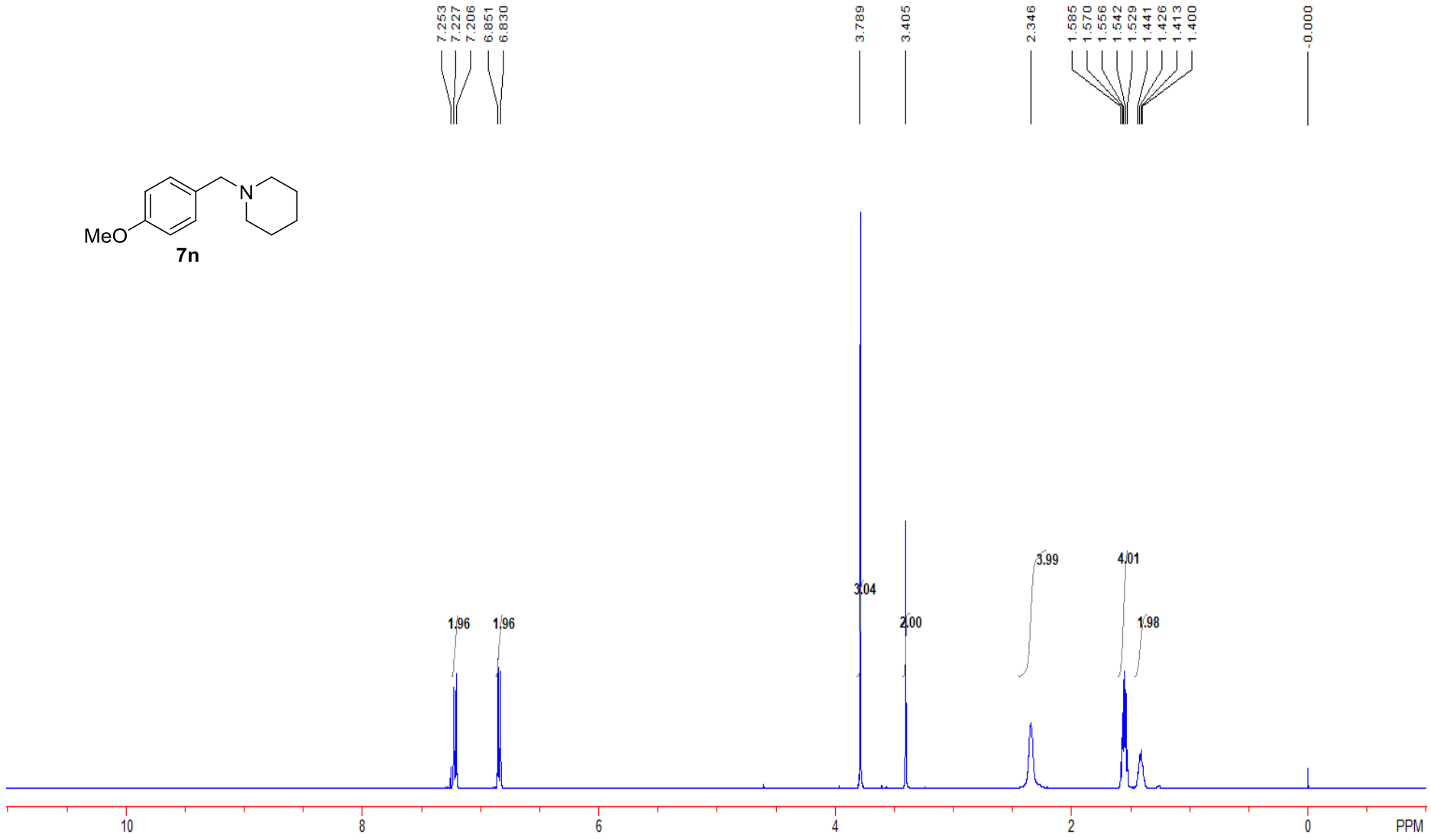
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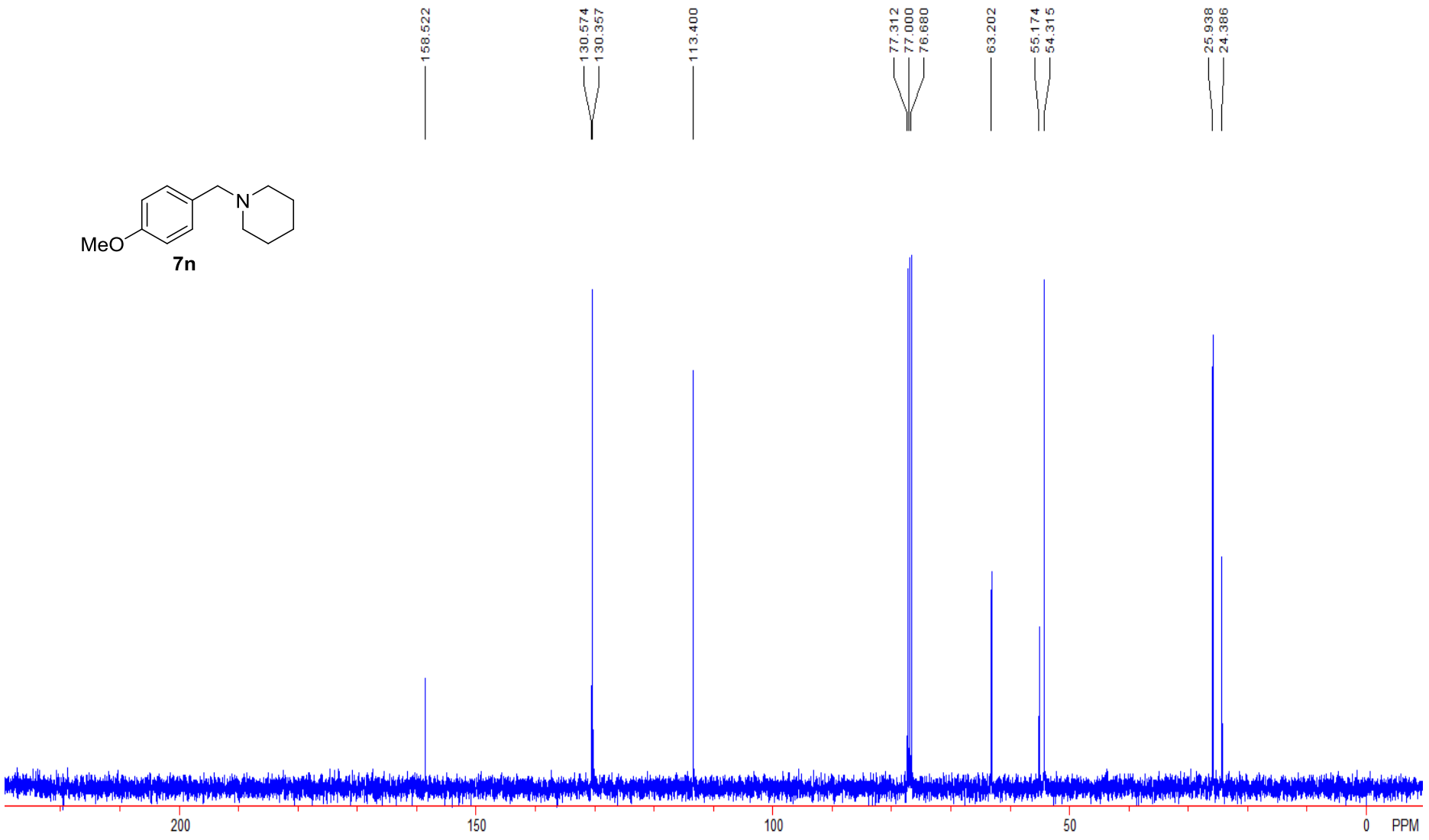
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