SUPPLEMENTARY INFORMATION

Switching the regioselectivity of acid-catalytic reactions of arylnaphtho[2,1-b]furans *via* [1,2]-aryl shift

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I. General information

^{1}H and ^{13}C NMR spectra were recorded in deuterated solvents on a spectrometers Bruker Fourier 300 HD and Bruker Avance Neo 300 working at 300 MHz for ^{1}H and 75 MHz for ^{13}C. ^{1}H and ^{13}C spectra reported in parts per million (ppm) at 293 K. Data are represented as follows: chemical shift, multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; dd, doublet of doublets; ddd, doublet of doublets of doublets; m, multiplet; br, broad), coupling constant in hertz (Hz). Melting points (mp) were recorded using an apparatus and not corrected. High resolution mass spectra (HRMS) were recorded on a TOF mass spectrometer Bruker MicroTOF via ESI mode. All starting chemicals and solvents were purchased from commercial sources and used without further purification. Silica column chromatography was performed using silica gel 60 (70−230 mesh); TLC analysis was conducted on silica gel 60 F_{254} plates.

UV/Vis absorption spectra were recorded on a spectrometer Agilent Cary 60 UV-Vis. Fluorescence spectra were recorded on an Agilent Cary Eclipse Fluorescence Spectrometer. The experimental measurements were performed at ambient temperature in the presence of air in 1.0 cm quartz cuvettes in acetonitrile solution. Relative fluorescence quantum yields were determined by the Parker-Rees method using anthracene (Φ_{fl} = 0.27, EtOH) as the standard using following equation (1):

$$\Phi_a = \Phi_s \left(\frac{G_a}{G_s}\right)\left(\frac{\eta_a}{\eta_s}\right)^2 \quad (1)$$

where Φ_a and Φ_s is the quantum yield of the analyzed sample and standard, respectively; G_a and G_s is the slope of the linear fit for the integrated fluorescence intensity of the analyzed sample and standard as a function of absorbance, respectively; and η_a and η_s are the refractive indices of the analyzed sample and the standard solutions, respectively.

X-ray diffraction data were collected at 100K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area-detector (kappa geometry, shutterless ω-scan technique), using graphite monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[1] The structure was solved by direct methods using SHELXT[2] and refined on F^2 using SHELXL-2018[3] in the OLEX2 program.[4] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. All hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters. The Mercury program suite[5] was used for molecular graphics. Full crystallographic data have been deposited with the Cambridge

[1] CrysAlisPro. Version 1.171.41.106a. *Rigaku Oxford Diffraction*, **2021**.

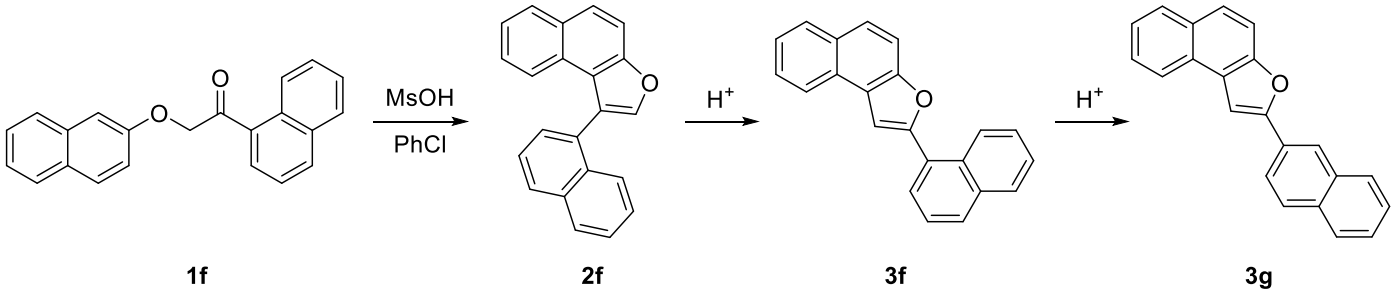
[2] Sheldrick, G. M. SHELXT - Integrated space-group and crystal-structure determination. *Acta Cryst.* **2015**, A71(1), 3-8.

[3] Sheldrick, G. M. Crystal structure refinement with SHELXL. *Acta Cryst.* **2015**, C71(1), 3-8.

[4] Dolomanov O. V.; Bourhis L. J.; Gildea R. J.; Howard J. A. K.; Puschmann H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.* **2009**, 42(2), 339-341.

[5] Macrae, C. F.; Edgington, P. R.; McCabe, P.; Pidcock, E.; Shields, G. P.; Taylor, R.; Towler, M.; van de Streek, J. Mercury: Visualization and Analysis of Crystal Structures. *J. Appl. Crystallogr*. **2006**, 39, 453–457.

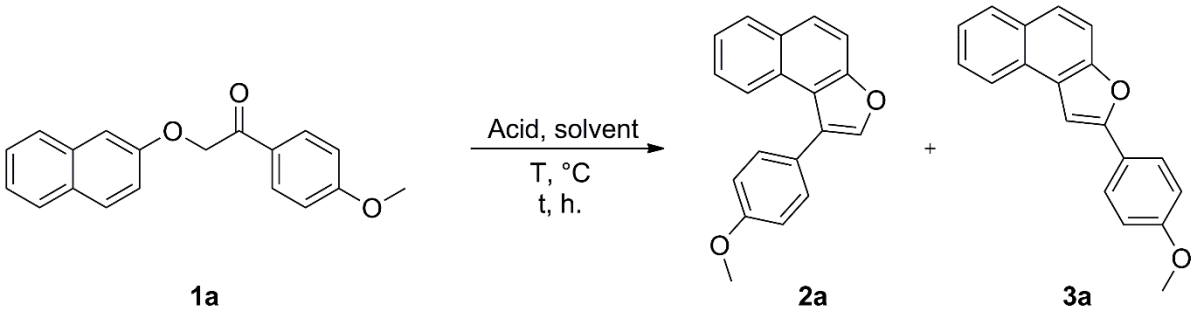
Crystallographic Data Center, CCDC 2363841. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk.



Scheme S1. Double [1,2]-aryl shift for *in situ* formed compound **2f**

II. [1,2]-Aryl shift optimization studies

Table S1. Reaction conditions optimization for the preparation of naphtho[2,1-*b*]furans **2a** and **3a**[a)]

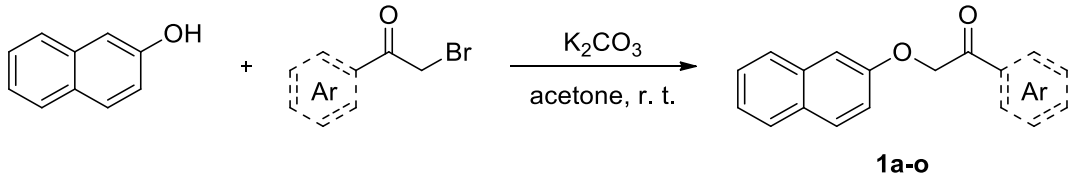


Entry	Solvent	Acid	Acid amount, eq.	T, °C	t, h	Ratio 1a / 2a / 3a
1	CH_2Cl_2	MsOH	0.1	22	18	1 / 0 / 0
2	CH_2Cl_2	MsOH	0.5	22	18	1 / 0.06 / 0
3	CH_2Cl_2	MsOH	1	22	18	1 / 0.43 / 0
4	CH_2Cl_2	MsOH	2	22	18	0.03 / 1 / 0
5	CH_2Cl_2	MsOH	3	22	18	0.02 / 1 / 0
6	CH_2Cl_2	MsOH	4	22	18	0 / 1 / 0
7	CH_2Cl_2	MsOH	5	22	18	0 / 1 / 0
8	CH_2Cl_2	MsOH	10	22	18	0 / 1 / 0.06
9	MsOH	-	-	22	18	0 / 1 / 0.9
10	CH_2Cl_2	MsOH	10	40	4	0 / 1 / 0.09
11	$CHCl_3$	MsOH	10	60	4	0 / 1 / 0.14
12	$ClCH_2$-CH_2Cl	MsOH	10	80	4	0 / 0.16 / 1
13	$ClCH_2$-CH_2Cl	MsOH	10	80	6	0 / 0 / 1
14	PhCl	MsOH	10	130	2	0 / 0 / 1
15	PPA	-	-	22	4	0.76 / 1 / 0
16	PPA	-	-	22	18	0.8 / 1 / 0

17	PPA	-	-	50	4	0.15 / 1 / 0.24
18	PPA	-	-	80	4	0 / 0.08 / 1
19	PPA	-	-	120	4	0 / 0.24 / 1
20	PPA	-	-	150	4	0 / 0.6 / 1
21	CH_2Cl_2	CF_3COOH	1	22	18	1 / 0 / 0
22	CH_2Cl_2	CF_3COOH	5	22	18	1 / 0 / 0
23	CH_2Cl_2	CF_3COOH	10	22	18	1 / 0 / 0
24	CH_2Cl_2	CF_3COOH	10	40	6	1 / 0.07 / 0
25	CF_3COOH	-	-	70	6	0 / 1 / 0.68
26	CH_3COOH	-	-	115	4	1 / 0 / 0
27	CH_2Cl_2	$BF_3{\cdot}Et_2O$	0.1	22	18	1 / 0.12 / 0
28	CH_2Cl_2	$BF_3{\cdot}Et_2O$	0.5	22	18	1 / 0.46 / 0
29	CH_2Cl_2	$BF_3{\cdot}Et_2O$	1	22	18	0.06 / 1 / 0
30	CH_2Cl_2	$BF_3{\cdot}Et_2O$	2	22	18	0 / 1 / 0
31	CH_2Cl_2	$BF_3{\cdot}Et_2O$	3	22	18	0 / 1 / 0
32	CH_2Cl_2	$BF_3{\cdot}Et_2O$	4	22	18	0 / 1 / 0
33	CH_2Cl_2	$BF_3{\cdot}Et_2O$	5	22	18	0 / 1 / 0
34	$ClCH_2$-CH_2Cl	$BF_3{\cdot}Et_2O$	10	80	6	0 / 1 / 0.22
35	CH_2Cl_2	$SnCl_4$	5	22	18	1 / 0 / 0
36	$ClCH_2$-CH_2Cl	$SnCl_4$	5	80	6	1 / 0 / 0
37	CH_2Cl_2	$TiCl_4$	5	22	18	1 / 0 / 0
38	$ClCH_2$-CH_2Cl	$TiCl_4$	5	80	6	0 / 1 / 0.13
39	CH_2Cl_2	$AlCl_3$	5	22	18	0.75 / 1 / 0
40	$ClCH_2$-CH_2Cl	$AlCl_3$	5	80	6	Tarring
41	CH_2Cl_2	$FeCl_3$	5	22	18	Tarring
42	CH_3COOH	MsOH	4	22	18	1 / 0 / 0
43	DCM	H_2SO_4	4	22	18	0/1/0
44	1,2-DCE	H_2SO_4	10	80	6	Tarring
45	DCM	HCl (sat.)	-	22	18	1/0.34/0
46	DCE	H_3PO_4	10	80	6	1/0/0
47	DCM	$HClO_4$	4	22	18	1/0/0

[a] **1a** (0.11 M solution)

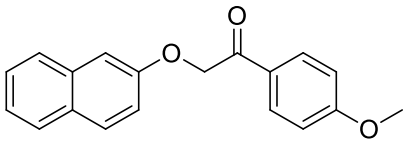
III. Synthesis of ketoethers 1a-o



1a-o

2-Naphthol (2.5 g, 17.4 mmol) was dissolved in 50 ml of acetone, K_2CO_3 (2.635 g, 19.1 mmol) was added and the mixture was stirred at room temperature for 30 minutes. To this mixture the corresponding 1-aryl-2-bromoethanone (17.4 mmol) was added. The reaction mixture was stirred at room temperature for 24 hours. After completion of the reaction, the mixture was filtered and the solvent was evaporated in vacuum. The residue was recrystallized twice from ethanol to obtain the desired ketoether **1**.

1-(4-Methoxyphenyl)-2-(naphthalen-2-yloxy)ethanone (1a)



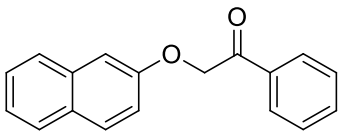
Beige crystals (4.613 g, 91 %, mp = 96-97 °C (lit.[1] 96-98°C)).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.07 (d, J = 8.7 Hz, 2H), 7.79 (m, 2H), 7.73 (d, J = 8.1 Hz, 1H), 7.45 (ddd, J = 8.2, 6.9, 1.3 Hz, 1H), 7.36 (ddd, J = 8.2, 6.9, 1.3 Hz, 1H), 7.29 (dd, J = 9.0, 2.6 Hz, 1H), 7.15 (d, J = 2.5 Hz, 1H), 6.99 (d, J = 8.7 Hz, 2H), 5.34 (s, 2H, CH_2), 3.90 (s, 3H, OMe).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 193.0, 164.1, 156.1, 134.3, 130.6, 129.7, 129.4, 127.7, 127.7, 126.9, 126.5, 124.0, 118.7, 114.1, 107.4, 70.8, 55.5.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{19}H_{17}O_3^+$: 293.1172, found: 293.1177

2-(Naphthalen-2-yloxy)-1-phenylethanone (1b)



Beige crystals (3.912 g, 86 %, mp = 105-106 °C (lit.[1] 105-107 °C)).

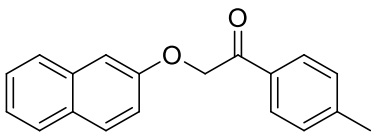
^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.11 – 8.04 (m, 2H), 7.82 – 7.77 (m, 2H), 7.73 (d, J = 8.2 Hz, 1H), 7.69 – 7.62 (m, 1H), 7.58 – 7.50 (m, 2H), 7.46 (ddd, J = 8.0, 6.9. 1.2 Hz, 1H), 7.38 (ddd, J = 8.0, 6.9. 1.2 Hz, 1H), 7.30 (dd, J = 9.1, 2.6 Hz, 1H), 7.16 (d, J = 2.4 Hz, 1H), 5.39 (s, 2H, CH_2).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 194.4, 156.0, 134.7, 134.3, 133.9, 129.8, 129.4, 128.9, 128.2, 127.7, 126.9, 126.5, 124.1, 118.7, 107.4, 70.9.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{18}H_{15}O_2^+$: 263.1067, found: 263.1074.

[1] T. B. Mete, D. Laha, R. G. Bhat, *ChemistrySelect*, **2018**, 3, 7656

2-(Naphthalen-2-yloxy)-1-(*p*-tolyl)ethanone (1c)



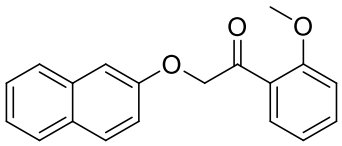
Beige crystals (3.833 g, 80 %, mp = 70-71 °C (lit.[1] 72 °C))

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 7.98 (d, J = 8.2 Hz, 2H), 7.83 – 7.77 (m, 2H), 7.73 (d, J = 8.1 Hz, 1H), 7.46 (ddd, J = 8.0, 6.9. 1.2 Hz, 1H), 7.41 – 7.29 (m, 4H), 7.16 (d, J = 2.5 Hz, 1H), 5.38 (s, 2H), 2.46 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 194.0, 156.0, 144.9, 134.3, 132.2, 129.7, 129.5, 129.4, 128.3, 127.7, 126.9, 126.5, 124.0, 118.7, 107.4, 70.8, 21.8.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{19}H_{17}O_2^+$: 277.1223, found: 277.1224.

1-(2-Methoxyphenyl)-2-(naphthalen-2-yloxy)ethanone (1d)



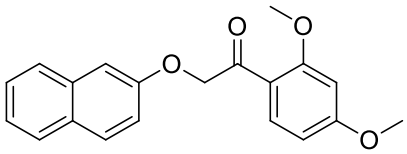
Brown powder (3.701 g, 73 %, mp = 90-91 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 7.98 (dd, J = 7.7, 1.7 Hz, 1H), 7.83 – 7.77 (m, 2H), 7.71 (d, J = 8.1 Hz, 1H), 7.62 – 7.54 (m, 1H), 7.44 (ddd, J = 8.1, 7.0, 1.0 Hz, 1H), 7.36 (ddd, J = 7.9, 6.9, 1.0 Hz, 1H), 7.30 (dd, J = 9.3, 2.8 Hz, 1H), 7.14 – 7.04 (m, 3H), 5.39 (s, 2H), 4.01 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 195.4, 159.3, 156.3, 134.8, 134.4, 131.0, 129.6, 129.3, 127.7, 126.8, 126.3, 125.1, 123.8, 121.2, 118.9, 111.6, 107.3, 74.3, 55.7.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{19}H_{17}O_3^+$: 293.1172, found: 293.1179.

1-(2,4-Dimethoxyphenyl)-2-(naphthalen-2-yloxy)ethanone (1e)



White crystals (4.416 g, 79 %, mp = 98-99 °C).

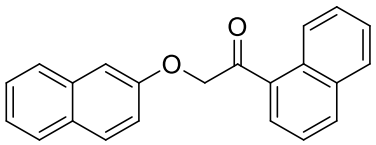
^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.05 (d, J = 8.8 Hz, 1H), 7.81 – 7.75 (m, 2H), 7.70 (d, J = 8.1 Hz, 1H), 7.43 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H), 7.38 – 7.29 (m, 2H), 7.08 (d, J = 2.4 Hz, 1H), 6.63 (dd, J = 8.8, 2.2 Hz, 1H), 6.54 (d, J = 2.2 Hz, 1H), 5.34 (s, 2H), 3.99 (s, 3H), 3.91 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 193.2, 165.4, 161.4, 156.5, 134.4, 133.2, 129.5, 129.2, 127.6, 126.8, 126.3, 123.7, 118.9, 118.3, 107.3, 105.9, 98.2, 74.2, 55.7, 55.7.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{20}H_{19}O_4^+$: 323.1278, found: 323.1275.

[1] Mohamed, M. I. Fazal; Arunadevi, S.; Koperuncholan, M.; Mubarak, M. *Seeni Chemica Sinica*, **2011**, 2(2), 52-57

1-(Naphthalen-1-yl)-2-(naphthalen-2-yloxy)ethanone (1f)



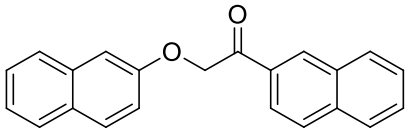
Beige crystals (4.821 g, 89%, mp = 110-111°C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.73 (d, J = 8.7 Hz, 1H), 8.08 (d, J = 8.2 Hz, 1H), 8.03 (dd, J = 7.2, 1.1 Hz, 1H), 7.92 (dd, J = 7.7, 1.6 Hz, 1H), 7.82 – 7.77 (m, 2H), 7.72 (d, J = 8.1 Hz, 1H), 7.68 – 7.54 (m, 3H), 7.46 (ddd, J = 8.2, 7.0, 1.3 Hz, 1H), 7.38 (ddd, J = 8.1, 6.9, 1.3 Hz, 1H), 7.29 (dd, J = 9.0, 2.6 Hz, 1H), 7.19 (d, J = 2.5 Hz, 1H), 5.42 (s, 2H, CH_2).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 198.2, 156.0, 134.3, 134.1, 133.7, 132.5, 130.4, 129.8, 129.4, 128.6, 128.4, 128.1, 127.7, 126.9, 126.7, 126.5, 125.6, 124.2, 124.1, 118.7, 107.4, 72.1.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{22}H_{17}O_2^+$: 313.1223, found: 313.1231.

1-(Naphthalen-2-yl)-2-(naphthalen-2-yloxy)ethanone (1g)



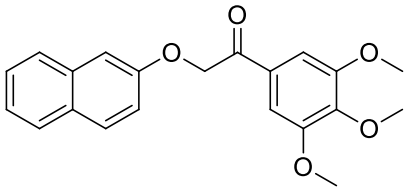
Brown powder (4.713 g, 87 %, mp =130-131 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.62 (s, 1H), 8.11 (dd, J = 8.6, 1.6 Hz, 1H), 8.03 (d, J = 7.8 Hz, 1H), 7.96 (d, J = 8.7 Hz, 1H), 7.92 (d, J = 7.9 Hz, 1H), 7.84 – 7.78 (m, 2H), 7.75 (d, J = 8.2 Hz, 1H), 7.75 (d, J = 8.2 Hz, 2H), 7.70 – 7.58 (m, 1H), 7.47 (ddd, J = 8.2, 6.8, 1.2 Hz, 1H), 7.42 – 7.36 (m, 1H), 7.33 (dd, J = 9.0, 2.6 Hz, 1H), 7.22 (d, J = 2.4 Hz, 1H), 5.52 (s, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 194.4, 156.0, 136.0, 134.3, 132.5, 131.9, 130.1, 129.8, 129.7, 129.4, 128.9, 128.8, 127.9, 127.7, 127.1, 126.9, 126.5, 124.1, 123.7, 118.8, 107.4, 71.0.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{22}H_{17}O_2^+$: 313.1223, found: 313.1231.

2-(Naphthalen-2-yloxy)-1-(3,4,5-trimethoxyphenyl)ethanone (1h)



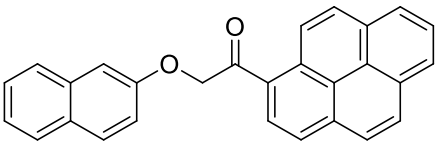
White crystals (3.789 g, 62 %, mp = 110-111 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 7.82 – 7.77 (m, 2H), 7.73 (d, J = 8.1 Hz, 1H), 7.46 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H), 7.41 – 7.33 (m, 3H), 7.28 (dd, J = 9.0, 2.6 Hz, 1H), 7.15 (d, J = 2.4 Hz, 1H), 5.35 (s, 2H), 3.96 (s, 3H), 3.94 (s, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 193.5, 155.9, 153.2, 143.4, 134.3, 129.8, 129.7, 129.4, 127.7, 126.9, 126.6, 124.1, 118.6, 107.4, 105.9, 71.1, 61.0, 56.4.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{21}O_5^+$: 353.1384, found: 353.1378.

2-(Naphthalen-2-yloxy)-1-(pyren-1-yl)ethanone (1i)



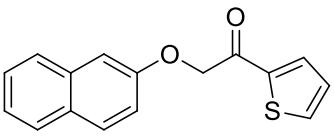
Yellow powder (5.294 g, 79 %, mp = 130-131°C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 9.05 (d, J = 9.4 Hz, 1H), 8.42 (d, J = 8.1 Hz, 1H), 8.28 – 8.21 (m, 3H), 8.21 – 8.16 (m, 2H), 8.11 – 8.03 (m, 2H), 7.81 – 7.76 (m, 2H), 7.74 (d, J = 8.2 Hz, 1H), 7.46 (ddd, J = 8.2, 6.8, 1.4 Hz, 1H), 7.37 (ddd, J = 8.0, 6.8, 1.3 Hz, 1H), 7.30 (dd, J = 9.0, 2.6 Hz, 1H), 7.25 (d, J = 2.6 Hz, 1H), 5.56 (s, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 198.5, 156.0, 134.5, 134.3, 131.0, 130.5, 130.2, 130.2, 130.1, 129.8, 129.4, 128.7, 127.7, 127.0, 126.9, 126.6, 126.5, 126.5, 126.4, 126.3, 125.0, 124.5, 124.1, 124.0, 123.9, 118.7, 107.4, 72.3.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{28}H_{19}O_2^+$: 387.1380, found: 387.1368.

2-(Naphthalen-2-yloxy)-1-(thiophen-2-yl)ethanone (1j)



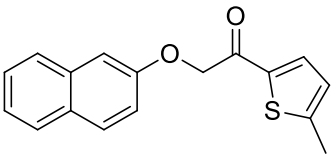
White crystals (3.490 g, 75 %, mp = 80-81 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.04 (dd, J = 3.8, 0.8 Hz, 1H), 7.83 – 7.79 (m, 2H), 7.77 – 7.71 (m, 2H), 7.47 (ddd, J = 8.1, 6.9, 1.0 Hz, 1H), 7.38 (ddd, J = 7.9, 6.9, 1.1 Hz, 1H), 7.31 (dd, J = 9.1, 2.7 Hz, 1H), 7.21 – 7.17 (m, 2H), 5.22 (s, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 188.2, 155.8, 140.6, 134.7, 134.3, 133.3, 129.9, 129.5, 128.3, 127.7, 127.0, 126.6, 124.2, 118.5, 107.4, 71.6.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{16}H_{13}O_2S^+$: 269.0631, found: 269.0639.

1-(5-Methylthiophen-2-yl)-2-(naphthalen-2-yloxy)ethanone (1k)



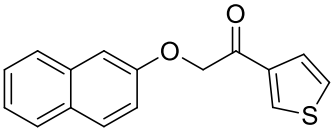
White crystals (3.819 g, 78 %, mp = 75-76 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 7.86 (d, J = 3.8 Hz, 1H), 7.82 – 7.78 (m, 2H), 7.74 (d, J = 8.1 Hz, 1H), 7.46 (ddd, J = 8.1, 6.8, 1.0 Hz, 1H), 7.38 (ddd, J = 7.8, 6.8, 0.9 Hz, 1H), 7.30 (dd, J = 9.2, 2.3 Hz, 1H), 7.17 (d, J = 2.5 Hz, 1H), 6.85 (d, J = 3.7 Hz, 1H), 5.17 (s, 2H), 2.57 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 187.7, 155.9, 151.0, 138.5, 134.3, 134.0, 129.8, 129.4, 127.7, 127.1, 127.0, 126.5, 124.1, 118.6, 107.4, 71.4, 16.0.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{17}H_{15}O_2S^+$: 283.0787, found: 283.0777.

2-(Naphthalen-2-yloxy)-1-(thiophen-3-yl)ethanone (1l)



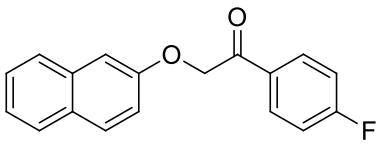
White crystals (4.281 g, 92 %, mp = 85-86 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.36 (dd, J = 2.9, 1.2 Hz, 1H), 7.83 – 7.77 (m, 2H), 7.74 (d, J = 8.2 Hz, 1H), 7.69 (dd, J = 5.1, 1.2 Hz, 1H), 7.47 (ddd, J = 8.2, 6.9, 1.3 Hz, 1H), 7.41 – 7.35 (m, 2H), 7.29 (dd, J = 8.9, 2.7 Hz, 1H), 7.16 (d, J = 2.5 Hz, 1H), 5.22 (s, 2H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 189.4, 155.9, 139.1, 134.3, 133.4, 129.8, 129.4, 127.7, 127.1, 126.9, 126.6, 126.5, 124.1, 118.6, 107.3, 71.8.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{16}H_{13}O_2S^+$: 269.0631, found: 269.0634.

1-(4-Fluorophenyl)-2-(naphthalen-2-yloxy)ethanone (1m)



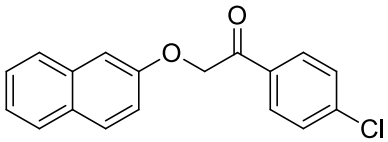
White crystals (4.132 g, 85 %, mp = 99-101 °C (lit.[1] 99-101 °C)).

^1H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.15 – 8.07 (m, 2H), 7.84 – 7.76 (m, 2H), 7.74 (d, J = 8.1 Hz, 1H), 7.47 (ddd, J = 8.1, 7.0, 1.2 Hz, 1H), 7.38 (ddd, J = 8.0, 7.0, 1.2 Hz, 1H), 7.28 (dd, J = 8.9, 2.6 Hz, 1H), 7.24 – 7.16 (m, 2H), 7.15 (d, J = 2.5 Hz, 1H), 5.34 (s, 2H, CH_2).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 193.2, 166.2 (d, J_{C-F} = 256.2 Hz), 155.8, 134.3, 131.1 (d, J_{C-F} = 3.2 Hz), 131.1 (d, J_{C-F} = 9.4 Hz), 129.8, 129.42, 127.70, 126.88, 126.6, 124.2, 118.6, 116.1 (d, J_{C-F} = 22.0 Hz), 107.3, 70.9.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{18}H_{14}FO_2^+$: 281.0972, found: 281.0969.

1-(4-Chlorophenyl)-2-(naphthalen-2-yloxy)ethanone (1n)



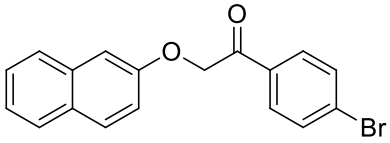
White crystals (4.324 g, 84 %, mp = 104-105 °C (lit.[1] 110-112 °C)).

^1H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.01 (d, J = 8.5 Hz, 2H), 7,83 – 7.76 (m, 2H), 7.73 (d, J = 8.1 Hz, 1H), 7.54 – 7.42 (m, 3H), 7.42 – 7.34 (m, 1H), 7.30 – 7.23 (m, 1H), 7.14 (d, J = 2.2 Hz, 1H), 5.33 (s, 2H, CH_2).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 193.6, 155.8, 140.4, 134.3, 132.9, 129.8, 129.8, 129.4, 129.2, 127.7, 126.9, 126.6, 124.2, 118.6, 107.3, 71.0.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{18}H_{14}ClO_2^+$: 297.0677, found: 297.0680.

1-(4-Bromophenyl)-2-(naphthalen-2-yloxy)ethanone (1o)



White crystals (4.973 g, 84 %, mp = 119-120 °C).

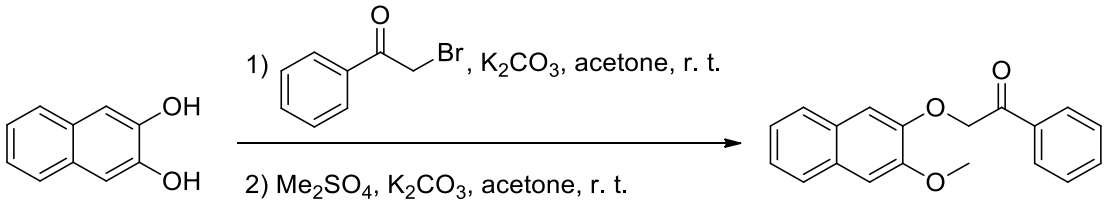
^1H NMR (300 MHz, $CDCl_3$), δ, ppm: 7.93 (d, *J* = 8.5 Hz, 2H), 7.79 (m, 2H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.50 – 7.42 (m, 1H), 7.41 – 7.34 (m, 1H), 7.26 (dd, *J* = 9.1, 2.3 Hz, 1H), 7.14 (d, *J* = 2.3 Hz, 1H), 5.32 (s, 2H, CH_2).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 193.8, 155.8, 134.3, 133.3, 132.2, 129.9, 129.8, 129.4, 129.2, 127.7, 126.9, 126.6, 124.2, 118.6, 107.3, 70.9.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{18}H_{14}BrO_2^+$: 341.0172, found: 341.0183.

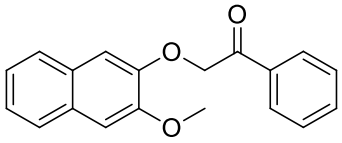
[1] T. B. Mete, D. Laha, R. G. Bhat, *ChemistrySelect*, **2018**, 3, 7656

IV. Synthesis of ketoether 1p



1p

2,3-Dihydroxynaphthalene (5 g, 31.25 mmol) was dissolved in 55 ml of acetone, K_2CO_3 (4.744 g, 34.38 mmol) was added and the mixture was stirred at room temperature for 30 minutes. Then 2-bromo-1-phenylethanone (6.219 g, 31.25 mmol) was added and the reaction mixture was stirred at room temperature for 24 hours. After that, K_2CO_3 (4.313 g, 31.25 mmol) and Me_2SO_4 (2.96 ml, 31.25 mmol) were added and this mixture was stirred again for 24 hours. The resulting mixture was filtered; the solvent was evaporated in vacuo. Ketoether **1p** was isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 4:1).



2-((3-Methoxynaphthalen-2-yl)oxy)-1-phenylethanone (1p)

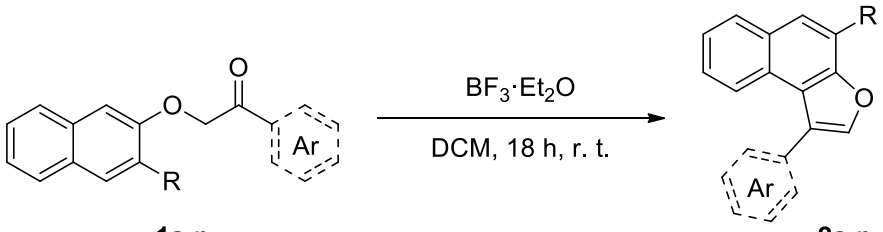
White powder (3.65 g, 40 %, mp = 101-102 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.10 – 8.05 (m, 2H), 7.70 (d, J = 7.9 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.56 – 7.49 (m, 2H), 7.40 – 7.29 (m, 2H), 7.17 (s, 1H), 7.09 (s, 1H), 5.47 (s, 2H), 4.02 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 194.0, 149.7, 147.9, 134.6, 133.9, 129.8, 128.9, 128.8, 128.2, 126.5, 126.3, 124.6, 124.2, 108.9, 107.0, 71.5, 55.9.

HRMS (ESI-TOF): m/z $[M+Na]^+$ calcd for $C_{19}H_{16}O_3Na^+$: 315.0992, found: 315.0993.

V. Synthesis of 1-arylnaphtho[2,1-*b*]furans 2a-p

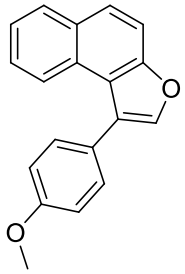


1a-p
R = H, OMe

2a-p

Ketoether **1a-p** (3.43 mmol) was dissolved in 30 ml of DCM, $BF_3 \cdot Et_2O$ (0.85 ml, 6.86 mmol) was added and the reaction mixture was stirred at room temperature for 18 hours. After completion of the reaction, the resulting solution was poured into ice and left for 24 hours. Then the organic phase was separated, washed successively with a saturated solution of $NaHCO_3$, a saturated solution of NaCl and dried over $CaCl_2$. 1-Arylnaphtho[2,1-*b*]furan **2a-p** was isolated using flash chromatography on silica gel.

1-(4-Methoxyphenyl)naphtho[2,1-*b*]furan (2a)



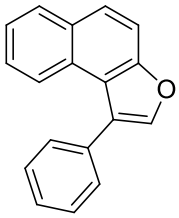
Colourless oil (714 mg, 76 %, petroleum ether/ethyl acetate = 20:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.06 (d, J = 8.2 Hz, 1H), 7.98 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 9.0 Hz, 1H), 7.73 (d, J = 9.0 Hz, 1H), 7.70 (s, 1H), 7.55 (d, J = 8.7 Hz, 1H), 7.48 (ddd, J = 8.1, 7.0, 1.5 Hz, 1H), 7.41 (ddd, J = 8.1, 7.0, 1.5 Hz, 1H), 7.09 (d, J = 8.7 Hz, 1H), 3.95 (s, 3H, OMe).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 159.5, 153.1, 141.6, 131.0, 130.8, 128.9, 128.4, 126.0, 125.8, 125.2, 124.3, 124.0, 123.4, 121.0, 114.0, 112.7, 55.4.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{19}H_{15}O_2^+$: 275.1067, found: 275.1068.

1-Phenylnaphtho[2,1-*b*]furan (2b)



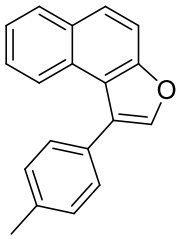
Colourless oil (795 mg, 95 %, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.04 (d, J = 8.3 Hz, 1H), 7.98 (d, J = 7.6 Hz, 1H), 7.81 (d, J = 9.0 Hz, 1H), 7.74 (d, J = 8.8 Hz, 1H), 7.73 (s, 1H), 7.68 – 7.63 (m, 2H), 7.60 – 7.51 (m, 3H), 7.47 (ddd, J = 8.2, 6.9, 1.4 Hz, 1H), 7.40 (ddd, J = 8.3, 7.0, 1.5 Hz, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 153.2, 141.7, 133.2, 130.9, 129.9, 128.9, 128.6, 128.4, 127.9, 126.0, 126.0, 124.5, 124.4, 123.4, 120.8, 112.7.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{18}H_{13}O^+$: 245.0961, found: 245.0965.

1-(*p*-Tolyl)naphtho[2,1-*b*]furan (2c)



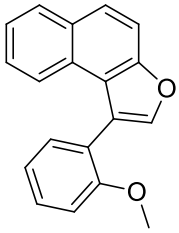
Colourless oil (646 mg, 73 %, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.08 (d, J = 8.2 Hz, 1H), 7.98 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 9.0 Hz, 1H), 7.73 (d, J = 9.0 Hz, 1H), 7.71 (s, 1H), 7.54 (d, J = 8.0 Hz, 2H), 7.48 (ddd, J = 8.1, 7.0, 1.4 Hz, 1H), 7.44 – 7.35 (m, 3H), 2.52 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 153.1, 141.6, 137.6, 130.8, 130.0, 129.8, 129.3, 128.9, 128.4, 125.9, 125.9, 124.4, 124.3, 123.4, 120.9, 112.7, 21.4.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{19}H_{15}O^+$: 259.1117, found: 259.1007.

1-(2-Methoxyphenyl)naphtho[2,1-*b*]furan (2d)



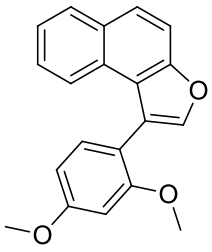
Yellowish oil (620 mg, 66 %, petroleum ether/ethyl acetate = 20:1)

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 7.96 (d, J = 8.0 Hz, 1H), 7.82 – 7.72 (m, 4H), 7.56 – 7.42 (m, 3H), 7.37 (ddd, J = 8.2, 7.0, 1.4 Hz, 1H), 7.18 – 7.09 (m, 2H), 3.75 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 157.9, 152.9, 141.9, 131.9, 130.7, 129.7, 128.8, 128.6, 125.8, 125.6, 124.2, 123.4, 122.1, 121.7, 120.7, 120.4, 112.7, 110.9, 55.5.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{19}H_{15}O_2^+$: 275.1067, found: 275.1064.

1-(2,4-Dimethoxyphenyl)naphtho[2,1-*b*]furan (2e)



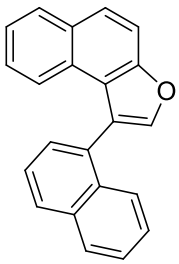
(646 mg, 62 %, petroleum ether/ethyl acetate = 10:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 7.96 (d, J = 8.3 Hz, 1H), 7.82 (d, J = 8.2 Hz, 1H), 7.78 (d, J = 9.4 Hz, 1H), 7.75 – 7.71 (m, 2H), 7.45 (ddd, J = 8.2, 7.1, 1.4 Hz, 1H), 7.42 – 7.35 (m, 2H), 6.71 (d, J = 2.3 Hz, 1H), 6.66 (dd, J = 8.2, 2.4 Hz, 1H), 3.96 (s, 3H), 3.73 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 161.3, 158.9, 152.9, 141.9, 132.2, 130.7, 128.8, 128.6, 125.7, 125.5, 124.1, 123.4, 121.9, 120.1, 114.5, 112.7, 104.3, 99.0, 55.5, 55.5.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{20}H_{17}O_3^+$: 305.1172, found: 305.1169.

1-(Naphthalen-1-yl)naphtho[2,1-*b*]furan (2f)



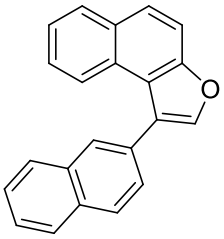
Colourless oil (928 mg, 92 %, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.10 – 8.01 (m, 2H), 7.98 (d, J = 8.1 Hz, 1H), 7.90 – 7.80 (m, 4H), 7.74 – 7.62 (m, 2H), 7.61 – 7.53 (m, 1H), 7.45 – 7.32 (m, 3H), 7.19 – 7.11 (m, 1H).

^{13}C{^{1}H} NMR (75 MHz, CDCl3), δ, ppm: 153.0, 142.5, 133.7, 133.1, 130.8, 130.6, 128.8, 128.7, 128.3, 128.3, 126.5, 126.4, 126.2, 126.1, 126.1, 126.1, 125.6, 124.4, 123.5, 122.2, 122.0, 112.7.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{22}H_{15}O^+$: 295.1117, found: 295.1121.

1-(Naphthalen-2-yl)naphtho[2,1-*b*]furan (2g)



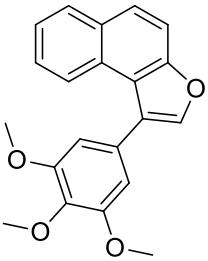
Colourless oil (706 mg, 70 %, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.11 (s, 1H), 8.09 – 7.93 (m, 5H), 7.87 – 7.75 (m, 4H), 7.65 – 7.57 (m, 2H), 7.48 (ddd, J = 8.1, 7.0, 1.1 Hz, 1H), 7.36 (ddd, J = 8.2, 7.0, 1.3 Hz, 1H).

^{13}C{^{1}H} NMR (75 MHz, CDCl3), δ, ppm: 153.3, 141.9, 133.5, 132.9, 130.9, 130.6, 129.0, 128.5, 128.4, 128.2, 128.1, 128.1, 127.9, 126.5, 126.3, 126.1, 126.1, 124.5, 124.4, 123.5, 120.9, 112.7.

HRMS (ESI-TOF): m/z $[M+H+O_2]^+$ calcd for $C_{22}H_{15}O_3^+$: 327.1016, found: 327.1018.

1-(3,4,5-Trimethoxyphenyl)naphtho[2,1-*b*]furan (2h)



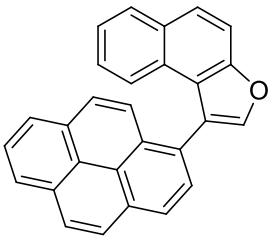
Colourless oil (859 mg, 75 %, petroleum ether/ethyl acetate = 10:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.15 – 8.10 (m, 1H), 8.01 – 7.96 (m, 1H), 7.80 (d, J = 9.0 Hz, 1H), 7.74 (s, 1H), 7.72 (d, J = 9.0 Hz, 1H), 7.53 – 7.40 (m, 2H), 6.85 (s, 2H), 4.01 (s, 3H), 3.91 (s, 6H).

^{13}C{^{1}H} NMR (75 MHz, CDCl3), δ, ppm: 153.3, 153.1, 141.6, 137.8, 130.8, 129.0, 128.5, 128.2, 126.0, 126.0, 124.5, 124.4, 123.5, 120.7, 112.7, 107.0, 61.1, 56.2.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{19}O_4^+$: 335.1278, found: 335.1283.

1-(Pyren-1-yl)naphtho[2,1-*b*]furan (2i)



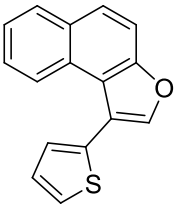
Yellow powder (985 mg, 78 %, mp = 75-76 °C, petroleum ether/ethyl acetate = 10:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.34 (d, J = 7.8 Hz, 1H), 8.29 (dd, J = 7.6, 1.0 Hz, 1H), 8.23 – 8.16 (m, 4H), 8.08 (d, J = 7.6 Hz, 1H), 8.06 – 8.03 (m, 1H), 7.99 – 7.94 (m, 2H), 7.92 (s, 1H), 7.91 – 7.83 (m, 2H), 7.35 (ddd, J = 8.1, 6.9, 1.1 Hz, 1H), 7.27 (d, J = 8.3 Hz, 1H), 7.00 (ddd, J = 8.3, 6.9, 1.2 Hz, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 153.1, 142.8, 131.4, 131.4, 131.1, 130.8, 130.5, 128.7, 128.6, 128.3, 128.0, 127.8, 127.8, 127.5, 126.2, 126.2, 126.1, 125.5, 125.4, 125.3, 124.9, 124.9, 124.8, 124.4, 123.4, 122.4, 122.3, 112.7.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{28}H_{17}O^+$: 369.1274, found: 369.1272.

1-(Thiophen-2-yl)naphtho[2,1-*b*]furan (2j)



Colourless oil (763 mg, 89%, petroleum ether).

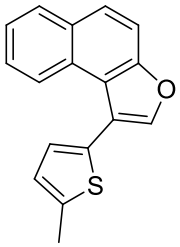
^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.24 – 8.19 (m, 1H), 8.01 – 7.97 (m, 1H), 7.82 (s, 1H), 7.82 (d, J = 8.9 Hz, 1H), 7.72 (d, J = 9.0 Hz, 1H), 7.54 – 7.43 (m, 3H), 7.35 (dd, J =

3.5, 1.2 Hz, 1H), 7.27 (dd, J = 5.2, 3.5 Hz, 1H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 153.1, 143.0, 133.2, 130.9, 128.9, 128.2, 127.6, 126.3, 126.2, 126.2, 126.2, 124.6, 123.2, 121.0, 116.9, 112.6.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{16}H_{11}OS^+$: 251.0525, found: 251.0532.

1-(5-Methylthiophen-2-yl)naphtho[2,1-*b*]furan (2k)



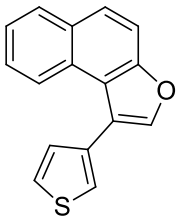
Colourless oil (815 mg, 90%, petroleum ether).

^1H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.33 – 8.25 (m, 1H), 8.01 – 7.93 (m, 1H), 7.82 – 7.77 (m, 2H), 7.70 (d, J = 8.9 Hz, 1H), 7.53 – 7.44 (m, 2H), 7.11 (d, J = 3.4 Hz, 1H), 6.89 (dd, J = 3.3, 1.0 Hz, 1H), 2.63 (s, 3H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 153.1, 142.9, 140.7, 130.9, 130.7, 128.8, 128.3, 128.1, 126.1, 126.1, 125.7, 124.5, 123.3, 121.0, 117.3, 112.5, 15.4.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{17}H_{13}OS^+$: 265.0682, found: 265.0687.

1-(Thiophen-3-yl)naphtho[2,1-*b*]furan (2l)



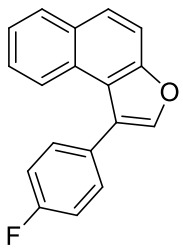
Colourless oil (755 mg, 88%, petroleum ether).

^1H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.12 – 8.07 (m, 1H), 8.01 – 7.96 (m, 1H), 7.80 (d, J = 9.0 Hz, 1H), 7.76 (s, 1H), 7.72 (d, J = 9.0 Hz, 1H), 7.56 (dd, J = 4.9, 3.0 Hz, 1H), 7.52 – 7.42 (m, 3H), 7.39 (dd, J = 4.9, 1.3 Hz, 1H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 153.1, 141.9, 132.8, 130.8, 129.4, 128.9, 128.4, 126.2, 126.1, 126.0, 124.5, 123.9, 123.4, 121.0, 119.1, 112.7.

HRMS (ESI-TOF): m/z $[M+O_2+H]^+$ calcd for $C_{16}H_{11}O_3S^+$: 283.0423, found: 283.0428.

1-(4-Fluorophenyl)naphtho[2,1-*b*]furan (2m)



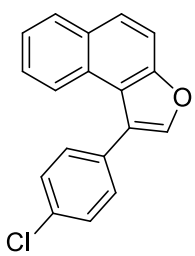
Colourless oil (818 mg, 91 %, petroleum ether).

^1H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.01 – 7.95 (m, 2H), 7.81 (d, J = 9.0 Hz, 1H), 7.74 (d, J = 9.0 Hz, 1H), 7.71 (s, 1H), 7.64 – 7.56 (m, 2H), 7.49 (ddd, J = 8.1, 7.0, 1.4 Hz, 1H), 7.42 (ddd, J = 8.3, 7.0, 1.4 Hz, 1H), 7.30 – 7.20 (m, 2H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 162.7 (d, J_{C-F} = 246.9 Hz), 153.2, 141.7, 131.5 (d, J_{C-F} = 8.0 Hz), 130.8, 129.0, 129.0, 129.0 (d, J_{C-F} = 3.6 Hz), 128.2, 126.1, 124.5, 123.4, 123.1, 120.7, 115.6 (d, J_{C-F} = 21.5 Hz), 112.7.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{18}H_{11}FO^+$: 262.0788, found: 262.0776.

1-(4-Chlorophenyl)naphtho[2,1-*b*]furan (2n)



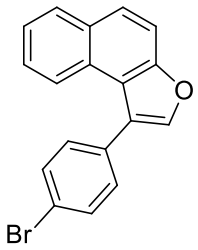
Colourless oil (850 mg, 89%, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.01 – 7.95 (m, 2H), 7.81 (d, J = 9.0 Hz, 1H), 7.73 (d, J = 9.0 Hz, 1H), 7.70 (s, 1H), 7.57 (d, J = 8.5 Hz, 2H), 7.53 (d, J = 8.5 Hz, 2H), 7.49 (ddd, J = 8.0, 7.1 Hz, 1.3 Hz 1H), 7.42 (ddd, J = 8.0, 7.1 Hz, 1.3 Hz, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 153.3, 141.8, 134.0, 131.6, 131.2, 130.9, 129.1, 128.9, 128.2, 126.2, 126.2, 124.5, 123.3, 123.2, 120.5, 112.7.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{18}H_{12}ClO^+$: 279.0571, found: 279.0572.

1-(4-Bromophenyl)naphtho[2,1-*b*]furan (2o)



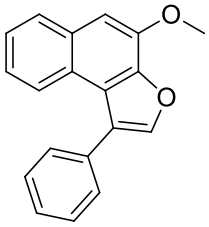
Colourless oil (1008 mg, 91%, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.01 – 7.95 (m, 2H), 7.81 (d, *J* = 9.0 Hz, 1H), 7.73 (d, *J* = 9.0 Hz, 1H), 7.71 – 7.66 (m, 3H), 7.54 – 7.46 (m, 3H), 7.45 – 7.39 (m, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 153.3, 141.7, 132.1, 131.8, 131.5, 130.9, 129.0, 128.2, 126.2, 126.2, 124.5, 123.4, 123.4, 122.1, 120.4, 112.6.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{18}H_{12}BrO^+$: 323.0066, found: 323.0069.

4-Methoxy-1-phenylnaphtho[2,1-*b*]furan (2p)



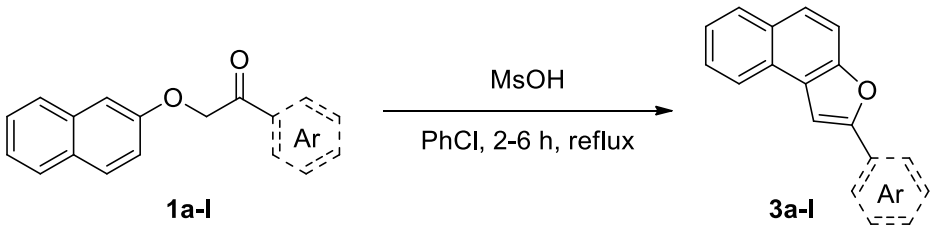
Colourless oil (752 mg, 80 %, petroleum ether/ethyl acetate = 20:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 7.93 (d, J = 8.3 Hz, 1H), 7.86 (d, J = 8.1 Hz, 1H), 7.73 (s, 1H), 7.66 – 7.60 (m, 2H), 7.58 – 7.49 (m, 3H), 7.43 (ddd, J = 8.1, 7.0, 1.1 Hz, 1H), 7.25 (ddd, J = 8.1, 7.0, 1.1 Hz, 1H), 7.13 (s, 1H), 4.16 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 145.8, 144.8, 142.0, 132.7, 132.1, 129.9, 128.6, 128.0, 127.7, 124.9, 124.8, 124.0, 123.8, 123.2, 122.5, 103.4, 55.9.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{19}H_{14}O_2^+$: 274.0988, found: 274.0990.

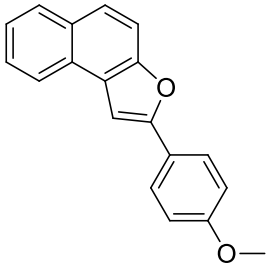
VI. Synthesis of 2-arylnaphtho[2,1-*b*]furans 3a-l



1a-l **3a-l**

Ketoether **1a-l** (3.43 mmol) was dissolved in 30 ml of PhCl, MsOH (2.23 ml, 34.3 mmol) was added and the reaction mixture was refluxed for 2-6 hours (TLC monitoring). After completion of the reaction, the resulting solution was poured into water (300 ml) and neutralized to pH = 7 by $NaHCO_3$. Then the organic phase was separated, washed with water and dried over $CaCl_2$. The solvent was evaporated in vacuum, 2-arylnaphtho[2,1-*b*]furan **3a-l** was isolated using flash chromatography on silica gel.

2-(4-Methoxyphenyl)naphtho[2,1-*b*]furan (3a)



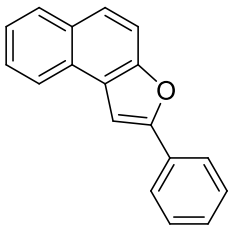
Yellowish powder (686 mg, 73 %, mp = 147-148 °C, petroleum ether/ethyl acetate = 20:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.19 (d, J = 8.1 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.93 – 7.86 (m, 2H), 7.76 – 7.67 (m, 2H), 7.61 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.51 (ddd, J = 8.1, 7.0, 1.1 Hz, 1H), 7.41 (s, 1H), 7.07 – 7.00 (m, 2H), 3.90 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 159.8, 155.6, 152.1, 130.5, 128.8, 127.5, 126.2, 126.1, 124.8, 124.6, 124.5, 123.6, 123.5, 114.3, 112.2, 98.9, 55.4.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{19}H_{14}O_2^+$: 274.0986, found: 274.0988.

2-Phenylnaphtho[2,1-*b*]furan (3b)



White powder (762 mg, 91 %, mp = 142-143 °C (lit.[1] 143-145 °C), petroleum ether).

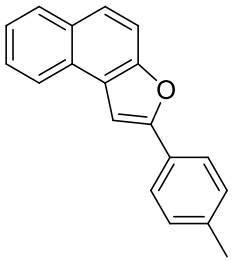
^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.21 (d, J = 8.2 Hz, 1H), 8.02 – 7.94 (m, 3H), 7.76 (d, J = 9.0 Hz, 1H), 7.72 (d, J = 9.1 Hz, 1H), 7.63 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.57 – 7.48 (m, 4H), 7.42 – 7.36 (m, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 155.4, 152.4, 130.7, 130.5, 128.9, 128.9, 128.3, 127.7, 126.3, 125.2, 124.7, 124.6, 124.6, 123.5, 112.3, 100.5.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{18}H_{12}O^+$: 244.0883, found: 244.0893.

[1] Upendra Sharma, Togati Naveen, Arun Maji, Srimanta Manna, Debabrata Maiti, *Angew. Chem. Int. Ed.* **2013**, 52, 12669 –12673

2-(*p*-Tolyl)naphtho[2,1-*b*]furan (3c)



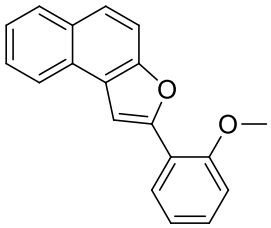
White powder (619 mg, 70 %, mp = 147-148 °C, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.20 (d, J = 8.1 Hz, 1H), 7.99 (d, J = 8.1 Hz, 1H), 7.87 (d, J = 8.0 Hz, 2H), 7.79 – 7.70 (m, 2H), 7.67 – 7.60 (m, 1H), 7.58 – 7.50 (m, 1H), 7.49 (s, 1H), 7.32 (d, J = 8.0 Hz, 2H), 2.46 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 155.7, 152.2, 138.3, 130.5, 129.6, 128.8, 128.0, 127.6, 126.2, 124.9, 124.7, 124.5, 123.5, 112.3, 99.8, 21.4.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{19}H_{14}O^+$: 258.1039, found: 258.1038.

2-(2-Methoxyphenyl)naphtho[2,1-*b*]furan (3d)



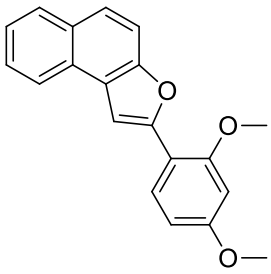
Yellowish powder (583 mg, 62 %, mp = 130-131 °C, petroleum ether/ethyl acetate = 20:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.28 (d, J = 8.1 Hz, 1H), 8.18 (dd, J = 7.8, 1.7 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H), 7.89 (s, 1H), 7.77 (d, J = 9.1 Hz, 1H), 7.73 (d, J = 9.1 Hz, 1H), 7.64 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.53 (ddd, J = 8.1, 7.0, 1.2 Hz, 1H), 7.37 (ddd, J = 8.3, 7.5, 1.7 Hz, 1H), 7.19 – 7.12 (m, 1H), 7.08 (d, J = 8.3 Hz, 1H), 4.09 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 156.2, 151.8, 151.4, 130.4, 129.0, 128.8, 127.9, 126.8, 126.1, 125.0, 1245.0, 124.4, 123.6, 120.9, 119.6, 112.2, 111.1, 105.5, 55.6.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{19}H_{15}O_2^+$: 275.1067, found: 275.1069.

2-(2,4-Dimethoxyphenyl)naphtho[2,1-*b*]furan (3e)



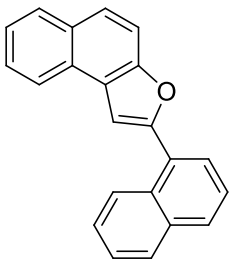
Yellowish powder (594 mg, 57 %, mp = 134-135 °C, petroleum ether/ethyl acetate = 20:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.26 (d, J = 8.1 Hz, 1H), 8.07 (d, J = 8.6 Hz, 1H), 7.98 (d, J = 8.1 Hz, 1H), 7.73 – 7.72 (m, 3H), 7.61 (ddd, J = 8.1, 7.0, 1.0 Hz, 1H), 7.51 (ddd, J = 7.9, 7.0, 1.0 Hz, 1H), 6.68 (dd, J = 8.6, 2.3 Hz, 1H), 6.63 (d, J = 2.2 Hz, 1H), 4.06 (s, 3H), 3.90 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 160.7, 157.5, 152.0, 151.0, 130.4, 128.7, 127.8, 127.7, 125.9, 125.1, 124.4, 124.3, 123.7, 113.0, 112.1, 104.9, 103.4, 98.8, 55.6, 55.5.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{20}H_{16}O_3^+$: 304.1094, found: 304.1083.

2-(Naphthalen-1-yl)naphtho[2,1-*b*]furan (3f)



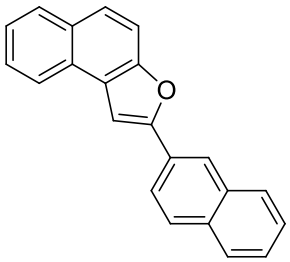
White powder (726 mg, 72 %, mp = 153-154 °C, petroleum ether/ethyl acetate = 30:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.61 (d, J = 8.1 Hz, 1H), 8.27 (d, J = 8.2 Hz, 1H), 8.04 – 7.94 (m, 4H), 7.82 – 7.79 (m, 2H), 7.69 – 7.59 (m, 5H), 7.55 (ddd, J = 8.1, 7.0, 1.2 Hz, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 155.1, 152.6, 134.1, 130.7, 130.5, 129.4, 128.9, 128.7, 128.4, 127.7, 127.2, 127.0, 126.4, 126.2, 125.6, 125.4, 125.3, 124.6, 124.4, 123.5, 112.4, 105.0.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{22}H_{14}O^+$: 294.1039, found: 294.1029.

2-(Naphthalen-2-yl)naphtho[2,1-*b*]furan (3g)



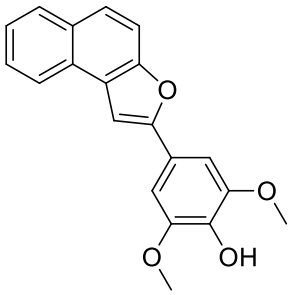
White powder (686 mg, 68 %, mp = 153-154 °C, petroleum ether/ethyl acetate = 30:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.45 (s, 1H), 8.23 (d, J = 8.0 Hz, 1H), 8.08 – 7.93 (m, 4H), 7.89 (d, J = 7.0 Hz, 1H), 7.83 – 7.73 (m, 2H), 7.69 – 7.60 (m, 2H), 7.59 – 7.50 (m, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 155.5, 152.6, 133.6, 133.2, 130.5, 128.9, 128.6, 128.4, 127.9, 127.8, 127.6, 126.7, 126.4, 126.3, 125.4, 124.7, 124.6, 123.5, 123.4, 122.7, 112.3, 101.1.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{22}H_{14}O^+$: 294.1039, found: 294.1037.

2,6-dimethoxy-4-(naphtho[2,1-b]furan-2-yl)phenol (3h)



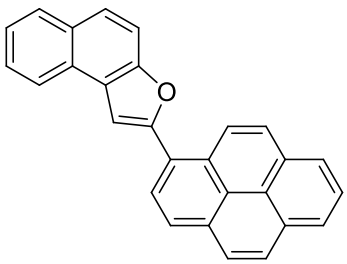
Beige powder (439 mg, 40 %, mp = 158-159 °C, petroleum ether/ethyl acetate = 4:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.18 (d, J = 8.1 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 9.1 Hz, 1H), 7.70 (d, J = 9.1 Hz, 1H), 7.62 (ddd, J = 8.1, 6.9, 0.9 Hz, 1H), 7.52 (ddd, J = 8.0, 7.0, 0.9 Hz, 1H), 7.41 (s, 1H), 7.18 (s, 2H), 5.70 (s, 1H, OH), 4.04 (s, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 155.5, 152.0, 147.4, 135.3, 130.4, 128.8, 127.5, 126.2, 124.8, 124.7, 124.6, 123.5, 122.2, 112.2, 101.7, 99.3, 56.4.

HRMS (ESI-TOF): m/z $[M+Na]^+$ calcd for $C_{20}H_{16}O_4Na^+$: 343.0941, found: 343.0939.

2-(Pyren-1-yl)naphtho[2,1-*b*]furan (3i)



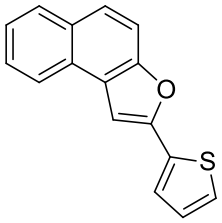
Yellow powder (884 mg, 70 %, mp = 157-158 °C, petroleum ether/ethyl acetate = 20:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.92 (d, J = 9.4 Hz, 1H), 8.50 (d, J = 8.0 Hz, 1H), 8.35 – 8.22 (m, 4H), 8.19 – 8.11 (m, 2H), 8.11 – 8.02 (m, 3H), 7.89 – 7.81 (m, 2H), 7.77 (s, 1H), 7.68 (ddd, J = 8.1, 7.0, 1.0 Hz, 1H), 7.57 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H).

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 155.5, 152.9, 131.5, 131.5, 131.1, 130.9, 130.5, 128.9, 128.5, 128.3, 128.1, 127.7, 127.4, 126.7, 126.4, 126.2, 125.9, 125.7, 125.4, 125.3, 125.0, 124.9, 124.9, 124.7, 124.6, 123.6, 112.4, 105.5.

HRMS (ESI-TOF): m/z $[M+O_2+H]^+$ calcd for $C_{28}H_{17}O_3^+$: 401.1172, found: 401.1163.

2-(Thiophen-2-yl)naphtho[2,1-*b*]furan (3j)



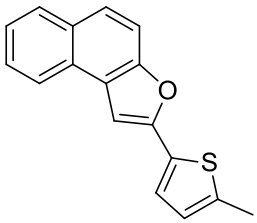
Beige powder (480 mg, 56 %, mp = 115-116 °C, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.17 (d, J = 8.1 Hz, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.76 (d, J = 9.0 Hz, 1H), 7.70 (d, J = 9.0 Hz, 1H), 7.63 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.58 – 7.50 (m, 2H), 7.40 – 7.37 (m, 2H), 7.16 (dd, J = 5.0, 3.7 Hz, 1H).

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 152.0, 150.9, 133.6, 130.5, 128.8, 128.0, 127.5, 126.3, 125.5, 125.3, 124.7, 124.5, 124.2, 123.5, 112.2, 100.4.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{16}H_{10}OS^+$: 250.0447, found: 250.0445.

2-(5-Methylthiophen-2-yl)naphtho[2,1-*b*]furan (3k)



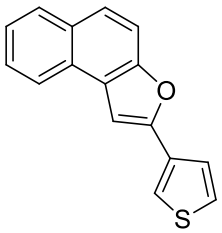
Brown powder (661 mg, 73 %, mp = 122-123 °C, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.15 (d, J = 8.1 Hz, 1H), 7.96 (d, J = 7.9 Hz, 1H), 7.72 (d, J = 8.9 Hz, 1H), 7.67 (d, J = 9.0 Hz, 1H), 7.60 (ddd, J = 8.1, 7.1, 1.1 Hz, 1H), 7.50 (ddd, J = 7.9, 7.0, 1.0 Hz, 1H), 7.34 (d, J = 3.5 Hz, 1H), 6.80 (d, J = 3.5 Hz, 1H), 2.58 (s, 3H).

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 151.8, 151.1, 140.5, 131.2, 130.5, 128.8, 127.4, 126.2, 126.2, 124.9, 124.6, 124.6, 124.2, 123.5, 112.1, 99.6, 15.4.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{17}H_{12}OS^+$: 264.0603, found: 264.0599.

2-(Thiophen-3-yl)naphtho[2,1-*b*]furan (3l)



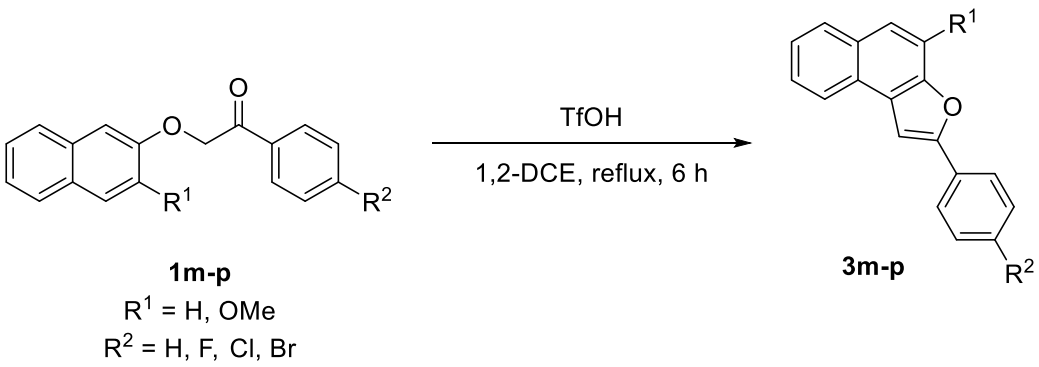
Gray powder (695 mg, 81 %, mp = 132-133 °C, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.18 (d, J = 8.1 Hz, 1H), 7.98 (d, J = 8.1 Hz, 1H), 7.78 (dd, J = 2.8, 1.0 Hz, 1H), 7.75 (d, J = 9.0 Hz, 1H), 7.70 (d, J = 9.0 Hz, 1H), 7.62 (ddd, J = 8.2, 7.1, 1.1 Hz, 1H), 7.56 (dd, J = 5.1, 1.0 Hz, 1H), 7.52 (ddd, J = 8.0, 7.2, 1.1 Hz, 1H), 7.45 (dd, J = 5.0, 3.0 Hz, 1H), 7.36 (s, 1H).

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 152.3, 151.9, 132.4, 130.5, 128.8, 127.6, 126.6, 126.2, 125.1, 125.0, 124.6, 124.4, 123.5, 120.8, 112.2, 100.3.

HRMS (ESI-TOF): m/z $[M+O_2+H]^+$ calcd for $C_{16}H_{11}O_3S^+$: 283.0428, found: 283.0423.

VII. Synthesis of 2-arylnaphtho[2,1-*b*]furans 3m-p

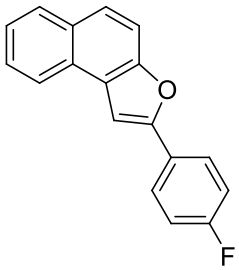


1m-p
R^1 = H, OMe
R^2 = H, F, Cl, Br

3m-p

Ketoether **1m-p** (3.43 mmol) was dissolved in 30 ml of 1,2-DCE, TfOH (0.61 ml, 6.86 mmol) was added and the reaction mixture was refluxed for 6 hours (TLC monitoring). After completion of the reaction, the resulting solution was poured into water (300 ml) and neutralized to pH = 7 by $NaHCO_3$. Then the organic phase was separated, washed with water and dried over $CaCl_2$. The solvent was evaporated in vacuum, 2-arylnaphtho[2,1-*b*]furan **3m-p** was isolated using flash chromatography on silica gel.

2-(4-Fluorophenyl)naphtho[2,1-*b*]furan (3m)



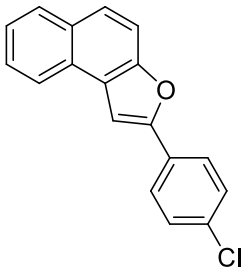
White powder (548 mg, 61 %, mp = 120-121 °C (lit.[1] 121-122 °C), petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.18 (d, J = 8.1 Hz, 1H), 7.98 (d, J = 8.2 Hz, 1H), 7.96 – 7.87 (m, 2H), 7.76 (d, J = 9.0 Hz, 1H), 7.70 (d, J = 9.1 Hz, 1H), 7.63 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.53 (ddd, J = 8.1, 7.0, 1.2 Hz, 1H), 7.46 (s, 1H), 7.24 – 7.15 (m, 2H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 162.7 (d, J_{C-F} = 248.4 Hz), 154.5, 152.3, 130.5, 128.8, 127.6, 127.0 (d, J_{C-F} = 3.3 Hz), 126.5 (d, J_{C-F} = 8.2 Hz), 126.3, 125.2, 124.6, 124.5, 123.4, 116.0 (d, J_{C-F} = 22.0 Hz), 112.2, 100.2.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{18}H_{11}FO^+$: 262.0788, found: 262.0793.

2-(4-Chlorophenyl)naphtho[2,1-*b*]furan (3n)



White powder (564 mg, 59 %, mp = 150-151 °C (lit.[2] 152.5-153.5 °C), petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.17 (d, J = 8.2 Hz, 1H), 7.98 (d, J = 8.1 Hz, 1H), 7.88 – 7.82 (m, 2H), 7.76 (d, J = 9.0 Hz, 1H), 7.69 (d, J = 9.0 Hz, 1H), 7.63 (ddd, J = 8.2, 7.1, 1.3 Hz, 1H), 7.53 (ddd, J = 8.2, 7.0, 1.3 Hz, 1H), 7.50 (s, 1H), 7.49 – 7.43 (m, 2H).

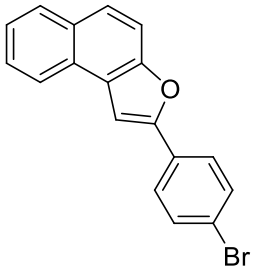
[1] Long Liu, Xuyu Ji, Jianyu Dong, Yongbo Zhou, Shuang-Feng Yin, *Org. Lett.* **2016**, 18, 13, 3138–3141

[2] Paul D. Seemuth, Hans Zimmer, *J. Org. Chem.* **1978**, 43, 15, 3063–3065

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 154.2, 152.5, 134.0, 130.5, 129.1, 129.1, 128.9, 127.6, 126.4, 125.8, 125.5, 124.7, 124.5, 123.4, 112.2, 100.9.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{18}H_{11}ClO^+$: 278.0493, found: 278.0494.

2-(4-Bromophenyl)naphtho[2,1-*b*]furan (3o)



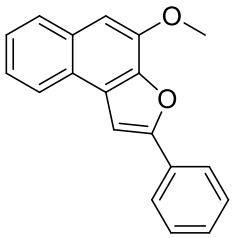
White powder (720 mg, 65 %, mp = 136-137 °C, petroleum ether).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.17 (d, J = 8.1 Hz, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.81 – 7.74 (m, 3H), 7.69 (d, J = 9.0 Hz, 1H), 7.66 – 7.58 (m, 3H), 7.56 – 7.49 (m, 2H).

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 154.2, 152.5, 132.0, 130.5, 129.6, 128.9, 127.6, 126.4, 126.1, 125.6, 124.7, 124.4, 123.4, 122.2, 112.2, 101.0.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{18}H_{11}BrO^+$: 321.9988, found: 321.9988.

4-Methoxy-2-phenylnaphtho[2,1-*b*]furan (3p)



White powder (564 mg, 60 %, mp = 152-153 °C, petroleum ether/ethyl acetate = 15:1).

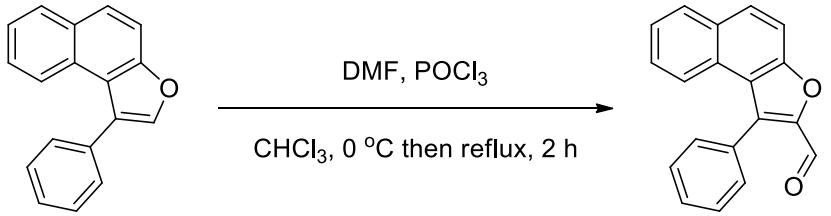
^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.16 – 8.07 (m, 1H), 8.01 – 7.96 (m, 2H), 7.89 – 7.83 (m, 1H), 7.54 – 7.46 (m, 5H), 7.38 (ddd, J = 8.2, 7.0, 1.3 Hz, 1H), 7.09 (s, 1H).

$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 155.8, 145.8, 143.9, 131.8, 130.4, 128.8, 128.4, 127.5, 126.4, 125.2, 124.9, 124.1, 123.3, 123.3, 103.1, 100.7, 55.9.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{19}H_{14}O_2^+$: 274.0988, found: 274.0998.

VIII. Derivatization experiments

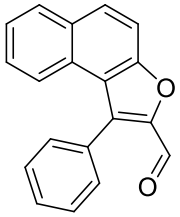
VIII.a. Synthesis of aldehyde 4



2b **4**

DMF (4.12 ml, 53.3 mmol) was dissolved in chloroform (4.1 ml) and cooled to 0 °C with ice and salt. $POCl_3$ (6.78 ml, 44.3 mmol) was added dropwise to the resulting solution at 0-5 °C and the mixture was stirred for 30 min at 0 °C. After that, a solution of **2b** (1 g, 4.1 mmol) in chloroform (16.5 ml) was added dropwise to the formed Vilsmeier-Haack reagent at 0 °C. The resulting reaction mixture was removed from the ice bath and refluxed for 2 h. After completion of the reaction, chloroform was evaporated in a vacuum, and the resulting viscous residue was poured into cold water (100 ml). The acids released during hydrolysis were neutralized with 5% NaOH solution to pH = 7. The resulting precipitate of aldehyde **4** was filtered, thoroughly washed with water and dried in a vacuum.

1-Phenylnaphtho[2,1-*b*]furan-2-carbaldehyde (4)



Yellowish powder (1.014 g, 91 %, mp = 108-109 °C (lit.[1] 108-110 °C)).

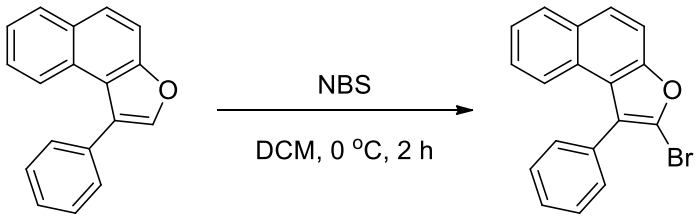
^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 9.63 (s, 1H), 8.04 – 7.94 (m, 2H), 7.81 (d, J = 8.3 Hz, 1H), 7.76 (d, J = 9.1 Hz, 1H), 7.69 – 7.60 (m, 5H), 7.52 (ddd, J = 8.1, 7.1, 1.2 Hz, 1H), 7.41 (ddd, J = 8.2, 7.2, 1.2 Hz, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 178.9, 154.2, 148.4, 136.1, 131.9, 131.1, 130.3, 130.3, 129.5, 129.4, 129.0, 128.8, 127.4, 125.5, 123.1, 121.3, 112.9.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{19}H_{13}O_2^+$: 273.0910, found: 273.0904.

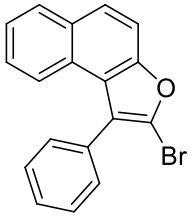
[1] Jun-Dan Fang, Xiao-Biao Yan, Wu-Jie Lin, Yi-Chuan Zhao, Xue-Yuan Liu, *Org. Lett.* **2019**, 21, 18, 7635–7638

VIII.b. Synthesis of bromide 5



2b **5**

1-Phenylnaphtho[2,1-*b*]furan **2b** (1 g, 4.1 mmol) was dissolved in dry dichloromethane (30 ml). The resulting solution was cooled to 0 °C with ice and salt. Then, NBS (0.803 g, 4.51 mmol) was added in portions to the cooled solution. The reaction mixture was stirred for 2 hours at 0 °C. After that the solution was washed successively with water, saturated NaCl solution and dried over anhydrous $CaCl_2$. The solvent was evaporated in vacuum and the residue was dried in vacuum.



2-Bromo-1-phenylnaphtho[2,1-*b*]furan (5)

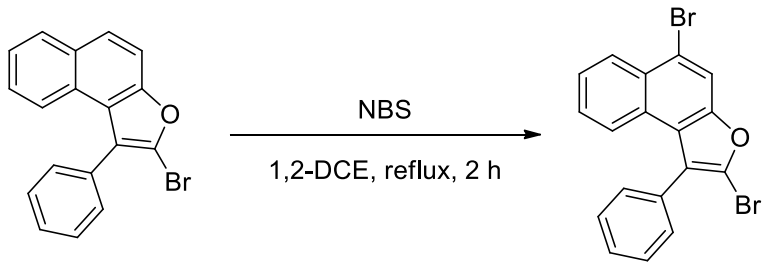
Colourless oil (1.072 g, 81%).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 7.95 (dd, J = 8.1, 1.1 Hz, 1H), 7.80 – 7.76 (m, 2H), 7.69 (d, J = 9.0 Hz, 1H), 7.61 – 7.55 (m, 5H), 7.46 (ddd, J = 8.1, 7.0, 1.2 Hz, 1H), 7.35 (ddd, J = 8.1, 7.0, 1.2 Hz, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 153.1, 132.3, 130.9, 130.4, 129.0, 128.8, 128.5, 127.3, 126.3, 125.9, 125.9, 124.8, 123.1, 123.0, 122.2, 111.9.

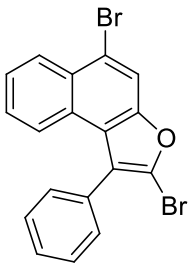
HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{18}H_{12}BrO^+$: 323.0066, found: 323.0062.

VIII.c. Synthesis of dibromide 6



5 **6**

2-Bromo-1-phenylnaphtho[2,1-*b*]furan **5** (500 mg, 1.55 mmol) was dissolved in dry 1,2-dichloroethane (11 ml). Then, NBS (303 mg, 1.7 mmol) was added and the resulting mixture was refluxed for 2 hours. After that the solution was washed successively with water, saturated NaCl solution and dried over anhydrous $CaCl_2$. The solvent was evaporated in vacuum and the residue was dried in vacuum.



2,5-Dibromo-1-phenylnaphtho[2,1-*b*]furan (6)

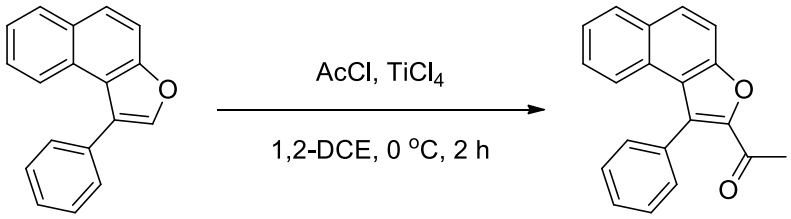
Colourless crystals (517 mg, 83%, mp = 165-166 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.37 (d, J = 8.3 Hz, 1H), 8.04 (s, 1H), 7.78 (d, J = 8.4 Hz, 1H), 7.63 – 7.52 (m, 6H), 7.39 (ddd, J = 8.2, 7.0, 1.1 Hz, 1H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 152.2, 131.8, 130.3, 129.0, 128.9, 128.7, 128.3, 127.6, 127.1, 126.7, 126.0, 123.5, 123.0, 122.2, 119.7, 116.1.

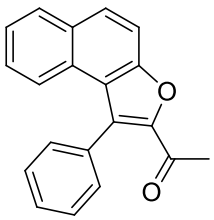
HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{18}H_{10}Br_2O^+$: 399.9093, found: 399.9087.

VIII.d. Synthesis of ketone 7



2b **7**

1-Phenylnaphtho[2,1-*b*]furan **2b** (1 g, 4.1 mmol) was dissolved in dry 1,2-dichloroethane (7 ml). The resulting solution was cooled to 0 °C with ice and salt. Then, $TiCl_4$ (0.5 ml, 4.51 mmol) was added to the cooled solution with stirring, and the solution of acetyl chloride (0.32 ml, 4.51 mmol) in dry 1,2-dichloroethane (7 ml) was added dropwise at 0 °C. After dropping the reaction mixture was stirred for 2 hours at 0 °C. Then the reaction mixture was poured into ice and left for 24 hours. After that the organic phase was separated, washed with saturated $NaHCO_3$ solution, saturated NaCl solution and dried over anhydrous $CaCl_2$. The solvent was evaporated in vacuum, the residue was triturated with petroleum ether, filtered off and dried in vacuum.



1-(1-Phenylnaphtho[2,1-*b*]furan-2-yl)ethanone (7)

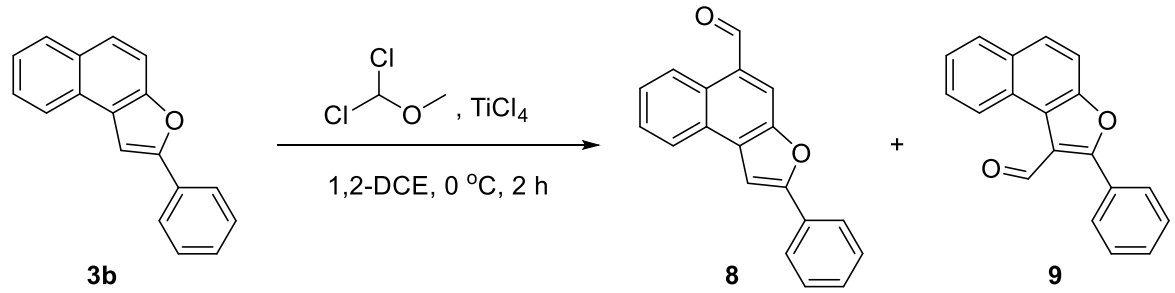
Beige powder (0.938 g, 80%, mp = 132-133 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 7.96 (d, J = 7.9 Hz, 1H), 7.94 (d, J = 9.0 Hz, 1H), 7.76 (d, J = 9.1 Hz, 1H), 7.64 – 7.58 (m, 3H), 7.58 – 7.53 (m, 2H), 7.52 – 7.44 (m, 2H), 7.33 (ddd, J = 9.3, 5.3, 1.7 Hz, 1H), 2.32 (s, 3H, Me).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 188.4, 152.8, 147.9, 133.2, 131.0, 130.6, 130.1, 129.5, 129.3, 129.1, 128.9, 128.8, 127.1, 125.2, 122.9, 122.3, 112.7, 28.2.

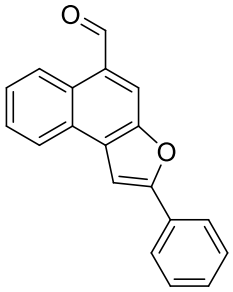
HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{20}H_{15}O_2^+$: 287.1067, found: 287.1072.

VIII.e. Synthesis of aldehydes 8 and 9



2-Phenylnaphtho[2,1-*b*]furan **3b** (500 mg, 2.05 mmol) was dissolved in dry 1,2-dichloroethane (5 ml). The resulting solution was cooled to 0 °C with ice and salt. Then, $TiCl_4$ (0.41 ml, 3.69 mmol) was added to the cooled solution with stirring, and the solution of dichloromethyl methyl ether (0.2 ml, 2.25 mmol) in dry 1,2-dichloroethane (5 ml) was added dropwise at 0 °C. After dropping the reaction mixture was stirred for 2 hours at 0 °C. Then the reaction mixture was poured into ice and left for 24 hours. After that the organic phase was separated, washed with saturated $NaHCO_3$ solution, saturated NaCl solution and dried over anhydrous $CaCl_2$. The solvent was evaporated in vacuum. Aldehydes **8** and **9** were isolated using column chromatography on silica gel (petroleum ether/ethyl acetate = 15:1).

2-Phenylnaphtho[2,1-*b*]furan-5-carbaldehyde (8)



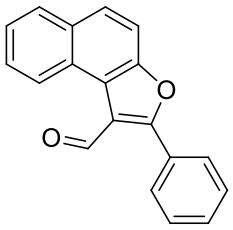
Yellow powder (301 mg, 54 %, mp = 120-121 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 10.43 (s, 1H), 9.44 – 9.34 (m, 1H), 8.28 – 8.21 (m, 1H), 8.19 (s, 1H), 8.02 – 7.95 (m, 2H), 7.75 – 7.67 (m, 2H), 7.59 – 7.51 (m, 3H), 7.46 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H)

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 192.1, 159.6, 150.7, 130.9, 129.6, 129.5, 129.0, 128.3, 128.1, 127.6, 127.4, 127.2, 125.9, 125.2, 123.8, 122.0, 100.9.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{19}H_{13}O_2^+$: 273.0910, found: 273.0916.

2-Phenylnaphtho[2,1-*b*]furan-1-carbaldehyde (9)



White powder (229 mg, 41 %, mp = 125-126 °C (lit.[1] 126-127 °C)).

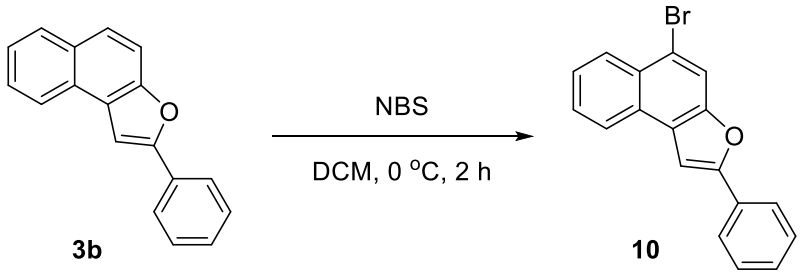
^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 10.36 (s, 1H), 9.59 (d, J = 8.5 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H), 7.90 (d, J = 8.9 Hz, 1H), 7.88 – 7.82 (m, 2H), 7.74 (d, J = 9.0 Hz, 1H), 7.75 – 7.69 (m, 1H), 7.65 – 7.56 (m, 4H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 186.8, 167.1, 152.6, 131.5, 130.9, 129.9, 129.0, 128.7, 128.6, 128.5, 128.3, 127.8, 126.9, 125.5, 120.4, 120.2, 111.7.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{19}H_{13}O_2^+$: 273.0910, found: 273.0915.

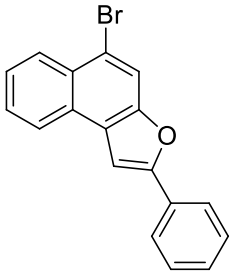
[1] Huiwen Zhang, Chunmei Ma, Ziwei Zheng, Rengwei Sun, Xinhong Yu, Jianhong Zhao, *Chem. Commun.* **2018**, 54, 4935-4938

VIII.f. Synthesis of bromide 10



2-Phenylnaphtho[2,1-*b*]furan **3b** (1 g, 4.1 mmol) was dissolved in dry dichloromethane (30 ml). The resulting solution was cooled to 0 °C with ice and salt. Then, NBS (0.803 g, 4.51 mmol) was added in portions to the cooled solution. The reaction mixture was stirred for 2 hours at 0 °C. After that the solution was washed successively with water, saturated NaCl solution and dried over anhydrous $CaCl_2$. The solvent was evaporated in vacuum and the residue was dried in vacuum.

5-Bromo-2-phenylnaphtho[2,1-*b*]furan (10)



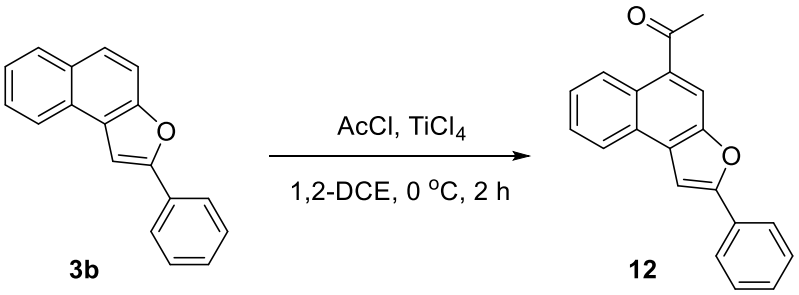
Brown powder (1.046 g, 79 %, mp = 148-149 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 9.29 – 9.24 (m, 1H), 8.45 – 8.40 (m, 1H), 8.22 – 8.16 (m, 2H), 8.06 (s, 1H), 7.76 – 7.63 (m, 2H), 7.59 – 7.44 (m, 4H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 150.5, 150.4, 129.3, 129.1, 129.0, 128.6, 128.3, 128.2, 127.1, 127.1, 126.1, 122.5, 121.0, 120.5, 116.4, 93.8.

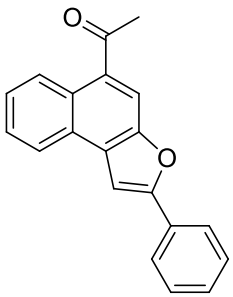
HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{18}H_{12}BrO^+$: 323.0066, found: 323.0051.

VIII.g. Synthesis of ketone 12



2-Phenylnaphtho[2,1-*b*]furan **3b** (1 g, 4.1 mmol) was dissolved in dry 1,2-dichloroethane (7 ml). The resulting solution was cooled to 0 °C with ice and salt. Then, $TiCl_4$ (0.5 ml, 4.51 mmol) was added to the cooled solution with stirring, and the solution of acetyl chloride (0.32 ml, 4.51 mmol) in dry 1,2-dichloroethane (7 ml) was added dropwise at 0 °C. After dropping the reaction mixture was stirred for 2 hours at 0 °C. Then the reaction mixture was poured into ice and left for 24 hours. After that the organic phase was separated, washed with saturated $NaHCO_3$ solution, saturated NaCl solution and dried over anhydrous $CaCl_2$. The solvent was evaporated in vacuum, the residue was triturated with petroleum ether, filtered off and dried in vacuum.

1-(2-Phenylnaphtho[2,1-*b*]furan-5-yl)ethanone (12)



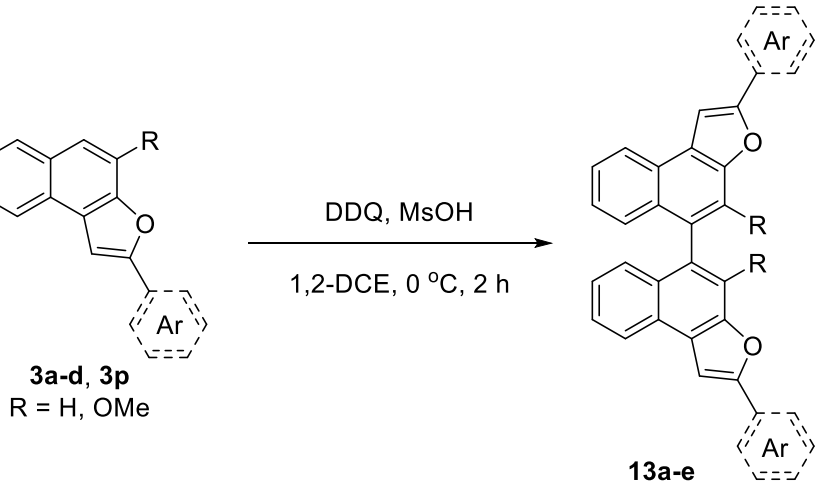
White powder (703 mg, 60 %, mp = 137-138 °C).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 9.02 – 8.96 (m, 1H), 8.27 – 8.18 (m, 2H), 8.02 – 7.93 (m, 2H), 7.70 – 7.59 (m, 2H), 7.58 – 7.49 (m, 3H), 7.47 – 7.40 (m, 1H), 2.84 (s, 3H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 200.6, 158.4, 150.2, 131.7, 129.9, 129.1, 129.0, 129.0, 127.9, 127.8, 127.4, 126.7, 126.6, 125.0, 123.7, 115.6, 100.7, 29.8.

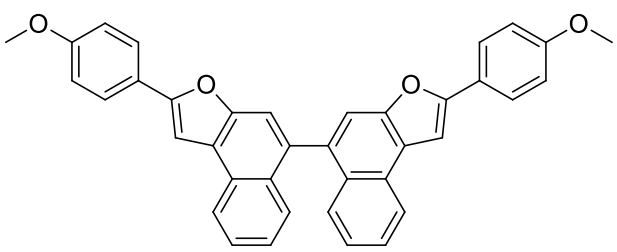
HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{20}H_{15}O_2^+$: 287.1067, found: 287.1072.

IX. Synthesis of binaphtho[2,1-*b*]furans 13a-e



2-Arylnaphtho[2,1-*b*]furan **3a-d** or **3p** (0.8 mmol) was dissolved in 1,2-dichloroethane (8 ml) and to this solution DDQ (100 mg, 0.44 mmol) was added. The reaction mixture was cooled to 0 °C and MsOH (0.16 ml, 2.4 mmol) was added with stirring. The resulting solution was stirred at 0 °C for 2 hours. After completion of the reaction, the organic phase was successively washed with water, saturated $NaHCO_3$ solution and dried over anhydrous $CaCl_2$. The solvent was evaporated in vacuum. The products were isolated using flash chromatography on silica gel.

2,2'-Bis(4-methoxyphenyl)-5,5'-binaphtho[2,1-*b*]furan (13a)



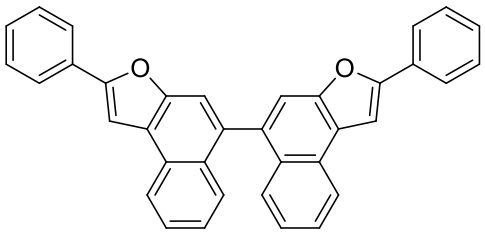
White powder (114 mg, 52 %, decomp. at 250 °C, petroleum ether/ethyl acetate = 10:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.30 (d, J = 8.0 Hz, 2H), 7.93 (d, J = 8.7 Hz, 4H), 7.80 (s, 2H), 7.64 – 7.56 (m, 2H), 7.56 – 7.51 (m, 4H), 7.33 – 7.27 (m, 2H), 7.05 (d, J = 8.7 Hz, 4H), 3.91 (s, 6H).

^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$), δ, ppm: 159.9, 155.9, 151.6, 135.3, 130.3, 127.8, 127.5, 126.3, 126.3, 126.1, 124.8, 124.6, 123.7, 123.6, 114.4, 98.9, 55.4.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{38}H_{27}O_4^+$: 547.1904, found: 547.1917.

2,2'-Diphenyl-5,5'-binaphtho[2,1-*b*]furan (13b)



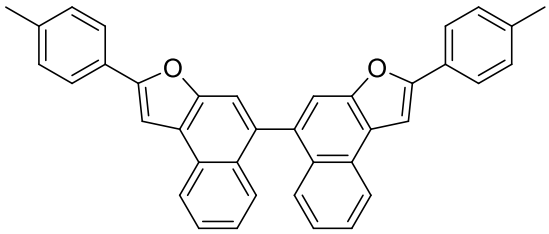
White powder (152 mg, 78 %, mp = 176-177 °C, petroleum ether/ethyl acetate = 30:1).

^{1}H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.33 (d, J = 8.1 Hz, 2H), 8.05 – 7.99 (m, 4H), 7.84 (s, 2H), 7.67 (s, 2H), 7.63 (ddd, J = 8.1, 7.1, 1.0 Hz, 2H), 7.59 – 7.50 (m, 6H), 7.45 – 7.38 (m, 2H), 7.33 (ddd, J = 8.3, 6.9, 1.2 Hz, 2H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 155.8, 151.9, 135.9, 130.6, 130.3, 128.9, 128.4, 127.8, 127.6, 126.3, 124.8, 124.6, 123.7, 114.5, 100.5.

HRMS (ESI-TOF): m/z $[M]^+$ calcd for $C_{36}H_{22}O_2^+$: 486.1614, found: 486.1641.

2,2'-Di-*p*-tolyl-5,5'-binaphtho[2,1-*b*]furan (13c)



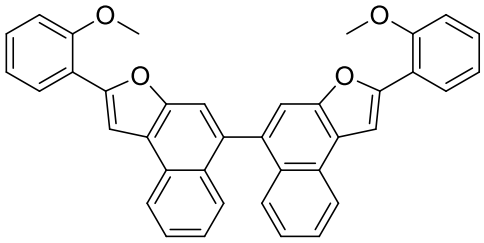
White powder (115 mg, 56 %, mp = 170-171 °C, petroleum ether/ethyl acetate = 30:1).

^1H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.30 (d, J = 7.9 Hz, 2H), 7.90 (d, J = 8.2 Hz, 4H), 7.81 (s, 2H), 7.64 – 7.58 (m, 4H), 7.53 (d, J = 8.3 Hz, 2H), 7.36 – 7.30 (m, 6H), 2.46 (s, 6H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 156.0, 151.7, 138.4, 135.6, 132.1, 130.3, 129.6, 127.9, 127.8, 127.6, 126.2, 124.7, 124.7, 123.7, 114.4, 99.8, 21.4.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{38}H_{27}O_2^+$: 515.2006, found: 515.1984.

2,2'-Bis(2-methoxyphenyl)-5,5'-binaphtho[2,1-*b*]furan (13d)

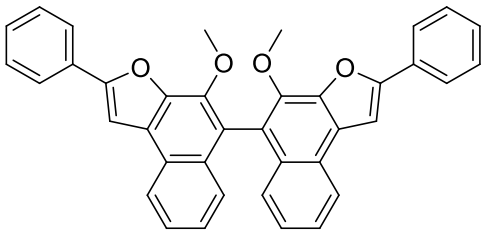


White powder (111 mg, 51 %, decomp. at 250 °C, petroleum ether/ethyl acetate = 10:1).

^1H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.39 (d, J = 8.0 Hz, 2H), 8.20 (dd, J = 7.8, 1.5 Hz, 2H), 8.00 (s, 2H), 7.85 (s, 2H), 7.63 (ddd, J = 8.2, 6.9, 0.9 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H), 7.42 – 7.35 (m, 2H), 7.35 – 7.29 (m, 2H), 7.19 – 7.13 (m, 2H), 7.11 (d, J = 8.3 Hz, 2H), 4.14 (s, 6H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 156.3, 152.1, 150.9, 135.8, 130.3, 129.1, 127.9, 127.8, 126.9, 126.1, 125.0, 124.5, 123.8, 120.9, 119.6, 114.3, 111.1, 105.5, 55.6.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{38}H_{27}O_4^+$: 547.1904, found: 547.1889.



4,4'-Dimethoxy-2,2'-diphenyl-5,5'-binaphtho[2,1-*b*]furan (13e)

White powder (124 mg, 57 %, mp = 190-191 °C, petroleum ether/ethyl acetate = 15:1).

^1H NMR (300 MHz, $CDCl_3$), δ, ppm: 8.25 (d, J = 8.1 Hz, 2H), 8.03 – 7.99 (m, 4H), 7.68 (s, 2H), 7.58 – 7.48 (m, 6H), 7.41 (ddd, 8.2, 6.9, 0.9 Hz, 2H), 7.33 – 7.23 (m, 4H), 4.11 (s, 6H).

$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$), δ, ppm: 155.6, 145.6, 143.4, 131.6, 130.5, 128.9, 128.5, 127.3, 126.7, 125.2, 124.8, 124.7, 124.5, 123.4, 119.7, 100.9, 60.8.

HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{38}H_{27}O_4^+$: 547.1904, found: 547.1910.

X. Spectral properties

Table S2. Spectral characteristics of **2d**, **3d** and **13d** in MeCN

Compound	λ_{abs}**, nm (**$\varepsilon \cdot 10^{-3}$**, M^{-1}·cm^{-1})**	λ_{em}**, nm**	**Stokes' shift, cm^{-1}**	Φ_{flu}[a] **(**λ_{exc}**, nm)**
2d	284 (14.1), 291 (14.3), 303_{sh} (11.1), 309 (9.9), 316_{sh} (6.9), 323 (7.7)	328, 341, 357_{sh}	1634	0.14 ± 0.01 (291)
3d	254 (16.1), 263 (16.5), 291 (15.3), 313_{sh} (16.5), 319 (17.4), 334 (29.8), 350 (36.1)	356, 374, 395_{sh}	1833	0.22 ± 0.02 (319)
13d	256 (12.9), 266 (12.6), 292 (10.3), 316_{sh} (11.3), 327_{sh} (13.4), 344 (23.5), 361 (32.2)	431	4499	0.31 ± 0.03 (344)

[a] Determined in MeCN solution according to the standard (anthracene in EtOH, Φ_{flu} = 0.27)

XI. Crystallographic data for 13b

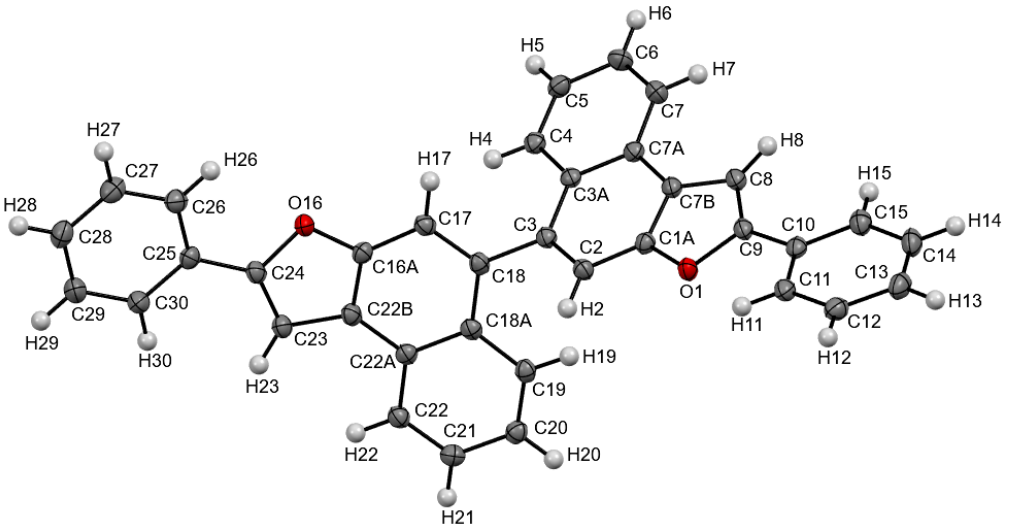


Fig. S1. ORTEP diagram of **13b** with ellipsoids shown at 50% probability level (CCDC No. 2363841)

Table S3. Crystal data and structure refinement for **13b**

Identification code	ME-209	
Empirical formula	$C_{36}H_{22}O_2$	
Formula weight	486.53	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 11.43259(10) Å	α = 90°
	b = 24.93811(18) Å	β = 96.9186(7)°
	c = 8.39634(6) Å	γ = 90°
Volume	2376.42(3) $Å^3$	
Z	4	
Density (calculated)	1.360 g/cm^3	
Absorption coefficient	0.650 mm^{-1}	
F(000)	1016	
Crystal size	0.27 × 0.08 × 0.05 mm^3	
Theta range for data collection	3.545 to 79.775°	
Index ranges	$-14 \le h \le 14$, $-31 \le k \le 31$, $-10 \le l \le 9$	
Reflections collected	28404	
Independent reflections	5163 [R(int) = 0.0236]	
Observed reflections	4778	

Table S3. *(continued)*

Completeness to theta = 67.684°	100.0 %
Absorption correction	Gaussian
Max. and min. transmission	1.000 and 0.784
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5163 / 0 / 343
Goodness-of-fit on F^2	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0908
R indices (all data)	R1 = 0.0380, wR2 = 0.0927
Largest diff. peak and hole	0.216 and -0.228 e.$Å^{-3}$

Table S4. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **13b**.

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
O(1)	7084(1)	5739(1)	2044(1)	22(1)
O(16)	7764(1)	8957(1)	2709(1)	22(1)
C(1A)	6767(1)	6189(1)	2830(1)	20(1)
C(2)	7458(1)	6652(1)	3105(1)	21(1)
C(3)	7017(1)	7070(1)	3928(1)	20(1)
C(3A)	5860(1)	7031(1)	4447(1)	19(1)
C(4)	5368(1)	7450(1)	5307(1)	21(1)
C(5)	4270(1)	7401(1)	5797(1)	24(1)
C(6)	3583(1)	6939(1)	5419(2)	27(1)
C(7)	4031(1)	6525(1)	4608(1)	25(1)
C(7A)	5174(1)	6555(1)	4137(1)	20(1)
C(7B)	5674(1)	6123(1)	3340(1)	20(1)
C(8)	5304(1)	5590(1)	2876(1)	22(1)
C(9)	6166(1)	5378(1)	2098(1)	21(1)
C(10)	6302(1)	4860(1)	1332(1)	22(1)
C(11)	7123(1)	4791(1)	249(1)	24(1)
C(12)	7274(1)	4294(1)	-441(2)	27(1)
C(13)	6618(1)	3857(1)	-34(2)	30(1)
C(14)	5782(1)	3922(1)	1020(2)	30(1)

Atom	x	y	z	U(eq)
C(15)	5612(1)	4420(1)	1694(1)	26(1)
C(16A)	8000(1)	8494(1)	3580(1)	21(1)
C(17)	7279(1)	8039(1)	3461(1)	21(1)
C(18)	7726(1)	7574(1)	4191(1)	20(1)
C(18A)	8880(1)	7570(1)	5117(1)	20(1)
C(19)	9382(1)	7102(1)	5877(1)	21(1)
C(20)	10466(1)	7114(1)	6782(1)	23(1)
C(21)	11110(1)	7595(1)	6998(1)	23(1)
C(22)	10665(1)	8055(1)	6259(1)	22(1)
C(22A)	9559(1)	8053(1)	5300(1)	20(1)
C(22B)	9101(1)	8517(1)	4451(1)	21(1)
C(23)	9584(1)	9026(1)	4084(1)	22(1)
C(24)	8765(1)	9271(1)	3019(1)	22(1)
C(25)	8788(1)	9773(1)	2138(1)	22(1)
C(26)	7883(1)	9915(1)	937(1)	25(1)
C(27)	7952(1)	10389(1)	100(1)	29(1)
C(28)	8911(1)	10732(1)	435(2)	30(1)
C(29)	9812(1)	10593(1)	1622(2)	30(1)
C(30)	9754(1)	10118(1)	2465(2)	26(1)

Table S5. Bond lengths [Å] for **13b**.

O(1)-C(1A)	1.3728(12)	**C(14)-C(15)**	1.3893(16)
O(1)-C(9)	1.3881(12)	**C(15)-H(15)**	0.9500
O(16)-C(16A)	1.3753(13)	**C(16A)-C(17)**	1.3986(15)
O(16)-C(24)	1.3857(13)	**C(16A)-C(22B)**	1.3784(15)
C(1A)-C(2)	1.4015(14)	**C(17)-H(17)**	0.9500
C(1A)-C(7B)	1.3792(15)	**C(17)-C(18)**	1.3806(15)
C(2)-H(2)	0.9500	**C(18)-C(18A)**	1.4491(15)
C(2)-C(3)	1.3802(15)	**C(18A)-C(19)**	1.4189(15)
C(3)-C(3A)	1.4443(15)	**C(18A)-C(22A)**	1.4308(14)
C(3)-C(18)	1.4968(14)	**C(19)-H(19)**	0.9500
C(3A)-C(4)	1.4239(15)	**C(19)-C(20)**	1.3738(16)
C(3A)-C(7A)	1.4292(14)	**C(20)-H(20)**	0.9500
C(4)-H(4)	0.9500	**C(20)-C(21)**	1.4078(16)
C(4)-C(5)	1.3730(16)	**C(21)-H(21)**	0.9500
C(5)-H(5)	0.9500	**C(21)-C(22)**	1.3726(16)
C(5)-C(6)	1.4093(16)	**C(22)-H(22)**	0.9500
C(6)-H(6)	0.9500	**C(22)-C(22A)**	1.4151(15)
C(6)-C(7)	1.3691(17)	**C(22A)-C(22B)**	1.4238(15)
C(7)-H(7)	0.9500	**C(22B)-C(23)**	1.4322(15)
C(7)-C(7A)	1.4114(15)	**C(23)-H(23)**	0.9500
C(7A)-C(7B)	1.4245(15)	**C(23)-C(24)**	1.3595(16)
C(7B)-C(8)	1.4341(14)	**C(24)-C(25)**	1.4563(15)
C(8)-H(8)	0.9500	**C(25)-C(26)**	1.4008(16)
C(8)-C(9)	1.3546(16)	**C(25)-C(30)**	1.4007(15)
C(9)-C(10)	1.4589(15)	**C(26)-H(26)**	0.9500
C(10)-C(11)	1.3939(16)	**C(26)-C(27)**	1.3832(17)
C(10)-C(15)	1.4050(15)	**C(27)-H(27)**	0.9500
C(11)-H(11)	0.9500	**C(27)-C(28)**	1.3912(18)
C(11)-C(12)	1.3884(16)	**C(28)-H(28)**	0.9500
C(12)-H(12)	0.9500	**C(28)-C(29)**	1.3883(18)
C(12)-C(13)	1.3887(17)	**C(29)-H(29)**	0.9500
C(13)-H(13)	0.9500	**C(29)-C(30)**	1.3854(16)
C(13)-C(14)	1.3886(19)	**C(30)-H(30)**	0.9500
C(14)-H(14)	0.9500		

Table S6. Angles [°] for **13b**

C(1A)-O(1)-C(9)	105.77(8)	**C(9)-C(8)-H(8)**	126.7
C(16A)-O(16)-C(24)	105.67(8)	**O(1)-C(9)-C(10)**	116.03(9)
O(1)-C(1A)-C(2)	125.22(10)	**C(8)-C(9)-O(1)**	110.97(9)
O(1)-C(1A)-C(7B)	110.64(9)	**C(8)-C(9)-C(10)**	133.00(10)
C(7B)-C(1A)-C(2)	124.14(10)	**C(11)-C(10)-C(9)**	120.83(10)
C(1A)-C(2)-H(2)	120.9	**C(11)-C(10)-C(15)**	119.02(10)
C(3)-C(2)-C(1A)	118.14(10)	**C(15)-C(10)-C(9)**	120.14(10)
C(3)-C(2)-H(2)	120.9	**C(10)-C(11)-H(11)**	119.7
C(2)-C(3)-C(3A)	120.25(9)	**C(12)-C(11)-C(10)**	120.63(11)
C(2)-C(3)-C(18)	118.93(9)	**C(12)-C(11)-H(11)**	119.7
C(3A)-C(3)-C(18)	120.73(9)	**C(11)-C(12)-H(12)**	120.0
C(4)-C(3A)-C(3)	122.39(10)	**C(11)-C(12)-C(13)**	120.01(11)
C(4)-C(3A)-C(7A)	117.36(10)	**C(13)-C(12)-H(12)**	120.0
C(7A)-C(3A)-C(3)	120.23(9)	**C(12)-C(13)-H(13)**	120.0
C(3A)-C(4)-H(4)	119.4	**C(14)-C(13)-C(12)**	119.95(11)
C(5)-C(4)-C(3A)	121.20(10)	**C(14)-C(13)-H(13)**	120.0
C(5)-C(4)-H(4)	119.4	**C(13)-C(14)-H(14)**	119.8
C(4)-C(5)-H(5)	119.7	**C(13)-C(14)-C(15)**	120.31(11)
C(4)-C(5)-C(6)	120.69(10)	**C(15)-C(14)-H(14)**	119.8
C(6)-C(5)-H(5)	119.7	**C(10)-C(15)-H(15)**	120.0
C(5)-C(6)-H(6)	120.1	**C(14)-C(15)-C(10)**	120.02(11)
C(7)-C(6)-C(5)	119.75(10)	**C(14)-C(15)-H(15)**	120.0
C(7)-C(6)-H(6)	120.1	**O(16)-C(16A)-C(17)**	124.52(10)
C(6)-C(7)-H(7)	119.5	**O(16)-C(16A)-C(22B)**	110.82(9)
C(6)-C(7)-C(7A)	120.93(10)	**C(22B)-C(16A)-C(17)**	124.29(10)
C(7A)-C(7)-H(7)	119.5	**C(16A)-C(17)-H(17)**	121.1
C(7)-C(7A)-C(3A)	119.97(10)	**C(18)-C(17)-C(16A)**	117.84(10)
C(7)-C(7A)-C(7B)	121.93(10)	**C(18)-C(17)-H(17)**	121.1
C(7B)-C(7A)-C(3A)	118.10(10)	**C(17)-C(18)-C(3)**	118.35(9)
C(1A)-C(7B)-C(7A)	119.07(10)	**C(17)-C(18)-C(18A)**	120.47(9)
C(1A)-C(7B)-C(8)	105.98(9)	**C(18A)-C(18)-C(3)**	121.10(9)
C(7A)-C(7B)-C(8)	134.96(10)	**C(19)-C(18A)-C(18)**	122.62(10)
C(7B)-C(8)-H(8)	126.7	**C(19)-C(18A)-C(22A)**	117.41(10)
C(9)-C(8)-C(7B)	106.62(9)	**C(22A)-C(18A)-C(18)**	119.97(9)

Table S6. *(continued)*

C(18A)-C(19)-H(19)	119.3	**O(16)-C(24)-C(25)**	117.13(9)
C(20)-C(19)-C(18A)	121.32(10)	**C(23)-C(24)-O(16)**	110.88(9)
C(20)-C(19)-H(19)	119.3	**C(23)-C(24)-C(25)**	131.92(10)
C(19)-C(20)-H(20)	119.6	**C(26)-C(25)-C(24)**	121.72(10)
C(19)-C(20)-C(21)	120.83(10)	**C(26)-C(25)-C(30)**	118.84(10)
C(21)-C(20)-H(20)	119.6	**C(30)-C(25)-C(24)**	119.41(10)
C(20)-C(21)-H(21)	120.2	**C(25)-C(26)-H(26)**	120.0
C(22)-C(21)-C(20)	119.65(10)	**C(27)-C(26)-C(25)**	119.96(11)
C(22)-C(21)-H(21)	120.2	**C(27)-C(26)-H(26)**	120.0
C(21)-C(22)-H(22)	119.6	**C(26)-C(27)-H(27)**	119.5
C(21)-C(22)-C(22A)	120.80(10)	**C(26)-C(27)-C(28)**	120.97(11)
C(22A)-C(22)-H(22)	119.6	**C(28)-C(27)-H(27)**	119.5
C(22)-C(22A)-C(18A)	119.94(10)	**C(27)-C(28)-H(28)**	120.3
C(22)-C(22A)-C(22B)	122.15(10)	**C(29)-C(28)-C(27)**	119.35(11)
C(22B)-C(22A)-C(18A)	117.87(10)	**C(29)-C(28)-H(28)**	120.3
C(16A)-C(22B)-C(22A)	119.30(10)	**C(28)-C(29)-H(29)**	119.9
C(16A)-C(22B)-C(23)	105.88(9)	**C(30)-C(29)-C(28)**	120.20(11)
C(22A)-C(22B)-C(23)	134.31(10)	**C(30)-C(29)-H(29)**	119.9
C(22B)-C(23)-H(23)	126.6	**C(25)-C(30)-H(30)**	119.7
C(24)-C(23)-C(22B)	106.71(10)	**C(29)-C(30)-C(25)**	120.69(11)
C(24)-C(23)-H(23)	126.6	**C(29)-C(30)-H(30)**	119.7

Table S7. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **13b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	22(1)	16(1)	27(1)	-3(1)	4(1)	-3(1)
O(16)	21(1)	17(1)	28(1)	-1(1)	0(1)	-2(1)
C(1A)	22(1)	16(1)	22(1)	-1(1)	2(1)	0(1)
C(2)	20(1)	19(1)	24(1)	0(1)	4(1)	-2(1)
C(3)	20(1)	18(1)	21(1)	0(1)	1(1)	-2(1)
C(3A)	19(1)	20(1)	19(1)	2(1)	0(1)	0(1)
C(4)	22(1)	20(1)	21(1)	1(1)	1(1)	1(1)
C(5)	24(1)	22(1)	27(1)	1(1)	4(1)	5(1)
C(6)	20(1)	29(1)	34(1)	2(1)	8(1)	1(1)
C(7)	21(1)	22(1)	32(1)	1(1)	4(1)	-3(1)
C(7A)	20(1)	19(1)	21(1)	2(1)	1(1)	0(1)
C(7B)	20(1)	18(1)	22(1)	2(1)	0(1)	-2(1)
C(8)	21(1)	19(1)	25(1)	1(1)	0(1)	-3(1)
C(9)	21(1)	18(1)	23(1)	2(1)	-1(1)	-4(1)
C(10)	23(1)	18(1)	23(1)	0(1)	-4(1)	0(1)
C(11)	22(1)	20(1)	28(1)	-1(1)	-2(1)	-1(1)
C(12)	25(1)	24(1)	32(1)	-4(1)	-1(1)	3(1)
C(13)	34(1)	18(1)	36(1)	-4(1)	-4(1)	1(1)
C(14)	35(1)	19(1)	34(1)	1(1)	-2(1)	-6(1)
C(15)	29(1)	22(1)	27(1)	1(1)	-1(1)	-4(1)
C(16A)	21(1)	17(1)	23(1)	-2(1)	4(1)	1(1)
C(17)	19(1)	21(1)	24(1)	-3(1)	2(1)	-1(1)
C(18)	20(1)	19(1)	22(1)	-3(1)	5(1)	-2(1)
C(18A)	20(1)	20(1)	20(1)	-2(1)	6(1)	-1(1)
C(19)	23(1)	19(1)	22(1)	-2(1)	6(1)	-2(1)
C(20)	24(1)	22(1)	23(1)	2(1)	5(1)	2(1)
C(21)	20(1)	26(1)	24(1)	-1(1)	2(1)	1(1)
C(22)	21(1)	22(1)	25(1)	-2(1)	3(1)	-3(1)
C(22A)	20(1)	20(1)	21(1)	-2(1)	5(1)	0(1)
C(22B)	20(1)	18(1)	23(1)	-4(1)	4(1)	-2(1)
C(23)	22(1)	18(1)	26(1)	-3(1)	1(1)	-2(1)
C(24)	21(1)	18(1)	27(1)	-5(1)	2(1)	-3(1)

Table S7. *(continued)*

C(25)	23(1)	17(1)	25(1)	-3(1)	4(1)	1(1)
C(26)	24(1)	21(1)	28(1)	-6(1)	0(1)	0(1)
C(27)	33(1)	25(1)	26(1)	-2(1)	-1(1)	5(1)
C(28)	36(1)	21(1)	32(1)	4(1)	7(1)	2(1)
C(29)	26(1)	22(1)	42(1)	1(1)	4(1)	-3(1)
C(30)	22(1)	21(1)	34(1)	0(1)	-1(1)	-1(1)

Table S8. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **13b**.

Atom	x	y	z	U(eq)
H(2)	8210	6677	2735	25
H(4)	5808	7769	5547	25
H(5)	3970	7682	6396	29
H(6)	2811	6914	5726	33
H(7)	3567	6213	4360	30
H(8)	4592	5420	3074	26
H(11)	7584	5087	-19	28
H(12)	7826	4252	-1192	32
H(13)	6741	3514	-477	36
H(14)	5324	3624	1283	36
H(15)	5028	4464	2399	32
H(17)	6508	8050	2896	25
H(19)	8960	6773	5757	26
H(20)	10785	6793	7269	27
H(21)	11849	7601	7651	28
H(22)	11104	8378	6393	27
H(23)	10331	9165	4505	27
H(26)	7222	9685	696	30
H(27)	7336	10483	-715	34
H(28)	8948	11058	-143	35
H(29)	10470	10824	1856	36
H(30)	10376	10026	3273	31

Table S9. Torsion angles [°] for **13b**.

O(1)-C(1A)-C(2)-C(3)	-179.51(10)	**C(18)-C(18A)-C(22A)-C(22)**	177.36(9)
O(1)-C(1A)-C(7B)-C(7A)	-177.91(9)	**C(5)-C(6)-C(7)-C(7A)**	-0.28(18)
O(1)-C(1A)-C(7B)-C(8)	1.62(12)	**C(6)-C(7)-C(7A)-C(3A)**	-2.55(16)
O(1)-C(9)-C(10)-C(11)	-17.16(15)	**C(6)-C(7)-C(7A)-C(7B)**	177.85(11)
O(1)-C(9)-C(10)-C(15)	162.19(10)	**C(7)-C(7A)-C(7B)-C(1A)**	176.36(10)
O(16)-C(16A)-C(17)-C(18)	168.76(9)	**C(7)-C(7A)-C(7B)-C(8)**	-2.99(19)
O(16)-C(16A)-C(22B)-C(22A)	-173.45(9)	**C(7A)-C(3A)-C(4)-C(5)**	-0.95(15)
O(16)-C(16A)-C(22B)-C(23)	-0.49(12)	**C(7A)-C(7B)-C(8)-C(9)**	178.05(12)
O(16)-C(24)-C(25)-C(26)	-5.02(15)	**C(7B)-C(1A)-C(2)-C(3)**	-0.48(16)
O(16)-C(24)-C(25)-C(30)	176.83(10)	**C(7B)-C(8)-C(9)-O(1)**	0.65(12)
C(1A)-O(1)-C(9)-C(8)	0.32(11)	**C(7B)-C(8)-C(9)-C(10)**	-179.16(11)
C(1A)-O(1)-C(9)-C(10)	-179.83(9)	**C(8)-C(9)-C(10)-C(11)**	162.65(12)
C(1A)-C(2)-C(3)-C(3A)	-1.54(15)	**C(8)-C(9)-C(10)-C(15)**	-18.00(18)
C(1A)-C(2)-C(3)-C(18)	-178.22(9)	**C(9)-O(1)-C(1A)-C(2)**	177.91(10)
C(1A)-C(7B)-C(8)-C(9)	-1.36(12)	**C(9)-O(1)-C(1A)-C(7B)**	-1.23(11)
C(2)-C(1A)-C(7B)-C(7A)	2.94(16)	**C(9)-C(10)-C(11)-C(12)**	178.14(10)
C(2)-C(1A)-C(7B)-C(8)	-177.53(10)	**C(9)-C(10)-C(15)-C(14)**	-177.01(10)
C(2)-C(3)-C(3A)-C(4)	179.62(10)	**C(10)-C(11)-C(12)-C(13)**	-1.07(17)
C(2)-C(3)-C(3A)-C(7A)	1.09(15)	**C(11)-C(10)-C(15)-C(14)**	2.35(17)
C(2)-C(3)-C(18)-C(17)	114.63(11)	**C(11)-C(12)-C(13)-C(14)**	2.24(18)
C(2)-C(3)-C(18)-C(18A)	-62.12(14)	**C(12)-C(13)-C(14)-C(15)**	-1.10(18)
C(3)-C(3A)-C(4)-C(5)	-179.52(10)	**C(13)-C(14)-C(15)-C(10)**	-1.20(18)
C(3)-C(3A)-C(7A)-C(7)	-178.29(10)	**C(15)-C(10)-C(11)-C(12)**	-1.21(16)
C(3)-C(3A)-C(7A)-C(7B)	1.33(14)	**C(16A)-O(16)-C(24)-C(23)**	-2.06(12)
C(3)-C(18)-C(18A)-C(19)	-2.70(15)	**C(16A)-O(16)-C(24)-C(25)**	175.34(9)
C(3)-C(18)-C(18A)-C(22A)	177.64(9)	**C(16A)-C(17)-C(18)-C(3)**	-173.64(9)
C(3A)-C(3)-C(18)-C(17)	-62.02(14)	**C(16A)-C(17)-C(18)-C(18A)**	3.13(15)
C(3A)-C(3)-C(18)-C(18A)	121.23(11)	**C(16A)-C(22B)-C(23)-C(24)**	-0.78(12)
C(3A)-C(4)-C(5)-C(6)	-1.84(16)	**C(17)-C(16A)-C(22B)-C(22A)**	-0.12(16)
C(3A)-C(7A)-C(7B)-C(1A)	-3.24(15)	**C(17)-C(16A)-C(22B)-C(23)**	172.84(10)
C(3A)-C(7A)-C(7B)-C(8)	177.40(11)	**C(17)-C(18)-C(18A)-C(19)**	-179.39(10)
C(4)-C(3A)-C(7A)-C(7)	3.11(15)	**C(17)-C(18)-C(18A)-C(22A)**	0.96(15)
C(4)-C(3A)-C(7A)-C(7B)	-177.28(9)	**C(18)-C(3)-C(3A)-C(4)**	-3.76(15)
C(4)-C(5)-C(6)-C(7)	2.49(17)	**C(18)-C(3)-C(3A)-C(7A)**	177.71(9)

Table S9. *(continued)*

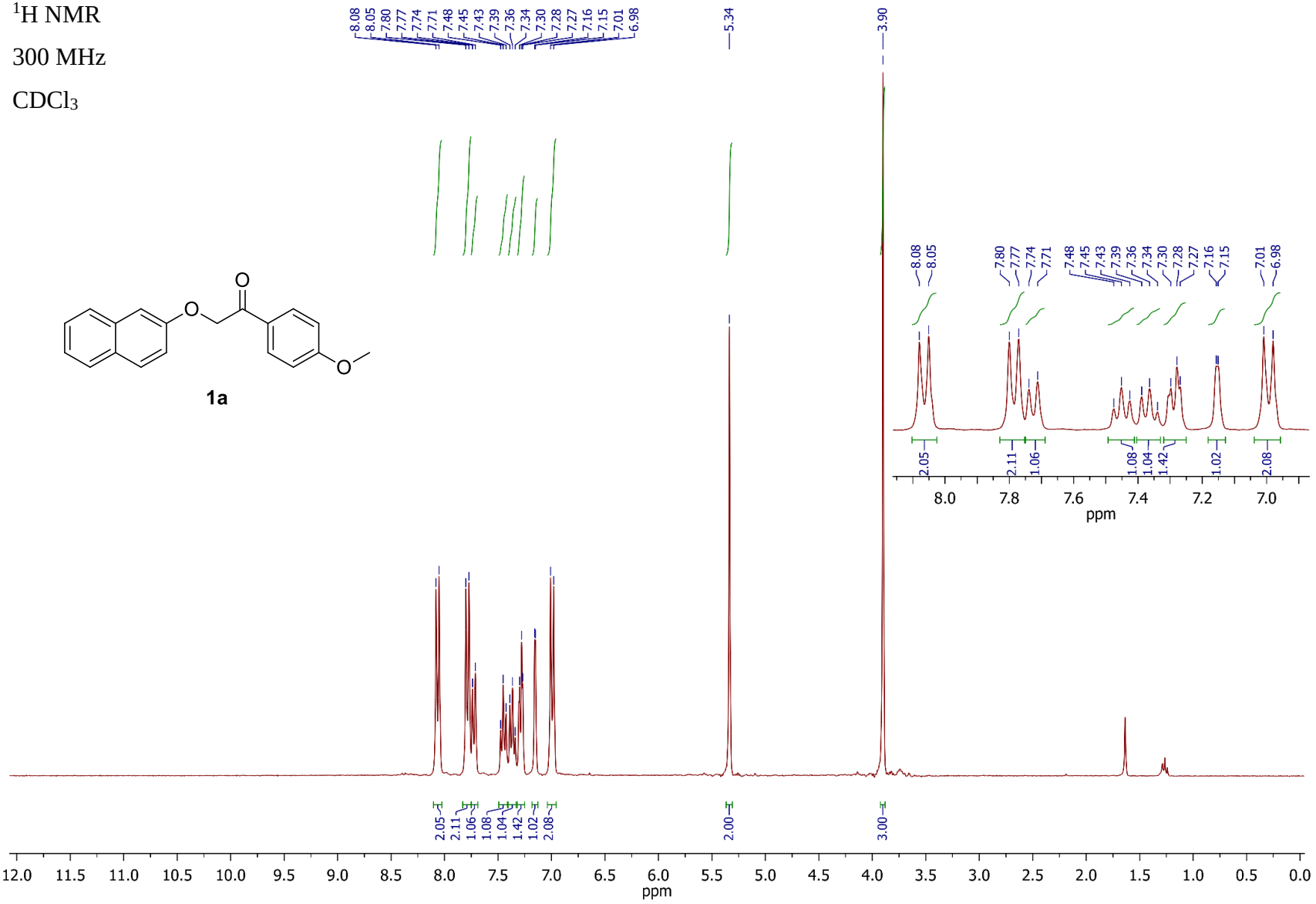
C(18)-C(18A)-C(19)-C(20)	-178.26(10)	**C(22A)-C(22B)-C(23)-C(24)**	170.63(11)
C(22B)-C(16A)-C(17)-C(18)	-3.67(16)	**C(22B)-C(23)-C(24)-O(16)**	1.78(12)
C(18)-C(18A)-C(22A)-C(22B)	-4.67(14)	**C(22B)-C(23)-C(24)-C(25)**	-175.11(11)
C(18A)-C(19)-C(20)-C(21)	0.63(16)	**C(23)-C(24)-C(25)-C(26)**	171.72(12)
C(18A)-C(22A)-C(22B)-C(16A)	4.26(15)	**C(23)-C(24)-C(25)-C(30)**	-6.43(18)
C(18A)-C(22A)-C(22B)-C(23)	-166.26(11)	**C(24)-O(16)-C(16A)-C(17)**	-171.77(10)
C(19)-C(18A)-C(22A)-C(22)	-2.31(15)	**C(24)-O(16)-C(16A)-C(22B)**	1.53(11)
C(19)-C(18A)-C(22A)-C(22B)	175.66(9)	**C(24)-C(25)-C(26)-C(27)**	-178.36(10)
C(19)-C(20)-C(21)-C(22)	-1.78(16)	**C(24)-C(25)-C(30)-C(29)**	178.57(11)
C(20)-C(21)-C(22)-C(22A)	0.83(16)	**C(25)-C(26)-C(27)-C(28)**	-0.13(18)
C(21)-C(22)-C(22A)-C(18A)	1.23(16)	**C(26)-C(25)-C(30)-C(29)**	0.37(17)
C(21)-C(22)-C(22A)-C(22B)	-176.65(10)	**C(26)-C(27)-C(28)-C(29)**	0.31(18)
C(22)-C(22A)-C(22B)-C(16A)	-177.82(10)	**C(27)-C(28)-C(29)-C(30)**	-0.14(19)
C(22)-C(22A)-C(22B)-C(23)	11.66(18)	**C(28)-C(29)-C(30)-C(25)**	-0.20(19)
C(22A)-C(18A)-C(19)-C(20)	1.40(15)	**C(30)-C(25)-C(26)-C(27)**	-0.20(16)

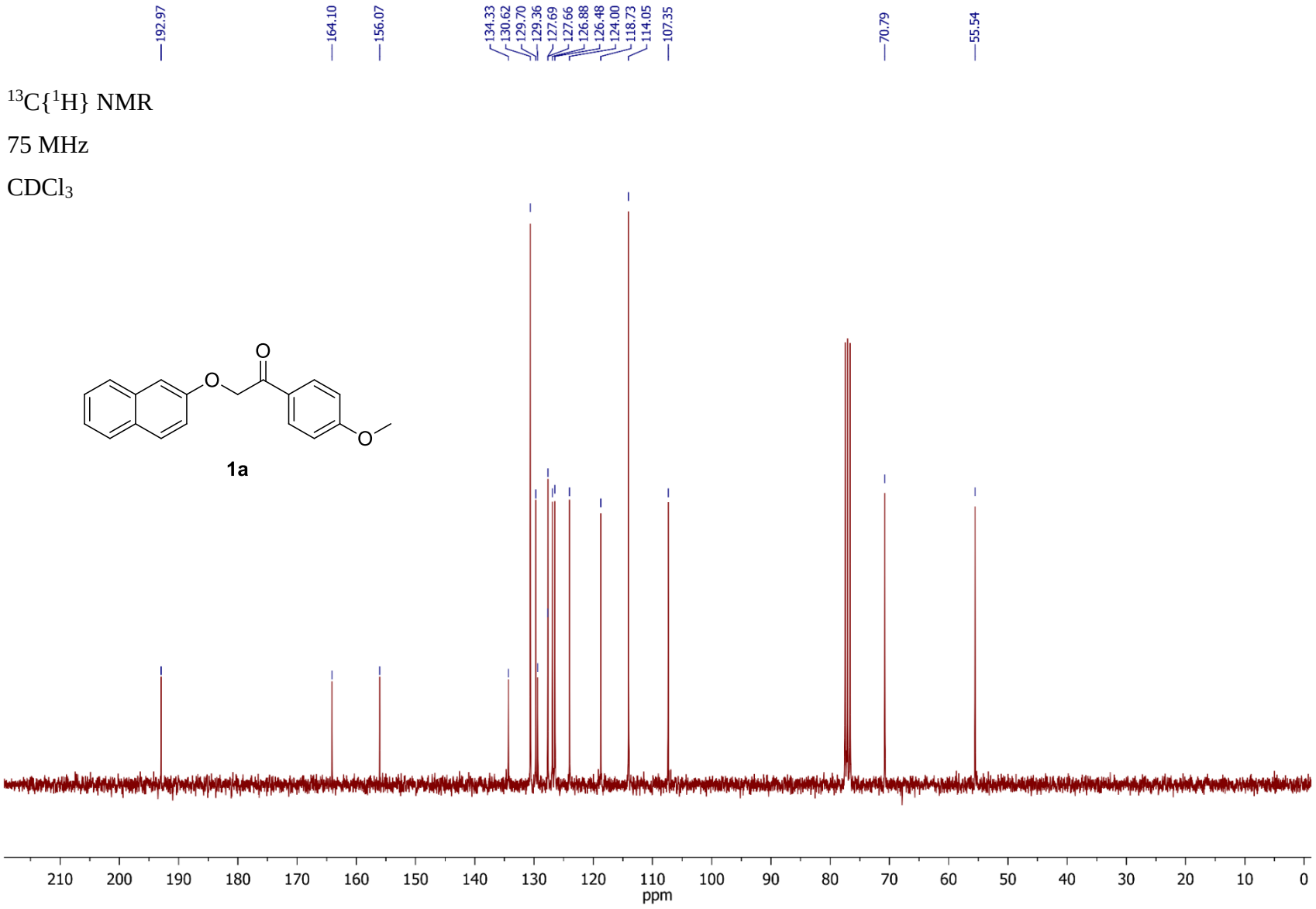
XII. Copies of ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra

^{1}H NMR

300 MHz

$CDCl_3$





$^{13}C\{^{1}H\}$ NMR

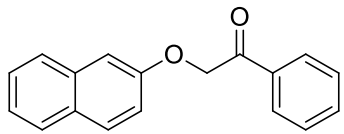
75 MHz

$CDCl_3$

^{1}H NMR

300 MHz

$CDCl_3$



1b

$^{13}C\{^{1}H\}$ NMR

75 MHz

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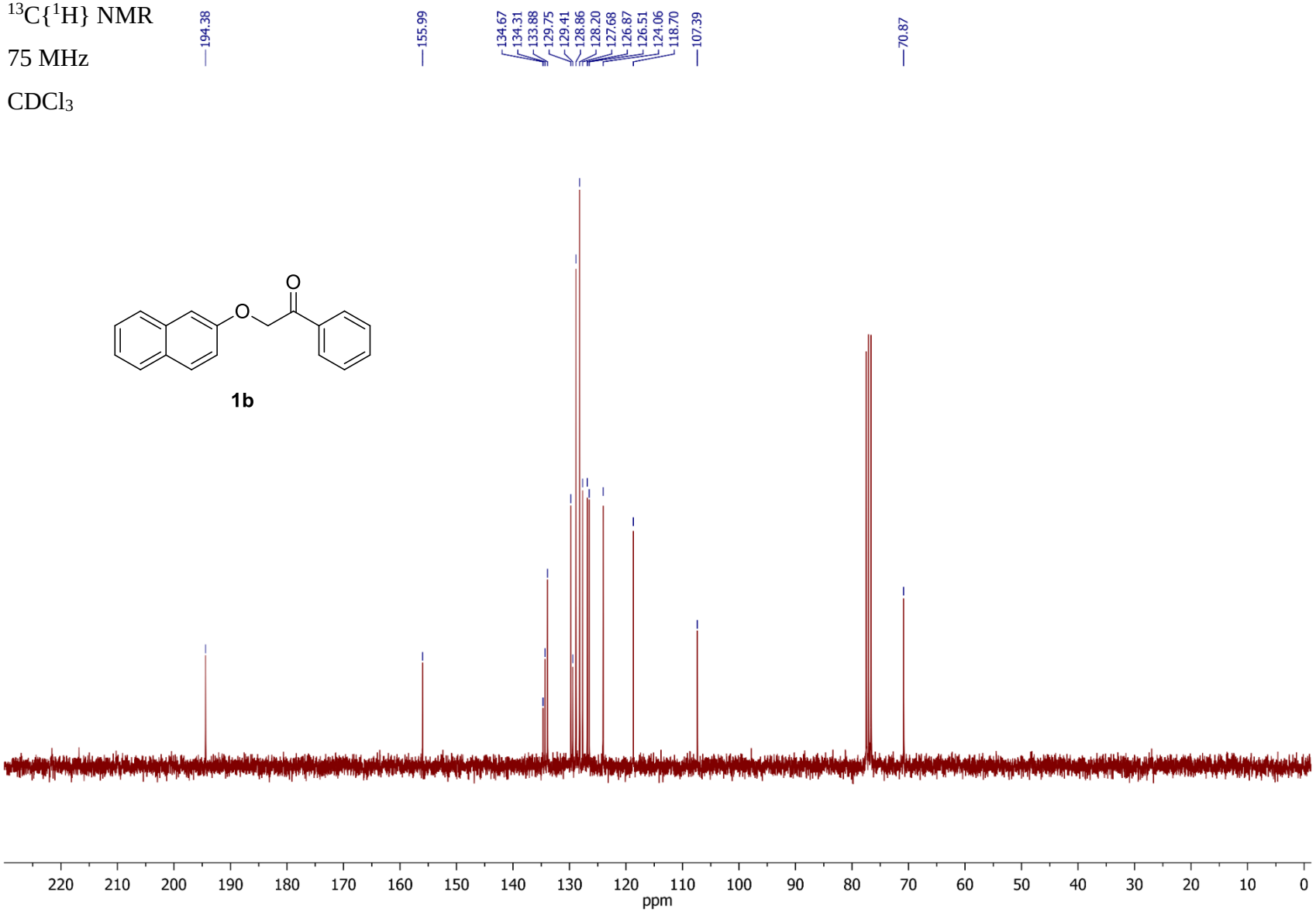
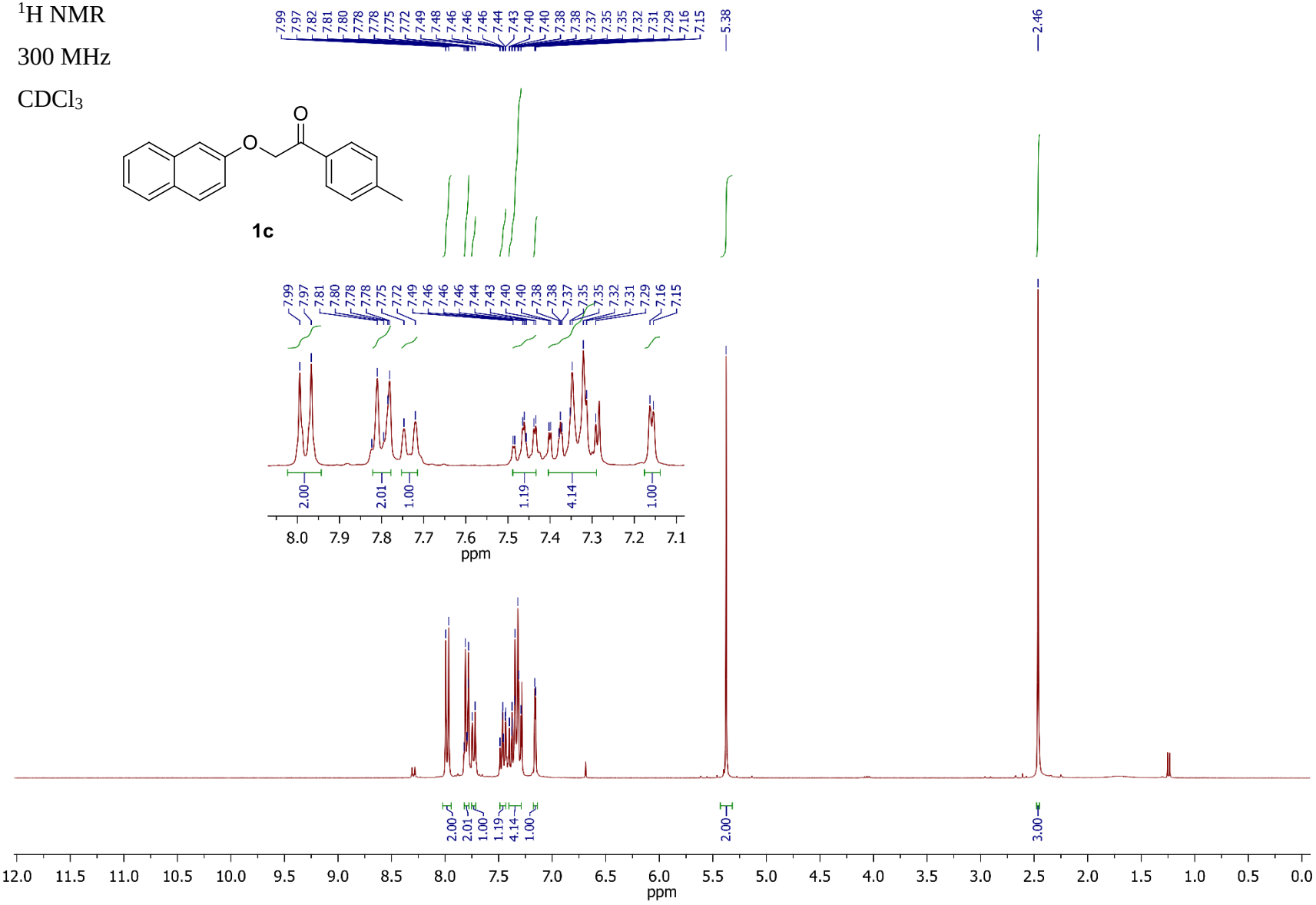


^{1}H NMR

300 MHz

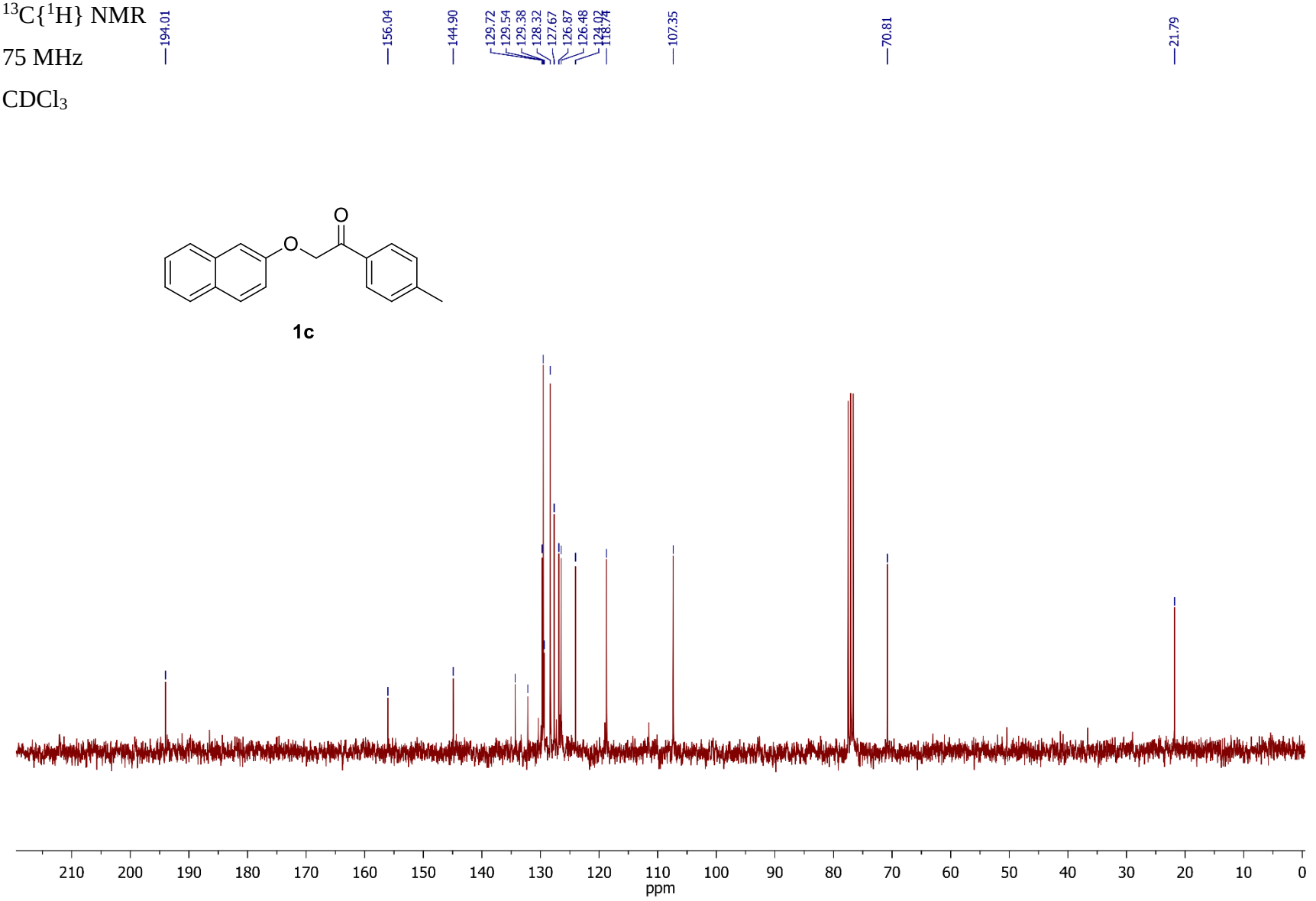
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

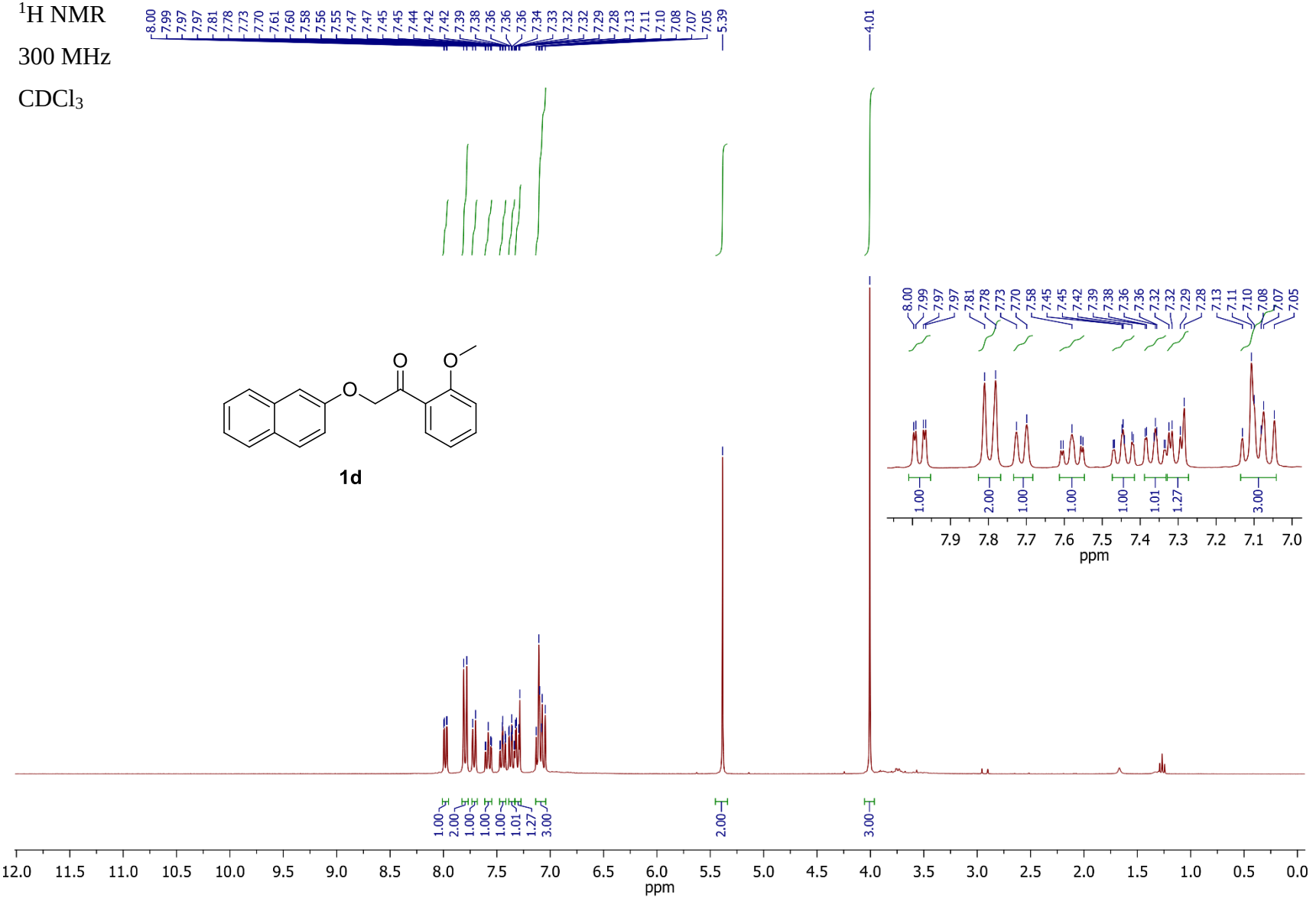
$CDCl_3$



^{1}H NMR

300 MHz

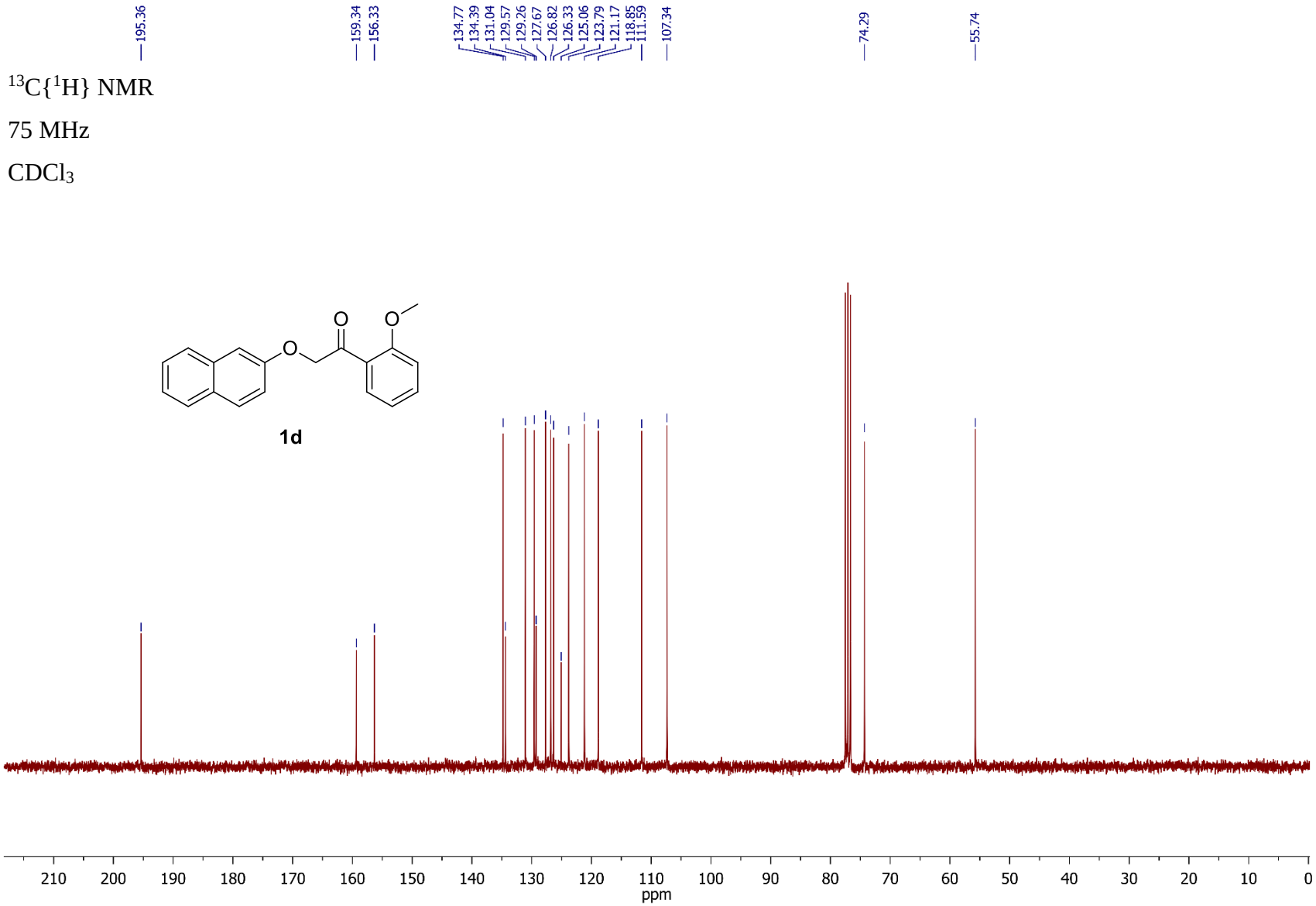
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

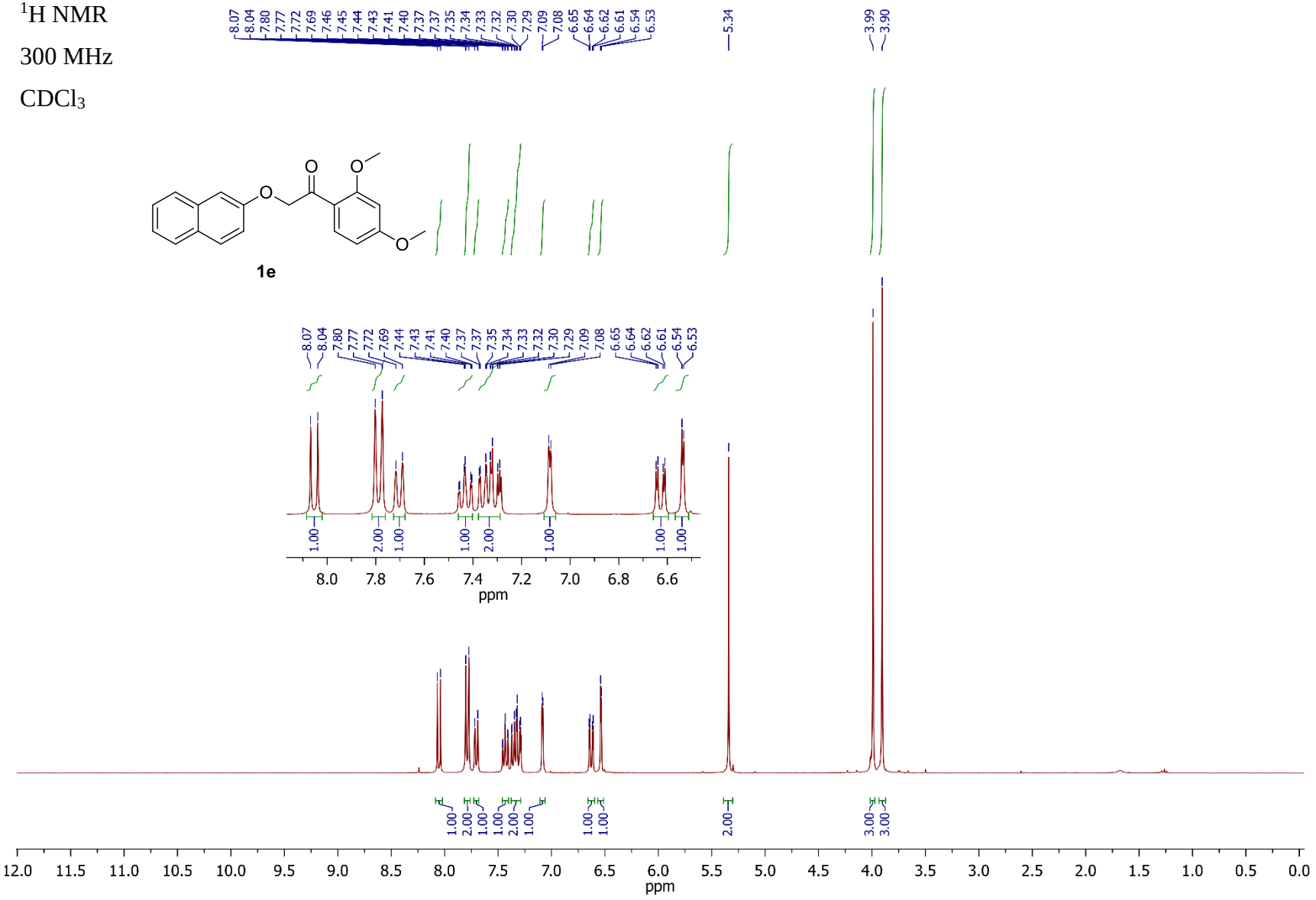
$CDCl_3$



^{1}H NMR

300 MHz

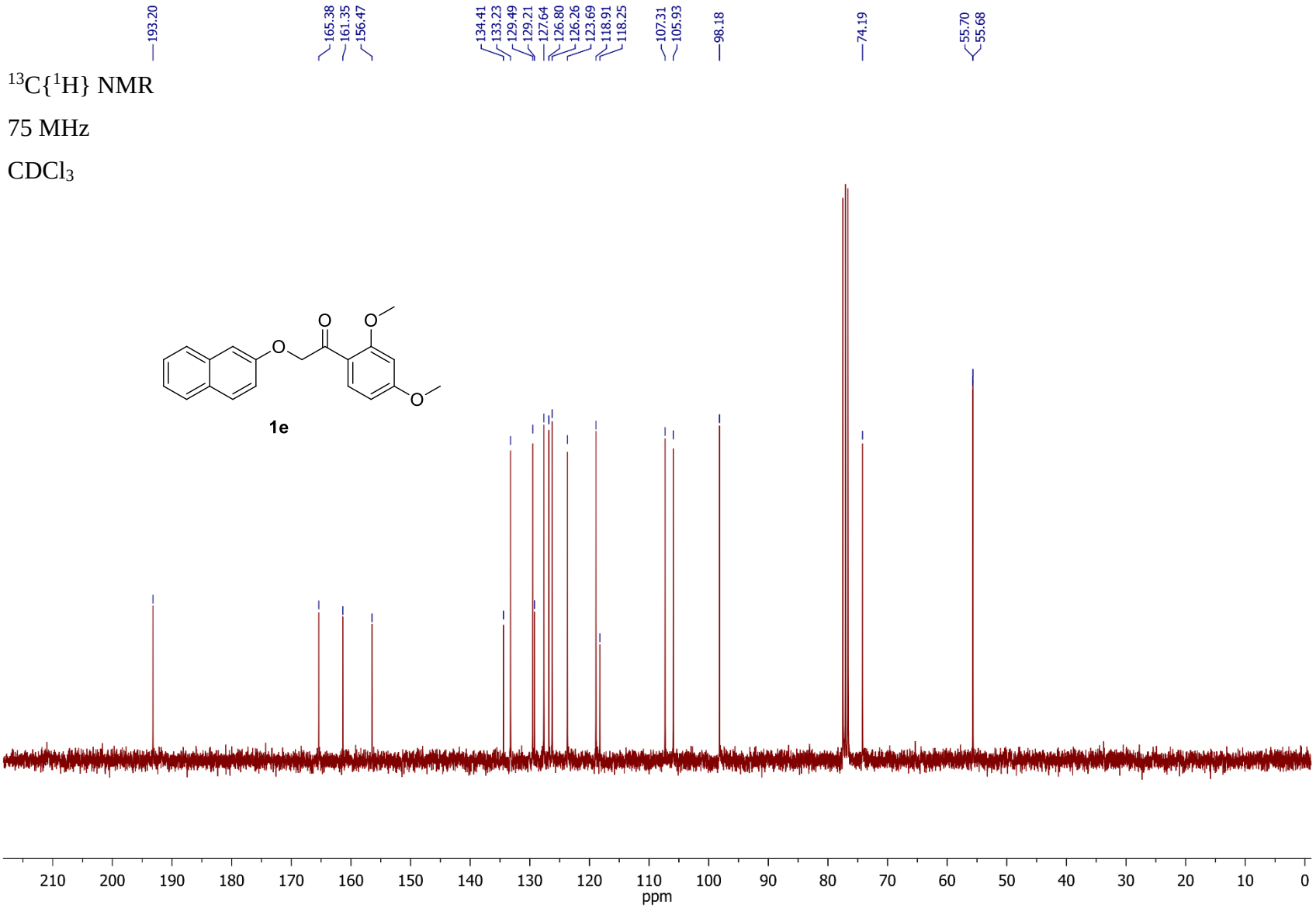
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

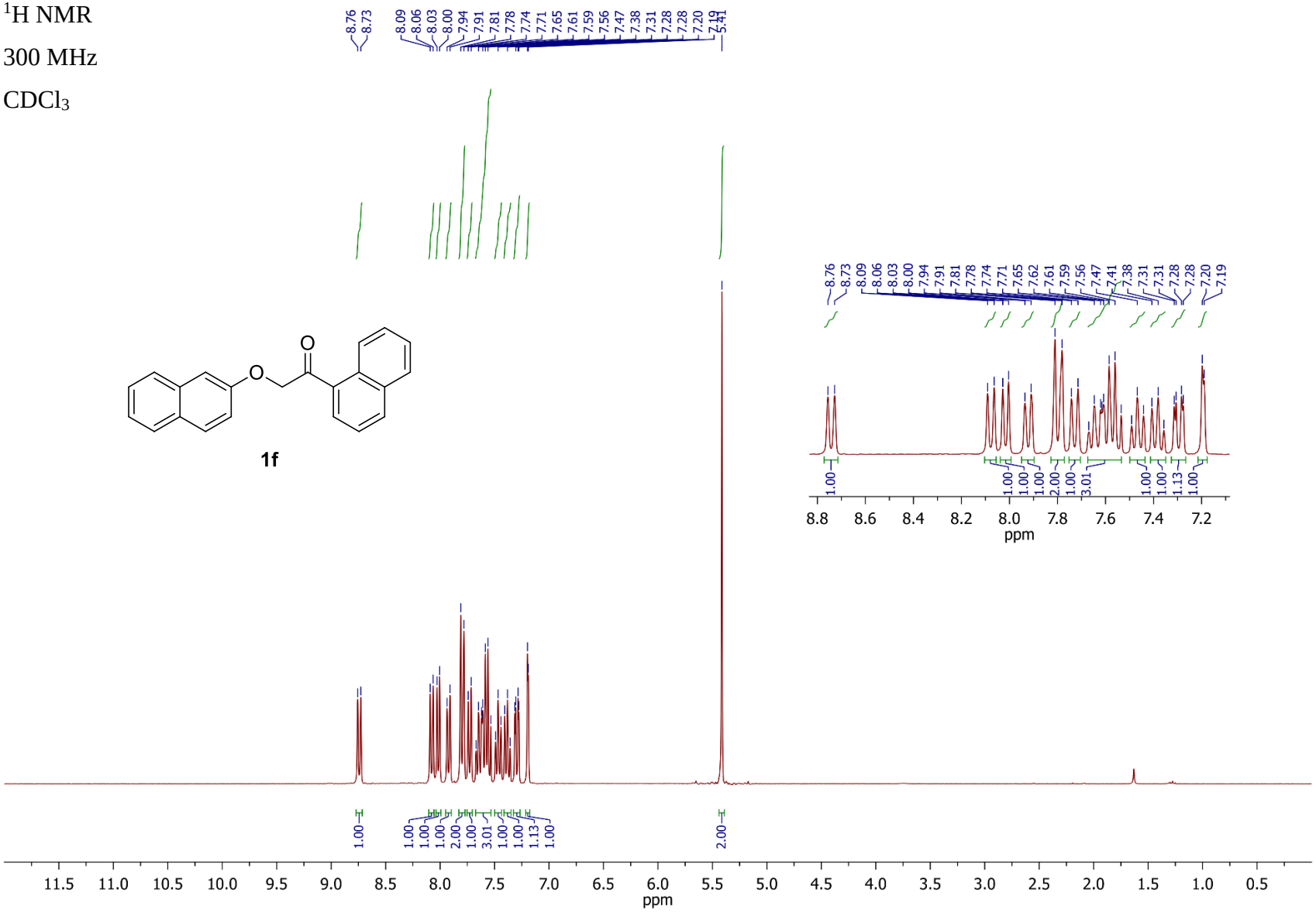
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$

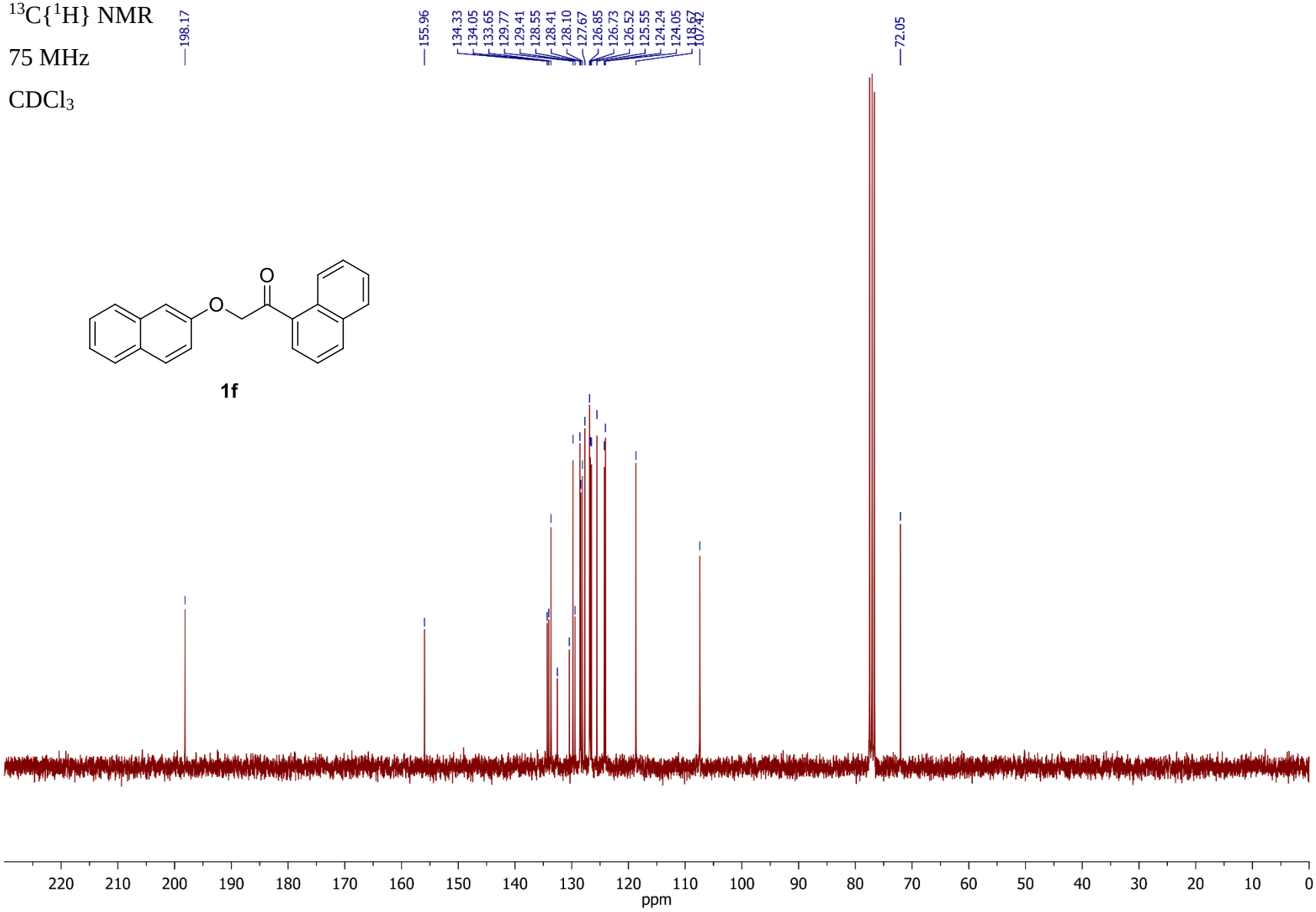


1f

$^{13}C\{^{1}H\}$ NMR

75 MHz

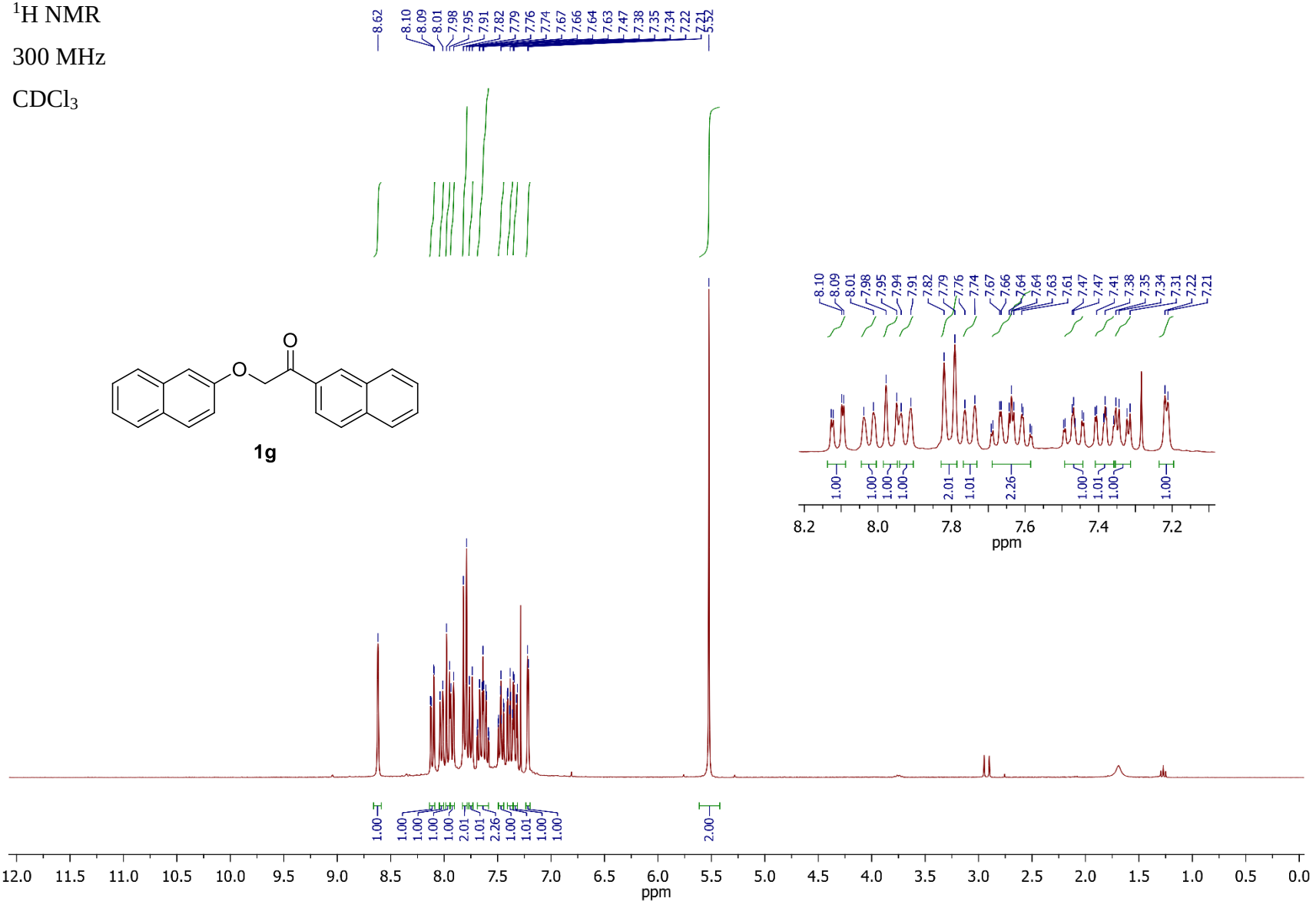
$CDCl_3$



^{1}H NMR

300 MHz

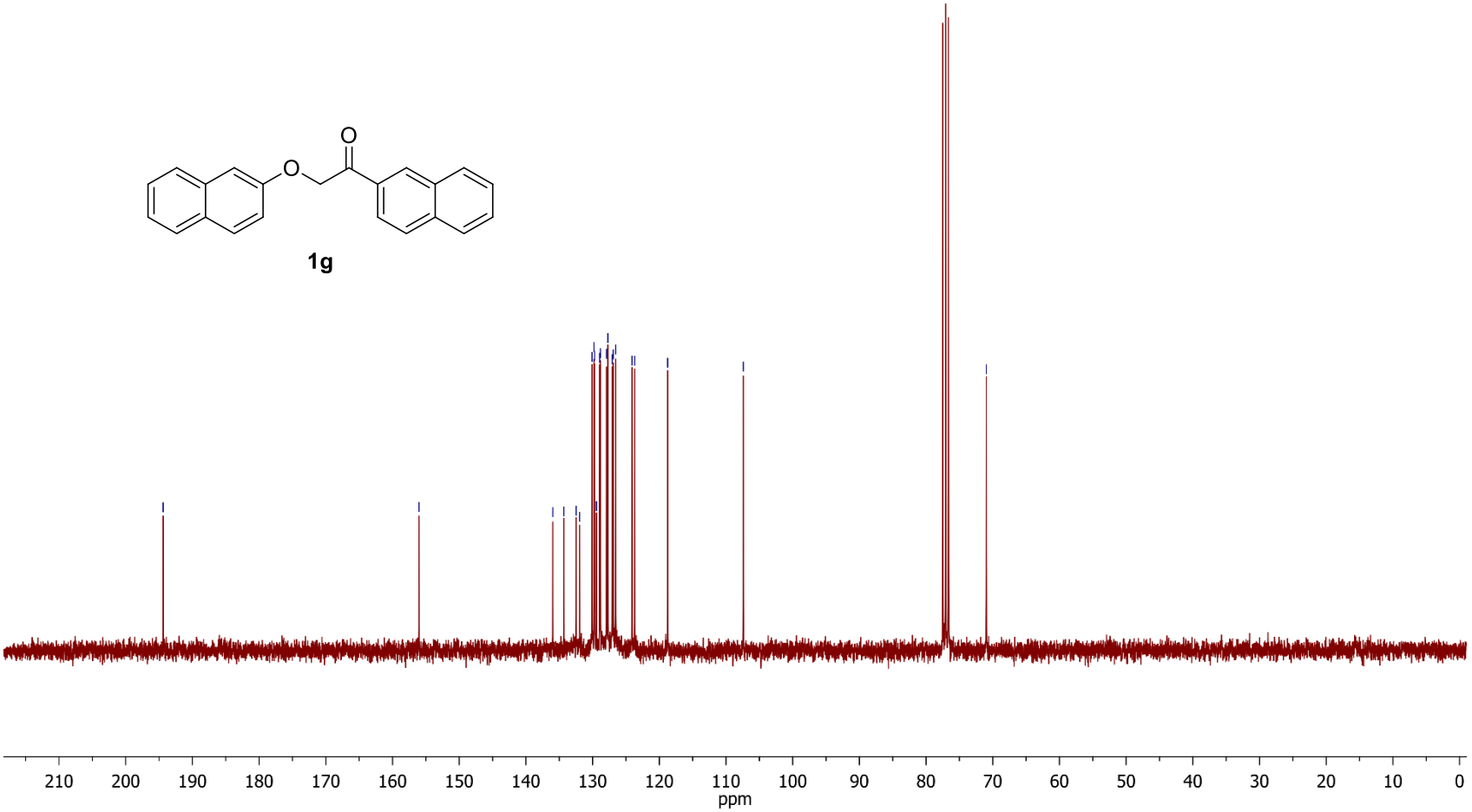
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

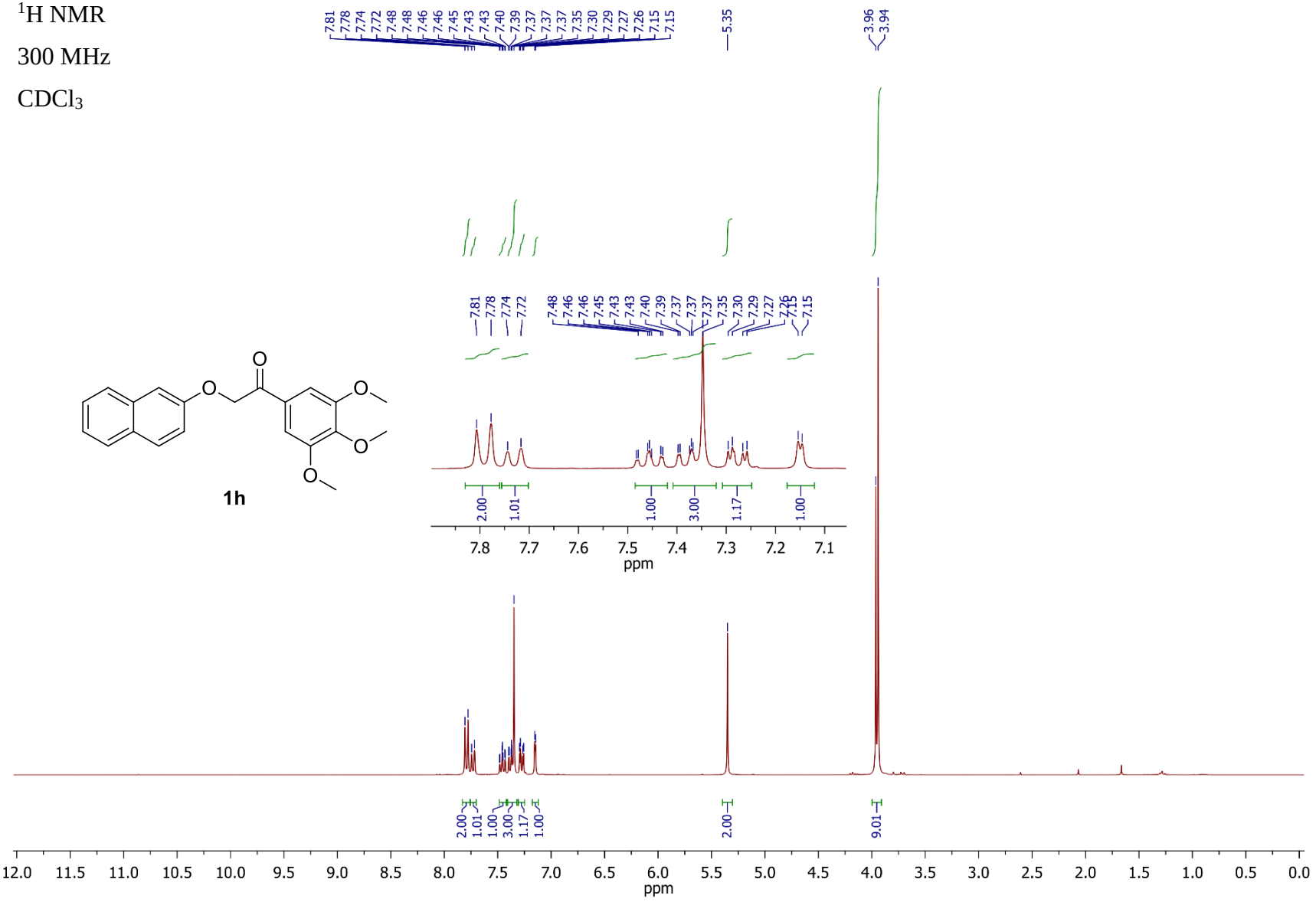
$CDCl_3$



^{1}H NMR

300 MHz

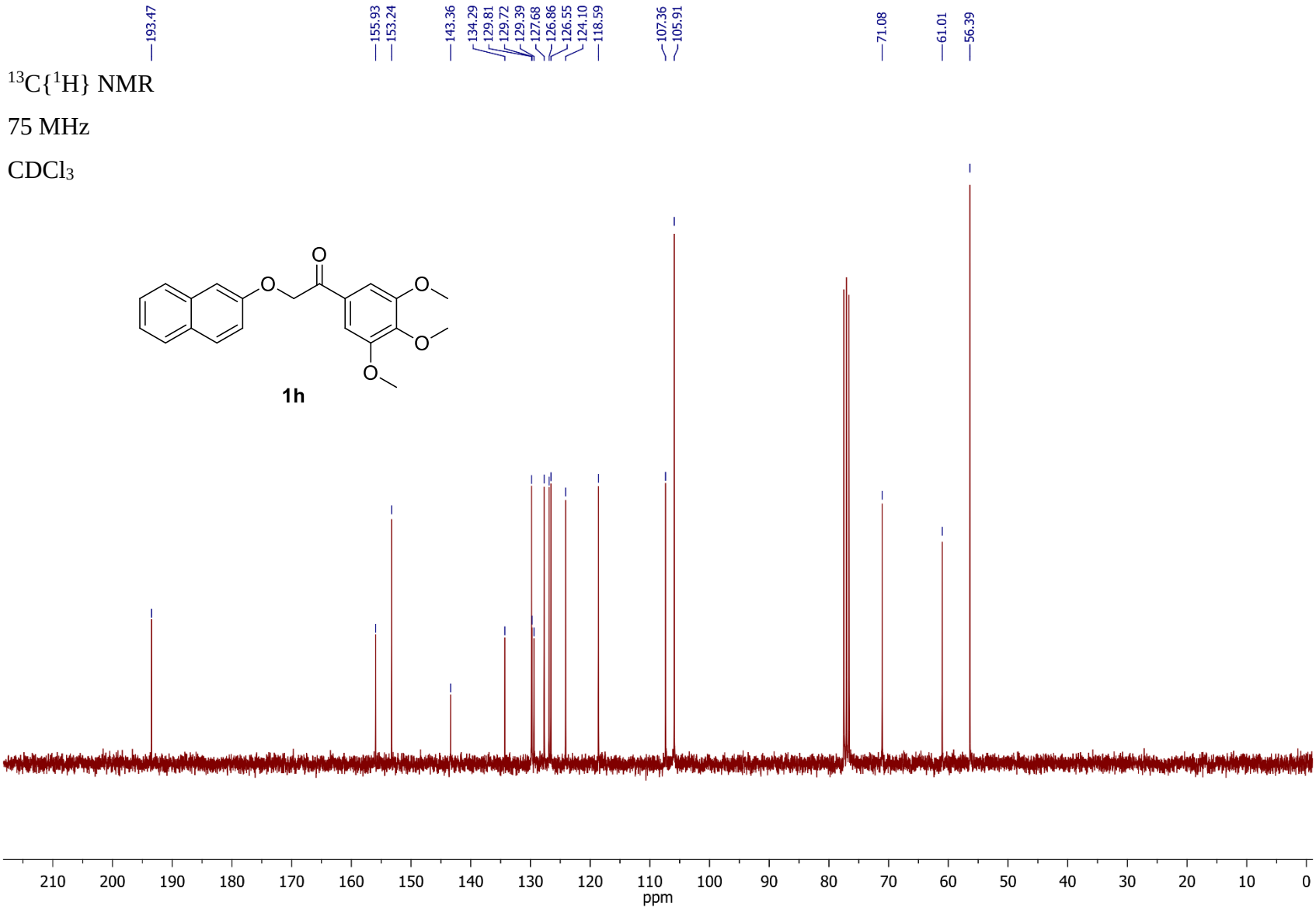
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

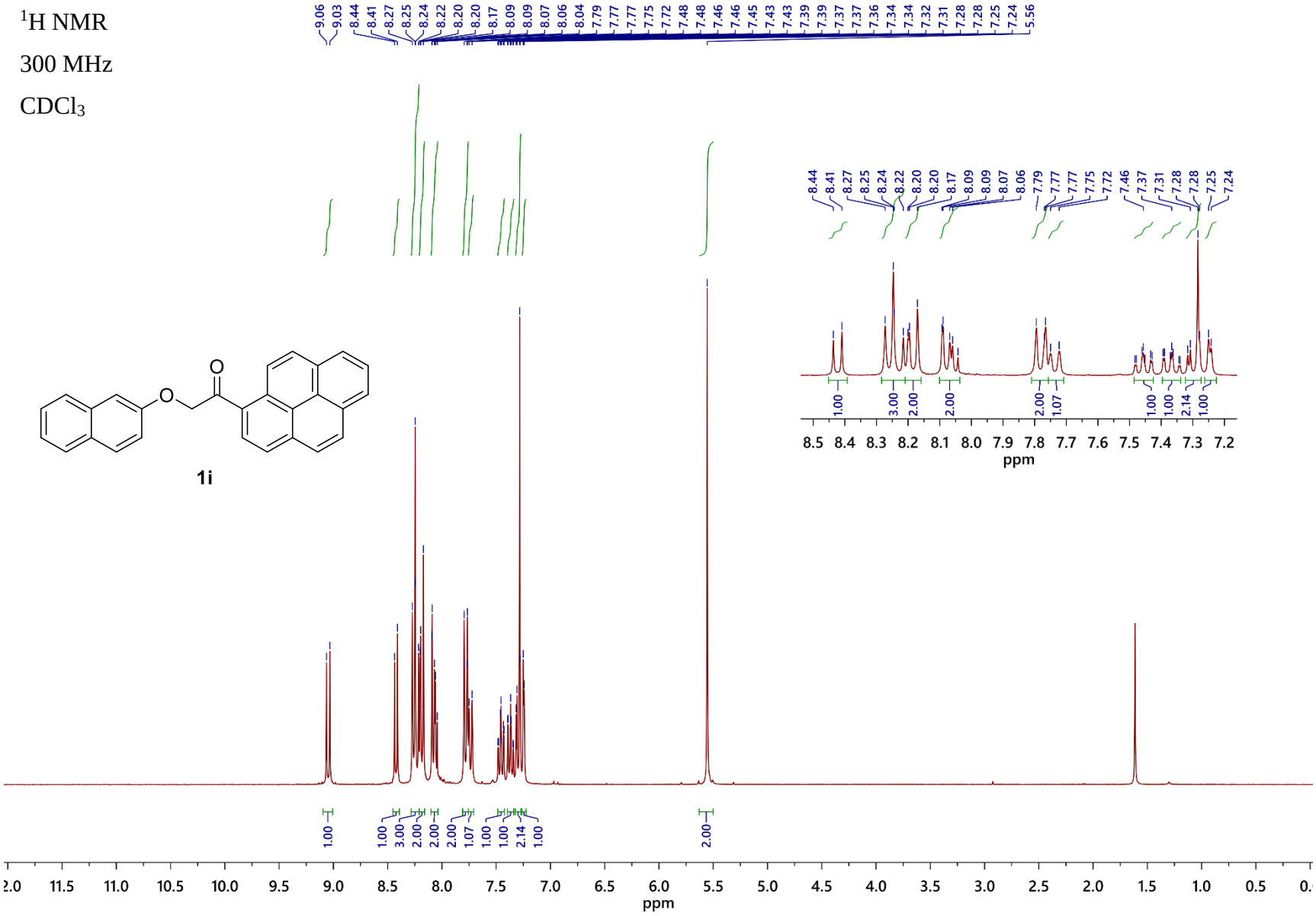
$CDCl_3$

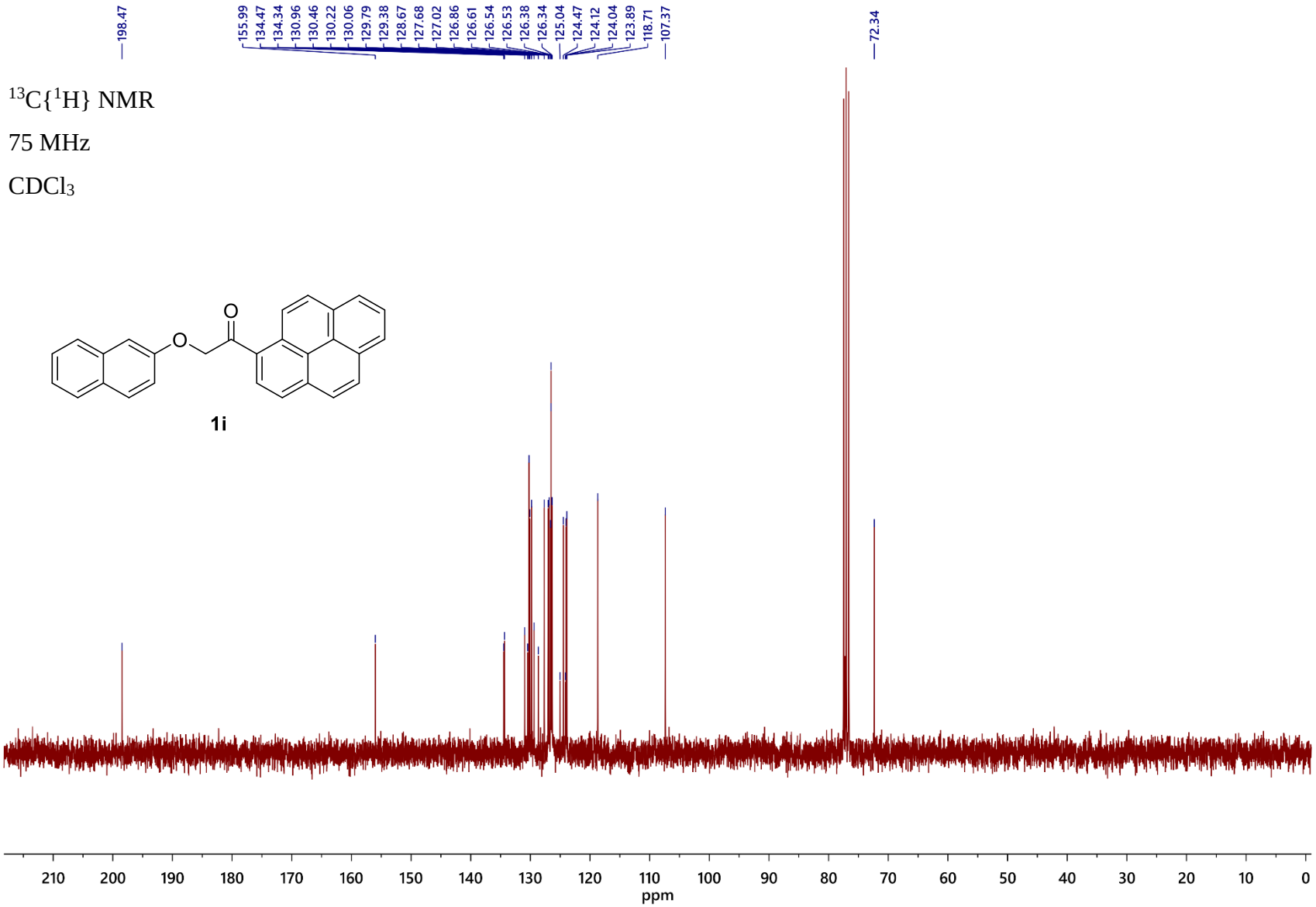


^{1}H NMR

300 MHz

$CDCl_3$

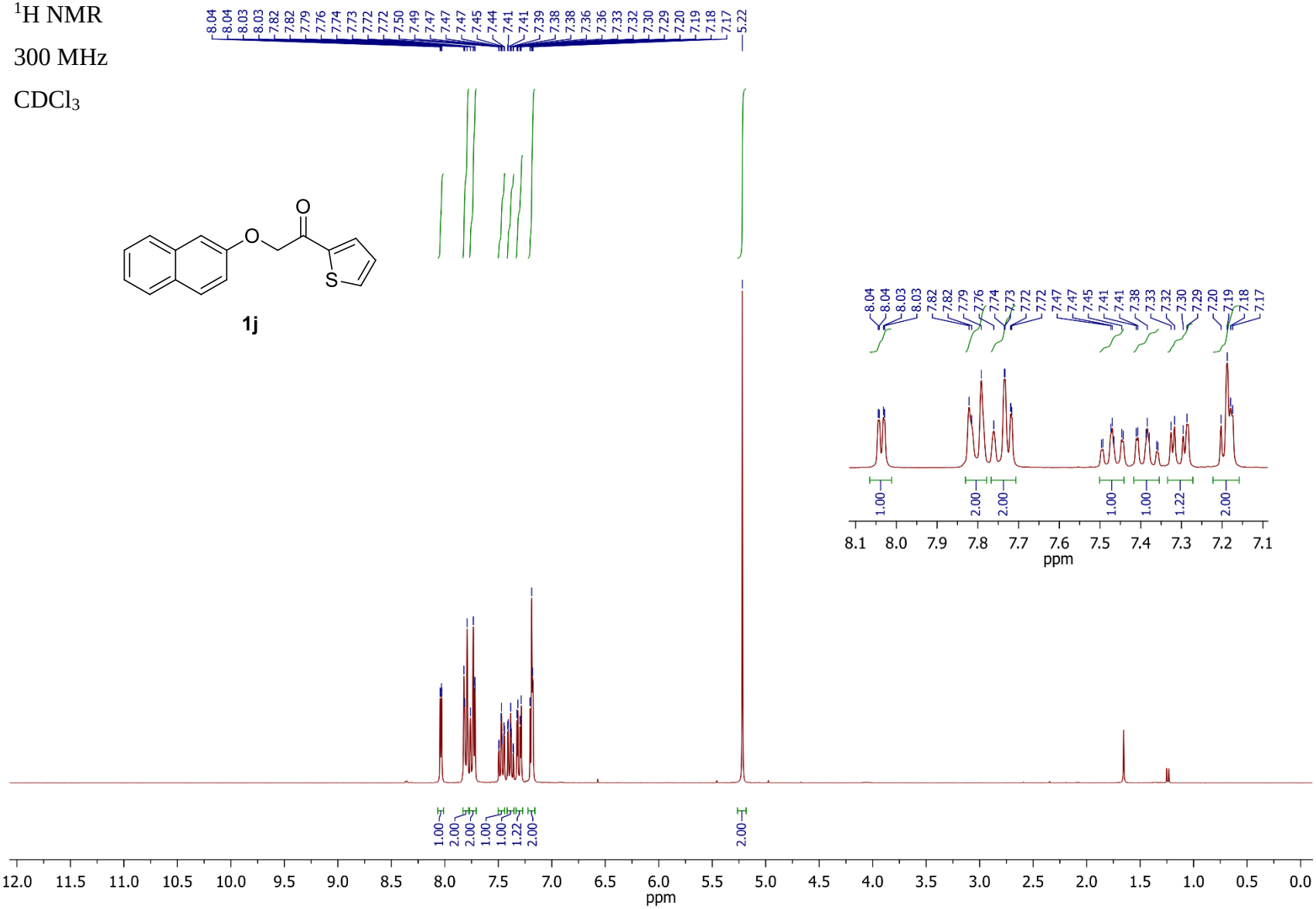



198.47
155.99
134.47
134.34
130.96
130.46
130.22
130.06
129.79
129.38
128.67
127.68
127.02
126.86
126.61
126.54
126.53
126.38
126.34
125.04
124.47
124.12
124.04
123.89
118.71
107.37
72.34
13C{1H} NMR
75 MHz
CDCl3
O
O
1i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

^{1}H NMR

300 MHz

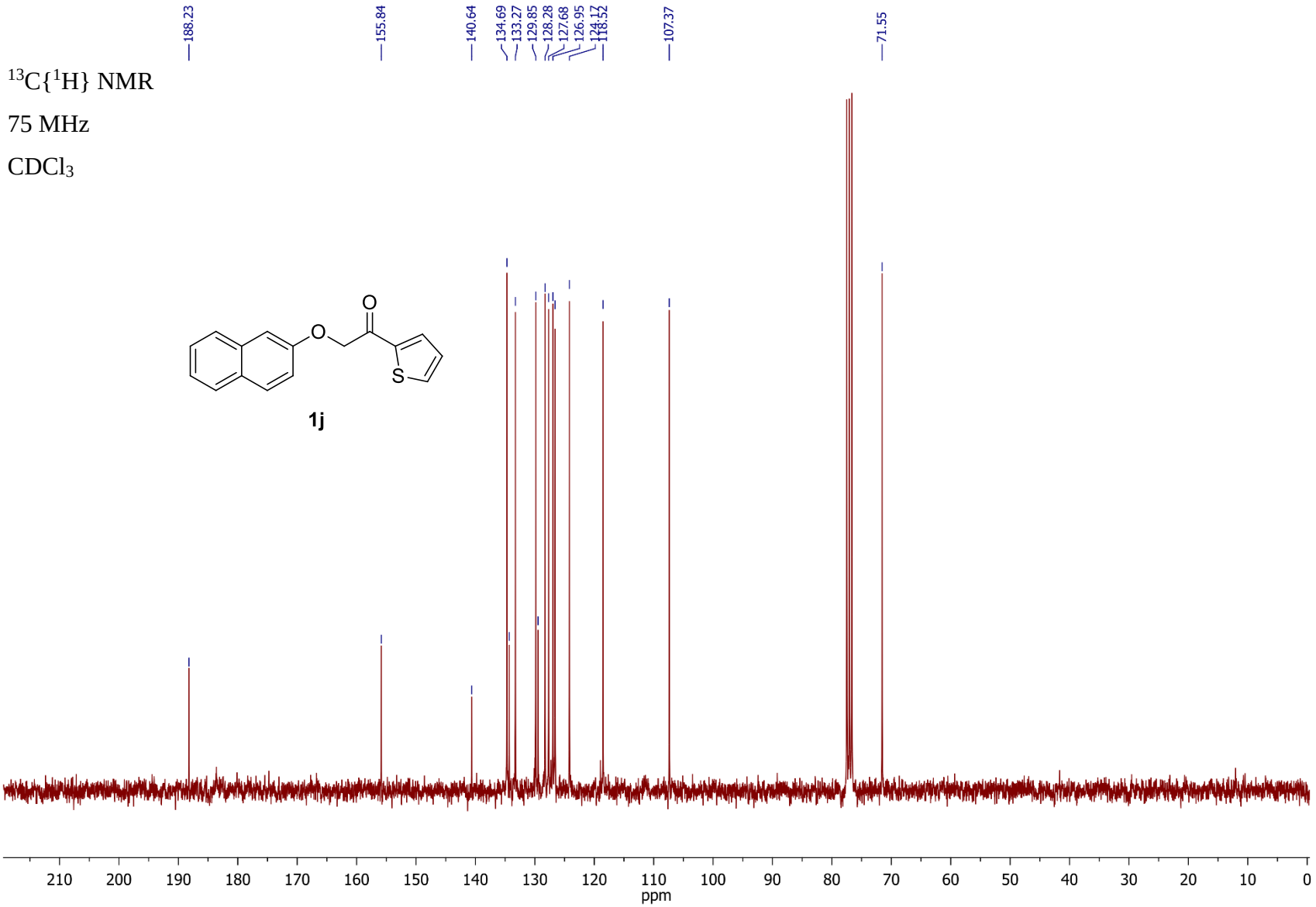
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

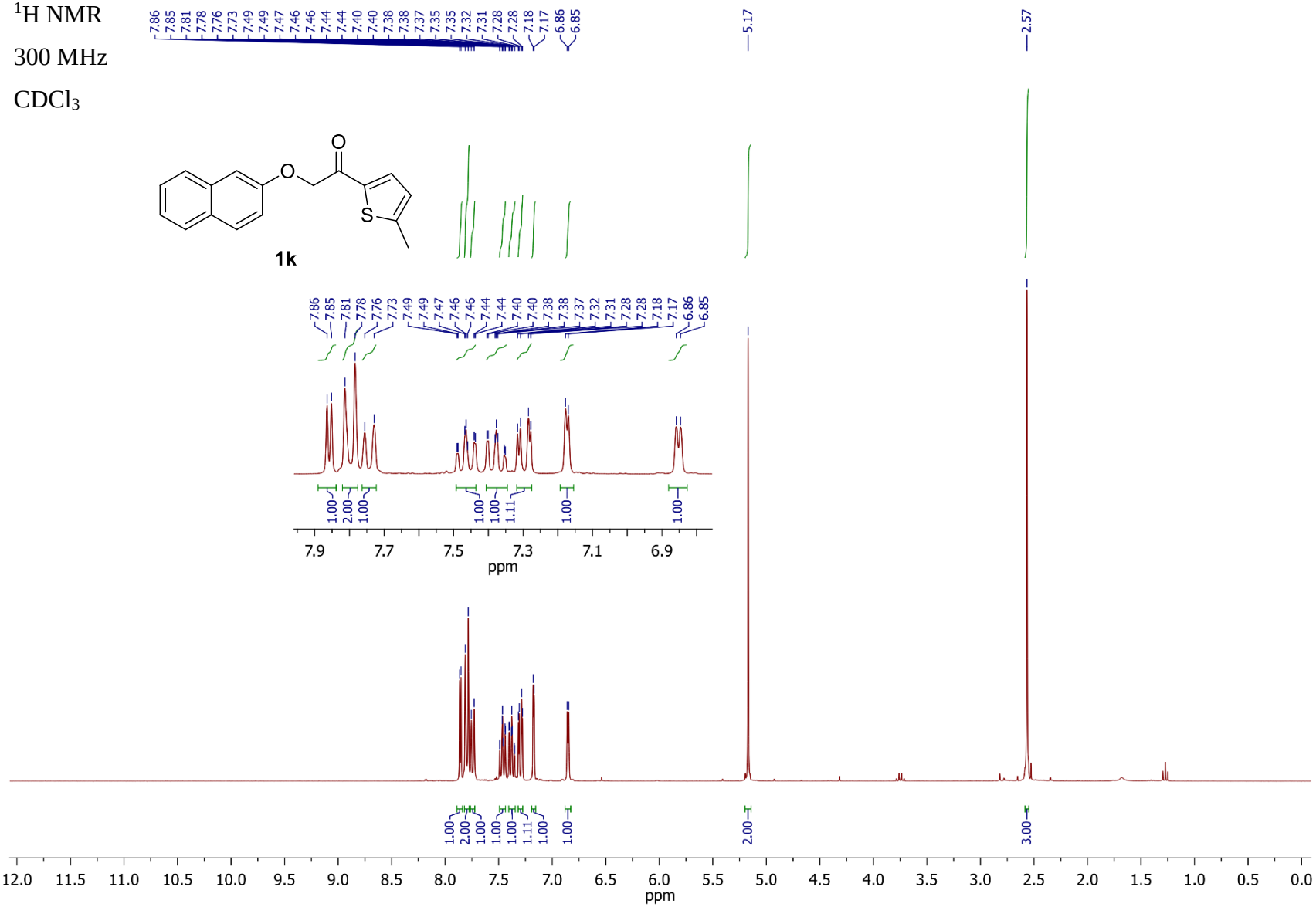
$CDCl_3$



^{1}H NMR

300 MHz

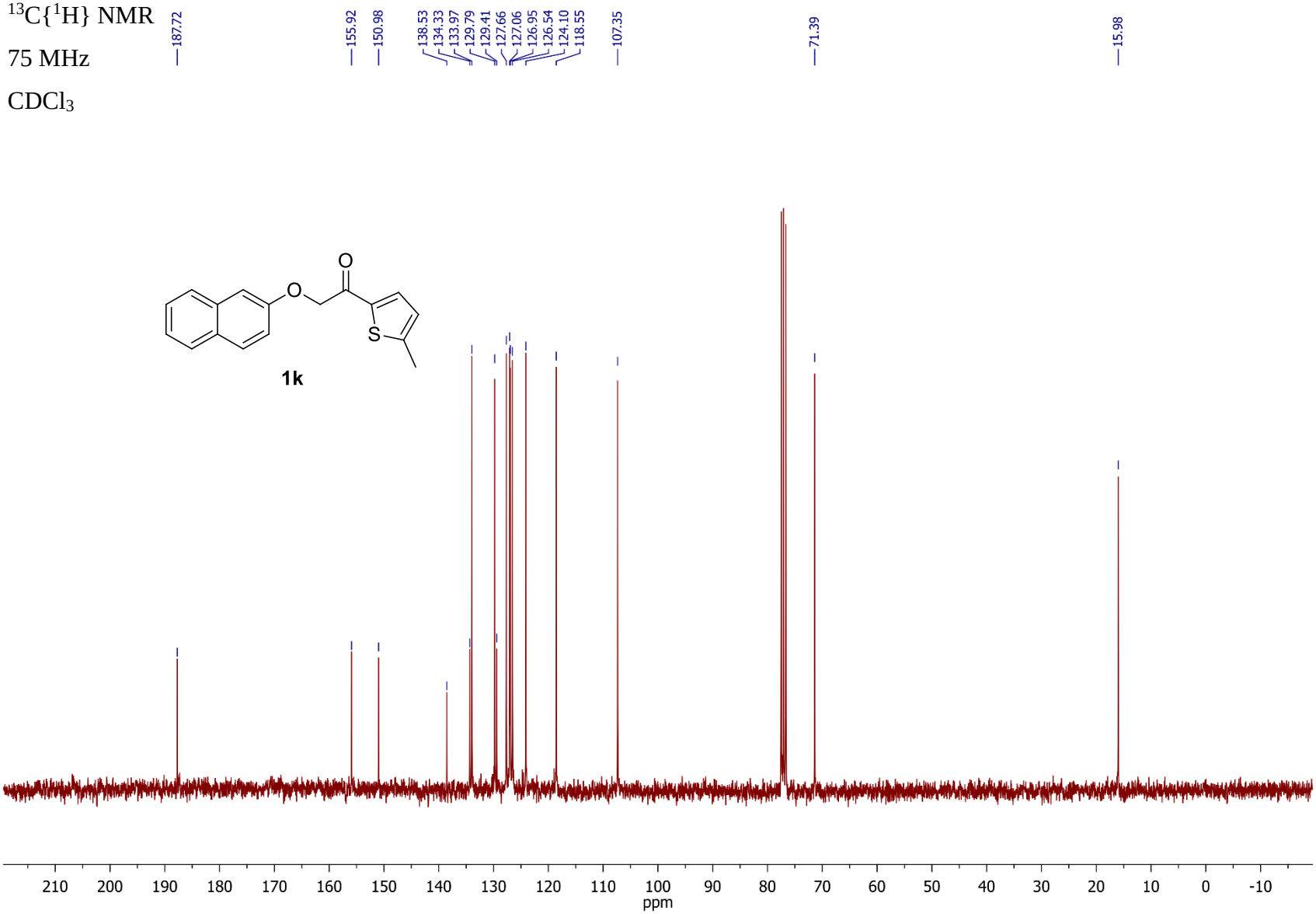
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

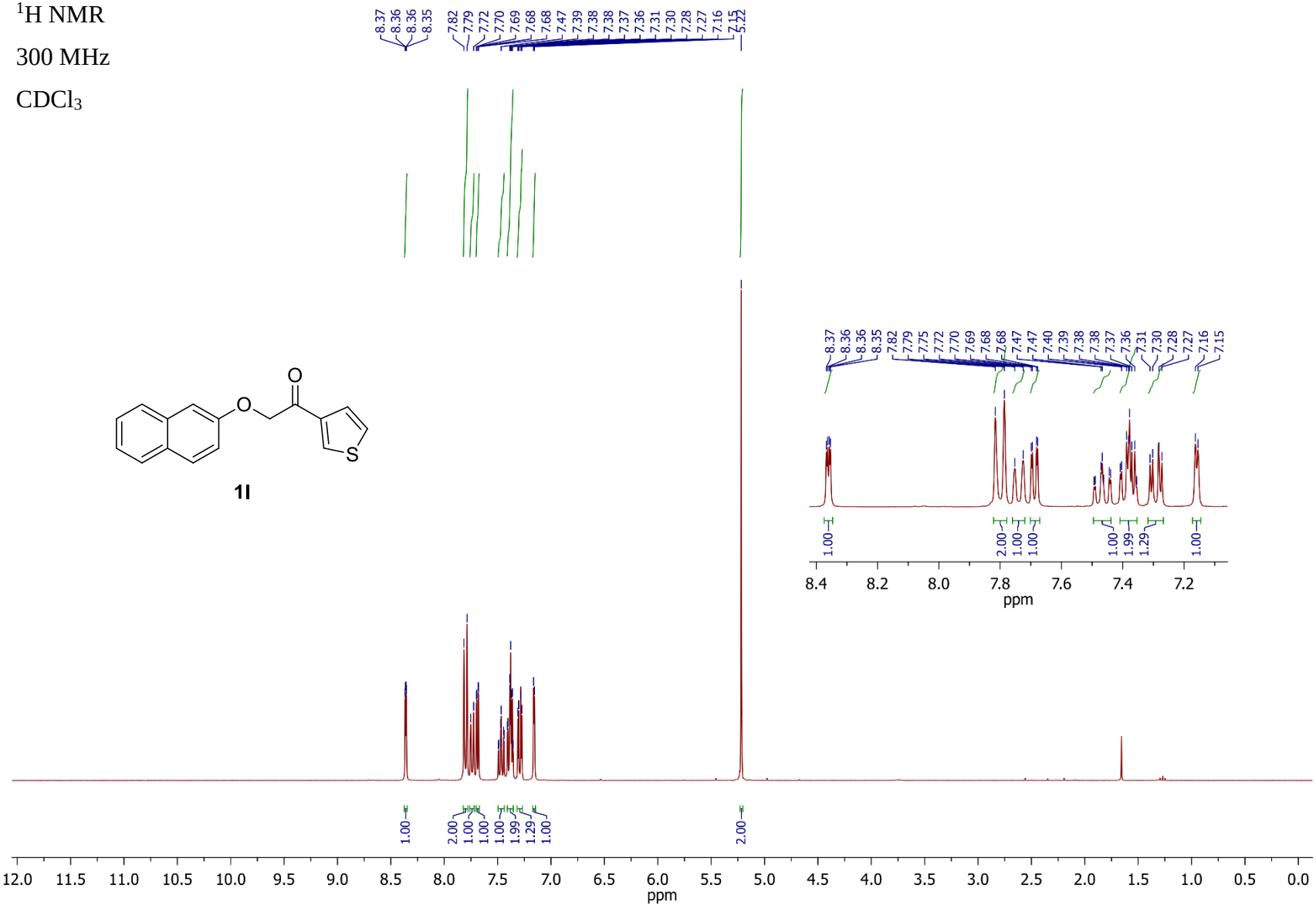
$CDCl_3$



^{1}H NMR

300 MHz

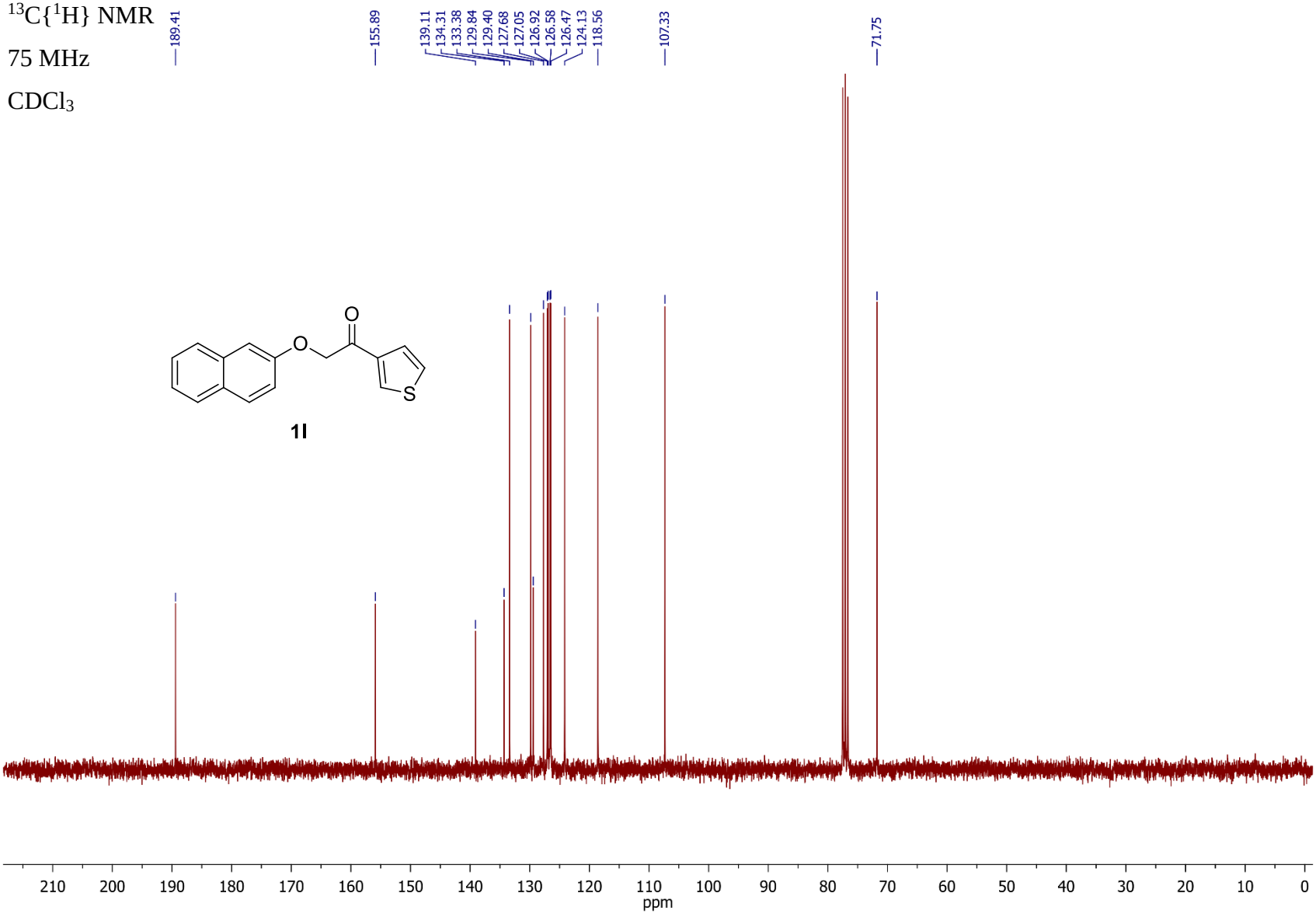
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

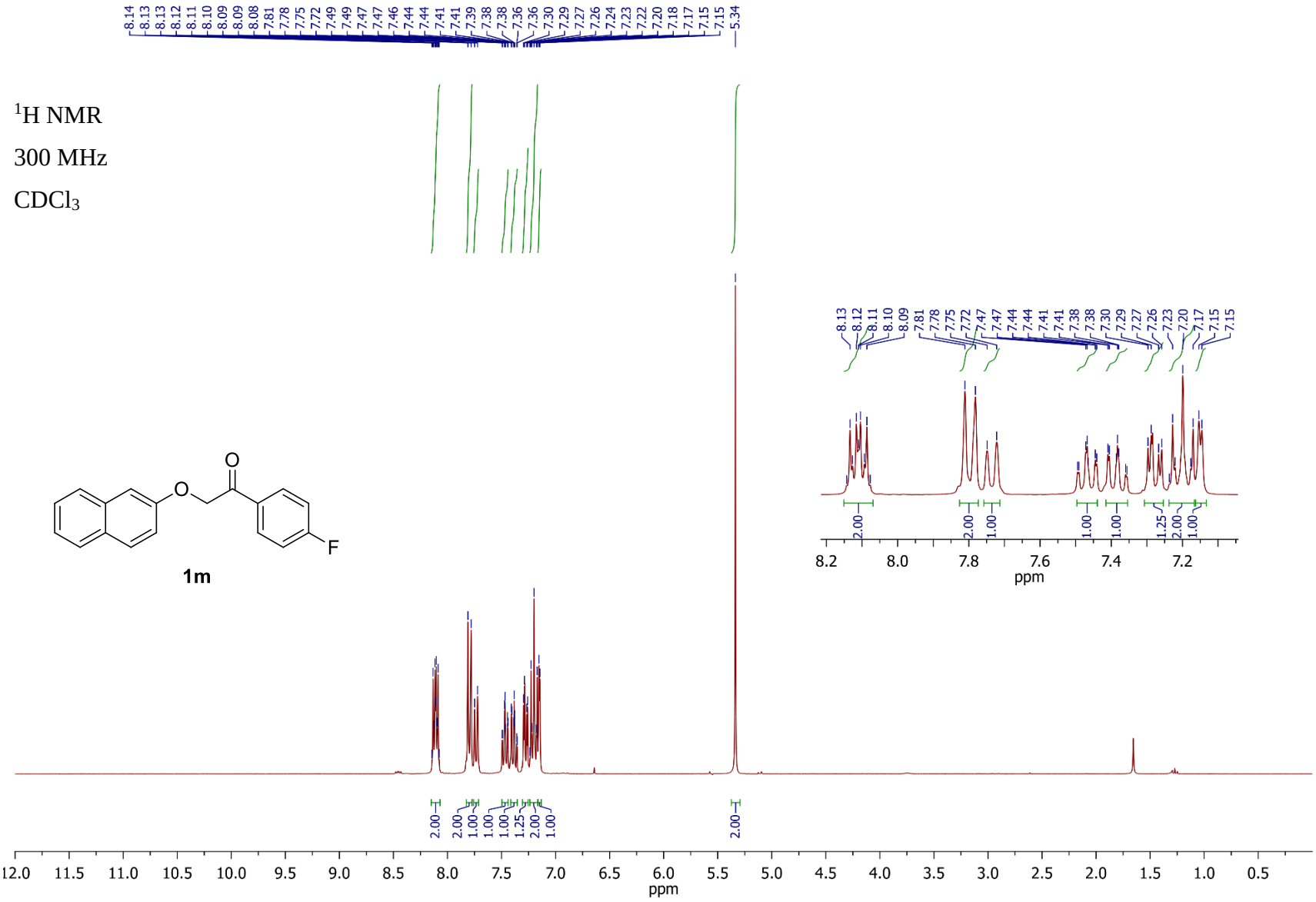
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$

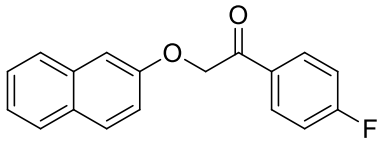


193.15
167.85
164.46
155.84
134.27
131.14
131.10
131.06
131.02
129.83
129.42
127.70
126.88
126.59
124.15
118.61
116.21
115.92
107.32
70.91

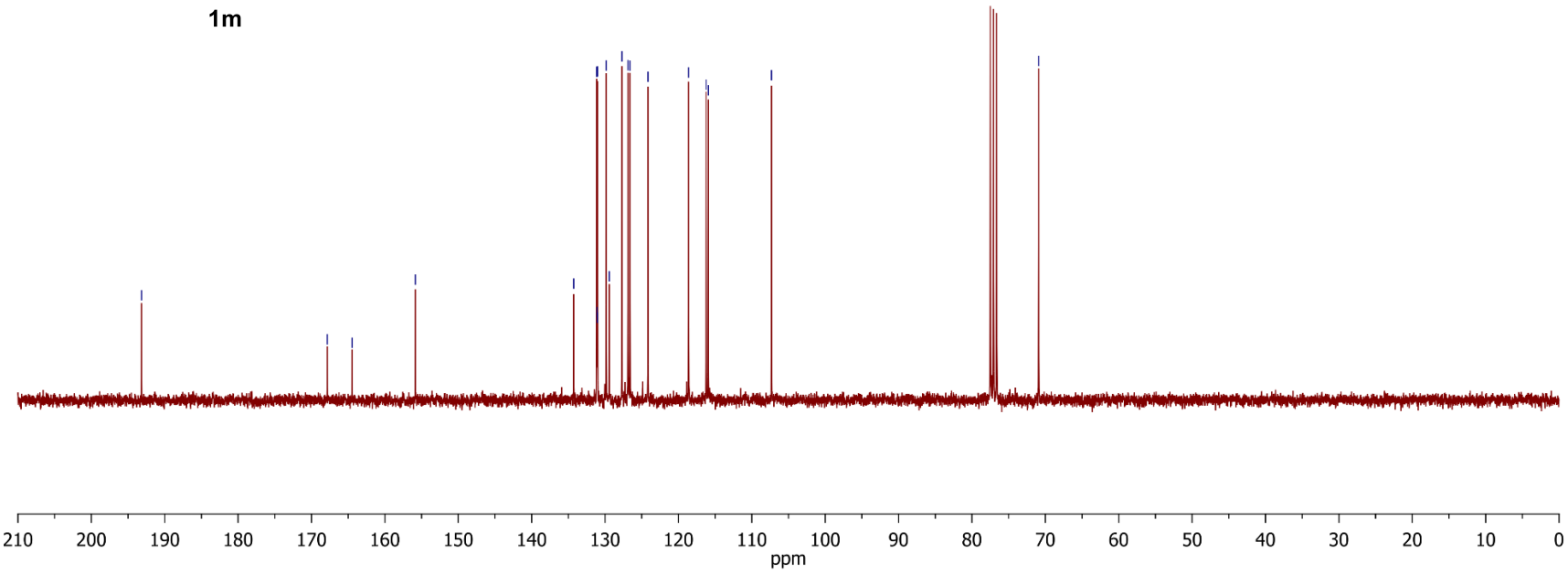
$^{13}C\{^{1}H\}$ NMR

75 MHz

$CDCl_3$



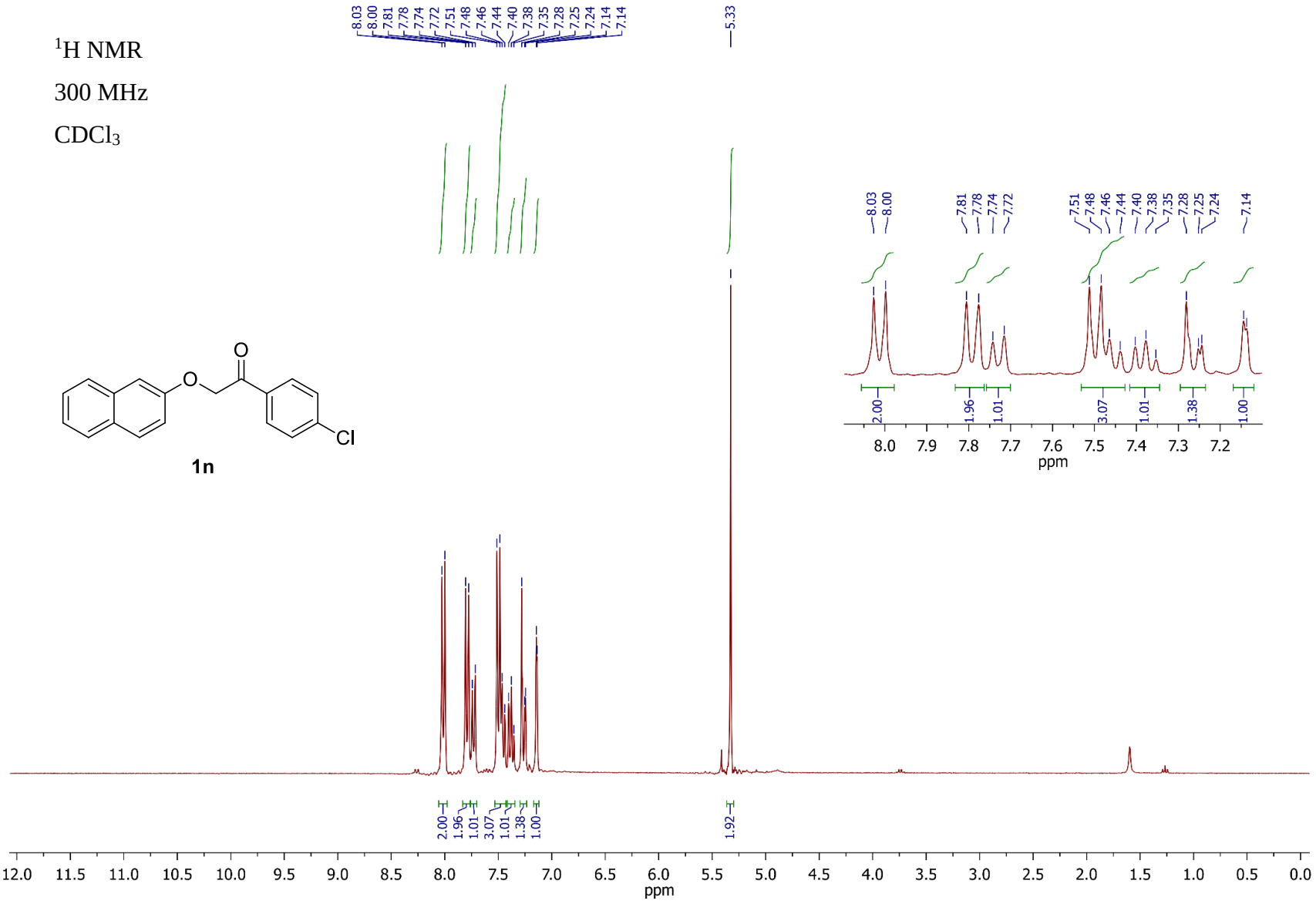
1m



^{1}H NMR

300 MHz

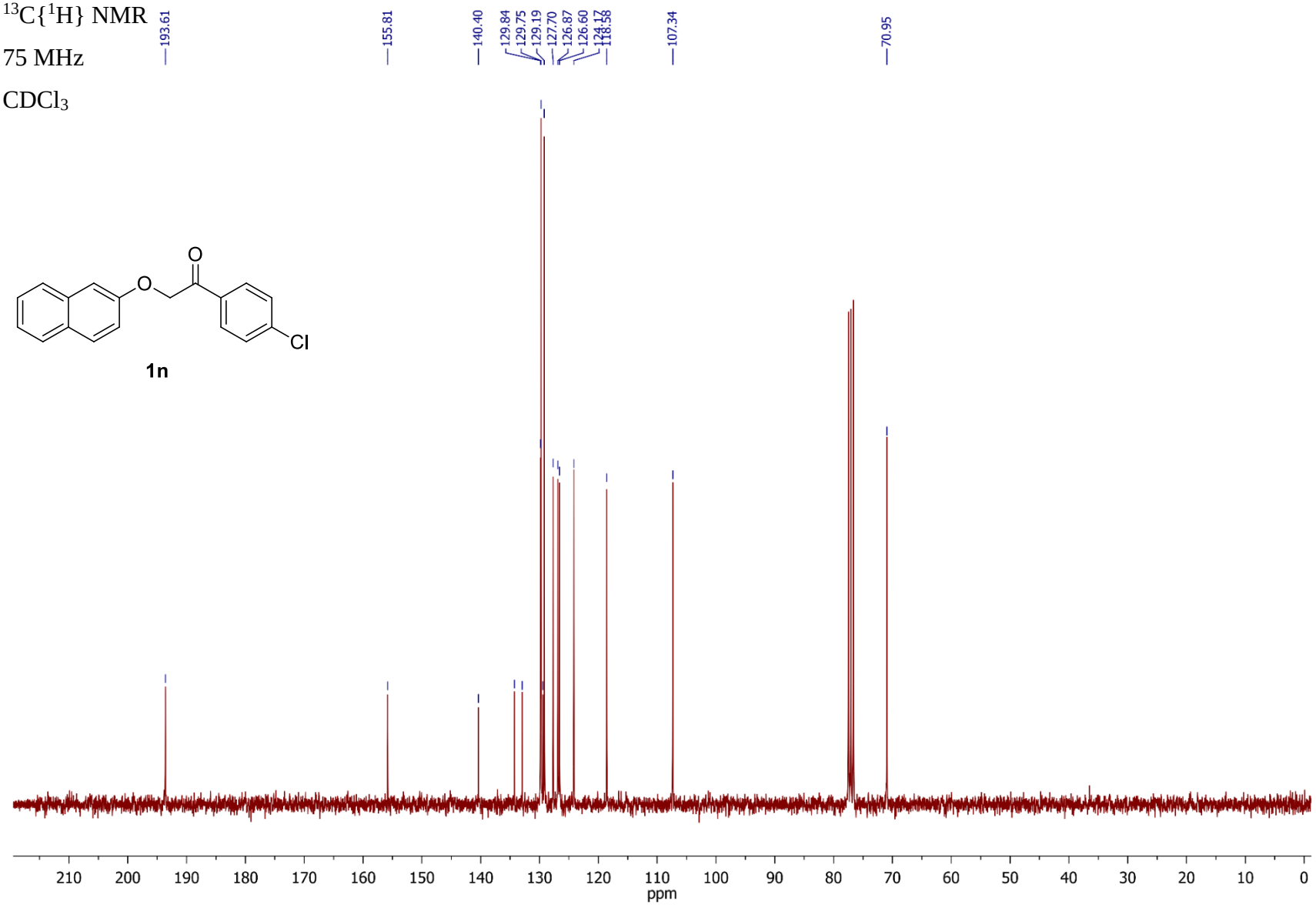
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

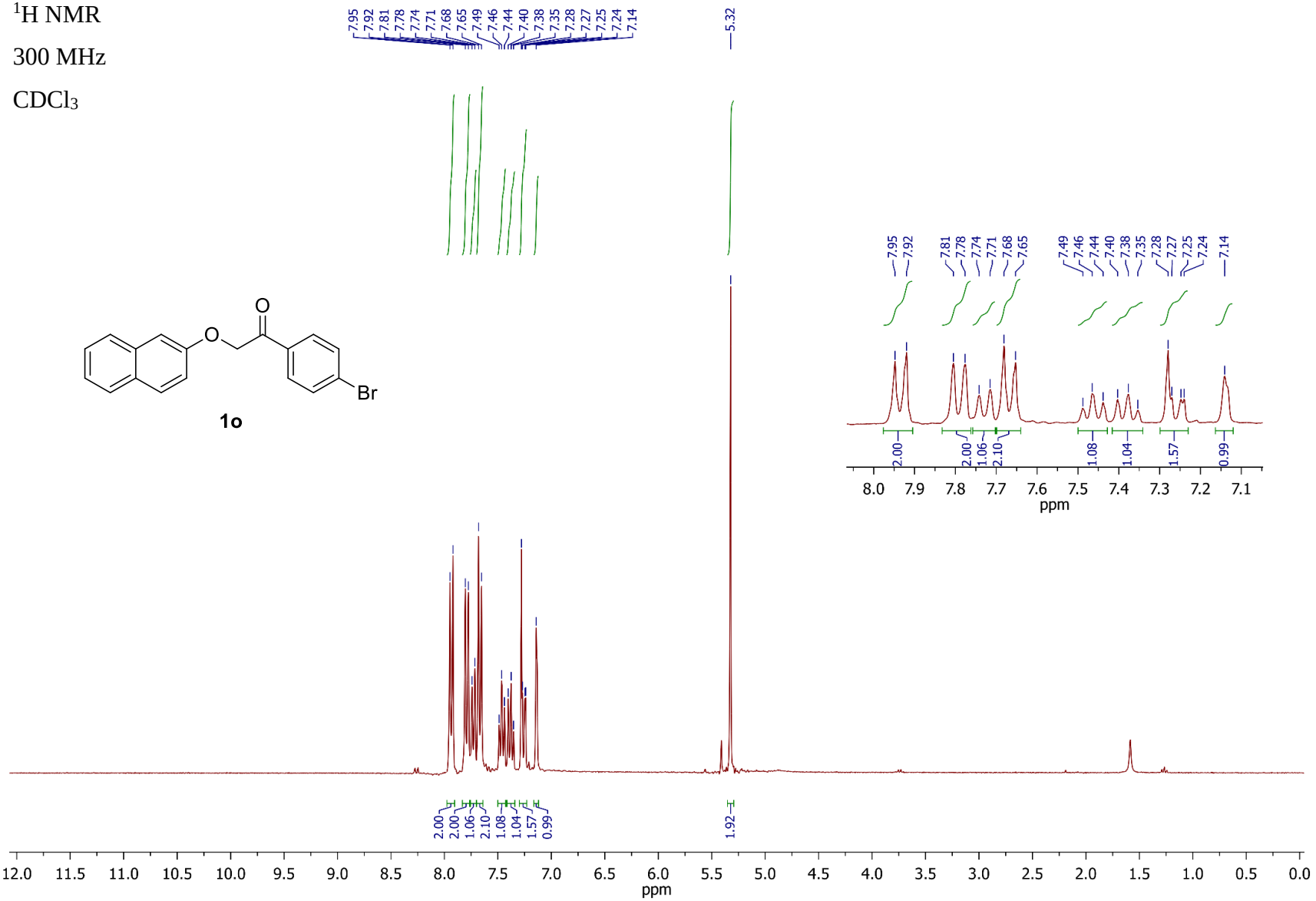
$CDCl_3$



^{1}H NMR

300 MHz

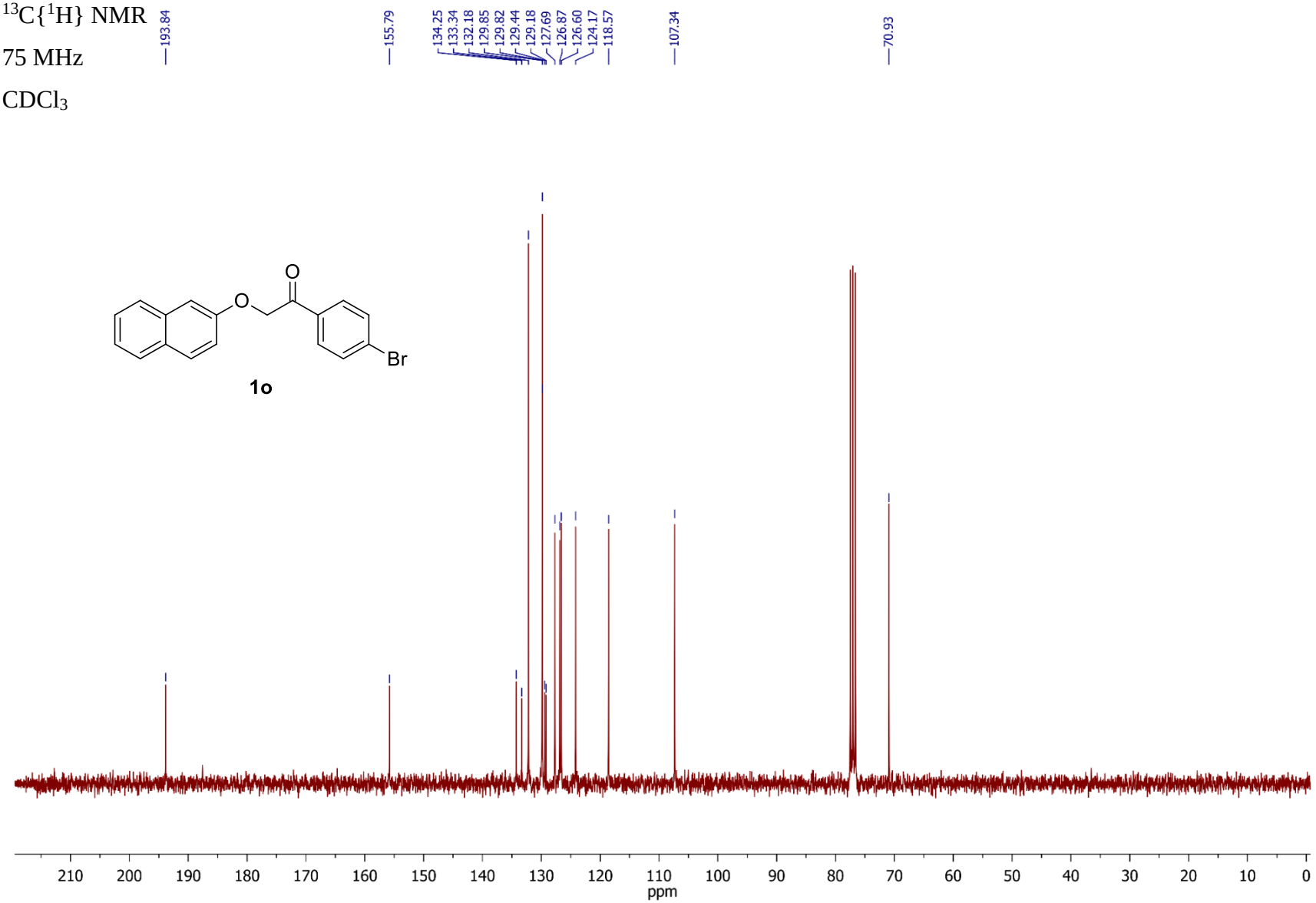
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

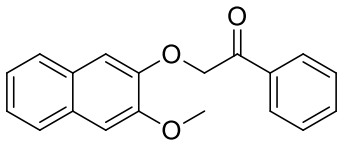
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$

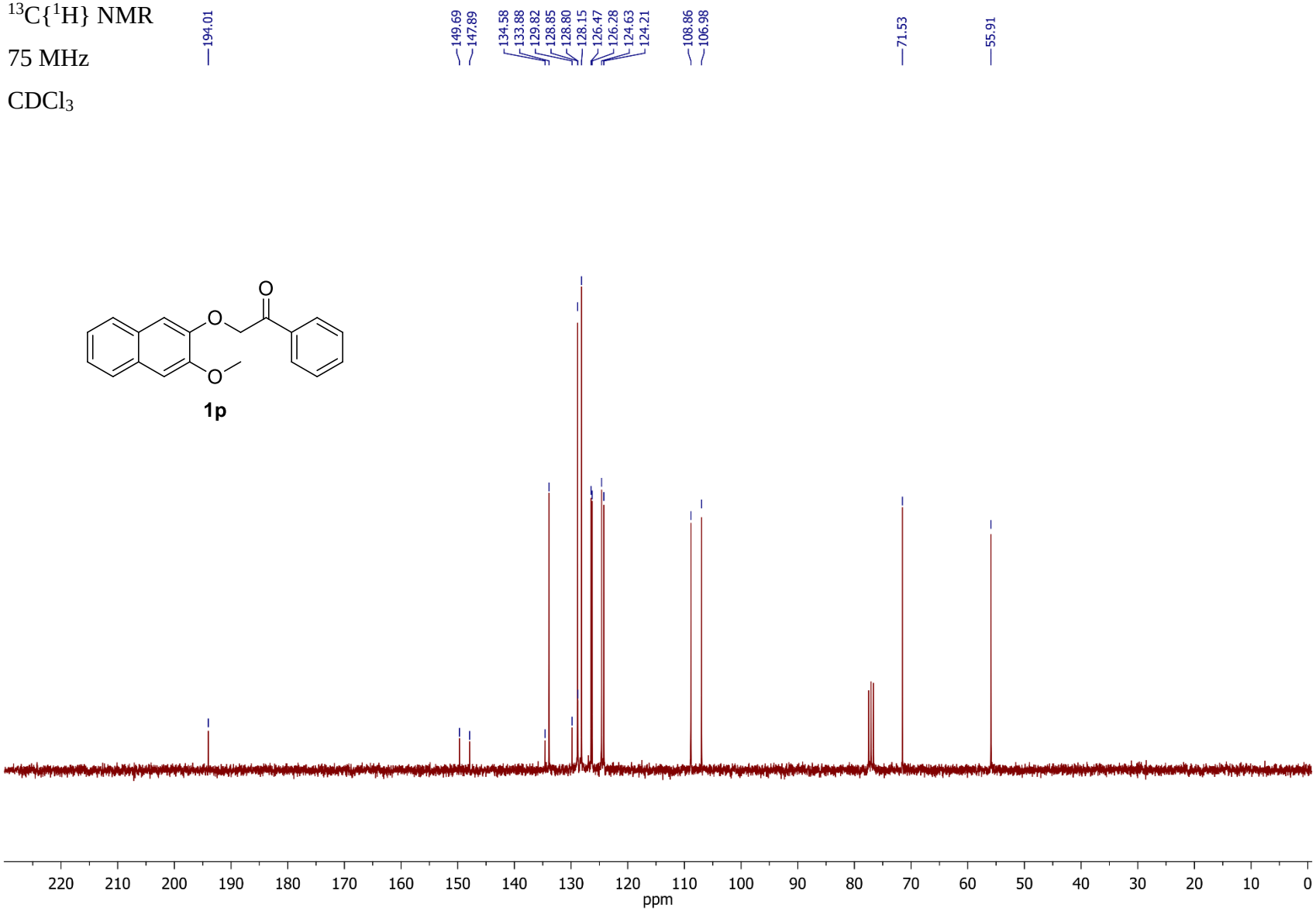


1p

$^{13}C\{^{1}H\}$ NMR

75 MHz

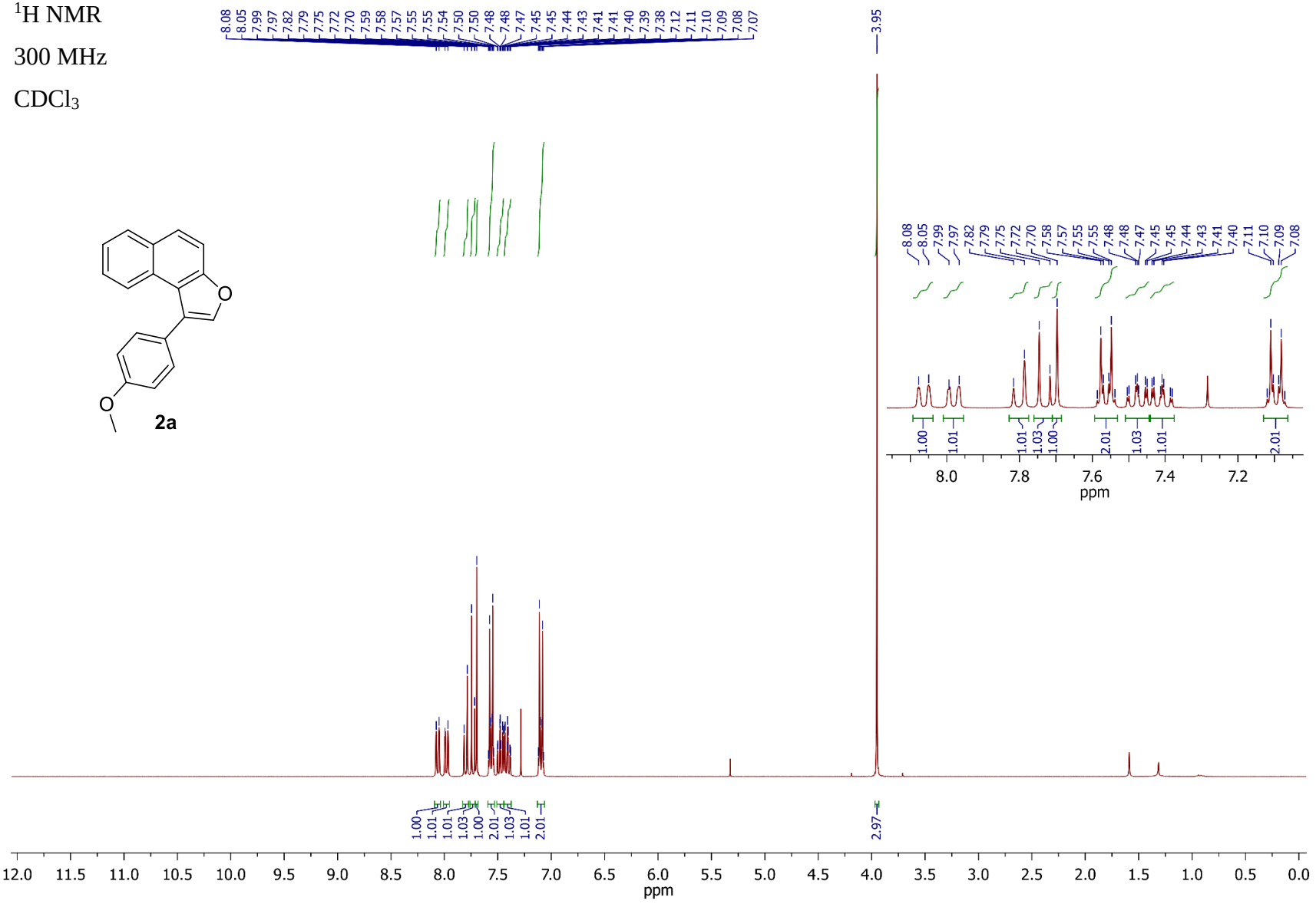
$CDCl_3$



^{1}H NMR

300 MHz

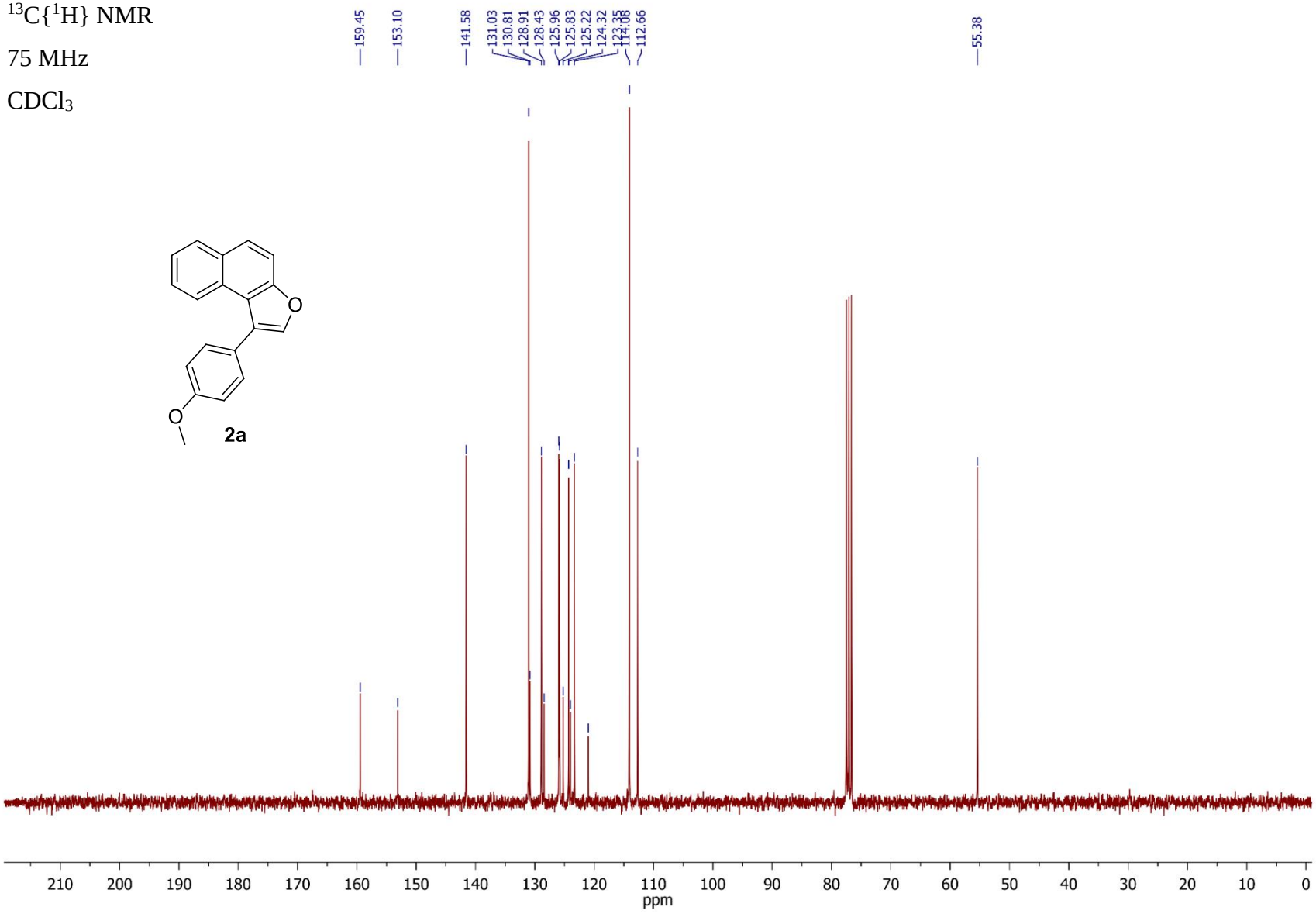
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

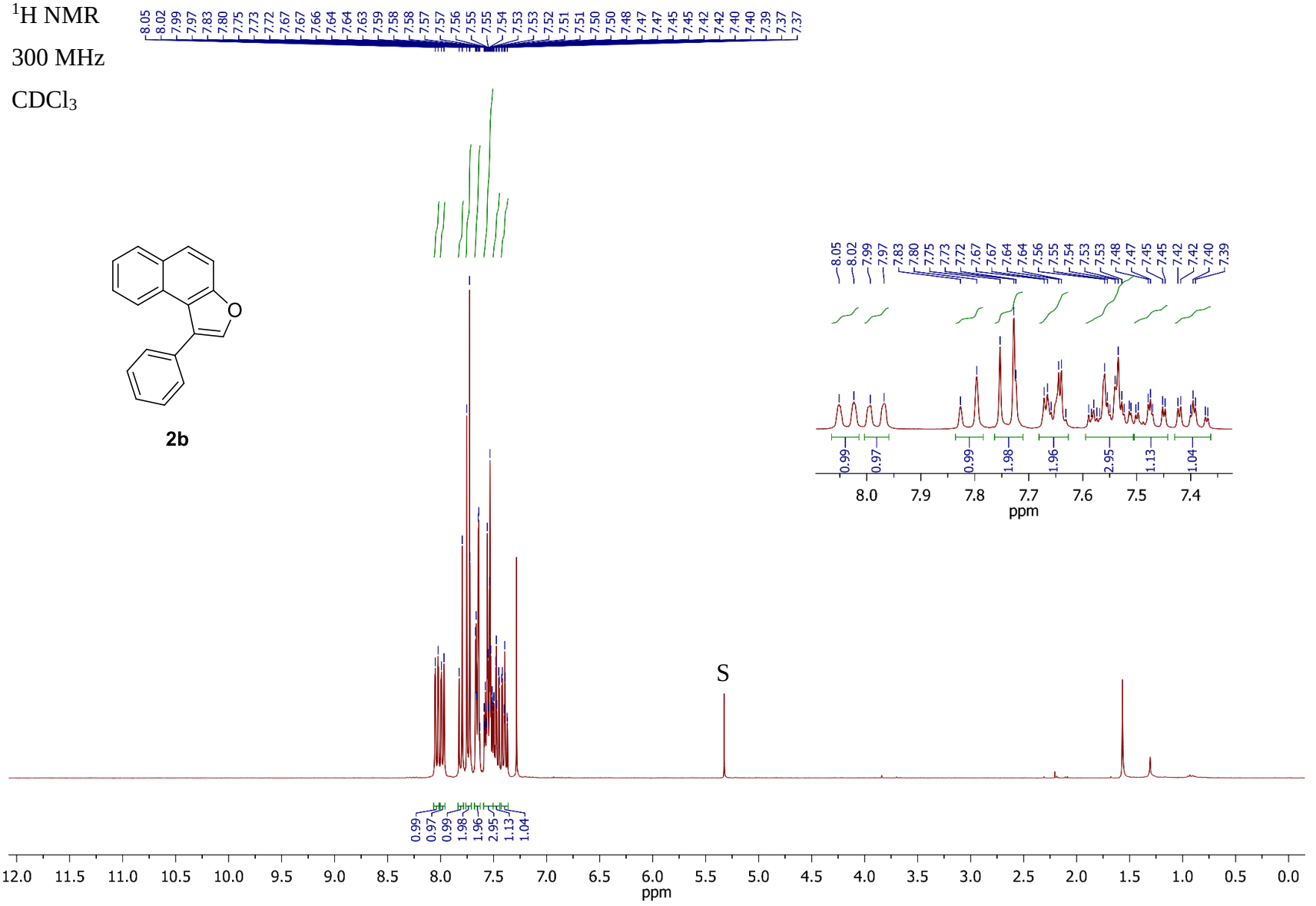
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$

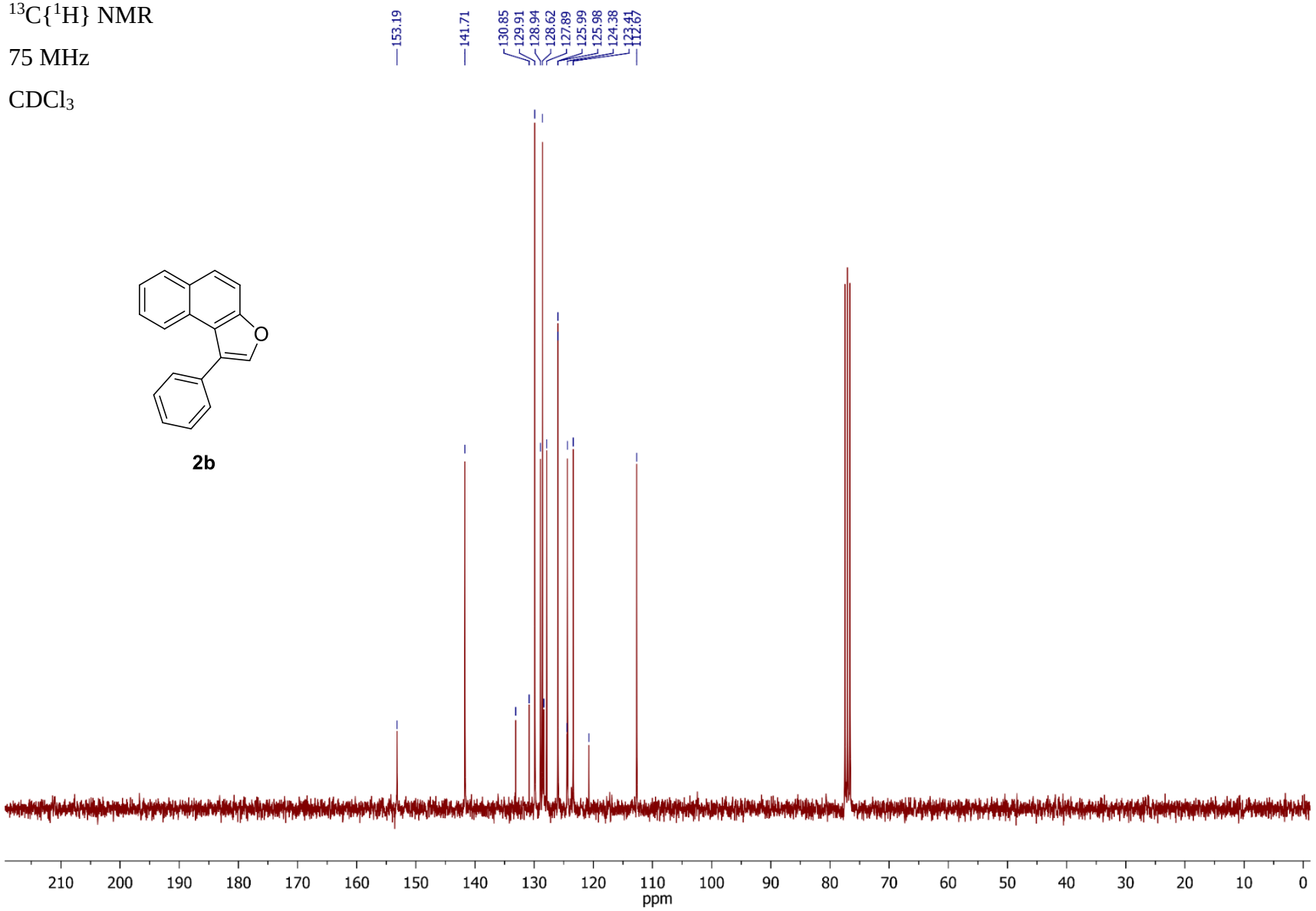


S – peak of dichloromethane (5.30 ppm)

$^{13}C\{^{1}H\}$ NMR

75 MHz

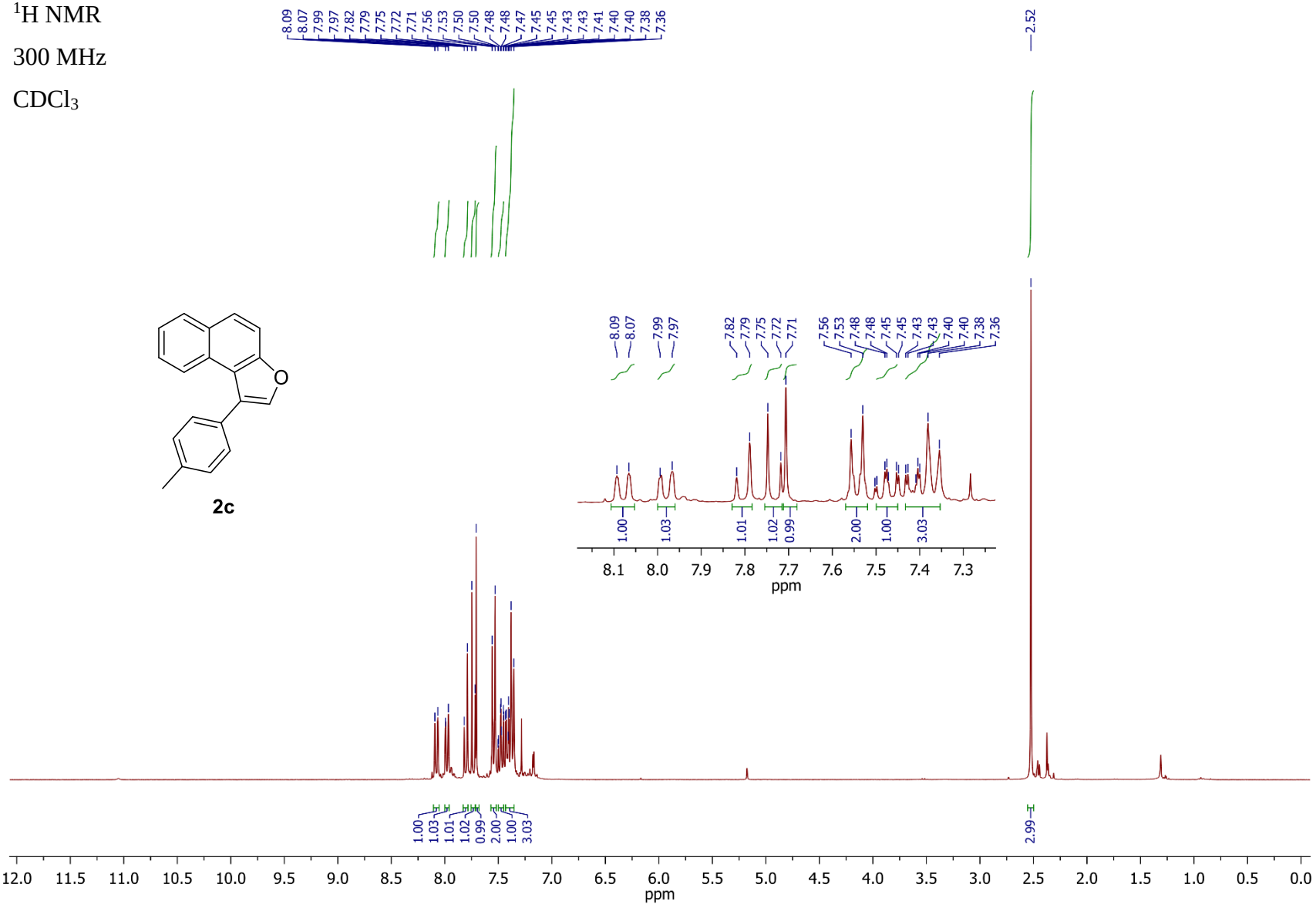
$CDCl_3$



^{1}H NMR

300 MHz

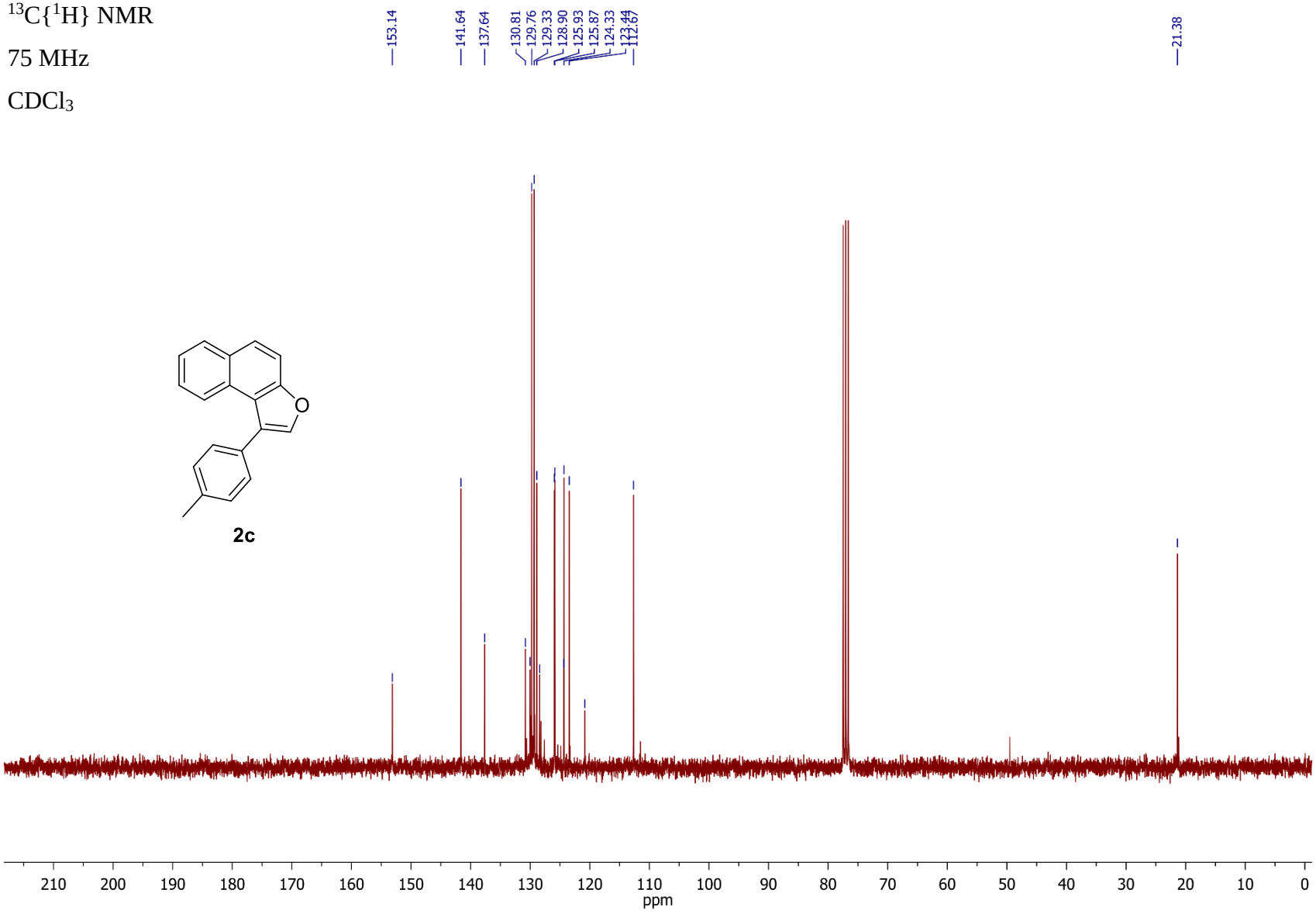
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

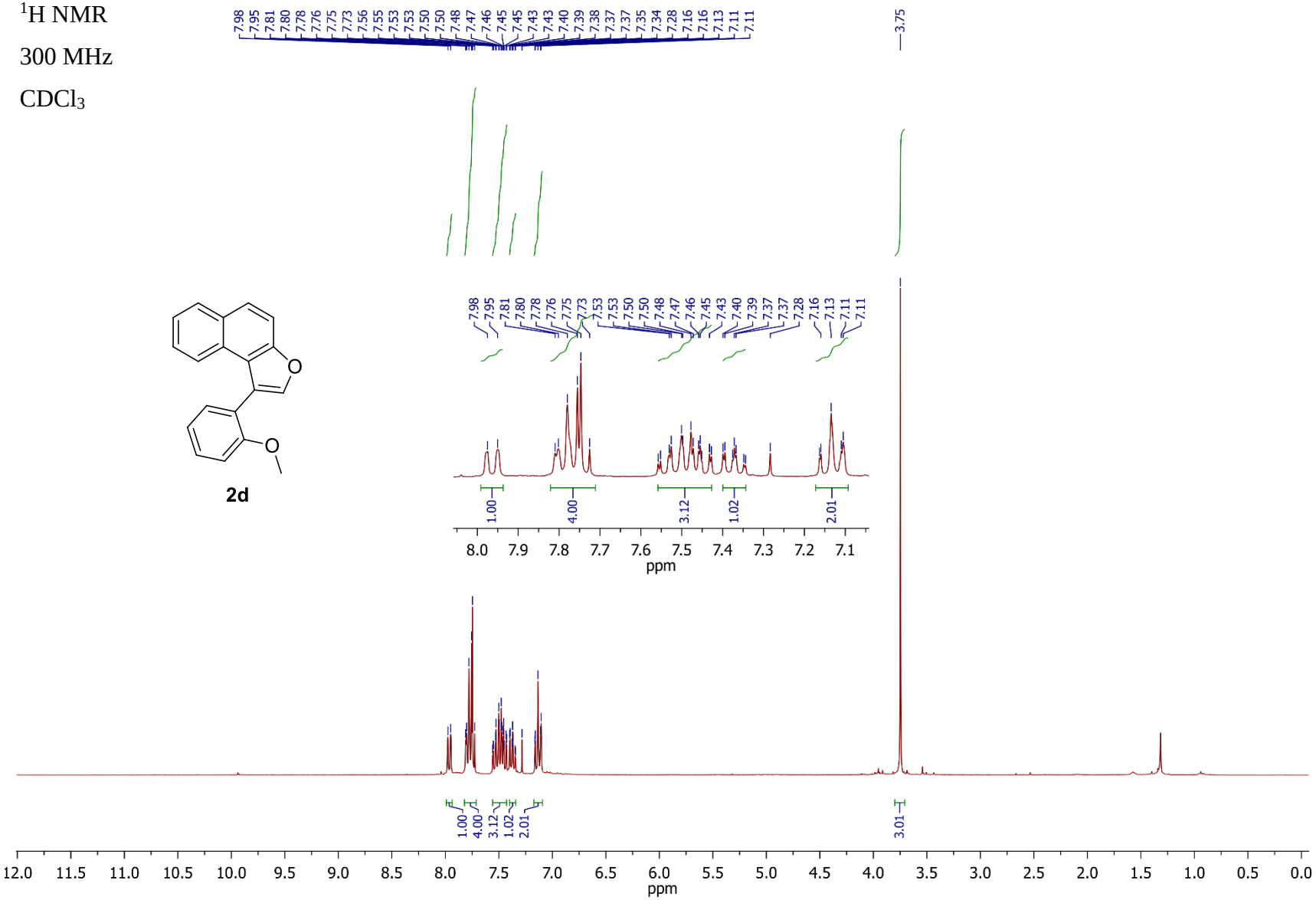
$CDCl_3$



^{1}H NMR

300 MHz

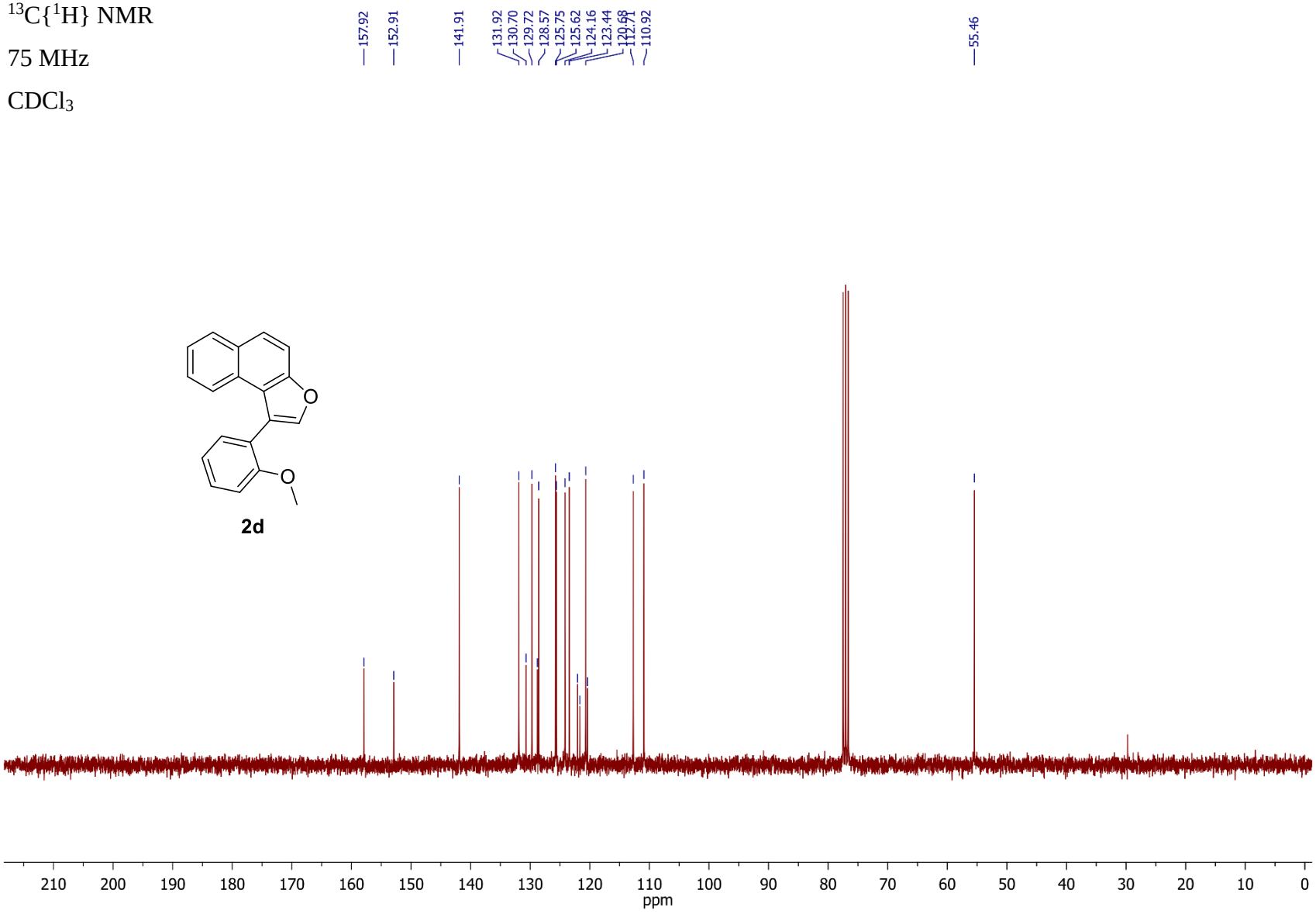
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

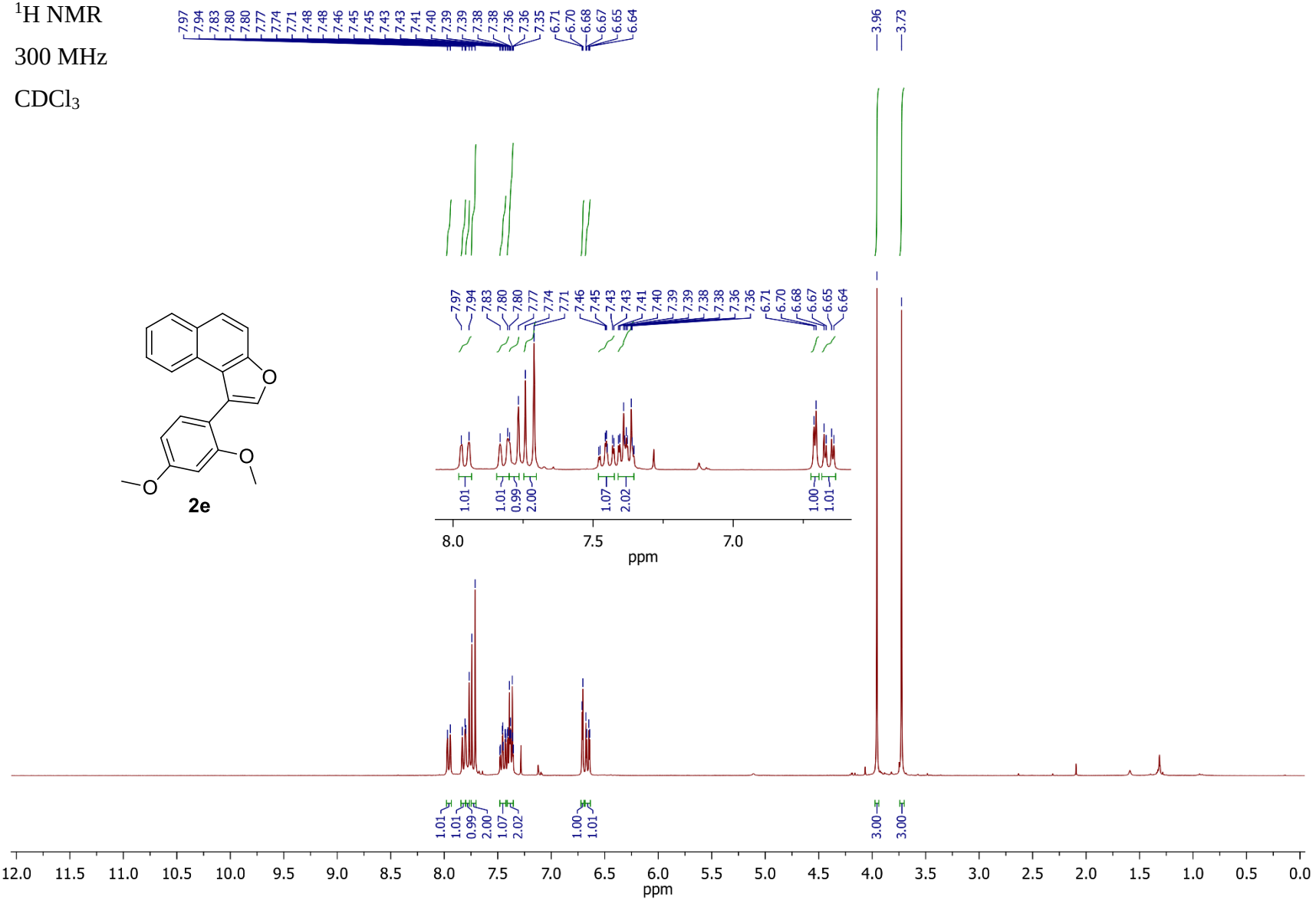
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$

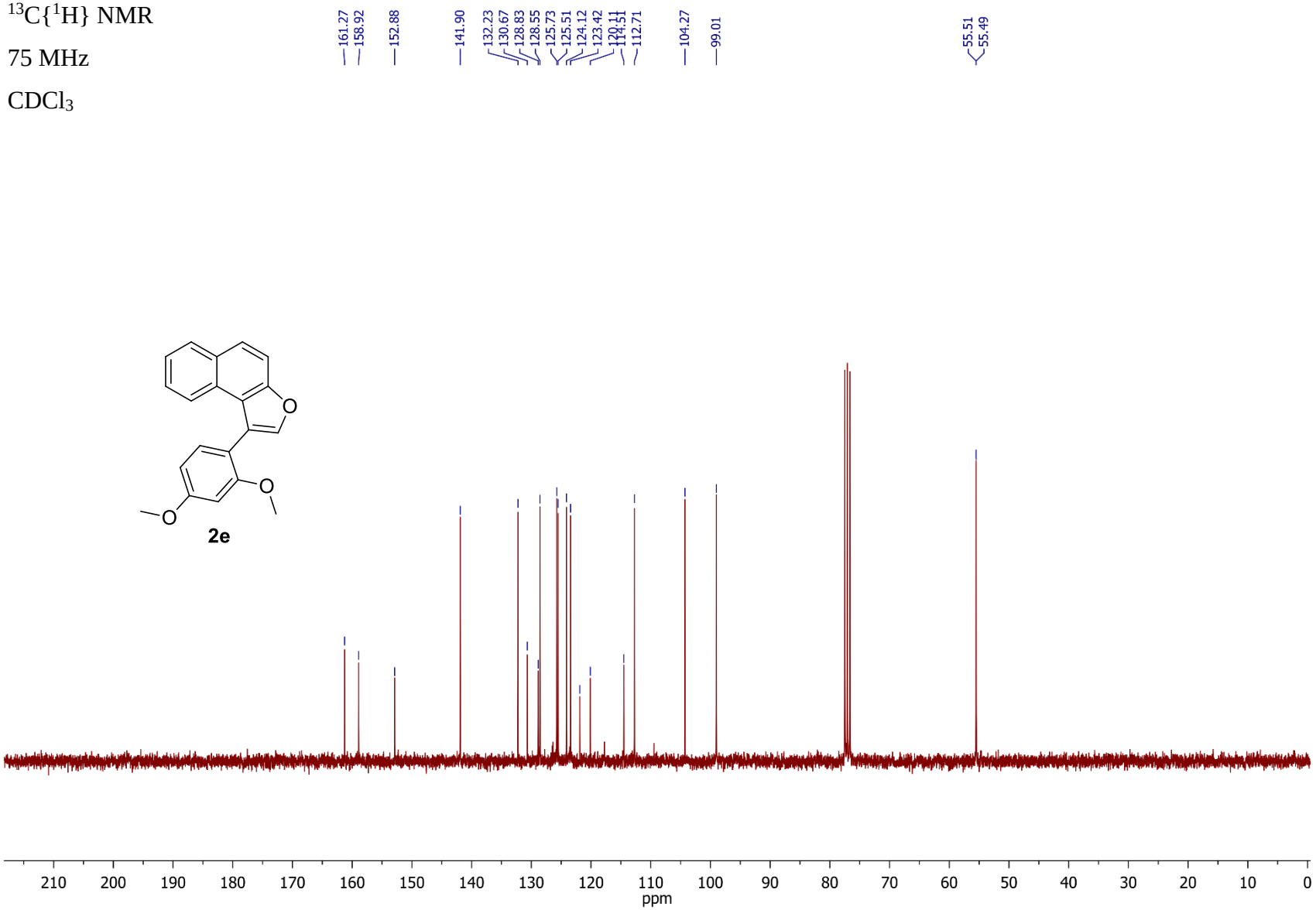


2e

$^{13}C\{^{1}H\}$ NMR

75 MHz

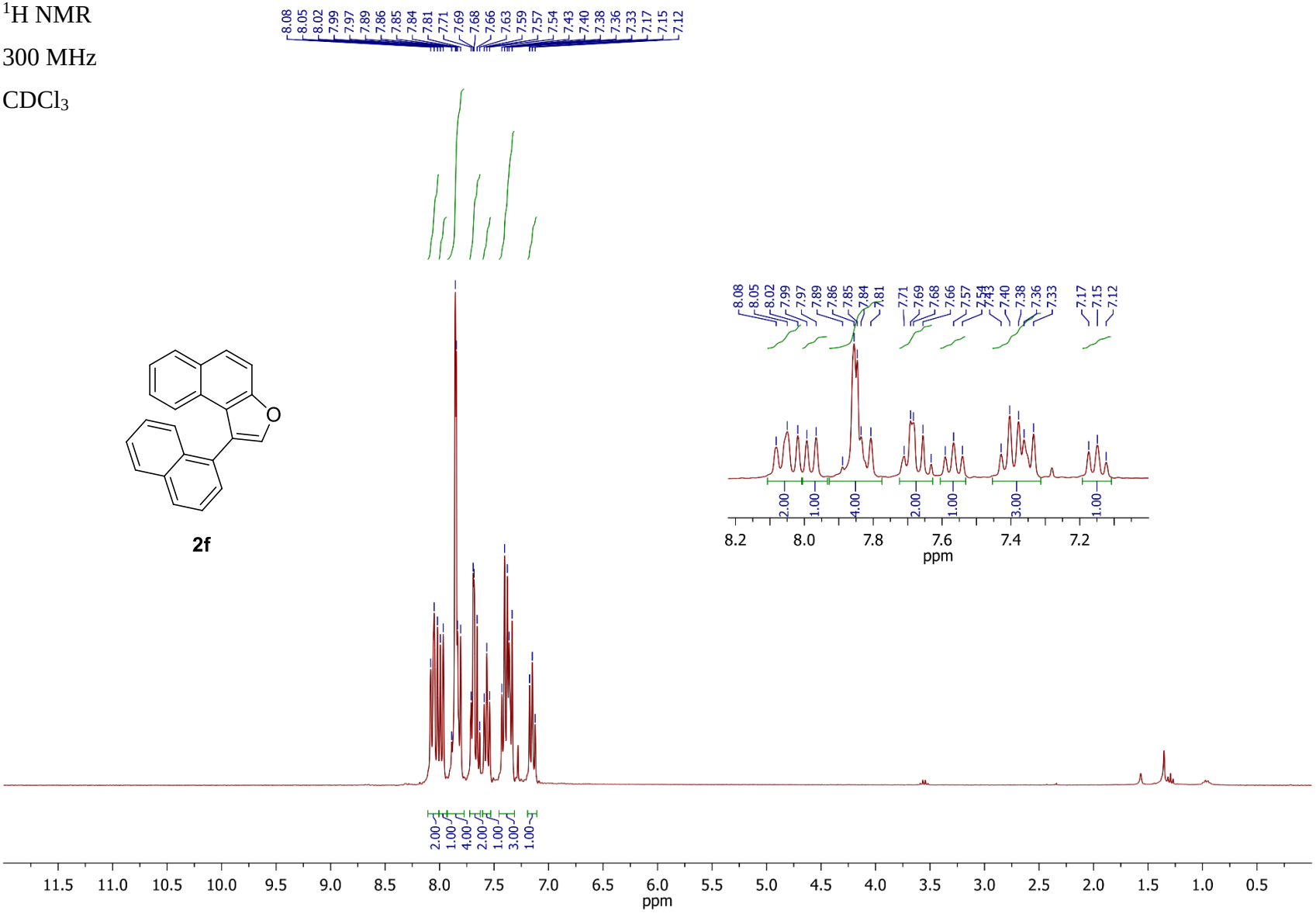
$CDCl_3$



^{1}H NMR

300 MHz

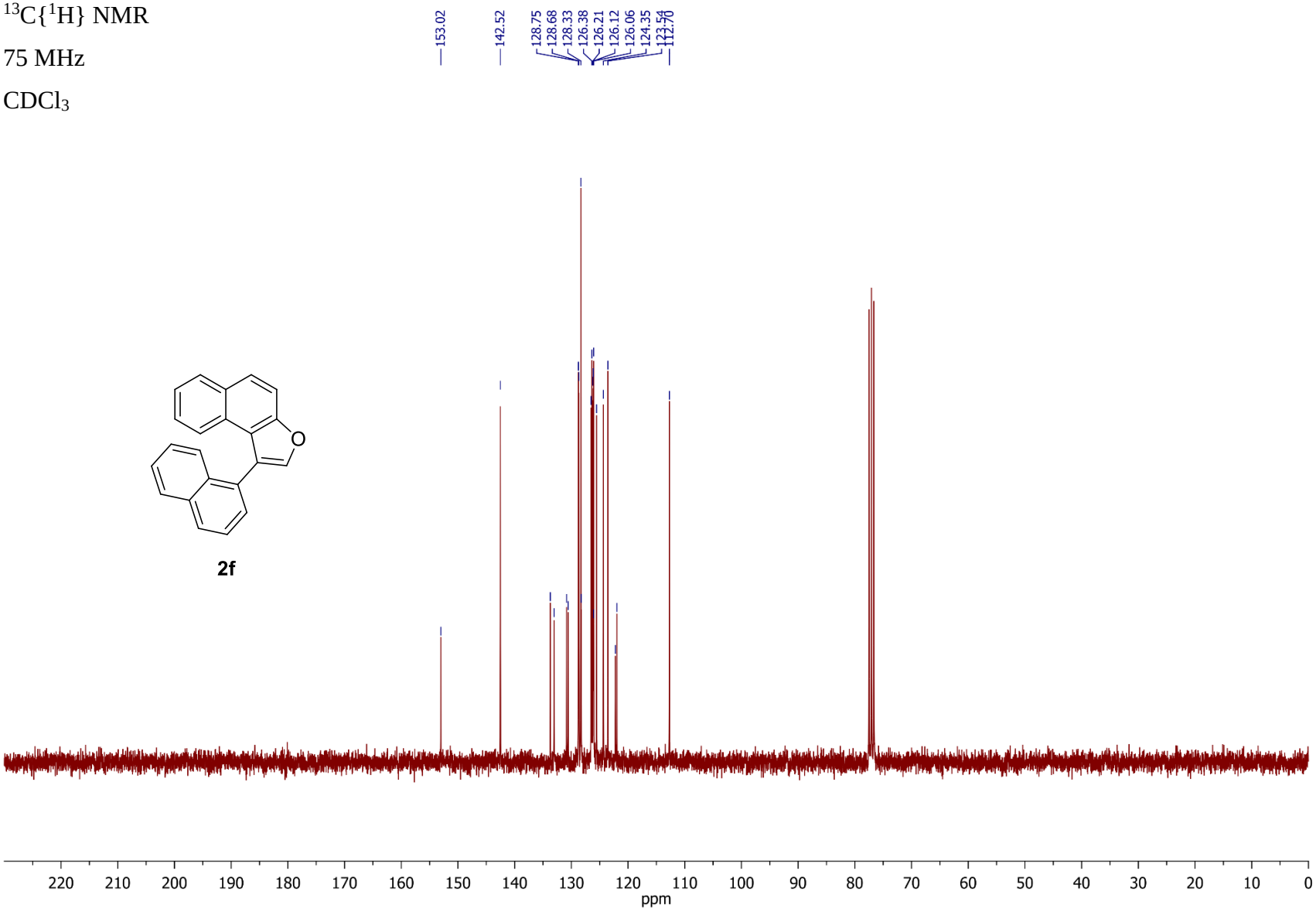
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

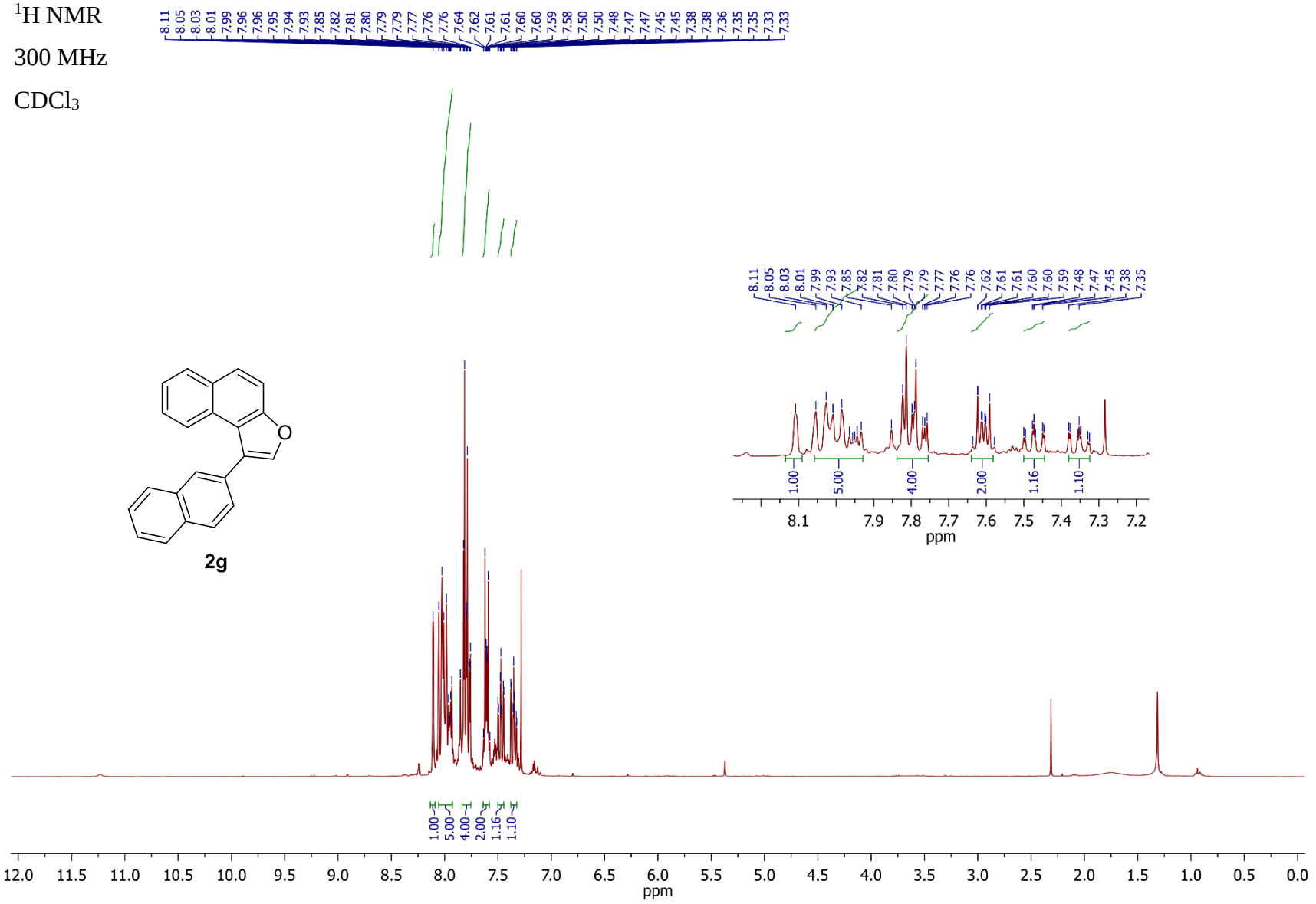
$CDCl_3$



^{1}H NMR

300 MHz

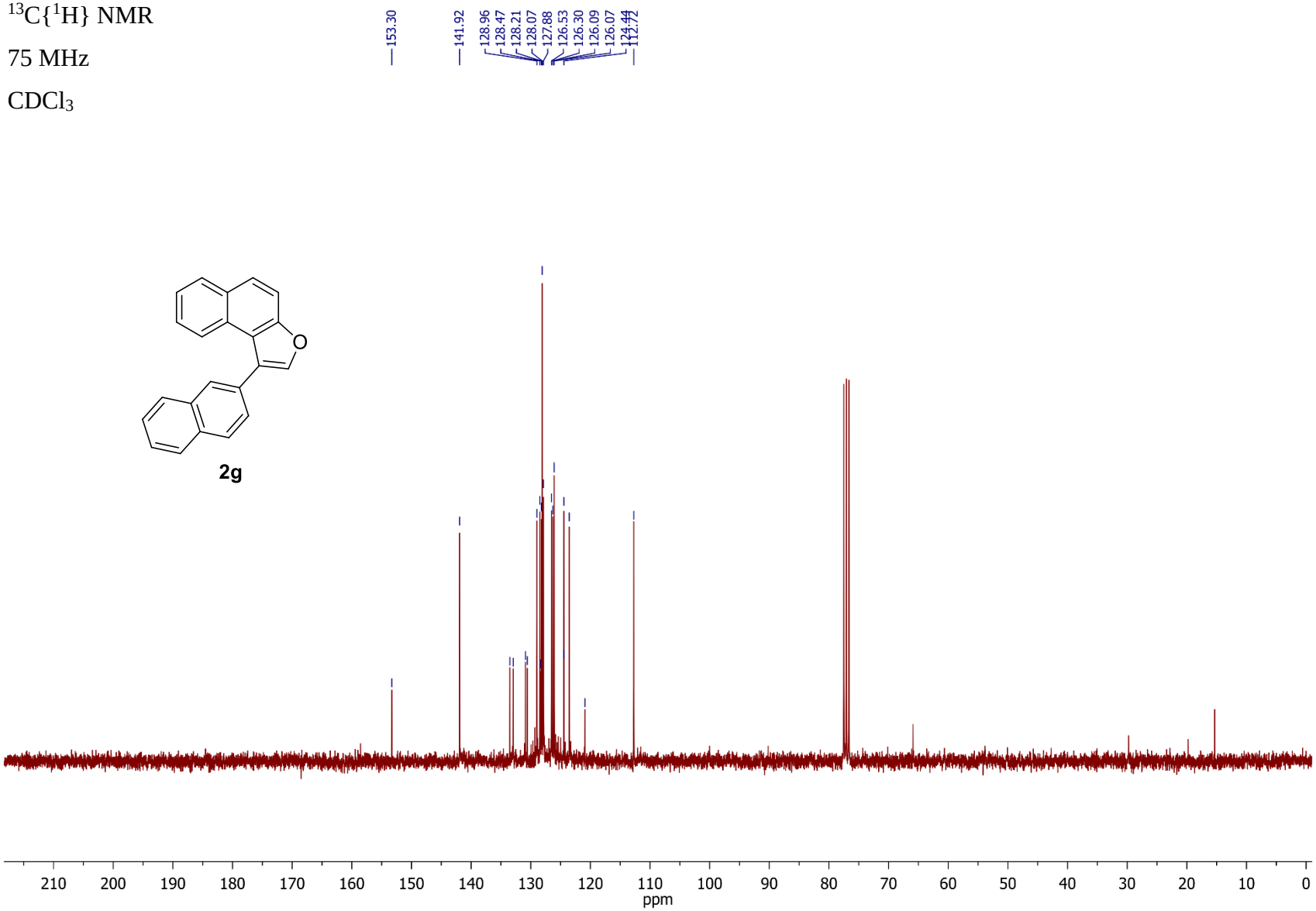
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

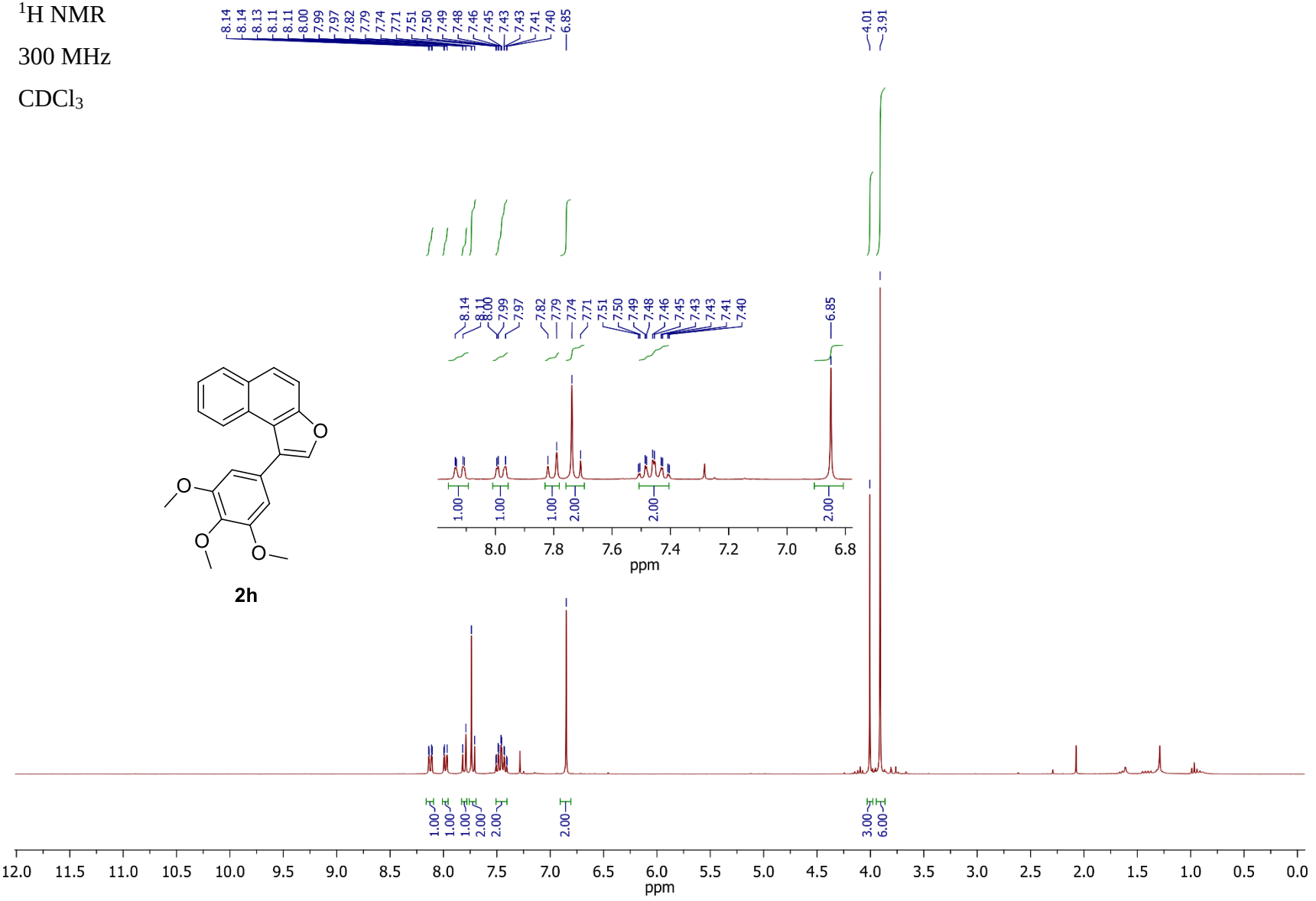
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$

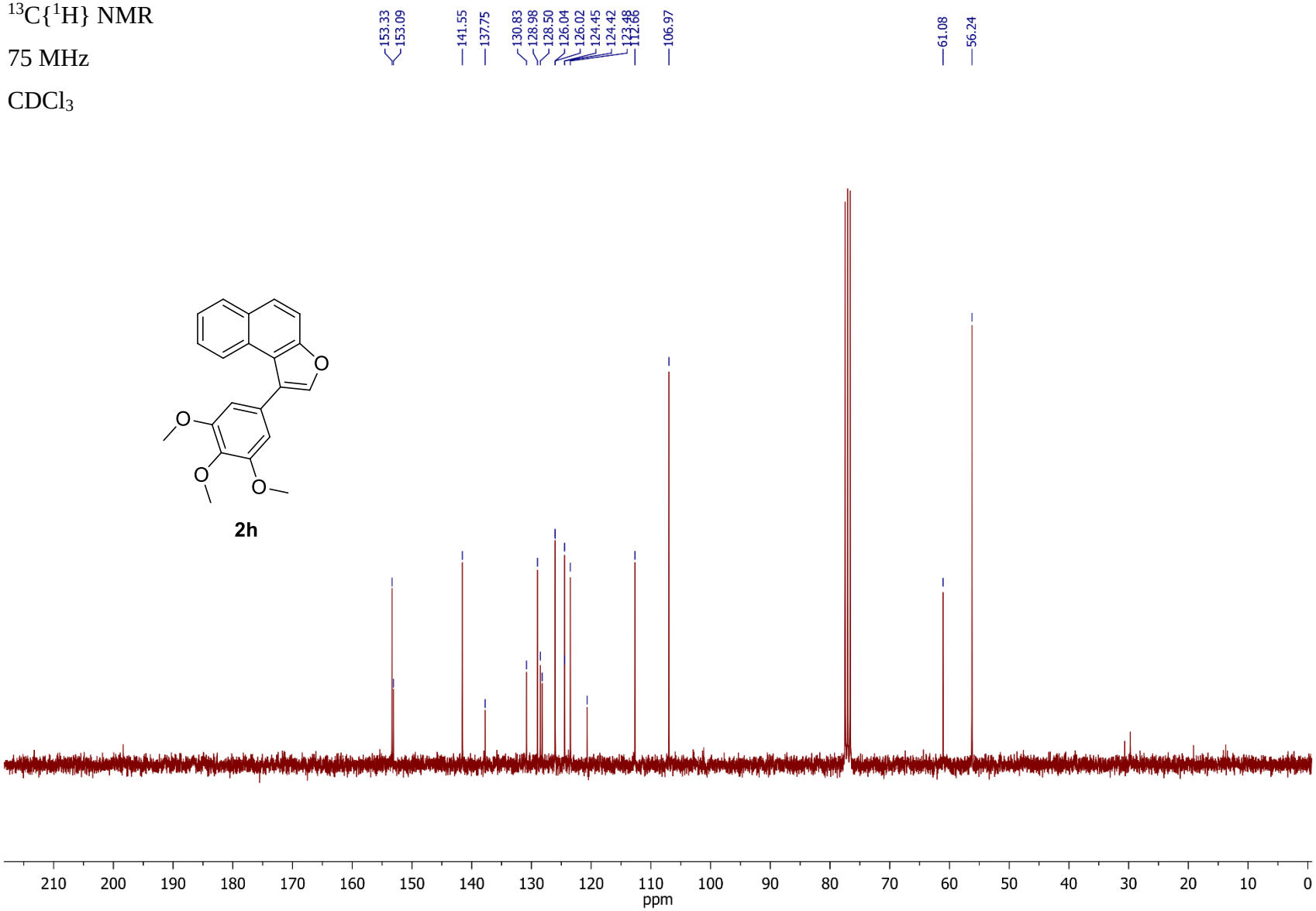


2h

$^{13}C\{^{1}H\}$ NMR

75 MHz

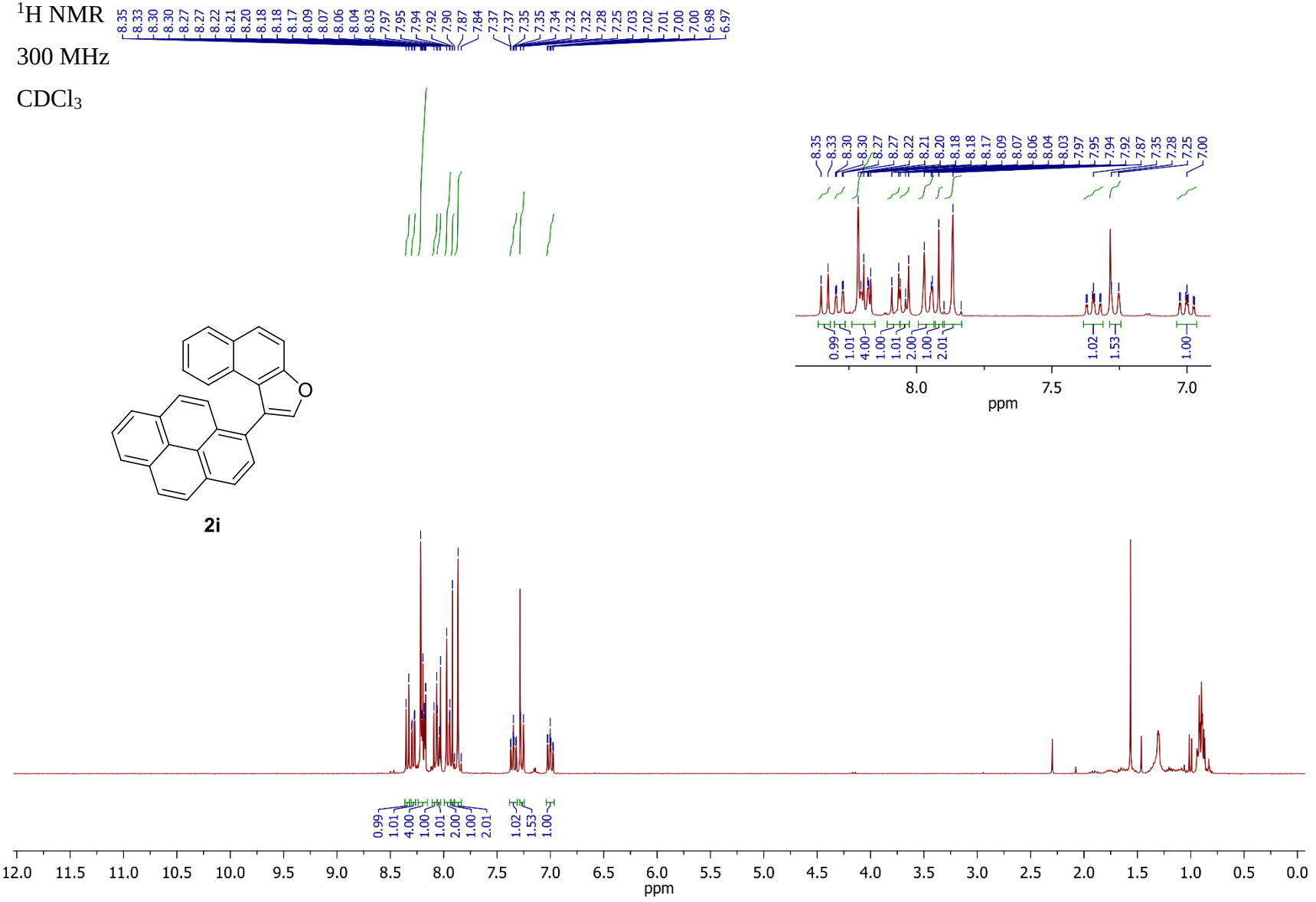
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$

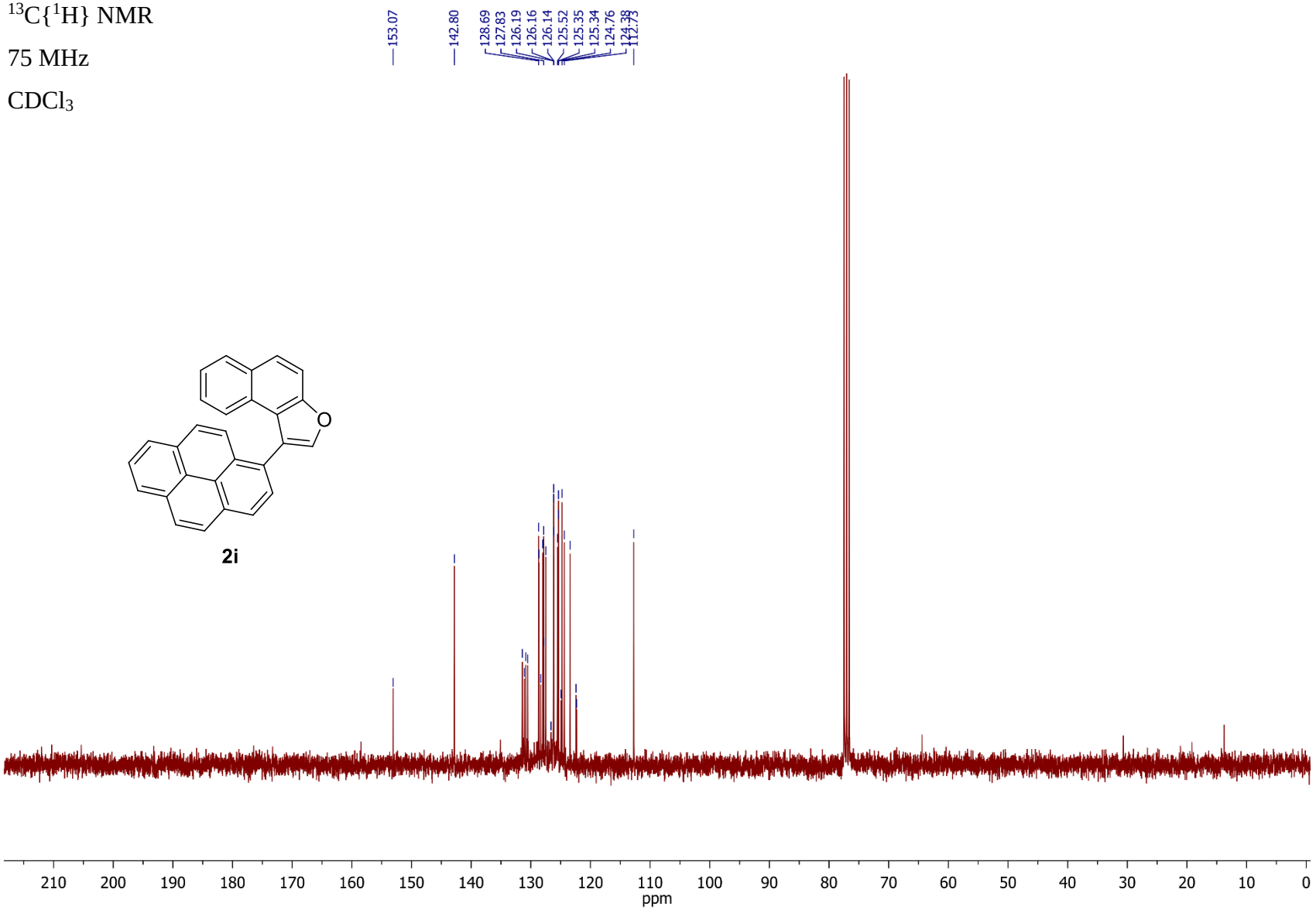


2i

$^{13}C\{^{1}H\}$ NMR

75 MHz

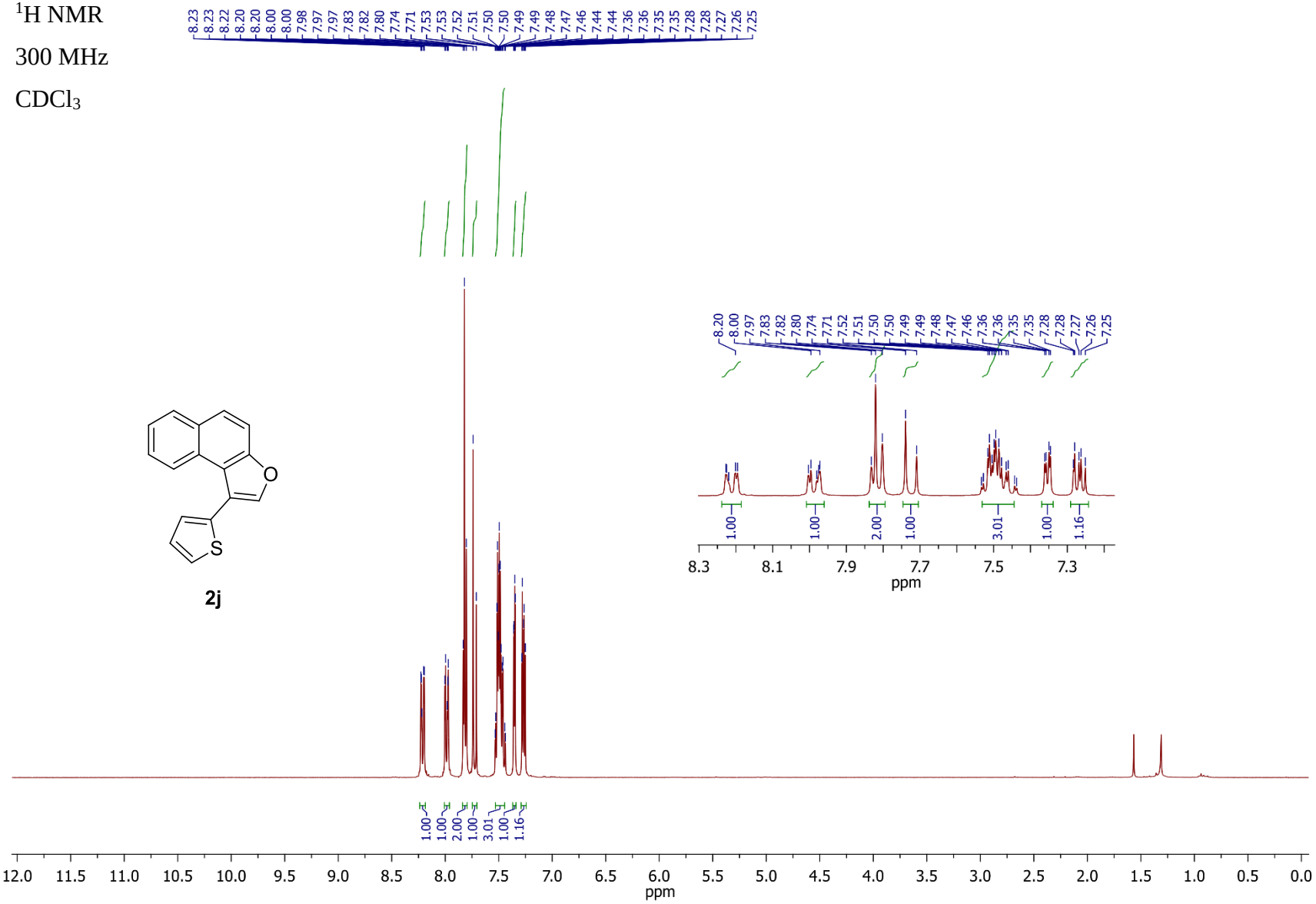
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$

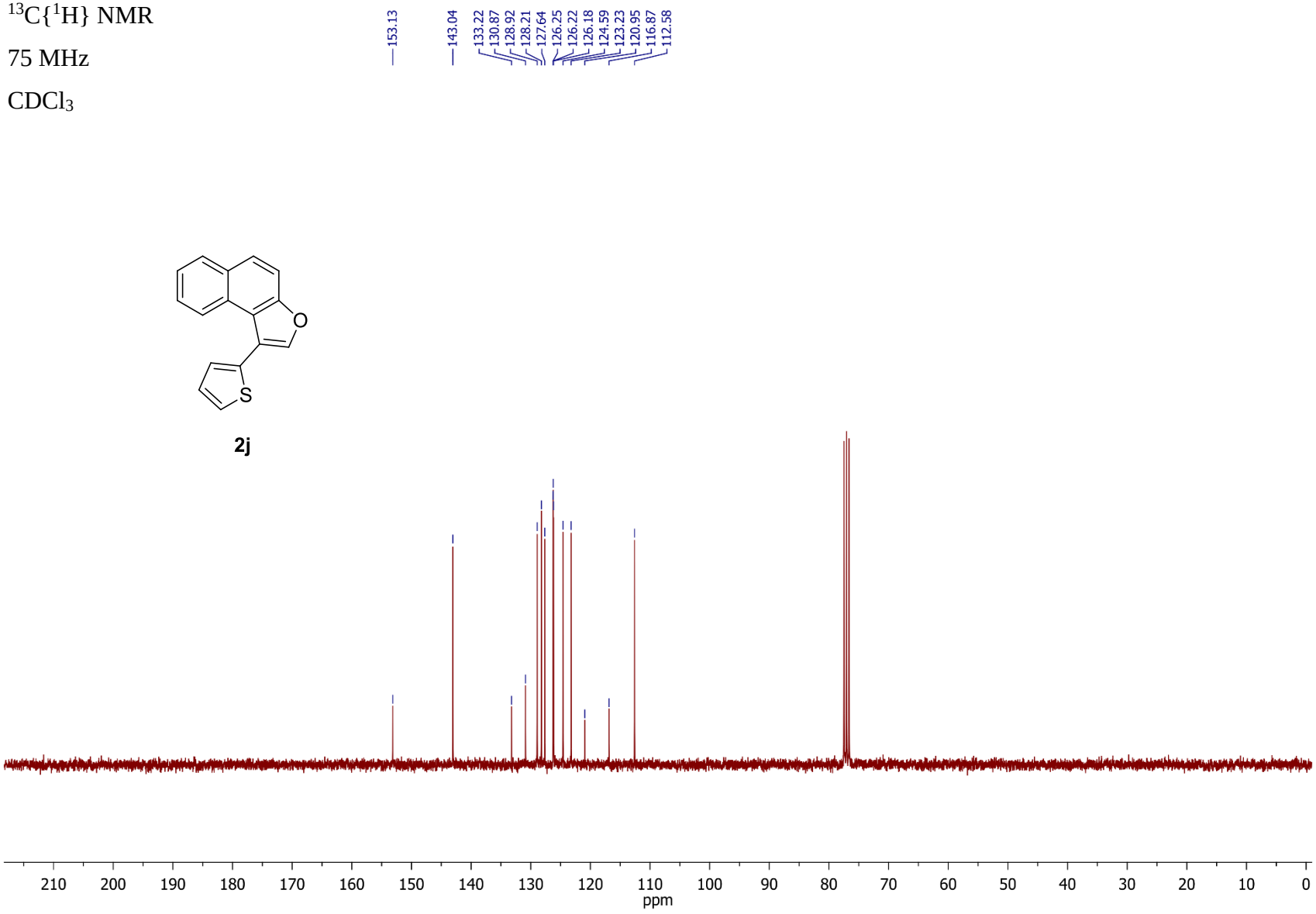


2j

$^{13}C\{^{1}H\}$ NMR

75 MHz

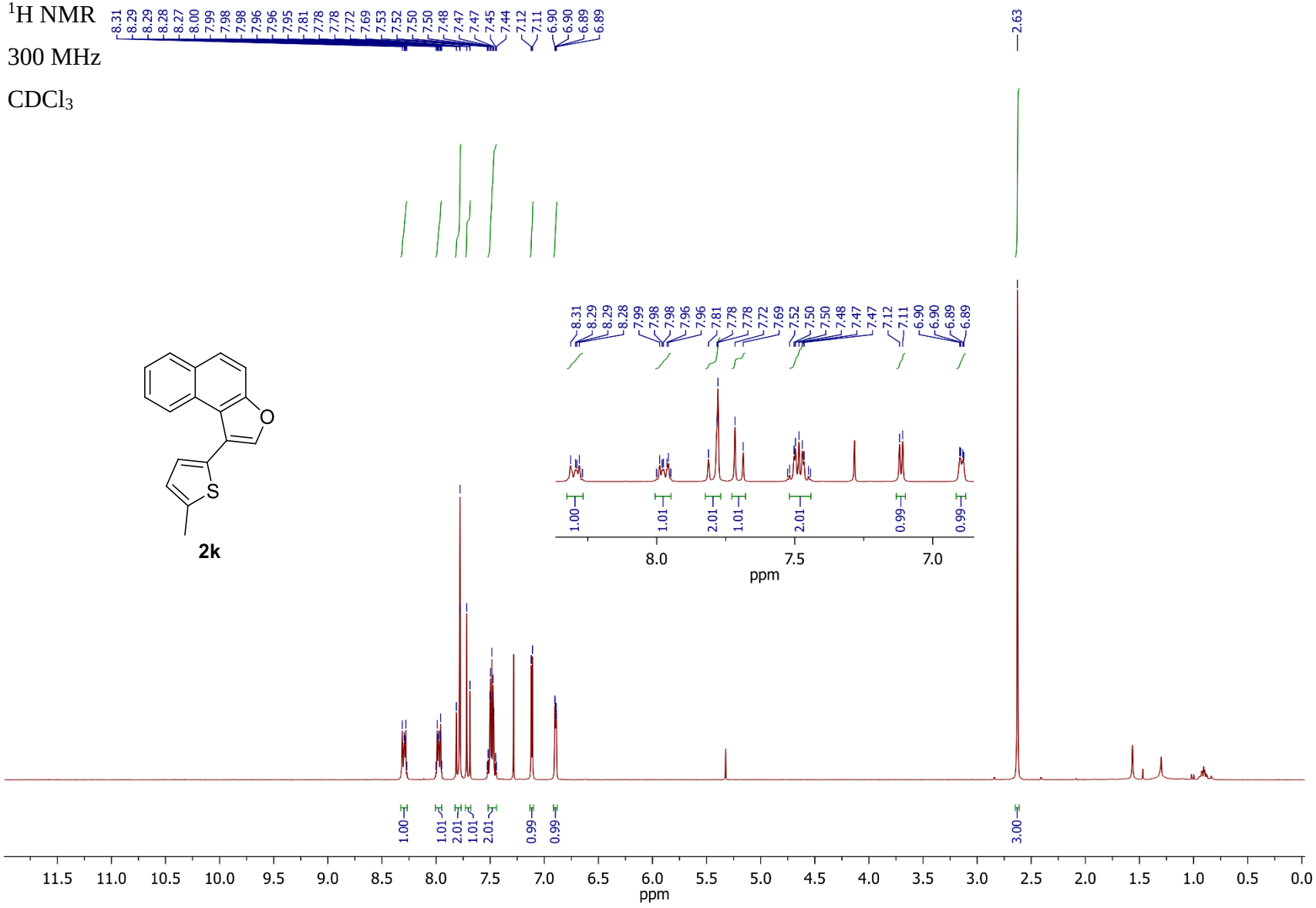
$CDCl_3$



^{1}H NMR

300 MHz

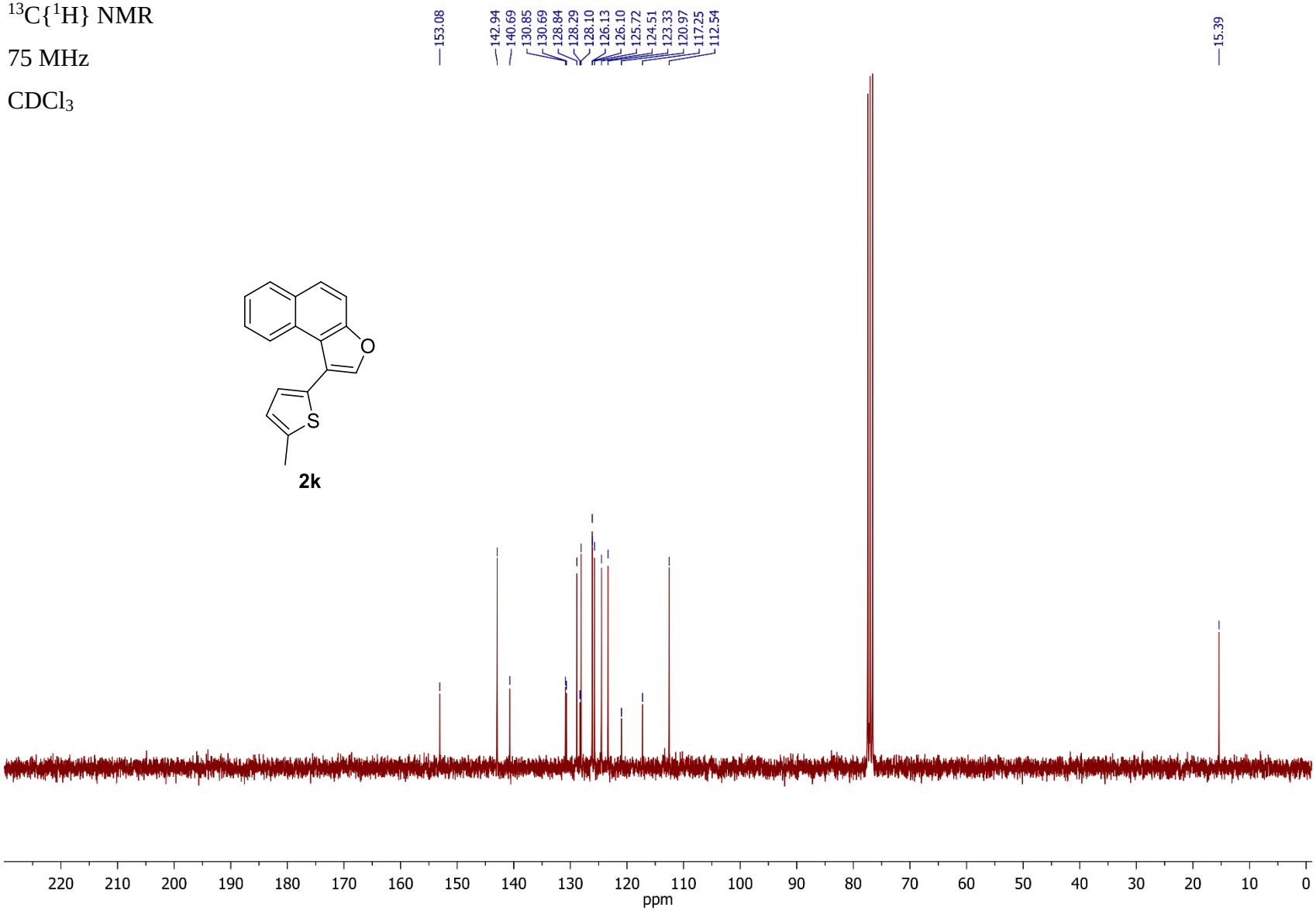
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

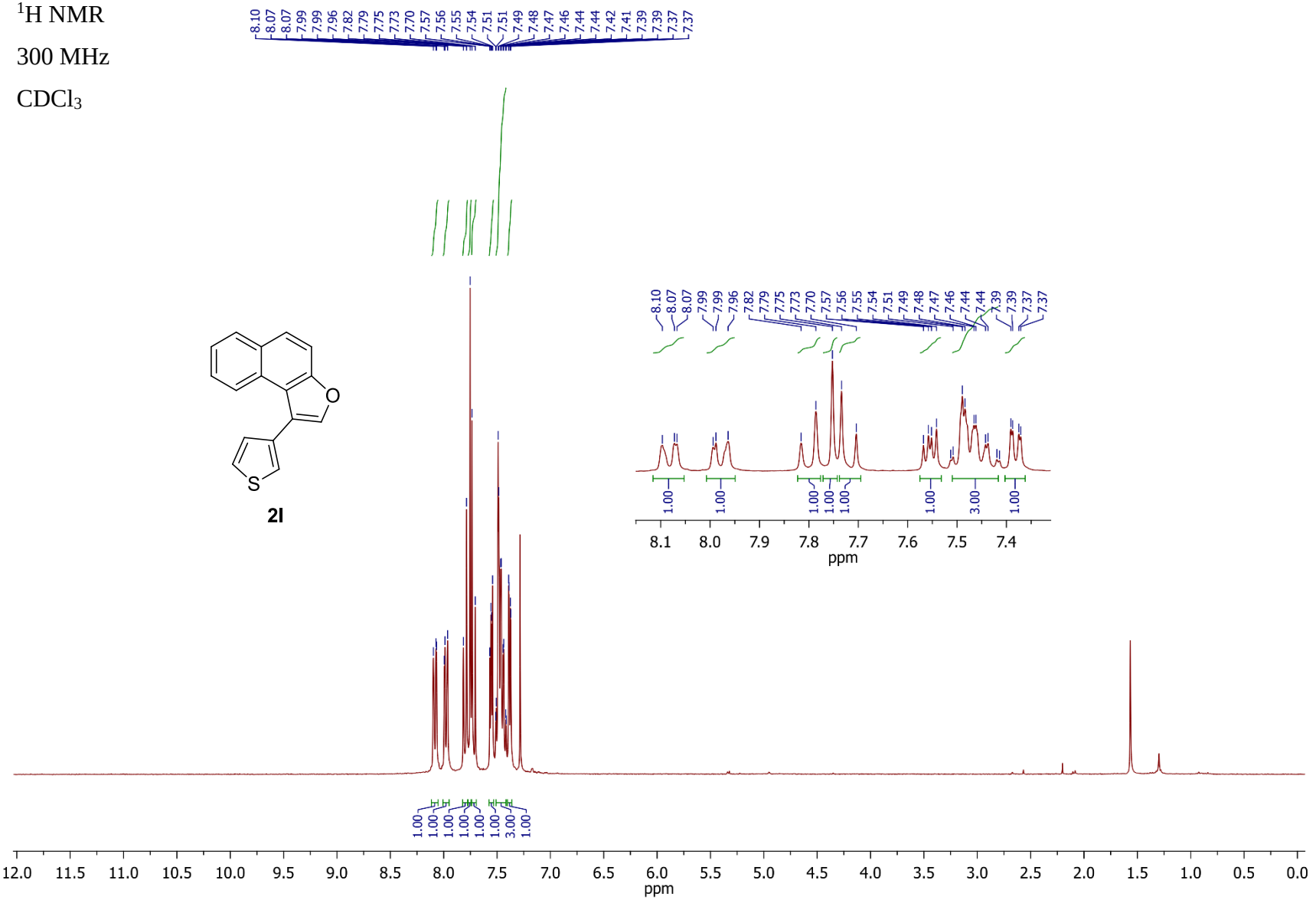
$CDCl_3$



^{1}H NMR

300 MHz

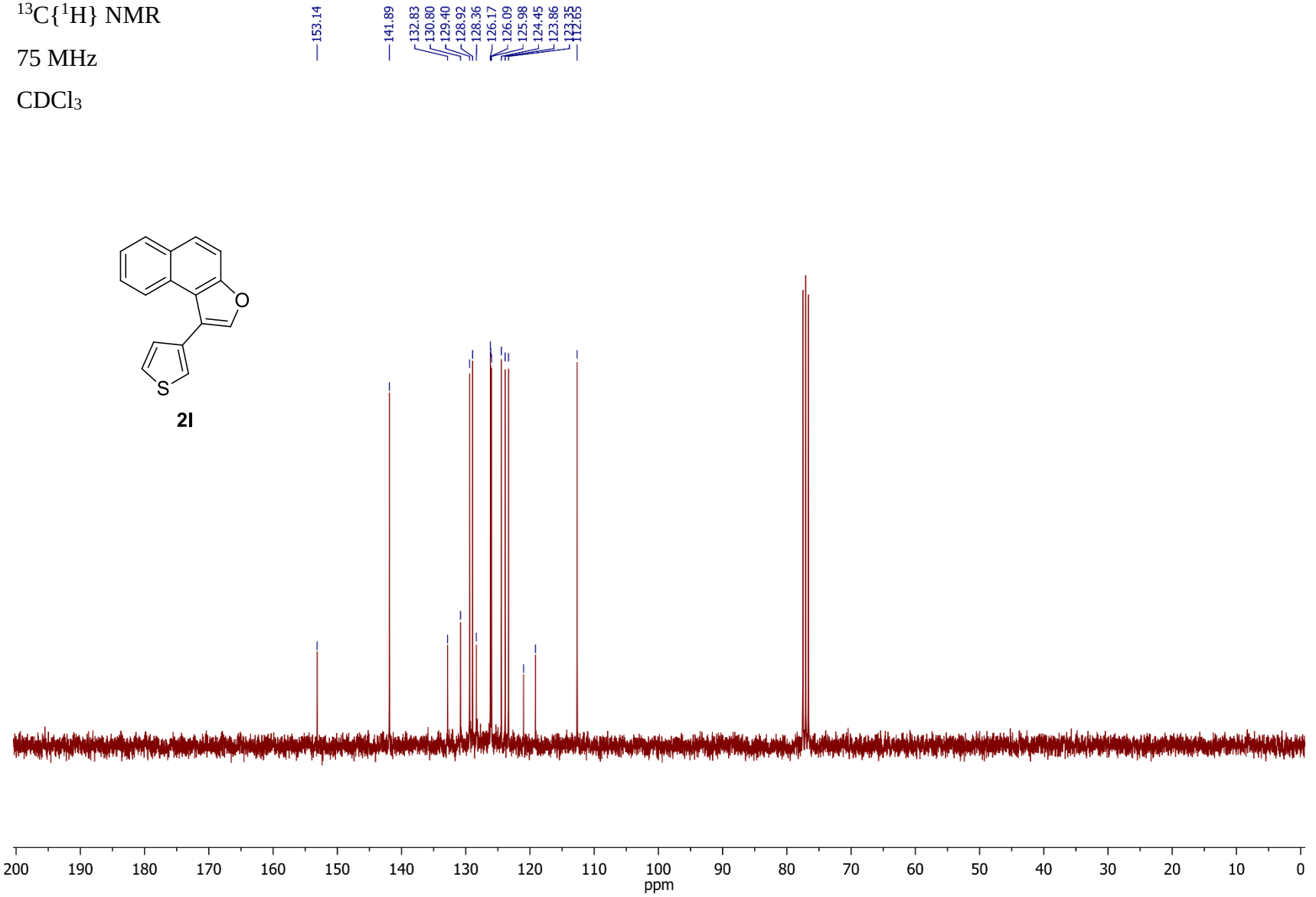
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

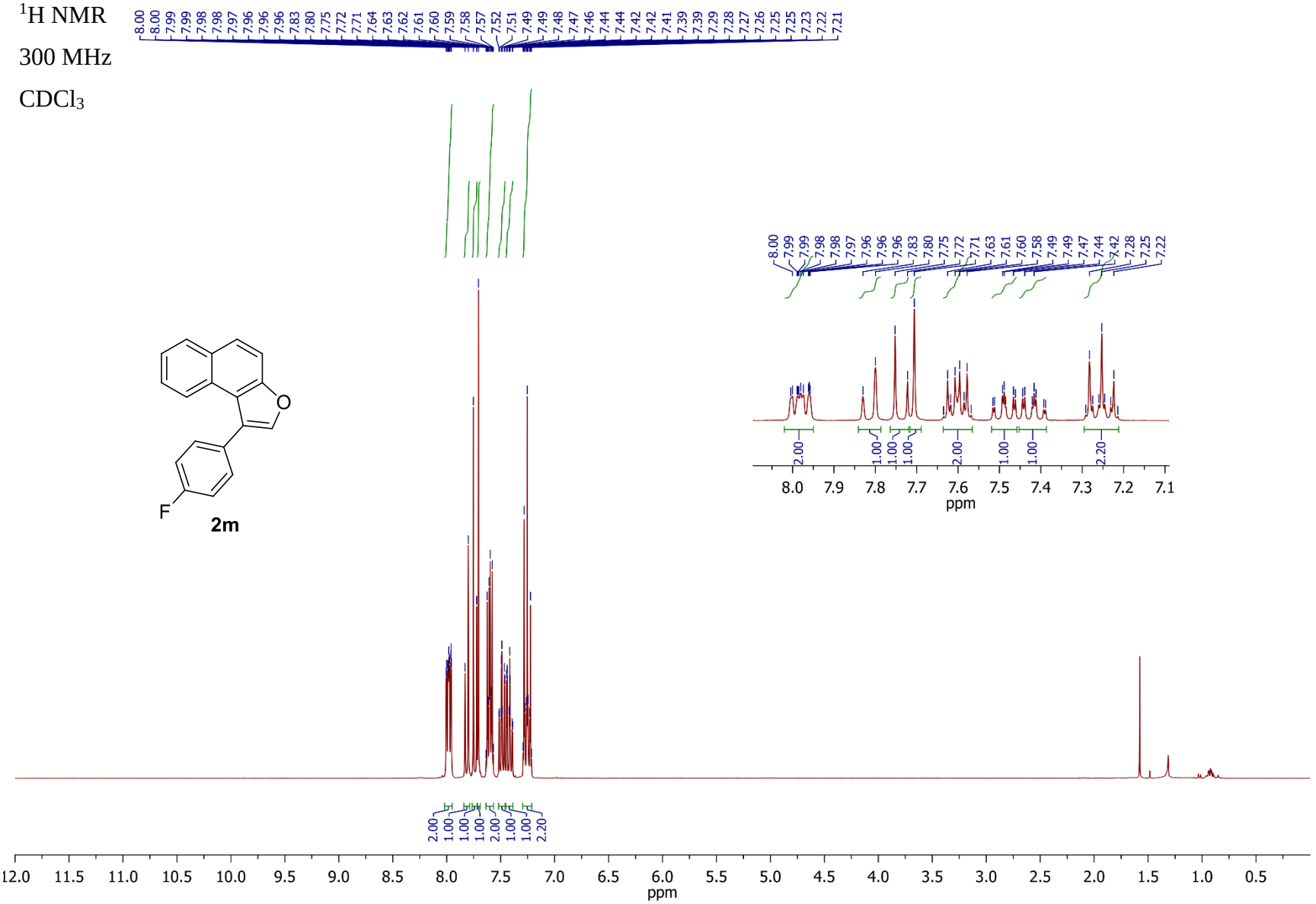
$CDCl_3$



^{1}H NMR

300 MHz

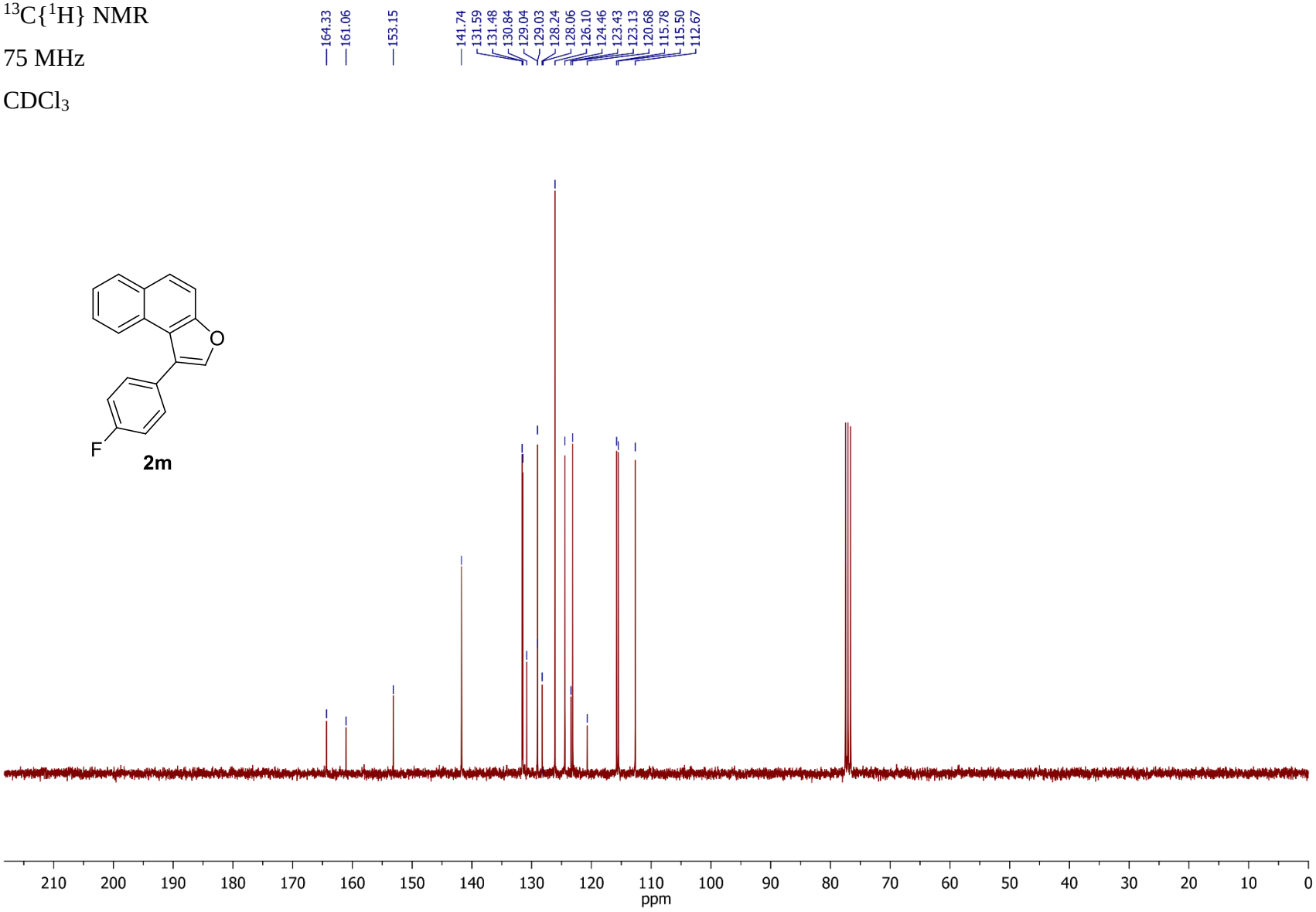
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

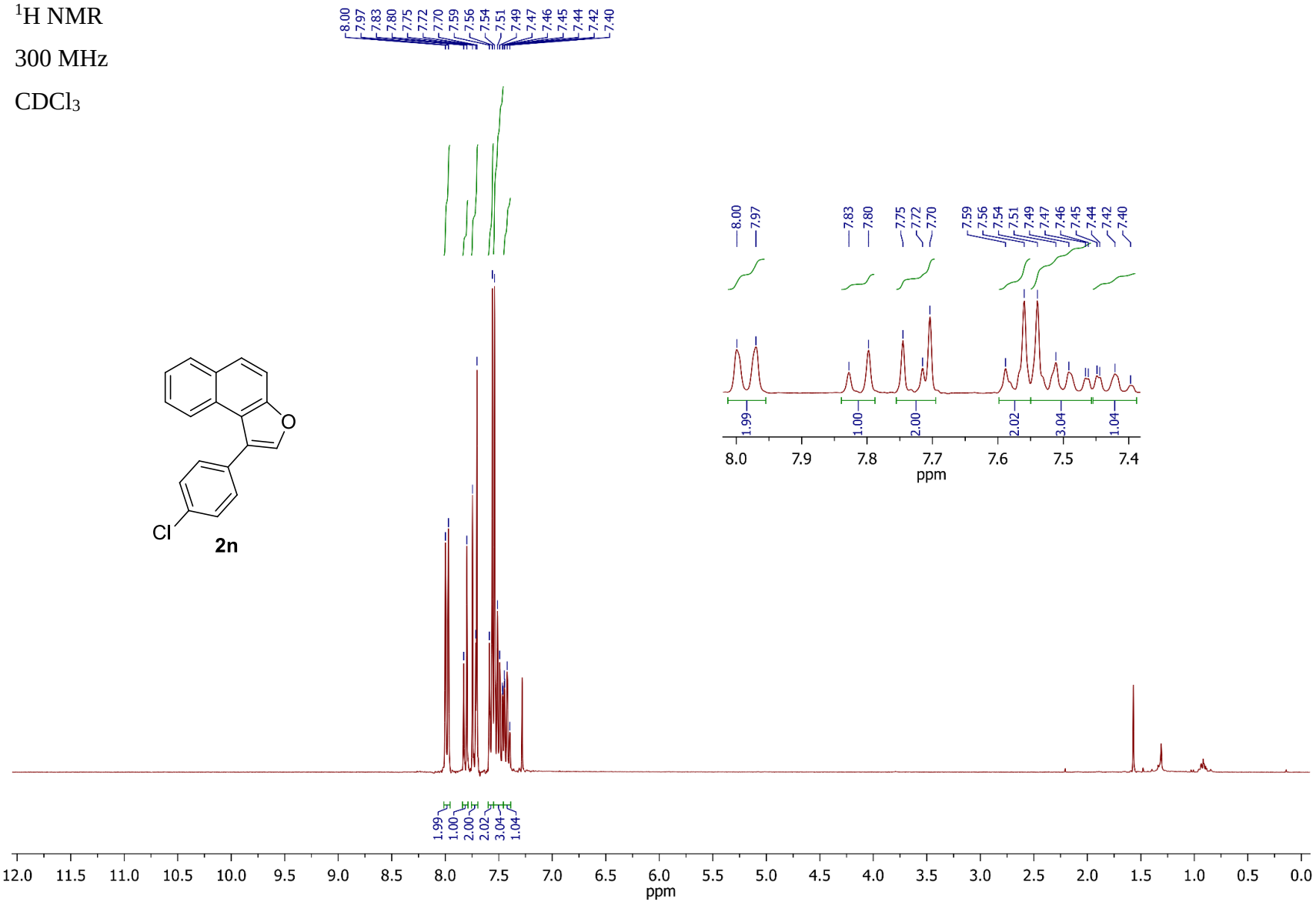
$CDCl_3$



^{1}H NMR

300 MHz

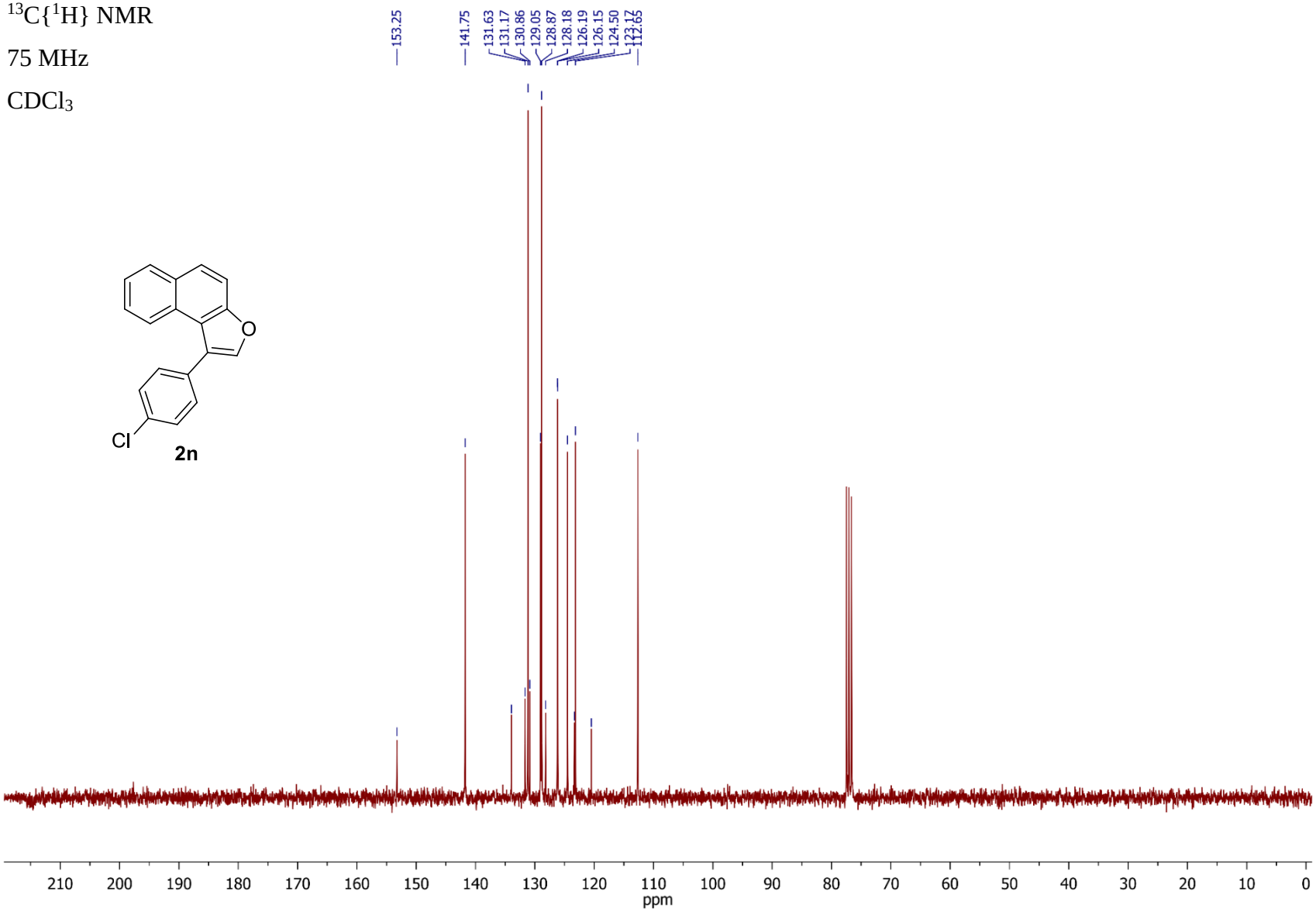
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

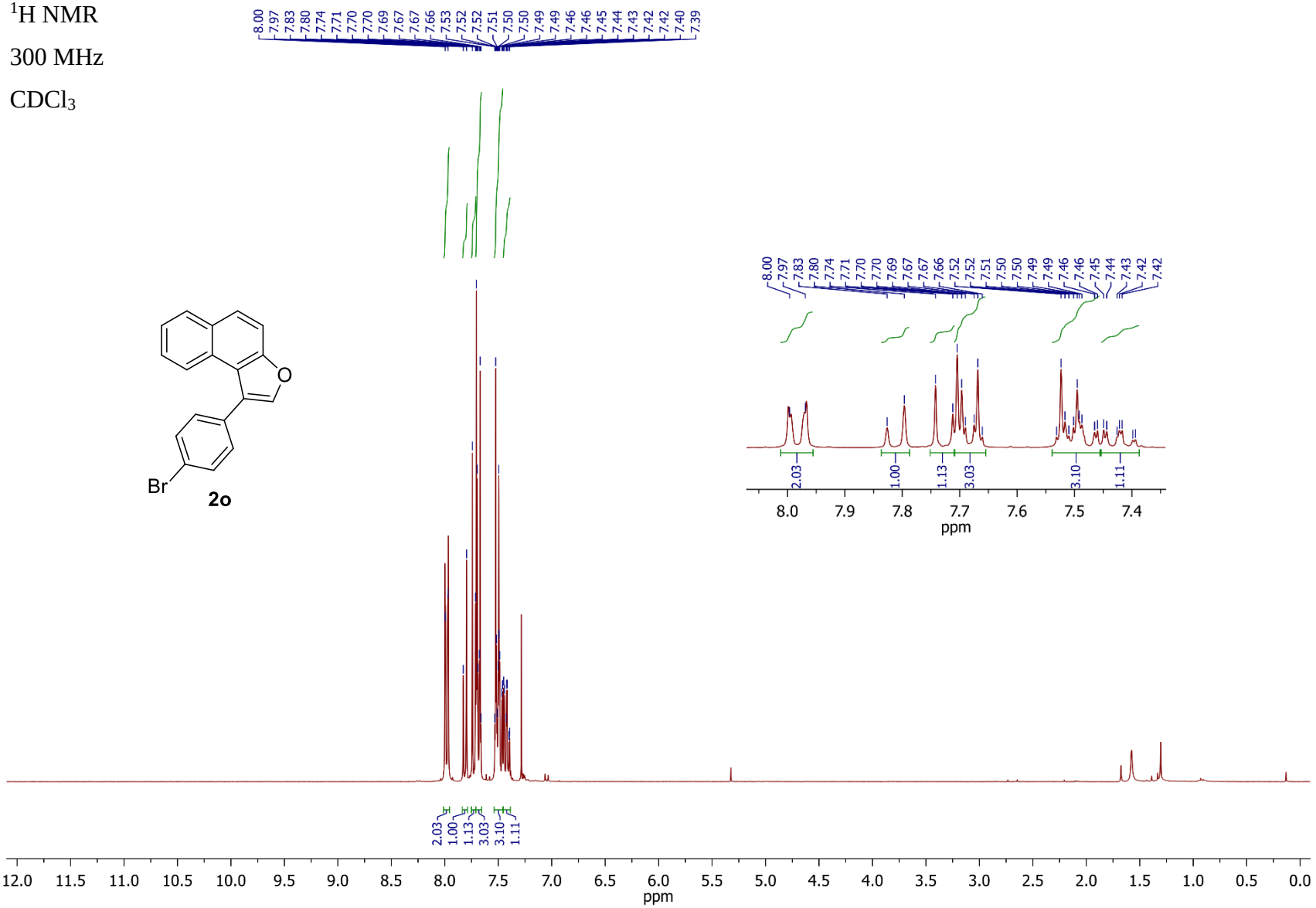
$CDCl_3$



^{1}H NMR

300 MHz

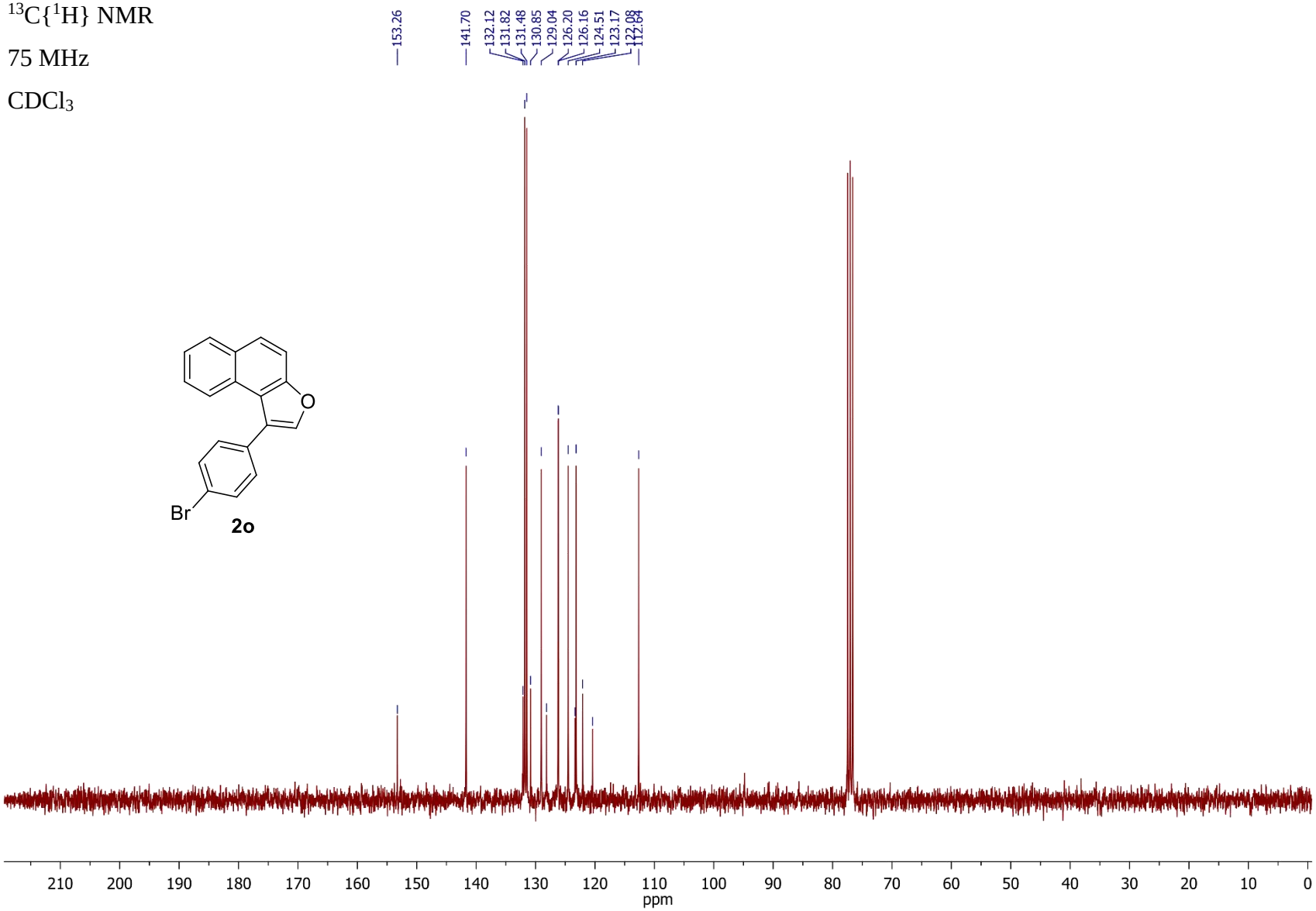
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

$CDCl_3$



^{1}H NMR

300 MHz

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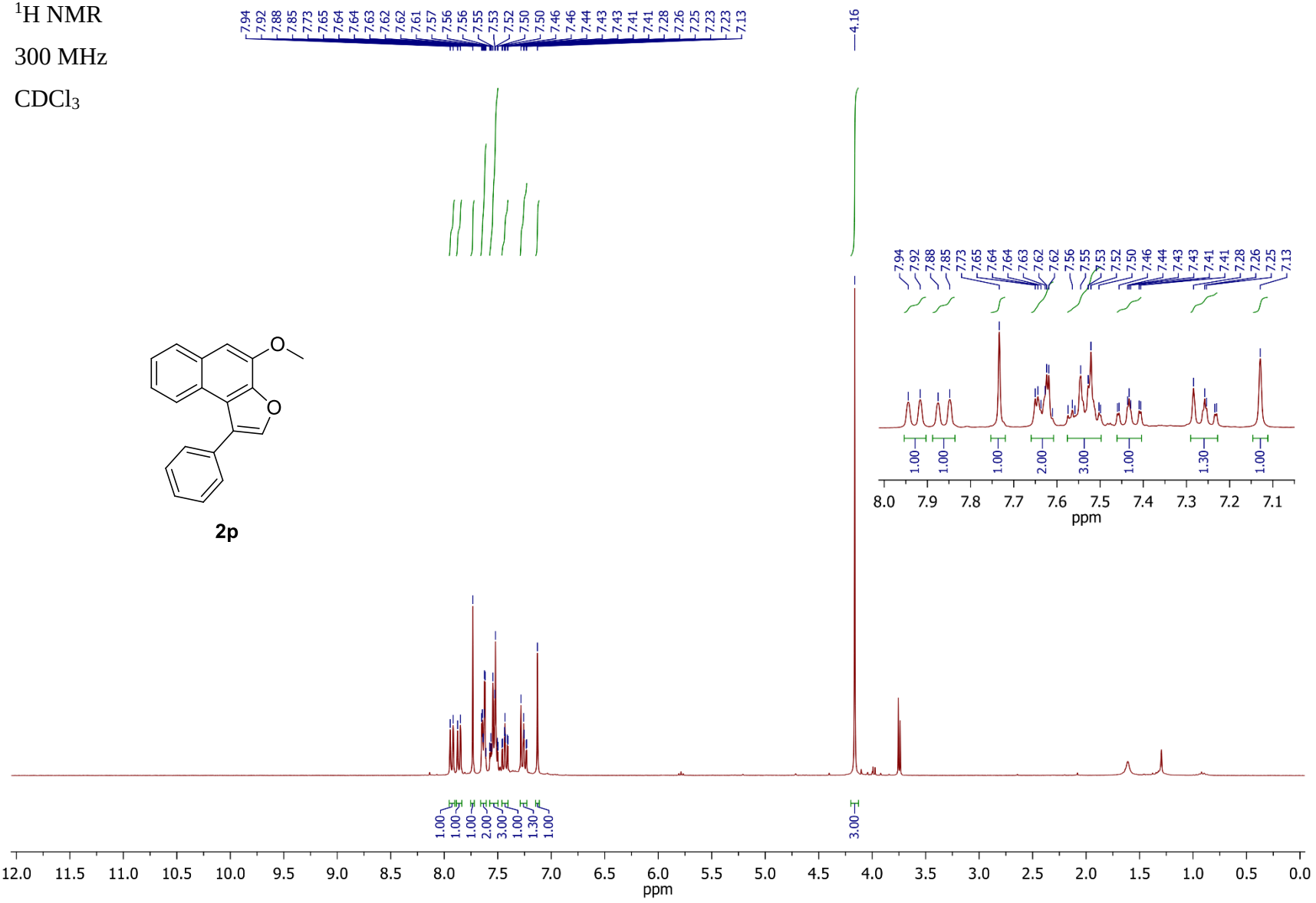
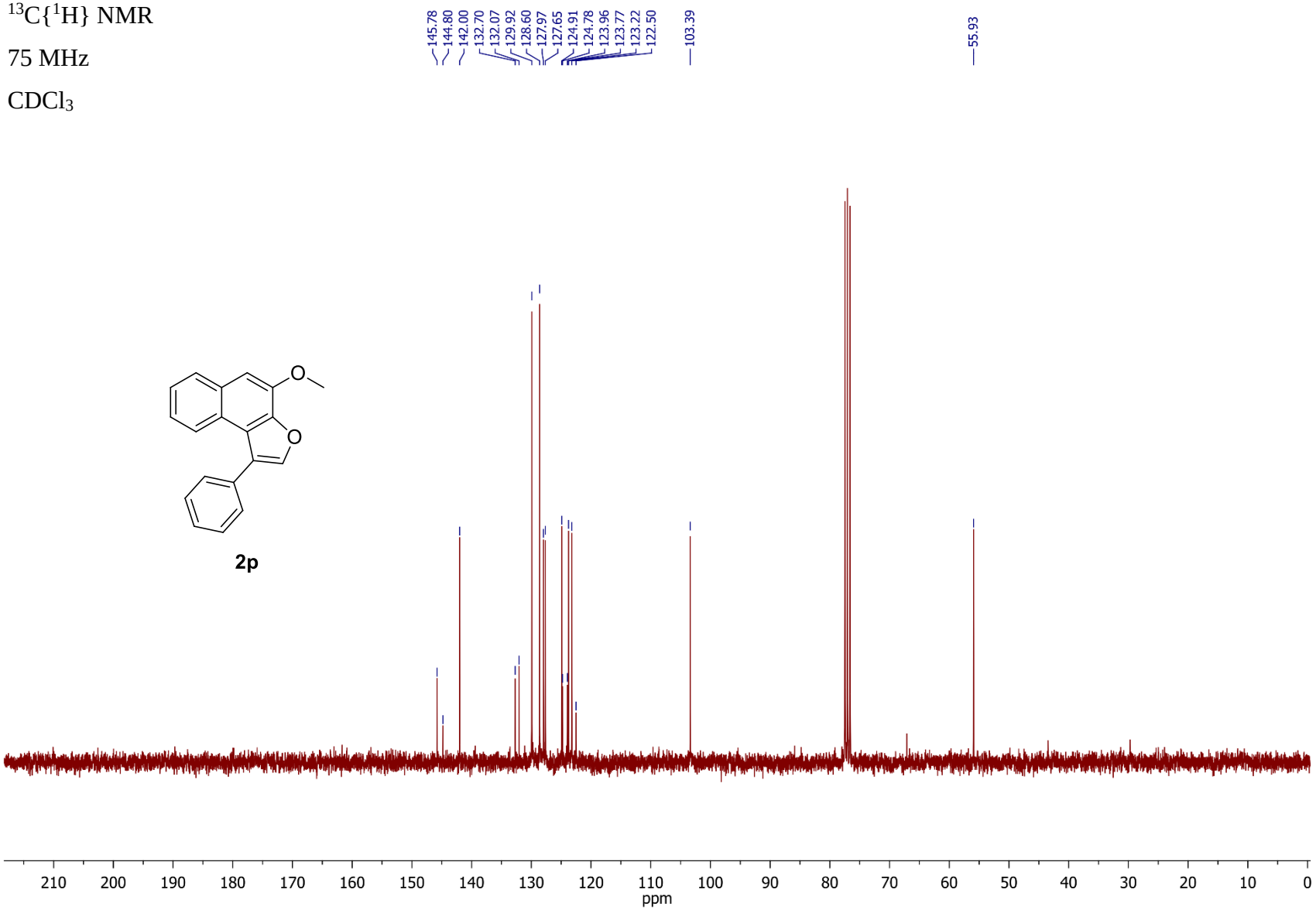
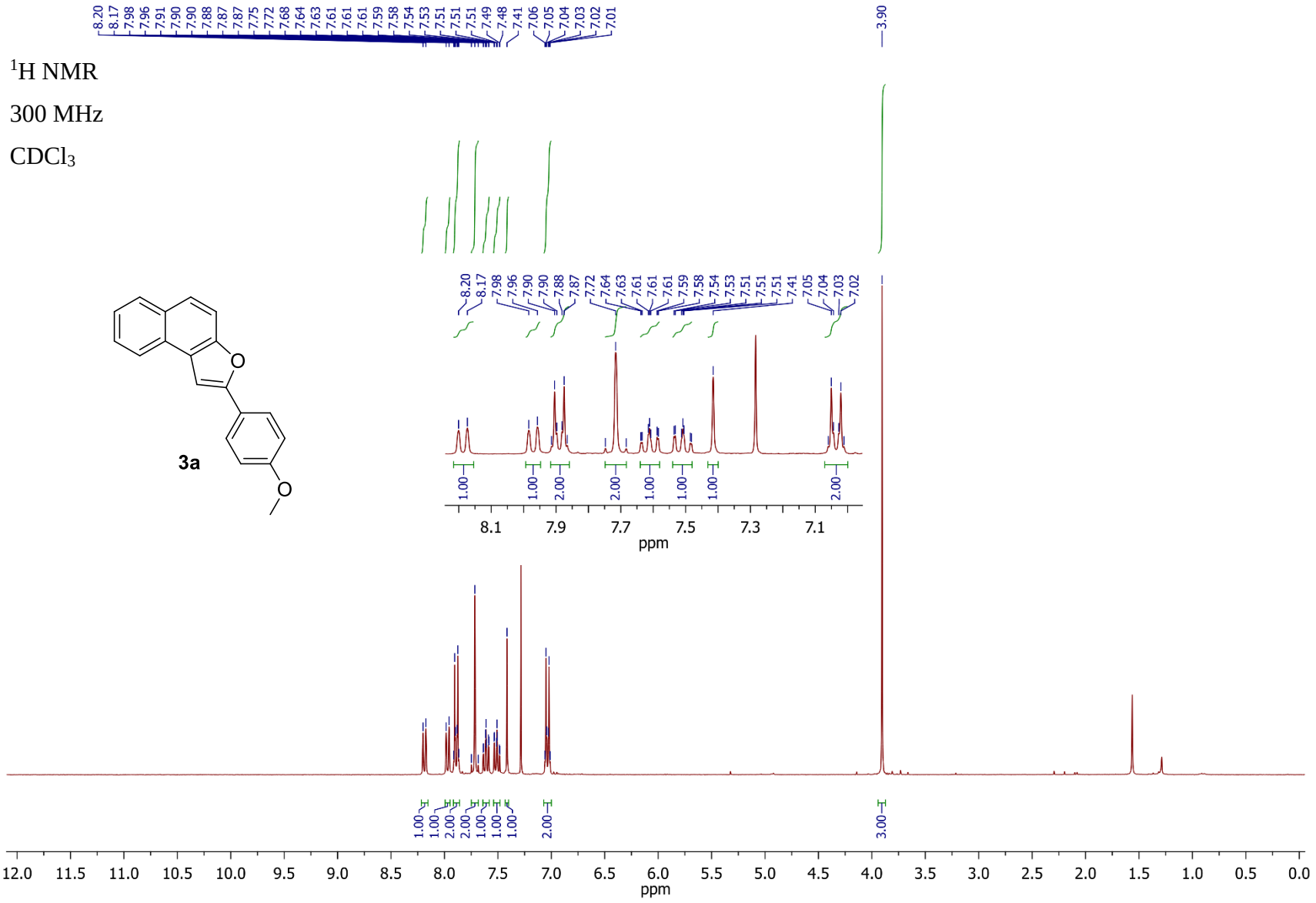


$^{13}C\{^{1}H\}$ NMR

75 MHz

$CDCl_3$

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7.48
7.41
7.06
7.05
7.04
7.03
7.02
7.01
3.90
1H NMR
300 MHz
CDCl3
3a
O
O
1.00
1.00
2.00
2.00
1.00
1.00
1.00
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8.1
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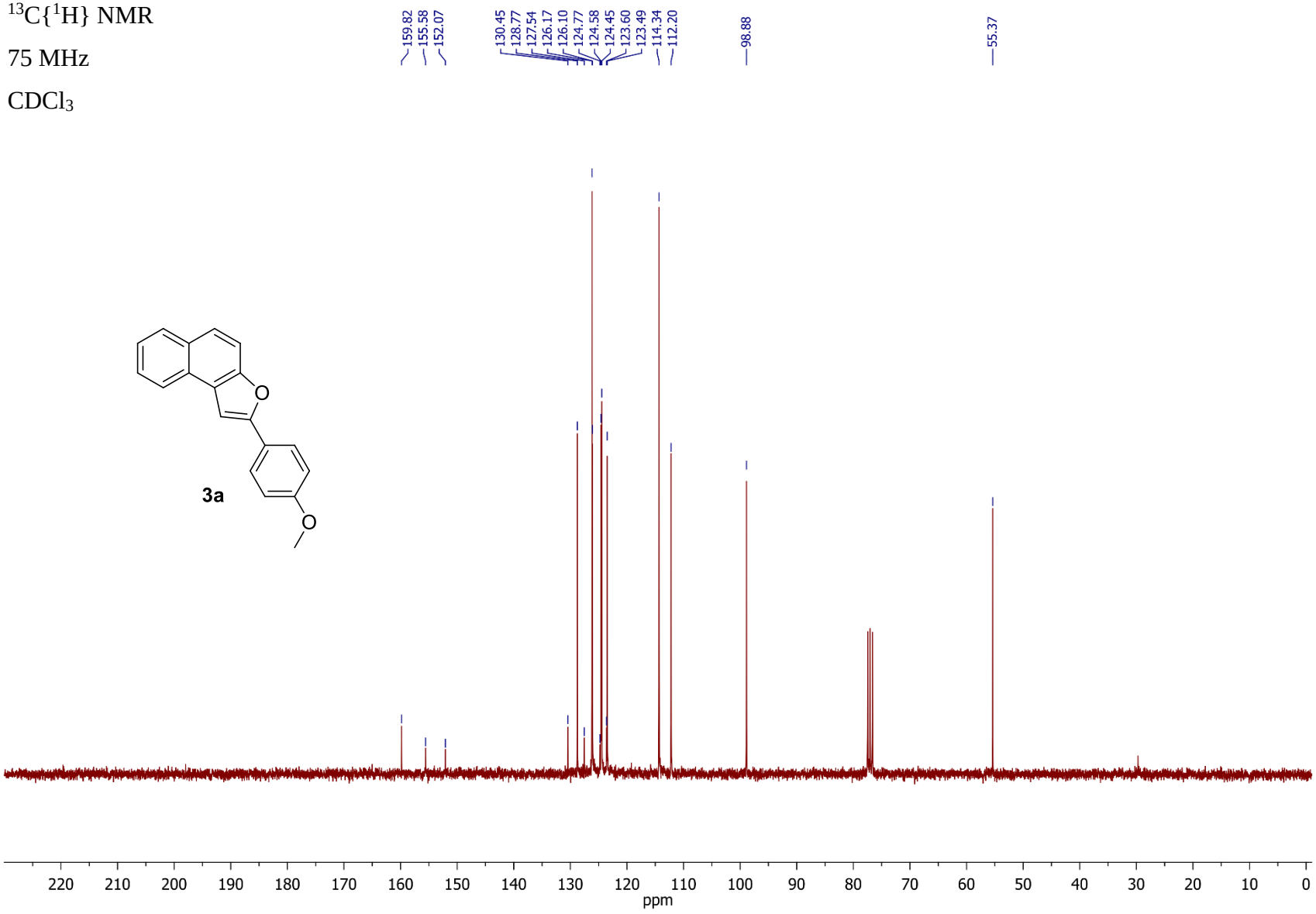
ppm

$^{13}C\{^{1}H\}$ NMR

75 MHz

$CDCl_3$



^{1}H NMR

300 MHz

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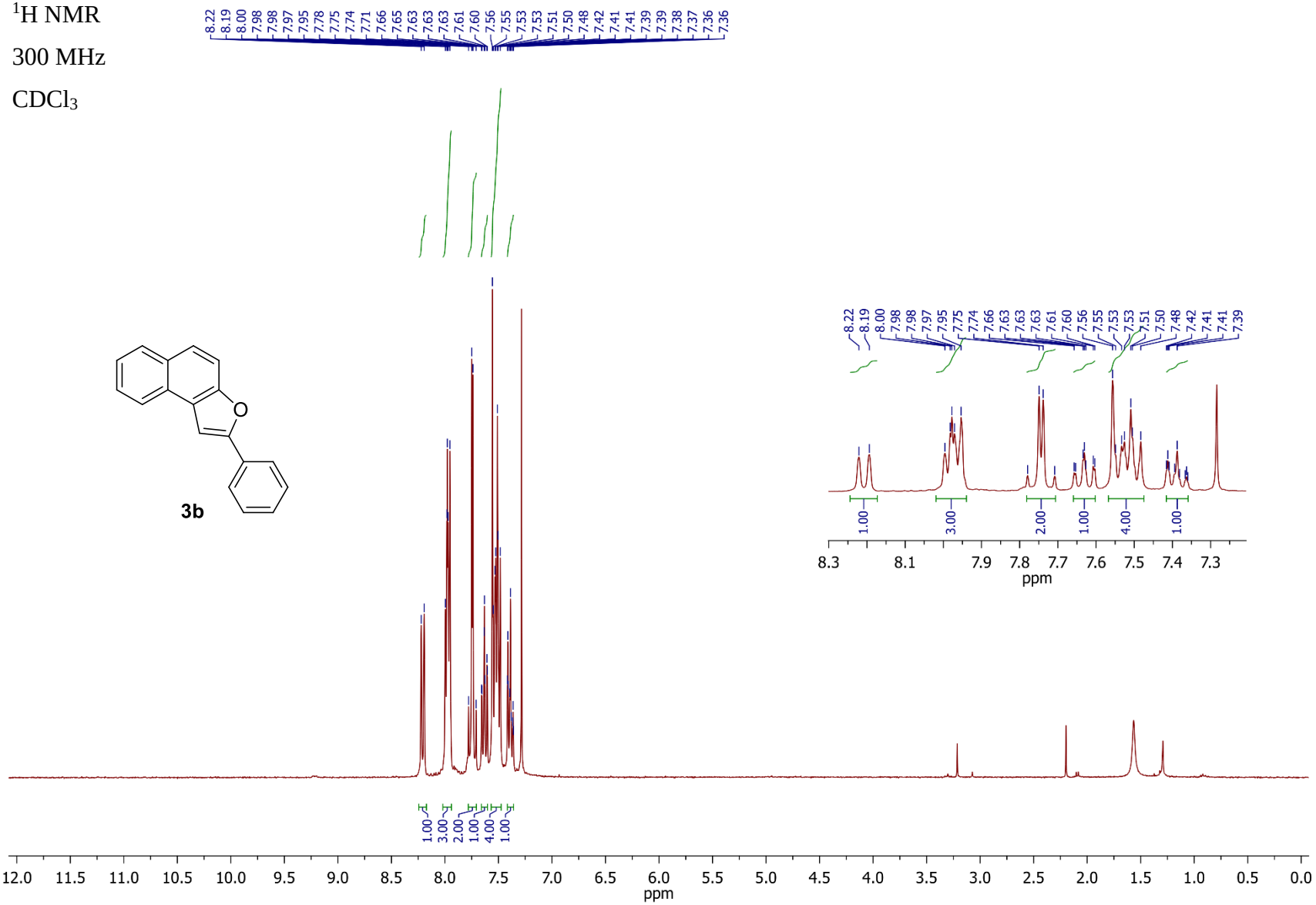

$^{13}C\{^{1}H\}$ NMR

75 MHz

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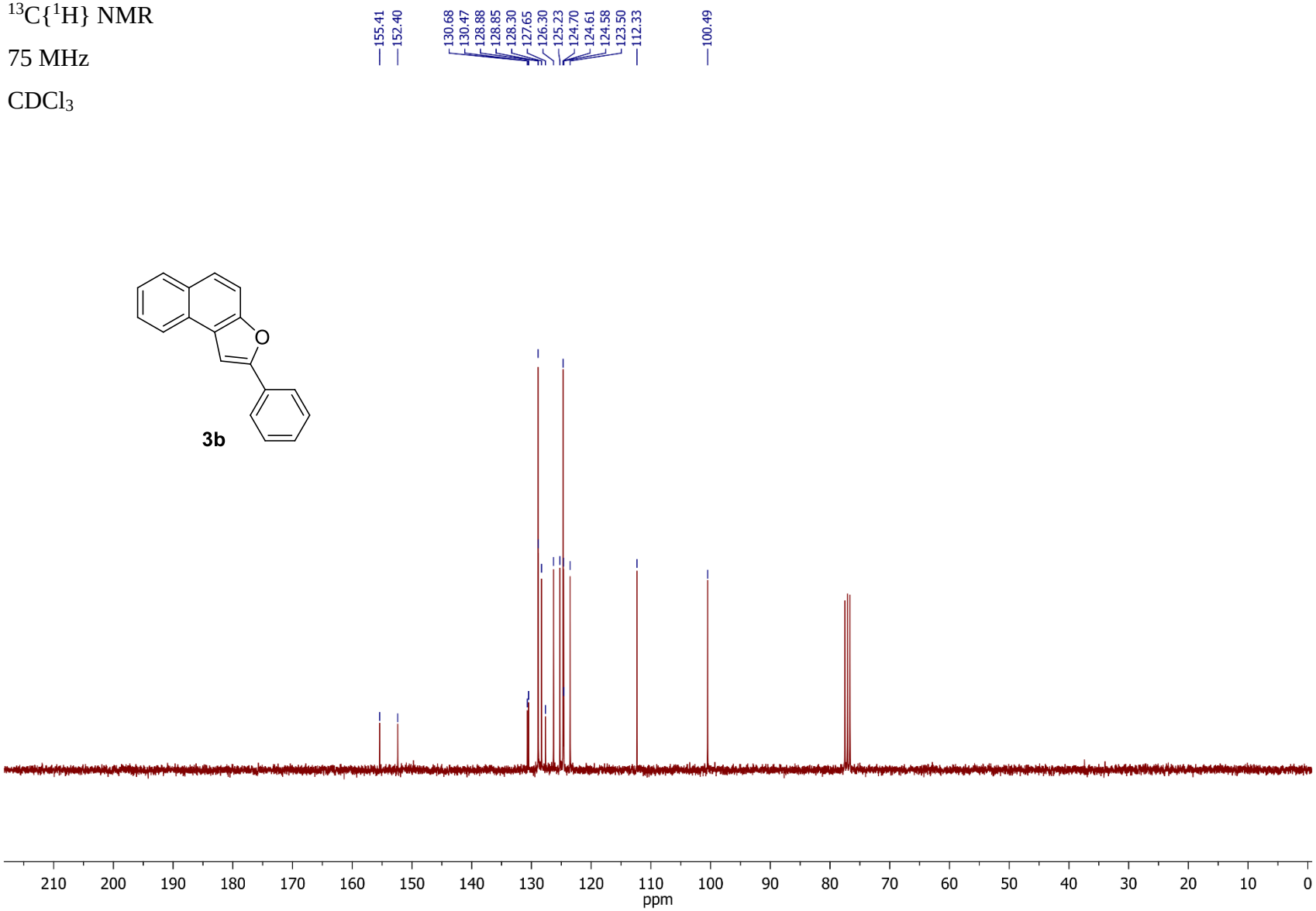

^{1}H NMR

300 MHz

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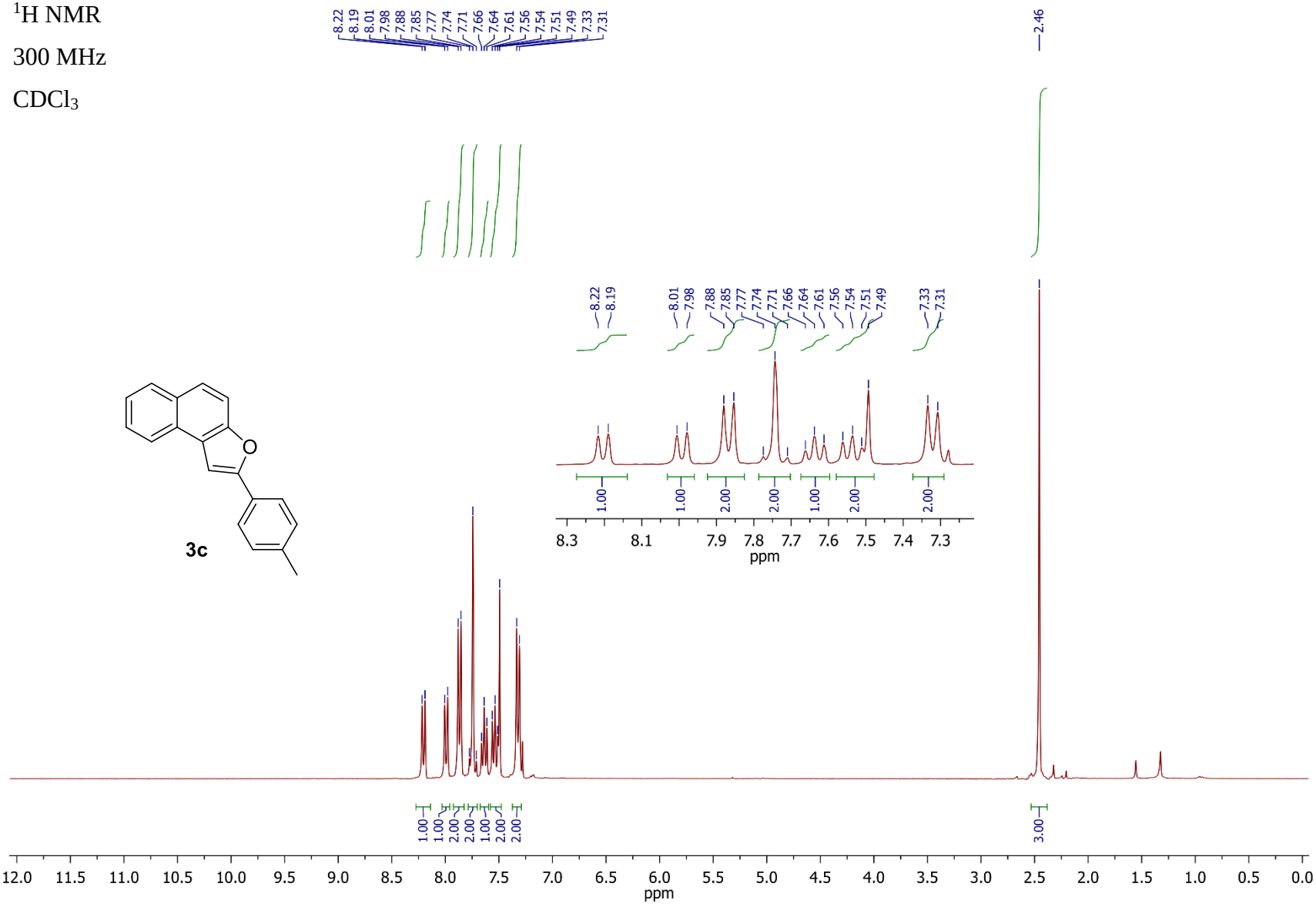
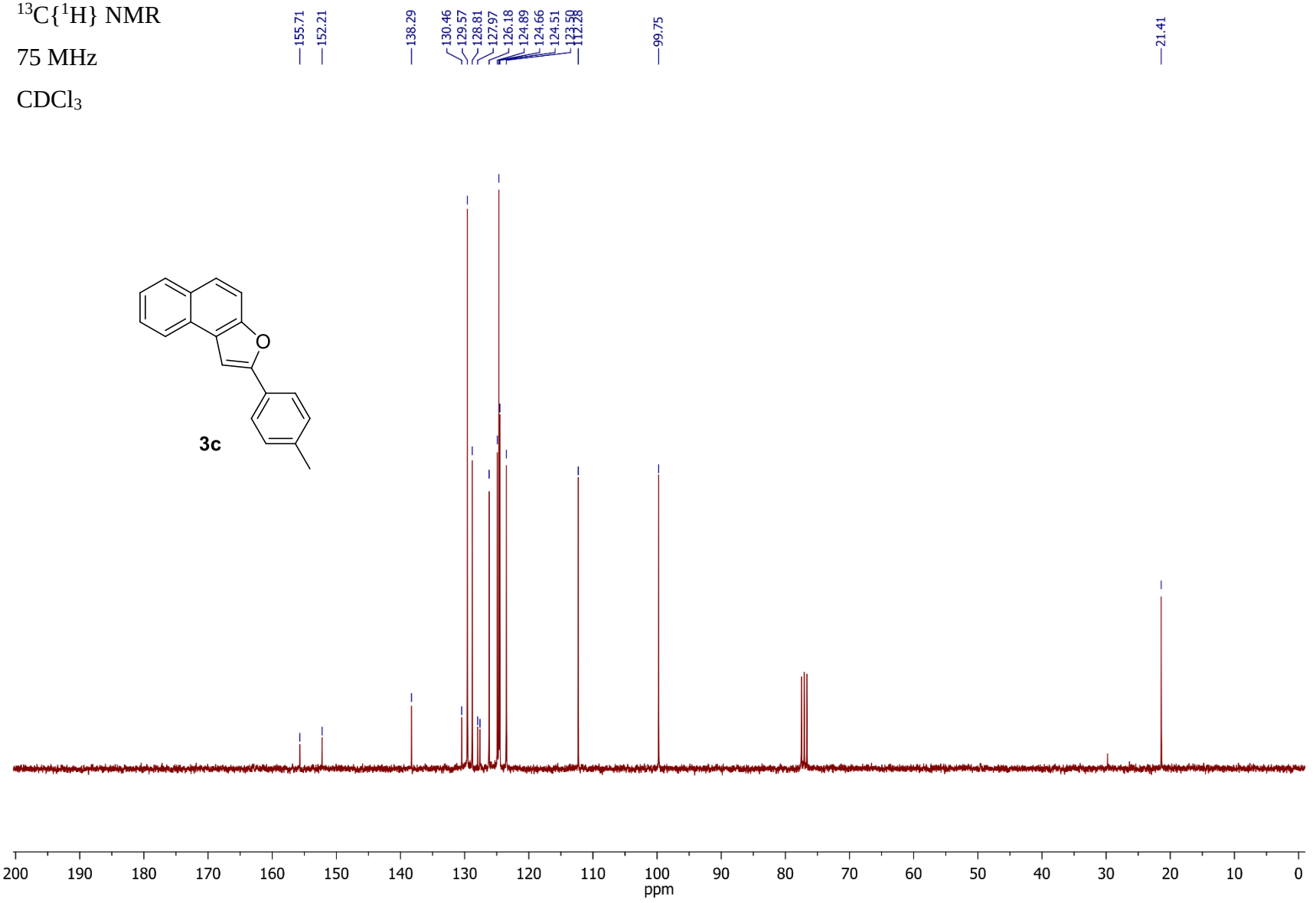


$^{13}C\{^{1}H\}$ NMR

75 MHz

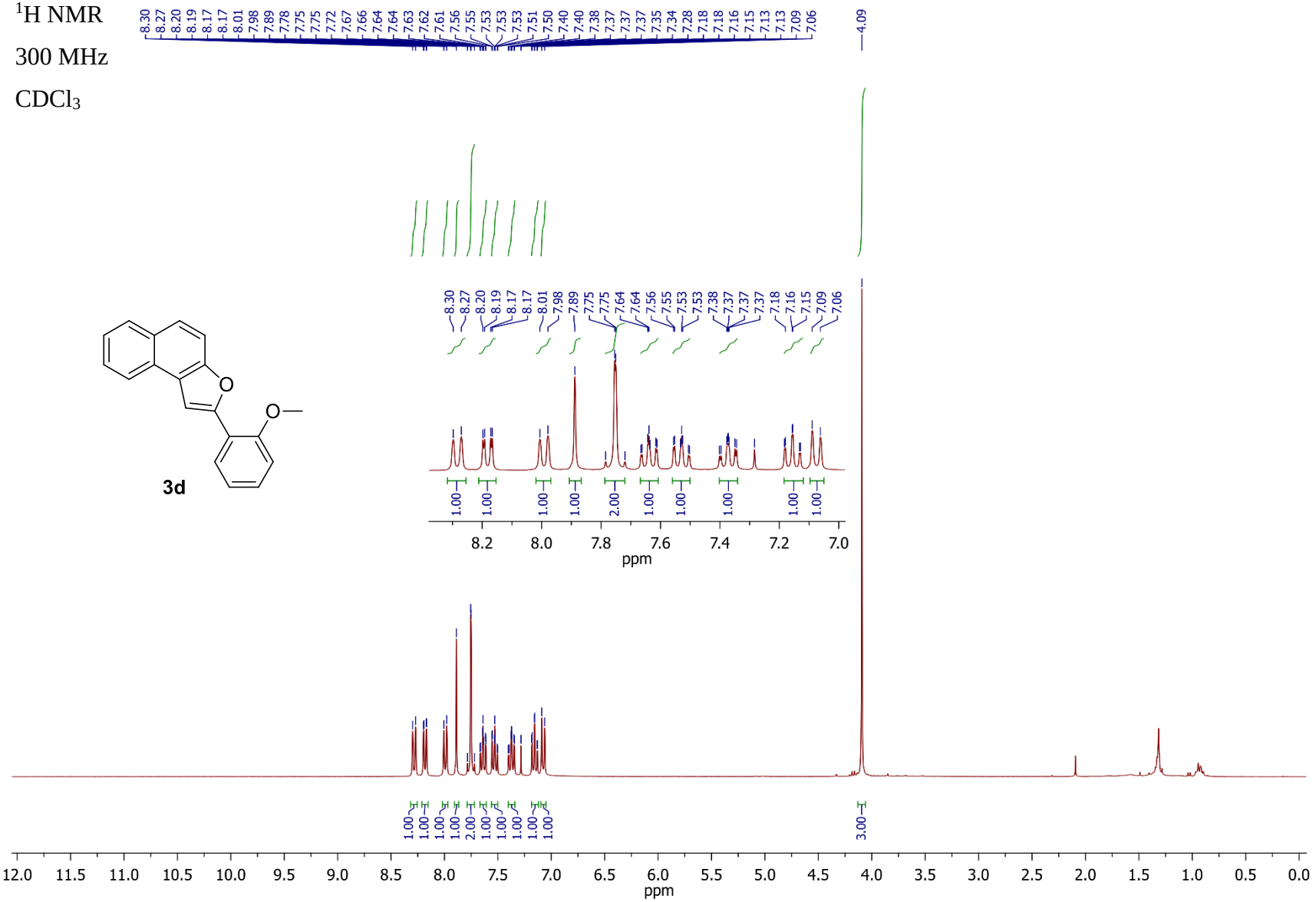
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

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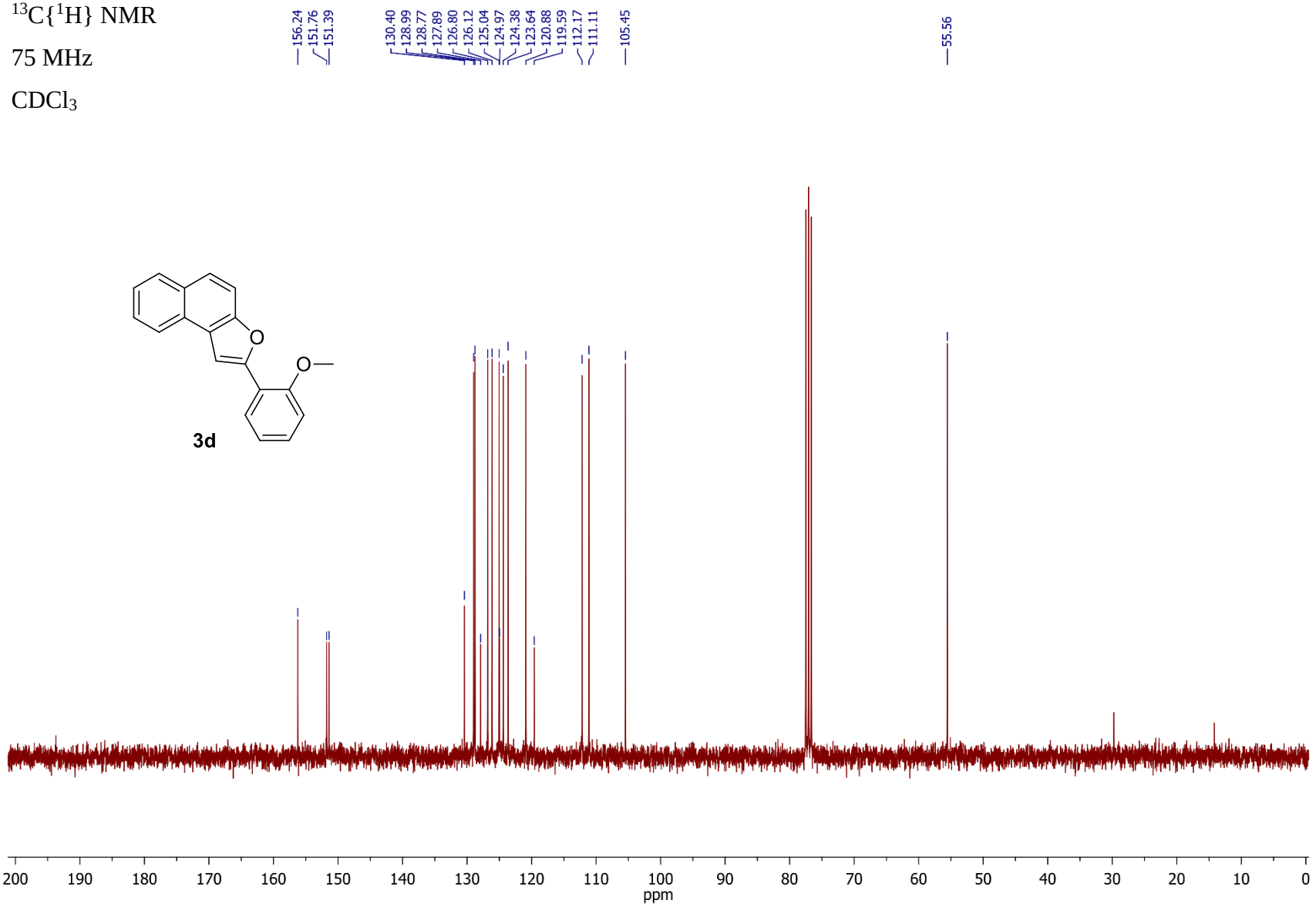

^{1}H NMR

300 MHz

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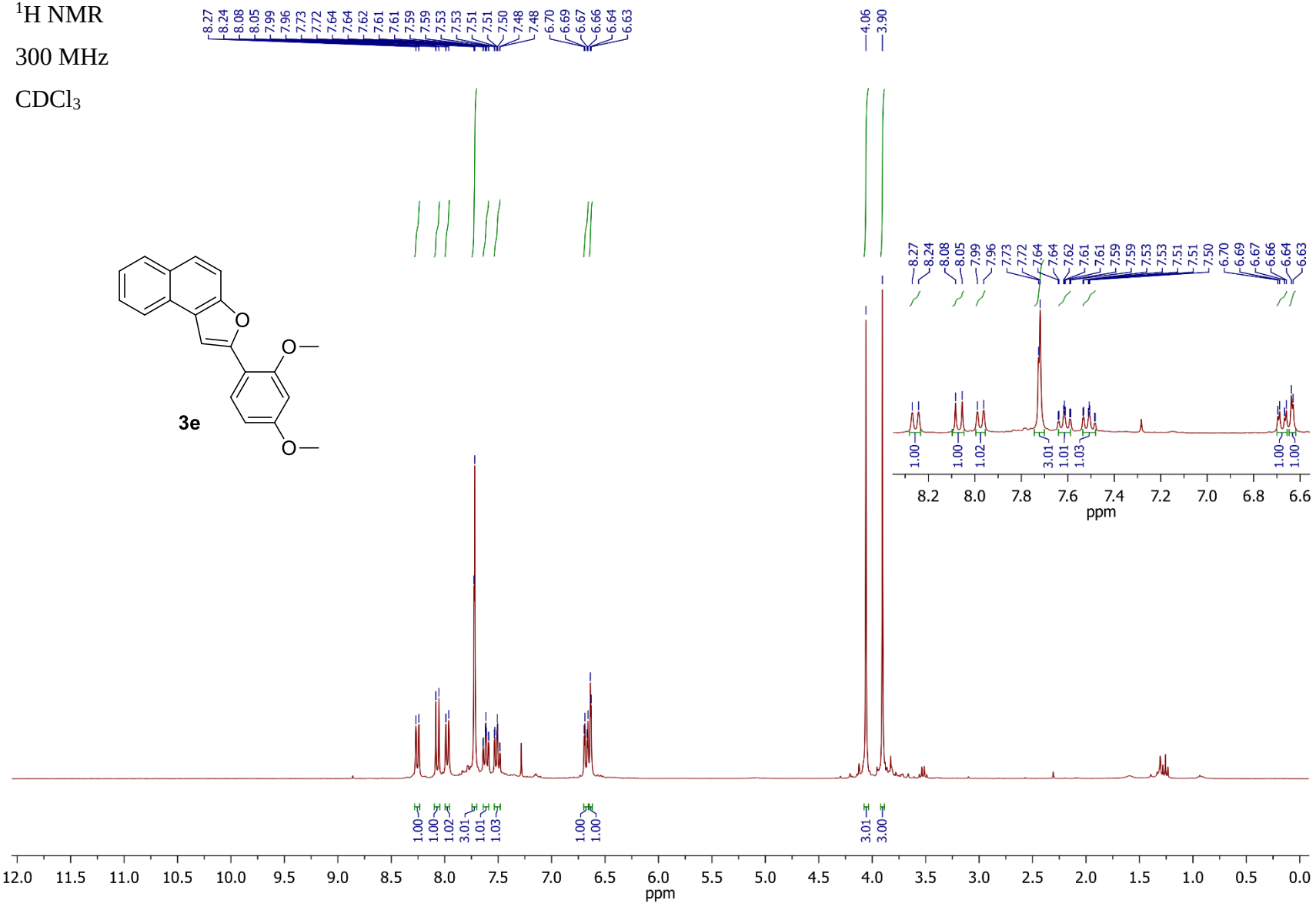

$^{13}C\{^{1}H\}$ NMR

75 MHz

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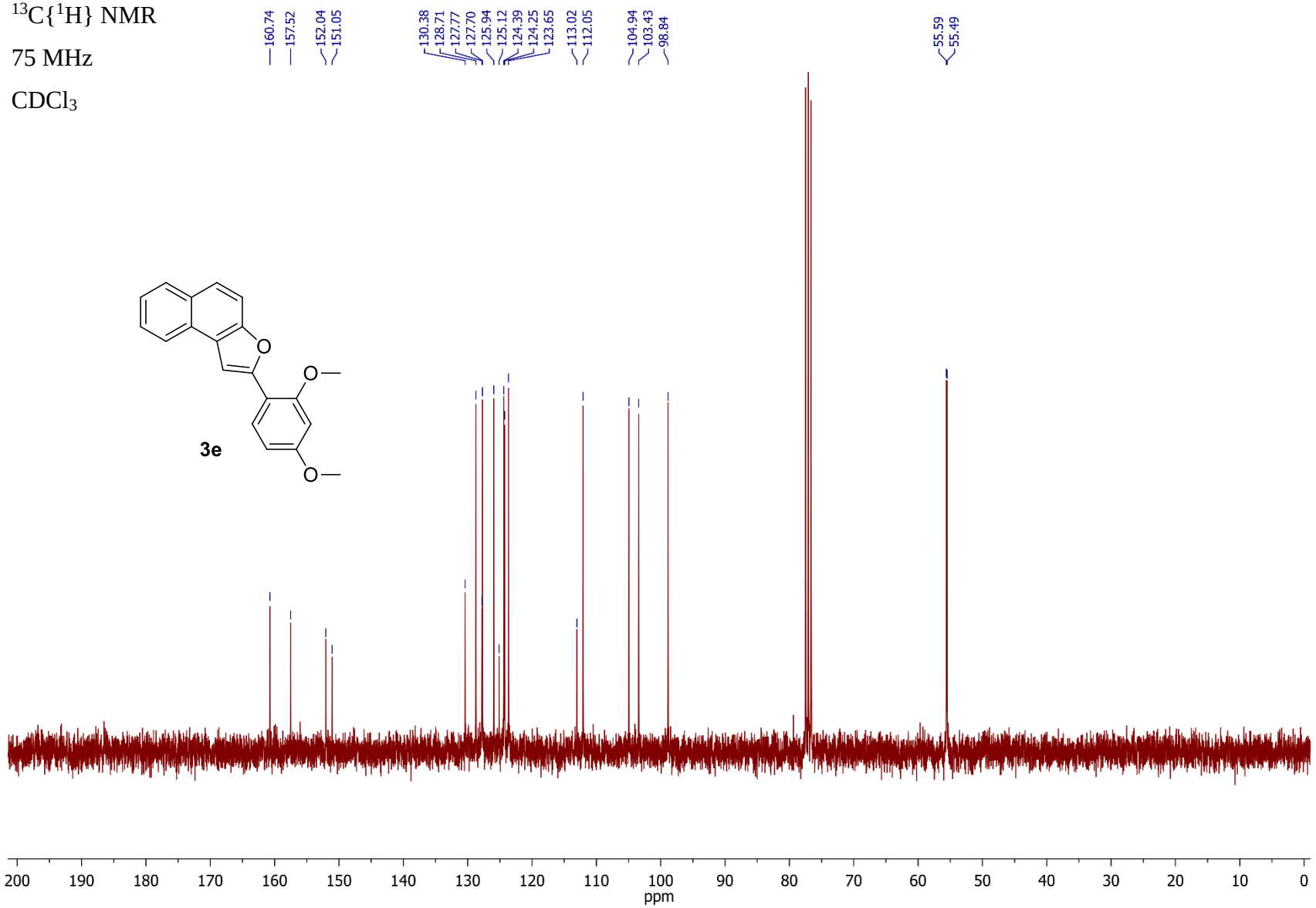

^{1}H NMR

300 MHz

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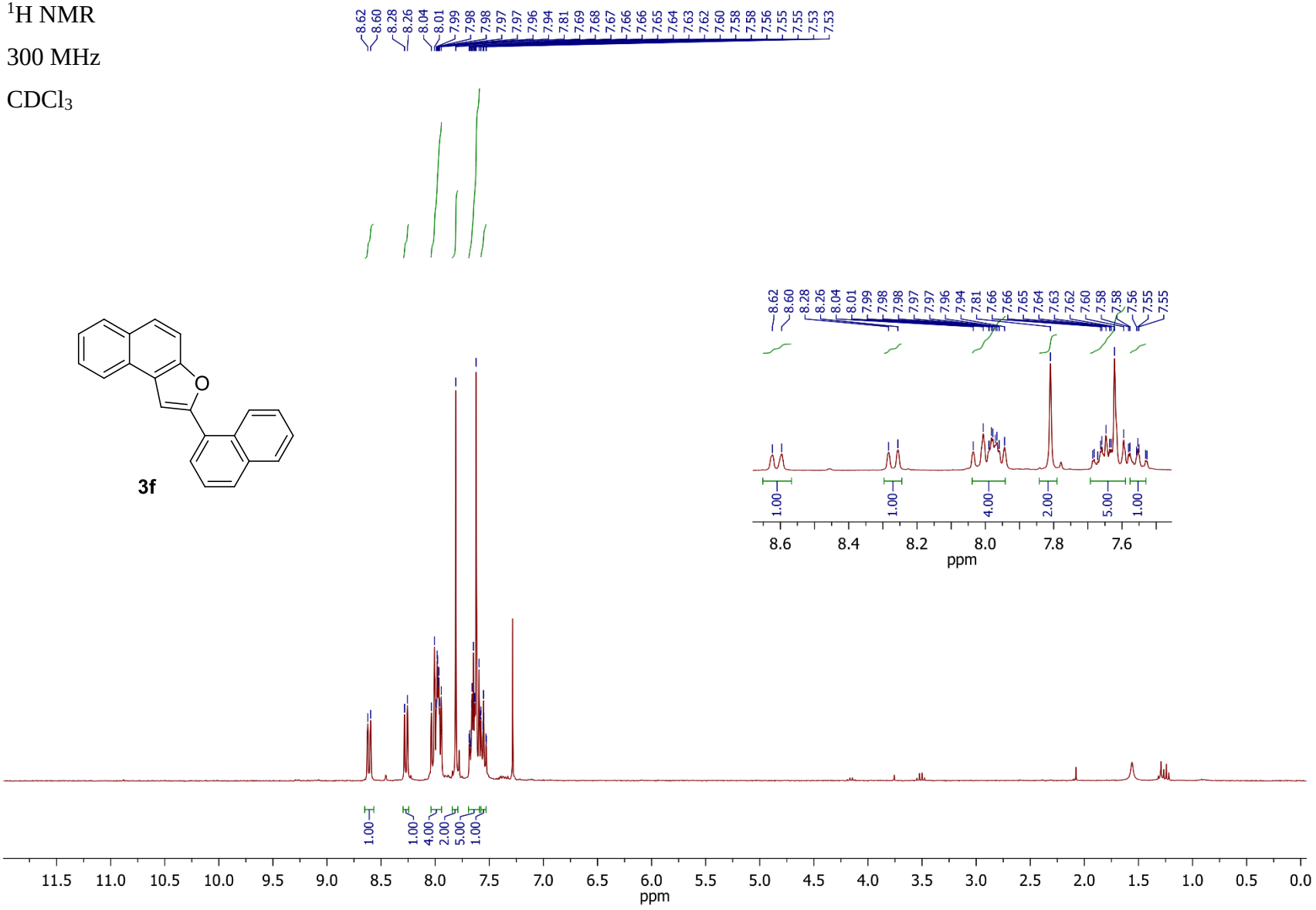
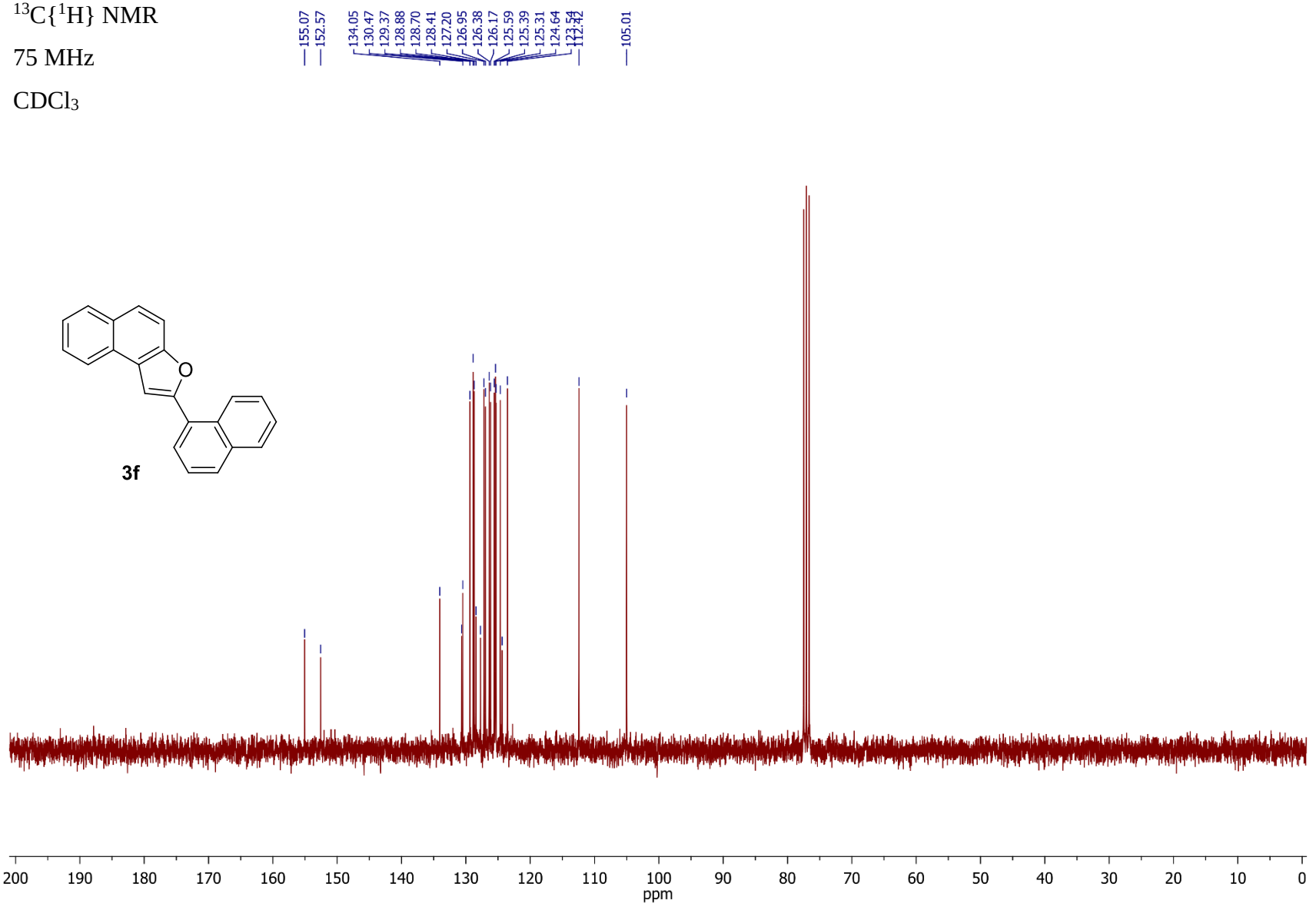


$^{13}C\{^{1}H\}$ NMR

75 MHz

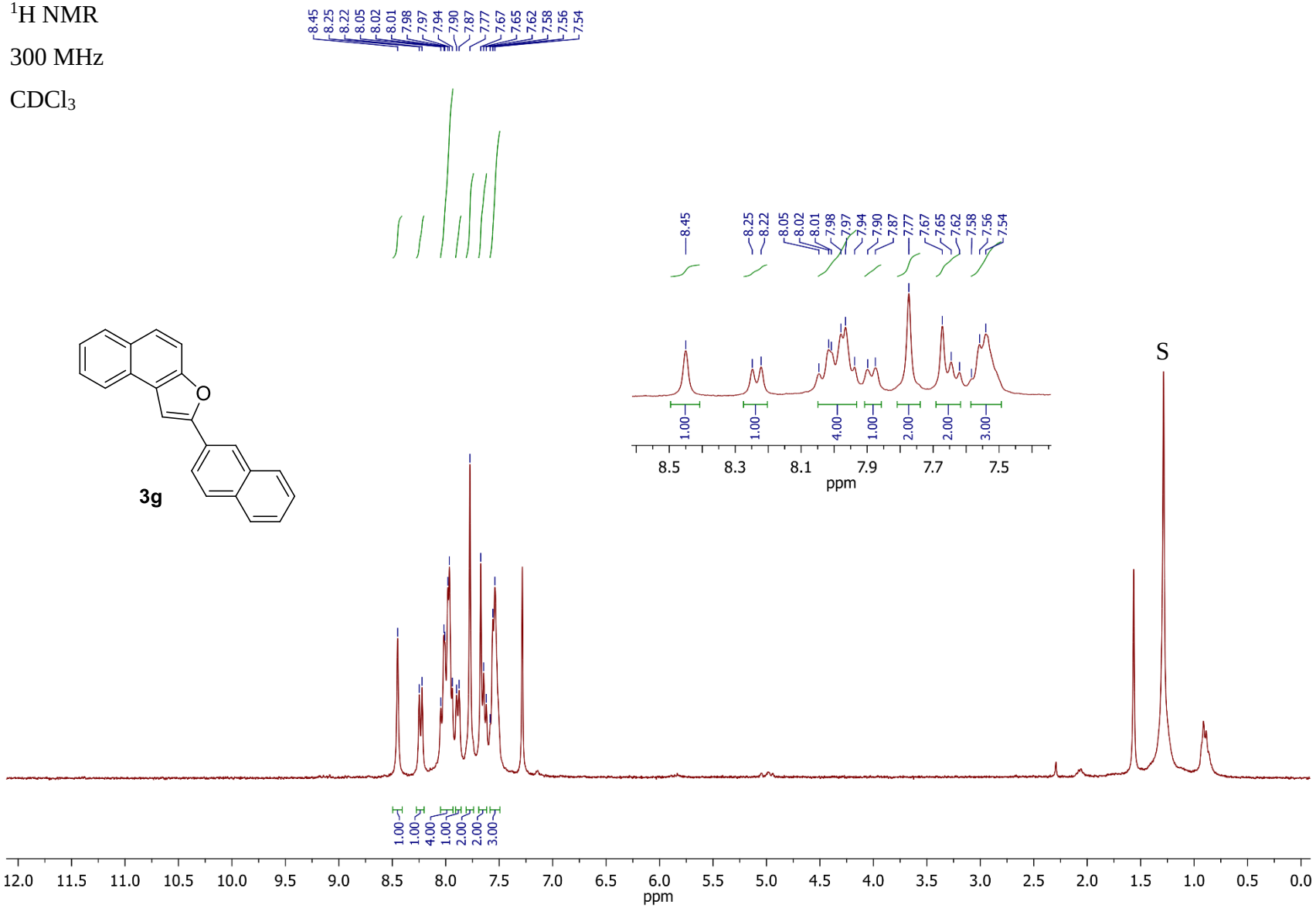
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$

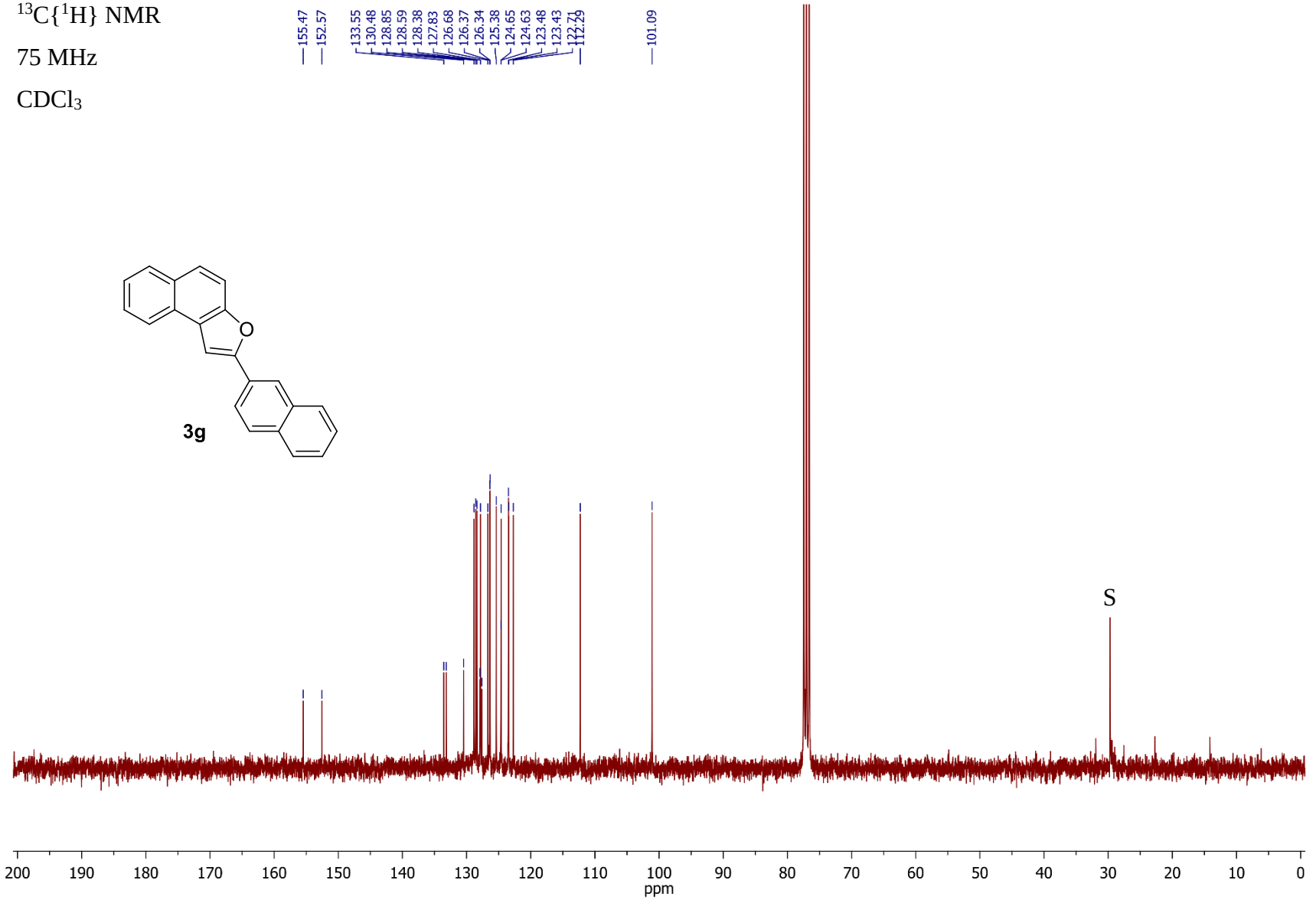


S – peak of grease (1.26 ppm)

$^{13}C\{^{1}H\}$ NMR

75 MHz

$CDCl_3$

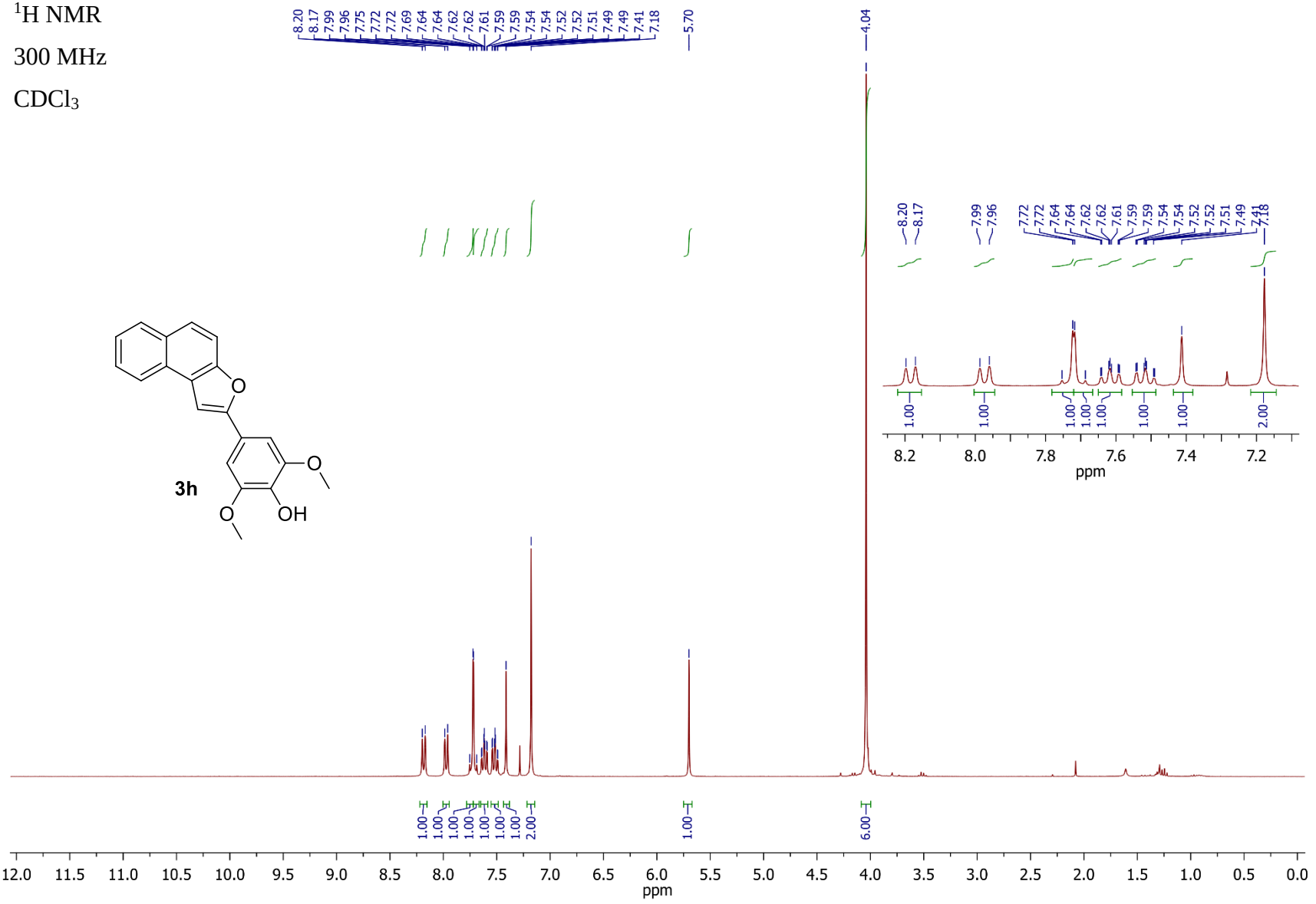


S – peak of grease (29.8 ppm)

^{1}H NMR

300 MHz

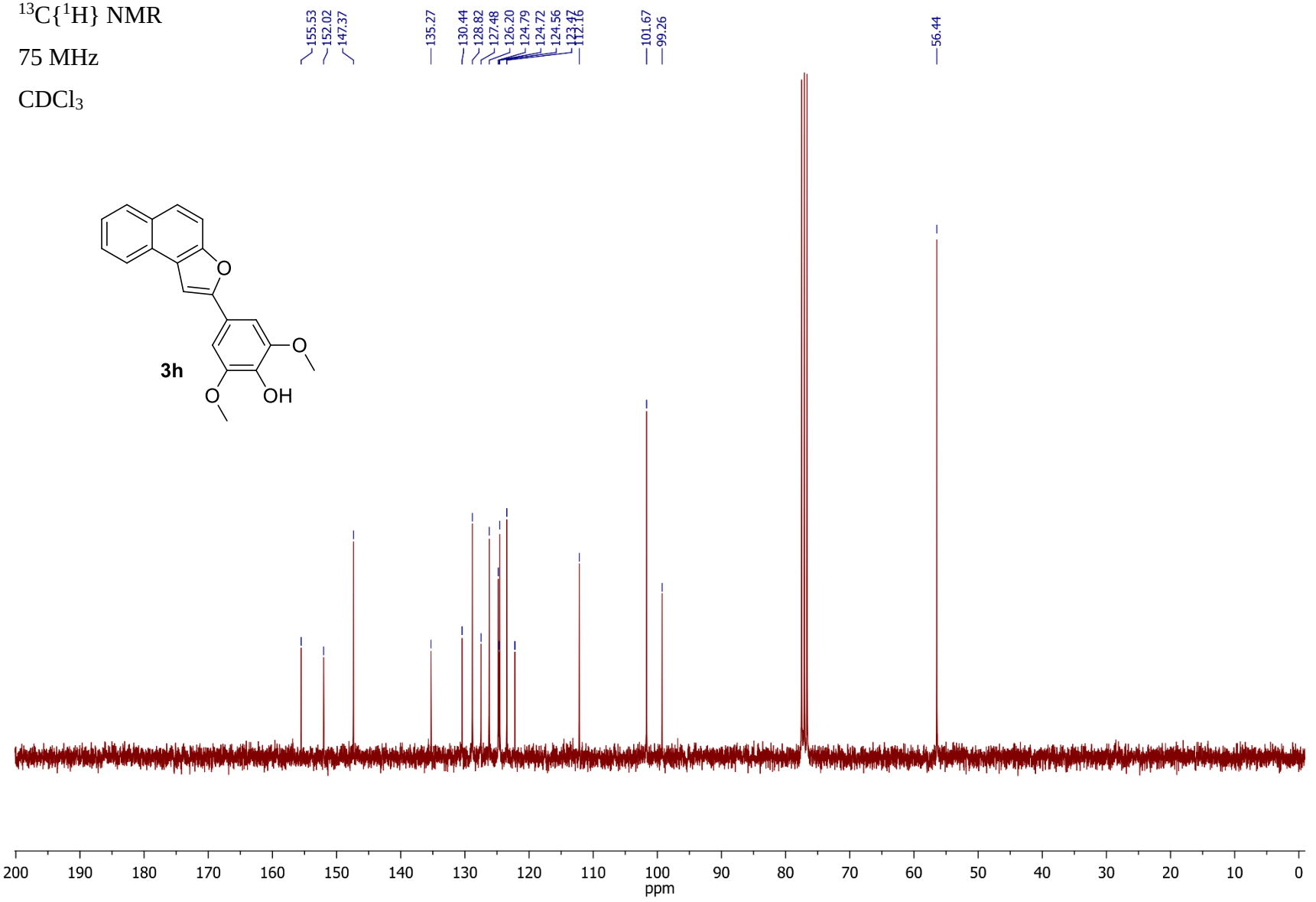
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

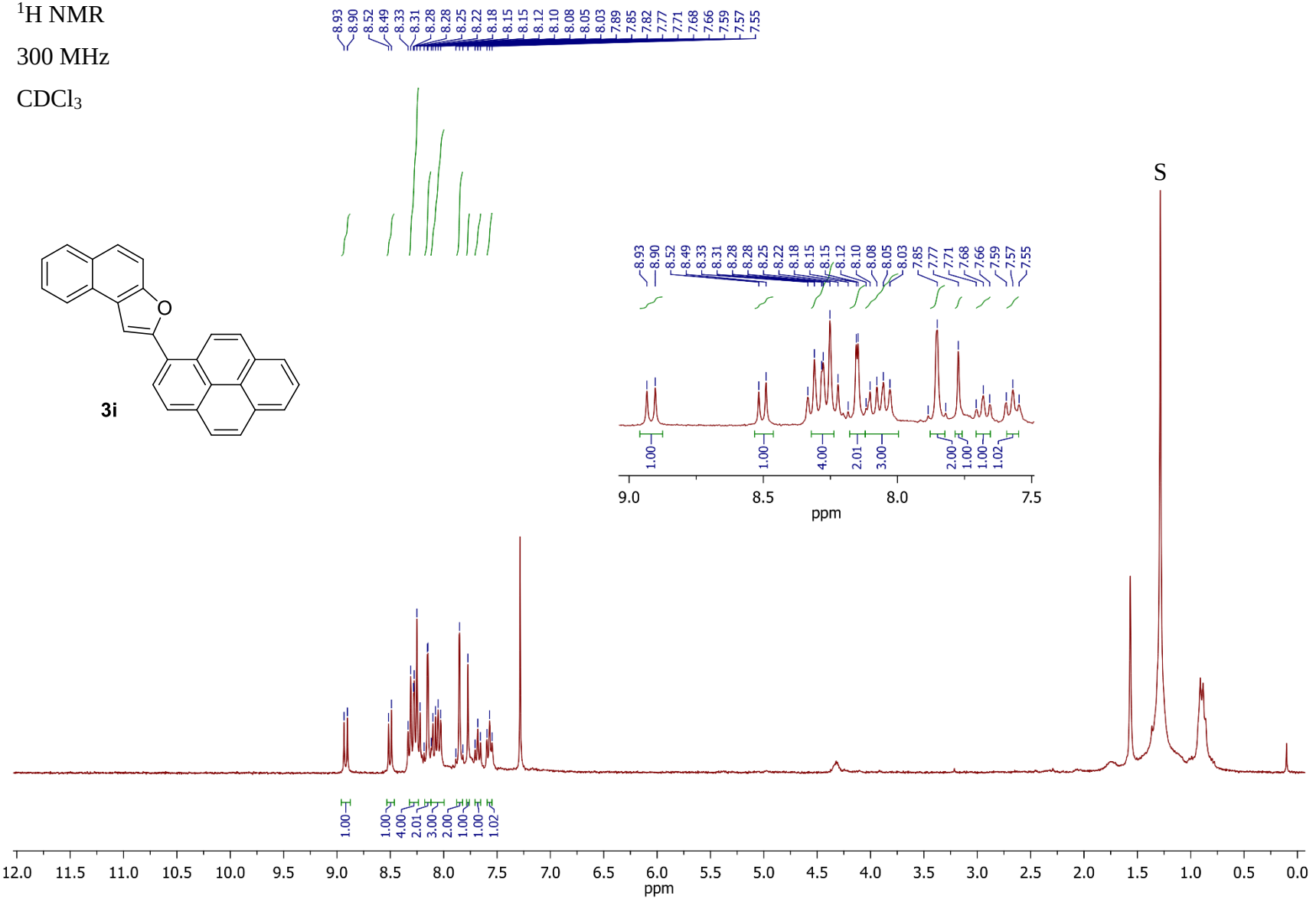
$CDCl_3$



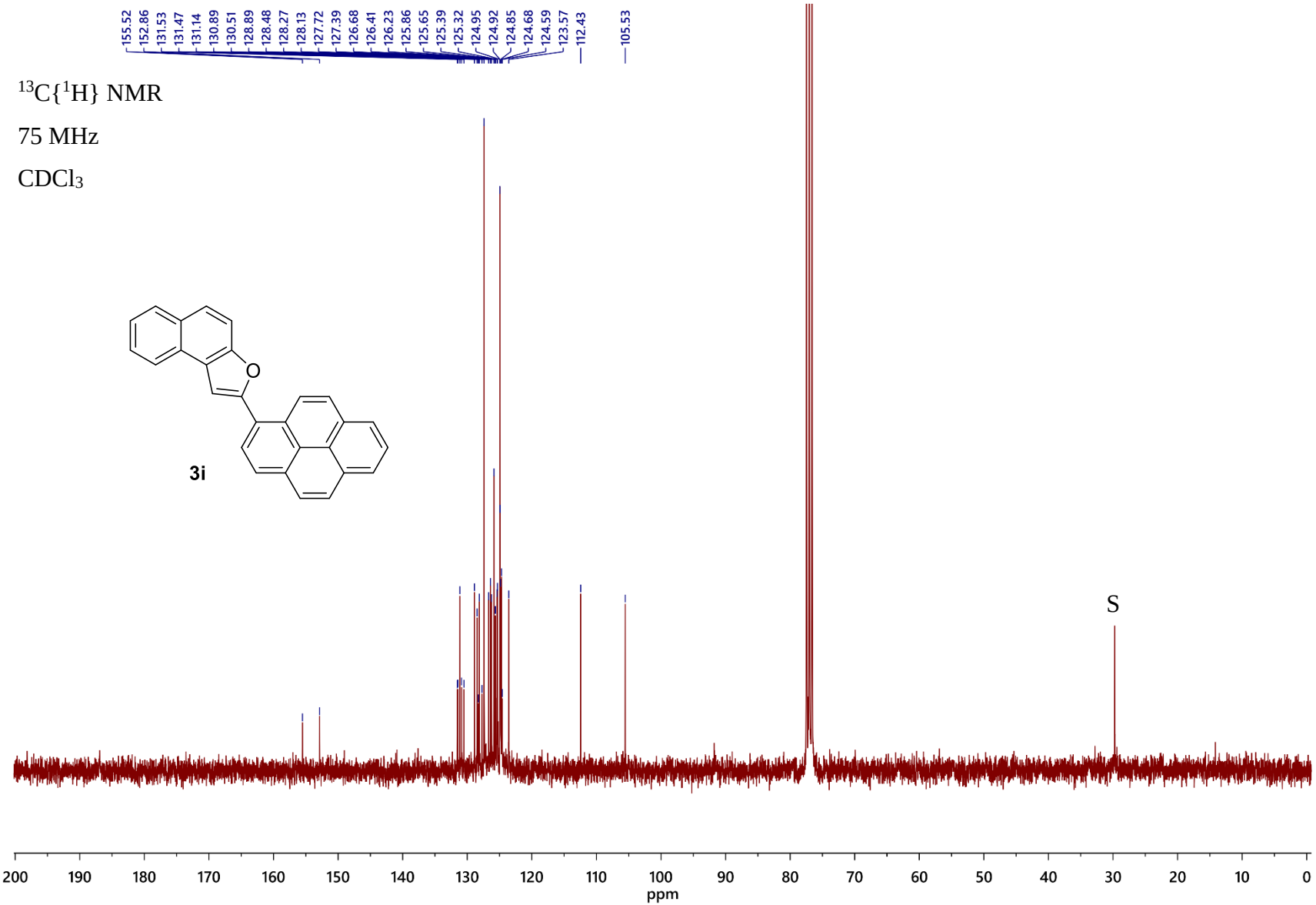
^{1}H NMR

300 MHz

$CDCl_3$



S – peak of grease (1.26 ppm)

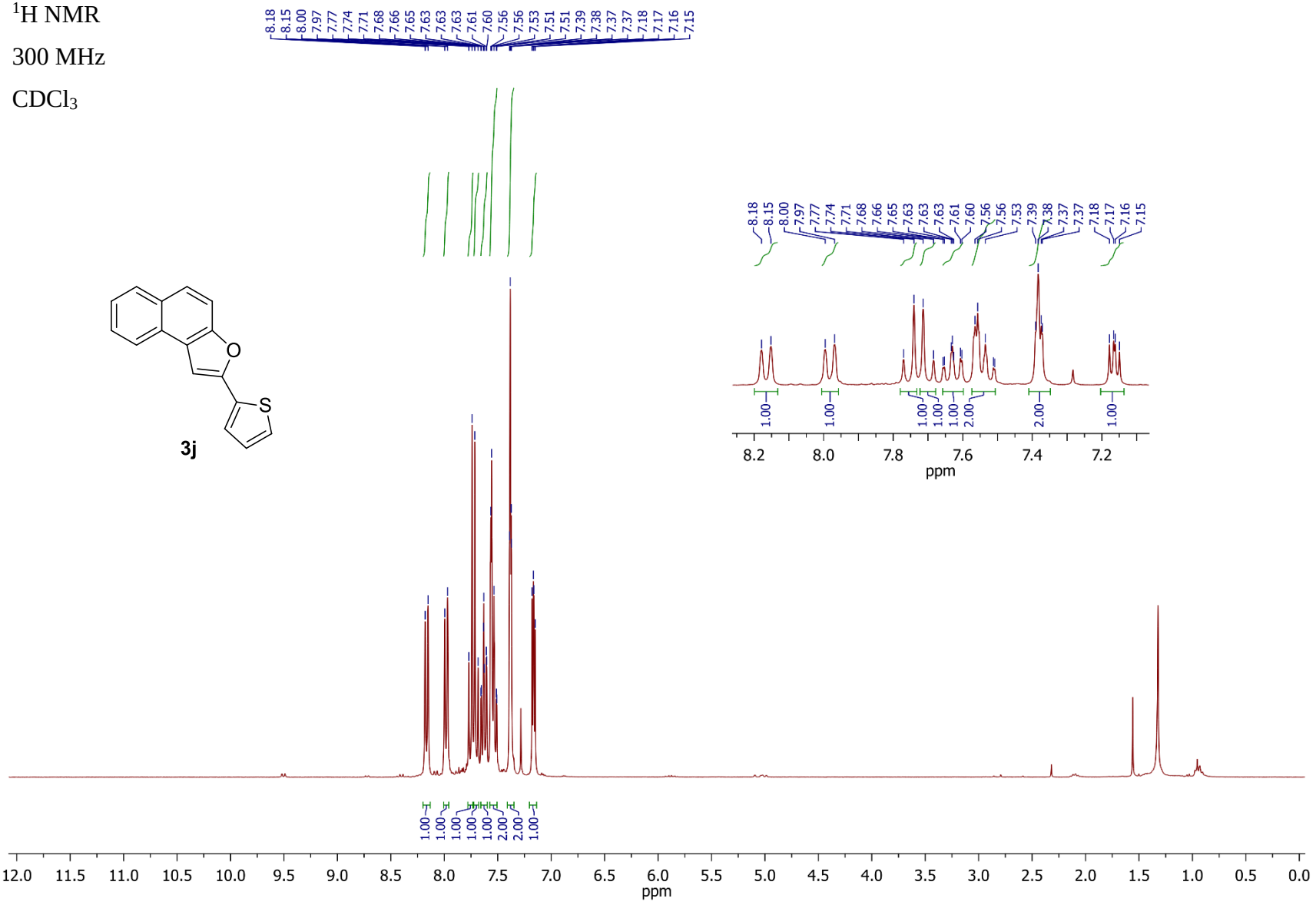


S – peak of grease (29.8 ppm)

^{1}H NMR

300 MHz

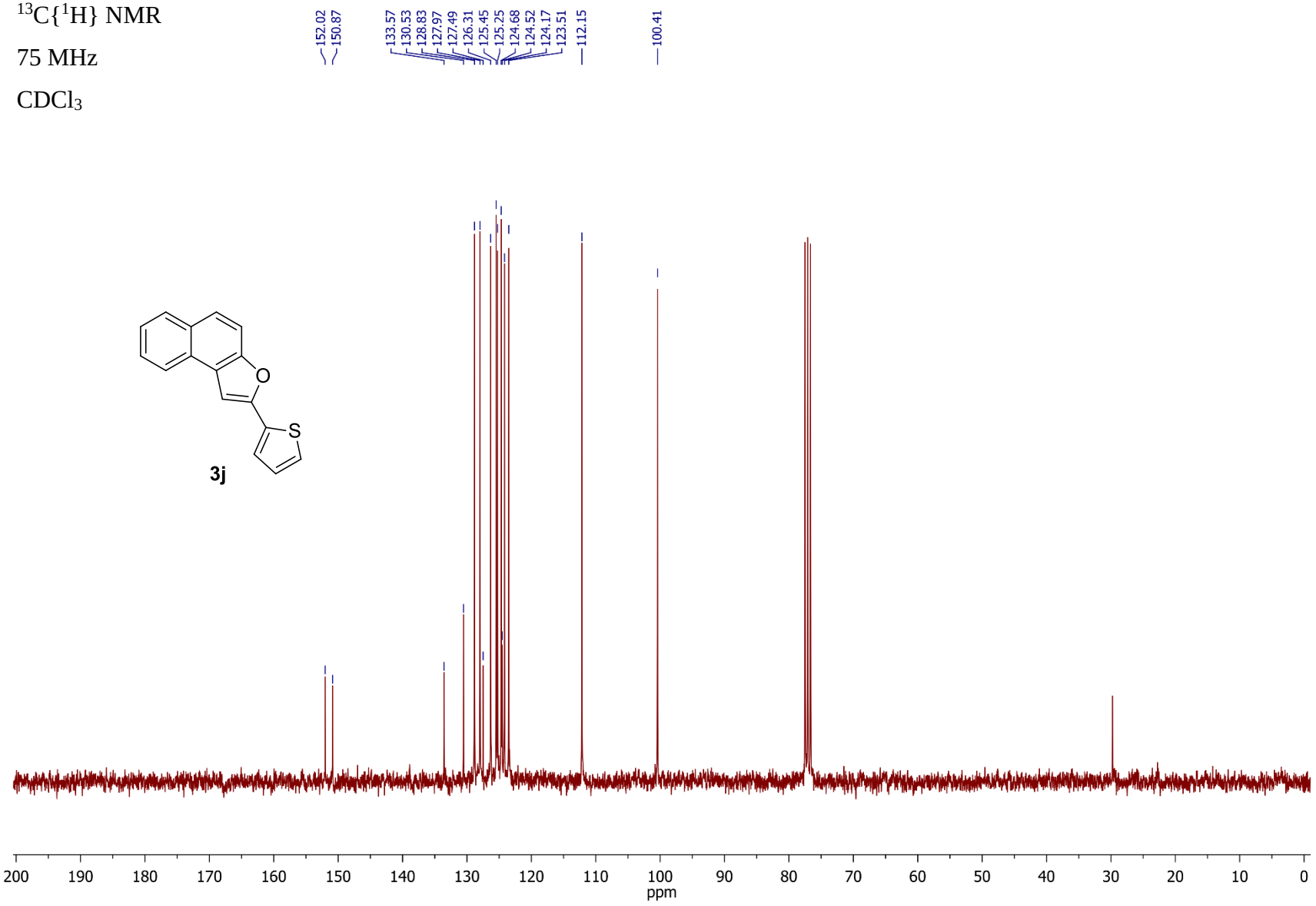
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

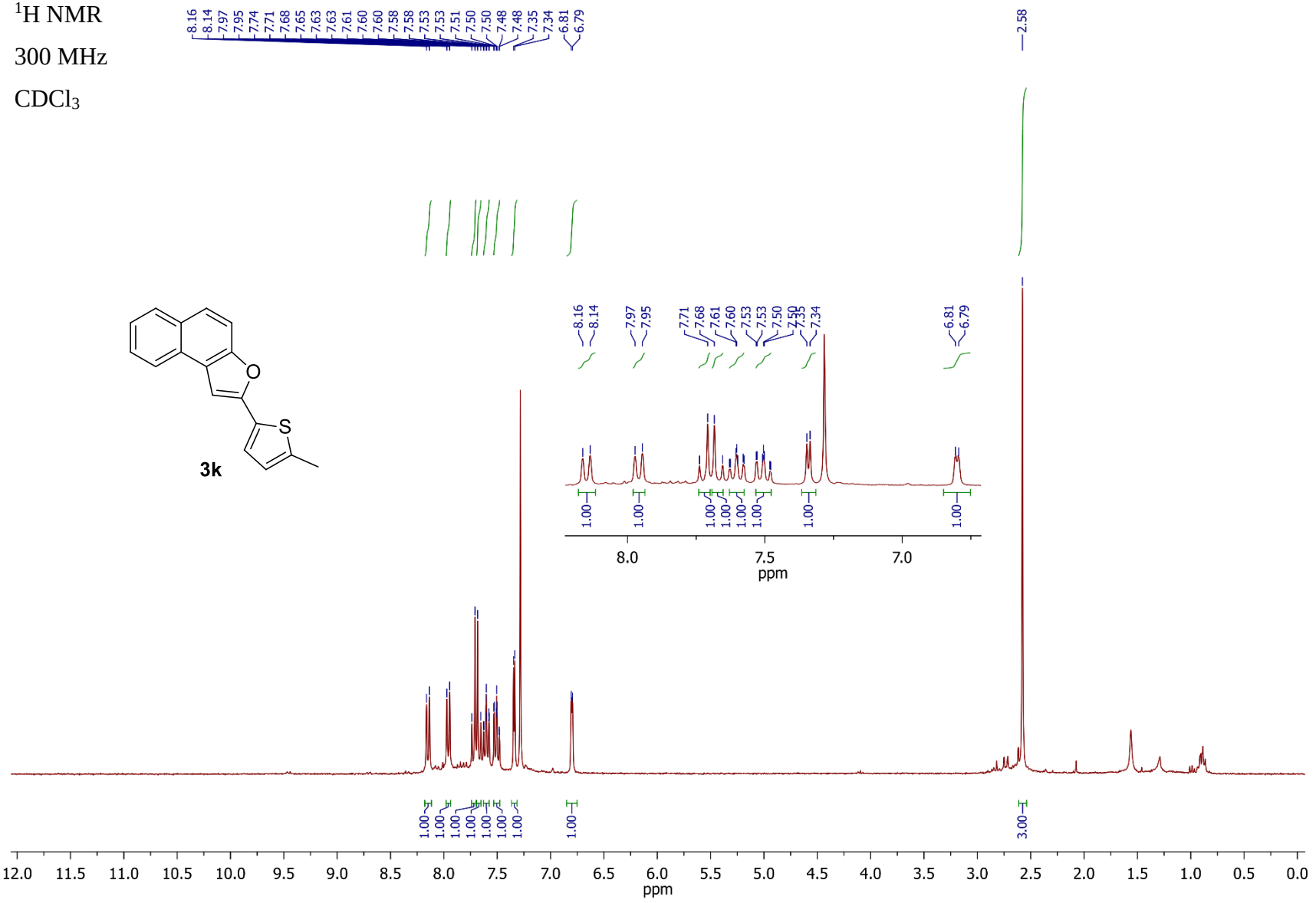
$CDCl_3$



^{1}H NMR

300 MHz

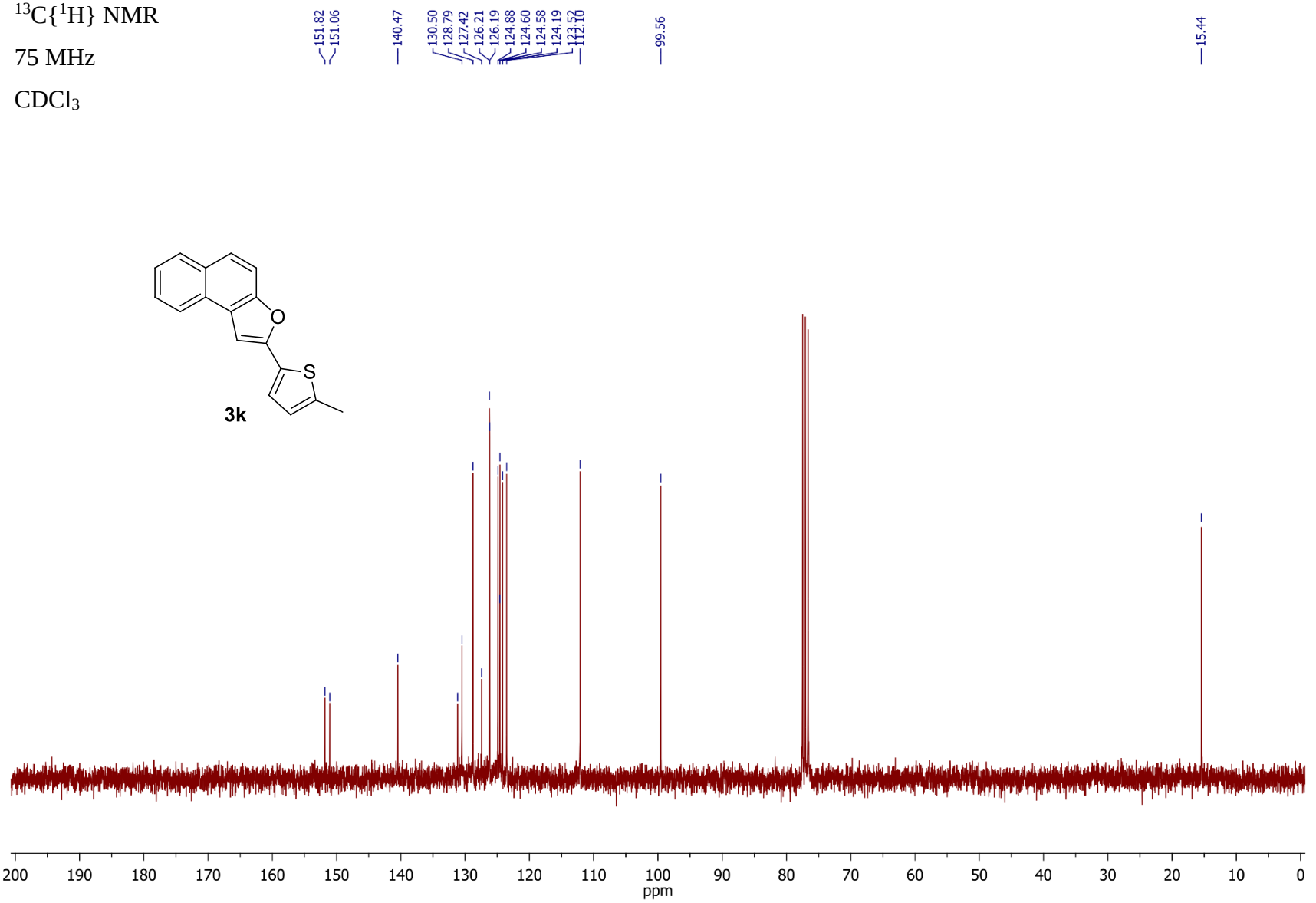
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

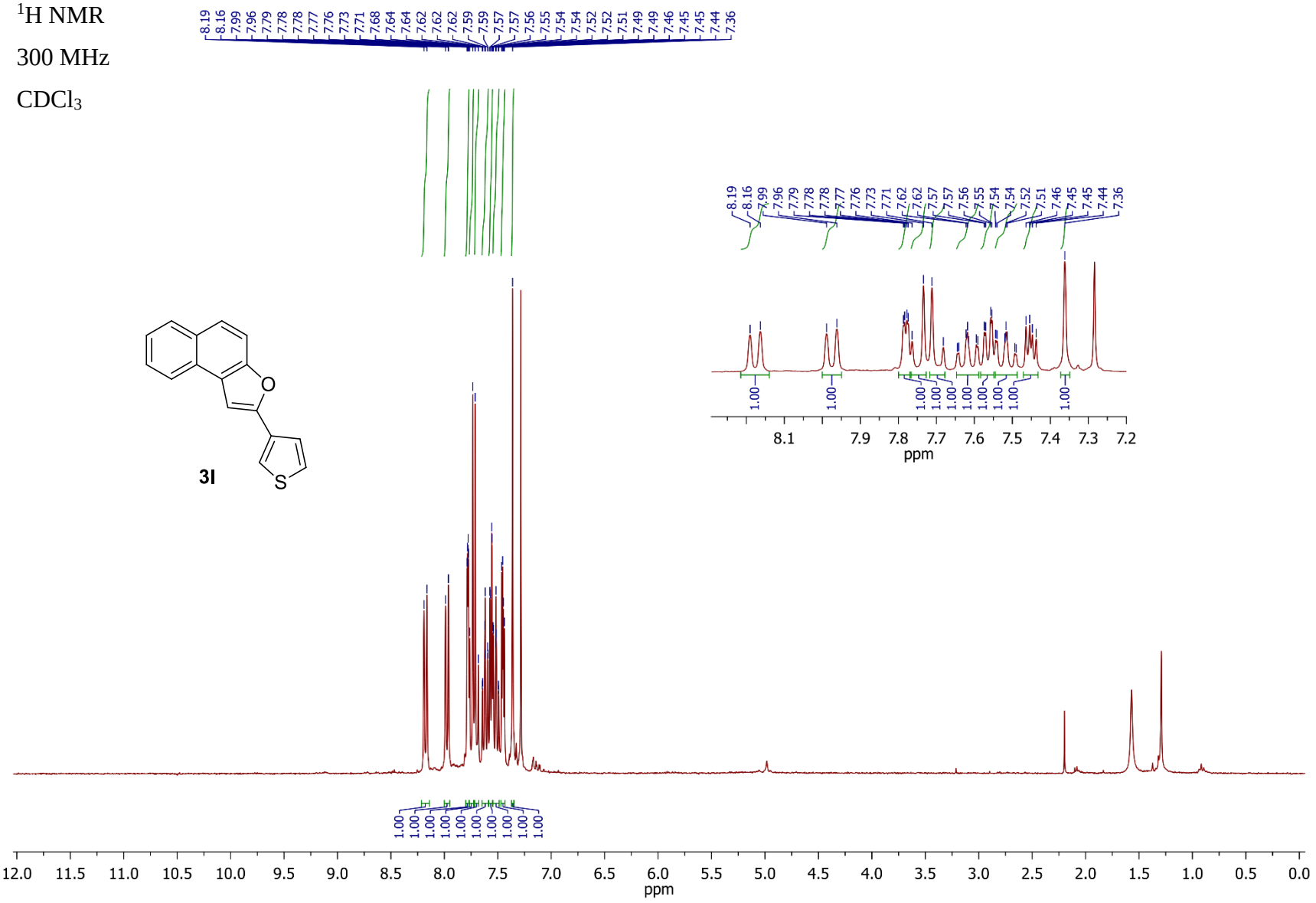
$CDCl_3$



^{1}H NMR

300 MHz

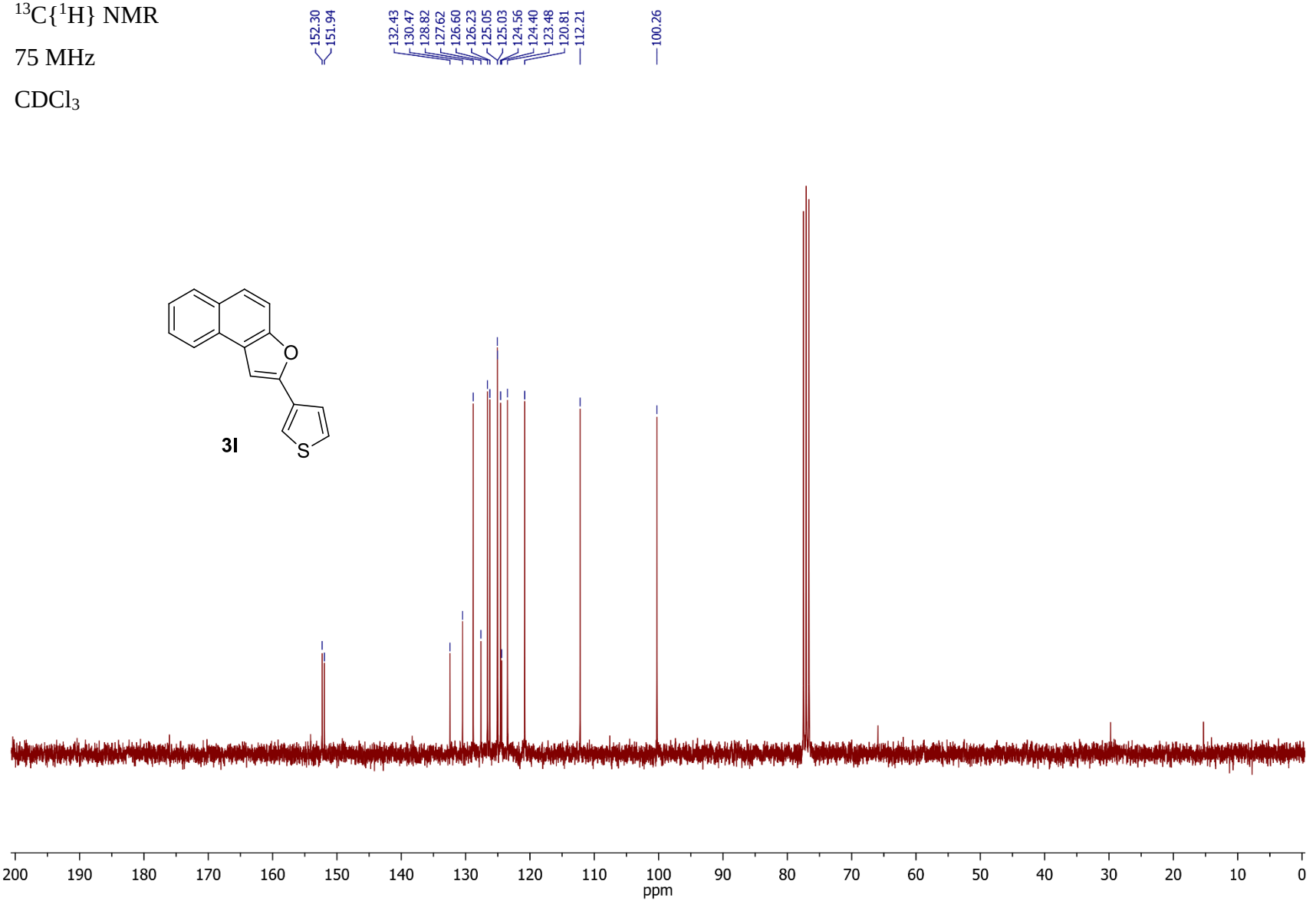
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

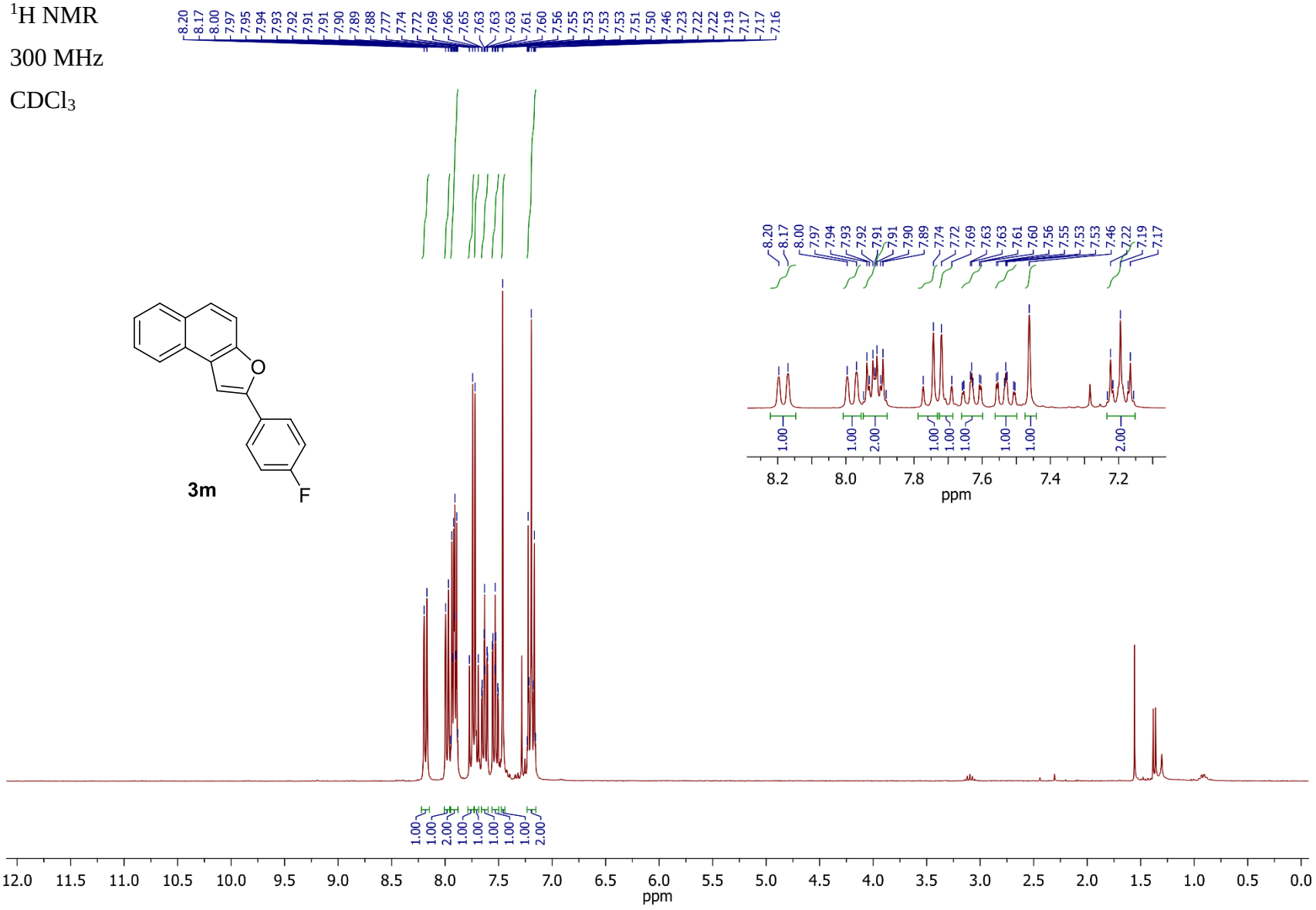
$CDCl_3$



^{1}H NMR

300 MHz

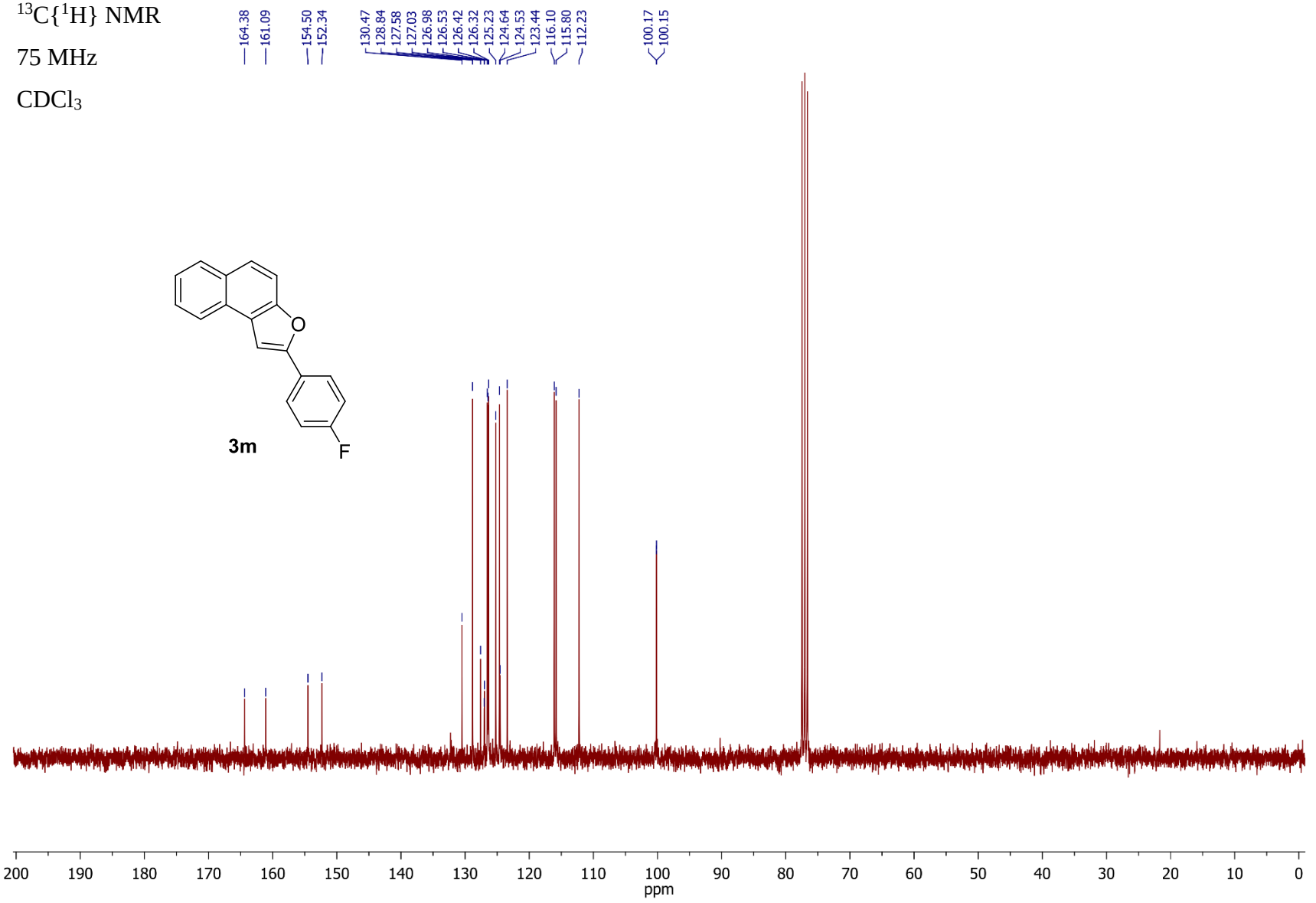
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

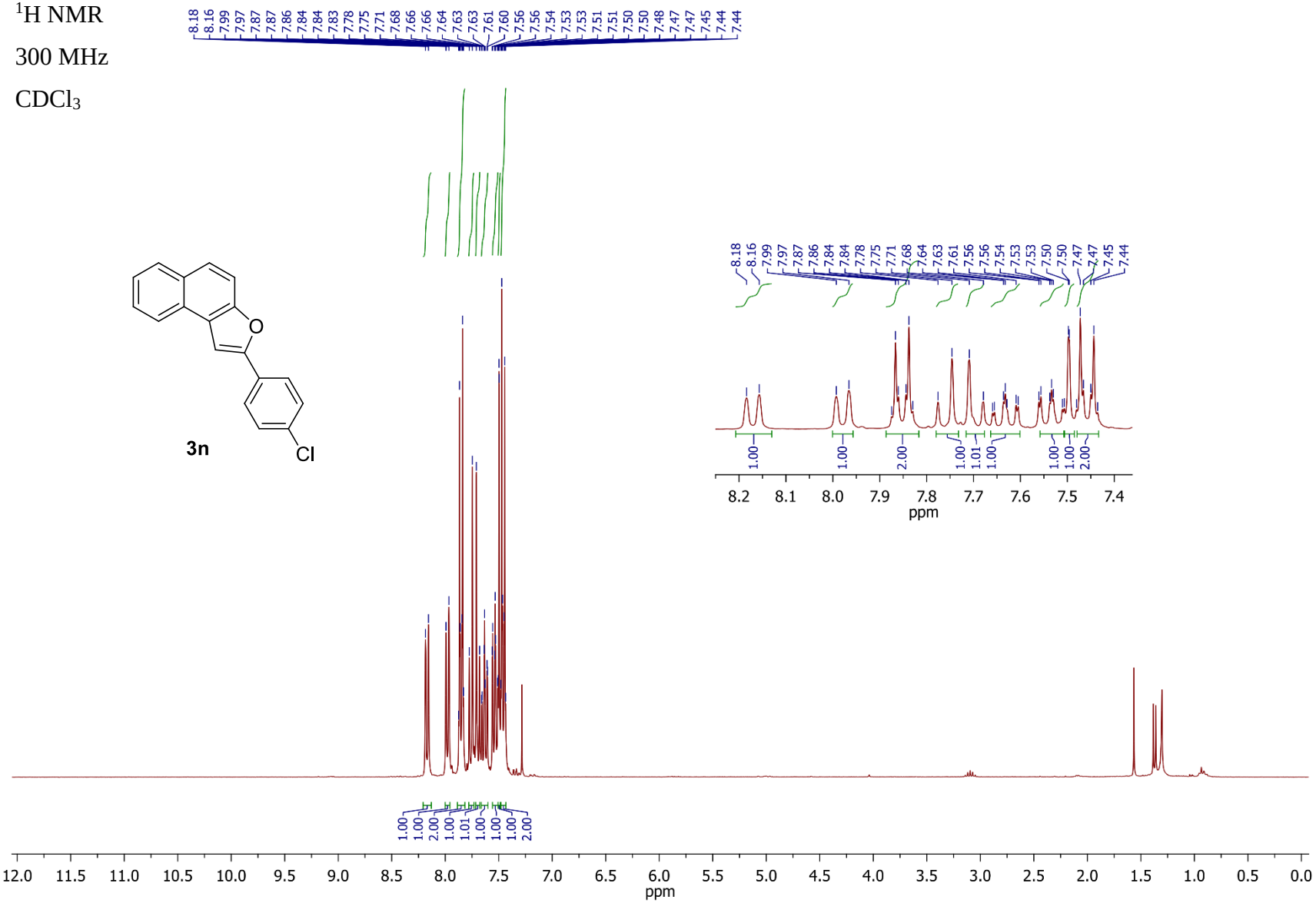
$CDCl_3$



^{1}H NMR

300 MHz

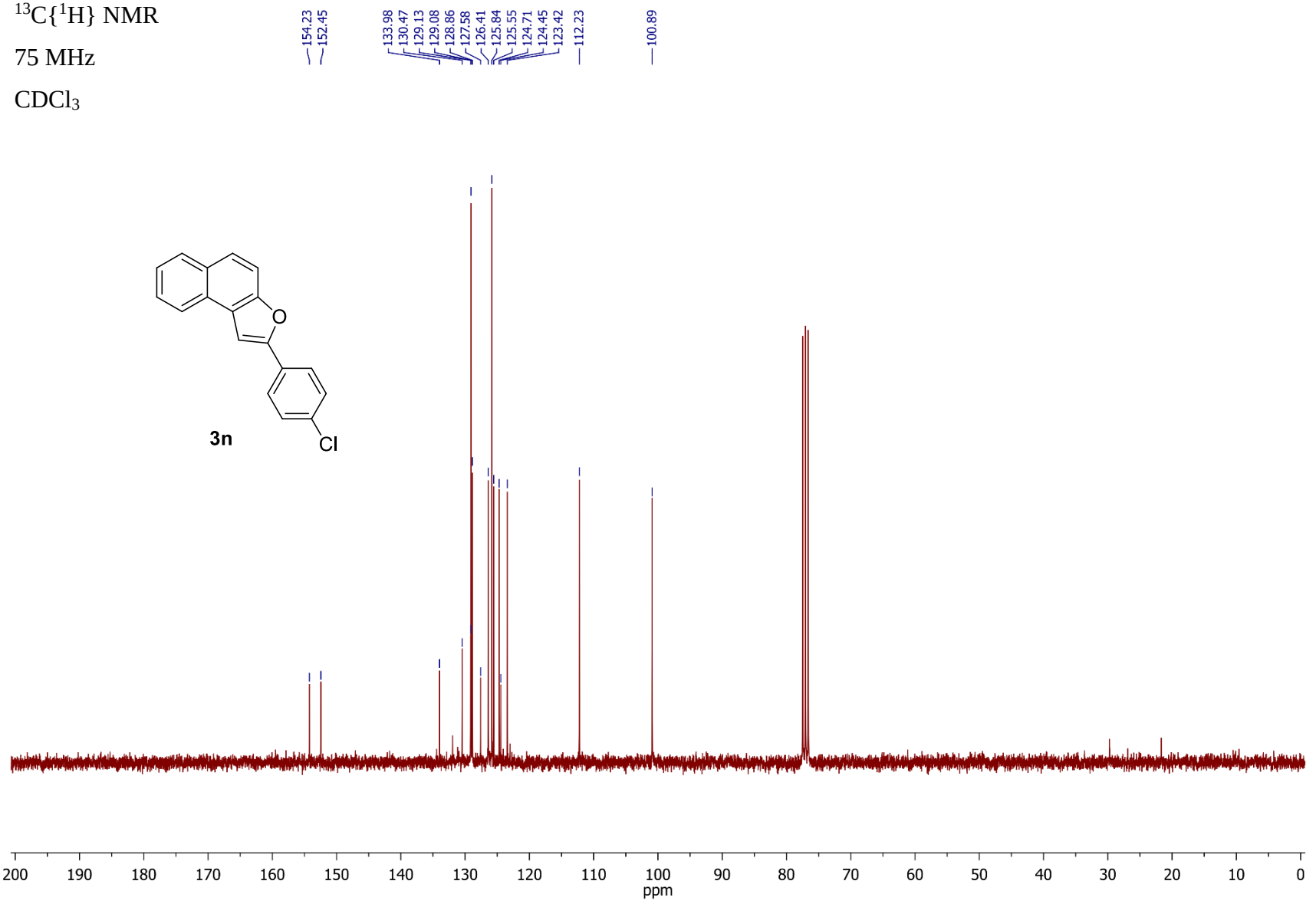
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

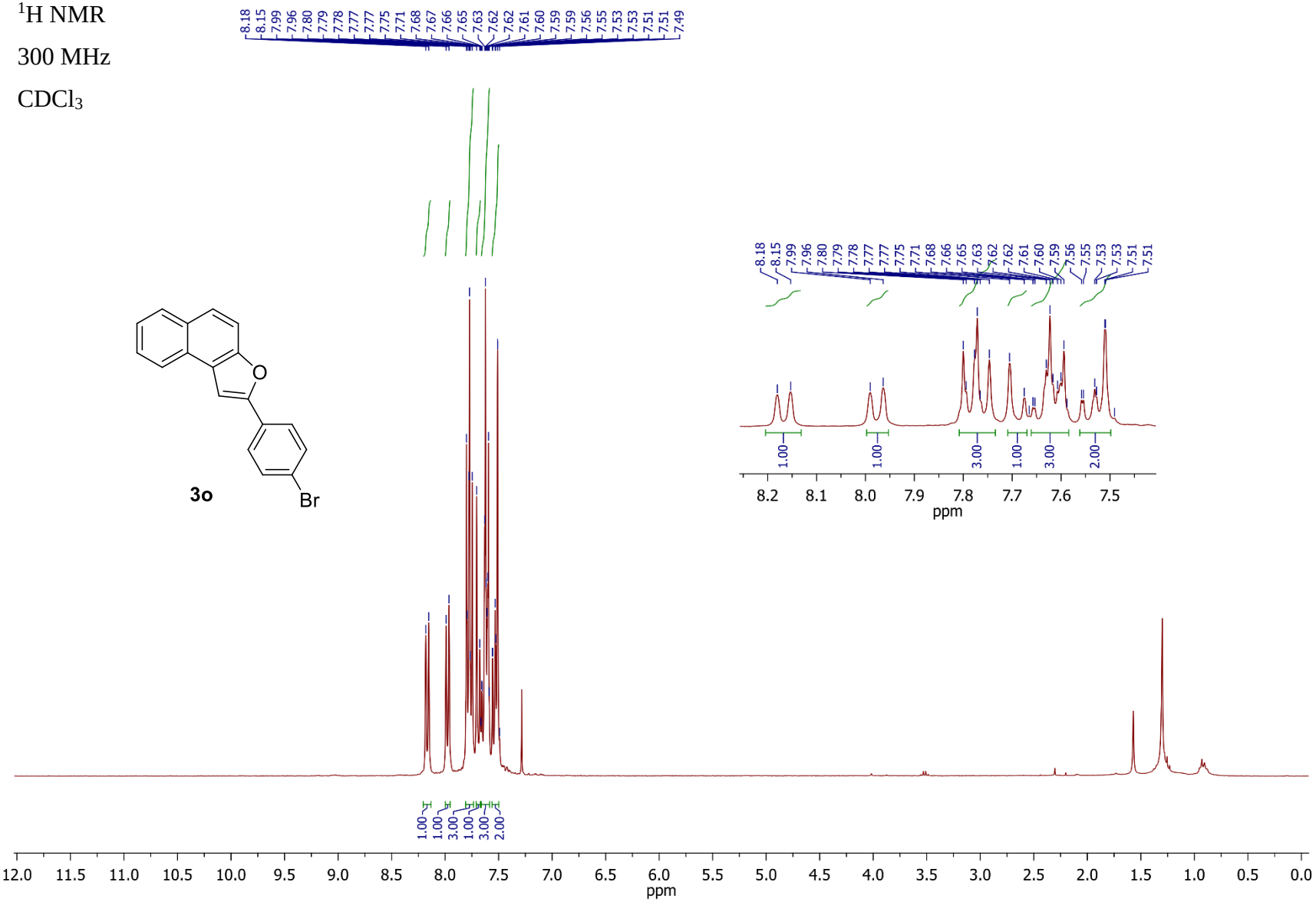
$CDCl_3$



^{1}H NMR

300 MHz

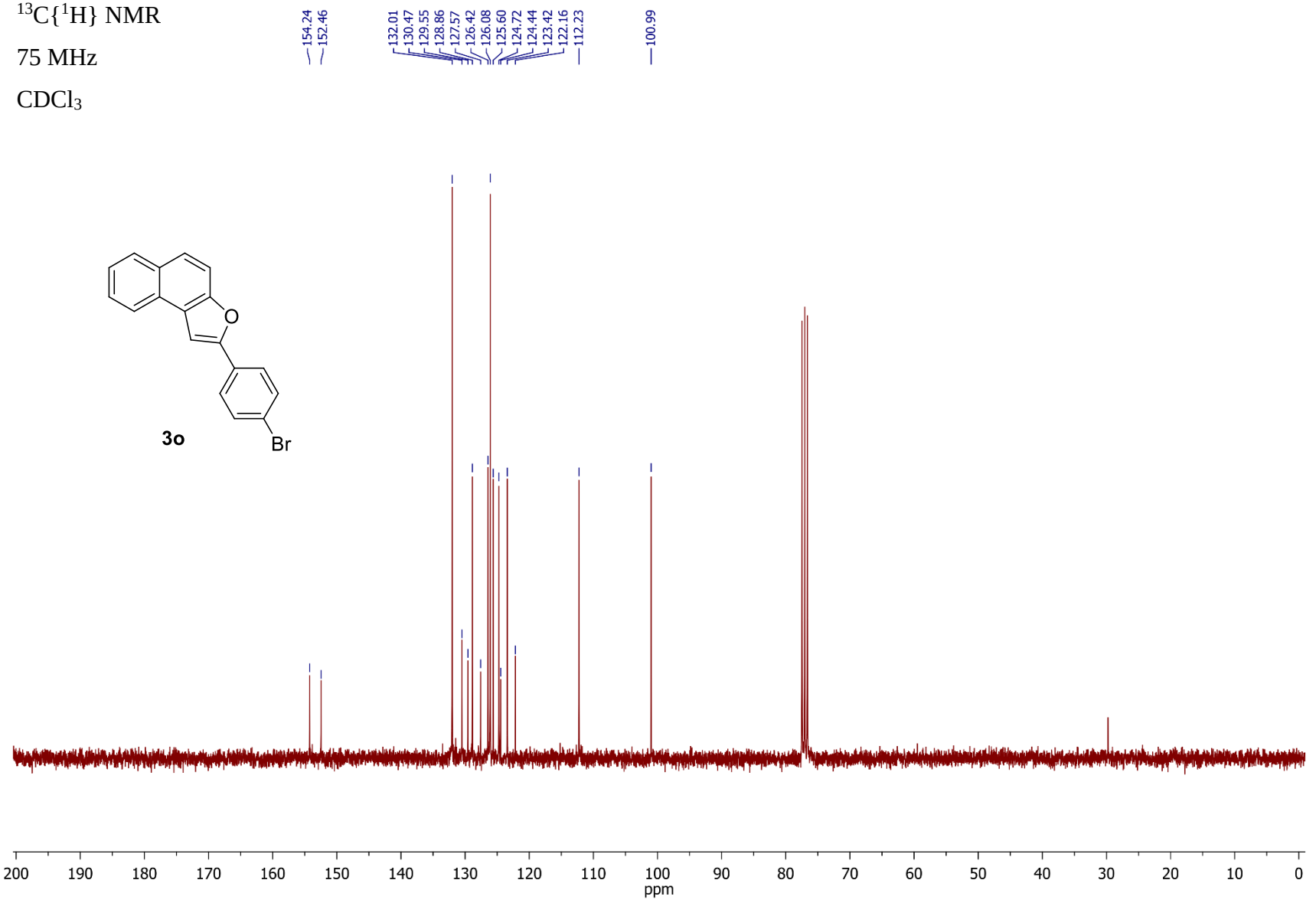
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

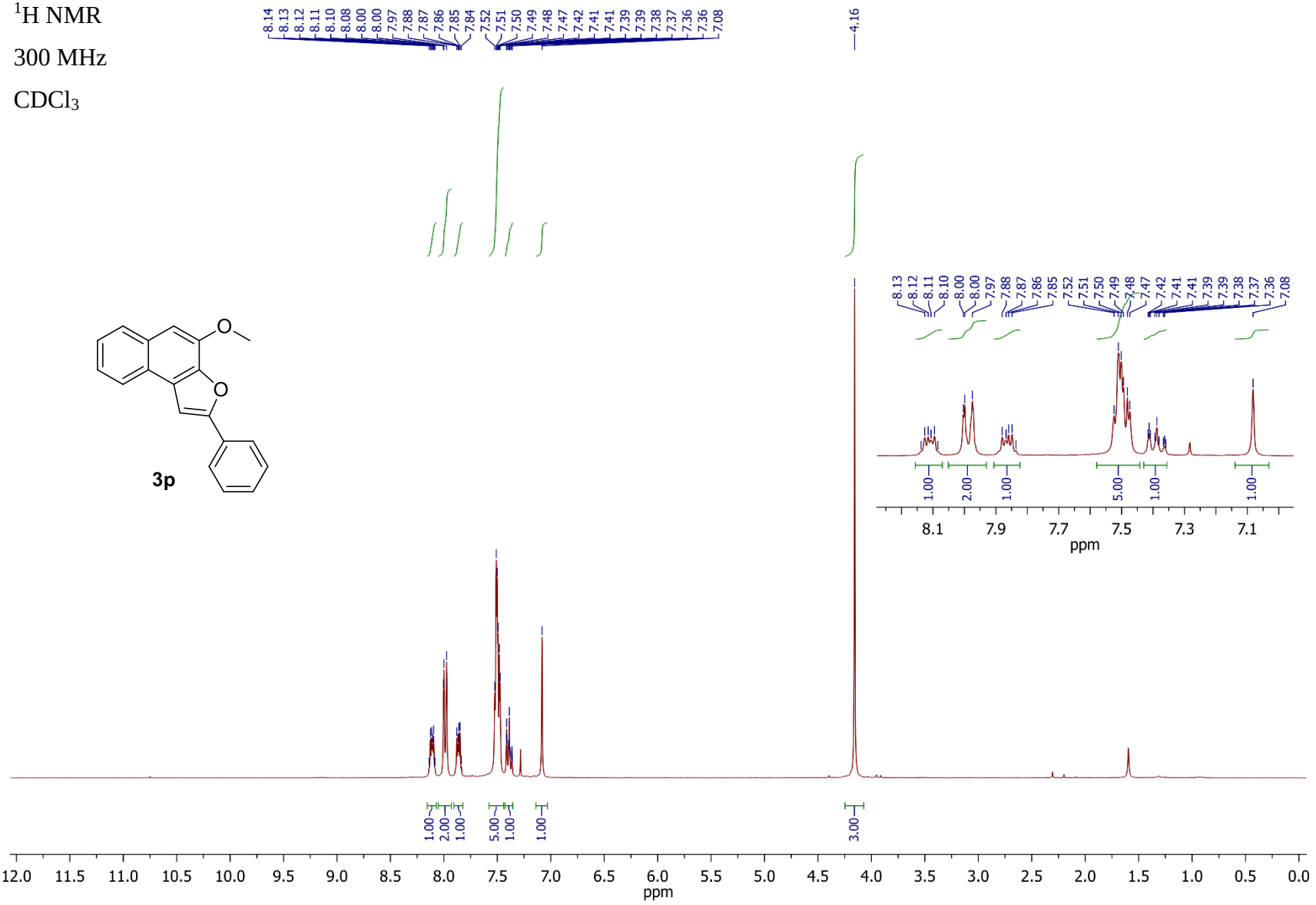
$CDCl_3$



^{1}H NMR

300 MHz

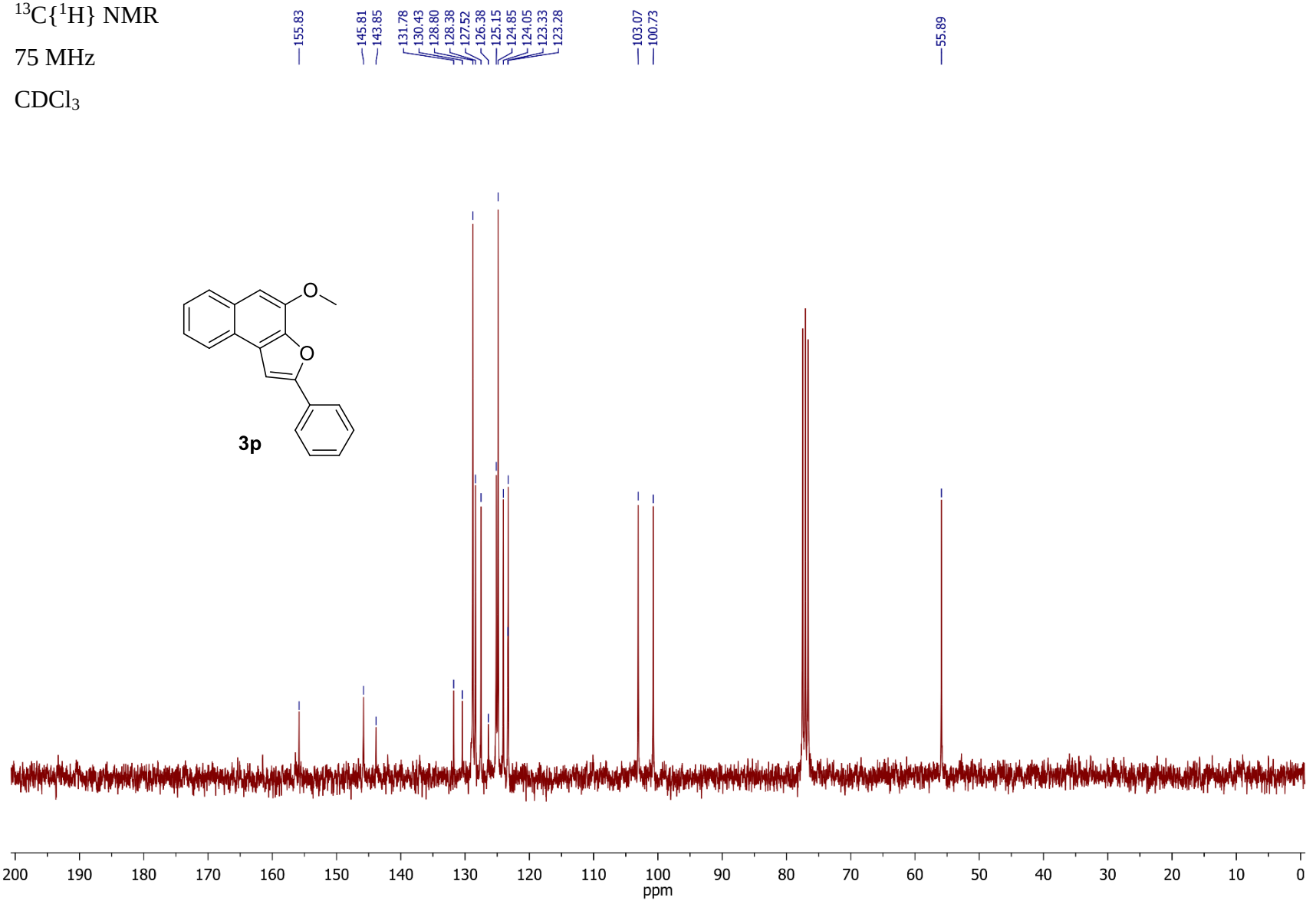
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

$CDCl_3$



^{1}H NMR

300 MHz

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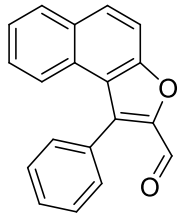

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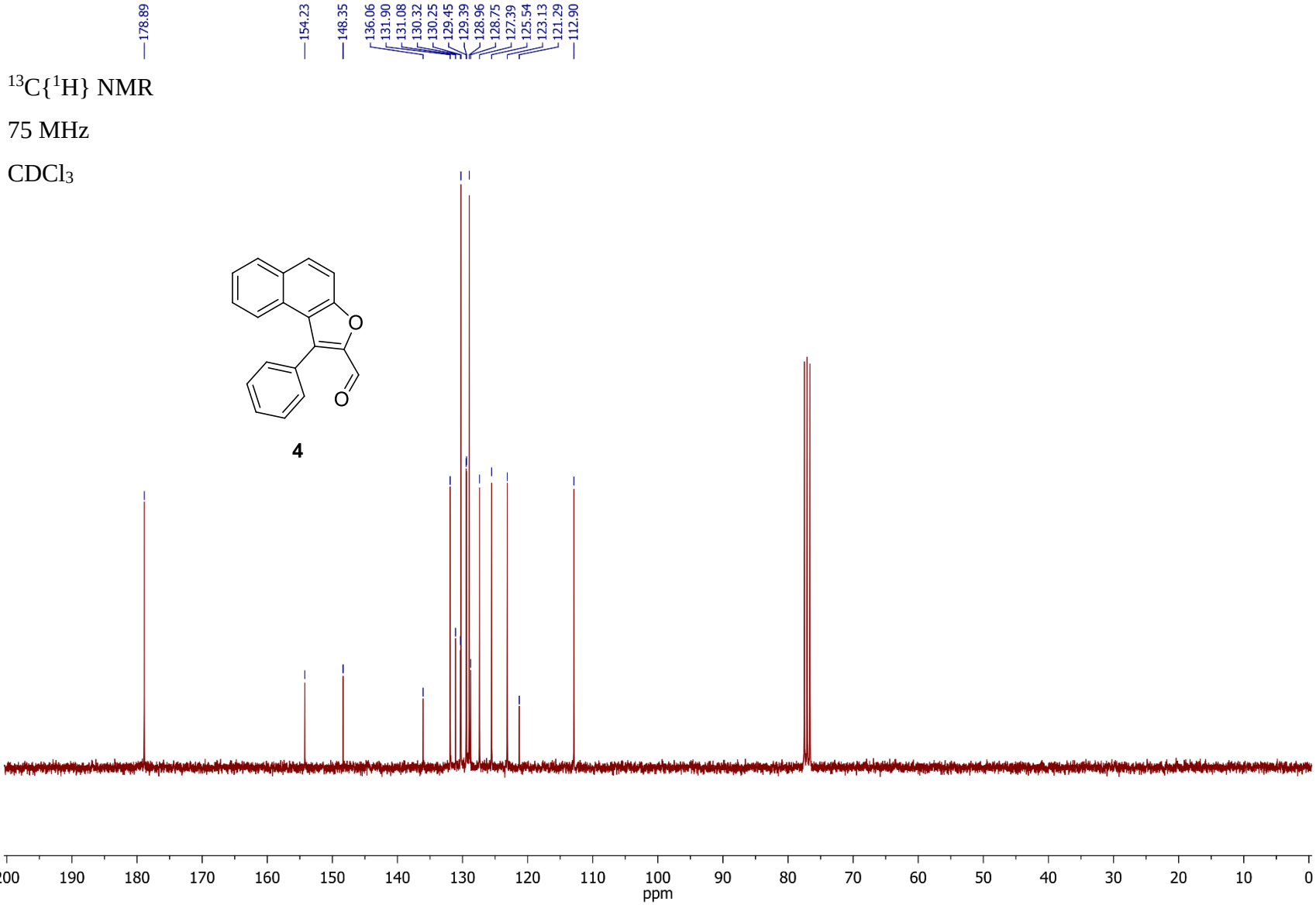


$^{13}C\{^{1}H\}$ NMR

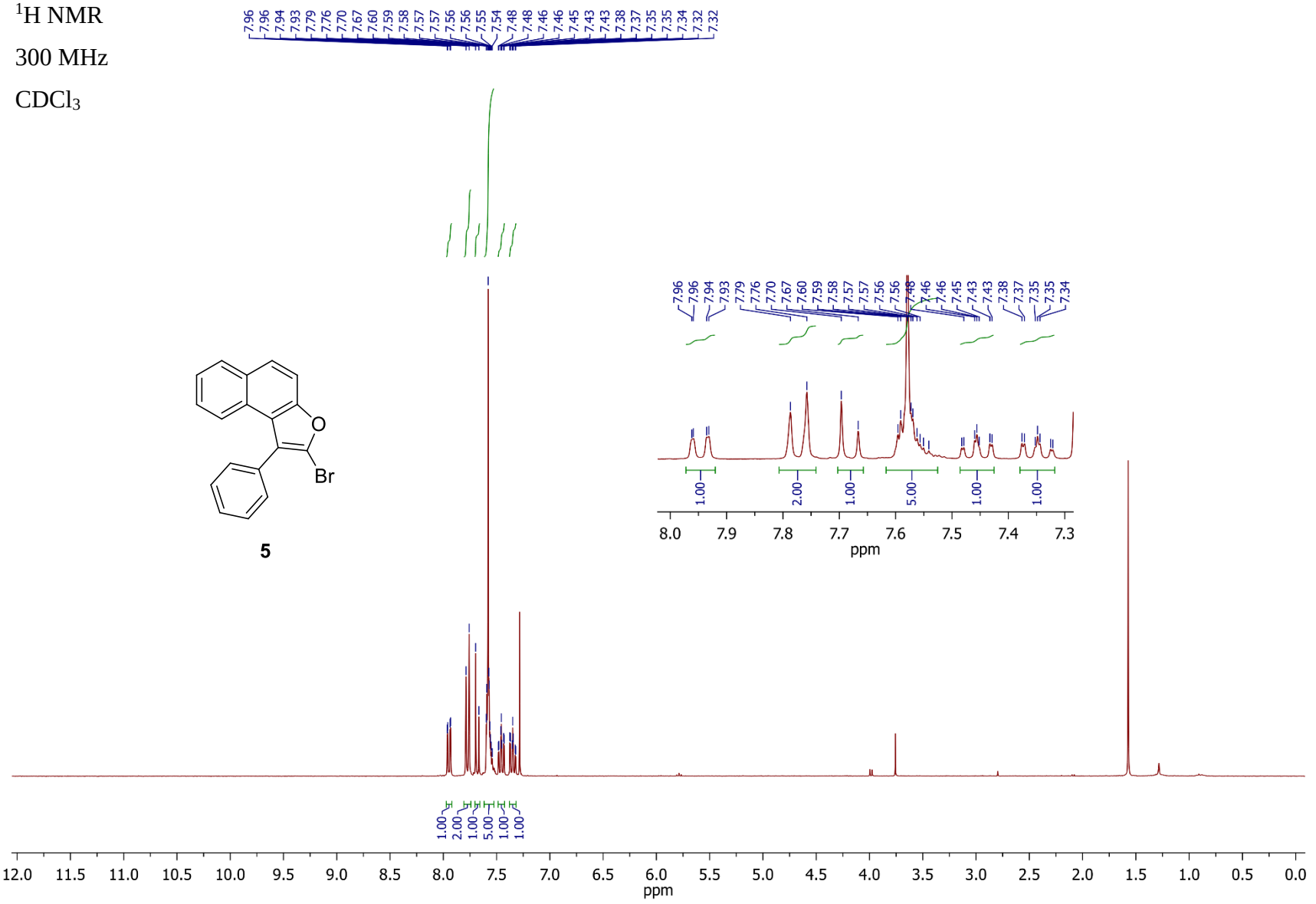
75 MHz

$CDCl_3$

^{1}H NMR

300 MHz

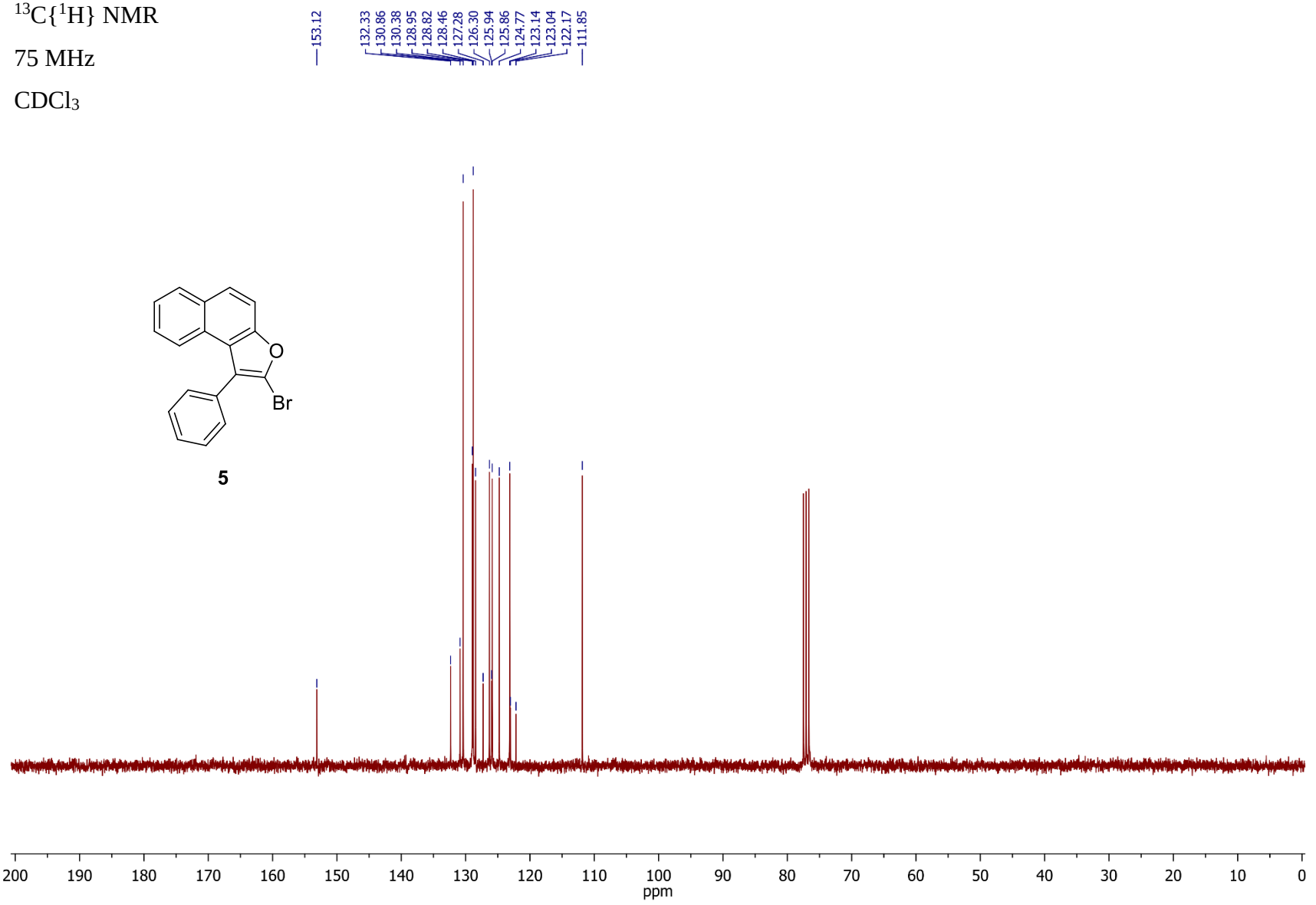
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

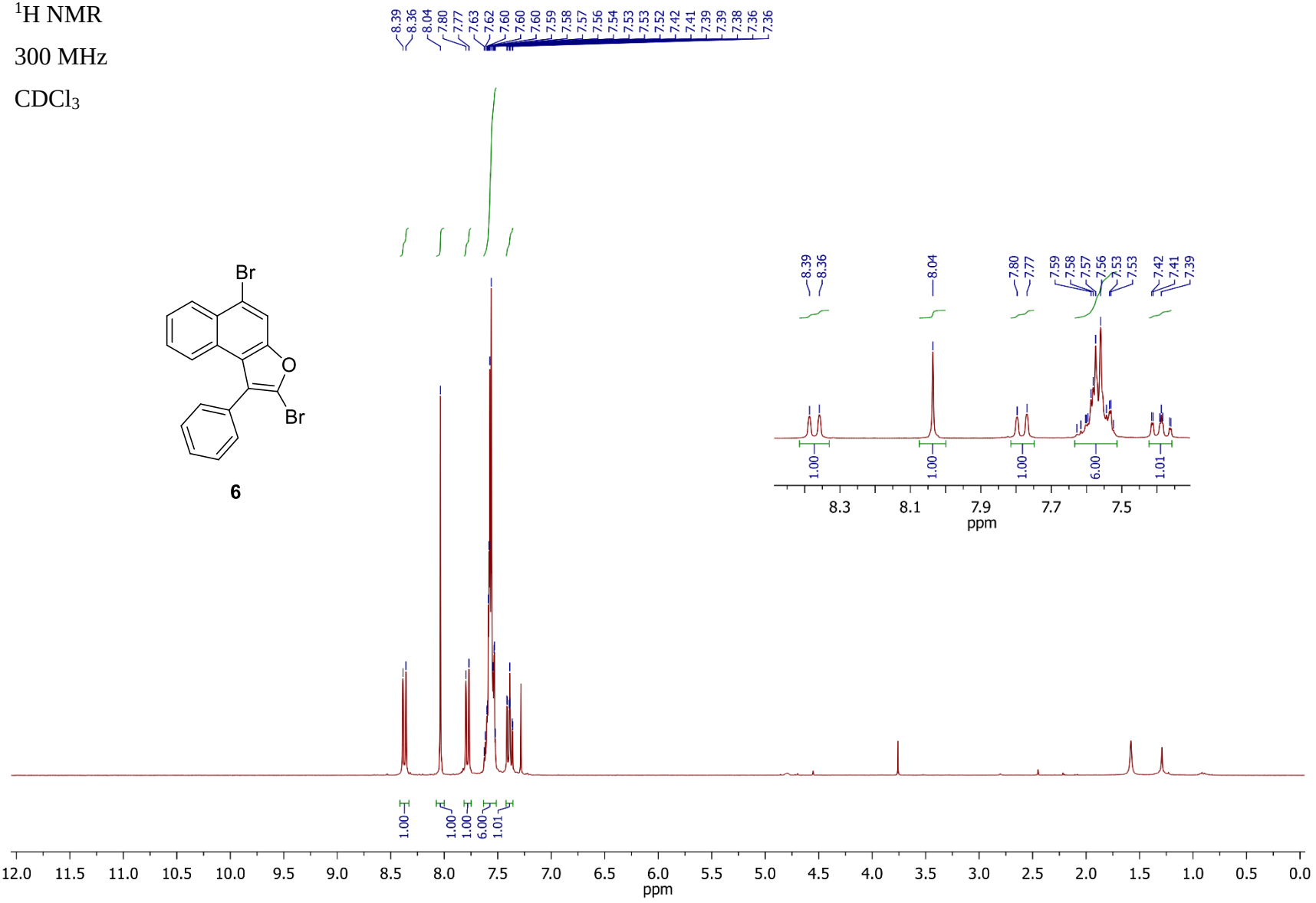
$CDCl_3$



^{1}H NMR

300 MHz

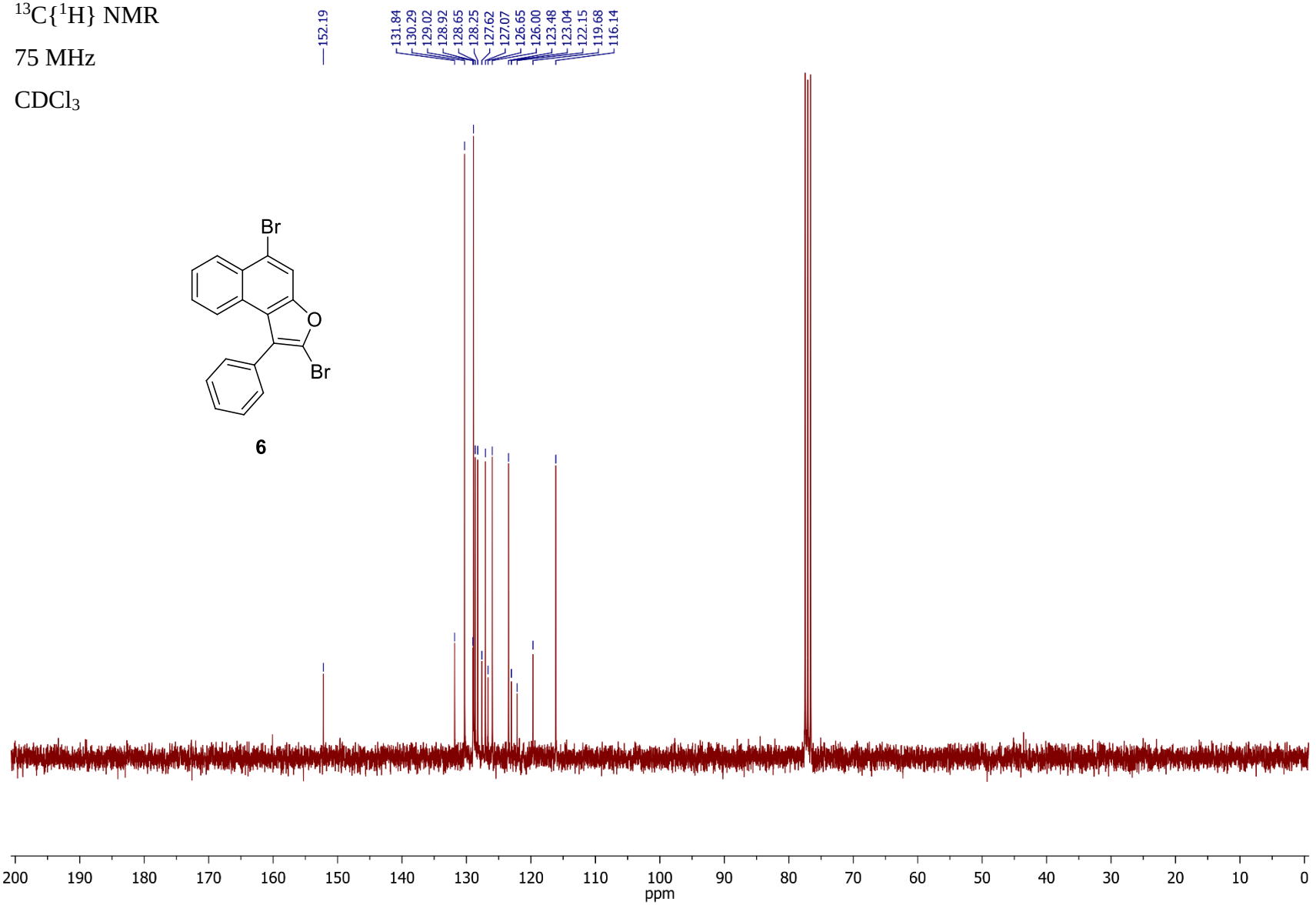
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

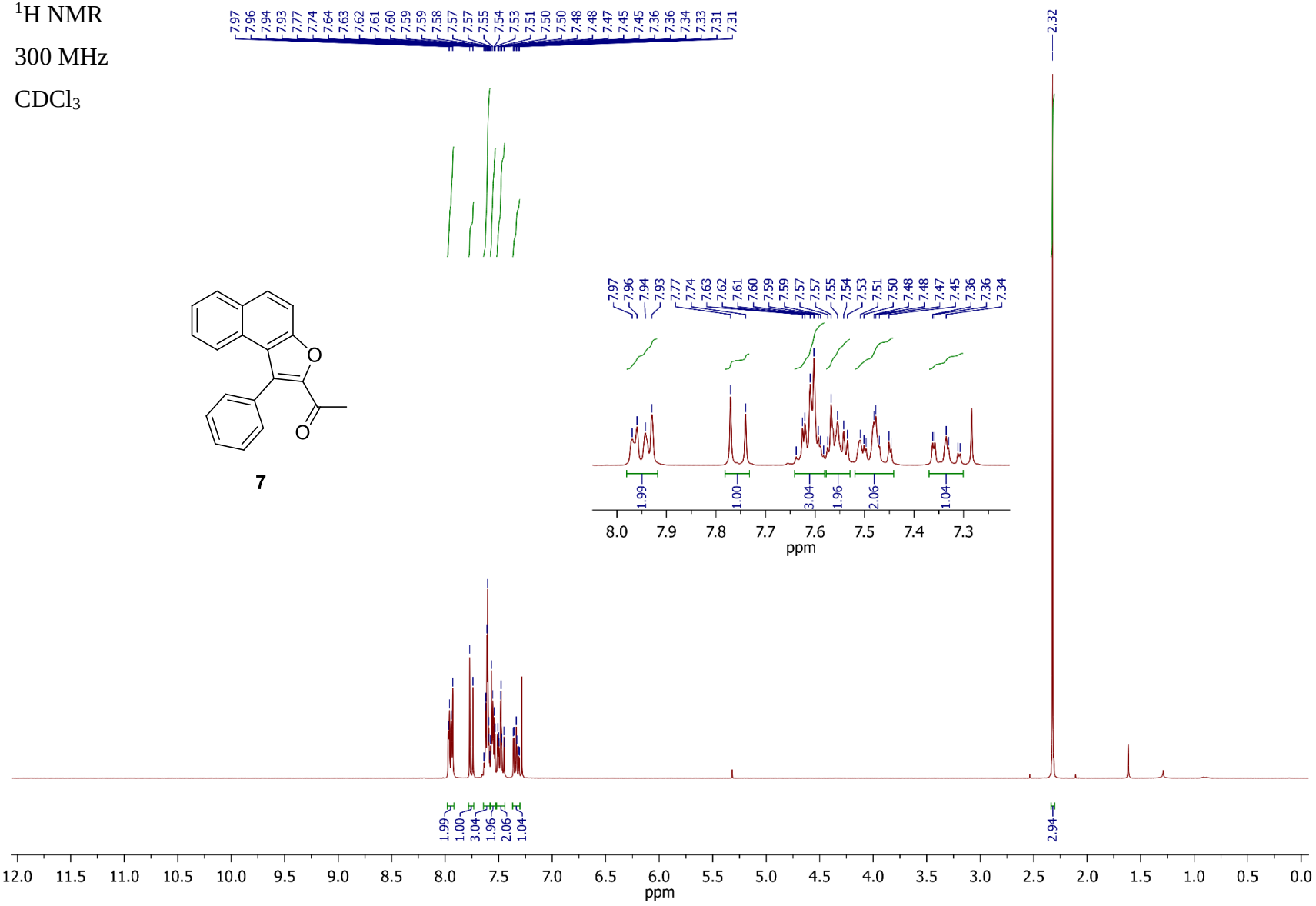
$CDCl_3$



^{1}H NMR

300 MHz

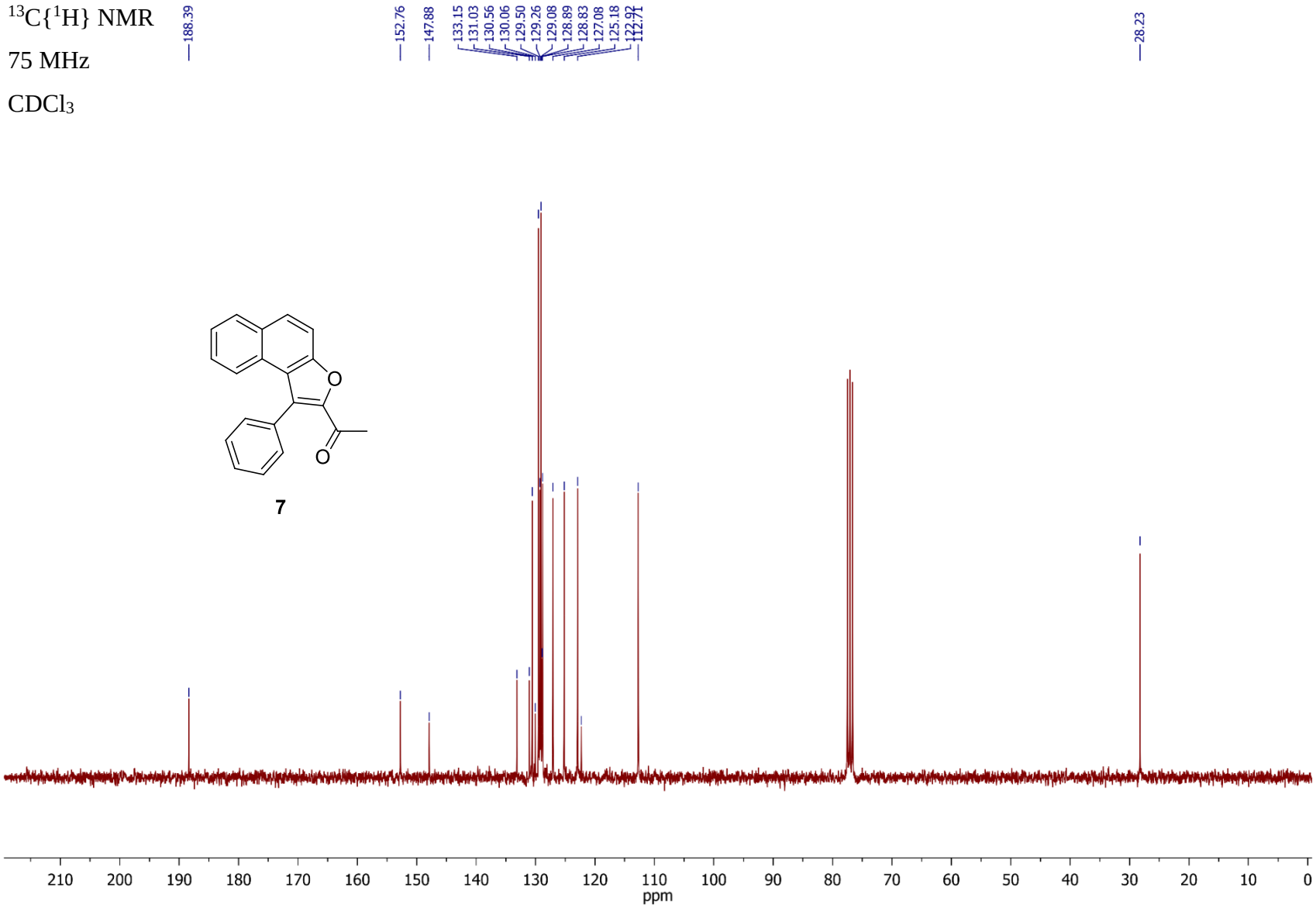
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

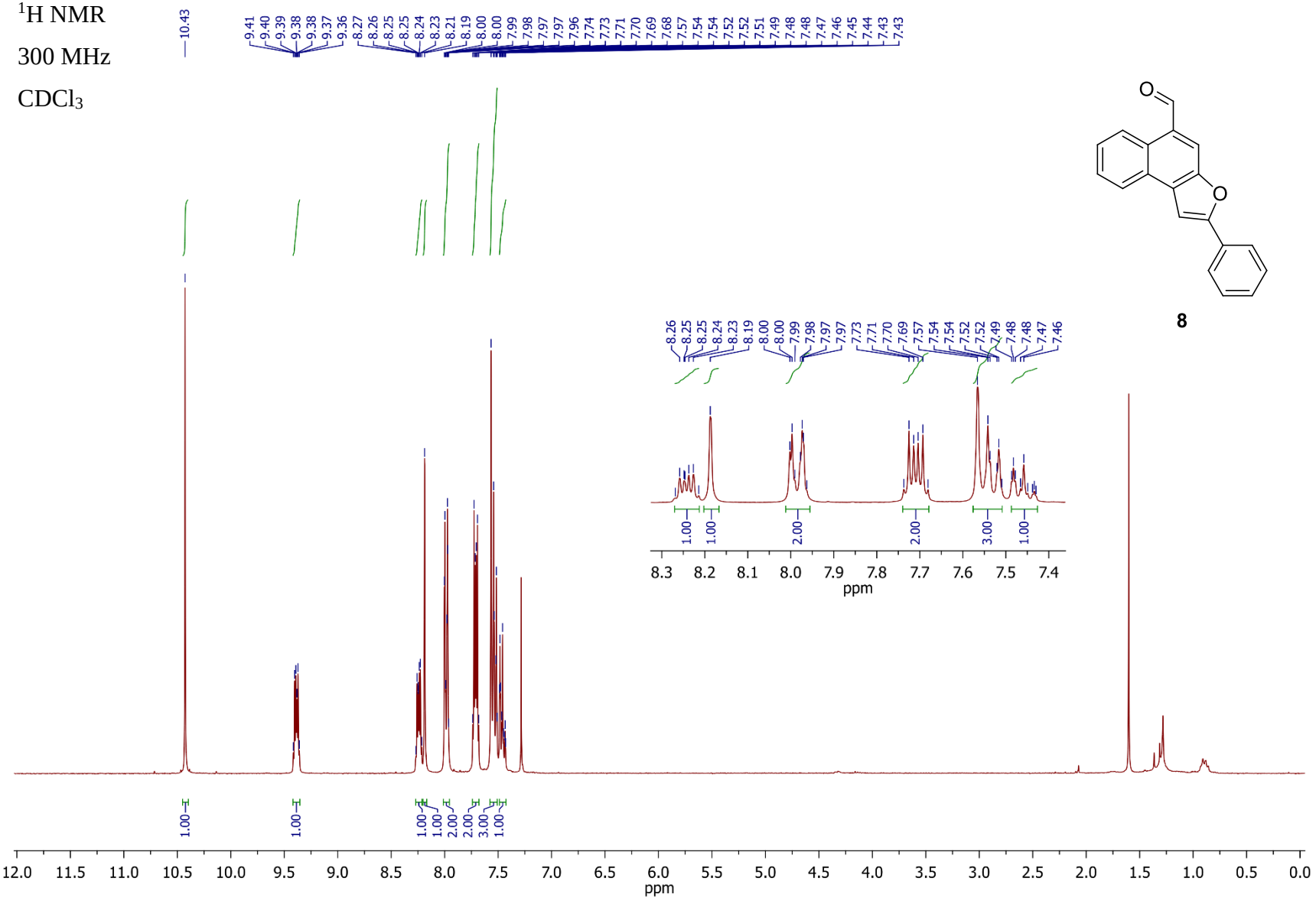
$CDCl_3$



^{1}H NMR

300 MHz

$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

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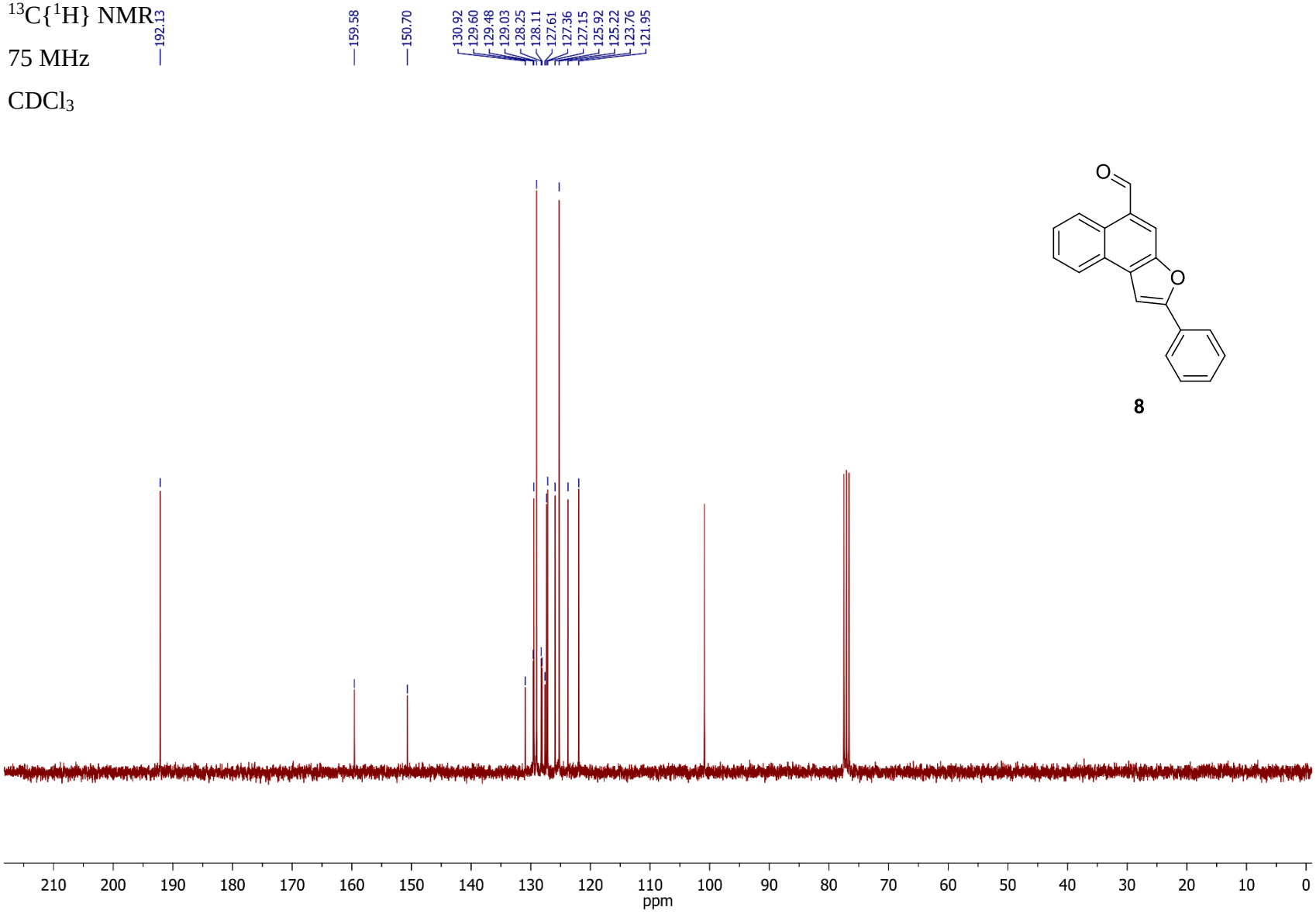
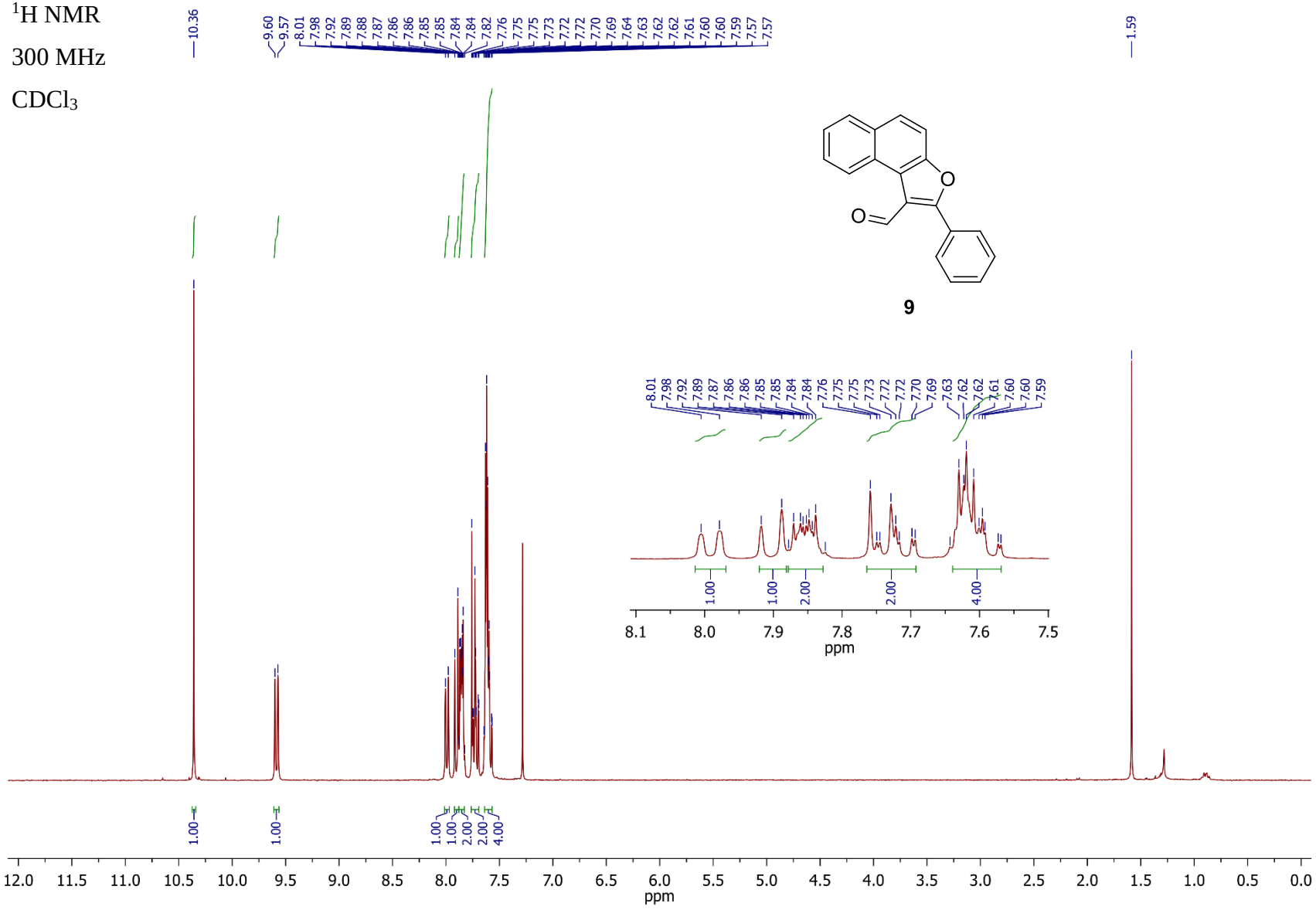


^{1}H NMR

300 MHz

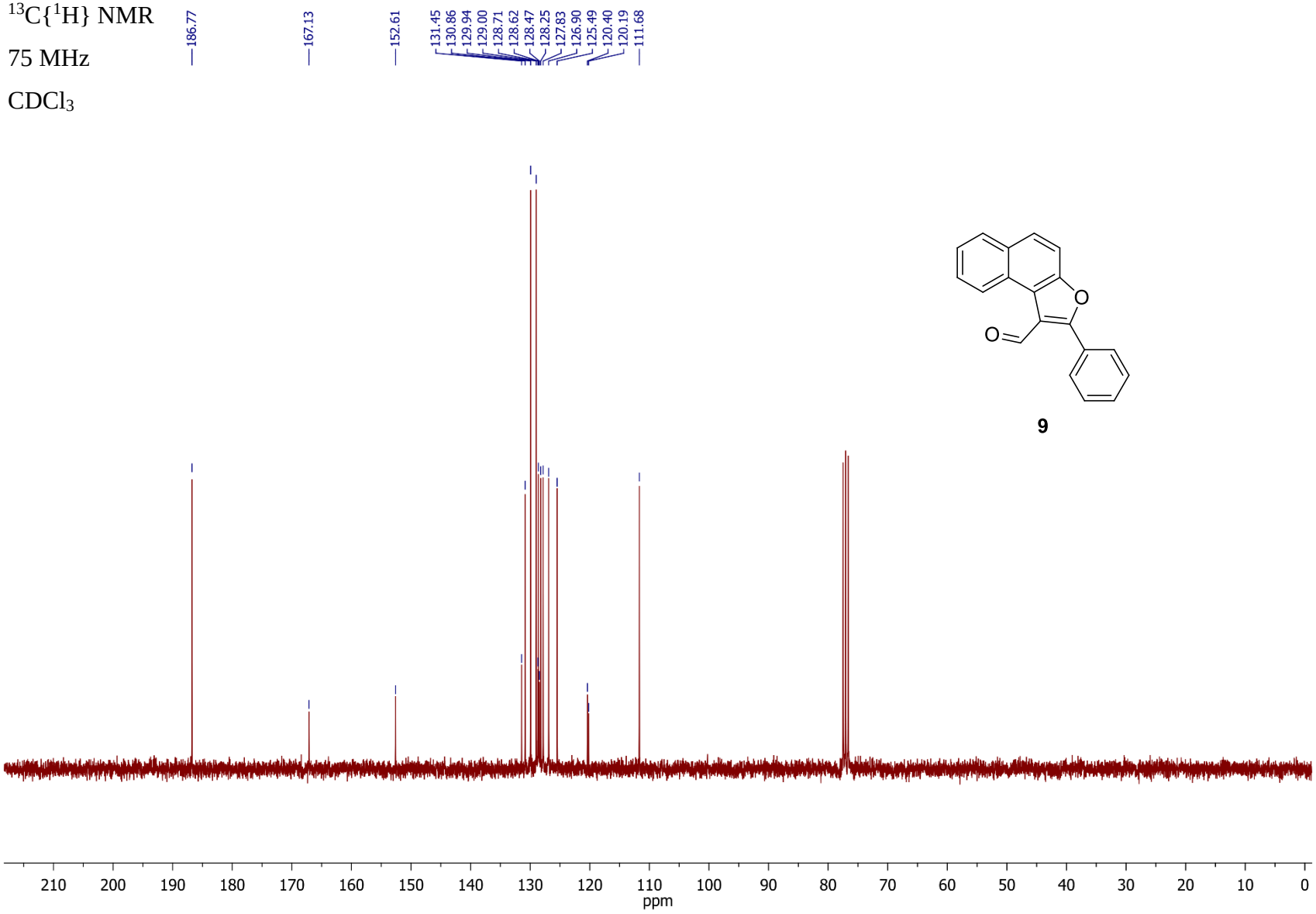
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

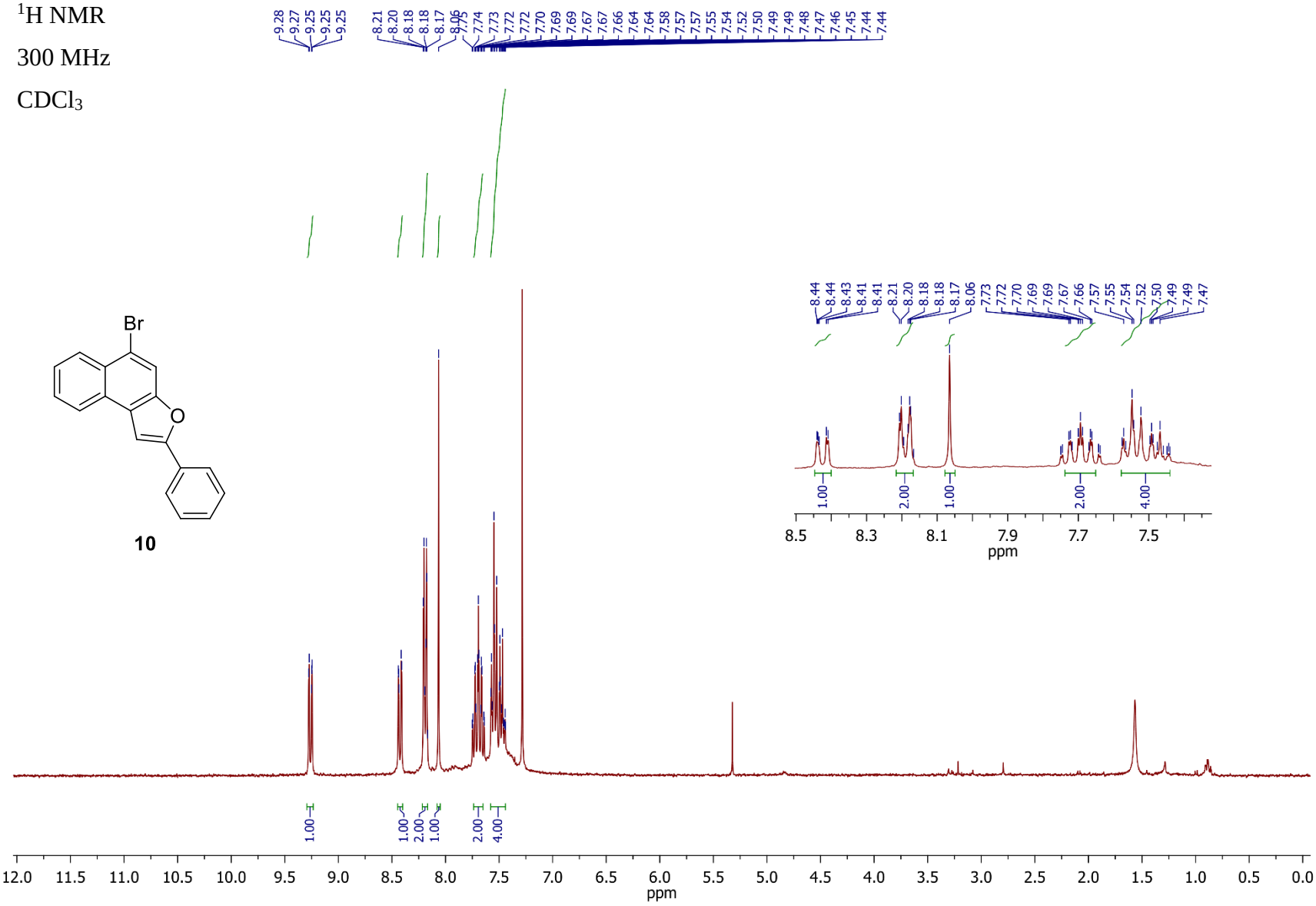
$CDCl_3$



^{1}H NMR

300 MHz

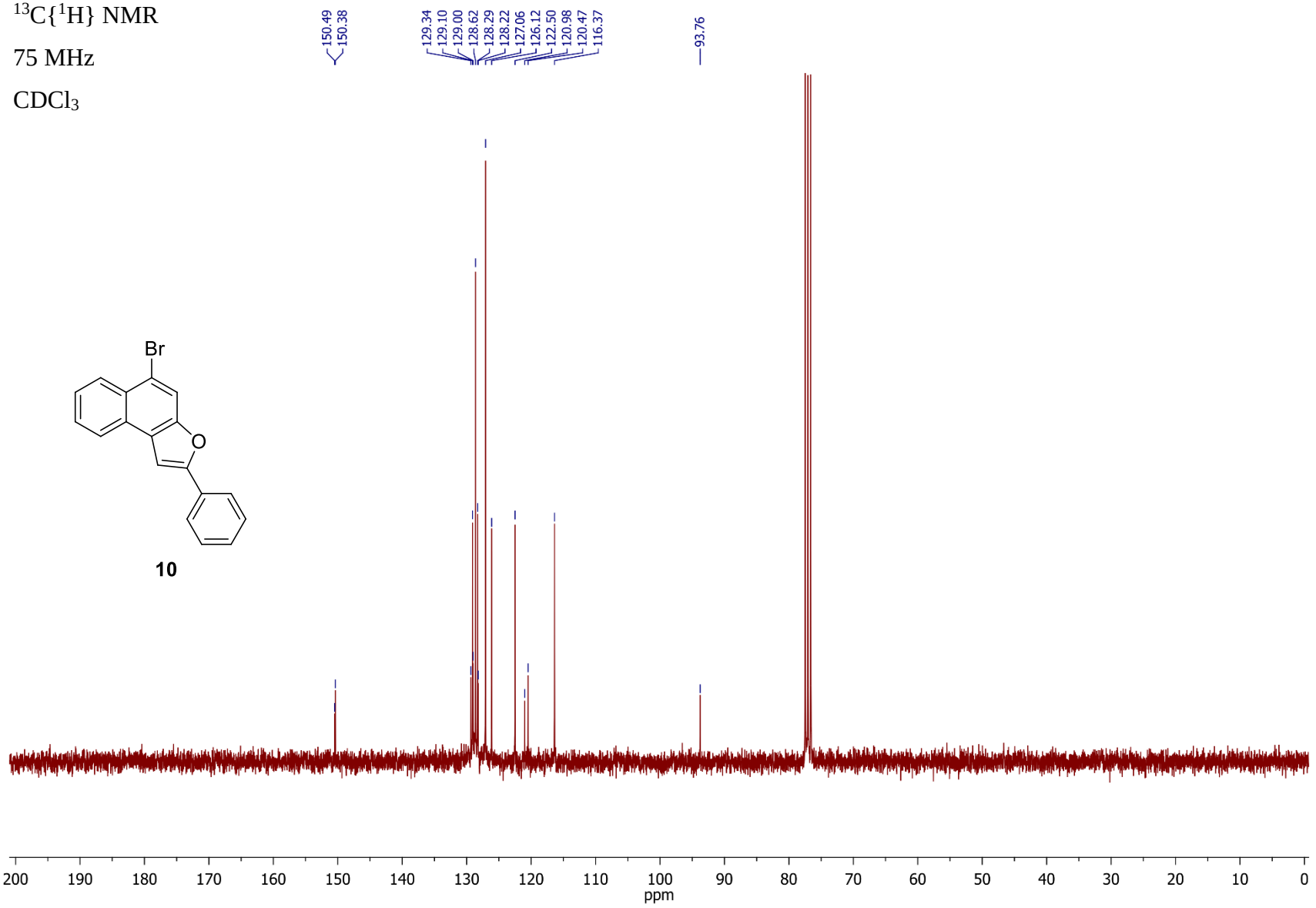
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

$CDCl_3$

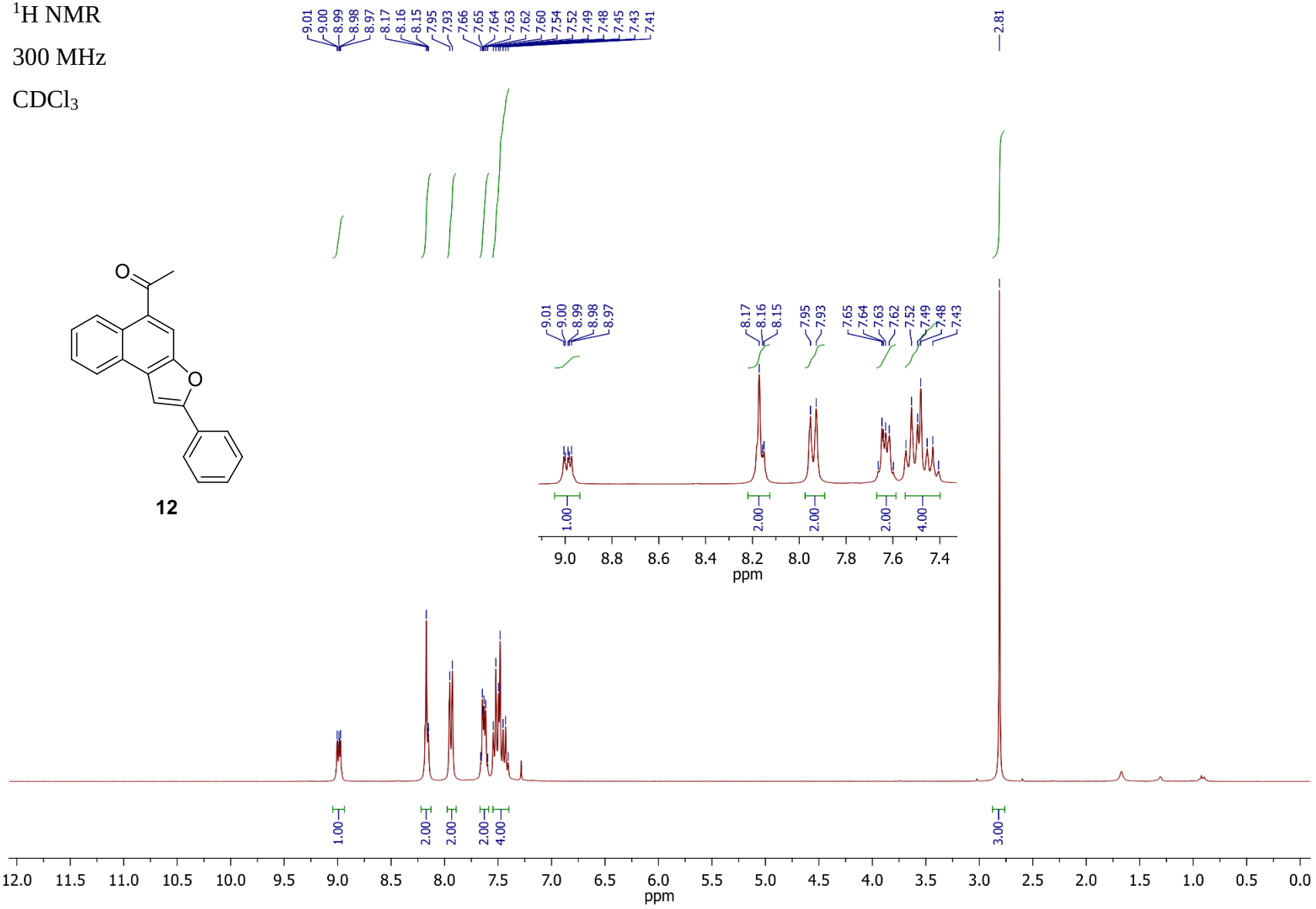


10

^{1}H NMR

300 MHz

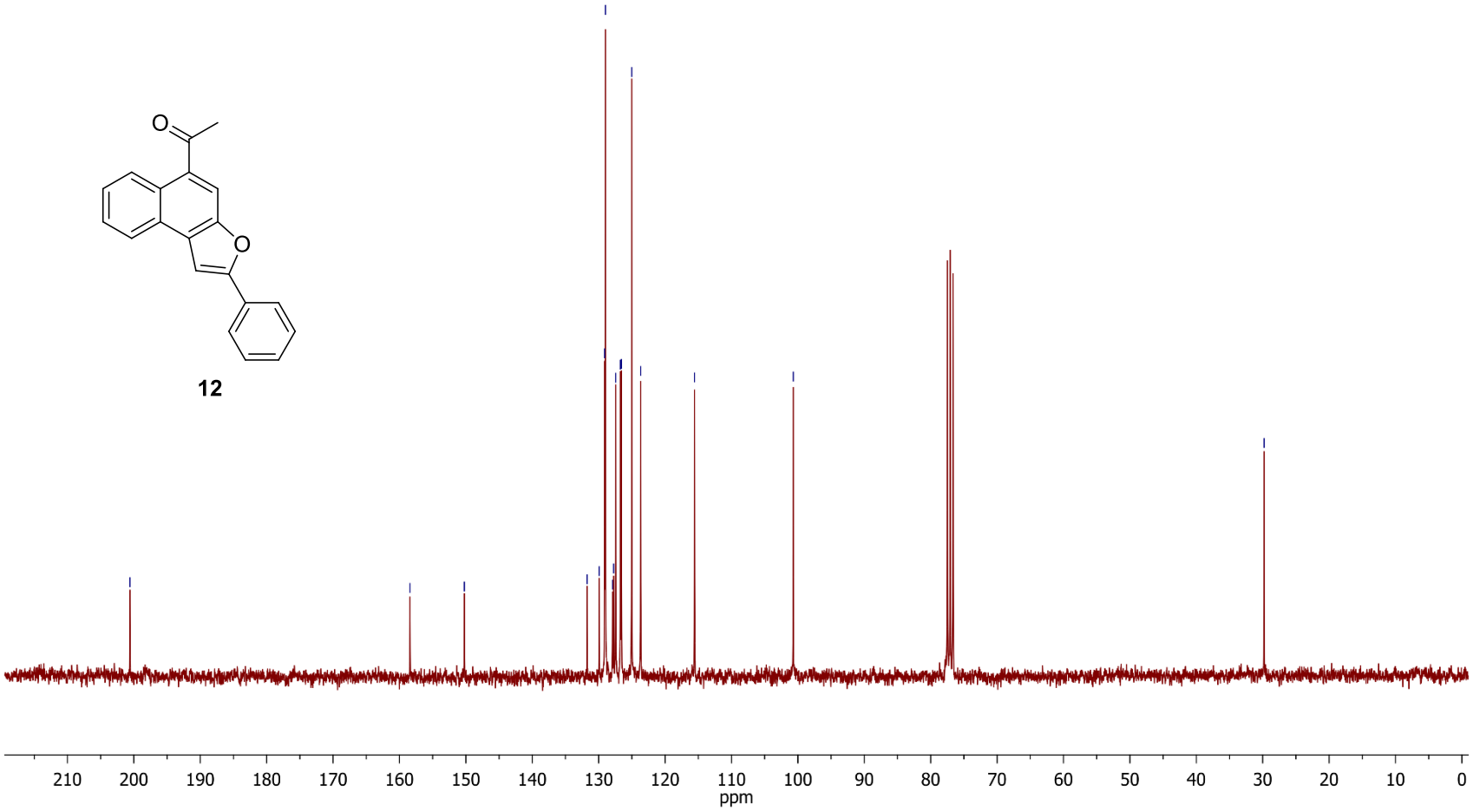
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

$CDCl_3$

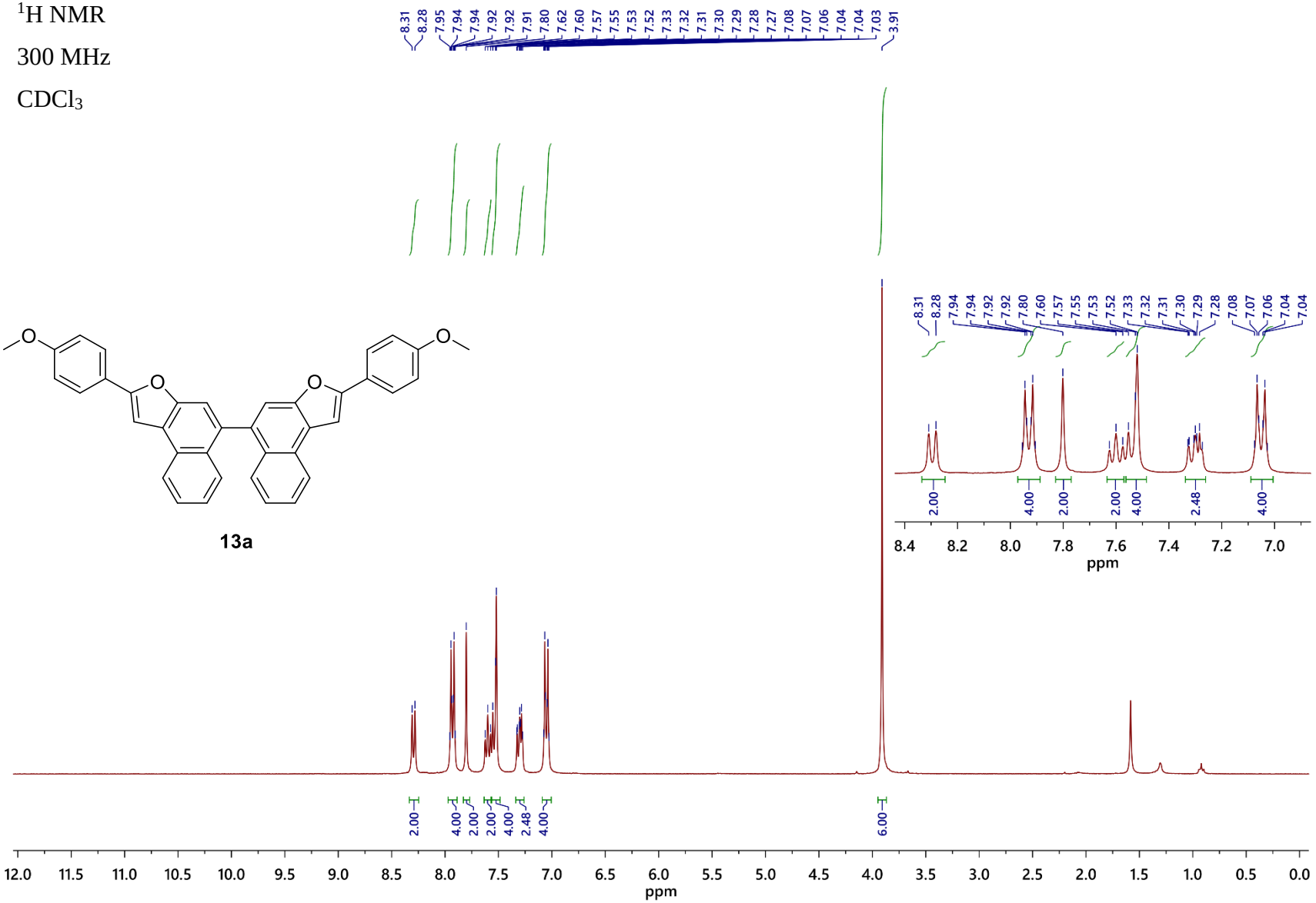


12

^{1}H NMR

300 MHz

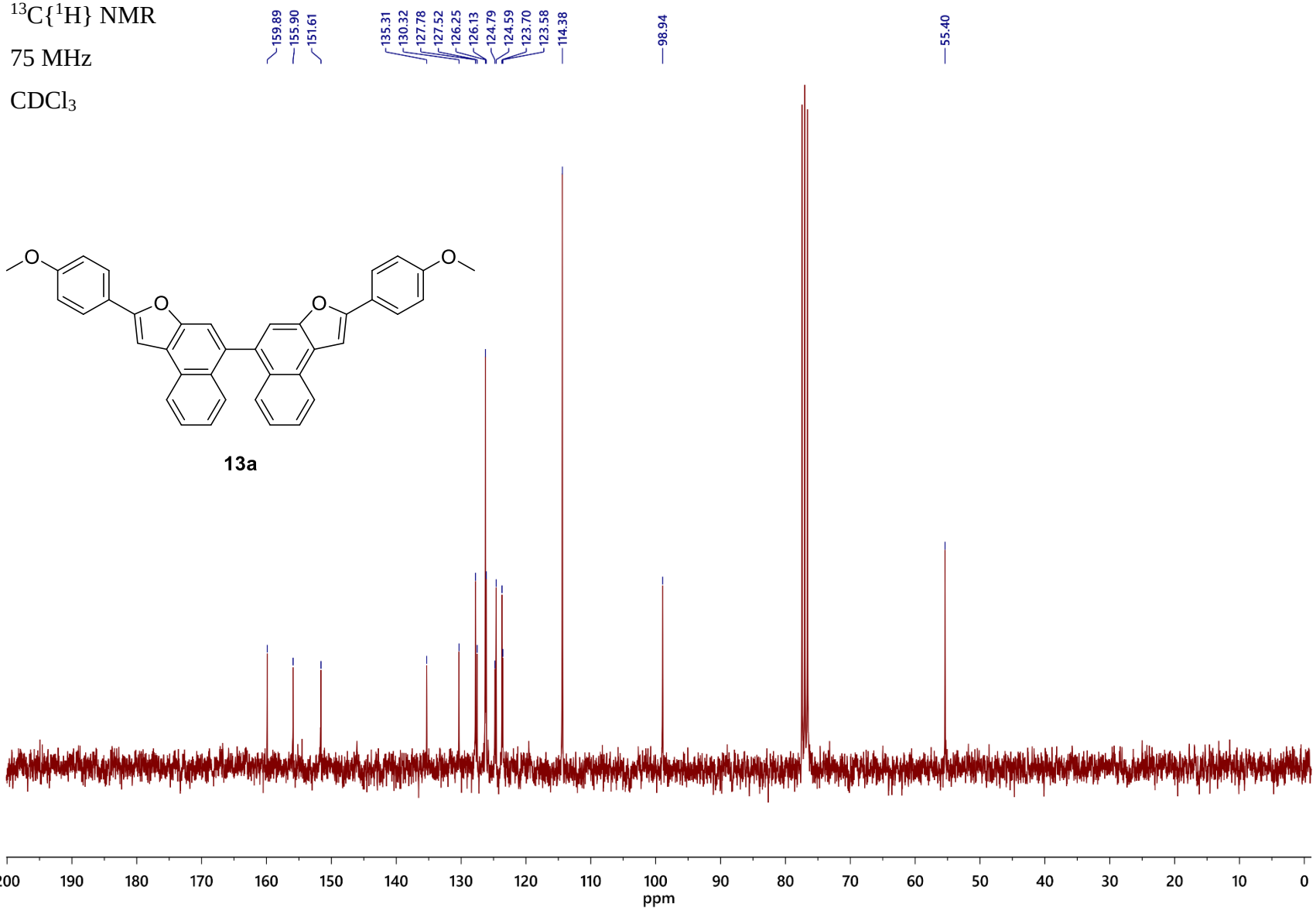
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

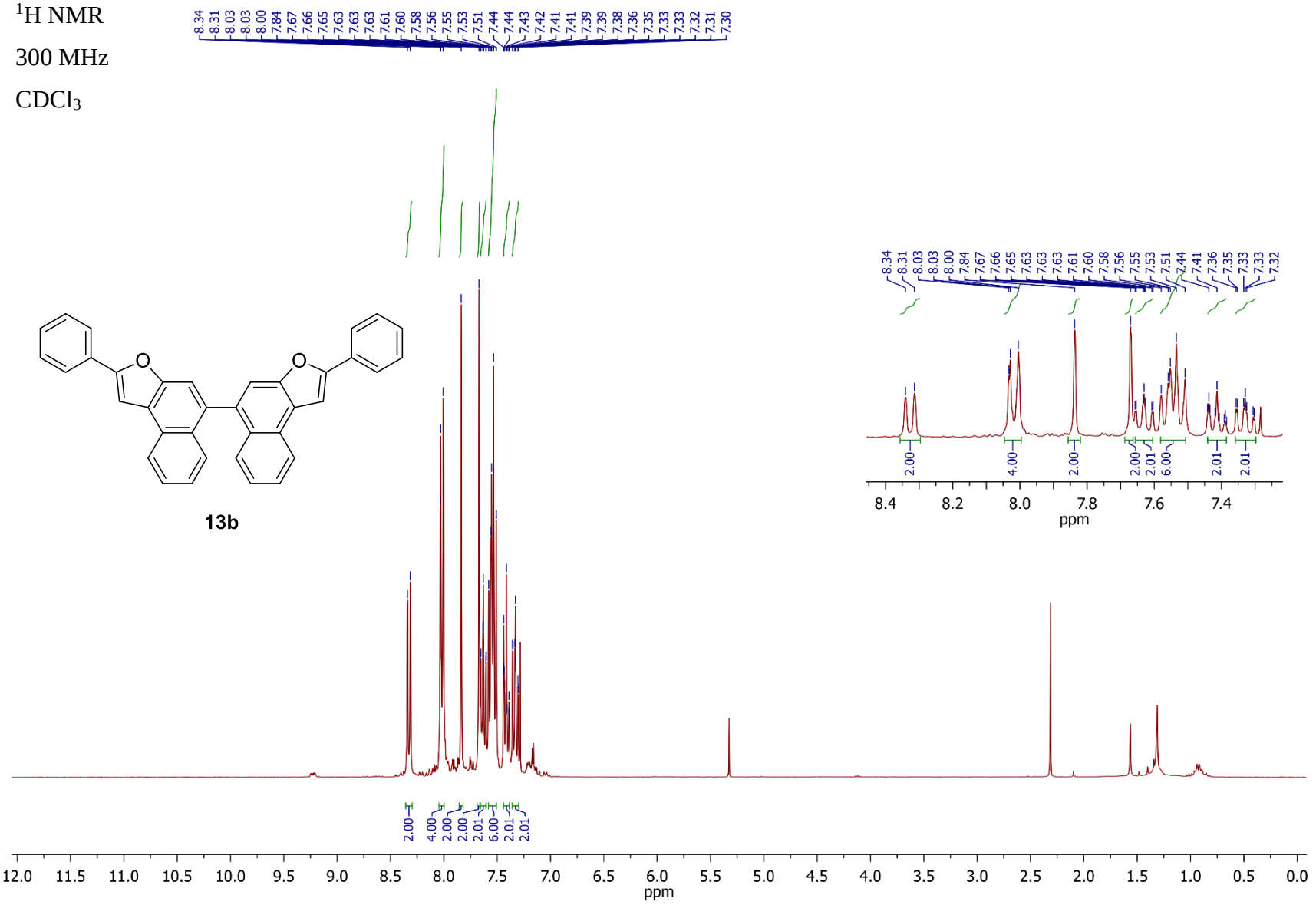
$CDCl_3$



^{1}H NMR

300 MHz

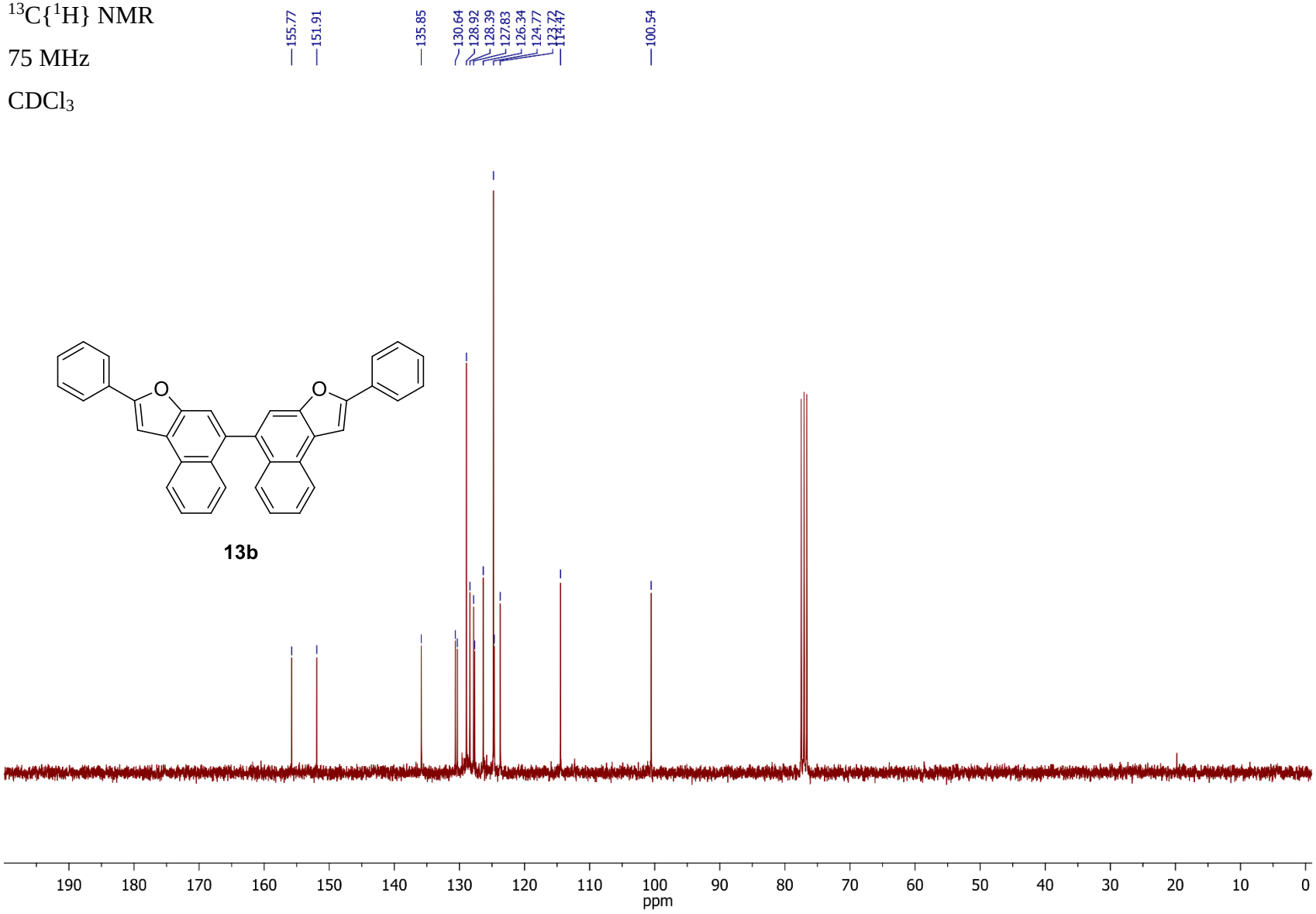
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

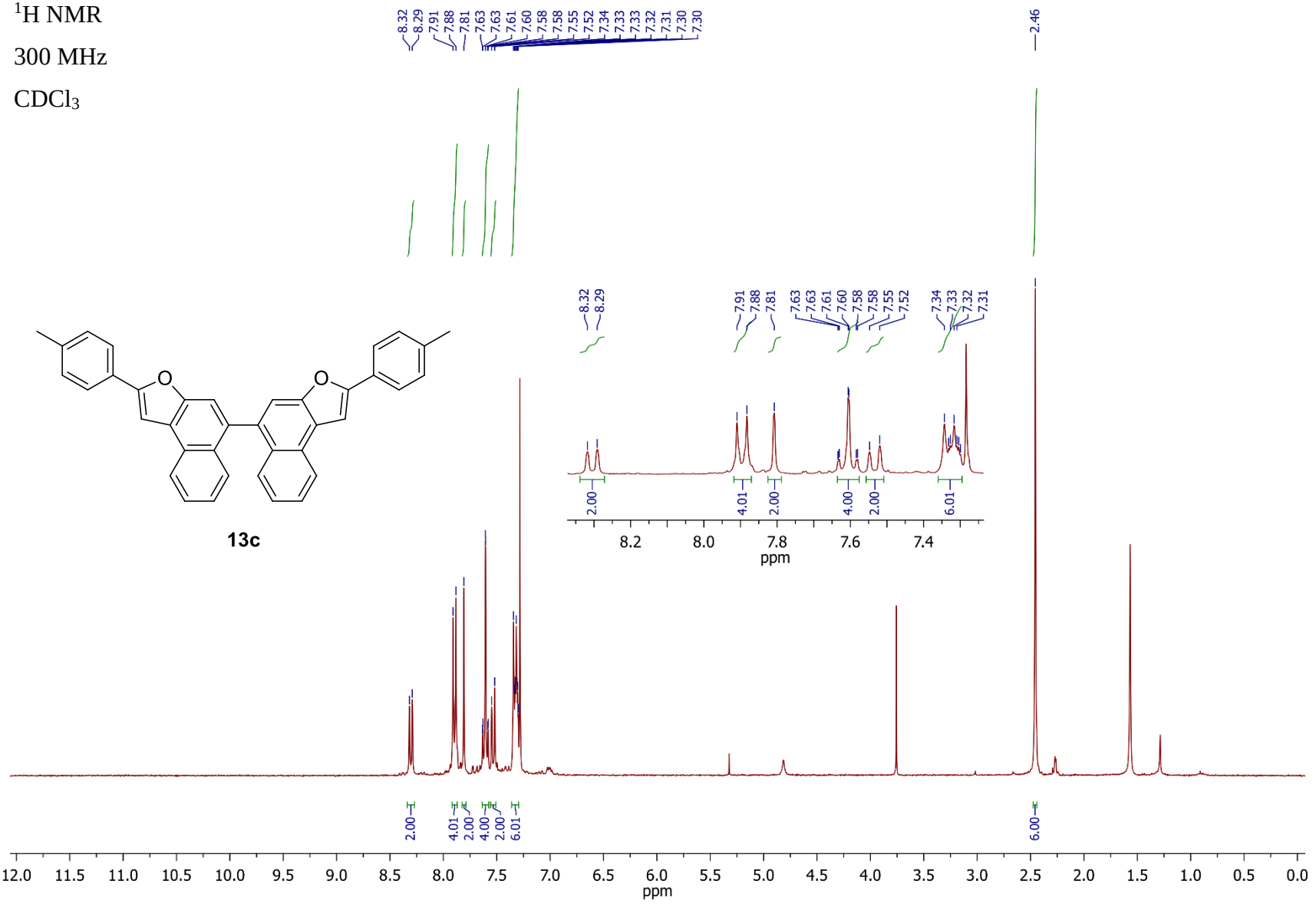
$CDCl_3$



^{1}H NMR

300 MHz

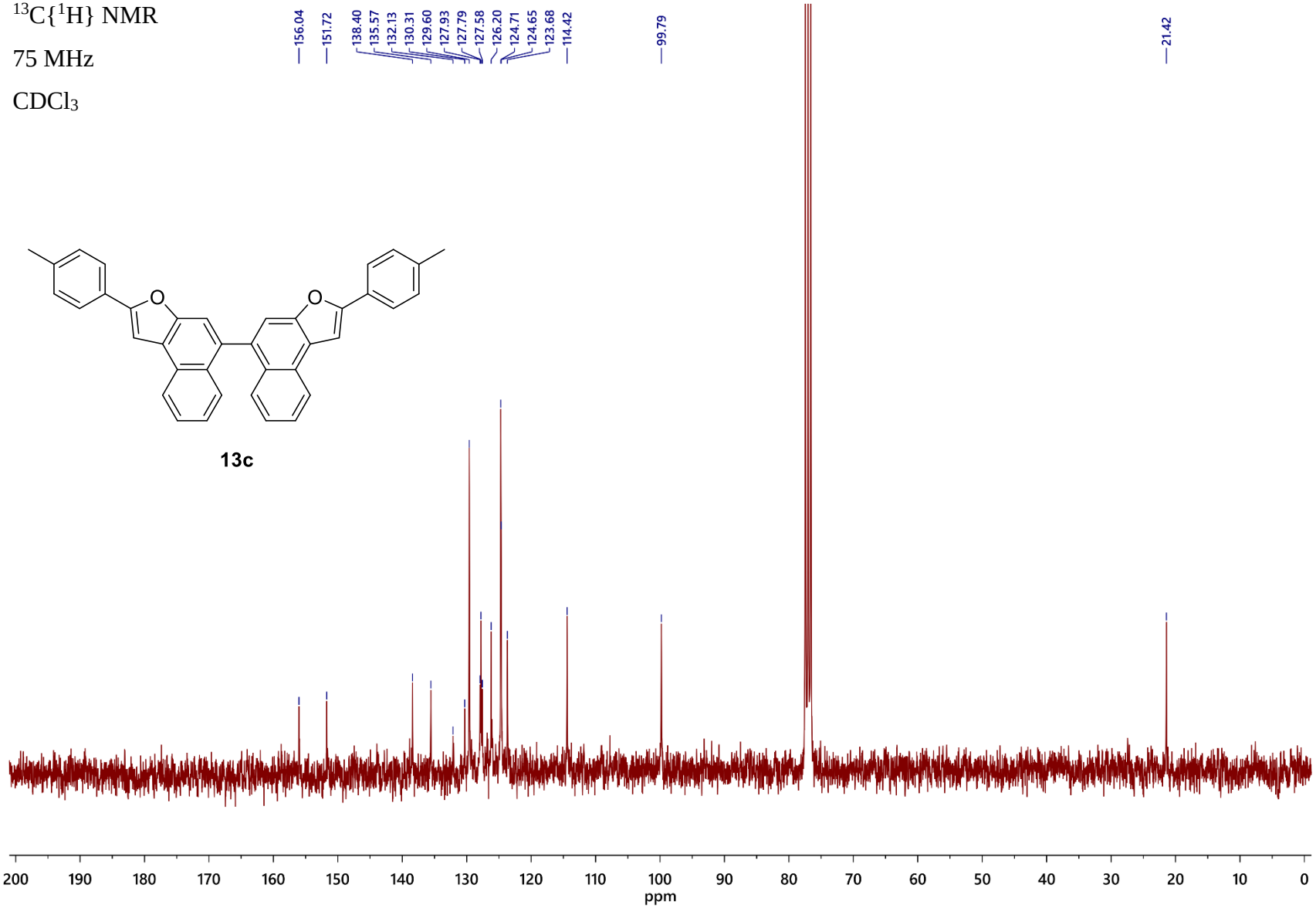
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

$CDCl_3$

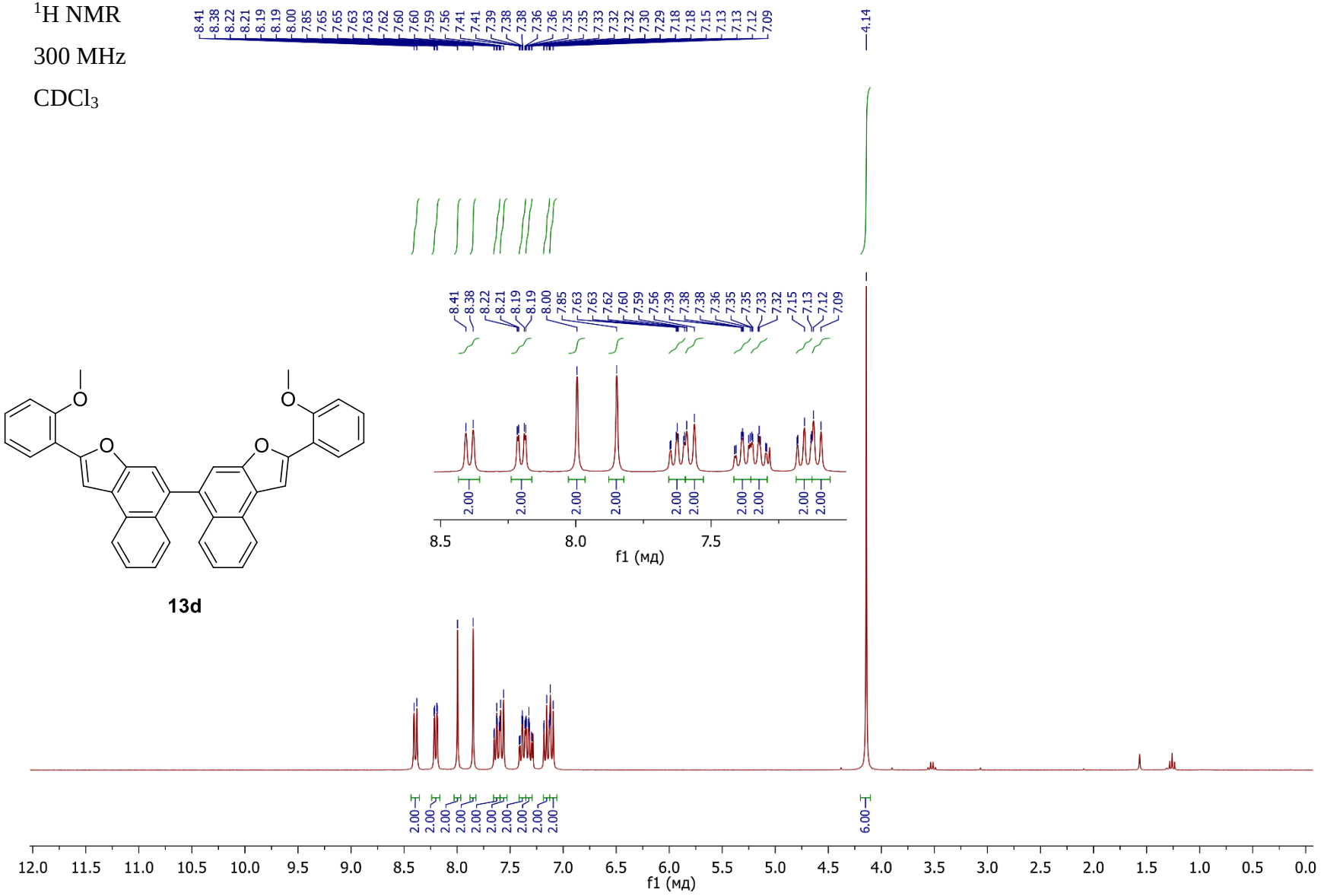


13c

^{1}H NMR

300 MHz

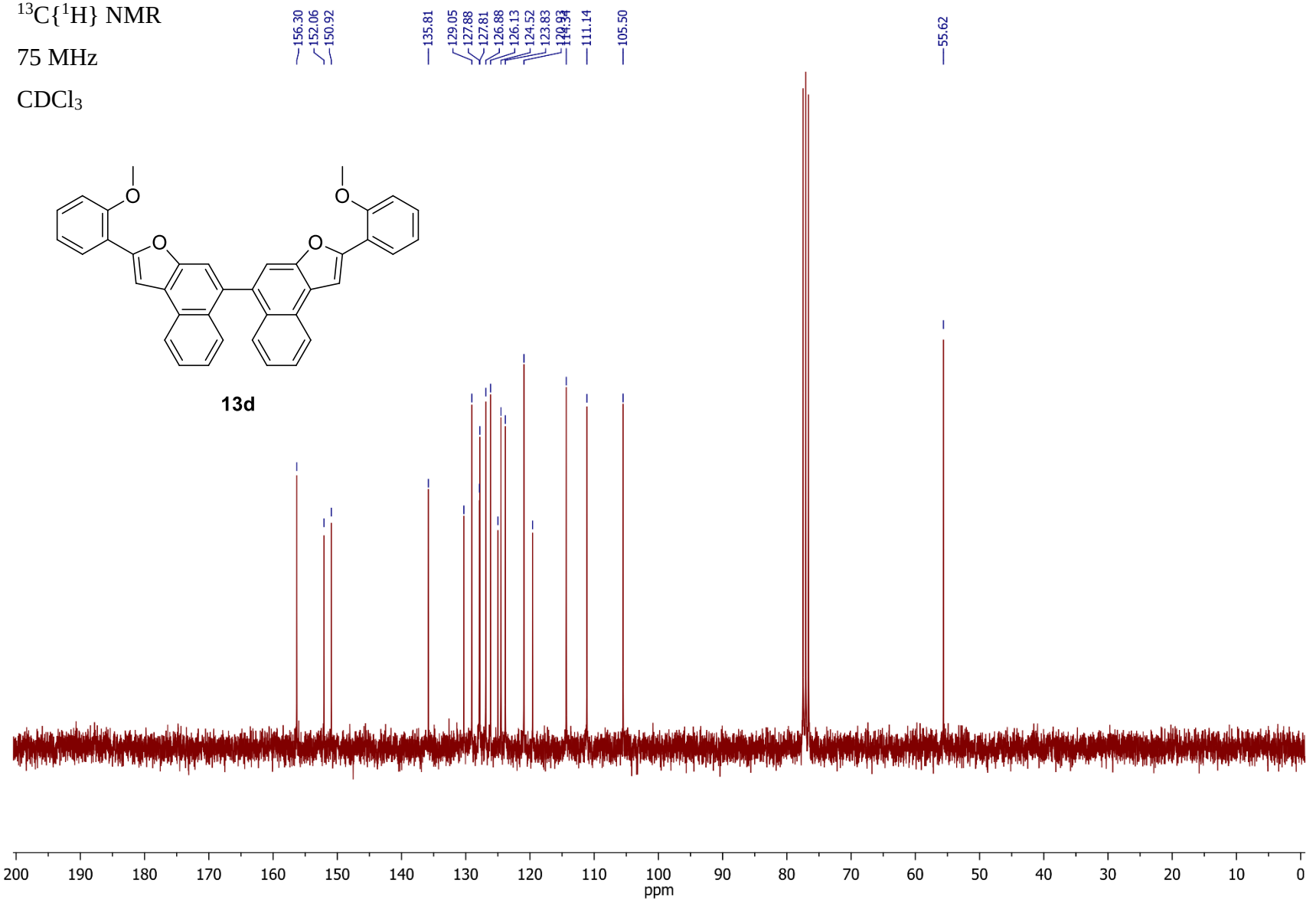
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

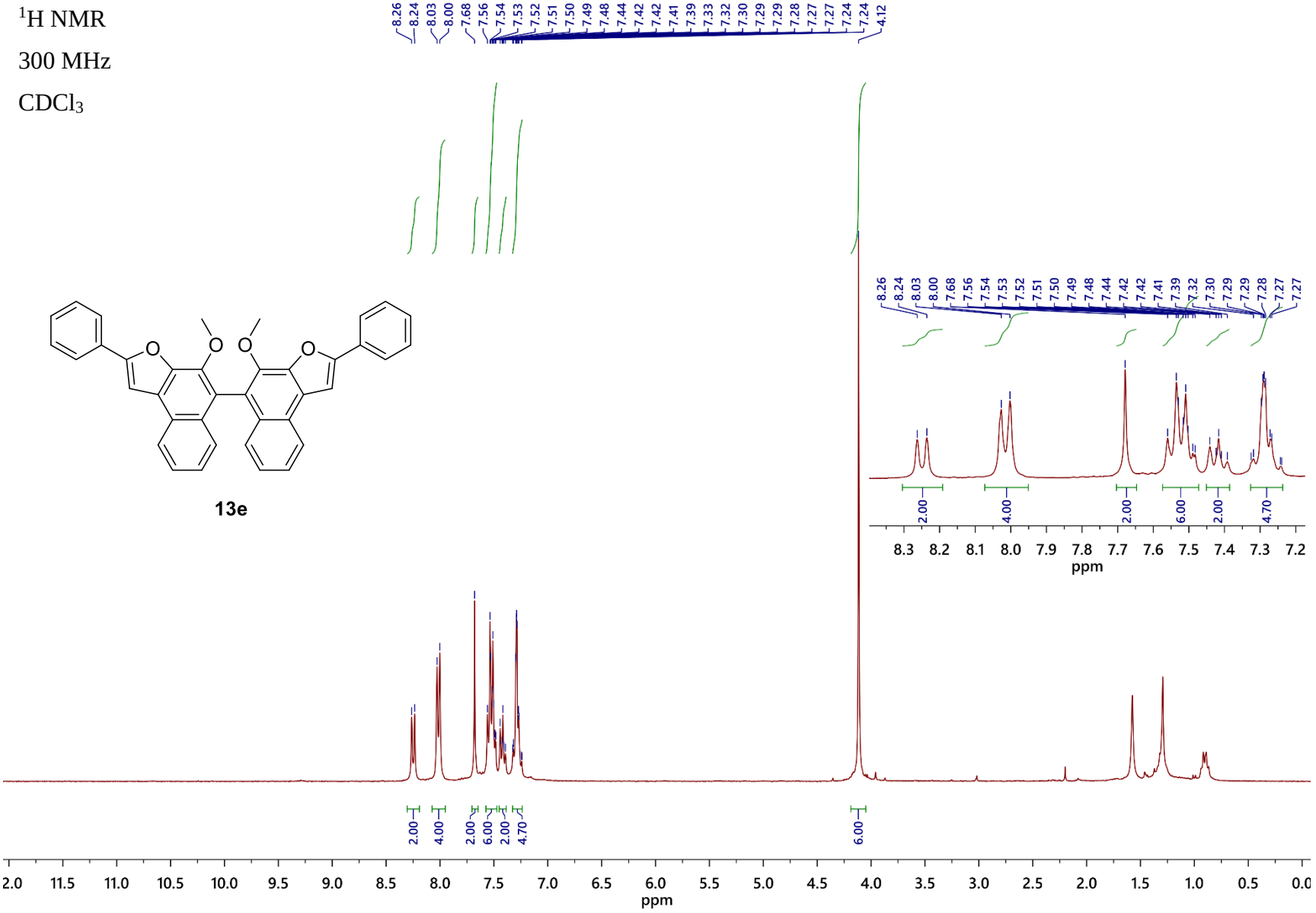
$CDCl_3$



^{1}H NMR

300 MHz

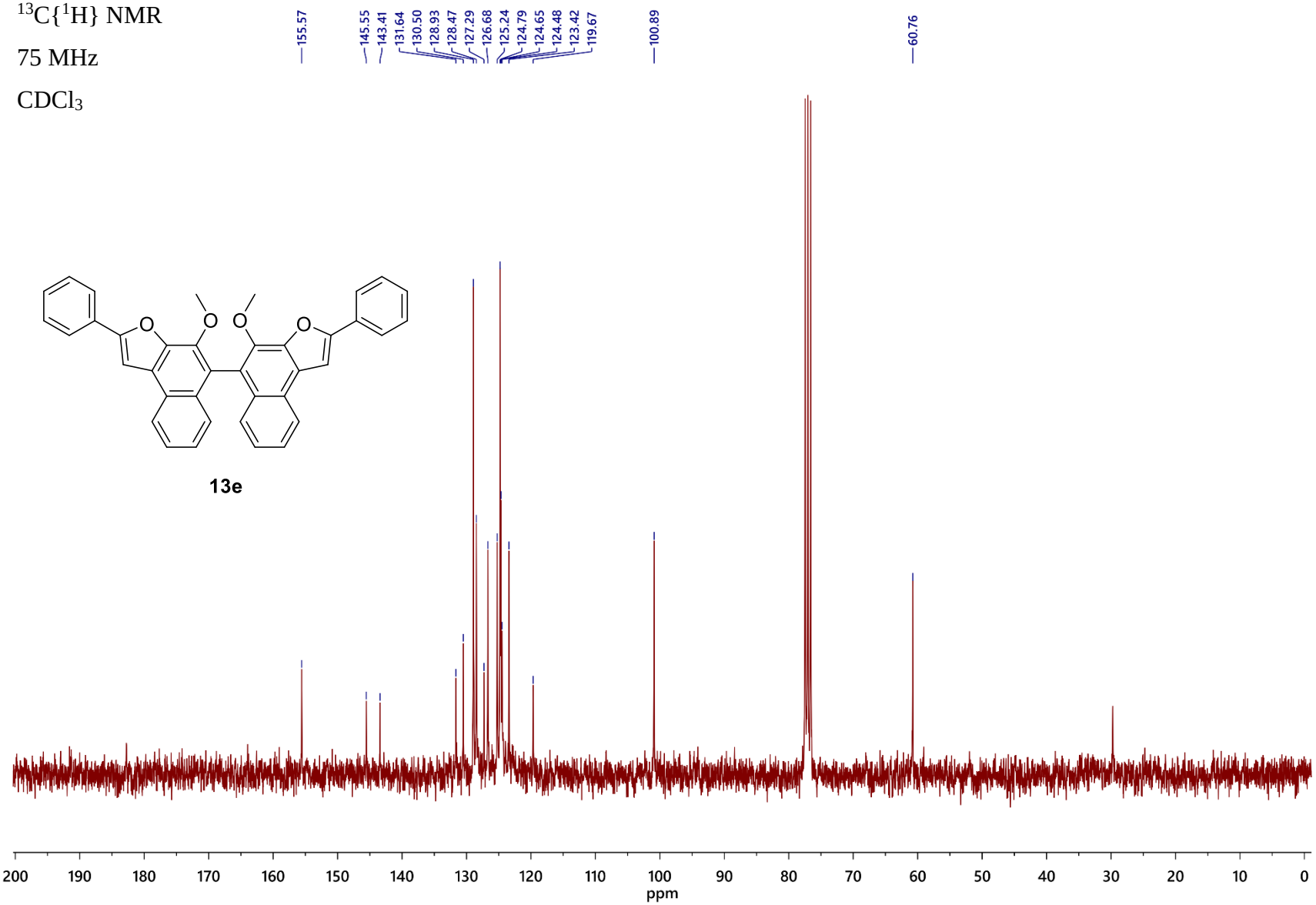
$CDCl_3$



$^{13}C\{^{1}H\}$ NMR

75 MHz

$CDCl_3$

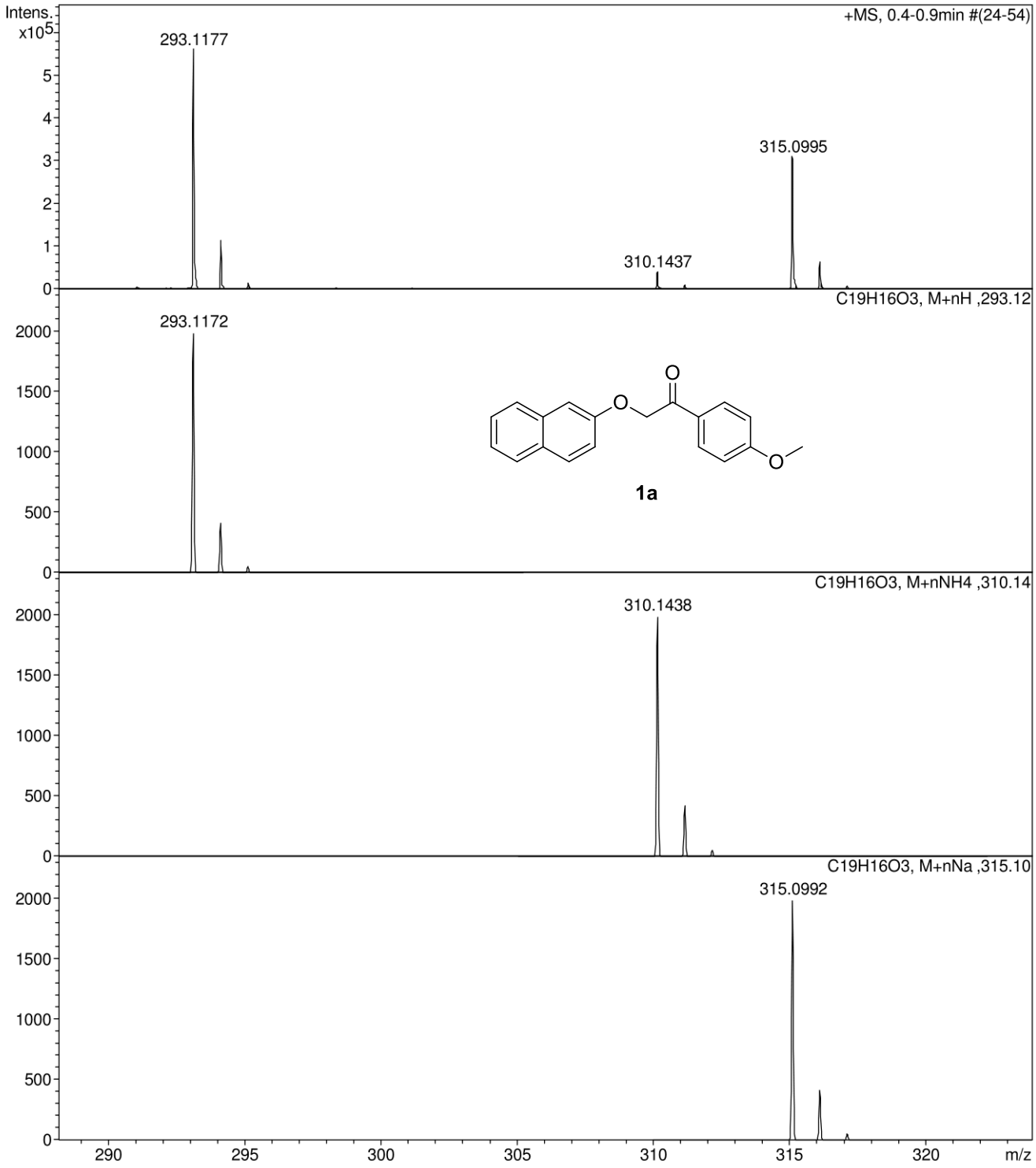


13e

XIII. Copies of HRMS spectra

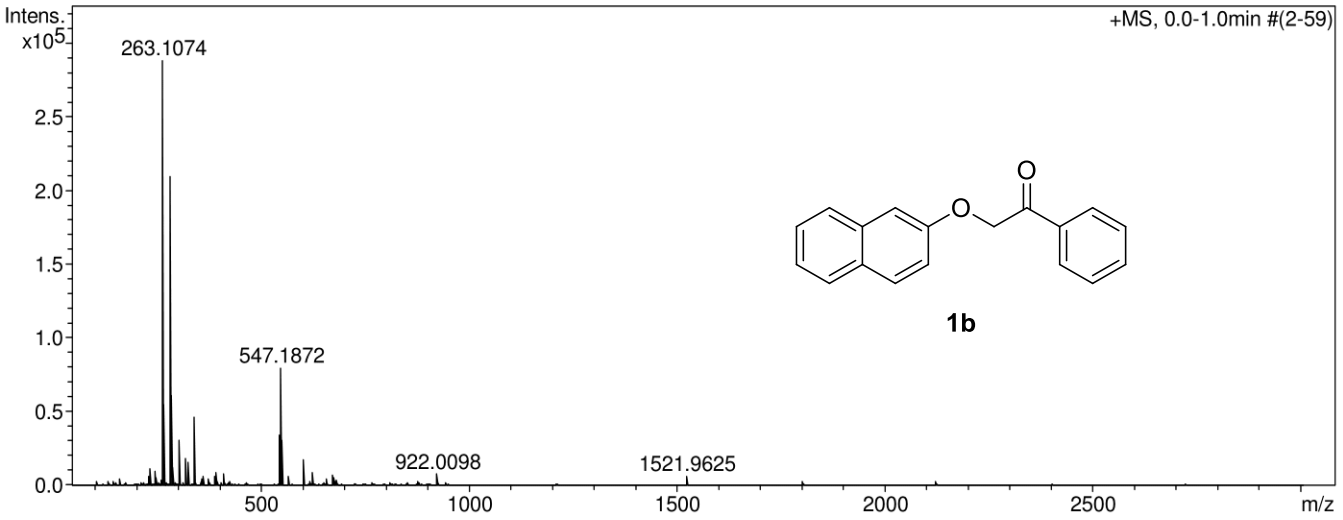
Acquisition Parameter

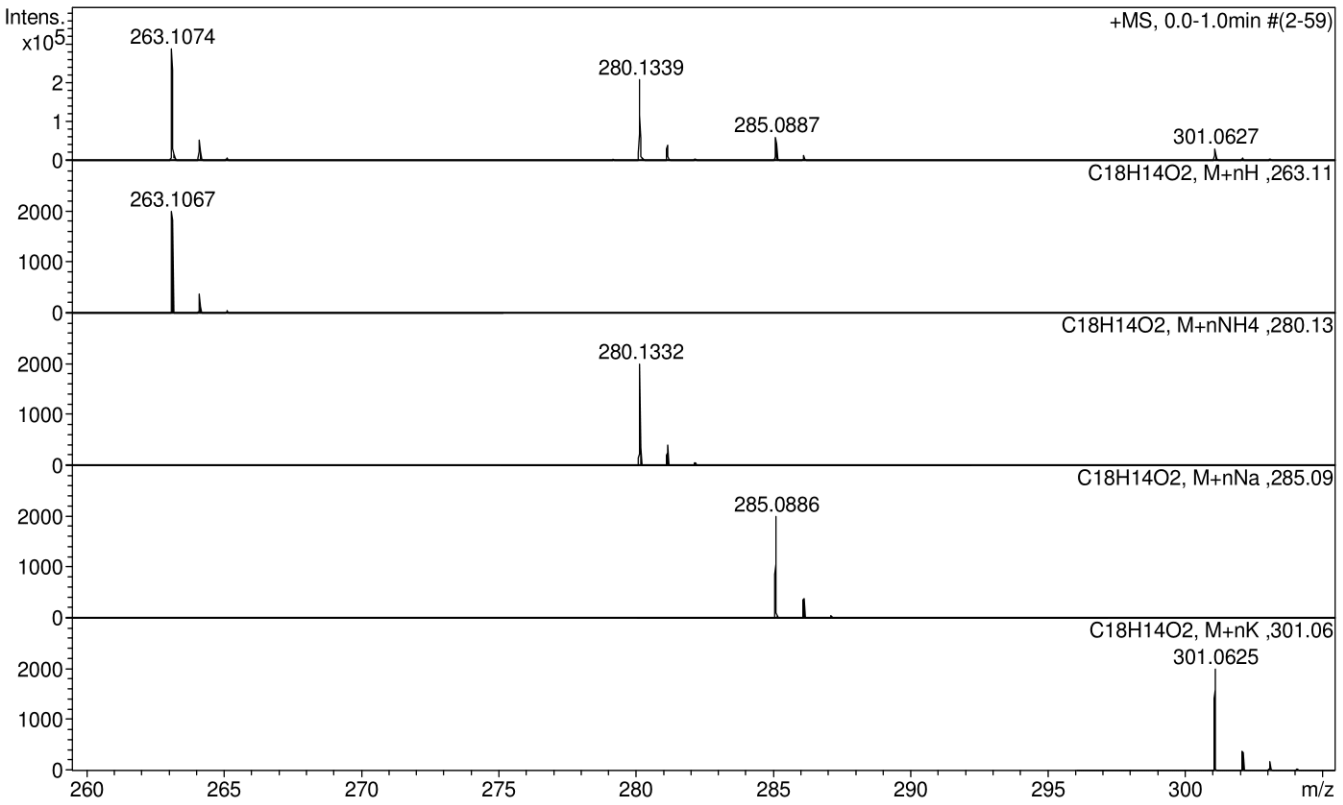
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





Acquisition Parameter

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Focus	Not active			Set Dry Heater	180 °C
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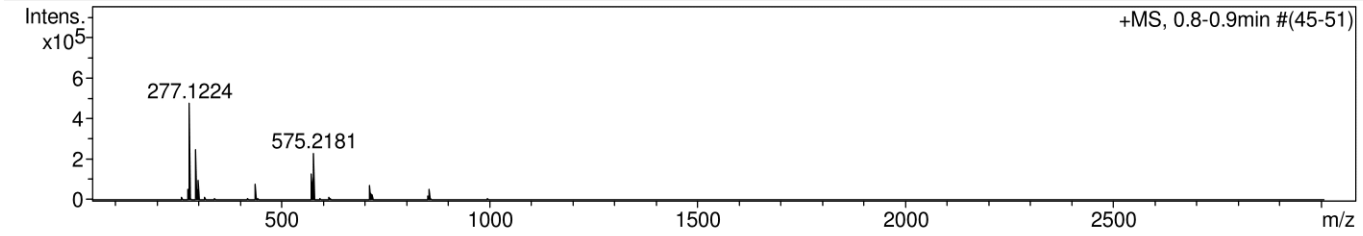
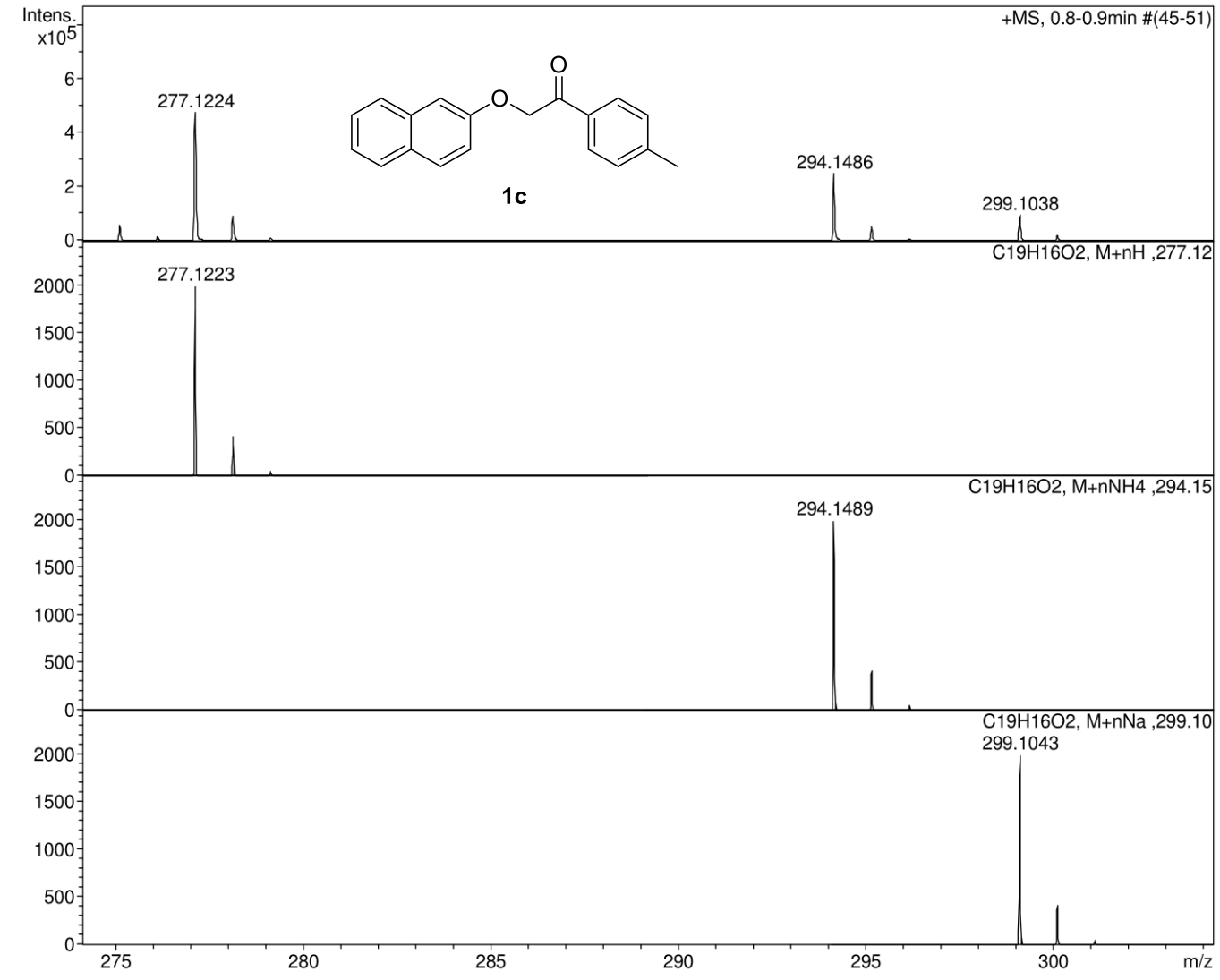
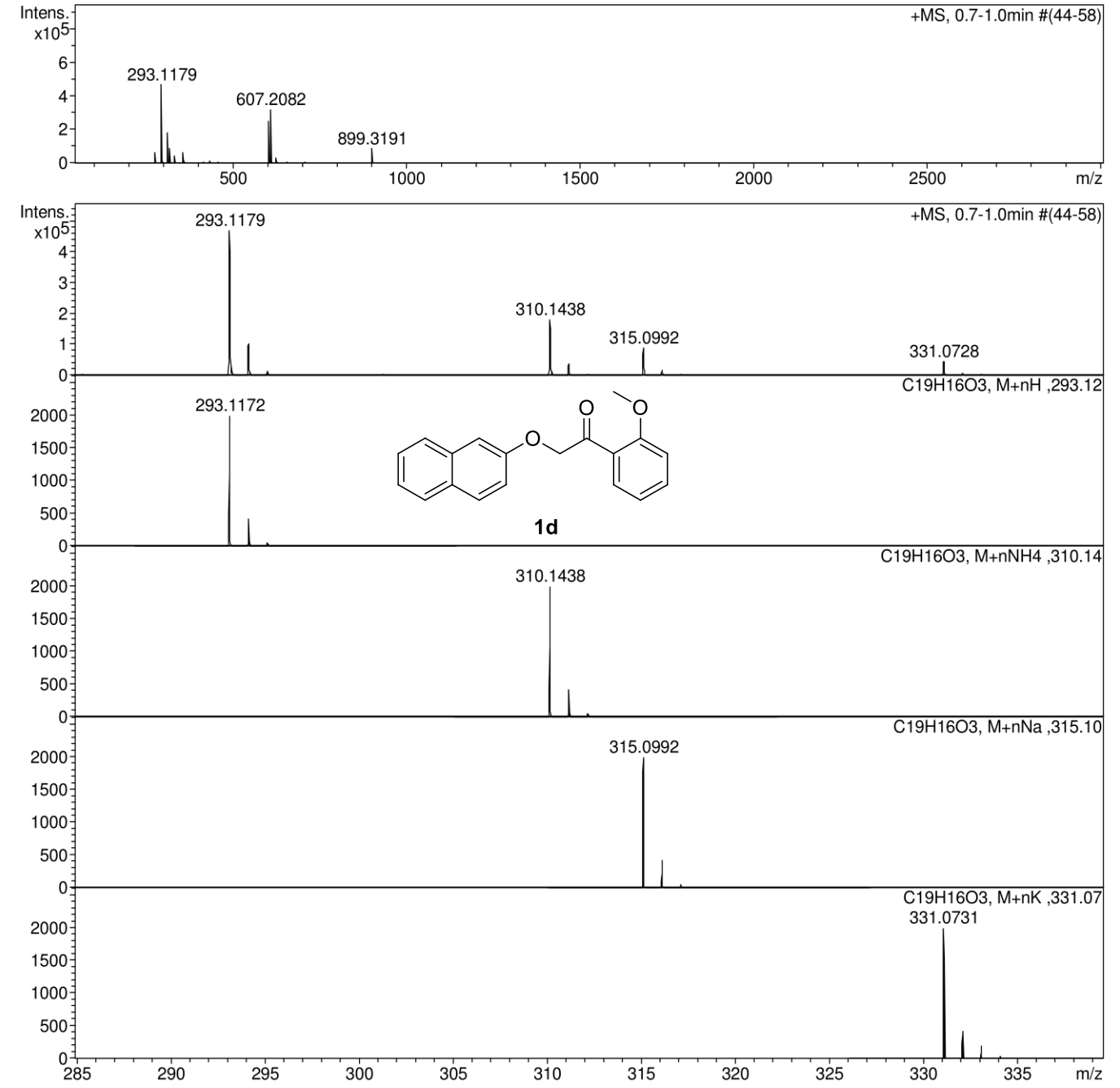
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
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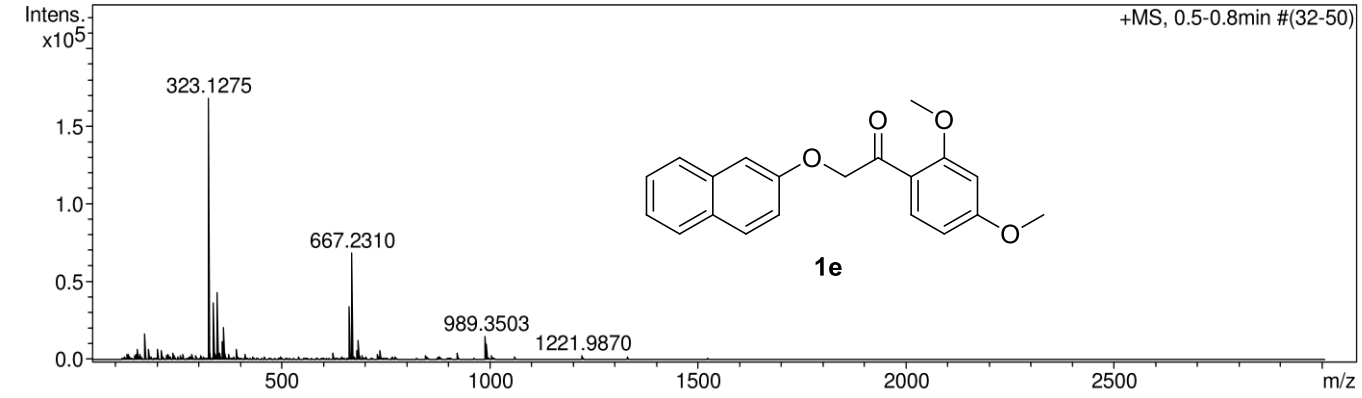

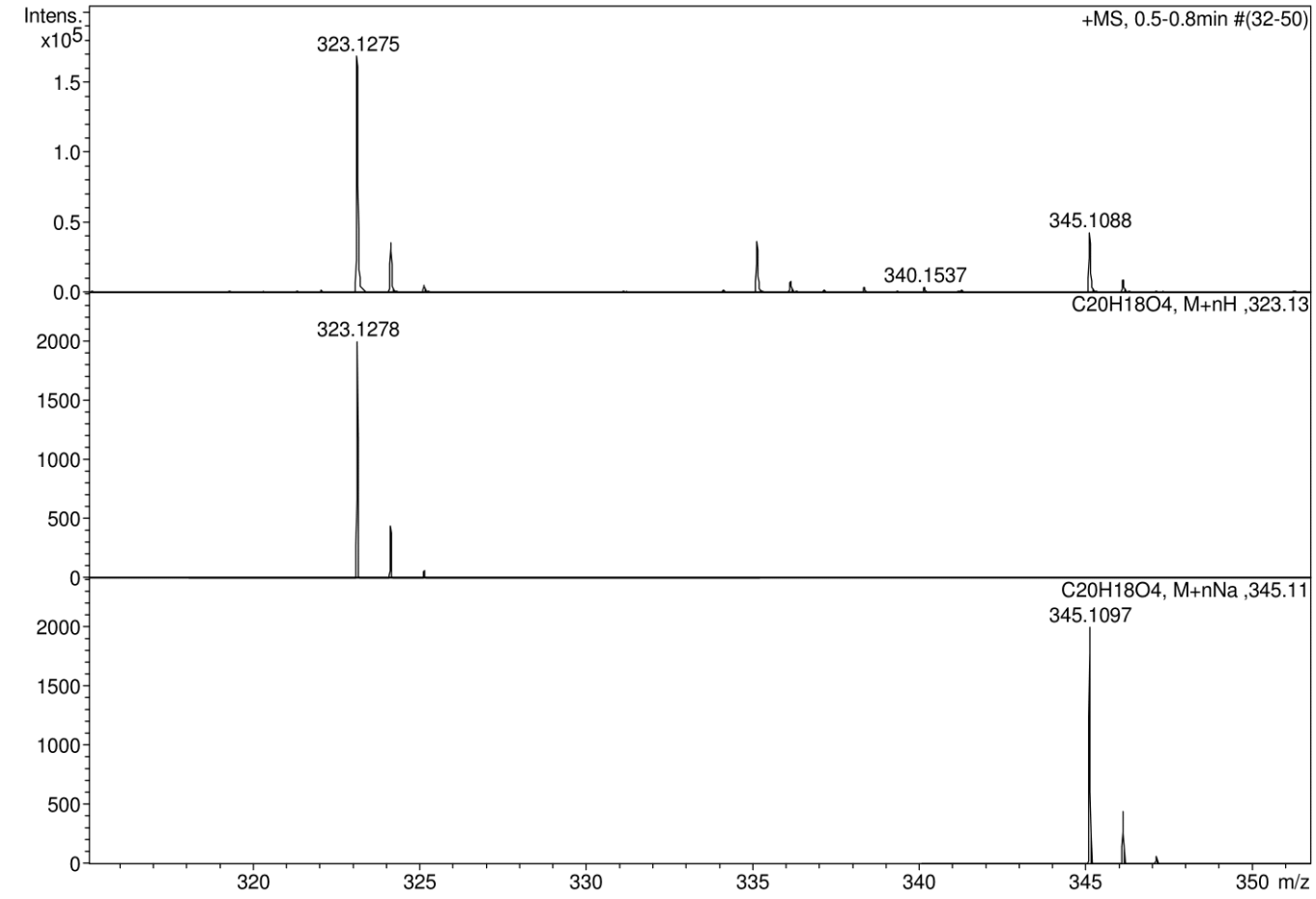

Acquisition Parameter

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Focus	Not active			Set Dry Heater	180 °C
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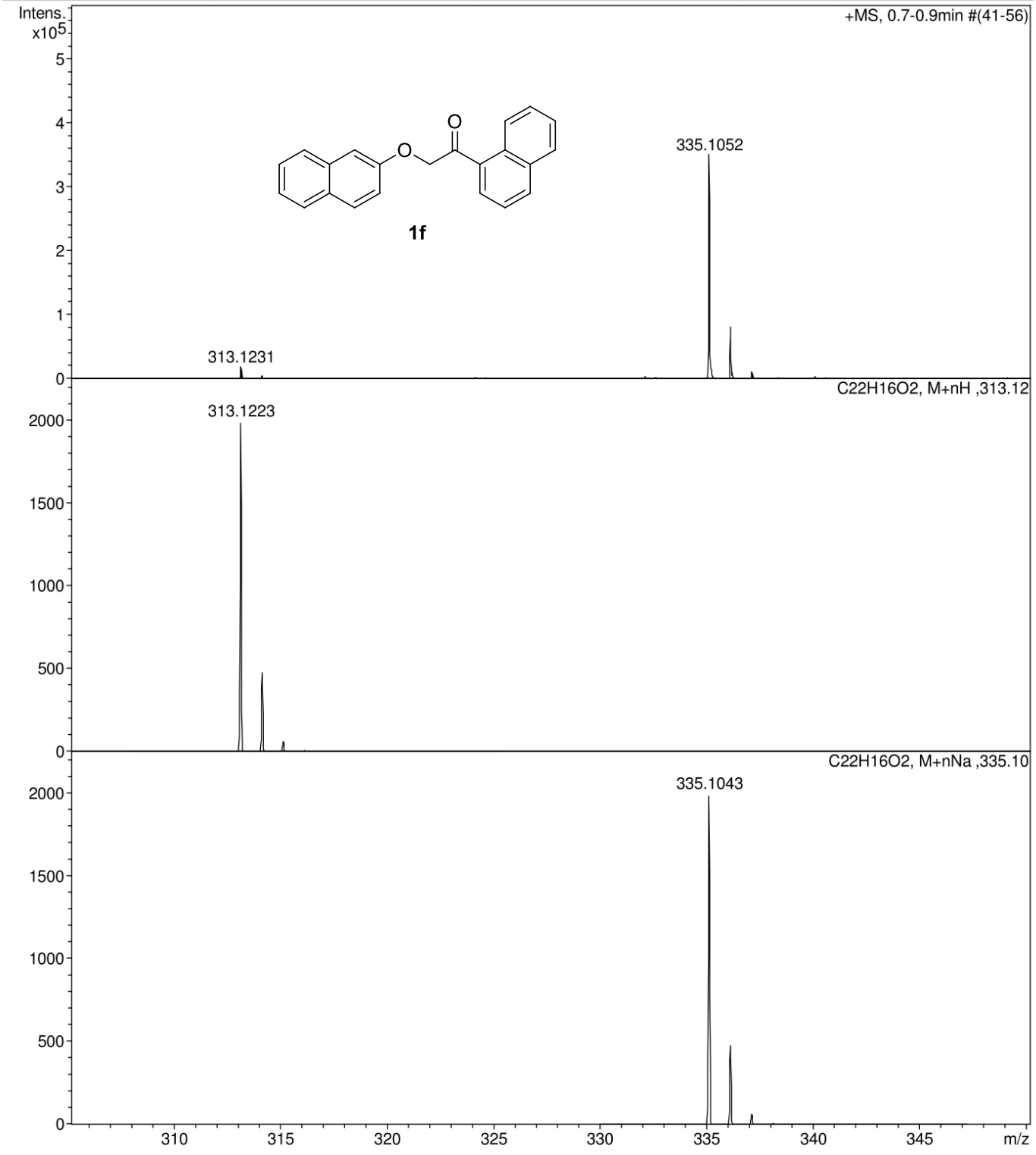

Acquisition Parameter

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Focus	Not active			Set Dry Heater	180 °C
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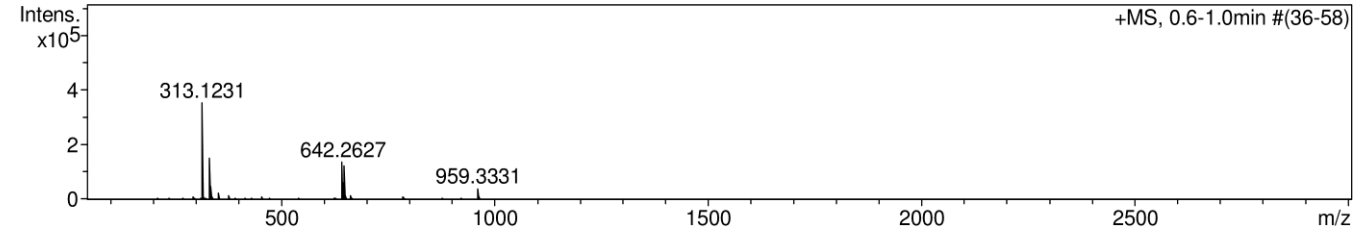

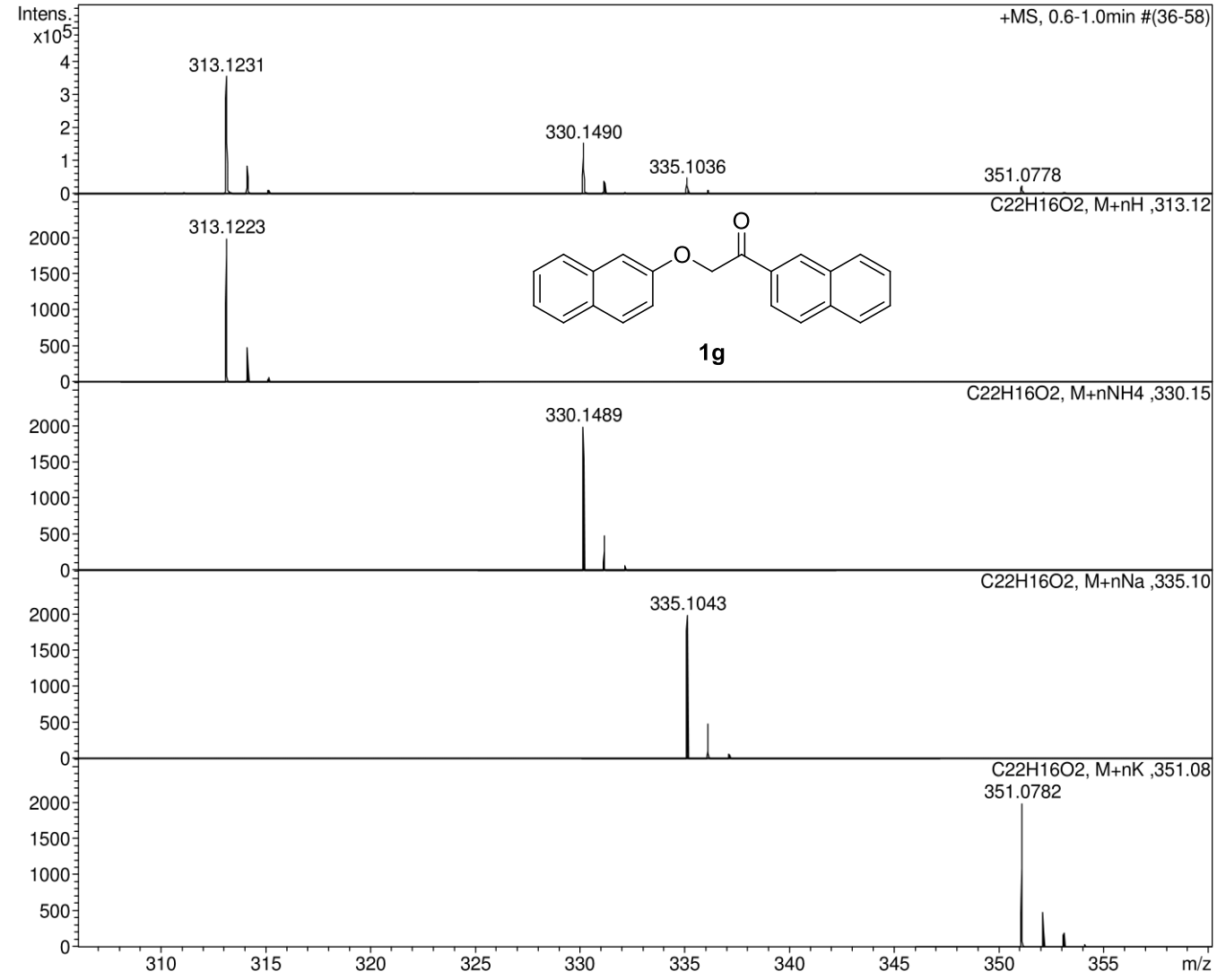

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
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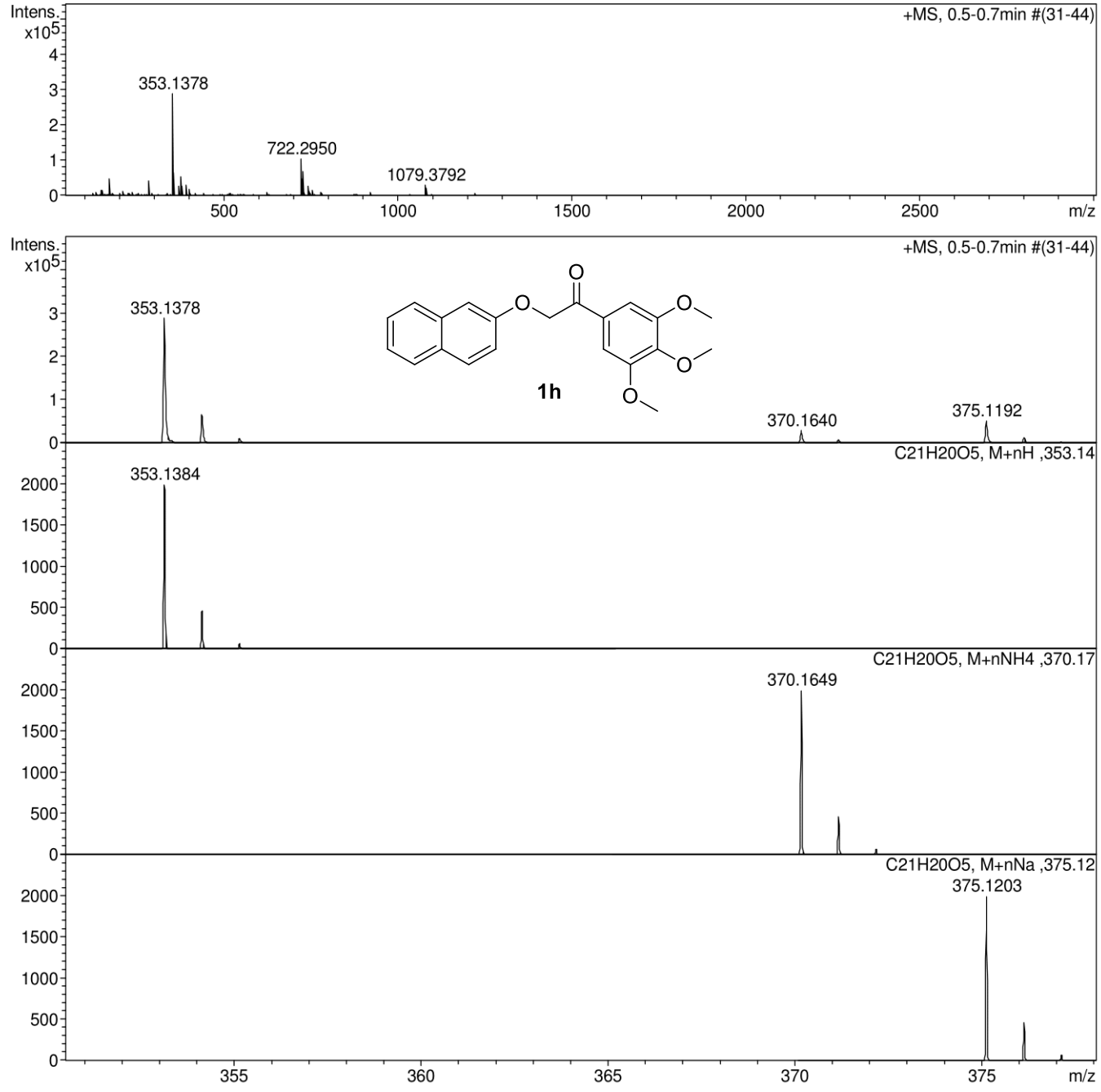

Acquisition Parameter

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Focus	Not active			Set Dry Heater	180 °C
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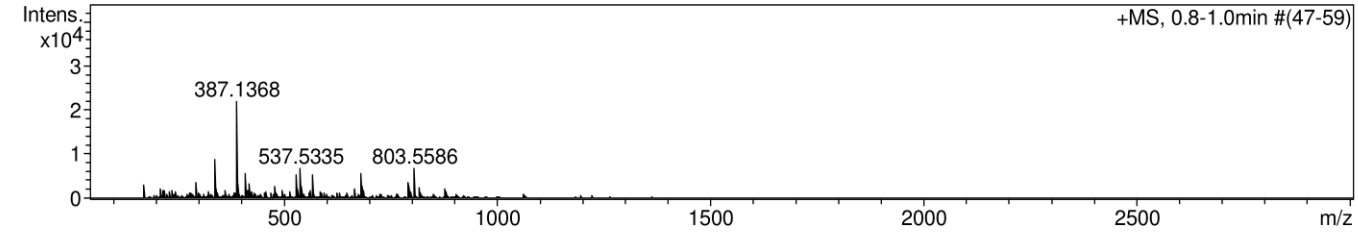

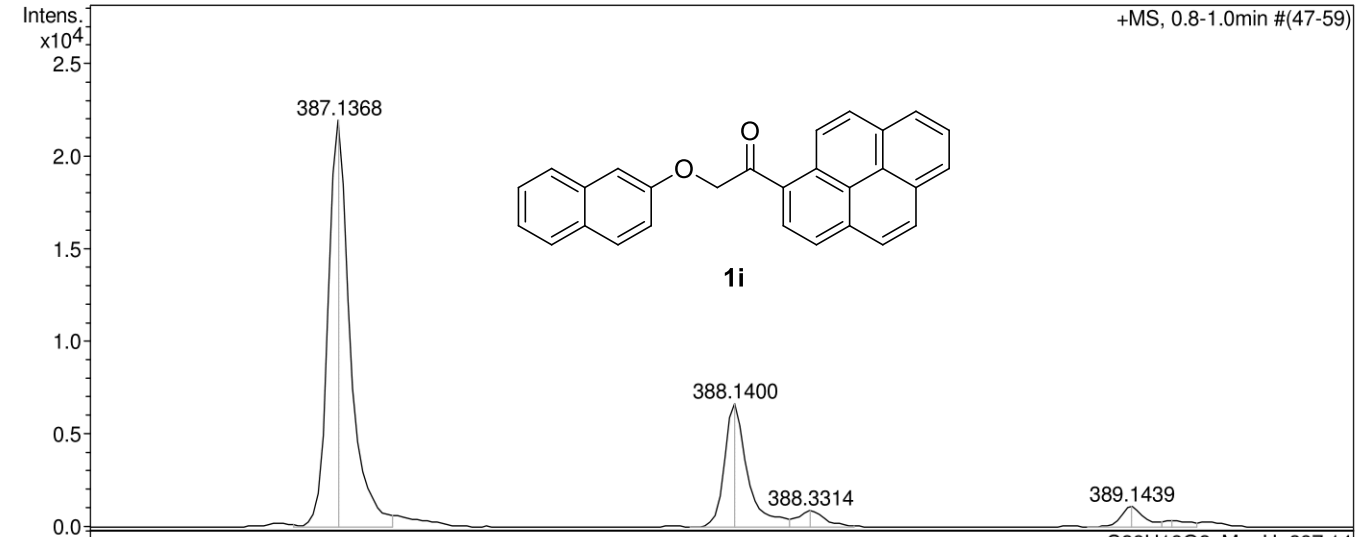

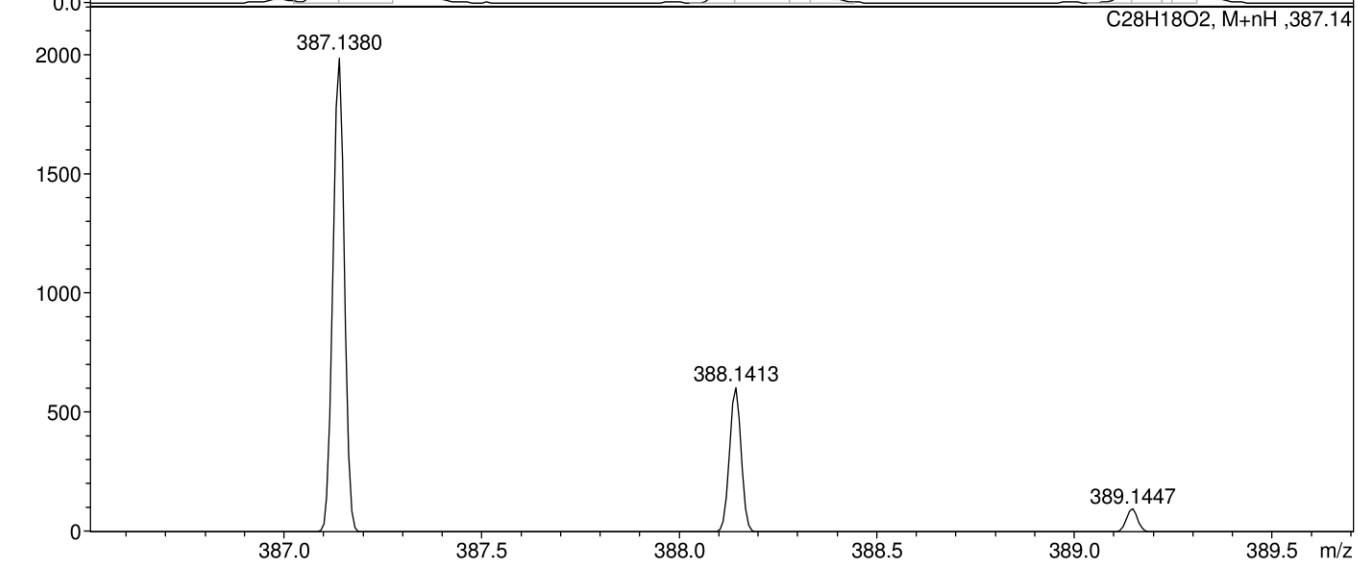

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
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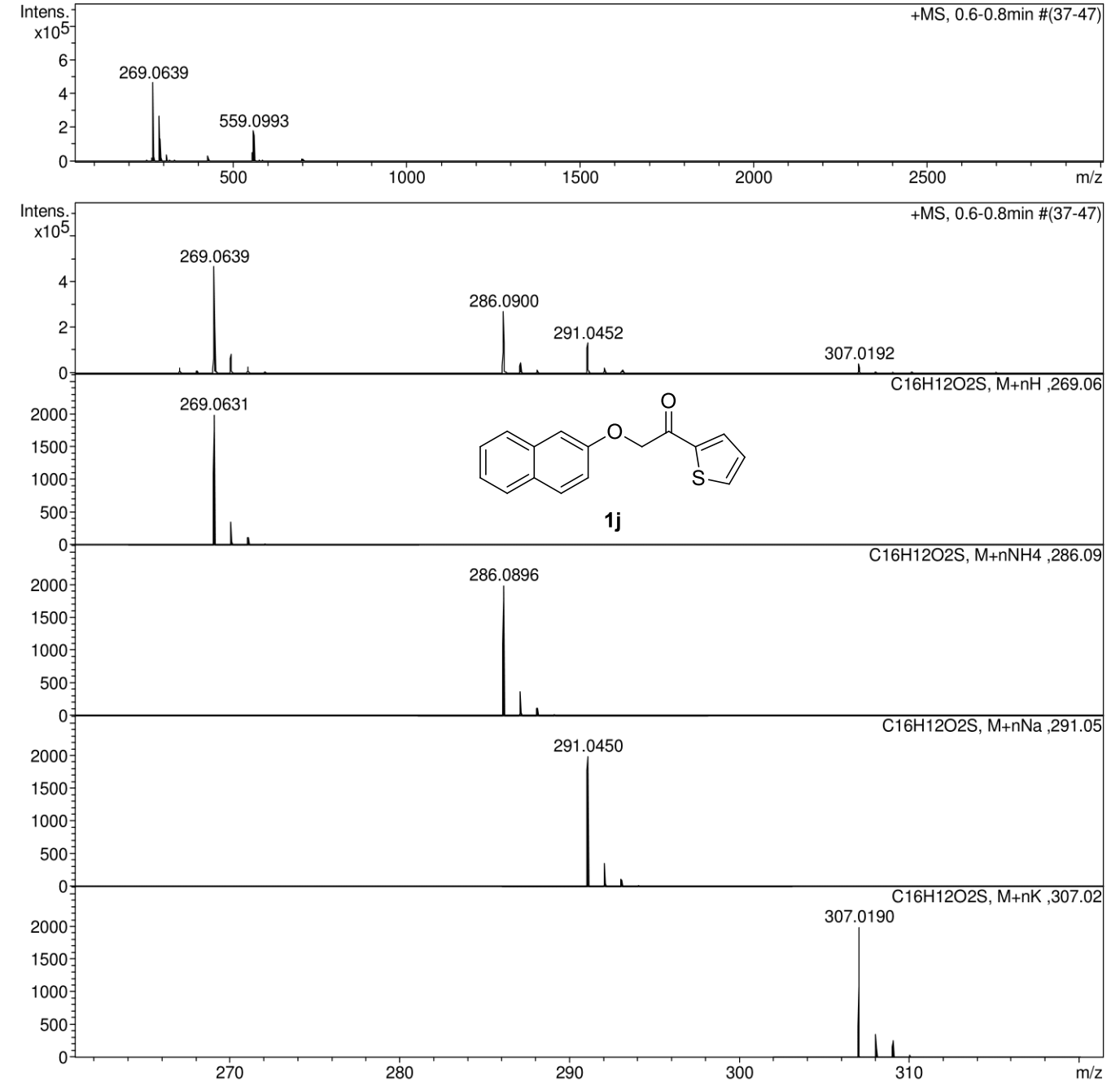

Acquisition Parameter

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Focus	Not active			Set Dry Heater	180 °C
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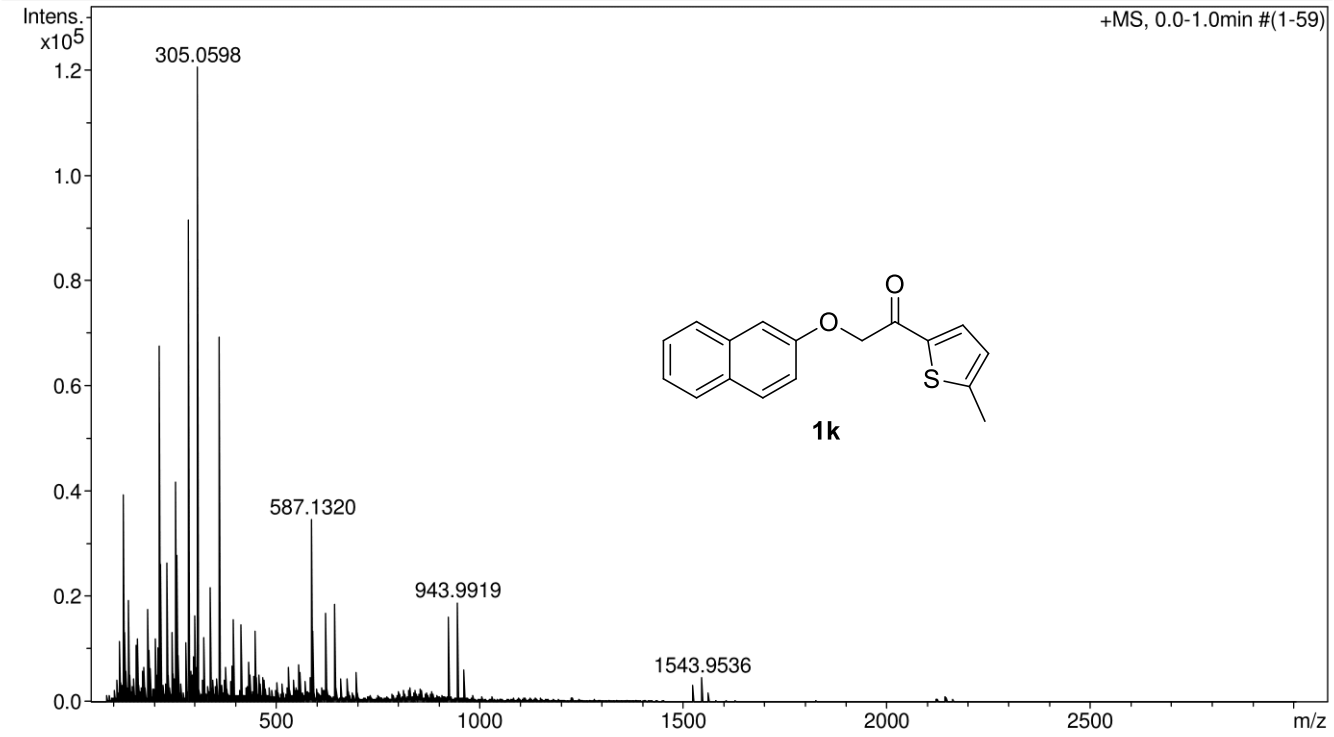

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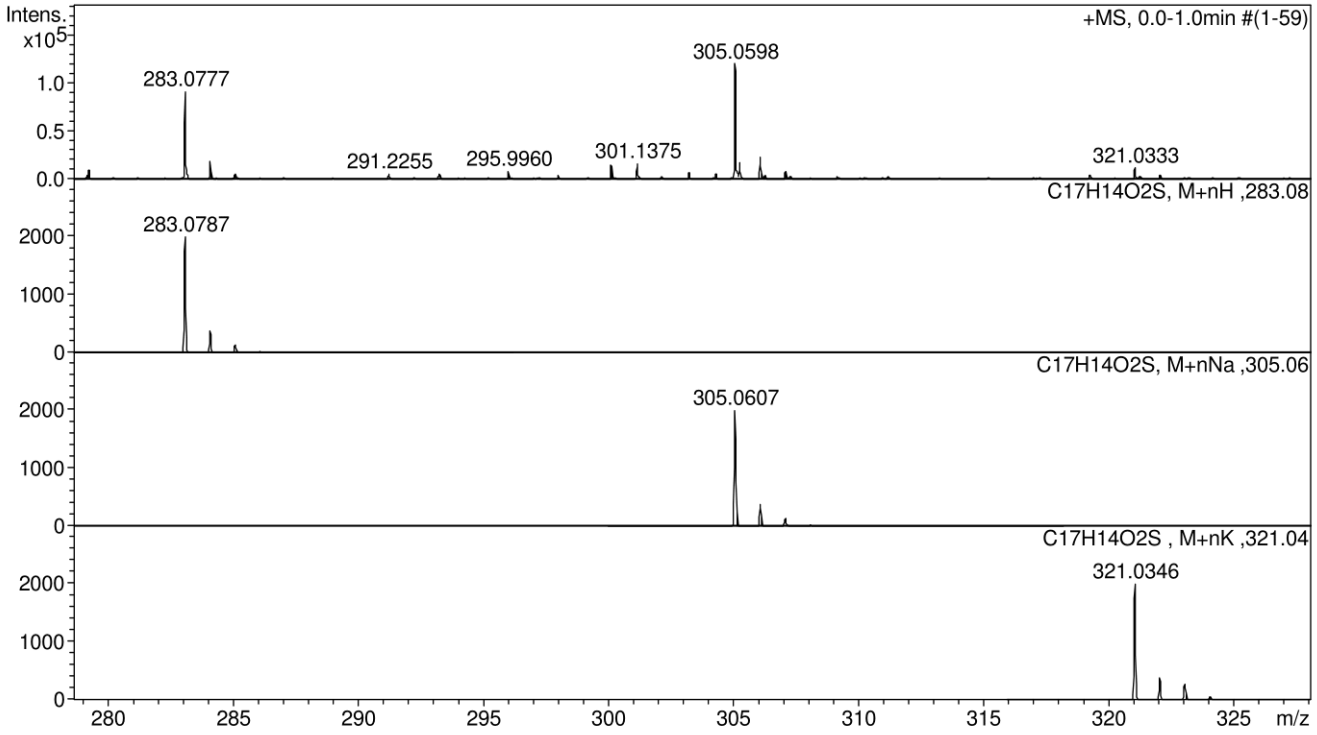

Acquisition Parameter

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Focus	Not active			Set Dry Heater	180 °C
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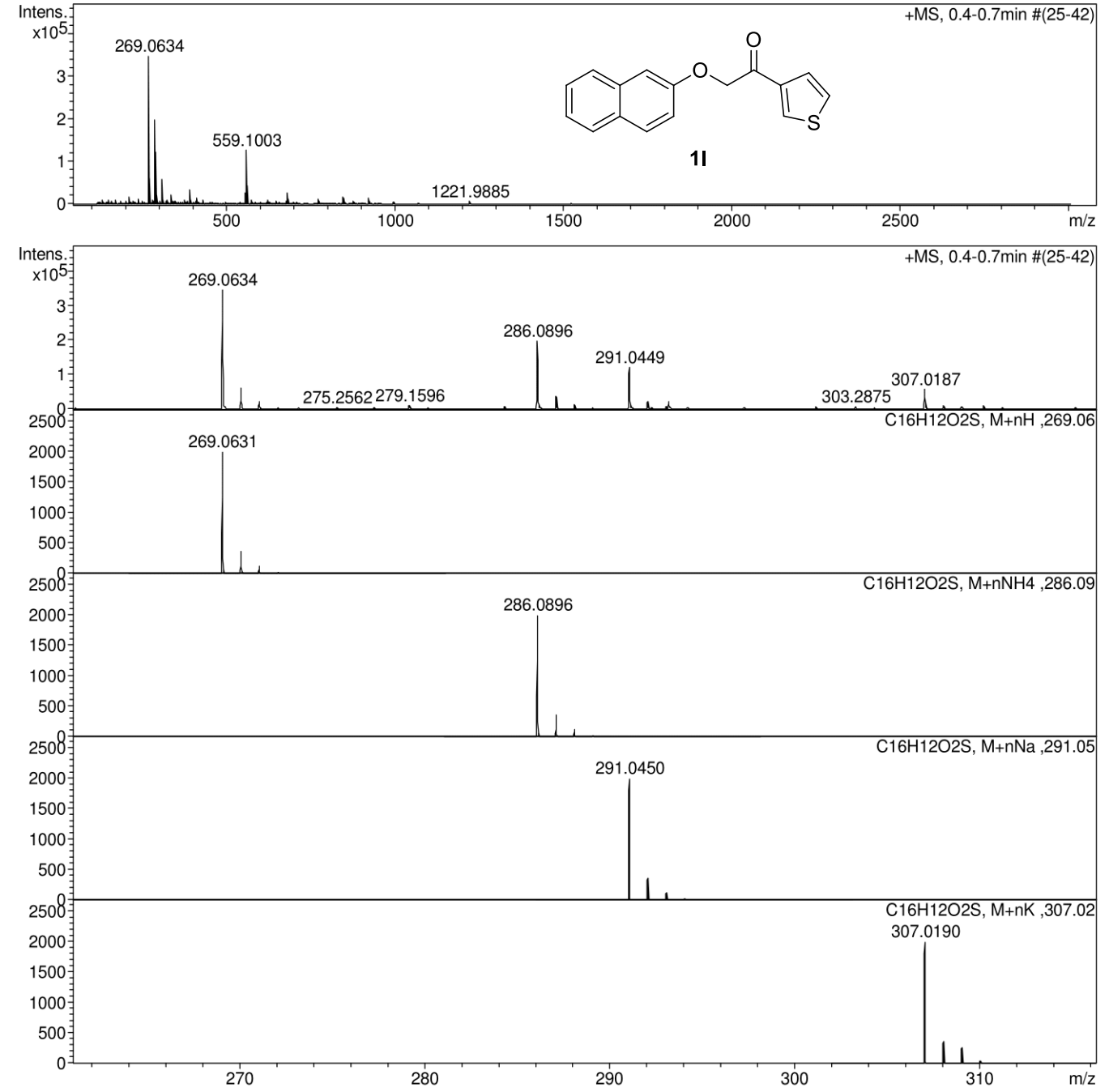

Acquisition Parameter

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Focus	Not active			Set Dry Heater	180 °C
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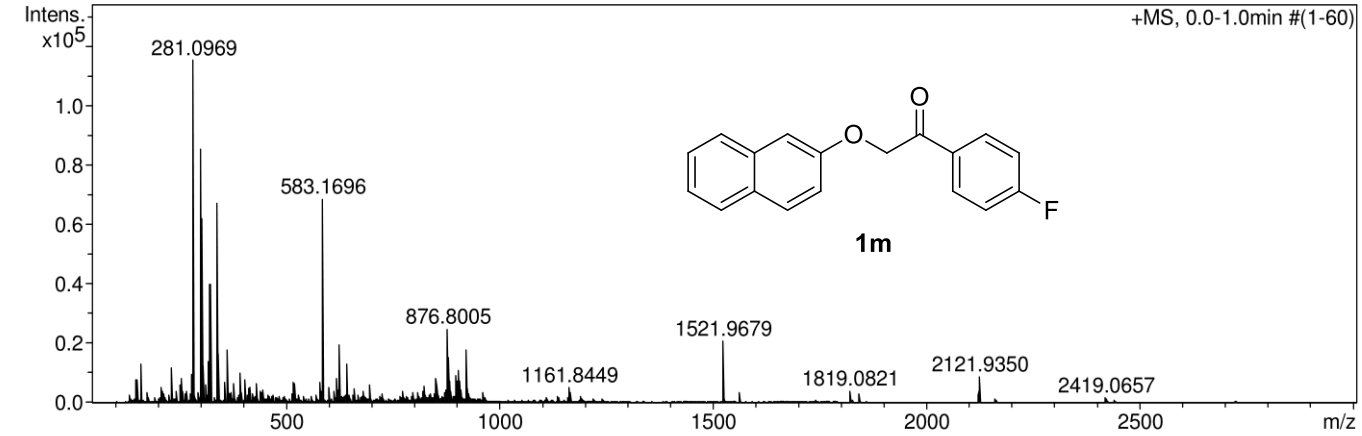

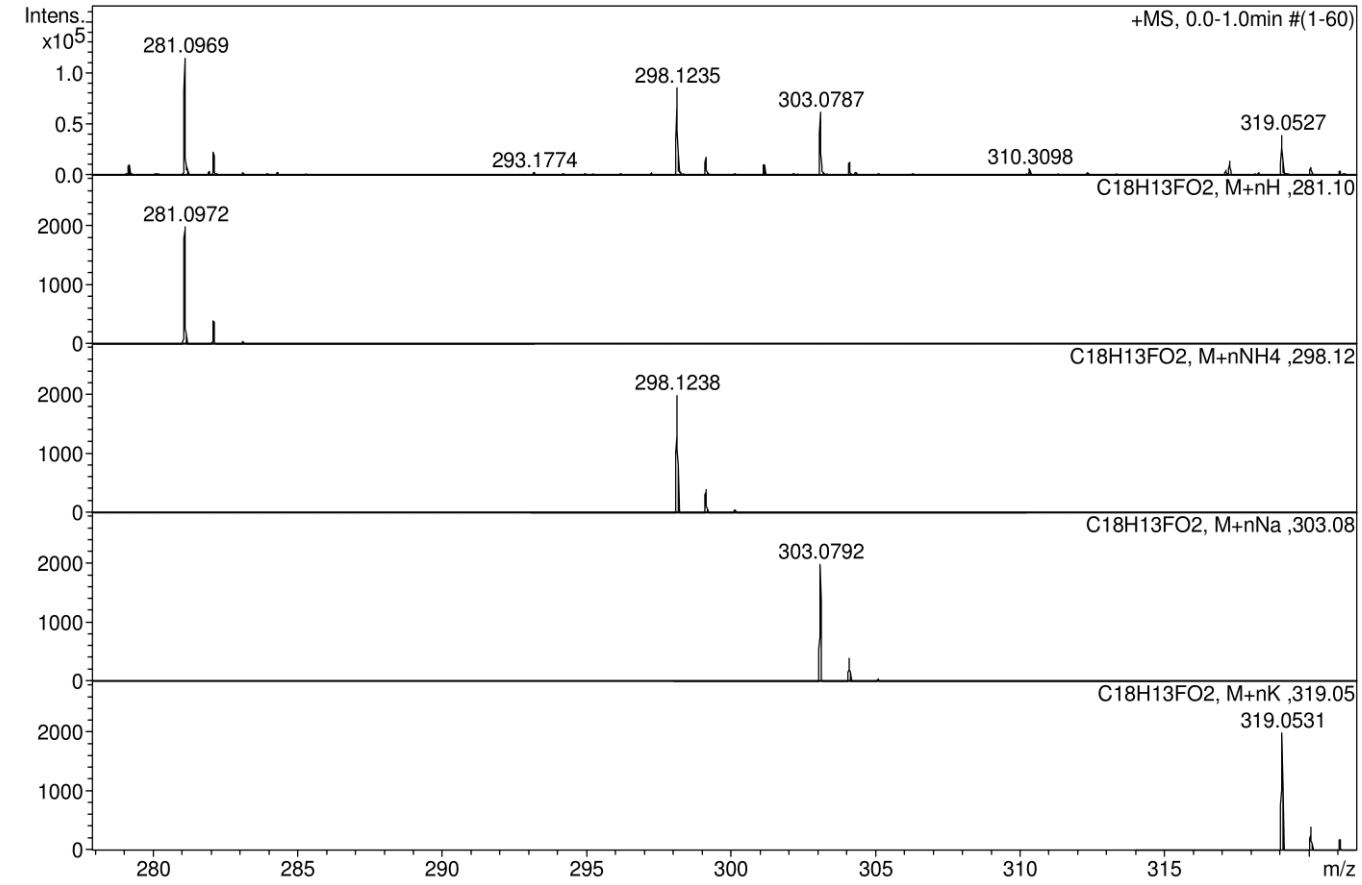

Acquisition Parameter

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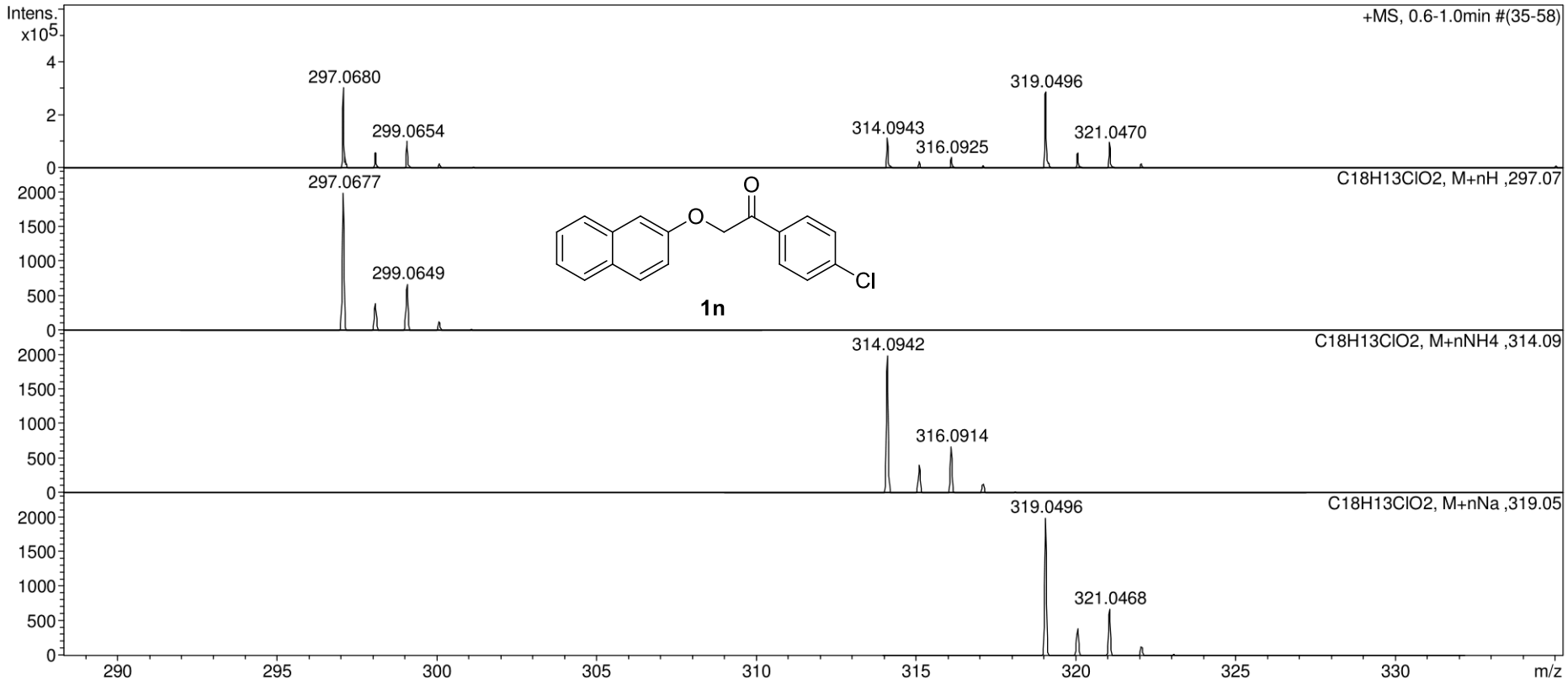

Acquisition Parameter

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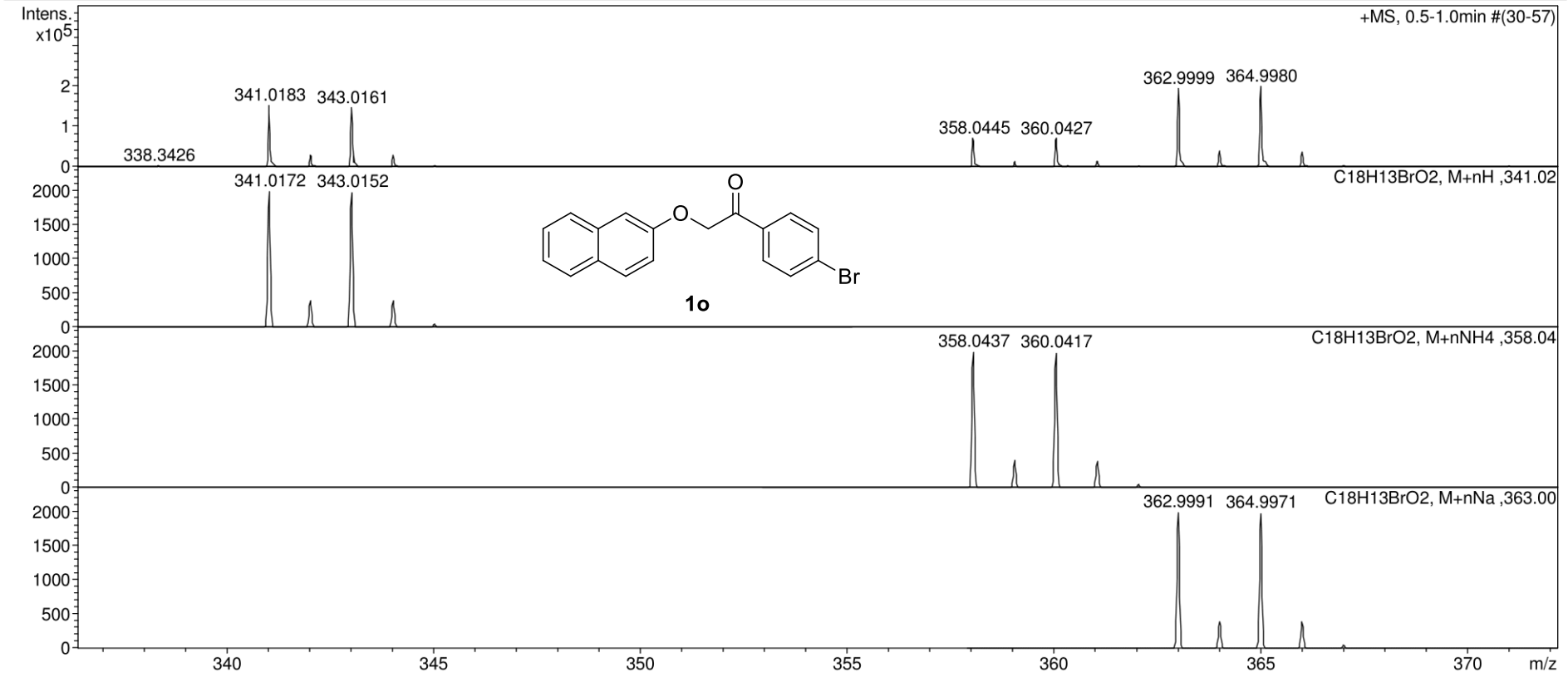
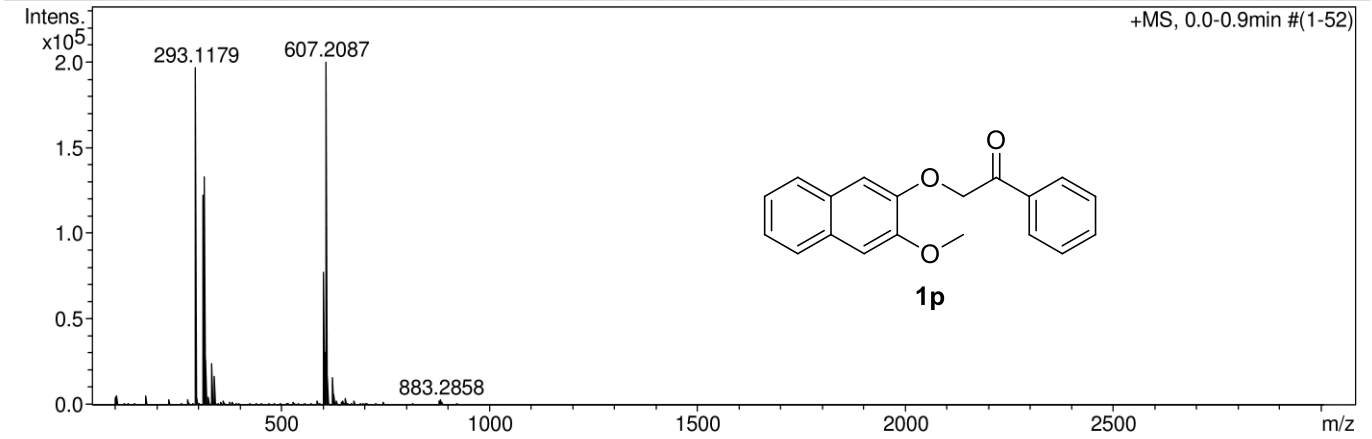
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



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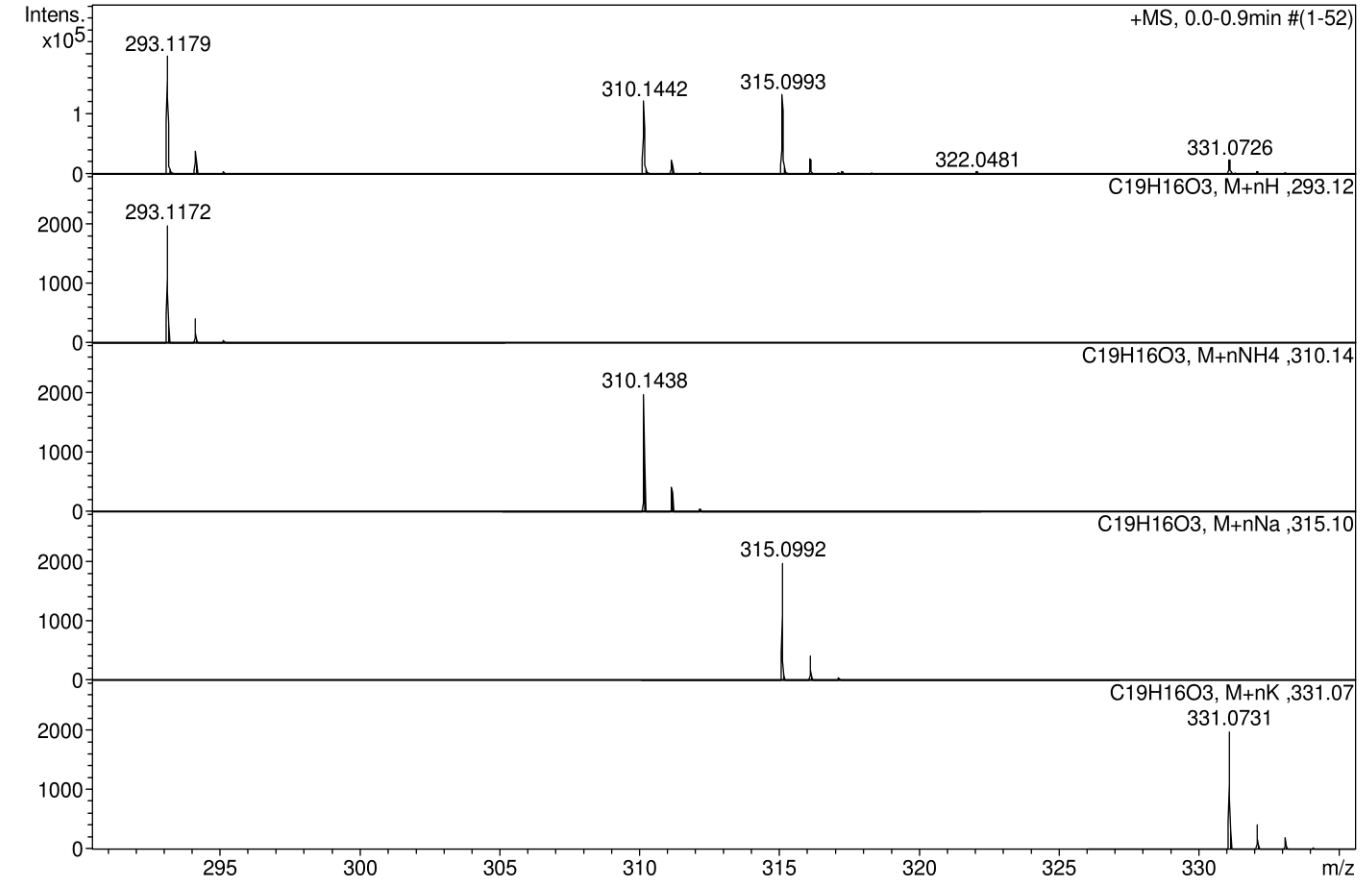
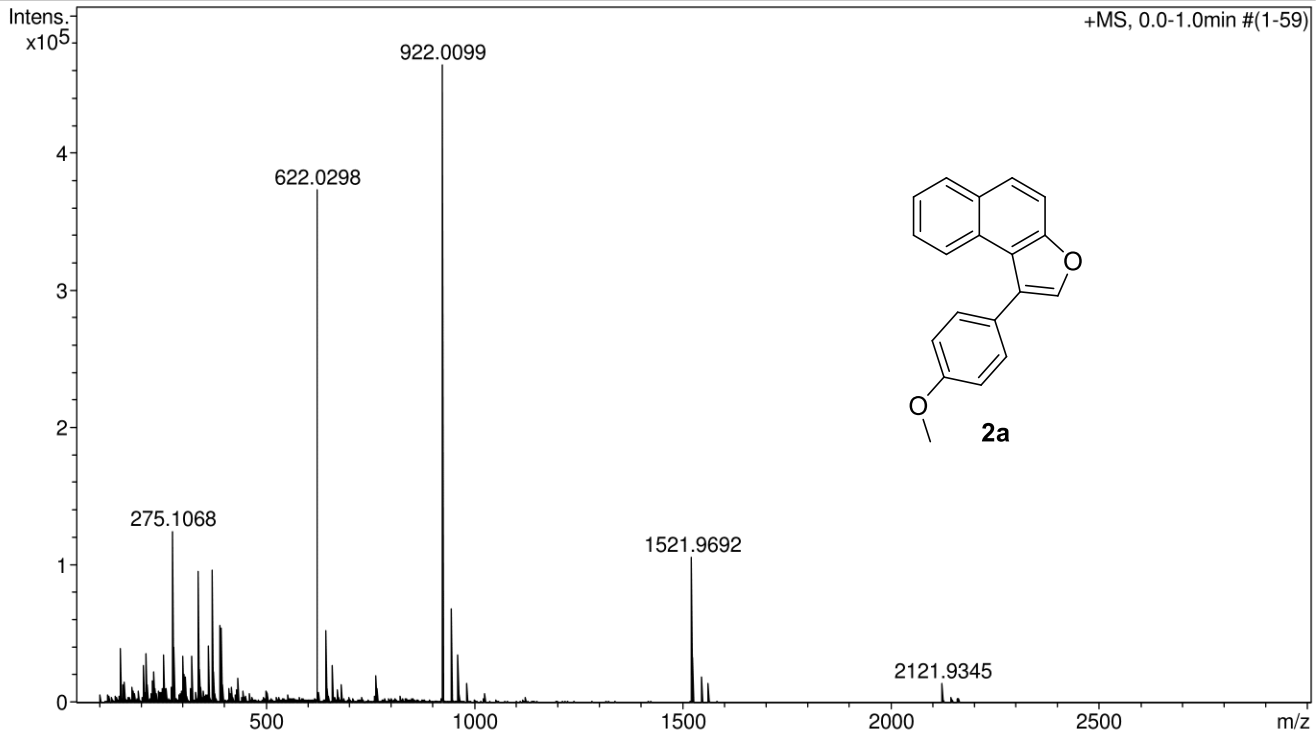
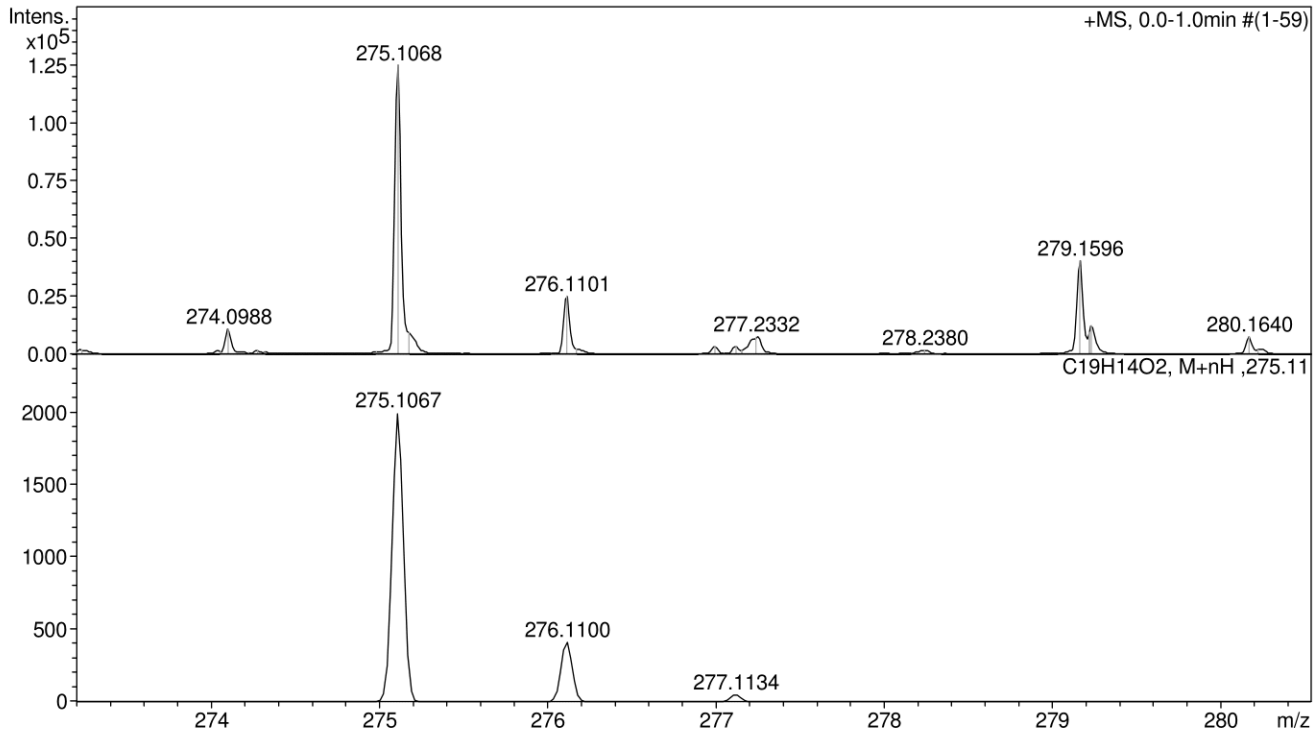


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 ℃
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





Acquisition Parameter

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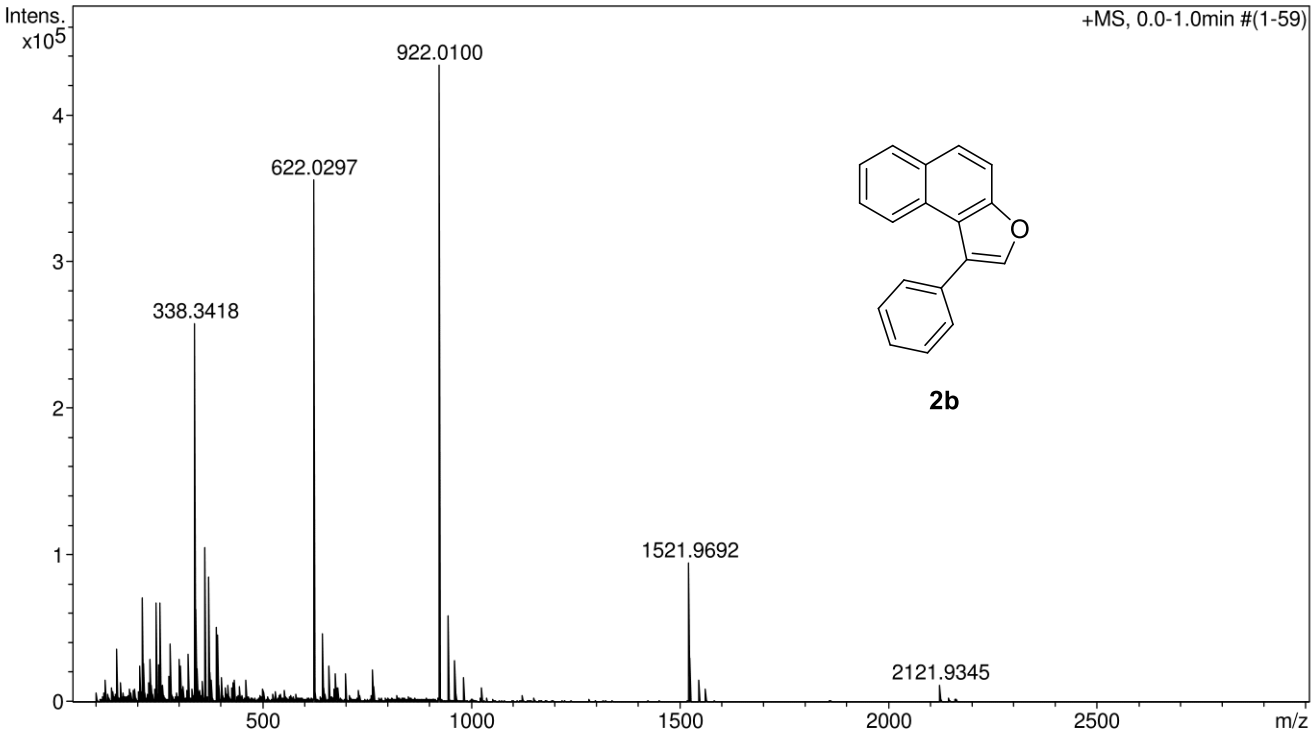
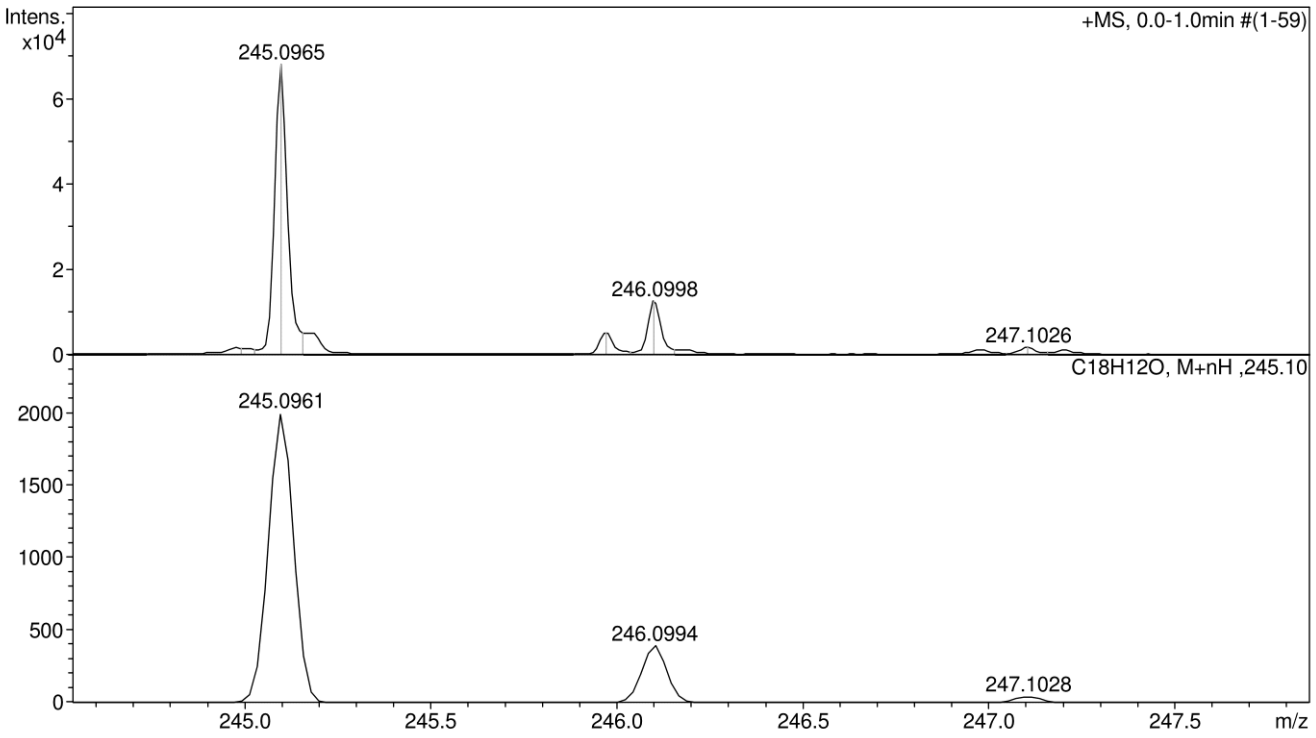
Focus	Not active			Set Dry Heater	180 ℃
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 ℃
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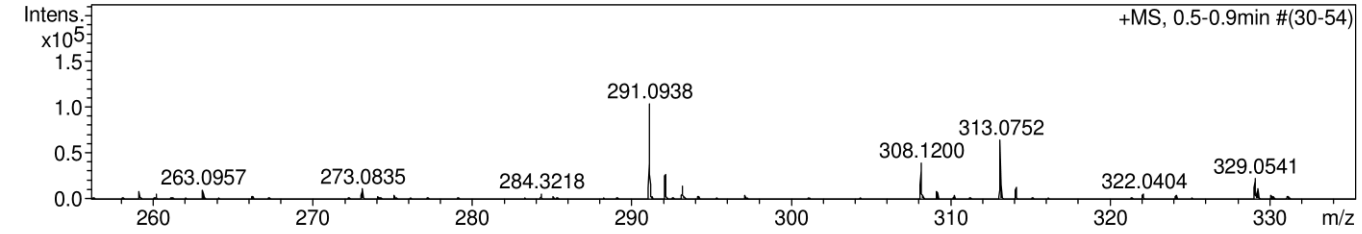
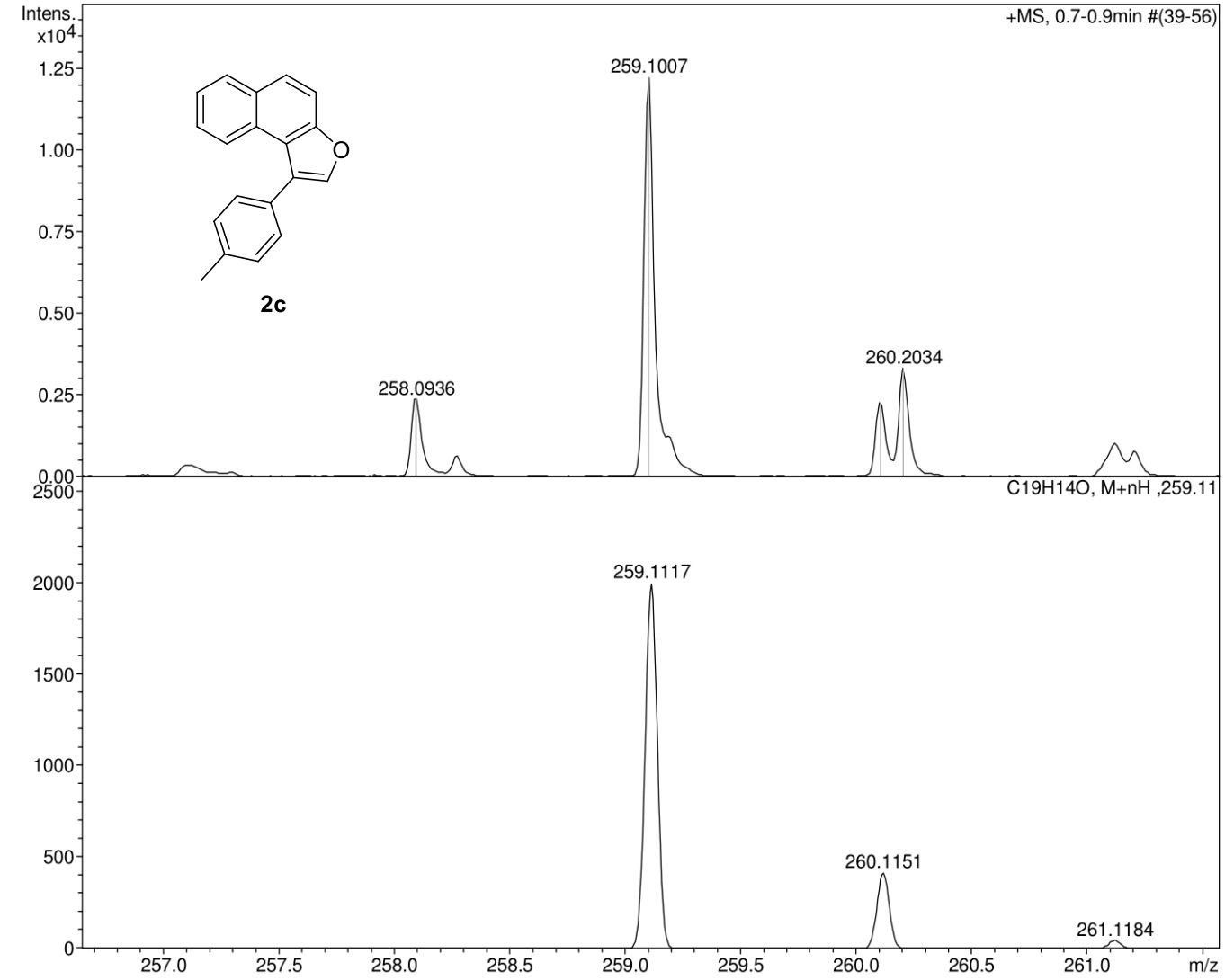
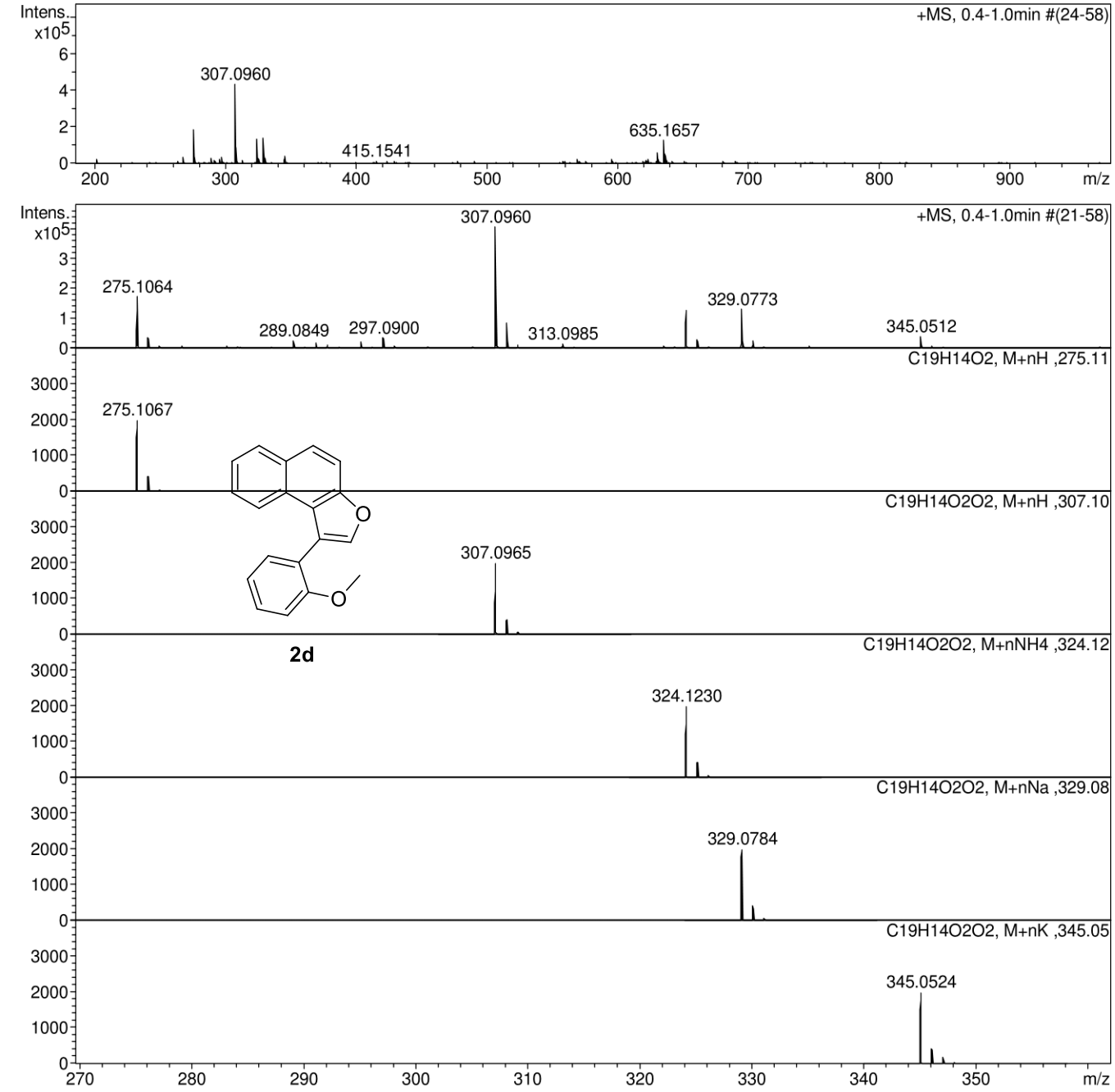
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





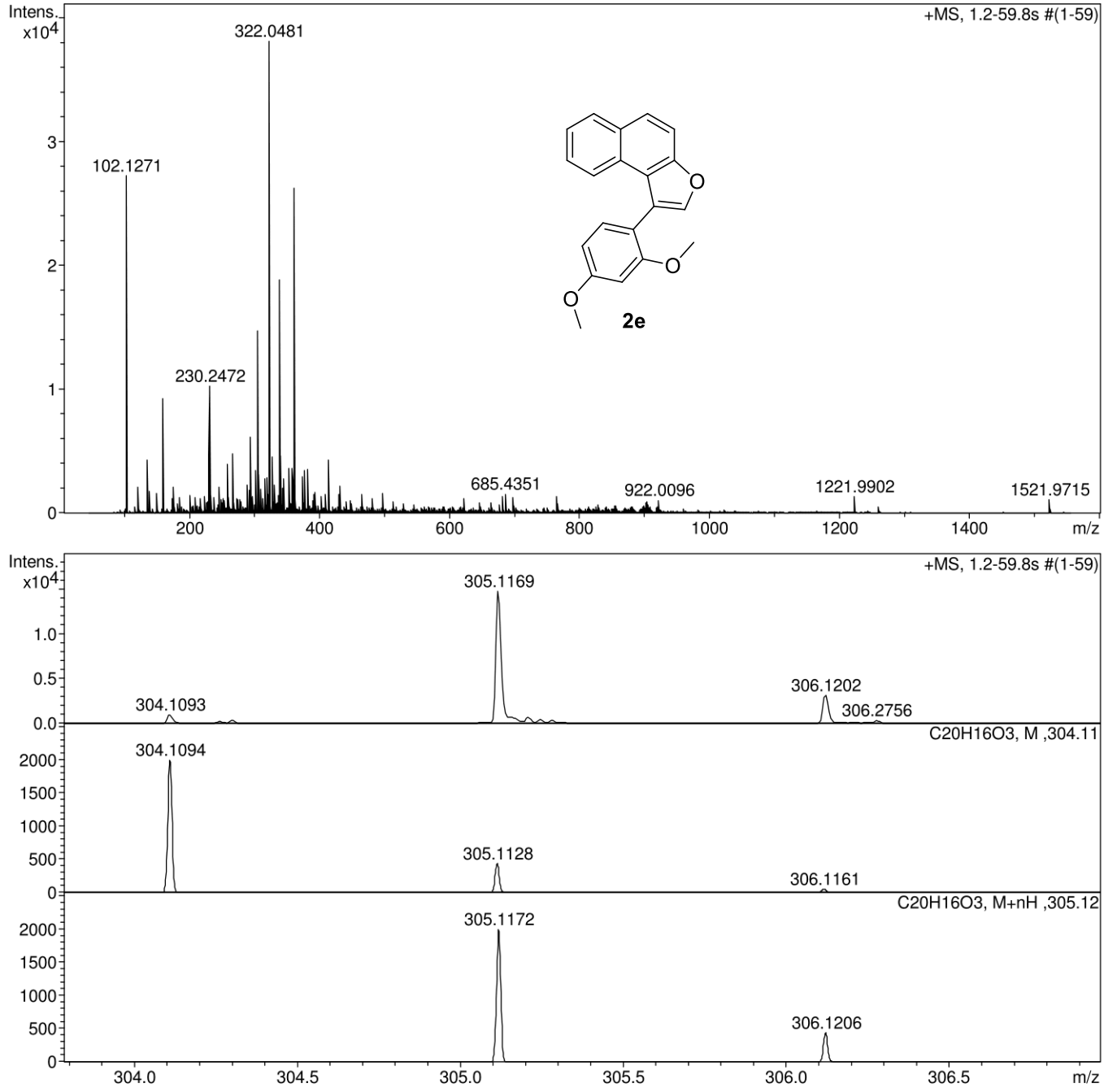
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 ℃
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



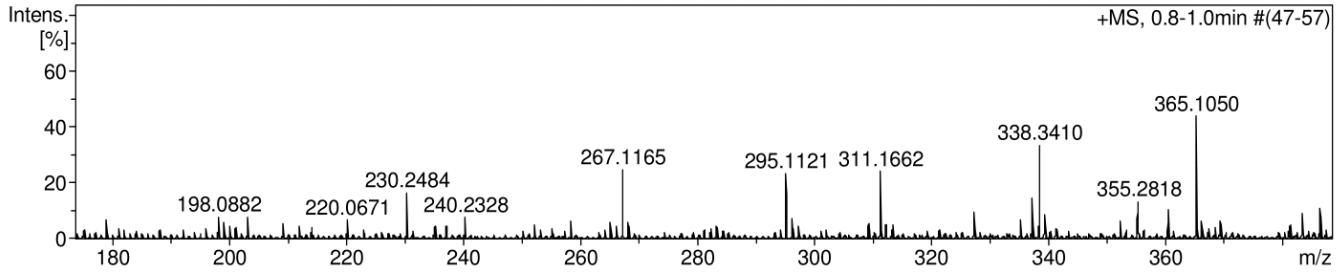
Acquisition Parameter

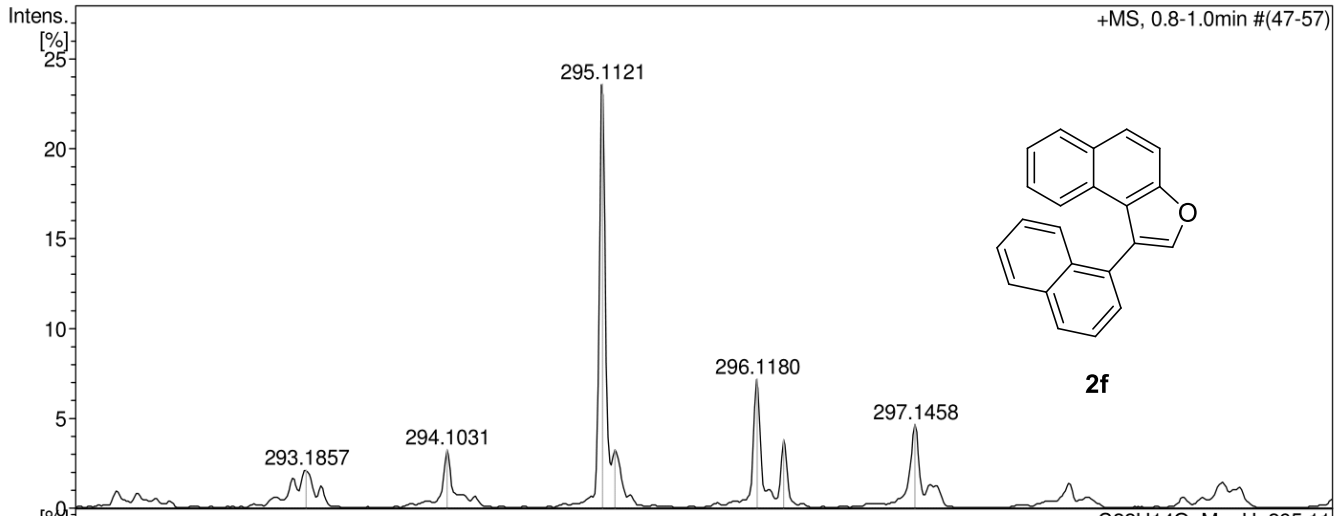
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1550 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

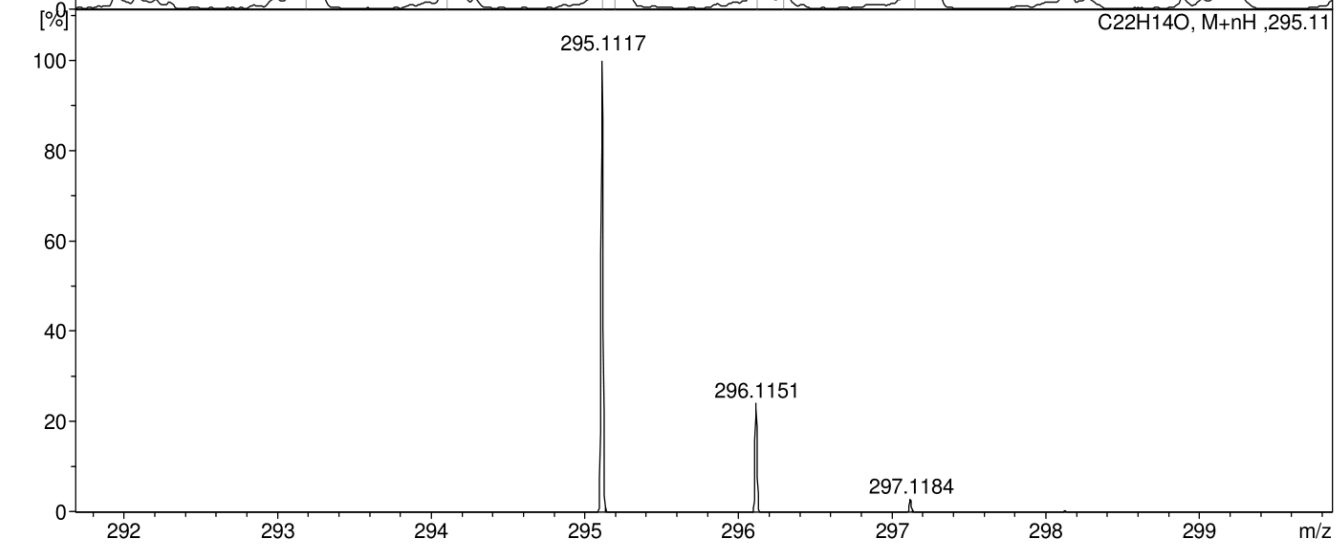


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

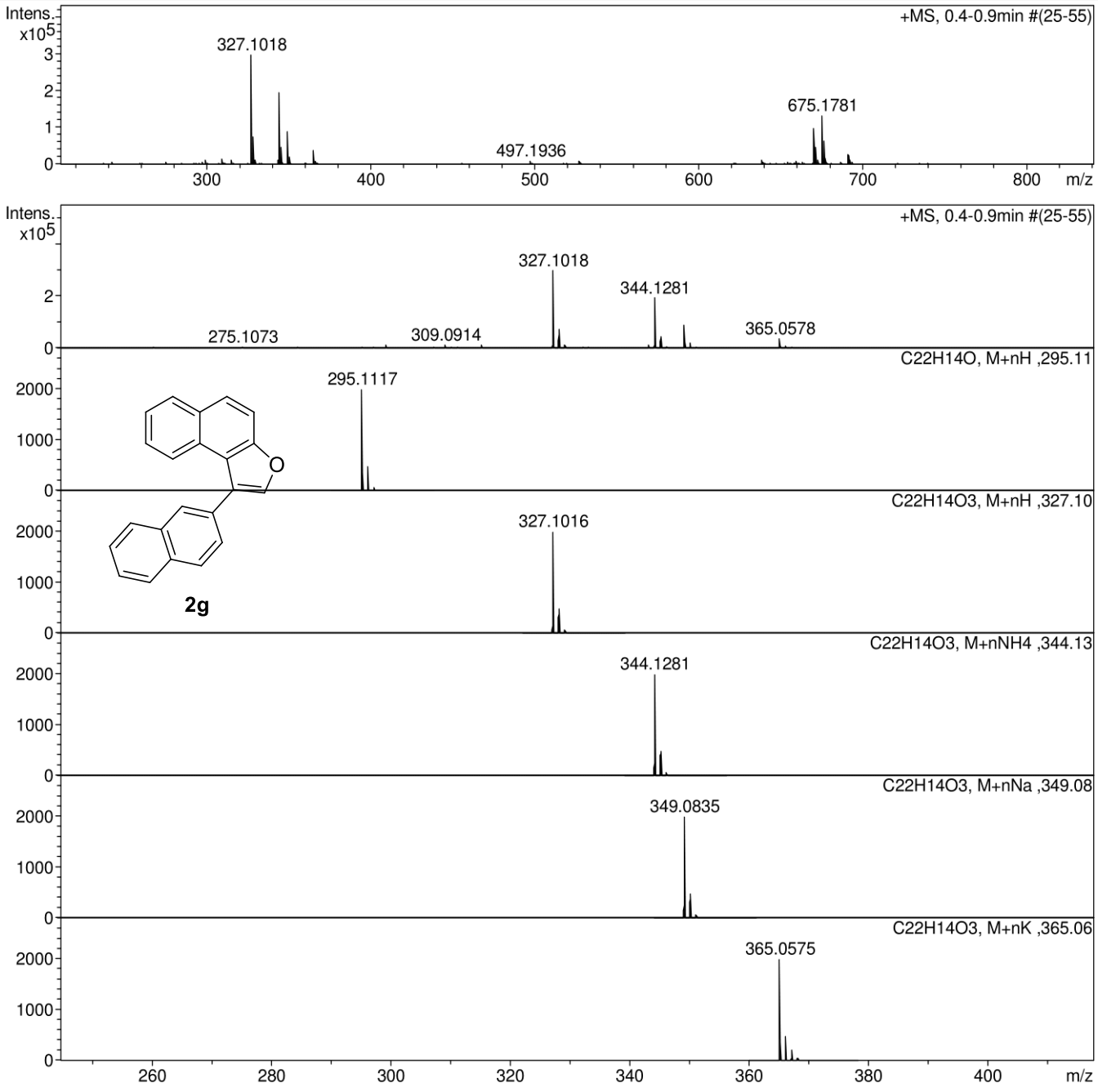






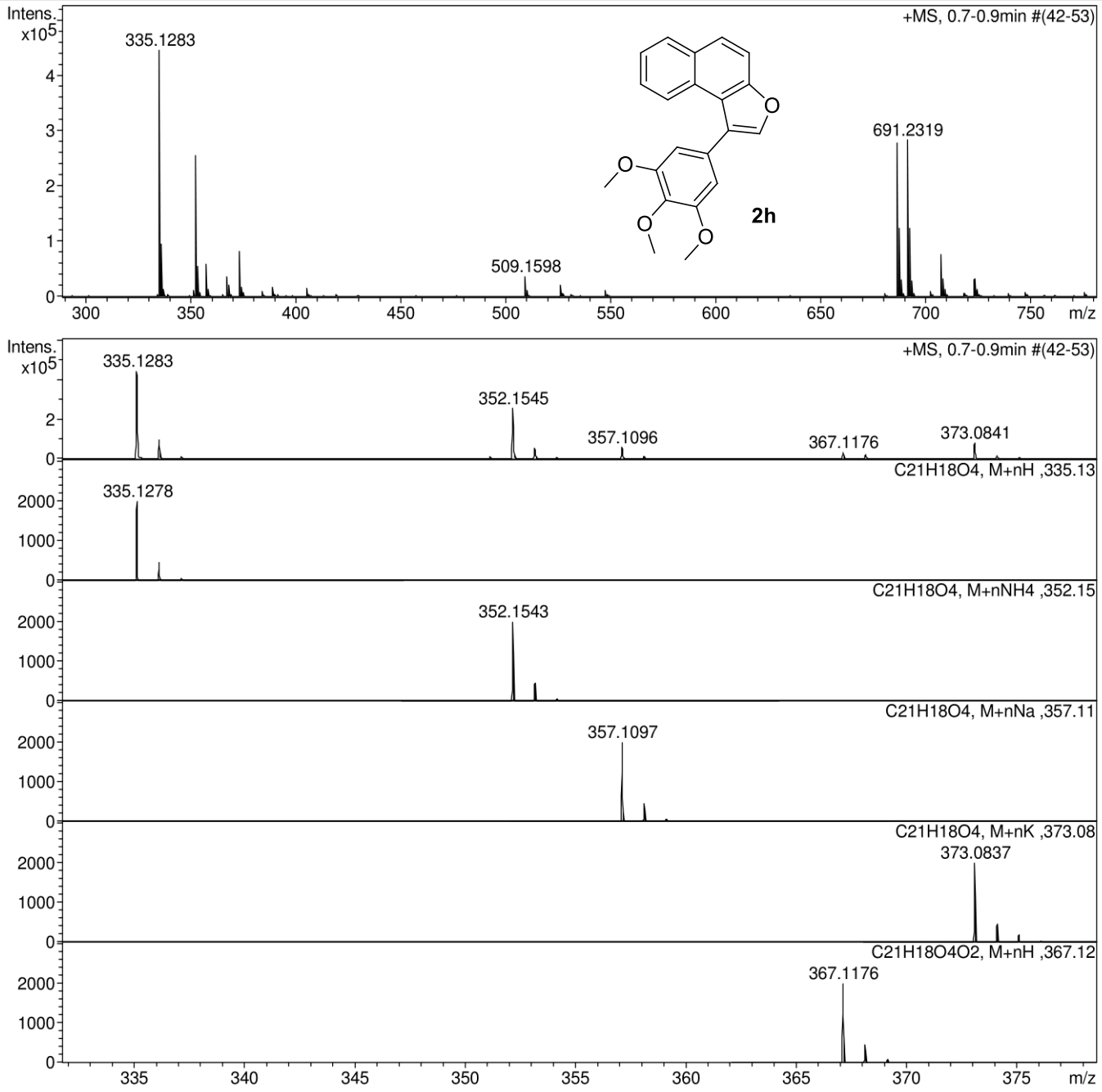
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



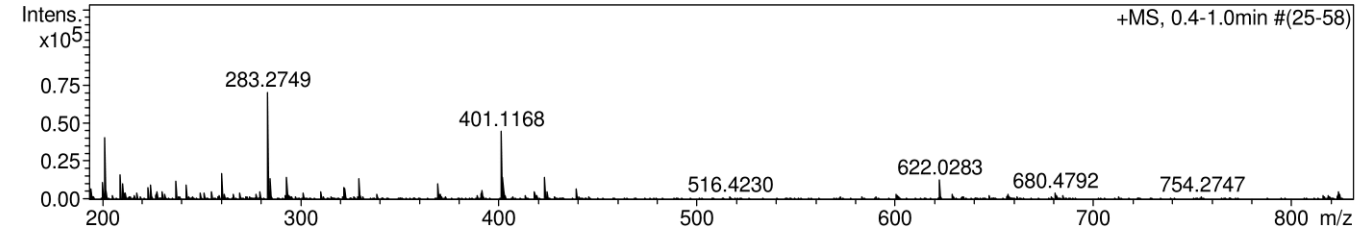
Acquisition Parameter

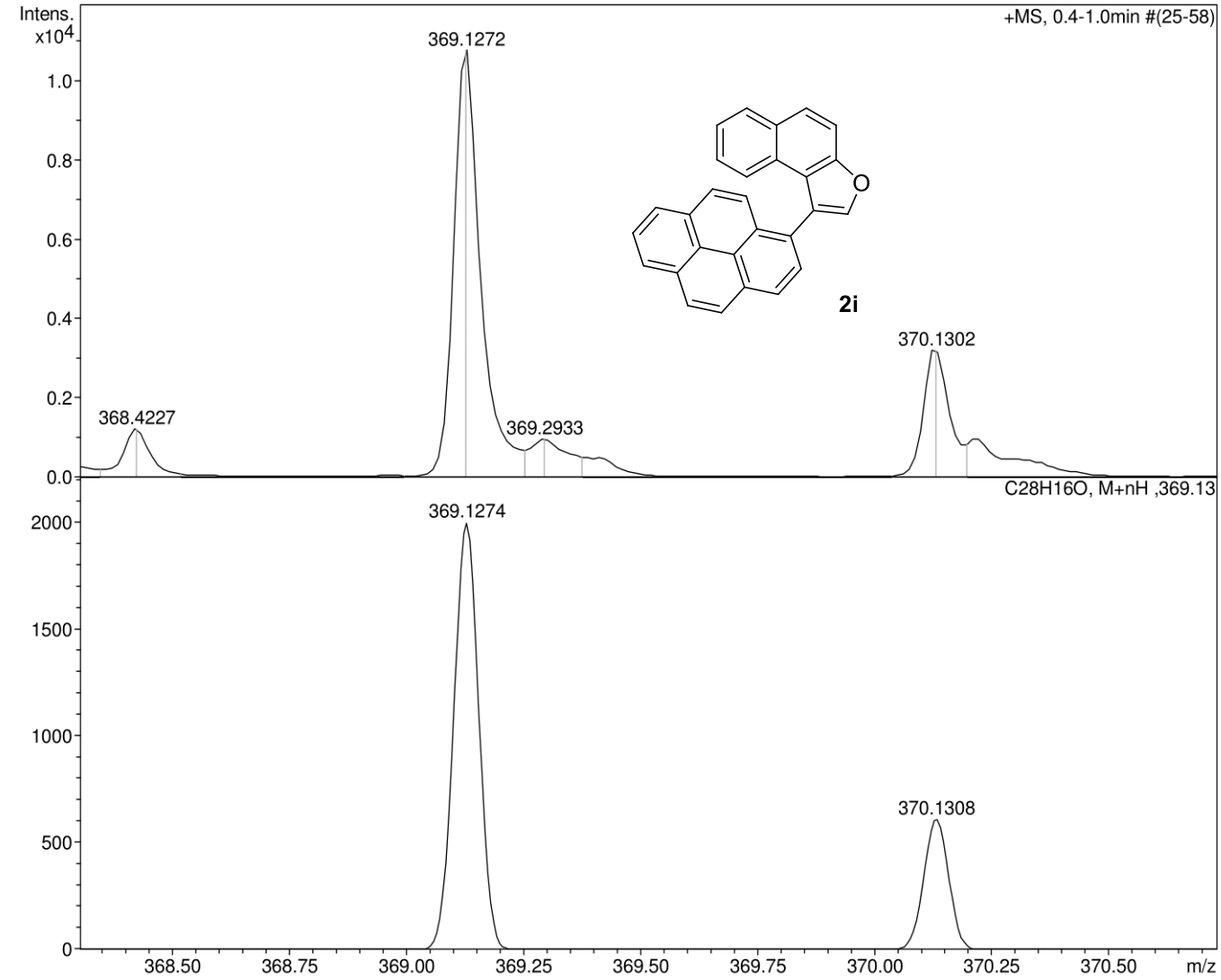
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Acquisition Parameter

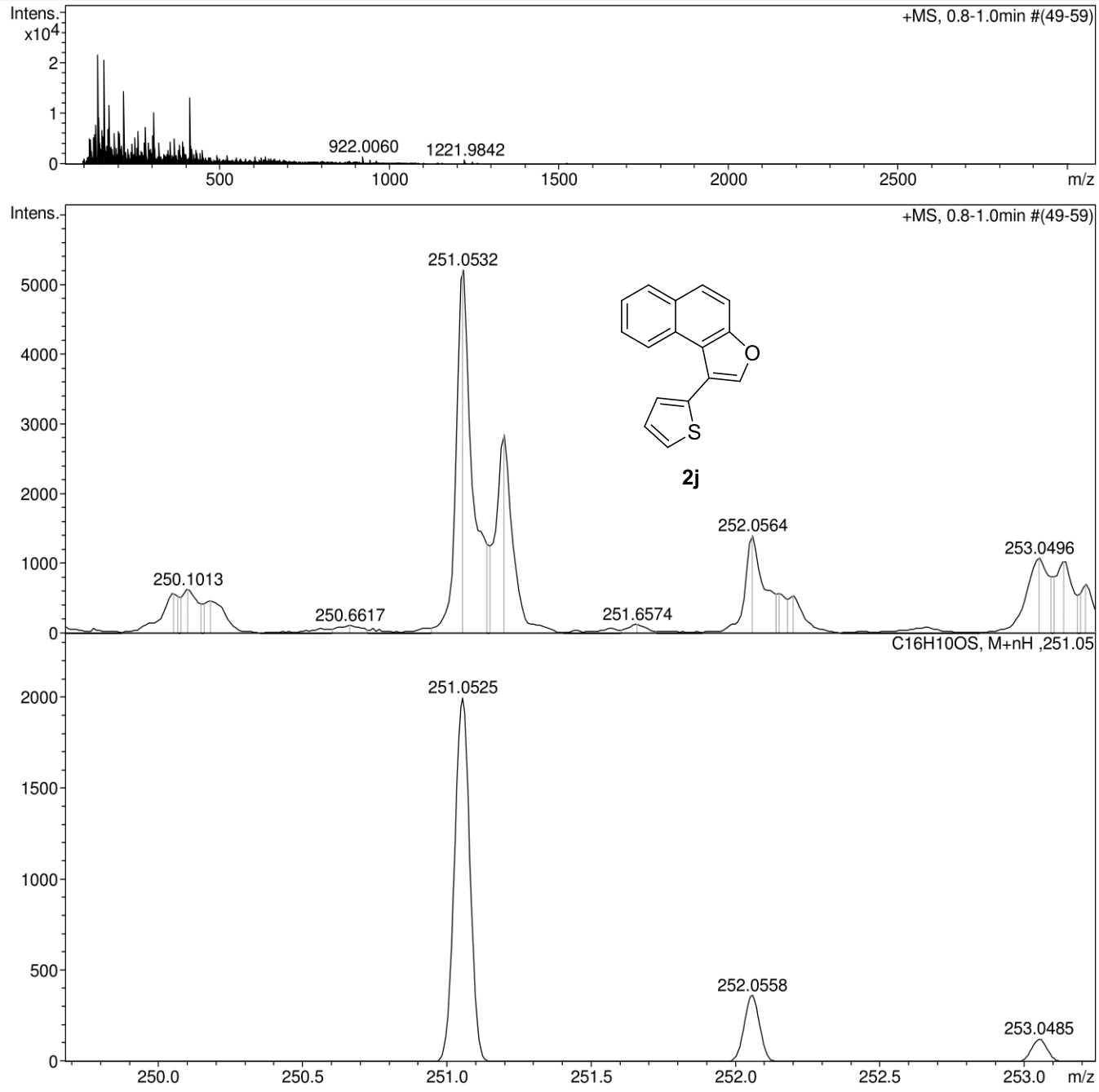
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





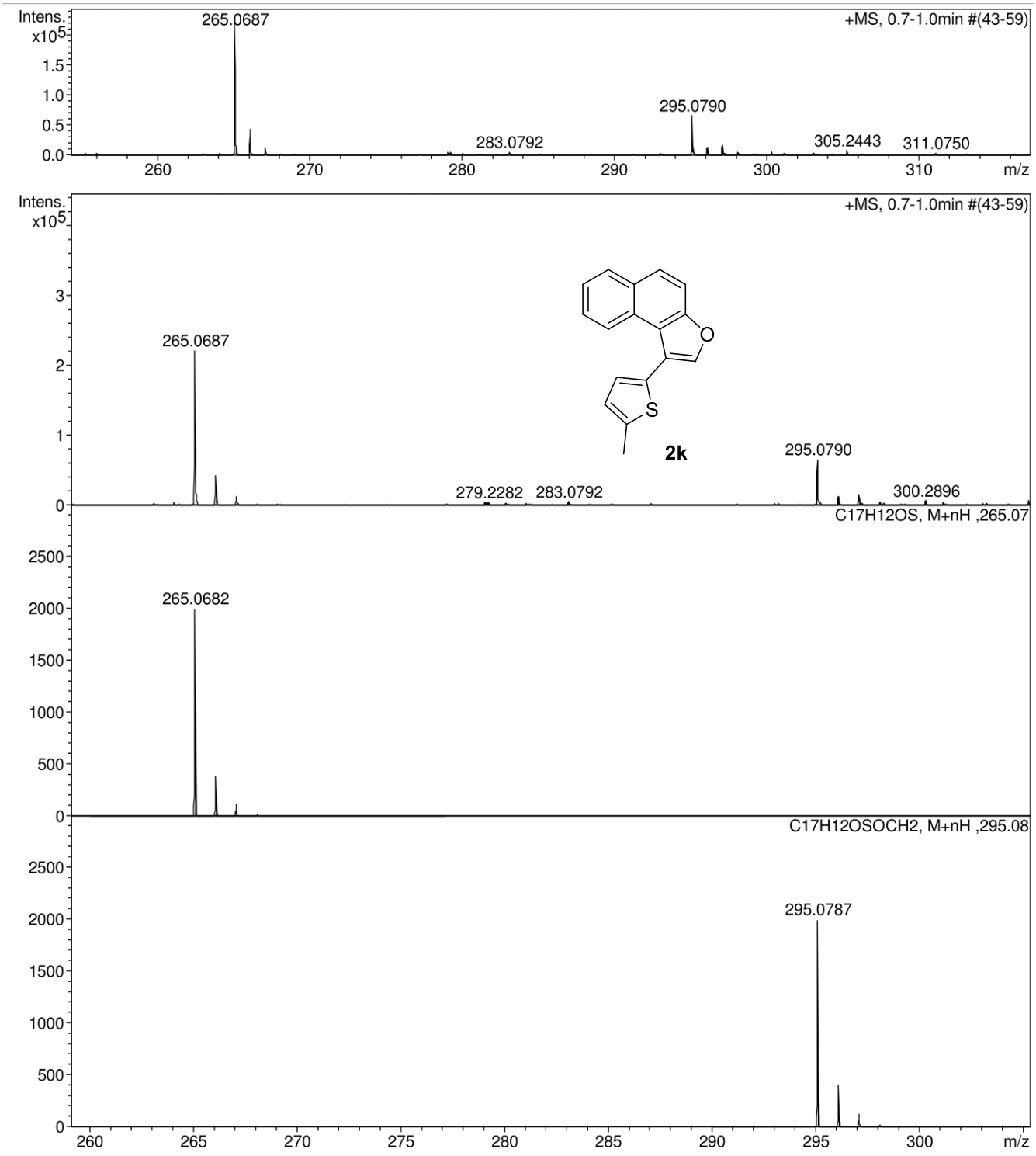
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



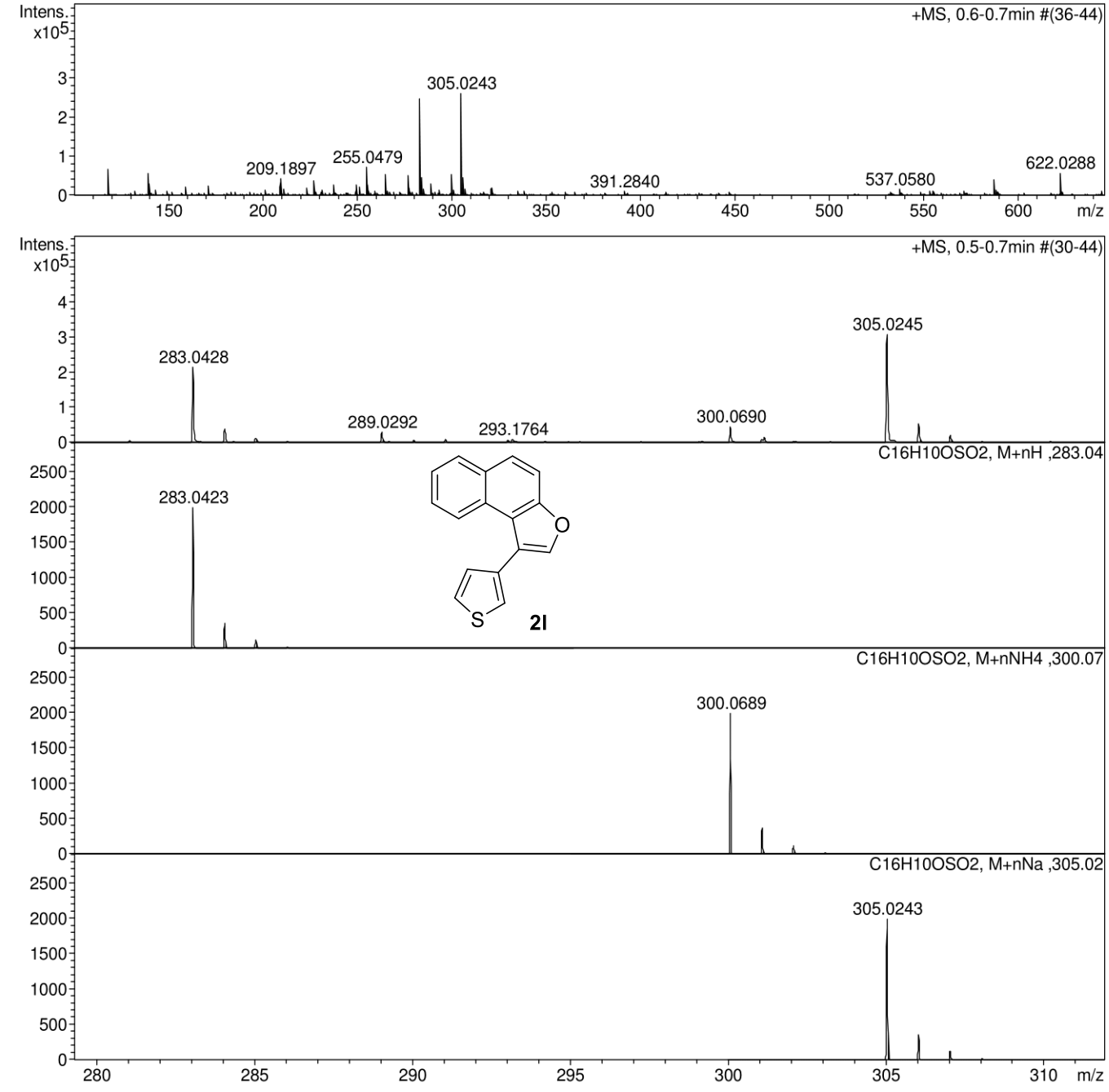
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



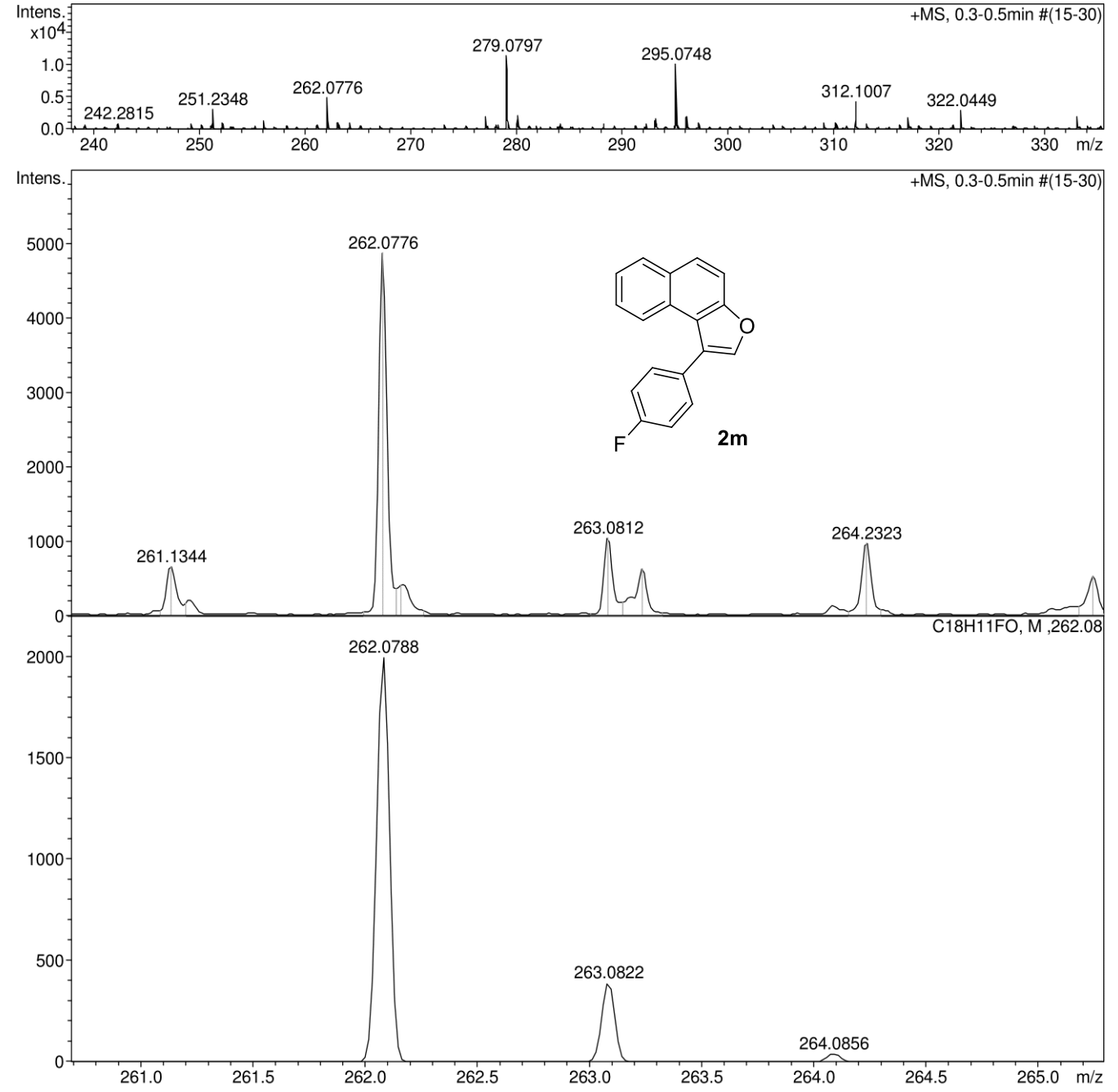
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



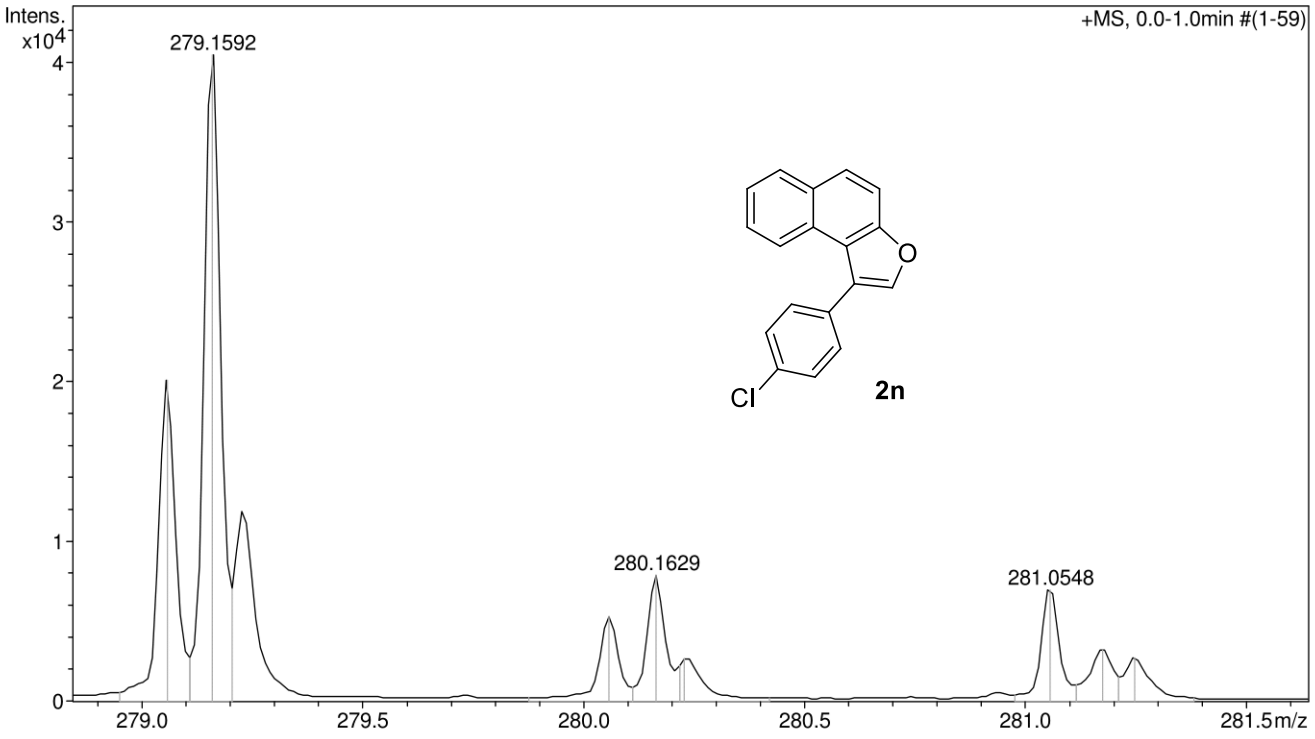
Acquisition Parameter

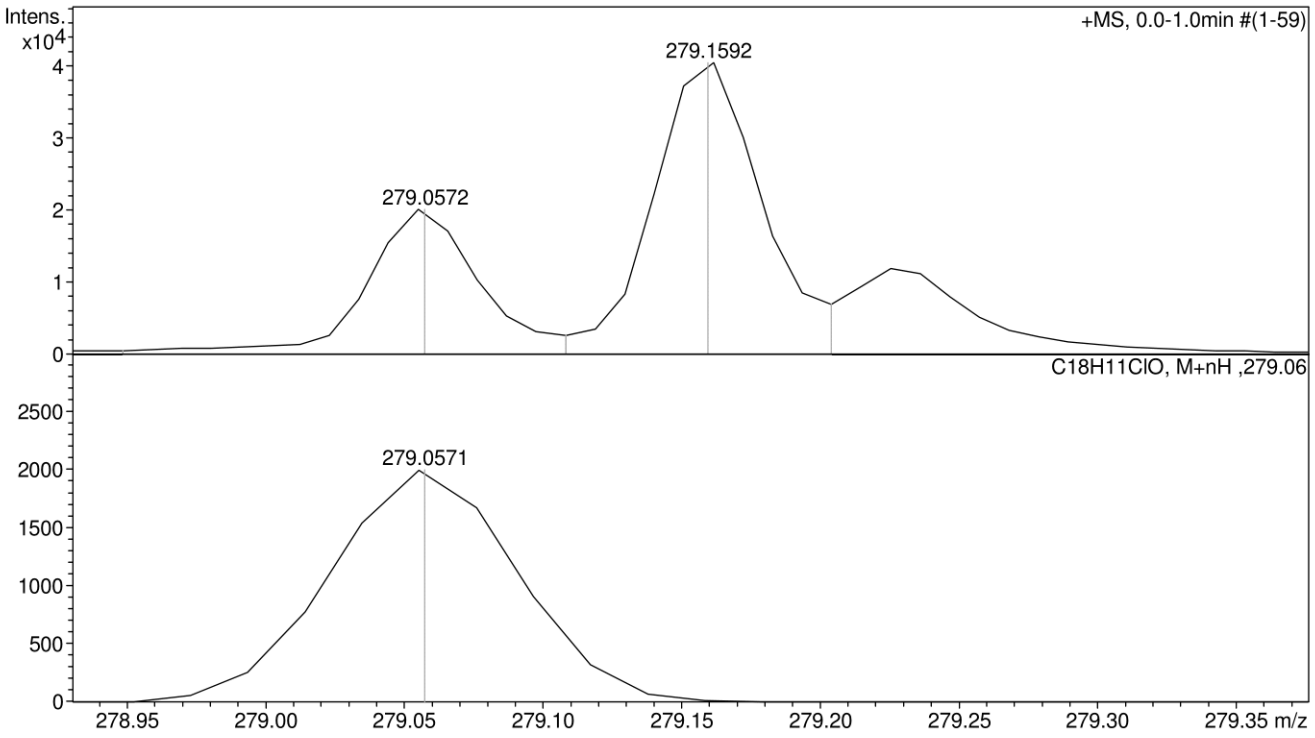
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Acquisition Parameter

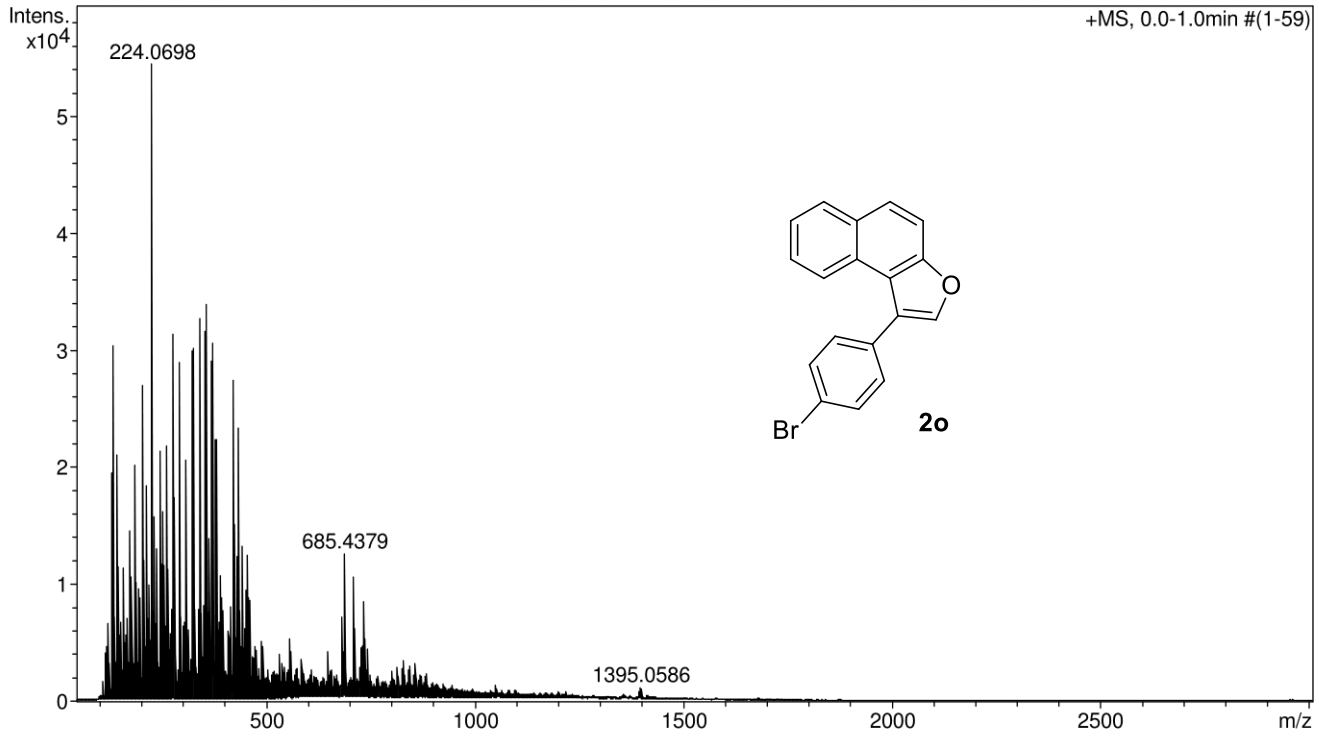
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 ℃
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

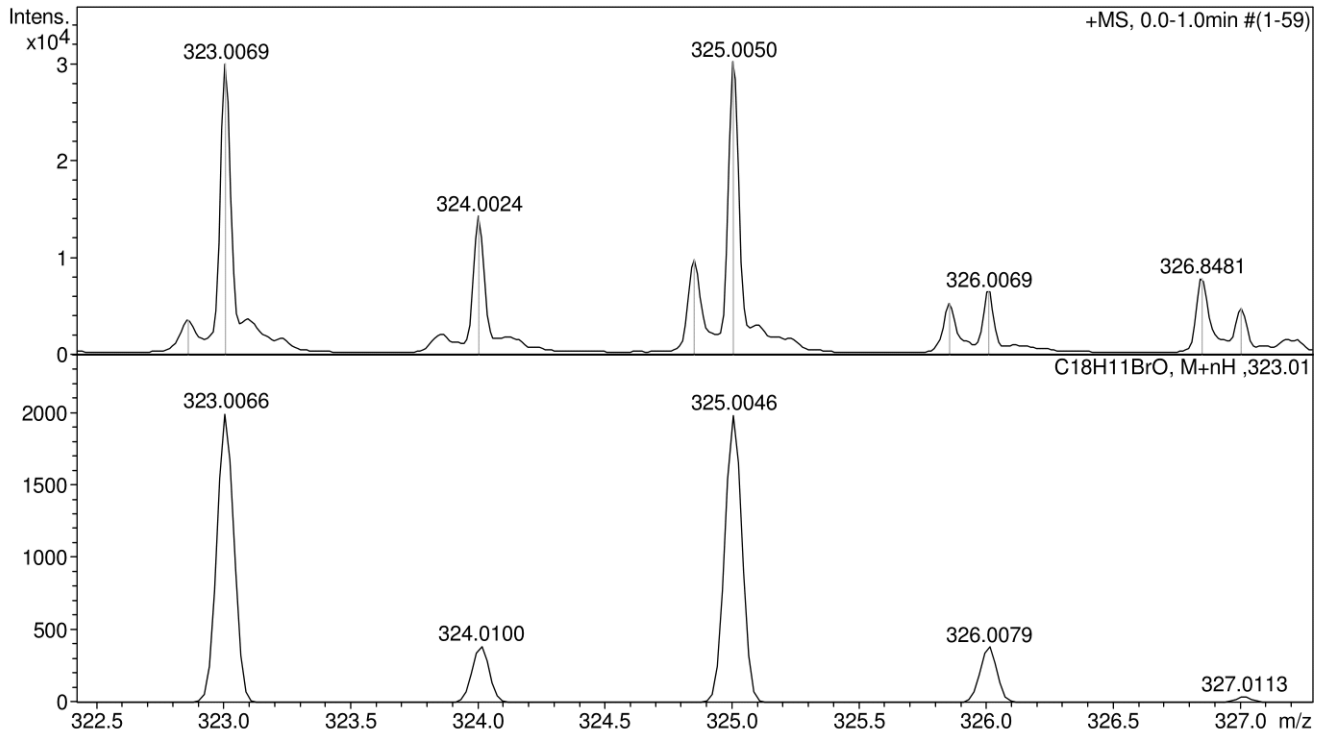




Acquisition Parameter

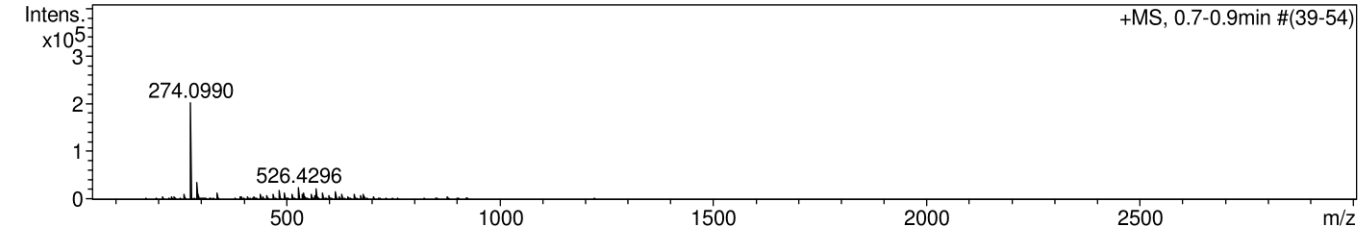
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

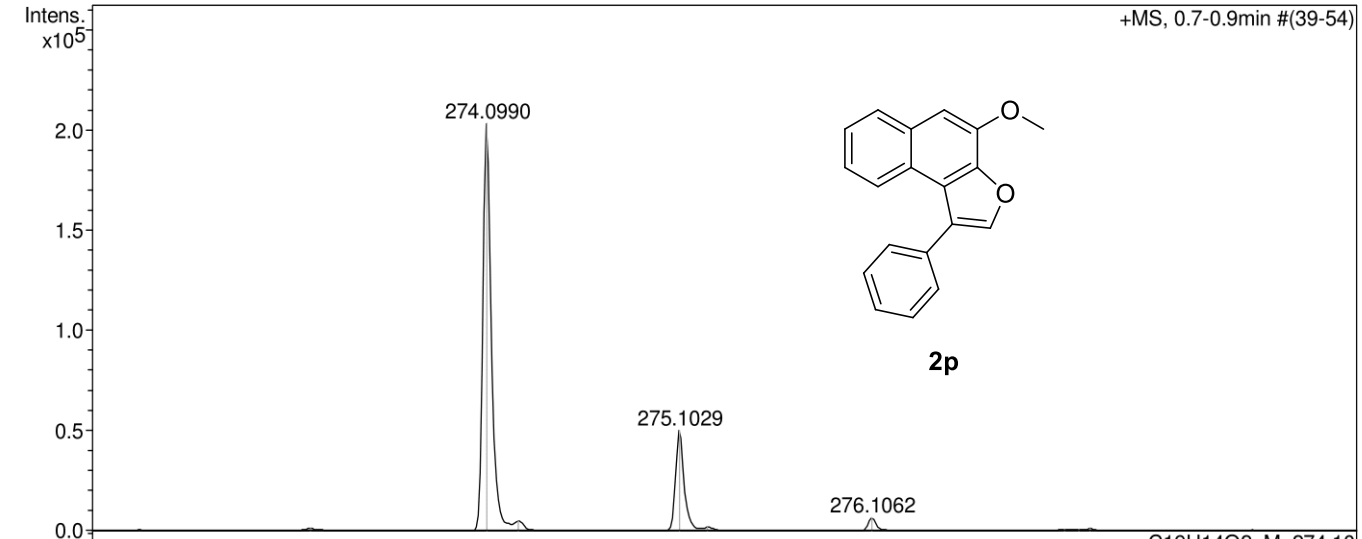




Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





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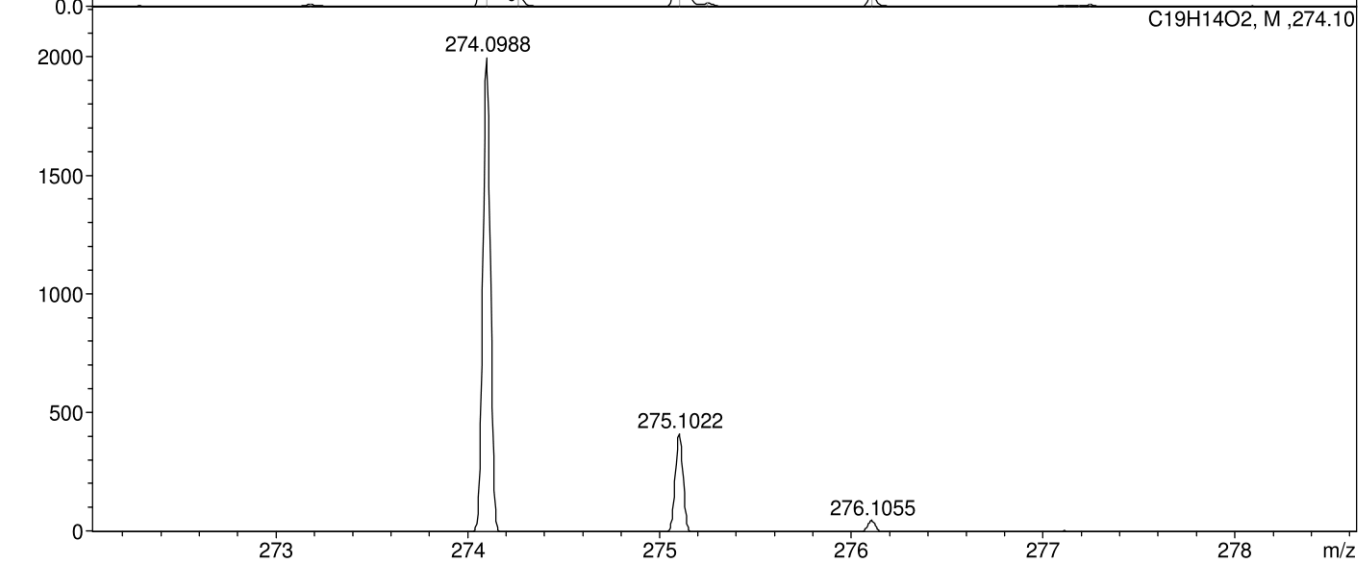
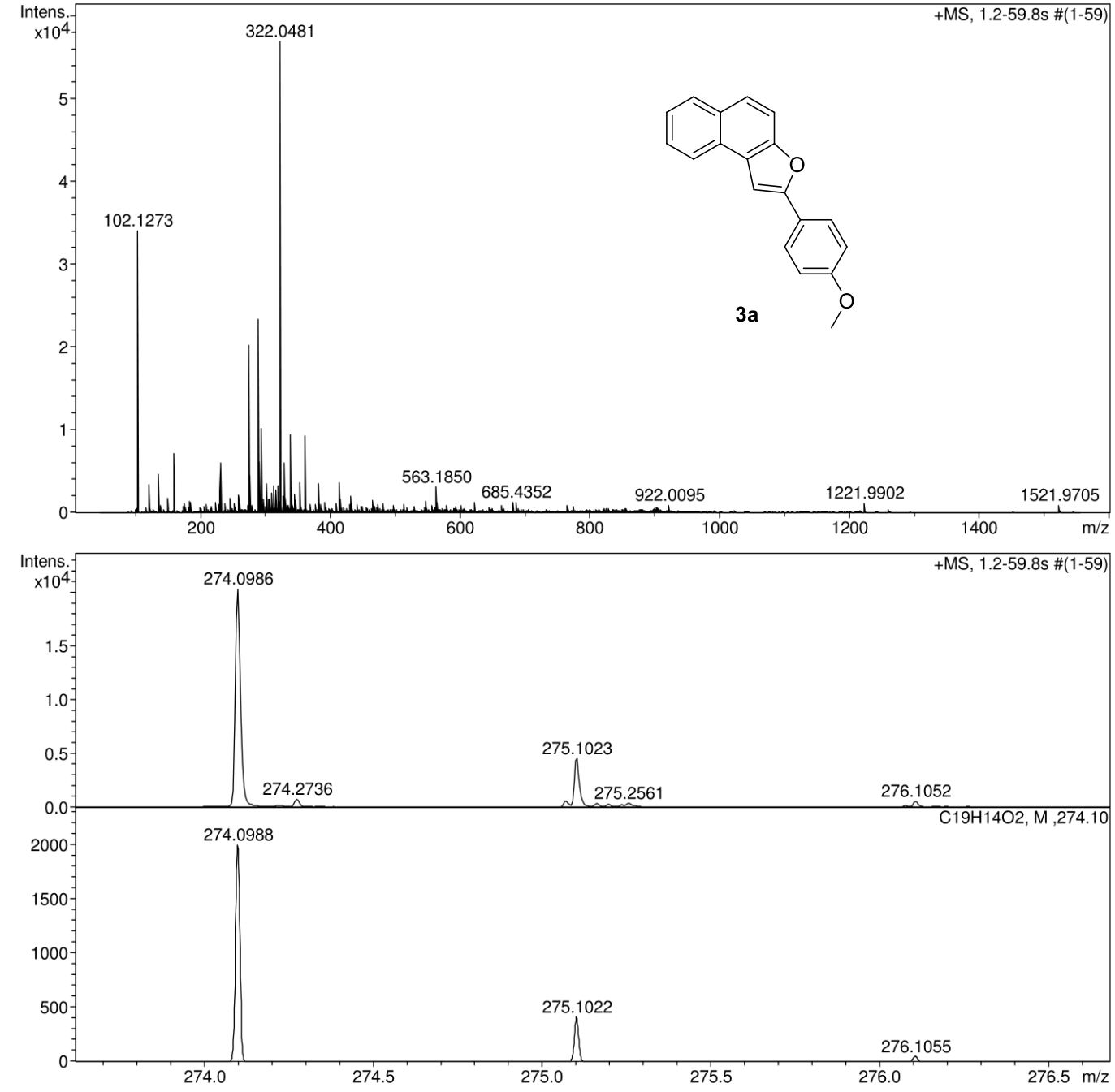


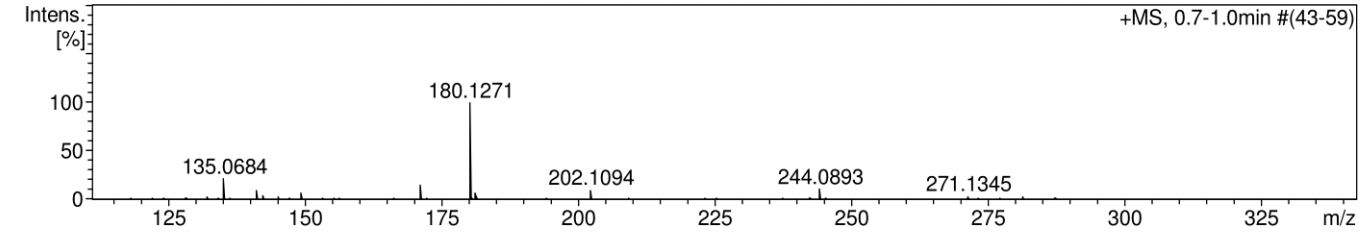
Acquisition Parameter

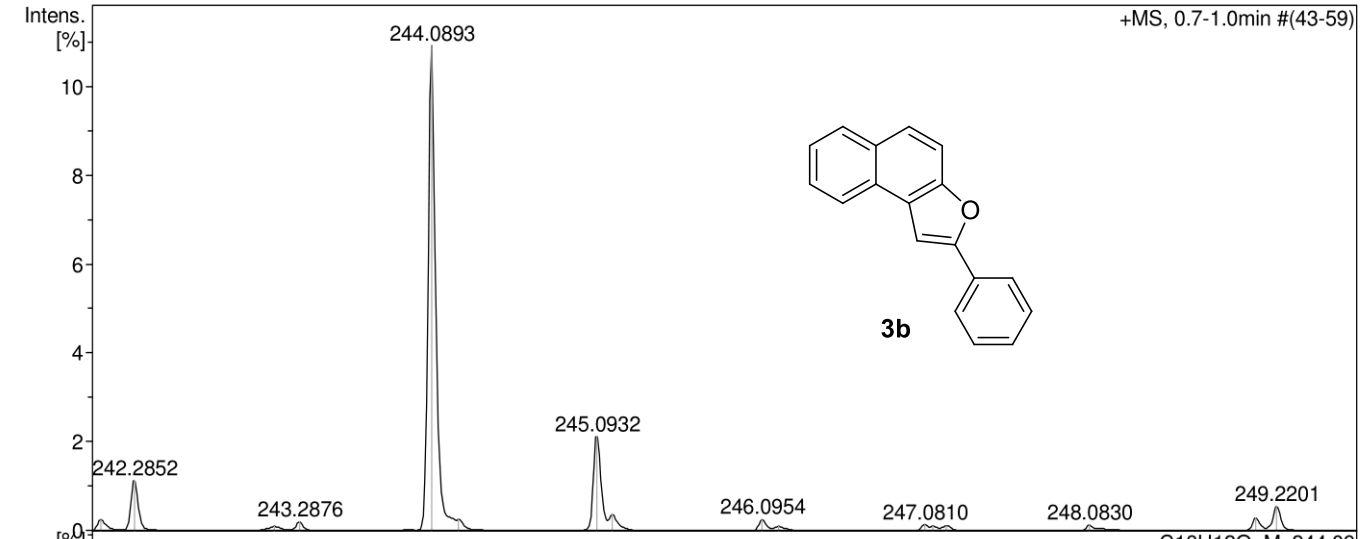
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1550 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

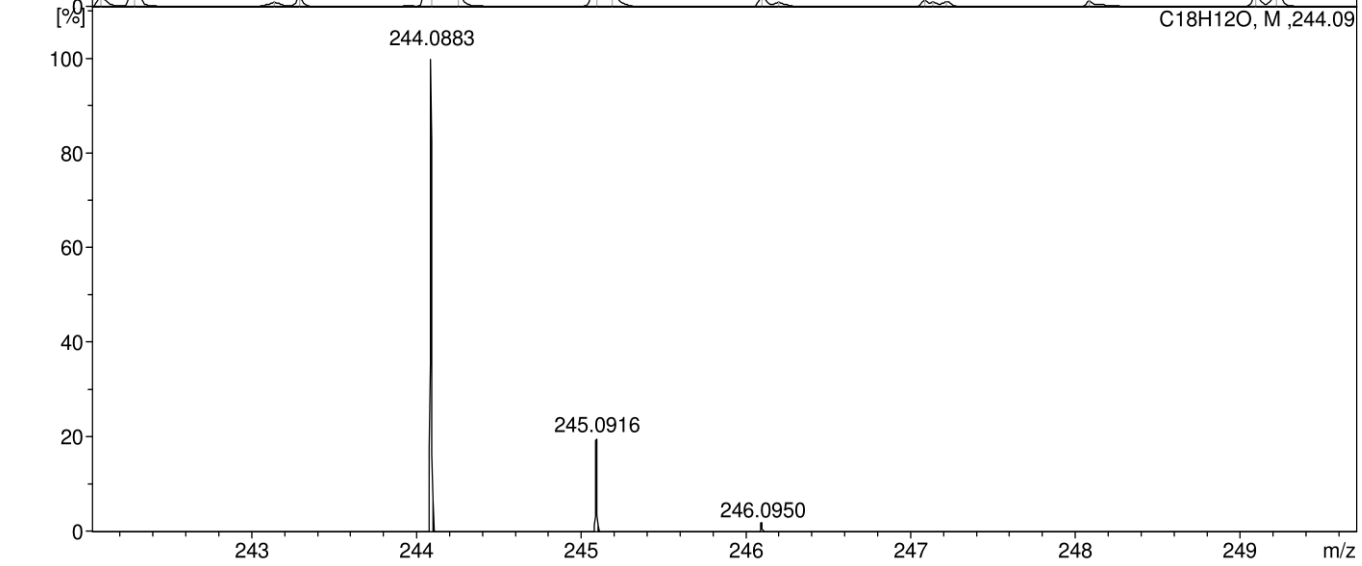


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

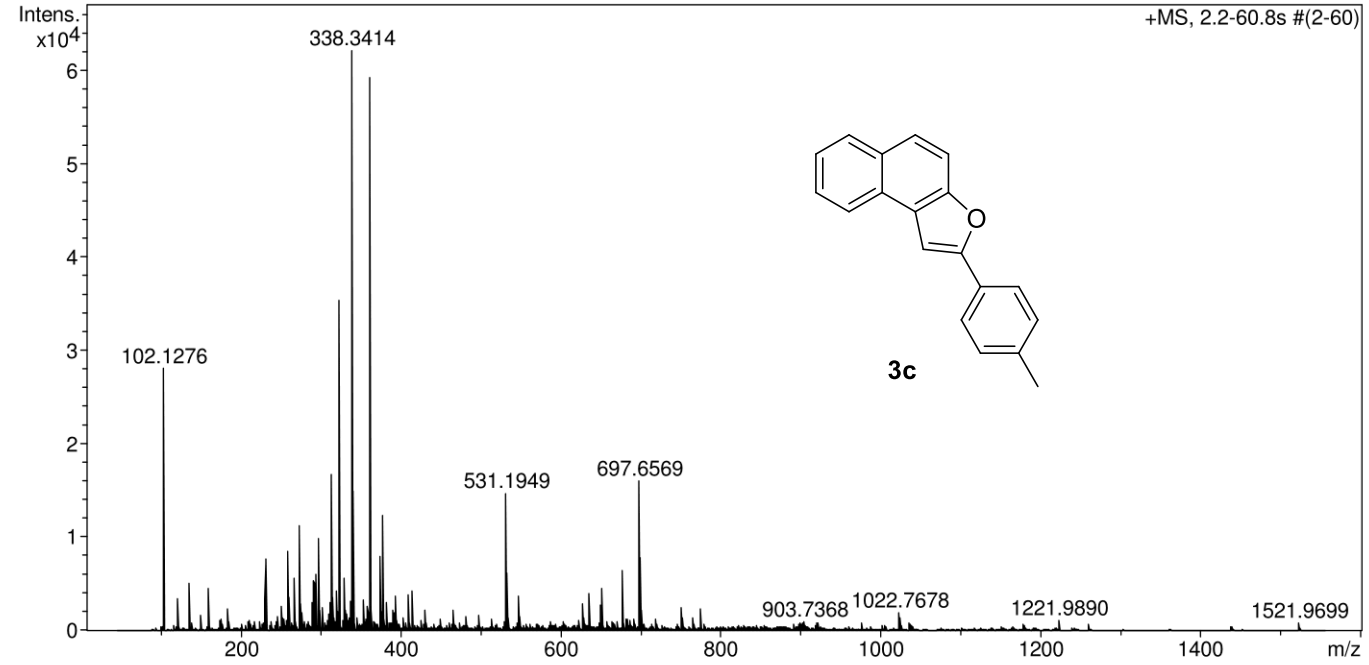


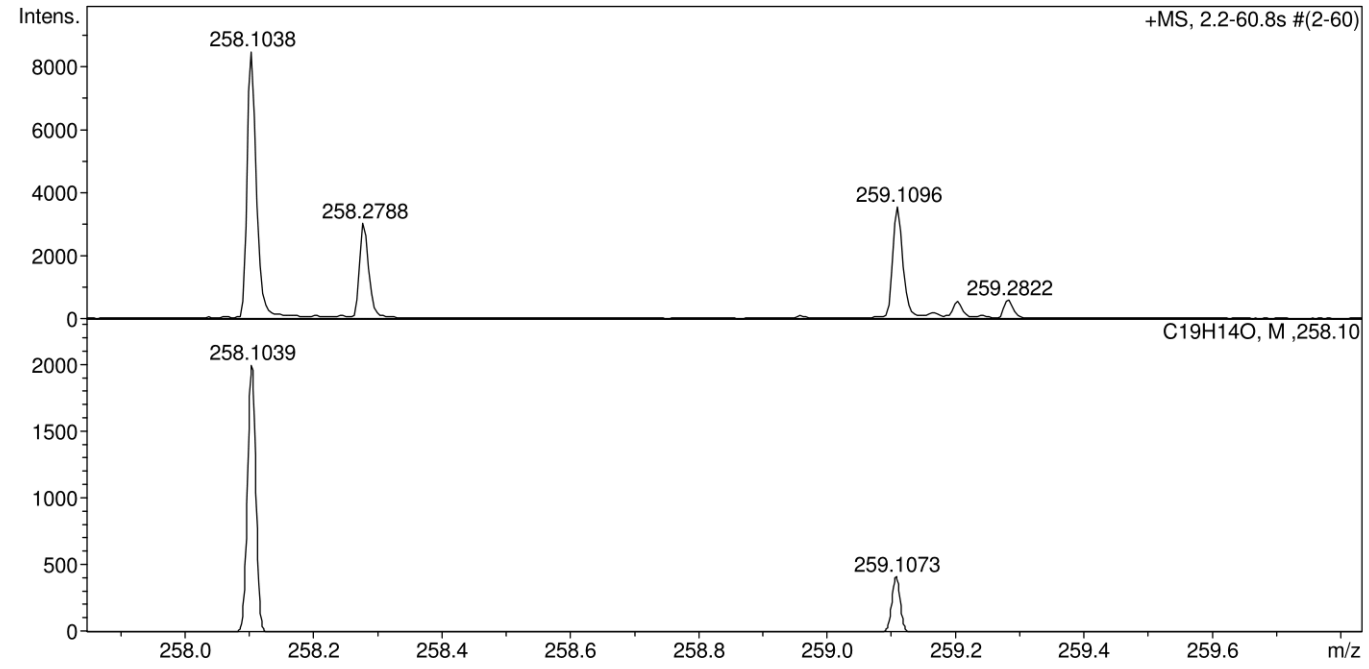




Acquisition Parameter

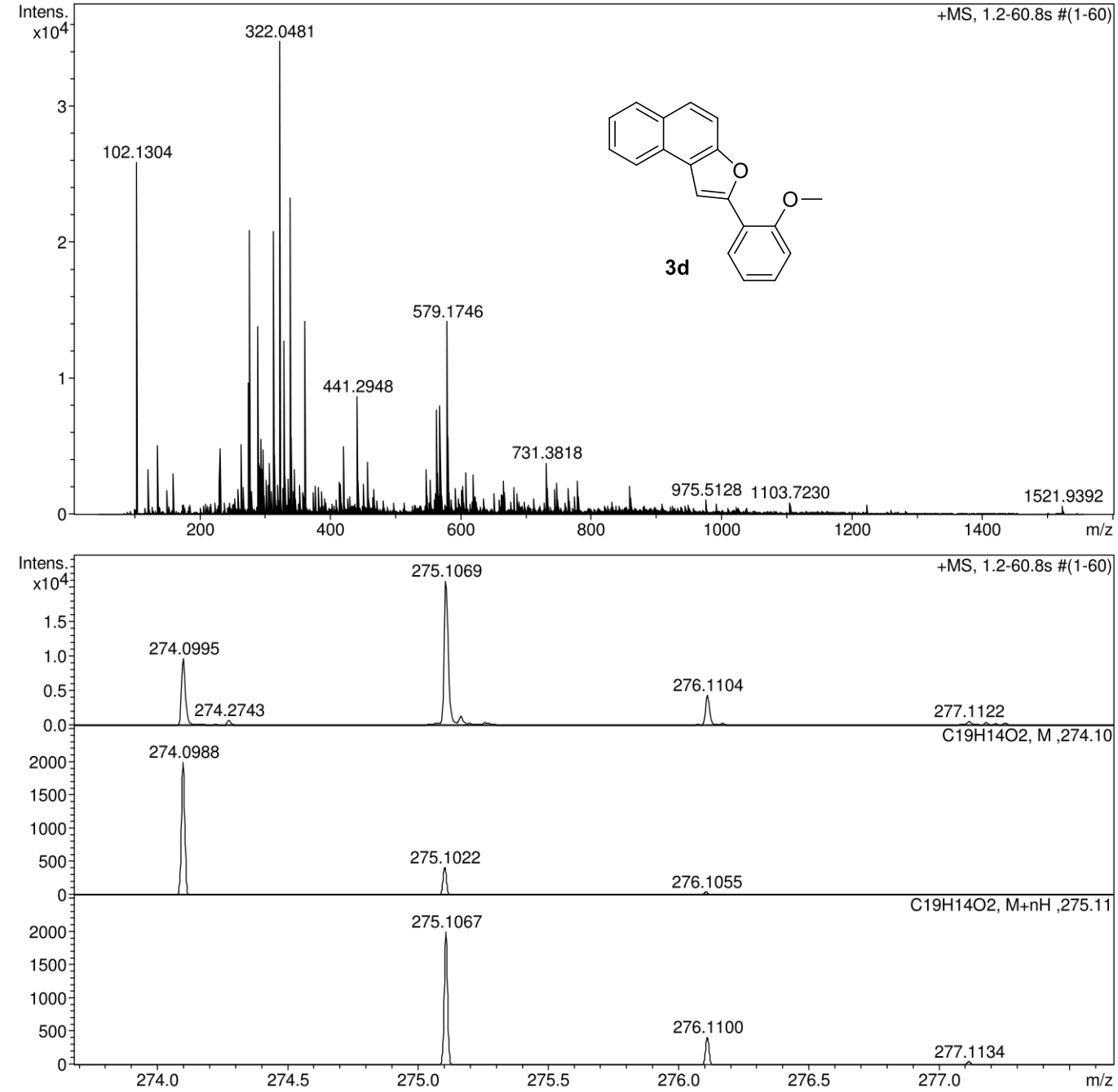
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1550 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source





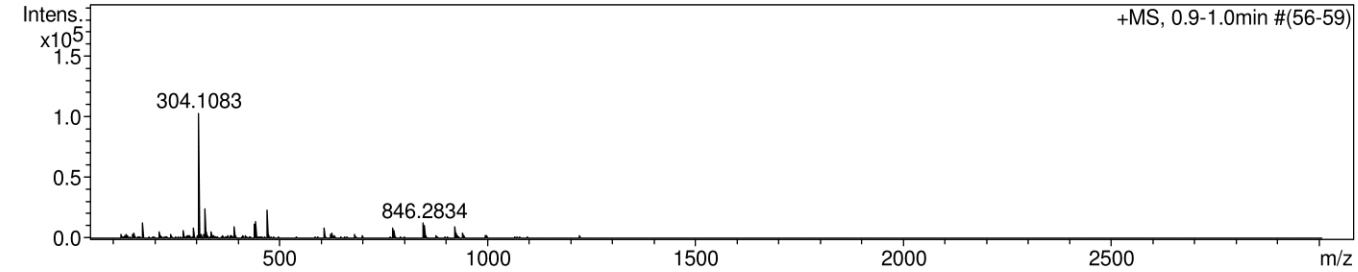
Acquisition Parameter

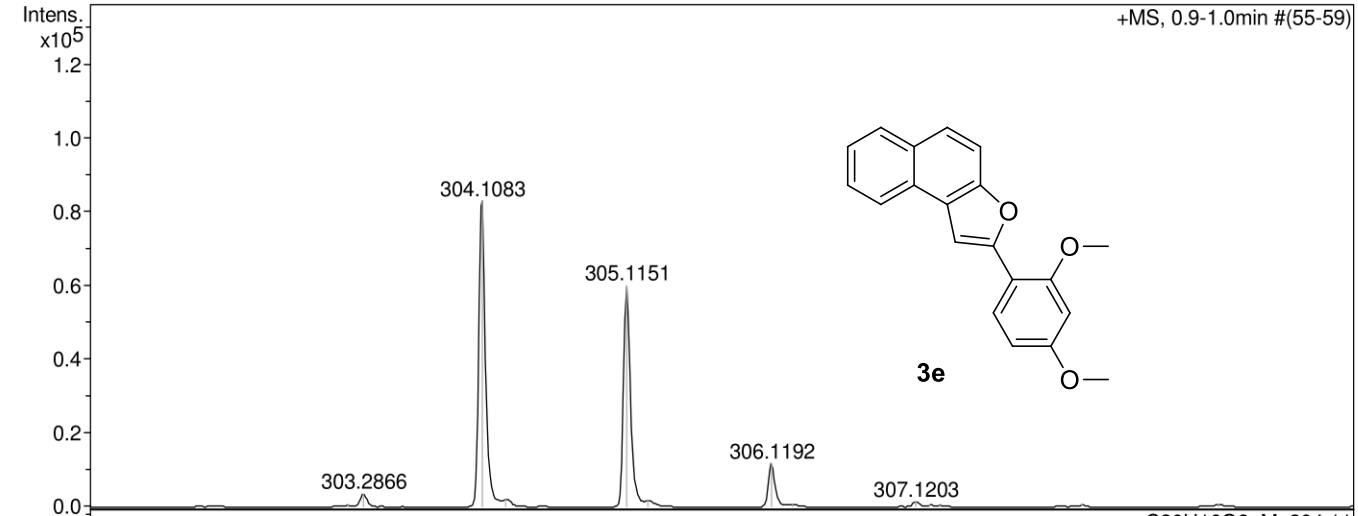
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1550 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 ℃
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





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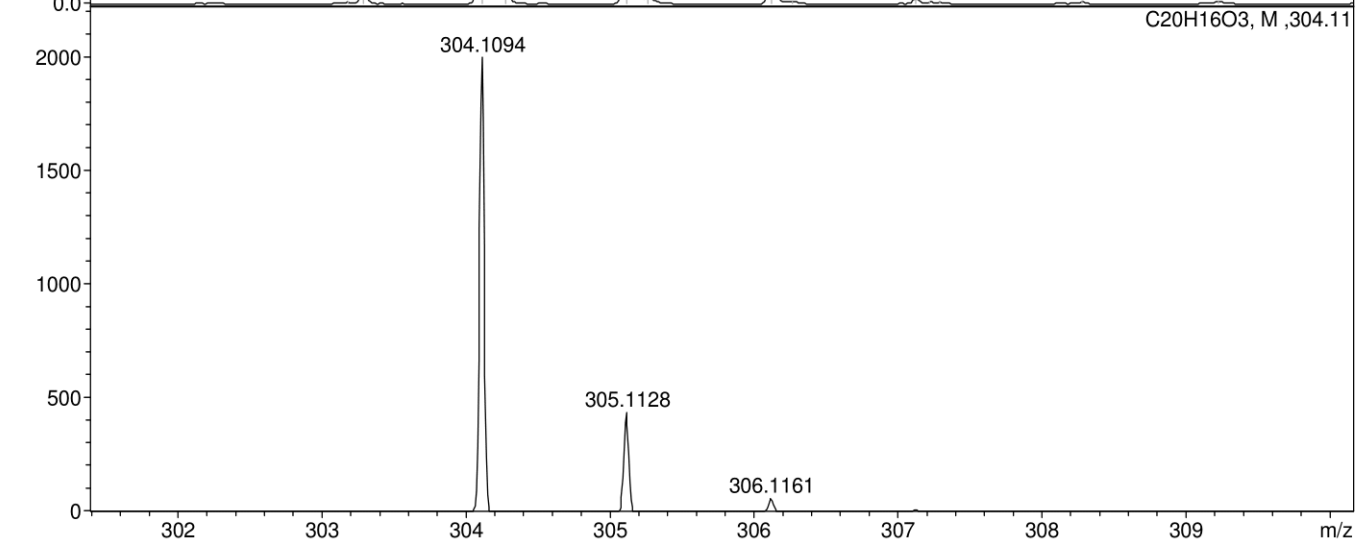
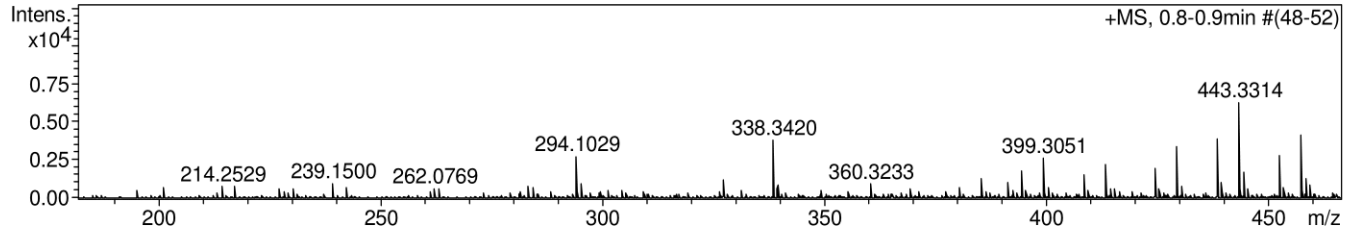
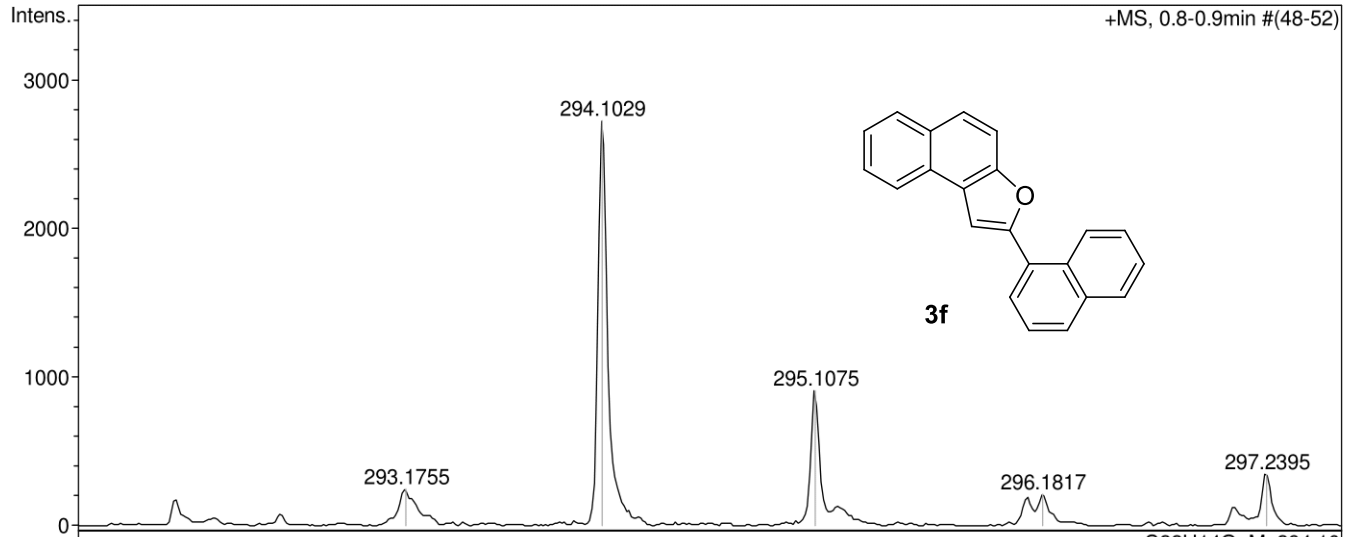
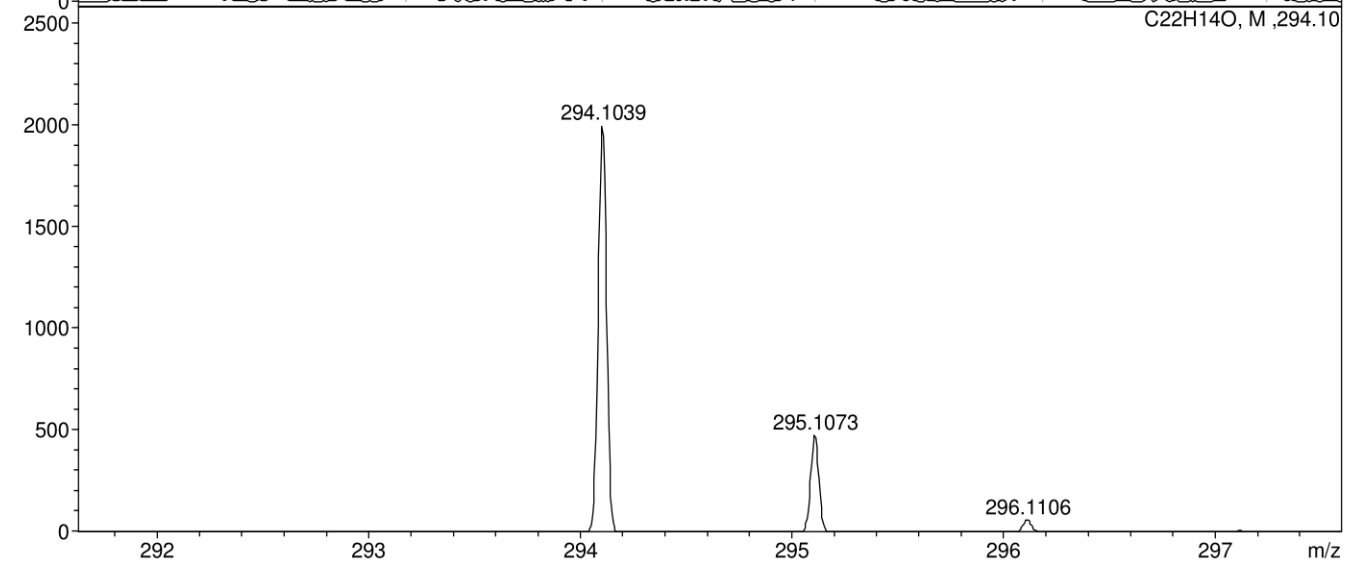


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

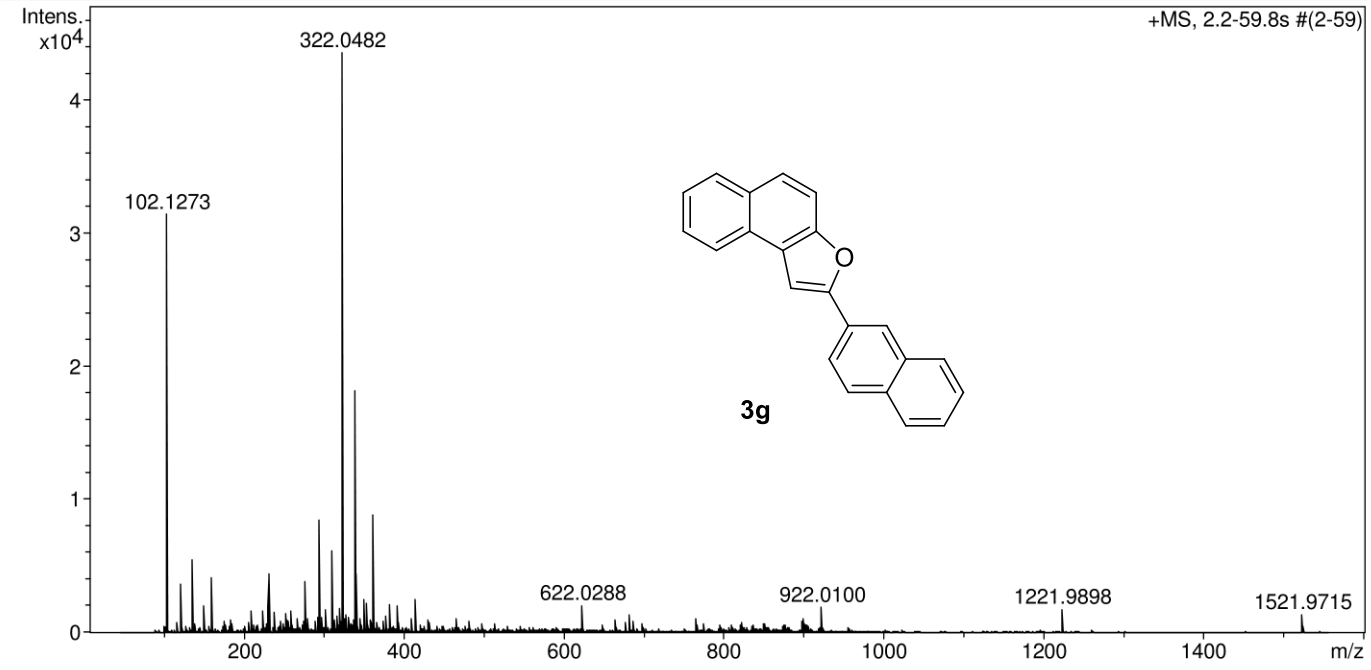


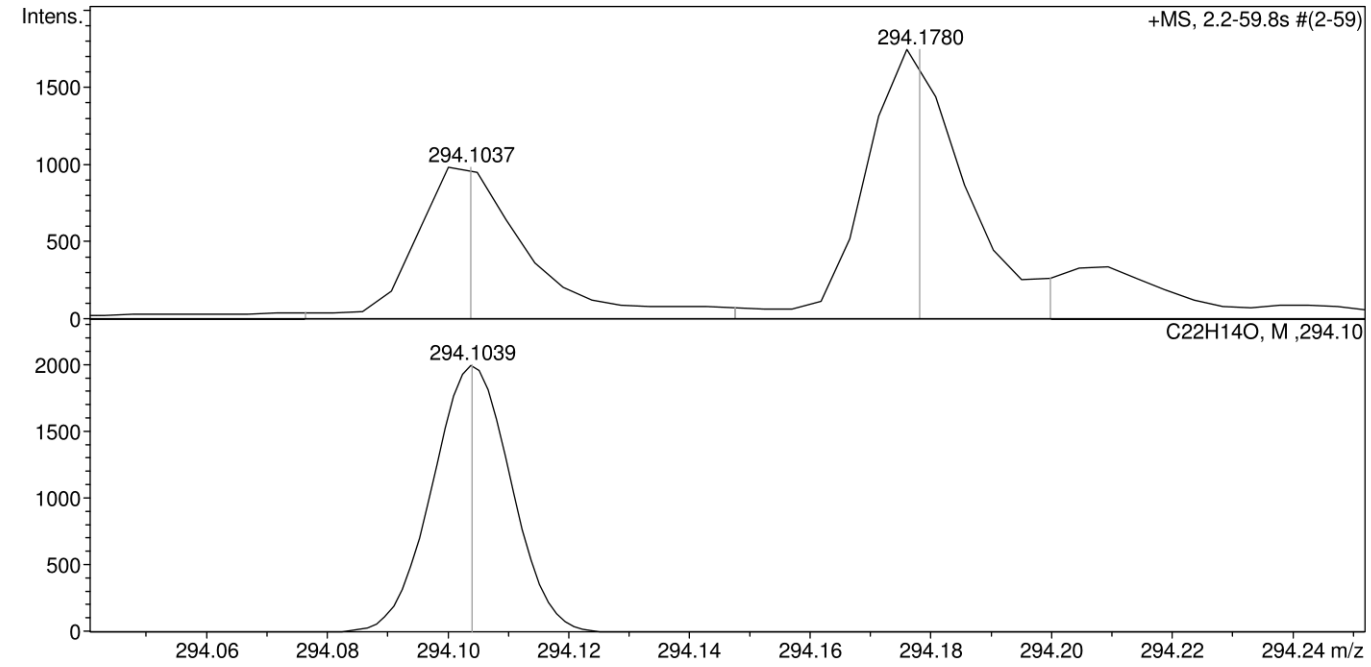




Acquisition Parameter

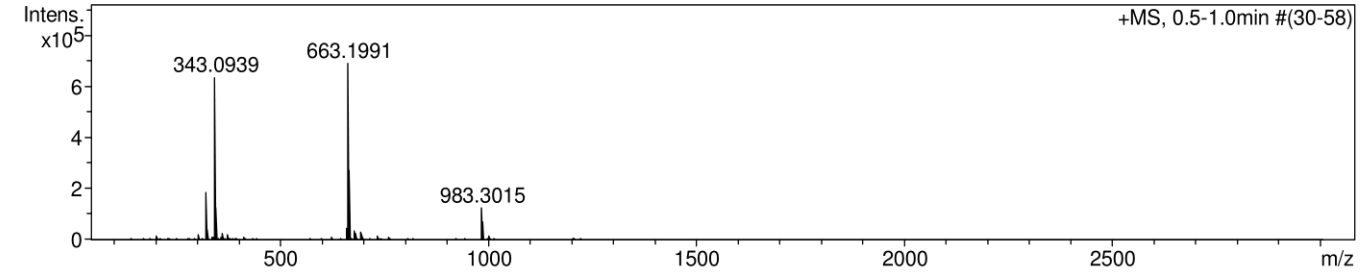
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1550 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

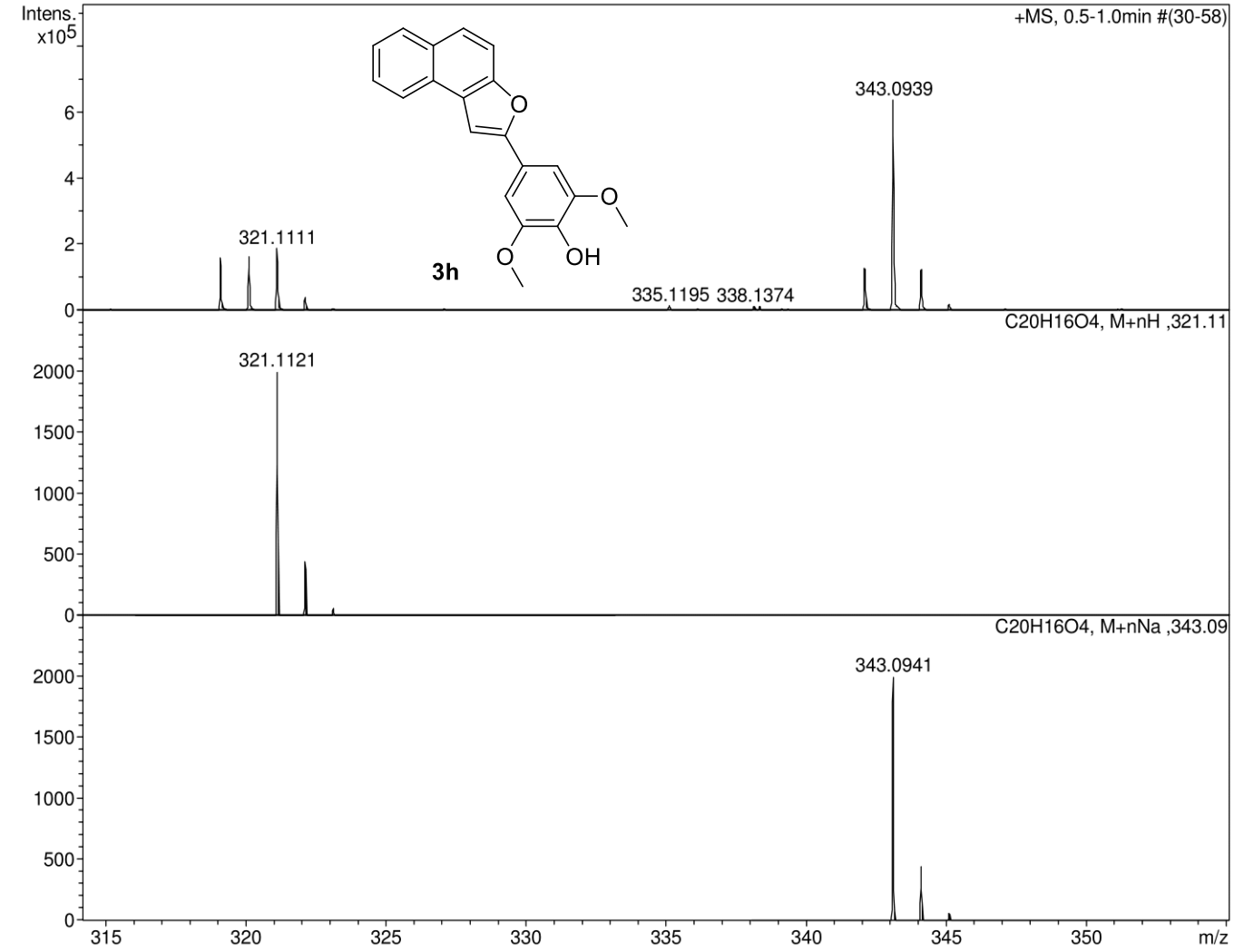




Acquisition Parameter

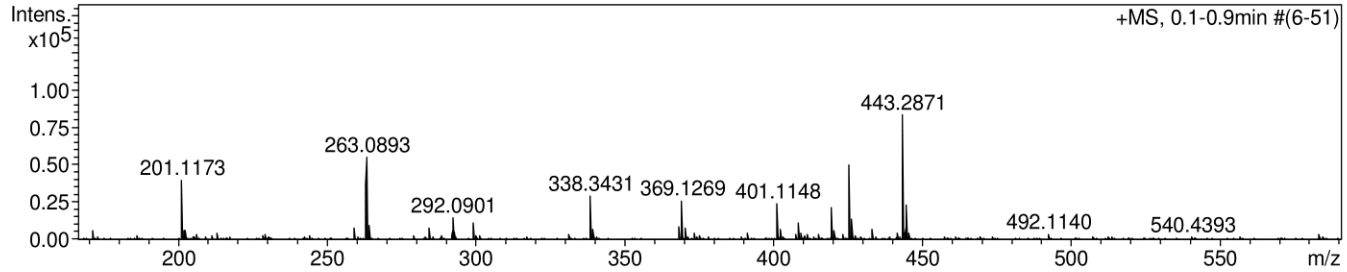
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

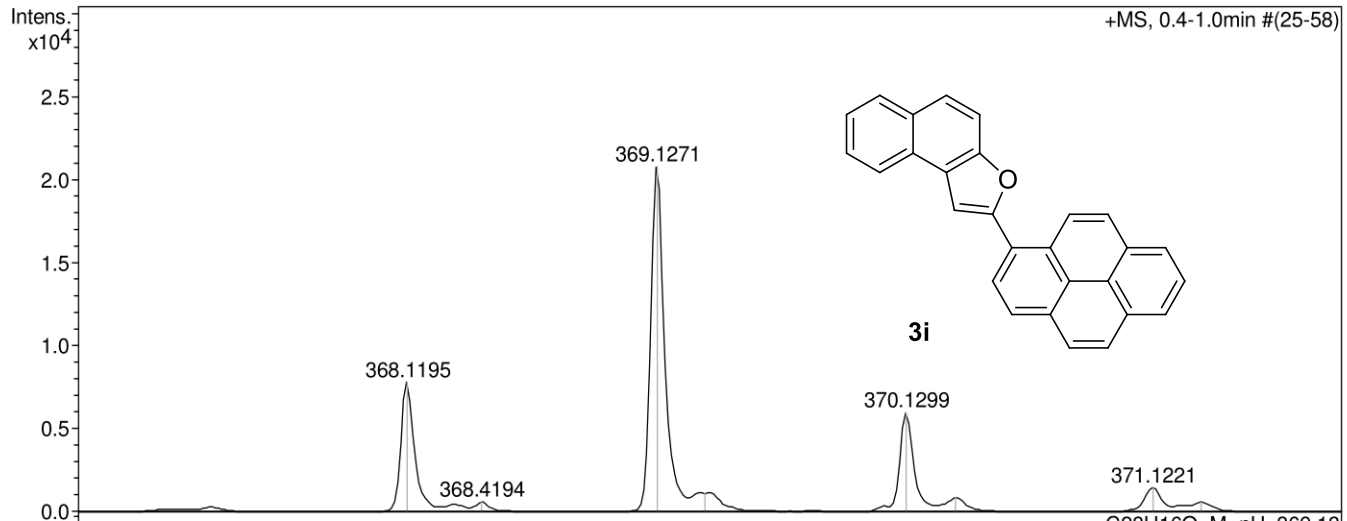


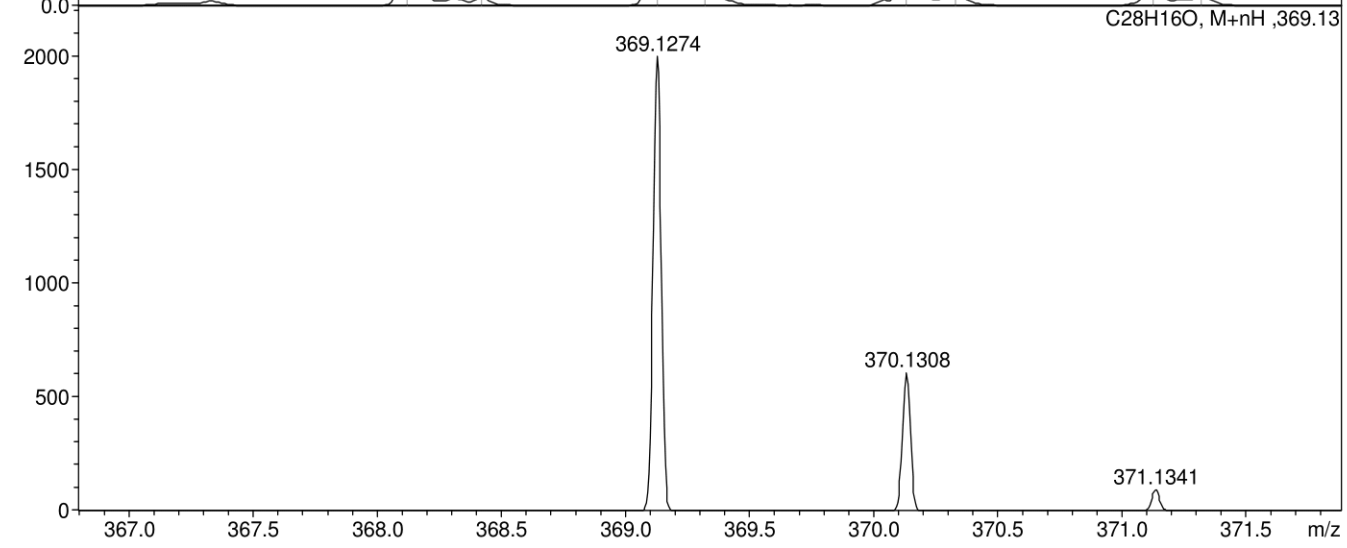


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

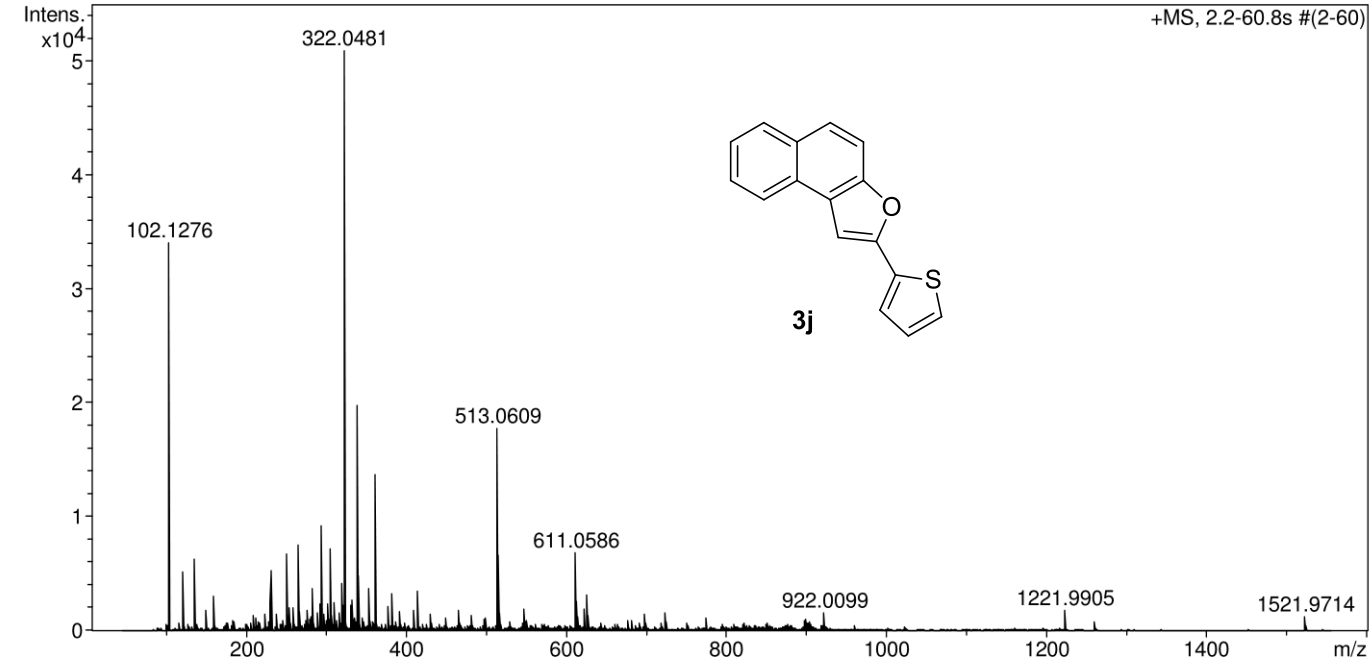


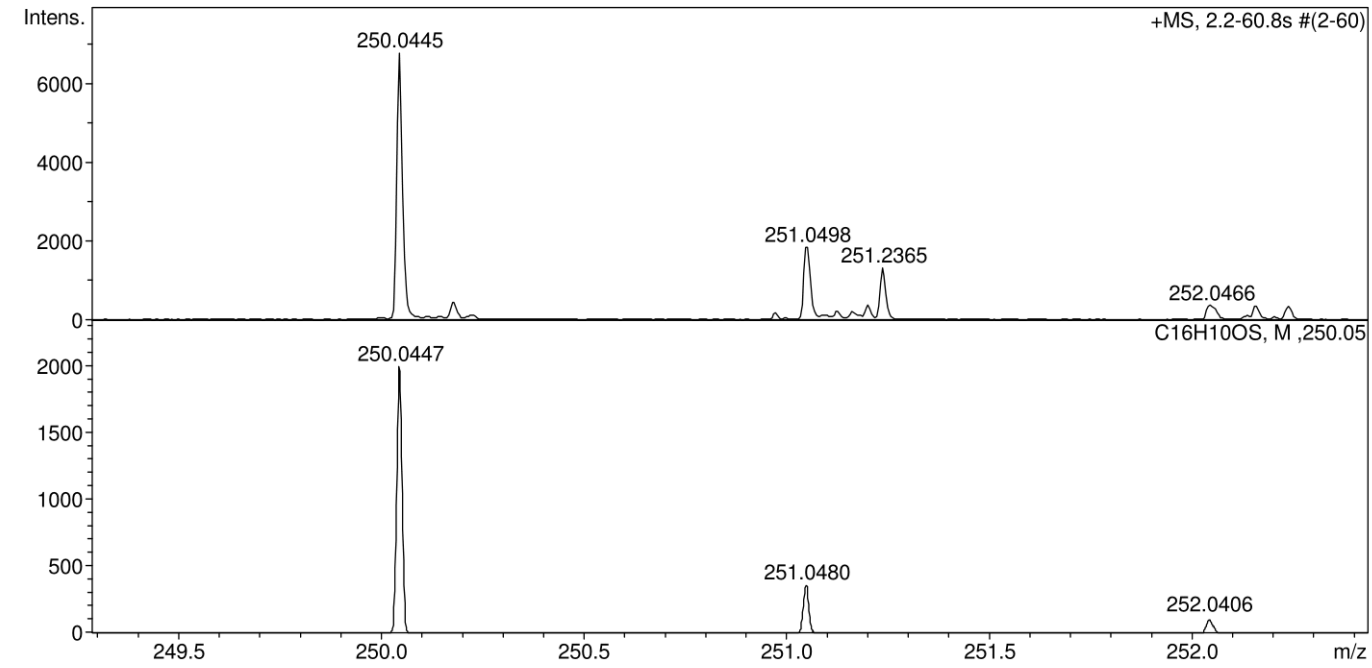




Acquisition Parameter

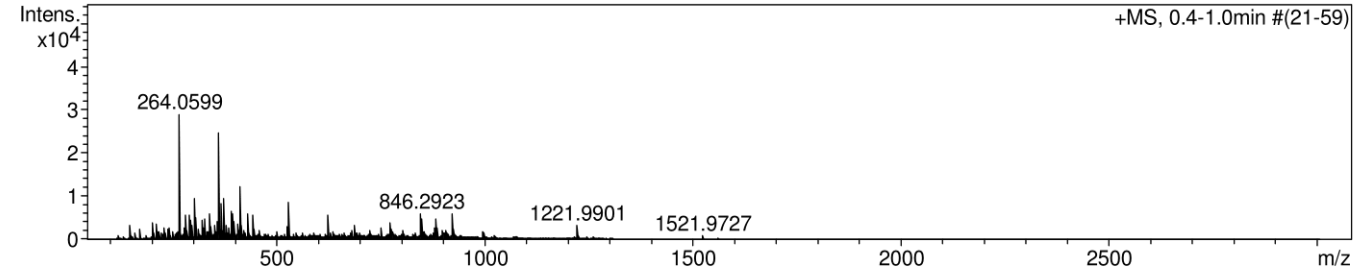
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1550 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

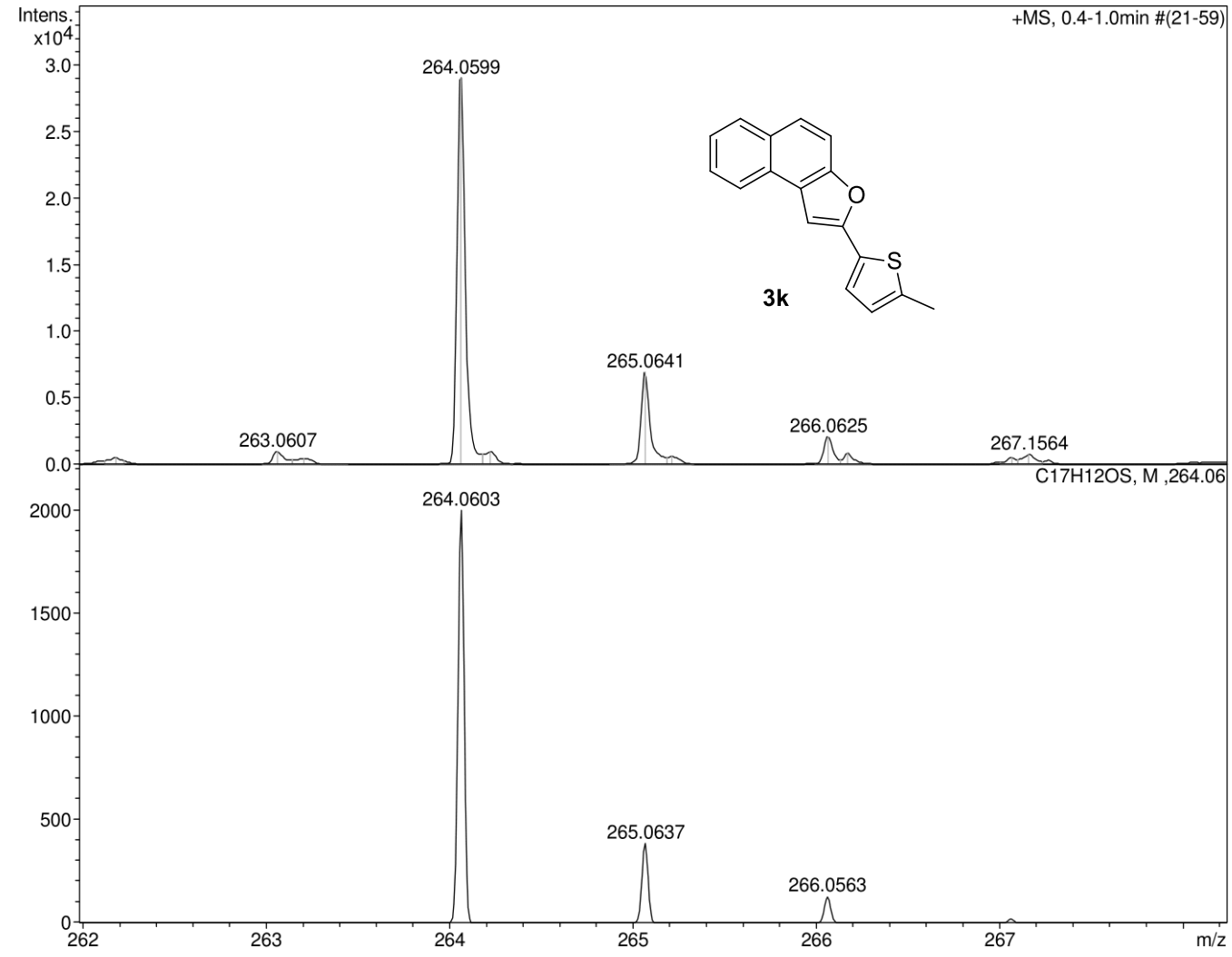




Acquisition Parameter

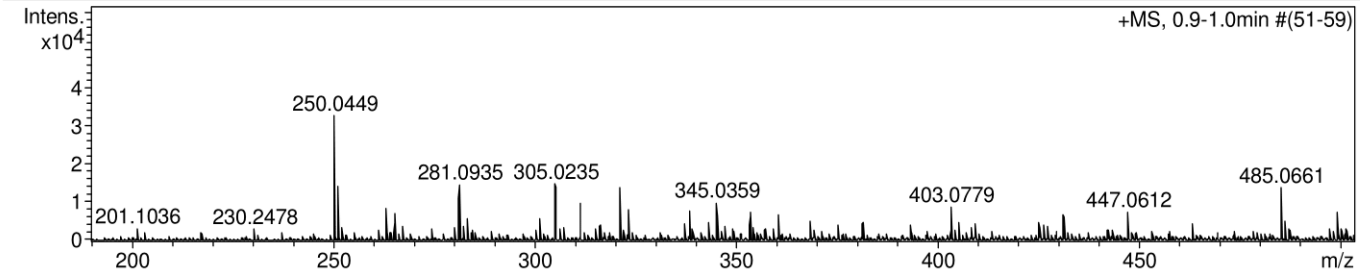
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

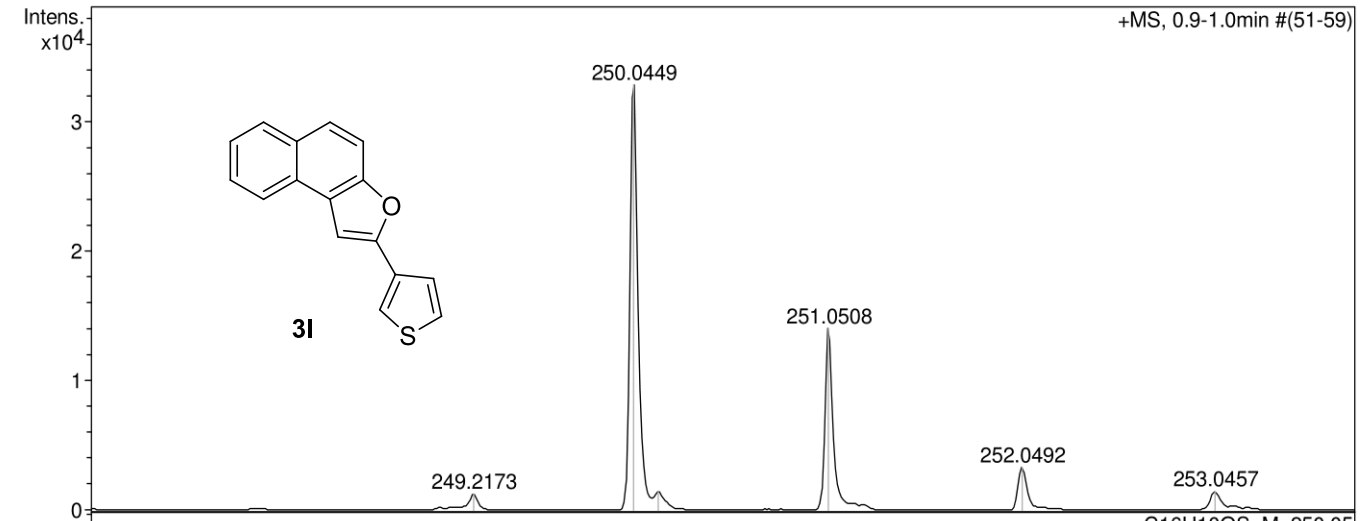


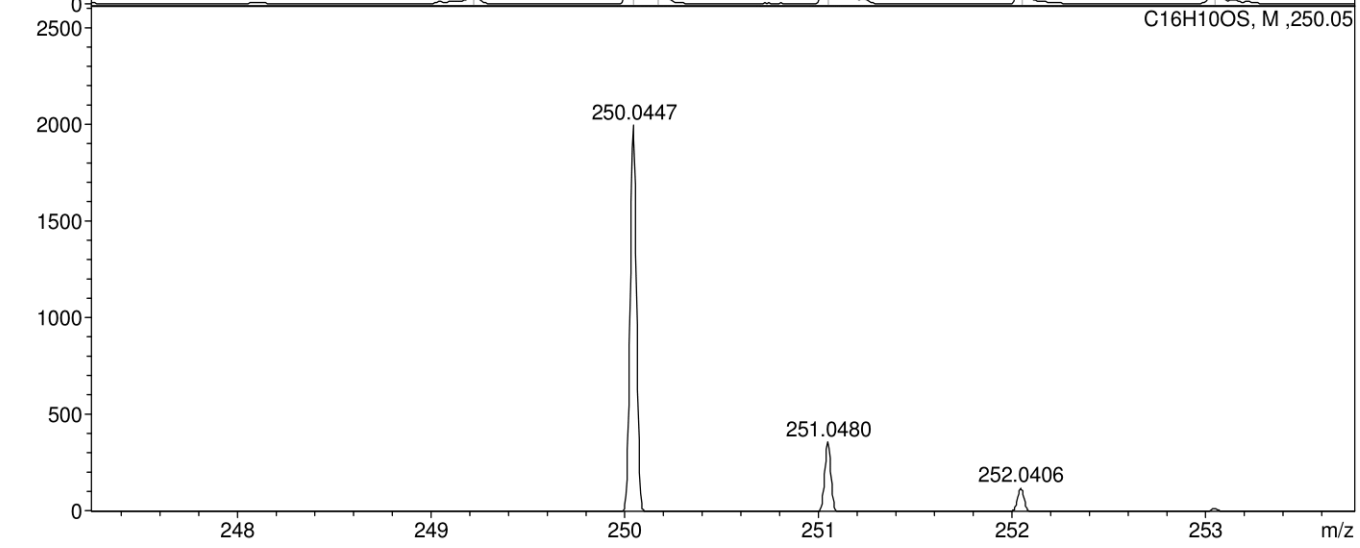


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

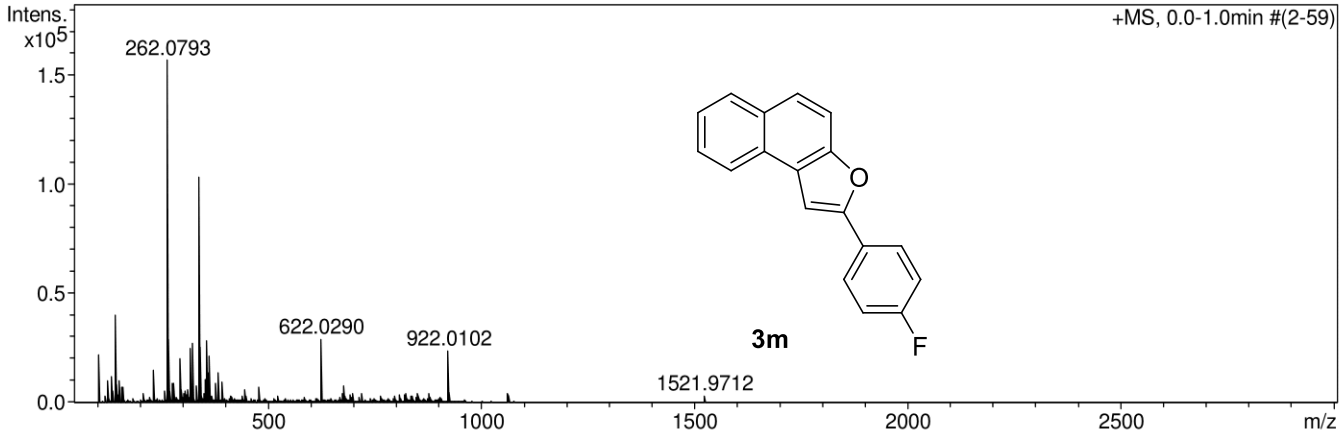


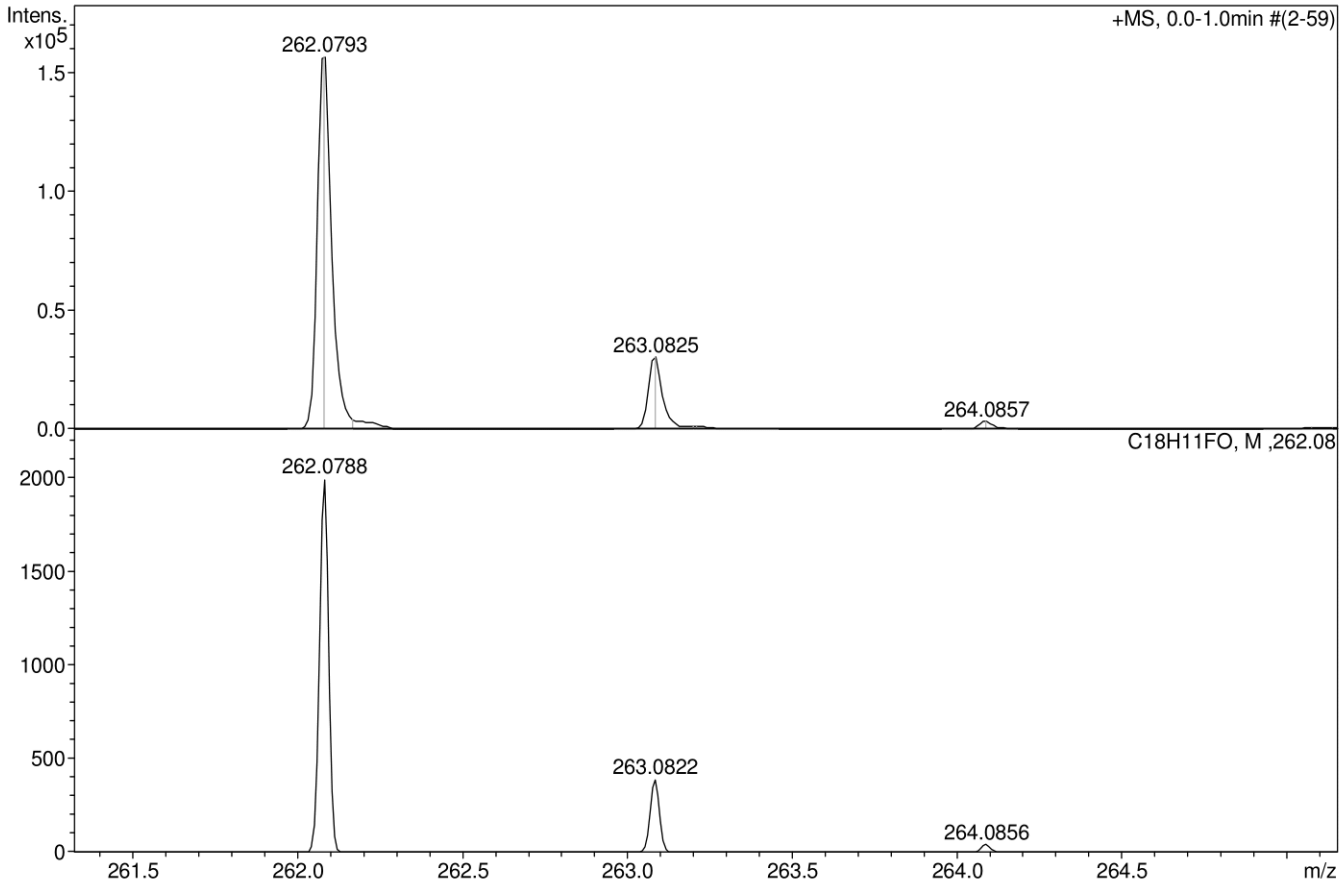




Acquisition Parameter

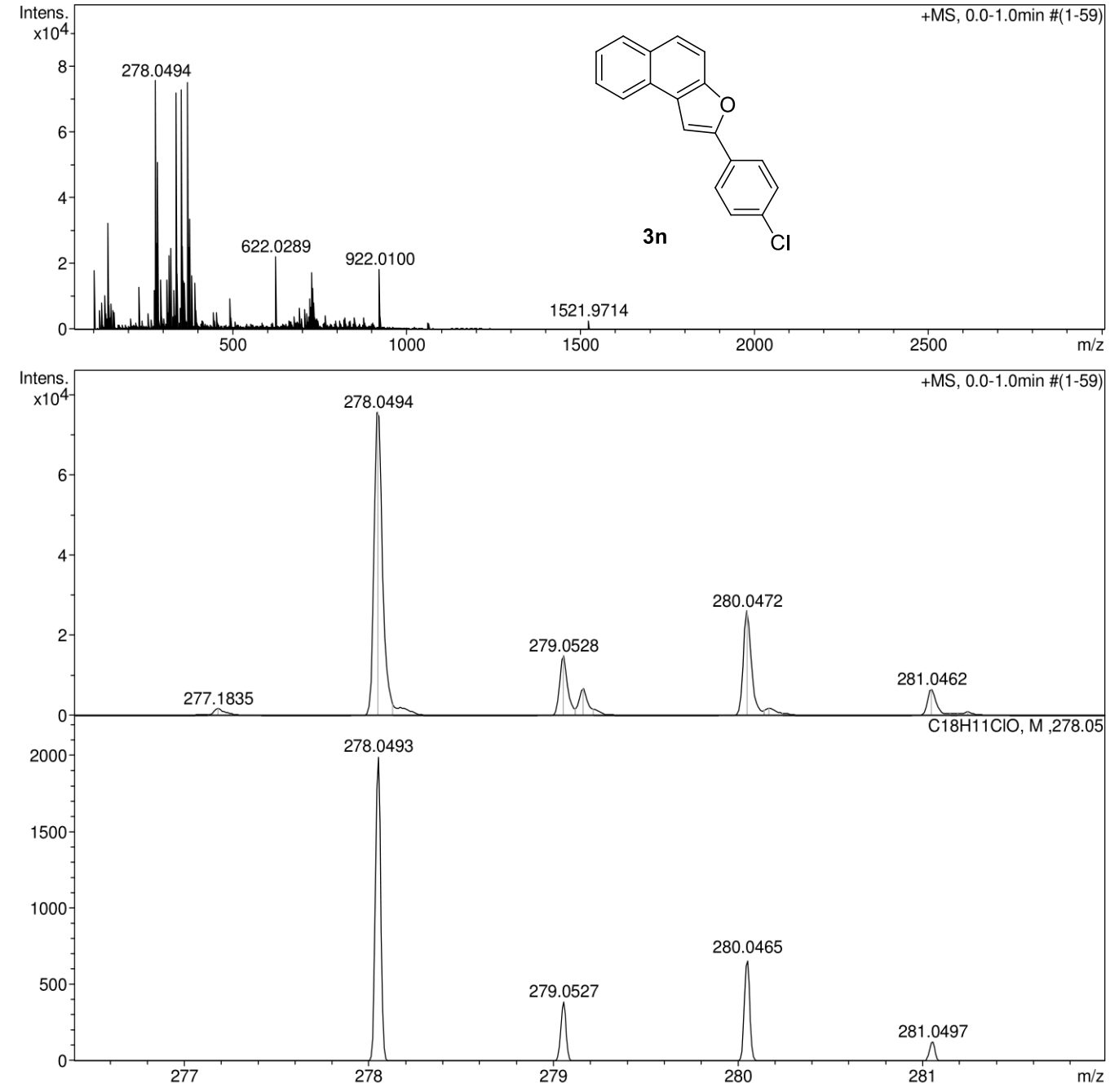
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





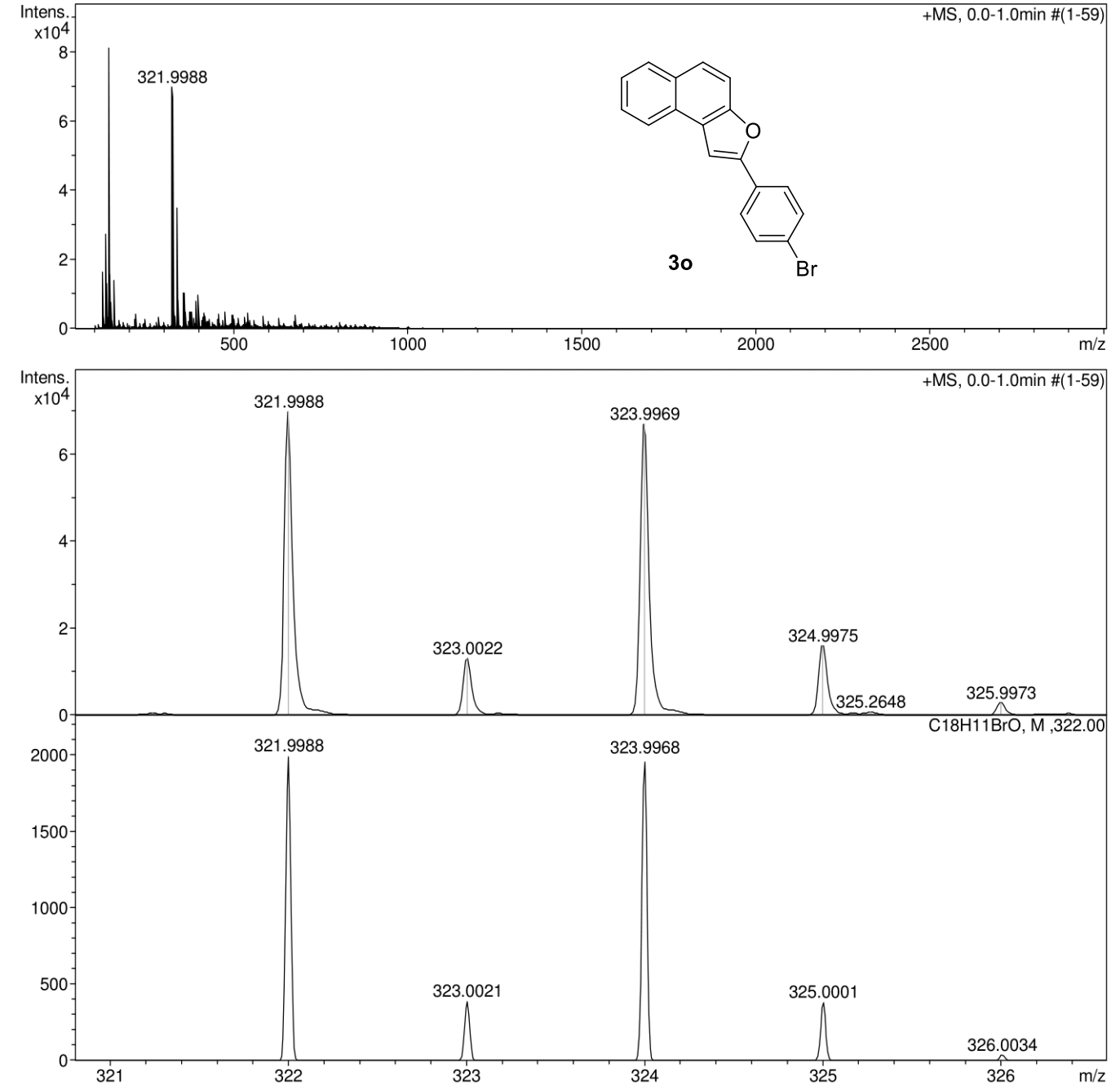
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



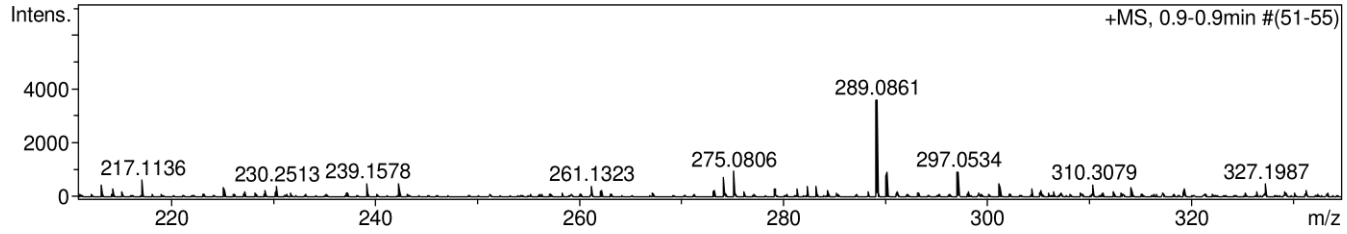
Acquisition Parameter

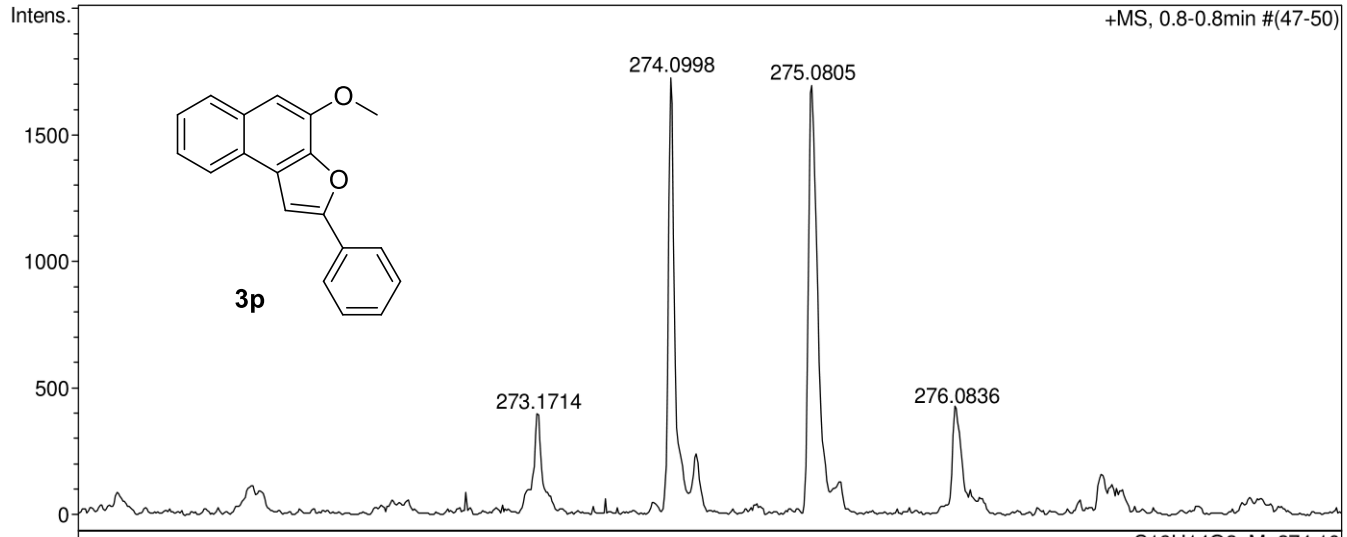
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

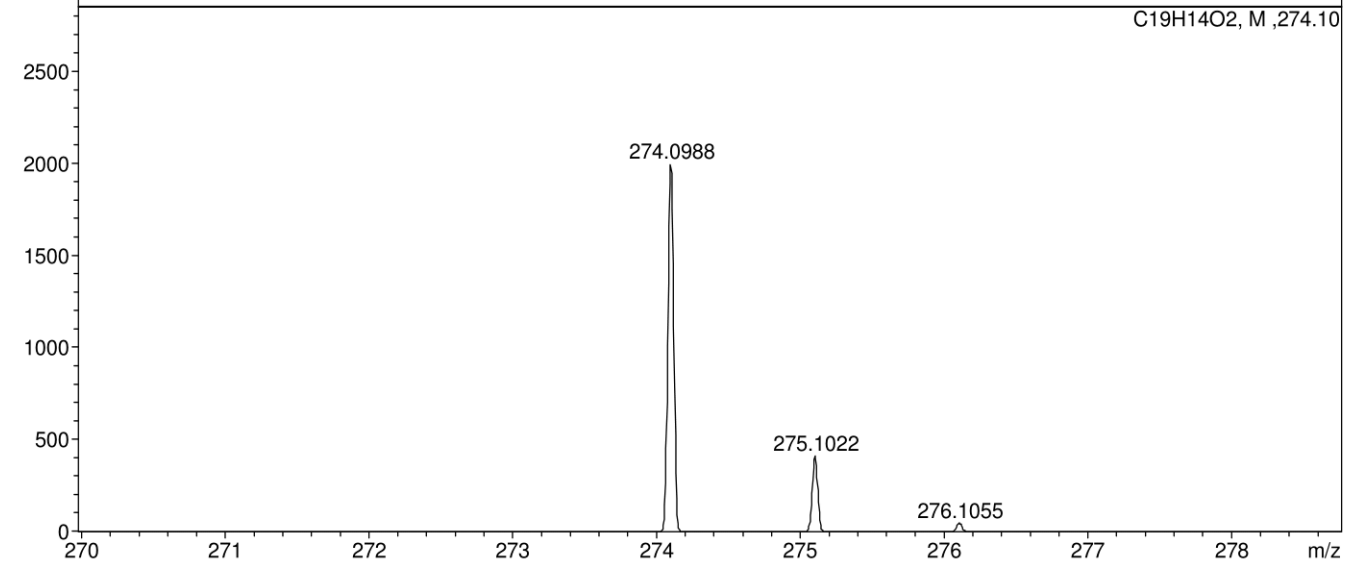


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

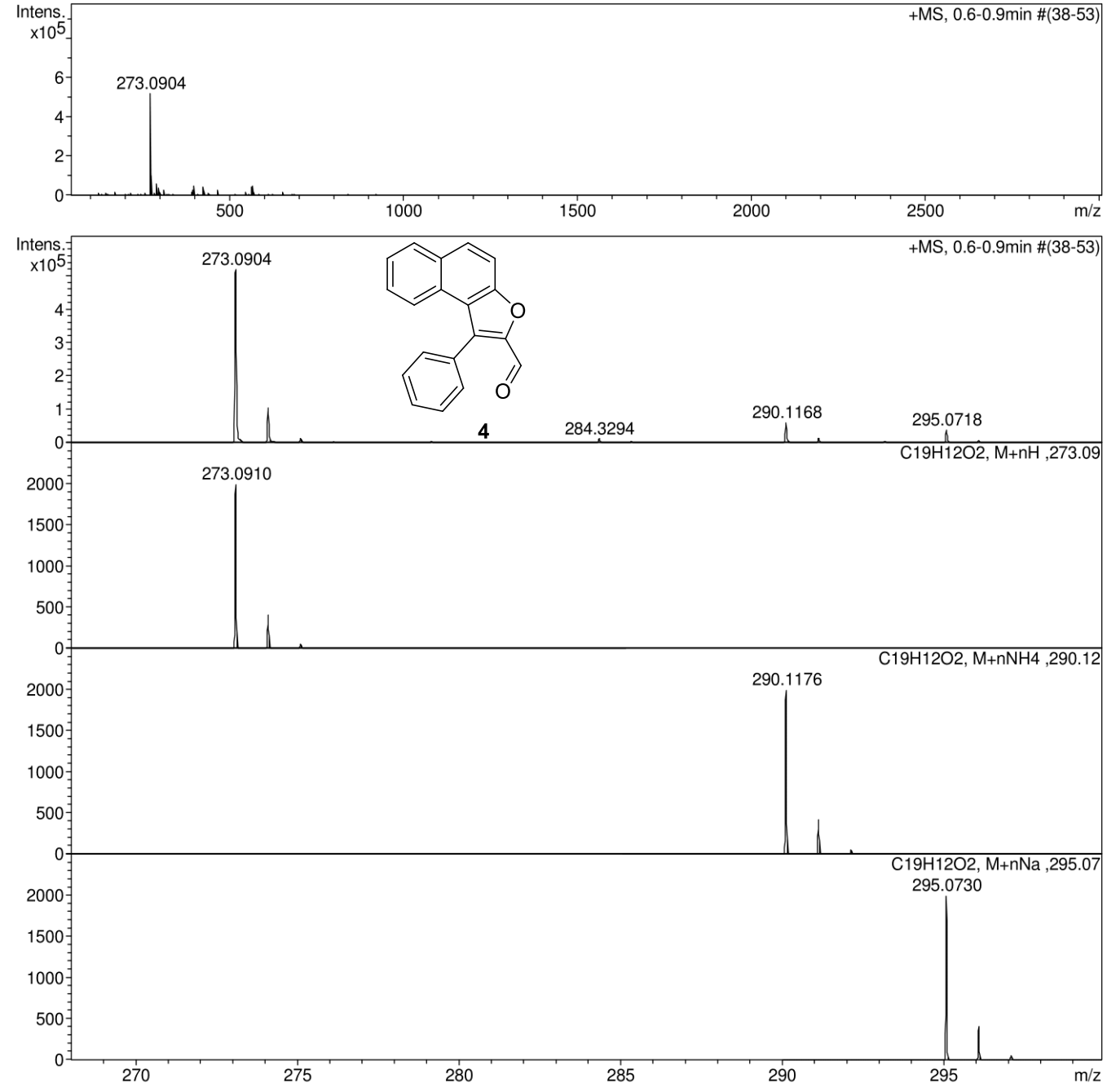






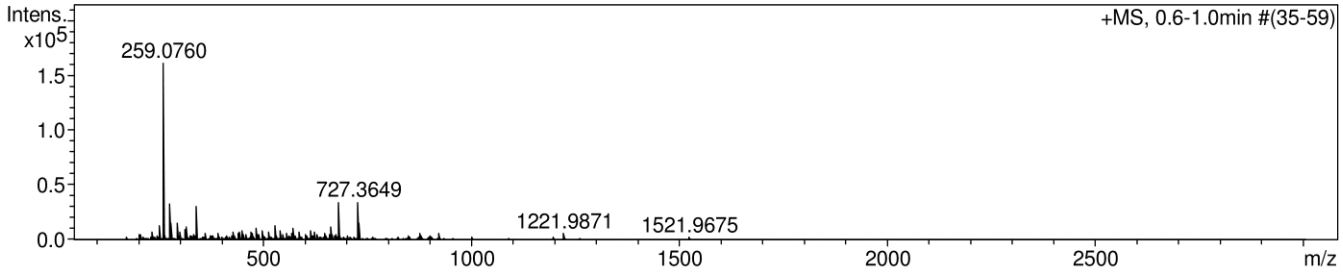
Acquisition Parameter

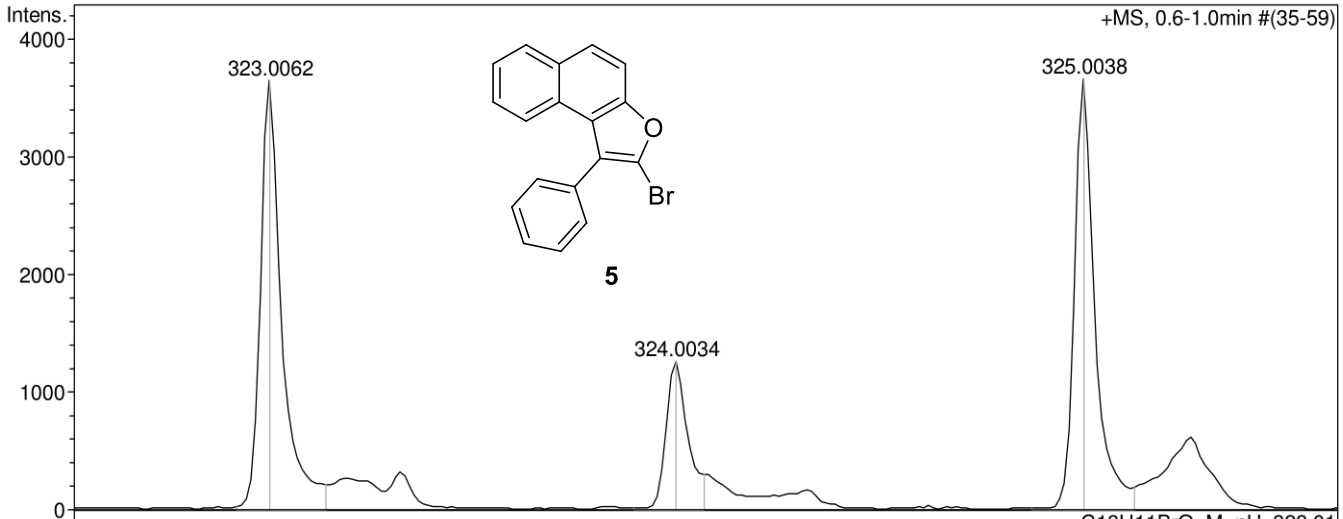
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

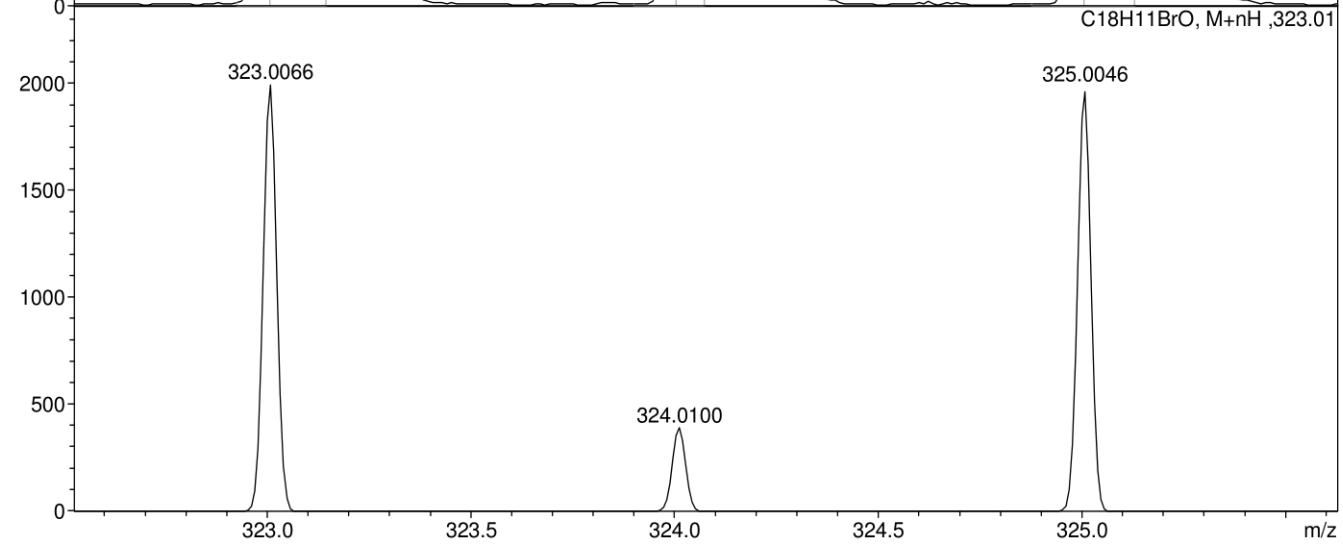


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

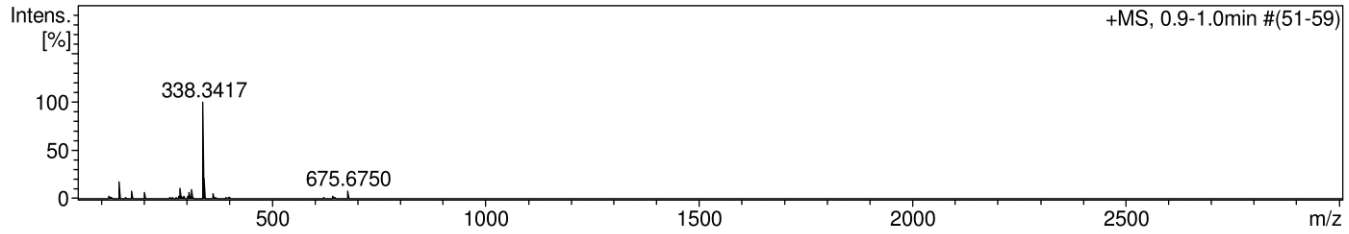


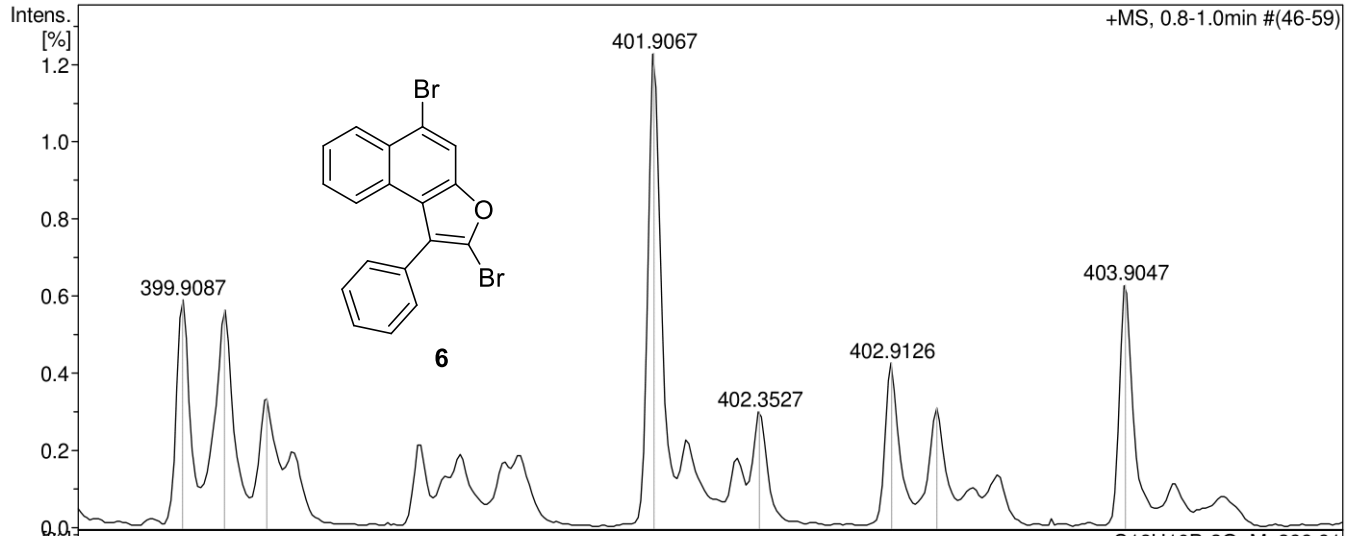


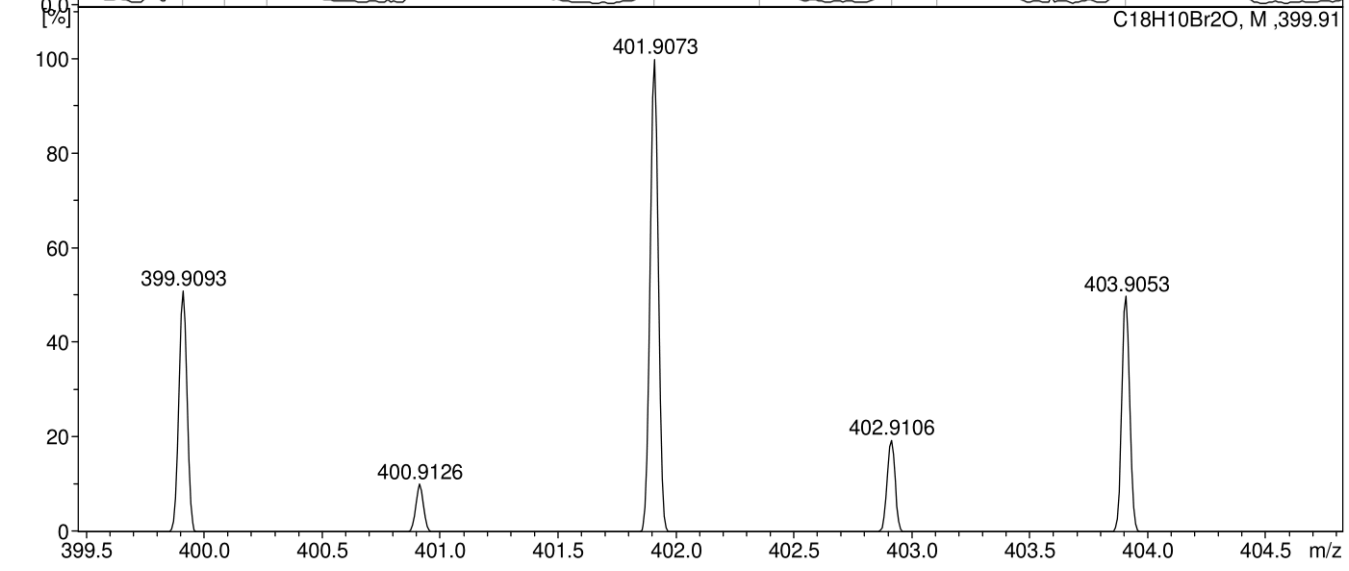


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

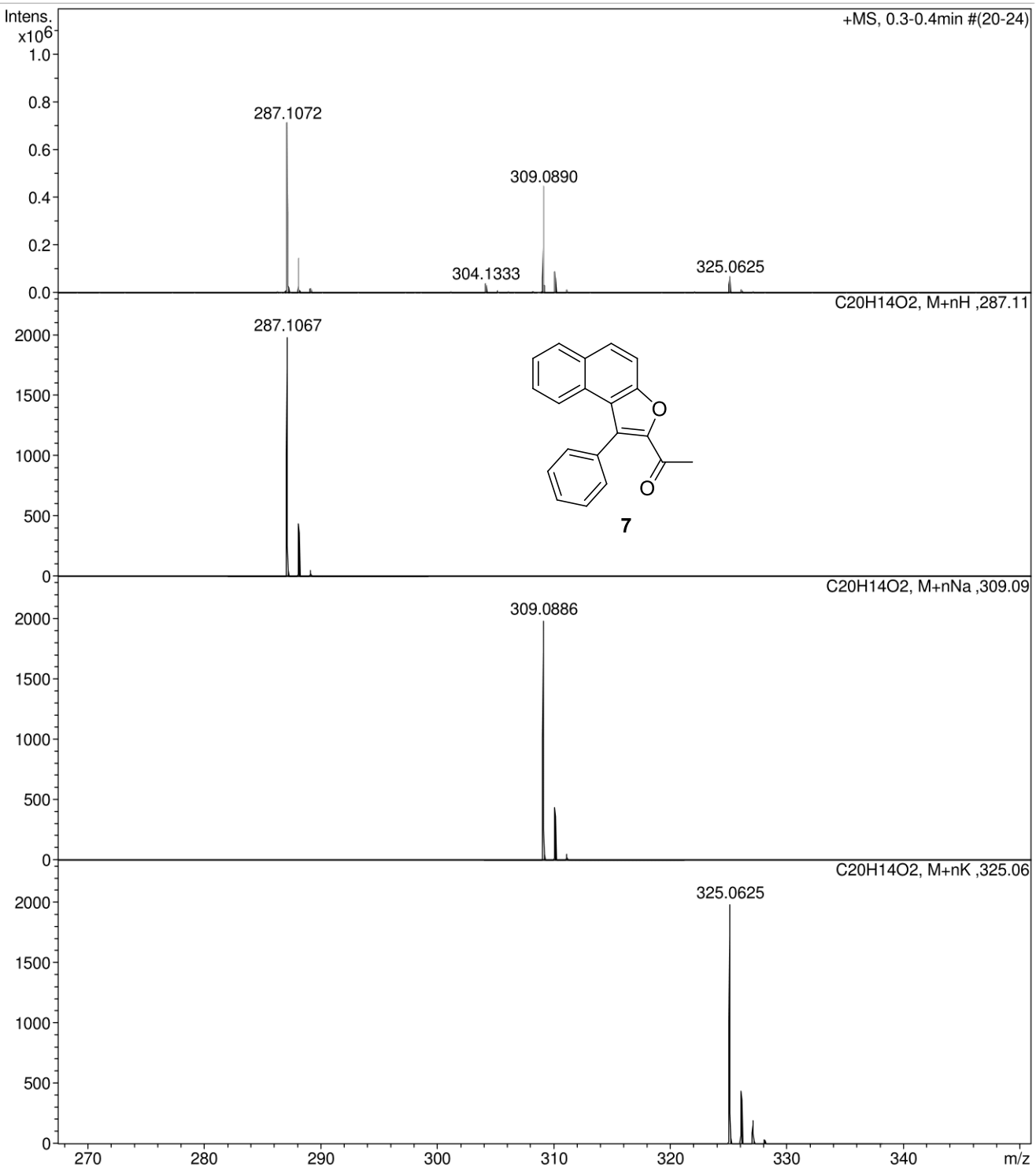






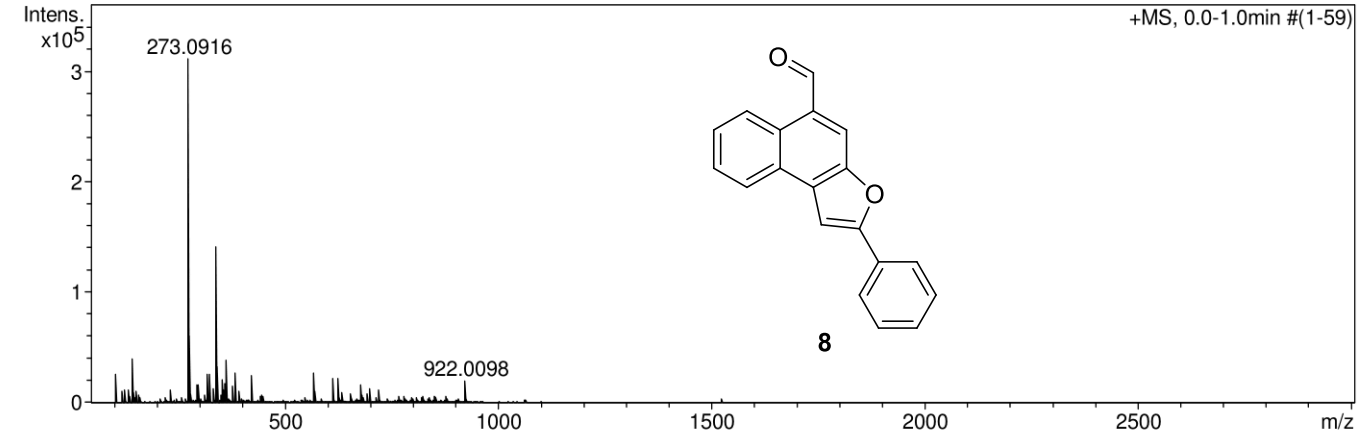
Acquisition Parameter

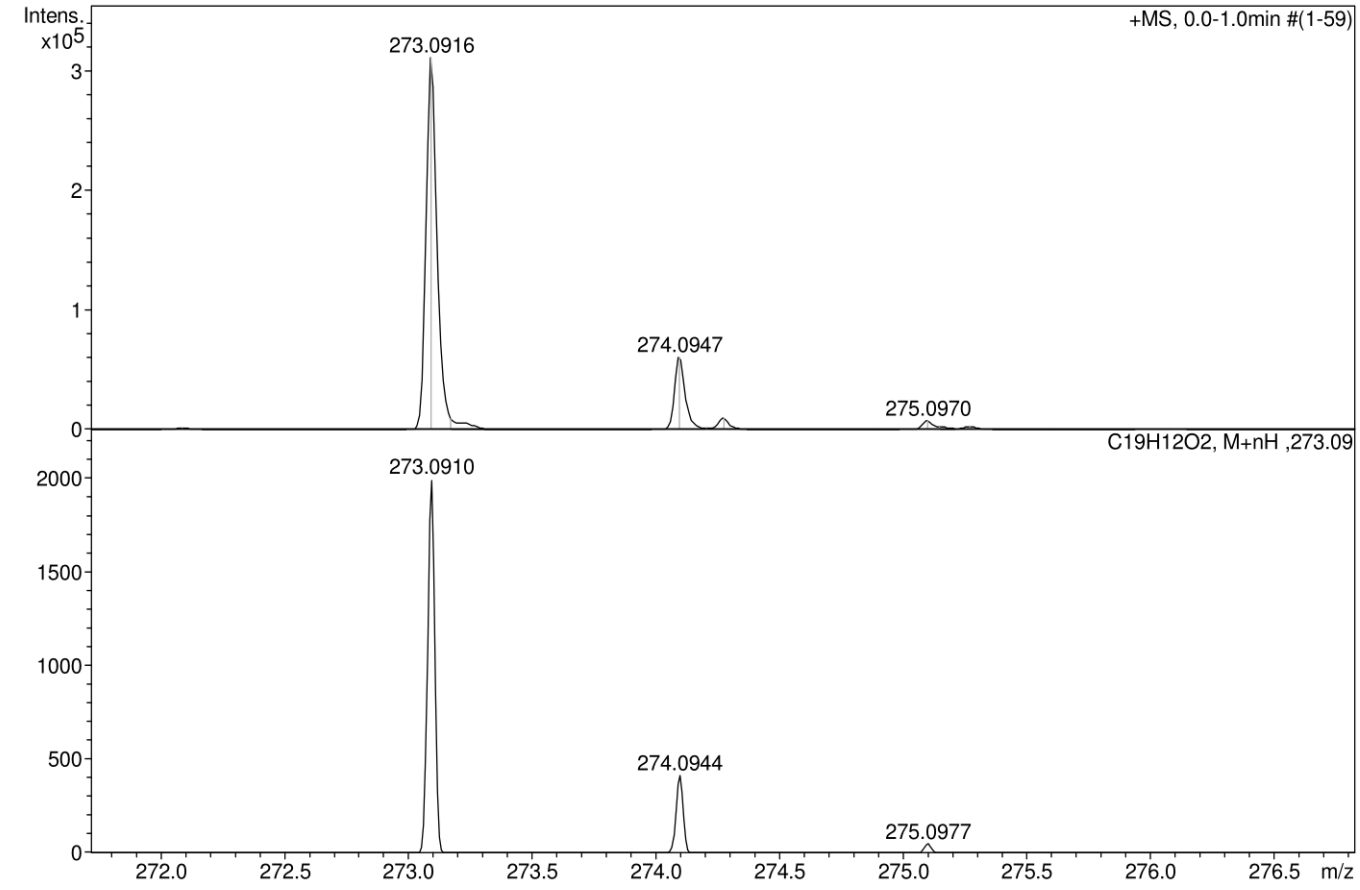
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Acquisition Parameter

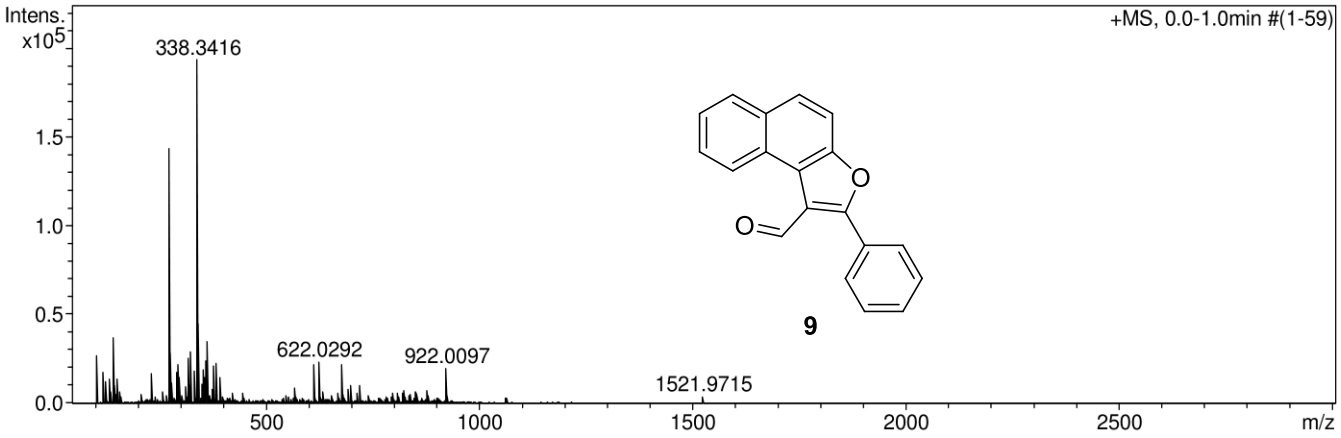
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



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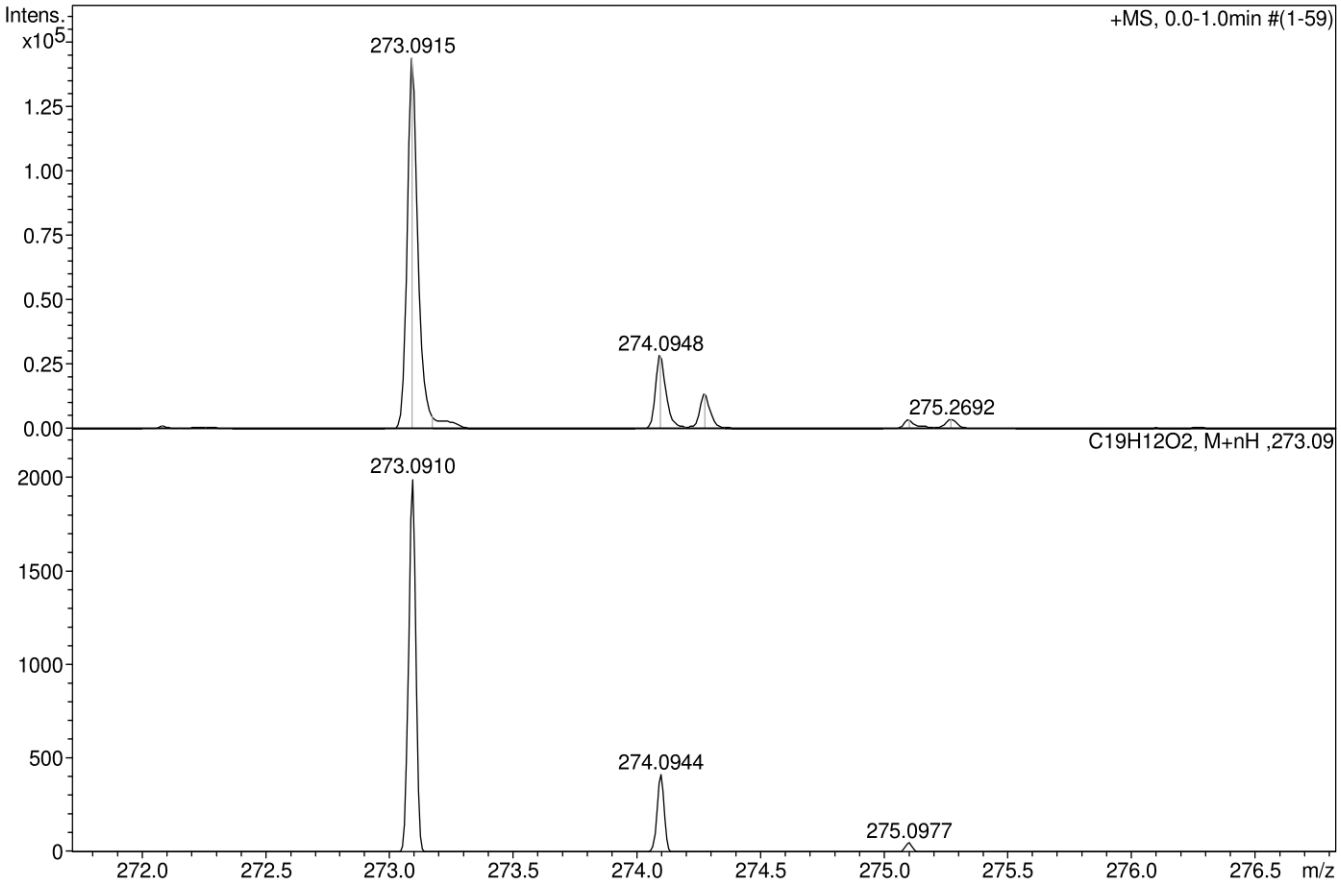
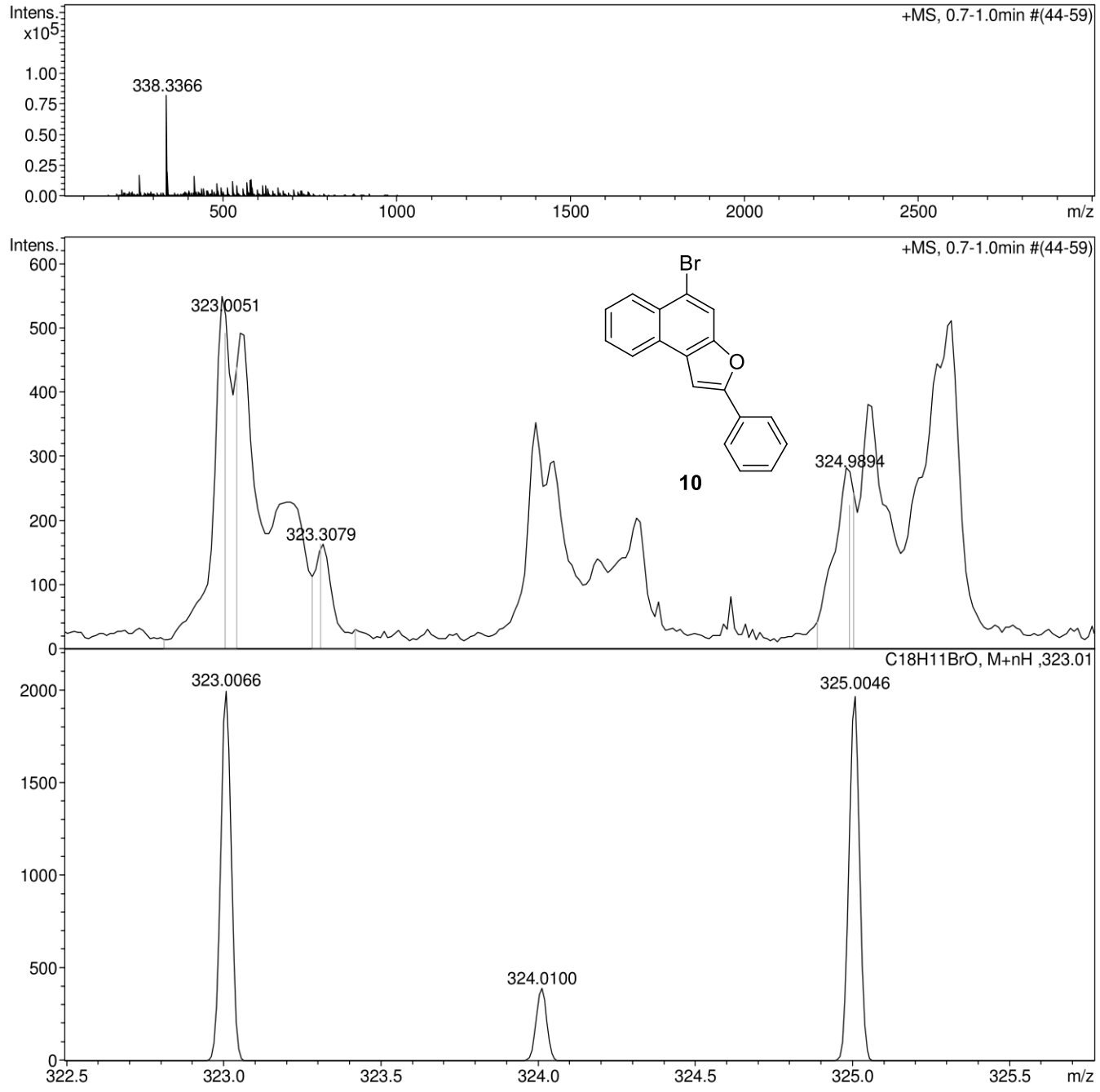


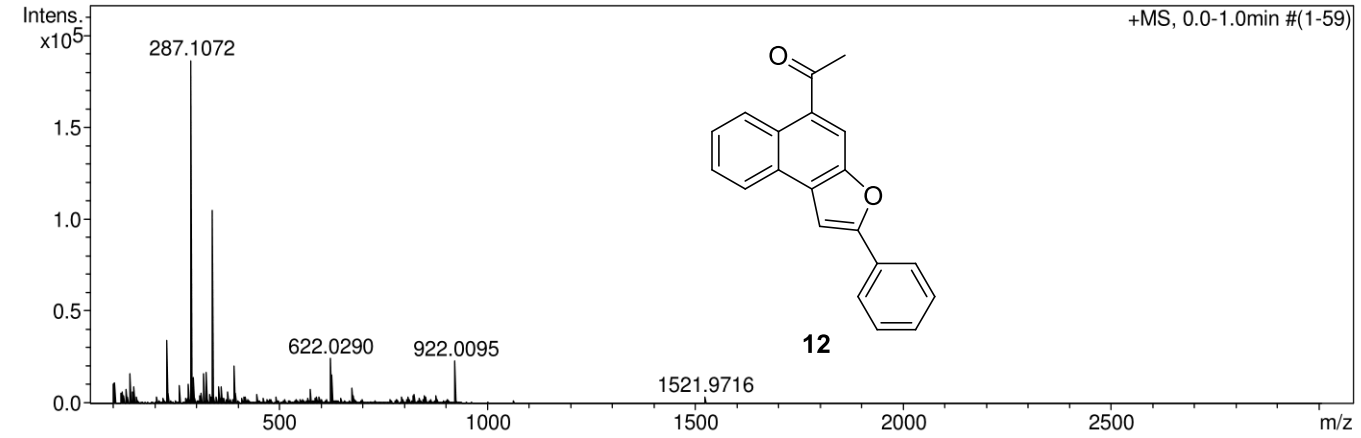
Acquisition Parameter

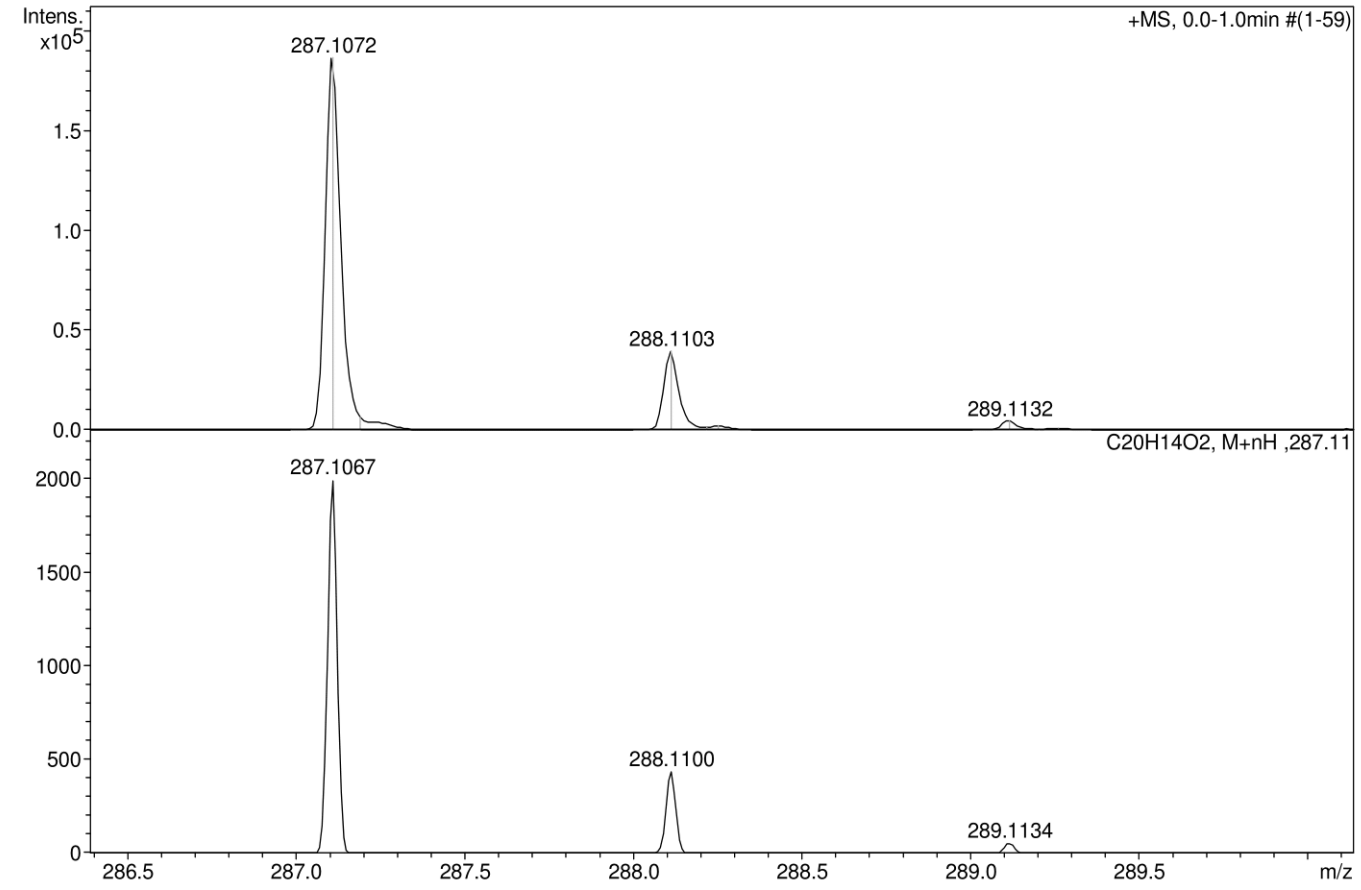
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Acquisition Parameter

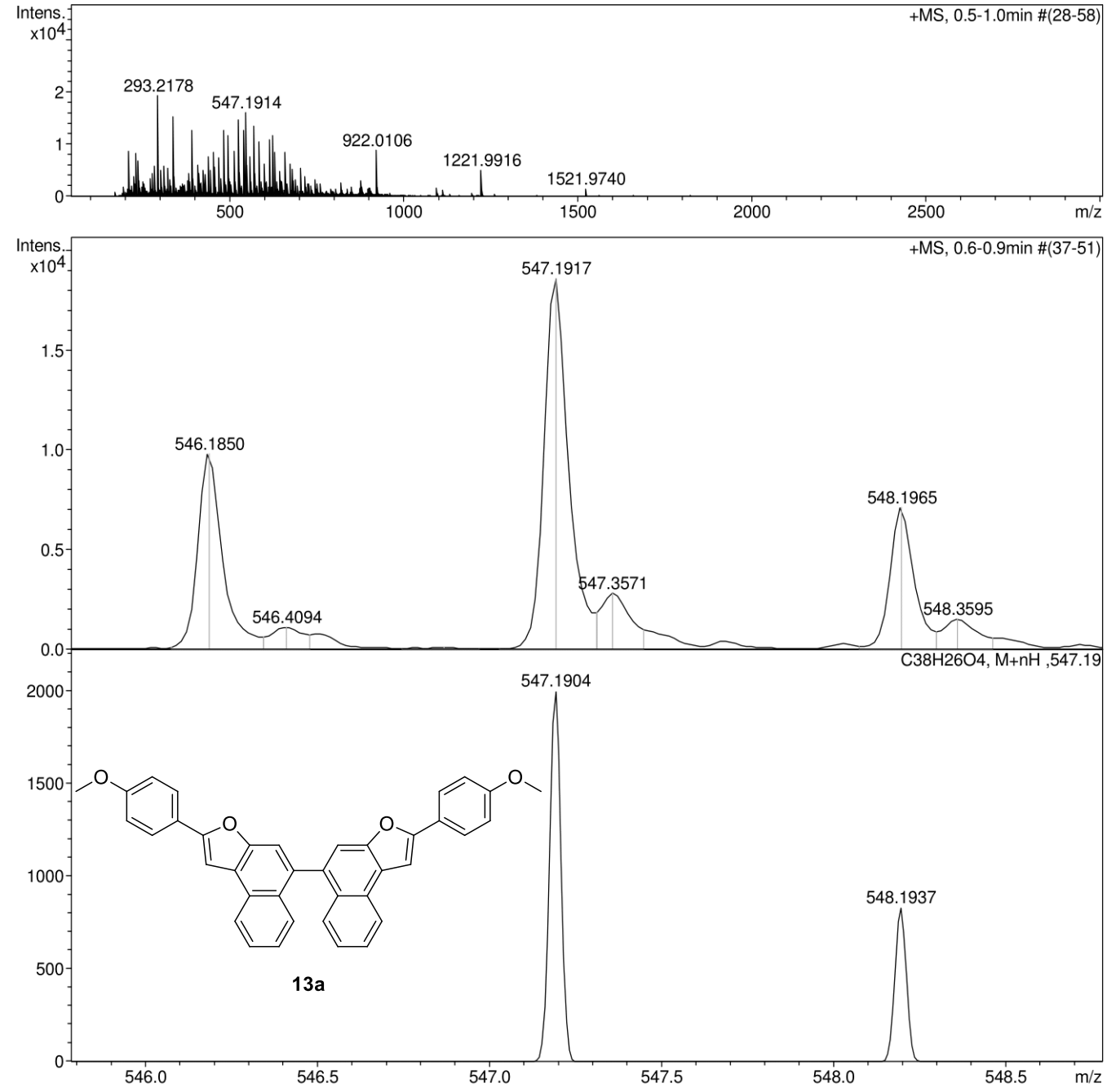
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





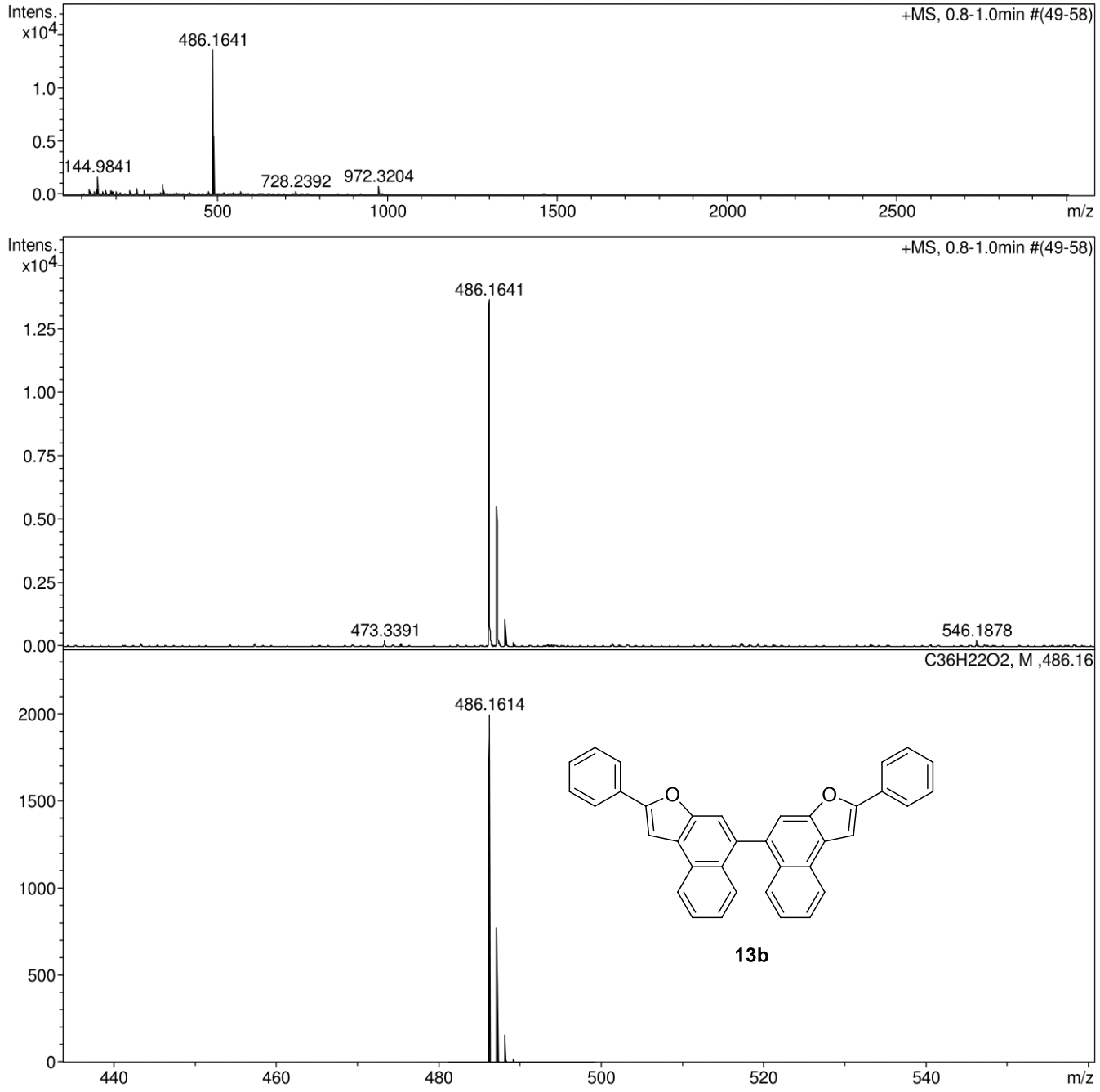
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



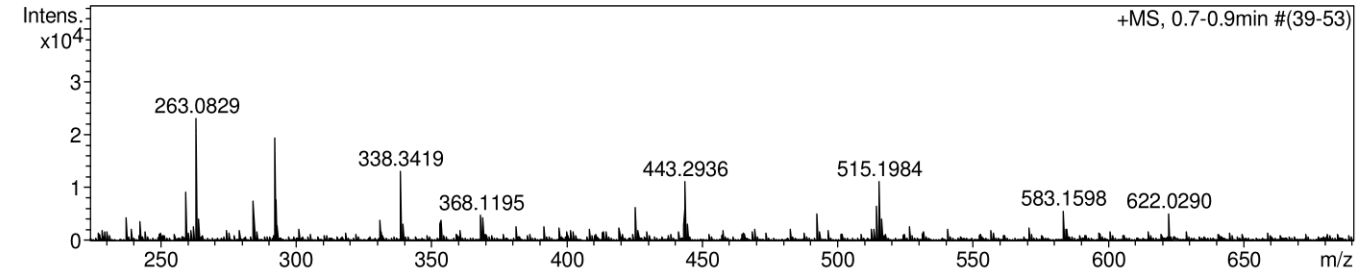
Acquisition Parameter

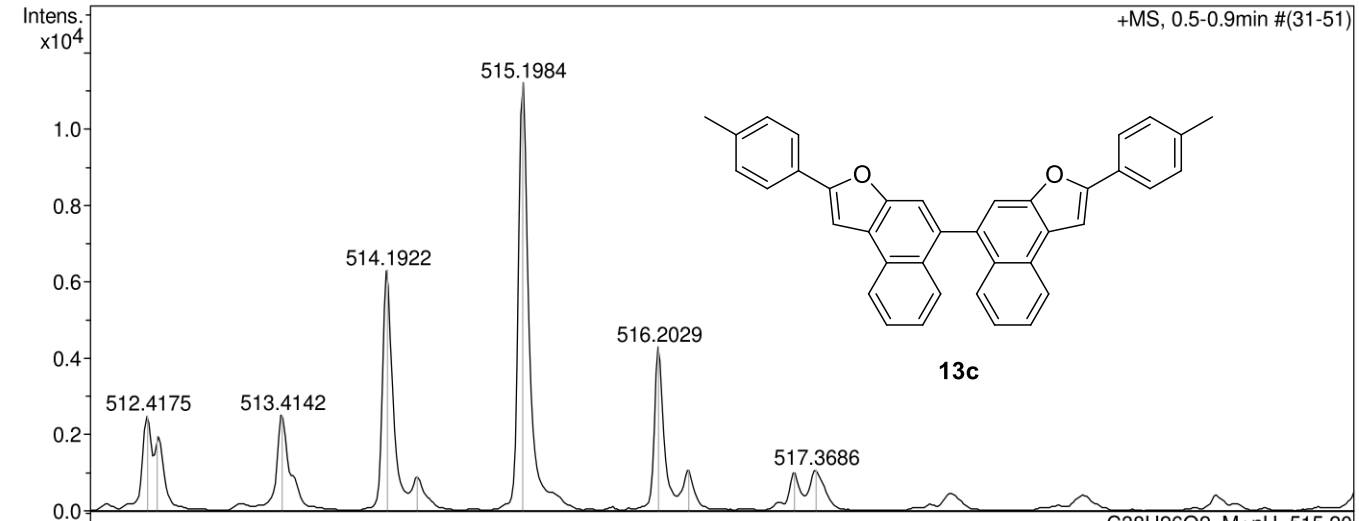
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

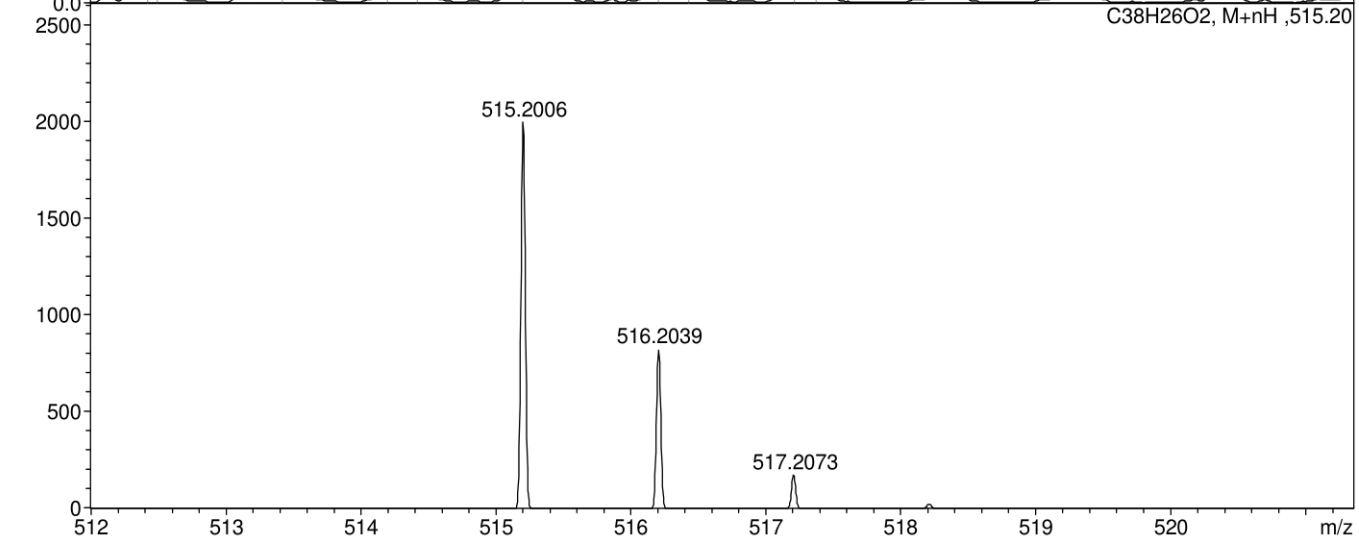


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

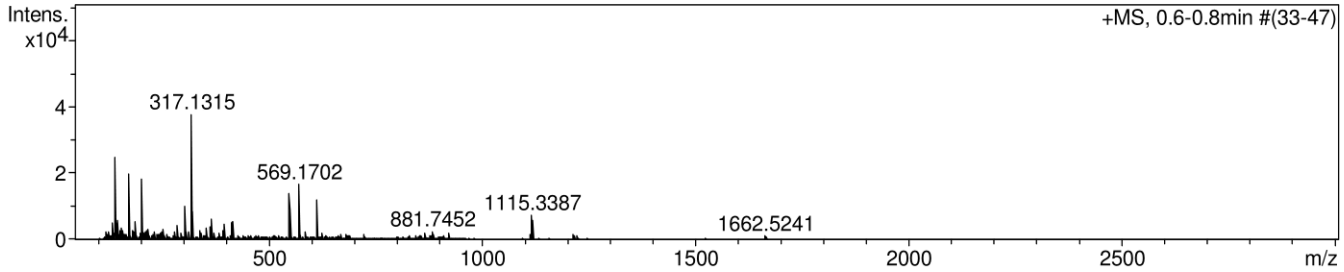


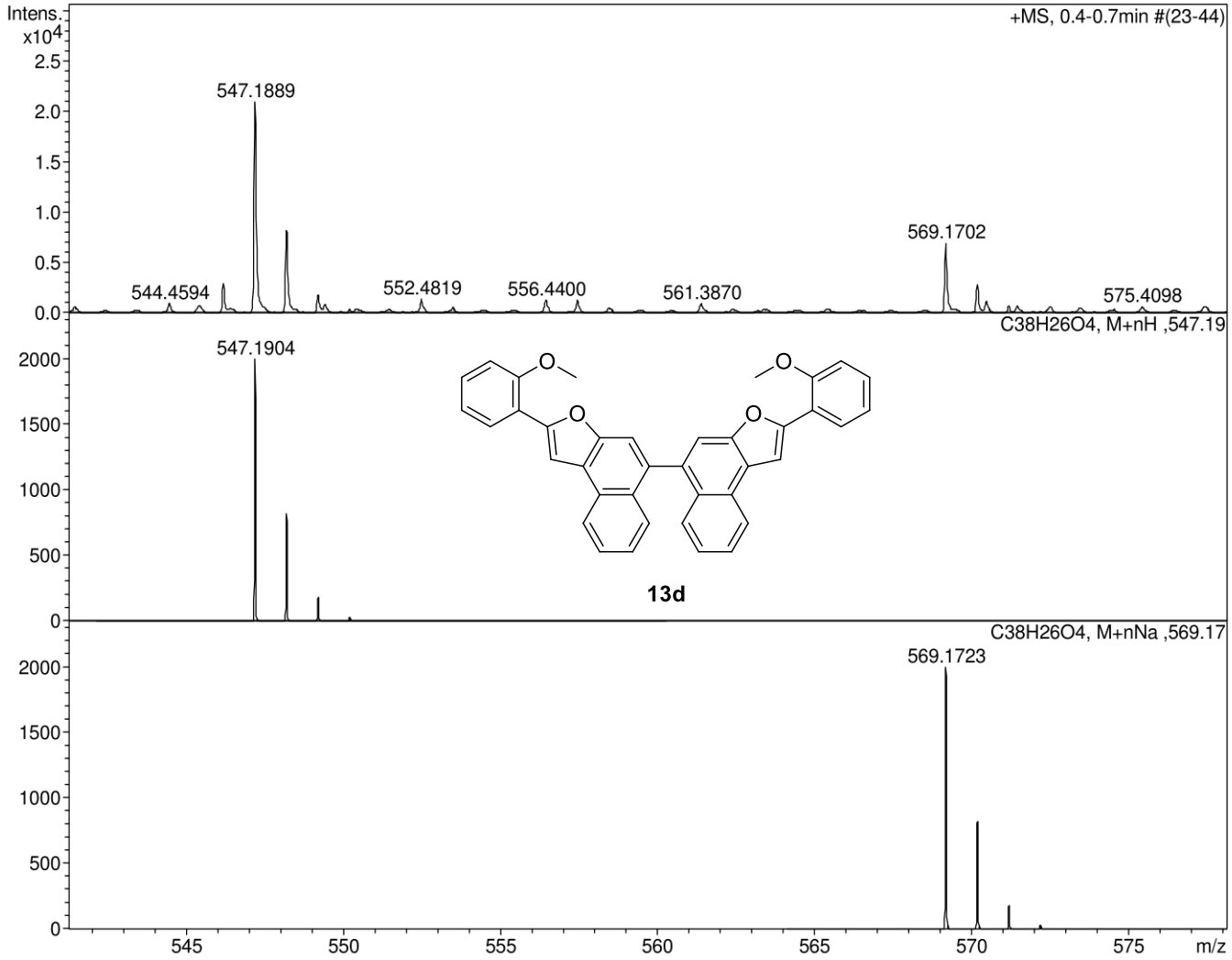




Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





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Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste