Electronic Supplementary Information

Nitroso-azomethine(ene) reaction enabled annulations of nitrosoarenes, azomethines and alkenes

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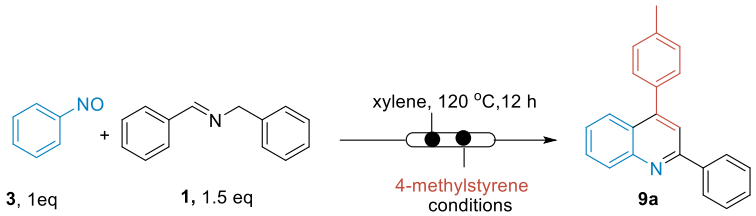
Experimental Section:

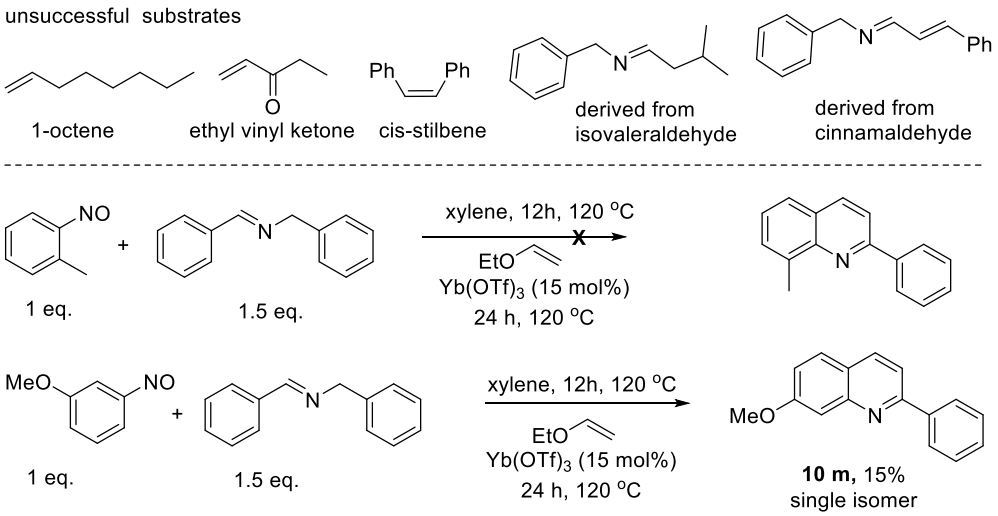
General: All reactions involving air- or moisture-sensitive reagents or intermediates were carried out in oven-dried glassware under an argon atmosphere. Dichloromethane (CH_2Cl_2) was freshly distilled from phosphorus(V)oxide (P_2O_5). Commercial grade xylene, benzene and toluene were distilled over CaH_2 before use. All other solvents and reagents were purified according to standard procedures or were used as received from Aldrich, Acros, Merck and Spectrochem. ^1H, ^{13}C NMR spectroscopy, *Bruker 400, 500, 600 MHz* (at 298 K). Chemical shifts, δ (in ppm), are reported relative to TMS δ (^1H) 0.0 ppm, δ (^{13}C) 0.0 ppm) which was used as the inner reference. Otherwise, the solvents residual proton resonance and carbon resonance ($CHCl_3$, δ (^1H) 7.26 ppm, δ (^{13}C) 77.2 ppm) were used for calibration. Column chromatography: Merck or Spectrochem silica gel 60-120 under gravity. Flash chromatography: Merck or Spectrochem silica gel 230-400. IR: spectra were recorded on Perkin Elmer Instrument at normal temperature. MS (ESI-HRMS): Mass spectra were recorded on an Agilent Accurate-Mass Q-TOF LC/MS 6520, and peaks are given in *m/z* (% of basis peak). Nitrosoarenes were prepared by following literature procedures.

Table S1: Variation of reaction conditions towards the better yield of arylquinoline **9a**.

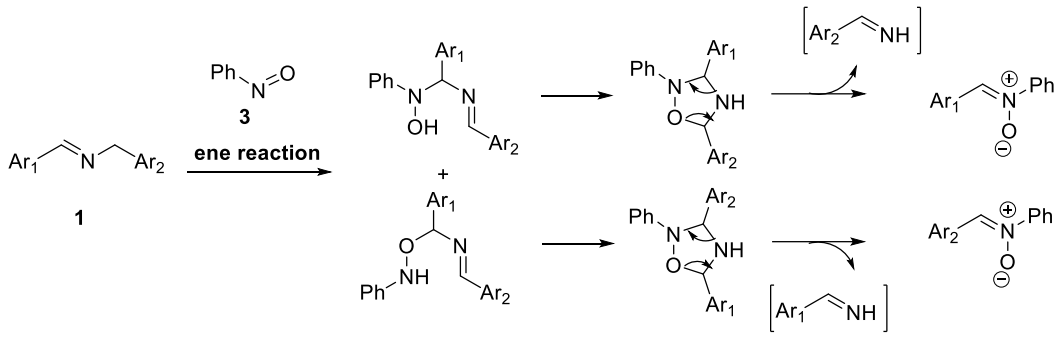


Entry	Equiv. of 4-methyl styrene	Acid	Solvent	Time	Temp.	Yield[b] (%)
1.	1	$Yb(OTf)_3$	xylene	12 h	120 °C	49
2.	1.5	$Yb(OTf)_3$	xylene	12 h	120 °C	55
3.	2	$Yb(OTf)_3$	xylene	12 h	120 °C	61
4.	2	-	xylene	12 h	120 °C	-
5.	2	$Sc(OTf)_3$	xylene	12 h	120 °C	66
6.	2	$Cu(OTf)_2$	xylene	12 h	120 °C	56
7.	2	$Yb(OTf)_3$	xylene	6 h	120 °C	35
8.	2	$Yb(OTf)_3$	xylene	24 h	120 °C	64
9.	2	$Yb(OTf)_3$	CCl_4	24 h	80 °C	55
10.	2	$Yb(OTf)_3$	toluene	24 h	110 °C	60
11.	2	$Yb(OTf)_3$	DCE	24 h	90 °C	62
12.[a]	2	$Yb(OTf)_3$	xylene	24 h	120 °C	68
13.	2	TfOH	xylene	24 h	120 °C	32
14.	2	$Cu(OAc)_2$	xylene	24 h	120 °C	-

All reactions were carried out with nitrosobenzene (0.28 mmol, 1 eq.) in solvent (3 mL), imine (0.42, 1.5 eq.) and Lewis acid (15 mol%). TfOH = Triflic acid. [a] = 30 mol% of Lewis acid was used. [b] = isolated yields.



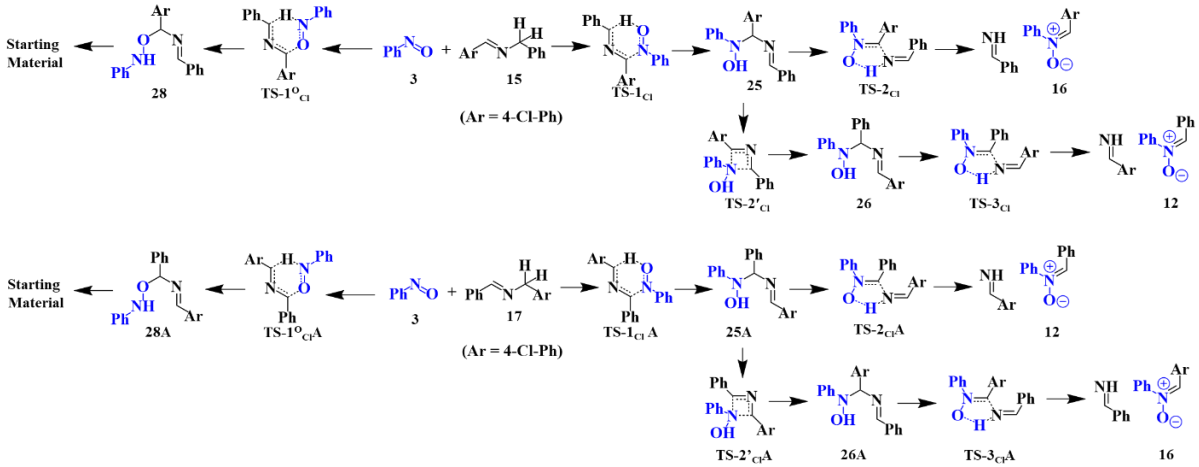
Scheme S1: Unsuccessful substrates and reaction with 3-methoxy nitroso benzene.



Scheme S2: Alternative anticipated mechanism for the formation of a mixture of nitrones from imines containing two different aryl moieties.

Computational details:

In this work, all density functional theory (DFT) calculations were carried out using G16 software.[1] For geometry optimization, the M06-2X/6-31+G(D, P) level of theory was used, unless specified otherwise.[2,3] To simulate the effects of xylene solvents, the SMD solvation model was implemented as an implicit solvation model.[3] Subsequent to the geometry optimizations, frequency calculations were executed to confirm the absence of a saddle point in the intermediate structure and to ensure the presence of one imaginary frequency for the transition state.



Scheme-s2: Plausible Mechanism for the formation of mixture nitrones from **15** & **17**.

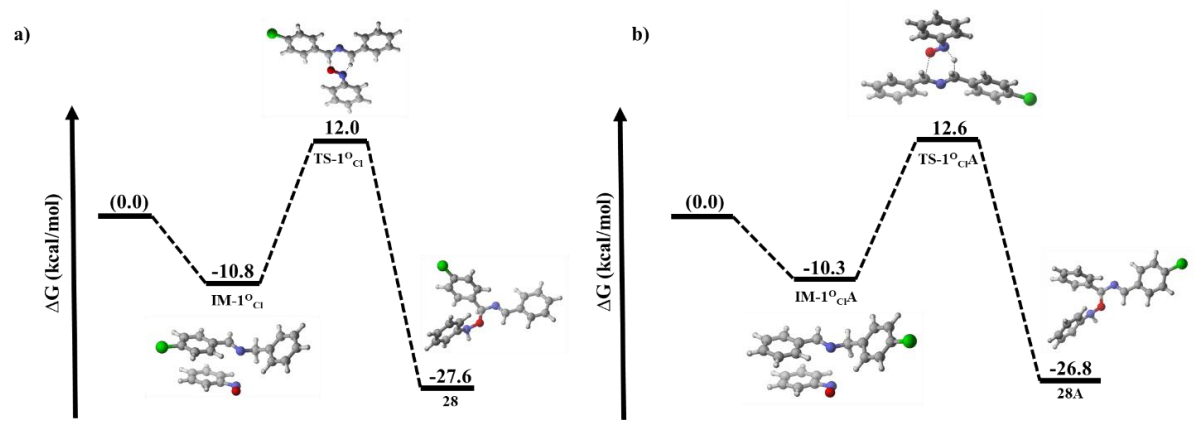


Figure-S1: a) Reaction profile for the formation of O-nitroso ene adduct from **15**. b) Reaction profile for the formation of O-nitoso ene adduct from **17**.

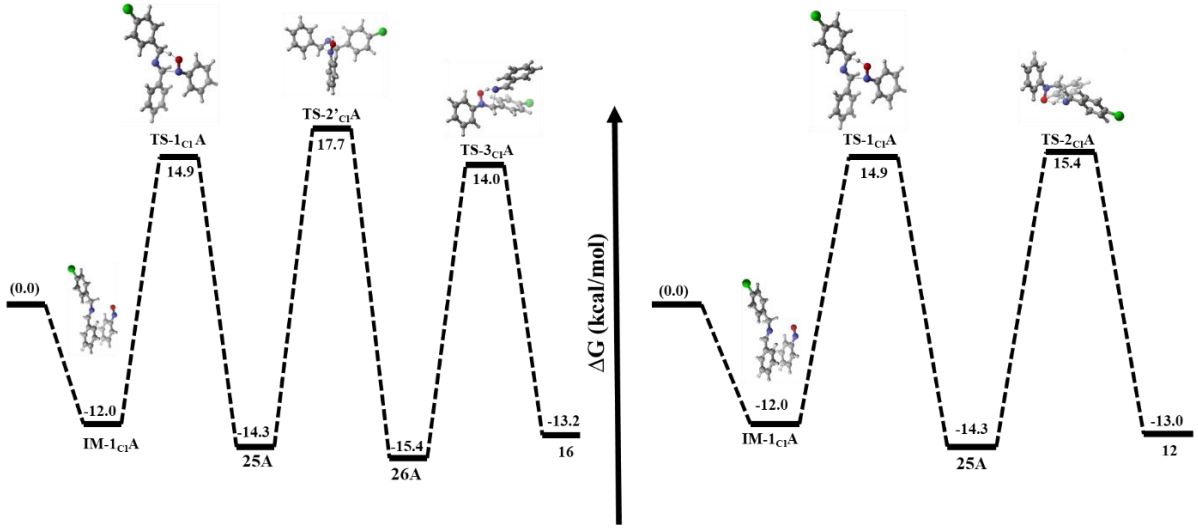
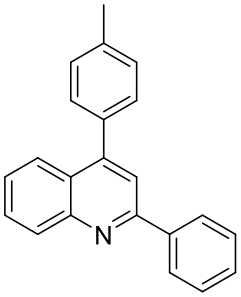


Figure-S2: Reaction profile for the formation of mixture nitrones from **17**.

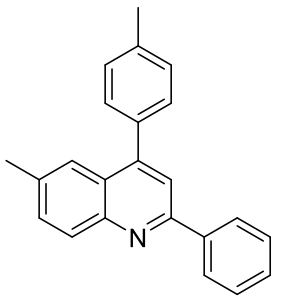
General procedure for the synthesis of quinolines (I):

Nitrosoarene (1 eq.) was added to a solution of azomethine (1.5 eq.) in xylene (3mL). The mixture was heated at 120 ^{o}C for 12 h under argon balloon. After that, the reaction mixture was cooled down to room temperature. Styrene derivatives (2 eq.) and $Yb(OTf)_3$ (15 mol%) were added to the reaction mixture. Then the reaction mixture was heated at 120 ^{o}C for another 24 under argon balloon. After the completion of reaction, the solvent was evaporated under reduced pressure. The reaction mixture was diluted with water (1x20 mL) and extracted with DCM (3x20 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The crude mixture was subjected to column chromatography (neutral alumina) to afford analytically pure products.

2-phenyl-4-(*p*-tolyl)quinoline (9a):[4] According to GP I: Nitrosobenzene (30 mg, 0.28 mmol), (*E*)-*N*-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, 4-methylstyrene (66 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **9a** as yellow gum (53 mg, 64%). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.33 (d, *J* = 7.5 Hz, 1H), 8.21 (d, *J* = 8.0 Hz, 2H), 7.95 (d, *J* = 8.5 Hz, 1H), 7.82 (s, 1H), 7.74 (t, *J* = 7.5 Hz, 1H), 7.55 – 7.47 (m, 6H), 7.37 (d, *J* = 8.0 Hz, 2H), 2.49 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ = 157.2, 149.4, 149.1, 140.0, 138.6, 135.7, 130.3, 129.71, 129.68, 129.5, 129.1, 127.8, 126.5, 126.1, 125.9, 119.6, 21.5 ppm. HRMS: Exact mass calculated for $C_{22}H_{18}N$ ($[M+H]^+$): 296.1434, Found: 296.1441.



6-methyl-2-phenyl-4-(*p*-tolyl) quinoline (9b):[5] According to GP I: 1-methy-4-nitrosobenzene (34 mg, 0.28 mmol), (*E*)-*N*-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, 4-methylstyrene (66 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **9b** as yellow gum (54 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.18 – 8.13 (m, 3H), 7.77 (s, 1H), 7.68 (s, 1H), 7.58 – 7.55 (m, 1H), 7.54 – 7.50 (m, 2H), 7.48 – 7.45 (m, 3H), 7.37 (d, *J* = 8.0 Hz, 2H), 2.50 (s, 3H), 2.48 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ = 156.3, 148.7, 147.6, 140.1, 138.4, 136.4, 135.9, 131.9, 130.0, 129.7, 129.5, 129.3, 129.0, 127.7, 126.1, 124.7, 119.6, 22.0, 21.5 ppm. HRMS: Exact mass calculated for $C_{23}H_{20}N$ ($[M+H]^+$): 310.1590, Found: 310.1595.



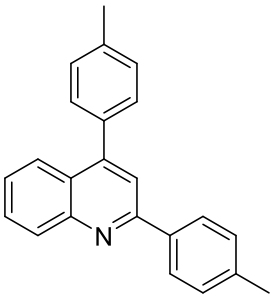
6-ethyl-2-phenyl-4-(*p*-tolyl) quinoline (9c): According to GP I: 1-ethy-4-Nitrosobenzene (38 mg, 0.28 mmol), (*E*)-*N*-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, 4-methylstyrene (66 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **9c** as yellow gum (51 mg, 56%). FT-IR ($\tilde{\nu}$) = 2965, 2927, 1603, 1517, 1491, 1344, 1276, 839, 695 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.20 – 8.16 (m, 3H), 7.77 (s, 1H), 7.71 (s, 1H), 7.63 – 7.60 (m, 1H), 7.54 – 7.51 (m, 2H), 7.49 – 7.46 (m, 3H), 7.38 (d, *J* = 7.6 Hz, 2H), 2.78 (q, *J* = 7.6 Hz, 2H), 2.50 (s, 3H), 1.27 (t, *J* = 7.6 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ = 156.3, 149.0,

147.6, 142.7, 139.9, 138.5, 135.9, 130.9, 130.0, 129.7, 129.5, 129.4, 129.0, 127.8, 126.0, 123.5, 119.7, 29.4, 21.6, 15.8 ppm. HRMS: Exact mass calculated for $C_{24}H_{22}N$ ($[M+H]^+$): 324.1747, Found: 324.1753.

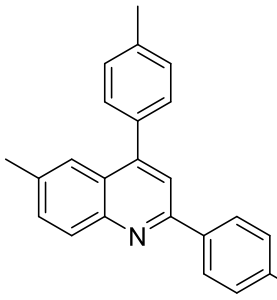
6-isopropyl-2-phenyl-4-(*p*-tolyl)quinoline (9d): According to GP I: 1-isopropyl-4-Nitrosobenzene (42 mg, 0.28 mmol), (*E*)-N-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, 4-methylstyrene (66 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **9d** as yellow gum (49 mg, 52%). FT-IR ($\tilde{\nu}$) = 2960, 2928, 2876, 1588, 1494, 1357, 1259, 1026, 833, 822, 769, 584 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ = 8.19 – 8.16 (m, 3H), 7.77 (s, 1H), 7.74 (s, 1H), 7.67 – 7.64 (m, 1H), 7.54 – 7.45 (m, 5H), 7.38 (d, *J* = 7.5 Hz, 2H), 3.07 – 3.01 (m, 1H), 2.50 (s, 3H), 1.29 (d, *J* = 6.5 Hz, 6H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 156.4, 149.0, 148.0, 147.1, 140.2, 138.4, 136.0, 130.3, 129.7, 129.5, 129.3, 129.2, 129.0, 127.7, 126.0, 122.2, 119.7, 34.6, 24.1, 21.5 ppm. HRMS: Exact mass calculated for $C_{25}H_{24}N$ ($[M+H]^+$): 338.1903, Found: 338.1904.

6-(*tert*-butyl)-2-phenyl-4-(*p*-tolyl)quinoline (9e): According to GP I: 1-*tert*-butyl-4-Nitrosobenzene (46 mg, 0.28mmol), (*E*)-N-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, 4-methylstyrene (66 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **9e** as yellow gum (55 mg, 56%). FT-IR ($\tilde{\nu}$) = 2958, 2928, 1617, 1588, 1494, 1360, 966, 823, 769, 590 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$) δ = 8.31 (d, *J* = 9.0 Hz, 1H), 8.18 (d, *J* = 7.2 Hz, 2H), 7.93 (s, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.78 (s, 1H), 7.55 – 7.47 (m, 5H), 7.38 (d, *J* = 6.6 Hz, 2H), 2.50 (s, 3H), 1.36 (s, 9H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$) δ = 156.3, 150.0, 149.6, 146.8, 139.3, 138.7, 135.7, 129.7, 129.6, 129.3, 129.1, 129.0, 127.9, 125.6, 120.9, 119.8, 35.3, 31.4, 21.6 ppm. Total count of 13C is less than expected due to the merging of signals in the aromatic region. HRMS: Exact mass calculated for $C_{26}H_{26}N$ ($[M+H]^+$): 352.2060, Found: 352.2067.

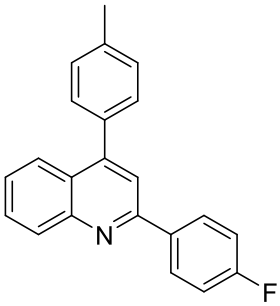
2-phenyl-4-(*p*-tolyl)quinoline (9f):[6] According to GP I: Nitrosobenzene (30 mg ,0.28mmol), (*E*)-*N*-(4-methylbenzyl)-1-(*p*-tolyl)methanimine (94 mg, 0.42 mmol) were reacted for 12 h, 4-methylstyrene (66 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were reacted further 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **9f** as yellow gum (50 mg, 58%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.27 (d, *J* = 7.8 Hz, 1H), 8.10 (d, *J* = 7.8 Hz, 2H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.80 (s, 1H), 7.74 – 7.72 (m, 1H), 7.48 – 7.46 (m, 3H), 7.37 – 7.33 (m, 4H), 2.49 (s, 3H), 2.44 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ = 156.9, 149.9, 148.5, 139.9, 138.7, 136.6, 135.6, 129.9, 129.8, 129.7, 129.5, 127.8, 126.4, 126.02, 125.95, 119.5, 21.6, 21.5 ppm. HRMS: Exact mass calculated for $C_{23}H_{20}N$ ($[M+H]^+$): 310.1590, Found: 310.1591.



6-methyl-2,4-di-*p*-tolylquinoline (9g):[7] According to GP I: 1-methyl-4-Nitrosobenzene (34 mg, 0.28 mmol), (*E*)-N-(4-methylbenzyl)-1-(p-tolyl)methanimine (94 mg, 0.42 mmol) were reacted for 12 h, 4-methylstyrene (66 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **9g** as yellow gum (53 mg, 59%). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.18 (d, *J* = 8.0 Hz, 1H), 8.09 (d, *J* = 8.0 Hz, 2H), 7.75 (s, 1H), 7.67 (s, 1H), 7.56 (d, *J* = 8.5 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.38 - 7.32 (m, 4H), 2.49 (s, 3H), 2.48 (s, 3H), 2.43 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$) δ = 156.2, 148.6, 147.6, 139.4, 138.4, 137.2, 136.2, 136.0, 131.8, 129.9, 129.74, 129.67, 129.48, 127.54, 125.9, 124.7, 119.5, 22.03, 21.6 ppm. HRMS: Exact mass calculated for $C_{24}H_{22}N$ ($[M+H]^+$): 324.1747, Found: 324.1739.

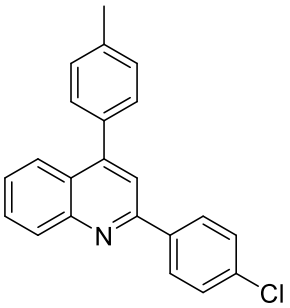


2-(4-fluorophenyl)-4-(*p*-tolyl)quinoline (9h): According to GP I: Nitrosobenzene (30 mg, 0.28 mmol), (*E*)-*N*-(4-fluorobenzyl)-1-(4-fluorophenyl)methanimine (97 mg, 0.42 mmol) were reacted for 12 h, 4-methylstyrene (66 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **9h** as colorless gum (41 mg, 47%). FT-IR ($\tilde{\nu}$) = 2923, 2854, 1592, 1497, 1358, 1230, 1156, 838, 764 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.28 (d, *J* = 6.6 Hz, 1H), 8.21 – 8.19 (m, 2H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.76 – 7.74 (m, 2H), 7.50 – 7.46 (m, 3H), 7.37 (d, *J* = 7.8 Hz, 2H), 7.22 (t, *J* = 8.4 Hz, 2H), 2.49 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$) δ = 164.1 (d, *J* = 249.5 Hz),

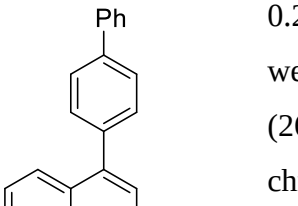


155.9, 149.3 (d, *J* = 186.3 Hz), 138.7, 135.7, 135.5, 129.9, 129.7 (d, *J* = 8.5 Hz), 129.65, 129.55, 126.6, 125.99, 125.97, 119.2, 116.0 (d, *J* = 21.6 Hz), 21.5 ppm. HRMS: Exact mass calculated for $C_{22}H_{17}NF$ ($[M+H]^+$): 314.1340, Found: 314.1342.

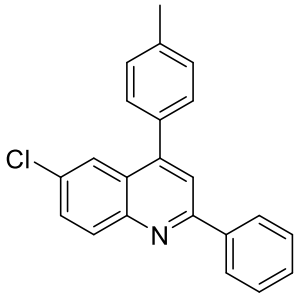
2-(4-chlorophenyl)-4-(*p*-tolyl)quinoline (9i):[8] According to GP I: Nitrosobenzene (30 mg, 0.28 mmol), (*E*)-*N*-(4-chlorobenzyl)-1-(4-chlorophenyl)methanimine (0.11 g, 0.42 mmol) were reacted for 12 h, 4-methylstyrene (66 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **9i** as colorless gum (41 mg, 45%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.25 (d, *J* = 8.4 Hz, 1H), 8.15 (d, *J* = 8.4 Hz, 2H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.77 (s, 1H), 7.76 – 7.73 (m, 1H), 7.51 – 7.45 (m, 5H), 7.37 (d, *J* = 7.8 Hz, 2H), 2.49 (s, 3H) ppm. HRMS: Exact mass calculated for $C_{22}H_{17}NCl$ ($[M+H]^+$): 330.1044, Found: 330.1043.



4-([1,1'-biphenyl]-4-yl)-2-phenylquinoline (9j):[9] According to GP I: Nitrosobenzene (30 mg, 0.28mmol), (*E*)-N-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, 4-vinyl-1,1'-biphenyl (0.1 g, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:50) gave **9j** as colorless gum (50 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.30 (d, *J* = 8.4 Hz, 1H), 8.24 (d, *J* = 7.6 Hz, 2H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.89 (s, 1H), 7.81 – 7.77 (m, 3H), 7.75 – 7.72 (m, 2H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.58 - 7.51 (m, 6H), 7.45 – 7.41 (m, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 157.1, 149.1, 149.0, 141.5, 140.7, 139.9, 137.5, 130.4, 130.2, 129.8, 129.6, 129.1, 129.0, 127.9, 127.8, 127.5, 127.4, 126.6, 126.0, 125.8, 119.5 ppm. HRMS: Exact mass calculated for $C_{27}H_{20}N$ ($[M+H]^+$): 358.1590, Found: 358.1592.

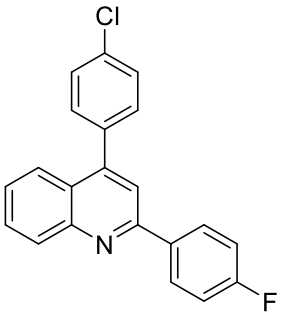


6-chloro-2-phenyl-4-(*p*-tolyl)quinoline (9k):[10] According to GP I: 1-chloro-4-Nitrosobenzene (40 mg, 0.28mmol), (*E*)-N-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, 4-methylstyrene (66 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:50) gave **9k** as colorless gum (37 mg, 40%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.21 –



8.17 (m, 3H), 7.90 (s, 1H), 7.83 (s, 1H), 7.67 (d, *J* = 9.0 Hz, 1H), 7.55 – 7.52 (m, 2H), 7.49 – 7.44 (m, 3H), 7.39 (d, *J* = 7.8 Hz, 2H), 2.50 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$) δ = 157.3, 148.9, 147.3, 139.3, 139.0, 134.9, 132.4, 131.8, 130.7, 129.8, 129.7, 129.6, 129.1, 127.8, 126.8, 124.8, 120.3, 21.6 ppm. HRMS: Exact mass calculated for $C_{22}H_{27}NCl$ ($[M+H]^+$): 330.1044, Found: 330.1049.

4-(4-chlorophenyl)-2-(4-fluorophenyl)quinoline (9l): According to GP I: Nitrosobenzene

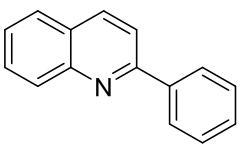


(30 mg, 0.28 mmol), (*E*)-*N*-(4-fluorobenzyl)-1-(4-fluorophenyl)methanimine (97 mg, 0.42 mmol) were reacted for 12 h, 4-chlorostyrene (78 mg, 0.56 mmol), $Yb(OTf)_3$ (26 mg, 0.042 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **9l** as colorless gum (33 mg, 35%). FT-IR ($\tilde{\nu}$) = 2962, 2925, 2854, 1598, 1496, 1357, 1156, 1015, 830, 763, 584 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.24 (d, *J* = 8.4 Hz, 1H), 8.20 – 8.18 (m, 2H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.77 – 7.74 (m, 2H), 7.55 – 7.49 (m, 5H), 7.22 (t, *J* = 8.4 Hz, 2H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$) δ = 164.2 (d, *J* = 250.1 Hz), 155.8, 148.6 (d, *J* = 35.9 Hz), 136.7, 135.3, 135.1, 131.0, 130.3, 130.0, 129.8 (d, *J* = 8.2 Hz), 127.0, 125.64, 125.55, 119.2, 116.1 (d, *J* = 21.6 Hz) ppm. HRMS: Exact mass calculated for $C_{21}H_{14}NClF$ ($[M+H]^+$): 334.0793, Found: 334.0792.

General procedure for the synthesis of 2-aryl quinolines(II):

Nitrosoarene (1 eq.) was added to a solution of azomethine (1.5 eq.) in xylene (3mL). The mixture was heated at 120 ^{o}C for 12 h under argon balloon. After that, the reaction mixture was cooled down to room temperature. Ethylvinylether (2 eq.) and $Cu(OTf)_2$ (20 mol%) were added to the reaction mixture. Then the reaction mixture was heated at 120 ^{o}C for another 24 under argon balloon. Then the solvent was evaporated under reduced pressure. Then the reaction mixture was diluted with water (1x20 mL) and extracted with DCM (3x20 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The crude mixture was subjected to column chromatography (neutral alumina) to afford analytically pure products.

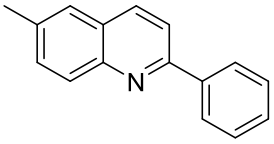
2-phenylquinoline (10a):[11] According to GP II: Nitrosobenzene (30 mg, 0.28 mmol), (*E*)-*N*-



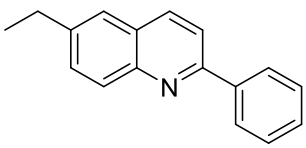
benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10a** as colorless gum (36 mg, 62%). ^{1}H

NMR (400 MHz, $CDCl_3$) δ = 8.23 (t, *J* = 8.4 Hz, 2H), 8.18 – 8.16 (m, 2H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 7.6 Hz, 1H), 7.76 – 7.72 (m, 1H), 7.56 – 7.52 (m, 3H), 7.49 – 7.46 (m, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ = 157.6, 148.3, 139.7, 137.2, 130.0, 129.8, 129.6, 129.1, 127.8, 127.7, 127.4, 126.6, 119.3 ppm. HRMS: Exact mass calculated for $C_{15}H_{12}N$ ($[M+H]^+$): 206.0964, Found: 206.0974.

6-methyl-2-phenylquinoline (10b):[12] According to GP II: 1-methyl-4-nitrosobenzene (34 mg, 0.28 mmol), (*E*)-*N*-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10b** as colorless gum (35 mg, 57%). ^1H NMR (400 MHz, $CDCl_3$) δ = 8.17 – 8.12 (m, 3H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.59 – 7.51 (m, 4H), 7.47 – 7.44 (m, 1H), 2.55 (s, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 156.8, 147.1, 140.0, 136.4, 136.3, 132.2, 129.6, 129.3, 129.0, 127.7, 127.4, 126.5, 119.2, 21.8 ppm. HRMS: Exact mass calculated for $C_{16}H_{14}N$ ($[M+H]^+$): 220.1121, Found: 220.1121.



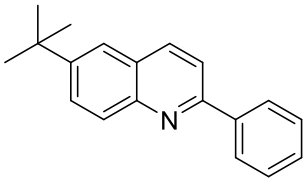
6-ethyl-2-phenylquinoline (10c):[13] According to GP II: 1-ethyl-4-nitrosobenzene (38 mg, 0.28 mmol), (*E*)-*N*-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10c** as colorless gum (35 mg, 54%). ^1H NMR (500 MHz, $CDCl_3$) δ = 8.18 – 8.16 (m, 4H), 7.85 (d, *J* = 8.5 Hz, 1H), 7.62 – 7.60 (m, 2H), 7.53 (t, *J* = 7.5 Hz, 2H), 7.46 (t, *J* = 7.0 Hz, 1H), 2.88 – 2.84 (m, 2H), 1.36 (t, *J* = 7.5 Hz, 3H) ppm. HRMS: Exact mass calculated for $C_{17}H_{16}N$ ($[M+H]^+$): 234.1277, Found: 234.1272.



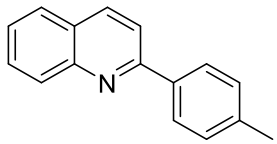
6-isopropyl-2-phenylquinoline (10d):[14] According to GP II: 1-isopropyl-4-nitrosobenzene (42 mg, 0.28 mmol), (*E*)-*N*-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10d** as colorless gum (42 mg, 60%). ^1H NMR (400 MHz, $CDCl_3$) = δ 8.18 – 8.11 (m, 4H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.66 – 7.62 (m, 2H), 7.55 – 7.51 (m, 2H), 7.48 – 7.44 (m, 1H), 3.15 – 3.08 (m, 1H), 1.37 (d, *J* = 7.2 Hz, 6H) ppm. ^{13}C

NMR (126 MHz, $CDCl_3$) δ = 156.9, 147.4, 147.12, 140.1, 136.6, 129.8, 129.3, 129.0, 127.7, 127.4, 123.8, 119.2, 34.3, 24.1 ppm. HRMS: Exact mass calculated for $C_{18}H_{18}N$ ($[M+H]^+$): 248.1434, Found: 248.1434.

6-*tert*butyl-2-phenylquinoline (10e):[15] According to GP II: 1-*tert*butyl-4-nitrosobenzene (46 mg, 0.28 mmol), (*E*)-*N*-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10e** as white gum (45 mg, 61%). ^1H NMR (400 MHz, $CDCl_3$) δ = 8.20 – 8.11 (m, 4H), 7.86 – 7.82 (m, 2H), 7.75 (d, *J* = 2.0 Hz, 1H), 7.55 – 7.51 (m, 2H), 7.47 – 7.44 (m, 1H), 1.45 (s, 9H). ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 157.0, 149.4, 147.1, 140.1, 137.0, 129.5, 129.3, 129.0, 128.8, 127.7, 127.1, 122.6, 119.2, 35.1, 31.4 ppm. HRMS: Exact mass calculated for $C_{19}H_{20}N$ ($[M+H]^+$): 262.1590, Found: 262.1599.

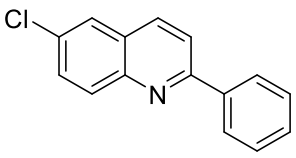


2-(p-tolyl)quinoline (10f):[12] According to GP II: Nitrosobenzene (30 mg, 0.28 mmol), (*E*)-N-(4-methylbenzyl)-1-(p-tolyl)methanimine (94 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10f** as colorless gum (33 mg, 53%). ^1H NMR (500 MHz, $CDCl_3$) δ = 8.34 (d, *J* = 8.0 Hz, 1H), 8.26 (d, *J* = 8.5 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 2H), 7.89 – 7.83 (m, 2H), 7.77 – 7.74 (m, 1H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H) ppm. HRMS: Exact mass calculated for $C_{16}H_{14}N$ ($[M+H]^+$): 220.1121, Found: 220.1123.

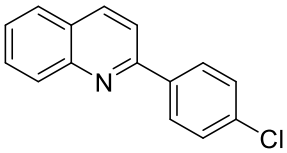


6-methyl-2-(*p*-tolyl)lquinoline (10g):[16] According to GP II: 1-methyl-4-nitrosobenzene (34 mg, 0.28 mmol), (*E*)-N-(4-methylbenzyl)-1-(p-tolyl)methanimine (94 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10g** as colorless gum (36 mg, 55%). ^1H NMR (600 MHz, $CDCl_3$) δ = 8.12 (d, *J* = 9.0 Hz, 1H), 8.08 – 8.04 (m, 3H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.58 – 7.55 (m, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 2.54 (s, 3H), 2.43 (s, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 156.7, 147.1, 139.4, 137.2, 136.2, 136.1, 132.1, 129.8, 129.6, 127.6, 127.3, 126.5, 119.1, 21.8, 21.5 ppm. HRMS: Exact mass calculated for $C_{17}H_{16}N$ ($[M+H]^+$): 234.1277, Found: 234.1281.

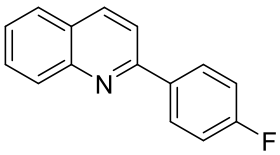
6-chloro-2-phenylquinoline (10h):[12] According to GP II: 1-Chloro-4-nitrosobenzene (40 mg, 0.28 mmol), (*E*)-*N*-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10h** as colorless gum (26 mg, 39%). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.30 (d, *J* = 7.5 Hz, 1H), 8.21 – 8.17 (m, 3H), 7.92 (d, *J* = 9.0 Hz, 1H), 7.84 (s, 1H), 7.70 (d, *J* = 7.0 Hz, 1H), 7.57 – 7.50 (m, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 157.8, 146.9, 139.5, 136.1, 132.2, 131.6, 130.8, 129.8, 129.1, 128.0, 127.8, 126.4, 120.1 ppm. HRMS: Exact mass calculated for $C_{15}H_{11}NCl$ ($[M+H]^+$): 240.0575, Found: 240.0576.



2-(4-chlorophenyl)quinoline (10i):[12] According to GP II: Nitrosobenzene (30 mg, 0.28 mmol), (*E*)-N-(4-chlorobenzyl)-1-(4-chlorophenyl)methanimine (0.11 g, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10i** as colorless gum (22 mg, 32%). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.38 (d, *J* = 6.5 Hz, 1H), 8.31 (d, *J* = 8.5 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 2H), 7.87 (d, *J* = 8.0 Hz, 2H), 7.79 (t, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 8.5 Hz, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 156.3, 148.5, 138.3, 137.2, 135.8, 130.1, 129.9, 129.3, 129.1, 127.7, 127.5, 126.7, 118.8 ppm. HRMS: Exact mass calculated for $C_{15}H_{11}NCl$ ($[M+H]^+$): 240.0575, Found: 240.0580.



2-(4-fluorophenyl)quinoline (10j):[12] According to GP II: Nitrosobenzene (30 mg, 0.28 mmol), (*E*)-*N*-(4-fluorobenzyl)-1-(4-fluorophenyl)methanimine (97 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10j** as colorless gum (23 mg, 37%). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.26 – 8.17 (m, 4H), 7.84 (d, *J* = 8.5 Hz, 2H), 7.76 – 7.73 (m, 1H), 7.56 – 7.53 (m, 1H), 7.22 (t, *J* = 8.0 Hz, 2H) ppm. HRMS: Exact mass calculated for $C_{15}H_{11}NF$ ($[M+H]^+$): 224.0870, Found: 224.0877.



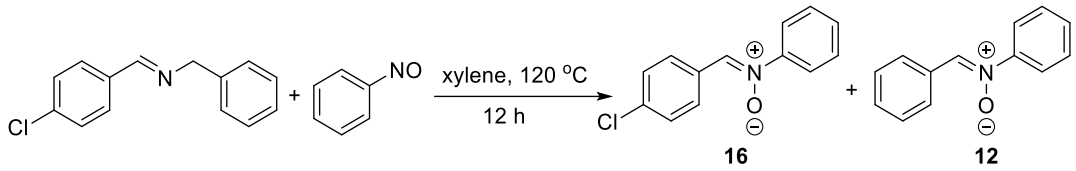
6-isopropyl-2-(*p*-tolyl)lquinoline (10k): According to GP II: 1-isopropyl-4-nitrosobenzene (42 mg, 0.28 mmol), (*E*)-N-(4-methylbenzyl)-1-(p-tolyl)methanimine (94 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc : hexane, 1:40) gave **10k** as colorless gum (37 mg, 50%). FT-IR ($\tilde{\nu}$) = 2960, 2925, 2872, 1596, 1494, 1459, 1189, 891, 784 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ = 8.14 (d, *J* = 9.0 Hz, 1H), 8.09 (d, *J* = 8.5 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 2H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.64 – 7.61 (m, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 3.14 – 3.08 (m, 1H), 2.43 (s, 3H), 1.36 (d, *J* = 7.0 Hz, 6H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 156.9, 147.4, 146.9, 139.4, 137.3, 136.5, 129.8, 129.71, 129.69, 127.6, 127.3, 123.8, 119.0, 34.3, 24.1, 21.5 ppm. HRMS: Exact mass calculated for $C_{19}H_{20}N$ ($[M+H]^+$): 262.1590, Found: 262.1596.

6-*tert*butyl-2-(*p*-tolyl)lquinoline (10l): According to GP II: 1-*tert*-butyl-4-nitrosobenzene (46 mg, 0.28mmol), (*E*)-N-(4-methylbenzyl)-1-(p-tolyl)methanimine (94 mg, 0.42 mmol) were reacted for 12 h, ethylvinyl ether (40 mg, 0.56 mmol), $Cu(OTf)_2$ (20 mg, 0.056 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc:hexane, 1:40) gave **10l** as colorless gum (39 mg, 51%). FT-IR ($\tilde{\nu}$)= 2955, 2920, 2862, 1595,1491, 1361, 1261, 1182, 910, 610 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ = 8.16 (d, *J* = 8.5 Hz, 1H), 8.10 (d, *J* = 9.0 Hz, 1H), 8.06 (d, *J* = 8.0 Hz, 2H), 7.84 – 7.81 (m, 2H), 7.73 (s, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H), 1.45 (s, 9H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 157.0, 149.2, 147.1, 139.4, 137.3, 136.8, 129.8, 129.4, 128.7, 127.6, 127.0, 122.6, 119.0, 35.1, 31.4, 21.5 ppm. HRMS: Exact mass calculated for $C_{20}H_{22}N$ ($[M+H]^+$): 276.1747, Found: 276.1740.

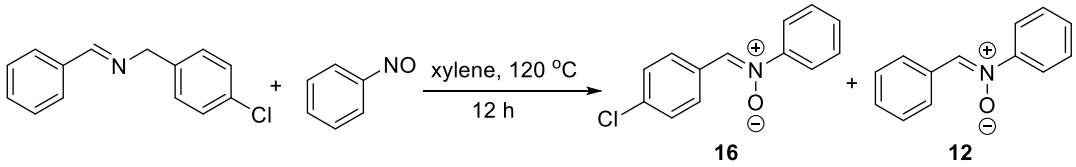
7-methoxy-2-phenylquinoline (10m):[17] 1-methoxy-3-nitrosobenzene (50 mg, 0.36 mmol), (*E*)-*N*-benzyl-1-phenylmethanimine (0.10 g, 0.54 mmol) were reacted for 12 h, ethylvinyl ether (52 mg, 0.72 mmol), $Yb(OTf)_3$ (33 mg, 0.054 mmol) were added and reacted further for 24 h and column chromatography of crude product (neutral alumina; EtOAc:hexane, 1:40) gave **10m** as colorless gum (13 mg, 15%). ^1H NMR (600 MHz, $CDCl_3$) δ = 8.14 (d, *J* = 8.4 Hz, 3H), 7.74 – 7.70 (m, 2H), 7.54 – 7.51 (m, 3H), 7.47 – 7.45 (m, 1H), 7.20 – 7.18 (m, 1H), 3.98 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$) δ = 161.1, 157.9, 150.2,

140.1, 136.6, 129.4, 129.0, 128.7, 127.7, 122.6, 119.7, 117.2, 107.8, 55.8 ppm. HRMS: Exact mass calculated for $C_{16}H_{14}NO$ ($[M+H]^+$): 236.1070, Found: 236.1073.

(*Z*)-N-(benzylidene)aniline oxide (12):[18] Nitrosobenzene (30 mg, 0.28 mmol, 1 eq.) was added to a solution of (*E*)-*N*-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol, 1.5 eq.) in xylene (3 mL). The mixture was heated at 120 °C for 12 h under argon balloon. Then the solvent was evaporated under reduced pressure. The crude mixture was subjected to flash chromatography (silica gel 230-400; EtOAc : hexane, 1:5) gave **12** as white solid (40 mg, 73%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.41 – 8.39 (m, 2H), 7.93 (s, 1H), 7.78 – 7.77 (m, 2H), 7.50 – 7.46 (m, 6H) ppm. HRMS: Exact mass calculated for $C_{13}H_{12}NO$ ($[M+H]^+$): 198.0913, Found: 198.0906.



Nitrosobenzene (35 mg, 0.33 mmol), (*E*)-*N*-benzyl-1-(4-chlorophenyl)methanimine (0.11 g, 0.49 mmol) were reacted for 12 h, and flash chromatography of crude product (silica gel 230-400; EtOAc: hexane, 1:5) gave **16** as white solid (39 mg, 52 %) and **12** as white solid (9 mg, 14 %). ^{1}H NMR of **16**:[18] (400 MHz, $CDCl_3$) δ = 8.35 (d, *J* = 8.4 Hz, 2H), 7.90 (s, 1H), 7.76 – 7.74 (m, 2H), 7.49 – 7.47 (m, 3H), 7.44 (d, *J* = 8.8 Hz, 2H) ppm. HRMS: Exact mass calculated for $C_{13}H_{11}NClO$ ($[M+H]^+$): 232.0524, Found: 232.0519.



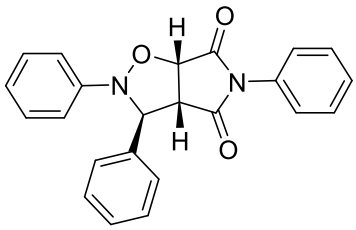
Nitrosobenzene (35 mg, 0.33 mmol), (*E*)-*N*-(4-chlorobenzyl)-1-phenylmethanimine (0.11 g, 0.49 mmol) were reacted for 12 h, and flash chromatography of crude product (silica gel 230-400; EtOAc: hexane, 1:5) gave **16** as white solid (23 mg, 30 %) and **12** as white solid (20 mg, 32 %).

General procedure for the synthesis of isoxazolidine(III):

Nitrosoarene (1 eq.) was added to a solution of imine derivative (1.5 eq.) in xylene (3mL) followed by the addition of *N*-phenyl maleimide (1 eq.). The mixture was heated at 120 °C for 12 h under argon balloon. After that, the reaction mixture was cooled down to room

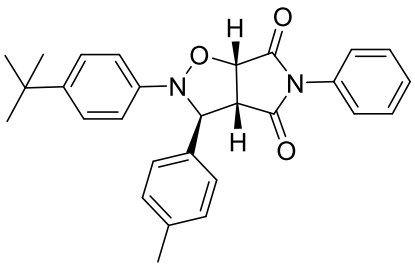
temperature. Then the solvent was evaporated under reduced pressure. The crude mixture was subjected to flash chromatography (silica gel) to afford analytically pure products.

(3S,3aR,6aS)-2,3,5-triphenyltetrahydro-4H-pyrrolo[3,4-d]isoxazole-4,6(5*H*)-dione (27a):

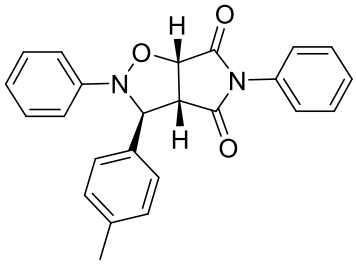


According to GP III: Nitrosobenzene (30 mg, 0.28 mmol), (*E*)-*N*-benzyl-1-phenylmethanimine (82 mg, 0.42 mmol) and *N*-phenyl maleimide (48 mg, 0.28 mmol) were reacted for 12 h, flash chromatography of crude product (silica gel; EtOAc : hexane, 1:3) gave **27a** as white solid (64 mg, 62%). M.p. = 152 – 155 ^{o}C. FT-IR ($\tilde{\nu}$) = 3068, 3036, 2986, 1713, 1595, 1493, 1381, 1265, 1197, 1029, 730, 575 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.60 (d, *J* = 7.2 Hz, 2H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.39 – 7.34 (m, 4H), 7.29 – 7.27 (m, 2H), 7.18 (d, *J* = 7.8 Hz, 2H), 7.02 (t, *J* = 7.2 Hz, 1H), 6.64 – 6.62 (m, 2H), 5.79 (s, 1H), 5.11 (d, *J* = 7.8 Hz, 1H), 4.02 (d, *J* = 7.8 Hz, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ = 174.3, 172.8, 149.0, 138.8, 131.1, 129.6, 129.2, 129.1, 128.3, 126.7, 126.3, 123.1, 114.5, 77.5, 70.1, 57.5 ppm. Total count of 13C is less than expected due to the merging of signals in the aromatic region. HRMS: Exact mass calculated for $C_{23}H_{19}N_2O_3$ ($[M+H]^+$): 371.1390, Found: 371.1381.

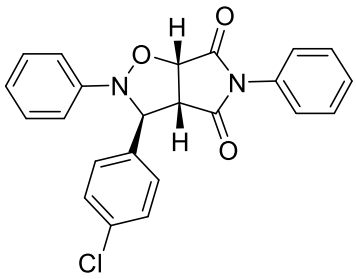
(3S,3aR,6aS)-2-(4-(*tert*-butyl)phenyl)-5-phenyl-3-(*p*-tolyl)tetrahydro-4H-pyrrolo[3,4-d]isoxazole-4,6(5*H*)-dione (27b):



According to GP III: 1-*tert*-butyl-4-nitrosobenzene (46 mg, 0.28 mmol), (*E*)-*N*-(4-methylbenzyl)-1-(*p*-tolyl)methanimine (94 mg, 0.42 mmol) and *N*-phenyl maleimide (48 mg, 0.28 mmol) were reacted for 12 h, flash chromatography of crude product (silica gel; EtOAc : hexane, 1:3) gave **27b** as colorless gum (71 mg, 58%). FT-IR ($\tilde{\nu}$) = 3061, 3033, 2987, 1715, 1602, 1498, 1375, 1210, 1155, 1021, 722, 578 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.51 (d, *J* = 7.8 Hz, 2H), 7.34 – 7.26 (m, 7H), 7.13 (d, *J* = 8.4 Hz, 2H), 6.51 (d, *J* = 6.6 Hz, 2H), 5.82 (s, 1H), 5.09 (d, *J* = 7.8 Hz, 1H), 4.03 (d, *J* = 7.8 Hz, 1H), 2.41 (s, 3H), 1.31 (s, 9H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$) δ = 174.5, 173.0, 146.8, 146.0, 138.0, 136.1, 131.0, 129.8, 129.19, 129.16, 126.50, 126.47, 126.4, 114.0, 77.7, 69.6, 57.5, 34.4, 31.6, 21.3 ppm. HRMS: Exact mass calculated for $C_{28}H_{29}N_2O_3$ ($[M+H]^+$): 441.2173, Found: 441.2174.

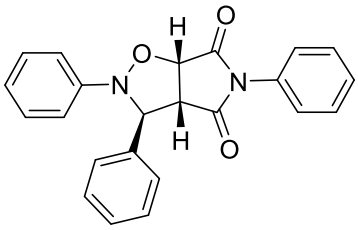
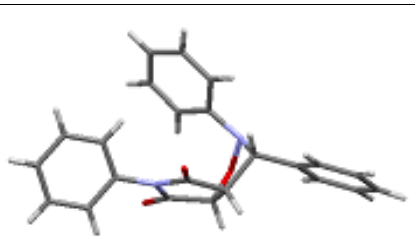
(3S,3aR,6aS)-2,5-diphenyl-3-(*p*-tolyl)tetrahydro-4*H*-pyrrolo[3,4-*d*]isoxazole-4,6(5*H*)-dione (27c): 

According to GP III: Nitrosobenzene (30 mg, 0.28 mmol), (*E*)-N-(4-methylbenzyl)-1-(*p*-tolyl)methanimine (94 mg, 0.42 mmol) and *N*-phenyl maleimide (48 mg, 0.28 mmol) were reacted for 12 h, flash chromatography of crude product (silica gel; EtOAc : hexane, 1:3) gave **27c** as white gum (59 mg, 55%). FT-IR ($\tilde{\nu}$) = 2960, 2925, 2857, 1714, 1595, 1489, 1380, 1265, 1020, 801, 757, 508 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.47 (d, *J* = 7.8 Hz, 2H), 7.36 – 7.35 (m, 3H), 7.28 – 7.24 (m, 4H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.00 (t, *J* = 7.2 Hz, 1H), 6.69 – 6.65 (m, 2H), 5.75 (s, 1H), 5.14 (d, *J* = 7.8 Hz, 1H), 4.03 (d, *J* = 7.8 Hz, 1H), 2.39 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$) δ = 174.4, 172.9, 149.1, 138.2, 135.8, 131.1, 129.8, 129.6, 129.21, 129.19, 126.7, 126.4, 123.1, 114.6, 77.5, 70.0, 57.5, 21.3 ppm. HRMS: Exact mass calculated for $C_{24}H_{21}N_2O_3$ ($[M+H]^+$): 385.1547, Found: 385.1544.

(3S,3aR,6aS)-3-(4-chlorophenyl)-2,5-diphenyltetrahydro-4*H*-pyrrolo[3,4-*d*]isoxazole-4,6(5*H*)-dione (27d): 

According to GP III: Nitrosobenzene (30 mg, 0.28 mmol), (*E*)-*N*-(4-chlorobenzyl)-1-(4-chlorophenyl)methanimine (0.11 g, 0.42 mmol) and *N*-phenyl maleimide (48 mg, 0.28 mmol) were reacted for 12 h, flash chromatography of crude product (silica gel; EtOAc : hexane, 1:3) gave **27d** as white solid (52 mg, 46%). M.p. – 202 - 204 ºC. FT-IR ($\tilde{\nu}$) = 3065, 3036, 1717, 1595, 1455, 1384, 1199, 1090, 827, 692 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.51 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.33 – 7.32 (m, 3H), 7.27 – 7.24 (m, 2H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.01 – 7.00 (m, 1H), 6.63 – 6.61 (m, 2H), 5.72 (s, 1H), 5.09 (d, *J* = 7.2 Hz, 1H), 3.96 (d, *J* = 7.8 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$) δ = 174.1, 172.6, 148.7, 137.3, 134.3, 131.0, 129.7, 129.32, 129.26, 129.2, 128.2, 126.3, 123.3, 114.6, 77.4, 69.5, 57.5 ppm. HRMS: Exact mass calculated for $C_{23}H_{18}ClN_2O_3$ ($[M+H]^+$): 405.1000, Found: 405.1003.

Crystallographic data of 27a:

	
Empirical formula	$C_{23}H_{18}N_2O_3$
Formula weight	370.39
Crystal size (mm^3), color	0.28 x 0.23 x 0.18, colorless
Crystal system	Orthorhombic
Space group	P 21 21 21
a (Å)	6.840(10)
b (Å)	11.120(16)
c (Å)	24.67(4)
α (deg)	90
β (deg)	90
γ (deg)	90
V ($Å^3$)	1876(5)
Z	4
ρ_{calc} (g cm^{-3})	1.311
μ (M_0 Kα) (mm^{-1})	0.088
F (000)	776.0
T(K)	296(2)
Range of indices (h; k; l)	-8, 8; -13, 13; -29, 29
Number of reflections collected	41325
Unique reflection	3279
Completeness to 2θ	99.9
R_{int}	0.5508
Refinement method	SHELXL-2018/3 (Sheldrick, 2018)
Data / restraints / parameters	3279/0/254
goodness-of-fit	0.904
$R_1[I \geq 2\sigma(I)]$	0.0776
$wR_2[I \geq 2\sigma(I)]$	0.1597
R_1 (all data)	0.2613
wR_2 (all data)	0.2428
Δ_r (max, min) e $Å^{-3}$	0.204/-0.233

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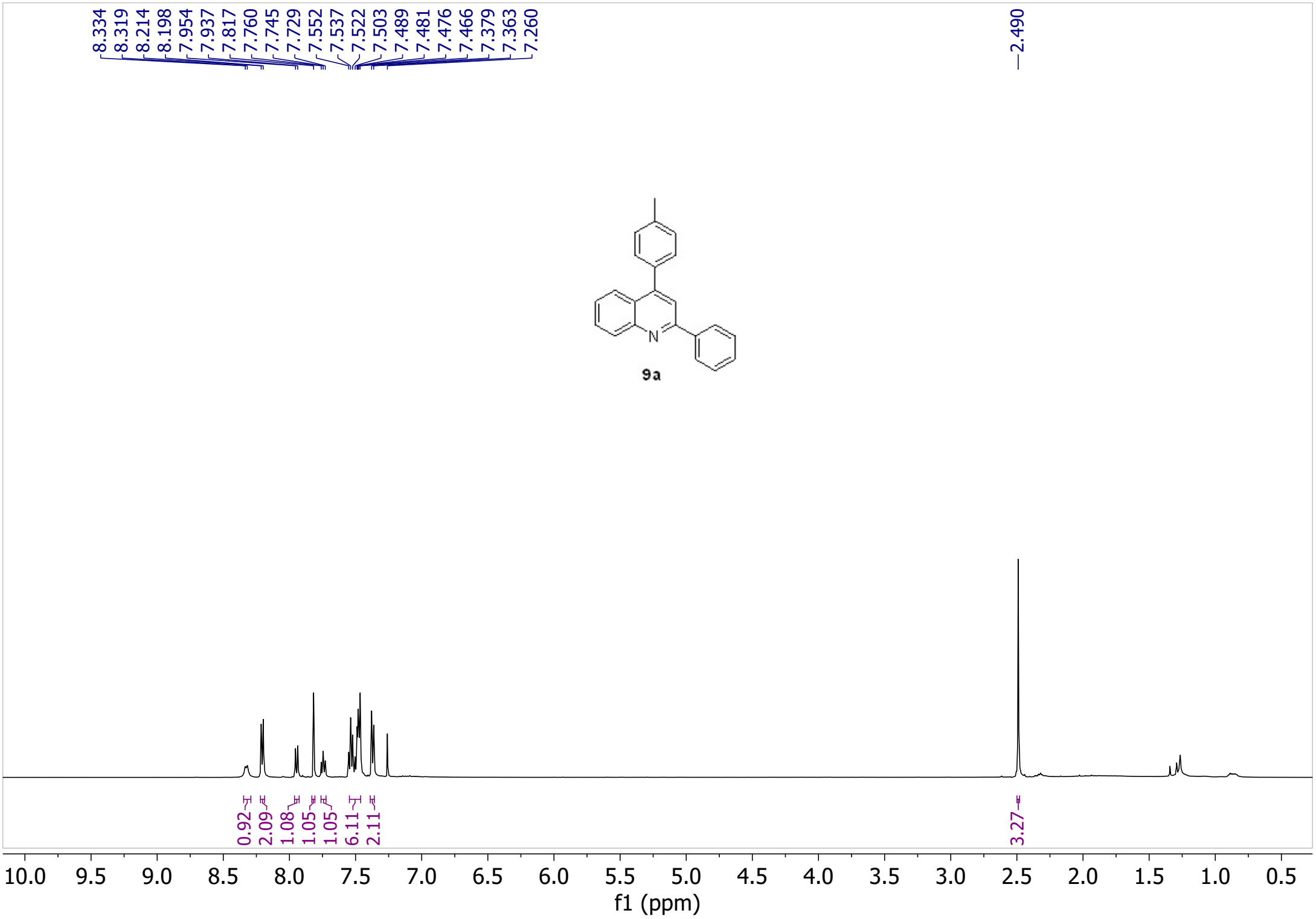
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1.08
1.05
1.05
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2.11
3.27
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8.5
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7.5
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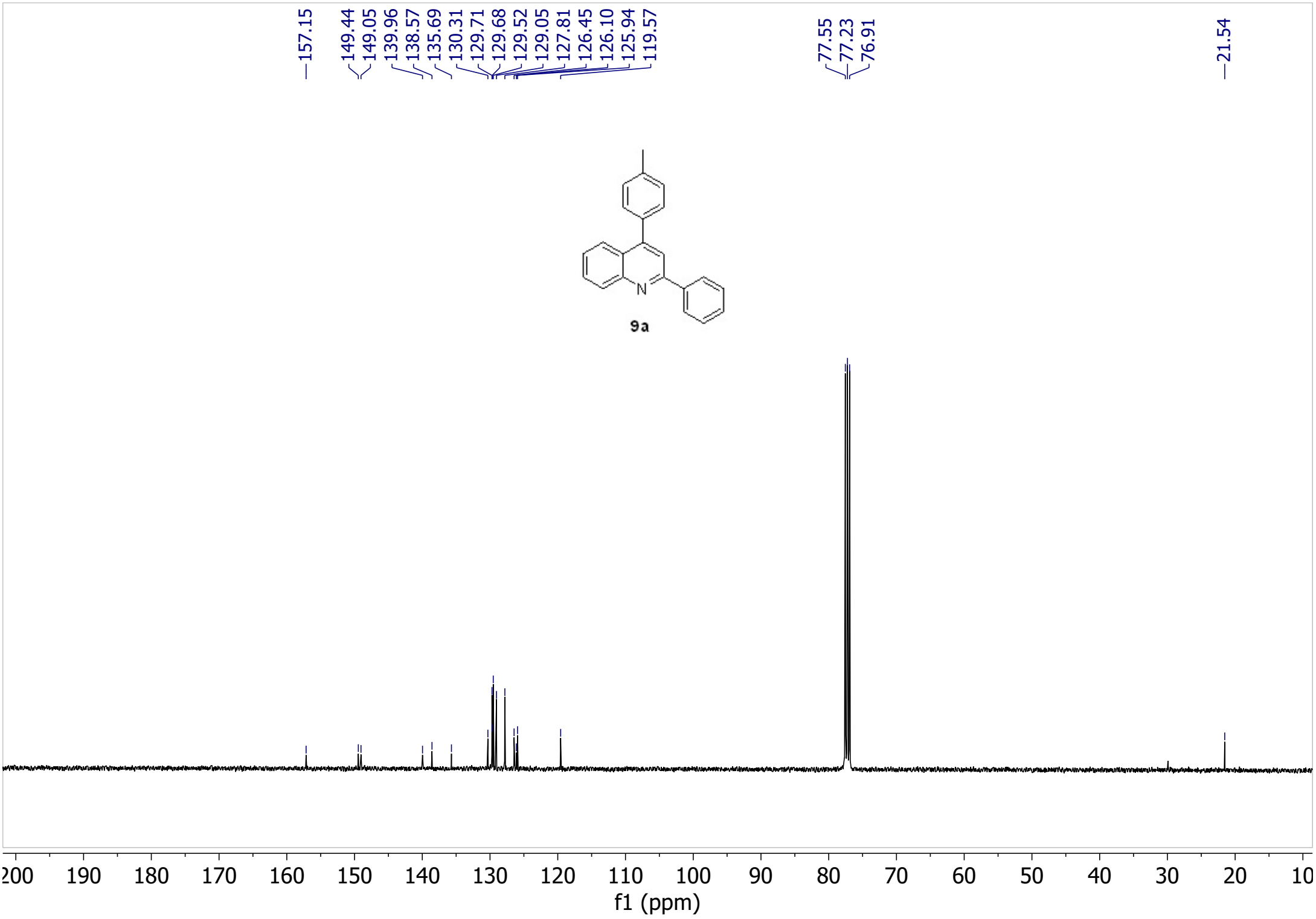
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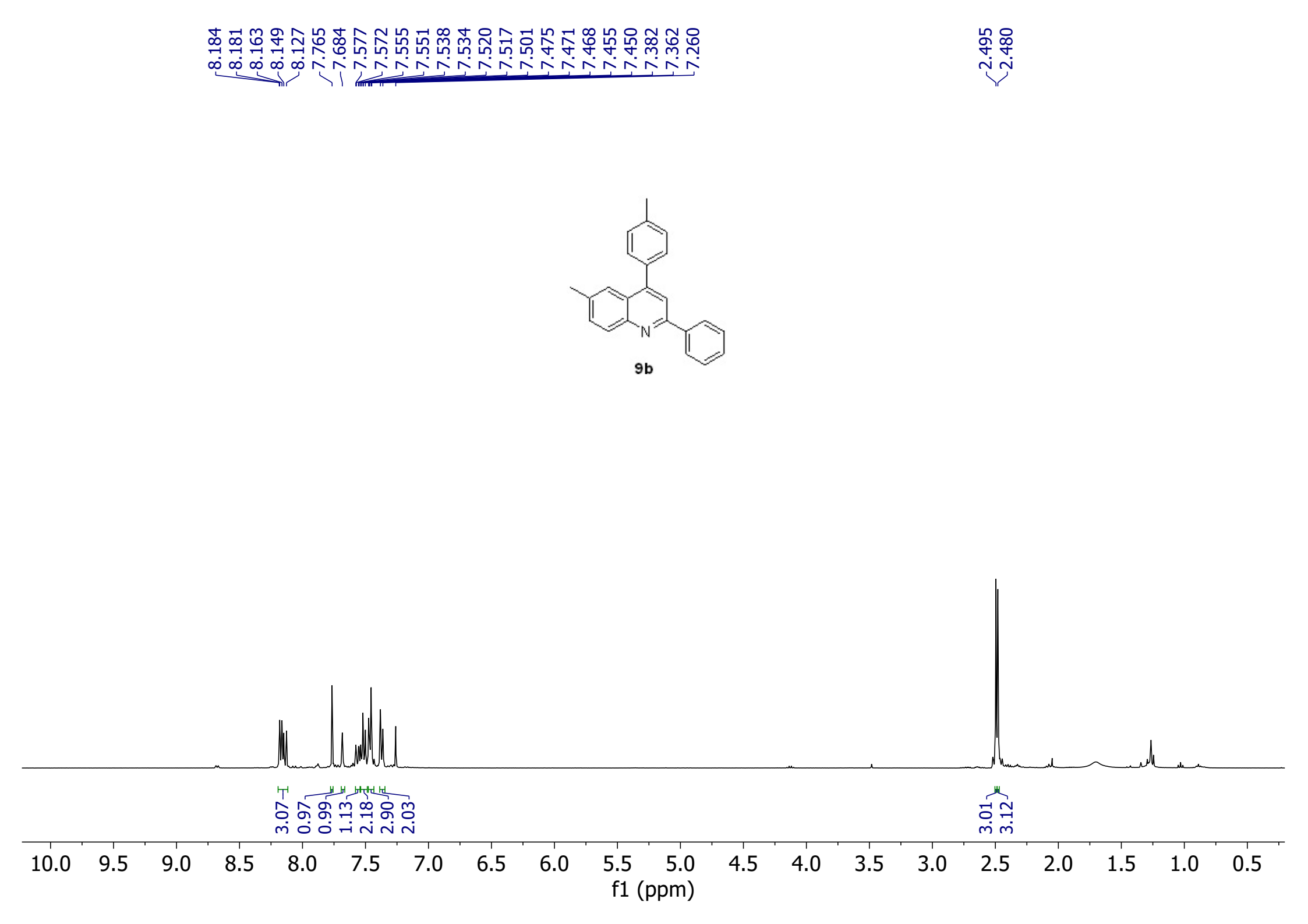
f1 (ppm)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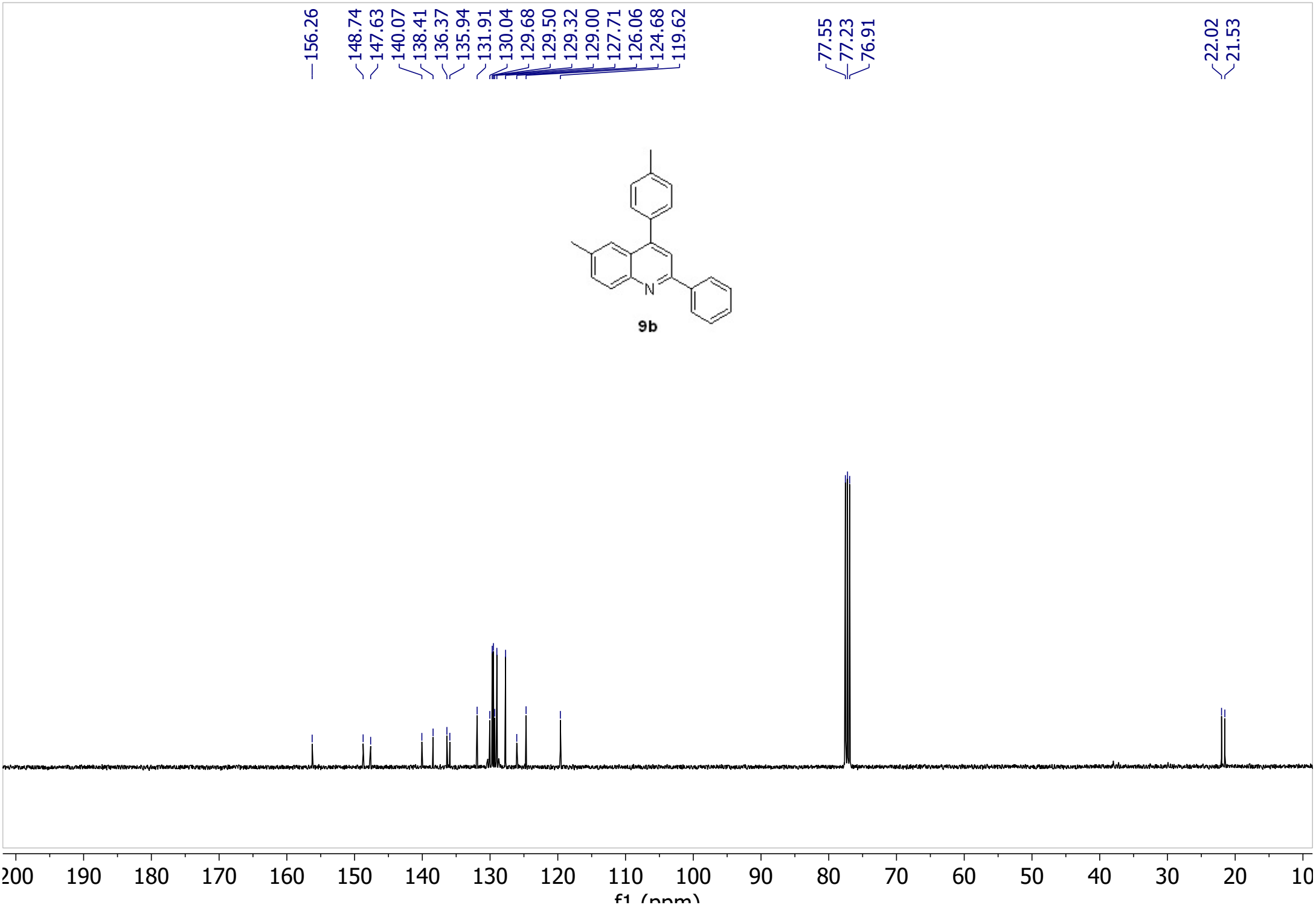
f1 (ppm)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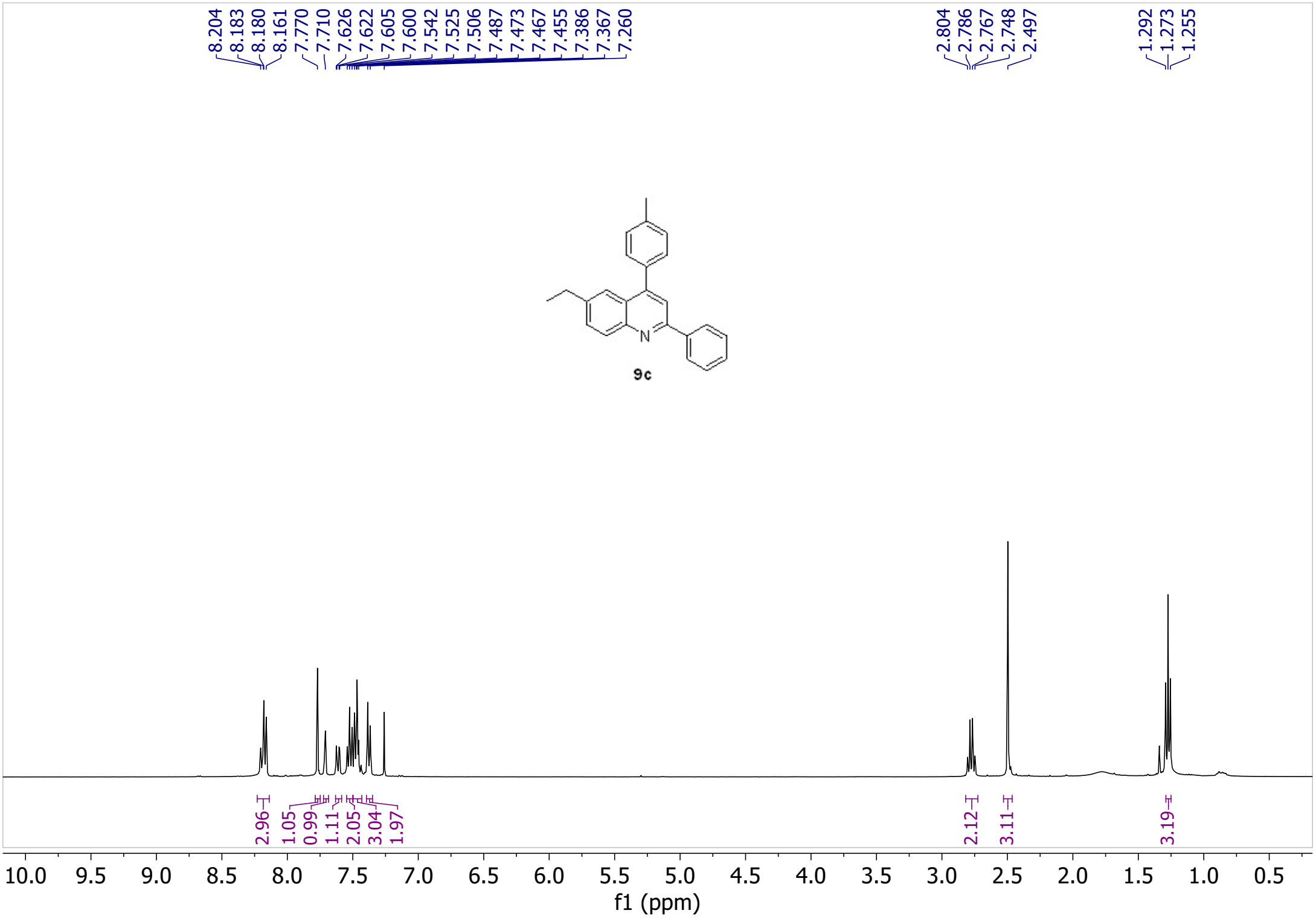
f1 (ppm)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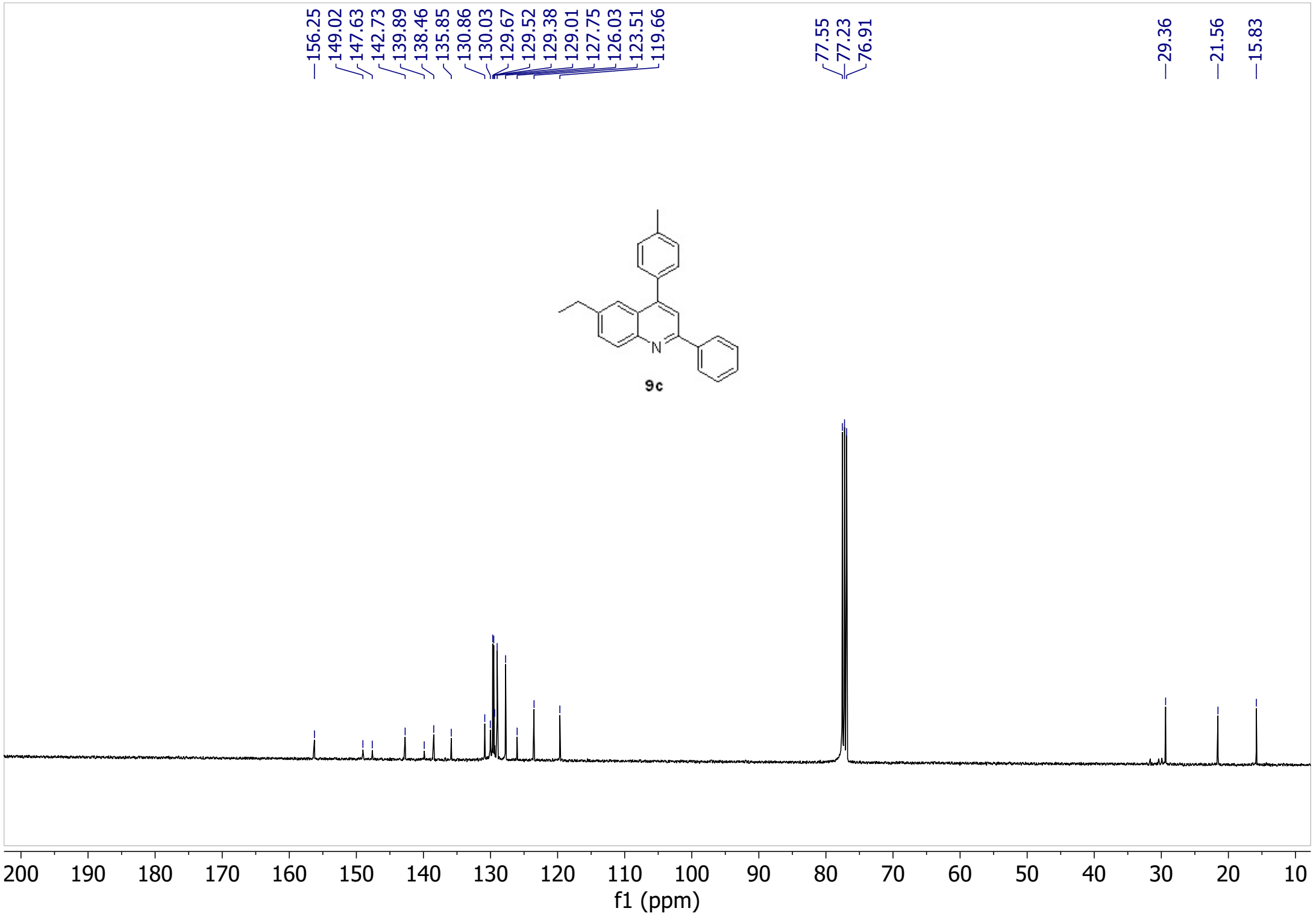
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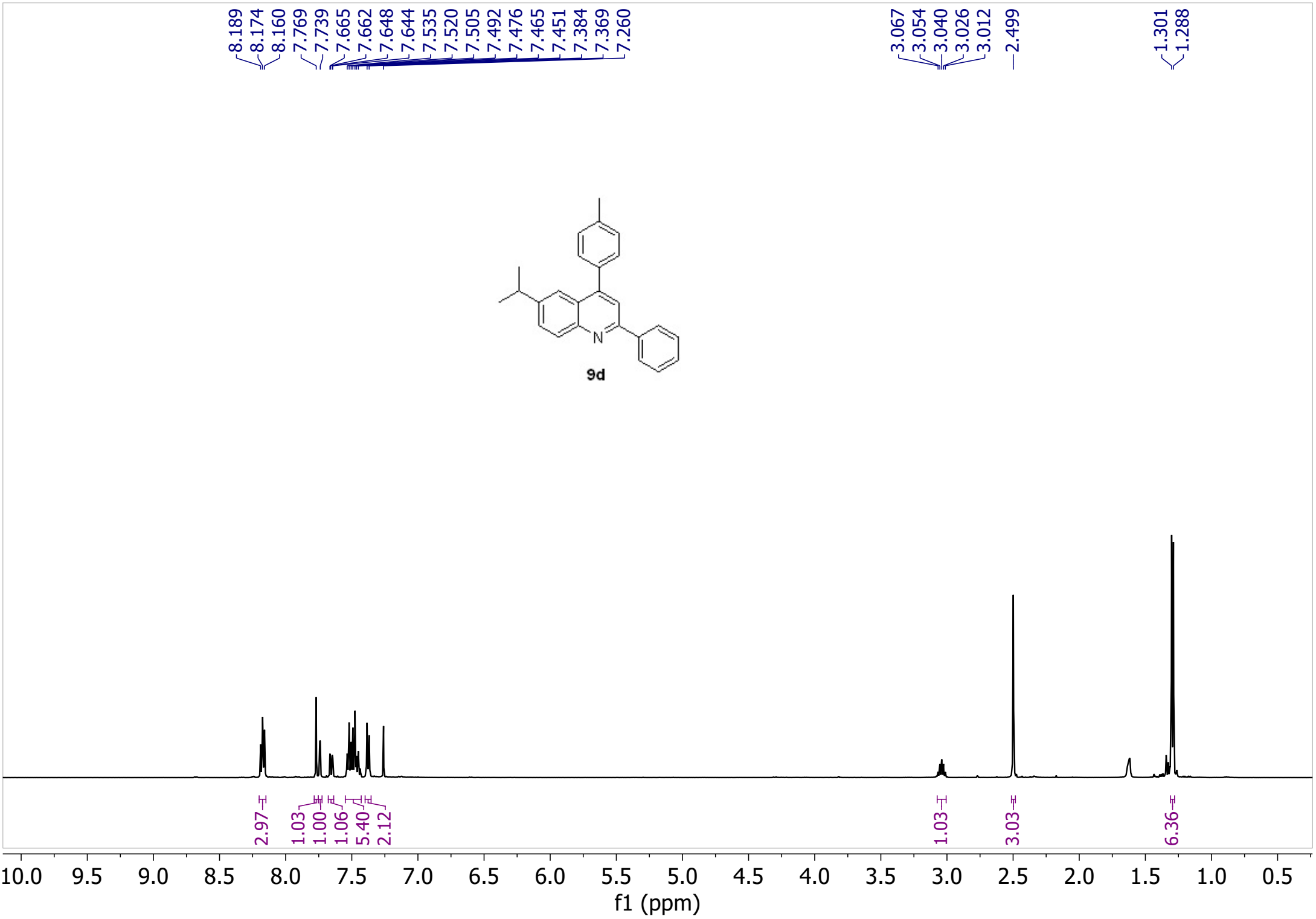
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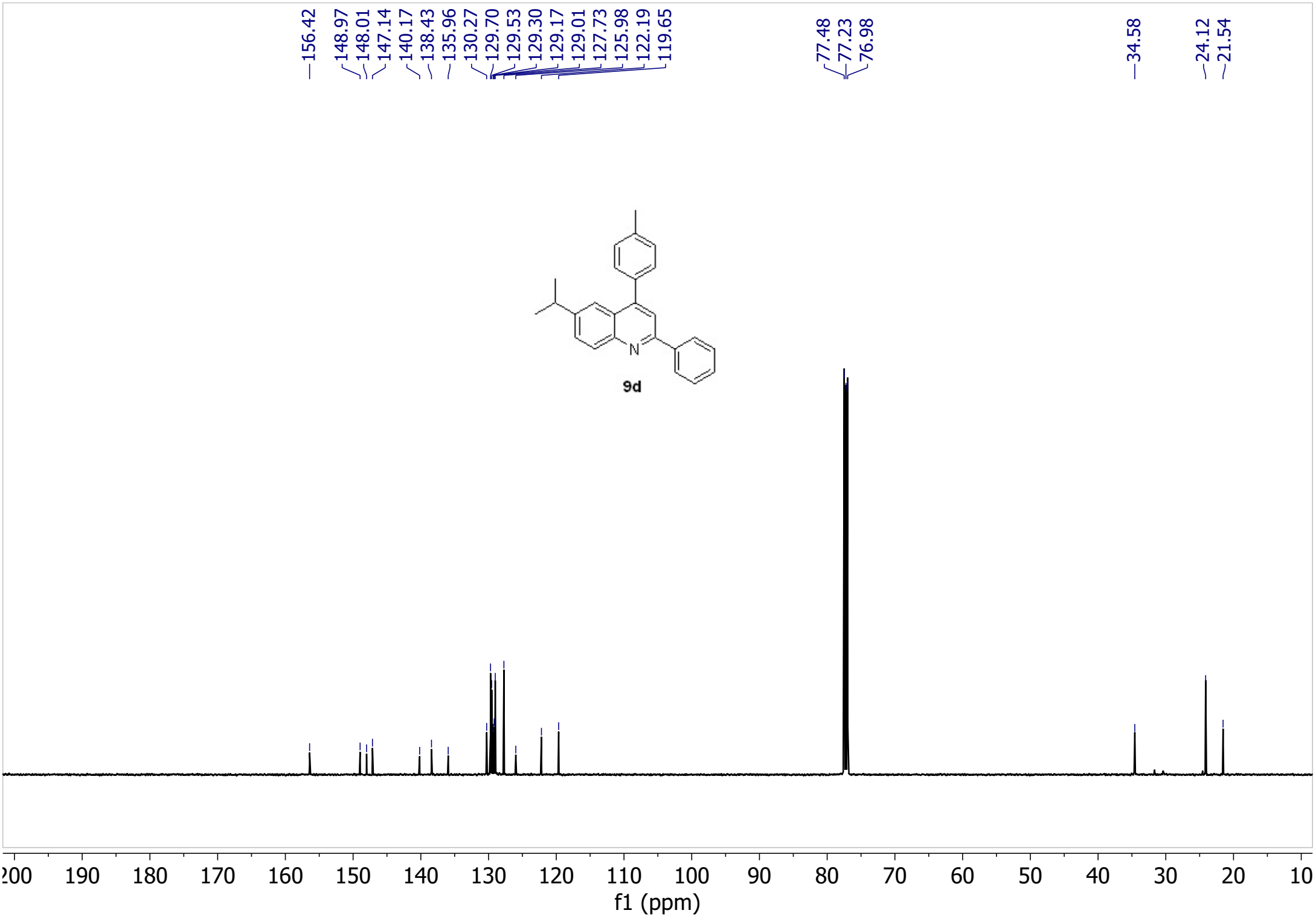
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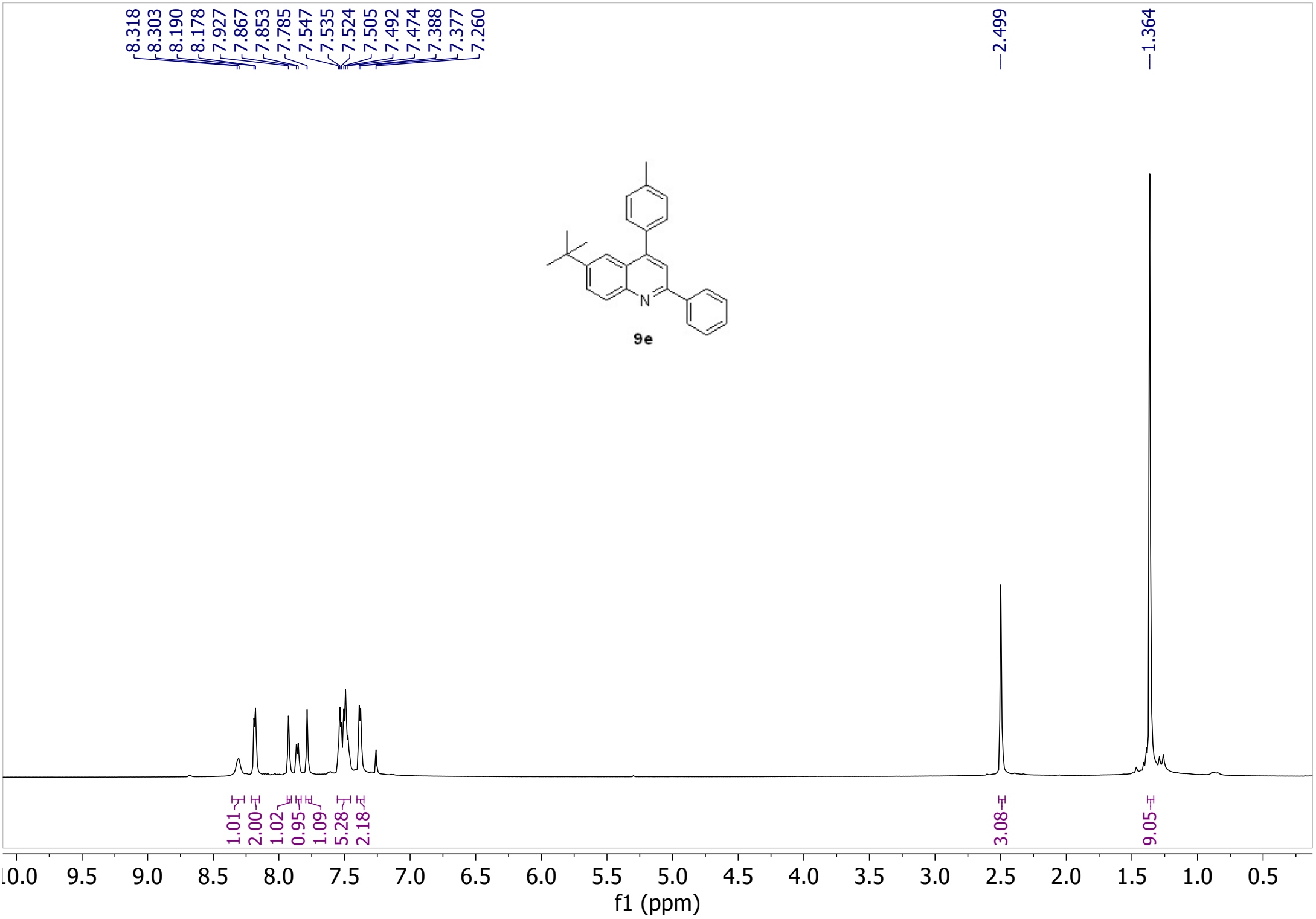
f1 (ppm)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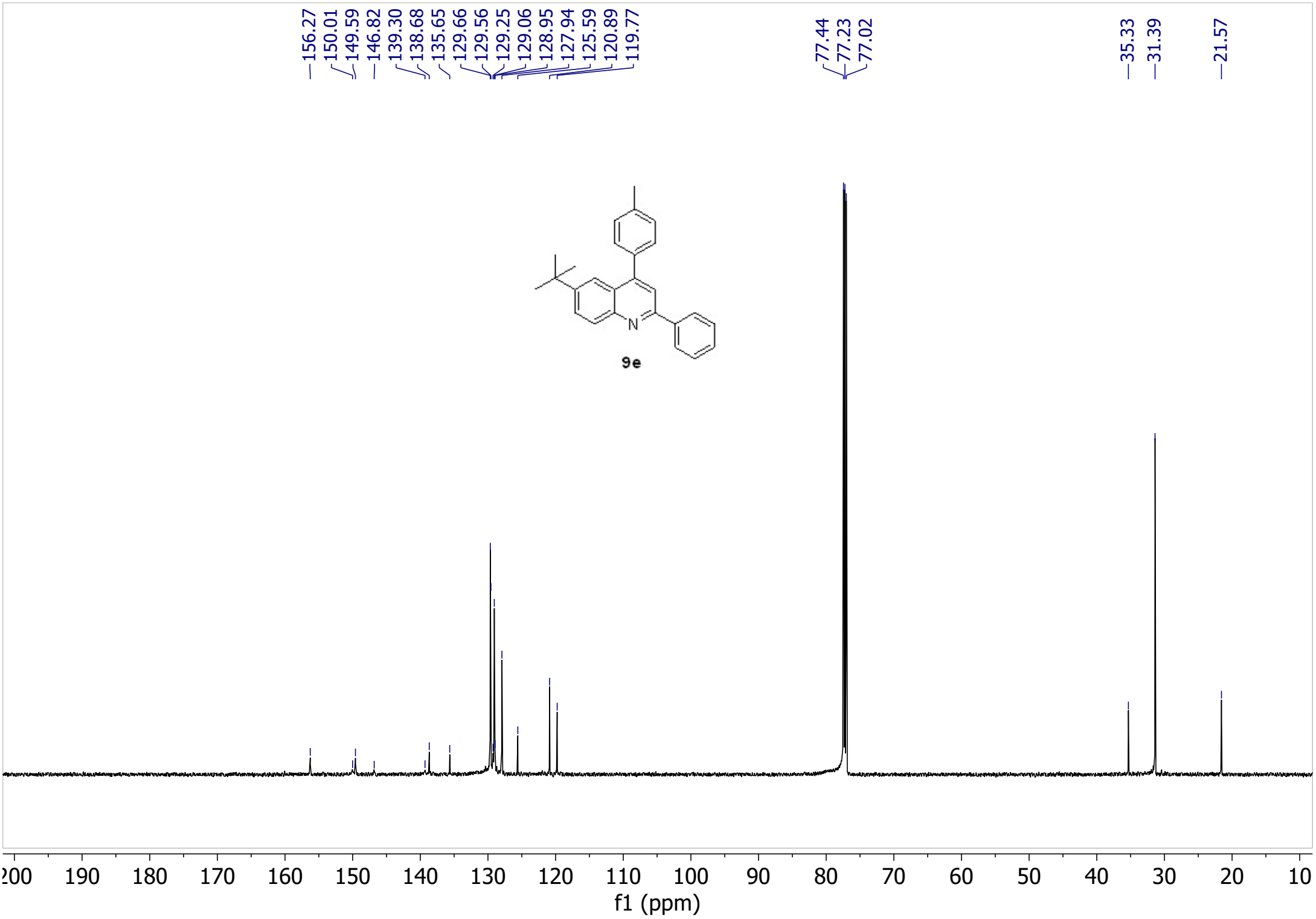
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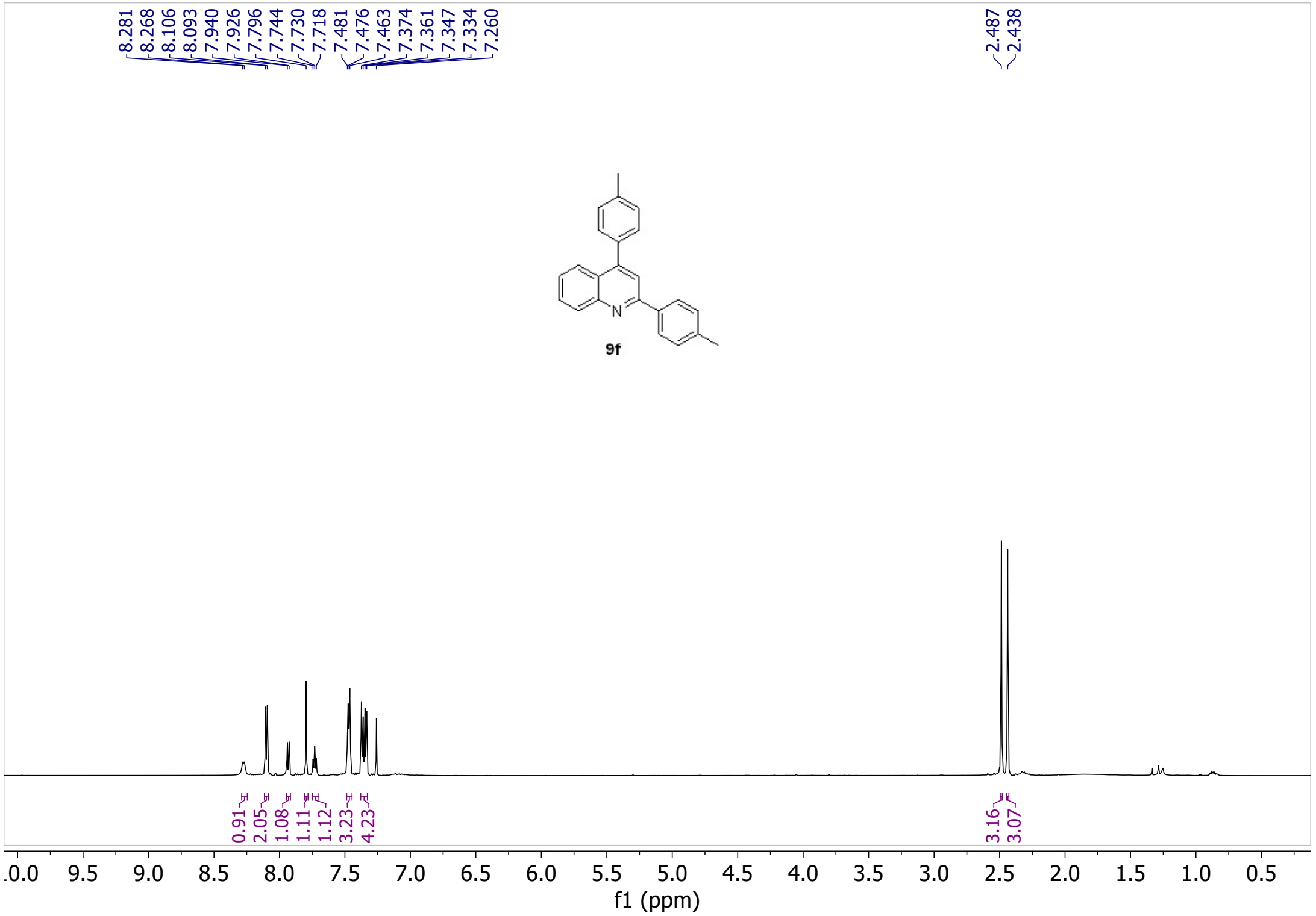
30
20
10
f1 (ppm)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7.744
7.730
7.718
7.481
7.476
7.463
7.374
7.361
7.347
7.334
7.260
2.487
2.438
N
9f
0.91
2.05
1.08
1.11
1.12
3.23
4.23
3.16
3.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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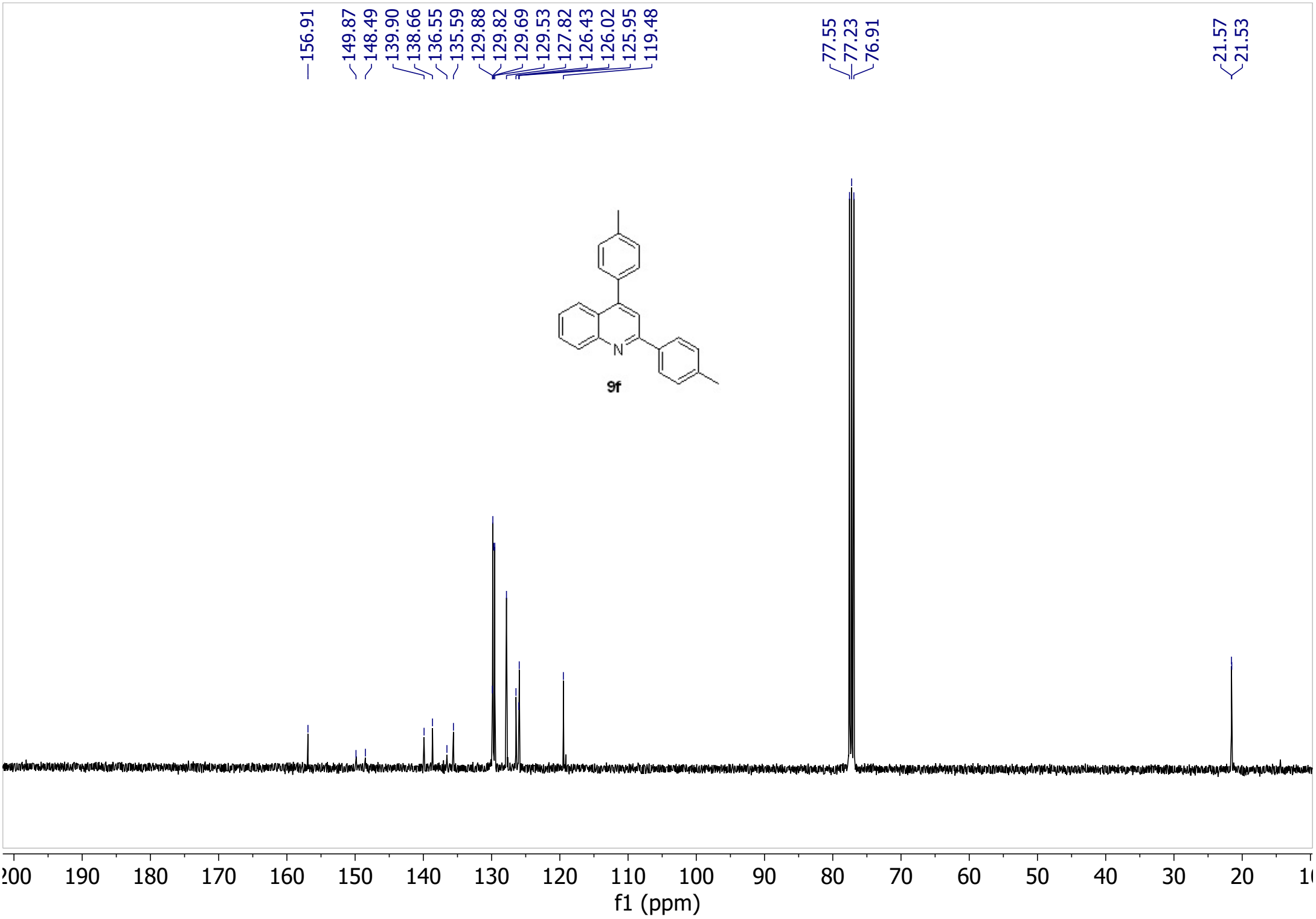
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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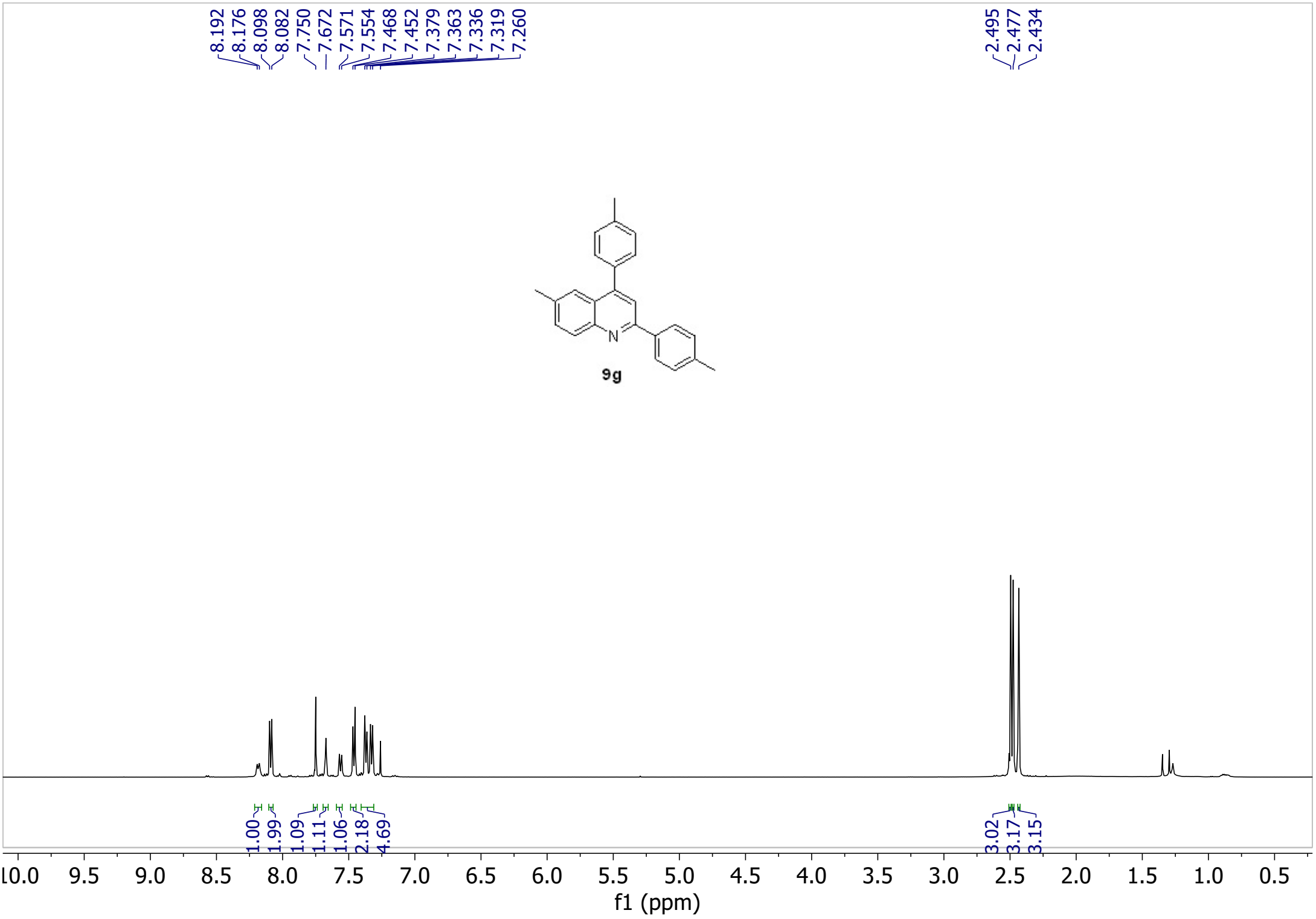
129.53
127.82
126.43
126.02
125.95
119.48
77.55
77.23
76.91
21.57
21.53
N
9f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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7.571
7.554
7.468
7.452
7.379
7.363
7.336
7.319
7.260
2.495
2.477
2.434
N
9g
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1.99
1.09
1.11
1.06
2.18
4.69
3.02
3.17
3.15
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
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3.0
2.5
2.0
1.5
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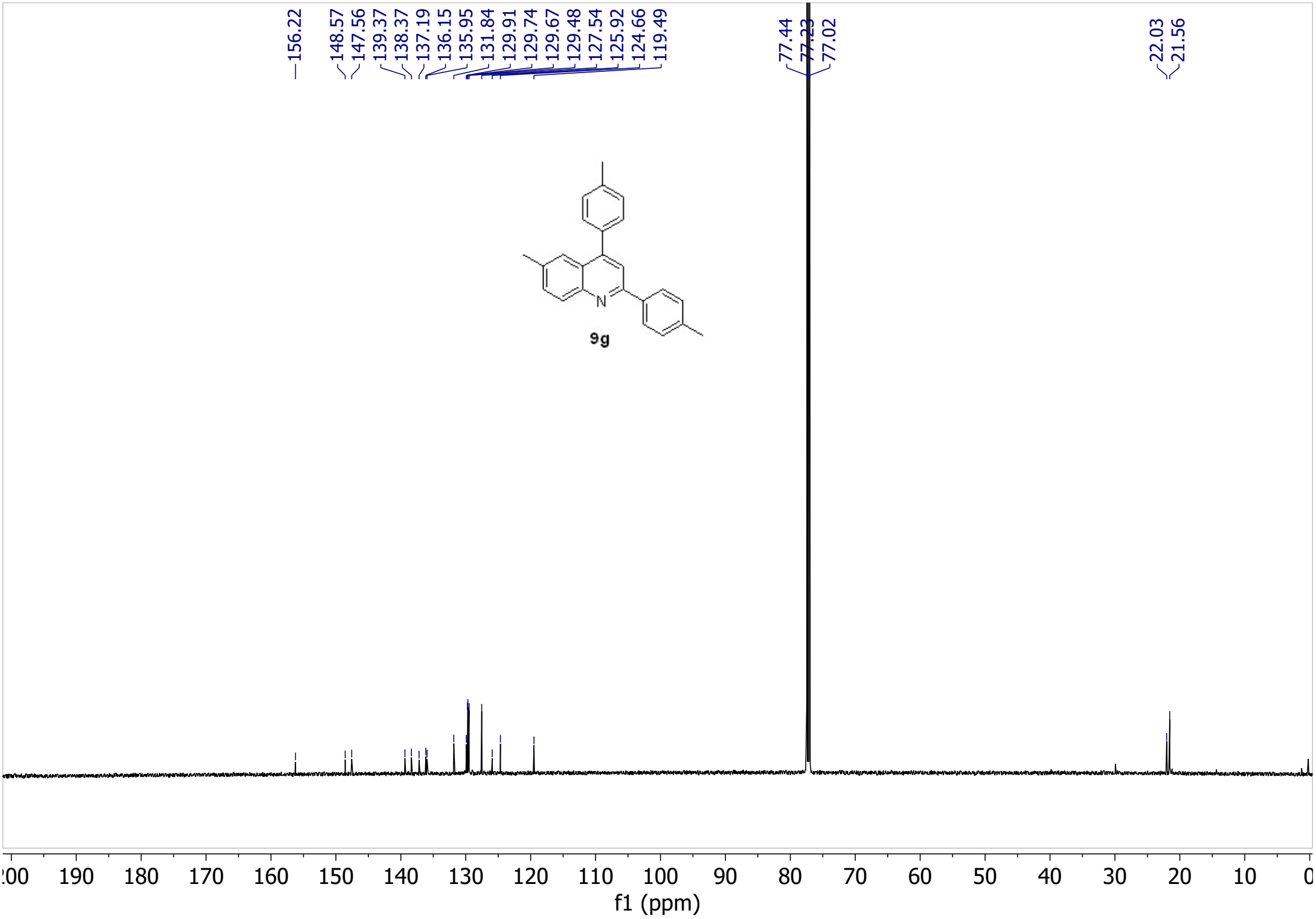
0.5
f1 (ppm)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135.95
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129.91
129.74
129.67
129.48
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124.66
119.49
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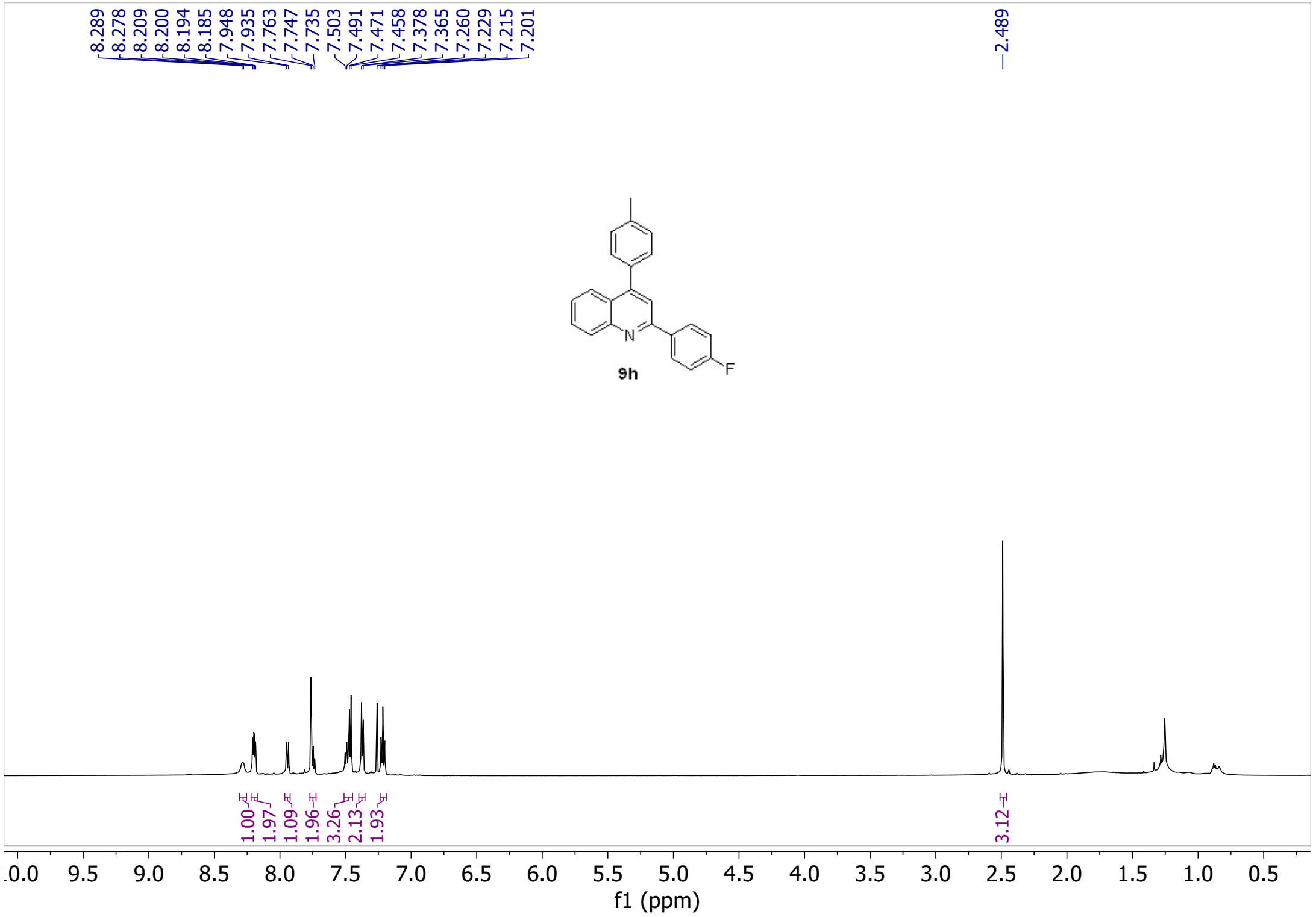
77.23
77.02
22.03
21.56
N
9g
f1 (ppm)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8.200
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8.185
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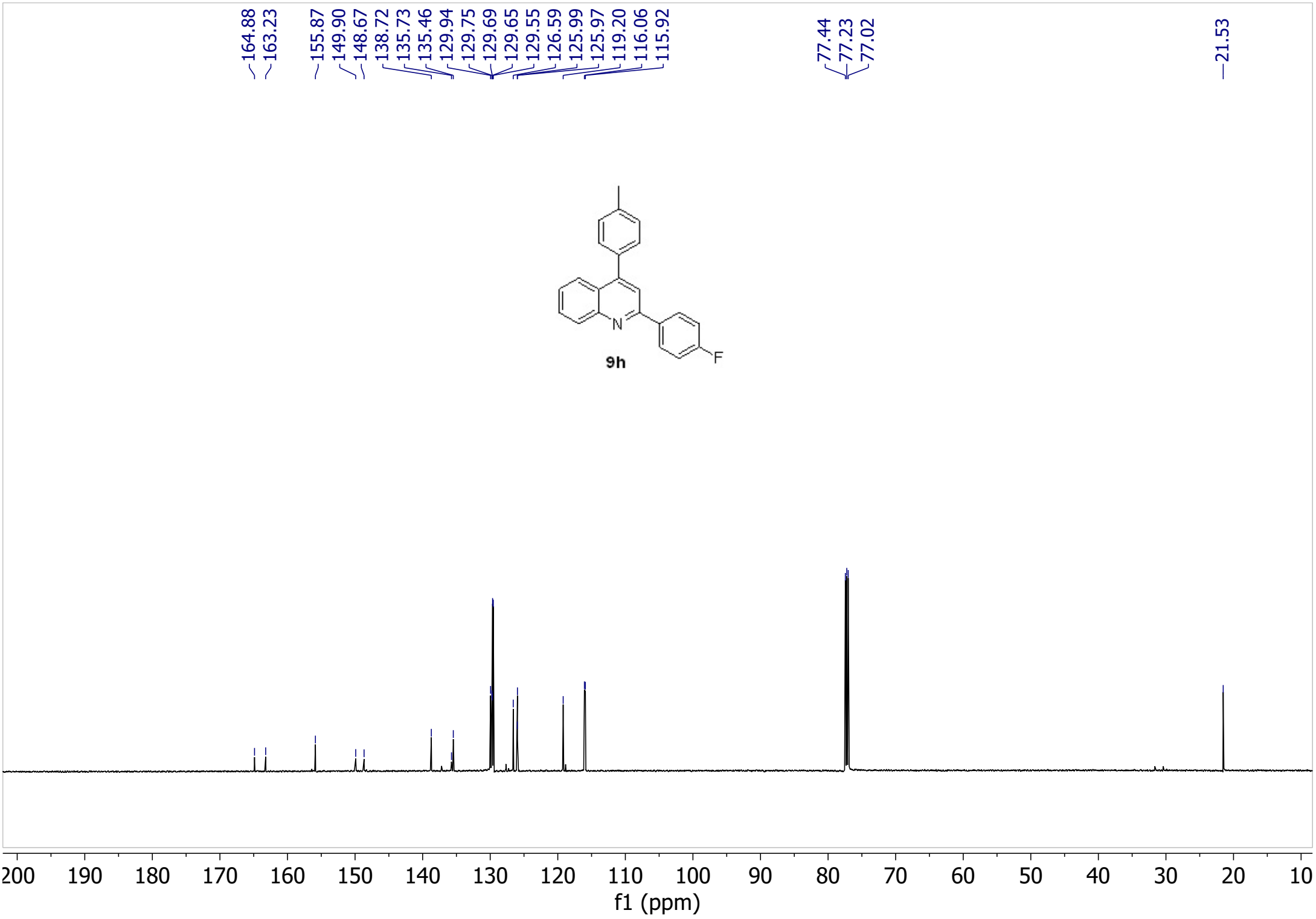
7.935
7.763
7.747
7.735
7.503
7.491
7.471
7.458
7.378
7.365
7.260
7.229
7.215
7.201
2.489
N
F
9h
1.00
1.97
1.09
1.96
3.26
2.13
1.93
3.12
f1 (ppm)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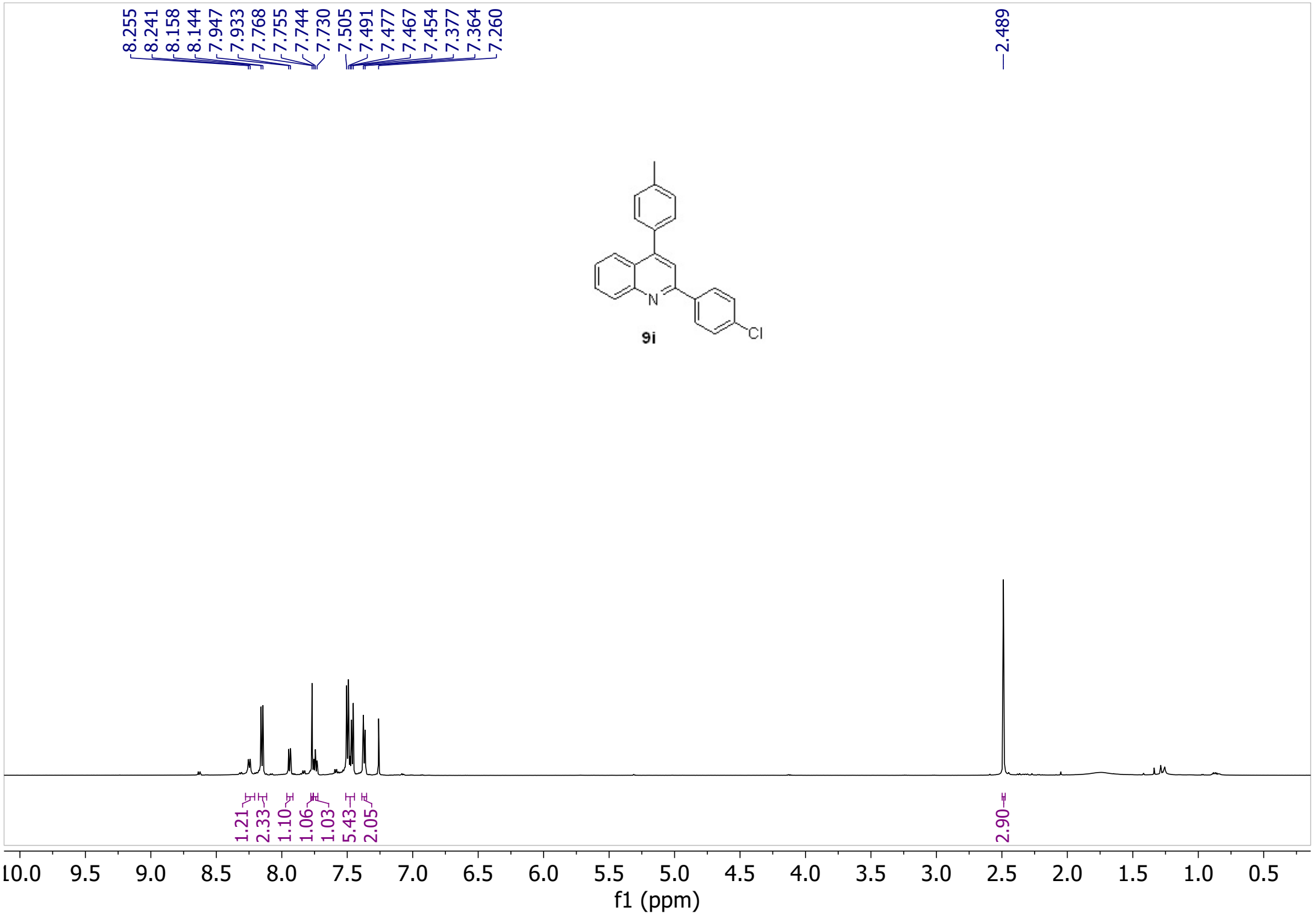
138.72
135.73
135.46
129.94
129.75
129.69
129.65
129.55
126.59
125.99
125.97
119.20
116.06
115.92
77.44
77.23
77.02
21.53
N
F
9h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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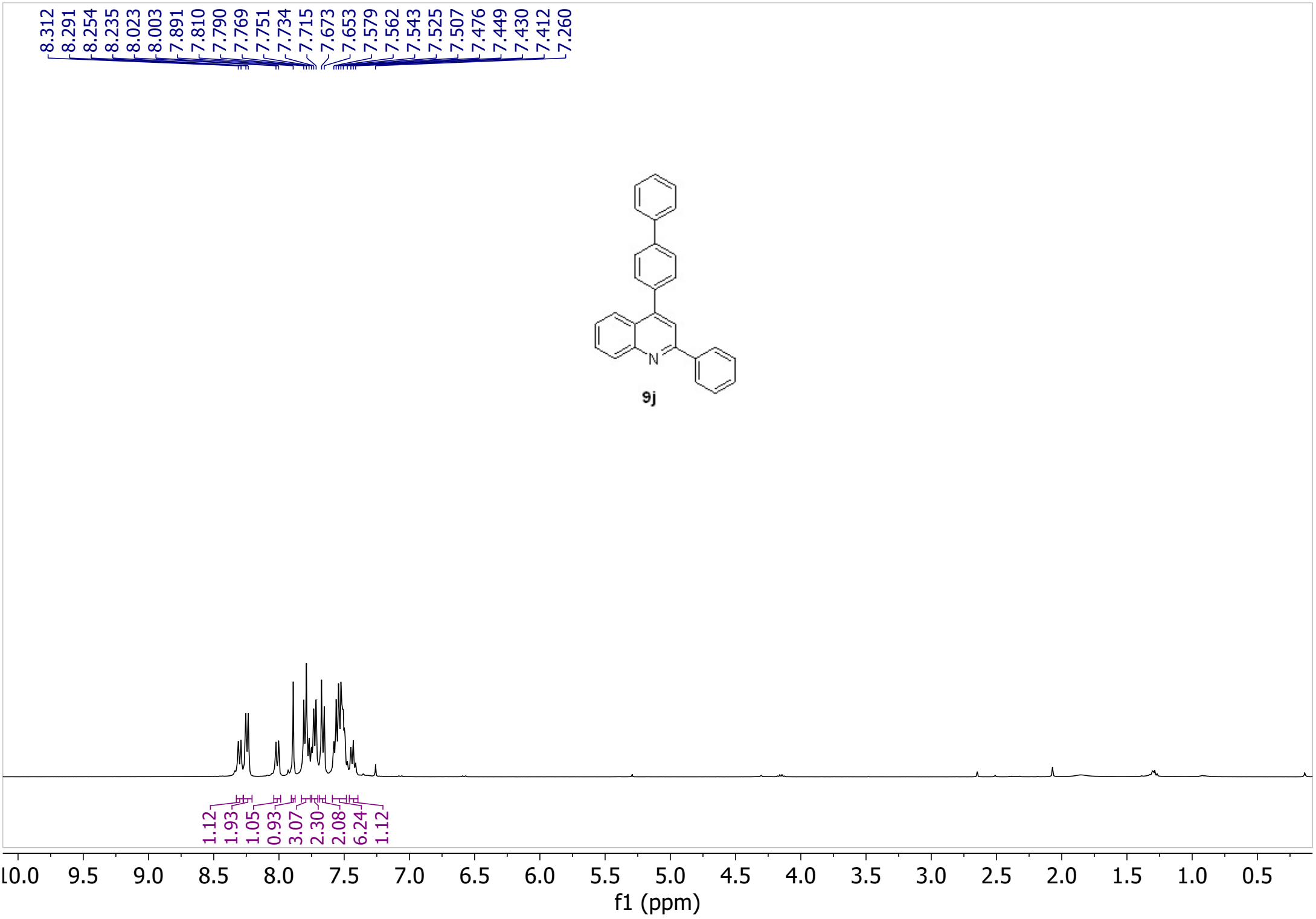
7.768
7.755
7.744
7.730
7.505
7.491
7.477
7.467
7.454
7.377
7.364
7.260
2.489
N
Cl
9i
1.21
2.33
1.10
1.06
1.03
5.43
2.05
2.90
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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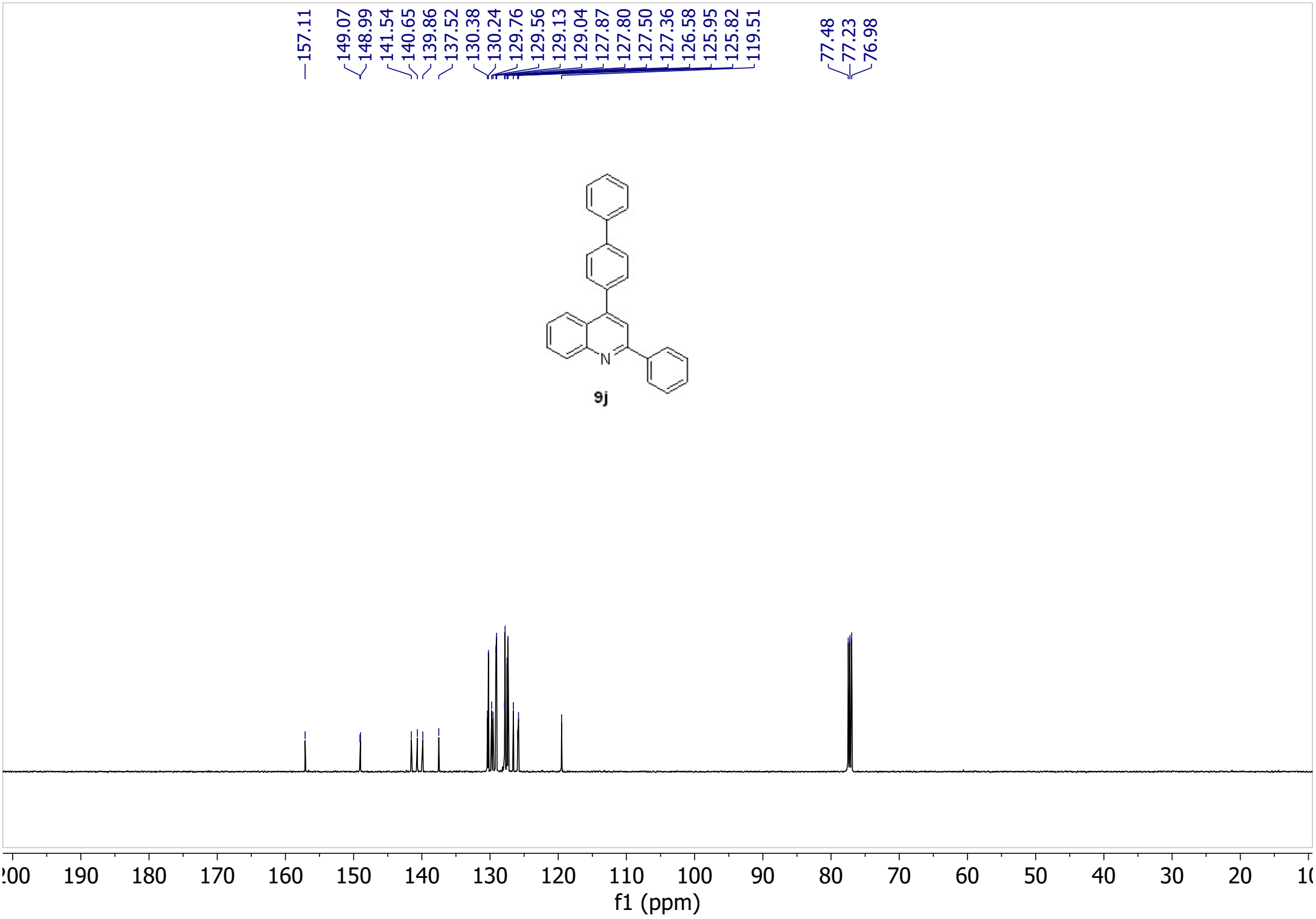
8.235
8.023
8.003
7.891
7.810
7.790
7.769
7.751
7.734
7.715
7.673
7.653
7.579
7.562
7.543
7.525
7.507
7.476
7.449
7.430
7.412
7.260
N
9j
1.12
1.93
1.05
0.93
3.07
2.30
2.08
6.24
1.12
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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140.65
139.86
137.52
130.38
130.24
129.76
129.56
129.13
129.04
127.87
127.80
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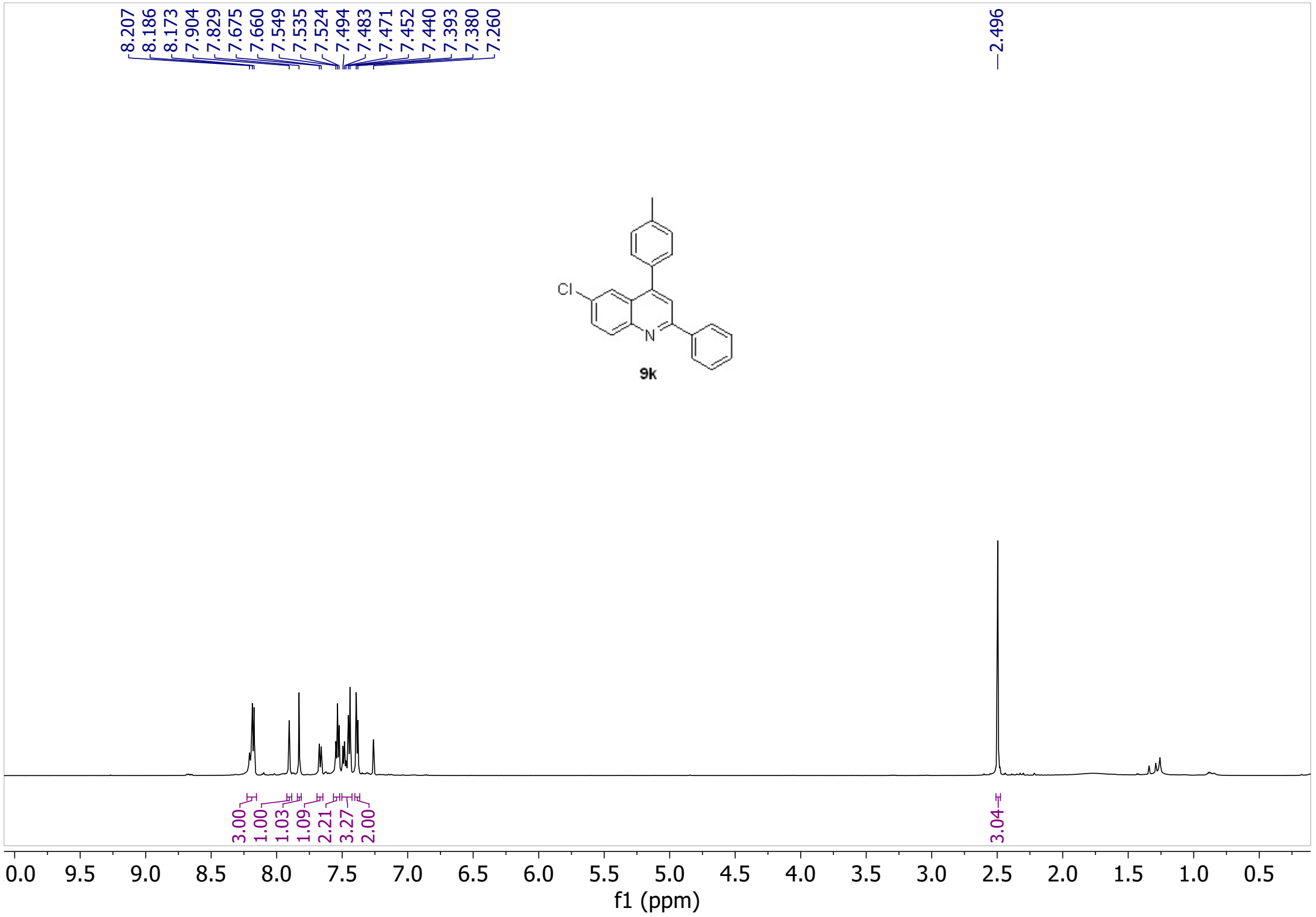
127.36
126.58
125.95
125.82
119.51
77.48
77.23
76.98
N
9j
f1 (ppm)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7.675
7.660
7.549
7.535
7.524
7.494
7.483
7.471
7.452
7.440
7.393
7.380
7.260
2.496
Cl
N
9k
3.00
1.00
1.03
1.09
2.21
3.27
2.00
3.04
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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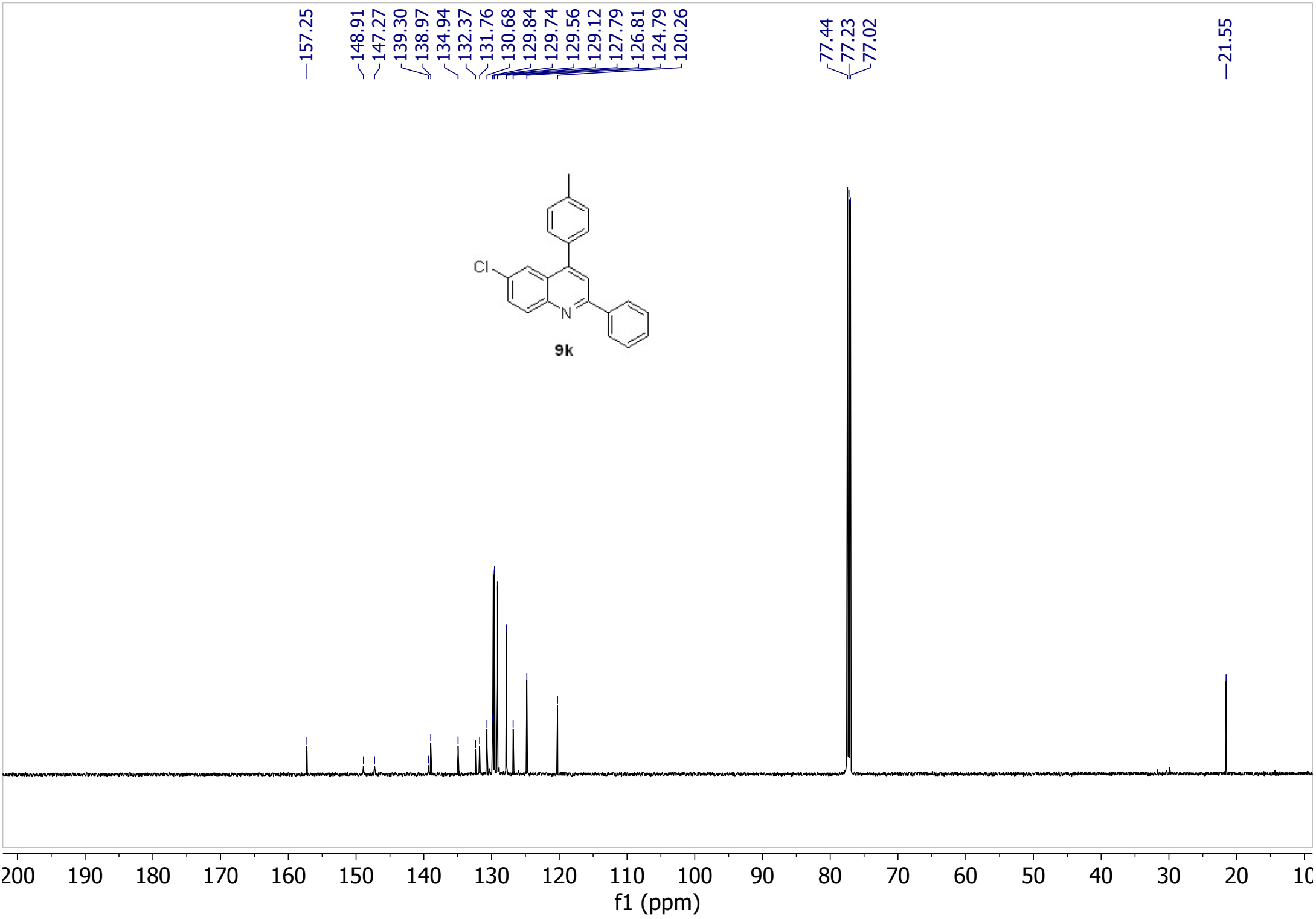
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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134.94
132.37
131.76
130.68
129.84
129.74
129.56
129.12
127.79
126.81
124.79
120.26
77.44
77.23
77.02
21.55
Cl
N
9k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

8.248
8.234
8.199
8.190
8.185
8.176
7.852
7.838
7.768
7.755
7.740
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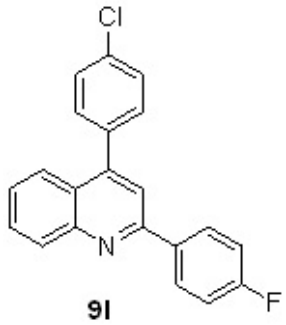
7.506
7.492
7.260
7.230
7.216
7.202

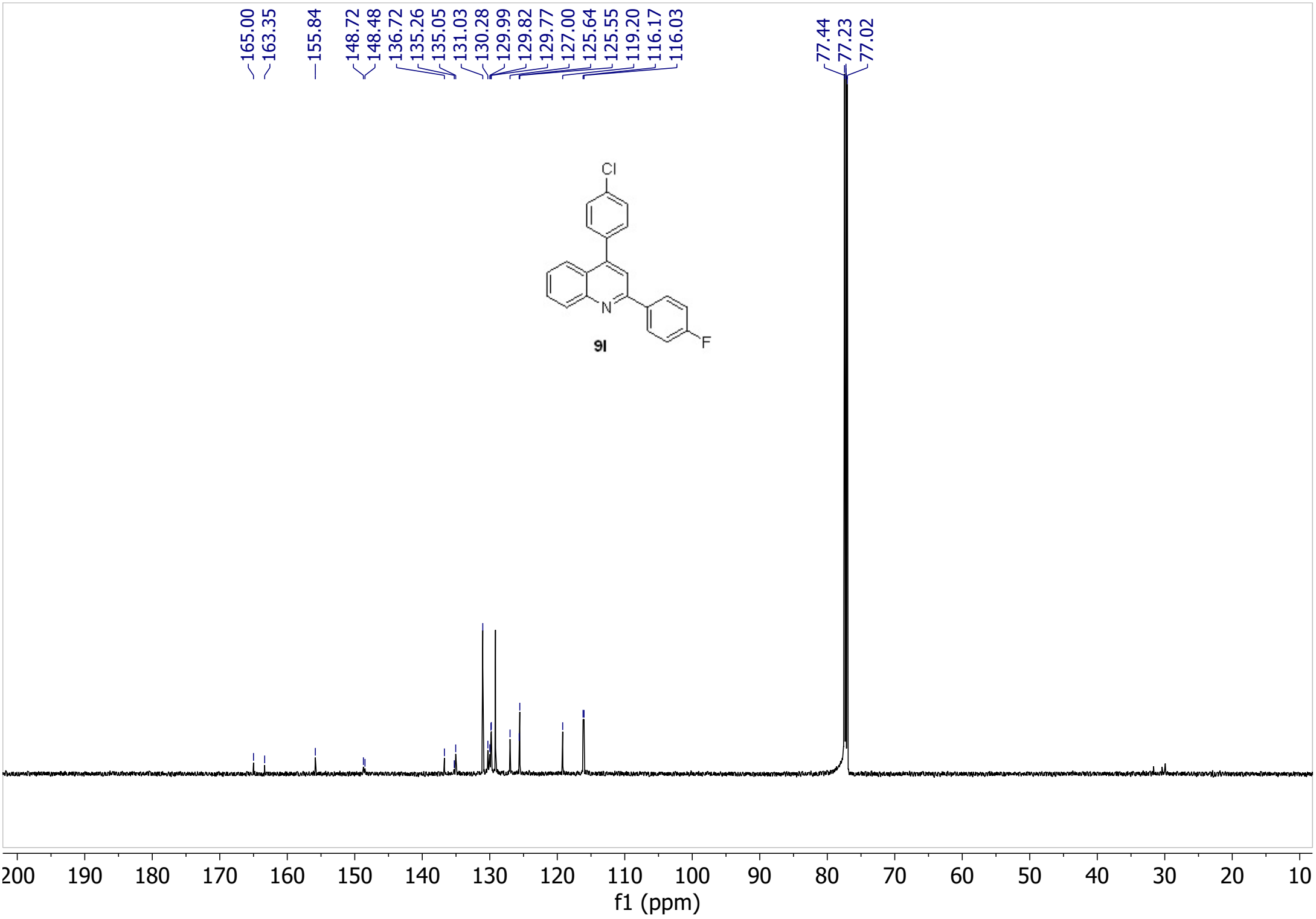


9l

1.00
1.90
1.14
2.14
5.17
1.89

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

f1 (ppm)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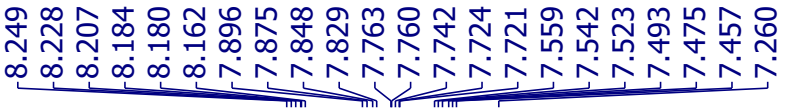
136.72
135.26
135.05
131.03
130.28
129.99
129.82
129.77
127.00
125.64
125.55
119.20
116.17
116.03
77.44
77.23
77.02
Cl
N
F
9l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.875
7.848
7.829
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7.724
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7.542
7.523
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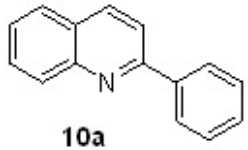
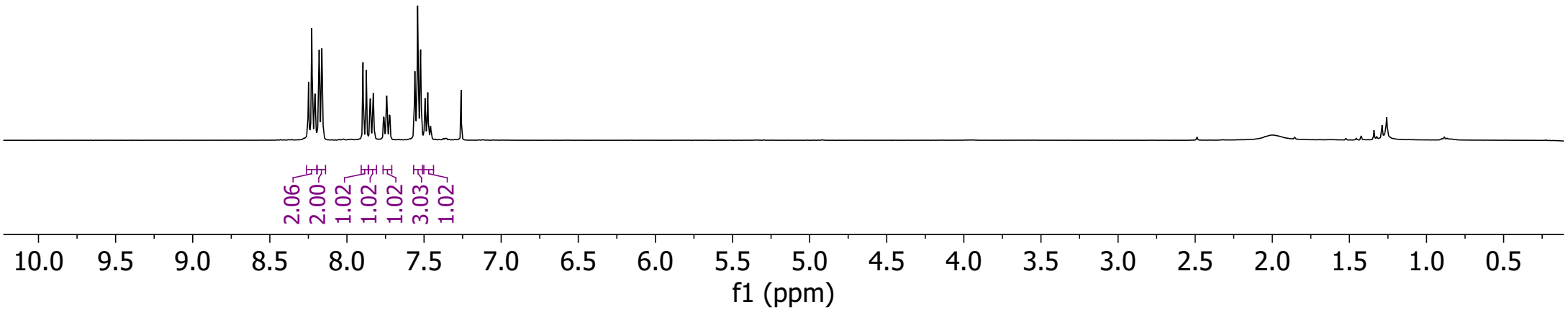
7.475
7.457
7.260


N

10a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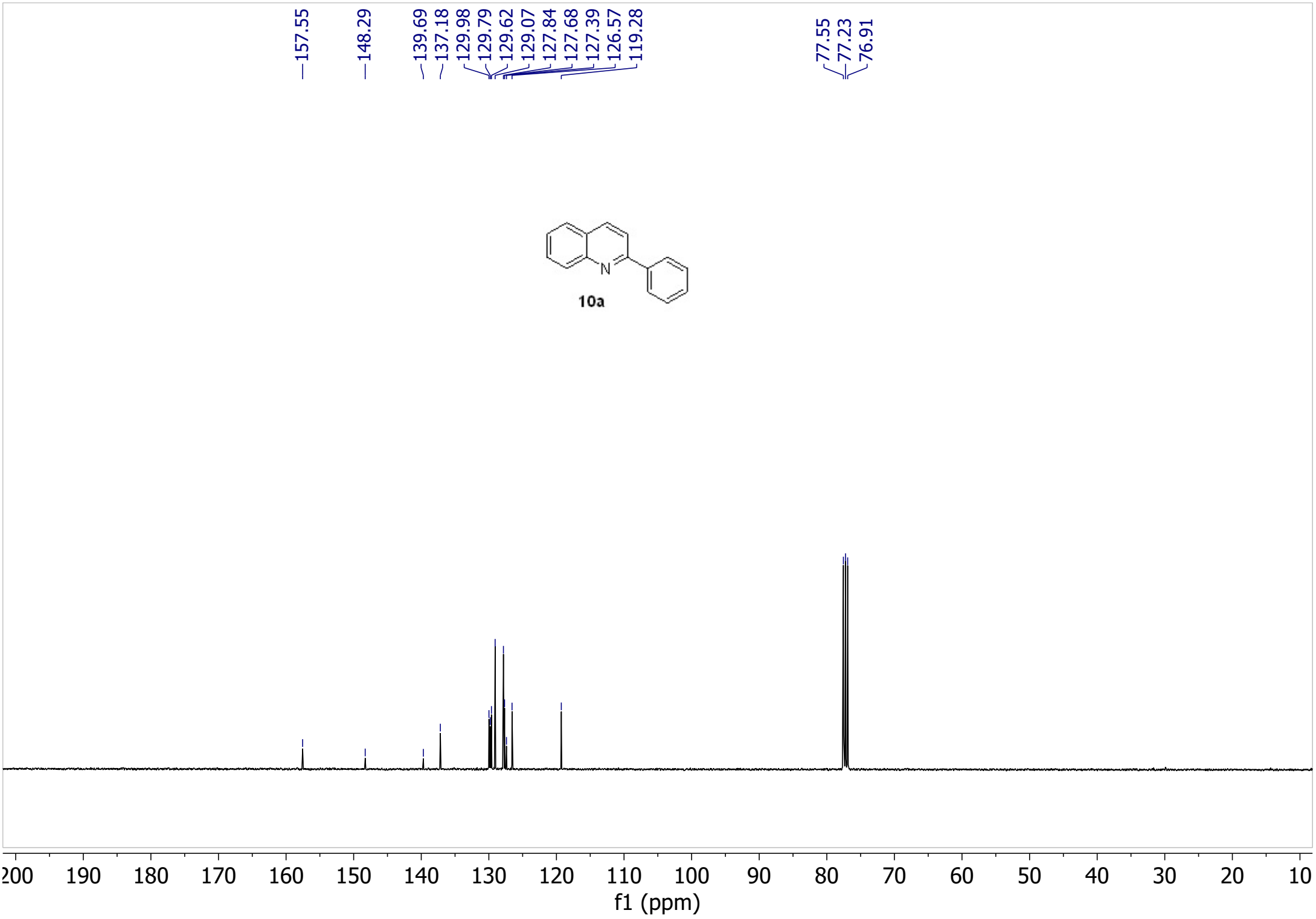
2.00
1.02
1.02
1.02
3.03
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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137.18
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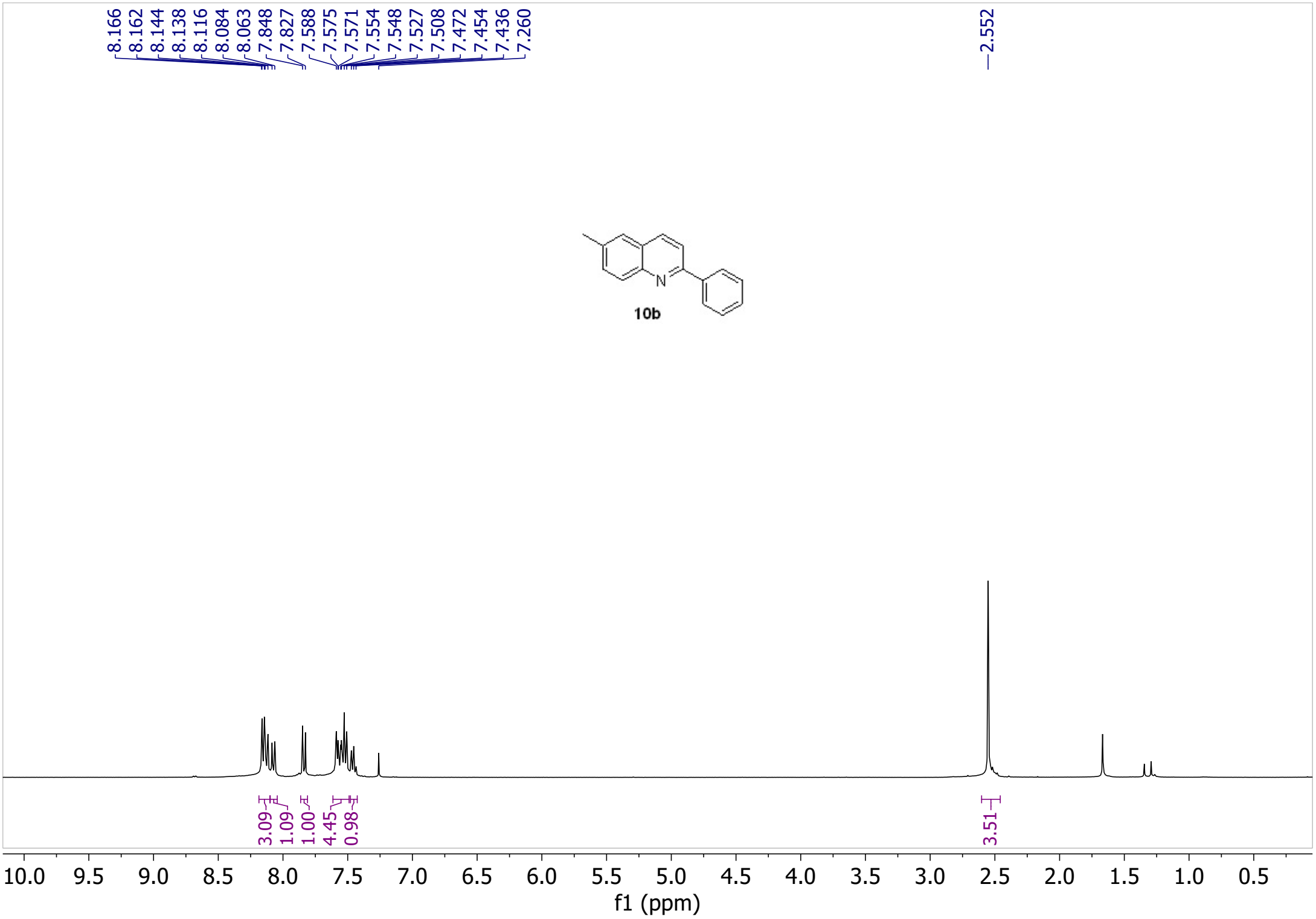
129.79
129.62
129.07
127.84
127.68
127.39
126.57
119.28
77.55
77.23
76.91
N
10a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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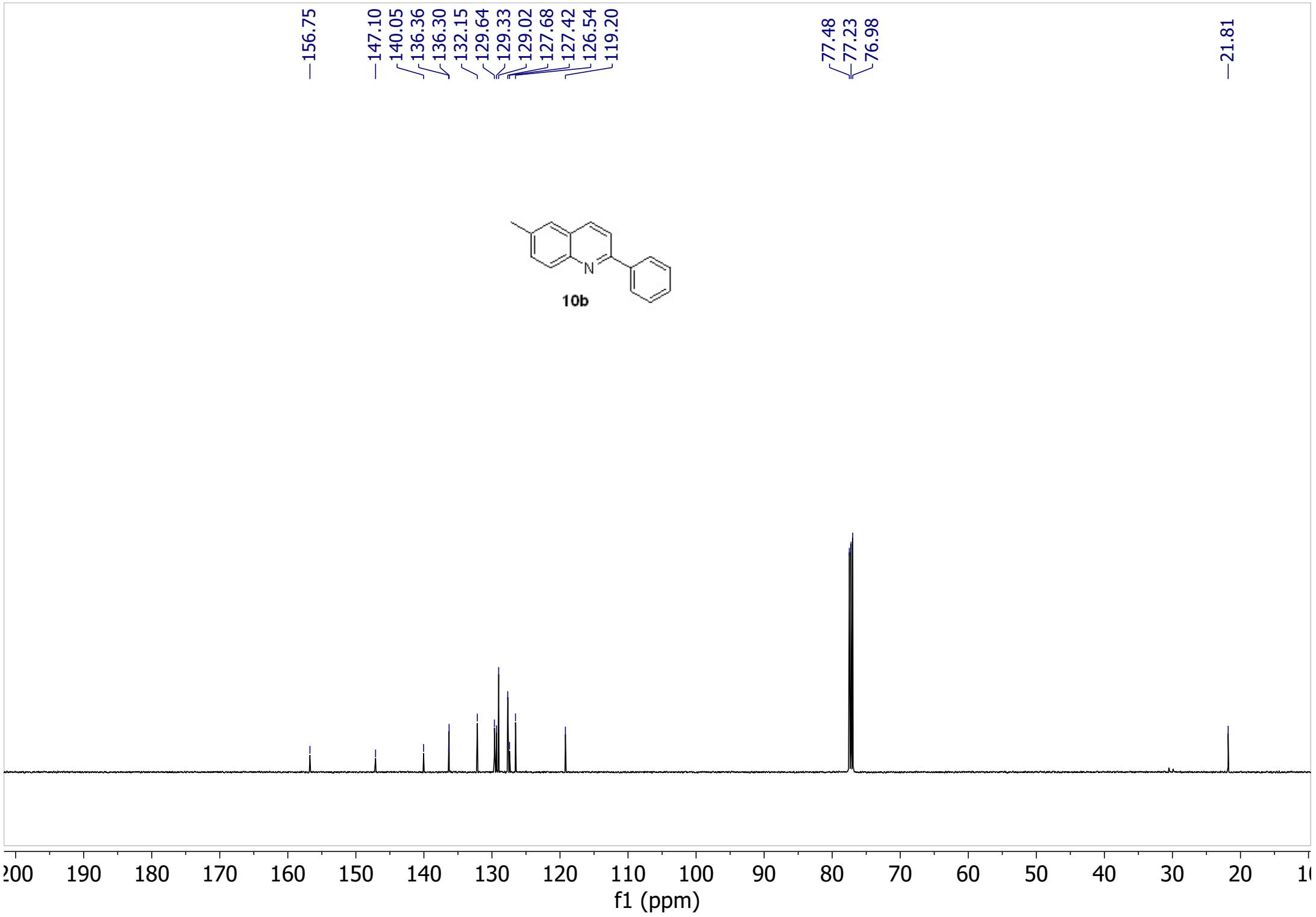
7.571
7.554
7.548
7.527
7.508
7.472
7.454
7.436
7.260
2.552
10b
3.09
1.09
1.00
4.45
0.98
3.51
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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132.15
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129.33
129.02
127.68
127.42
126.54
119.20
77.48
77.23
76.98
21.81
N
10b
200
190
180
170
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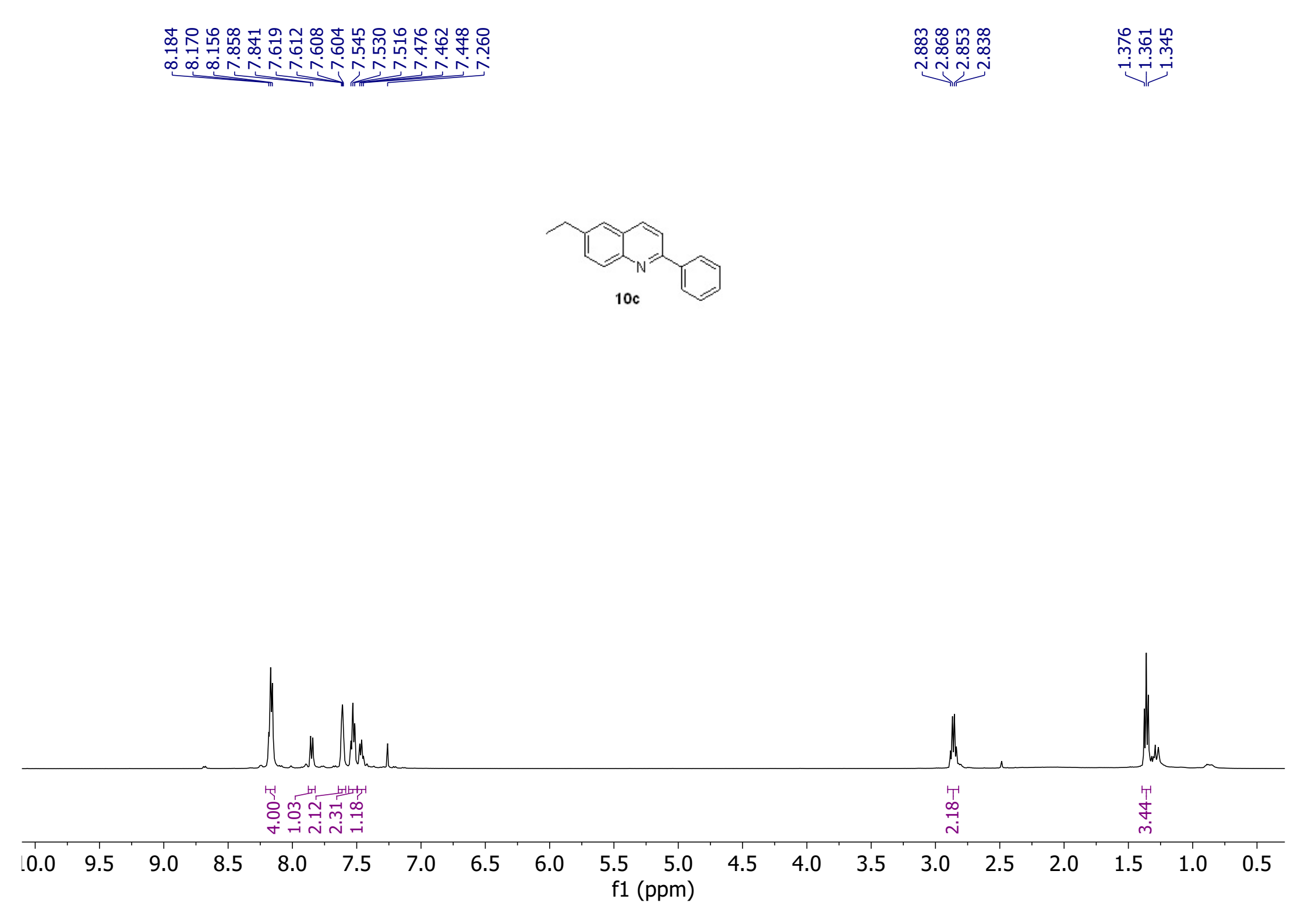
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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7.530
7.516
7.476
7.462
7.448
7.260
2.883
2.868
2.853
2.838
1.376
1.361
1.345
N
10c
4.00
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2.12
2.31
1.18
2.18
3.44
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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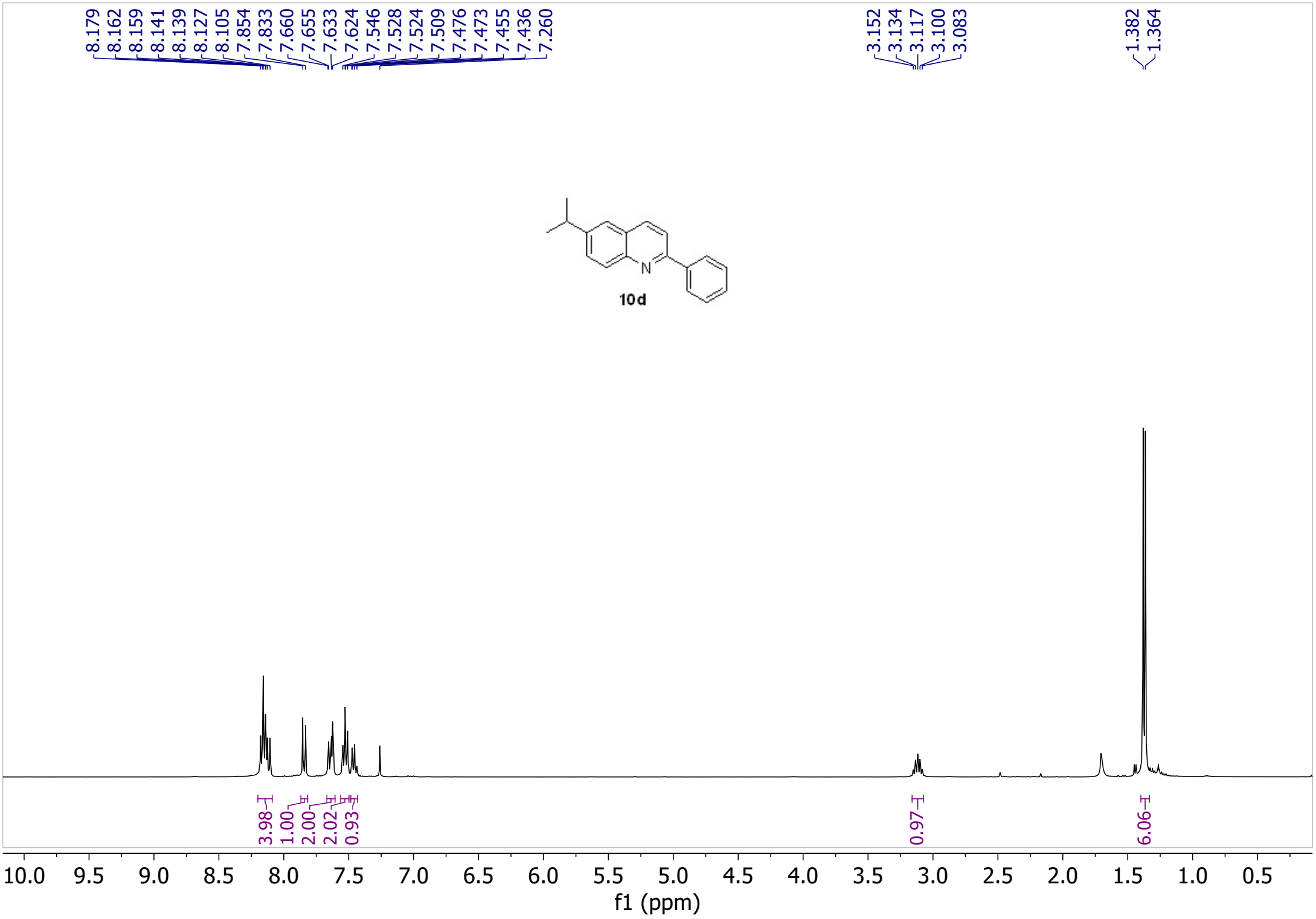
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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7.624
7.546
7.528
7.524
7.509
7.476
7.473
7.455
7.436
7.260
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3.134
3.117
3.100
3.083
1.382
1.364
N
10d
3.98
1.00
2.00
2.02
0.93
0.97
6.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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4.0
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3.0
2.5
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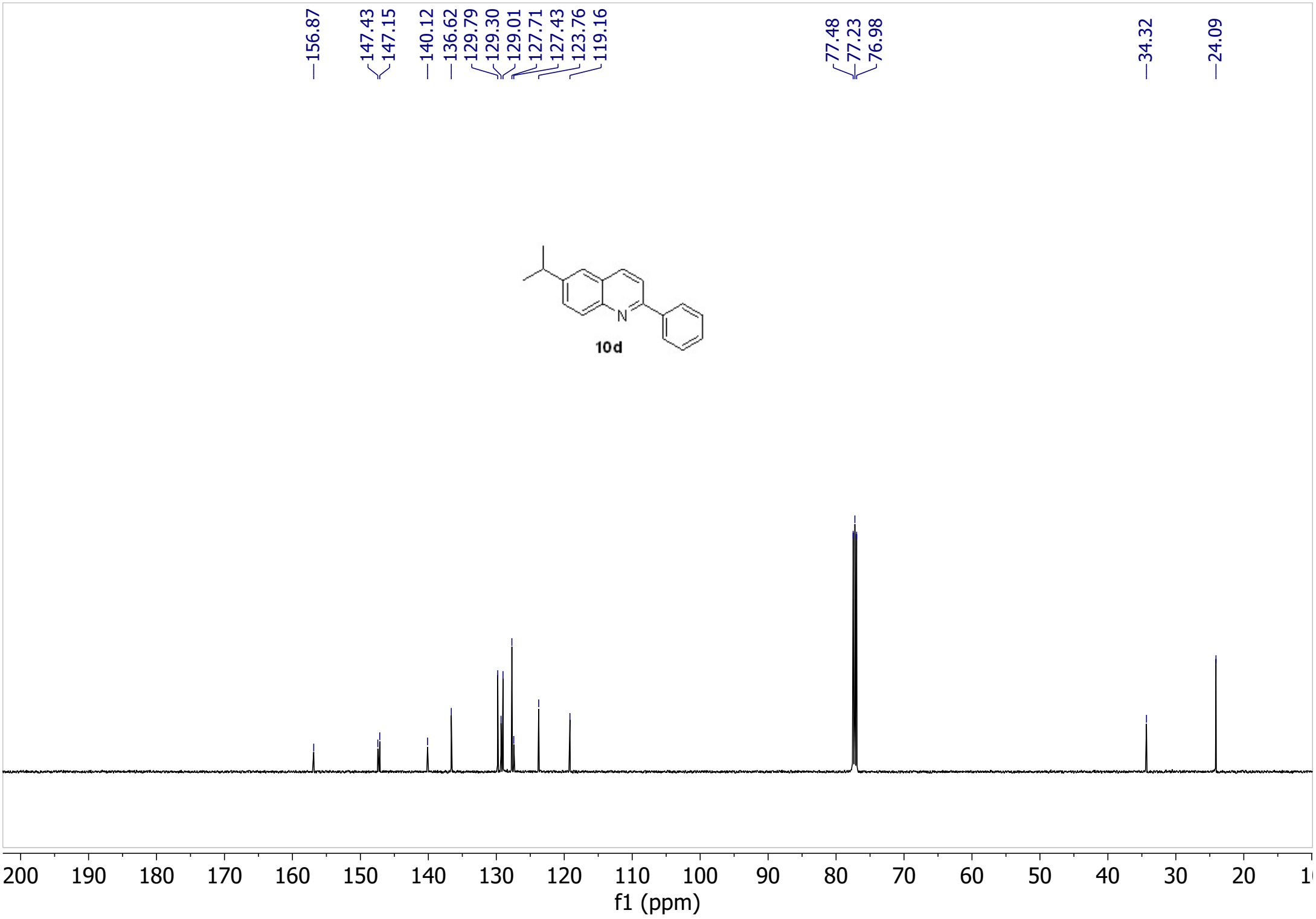
1.5
1.0
0.5
f1 (ppm)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136.62
129.79
129.30
129.01
127.71
127.43
123.76
119.16
77.48
77.23
76.98
34.32
24.09
N
10d
200
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180
170
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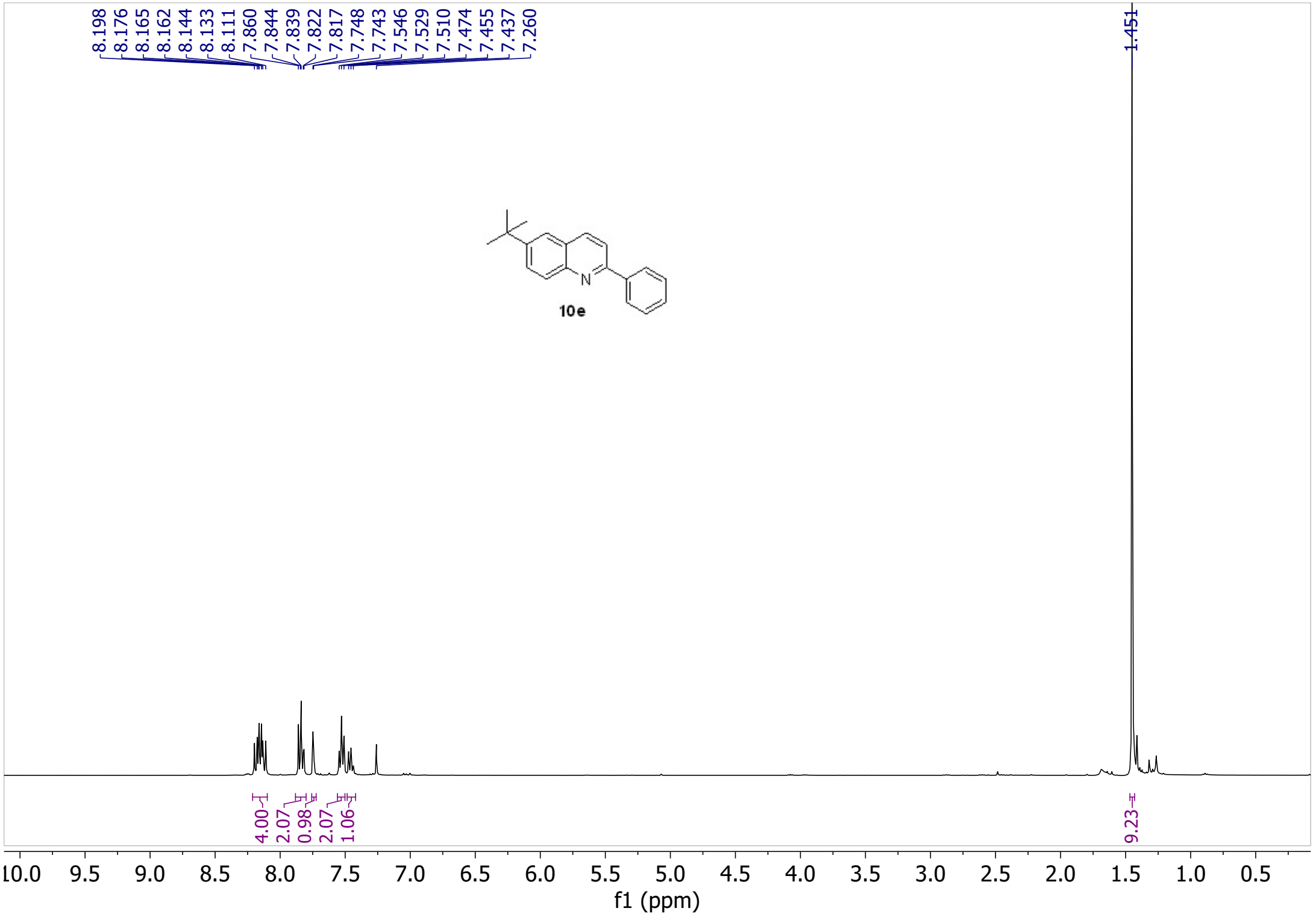
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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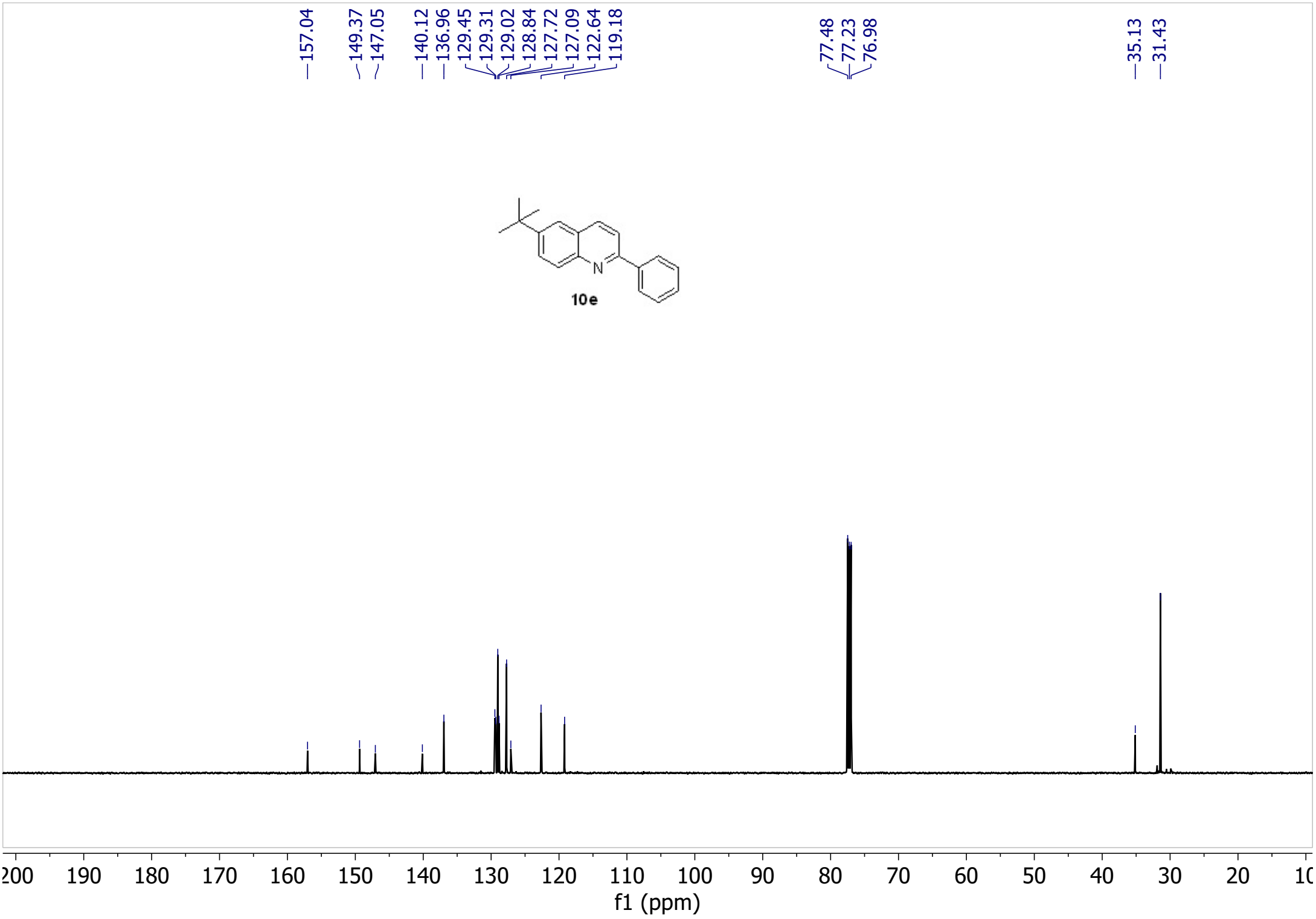
7.839
7.822
7.817
7.748
7.743
7.546
7.529
7.510
7.474
7.455
7.437
7.260
1.451
N
10e
4.00
2.07
0.98
2.07
1.06
9.23
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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140.12
136.96
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129.31
129.02
128.84
127.72
127.09
122.64
119.18
77.48
77.23
76.98
35.13
31.43
N
10e
200
190
180
170
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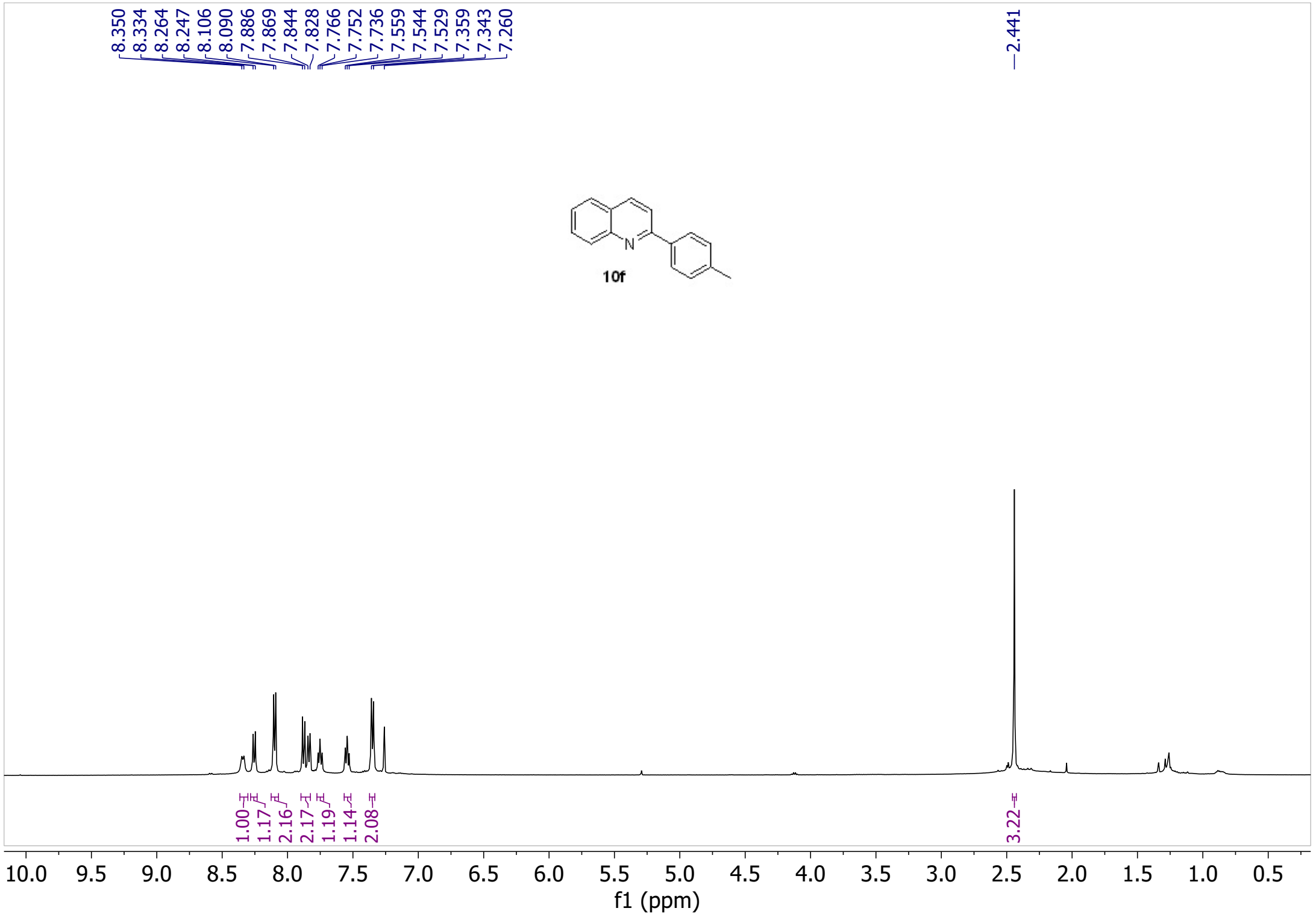
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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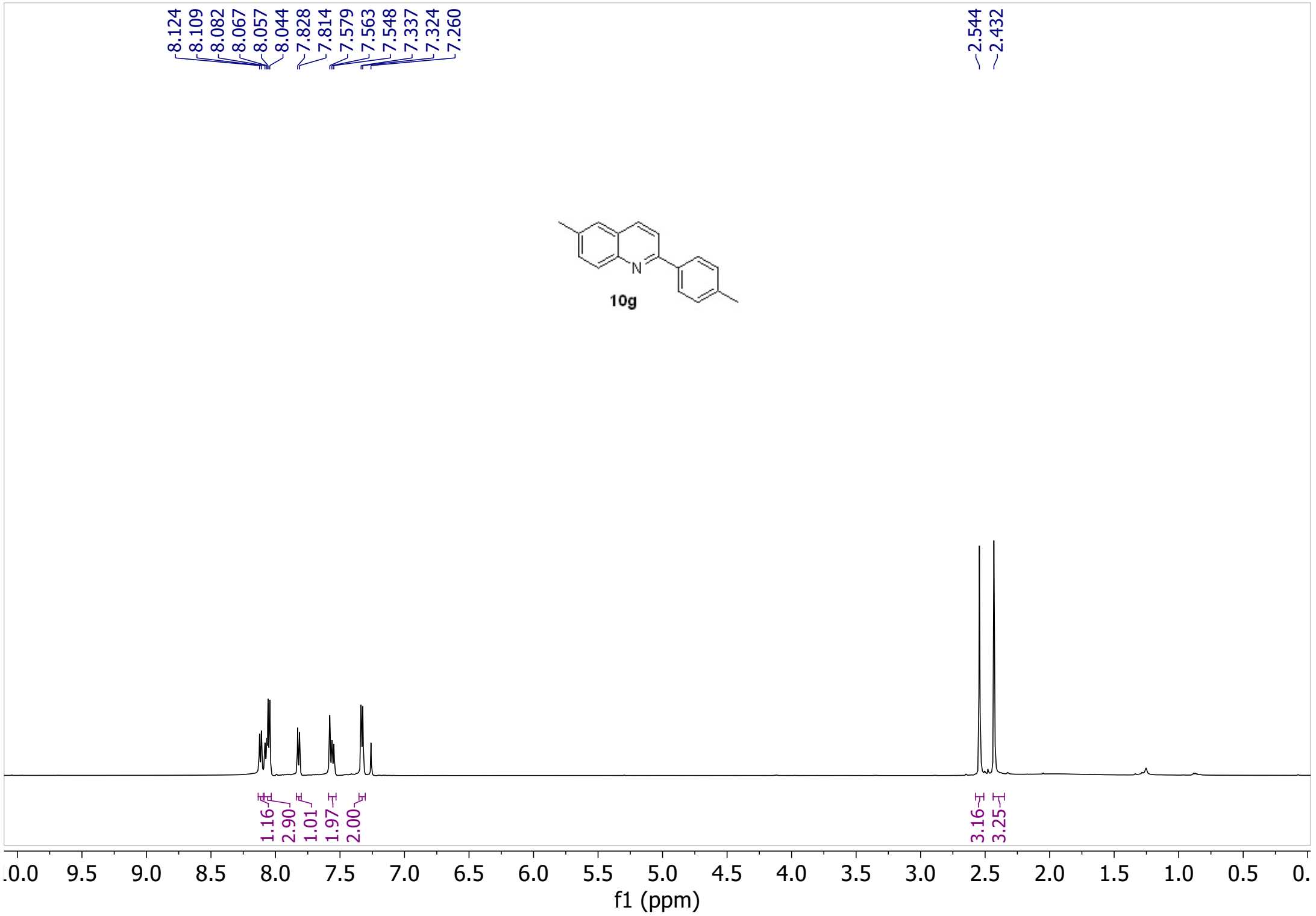
7.544
7.529
7.359
7.343
7.260
2.441
10f
1.00
1.17
2.16
2.17
1.19
1.14
2.08
3.22
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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7.828
7.814
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7.563
7.548
7.337
7.324
7.260
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10g
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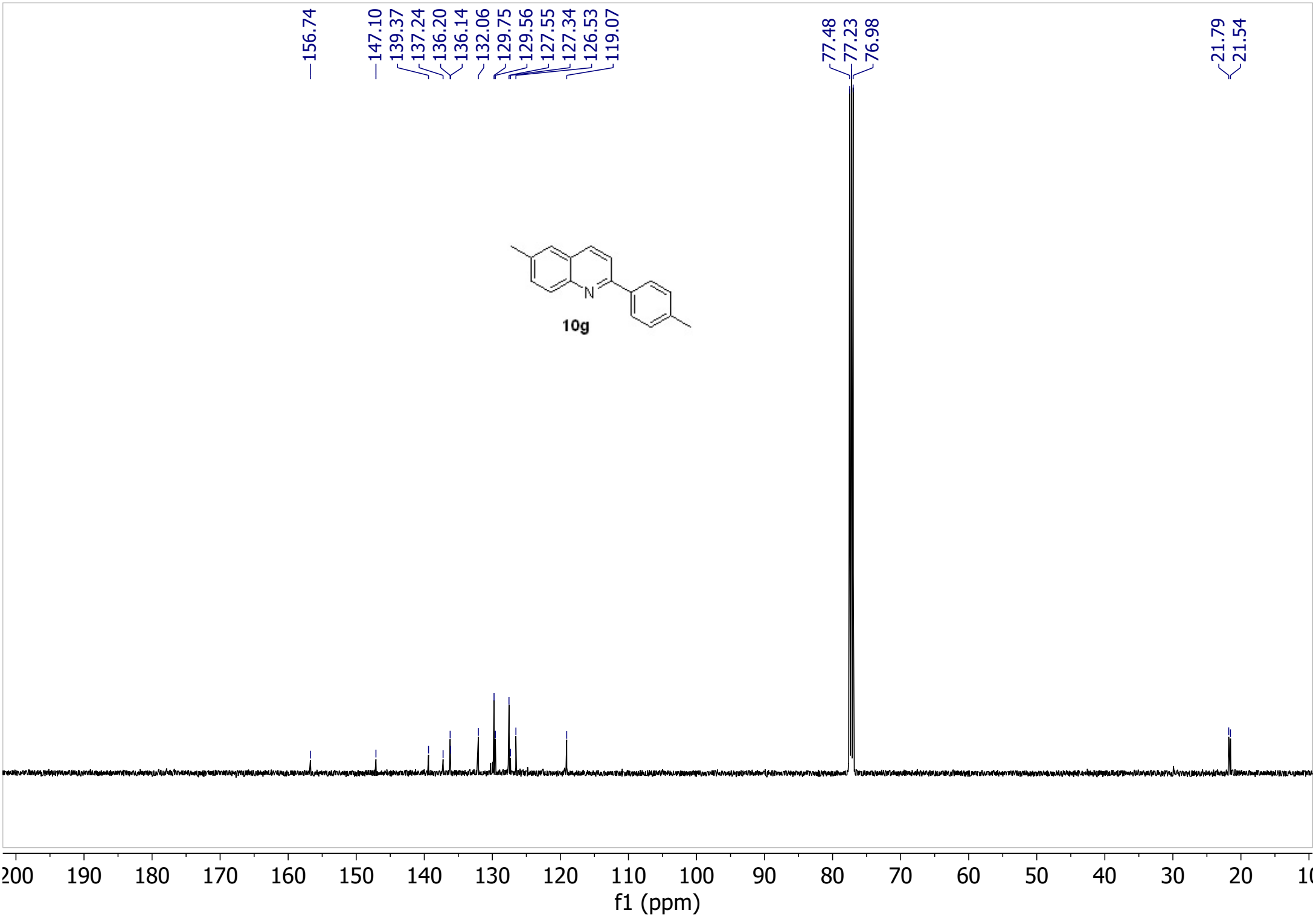
2.90
1.01
1.97
2.00
3.16
3.25
f1 (ppm)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147.10
139.37
137.24
136.20
136.14
132.06
129.75
129.56
127.55
127.34
126.53
119.07
77.48
77.23
76.98
21.79
21.54
N
10g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
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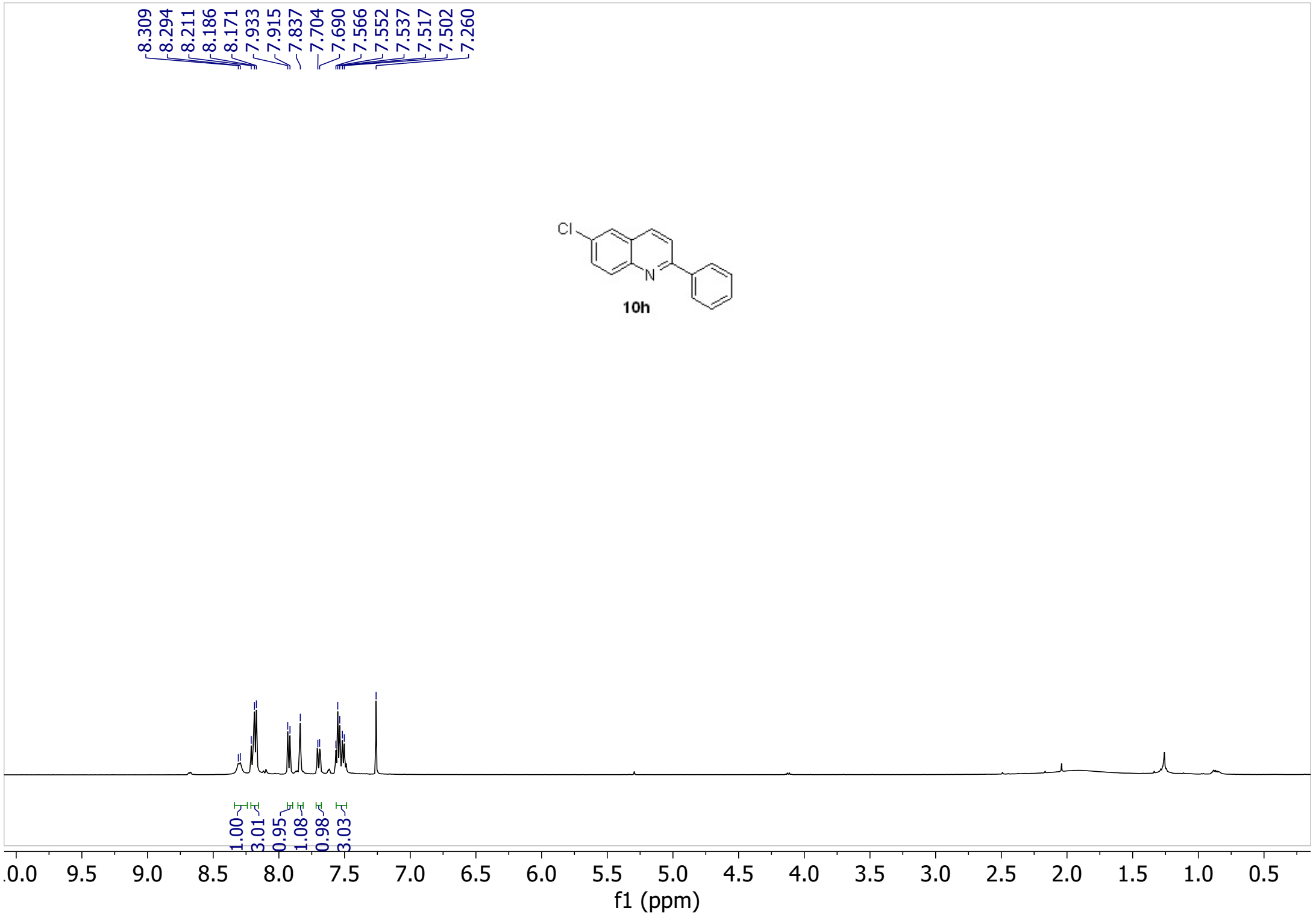
30
20
f1 (ppm)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7.566
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7.537
7.517
7.502
7.260
Cl
N
10h
1.00
3.01
0.95
1.08
0.98
3.03
.0.0
9.5
9.0
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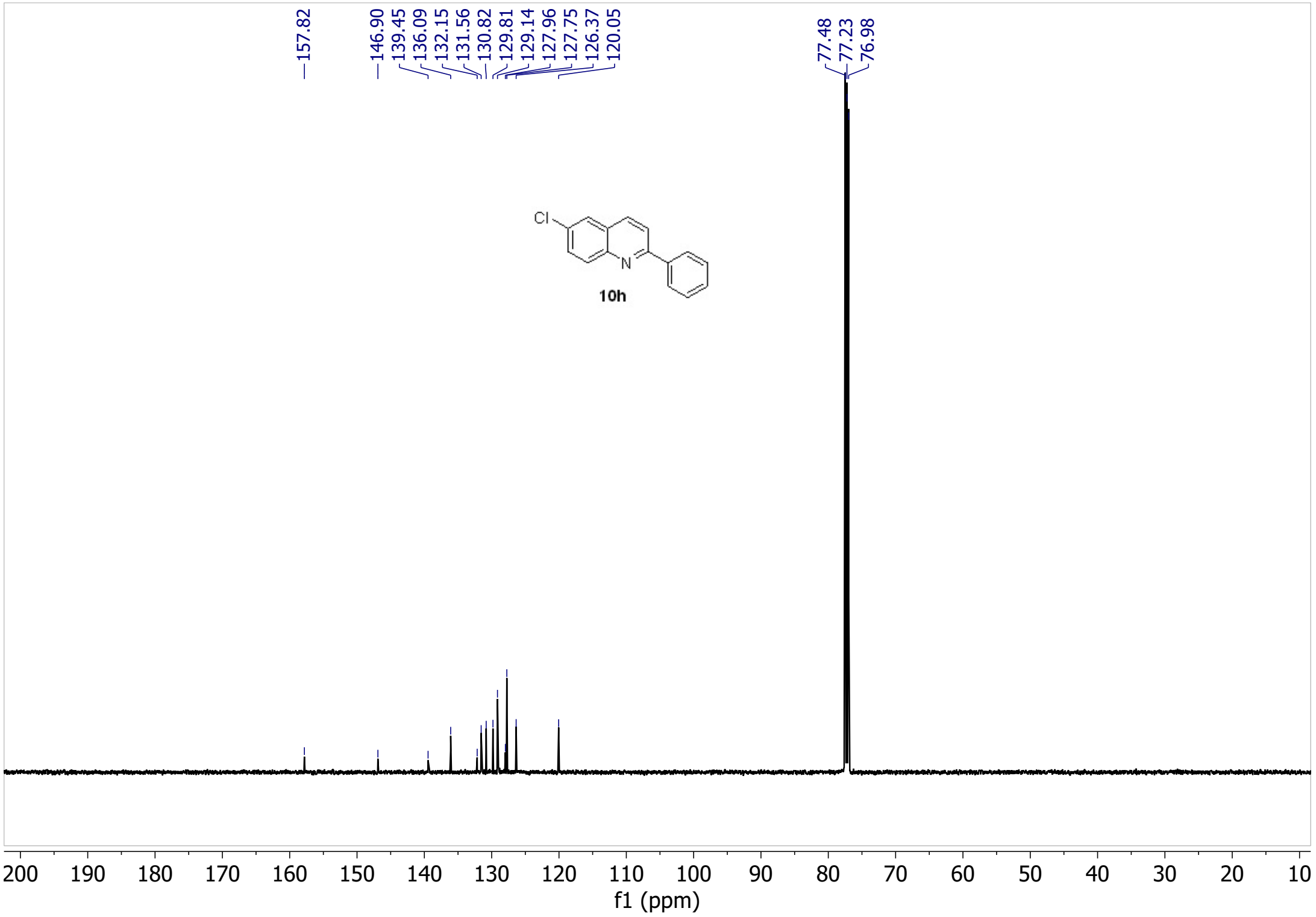
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127.75
126.37
120.05
77.48
77.23
76.98
Cl
N
10h
200
190
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120
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100
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80
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60
50
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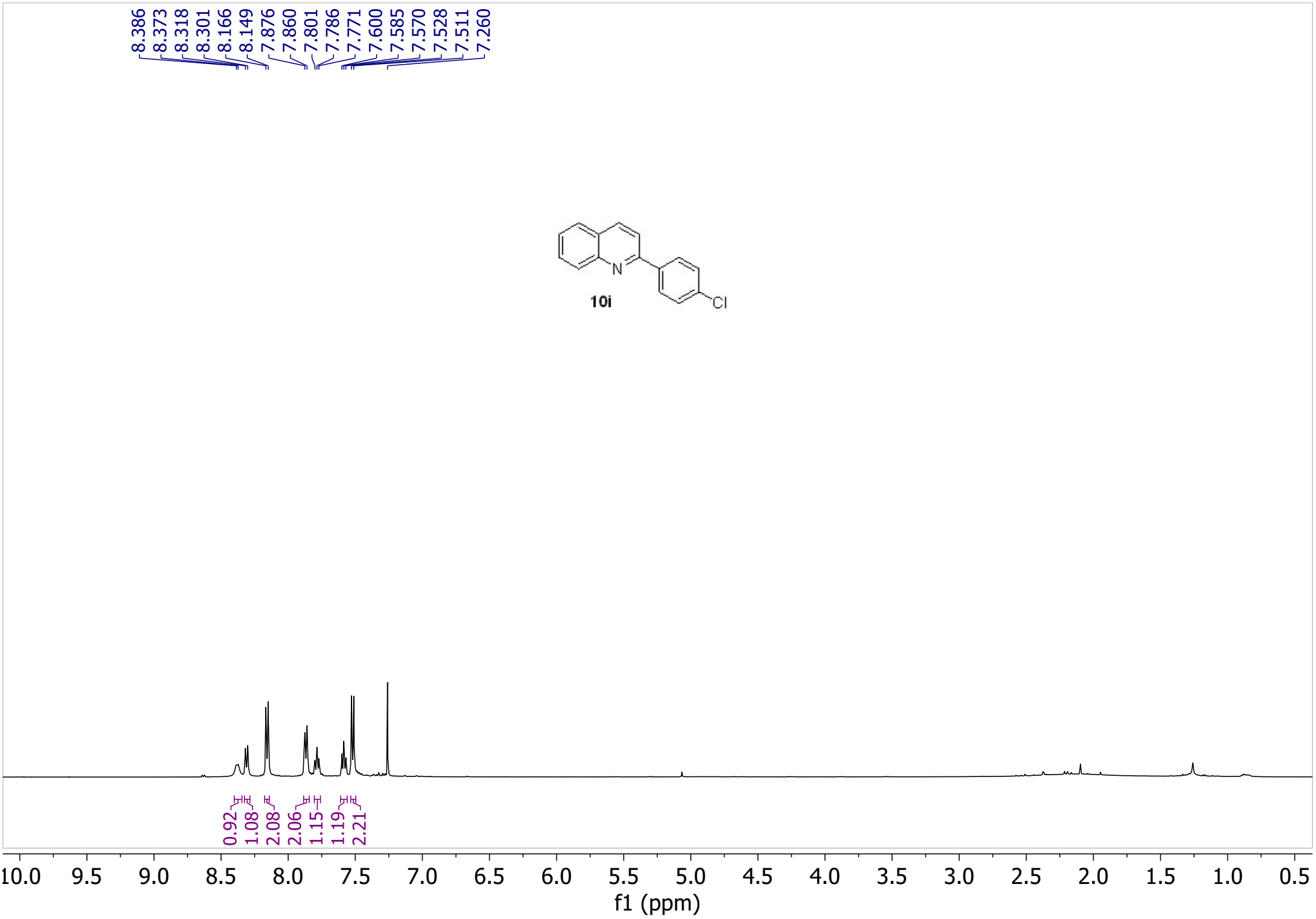
20
10
f1 (ppm)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7.860
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7.771
7.600
7.585
7.570
7.528
7.511
7.260
N
Cl
10i
0.92
1.08
2.08
2.06
1.15
1.19
2.21
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
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3.0
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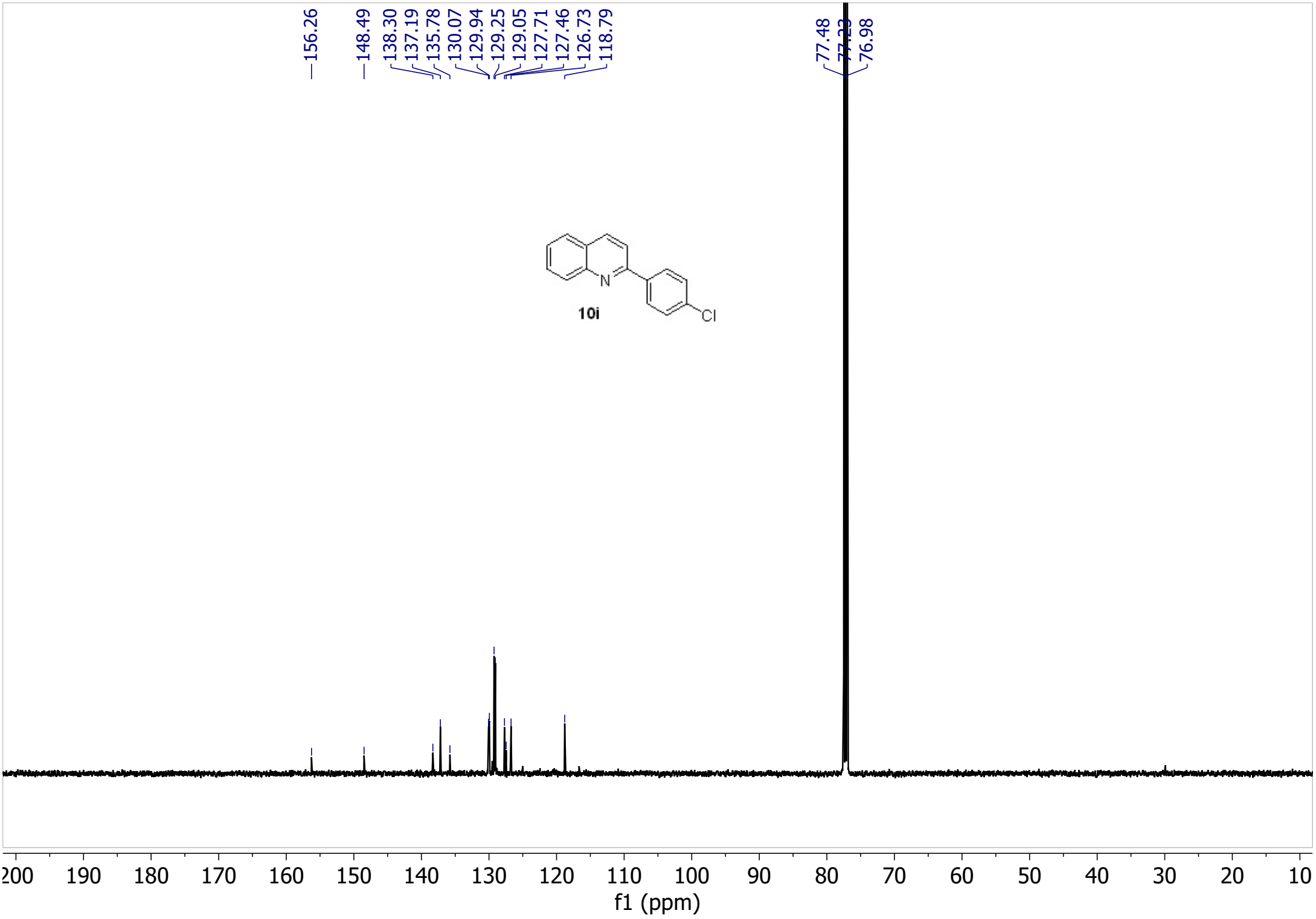
2.0
1.5
1.0
0.5
f1 (ppm)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130.07
129.94
129.25
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127.71
127.46
126.73
118.79
77.48
77.23
76.98
N
Cl
10i
200
190
180
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160
150
140
130
120
110
100
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80
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50
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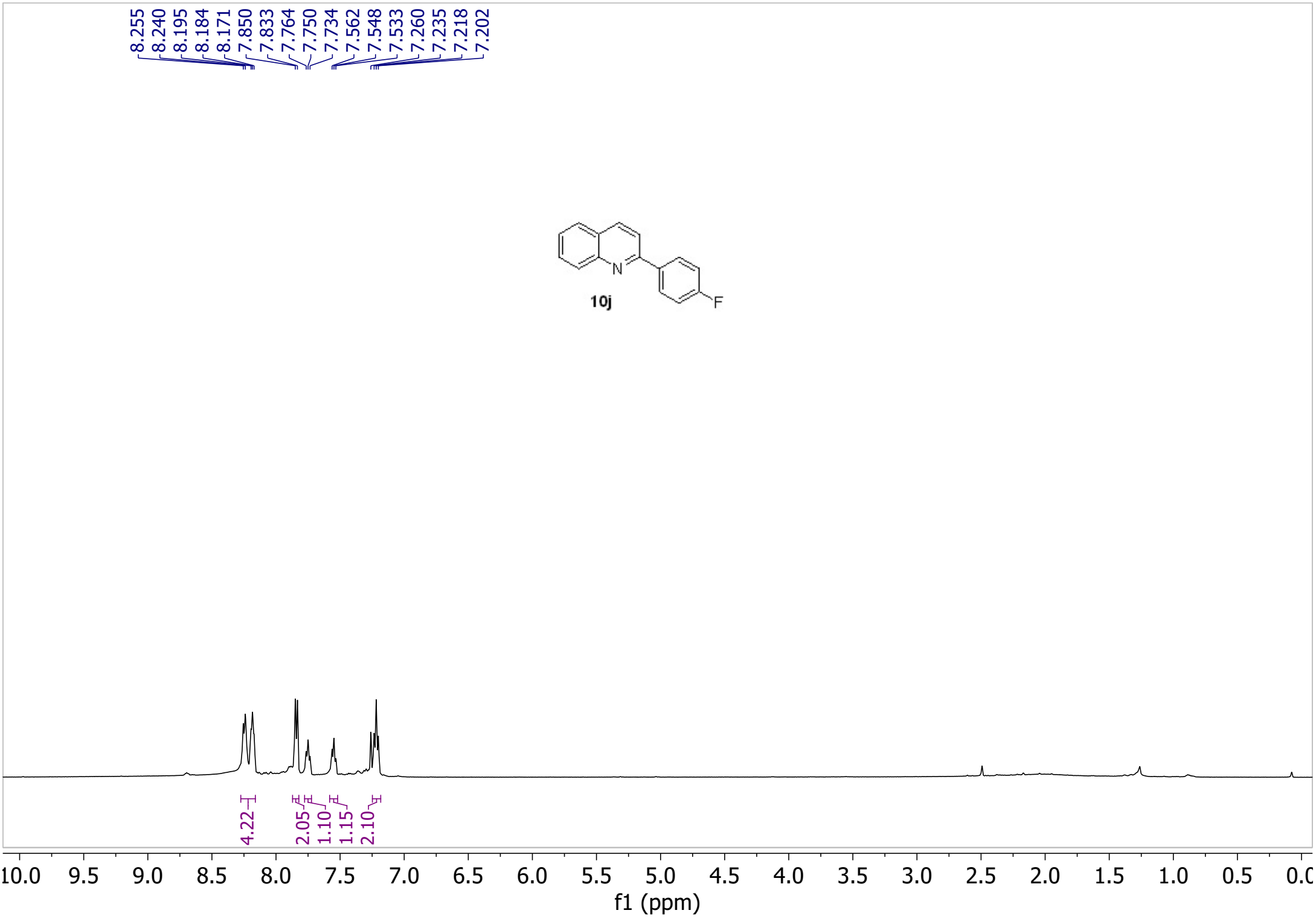
20
10
f1 (ppm)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7.764
7.750
7.734
7.562
7.548
7.533
7.260
7.235
7.218
7.202
N
F
10j
4.22
2.05
1.10
1.15
2.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
1.5
1.0
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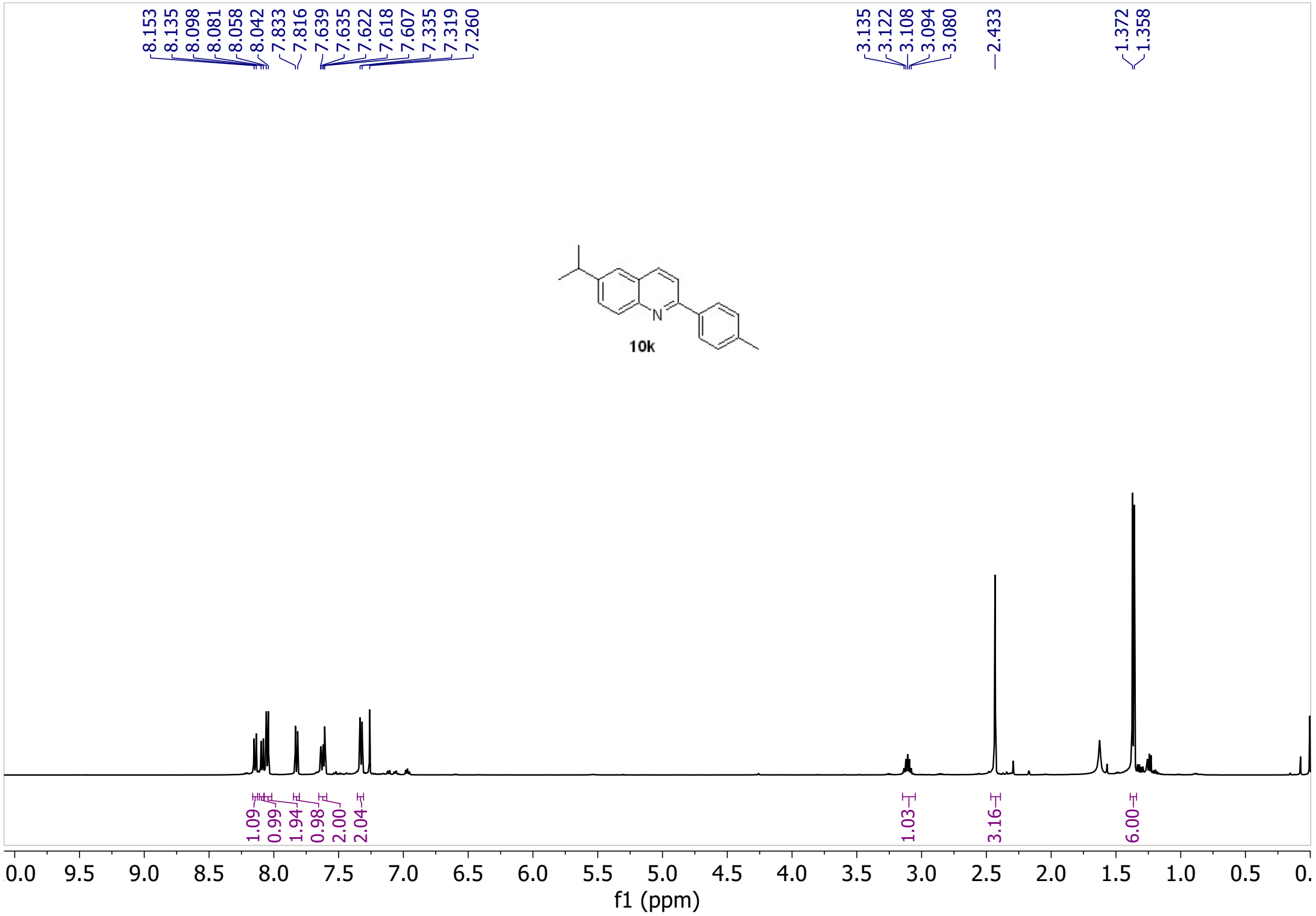
0.0
f1 (ppm)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8.058
8.042
7.833
7.816
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7.635
7.622
7.618
7.607
7.335
7.319
7.260
3.135
3.122
3.108
3.094
3.080
2.433
1.372
1.358
10k
1.09
0.99
1.94
0.98
2.00
2.04
1.03
3.16
6.00
0.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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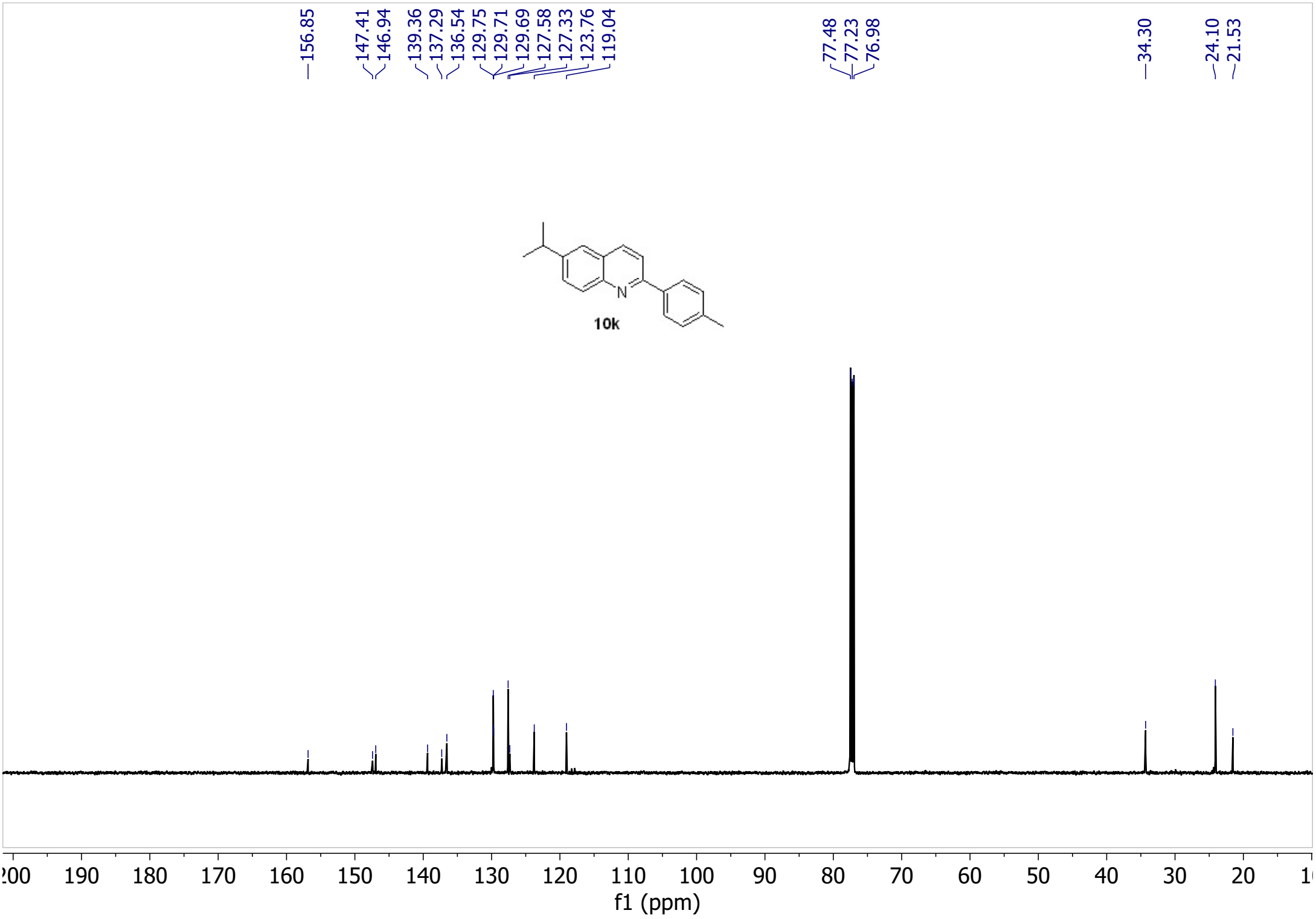
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)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136.54
129.75
129.71
129.69
127.58
127.33
123.76
119.04
77.48
77.23
76.98
34.30
24.10
21.53
N
10k
200
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180
170
160
150
140
130
120
110
100
90
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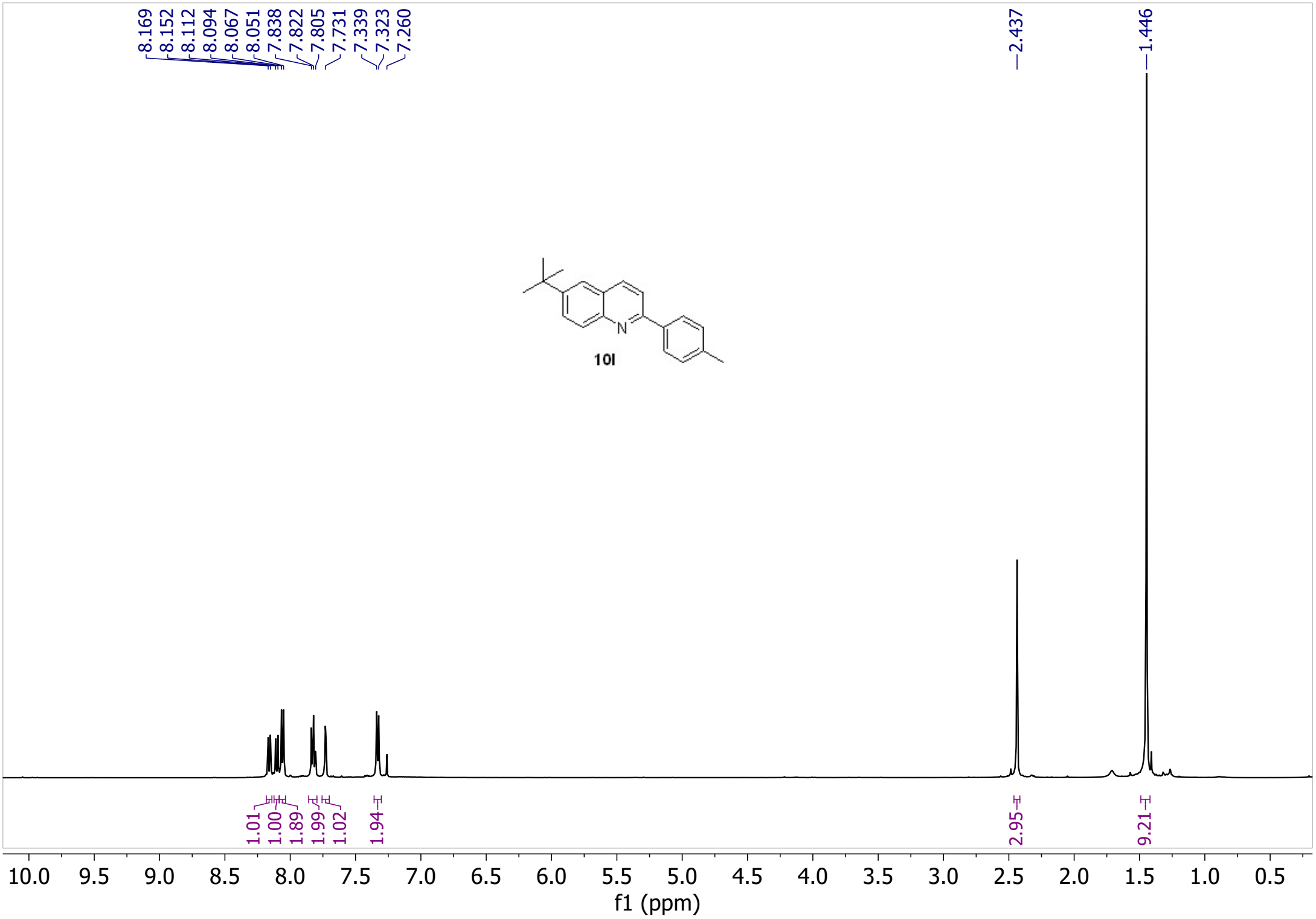
70
60
50
40
30
20
f1 (ppm)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7.323
7.260
2.437
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1.00
1.89
1.99
1.02
1.94
2.95
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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4.0
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3.0
2.5
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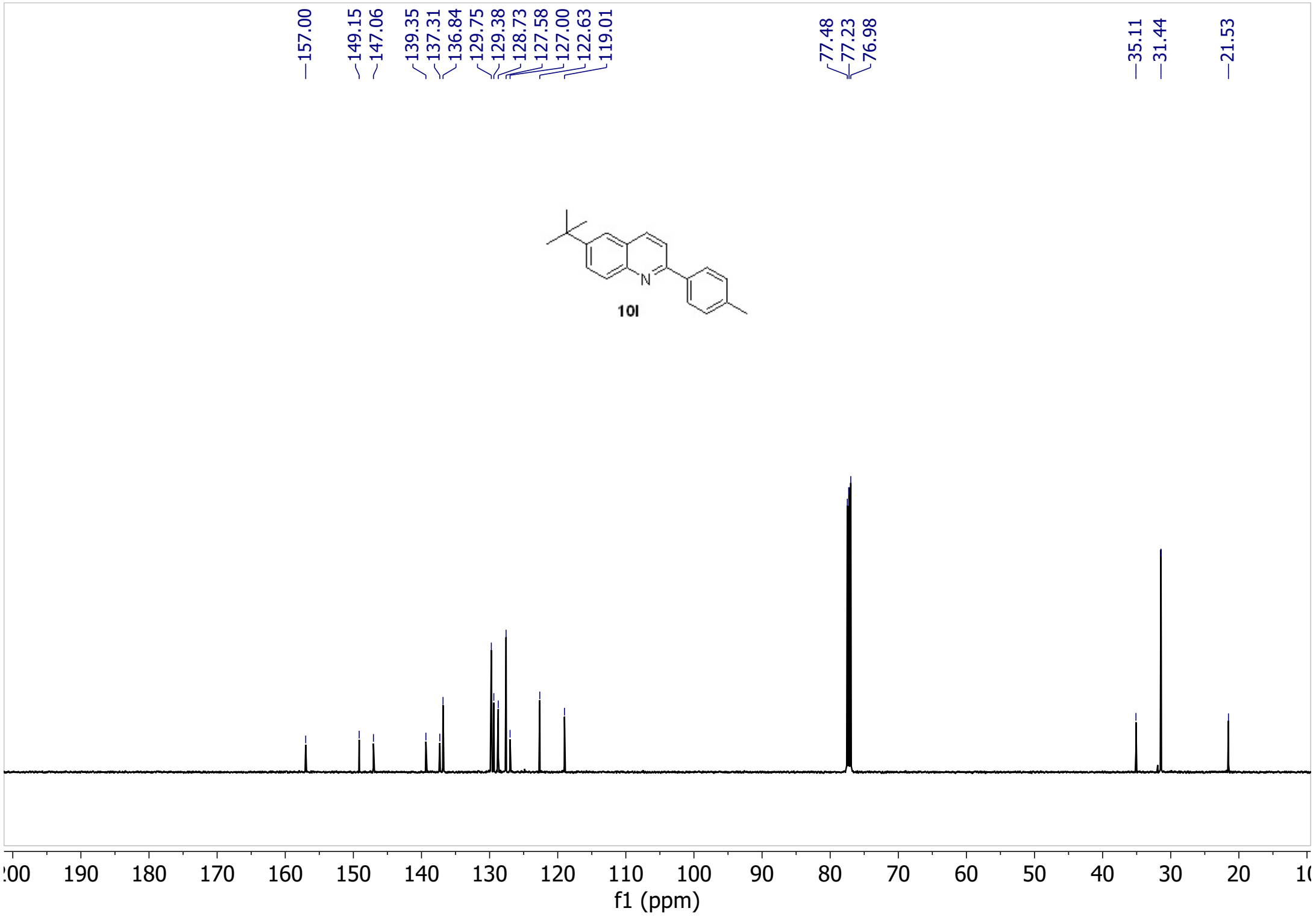
0.5
f1 (ppm)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119.01
77.48
77.23
76.98
35.11
31.44
21.53
N
10l
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180
170
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150
140
130
120
110
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70
60
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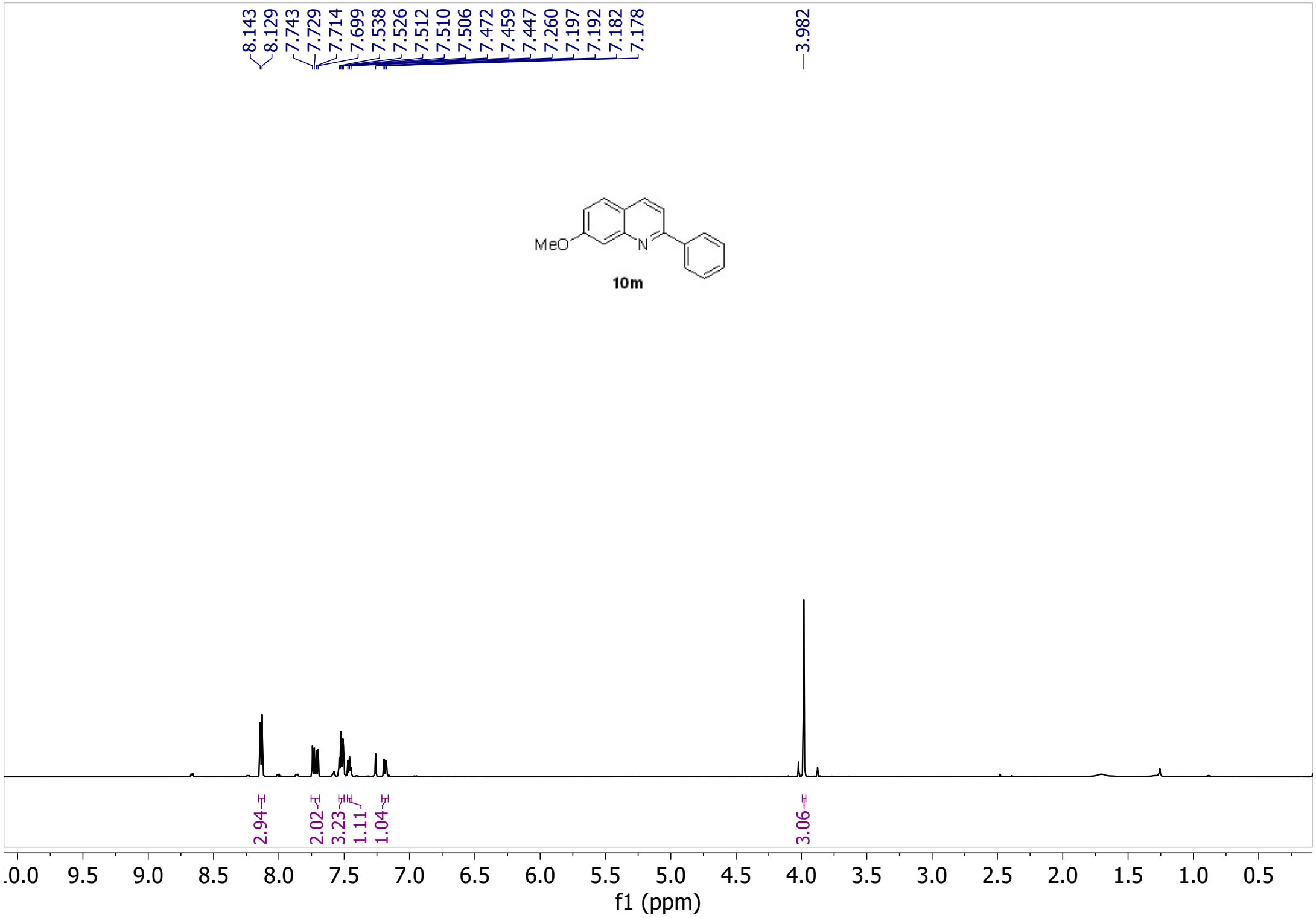
40
30
20
f1 (ppm)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7.510
7.506
7.472
7.459
7.447
7.260
7.197
7.192
7.182
7.178
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MeO
N
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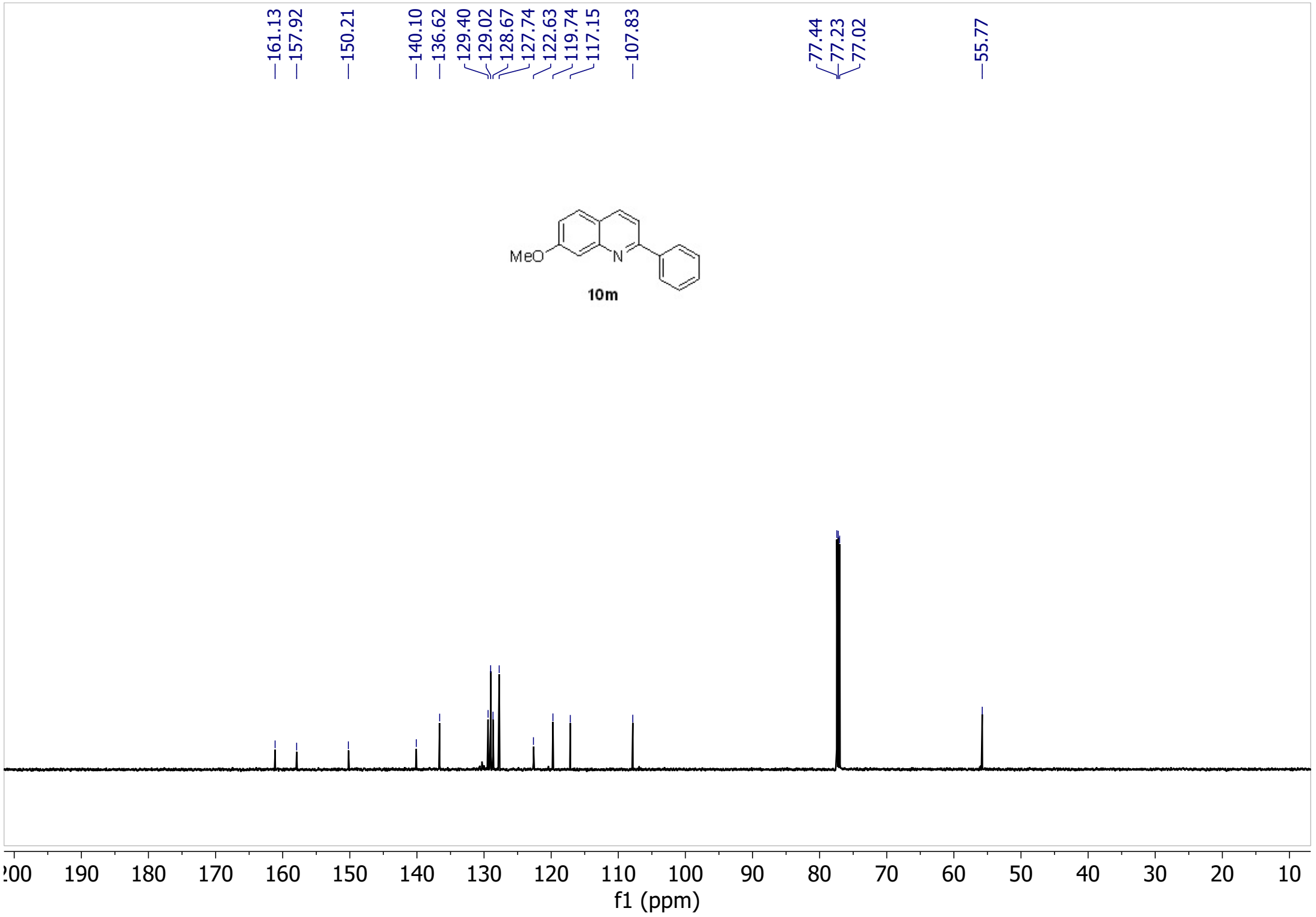
2.94
2.02
3.23
1.11
1.04
3.06
f1 (ppm)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122.63
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117.15
107.83
77.44
77.23
77.02
55.77
MeO
N
10m
200
190
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170
160
150
140
130
120
110
100
90
80
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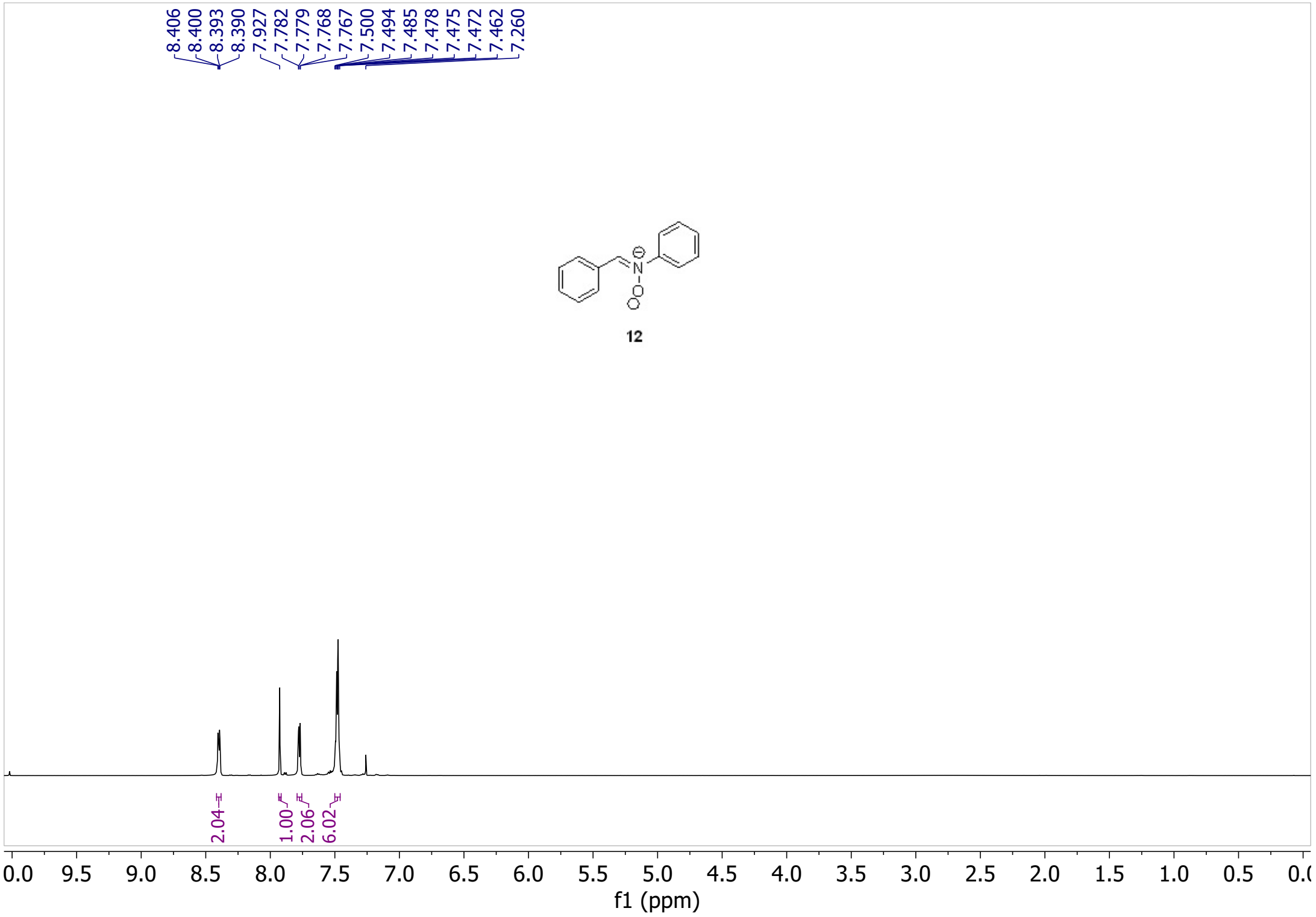
60
50
40
30
20
10
f1 (ppm)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7.478
7.475
7.472
7.462
7.260
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2.04
1.00
2.06
6.02
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9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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4.0
3.5
3.0
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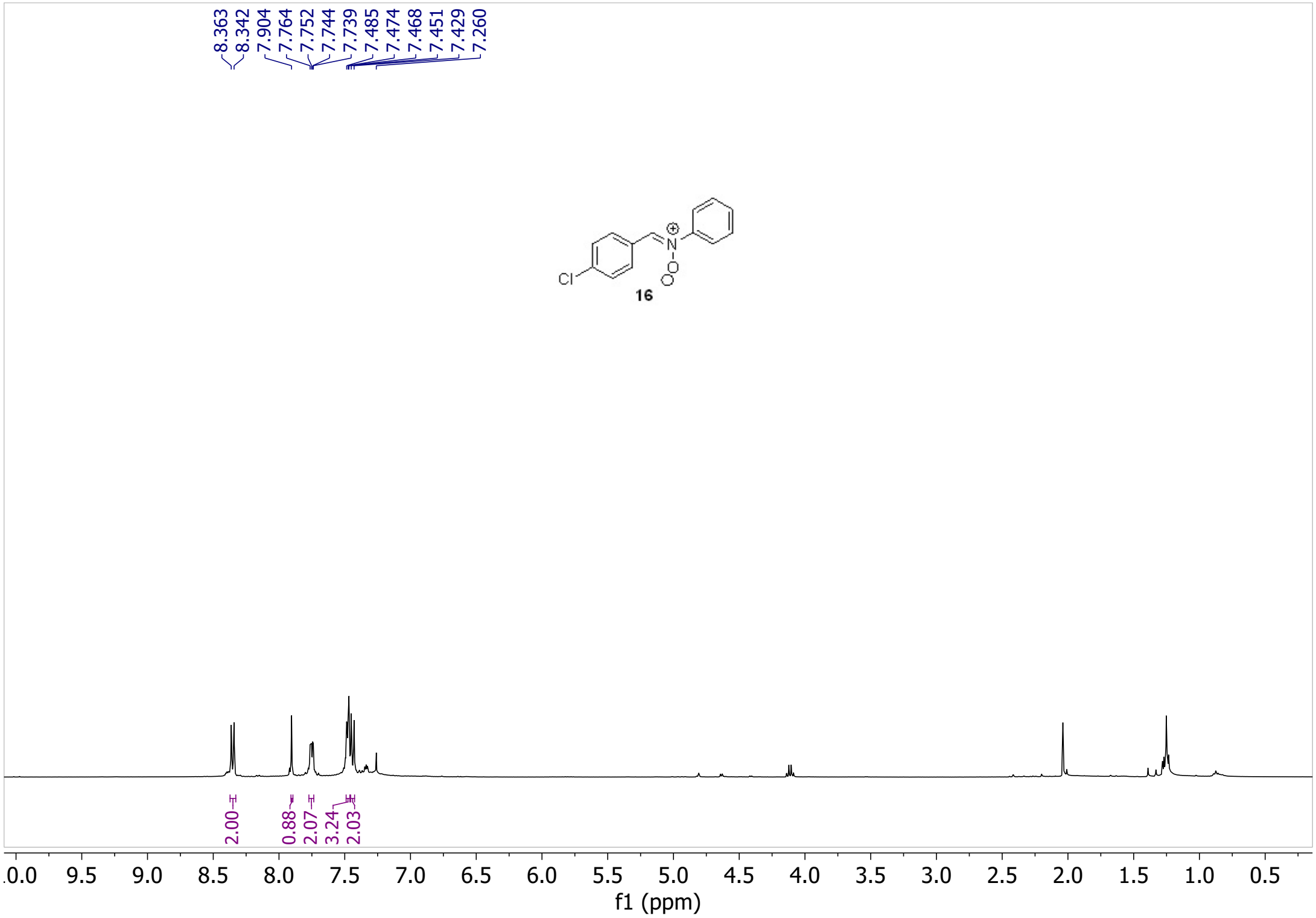
2.0
1.5
1.0
0.5
f1 (ppm)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7.260
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O
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4.0
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3.0
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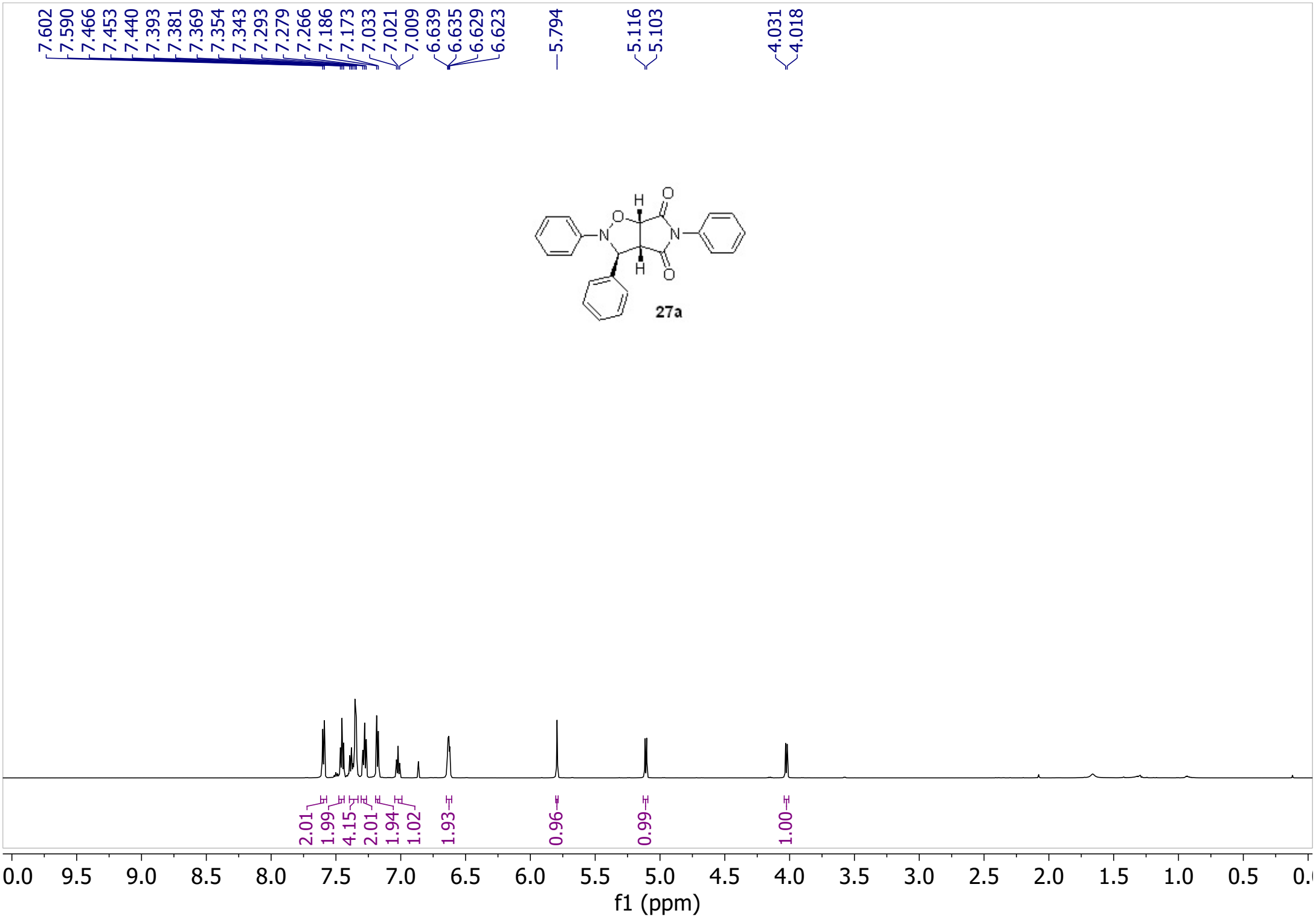
f1 (ppm)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7.021
7.009
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6.635
6.629
6.623
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5.116
5.103
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O
O
N
N
H
O
27a
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4.15
2.01
1.94
1.02
1.93
0.96
0.99
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8.0
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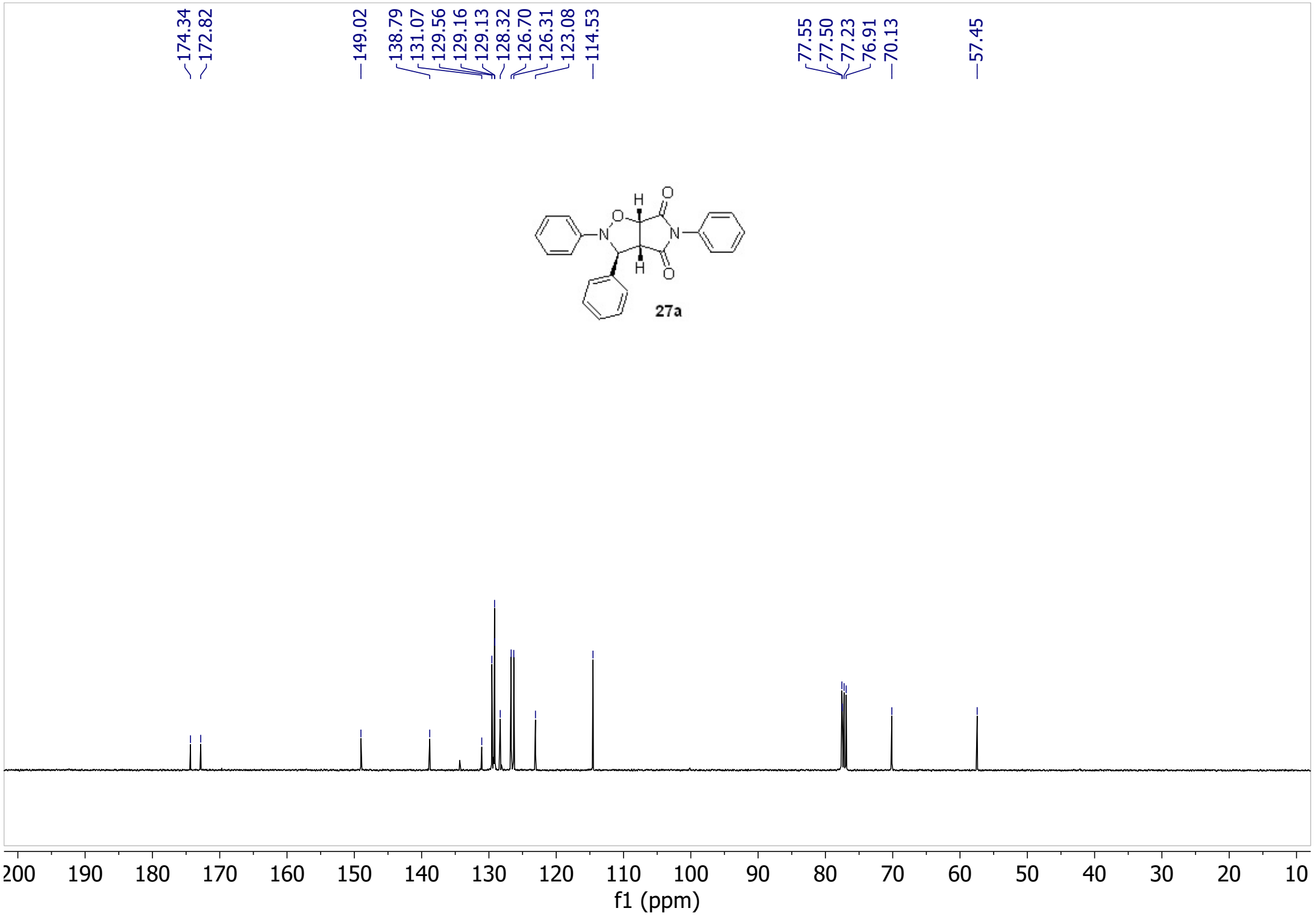
f1 (ppm)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129.16
129.13
128.32
126.70
126.31
123.08
114.53
77.55
77.50
77.23
76.91
70.13
57.45
27a
200
190
180
170
160
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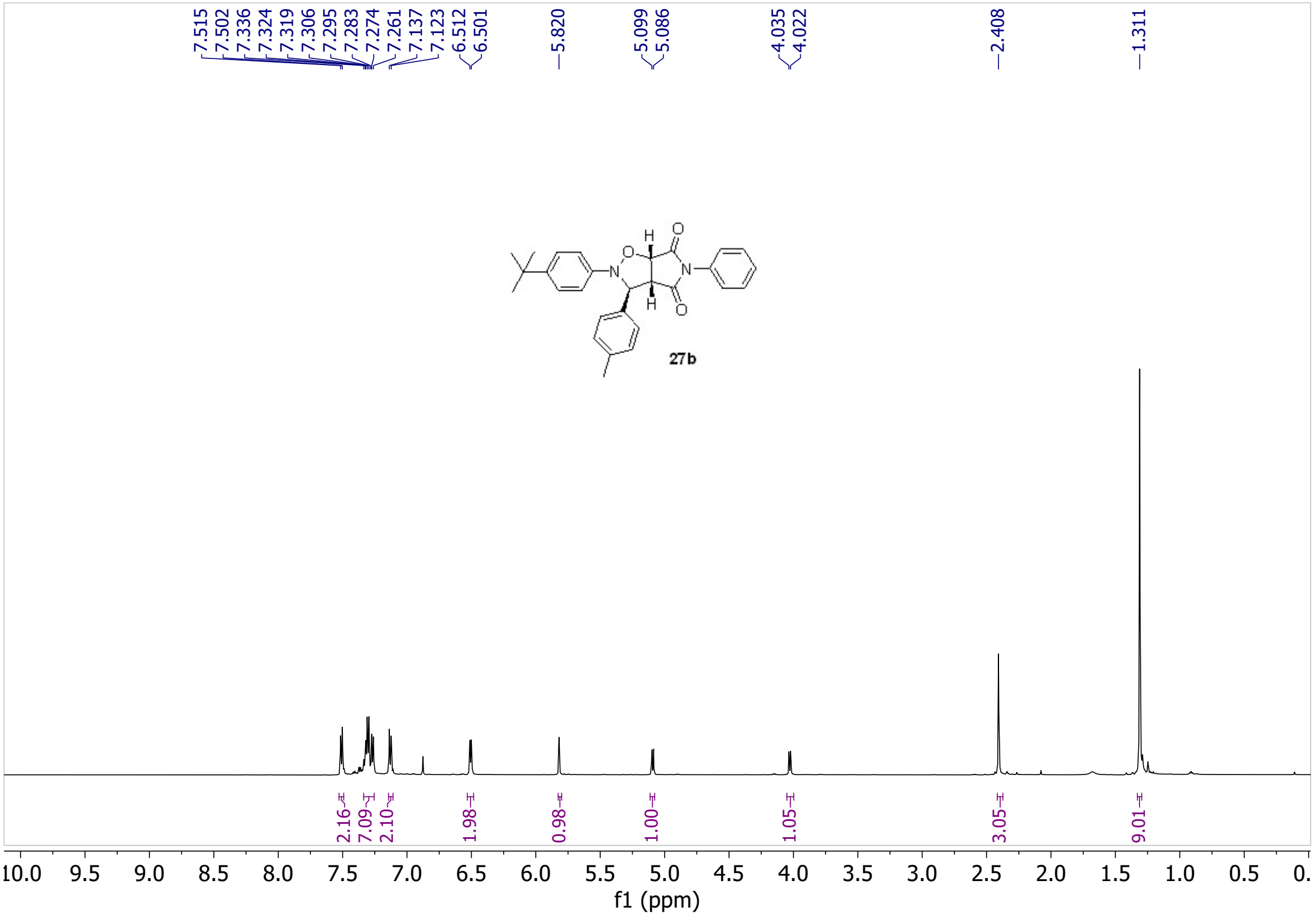
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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6.501
5.820
5.099
5.086
4.035
4.022
2.408
1.311
27b
2.16
7.09
2.10
1.98
0.98
1.00
1.05
3.05
9.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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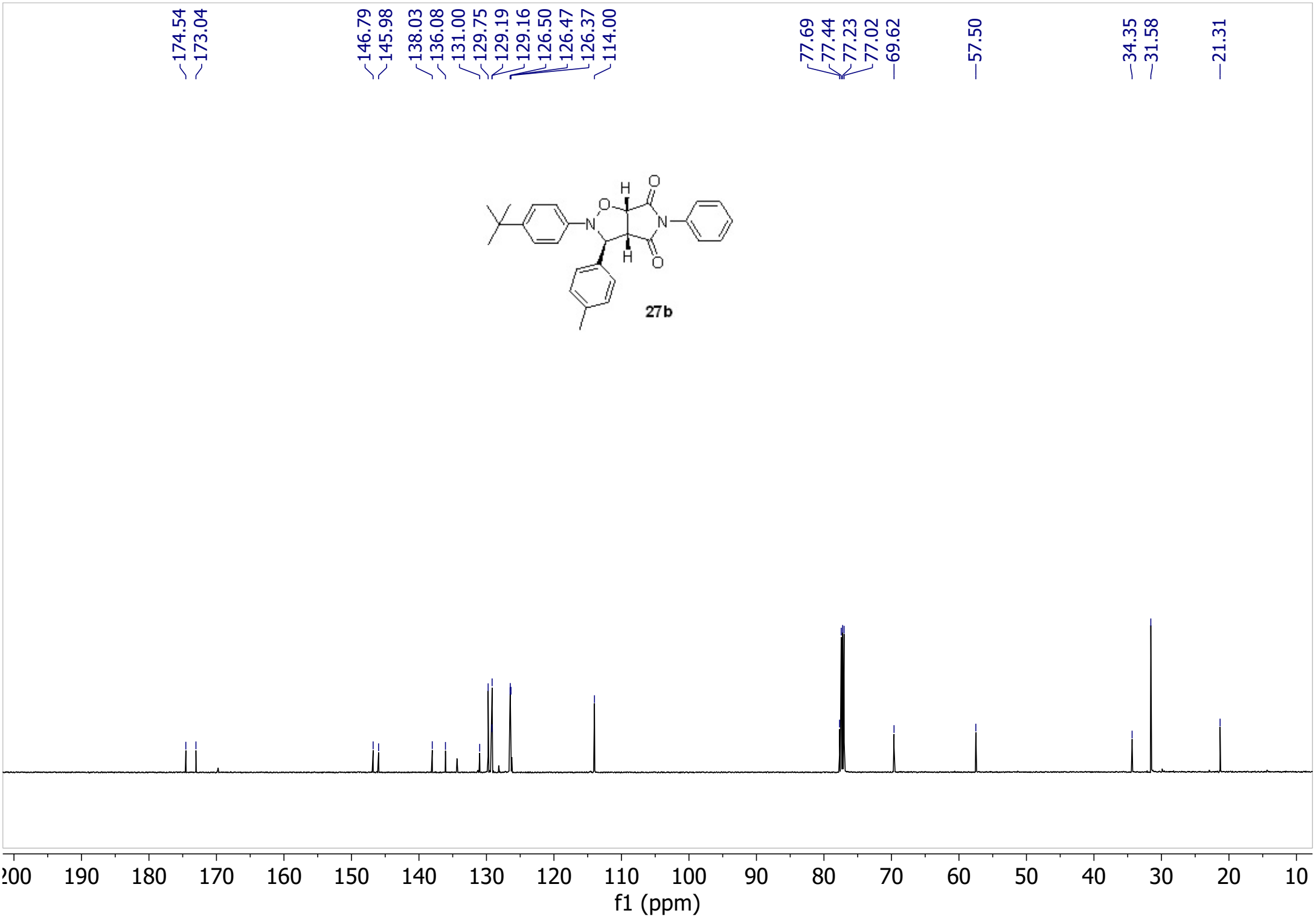
f1 (ppm)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126.47
126.37
114.00
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77.44
77.23
77.02
69.62
57.50
34.35
31.58
21.31
O
H
O
N
N
H
O
27b
200
190
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120
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100
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60
50
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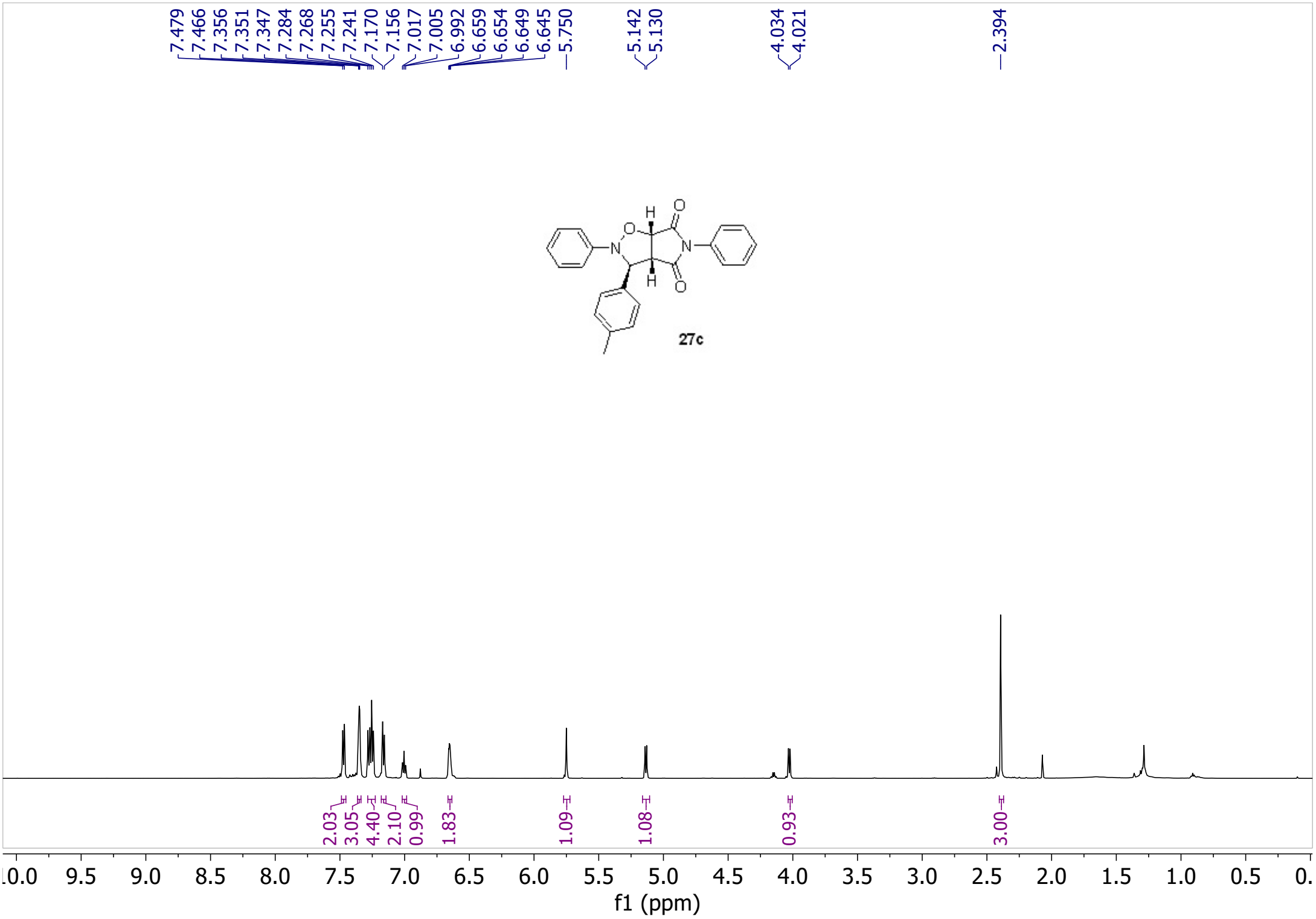
30
20
10
f1 (ppm)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6.659
6.654
6.649
6.645
5.750
5.142
5.130
4.034
4.021
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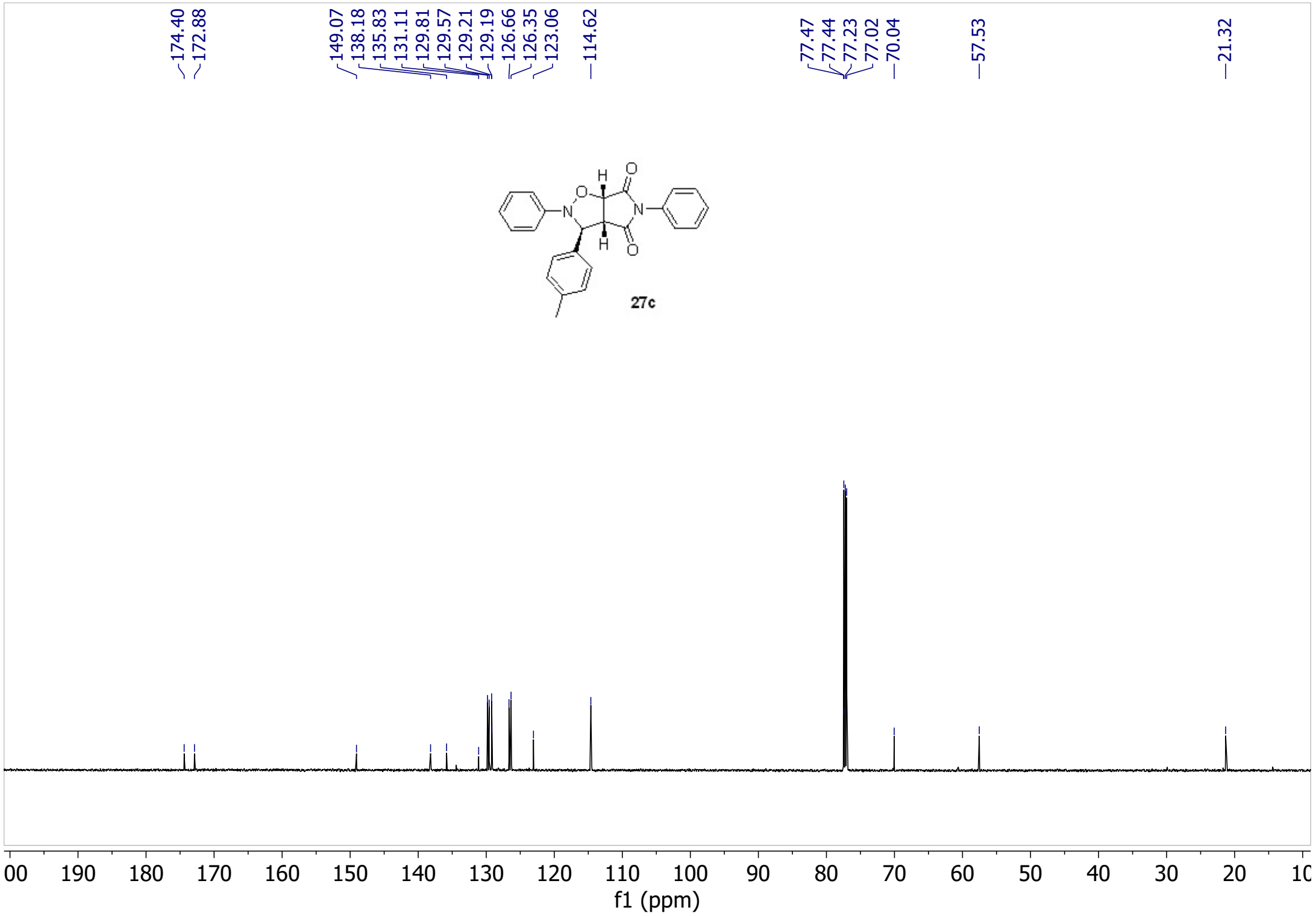
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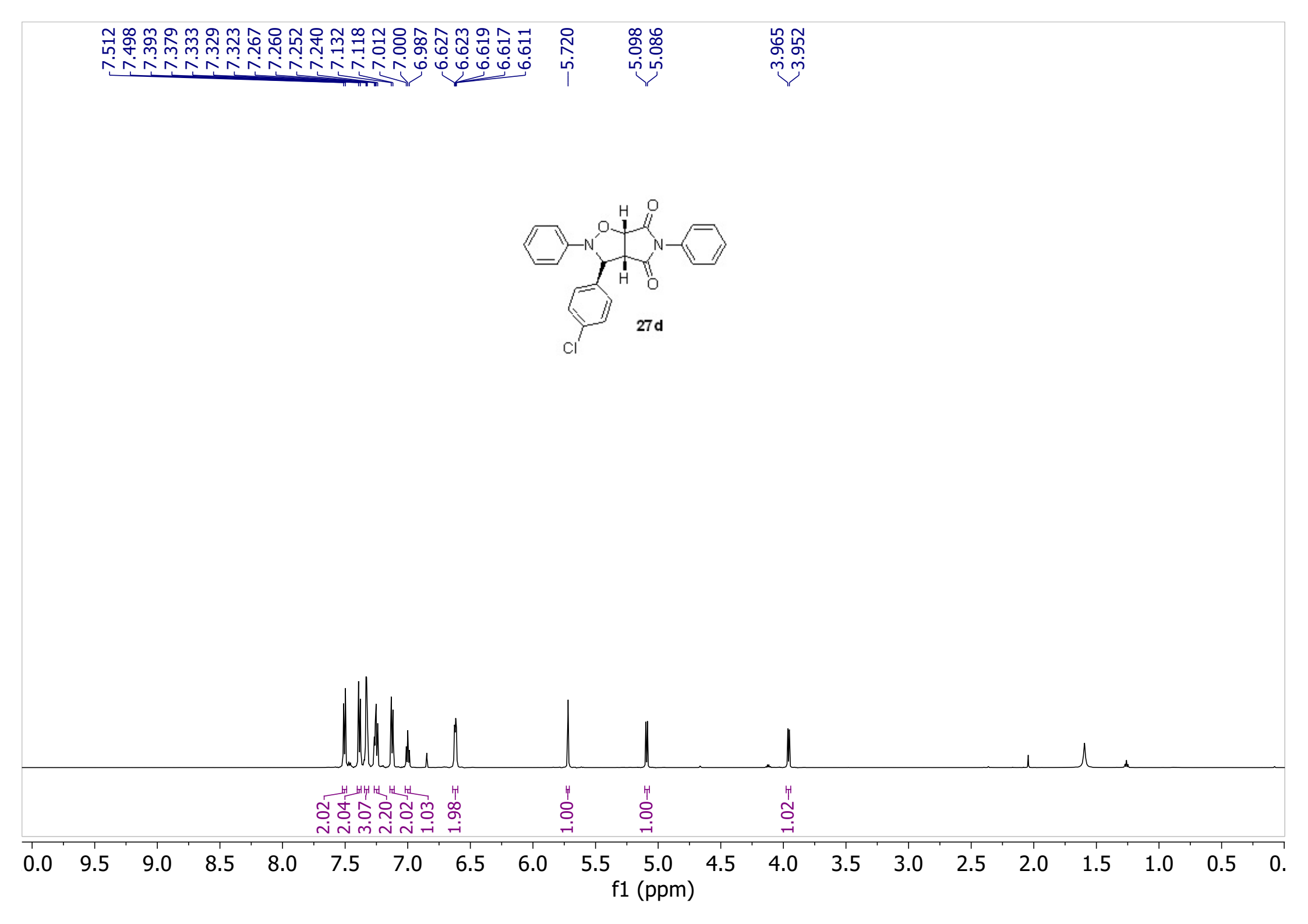
77.47
77.44
77.23
77.02
70.04
57.53
21.32
27c
f1 (ppm)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7.012
7.000
6.987
6.627
6.623
6.619
6.617
6.611
5.720
5.098
5.086
3.965
3.952
H
O
N
O
N
H
O
Cl
27d
2.02
2.04
3.07
2.20
2.02
1.03
1.98
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1.00
1.02
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9.0
8.5
8.0
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7.0
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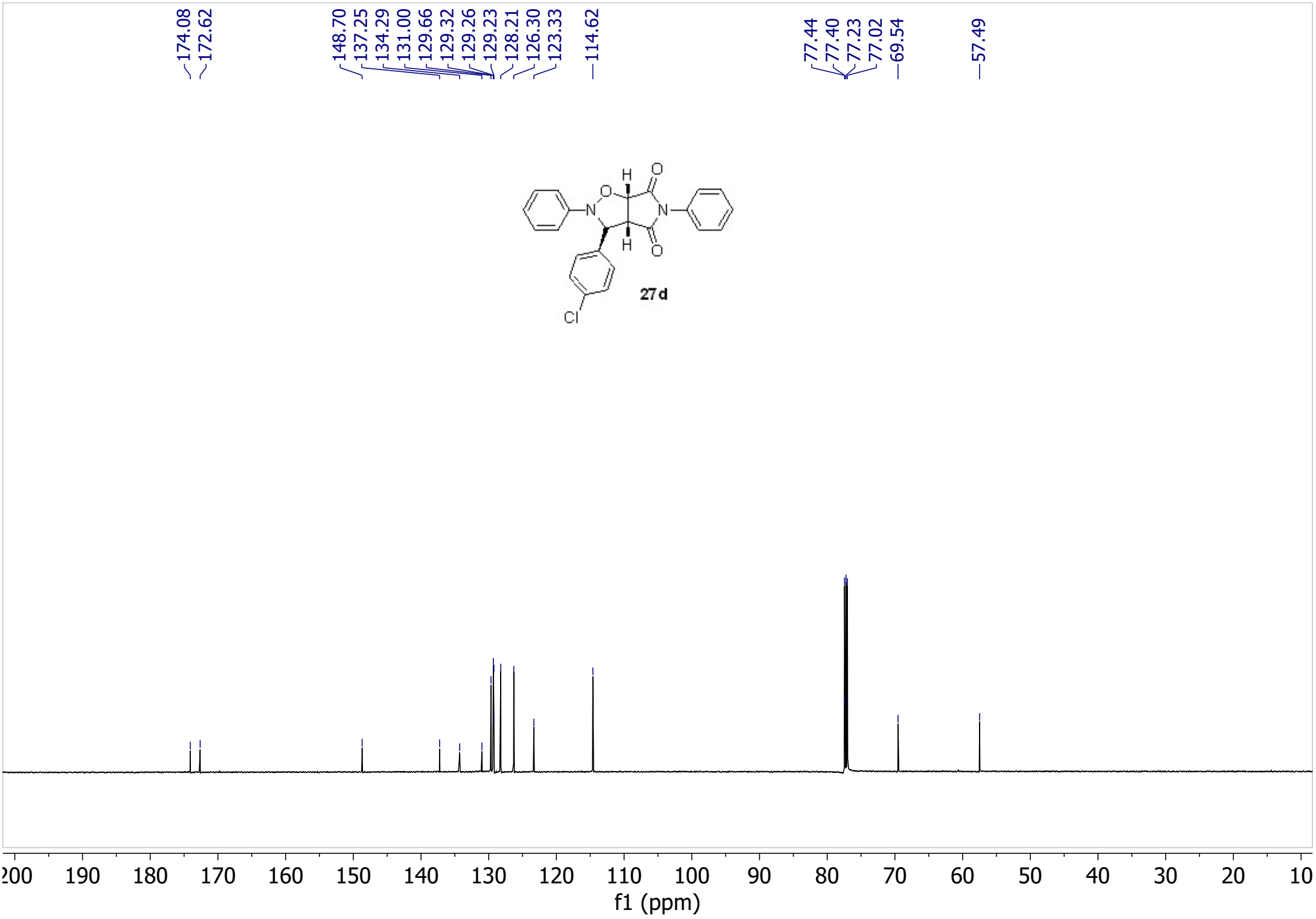
f1 (ppm)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128.21
126.30
123.33
114.62
77.44
77.40
77.23
77.02
69.54
57.49
H
O
O
N
N
O
H
O
Cl
27d
200
190
180
170
160
150
140
130
120
110
100
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80
70
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40
30
20
10
f1 (ppm)

Coordinate File:

- TS_p-1:

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C	-1.500507000000	0.804176000000	-0.116607000000
C	-1.686745000000	-0.550804000000	0.214193000000
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C	-4.070147000000	-0.294628000000	0.038533000000
H	-4.791752000000	1.661805000000	-0.481982000000
H	-2.519234000000	2.638277000000	-0.618829000000
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H	-3.097889000000	-2.144605000000	0.542089000000
C	-0.184862000000	1.405889000000	-0.212969000000
H	-0.103627000000	2.460578000000	-0.484722000000
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C	2.188248000000	1.249481000000	0.183918000000
H	1.345327000000	0.507113000000	1.072728000000
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C	4.618517000000	0.875282000000	0.403316000000
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H	4.712109000000	1.902905000000	0.745230000000
C	4.377464000000	-1.758677000000	-0.460389000000
H	2.281279000000	-1.330222000000	-0.711350000000
C	5.630557000000	-1.259001000000	-0.105746000000
H	6.716263000000	0.469839000000	0.585949000000
H	4.281726000000	-2.781501000000	-0.811967000000
H	6.510527000000	-1.890338000000	-0.170920000000
Cl	-5.669737000000	-0.983057000000	0.134252000000

- 2:

C	-2.648743000000	1.603819000000	-0.373506000000
C	-1.485798000000	0.894924000000	-0.001488000000
C	-1.651323000000	-0.440435000000	0.425321000000
C	-2.901272000000	-1.048482000000	0.430079000000
C	-4.022127000000	-0.324174000000	0.038663000000
C	-3.900026000000	1.008697000000	-0.352753000000
H	-2.557141000000	2.636679000000	-0.697422000000
H	-0.808830000000	-1.014561000000	0.803013000000
H	-3.010767000000	-2.075782000000	0.760880000000
H	-4.782057000000	1.567885000000	-0.646057000000
C	-0.210683000000	1.553308000000	-0.077736000000
H	-0.139094000000	2.625762000000	-0.208123000000
N	0.941003000000	0.876696000000	-0.004210000000
H	0.836427000000	-0.137892000000	-0.023018000000

C	2.204284000000	1.296395000000	0.086291000000
H	2.355976000000	2.356889000000	0.245680000000
C	3.318923000000	0.389036000000	-0.007033000000
C	4.595946000000	0.831577000000	0.397503000000
C	3.204812000000	-0.935276000000	-0.480414000000
C	5.693709000000	-0.015845000000	0.359943000000
H	4.710502000000	1.850681000000	0.757012000000
C	4.306288000000	-1.784326000000	-0.497842000000
H	2.263202000000	-1.303507000000	-0.881644000000
C	5.557641000000	-1.335722000000	-0.077582000000
H	6.663461000000	0.352162000000	0.680904000000
H	4.189112000000	-2.798998000000	-0.866145000000
H	6.416051000000	-1.998240000000	-0.103774000000
Cl	-5.593745000000	-1.079937000000	0.058323000000

- 3:

C	1.705778000000	1.052414000000	0.000001000000
C	2.167808000000	-0.262688000000	0.000000000000
C	1.268290000000	-1.335577000000	0.000000000000
C	-0.099555000000	-1.097970000000	0.000001000000
C	-0.550611000000	0.224629000000	-0.000001000000
C	0.334363000000	1.299243000000	-0.000001000000
H	2.409482000000	1.877848000000	0.000002000000
H	3.235462000000	-0.458541000000	-0.000002000000
H	1.642688000000	-2.354009000000	-0.000003000000
H	-0.823860000000	-1.905473000000	0.000002000000
H	-0.069112000000	2.307221000000	0.000000000000
N	-1.951637000000	0.583113000000	0.000000000000
O	-2.711205000000	-0.353644000000	0.000000000000

- 11:

C	-3.315777000000	-0.866701000000	0.891397000000
C	-2.308253000000	-0.393235000000	0.047261000000
C	-2.569429000000	0.689796000000	-0.801576000000
C	-3.823841000000	1.287289000000	-0.798597000000
C	-4.828300000000	0.810779000000	0.048453000000
C	-4.573877000000	-0.266928000000	0.893501000000
H	-3.111640000000	-1.707827000000	1.549715000000
H	-1.776214000000	1.042468000000	-1.453175000000
H	-4.024287000000	2.126493000000	-1.457300000000
H	-5.807082000000	1.280302000000	0.047307000000
H	-5.351837000000	-0.639691000000	1.552061000000
C	-0.982809000000	-1.042583000000	0.068670000000
H	-0.877256000000	-1.894467000000	0.761047000000
N	-0.017264000000	-0.652628000000	-0.655553000000

C	1.235288000000	-1.370698000000	-0.556066000000
H	1.435045000000	-1.823019000000	-1.535753000000
H	1.180412000000	-2.192341000000	0.178515000000
C	2.399207000000	-0.464143000000	-0.203442000000
C	2.213113000000	0.868781000000	0.162217000000
C	3.696602000000	-0.986473000000	-0.227357000000
C	3.307920000000	1.666138000000	0.500192000000
H	1.209328000000	1.280880000000	0.172300000000
C	4.788467000000	-0.193496000000	0.111382000000
H	3.850697000000	-2.024635000000	-0.514476000000
C	4.596384000000	1.139728000000	0.477164000000
H	3.149601000000	2.702891000000	0.781295000000
H	5.789418000000	-0.613455000000	0.087958000000
H	5.446499000000	1.761269000000	0.740189000000

- IM-1:

N	0.048128000000	-2.613694000000	-0.071226000000
O	0.661360000000	-2.539379000000	-1.108523000000
C	-2.134159000000	2.575935000000	-0.771214000000
C	-1.187650000000	1.721249000000	-0.200453000000
C	-1.441985000000	1.142722000000	1.048876000000
C	-2.632984000000	1.415298000000	1.709875000000
C	-3.584043000000	2.258772000000	1.129498000000
C	-3.334364000000	2.838757000000	-0.112715000000
H	-1.931180000000	3.030962000000	-1.737995000000
H	-0.693735000000	0.483475000000	1.478650000000
H	-2.826736000000	0.965388000000	2.679027000000
H	-4.067922000000	3.499565000000	-0.563906000000
C	0.061749000000	1.429464000000	-0.930825000000
N	0.829515000000	0.473719000000	-0.604962000000
C	2.041640000000	0.277788000000	-1.386438000000
H	1.947629000000	-0.691964000000	-1.889913000000
H	2.165757000000	1.054870000000	-2.157157000000
C	3.251007000000	0.247853000000	-0.478944000000
C	4.243420000000	1.222262000000	-0.573823000000
C	3.374861000000	-0.763102000000	0.479931000000
C	5.353453000000	1.189353000000	0.271956000000
H	4.149588000000	2.013015000000	-1.314299000000
C	4.478829000000	-0.795923000000	1.326149000000
H	2.597906000000	-1.519563000000	0.555308000000
C	5.472190000000	0.180342000000	1.223610000000
H	6.120989000000	1.952528000000	0.186869000000
H	4.567991000000	-1.585656000000	2.065884000000
H	6.333859000000	0.152066000000	1.883387000000
H	0.284273000000	2.084679000000	-1.789277000000
C	-1.307049000000	-2.125566000000	-0.133046000000

C	-2.072566000000	-2.356683000000	1.008061000000
C	-1.829161000000	-1.455110000000	-1.241343000000
C	-3.395218000000	-1.922391000000	1.040085000000
H	-1.616572000000	-2.875201000000	1.846363000000
C	-3.142054000000	-1.006485000000	-1.193402000000
H	-1.191649000000	-1.281708000000	-2.102090000000
C	-3.923352000000	-1.243379000000	-0.057136000000
H	-4.007386000000	-2.098859000000	1.918503000000
H	-3.561411000000	-0.460902000000	-2.032691000000
H	-4.946990000000	-0.882691000000	-0.026580000000
H	-4.514171000000	2.467923000000	1.649207000000

- TS-1:

N	-0.589487000000	-0.765102000000	1.229501000000
O	0.550003000000	-1.361340000000	1.303865000000
C	-2.572961000000	1.503626000000	-1.125319000000
C	-1.344617000000	1.614150000000	-0.465947000000
C	-1.130100000000	2.672377000000	0.427024000000
C	-2.131430000000	3.609603000000	0.644054000000
C	-3.356263000000	3.499401000000	-0.022333000000
C	-3.576224000000	2.446619000000	-0.907225000000
H	-2.740870000000	0.673770000000	-1.807773000000
H	-0.178918000000	2.731380000000	0.945963000000
H	-1.965369000000	4.426358000000	1.339397000000
H	-4.525860000000	2.357568000000	-1.425283000000
C	-0.320207000000	0.591476000000	-0.691179000000
N	0.936190000000	0.785306000000	-0.402934000000
C	1.785096000000	-0.258656000000	-0.593572000000
H	1.323221000000	-0.914581000000	0.531326000000
H	1.520370000000	-1.013510000000	-1.347864000000
C	3.231737000000	-0.081365000000	-0.350900000000
C	4.132670000000	-1.045033000000	-0.819238000000
C	3.717148000000	1.016376000000	0.371872000000
C	5.497109000000	-0.913077000000	-0.577634000000
H	3.759369000000	-1.899561000000	-1.378647000000
C	5.081001000000	1.147060000000	0.608783000000
H	3.012447000000	1.758189000000	0.732804000000
C	5.975304000000	0.184206000000	0.137203000000
H	6.186660000000	-1.664677000000	-0.948821000000
H	5.450286000000	2.002749000000	1.165473000000
H	7.038947000000	0.289576000000	0.325847000000
H	-0.624498000000	-0.272940000000	-1.297798000000
C	-1.597488000000	-1.606067000000	0.688259000000
C	-2.904791000000	-1.113704000000	0.788127000000
C	-1.349794000000	-2.852825000000	0.096297000000
C	-3.964143000000	-1.865207000000	0.288657000000

H	-3.062388000000	-0.149990000000	1.263247000000
C	-2.415391000000	-3.590470000000	-0.404487000000
H	-0.332141000000	-3.224598000000	0.047451000000
C	-3.722121000000	-3.100751000000	-0.312069000000
H	-4.978503000000	-1.487451000000	0.369293000000
H	-2.231950000000	-4.556354000000	-0.864841000000
H	-4.548553000000	-3.686845000000	-0.701328000000
H	-4.136417000000	4.233793000000	0.152426000000

- 19:

C	-0.944528000000	1.398250000000	-0.328764000000
C	-0.347306000000	2.381803000000	0.460561000000
C	-0.996931000000	3.592952000000	0.683197000000
C	-2.250394000000	3.830510000000	0.118648000000
C	-2.850688000000	2.852216000000	-0.670985000000
C	-2.198400000000	1.640436000000	-0.893788000000
H	0.630052000000	2.191942000000	0.893192000000
H	-0.524503000000	4.353589000000	1.297093000000
H	-3.823830000000	3.031197000000	-1.117442000000
H	-2.669469000000	0.876894000000	-1.509152000000
C	-0.277385000000	0.049021000000	-0.539033000000
H	-0.592631000000	-0.338653000000	-1.514309000000
N	1.159405000000	0.193347000000	-0.595126000000
C	1.917173000000	-0.624871000000	0.008455000000
H	1.519110000000	-1.464351000000	0.594040000000
C	3.388554000000	-0.513758000000	-0.051299000000
C	4.010034000000	0.523566000000	-0.757886000000
C	4.171577000000	-1.461401000000	0.612653000000
C	5.396511000000	0.604676000000	-0.795175000000
H	3.386216000000	1.251225000000	-1.267346000000
C	5.562465000000	-1.380137000000	0.573931000000
H	3.687479000000	-2.266954000000	1.159858000000
C	6.175534000000	-0.346320000000	-0.129962000000
H	5.876220000000	1.409858000000	-1.342785000000
H	6.164335000000	-2.120503000000	1.091173000000
H	7.258547000000	-0.278909000000	-0.161789000000
N	-0.744986000000	-0.960128000000	0.446019000000
C	-2.083507000000	-1.407177000000	0.217297000000
C	-3.145049000000	-1.050497000000	1.049347000000
C	-2.309780000000	-2.231233000000	-0.890816000000
C	-4.429031000000	-1.511824000000	0.760097000000
H	-2.958538000000	-0.409302000000	1.902021000000
C	-3.597169000000	-2.671283000000	-1.178639000000
H	-1.470961000000	-2.532758000000	-1.512106000000
C	-4.664947000000	-2.313990000000	-0.353707000000
H	-5.252217000000	-1.228699000000	1.408896000000

H	-3.763689000000	-3.308976000000	-2.041245000000
H	-5.667566000000	-2.665141000000	-0.574276000000
O	-0.621899000000	-0.379668000000	1.730587000000
H	-0.130096000000	-1.037835000000	2.238142000000
H	-2.754596000000	4.776560000000	0.290295000000

- TS-2:

C	0.204035000000	2.122900000000	0.230746000000
C	-0.634839000000	2.453197000000	1.305373000000
C	-1.453226000000	3.577650000000	1.249736000000
C	-1.437819000000	4.389394000000	0.117985000000
C	-0.606578000000	4.066290000000	-0.957015000000
C	0.204328000000	2.938346000000	-0.913474000000
H	-0.645247000000	1.818513000000	2.188122000000
H	-2.098285000000	3.817894000000	2.088550000000
H	-0.594734000000	4.696425000000	-1.840510000000
H	0.835817000000	2.678248000000	-1.754437000000
C	1.032909000000	0.933101000000	0.393113000000
H	1.154562000000	0.558398000000	1.406763000000
N	-0.372134000000	-0.607896000000	-0.572835000000
C	-1.565025000000	-0.256687000000	-0.361669000000
H	-1.890442000000	0.806536000000	-0.316834000000
C	-2.687229000000	-1.211277000000	-0.136575000000
C	-2.465232000000	-2.592938000000	-0.118096000000
C	-3.979555000000	-0.719146000000	0.059734000000
C	-3.525788000000	-3.465836000000	0.094155000000
H	-1.451366000000	-2.950697000000	-0.271305000000
C	-5.044401000000	-1.593880000000	0.271184000000
H	-4.146830000000	0.355909000000	0.044189000000
C	-4.817848000000	-2.968597000000	0.288644000000
H	-3.351328000000	-4.537495000000	0.109259000000
H	-6.046778000000	-1.204864000000	0.421759000000
H	-5.644271000000	-3.653250000000	0.453571000000
N	1.957737000000	0.513510000000	-0.470102000000
C	2.954431000000	-0.435588000000	-0.107710000000
C	3.217517000000	-1.518920000000	-0.944816000000
C	3.674975000000	-0.244981000000	1.072043000000
C	4.194168000000	-2.435768000000	-0.570301000000
H	2.649219000000	-1.629714000000	-1.859793000000
C	4.641115000000	-1.177990000000	1.438617000000
H	3.500806000000	0.637569000000	1.680174000000
C	4.903173000000	-2.275550000000	0.620782000000
H	4.397571000000	-3.286740000000	-1.212300000000
H	5.202124000000	-1.033651000000	2.356202000000
H	5.662925000000	-2.996258000000	0.904377000000
O	1.507628000000	0.477286000000	-1.738665000000

H	0.523412000000	-0.005493000000	-1.452422000000
H	-2.072055000000	5.268771000000	0.069774000000

- 12:

C	-2.128138000000	-0.673457000000	-0.598119000000
C	-2.794590000000	0.417259000000	-1.191647000000
C	-4.169254000000	0.565391000000	-1.074059000000
C	-4.911743000000	-0.377330000000	-0.359331000000
C	-4.264539000000	-1.461946000000	0.228251000000
C	-2.883809000000	-1.620179000000	0.118970000000
H	-2.215530000000	1.154029000000	-1.743527000000
H	-4.663422000000	1.412735000000	-1.538888000000
H	-4.838503000000	-2.198885000000	0.781437000000
H	-2.380477000000	-2.460481000000	0.576184000000
C	-0.686028000000	-0.703907000000	-0.762418000000
H	-0.217534000000	0.109129000000	-1.302404000000
N	0.385719000000	-0.303644000000	2.623985000000
C	-0.347559000000	0.563924000000	2.051813000000
H	-1.444497000000	0.562205000000	2.121253000000
C	0.223078000000	1.625528000000	1.192841000000
C	1.595457000000	1.669345000000	0.916413000000
C	-0.632386000000	2.554507000000	0.594004000000
C	2.096914000000	2.624686000000	0.039373000000
H	2.246380000000	0.936486000000	1.384271000000
C	-0.128181000000	3.514840000000	-0.281719000000
H	-1.698739000000	2.510940000000	0.805222000000
C	1.236824000000	3.546524000000	-0.563997000000
H	3.159728000000	2.647684000000	-0.181265000000
H	-0.797700000000	4.233865000000	-0.743787000000
H	1.631898000000	4.289379000000	-1.250186000000
N	0.132125000000	-1.585336000000	-0.243766000000
C	1.562549000000	-1.429174000000	-0.451495000000
C	2.397685000000	-1.816149000000	0.591537000000
C	2.072336000000	-0.911636000000	-1.639533000000
C	3.770391000000	-1.632040000000	0.455323000000
H	1.952576000000	-2.223500000000	1.490192000000
C	3.448344000000	-0.737514000000	-1.764244000000
H	1.414063000000	-0.666406000000	-2.465967000000
C	4.297888000000	-1.087006000000	-0.715616000000
H	4.429459000000	-1.912859000000	1.270294000000
H	3.854704000000	-0.339125000000	-2.688139000000
H	5.369598000000	-0.948570000000	-0.816763000000
O	-0.223069000000	-2.552861000000	0.507932000000
H	-0.186475000000	-0.985075000000	3.123846000000
H	-5.987332000000	-0.265788000000	-0.264849000000

- IM-1^{O} :

C	3.405538000000	0.018440000000	-1.312561000000
C	2.423084000000	-0.803992000000	-0.756869000000
C	2.700904000000	-1.518380000000	0.413799000000
C	3.943717000000	-1.396856000000	1.023700000000
C	4.921516000000	-0.565085000000	0.469673000000
C	4.653221000000	0.139234000000	-0.702462000000
H	3.185569000000	0.575214000000	-2.220831000000
H	1.922071000000	-2.146524000000	0.834875000000
H	4.155640000000	-1.947907000000	1.934867000000
H	5.411455000000	0.781727000000	-1.138912000000
C	1.088456000000	-0.859701000000	-1.385702000000
N	0.155241000000	-1.597283000000	-0.945734000000
C	-1.119855000000	-1.551166000000	-1.638606000000
H	-1.128965000000	-0.799235000000	-2.444267000000
H	-1.273827000000	-2.534563000000	-2.103040000000
C	-2.261369000000	-1.279032000000	-0.680859000000
C	-3.336165000000	-0.484813000000	-1.081695000000
C	-2.257819000000	-1.819467000000	0.609199000000
C	-4.392113000000	-0.224651000000	-0.207787000000
H	-3.338102000000	-0.041057000000	-2.074007000000
C	-3.310154000000	-1.560345000000	1.483120000000
H	-1.410282000000	-2.419385000000	0.926065000000
C	-4.380236000000	-0.759037000000	1.078723000000
H	-5.212279000000	0.409525000000	-0.529327000000
H	-3.295437000000	-1.980813000000	2.484540000000
H	-5.196920000000	-0.552202000000	1.763416000000
H	0.943560000000	-0.203391000000	-2.260058000000
O	-2.208249000000	2.385676000000	-1.335223000000
N	-1.003472000000	2.460230000000	-1.277386000000
C	-0.425678000000	1.995253000000	-0.042238000000
C	0.955251000000	2.162475000000	0.061911000000
C	-1.168040000000	1.376167000000	0.967604000000
C	1.615505000000	1.706357000000	1.198668000000
H	1.488279000000	2.635848000000	-0.758159000000
C	-0.498594000000	0.913654000000	2.092725000000
H	-2.239479000000	1.246276000000	0.845654000000
C	0.886179000000	1.078681000000	2.207525000000
H	2.693722000000	1.805080000000	1.282323000000
H	-1.053451000000	0.408943000000	2.877357000000
H	1.401511000000	0.701260000000	3.085701000000
H	5.890468000000	-0.471255000000	0.950216000000

- TS-1^{O} :

C	3.718674000000	0.111668000000	-0.812039000000
C	2.692874000000	-0.731607000000	-0.374867000000

C	3.012502000000	-1.940373000000	0.254831000000
C	4.343198000000	-2.299750000000	0.431908000000
C	5.365037000000	-1.456617000000	-0.011389000000
C	5.051621000000	-0.249145000000	-0.633010000000
H	3.467192000000	1.053723000000	-1.293927000000
H	2.204736000000	-2.578573000000	0.597270000000
H	4.589000000000	-3.237352000000	0.920561000000
H	5.843235000000	0.409192000000	-0.976404000000
C	1.296244000000	-0.324312000000	-0.569016000000
N	0.302985000000	-1.142127000000	-0.363274000000
C	-0.950239000000	-0.613890000000	-0.465321000000
H	-0.969395000000	0.073738000000	0.707896000000
H	-1.098140000000	0.234487000000	-1.150836000000
C	-2.126150000000	-1.507826000000	-0.329658000000
C	-3.373790000000	-1.077684000000	-0.795234000000
C	-2.020165000000	-2.754792000000	0.297838000000
C	-4.500150000000	-1.882611000000	-0.642869000000
H	-3.456280000000	-0.112036000000	-1.289506000000
C	-3.145533000000	-3.558893000000	0.443949000000
H	-1.048488000000	-3.078219000000	0.656733000000
C	-4.388239000000	-3.125911000000	-0.022757000000
H	-5.462230000000	-1.542518000000	-1.013128000000
H	-3.055843000000	-4.527307000000	0.926295000000
H	-5.263954000000	-3.756265000000	0.094995000000
H	1.135813000000	0.642995000000	-1.066132000000
O	0.874630000000	0.646830000000	1.380580000000
N	-0.336189000000	0.968721000000	1.372217000000
C	-0.624283000000	2.219784000000	0.705514000000
C	-1.969235000000	2.551913000000	0.533071000000
C	0.390132000000	3.088163000000	0.307761000000
C	-2.302043000000	3.762705000000	-0.063111000000
H	-2.735240000000	1.856257000000	0.868300000000
C	0.045773000000	4.303515000000	-0.280975000000
H	1.423229000000	2.804959000000	0.480337000000
C	-1.294147000000	4.640333000000	-0.470831000000
H	-3.344817000000	4.027574000000	-0.204979000000
H	0.826090000000	4.992508000000	-0.588417000000
H	-1.555128000000	5.588542000000	-0.929645000000
H	6.403127000000	-1.740524000000	0.130563000000

- 24 :

C	3.218063000000	-0.301709000000	-1.334213000000
C	2.570470000000	-0.431231000000	-0.107371000000
C	3.141029000000	-1.211237000000	0.901623000000
C	4.353864000000	-1.854839000000	0.679479000000
C	5.000576000000	-1.726669000000	-0.551597000000

C	4.432450000000	-0.950490000000	-1.558573000000
H	2.773602000000	0.309357000000	-2.115911000000
H	2.627031000000	-1.300354000000	1.853504000000
H	4.797880000000	-2.457822000000	1.465338000000
H	4.933623000000	-0.846055000000	-2.515677000000
C	1.247622000000	0.247704000000	0.130695000000
N	0.199211000000	-0.723832000000	0.386912000000
C	-0.760026000000	-0.754063000000	-0.447447000000
H	-0.387467000000	0.787828000000	2.046254000000
H	-0.789346000000	-0.072159000000	-1.312440000000
C	-1.907212000000	-1.668271000000	-0.312705000000
C	-2.989262000000	-1.530619000000	-1.186521000000
C	-1.937366000000	-2.654384000000	0.681502000000
C	-4.098067000000	-2.366001000000	-1.068852000000
H	-2.961190000000	-0.762244000000	-1.955418000000
C	-3.042604000000	-3.488568000000	0.795445000000
H	-1.085047000000	-2.750446000000	1.346701000000
C	-4.124345000000	-3.345045000000	-0.077948000000
H	-4.937071000000	-2.253937000000	-1.747906000000
H	-3.064821000000	-4.255179000000	1.563448000000
H	-4.985532000000	-3.999410000000	0.014639000000
H	0.990734000000	0.888622000000	-0.729794000000
O	1.408270000000	1.064276000000	1.295767000000
N	0.187652000000	1.579513000000	1.764094000000
C	-0.477446000000	2.421090000000	0.848283000000
C	-1.873627000000	2.386440000000	0.764543000000
C	0.242638000000	3.330689000000	0.066152000000
C	-2.542849000000	3.268173000000	-0.080418000000
H	-2.430934000000	1.665749000000	1.358679000000
C	-0.436746000000	4.194662000000	-0.787399000000
H	1.325149000000	3.348252000000	0.141783000000
C	-1.830020000000	4.174045000000	-0.864473000000
H	-3.626792000000	3.235610000000	-0.133512000000
H	0.128942000000	4.896404000000	-1.392724000000
H	-2.352595000000	4.854256000000	-1.528537000000
H	5.946781000000	-2.230509000000	-0.722847000000

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C	-3.664470000000	-1.006840000000	0.658656000000
C	-2.363774000000	-1.483035000000	0.513785000000
C	-1.390699000000	-0.721298000000	-0.136323000000
C	-1.733167000000	0.535958000000	-0.648438000000
C	-3.025564000000	1.023258000000	-0.511713000000
C	-3.980985000000	0.244700000000	0.142503000000
H	-4.423628000000	-1.593867000000	1.163302000000
H	-2.104448000000	-2.459949000000	0.913880000000

H	-0.969525000000	1.119310000000	-1.152448000000
H	-3.300872000000	1.995787000000	-0.904674000000
C	-0.020871000000	-1.253233000000	-0.271497000000
H	0.149378000000	-2.253458000000	0.159437000000
N	0.908404000000	-0.608343000000	-0.844158000000
C	2.216683000000	-1.232455000000	-0.919142000000
H	2.441429000000	-1.384075000000	-1.983262000000
H	2.234129000000	-2.221636000000	-0.434266000000
C	3.292674000000	-0.352273000000	-0.315767000000
C	4.359872000000	-0.928103000000	0.375425000000
C	3.251913000000	1.036610000000	-0.467461000000
C	5.378645000000	-0.133394000000	0.900126000000
H	4.394367000000	-2.006916000000	0.507685000000
C	4.266756000000	1.831850000000	0.059547000000
H	2.414049000000	1.485677000000	-0.991251000000
C	5.334367000000	1.249993000000	0.743174000000
H	6.201569000000	-0.595546000000	1.436646000000
H	4.223286000000	2.909917000000	-0.061984000000
H	6.123390000000	1.871595000000	1.154585000000
Cl	-5.604130000000	0.854183000000	0.315541000000

- IM-1_{Cl}:

N	0.077861000000	2.402227000000	1.710690000000
O	-0.972248000000	2.862318000000	1.334136000000
C	1.735445000000	-0.945198000000	-1.510434000000
C	0.764886000000	-0.793958000000	-0.519451000000
C	1.032191000000	-1.245636000000	0.779551000000
C	2.253870000000	-1.830451000000	1.082999000000
C	3.213511000000	-1.959416000000	0.077817000000
C	2.966454000000	-1.529397000000	-1.220405000000
H	1.533866000000	-0.590994000000	-2.518515000000
H	0.270801000000	-1.114903000000	1.542929000000
H	2.472971000000	-2.179656000000	2.086276000000
H	3.727422000000	-1.644158000000	-1.984508000000
C	-0.515823000000	-0.136942000000	-0.846245000000
N	-1.424642000000	0.041937000000	0.019688000000
C	-2.635045000000	0.719604000000	-0.395577000000
H	-2.729083000000	1.624945000000	0.215540000000
H	-2.580354000000	1.036557000000	-1.451870000000
C	-3.871837000000	-0.133563000000	-0.194519000000
C	-5.126614000000	0.482252000000	-0.160289000000
C	-3.796553000000	-1.521834000000	-0.078273000000
C	-6.286339000000	-0.274814000000	-0.022304000000
H	-5.192962000000	1.565108000000	-0.238650000000
C	-4.957677000000	-2.282128000000	0.065091000000
H	-2.825122000000	-2.006244000000	-0.086402000000

C	-6.204734000000	-1.663026000000	0.091109000000
H	-7.253282000000	0.218205000000	0.004345000000
H	-4.884582000000	-3.361325000000	0.159530000000
H	-0.630506000000	0.202437000000	-1.889420000000
C	1.112912000000	2.363198000000	0.703744000000
C	2.318735000000	1.802542000000	1.116595000000
C	0.929991000000	2.827541000000	-0.601365000000
C	3.369888000000	1.696191000000	0.208007000000
H	2.406152000000	1.446826000000	2.138995000000
C	1.982776000000	2.723171000000	-1.500325000000
H	-0.027984000000	3.253546000000	-0.882921000000
C	3.198769000000	2.158583000000	-1.095245000000
H	4.310566000000	1.247298000000	0.510572000000
H	1.865057000000	3.078874000000	-2.519163000000
H	4.014536000000	2.074388000000	-1.807091000000
H	-7.107281000000	-2.255389000000	0.203975000000
Cl	4.760376000000	-2.667266000000	0.461633000000

- TS-1_{Cl} :

N	-0.162343000000	1.166344000000	1.221595000000
O	-1.423877000000	1.406503000000	1.317633000000
C	2.358737000000	-0.388296000000	-1.185588000000
C	1.217768000000	-0.859013000000	-0.529606000000
C	1.326573000000	-1.949017000000	0.343717000000
C	2.552887000000	-2.564205000000	0.548899000000
C	3.678221000000	-2.081615000000	-0.122187000000
C	3.595469000000	-0.998715000000	-0.989809000000
H	2.281141000000	0.465888000000	-1.853522000000
H	0.438761000000	-2.292484000000	0.864277000000
H	2.649747000000	-3.405039000000	1.226743000000
H	4.483492000000	-0.641379000000	-1.499081000000
C	-0.059838000000	-0.172415000000	-0.729381000000
N	-1.201188000000	-0.727305000000	-0.433790000000
C	-2.319408000000	0.029018000000	-0.591683000000
H	-2.047154000000	0.767493000000	0.544380000000
H	-2.296274000000	0.843049000000	-1.330230000000
C	-3.648733000000	-0.564272000000	-0.339676000000
C	-4.796364000000	0.107113000000	-0.777837000000
C	-3.785475000000	-1.769563000000	0.361492000000
C	-6.060769000000	-0.418420000000	-0.527872000000
H	-4.694207000000	1.044028000000	-1.320280000000
C	-5.049809000000	-2.293608000000	0.606799000000
H	-2.891643000000	-2.283470000000	0.699267000000
C	-6.190875000000	-1.621138000000	0.165148000000
H	-6.943466000000	0.108902000000	-0.875525000000
H	-5.147966000000	-3.230463000000	1.146321000000

H	-7.175807000000	-2.033340000000	0.360084000000
H	-0.025426000000	0.753899000000	-1.319271000000
Cl	5.220099000000	-2.850948000000	0.138920000000
C	0.553580000000	2.272414000000	0.692425000000
C	1.948402000000	2.177876000000	0.776639000000
C	-0.050359000000	3.403900000000	0.125661000000
C	2.740200000000	3.211878000000	0.286214000000
H	2.383122000000	1.294785000000	1.235526000000
C	0.751249000000	4.426317000000	-0.366681000000
H	-1.132524000000	3.466113000000	0.089409000000
C	2.144729000000	4.334007000000	-0.290277000000
H	3.821158000000	3.143381000000	0.356234000000
H	0.291703000000	5.305392000000	-0.807671000000
H	2.762273000000	5.140583000000	-0.672393000000

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C	0.731534000000	-0.531763000000	0.609731000000
C	1.915333000000	-0.671480000000	1.332728000000
C	2.801788000000	-1.708554000000	1.056658000000
C	2.488097000000	-2.609779000000	0.044558000000
C	1.306280000000	-2.496763000000	-0.682221000000
C	0.429644000000	-1.455905000000	-0.389992000000
H	2.163779000000	0.050972000000	2.105924000000
H	3.726546000000	-1.815951000000	1.612457000000
H	1.077616000000	-3.216977000000	-1.460043000000
H	-0.498211000000	-1.363360000000	-0.946427000000
C	-0.188232000000	0.648332000000	0.866372000000
H	0.027258000000	1.026364000000	1.885446000000
N	-1.562139000000	0.199467000000	0.879758000000
C	-2.360236000000	0.560778000000	-0.042004000000
H	-2.054626000000	1.243785000000	-0.842111000000
C	-3.753090000000	0.074233000000	-0.088336000000
C	-4.240889000000	-0.835789000000	0.858115000000
C	-4.595727000000	0.529930000000	-1.105836000000
C	-5.556046000000	-1.277388000000	0.783079000000
H	-3.571906000000	-1.181124000000	1.639953000000
C	-5.914900000000	0.086339000000	-1.180421000000
H	-4.213947000000	1.237023000000	-1.838203000000
C	-6.395402000000	-0.817562000000	-0.235781000000
H	-5.932472000000	-1.982848000000	1.517252000000
H	-6.564472000000	0.445174000000	-1.972389000000
H	-7.422220000000	-1.165718000000	-0.290938000000
N	0.079291000000	1.742834000000	-0.096243000000
Cl	3.592316000000	-3.911011000000	-0.314730000000
C	1.468576000000	2.085643000000	-0.237632000000
C	2.202853000000	1.434440000000	-1.230774000000

C	2.097327000000	3.015298000000	0.591601000000
C	3.564980000000	1.680647000000	-1.365309000000
H	1.694079000000	0.730022000000	-1.880722000000
C	3.460554000000	3.269473000000	0.443181000000
H	1.532904000000	3.559415000000	1.342222000000
C	4.200286000000	2.597344000000	-0.526773000000
H	4.129454000000	1.162094000000	-2.133727000000
H	3.942291000000	3.997205000000	1.088703000000
H	5.261307000000	2.795561000000	-0.638103000000
O	-0.678190000000	2.863008000000	0.301933000000
H	-0.537675000000	3.000522000000	1.255379000000

- TS-2_{Cl}:

C	0.548965000000	-1.560712000000	0.230520000000
C	1.439481000000	-1.353177000000	1.293429000000
C	2.747770000000	-1.821509000000	1.238326000000
C	3.166340000000	-2.509871000000	0.105025000000
C	2.300898000000	-2.727438000000	-0.967028000000
C	0.999814000000	-2.246694000000	-0.909613000000
H	1.104378000000	-0.814214000000	2.175877000000
H	3.434236000000	-1.657411000000	2.061218000000
H	2.651112000000	-3.265119000000	-1.841103000000
H	0.327603000000	-2.396430000000	-1.745808000000
C	-0.803530000000	-1.040820000000	0.395912000000
H	-1.112148000000	-0.794211000000	1.409000000000
N	-0.509936000000	1.014691000000	-0.576641000000
C	0.670144000000	1.406032000000	-0.363474000000
H	1.543553000000	0.717703000000	-0.316802000000
C	1.047638000000	2.829621000000	-0.139025000000
C	0.075715000000	3.836356000000	-0.116706000000
C	2.390127000000	3.163613000000	0.053217000000
C	0.447895000000	5.158437000000	0.095428000000
H	-0.961237000000	3.550937000000	-0.266967000000
C	2.764597000000	4.489845000000	0.264260000000
H	3.142255000000	2.377567000000	0.034089000000
C	1.792997000000	5.488311000000	0.285799000000
H	-0.307585000000	5.938134000000	0.113671000000
H	3.809956000000	4.743239000000	0.411269000000
H	2.080515000000	6.522254000000	0.450516000000
N	-1.804248000000	-1.218558000000	-0.465957000000
Cl	4.798671000000	-3.105378000000	0.019989000000
C	-3.162481000000	-0.992311000000	-0.104904000000
C	-3.989131000000	-0.249668000000	-0.946523000000
C	-3.650081000000	-1.547677000000	1.078702000000
C	-5.311959000000	-0.038034000000	-0.572372000000
H	-3.582213000000	0.155821000000	-1.864341000000

C	-4.973281000000	-1.316811000000	1.444660000000
H	-3.009925000000	-2.176401000000	1.690269000000
C	-5.807276000000	-0.561436000000	0.622480000000
H	-5.958972000000	0.547286000000	-1.217642000000
H	-5.355668000000	-1.745824000000	2.365076000000
H	-6.840560000000	-0.390593000000	0.905558000000
O	-1.450383000000	-0.943104000000	-1.735284000000
H	-0.908193000000	0.014260000000	-1.451933000000

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C	1.499909000000	-0.645657000000	0.564669000000
C	2.170295000000	0.451023000000	1.141140000000
C	3.541604000000	0.609486000000	1.012371000000
C	4.264861000000	-0.342979000000	0.295668000000
C	3.632238000000	-1.438657000000	-0.280747000000
C	2.254209000000	-1.594080000000	-0.151312000000
H	1.598697000000	1.193371000000	1.692505000000
H	4.050843000000	1.456529000000	1.458627000000
H	4.215580000000	-2.169203000000	-0.830464000000
H	1.753230000000	-2.441467000000	-0.597935000000
C	0.060618000000	-0.681502000000	0.742250000000
H	-0.409398000000	0.133640000000	1.277676000000
N	-0.995154000000	-0.289180000000	-2.613923000000
C	-0.251407000000	0.602241000000	-2.094672000000
H	0.838704000000	0.629722000000	-2.232794000000
C	-0.797190000000	1.655627000000	-1.209973000000
C	-2.157436000000	1.683008000000	-0.876390000000
C	0.071809000000	2.592751000000	-0.644705000000
C	-2.631942000000	2.627980000000	0.026313000000
H	-2.819781000000	0.945780000000	-1.320948000000
C	-0.405605000000	3.542941000000	0.257039000000
H	1.128279000000	2.564837000000	-0.903055000000
C	-1.757327000000	3.556620000000	0.598019000000
H	-3.684840000000	2.638069000000	0.291036000000
H	0.274323000000	4.268571000000	0.692793000000
H	-2.131295000000	4.291674000000	1.304103000000
N	-0.753189000000	-1.573831000000	0.235529000000
Cl	5.988040000000	-0.153493000000	0.122213000000
C	-2.183346000000	-1.429009000000	0.450752000000
C	-3.020849000000	-1.822347000000	-0.587913000000
C	-2.689467000000	-0.915668000000	1.641935000000
C	-4.394089000000	-1.650062000000	-0.443180000000
H	-2.577260000000	-2.224760000000	-1.489586000000
C	-4.066289000000	-0.753827000000	1.775281000000
H	-2.027727000000	-0.665091000000	2.464059000000
C	-4.918919000000	-1.110507000000	0.731664000000

H	-5.055883000000	-1.935820000000	-1.254152000000
H	-4.470614000000	-0.359849000000	2.701931000000
H	-5.991142000000	-0.981704000000	0.839486000000
O	-0.392565000000	-2.544906000000	-0.508039000000
H	-0.439532000000	-0.958870000000	-3.147074000000

- TS-2'$_{Cl}$:

C	-1.803718000000	-0.397203000000	0.809326000000
C	-2.305681000000	-1.648107000000	0.449275000000
C	-3.604820000000	-1.770459000000	-0.035352000000
C	-4.385444000000	-0.625927000000	-0.173258000000
C	-3.900211000000	0.632594000000	0.173497000000
C	-2.606499000000	0.737448000000	0.674051000000
H	-1.664706000000	-2.516016000000	0.573481000000
H	-4.013068000000	-2.738101000000	-0.305563000000
H	-4.530147000000	1.507324000000	0.056747000000
H	-2.215430000000	1.712209000000	0.957687000000
C	-0.405195000000	-0.269362000000	1.310583000000
H	-0.327986000000	0.519922000000	2.086898000000
N	0.398808000000	-1.407097000000	1.415614000000
C	1.567229000000	-0.680908000000	1.146649000000
H	1.932996000000	0.040722000000	1.905456000000
C	2.703359000000	-1.339352000000	0.438001000000
C	2.604745000000	-2.674794000000	0.045453000000
C	3.857260000000	-0.608333000000	0.144066000000
C	3.662188000000	-3.278062000000	-0.632423000000
H	1.700179000000	-3.220347000000	0.298056000000
C	4.905679000000	-1.206606000000	-0.549260000000
H	3.928283000000	0.431767000000	0.456360000000
C	4.808839000000	-2.544134000000	-0.935138000000
H	3.592343000000	-4.320788000000	-0.926135000000
H	5.798259000000	-0.635206000000	-0.783514000000
H	5.629034000000	-3.014219000000	-1.468939000000
N	0.675414000000	0.359665000000	0.182446000000
Cl	-6.010449000000	-0.770149000000	-0.790361000000
C	0.952509000000	1.758189000000	-0.030693000000
C	0.953189000000	2.299022000000	-1.316155000000
C	1.216181000000	2.565109000000	1.081557000000
C	1.219643000000	3.656765000000	-1.483904000000
H	0.748321000000	1.661497000000	-2.165762000000
C	1.480189000000	3.918421000000	0.896735000000
H	1.217962000000	2.150136000000	2.082588000000
C	1.482929000000	4.469334000000	-0.384529000000
H	1.220178000000	4.076709000000	-2.484495000000
H	1.684620000000	4.542437000000	1.760499000000
H	1.689599000000	5.525487000000	-0.522425000000

O	0.446280000000	-0.259179000000	-1.036329000000
H	0.283178000000	-1.187356000000	-0.751485000000

- 26:

C	-2.673299000000	0.465868000000	0.006046000000
C	-3.283010000000	-0.578135000000	0.712641000000
C	-4.665986000000	-0.689490000000	0.747938000000
C	-5.442514000000	0.251859000000	0.071035000000
C	-4.859703000000	1.296887000000	-0.637018000000
C	-3.470766000000	1.395600000000	-0.664490000000
H	-2.652981000000	-1.295170000000	1.229234000000
H	-5.148274000000	-1.494587000000	1.291300000000
H	-5.483825000000	2.016337000000	-1.155148000000
H	-3.003030000000	2.208814000000	-1.213795000000
C	-1.203858000000	0.598661000000	-0.044397000000
H	-0.812461000000	1.440367000000	-0.630609000000
N	-0.442828000000	-0.207896000000	0.569982000000
C	0.993034000000	-0.047931000000	0.526917000000
H	1.293857000000	0.343274000000	1.505341000000
C	1.676224000000	-1.390180000000	0.324517000000
C	1.104524000000	-2.375701000000	-0.481170000000
C	2.920266000000	-1.623078000000	0.914378000000
C	1.769689000000	-3.580011000000	-0.694899000000
H	0.135237000000	-2.193017000000	-0.934618000000
C	3.588095000000	-2.827961000000	0.700518000000
H	3.371527000000	-0.857548000000	1.542004000000
C	3.013174000000	-3.808425000000	-0.105125000000
H	1.317257000000	-4.342300000000	-1.321630000000
H	4.553412000000	-2.999911000000	1.166237000000
H	3.529443000000	-4.749154000000	-0.269842000000
N	1.457730000000	0.967187000000	-0.452692000000
Cl	-7.178901000000	0.112764000000	0.113990000000
C	2.793180000000	1.420842000000	-0.212089000000
C	3.865461000000	1.059164000000	-1.027758000000
C	3.003088000000	2.254296000000	0.891836000000
C	5.144694000000	1.525830000000	-0.726302000000
H	3.691086000000	0.410073000000	-1.877106000000
C	4.285870000000	2.699590000000	1.192361000000
H	2.155607000000	2.558462000000	1.499996000000
C	5.364488000000	2.337803000000	0.383713000000
H	5.976719000000	1.239175000000	-1.362095000000
H	4.440328000000	3.344662000000	2.051681000000
H	6.363497000000	2.693012000000	0.613931000000
O	1.349100000000	0.385142000000	-1.738494000000
H	0.880885000000	1.051439000000	-2.257687000000

- TS-3_{Cl}:

C	2.092052000000	0.448822000000	0.195846000000
C	2.842056000000	-0.641197000000	0.651855000000
C	4.226248000000	-0.639065000000	0.542622000000
C	4.860975000000	0.465253000000	-0.027055000000
C	4.137502000000	1.559909000000	-0.487444000000
C	2.749213000000	1.541608000000	-0.372585000000
H	2.311402000000	-1.481845000000	1.088996000000
H	4.817623000000	-1.478695000000	0.891527000000
H	4.654523000000	2.406103000000	-0.926468000000
H	2.169156000000	2.390221000000	-0.728096000000
C	0.607715000000	0.449009000000	0.311798000000
H	0.136389000000	1.346489000000	-0.143486000000
N	-0.045734000000	-0.477355000000	0.877601000000
C	-1.892891000000	-0.595191000000	-0.397371000000
H	-1.646834000000	-0.158173000000	-1.363257000000
C	-1.867578000000	-2.056953000000	-0.316259000000
C	-1.096816000000	-2.734326000000	-1.269426000000
C	-2.597993000000	-2.786861000000	0.631224000000
C	-1.049584000000	-4.123744000000	-1.277959000000
H	-0.523702000000	-2.164814000000	-1.996747000000
C	-2.559893000000	-4.176177000000	0.606698000000
H	-3.181477000000	-2.261085000000	1.378209000000
C	-1.784478000000	-4.847372000000	-0.340110000000
H	-0.443322000000	-4.639990000000	-2.014961000000
H	-3.132627000000	-4.739522000000	1.336252000000
H	-1.753302000000	-5.932327000000	-0.345647000000
N	-2.573563000000	0.204920000000	0.425479000000
Cl	6.600437000000	0.470689000000	-0.166559000000
C	-2.859755000000	1.561517000000	0.102720000000
C	-2.689951000000	2.553024000000	1.068967000000
C	-3.337073000000	1.874116000000	-1.171870000000
C	-2.960053000000	3.875636000000	0.730992000000
H	-2.345295000000	2.273630000000	2.056866000000
C	-3.592041000000	3.203276000000	-1.496706000000
H	-3.532015000000	1.084580000000	-1.891182000000
C	-3.401321000000	4.208503000000	-0.549788000000
H	-2.821009000000	4.652378000000	1.476017000000
H	-3.959878000000	3.448907000000	-2.487601000000
H	-3.609901000000	5.242377000000	-0.803663000000
O	-2.342302000000	-0.080256000000	1.724544000000
H	-1.231682000000	-0.279565000000	1.569937000000

- 12:

C	0.914993000000	-0.745011000000	-1.447401000000
C	2.110508000000	-0.036119000000	-1.609824000000

C	3.273093000000	-0.468085000000	-0.987105000000
C	3.232558000000	-1.613149000000	-0.192177000000
C	2.059636000000	-2.341557000000	-0.025829000000
C	0.901391000000	-1.898461000000	-0.661571000000
H	2.100431000000	0.869581000000	-2.208165000000
H	4.201131000000	0.083560000000	-1.091843000000
H	2.056298000000	-3.232018000000	0.593217000000
H	-0.028192000000	-2.448860000000	-0.531275000000
C	-0.346249000000	-0.229312000000	-2.021954000000
H	-1.236466000000	-0.848356000000	-1.834052000000
N	-0.385156000000	0.880307000000	-2.639825000000
C	-0.992912000000	0.689547000000	0.878538000000
H	-1.000107000000	-0.223305000000	1.460969000000
C	0.234637000000	1.462420000000	0.846877000000
C	1.290256000000	0.970328000000	1.639045000000
C	0.447424000000	2.607024000000	0.058497000000
C	2.524505000000	1.602645000000	1.655283000000
H	1.137480000000	0.072587000000	2.233604000000
C	1.692436000000	3.232993000000	0.081363000000
H	-0.352223000000	2.976065000000	-0.568238000000
C	2.728755000000	2.741108000000	0.872508000000
H	3.329223000000	1.202699000000	2.264438000000
H	1.851763000000	4.113388000000	-0.533305000000
H	3.694097000000	3.238056000000	0.877670000000
N	-2.106218000000	0.953431000000	0.239490000000
Cl	4.683259000000	-2.131116000000	0.627536000000
C	-3.231316000000	0.040406000000	0.371016000000
C	-4.031788000000	-0.142463000000	-0.752552000000
C	-3.514502000000	-0.600854000000	1.574271000000
C	-5.106835000000	-1.023077000000	-0.680953000000
H	-3.804280000000	0.419349000000	-1.651247000000
C	-4.598717000000	-1.473610000000	1.635192000000
H	-2.922541000000	-0.399962000000	2.460726000000
C	-5.389913000000	-1.693393000000	0.509018000000
H	-5.729504000000	-1.179548000000	-1.555652000000
H	-4.832800000000	-1.968952000000	2.571722000000
H	-6.234159000000	-2.372775000000	0.563208000000
O	-2.281532000000	1.935009000000	-0.558841000000
H	-1.341436000000	1.122947000000	-2.900276000000

- 17:

C	-5.373519000000	-0.217746000000	-0.983110000000
C	-4.198356000000	0.529780000000	-1.034388000000
C	-3.170895000000	0.294679000000	-0.117378000000
C	-3.328192000000	-0.697202000000	0.858983000000
C	-4.499910000000	-1.442018000000	0.909054000000

C	-5.524451000000	-1.204305000000	-0.011398000000
H	-6.167640000000	-0.030295000000	-1.698662000000
H	-4.075235000000	1.300855000000	-1.791223000000
H	-2.521928000000	-0.863401000000	1.566380000000
H	-4.620205000000	-2.210147000000	1.666508000000
H	-6.438558000000	-1.788200000000	0.031630000000
C	-1.934379000000	1.096261000000	-0.196089000000
H	-1.910737000000	1.866048000000	-0.985301000000
N	-0.952215000000	0.918708000000	0.587206000000
C	0.204557000000	1.772633000000	0.426274000000
H	0.298334000000	2.377461000000	1.337226000000
H	0.087258000000	2.471372000000	-0.419602000000
C	1.485553000000	0.981662000000	0.246856000000
C	2.709092000000	1.658144000000	0.237151000000
C	1.481331000000	-0.402004000000	0.075594000000
C	3.907041000000	0.975292000000	0.058061000000
H	2.728958000000	2.737165000000	0.372555000000
C	2.674380000000	-1.102236000000	-0.103639000000
H	0.537783000000	-0.937174000000	0.091935000000
C	3.876540000000	-0.406706000000	-0.110881000000
H	4.855237000000	1.501579000000	0.051989000000
H	2.671471000000	-2.178849000000	-0.234773000000
Cl	5.374590000000	-1.276164000000	-0.331155000000

- IM-1$_{Cl}$A:

N	-1.659127000000	-2.055507000000	1.740484000000
O	-0.741180000000	-2.725534000000	1.334339000000
C	-2.638102000000	1.800467000000	-1.331622000000
C	-1.702805000000	1.333928000000	-0.406018000000
C	-1.791202000000	1.740452000000	0.931977000000
C	-2.805250000000	2.602691000000	1.330229000000
C	-3.741019000000	3.064955000000	0.399824000000
C	-3.656170000000	2.664884000000	-0.931703000000
H	-2.571046000000	1.477675000000	-2.368204000000
H	-1.061767000000	1.358257000000	1.640290000000
H	-2.871572000000	2.916575000000	2.367431000000
H	-4.380002000000	3.023728000000	-1.656788000000
C	-0.646343000000	0.403646000000	-0.850017000000
N	0.228457000000	-0.063096000000	-0.058869000000
C	1.198659000000	-0.993452000000	-0.593890000000
H	1.051306000000	-1.951025000000	-0.078463000000
H	1.044836000000	-1.170851000000	-1.672657000000
C	2.625084000000	-0.536003000000	-0.363715000000
C	3.676590000000	-1.407254000000	-0.663675000000
C	2.924606000000	0.736319000000	0.121308000000
C	5.001417000000	-1.021128000000	-0.493141000000

H	3.458249000000	-2.405692000000	-1.035462000000
C	4.248104000000	1.138639000000	0.300590000000
H	2.115687000000	1.415223000000	0.369933000000
C	5.274533000000	0.256256000000	-0.010514000000
H	5.815736000000	-1.698561000000	-0.725835000000
H	4.481020000000	2.127749000000	0.679772000000
H	-0.669965000000	0.125247000000	-1.917222000000
H	-4.531447000000	3.739487000000	0.714697000000
Cl	6.934681000000	0.753231000000	0.206835000000
C	-2.664455000000	-1.748133000000	0.750522000000
C	-3.710400000000	-0.946140000000	1.199212000000
C	-2.596897000000	-2.190440000000	-0.573227000000
C	-4.713223000000	-0.569334000000	0.308271000000
H	-3.709751000000	-0.618369000000	2.234502000000
C	-3.600148000000	-1.813055000000	-1.455182000000
H	-1.761405000000	-2.810626000000	-0.883089000000
C	-4.654691000000	-1.003654000000	-1.013981000000
H	-5.525791000000	0.068897000000	0.638869000000
H	-3.568507000000	-2.143807000000	-2.488607000000
H	-5.430764000000	-0.706203000000	-1.712872000000

- TS-1_{Cl}A:

N	1.252597000000	0.798659000000	1.196059000000
O	0.145573000000	1.458334000000	1.198818000000
C	3.245841000000	-1.517500000000	-1.112726000000
C	1.999422000000	-1.605153000000	-0.484339000000
C	1.746513000000	-2.653513000000	0.410582000000
C	2.727791000000	-3.603793000000	0.659434000000
C	3.970384000000	-3.516969000000	0.022887000000
C	4.228546000000	-2.474221000000	-0.863506000000
H	3.444219000000	-0.694123000000	-1.794881000000
H	0.782259000000	-2.694304000000	0.906598000000
H	2.532198000000	-4.412640000000	1.356299000000
H	5.192213000000	-2.403032000000	-1.357789000000
C	1.000461000000	-0.565820000000	-0.739074000000
N	-0.264086000000	-0.726852000000	-0.468148000000
C	-1.087634000000	0.331802000000	-0.687003000000
H	-0.625291000000	0.998180000000	0.441140000000
H	-0.799423000000	1.069652000000	-1.448731000000
C	-2.538653000000	0.183835000000	-0.459415000000
C	-3.420041000000	1.157996000000	-0.941955000000
C	-3.053639000000	-0.899078000000	0.265183000000
C	-4.788981000000	1.058062000000	-0.717563000000
H	-3.031736000000	2.003844000000	-1.503546000000
C	-4.419439000000	-1.011352000000	0.492594000000
H	-2.369589000000	-1.653123000000	0.639714000000

C	-5.277126000000	-0.029930000000	-0.000442000000
H	-5.473004000000	1.810329000000	-1.094399000000
H	-4.823372000000	-1.850335000000	1.048531000000
H	1.335013000000	0.289637000000	-1.342771000000
H	4.734569000000	-4.261714000000	0.222429000000
Cl	-6.991201000000	-0.168586000000	0.284054000000
C	2.332613000000	1.569773000000	0.695761000000
C	3.601877000000	1.004303000000	0.872482000000
C	2.189669000000	2.819059000000	0.074105000000
C	4.728350000000	1.685682000000	0.421616000000
H	3.677496000000	0.040490000000	1.367206000000
C	3.321362000000	3.485414000000	-0.377968000000
H	1.199386000000	3.247452000000	-0.035178000000
C	4.590853000000	2.922846000000	-0.207526000000
H	5.713103000000	1.251324000000	0.561758000000
H	3.219614000000	4.452241000000	-0.860975000000
H	5.469587000000	3.454109000000	-0.559011000000

- 25A:

C	-1.606220000000	1.136531000000	-0.480516000000
C	-1.124349000000	1.883561000000	0.594837000000
C	-1.771825000000	3.054551000000	0.982693000000
C	-2.901391000000	3.491067000000	0.291155000000
C	-3.377497000000	2.755059000000	-0.792528000000
C	-2.729877000000	1.582946000000	-1.176056000000
H	-0.240376000000	1.547616000000	1.129422000000
H	-1.391585000000	3.628845000000	1.821804000000
H	-4.254775000000	3.090060000000	-1.336735000000
H	-3.112438000000	0.997175000000	-2.007992000000
C	-0.957306000000	-0.183806000000	-0.858273000000
H	-1.260041000000	-0.445256000000	-1.883848000000
N	0.480369000000	-0.028114000000	-0.882985000000
C	1.204215000000	-0.571199000000	0.005633000000
H	0.780829000000	-1.187266000000	0.809445000000
C	2.669620000000	-0.392134000000	0.023329000000
C	3.316973000000	0.387249000000	-0.943311000000
C	3.425143000000	-1.007359000000	1.023715000000
C	4.695395000000	0.546084000000	-0.910967000000
H	2.719240000000	0.861158000000	-1.715178000000
C	4.809012000000	-0.856402000000	1.069104000000
H	2.927816000000	-1.612227000000	1.777834000000
C	5.429457000000	-0.078931000000	0.097810000000
H	5.206526000000	1.146751000000	-1.655272000000
H	5.400431000000	-1.332255000000	1.843294000000
H	-3.404836000000	4.404357000000	0.592553000000
Cl	7.160457000000	0.120105000000	0.140062000000

N	-1.424269000000	-1.273400000000	0.038934000000
C	-2.856771000000	-1.301293000000	0.201173000000
C	-3.403676000000	-0.647908000000	1.305315000000
C	-3.687780000000	-1.932330000000	-0.725737000000
C	-4.785606000000	-0.596516000000	1.464992000000
H	-2.738390000000	-0.171508000000	2.018370000000
C	-5.069956000000	-1.888357000000	-0.551482000000
H	-3.246054000000	-2.459146000000	-1.564609000000
C	-5.623035000000	-1.214935000000	0.536752000000
H	-5.207702000000	-0.077729000000	2.319862000000
H	-5.716449000000	-2.380468000000	-1.271638000000
H	-6.700039000000	-1.179807000000	0.665966000000
O	-1.017351000000	-2.466298000000	-0.629749000000
H	-0.670963000000	-3.026357000000	0.076203000000

- TS-2'$_{Cl}$A:

C	-2.703507000000	-1.339103000000	0.437710000000
C	-2.605088000000	-2.674597000000	0.045307000000
C	-3.662657000000	-3.277803000000	-0.632435000000
C	-4.809221000000	-2.543749000000	-0.935173000000
C	-4.905857000000	-1.206162000000	-0.549447000000
C	-3.857328000000	-0.607959000000	0.143776000000
H	-1.700547000000	-3.220206000000	0.297876000000
H	-3.592967000000	-4.320568000000	-0.926045000000
H	-5.798372000000	-0.634667000000	-0.783714000000
H	-3.928211000000	0.432171000000	0.455999000000
C	-1.567275000000	-0.680825000000	1.146385000000
H	-1.933067000000	0.040744000000	1.905267000000
N	-0.398961000000	-1.407191000000	1.415608000000
C	0.404992000000	-0.269345000000	1.310428000000
H	0.327902000000	0.519819000000	2.086905000000
C	1.803583000000	-0.397210000000	0.809258000000
C	2.305594000000	-1.648181000000	0.449526000000
C	2.606338000000	0.737431000000	0.673782000000
C	3.604759000000	-1.770607000000	-0.035022000000
H	1.664632000000	-2.516072000000	0.573939000000
C	3.900076000000	0.632498000000	0.173304000000
H	2.215251000000	1.712240000000	0.957227000000
C	4.385352000000	-0.626084000000	-0.173165000000
H	4.013050000000	-2.738300000000	-0.304984000000
H	4.529997000000	1.507219000000	0.056397000000
H	-5.629511000000	-3.013781000000	-1.468876000000
Cl	6.010382000000	-0.770400000000	-0.790188000000
N	-0.675351000000	0.359469000000	0.182537000000
C	-0.952328000000	1.758088000000	-0.030587000000
C	-1.216697000000	2.564860000000	1.081589000000

C	-0.952046000000	2.299069000000	-1.315976000000
C	-1.480508000000	3.918211000000	0.896757000000
H	-1.219145000000	2.149756000000	2.082562000000
C	-1.218340000000	3.656844000000	-1.483738000000
H	-0.746538000000	1.661663000000	-2.165516000000
C	-1.482356000000	4.469278000000	-0.384440000000
H	-1.685472000000	4.542134000000	1.760460000000
H	-1.218165000000	4.076914000000	-2.484275000000
H	-1.688895000000	5.525455000000	-0.522346000000
O	-0.446036000000	-0.259267000000	-1.036274000000
H	-0.282874000000	-1.187448000000	-0.751533000000

- 26A:

C	3.809141000000	0.069221000000	-0.033711000000
C	4.166724000000	-1.071639000000	-0.763241000000
C	5.491916000000	-1.487517000000	-0.795365000000
C	6.471685000000	-0.770451000000	-0.102699000000
C	6.121479000000	0.365302000000	0.623630000000
C	4.792066000000	0.782331000000	0.657405000000
H	3.390697000000	-1.613070000000	-1.295071000000
H	5.767166000000	-2.372244000000	-1.360826000000
H	6.880068000000	0.924605000000	1.161770000000
H	4.512993000000	1.669171000000	1.221602000000
C	2.409799000000	0.536520000000	0.019867000000
H	2.223564000000	1.438371000000	0.618274000000
N	1.479749000000	-0.059728000000	-0.603455000000
C	0.124658000000	0.440031000000	-0.556482000000
H	-0.065651000000	0.927272000000	-1.519359000000
C	-0.862552000000	-0.704105000000	-0.402202000000
C	-0.545634000000	-1.832893000000	0.353687000000
C	-2.129725000000	-0.604431000000	-0.978808000000
C	-1.476800000000	-2.850739000000	0.534986000000
H	0.441028000000	-1.914449000000	0.798358000000
C	-3.074127000000	-1.614075000000	-0.806410000000
H	-2.390221000000	0.271478000000	-1.568446000000
C	-2.734857000000	-2.728602000000	-0.048156000000
H	-1.234771000000	-3.731054000000	1.120160000000
H	-4.058315000000	-1.540665000000	-1.255442000000
H	7.505940000000	-1.098968000000	-0.131095000000
Cl	-3.907699000000	-4.003521000000	0.171419000000
N	-0.094964000000	1.498516000000	0.462202000000
C	-1.280970000000	2.266795000000	0.241161000000
C	-1.282220000000	3.156804000000	-0.838576000000
C	-2.410843000000	2.150543000000	1.051116000000

C	-2.420283000000	3.904254000000	-1.121647000000
H	-0.384908000000	3.266926000000	-1.441312000000
C	-3.540586000000	2.917752000000	0.767226000000
H	-2.399244000000	1.457012000000	1.882933000000
C	-3.556771000000	3.788569000000	-0.319529000000
H	-2.413224000000	4.591212000000	-1.962139000000
H	-4.418633000000	2.821217000000	1.398360000000
H	-4.441192000000	4.378415000000	-0.536315000000
O	-0.138239000000	0.859602000000	1.723827000000
H	0.495406000000	1.354293000000	2.259082000000

- TS-3_{Cl}A:

C	0.548965000000	-1.560712000000	0.230520000000
C	1.439481000000	-1.353177000000	1.293429000000
C	2.747770000000	-1.821509000000	1.238326000000
C	3.166340000000	-2.509871000000	0.105025000000
C	2.300898000000	-2.727438000000	-0.967028000000
C	0.999814000000	-2.246694000000	-0.909613000000
H	1.104378000000	-0.814214000000	2.175877000000
H	3.434236000000	-1.657411000000	2.061218000000
H	2.651112000000	-3.265119000000	-1.841103000000
H	0.327603000000	-2.396430000000	-1.745808000000
C	-0.803530000000	-1.040820000000	0.395912000000
H	-1.112148000000	-0.794211000000	1.409000000000
N	-0.509936000000	1.014691000000	-0.576641000000
C	0.670144000000	1.406032000000	-0.363474000000
H	1.543553000000	0.717703000000	-0.316802000000
C	1.047638000000	2.829621000000	-0.139025000000
C	0.075715000000	3.836356000000	-0.116706000000
C	2.390127000000	3.163613000000	0.053217000000
C	0.447895000000	5.158437000000	0.095428000000
H	-0.961237000000	3.550937000000	-0.266967000000
C	2.764597000000	4.489845000000	0.264260000000
H	3.142255000000	2.377567000000	0.034089000000
C	1.792997000000	5.488311000000	0.285799000000
H	-0.307585000000	5.938134000000	0.113671000000
H	3.809956000000	4.743239000000	0.411269000000
H	2.080515000000	6.522254000000	0.450516000000
N	-1.804248000000	-1.218558000000	-0.465957000000
Cl	4.798671000000	-3.105378000000	0.019989000000
C	-3.162481000000	-0.992311000000	-0.104904000000
C	-3.989131000000	-0.249668000000	-0.946523000000
C	-3.650081000000	-1.547677000000	1.078702000000
C	-5.311959000000	-0.038034000000	-0.572372000000
H	-3.582213000000	0.155821000000	-1.864341000000
C	-4.973281000000	-1.316811000000	1.444660000000

H	-3.009925000000	-2.176401000000	1.690269000000
C	-5.807276000000	-0.561436000000	0.622480000000
H	-5.958972000000	0.547286000000	-1.217642000000
H	-5.355668000000	-1.745824000000	2.365076000000
H	-6.840560000000	-0.390593000000	0.905558000000
O	-1.450383000000	-0.943104000000	-1.735284000000
H	-0.908193000000	0.014260000000	-1.451933000000

- TS-2$_{Cl}$A:

C	2.092052000000	0.448822000000	0.195846000000
C	2.842056000000	-0.641197000000	0.651855000000
C	4.226248000000	-0.639065000000	0.542622000000
C	4.860975000000	0.465253000000	-0.027055000000
C	4.137502000000	1.559909000000	-0.487444000000
C	2.749213000000	1.541608000000	-0.372585000000
H	2.311402000000	-1.481845000000	1.088996000000
H	4.817623000000	-1.478695000000	0.891527000000
H	4.654523000000	2.406103000000	-0.926468000000
H	2.169156000000	2.390221000000	-0.728096000000
C	0.607715000000	0.449009000000	0.311798000000
H	0.136389000000	1.346489000000	-0.143486000000
N	-0.045734000000	-0.477355000000	0.877601000000
C	-1.892891000000	-0.595191000000	-0.397371000000
H	-1.646834000000	-0.158173000000	-1.363257000000
C	-1.867578000000	-2.056953000000	-0.316259000000
C	-1.096816000000	-2.734326000000	-1.269426000000
C	-2.597993000000	-2.786861000000	0.631224000000
C	-1.049584000000	-4.123744000000	-1.277959000000
H	-0.523702000000	-2.164814000000	-1.996747000000
C	-2.559893000000	-4.176177000000	0.606698000000
H	-3.181477000000	-2.261085000000	1.378209000000
C	-1.784478000000	-4.847372000000	-0.340110000000
H	-0.443322000000	-4.639990000000	-2.014961000000
H	-3.132627000000	-4.739522000000	1.336252000000
H	-1.753302000000	-5.932327000000	-0.345647000000
N	-2.573563000000	0.204920000000	0.425479000000
Cl	6.600437000000	0.470689000000	-0.166559000000
C	-2.859755000000	1.561517000000	0.102720000000
C	-2.689951000000	2.553024000000	1.068967000000
C	-3.337073000000	1.874116000000	-1.171870000000
C	-2.960053000000	3.875636000000	0.730992000000
H	-2.345295000000	2.273630000000	2.056866000000
C	-3.592041000000	3.203276000000	-1.496706000000
H	-3.532015000000	1.084580000000	-1.891182000000
C	-3.401321000000	4.208503000000	-0.549788000000
H	-2.821009000000	4.652378000000	1.476017000000

H	-3.959878000000	3.448907000000	-2.487601000000
H	-3.609901000000	5.242377000000	-0.803663000000
O	-2.342302000000	-0.080256000000	1.724544000000
H	-1.231682000000	-0.279565000000	1.569937000000

- IM-1$^{O}_{Cl}$:

C	-2.042650000000	0.964482000000	-1.696448000000
C	-0.932461000000	0.909891000000	-0.852289000000
C	-1.067875000000	1.296168000000	0.487297000000
C	-2.296145000000	1.719670000000	0.977087000000
C	-3.396493000000	1.742404000000	0.120499000000
C	-3.284270000000	1.373155000000	-1.215577000000
H	-1.942521000000	0.666583000000	-2.737326000000
H	-0.196062000000	1.248943000000	1.133615000000
H	-2.410910000000	2.022628000000	2.012281000000
H	-4.153974000000	1.405573000000	-1.862593000000
C	0.359488000000	0.415470000000	-1.367171000000
N	1.305801000000	0.101256000000	-0.585367000000
C	2.530912000000	-0.431044000000	-1.156027000000
H	2.537270000000	-1.506841000000	-0.931467000000
H	2.569798000000	-0.310082000000	-2.250090000000
C	3.741095000000	0.202797000000	-0.508779000000
C	4.703266000000	0.864831000000	-1.269121000000
C	3.900766000000	0.119903000000	0.878504000000
C	5.820192000000	1.435817000000	-0.656232000000
H	4.580277000000	0.937084000000	-2.347085000000
C	5.011893000000	0.690696000000	1.490929000000
H	3.143987000000	-0.391146000000	1.468885000000
C	5.975512000000	1.349872000000	0.724403000000
H	6.563722000000	1.949253000000	-1.258113000000
H	5.129200000000	0.620921000000	2.568000000000
H	6.842242000000	1.794295000000	1.203764000000
H	0.440561000000	0.305967000000	-2.461104000000
Cl	-4.948616000000	2.242589000000	0.739272000000
O	0.802584000000	-1.693904000000	2.265249000000
N	0.763471000000	-2.206815000000	1.174124000000
C	-0.550028000000	-2.253971000000	0.573005000000
C	-0.593893000000	-2.785119000000	-0.713960000000
C	-1.699056000000	-1.776271000000	1.205418000000
C	-1.808800000000	-2.828822000000	-1.392374000000
H	0.328429000000	-3.142807000000	-1.163593000000
C	-2.910158000000	-1.828672000000	0.526078000000
H	-1.620689000000	-1.364227000000	2.206156000000
C	-2.962441000000	-2.349241000000	-0.770445000000
H	-1.859179000000	-3.233766000000	-2.397848000000
H	-3.813574000000	-1.451434000000	0.995464000000

H	-3.910793000000	-2.376902000000	-1.298657000000

- TS-1$^{O}_{Cl}$:

C	-2.639475000000	-1.326385000000	-0.195151000000
C	-2.112116000000	-0.191686000000	0.432139000000
C	-2.977914000000	0.812158000000	0.874070000000
C	-4.353924000000	0.691019000000	0.706969000000
C	-4.855845000000	-0.448734000000	0.086979000000
C	-4.010516000000	-1.460513000000	-0.367402000000
H	-1.957900000000	-2.094595000000	-0.544478000000
H	-2.571611000000	1.699216000000	1.353756000000
H	-5.031175000000	1.465438000000	1.049302000000
H	-4.429677000000	-2.335065000000	-0.852555000000
C	-0.665244000000	-0.029619000000	0.611620000000
N	0.167596000000	-1.006807000000	0.393401000000
C	1.495209000000	-0.703497000000	0.472104000000
H	1.610947000000	-0.035048000000	-0.707182000000
H	1.798342000000	0.109708000000	1.148986000000
C	2.496720000000	-1.787284000000	0.324748000000
C	3.805419000000	-1.578143000000	0.774056000000
C	2.169121000000	-2.998028000000	-0.297092000000
C	4.773700000000	-2.566014000000	0.611706000000
H	4.059594000000	-0.640491000000	1.263717000000
C	3.136631000000	-3.984881000000	-0.453106000000
H	1.152185000000	-3.149647000000	-0.644075000000
C	4.440888000000	-3.772334000000	-0.002218000000
H	5.784393000000	-2.396810000000	0.969628000000
H	2.875019000000	-4.924014000000	-0.930626000000
H	5.192840000000	-4.544980000000	-0.127281000000
H	-0.335039000000	0.896237000000	1.103335000000
Cl	-6.577423000000	-0.614861000000	-0.129626000000
O	-0.115340000000	0.851999000000	-1.351629000000
N	1.132821000000	0.955759000000	-1.364521000000
C	1.648933000000	2.138392000000	-0.711377000000
C	3.034296000000	2.226733000000	-0.563038000000
C	0.811320000000	3.173732000000	-0.301629000000
C	3.586561000000	3.360124000000	0.022197000000
H	3.659000000000	1.405781000000	-0.907870000000
C	1.375727000000	4.309548000000	0.275998000000
H	-0.258305000000	3.079030000000	-0.457168000000
C	2.757185000000	4.403093000000	0.442681000000
H	4.661988000000	3.435975000000	0.145757000000
H	0.735352000000	5.126634000000	0.592721000000
H	3.189992000000	5.290526000000	0.893026000000

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C	-0.437564000000	0.768566000000	-0.857929000000

C	-0.169107000000	1.579208000000	0.246039000000
C	-1.104847000000	2.511275000000	0.685047000000
C	-2.314078000000	2.627490000000	0.004676000000
C	-2.595693000000	1.841343000000	-1.107137000000
C	-1.648663000000	0.914187000000	-1.534602000000
H	0.780268000000	1.484413000000	0.764742000000
H	-0.902694000000	3.144746000000	1.541843000000
H	-3.543055000000	1.950572000000	-1.623121000000
H	-1.865164000000	0.279255000000	-2.388750000000
C	0.515213000000	-0.341161000000	-1.260374000000
H	0.423951000000	-0.526671000000	-2.337895000000
N	1.872614000000	0.018817000000	-0.986836000000
C	2.594790000000	-0.697087000000	-0.223046000000
H	2.217637000000	-1.608529000000	0.252552000000
C	3.996918000000	-0.338190000000	0.068774000000
C	4.585017000000	0.807344000000	-0.482193000000
C	4.746876000000	-1.161427000000	0.912819000000
C	5.907149000000	1.117938000000	-0.189233000000
H	3.988231000000	1.435817000000	-1.135682000000
C	6.073309000000	-0.849418000000	1.205583000000
H	4.287652000000	-2.049683000000	1.339989000000
C	6.653783000000	0.290614000000	0.654446000000
H	6.361622000000	2.005876000000	-0.617359000000
H	6.650733000000	-1.493412000000	1.861084000000
H	7.686715000000	0.536749000000	0.880184000000
Cl	-3.494200000000	3.790654000000	0.551160000000
O	0.156217000000	-1.561316000000	-0.580480000000
N	-1.005243000000	-2.096215000000	-1.158600000000
H	-0.740298000000	-3.009502000000	-1.519304000000
C	-2.089236000000	-2.202215000000	-0.248569000000
C	-3.156188000000	-3.031790000000	-0.612845000000
C	-2.154590000000	-1.461183000000	0.931438000000
C	-4.280553000000	-3.115214000000	0.199950000000
H	-3.104944000000	-3.599631000000	-1.538621000000
C	-3.291279000000	-1.550477000000	1.734224000000
H	-1.325987000000	-0.822788000000	1.211671000000
C	-4.357604000000	-2.372014000000	1.378758000000
H	-5.101929000000	-3.762268000000	-0.091889000000
H	-3.336785000000	-0.966223000000	2.648170000000
H	-5.237801000000	-2.434243000000	2.009605000000

- IM-1$^{O}_{Cl}$A:

C	-3.116532000000	1.890625000000	-1.120145000000
C	-1.946042000000	1.493771000000	-0.469935000000
C	-1.826507000000	1.676901000000	0.913893000000
C	-2.870917000000	2.246577000000	1.632339000000

C	-4.046441000000	2.627903000000	0.979900000000
C	-4.169238000000	2.448842000000	-0.396786000000
H	-3.207358000000	1.747368000000	-2.194458000000
H	-0.909274000000	1.360755000000	1.402813000000
H	-2.772830000000	2.393179000000	2.703660000000
H	-5.079719000000	2.748056000000	-0.906611000000
C	-0.860299000000	0.859028000000	-1.242665000000
N	0.098550000000	0.258015000000	-0.671484000000
C	1.098840000000	-0.394685000000	-1.496481000000
H	0.880973000000	-1.471705000000	-1.461307000000
H	1.051673000000	-0.073960000000	-2.548954000000
C	2.484059000000	-0.172122000000	-0.935064000000
C	3.514062000000	0.333936000000	-1.724596000000
C	2.744477000000	-0.491627000000	0.401643000000
C	4.794257000000	0.518706000000	-1.201239000000
H	3.322078000000	0.592547000000	-2.762732000000
C	4.014102000000	-0.311556000000	0.938755000000
H	1.940996000000	-0.879624000000	1.022616000000
C	5.029153000000	0.192960000000	0.128137000000
H	5.596851000000	0.914440000000	-1.813870000000
H	4.221263000000	-0.558544000000	1.974259000000
H	-0.947218000000	0.911413000000	-2.340557000000
O	-0.384007000000	-1.733071000000	2.020406000000
N	-0.613279000000	-2.113911000000	0.898610000000
C	-1.967940000000	-1.894337000000	0.448105000000
C	-2.223427000000	-2.275996000000	-0.866865000000
C	-2.954422000000	-1.309037000000	1.243828000000
C	-3.487331000000	-2.056191000000	-1.407687000000
H	-1.422648000000	-2.728575000000	-1.445309000000
C	-4.215832000000	-1.098707000000	0.700775000000
H	-2.712503000000	-1.019253000000	2.260926000000
C	-4.478568000000	-1.466367000000	-0.622198000000
H	-3.700834000000	-2.341543000000	-2.432533000000
H	-4.992584000000	-0.632124000000	1.298037000000
H	-5.463660000000	-1.287769000000	-1.042605000000
H	-4.861356000000	3.071041000000	1.544255000000
Cl	6.625799000000	0.423436000000	0.798056000000

- TS-1$^{O}_{Cl}$A:

C	-4.092665000000	-1.235047000000	0.804196000000
C	-2.814130000000	-1.598593000000	0.370849000000
C	-2.622887000000	-2.832390000000	-0.262293000000
C	-3.699292000000	-3.691795000000	-0.446206000000
C	-4.974132000000	-3.326951000000	-0.006599000000
C	-5.170537000000	-2.096703000000	0.618319000000
H	-4.239399000000	-0.272429000000	1.288727000000

H	-1.626637000000	-3.094842000000	-0.602313000000
H	-3.549181000000	-4.647913000000	-0.937633000000
H	-6.160284000000	-1.809512000000	0.958614000000
C	-1.697326000000	-0.668226000000	0.571008000000
N	-0.457984000000	-1.023571000000	0.378637000000
C	0.479743000000	-0.040084000000	0.484121000000
H	0.233949000000	0.595284000000	-0.698433000000
H	0.274200000000	0.801931000000	1.162334000000
C	1.913343000000	-0.397500000000	0.363663000000
C	2.888954000000	0.495246000000	0.819468000000
C	2.314037000000	-1.594920000000	-0.240441000000
C	4.243056000000	0.203907000000	0.684162000000
H	2.586474000000	1.424575000000	1.296542000000
C	3.663014000000	-1.899210000000	-0.376902000000
H	1.554041000000	-2.284106000000	-0.593421000000
C	4.617191000000	-0.994843000000	0.085582000000
H	5.001522000000	0.890934000000	1.042633000000
H	3.980016000000	-2.827730000000	-0.838993000000
H	-1.939403000000	0.284382000000	1.063234000000
O	-1.677455000000	0.376435000000	-1.382201000000
N	-0.698093000000	1.157637000000	-1.368557000000
C	-0.941310000000	2.421991000000	-0.709867000000
C	0.155644000000	3.268041000000	-0.537293000000
C	-2.220788000000	2.809606000000	-0.317149000000
C	-0.028491000000	4.511931000000	0.055104000000
H	1.137405000000	2.939863000000	-0.871296000000
C	-2.396124000000	4.062225000000	0.268022000000
H	-3.052364000000	2.134520000000	-0.490708000000
C	-1.305486000000	4.910201000000	0.458909000000
H	0.818879000000	5.174854000000	0.196789000000
H	-3.388573000000	4.379452000000	0.572058000000
H	-1.449566000000	5.884272000000	0.915047000000
H	-5.812502000000	-4.000555000000	-0.154232000000
Cl	6.310160000000	-1.374367000000	-0.084813000000

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C	-1.371766000000	1.405034000000	-0.605516000000
C	-0.905204000000	1.956797000000	0.589314000000
C	-1.647946000000	2.935177000000	1.245716000000
C	-2.859961000000	3.370766000000	0.709692000000
C	-3.321162000000	2.832111000000	-0.489788000000
C	-2.576865000000	1.853947000000	-1.146916000000
H	0.041698000000	1.621392000000	1.002306000000
H	-1.279571000000	3.360433000000	2.174181000000
H	-4.262718000000	3.168527000000	-0.912148000000
H	-2.942050000000	1.416500000000	-2.071844000000

C	-0.645414000000	0.245881000000	-1.262432000000
H	-0.836314000000	0.259552000000	-2.342618000000
N	0.768697000000	0.342488000000	-1.062443000000
C	1.401413000000	-0.568941000000	-0.442122000000
H	0.906537000000	-1.461835000000	-0.046231000000
C	2.856878000000	-0.469998000000	-0.215297000000
C	3.591544000000	0.629753000000	-0.675364000000
C	3.512421000000	-1.490039000000	0.477796000000
C	4.958487000000	0.707014000000	-0.447575000000
H	3.071341000000	1.417226000000	-1.211311000000
C	4.883402000000	-1.425545000000	0.713904000000
H	2.946121000000	-2.344968000000	0.838298000000
C	5.592185000000	-0.324327000000	0.246749000000
H	5.537144000000	1.553858000000	-0.799754000000
H	5.397915000000	-2.213968000000	1.251728000000
O	-1.151852000000	-1.003373000000	-0.749890000000
N	-2.413595000000	-1.263914000000	-1.306385000000
H	-2.310180000000	-2.124987000000	-1.837669000000
C	-3.440573000000	-1.385640000000	-0.335884000000
C	-4.618148000000	-2.038469000000	-0.718832000000
C	-3.340793000000	-0.818191000000	0.934773000000
C	-5.687958000000	-2.118689000000	0.164995000000
H	-4.694543000000	-2.472669000000	-1.712738000000
C	-4.422786000000	-0.904373000000	1.809714000000
H	-2.428524000000	-0.313939000000	1.228710000000
C	-5.598671000000	-1.550053000000	1.436224000000
H	-6.595834000000	-2.628391000000	-0.142504000000
H	-4.338095000000	-0.457245000000	2.795445000000
H	-6.434769000000	-1.611981000000	2.124557000000
H	-3.439726000000	4.131410000000	1.223237000000
Cl	7.308011000000	-0.227955000000	0.534373000000

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