Electronic Supplementary Material (ESI) for ChemComm.
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1. General: All the chemicals used here were received from commercial sources, otherwise mentioned. HPLC grade chloroform, reagent grade 2, 2, 2 - trifluoro ethanol (TFE), methanol, Dichloroethane (DCE), 1,4 Dioxane, ethanol, ^{t}Amyl alcohol, Dimethyl formamide (DMF) used as such. All reactions were carried out under argon atmosphere unless otherwise stated. ^{1}H and ^{13}C NMR were recorded on JEOL (400 and 500 MHz) using $CDCl_3$ and DMSO-d_6 as a solvent. Chemical shifts (δ) are given in ppm relative to TMS, coupling constants (J) in Hz. The solvent signals used as a references and the chemicals shifts converted to TMS scale ($CDCl_3$: δC = 77 ppm; residual $CHCl_3$ in $CDCl_3$: δH = 7.26 ppm) and (DMSO-d_6: δC = 40 ppm; δH = 2.5 ppm). All the reactions were monitored by analytical thin layer chromatography (TLC) using commercial aluminium sheets precoated with silica gel. Column Chromatography was conducted on silica gel (Merck, 100-200 mesh). EI-MS/ESI-MS was recorded on a Waters-Micromass Quattro Micro triplequadrupole mass spectrometers. GC–MS was used to analyze our samples on a Shimadzu GC 2010 plus and MS 2010SE system. All other chemicals were received and used as such from the commercial sources.

All Quinoline-N-oxide were prepared according to the reported literature.[1] 2-Methyl quinaxalin-N-Oxide were prepared based on the literatrue procedure.[2]

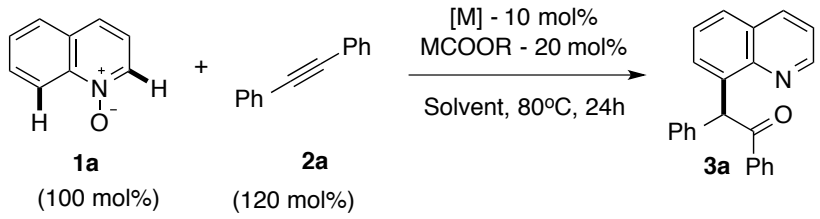
All the alkynes were prepared according to the reported literature.[3]

Compound **5** was prepared according to the literature procedure.[4]

[1] H. Hwang, J. Kim, J. Jeong, S. Chang, *J. Am. Chem. Soc.*, **2014**, *136,* 10770–10776.
[2] T. Nishida, H. Ida, Y. Kuninobu, M. Kanai, *Nat. Commun*. **2014**, 5, 3387.
[3] (a) Y. Wang, C. Chen, S. Zhang, Z. Lou, X. Su, L. Wen, M. Li, *Org. Lett*. **2013**, *15*, 4794-4797; (b) B. E. Moulton, A. C. Whitwood, A. K. D-. Klair, J. M. Lynam*, J. Org. Chem*. **2011**, *76*, 5320-5334.
[4] T. Shibata, Y. Matsuo, *Adv. Synth. Catal.* **2014**, *356*, 1516-1520

2. Optimization for C-(8)H bond functionalization:

Table S1. Optimization of Reaction Conditions[a]



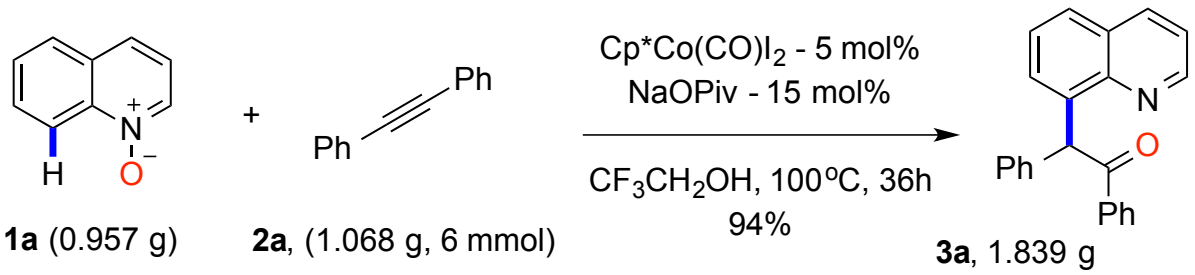
1a (100 mol%) + **2a** (120 mol%) → **3a**

Entry	[M]	MCOOR	Solvent	Yield[b]
1	$Cp^*Co(CO)I_2$	NaOAc	Dioxane	-
2	$Cp^*Co(CO)I_2$	NaOAc	CF_3CH_2OH	80
3	$Cp^*Co(CO)I_2$	NaOAc	$(CH_2)_2Cl_2$	-
4	$Cp^*Co(CO)I_2$	NaOAc	MeOH	-
5	$Cp^*Co(CO)I_2$	NaOAc	EtOH	-
6	$Cp^*Co(CO)I_2$	NaOAc	tAmOH	-
7	$Cp^*Co(CO)I_2$	NaOAc	Dioxane	-
8	$Cp^*Co(CO)I_2$	NaOAc	DMF	-
9	$Cp^*Co(CO)I_2$	KOAc	TFE	69
10	$Cp^*Co(CO)I_2$	CsOAc	TFE	66
11	$Cp^*Co(CO)I_2$	AgOPiv	TFE	74
12	$Cp^*Co(CO)I_2$	$Cu(OAc)_2.H_2O$	TFE	68
13	$Cp^*Co(CO)I_2$	AcOH	TFE	8
14	$Cp^*Co(CO)I_2$	NaOPiv	TFE	86
15	$Cp^*Co(CO)I_2$	NaOPiv	TFE	86[c]
16	$Cp^*Co(CO)I_2$	NaOPiv	TFE	72[d]
17	$Cp^*Co(CO)I_2$	NaOPiv	TFE	67[d,e]
18	-	NaOPiv	TFE	-
19	$Cp^*Co(CO)I_2$	-	TFE	-
20	$Cp^*Co(CO)I_2$	NaOPiv	TFE	13[f]
21	$Cp^*Co(CO)I_2$	NaOPiv	TFE	-[g]
22	$Cp^*Co(CO)I_2$	NaOPiv	TFE	-[e,g]
23	$Co(acac)_3$	NaOAc	TFE	-
24	$CoCl_2$	NaOAc	TFE	-
25	$[Cp^*RhCl_2]_2$	NaOPiv	TFE	9[d]
27	$[Cp^*IrCl_2]_2$	NaOPiv	TFE	-[d]
26	$[Ru(p\text{-}cym)Cl_2]_2$	NaOPiv	TFE	-[d]
28	$Cp^*Co(CO)I_2$	NaOPiv	TFE	94[h]
29	$Cp^*Co(CO)I_2$	NaOPiv	TFE	90[h,i]

[a] All reactions were conducted under Ar atmosphere at 80°C on 0.3 mmol scale for 24h. [b]Isolated yield of **3a**. [c] reaction performed at 100°C. [d] 5 mol% of [M] catalyst and 10 mo% of NaOPiv was used. [e]10 mol% of $AgSbF_6$ was added. [f] reaction performed at 50°C [g] reaction conducted at ambient temperature. [h] 120 mol% of **1a** and 100 mol% of **2a** was used. [i] reaction performed for 12h at 100°C.

3. Large scale reaction

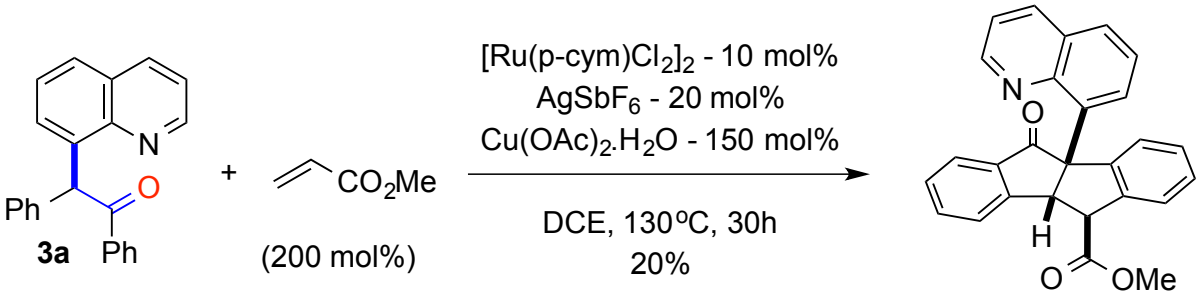
Scheme S1: Gram scale reaction



1a (0.957 g) **2a**, (1.068 g, 6 mmol) **3a**, 1.839 g

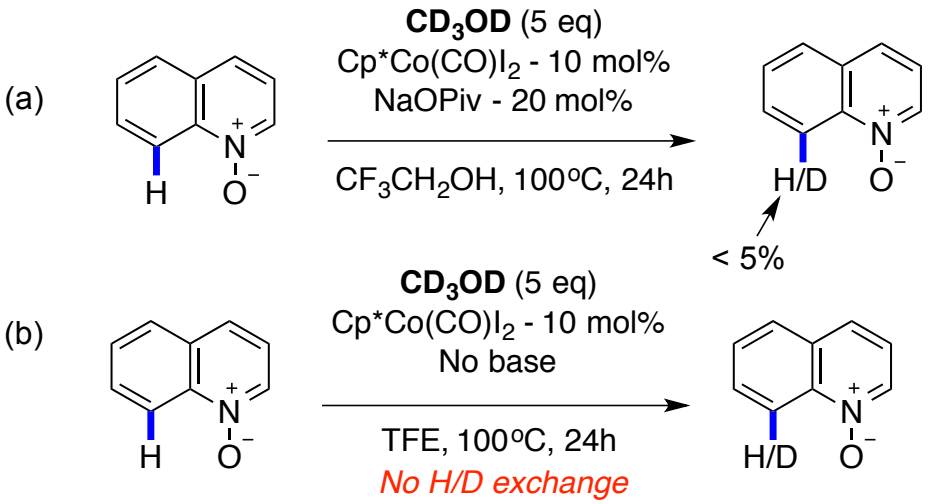
4. Application of 3a.

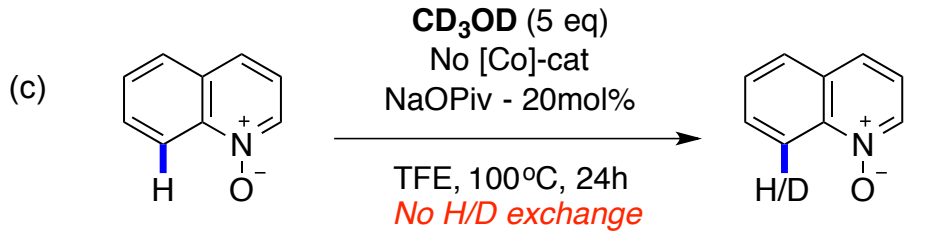
Scheme S2: Application of 3a for cascade C-H bond functionalization

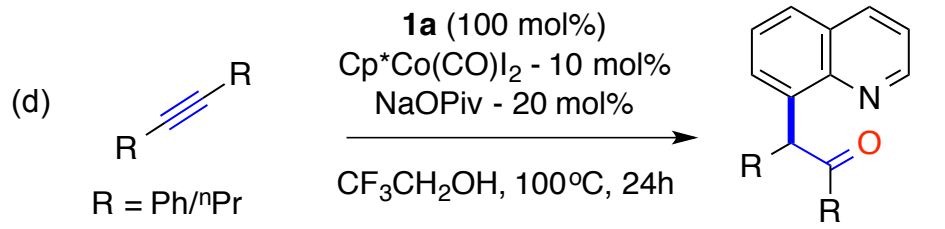


5. Scheme for control experiments

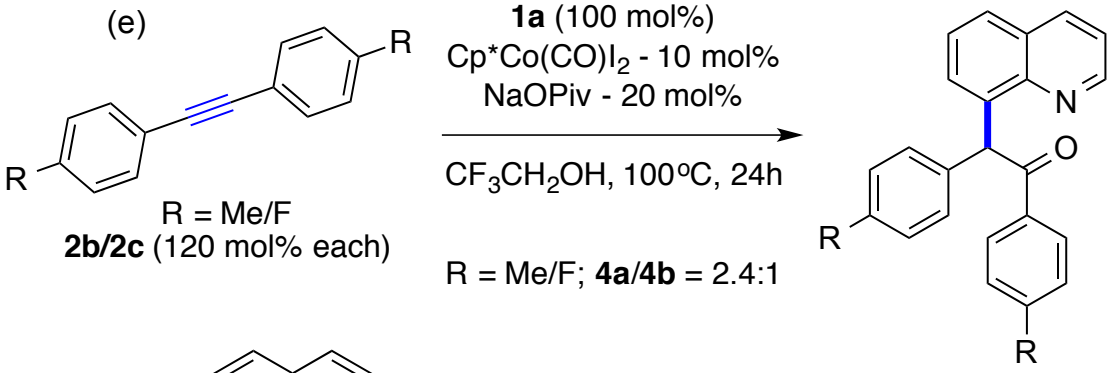
Scheme S3: Control experiments

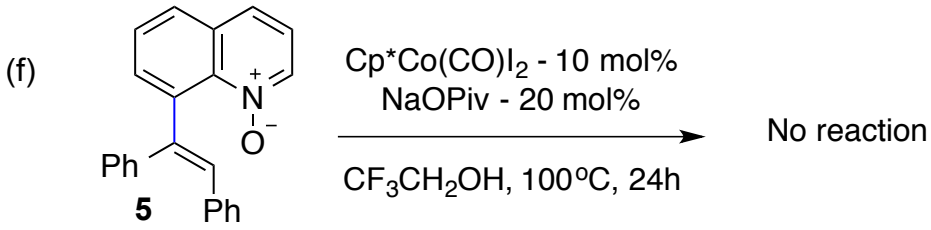






R = Ph; (**3a**) 50%
R = n-propyl; (**4e**) 46%



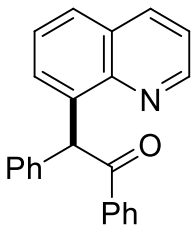


6. Genaral procedure for catalytic C-H activation and OAT of various quinoline-N-oxide (1) with diphenylacetylene (2a):

Procedure A:

An oven dried schlenk was charged with Teflon coated magnetic stir bar under argon atmosphere added Cp*Co(CO)I_2 (14.2 mg, 0.03 mmol, 10 mol%), and sodium pivalate (7.44 mg, 0.06 mmol, 20 mol%) followed by 2, 2, 2 - trifluoro ethanol (TFE 1 mL). Subsequently quinoline N-Oxide **1a** (52.2 mg, 0.36 mmol, 120 mol%), and diphenylacetylene **2a** (53.4 mg, 0.3 mmol, 100 mol%) were added. The closed schlenk tube containing reaction mixture were placed in preheated oil bath at 100 °C for 24 hours. After 24h the reaction mixture was allowed to cool to room temperature. Removal of solvent followed by column chromatography (EtOAc/Hexane) on silica gel afforded functionalized quinoline **3a** in good yields.

1,2-diphenyl-2-(quinolin-8-yl)ethanone (3a): Compound **3a** was prepared according to the general procedure **A** from **1a** (52.2 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 94% (92 mg) as a white solid.

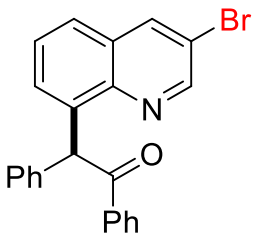


^{1}H NMR (500 MHz, $CDCl_3$): δ 8.85 (d, *J* = 2.4 Hz, 1H), 8.14 (t, *J* = 14.5, 6.9 Hz, 3H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.50-7.45 (q, *J* = 15.6, 7.5 *Hz*, 5H), 7.43-7.36 (m, 6H), 7.29 (t, *J* = 14.7, 7.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 198.5, 148.9, 145.1, 138.3, 137.7, 136.8, 135.7, 132.0, 129.3, 128.4, 128.2, 127.9, 126.6, 125.7, 120.6, 53.3.

HRMS: $[M+H]^+$ calculated for $C_{23}H_{18}NO$: 324.1388, found 324.1388.

2-(3-bromoquinolin-8-yl)-1,2-diphenylethanone (3b): Compound **3b** was prepared according to the general procedure **A** from **1b** (80.24 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 76% (92 mg) as a light yellow colour solid.

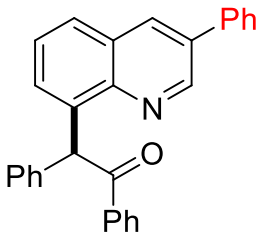


^{1}H NMR (500 MHz, $CDCl_3$): δ 8.83 (d, *J* = 2.1 Hz, 1H), 8.28 (d, *J* = 2.2 Hz, 1H), 8.12 (m, 2H), 7.64-7.62 (m, 1H), 7.51-7.45 (m, 4H), 7.44-7.35 (m, 6H), 7.29 (t, *J* = 14.9, 7.4 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 198.9, 150.5, 143.9, 139.4, 137.8, 137.5, 137.3, 132.8, 130.3, 129.9, 129.4, 129.08, 129.03, 128.6, 127.6, 127.4, 126.3, 117.6, 53.9.

HRMS: $[M + H]^+$ calculated for $C_{23}H_{17}BrNO$: 402.0494, found 402.0494.

1,2-diphenyl-2-(3-phenylquinolin-8-yl)ethanone (3c): Compound **3c** was prepared according to the general procedure **A** from **1c** (79.56 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.4) yielded 88% (106 mg) as a light yellow colour solid.

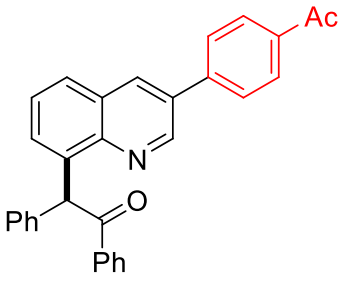


^{1}H NMR (400 MHz, $CDCl_3$): δ 9.13 (s, 1H), 8.28 (d, *J* = 2.3 Hz, 1H), 8.20-8.17 (m, 2H), 7.79-7.77(dd, *J* = 8.0, 1.0 Hz, 1H), 7.70-7.68 (m, 2H), 7.53-7.47 (m, 7H), 7.44-7.38 (m, 6H), 7.33-7.29 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 199.2, 149.1, 144.9, 139.0, 138.3, 138.0, 137.5, 133.9, 133.5, 132.7, 130.0, 129.8, 129.2, 129.1, 128.9, 128.6, 128.2, 128.1, 127.5, 127.4, 127.3, 126.8, 54.1.

HRMS: $[M + H]^+$ calculated for $C_{29}H_{22}NO$: 400.1701, found 400.1703.

2-(3-acetylquinolin-8-yl)-1,2-diphenylethanone (3d): Compound **3d** was prepared according to the general procedure **A** from **1d** (94.68 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (4% EtOAc/Hexane, R_f = 0.2) yielded 80% (106 mg) as a white colour solid.

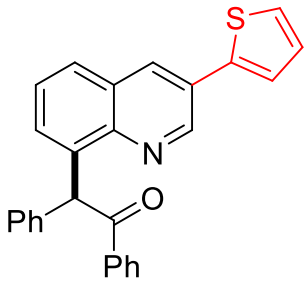


^{1}H NMR (400 MHz, $CDCl_3$): δ 9.10 (d, *J* = 2.4 Hz, 1H), 8.30 (d, *J* = 2.5 Hz, 1H), 8.19-8.17 (m, 2H), 8.08-8.06 (m, 2H), 7.78-7.73 (m, 3H), 7.52-7.46 (m, 5H), 7.43-7.37 (m, 5H), 7.33-7.29 (m, 1H), 2.64 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 198.9, 197.4, 148.4, 145.0, 142.2, 138.9, 137.8, 137.2, 136.2, 133.8, 132.6, 132.3, 130.2, 129.8, 129.0, 128.9, 128.8, 128.4, 127.8, 127.35, 127.33, 127.2, 126.9, 53.9, 26.5.

HRMS: $[M + H]^+$ calculated for $C_{31}H_{24}NO_2$: 442.1807, found 442.1806.

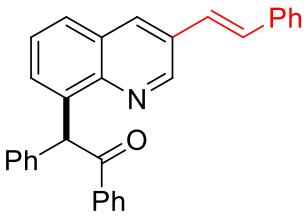
1,2-diphenyl-2-(3-(thiophen-2-yl)quinolin-8-yl)ethanone (3e): Compound **3e** was prepared according to the general procedure **A** from **1e** (81.72 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (4% EtOAc/Hexane, R_f = 0.3) yielded 95% (116 mg) as a white colour solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.16 (d, *J* = 2.3 Hz, 1H), 8.26 (d, *J* = 2.3 Hz, 1H), 8.21-8.19 (m, 2H), 7.74-7.42 (dd, *J* = 8.15, 1.4 Hz, 1H), 7.53-7.30 (m, 13H), 7.15-7.13 (dd, *J* = 5.0, 3.6 Hz, 1H).



^{13}C NMR (125 MHz, $CDCl_3$): δ 198.9, 147.6, 144.6, 140.5, 138.8, 138.0, 137.2, 132.5, 131.5, 129.8, 129.6, 128.9, 128.7, 128.4, 128.3, 127.9, 127.5, 127.1, 127.0, 126.9, 125.9, 124.2, 53.8.

HRMS: $[M + H]^+$ calculated for $C_{31}H_{22}NO$: 406.1266, found 406.1266.

(*E*)-1,2-diphenyl-2-(3-styrylquinolin-8-yl)ethanone(3f): Compound **3f** was prepared according to the general procedure **A** from **1f** (88.92 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 65% (84 mg) as a white colour solid.

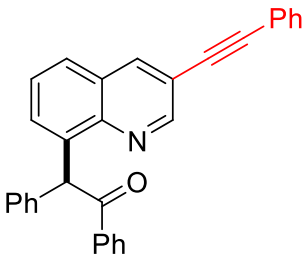


^{1}H NMR (500 MHz, $CDCl_3$): δ 9.07 (s, 1H), 8.15 (t, *J* = 15.4, 7.6 Hz, 3H), 7.72 (d, *J* = 8.2 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 2H), 7.51-7.45 (m, 5H), 7.43-7.36 (m, 7H), 7.32-7.28 (m, 3H), 7.22 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 199.1, 148.5, 144.9, 138.9, 138.2, 137.4, 136.8, 132.8, 132.7, 131.0, 130.4, 129.9, 129.7, 129.1, 128.9, 128.5, 128.3, 127.29, 127.27, 126.9, 126.8, 125.2, 54.0.

HRMS: $[M + H]^+$ calculated for $C_{31}H_{24}NO$: 426.1858, found 426.1858.

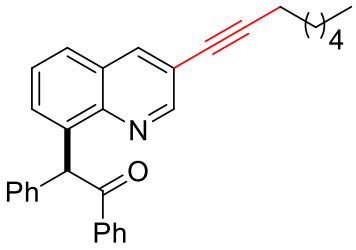
1,2-diphenyl-2-(3-(phenylethynyl)quinolin-8-yl)ethanone (3g): Compound **3g** was prepared according to the general procedure **A** from **1g** (88.2 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (4% EtOAc/Hexane, R_f = 0.3) yielded 65% (83 mg) as a light yellow colour solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.93 (d, J = 2.0 Hz, 1H), 8.28 (d, J = 2.1 Hz, 1H), 8.13-8.11 (m, 2H), 7.70-7.68 (dd, J = 8.4, 1.3 Hz, 1H), 7.58-7.56 (m, 2H), 7.51-7.44 (m, 4H), 7.42-7.36 (m, 9H), 7.30-7.26 (m, 1H).



^{13}C NMR (125 MHz, $CDCl_3$): δ 198.9, 151.2, 144.2, 139.0, 138.4, 138.0, 137.3, 132.6, 131.7, 130.5, 129.8, 128.9, 128.8, 128.7, 128.4, 127.3, 127.2, 127.0, 126.8, 122.6, 117.5, 92.6, 86.6, 53.7.

HRMS: $[M + H]^+$ calculated for $C_{31}H_{22}NO$: 424.1701, found 424.1707.

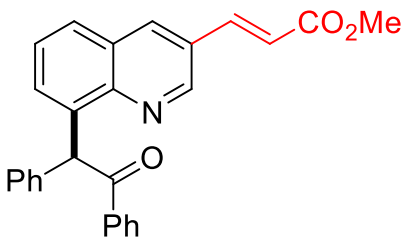
2-(3-(oct-1-ynyl)quinolin-8-yl)-1,2-diphenylethanone (3h): Compound **3h** was prepared according to the general procedure **A** from **1h** (91.08 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 65% (85 mg) as a light yellow colour liquid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.80 (m, 1H), 8.13 (m, 2H), 8.10 (m, 1H), 7.64 (d, J = 8.4 Hz, 1H), 7.49-7.45 (m, 2H), 7.43- 7.41 (m, 2H), 7.40 (m, 2H), 7.38 (m, 2H), 7.35-7.33 (m, 2H), 7.29-7.25 (m, 1H), 2.46 (t, J = 14.0, 6.9 Hz, 2H), 1.67-1.60 (dt, J = 14.1, 7.0 Hz, 2H), 1.51-1.60 (m, 2H), 1.36-1.32 (m, 4H), 0.94-0.90 (m, 3H).



^{13}C NMR (125 MHz, $CDCl_3$): δ 198.9, 151.7, 143.9, 138.9, 138.09,138.02, 137.3, 132.5, 129.9, 129.7, 128.9, 128.7, 128.4, 127.4, 127.1, 126.7, 126.6, 118.3, 94.1, 77.9, 53.7, 31.3, 28.57, 28.55, 22.5, 19.5, 14.0.

HRMS: $[M + H]^+$ calculated for $C_{31}H_{30}NO$: 432.2327, found 432.2321.

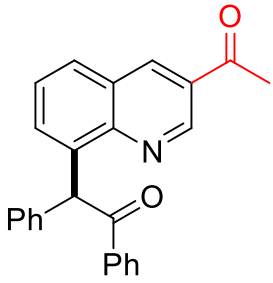
(*E*)-methyl 3-(8-(2-oxo-1,2-diphenylethyl)quinolin-3-yl)acrylate (3i): Compound **3i** was prepared according to the general procedure **A** from **1i** (82.44 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 70% (86 mg) as a white colour solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.00 (d, J = 1.4 Hz, 1H), 8.20 (d, J = 1.4 Hz, 1H), 8.13 (d, J = 7.5 Hz, 2H), 7.82 (d, J = 16.0 Hz, 1H), 7.73 (d, J = 7.7 Hz, 1H), 7.52-7.36 (m, 10H), 7.31-7.28 (t, J = 14.6, 7.6 Hz, 1H), 6.63 (d, J = 16.0 Hz, 1H), 3.84 (s, 3H).



^{13}C NMR (100 MHz, $CDCl_3$): δ 198.9, 167.0, 148.4, 146.1, 141.5, 139.3, 137.9, 137.3, 135.8, 132.8, 131.1, 129.9, 129.08, 129.03, 128.6, 127.8, 127.6, 127.48, 127.41, 127.3, 119.7, 54.0, 52.0.

HRMS: $[M + H]^+$ calculated for $C_{27}H_{22}NO_3$: 408.1600, found 408.1606.

2-(3-Acetylquinolin-8-yl)-1,2-diphenylethanone (3j): Compound **3j** was prepared according to the general procedure **A** from **1j** (67.32 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (4% EtOAc/Hexane, R_f = 0.3) yielded 84% (92 mg) as a white colour solid.

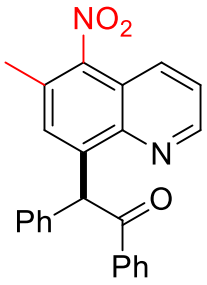


^{1}H NMR (500 MHz, $CDCl_3$): δ 9.34 (d, J = 2.3 Hz, 1H), 8.68 (d, J = 1.4 Hz, 1H), 8.12 (d, J = 7.4 Hz, 2H), 7.83 (d, J = 7.3 Hz, 2H), 7.53-7.48 (m, 3H), 7.45-7.36 (m, 7H), 7.29 (m, 1H), 2.64 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 198.9, 196.8, 148.4, 147.4, 139.5, 137.8, 137.6, 137.3, 132.8, 132.5, 129.9, 129.4, 129.0, 128.6, 127.48, 127.44, 127.0, 54.0, 26.9.

HRMS: $[M + H]^+$ calculated for $C_{25}H_{20}NO_2$: 366.1494, found 366.1492.

2-(6-methyl-5-nitroquinolin-8-yl)-1,2-diphenylethanone (3k): Compound **3k** was prepared according to the general procedure **A** from **1k** (73.44 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (10% EtOAc/Hexane, R_f = 0.2) yielded 65% (75 mg) as a white colour solid.

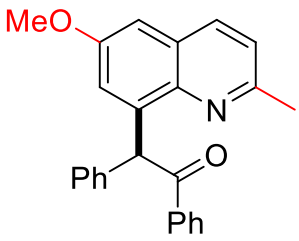


^{1}H NMR (500 MHz, $CDCl_3$): δ 8.84 (dd, J = 4.0, 1.7 Hz, 1H), 8.13-8.09 (m, 3H), 7.54-7.48 (m, 2H), 7.46-7.39 (m, 7H), 7.36-7.31 (m, 1H), 7.23 (s, 1H), 2.45 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 198.3, 149.9, 145.9, 144.0, 142.7, 137.0, 133.0, 132.4, 130.4, 129.8, 129.3, 129.1, 128.9, 128.7, 127.8, 123.2, 120.5, 54.1, 18.5.

HRMS: $[M + H]^+$ calculated for $C_{24}H_{19}N_2O_3$: 383.1396, found 383.1394.

2-(6-methoxy-2-methylquinolin-8-yl)-1,2-diphenylethanone (3l): Compound **3l** was prepared according to the general procedure **A** from **1l** (68.04 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (4% EtOAc/Hexane, R_f = 0.25) yielded 86% (95 mg) as a white colour solid.

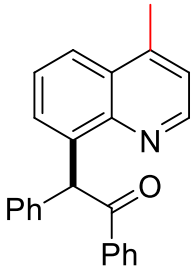


^{1}H NMR (500 MHz, $CDCl_3$): δ 8.18 (d, J = 8.3, 2H), 7.88 (d, J = 8.2 Hz, 1H), 7.52-7.48 (m, 3H), 7.44-7.37 (m, 5H), 7.30 (t, J = 14.7, 7.3 Hz, 1H), 7.17 (d, J = 8.5 Hz, 1H), 6.98 (s, 1H), 6.92 (d, J = 2.7 Hz, 1H), 3.81 (s, 3H), 2.48 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 199.4, 156.9, 155.3, 141.4, 141.0, 138.0, 137.4, 135.1, 132.4, 130.1, 129.0, 128.9, 128.4, 127.47, 127.41, 122.6, 122.2, 104.1, 55.3, 54.4, 24.8.

HRMS: $[M + H]^+$ calculated for $C_{25}H_{22}NO_2$: 368.1651, found 368.1659.

2-(4-methylquinolin-8-yl)-1,2-diphenylethanone (3m): Compound **3m** was prepared according to the general procedure **A** from **1m** (57.24 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 87% (88 mg) as a light yellow solid.

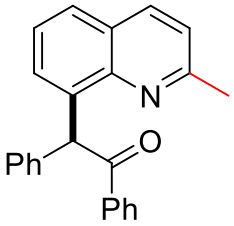


^{1}H NMR (400 MHz, $CDCl_3$): δ 8.72 (d, *J* = 4.3, 1H), 8.17-8.14 (m, 2H), 7.94-7.92 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.50-7.46 (m, 5H), 7.42-7.40 (m, 5H), 7.31-7.27 (m, 1H), 7.23-7.21 (dd, *J* = 4.4, 0.9 Hz, 1H), 2.69 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 199.1, 149.0, 145.3, 144.4, 139.3, 138.3, 137.4, 132.4, 129.8, 129.4, 128.7, 128.36, 128.32, 127.0, 125.8, 123.0, 121.9, 54.1, 18.8.

HRMS: $[M + H]^+$ calculated for $C_{24}H_{20}NO$: 338.1545, found 338.1533.

2-(2-methylquinolin-8-yl)-1,2-diphenylethanone (3n): Compound **3n** was prepared according to the general procedure **A** from **1n** (57.24 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 85% (86 mg) as a white solid.

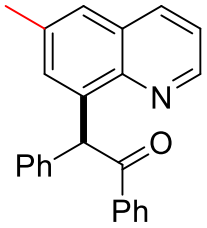


^{1}H NMR (500 MHz, $CDCl_3$): δ 8.20- 8.18 (m, 2H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.67 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.53-7.48 (m, 3H), 7.44-7.36 (m, 6H), 7.33-7.30 (m, 2H), 7.23 (d, *J* = 8.5 Hz, 1H), 2.54 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 199.7, 158.1, 145.2, 139.1, 138.0, 137.9, 136.3, 132.4, 130.2, 129.5, 129.0, 128.9, 128.4, 127.2, 126.7, 126.5, 125.4, 122.0, 54.3, 25.2.

HRMS: $[M + H]^+$ calculated for $C_{24}H_{20}NO$: 338.1545, found 338.1541.

2-(6-methylquinolin-8-yl)-1,2-diphenylethanone (3o): Compound **3o** was prepared according to the general procedure **A** from **1o** (57.24 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 96% (87 mg) as a white solid.

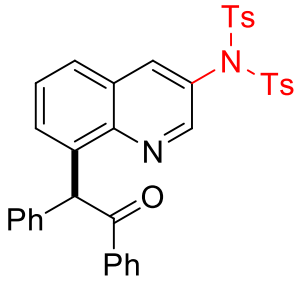


^{1}H NMR (500 MHz, $CDCl_3$): δ 8.80 (d, *J* = 3.0 Hz, 1H), 8.16 (d, *J* = 7.3 Hz, 2H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.49-7.47 (m, 5H), 7.41-7.29 (m, 7H), 2.45 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 199.3, 148.7, 144.4, 138.4, 137.5, 136.1, 135.6, 132.6, 132.1, 129.9, 129.1, 128.8, 128.6, 128.5, 127.2, 126.1, 121.3, 53.7, 21.9.

HRMS: $[M + H]^+$ calculated for $C_{24}H_{20}NO$: 338.1545, found 338.1551.

4-methyl-N-(8-(2-oxo-1,2-diphenylethyl)quinolin-3-yl)-N-tosylbenzenesulfonamide (3p):



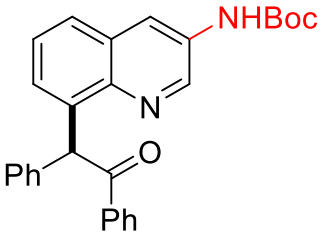
Compound **3p** was prepared according to the general procedure **A** from **1p** (168.48 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (10% EtOAc/Hexane, R_f = 0.2) yielded 40% (79 mg) as a light yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (d, J = 2.5 Hz, 1H), 8.11-8.08 (m, 2H), 7.83-7.78 (dd, J = 13.8, 2.5 Hz, 5H), 7.65 (dd, J = 8.0, 1.8 Hz, 1H), 7.52-7.46 (m, 3H), 7.45-7.37 (m, 7H), 7.35-7.27 (m, 5H), 2.46 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 198.7, 150.7, 145.5, 139.3, 138.7, 138.0, 137.3, 132.7, 131.8, 130.0, 129.8, 129.0, 128.7, 128.5, 128.2, 127.8, 127.5, 127.4, 53.8, 21.8.

HRMS: $[M + H]^+$ calculated for $C_{37}H_{31}N_2O_5S_2$: 647.1674, found 647.1686.

***tert*-butyl 8-(2-oxo-1,2-diphenylethyl)quinolin-3-ylcarbamate (3q):** Compound **3q** was



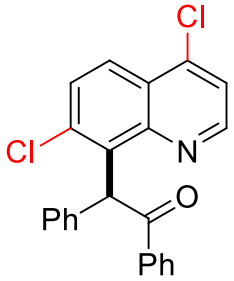
prepared according to the general procedure **A** from **1q** (93.6 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (10% EtOAc/Hexane, R_f = 0.2) yielded 38% (50 mg) as a light yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.37 (s, 1H), 8.09 (dd, J = 8.01, 0.7 Hz, 2H), 7.66-7.64 (dd, J = 8.2, 1.3 Hz, 1H), 7.50-7.47 (m, 1H), 7.46-7.42 (m, 3H), 7.46-7.42 (m, 3H), 7.41-7.39 (m, 2H), 7.37-7.34 (m, 3H), 7.33 (s, 1H), 7.29-7.24 (m, 2H), 1.55 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 199.3, 172.3, 152.8, 142.6, 138.5, 138.1, 137.4, 132.6, 132.2, 129.9, 129.0, 128.8, 128.6, 128.5, 128.2, 127.2, 127.0, 126.9, 122.16, 81.3, 54.0, 28.4.

HRMS: $[M + H]^+$ calculated for $C_{28}H_{27}N_2O_3$: 439.2022, found 439.2020.

2-(4,7-dichloroquinolin-8-yl)-1,2-diphenylethanone (3r): Compound **3r** was prepared



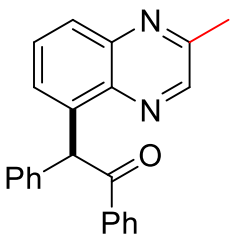
according to the general procedure **A** from **1r** (76.32 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (6% EtOAc/Hexane, R_f = 0.3) yielded 38% (19 mg) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.72 (d, J = 4.6 Hz, 1H), 8.08 (d, J = 9.0 Hz, 1H), 7.73-7.70 (m, 2H), 7.64 (d, J = 9.0 Hz, 1H), 7.41 (d, J = 4.6 Hz, 1H), 7.39-7.37 (m, 2H), 7.30-7.26 (m, 2H), 7.26-7.21 (m, 2H), 7.19-7.15 (m, 2H), 6.59 (s, 1H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 193.9, 149.6, 147.0, 142.9, 138.4, 137.6, 137.3, 136.6, 131.6, 130.3, 129.8, 128.2, 128.0, 127.7, 127.1, 125.6, 124.6, 121.6, 56.1.

HRMS: $[M + H]^+$ calculated for $C_{23}H_{16}Cl_2NO$: 392.0609, found 392.0599.

2-(2-methylquinoxalin-5-yl)-1,2-diphenylethanone (3s): Compound **3s** was prepared according to the general procedure **A** from **1s** (57.6 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (4% EtOAc/Hexane, R_f = 0.3) yielded 70% (71 mg) as a white solid.

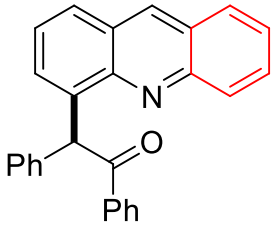


^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (s, 1H), 8.14-8.11 (m, 2H), 8.00-7.97 (dd, J = 8.4, 1.1 Hz, 1H), 7.62-7.58 (m, 1H), 7.53-7.46 (m, 3H), 7.44-7.36 (m, 5H), 7.33-7.29 (m, 1H), 7.26 (s, 1H), 2.60 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 199.1, 152.9, 145.8, 141.0, 139.7, 139.2, 137.52, 137.50, 132.7, 130.2, 130.0, 129.0, 128.9, 128.7, 128.5, 128.2, 127.5, 53.8, 22.6.

HRMS: $[M + H]^+$ calculated for $C_{23}H_{19}N_2O$: 339.1497, found 339.1494.

2-(acridin-4-yl)-1,2-diphenylethanone (3t): Compound **3t** was prepared according to the general procedure **A** from **1t** (70.2 mg, 0.36 mmol, 120 mol%) and **2a** (53.4 mg, 0.3 mmol, 100 mol%). Reaction mixture was purified by flash column chromatography (6% EtOAc/Hexane, R_f = 0.3) yielded 46% (52 mg) as a yellow solid.



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (s, 1H), 8.25-8.23 (m, 2H), 7.94 (d, J = 8.4 Hz, 1H), 7.89-7.85 (m, 2H), 7.67-7.63 (m, 1H), 7.58-7.52 (m, 3H), 7.49-7.39 (m, 7H), 7.36-7.30 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 199.6, 148.2, 146.6, 139.9, 138.1, 137.6, 136.0, 132.5, 130.2, 129.9, 129.7, 129.04, 129.01, 128.5, 128.0, 127.46, 127.42, 126.7, 126.6, 125.8, 125.5, 54.8.

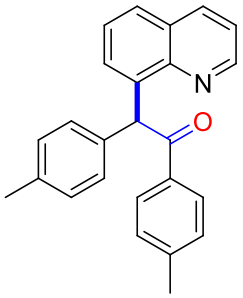
HRMS: $[M + H]^+$ calculated for $C_{27}H_{20}NO$: 374.1545, found 375.1544.

7. General procedure for catalytic reaction of quinoline N-oxides with various alkynes:

Procedure B:

An oven dried schlenk was charged with Teflon coated magnetic stir bar under argon atmosphere added Cp*Co(CO)I_2 (14.2 mg, 0.03 mmol, 10 mol%), and quinoline N-Oxide **1** (43.5 mg, 0.3 mmol, 1.0 eq). followed by 2, 2, 2 - trifluoro ethanol (TFE 1 mL). Subsequently added sodium pivalate (7.44 mg, 0.06 mmol, 20 mol%), and alkyne **2** (80.4 mg, 0.45 mmol, 1.5 eq). The closed schlenk tube containing reaction mixture were placed in preheated oil bath at 100 °C for 24 hours. After 24h the reaction mixture was allowed to cool to room temperature. Removal of solvent followed by column chromatography (EtOAc/Hexane) on silica gel afforded functionalized quinoline **4a** in good yields.

2-(quinolin-8-yl)-1,2-dip-tolylethanone (4a): Compound **4a** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2a** (92.7 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.35) yielded 60% (64 mg) as a yellow colour oily compound.

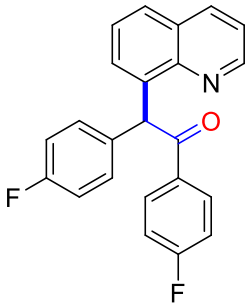


^{1}H NMR (400 MHz, $CDCl_3$): δ 8.85 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.13 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 2H), 7.73-7.71 (dd, *J* = 7.7, 1.9 Hz, 1H), 7.48-7.43 (m, 3H), 7.39-7.34 (m, 3H), 7.19 (t, *J* = 15.2, 7.8, Hz, 4H), 2.36 (s, 3H), 2.34 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 198.9, 149.6, 145.9, 143.3, 139.3, 136.7, 136.3, 135.4, 134.9, 129.9, 129.8, 129.6, 129.2, 128.4, 127.0, 126.3, 121.2, 53.4, 21.7, 21.2.

HRMS: $[M + H]^+$ calculated for $C_{25}H_{22}NO$: 352.1701, found 352.1702.

1,2-bis(4-fluorophenyl)-2-(quinolin-8-yl)ethanone (4b): Compound **4b** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2b** (96.3 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (4% EtOAc/Hexane, R_f = 0.35) yielded 85% (92 mg) as a white colour compound.



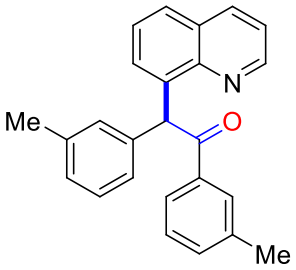
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.87-8.86 (dd, *J* = 4.4, 1.7 Hz, 1H), 8.15-8.13 (m, 3H), 7.75-7.73 (m, 1H), 7.49-7.46 (t, *J* = 15.6, 7.6 Hz, 1H), 7.42-7.39 (m, 5H), 7.07-7.03 (m, 4H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 197.6, 166.5, 164.5, 163.1, 161.1, 149.8, 145.6, 138.5, 136.4, 133.9, 133.6, 131.7, 131.6, 131.48, 131.42, 129.6, 128.6, 127.5, 126.4, 121.4, 115.8, 115.7, 115.6, 52.8.

^{19}F NMR ($CDCl_3$, 377 MHz): δ = -115.27, -105.55.

HRMS: $[M + H]^+$ calculated for $C_{23}H_{16}F_2NO$: 360.1200, found 360.1207.

2-(quinolin-8-yl)-1,2-di*m*-tolylethanone (4c): Compound **4c** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2c** (92.7 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.35) yielded 87% (92 mg) as a white colour compound.

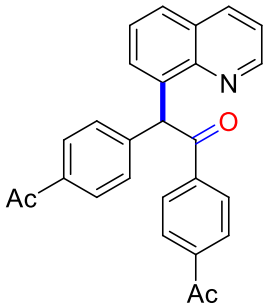


^{1}H NMR (500 MHz, $CDCl_3$): δ 8.86-8.84 (dd, *J* = 3.9, 1.6 Hz, 1H), 8.14-8.12 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.97 (s, 2H), 7.72 (d, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 15.2, 7.4 Hz, 1H), 7.42-7.36 (m, 3H), 7.30-7.25 (m, 5H), 7.10 (m, 1H), 2.36 (s, 3H), 2.34 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 199.4, 149.5, 145.8, 139.2, 138.5, 138.27, 138.23, 137.5, 136.4, 133.4, 130.6, 130.1, 129.6, 128.7, 128.47, 128.41, 128.0, 127.1, 127.0, 126.4, 126.4, 121.2, 53.9, 21.6, 21.5.

HRMS: $[M + H]^+$ calculated for $C_{25}H_{22}NO$: 352.1701, found 352.1701.

2-(quinolin-8-yl)-1,2-di*p*-acetylethanone (4d): Compound **4d** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2d** (117.9 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (10% EtOAc/Hexane, R_f = 0.2) yielded 75% (92 mg) as a yellow colour compound.

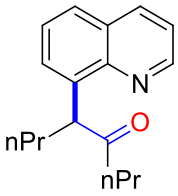


^{1}H NMR (400 MHz, $CDCl_3$): δ 8.86 (dd, *J* = 4.1, 1.1 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 3H), 7.94 (dd, *J* = 8.1, 1.6 Hz, 4H), 7.76 (d, *J* = 7.7 Hz, 1H), 7.55-7.37 (m, 6H), 2.58 (s, 3H), 2.57 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 198.1, 197.7, 197.5, 149.8, 145.4, 143.3, 140.4, 139.9, 137.7, 136.5, 136.2, 130.1, 129.6, 129.1, 128.8, 128.6, 128.5, 127.8, 126.4, 121.5, 54.1, 26.9, 26.6.

HRMS: $[M + H]^+$ calculated for $C_{27}H_{22}NO_3$: 408.1600, found 408.1600.

5-(quinolin-8-yl)octan-4-one (4e): Compound **4e** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2e** (49.59 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 70% (58 mg) as a yellow oily compound.

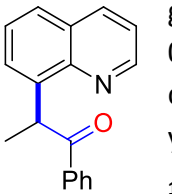


^{1}H NMR (500 MHz, $CDCl_3$): δ 8.94 (d, *J* = 3.0 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.2 Hz, 1H), 7.56 (d, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 15.1, 7.8 Hz, 1H), 7.42-7.39 (dd, *J* = 8.0, 4.1 Hz, 1H), 5.32 (t, *J* = 14.7, 7.5 Hz, 1H), 2.40-2.25 (m, 2H), 2.20-2.13 (m, 1H), 1.80-1.73 (m, 1H), 1.56-1.42 (dq, 2H), 1.32-1.24 (m, 2H), 0.86 (t, *J* = 14.5, 7.2 Hz, 3H), 0.72 (t, *J* = 14.8, 7.8 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 211.6, 149.6, 146.3, 138.6, 136.6, 128.6, 128.2, 126.8, 126.5, 121.1, 50.8, 44.2, 34.4, 20.9, 17.3, 14.2, 13.6.

HRMS: $[M + H]^+$ calculated for $C_{17}H_{22}NO$: 256.1701, found 256.1703.

1-phenyl-2-(quinolin-8-yl)propan-1-one (4f): Compound **4f** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2f** (52.2 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 57% (45 mg) as a light yellow oily compound.

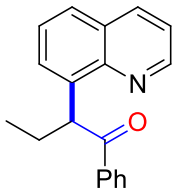


^{1}H NMR (500 MHz, $CDCl_3$): δ 9.02 (dd, *J* = 4.2, 1.9 Hz, 1H), 8.16 (dd, *J* = 8.06, 1.3 Hz, 1H), 8.05 (dd, *J* = 8.0, 0.8 Hz, 2H), 7.68 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.55-7.53 (dd, *J* = 7.4, 1.5 Hz, 1H), 7.46-7.43 (m, 2H), 7.38 (t, *J* = 14.9, 7.3 Hz, 1H), 7.27 (m, 2H), 6.28 (q, *J* = 20.9, 14.0, 7.1 Hz, 1H), 1.61 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 201.8, 149.7, 145.0, 140.5, 136.7, 132.6, 128.9, 128.8, 128.4, 128.0, 126.9, 126.7, 121.3, 100.0, 41.0, 18.7.

HRMS: $[M + H]^+$ calculated for $C_{18}H_{16}NO$: 262.1232, found 262.1231.

1-phenyl-2-(quinolin-8-yl)butan-1-one (4g): Compound **4g** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2g** (58.5 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 89% (74 mg) as a light yellow oily compound.

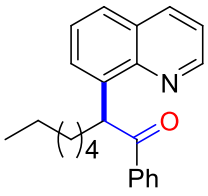


^{1}H NMR (500 MHz, $CDCl_3$); δ 9.05-9.03 (dd, *J* = 4.0, 1.7 Hz, 1H), 8.14-8.11 (m, 3H), 7.66-7.61 (m, 2H), 7.44-7.41 (m, 2H), 7.37 (t, *J* = 14.5, 7.0 Hz, 1H), 7.27 (t, *J* = 15.1, 7.6 Hz, 2H), 6.26 (t, *J* = 14.4, 6.9 Hz, 1H), 2.33 (h, *J* = 21.4, 15.2, 7.2 Hz, 1H), 1.94 (h, *J* = 21.3, 14.3, 7.3 Hz, 1H), 0.93 (t, *J* = 14.2, 7.8 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 201.4, 149.7, 145.6, 138.9, 137.2, 136.7, 132.6, 128.9, 128.7, 128.3, 128.1, 126.9, 126.6, 121.2, 47.3, 27.4, 12.5.

HRMS: $[M + H]^+$ calculated for $C_{19}H_{18}NO$: 276.1388, found 276.1387.

1-phenyl-2-(quinolin-8-yl)octan-1-one (4h): Compound **4h** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2h** (83.7 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.35) yielded 94% (94 mg) as a light yellow oily compound.

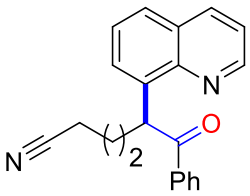


^{1}H NMR (500 MHz, $CDCl_3$): δ 9.05-9.03 (dd, *J* = 4.1, 1.7 Hz, 1H), 8.14 (m, 3H), 7.67-7.62 (ddd, *J* = 16.7, 15.5, 9.5, 8.1, 1.3 Hz, 2H), 7.45-7.36 (m, 3H), 7.29-7.26 (m, 2H), 6.33 (t, *J* = 14.3, 7.0 Hz, 1H), 2.33-2.26 (m, 1H), 1.41-1.18 (m, 8H), 0.82 (t, *J* = 14.0, 6.8 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 201.5, 149.7, 145.6, 139.1, 137.2, 136.6, 132.6, 128.9, 128.7, 128.3, 128.1, 126.9, 126.6, 121.2, 45.7, 34.4, 31.7, 29.5, 27.9, 22.6, 14.1.

HRMS: $[M + H]^+$ calculated for $C_{23}H_{26}NO$: 332.2014, found 332.2018.

6-oxo-6-phenyl-5-(quinolin-8-yl)hexanenitrile (4i): Compound **4i** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2i** (76.05 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (8% EtOAc/Hexane, R_f = 0.2) yielded 80% (76 mg) as oily compound.

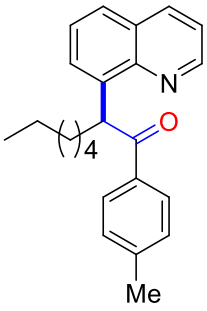


^{1}H NMR (500 MHz, $CDCl_3$): δ 9.06 (dd, *J* = 4.1, 1.8 Hz, 1H), 8.17-8.15 (dd, *J* = 7.8, 1.8 Hz, 1H), 8.05 (d, *J* = 7.4 Hz, 2H), 7.69-7.67 (m, 1H), 7.55 (m, 1H), 7.48-7.46 (dd, *J* = 8.1, 4.2 Hz, 1H), 7.44-7.35 (m, 2H), 7.26-7.23 (t, *J* = 15.7, 7.4 Hz, 2H), 6.34 (t, *J* = 14.5, 6.9 Hz, 1H), 2.34-2.32 (m, 3H), 2.10-2.03 (m, 1H), 1.72-1.64 (m, 1H), 1.61-1.52 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 200.1, 149.9, 145.1, 137.8, 136.7, 136.3, 132.7, 128.7, 128.3, 128.2, 127.8, 127.2, 126.5, 121.3, 119.6, 44.5, 32.8, 23.3, 17.0.

HRMS: $[M + H]^+$ calculated for $C_{21}H_{19}N_2O$: 315.1497, found 315.1487.

2-(quinolin-8-yl)-1-*p*-tolyloctan-1-one (4j): Compound **4j** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2j** (90 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.35) yielded 59% (62 mg) as oily compound.

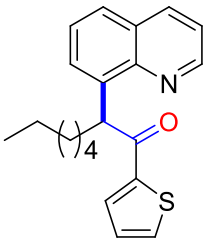


^{1}H NMR (500 MHz, $CDCl_3$): δ 9.04 (dd, *J* = 4.0, 1.9 Hz, 1H), 8.14-8.12 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 2H), 7.66-7.62 (t, *J* = 16.2, 8.2 Hz, 2H), 7.45-7.42 (m, 2H), 7.08 (d, *J* = 7.6 Hz, 2H), 6.31 (t, *J* = 14.3, 7.4 Hz, 1H), 2.32-2.28 (m, 1H), 2.27 (s, 3H), 1.90-1.83 (m, 1H), 1.26-1.18 (m, 8H), 0.82 (t, *J* = 13.8, 6.9 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 201.1, 149.6, 145.5, 143.3, 139.3, 136.6, 134.7, 129.0, 128.7, 128.1, 126.8, 126.7, 121.1, 45.5, 34.4, 31.7, 29.5, 27.9, 22.6, 21.5, 14.1.

HRMS: $[M + H]^+$ calculated for $C_{24}H_{28}NO$: 346.2171, found 346.2173.

2-(quinolin-8-yl)-1-(thiophen-2-yl)octan-1-one (4k): Compound **4k** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2k** (86.4 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.35) yielded 67% (68 mg) as oily compound.

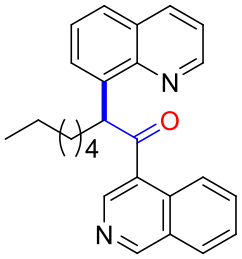


^{1}H NMR (500 MHz, $CDCl_3$): δ 9.03 (d, *J* = 3.0 Hz, 1H), 8.14 (d , *J* = 8.0 Hz, 1H), 7.98 (d, *J* = 3.8 Hz, 1H), 7.74 (d, *J* = 7.4 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.48-7.41 (m, 3H), 6.91 (t, *J* = 8.7, 4.2 Hz, 1H), 6.25 (t, *J* = 14.3, 7.4 Hz, 1H), 2.34-2.27 (m, 1H), 1.92-1.85 (m, 1H), 1.28-1.20 (m, 8H), 0.82 (t, *J* = 14.1, 6.8 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 194.5, 149.7, 145.7, 145.1, 139.1, 136.6, 133.5, 133.1, 128.7, 128.05, 128.00, 126.9, 126.7, 121.2, 46.4, 34.2, 31.7, 29.4, 27.8, 22.6, 14.1.

HRMS: $[M + H]^+$ calculated for $C_{21}H_{24}NOS$: 338.1579, found 338.1097.

1-(quinolin-3-yl)-2-(quinolin-8-yl)octan-1-one (4l): Compound **4l** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2l** (106.65 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (5% EtOAc/Hexane, R_f = 0.3) yielded 72% (68 mg) as a yellow semi solid compound.

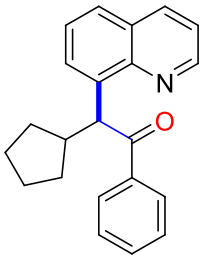


^{1}H NMR (400 MHz, $CDCl_3$): δ 9.51 (s, 1H), 9.09 (dd, *J* = 4.0, 1.9 Hz, 1H), 9.04 (d, *J* = 1.9 Hz, 1H), 8.14-8.11 (dd, *J* = 8.4, 2.0 Hz, 1H), 8.01 (d, *J* = 8.6 Hz, 1H)7.76-7.64 (m, 4H), 7.50-7.42 (m, 3H), 6.42 (t, *J* = 14.3, 7.5 Hz, 1H), 2.41-2.32 (m, 1H), 1.99-1.92 (m, 1H), 1.35-1.19 (m, 8H), 0.81 (t, *J* = 13.9, 6.9 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 200.1, 149.8, 149.7, 149.3, 145.3, 138.3, 138.1, 136.6, 131.5, 129.4, 129.3, 129.0, 128.7, 128.1, 127.1, 127.0, 126.9, 126.6, 121.3, 46.1, 33.7, 31.6, 29.3, 27.6, 22.5, 14.0.

HRMS: $[M + H]^+$ calculated for $C_{26}H_{27}N_2O$: 383.2123, found 383.2124.

2-cyclopentyl-1-phenyl-2-(quinolin-8-yl)ethanone (4m): Compound **4m** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2m** (76.5 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 84% (80 mg) as oily compound.

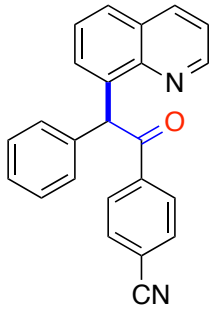


^{1}H NMR (500 MHz, $CDCl_3$): δ 9.07 (dd, J = 4.0, 1.5 Hz, 1H), 8.23 (m, 2H), 7.79-7.77 (m, 1H), 7.64 (d, J = 8.7 Hz, 1H), 7.47-7.34 (m, 7H), 6.31 (d, J = 10.4 Hz, 1H), 2.95-2.86 (h, J = 9.2, 8.8, 8.3 Hz, 1H), 2.13-2.05 (m, 2H), 1.82-1.71 (m, 2H) 1.45-1.31 (m, 2H), 1.21-1.12 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 212.1, 201.6, 149.6, 149.3, 145.9, 139.0, 138.5, 138.1, 137.4, 136.7, 136.3, 132.7, 132.0, 129.6, 129.0, 128.8, 128.7, 128.3, 127.2, 126.9, 126.8, 126.6, 121.2, 121.1, 58.2, 52.0, 50.5, 45.4, 32.2, 30.3, 30.1, 29.9, 26.1, 26.0, 25.4, 24.9.

HRMS: $[M + H]^+$ calculated for $C_{22}H_{22}NO$: 316.1701, found 316.1701.

4-(2-oxo-2-phenyl-1-(quinolin-8-yl)ethyl)benzonitrile (4n major): Compound **4n** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2n** (91.35 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (10% EtOAc/Hexane, R_f = 0.2) yielded 58% (61 mg) as light yellow compound.

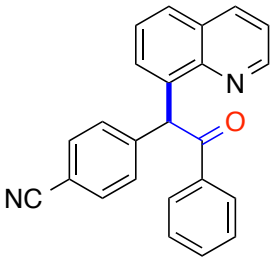


^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79 (dd, J = 4.2, 1.8 Hz, 1H), 8.20-8.15 (m, 3H), 7.75 (dd, J = 8.1, 1.3 Hz, 1H), 7.71-7.68 (m, 2H), 7.48-7.38 (m, 6H), 7.35-7.32 (m, 1H), 7.31-7.29 (m, 1H), 7.25 (s, 1H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 198.1, 149.5, 145.5, 141.0, 138.7, 136.8, 136.4, 132.4, 130.0, 129.8, 129.3, 129.2, 128.4, 127.7, 127.5, 126.4, 121.4, 118.2, 115.7, 54.7.

HRMS: $[M + H]^+$ calculated for $C_{24}H_{17}N_2O$: 349.1341, found 349.1342.

4-(2-phenyl-2-(quinolin-8-yl)acetyl)benzonitrile (4n' miner): Compound **4n'** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2n** (91.35 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (10% EtOAc/Hexane, R_f = 0.2) yielded 20% (21 mg) as light yellow compound.

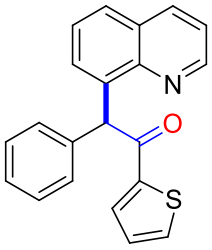


.**H NMR** (400 MHz, $CDCl_3$): δ 8.91 (dd, J = 4.1, 1.6 Hz, 1H), 8.18-8.15 (m, 1H), 8.06-8.03 (m, 2H), 7.71-7.75 (m, 1H), 7.62-7.60 (m, 3H), 7.54-7.52 (m, 2H), 7.48-7.42 (m, 4H), 7.38-7.34 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 198.1, 149.9, 144.3, 137.0, 136.8, 136.6, 132.4, 133.2, 132.2, 130.6, 129.6, 129.0, 128.8, 128.7, 127.9, 126.5, 121.6, 118.9, 110.9, 53.1.

HRMS: $[M + H]^+$ calculated for $C_{24}H_{17}N_2O$: 349.1341, found 349.1342.

1-phenyl-2-(quinolin-8-yl)-2-(thiophen-2-yl)ethanone (4o): Compound **4o** was prepared according to the general procedure **B** from **1a** (43.5 mg, 0.3 mmol, 100 mlo%) and **2o** (82.8 mg, 0.45 mmol, 150 mol%). Reaction mixture was purified by flash column chromatography (2% EtOAc/Hexane, R_f = 0.3) yielded 93% (92 mg) as light yellow compound.

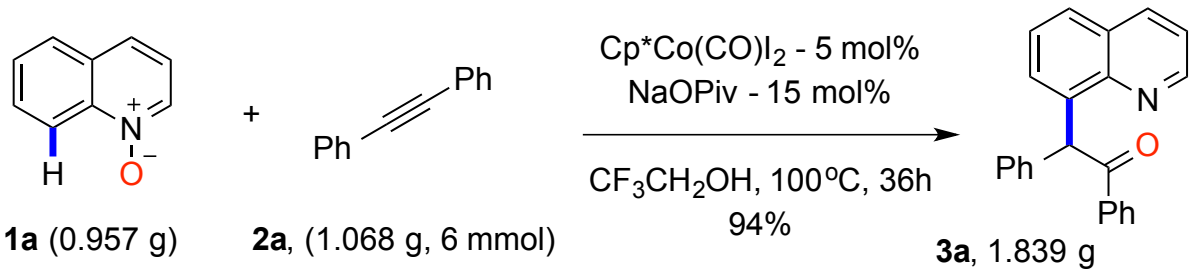


^{1}H NMR (500 MHz, $CDCl_3$): δ 8.89 (d, *J* = 2.8, 1H), 8.13 (d, *J* = 7.4 Hz, 1H), 7.92 (d, *J* = 2.8 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.56-7.46 (m, 5H), 7.41-7.35 (m, 4H), 7.30-7.27 (t, *J* = 14.3, 7.1 Hz, 1H), 7.03(t, *J* = 8.6, 4.6 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 191.9, 149.7, 144.6, 138.5, 138.3, 136.4, 133.4, 132.9, 129.9, 129.7, 128.8, 128.5, 128.1, 127.3, 127.2, 126.4, 54.5.

HRMS: $[M + H]^+$ calculated for $C_{21}H_{16}NOS$: 330.0953, found 330.0960.

8. Gram scale reaction of 1,2-diphenyl-2-(quinolin-8-yl)ethanone (3a):

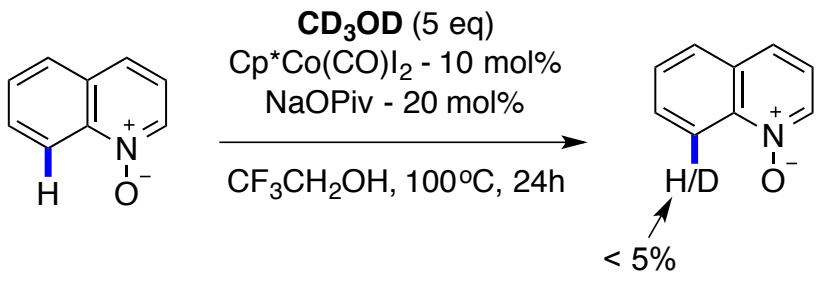


1a (0.957 g) **2a**, (1.068 g, 6 mmol) **3a**, 1.839 g

An oven dried schlenk was charged with Teflon coated magnetic stir bar under argon atmosphere added $Cp^*Co(CO)I_2$ (142.5 mg, 0.3 mmol, 5 mol%), and quinoline N-Oxide **1a** (0.957 mg, 6.6 mmol, 1.1 eq) followed by 2, 2, 2 - trifluoro ethanol (TFE 15 mL). Subsequently added sodium pivalate (111.6 mg, 0.9 mmol, 15 mol%), and alkyne **2a** (1068 mg, 6 mmol, 1.0 eq). The closed schlenk tube containing reaction mixture were placed in preheated oil bath at 100 °C for 36 hours. The reaction mixture was allowed to cool to room temperature after above mentioned time. Removal of solvent followed by column chromatography (2% EtOAc/Hexane; R_f=0.3) on silica gel afforded functionalized quinoline **3a** with 94% (1.839g) as whilte solid.

9. Control experiments: (detailed procedure)

9.1. Deuterium labelled experiment:

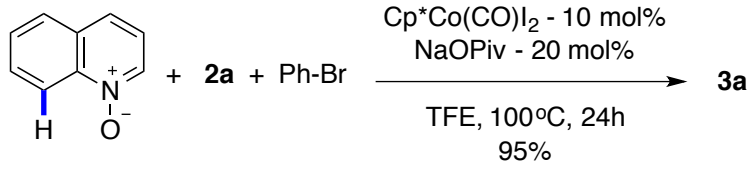


An oven dried schlenk was charged with Teflon coated magnetic stir bar under argon atmosphere added $Cp^*Co(CO)I_2$ (14.2 mg, 0.03 mmol, 10 mol%), and quinoline N-Oxide

(43.5 mg, 0.3 mmol, 1.0 eq) followed by 2, 2, 2 - trifluoro ethanol (TFE 1 mL). Subsequently added sodium pivalate (7.44 mg, 0.06 mmol, 20 mol%), and CD_3OD (54 mg, 1.5 mmol, 5.0 eq). Finally closed schlenk tube and placed in preheated oil bath at 100 °C for 24 hours. After completion of reaction time, the reaction mixture was allowed to cool down to room temperature. Removal of solvent followed by column chromatography (3% EtOAc/methanol) on silica gel gave compound **1a**. The ^{1}HNMR analysis revealed that there is no ^{2}H-incoroporation in compound **1a**.

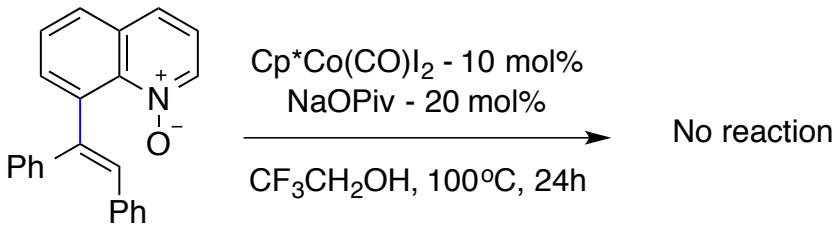
9.2 Competittive experiments with Ph-Br:

An oven dried schlenk was charged with Teflon coated magnetic stir bar under argon atmosphere added $Cp^*Co(CO)I_2$ (14.2 mg, 0.03 mmol, 10 mol%), and quinoline N-Oxide **1a** (65.25 mg, 0.45 mmol, 1.5 eq). followed by 2, 2, 2 - trifluoro ethanol (TFE 1 mL). Subsequently added sodium pivalate (7.44 mg, 0.06 mmol, 20 mol%), and **2a** diphenyl acetylene (53.4 mg, 0.3 mmol, 100 mol%), **2c** bromo benzene (47.1 mg, 0.3 mmol, 100 mol%) and Finally closed schlenk tube and placed in preheated oil bath at 100 °C for 24 hours. After completion of reaction time allowed to cool down to room temperature. Remove solvent from reaction mixture and subjected to column chromatography (2% EtOAc/Hexane) on silica gel afforded intra molecular oxygen transferred quinoline .



9.3 Intramolecular oxygen atom transfer reaction with 5:

An oven dried schlenk was charged with Teflon coated magnetic stir bar under argon atmosphere added $Cp^*Co(CO)I_2$ (7.35 mg, 0.015 mmol, 10 mol%), and (*E*)-8-(1,2-diphenylvinyl)quinoline 1-oxide **5** (50 mg, 0.15 mmol, 1.0 eq). followed by 2, 2, 2 - trifluoro ethanol (TFE 1 mL). Subsequently sodium pivalate (3.8. mg, 0.03 mmol, 20 mol%) was added. The resultant mixture was in a closed schlenk tube and placed in preheated oil bath at 100 °C for 12 hours. After completion of reaction time allowed to cool down to room temperature. Removal of solvent followed by column chromatography (50% EtOAc/Hexane) on silica gel gave compound which after ^{1}HNMR analysis revealed that there is no formation of oxygen transfer product.

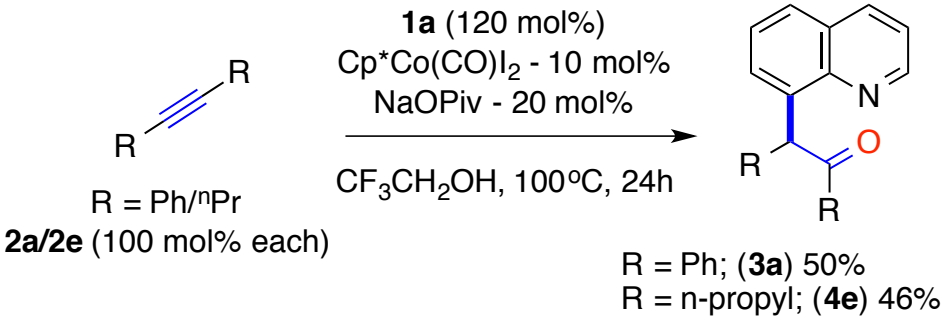


^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (dd, *J* = 6.0, 1.0 Hz, 1H), 7.85-7.83 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.71-7.69 (dd, *J* = 8.4, 0.8, 1H), 7.52- 7.49 (m, 1H), 7.42-7.40 (dd, *J* = 7.2, 1.5 Hz, 1H), 7.28-7.19 (m, 6H), 7.06-6.99 (m, 4H), 6.95-6.92 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 143.68, 143.65, 141.5, 137.8, 136.8, 134.6, 133.5, 132.4, 129.6, 128.5, 128.3, 128.2, 127.9, 127.0, 126.8, 126.3, 126.2, 125.6, 125.3, 121.3.

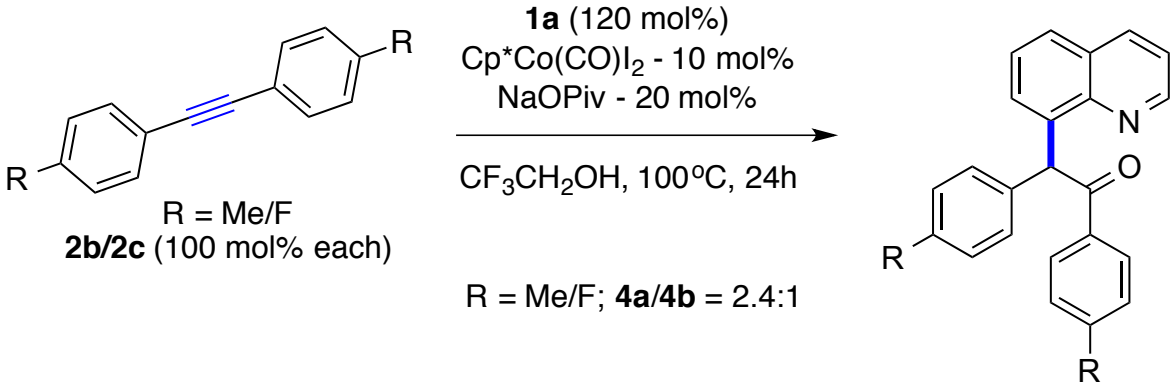
9.4 Competitive experiment of aromatic and aliphatic alkynes with quinoline:

An oven dried schlenk was charged with Teflon coated magnetic stir bar under argon atmosphere added $Cp^*Co(CO)I_2$ (14.2 mg, 0.03 mmol, 10 mol%), and quinoline N-Oxide **1a** (43.5 mg, 0.3 mmol, 1.0 eq). followed by 2, 2, 2 - trifluoro ethanol (TFE 1 mL). Subsequently sodium pivalate (7.44 mg, 0.06 mmol, 20 mol%), diphenyl acetylene **2a** (64.08 mg) and 4-octyne **2e** (39.6 mg), 0.36 mmol, 1.2 eq) were added. The resultant reaction mixture in a closed schlenk tube were placed in preheated oil bath at 100 °C for 24 hours. After completion of reaction time, it was allowed to cool down to room temperature. Removal of solvent followed by column chromatography (2% EtOAc/Hexane) on silica gel afforded **3a** with 50% and **4e** with 46% yields respectively.

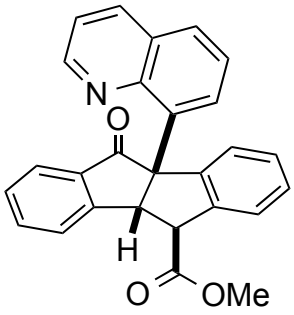


9.5 Competitive experiment of aromatic alkynes (2b vs 2c):

An oven dried schlenk was charged with Teflon coated magnetic stir bar under argon atmosphere added $Cp^*Co(CO)I_2$ (14.2 mg, 0.03 mmol, 10 mol%), and quinoline N-Oxide **1a** (43.5 mg, 0.3 mmol, 1.0 eq). followed by 2, 2, 2 - trifluoro ethanol (TFE 1 mL). Subsequently added sodium pivalate (7.44 mg, 0.06 mmol, 20 mol%), and alkynes **2b/2c** {(para methyl(74.16 mg), para flouro(77.04 mg), 0.36 mmol, 1.2 eq)}. Finally closed schlenk tube and placed in preheated oil bath at 100 °C for 24 hours. After completion of reaction time allowed to cool down to room temperature. Remove solvent from reaction mixture and subjected to column chromatography (2% EtOAc/Hexane) on silica gel afforded **4a** and **4b** in 2.4:1 ratio respectively.



10. Application: An oven dried schlenk was charged with Teflon coated magnetic stir bar under argon atmosphere added $[Ru(p\text{-}cym)Cl_2]_2$ (30.60 mg, 0.05 mmol, 10 mol%), and $AgSbF_6$ (34.30 mg, 0.1 mmol, 20mol%) followed by 1, 2 Dichloro ethane (DCE 1.5 mL). Subsequently **3a** (1,2-diphenyl-2-(quinolin-8-yl)ethanone) (161.5 mg, 0.5 mmol, 1 eq) and methyl acrylate (86.03 mg, 1 mmol, 2 eq) and finally added $Cu(OAc)_2.H_2O$ (149.7 mg, 0.75 mmol, 1.5 eq) were added under Ar. The resultant reaction mixture in a closed schlenk tube was placed in preheated oil bath at 130 °C for 30 hours. After 30h, the reaction mixture was allowed to cool down to room temperature. Removal of solvent followed by column chromatography (20% EtOAc/Hexane) on silica gel gave white solid in 20% yield as a single diastereomer.



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.43-8.41 (dd, *J* = 4.4, 1.2 Hz, 1H), 8.10-8.08 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.73-7.71 (m, 2H), 7.65-7.62 (m, 1H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.45-7.42 (m, 2H), 7.41-7.34 (m, 3H), 7.27-7.25 (m, 1H), 7.22-7.20 (dd, *J* = 6.7, 1.0 Hz, 1H), 4.59 (s, 1H), 4.34 (s, 1H), 3.50 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 204.3, 173.0, 153.9, 148.5, 145.7, 141.9, 141.6, 140.9, 137.2, 136.1, 134.1, 130.4, 129.0, 128.6, 128.0, 127.6, 127.5, 126.5, 125.9, 125.2, 124.2, 121.0, 70.5, 56.6, 56.0, 52.2.

HRMS: $[M + H]^+$ calculated for $C_{27}H_{19}NO_3$: 406.1443, found 406.1456.

11. **Crystallographic Summary:**

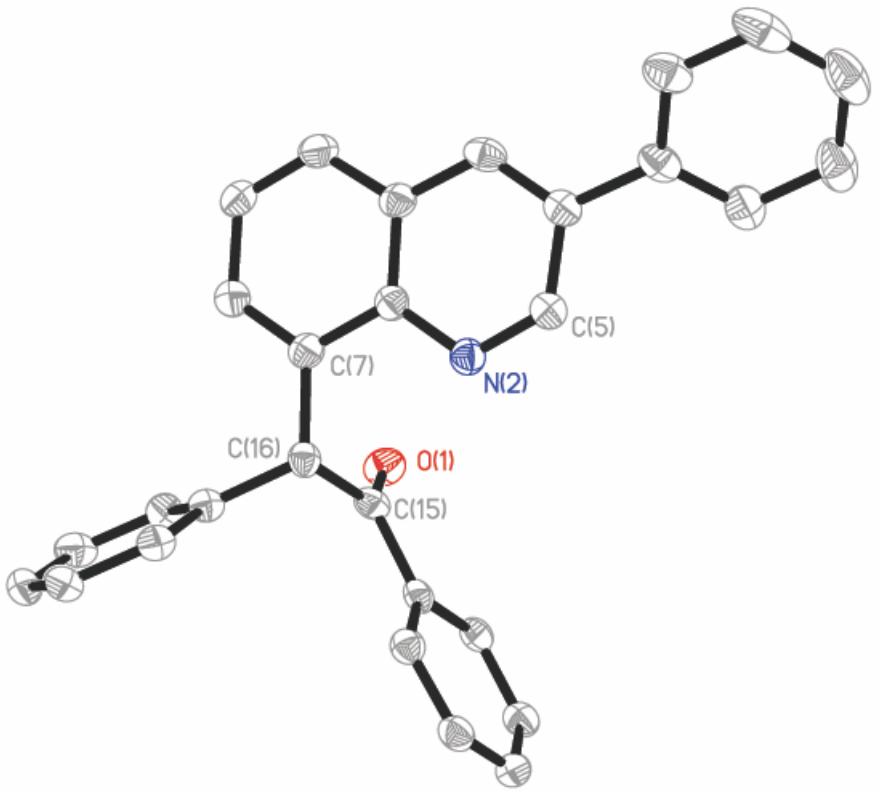


Figure S1: Structure of compound **3c** in solid state. Hydrogen atoms are omitted for clarity.

X-ray Crystal Structure Analysis : C29H21NO, MW = 399.47 g.mol-1 , yellow, crystal size = 0.20 x 0.15 x 0.13 mm, orthorhombic, space group P 2_1 2_1 2_1 , a = 9.0018(2) Å, b = 13.225(3) Å, c = 17.293(4) Å , T = 100 K, Z = 4, Dcalc = 1.29 g.cm-1 , λ = 0.71073 Å (Mo-Kα), CCD Bruker SMART APEX diffractometer, 1.9 < q < 25.4, 3766 measured reflections, structures were solved by direct methods and refined (SHELXL-97) by full matrix least squares based on F^2.

12. **Computational details:**

DFT calculations were performed to search all intermediates and transition structures on potential energy surfaces using the Gaussian 09 program.[5] DFT method B3LYP[6] with a standard 6-311G(d) basis set (LANL2DZ basis set for Co) was used for the geometry optimizations. Intrinsic reaction coordinate (IRC) calculations and subsequent geometry optimizations were carried out to confirm the minima linked by each transition state. The M11L functional, proposed by Truhlar et al.,[7] was used with a 6-311+G(d) basis set (SDD basis set for Co) to calculate the single-point energies because which has been demonstrated to provide a reliable energetic information.[8,9] Solvent effects of 2,2,2-trifluoroethanol (ε =26.726) and 1,4-dioxane (ε =2.209) were evaluated with single-point energy calculations at the gas phase-optimized geometries (B3LYP) using the SMD continuum solvation model.[10]

The energy profiles of the reaction pathways are presented as Gibbs free energy changes (ΔG's) involving zero-point vibrational energy (ZPVE) and thermal corrections obtained at 298.15 K and 1 atm pressure. To estimate the Gibbs free energies, the ZPVE and thermal corrections obtained from the gas phase computations at the B3LYP/6-311G(d),LANL2DZ(Co) level of theory have been applied to the M11L/6-311+G(d) energies in the solvent phase.

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Results and discussion:

The free energy profiles for the C-H bond functionalization, alkyne insertion (C-C bond formation), N-O bond cleavage (oxygen atom transfer) and catalyst regeneration are shown in Figures 1-3. It has been shown that the metal center ligated by solvent molecules exothermically.[9,11] The energetic trends of $SMD_{(1,4\text{-dioxane})}$/M11L/6-311+G(d),SDD(Co) are found to be similar to that of $SMD_{(2,2,2\text{-Trifluoroethanol})}$/M11L/6-311+G(d),SDD(Co) calculations. However, the discussions in the text are presented using the $SMD_{(1,4\text{-dioxane})}$/M11L/6-311+G(d),SDD(Co) level of theory to compare with the Rh-catalyzed reactions.[9] 2,2,2-trifluoroethanol and acetate molecules ligate the $CoCp^*(CO)I_2$ to form $[CoCp^*(OAc)(CF_3CH_2OH)]$ **1**, which was set to be a reference starting point. The coordination of quinoline N-oxide **2**, with **1** gives the intermediate **3** releasing 14.7 kcal/mol of free energy. The abstraction of hydrogen atom at C8 position and the formation of C-Co bond occur through the transition state **4ts**, with an activation free energy of 26.7 kcal/mol. Resulting intermediate **5'** of this concerted metallation-deprotonation step is endothermic by 14.5 kcal/mol. Intermediate **5'** then coordinates with the diphenylalkyne with a release of acetic acid (Figure S2) to form the complex **6** with an energetic span of 9.0 kcal/mol.

As shown by Li et al.,[9] (for Rh catalyzed reactions) four possible pathways were taken into account for the Co catalyzed reactions. The free energy profiles of the C-C bond formation, N-O bond cleavage (oxygen atom transfer) are shown in Figure S3. Similar to the reported Rh catalyzed reactions Co also undergoes a blue pathway as a lowest-energy pathway. The alkyne-coordinated complex **6** exothermically (0.4 kcal/mol) undergoes C-C bond formation through a transition state of **7ts** leading to a seven membered alkenyl cyclic intermediate **8** (which corresponds to intermediate V (scheme 5) in the manuscript). A subsequent reductive elimination step proceeds through a transition state **9ts** leading to the complex **10** with an energetic span of 29.1 kcal/mol. This is found to be the rate-limiting step for the whole catalytic cycle. The formation of highly exothermic (66.1 kcal/mol) Co-complex **12** facilitated by N-O bond cleavage obtained through **11ts** with an energetic span of 3.2 kcal/mol. As shown in the Figure 2 other pathways are proceeds through high-energy barriers. Our detailed computational investigation revealed that Co-catalyzed C-H

[11] J. Jiang, R. Ramozzi, K. Morokuma, *Chem*. *Eur*. *J*. **2015**, *21*, 11158–11164.

activation/OAT reaction is energetically feasible and follows reactions pathways similar to the reported Rh-catalyzed C-H activation/OAT reactions reported by Li et al.[9]

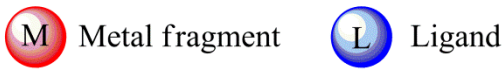
The free energy profiles for the protonation step of complex **13** are shown in the Figure S4. (For simplicity, we took acetic acid instead of Pivalic acid although both NaOAc and NaOPiv gave expected product). The coordination of acetic acid leads to the formation of intermediate **23** with an energy span of 5.2 kcal/mol, which is protonated by an acetic acid through transition state **24ts** to form enol-coordinated cobalt complex **25**. This step occurs with an energetic span of 3.6 kcal/mol. Further, elimination of active catalyst **1**, from **25** the desired product **26** was obtained. Overall the formation of product **26** from quinoline-N-oxide **1** is highly exothermic with an energy gain of 60.4 kcal/mol. Comparing the results of Rh and Co catalyzed reactions, the former one found to have lower energy barriers in all reaction steps (Table S2). The results indicate that the Rh catalyzed reactions are relatively faster compared to the Co catalyzed reactions with diarylalkynes. But surprisingly, our experimental results disclose that [Cp*Rh^{III}] was in efficient with dialkylacetylene (0% conversion) compare to its congener [Cp*Co^{III}] higher yield (see manuscript). To understand the contrast in reactivity patterns we have calculated the stabilization energies due to the charge transfer interaction between metal fragment to acetylene (M→L) and acetylene to metal fragment (L→M) as shown in the Table S3. It is interesting to note that the L→M charge transfer stabilization is substantially higher in case of di-propyl-acetylene to Co (27.5 kcal/mol) compared to others (Table S3). This may be the cause for the feasibility of Co catalysed reactions with di-alkyl-acetylene. However, there may be other reasons for this special property of Co catalyst as this is the preliminary result and we anticipate more investigations will be done to evaluate the reactivity pattern.

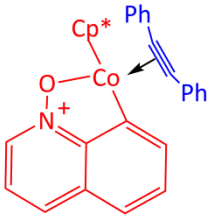
Furthermore, the regioselectivity of non-symmetrical alkyne, prop-1-yn-1-ylbenzene (Scheme S1) has been explained using the free energy profiles shown in the Figure S5. A comparison of the relative free energies of transition states **30ts** and **36ts** revealed that the later was 11.3 kcal/mol higher in energy than the former. This is due to the better conjugation between the phenyl group and the enolate moiety in the **30ts**. This result is consistent with the experimental observations.

Table S2. B3LYP and M11L free energies for Co and Rh catalyzed C-H functionalization reaction of quinoline N-oxide

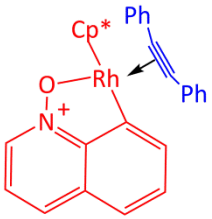
	Co-complexes			Rh-reported[5]	
	M11L 1,4-dioxane	M11L TFE	B3LYP GAS	B3LYP GAS	M11L 1,4-dioxane
1	0.0	0.0	0.0	0.0	0.0
3	-14.7	-7.5	-17.8	-15.1	-10.2
4ts	12.0	18.6	11.6	10.6	13.1
5'	-0.2	8.5	-5.4	-	-
5	10.5	15.3	11.7	-6.9	-2.8
6	8.8	19.2	7.6	0.6	-4.0
7ts	23.2	32.5	22.1	21.1	14.1
8	8.4	15.9	5.9	1.7	-7.8
9ts	37.5	46.1	33.4	29.2	16.8
10	15.5	24.6	11.3	6.7	-7.4
11ts	18.7	20.4	19.3	12.0	-5.3
12	-66.1	-54.5	-66.0	-55.0	-70.0
13	-52.6	-43.8	-56.1	-60.1	-76.2
14ts	26.9	37.2	23.7	18.9	17.8
15	25.7	34.6	20.1	18.7	19.6
16ts	43.7	50.0	38.2	26.8	28.7
17	-16.3	-5.0	-14.2	-13.3	-19.8
18ts	-13.1	-2.1	-11.1	-4.9	-11.8
19ts	48.6	55.1	46.8	47.7	38.0
20	21.0	27.1	20.1	16.3	3.8
20'	-13.5	-5.5	-8.08	-	-
21ts	48.6	52.5	48.1	40.2	26.9
22ts	56.5	62.5	49.2	42.9	42.9
23	-47.4	-37.8	-60.7	-47.5	-55.7
24ts	-43.8	-34.9	-53.8	-46.4	-52.9
25	-44.2	-36.2	-55.3	-41.5	-54.3
26	-60.4	-59.6	-66.4	-51.7	-63.5
27	5.0	18.4	5.0	1.7	-2.0
28ts	21.8	31.4	18.8	21.1	15.7
29	8.0	16.3	3.0	1.4	-6.2
30ts	31.3	46.6	31.3	31.1	19.1
31	14.9	18.5	7.0	-	-
32ts	16.1	18.1	14.5	11.8	-3.5
33	-42.0	-36.4	-46.7	-60.5	-72.9
34ts	25.1	34.7	21.1	22.2	17.4
35	11.8	17.8	9.1	6.5	0.5
36ts	42.6	48.2	35.4	33.4	27.1
37	14.6	18.9	7.0	4.2	-6.3
38ts	16.9	19.5	14.6	10.9	-3.8
39	-45.3	-40.1	-49.1	-58.7	-73.9

Table S3. The ligand to metal (L-M) and metal to ligand (M-L) charge transfer stabilization energies calculated by using the B3LYP method

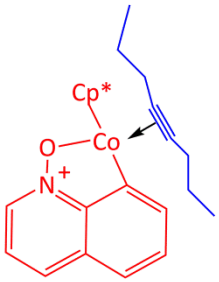




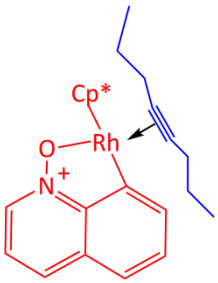
6-Co



6-Rh



6'-Co



6'-Rh

	L-M	M-L
6-Co	19.4	7.3
6-Rh	19.4	14.5
6'-Co	27.5	7.6
6'-Rh	19.5	14.1

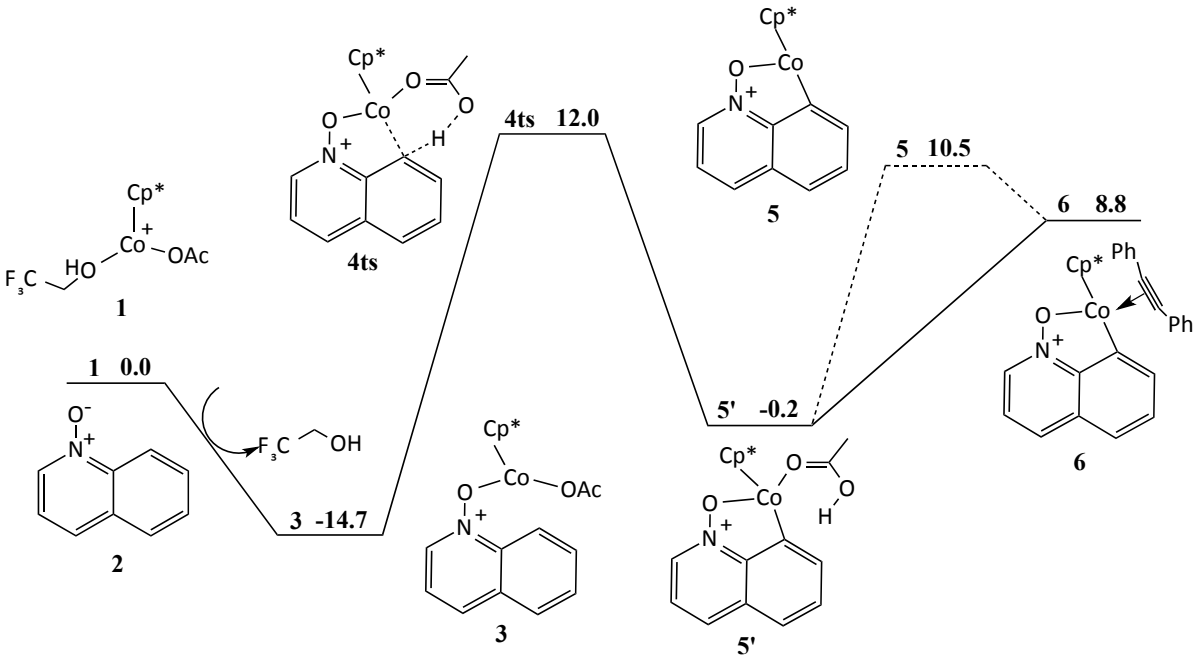


Figure S2. Free energy profiles for the cobalt-catalyzed C-H bond functionalization of quinoline N-oxide. The relative free energies are shown in kcal/mol M11L method in 1,4-dioxane

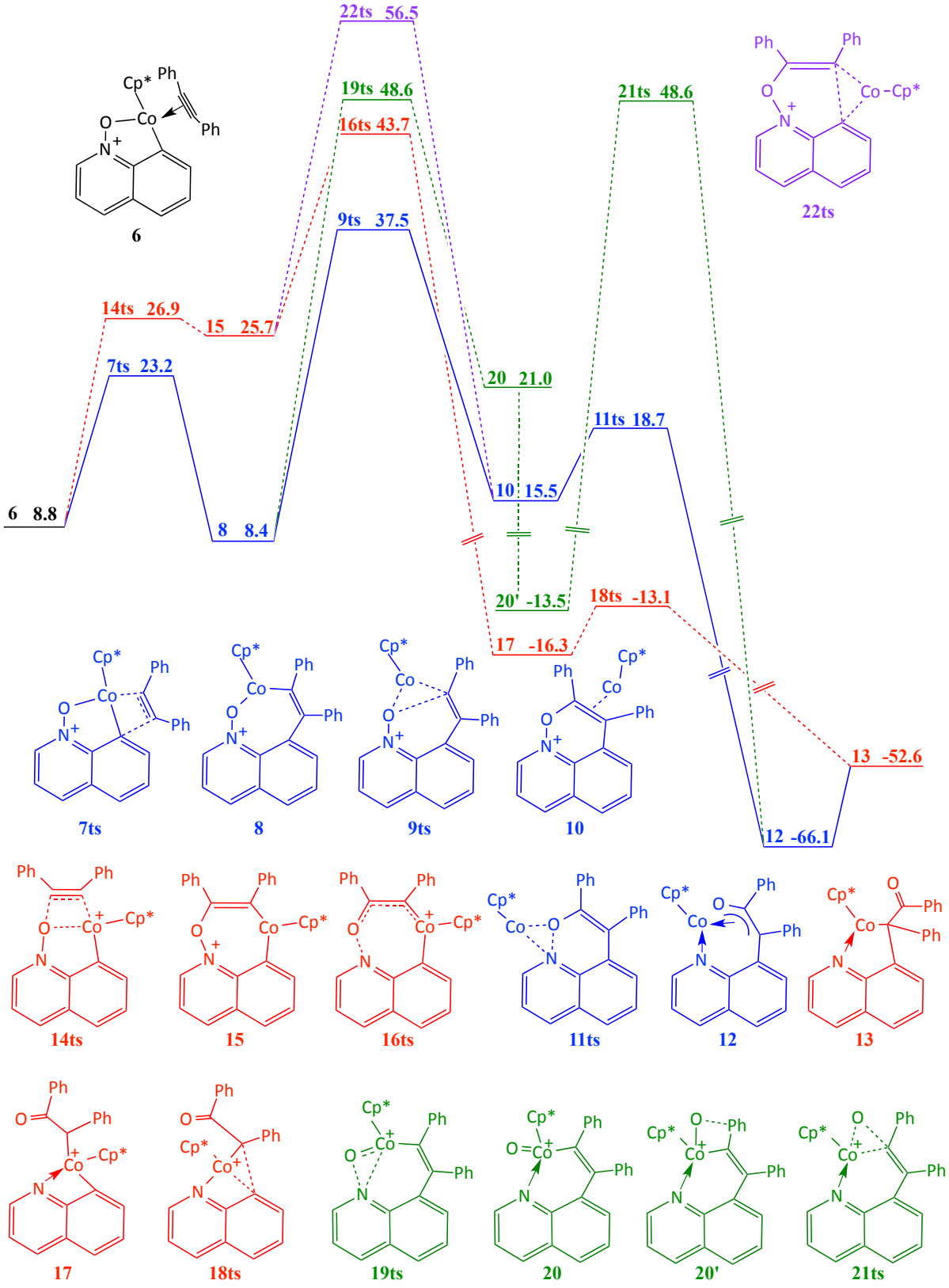


Figure S3. Free energy profiles for the cobalt-catalyzed C-C bond formation and N-O bond cleavage of quinoline N-oxide. The relative free energies are shown in kcal/mol M11L method in 1,4-dioxane.

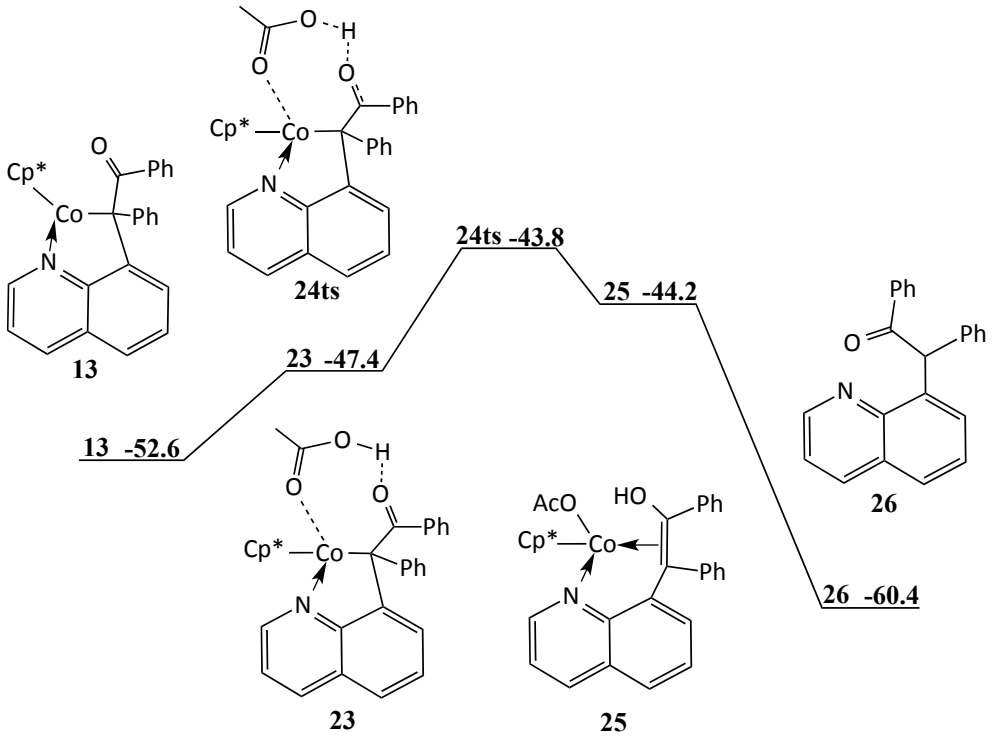
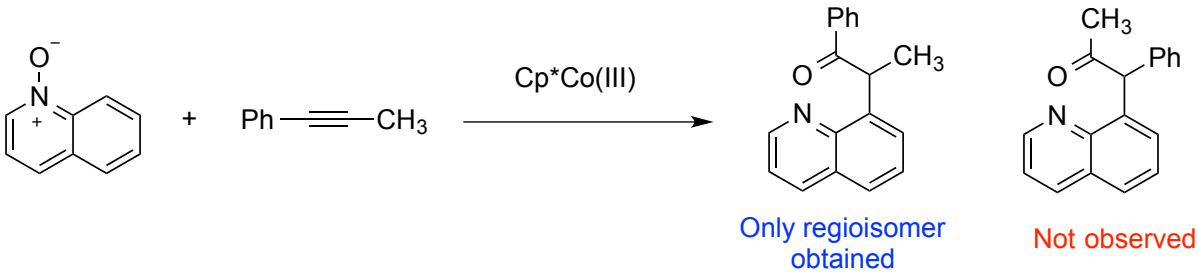


Figure S4. Free energy profiles for the protonation steps in the cobalt-catalyzed C-H bond functionalization of quinoline N-oxide. The relative free energies are shown in kcal/mol M11L method in 1,4-dioxane.

Origin of regioselectivity with unsymmetrical alkyne:



Scheme S1. The cobalt catalysed C-C bond formation of quinoline N-oxide and non-symmetrical alkyne.

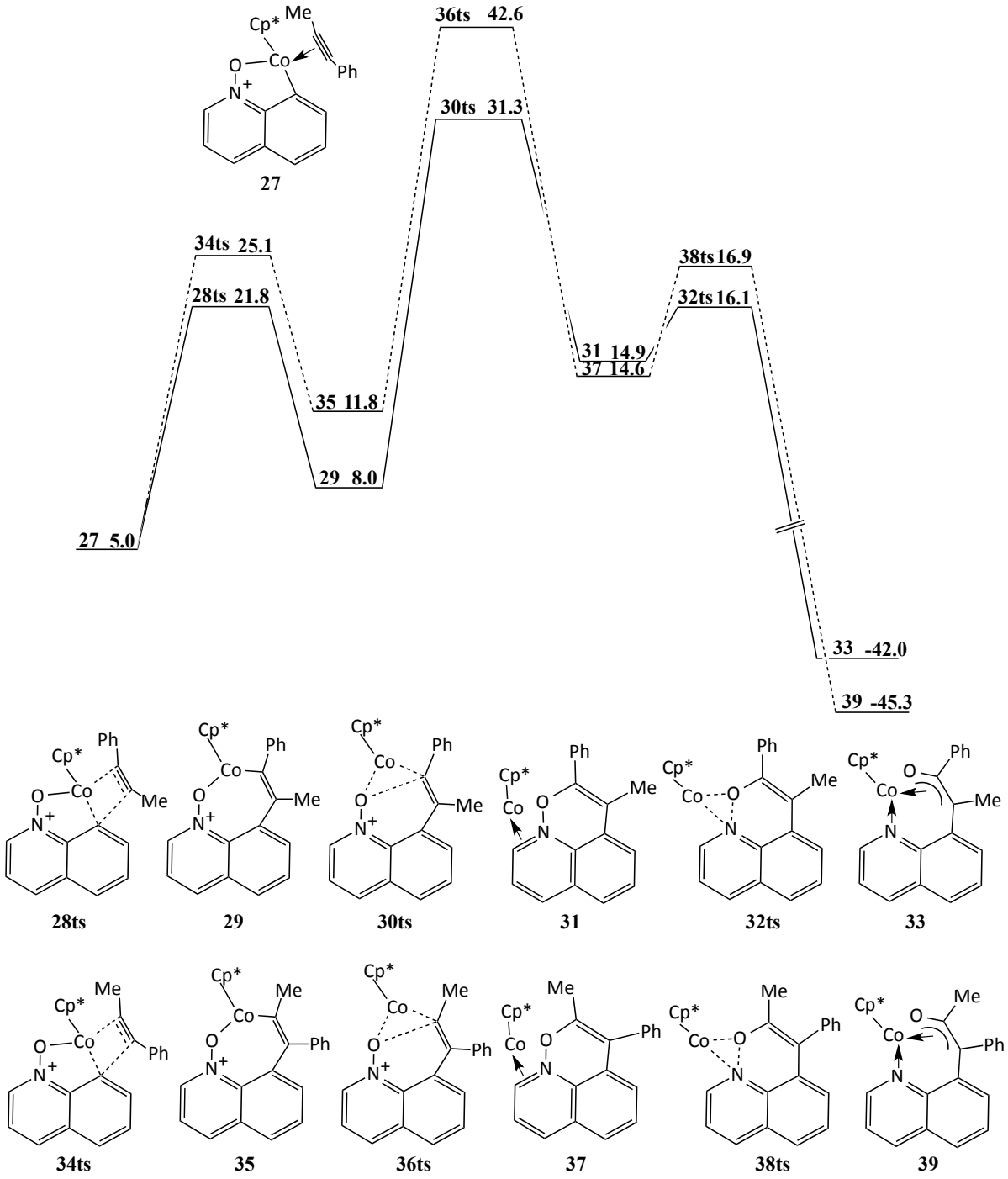


Figure S5. Free energy profiles for the regioselectivity of the cobalt-catalyzed C-H bond functionalization of quinoline N-oxide with prop-1-yn-1ylbenzene. The relative free energies are shown in kcal/mol M11L method in 1,4-dioxane.

B3LYP geometries for all the optimized intermediates and transition states in the study:

1

Ni	0.667224000	0.183881000	-0.059575000
C	1.755386000	-1.021828000	1.284240000
C	0.665826000	-1.754184000	0.746106000
C	2.552334000	-0.540399000	0.181852000
C	0.836494000	-1.817979000	-0.700446000
C	2.014938000	-1.108972000	-1.036688000
C	-0.422825000	-2.444346000	1.503687000
H	-0.182344000	-3.507474000	1.612052000
H	-0.549731000	-2.039133000	2.507621000
H	-1.382447000	-2.386896000	0.988419000
C	2.003273000	-0.687472000	2.717474000
H	1.203838000	-1.037072000	3.368738000
H	2.933431000	-1.158483000	3.051114000
H	2.111986000	0.389513000	2.862080000
C	3.814163000	0.252619000	0.292516000
H	3.807565000	0.909737000	1.162921000
H	4.671642000	-0.420984000	0.399252000
H	3.989185000	0.862240000	-0.594515000
C	2.583675000	-0.882924000	-2.398094000
H	2.796868000	0.173607000	-2.572540000
H	3.528373000	-1.427503000	-2.497970000
H	1.919023000	-1.228789000	-3.188266000
C	-0.082474000	-2.545677000	-1.626357000
H	-1.129857000	-2.367756000	-1.378208000
H	0.071861000	-2.265898000	-2.667946000
H	0.089712000	-3.624430000	-1.547789000
C	0.814051000	2.520123000	-0.060109000
O	0.931893000	1.829592000	-1.129249000
O	0.601418000	1.852228000	1.004945000
C	0.936287000	4.006892000	-0.059497000
H	0.435472000	4.435032000	0.807863000
H	1.995921000	4.275607000	-0.009227000
H	0.535564000	4.424241000	-0.983455000
C	-2.336462000	0.724372000	0.438087000
H	-2.453138000	1.807818000	0.486180000
H	-2.037641000	0.352947000	1.414605000
O	-1.313530000	0.348565000	-0.496844000
H	-1.420712000	0.830799000	-1.328419000
C	-3.652820000	0.087795000	0.020565000
F	-3.570156000	-1.257043000	0.018028000
F	-3.983273000	0.477576000	-1.226856000
F	-4.624231000	0.453565000	0.860513000

2

C	2.020728000	1.432920000	-0.000001000
C	0.727724000	1.896834000	-0.000024000
C	-0.331960000	0.956389000	0.000036000
C	-0.032703000	-0.432537000	0.000018000
C	2.292661000	0.061085000	-0.000048000
H	-1.950897000	2.385475000	0.000069000
H	2.862487000	2.115961000	-0.000132000
H	0.509759000	2.958761000	0.000105000
C	-1.701093000	1.329092000	0.000028000
C	-1.051416000	-1.401070000	-0.000008000
H	3.286710000	-0.362654000	0.000156000
C	-2.366801000	-0.996557000	-0.000043000
C	-2.693057000	0.377752000	0.000009000
H	-3.158392000	-1.738062000	-0.000112000
H	-3.734576000	0.682102000	-0.000013000
O	1.574644000	-2.109886000	0.000055000
N	1.309118000	-0.866198000	-0.000053000
H	-0.760565000	-2.442560000	0.000052000

3

C	-3.003173000	-2.155204000	-1.438524000
C	-4.077419000	-1.524335000	-0.854658000
C	-3.923075000	-0.230370000	-0.307976000
C	-2.646901000	0.400857000	-0.371613000
C	-1.766684000	-1.507015000	-1.490845000
H	-5.964723000	0.007748000	0.358128000
H	-3.088378000	-3.144731000	-1.868923000
H	-5.046523000	-2.009280000	-0.812710000
C	-4.988598000	0.477535000	0.305980000
C	-2.448796000	1.688282000	0.157662000
H	-0.881005000	-1.934697000	-1.935636000
C	-3.510336000	2.337963000	0.744618000
C	-4.786236000	1.734088000	0.819808000
H	-3.365941000	3.330178000	1.157091000
H	-5.605402000	2.269584000	1.285809000
Ni	1.112529000	-0.084987000	0.034021000
O	-0.426851000	0.331404000	-1.120020000
N	-1.602249000	-0.283882000	-0.979771000
C	2.433953000	1.479027000	0.492300000
C	2.984504000	0.191097000	0.872390000
C	2.208002000	1.463660000	-0.905758000
C	3.135293000	-0.587310000	-0.316967000
C	2.588457000	0.158926000	-1.406924000
C	3.422027000	-0.182133000	2.252720000
H	4.433932000	0.191370000	2.443352000
H	2.767083000	0.246216000	3.012233000
H	3.442697000	-1.262510000	2.398389000
C	2.145055000	2.588758000	1.450366000
H	1.603049000	2.227511000	2.326811000
H	3.080912000	3.033138000	1.804786000
H	1.554842000	3.383268000	0.994910000
C	1.624783000	2.547741000	-1.749964000
H	1.403209000	3.445329000	-1.173779000
H	2.327095000	2.827261000	-2.540900000
H	0.701851000	2.213958000	-2.230699000
C	2.534122000	-0.254593000	-2.842891000
H	1.633084000	0.118130000	-3.332381000
H	3.394721000	0.147922000	-3.388247000
H	2.557662000	-1.338687000	-2.957786000
C	3.677019000	-1.975805000	-0.396796000
H	3.602097000	-2.501815000	0.554109000
H	3.162645000	-2.572529000	-1.150635000
H	4.736694000	-1.939599000	-0.673039000
H	-1.468906000	2.136566000	0.096726000
C	-0.077525000	-1.443762000	1.545187000
O	0.481730000	-1.913551000	0.497249000
O	0.014914000	-0.189134000	1.718399000
C	-0.781608000	-2.331365000	2.522211000
H	-1.513912000	-1.765037000	3.096211000
H	-1.256734000	-3.167402000	2.008895000
H	-0.048100000	-2.746052000	3.220120000

4ts

C	3.938410000	0.070885000	-2.040131000
C	4.361559000	-0.070792000	-0.737752000
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C	2.066693000	0.296244000	-0.003496000
C	2.581753000	0.269527000	-2.321834000
H	4.774427000	-0.289368000	1.973270000
H	4.631081000	0.007779000	-2.869644000
H	5.405209000	-0.258942000	-0.512266000
C	3.746246000	-0.087712000	1.692758000
C	1.050554000	0.498516000	0.967773000
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C	2.775072000	0.065168000	2.655188000
H	0.730788000	0.598200000	3.080716000
H	3.038374000	-0.016104000	3.704008000
Ni	-0.757287000	0.018007000	-0.093106000
O	0.394596000	0.476782000	-1.611196000
N	1.690750000	0.350658000	-1.329744000

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C	-2.355749000	-1.027592000	-0.896670000
C	-1.212933000	-1.894102000	-0.953592000
C	-3.818907000	0.001310000	0.993178000
H	-4.731691000	-0.593334000	0.878883000
H	-3.725658000	0.260811000	2.047404000
H	-3.949711000	0.921739000	0.423700000
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H	-0.558957000	-1.596258000	3.133610000
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H	0.937448000	-2.540015000	1.669528000
H	0.063512000	-3.931430000	1.036997000
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H	-1.294826000	-3.197249000	-2.633665000
H	-0.501785000	-1.658149000	-2.962789000
C	-3.186710000	-0.568812000	-2.050223000
H	-3.491018000	0.470873000	-1.924826000
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H	-4.094509000	-1.175963000	-2.135409000
H	0.370382000	1.547189000	0.799817000
C	-1.124376000	2.827055000	0.059067000
O	-1.660724000	1.728858000	-0.309370000
O	-0.030772000	2.883239000	0.671616000
C	-1.851166000	4.108316000	-0.261092000
H	-2.820518000	3.913426000	-0.714794000
H	-1.972150000	4.697223000	0.649794000
H	-1.240322000	4.699139000	-0.947708000

5

C	4.065194000	-1.984457000	-0.049788000
C	4.452656000	-0.659684000	-0.033594000
C	3.474983000	0.361810000	-0.033826000
C	2.108379000	-0.014933000	-0.046395000
C	2.706001000	-2.318363000	-0.071677000
H	4.774780000	2.096232000	-0.019139000
H	4.793087000	-2.785386000	-0.050291000
H	5.505120000	-0.397832000	-0.023586000
C	3.746097000	1.752957000	-0.028806000
C	1.009302000	0.874453000	-0.044754000
H	2.320844000	-3.328525000	-0.094064000
C	1.353125000	2.217993000	-0.043537000
C	2.702446000	2.651342000	-0.039415000
H	0.582289000	2.980615000	-0.045725000
H	2.913703000	3.715363000	-0.041552000
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O	0.480825000	-1.648813000	-0.109654000
N	1.791489000	-1.350006000	-0.071749000
C	-2.080747000	1.230507000	0.492089000
C	-2.258802000	0.857029000	-0.864707000
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C	-2.532501000	-0.577042000	-0.907280000
C	-2.476053000	-1.079670000	0.406461000
C	-2.277495000	1.761075000	-2.054916000
H	-3.310926000	2.007446000	-2.323118000
H	-1.754810000	2.698896000	-1.868242000
H	-1.821135000	1.294449000	-2.929446000
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H	-1.990971000	-2.762044000	1.661348000
H	-3.686034000	-2.656963000	1.194432000
H	-2.480067000	-3.202710000	0.030405000
C	-2.786385000	-1.347456000	-2.161863000
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H	-2.676361000	-2.421285000	-2.016273000
H	-3.807907000	-1.164428000	-2.513041000

5'

C	4.012231000	-0.622836000	-1.932963000
C	4.404434000	-0.488005000	-0.620295000
C	3.430220000	-0.260738000	0.381953000
C	2.066443000	-0.193924000	-0.002770000
C	2.657511000	-0.532074000	-2.280701000
H	4.742524000	-0.116025000	2.099856000
H	4.733379000	-0.793228000	-2.722216000
H	5.452648000	-0.546502000	-0.349119000
C	3.713930000	-0.073284000	1.759053000
C	0.982309000	0.025782000	0.883712000
H	2.277868000	-0.611376000	-3.289794000
C	1.337063000	0.222660000	2.207938000
C	2.689289000	0.175099000	2.640982000
H	0.572917000	0.417375000	2.953456000
H	2.911096000	0.333944000	3.691016000
Ni	-0.705564000	-0.051096000	-0.094973000
O	0.451240000	-0.212213000	-1.659476000
N	1.738818000	-0.324683000	-1.336238000
C	-1.669201000	-1.336558000	1.303878000
C	-2.513864000	-0.245235000	0.975910000
C	-1.325798000	-2.000354000	0.075111000
C	-2.838429000	-0.334312000	-0.444077000
C	-2.137180000	-1.422819000	-0.983483000
C	-3.128057000	0.734641000	1.925006000
H	-4.135829000	0.411379000	2.207696000
H	-2.550843000	0.836974000	2.844756000
H	-3.222423000	1.724771000	1.476404000
C	-1.262221000	-1.773090000	2.673250000
H	-1.302491000	-0.962520000	3.401095000
H	-1.957858000	-2.545807000	3.019246000
H	-0.261612000	-2.203978000	2.695809000
C	-0.488018000	-3.231981000	-0.062471000
H	0.294806000	-3.282074000	0.695525000
H	-1.105821000	-4.130414000	0.045826000
H	-0.011875000	-3.284638000	-1.042644000
C	-2.122825000	-1.893228000	-2.401514000
H	-1.111135000	-1.866471000	-2.812587000
H	-2.477925000	-2.926533000	-2.462002000
H	-2.760644000	-1.286026000	-3.042494000
C	-3.766290000	0.597944000	-1.153039000
H	-3.533935000	1.639092000	-0.923612000
H	-3.720150000	0.478980000	-2.234958000
H	-4.800188000	0.415642000	-0.842015000
H	1.004244000	2.150527000	0.766771000
C	-0.315151000	2.979541000	-0.303351000
O	-0.969032000	1.948723000	-0.456819000
O	0.806548000	3.032589000	0.390356000
C	-0.728353000	4.297353000	-0.878519000
H	-1.600834000	4.177367000	-1.515448000
H	-0.953452000	4.995013000	-0.067871000
H	0.097720000	4.726611000	-1.448889000

6

C	-2.084545000	-3.049752000	-3.081356000
C	-3.231071000	-2.499829000	-2.553631000
C	-3.148434000	-1.642347000	-1.430338000

C	-1.866170000	-1.376287000	-0.876113000
C	-0.837510000	-2.766414000	-2.508719000
H	-5.252941000	-1.191088000	-1.193260000
H	-2.117070000	-3.706667000	-3.941217000
H	-4.198267000	-2.715695000	-2.994103000
C	-4.254579000	-1.014148000	-0.808546000
C	-1.627308000	-0.538868000	0.234455000
H	0.102450000	-3.161498000	-2.867208000
C	-2.746913000	0.057483000	0.778861000
C	-4.046957000	-0.183358000	0.267710000
H	-2.650706000	0.744614000	1.611878000
H	-4.893402000	0.307056000	0.737240000
Ni	0.272643000	-0.485567000	0.654791000
O	0.422922000	-1.686820000	-0.894262000
N	-0.758830000	-1.960783000	-1.449206000
C	0.738168000	0.200124000	2.628719000
C	-0.115576000	-0.933183000	2.726842000
C	1.987800000	-0.230398000	2.023326000
C	0.519997000	-2.012794000	2.033161000
C	1.855100000	-1.583425000	1.662763000
C	0.129817000	1.630135000	-0.412189000
C	1.173748000	1.045535000	-0.705569000
C	2.481031000	0.936538000	-1.309315000
C	2.948269000	-0.233111000	-1.926484000
C	3.293624000	2.086509000	-1.318738000
C	4.199195000	-0.248810000	-2.535778000
H	2.319955000	-1.112587000	-1.929633000
C	4.540864000	2.060545000	-1.930384000
H	2.934289000	2.998132000	-0.854526000
C	4.999412000	0.892284000	-2.538328000
H	4.548948000	-1.156340000	-3.016435000
H	5.154265000	2.955058000	-1.935611000
H	5.972730000	0.874363000	-3.016500000
C	-0.971590000	2.544886000	-0.378242000
C	-1.043398000	3.554778000	0.596547000
C	-1.952152000	2.496851000	-1.385217000
C	-2.071812000	4.490005000	0.563441000
H	-0.280826000	3.615140000	1.362909000
C	-2.973017000	3.437932000	-1.414466000
H	-1.895732000	1.727291000	-2.145968000
C	-3.038642000	4.433260000	-0.439364000
H	-2.112355000	5.271156000	1.314742000
H	-3.716921000	3.399151000	-2.202681000
H	-3.835675000	5.168348000	-0.466451000
C	3.216550000	0.614956000	1.928796000
H	2.989561000	1.645512000	1.653866000
H	3.713047000	0.643165000	2.905239000
H	3.933104000	0.230322000	1.205244000
C	0.523364000	1.525171000	3.290083000
H	0.874915000	1.489178000	4.327418000
H	1.078887000	2.320714000	2.792906000
H	-0.528195000	1.813263000	3.315513000
C	-1.388952000	-1.023798000	3.502432000
H	-1.169256000	-1.443609000	4.490745000
H	-1.849719000	-0.049985000	3.666239000
H	-2.124930000	-1.672415000	3.028517000
C	0.002422000	-3.408599000	1.899636000
H	0.378608000	-4.034591000	2.716434000
H	-1.086866000	-3.447939000	1.934601000
H	0.328893000	-3.866403000	0.964982000
C	2.876091000	-2.462482000	1.015599000
H	3.284259000	-3.168972000	1.746309000
H	2.436540000	-3.047694000	0.205918000
H	3.708537000	-1.892952000	0.604505000

7ts

C	3.092229000	-1.283659000	3.411780000
C	3.979126000	-0.906644000	2.429043000
C	3.497045000	-0.566395000	1.141840000
C	2.095305000	-0.592882000	0.915021000
C	1.727204000	-1.391587000	3.123120000
H	5.400436000	-0.186128000	0.183777000
H	3.428937000	-1.542395000	4.407634000
H	5.044272000	-0.873424000	2.628658000
C	4.325027000	-0.209827000	0.047326000
C	1.486845000	-0.182417000	-0.304284000
H	0.981770000	-1.757729000	3.814690000
C	2.361302000	0.136519000	-1.335674000
C	3.760661000	0.096584000	-1.170186000
H	1.963329000	0.498879000	-2.276685000
H	4.397681000	0.354923000	-2.009152000
Ni	-0.389279000	-0.946217000	-0.321093000
O	-0.003226000	-1.293203000	1.597460000
N	1.271654000	-1.086589000	1.903657000
C	-0.976974000	-1.341287000	-2.301400000
C	-0.077237000	-2.407935000	-1.913935000
C	-2.141739000	-1.409915000	-1.465337000
C	-0.619728000	-3.029196000	-0.773366000
C	-1.893684000	-2.389909000	-0.467522000
C	0.138685000	1.196584000	-0.105593000
C	-1.011376000	0.790155000	0.290137000
C	-2.244665000	1.268922000	0.887888000
C	-2.800603000	0.603976000	1.992640000
C	-2.884968000	2.416159000	0.390353000
C	-3.963992000	1.080917000	2.587144000
H	-2.297521000	-0.270104000	2.388066000
C	-4.054358000	2.880739000	0.983879000
H	-2.461572000	2.944989000	-0.455927000
C	-4.597431000	2.215920000	2.081817000
H	-4.377038000	0.566946000	3.448698000
H	-4.539514000	3.767779000	0.590798000
H	-5.506968000	2.583115000	2.544683000
C	0.810031000	2.459220000	-0.438422000
C	0.398536000	3.192640000	-1.560242000
C	1.812216000	2.984011000	0.390528000
C	0.977822000	4.426514000	-1.846059000
H	-0.375785000	2.793359000	-2.206236000
C	2.377999000	4.221546000	0.108466000
H	2.130648000	2.429489000	1.266236000
C	1.966585000	4.943330000	-1.012488000
H	0.651062000	4.985952000	-2.716012000
H	3.139101000	4.627590000	0.766019000
H	2.413125000	5.907047000	-1.231736000
C	-3.393370000	-0.614062000	-1.652673000
H	-3.193190000	0.392477000	-2.021452000
H	-4.031350000	-1.109890000	-2.392709000
H	-3.968789000	-0.519575000	-0.733070000
C	-0.839367000	-0.490228000	-3.525782000
H	-1.309927000	-0.983030000	-4.383932000
H	-1.323702000	0.480027000	-3.408604000
H	0.203344000	-0.315226000	-3.793612000
C	1.173793000	-2.795476000	-2.635634000
H	0.930513000	-3.461325000	-3.470722000
H	1.695937000	-1.934572000	-3.055013000
H	1.876154000	-3.324719000	-1.991247000
C	-0.043735000	-4.168133000	0.004622000
H	-0.593636000	-5.091393000	-0.206941000
H	1.002822000	-4.349472000	-0.241393000
H	-0.114648000	-3.988402000	1.078837000
C	-2.823762000	-2.838004000	0.614682000
H	-3.324431000	-3.767586000	0.322454000
H	-2.289657000	-3.035705000	1.545856000
H	-3.597185000	-2.099386000	0.822134000

8			
Ni	-1.305467000	-0.191262000	-0.093175000
C	-3.003597000	0.120990000	1.158950000
C	-3.431038000	-0.751977000	0.073714000
C	-1.976583000	-0.532807000	1.891126000
C	-2.636893000	-1.900735000	0.109601000
C	-1.674826000	-1.752744000	1.201420000
C	-3.725528000	1.371435000	1.547695000
H	-4.689693000	1.107049000	1.996651000
H	-3.176261000	1.959274000	2.281473000
H	-3.933455000	2.013856000	0.691451000
C	-4.551531000	-0.443395000	-0.870048000
H	-4.521326000	-1.068404000	-1.763029000
H	-5.518479000	-0.615940000	-0.384507000
H	-4.535974000	0.600005000	-1.191309000
C	-2.752727000	-3.089132000	-0.791849000
H	-3.495994000	-3.790609000	-0.397631000
H	-3.069906000	-2.812652000	-1.798572000
H	-1.814448000	-3.638609000	-0.872896000
C	-0.769584000	-2.831830000	1.708651000
H	-1.307846000	-3.456510000	2.430816000
H	-0.424260000	-3.496061000	0.915986000
H	0.106559000	-2.430567000	2.218767000
C	-1.350164000	-0.060749000	3.165781000
H	-1.320433000	1.027591000	3.228984000
H	-1.926283000	-0.421276000	4.025227000
H	-0.329242000	-0.426175000	3.280003000
O	-0.154085000	-0.935198000	-1.499463000
C	1.758517000	-1.793116000	-0.289752000
C	0.643087000	-2.957376000	-2.066069000
C	2.048934000	-0.616039000	0.472575000
C	2.561910000	-2.972549000	-0.103051000
C	1.470192000	-4.071524000	-1.952502000
H	-0.156661000	-2.875313000	-2.787268000
C	3.052821000	-0.715065000	1.429598000
C	3.550282000	-2.998321000	0.909783000
C	2.402673000	-4.094352000	-0.947930000
H	1.334272000	-4.899089000	-2.636780000
C	3.776848000	-1.890262000	1.682206000
H	3.297215000	0.179150000	1.991083000
H	4.131651000	-3.903784000	1.043331000
H	3.037700000	-4.959931000	-0.796784000
H	4.533173000	-1.900896000	2.458668000
N	0.749928000	-1.889393000	-1.263090000
C	0.164873000	0.960305000	0.185572000
C	1.475709000	0.747428000	0.251538000
C	-0.672264000	2.018949000	-0.342974000
C	-1.152143000	3.131050000	0.392711000
C	-1.180300000	1.808796000	-1.654342000
C	-2.059419000	4.005276000	-0.170265000
H	-0.773566000	3.307364000	1.392638000
C	-2.137541000	2.684943000	-2.190921000
H	-0.732627000	1.050228000	-2.284032000
C	-2.572005000	3.776824000	-1.460215000
H	-2.381778000	4.878582000	0.387209000
H	-2.495993000	2.526010000	-3.202363000
H	-3.285932000	4.472304000	-1.887803000
C	2.471822000	1.851557000	0.076619000
C	2.412824000	3.014678000	0.854193000
C	3.483720000	1.743539000	-0.889433000
C	3.328300000	4.047683000	0.663167000
H	1.659403000	3.100159000	1.629364000
C	4.393073000	2.777555000	-1.084887000
H	3.550802000	0.849867000	-1.502049000
C	4.318259000	3.933954000	-0.309064000
H	3.270992000	4.938490000	1.279928000
H	5.161623000	2.681887000	-1.844758000
H	5.031366000	4.737493000	-0.458334000

9ts			
C	-0.799291000	-4.305025000	-1.631659000
C	-1.965981000	-4.371230000	-0.908817000
C	-2.519575000	-3.212885000	-0.309614000
C	-1.823880000	-1.958200000	-0.446373000
C	-0.142072000	-3.081492000	-1.748595000
H	-4.271921000	-4.175066000	0.489343000
H	-0.371687000	-5.175554000	-2.111967000
H	-2.492846000	-5.313285000	-0.804971000
C	-3.749849000	-3.233359000	0.368681000
C	-2.366131000	-0.731390000	0.057923000
H	0.782888000	-2.928142000	-2.283819000
C	-3.631932000	-0.831744000	0.666300000
C	-4.291331000	-2.047187000	0.832919000
H	-4.104567000	0.075989000	1.017022000
H	-5.254697000	-2.056382000	1.330944000
Ni	1.414239000	-0.138949000	-0.073834000
O	0.054815000	-0.843113000	-1.465540000
N	-0.655319000	-1.987764000	-1.170643000
C	-1.698946000	0.518139000	-0.164771000
C	-0.388533000	0.537431000	-0.591846000
C	0.538877000	1.555215000	-1.031557000
C	1.601957000	1.185034000	-1.911626000
C	0.549958000	2.868450000	-0.465267000
C	2.619417000	2.123940000	-2.209518000
H	1.512539000	0.319435000	-2.554143000
C	1.541961000	3.755732000	-0.796590000
H	-0.248509000	3.167535000	0.199627000
C	2.595931000	3.385203000	-1.664926000
H	3.391374000	1.847576000	-2.919505000
H	1.512106000	4.761203000	-0.390449000
H	3.362362000	4.108343000	-1.921293000
C	-2.437552000	1.809475000	-0.003205000
C	-2.866337000	2.521495000	-1.130984000
C	-2.714323000	2.333457000	1.267409000
C	-3.551506000	3.726249000	-0.992178000
H	-2.663593000	2.125806000	-2.120946000
C	-3.405097000	3.535780000	1.406211000
H	-2.382078000	1.797642000	2.151329000
C	-3.823321000	4.236079000	0.276101000
H	-3.878881000	4.263668000	-1.875909000
H	-3.613260000	3.926731000	2.396711000
H	-4.360020000	5.172516000	0.383533000
C	2.652694000	0.528413000	1.459622000
C	1.588530000	-0.225150000	2.048956000
C	3.453158000	-0.362995000	0.633778000
C	1.631221000	-1.525165000	1.471719000
C	2.817611000	-1.613891000	0.622852000
C	4.738346000	0.007658000	-0.037430000
H	4.702993000	1.012489000	-0.462493000
H	5.563113000	-0.006629000	0.683889000
H	4.997539000	-0.684953000	-0.839489000
C	3.307568000	-2.855833000	-0.059616000
H	3.824727000	-2.637827000	-0.996016000
H	4.017122000	-3.389343000	0.582440000
H	2.498324000	-3.554763000	-0.277574000
C	0.763233000	-2.682717000	1.859931000
H	0.639627000	-3.404434000	1.050739000
H	1.216726000	-3.226213000	2.696425000
H	-0.227909000	-2.364055000	2.184627000
C	0.606873000	0.264480000	3.066976000
H	-0.368836000	-0.212935000	2.958964000
H	0.963993000	0.048102000	4.079963000
H	0.456186000	1.343070000	3.002864000
C	3.047047000	1.927228000	1.815714000
H	2.207304000	2.513687000	2.188072000
H	3.807749000	1.907455000	2.604422000
H	3.474045000	2.462030000	0.966882000

10			
C	-3.567280000	-1.475369000	-2.547703000
C	-4.013531000	-0.297830000	-2.011163000
C	-3.100409000	0.652704000	-1.472316000
C	-1.707586000	0.268275000	-1.323364000
C	-2.183892000	-1.749881000	-2.557676000
H	-4.509838000	2.253342000	-1.291877000
H	-4.239789000	-2.191578000	-3.000709000
H	-5.066965000	-0.042418000	-2.055542000
C	-3.465645000	1.970371000	-1.218753000
C	-0.699238000	1.274121000	-1.013008000
H	-1.741560000	-2.634983000	-2.993868000
C	-1.146532000	2.622596000	-0.922246000
C	-2.484554000	2.947150000	-0.987061000
H	-0.401916000	3.402768000	-0.821700000
H	-2.783152000	3.985810000	-0.898898000
Ni	-0.583498000	-0.096570000	0.536123000
O	-0.020527000	-1.191783000	-2.080686000
N	-1.341290000	-0.902575000	-2.005669000
C	0.644375000	0.800798000	-0.790179000
C	0.714740000	-0.640021000	-0.904850000
C	1.921122000	-1.481930000	-0.717431000
C	2.019675000	-2.750103000	-1.315150000
C	2.991427000	-1.053314000	0.087211000
C	3.141358000	-3.551061000	-1.118939000
H	1.221866000	-3.115519000	-1.947058000
C	4.109158000	-1.857462000	0.280644000
H	2.960156000	-0.083599000	0.562344000
C	4.193033000	-3.112046000	-0.320651000
H	3.190703000	-4.523095000	-1.598179000
H	4.922996000	-1.495468000	0.900236000
H	5.067914000	-3.735251000	-0.171647000
C	1.786392000	1.749444000	-0.681620000
C	2.764241000	1.732990000	-1.686385000
C	1.892903000	2.696074000	0.344436000
C	3.819711000	2.639047000	-1.662265000
H	2.696185000	1.005332000	-2.487823000
C	2.951786000	3.601673000	0.369154000
H	1.147980000	2.718502000	1.131493000
C	3.918017000	3.575131000	-0.634034000
H	4.566679000	2.613816000	-2.448343000
H	3.022491000	4.326258000	1.173573000
H	4.742913000	4.278979000	-0.614673000
C	0.140190000	-0.247675000	2.522648000
C	-0.961913000	0.659724000	2.542271000
C	-0.341097000	-1.532793000	2.053190000
C	-2.096745000	-0.029975000	2.031290000
C	-1.719770000	-1.394996000	1.738388000
C	0.440502000	-2.807839000	2.050245000
H	1.494973000	-2.651711000	1.827671000
H	0.380255000	-3.276905000	3.038980000
H	0.055120000	-3.526226000	1.326155000
C	-2.646196000	-2.494875000	1.313633000
H	-2.123433000	-3.279250000	0.763535000
H	-3.106793000	-2.969628000	2.187204000
H	-3.457275000	-2.130245000	0.681736000
C	-3.481189000	0.534116000	1.966772000
H	-4.138983000	-0.049576000	1.323020000
H	-3.926812000	0.533810000	2.967752000
H	-3.492435000	1.566784000	1.612644000
C	-0.963198000	2.063161000	3.068774000
H	-1.497389000	2.754145000	2.411326000
H	-1.459590000	2.105267000	4.044471000
H	0.047403000	2.447533000	3.210705000
C	1.494691000	0.012603000	3.106610000
H	1.887924000	0.993698000	2.835444000
H	1.437720000	-0.022332000	4.200417000
H	2.223067000	-0.735443000	2.798644000

11ts			
C	-2.772764000	1.455655000	-2.492928000
C	-2.376433000	2.714273000	-2.167875000
C	-1.222596000	2.933083000	-1.336474000
C	-0.481262000	1.809646000	-0.878563000
C	-2.086394000	0.334604000	-1.924448000
H	-1.367188000	5.080607000	-1.218553000
H	-3.583568000	1.273315000	-3.188149000
H	-2.898082000	3.577417000	-2.566902000
C	-0.804138000	4.204254000	-0.917138000
C	0.753253000	1.919446000	-0.183103000
H	-2.063548000	-0.621914000	-2.455250000
C	1.084208000	3.214195000	0.251025000
C	0.310563000	4.323306000	-0.098190000
H	1.976385000	3.361581000	0.844711000
H	0.609456000	5.303296000	0.257797000
Ni	-2.072478000	-0.645882000	-0.193250000
O	0.360200000	-0.604781000	-1.581472000
N	-0.981370000	0.550256000	-1.108966000
C	1.651474000	0.771909000	-0.084598000
C	1.457648000	-0.341443000	-0.880681000
C	2.473401000	-1.395679000	-1.153246000
C	3.772791000	-1.087283000	-1.579551000
C	2.091127000	-2.743175000	-1.053741000
C	4.673573000	-2.104645000	-1.870512000
H	4.074122000	-0.053902000	-1.689386000
C	2.999965000	-3.757973000	-1.330581000
H	1.080581000	-2.989231000	-0.747957000
C	4.293424000	-3.440549000	-1.740658000
H	5.675639000	-1.855122000	-2.201986000
H	2.699066000	-4.795664000	-1.233603000
H	5.002064000	-4.230731000	-1.964253000
C	-2.071289000	-1.946415000	1.491783000
C	-1.934147000	-0.614036000	1.930558000
C	-3.319746000	-2.058630000	0.740138000
C	-3.051772000	0.134686000	1.384984000
C	-3.950994000	-0.796507000	0.727963000
C	-3.833086000	-3.329320000	0.136388000
H	-3.050123000	-3.885517000	-0.384540000
H	-4.222382000	-3.989487000	0.918960000
H	-4.642230000	-3.151299000	-0.571692000
C	-5.280904000	-0.443813000	0.139942000
H	-5.604669000	-1.164680000	-0.610967000
H	-6.044887000	-0.425248000	0.924783000
H	-5.272498000	0.543438000	-0.324803000
C	-3.324990000	1.583290000	1.623834000
H	-3.866074000	2.040287000	0.793907000
H	-3.944636000	1.702436000	2.520360000
H	-2.408358000	2.151155000	1.785375000
C	-0.860254000	-0.046782000	2.802512000
H	-0.503995000	0.920775000	2.446110000
H	-1.244879000	0.101589000	3.817589000
H	0.000077000	-0.710551000	2.874217000
C	-1.146928000	-3.087800000	1.777845000
H	-0.122123000	-2.756851000	1.947373000
H	-1.473078000	-3.620909000	2.677882000
H	-1.134021000	-3.817389000	0.966253000
C	2.911708000	0.897432000	0.716473000
C	3.922228000	1.804834000	0.363973000
C	3.109279000	0.096844000	1.847429000
C	5.087125000	1.907988000	1.119716000
H	3.804671000	2.421041000	-0.522076000
C	4.274031000	0.196684000	2.605142000
H	2.345029000	-0.619509000	2.129952000
C	5.265912000	1.104903000	2.244806000
H	5.859429000	2.610711000	0.824731000
H	4.406758000	-0.436591000	3.476130000
H	6.173852000	1.184330000	2.832922000

12			
Ni	-1.225710000	-0.128163000	0.433027000
C	-1.977238000	-1.993817000	1.037146000
C	-2.774735000	-0.978188000	1.702846000
C	-2.210645000	-1.885916000	-0.364881000
C	-3.412448000	-0.212230000	0.713425000
C	-2.984037000	-0.706443000	-0.584862000
C	-1.245418000	-3.093302000	1.742665000
H	-1.946856000	-3.866565000	2.075000000
H	-0.512695000	-3.574356000	1.095447000
H	-0.723628000	-2.729191000	2.630190000
C	-2.863409000	-0.815612000	3.187885000
H	-3.403663000	0.087099000	3.473902000
H	-3.386766000	-1.666188000	3.636791000
H	-1.872017000	-0.770316000	3.645092000
C	-4.451583000	0.845263000	0.920891000
H	-5.445044000	0.384763000	0.880122000
H	-4.372699000	1.335549000	1.892804000
H	-4.433523000	1.610743000	0.144068000
C	-3.498771000	-0.221444000	-1.906058000
H	-4.478183000	-0.660077000	-2.127220000
H	-3.619499000	0.863261000	-1.925327000
H	-2.830814000	-0.490726000	-2.725159000
C	-1.808342000	-2.874314000	-1.406203000
H	-0.899038000	-3.414161000	-1.148510000
H	-2.610455000	-3.614658000	-1.511016000
H	-1.662940000	-2.417434000	-2.383830000
O	0.195814000	0.089389000	1.788877000
C	-0.070732000	2.104348000	-0.901834000
C	-1.823809000	2.793410000	0.451455000
C	0.814223000	1.050388000	-1.242796000
C	0.085043000	3.413344000	-1.438837000
C	-1.707149000	4.122687000	0.005064000
H	-2.557453000	2.533627000	1.201084000
C	1.784642000	1.314403000	-2.193758000
C	1.090367000	3.628045000	-2.412891000
C	-0.776332000	4.426814000	-0.958411000
H	-2.362520000	4.878980000	0.419409000
C	1.906926000	2.589328000	-2.789747000
H	2.479950000	0.537521000	-2.486781000
H	1.205926000	4.614022000	-2.850105000
H	-0.682949000	5.437330000	-1.342862000
H	2.676490000	2.748868000	-3.536975000
N	-1.067421000	1.807934000	-0.008402000
C	1.154538000	0.037351000	0.984858000
C	0.667252000	-0.222777000	-0.439117000
C	2.522391000	0.274610000	1.452078000
C	3.632527000	0.138540000	0.601360000
C	2.724453000	0.640786000	2.797220000
C	4.913893000	0.366059000	1.085291000
H	3.495100000	-0.162795000	-0.427872000
C	4.006090000	0.868336000	3.273695000
H	1.867090000	0.745610000	3.450800000
C	5.101978000	0.731529000	2.418398000
H	5.767965000	0.254949000	0.426810000
H	4.156970000	1.152465000	4.309104000
H	6.104467000	0.908813000	2.792996000
C	1.146648000	-1.489529000	-1.069945000
C	1.028407000	-1.698473000	-2.456532000
C	1.715515000	-2.528083000	-0.309608000
C	1.478417000	-2.871675000	-3.053811000
H	0.573287000	-0.935503000	-3.077809000
C	2.158789000	-3.705255000	-0.906213000
H	1.827716000	-2.420299000	0.763989000
C	2.049614000	-3.882765000	-2.283819000
H	1.377795000	-2.996975000	-4.126968000
H	2.600706000	-4.481938000	-0.290774000
H	2.404516000	-4.795182000	-2.750042000

13			
C	-3.086199000	2.190396000	2.166402000
C	-2.789323000	3.277432000	1.379349000
C	-1.707884000	3.216493000	0.466751000
C	-0.962502000	2.006500000	0.378072000
C	-1.280458000	0.892092000	1.180154000
C	-2.331568000	1.000806000	2.069238000
H	-1.860248000	5.229378000	-0.323303000
H	-3.908646000	2.239007000	2.871143000
H	-3.370315000	4.190589000	1.452175000
C	-1.312366000	4.293350000	-0.359150000
H	-2.591142000	0.158347000	2.701080000
C	0.463999000	2.916318000	-1.204176000
C	-0.227330000	4.142121000	-1.187805000
H	1.335787000	2.804698000	-1.829952000
H	0.116288000	4.948224000	-1.824467000
Ni	1.037273000	0.076306000	-0.337307000
C	-0.433068000	-0.343466000	1.039936000
N	0.115441000	1.870823000	-0.466827000
C	-1.183709000	-1.624616000	0.817920000
O	-0.731551000	-2.713392000	1.155827000
C	-2.533991000	-1.607315000	0.151553000
C	-2.924249000	-0.682885000	-0.826916000
C	-3.418575000	-2.640435000	0.493618000
C	-4.167417000	-0.787263000	-1.443095000
H	-2.252273000	0.111517000	-1.126801000
C	-4.670966000	-2.729220000	-0.103564000
H	-3.107620000	-3.370558000	1.231150000
C	-5.048047000	-1.803973000	-1.075528000
H	-4.452061000	-0.073377000	-2.208981000
H	-5.350396000	-3.524364000	0.183693000
H	-6.021893000	-1.876410000	-1.547917000
C	0.819356000	-0.325494000	1.841094000
C	1.569553000	0.887889000	1.907154000
C	1.363932000	-1.447814000	2.536594000
C	2.800894000	0.951727000	2.583406000
H	1.136910000	1.825286000	1.599417000
C	2.550798000	-1.349440000	3.228553000
H	0.805747000	-2.369318000	2.547784000
C	3.296601000	-0.155120000	3.239152000
H	3.326020000	1.899726000	2.629723000
H	2.907725000	-2.208359000	3.787530000
H	4.227165000	-0.097765000	3.793374000
C	1.999487000	-1.775423000	-0.877525000
C	0.938035000	-1.529709000	-1.799768000
C	2.954198000	-0.701707000	-1.000354000
C	1.177028000	-0.256895000	-2.406913000
C	2.459359000	0.233820000	-1.937393000
C	0.356783000	0.330919000	-3.511790000
H	0.442445000	1.415577000	-3.574286000
H	0.691364000	-0.072891000	-4.474012000
H	-0.700650000	0.085360000	-3.409944000
C	-0.131487000	-2.502968000	-2.173280000
H	-1.029483000	-2.018966000	-2.554946000
H	0.249750000	-3.154999000	-2.968479000
H	-0.417138000	-3.145334000	-1.341126000
C	2.222115000	-3.061967000	-0.147196000
H	1.297883000	-3.461356000	0.267642000
H	2.624892000	-3.805484000	-0.844686000
H	2.940210000	-2.954536000	0.664431000
C	4.276072000	-0.637095000	-0.309216000
H	4.218157000	-0.973951000	0.726423000
H	4.989318000	-1.293327000	-0.821367000
H	4.693880000	0.369767000	-0.313742000
C	3.243015000	1.391621000	-2.486077000
H	2.680481000	1.960026000	-3.227347000
H	3.587431000	2.082121000	-1.712322000
H	4.135872000	1.020420000	-2.998617000

14ts			
C	-3.035571000	-3.351443000	0.275190000
C	-2.417302000	-3.644219000	1.472220000
C	-1.207719000	-3.005534000	1.831611000
C	-0.635638000	-2.069665000	0.920873000
C	-2.467866000	-2.407064000	-0.586202000
H	-0.914988000	-3.929013000	3.768478000
H	-3.960907000	-3.830229000	-0.017587000
H	-2.858282000	-4.367275000	2.150311000
C	-0.516029000	-3.225470000	3.046384000
C	0.578039000	-1.372417000	1.127933000
H	-2.892464000	-2.106601000	-1.533132000
C	1.184280000	-1.625770000	2.346800000
C	0.647948000	-2.535344000	3.292193000
H	2.108497000	-1.119916000	2.607480000
H	1.174681000	-2.691619000	4.228031000
Ni	1.054056000	-0.336067000	-0.434132000
O	-0.799206000	-0.865228000	-1.072861000
N	-1.321524000	-1.818121000	-0.250101000
C	3.102609000	0.057742000	-0.364687000
C	2.935903000	-1.323824000	-0.755477000
C	2.555118000	0.880038000	-1.417159000
C	2.181749000	-1.342392000	-1.951923000
C	1.939326000	0.026909000	-2.360620000
C	-0.089134000	1.166889000	0.169055000
C	-1.234281000	0.857259000	-0.336650000
C	-2.636703000	1.010824000	-0.575321000
C	-3.144371000	1.184628000	-1.878590000
C	-3.522039000	1.042519000	0.519481000
C	-4.502846000	1.384275000	-2.075859000
H	-2.463121000	1.164027000	-2.721652000
C	-4.879087000	1.266085000	0.313200000
H	-3.131869000	0.916308000	1.522900000
C	-5.370296000	1.430114000	-0.980811000
H	-4.889393000	1.520709000	-3.079864000
H	-5.553698000	1.308572000	1.161083000
H	-6.429837000	1.599710000	-1.139311000
C	0.230683000	2.409510000	0.894847000
C	-0.192935000	3.659757000	0.417321000
C	0.952787000	2.354619000	2.095655000
C	0.102400000	4.822162000	1.122877000
H	-0.746707000	3.719187000	-0.513555000
C	1.230557000	3.518541000	2.806737000
H	1.275002000	1.393275000	2.477391000
C	0.811723000	4.756120000	2.320875000
H	-0.226616000	5.781590000	0.737840000
H	1.778652000	3.459124000	3.741233000
H	1.036721000	5.662813000	2.871811000
C	3.954569000	0.553849000	0.762951000
H	4.987536000	0.697469000	0.426172000
H	3.603615000	1.510835000	1.150294000
H	3.989041000	-0.151426000	1.594770000
C	3.513621000	-2.507726000	-0.047398000
H	4.536367000	-2.686076000	-0.397021000
H	3.562924000	-2.360882000	1.031553000
H	2.942431000	-3.418444000	-0.229635000
C	1.726814000	-2.545653000	-2.716661000
H	2.330757000	-2.677583000	-3.620688000
H	1.812617000	-3.462413000	-2.132763000
H	0.687331000	-2.447153000	-3.038789000
C	1.229647000	0.429840000	-3.616572000
H	1.887293000	0.317952000	-4.485349000
H	0.348391000	-0.188766000	-3.800342000
H	0.907036000	1.471282000	-3.587995000
C	2.665843000	2.368986000	-1.495882000
H	1.854792000	2.817460000	-2.070340000
H	2.673444000	2.836273000	-0.511817000
H	3.604742000	2.638416000	-1.992689000

15			
C	-1.860355000	-4.155058000	0.066034000
C	-1.189781000	-4.295331000	1.265206000
C	-0.248181000	-3.332102000	1.690025000
C	0.017364000	-2.212689000	0.841222000
C	-1.621567000	-3.029339000	-0.724326000
H	0.289730000	-4.234558000	3.583160000
H	-2.582424000	-4.886267000	-0.272447000
H	-1.385619000	-5.155774000	1.896685000
C	0.461887000	-3.401155000	2.911554000
C	0.970094000	-1.199026000	1.106201000
H	-2.125508000	-2.814308000	-1.654882000
C	1.600812000	-1.327447000	2.334702000
C	1.352540000	-2.401686000	3.224325000
H	2.323093000	-0.580354000	2.646532000
H	1.887945000	-2.437174000	4.167392000
Ni	1.201116000	0.013115000	-0.382227000
O	-0.546360000	-0.973316000	-1.087984000
N	-0.727387000	-2.134152000	-0.315317000
C	2.980388000	1.041102000	-0.154090000
C	3.324464000	-0.287803000	-0.619251000
C	2.252625000	1.704553000	-1.211721000
C	2.689253000	-0.480231000	-1.862072000
C	2.013676000	0.754652000	-2.227202000
C	-0.417022000	0.960933000	0.141952000
C	-1.317835000	0.188665000	-0.454196000
C	-2.767166000	0.105706000	-0.642935000
C	-3.319027000	-0.179593000	-1.903960000
C	-3.630777000	0.340695000	0.438118000
C	-4.698375000	-0.232046000	-2.074659000
H	-2.663046000	-0.337828000	-2.754097000
C	-5.009938000	0.299507000	0.258429000
H	-3.215370000	0.562147000	1.414590000
C	-5.547335000	0.009307000	-0.994449000
H	-5.112658000	-0.444341000	-3.054580000
H	-5.666668000	0.488023000	1.100846000
H	-6.622784000	-0.023908000	-1.130775000
C	-0.673044000	2.222460000	0.840287000
C	-1.483138000	3.224407000	0.278975000
C	-0.094961000	2.456956000	2.098697000
C	-1.708945000	4.417459000	0.958099000
H	-1.930478000	3.066573000	-0.696410000
C	-0.338073000	3.643922000	2.783183000
H	0.530195000	1.691695000	2.544821000
C	-1.141448000	4.630684000	2.213523000
H	-2.332272000	5.182191000	0.506688000
H	0.103855000	3.801555000	3.761584000
H	-1.322199000	5.559800000	2.743115000
C	3.547576000	1.720151000	1.053536000
H	4.495270000	2.210149000	0.801867000
H	2.879621000	2.489596000	1.441709000
H	3.760723000	1.019064000	1.861793000
C	4.233171000	-1.248123000	0.080265000
H	5.274679000	-1.030054000	-0.180049000
H	4.154477000	-1.179379000	1.165446000
H	4.037457000	-2.283768000	-0.199651000
C	2.723577000	-1.712237000	-2.712827000
H	3.434382000	-1.590043000	-3.537169000
H	3.030183000	-2.593638000	-2.148770000
H	1.750972000	-1.923412000	-3.163527000
C	1.273746000	0.974512000	-3.510935000
H	1.972739000	1.184100000	-4.327828000
H	0.695260000	0.095623000	-3.803786000
H	0.585863000	1.818192000	-3.447990000
C	1.866987000	3.149080000	-1.217998000
H	1.025516000	3.351584000	-1.880502000
H	1.599983000	3.509611000	-0.225084000
H	2.712377000	3.751095000	-1.569706000

16ts			
C	2.401048000	4.148828000	-0.236290000
C	1.773797000	4.322915000	0.974549000
C	0.772269000	3.423481000	1.413137000
C	0.396805000	2.323614000	0.562374000
C	2.057045000	3.023622000	-1.003211000
H	0.369263000	4.430135000	3.283370000
H	3.168094000	4.825546000	-0.591127000
H	2.042108000	5.158170000	1.613543000
C	0.099422000	3.595389000	2.645246000
C	-0.667808000	1.435468000	0.900284000
H	2.556367000	2.760604000	-1.928011000
C	-1.278182000	1.681036000	2.126444000
C	-0.898843000	2.723927000	3.000907000
H	-2.110391000	1.054952000	2.440451000
H	-1.422160000	2.848658000	3.943086000
Ni	-1.399332000	-0.078944000	-0.069875000
O	1.075799000	0.709863000	-1.508662000
N	1.107798000	2.211981000	-0.601313000
C	-2.860151000	-1.418154000	-0.919690000
C	-3.552807000	-0.340850000	-0.217209000
C	-2.086616000	-0.842051000	-1.943208000
C	-3.189271000	0.886168000	-0.794789000
C	-2.203744000	0.599522000	-1.819532000
C	0.328866000	-0.890219000	-0.063723000
C	1.395500000	-0.311401000	-0.723051000
C	2.843378000	-0.618834000	-0.580634000
C	3.410437000	-0.950709000	0.658200000
C	3.682355000	-0.527817000	-1.702633000
C	4.776664000	-1.192429000	0.769261000
H	2.783702000	-1.010038000	1.540656000
C	5.046186000	-0.775784000	-1.591005000
H	3.255970000	-0.272382000	-2.666976000
C	5.597188000	-1.109265000	-0.353937000
H	5.201833000	-1.441318000	1.735751000
H	5.679745000	-0.714508000	-2.469586000
H	6.660969000	-1.302605000	-0.266454000
C	0.380575000	-2.141199000	0.687609000
C	1.016400000	-3.290243000	0.174090000
C	-0.286688000	-2.244951000	1.925685000
C	0.973342000	-4.491913000	0.869690000
H	1.533907000	-3.234218000	-0.776532000
C	-0.299186000	-3.442100000	2.632256000
H	-0.749803000	-1.362787000	2.359089000
C	0.322519000	-4.572083000	2.101770000
H	1.459954000	-5.368588000	0.455779000
H	-0.791624000	-3.494869000	3.597382000
H	0.305185000	-5.509137000	2.647428000
C	-1.290563000	-1.560125000	-2.985403000
H	-1.901792000	-1.709519000	-3.882375000
H	-0.407345000	-0.995417000	-3.283043000
H	-0.964447000	-2.544275000	-2.647525000
C	-3.050400000	-2.877460000	-0.643446000
H	-3.958985000	-3.242367000	-1.135342000
H	-2.216777000	-3.475737000	-1.011158000
H	-3.157359000	-3.085155000	0.422764000
C	-4.494030000	-0.559290000	0.925429000
H	-5.438462000	-0.978056000	0.561003000
H	-4.098067000	-1.272632000	1.652973000
H	-4.731331000	0.365961000	1.450327000
C	-3.722208000	2.243849000	-0.458058000
H	-4.558958000	2.495553000	-1.118380000
H	-4.089256000	2.302620000	0.567197000
H	-2.966805000	3.020621000	-0.579901000
C	-1.643652000	1.602017000	-2.773349000
H	-2.339066000	1.738886000	-3.610406000
H	-1.505406000	2.576827000	-2.304749000
H	-0.685985000	1.286042000	-3.180731000

17			
C	-2.277399000	-3.336750000	-0.703025000
C	-2.393153000	-3.470323000	0.665655000
C	-1.567854000	-2.692933000	1.515878000
C	-0.666890000	-1.822826000	0.867218000
C	-1.341824000	-2.431909000	-1.257581000
H	-2.198164000	-3.316527000	3.503347000
H	-2.901617000	-3.917687000	-1.371412000
H	-3.113181000	-4.164424000	1.088240000
C	-1.533689000	-2.673567000	2.935767000
C	0.246905000	-0.970060000	1.508389000
H	-1.250263000	-2.308561000	-2.331629000
C	0.245621000	-0.972739000	2.881867000
C	-0.651796000	-1.834673000	3.583300000
H	0.914375000	-0.347025000	3.466812000
H	-0.631227000	-1.827245000	4.668591000
Ni	1.029517000	-0.382860000	-0.207758000
O	-0.750388000	1.202965000	-2.457032000
N	-0.559364000	-1.701953000	-0.486649000
C	2.661366000	0.470602000	-1.327133000
C	3.060078000	0.190004000	0.028154000
C	2.242568000	-0.753820000	-1.917592000
C	2.998066000	-1.240276000	0.221118000
C	2.480786000	-1.817028000	-0.958819000
C	-0.024609000	1.145323000	-0.278640000
C	-1.125813000	1.071272000	-1.298199000
C	-2.543891000	0.908111000	-0.914603000
C	-2.947253000	0.849042000	0.426952000
C	-3.507261000	0.842404000	-1.933741000
C	-4.296163000	0.726249000	0.743381000
H	-2.214166000	0.902824000	1.224082000
C	-4.851766000	0.721213000	-1.613064000
H	-3.182280000	0.897271000	-2.966365000
C	-5.247113000	0.663631000	-0.274282000
H	-4.606782000	0.685458000	1.781514000
H	-5.595365000	0.676452000	-2.401168000
H	-6.299214000	0.574013000	-0.025283000
C	0.153312000	2.423829000	0.349200000
C	-0.412823000	3.608443000	-0.196428000
C	0.857955000	2.525747000	1.573629000
C	-0.248792000	4.827332000	0.438492000
H	-0.945823000	3.566679000	-1.138514000
C	0.979534000	3.741514000	2.225465000
H	1.255033000	1.622997000	2.014124000
C	0.438133000	4.895675000	1.653903000
H	-0.665323000	5.726467000	-0.001085000
H	1.496008000	3.798897000	3.177146000
H	0.544826000	5.849439000	2.159556000
C	1.780675000	-0.925739000	-3.331263000
H	2.641300000	-0.975952000	-4.007583000
H	1.216348000	-1.849161000	-3.467604000
H	1.150199000	-0.096975000	-3.653054000
C	2.745860000	1.792609000	-2.022656000
H	3.711789000	1.877005000	-2.533034000
H	1.962828000	1.906045000	-2.772060000
H	2.674259000	2.630297000	-1.328207000
C	3.767890000	1.138149000	0.946760000
H	4.849172000	1.070486000	0.780270000
H	3.481892000	2.175575000	0.778622000
H	3.595763000	0.905451000	1.999131000
C	3.480991000	-1.972414000	1.433184000
H	4.563807000	-2.127318000	1.365827000
H	3.289106000	-1.420476000	2.353655000
H	3.017947000	-2.954019000	1.533452000
C	2.275247000	-3.279315000	-1.204931000
H	3.203470000	-3.735340000	-1.565855000
H	1.984033000	-3.811320000	-0.297955000
H	1.511548000	-3.466824000	-1.959411000

18ts			
C	-2.029778000	-3.591935000	-0.430000000
C	-2.444597000	-3.328815000	0.858555000
C	-1.857819000	-2.254125000	1.571972000
C	-0.871155000	-1.521147000	0.881648000
C	-1.010987000	-2.811744000	-1.025041000
H	-2.900559000	-2.336564000	3.477924000
H	-2.470222000	-4.400608000	-1.000728000
H	-3.215218000	-3.936715000	1.322104000
C	-2.146079000	-1.820994000	2.893035000
C	-0.174471000	-0.416310000	1.407840000
H	-0.668976000	-3.016240000	-2.033607000
C	-0.490505000	-0.019336000	2.688155000
C	-1.471421000	-0.740852000	3.424735000
H	-0.025386000	0.841167000	3.157784000
H	-1.699810000	-0.419720000	4.435761000
Ni	1.127868000	-0.464729000	-0.146092000
O	-0.704636000	0.759615000	-2.487421000
N	-0.442939000	-1.812139000	-0.377486000
C	3.143725000	0.035486000	0.360894000
C	2.975862000	-1.380036000	0.608742000
C	2.915371000	0.278192000	-1.033336000
C	2.610943000	-1.988979000	-0.605779000
C	2.510419000	-0.955243000	-1.625236000
C	-0.002023000	0.990942000	-0.321518000
C	-1.112819000	0.780195000	-1.335603000
C	-2.554818000	0.698935000	-1.005751000
C	-3.066586000	1.057866000	0.249265000
C	-3.438250000	0.306798000	-2.024940000
C	-4.437975000	1.022922000	0.479537000
H	-2.400419000	1.380086000	1.039389000
C	-4.804467000	0.261205000	-1.786986000
H	-3.034459000	0.050318000	-2.997361000
C	-5.306247000	0.621083000	-0.534237000
H	-4.830482000	1.314864000	1.447427000
H	-5.482229000	-0.045000000	-2.576295000
H	-6.375331000	0.594275000	-0.351622000
C	0.194891000	2.371984000	0.088544000
C	-0.383681000	3.437152000	-0.644924000
C	0.972785000	2.701826000	1.219252000
C	-0.166595000	4.756971000	-0.275125000
H	-0.974533000	3.232447000	-1.528866000
C	1.157254000	4.019927000	1.605490000
H	1.404466000	1.904112000	1.804514000
C	0.595211000	5.054611000	0.854368000
H	-0.602311000	5.556444000	-0.863834000
H	1.740656000	4.247164000	2.491237000
H	0.746722000	6.086569000	1.151572000
C	3.104548000	1.575794000	-1.752675000
H	4.134577000	1.651563000	-2.118393000
H	2.442155000	1.660100000	-2.614323000
H	2.924692000	2.435784000	-1.106506000
C	3.784064000	0.979413000	1.332289000
H	4.858670000	0.768958000	1.379462000
H	3.675007000	2.021911000	1.038419000
H	3.398899000	0.864209000	2.347627000
C	3.228456000	-2.061012000	1.918641000
H	4.301817000	-2.228125000	2.062527000
H	2.878735000	-1.465171000	2.763394000
H	2.740287000	-3.034450000	1.975271000
C	2.406959000	-3.455466000	-0.825488000
H	3.373180000	-3.939594000	-1.004093000
H	1.954244000	-3.946712000	0.037240000
H	1.785262000	-3.662590000	-1.696079000
C	2.205220000	-1.164597000	-3.076563000
H	3.130947000	-1.239362000	-3.657747000
H	1.645319000	-2.084835000	-3.248741000
H	1.616900000	-0.342839000	-3.485763000

19ts			
Ni	1.147711000	-0.596510000	-0.160533000
C	1.605139000	-2.573725000	0.453780000
C	2.871055000	-2.092552000	-0.085941000
C	1.279462000	-1.783472000	1.611212000
C	3.271806000	-0.998736000	0.678829000
C	2.226383000	-0.736606000	1.675487000
C	0.962065000	-3.854775000	0.038635000
H	1.495540000	-4.689347000	0.511614000
H	-0.082112000	-3.918210000	0.336952000
H	1.014331000	-4.008607000	-1.039455000
C	3.571757000	-2.712565000	-1.253963000
H	4.483135000	-2.176355000	-1.518979000
H	3.854567000	-3.746550000	-1.034044000
H	2.930524000	-2.734615000	-2.139014000
C	4.585557000	-0.280868000	0.629512000
H	5.254611000	-0.708077000	1.385266000
H	5.088985000	-0.384241000	-0.332306000
H	4.497316000	0.782142000	0.857388000
C	2.300778000	0.308686000	2.744171000
H	2.906379000	-0.050592000	3.584181000
H	2.760129000	1.233553000	2.391698000
H	1.314061000	0.554220000	3.137604000
C	0.235340000	-2.080252000	2.639736000
H	-0.521483000	-2.767545000	2.269194000
H	0.708176000	-2.549743000	3.509127000
H	-0.268951000	-1.178688000	2.990780000
O	1.015397000	-0.102156000	-1.844266000
C	0.744070000	2.345616000	-0.362932000
C	2.761384000	1.497580000	-1.305509000
C	-0.577069000	2.161529000	0.144364000
C	1.309008000	3.666756000	-0.443333000
C	3.332100000	2.759252000	-1.411221000
H	3.260211000	0.612382000	-1.663124000
C	-1.240552000	3.315800000	0.576962000
C	0.579669000	4.781082000	0.028075000
C	2.601007000	3.843253000	-0.979588000
H	4.319854000	2.862925000	-1.841729000
C	-0.680148000	4.598609000	0.540136000
H	-2.248875000	3.210542000	0.952924000
H	1.034936000	5.764244000	-0.016480000
H	3.003706000	4.847740000	-1.056233000
H	-1.254356000	5.441267000	0.907706000
N	1.539274000	1.295686000	-0.781202000
C	-0.753714000	-0.334819000	-0.037197000
C	-1.314233000	0.882664000	0.115396000
C	-1.533697000	-1.555005000	-0.342493000
C	-2.441373000	-2.134072000	0.560573000
C	-1.411682000	-2.129240000	-1.620216000
C	-3.195798000	-3.246051000	0.198100000
H	-2.578692000	-1.694173000	1.540080000
C	-2.185860000	-3.224211000	-1.988786000
H	-0.717290000	-1.693276000	-2.330262000
C	-3.072998000	-3.795284000	-1.077479000
H	-3.895702000	-3.673258000	0.908667000
H	-2.092542000	-3.635812000	-2.988399000
H	-3.667931000	-4.657092000	-1.360144000
C	-2.818968000	1.007745000	0.141911000
C	-3.528691000	0.986068000	1.347611000
C	-3.525941000	1.169246000	-1.054002000
C	-4.916206000	1.118988000	1.358265000
H	-2.992319000	0.867363000	2.284767000
C	-4.913243000	1.296107000	-1.044675000
H	-2.987357000	1.185596000	-1.995955000
C	-5.611703000	1.272227000	0.160866000
H	-5.452770000	1.099720000	2.301224000
H	-5.448766000	1.412257000	-1.981064000
H	-6.691837000	1.371596000	0.167251000

20			
Ni	1.203313000	-0.745699000	-0.318213000
C	1.274752000	-2.503233000	1.066752000
C	2.520766000	-2.349315000	0.420251000
C	1.031902000	-1.315895000	1.881595000
C	3.014329000	-1.033952000	0.740692000
C	2.099697000	-0.423570000	1.685234000
C	0.456864000	-3.752067000	1.049451000
H	0.867140000	-4.465366000	1.774391000
H	-0.583878000	-3.576510000	1.312357000
H	0.479818000	-4.229781000	0.069864000
C	3.155889000	-3.343399000	-0.493134000
H	4.223197000	-3.157268000	-0.616409000
H	3.036285000	-4.358379000	-0.109146000
H	2.682895000	-3.291794000	-1.479679000
C	4.357004000	-0.500441000	0.366707000
H	5.094361000	-0.833457000	1.107096000
H	4.690451000	-0.861193000	-0.606344000
H	4.386080000	0.588841000	0.358649000
C	2.330531000	0.863342000	2.413064000
H	2.894973000	0.674701000	3.333101000
H	2.908906000	1.575117000	1.823648000
H	1.396484000	1.348113000	2.696604000
C	-0.060176000	-1.166325000	2.886510000
H	-0.935373000	-1.761386000	2.633359000
H	0.296876000	-1.512969000	3.863152000
H	-0.370743000	-0.127867000	3.004009000
O	1.367888000	-1.314919000	-1.859688000
C	0.949067000	2.191199000	-0.399930000
C	2.545888000	1.230581000	-1.809956000
C	-0.309693000	2.086899000	0.268656000
C	1.567321000	3.472095000	-0.557002000
C	3.134055000	2.471734000	-2.091540000
H	2.903397000	0.319946000	-2.269695000
C	-0.794215000	3.229622000	0.891602000
C	1.033570000	4.595615000	0.121245000
C	2.679176000	3.580690000	-1.422099000
H	3.953047000	2.523532000	-2.798113000
C	-0.109489000	4.460203000	0.865327000
H	-1.759158000	3.190942000	1.379347000
H	1.529264000	5.555441000	0.023330000
H	3.147442000	4.549294000	-1.564510000
H	-0.529789000	5.312075000	1.387620000
N	1.534732000	1.088832000	-0.958855000
C	-0.748512000	-0.349254000	-0.190383000
C	-1.171197000	0.891636000	0.097043000
C	-1.567981000	-1.533561000	-0.492998000
C	-2.597874000	-1.941784000	0.380912000
C	-1.395797000	-2.253006000	-1.688580000
C	-3.431942000	-3.004258000	0.054792000
H	-2.770626000	-1.396331000	1.298668000
C	-2.246192000	-3.299185000	-2.022417000
H	-0.576963000	-1.988001000	-2.349428000
C	-3.262748000	-3.686449000	-1.149150000
H	-4.224309000	-3.291683000	0.737746000
H	-2.103839000	-3.826087000	-2.959756000
H	-3.912680000	-4.517325000	-1.401678000
C	-2.655548000	1.179570000	0.085609000
C	-3.397467000	1.226179000	1.271215000
C	-3.301064000	1.431821000	-1.128271000
C	-4.760011000	1.517411000	1.242915000
H	-2.911304000	1.030228000	2.222713000
C	-4.664012000	1.718191000	-1.156271000
H	-2.735648000	1.395861000	-2.053539000
C	-5.396480000	1.762602000	0.028057000
H	-5.323323000	1.548789000	2.169680000
H	-5.153584000	1.905732000	-2.105973000
H	-6.457549000	1.986036000	0.004803000

20'			
Ni	-0.825442000	-0.597244000	-0.400746000
C	-1.280504000	-2.618338000	-0.967372000
C	-2.080061000	-1.665792000	-1.710299000
C	0.074660000	-2.387969000	-1.284717000
C	-1.197049000	-0.903606000	-2.536379000
C	0.135463000	-1.301345000	-2.247546000
C	-1.852431000	-3.675021000	-0.082855000
H	-2.307862000	-4.464970000	-0.690083000
H	-1.098035000	-4.144528000	0.548310000
H	-2.629800000	-3.256007000	0.556944000
C	-3.572256000	-1.622807000	-1.673967000
H	-3.980887000	-0.796545000	-2.256996000
H	-3.993572000	-2.545416000	-2.086352000
H	-3.921482000	-1.534213000	-0.642168000
C	-1.596509000	0.123048000	-3.547814000
H	-1.723026000	-0.353035000	-4.526440000
H	-2.544255000	0.603370000	-3.302763000
H	-0.843085000	0.903350000	-3.664316000
C	1.343883000	-0.887077000	-3.027067000
H	1.355613000	-1.404235000	-3.993221000
H	1.357136000	0.184169000	-3.239758000
H	2.270115000	-1.141269000	-2.516220000
C	1.241940000	-3.195406000	-0.818036000
H	1.037939000	-3.703683000	0.124552000
H	1.475767000	-3.966965000	-1.560502000
H	2.139064000	-2.591974000	-0.686374000
O	-2.114380000	-0.802080000	0.988449000
C	-0.223967000	2.255170000	-0.340288000
C	-2.478532000	1.713182000	-0.584544000
C	1.109267000	1.846189000	-0.018102000
C	-0.519222000	3.639446000	-0.513570000
C	-2.849280000	3.061229000	-0.721666000
H	-3.221874000	0.927990000	-0.568199000
C	2.092400000	2.822224000	0.050073000
C	0.530648000	4.590661000	-0.450356000
C	-1.866794000	4.018462000	-0.718711000
H	-3.895472000	3.316822000	-0.835325000
C	1.812002000	4.184049000	-0.183719000
H	3.097046000	2.544494000	0.341016000
H	0.299708000	5.639522000	-0.603070000
H	-2.109424000	5.068092000	-0.848148000
H	2.615826000	4.908342000	-0.118365000
N	-1.220788000	1.321429000	-0.452193000
C	0.427169000	-0.130237000	1.225222000
C	1.391755000	0.463482000	0.469539000
C	-0.221304000	-0.353456000	2.363761000
C	0.204704000	0.145039000	3.665443000
C	-1.547375000	-1.083587000	2.239607000
C	-0.683668000	0.195043000	4.681180000
H	1.209060000	0.539152000	3.779982000
C	-2.497202000	-0.775027000	3.369465000
H	-1.321596000	-2.169130000	2.327765000
C	-2.072736000	-0.219578000	4.512865000
H	-0.377541000	0.595399000	5.642430000
H	-3.526611000	-1.089332000	3.230868000
H	-2.759465000	-0.061495000	5.338103000
C	2.743004000	-0.123490000	0.314623000
C	3.606745000	0.234166000	-0.736537000
C	3.208015000	-1.036600000	1.279489000
C	4.888183000	-0.299959000	-0.816357000
H	3.274608000	0.928346000	-1.498228000
C	4.492423000	-1.559185000	1.204436000
H	2.554679000	-1.325089000	2.094646000
C	5.336346000	-1.194549000	0.154865000
H	5.539275000	-0.016418000	-1.636081000
H	4.838120000	-2.249467000	1.965993000
H	6.339232000	-1.603227000	0.095908000

21ts			
Ni	-0.816341000	-0.654789000	0.087078000
C	-0.967257000	-2.739064000	-0.469311000
C	-2.362098000	-2.415099000	-0.271879000
C	-0.506362000	-2.002927000	-1.604399000
C	-2.699557000	-1.391150000	-1.183038000
C	-1.543509000	-1.086288000	-1.976991000
C	-0.255753000	-3.856545000	0.221661000
H	-0.558179000	-4.822292000	-0.199045000
H	0.827680000	-3.781293000	0.121563000
H	-0.497705000	-3.871476000	1.284825000
C	-3.141792000	-2.884045000	0.884647000
H	-4.208659000	-2.672814000	0.811670000
H	-3.005759000	-3.948197000	1.085781000
H	-2.697804000	-2.319648000	1.742611000
C	-4.038079000	-0.749486000	-1.363723000
H	-4.518481000	-1.132955000	-2.270877000
H	-4.713815000	-0.955306000	-0.533540000
H	-3.964051000	0.333777000	-1.483782000
C	-1.547091000	-0.183665000	-3.171371000
H	-2.048041000	-0.670191000	-4.016276000
H	-2.083132000	0.748125000	-2.977295000
H	-0.539209000	0.069584000	-3.497090000
C	0.709460000	-2.327873000	-2.404603000
H	1.548119000	-2.651033000	-1.788824000
H	0.462473000	-3.163647000	-3.071092000
H	1.042642000	-1.504860000	-3.032874000
O	-1.217143000	-1.065955000	1.808526000
C	-0.930696000	2.212151000	0.383447000
C	-2.877563000	1.174105000	1.090650000
C	0.394600000	2.048667000	-0.089130000
C	-1.432999000	3.497939000	0.727188000
C	-3.449508000	2.405341000	1.461857000
H	-3.383203000	0.238809000	1.277971000
C	1.176654000	3.179510000	-0.259339000
C	-0.600075000	4.626556000	0.528519000
C	-2.739574000	3.564937000	1.265424000
H	-4.440226000	2.416029000	1.899530000
C	0.673342000	4.464414000	0.037435000
H	2.197526000	3.083234000	-0.608436000
H	-0.977857000	5.613552000	0.773306000
H	-3.159520000	4.528274000	1.535786000
H	1.313452000	5.326848000	-0.110344000
N	-1.685638000	1.089026000	0.525060000
C	0.803448000	-0.238369000	0.807179000
C	0.924589000	0.662382000	-0.280370000
C	1.621764000	-0.534840000	1.912751000
C	2.793071000	0.246844000	2.137786000
C	1.307640000	-1.583090000	2.820821000
C	3.609164000	-0.015357000	3.219732000
H	3.031916000	1.057094000	1.459623000
C	2.143409000	-1.842266000	3.891946000
H	0.369112000	-2.094777000	2.654633000
C	3.287421000	-1.063617000	4.092732000
H	4.492962000	0.586755000	3.396784000
H	1.903520000	-2.638970000	4.586759000
H	3.932698000	-1.266578000	4.941343000
C	1.937471000	0.460191000	-1.349018000
C	1.828708000	1.173637000	-2.558848000
C	3.038691000	-0.399373000	-1.188333000
C	2.785997000	1.040457000	-3.557008000
H	0.989316000	1.840643000	-2.713846000
C	4.000631000	-0.522762000	-2.186190000
H	3.158272000	-0.972023000	-0.277426000
C	3.879992000	0.193899000	-3.374214000
H	2.680321000	1.601779000	-4.479141000
H	4.847873000	-1.182317000	-2.032532000
H	4.630734000	0.096354000	-4.150582000

22ts			
C	0.189086000	4.768631000	0.209215000
C	-0.500925000	4.480559000	1.369265000
C	-0.781946000	3.142621000	1.738796000
C	-0.402210000	2.100604000	0.832192000
C	0.659901000	3.726058000	-0.583346000
H	-1.737723000	3.544665000	3.634170000
H	0.425563000	5.786481000	-0.072603000
H	-0.813251000	5.283208000	2.028316000
C	-1.410525000	2.773643000	2.947002000
C	-0.683293000	0.715095000	1.063301000
H	1.298151000	3.837884000	-1.446969000
C	-1.210976000	0.425198000	2.344470000
C	-1.579460000	1.431394000	3.243267000
H	-1.385327000	-0.607969000	2.623414000
H	-2.036624000	1.147183000	4.185335000
Ni	-1.258456000	-0.603115000	-0.220885000
O	0.817629000	1.474889000	-1.098603000
N	0.342370000	2.467050000	-0.249622000
C	-2.091323000	-2.132256000	-1.510597000
C	-3.092840000	-1.525402000	-0.635654000
C	-1.541762000	-1.109343000	-2.294254000
C	-3.221264000	-0.151710000	-0.952727000
C	-2.188480000	0.142799000	-1.902103000
C	0.604782000	-0.350657000	0.363354000
C	1.460581000	0.395070000	-0.393204000
C	2.887925000	0.315101000	-0.689899000
C	3.775619000	-0.445313000	0.099669000
C	3.416982000	0.999875000	-1.805287000
C	5.127635000	-0.502766000	-0.210888000
H	3.414947000	-0.977285000	0.967709000
C	4.768790000	0.926995000	-2.113125000
H	2.761590000	1.577071000	-2.444675000
C	5.633717000	0.178344000	-1.317032000
H	5.792013000	-1.083216000	0.420094000
H	5.148489000	1.455723000	-2.980853000
H	6.690093000	0.125561000	-1.556146000
C	1.011106000	-1.525985000	1.182251000
C	1.098990000	-2.789703000	0.575403000
C	1.322881000	-1.415824000	2.547748000
C	1.490594000	-3.905770000	1.308016000
H	0.875660000	-2.885264000	-0.480393000
C	1.705589000	-2.537267000	3.279566000
H	1.291012000	-0.446392000	3.031133000
C	1.789105000	-3.785099000	2.664431000
H	1.565278000	-4.870709000	0.817981000
H	1.949125000	-2.432652000	4.331577000
H	2.090728000	-4.655685000	3.236491000
C	-0.495918000	-1.226900000	-3.358417000
H	-0.948209000	-1.151579000	-4.353504000
H	0.249531000	-0.432290000	-3.284476000
H	0.032377000	-2.179490000	-3.312554000
C	-1.792734000	-3.599935000	-1.565777000
H	-2.629258000	-4.144854000	-2.016459000
H	-0.908671000	-3.814938000	-2.167138000
H	-1.630329000	-4.030443000	-0.574653000
C	-3.897345000	-2.289321000	0.370021000
H	-4.712871000	-2.829069000	-0.124573000
H	-3.296801000	-3.038690000	0.891751000
H	-4.349139000	-1.638079000	1.119395000
C	-4.202700000	0.820235000	-0.372559000
H	-5.117814000	0.857164000	-0.973630000
H	-4.496072000	0.549462000	0.643298000
H	-3.800770000	1.834489000	-0.335986000
C	-1.988459000	1.456074000	-2.591174000
H	-2.653529000	1.525773000	-3.459793000
H	-2.225715000	2.302342000	-1.943362000
H	-0.968509000	1.576992000	-2.954382000

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C	2.704129000	1.794049000	2.885912000
C	2.388418000	0.777301000	3.755635000
C	1.393796000	-0.166276000	3.404149000
C	0.723299000	-0.015827000	2.153145000
C	1.073922000	1.008702000	1.250116000
C	2.053435000	1.904330000	1.638863000
H	1.533485000	-1.413958000	5.169460000
H	3.469485000	2.515692000	3.149123000
H	2.897003000	0.681823000	4.709169000
C	1.045176000	-1.273928000	4.210341000
H	2.336194000	2.706401000	0.966793000
C	-0.512360000	-1.947251000	2.517173000
C	0.111996000	-2.174451000	3.757051000
H	-1.239345000	-2.650873000	2.138008000
H	-0.157993000	-3.051251000	4.332843000
Ni	-1.094259000	-0.538444000	0.007626000
C	0.379609000	1.054591000	-0.098460000
N	-0.254200000	-0.893470000	1.758638000
C	1.148558000	0.467599000	-1.241826000
O	0.602132000	0.395051000	-2.355370000
C	2.578827000	0.014284000	-1.160272000
C	3.136893000	-0.762077000	-0.134292000
C	3.395064000	0.383785000	-2.243402000
C	4.471027000	-1.153568000	-0.192715000
H	2.529559000	-1.098041000	0.693647000
C	4.736485000	0.021490000	-2.280022000
H	2.969169000	0.966146000	-3.051506000
C	5.278127000	-0.752513000	-1.255911000
H	4.882888000	-1.769965000	0.599382000
H	5.355833000	0.335308000	-3.113181000
H	6.321891000	-1.046031000	-1.287982000
C	-0.097720000	2.472419000	-0.376585000
C	-0.646885000	3.221214000	0.682122000
C	0.078849000	3.139944000	-1.600884000
C	-1.018247000	4.551708000	0.525276000
H	-0.769627000	2.760253000	1.654937000
C	-0.283381000	4.477285000	-1.755532000
H	0.496460000	2.621076000	-2.451888000
C	-0.839236000	5.192311000	-0.700163000
H	-1.438347000	5.092543000	1.367321000
H	-0.121828000	4.960489000	-2.713662000
H	-1.118470000	6.232883000	-0.824254000
C	-3.144725000	-1.130759000	0.617136000
C	-2.988919000	0.296210000	0.425357000
C	-2.834685000	-1.770781000	-0.591655000
C	-2.753452000	0.518621000	-0.977226000
C	-2.544643000	-0.740798000	-1.581545000
C	-2.868893000	1.810926000	-1.710385000
H	-2.162332000	1.883711000	-2.535348000
H	-3.877859000	1.869449000	-2.137349000
H	-2.733842000	2.679189000	-1.070455000
C	-3.407502000	1.322205000	1.431350000
H	-3.065914000	2.319453000	1.164160000
H	-4.501327000	1.356651000	1.496417000
H	-3.034638000	1.094342000	2.432236000
C	-3.670772000	-1.760144000	1.867862000
H	-3.260863000	-1.310227000	2.773496000
H	-4.756114000	-1.613657000	1.909637000
H	-3.499088000	-2.836593000	1.905767000
C	-2.890001000	-3.240267000	-0.866108000
H	-2.672741000	-3.840460000	0.018988000
H	-3.892008000	-3.520527000	-1.209689000
H	-2.193957000	-3.537869000	-1.650356000
C	-2.338374000	-0.973499000	-3.045842000
H	-1.726495000	-0.191529000	-3.493757000
H	-1.864190000	-1.932145000	-3.255870000
H	-3.305159000	-0.974283000	-3.562266000
H	-2.119502000	-3.351829000	2.620911000
C	-1.970681000	-3.911201000	-0.165348000
H	-1.337389000	-4.294910000	0.635778000
C	0.618499000	-2.739133000	-1.612413000
O	0.811122000	-2.222488000	-2.803793000
O	0.134567000	-2.133104000	-0.650916000
C	1.068021000	-4.166136000	-1.507673000
H	2.161411000	-4.188730000	-1.508727000
H	0.701084000	-4.620911000	-0.590646000
H	0.736833000	-4.734085000	-2.378431000
H	0.676659000	-1.237078000	-2.813247000

24ts

C	2.329721000	2.927819000	2.388750000
C	2.426401000	1.946021000	3.344807000
C	1.768446000	0.707413000	3.154760000
C	0.975076000	0.521365000	1.981907000
C	0.906129000	1.525096000	0.989136000
C	1.582054000	2.710906000	1.213074000
H	2.497077000	-0.265813000	4.946379000
H	2.844839000	3.872337000	2.523172000
H	3.017670000	2.098453000	4.241517000
C	1.900241000	-0.381192000	4.047349000
H	1.544614000	3.490758000	0.461139000
C	0.522152000	-1.679123000	2.581437000
C	1.304243000	-1.581030000	3.746185000
H	0.054774000	-2.616496000	2.316065000
H	1.416608000	-2.449109000	4.383953000
Ni	-0.830614000	-0.821503000	0.151171000
C	0.138505000	1.263588000	-0.281609000
N	0.318521000	-0.664523000	1.755633000
C	0.828411000	0.572205000	-1.329253000
O	0.201193000	0.297251000	-2.430497000
C	2.298024000	0.288913000	-1.342992000
C	3.062984000	-0.298017000	-0.325489000
C	2.955011000	0.713501000	-2.513561000
C	4.438904000	-0.440837000	-0.469941000
H	2.586392000	-0.702602000	0.552693000
C	4.333962000	0.592101000	-2.641265000
H	2.378600000	1.152620000	-3.318275000
C	5.082283000	0.014016000	-1.619671000
H	5.010797000	-0.916328000	0.319860000
H	4.819942000	0.941617000	-3.545539000
H	6.156878000	-0.091649000	-1.721970000
C	-0.794435000	2.390290000	-0.639093000
C	-1.422746000	3.113102000	0.392561000
C	-0.960594000	2.868181000	-1.951377000
C	-2.190521000	4.242401000	0.129925000
H	-1.293118000	2.800471000	1.421429000
C	-1.722411000	4.004796000	-2.212001000
H	-0.496310000	2.353083000	-2.779597000
C	-2.347595000	4.696464000	-1.178574000
H	-2.657994000	4.774916000	0.951886000
H	-1.820123000	4.352359000	-3.235201000
H	-2.938886000	5.581522000	-1.386431000
C	-2.512065000	-1.772195000	1.194249000
C	-2.802107000	-0.394623000	0.884591000
C	-2.263327000	-2.454056000	-0.016298000
C	-2.878441000	-0.284804000	-0.546433000
C	-2.443692000	-1.511851000	-1.105924000
C	-3.449862000	0.844441000	-1.330610000
H	-2.911271000	1.018071000	-2.260752000
H	-4.480768000	0.580185000	-1.598076000
H	-3.484058000	1.778544000	-0.776415000
C	-3.295360000	0.602089000	1.887391000
H	-3.332536000	1.609350000	1.479180000
H	-4.311042000	0.340361000	2.205271000
H	-2.675830000	0.624932000	2.786539000
C	-2.598911000	-2.374377000	2.559779000
H	-2.177576000	-1.730979000	3.333670000
H	-3.654189000	-2.524658000	2.815201000
H	-4.483765000	-0.399495000	-1.486574000
H	-3.817818000	0.991398000	-0.629675000
C	-3.218635000	-0.019786000	2.027988000

H	-2.907660000	-4.479161000	-0.140427000
H	-1.483550000	-4.135846000	-1.112600000
C	-2.457486000	-1.848321000	-2.564139000
H	-2.194856000	-0.987822000	-3.178318000
H	-1.766277000	-2.650363000	-2.816332000
H	-3.462304000	-2.171954000	-2.859270000
C	0.957377000	-2.578875000	-1.649823000
O	0.817035000	-2.014079000	-2.772845000
O	0.531110000	-2.139009000	-0.534948000
C	1.737815000	-3.871075000	-1.628933000
H	2.804101000	-3.626760000	-1.644043000
H	1.529066000	-4.453517000	-0.733117000
H	1.526911000	-4.453667000	-2.526024000
H	0.494153000	-0.765947000	-2.728380000

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C	1.767920000	3.565080000	2.101814000
C	2.061999000	2.687864000	3.116245000
C	1.657161000	1.335086000	3.023597000
C	0.904735000	0.907653000	1.885040000
C	0.630254000	1.816357000	0.834215000
C	1.061865000	3.124572000	0.965173000
H	2.582722000	0.672245000	4.864267000
H	2.090750000	4.598305000	2.160393000
H	2.621005000	3.011783000	3.987757000
C	2.013065000	0.368457000	3.991963000
H	0.859627000	3.827122000	0.164954000
C	0.914625000	-1.285581000	2.659961000
C	1.669719000	-0.945234000	3.795626000
H	0.654103000	-2.316156000	2.470099000
H	1.961939000	-1.722378000	4.490998000
Ni	-0.587889000	-1.011426000	0.209696000
C	-0.099178000	1.370721000	-0.397798000
N	0.497469000	-0.401247000	1.766602000
C	0.603461000	0.634604000	-1.363140000
O	-0.040986000	0.249614000	-2.473706000
C	2.097333000	0.557573000	-1.453227000
C	2.996488000	0.197009000	-0.440978000
C	2.623680000	0.980986000	-2.689094000
C	4.369655000	0.275562000	-0.652082000
H	2.638789000	-0.206633000	0.491269000
C	3.996196000	1.072962000	-2.888683000
H	1.949846000	1.254127000	-3.491327000
C	4.877322000	0.722259000	-1.869794000
H	5.046519000	-0.024152000	0.141095000
H	4.373930000	1.414669000	-3.846184000
H	5.948718000	0.785616000	-2.026141000
C	-1.276189000	2.226447000	-0.739109000
C	-2.017005000	2.830352000	0.294983000
C	-1.579654000	2.604388000	-2.060225000
C	-3.026713000	3.746750000	0.025832000
H	-1.786612000	2.594428000	1.326794000
C	-2.583475000	3.531665000	-2.326706000
H	-1.027482000	2.178993000	-2.885315000
C	-3.318141000	4.102183000	-1.290694000
H	-3.578446000	4.194035000	0.846139000
H	-2.785236000	3.813504000	-3.354723000
H	-4.098475000	4.824602000	-1.503813000
C	-1.995417000	-2.202260000	1.329300000
C	-2.596770000	-0.930893000	1.015128000
C	-1.694095000	-2.866028000	0.109171000
C	-2.748020000	-0.874148000	-0.403564000
C	-2.095916000	-2.009654000	-0.974761000
C	-3.552372000	0.098741000	-1.189823000
H	-3.048485000	0.402934000	-2.105787000
H	-3.491749000	0.941899000	1.599205000
H	-4.133869000	-0.471135000	2.426917000
H	-2.557623000	0.165809000	2.877510000
C	-1.905761000	-2.791622000	2.699645000
H	-1.650921000	-2.054535000	3.462121000
H	-2.884971000	-3.202187000	2.972893000
H	-1.194046000	-3.615921000	2.758414000
C	-1.129780000	-4.241870000	-0.018083000
H	-0.320585000	-4.424954000	0.689738000
H	-1.916726000	-4.977750000	0.182827000
H	-0.750595000	-4.436073000	-1.019957000
C	-2.136110000	-2.378115000	-2.425319000
H	-2.131842000	-1.494778000	-3.062932000
H	-1.290509000	-2.993917000	-2.722121000
H	-3.056962000	-2.933404000	-2.638742000
C	1.407638000	-2.500783000	-1.411723000
O	0.993275000	-2.134145000	-2.521984000
O	0.977048000	-2.082608000	-0.264805000
C	2.546054000	-3.498402000	-1.337739000
H	3.485193000	-2.955170000	-1.477119000
H	2.583848000	-4.010156000	-0.376965000
H	2.461747000	-4.218398000	-2.152062000
H	0.348377000	-0.637301000	-2.736830000

26

O	-0.213892000	-2.229588000	-1.244526000
C	0.209369000	1.515679000	-0.142367000
C	0.934858000	1.753653000	-2.314713000
C	-0.328052000	0.672643000	0.877709000
C	0.507691000	2.884017000	0.153468000
C	1.262531000	3.116447000	-2.124892000
H	1.098778000	1.284365000	-3.282577000
C	-0.547092000	1.217783000	2.127053000
C	0.260331000	3.391855000	1.451637000
C	1.046800000	3.674894000	-0.891302000
H	1.675291000	3.693852000	-2.944778000
C	-0.259509000	2.568711000	2.418900000
H	-0.964605000	0.592490000	2.910922000
H	0.485980000	4.432052000	1.667040000
H	1.284075000	4.717620000	-0.700285000
H	-0.453429000	2.949988000	3.416169000
N	0.431123000	0.986036000	-1.375615000
C	0.227427000	-1.586423000	-0.319351000
C	-0.714911000	-0.784402000	0.616930000
C	1.693259000	-1.665738000	0.019171000
C	2.539058000	-2.257822000	-0.928733000
C	2.239448000	-1.233004000	1.233117000
C	3.897203000	-2.400417000	-0.677219000
H	2.101914000	-2.603406000	-1.857891000
C	3.600464000	-1.385503000	1.490407000
H	1.613062000	-0.774347000	1.988141000
C	4.432400000	-1.964648000	0.535860000
H	4.540993000	-2.855105000	-1.423507000
H	4.010003000	-1.050295000	2.437988000
H	5.493219000	-2.078616000	0.736059000
C	-2.178278000	-0.904155000	0.208150000
C	-2.633152000	-0.454434000	-1.036157000
C	-3.102908000	-1.452894000	1.099669000
C	-3.980284000	-0.547267000	-1.370562000
H	-1.923428000	-0.043971000	-1.743272000
C	-4.453615000	-1.547138000	0.766621000
H	-2.766255000	-1.818757000	2.066246000
C	-4.896718000	-1.091564000	-0.471006000
H	-4.316345000	-0.198488000	-2.342265000
H	-5.154951000	-1.979336000	1.473750000

H	-5.946867000	-1.163705000	-0.736316000
H	-0.622087000	-1.291537000	1.585757000

27

Ni	0.082646000	0.612007000	0.070994000
C	-1.517307000	2.020346000	0.616292000
C	-0.989820000	1.418634000	1.774006000
C	-0.426940000	2.670058000	-0.092472000
C	0.433542000	1.693023000	1.807677000
C	0.743553000	2.559443000	0.711038000
C	-2.952610000	2.096390000	0.209410000
H	-3.368004000	3.058429000	0.530195000
H	-3.077066000	2.039281000	-0.872180000
H	-3.558321000	1.310953000	0.658240000
C	-1.728269000	0.630546000	2.807126000
H	-1.856246000	1.225670000	3.717504000
H	-2.717956000	0.330224000	2.464800000
H	-1.180220000	-0.272633000	3.080424000
C	1.361210000	1.302019000	2.912408000
H	1.299967000	2.020748000	3.737057000
H	1.108940000	0.321476000	3.317348000
H	2.399975000	1.272880000	2.581265000
C	2.033237000	3.287853000	0.517735000
H	2.031135000	4.179458000	1.155017000
H	2.900401000	2.690459000	0.797132000
H	2.172078000	3.631617000	-0.506712000
C	-0.594418000	3.528178000	-1.307465000
H	-1.315635000	3.106494000	-2.008988000
H	-0.963566000	4.520122000	-1.024682000
H	0.345031000	3.677076000	-1.840948000
O	0.212344000	-1.132855000	0.971787000
C	2.257661000	-1.112271000	-0.103267000
C	1.603241000	-2.962784000	1.239099000
C	1.861252000	0.153830000	-0.588270000
C	3.499092000	-1.740719000	-0.395403000
C	2.813471000	-3.614033000	0.967159000
H	0.820994000	-3.366680000	1.865966000
C	2.777788000	0.785337000	-1.406033000
C	4.391880000	-1.032646000	-1.235955000
C	3.756033000	-3.016686000	0.161436000
H	2.981796000	-4.589139000	1.406241000
C	4.029848000	0.200615000	-1.724568000
H	2.552068000	1.754797000	-1.836433000
H	5.350800000	-1.472961000	-1.485809000
H	4.694360000	-3.516342000	-0.052448000
H	4.712714000	0.742664000	-2.370726000
N	1.359428000	-1.761961000	0.713231000
C	-1.411265000	-0.464768000	-1.281922000
C	-0.552781000	0.043377000	-2.000096000
C	0.156411000	0.384718000	-3.239250000
H	1.068812000	-0.201240000	-3.353370000
H	-0.497983000	0.169528000	-4.088506000
H	0.429594000	1.440496000	-3.283654000
C	-2.619960000	-1.102010000	-0.833001000
C	-3.794697000	-0.858341000	-1.571747000
C	-2.670408000	-1.985602000	0.256375000
C	-4.984307000	-1.488003000	-1.227809000
H	-3.762993000	-0.183141000	-2.419508000
C	-3.868490000	-2.604791000	0.596554000
H	-1.769040000	-2.170101000	0.823448000
C	-5.025977000	-2.360513000	-0.140968000
H	-5.879829000	-1.297451000	-1.809177000
H	-3.897982000	-3.287294000	1.439228000
H	-5.955840000	-2.850209000	0.126987000

28ts

Ni	-0.039604000	0.614103000	0.091245000
C	-1.572545000	2.113169000	0.131773000
C	-1.079750000	1.830905000	1.433569000
C	-0.457648000	2.526786000	-0.672953000
C	0.327374000	2.206255000	1.470602000
C	0.696225000	2.664793000	0.190278000
C	-2.995721000	2.042238000	-0.319281000
H	-3.466723000	3.022111000	-0.182129000
H	-3.085477000	1.787359000	-1.375622000
H	-3.577060000	1.316683000	0.247771000
C	-1.872196000	1.388310000	2.622151000
H	-2.156287000	2.252829000	3.232374000
H	-2.788835000	0.873994000	2.334145000
H	-1.296562000	0.715676000	3.259961000
C	1.185859000	2.133924000	2.692158000
H	0.918643000	2.932420000	3.392486000
H	1.050629000	1.185783000	3.215737000
H	2.245063000	2.245930000	2.459605000
C	2.020423000	3.236048000	-0.204414000
H	2.002954000	4.325320000	-0.090512000
H	2.835674000	2.856604000	0.412142000
H	2.269467000	3.028250000	-1.245241000
C	-0.544443000	2.979348000	-2.098215000
H	-1.242426000	2.374686000	-2.679355000
H	-0.897431000	4.015375000	-2.146718000
H	0.423426000	2.951580000	-2.600635000
O	0.397550000	-0.789328000	1.428421000
C	2.205595000	-1.048550000	0.005164000
C	2.031788000	-2.313830000	2.008824000
C	1.536270000	-0.163856000	-0.888447000
C	3.523353000	-1.531526000	-0.205044000
C	3.290534000	-2.881561000	1.782808000
H	1.413172000	-2.518542000	2.871015000
C	2.301679000	0.318126000	-1.942804000
C	4.233955000	-1.014900000	-1.318837000
C	4.048496000	-2.479082000	0.706821000
H	3.660734000	-3.609466000	2.493581000
C	3.639588000	-0.085222000	-2.141283000
H	1.847979000	0.979499000	-2.672741000
H	5.245398000	-1.357485000	-1.506165000
H	5.045444000	-2.876314000	0.553044000
H	4.193413000	0.322633000	-2.980084000
N	1.540167000	-1.407600000	1.157173000
C	-1.154255000	-0.764381000	-0.731926000
C	-0.154012000	-0.872079000	-1.517567000
C	0.182841000	-1.523133000	-2.818170000
H	1.087946000	-2.129586000	-2.759136000
H	-0.656379000	-2.168035000	-3.093363000
H	0.320432000	-0.792258000	-3.618438000
C	-2.485019000	-1.275466000	-0.468960000
C	-3.445505000	-1.326678000	-1.493355000
C	-2.823922000	-1.751400000	0.807980000
C	-4.711948000	-1.846188000	-1.243340000
H	-3.197477000	-0.956898000	-2.482606000
C	-4.089451000	-2.275961000	1.047597000
H	-2.080427000	-1.717594000	1.595494000
C	-5.037636000	-2.321541000	0.025649000
H	-5.444995000	-1.881350000	-2.042140000
H	-4.337304000	-2.651643000	2.034682000
H	-6.024812000	-2.727809000	0.216972000

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C	-3.876528000	-1.529105000	-1.953083000
C	-4.598559000	-0.834935000	-1.017418000
C	-3.970845000	0.160327000	-0.234585000
C	-2.577280000	0.468260000	-0.415741000
C	-2.509817000	-1.284598000	-2.052587000
H	-5.779874000	0.624335000	0.842422000
H	-4.323401000	-2.281809000	-2.589743000
H	-5.655808000	-1.026858000	-0.873902000
C	-4.735709000	0.885212000	0.711162000
C	-2.009233000	1.590920000	0.271992000
H	-1.850575000	-1.827117000	-2.714088000
C	-2.830053000	2.258589000	1.172859000
C	-4.164888000	1.903681000	1.425513000
H	-2.416150000	3.110003000	1.700009000
H	-4.741877000	2.460306000	2.155142000
Ni	0.763950000	-0.394131000	-0.071169000
O	-0.561903000	-0.309067000	-1.518672000
N	-1.878950000	-0.365619000	-1.307089000
C	-0.669935000	2.190328000	-0.006718000
C	0.436423000	1.462029000	0.010504000
C	1.781245000	1.656048000	-0.493029000
C	2.093264000	1.012306000	-1.721094000
C	2.826812000	2.286239000	0.225274000
C	3.416352000	0.994480000	-2.190546000
H	1.291998000	0.647855000	-2.352848000
C	4.112712000	2.296837000	-0.277604000
H	2.596466000	2.787999000	1.158805000
C	4.418359000	1.632491000	-1.479208000
H	3.638659000	0.518681000	-3.139753000
H	4.896472000	2.821552000	0.258828000
H	5.434086000	1.646015000	-1.859053000
C	2.193524000	-1.149889000	1.311224000
C	0.964680000	-0.898748000	1.978297000
C	1.977538000	-2.190899000	0.312901000
C	-0.041286000	-1.680397000	1.321572000
C	0.621506000	-2.526526000	0.329507000
C	3.054850000	-2.782269000	-0.541890000
H	3.751310000	-2.021496000	-0.899195000
H	3.639461000	-3.511140000	0.030303000
H	2.651327000	-3.301779000	-1.411551000
C	-0.051913000	-3.568574000	-0.506326000
H	0.431955000	-3.692994000	-1.476109000
H	-0.022826000	-4.539422000	0.000123000
H	-1.102963000	-3.336815000	-0.682587000
C	-1.452207000	-1.848798000	1.792515000
H	-2.124030000	-2.171339000	0.996405000
H	-1.491415000	-2.621591000	2.568984000
H	-1.856571000	-0.934507000	2.227714000
C	0.753962000	-0.010822000	3.164241000
H	-0.244598000	0.427120000	3.173393000
H	0.870735000	-0.584264000	4.090575000
H	1.473502000	0.807842000	3.196645000
C	3.544078000	-0.640722000	1.703544000
H	3.487352000	0.246673000	2.332297000
H	4.070337000	-1.413401000	2.275506000
H	4.165204000	-0.399698000	0.840170000
C	-0.667346000	3.663716000	-0.375094000
H	-0.979648000	4.303608000	0.455765000
H	0.329543000	3.984913000	-0.677546000
H	-1.355699000	3.859660000	-1.203253000

30ts			
C	-3.391846000	-2.065574000	-1.809060000
C	-4.330785000	-1.469667000	-1.000189000
C	-4.027707000	-0.287007000	-0.281519000
C	-2.707014000	0.274251000	-0.395538000
C	-2.115060000	-1.514906000	-1.889807000
H	-5.973892000	-0.034009000	0.605208000
H	-3.611513000	-2.958911000	-2.379261000
H	-5.327052000	-1.889574000	-0.917279000
C	-4.981627000	0.388359000	0.500891000
C	-2.359969000	1.524262000	0.208130000
H	-1.302913000	-1.922267000	-2.472960000
C	-3.382477000	2.154010000	0.942513000
C	-4.649128000	1.592059000	1.096587000
H	-3.171124000	3.103272000	1.417428000
H	-5.387742000	2.117099000	1.692332000
Ni	0.958302000	-0.346148000	-0.086013000
O	-0.547421000	0.061597000	-1.443700000
N	-1.822945000	-0.404178000	-1.197972000
C	-1.082679000	2.125820000	-0.031278000
C	-0.049928000	1.348414000	-0.504455000
C	1.318132000	1.582637000	-0.894432000
C	1.925707000	0.712633000	-1.850825000
C	2.149377000	2.526157000	-0.210100000
C	3.310963000	0.835655000	-2.123637000
H	1.319329000	0.159595000	-2.555590000
C	3.480882000	2.630647000	-0.519729000
H	1.720121000	3.166941000	0.548371000
C	4.076297000	1.776491000	-1.479012000
H	3.748243000	0.206795000	-2.891527000
H	4.087006000	3.378279000	-0.019428000
H	5.128724000	1.884958000	-1.716753000
C	2.311666000	-0.704004000	1.457872000
C	0.996001000	-0.710934000	2.019283000
C	2.427039000	-1.815239000	0.525074000
C	0.256776000	-1.711804000	1.329511000
C	1.163512000	-2.419398000	0.428112000
C	3.690828000	-2.235085000	-0.156771000
H	4.282287000	-1.378669000	-0.486479000
H	4.319158000	-2.813671000	0.529663000
H	3.499818000	-2.863006000	-1.028031000
C	0.811643000	-3.632471000	-0.380273000
H	1.421990000	-3.719029000	-1.280751000
H	0.971672000	-4.543694000	0.206685000
H	-0.236649000	-3.637770000	-0.685025000
C	-1.141598000	-2.145175000	1.647394000
H	-1.655730000	-2.565888000	0.781655000
H	-1.122907000	-2.931424000	2.410496000
H	-1.750122000	-1.331045000	2.042763000
C	0.494448000	0.173842000	3.117638000
H	-0.578622000	0.356829000	3.042559000
H	0.677962000	-0.286233000	4.095037000
H	0.994847000	1.143602000	3.122122000
C	3.462406000	0.124363000	1.936761000
H	3.140887000	1.079521000	2.352049000
H	3.997434000	-0.411663000	2.729073000
H	4.182844000	0.333048000	1.145702000
C	-0.906180000	3.610146000	0.191271000
H	-0.684897000	3.869352000	1.233830000
H	-0.103348000	4.012323000	-0.426218000
H	-1.818071000	4.146811000	-0.084393000

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C	-2.181689000	1.004275000	-2.392184000
C	-2.399700000	2.227033000	-1.861408000
C	-1.504133000	2.774156000	-0.861583000
C	-0.386155000	2.031392000	-0.460231000
C	-1.099008000	0.157527000	-1.935943000
H	-2.518350000	4.653910000	-0.568075000
H	-2.800661000	0.621234000	-3.195583000
H	-3.217399000	2.844313000	-2.216595000
C	-1.665156000	4.047060000	-0.284832000
C	0.586876000	2.498243000	0.430811000
H	-0.562590000	-0.441672000	-2.673256000
C	0.383015000	3.767525000	0.982857000
C	-0.738016000	4.524535000	0.629767000
H	1.105350000	4.178101000	1.677735000
H	-0.874397000	5.506941000	1.067830000
Ni	-1.051847000	-0.913488000	-0.327480000
O	1.167559000	0.398200000	-1.266998000
N	-0.213135000	0.701364000	-0.941696000
C	1.773021000	1.665874000	0.675646000
C	2.059911000	0.692852000	-0.219319000
C	3.275439000	-0.123523000	-0.363993000
C	4.548771000	0.446022000	-0.208459000
C	3.182425000	-1.481831000	-0.708719000
C	5.692673000	-0.329911000	-0.361024000
H	4.643530000	1.504435000	0.002143000
C	4.327274000	-2.254976000	-0.858644000
H	2.207380000	-1.931315000	-0.859441000
C	5.585857000	-1.682114000	-0.680800000
H	6.669748000	0.125911000	-0.244514000
H	4.240371000	-3.304296000	-1.119298000
H	6.479478000	-2.284371000	-0.802599000
C	-0.955721000	-2.300445000	1.312795000
C	-1.453679000	-1.076598000	1.778690000
C	-1.831522000	-2.774321000	0.234478000
C	-2.603995000	-0.735673000	0.951976000
C	-2.885935000	-1.853794000	0.071317000
C	-1.642873000	-4.069437000	-0.493106000
H	-0.597369000	-4.246552000	-0.757124000
H	-1.953424000	-4.908100000	0.139697000
H	-2.231120000	-4.117352000	-1.409448000
C	-4.075827000	-1.971326000	-0.828154000
H	-3.897739000	-2.649575000	-1.663085000
H	-4.933033000	-2.361476000	-0.268651000
H	-4.373524000	-1.005386000	-1.239245000
C	-3.493176000	0.445598000	1.161917000
H	-3.994020000	0.754090000	0.243924000
H	-4.274649000	0.190953000	1.887913000
H	-2.952530000	1.305244000	1.558545000
C	-0.935325000	-0.240666000	2.906537000
H	-0.925861000	0.822464000	2.658242000
H	-1.575630000	-0.358794000	3.787427000
H	0.075728000	-0.525034000	3.197097000
C	0.229731000	-3.055806000	1.827557000
H	0.907871000	-2.421414000	2.397983000
H	-0.097344000	-3.866192000	2.488329000
H	0.806151000	-3.519855000	1.024322000
C	2.640966000	1.972471000	1.868662000
H	2.025208000	2.118754000	2.760679000
H	3.344491000	1.168693000	2.077749000
H	3.221387000	2.890536000	1.729426000

32ts			
C	-2.100707000	1.436163000	-2.503145000
C	-2.102488000	2.681304000	-1.956706000
C	-1.214674000	3.010620000	-0.874190000
C	-0.325592000	2.015761000	-0.388987000
C	-1.265812000	0.420800000	-1.936858000
H	-1.878902000	5.039328000	-0.566745000
H	-2.699340000	1.193457000	-3.372982000
H	-2.742485000	3.459104000	-2.358729000
C	-1.191054000	4.265350000	-0.244764000
C	0.678074000	2.268251000	0.579787000
H	-0.914007000	-0.409913000	-2.556335000
C	0.633007000	3.533449000	1.186901000
C	-0.294795000	4.500171000	0.788669000
H	1.353989000	3.785986000	1.953862000
H	-0.291114000	5.466260000	1.281718000
Ni	-1.274122000	-0.833413000	-0.377013000
O	1.251267000	0.064210000	-1.200510000
N	-0.421805000	0.734495000	-0.881777000
C	1.767258000	1.323249000	0.783770000
C	2.058017000	0.394874000	-0.192830000
C	3.356393000	-0.318207000	-0.337362000
C	4.578197000	0.368303000	-0.283204000
C	3.362078000	-1.694659000	-0.612722000
C	5.775684000	-0.313121000	-0.468790000
H	4.587359000	1.438801000	-0.115444000
C	4.561805000	-2.375531000	-0.785648000
H	2.420582000	-2.226707000	-0.685886000
C	5.771223000	-1.686363000	-0.713419000
H	6.714430000	0.228681000	-0.429667000
H	4.555152000	-3.441906000	-0.984365000
H	6.707446000	-2.215157000	-0.855781000
C	-1.126225000	-2.360618000	1.092725000
C	-1.466355000	-1.141786000	1.714796000
C	-2.158299000	-2.678784000	0.108996000
C	-2.668568000	-0.649031000	1.068020000
C	-3.134327000	-1.659438000	0.135889000
C	-2.165886000	-3.910995000	-0.741620000
H	-1.181082000	-4.129420000	-1.161443000
H	-2.454156000	-4.781652000	-0.142713000
H	-2.871924000	-3.836026000	-1.568329000
C	-4.409051000	-1.594051000	-0.645441000
H	-4.386989000	-2.234702000	-1.527169000
H	-5.246839000	-1.925912000	-0.022579000
H	-4.635247000	-0.579045000	-0.975727000
C	-3.404988000	0.595534000	1.442540000
H	-4.012234000	0.978175000	0.621444000
H	-4.083916000	0.386038000	2.277556000
H	-2.731566000	1.390253000	1.766011000
C	-0.748655000	-0.466051000	2.838803000
H	-0.757456000	0.619619000	2.736296000
H	-1.237870000	-0.707245000	3.789219000
H	0.290136000	-0.785710000	2.912964000
C	0.047210000	-3.231952000	1.412894000
H	0.892756000	-2.661380000	1.797905000
H	-0.228547000	-3.965556000	2.178792000
H	0.389928000	-3.796374000	0.544096000
C	2.689350000	1.552675000	1.960218000
H	2.109205000	1.681721000	2.879395000
H	3.361635000	0.711603000	2.118156000
H	3.309952000	2.449207000	1.852408000

33			
C	-2.779895000	1.490489000	-2.487022000
C	-3.089604000	2.497882000	-1.607500000
C	-2.290387000	2.711985000	-0.458406000
C	-1.145265000	1.869688000	-0.262942000
C	-1.773205000	0.586215000	-2.117549000
H	-3.449510000	4.367272000	0.314235000
H	-3.333057000	1.339448000	-3.405724000
H	-3.930649000	3.158596000	-1.792437000
C	-2.563510000	3.757425000	0.454162000
C	-0.115470000	2.276902000	0.660642000
H	-1.596286000	-0.307352000	-2.703767000
C	-0.463852000	3.307459000	1.537765000
C	-1.685027000	3.998869000	1.481575000
H	0.264034000	3.633547000	2.269235000
H	-1.886782000	4.780706000	2.205225000
Ni	-0.560165000	-0.931498000	-0.024713000
O	1.117840000	-0.439948000	0.283776000
N	-1.032643000	0.725158000	-1.023388000
C	1.315001000	1.921828000	0.520259000
C	1.815367000	0.683840000	0.206891000
C	3.245861000	0.421412000	-0.139345000
C	3.825202000	1.009625000	-1.270045000
C	4.001841000	-0.480286000	0.619358000
C	5.138784000	0.713351000	-1.625332000
H	3.242222000	1.695945000	-1.875972000
C	5.318486000	-0.765339000	0.270992000
H	3.559708000	-0.943682000	1.494870000
C	5.889611000	-0.170798000	-0.853421000
H	5.574889000	1.172675000	-2.506109000
H	5.901055000	-1.450788000	0.877619000
H	6.914778000	-0.396379000	-1.126832000
C	-0.613506000	-2.486672000	1.362987000
C	-1.837066000	-1.716648000	1.412376000
C	-0.493176000	-3.024795000	0.057226000
C	-2.488520000	-1.832315000	0.142329000
C	-1.646886000	-2.599516000	-0.713542000
C	0.630047000	-3.867775000	-0.450700000
H	1.580183000	-3.596811000	0.009432000
H	0.439183000	-4.922057000	-0.219619000
H	0.746615000	-3.788036000	-1.531830000
C	-1.931650000	-3.031438000	-2.117446000
H	-1.057406000	-2.935307000	-2.765276000
H	-2.220266000	-4.087924000	-2.129265000
H	-2.751882000	-2.472476000	-2.567154000
C	-3.835690000	-1.269112000	-0.185355000
H	-4.018594000	-1.223631000	-1.257885000
H	-4.613775000	-1.905473000	0.248854000
H	-3.976519000	-0.266031000	0.220388000
C	-2.370319000	-1.006586000	2.613423000
H	-3.073406000	-0.217676000	2.346255000
H	-2.903662000	-1.715882000	3.257094000
H	-1.575660000	-0.561633000	3.213342000
C	0.358120000	-2.670244000	2.483023000
H	0.292313000	-1.867147000	3.217035000
H	0.155472000	-3.611184000	3.005479000
H	1.385375000	-2.706865000	2.120395000
C	2.276907000	3.062352000	0.798149000
H	2.320427000	3.297494000	1.867791000
H	3.291728000	2.818944000	0.497679000
H	1.976520000	3.978832000	0.282397000

34ts			
Ni	1.057980000	-0.284215000	-0.155673000
C	2.438537000	-1.900072000	0.134242000
C	3.080087000	-0.747016000	-0.392727000
C	1.814200000	-1.523685000	1.369314000
C	2.970373000	0.313522000	0.601275000
C	2.217815000	-0.171467000	1.689069000
C	2.434968000	-3.282657000	-0.438623000
H	3.097018000	-3.924329000	0.152378000
H	1.445095000	-3.743018000	-0.417655000
H	2.800221000	-3.306399000	-1.464582000
C	3.865199000	-0.636540000	-1.662184000
H	4.940469000	-0.649109000	-1.454762000
H	3.655851000	-1.458305000	-2.347176000
H	3.644959000	0.295079000	-2.187064000
C	3.587577000	1.666163000	0.451919000
H	4.671001000	1.606229000	0.600663000
H	3.418809000	2.068369000	-0.548340000
H	3.197798000	2.381316000	1.176619000
C	1.915023000	0.546113000	2.965907000
H	2.617099000	0.236720000	3.747419000
H	2.000665000	1.627948000	2.861041000
H	0.910097000	0.329790000	3.331473000
C	1.093874000	-2.462603000	2.287146000
H	0.485576000	-3.186626000	1.742535000
H	1.814637000	-3.032048000	2.884700000
H	0.444906000	-1.938320000	2.988974000
O	1.028570000	1.219474000	-1.452794000
C	-0.682875000	1.897074000	-0.050225000
C	0.092861000	3.301591000	-1.803641000
C	-0.629106000	0.595981000	0.524679000
C	-1.494879000	2.947847000	0.453665000
C	-0.765696000	4.326350000	-1.390315000
H	0.780939000	3.375841000	-2.633800000
C	-1.340319000	0.430998000	1.706784000
C	-2.206524000	2.699095000	1.654951000
C	-1.532234000	4.171657000	-0.257627000
H	-0.778383000	5.247171000	-1.959487000
C	-2.096376000	1.476249000	2.276972000
H	-1.376648000	-0.546166000	2.174741000
H	-2.829414000	3.482123000	2.072717000
H	-2.160223000	4.980103000	0.099501000
H	-2.630761000	1.293605000	3.203021000
N	0.141429000	2.151193000	-1.124177000
C	-0.022619000	-1.177993000	-1.481602000
C	-1.000636000	-0.866621000	-0.716789000
C	-2.369123000	-1.323114000	-0.453569000
C	-2.593230000	-2.684527000	-0.198698000
C	-3.469593000	-0.456706000	-0.542487000
C	-3.888960000	-3.168099000	-0.036571000
H	-1.748366000	-3.361150000	-0.132323000
C	-4.760881000	-0.945634000	-0.390632000
H	-3.311698000	0.595946000	-0.747809000
C	-4.973889000	-2.300620000	-0.131887000
H	-4.049427000	-4.222495000	0.160626000
H	-5.605537000	-0.270811000	-0.477905000
H	-5.983427000	-2.677314000	-0.008545000
C	0.269702000	-1.802793000	-2.787105000
H	0.762334000	-1.081835000	-3.445566000
H	0.935038000	-2.662143000	-2.690680000
H	-0.652293000	-2.135479000	-3.273399000

35			
Ni	1.121959000	-0.530618000	-0.149647000
C	2.302144000	-2.183655000	0.392738000
C	2.888551000	-1.376831000	-0.646038000
C	2.107929000	-1.335726000	1.511243000
C	3.250239000	-0.084534000	-0.060858000
C	2.757545000	-0.051889000	1.243973000
C	2.020669000	-3.650592000	0.331704000
H	2.870985000	-4.196637000	0.755134000
H	1.139065000	-3.932315000	0.908699000
H	1.888233000	-4.006971000	-0.688963000
C	3.286357000	-1.831585000	-2.012671000
H	4.333264000	-2.156605000	-2.016870000
H	2.683092000	-2.672109000	-2.356305000
H	3.190733000	-1.030132000	-2.746804000
C	3.963589000	0.996832000	-0.806791000
H	5.007383000	0.715940000	-0.980011000
H	3.509778000	1.167149000	-1.785483000
H	3.965697000	1.942012000	-0.263477000
C	2.831844000	1.072890000	2.229804000
H	3.552982000	0.841578000	3.020769000
H	3.147181000	2.007259000	1.765355000
H	1.871550000	1.250988000	2.720082000
C	1.501238000	-1.721505000	2.823520000
H	0.822565000	-2.569133000	2.727700000
H	2.285135000	-2.008502000	3.533399000
H	0.947080000	-0.897500000	3.277120000
O	0.754059000	0.684782000	-1.646610000
C	-0.555864000	1.906123000	-0.119197000
C	0.570938000	2.939157000	-1.957368000
C	-1.112326000	0.726825000	0.478279000
C	-0.799066000	3.203588000	0.429818000
C	0.212269000	4.215604000	-1.517580000
H	1.174459000	2.744384000	-2.832574000
C	-1.703816000	0.910948000	1.728511000
C	-1.441145000	3.303250000	1.686617000
C	-0.416937000	4.352528000	-0.305219000
H	0.495765000	5.071738000	-2.116141000
C	-1.839331000	2.165595000	2.345179000
H	-2.151119000	0.046824000	2.206146000
H	-1.613679000	4.286048000	2.110918000
H	-0.633541000	5.334345000	0.100169000
H	-2.317028000	2.232996000	3.316053000
N	0.245858000	1.848564000	-1.256598000
C	-0.450778000	-1.396658000	-0.717899000
C	-1.409981000	-0.597577000	-0.221037000
C	-2.867887000	-0.950791000	-0.229488000
C	-3.316983000	-2.190105000	0.244266000
C	-3.813578000	-0.043409000	-0.730610000
C	-4.670167000	-2.520412000	0.206048000
H	-2.602189000	-2.895732000	0.654553000
C	-5.163357000	-0.375480000	-0.774078000
H	-3.489463000	0.923451000	-1.103308000
C	-5.596668000	-1.615379000	-0.304897000
H	-4.999641000	-3.483990000	0.580283000
H	-5.879124000	0.332707000	-1.178284000
H	-6.650129000	-1.871569000	-0.335562000
C	-0.632087000	-2.611321000	-1.560977000
H	0.023503000	-2.562549000	-2.436597000
H	-0.379265000	-3.531581000	-1.028534000
H	-1.659683000	-2.708961000	-1.919891000

36ts			
C	-0.818681000	4.234236000	-1.011744000
C	0.224107000	4.545641000	-0.172457000
C	1.136108000	3.550697000	0.264235000
C	0.938740000	2.192624000	-0.175529000
C	-0.992054000	2.912768000	-1.421382000
H	2.391396000	4.855841000	1.426630000
H	-1.512704000	4.985551000	-1.365633000
H	0.374284000	5.568155000	0.155726000
C	2.241860000	3.840850000	1.078462000
C	1.855305000	1.141468000	0.161529000
H	-1.775817000	2.564477000	-2.077628000
C	2.954610000	1.525950000	0.957212000
C	3.132410000	2.829782000	1.407619000
H	3.674590000	0.766355000	1.232874000
H	3.989627000	3.055358000	2.032564000
Ni	-1.406978000	-0.670285000	-0.461587000
O	-0.367863000	0.731603000	-1.568314000
N	-0.137633000	1.972242000	-0.997831000
C	1.663057000	-0.187105000	-0.327055000
C	0.436712000	-0.523312000	-0.888902000
C	2.744853000	-1.209805000	-0.262925000
C	3.961676000	-0.991031000	-0.928858000
C	2.573796000	-2.416567000	0.429449000
C	4.968254000	-1.951414000	-0.905616000
H	4.112826000	-0.066589000	-1.476852000
C	3.580251000	-3.380520000	0.448847000
H	1.652037000	-2.590223000	0.974947000
C	4.780151000	-3.150622000	-0.219018000
H	5.899007000	-1.766575000	-1.431520000
H	3.430248000	-4.306126000	0.994712000
H	5.565771000	-3.898124000	-0.202465000
C	-2.234890000	-2.113121000	0.756795000
C	-1.723502000	-1.078270000	1.594862000
C	-3.340168000	-1.571082000	-0.037279000
C	-2.354196000	0.132263000	1.174217000
C	-3.408480000	-0.197287000	0.212950000
C	-4.231630000	-2.377885000	-0.931716000
H	-3.689802000	-3.165552000	-1.459646000
H	-5.012842000	-2.872562000	-0.343953000
H	-4.730958000	-1.761630000	-1.680361000
C	-4.397162000	0.777574000	-0.351295000
H	-4.787219000	0.457860000	-1.318686000
H	-5.253449000	0.889415000	0.322932000
H	-3.967386000	1.773337000	-0.478287000
C	-2.156872000	1.475460000	1.806060000
H	-2.332748000	2.296468000	1.108181000
H	-2.864523000	1.609542000	2.632007000
H	-1.153988000	1.589218000	2.220077000
C	-0.692121000	-1.201889000	2.672034000
H	0.094643000	-0.449200000	2.581087000
H	-1.152088000	-1.075399000	3.657727000
H	-0.213600000	-2.181364000	2.667627000
C	-1.870371000	-3.566028000	0.814479000
H	-0.855551000	-3.723893000	1.181905000
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H	0.606203000	-2.541403000	-1.574152000
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37			
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39

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2,2,2-trifluoroethanol

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F	-0.452999000	-0.987568000	-0.905628000
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Acetic acid

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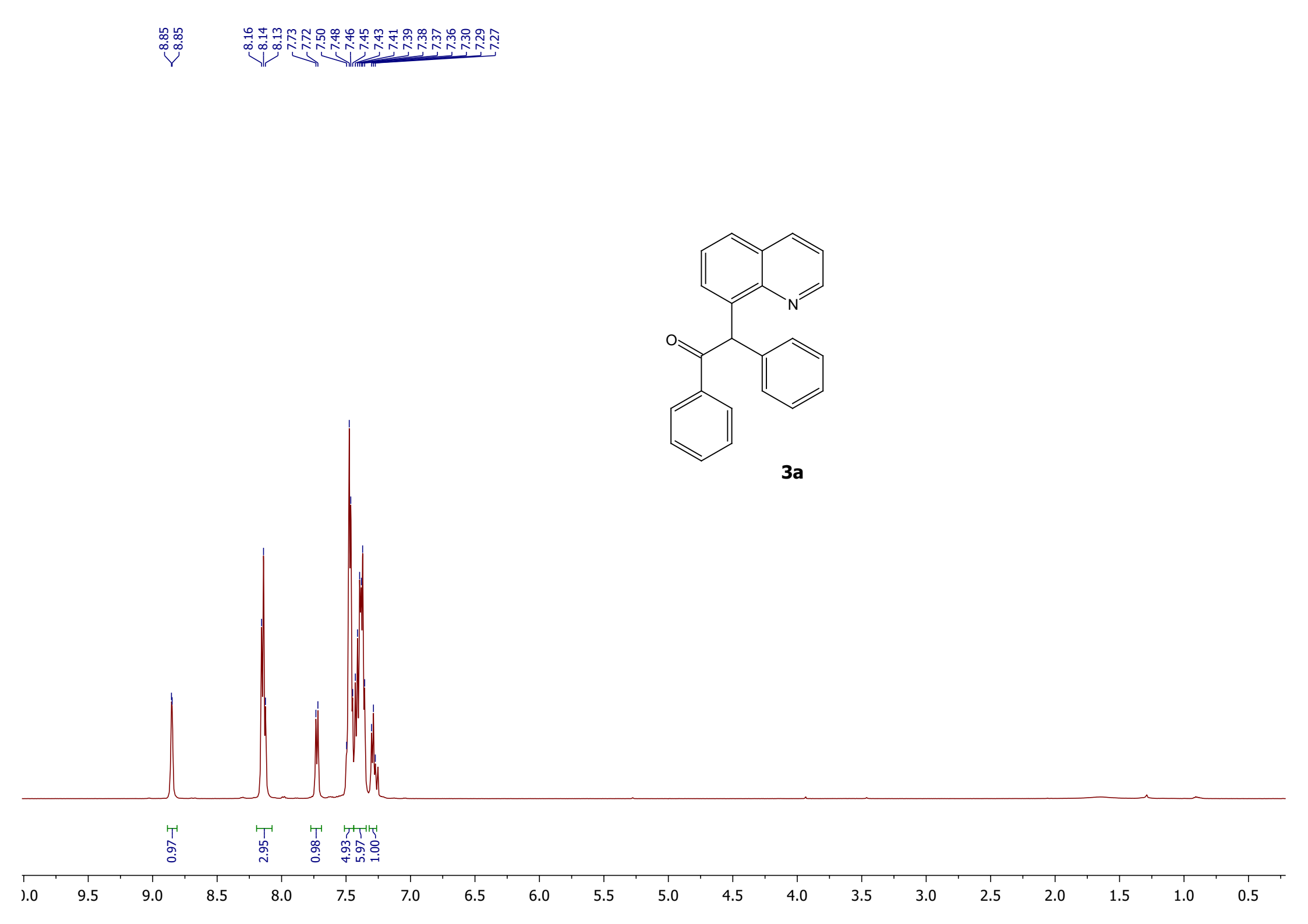
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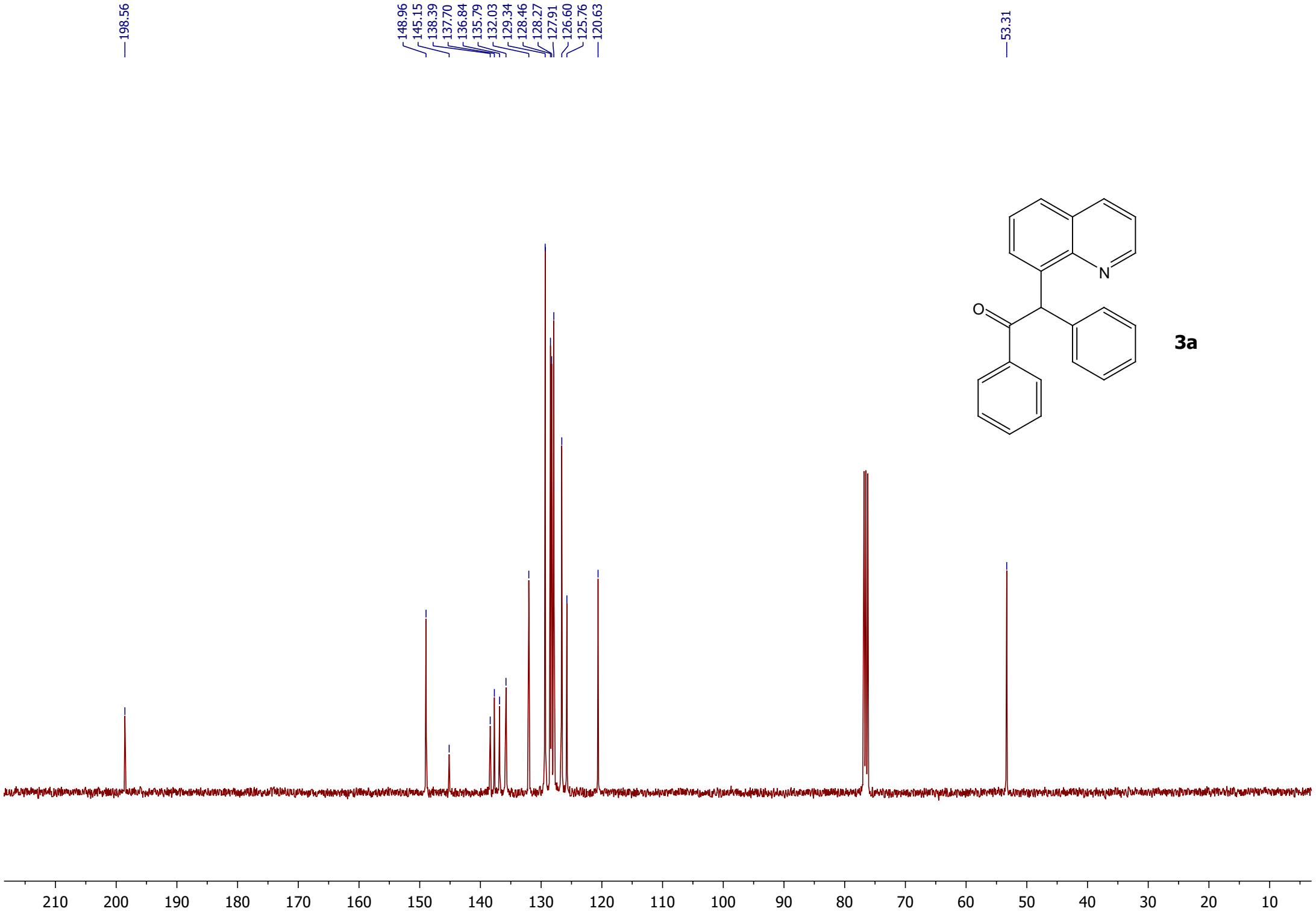
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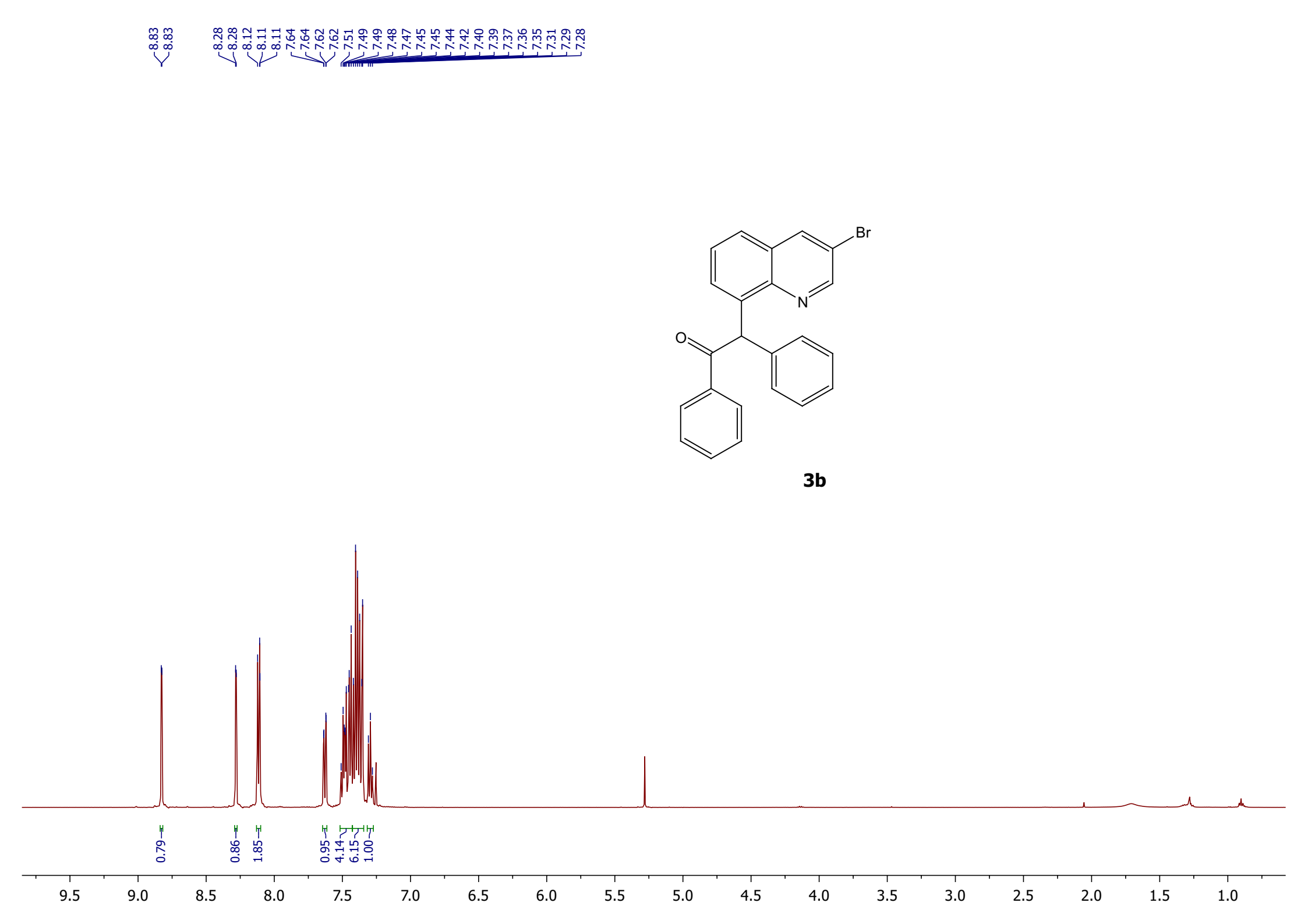
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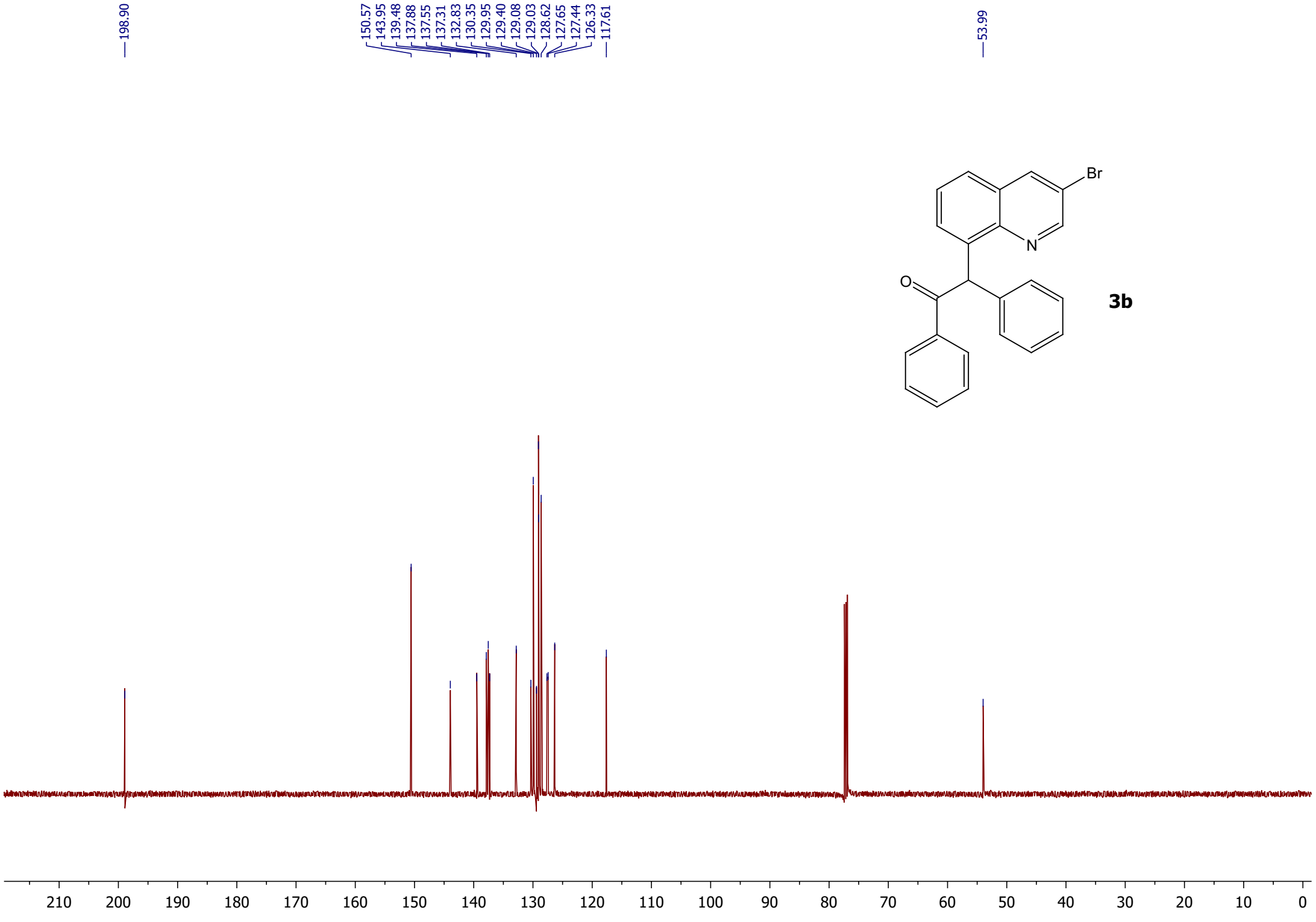
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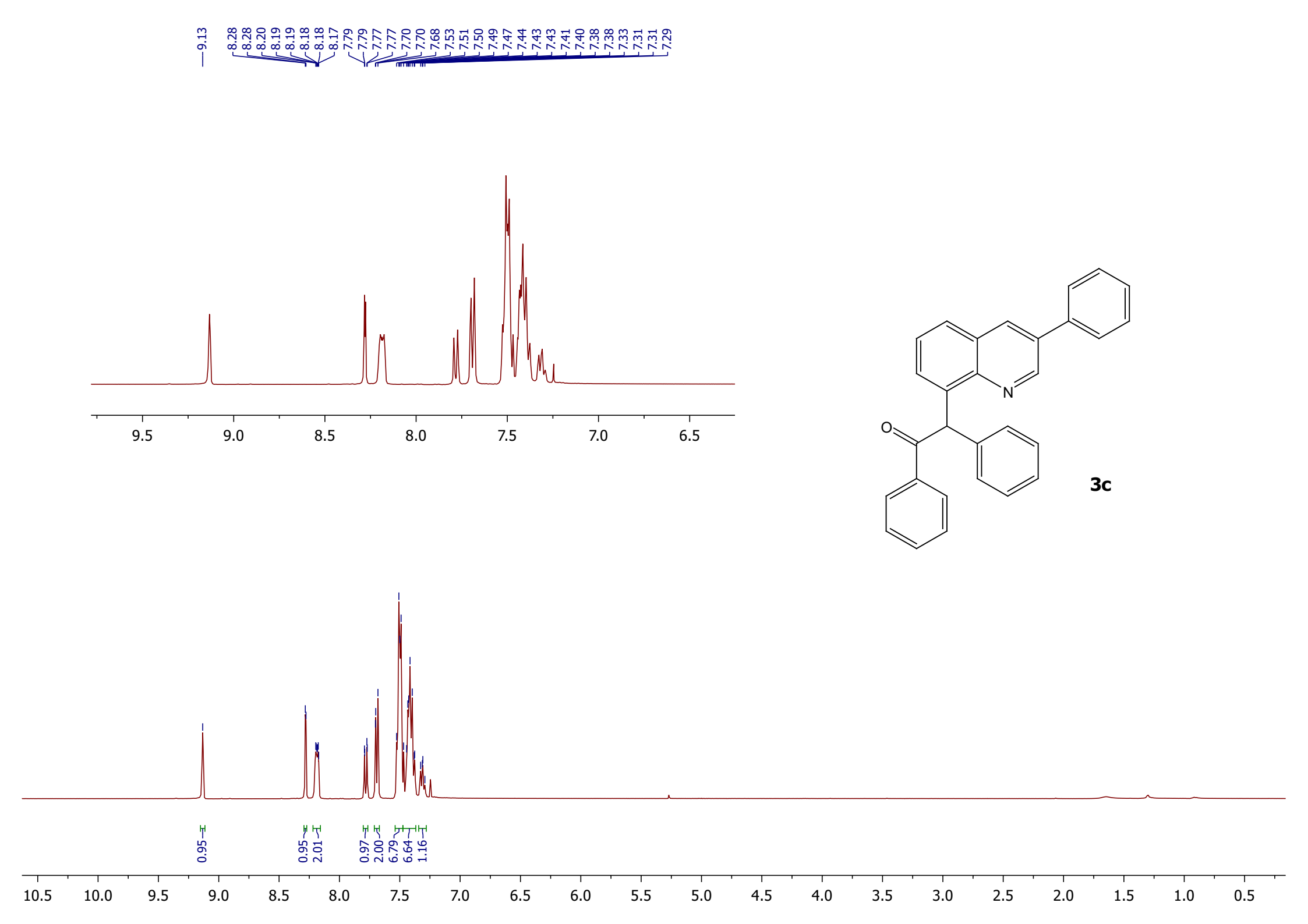
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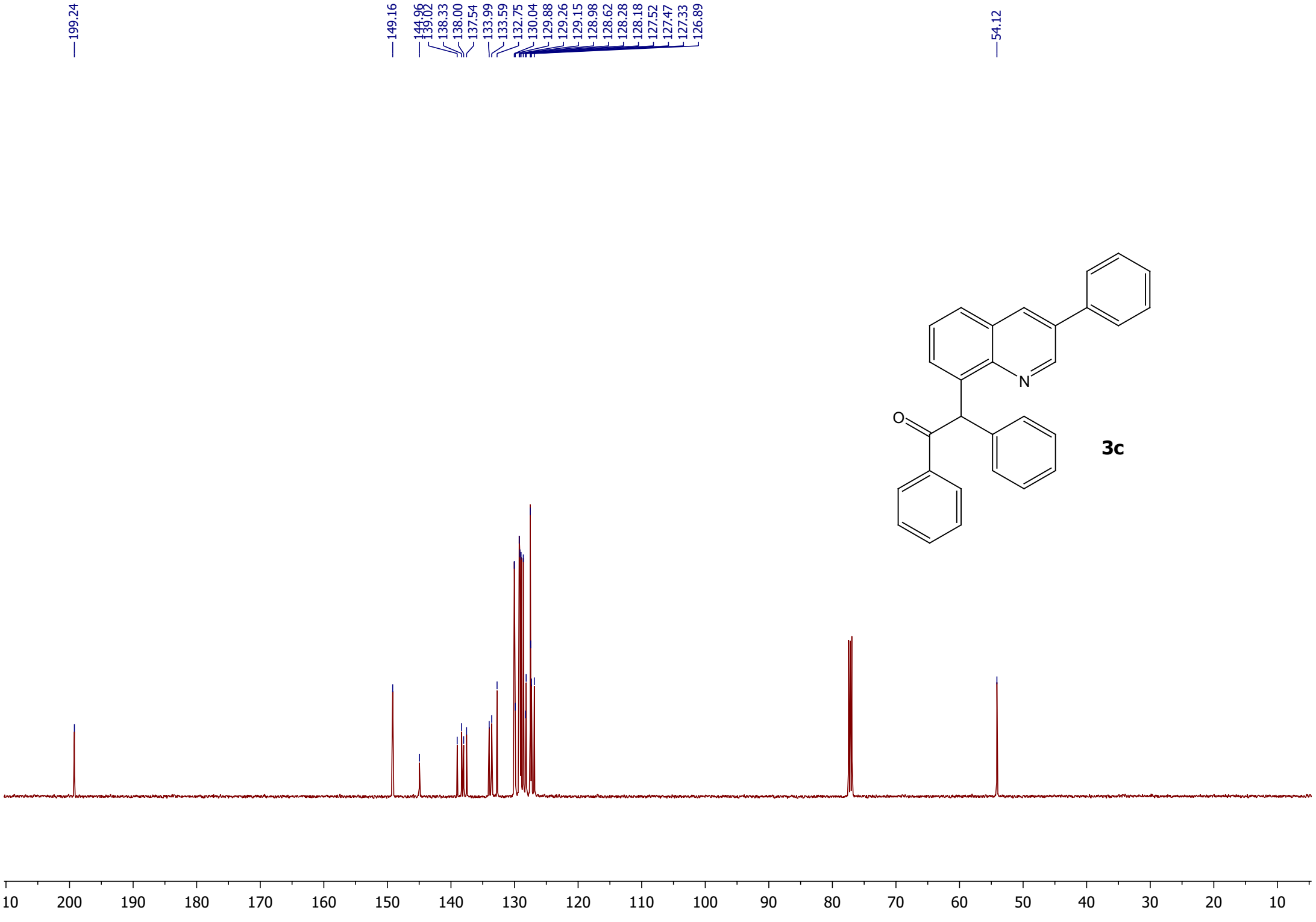
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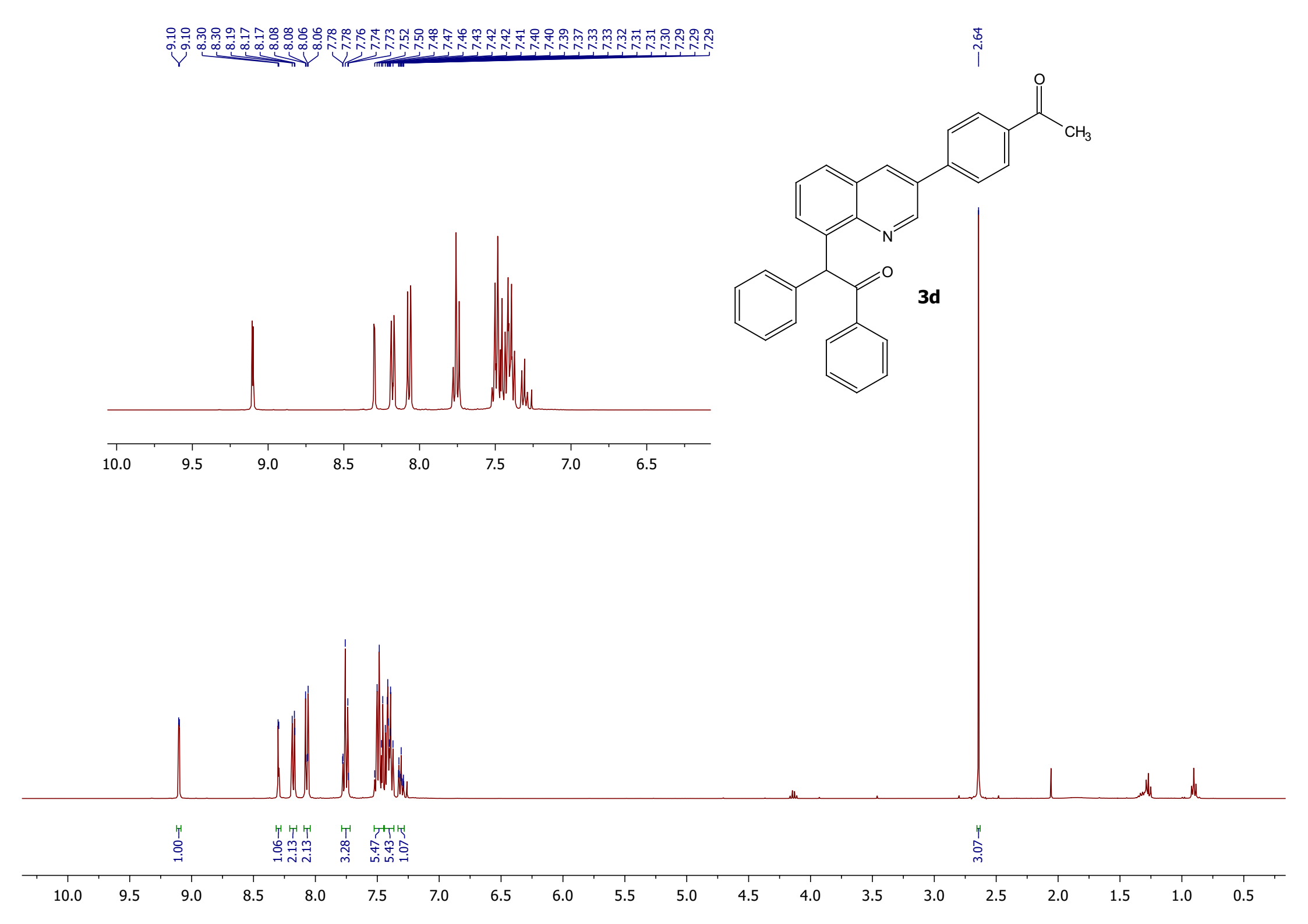
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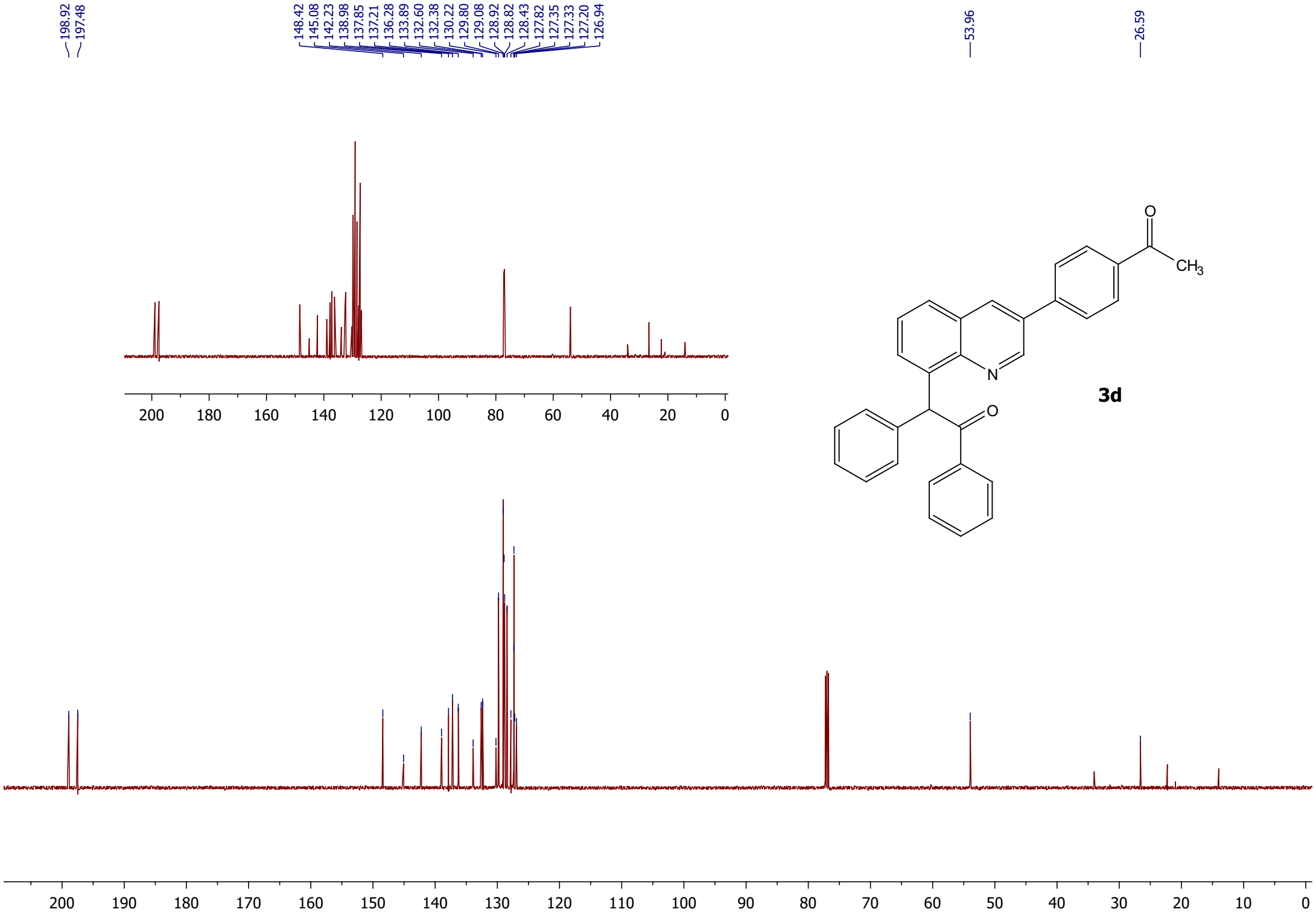
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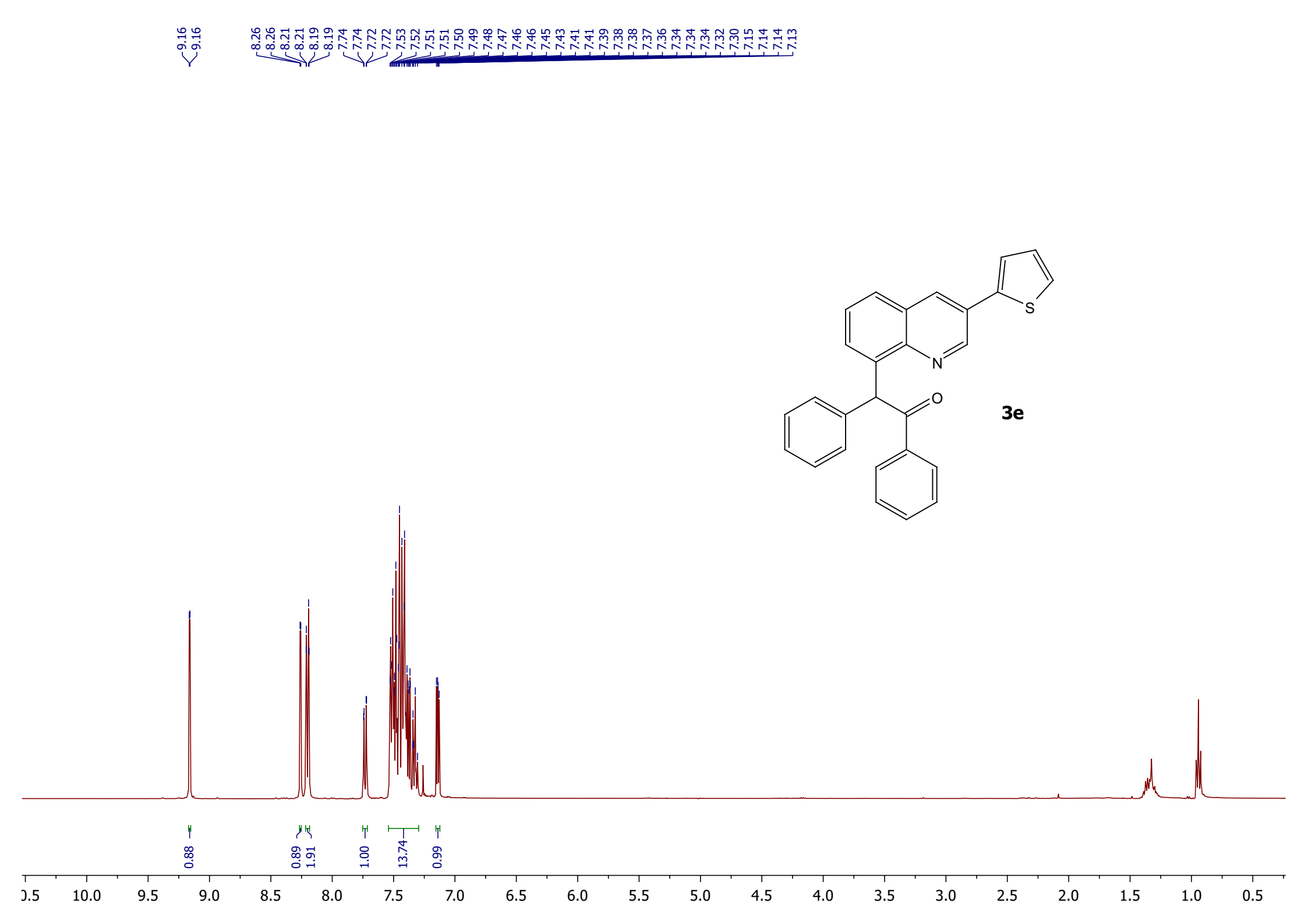
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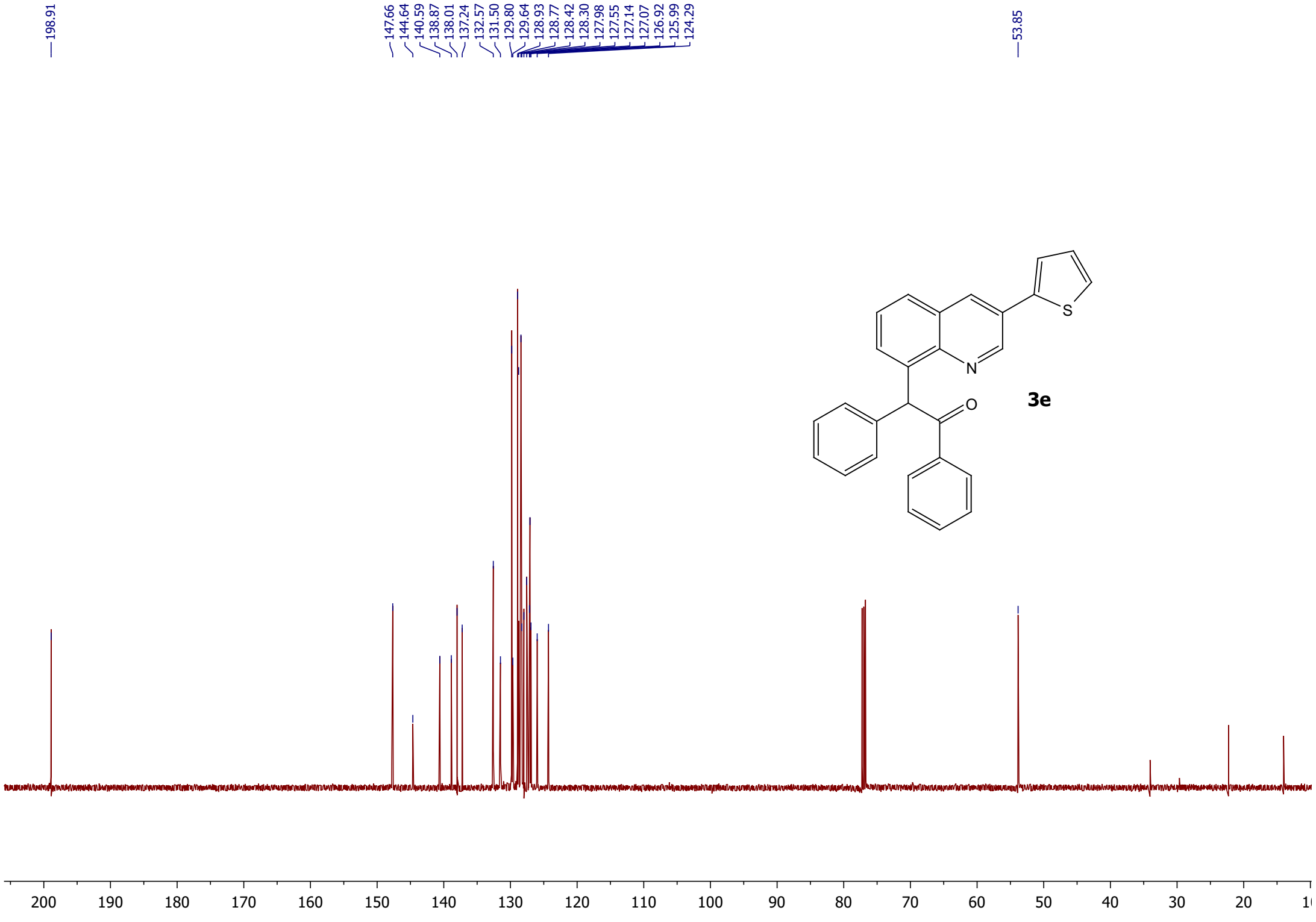
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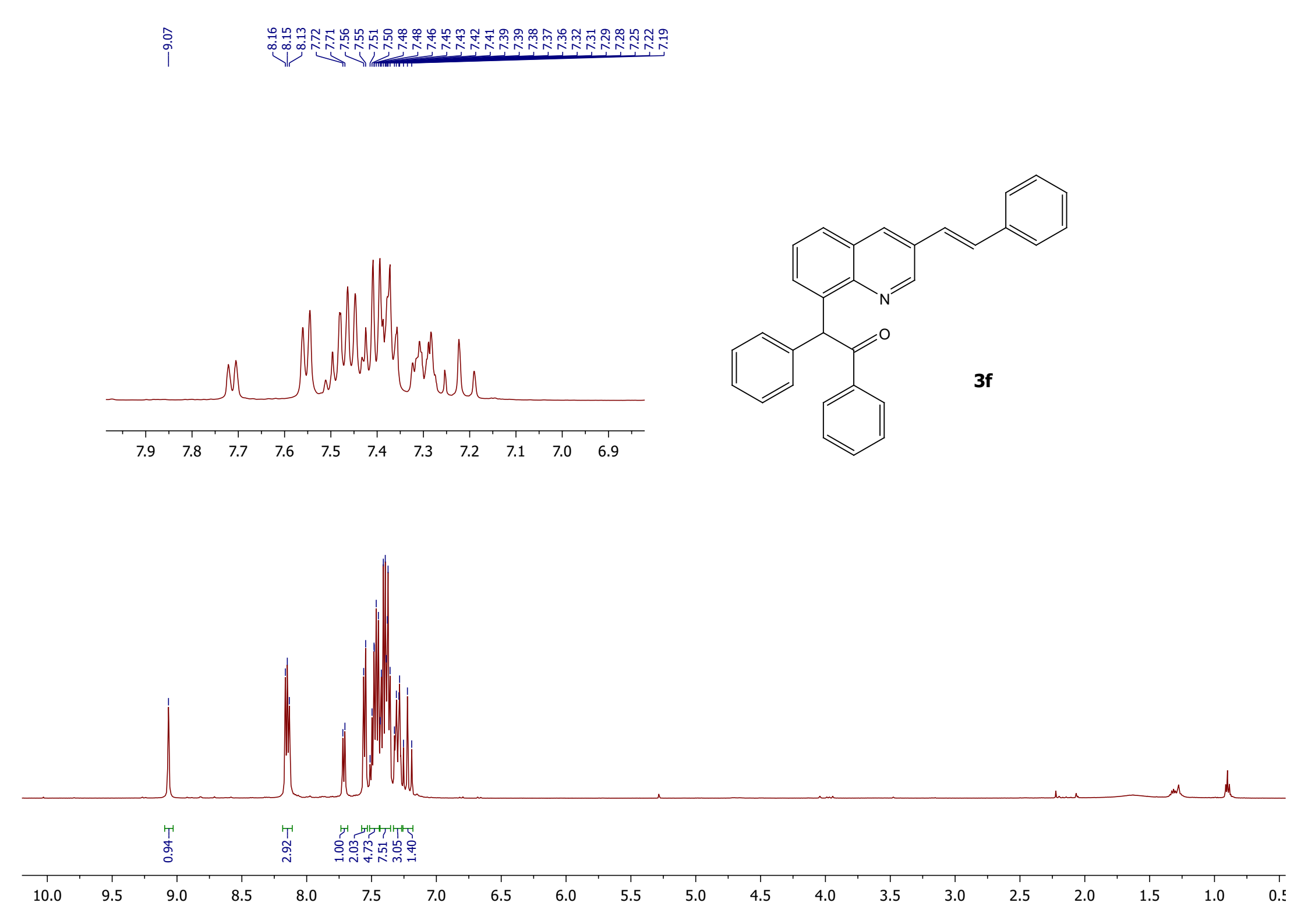
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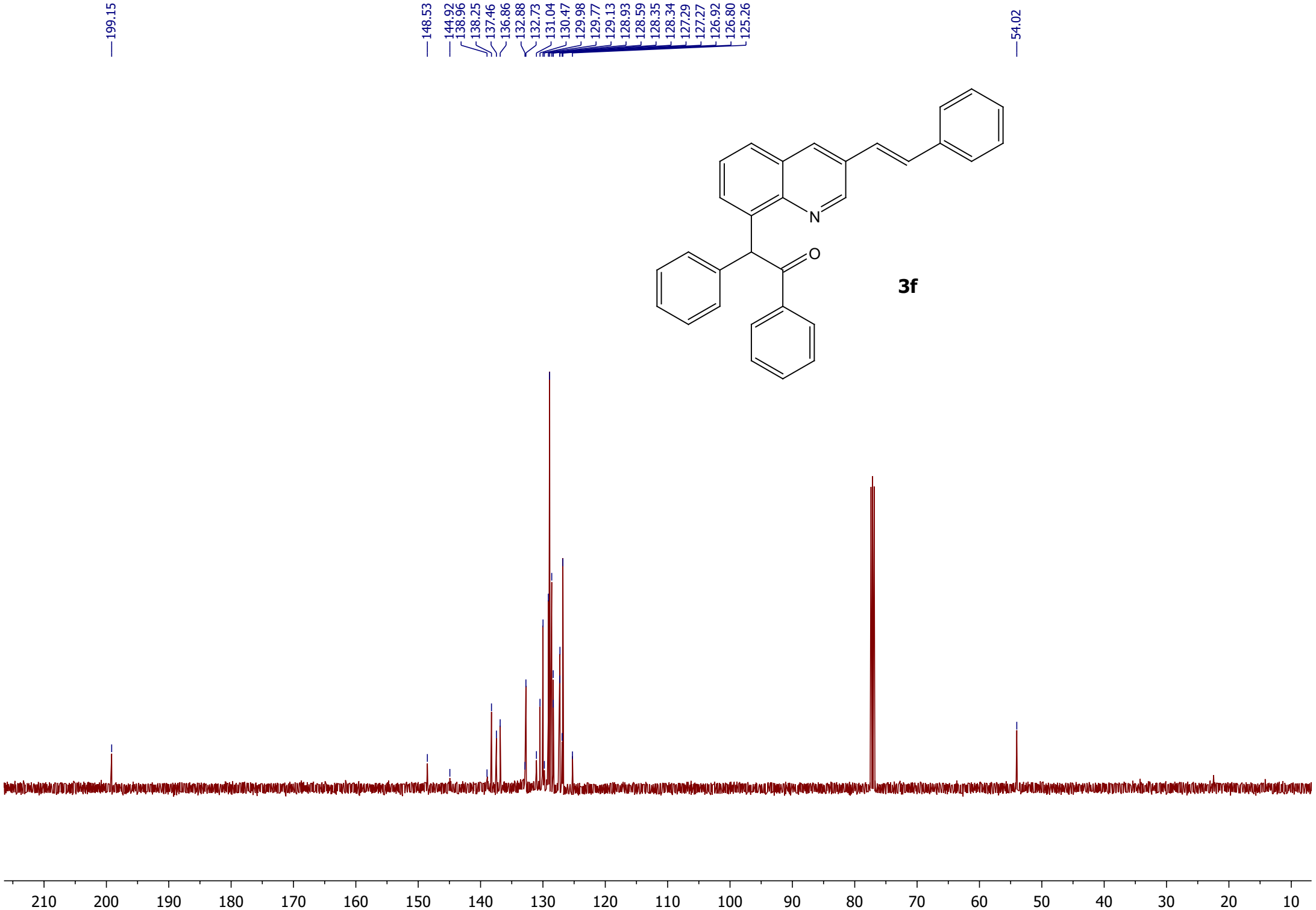
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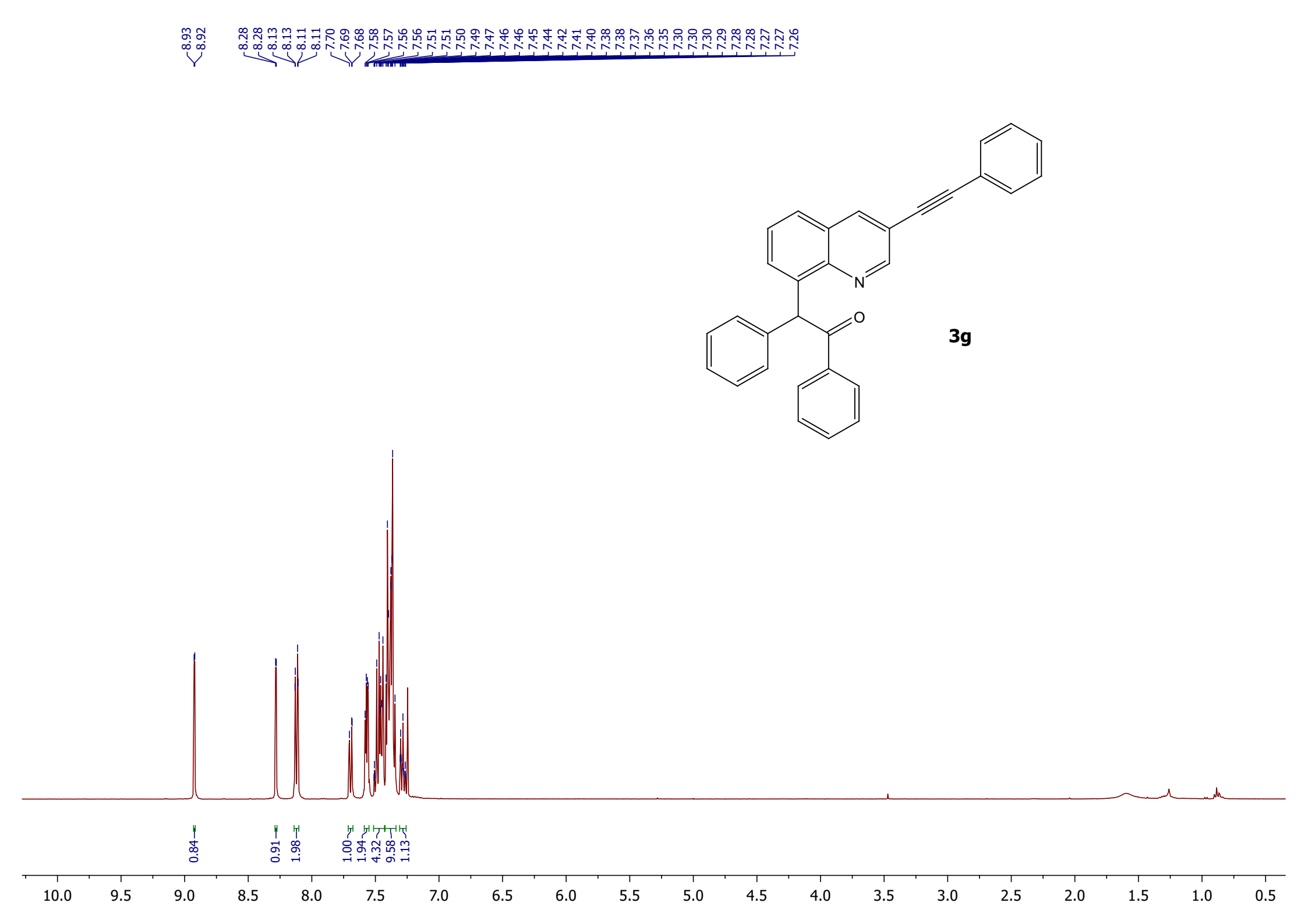
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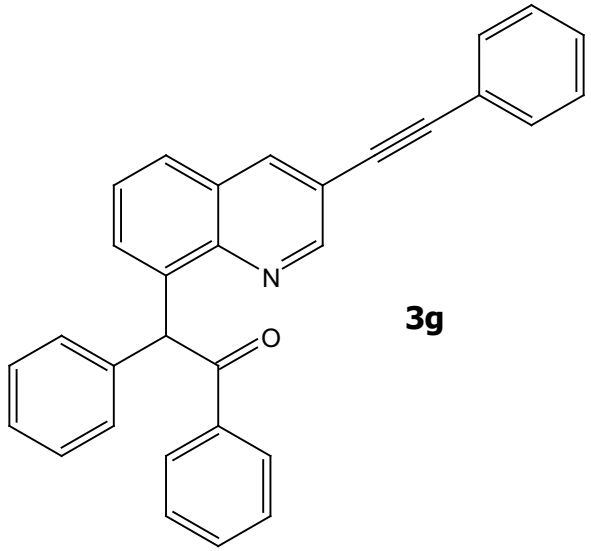

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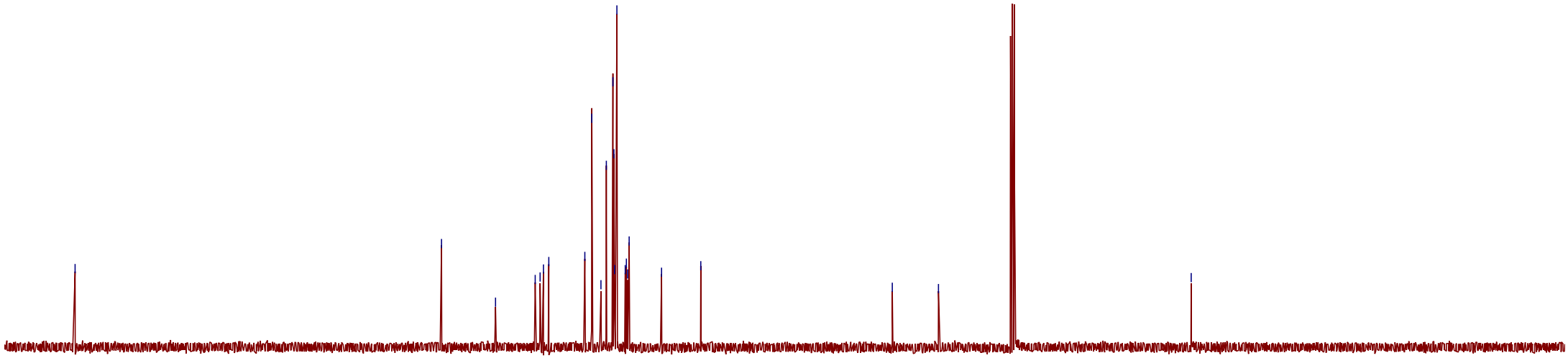

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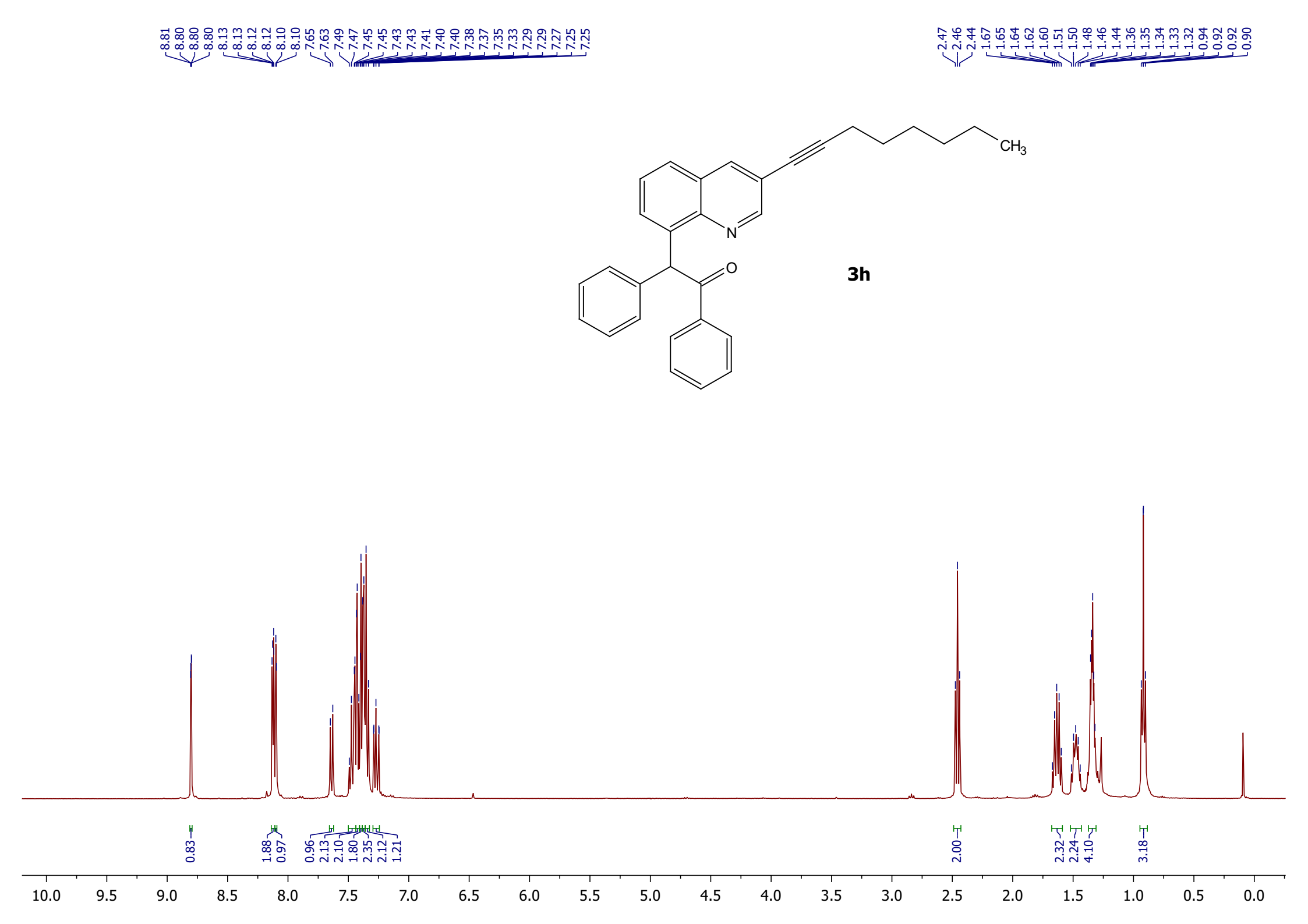
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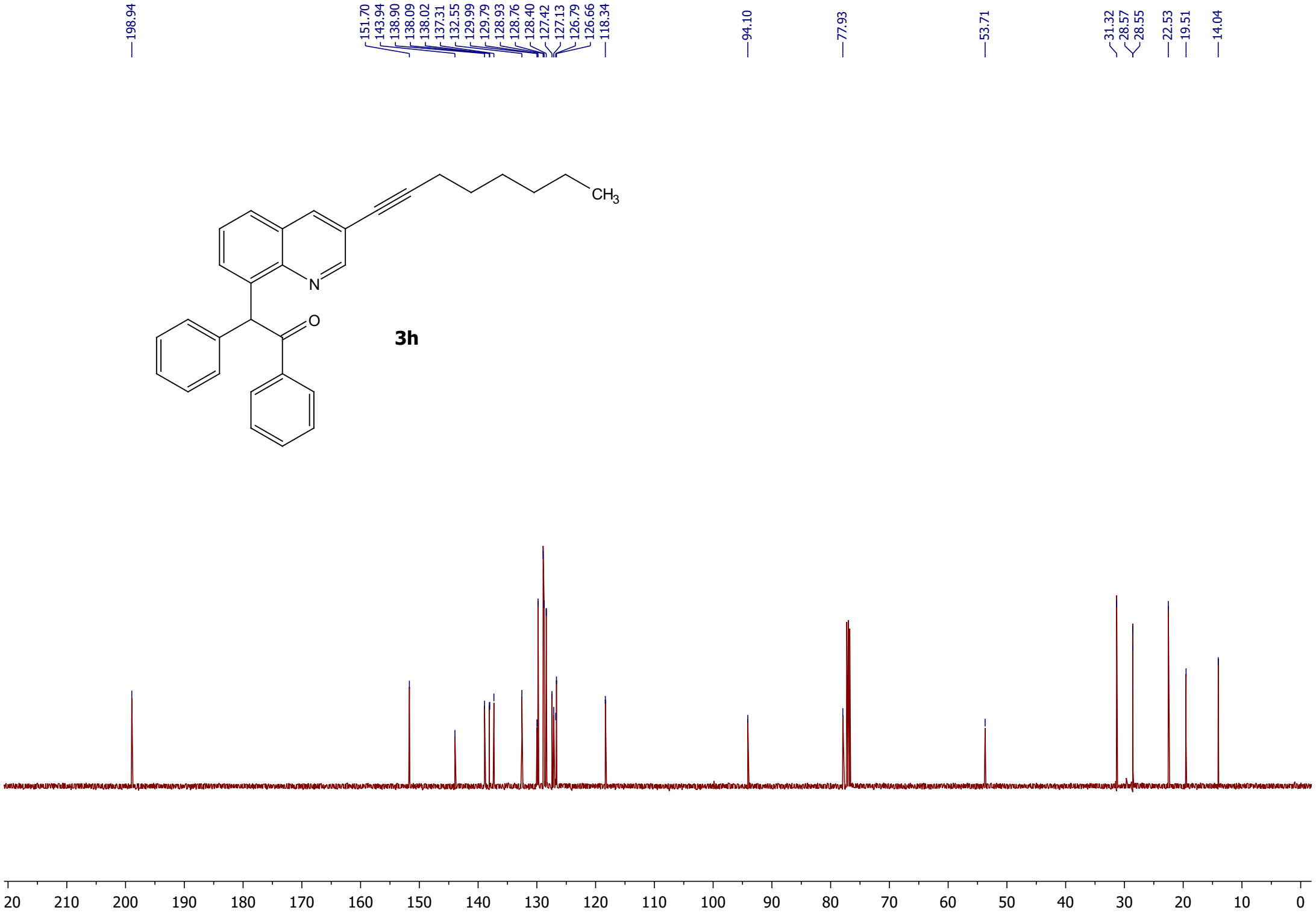
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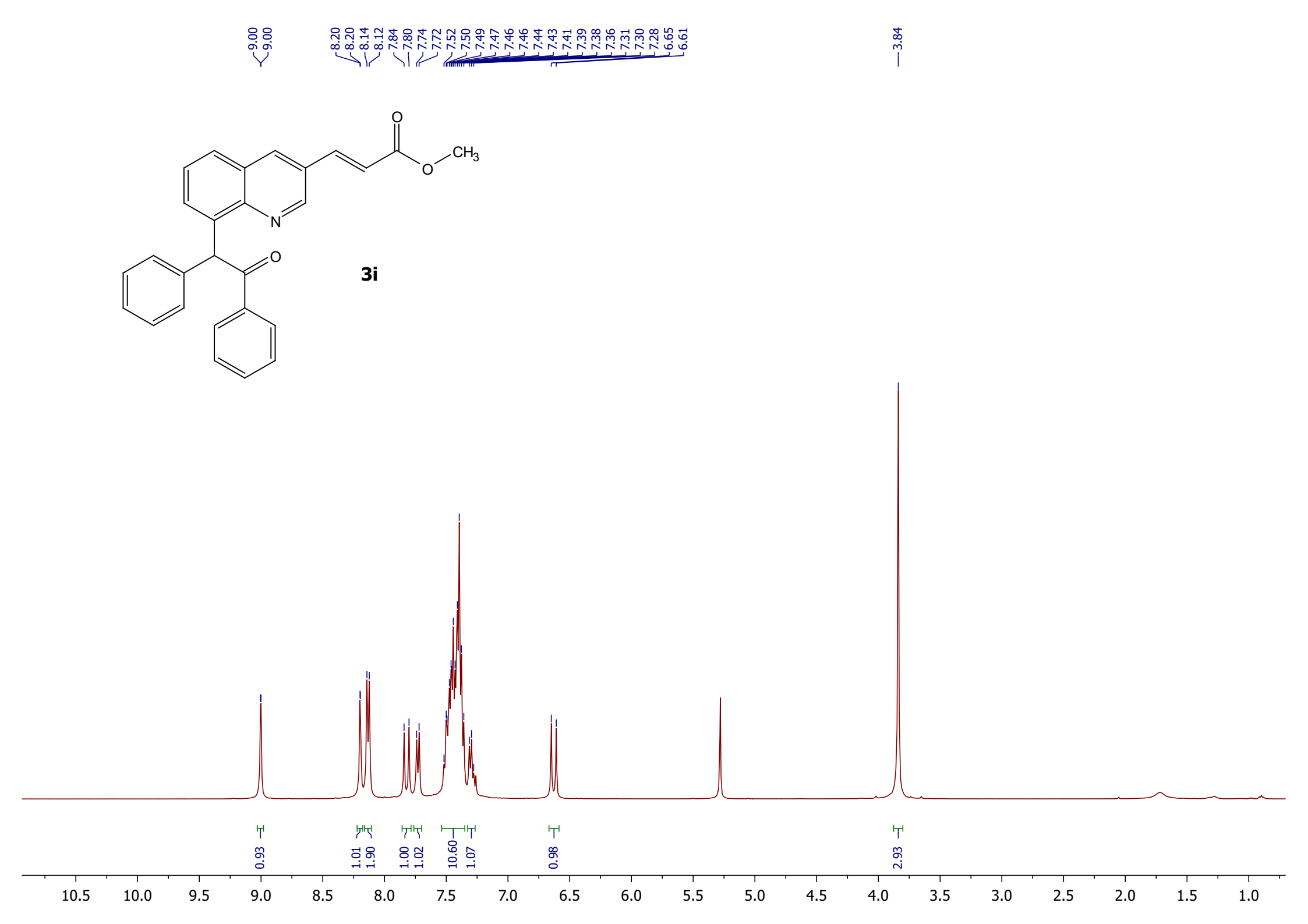
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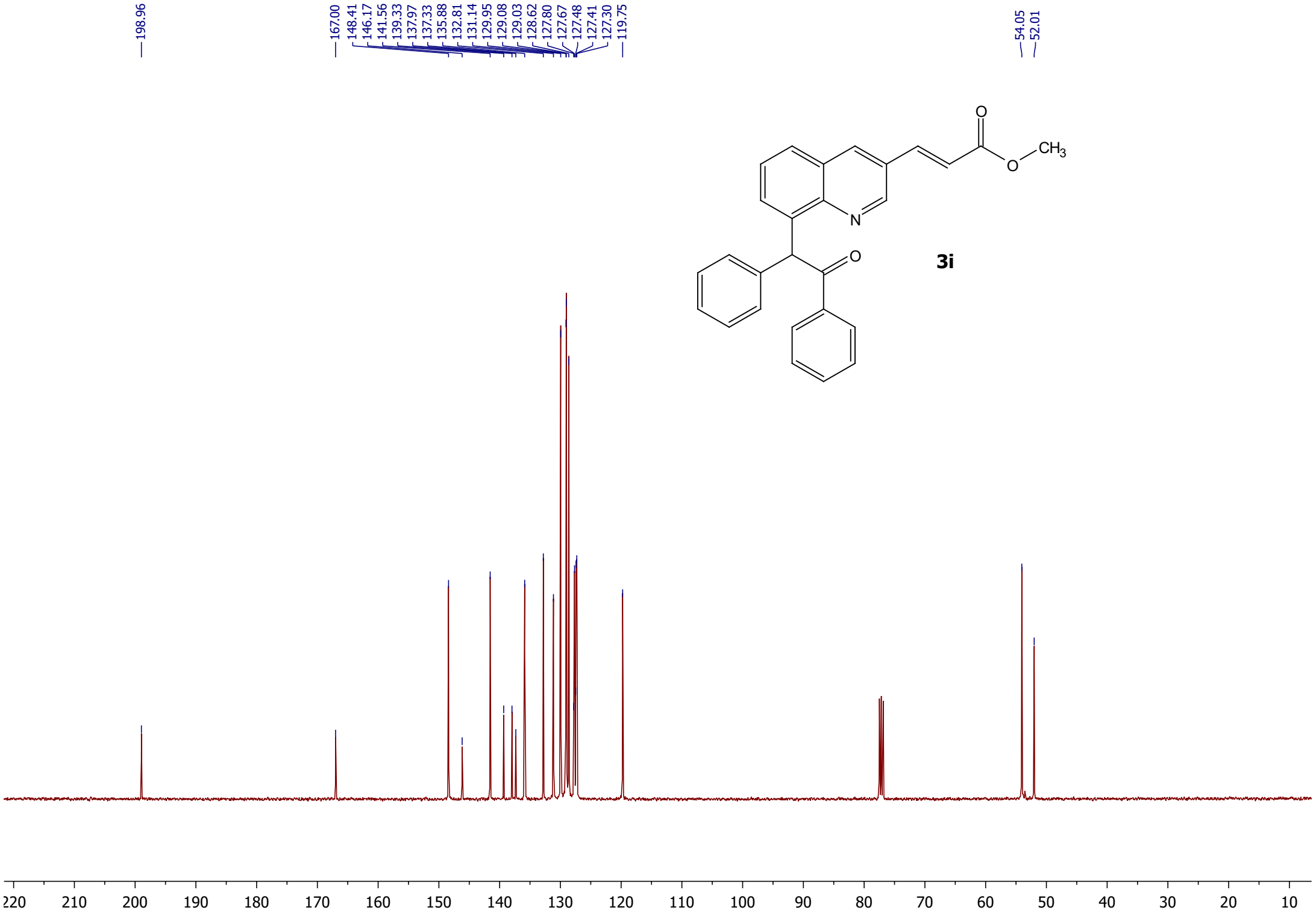
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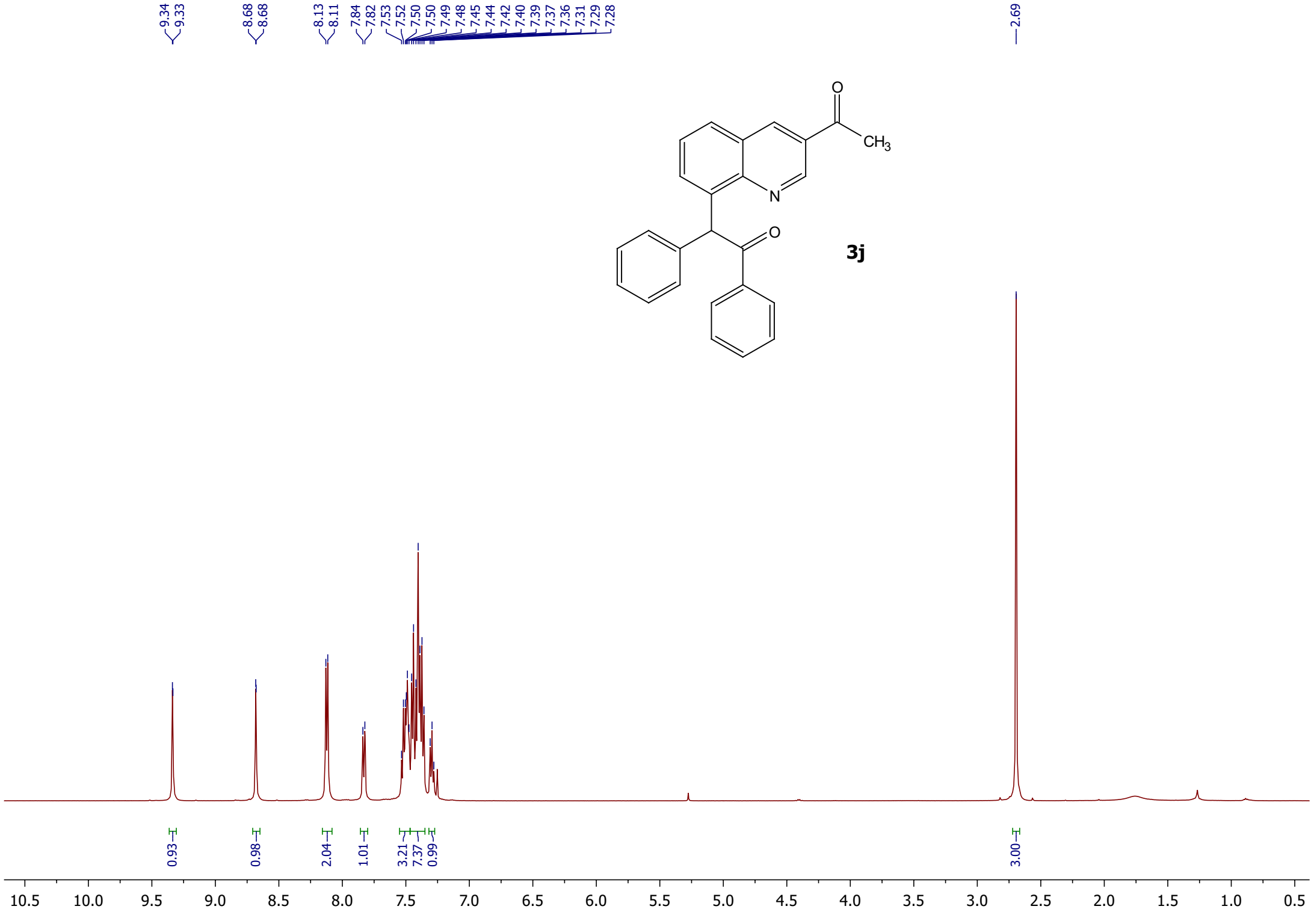
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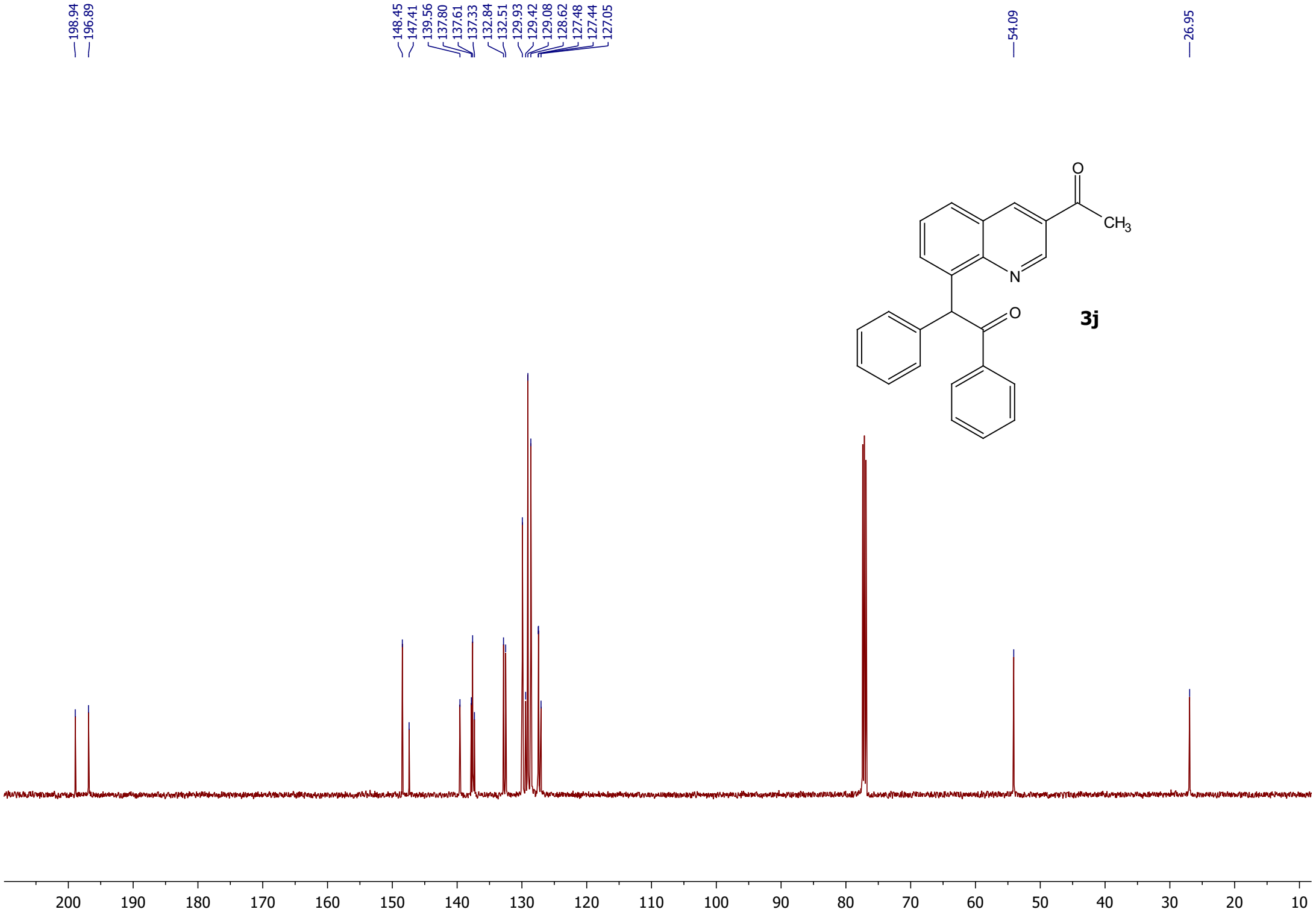
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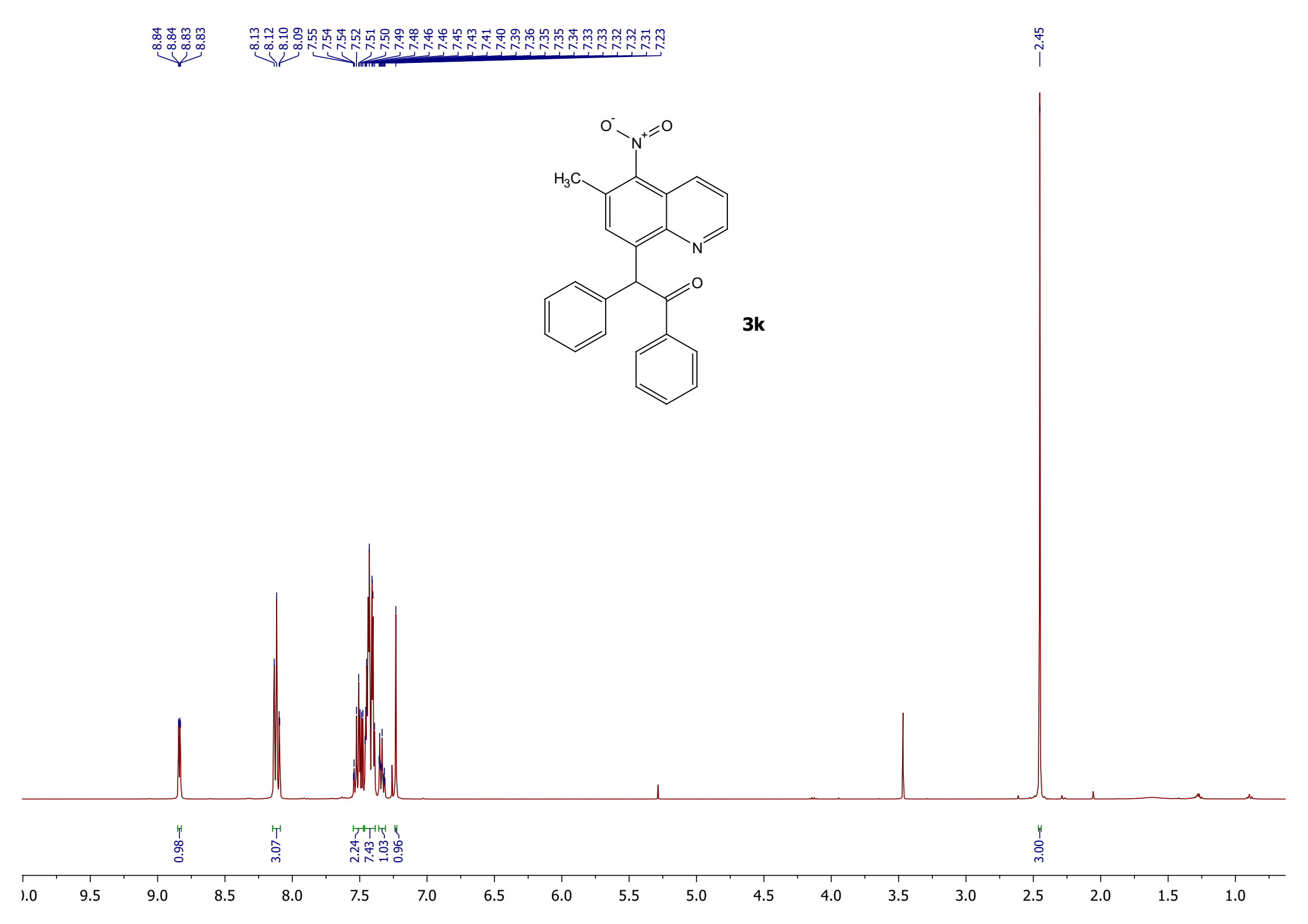
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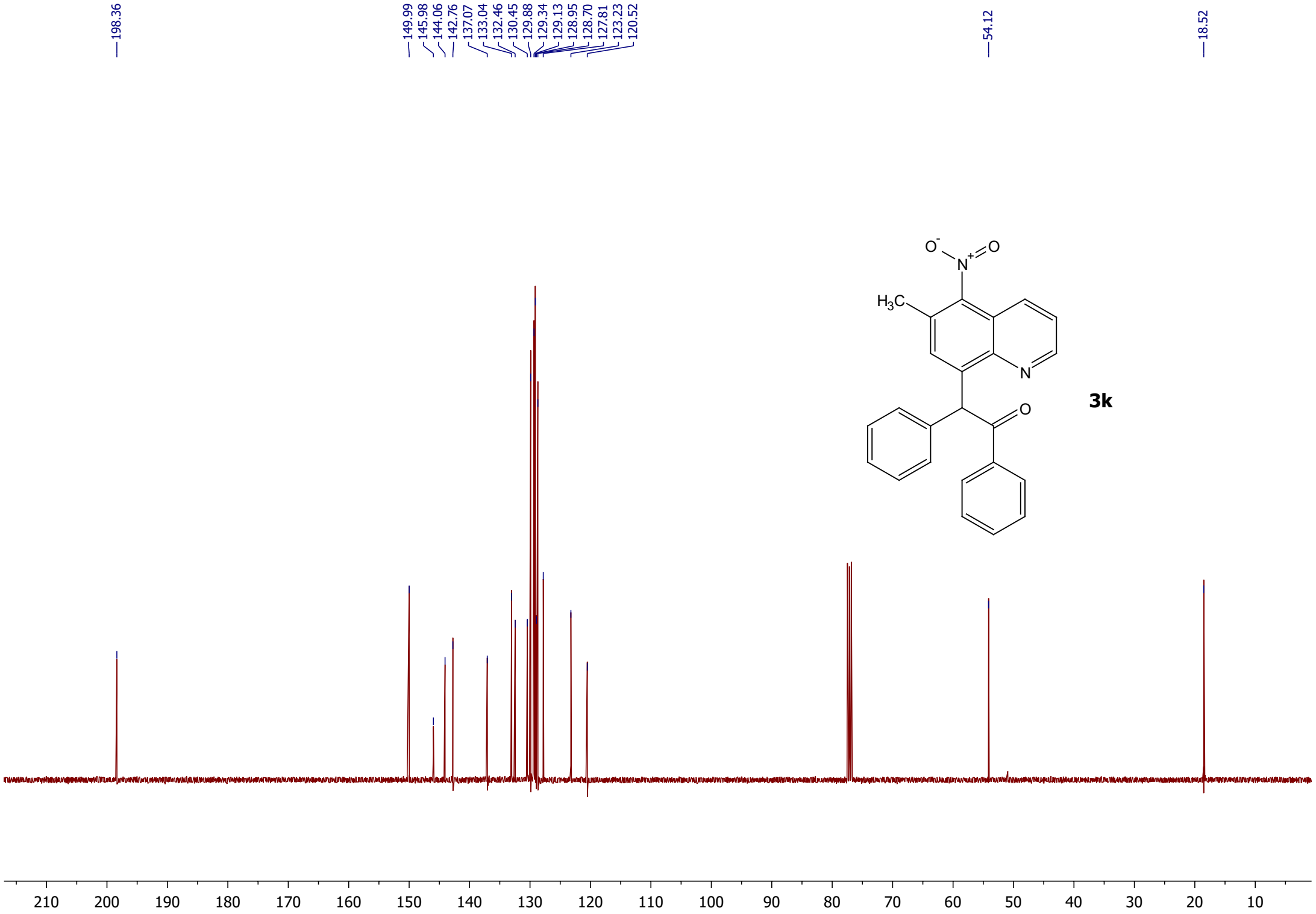
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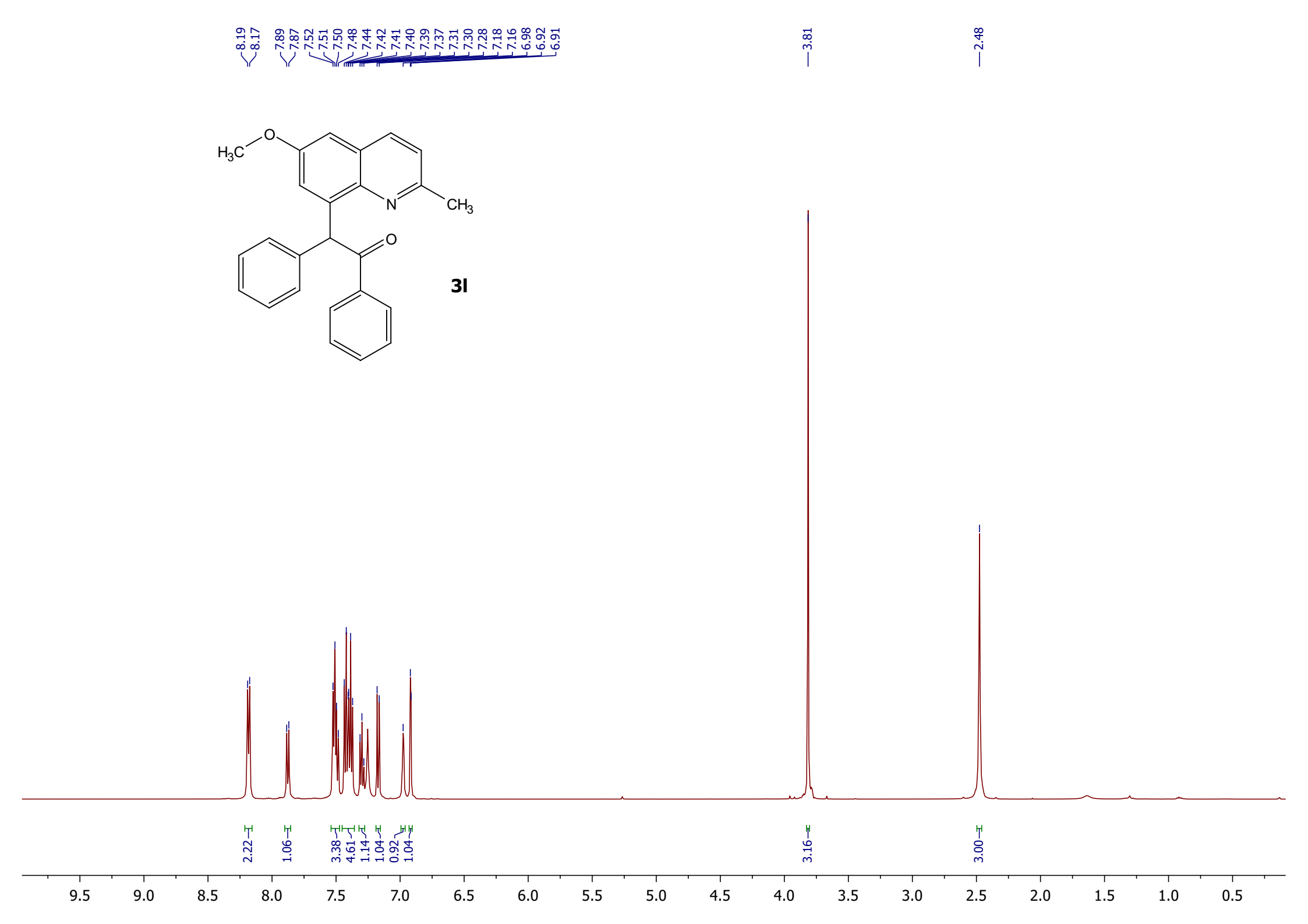
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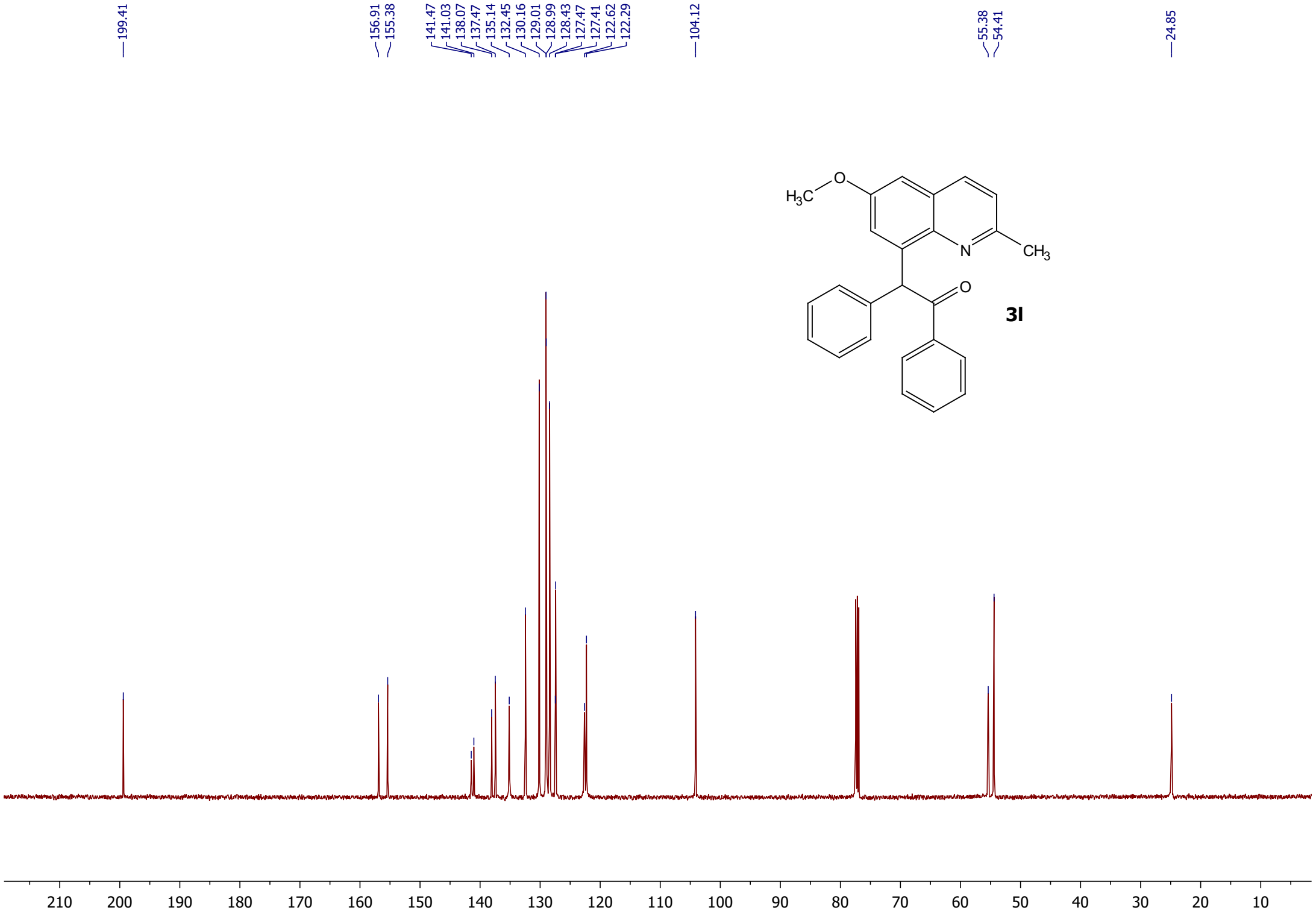
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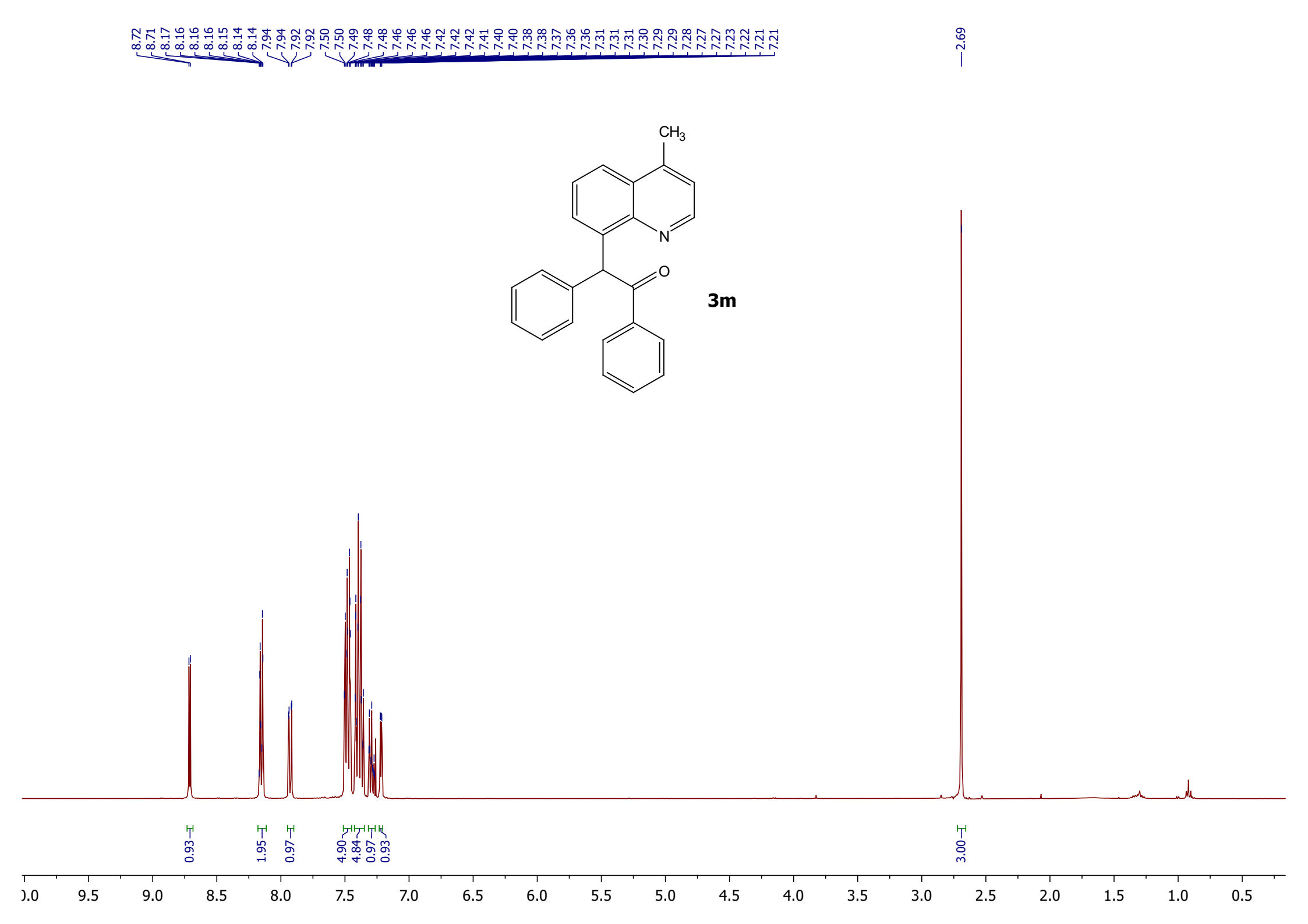
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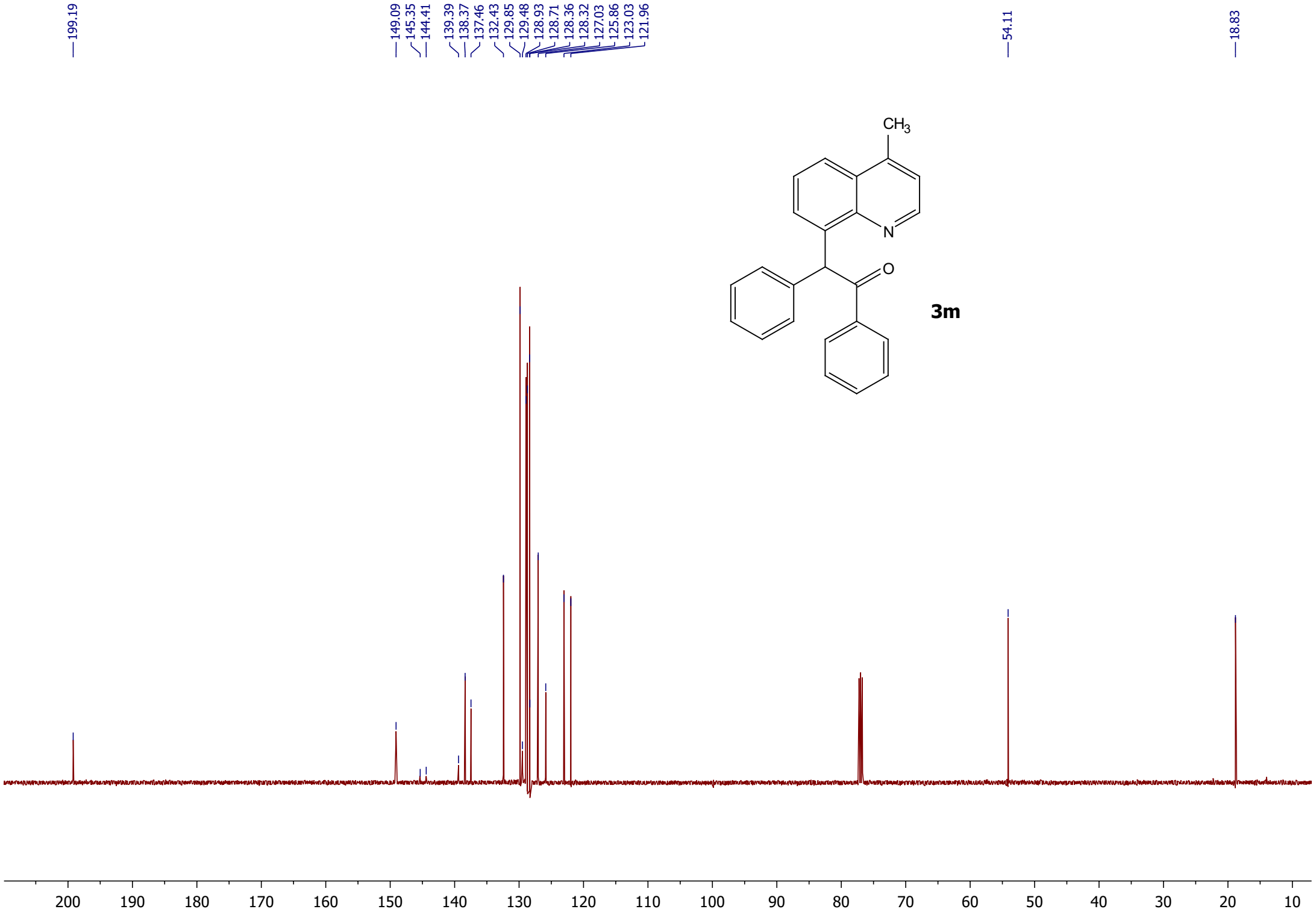
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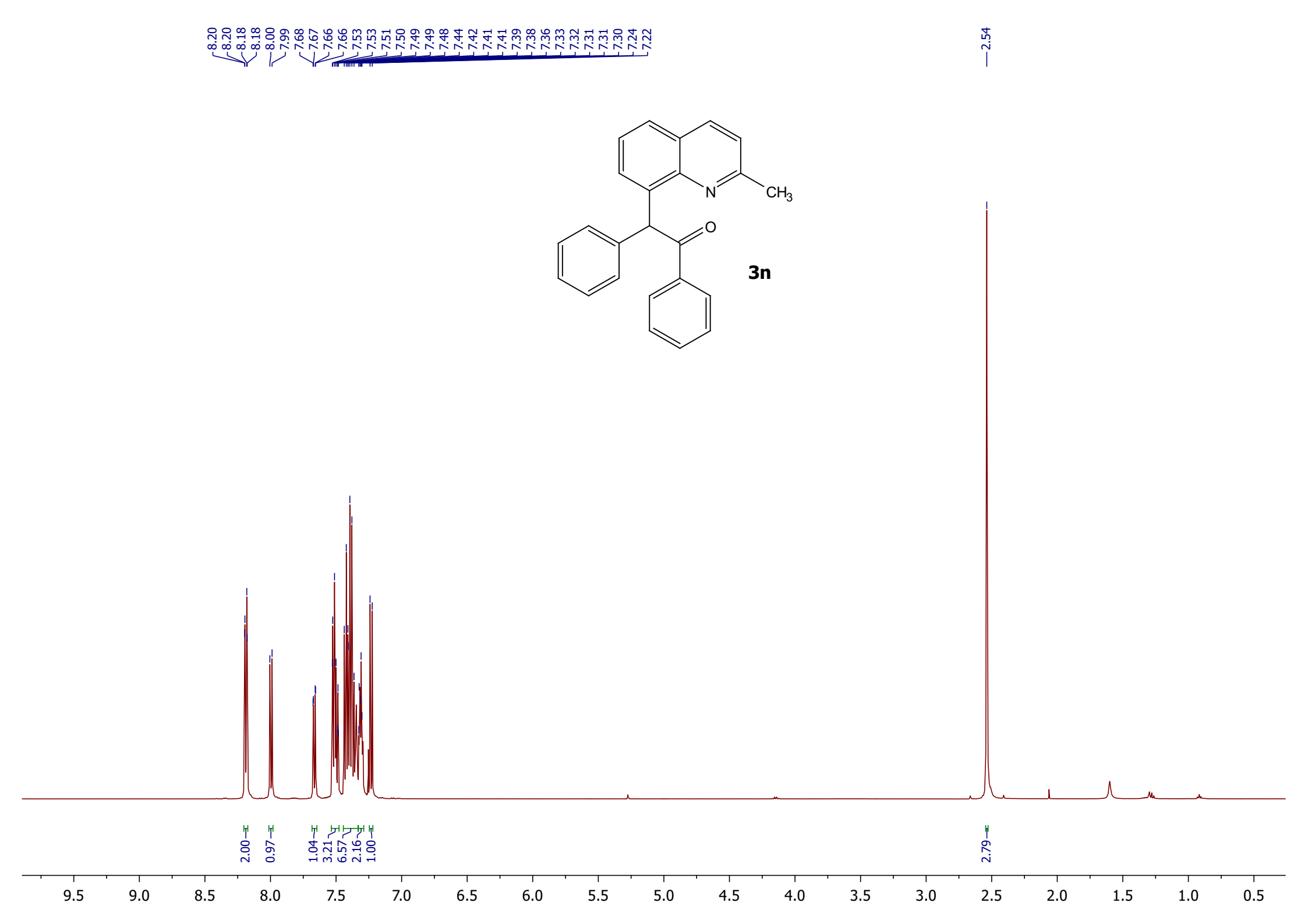
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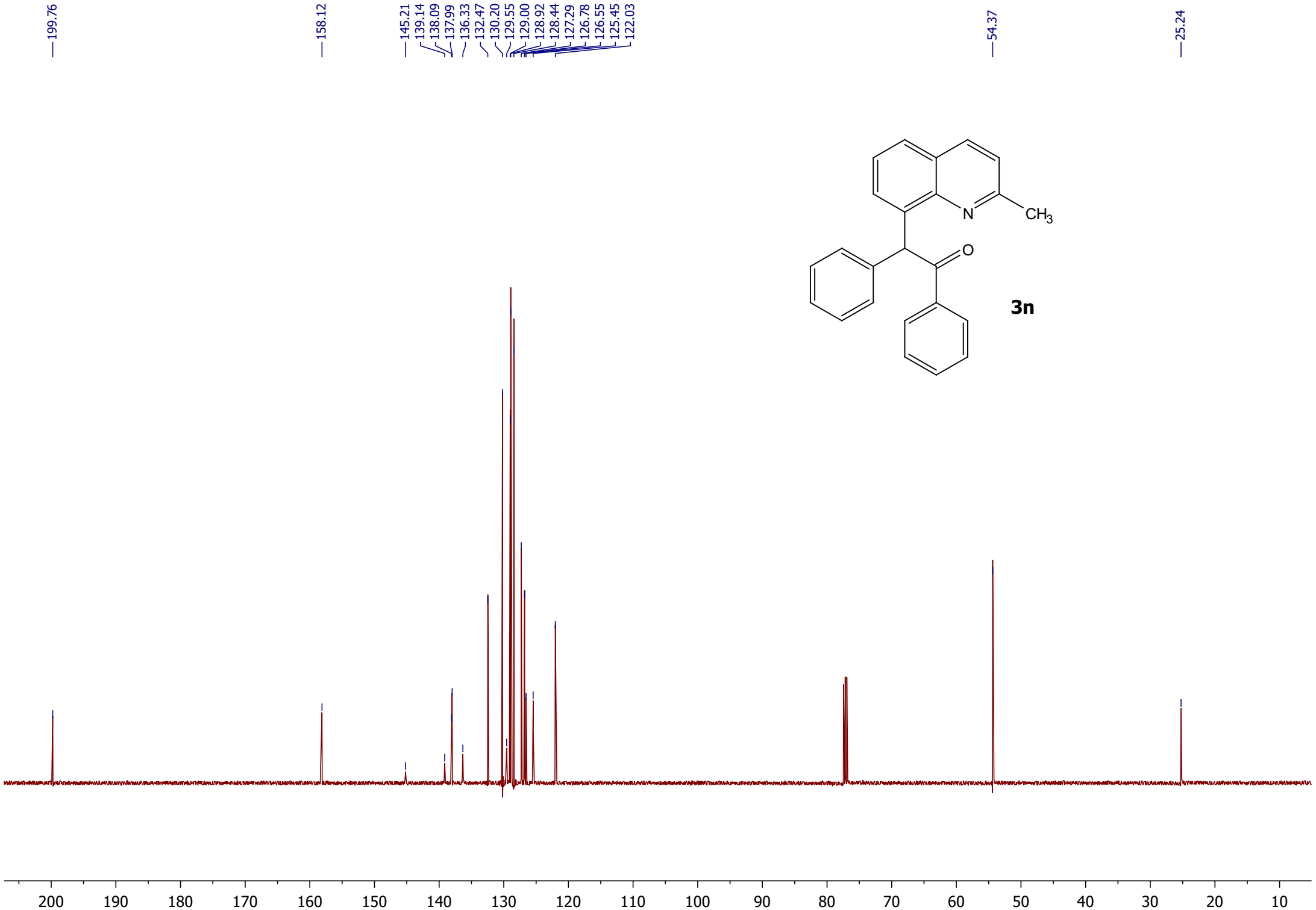
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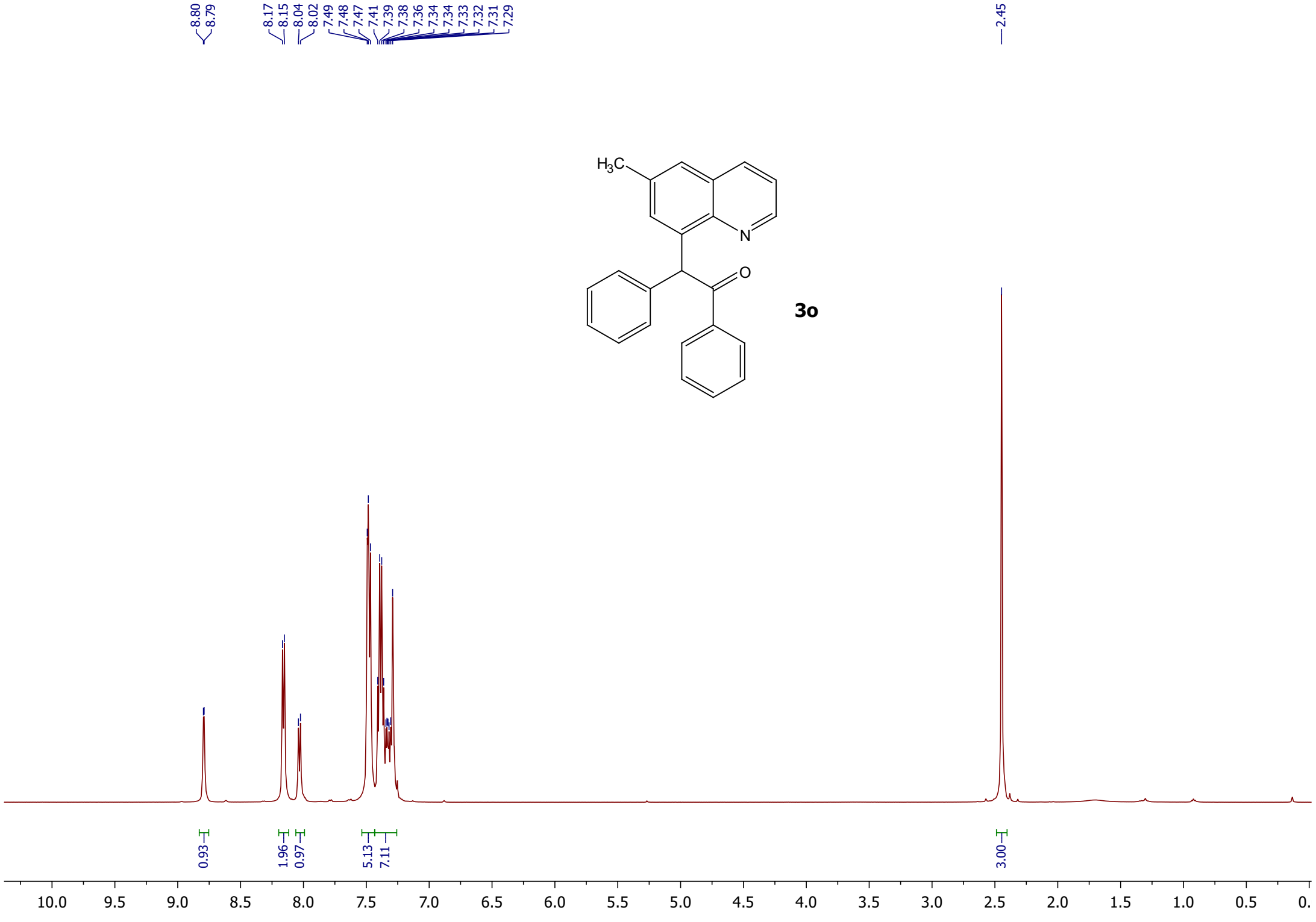
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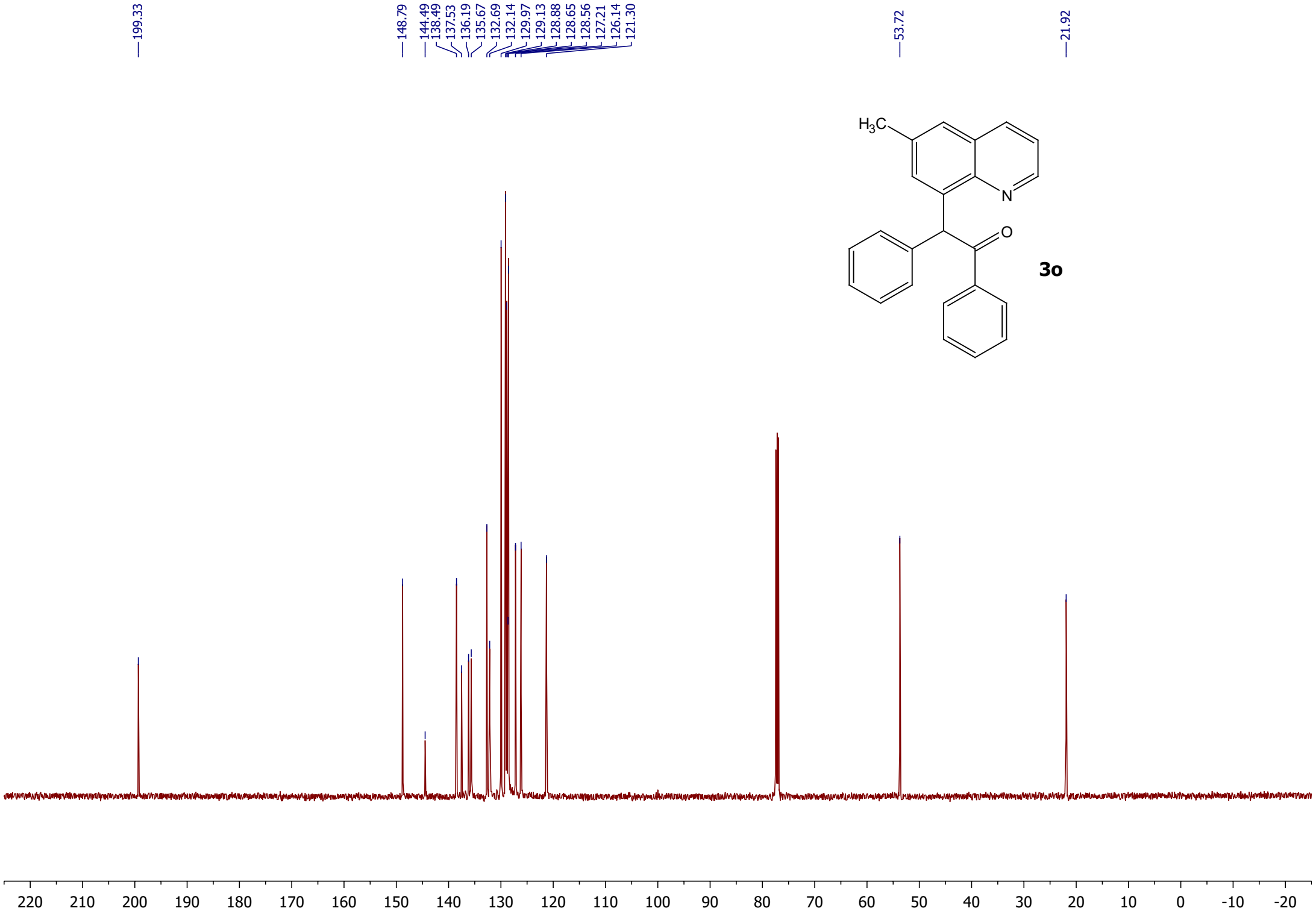
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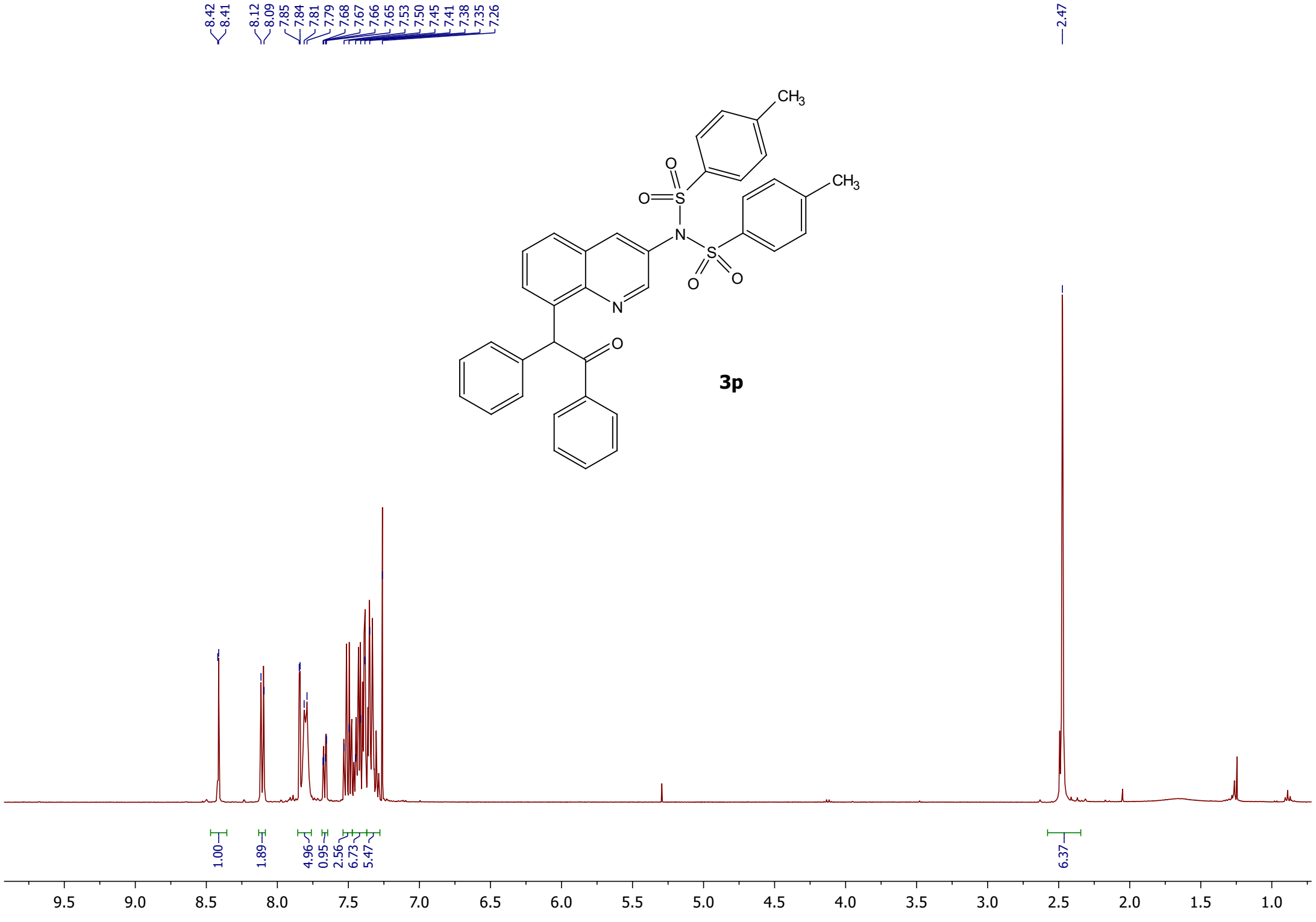
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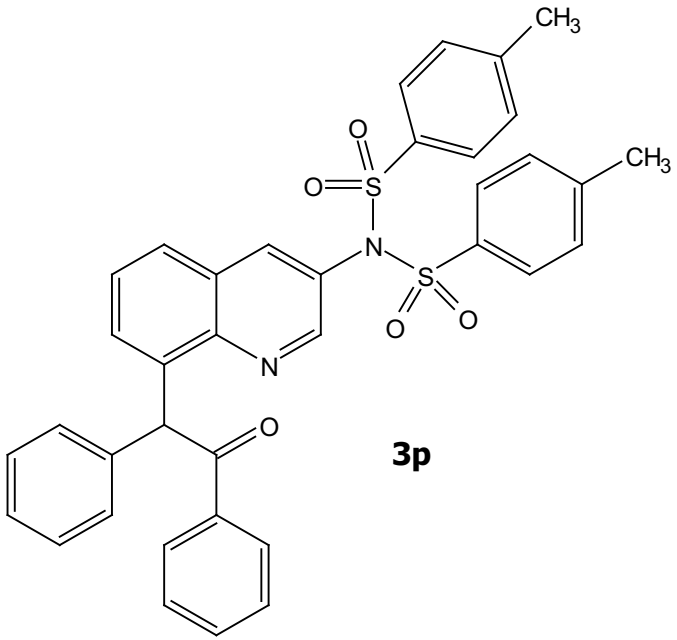

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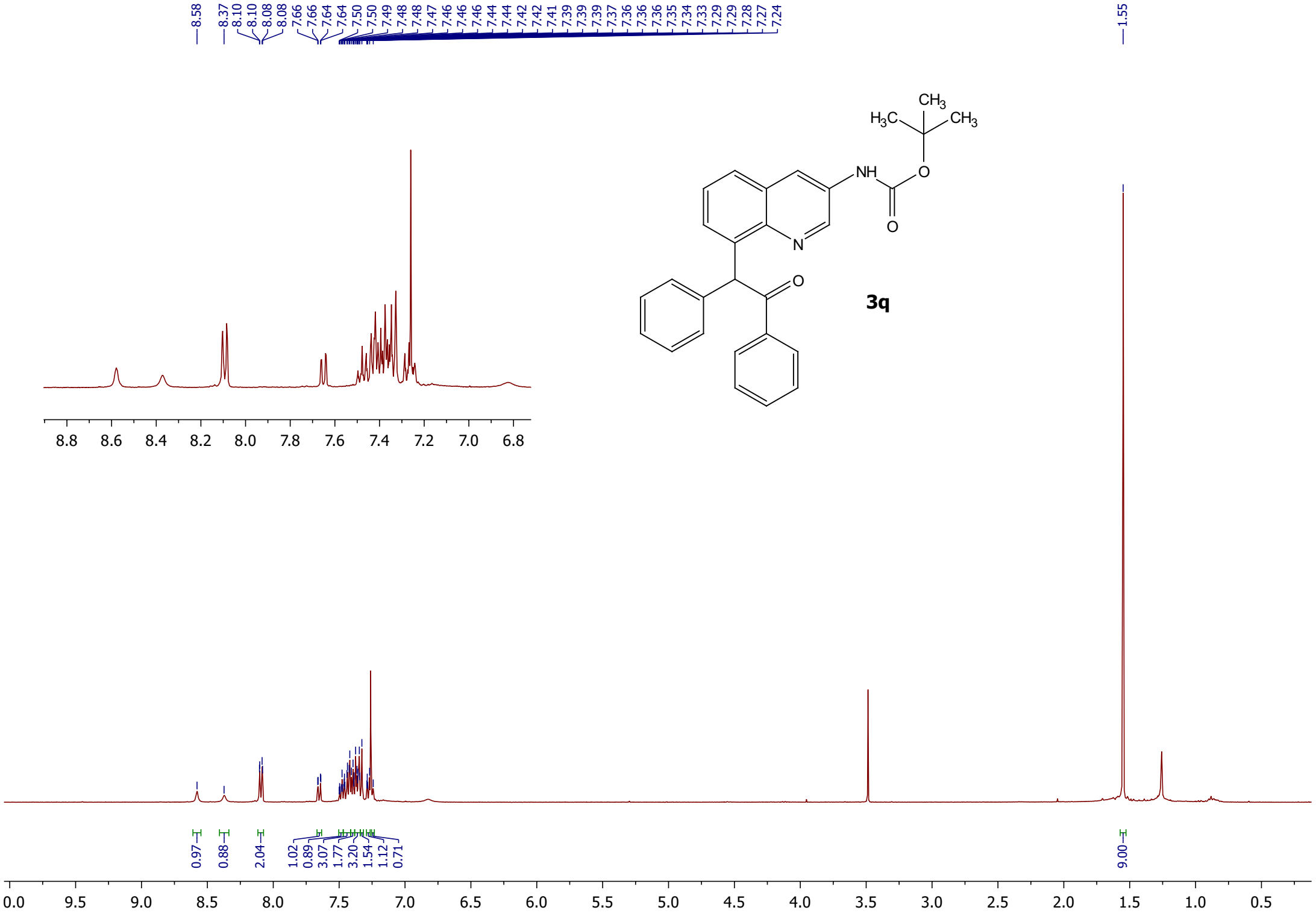
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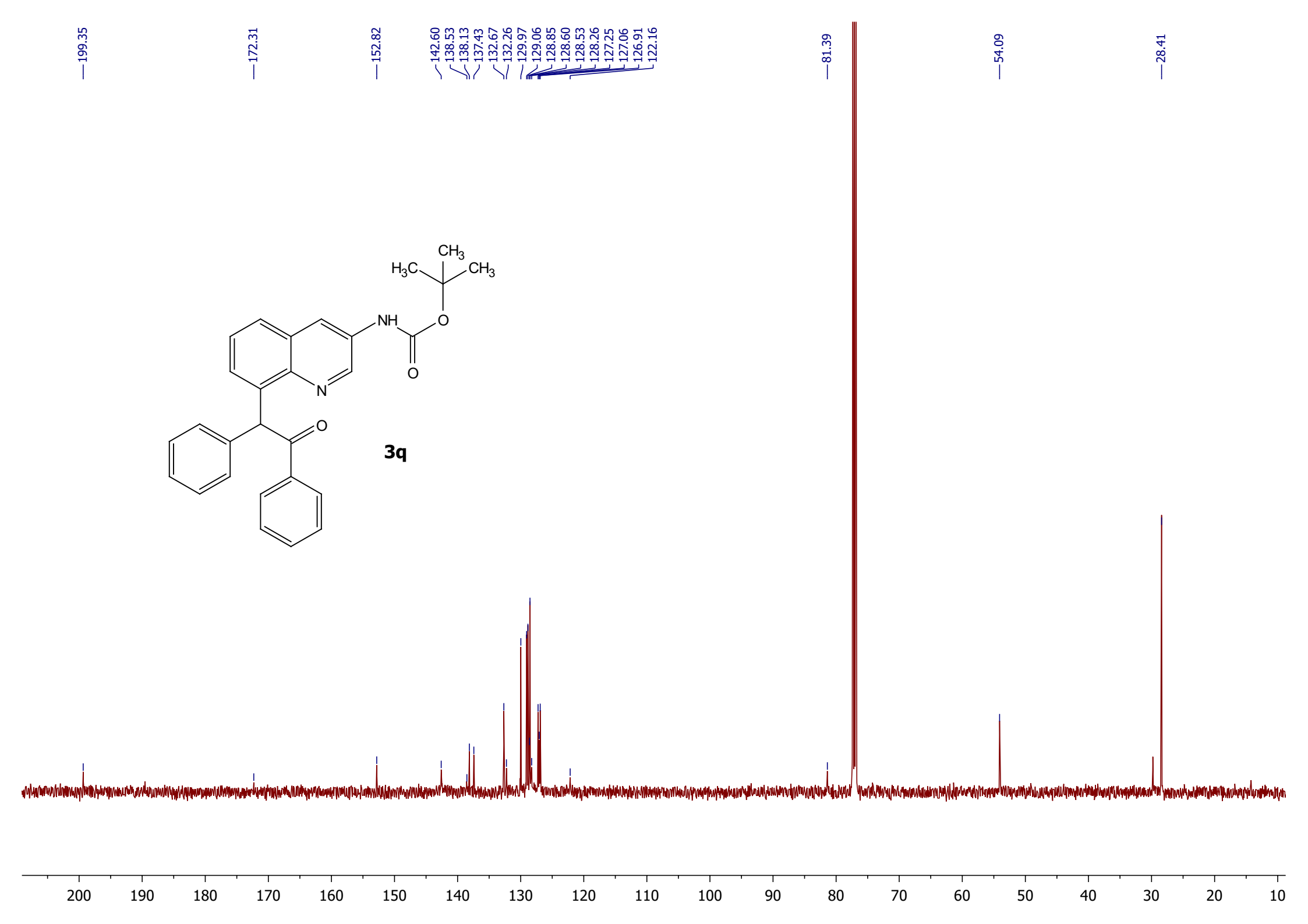
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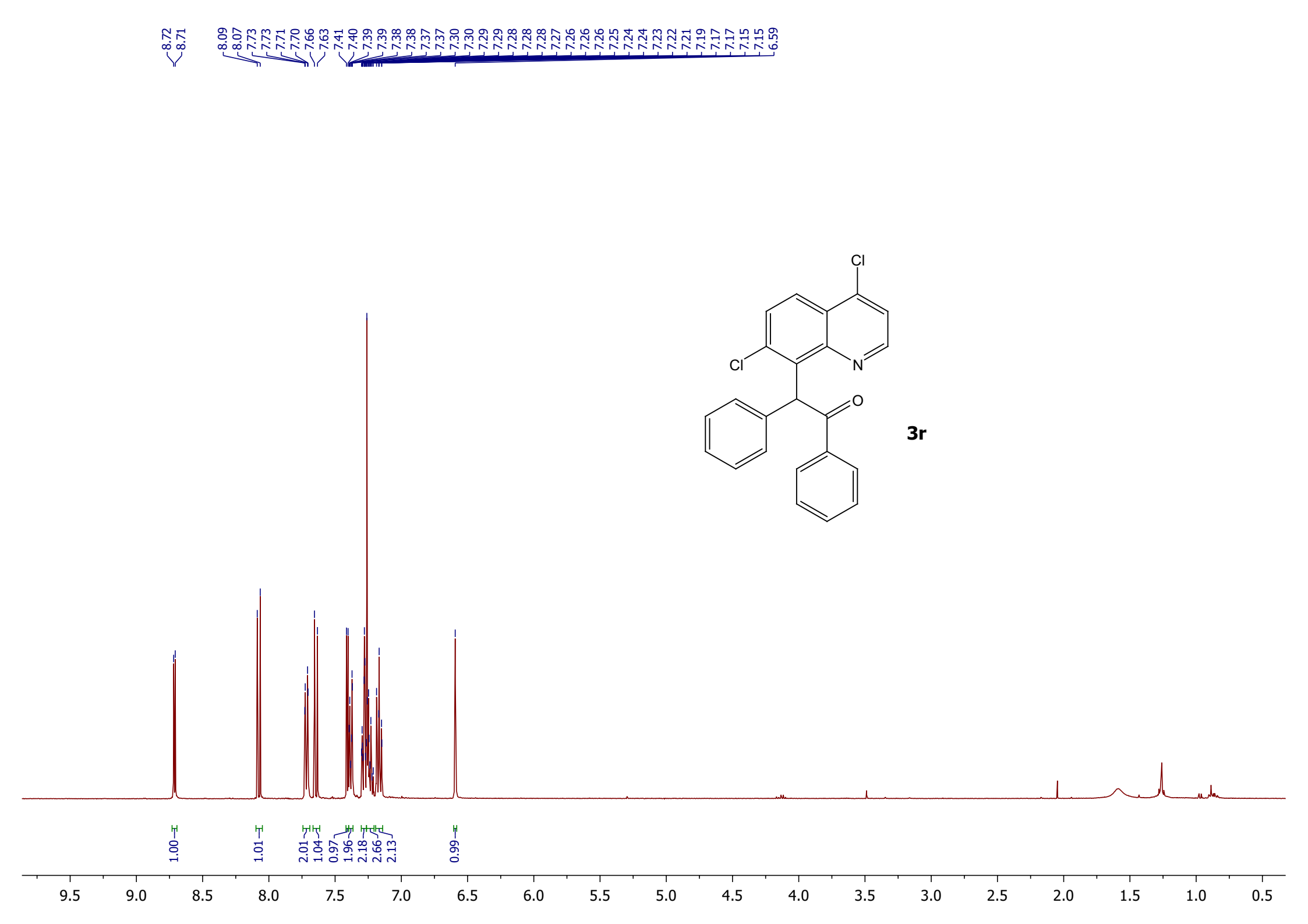
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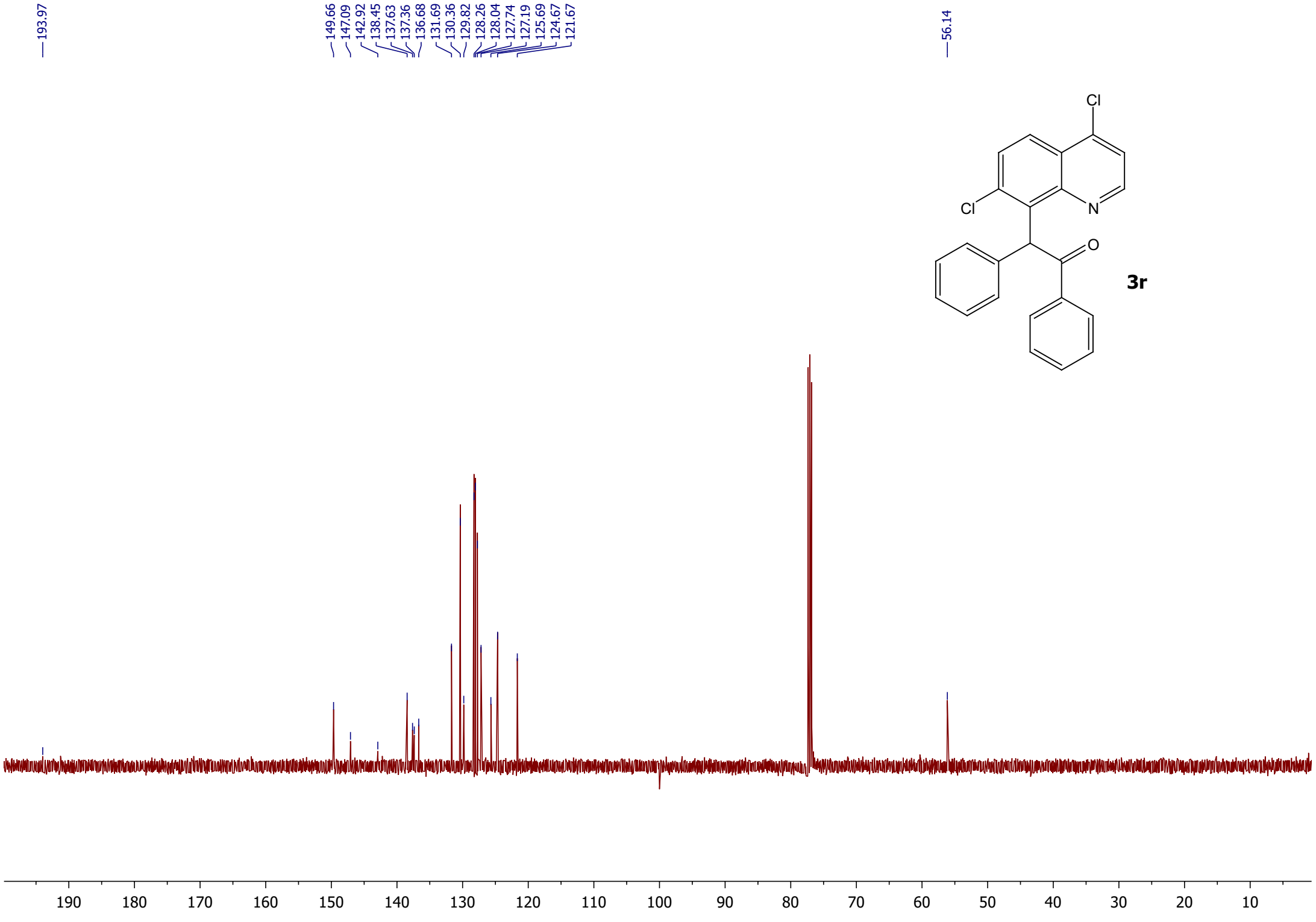
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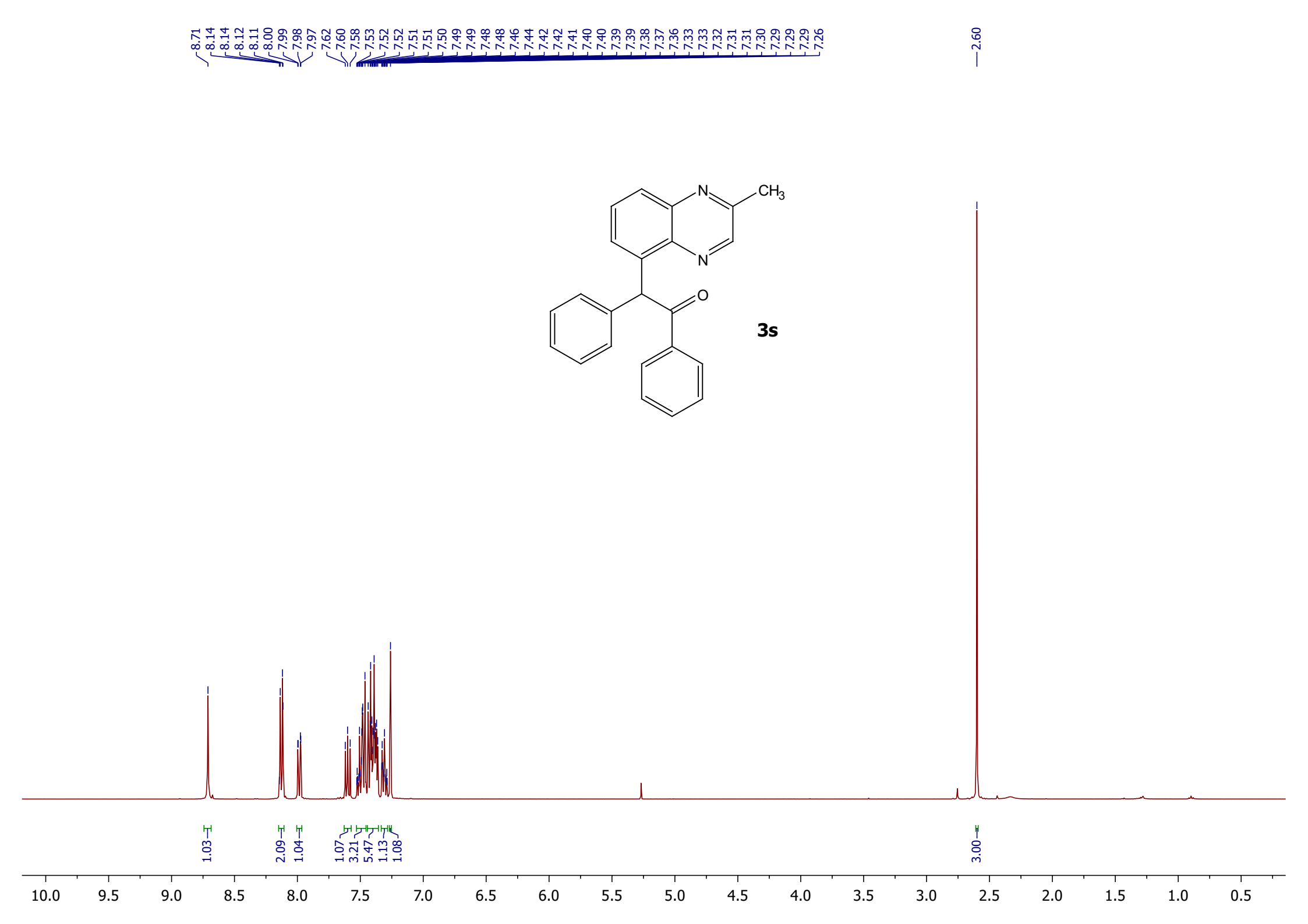
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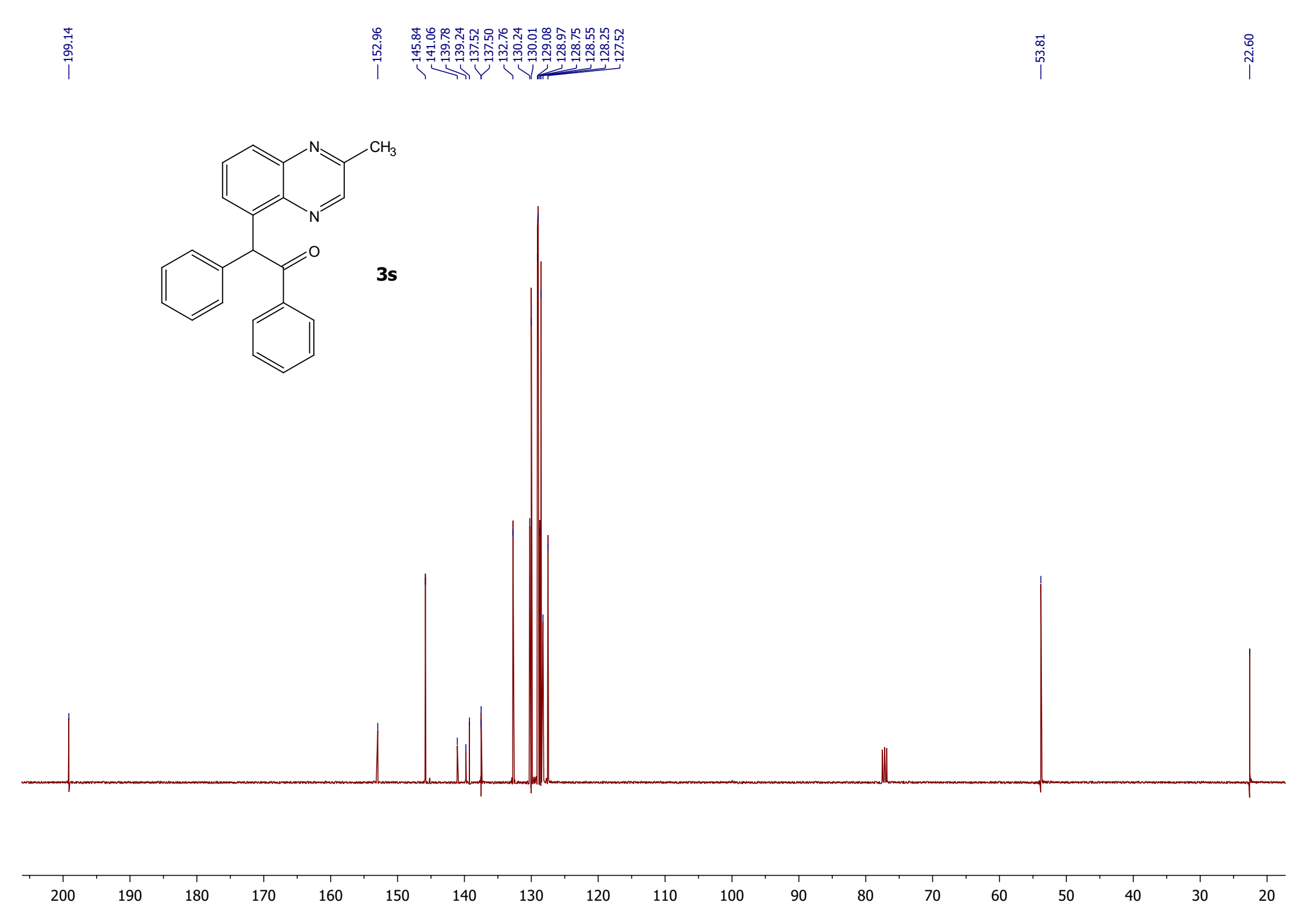
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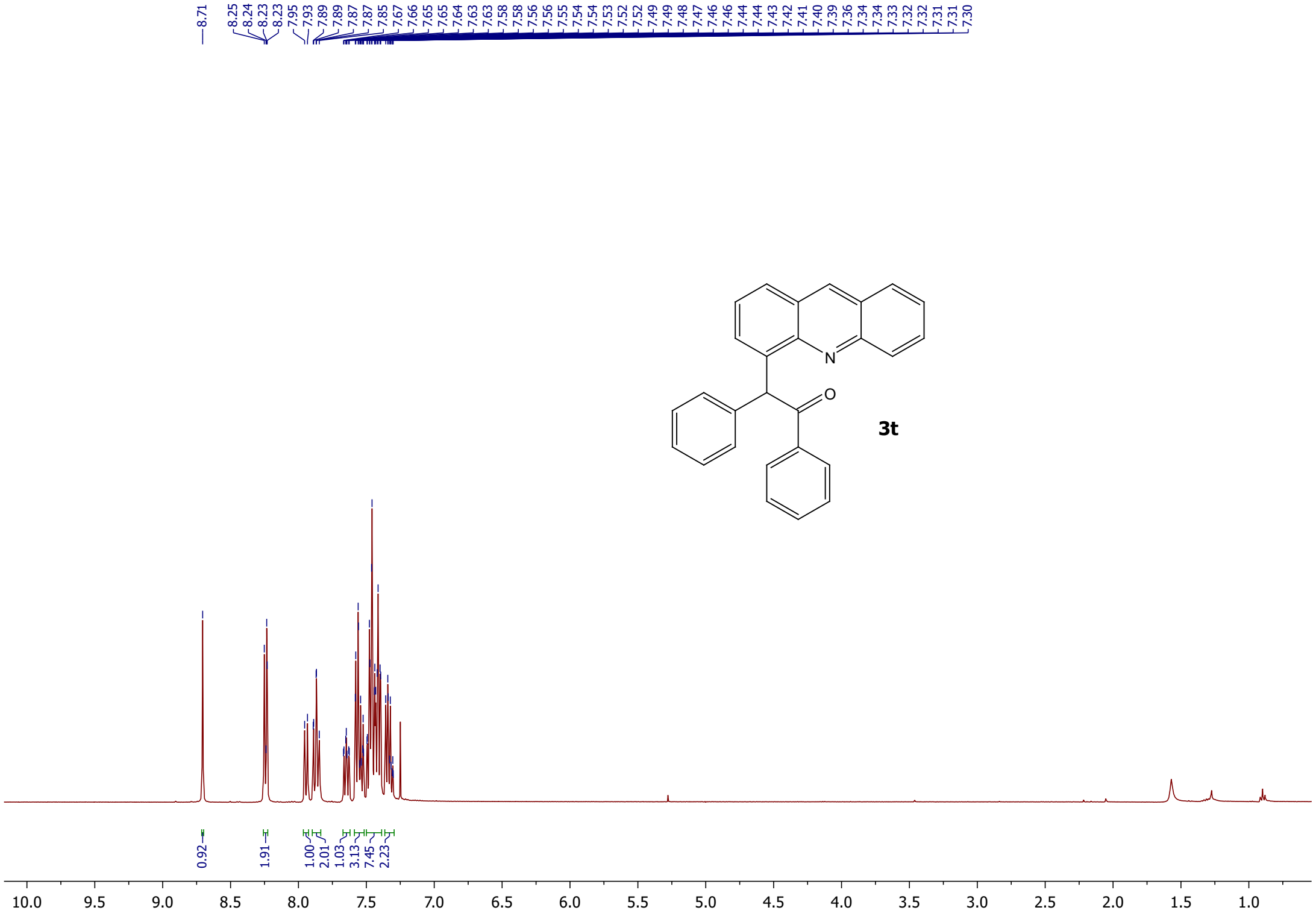
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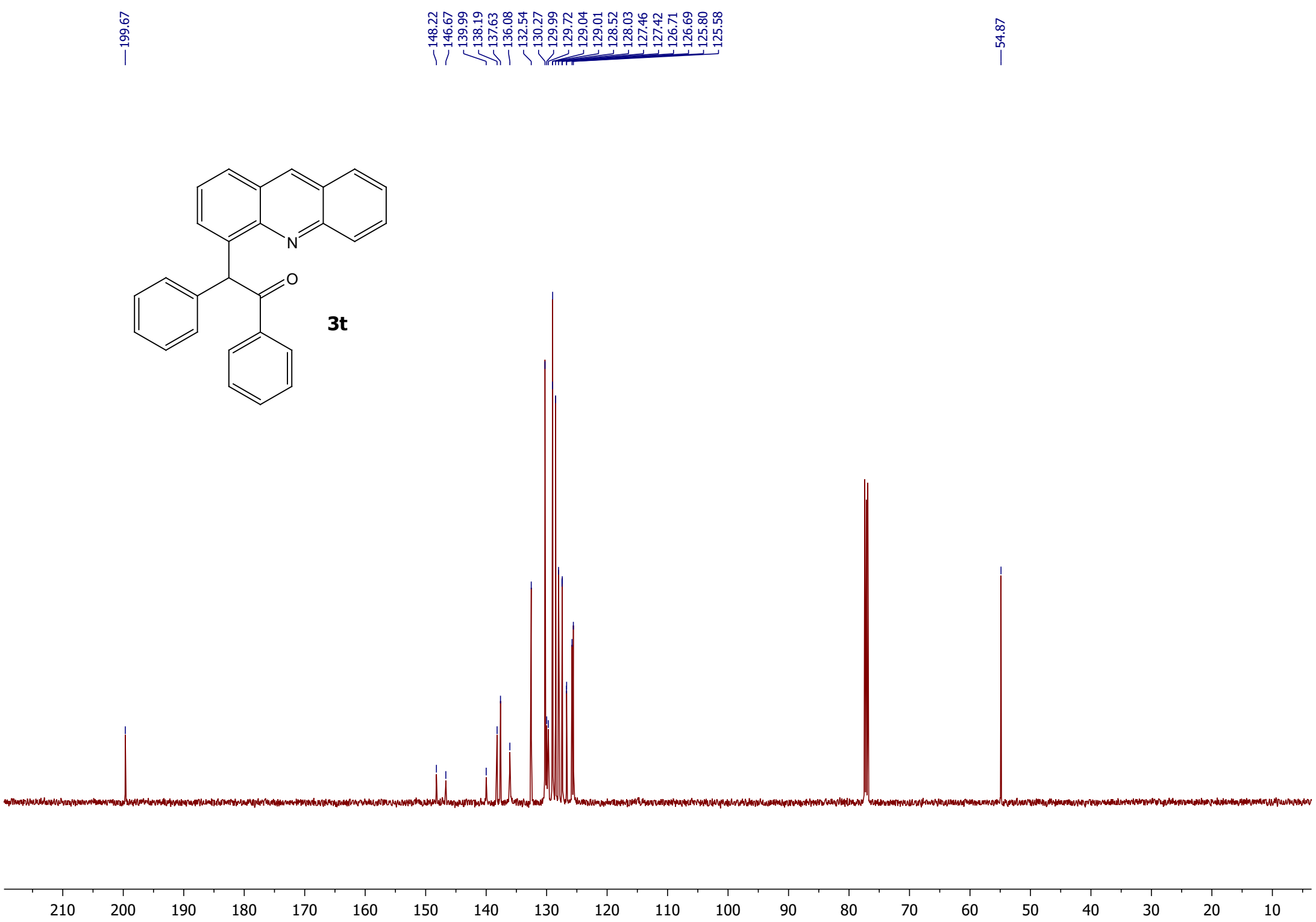
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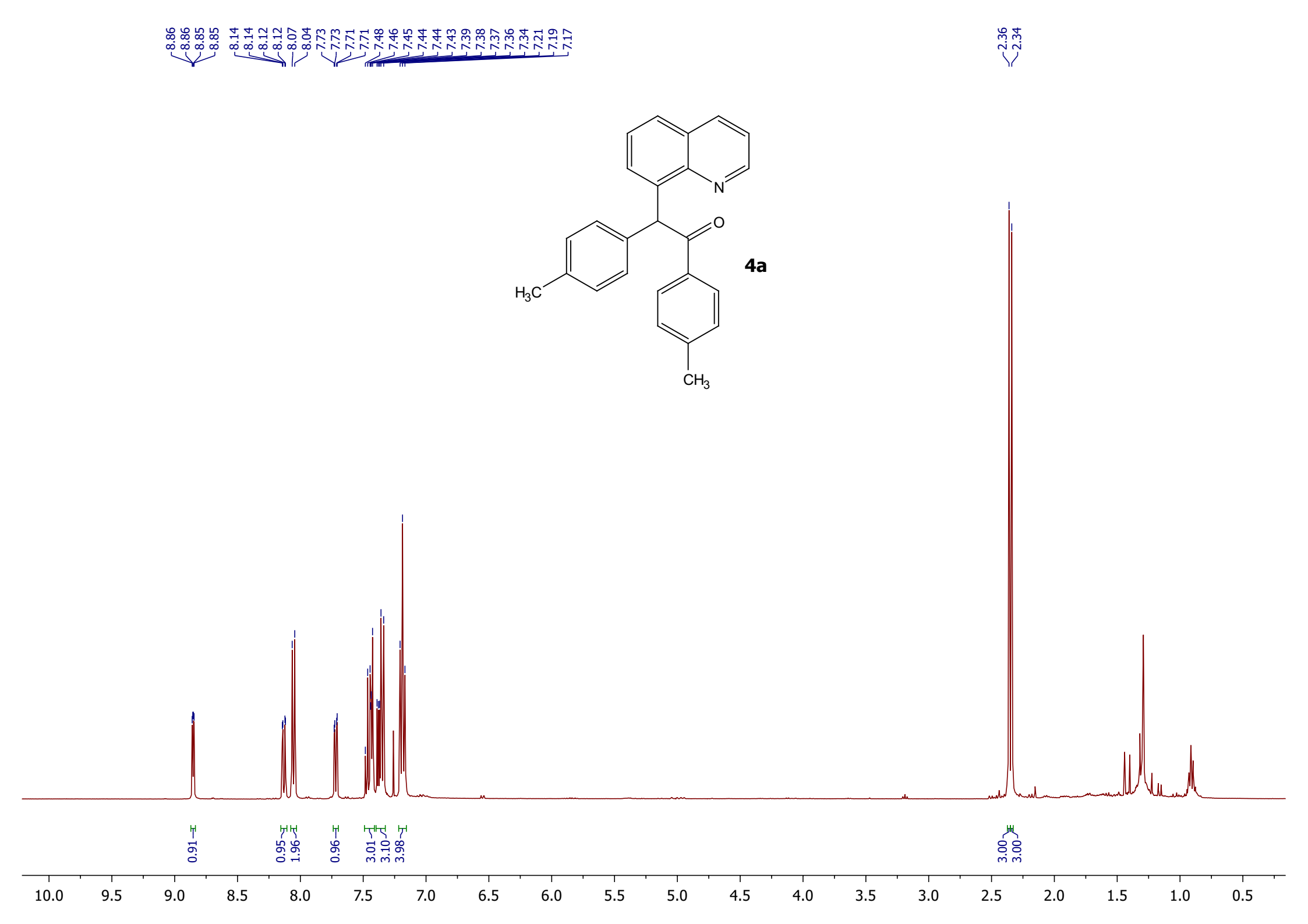
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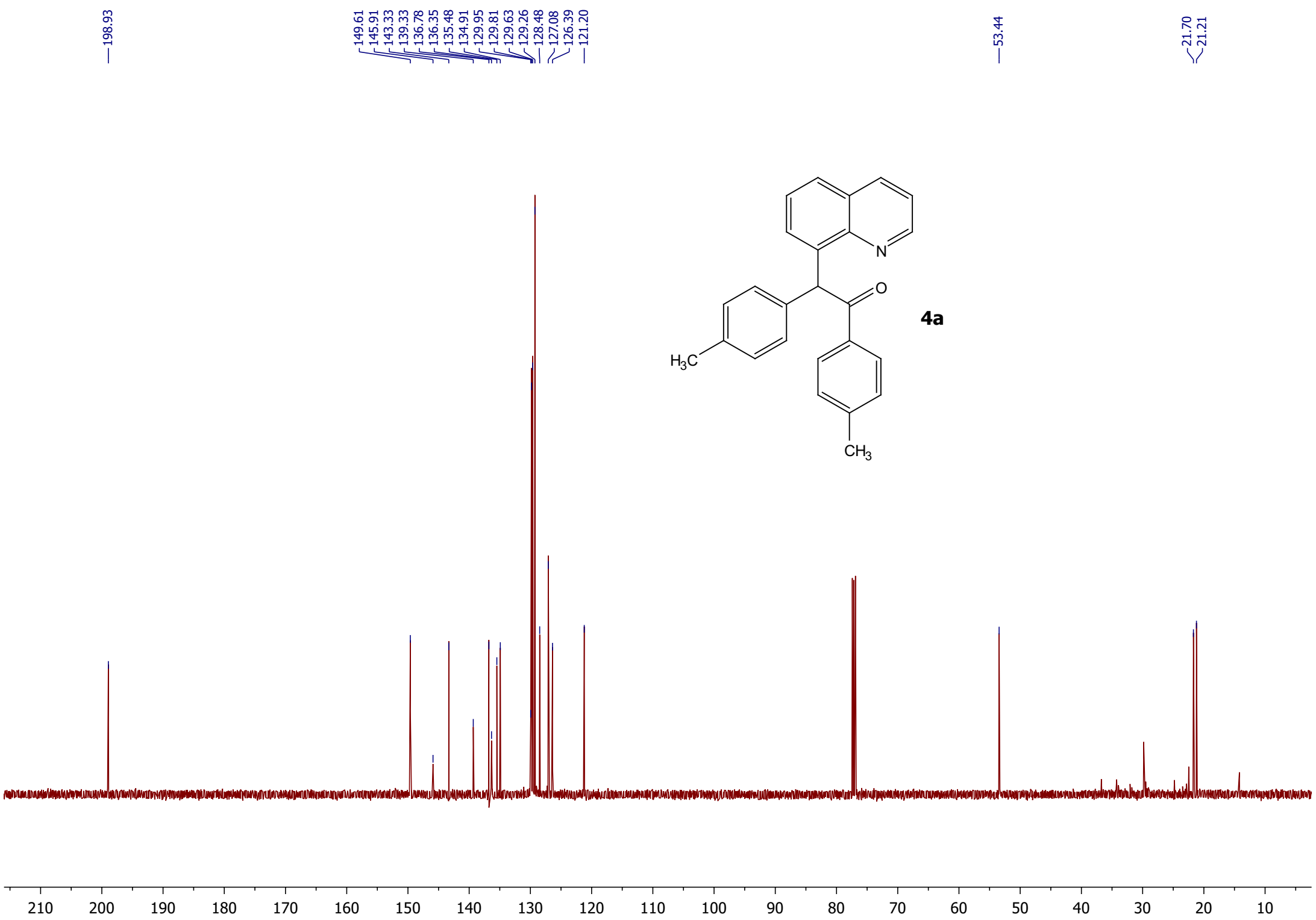
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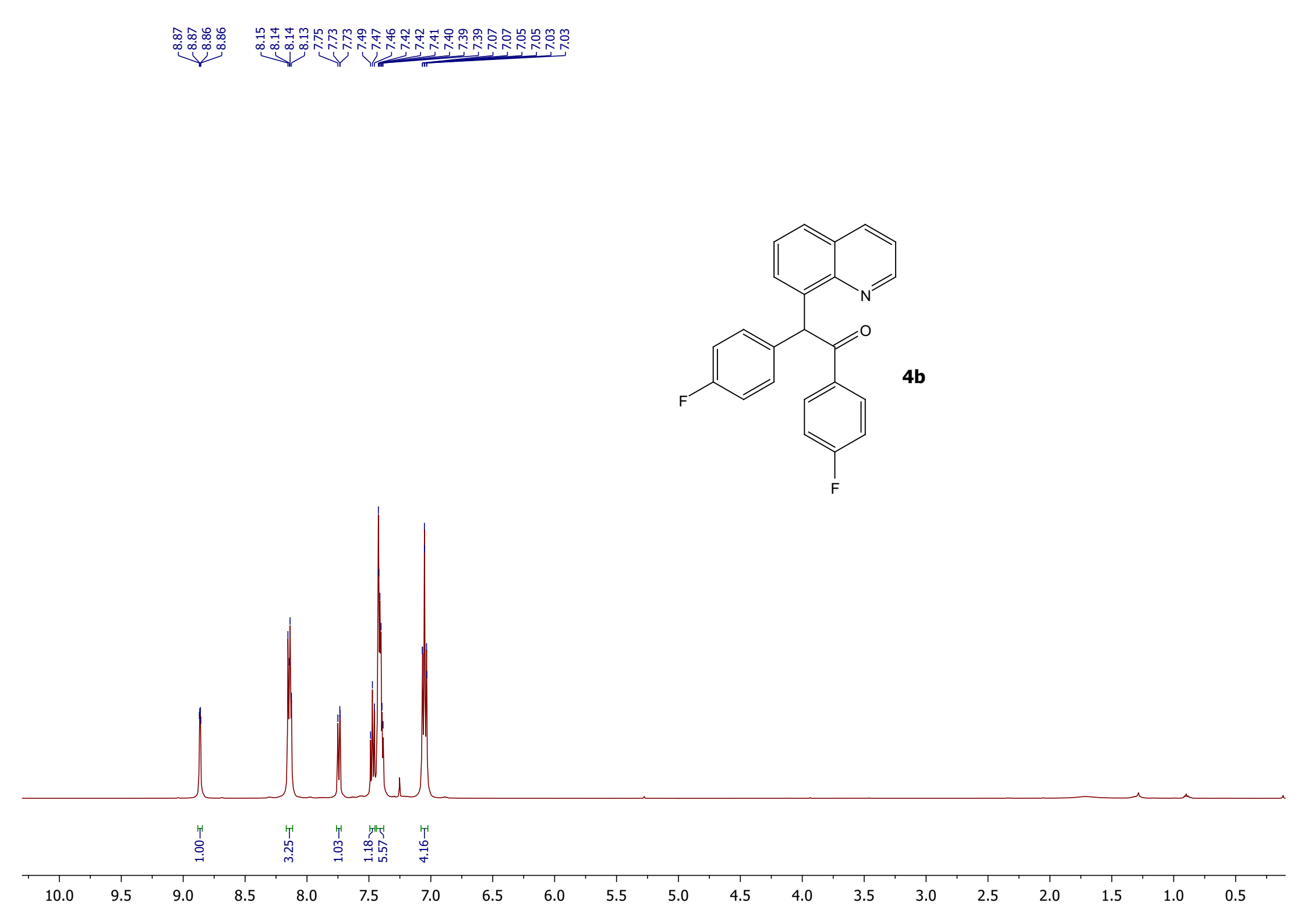
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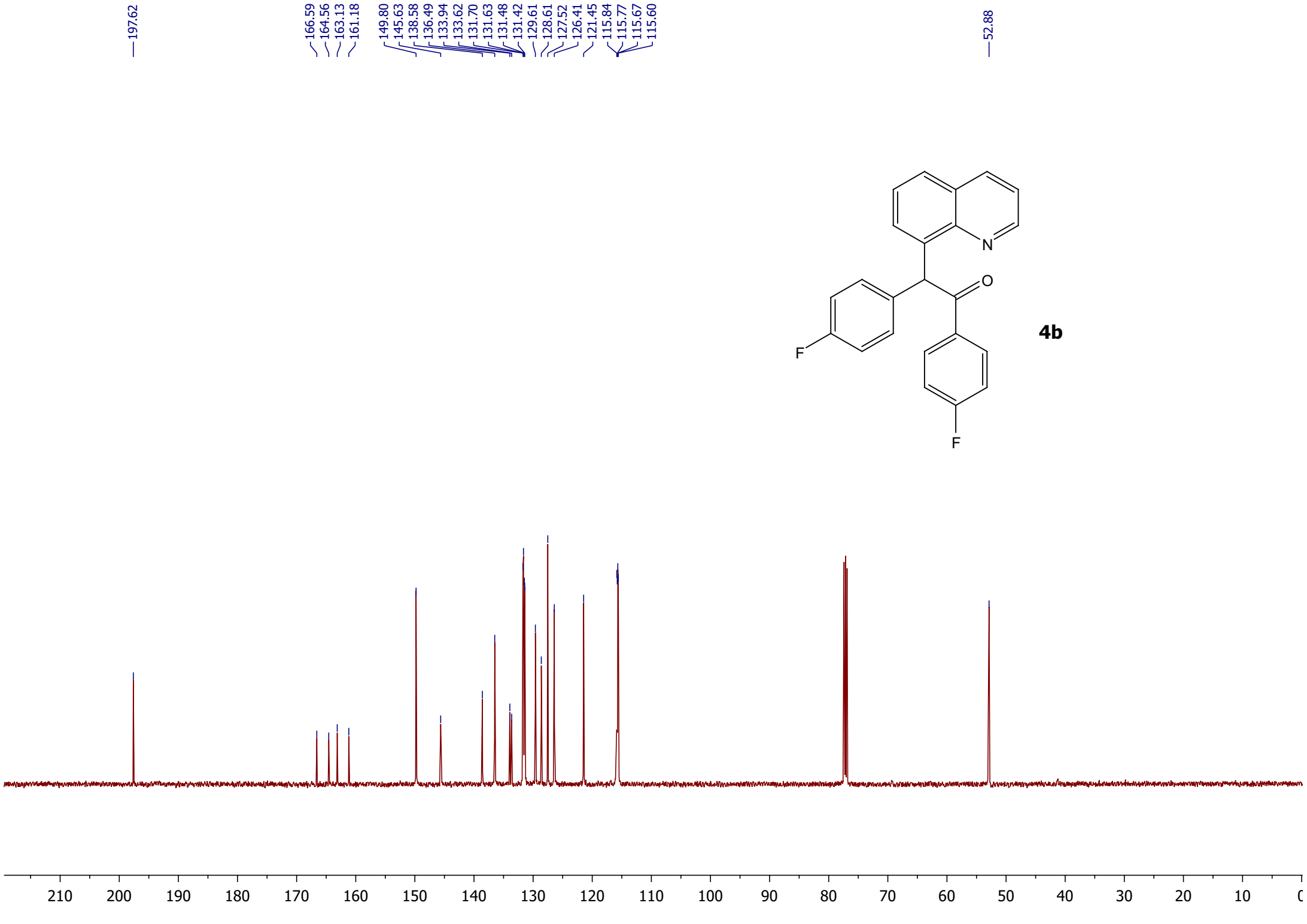
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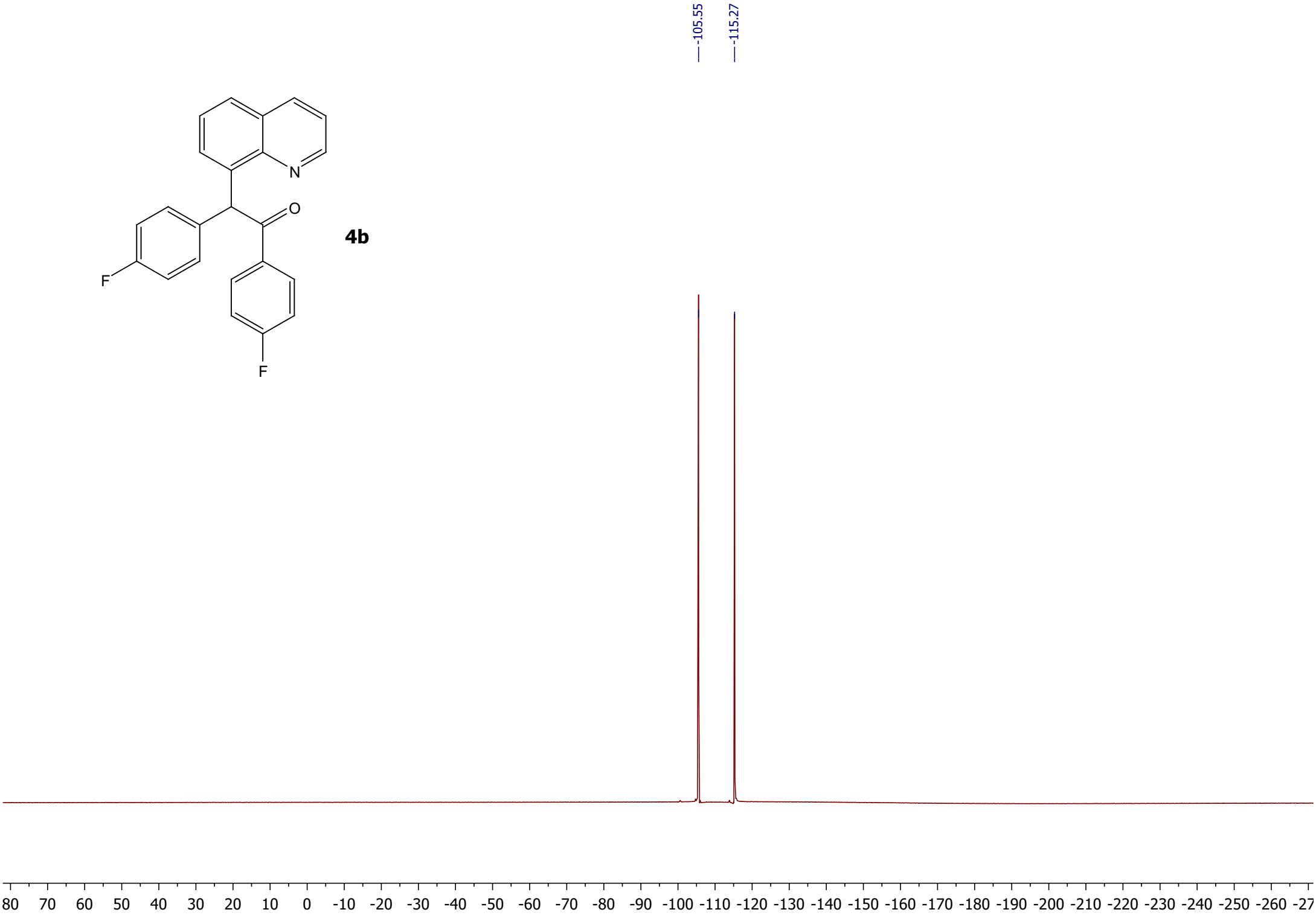
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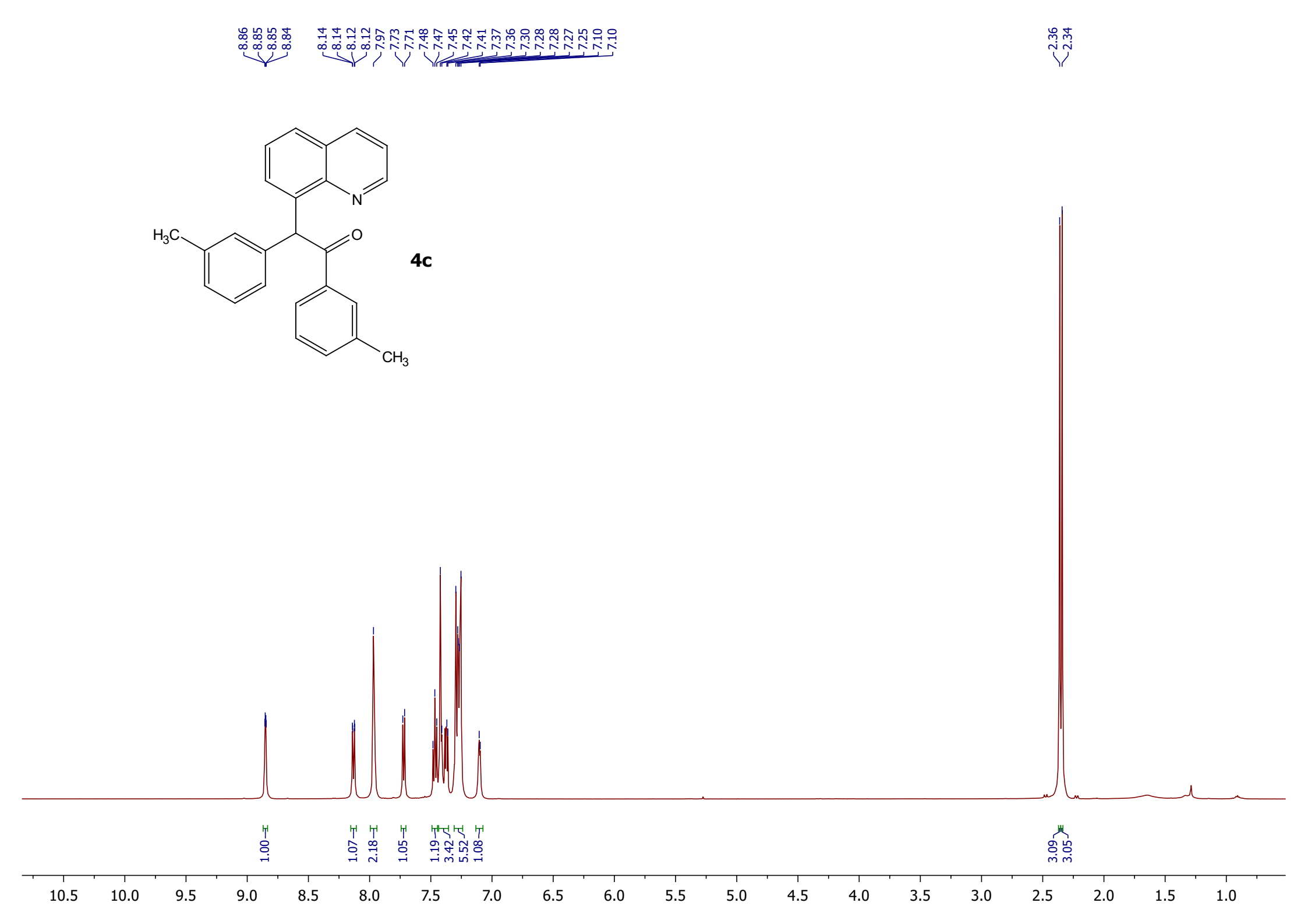
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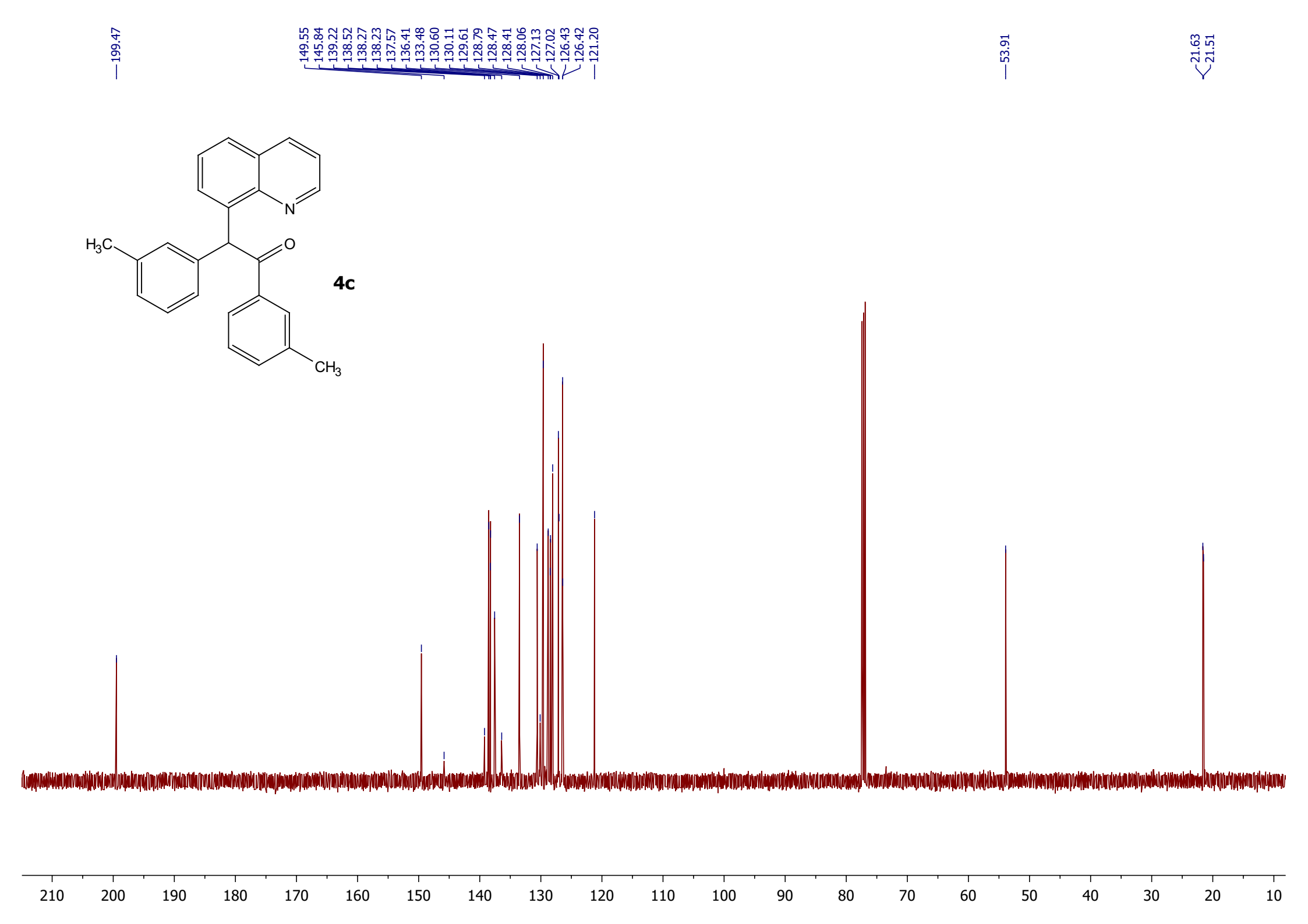
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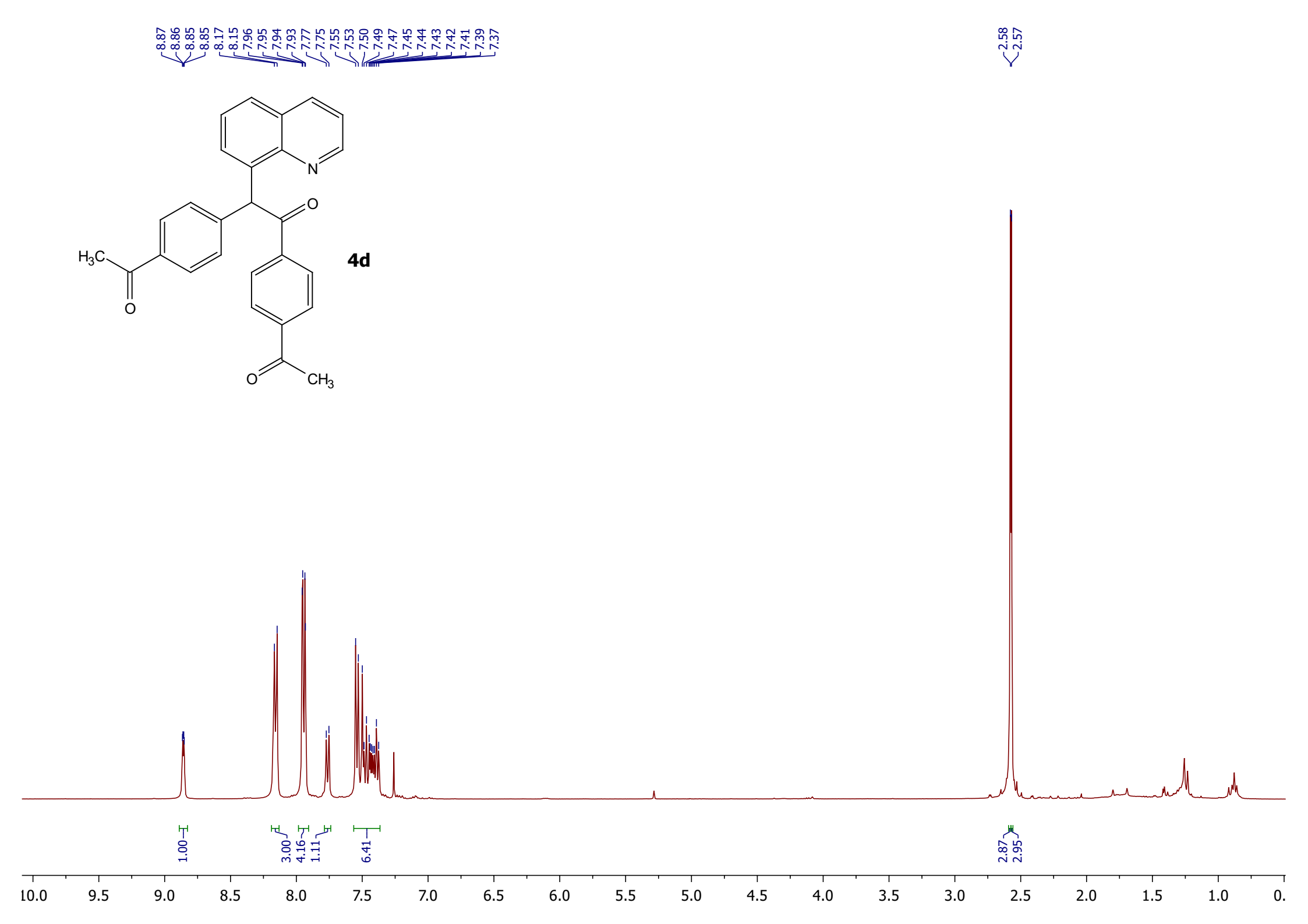
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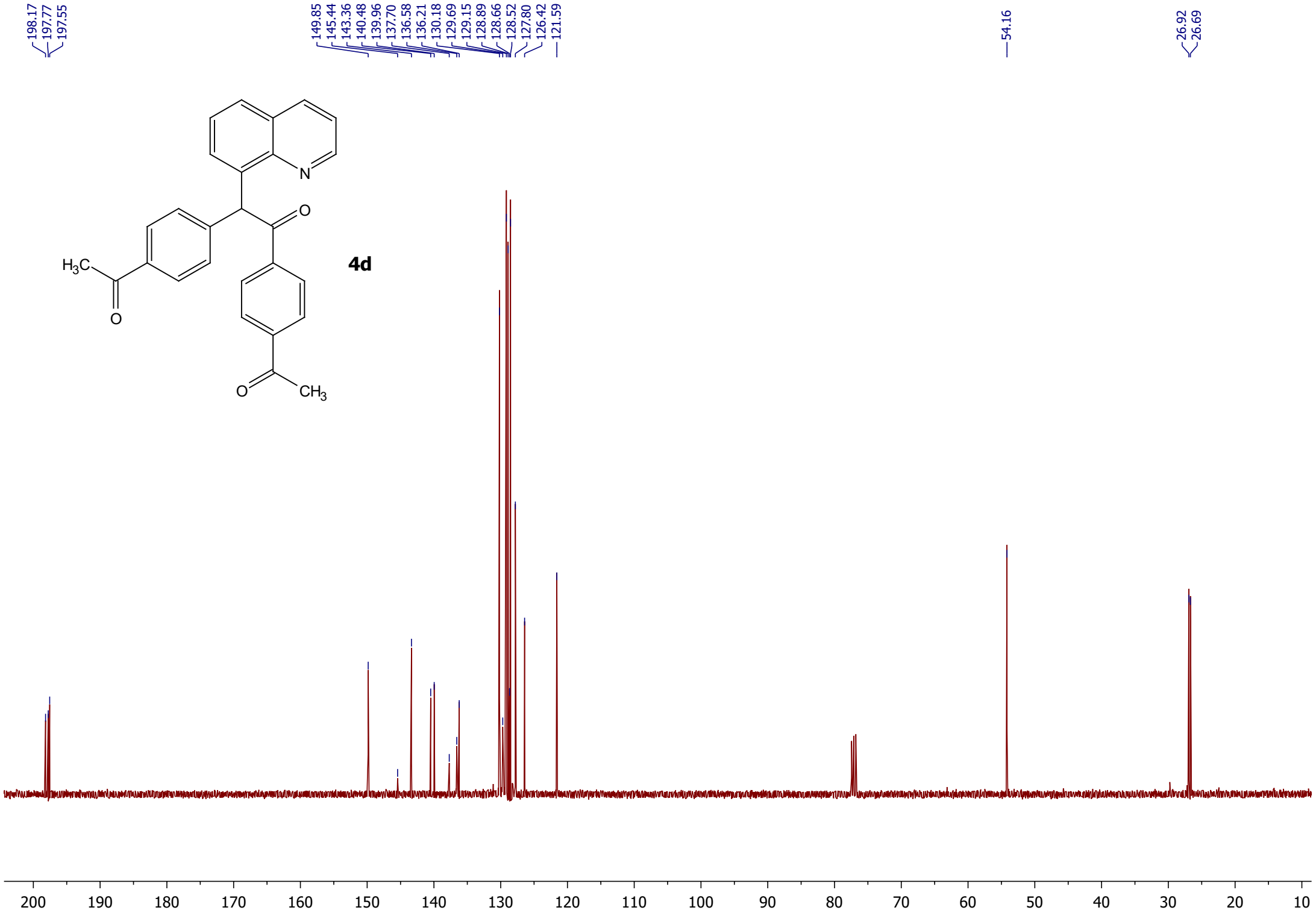
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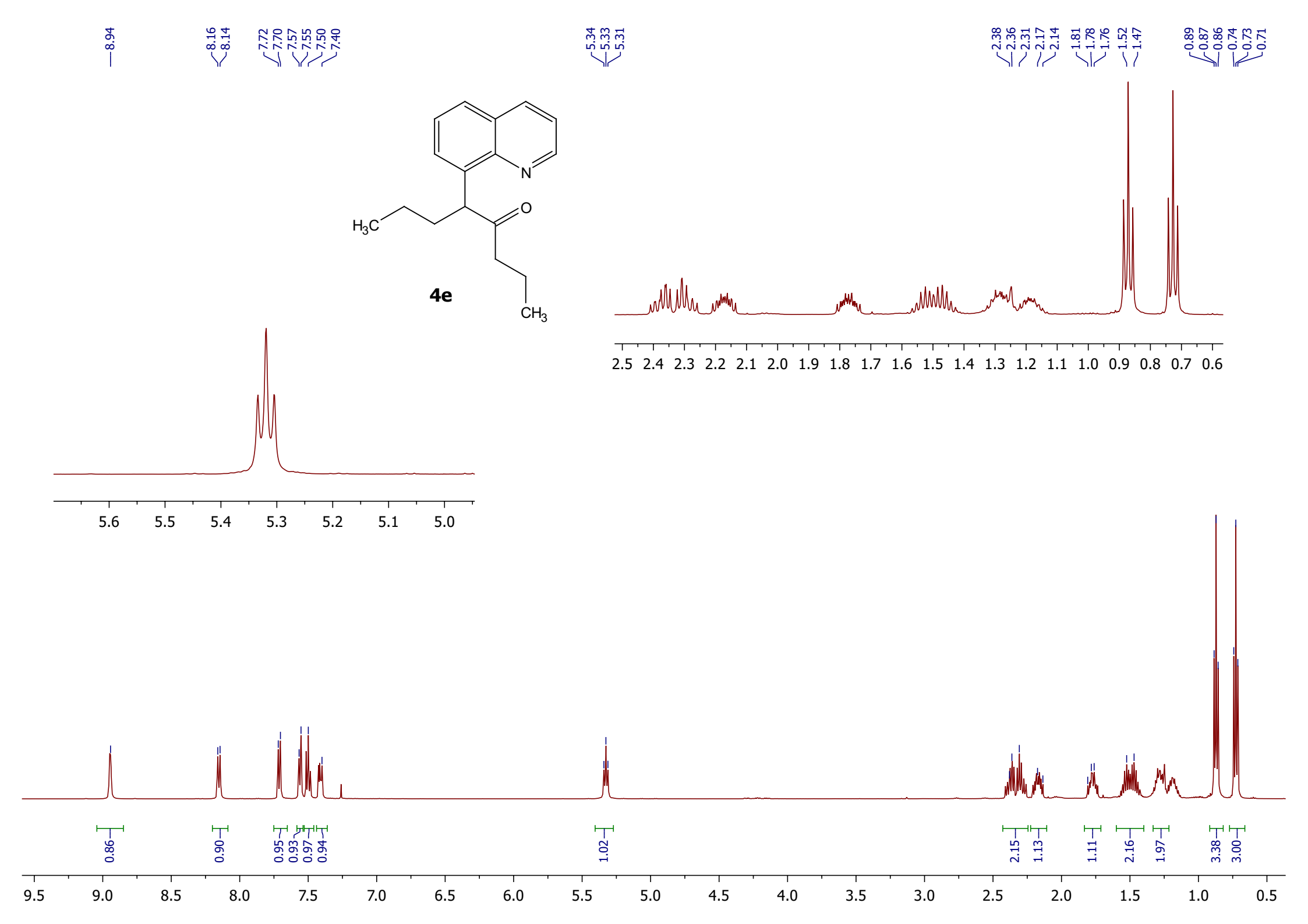
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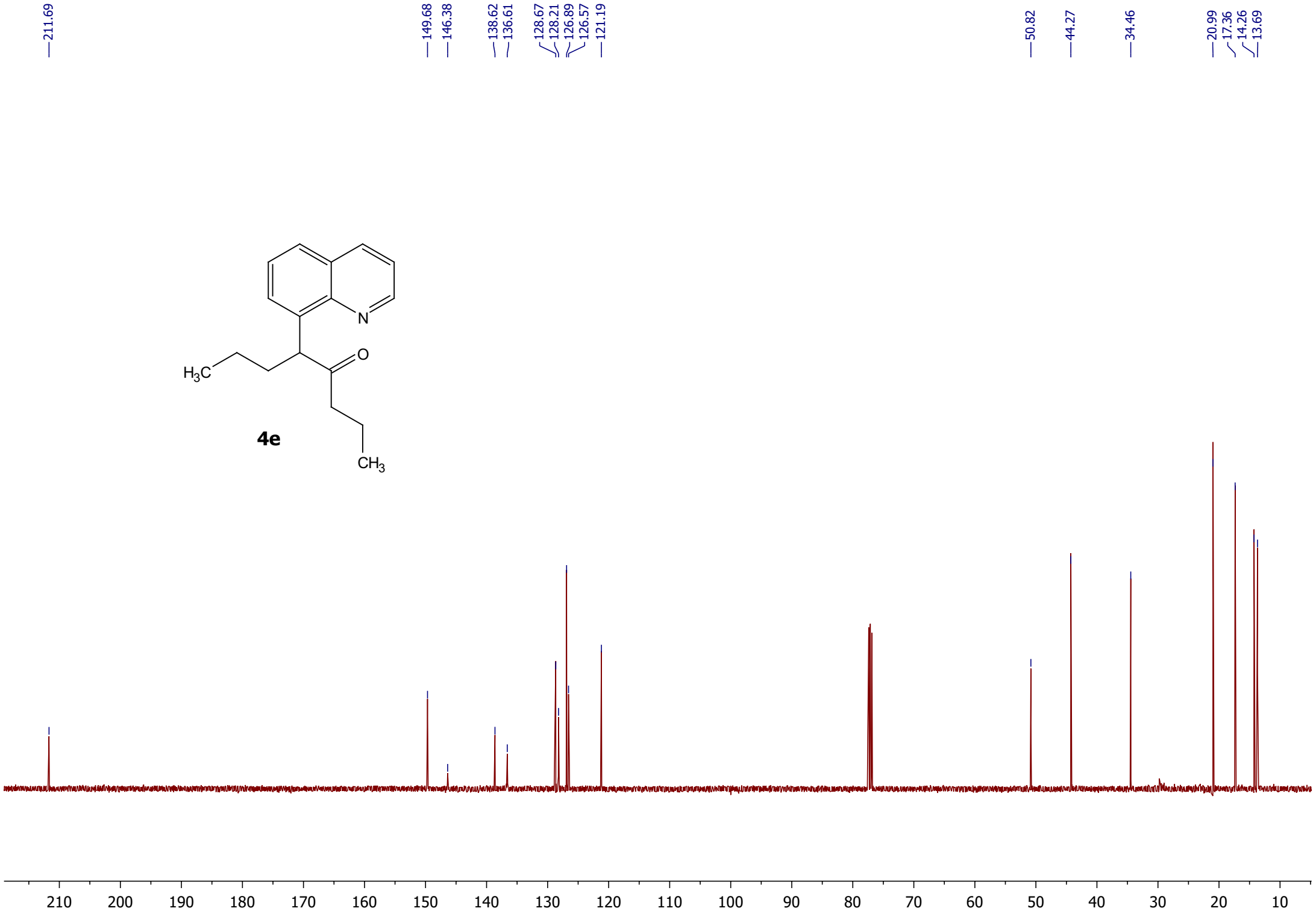
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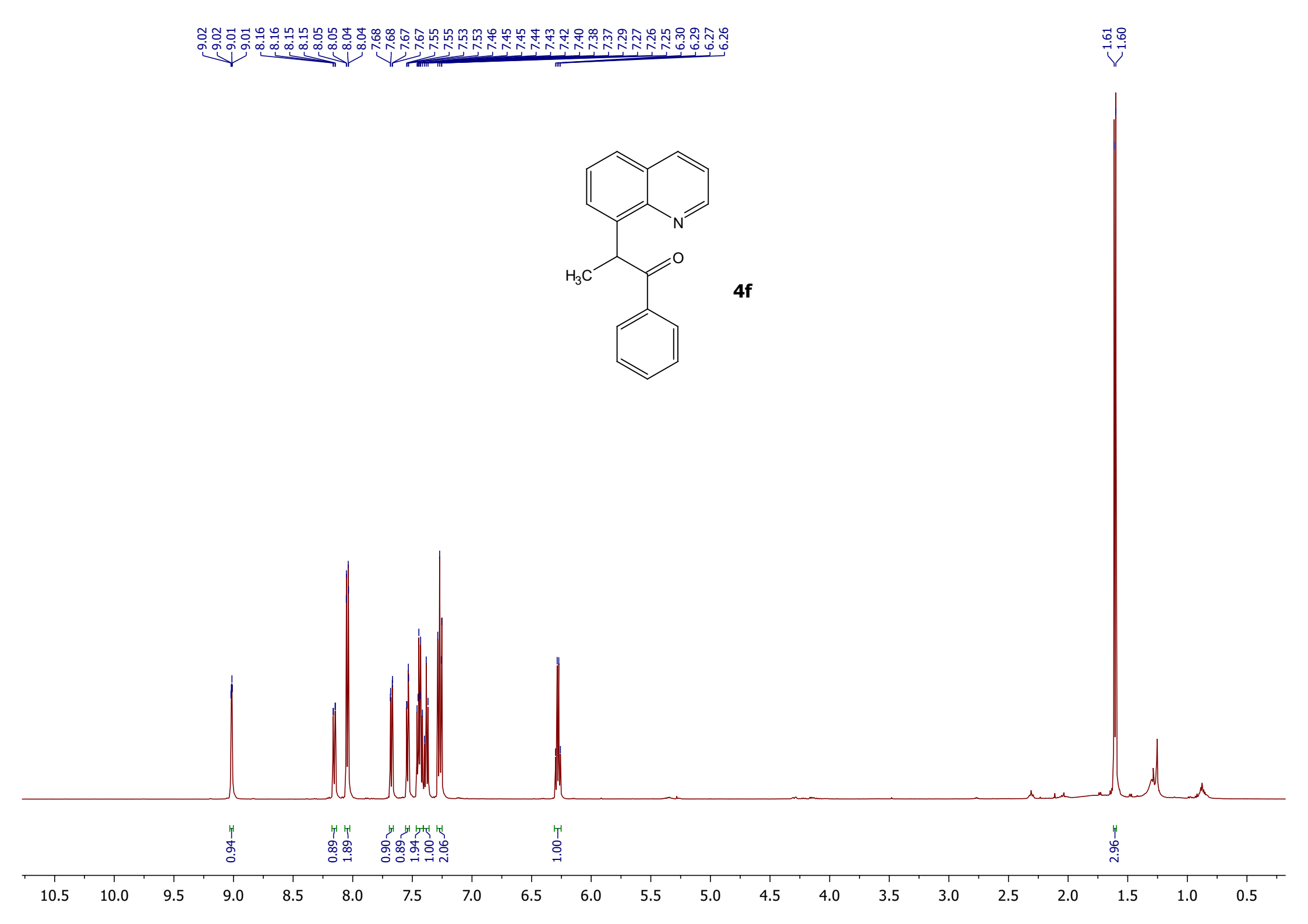
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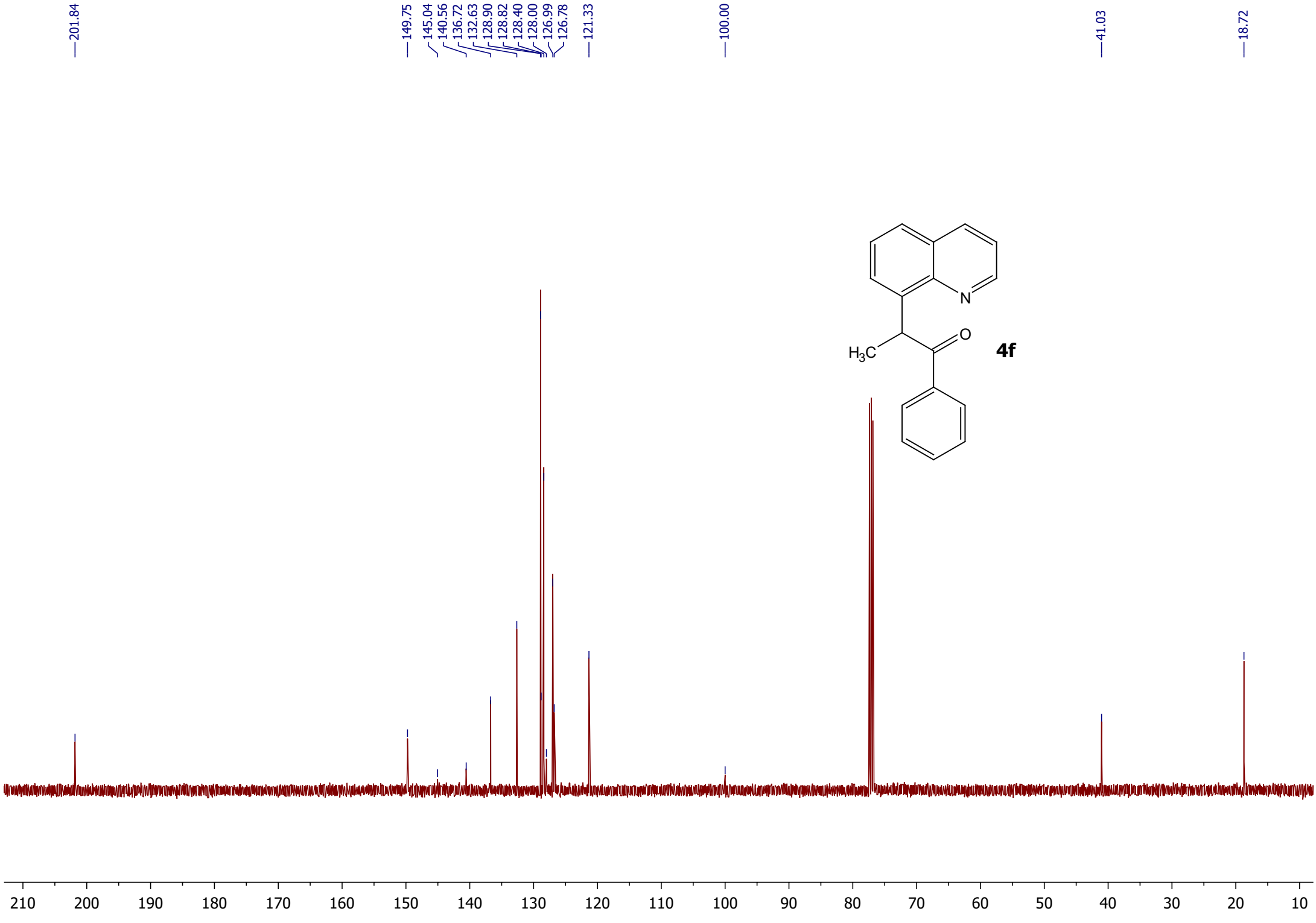
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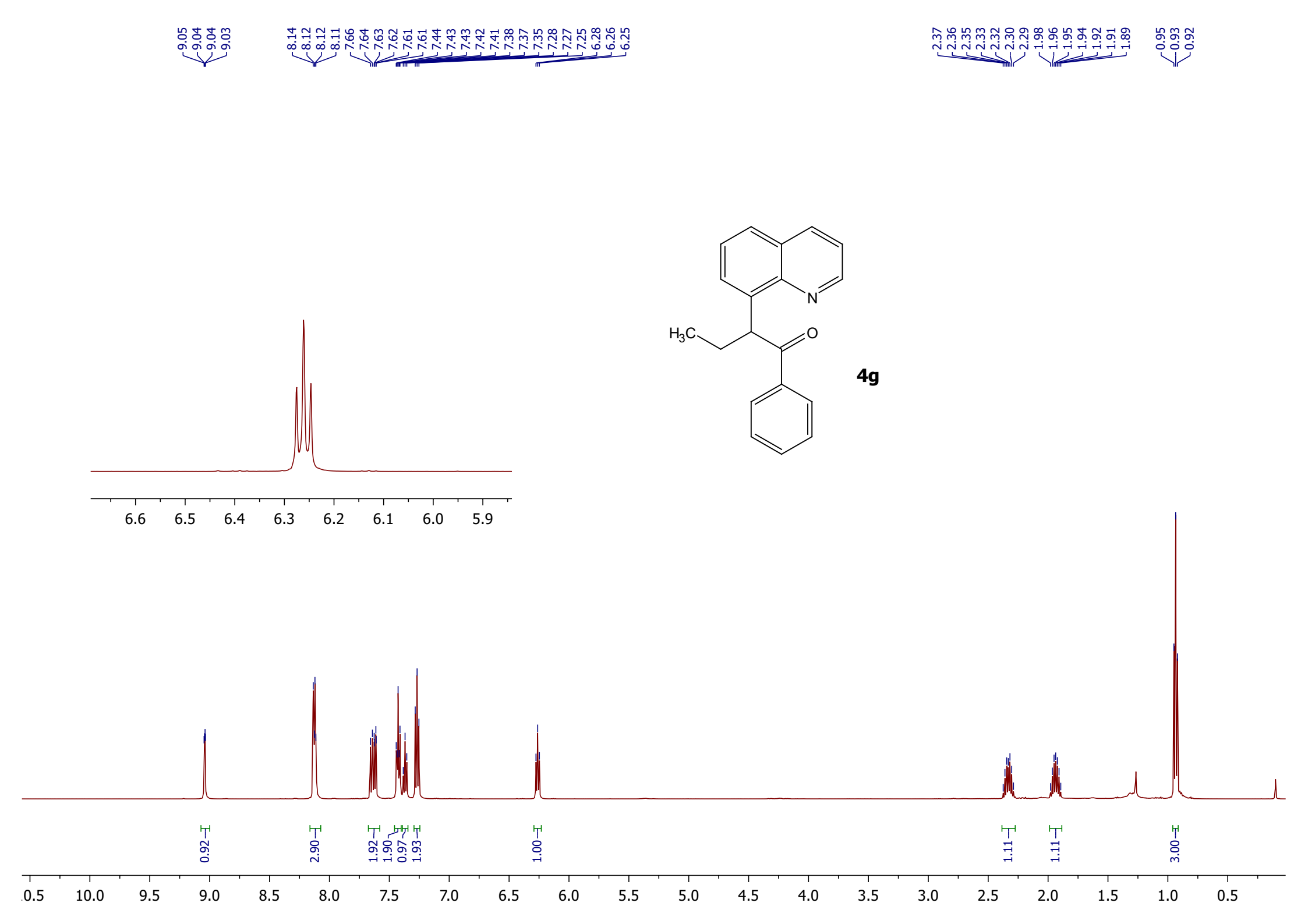
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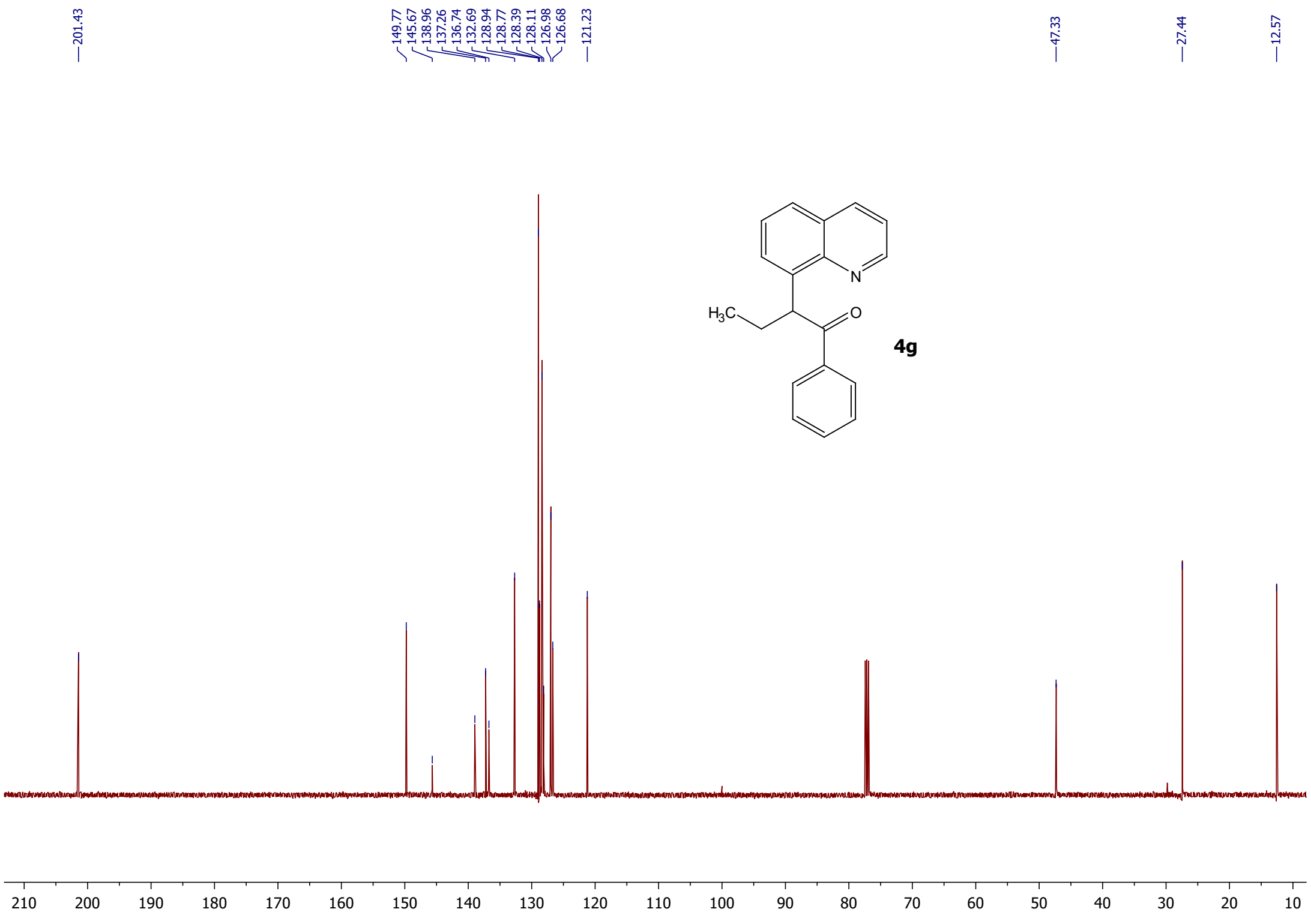
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N
H3C
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4g
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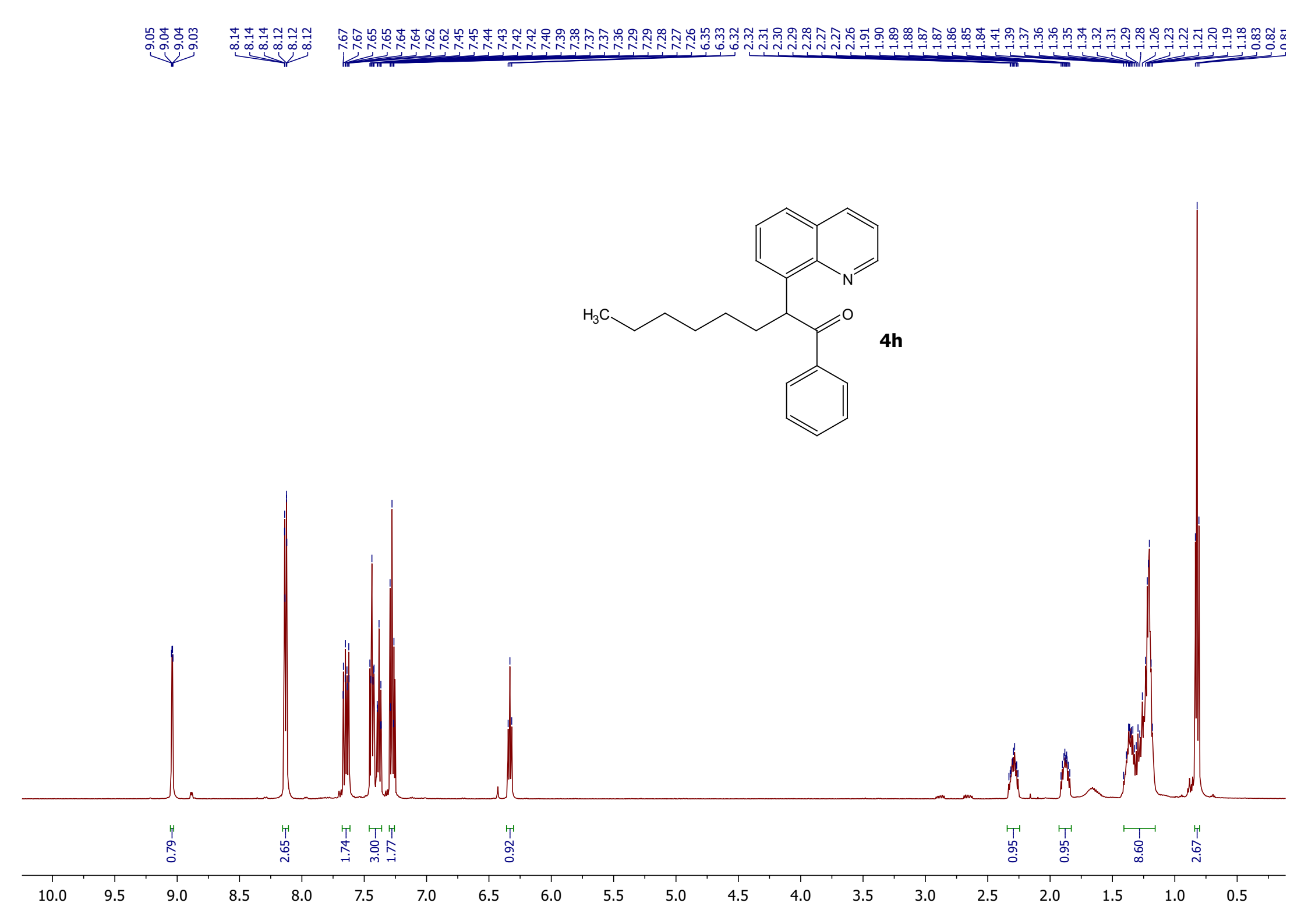
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O
H3C
4h
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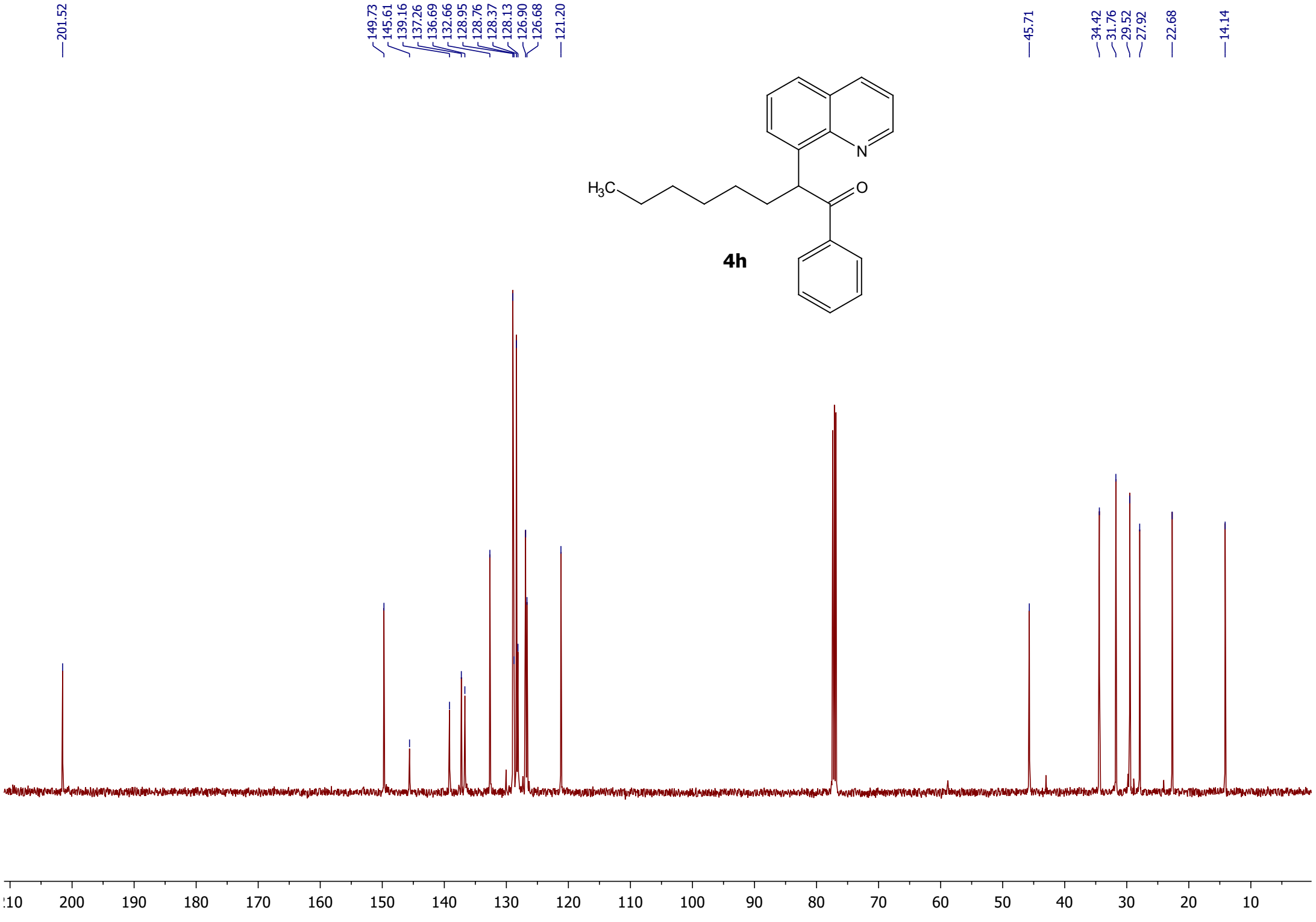
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H3C
N
O
4h
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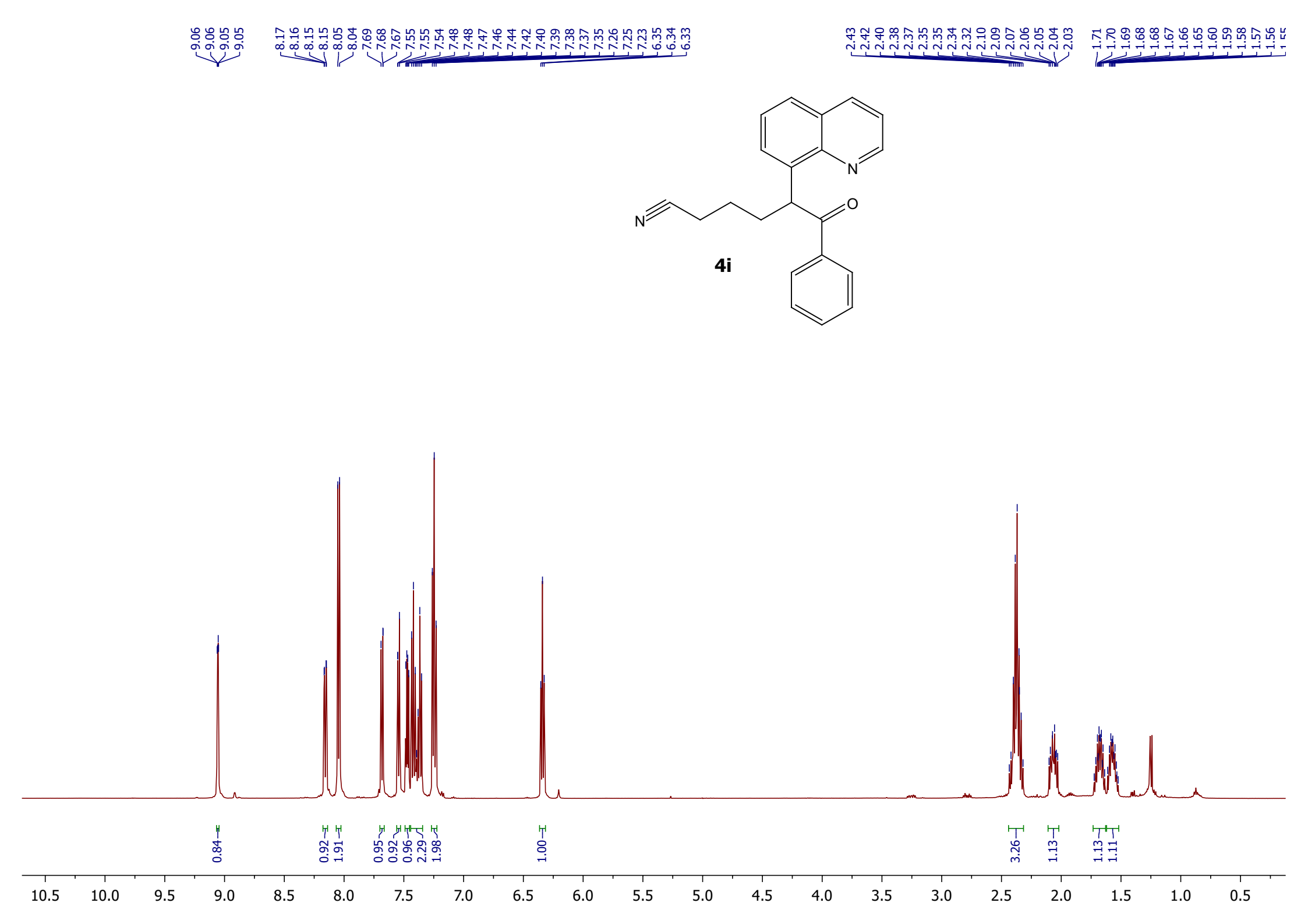
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2.43 2.42 2.40 2.38 2.37 2.35 2.35 2.34 2.32 2.10 2.09 2.07 2.06 2.05 2.04 2.03
1.71 1.70 1.69 1.68 1.68 1.67 1.66 1.65 1.60 1.59 1.58 1.57 1.56
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O
N
4i
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1.13
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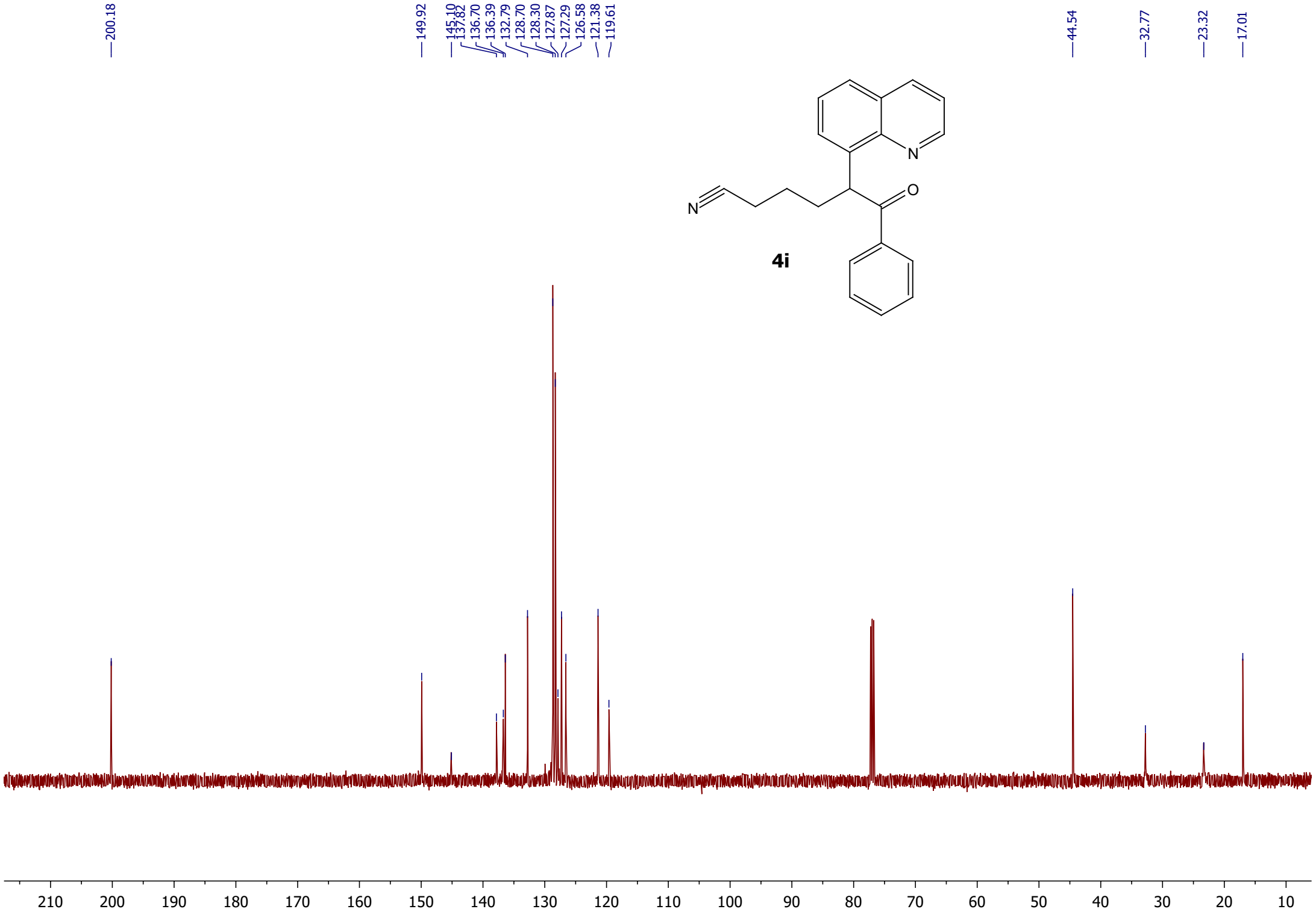
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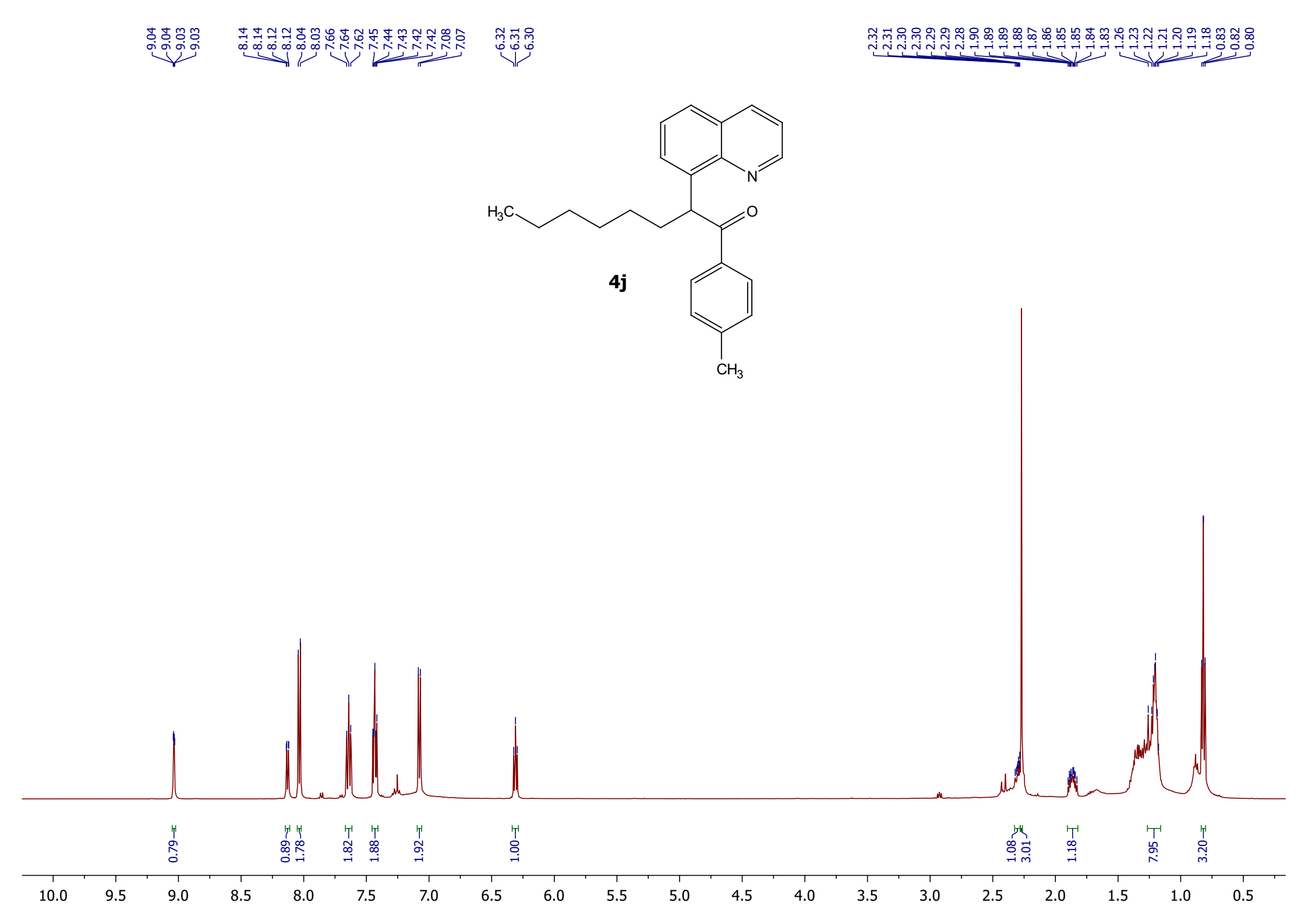
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H3C
CH3
4j
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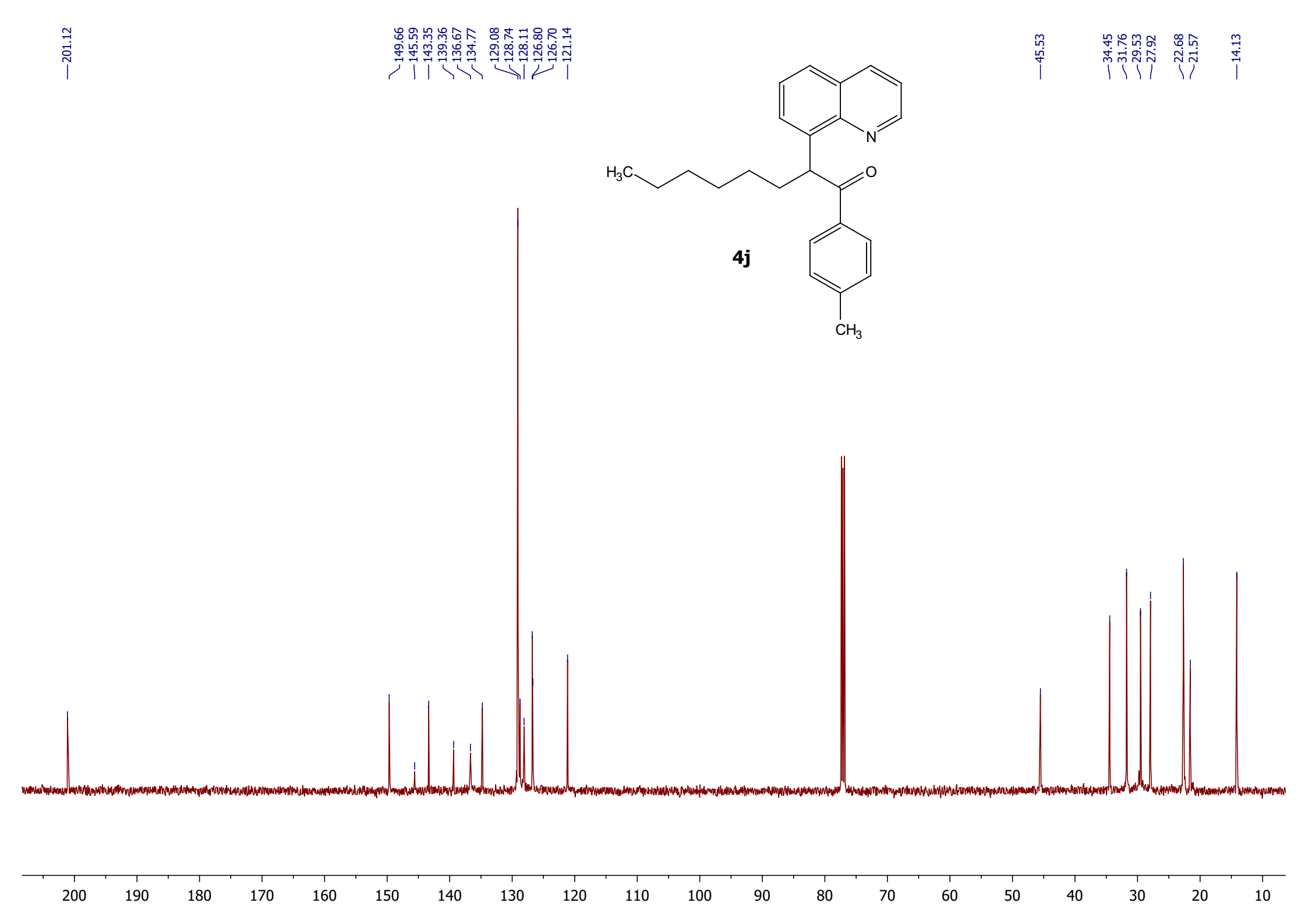
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4j
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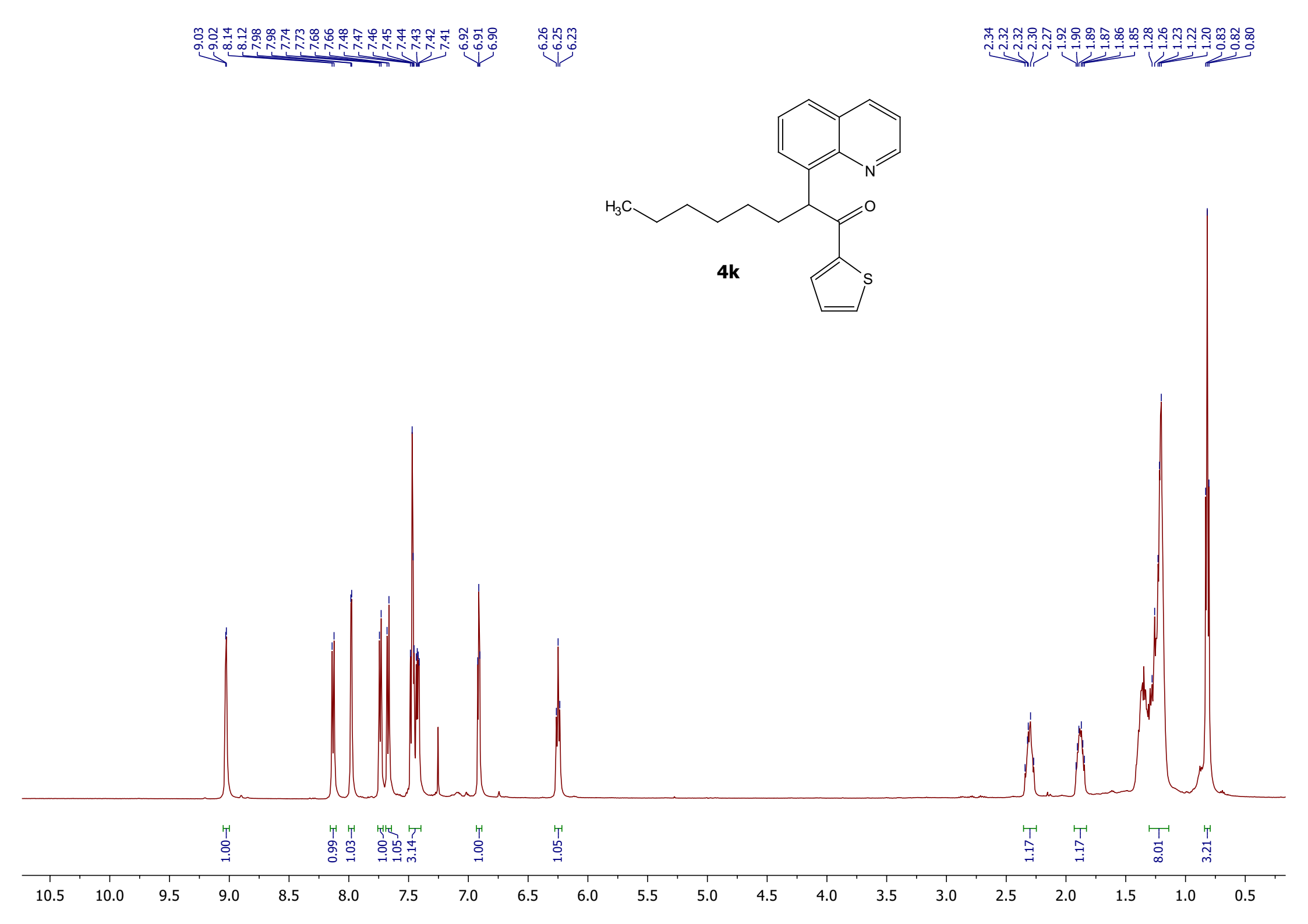
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1.20
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0.80
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O
S
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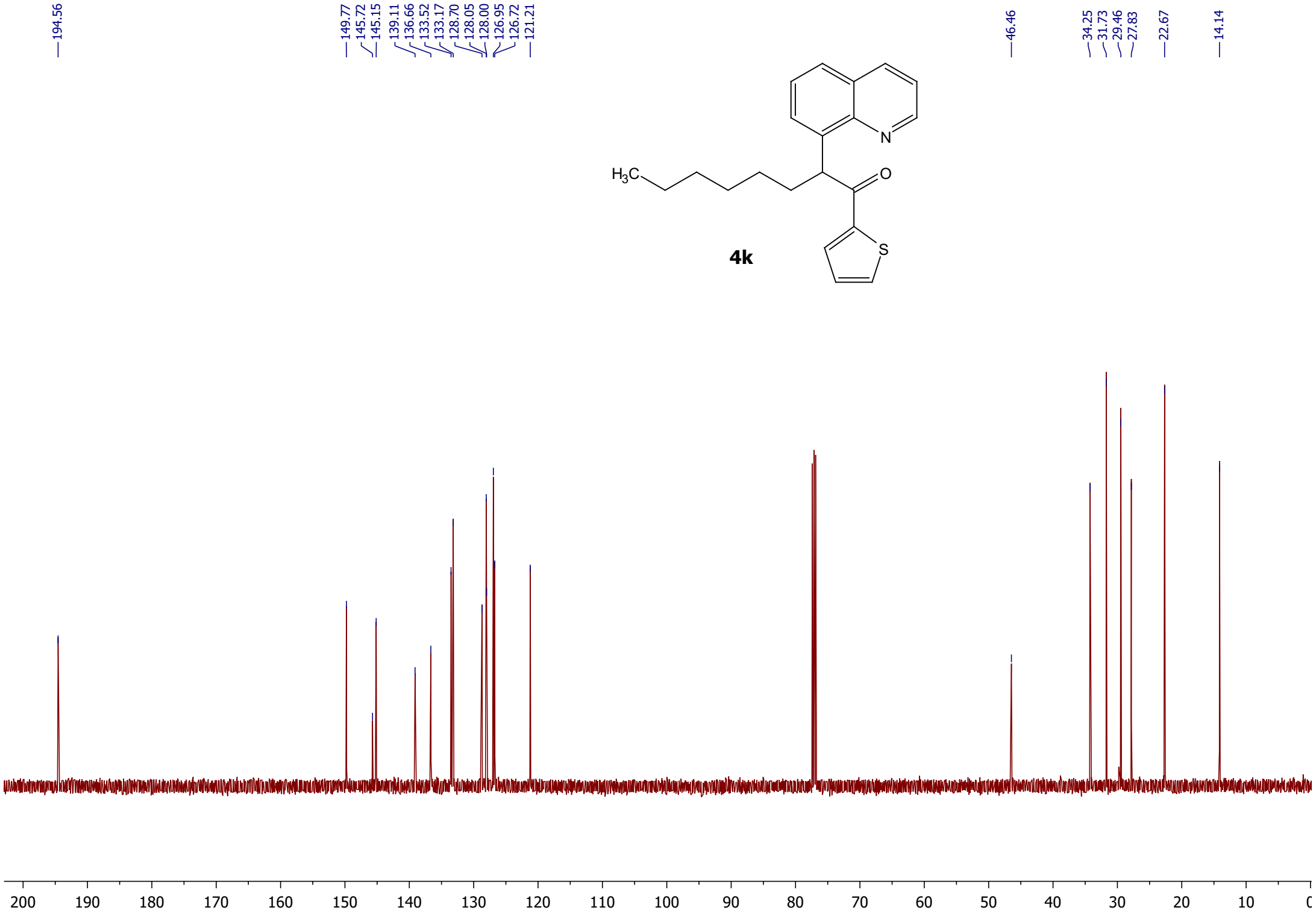
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S
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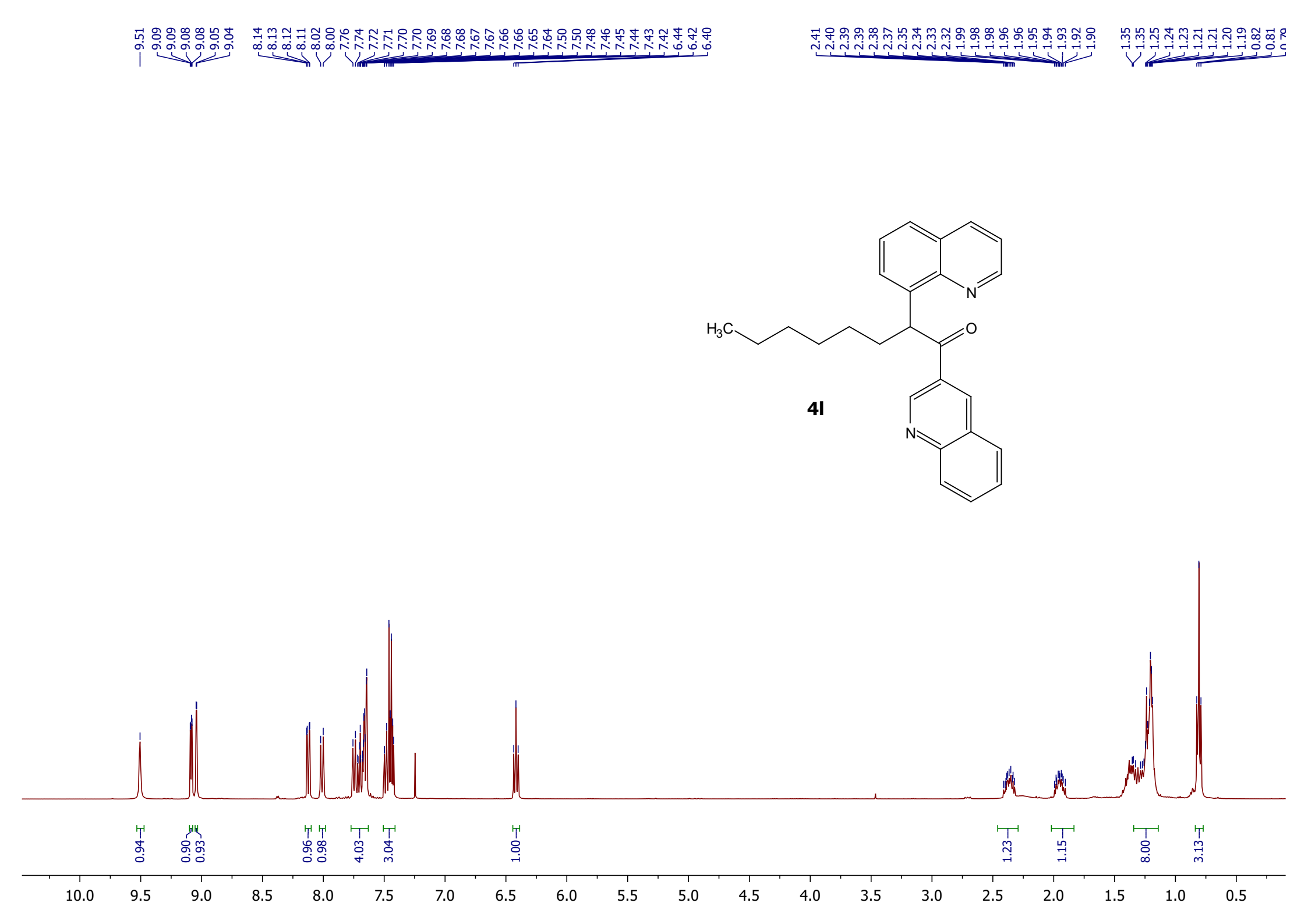
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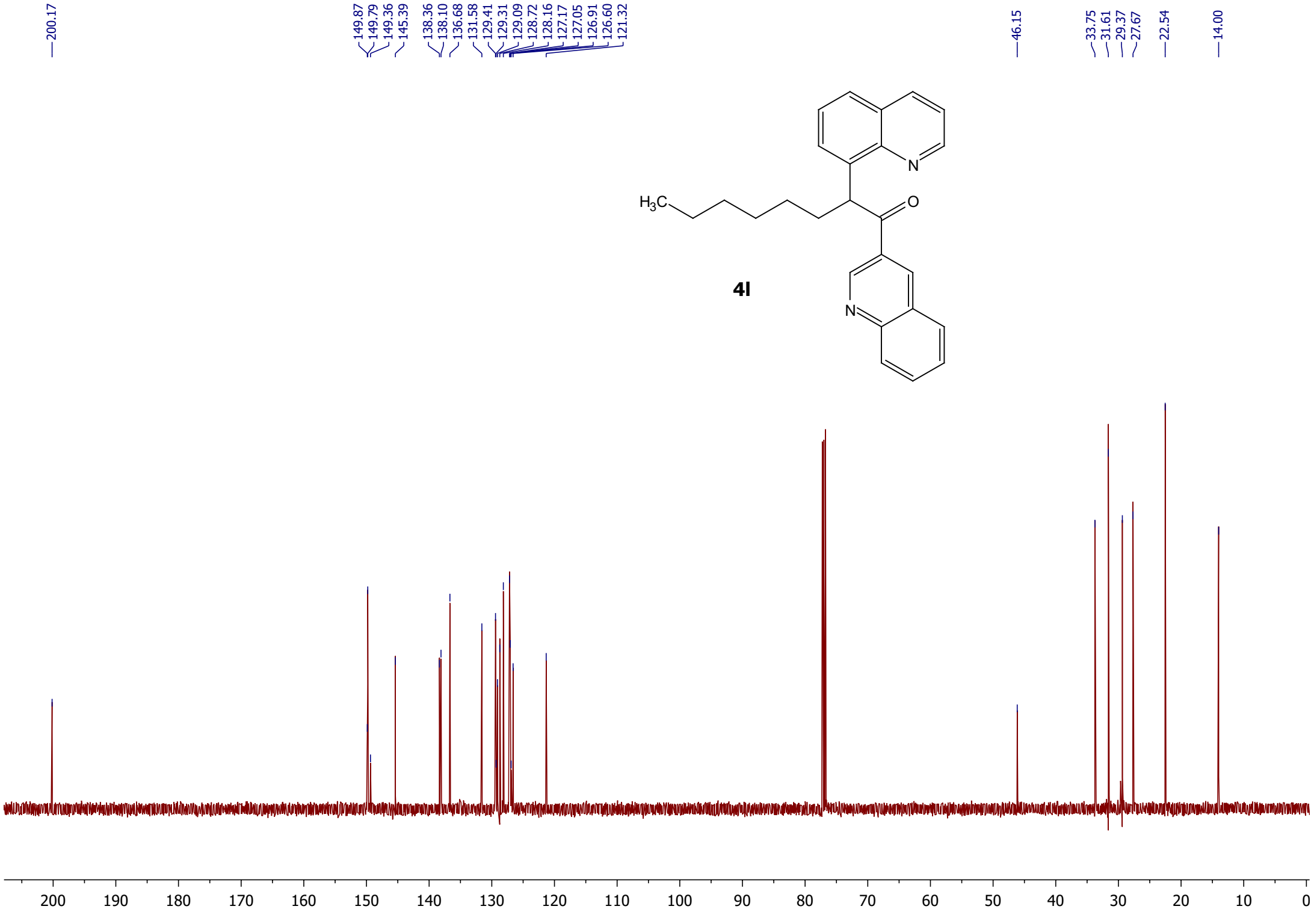
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H3C
O
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N
4l
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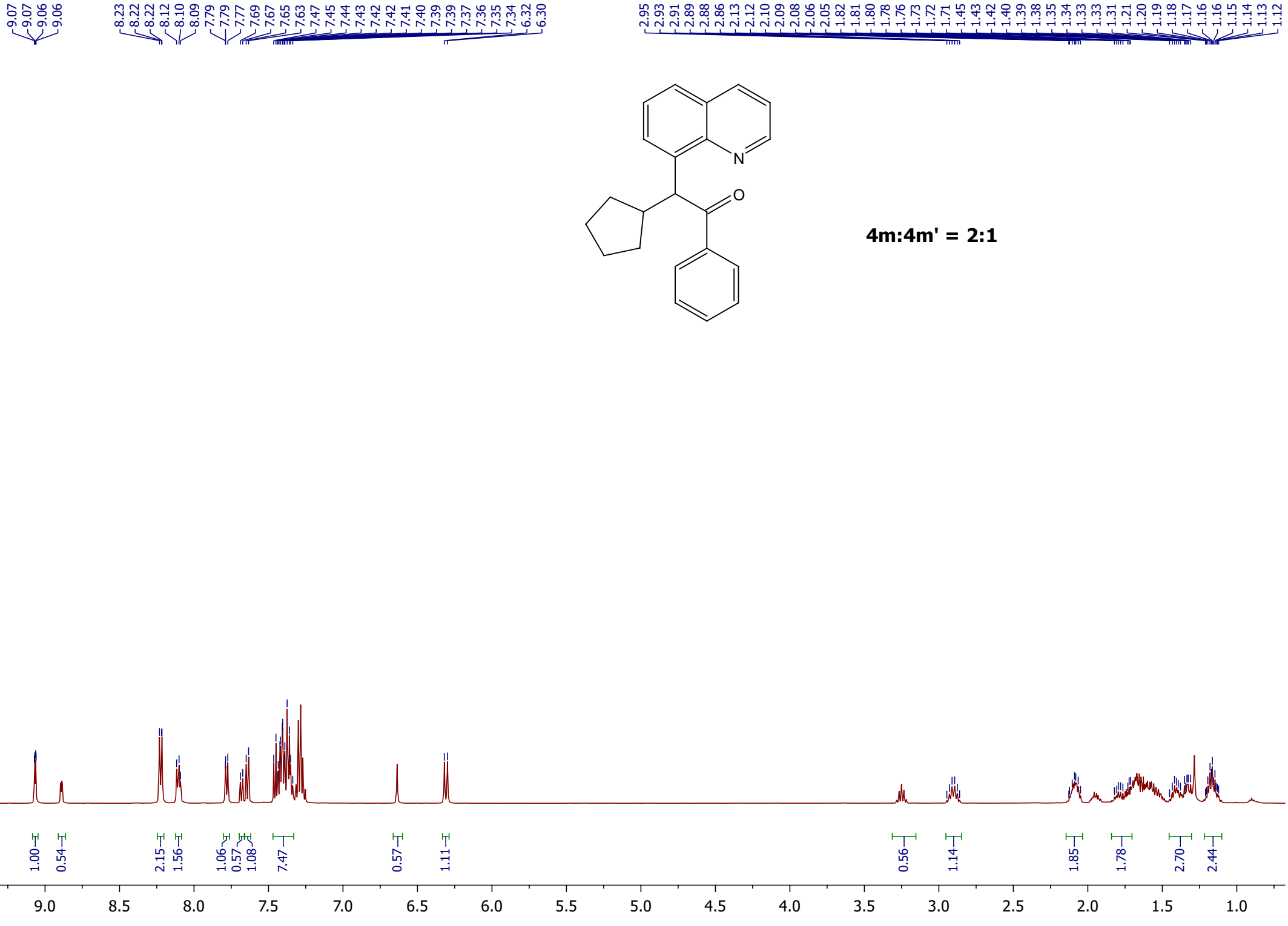
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2.95 2.93 2.91 2.89 2.88 2.86 2.13 2.12 2.10 2.09 2.08 2.06 2.05 1.82 1.81 1.80 1.78 1.76 1.73 1.72 1.71 1.45 1.43 1.42 1.40 1.39 1.38 1.35 1.34 1.33 1.33 1.31 1.21 1.20 1.19 1.18 1.17 1.16 1.16 1.15 1.14 1.13 1.12
N
O
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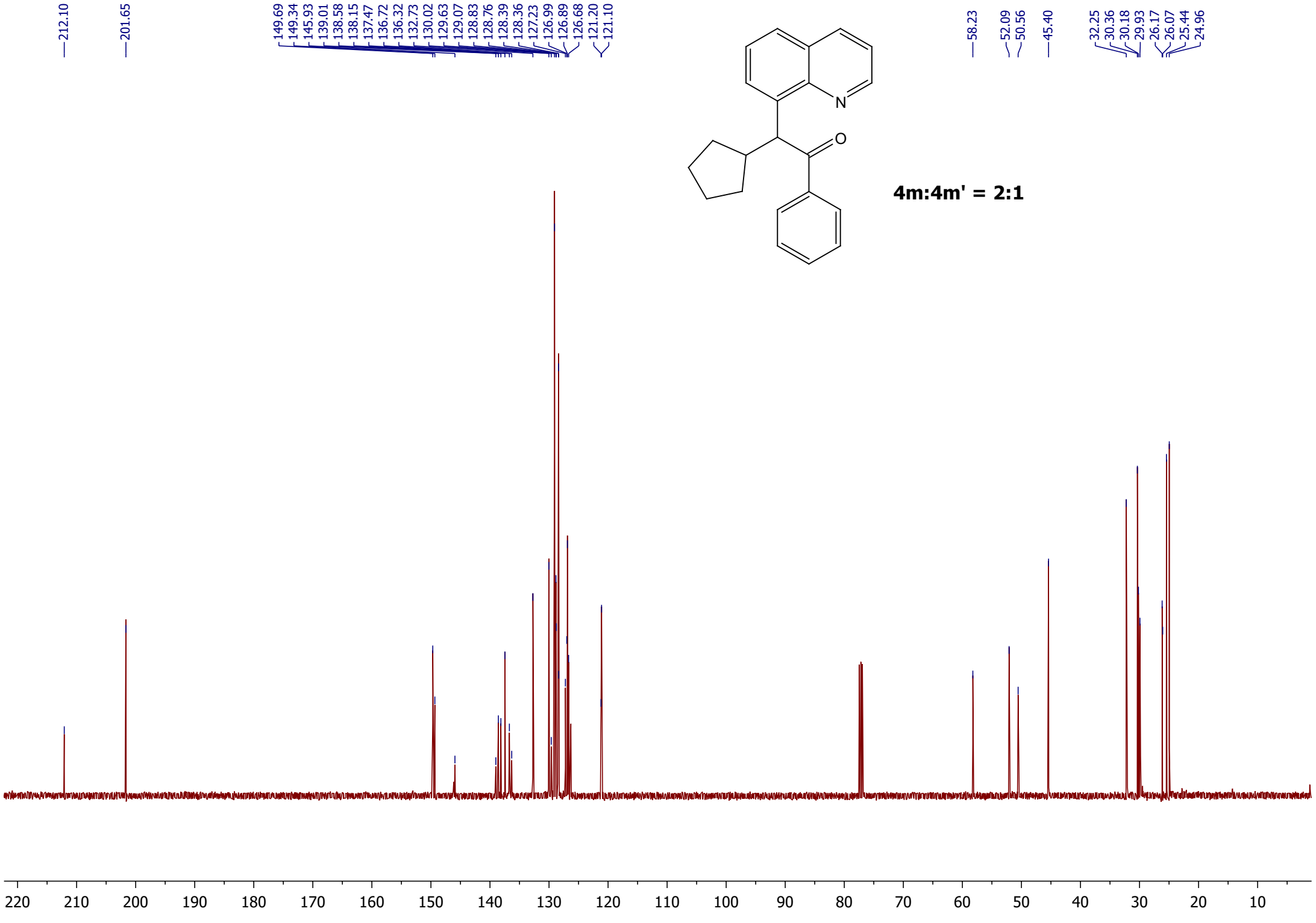
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45.40
32.25
30.36
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26.17
26.07
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O
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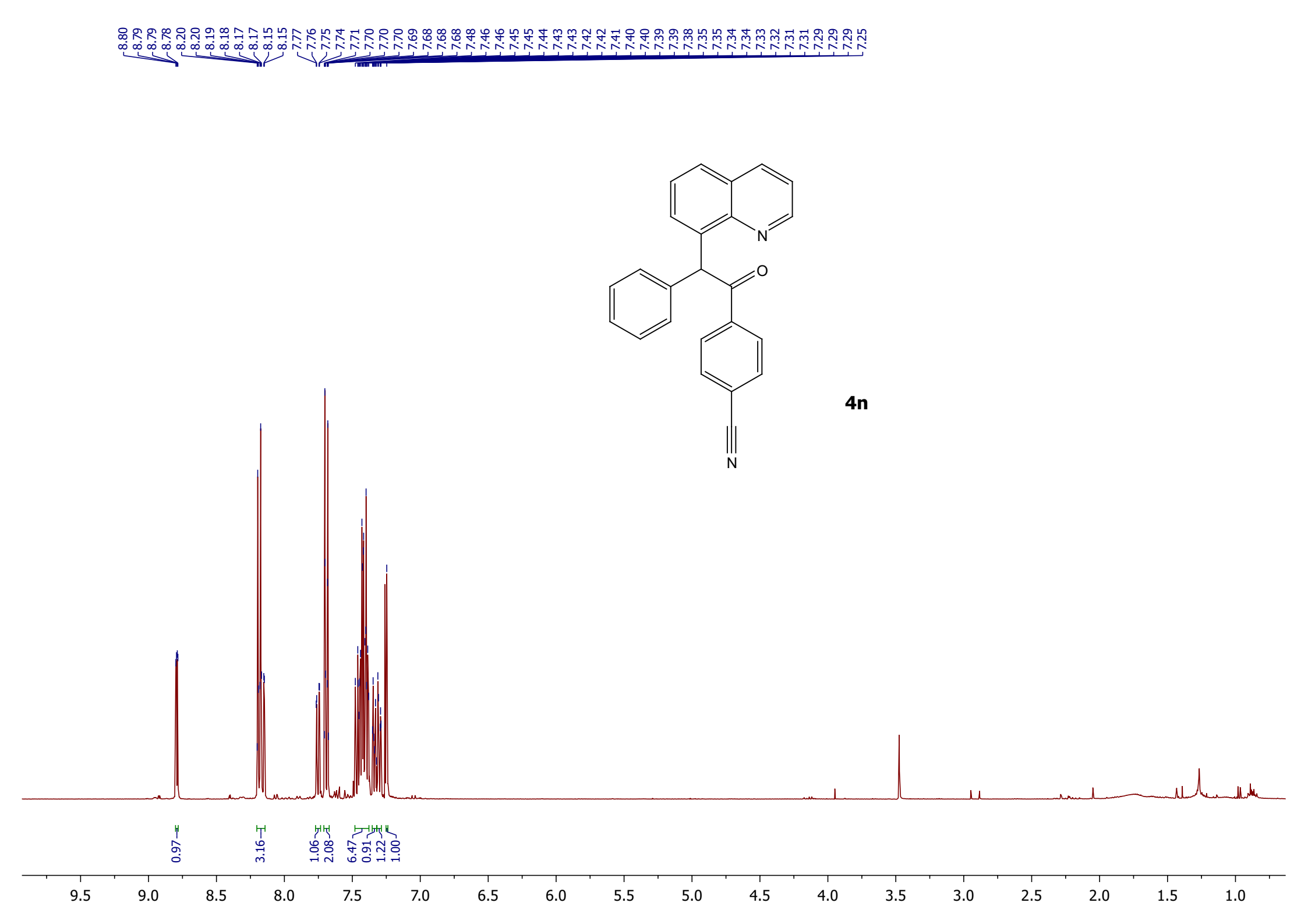
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N
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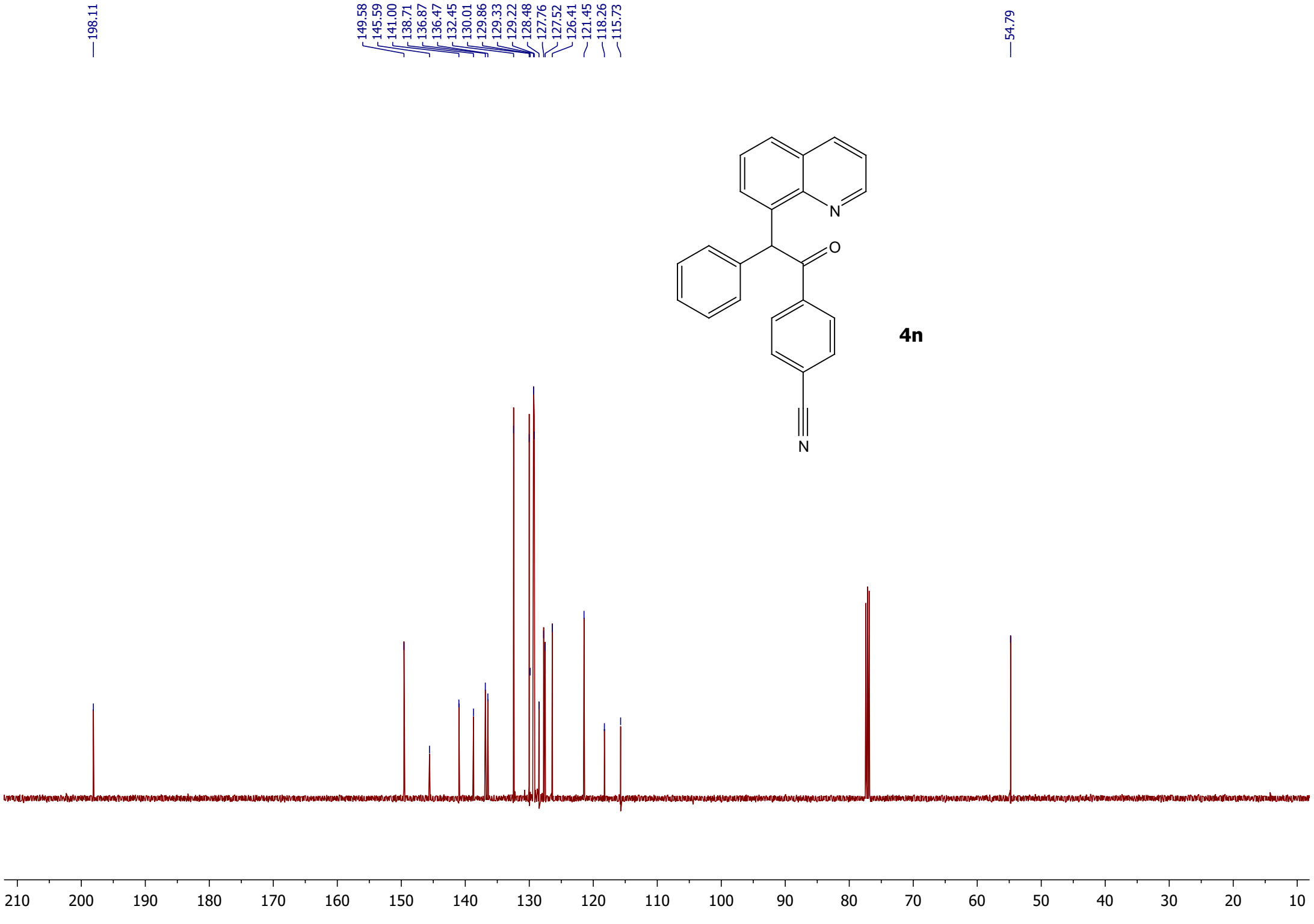
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54.79
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O
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4n
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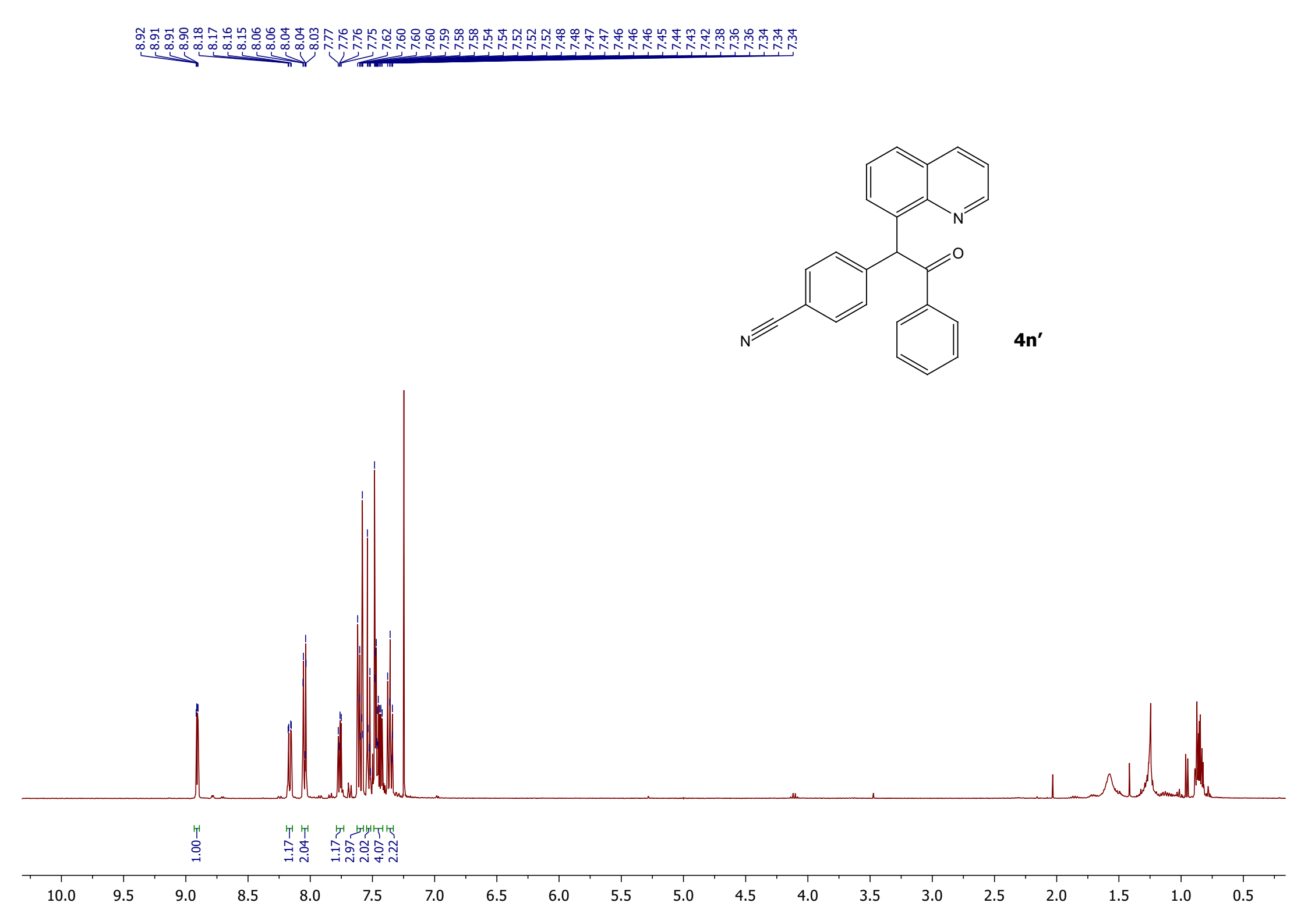
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N
O
N
4n′
1.00 1.17 2.04 1.17 2.97 2.02 4.07 2.22
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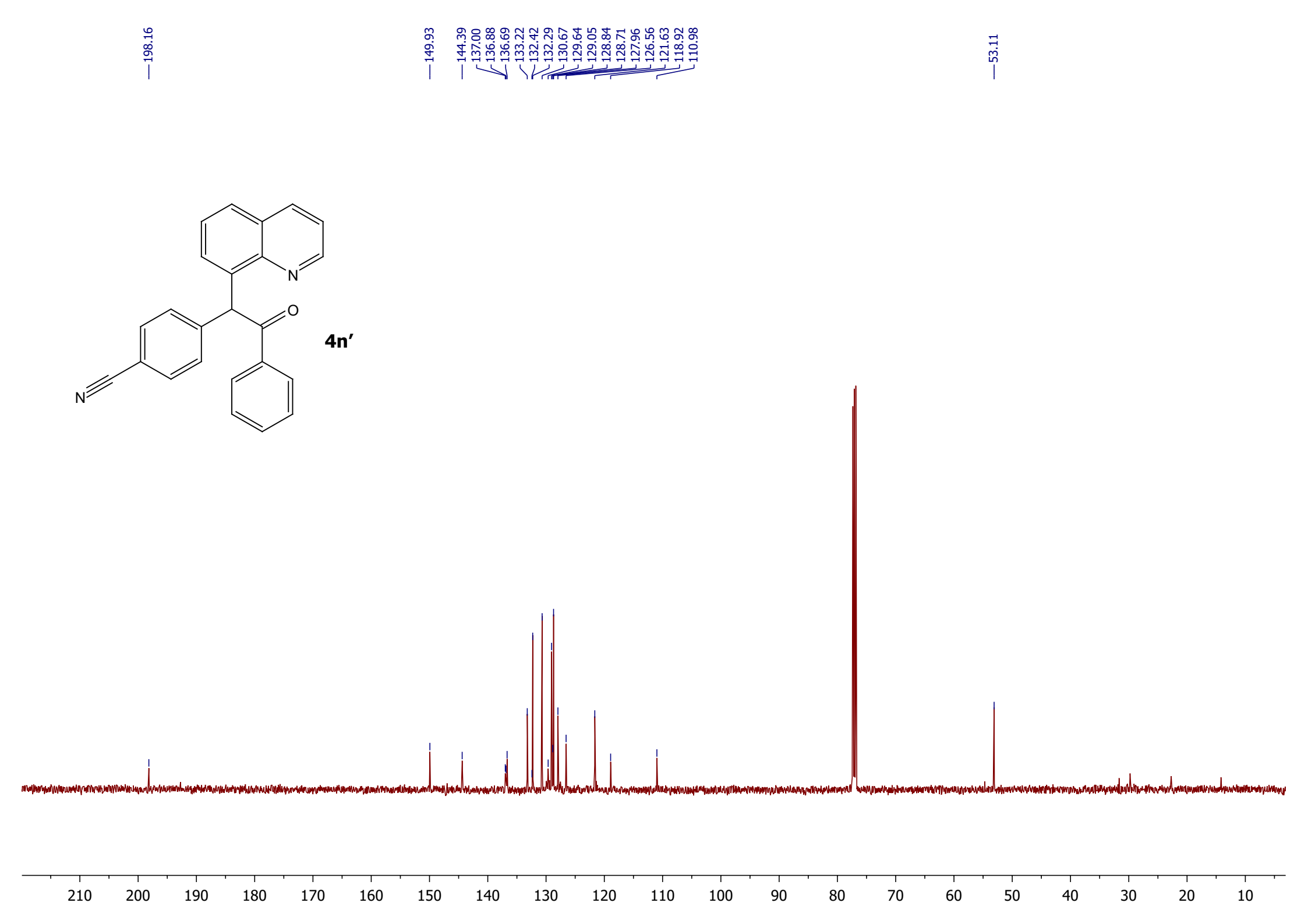
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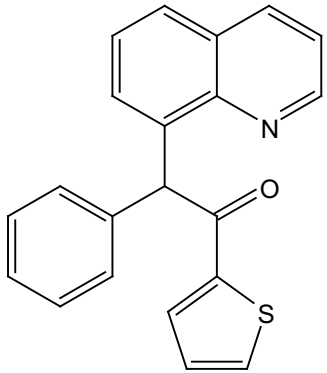
7.02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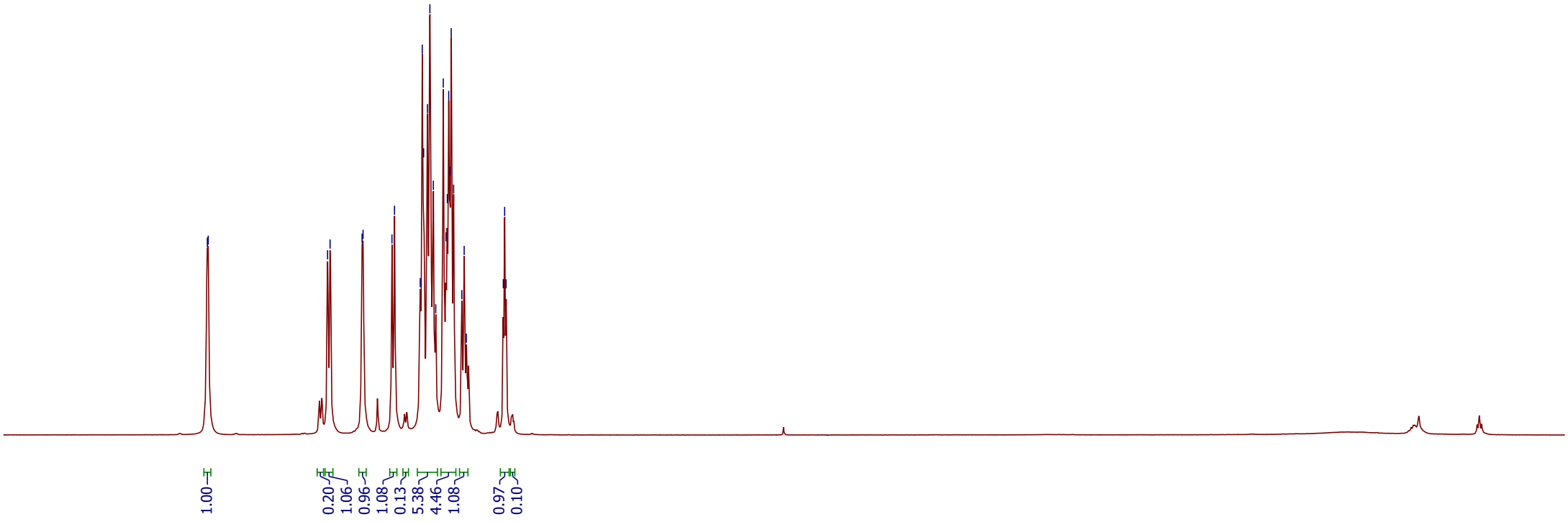
S

4o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9.5
9.0
8.5
8.0
7.5
7.0
6.5
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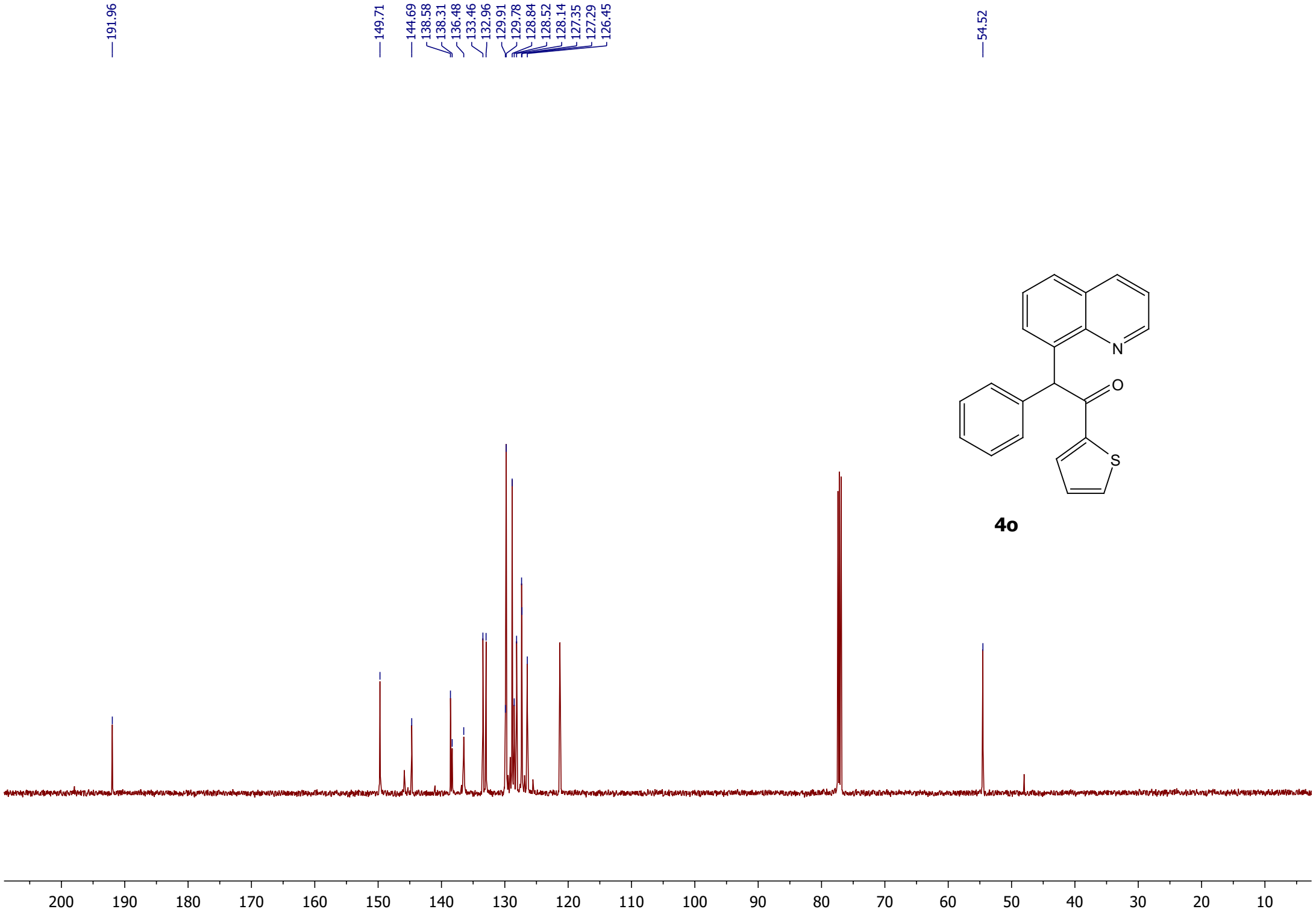
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128.52
128.14
127.35
127.29
126.45
54.52
N
O
S
4o
200
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150
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130
120
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100
90
80
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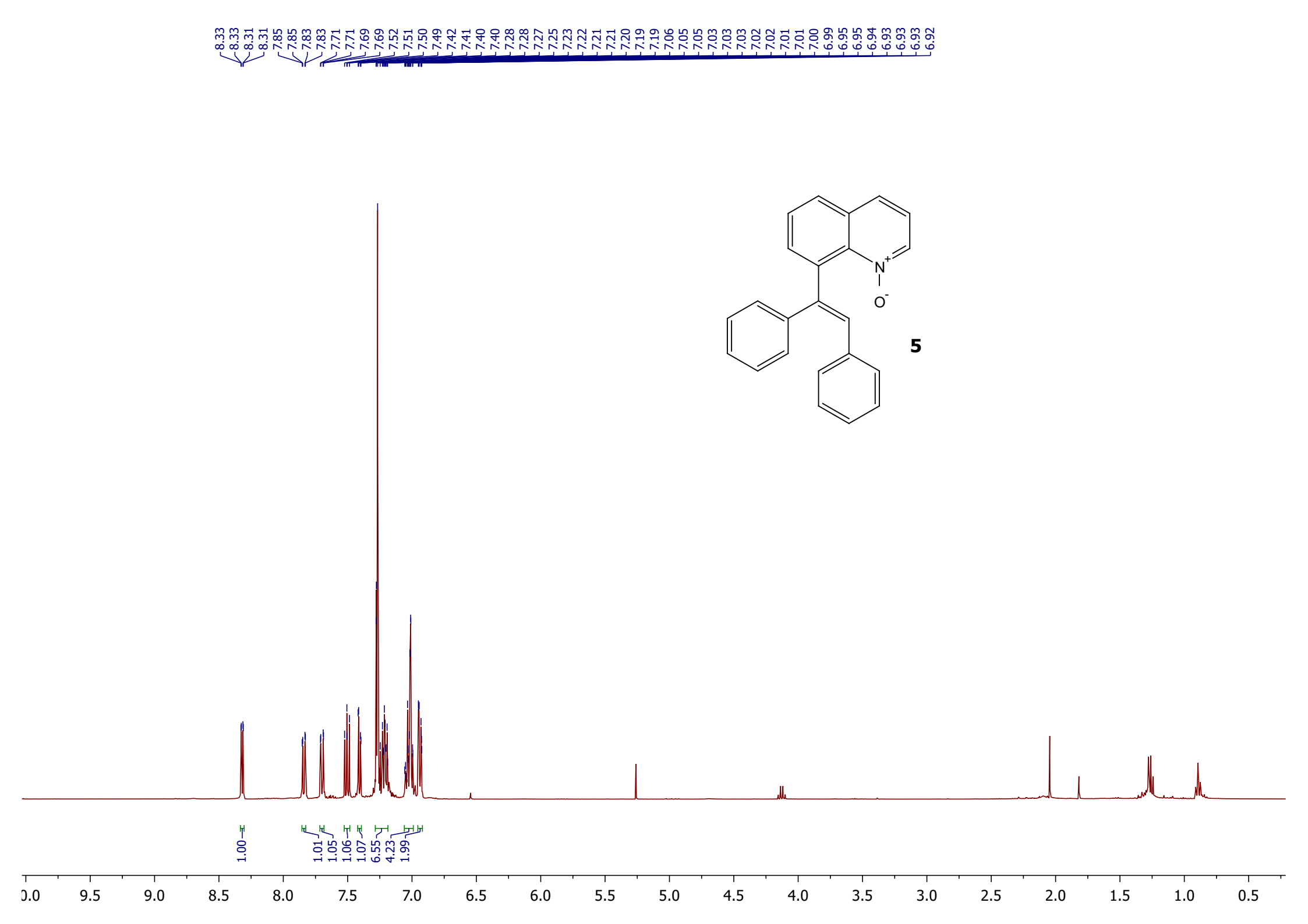
20
10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8.31
8.31
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7.69
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7.51
7.50
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7.42
7.41
7.40
7.40
7.28
7.28
7.27
7.25
7.23
7.22
7.21
7.21
7.20
7.19
7.19
7.06
7.05
7.05
7.03
7.03
7.03
7.02
7.02
7.01
7.01
7.00
6.99
6.95
6.95
6.94
6.93
6.93
6.92
N+
O-
5
1.00
1.01
1.05
1.06
1.07
6.55
4.23
1.99
0.0
9.5
9.0
8.5
8.0
7.5
7.0
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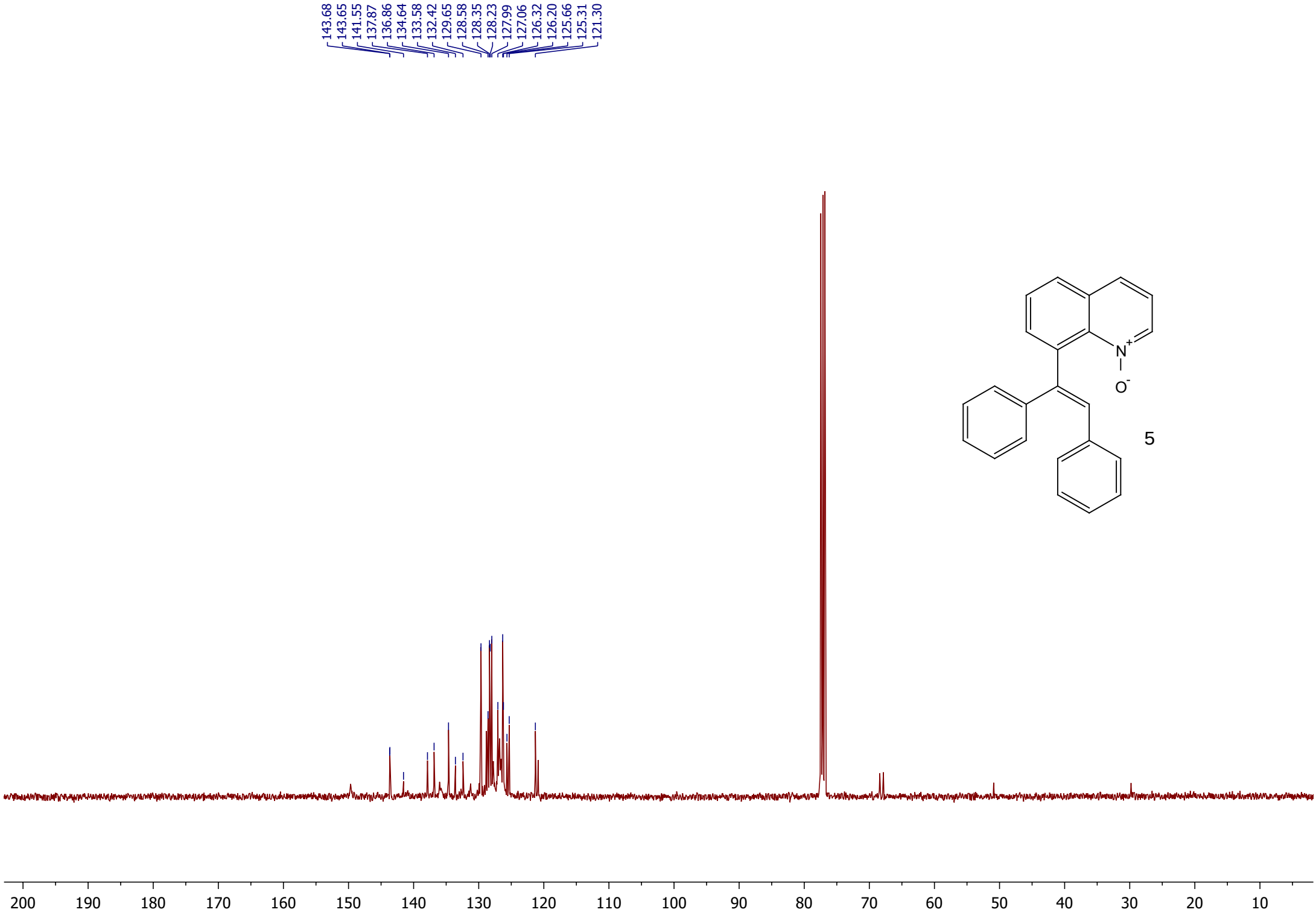
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136.86
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133.58
132.42
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128.35
128.23
127.99
127.06
126.32
126.20
125.66
125.31
121.30
N+
O-
5
200
190
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170
160
150
140
130
120
110
100
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80
70
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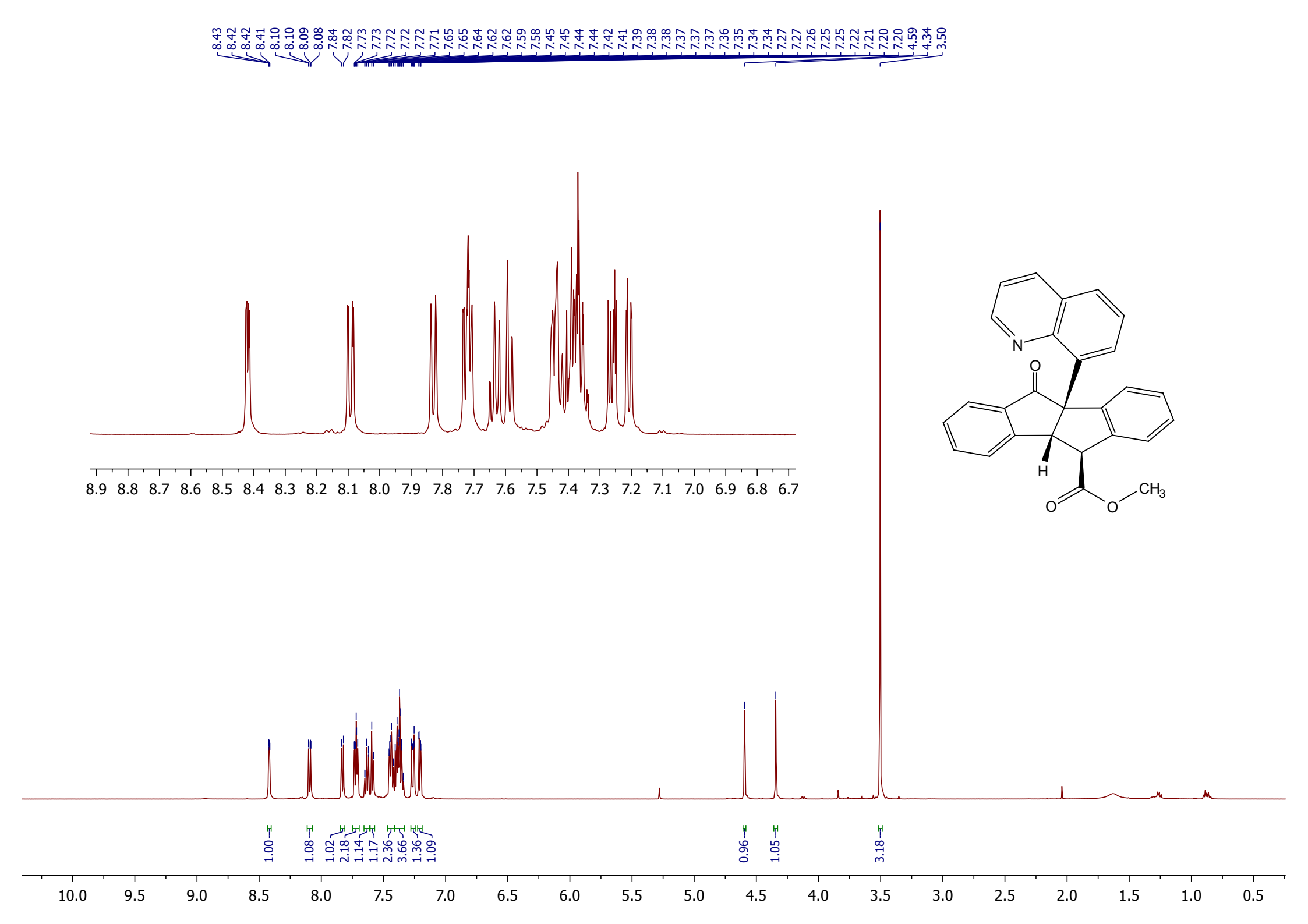
30
20
10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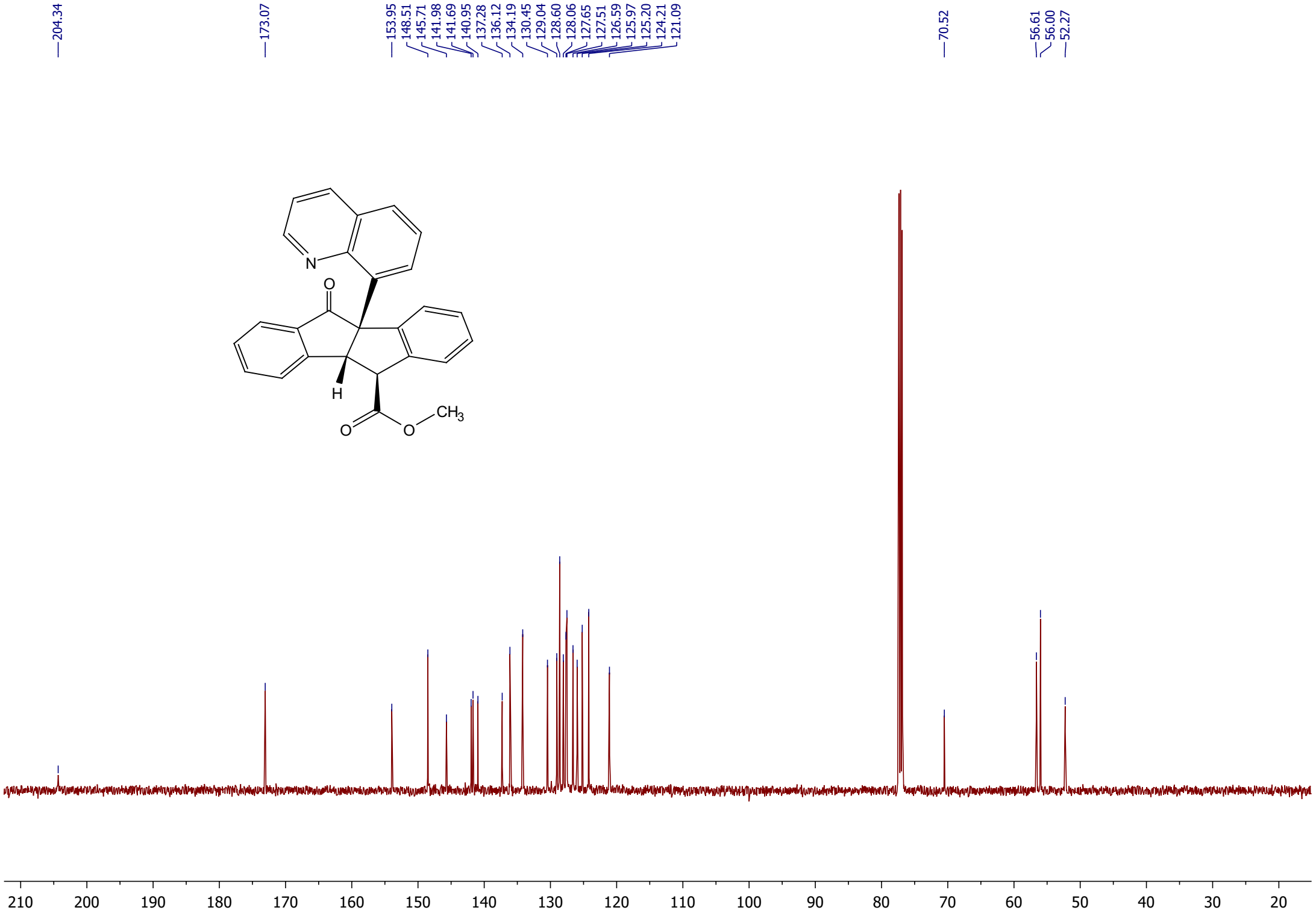
8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
N
O
H
O
O
CH3
1.00 1.08 1.02 2.18 1.14 1.17 2.36 3.66 1.36 1.09 0.96 1.05 3.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5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140.95
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134.19
130.45
129.04
128.60
128.06
127.65
127.51
126.59
125.97
125.20
124.21
121.09
70.52
56.61
56.00
52.27
N
O
H
O
O
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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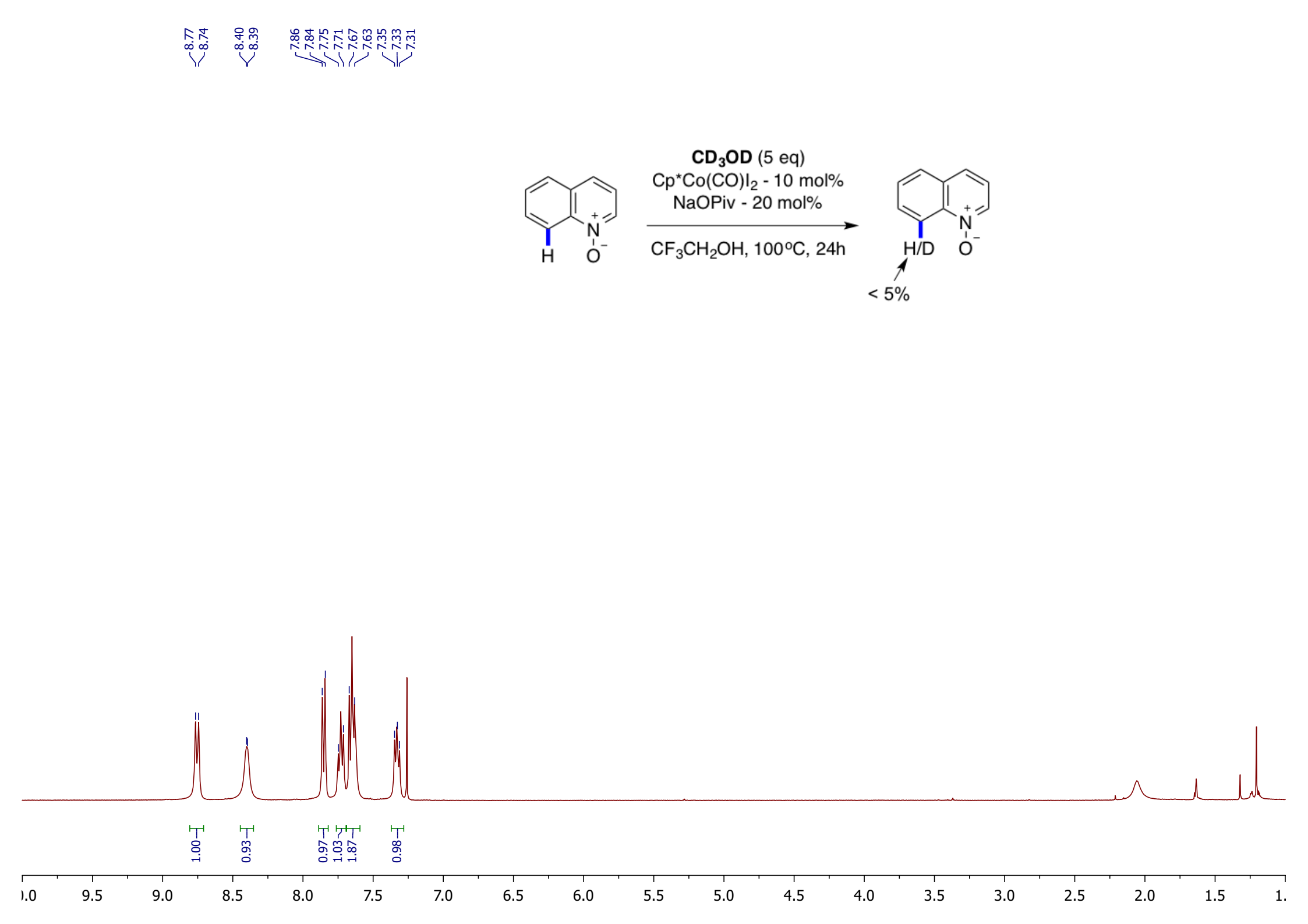
30
20


8.77
8.74
8.40
8.39
7.86
7.84
7.75
7.71
7.67
7.63
7.35
7.33
7.31
CD3OD (5 eq)
Cp*Co(CO)I2 - 10 mol%
NaOPiv - 20 mol%
CF3CH2OH, 100ºC, 24h
H
N
O
H/D
< 5%
1.00
0.93
0.97
1.03
1.87
0.98
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