Supporting Information

Selective C−C Bond Formation from Rhodium-Catalyzed C−H Activation Reaction of 2-Arylpyridines with 3-Ary-2*H*-azirines

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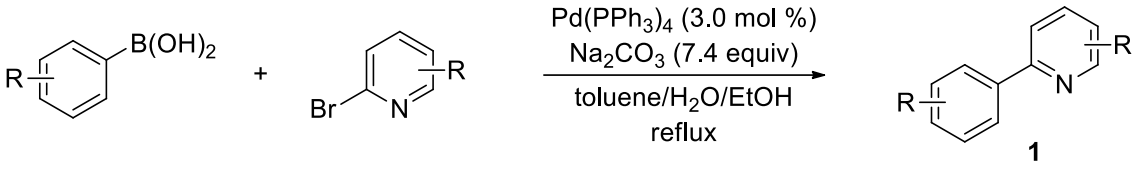
Contents

1. Experimental Section

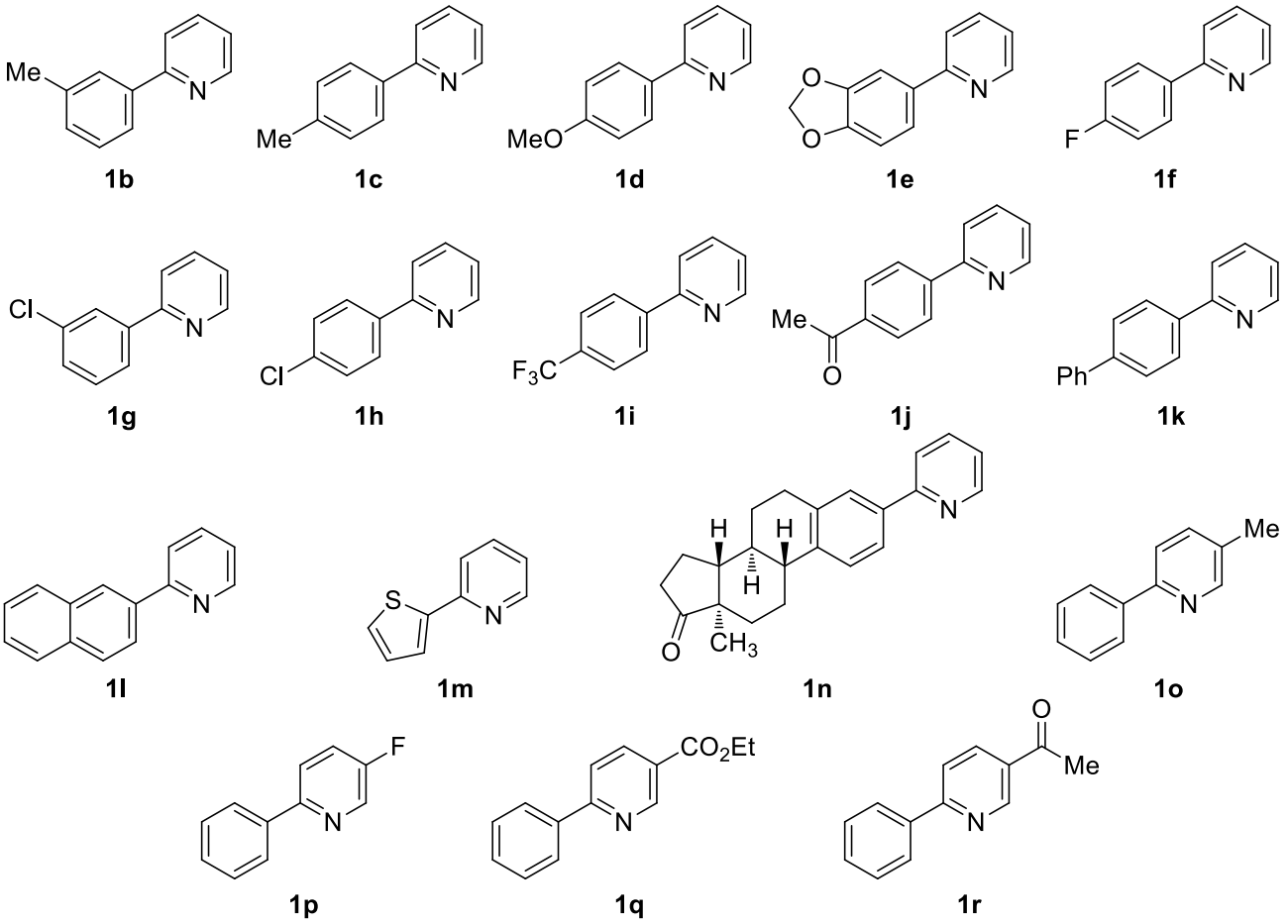
General: Commercial available reagents were used without purification. All reaction mixtures were stirred magnetically and were monitored by thin-layer chromatography using silica gel pre-coated glass plates, which were visualized with UV light and then, developed using either iodine or a solution of anisaldehyde. Flash column chromatography was carried out using silica gel (230-400 mesh). ^{1}H NMR (400 MHz), ^{13}C{^{1}H} NMR (100 MHz), and ^{19}F NMR (377 MHz) spectra were recorded on NMR spectrometer. Deuterated chloroform was used as the solvent and chemical shift values (δ) are reported in parts per million relative to the residual signals of this solvent [δ 7.26 for ^{1}H (chloroform-*d*), and δ 77.2 for ^{13}C{^{1}H} (chloroform-*d*)]. Infrared spectra were recorded on FT-IR spectrometer as either a thin film pressed between two sodium chloride plates or as a solid suspended in a potassium bromide disk. High resolution mass spectra (HRMS) were obtained by electron impact (EI) ionization technique (magnetic sector - electric sector double focusing mass analyzer) from the KBSI (Korea Basic Science Institute Daegu Center). Melting points were determined in open capillary tube.

2. General Procedure for the Preparation of Starting Materials

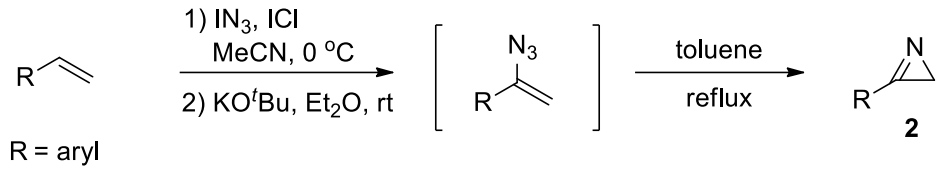
1) Preparation of 2-arylpyridines[1, 2]



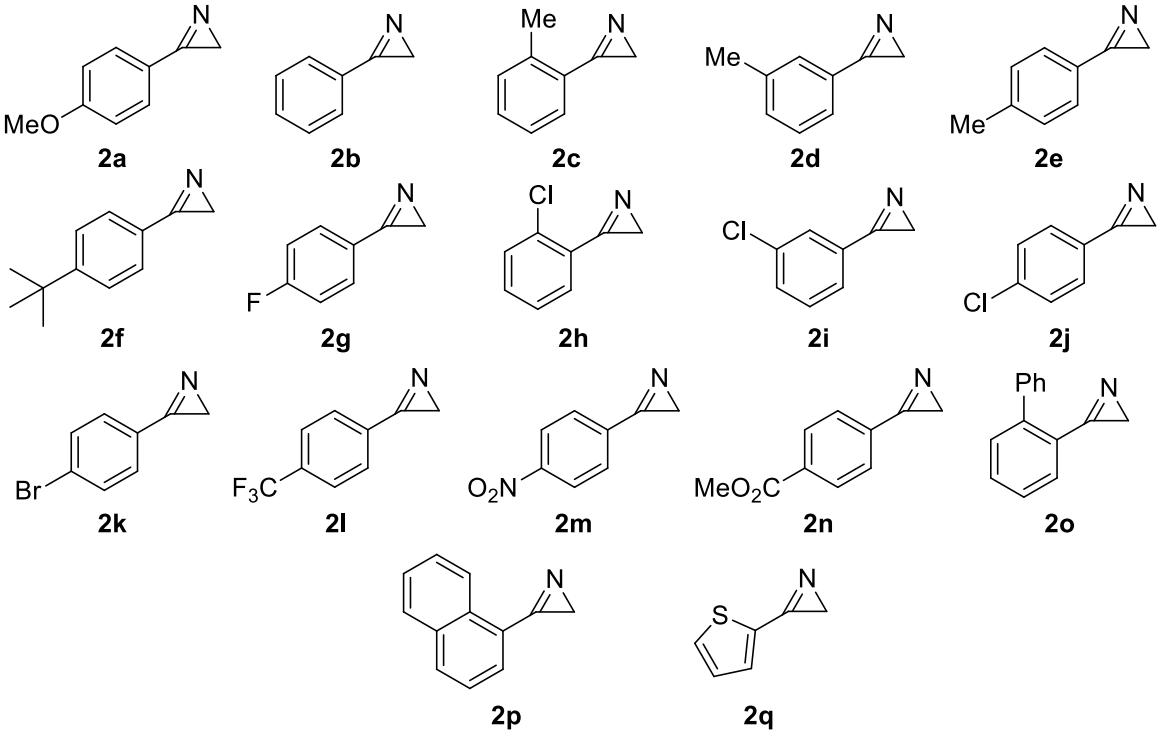
2-Bromopyridine (2.0 mmol, 1.0 equiv) was added to a solution of arylboronic acid (1.3 equiv), Na_2CO_3 (7.4 equiv), and $Pd(PPh_3)_4$ (3.0 mol %) in toluene (7.0 mL), ethanol (1.5 mL), and H_2O (7.0 mL) in 50 mL two-necked flask under a nitrogen atmosphere. After being refluxed at 110 ^oC for overnight, the reaction mixture was cooled to room temperature. The reaction mixture was quenched by aqueous NH_4Cl, extracted by EtOAc (3 x 20 mL, 60 mL), dried over $MgSO_4$, and evaporated in vacuo to afford the crude product, which was further purified by flash chromatography on silica gel with EtOAc and hexane to give the corresponding 2-arylpyridine in good yield.



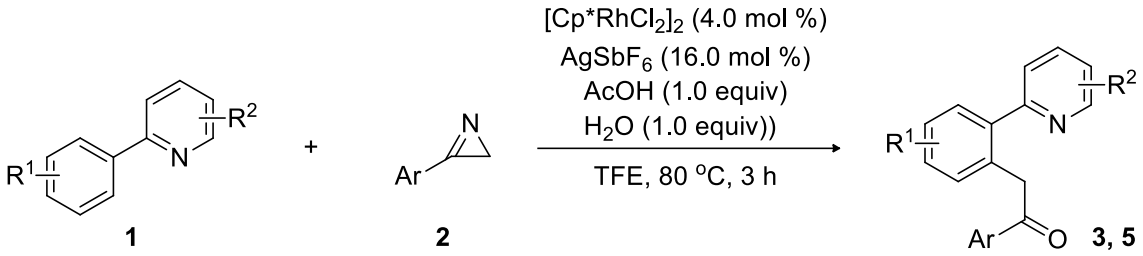
2) Preparation of azirines[3]



ICl 1.0 M solution (2.2 mmol, 1.1 equiv, 2.2 mL) was added to a solution of NaN_3 (4.0 mmol, 2.0 equiv, 260 mg) in MeCN (4.0 mL) at 0 °C. After being stirred at room temperature for 1.5 h, styrene (2.0 mmol, 1.0 equiv) in MeCN (4.0 mL) was added to the reaction mixture, which was stirred for 5 h. After the mixture was partitioned between ether and H_2O, the organic phase was separated, dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was dissolved in Et_2O (6.0 mL) and then, KO*t*-Bu (3.1 mmol, 350 mg) was added to reaction mixture. After being stirred for 5 h at room temperature, it was partitioned between ethyl acetate and H_2O and then, the organic phase was separated, dried with $MgSO_4$ and concentrated under reduced pressure. The crude product were purified by silica gel flash column chromatography (eluant: hexane) to give the corresponding vinyl azide. A solution of vinyl azide in toluene (0.5 M) was heated to 110 °C for 3 h. After the reaction mixture was cooled to room temperature, toluene was evaporated. The crude product was purified by flash column chromatography to give 2*H*-azirine in good yield.

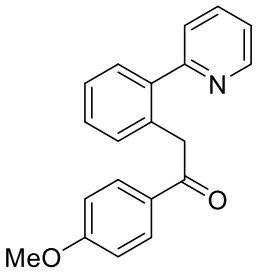


3. Procedure of the Rh-Catalyzed Acylmethylation of 2*H*-Azirines



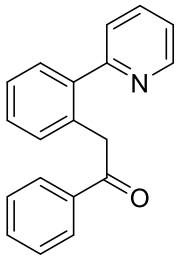
A dried test tube equipped with a magnetic stirrer was charged with 2-arylpyridine **1** (2.0 equiv), $[Cp^*RhCl_2]_2$ (4.0 mol %), $AgSbF_6$ (16.0 mol %), and TFE (1.0 mL) under a nitrogen atmosphere. 2*H*-Azirine **2** (0.2 mmol, 1.0 equiv) in TFE (1.0 mL), H_2O (1.0 equiv), and AcOH (1.0 equiv) were added to reaction mixture. After being stirred at 80 °C for 3 h, the reaction mixture was cooled to room temperature, filtered through a pad of Celite and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel.

1-(4-Methoxyphenyl)-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3a)[4]: Yield: 52.4 mg (86%); R_f = 0.3 (EtOAc: Hexane = 1:5); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (dq, *J* = 4.9 Hz, *J* = 0.9 Hz, 1H), 7.87 (dt, *J* = 9.7 Hz, *J* = 2.5 Hz, 2H), 7.68 (td, *J* = 11.6 Hz, *J* = 1.9 Hz, 1H), 7.48-7.46 (m, 1H), 7.44 (dt, *J* = 7.9 Hz, *J* = 1.0 Hz, 1H), 7.40-7.35 (m, 2H), 7.34-7.30 (m, 1H), 7.16 (ddd, *J* = 7.6 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 6.88 (dt, *J* = 9.7 Hz, *J* = 2.5 Hz, 2H), 4.46 (s, 2H), 3.85 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 196.7, 163.3, 159.7, 148.9, 140.2, 136.7, 133.7, 131.7, 130.7, 130.2, 130.0, 128.6, 127.2, 124.0, 121.8, 113.7, 55.5, 43.2.



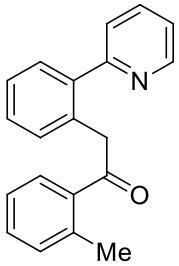
3a

1-Phenyl-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3b)[5]: Yield: 46.0 mg (84%); R_f = 0.3 (EtOAc: Hexane = 1:5); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (dq, *J* = 4.8 Hz, *J* = 0.8 Hz, 1H), 7.90-7.88 (m, 2H), 7.67 (td, *J* = 11.6 Hz, *J* = 1.7 Hz, 1H), 7.53-7.48 (m, 2H), 7.45 (dt, *J* = 7.9 Hz, *J* = 0.9 Hz, 1H), 7.42-7.37 (m, 4H), 7.35-7.31 (m, 1H), 7.12 (ddd, *J* = 7.5 Hz, *J* = 4.9 Hz, *J* = 0.9 Hz, 1H), 4.51 (s, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 198.0, 159.6, 148.7, 140.1, 137.2, 136.7, 133.4, 132.8, 132.0, 129.9, 128.7, 128.5, 128.3, 127.4, 123.9, 121.8, 43.7.



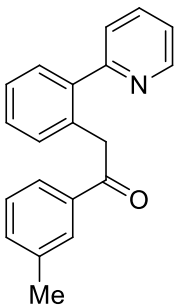
3b

2-(2-(Pyridin-2-yl)phenyl)-1-(*o*-tolyl)ethanone (3c): Yield: 52.3 mg (89%); R_f = 0.3 (EtOAc: Hexane = 1:5); Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40-8.39 (m, 1H), 7.67 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.49-7.47 (m, 1H), 7.45-7.38 (m, 3H), 7.36-7.30 (m, 2H), 7.21-7.12 (m, 3H), 4.45 (s, 2H), 2.37 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 201.5, 159.7, 148.6, 140.1, 138.4, 138.3, 136.7, 133.5, 132.2, 131.8, 131.0, 130.0, 128.7, 128.3, 127.4, 125.6, 124.0, 121.8, 46.7, 21.1; IR (film): 3063, 2968, 1688, 1587, 1426, 1321, 1216, 988, 751 cm^{-1}; HRMS (EI) *m/z*: [M]$^+$ Calcd for $C_{20}H_{17}NO$ 287.1310; Found 287.1307.



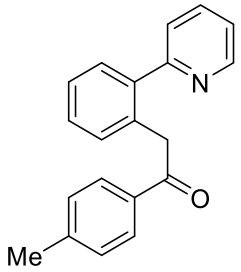
3c

2-(2-(Pyridin-2-yl)phenyl)-1-(*m*-tolyl)ethan-1-one (3d): Yield: 50.7 mg (88%); R_f = 0.3 (EtOAc: Hexane = 1:5); Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (dq, J = 4.8 Hz, J = 0.8 Hz, 1H), 7.71-7.66 (m, 3H), 7.49-7.47 (m, 1H), 7.45 (dt, J = 7.9 Hz, J = 0.9 Hz, 1H), 7.39-7.37 (m, 2H), 7.34-7.27 (m, 3H), 7.14 (ddd, J = 7.5 Hz, J = 4.9 Hz, J = 1.0 Hz, 1H), 4.51 (s, 2H), 2.37 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 198.2, 159.7, 148.8, 140.2, 138.3, 137.3, 136.7, 133.6, 133.5, 131.9, 130.0, 128.9, 128.7, 128.4, 127.3, 125.6, 124.0, 121.8, 43.6, 21.5; IR (film): 3058, 2918, 1685, 1586, 1426, 1245, 1157, 1024, 794, 752, 691 cm^{-1}; HRMS (EI) *m/z*: [M]$^+$ Calcd for $C_{20}H_{17}NO$ 287.1310; Found 287.1311.



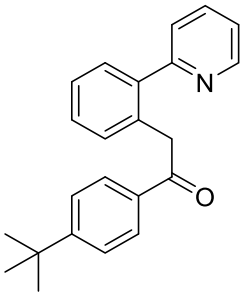
3d

2-(2-(Pyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (3e)[6]: Yield: 52.4 mg (91%); R_f = 0.3 (EtOAc: Hexane = 1:5); Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (dq, J = 4.8 Hz, J = 0.9 Hz, 1H), 7.78 (dt, J = 8.5 Hz, J = 1.8 Hz, 2H), 7.67 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.49-7.47 (m, 1H), 7.44 (dt, J = 7.9 Hz, J = 1.0 Hz, 1H), 7.40-7.35 (m, 2H), 7.34-7.30 (m, 1H), 7.20 (d, J = 8.0 Hz, 2H), 7.14 (ddd, J = 7.6 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 4.48 (s, 2H), 2.38 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.7, 159.7, 148.9, 143.5, 140.2, 136.7, 134.7, 133.6, 131.9, 130.0, 129.2, 128.7, 128.5, 127.3, 124.0, 121.8, 43.5, 21.7.



3e

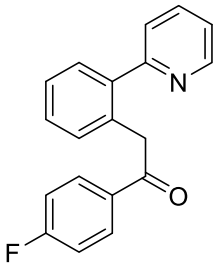
1-(4-(*tert*-Butyl)phenyl)-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3f): Yield: 47.9 mg (73%); R_f = 0.4 (EtOAc: Hexane = 1:5); Red oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (dq, J = 4.8 Hz, J = 0.8 Hz, 1H), 7.83 (dt, J = 9.1 Hz, J = 2.1 Hz, 2H), 7.67 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.50-7.42 (m, 3H), 7.41-7.39 (m, 1H), 7.38-7.34 (m, 2H), 7.33-7.29 (m, 1H), 7.15 (ddd, J = 7.5 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 4.50 (s, 2H), 1.32 (s, 9H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.7, 159.7, 156.5, 148.9, 140.3, 136.6, 134.6, 133.5, 131.7, 130.0, 128.6, 128.4, 127.3, 125.5, 124.0, 121.8, 43.5, 35.2, 31.2; IR (film): 3058, 2963, 1684, 1604, 1471, 1331, 1222, 995, 752 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{23}H_{23}NO$ 329.1780; Found 329.1780.



3f

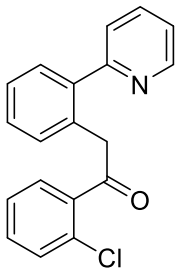
1-(4-Fluorophenyl)-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3g): Yield: 44.8 mg (77%); R_f = 0.3 (EtOAc: Hexane = 1:5); Beige solid; Melting point: 63-65 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (dq, J = 4.8 Hz, J = 0.9 Hz, 1H), 7.94-7.89 (m, 2H), 7.68 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.51-7.48 (m, 1H), 7.45 (dt, J = 7.9 Hz, J = 0.9 Hz, 1H), 7.40-7.35 (m, 2H), 7.34-7.30 (m, 1H), 7.13 (ddd, J =

7.5 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 7.09-7.04 (m, 2H), 4.48 (s, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 196.5, 165.6 (d, *J* = 254.0 Hz), 159.5, 148.7, 139.9, 136.7, 133.6 (d, *J* = 2.9 Hz), 133.3, 131.9, 131.0 (d, *J* = 9.1 Hz), 130.0, 128.7, 127.4, 123.9, 121.9, 115.6 (d, *J* = 21.7 Hz), 43.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.94; IR (film): 3063, 2911, 1687, 1597, 1331, 1220, 1156, 997, 835, 752 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{19}H_{14}FNO$ 291.1059; Found 291.1062.



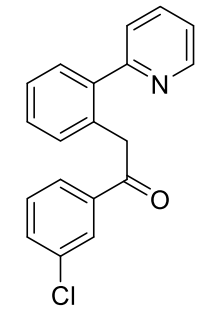
3g

1-(2-Chlorophenyl)-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3h): Yield: 35.2 mg (57%); R_f = 0.3 (EtOAc: Hexane = 1:5); Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (dq, *J* = 4.9 Hz, *J* = 0.9 Hz, 1H), 7.68 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.47-7.45 (m, 1H), 7.43-7.37 (m, 4H), 7.36-7.29 (m, 3H), 7.26-7.22 (m, 1H), 7.15 (ddd, *J* = 7.5 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 4.49 (s, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 200.5, 159.5, 148.6, 140.2, 139.7, 136.7, 132.7, 132.4, 131.4, 130.8, 130.4, 129.9, 129.4, 128.7, 127.6, 126.7, 123.9, 121.9, 48.0; IR (film): 3062, 1699, 1587, 1427, 1324, 1211, 1066, 991, 753 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{19}H_{14}ClNO$ 307.0764; Found 307.0765.



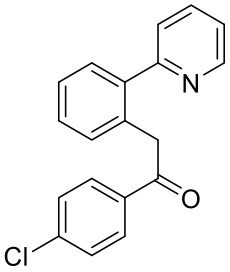
3h

1-(3-Chlorophenyl)-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3i): Yield: 40.7 mg (66%); R_f = 0.2 (EtOAc: Hexane = 1:5); Beige solid; Melting point: 85-87 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dq, *J* = 4.8 Hz, *J* = 0.9 Hz, 1H), 7.86 (t, *J* = 1.8 Hz, 1H), 7.77 (dt, *J* = 7.8 Hz, *J* = 1.3 Hz, 1H), 7.69 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.51-7.45 (m, 3H), 7.41-7.38 (m, 2H), 7.37-7.31 (m, 2H), 7.14 (ddd, *J* = 7.5 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 4.50 (s, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 196.7, 159.4, 148.6, 139.8, 138.9, 136.8, 134.8, 133.0, 132.7, 132.1, 130.0, 129.9, 128.8, 128.5, 127.6, 126.4, 123.8, 121.9, 43.8; IR (film): 3064, 2923, 1692, 1587, 1425, 1329, 1211, 997, 788, 750 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{19}H_{14}ClNO$ 307.0764; Found 307.0761.



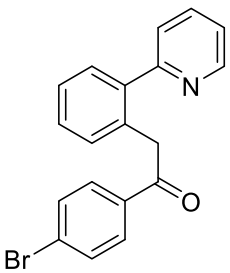
3i

1-(4-Chlorophenyl)-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3j): Yield: 38.2 mg (62%); R_f = 0.3 (EtOAc: Hexane = 1:5); Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (dq, J = 4.9 Hz, J = 0.9 Hz, 1H), 7.84 (dt, J = 9.1 Hz, J = 2.1 Hz, 2H), 7.69 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.51-7.48 (m, 1H), 7.46 (dt, J = 7.9 Hz, J = 0.9 Hz, 1H), 7.40-7.37 (m, 4H), 7.33-7.30 (m, 1H), 7.14 (ddd, J = 7.6 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 4.47 (s, 2H) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 196.8, 159.5, 148.7, 139.8, 139.1, 136.8, 135.6, 133.2, 132.0, 130.0, 129.8, 128.9, 128.8, 127.5, 123.9, 121.9, 43.7; IR (film): 3060, 2905, 1688, 1587, 1426, 1331, 1213, 1090, 996, 803, 753 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{19}H_{14}ClNO$ 307.0764; Found 307.0766.



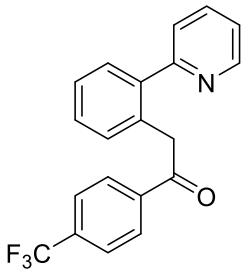
3j

1-(4-Bromophenyl)-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3k)[4]: Yield: 52.6 mg (75%); R_f = 0.3 (EtOAc: Hexane = 1:5); Brown solid; Melting point: 86-88 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (dq, J = 4.9 Hz, J = 0.8 Hz, 1H), 7.76 (dt, J = 9.0 Hz, J = 2.1 Hz, 2H), 7.68 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.54 (dt, J = 9.0 Hz, J = 2.1 Hz, 2H), 7.51-7.48 (m, 1H), 7.45 (dt, J = 7.9 Hz, J = 0.9 Hz, 1H), 7.40-7.36 (m, 2H), 7.33-7.30 (m, 1H), 7.13 (ddd, J = 7.5 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 4.46 (s, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.0, 159.4, 148.7, 139.8, 136.8, 136.0, 133.2, 132.0, 131.8, 129.9 (2C), 128.8, 127.8, 127.5, 123.8, 121.9, 43.7.



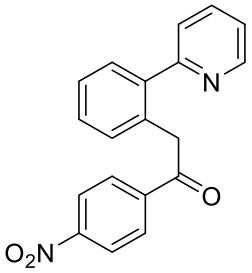
3k

2-(2-(Pyridin-2-yl)phenyl)-1-(4-(trifluoromethyl)phenyl)ethan-1-one (3l): Yield: 36.6 mg (54%); R_f = 0.4 (EtOAc: Hexane = 1:5); Beige solid; Melting point: 98-100 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.28 (dq, J = 4.9 Hz, J = 0.9 Hz, 1H), 8.01 (d, J = 8.1 Hz, 2H), 7.73-7.67 (m, 3H), 7.54-7.51 (m, 1H), 7.48 (dt, J = 7.9 Hz, J = 1.0 Hz, 1H), 7.43-7.38 (m, 2H), 7.36-7.32 (m, 1H), 7.13 (ddd, J = 7.6 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 4.53 (s, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 197.0, 159.4, 148.6, 140.1, 139.6, 136.9, 134.0 (q, J = 32.6 Hz), 133.0, 132.2, 130.0, 128.9, 128.7, 127.7, 125.6 (q, J = 3.7 Hz), 123.82 (q, J = 272.4 Hz), 123.81, 122.0, 44.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.02; IR (film): 3062, 2921, 1693, 1587, 1322, 1127, 1066, 834, 752 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{20}H_{14}F_3NO$ 341.1027; Found 341.1030.



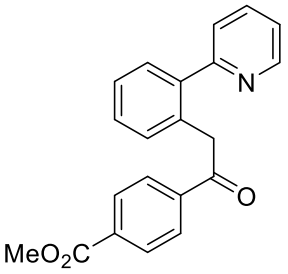
3l

1-(4-Nitrophenyl)-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3m): Yield: 26.9 mg (42%); R_f = 0.2 (EtOAc: Hexane = 1:5); Orange solid; Melting point: 128-130 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.27 (dt, J = 9.1 Hz, J = 2.1 Hz, 2H), 8.20 (dq, J = 4.8 Hz, J = 0.8 Hz, 1H), 8.07 (dt, J = 9.1 Hz, J = 2.1 Hz, 2H), 7.71 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.55-7.50 (m, 2H), 7.44-7.40 (m, 2H), 7.37-7.33 (m, 1H), 7.12 (ddd, J = 7.5 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 4.53 (s, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 196.4, 159.1, 150.1, 148.3, 142.1, 139.2, 137.0, 132.7, 132.3, 130.0, 129.3, 128.9, 127.8, 123.8, 123.7, 122.0, 44.5; IR (film): 2924, 1693, 1522, 1346, 1211, 999, 855, 750 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{19}H_{14}N_2O_3$ 318.1004; Found 318.1008.



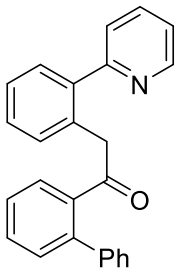
3m

Methyl 4-(2-(2-(pyridin-2-yl)phenyl)acetyl)benzoate (3n): Yield: 33.2 mg (50%); R_f = 0.2 (EtOAc: Hexane = 1:5); Ivory solid; Melting point: 63-65 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (dq, J = 4.9 Hz, J = 0.9 Hz, 1H), 8.08 (dt, J = 8.3 Hz, J = 1.7 Hz, 2H), 7.94 (dt, J = 8.3 Hz, J = 1.7 Hz, 2H), 7.68 (td, J = 11.6 Hz, J = 1.9 Hz, 1H), 7.53-7.49 (m, 1H), 7.47 (dt, J = 7.9 Hz, J = 1.0 Hz, 1H), 7.43-7.37 (m, 2H), 7.37-7.32 (m, 1H), 7.11 (ddd, J = 7.5 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 4.52 (s, 2H), 3.94 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.5, 166.5, 159.4, 148.6, 140.8, 139.7, 136.8, 133.5, 133.2, 132.2, 129.9, 129.8, 128.8, 128.2, 127.6, 123.8, 121.9, 52.5, 44.2; IR (film): 3059, 2951, 1724, 1692, 1427, 1280, 1213, 1109, 997, 753 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{21}H_{17}NO_3$ 331.1208; Found 331.1210.



3n

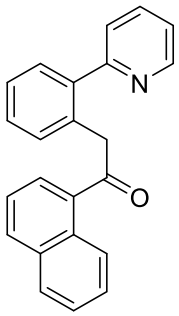
1-([1,1'-Biphenyl]-2-yl)-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3o): Yield: 58.0 mg (83%); R_f = 0.2 (EtOAc: Hexane = 1:5); Ruby solid; Melting point: 101-103 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (dq, J = 4.8 Hz, J = 0.8 Hz, 1H), 7.63 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.42 (td, J = 11.1 Hz, J = 1.7 Hz, 1H), 7.38-7.33 (m, 4H), 7.32-7.31 (m, 1H), 7.30-7.23 (m, 7H), 7.14 (ddd, J = 7.6 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 6.97-6.95 (m, 1H), 3.81 (s, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 204.7, 159.6, 148.7, 141.0, 140.7, 140.4, 139.9, 136.5, 132.8, 131.7, 130.2, 130.1, 129.8, 129.0, 128.7, 128.4, 128.0, 127.9, 127.3, 127.2, 123.9, 121.7, 47.5; IR (film): 3058, 2919, 1693, 1587, 1471, 1426, 1209, 990, 749, 701 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{25}H_{19}NO$ 349.1467; Found 349.1464.



3o

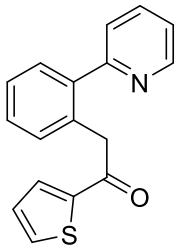
1-(Naphthalen-1-yl)-2-(2-(pyridin-2-yl)phenyl)ethan-1-one (3p): Yield: 54.3 mg (84%); R_f = 0.2 (EtOAc: Hexane = 1:5); Orange oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45-8.41 (m, 1H), 8.19 (dq, J = 4.9 Hz, J = 0.9 Hz, 1H), 7.92 (d, J = 8.2 Hz, 1H), 7.85-7.81 (m, 1H), 7.75 (dd, J = 7.2 Hz, J = 1.1 Hz,

1H), 7.61 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.51-7.46 (m, 3H), 7.45-7.37 (m, 5H), 7.03 (ddd, *J* = 7.5 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 4.60 (s, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 201.4, 159.6, 148.6, 140.1, 136.65, 136.58, 134.0, 133.6, 132.3, 132.2, 130.3, 130.0, 128.7, 128.3, 127.7, 127.5, 127.0, 126.4, 126.2, 124.4, 123.9, 121.8, 47.4; IR (film): 3049, 2922, 1689, 1587, 1426, 1231, 1093, 948, 779, 752 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{23}H_{17}NO$ 323.1310; Found 323.1311.



3p

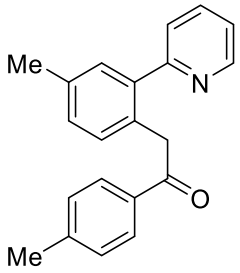
2-(2-(Pyridin-2-yl)phenyl)-1-(thiophen-2-yl)ethan-1-one (3q)[4]: Yield: 39.4 mg (71%); R_f = 0.1 (EtOAc: Hexane = 1:5); Moss green solid; Melting point: 78-80 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (dq, *J* = 4.8 Hz, *J* = 0.9 Hz, 1H), 7.69 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.60 (dd, *J* = 3.8 Hz, *J* = 1.1 Hz, 1H), 7.56 (dd, *J* = 5.0 Hz, *J* = 1.1 Hz, 1H), 7.49-7.44 (m, 2H), 7.40-7.34 (m, 3H), 7.17 (ddd, *J* = 7.6 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 7.05 (dd, *J* = 4.9 Hz, *J* = 3.8 Hz, 1H), 4.44 (s, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 190.8, 159.6, 148.8, 144.3, 140.3, 136.7, 133.4, 133.0, 132.1, 131.8, 130.0, 128.7, 128.0, 127.5, 124.1, 121.9, 44.2.



3q

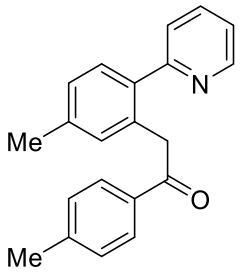
2-(4-Methyl-2-(pyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (5a): Yield: 47.6 mg (79%); R_f = 0.4 (EtOAc: Hexane = 1:5); Ivory solid; Melting point: 99-101 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (dq, *J* = 4.9 Hz, *J* = 0.8 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 2H), 7.65 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.43 (dt, *J* = 7.9 Hz, *J* = 0.9 Hz, 1H), 7.29 (s, 1H), 7.19-7.17 (m, 4H), 7.13 (ddd, *J* = 7.5 Hz, *J* = 4.9 Hz, *J* = 1.0 Hz, 1H), 4.42 (s, 2H), 2.382 (s, 3H), 2.375 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 197.9, 159.8, 148.9, 143.5, 140.1, 136.8, 136.5, 134.7, 131.6, 130.7, 130.4, 129.4, 129.2, 128.5, 124.0,

121.8, 43.1, 21.7, 21.2; IR (film): 3017, 2919, 1685, 1606, 1427, 1330, 1223, 1000, 779 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{21}H_{19}NO$ 301.1467; Found 301.1465.



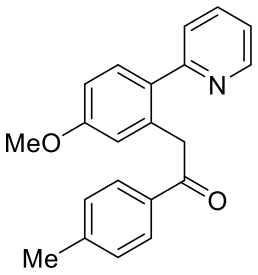
5a

2-(5-Methyl-2-(pyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (5b): Yield: 53.0 mg (88%); R_f = 0.3 (EtOAc: Hexane = 1:5); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (dq, *J* = 4.8 Hz, *J* = 0.9 Hz, 1H), 7.79 (dt, *J* = 8.4 Hz, *J* = 1.8 Hz, 2H), 7.65 (td, *J* = 11.6 Hz, *J* = 1.9 Hz, 1H), 7.42 (dt, *J* = 7.9 Hz, *J* = 1.0 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.20-7.16 (m, 3H), 7.13-7.09 (m, 2H), 4.46 (s, 2H), 2.383 (s, 3H), 2.375 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.9, 159.7, 148.8, 143.5, 138.5, 137.4, 136.6, 134.8, 133.4, 132.6, 129.9, 129.2, 128.5, 128.1, 123.9, 121.6, 43.5, 21.7, 21.3; IR (film): 3049, 2919, 1685, 1606, 1467, 1331, 1181, 1012, 780, 748 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{21}H_{19}NO$ 301.1467; Found 301.1469.



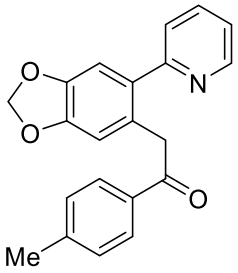
5b

2-(5-Methoxy-2-(pyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (5c): Yield: 56.4 mg (89%); R_f = 0.2 (EtOAc: Hexane = 1:5); Brown solid; Melting point: 55-57 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (dq, *J* = 4.9 Hz, *J* = 0.8 Hz, 1H), 7.79 (dt, *J* = 8.5 Hz, *J* = 1.9 Hz, 2H), 7.64 (td, *J* = 11.6 Hz, *J* = 1.9 Hz, 1H), 7.44-7.40 (m, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 7.09 (ddd, *J* = 7.5 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 6.90 (dd, *J* = 8.5 Hz, *J* = 2.6 Hz, 1H), 6.85 (d, *J* = 2.6 Hz, 1H), 4.49 (s, 2H), 3.38 (s, 3H), 2.39 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.6, 159.8, 159.4, 148.8, 143.5, 136.6, 135.2, 134.7, 132.9, 131.2, 129.3, 128.6, 123.7, 121.4, 117.3, 112.8, 55.4, 43.8, 21.7; IR (film): 3004, 2922, 1685, 1607, 1466, 1241, 1181, 1045, 782 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{21}H_{19}NO_2$ 317.1416; Found 317.1413.



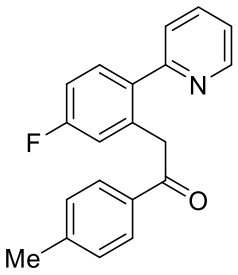
5c

2-(6-(Pyridin-2-yl)benzo[d][1,3]dioxol-5-yl)-1-(*p*-tolyl)ethan-1-one (5d): Yield: 58.9 mg (89%); R_f = 0.3 (EtOAc: Hexane = 1:5); Beige solid; Melting point: 119-121 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.34 (dq, *J* = 4.8 Hz, *J* = 0.9 Hz, 1H), 7.84 (dt, *J* = 8.4 Hz, *J* = 1.8 Hz, 2H), 7.62 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.41 (dt, *J* = 7.9 Hz, *J* = 1.0 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.07 (ddd, *J* = 7.5 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 5.99 (s, 2H), 4.50 (s, 2H), 2.40 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 196.4, 159.0, 148.7, 147.7, 147.4, 143.6, 136.6, 134.7, 134.6, 129.3, 128.4, 123.60, 123.57, 121.5, 115.9, 107.2, 101.4, 37.2, 21.8; IR (film): 3051, 2899, 1685, 1586, 1455, 1255, 1056, 932, 781 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{21}H_{17}NO_3$ 331.1208; Found 331.1207.



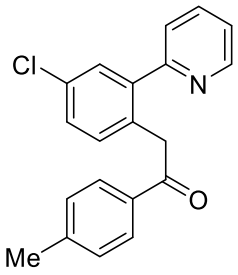
5d

2-(5-Fluoro-2-(pyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (5e): Yield: 50.7 mg (83%); R_f = 0.4 (EtOAc: Hexane = 1:5); Ivory solid; Melting point: 88-90 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.41 (dq, *J* = 4.8 Hz, *J* = 0.8 Hz, 1H), 7.77 (dt, *J* = 8.5 Hz, *J* = 1.8 Hz, 2H), 7.66 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.45 (dd, *J* = 8.3 Hz, *J* = 5.9 Hz, 1H), 7.40 (dt, *J* = 7.9 Hz, *J* = 1.0 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.13 (ddd, *J* = 7.5 Hz, *J* = 4.9 Hz, *J* = 1.0 Hz, 1H), 7.08-7.02 (m, 2H), 4.47 (s, 2H), 2.39 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 197.0, 162.7 (d, *J* = 247.8 Hz), 158.8, 148.9, 143.8, 136.8, 136.4 (d, *J* = 3.4 Hz), 136.1 (d, *J* = 8.0 Hz), 134.5, 131.6 (d, *J* = 8.4 Hz), 129.3, 128.5, 123.9, 121.9, 118.7 (d, *J* = 21.6 Hz), 114.2 (d, *J* = 21.1 Hz), 43.4, 21.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.82; IR (film): 3053, 2920, 1684, 1607, 1430, 1330, 1227, 1006, 782 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{20}H_{16}FNO$ 305.1216; Found 305.1214.



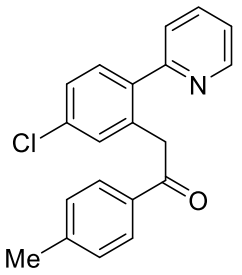
5e

2-(4-Chloro-2-(pyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (5f): Yield: 39.3 mg (61%); R_f = 0.4 (EtOAc: Hexane = 1:5); Ivory solid; Melting point: 107-109 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (dq, *J* = 4.8 Hz, *J* = 0.8 Hz, 1H), 7.77 (d, *J* = 8.1 Hz, 2H), 7.68 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.48 (d, *J* = 2.2 Hz, 1H), 7.43 (dt, *J* = 7.9 Hz, *J* = 0.9 Hz, 1H), 7.35 (dd, *J* = 8.2 Hz, *J* = 2.2 Hz, 1H), 7.23-7.15 (m, 4H), 4.45 (s, 2H), 2.39 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.2, 158.4, 149.0, 143.8, 141.8, 136.9, 134.5, 133.3, 133.0, 132.2, 129.9, 129.3, 128.6, 128.5, 123.9, 122.3, 42.9, 21.8; IR (film): 3053, 2919, 1683, 1606, 1427, 1329, 1222, 1000, 777 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{20}H_{16}ClNO$ 321.0920; Found 321.0921.



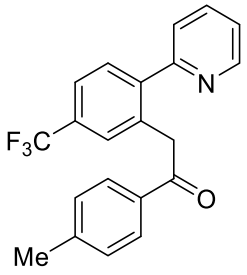
5f

2-(5-Chloro-2-(pyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (5g): Yield: 45.1 mg (70%); R_f = 0.4 (EtOAc: Hexane = 1:5); Yellow solid; Melting point: 108-110 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (dq, *J* = 4.8 Hz, *J* = 0.9 Hz, 1H), 7.78 (dt, *J* = 8.5 Hz, *J* = 1.8 Hz, 2H), 7.67 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.43-7.40 (m, 2H), 7.36-7.31 (m, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.14 (ddd, *J* = 7.6 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 4.47 (s, 2H), 2.39 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 196.9, 158.6, 148.9, 143.8, 138.7, 136.8, 135.6, 134.5, 134.4, 132.0, 131.1, 129.3, 128.5, 127.5, 123.9, 122.1, 43.3, 21.8; IR (film): 3054, 2919, 1684, 1587, 1465, 1328, 1222, 1002, 808, 779 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{20}H_{16}ClNO$ 321.0920; Found 321.0918.



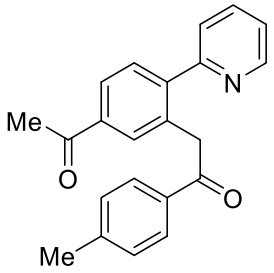
5g

2-(2-(Pyridin-2-yl)-5-(trifluoromethyl)phenyl)-1-(*p*-tolyl)ethan-1-one (5h): Yield: 46.2 mg (65%); R_f = 0.2 (EtOAc: Hexane = 1:5); Beige solid; Melting point: 97-99 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.42 (dq, *J* = 4.8 Hz, *J* = 0.8 Hz, 1H), 7.78 (dt, *J* = 8.5 Hz, *J* = 1.7 Hz, 2H), 7.70 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.63 (dd, *J* = 8.1 Hz, *J* = 1.2 Hz, 1H), 7.59 (d, *J* = 7.9 Hz, 2H), 7.46 (dt, *J* = 7.9 Hz, *J* = 0.9 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.17 (ddd, *J* = 7.6 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 4.56 (s, 2H), 2.40 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 196.7, 158.4, 149.0, 143.9, 143.7, 136.9, 134.7, 134.4, 130.6 (q, *J* = 32.5 Hz), 130.3, 129.4, 129.0 (q, *J* = 3.7 Hz), 128.4, 124.21 (q, *J* = 272.3 Hz), 124.19 (q, *J* = 3.8 Hz), 124.0, 122.5, 43.4, 21.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.50; IR (film): 3054, 2920, 1685, 1607, 1468, 1334, 1124, 1002, 781 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{21}H_{16}F_3NO$ 355.1184; Found 355.1188.



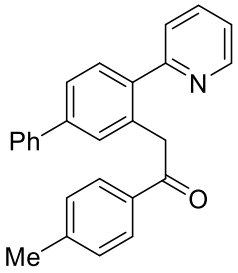
5h

2-(5-Acetyl-2-(pyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (5i): Yield: 48.8 mg (74%); R_f = 0.1 (EtOAc: Hexane = 1:5); Brown solid; Melting point: 100-102 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.41 (dq, *J* = 4.8 Hz, *J* = 0.9 Hz, 1H), 7.96 (dd, *J* = 8.0 Hz, *J* = 1.8 Hz, 1H), 7.91 (d, *J* = 1.7 Hz, 1H), 7.79 (dt, *J* = 8.5 Hz, *J* = 1.8 Hz, 2H), 7.69 (td, *J* = 11.6 Hz, *J* = 1.8 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.48 (dt, *J* = 7.9 Hz, *J* = 1.0 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.16 (ddd, *J* = 7.6 Hz, *J* = 4.9 Hz, *J* = 1.1 Hz, 1H), 4.58 (s, 2H), 2.63 (s, 3H), 2.40 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 197.9, 197.0, 158.6, 149.0, 144.6, 143.8, 136.93, 136.90, 134.5, 134.3, 132.2, 130.2, 129.3, 128.4, 127.3, 124.0, 122.4, 43.5, 26.9, 21.7; IR (film): 3052, 2920, 1681, 1606, 1467, 1276, 1223, 1004, 841, 781, 693 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{22}H_{19}NO_2$ 329.1416; Found 329.1418.



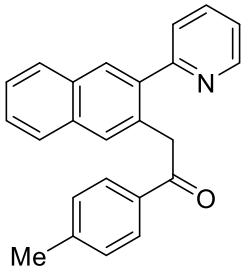
5i

2-(4-(Pyridin-2-yl)-[1,1'-biphenyl]-3-yl)-1-(*p*-tolyl)ethan-1-one (5j): Yield: 53.8 mg (74%); R_f = 0.3 (EtOAc: Hexane = 1:5); Gray solid; Melting point: 120-122 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.43 (dq, J = 4.8 Hz, J = 0.9 Hz, 1H), 7.81 (d, J = 8.2 Hz, 2H), 7.68 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.64-7.61 (m, 2H), 7.60-7.54 (m, 3H), 7.50 (dt, J = 8.0 Hz, J = 0.9 Hz, 1H), 7.43 (t, J = 7.5 Hz, 2H), 7.36-7.32 (m, 1H), 7.20 (d, J = 8.0 Hz, 2H), 7.14 (ddd, J = 7.5 Hz, J = 4.9 Hz, J = 1.0 Hz, 1H), 4.58 (s, 2H), 2.39 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 197.6, 159.4, 148.9, 143.6, 141.4, 140.7, 139.1, 136.7, 134.7, 134.0, 130.8, 130.4, 129.3, 128.8, 128.5, 127.5, 127.4, 126.0, 123.9, 121.8, 43.7, 21.7; IR (film): 3054, 2918, 1684, 1586, 1466, 1331, 1222, 1002, 761, 698 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{26}H_{21}NO$ 363.1623; Found 363.1621.



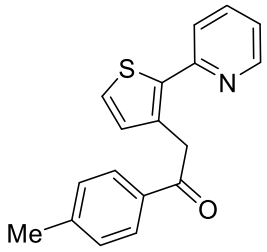
5j

2-(3-(Pyridin-2-yl)naphthalen-2-yl)-1-(*p*-tolyl)ethan-1-one (5k): Yield: 55.7 mg (83%); R_f = 0.4 (EtOAc: Hexane = 1:5); Ivory solid; Melting point: 157-159 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.42 (dq, J = 4.8 Hz, J = 0.8 Hz, 1H), 7.95 (s, 1H), 7.87-7.84 (m, 1H), 7.83-7.77 (m, 4H), 7.71 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.58 (dt, J = 7.9 Hz, J = 0.9 Hz, 1H), 7.50-7.44 (m, 2H), 7.20 (d, J = 8.0 Hz, 2H), 7.14 (ddd, J = 7.5 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 4.68 (s, 2H), 2.38 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 197.8, 159.8, 148.7, 143.5, 138.5, 136.8, 134.7, 133.4, 132.7, 131.6, 130.8, 129.5, 129.2, 128.5, 128.0, 127.5, 126.6, 126.2, 124.2, 121.9, 43.9, 21.7; IR (film): 3054, 2919, 1683, 1606, 1426, 1326, 1221, 1008, 893, 746 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{24}H_{19}NO$ 337.1467; Found 337.1464.



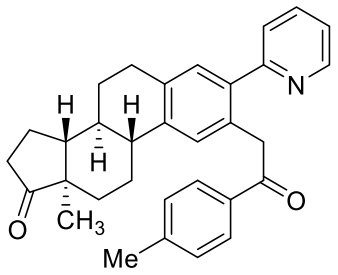
5k

2-(2-(Pyridin-2-yl)thiophen-3-yl)-1-(*p*-tolyl)ethan-1-one (5l): Yield: 35.2 mg (60%); R_f = 0.5 (EtOAc: Hexane = 1:5); Ruby oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (dq, J = 4.8 Hz, J = 0.8 Hz, 1H), 7.93 (dt, J = 8.4 Hz, J = 1.8 Hz, 1H), 7.64 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.53 (d, J = 8.0 Hz, 1H), 7.31 (d, J = 5.1 Hz, 1H), 7.24 (d, J = 8.4 Hz, 2H), 7.11 (ddd, J = 7.5 Hz, J = 4.9 Hz, J = 1.0 Hz, 1H), 7.00 (d, J = 5.1 Hz, 1H), 4.72 (s, 2H), 2.41 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.5, 153.4, 149.4, 143.8, 138.5, 136.8, 134.8, 133.6, 131.8, 129.4, 128.8, 125.3, 122.1, 121.7, 39.8, 21.8; IR (film): 3106, 2919, 1683, 1606, 1470, 1329, 1181, 1007, 778 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{18}H_{15}NOS$ 293.0874; Found 293.0871.



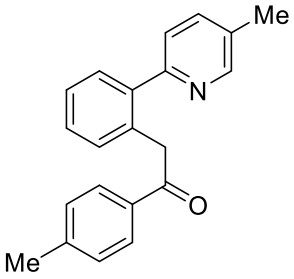
5l

(8*S*,9*R*,13*R*,14*R*)-13-Methyl-2-(2-oxo-2-(*p*-tolyl)ethyl)-3-(pyridin-2-yl)-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[*a*]phenanthren-17-one (5m): Yield: 74.0 mg (80%); R_f = 0.4 (EtOAc: Hexane = 1:5); Brown solid; Melting point: 172-174 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (dq, J = 4.9 Hz, J = 0.8 Hz, 1H), 7.79 (dt, J = 8.5 Hz, J = 1.8 Hz, 2H), 7.64 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.43 (dt, J = 7.9 Hz, J = 0.9 Hz, 1H), 7.23 (d, J = 2.0 Hz, 2H), 7.20 (d, J = 8.0 Hz, 2H), 7.11 (ddd, J = 7.5 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 4.45 (q, J = 15.8 Hz, 2H), 2.97-2.95 (m, 2H), 2.51 (q, J = 9.1 Hz, 1H), 2.46-2.42 (m, 1H), 2.38 (s, 3H), 2.36-2.33 (m, 1H), 2.22-2.12 (m, 1H), 2.10-2.01 (m, 2H), 1.96 (dt, J = 12.5 Hz, J = 2.9 Hz, 1H), 1.69-1.57 (m, 3H), 1.55-1.42 (m, 3H), 0.92 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 220.9, 197.9, 159.6, 148.8, 143.5, 140.1, 137.8, 136.5, 135.4, 134.7, 130.6, 130.5, 129.2, 128.9, 128.5, 123.7, 121.6, 50.6, 48.1, 44.4, 43.3, 38.2, 36.0, 31.7, 29.2, 26.6, 25.8, 21.7 (2C), 14.0; IR (film): 2927, 2865, 1736, 1685, 1587, 1469, 1427, 1222, 808, 733 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{32}H_{33}NO_2$ 463.2511; Found 463.2508.



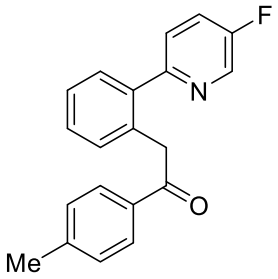
5m

2-(2-(5-Methylpyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (5n): Yield: 49.8 mg (83%); R_f = 0.3 (EtOAc: Hexane = 1:5); Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.78 (d, J = 8.2 Hz, 2H), 7.50-7.47 (m, 1H), 7.47-7.43 (m, 1H), 7.37-7.31 (m, 3H), 7.30-7.28 (m, 1H), 7.19 (d, J = 8.2 Hz, 2H), 4.48 (s, 2H), 2.38 (s, 3H), 2.29 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.8, 156.8, 149.2, 143.5, 140.2, 137.3, 134.7, 133.5, 131.7, 131.3, 129.9, 129.2, 128.5, 128.4, 127.2, 123.5, 43.5, 21.7, 18.2; IR (film): 3027, 2920, 1685, 1605, 1478, 1330, 1222, 1000, 808, 746 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{21}H_{19}NO$ 301.1467; Found 301.1464.



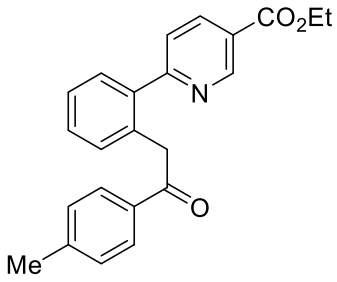
4n

2-(2-(5-Fluoropyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (5o): Yield: 27.4 mg (45%); R_f = 0.4 (EtOAc: Hexane = 1:5); Brown solid; Melting point: 77-79 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 2.8 Hz, 1H), 7.79 (d J = 8.2 Hz, 2H), 7.47-7.43 (m, 2H), 7.42-7.36 (m, 3H), 7.32-7.29 (m, 1H), 7.21 (d, J = 8.0 Hz, 2H), 4.46 (s, 2H), 2.40 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.5, 158.5 (d, J = 256.4 Hz), 155.9 (d, J = 4.2 Hz), 143.7, 139.2, 136.9 (d, J = 23.2 Hz), 134.6, 133.7, 132.1, 129.9, 129.3, 128.8, 128.5, 127.4, 124.9 (d, J = 4.1 Hz), 123.6 (d, J = 18.3 Hz), 43.5, 21.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -129.67; IR (film): 3027, 2920, 1684, 1606, 1476, 1330, 1224, 841, 744 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{20}H_{16}FNO$ 305.1216; Found 305.1217.



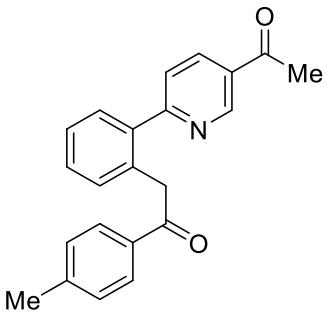
5o

Ethyl 6-(2-(2-oxo-2-(p-tolyl)ethyl)phenyl)nicotinate (5p): Yield: 48.1 mg (67%); R_f = 0.4 (EtOAc: Hexane = 1:5); Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.015-9.008 (m, 1H), 8.28 (dd, *J* = 8.2 Hz, *J* = 2.2 Hz, 1H), 7.79 (d, *J* = 8.2 Hz, 2H), 7.55 (d, *J* = 8.2 Hz, 1H), 7.52-7.50 (m, 1H), 7.44-7.37 (m, 2H), 7.35-7.31 (m, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 4.54 (s, 2H), 4.39 (q, *J* = 7.1 Hz, 2H), 2.40 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.4, 165.4, 163.5, 150.1, 143.7, 139.4, 137.8, 134.6, 133.9, 132.2, 130.1, 129.3 (2C), 128.5, 127.5, 124.3, 123.5, 61.4, 43.6, 21.8, 14.4; IR (film): 3061, 2981, 1718, 1594, 1370, 1284, 1120, 1021, 810, 754 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{23}H_{21}NO_3$ 359.1521; Found 359.1523.



5p

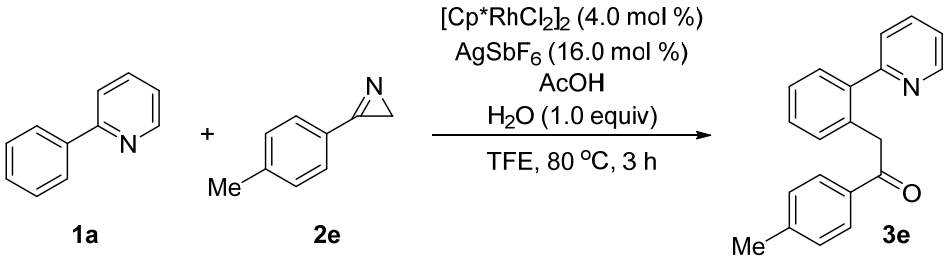
2-(2-(5-Acetylpyridin-2-yl)phenyl)-1-(*p*-tolyl)ethan-1-one (5q): Yield: 44.9 mg (68%); R_f = 0.2 (EtOAc: Hexane = 1:5); Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (dd, *J* = 2.3 Hz, *J* = 0.8 Hz, 1H), 8.22 (dd, *J* = 8.2 Hz, *J* = 2.3 Hz, 1H), 7.80 (dt, *J* = 8.5 Hz, *J* = 1.8 Hz, 2H), 7.59 (dd, *J* = 8.2 Hz, *J* = 0.8 Hz, 1H), 7.53-7.50 (m, 1H), 7.45-7.38 (m, 2H), 7.34-7.32 (m, 1H), 7.22 (d, *J* = 7.9 Hz, 2H), 4.54 (s, 2H), 2.56 (s, 3H), 2.40 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.3, 196.6, 163.7, 149.1, 143.8, 139.2, 136.3, 134.6, 134.0, 132.3, 130.2, 130.0, 129.4, 129.3, 128.4, 127.5, 123.8, 43.6, 26.8, 21.7; IR (film): 3027, 2920, 1685, 1590, 1373, 1272, 1020, 810, 748 cm^{-1}; HRMS (EI) *m/z*: $[M]^+$ Calcd for $C_{22}H_{19}NO_2$ 329.1416; Found 329.1413.



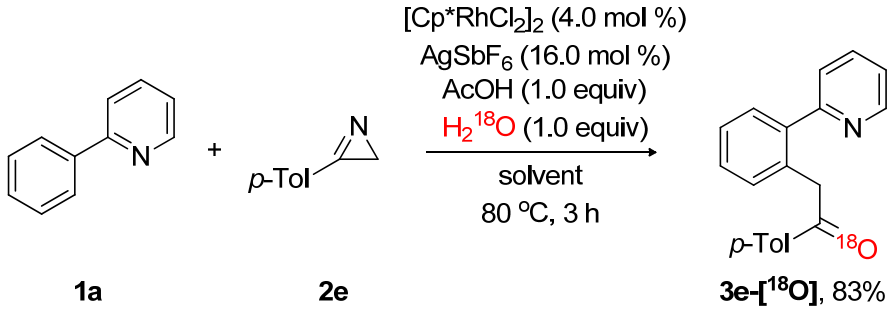
5q

4. Mechanistic Studies

Table S1. Examination of the Amount of Acetic Acid.

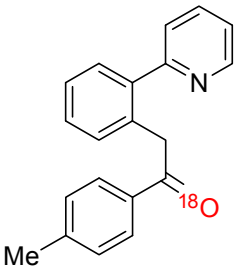


entry	AcOH (mol %)	yield (%)
1	10	55
2	50	80
3	100	91
4	200	40

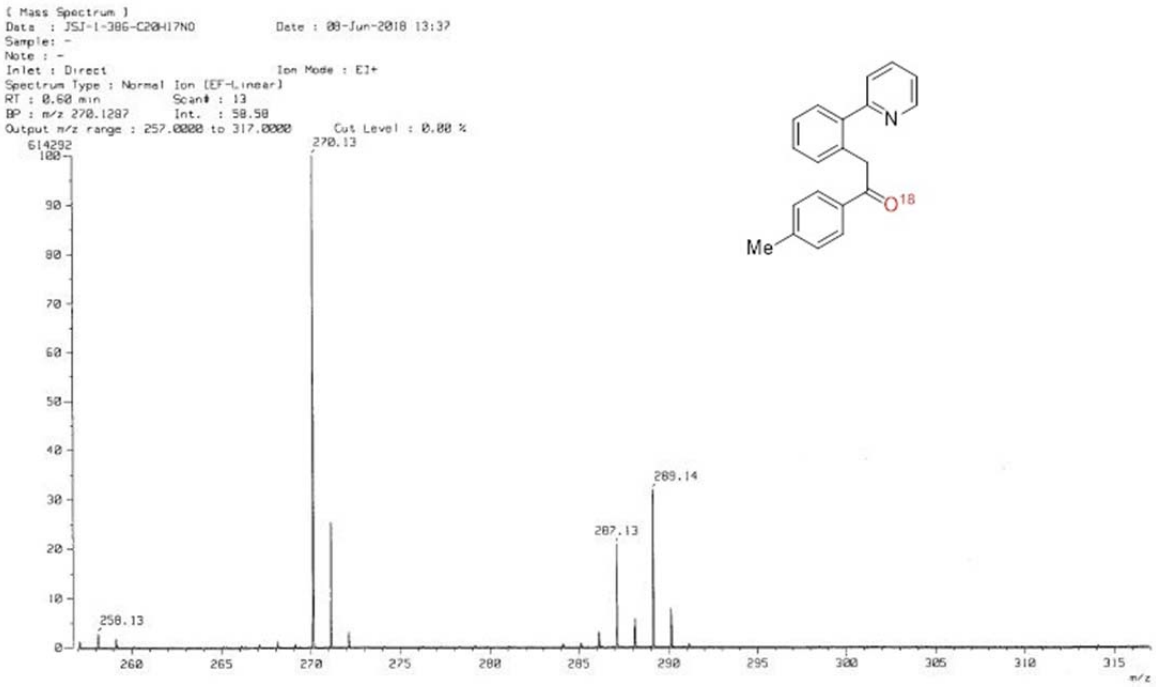


A dried test tube equipped with a magnetic stirrer was charged with 2-arylpyridine **1** (2.0 equiv), $[Cp^*RhCl_2]_2$ (4.0 mol %), $AgSbF_6$ (16.0 mol %), and TFE (1.0 mL) under a nitrogen atmosphere. 3-(*p*-tolyl)-2*H*-azirine **2e** (0.2 mmol, 1.0 equiv) in TFE (1.0 mL), $H_2{}^{18}O$ (1.0 equiv), and AcOH (1.0 equiv) were added to reaction mixture. After being stirred at 80 °C for 3 h, the reaction mixture was cooled to room temperature, filtered through a pad of Celite and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel.

2-(2-(Pyridin-2-yl)phenyl)-1-(*p*-tolyl)ethanone (3e-[^{18}O]) : Yield: 48.1 mg (83%); R_f = 0.3 (EtOAc: Hexane = 1:5); Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (dq, J = 4.8 Hz, J = 0.9 Hz, 1H), 7.78 (dt, J = 8.5 Hz, J = 1.8 Hz, 2H), 7.67 (td, J = 11.6 Hz, J = 1.8 Hz, 1H), 7.49-7.47 (m, 1H), 7.44 (dt, J = 7.9 Hz, J = 1.0 Hz, 1H), 7.40-7.35 (m, 2H), 7.34-7.30 (m, 1H), 7.20 (d, J = 8.0 Hz, 2H), 7.14 (ddd, J = 7.6 Hz, J = 4.9 Hz, J = 1.1 Hz, 1H), 4.48 (s, 2H), 2.38 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 197.7, 159.7, 148.9, 143.5, 140.2, 136.7, 134.7, 133.6, 131.9, 130.0, 129.2, 128.7, 128.5, 127.3, 124.0, 121.8, 43.5, 21.7; IR (neat) 3024, 2862, 2721, 1684, 1632, 1225, 990, 745 cm^{-1}; HRMS (EI) calcd for $C_{17}H_{19}N^{18}O$ 289.1352, found 289.1350.



3e-[^{18}O]

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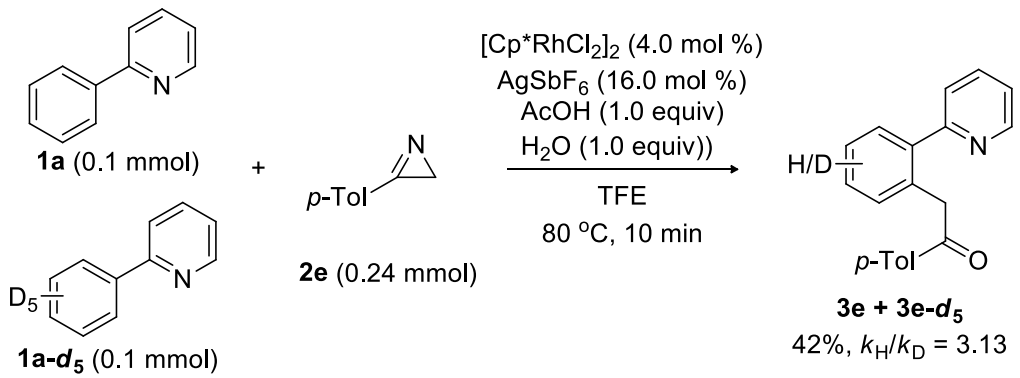
[ Elemental Composition ]
Data  : JSJ-1-386-C20H17NO          Date : 08-Jun-2018 13:37
Sample: -
Note : -
Inlet : Direct                      Ion Mode : EI+
RT : 0.60 min                       Scan#: 13
Elements : C 20/0, H 17/0, N 1/0, O 1/0(16O 1/0, 18O 1/0)
Mass Tolerance      : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z  Int%   Err[ppm / mmu]    U.S.  Composition
  270.1287   100.0     +1.5 /  +0.4    13.5  C 20 H 16 N

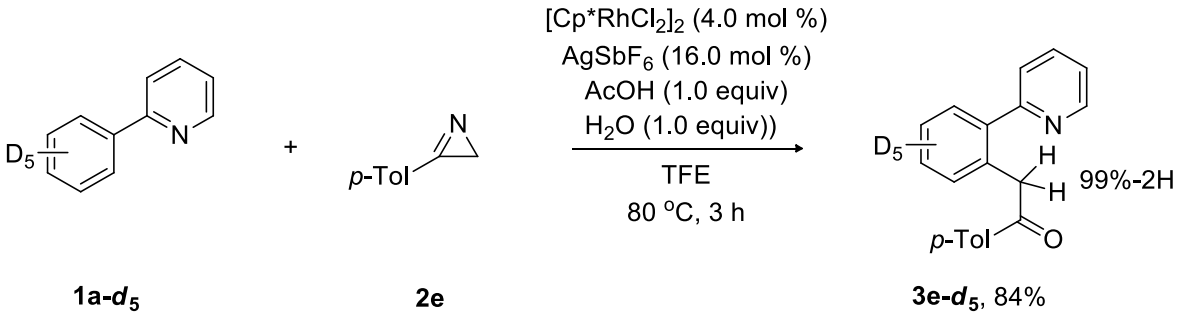
  271.1319    25.4

  287.1308    21.0     -0.8 /  -0.2    13.0  C 20 H 17 N 16O

  289.1350    32.1     -0.9 /  -0.2    13.0  C 20 H 17 N 18O
```

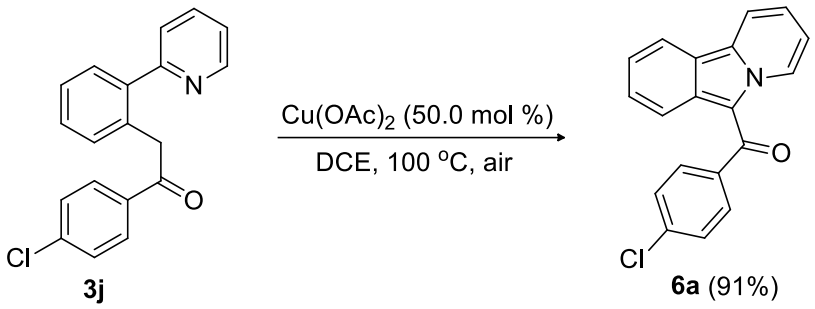


A dried test tube equipped with a magnetic stirrer was charged with 2-phenylpyridine **1a** (0.1 mmol), **1a-*d*$_5$** (0.1 mmol), [Cp*RhCl$_2$]$_2$ (4.0 mol %), AgSbF$_6$ (16.0 mol %), and TFE (1.0 mL) under a nitrogen atmosphere. 3-(*p*-tolyl)-2*H*-azirine **2e** (0.24 mmol, 2.0 equiv) in TFE (1.0 mL), H$_2$O (1.0 equiv), and AcOH (1.0 equiv) were added to reaction mixture. After being stirred at 80 °C for 3 h, the reaction mixture was cooled to room temperature, filtered through a pad of Celite and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel.



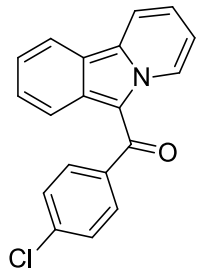
A dried test tube equipped with a magnetic stirrer was charged with 2-phenylpyridine **1a-*d*$_5$** (2.0 equiv), [Cp*RhCl$_2$]$_2$ (4.0 mol %), AgSbF$_6$ (16.0 mol %), and TFE (1.0 mL) under a nitrogen atmosphere. 3-(*p*-tolyl)-2*H*-azirine **2e** (0.2 mmol, 1.0 equiv) in TFE (1.0 mL), H$_2$O (1.0 equiv), and AcOH (1.0 equiv) were added to reaction mixture. After being stirred at 80 °C for 3 h, the reaction mixture was cooled to room temperature, filtered through a pad of Celite and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel.

5. Synthetic Applications

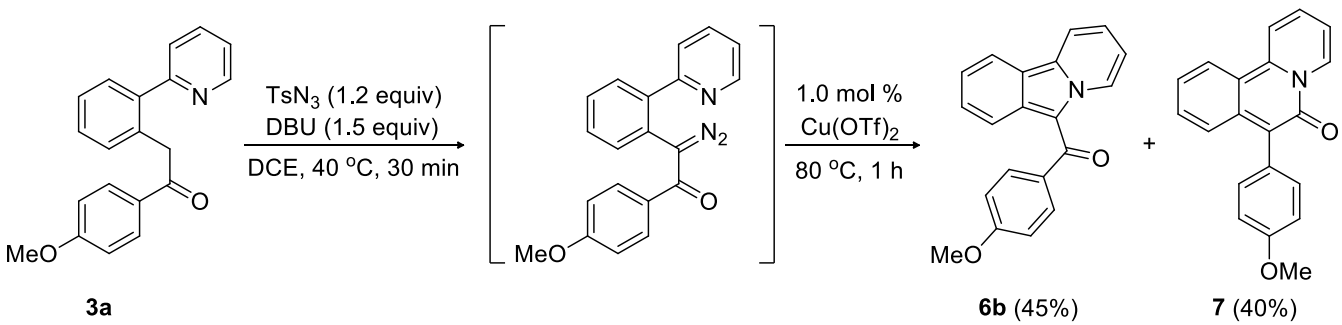


A test tube equipped with a magnetic stirrer was charged with 1-(4-chlorophenyl)-2-(2-(pyridin-2-yl)phenyl)ethanone **3j** (1.0 equiv, 0.1 mmol, 31.0 mg), $Cu(OAc)_2$ (50.0 mol %, 9.1 mg), and DCE (1.0 mL) under air. After being stirred at 100 °C for 12 h, the reaction mixture was cooled to room temperature, filtered through a pad of Celite and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel.

(4-Chlorophenyl)(pyrido[2,1-*a*]isoindol-6-yl)methanone (6a)[7a] : Yield: 55.7 mg (91%); R_f = 0.3 (EtOAc: Hexane = 1:5); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (d, J = 7.0 Hz, 1H), 8.24 (d, J = 8.5 Hz, 1H), 8.12 (d, J = 7.9 Hz, 1H), 7.65 (d, J = 8.3 Hz, 2H), 7.57 (t, J = 7.7 Hz, 1H), 7.50 (d, J = 8.3 Hz, 2H), 7.41-7.37 (m, 1H), 7.32-7.23 (m, 2H), 6.92 (d, J = 8.3 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 181.6, 140.8, 136.3, 135.1, 132.4, 129.8, 129.5, 128.9, 128.5, 125.6, 121.5, 120.1, 119.9, 119.0, 118.6, 117.3, 114.0



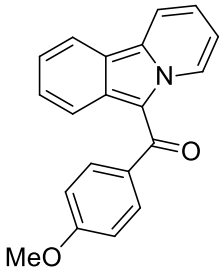
6a



In a dried test tube, 1-(4-methoxyphenyl)-2-(2-(pyridin-2-yl)phenyl)ethanone **3a** (1.0 equiv, 0.2 mmol, 60.6 mg) and tosyl azide (0.24 mmol, 1.2 equiv.) were dissolved in MeCN (1.0 mL) under air.

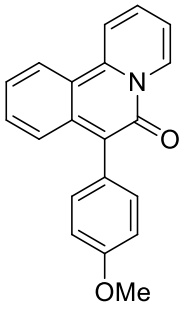
After 5 min, DBU (0.3 mmol, 1.5 equiv.) was added. The reaction mixture was stirred for 30 min at 40 °C and then, $Cu(OTf)_2$ (1.0 mol %) was added to the reaction mixture. It was stirred at 80 °C for 1 h. Then, the solvent was removed under reduced pressure and the residue was purified by silica gel flash column chromatography to give desired products.

(4-Methoxyphenyl)(pyrido[2,1-*a*]isoindol-6-yl)methanone (6b)[7a] : Yield: 27.1 mg (45%); R_f = 0.3 (EtOAc: Hexane = 1:5); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.51 (d, *J* = 7.0 Hz, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 7.0 Hz, 2H), 7.50-7.46 (m, 1H), 7.35-7.20 (m, 4H), 7.08 (d, *J* = 8.4 Hz, 1H), 7.02 (d, *J* = 7.1 Hz, 2H), 3.92 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 183.0, 161.6, 134.9, 134.4, 132.3, 130.5, 129.1, 128.0, 124.6, 121.1, 120.0, 119.4, 118.2, 117.3, 114.3, 113.7, 55.4



6b

7-(4-Methoxyphenyl)-6*H*-pyrido[2,1-*a*]isoquinolin-6-one (7) : Yield: 24.1 mg (40%); R_f = 0.2 (EtOAc: Hexane = 3:1); red solid; Melting point: 162-165 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.97 (d, *J* = 7.0 Hz, 1H), 8.74 (d, *J* = 8.8 Hz, 1H), 8.38 (d, *J* = 8.6 Hz, 1H), 7.96-7.91 (m, 1H), 7.61-7.54 (m, 2H), 7.47-7.41 (m, 3H), 7.23-7.19 (m, 1H), 7.06 (d, *J* = 8.7 Hz, 2H), 3.89 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.6, 153.6, 141.5, 138.0, 132.6, 132.6, 131.0, 130.7, 129.1, 123.9, 123.7, 121.3, 120.8, 118.8, 114.1, 114.0, 109.7, 55.4; IR (neat) 2924, 2742, 2623, 1744, 1710, 1242, 1021, 842 cm^{-1}; HRMS (EI) calcd for $C_{20}H_{15}NO_2$ 301.1103, found 301.1105.



7

6. Computational details

Geometry optimizations of all the ground state structures were completed using density functional theory as implemented in the Jaguar 9.1[8] with the M06[9] level of theory and the LACV3P** basis set[10] for the Rh center. Single-point calculation were performed with triple-ζ-quality basis set, cc-pVTZ(-f).[11] Transition state structures were obtained from the quadratic synchronous transit search methods (QST).[12] The nature of all stationary points was verified by the number of imaginary frequencies (negative eigenvalue from the frequency calculation): zero for the ground states to be local minima and one for the transition states to be first-order saddle point. The Gibbs free energies were calculated at 353.15 K based upon ideal gas-phase conditions. Solvation energies were computed by single-point calculations on the optimized gas-phase geometries using a self-consistent reaction field(SCRF)[13] based on numerical solutions of the Poisson–Boltzmann equation with a dielectric constant, $\varepsilon = 26.73$ for TFE (2,2,2-trifluoroethanol). The Gibbs free energy was computed according to the protocols below:

$$G(sol) = G(gas) + G(solv) \quad (1)$$

$$G(gas) = H(gas) - TS(gas) \quad (2)$$

$$H(gas) = E(SCF) + ZPE \quad (3)$$

$$\Delta G(sol) = \Sigma G(sol) \text{ for products} - \Sigma G(sol) \text{ for reactants} \quad (4)$$

where G(gas) is the free energy in the gas phase; G(solv) is the free energy of solvation, which is obtained using the continuum solvation model; the enthalpic and entropic components in the gas phase are denoted as H(gas) and S(gas); T is the temperature (353.15 K); E(SCF) is the self-consistent field energy in gas phase, and ZPE is the zero-point energy.

7. Computational results

Table S1. Computed Energy Components for DFT-Optimized Structures

	E(SCF)/(eV)	**ZPE/(kcal/mol)**	**S(gas)/(cal·mol^{-1}·K^{-1})**	**G(solv)/(kcal/mol)**
	cc-pVTZ(-f)/LACV3P**	6-31G**/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**
3a'	–26047.816	208.92	140.38	–13.91
4	–26047.633	208.21	147.25	–11.95
A	–32839.766	278.92	186.60	–41.48
A-TS	–32838.906	275.59	181.95	–42.06
B	–32839.492	278.95	189.69	–39.51
C	–39616.805	340.34	208.56	–37.52
C-TS	–39615.707	339.15	210.60	–38.17
^{1}D	–39616.152	337.84	202.46	–39.49
^{3}D	–39615.504	338.08	210.31	–39.50
^{1}D-TS	–39615.730	339.91	206.44	–39.67
E	–39617.332	341.23	211.12	–41.28
F	–45850.438	381.18	233.60	–43.06
F-TS	–45850.406	379.37	228.57	–41.36
G	–45851.121	382.65	232.67	–43.37
^{1}D-TS'	–39615.184	339.25	198.12	–41.02
^{3}D-TS	–39614.949	337.77	212.93	–38.70
H	–39617.750	341.04	193.87	–38.05
I	–45850.656	381.07	236.74	–40.50
I-TS	–45849.918	378.92	227.02	–42.21
J	–45850.500	381.97	227.00	–43.76
ppy	–13037.124	106.12	95.35	–6.15
Azirine	–13008.934	99.78	97.93	–8.52
Nitrene	–13007.624	97.62	100.84	–8.23
Acetate	–6216.633	29.91	64.22	–73.67
Acetic Acid	–6232.402	38.98	68.87	–8.91

8. XYZ Coordinates

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3'

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C	-0.799001634	-4.575531006	0.160575405
C	-1.925934076	-4.296079636	-0.602904320
C	-2.368060827	-5.272033215	-1.487609982
N	-1.760930419	-6.441876888	-1.655764222
C	-0.681029201	-6.716727257	-0.918284893
C	-0.170883447	-5.802184105	0.010563510
H	-0.421054900	-3.849701405	0.877247930
H	-2.455037832	-3.351877213	-0.508861065
H	-3.261991262	-5.107173443	-2.093202829
H	0.691048741	-6.065920353	0.618598163
C	-0.036809180	-8.033007622	-1.119592786
C	-0.779271245	-9.217520714	-1.304775238
C	1.360062361	-8.092360497	-1.104663849
C	-0.072402537	-10.414256096	-1.434149146
C	2.039787292	-9.290857315	-1.261073112
C	1.315019846	-10.463893890	-1.420692205
H	1.921872735	-7.166504383	-0.990158200
H	-0.636233032	-11.341742516	-1.537464023
H	3.127024174	-9.306639671	-1.257439137
H	1.825849533	-11.417719841	-1.530726314
C	-2.287127256	-9.278088570	-1.285547972
N	-4.238152027	-8.323886871	-2.265160322
C	-3.055534601	-8.752701759	-2.486080647
H	-2.579846382	-10.330808640	-1.150501251
H	-2.699014902	-8.743630409	-0.421318859
C	-2.438196659	-8.807008743	-3.834327459
C	-2.549689293	-7.699789047	-4.684442997
C	-1.790183544	-9.940742493	-4.316951752
C	-2.039283276	-7.727410793	-5.967059612
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H	-1.690306664	-10.817214966	-3.680089712
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H	-4.678684711	-8.062815666	-3.151454687
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C	-0.316443533	-9.944746971	-8.248161316
H	0.591804981	-10.212868690	-7.689144611
H	-0.992274225	-10.812047958	-8.262503624
H	-0.040179495	-9.692442894	-9.274288177

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4

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C	-3.243716240	-6.927994728	-0.329230428
C	-3.455450535	-5.614214897	-0.727401853
C	-2.484048843	-5.007461071	-1.516194344
N	-1.366148710	-5.608494282	-1.915665865
C	-1.176296234	-6.881134510	-1.546785116
C	-2.088602066	-7.572755814	-0.744246185
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H	-4.350453377	-5.070328712	-0.438082546
H	-2.615991116	-3.974775553	-1.845400810
H	-1.896700263	-8.610968590	-0.481991440
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C	0.463442534	-7.543035030	-3.360603333
C	0.857772946	-8.216347694	-1.077952981
C	1.682018042	-8.130393028	-3.708600998
C	2.066482306	-8.803321838	-1.432663202
C	2.486188173	-8.740241051	-2.755669832
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C	-3.203862906	-6.382854939	-6.436313152
C	-1.926388741	-4.746494770	-5.232523441

C	-3.797572374	-5.379310608	-7.195414066
C	-2.508335114	-3.738798857	-5.978631020
C	-3.446849108	-4.048293114	-6.967417240
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H	-4.514319420	-5.645309925	-7.967059612
H	-2.260059357	-2.692822933	-5.816247940
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O	-3.950965881	-2.991507053	-7.650447845
C	-4.892582417	-3.250802279	-8.659893036
H	-4.469938755	-3.874785185	-9.460885048
H	-5.790749073	-3.745780945	-8.262877464
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A

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C	-0.234979913	-4.539167404	-4.188413620
C	1.161340714	-4.883155346	-4.064401150
C	1.856752992	-3.739825010	-3.548511505
Rh	0.395596564	-4.355616093	-2.099884272
C	0.155504704	-3.413752079	0.276661277
O	1.302701235	-3.643096209	-0.224384621
O	-0.869530380	-3.616978884	-0.443906426
C	0.027638162	-2.920062780	1.678015113
H	-1.015322089	-2.930002928	1.999885321
H	0.636523068	-3.537740946	2.344749689
H	0.416137695	-1.898047686	1.740456223
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C	1.726086259	-6.547513485	-0.572635591
N	0.534338951	-6.333588600	-1.164654970
C	-0.332454175	-7.362630367	-1.296130657
C	0.015588783	-8.637454987	-0.837289929
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H	2.367918491	-5.675400734	-0.469970107
H	-0.710468113	-9.440289497	-0.924574256
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C	-3.426759005	-7.958613396	-3.356156111
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H	-3.798619986	-8.700030327	-4.058999538
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C	-1.679902673	-2.442184687	-3.645142555
H	-1.787658691	-1.743784547	-4.494085312
H	-2.533701658	-3.136726379	-3.658415556
H	-1.730567098	-1.857164383	-2.712455034
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H	0.297397166	-0.857111871	-2.378106356
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C	3.298540354	-3.644382000	-3.207643986
H	3.437347174	-3.186842442	-2.221039057
H	3.782137632	-4.625556469	-3.201282740
H	3.823312521	-3.015817404	-3.938711405
C	1.756493807	-6.204149723	-4.399163246
H	2.658168793	-6.403797150	-3.811161280
H	1.046340466	-7.016810894	-4.209097862
H	2.033007860	-6.244591713	-5.460093498
C	-1.295947075	-5.373477936	-4.806124210
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H	-1.038093090	-6.435882092	-4.794657230
H	-2.256927252	-5.261873722	-4.293238163

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A-TS

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C	2.099580050	-3.483887196	-1.597568154
C	1.190732241	-3.805766821	-0.512107670
C	-0.039286152	-3.108957291	-0.752733231

C	0.081466161	-2.388165236	-1.996053100
C	1.417075872	-2.609214067	-2.497117043
Rh	0.328241497	-4.514739990	-2.393666267
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O	0.004641665	-4.504362106	-4.507260799
O	0.426181316	-6.695856571	-4.636405945
C	-0.114319921	-5.551270008	-6.638439655
H	0.812518895	-5.820154190	-7.154639721
H	-0.858530819	-6.306885719	-6.906255245
H	-0.444997847	-4.564024925	-6.963908672
C	-3.887496471	-6.958267212	-1.976907730
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C	-2.692180872	-5.053000927	-2.772901058
N	-1.543530107	-5.550464630	-2.301246405
C	-1.512176037	-6.758299828	-1.695249557
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H	-2.624208450	-4.092905998	-3.282198668
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C	0.905544519	-6.663828850	-2.053568363
C	0.051927876	-8.188176155	-0.342318267
C	2.199926376	-7.117088795	-1.770606041
C	1.352042437	-8.604167938	-0.070960276
C	2.424957037	-8.081067085	-0.792664230
H	-0.777802229	-8.602054596	0.228371501
H	3.036405325	-6.739823818	-2.358615160
H	1.529083133	-9.351041794	0.698841155
H	3.433648825	-8.437577248	-0.596841216
H	0.687420249	-6.519483089	-3.322445631
C	1.517596245	-4.615262985	0.692339242
H	0.616747081	-5.029578209	1.156033754
H	2.178620338	-5.453610897	0.449244916
H	2.023228168	-3.994539499	1.443317533
C	-1.239508629	-3.161051989	0.121770978
H	-2.155182123	-2.929126501	-0.430110127
H	-1.359040737	-4.150285244	0.577199578
H	-1.148032188	-2.430493593	0.935593367
C	3.521255493	-3.907589197	-1.707253456
H	3.728912830	-4.786751747	-1.091079831
H	3.794670820	-4.145699501	-2.740839481
H	4.182856083	-3.100101948	-1.367856860
C	1.942221165	-2.049162626	-3.768042803
H	2.953636646	-2.404759407	-3.979723454
H	1.296873212	-2.331640244	-4.608544827
H	1.970376611	-0.953556180	-3.718178988
C	-0.934053719	-1.516532063	-2.645249367
H	-0.949706197	-1.677109003	-3.729601383
H	-1.941046000	-1.702998281	-2.258589506
H	-0.708525002	-0.456153810	-2.471333504

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B

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C	1.721335292	-3.627520800	-1.202549696
C	0.451289803	-3.518721342	-0.528332949
C	-0.407441676	-2.622256994	-1.312870860
C	0.259304255	-2.335791349	-2.507162809
C	1.564787149	-3.010233641	-2.478205681
Rh	0.109174758	-4.622282505	-2.326591015
C	-0.647055030	-5.776604176	-5.172595978
O	-0.016982144	-4.918220043	-4.555993080
O	-1.455014229	-6.633557796	-4.583570957
C	-0.573225915	-5.947727680	-6.647747040
H	-0.153740585	-6.933571815	-6.873729229
H	-1.580732584	-5.922839165	-7.073429108
H	0.048043605	-5.169479370	-7.089761257
C	-3.394333124	-7.277074337	-0.176279739
C	-3.775611877	-6.073717594	-0.769744992
C	-2.834274054	-5.383741856	-1.509101510
N	-1.577509522	-5.833044052	-1.675501466
C	-1.200522542	-7.020112038	-1.125703454
C	-2.108884811	-7.754358292	-0.360574186
H	-4.103783607	-7.842167854	0.422567397
H	-4.781139374	-5.680211067	-0.661917388
H	-3.069791079	-4.438135147	-1.993902802
H	-1.798486233	-8.692335129	0.090178214

C	0.161248580	-7.423113823	-1.456242561
C	0.939878106	-6.473682404	-2.148850918
C	0.668529570	-8.703261375	-1.205421567
C	2.193514824	-6.841631413	-2.623793364
C	1.933757663	-9.045855522	-1.656484842
C	2.687514544	-8.122144699	-2.378286123
H	0.070465863	-9.442623138	-0.675389111
H	2.795264244	-6.131648064	-3.191540003
H	2.327877998	-10.039775848	-1.463303685
H	3.669823170	-8.402701378	-2.752282858
H	-1.449376702	-6.455525875	-3.621990204
C	0.140649334	-4.032482624	0.833127439
H	-0.924080253	-4.269646168	0.938872635
H	0.709501445	-4.942163944	1.051446319
H	0.390457004	-3.288403034	1.600650907
C	-1.745559573	-2.139503241	-0.878181338
H	-2.370134354	-1.843755007	-1.727374673
H	-2.286138773	-2.900248528	-0.304201096
H	-1.641917825	-1.263476610	-0.225118637
C	2.942134142	-4.273176193	-0.654372752
H	2.697304726	-5.137886047	-0.030932913
H	3.617958784	-4.614221096	-1.443649054
H	3.491935492	-3.554925203	-0.032797568
C	2.580131531	-2.899795771	-3.558961391
H	3.407070398	-3.600714922	-3.411153555
H	2.133114576	-3.104450226	-4.537954807
H	3.003365755	-1.887255073	-3.591364145
C	-0.229838133	-1.537740231	-3.660969496
H	-0.104332313	-2.092727423	-4.597051144
H	-1.287005067	-1.277455211	-3.558710337
H	0.338375300	-0.603484571	-3.755080223

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C

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C	1.331882834	-3.260162592	-1.082685351
C	-0.063435987	-3.363203764	-0.761465788
C	-0.826940835	-2.761426449	-1.857576251
C	0.071204878	-2.449659824	-2.885729551
C	1.418777704	-2.814504862	-2.437742233
Rh	0.302037269	-4.691288471	-2.430402994
C	-3.087656736	-8.161752701	-1.720400333
C	-3.488063097	-6.950172424	-2.282170534
C	-2.521949291	-5.983828545	-2.505715847
N	-1.231673717	-6.170277596	-2.202610731
C	-0.821137190	-7.352070332	-1.680259109
C	-1.750963807	-8.364941597	-1.425241590
H	-3.815986156	-8.944893837	-1.521098852
H	-4.524303913	-6.755769730	-2.540942430
H	-2.776812315	-5.016682148	-2.939419508
H	-1.419049501	-9.307497025	-0.997576892
C	0.619677246	-7.449581623	-1.476684332
C	1.374126077	-6.308271408	-1.816319108
C	1.262635112	-8.617548943	-1.047889829
C	2.763373375	-6.380503654	-1.777113676
C	2.646542311	-8.663268089	-0.977336884
C	3.396302700	-7.549403191	-1.355325341
H	0.684470057	-9.501296997	-0.779031456
H	3.368518353	-5.527090549	-2.087345123
H	3.143394947	-9.571267128	-0.644280851
H	4.483387947	-7.592724800	-1.322704911
C	1.596509099	-6.354291439	-5.146966457
N	0.690633595	-5.436724186	-4.395038128
C	0.310028613	-5.803003311	-5.547958374
H	2.527303696	-5.924019337	-5.521466732
H	1.661767364	-7.384243488	-4.788123608
C	-0.745762587	-5.679543495	-6.496365547
C	-1.872811079	-4.885826111	-6.209992886
C	-0.661522567	-6.338859558	-7.727567673
C	-2.882202387	-4.760755539	-7.135468483
C	-1.673309445	-6.220671177	-8.666011810
C	-2.789809465	-5.426995277	-8.372822762
H	-1.924184084	-4.367963314	-5.250663757
H	0.213412806	-6.949540615	-7.942099571
H	-3.763894558	-4.152715683	-6.952167988
H	-1.591155529	-6.738486767	-9.616690636
C	2.659368753	-2.578668356	-3.228091240
H	3.503740311	-3.154977322	-2.835393667

H	2.521311760	-2.863253832	-4.277449131
H	2.945833445	-1.518413782	-3.209070206
C	-0.230596006	-1.863042474	-4.220716476
H	0.280025572	-2.409085035	-5.022987843
H	-1.303804994	-1.872004867	-4.438003063
H	0.106455937	-0.819665194	-4.274507999
C	-2.298289061	-2.540843725	-1.837808251
H	-2.715019941	-2.447164774	-2.847193480
H	-2.825647354	-3.353731155	-1.325311184
H	-2.540278435	-1.616164565	-1.297995329
C	-0.625899613	-3.788235664	0.550729156
H	-1.637543201	-4.194653034	0.440789044
H	-0.007760534	-4.566254139	1.011958838
H	-0.682219923	-2.944610119	1.251403570
C	2.452438354	-3.555120230	-0.150566131
H	2.252139807	-4.440186024	0.462547868
H	3.397601366	-3.721513271	-0.675843060
H	2.599008083	-2.704197168	0.527592540
O	-3.820237875	-5.237282753	-9.203061104
C	-3.796055555	-5.858253002	-10.477577209
H	-2.936892033	-5.516220093	-11.069005966
H	-3.769107342	-6.951865196	-10.386250496
H	-4.718576908	-5.561586380	-10.978014946

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C-TS

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C	0.900207698	-3.565893888	-0.818983555
C	-0.506614149	-3.228496313	-0.998464644
C	-0.671088457	-2.649412632	-2.267979383
C	0.635916710	-2.636358976	-2.908843994
C	1.615980625	-3.092187643	-1.974928379
Rh	0.289064407	-4.802423954	-2.512571812
C	-2.315804958	-8.411541939	-0.579436064
C	-2.983516932	-7.342980385	-1.176024556
C	-2.229283571	-6.349800110	-1.774268985
N	-0.890460849	-6.393030643	-1.786650062
C	-0.222569555	-7.434455395	-1.238621712
C	-0.933080554	-8.462663651	-0.615682304
H	-2.876589775	-9.207123756	-0.095509388
H	-4.067083836	-7.281504631	-1.180515885
H	-2.681057453	-5.493013859	-2.271650314
H	-0.398295015	-9.297118187	-0.171005279
C	1.219538450	-7.370074749	-1.428039670
C	1.697832584	-6.252019405	-2.142795563
C	2.100734949	-8.378181458	-1.022091508
C	3.040911198	-6.211448669	-2.499274254
C	3.446843147	-8.297510147	-1.341557860
C	3.911968231	-7.223165512	-2.095419407
H	1.733740330	-9.237840652	-0.464056075
H	3.430419207	-5.388237953	-3.097092628
H	4.130108356	-9.079874039	-1.022264600
H	4.962627411	-7.171133995	-2.373796463
C	0.577127814	-5.681674957	-4.710268497
N	-1.092027545	-4.936831474	-4.303860664
C	-0.660622716	-5.415746689	-5.400004387
H	1.437002659	-5.044267178	-4.918928623
H	0.770254850	-6.707827568	-4.404541969
C	-1.205307364	-5.596106052	-6.717656612
C	-2.509568453	-5.189059734	-7.015948772
C	-0.421573043	-6.192675114	-7.716831207
C	-3.031869411	-5.369832516	-8.284020424
C	-0.930488944	-6.377361298	-8.982943535
C	-2.240217924	-5.968084335	-9.276092529
H	-3.113973618	-4.727223873	-6.236636162
H	0.593081355	-6.511661530	-7.483110428
H	-4.046124935	-5.049624920	-8.500301361
H	-0.347851485	-6.837202549	-9.776145935
C	-1.556013703	-3.495740891	0.021476086
H	-2.565716982	-3.397578955	-0.388048381
H	-1.457652211	-4.503311157	0.443609267
H	-1.463556886	-2.789692879	0.856963694
C	-1.933186769	-2.225537539	-2.923485518
H	-2.205487728	-2.940301180	-3.718579769
H	-2.763431787	-2.172797680	-2.212677717
H	-1.831260681	-1.238481879	-3.389830589
C	1.491771221	-4.084316254	0.445910245
H	1.646300554	-3.273134708	1.169572830

H	0.834119380	-4.824783325	0.916045964
H	2.457524300	-4.568822384	0.270512551
O	-2.645285368	-6.191522121	-10.531966209
C	-3.956027269	-5.810563087	-10.905010223
H	-4.710066795	-6.343960285	-10.311803818
H	-4.102641106	-4.728078365	-10.796888351
H	-4.065112591	-6.084722996	-11.954920769
C	0.898450673	-2.059902906	-4.255172729
H	1.872612596	-2.366677523	-4.649570942
H	0.124640025	-2.354556322	-4.973066330
H	0.895526350	-0.962642014	-4.204936981
C	3.091407537	-2.971158266	-2.117126703
H	3.414497614	-1.972723722	-1.794829249
H	3.624287367	-3.703292847	-1.503645658
H	3.418605804	-3.096224070	-3.155916691

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C	1.243504763	-3.546415091	-1.084694982
C	-0.160581574	-3.415860415	-0.861235321
C	-0.751023710	-2.857754230	-2.037197828
C	0.297943473	-2.639178514	-3.002247334
C	1.535940647	-3.067145348	-2.415421963
Rh	0.197128639	-4.859279156	-2.692819834
C	-2.670999050	-8.183874130	-0.600371540
C	-3.255745888	-7.176863194	-1.365953326
C	-2.429702759	-6.292107105	-2.038144350
N	-1.094905019	-6.383154869	-1.964022875
C	-0.506152570	-7.360147476	-1.236642718
C	-1.290985107	-8.280035019	-0.539143085
H	-3.290998697	-8.894824028	-0.059155405
H	-4.333754063	-7.080062866	-1.449557662
H	-2.812708616	-5.500802517	-2.680251122
H	-0.815650761	-9.063509941	0.045007125
C	0.948348284	-7.350175858	-1.301483750
C	1.535058022	-6.320528507	-2.061436892
C	1.754758596	-8.337506294	-0.722109675
C	2.902174234	-6.352666378	-2.299276590
C	3.127047539	-8.321118355	-0.913486302
C	3.698558807	-7.338130951	-1.718765616
H	1.305779934	-9.134442329	-0.131046861
H	3.370868683	-5.624938488	-2.959711552
H	3.748481274	-9.089336395	-0.460473955
H	4.769926071	-7.343462944	-1.907932281
C	0.792263031	-5.649844170	-4.583615303
N	-1.225430965	-4.790039539	-4.216864586
C	-0.527258396	-5.307623863	-5.165585518
H	1.652334929	-5.084966660	-4.960435390
H	1.005272269	-6.718829155	-4.511259556
C	-0.978671193	-5.506891727	-6.537519455
C	-2.209918022	-4.991147041	-6.964832783
C	-0.192408219	-6.231640339	-7.445119858
C	-2.661117554	-5.194760323	-8.258762360
C	-0.630395353	-6.443486691	-8.737189293
C	-1.870262027	-5.930238724	-9.152924538
H	-2.817535400	-4.421258450	-6.262327194
H	0.768460810	-6.640541553	-7.125535011
H	-3.620143890	-4.783190727	-8.568397522
H	-0.041739278	-7.007866859	-9.456016541
C	-0.864767015	-3.829322100	0.382925868
H	-1.928935885	-4.017549992	0.207671195
H	-0.425781459	-4.743983746	0.800606370
H	-0.788234890	-3.051400900	1.153499722
C	-2.178111076	-2.521715879	-2.266666651
H	-2.543239117	-3.035684586	-3.168815136
H	-2.810299397	-2.806680918	-1.419993758
H	-2.301849365	-1.443372250	-2.429186821
C	2.248573303	-3.962331295	-0.069525123
H	2.414916754	-3.146386623	0.647414804
H	1.919189572	-4.839468956	0.501156211
H	3.211366177	-4.205840111	-0.528710961
O	-2.212913275	-6.192961693	-10.424501419
C	-3.463525534	-5.729065895	-10.901416779
H	-4.296582699	-6.153138161	-10.321535110
H	-3.522112608	-4.630560398	-10.875326157
H	-3.541248560	-6.066488743	-11.935984612
C	0.110539638	-1.988834500	-4.326554775

H	0.897019804	-2.268079042	-5.035931587
H	-0.850834608	-2.271544456	-4.770734310
H	0.126854077	-0.895390213	-4.221223354
C	2.897410870	-2.788830757	-2.950177431
H	3.360417843	-1.861339211	-2.287180185
H	3.639460802	-3.768362522	-2.817574501
H	2.811160803	-2.467458248	-4.121446609

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C	1.912228703	-3.625456333	-2.141067266
C	1.128922105	-3.385325909	-0.967700183
C	-0.045942601	-2.611412048	-1.362850904
C	-0.046896052	-2.497445107	-2.764902115
C	1.140573382	-3.185940027	-3.266146660
Rh	-0.035742696	-4.740133762	-2.248654604
C	-2.932682276	-7.008136749	0.963524461
C	-3.333167553	-5.770285130	0.463141024
C	-2.510928154	-5.141037941	-0.455151141
N	-1.354303360	-5.679657936	-0.860857368
C	-0.967553377	-6.899055004	-0.419629306
C	-1.753137112	-7.578379631	0.515805960
H	-3.548812389	-7.531406879	1.691581726
H	-4.262461662	-5.303406715	0.774670660
H	-2.767707586	-4.175020218	-0.889549196
H	-1.440642715	-8.554067612	0.877565861
C	0.250669152	-7.403103352	-1.043946266
C	0.831632495	-6.585511684	-2.033097982
C	0.808183491	-8.654784203	-0.756597459
C	1.919136524	-7.060138226	-2.756855011
C	1.916289926	-9.104421616	-1.459638119
C	2.462063074	-8.312488556	-2.468408823
H	0.372531950	-9.287075996	0.016219504
H	2.361628532	-6.456474781	-3.550218821
H	2.346179724	-10.076611519	-1.233014464
H	3.318655968	-8.671488762	-3.035890579
C	-0.589966238	-6.822099686	-5.618989468
N	-1.083904147	-5.495942593	-3.766316414
C	-1.526445270	-6.215610027	-4.762749672
H	0.471215367	-6.727535725	-5.400266647
H	-0.897663653	-7.379489899	-6.500015736
C	-2.993235350	-6.338371754	-4.948010445
C	-3.850145817	-5.403458595	-4.347369671
C	-3.556048870	-7.383334637	-5.681441784
C	-5.218603611	-5.506239891	-4.487598896
C	-4.933349133	-7.499512196	-5.830937386
C	-5.773400307	-6.556797028	-5.233676434
H	-3.420066118	-4.577118874	-3.777922392
H	-2.918644190	-8.142335892	-6.131585598
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H	-5.340849400	-8.327633858	-6.404910564
C	-1.034244299	-2.042188883	-0.408205032
H	-1.991941214	-1.813564897	-0.888521075
H	-1.223746896	-2.715507746	0.436085880
H	-0.650886774	-1.103069067	0.013802404
C	-1.067211151	-1.836871743	-3.624780655
H	-1.295955658	-2.443556309	-4.509074211
H	-2.005586863	-1.670660615	-3.085061550
H	-0.711335123	-0.861029804	-3.980931997
C	1.533231616	-3.252123117	-4.701474190
H	2.268675566	-4.043322086	-4.881955624
H	0.665196955	-3.451553106	-5.340548515
H	1.977413177	-2.303665161	-5.032742500
C	3.286859035	-4.189590454	-2.161104918
H	3.403834581	-5.019279480	-1.456053495
H	3.571598530	-4.548750401	-3.154818535
H	4.005110741	-3.408141375	-1.879371524
C	1.534069180	-3.686333418	0.433615059
H	0.664293528	-3.885721207	1.069954872
H	2.183653116	-4.566921234	0.478337288
H	2.081103086	-2.842625380	0.876386106
O	-7.115292072	-6.568605900	-5.314110756
C	-7.734804153	-7.591174126	-6.068784714
H	-7.416452408	-7.562099934	-7.120393276
H	-7.520789146	-8.585070610	-5.650732517
H	-8.808778763	-7.404663563	-6.014686108

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C	-0.744295835	-2.838408232	-1.623854160
C	0.174479142	-2.397630692	-2.629749060
C	1.469642639	-2.889261723	-2.269383192
Rh	0.096235320	-4.657049179	-2.531260490
C	-2.900480986	-8.234945297	-1.155603528
C	-3.455513954	-7.073405266	-1.689139843
C	-2.601300716	-6.075454712	-2.123867512
N	-1.271999478	-6.194629669	-2.019380808
C	-0.711307228	-7.317401886	-1.517058969
C	-1.524048924	-8.364946365	-1.079241276
H	-3.542381525	-9.043202400	-0.814842165
H	-4.529757023	-6.947499752	-1.779641747
H	-2.961820841	-5.157644749	-2.583921432
H	-1.074449658	-9.277281761	-0.697960436
C	0.746453643	-7.315242767	-1.512023687
C	1.397458553	-6.309182644	-2.266179085
C	1.509369373	-8.240939140	-0.794191599
C	2.792030096	-6.277773857	-2.293095827
C	2.895158291	-8.191157341	-0.820908368
C	3.533202887	-7.205920219	-1.571374655
H	1.011449933	-8.997763634	-0.190548778
H	3.305644751	-5.529436588	-2.895451307
H	3.477112293	-8.916177750	-0.259046644
H	4.619605064	-7.162414074	-1.601480126
C	0.837969065	-6.033634186	-4.186393261
N	-0.985962093	-4.583400726	-4.259780884
C	-0.325724632	-5.437474728	-4.946630001
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C	-1.762891769	-5.289751053	-6.965735912
C	0.188015312	-6.702017784	-7.034525871
C	-2.063316345	-5.634035587	-8.263471603
C	-0.102062739	-7.057052135	-8.346347809
C	-1.233121634	-6.521028996	-8.967058182
H	-2.402570963	-4.603178024	-6.415105820
H	1.076501250	-7.122757912	-6.565323830
H	-2.936425447	-5.237473011	-8.775039673
H	0.553021491	-7.743220329	-8.873988152
O	-1.613050818	-6.790545464	-10.226507187
C	-0.822362125	-7.673416138	-10.994680405
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H	-1.304646015	-7.747128963	-11.970451355
C	-0.192778632	-1.628653407	-3.845785856
H	0.679413736	-1.410327196	-4.468655586
H	-0.915918946	-2.189431429	-4.454180241
H	-0.655680478	-0.674044549	-3.565920115
C	2.720819235	-2.632648230	-3.036391735
H	3.544094801	-3.273644686	-2.706331730
H	2.572238207	-2.796452284	-4.109995842
H	3.046864033	-1.592290163	-2.905602694
C	2.500819683	-3.977975130	-0.097807027
H	2.314998865	-4.998380661	0.261863202
H	3.452662945	-3.988244534	-0.635896504
H	2.628120899	-3.337130785	0.784066796
C	-0.521013021	-4.023943424	0.710279226
H	-1.567160368	-4.330067635	0.603578627
H	0.054557797	-4.897523880	1.038834453
H	-0.477834761	-3.280952930	1.517614365
C	-2.199494362	-2.527767658	-1.599098206
H	-2.633028746	-2.597079754	-2.603575706
H	-2.751333475	-3.204021692	-0.937192798
H	-2.372536421	-1.506174922	-1.235271335

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C	-0.379644603	-2.991727352	-3.463880777
C	0.928219795	-3.439653635	-3.144256830

Rh	-0.512309492	-4.948710918	-2.424431324
C	-2.803255320	-7.737485409	0.875788689
C	-3.571093321	-6.723600388	0.312586725
C	-3.010354042	-5.936732769	-0.684665620
N	-1.760532618	-6.138085365	-1.107137203
C	-1.024340391	-7.141423702	-0.598493516
C	-1.509625673	-7.957959175	0.413049012
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H	-4.590112686	-6.541188717	0.639695585
H	-3.558458090	-5.127028942	-1.164802670
H	-0.888444602	-8.756912231	0.810118079
C	0.306443304	-7.238378048	-1.237177730
C	0.382535368	-7.387631893	-2.647830725
C	1.469484091	-7.139601231	-0.466047555
C	1.661553144	-7.330052853	-3.231592894
C	2.715355635	-7.136972427	-1.073504806
C	2.808557272	-7.197954178	-2.466048002
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H	1.740700245	-7.453097343	-4.311913013
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H	3.783282280	-7.182974815	-2.948634386
C	-0.764324427	-7.923809528	-3.480024099
N	-1.647743344	-5.667912960	-3.930835009
C	-1.621907711	-6.912085533	-4.220046043
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H	-1.428833127	-8.536501884	-2.851652622
C	-2.488721132	-7.435332298	-5.307691097
C	-3.296790123	-6.543641090	-6.033742905
C	-2.550829172	-8.789382935	-5.646361828
C	-4.115863800	-6.981769562	-7.050132275
C	-3.374020815	-9.249763489	-6.669332981
C	-4.158967018	-8.343029976	-7.382516861
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H	-3.397464991	-10.310832024	-6.898884296
C	2.034156799	-3.699921846	-4.103825569
H	2.733002901	-4.446806431	-3.710911989
H	1.651615500	-4.069055080	-5.060670376
H	2.605045795	-2.781764030	-4.296116829
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H	2.186044693	-3.877454281	0.100065403
H	2.871863365	-4.567285061	-1.382191658
H	3.011296511	-2.834278822	-1.069377661
C	-0.505233169	-3.047225952	0.331334561
H	-1.550010681	-3.320519209	0.516609907
H	0.120773546	-3.727766752	0.919532418
H	-0.358860224	-2.033311129	0.723657966
C	-2.529582977	-2.487087250	-2.108383179
H	-3.135167122	-2.963699341	-2.888372898
H	-2.957083941	-2.733815670	-1.131054521
H	-2.619654179	-1.399934769	-2.239658833
C	-0.969941974	-2.775284529	-4.805918694
H	-0.204137221	-2.765477419	-5.585571766
H	-1.680876493	-3.585690975	-5.030182362
H	-1.506427169	-1.819815397	-4.844886303
O	-4.988523006	-8.669656754	-8.388830185
C	-5.064147472	-10.021009445	-8.784350395
H	-4.088438988	-10.397897720	-9.120655060
H	-5.435032845	-10.658121109	-7.969626427
H	-5.766694069	-10.060411453	-9.618511200

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C	0.719102383	-3.453485727	-1.483843803
C	-0.517891228	-3.337360382	-0.837126791
C	-1.536394119	-3.117602825	-1.862021208
C	-0.874413311	-3.023609161	-3.147426128
C	0.494287908	-3.325830936	-2.928884029
Rh	-0.727308512	-5.046705246	-2.293396473
C	-2.034508467	-8.453861237	0.955200911
C	-3.036757946	-7.572392464	0.572689712
C	-2.770480394	-6.629237652	-0.413829207
N	-1.568266034	-6.563032627	-0.993299484
C	-0.604156554	-7.444113731	-0.666861713
C	-0.796954572	-8.399469376	0.319461733
H	-2.218262434	-9.194580078	1.729324937

H	-4.022892952	-7.608200550	1.025127172
H	-3.528595924	-5.941542149	-0.787979901
H	0.001569332	-9.095333099	0.562689006
C	0.628209829	-7.277802944	-1.467573643
C	0.552508354	-7.335628986	-2.884184599
C	1.854133844	-7.053602219	-0.830857635
C	1.727138400	-7.060861588	-3.604641914
C	3.003730774	-6.829792976	-1.571958184
C	2.930412769	-6.802219391	-2.966846704
H	1.885708332	-7.044611931	0.258204669
H	1.690684438	-7.112037182	-4.692754745
H	3.954714537	-6.670480728	-1.069368124
H	3.826134443	-6.620990276	-3.556782484
C	-0.613967240	-7.955933094	-3.620900869
N	-1.870375276	-5.834311485	-3.769172192
C	-1.659286737	-7.017518997	-4.204855919
H	-0.203224227	-8.572911263	-4.430273056
H	-1.139067173	-8.657602310	-2.954914331
C	-2.473628759	-7.549260139	-5.323935986
C	-3.080820799	-6.659257889	-6.225708485
C	-2.670734882	-8.917870522	-5.521356583
C	-3.856431246	-7.118354797	-7.267558098
C	-3.458650827	-9.395891190	-6.562533379
C	-4.057215214	-8.493031502	-7.443562508
H	-2.919860125	-5.590735435	-6.101008892
H	-2.223325968	-9.643236160	-4.843925953
H	-4.319243431	-6.436883450	-7.976710796
H	-3.599799871	-10.466218948	-6.678179264
H	-3.470628023	-5.086138725	-3.890455961
O	-4.335952282	-4.625988483	-4.112190247
O	-4.954063892	-5.288212776	-2.063695431
C	-5.219232559	-4.770968437	-3.132107496
C	-6.559985638	-4.205951214	-3.482791901
H	-6.981229782	-4.751211166	-4.333418369
H	-7.232502460	-4.279621124	-2.627546787
H	-6.457099915	-3.161529303	-3.794989824
C	-2.958554983	-2.788102388	-1.590547204
H	-3.538951159	-2.748619080	-2.516154289
H	-3.437068462	-3.516937494	-0.927262783
H	-3.020529985	-1.804565430	-1.104241967
C	-1.525759578	-2.707008362	-4.443543434
H	-0.971843719	-3.136292934	-5.284014702
H	-2.549151182	-3.093978882	-4.489321232
H	-1.568400264	-1.619540691	-4.585981846
C	-0.791301608	-3.464989662	0.619722188
H	-1.785502553	-3.887576103	0.800813913
H	-0.057096861	-4.117338181	1.105464101
H	-0.755181372	-2.488318920	1.118151546
C	2.054395914	-3.614673138	-0.859570146
H	1.987115979	-3.975392580	0.171409667
H	2.682346582	-4.310609818	-1.425959587
H	2.574631453	-2.647439718	-0.842313290
C	1.573506832	-3.357714176	-3.949409723
H	2.315947294	-4.131153107	-3.722686529
H	1.172630310	-3.553109646	-4.947989464
H	2.098773718	-2.393449068	-3.978406668
O	-4.829967976	-8.839330673	-8.488800049
C	-5.055246830	-10.210596085	-8.731880188
H	-4.115662098	-10.742998123	-8.933480263
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H	-5.693363667	-10.264950752	-9.615364075

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C	0.554756522	-3.645280123	-2.051550865
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C	-1.264176607	-3.123777151	-3.401498795
C	0.074892476	-3.639034510	-3.411138773
Rh	-1.210035920	-4.917553425	-2.216984034
C	-1.787600398	-8.550342560	1.045217395
C	-2.454031229	-7.339095116	1.172946095
C	-2.085361719	-6.289349079	0.347052544
N	-1.101109028	-6.388214588	-0.561822116
C	-0.418033928	-7.548808575	-0.655397713
C	-0.750603020	-8.649814606	0.127504274
H	-2.057549953	-9.400512695	1.666424155

H	-3.254296780	-7.203067303	1.893811464
H	-2.613864183	-5.340487003	0.379998475
H	-0.168371007	-9.561917305	0.023177257
C	0.839973629	-7.549583912	-1.451674342
C	0.905044436	-7.837227821	-2.819700480
C	2.010253429	-7.251171589	-0.747414410
C	2.139804363	-7.728004932	-3.464813232
C	3.239106655	-7.197406769	-1.392636180
C	3.298742771	-7.409382820	-2.766733885
H	1.948780537	-7.082115650	0.327573389
H	2.194575071	-7.950879574	-4.530336380
H	4.142953873	-6.983722210	-0.827369213
H	4.251235008	-7.361609936	-3.289241552
C	-0.262094855	-8.389175415	-3.578868151
N	-1.646737099	-6.317859173	-3.690765381
C	-1.268416286	-7.427746296	-4.190367222
H	0.131983668	-9.033583641	-4.372842789
H	-0.844877660	-9.055287361	-2.921261311
C	-1.897672534	-7.894791126	-5.457370758
C	-2.369512081	-6.947780132	-6.381909847
C	-2.025297403	-9.245875359	-5.790450096
C	-2.952811003	-7.330950737	-7.570904255
C	-2.619644403	-9.650998116	-6.979530811
C	-3.098741293	-8.690329552	-7.873660088
H	-2.245714903	-5.889557362	-6.159617424
H	-1.670168281	-10.016445160	-5.108703136
H	-3.307314396	-6.603609562	-8.296628952
H	-2.710850477	-10.710878372	-7.196844578
H	-2.906160116	-5.908323765	-3.952360392
O	-4.001851559	-5.603144169	-3.917271376
O	-3.484859467	-5.108376026	-1.791439533
C	-4.309000015	-5.242065430	-2.725952148
C	-5.756505013	-4.932532787	-2.495623827
H	-6.354092598	-5.838161945	-2.639216185
H	-5.920693398	-4.536832809	-1.491818547
H	-6.091043949	-4.208670139	-3.246577024
C	-2.856051683	-2.150678396	-1.561106443
H	-3.600398540	-2.110823393	-2.360878229
H	-3.286859512	-2.725455999	-0.733277321
H	-2.684462309	-1.125414491	-1.209200621
C	-2.127246857	-2.894155741	-4.590459824
H	-1.892139554	-3.601221323	-5.392081738
H	-3.189374208	-3.016831398	-4.355526924
H	-1.982870936	-1.879716754	-4.984211922
C	-0.368445605	-2.870024920	0.266997546
H	-1.357202053	-2.804043770	0.732970178
H	0.175025836	-3.691060543	0.747908592
H	0.167430148	-1.939536095	0.496202290
C	1.927084923	-4.006539822	-1.626004577
H	1.976842523	-4.227183342	-0.555329621
H	2.316436529	-4.867975712	-2.175579309
H	2.599538088	-3.157744169	-1.816615343
C	0.847312927	-4.091840267	-4.597468853
H	1.492265463	-4.941845894	-4.347315311
H	0.184628010	-4.408452988	-5.408438206
H	1.481557012	-3.279610157	-4.975985527
O	-3.687377453	-8.965298653	-9.051479340
C	-3.809689760	-10.315877914	-9.443457603
H	-2.826050758	-10.794652939	-9.545185089
H	-4.420520306	-10.889047623	-8.733090401
H	-4.305397987	-10.309906006	-10.415646553

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C	0.245995000	-3.713557720	-1.471642017
C	-1.017338395	-3.195060730	-1.004137993
C	-1.793200493	-2.821727753	-2.157910824
C	-1.060580850	-3.205330849	-3.323031902
C	0.219156548	-3.754009485	-2.899845362
Rh	-1.420459032	-5.003213882	-2.150201321
C	-0.249286771	-7.950836182	1.640012980
C	-1.374689221	-7.137045383	1.613891363
C	-1.678467155	-6.467775345	0.441747636
N	-0.929270625	-6.559939861	-0.670700073
C	0.152240098	-7.366728306	-0.664228082
C	0.510769486	-8.069630623	0.488481224
H	0.024483019	-8.496205330	2.539424181

H	-2.015757561	-7.021555901	2.482210636
H	-2.551563025	-5.823846340	0.364757061
H	1.380913019	-8.719626427	0.452957362
C	0.996150911	-7.512553692	-1.871591091
C	0.490361035	-7.978294849	-3.091792822
C	2.370672703	-7.267724037	-1.746362567
C	1.368374228	-8.136843681	-4.167418957
C	3.229140759	-7.420063019	-2.825308561
C	2.720834494	-7.851287365	-4.047742844
H	2.762939930	-6.948638916	-0.780807078
H	0.974628508	-8.510913849	-5.112953186
H	4.290825367	-7.216735363	-2.710310936
H	3.382502079	-7.984242916	-4.900167942
C	-0.956933796	-8.358427048	-3.281516075
N	-1.772194862	-6.198740482	-3.911247015
C	-1.600548267	-7.425766468	-4.266241550
H	-0.998624980	-9.388854027	-3.647992134
H	-1.542079091	-8.296683311	-2.357725143
C	-1.935935378	-7.891620636	-5.618210793
C	-1.854694247	-7.007756233	-6.710910320
C	-2.320128441	-9.212620735	-5.870761395
C	-2.145876646	-7.424176216	-7.990527153
C	-2.633208752	-9.643013954	-7.151766300
C	-2.541202545	-8.749667168	-8.224060059
H	-1.505780578	-5.986702442	-6.556282043
H	-2.412728548	-9.919735909	-5.049556255
H	-2.059277296	-6.757521152	-8.844308853
H	-2.943467140	-10.671490669	-7.307523727
H	-2.267264128	-5.652637959	-4.615450382
O	-3.528710127	-7.526681900	-1.824987769
O	-3.463714123	-5.274762154	-1.700584054
C	-4.068314075	-6.434369087	-1.705281615
C	-5.570305347	-6.322835445	-1.549736738
H	-5.946466446	-7.196059704	-1.011097312
H	-5.868257046	-5.402169228	-1.042609453
H	-6.028434277	-6.327573299	-2.545350075
C	-3.165223122	-2.260471344	-2.110358477
H	-3.478180408	-1.858082533	-3.077928305
H	-3.870680332	-3.053789616	-1.818550825
H	-3.231643915	-1.457713246	-1.367348909
C	-1.505790830	-2.987253189	-4.725511074
H	-0.939198315	-3.601634741	-5.432822227
H	-2.572943211	-3.208583355	-4.848864555
H	-1.358568430	-1.939185619	-5.016936302
C	-1.414637327	-2.941669226	0.407589614
H	-2.488581419	-3.112675428	0.547650933
H	-0.874765515	-3.588566303	1.106973767
H	-1.206374526	-1.901571870	0.693265021
C	1.373366475	-4.109791279	-0.589471400
H	1.033780694	-4.707192898	0.266070813
H	2.127203703	-4.685152054	-1.132753015
H	1.859010696	-3.211715937	-0.186023325
C	1.304534197	-4.201663971	-3.813144207
H	2.005023956	-4.880237103	-3.313986301
H	0.897247732	-4.740846634	-4.676469326
H	1.873808980	-3.343587399	-4.193626404
O	-2.792788029	-9.062638283	-9.501950264
C	-3.160692692	-10.391548157	-9.816164970
H	-2.372082472	-11.101505280	-9.533654213
H	-4.100247383	-10.674438477	-9.323746681
H	-3.300147772	-10.422628403	-10.897553444

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^{1}D-TS'

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C	1.259085774	-3.577841759	-0.729226053
C	-0.150382251	-3.619013786	-0.508157134
C	-0.795783281	-2.754477978	-1.464942575
C	0.230533034	-2.196634054	-2.297541857
C	1.497320771	-2.730854750	-1.864470243
Rh	0.193499446	-4.402793407	-2.630498171
C	-2.532255650	-8.457469940	-2.252181053
C	-3.172462225	-7.217185020	-2.262658119
C	-2.394845486	-6.082413197	-2.382646322
N	-1.054951787	-6.134137154	-2.461886883
C	-0.415078282	-7.327092648	-2.420217991
C	-1.155262947	-8.512681007	-2.336888790
H	-3.111095190	-9.374738693	-2.180035114

H	-4.251829147	-7.132374287	-2.187455177
H	-2.840351582	-5.089483261	-2.411317110
H	-0.640279889	-9.468411446	-2.344468594
C	1.028425097	-7.242361069	-2.434366465
C	1.610238433	-5.992990971	-2.729596615
C	1.863144279	-8.321040154	-2.085913181
C	2.999260664	-5.839923859	-2.644965887
C	3.228660107	-8.160020828	-1.993458271
C	3.791829824	-6.905007362	-2.265129566
H	1.418411732	-9.285640717	-1.847124100
H	3.450063467	-4.898420811	-2.948604345
H	3.861414194	-8.995970726	-1.709254622
H	4.869775772	-6.770208359	-2.206451893
C	-0.886079967	-4.246253014	-4.474617958
N	1.196924567	-5.118443012	-4.356093407
C	0.118125029	-5.127997398	-5.098352909
H	-1.930653453	-4.569335938	-4.431520939
H	-0.780750215	-3.202236414	-4.779110909
C	0.020539574	-5.895534992	-6.319890499
C	0.948307157	-6.919147968	-6.559246540
C	-0.986423492	-5.655084133	-7.269568920
C	0.894885063	-7.675148964	-7.716461182
C	-1.052978992	-6.404566765	-8.423986435
C	-0.108702518	-7.416512489	-8.659860611
H	1.715577841	-7.113414288	-5.810328484
H	-1.711401820	-4.860678196	-7.096925735
H	1.623214006	-8.463693619	-7.879477024
H	-1.817236304	-6.234498501	-9.177375793
C	-0.803808272	-4.419759274	0.562851310
H	-1.872568607	-4.565963745	0.379343212
H	-0.338530630	-5.408764362	0.654875338
H	-0.701129973	-3.919823647	1.535015225
C	-2.244881868	-2.408575535	-1.512160778
H	-2.609651089	-2.319829702	-2.542759895
H	-2.858365536	-3.158442020	-1.000846148
H	-2.435298681	-1.448417783	-1.015759468
C	2.264734983	-4.286729336	0.109422214
H	2.281577349	-3.864437103	1.122411966
H	2.035366297	-5.356550217	0.202678993
H	3.274735689	-4.207345009	-0.300949335
O	-0.252921760	-8.086077690	-9.812508583
C	0.683588505	-9.097116470	-10.131318092
H	1.703131080	-8.693502426	-10.187682152
H	0.655385375	-9.914648056	-9.398374557
H	0.395809531	-9.483210564	-11.110258102
C	0.073091269	-1.143620968	-3.336659193
H	0.731712580	-1.325050831	-4.193900108
H	-0.956580818	-1.071920276	-3.700808048
H	0.342695892	-0.162527978	-2.922740698
C	2.811776400	-2.318701029	-2.430310965
H	3.643192768	-2.864812136	-1.976102829
H	2.850061178	-2.481564522	-3.514518023
H	2.984631300	-1.249478102	-2.251670122

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C	1.496215105	-3.313021183	-1.467175126
C	0.251318097	-3.053214550	-0.822359264
C	-0.655168593	-2.443414688	-1.794555306
C	0.009027543	-2.408185959	-3.036736250
C	1.325227618	-3.000312328	-2.860738277
Rh	-0.112675272	-4.581339359	-2.365404844
C	-3.283466816	-7.641040802	-0.196622133
C	-3.708123684	-6.345975876	-0.480675071
C	-2.808860302	-5.476218700	-1.074161172
N	-1.554288030	-5.836377144	-1.367828727
C	-1.134236932	-7.102043152	-1.127487183
C	-1.995294094	-8.025144577	-0.530977607
H	-3.960406542	-8.352668762	0.269080758
H	-4.716706276	-6.014360905	-0.255031556
H	-3.089982510	-4.457446098	-1.335385561
H	-1.657374024	-9.041849136	-0.350664675
C	0.211945266	-7.403808594	-1.603604794
C	0.810253441	-6.445970535	-2.460951090
C	0.917927682	-8.564288139	-1.287971139
C	2.074139833	-6.688168526	-3.015757322
C	2.184786320	-8.785085678	-1.817806959

C	2.759181976	-7.848906994	-2.682099104
H	0.490228623	-9.296557426	-0.605493128
H	2.499529839	-5.973474026	-3.719097614
H	2.726269245	-9.691498756	-1.560947180
H	3.745183229	-8.034066200	-3.102085829
C	-0.713012755	-8.031168938	-4.779631615
N	-0.412395537	-5.881334305	-3.849946260
C	-1.216687799	-6.799532890	-4.368247509
H	0.330857843	-8.281736374	-4.611388206
C	-2.659515381	-6.469552517	-4.483273983
C	-3.092732906	-5.147500038	-4.657087326
C	-3.619271517	-7.469028473	-4.328728676
C	-4.439256191	-4.843451500	-4.687041759
C	-4.978954792	-7.177463055	-4.354059219
C	-5.395889282	-5.857424259	-4.536840439
H	-2.352751970	-4.357549191	-4.780910015
H	-3.305459499	-8.497695923	-4.155976772
H	-4.793010712	-3.827025652	-4.842527866
H	-5.699748993	-7.979755402	-4.227512836
C	2.361998796	-3.076802969	-3.926969290
H	3.211267471	-3.695908546	-3.621887684
H	1.951327205	-3.493560314	-4.854347706
H	2.752957344	-2.078018188	-4.162164688
C	2.725276947	-3.864607334	-0.834348381
H	2.490031719	-4.440032005	0.066855192
H	3.265264750	-4.531440735	-1.515033603
H	3.410153866	-3.057634115	-0.545055032
C	-0.513913214	-1.891558409	-4.329564571
H	-0.260790020	-2.564419031	-5.157031059
H	-1.601464748	-1.768759012	-4.309998512
H	-0.074386396	-0.912596464	-4.562474251
C	-2.024052382	-1.933374763	-1.506248116
H	-2.710851669	-2.121939421	-2.340934992
H	-2.448184967	-2.393306255	-0.607154846
H	-2.010736942	-0.850348175	-1.329858541
C	-0.047584288	-3.251706839	0.622964203
H	-1.096969008	-3.519974470	0.787071228
H	0.566789627	-4.049314976	1.053242326
H	0.149445146	-2.334212780	1.192407131
H	-1.334752679	-8.734638214	-5.326270580
O	-6.680458069	-5.458966732	-4.578252792
C	-7.690538406	-6.441839695	-4.488897324
H	-7.608753204	-7.176239491	-5.301309586
H	-7.658977032	-6.965961456	-3.523604870
H	-8.641621590	-5.914661884	-4.577441692

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H

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C	0.882708430	-3.741567612	-0.641393065
C	-0.432979643	-3.176402330	-0.439740360
C	-0.647566378	-2.134058714	-1.399437428
C	0.523928225	-2.079617739	-2.237905502
C	1.470371604	-3.058037043	-1.745563030
Rh	-0.374106586	-4.040527821	-2.470248699
C	-3.450647354	-7.875472546	-1.725929737
C	-3.887111425	-6.559018612	-1.621836185
C	-2.964642525	-5.548259258	-1.824495077
N	-1.669489026	-5.781135082	-2.089267254
C	-1.228167176	-7.057309628	-2.183806658
C	-2.119666100	-8.122139931	-2.014997244
H	-4.145343304	-8.701616287	-1.598417163
H	-4.922771454	-6.316146851	-1.405533075
H	-3.254814625	-4.499393940	-1.782000422
H	-1.760526776	-9.138993263	-2.146230698
C	0.189930499	-7.331386089	-2.491020918
C	0.922758281	-6.532475471	-3.396070242
C	0.833585322	-8.418040276	-1.892873406
C	2.260494947	-6.819864750	-3.659354687
C	2.163424730	-8.709355354	-2.167827606
C	2.876094580	-7.909593582	-3.055275202
H	0.290517271	-9.026354790	-1.171673059
H	2.798743486	-6.180618286	-4.356636524
H	2.645038843	-9.552436829	-1.680200338
H	3.917667389	-8.130805016	-3.274474621
C	-1.323836446	-3.965400696	-4.442644119
N	0.338807583	-5.374588966	-3.933289766
C	-0.759183168	-5.288623810	-4.670041561

H	-2.391251564	-3.826441765	-4.622004509
H	-0.724107683	-3.161537647	-4.875069618
C	-1.384119868	-6.399808407	-5.379226208
C	-0.641413033	-7.520773888	-5.779920101
C	-2.760933161	-6.380329132	-5.667737007
C	-1.239071488	-8.592499733	-6.420932770
C	-3.372123957	-7.451350689	-6.282901764
C	-2.617022276	-8.568951607	-6.665458202
H	0.431652695	-7.549973965	-5.608239651
H	-3.362981558	-5.519433975	-5.386159420
H	-0.629909635	-9.434733391	-6.734040737
H	-4.437656879	-7.455407619	-6.494921684
C	1.494190812	-4.834066391	0.166280091
H	0.742208719	-5.569888592	0.474938929
H	2.262282133	-5.370416641	-0.401726484
H	1.966259480	-4.444603920	1.077575326
C	-1.367102385	-3.596755743	0.638760567
H	-2.397907972	-3.290693045	0.435847998
H	-1.354526758	-4.683234692	0.780618966
H	-1.069897413	-3.140570164	1.591969490
C	2.808470249	-3.336726665	-2.332389832
H	3.584283829	-2.751678944	-1.822099686
H	3.073058367	-4.396242619	-2.236077547
H	2.840930700	-3.078720808	-3.396156311
C	0.781397402	-1.093189955	-3.322569370
H	1.404716253	-1.518977761	-4.116375446
H	-0.151272193	-0.745861888	-3.778760195
H	1.304880738	-0.212241620	-2.929327726
C	-1.832034707	-1.236610770	-1.503823876
H	-2.097656965	-1.047169089	-2.549814224
H	-2.709270716	-1.668605328	-1.011921287
H	-1.635022759	-0.266099006	-1.030385137
O	-3.298221827	-9.557521820	-7.260200977
C	-2.591496468	-10.709578514	-7.680167198
H	-1.821787000	-10.460124969	-8.421680450
H	-2.125217676	-11.223146439	-6.828914165
H	-3.328515291	-11.370082855	-8.138319969

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C	1.038478017	-3.866888762	-0.912635088
C	-0.272448838	-3.368129730	-0.615249038
C	-0.614695370	-2.349644899	-1.579981327
C	0.499452561	-2.219158649	-2.481039524
C	1.507139921	-3.166978836	-2.080840349
Rh	-0.310323954	-4.255493641	-2.630050182
C	-3.927278042	-7.546842575	-1.783019423
C	-4.184525490	-6.182060242	-1.863087535
C	-3.118740559	-5.330029964	-2.090401888
N	-1.850690365	-5.757827759	-2.203029394
C	-1.582491040	-7.080245018	-2.111501455
C	-2.624777079	-7.994338512	-1.917192340
H	-4.737393379	-8.256165504	-1.634724498
H	-5.190505981	-5.783874512	-1.774001241
H	-3.265893698	-4.256586075	-2.201974392
H	-2.400145054	-9.057111740	-1.905977726
C	-0.193734914	-7.567095757	-2.227481842
C	0.746369898	-6.985554695	-3.107363224
C	0.214211464	-8.646855354	-1.437539458
C	2.047699928	-7.488364697	-3.160623789
C	1.507811308	-9.146916389	-1.501410007
C	2.425561428	-8.566925049	-2.370296955
H	-0.490396023	-9.082036018	-0.730805039
H	2.753652334	-7.029310703	-3.850912094
H	1.799673200	-9.979013443	-0.866412580
H	3.441032410	-8.950477600	-2.430168152
C	-0.961827040	-4.300251007	-4.778544903
N	0.447806239	-5.827105522	-3.855485916
C	-0.615157008	-5.678975582	-4.676384926
H	-1.926416278	-4.032267570	-5.207663536
H	-0.138004094	-3.639514208	-5.063970089
C	-1.374613881	-6.800034523	-5.220987797
C	-0.725363910	-8.006038666	-5.516028404
C	-2.752227306	-6.703168869	-5.483827114
C	-1.414705038	-9.090256691	-6.033588886
C	-3.455409288	-7.783726215	-5.971512318
C	-2.793360472	-8.989541054	-6.248933315

H	0.349681288	-8.090127945	-5.368000984
H	-3.282835007	-5.775923729	-5.274451256
H	-0.876134038	-10.002638817	-6.270622730
H	-4.524034977	-7.731362820	-6.161467075
H	1.819608092	-5.308529377	-5.087417603
O	2.486435413	-5.344409466	-5.813200951
O	1.926452160	-3.182291031	-5.975971222
C	2.580904007	-4.131476879	-6.364511967
C	3.566856623	-4.096865177	-7.487174034
H	3.249006271	-4.785079002	-8.277414322
H	3.645974159	-3.085050344	-7.885246754
H	4.544690609	-4.443084240	-7.136915207
C	2.828208208	-3.379062891	-2.730947495
H	3.614414930	-2.841728687	-2.184274197
H	3.100227833	-4.442543507	-2.733273268
H	2.823978662	-3.023653507	-3.766141891
C	0.607034326	-1.242978454	-3.598764658
H	1.218137383	-1.628553510	-4.421646595
H	-0.379859328	-0.990445733	-4.001871586
H	1.065992475	-0.311177731	-3.242260933
C	-1.837337971	-1.498197794	-1.580294251
H	-2.213709116	-1.336662889	-2.596647263
H	-2.642585993	-1.948426247	-0.990776598
H	-1.630354762	-0.511895299	-1.144688487
C	-1.122326612	-3.825077534	0.517422318
H	-2.186460733	-3.646575689	0.332865149
H	-0.989060521	-4.894874573	0.713176072
H	-0.852537811	-3.285111427	1.434259892
C	1.778088212	-4.932164669	-0.181521595
H	1.104347467	-5.549072742	0.422656476
H	2.299308538	-5.602664948	-0.876685917
H	2.530482054	-4.504630089	0.493428677
O	-3.562059402	-9.980258942	-6.722615719
C	-2.951460123	-11.214388847	-7.049257278
H	-2.196057558	-11.090702057	-7.836141586
H	-2.487225294	-11.676812172	-6.167928219
H	-3.748491526	-11.862047195	-7.416676044

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I-TS

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C	-0.151722193	-2.882554054	-0.596878052
C	0.026842669	-2.409895420	-1.964745879
C	1.040585160	-3.193495989	-2.582971334
C	1.449538946	-4.206301689	-1.641537666
C	0.740415871	-3.966689587	-0.395986736
Rh	-0.689861298	-4.497704983	-1.986852646
C	-1.748284698	-8.979291916	-0.327833831
C	-2.262707233	-7.849485397	0.300840169
C	-1.908861041	-6.609230042	-0.197972402
N	-1.087139606	-6.461740494	-1.247464418
C	-0.579692483	-7.547008038	-1.877590537
C	-0.908612728	-8.825767517	-1.418404937
H	-2.014035225	-9.973989487	0.020788200
H	-2.934049606	-7.924017906	1.150460839
H	-2.296239614	-5.686661243	0.234843224
H	-0.526747108	-9.692138672	-1.951923609
C	0.304476559	-7.371417999	-3.047042847
C	0.062280491	-6.345351219	-3.985816240
C	1.381872535	-8.238368988	-3.249710798
C	0.916802287	-6.192972183	-5.074911118
C	2.223787546	-8.085412025	-4.344405174
C	1.992379665	-7.057147026	-5.253824711
H	1.583529353	-9.023610115	-2.522321463
H	0.688211560	-5.424387455	-5.811045170
H	3.061198473	-8.763873100	-4.485051155
H	2.640585184	-6.938455105	-6.119208336
C	-3.376416683	-6.473999500	-3.353374958
N	-1.108460307	-5.548123837	-3.832489252
C	-2.281843901	-6.361572266	-4.110499859
H	-3.488934994	-5.989555359	-2.389627218
H	-4.213261127	-7.053265095	-3.734344006
C	-2.159198046	-7.056552887	-5.420333862
C	-2.036041737	-8.442324638	-5.489497662
C	-2.046633005	-6.315421104	-6.605617046
C	-1.786820889	-9.090252876	-6.697494507
C	-1.808484912	-6.943028450	-7.812823772
C	-1.661236644	-8.336136818	-7.865376949

H	-2.115583658	-9.027281761	-4.572434425
H	-2.146614313	-5.229541302	-6.570898533
H	-1.685990334	-10.172624588	-6.716481209
H	-1.725289106	-6.383756161	-8.741906166
O	-2.743663788	-3.716053963	-2.295551538
C	-2.967832327	-3.252738237	-3.440566778
O	-2.204293251	-3.429689407	-4.462393761
C	-4.178852081	-2.410062075	-3.677108288
H	-4.836660862	-2.920567036	-4.388203144
H	-4.715233803	-2.216620445	-2.747367859
H	-3.875501871	-1.467917919	-4.146633148
H	-1.521600485	-4.326854706	-4.306093693
C	1.569968700	-2.995434046	-3.956709385
H	2.300107956	-2.175398350	-3.963729143
H	2.071953058	-3.892344952	-4.331245899
H	0.772021413	-2.729650259	-4.660054207
C	-0.644279242	-1.219758749	-2.550569296
H	-0.785336614	-1.322268367	-3.631273508
H	-1.620957255	-1.041012526	-2.089109421
H	-0.031846270	-0.325070739	-2.375599623
C	-1.122275352	-2.306696892	0.370995611
H	-2.122496367	-2.240836620	-0.074142575
H	-1.196546555	-2.909737825	1.280801177
H	-0.822532296	-1.293177605	0.666977465
C	0.937560380	-4.750106335	0.851848841
H	0.082868256	-4.665484905	1.529788494
H	1.098218560	-5.812766552	0.640103340
H	1.823067546	-4.385412693	1.388476491
C	2.558049917	-5.177667618	-1.827756166
H	3.513206482	-4.722455978	-1.532152534
H	2.415821791	-6.072444439	-1.213535428
H	2.646856308	-5.499200821	-2.870758057
O	-1.399304628	-8.847866058	-9.086259842
C	-1.224134207	-10.243018150	-9.202158928
H	-0.377074122	-10.595804214	-8.595252991
H	-2.130986929	-10.790991783	-8.906788826
H	-1.014995098	-10.442010880	-10.254885674

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J

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C	0.308255374	-2.973847628	-0.548032463
C	0.077713333	-2.222861528	-1.754044175
C	0.826271057	-2.833595753	-2.812110901
C	1.593193769	-3.926549911	-2.238892317
C	1.269161940	-4.018168926	-0.856624842
Rh	-0.573644519	-4.306427479	-2.012830257
C	-2.349869251	-7.889195442	0.864802837
C	-2.754904985	-6.571269512	1.019803762
C	-2.242567062	-5.613162518	0.159061641
N	-1.356301665	-5.915469170	-0.804593861
C	-0.947634518	-7.190972805	-0.967656672
C	-1.447415352	-8.199874878	-0.140852243
H	-2.743391991	-8.673075676	1.506911159
H	-3.469359398	-6.279092312	1.783091307
H	-2.548009872	-4.567770004	0.210709438
H	-1.150217414	-9.229784012	-0.316218525
C	0.008337171	-7.542283058	-2.041571617
C	0.008718897	-6.954884529	-3.317914486
C	0.943026423	-8.556062698	-1.789992094
C	0.882784426	-7.416178703	-4.298537731
C	1.834035635	-8.992209435	-2.760082722
C	1.795280099	-8.427517891	-4.028908730
H	0.986019492	-8.993556023	-0.794702351
H	0.836322427	-6.972578526	-5.293488979
H	2.553485394	-9.771524429	-2.523965836
H	2.473213673	-8.767827988	-4.807135582
C	-2.925469637	-7.159347057	-3.594019175
N	-0.854221523	-5.851298809	-3.663346291
C	-2.190846205	-6.195477009	-4.152531624
H	-2.589672804	-7.761093616	-2.756177664
H	-3.916680098	-7.364160061	-3.984841347
C	-2.582252502	-5.463782787	-5.371263504
C	-3.207629204	-6.151955128	-6.413124084
C	-2.298072100	-4.100158691	-5.559274673
C	-3.559613943	-5.518570900	-7.598385811
C	-2.635241032	-3.461115837	-6.736631870
C	-3.269595385	-4.163442135	-7.768244743

H	-3.400805473	-7.217834949	-6.305721760
H	-1.869062185	-3.526157618	-4.739876270
H	-4.039181232	-6.092028618	-8.385894775
H	-2.435275793	-2.402633905	-6.887555599
O	-2.526202917	-3.861987829	-2.584366322
C	-3.363476038	-3.209161758	-1.840442657
O	-3.142733812	-2.804349422	-0.697245121
C	-4.689386845	-2.994921207	-2.530807972
H	-4.537442684	-2.459843874	-3.474654198
H	-5.125417233	-3.966749668	-2.788085222
H	-5.372489929	-2.436480284	-1.888196230
H	-0.407834768	-5.356645584	-4.435541153
C	0.911932170	-2.350876331	-4.216915607
H	1.738312006	-1.636892319	-4.329690933
H	1.091063023	-3.167588472	-4.925404072
H	-0.006498493	-1.839984775	-4.522716045
C	-0.797295988	-1.030214071	-1.874718189
H	-1.214270115	-0.934871793	-2.882728577
H	-1.628582120	-1.078385115	-1.165566921
H	-0.211525723	-0.123856194	-1.668422580
C	-0.259527892	-2.656080484	0.787351668
H	-1.322872639	-2.409687996	0.696230114
H	-0.155263871	-3.497557640	1.479177594
H	0.261661917	-1.797761798	1.231226921
C	1.830831051	-4.991852283	0.116318062
H	1.105253339	-5.244852066	0.896653831
H	2.136812449	-5.920607090	-0.376090765
H	2.713533401	-4.569706917	0.613187611
C	2.580590963	-4.764609337	-2.966834784
H	3.582492352	-4.324969292	-2.876118183
H	2.626969576	-5.784118176	-2.570498466
H	2.354580641	-4.829741478	-4.036748886
O	-3.553764820	-3.449820042	-8.873189926
C	-4.208378315	-4.103084087	-9.940681458
H	-3.599202871	-4.923325062	-10.344308853
H	-5.185478687	-4.497708321	-9.631073952
H	-4.354965210	-3.351031542	-10.717310905

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C	-0.659199953	0.017164590	-3.627709627
C	-0.719029367	1.201391697	-2.901327848
C	-0.765326738	1.104908586	-1.514261603
N	-0.762568414	-0.046508893	-0.851917803
C	-0.709890604	-1.193034053	-1.548361659
C	-0.651324809	-1.191195726	-2.949232817
H	-0.615127444	0.033109181	-4.715380669
H	-0.726531327	2.170933008	-3.391346216
H	-0.807955384	2.008894205	-0.902902007
H	-0.591903269	-2.121925354	-3.508672476
C	-0.711593270	-2.447006702	-0.757071137
C	-0.766788483	-3.712038517	-1.355489373
C	-0.659939349	-2.375076056	0.640541792
C	-0.763871670	-4.866109848	-0.583012164
C	-0.658032179	-3.528011799	1.412478209
C	-0.708472610	-4.779882908	0.805244923
H	-0.822882116	-3.812353611	-2.438273668
H	-0.622404933	-1.392322540	1.102980375
H	-0.808723330	-5.838789463	-1.069858789
H	-0.616228402	-3.448474884	2.497377157
H	-0.706759632	-5.683965683	1.409856677

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Azirine

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C	1.109040022	1.458641291	-1.614048958
N	0.388196498	1.601771474	-0.281293392
C	1.649499893	1.678825974	-0.297556520
H	1.111858010	0.462448955	-2.060975313
H	0.997834861	2.285223484	-2.318683863
C	2.783479929	1.863137364	0.573221147
C	2.583091021	2.045435429	1.946721673
C	4.080535889	1.860374451	0.051696219
C	3.668992996	2.218006372	2.788589001
C	5.169713020	2.034986258	0.891812563
C	4.959729195	2.215738773	2.258782387
H	1.565946817	2.045278072	2.333670378

H	4.218991280	1.723388791	-1.019314408
H	3.546199322	2.362067223	3.859161139
H	6.186799049	2.047988415	0.506063879
O	6.018081665	2.417060375	3.099158525
C	6.718819141	1.222909808	3.420075417
H	6.060313702	0.499196529	3.940782547
H	7.135134220	0.732728720	2.517873764
H	7.540678501	1.503013134	4.083918571

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Nitrene

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C	1.719873428	1.184247732	-1.629385591
N	0.499925166	2.260747671	0.052856673
C	1.644477606	1.771561027	-0.362373263
H	2.632938623	0.717989206	-1.988446116
H	0.839156210	1.166455269	-2.264419317
C	2.823869228	1.853824496	0.543923199
C	2.625504971	1.892207146	1.927732706
C	4.125278473	1.919238091	0.041921891
C	3.705716372	1.977877498	2.793624163
C	5.210574150	2.001438618	0.904336631
C	4.999706745	2.033791304	2.279759645
H	1.609816074	1.850454330	2.317048073
H	4.291805267	1.925915241	-1.033864379
H	3.562724829	2.011040211	3.871662617
H	6.230081558	2.057497263	0.529970229
O	6.074438095	2.144271135	3.120410919
C	6.478910923	0.899637759	3.671457291
H	5.670218468	0.430896997	4.267741680
H	6.786173820	0.187925234	2.878448248
H	7.332727432	1.099166512	4.324415684

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Acetate

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C	0.010304348	0.005157422	-0.097033061
O	0.830166280	-0.755463004	-0.655817509
C	-0.000350045	-0.019723658	1.466597199
H	-1.018351912	-0.419848293	1.817747355
H	0.841970503	-0.660805047	1.886005521
H	0.081373662	1.063637733	1.859645844
O	-0.825003982	0.794433713	-0.593056142

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Acetic Acid

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C	0.054775335	-0.046620309	-0.038383011
O	0.802732110	-0.691217303	-0.730650425
C	0.023511583	-0.036807694	1.457498550
H	-1.004219174	-0.109814271	1.823166490
H	0.628579199	-0.858118951	1.842532873
H	0.431497812	0.912428498	1.820423007
O	-0.868078053	0.791301787	-0.553456068
H	-0.764119983	0.737648606	-1.515870571

9. Frequencies

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7.12 24.82 42.16 54.02 79.44 84.84
102.14 121.33 132.93 156.93 191.07 244.76
259.09 275.77 288.01 293.17 311.02 367.94
402.48 417.66 420.89 435.94 465.81 495.22
503.64 517.04 554.88 566.32 588.48 621.91
637.45 642.46 650.13 682.56 728.91 743.96
759.48 760.59 771.40 807.78 812.81 830.45
836.66 864.26 885.96 898.49 904.30 930.10
945.27 953.39 956.42 970.63 985.04 1002.88
1008.40 1013.89 1037.43 1044.53 1082.50 1088.43
1112.80 1116.50 1122.68 1138.62 1158.61 1167.72
1168.14 1180.79 1192.17 1198.98 1214.75 1224.36
1281.41 1297.84 1306.49 1322.52 1327.95 1332.43
1344.66 1369.26 1374.89 1388.82 1441.05 1458.24
1460.04 1462.16 1465.40 1479.30 1483.78 1513.64
1542.47 1564.38 1636.20 1645.85 1654.51 1665.23
1681.05 1691.69 1718.69 2997.22 3025.39 3072.17
3100.93 3131.84 3144.84 3152.99 3167.97 3175.84
3177.92 3180.02 3183.14 3194.04 3194.97 3198.21
3202.45 3210.68 3469.59

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23.09 28.32 50.46 60.39 72.42 88.54
99.46 114.41 141.84 155.70 194.53 230.43
243.68 269.97 300.68 302.99 316.84 351.94
382.89 406.16 412.47 431.97 437.87 473.10
494.65 532.46 551.33 555.68 566.84 612.74
620.37 636.05 641.67 659.40 705.31 725.69
740.27 752.38 755.59 758.99 773.23 801.78
807.73 823.23 841.67 851.59 861.39 882.60
900.24 942.46 951.09 971.33 974.18 981.48
1000.34 1004.64 1006.66 1019.94 1044.37 1079.47
1083.14 1111.59 1114.75 1121.22 1127.13 1140.33
1156.22 1162.74 1168.04 1178.26 1198.43 1263.01
1284.91 1296.50 1304.95 1318.43 1327.64 1330.77
1339.09 1376.91 1386.40 1408.88 1454.40 1456.72
1461.72 1465.86 1466.14 1483.54 1507.77 1526.99
1546.47 1563.40 1636.86 1643.17 1654.17 1663.22
1679.14 1691.00 1703.46 2996.39 3071.02 3133.20
3143.53 3162.84 3164.90 3166.32 3173.03 3174.64
3175.69 3181.29 3189.14 3196.73 3197.11 3200.66
3207.00 3264.96 3624.30

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A

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10.38 32.82 55.15 63.88 71.63 73.41
84.25 97.86 101.32 113.28 121.94 135.13
137.86 142.00 148.90 157.27 158.62 166.97
179.50 184.95 192.46 210.95 228.62 243.81
255.81 280.75 288.26 296.92 311.52 319.21
322.05 332.14 379.06 414.79 429.54 443.48
453.51 461.25 467.67 511.10 532.61 536.82
548.12 556.54 577.21 588.40 602.63 617.44
621.84 634.01 647.76 685.70 712.16 754.39
766.21 770.86 800.07 809.81 814.12 868.55
903.13 946.43 955.77 966.48 973.43 975.53
990.79 1004.74 1010.68 1011.94 1018.58 1019.76
1022.54 1025.36 1028.75 1032.02 1037.53 1042.28
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1109.18 1130.87 1166.96 1170.19 1182.49 1186.56
1194.66 1295.92 1311.94 1331.06 1336.21 1368.27
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1442.34 1445.21 1447.94 1450.13 1453.34 1457.79
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3119.85 3121.19 3123.37 3139.10 3143.14 3144.24
3147.18 3154.48 3164.20 3177.07 3179.08 3189.54
3192.07 3196.44 3200.65 3204.11 3211.98 3217.59

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A-TS

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-1584.50 23.24 42.21 56.49 64.65 71.07
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248.11 252.47 268.01 287.56 301.24 313.44
317.17 320.05 356.01 409.14 420.62 435.59
437.93 444.98 457.46 497.46 530.81 536.19
543.26 545.63 559.58 589.62 592.22 599.10
621.76 631.74 643.97 661.95 685.91 743.39
756.70 770.10 770.29 805.86 806.52 814.43
892.85 898.54 953.96 959.54 965.35 968.03
970.23 1006.91 1014.96 1015.46 1022.05 1022.75
1024.07 1027.87 1028.59 1032.17 1037.95 1043.01
1056.18 1066.74 1083.97 1085.41 1090.28 1105.59
1124.54 1135.74 1165.55 1169.94 1181.96 1184.42

1218.71 1279.12 1299.48 1317.21 1332.00 1339.63
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B

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870.47 893.41 926.85 949.21 950.43 955.46
969.29 996.57 1013.74 1014.90 1018.51 1019.24
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1424.85 1430.34 1434.84 1435.89 1439.69 1440.97
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C

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318.18 343.49 365.75 384.43 418.65 422.78
429.14 433.94 442.32 477.50 480.67 491.86
501.67 522.14 530.53 539.74 546.34 550.66
564.33 597.02 600.09 615.53 630.90 634.13
645.71 667.60 669.95 723.22 723.53 744.57
766.71 773.34 804.16 804.42 811.73 825.61
828.29 850.00 868.92 892.39 946.45 950.26
952.32 953.51 960.98 963.71 972.41 992.53
998.87 1010.86 1015.46 1017.17 1021.56 1025.58
1028.27 1032.27 1033.46 1033.84 1044.70 1052.58
1074.15 1083.97 1084.93 1086.23 1088.57 1103.43
1114.40 1120.11 1127.81 1141.68 1154.81 1162.68
1163.82 1170.84 1178.35 1181.85 1189.13 1195.30
1253.37 1293.56 1303.01 1326.19 1332.97 1342.06
1357.59 1357.77 1371.27 1372.83 1391.48 1392.88
1396.50 1397.84 1426.99 1430.02 1439.77 1442.53
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C-TS

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559.83 562.44 594.60 601.35 607.99 633.43
640.11 643.68 663.95 673.06 720.79 723.54
743.55 767.17 772.42 779.18 802.08 809.53
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901.19 949.77 953.48 955.08 957.78 965.49
966.24 994.83 1009.25 1010.97 1014.36 1016.60
1022.33 1024.18 1031.49 1038.17 1040.91 1050.58

1062.98 1075.17 1083.87 1084.96 1088.58 1095.94
1105.97 1124.03 1128.35 1141.72 1142.92 1163.43
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1254.24 1293.12 1302.76 1338.62 1343.86 1344.30
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3173.28 3173.91 3174.96 3181.40 3182.53 3192.37
3201.44 3207.87 3209.81 3218.05 3219.50 3233.32

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^{1}D

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12.98 33.90 39.26 42.95 54.58 63.15
77.06 96.74 115.89 120.07 128.78 131.01
143.56 143.96 147.04 155.56 158.13 170.51
181.05 193.13 210.25 213.47 221.45 228.17
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292.82 305.49 313.88 320.24 347.52 365.55
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439.41 458.09 474.33 491.00 496.37 518.80
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602.24 603.43 622.83 632.98 638.78 641.57
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1479.86 1484.49 1495.63 1504.76 1514.68 1524.24
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2163.51 2996.12 3013.52 3028.82 3029.75 3032.35
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3166.51 3168.25 3169.72 3173.77 3183.76 3185.88
3188.79 3190.25 3199.95 3201.25 3204.21 3215.69

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^{3}D

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^{1}D-TS

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E

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12.55 18.48 23.41 41.58 59.10 68.90
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F

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F-TS

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1026.35 1029.11 1030.38 1032.11 1035.11 1055.14
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1317.28 1329.26 1335.02 1361.18 1364.10 1373.89
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G

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11.17 31.42 32.50 36.90 45.45 47.28
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430.77 436.31 446.55 474.14 500.32 507.78
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558.57 567.93 581.93 588.93 605.18 610.34
615.79 636.84 642.31 643.21 664.88 680.08
717.10 734.48 743.75 764.28 773.00 794.81
802.49 812.27 813.89 817.77 821.72 842.29
852.33 863.59 894.75 913.11 950.78 952.66
955.37 958.68 958.97 964.32 969.35 997.84
1002.84 1011.63 1013.20 1016.78 1019.17 1023.51
1026.20 1028.63 1031.22 1035.45 1040.83 1041.68
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1109.23 1118.60 1134.69 1138.62 1163.96 1167.17
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1447.90 1450.80 1452.79 1455.08 1457.78 1457.90
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1476.37 1479.37 1483.23 1490.78 1495.38 1507.87
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1649.26 1667.55 1669.30 1674.84 1693.60 1776.73
3014.10 3014.27 3030.22 3032.71 3033.54 3035.96
3052.10 3075.64 3097.83 3104.30 3108.41 3108.59
3109.91 3113.31 3132.61 3134.77 3134.82 3140.38
3140.52 3146.15 3157.27 3158.97 3159.99 3164.79
3165.52 3169.10 3187.51 3188.78 3189.99 3194.09
3200.76 3205.25 3206.55 3216.75 3219.10 3522.45

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^{1}D-TS'

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363.78 379.67 393.16 407.57 409.92 421.73
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562.00 586.54 596.82 600.82 620.36 625.80
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745.44 759.37 764.08 772.27 794.89 804.29
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^{3}D-TS

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161.68 175.66 182.25 187.05 188.16 205.85
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847.62 863.41 871.42 893.60 901.07 905.64
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1195.90 1241.21 1271.52 1279.56 1296.38 1309.35
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1377.88 1379.91 1387.04 1393.32 1395.53 1397.73
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1631.56 1640.63 1664.94 1667.67 1679.22 1840.83
3013.79 3027.87 3029.88 3032.29 3033.35 3037.42
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169.17 178.16 184.36 192.05 193.47 214.51
221.60 240.09 245.54 260.56 269.83 281.52
289.70 290.96 300.53 306.76 309.55 318.84
327.74 361.33 382.11 397.92 420.40 421.76
428.57 433.39 437.60 448.56 468.09 481.07
517.58 531.36 534.96 544.20 544.98 558.32
566.99 569.56 588.31 593.70 605.06 611.76
626.43 634.35 642.17 649.13 652.92 692.29
702.36 736.57 745.61 751.97 760.87 772.32
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1022.89 1023.48 1024.67 1026.63 1030.23 1031.53
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1376.61 1377.25 1385.62 1393.41 1393.59 1401.93
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1439.78 1442.52 1444.13 1449.03 1449.10 1453.78
1456.15 1460.49 1460.56 1464.96 1465.98 1466.66
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1652.10 1665.64 1674.28 1687.16 1729.78 1738.26
3009.59 3033.66 3034.60 3035.14 3037.57 3038.71
3047.64 3090.21 3111.27 3115.86 3118.55 3118.85
3119.86 3130.80 3137.49 3138.41 3141.94 3147.48
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1106.88 1117.41 1159.84 1165.27 1195.34 1294.23
1309.70 1331.34 1341.66 1378.16 1455.32 1486.30
1503.85 1539.85 1633.03 1656.15 1662.02 1678.63
3131.06 3162.16 3168.17 3170.08 3178.34 3190.83
3194.46 3202.03 3206.56

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Azirine

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71.83 81.99 100.81 131.88 192.54 266.02
305.95 364.72 409.23 421.97 490.81 500.80
571.35 637.36 652.80 745.78 824.80 839.03
868.30 905.10 961.28 973.08 992.38 1012.02
1022.74 1073.49 1103.61 1111.03 1154.60 1170.04
1176.24 1196.44 1288.75 1300.09 1350.83 1380.66
1454.32 1461.57 1463.79 1488.07 1495.56 1553.50
1643.63 1679.20 1858.56 2930.44 2997.90 3073.70
3135.54 3160.98 3176.30 3182.96 3193.41 3200.13

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Nitrene

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60.98 81.88 91.88 184.19 214.71 272.20
309.54 353.86 407.83 422.18 460.70 505.92
529.06 557.67 609.35 645.44 691.11 747.24
767.95 835.62 837.81 868.69 954.25 967.48
994.55 1022.63 1076.14 1108.34 1131.76 1167.17
1177.56 1197.47 1269.36 1295.58 1303.89 1357.83
1384.25 1453.18 1458.78 1463.17 1468.87 1489.13
1555.39 1646.35 1680.44 2924.83 2990.53 3131.98
3150.86 3174.57 3178.14 3192.38 3195.64 3264.45

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Acetate

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473.97 563.69 623.26 696.02 876.98 1077.88
1093.18 1364.86 1415.30 1487.36 1494.78 1816.96
2569.05 2639.02 2731.01

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Acetic Acid

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68.56 421.26 540.96 589.00 692.91 889.64
996.60 1057.51 1223.34 1343.25 1418.75 1447.86
1454.25 1905.61 3061.77 3147.40 3188.09 3819.55

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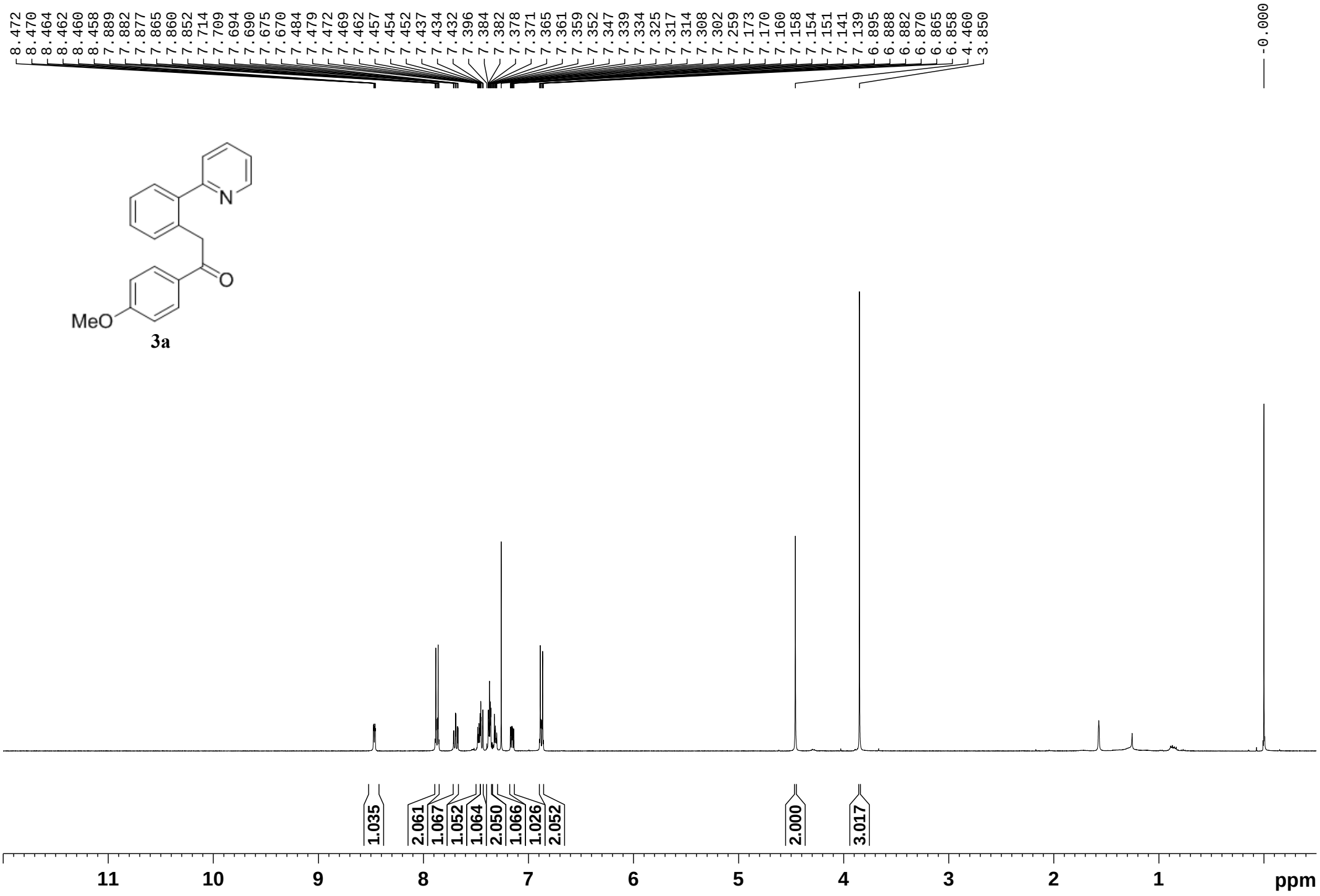
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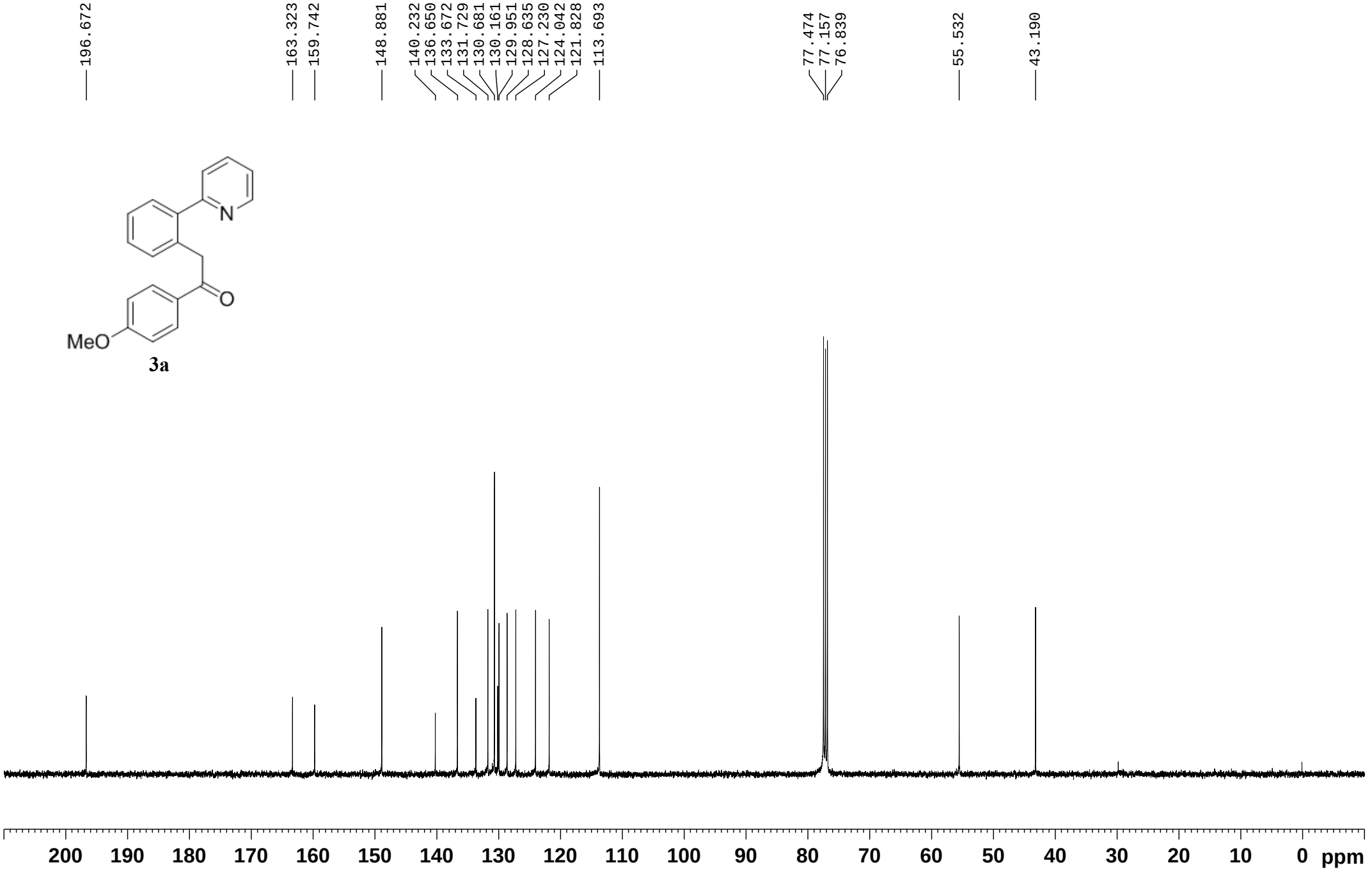
3a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55.532
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O
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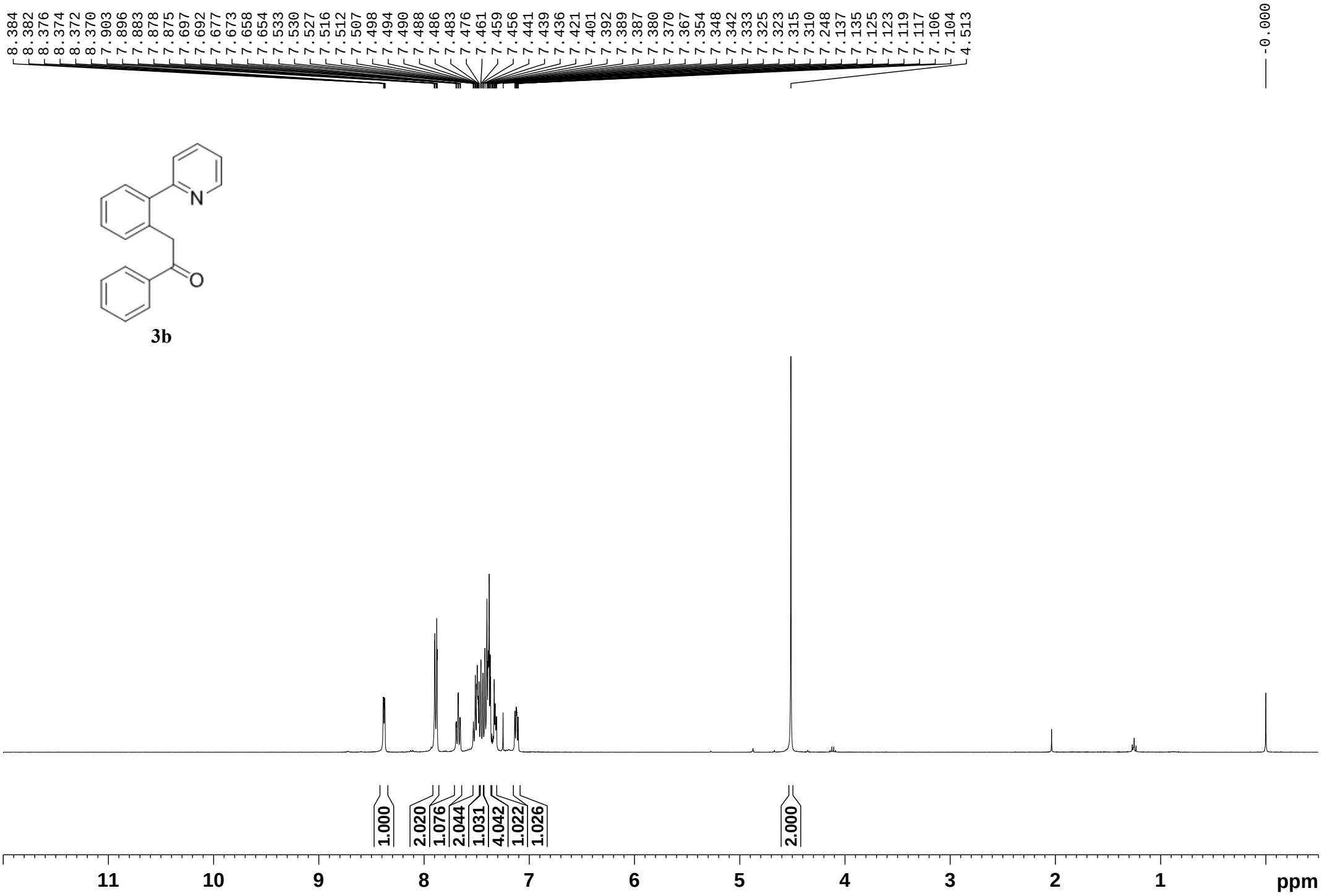
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O
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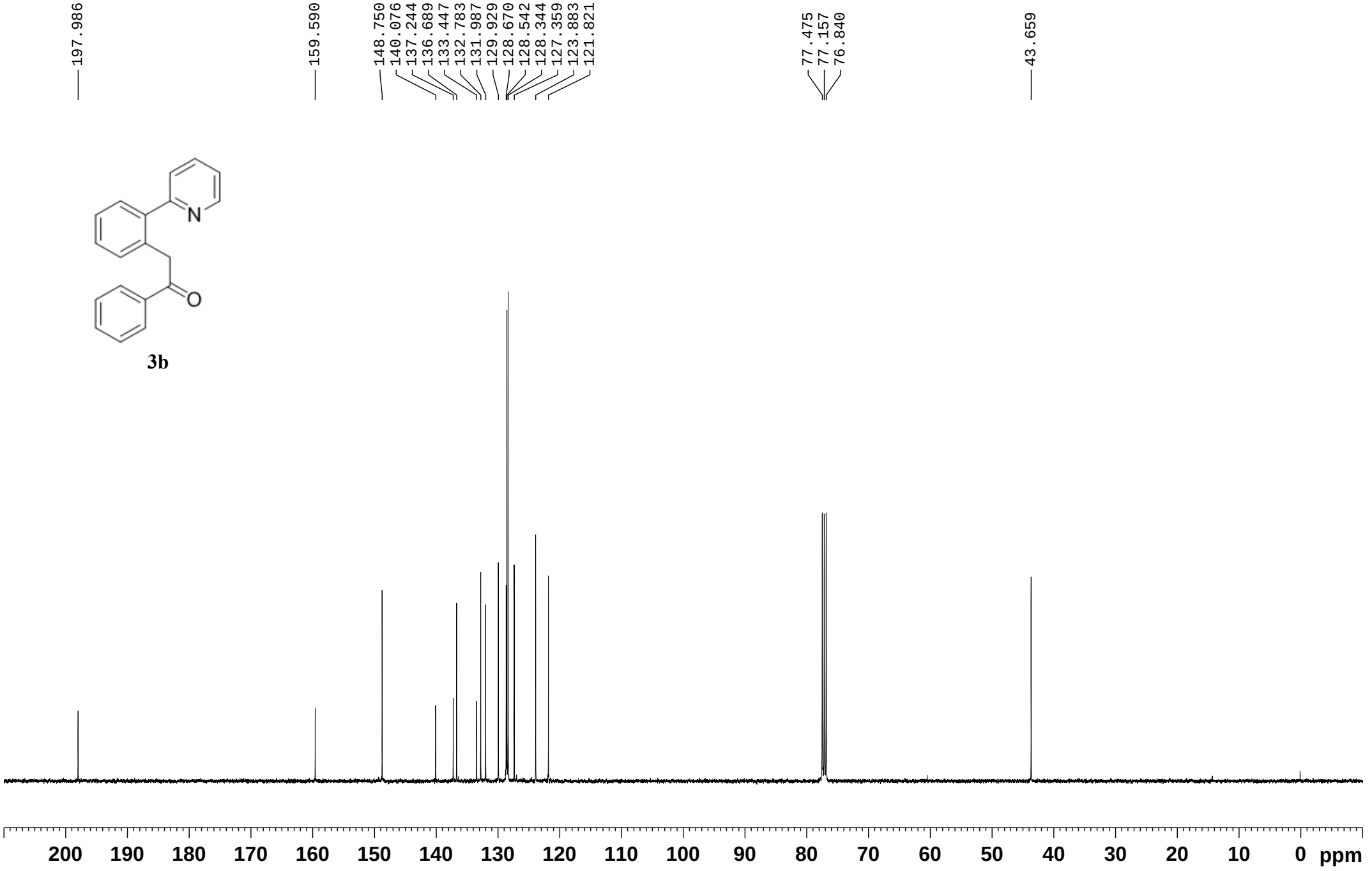
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N
O
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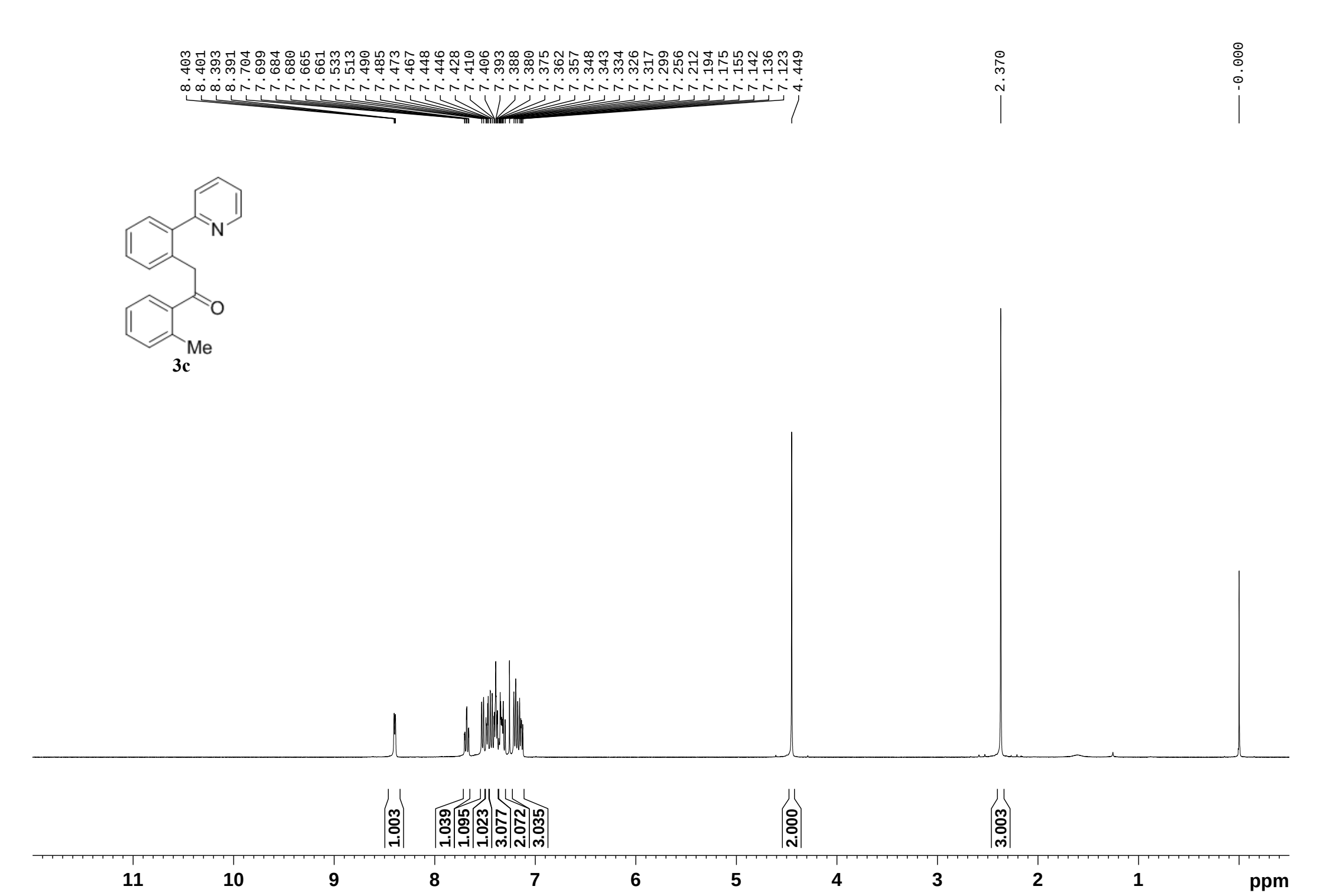
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7.406
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7.357
7.348
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7.334
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7.317
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7.155
7.142
7.136
7.123
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O
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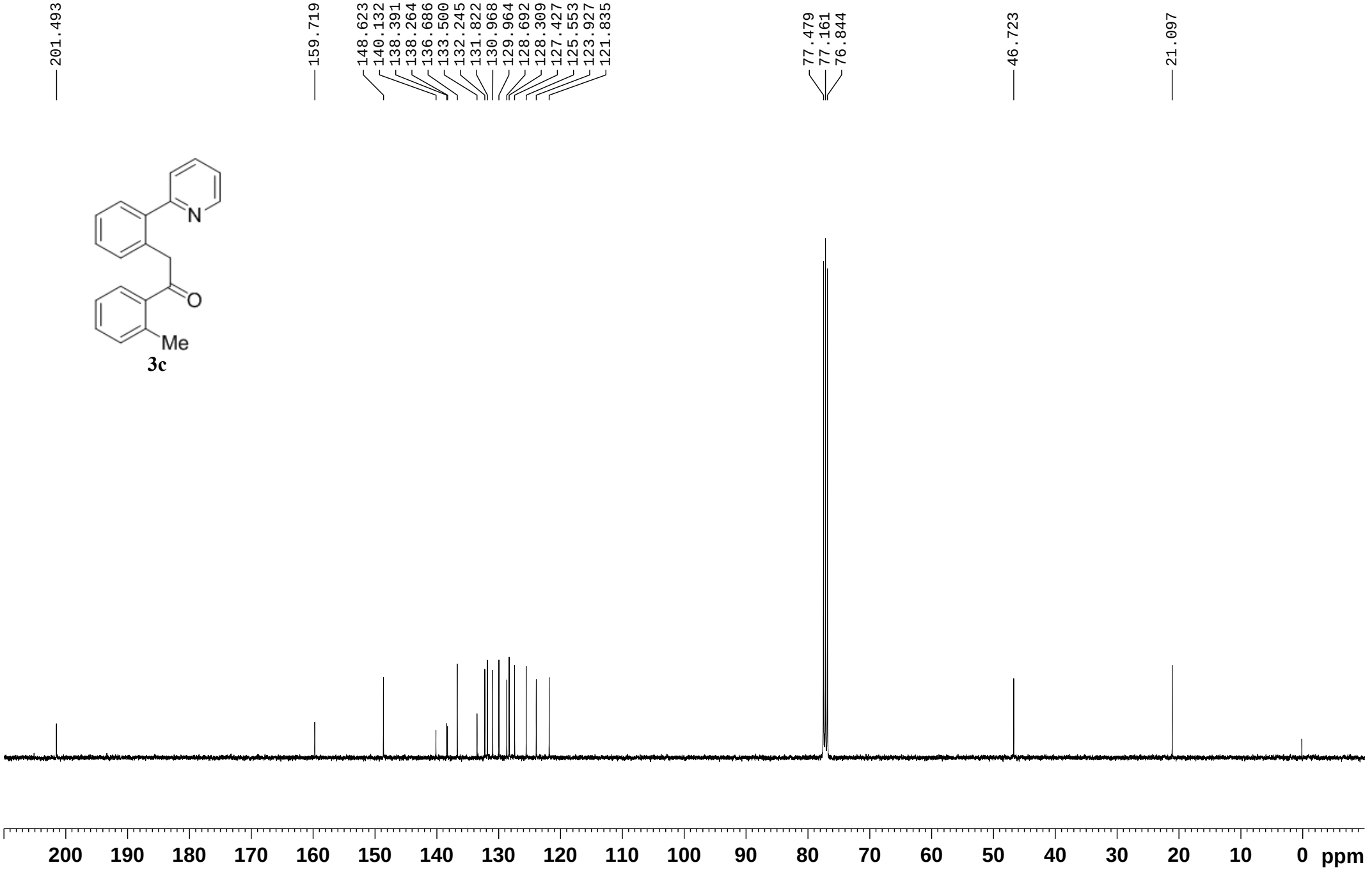
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O
Me
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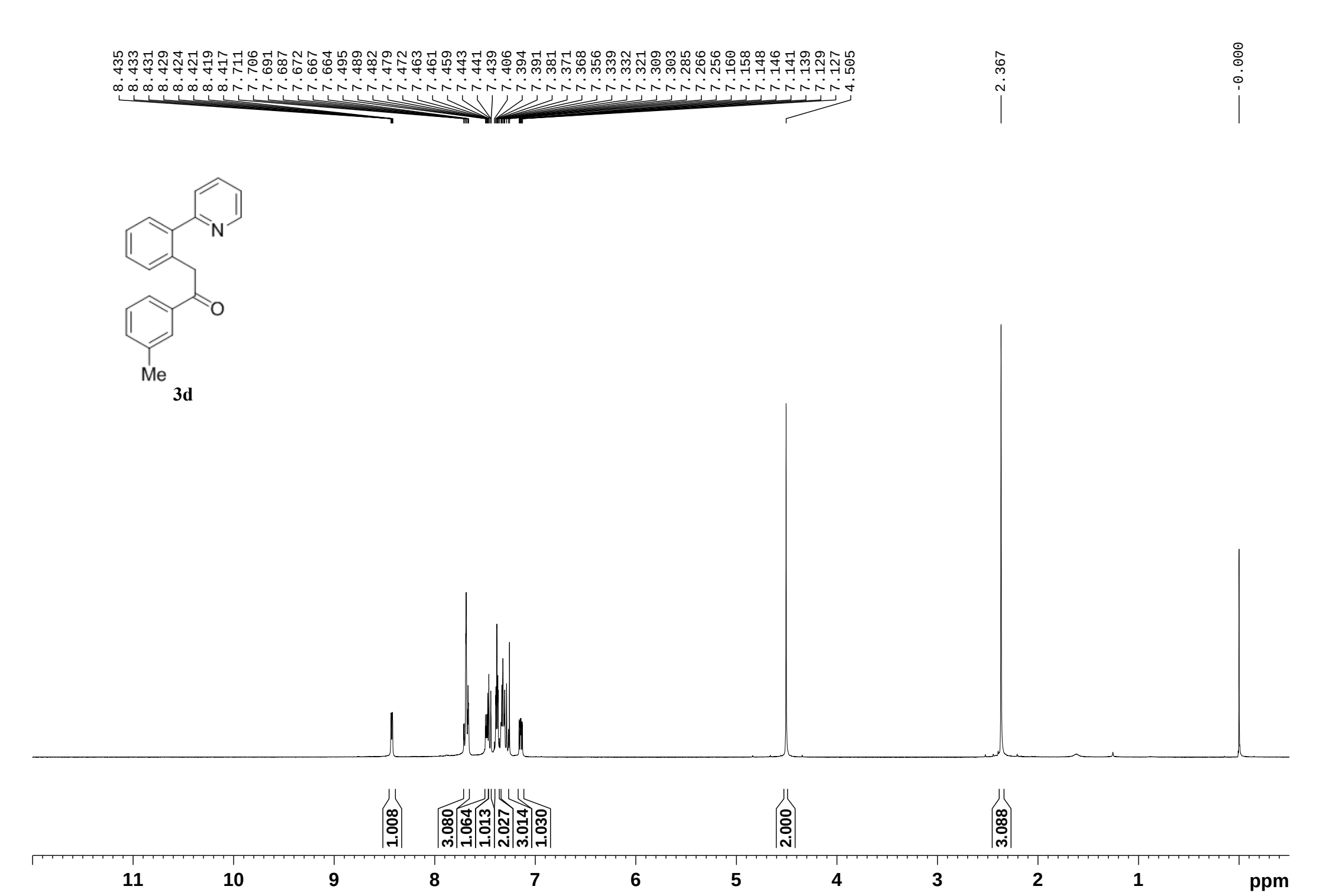
3c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7.667
7.664
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7.482
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7.459
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7.441
7.439
7.406
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7.391
7.381
7.371
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7.332
7.321
7.309
7.303
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7.266
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7.158
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7.139
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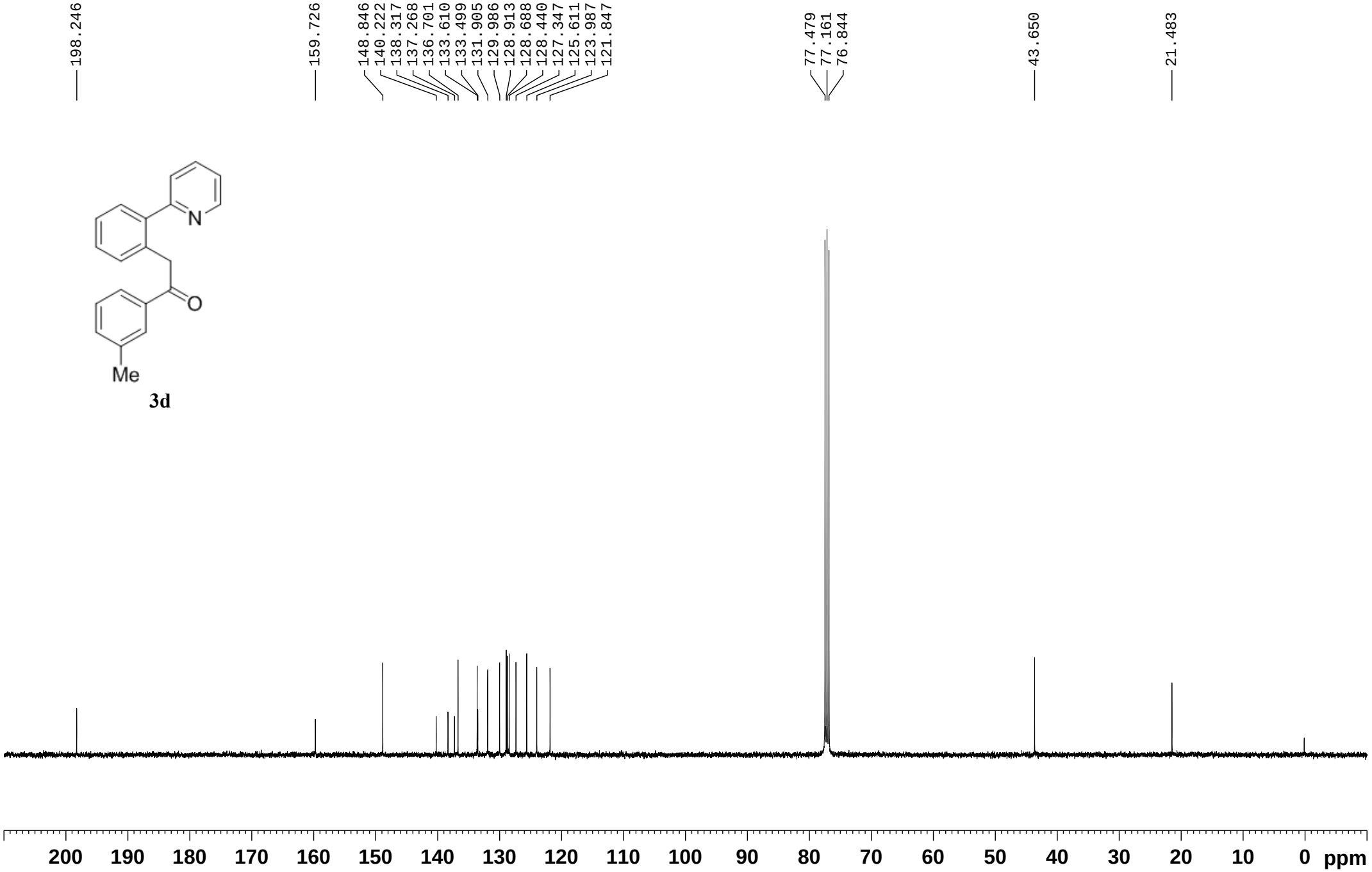
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127.347
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77.161
76.844
43.650
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O
Me
200
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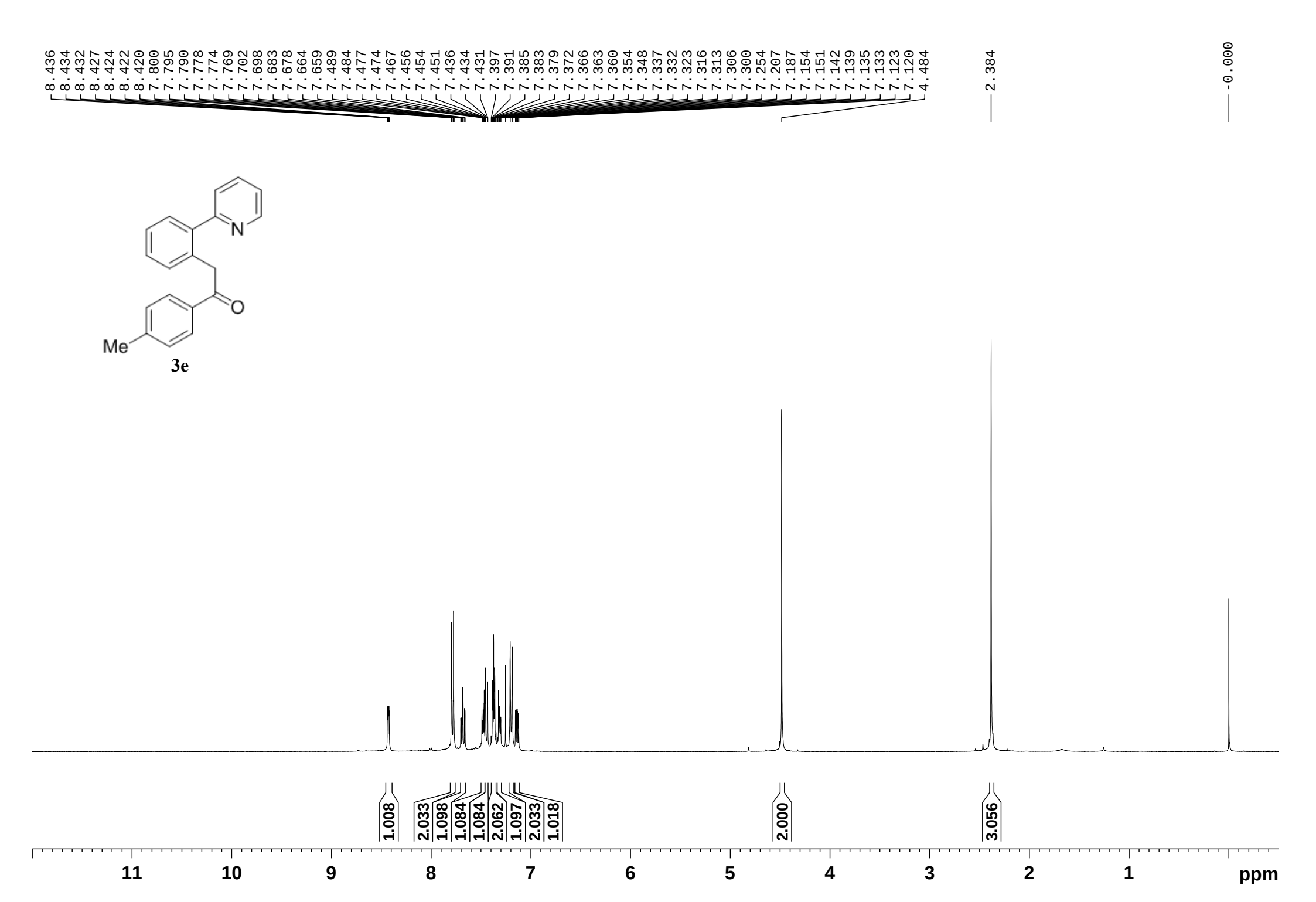
3d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7.379
7.372
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7.348
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7.332
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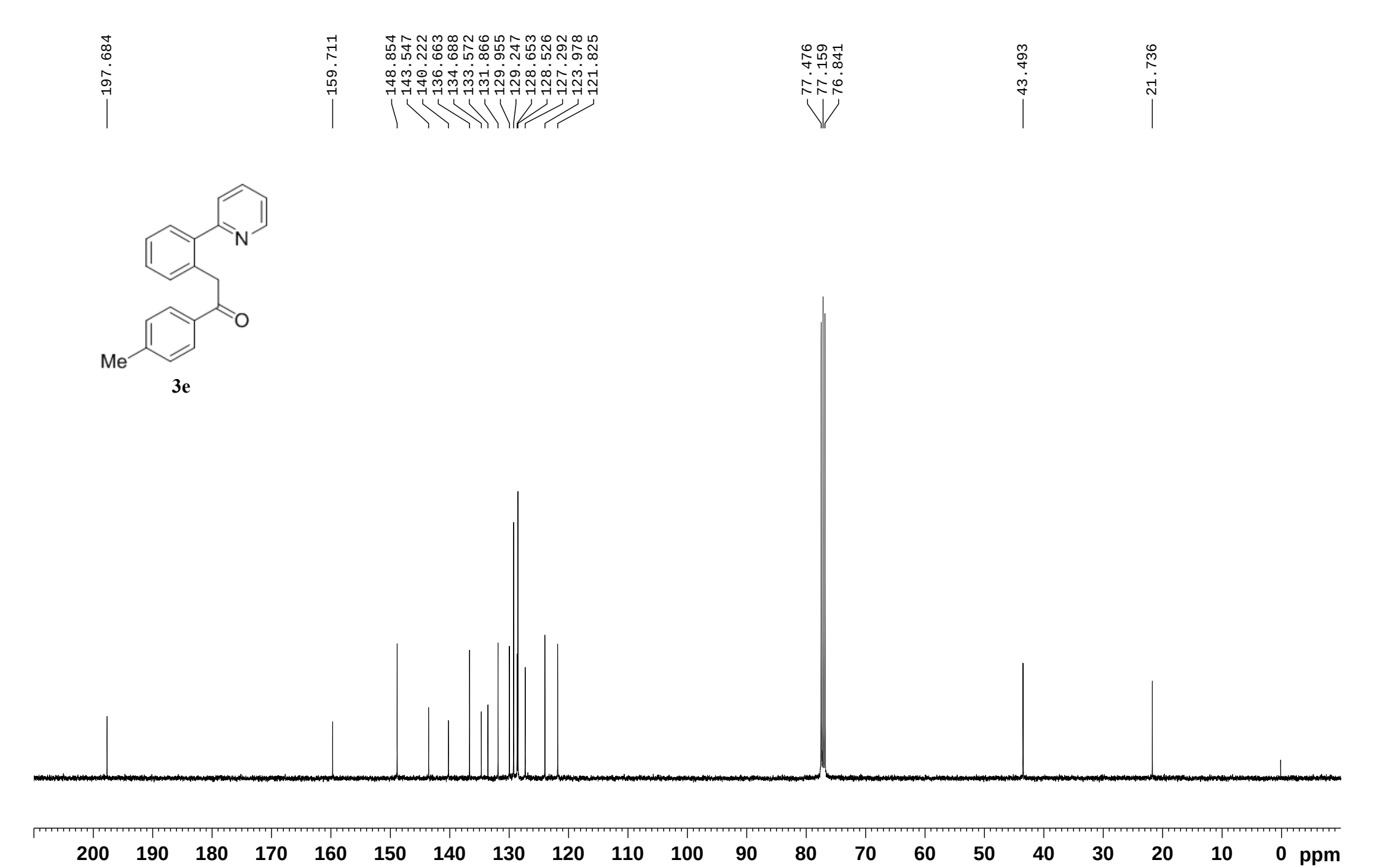
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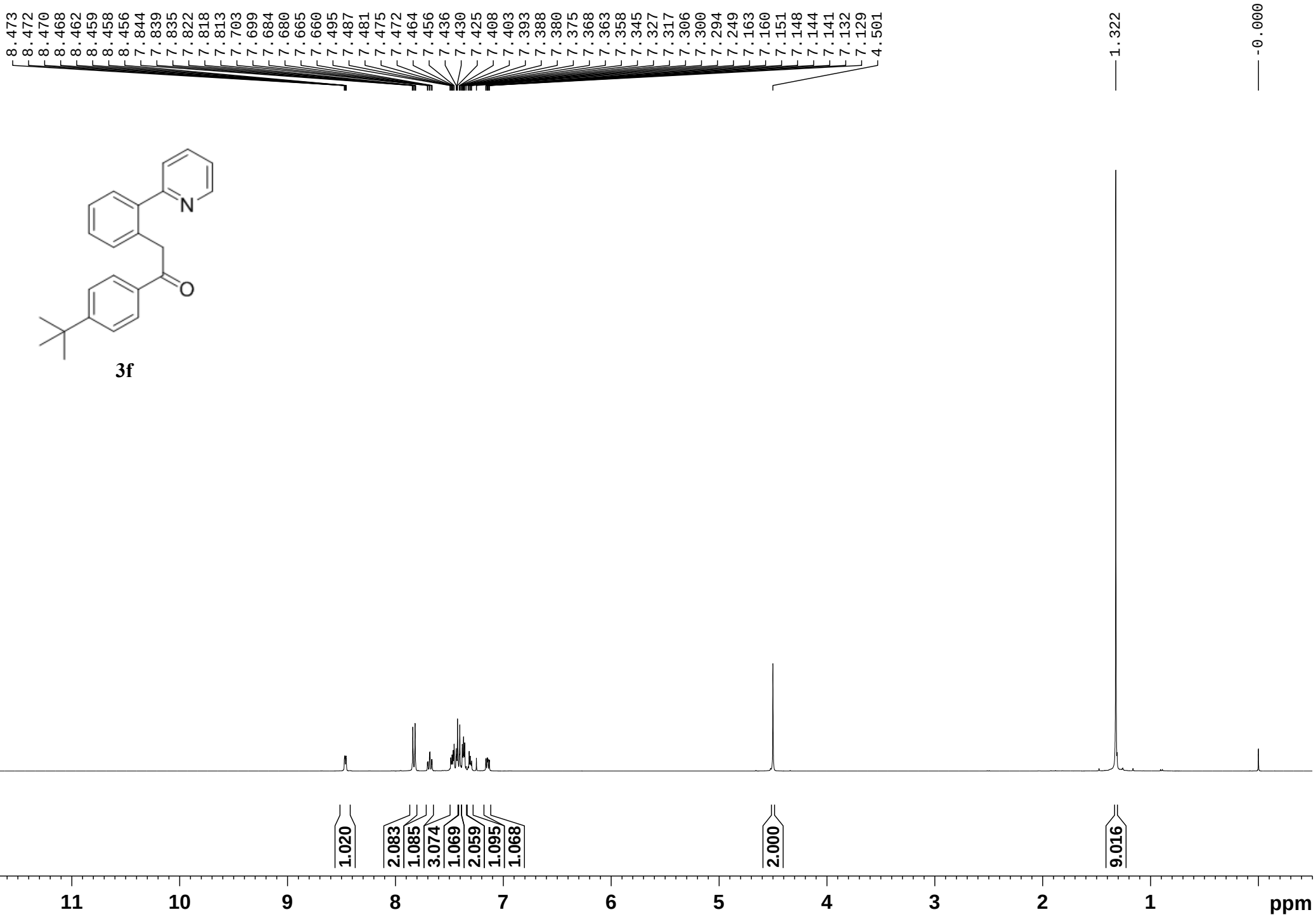
ppm

3e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7.699
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7.481
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7.472
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7.327
7.317
7.306
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7.148
7.144
7.141
7.132
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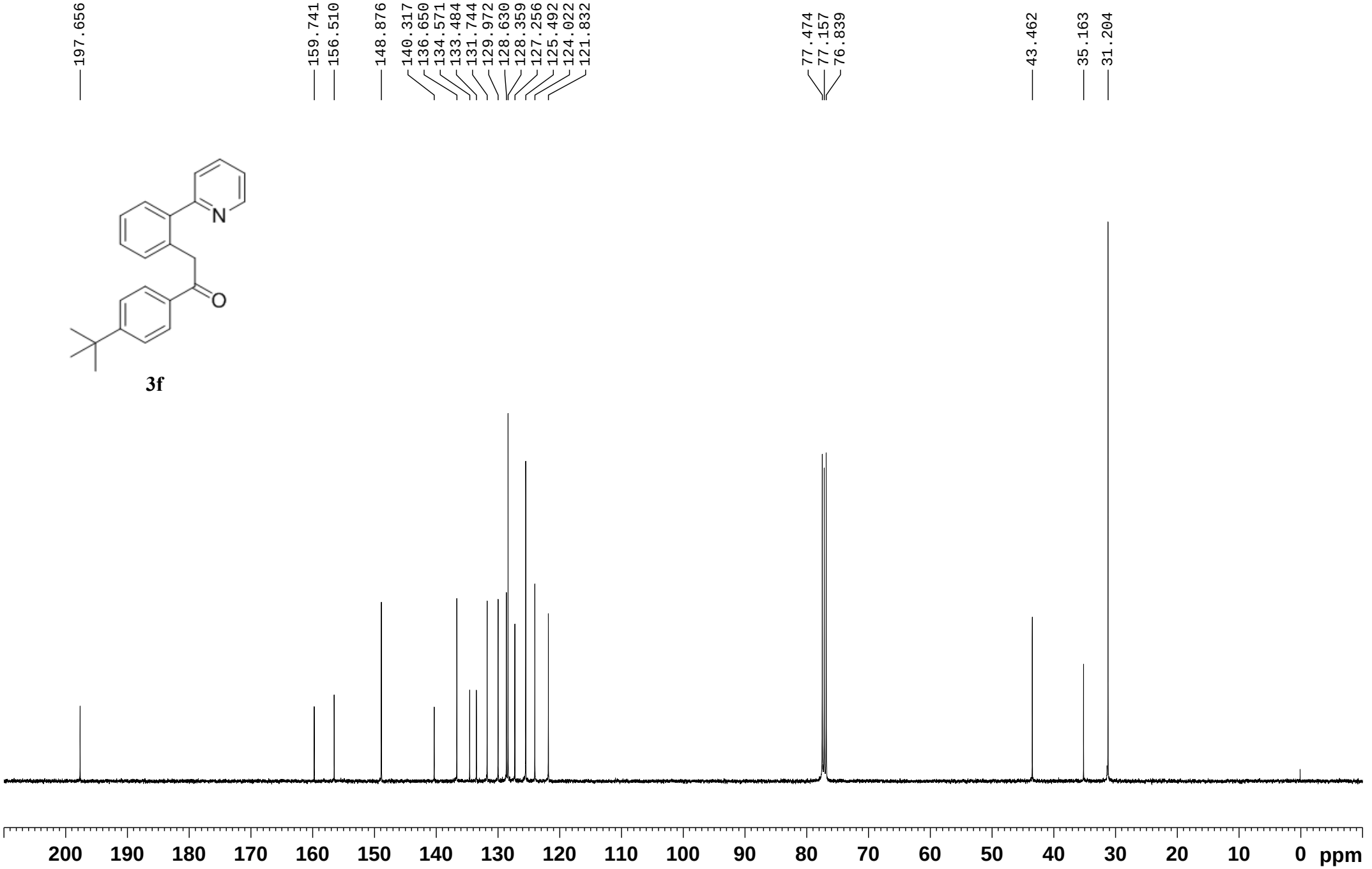
ppm

3f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31.204
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O
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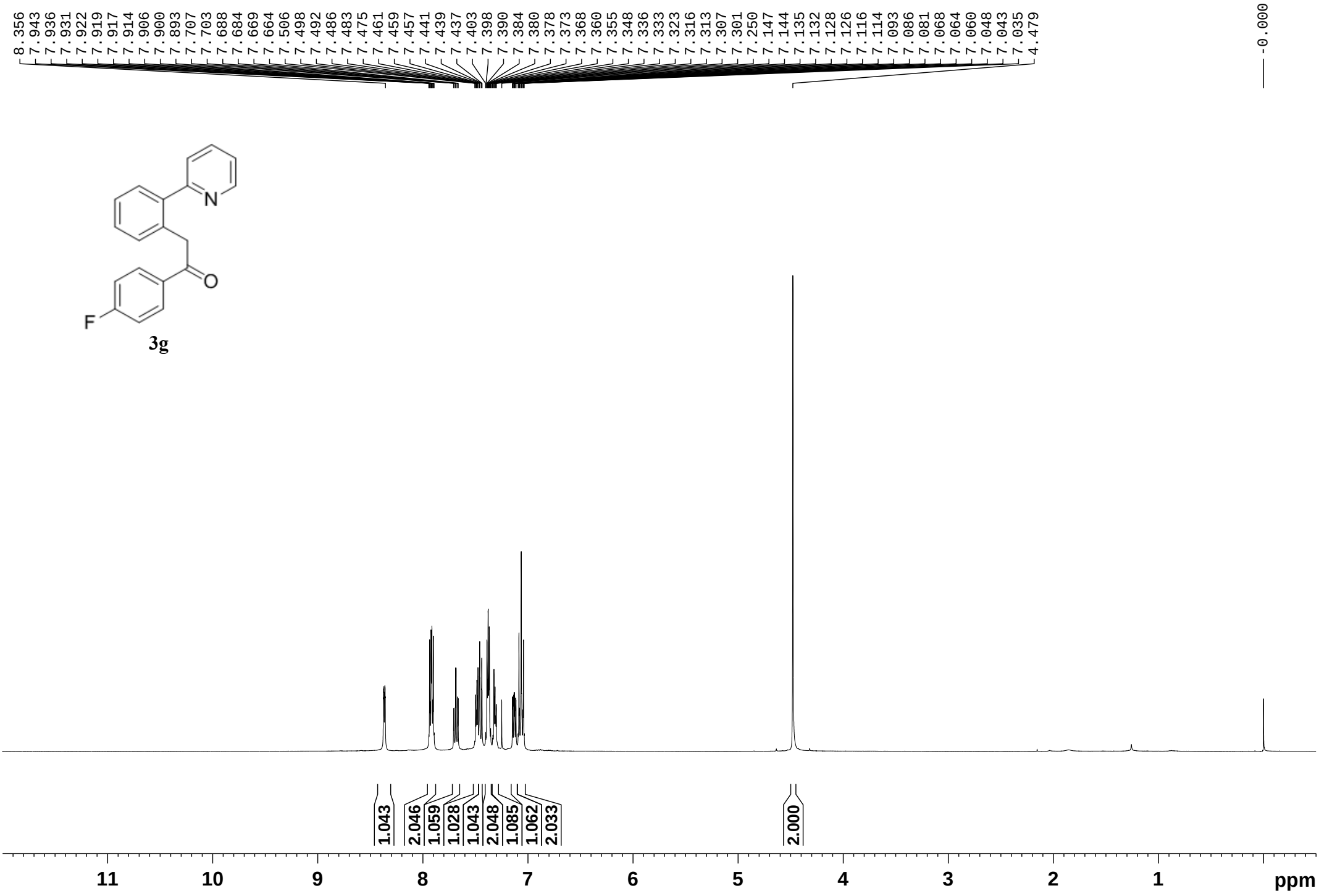
ppm

3f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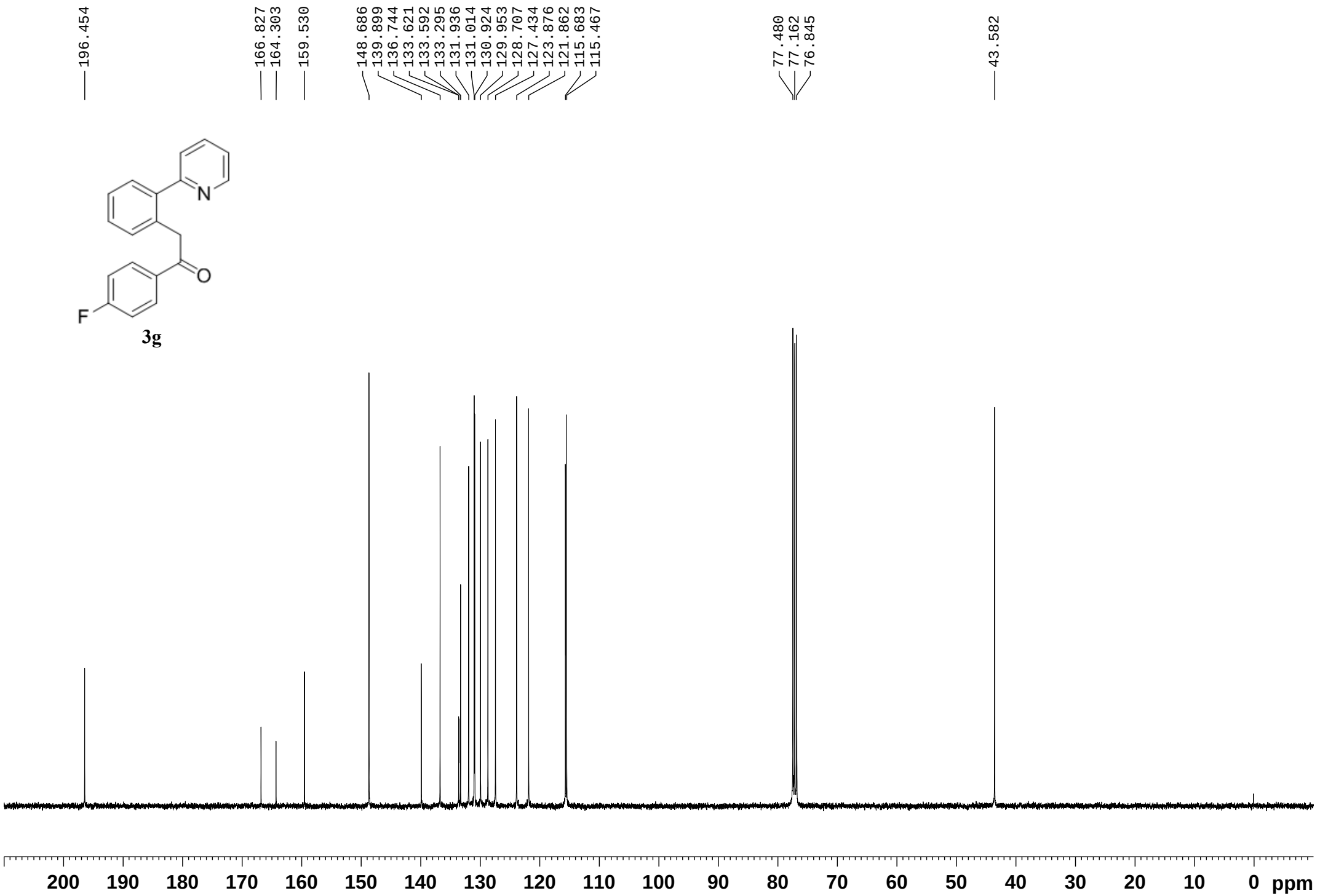
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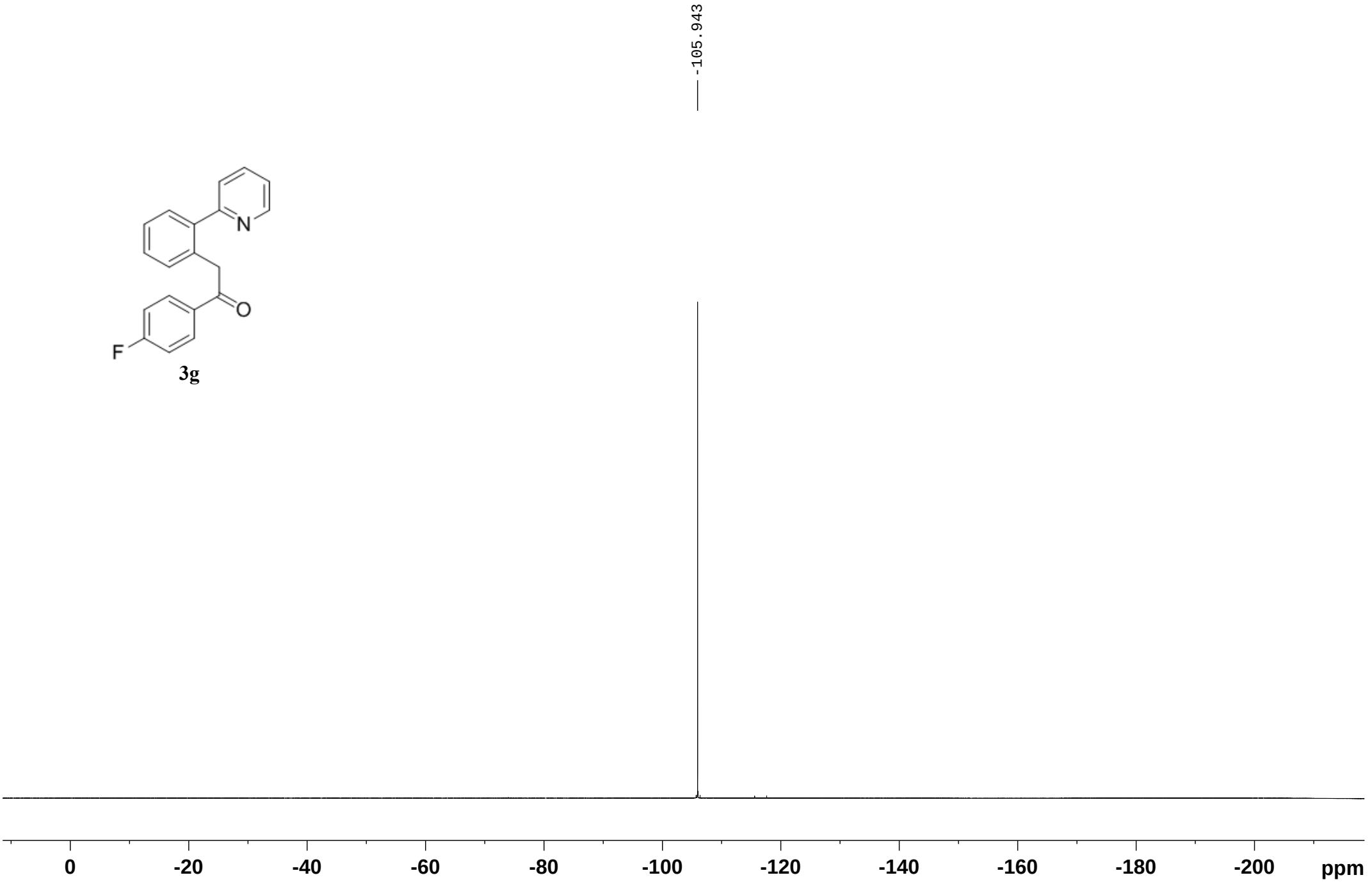
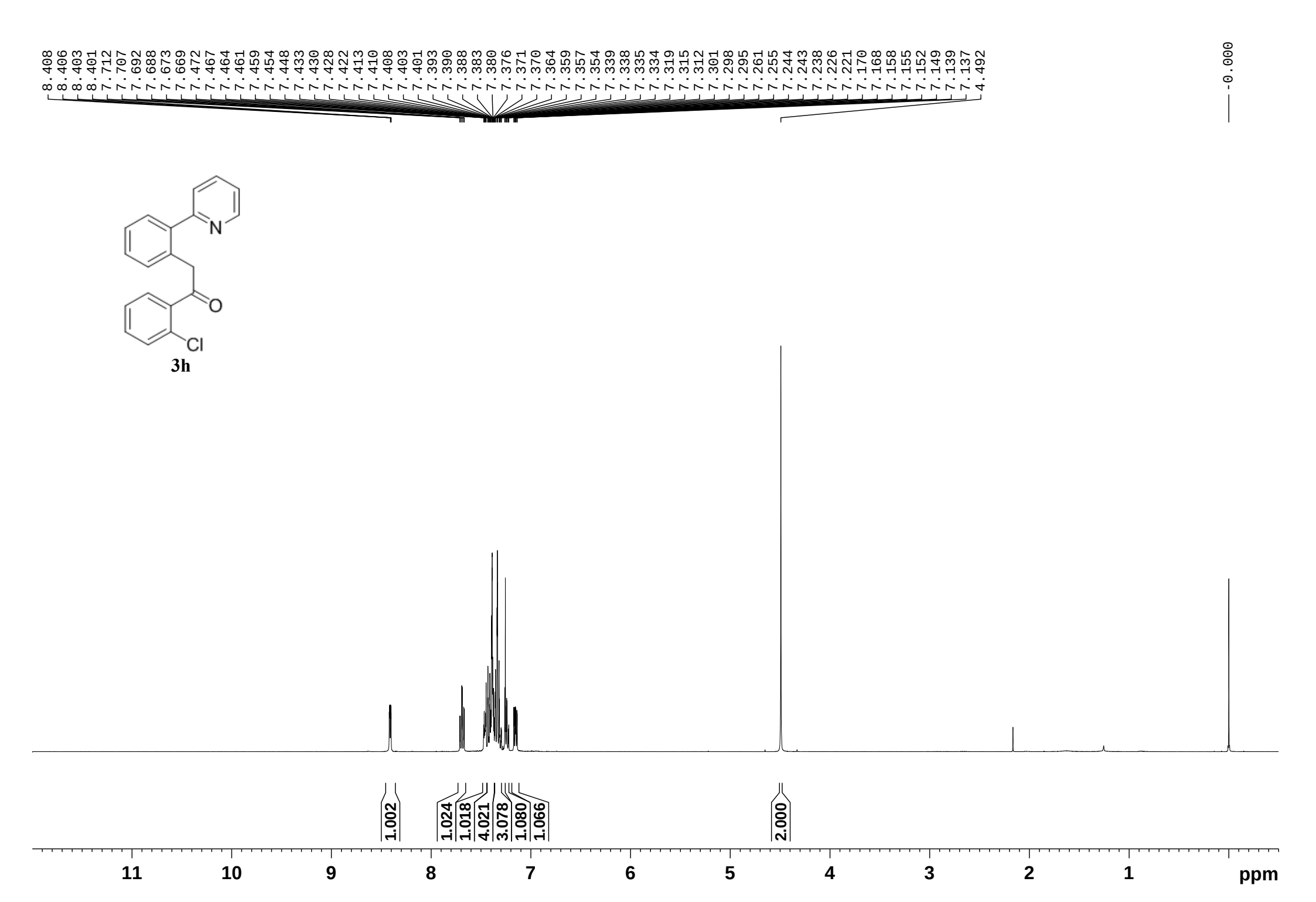
3g

3g

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7.401
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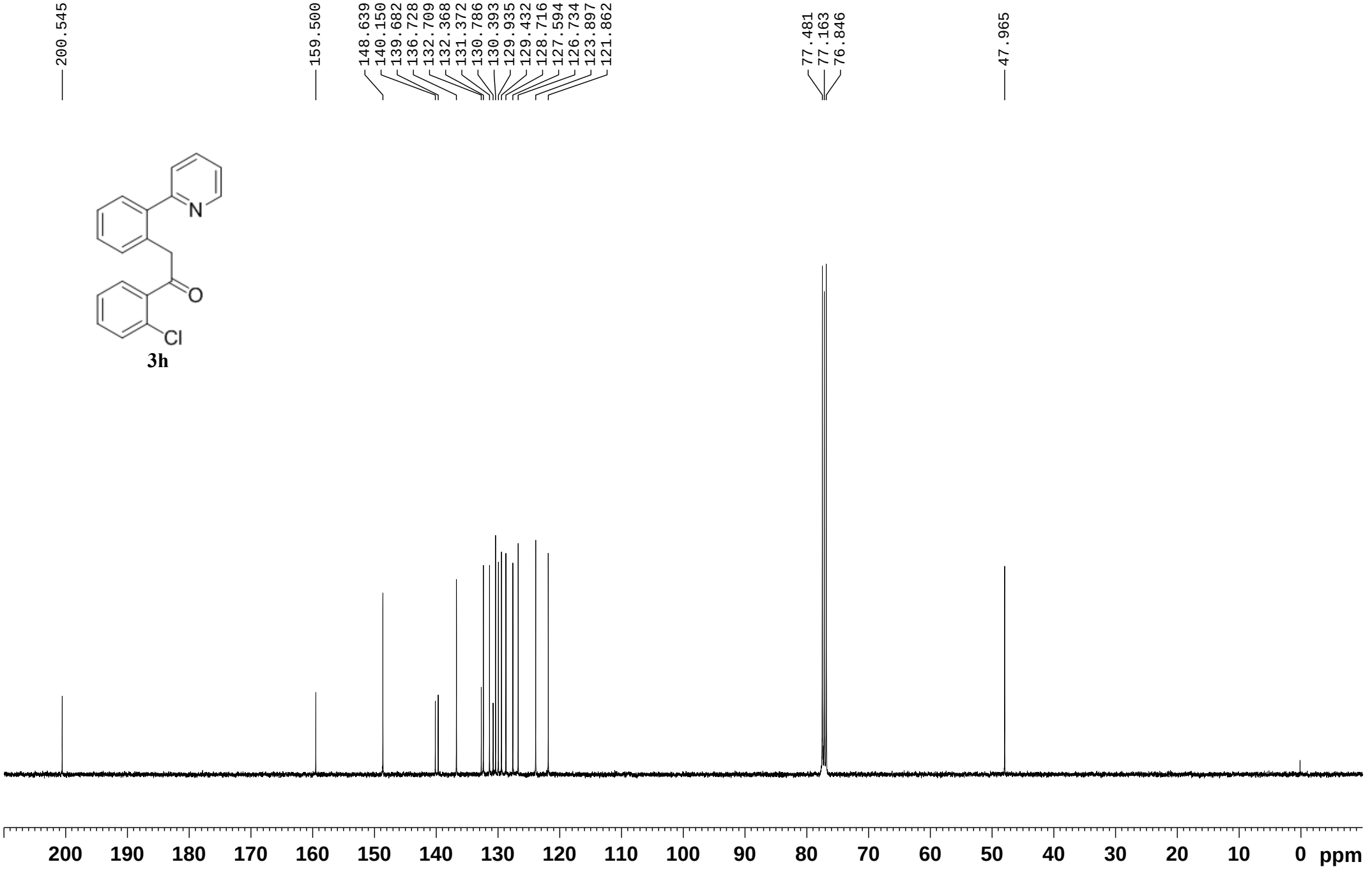
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Cl
3h
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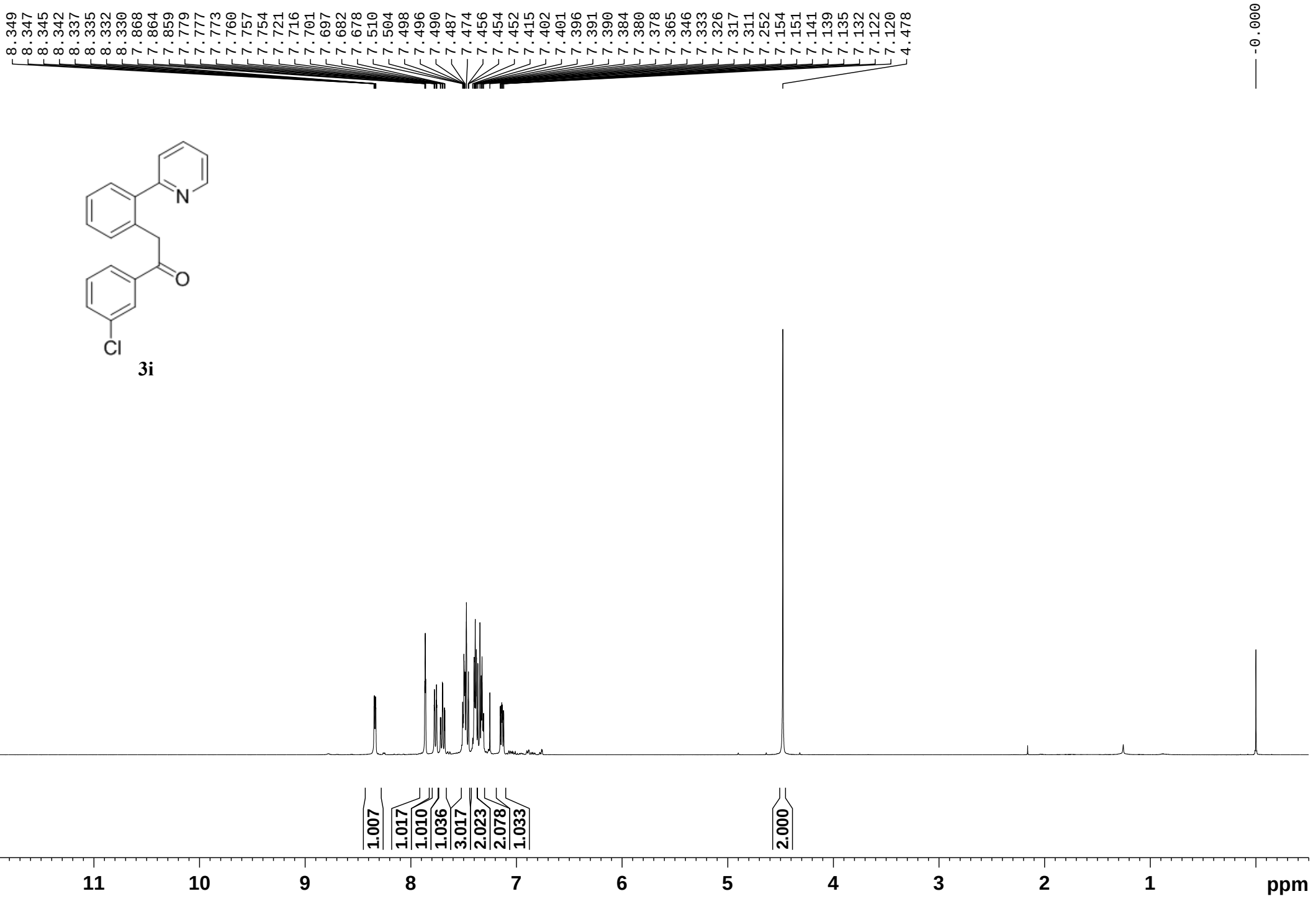
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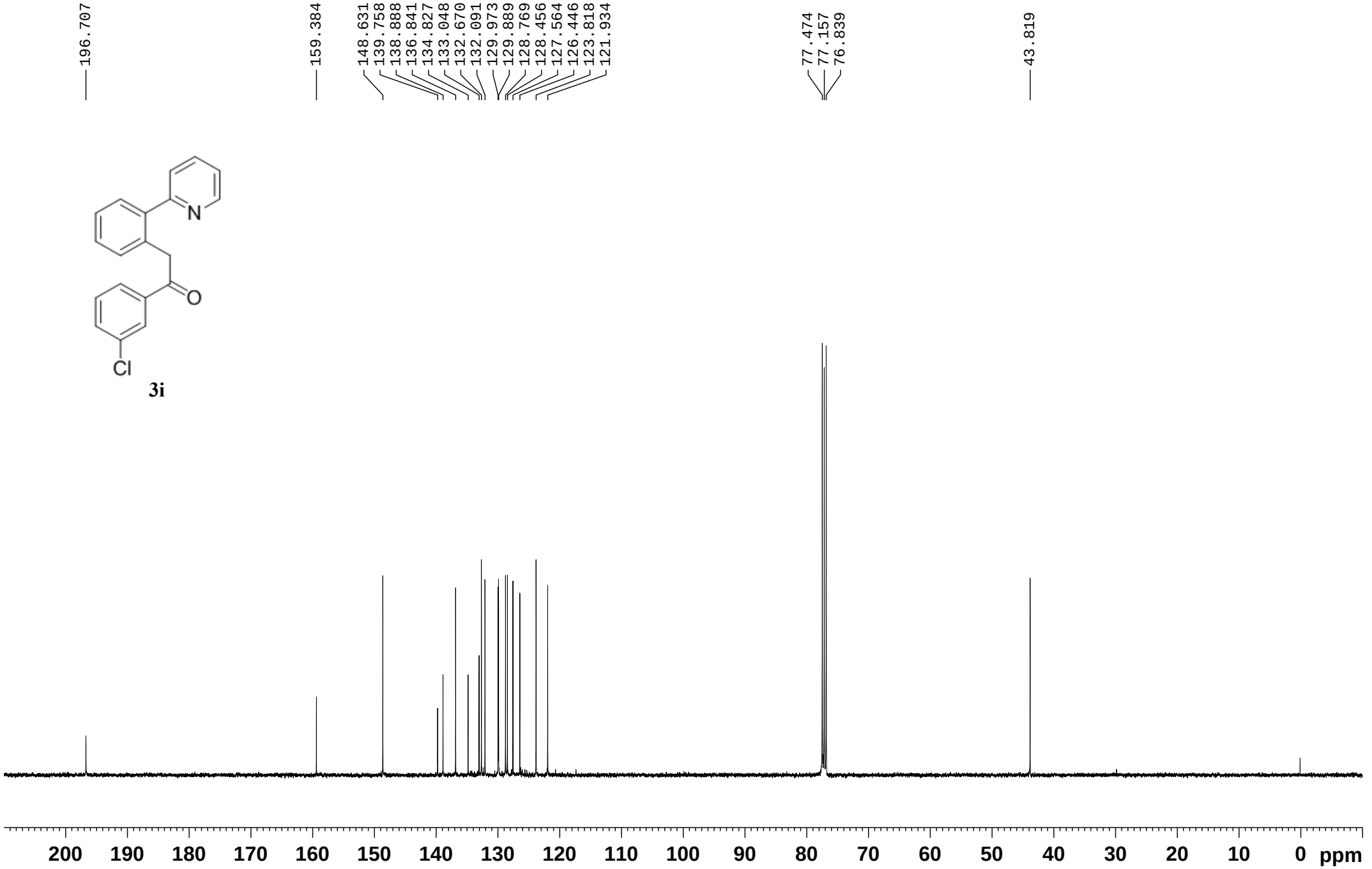
ppm

3i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77.157
76.839
43.819
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O
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10
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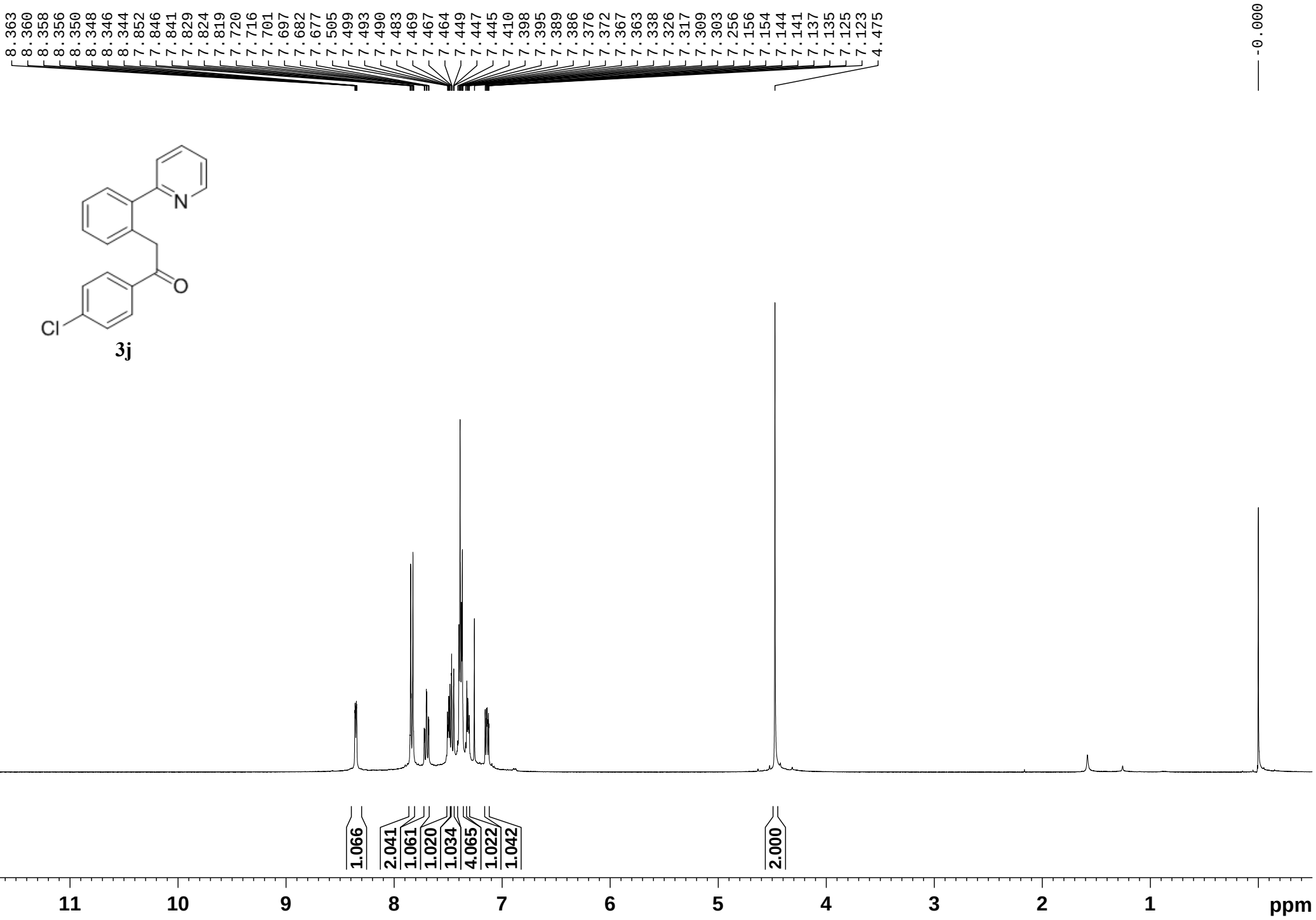
ppm

3i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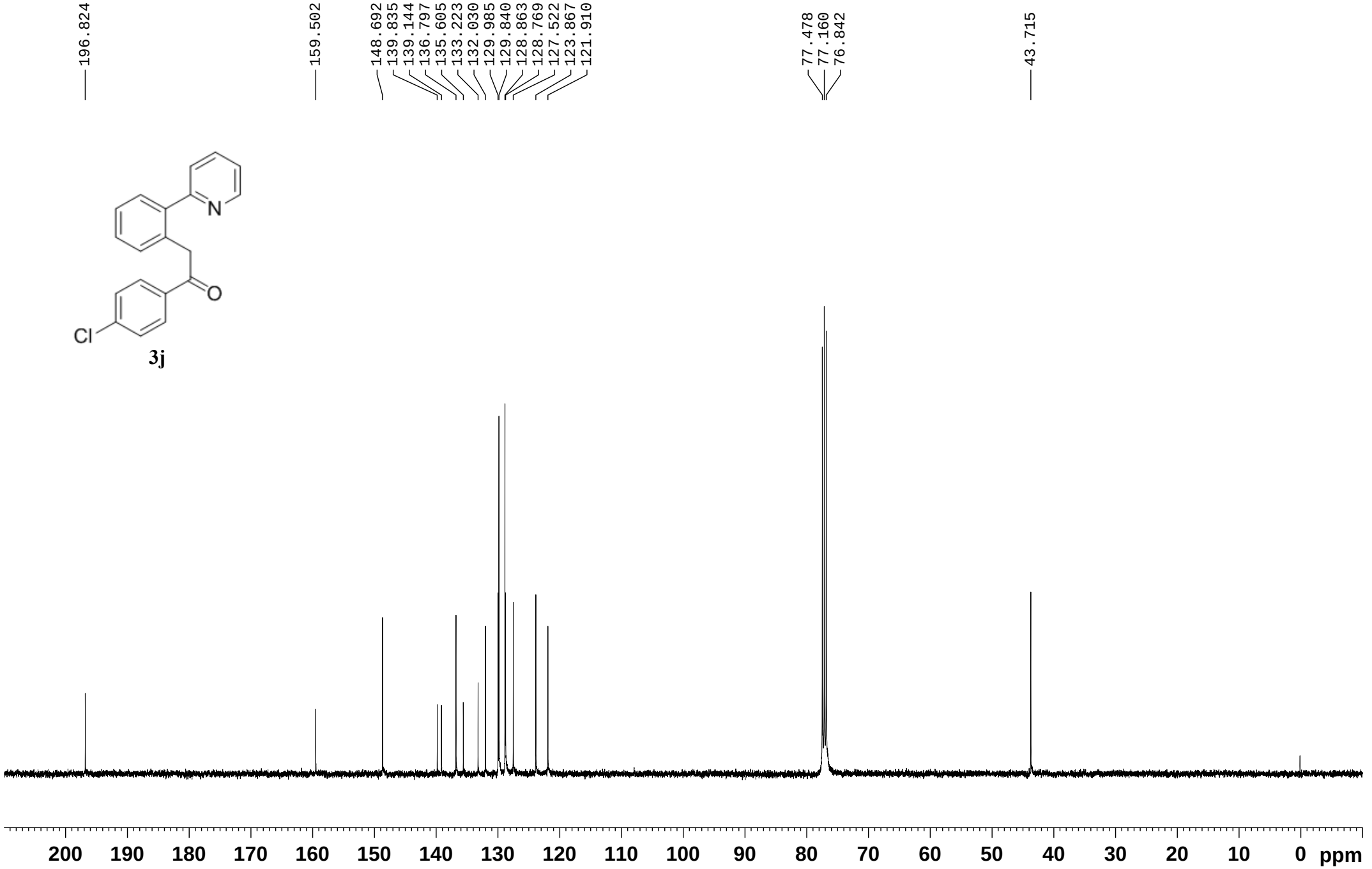
3j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10
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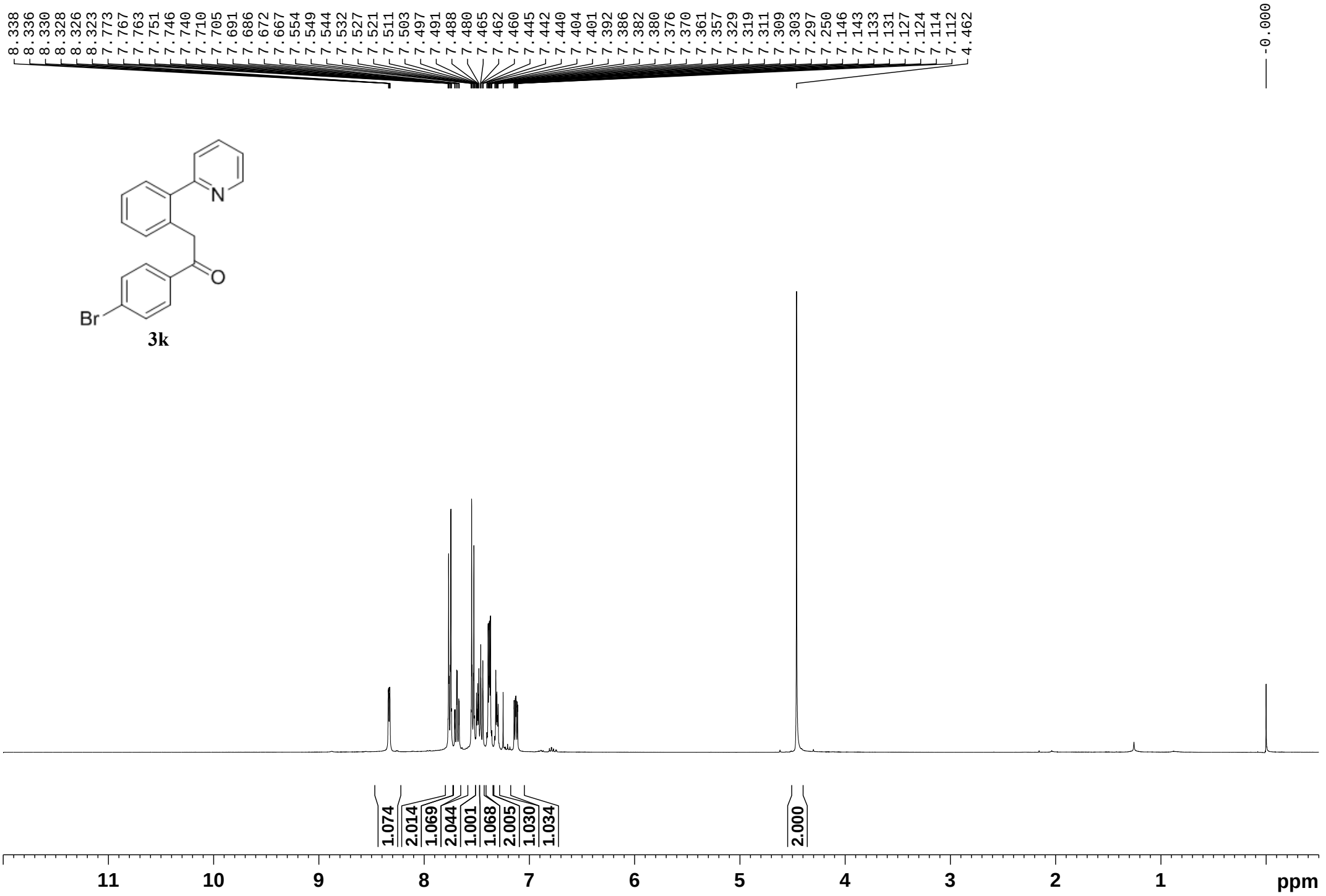
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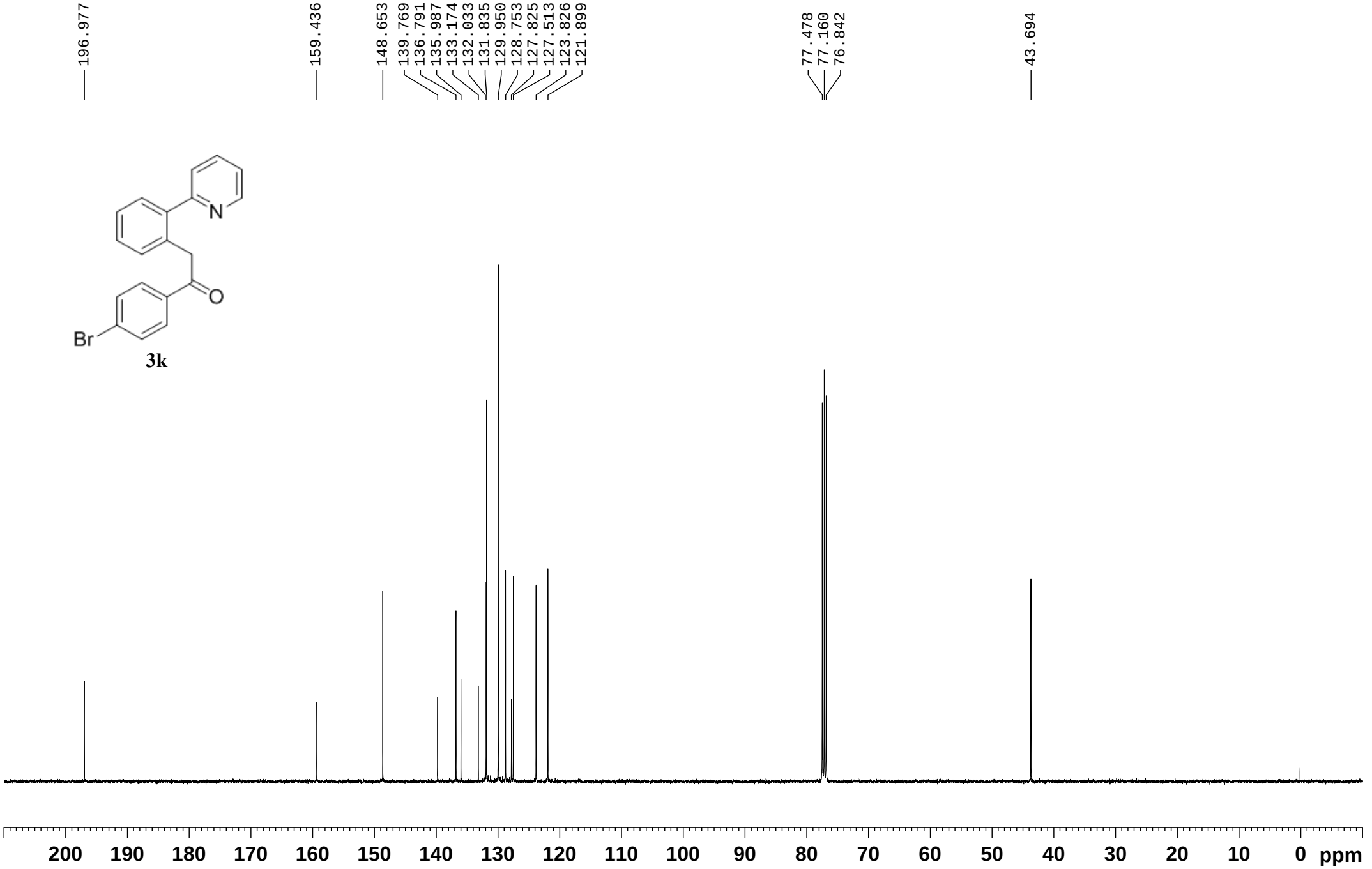
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76.842
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O
Br
3k
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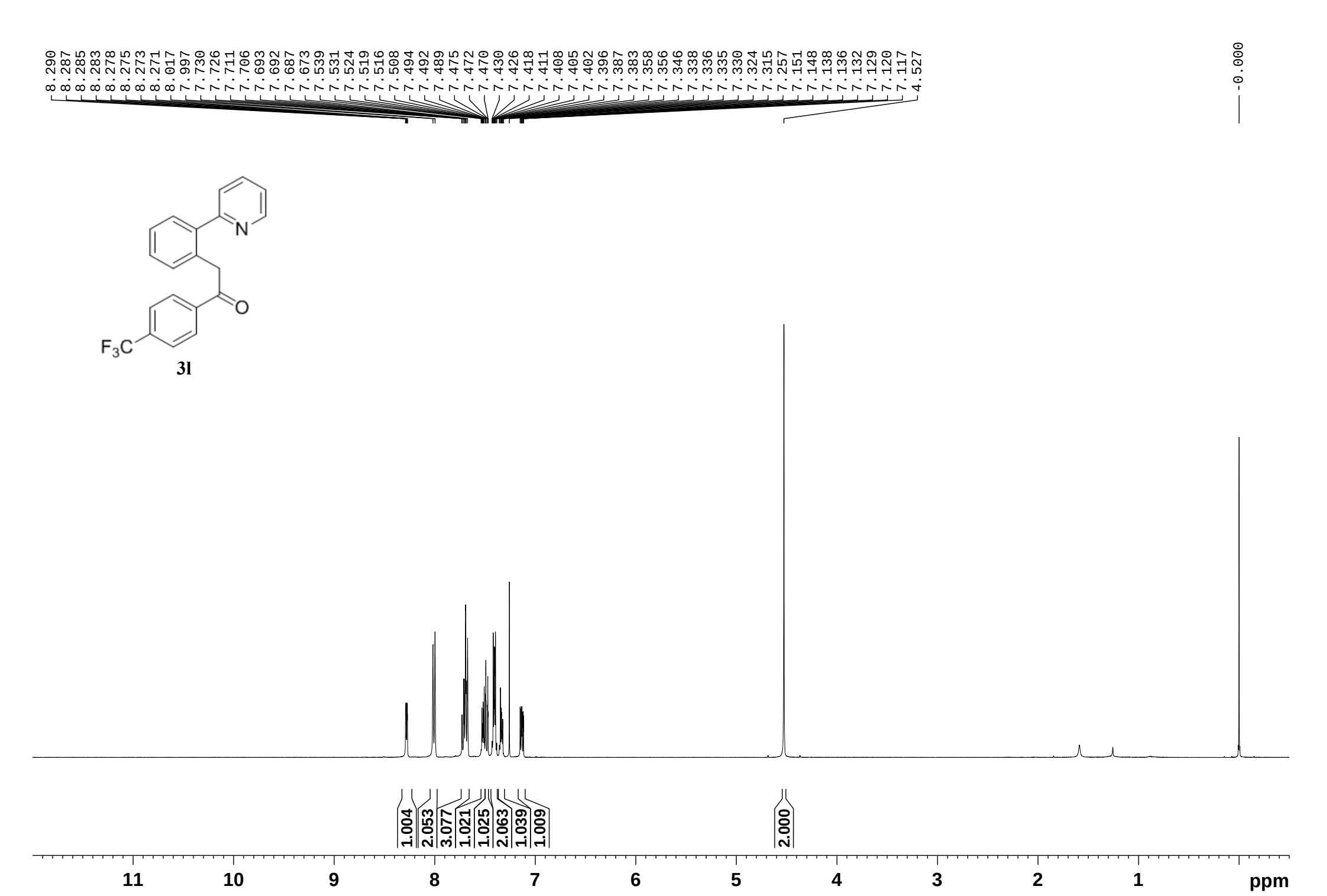
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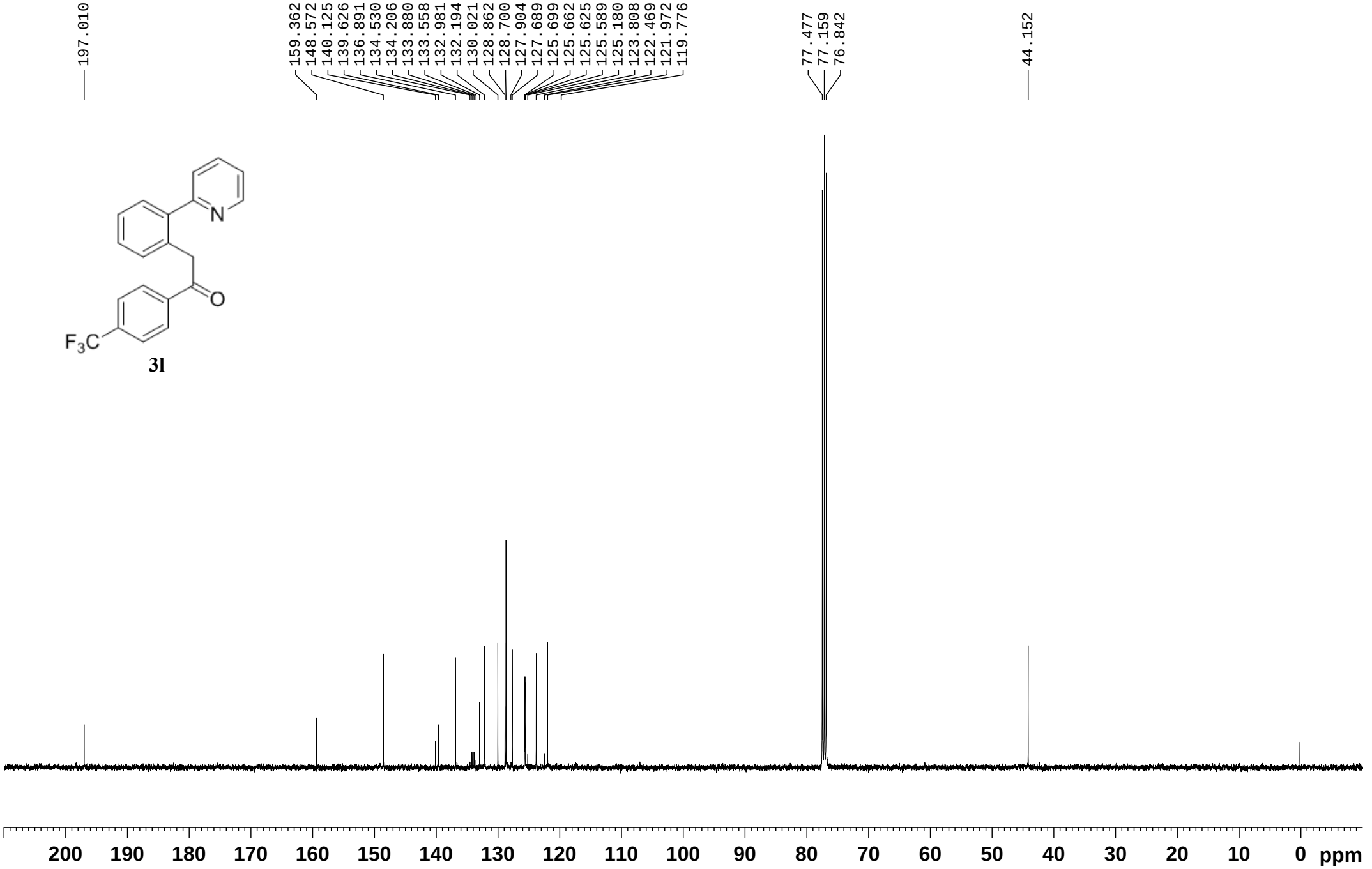
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O
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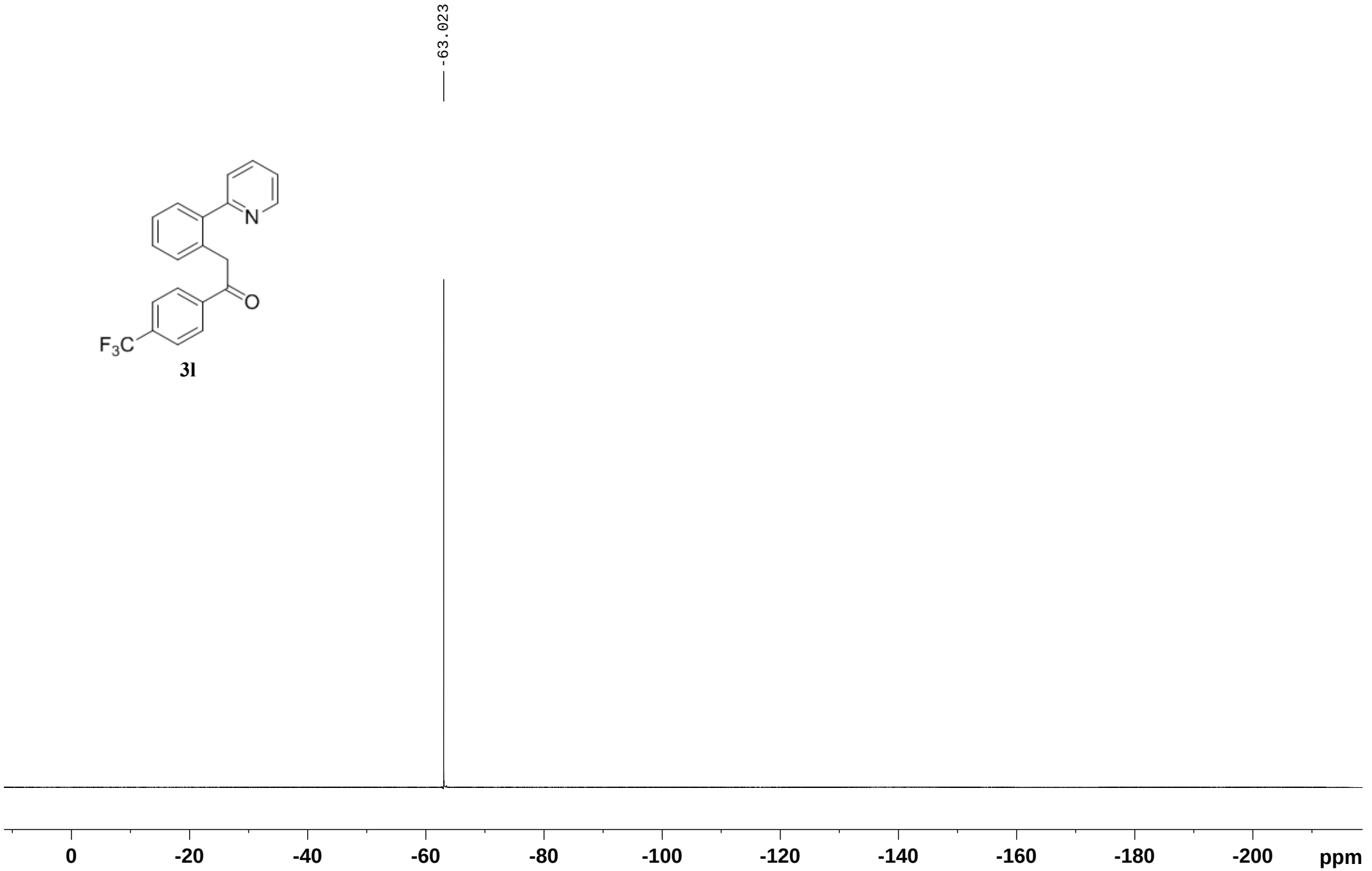
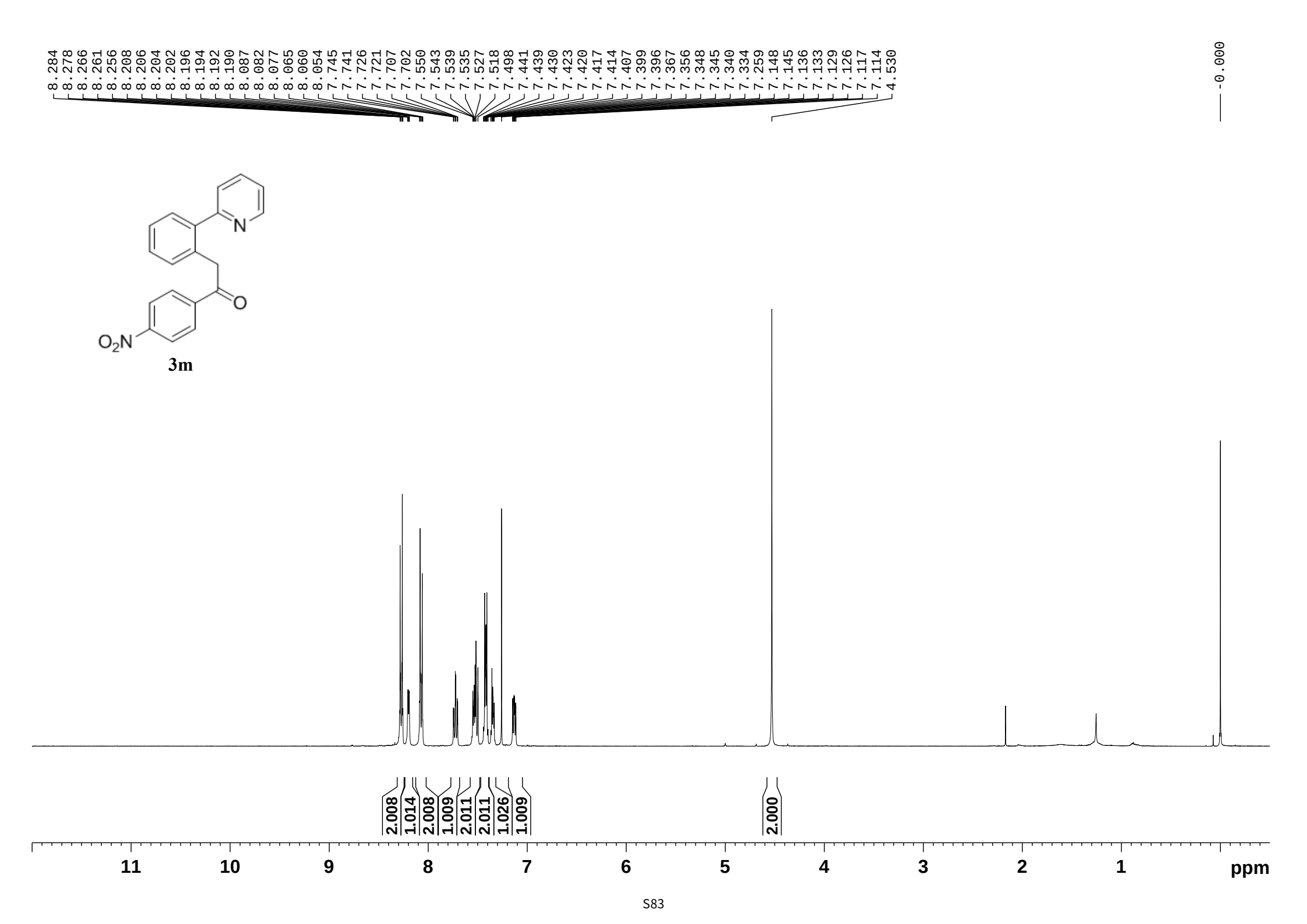
3l

3l

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7.334
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7.133
7.129
7.126
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7.114
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3m
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1.014
2.008
1.009
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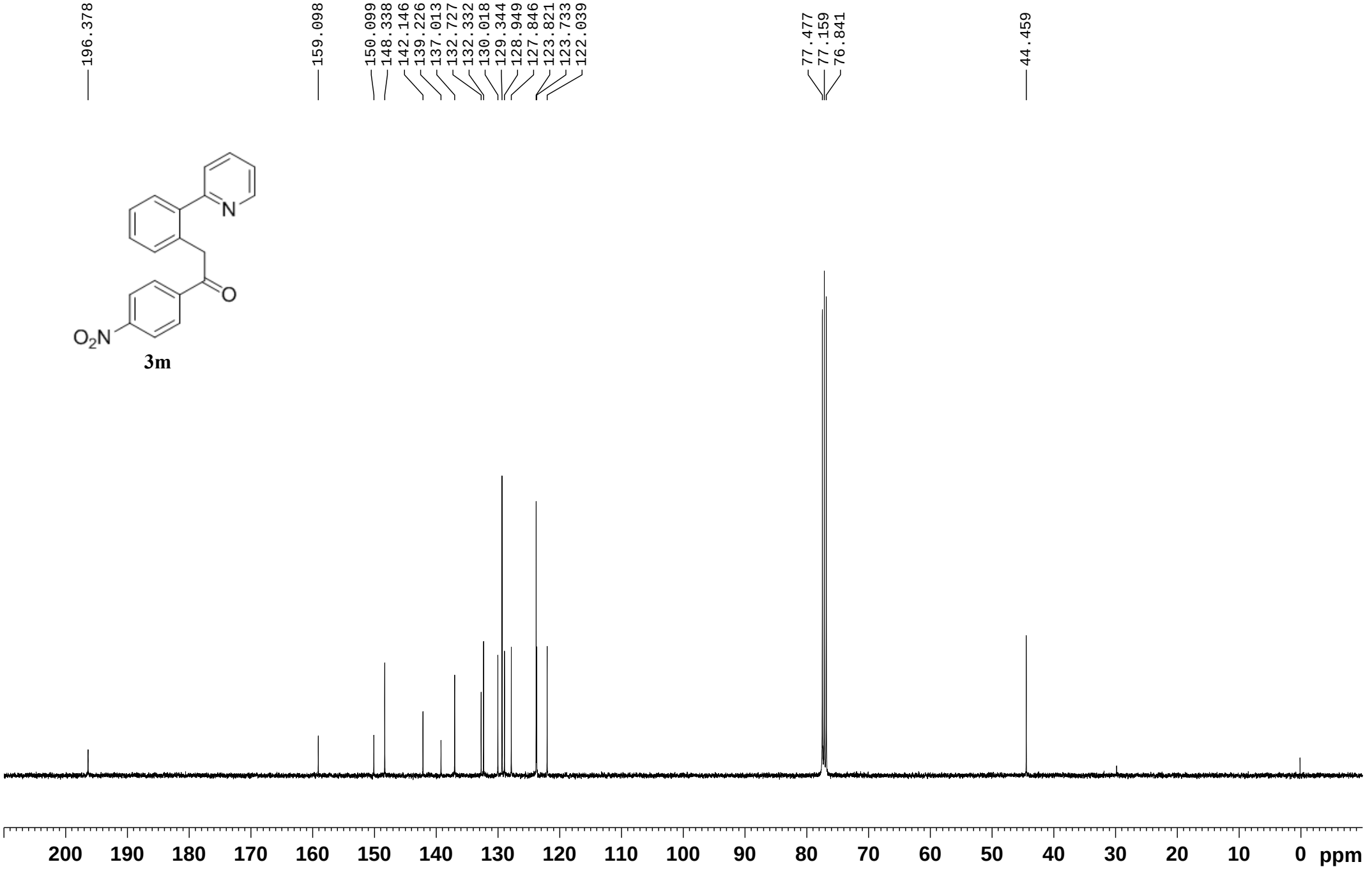
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O
O2N
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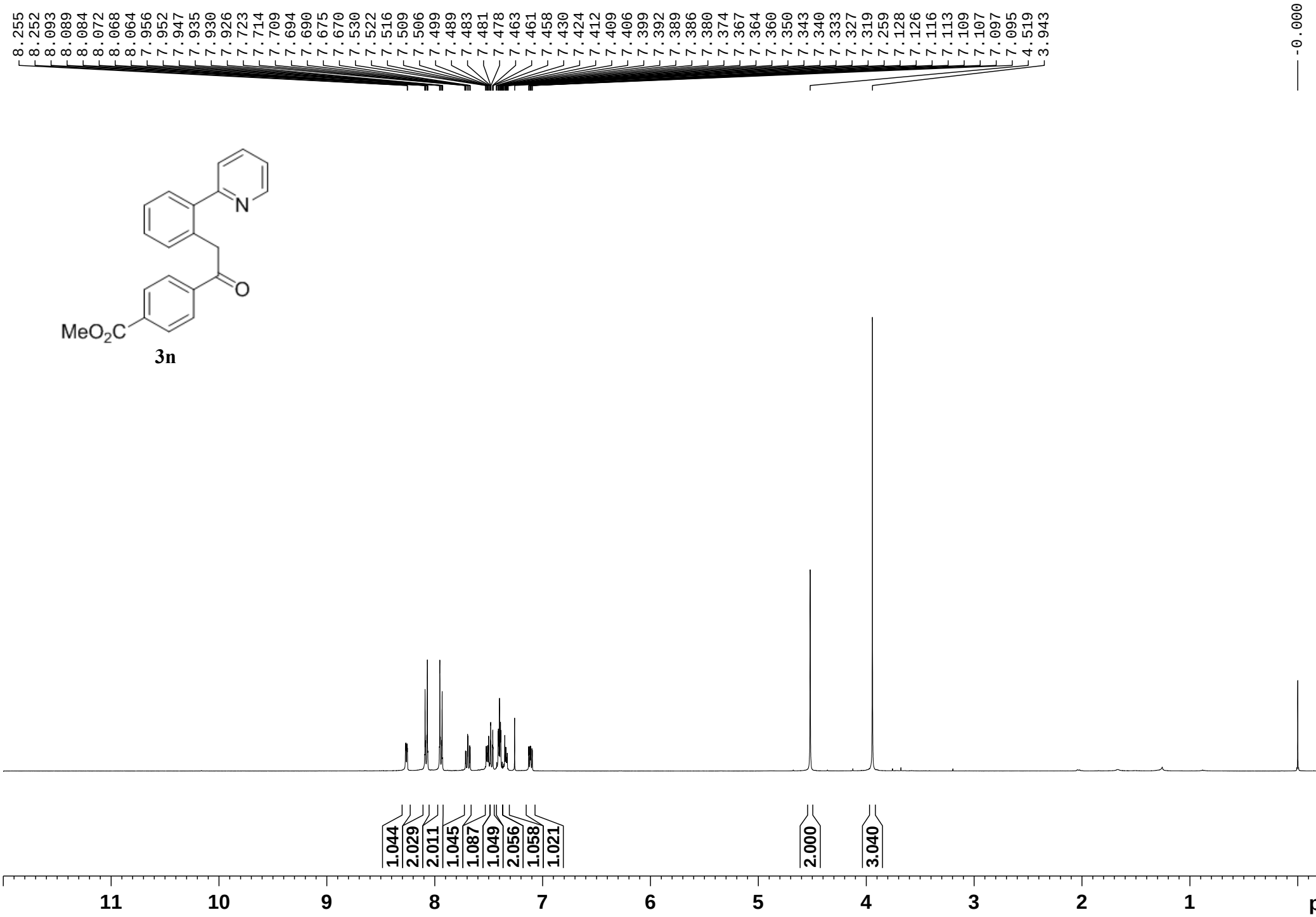
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7.327
7.319
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6
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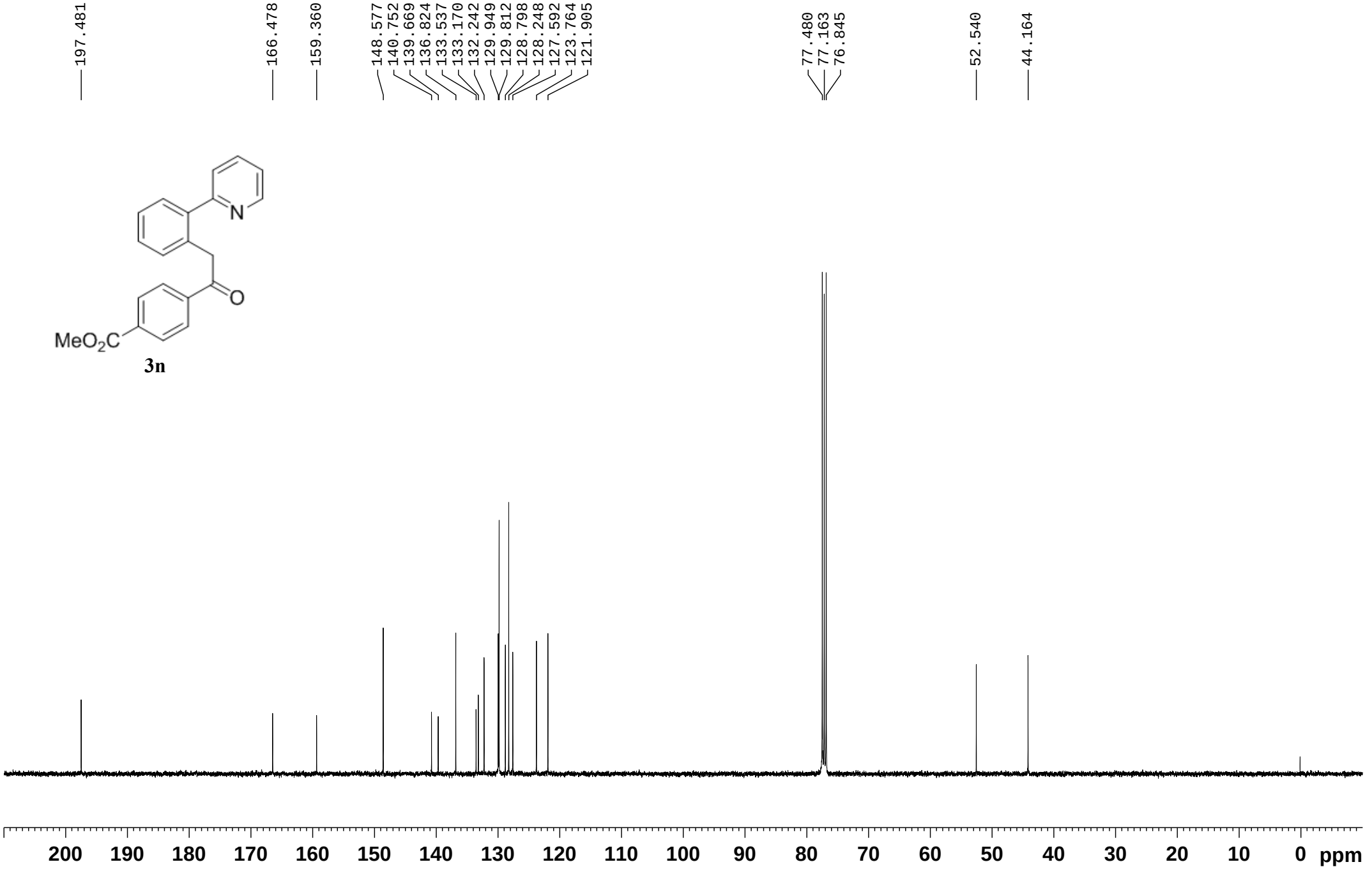
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O
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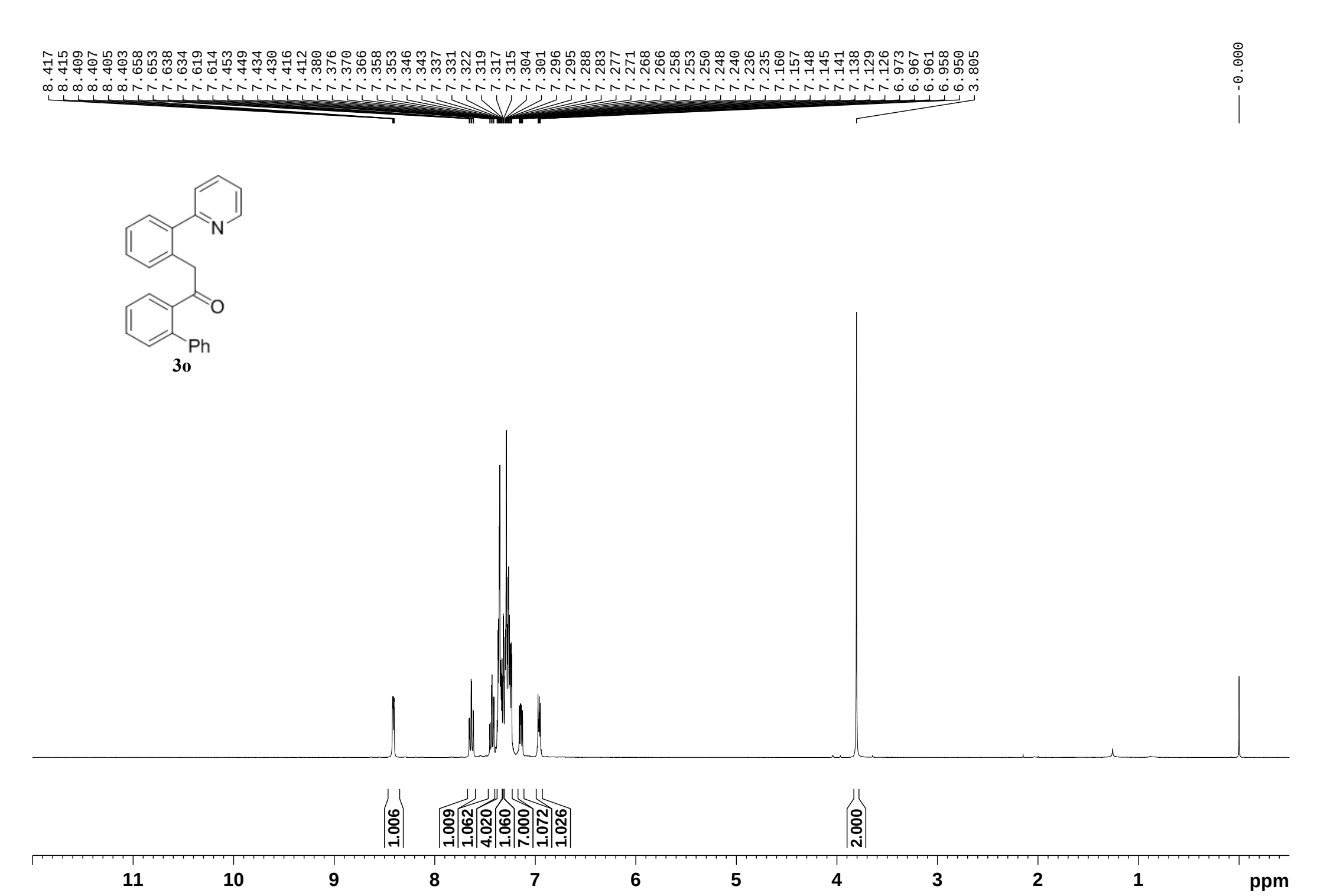
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7.157
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7.129
7.126
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6.958
6.950
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O
Ph
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1.009
1.062
4.020
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ppm

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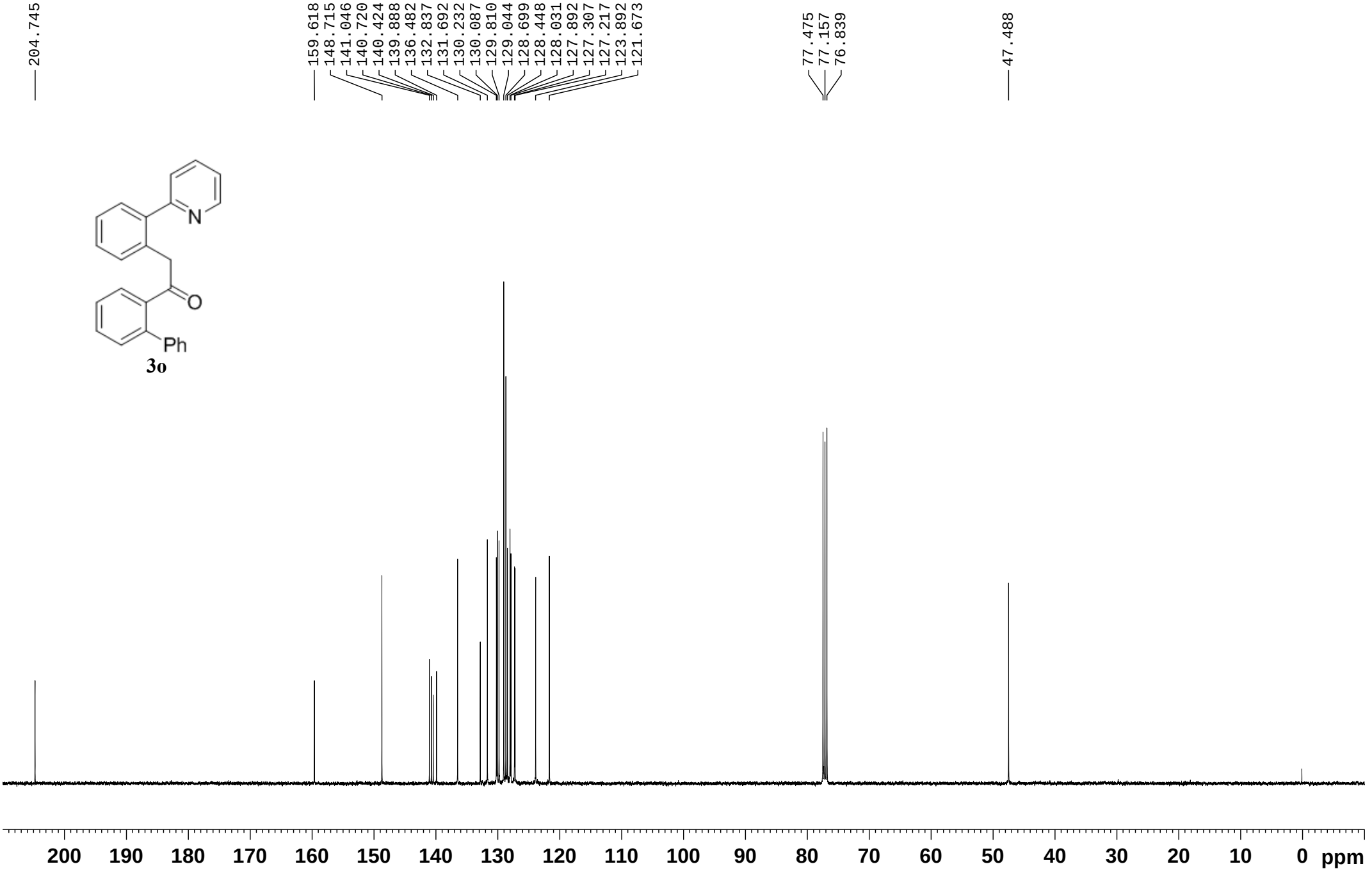
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128.448
128.031
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Ph
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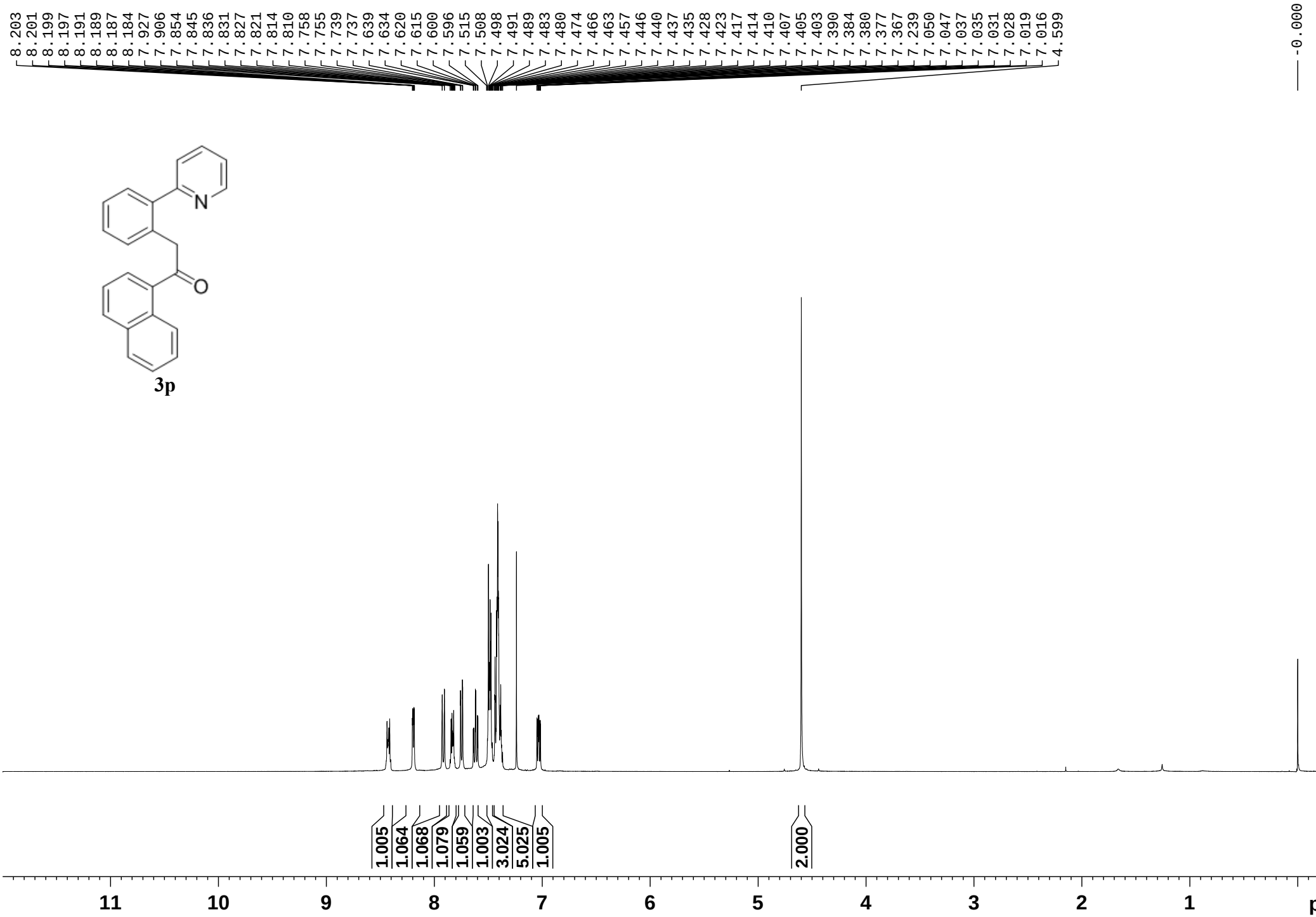
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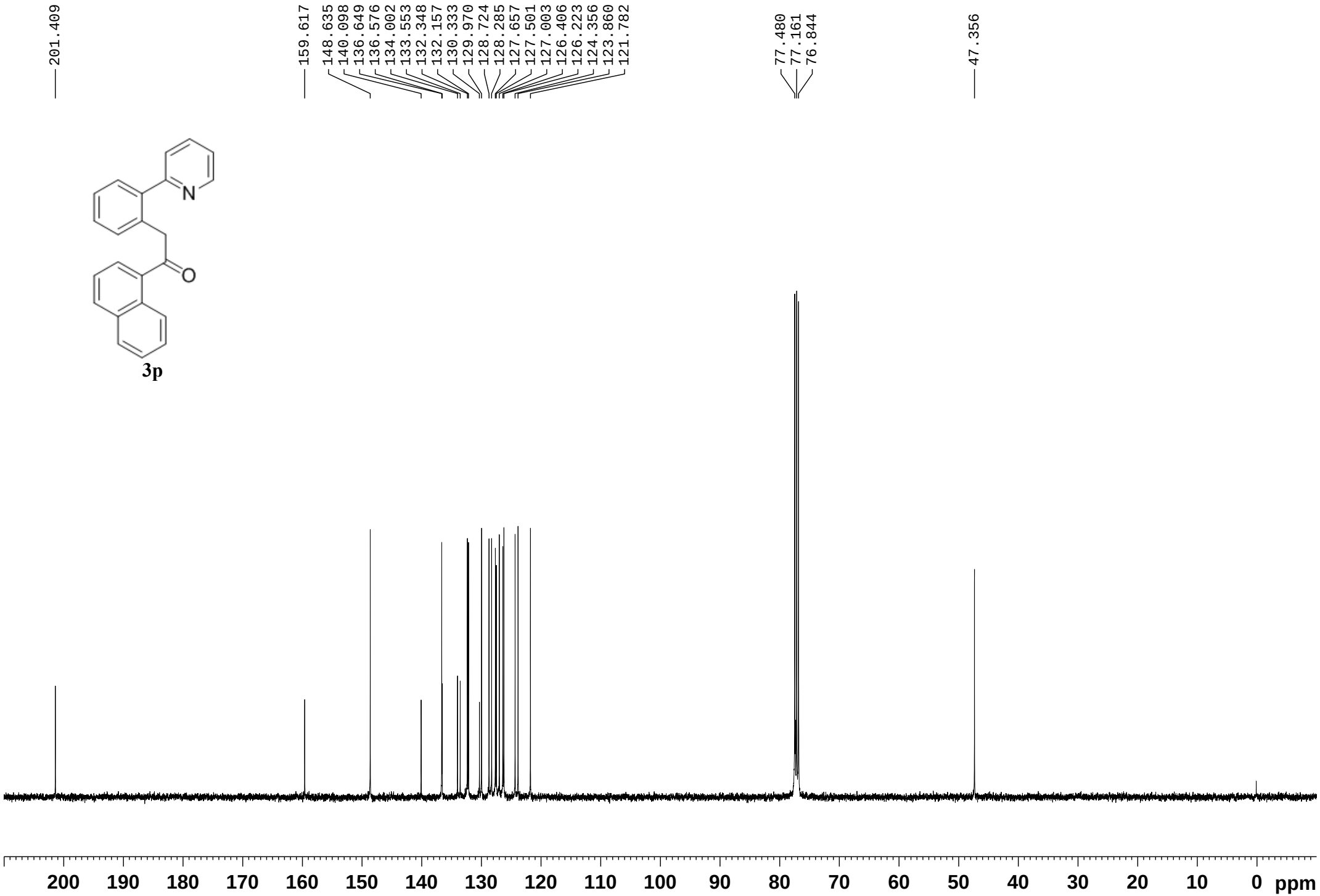
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127.003
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126.223
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47.356
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O
3p
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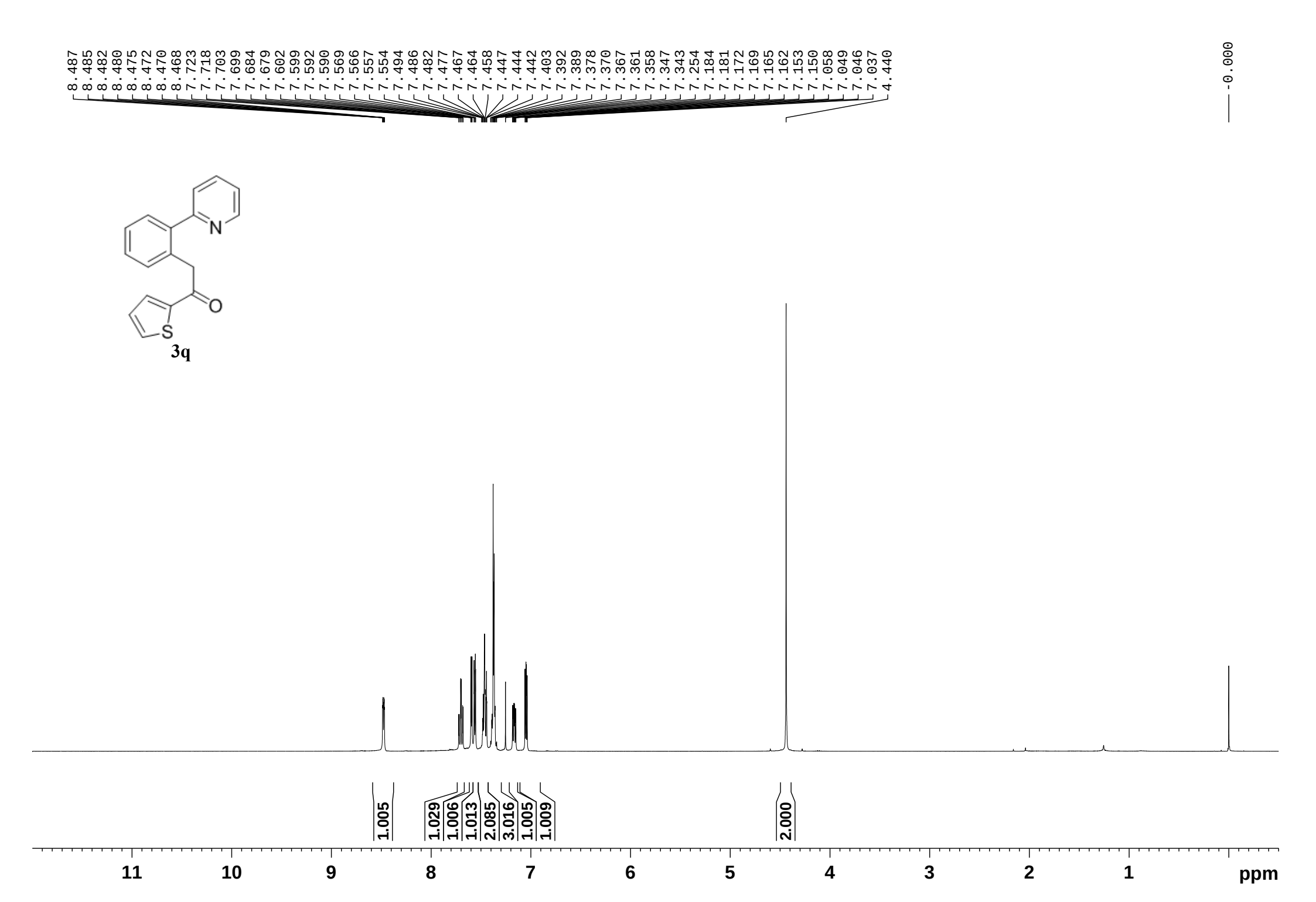
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7.679
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7.554
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1.013
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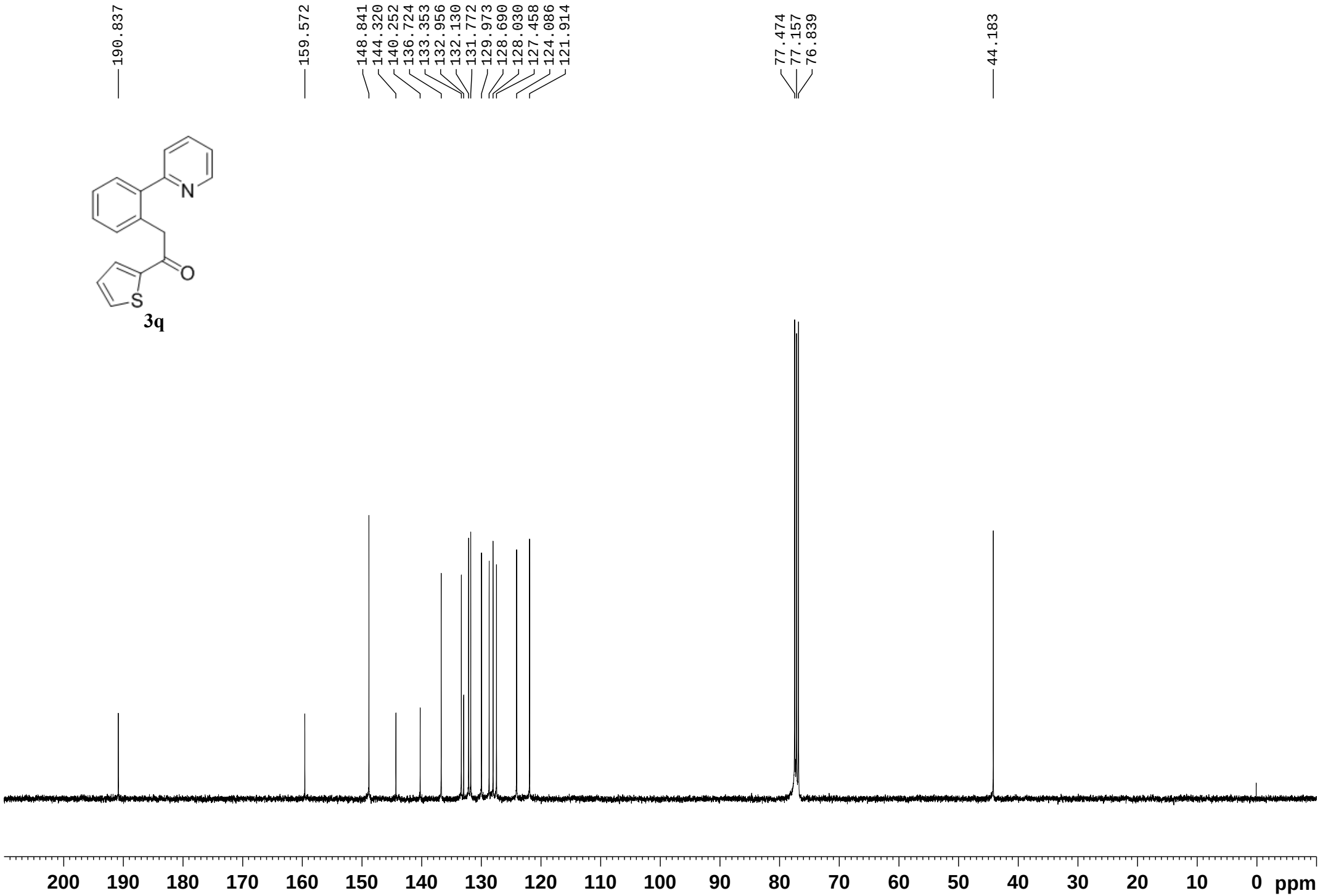
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S
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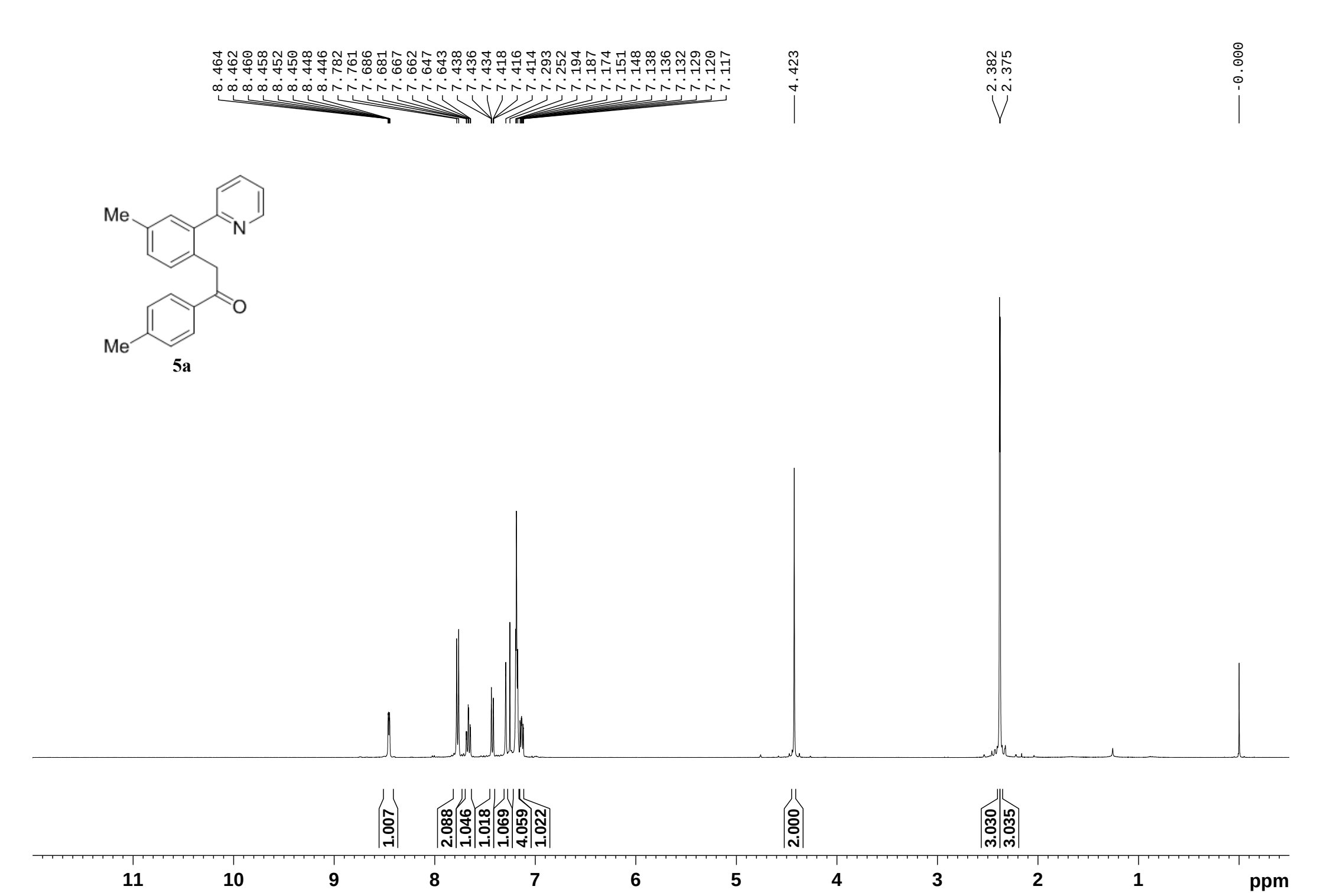
3q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7.117
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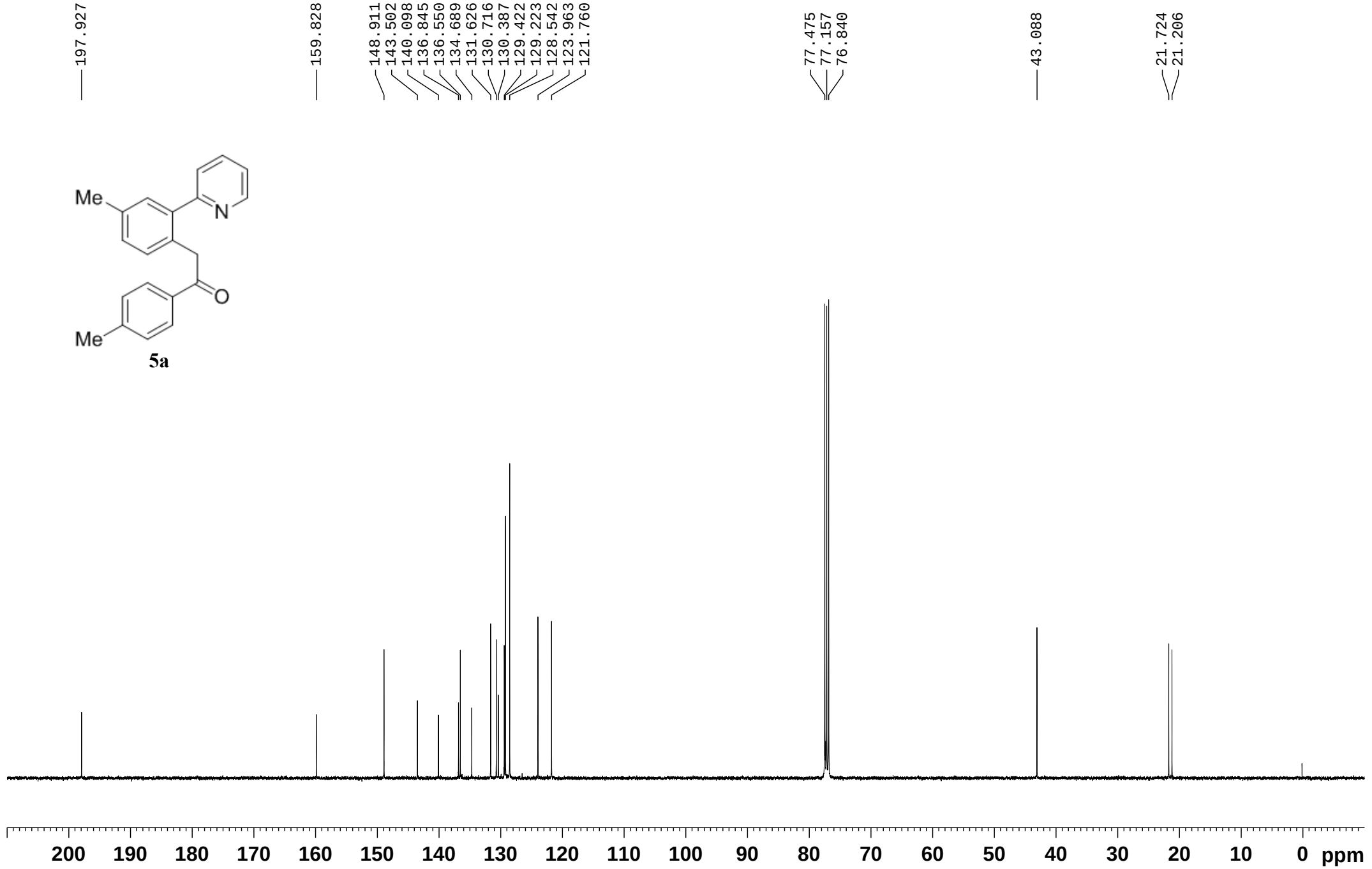
ppm

5a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128.542
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121.760
77.475
77.157
76.840
43.088
21.724
21.206
Me
N
O
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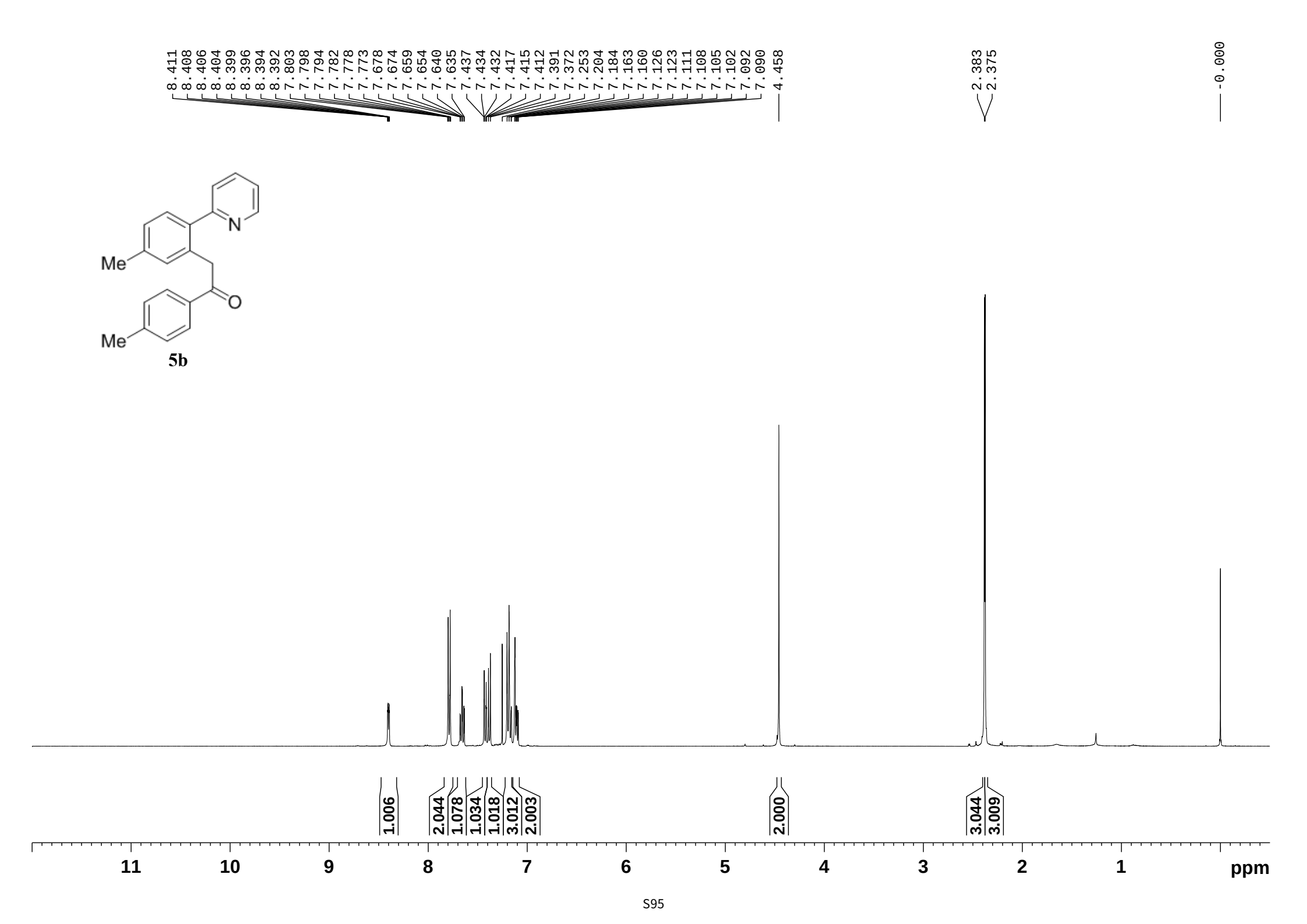
5a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7.160
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7.105
7.102
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7.090
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Me
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1.078
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3.009
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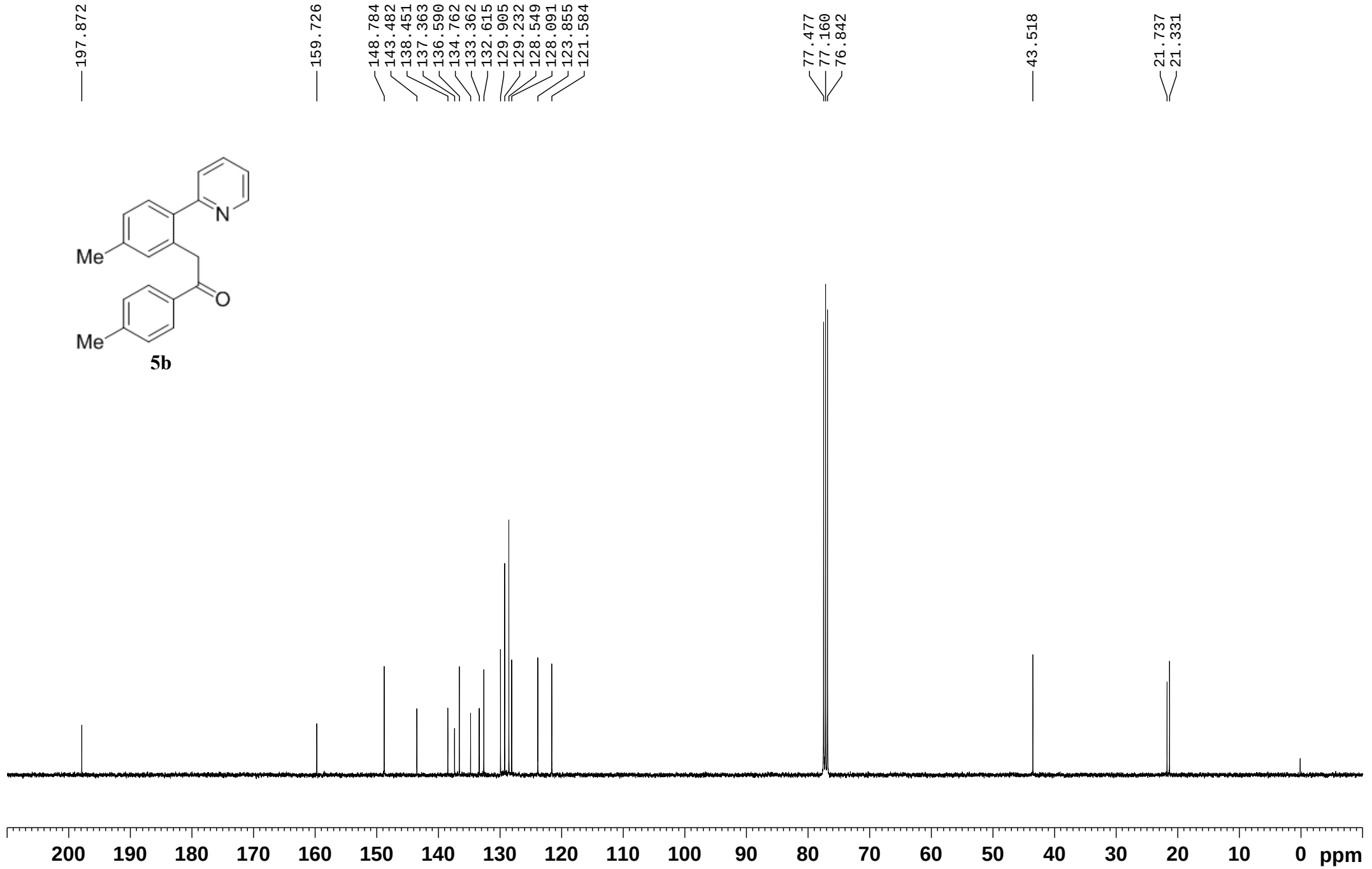
ppm

5b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76.842
43.518
21.737
21.331
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Me
O
Me
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50
40
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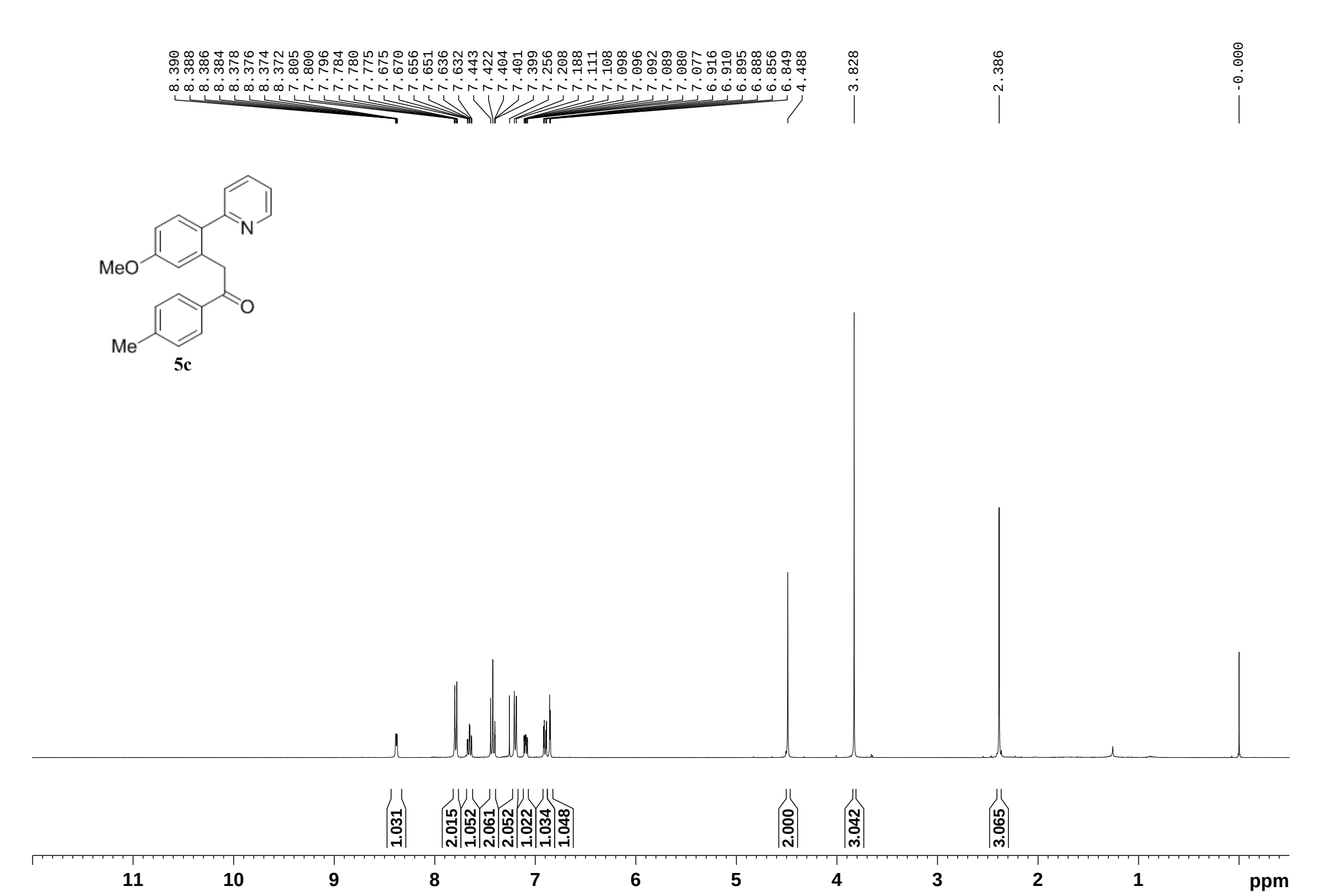
ppm

5b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O
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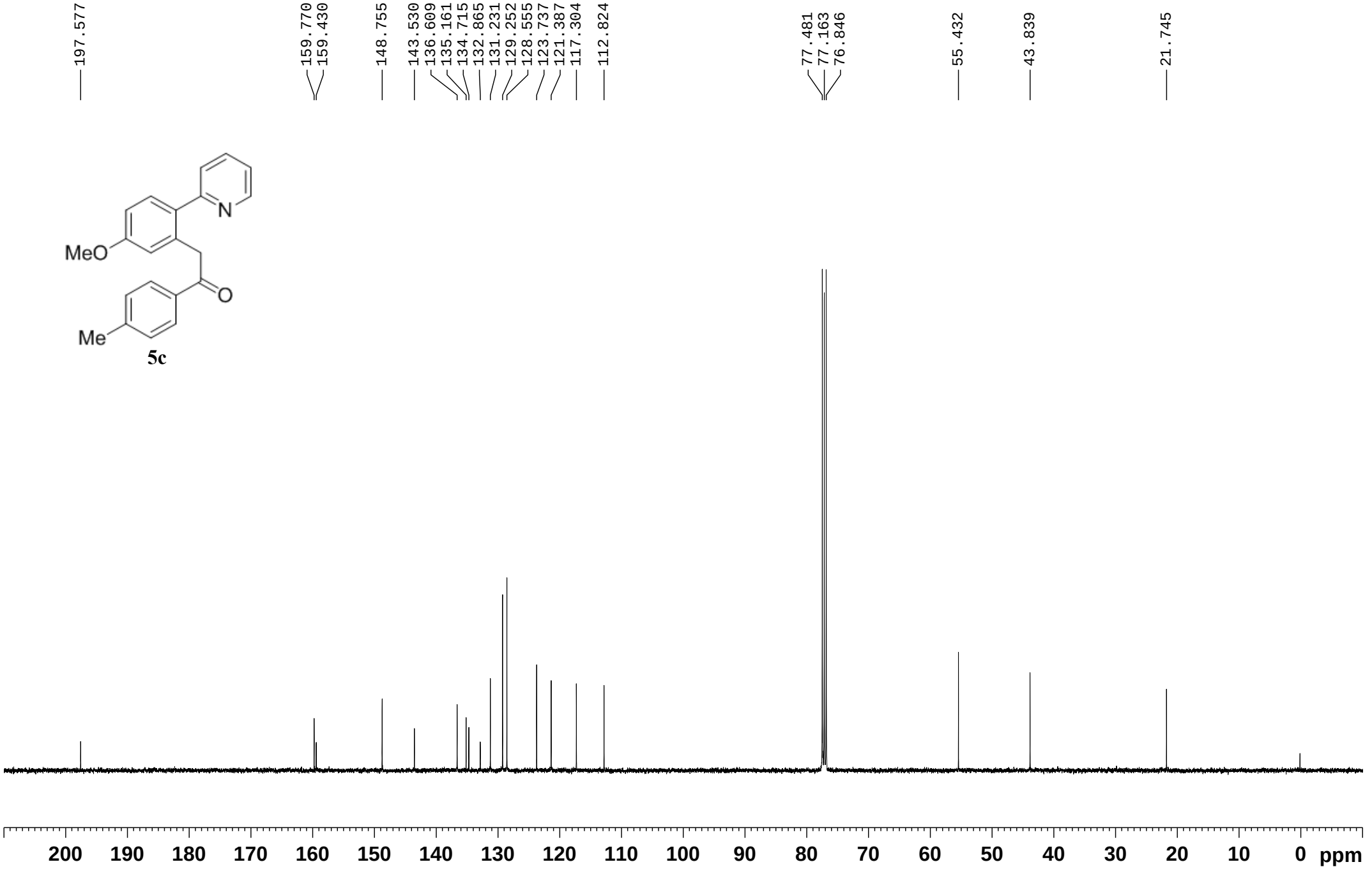
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77.163
76.846
55.432
43.839
21.745
MeO
N
O
Me
5c
200
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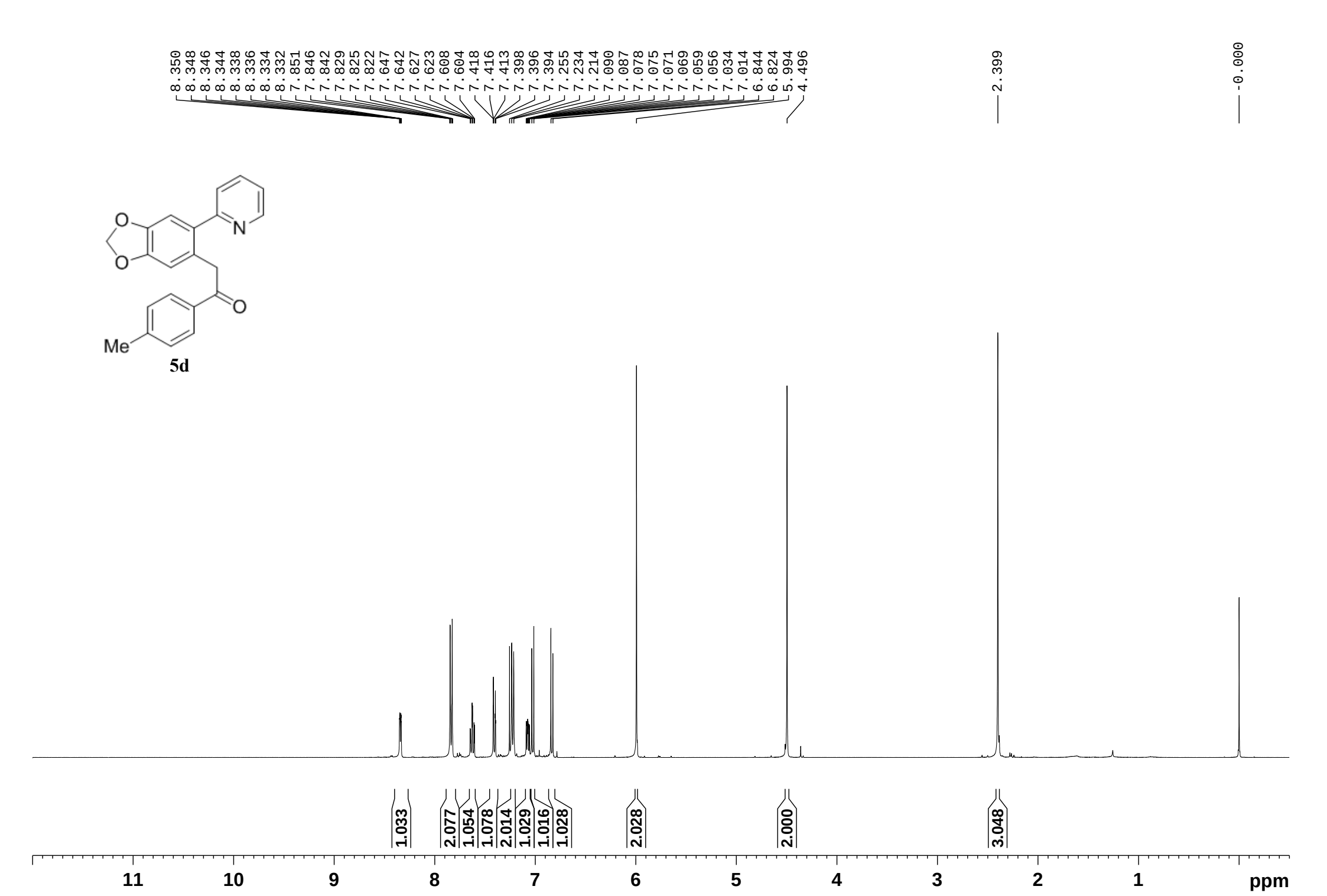
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7.604
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7.413
7.398
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7.394
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7.078
7.075
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7.056
7.034
7.014
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2.399
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O
O
N
O
Me
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1.054
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2.014
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1.016
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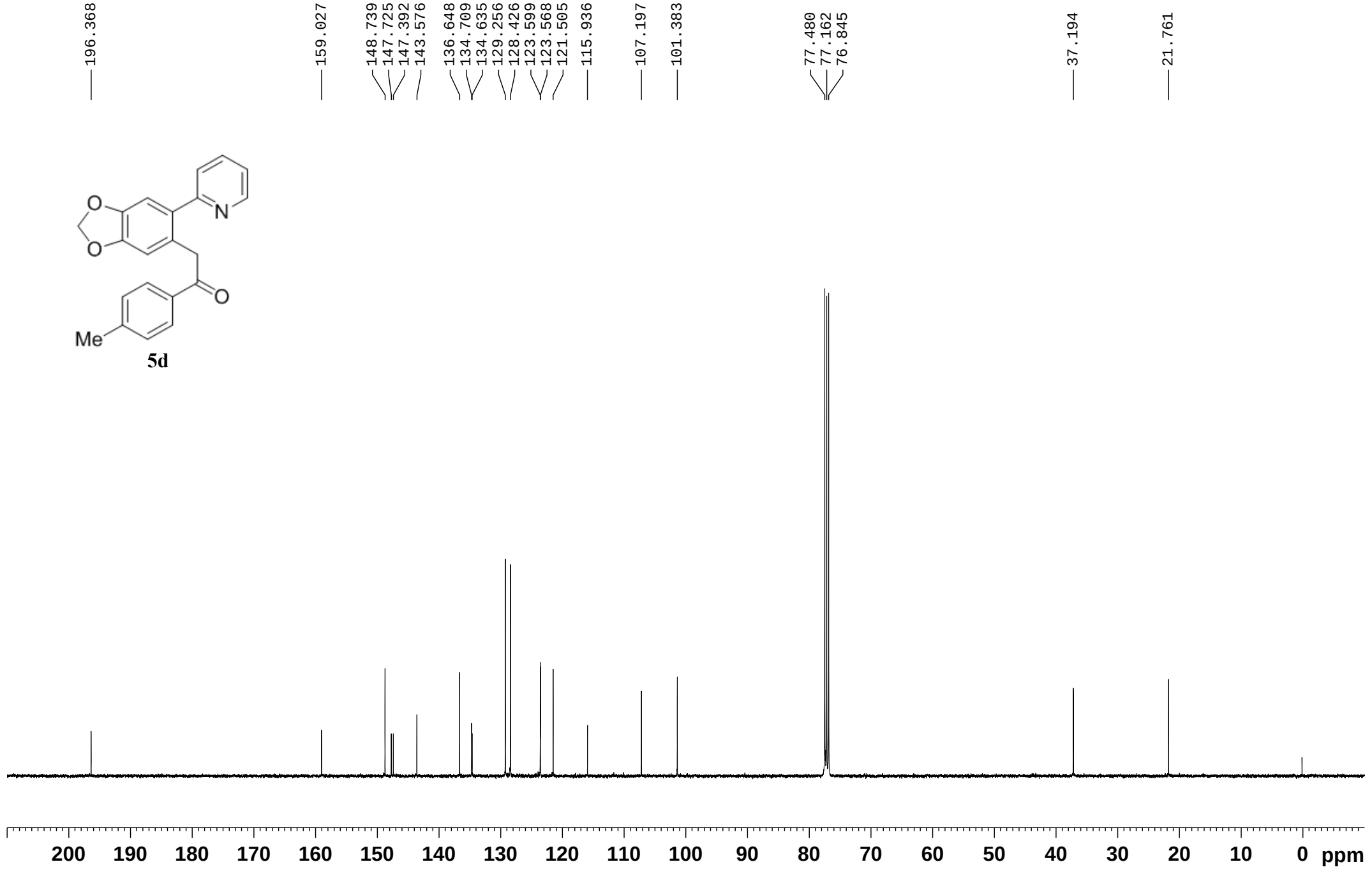
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123.568
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107.197
101.383
77.480
77.162
76.845
37.194
21.761
O
O
N
O
Me
200
190
180
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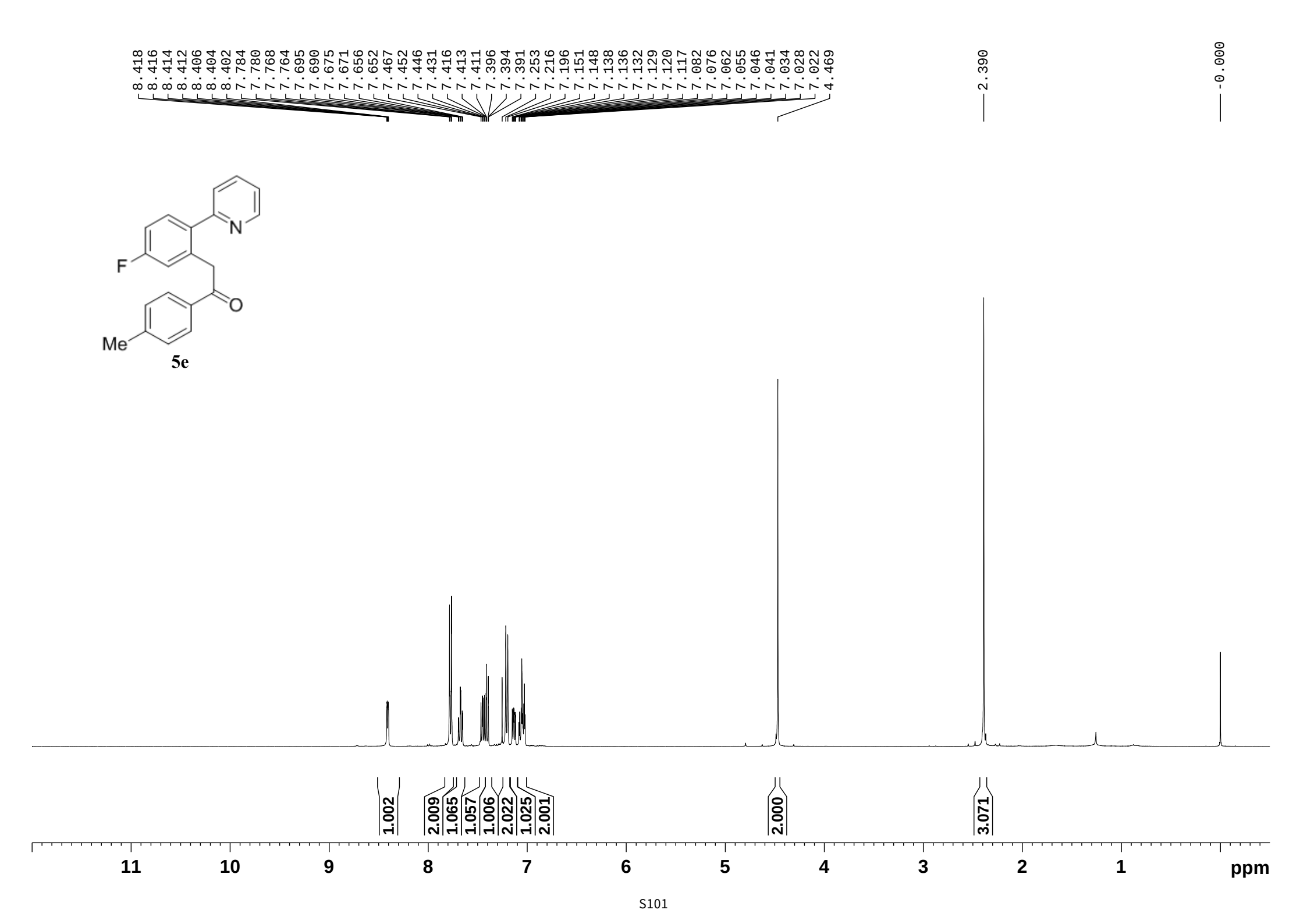
5d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7.138
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7.132
7.129
7.120
7.117
7.082
7.076
7.062
7.055
7.046
7.041
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N
O
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ppm

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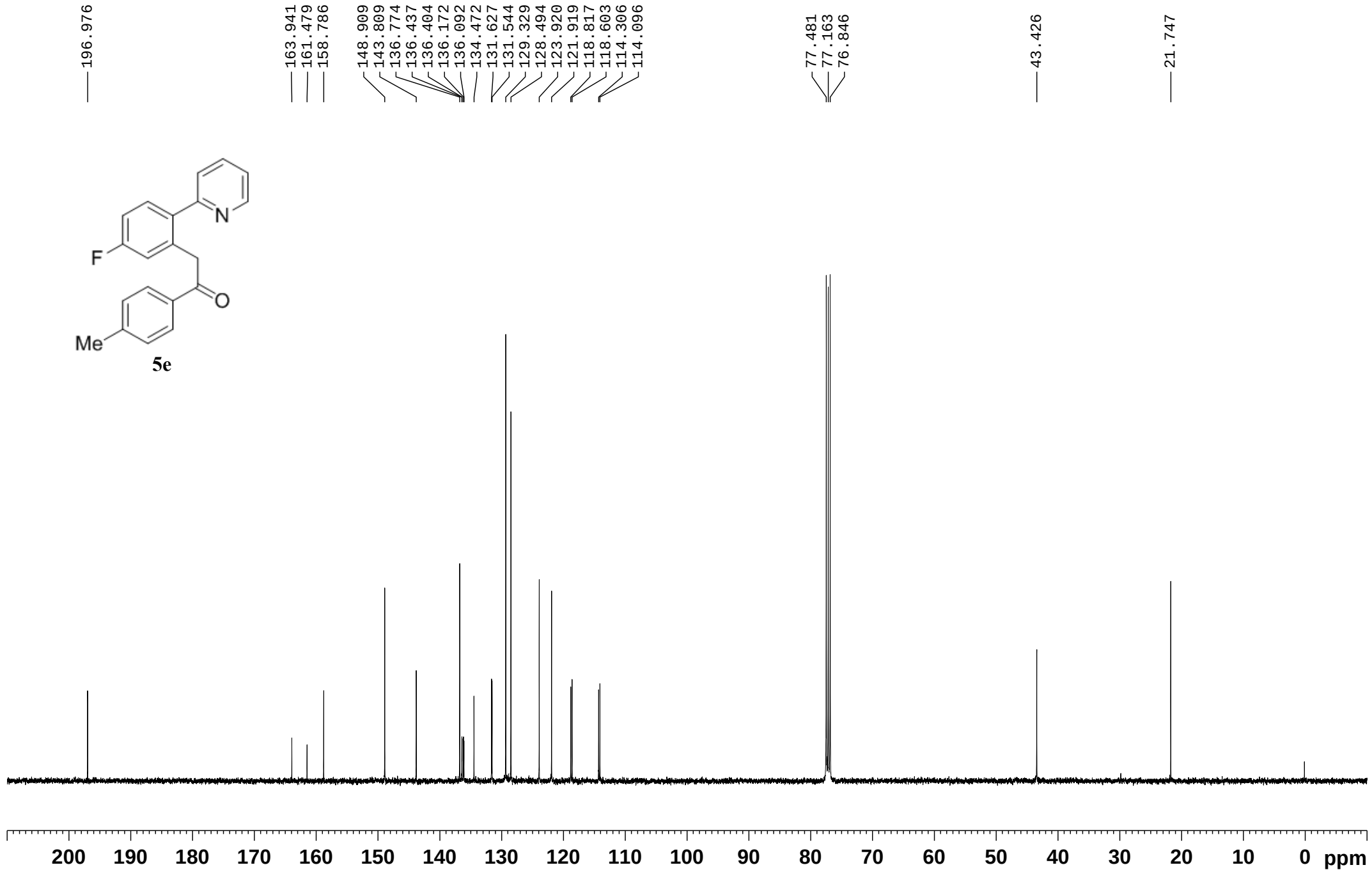
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121.919
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114.306
114.096
77.481
77.163
76.846
43.426
21.747
F
N
O
Me
200
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180
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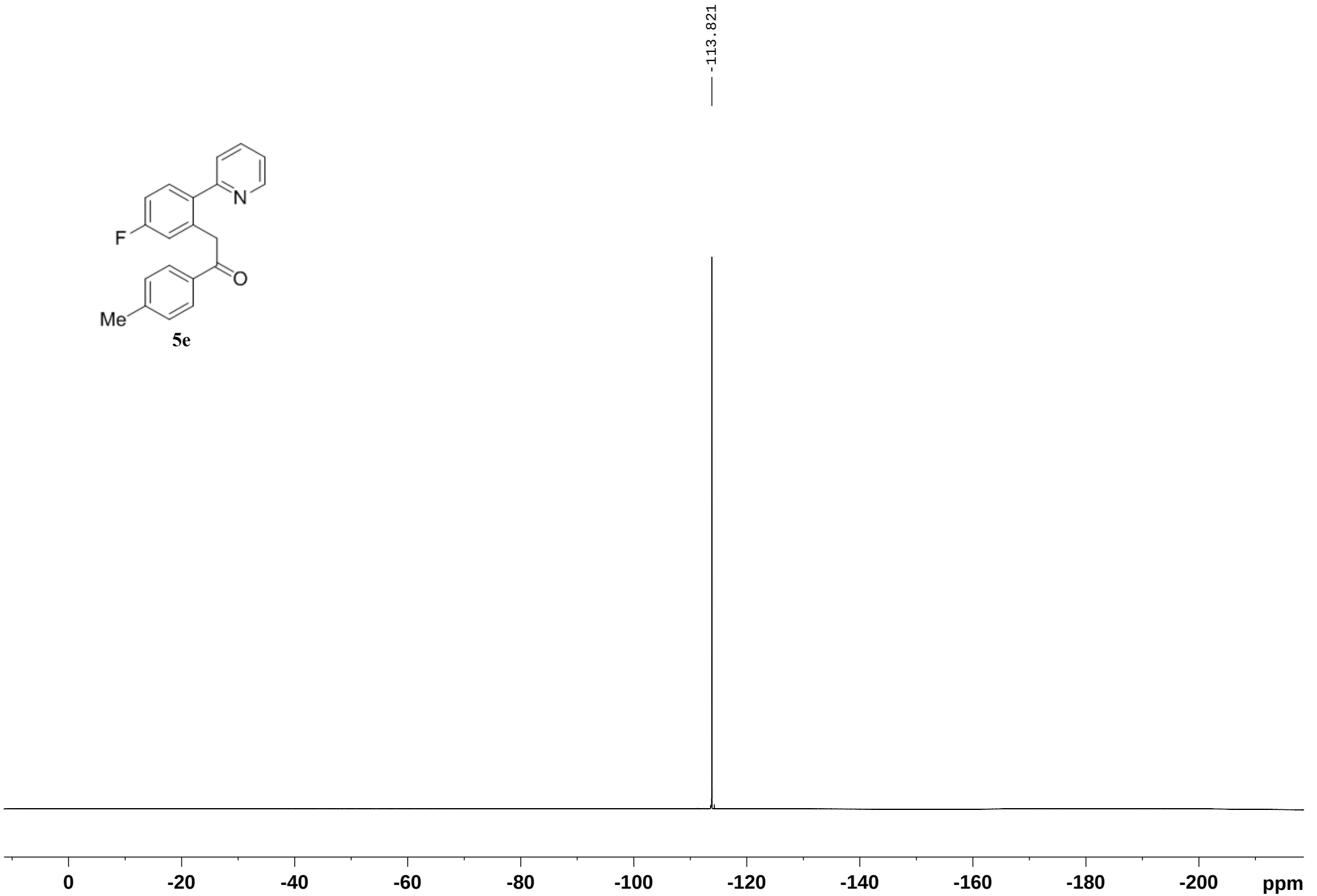
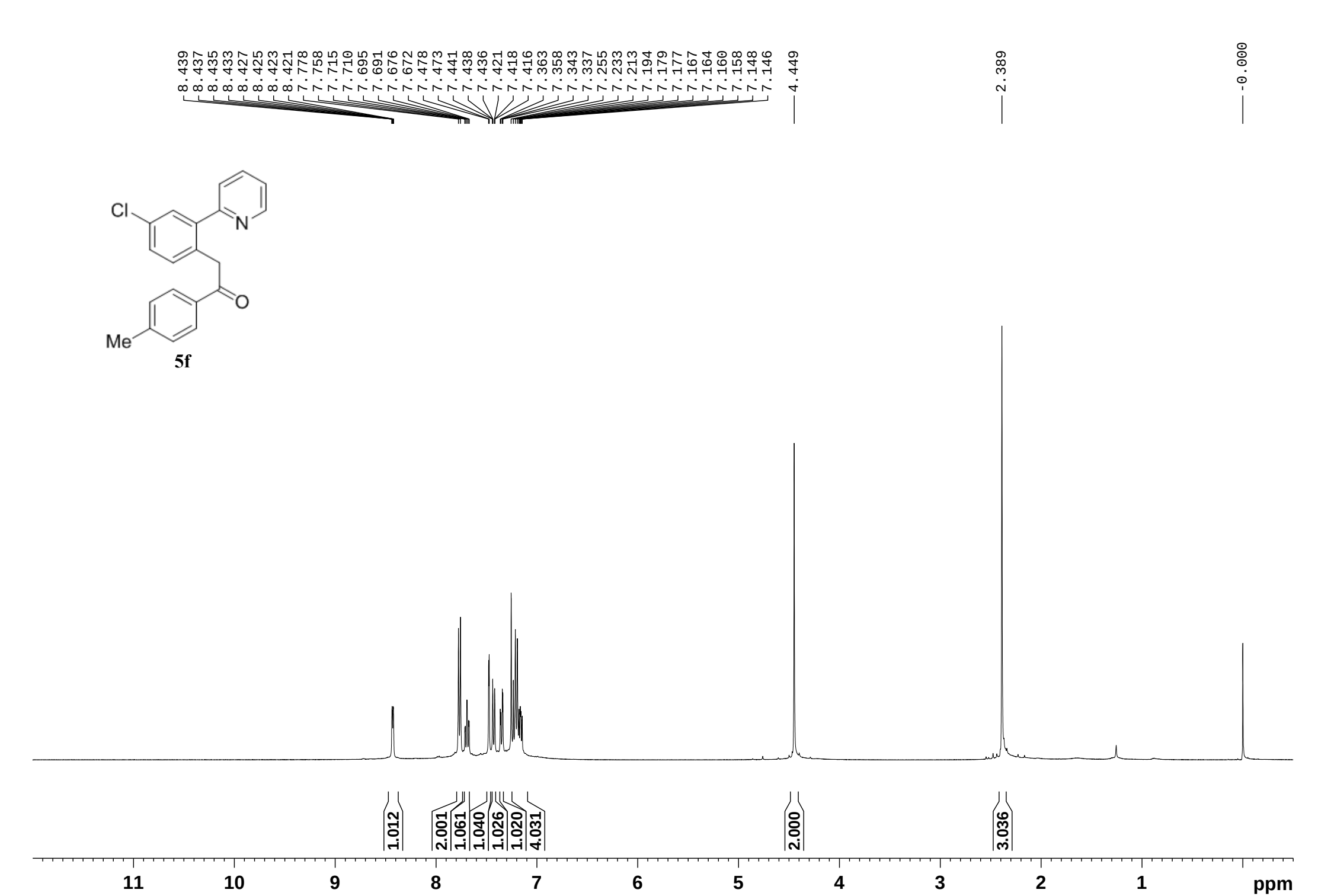
ppm

5e

5e

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7.672
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7.436
7.421
7.418
7.416
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7.358
7.343
7.337
7.255
7.233
7.213
7.194
7.179
7.177
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7.160
7.158
7.148
7.146
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Cl
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O
Me
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1.040
1.026
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2
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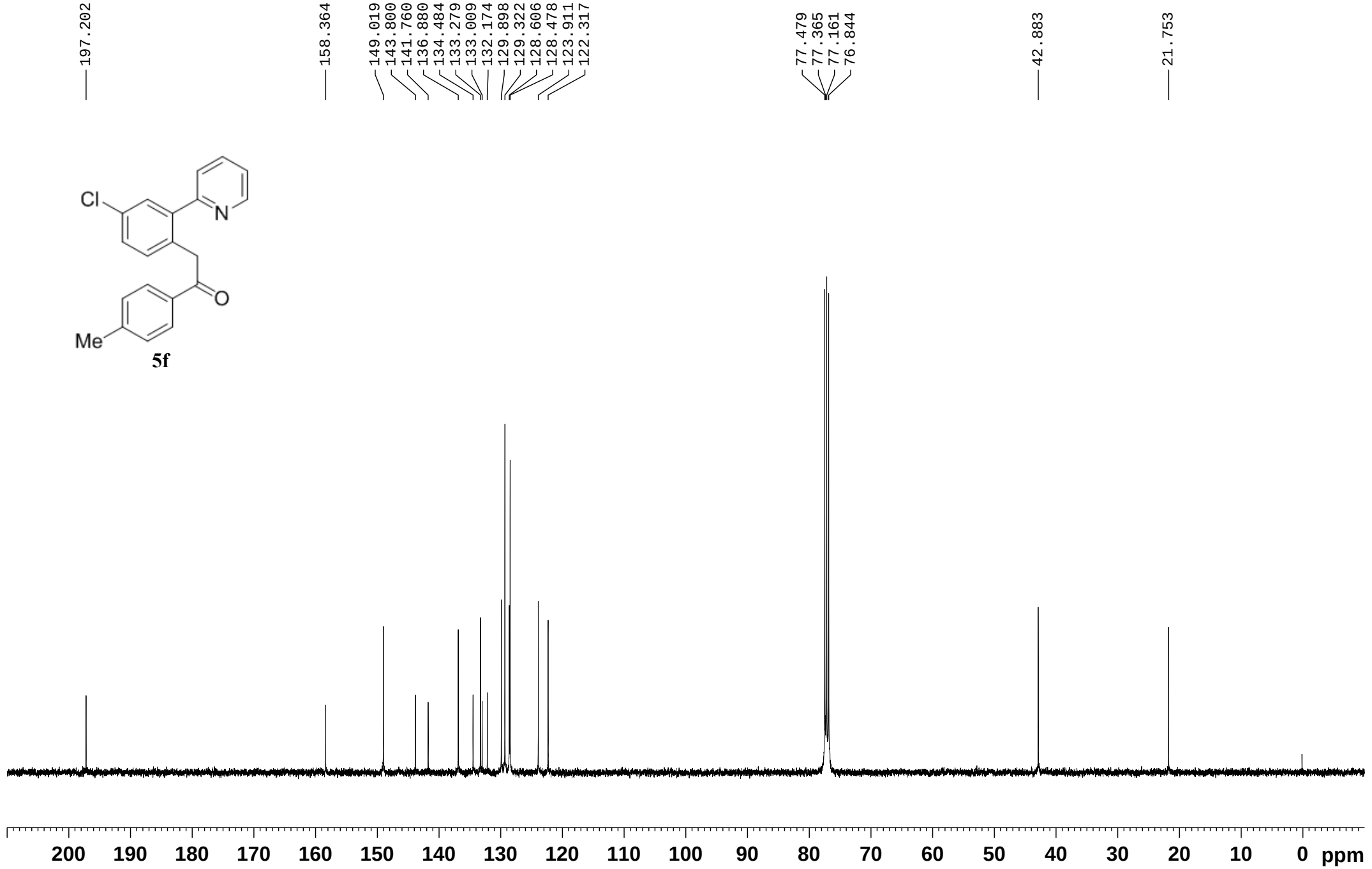
ppm

5f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128.478
123.911
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77.161
76.844
42.883
21.753
Cl
N
O
Me
5f
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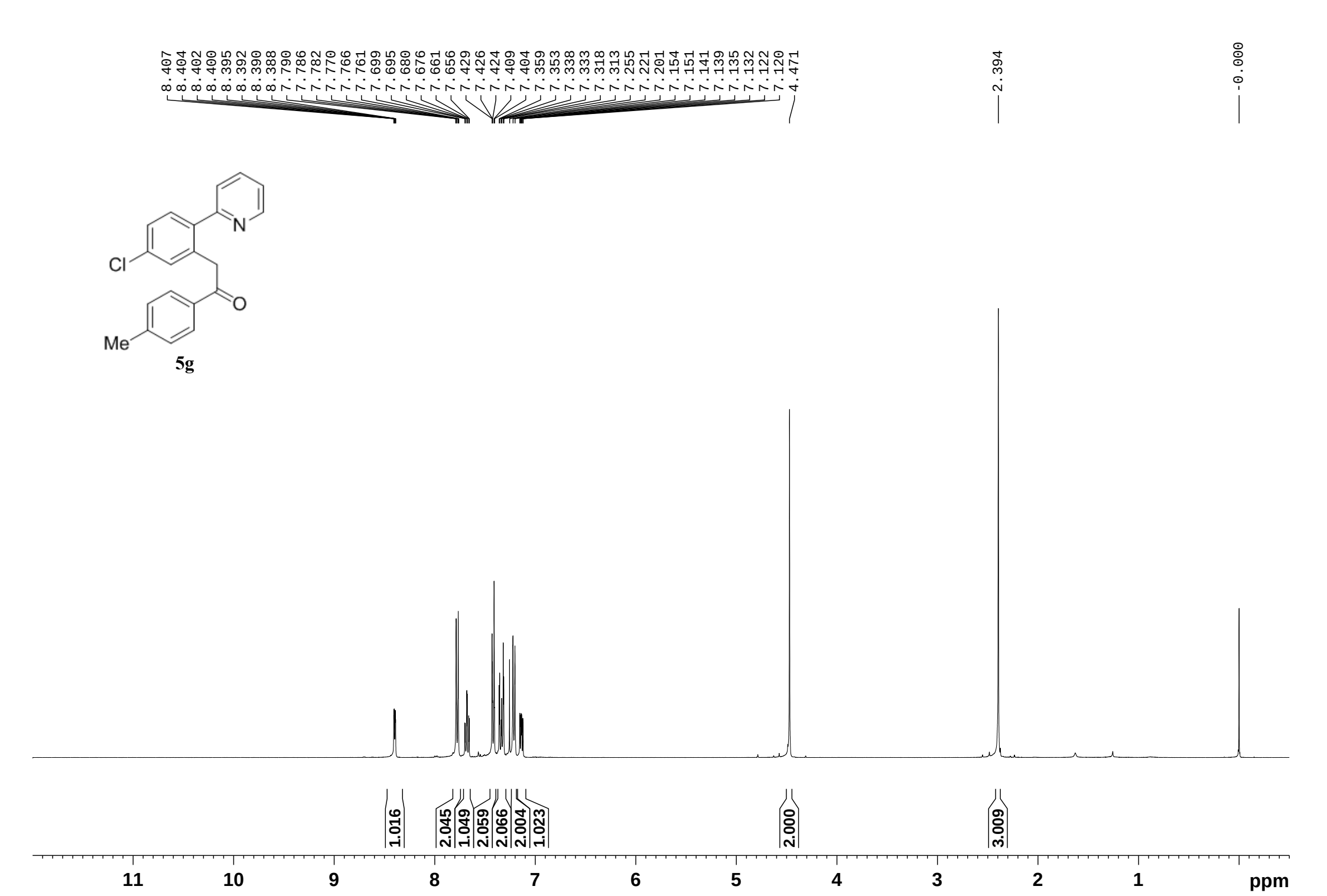
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Cl
O
Me
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2.059
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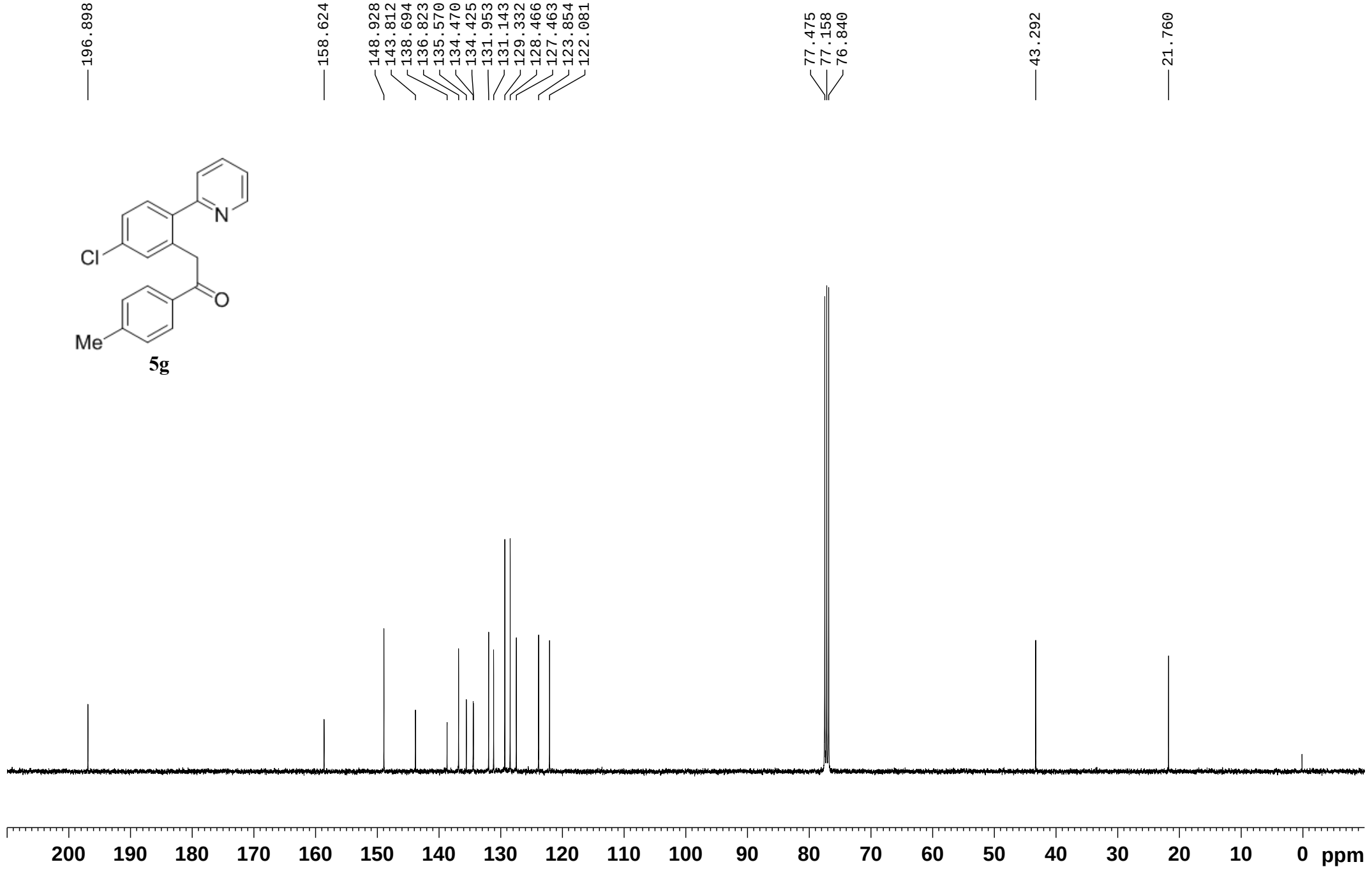
ppm

5g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127.463
123.854
122.081
77.475
77.158
76.840
43.292
21.760
Cl
N
O
Me
200
190
180
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130
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90
80
70
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50
40
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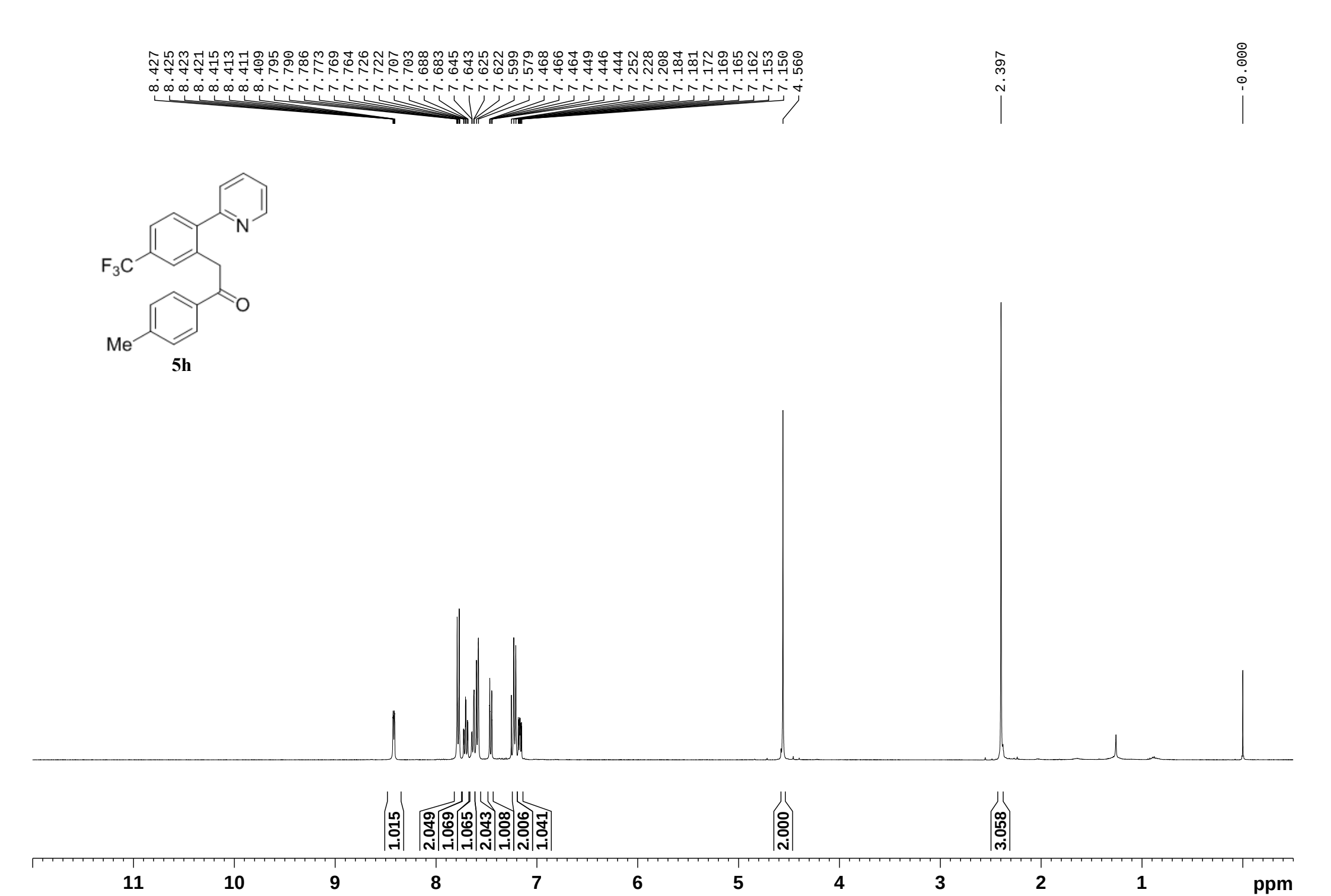
ppm

5g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7.764
7.726
7.722
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7.599
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7.162
7.153
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F3C
O
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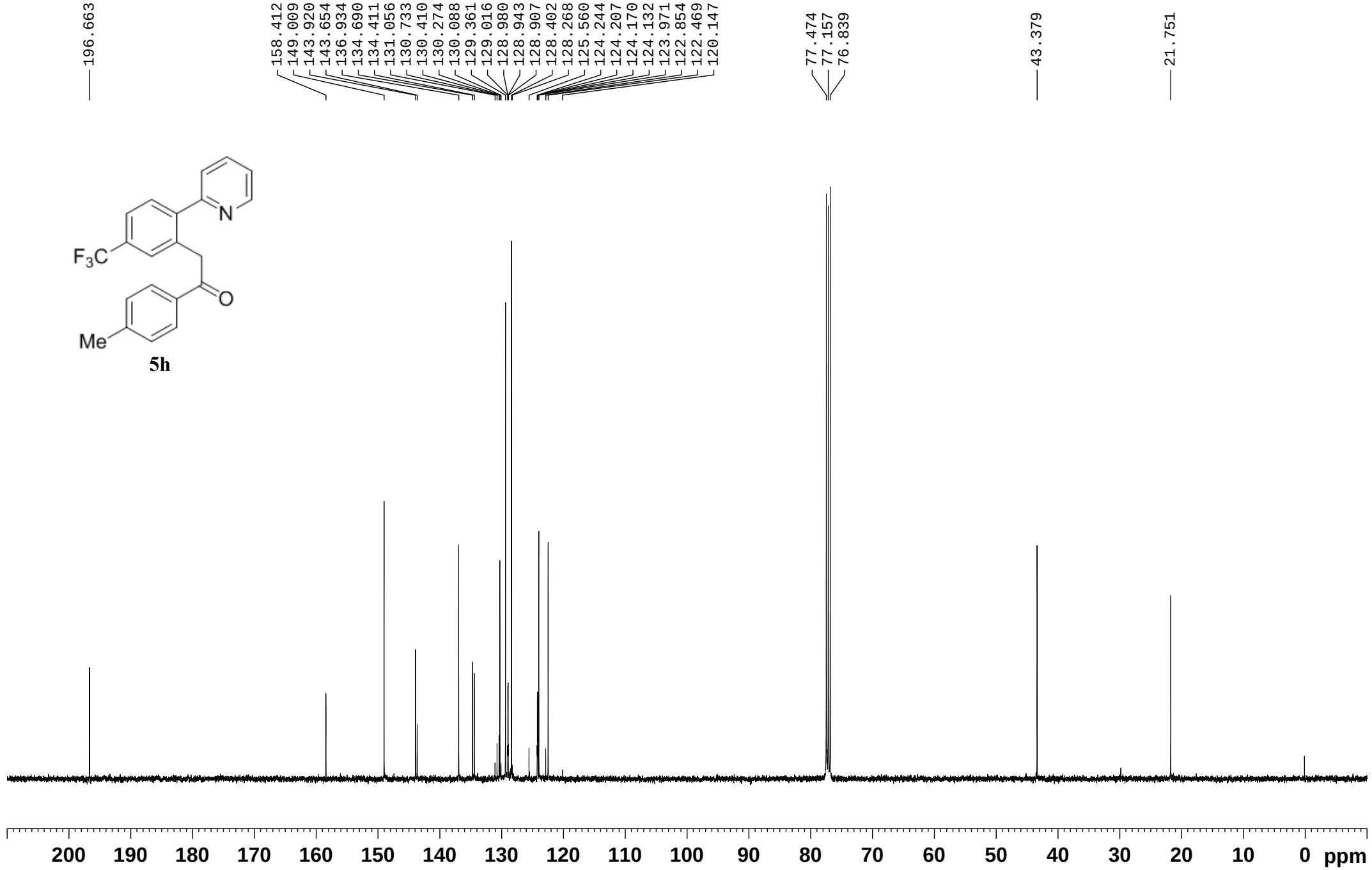
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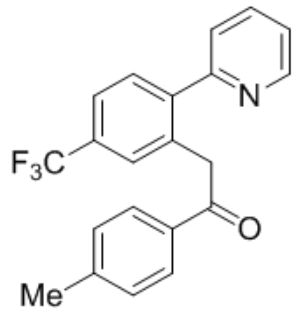
5h



5h

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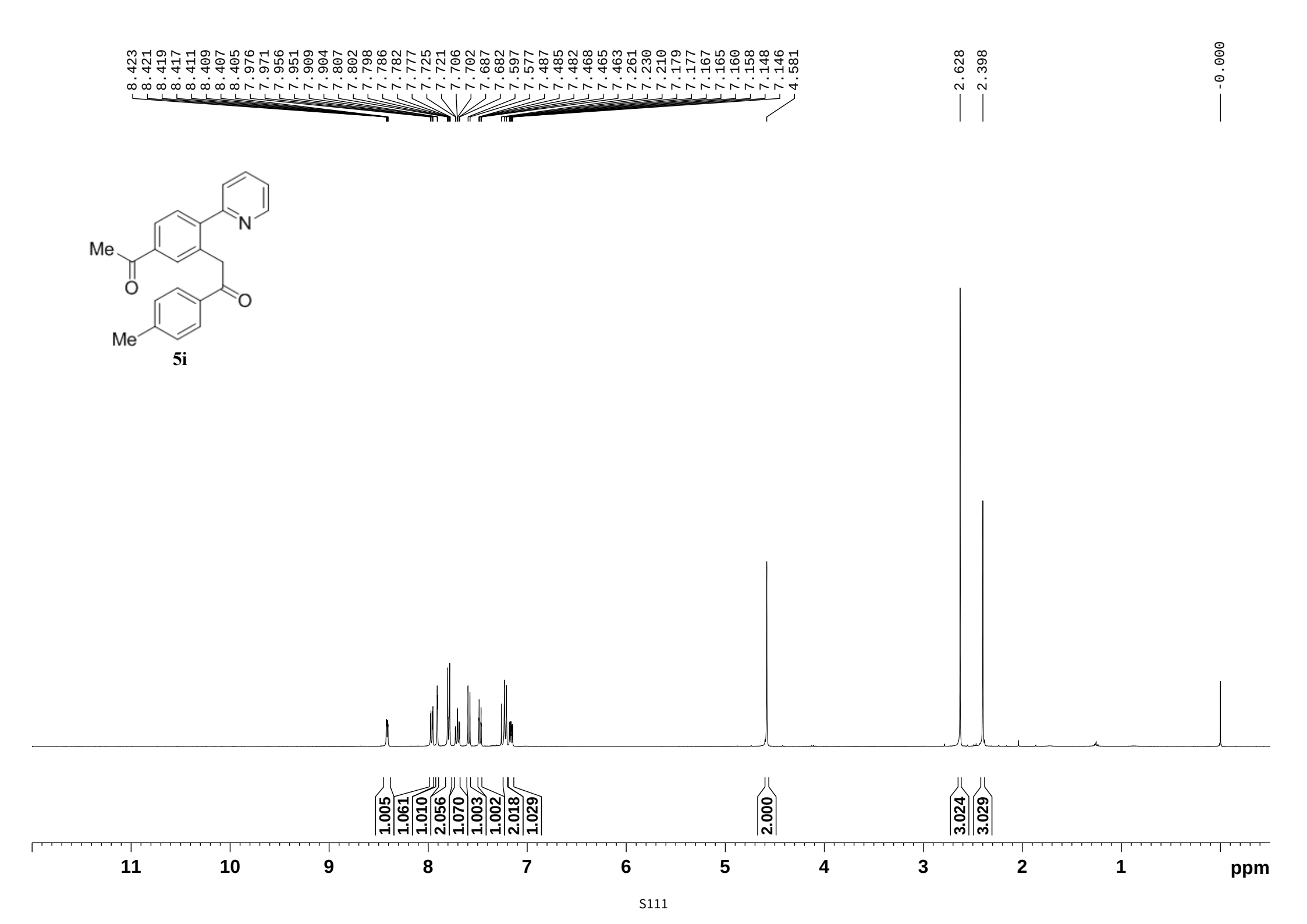
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7.148
7.146
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O
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O
Me
5i
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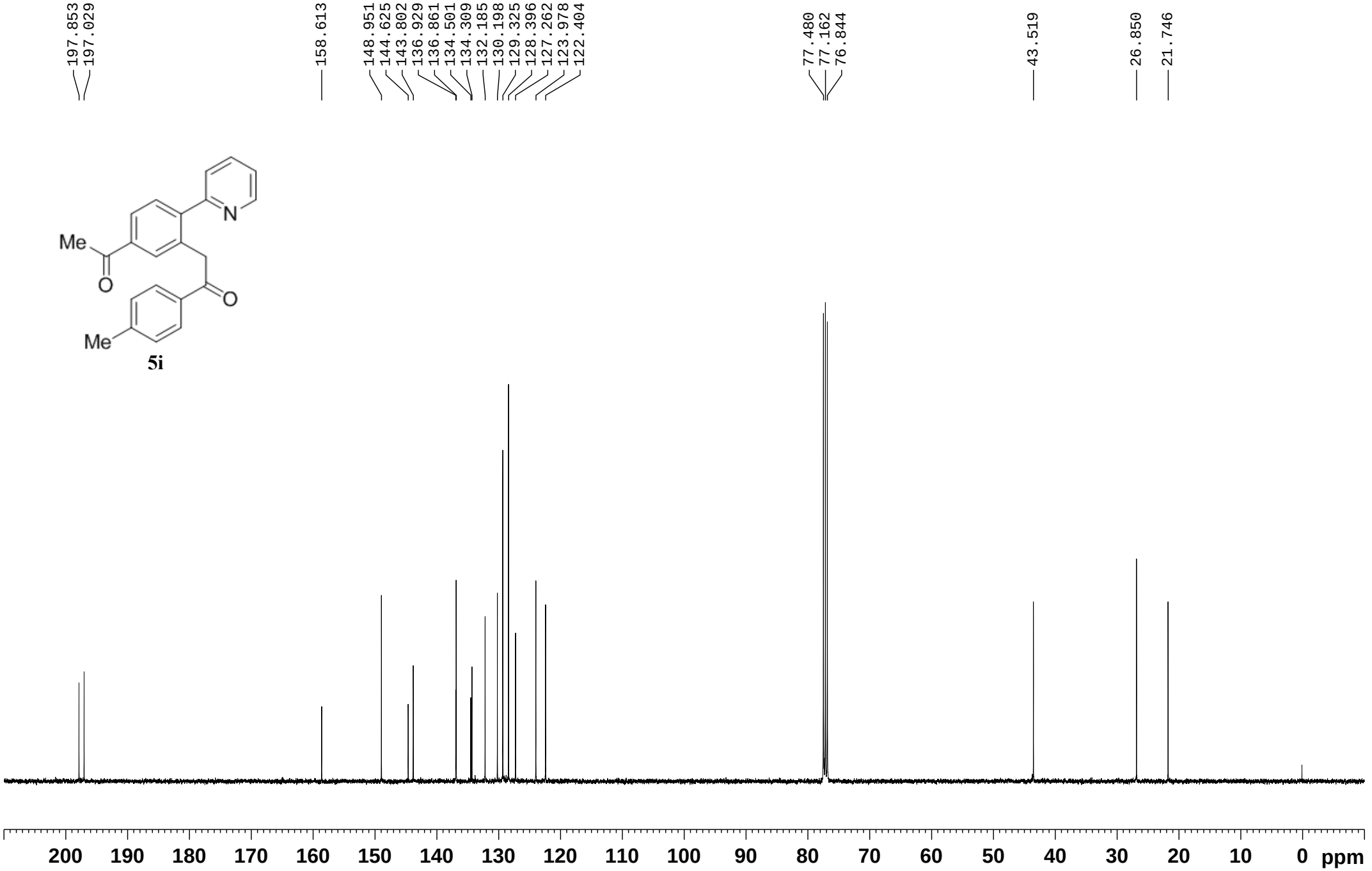
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122.404
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77.162
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Me
O
N
O
Me
200
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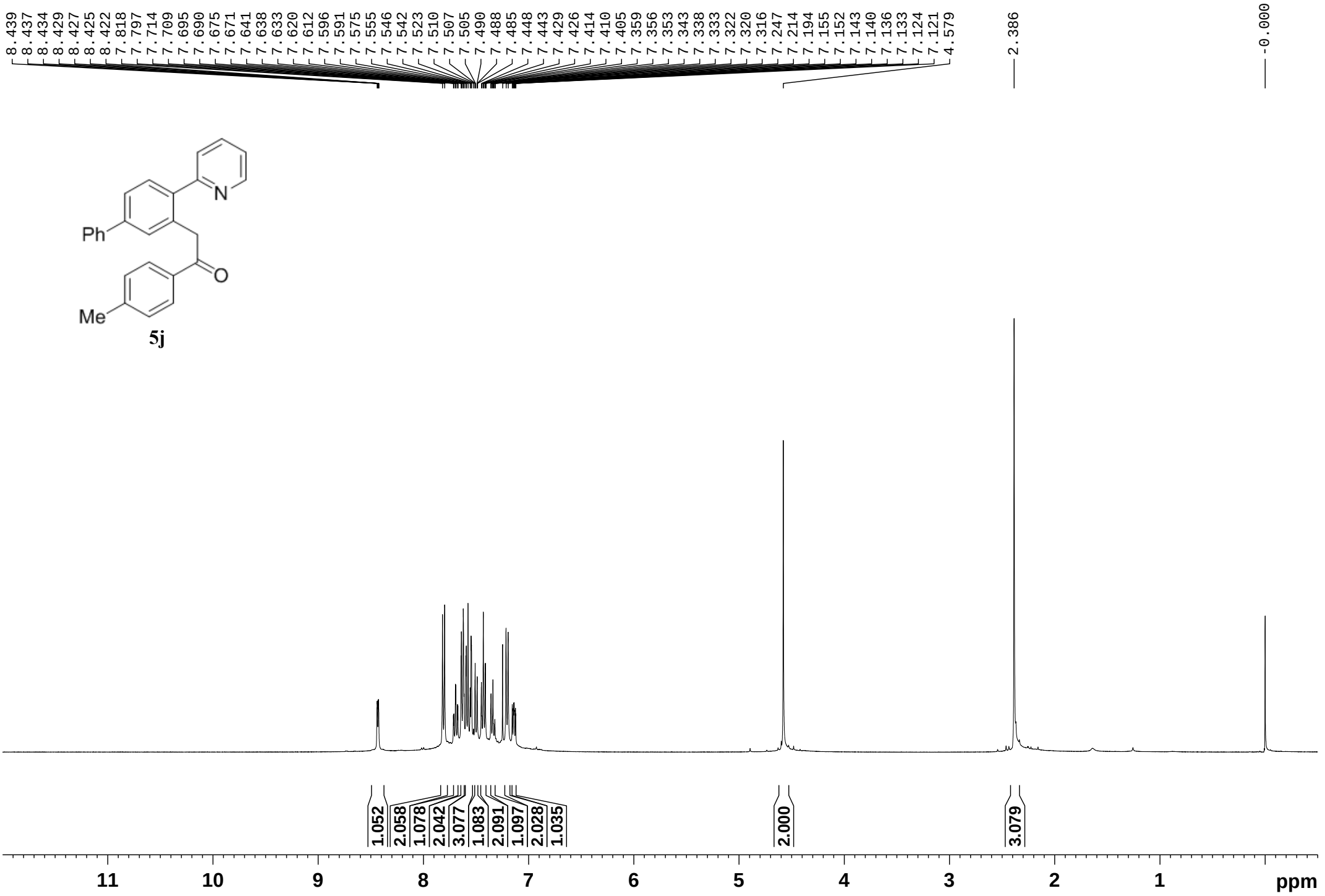
5i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Ph
O
Me
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1.078
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2
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ppm

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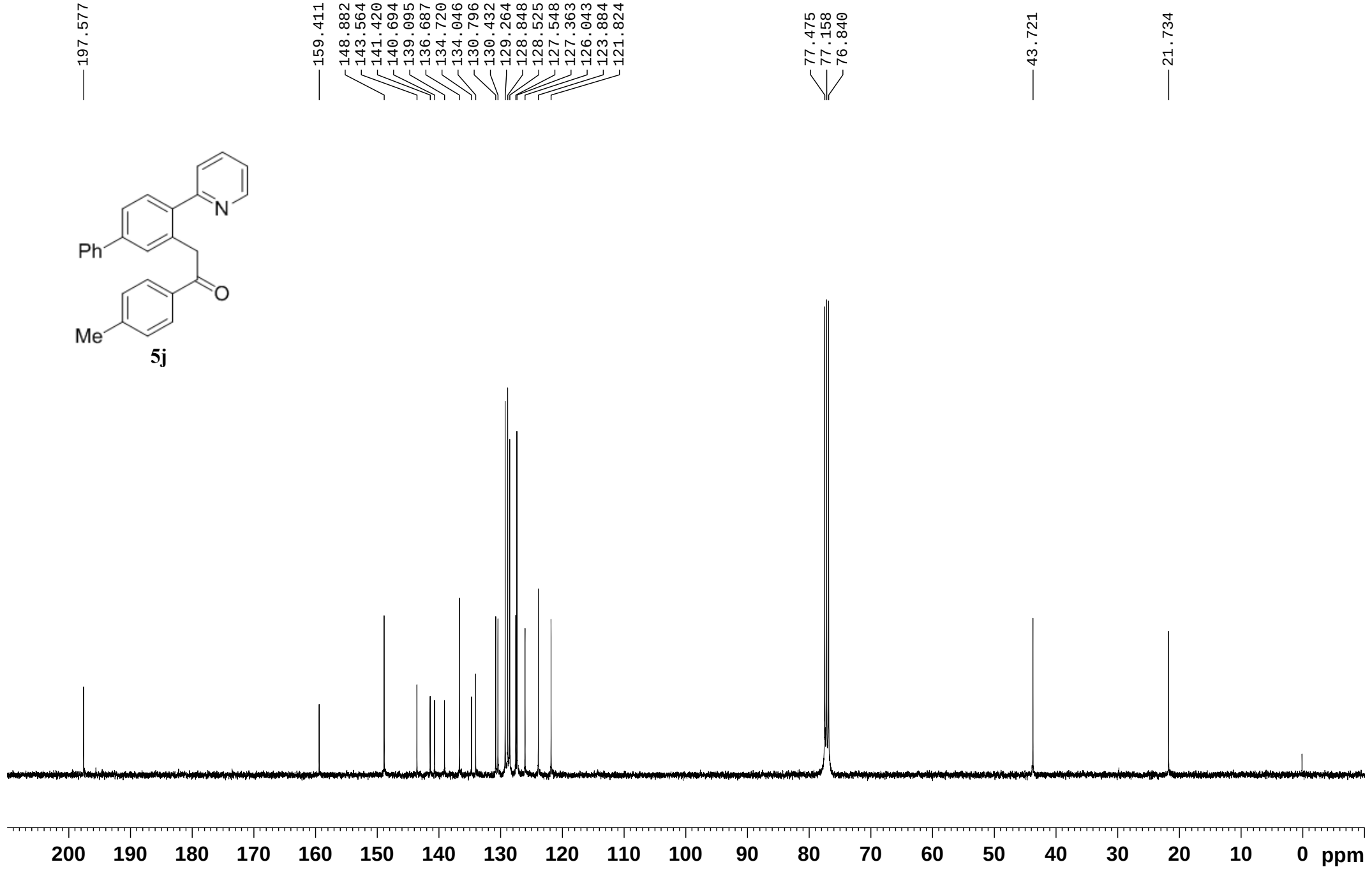
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127.363
126.043
123.884
121.824
77.475
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21.734
N
Ph
O
Me
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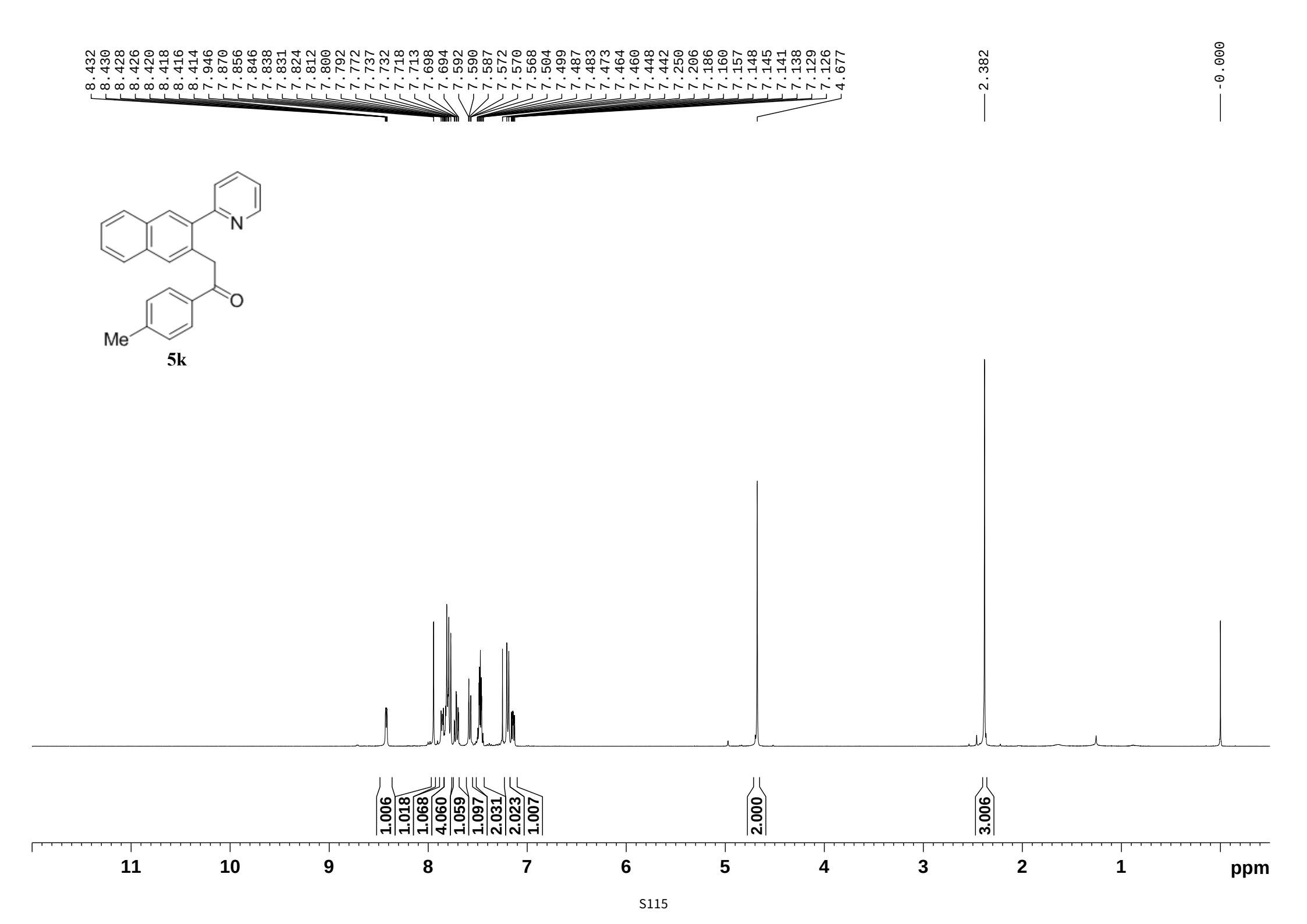
ppm

5j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7.694
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7.570
7.568
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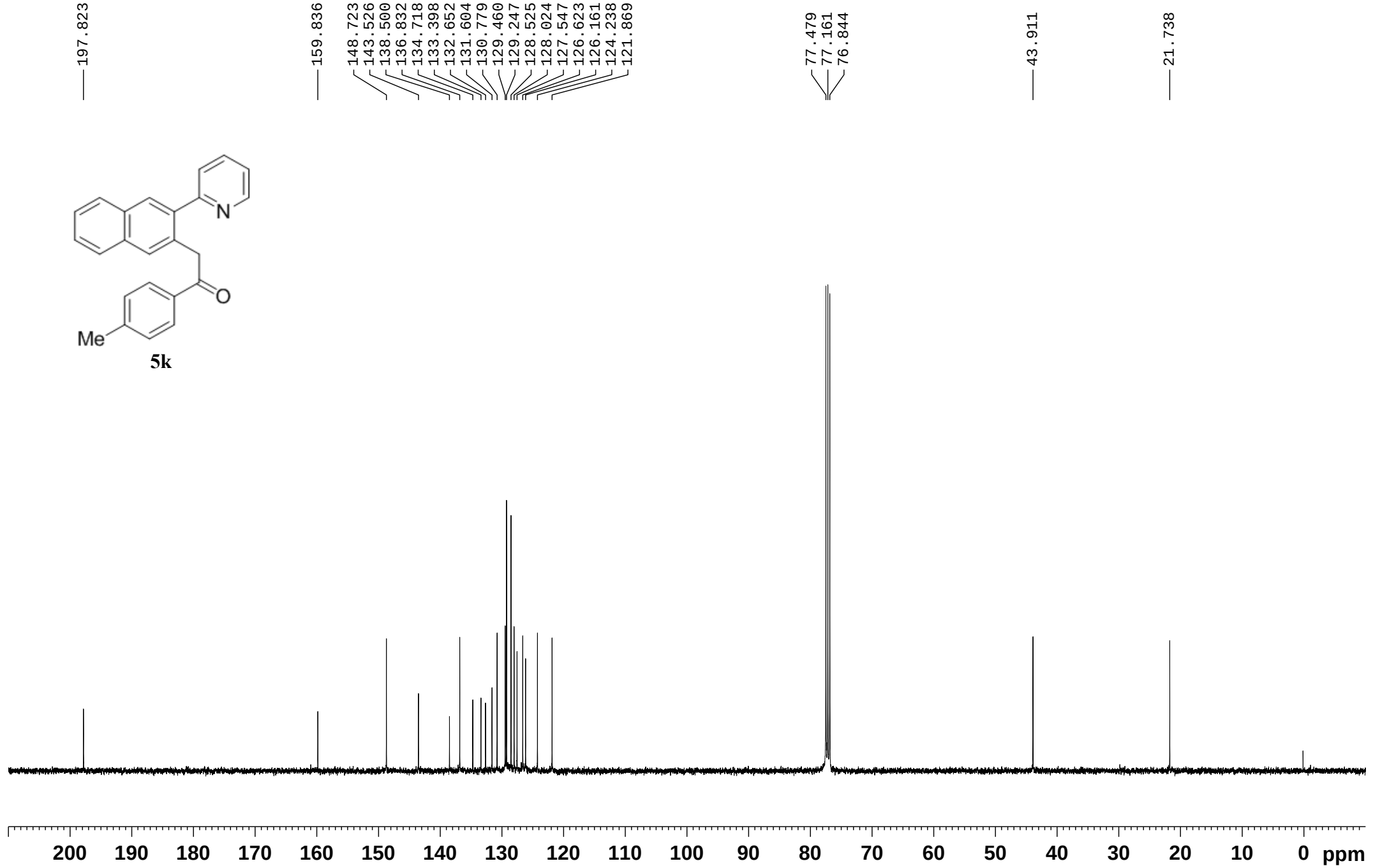
ppm

5k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77.161
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43.911
21.738
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O
Me
200
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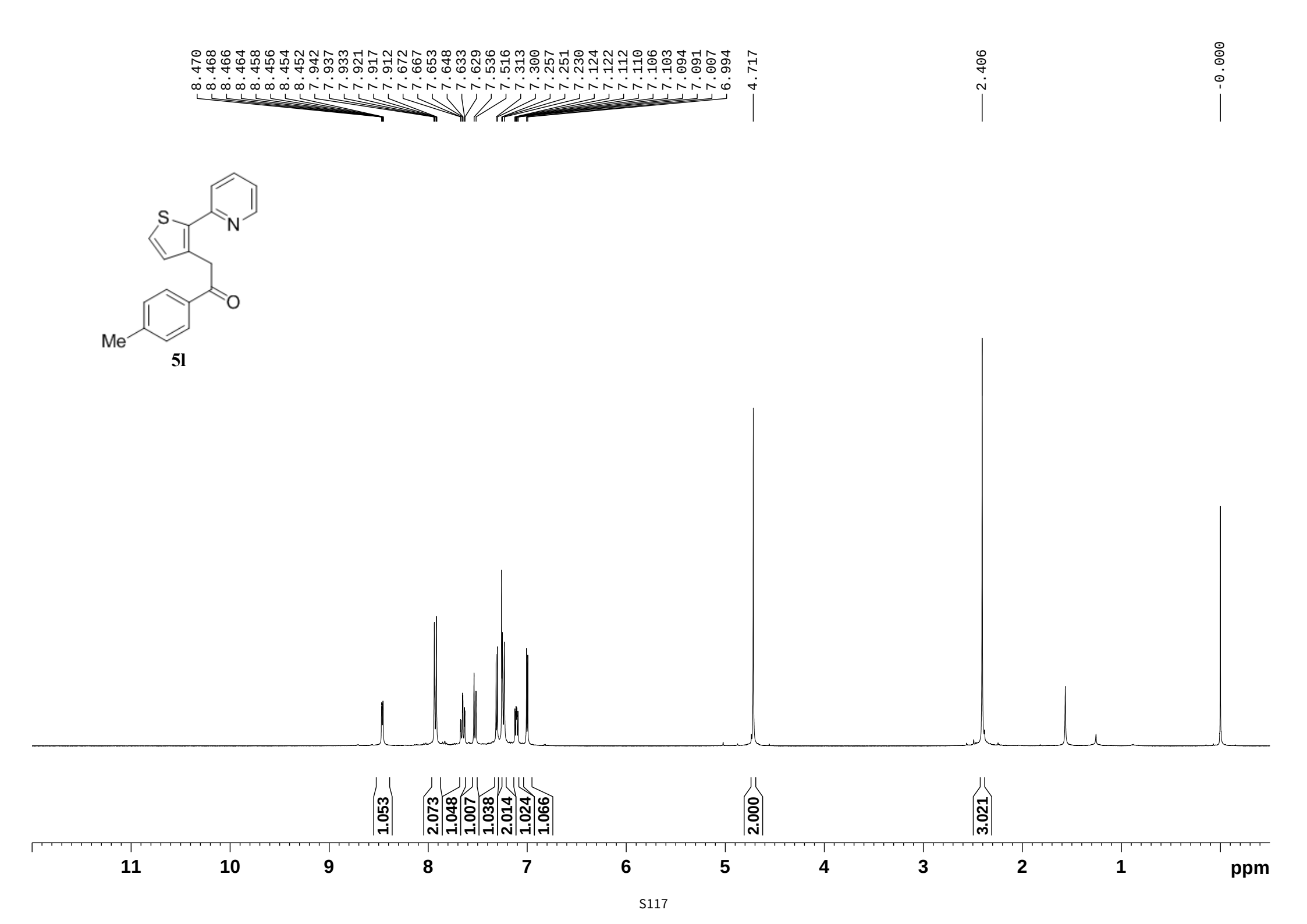
5k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7.516
7.313
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7.257
7.251
7.230
7.124
7.122
7.112
7.110
7.106
7.103
7.094
7.091
7.007
6.994
4.717
2.406
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S
N
O
Me
5l
1.053
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1.048
1.007
1.038
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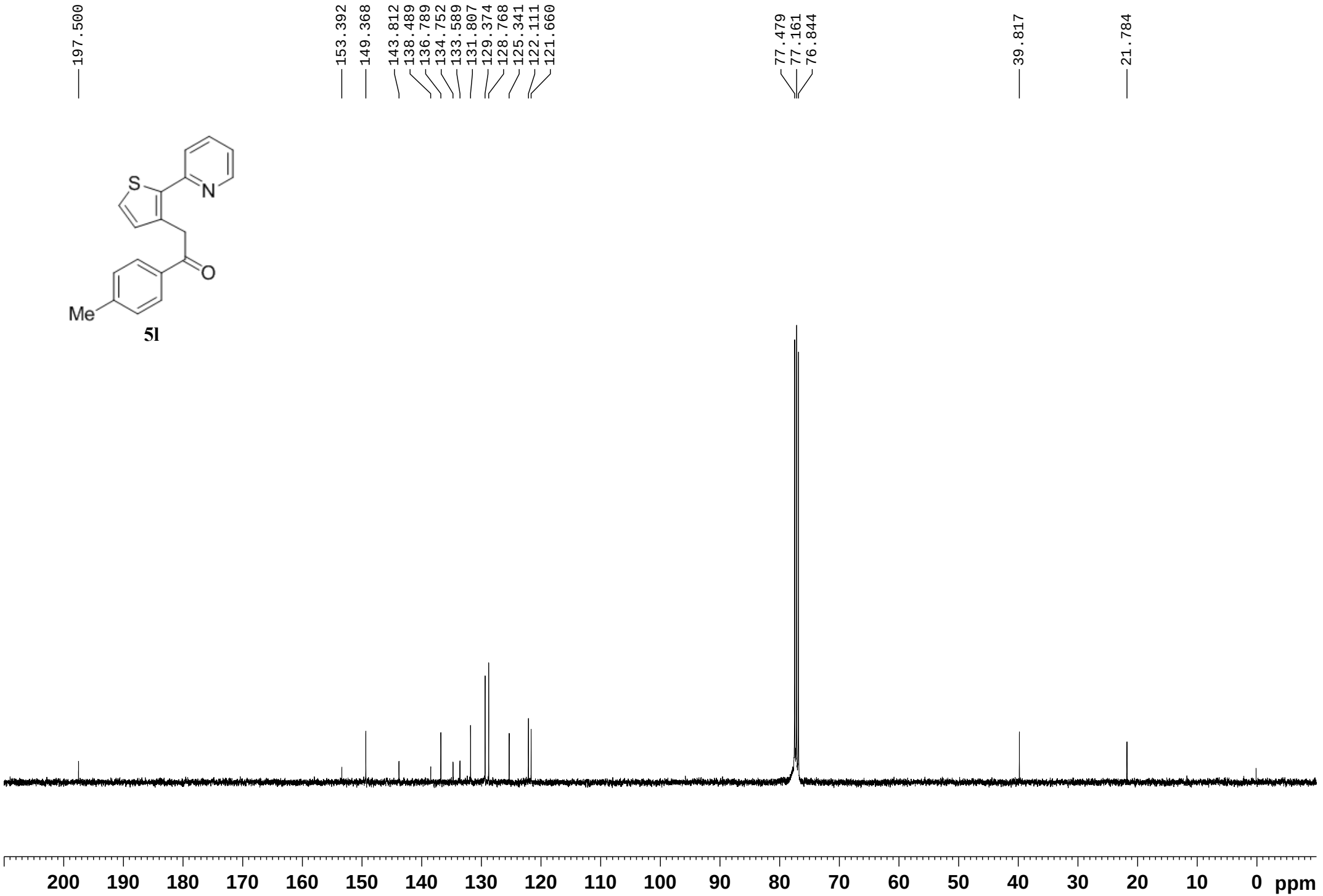
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122.111
121.660
77.479
77.161
76.844
39.817
21.784
S
N
O
Me
200
190
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150
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120
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100
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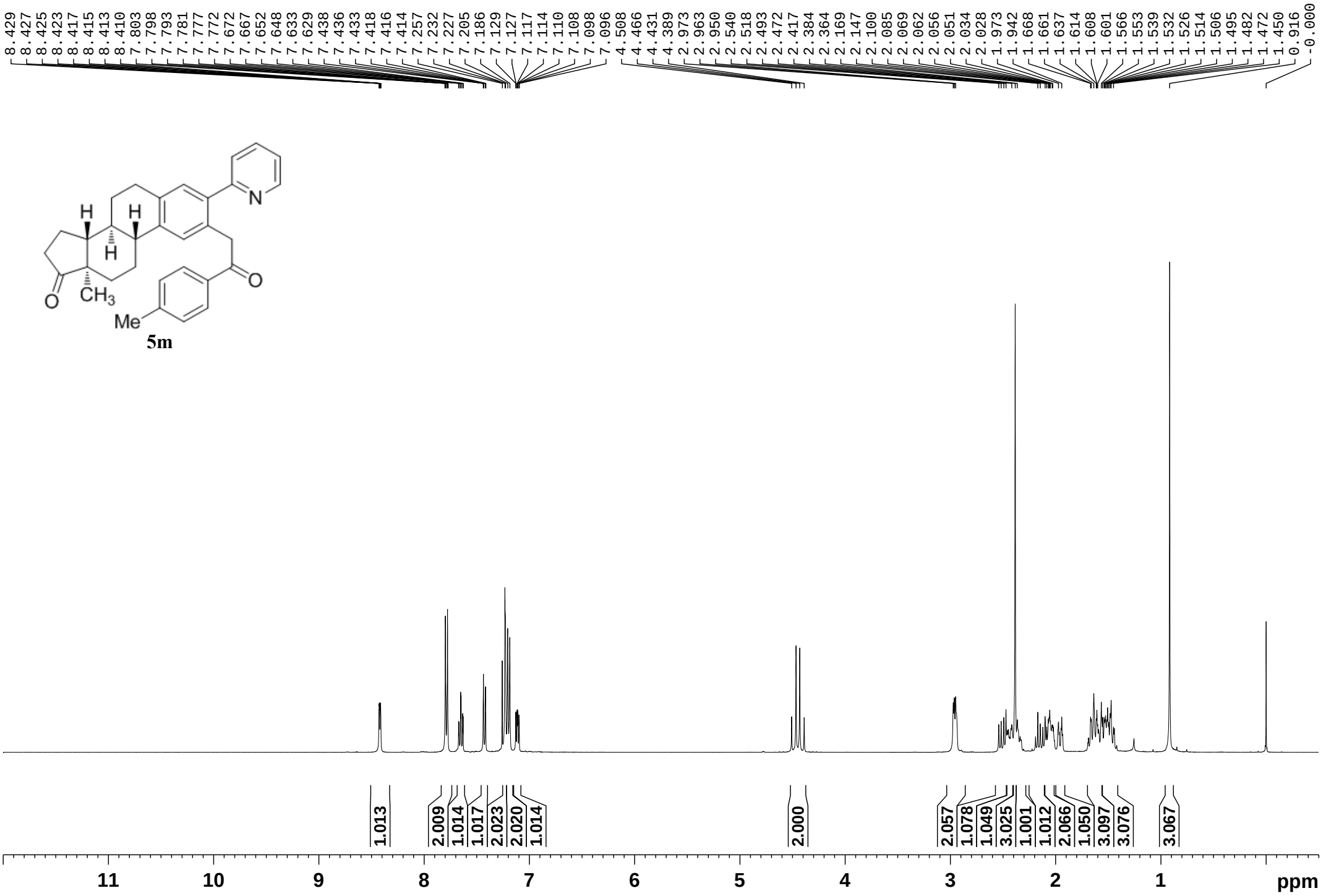
10
0
ppm

5l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7.777
7.772
7.672
7.667
7.652
7.648
7.633
7.629
7.438
7.436
7.433
7.418
7.416
7.414
7.257
7.232
7.227
7.205
7.186
7.129
7.127
7.117
7.114
7.110
7.108
7.098
7.096
4.508
4.466
4.431
4.389
2.973
2.963
2.950
2.540
2.518
2.493
2.472
2.417
2.384
2.364
2.169
2.147
2.100
2.085
2.069
2.062
2.056
2.051
2.034
2.028
1.973
1.942
1.668
1.661
1.637
1.614
1.608
1.601
1.566
1.553
1.539
1.532
1.526
1.514
1.506
1.495
1.482
1.472
1.450
0.916
-0.000
H
H
H
N
O
O
CH3
Me
5m
1.013
2.009
1.014
1.017
2.023
2.020
1.014
2.000
2.057
1.078
1.049
3.025
1.001
1.012
2.066
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3.076
3.067
11
10
9
8
7
6
5
4
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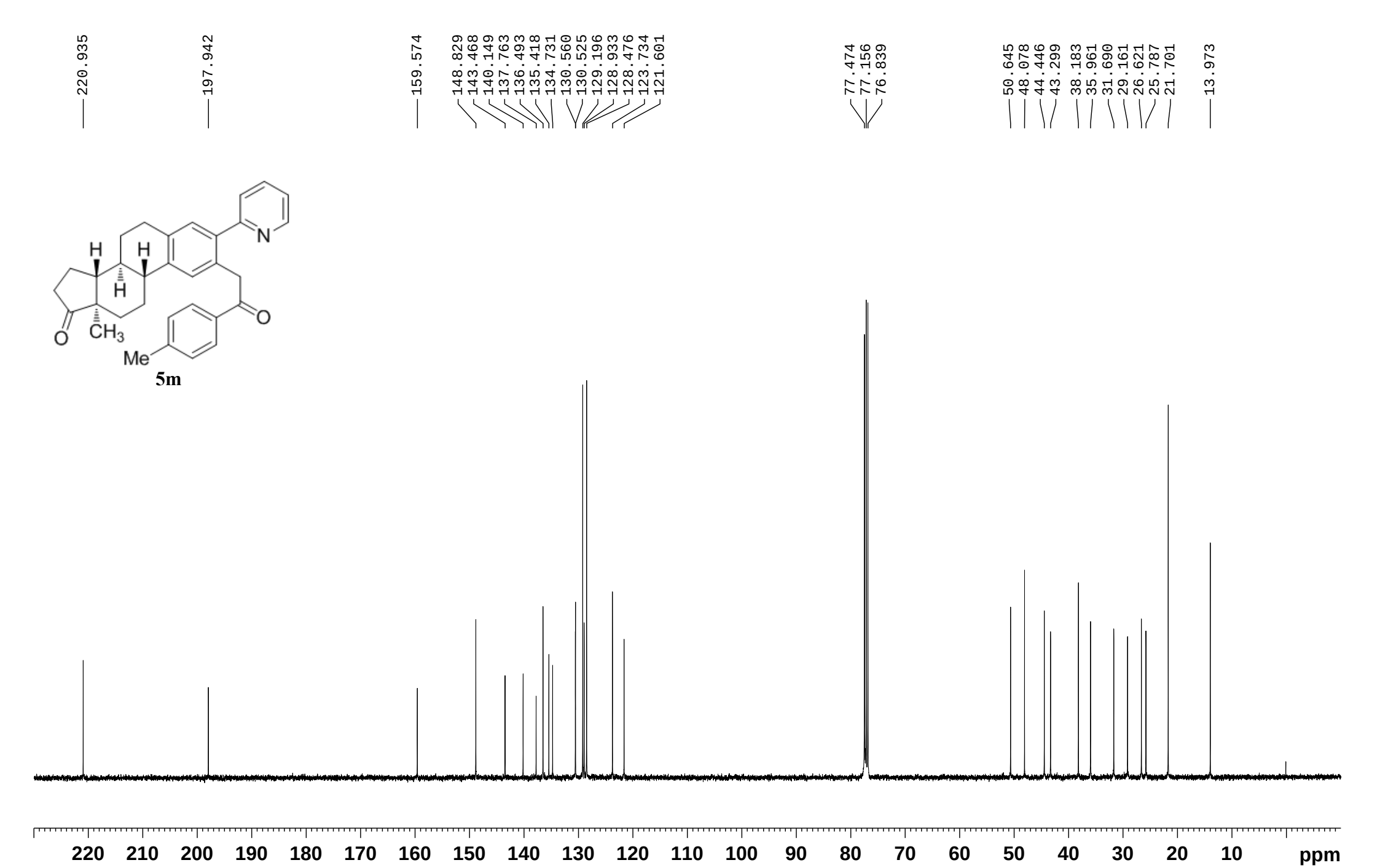
2
1
ppm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136.493
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130.525
129.196
128.933
128.476
123.734
121.601
77.474
77.156
76.839
50.645
48.078
44.446
43.299
38.183
35.961
31.690
29.161
26.621
25.787
21.701
13.973
H
H
H
N
O
O
CH3
Me
220
210
200
190
180
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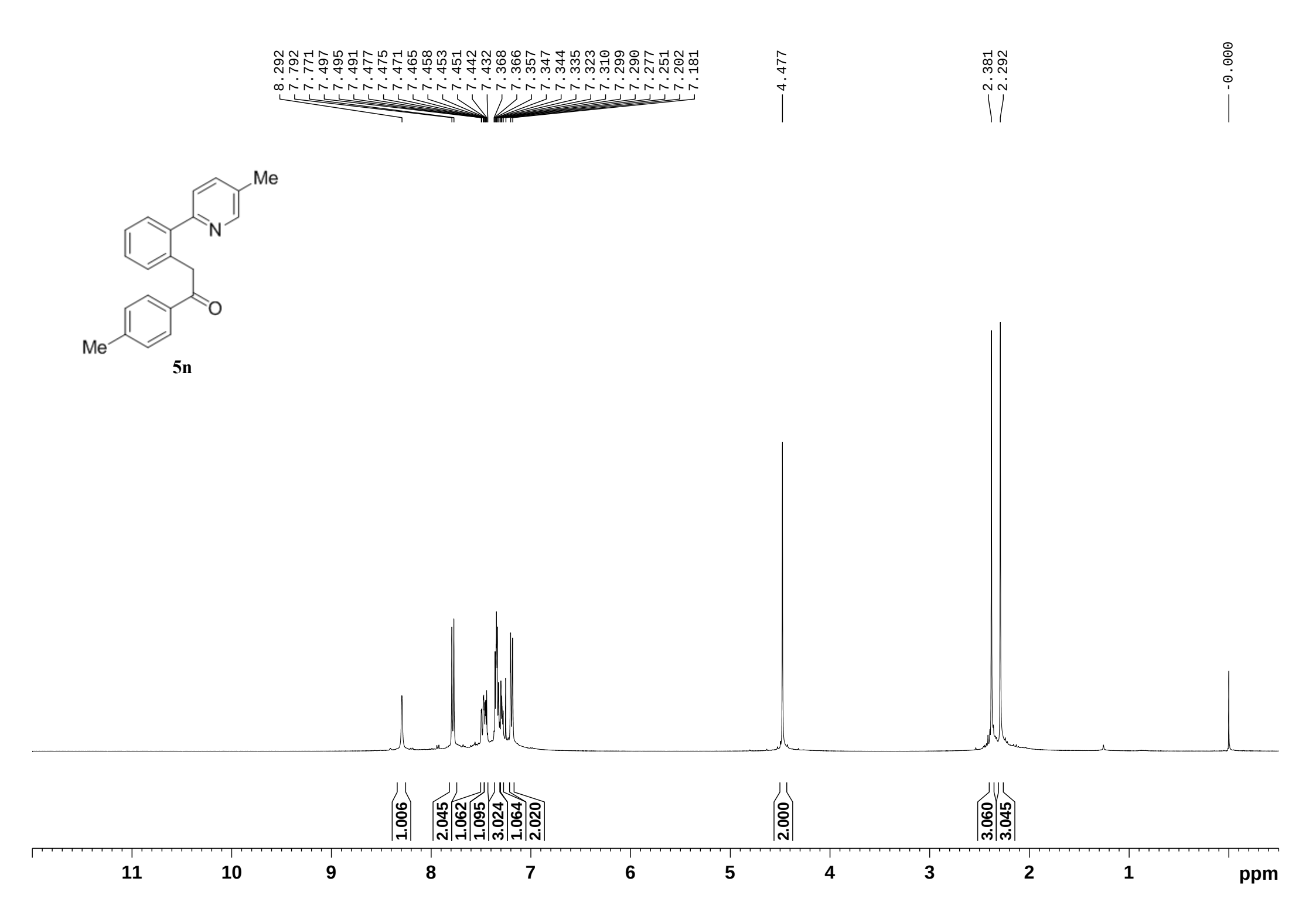
120
110
100
90
80
70
60
50
40
30
20
10
ppm

5m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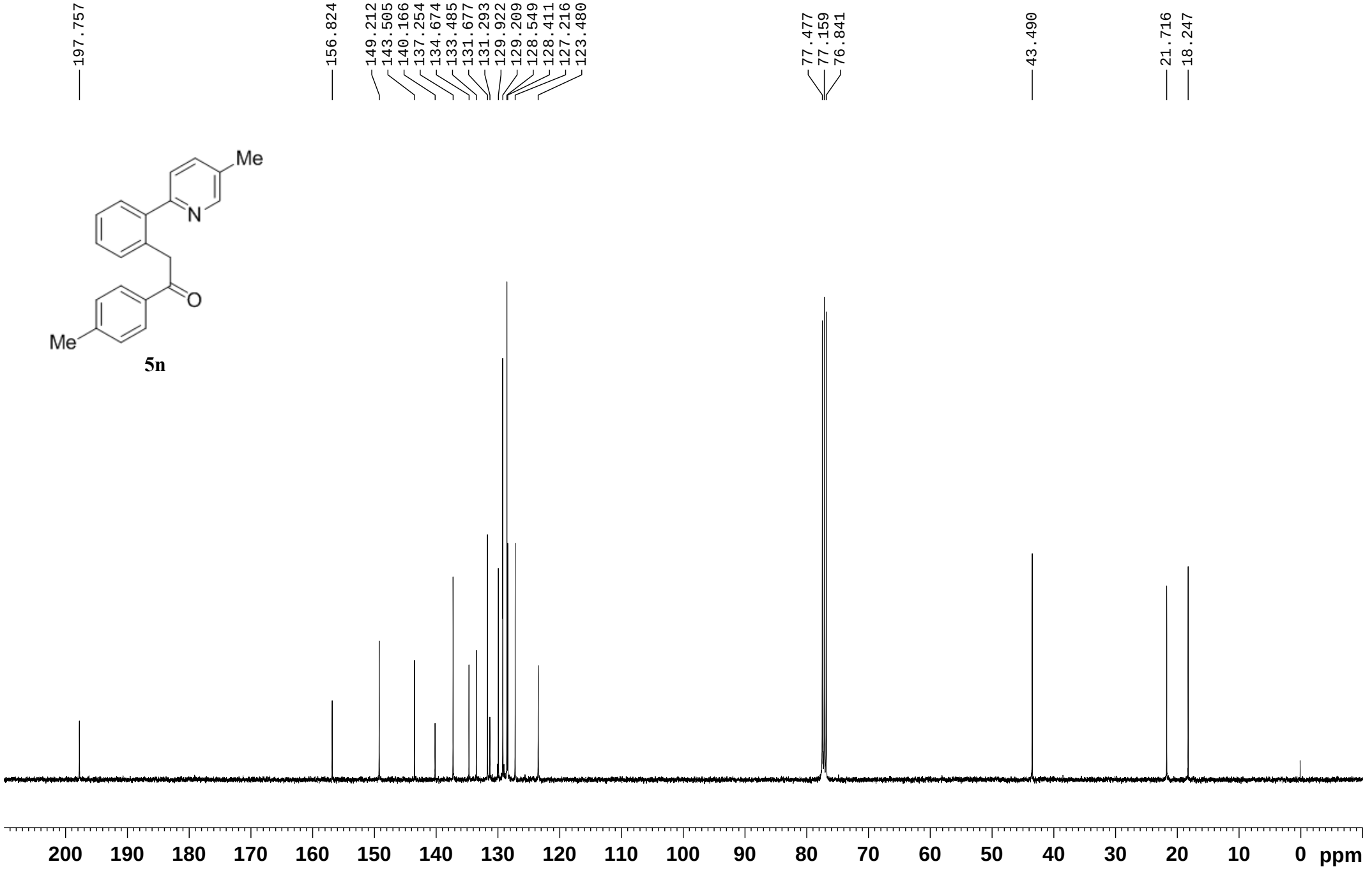
7.792
7.771
7.497
7.495
7.491
7.477
7.475
7.471
7.465
7.458
7.453
7.451
7.442
7.432
7.368
7.366
7.357
7.347
7.344
7.335
7.323
7.310
7.299
7.290
7.277
7.251
7.202
7.181
4.477
2.381
2.292
-0.000
Me
N
O
Me
1.006
2.045
1.062
1.095
3.024
1.064
2.020
2.000
3.060
3.045
11
10
9
8
7
6
5
4
3
2
1
ppm

5n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140.166
137.254
134.674
133.485
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131.293
129.922
129.209
128.549
128.411
127.216
123.480
77.477
77.159
76.841
43.490
21.716
18.247
Me
N
O
Me
200
190
180
170
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150
140
130
120
110
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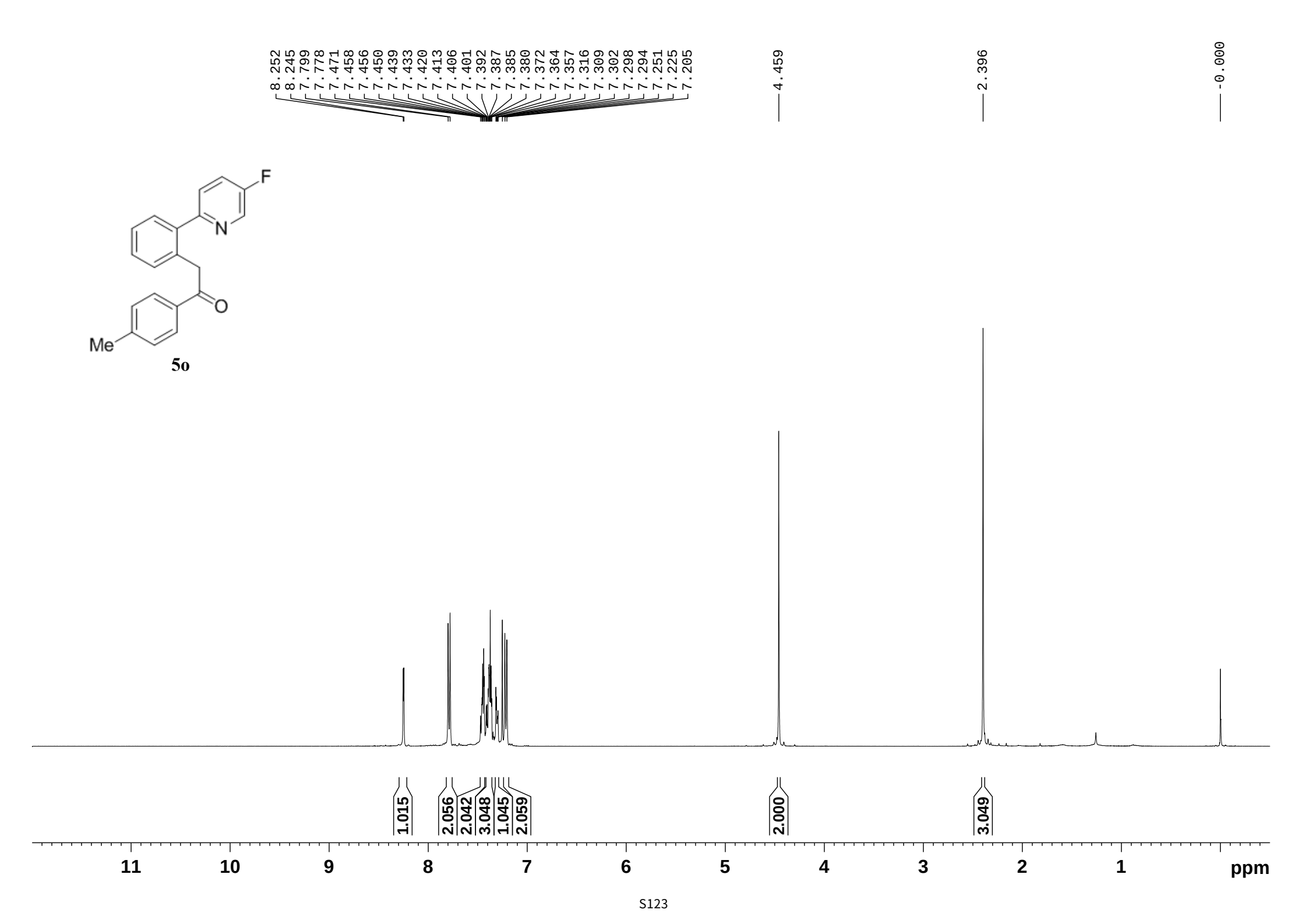
90
80
70
60
50
40
30
20
10
0
ppm

5n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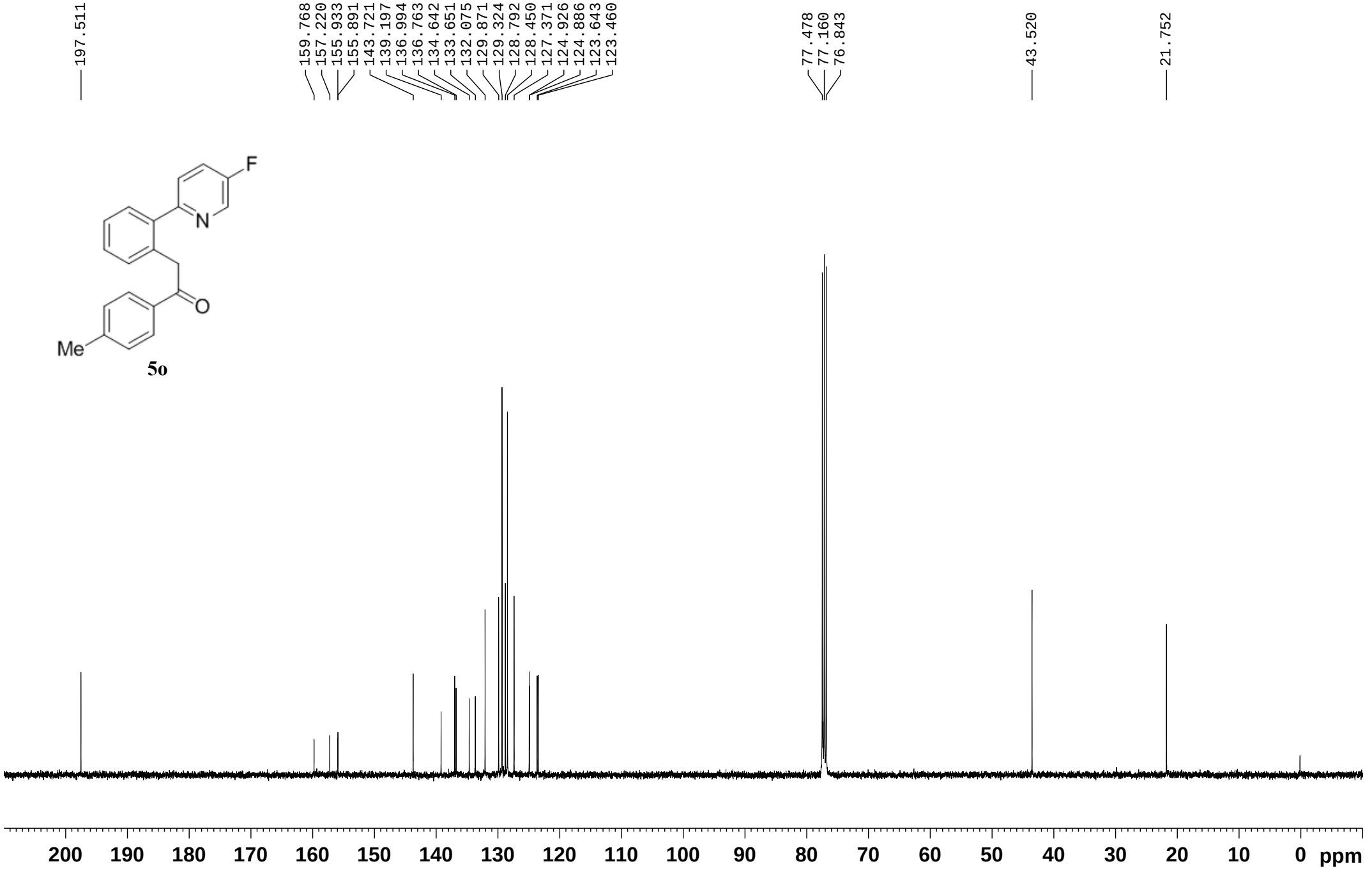
7.799
7.778
7.471
7.458
7.456
7.450
7.439
7.433
7.420
7.413
7.406
7.401
7.392
7.387
7.385
7.380
7.372
7.364
7.357
7.316
7.309
7.302
7.298
7.294
7.251
7.225
7.205
4.459
2.396
-0.000
F
N
O
Me
1.015
2.056
2.042
3.048
1.045
2.059
2.000
3.049
11
10
9
8
7
6
5
4
3
2
1
ppm

5o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155.933
155.891
143.721
139.197
136.994
136.763
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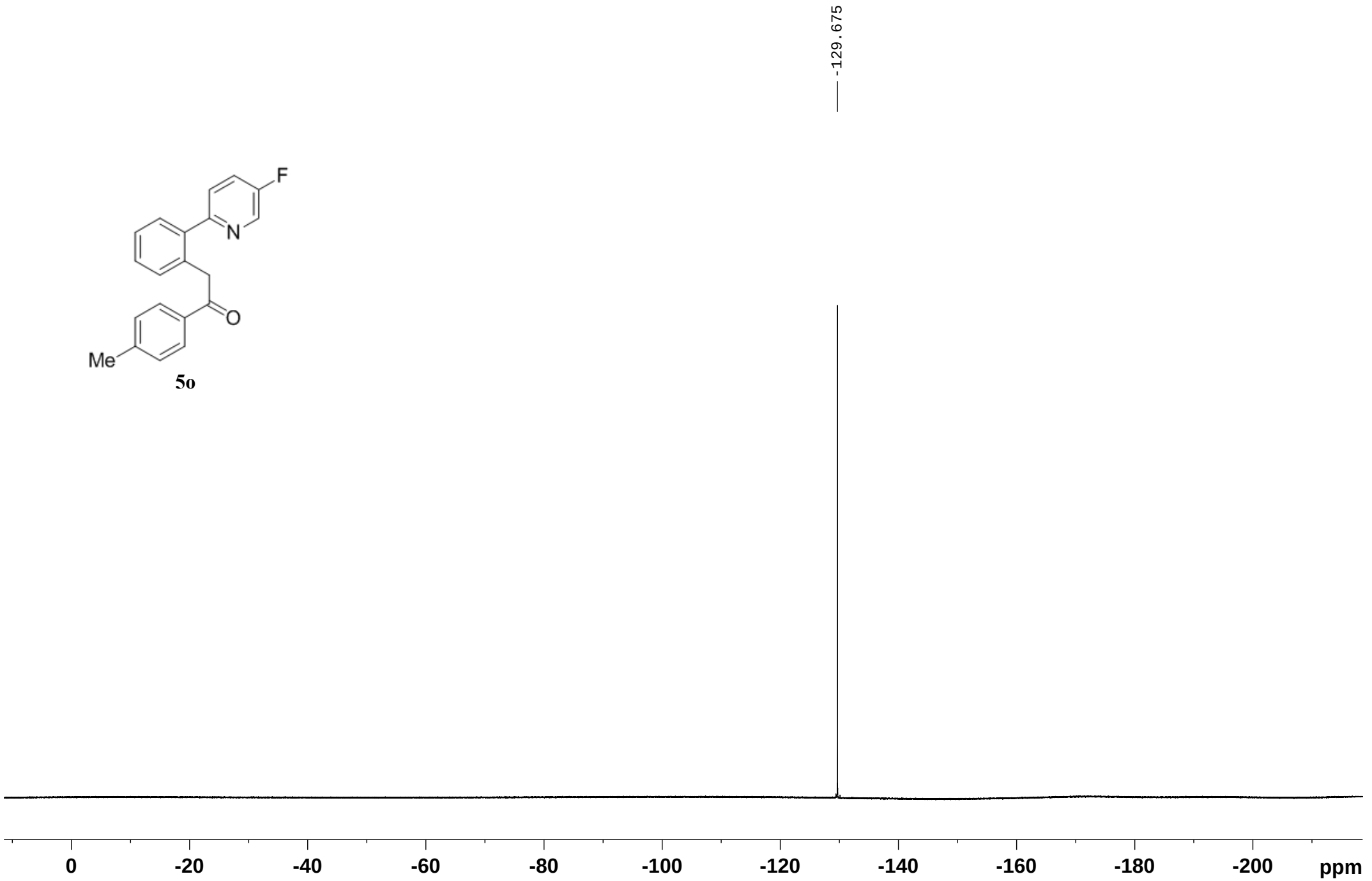
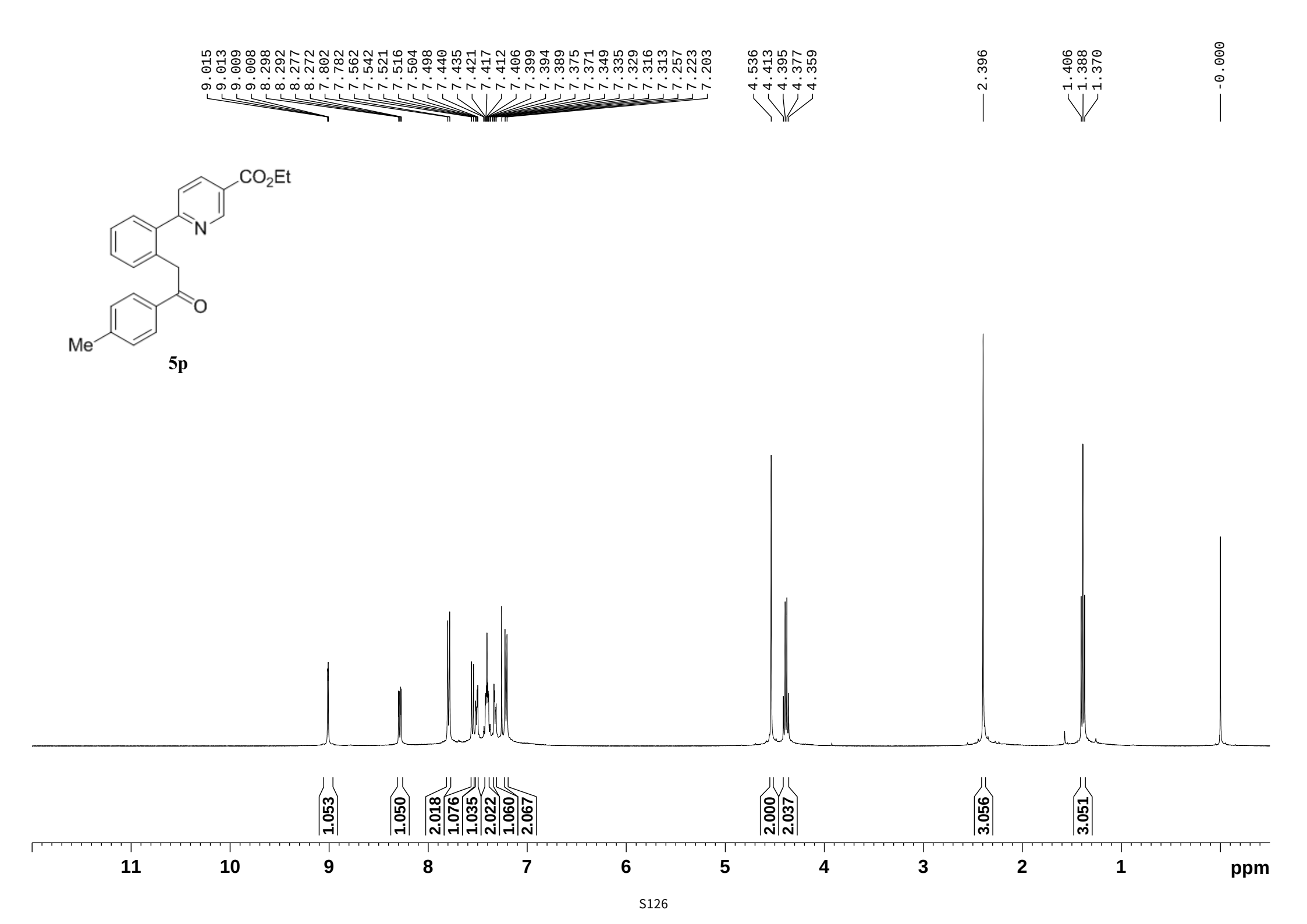
133.651
132.075
129.871
129.324
128.792
128.450
127.371
124.926
124.886
123.643
123.460
77.478
77.160
76.843
43.520
21.752
F
N
O
Me
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

5o

5o

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9.008
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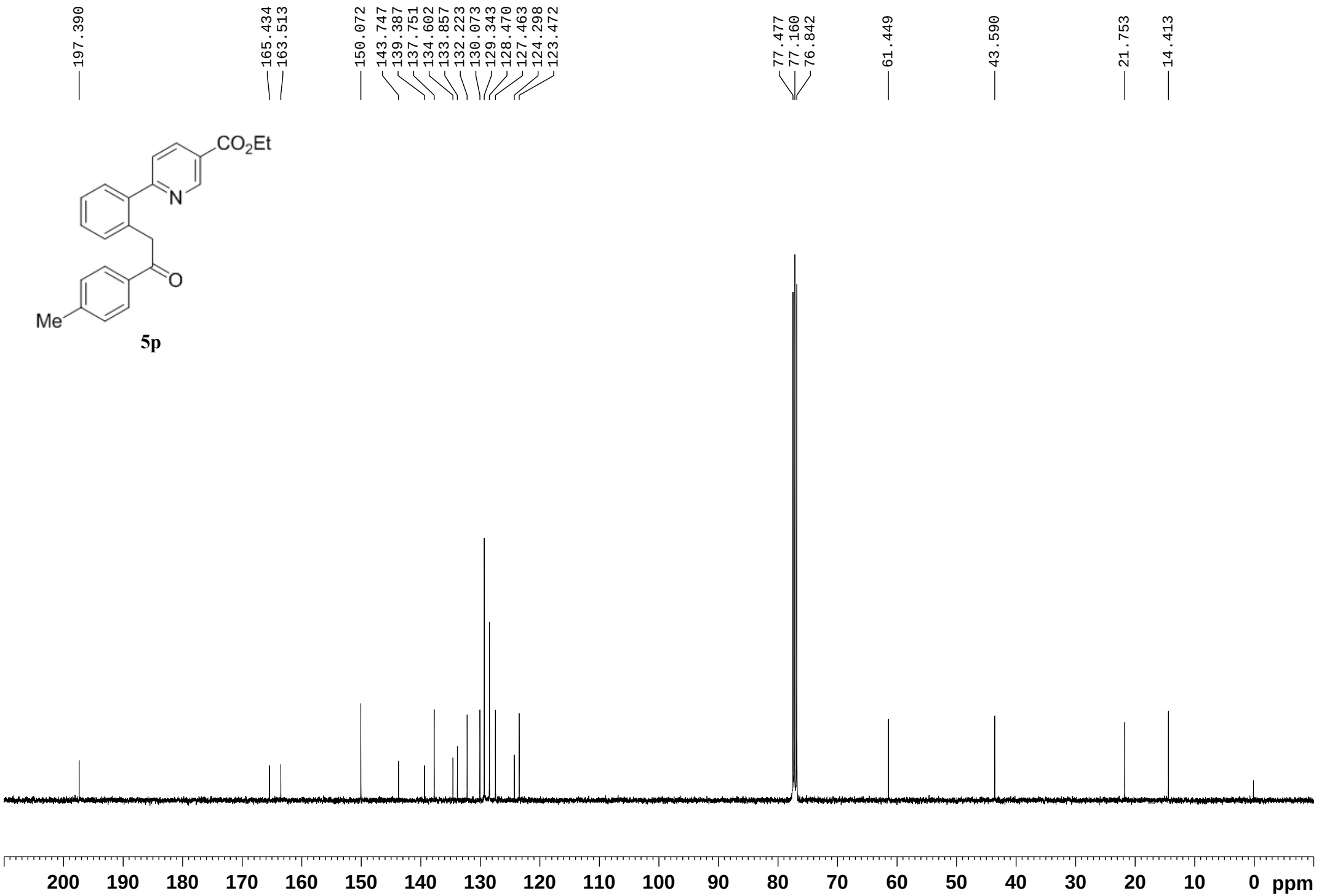
8.292
8.277
8.272
7.802
7.782
7.562
7.542
7.521
7.516
7.504
7.498
7.440
7.435
7.421
7.417
7.412
7.406
7.399
7.394
7.389
7.375
7.371
7.349
7.335
7.329
7.316
7.313
7.257
7.223
7.203
4.536
4.413
4.395
4.377
4.359
2.396
1.406
1.388
1.370
-0.000
CO2Et
N
O
Me
1.053
1.050
2.018
1.076
1.035
2.022
1.060
2.067
2.000
2.037
3.056
3.051
11
10
9
8
7
6
5
4
3
2
1
ppm

5p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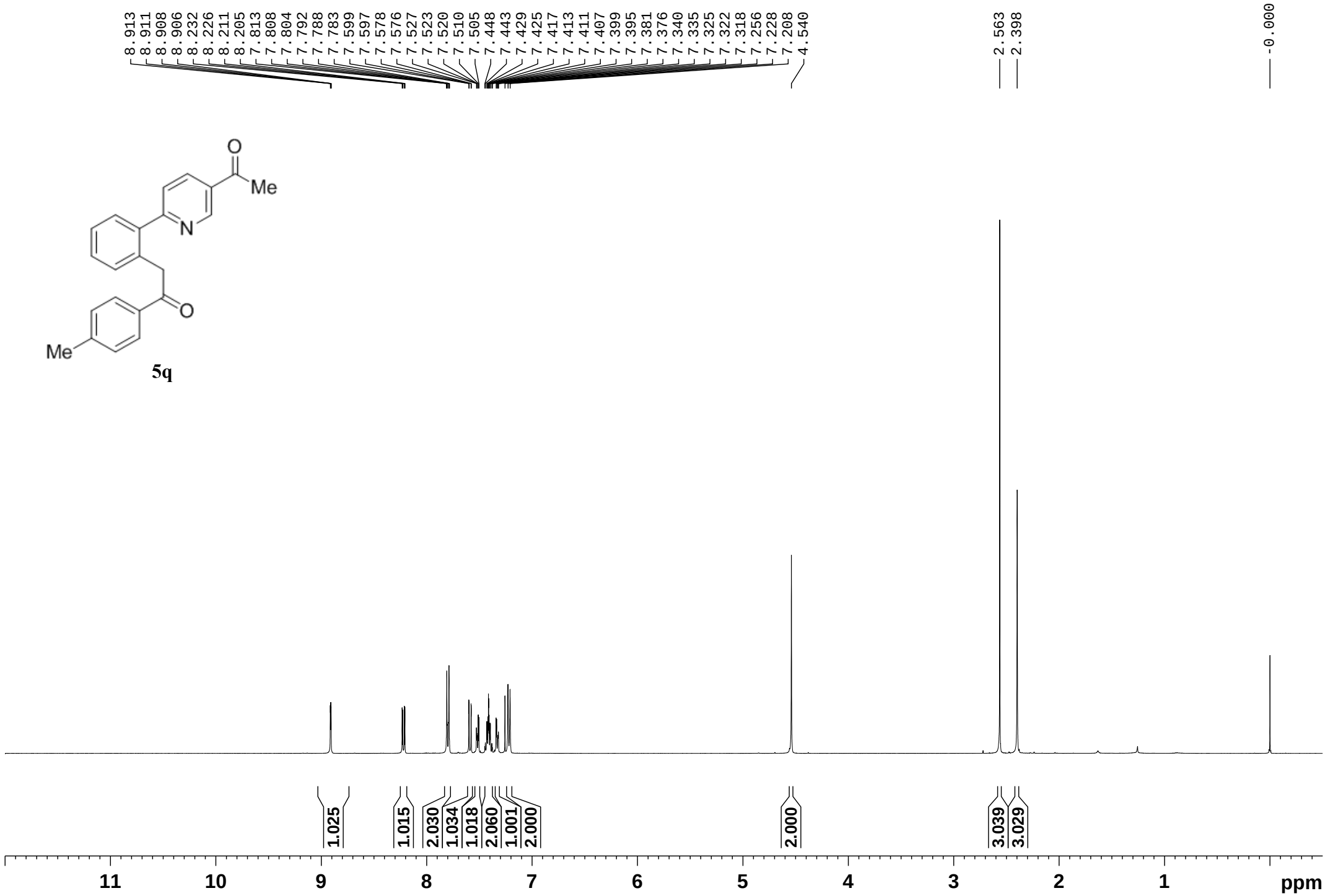
150.072
143.747
139.387
137.751
134.602
133.857
132.223
130.073
129.343
128.470
127.463
124.298
123.472
77.477
77.160
76.842
61.449
43.590
21.753
14.413
CO2Et
N
O
Me
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

5p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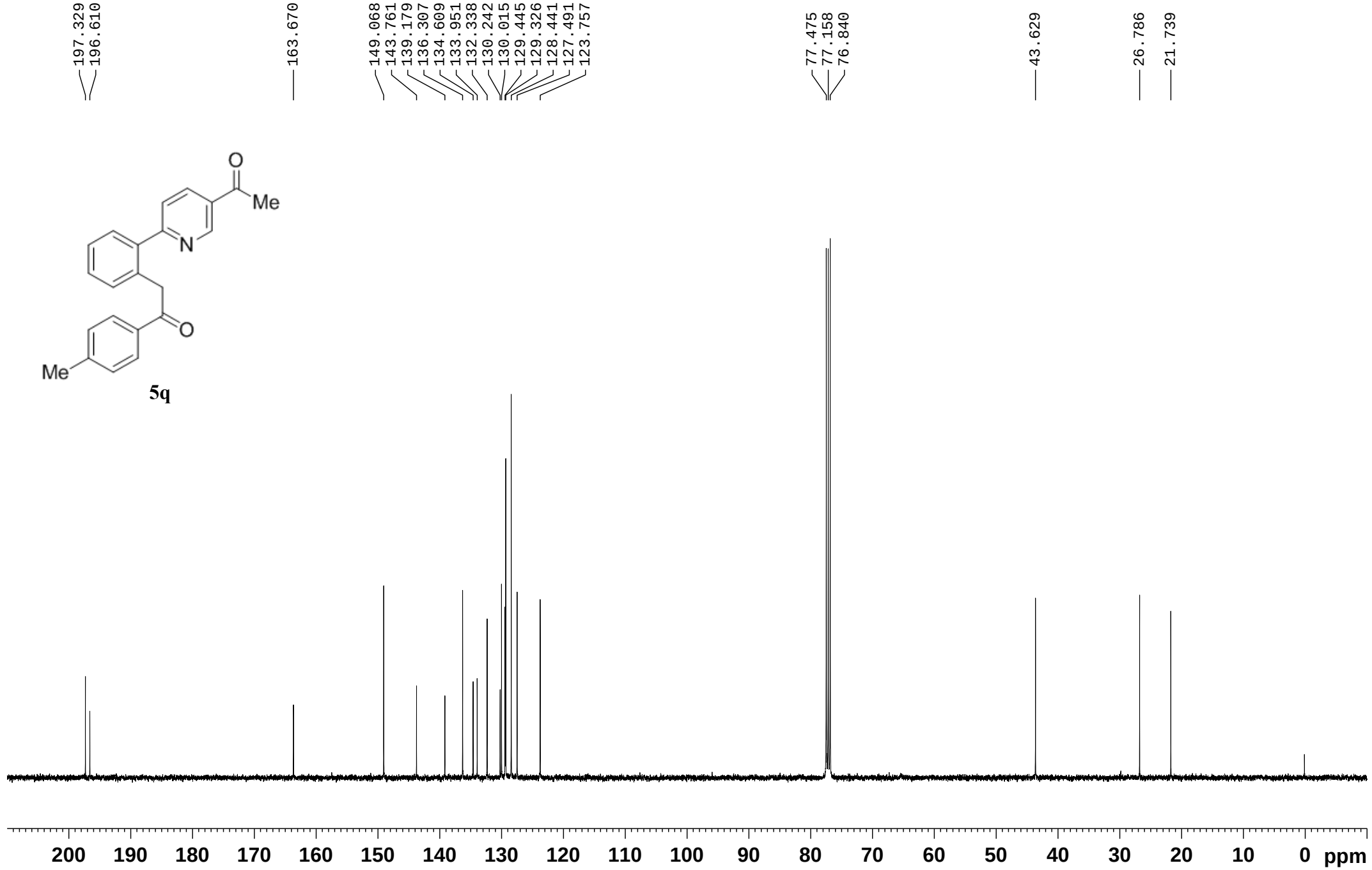
8.911
8.908
8.906
8.232
8.226
8.211
8.205
7.813
7.808
7.804
7.792
7.788
7.783
7.599
7.597
7.578
7.576
7.527
7.523
7.520
7.510
7.505
7.448
7.443
7.429
7.425
7.417
7.413
7.411
7.407
7.399
7.395
7.381
7.376
7.340
7.335
7.325
7.322
7.318
7.256
7.228
7.208
4.540
2.563
2.398
-0.000
O
Me
N
O
Me
1.025
1.015
2.030
1.034
1.018
2.060
1.001
2.000
2.000
3.039
3.029
11
10
9
8
7
6
5
4
3
2
1
ppm

5q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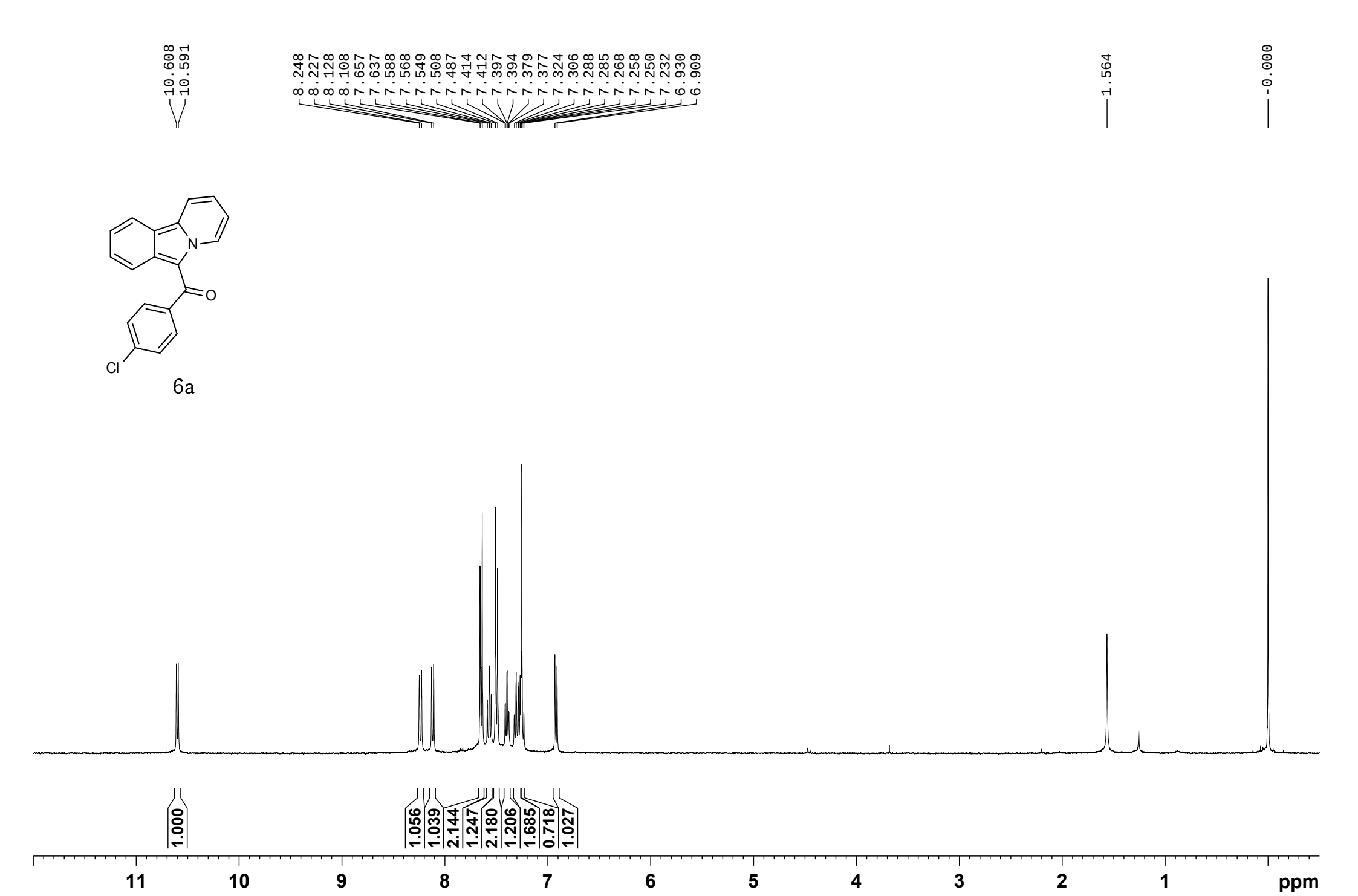
163.670
149.068
143.761
139.179
136.307
134.609
133.951
132.338
130.242
130.015
129.445
129.326
128.441
127.491
123.757
77.475
77.158
76.840
43.629
26.786
21.739
O
Me
N
O
Me
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

5q


10.608
10.591
8.248
8.227
8.128
8.108
7.657
7.637
7.588
7.568
7.549
7.508
7.487
7.414
7.412
7.397
7.394
7.379
7.377
7.324
7.306
7.288
7.285
7.268
7.258
7.250
7.232
6.930
6.909
1.564
-0.000
N
O
Cl
6a
1.000
1.056
1.039
2.144
1.247
2.180
1.206
1.685
0.718
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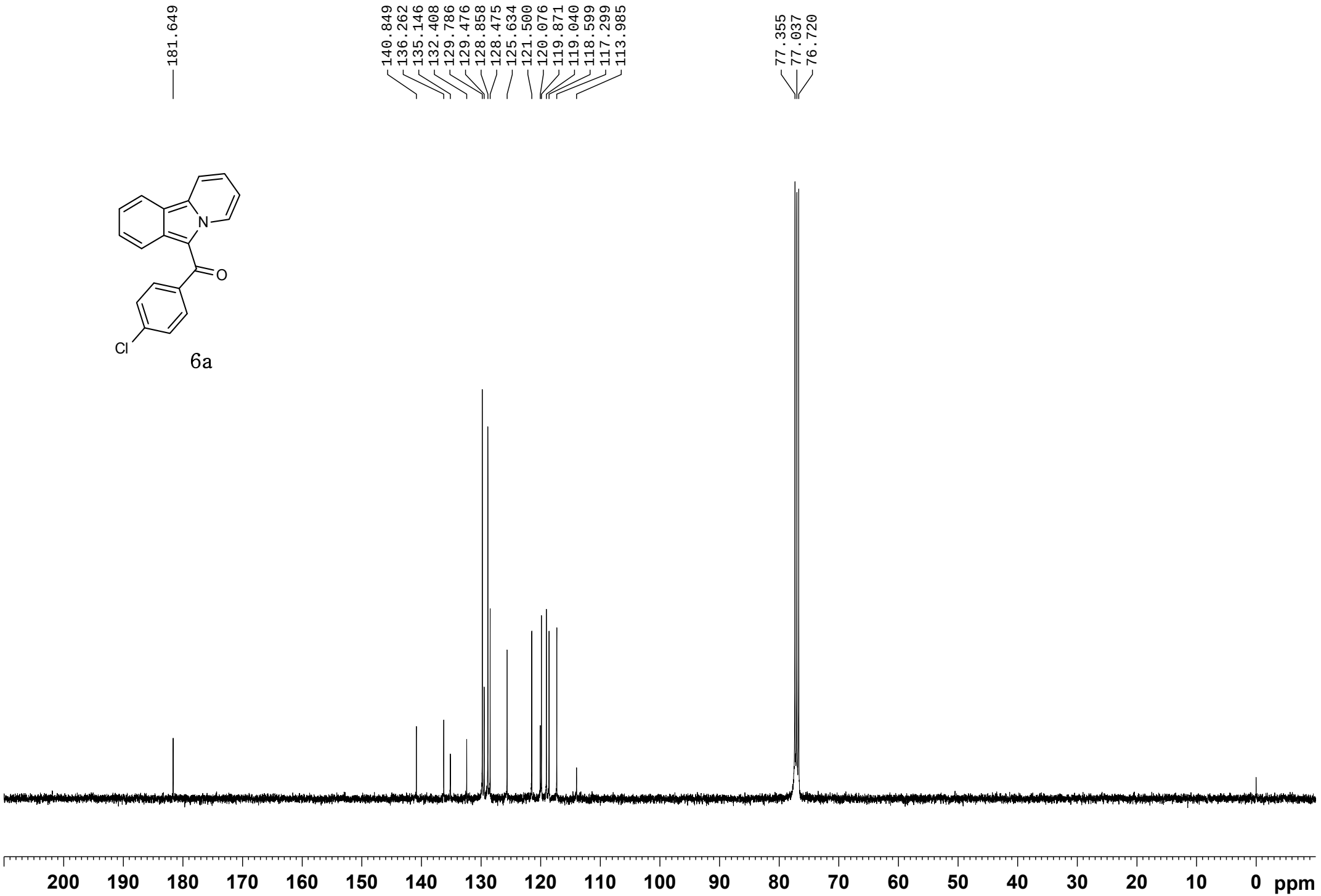
11
10
9
8
7
6
5
4
3
2
1
ppm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135.146
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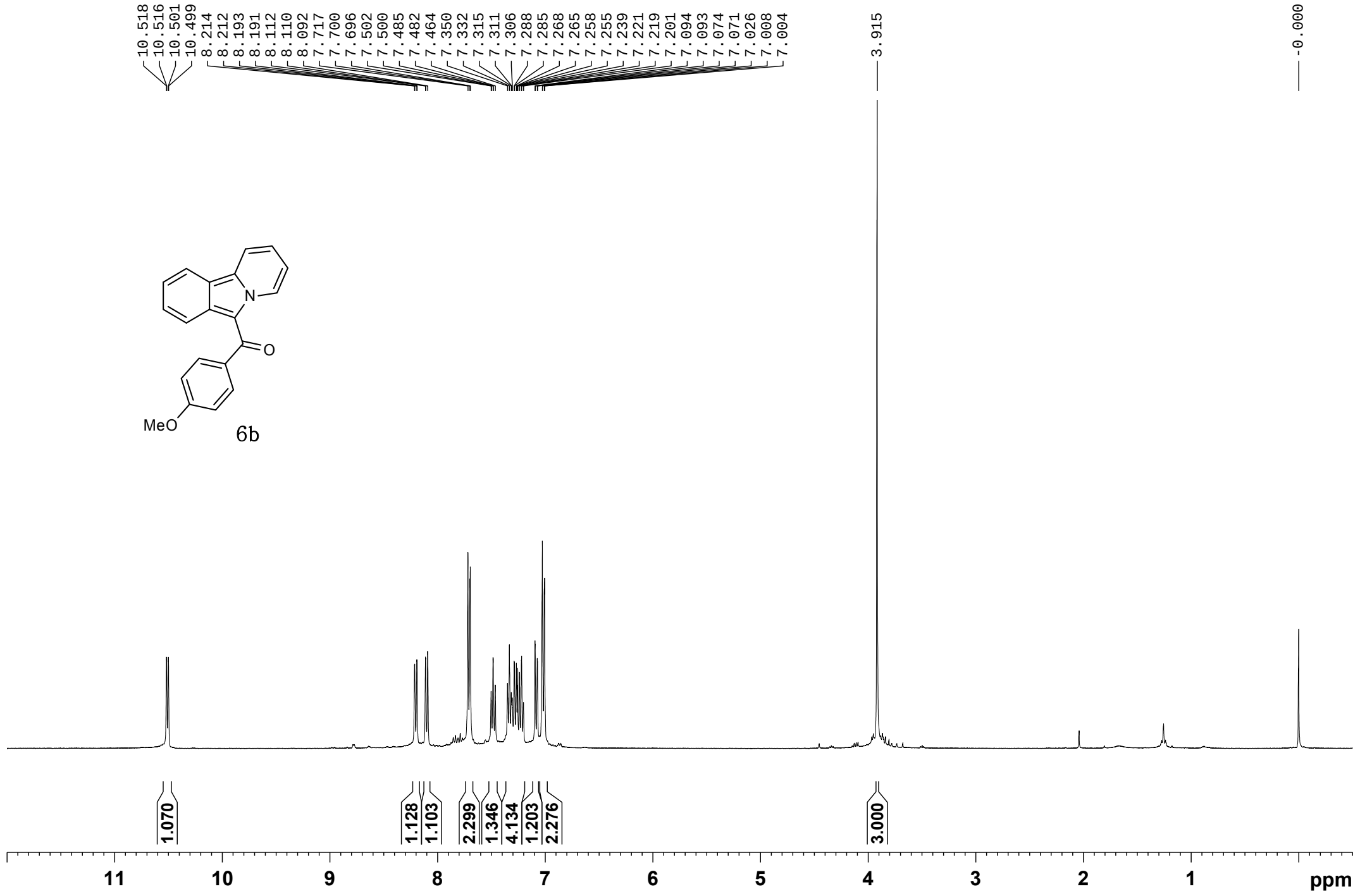
129.476
128.858
128.475
125.634
121.500
120.076
119.871
119.040
118.599
117.299
113.985
77.355
77.037
76.720
N
O
Cl
6a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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10.499
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8.212
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8.191
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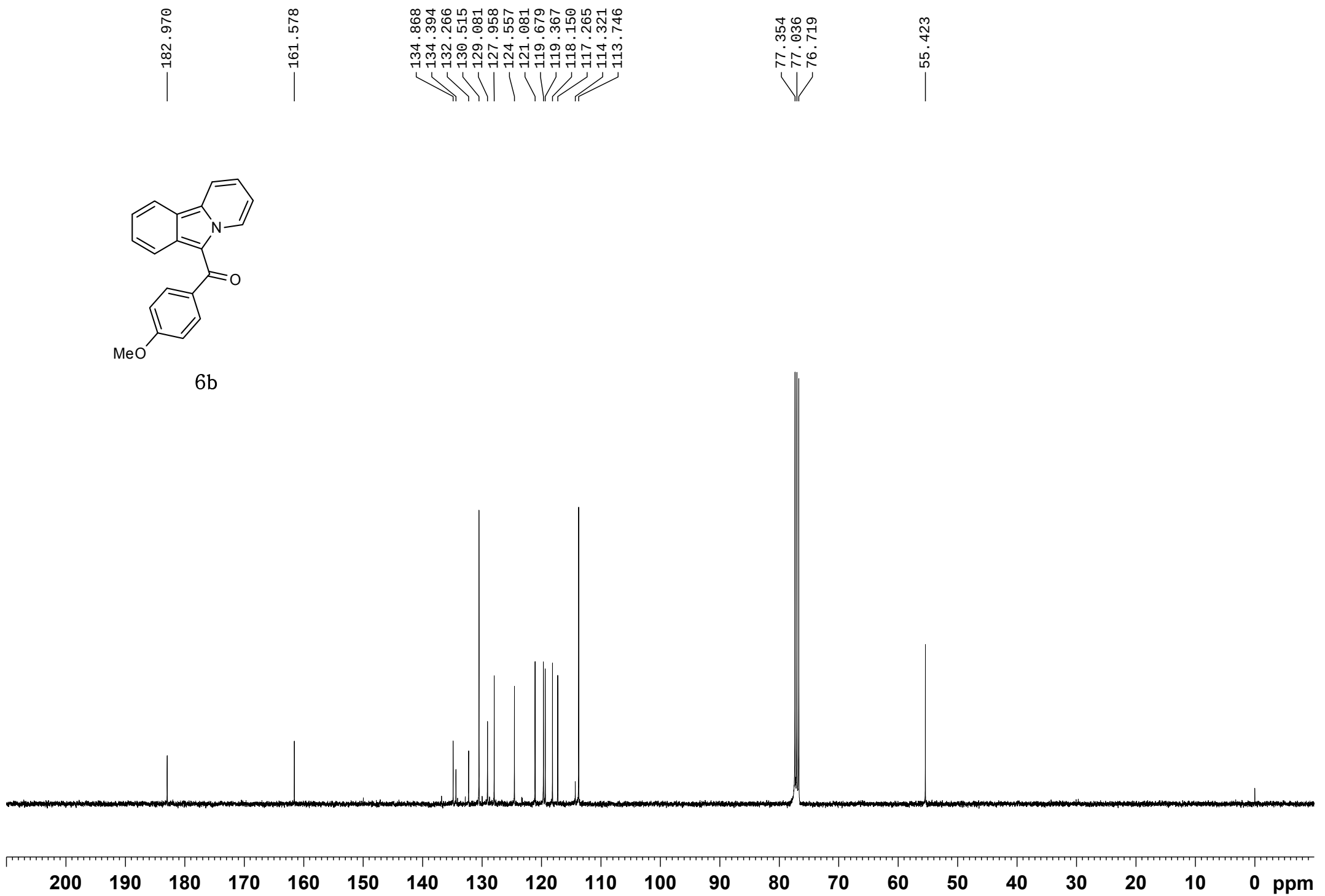
8.110
8.092
7.717
7.700
7.696
7.502
7.500
7.485
7.482
7.464
7.350
7.332
7.315
7.311
7.306
7.288
7.285
7.268
7.265
7.258
7.255
7.239
7.221
7.219
7.201
7.094
7.093
7.074
7.071
7.026
7.008
7.004
3.915
-0.000
N
O
MeO
6b
1.070
1.128
1.103
2.299
1.346
4.134
1.203
2.276
3.000
11
10
9
8
7
6
5
4
3
2
1
ppm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121.081
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119.367
118.150
117.265
114.321
113.746
77.354
77.036
76.719
55.423
N
O
MeO
200
190
180
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130
120
110
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90
80
70
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50
40
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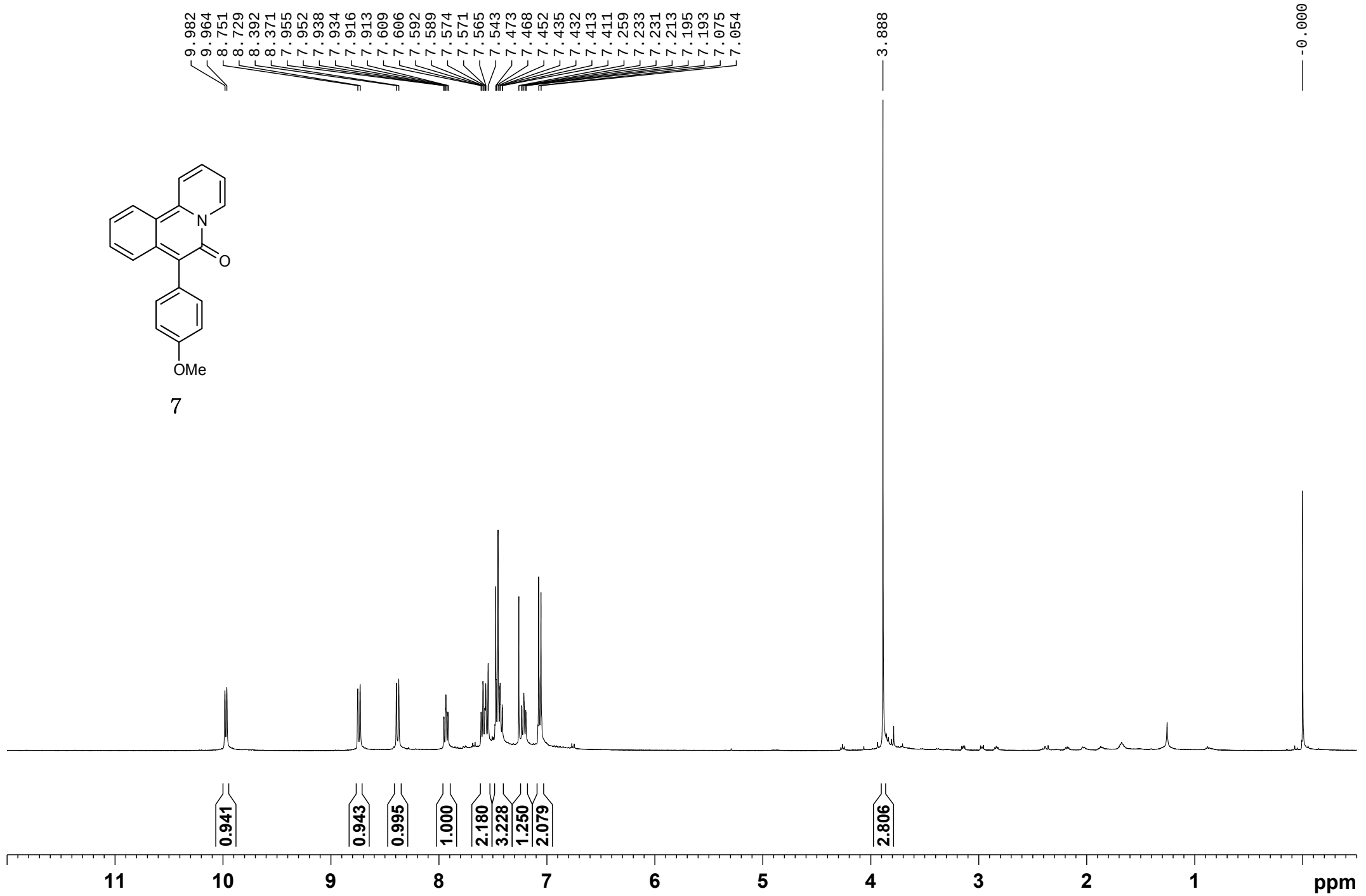
20
10
0
ppm

6b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7.952
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7.934
7.916
7.913
7.609
7.606
7.592
7.589
7.574
7.571
7.565
7.543
7.473
7.468
7.452
7.435
7.432
7.413
7.411
7.259
7.233
7.231
7.213
7.195
7.193
7.075
7.054
3.888
-0.000
N
O
OMe
0.941
0.943
0.995
1.000
2.180
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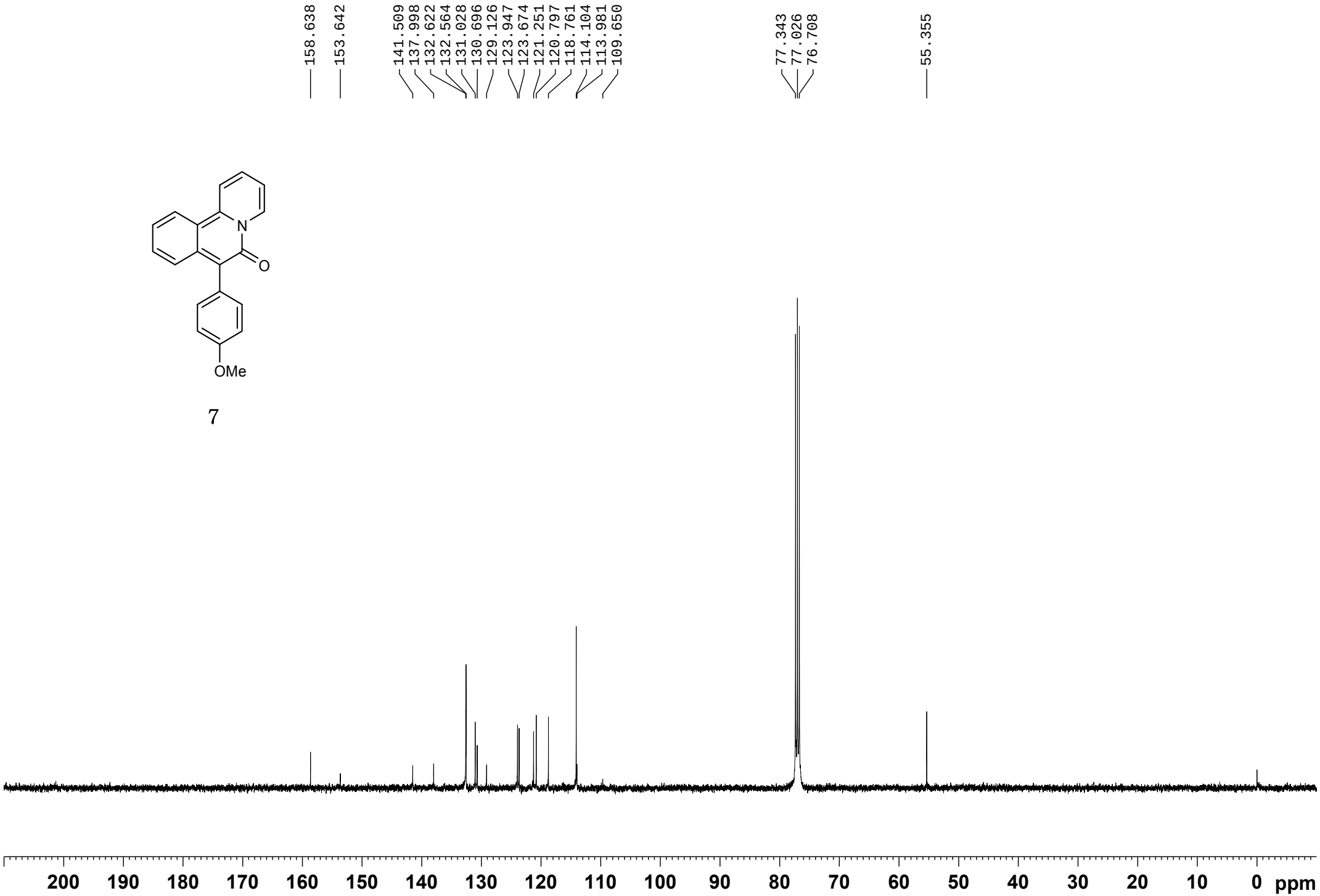
2.079
2.806
11
10
9
8
7
6
5
4
3
2
1
ppm

7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141.509
137.998
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131.028
130.696
129.126
123.947
123.674
121.251
120.797
118.761
114.104
113.981
109.650
77.343
77.026
76.708
55.355
N
O
OMe
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

7