Surpporting Information

A novel and one-pot method for the synthesis of substituted furopyridines: I_2-mediated oxidative reaction of enamines via tandem cyclization under metal-free conditions

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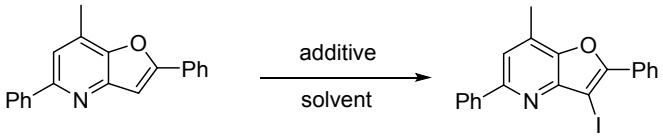
General remark

^{1}H NMR and ^{13}C NMR spectra were recorded on 400MHz and 100MHz in $CDCl_3$. All chemical shifts are given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. All compounds were further characterized by HRMS; copies of their ^{1}H NMR and ^{13}C NMR spectra are provided. Products were purified by flash chromatography on 100–200 mesh silica gels. All melting points were determined without correction. Unless otherwise noted, commercially available reagents and solvents were used without further purification.

Table 2. Optimization of Reaction Condition [a]



2a **3a**

entry	Additive/equiv	Acid	solvent	yield[b]
1	I_2 (1.2)	HOAc	DMSO	40
2	I_2 (1.2)	TsOH	DMSO	55
3	I_2 (1.2)	CF_3SO_3H	DMSO	52
4	I_2 (1.2)	CF_3COOH	DMSO	43
5	NIS (2.0)	CF_3SO_3H	DMSO	60
6	NIS (2.0)	TsOH	DMSO	68
7	NIS (2.0)	TsOH	DMF	56
8	NIS (2.0)	TsOH	THF	36
9	NIS (2.0)	TsOH	DCE	42

[a] Reaction conditions: **2a** (0.3 mmol), acid (0.3 mmol), solvent (2 mL), 120 °C. [b] Yields of isolated products.

Experimental Section

The substrate 1 was prepared according to following literatures1-3:

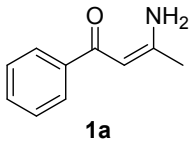
A mixture of 1-phenyl-1,3-butanedione **1a** (6.0 mmol), NH_4OAc (30.0 mmol) and MeOH (10 mL) was heated at 70 °C for 2 h. The mixture was cooled to room temperature. The solid was filtered and washed with water then MeOH to give the title product as a white solid.

(1) X. Fan, Y. He, L. Cui, S. Guo, J. Wang, X. Zhang. *Eur. J. Org. Chem.* **2012**, *4*, 673–677.

(2) Y. K. Ramtohul, A. Chartrand. *Org. Lett.*, **2007**, *9*, 1029.

(3)X. Sun, Y. Lyu, D. Zhang-Negrerie, Y. Du, K. Zhao. *Org. Lett.*, **2013**, *15*, 6222.

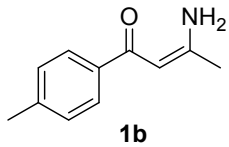
Characterization data of 1 .



1a

(Z)-3-amino-1-phenylbut-2-en-1-one(1a)[1]

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.13 (s, 1 H), 7.81-7.78 (m, 2 H), 7.37-7.31 (m, 3 H), 5.66 (s, 1 H), 5.22 (s, 1 H), 1.97 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 189.48, 162.97, 140.17, 130.77, 128.17, 127.06, 92.28, 22.83. HRMS calcd for $C_{10}H_{12}NO$ $[M+H]^+$ 162.0913; found: 162.0911

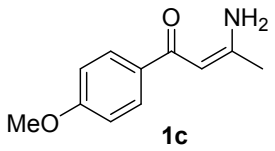


1b

(Z)-3-amino-1-(p-tolyl)but-2-en-1-one(1b)

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.18 (s, 1 H), 7.80-7.78 (d, *J* = 8.0 Hz , 2 H), 7.23-7.21 (d, *J* = 8.0 Hz , 2 H), 5.73 (s, 1 H), 5.28 (s, 1 H), 2.39 (s, 3 H), 2.04 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 189.28, 162.58, 141.10, 137.46, 128.86, 127.11, 92.08, 22.81,

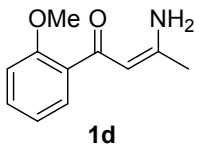
21.38. HRMS calcd for $C_{11}H_{14}NO$ $[M+H]^+$ 176.1069; found: 176.1065.



1c

(Z)-3-amino-1-(4-methoxyphenyl)but-2-en-1-one(1c)

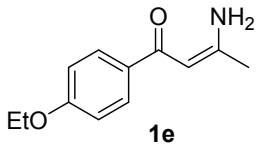
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.11 (s, 1 H), 7.87-7.85 (d, *J* = 8.0 Hz, 2 H), 6.91-6.89 (d, *J* = 8.0 Hz, 2 H), 5.69 (s, 1 H), 5.29 (s, 1 H), 3.83 (s, 3 H),2.02 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 188.48, 162.31, 161.78, 132.84, 128.91, 113.34, 91.71, 55.24, 22.77. HRMS calcd for $C_{11}H_{14}NO_2$ $[M+H]^+$ 192.1018; found: 191.1016.



1d

(Z)-3-amino-1-(2-methoxyphenyl)but-2-en-1-one(1d)

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.02 (s, 1 H), 7.51-7.48 (m, 1 H), 7.28-7.24 (m, 1 H), 6.91-6.83 (m, 2 H), 5.54 (s, 1 H), 5.21 (s, 1 H), 3.79 (s, 3 H), 1.92 (d, *J* = 1.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 190.43, 162.12, 162.03, 156.92, 131.33, 130.86, 129.56, 120.41, 111.42, 97.06, 97.05, 55.64, 22.67. HRMS calcd for $C_{11}H_{14}NO_2$ $[M+H]^+$ 192.1018; found: 192.1016.

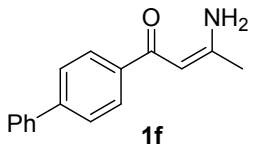


1e

(Z)-3-amino-1-(4-ethoxyphenyl)but-2-en-1-one(1e)

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.10 (s, 1 H), 7.85–7.83 (d, *J* = 8.0 Hz, 2 H), 6.89-6.87 (d, *J* = 8.0 Hz, 2 H), 5.68 (s, 1 H), 5.27 (s, 1 H), 4.08–4.03 (m, 2 H), 2.01 (s, 3 H), 1.42-1.39 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 188.53, 162.22, 161.20, 132.64, 128.91, 113.82, 91.71, 63.45, 22.78, 14.68. HRMS calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$ 206.1175;

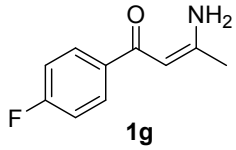
found: 206.1179.



1f

(Z)-1-([1,1'-biphenyl]-4-yl)-3-aminobut-2-en-1-one(1f)

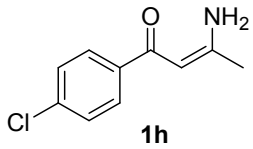
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.25 (brs, 1 H), 7.97-7.95 (d, *J* = 8.0 Hz, 2 H), 7.65 - 7.62 (m, 3 H), 7.47-7.45 (d, *J* = 8.0 Hz, 2 H), 7.39-7.35 (m, 1 H), 5.79 (s, 1 H), 5.24 (brs, 1 H), 2.08 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 188.99, 162.91, 143.52, 140.45, 138.90, 128.80, 127.69, 127.65, 127.18, 126.91, 92.35, 22.93. HRMS calcd for $C_{16}H_{16}NO$ $[M+H]^+$ 238.1226; found: 238.1223.



1g

(Z)-3-amino-1-(4-fluorophenyl)but-2-en-1-one (1g)

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.17 (brs, 1 H), 7.89-7.86 (m, 2 H), 7.09-7.04 (m, 2 H), 5.67 (s, 1 H), 5.21 (brs, 1 H), 2.05 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 188.03, 165.74-163.25 (d, *J* = 249 Hz, 1 C), 162.98, 136.40-136.37 (d, *J* = 3 Hz, 1 C), 129.38-129.29 (d, *J* = 9 Hz, 2 C), 115.19-114.97 (d, *J* = 22 Hz, 2 C), 91.94, 22.89. HRMS calcd for $C_{10}H_{11}FNO$ $[M+H]^+$ 180.0818; found: 180.0814.

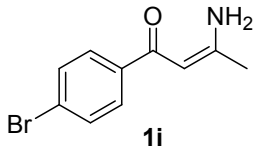


1h

(Z)-3-amino-1-(4-chlorophenyl)but-2-en-1-one(1h)

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.21 (brs, 1 H), 7.82-7.80 (d, *J* = 8.0 Hz, 2 H), 7.38-7.36 (d, *J* = 8.0 Hz, 2 H), 5.68 (s, 1 H), 5.30 (brs, 1 H), 2.06 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 187.98, 163.38, 138.52, 136.91, 128.54, 128.43, 92.01, 22.92. HRMS calcd

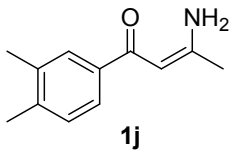
for $C_{10}H_{11}ClNO$ $[M+H]^+$ 196.0523; found: 196.0521.



1i

(Z)-3-amino-1-(4-bromophenyl)but-2-en-1-one (1i)

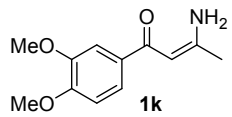
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.21 (brs, 1 H), 7.74-7.72 (d, *J* = 8.0 Hz, 2 H), 7.54-7.52 (d, *J* = 8.0 Hz, 2 H), 5.67 (s, 1 H), 5.34 (brs, 1 H), 2.05 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 188.00, 163.42, 138.95, 131.36, 128.71, 125.41, 91.93, 22.84. HRMS calcd for $C_{10}H_{11}BrNO$ $[M+H]^+$ 240.0018; found: 240.0015.



1j

(Z)-3-amino-1-(3,4-dimethylphenyl)but-2-en-1-one (1j)

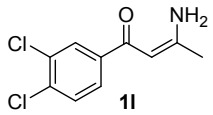
^{1}H NMR (400 MHz, CDCl3, ppm): δ = 10.15 (brs, 1 H), 7.66 (s, 1 H), 7.62-7.59(m, 1 H), 7.17 -7.15 (d, *J* = 8.0 Hz, 1 H), 5.72 (s, 1 H), 5.21 (brs, 1 H) 2.30 (s, 3 H), 2.29 (s, 3 H), 2.04 (s, 3 H); ^{13}C NMR (100 MHz, CDCl3, ppm): δ = 189.58, 162.43, 139.83, 137.87, 136.34, 129.44, 128.34, 124.64, 92.19, 22.82, 19.77, 19.75. HRMS calcd for $C_{12}H_{16}NO$ $[M+H]^+$ 190.1226; found: 190.1221.



1k

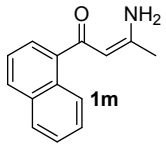
(Z)-3-amino-1-(3,4-dimethoxyphenyl)but-2-en-1-one (1k)

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.12 (brs, 1 H), 7.511-7.506 (d, *J* = 2.0 Hz, 1 H), 7.48- 7.45 (m, 1 H), 6.86-6.84 (d, *J* = 8.0 Hz, 1 H), 5.70 (s, 1 H), 5.16 (brs, 1 H), 3.94 (s, 3 H), 3.91 (s, 3 H), 2.04 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 188.45, 162.26, 151.42, 148.73, 133.09, 120.51, 110.05, 109.98, 91.76, 55.91, 55.86, 22.89. HRMS calcd for $C_{12}H_{16}NO_3$ $[M+H]^+$ 222.1124; found: 222.1123.



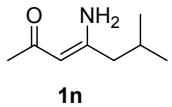
(Z)-3-amino-1-(3,4-dichlorophenyl)but-2-en-1-one (1l)

^{1}H NMR (400 MHz, CDCl3, ppm): δ = 10.16 (brs, 1 H), 7.89-7.88 (d, *J* = 4.0 Hz, 1 H), 7.62-7.61 (d, *J* = 4.0 Hz, 1 H), 7.42-7.40 (d, *J* = 8.0 Hz, 1 H), 5.58 (s, 1 H), 5.35 (brs, 1 H), 2.01 (s, 3 H); ^{13}C NMR (100 MHz, CDCl3, ppm): δ = 186.34, 164.00, 139.96, 134.85, 132.55, 130.21, 129.18, 126.24, 91.79, 22.85. HRMS calcd for $C_{10}H_{10}Cl_2NO$ $[M+H]^+$ 230.0133; found: 230.0137.



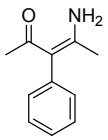
(Z)-3-amino-1-(naphthalen-1-yl)but-2-en-1-one (1m)

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.30 (brs, 1 H), 8.40 (s, 1 H), 8.02-8.00 (m, 1 H), 7.96 -7.93 (m, 1 H), 7.89-7.85 (m, 2 H), 7.532-7.525 (d, *J* =2.8 Hz, 2 H), 5.91 (s, 1 H), 5.24 (brs, 1 H), 2.12 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 189.34, 162.84, 137.48, 134.65, 132.85, 129.19, 127.89, 127.62, 127.51, 127.18, 126.21, 124.18, 92.57, 22.95. HRMS calcd for $C_{10}H_{14}NO$ $[M+H]^+$ 212.1069; found: 212.1066.



(Z)-4-amino-6-methylhept-3-en-2-one (1n)

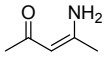
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 9.70 (brs, 1 H), 5.40 (brs, 1 H), 4.93 (s, 1 H), 2.06-2.05 (d, *J* = 4.0 Hz, 1 H), 1.96-1.95 (m, 1 H), 1.91-1.80 (m, 3 H), 0.88–0.83 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 196.65, 164.12, 95.91, 95.76, 51.68, 45.73, 29.26, 27.73, 22.28. HRMS calcd for $C_8H_{16}NO$ $[M+H]^+$ 142.1226; found: 142.1225.



1o

(Z)-4-amino-3-phenylpent-3-en-2-one (1o)

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 10.54 (brs, 1 H), 7.36-7.32 (m, 2 H), 7.29-7.25 (m, 1 H), 7.18-7.16 (m, 2 H), 5.15 (brs, 1 H), 1.84 (s, 3 H), 1.70 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 196.76, 159.52, 140.45, 131.85, 128.45, 126.58, 110.14, 29.28, 22.15. HRMS calcd for $C_{10}H_{14}NO$ $[M+H]^+$ 176.1069; found: 176.1065.



1q

(Z)-4-aminopent-3-en-2-one (1q)

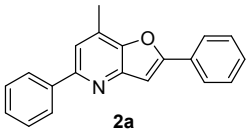
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 9.63 (brs, 1 H), 5.21 (brs, 1 H), 4.95 (s, 1 H), 1.95 (s, 3 H), 1.84 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 196.53, 161.12, 95.57, 29.08, 22.09. HRMS calcd for $C_5H_{10}NO$ $[M+H]^+$ 100.0756; found: 100.0754.

General procedure for the synthesis of the desired furaopyridines 2.

An oven-dried tube was charged with **1** (0.3 mmol), I_2 (0.36 mmol) and 2 mL CH_3CN. Then the reaction was stirred at 80 ^{o}C under air and the reaction time was monitored by TLC. After cooling to room temperature, the solvent was diluted with 20 ml of CH_2Cl_2 and washed with 10 ml of saturated solution of $NaHCO_3$, 10 ml of saturated solution of $Na_2S_2O_3$ successively, and dried over anhydrous Na_2SO_4. Then the solvent was evaporated in vacuo, the residues were purified by column chromatography, eluting with petroleum ether/EtOAc to afford the desired substituted furopyridines.

General procedure for the synthesis of the desired furaopyridines 3.

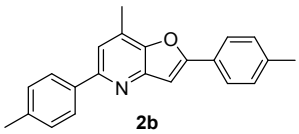
An oven-dried tube was charged with **2** (0.3 mmol), NIS (0.6 mmol), (0.3 mmol) TsOH and 2 mL DMSO. Then the reaction was stirred at 120 ^{o}C under air and the reaction time was monitored by TLC. After cooling to room temperature, the solvent was diluted with 30 ml of CH_2Cl_2, washed with 15 ml H_2O, and dried over anhydrous Na_2SO_4. Then the solvent was evaporated in vacuo, the residues were purified by column chromatography, eluting with petroleum ether/EtOAc to afford the disired products.



2a

7-methyl-2,5-diphenylfuro[3,2-b]pyridine (2a)

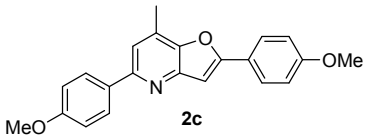
Yellow solid, melting point: 133-135 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.00 (d, *J* = 7.2 Hz, 2 H), 7.91 (d, *J* = 7.2 Hz, 2 H), 7.47-7.44(m, 5 H), 7.39 (d, *J* = 3.2 Hz, 2 H), 2.63 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.32, 154.56, 148.32, 147.26, 140.10, 129.99, 129.72, 129.32, 128.85, 128.64, 128.31, 127.17, 125.20, 118.31, 102.82, 14.95. HRMS calcd for $C_{20}H_{16}NO$ $[M+H]^+$ 286.1226; found: 286.1233.



2b

7-methyl-2,5-dip-tolylfuro[3,2-b]pyridine (2b)

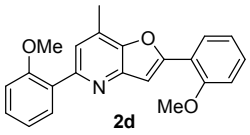
Yellow solid, melting point: 166-168 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.89 (d, *J* = 8.0 Hz, 2 H), 7.80 (d, *J* = 8.0 Hz, 2 H), 7.39 (s, 1 H), 7.27-7.23 (m, 4 H), 7.17(s, 1 H), 2.59 (s, 3 H), 2.39 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.47, 154.36, 148.32, 146.98, 139,43, 138.10, 137.27, 129.51, 129.49, 129,33, 127.27, 126.97, 125.09, 117.80, 102.03, 21.42, 21.19, 14.92. HRMS calcd for $C_{22}H_{20}NO$ $[M+H]^+$ 314.1539, found: 314.1543.



2c

2,5-bis(4-methoxyphenyl)-7-methylfuro[3,2-b]pyridine (2c)

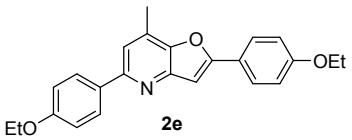
Yellow solid, melting point: 169-171 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.94 (d, *J* = 8.8 Hz, 2 H), 7.84 (d, *J* = 8.8 Hz, 2 H), 7.35 (s, 1 H), 7.09 (s, 1 H), 7.01-6.98 (m, 4 H), 3.87 (s, 3H), 3.86 (s, 3H), 2.60 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.54, 159.93, 159.36, 154.05, 148.52, 146.76, 132.89, 129.31, 128.32, 126.72, 122.89, 117.23, 114.31, 114.00, 101.17, 55.38, 55.33, 14.94. HRMS calcd for $C_{22}H_{20}NO_3$ $[M+H]^+$346.1437; found: 346.1440.



2d

2,5-bis(2-methoxyphenyl)-7-methylfuro[3,2-b]pyridine (2d)

Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.11-8.09 (m, 1 H), 7.74-7.72 (m, 1 H), 7.60 (s, 1 H), 7.47 (s, 1 H), 7.38-7.33 (m, 2 H), 7.11-7.06 (m, 2 H), 7.02-6.99 (m, 2 H), 3.98 (s, 3 H), 3.85 (s, 3 H), 2.62 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.83, 156.68, 155.07, 152.64, 148.49, 145.74, 131.41, 130.06, 129.95, 129.28, 128.21, 126.71, 122.07, 120.92, 120.60, 119.00, 111.25, 111.12, 107.88, 55.63, 55.45, 14.95. HRMS calcd for $C_{22}H_{20}NO_3$ $[M+H]^+$ 346.1437; found: 346.1434.

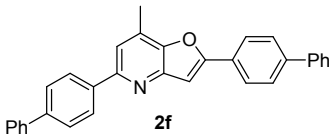


2e

2,5-bis(4-ethoxyphenyl)-7-methylfuro[3,2-b]pyridine (2e)

Yellow solid, melting point: 169-171 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.92 (d, *J* = 8.8 Hz, 2 H), 7.82 (d, *J* = 8.8 Hz, 2 H), 7.34 (s, 1 H), 7.07 (s, 1 H), 6.99-6.96 (m, 4 H), 4.11-4.05 (m, 4 H), 2.59 (s, 3 H), 1.46-1.42 (m, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =

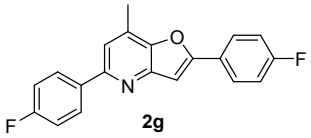
159.90, 159.39, 159.27, 154.05, 148.50, 146.69, 132.69, 129.26, 128.28, 126.68, 122.67, 117.16, 114.77, 114.53, 101.04, 63.57, 63.46, 14.92, 14.82, 14.74. HRMS calcd for $C_{24}H_{24}NO_3$ $[M+H]^+$374.1750; found: 374.1755.



2f

2,5-di([1,1'-biphenyl]-4-yl)-7-methylfuro[3,2-b]pyridine (2f)

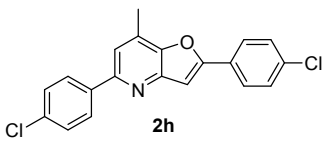
Yellow solid, melting point: 201-202 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm):δ = 8.09-8.07 (m, 2 H), 7.99-7.96 (m, 2 H), 7.72-7.63 (m, 8 H), 7.49-7.44 (m, 5 H), 7.40-7.34 (m, 2 H), 7.29 (s, 1 H), 2.65 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.16, 154.10, 148.43, 147.40, 142.06, 141.08, 140.72, 140.27, 138.99, 129.74, 128.93, 128.88, 128.81, 127.77, 127.54, 127.40, 127.38, 127.09, 127.03, 125.65, 118.25, 102.89, 15.02. HRMS calcd for $C_{32}H_{24}NO$ $[M+H]^+$438.1852; found: 438.1857.



2g

2,5-bis(4-fluorophenyl)-7-methylfuro[3,2-b]pyridine (2g)

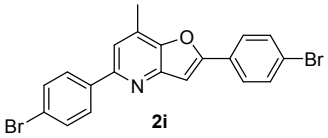
Yellow solid, melting point: 157-159 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.99-7.95 (m, 2 H), 7.91-7.88 (m, 2 H), 7.40 (s, 1 H), 7.20-7.13 (m, 5 H), 2.63 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 164.66-162.17 (d, *J* = 249 Hz, 1 C), 164.46-162.00 (d, *J* = 246 Hz, 1 C), 158.60, 153.64, 148.30, 147.19, 136.20-136.17 (d, *J* = 3 Hz, 1 C) , 129.88, 128.95-128.86 (d, *J* = 9 Hz, 2 C), 127.23-127.15 (d, *J* = 8 Hz, 2 C), 126.31-126.28 (d, *J* = 3 Hz, 1 C), 118.03, 116.19-115.97 (d, *J* = 22 Hz, 2 C), 115.65-115.43 (d, *J* = 22 Hz, 2 C), 102.48, 14.95. HRMS calcd for $C_{20}H_{14}F_2NO$ $[M+H]^+$322.1037; found: 322.1040.



2h

2,5-bis(3,4-dichlorophenyl)-7-methylfuro[3,2-b]pyridine (2h)

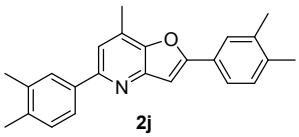
Yellow solid, melting point: 204-206 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.94 (d, *J* = 8.8 Hz, 2 H), 7.84 (d, *J* = 8.4 Hz, 2 H), 7.46-7.43 (m, 5 H), 7.22 (s, 1 H), 2.63 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 158.45, 153.42, 148.20, 147.41, 138.34, 135.39, 134.59, 130.04, 129.20, 128.84, 128.43,128.39, 126.46, 118.28, 103.12, 14.97. HRMS calcd for $C_{20}H_{14}Cl_2NO$ $[M+H]^+$ 354.0446; found: 354.0449.



2i

2,5-bis(4-bromophenyl)-7-methylfuro[3,2-b]pyridine(2i)

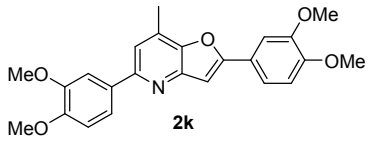
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.87 (d, *J* = 8.4 Hz, 2 H), 7.77 (d, *J* = 8.8 Hz, 2 H), 7.62-7.58 (m, 4 H), 7.43 (s, 1 H), 7.22 (s, 1 H), 2.63 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 158.40, 153.45, 148.20, 147.40, 138.81, 132.11, 131.77, 130.01, 128.77, 128.70, 126.63, 123.59, 122.84, 118.27, 103.18, 14.98. HRMS calcd for $C_{20}H_{14}Br_2NO$ $[M+H]^+$ 441.9436; found: 441.9439.



2j

2,5-bis(3,4-dimethylphenyl)-7-methylfuro[3,2-b]pyridine (2j)

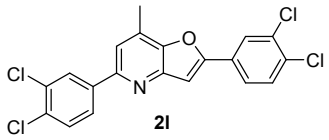
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.81 (s, 1 H), 7.70-7.63 (m, 3 H), 7.40 (s, 1 H), 7.22 (d, *J* = 5.6 Hz, 2 H), 7.17 (s, 1 H), 2.62 (s, 3 H), 2.36 (s, 3 H), 2.35 (s, 3 H), 2.31 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.58, 154.52, 148.36, 146.96, 138.19, 137.75, 137.11, 136.78, 130.08, 129.89, 129.40, 128.29, 128.10, 127.67, 126.22, 124.48, 122.72, 117.81, 101.97, 19.90, 19.85, 19.77, 19.54 14.96. HRMS calcd for $C_{24}H_{24}NO$ $[M+H]^+$ 342.1852; found: 342.1856



2k

2,5-bis(3,4-dimethoxyphenyl)-7-methylfuro[3,2-b]pyridine (2k)

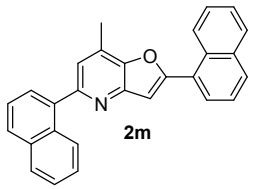
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.66 (d, *J* = Hz, 1 H), 7.51-7.49 (m, 2 H), 7.38 (d, *J* = 2 Hz, 2 H), 7.11 (s, 1 H), 6.97-6.94 (m, 2 H), 4.03 (s, 3 H), 4.00 (s, 3 H),3.95 (s, 3H), 3.94 (s, 3H), 2.62 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.30, 153.96, 150.17, 149.39, 149.19, 149.10, 148.34, 146.81, 133.08, 129.35, 122.96, 119.43, 118.43, 117.37, 111.29, 110.98, 110.22, 108.10, 101.41, 56.01, 55.95, 55.92, 55.90, 14.96. HRMS calcd for $C_{24}H_{24}NO_5$ $[M+H]^+$ 406.1648; found: 406.1660.



2l

2,5-bis(3,4-dichlorophenyl)-7-methylfuro[3,2-b]pyridine (2l)

Yellow solid, melting point: 204-206 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.12 (d, *J* = 2.4 Hz, 1 H), 7.97 (d, *J* = 2 Hz, 1 H), 7.84-7.81 (m, 1 H), 7.72-7.69 (m, 1 H), 7.55-7.51(m, 2 H), 7.43 (s, 1 H), 7.22 (s, 1 H), 2.64 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 157.22, 152.29, 148.05, 147.69, 139.73, 133.54, 133.44, 132.98, 132.70, 131.01, 130.61, 130.37, 129.71, 129.01, 126.84, 126.22, 124.37, 118.55, 104.00, 15.02. HRMS calcd for $C_{20}H_{12}Cl_4NO$ $[M+H]^+$ 421.9667; found: 421.9669.

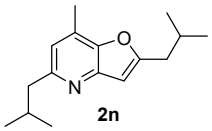


2m

7-methyl-2,5-di(naphthalen-1-yl)furo[3,2-b]pyridine (2m)

Yellow solid, melting point: 201-203 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.46 (s, 1 H), 8.38 (s, 1 H), 8.18-8.16 (m, 1 H), 7.96-7.82 (m, 7 H), 7.57 (s, 1 H), 7.52-7.48 (m, 4 H), 7.37 (s, 1 H), 2.67 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.40, 154.35, 148.46,

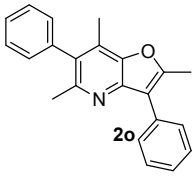
147.46, 137.36, 133.62, 133.57, 133.34, 133.26, 129.76, 128.65, 128.61, 128.53, 128.30, 127.83, 127.63, 127.21, 126.84, 126.75, 126.19, 126.15, 125.11, 124.31, 122.76, 118.65, 103.34, 103.31, 15.00. HRMS calcd for $C_{28}H_{20}NO$ $[M+H]^+$ 386.1539; found: 386.1554.



2n

2,5-diisopropyl-7-methylfuro[3,2-b]pyridine (2n)

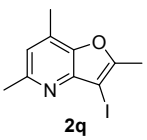
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.79 (s, 1 H), 6.59 (s, 1H), 2.70-2.66 (m, 4 H), 2.48 (s, 3 H), 2.15-2.08 (m, 2 H), 1.01 (s, 3 H), 1.00 (s, 3 H), 0.95 (s, 3 H), 0.94 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 162.92, 156.56, 147.05, 146.18, 129.44, 119.59, 103.96, 46.90, 38.02, 29.69, 27.63, 22.40, 22.43, 14.75. HRMS calcd for $C_{16}H_{24}NO$ $[M+H]^+$ 246.1852; found: 246.1855.



2o

2,5,7-trimethyl-3,6-diphenylfuro[3,2-b]pyridine(2o)

Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.80-7.77 (s, 2 H), 7.51-7.44 (s, 4 H),7.40-7.34 (m, 2 H), 7.21-7.19 (m, 2 H), 2.64 (s, 3 H), 2.35 (s, 3 H), 2.22 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 154.81, 152.31, 145.60, 144.84, 139.02, 132.29, 131.60, 131.06, 129.59, 129.10, 128.58, 127.20, 127.16, 126.95, 117.12, 24.41, 13.87, 12.71. HRMS calcd for $C_{22}H_{20}NO$ $[M+H]^+$ 314.1539; found: 314.1531.

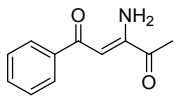


2q

6-iodo-2,5,7-trimethylfuro[3,2-b]pyridine (2q)

Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.89 (s, 1 H), 2.63 (s, 3 H), 2.58 (s, 3 H),

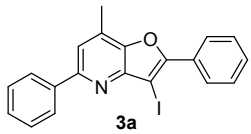
2.46 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 158.74, 154.83, 147.18, 145.59, 129.45, 120.77, 65.52, 24.25, 14.55, 14.24. HRMS calcd for $C_{10}H_{11}INO$ $[M+H]^+$287.9879; found: 287.9884.



2t

(Z)-3-amino-1-phenylpent-2-ene-1,4-dione(2t)

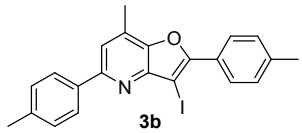
Yellow solid, melting point: 75-78 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.94-7.91 (m, 2 H), 7.52-7.44 (m, 3 H), 6.48 (s, 1 H), 2.53 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 195.79, 192.32, 151.13, 139.33, 131.90, 128.50, 127.26, 93.94, 24.97. HRMS calcd for $C_{11}H_{12}NO_2[M+H]^+$ 190.0862; found: 190.0865



3a

3-iodo-7-methyl-2,5-diphenylfuro[3,2-b]pyridine(3a)

Yellow solid, melting point: 188-200 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.26 (d, *J* = 7.2Hz, 2 H), 8.11 (d, *J* = 7.2Hz, 2 H), 7.56-7.46 (m, 6 H), 7.42-7.38 (m, 1 H), 2.64 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 155.95, 154.75, 148.56, 146.15, 139.54, 130.16, 129.85, 129.79, 128.76, 128.58, 127.62, 127.26, 119.34, 65.15, 14.65. HRMS calcd for $C_{20}H_{15}INO$ $[M+H]^+$ 412.0192; found: 412.0198.

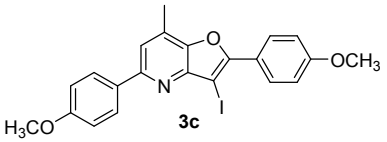


3b

3-iodo-7-methyl-2,5-di-p-tolylfuro[3,2-b]pyridine(3b)

Yellow solid, melting point: 185-189 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.14 (d, *J* = 8.0 Hz, 2 H), 8.00 (d, *J* = 8.0 Hz, 2 H), 7.51 (d, *J* = 0.4 Hz, 1 H), 7.32 (d, *J* = 8.0 Hz, 2 H),

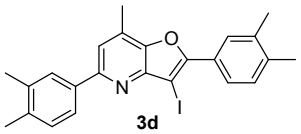
7.29-7.25 (m, 2 H), 2.61 (s, 3 H), 2.44 (s, 3 H), 2.41 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.13, 154.66, 148.54, 145.92, 140.01, 138.41, 136.81, 129.91, 129.36, 129.26, 127.54, 127.09, 118.84, 64.40, 21.52, 21.25, 14.62. HRMS calcd for $C_{22}H_{19}INO$ $[M+H]^+$ 440.0505; found: 440.0508.



3c

3-iodo-2,5-bis(4-methoxyphenyl)-7-methylfuro[3,2-b]pyridine(3c)

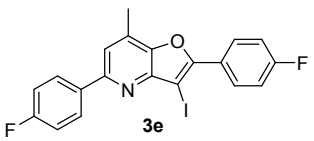
Yellow solid, melting point: 179-180 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.19 (d, *J* = 8.8 Hz, 2 H), 8.05 (d, *J* = 8.4 Hz, 2 H), 7.44 (s, 1 H), 7.03-6.98 (m, 4 H), 3.88 (s, 3 H), 3.86 (s, 3 H), 2.59 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.71, 160.13, 155.91, 154.20, 148.54, 145.60, 132.33, 129.71, 129.14, 128.40, 122.48, 118.20, 114.00, 113.97, 63.34, 55.38, 55.33, 14.60. HRMS calcd for $C_{25}H_{19}INO_3[M+H]^+$ 508.0403; found: 508.0399.



3d

2,5-bis(3,4-dimethylphenyl)-3-iodo-7-methylfuro[3,2-b]pyridine(3d)

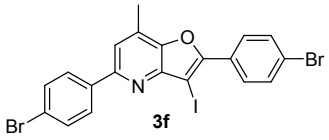
Yellow solid, melting point: 165-169 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.98 (d, *J* = 6.4 Hz, 2 H), 7.88 (s, 1 H), 7.80 (d, *J* = 8.0 Hz,1 H), 7.48 (s, 1 H), 7.26-7.20 (m, 2 H), 2.60 (s, 3 H), 2.36 (s, 6 H), 2.32 (s, 3 H), 2.31 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.10, 154.70, 148.45, 145.82, 138.69, 137.19, 137.02, 136.82, 136.71, 129.88, 129.77, 129.74, 128.48, 128.34, 127.41, 125.19, 124.57, 118.79, 64.27, 19.97, 19.90, 19.82, 19.58, 14.63. HRMS calcd for $C_{24}H_{23}INO$ $[M+H]^+$ 468.0818; found: 468.0822.



3e

2,5-bis(4-fluorophenyl)-3-iodo-7-methylfuro[3,2-b]pyridine(3e)

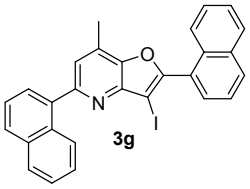
Yellow solid, melting point: 210-212 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.24-8.22 (m, 2 H), 8.09-8.05 (m, 2 H), 7.48 (s, 1 H), 7.25-7.13 (m, 5 H), 2.62 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 164.73-162.23 (d, *J* = 250 Hz, 1 C), 164.61-162.15 (d, *J* = 246 Hz, 1 C), 155.24, 153.76, 148.48, 146.00, 135.62-135.59 (d, *J* = 3 Hz, 1 C), 130.25, 129.72-129.64 (d, *J* = 8 Hz, 2 C), 129.01-128.93 (d, *J* = 8 Hz, 2 C), 126.03-126.00 (d, *J* = 3 Hz, 1 C), 118.99, 115.88-115.65 (d, *J* = 23 Hz, 2 C), 115.65-115.43 (d, *J* = 22 Hz, 2 C), 64.81, 14.64. HRMS calcd for $C_{20}H_{13}F_2INO$ $[M+H]^+$ 448.0004; found: 448.0008.



3f

2,5-bis(4-bromophenyl)-3-iodo-7-methylfuro[3,2-b]pyridine(3f)

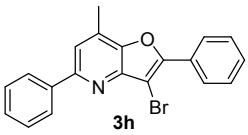
Yellow solid, melting point: 208-210 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.15 (d, *J* = 8.4 Hz, 2 H), 7.98 (d, *J* = 8.4 Hz, 2 H), 7.66 (d, *J* = 8.4 Hz, 2 H), 7.60 (d, *J* = 8.4 Hz, 2 H), 7.54 (s, 1 H), 2.64 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 155.11, 153.65, 148.56, 146.26, 138.28, 131.87, 131.80, 130.44, 128.95, 128.79, 128.64, 124.25, 123.14, 119.24, 65.62, 14.65. HRMS calcd for $C_{20}H_{13}Br_2INO$ $[M+H]^+$ 567.8402; found: 567.8405.



3g

3-iodo-7-methyl-2,5-di(naphthalen-1-yl)furo[3,2-b]pyridine(3g)

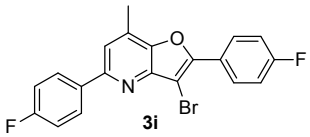
Yellow solid, melting point: 214-216 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.80 (s, 1 H),8.55 (s, 1 H), 8.37-8.31 (m, 2 H), 8.01-7.95 (m, 4 H), 7.90-7.87 (m, 2 H), 7.73 (d, *J* = 0.4 Hz, 1 H), 7.58-7.48 (m, 4 H), 2.72 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.04, 154.62, 148.78, 146.35, 136.89, 133.68, 133.56, 133.52, 132.94, 130.24, 128.76, 128.69, 128.35, 128.29, 127.79, 127.71, 127.66, 127.30, 127.20, 126.74, 126.30, 126.15, 125.19, 124.40, 119.65, 65.56, 14.76. HRMS calcd for $C_{28}H_{19}INO$ $[M+H]^+$ 512.0505; found: 512.0509.



3h

3-bromo-7-methyl-2,5-diphenylfuro[3,2-b]pyridine(3h)

Yellow solid, melting point: 207-209 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.25-8.23 (m, 2 H), 8.09-8.07 (m, 2 H), 7.53-7.44 (m, 6 H), 7.41-7.38 (m, 1 H), 2.63 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 155.05, 153.59, 146.05, 145.81, 139.56, 130.30, 129.67, 129.34, 128.67, 128.59, 127.29, 126.93, 119.37, 95.90, 14.65. HRMS calcd for $C_{20}H_{15}BrNO$ $[M+H]^+$ 364.0331; found: 364.0335.



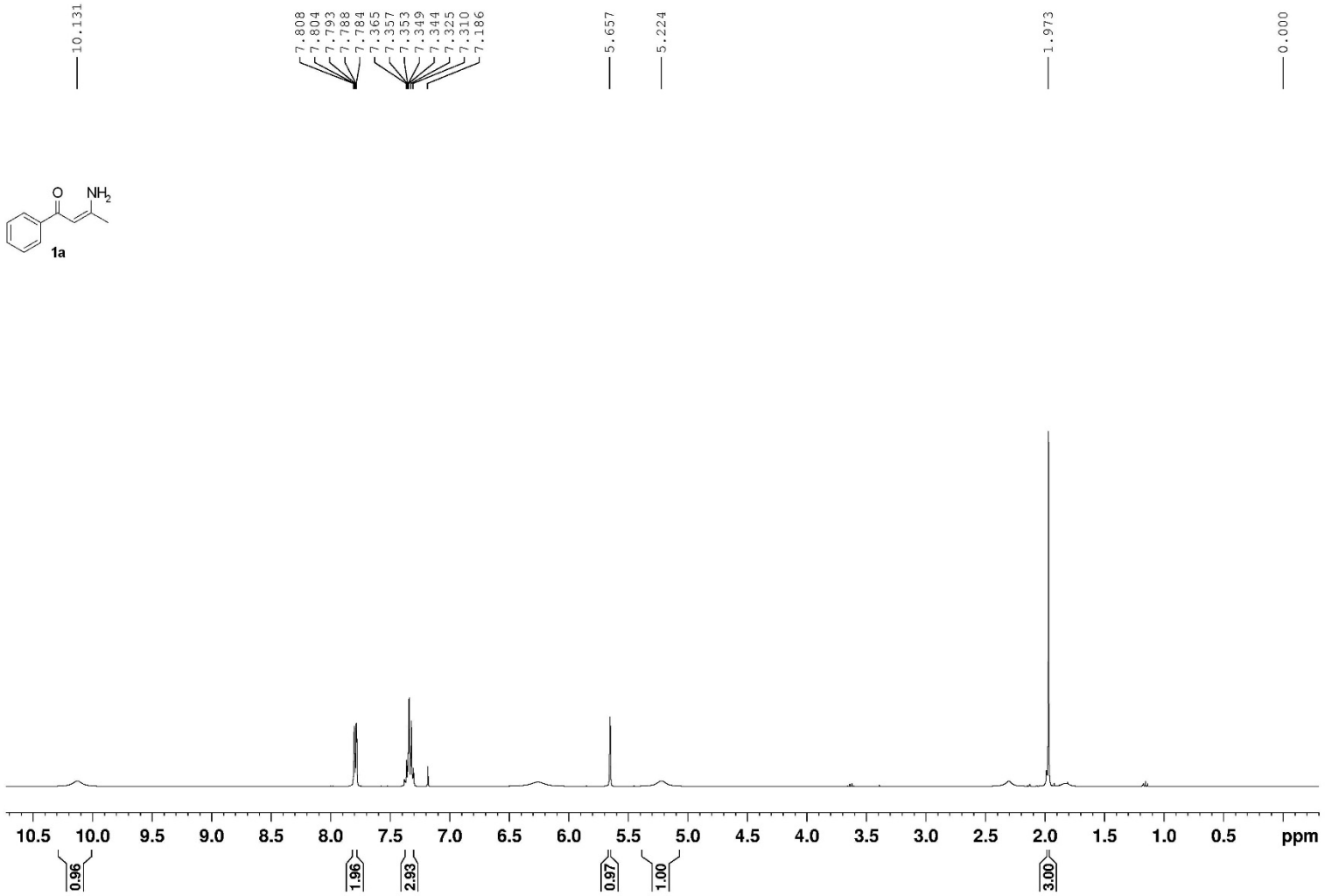
3i

3-bromo-2,5-bis(4-fluorophenyl)-7-methylfuro[3,2-b]pyridine(3i)

Yellow solid, melting point: 178-180 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.24-8.21 (m, 2 H), 8.07-8.03 (m, 2 H), 7.47 (s, 1 H), 7.25-7.13 (m, 5 H), 2.62 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 164.64-162.14 (d, J = 250 Hz, 1 C), 164.64-162.18 (d, J = 246 Hz, 1 C), 154.07, 152.89, 145.97, 145.67, 135.65-135.62 (d, J = 3 Hz, 1 C), 130.41, 129.06-128.97 (d, J = 9 Hz, 4 C), 125.55-125.51(d, J = 4 Hz, 1 C), 119.04, 116.00-115.78 (d, J = 22 Hz, 2 C), 115.67-115.45 (d, J = 22 Hz, 2 C), 95.51, 14.64. HRMS calcd for $C_{20}H_{13}BrF_2NO$ $[M+H]^+$ 400.0142; found: 400.0146.

Reference

(1) M. Sugiura, M.Kumahara, M. Nakajima *Chem. Comm*., 2009, **24**, 3585.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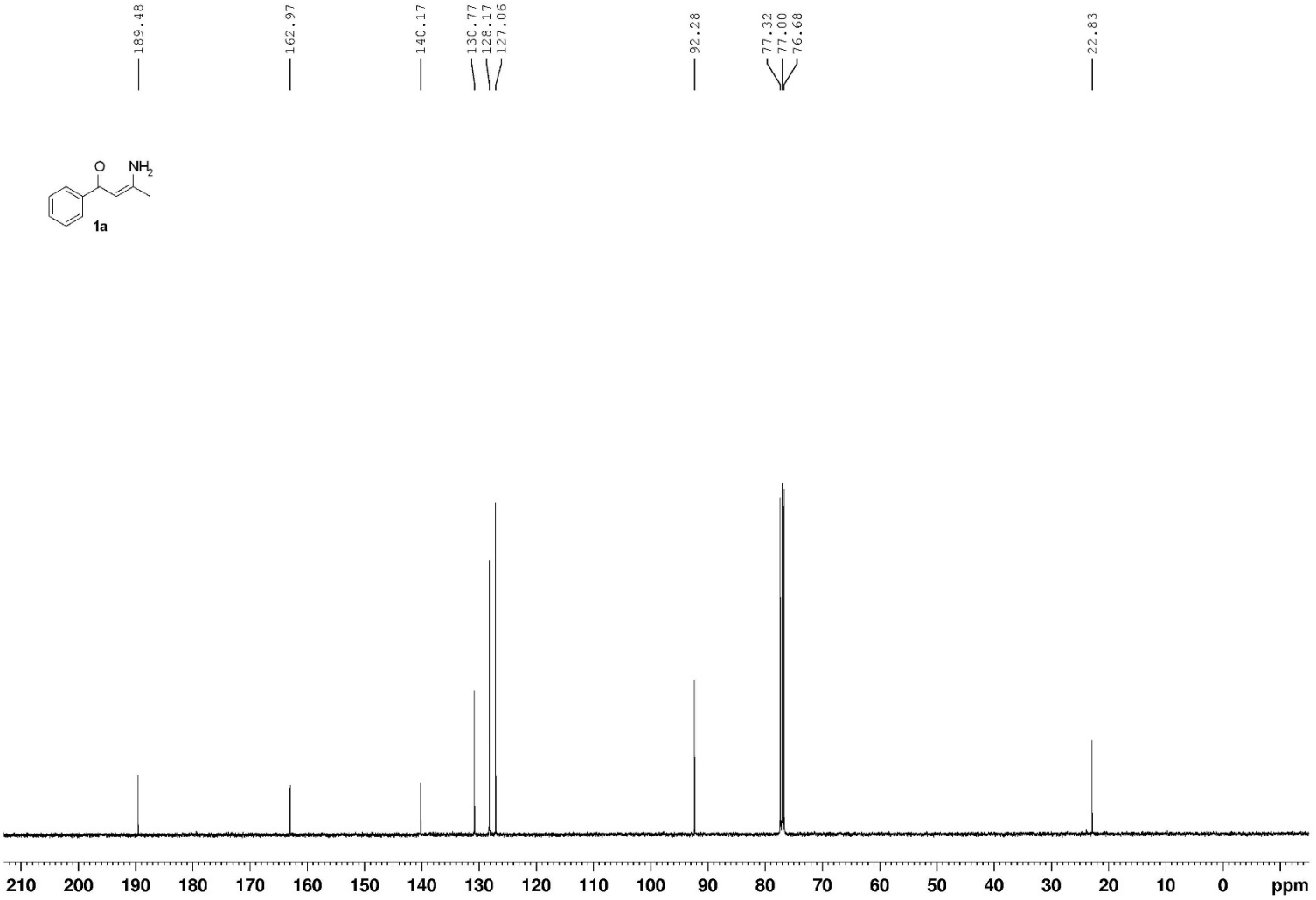
7.784
7.365
7.357
7.353
7.349
7.344
7.325
7.310
7.186
5.657
5.224
1.973
0.000
O
NH2
1a
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.96
1.96
2.93
0.97
1.00
3.00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162.97
140.17
130.77
128.17
127.06
92.28
77.32
77.00
76.68
22.83
O
NH2
1a
210
200
190
180
170
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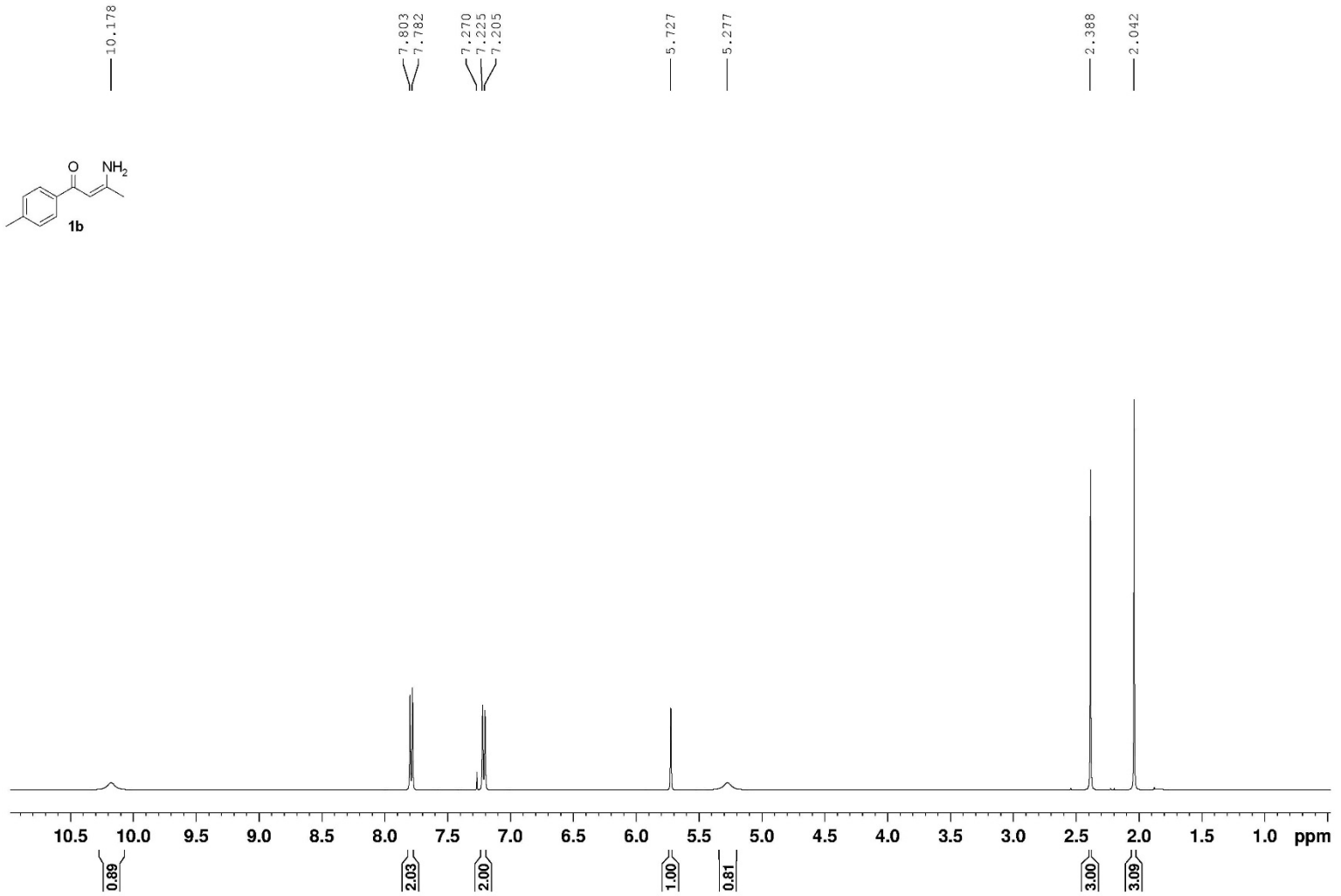
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.782
7.270
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7.205
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5.277
2.388
2.042
O
NH2
1b
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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1.5
1.0
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2.00
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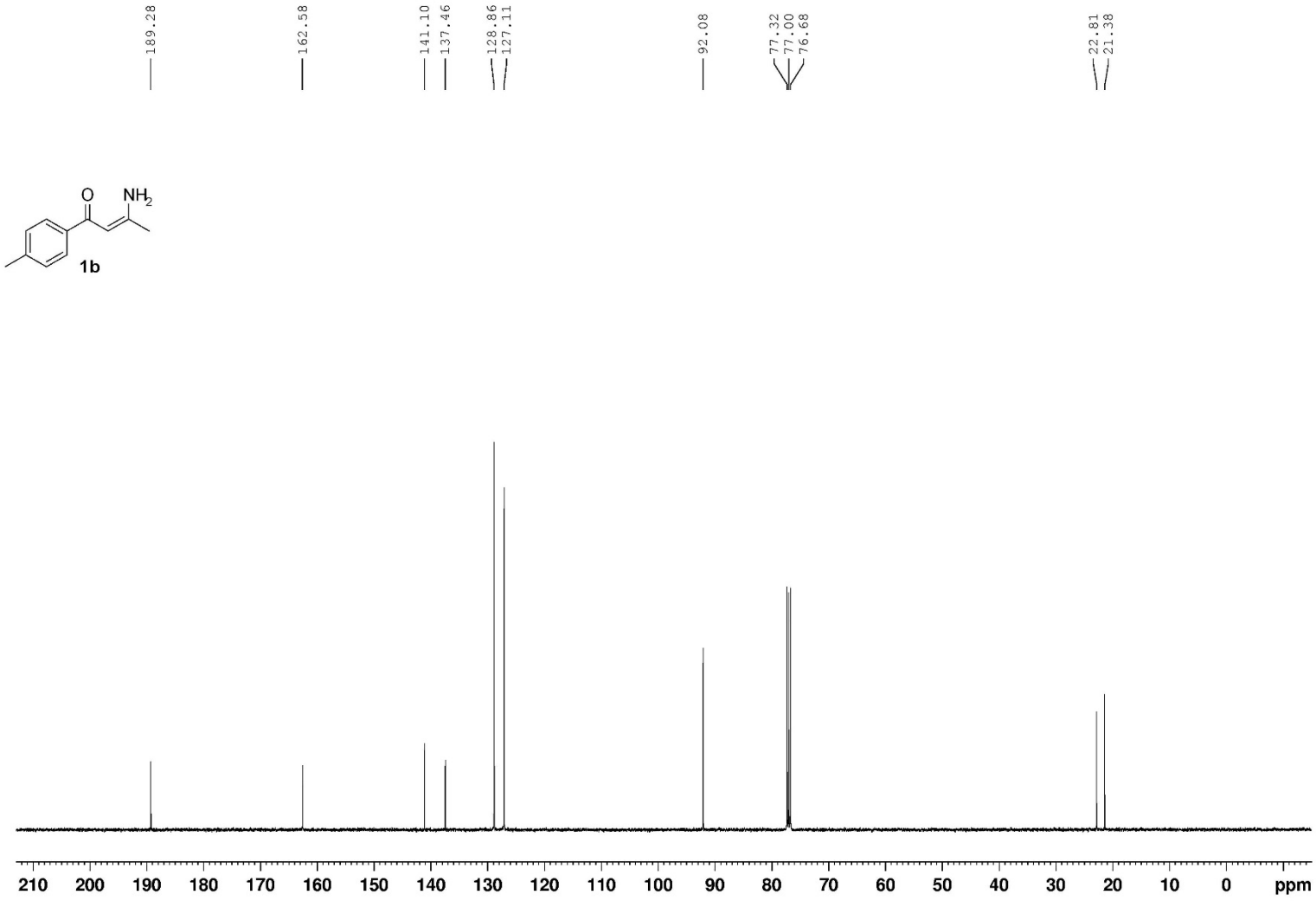
0.81
3.00
3.09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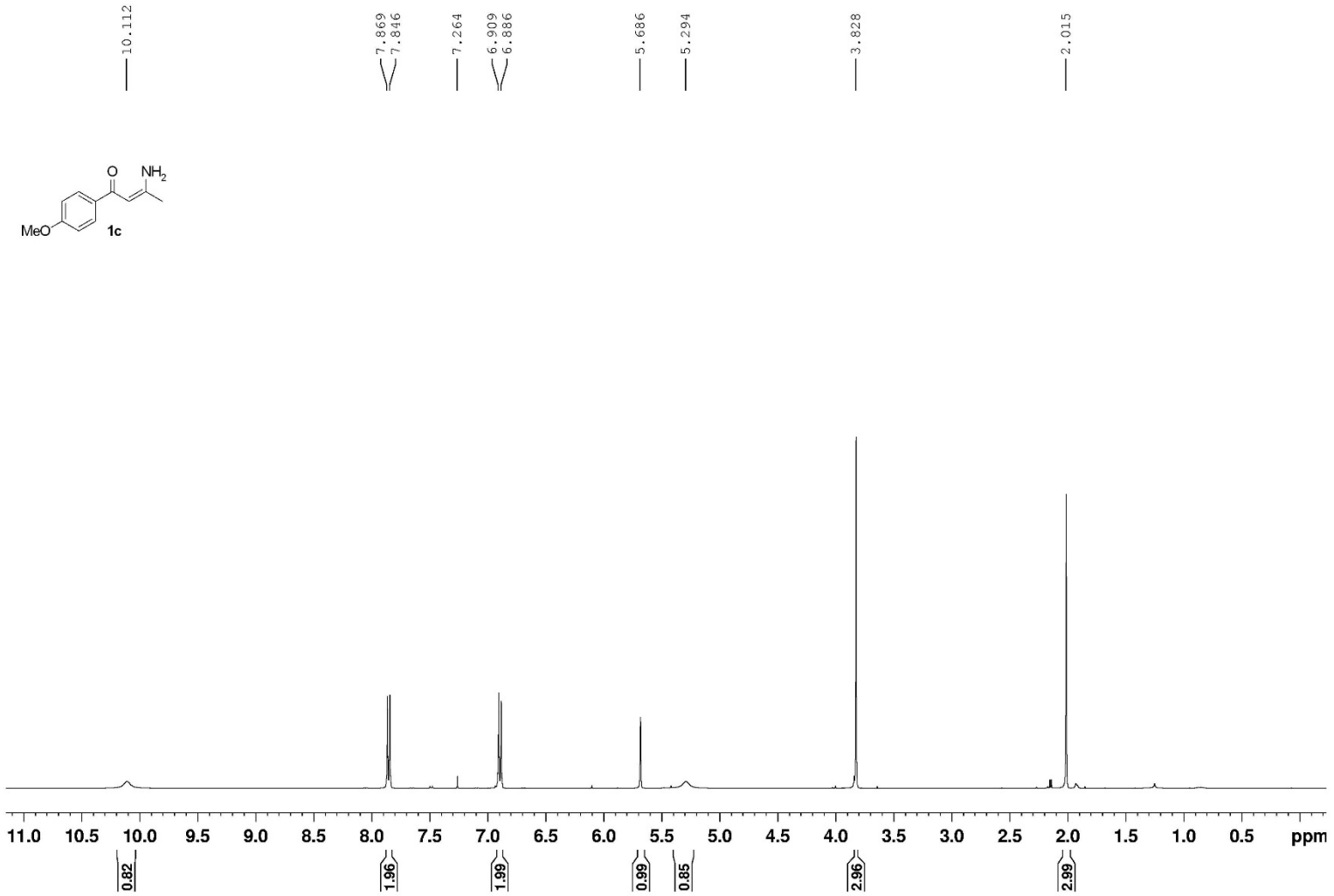
162.58
141.10
137.46
128.86
127.11
92.08
77.32
77.00
76.68
22.81
21.38
O
NH2
1b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.846
7.264
6.909
6.886
5.686
5.294
3.828
2.015
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NH2
MeO
1c
11.0
10.5
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
ppm
0.82
1.96
1.99
0.99
0.85
2.96
2.99


188.48
162.31
161.78
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113.34
91.71
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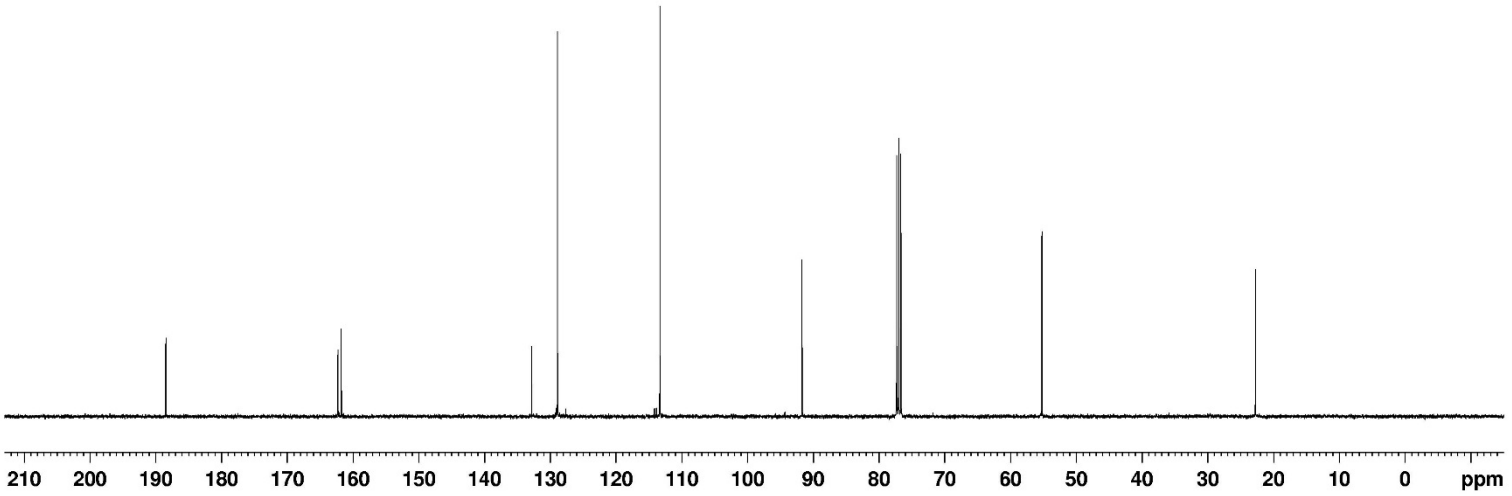
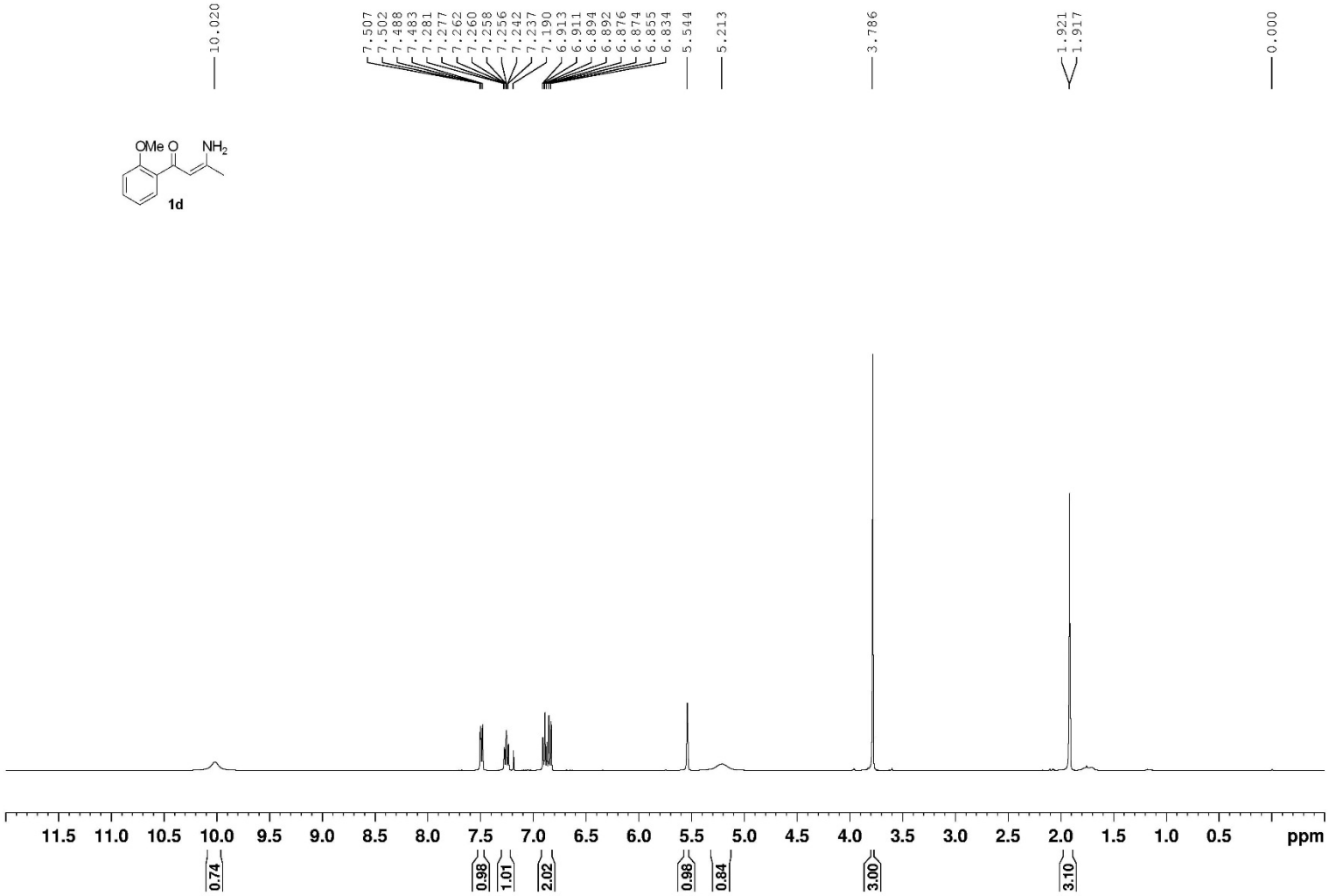
77.00
76.68
55.24
22.77
O
NH2
MeO
1c


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.258
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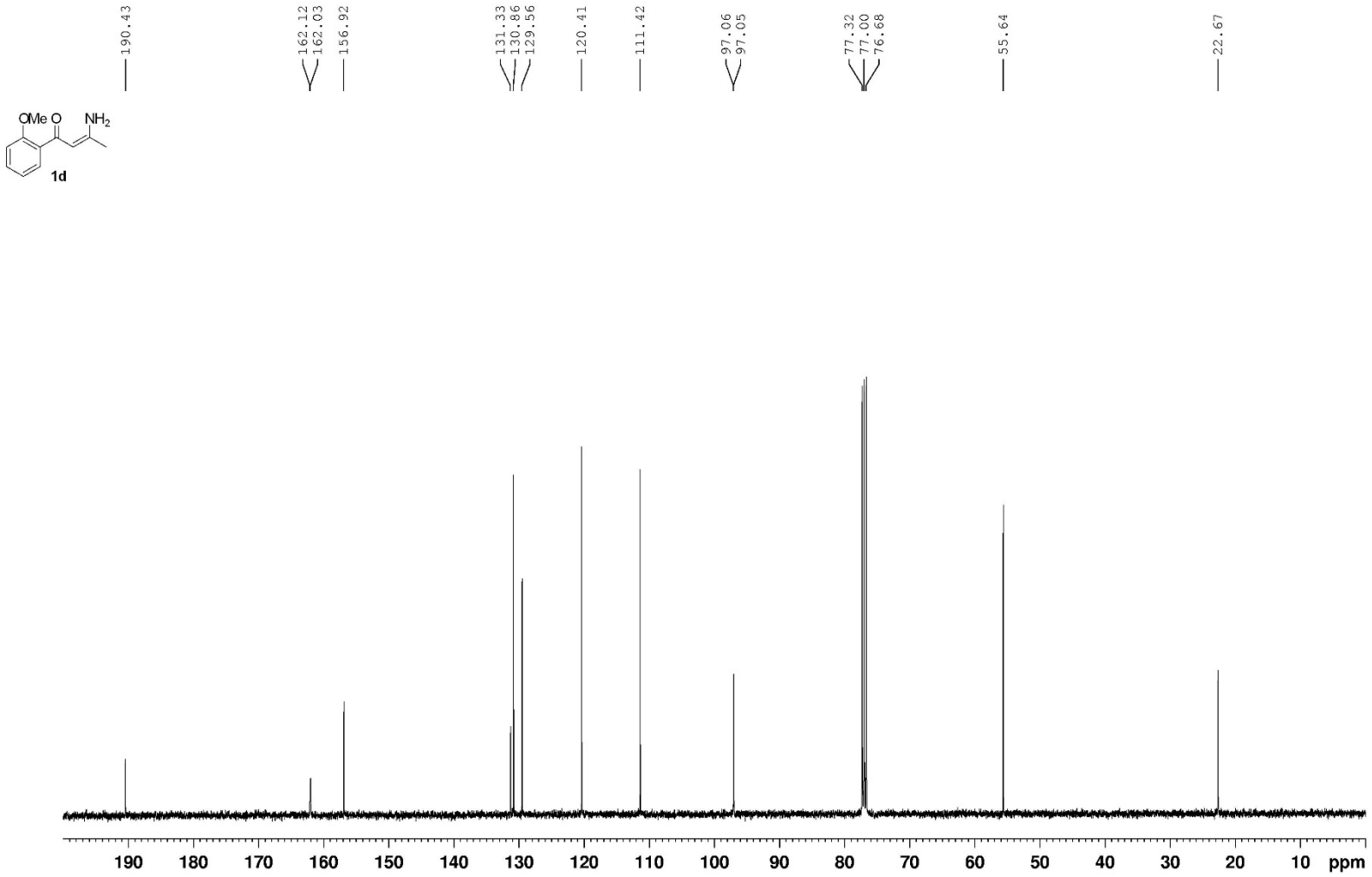
7.242
7.237
7.190
6.913
6.911
6.894
6.892
6.876
6.874
6.855
6.834
5.544
5.213
3.786
1.921
1.917
0.000
OMe O
NH2
1d
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.74
0.98
1.01
2.02
0.98
0.84
3.00
3.10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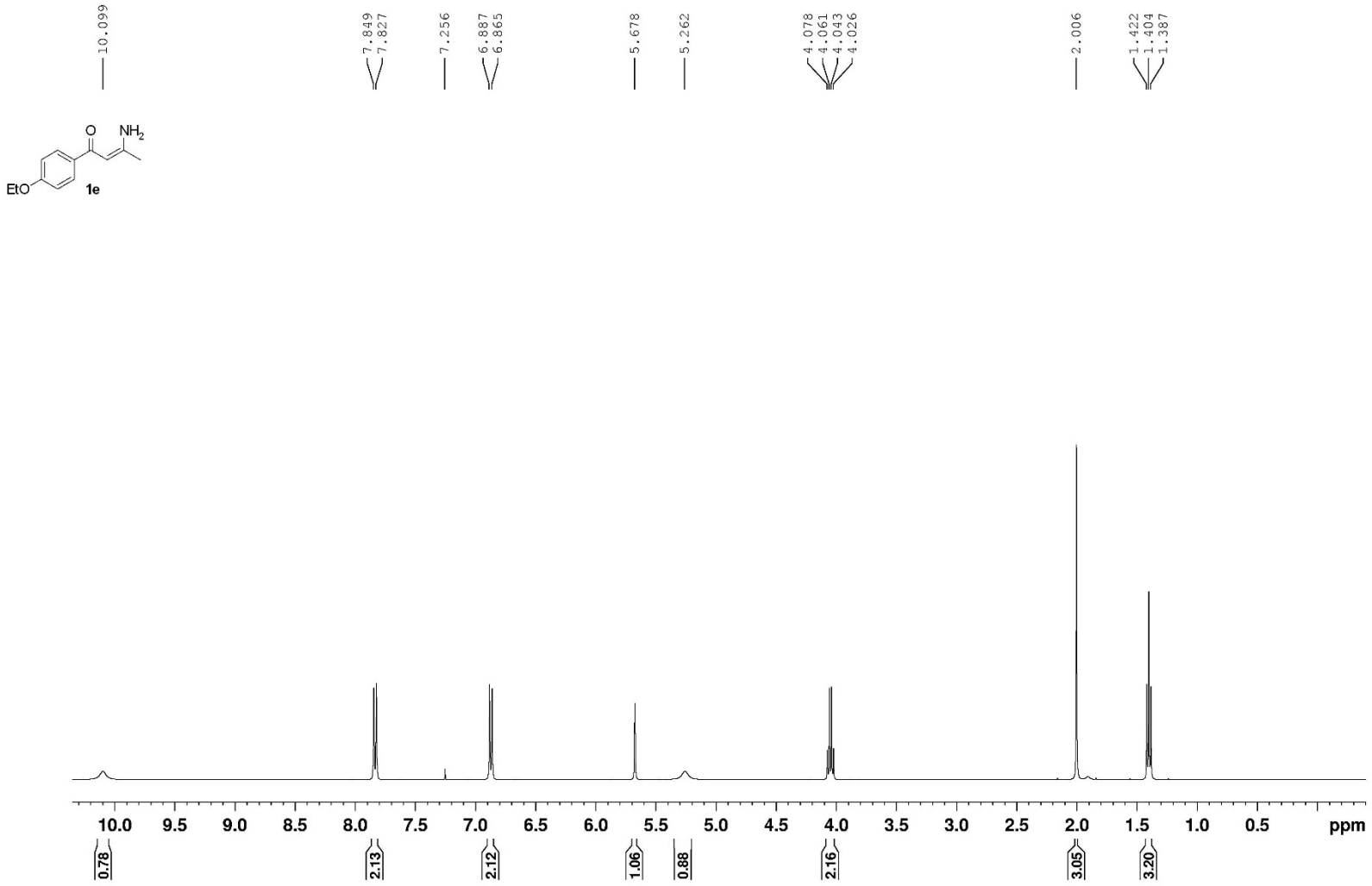
162.12
162.03
156.92
131.33
130.86
129.56
120.41
111.42
97.06
97.05
77.32
77.00
76.68
55.64
22.67
OMe O
NH2
1d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.827
7.256
6.887
6.865
5.678
5.262
4.078
4.061
4.043
4.026
2.006
1.422
1.404
1.387
O
NH2
EtO
1e
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
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0.5
ppm
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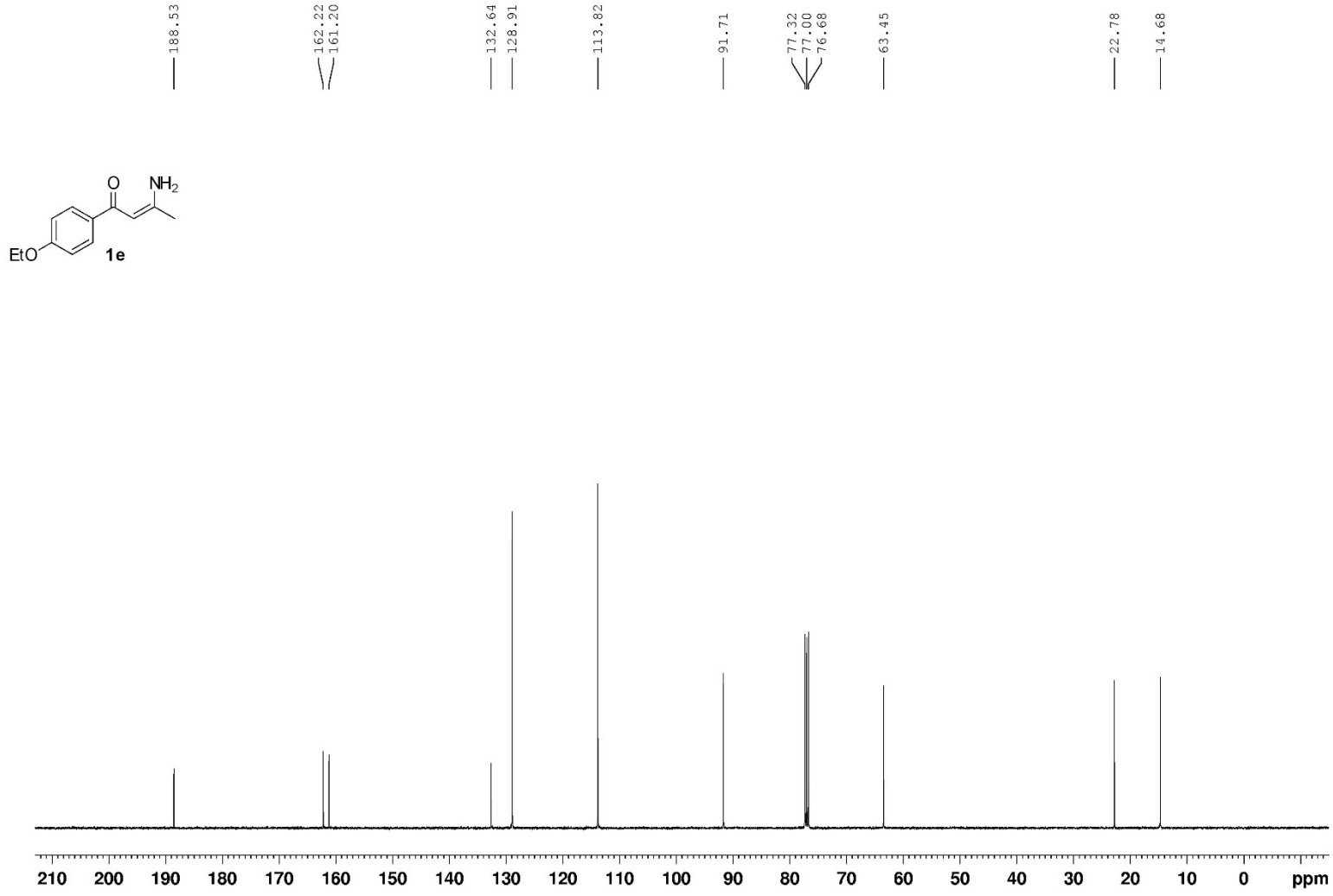
1.06
0.88
2.16
3.05
3.20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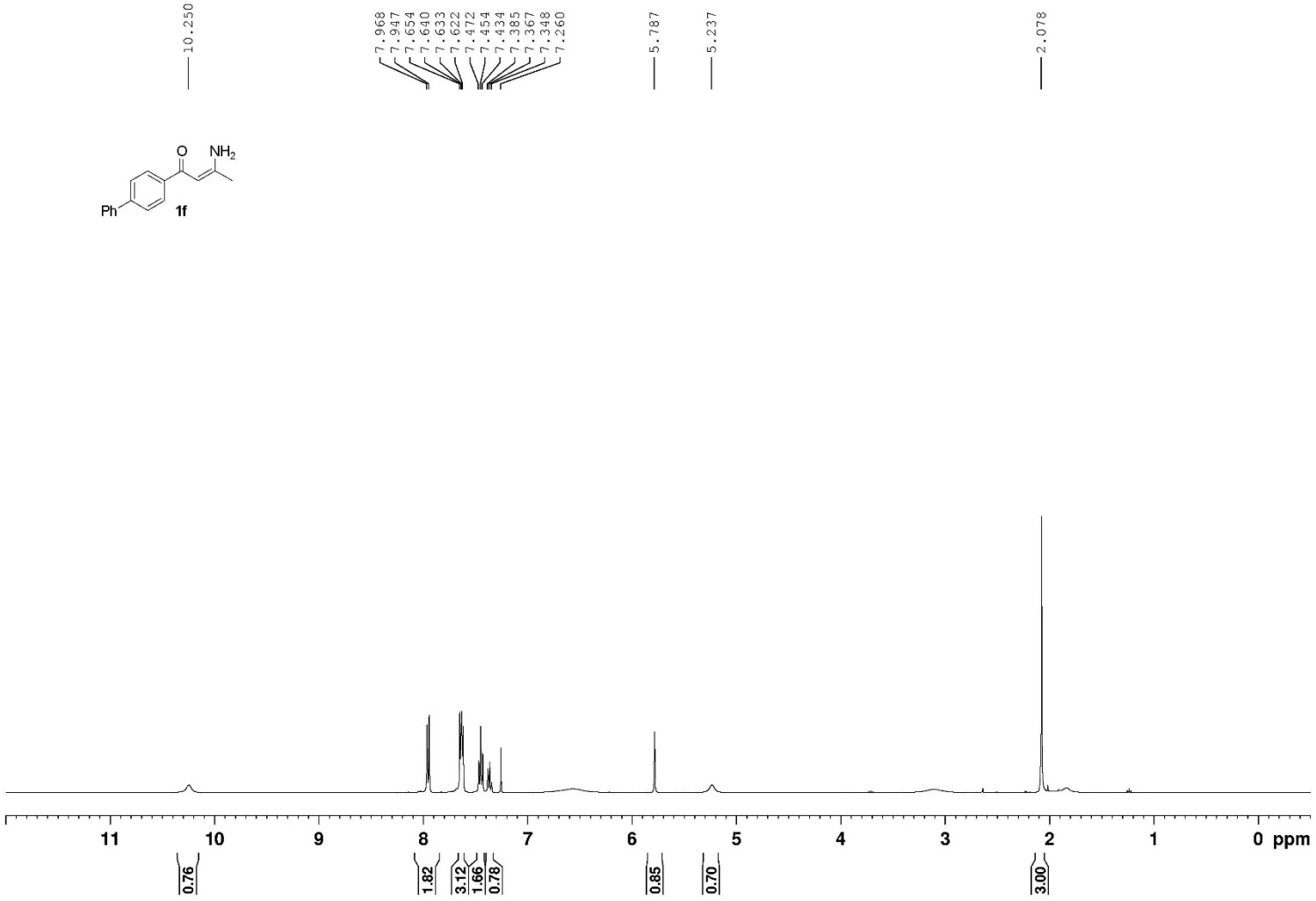
132.64
128.91
113.82
91.71
77.32
77.00
76.68
63.45
22.78
14.68
O
NH2
EtO
1e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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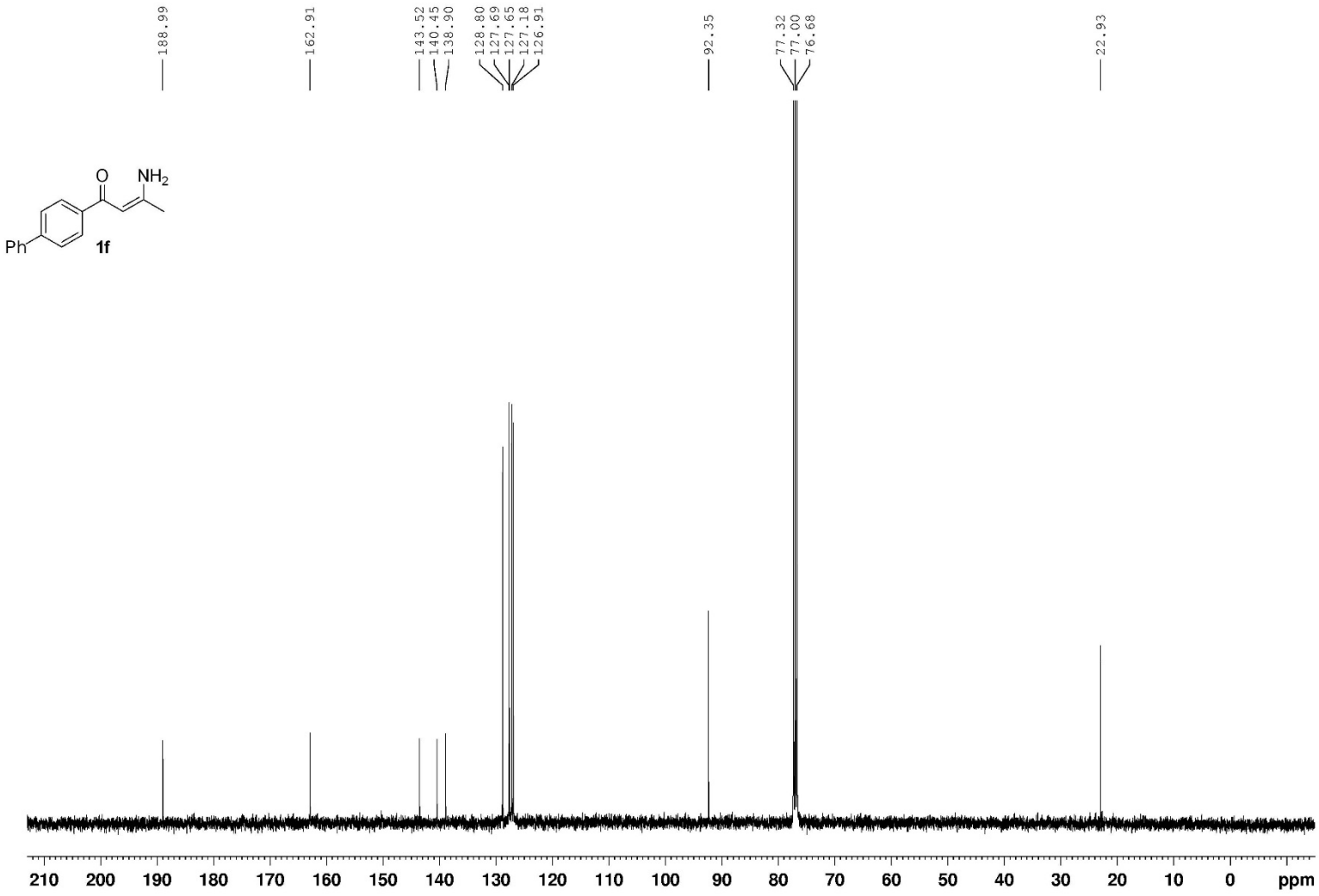
7.947
7.654
7.640
7.633
7.622
7.472
7.454
7.434
7.385
7.367
7.348
7.260
5.787
5.237
2.078
O
NH2
Ph
1f
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.76
1.82
3.12
1.66
0.78
0.85
0.70
3.00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143.52
140.45
138.90
128.80
127.69
127.65
127.18
126.91
92.35
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77.00
76.68
22.93
O
NH2
Ph
1f
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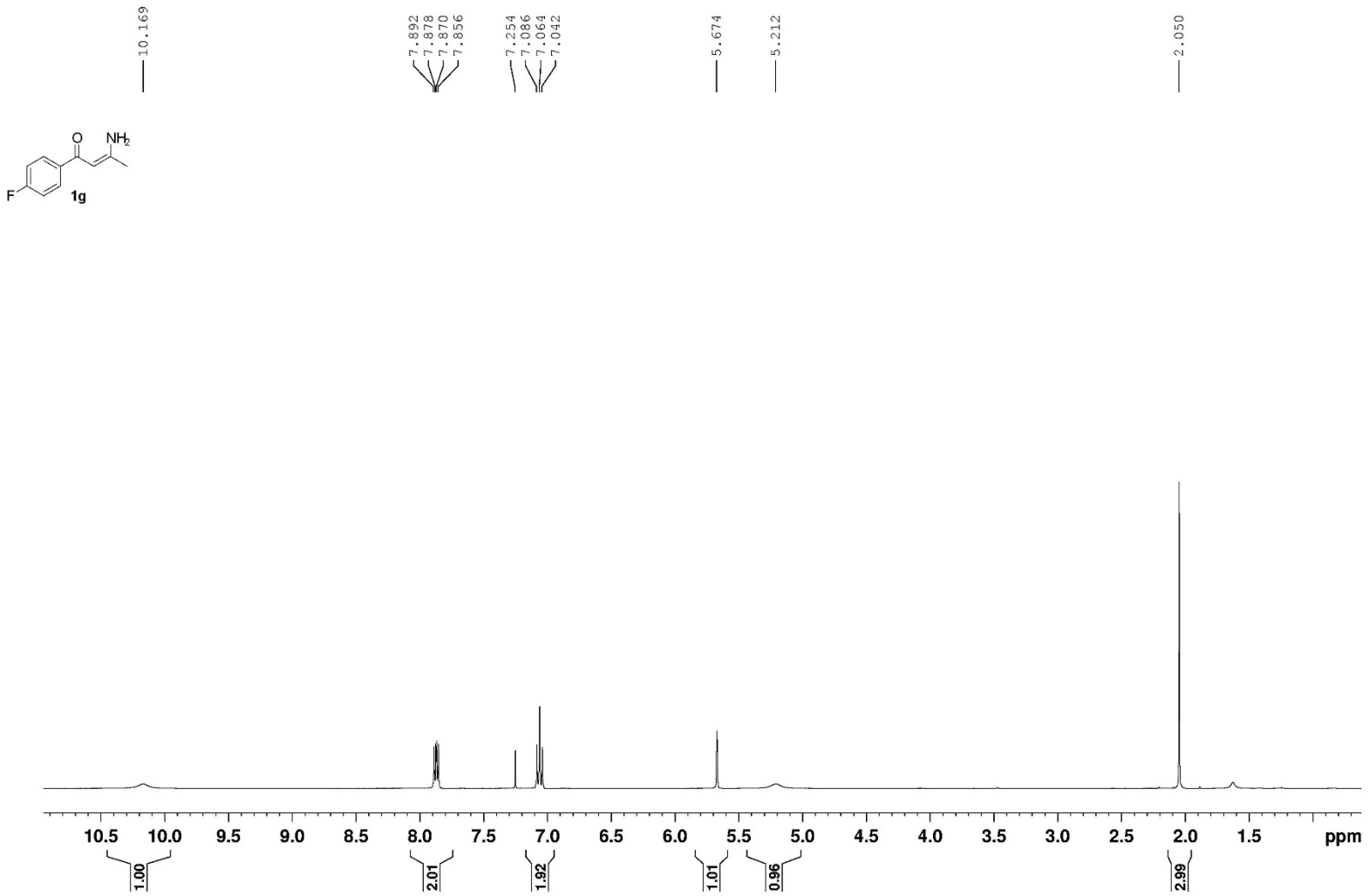
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7.870
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7.254
7.086
7.064
7.042
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5.212
2.050
O
NH2
F
1g
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
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2.01
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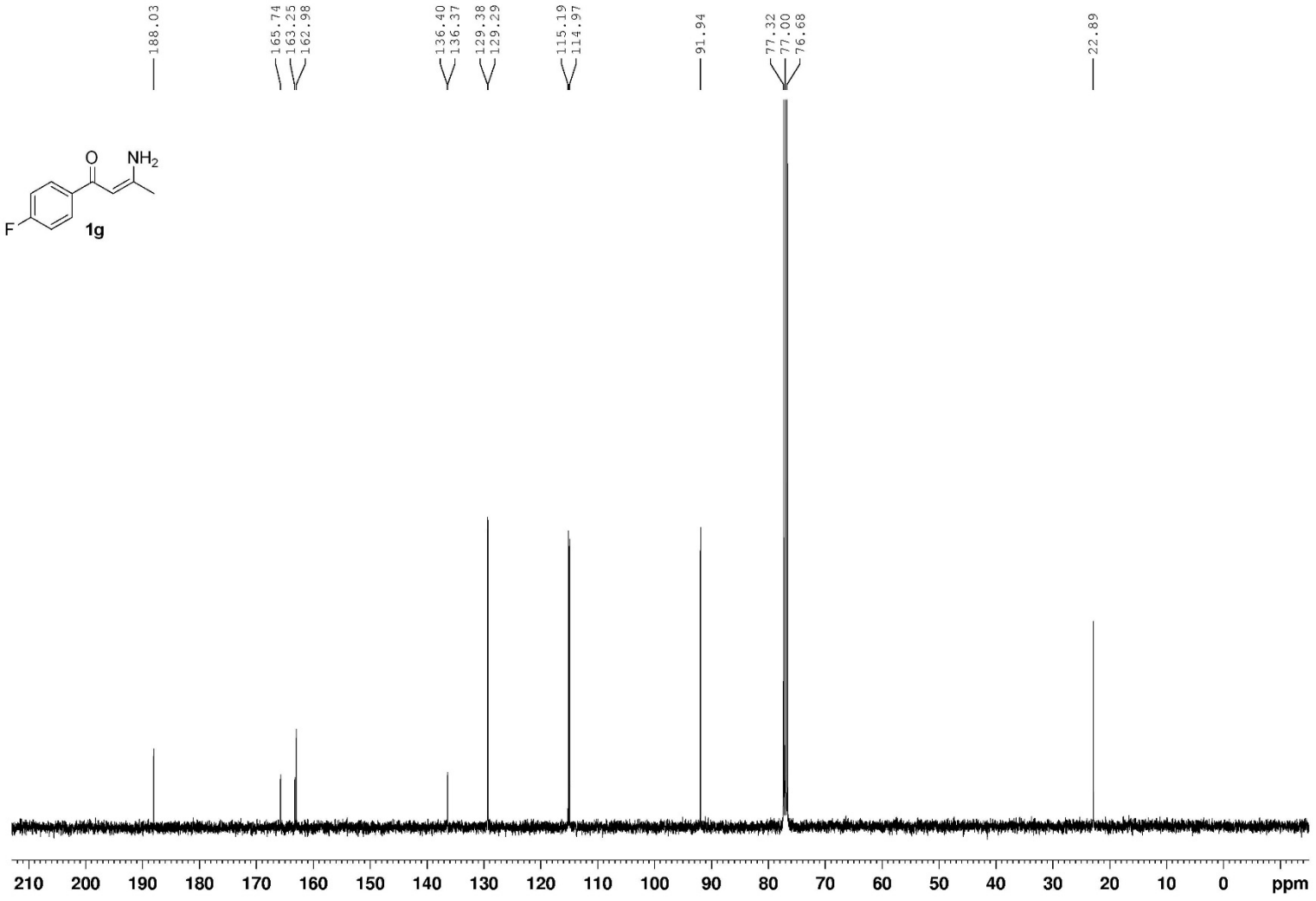
1.01
0.96
2.99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136.40
136.37
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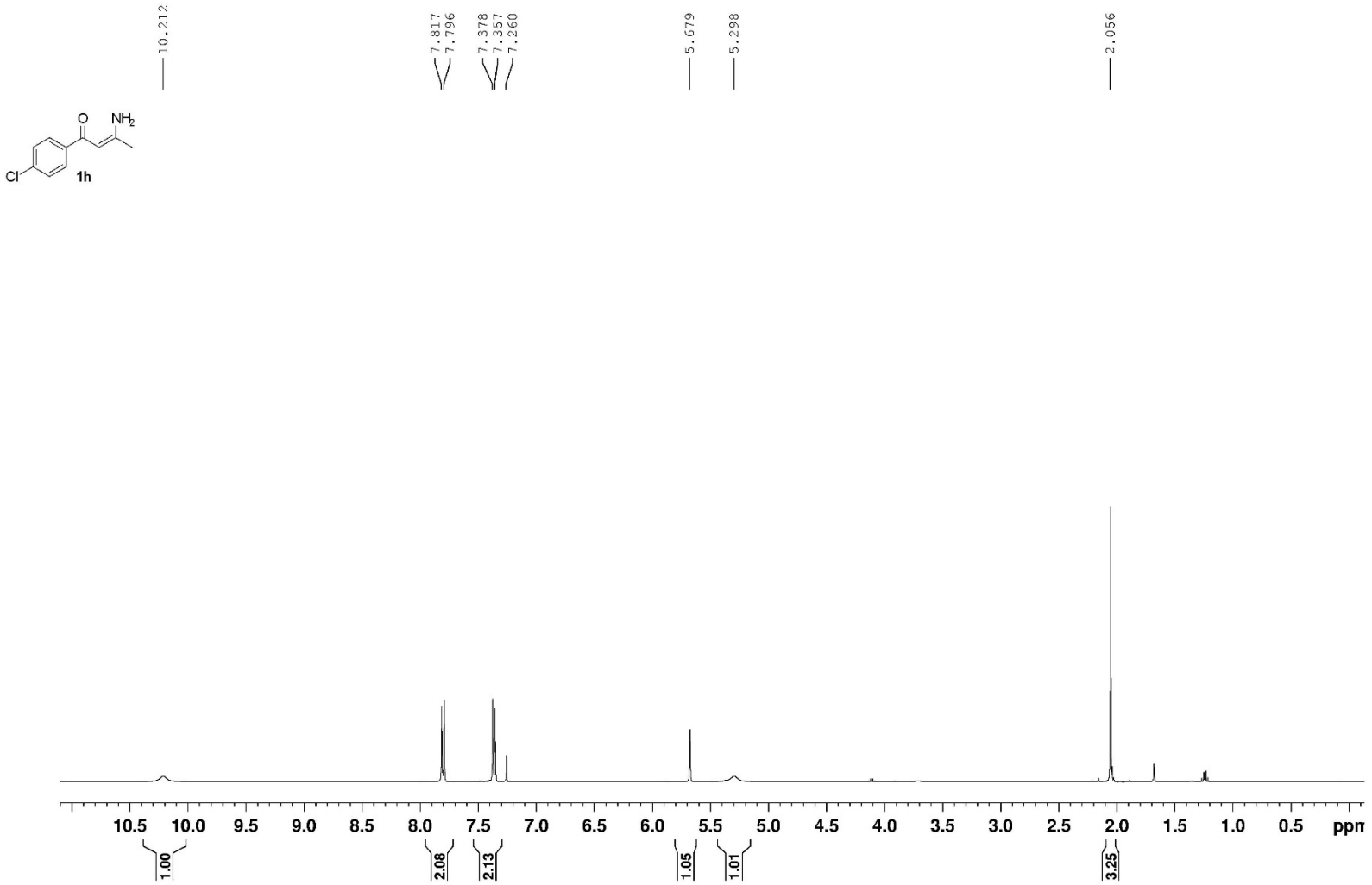
129.29
115.19
114.97
91.94
77.32
77.00
76.68
22.89
O
NH2
F
1g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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5.298
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O
NH2
Cl
1h
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10.0
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
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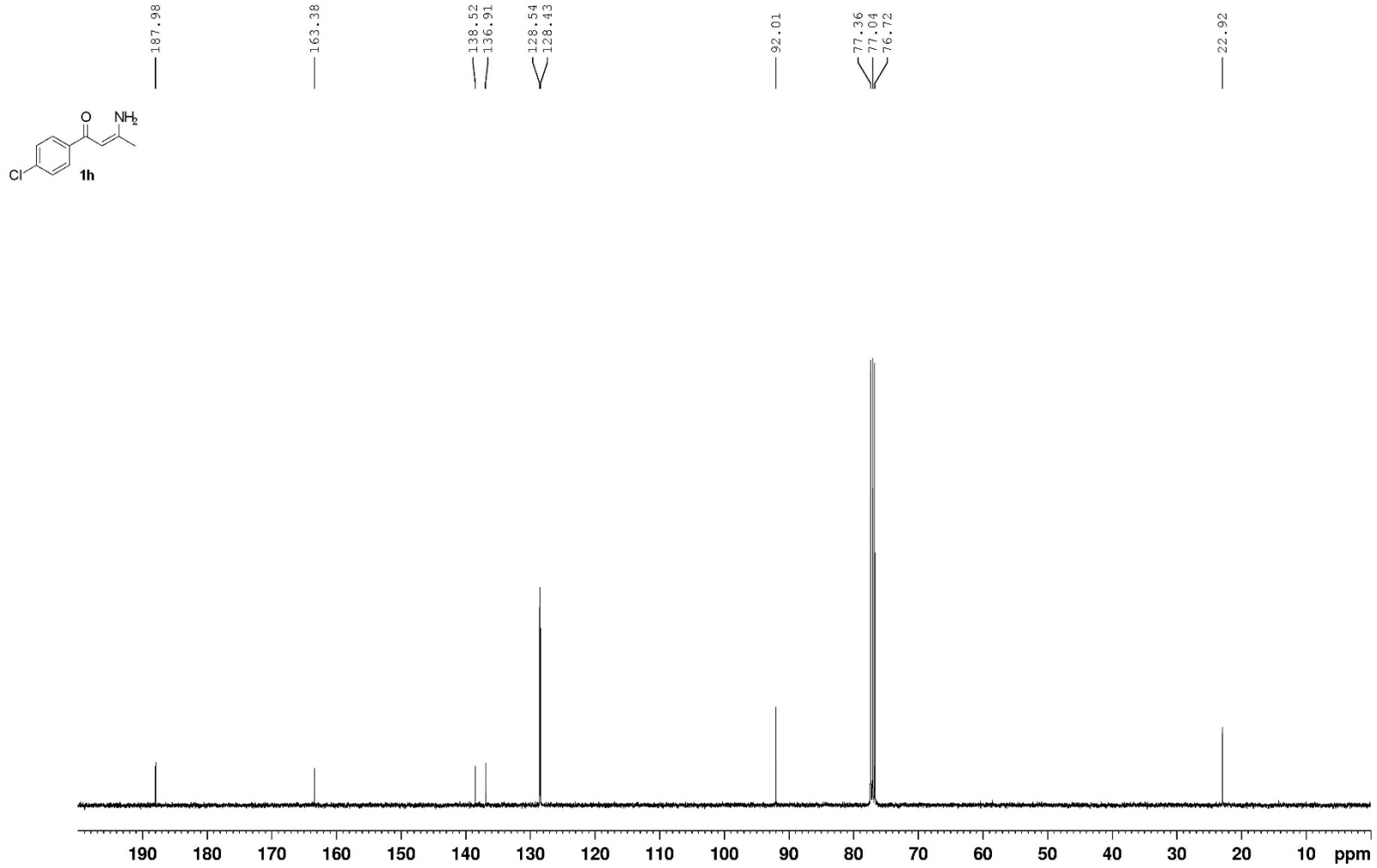
1.5
1.0
0.5
ppm
1.00
2.08
2.13
1.05
1.01
3.25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136.91
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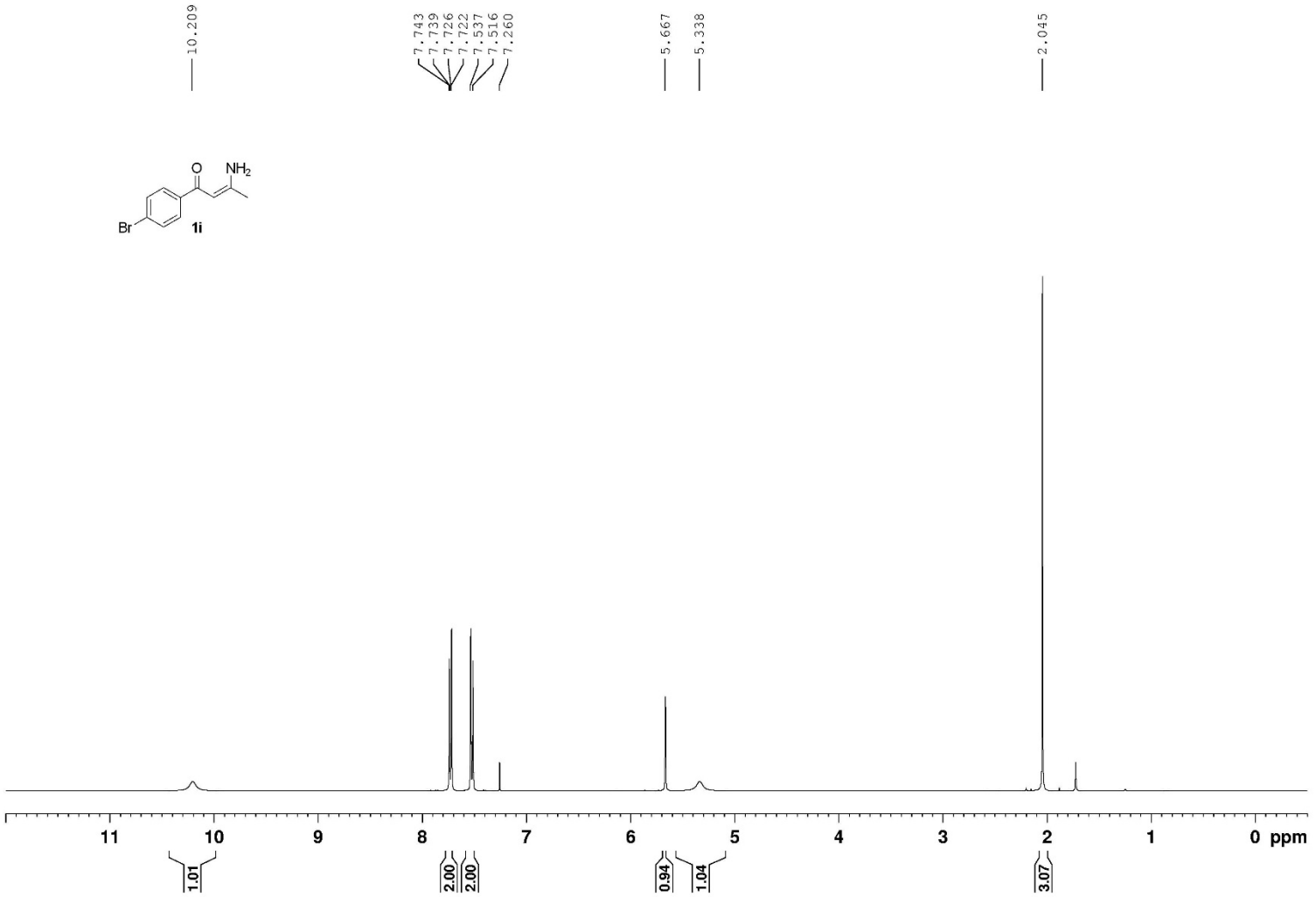
128.43
92.01
77.36
77.04
76.72
22.92
O
NH2
Cl
1h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.739
7.726
7.722
7.537
7.516
7.260
5.667
5.338
2.045
O
NH2
Br
1i
11
10
9
8
7
6
5
4
3
2
1
0 ppm
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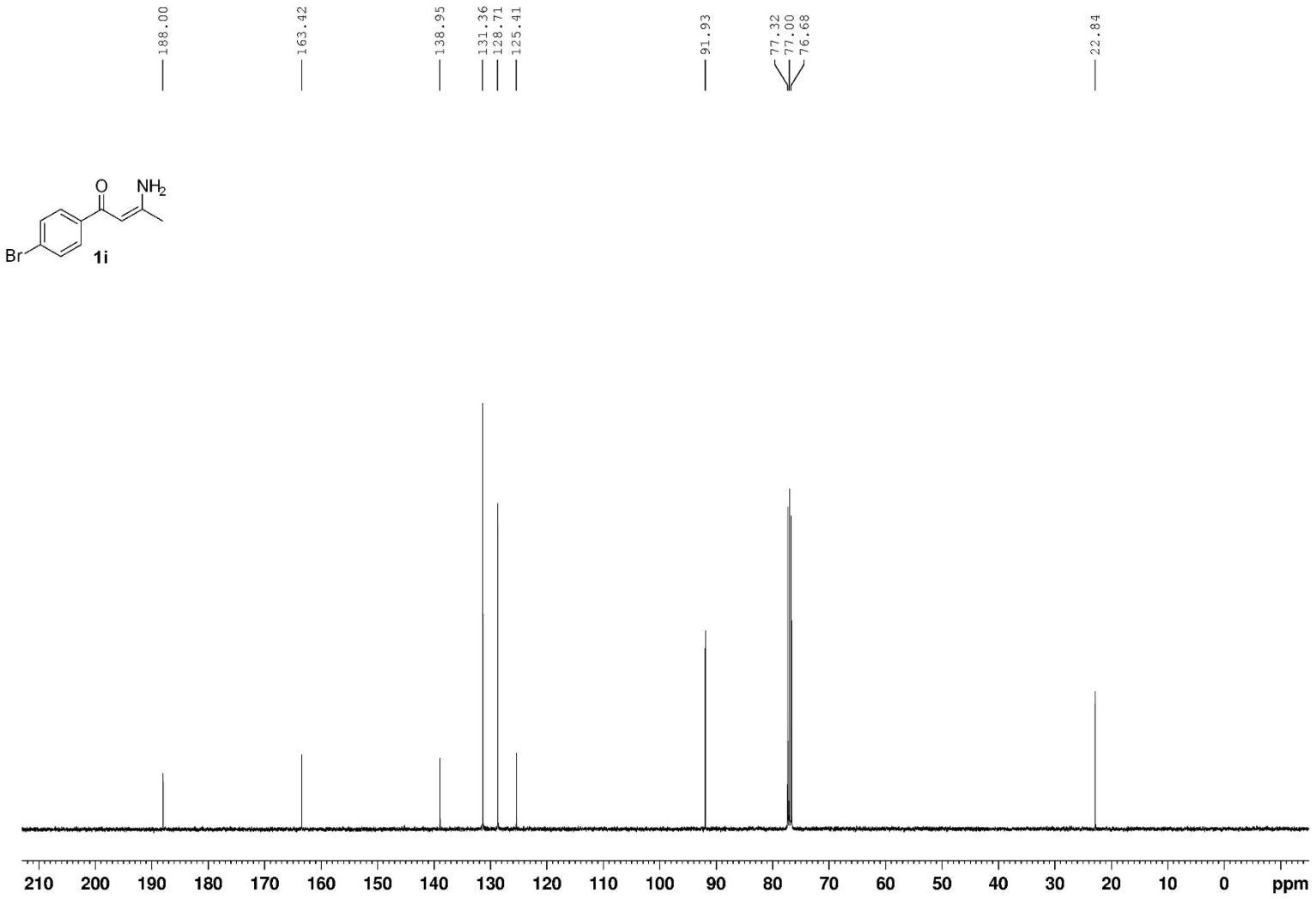
2.00
2.00
0.94
1.04
3.07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77.00
76.68
22.84
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NH2
Br
1i
210
200
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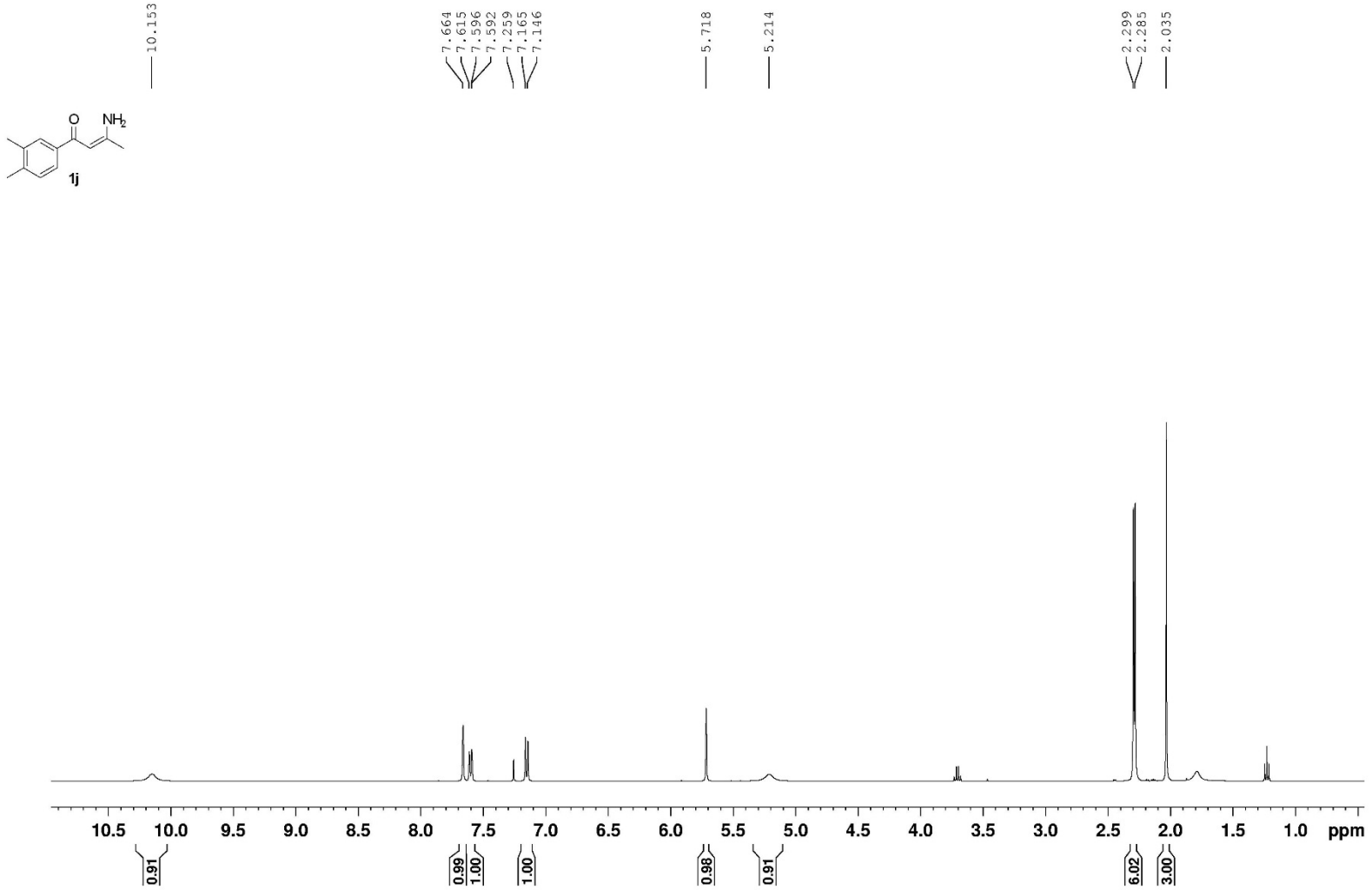
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.615
7.596
7.592
7.259
7.165
7.146
5.718
5.214
2.299
2.285
2.035
O
NH2
1j
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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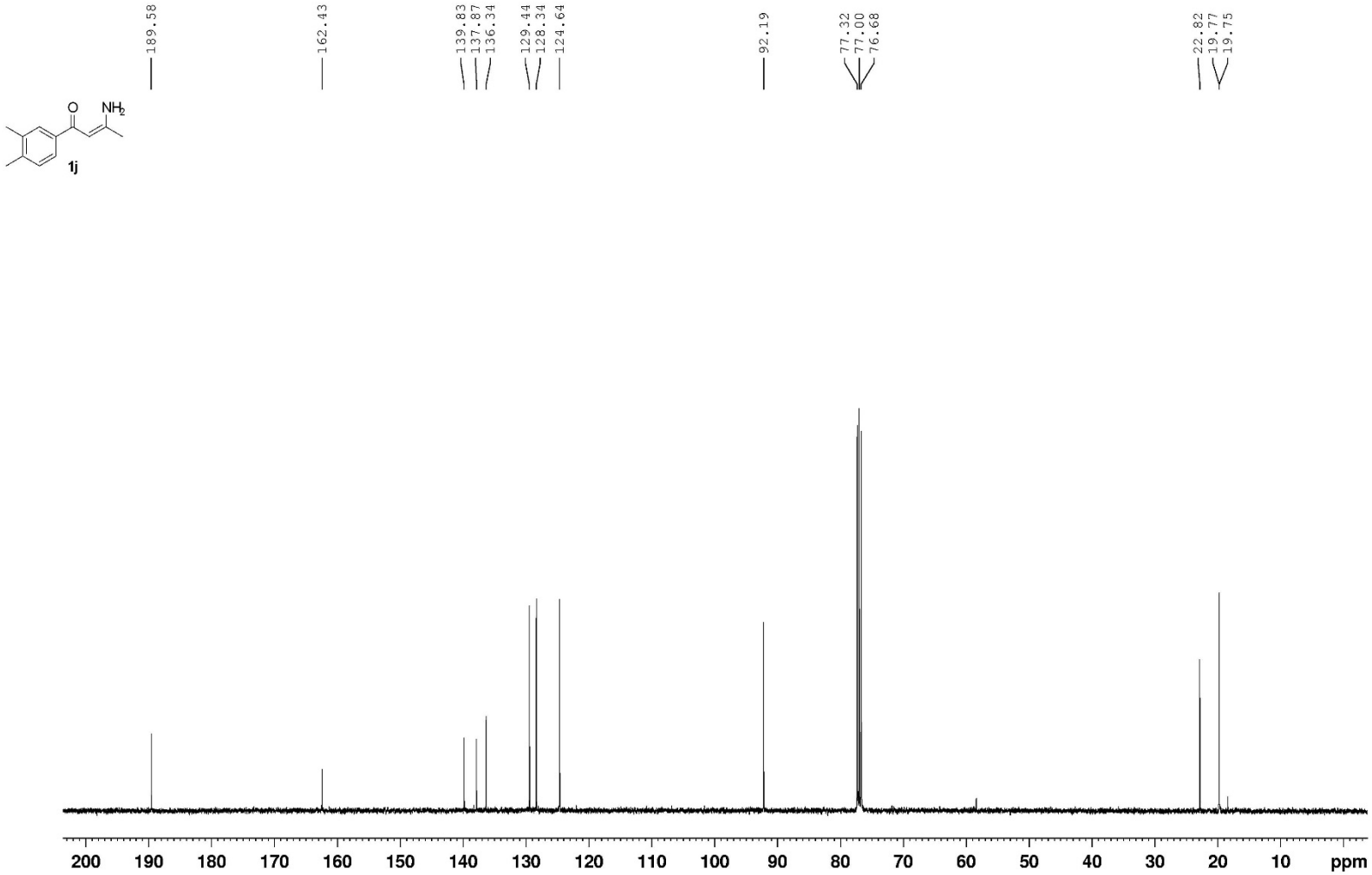
1.0
ppm
0.91
0.99
1.00
1.00
0.98
0.91
6.02
3.00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137.87
136.34
129.44
128.34
124.64
92.19
77.32
77.00
76.68
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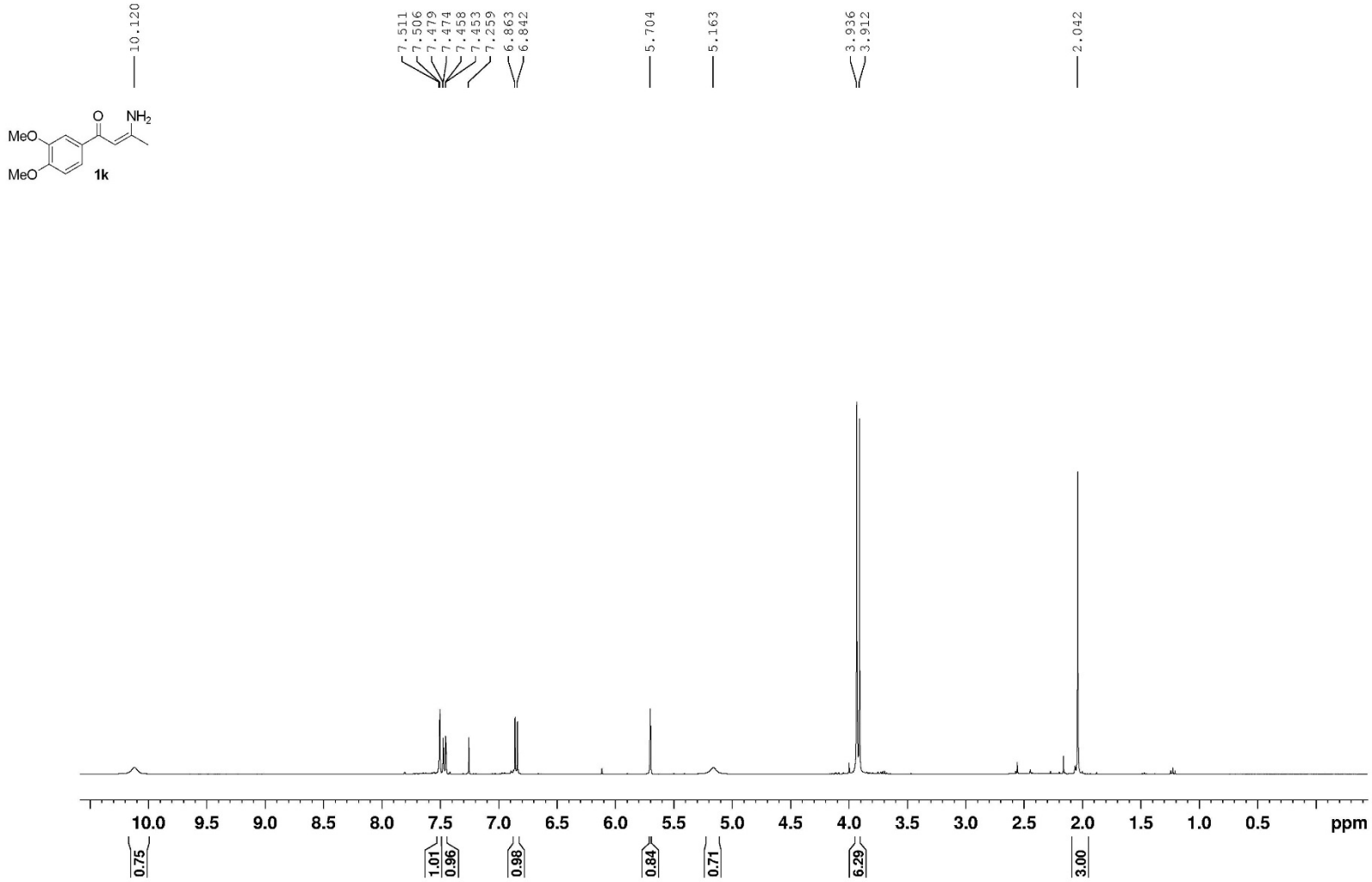
19.77
19.75
O
NH2
1j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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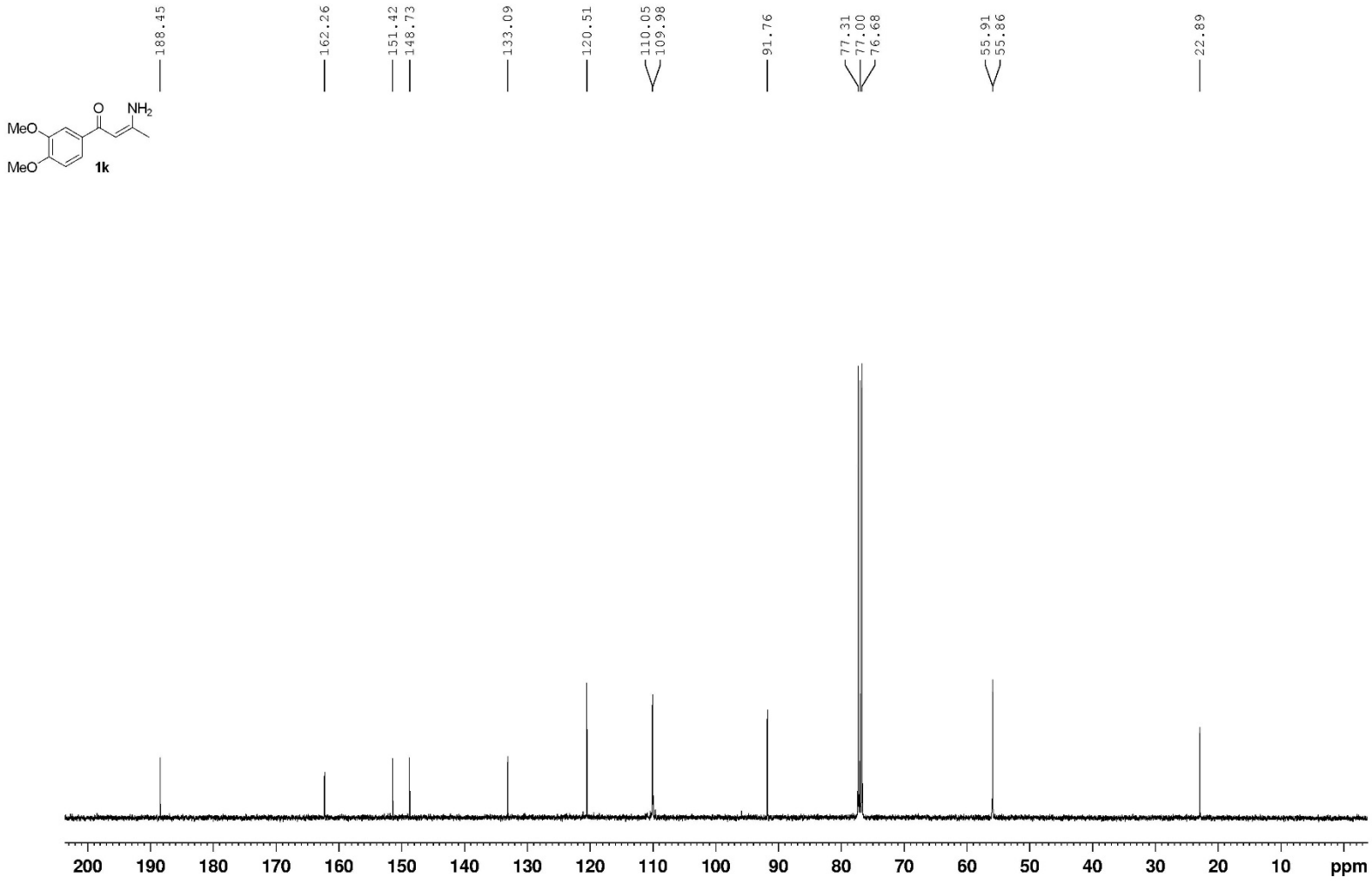
7.511
7.506
7.479
7.474
7.458
7.453
7.259
6.863
6.842
5.704
5.163
3.936
3.912
2.042
O
NH2
MeO
MeO
1k
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.75
1.01
0.96
0.98
0.84
0.71
6.29
3.00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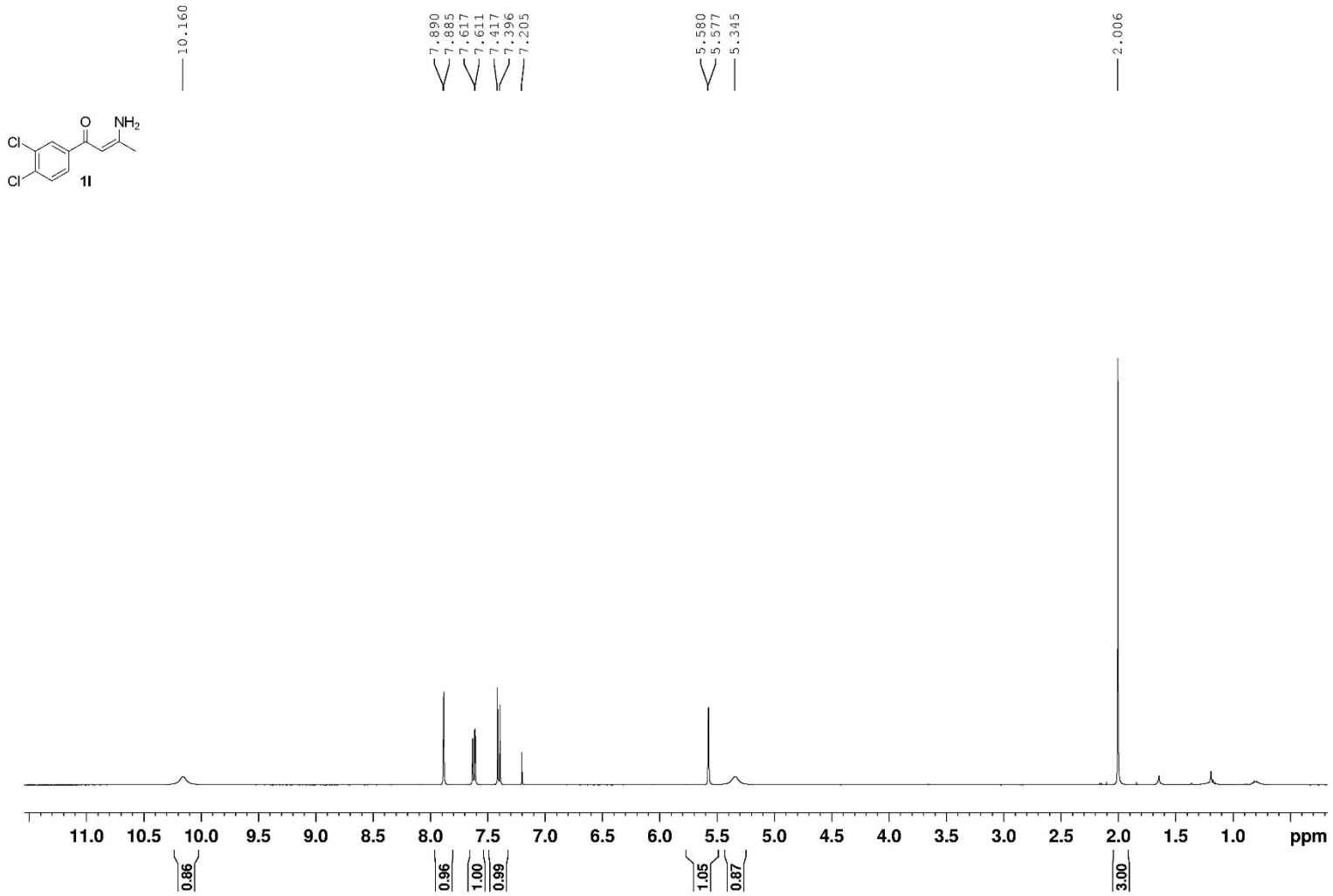
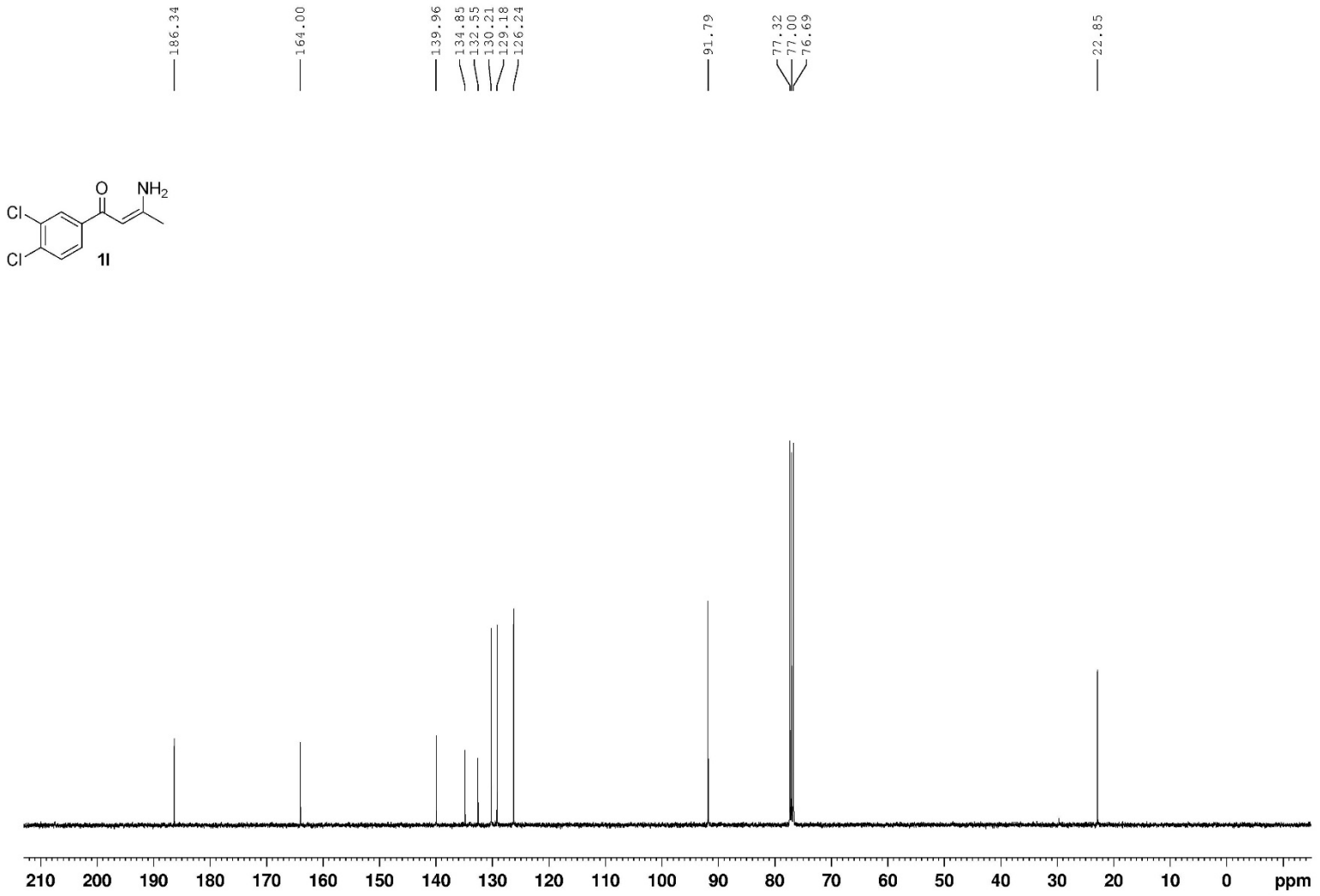
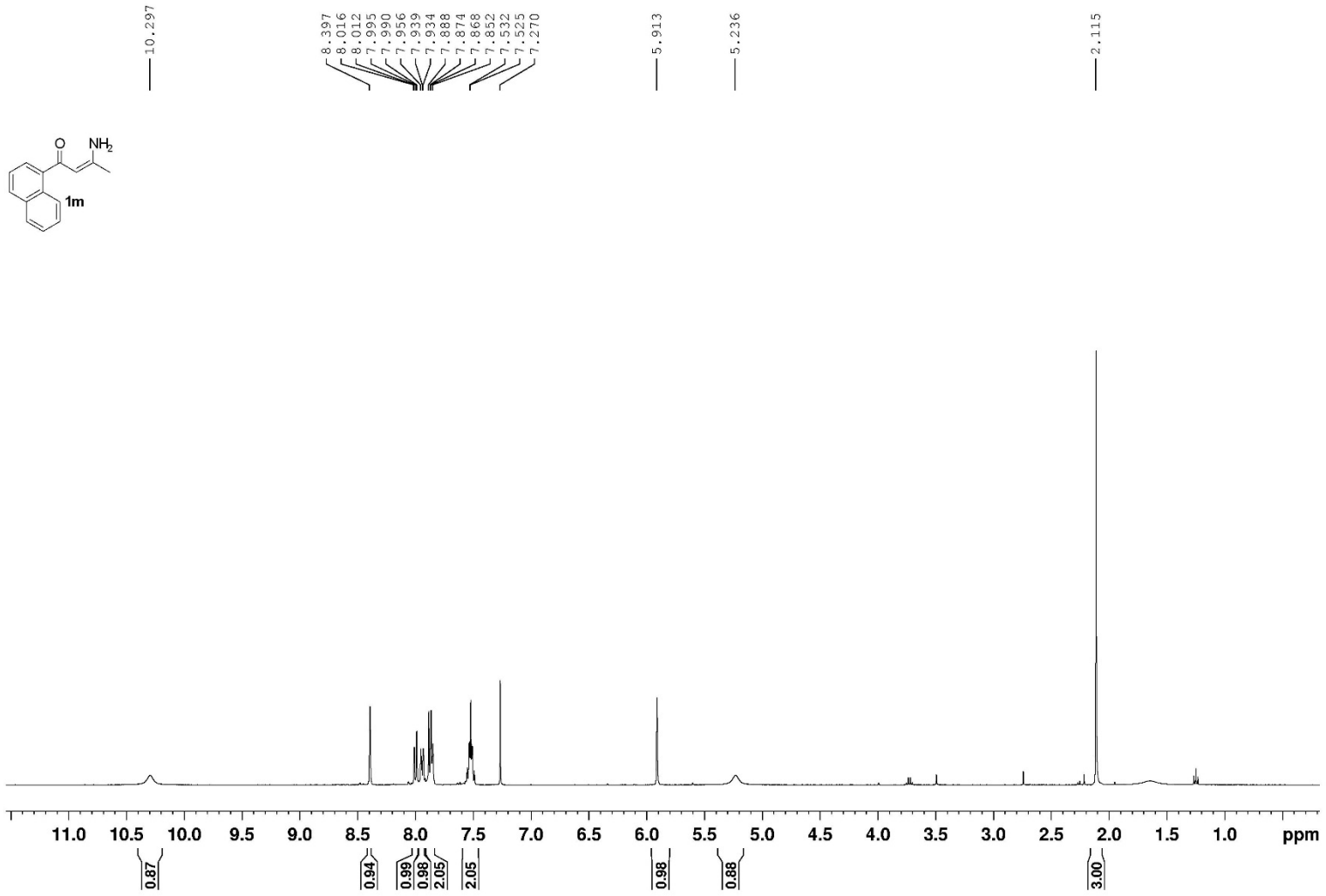
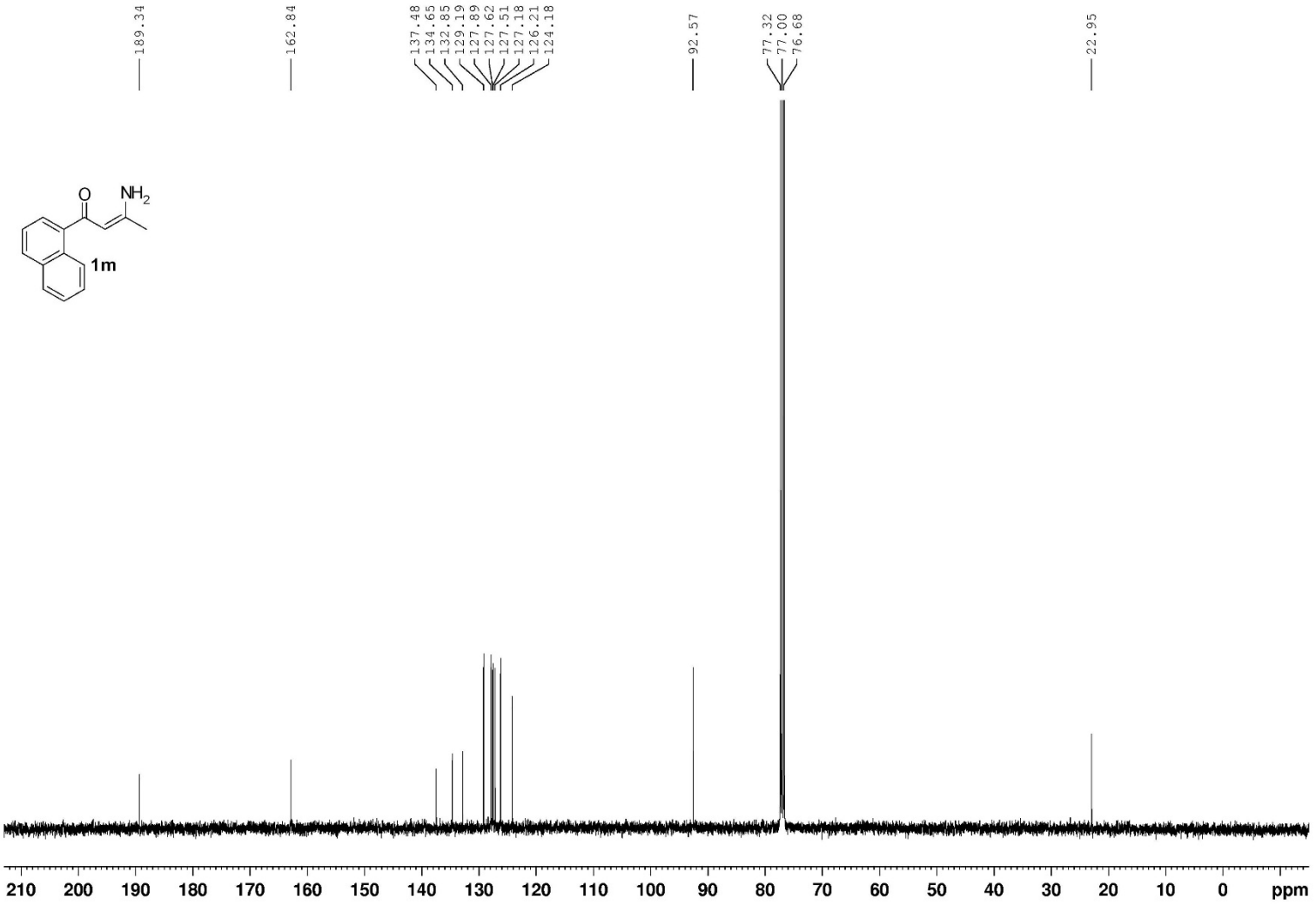
162.26
151.42
148.73
133.09
120.51
110.05
109.98
91.76
77.31
77.00
76.68
55.91
55.86
22.89
O
NH2
MeO
MeO
1k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


10.160
7.890
7.885
7.617
7.611
7.417
7.396
7.205
5.580
5.577
5.345
2.006
O
NH2
Cl
Cl
1l
11.0
10.5
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
ppm
0.86
0.96
1.00
0.99
1.05
0.87
3.00


186.34
164.00
139.96
134.85
132.55
130.21
129.18
126.24
91.79
77.32
77.00
76.69
22.85
O
NH2
Cl
Cl
1l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


10.297
8.397
8.016
8.012
7.995
7.990
7.956
7.939
7.934
7.888
7.874
7.868
7.852
7.532
7.525
7.270
5.913
5.236
2.115
O
NH2
1m
11.0
10.5
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
ppm
0.87
0.94
0.99
0.98
2.05
2.05
0.98
0.88
3.00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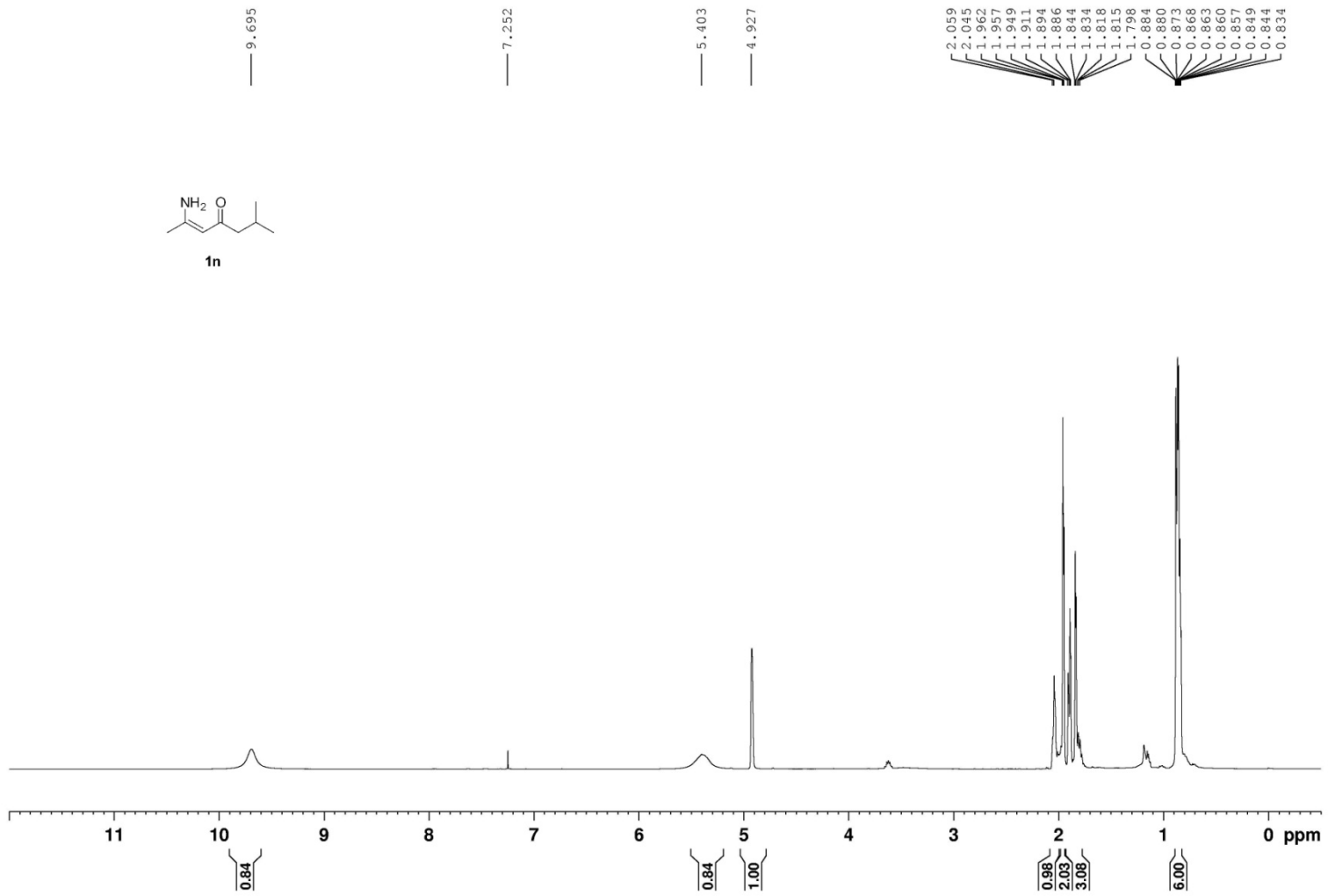
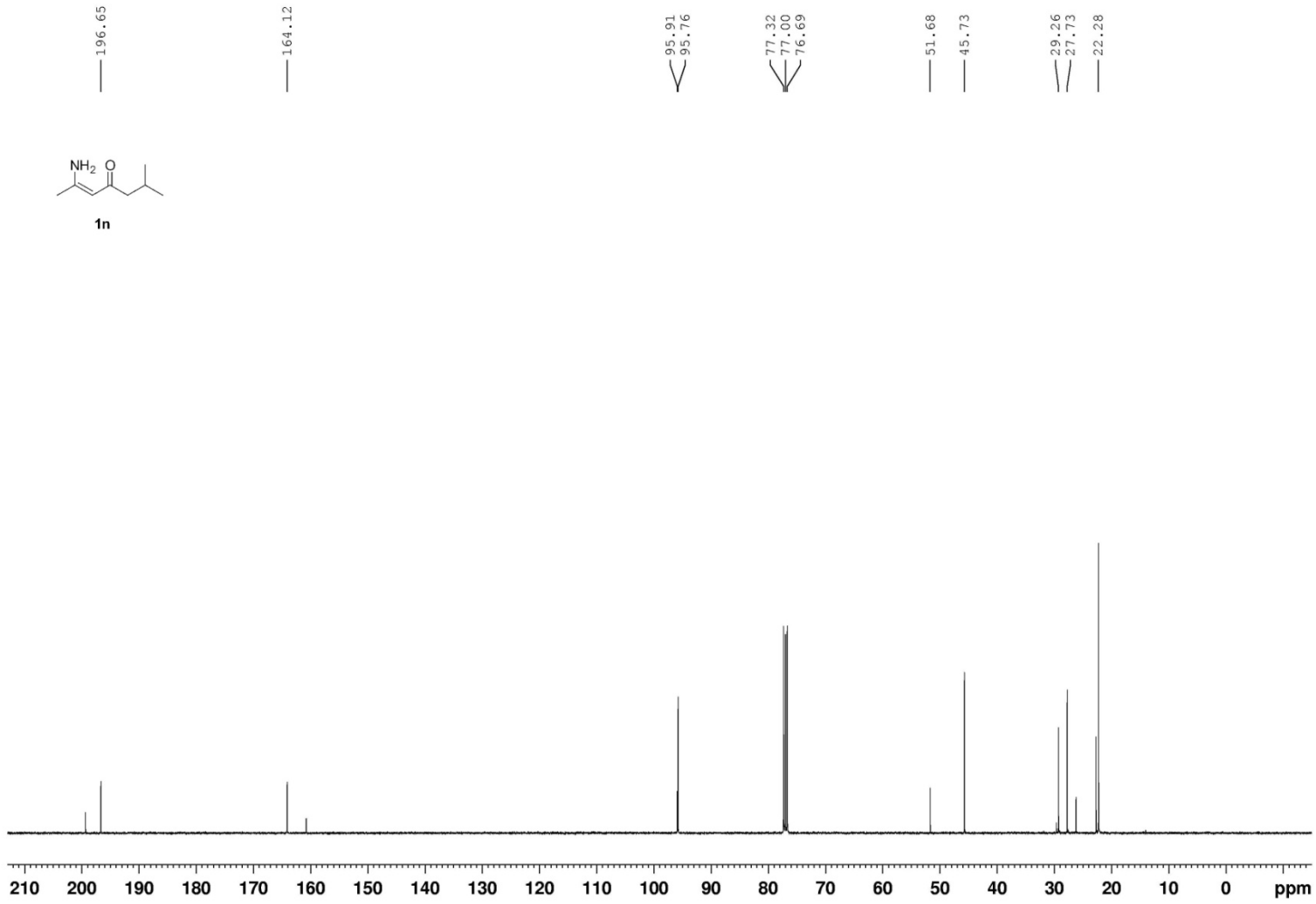
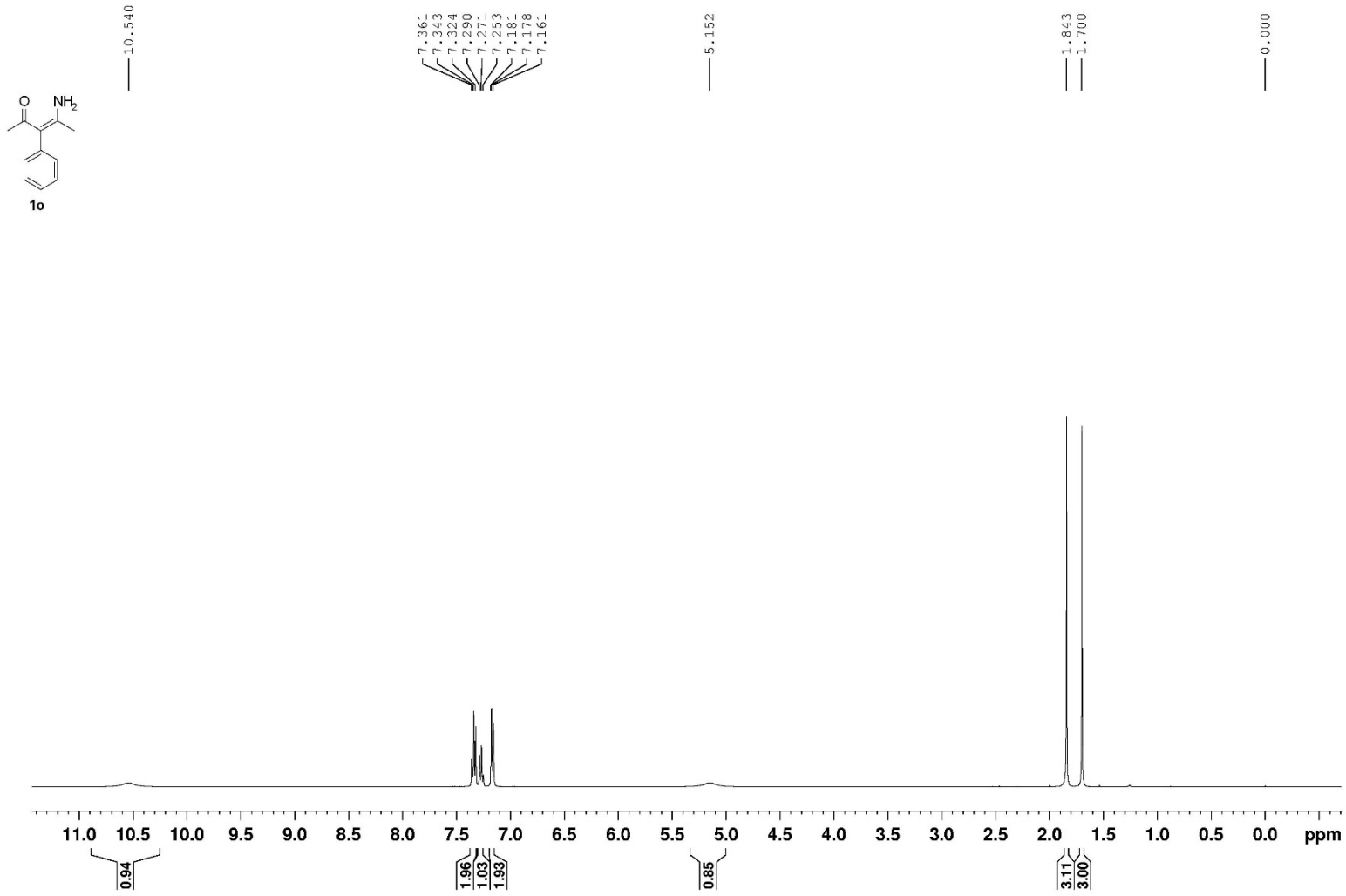
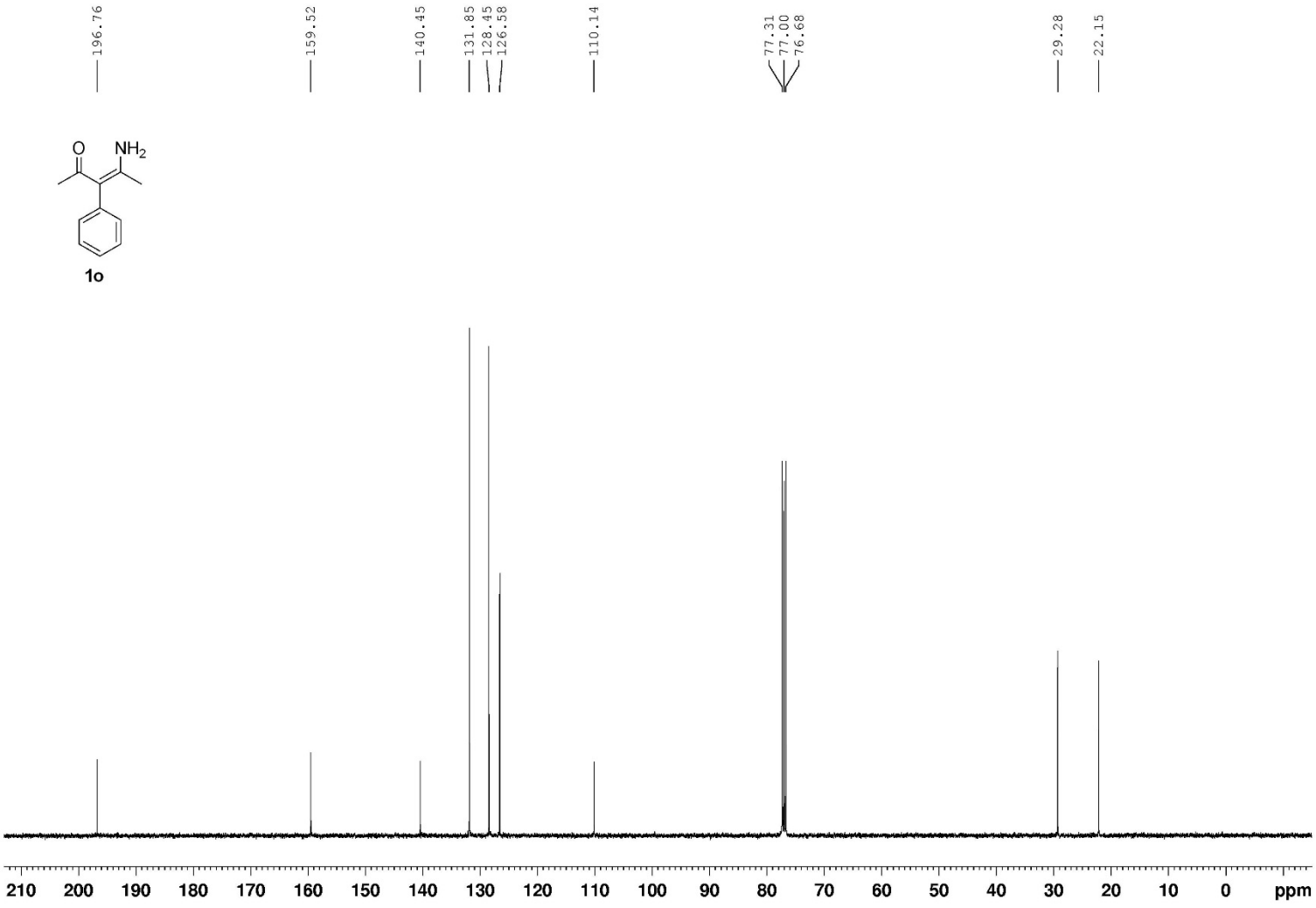
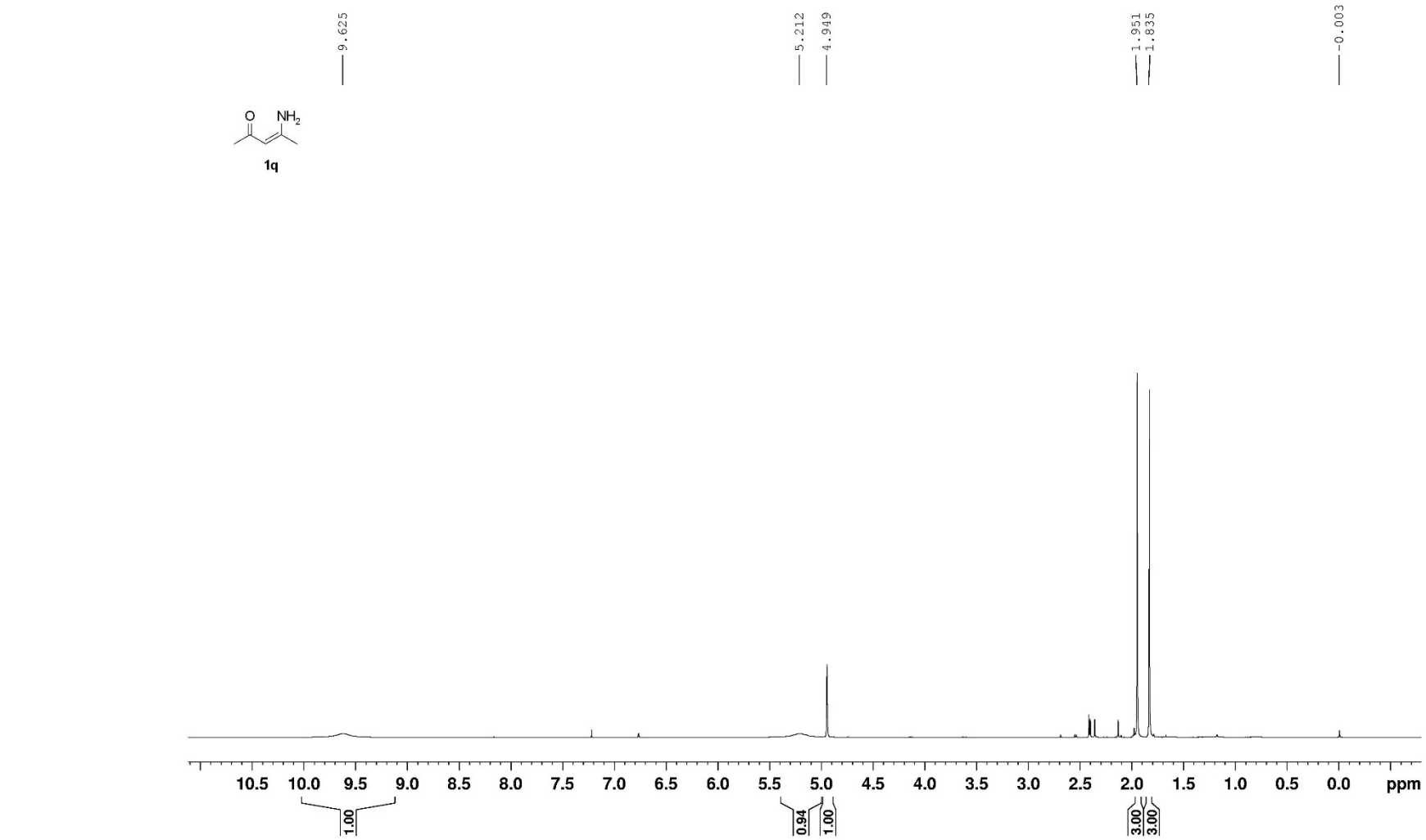
162.84
137.48
134.65
132.85
129.19
127.89
127.62
127.51
127.18
126.21
124.18
92.57
77.32
77.00
76.68
22.95
O
NH2
1m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

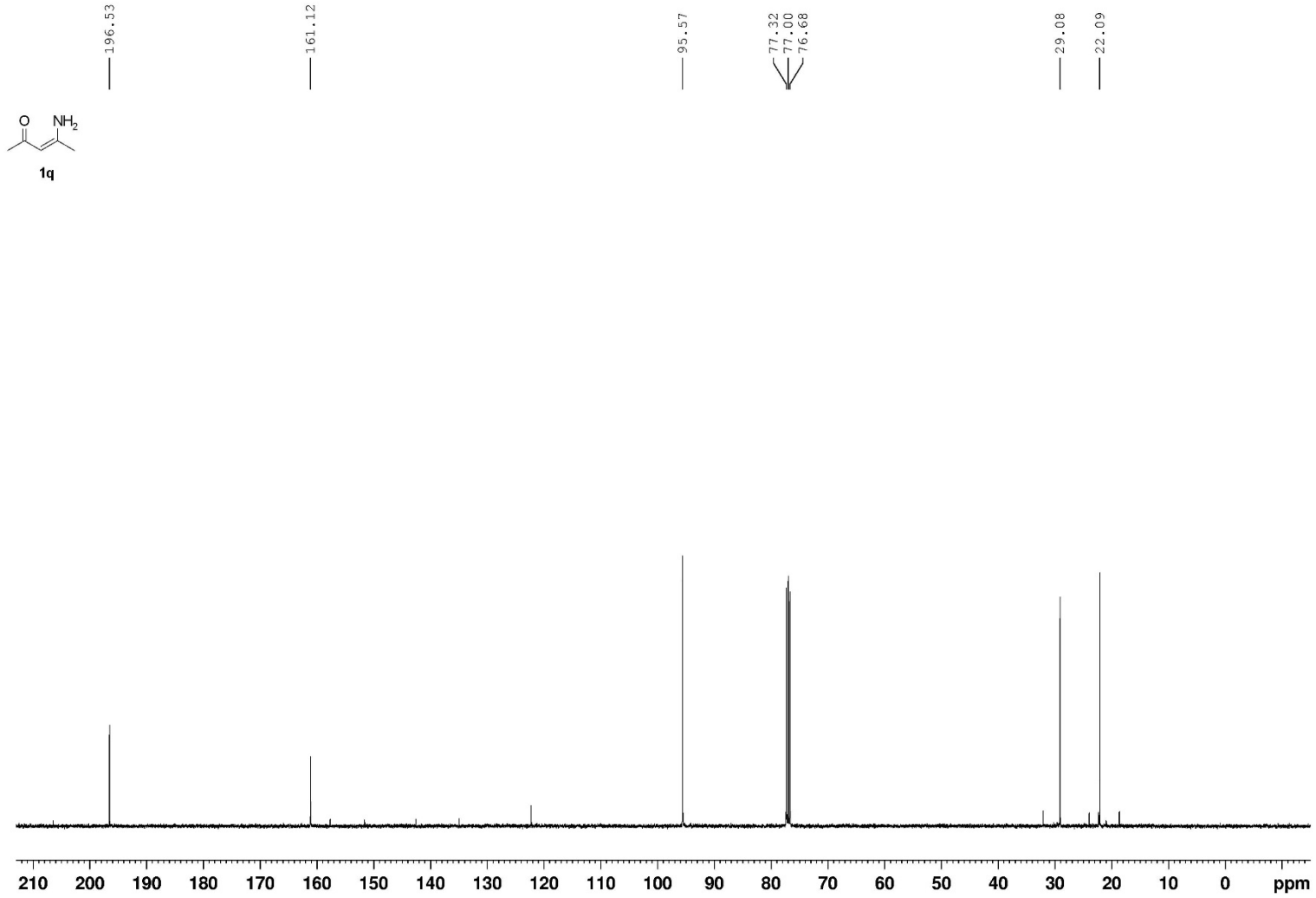

9.695
7.252
5.403
4.927
2.059
2.045
1.962
1.957
1.949
1.911
1.894
1.886
1.844
1.834
1.818
1.815
1.798
0.884
0.880
0.873
0.868
0.863
0.860
0.857
0.849
0.844
0.834
NH2
O
1n
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.84
0.84
1.00
0.98
2.03
3.08
6.00

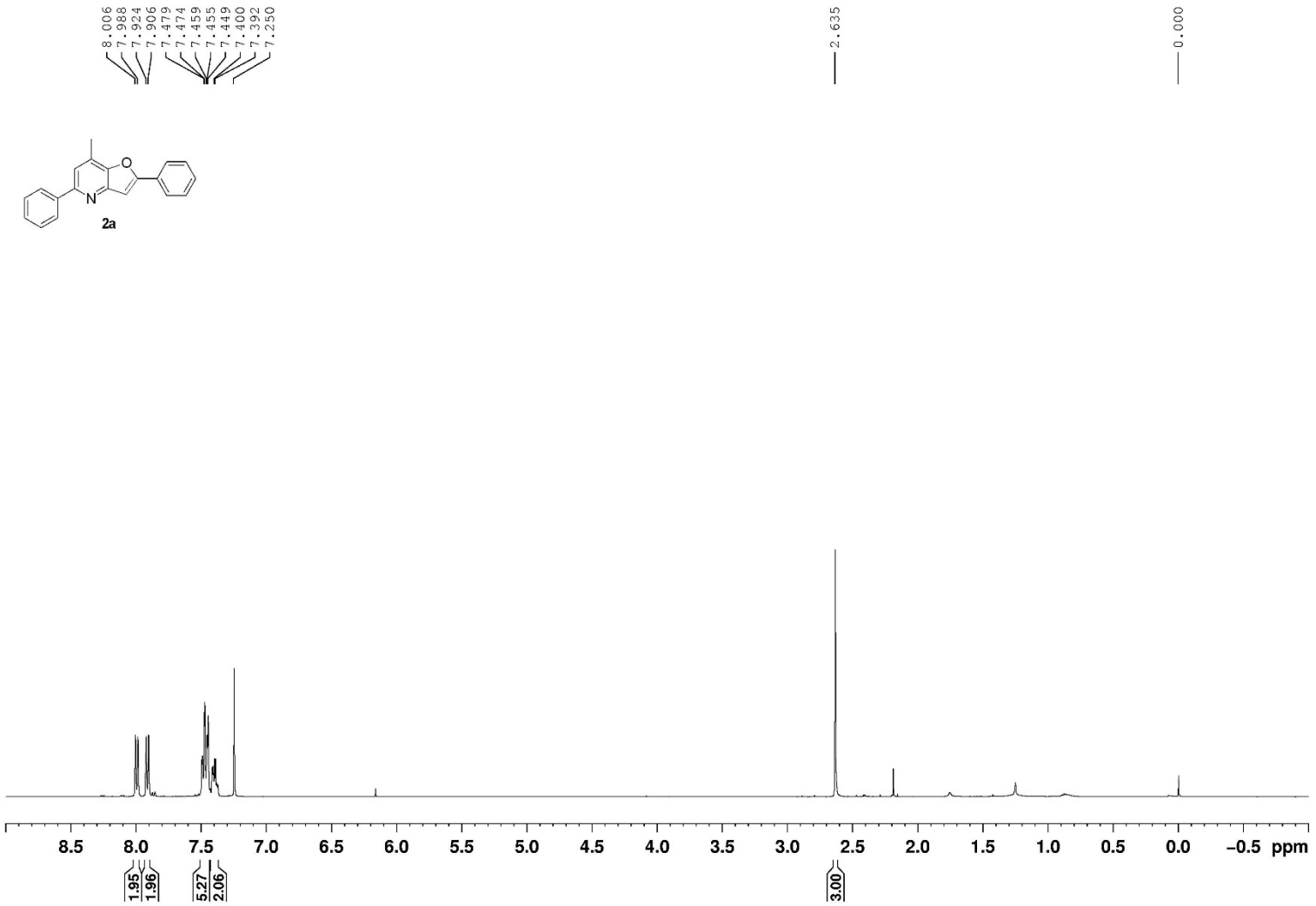

196.65
164.12
95.91
95.76
77.32
77.00
76.69
51.68
45.73
29.26
27.73
22.28
NH2
O
1n
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

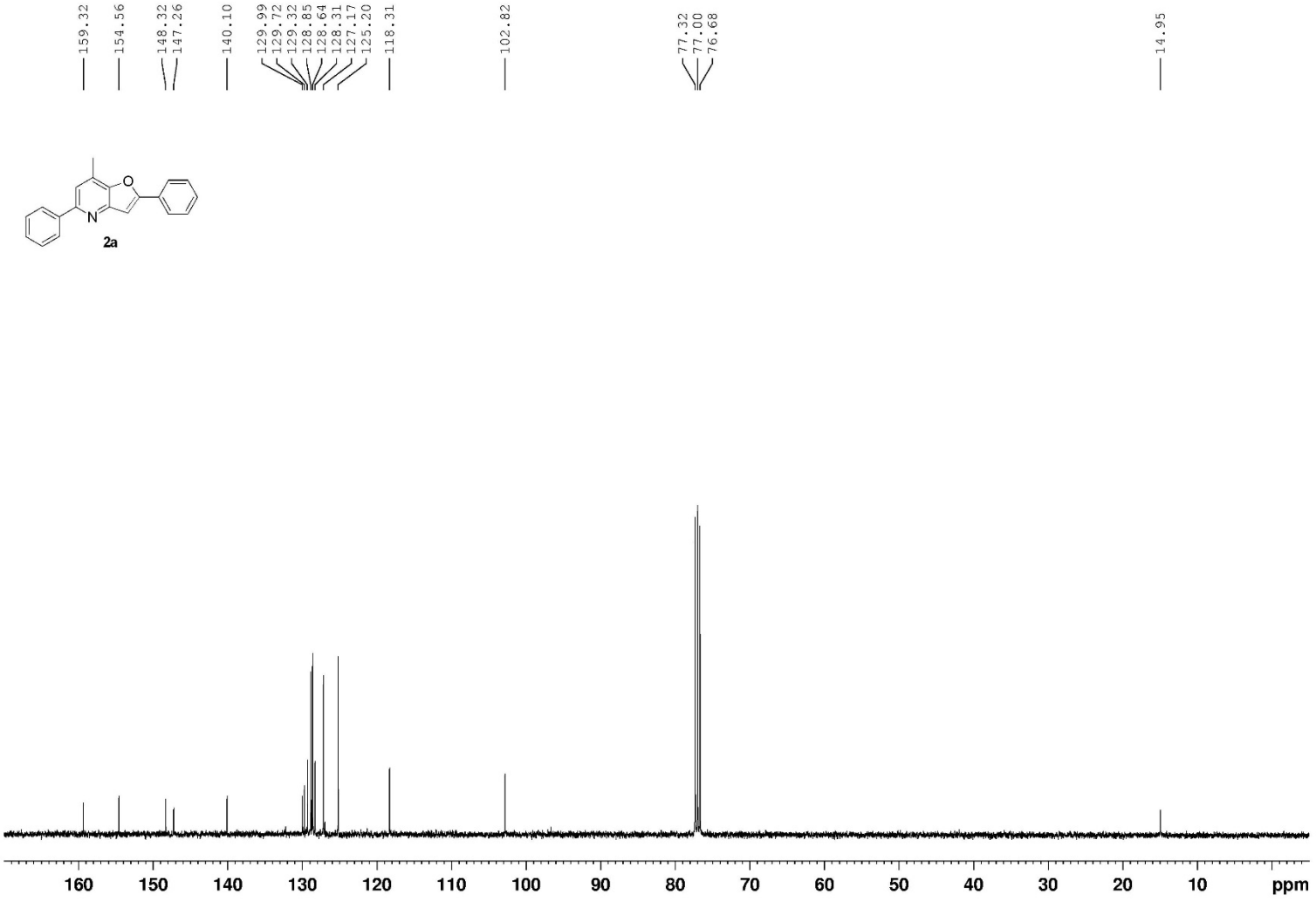

10.540
7.361
7.343
7.324
7.290
7.271
7.253
7.181
7.178
7.161
5.152
1.843
1.700
0.000
O
NH2
1o
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.94
1.96
1.03
1.93
0.85
3.11
3.00

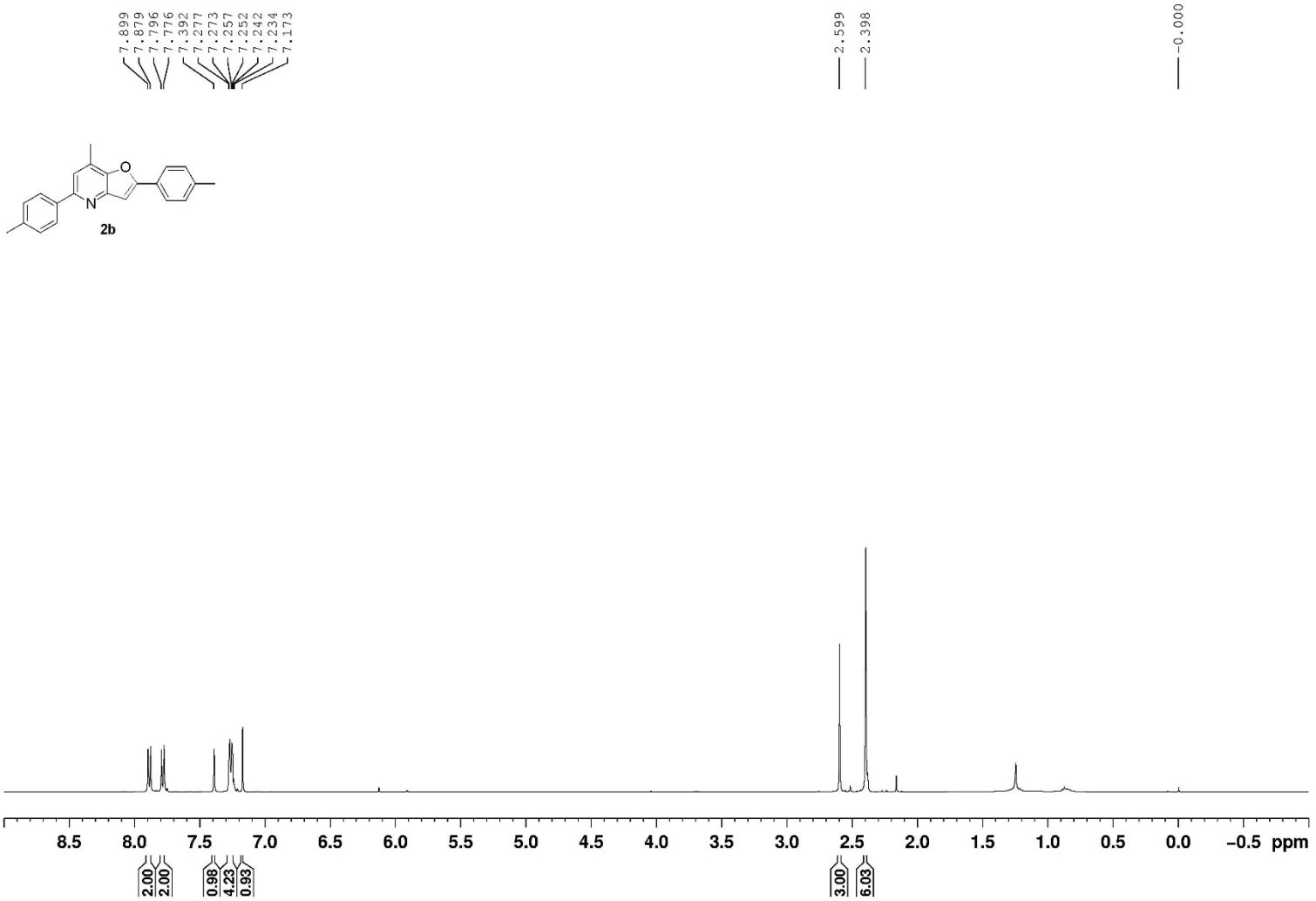

196.76
159.52
140.45
131.85
128.45
126.58
110.14
77.31
77.00
76.68
29.28
22.15
O
NH2
1o
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


9.625
5.212
4.949
1.951
1.835
-0.003
O
NH2
1q
10.5
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
0.0
ppm
1.00
0.94
1.00
3.00
3.00


196.53
161.12
95.57
77.32
77.00
76.68
29.08
22.09
O
NH2
1q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.006
7.988
7.924
7.906
7.479
7.474
7.459
7.455
7.449
7.400
7.392
7.250
2.635
0.000
O
N
2a
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
0.0
−0.5 ppm
1.95
1.96
5.27
2.06
3.00


159.32
154.56
148.32
147.26
140.10
129.99
129.72
129.32
128.85
128.64
128.31
127.17
125.20
118.31
102.82
77.32
77.00
76.68
14.95
O
N
2a
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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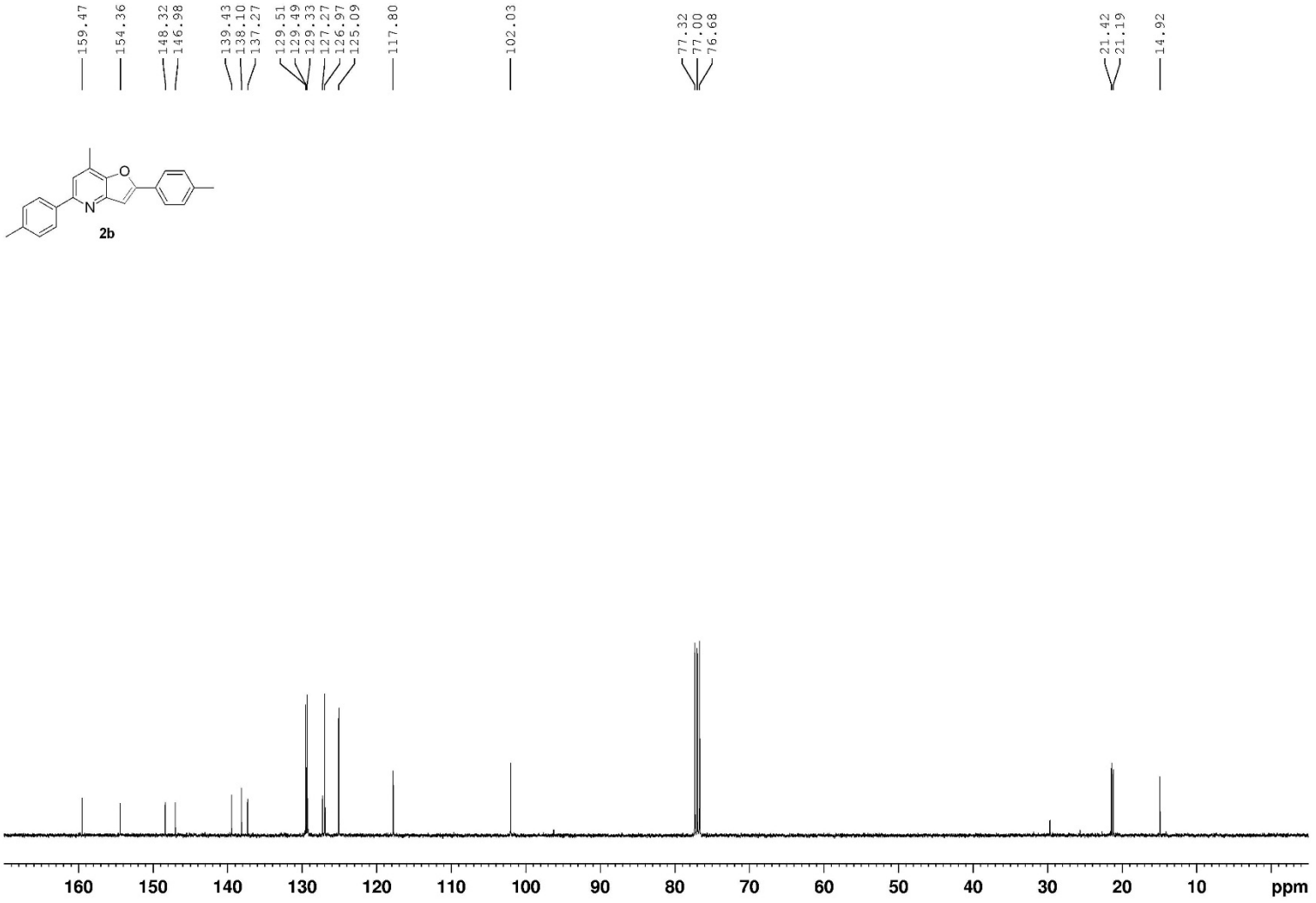
7.879
7.796
7.776
7.392
7.277
7.273
7.257
7.252
7.242
7.234
7.173
2.599
2.398
0.000
O
N
2b
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5 ppm
2.00
2.00
0.98
4.23
0.93
3.00
6.03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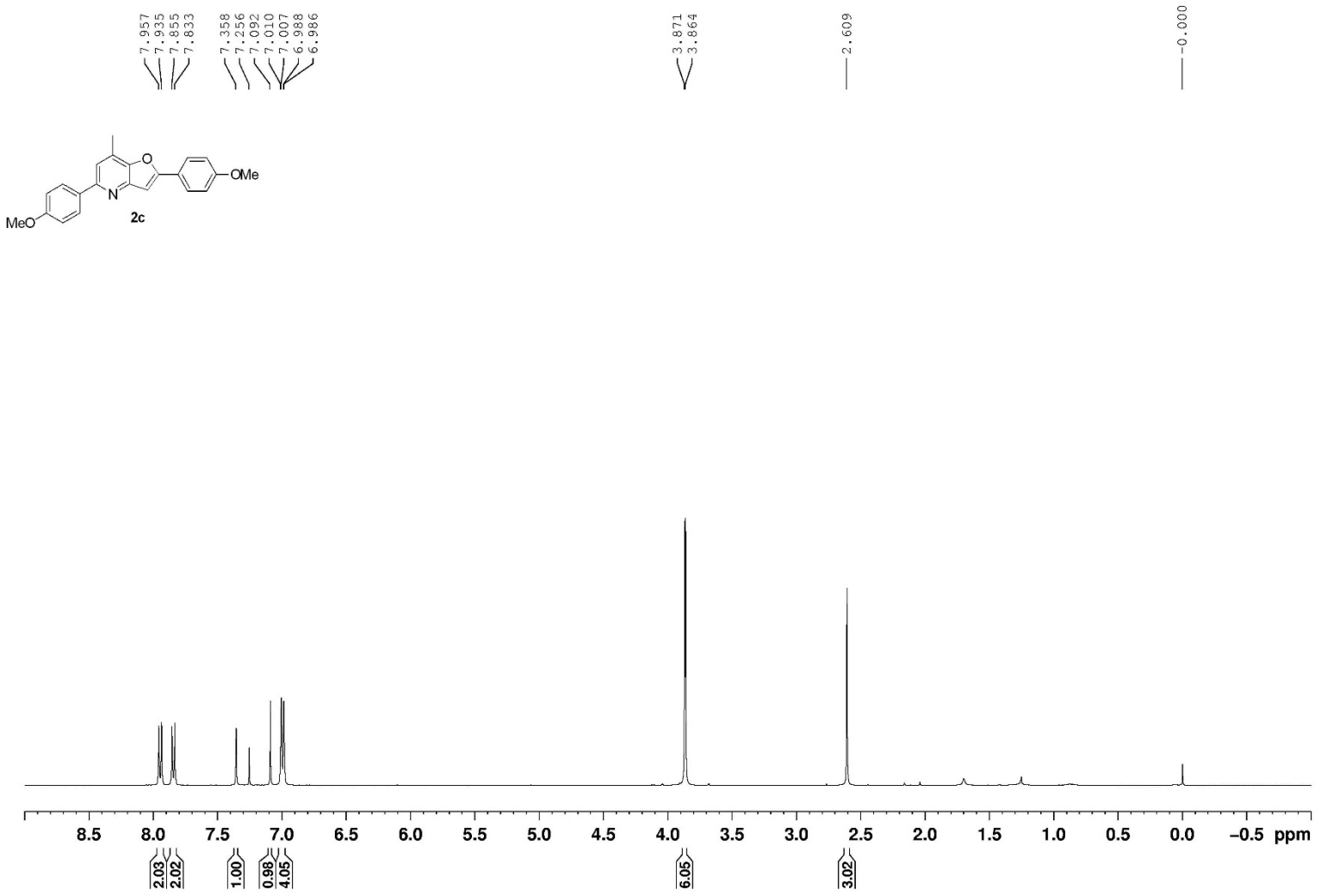
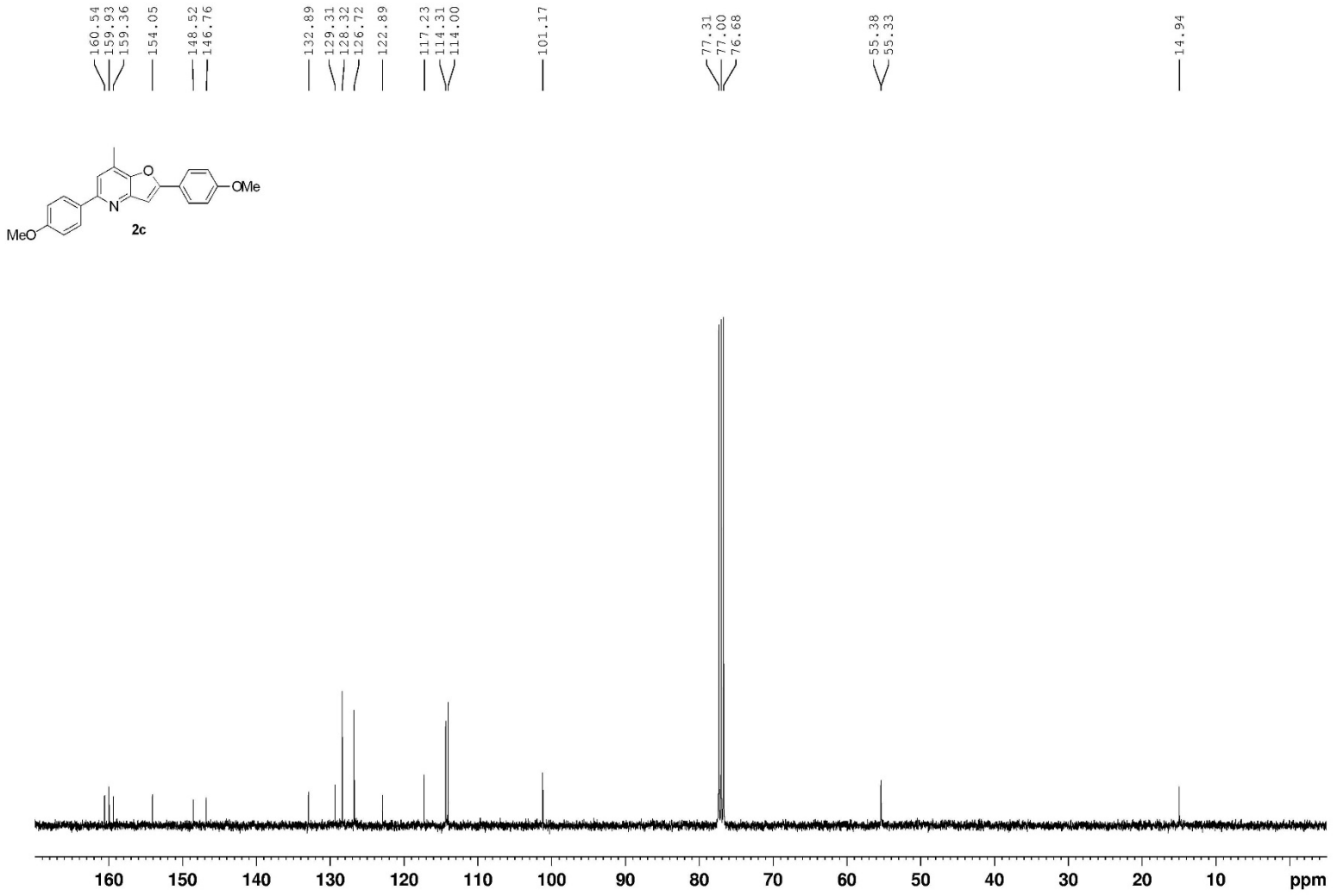
154.36
148.32
146.98
139.43
138.10
137.27
129.51
129.49
129.33
127.27
126.97
125.09
117.80
102.03
77.32
77.00
76.68
21.42
21.19
14.92
O
N
2b
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.957
7.935
7.855
7.833
7.358
7.256
7.092
7.010
7.007
6.988
6.986
3.871
3.864
2.609
-0.000
O
N
OMe
MeO
2c
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
0.0
-0.5 ppm
2.03
2.02
1.00
0.98
4.05
6.05
3.02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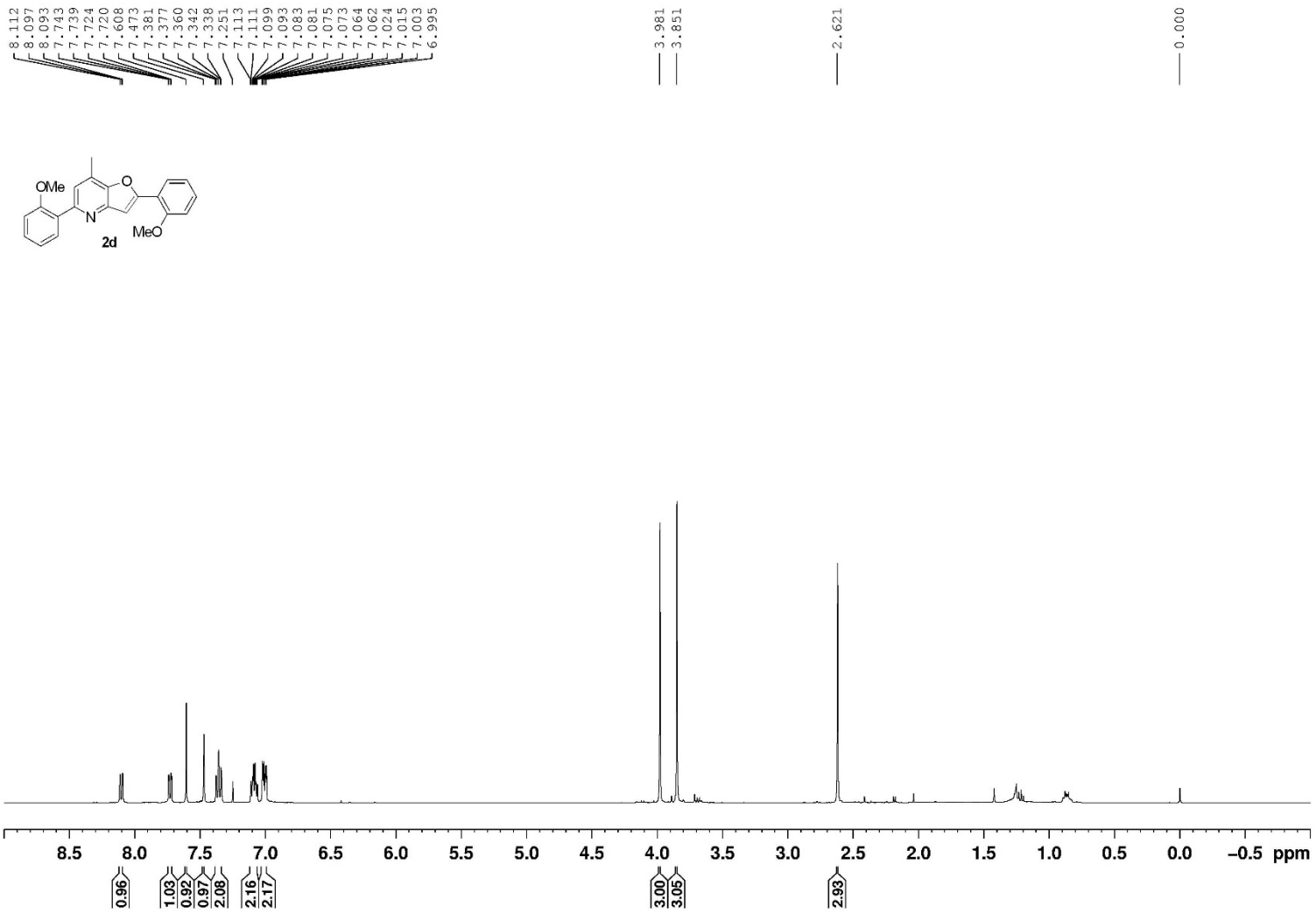
159.36
154.05
148.52
146.76
132.89
129.31
128.32
126.72
122.89
117.23
114.31
114.00
101.17
77.31
77.00
76.68
55.38
55.33
14.94
O
N
OMe
MeO
2c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.112
8.097
8.093
7.743
7.739
7.724
7.720
7.608
7.473
7.381
7.377
7.360
7.342
7.338
7.251
7.113
7.111
7.099
7.093
7.083
7.081
7.075
7.073
7.064
7.062
7.024
7.015
7.003
6.995
3.981
3.851
2.621
0.000
OMe
MeO
N
O
2d
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
0.0
−0.5 ppm
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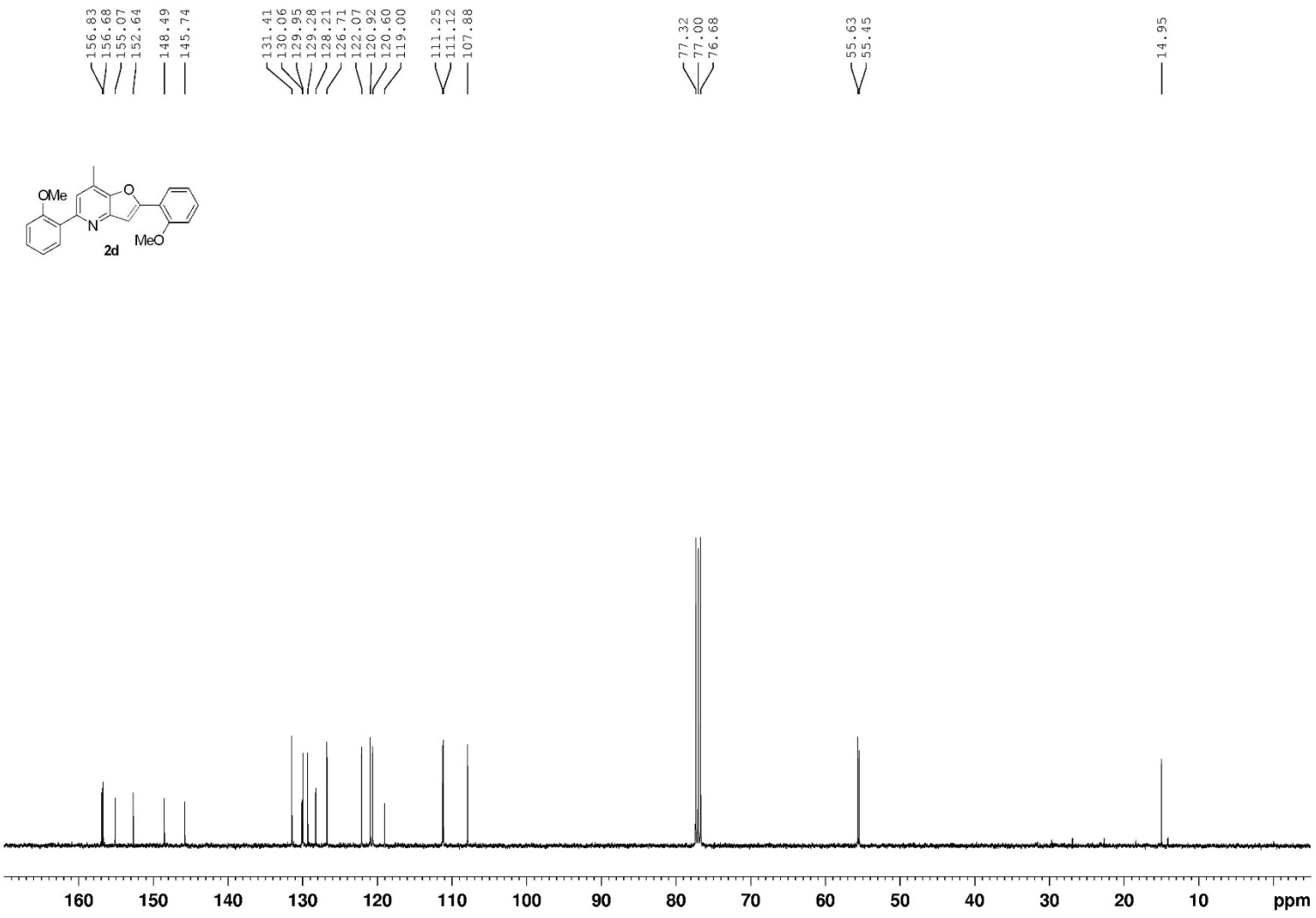
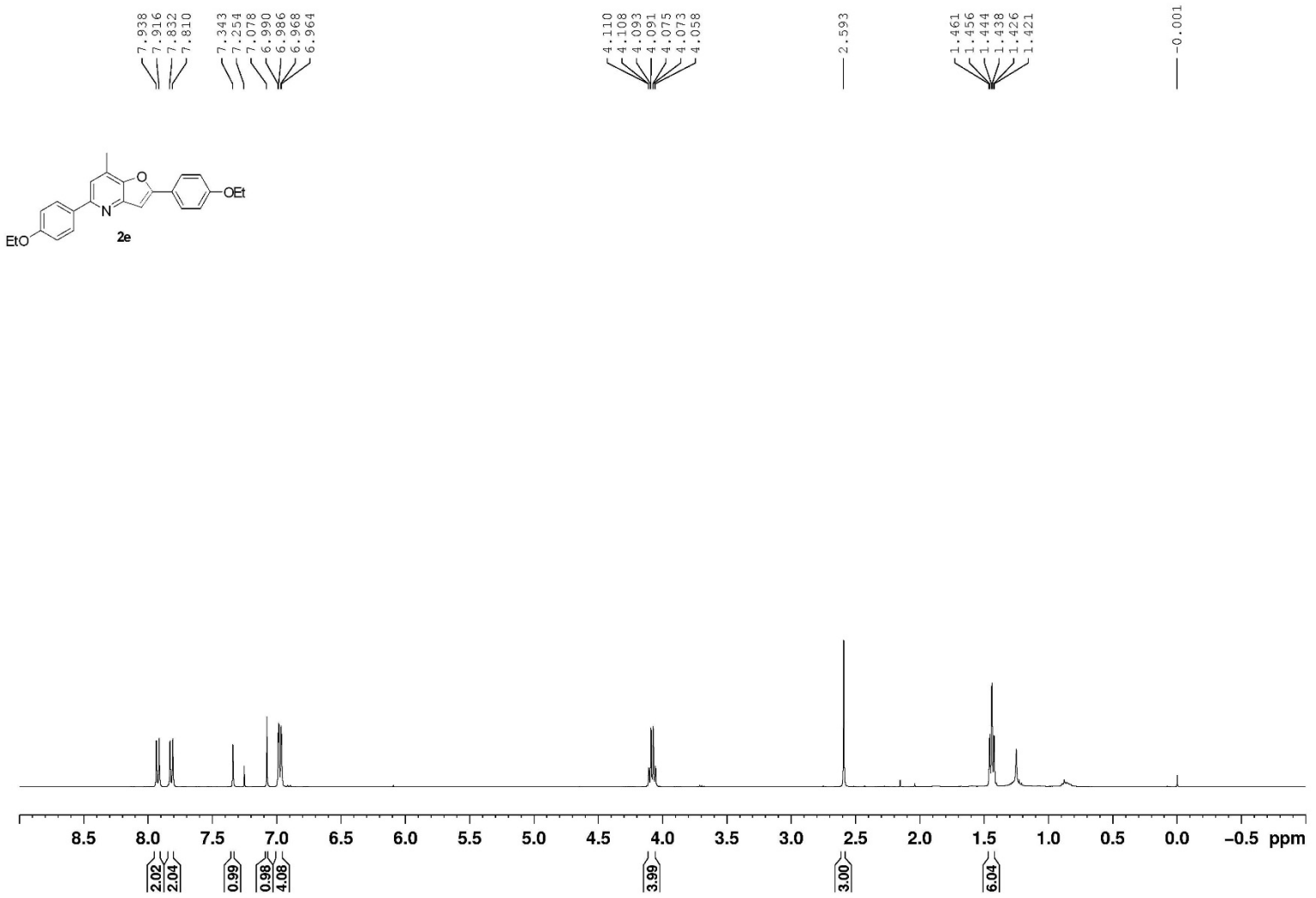
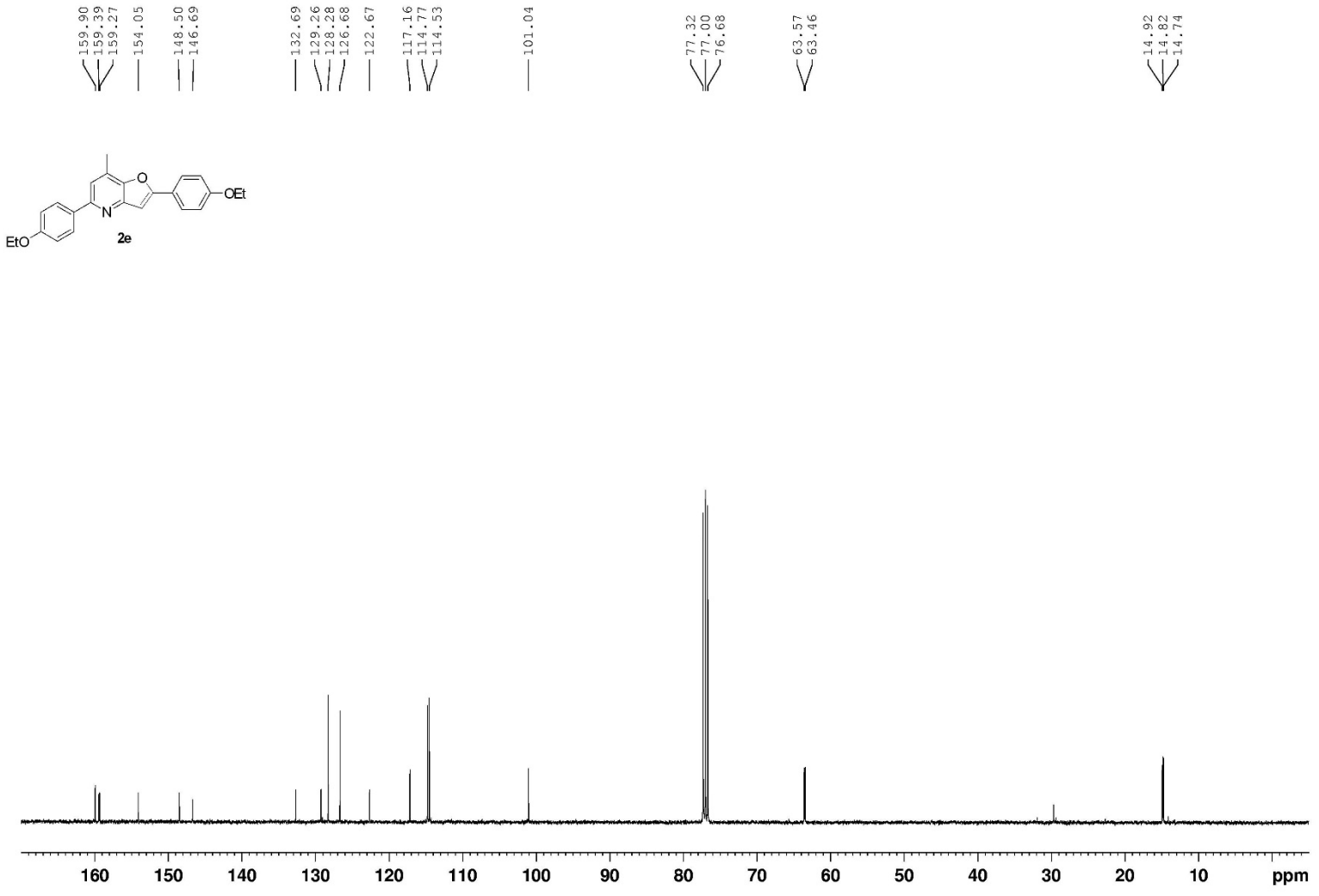
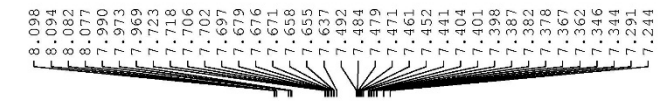
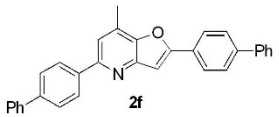
1.03
0.92
0.97
2.08
2.16
2.17
3.00
3.05
2.93


156.83
156.68
155.07
152.64
148.49
145.74
131.41
130.06
129.95
129.28
128.21
126.71
122.07
120.92
120.60
119.00
111.25
111.12
107.88
77.32
77.00
76.68
55.63
55.45
14.95
OMe
N
O
MeO
2d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.938
7.916
7.832
7.810
7.343
7.254
7.078
6.990
6.986
6.968
6.964
4.110
4.108
4.093
4.091
4.075
4.073
4.058
2.593
1.461
1.456
1.444
1.438
1.426
1.421
0.001
EtO
OEt
N
O
2e
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
0.0
-0.5 ppm
2.02
2.04
0.99
0.98
4.08
3.99
3.00
6.04


159.90
159.39
159.27
154.05
148.50
146.69
132.69
129.26
128.28
126.68
122.67
117.16
114.77
114.53
101.04
77.32
77.00
76.68
63.57
63.46
14.92
14.82
14.74
O
N
OEt
EtO
2e
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

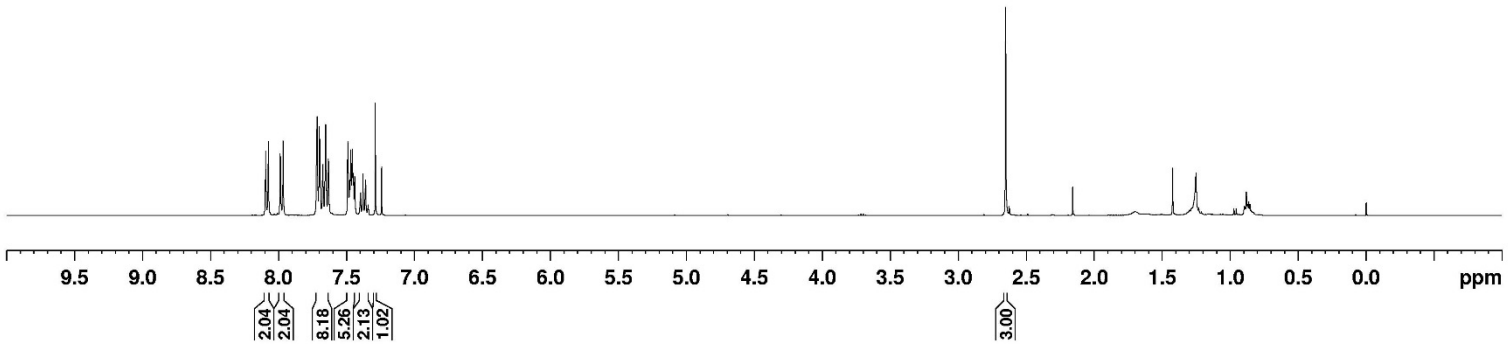

8.098
8.094
8.082
8.077
7.990
7.973
7.969
7.723
7.718
7.706
7.702
7.697
7.679
7.676
7.671
7.658
7.655
7.637
7.492
7.484
7.479
7.471
7.461
7.452
7.441
7.404
7.401
7.398
7.387
7.382
7.378
7.367
7.362
7.346
7.344
7.291
7.244

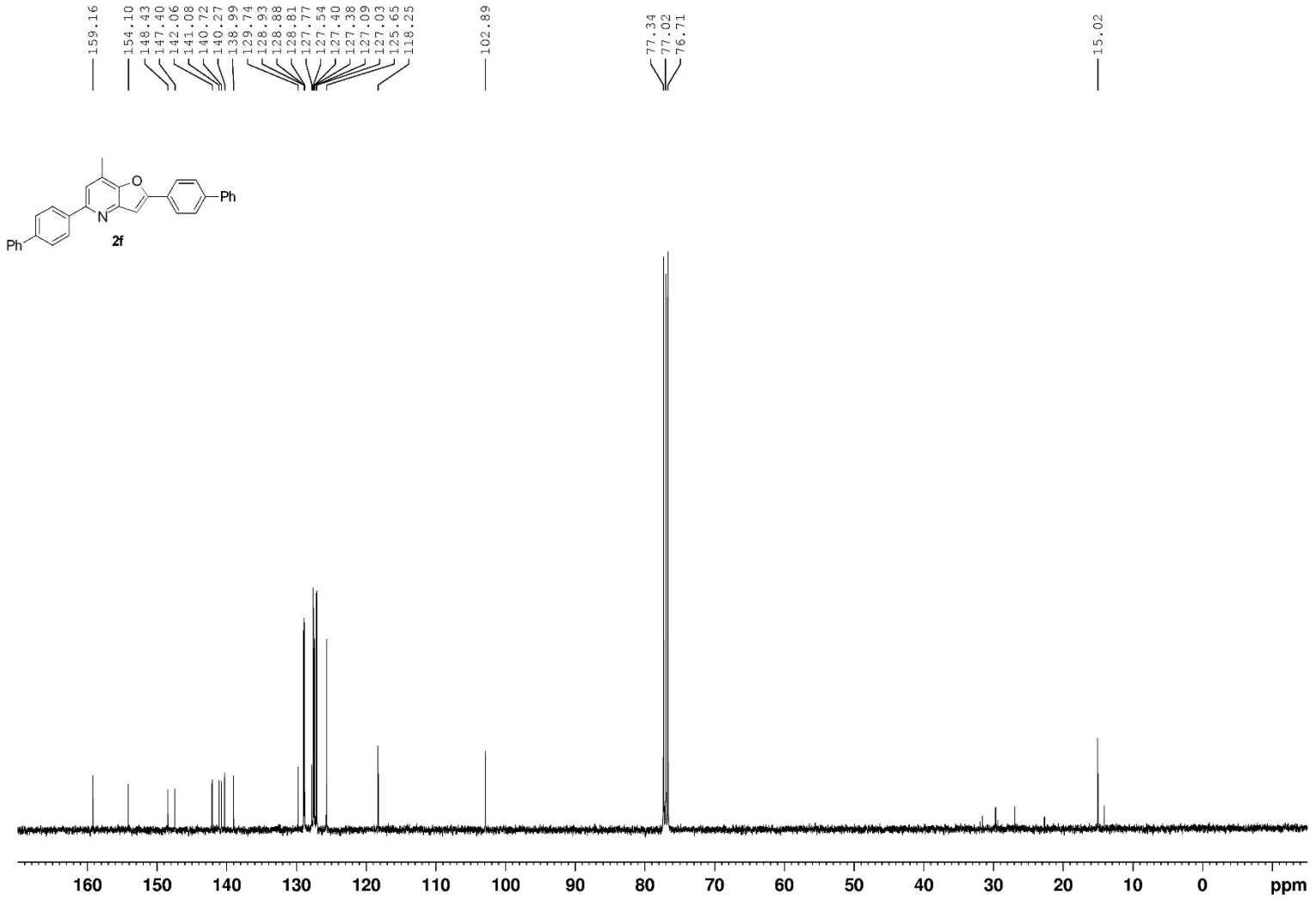

O
N
Ph
Ph

2f

2.653

0.000


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
0.0
ppm
2.04
2.04
8.18
5.26
2.13
1.02
3.00


159.16
154.10
148.43
147.40
142.06
141.08
140.72
140.27
138.99
129.74
128.93
128.88
128.81
127.77
127.54
127.40
127.38
127.09
127.03
125.65
118.25
102.89
77.34
77.02
76.71
15.02
O
N
Ph
Ph
2f
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140
130
120
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100
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80
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60
50
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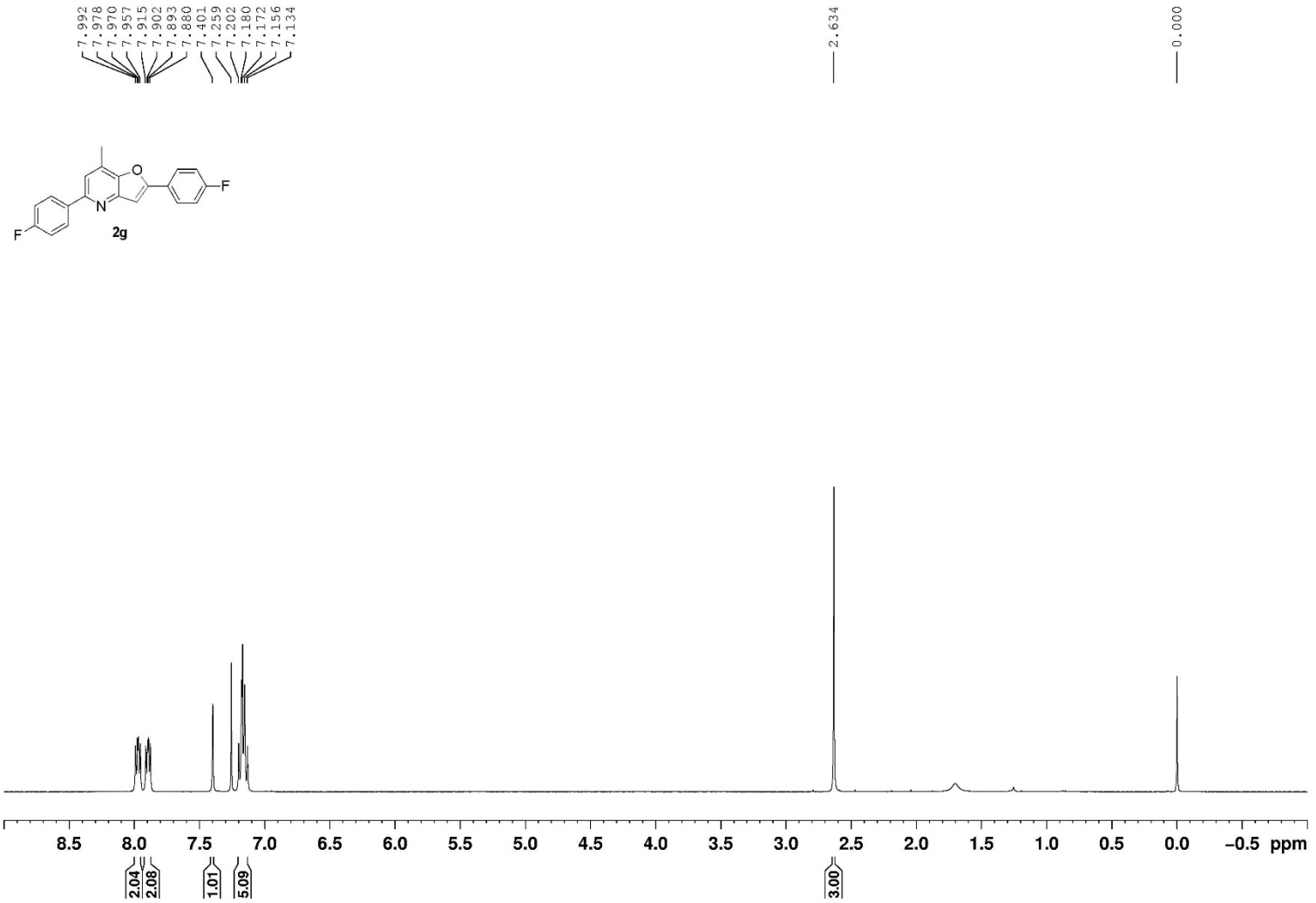
20
10
0
ppm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7.970
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7.902
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7.880
7.401
7.259
7.202
7.180
7.172
7.156
7.134
2.634
0.000
O
N
F
F
2g
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
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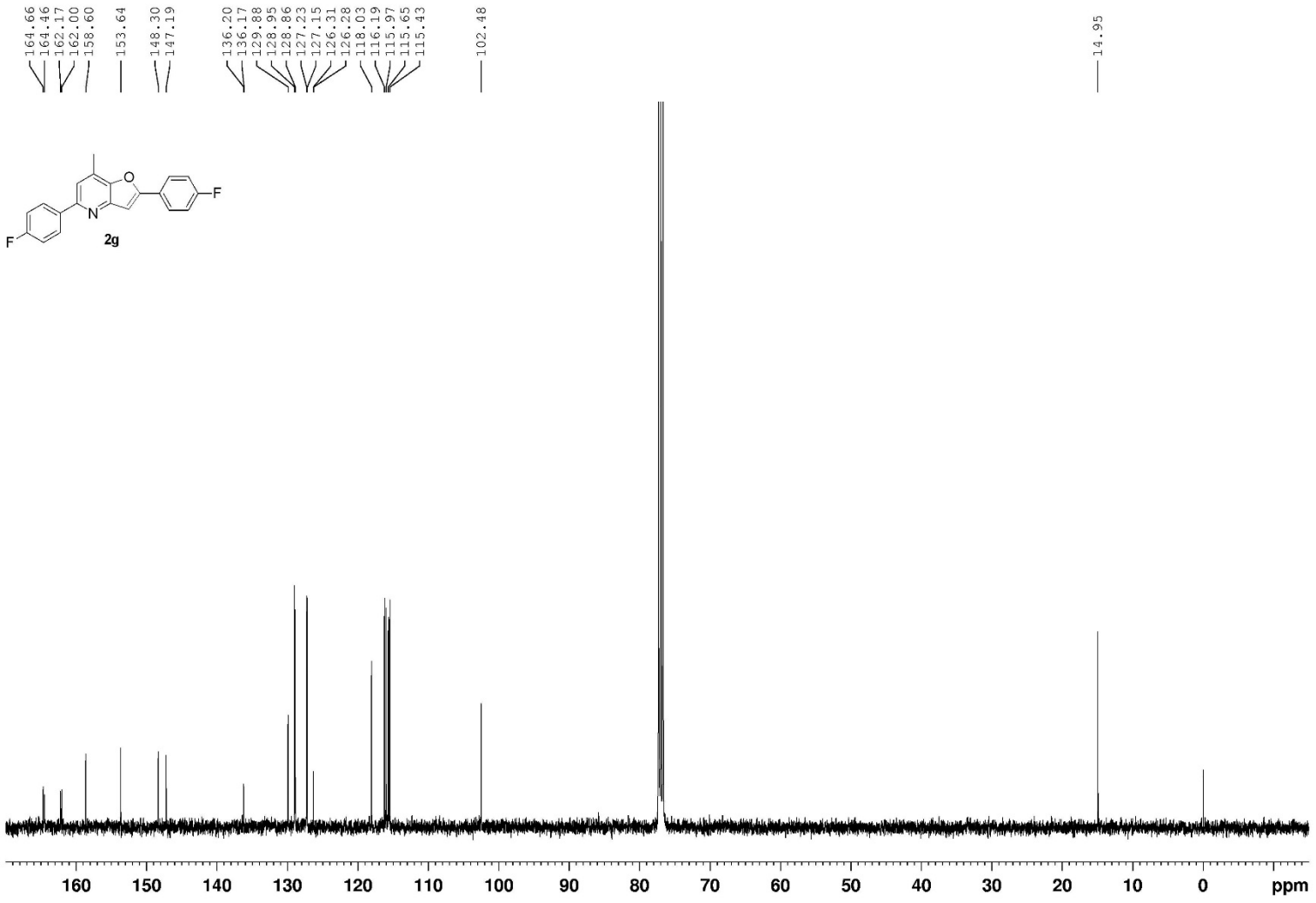
2.04
2.08
1.01
5.09
3.00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162.17
162.00
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153.64
148.30
147.19
136.20
136.17
129.88
128.95
128.86
127.23
127.15
126.31
126.28
118.03
116.19
115.97
115.65
115.43
102.48
14.95
O
N
F
F
2g
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150
140
130
120
110
100
90
80
70
60
50
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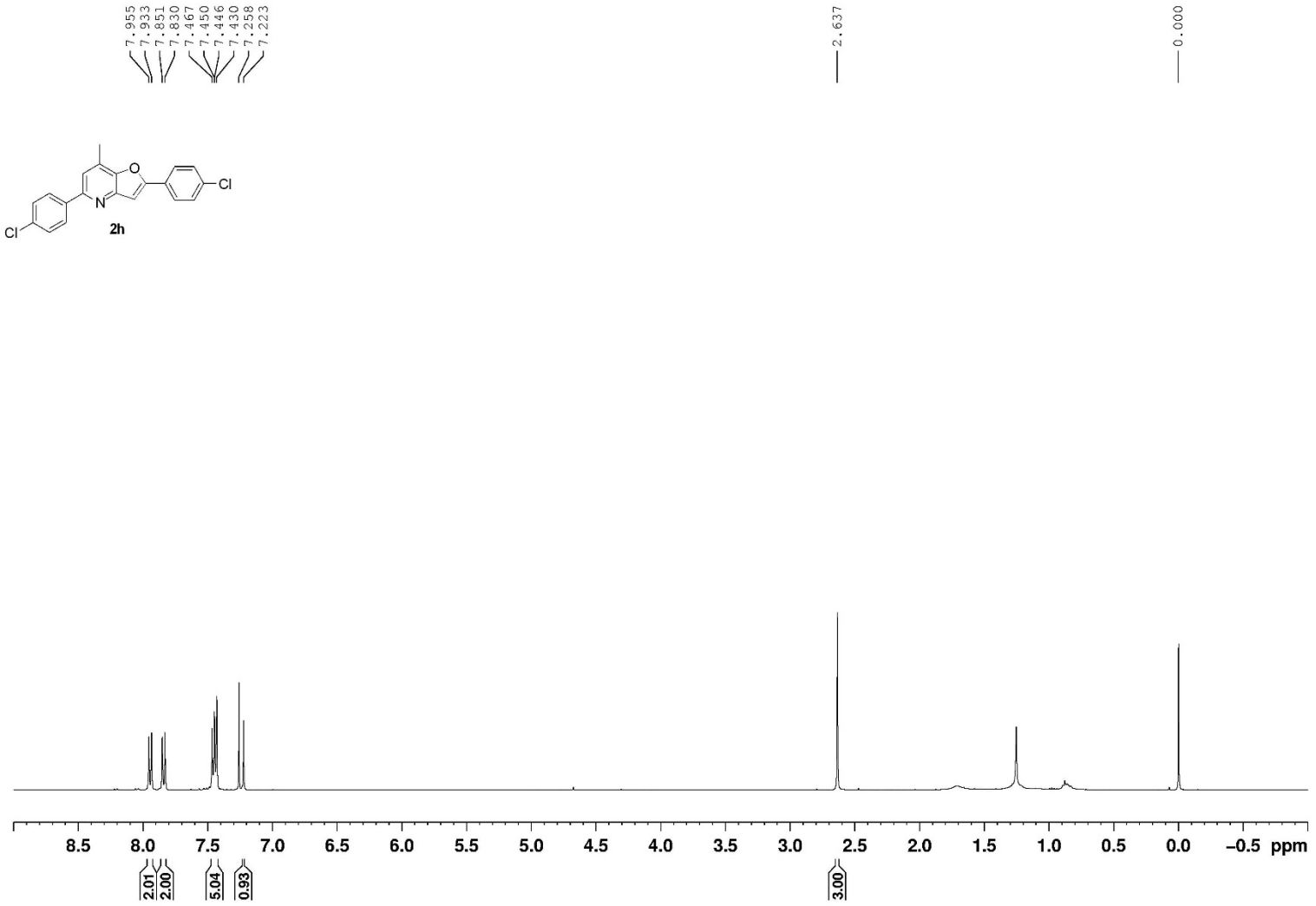
30
20
10
0
ppm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7.830
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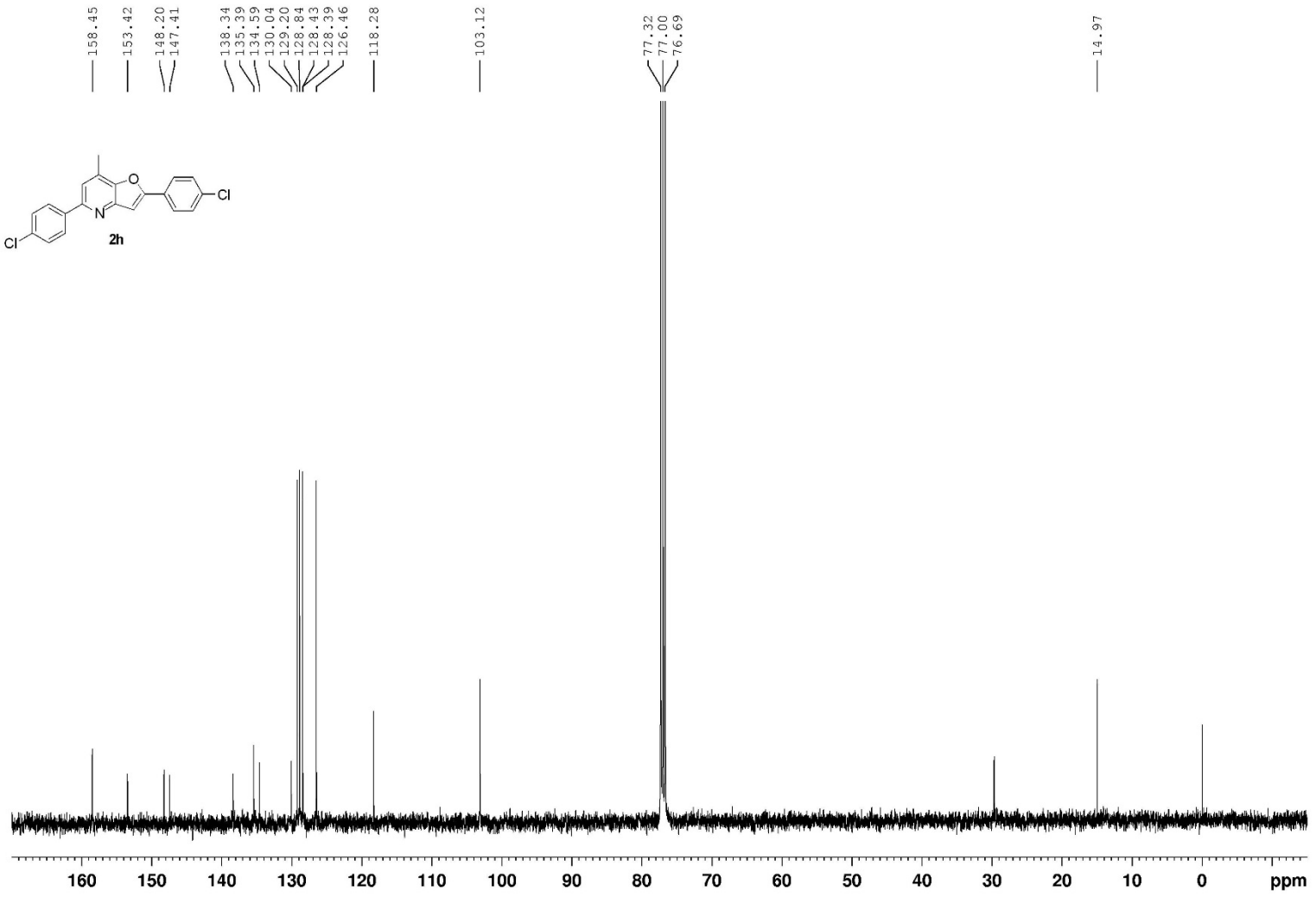
7.450
7.446
7.430
7.258
7.223
2.637
0.000
O
N
Cl
Cl
2h
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5 ppm
2.01
2.00
5.04
0.93
3.00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147.41
138.34
135.39
134.59
130.04
129.20
128.84
128.43
128.39
126.46
118.28
103.12
77.32
77.00
76.69
14.97
O
N
Cl
Cl
2h
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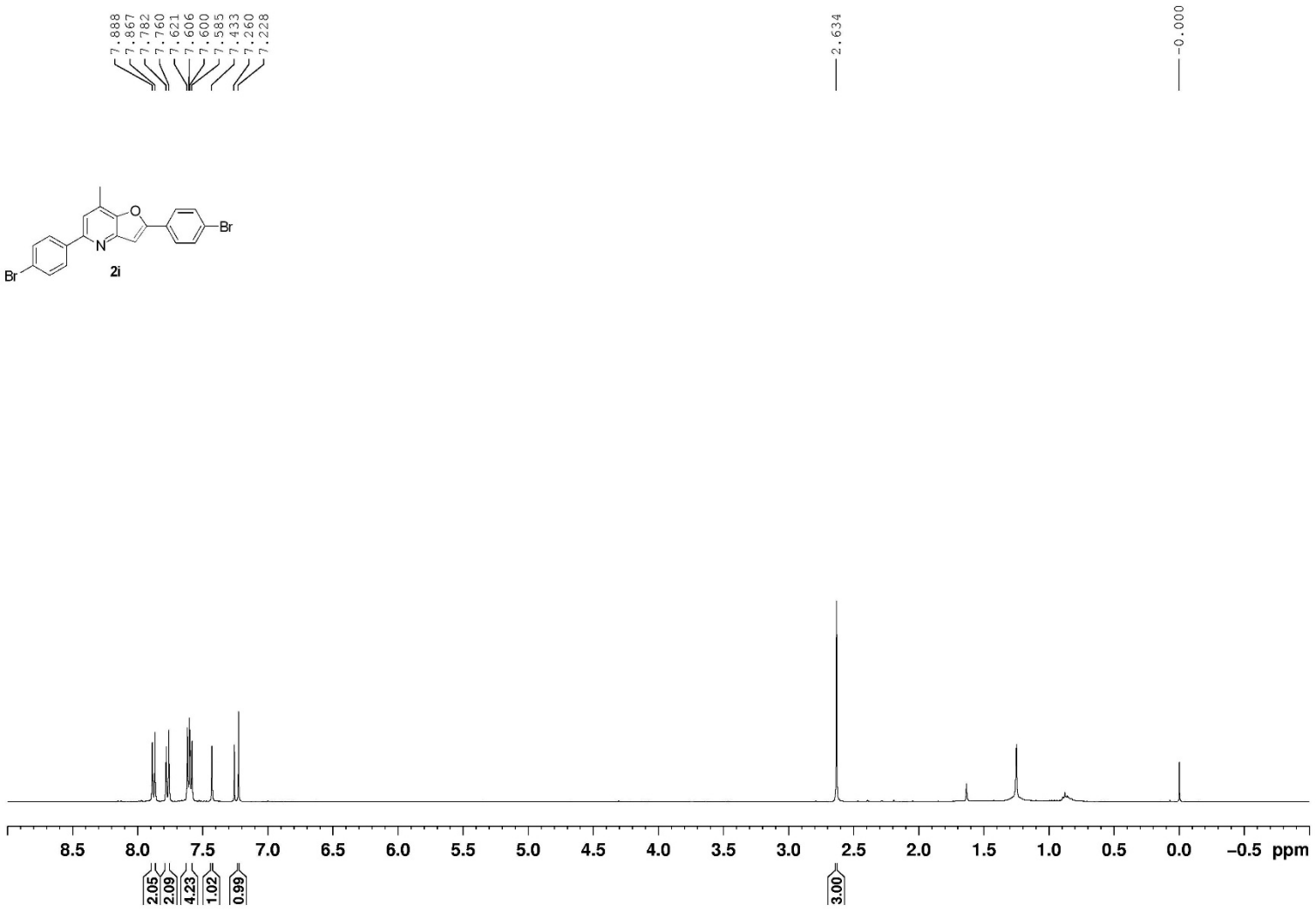
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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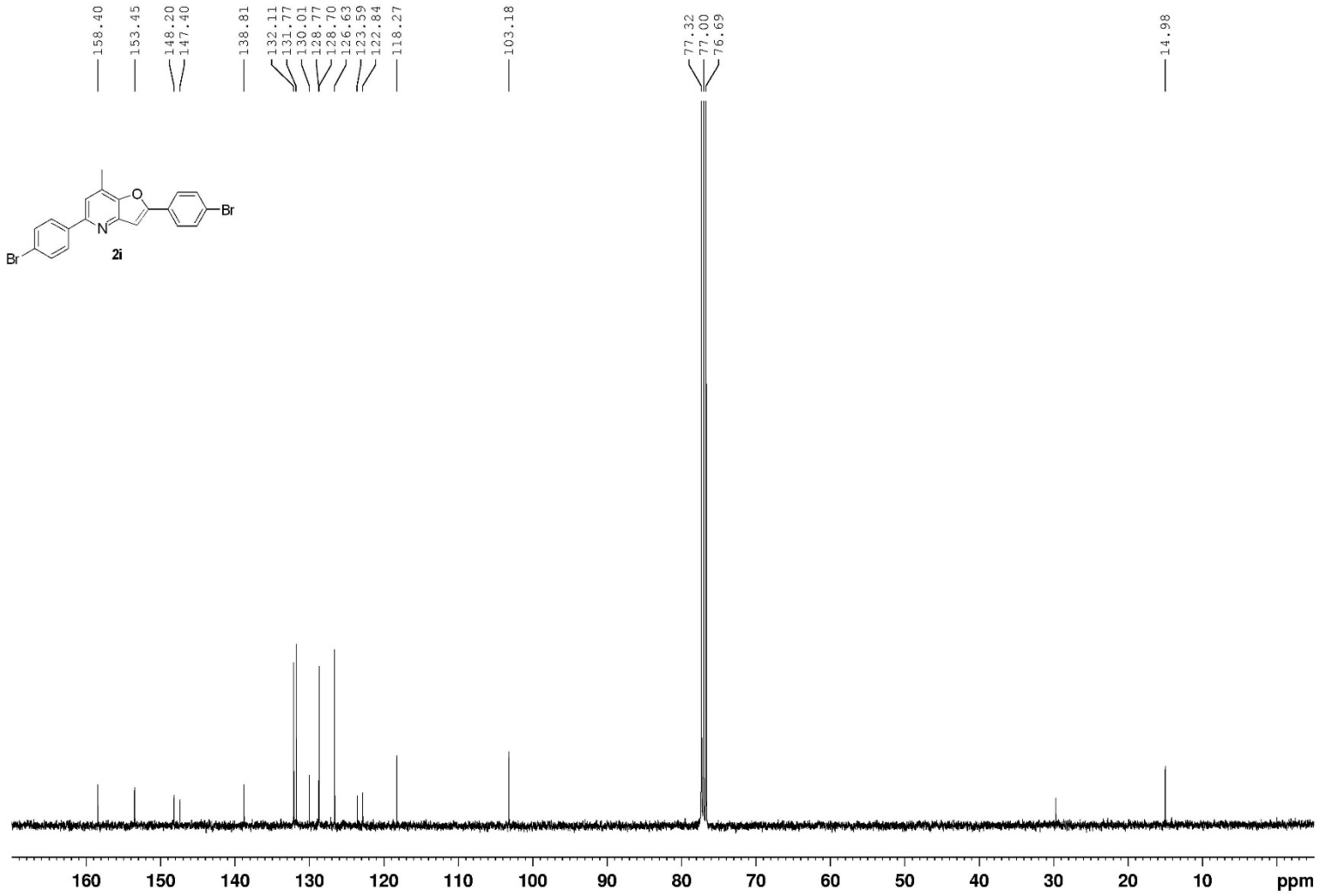
7.867
7.782
7.760
7.621
7.606
7.600
7.585
7.433
7.260
7.228
2.634
-0.000
Br
Br
O
N
2i
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5 ppm
2.05
2.09
4.23
1.02
0.99
3.00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153.45
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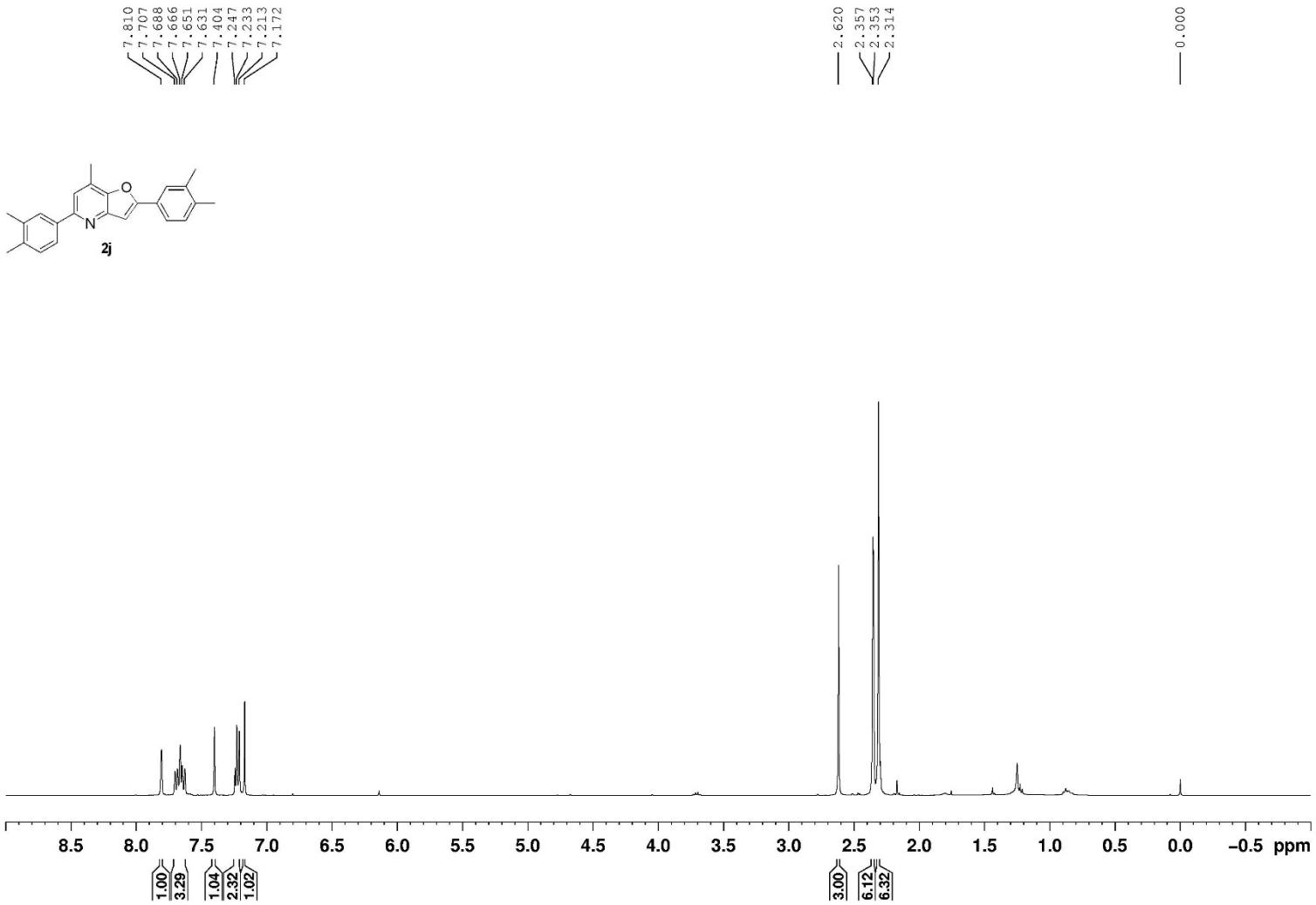
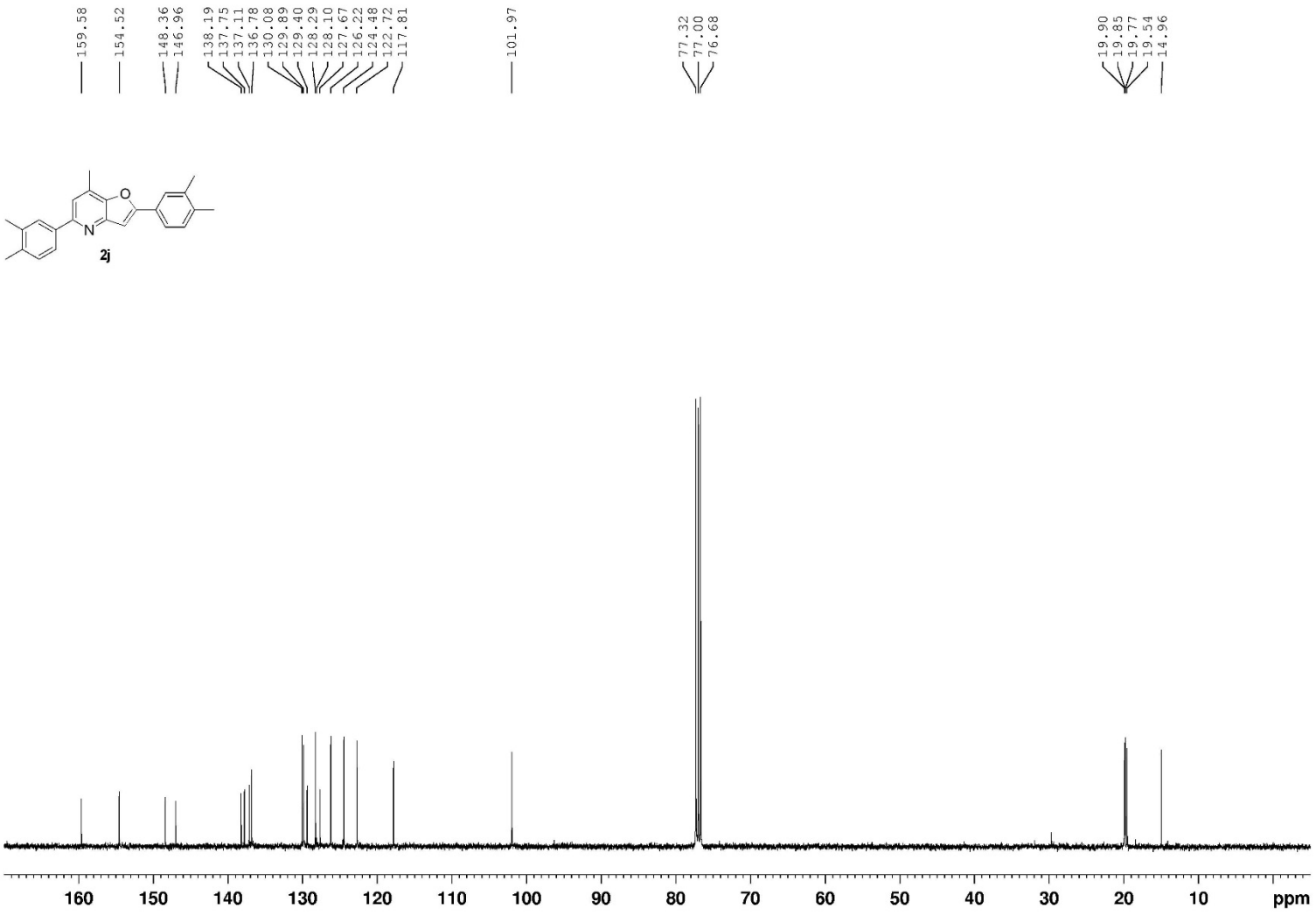
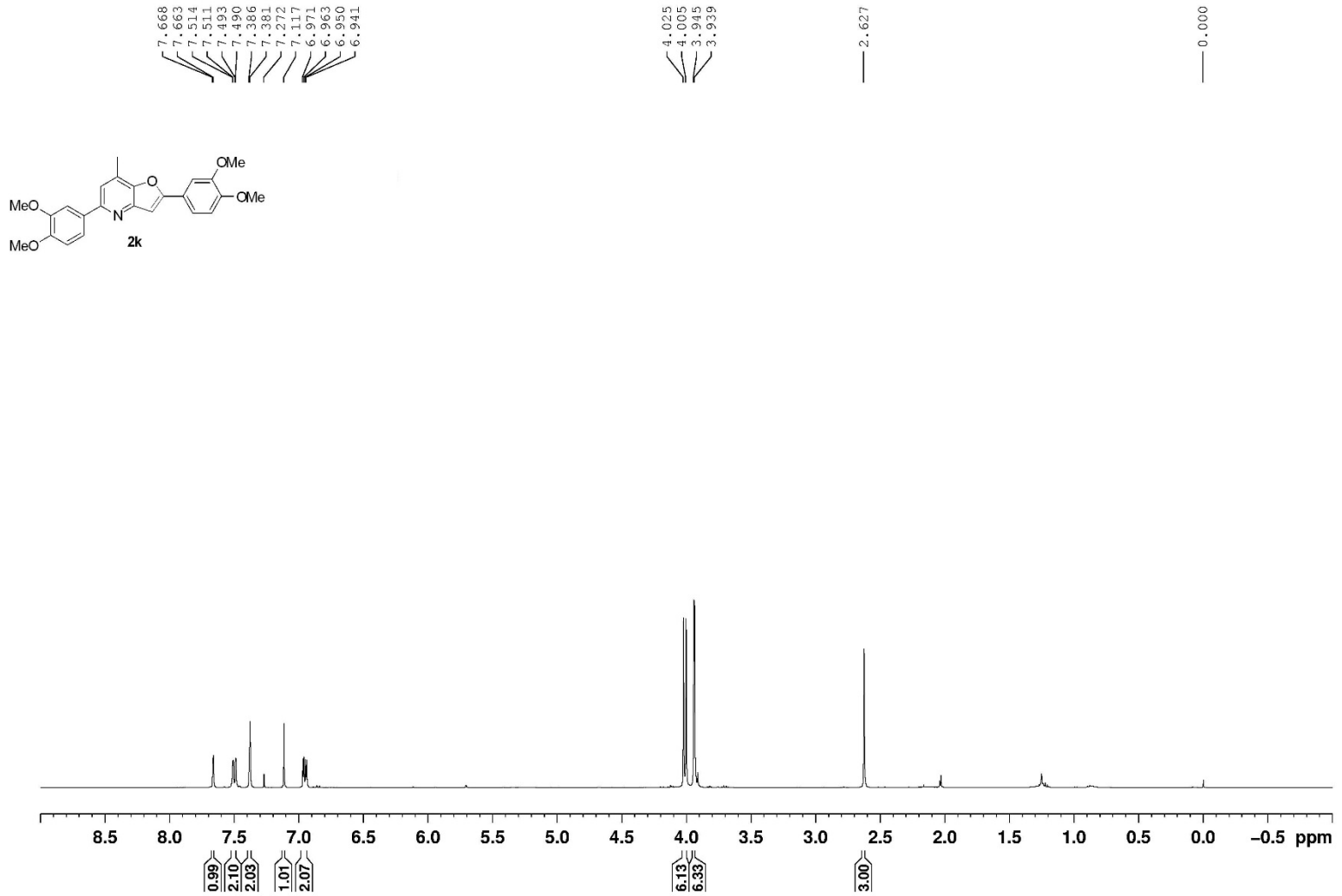
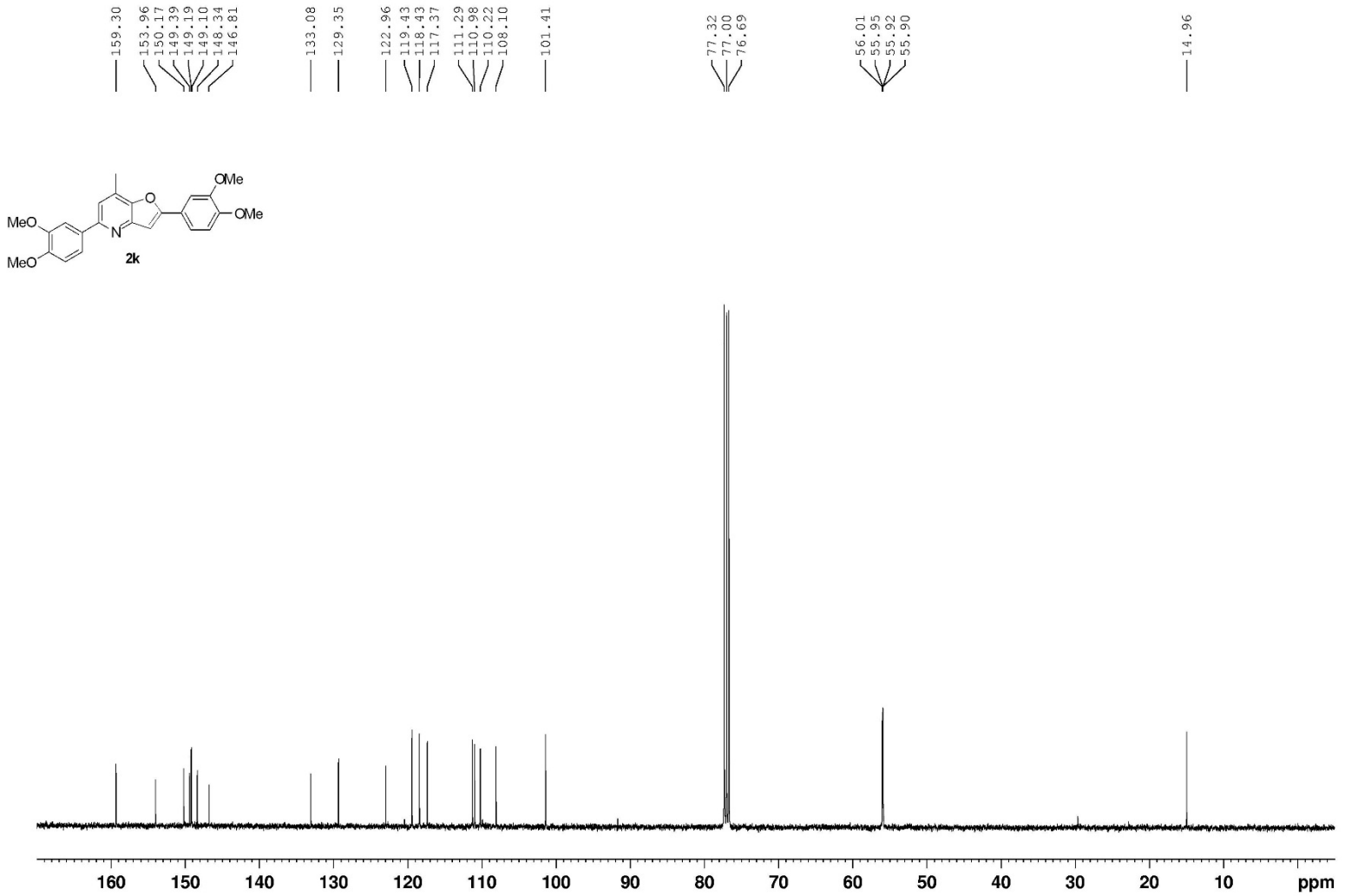
147.40
138.81
132.11
131.77
130.01
128.77
128.70
126.63
123.59
122.84
118.27
103.18
77.32
77.00
76.69
14.98
Br
Br
O
N
2i
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.810
7.707
7.688
7.666
7.651
7.631
7.404
7.247
7.233
7.213
7.172
2.620
2.357
2.353
2.314
0.000
O
N
2j
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
0.0
−0.5 ppm
1.00
3.29
1.04
2.32
1.02
3.00
6.12
6.32


159.58
154.52
148.36
146.96
138.19
137.75
137.11
136.78
130.08
129.89
129.40
128.29
128.10
127.67
126.22
124.48
122.72
117.81
101.97
77.32
77.00
76.68
19.90
19.85
19.77
19.54
14.96
O
N
2j
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.668
7.663
7.514
7.511
7.493
7.490
7.386
7.381
7.272
7.117
6.971
6.963
6.950
6.941
4.025
4.005
3.945
3.939
2.627
0.000
OMe
OMe
MeO
MeO
N
O
2k
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
0.0
−0.5 ppm
0.99
2.10
2.03
1.01
2.07
6.13
6.33
3.00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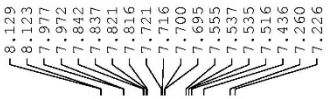
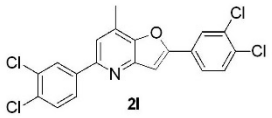
153.96
150.17
149.39
149.19
149.10
148.34
146.81
133.08
129.35
122.96
119.43
118.43
117.37
111.29
110.98
110.22
108.10
101.41
77.32
77.00
76.69
56.01
55.95
55.92
55.90
14.96
OMe
OMe
MeO
MeO
N
O
2k
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

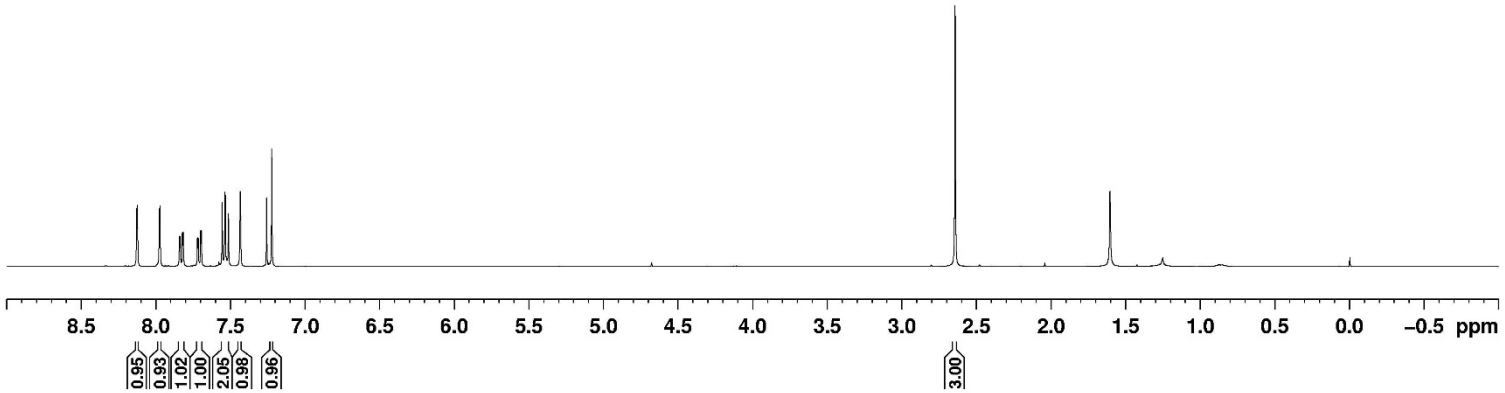

8.129
8.123
7.977
7.972
7.842
7.837
7.821
7.816
7.721
7.716
7.700
7.695
7.555
7.537
7.535
7.516
7.436
7.260
7.226


Cl
Cl
O
N
Cl
Cl

2l

2.645

0.000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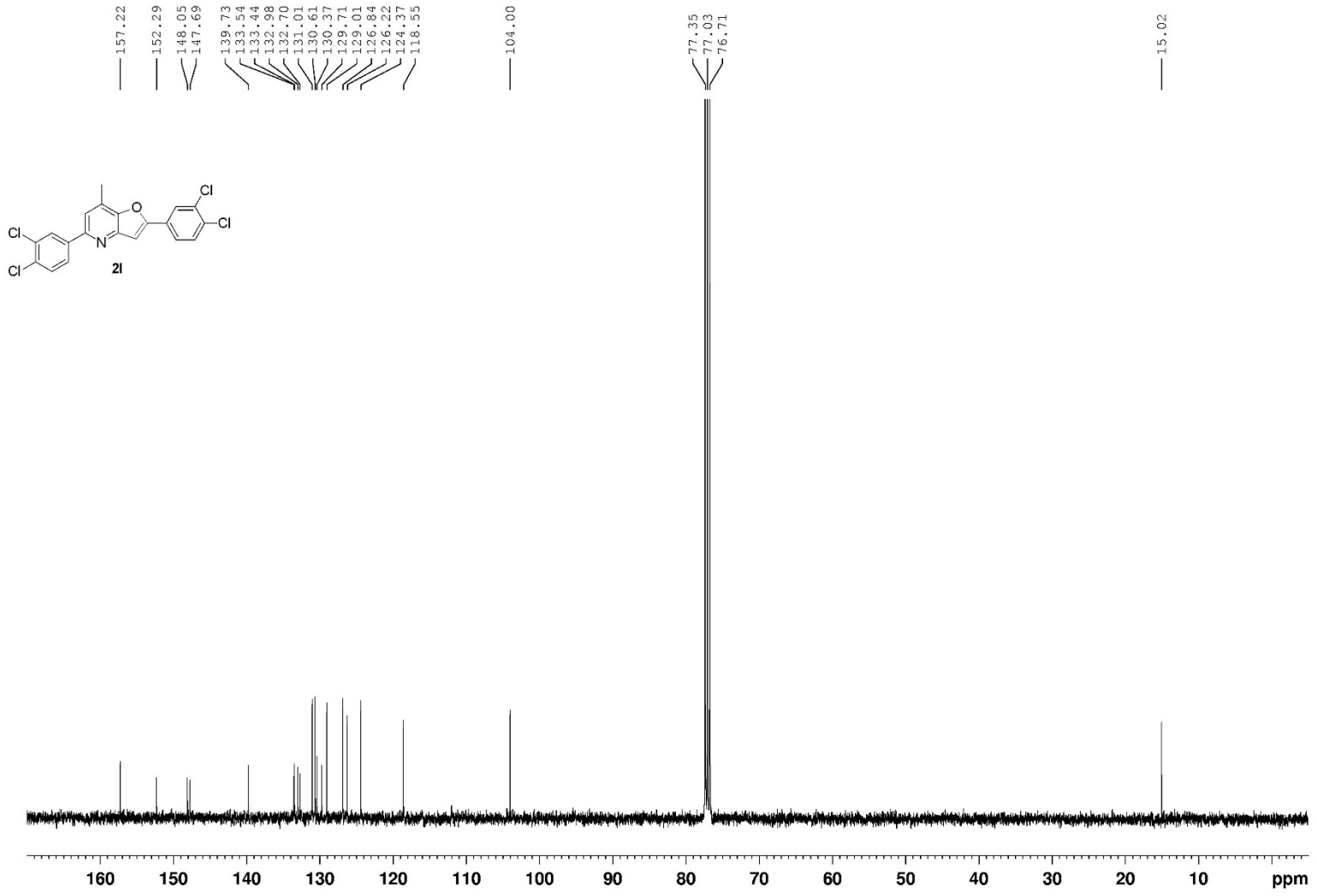
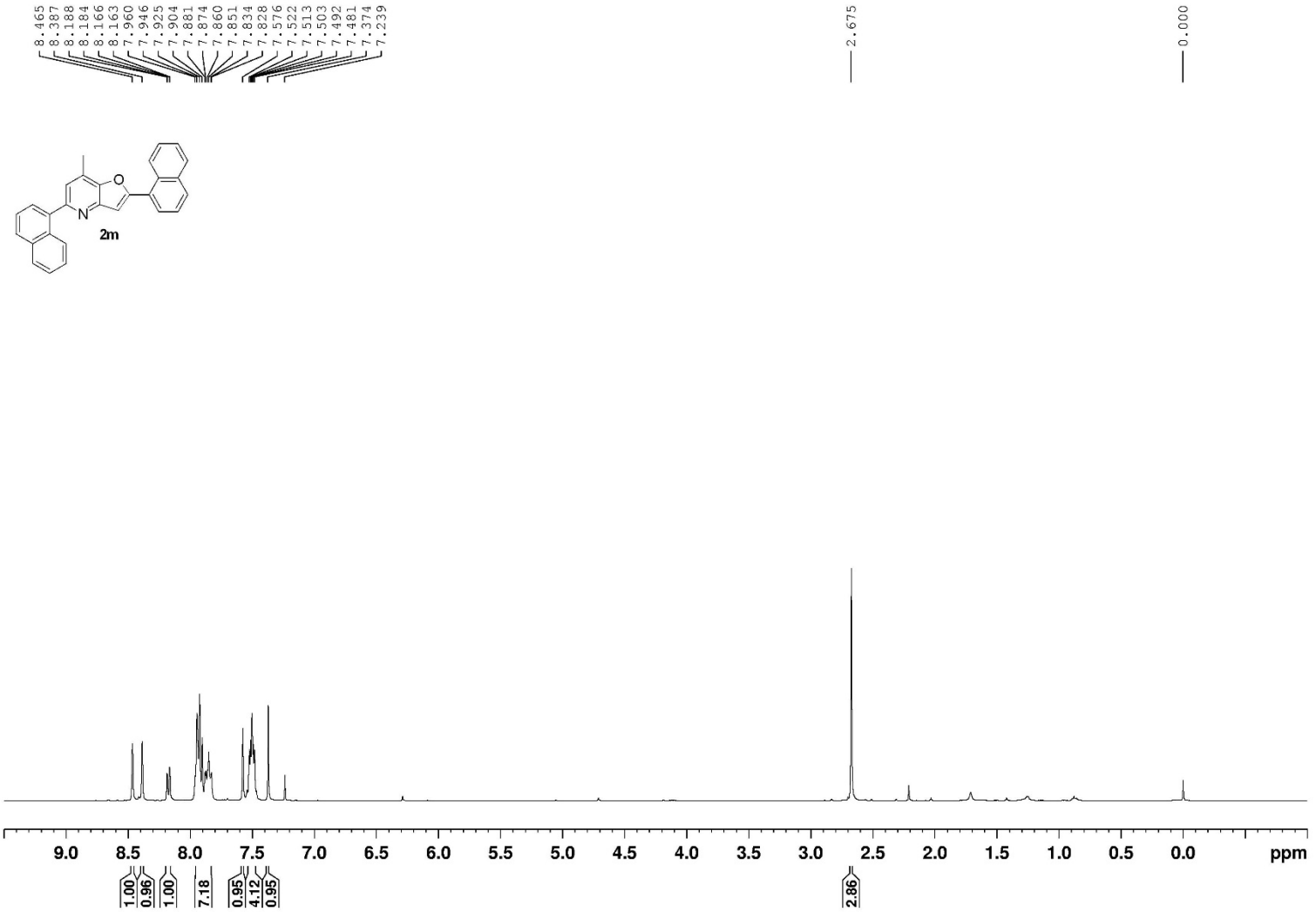
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5 ppm
0.95
0.93
1.02
1.00
2.05
0.98
0.96
3.00


157.22
152.29
148.05
147.69
139.73
133.54
133.44
132.98
132.70
131.01
130.61
130.37
129.71
129.01
126.84
126.22
124.37
118.55
104.00
77.35
77.03
76.71
15.02
Cl
Cl
Cl
Cl
O
N
2l
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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8.387
8.188
8.184
8.166
8.163
7.960
7.946
7.925
7.904
7.881
7.874
7.860
7.851
7.834
7.828
7.576
7.522
7.513
7.503
7.492
7.481
7.374
7.239
2.675
0.000
2m
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
0.0
ppm
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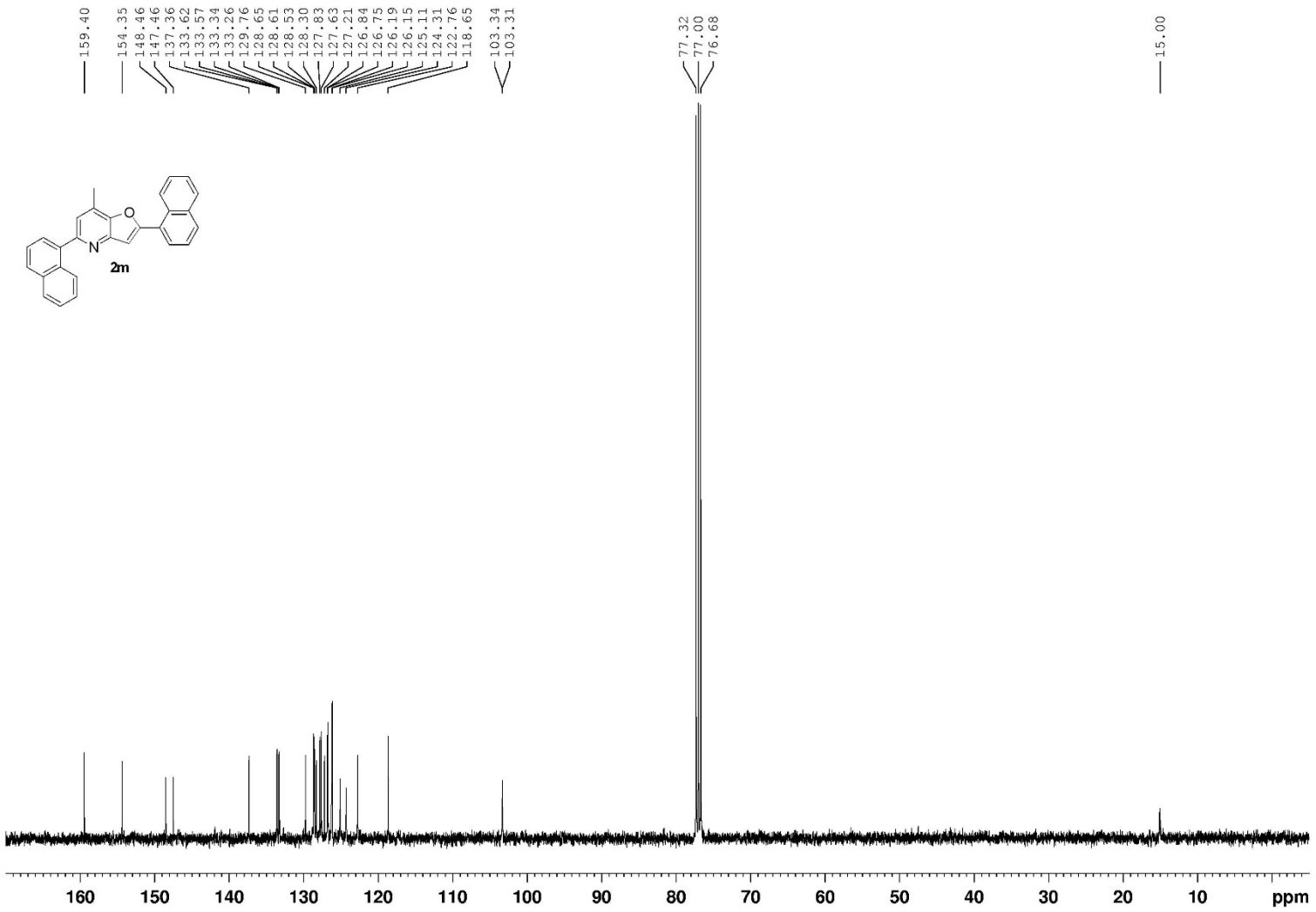
0.96
1.00
7.18
0.95
4.12
0.95
2.86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154.35
148.46
147.46
137.36
133.62
133.57
133.34
133.26
129.76
128.65
128.61
128.53
128.30
127.83
127.63
127.21
126.84
126.75
126.19
126.15
125.11
124.31
122.76
118.65
103.34
103.31
77.32
77.00
76.68
15.00
O
N
2m
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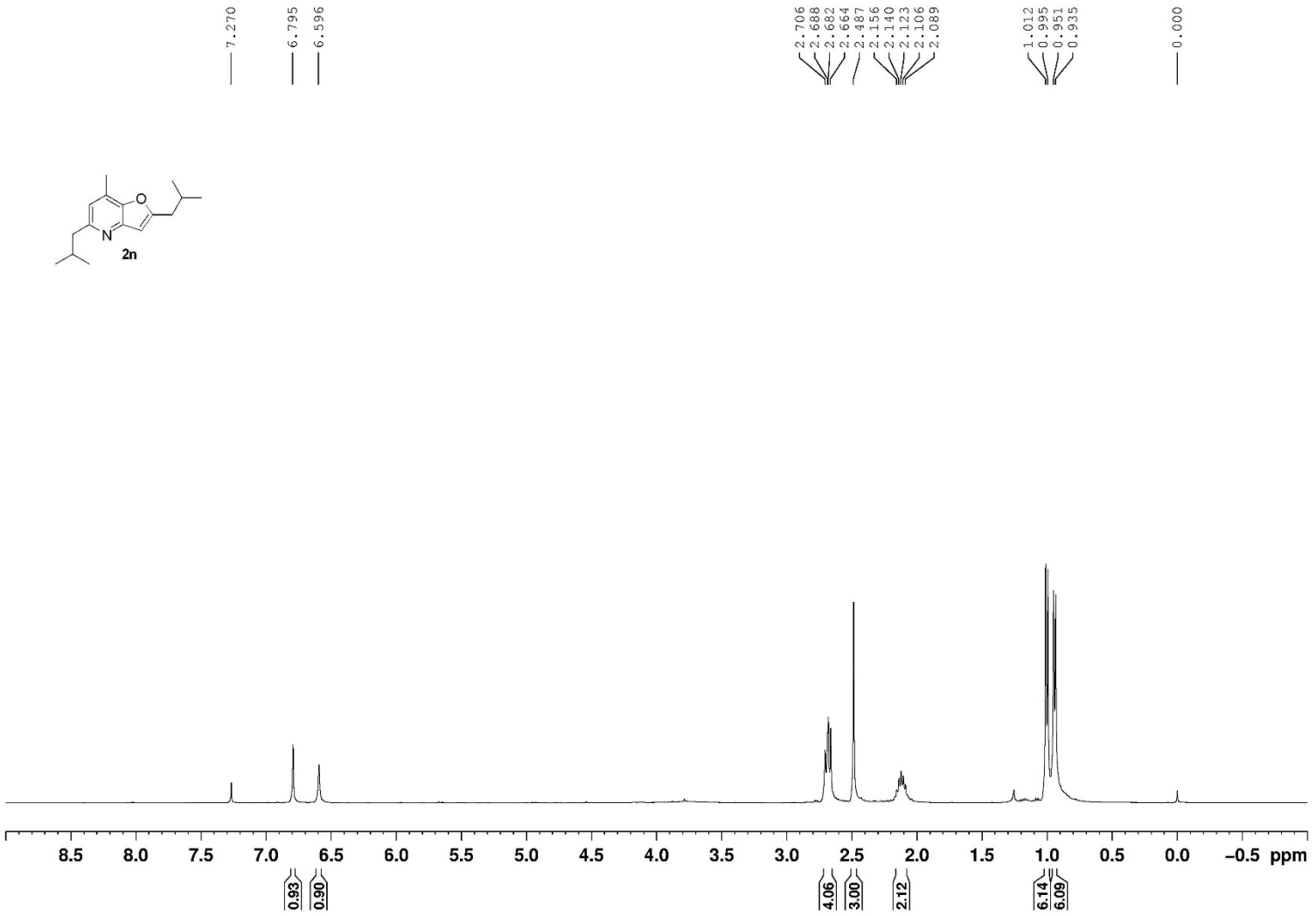
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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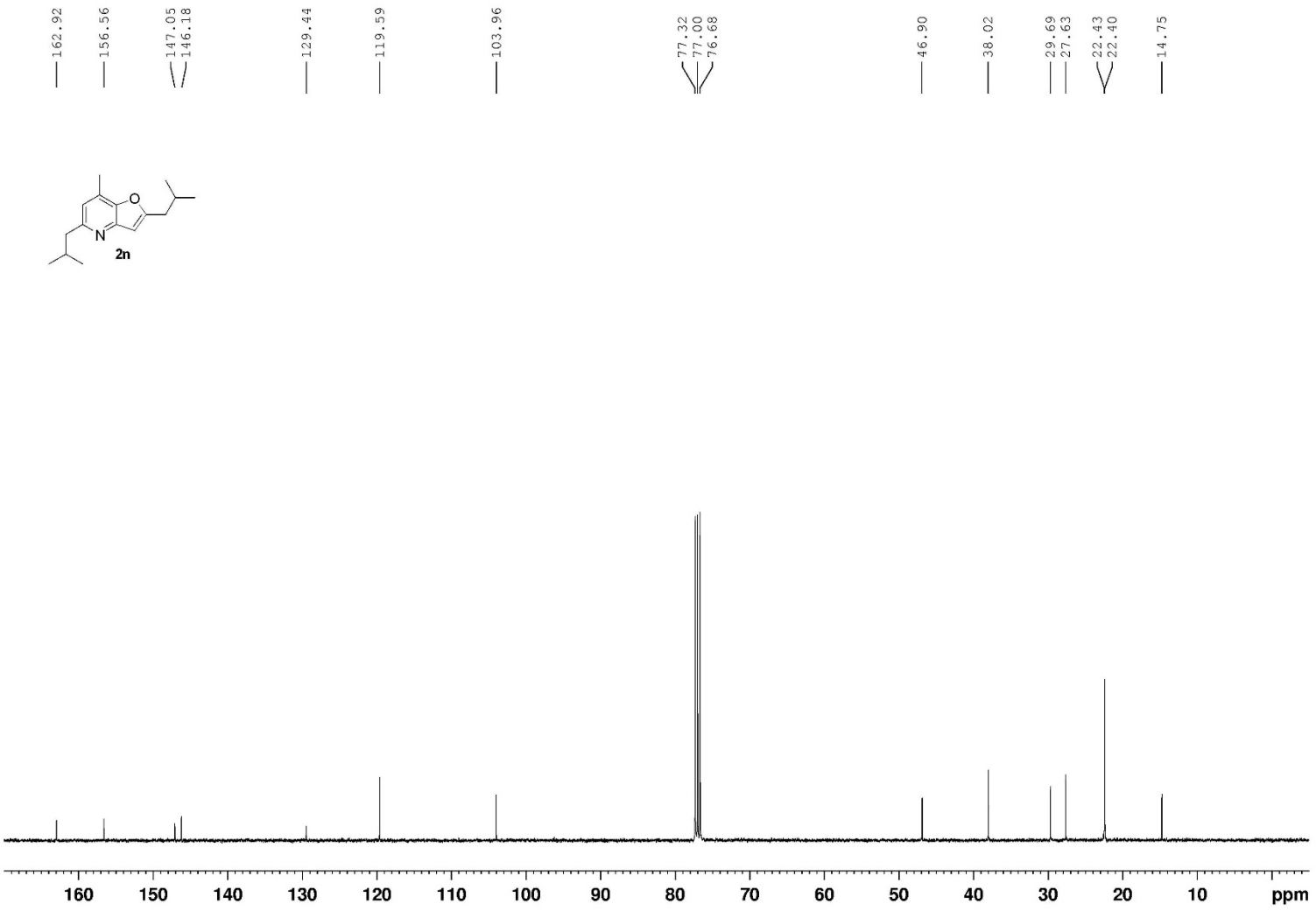
6.596
2.706
2.688
2.682
2.664
2.487
2.156
2.140
2.123
2.106
2.089
1.012
0.995
0.951
0.935
0.000
2n
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5 ppm
0.93
0.90
4.06
3.00
2.12
6.14
6.09


162.92
156.56
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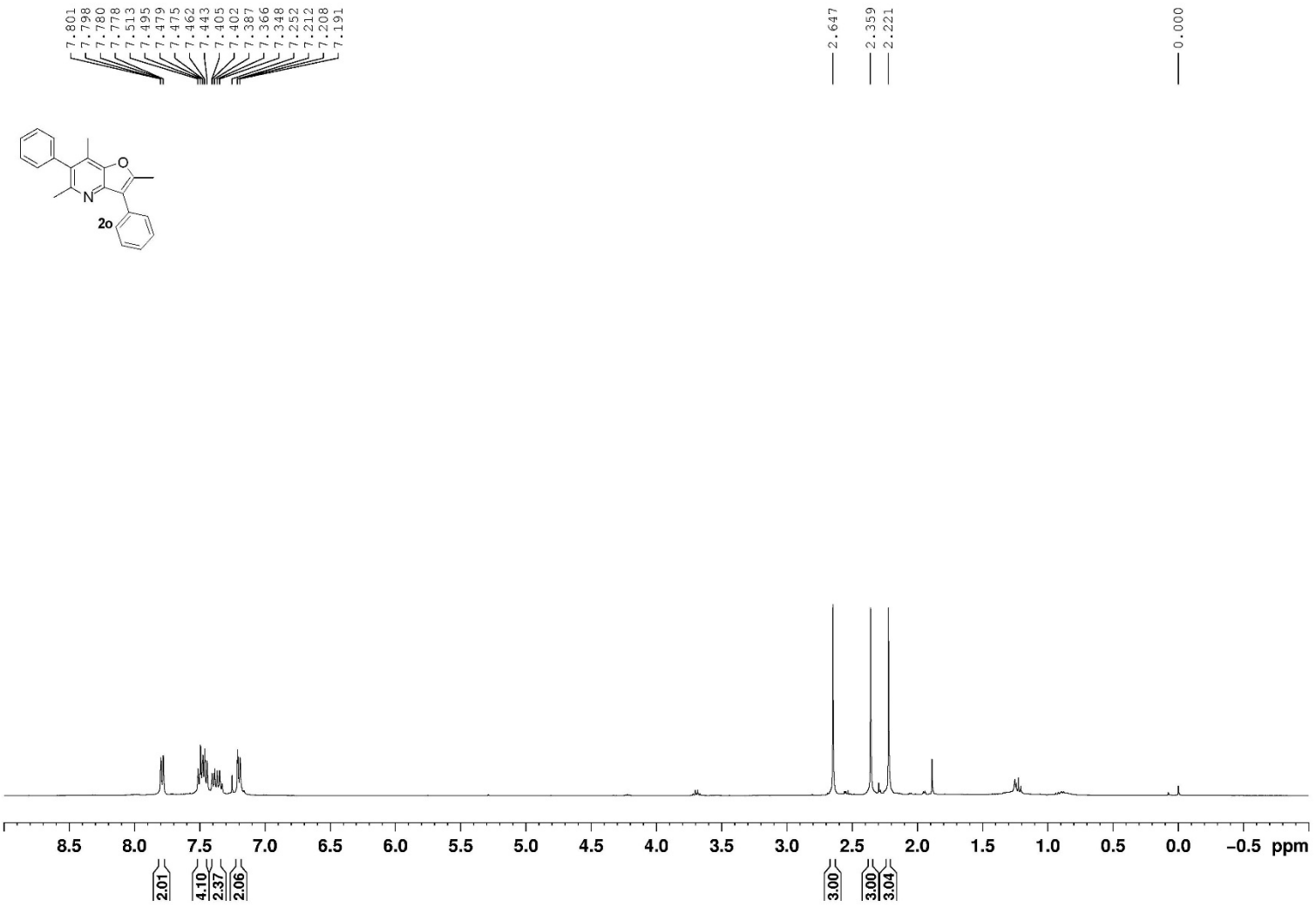
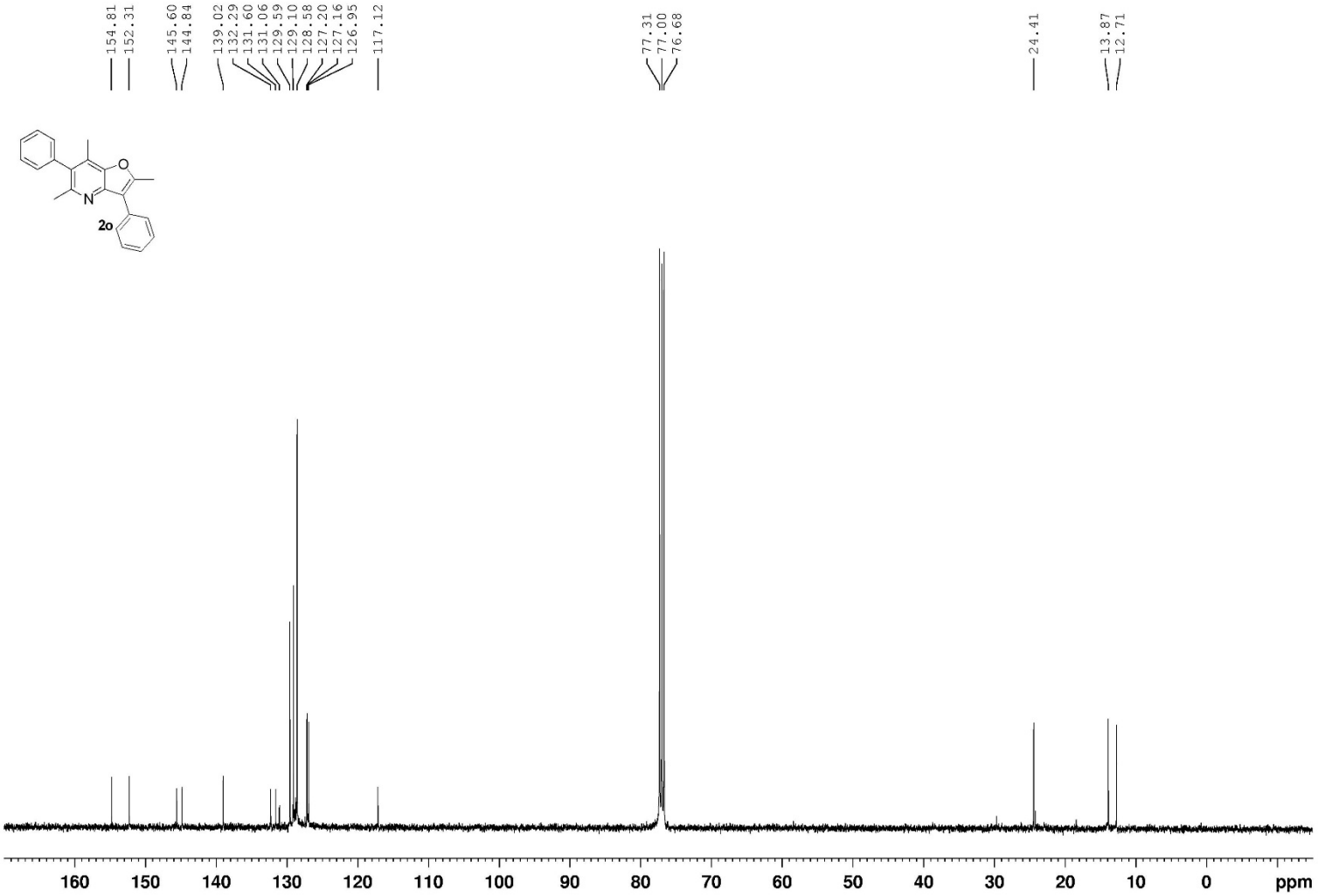
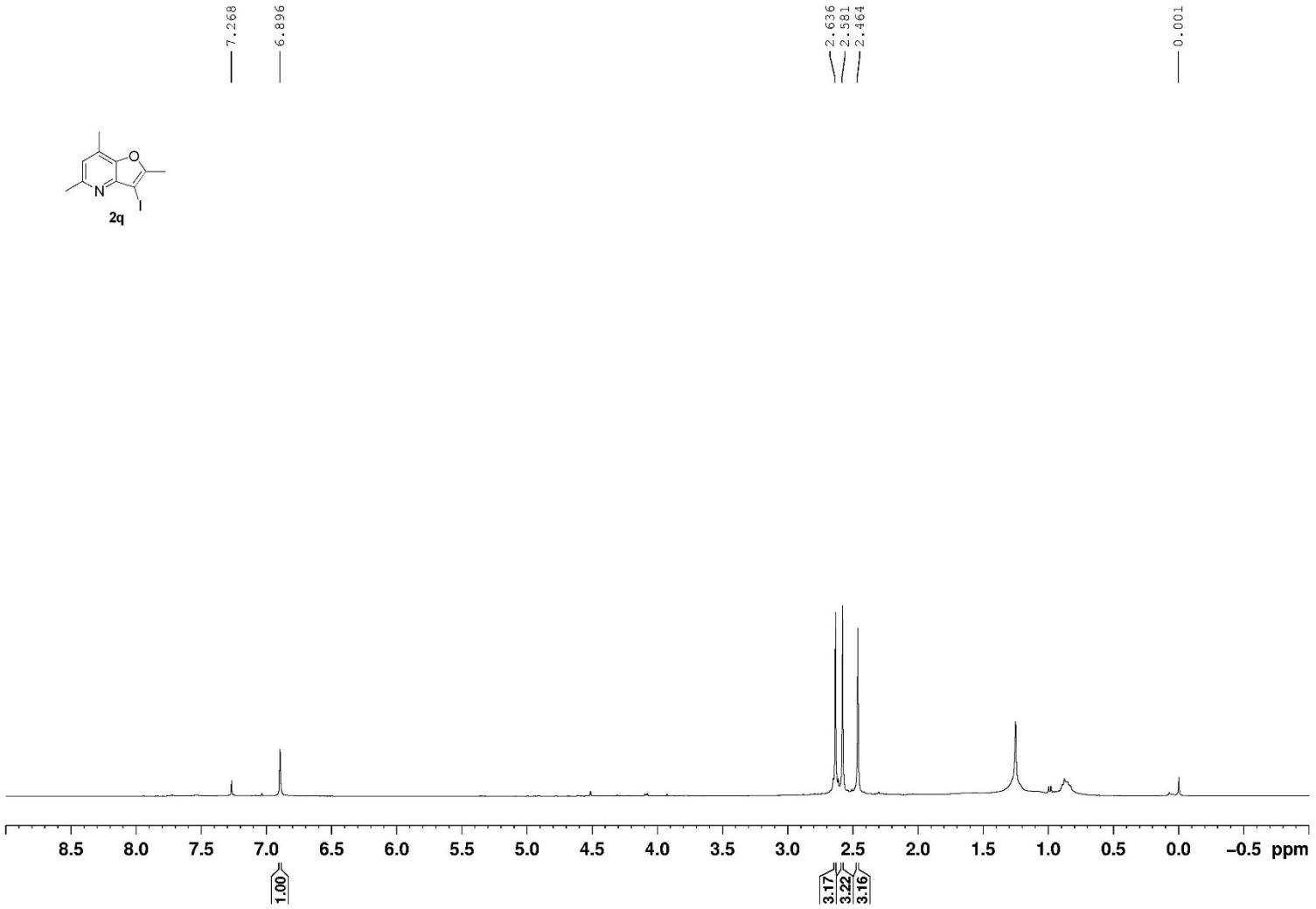
146.18
129.44
119.59
103.96
77.32
77.00
76.68
46.90
38.02
29.69
27.63
22.43
22.40
14.75
O
N
2n
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.801
7.798
7.780
7.778
7.513
7.495
7.479
7.475
7.462
7.443
7.405
7.402
7.387
7.366
7.348
7.252
7.212
7.208
7.191
2.647
2.359
2.221
0.000
O
N
2o
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
0.0
-0.5 ppm
2.01
4.10
2.37
2.06
3.00
3.00
3.04


154.81
152.31
145.60
144.84
139.02
132.29
131.60
131.06
129.59
129.10
128.58
127.20
127.16
126.95
117.12
77.31
77.00
76.68
24.41
13.87
12.71
O
N
2o
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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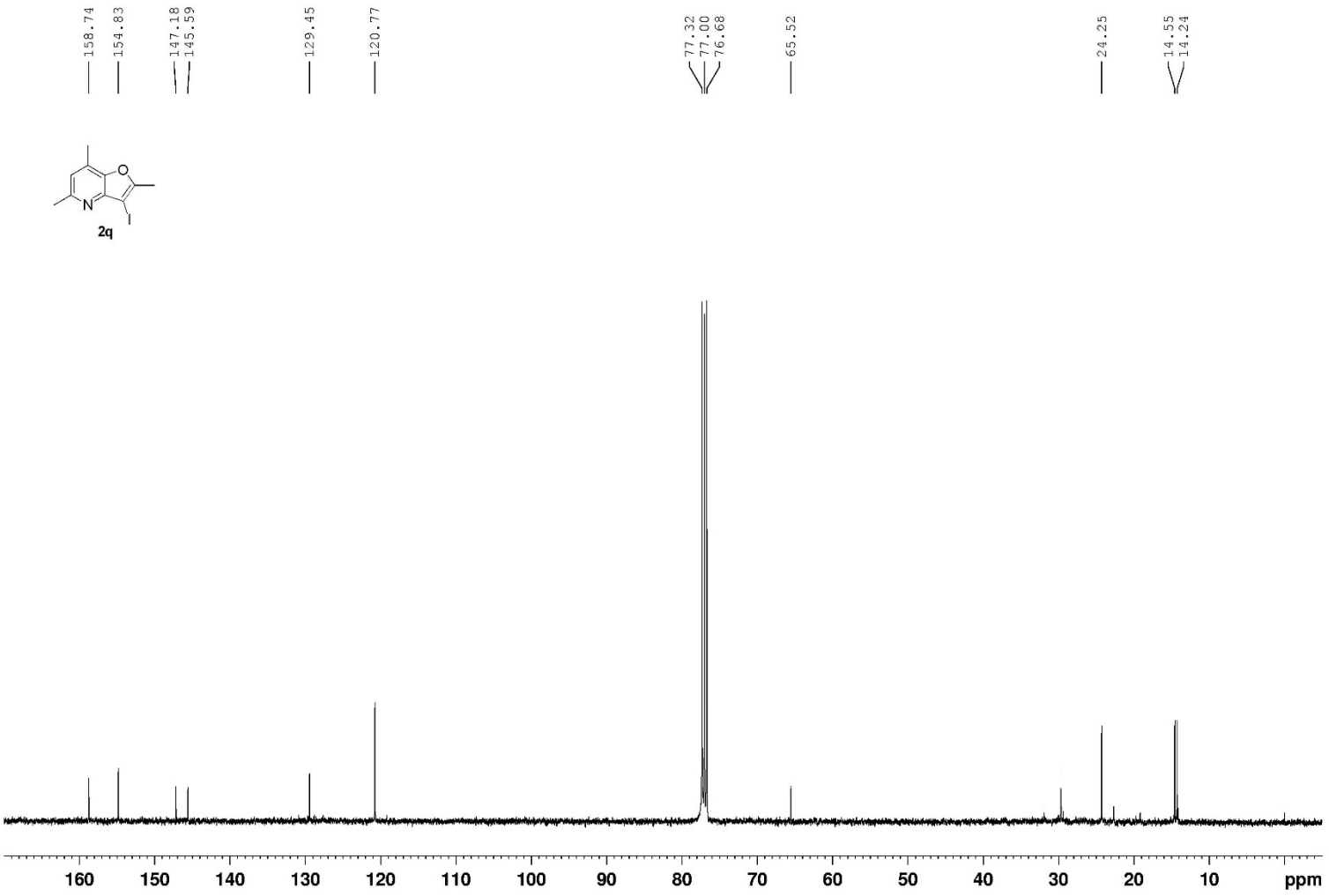
6.896
2.636
2.581
2.464
0.001
O
N
I
2q
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5 ppm
1.00
3.17
3.22
3.16


158.74
154.83
147.18
145.59
129.45
120.77
77.32
77.00
76.68
65.52
24.25
14.55
14.24
N
O
I
2q
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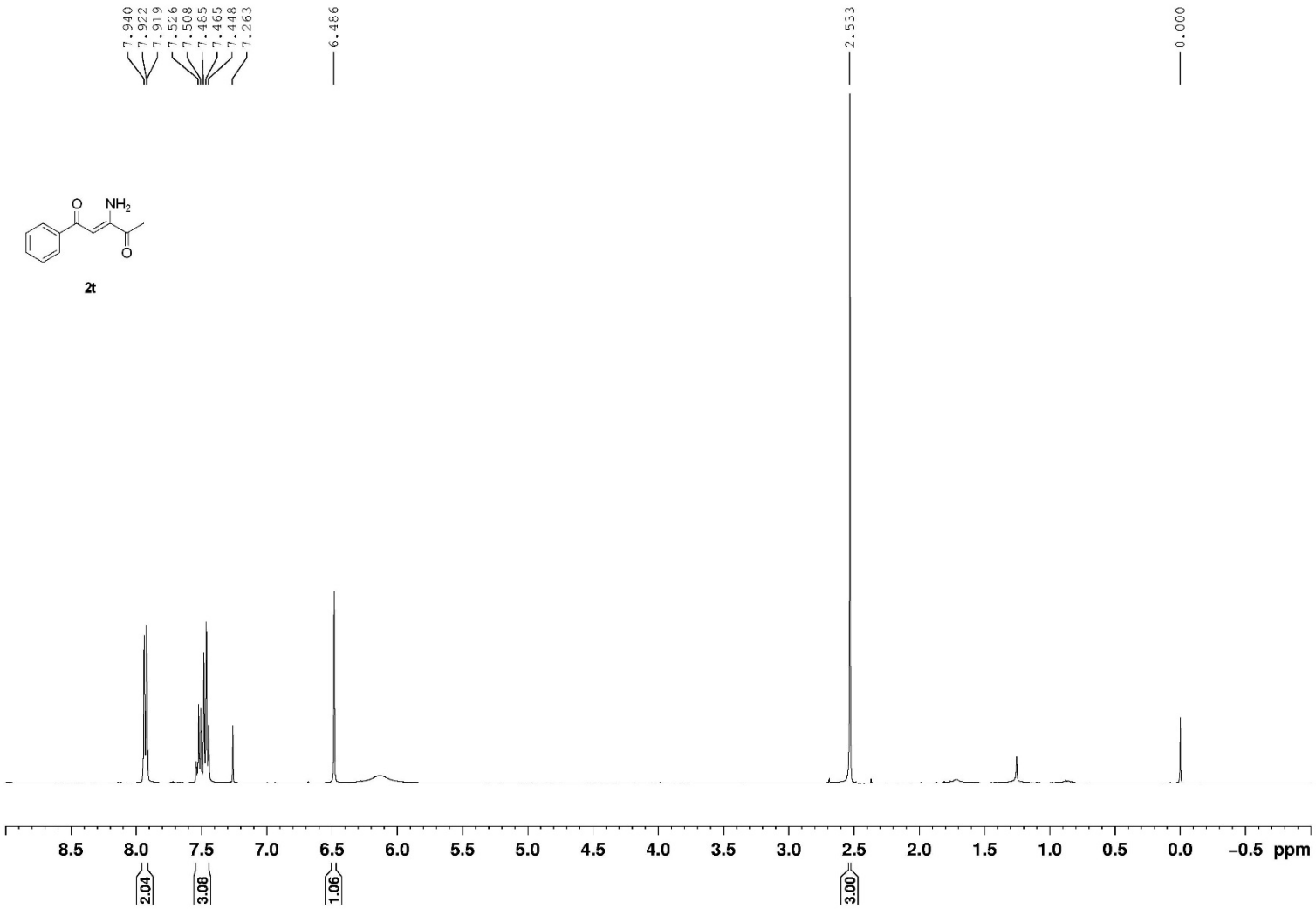
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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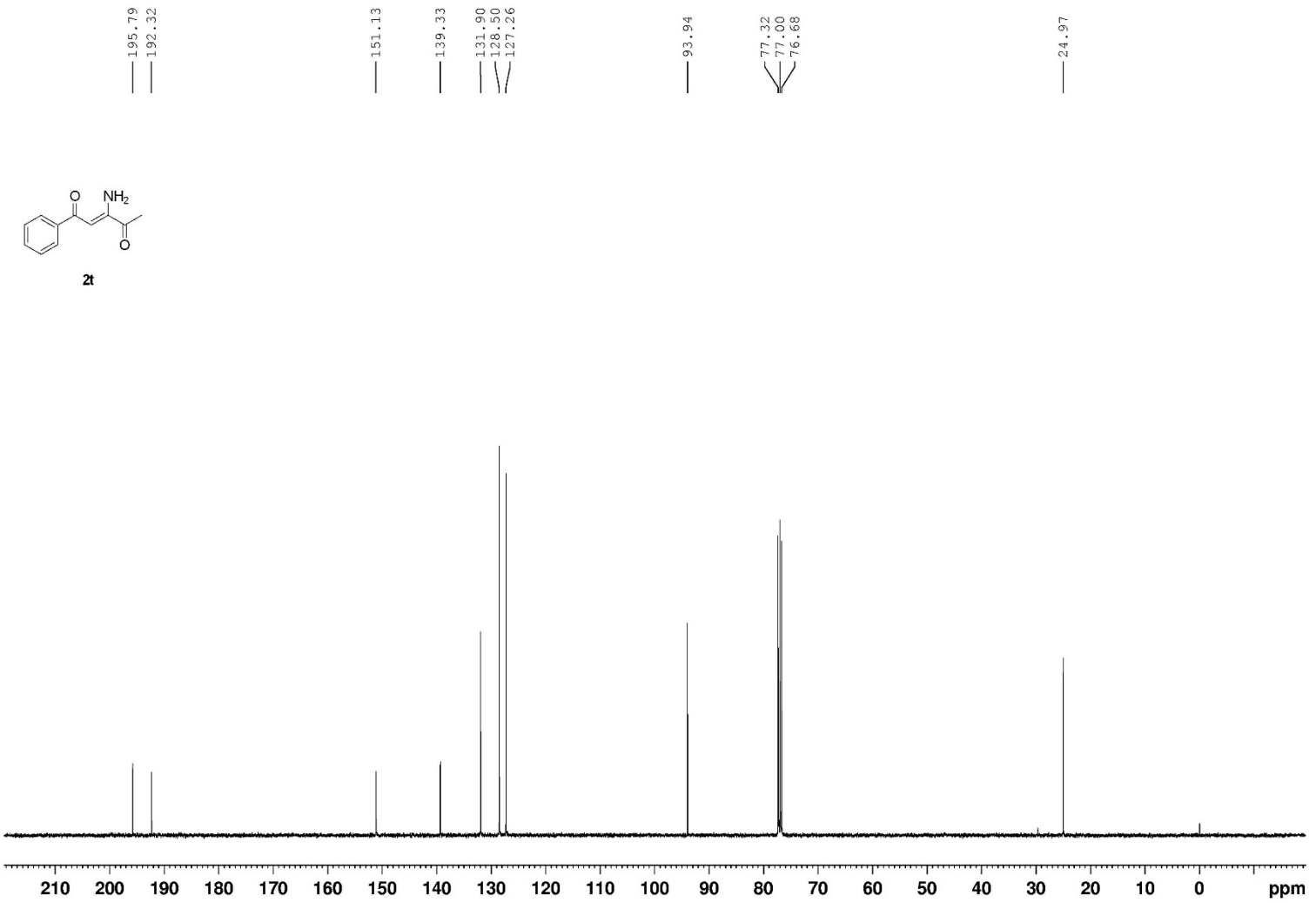
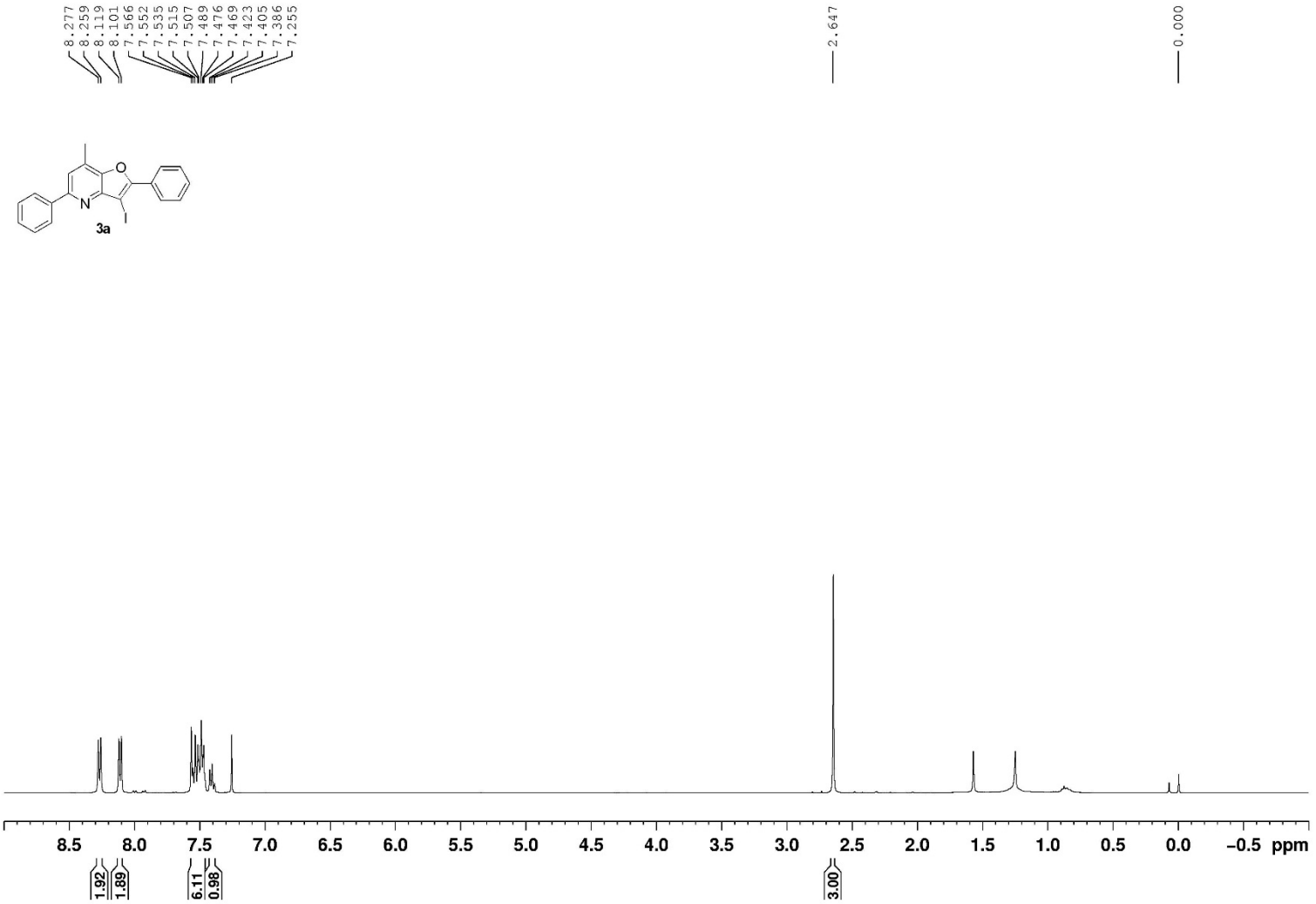
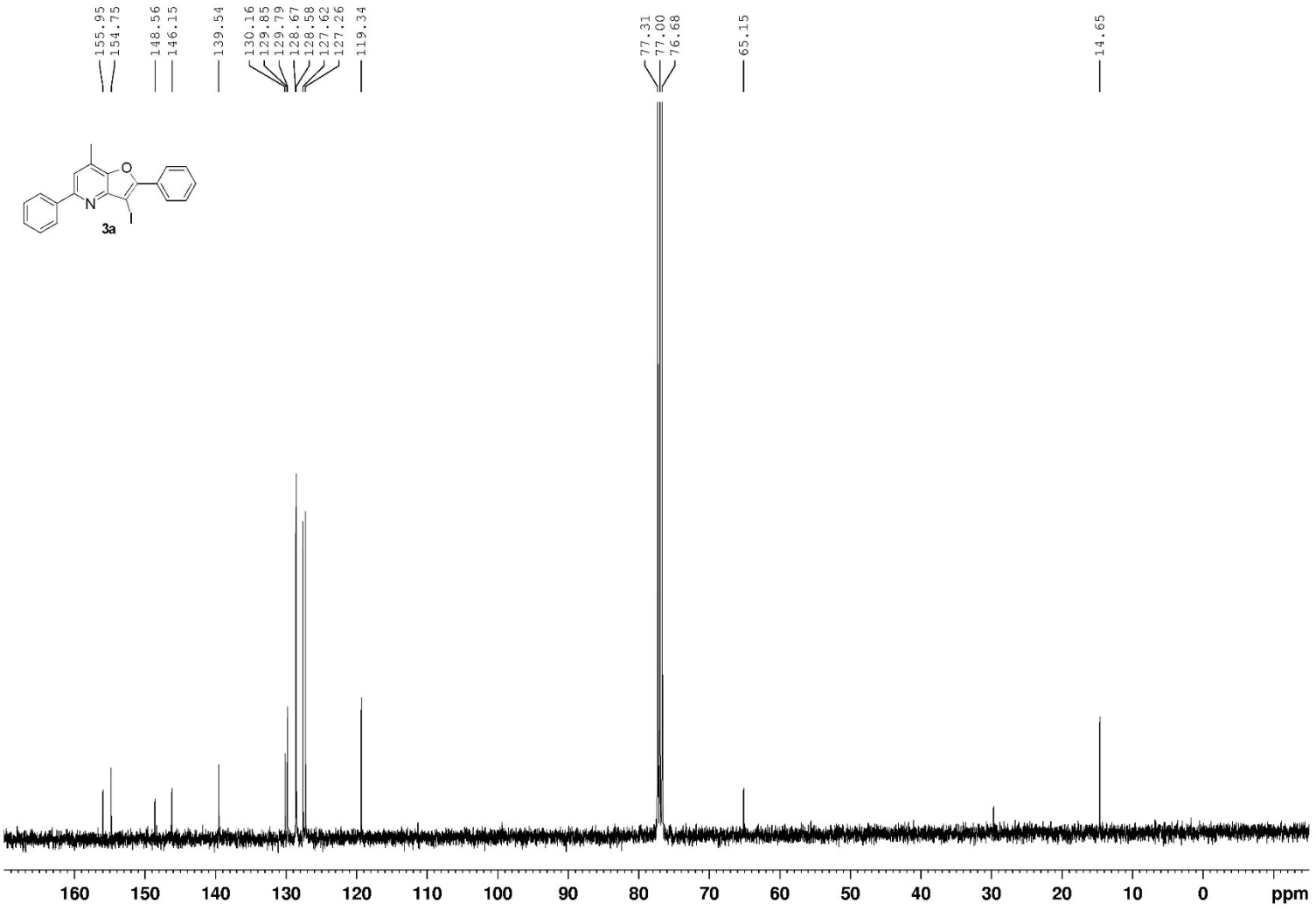
7.922
7.919
7.526
7.508
7.485
7.465
7.448
7.263
6.486
2.533
0.000
O
NH2
O
2t
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5 ppm
2.04
3.08
1.06
3.00


195.79
192.32
151.13
139.33
131.90
128.50
127.26
93.94
77.32
77.00
76.68
24.97
O
NH2
O
2t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.277
8.259
8.119
8.101
7.566
7.552
7.535
7.515
7.507
7.489
7.476
7.469
7.423
7.405
7.386
7.255
2.647
0.000
O
N
I
3a
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
0.0
-0.5 ppm
1.92
1.89
6.11
0.98
3.00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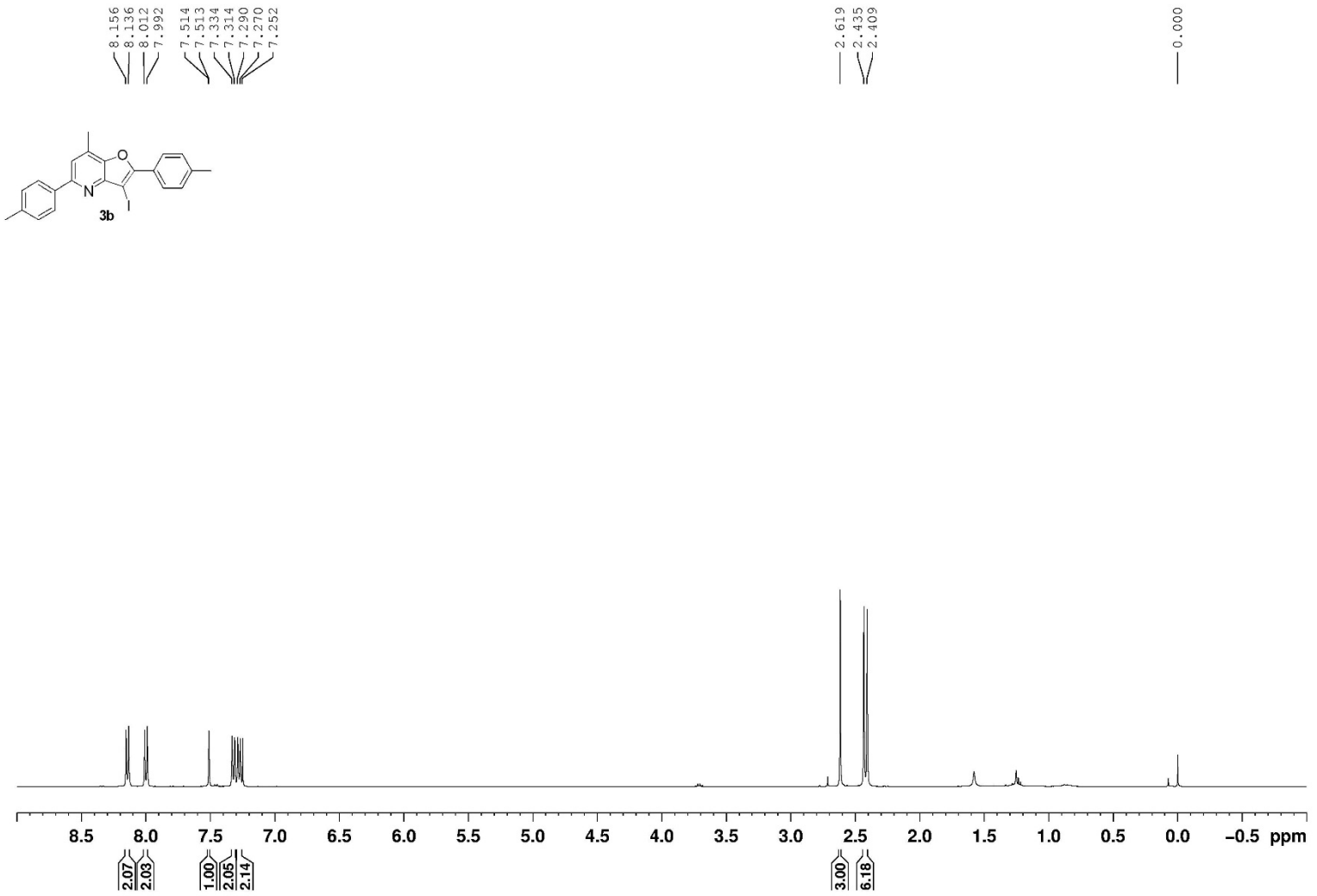
154.75
148.56
146.15
139.54
130.16
129.85
129.79
128.67
128.58
127.62
127.26
119.34
77.31
77.00
76.68
65.15
14.65
O
N
I
3a
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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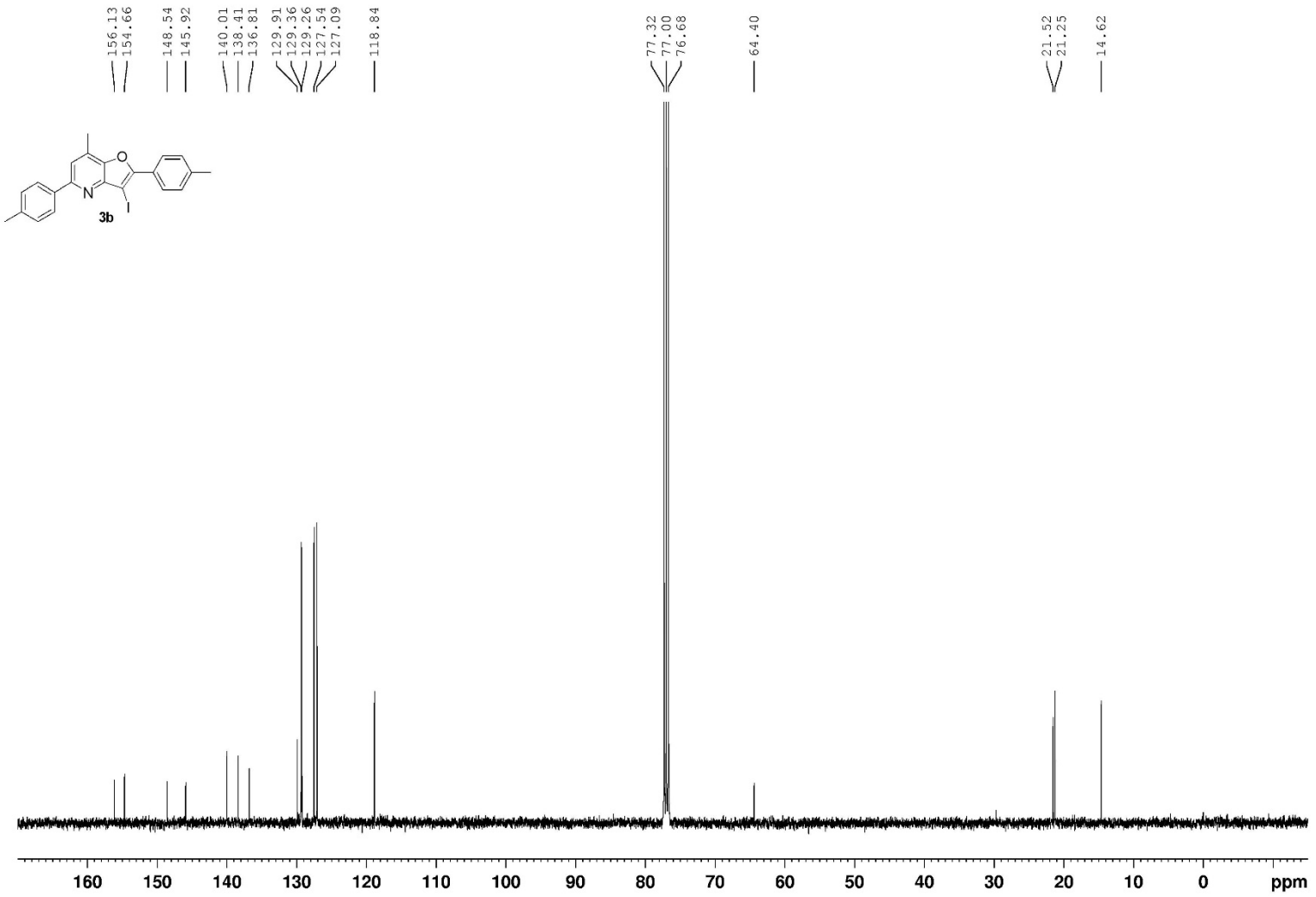
8.136
8.012
7.992
7.514
7.513
7.334
7.314
7.290
7.270
7.252
2.619
2.435
2.409
0.000
O
N
I
3b
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5 ppm
2.07
2.03
1.00
2.05
2.14
3.00
6.18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154.66
148.54
145.92
140.01
138.41
136.81
129.91
129.36
129.26
127.54
127.09
118.84
77.32
77.00
76.68
64.40
21.52
21.25
14.62
O
N
I
3b
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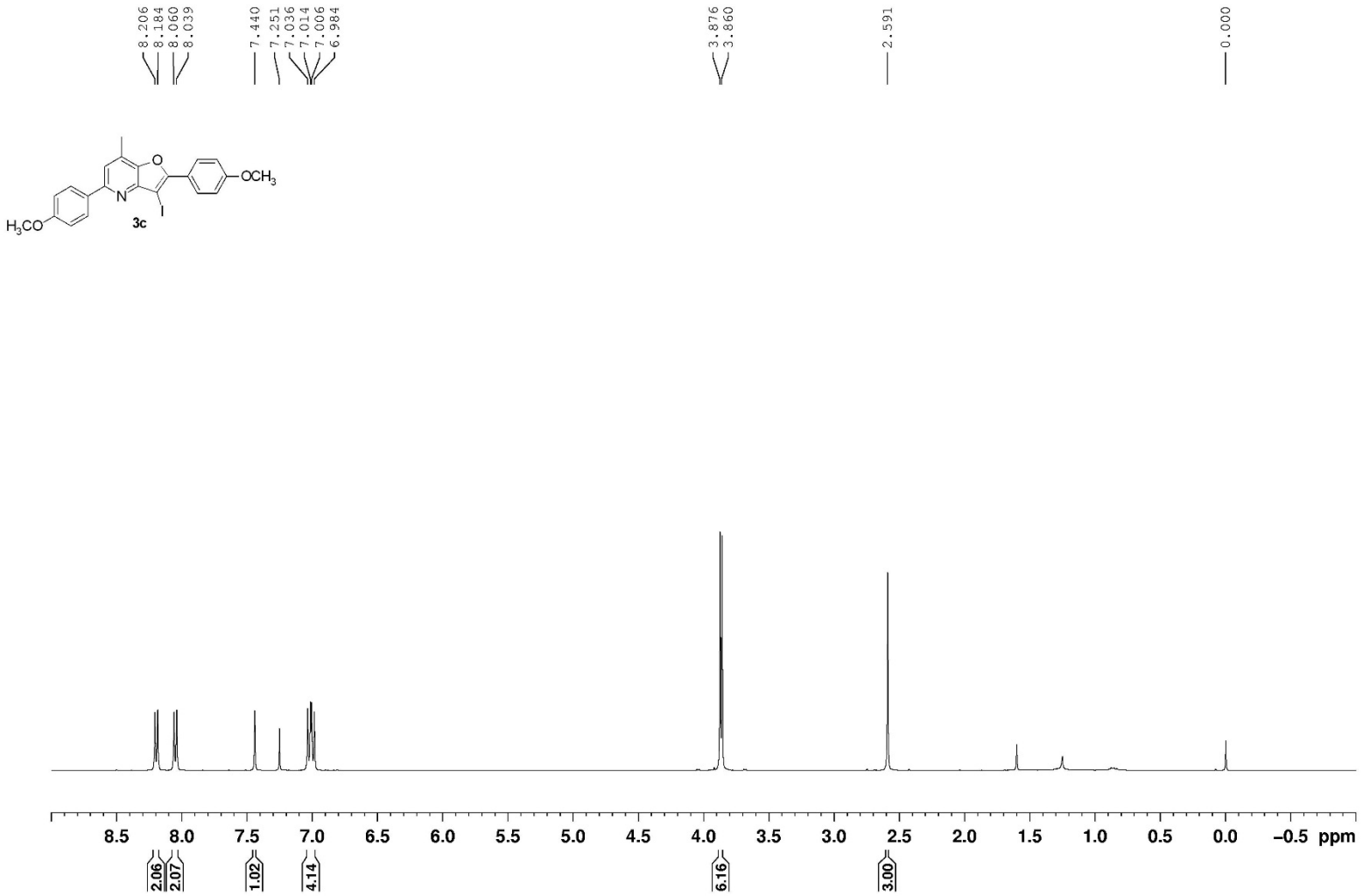
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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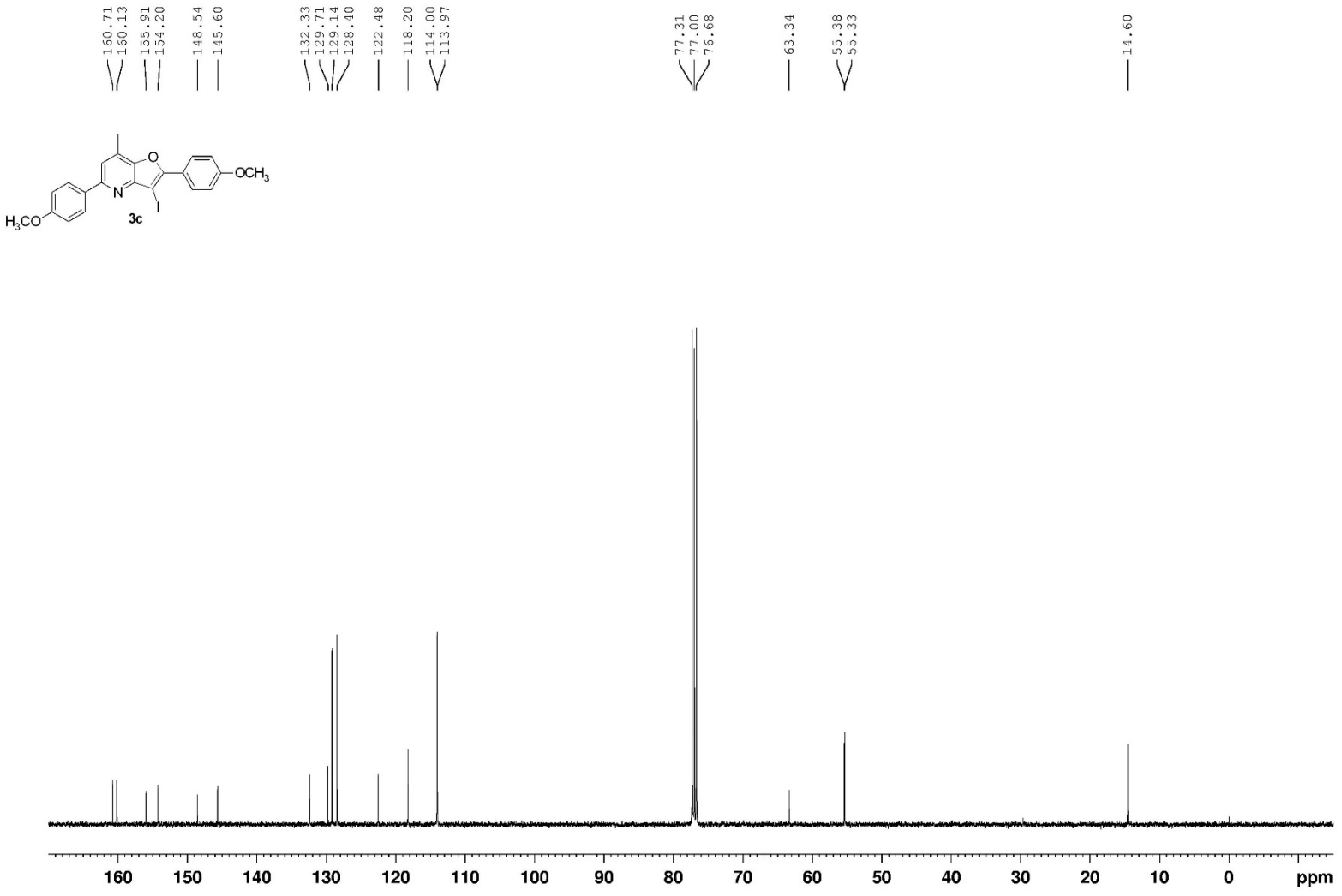
8.184
8.060
8.039
7.440
7.251
7.036
7.014
7.006
6.984
3.876
3.860
2.591
0.000
OCH3
H3CO
N
O
I
3c
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5 ppm
2.06
2.07
1.02
4.14
6.16
3.00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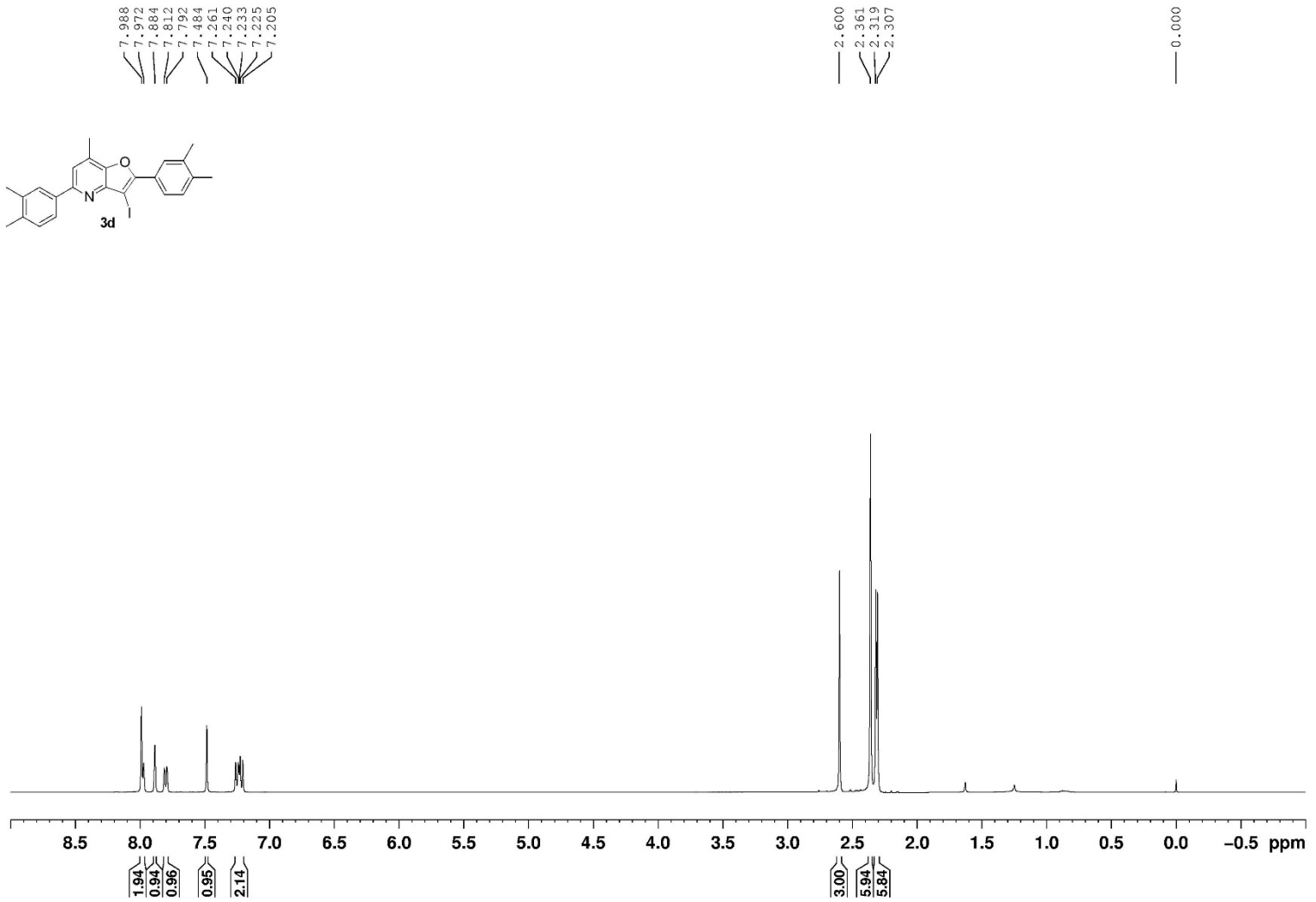
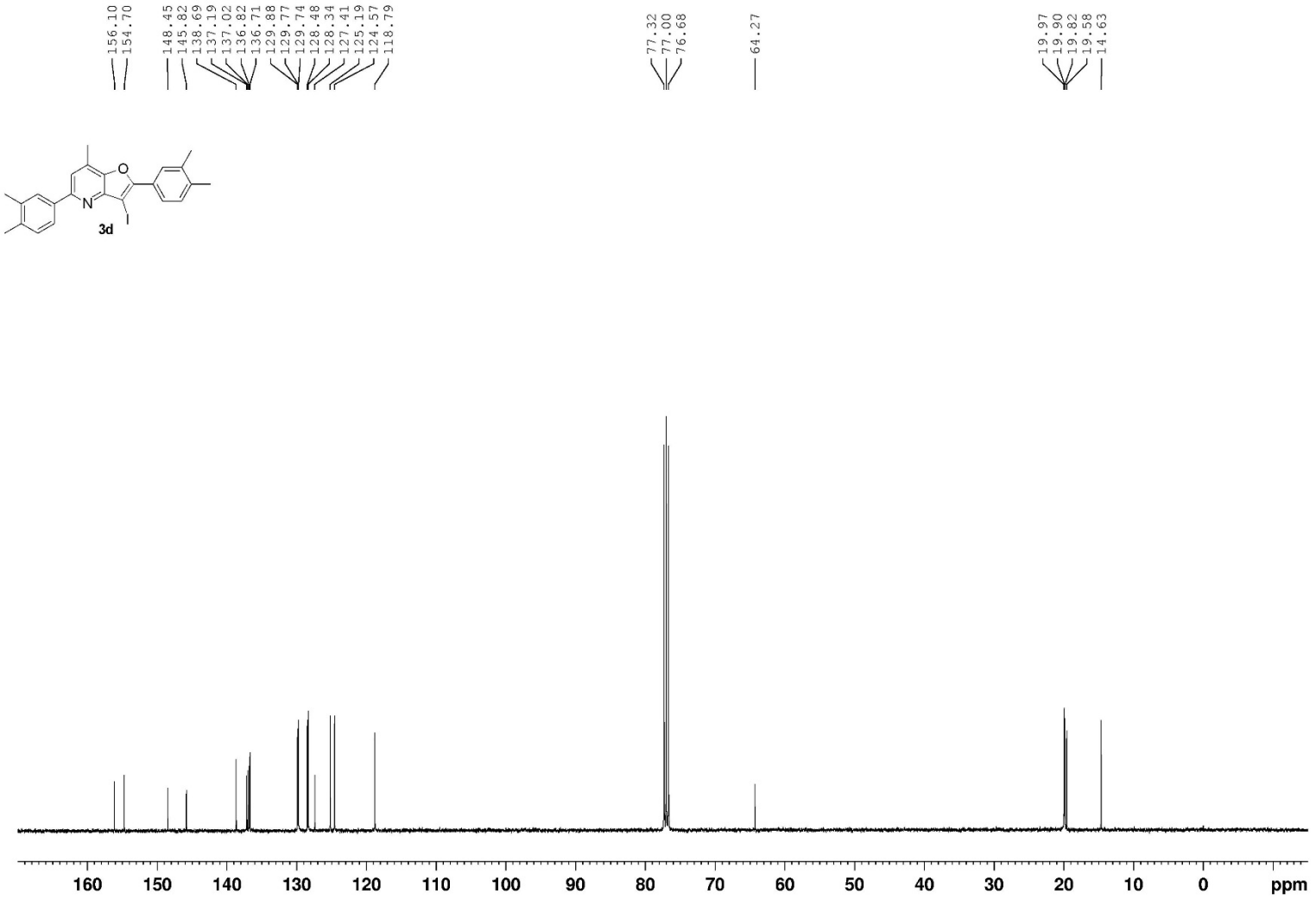
160.13
155.91
154.20
148.54
145.60
132.33
129.71
129.14
128.40
122.48
118.20
114.00
113.97
77.31
77.00
76.68
63.34
55.38
55.33
14.60
OCH3
H3CO
N
O
I
3c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.988
7.972
7.884
7.812
7.792
7.484
7.261
7.240
7.233
7.225
7.205
2.600
2.361
2.319
2.307
0.000
O
N
I
3d
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
0.0
−0.5 ppm
1.94
0.94
0.96
0.95
2.14
3.00
5.94
5.84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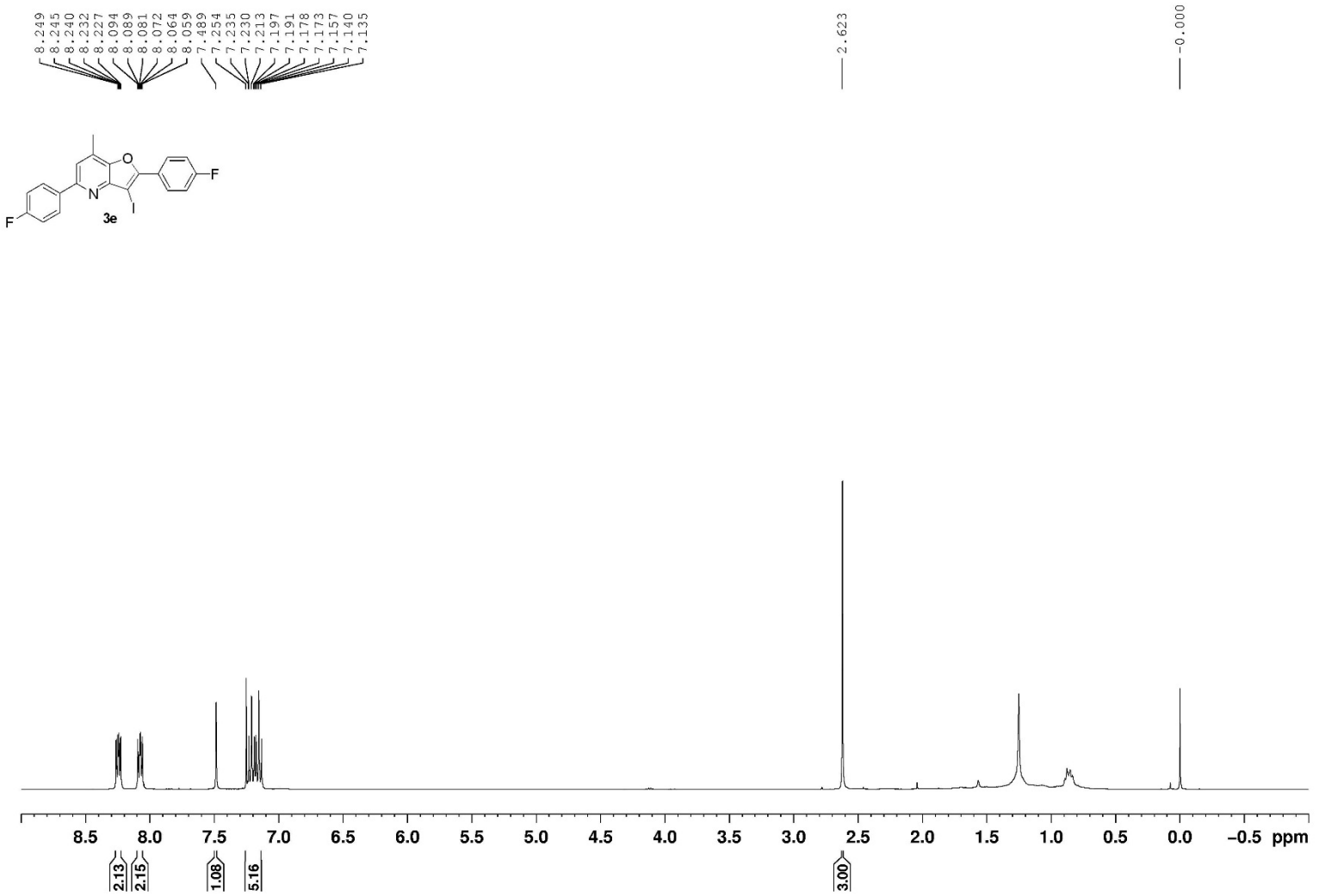
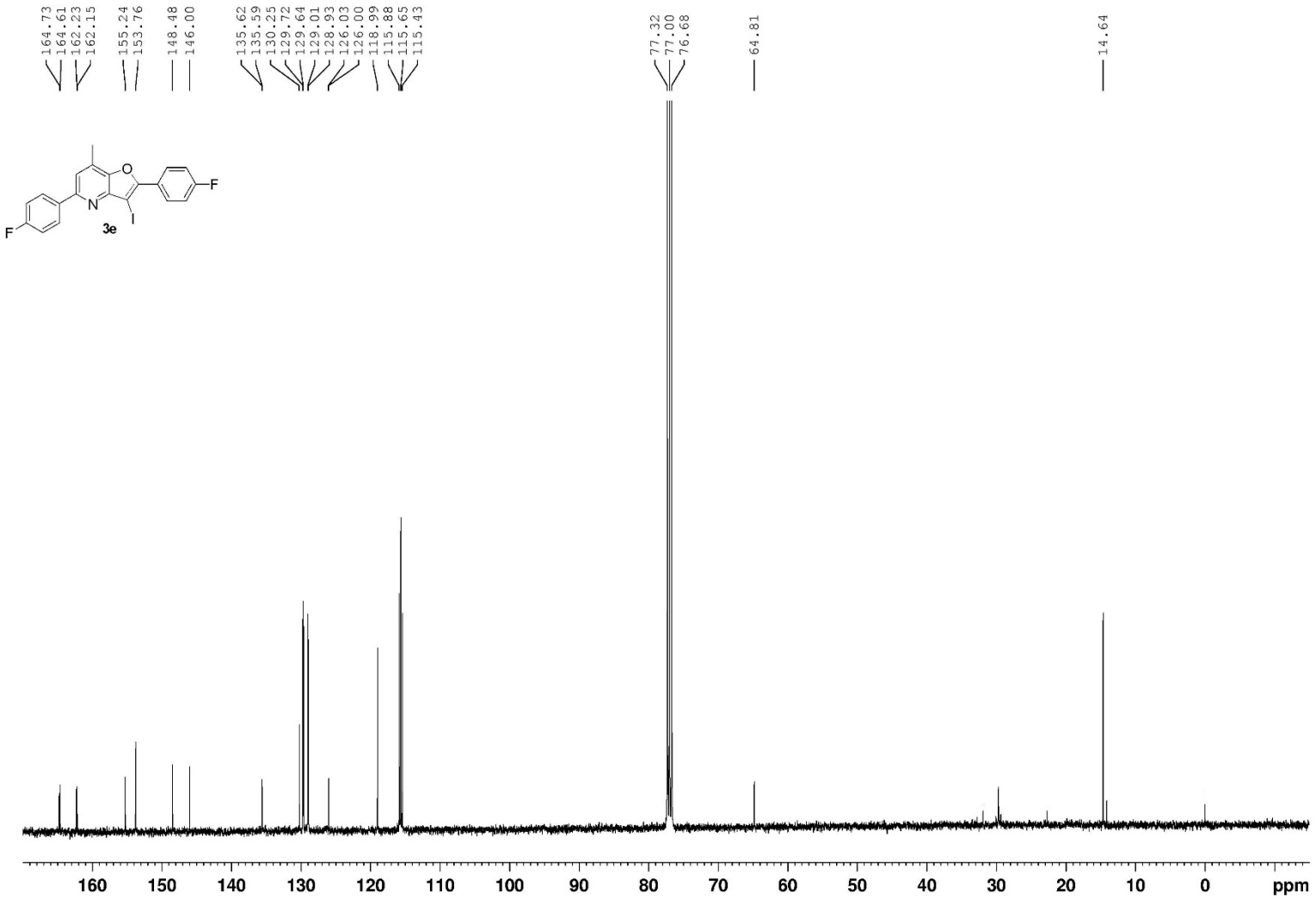
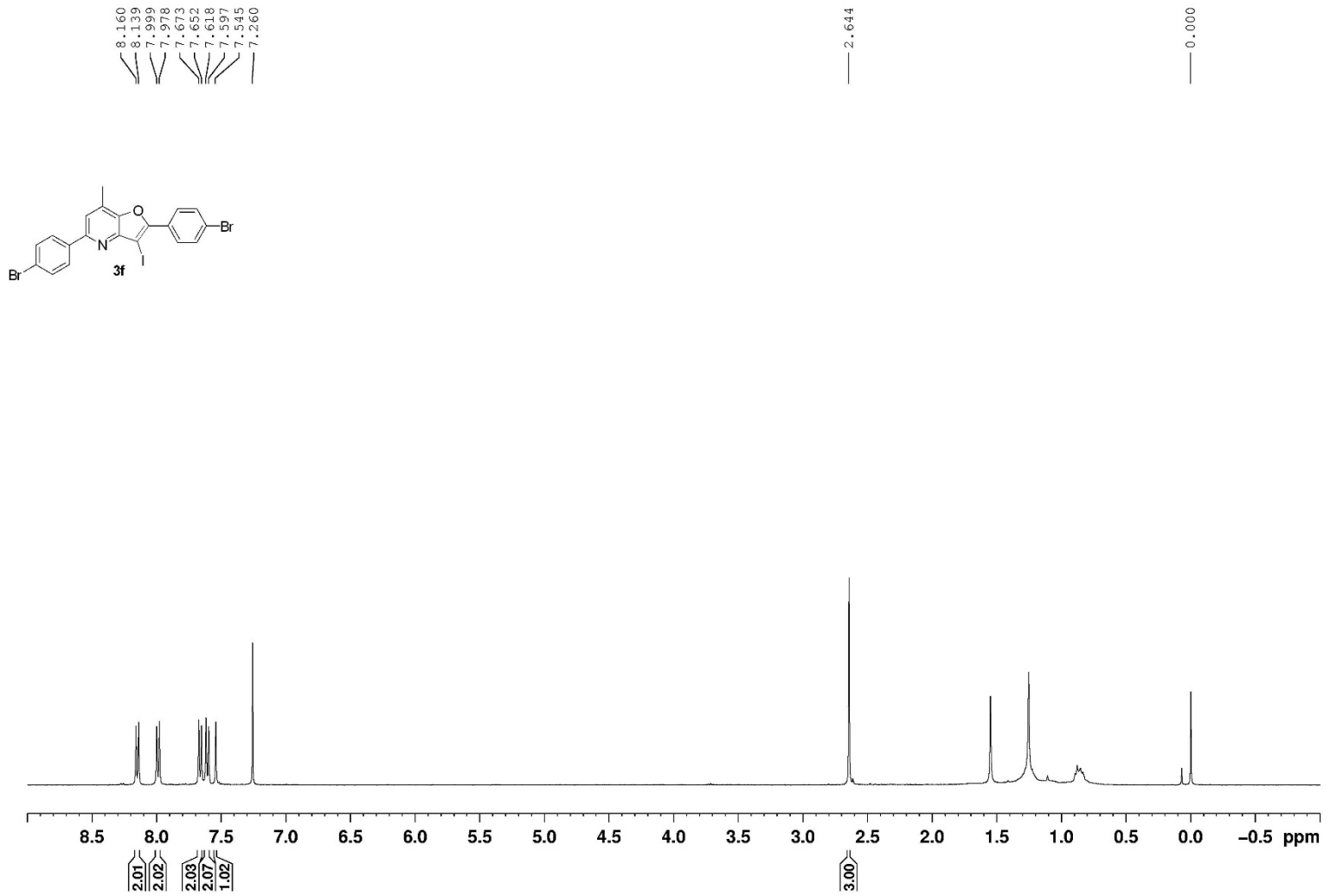
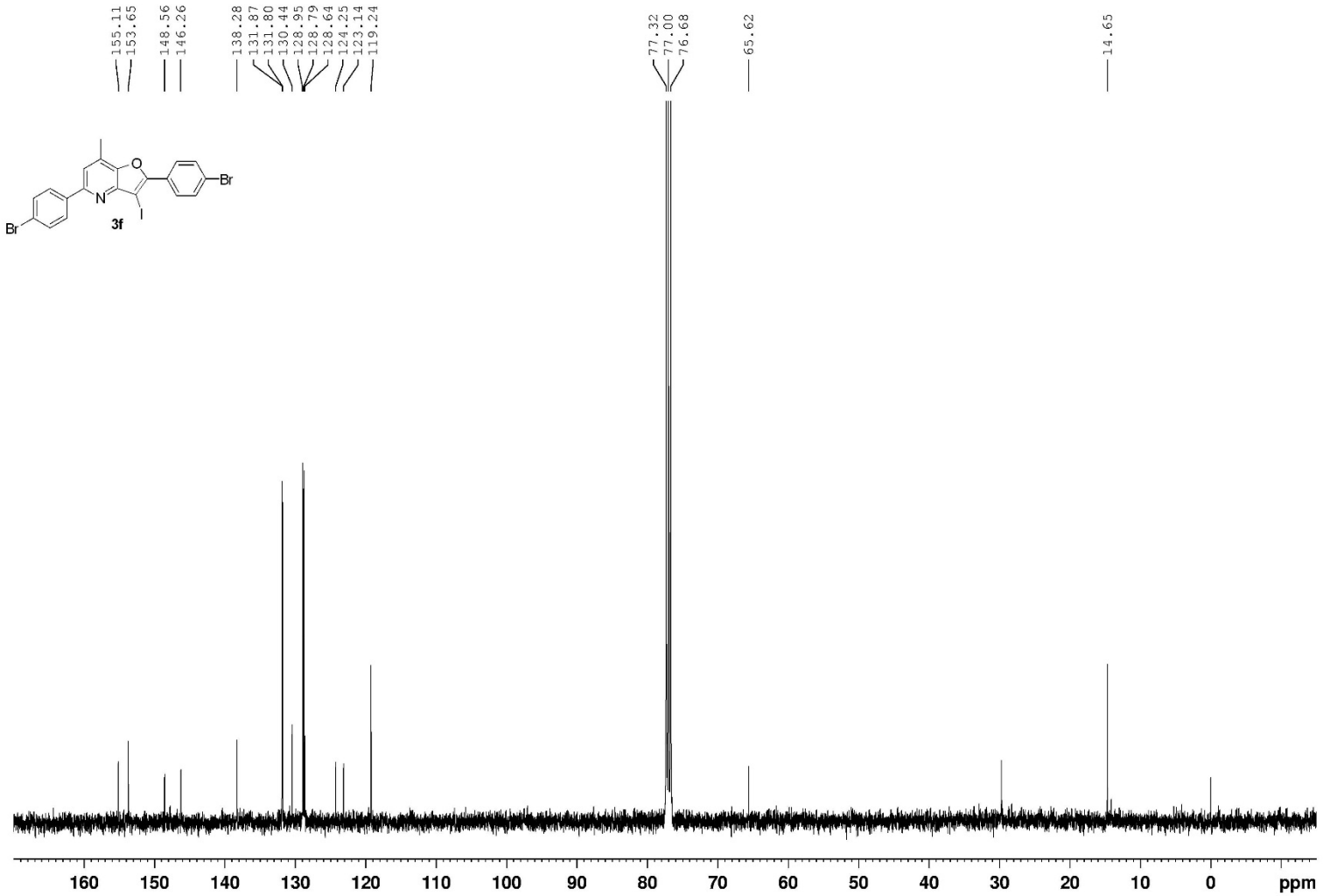
154.70
148.45
145.82
138.69
137.19
137.02
136.82
136.71
129.88
129.77
129.74
128.48
128.34
127.41
125.19
124.57
118.79
77.32
77.00
76.68
64.27
19.97
19.90
19.82
19.58
14.63
O
N
I
3d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.249
8.245
8.240
8.232
8.227
8.094
8.089
8.081
8.072
8.064
8.059
7.489
7.254
7.235
7.230
7.213
7.197
7.191
7.178
7.173
7.157
7.140
7.135
2.623
0.000
O
N
F
F
I
3e
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
0.0
−0.5 ppm
2.13
2.15
1.08
5.16
3.00


164.73
164.61
162.23
162.15
155.24
153.76
148.48
146.00
135.62
135.59
130.25
129.72
129.64
129.01
128.93
126.03
126.00
118.99
115.88
115.65
115.43
77.32
77.00
76.68
64.81
14.64
F
N
O
I
F
3e
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.160
8.139
7.999
7.978
7.673
7.652
7.618
7.597
7.545
7.260
2.644
0.000
Br
N
O
Br
I
3f
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
0.0
-0.5 ppm
2.01
2.02
2.03
2.07
1.02
3.00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148.56
146.26
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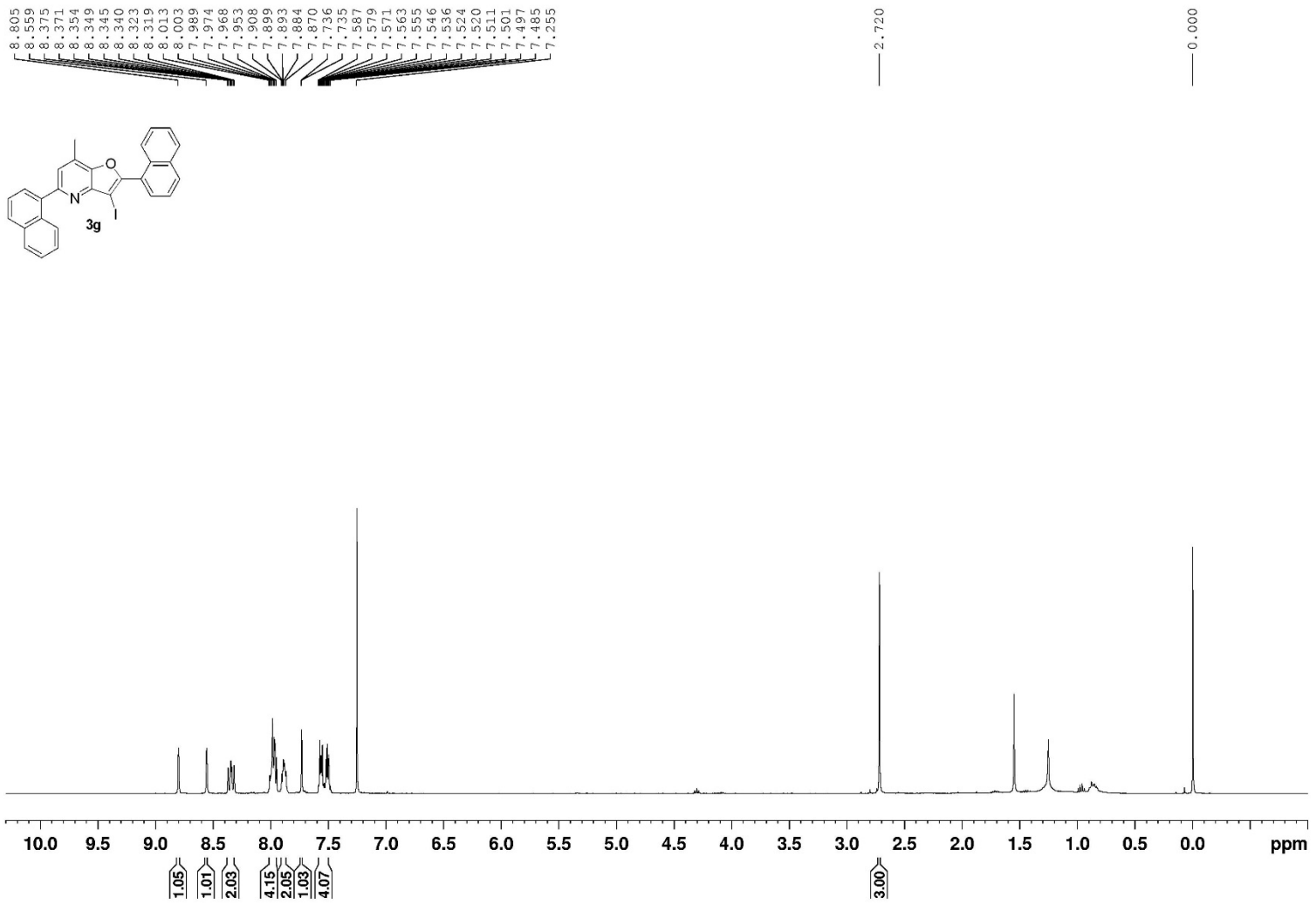
131.87
131.80
130.44
128.95
128.79
128.64
124.25
123.14
119.24
77.32
77.00
76.68
65.62
14.65
Br
Br
O
N
I
3f
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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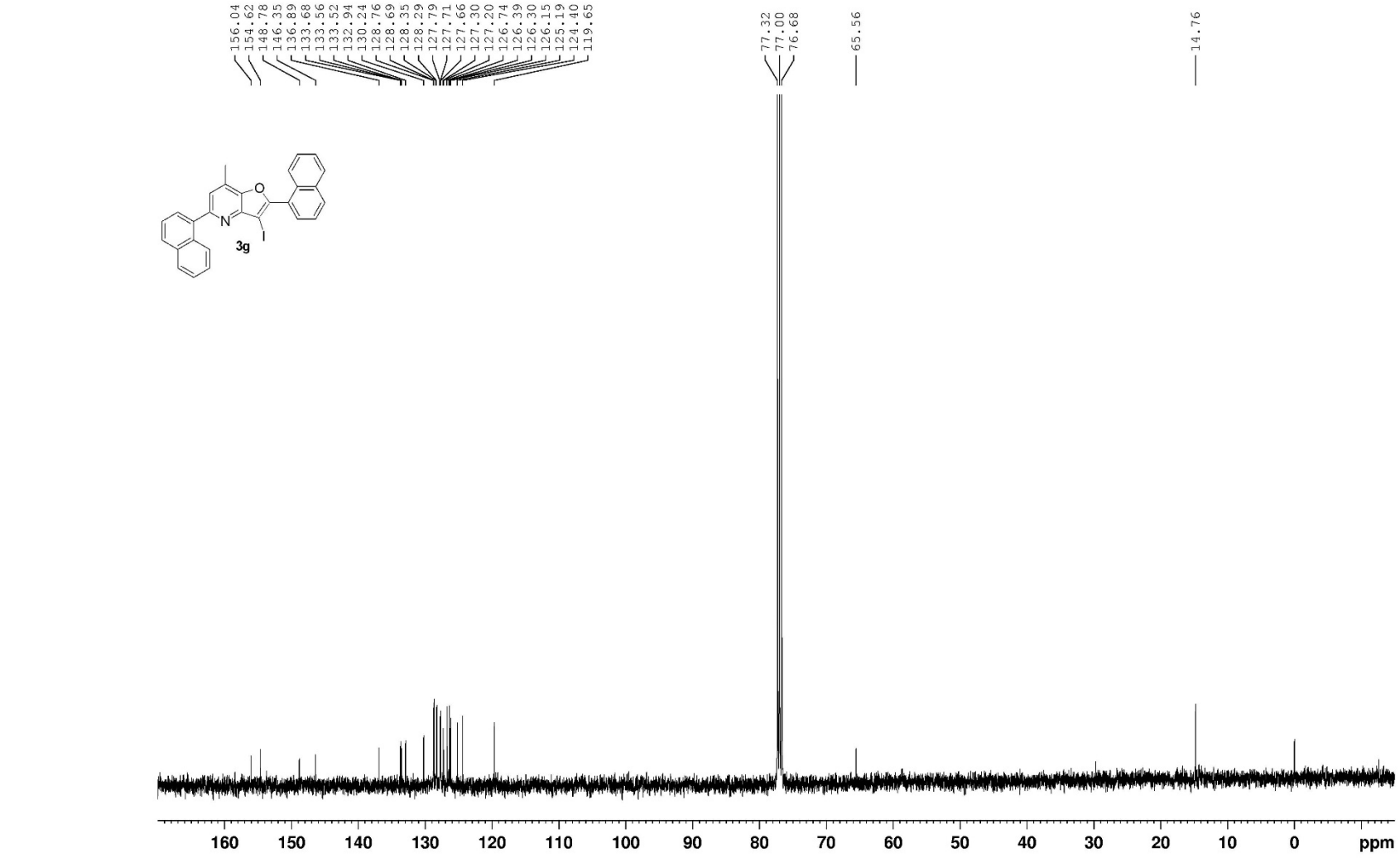
8.371
8.354
8.349
8.345
8.340
8.323
8.319
8.013
8.003
7.989
7.974
7.968
7.953
7.908
7.899
7.893
7.884
7.870
7.736
7.735
7.587
7.579
7.571
7.563
7.555
7.546
7.536
7.524
7.520
7.511
7.501
7.497
7.485
7.255
2.720
0.000
3g
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.05
1.01
2.03
4.15
2.05
1.03
4.07
3.00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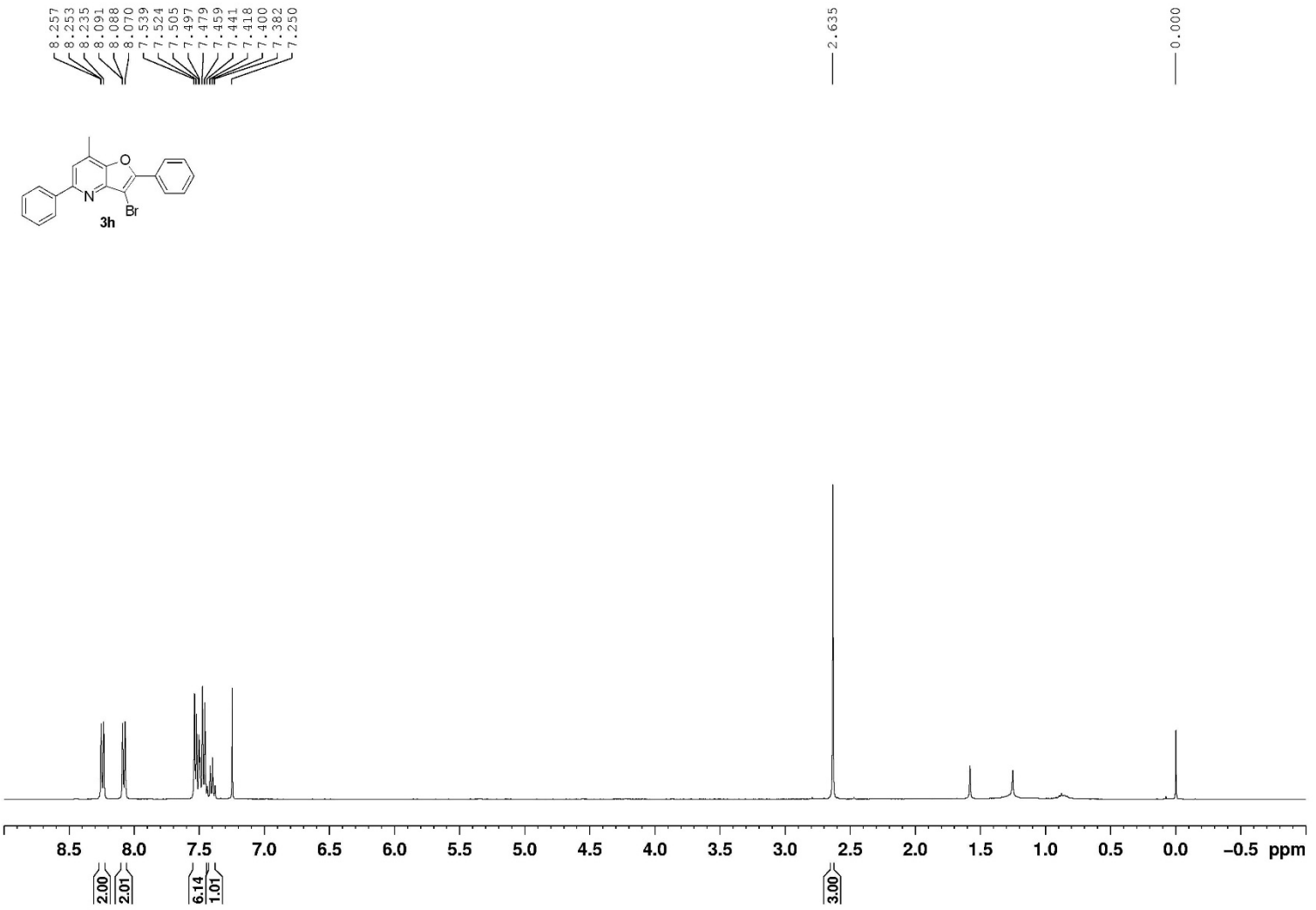
136.89
133.68
133.56
133.52
132.94
130.24
128.76
128.69
128.35
128.29
127.79
127.71
127.66
127.30
127.20
126.74
126.39
126.30
126.15
125.19
124.40
119.65
77.32
77.00
76.68
65.56
14.76
O
N
I
3g
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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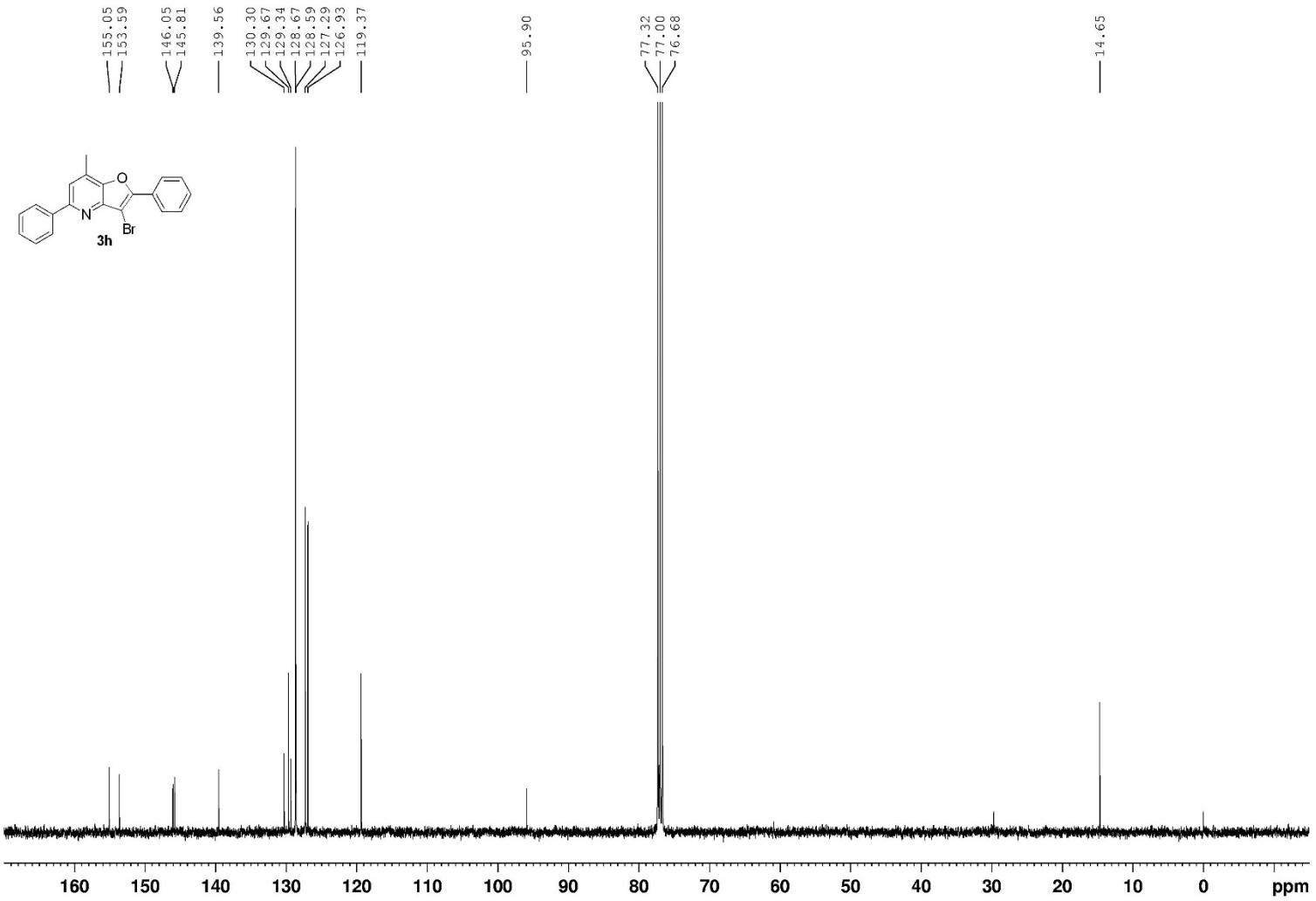
8.235
8.091
8.088
8.070
7.539
7.524
7.505
7.497
7.479
7.459
7.441
7.418
7.400
7.382
7.250
2.635
0.000
O
N
Br
3h
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5 ppm
2.00
2.01
6.14
1.01
3.00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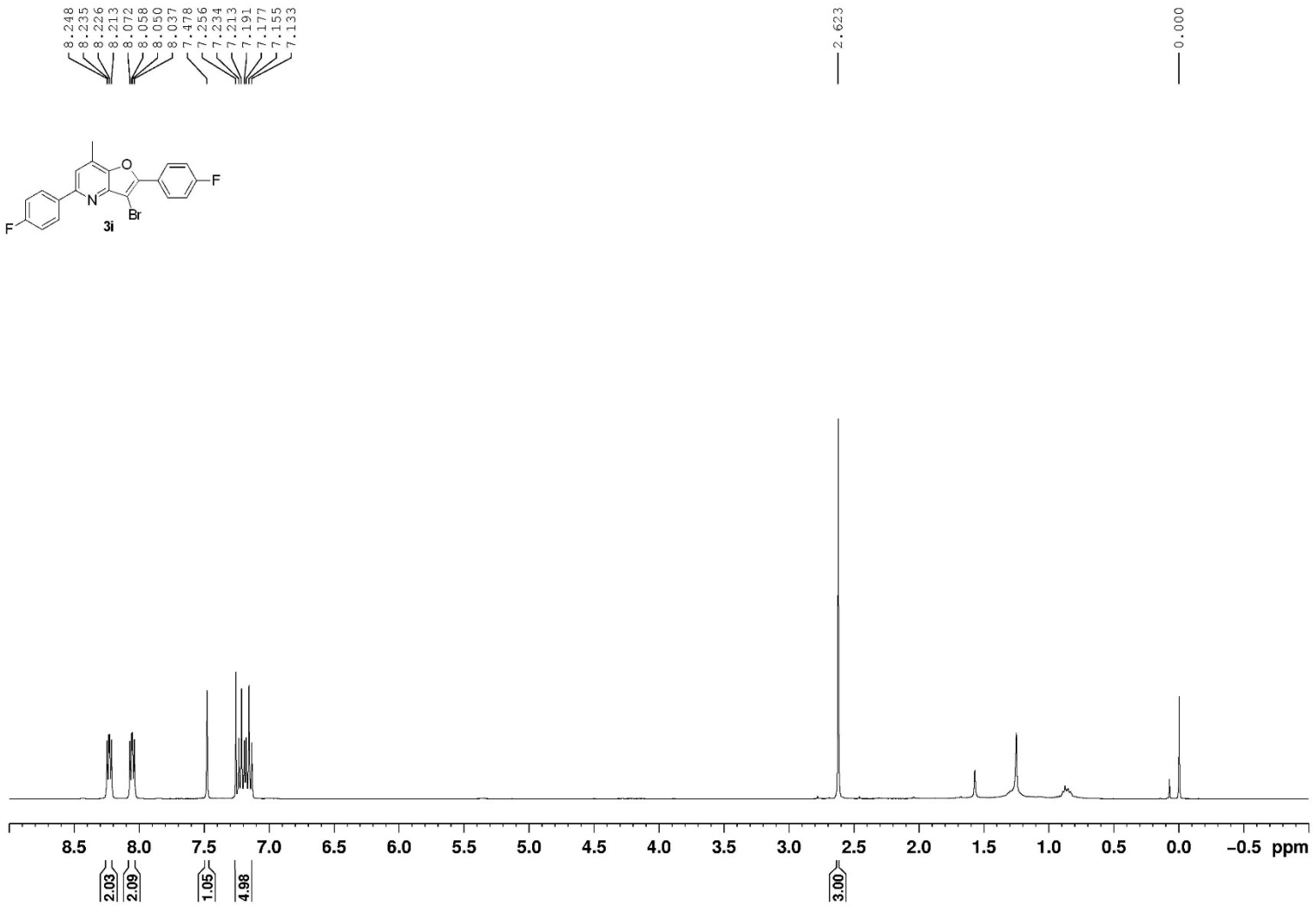
153.59
146.05
145.81
139.56
130.30
129.67
129.34
128.67
128.59
127.29
126.93
119.37
95.90
77.32
77.00
76.68
14.65
O
N
Br
3h
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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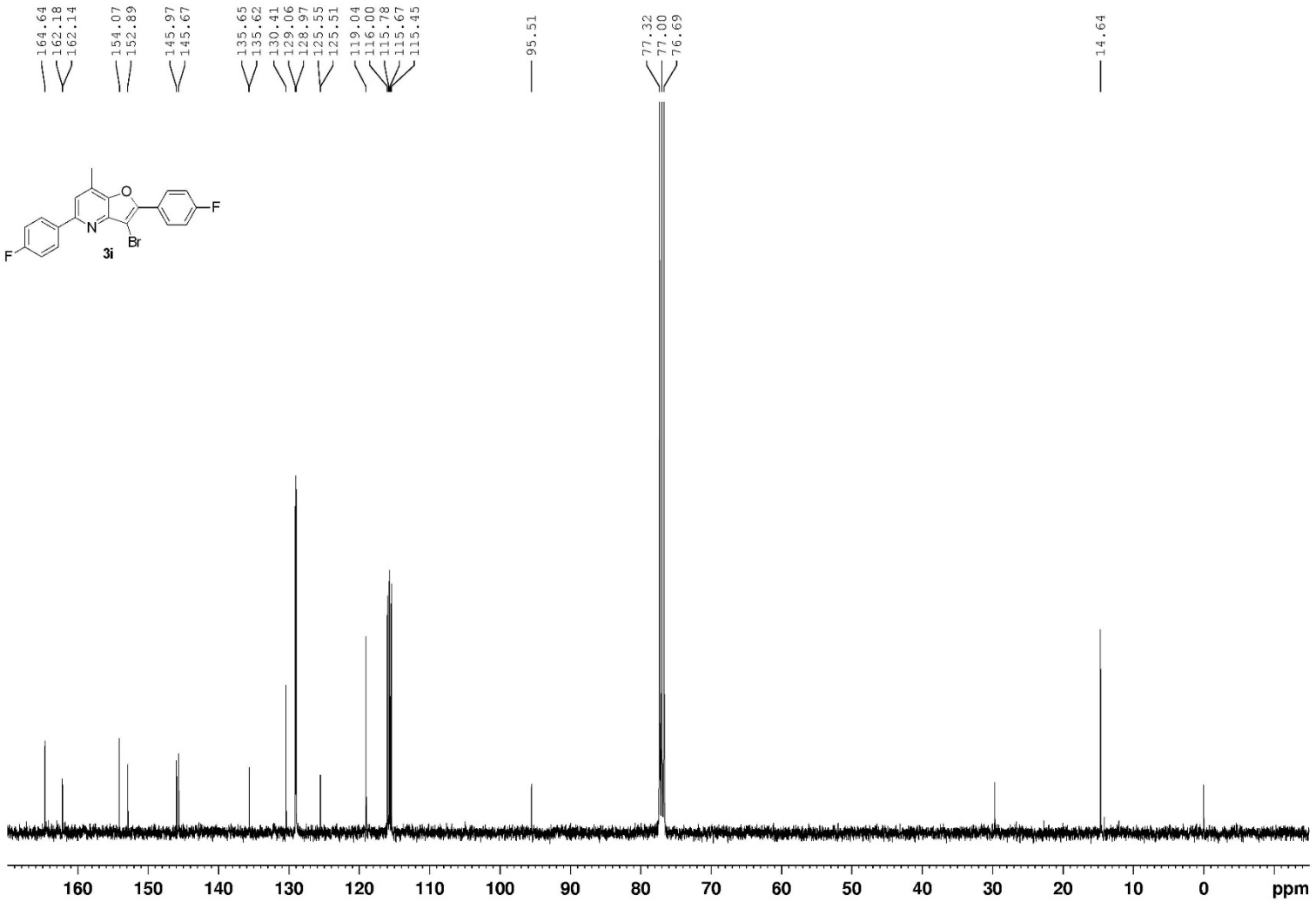
8.235
8.226
8.213
8.072
8.058
8.050
8.037
7.478
7.256
7.234
7.213
7.191
7.177
7.155
7.133
2.623
0.000
F
O
N
Br
F
3i
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5 ppm
2.03
2.09
1.05
4.98
3.00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162.18
162.14
154.07
152.89
145.97
145.67
135.65
135.62
130.41
129.06
128.97
125.55
125.51
119.04
116.00
115.78
115.67
115.45
95.51
77.32
77.00
76.69
14.64
O
N
F
Br
F
3i
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm