Supporting Information for

Electrochemical Dearomatization of 2-Naphthols for C–O Bond Formation

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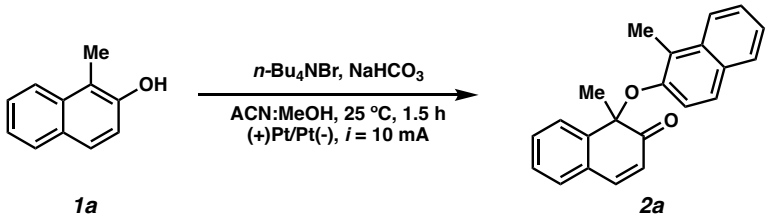
1. General Information

Unless otherwise noted, reagents and solvents were used as supplied commercially without further purification. 1-Methylnaphthalen-2-ol was purchased from BLD pharm and HPLC-grade methanol, and acetonitrile were purchased from Daejung. Electrolytes, alcohols, and bases were purchased from Sigma-Aldrich, Acros Organics, Alfa Aesar, Angene, BLD Pharm, TCI, and Combi-Blocks. Two different potentiostats, ElectraSyn 2.0, purchased from IKA and Vertex, were used for the electrochemical reactions. For gram-scale synthesis, potentiostat purchased from Ivium was used. All electrodes were purchased from IKA but Pt and Pt mesh were purchased from alfa for gram scales. Reactions were monitored by thin layer chromatography (TLC) using TLC Silica gel 60 F254 (Merck) and visualized by UV light (254nm) or exposure $KMnO_4$ solution followed by heating. Flash column chromatography was performed on silica gel 60 (particle size 230-400 mesh) and performed on Yamazen Automated Flash Chromatography System using Biotage® SNAP Ultra HP-Sphere C18 25 μm cartridges. All spectra were recorded on Bruker 400 MHz spectrometer in $CDCl_3$. ^1H NMR and ^{13}C NMR spectra chemical shifts are reported relative to the residual solvent peak. Data for ^1H, ^{13}C, and ^{19}F are reported in terms of chemical shifts (δ ppm).

Figure S1. Electrode and Ika electrasyn 2.0 set up. **(**Pt **:** 8.00 mm × 52.5 mm × 1.50 mm, graphite : 8.00 mm × 52.5 mm × 2.00 mm)

2. Optimization table of compound 2a[a]



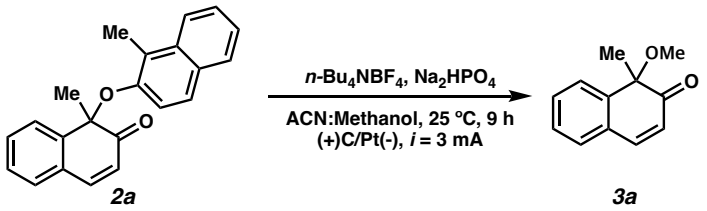
1a *2a*

entry	Electrolyte	Current (mA)	anode	Cathode	solvent	Base (equiv)	Time (h)	yield (%)
1	nBu$_4$NBF$_4$	10	C	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	44[b](30[c])

2	nBu$_4$NBF$_4$	10	C	Foiled Pt	MeCN	none	1.5	16[c]
3	nBu$_4$NBF$_4$	10	C	C	MeCN:MeOH (1:1)	none	1.5	51[b]
4	nBu$_4$NBF$_4$	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	74[b]
5	nBu$_4$NBF$_4$	10	C	RVC	MeCN:MeOH (1:1)	none	1.5	42[b]
6	nBu$_4$NBF$_4$	10	RVC	C	MeCN:MeOH (1:1)	none	1.5	50[b]
7	nBu$_4$NBF$_4$	10	Foiled Pt	RVC	MeCN:MeOH (1:1)	none	1.5	33[b]
8	nBu$_4$NBF$_4$	10	RVC	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	42[b]
9	nBu$_4$NBF$_4$	10	Foiled Pt	C	MeCN:MeOH (1:1)	none	1.5	18[b]
10	nBu$_4$NBF$_4$	5	RVC	RVC	MeCN:MeOH (1:1)	none	1.5	35[b]
11	nBu$_4$NBF$_4$	15	Plated Pt	Plated Pt	MeCN:MeOH (1:1)	none	1.5	40[b]
12	nBu$_4$NPF$_6$	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	38[b]
13	LiClO$_4$	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	20[b]
14	KI	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	49[b]
15	NaBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	75[b]
16	LiBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	74[b]
17	nEt$_4$NBF$_4$	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	49[b]
18	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	79[b]
19	NaPF$_6$	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	34[b]
20	LiBF$_4$	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	5[b]
21	KPF$_6$	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	30[b]
22	LiPF$_6$	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	25[b]
23	nBu$_4$NBr	15	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	47[b]
24	nBu$_4$NBr	5	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	none	1.5	39[b]
25	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeOH:CH$_2$Cl$_2$ (1:1)	none	1.5	75[b]
26	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeOH:THF (1:1)	none	1.5	65[b]
27	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeOH:DMF (1:1)	none	1.5	8[b]
28	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	Et$_3$N (0.5)	1.5	84[b]
29	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	Et$_3$N (1.5)	1.5	52[c]
30	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	t-BuOK (0.5)	1.5	52[b]
31	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	K$_2$CO$_3$ (0.5)	1.5	62[b]
32	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	NaOAc (0.5)	1.5	92[b]
33	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	NaOAc (1.5)	1.5	75[c]
34	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	NaHCO$_3$ (0.5)	1.5	80[b]
35	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	NaHCO$_3$ (1.5)	1.5	96[b](76[c])
36	nBu$_4$NBr	10	Foiled Pt	Foiled Pt	MeCN:MeOH (1:1)	NaHCO$_3$ (3.0)	1.5	75[b]

[a]1-Methylnaphthalen-2-ol **1a** (0.32 mmol, 1.0 equiv) and electrolyte (0.32 mmol, 1.0 equiv) were dissolved in solvent (0.05 M). [b]Determined by high-performance liquid chromatography (HPLC) using a 3-nitrophenol as the internal standard. [c]Isolated yield.

3. Optimization table of compound 3a[a]



2a *3a*

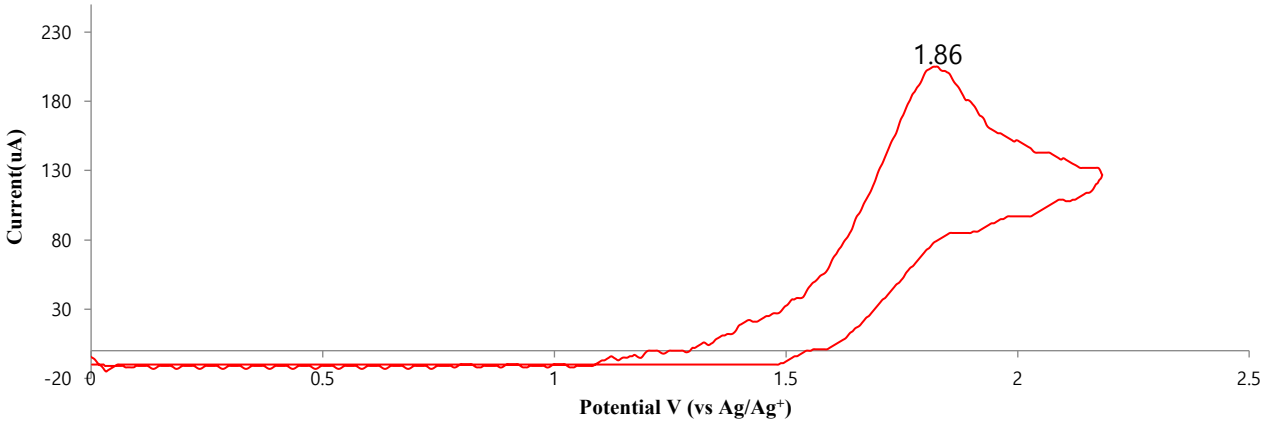
entry	Electrolyte	Current (mA)	anode	Cathode	solvent	Base (equiv)	Time (h)	yield (%)
1	nBu$_4$NPF$_6$	10	C	Foiled Pt	MeCN:MeOH (1:1)	NaHCO$_3$ (0.5)	4	60[b](40[c])
2	nBu$_4$NPF$_6$	5	C	Foiled Pt	MeCN:MeOH (1:1)	NaHCO$_3$ (0.5)	7.5	64[b]
3	nBu$_4$NPF$_6$	3	C	Foiled Pt	MeCN:MeOH (1:1)	NaHCO$_3$ (0.5)	9	66[b](51[c])
4	nBu$_4$NPF$_6$	3	C	Foiled Pt	MeCN:MeOH (1:1)	Na$_2$CO$_3$ (0.5)	9	27[b]
5	nBu$_4$NPF$_6$	3	C	Foiled Pt	MeCN:MeOH (1:1)	Na$_2$HPO$_4$ (0.5)	9	66[b](52[c])
6	nBu$_4$NPF$_6$	3	C	Foiled Pt	MeCN:MeOH (1:1)	Na$_2$HPO$_4$ (1.0)	9	61[c]
7	nBu$_4$NPF$_6$	3	C	Foiled Pt	MeCN:MeOH (1:1)	Na$_2$HPO$_4$ (1.5)	9	45[c]
8	nBu$_4$NPF$_6$	3	C	C	MeCN:MeOH (1:1)	Na$_2$HPO$_4$ (1.0)	9	47[c]
9	nBu$_4$NPF$_6$	3	C	Ni	MeCN:MeOH (1:1)	Na$_2$HPO$_4$ (1.0)	9	57[c]
10	nBu$_4$NPF$_6$	3	C	Ag	MeCN:MeOH (1:1)	Na$_2$HPO$_4$ (1.0)	9	59[c]
11	NaNPF$_6$	3	C	Foiled Pt	MeCN:MeOH (1:1)	Na$_2$HPO$_4$ (1.0)	9	52[c]
12	NaBF$_4$	3	C	Foiled Pt	MeCN:MeOH (1:1)	Na$_2$HPO$_4$ (1.0)	9	59[c]
13	nBu$_4$NBF$_4$	3	C	Foiled Pt	MeCN:MeOH (1:1)	Na$_2$HPO$_4$ (1.0)	9	69[c]
14	nBu$_4$NBF$_4$	3	C	Foiled Pt	MeOH	Na$_2$HPO$_4$ (1.0)	9	35[c]
15	nBu$_4$NBF$_4$	3	C	Foiled Pt	MeCN:MeOH (1:2)	Na$_2$HPO$_4$ (1.0)	9	44[c]

[a]1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1H)-one **2a** (0.16 mmol, 1.0 equiv) and electrolyte (0.16 mmol, 1.0 equiv) were dissolved in solvent (0.05 M). [b]NMR yield using BHT as the internal standard. [c]Isolated yield.

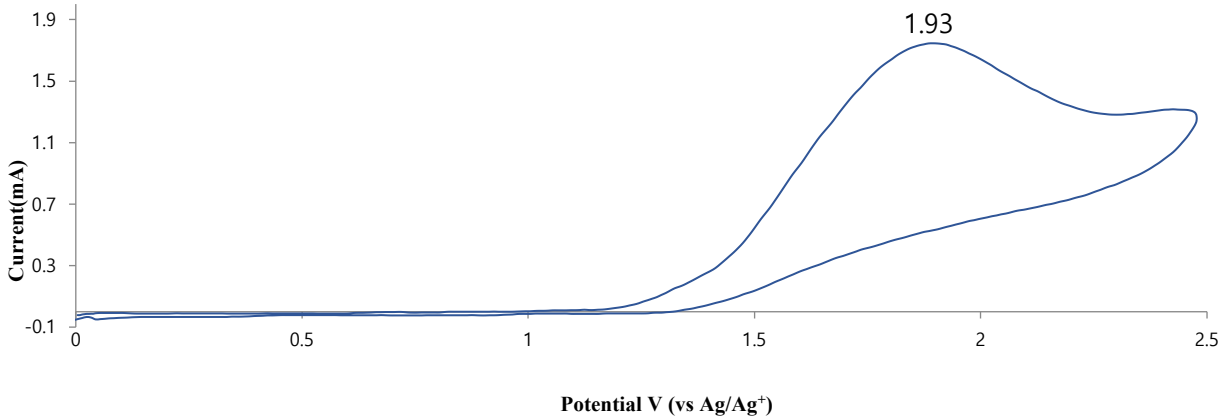
4. Cyclic voltammetry experiment

Cyclic voltammetry curve was recorded by IKA electrasyn 2.0 in a three-electrode cell at room temperature, using glassy carbon as working electrode, Ag/AgCl as reference electrode (filled with 3M KCl solutions), and plated Pt as the counter electrode. The starting point was at 0.0 V and measured in the positive direction. The initial potential was 0.0 V and switching potential was +2.5 V. The scan rate was 400 mV/s.

(a)



(b)



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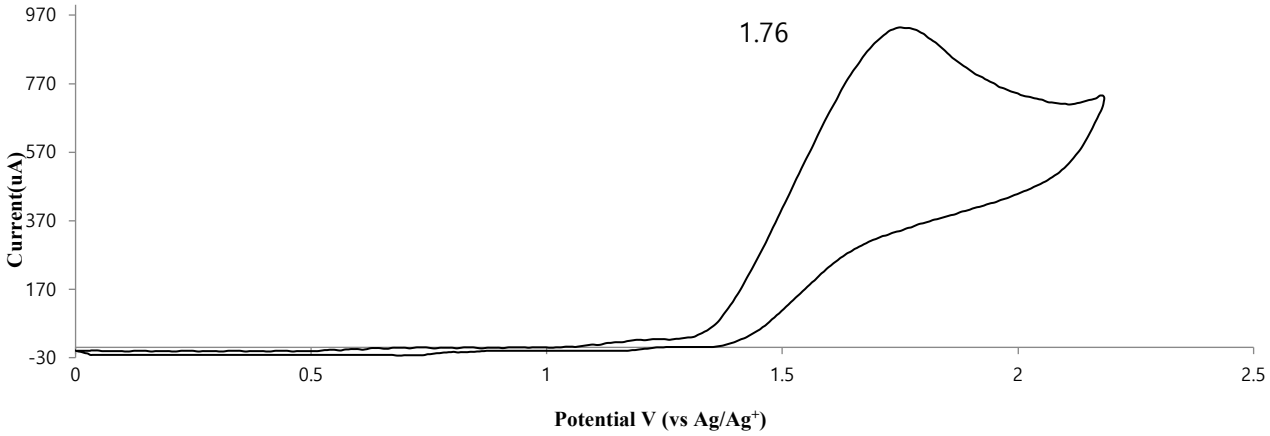
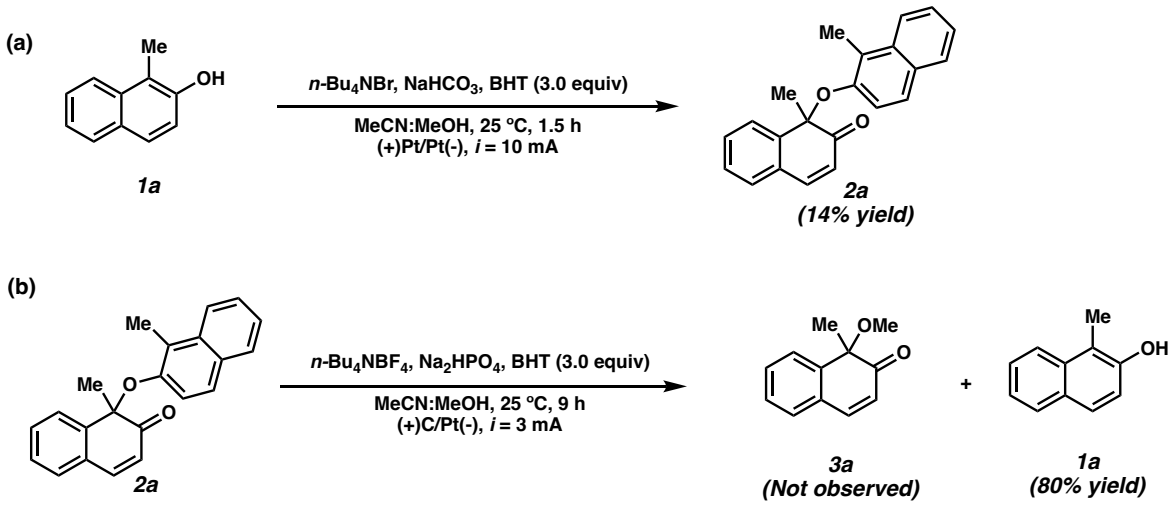


Figure S2. (a) **1a** in 0.1 M nBu$_4$NBF$_4$ in MeCN, (b) **2a** in 0.1 M nBu$_4$NBF$_4$ in MeCN, (c) **2a** + Na_2HPO_4 in 0.1 M nBu$_4$NBF$_4$ in MeCN.

5. Control experiment



Scheme S1. Control experiment with radical scavenger BHT.

To investigate whether radical intermediates were generated during the reaction, control experiments were conducted by adding the radical scavenger BHT under the optimized conditions. In the C–O homocoupling protocol, the addition of BHT significantly reduced the yield of the desired product **2a** (Scheme S1a). In addition, in the alkoxylation protocol, the addition of BHT completely suppressed the formation of the desired product (Scheme S1b). These results strongly suggest that radical intermediates were generated during the reactions.

6. Proposed mechanism[1-5]

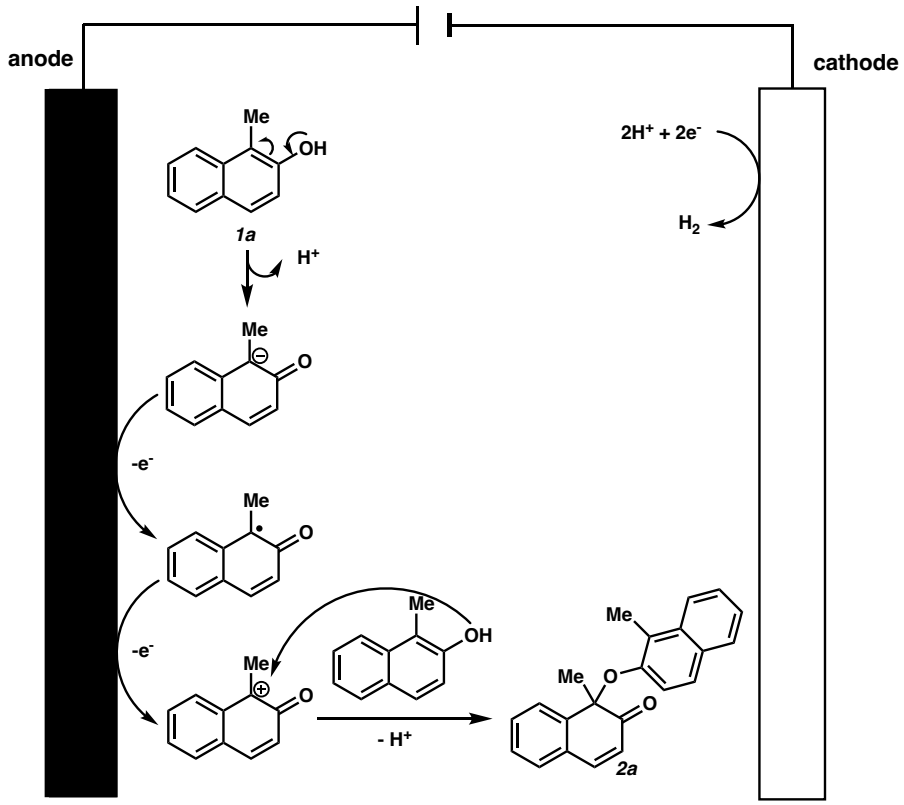


Figure S3. Plausible mechanism of the C–O homocoupling reaction.

Deprotonation of **1a** generates a carbanion intermediate, which undergoes two successive oxidations at the anode to form the corresponding carbocation. Nucleophilic attack by naphthol then affords the C–O homocoupled product **2a**. Protons released during the reaction are reduced at the cathode to produce hydrogen gas.

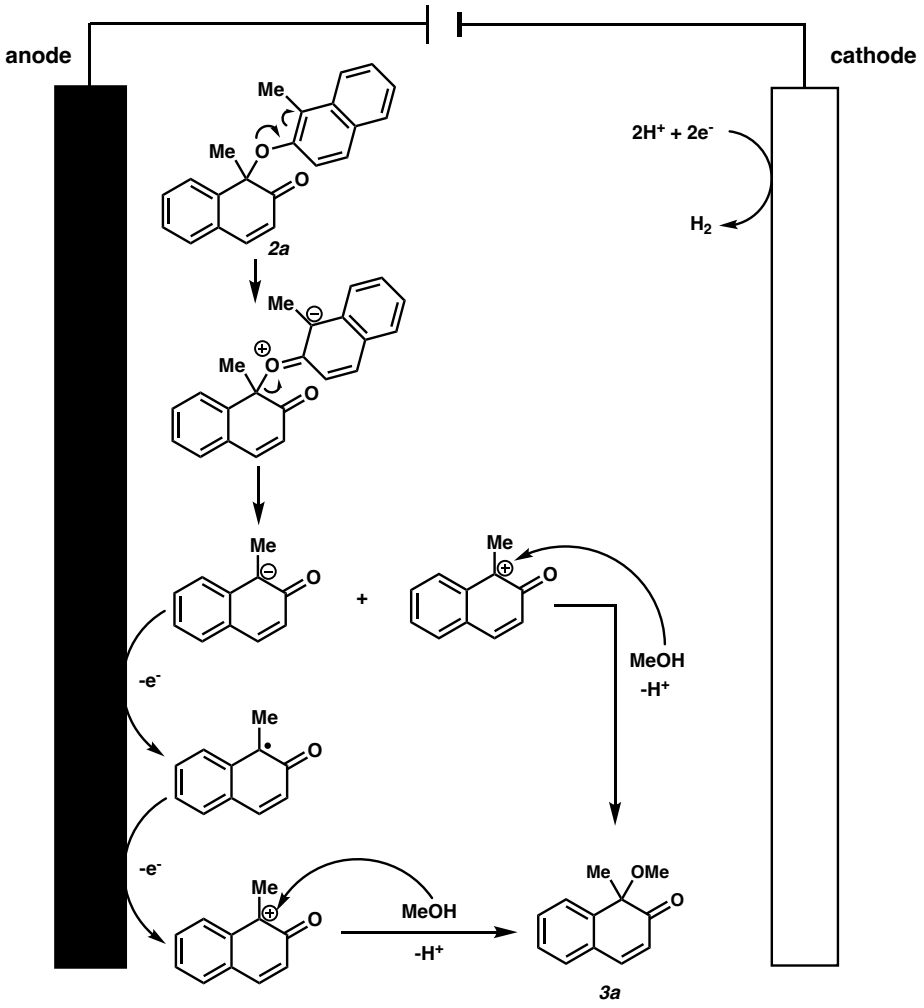
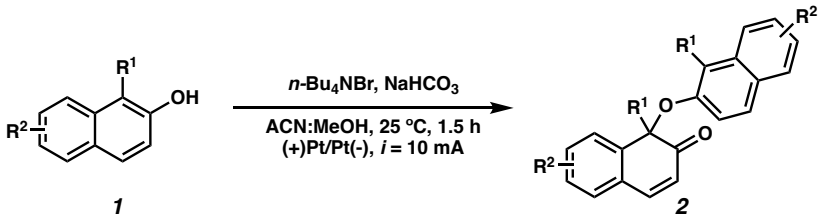


Figure S4. Plausible mechanism of the alkoxylation reaction.

The reaction proceeds via dearomatization followed by C–O bond cleavage to generate a carbanion intermediate. Two successive oxidations of the carbanion intermediate produce a tertiary carbocation intermediate. Nucleophilic attack of the carbocation by MeOH results in formation of the final product **3a**. The protons released during the process are reduced at the cathode, leading to the evolution of hydrogen gas.

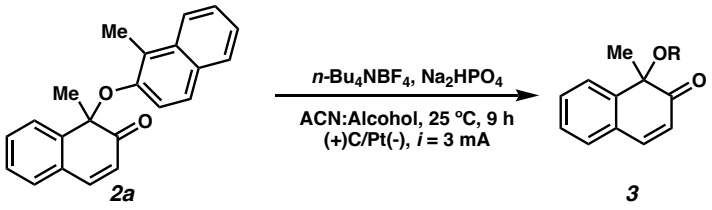
7. Experiment procedure

General Procedure 1

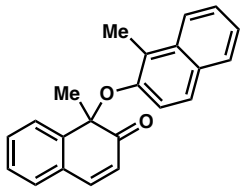


To a undivided cell with magnetic stir bar, tetrabutylammonium bromide (0.158 mmol, 1.00 equiv), sodium hydrogen carbonate (0.237 mmol, 1.50 equiv), naphthol **1** (0.158 mmol, 1.00 equiv) were added. The mixture was dissolved in MeCN:MeOH (1:1, 0.053 M). The cell was sealed using vial cap carrying a foiled platinum (8.00 mm x 52.5 mm x 1.50 mm) as working electrode and a foiled platinum (8.00 mm x 52.5 mm x 1.50 mm) as counter electrode. The reaction mixture was stirred at 25 °C for 1.5 h with constant current of 10 mA using IKA electrasyn 2.0. After the completion of reaction, the mixture was concentrated under reduced pressure and diluted with H_2O. The aqueous phase was extracted with EtOAc or CH_2Cl_2. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residues was purified by flash column chromatography or reverse phase medium pressure liquid chromatography.

General Procedure 2



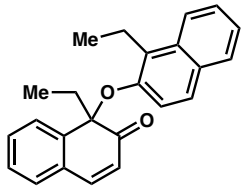
To a undivided cell with magnetic stir bar, tetrabutylammonium tetrafluoroborate (0.158 mmol, 1.00 equiv), sodium phosphate dibasic (0.158 mmol, 1.00 equiv), dimer **2** (0.158 mmol, 1.00 equiv) were added. The mixture was dissolved in MeCN:alcohol (1:1, 0.053 M) or MeCN:MeOH (1:1, 0.053M). The cell was sealed using vial cap carrying a graphite (8.00 mm × 52.5 mm × 2.00 mm) as working electrode and a foiled platinum (8.00 mm × 52.5 mm × 1.50 mm) as counter electrode. The reaction mixture was stirred at 25 °C for 9 h with constant current of 3 mA using IKA electrasyn 2.0. After the completion of reaction, the mixture was concentrated under reduced pressure and diluted with H_2O. The aqueous phase was extracted with EtOAc or CH_2Cl_2. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residues was purified by flash column chromatography or reverse phase medium pressure liquid chromatography.



2a

1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1H)-one (2a). Following the general procedure 1, 1-methylnaphthalen-2-ol (25.0 mg, 0.158 mmol), tetrabutylammonium bromide (51.0 mg, 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 18.8 mg (76%), yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.6 Hz, 1H), 7.63 – 7.56 (m, 2H), 7.47 – 7.40 (m, 3H), 7.34 – 7.22 (m, 4H), 6.38 (d, *J* = 9.9 Hz, 1H), 6.01 (d, *J* = 8.9 Hz, 1H), 2.76 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.1, 150.4, 145.2, 144.7, 133.9, 131.1, 130.0, 129.4, 128.8, 128.3, 128.2, 126.4, 126.1, 125.9, 125.1, 123.5, 123.4, 120.0, 115.8, 82.2, 31.8, 11.2; FT-IR (neat) 2955, 2918, 2850, 1676, 1262, 1233, 1083, 828, 797, 758 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{22}H_{18}NaO_2$: 337.1199, found: 337.1199.

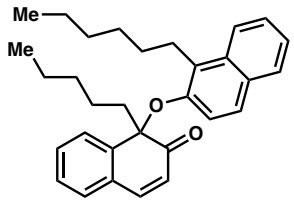


2b

1-ethyl-1-((1-ethylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one (2b).

Following the general procedure 1, 1-ethylnaphthalen-2-ol (27.0 mg, 0.158 mmol), tetrabutylammonum bromide (51.0 mg 0.158 mmol) and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by column chromatography on silica gel (1:4 EtOAc:hexanes) and then MPLC on C-18 silica gel (5–100% acetonitrile/water): 42.1 mg (78%), yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.7 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.58 (d, *J* = 10.0 Hz, 1H), 7.50 – 7.27 (m, 7H), 6.37 (d, *J* = 10.0 Hz, 1H), 6.05 (d, *J* = 9.0 Hz, 1H), 3.47 – 3.23 (m, 2H), 2.19 (ddq, *J* = 28.6, 14.5, 7.2 Hz, 2H), 1.46 (t, *J* = 7.5 Hz, 3H), 1.03 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.8, 149.9, 144.8, 143.7, 133.0, 130.5, 130.1, 129.9, 129.0, 128.5, 128.2, 126.4, 126.4, 126.1, 125.9, 125.9, 123.1, 116.1, 84.9, 38.2, 18.9, 14.5, 7.8; FT-IR (neat) 2917, 2359, 1675, 1592, 1512, 1467, 1239, 1148, 1055, 824, 744, 668, 624 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{24}H_{22}NaO_2$: 365.1518, found: 365.1514.

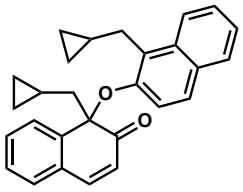


2c

1-hexyl-1-((1-hexylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one (2c).

Following the general procedure 1, 1-hexylnaphthalen-2-ol (36.0 mg, 0.158 mmol), tetrabutylammonum bromide (51.0 mg 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by column chromatography on silica gel (1:1:2 EtOAc:CH_2Cl_2:hexanes) and then MPLC on C-18 silica gel (5–100% acetonitrile/water): 72.2 mg (67%), yellow oil.

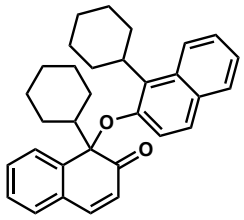
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.6 Hz, 1H), 7.67 – 7.55 (m, 2H), 7.52 – 7.27 (m, 7H), 6.37 (d, *J* = 9.9 Hz, 1H), 6.03 (d, *J* = 9.0 Hz, 1H), 3.32 (dddd, *J* = 37.2, 13.1, 10.3, 5.7 Hz, 2H), 2.13 (dddd, *J* = 35.3, 13.5, 11.7, 4.8 Hz, 2H), 1.36 – 1.24 (m, 2H), 1.98 – 1.75 (m, 2H), 1.71 – 1.60 (m, 2H), 1.58 – 1.37 (m, 6H), 1.36 – 1.24 (m, 6H), 0.99 (t, *J* = 7.0 Hz, 3H), 0.94 – 0.86 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.9, 150.1, 144.7, 144.0, 133.3, 130.5, 130.0, 129.9, 128.9, 128.5, 128.1, 126.4, 126.3, 126.0, 125.9, 124.8, 123.3, 123.1, 116.1, 84.8, 44.9, 32.0, 31.8, 30.3, 30.1, 29.5, 25.8, 23.0, 23.0, 22.7, 14.3, 14.2; FT-IR (neat) 2955, 2918, 2850, 1676, 1262, 1233, 1083, 828, 797, 758 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{31}H_{36}NaO_2$: 463.2613, found: 463.2629.



2d

1-(cyclopropylmethyl)-1-((1-(cyclopropylmethyl)naphthalen-2-yl)oxy)naphthalen-2(1*H*)-one (2d).
Following the general procedure 1, 1-(cyclopropylmethyl)naphthalen-2-ol (31.0 mg, 0.158 mmol), tetrabutylammonum bromide (51.0 mg 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by column chromatography on silica gel (1:8 EtOAc:hexanes) and then MPLC on C-18 silica gel (5–100% acetonitrile/water): 42.1 mg (78%), yellow sticky oil.

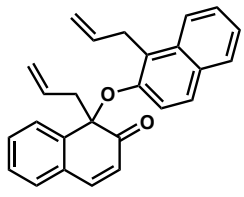
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 8.8, 3.6 Hz, 1H), 7.64 (dd, *J* = 8.1, 2.5 Hz, 1H), 7.59 – 7.40 (m, 5H), 7.36 – 7.26 (m, 4H), 6.41 (d, *J* = 9.9 Hz, 1H), 6.10 (dd, *J* = 9.4, 4.6 Hz, 1H), 3.46 – 3.24 (m, 2H), 2.14 (dddd, *J* = 23.8, 13.6, 7.0, 3.6 Hz, 2H), 1.34 (d, *J* = 15.9 Hz, 1H), 0.76 (dp, *J* = 12.6, 4.6, 3.8 Hz, 1H), 0.65 – 0.56 (m, 4H), 0.46 (s, 2H), 0.01 (qd, *J* = 11.4, 9.8, 5.2 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.9, 150.3, 150.3, 144.7, 144.7, 143.7, 133.6, 133.5, 130.4, 130.3, 129.7, 128.9, 128.4, 128.2, 126.6, 126.5, 126.1, 126.0, 123.8, 123.6, 123.1, 116.1, 85.0, 50.9, 29.3, 11.6, 11.6, 5.6, 5.5, 5.3, 4.9, 4.6; FT-IR (neat) 3074, 2359, 1711, 1675, 1592, 1512, 1260, 1241, 1123, 822, 765, 745 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{28}H_{26}NaO_2$: 417.1831, found: 417.1823.



2e

1-cyclohexyl-1-((1-cyclohexylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one (2e). Following the general procedure 1, 1-cyclohexylnaphthalen-2-ol (35.8 mg, 0.158 mmol), tetrabutylammonum bromide (51.0 mg 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by column chromatography on silica gel (1:8 EtOAc:hexanes) and then MPLC on C-18 silica gel (5–100% acetonitrile/water): 20.3 mg (28%), yellow oil.

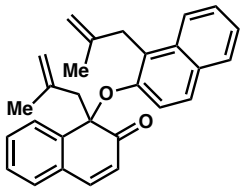
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.8 Hz, 1H), 7.61 – 7.50 (m, 2H), 7.46 – 7.28 (m, 4H), 7.27 – 7.15 (m, 2H), 6.33 (d, *J* = 10.1 Hz, 1H), 5.98 (d, *J* = 9.1 Hz, 1H), 3.60 (t, *J* = 12.1 Hz, 1H), 2.82 – 2.63 (m, 1H), 2.22 – 1.60 (m, 12H), 1.56 – 1.34 (m, 2H), 1.31 – 0.95 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.1, 151.6, 144.8, 142.5, 133.2, 131.2, 130.0, 129.5, 129.0, 128.7, 128.1, 127.6, 127.5, 126.9, 126.7, 126.1, 122.9, 122.9, 117.1, 87.6, 52.4, 38.7, 30.1, 29.8, 27.9, 27.7, 27.4, 26.8, 26.6, 26.5, 26.4; FT-IR (neat) 2924, 2852, 1673, 1451, 1263, 1231, 1080, 1026, 734, 701 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{32}H_{34}NaO_2$: 473.2457, found: 473.2401.



2f

1-allyl-1-((1-allylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one (2f). Following the general procedure 1, 1-allylnaphthalen-2-ol (29.0 mg, 0.158 mmol), tetrabutylammonum bromide (51.0 mg 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by column chromatography on silica gel (1:1:2 EtOAc:CH_2Cl_2:hexanes) and then MPLC on C-18 silica gel (5–100% acetonitrile/water): 20.3 mg (35%), yellow oil.

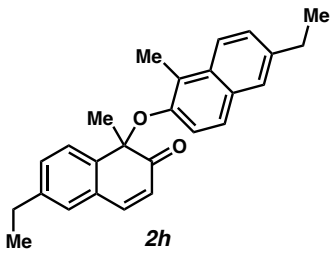
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 8.8, 3.6 Hz, 1H), 7.64 (dd, *J* = 8.1, 2.5 Hz, 1H), 7.59 – 7.40 (m, 5H), 7.36 – 7.26 (m, 4H), 6.41 (d, *J* = 9.9 Hz, 1H), 6.10 (dd, *J* = 9.4, 4.6 Hz, 1H), 3.46 – 3.24 (m, 2H), 2.14 (dddd, *J* = 23.8, 13.6, 7.0, 3.6 Hz, 2H), 1.34 (d, *J* = 15.9 Hz, 1H), 0.76 (dp, *J* = 12.6, 4.6, 3.8 Hz, 1H), 0.65 – 0.56 (m, 4H), 0.46 (s, 2H), 0.01 (qd, *J* = 11.4, 9.8, 5.2 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.9, 150.3, 150.3, 144.7, 144.7, 143.7, 133.6, 133.5, 130.4, 130.3, 129.7, 128.9, 128.4, 128.2, 126.6, 126.5, 126.1, 126.0, 123.8, 123.6, 123.1, 116.1, 85.0, 50.9, 29.3, 11.6, 11.6, 5.6, 5.5, 5.3, 4.9, 4.6; FT-IR (neat) 3070, 2918, 1672, 1593, 1511, 1240, 1085, 991, 914, 799, 742, 673 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{26}H_{22}NaO_2$: 389.1518, found: 389.1513.



2g

1-(2-methylallyl)-1-((1-(2-methylallyl)naphthalen-2-yl)oxy)naphthalen-2(1*H*)-one (2g). Following the general procedure 1, 1-(2-methylallyl)naphthalen-2-ol (31.0 mg, 0.158 mmol), tetrabutylammonum bromide (51.0 mg 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5-100% acetonitrile/water): 26.4 mg (42%), yellow oil.

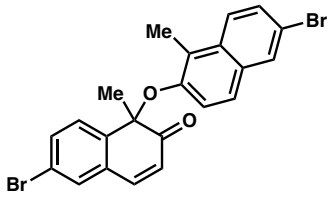
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.6 Hz, 1H), 7.68 – 7.49 (m, 2H), 7.39 (dd, *J* = 13.8, 7.3 Hz, 5H), 7.33 – 7.27 (m, 2H), 7.23 (d, *J* = 7.4 Hz, 1H), 6.33 (dd, *J* = 10.0, 1.9 Hz, 1H), 6.04 (dd, *J* = 9.0, 1.8 Hz, 1H), 4.89 – 4.80 (m, 2H), 4.48 (d, *J* = 12.3 Hz, 2H), 4.14 (d, *J* = 16.5 Hz, 1H), 3.90 (d, *J* = 16.6 Hz, 1H), 2.84 (d, *J* = 12.7 Hz, 1H), 2.77 (d, *J* = 12.9 Hz, 1H), 1.98 (s, 3H), 1.65 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.2, 150.6, 144.9, 144.5, 142.9, 139.2, 134.0, 130.3, 130.1, 129.8, 128.8, 128.3, 128.2, 127.1, 126.9, 126.2, 125.9, 123.9, 123.3, 121.2, 117.3, 116.1, 110.9, 85.4, 52.4, 33.7, 24.3, 23.6; FT-IR (neat) 2955, 2918, 2850, 1676, 1262, 1233, 1083, 828, 797, 758 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{28}H_{26}NaO_2$: 337.1199, found: 337.1199.



2h

6-ethyl-1-((6-ethyl-1-methylnaphthalen-2-yl)oxy)-1-methylnaphthalen-2-(1*H*)-one (2h). Following the general procedure 1, 6-ethyl-1-methylnaphthalen-2-ol (29.4 mg, 0.158 mmol), tetrabutylammonium bromide (51.0 mg, 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 24.6 mg (85%), yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.7 Hz, 1H), 7.57 (d, *J* = 10.0 Hz, 1H), 7.39 (d, *J* = 1.7 Hz, 1H), 7.32 (td, *J* = 6.8, 3.2 Hz, 2H), 7.24 (d, *J* = 1.8 Hz, 1H), 7.19 (d, *J* = 9.0 Hz, 1H), 7.10 (dd, *J* = 8.0, 1.9 Hz, 1H), 6.37 (d, *J* = 9.9 Hz, 1H), 6.02 (d, *J* = 8.9 Hz, 1H), 2.79 – 2.69 (m, 5H), 2.63 (q, *J* = 7.6 Hz, 2H), 1.81 (s, 3H), 1.24 (dt, *J* = 14.8, 7.6 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.5, 149.9, 145.5, 144.2, 141.9, 139.1, 132.3, 130.7, 129.4, 129.4, 129.3, 129.0, 127.3, 125.9, 125.9, 125.8, 125.0, 123.6, 119.8, 116.0, 82.0, 31.9, 28.8, 28.4, 15.7, 15.3, 11.3. FT-IR (neat) 2960, 2924, 2869, 1677, 1600, 1479, 1459, 1377, 1237, 1088, 816, 792, 699 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{26}H_{26}NaO_2$: 393.1824, found: 393.1825.

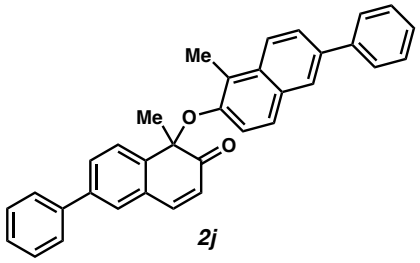


2i

6-bromo-1-((6-bromo-1-methylnaphthalen-2-yl)oxy)-1-methylnaphthalen-2(1*H*)-one (2i). Following the general procedure 1, 6-bromo-1-methylnaphthalen-2-ol (37.5 mg, 0.158 mmol), tetrabutylammonium bromide (51.0 mg, 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5→100% acetonitrile/water): 29.1 mg (76%), yellow solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 9.1 Hz, 1H), 7.76 (d, *J* = 2.1 Hz, 1H), 7.58 (d, *J* = 2.0 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.41 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.29 (d, *J* = 8.3 Hz, 1H), 7.17 (d, *J* = 9.1 Hz, 1H), 2.72 (s, 3H), 1.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.0, 150.4, 143.6, 143.2, 133.8, 132.6, 132.4, 131.2, 130.1, 130.0, 129.5, 127.5, 126.4, 125.6, 125.5, 122.2, 120.5, 117.4, 116.6, 82.1, 31.6, 11.3.

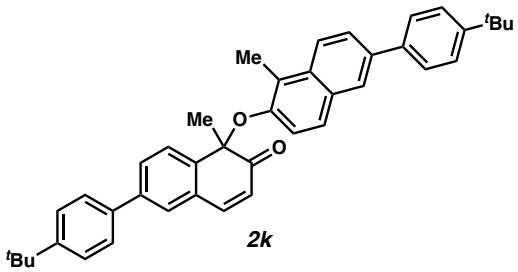
FT-IR (neat) 2956, 2917, 2850, 2359, 2343, 1664, 1457, 1051, 740, 691, 683 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{22}H_{16}Br_2NaO_2$: 492.9409, found: 492.9408.



2j

1-methyl-1-((1-methyl-6-phenylnaphthalen-2-yl-oxy)-6-phenylnaphthalen-2-(1*H*)-one (2j). Following the general procedure 1, 1-methyl-6-phenylnaphthalen-2-ol (37.0 mg, 0.158 mmol), tetrabutylammonium bromide (51.0 mg, 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 17.7 mg (48%), yellow solid.

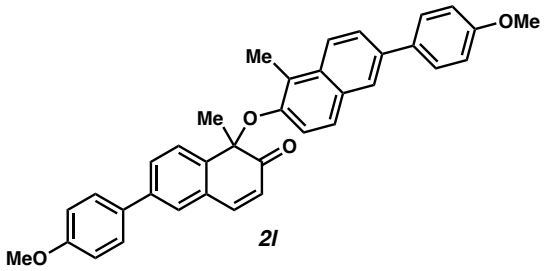
^1H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.9 Hz, 1H), 7.81 (s, 1H), 7.73 (d, *J* = 8.9 Hz, 1H), 7.70 – 7.62 (m, 4H), 7.56 (d, *J* = 7.5 Hz, 2H), 7.51 (d, *J* = 2.4 Hz, 2H), 7.47 – 7.41 (m, 4H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.33 (d, *J* = 9.2 Hz, 2H), 6.44 (d, *J* = 9.9 Hz, 1H), 6.11 (d, *J* = 9.0 Hz, 1H), 2.81 (s, 3H), 1.88 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.0, 150.6, 145.1, 143.4, 141.4, 141.3, 139.7, 136.1, 133.2, 129.9, 129.7, 129.2, 129.1, 129.1, 129.0, 128.9, 128.6, 128.0, 127.3, 127.1, 127.1, 126.8, 126.4, 126.2, 125.8, 125.6, 124.2, 120.1, 116.4, 82.2, 31.9, 11.3. FT-IR (neat) 2954, 2921, 2851, 1678, 1459, 1377, 1264, 738, 698 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{34}H_{26}NaO_2$: 489.1825, found: 489.1826.



2k

6-(4-tert-butyl)phenyl)-1-((6-(4-(tert-butyl)phenyl)-1-methylnaphthalen-2-yl)oxy)-1-methylnaphthalen-2(1*H*)-one (2k). Following the general procedure 1, 6-(4-(tert-butyl)phenyl)-1-methylnaphthalen-2-ol (45.9 mg, 0.158 mmol), tetrabutylammonium bromide (51.0 mg, 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 24.2 mg (53%), yellow solid.

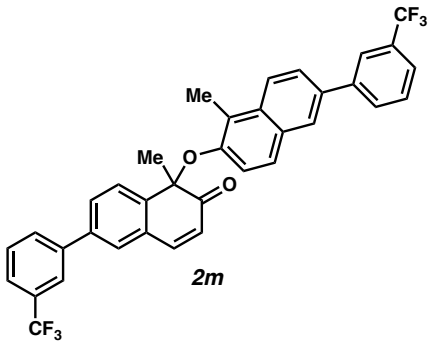
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.9 Hz, 1H), 7.80 (d, *J* = 2.2 Hz, 1H), 7.73 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.67 (d, *J* = 10.0 Hz, 1H), 7.64 – 7.57 (m, 3H), 7.52 – 7.44 (m, 8H), 7.32 (d, *J* = 8.8 Hz, 1H), 6.42 (d, *J* = 9.9 Hz, 1H), 6.09 (d, *J* = 8.9 Hz, 1H), 2.80 (s, 3H), 1.87 (s, 3H), 1.36 (s, 9H), 1.35 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.1, 151.1, 150.5, 150.1, 145.3, 143.0, 141.2, 138.3, 136.8, 135.9, 133.0, 129.8, 129.6, 129.1, 128.4, 126.9, 126.7, 126.7, 126.4, 126.0, 125.9, 125.9, 125.8, 125.4, 124.1, 120.0, 116.3, 82.2, 34.7, 34.6, 31.8, 31.5, 31.4, 11.3; FT-IR (neat) 2954, 2920, 2869, 1714, 1682, 1459, 1376, 1239, 827, 737 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{42}H_{42}NaO_2$: 601.3077, found: 601.3080.



2l

6-(4-methoxyphenyl)-1-((6-(4-methoxyphenyl)-1-methylnaphthalen-2-yl)oxy-1-methylnaphthalen-2(1*H*)-one (2l). Following the general procedure 1, 6-(4-methoxyphenyl)-1-methylnaphthalen-2-ol (41.8 mg, 0.158 mmol), tetrabutylammonium bromide (51.0 mg, 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 17.1 mg (41%), yellow sticky oil.

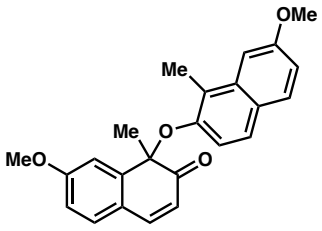
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 9.2 Hz, 1H), 7.74 (s, 1H), 7.68 (dd, *J* = 11.6, 9.5 Hz, 2H), 7.62 – 7.56 (m, 2H), 7.50 (s, 1H), 7.48 (d, *J* = 2.2 Hz, 1H), 7.46 (d, *J* = 1.2 Hz, 2H), 7.30 (d, *J* = 8.9 Hz, 1H), 7.00 – 6.95 (m, 4H), 6.42 (d, *J* = 9.9 Hz, 1H), 6.10 (d, *J* = 9.2 Hz, 1H), 3.84 (d, *J* = 0.9 Hz, 6H), 2.80 (s, 3H), 1.87 (s, 3H);^{13}C NMR (101 MHz, $CDCl_3$) δ 200.1, 159.7, 159.1, 150.4, 145.3, 142.7, 140.9, 135.7, 133.8, 132.8, 132.2, 129.9, 129.2, 129.2, 128.3, 128.2, 128.1, 126.6, 126.4, 125.7, 125.5, 124.1, 120.0, 116.4, 114.5, 114.4, 114.4, 82.2, 55.5, 31.8, 11.3; FT-IR (neat) 2955, 2918, 2850, 1737, 1679, 1519, 1464, 1377, 1248, 1181, 816, 720 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{36}H_{30}NaO_4$: 549.2036, found: 549.2034.



2m

1-methyl-1-((1-methyl-6-(3-(trifluoromethyl)phenyl)naphthalen-2-yl)oxy-6-(3-(trifluoromethyl)phenyl)naphthalen-2(1*H*)-one (2m). Following the general procedure 1, 1-methyl-6-(3-(trifluoromethyl)phenyl)naphthalen-2-ol (47.8 mg, 0.158 mmol), tetrabutylammonium bromide (51.0 mg, 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 41.9 mg (88%), yellow solid.

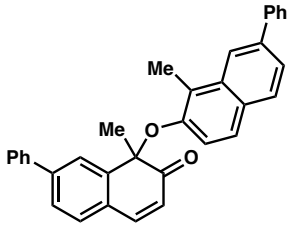
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.9 Hz, 1H), 7.88 (s, 1H), 7.84 – 7.79 (m, 3H), 7.74 – 7.68 (m, 3H), 7.67 – 7.62 (m, 2H), 7.59 – 7.54 (m, 3H), 7.54 – 7.50 (m, 2H), 7.35 (d, *J* = 9.1 Hz, 1H), 6.47 (d, *J* = 10.0 Hz, 1H), 6.11 (d, *J* = 9.0 Hz, 1H), 2.82 (s, 3H), 1.89 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.6, 150.9, 144.7, 144.2, 142.0, 140.6, 140.0, 134.6, 133.5, 131.6 (q, *J* = 32.3 Hz), 131.3 (q, *J* = 32.2 Hz), 130.5, 130.4 (q, *J* = 1.4 Hz), 130.2, 129.7, 129.6, 129.4, 129.1, 128.6, 126.9, 126.6, 126.5, 125.9, 125.4, 124.7 (q, *J* = 3.8 Hz), 124.6, 124.0 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 3.8 Hz), 120.2, 116.5, 82.3, 31.8, 11.3; ^{19}F NMR (377 MHz, $CDCl_3$) δ −62.58, −62.66; FT-IR (neat) 2954, 2917, 2869, 1714, 1458, 1376, 1330, 1219, 1125, 801, 700 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{36}H_{24}F_6NaO_2$: 625.1572, found: 625.1574.



2n

7-methoxy-1-((7-methoxy-1-methylnaphthalen-2-yl)oxy)-1-methylnaphthalen-2(1*H*)-one (2n). Following the general procedure 1, 7-methoxy-1-methylnaphthalen-2-ol (29.7 mg, 0.158 mmol), tetrabutylammonium bromide (51.0 mg, 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 15.0 mg (51%), yellow sticky oil.

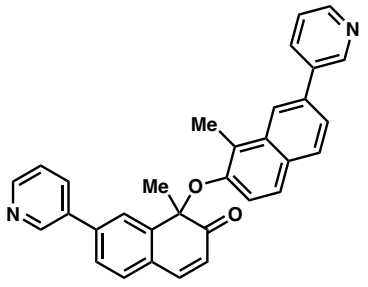
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 9.8 Hz, 1H), 7.51 (d, *J* = 8.9 Hz, 1H), 7.35 (d, *J* = 8.3 Hz, 1H), 7.22 – 7.17 (m, 2H), 6.98 (d, *J* = 2.6 Hz, 1H), 6.95 (dd, *J* = 8.9, 2.4 Hz, 1H), 6.80 (dd, *J* = 8.5, 2.6 Hz, 1H), 6.24 (d, *J* = 9.9 Hz, 1H), 5.93 (d, *J* = 9.1 Hz, 1H), 3.94 (s, 3H), 3.69 (s, 3H), 2.72 (s, 3H), 1.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.9, 162.1, 158.0, 151.0, 147.2, 145.0, 135.1, 131.7, 129.9, 126.2, 124.3, 122.6, 122.5, 118.7, 115.9, 113.5, 113.3, 112.0, 102.2, 82.1, 55.4, 55.3, 32.1, 11.4; FT-IR (neat) 2956, 2924, 2850, 1711, 1676, 1461, 1359, 1219, 1089, 828, 735, 701 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{24}H_{22}NaO_4$: 397.1411, found: 397.1413.



2o

1-methyl-1-((1-methyl-7-phenylnaphthalen-2-yl)oxy)-7-phenylnaphthalen-2(1*H*)-one (2o). Following the general procedure 1, 1-methyl-7-phenylnaphthalen-2-ol (37.0 mg, 0.158 mmol), tetrabutylammonium bromide (51.0 mg, 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 29.9 mg (81%), yellow sticky oil.

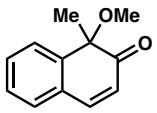
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 2.0 Hz, 1H), 7.73 (dd, *J* = 8.4, 1.5 Hz, 3H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 9.9 Hz, 1H), 7.57 – 7.52 (m, 2H), 7.50 (td, *J* = 7.9, 1.8 Hz, 3H), 7.44 – 7.29 (m, 7H), 6.40 (d, *J* = 9.9 Hz, 1H), 6.13 (d, *J* = 8.9 Hz, 1H), 2.86 (s, 3H), 1.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.9, 150.9, 145.3, 144.7, 143.8, 142.0, 139.8, 138.9, 134.2, 130.5, 129.0, 128.9, 128.9, 128.4, 128.3, 128.1, 127.7, 127.4, 127.2, 126.9, 126.3, 125.0, 124.6, 123.3, 121.8, 120.4, 116.0, 82.5, 32.1, 11.4. FT-IR (neat) 2952, 2920, 2850, 1668, 1443, 1372, 1310, 738, 698 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{34}H_{26}NaO_2$: 489.1825, found: 489.1824.



2p

1-methyl-1-((1-methyl-7-(pyridin-3-yl)naphthalen-2-yl)oxy)-7-(pyridin-3-yl)naphthalen-2(1*H*)-one (2p). Following the general procedure 1, 1-methyl-7-(pyridin-3-yl)naphthalen-2-ol (37.2 mg, 0.158 mmol), tetrabutylammonium bromide (51.0 mg, 0.158 mmol), and sodium hydrogen carbonate (20.0 mg, 0.237 mmol) were used and stirred for 1.5 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 30.0 mg (76%), yellow solid.

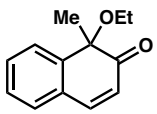
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (d, *J* = 2.4 Hz, 1H), 8.68 (d, *J* = 2.4 Hz, 1H), 8.64 – 8.58 (m, 1H), 8.57 – 8.47 (m, 1H), 8.13 (s, 1H), 8.00 (dt, *J* = 7.9, 2.0 Hz, 1H), 7.74 – 7.63 (m, 4H), 7.56 (s, 2H), 7.49 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.41 (dd, *J* = 7.9, 4.8 Hz, 1H), 7.30 (t, *J* = 8.5 Hz, 2H), 6.42 (dd, *J* = 9.9, 2.6 Hz, 1H), 6.20 – 6.01 (m, 1H), 2.83 (d, *J* = 2.6 Hz, 3H), 1.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.4, 151.0, 149.3, 148.6, 148.3, 148.2, 145.6, 144.4, 140.4, 137.4, 135.5, 135.3, 135.0, 134.4, 134.1, 130.8, 129.3, 129.1, 128.3, 127.0, 126.4, 125.6, 124.3, 123.8, 123.7, 122.8, 122.2, 120.5, 116.3, 82.4, 32.0, 11.4; FT-IR (neat) 3033, 2953, 2919, 2850, 1676, 1607, 1457, 1371, 1220, 1091, 805, 734, 710 cm^{-1}; HRMS (ESI) *m/z* ([M+H]$^+$) calcd for $C_{32}H_{25}N_2O_2$: 469.1910, found: 469.1911.



3a

1-methoxy-1-methylnaphthalen-2-(1*H*)-one (3a). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and methanol (1.5 ml) were used and stirred for 9 h. The product was purified by column chromatography on silica gel (1:1:4 EtOAc:CH_2Cl_2:hexanes): 41.0 mg (69%), yellow solid.

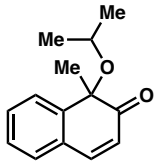
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.8 Hz, 1H), 7.52 – 7.45 (m, 1H), 7.42 (d, *J* = 9.9 Hz, 1H), 7.39 – 7.33 (m, 2H), 6.21 (d, *J* = 9.9 Hz, 1H), 3.06 (d, *J* = 1.8 Hz, 3H), 1.52 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.4, 145.2, 143.7, 130.7, 130.7, 129.7, 128.3, 126.4, 125.4, 82.8, 54.0, 31.1; FT-IR (neat) 2953, 2925, 2870, 1674, 1448, 1236, 1105, 1078, 836, 778 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{12}H_{12}NaO_2$: 211.0729, found: 211.0730.



3b

1-ethoxy-1-methylnaphthalen-2(1*H*)-one (3b). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and ethanol (1.5 ml) were used and stirred for 7 h. The product was purified by column chromatography on silica gel (1:1:4 EtOAc:CH_2Cl_2:hexanes): 30.0 mg (47%), yellow oil.

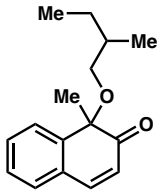
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.7 Hz, 1H), 7.48 – 7.42 (m, 2H), 7.40 (d, *J* = 10.0 Hz, 0H), 7.34 – 7.33 (m, 1H), 7.32 (s, 1H), 6.17 (d, *J* = 9.9 Hz, 1H), 3.24 (dq, *J* = 8.7, 6.9 Hz, 1H), 3.00 (dq, *J* = 8.8, 7.2 Hz, 1H), 1.50 (s, 3H), 1.18 (t, *J* = 7.0 Hz, 3H).). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.5, 145.1, 144.6, 130.6, 130.5, 129.6, 128.1, 126.3, 125.4, 82.2, 61.9, 31.2, 15.7; FT-IR (neat) 2953, 2920, 2869, 1727, 1672, 1453, 1376, 1264, 1101, 1079, 753, 699 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{13}H_{14}NaO_2$: 255.0886, found: 255.0887.



3c

1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one (3c). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and isopropanol (1.5 ml) were used and stirred for 10 h. The product was purified by column chromatography on silica gel (1:1:4 EtOAc:CH_2Cl_2:hexanes): 30.8 mg (45%), yellow oil.

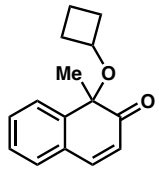
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.2 Hz, 1H), 7.49 – 7.39 (m, 2H), 7.35 – 7.30 (m, 2H), 6.21 (d, *J* = 9.9 Hz, 1H), 3.47 (p, *J* = 6.1 Hz, 1H), 1.48 (s, 3H), 1.05 (d, *J* = 6.1 Hz, 3H), 0.95 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.4, 145.1, 145.0, 130.2, 129.9, 129.5, 128.1, 127.9, 125.4, 80.0, 69.9, 31.6, 24.0, 23.7; FT-IR (neat) 2967, 2923, 2870, 1668, 1446, 1379, 1232, 1113, 1077, 992, 827, 757 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{14}H_{16}NaO_2$: 239.1042, found: 239.1043.



3d

1-methyl-1-(2-methylbutoxy)naphthalen-2(1*H*)-one (3d). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and 2-methyl-1-butanol (1.5 ml) were used and stirred for 10 h. The product was purified by column chromatography on silica gel (1:1:4 EtOAc:CH_2Cl_2:hexanes): 36.8 mg (48%), yellow oil.

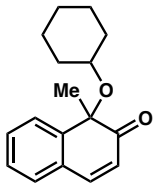
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 7.8, 3.4 Hz, 1H), 7.45 (ddd, *J* = 7.8, 5.5, 3.2 Hz, 1H), 7.41 (d, *J* = 9.9 Hz, 1H), 7.34 (d, *J* = 1.7 Hz, 1H), 7.33 (s, 2H), 6.18 (d, *J* = 9.9 Hz, 1H), 2.98 (ddd, *J* = 29.7, 8.3, 5.8 Hz, 1H), 2.80 – 2.65 (m, 1H), 1.67 (tdd, *J* = 12.6, 8.7, 5.3 Hz, 2H), 1.59 – 1.36 (m, 4H), 1.06 (dddd, *J* = 20.4, 10.9, 7.2, 3.7 Hz, 1H), 0.94 – 0.77 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.4, 145.0, 144.6, 144.6, 130.5, 130.5, 129.5, 128.1, 126.8, 126.7, 125.6, 81.5, 71.2, 71.0, 35.5, 35.5, 31.1, 31.1, 26.3, 26.2, 16.9, 16.4, 11.5, 11.3; FT-IR (neat) 2956, 2918, 2850, 1675, 1457, 1233, 1099, 1079, 826, 756 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{16}H_{20}NaO_2$: 267.1355, found: 267.1357.



3e

1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one (3e). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and cyclobutanol (1.5 ml) were used and stirred for 6 h. The product was purified by column chromatography on silica gel (1:8 EtOAc:hexanes): 30.3 mg (42%), yellow oil.

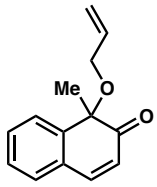
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.7 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.42 – 7.38 (m, 1H), 7.33 (dd, *J* = 5.7, 1.8 Hz, 2H), 6.17 (d, *J* = 9.9 Hz, 1H), 3.49 (p, *J* = 8.3, 7.7 Hz, 1H), 2.19 – 2.03 (m, 2H), 1.98 (q, *J* = 10.5, 10.0 Hz, 1H), 1.87 – 1.78 (m, 1H), 1.50 (m, 4H), 1.15 (tdd, *J* = 10.8, 7.8, 3.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.8, 145.2, 144.9, 130.3, 130.2, 129.5, 128.2, 127.0, 125.2, 82.2, 72.2, 33.0, 32.9, 30.8, 12.8; FT-IR (neat) 2950, 2925, 2871, 1672, 1234, 1133, 1105, 826, 757 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{15}H_{16}NaO_2$: 251.1042, found: 251.1043.



3f

1-(cyclohexyloxy)-1-methylnaphthalen-2(1*H*)-one (3f). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and cyclohexanol (1.5 ml) were used and stirred for 7 h. The product was purified by column chromatography on silica gel (1:8 EtOAc:hexanes): 30.0 mg (42%), yellow oil.

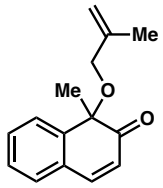
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.7 Hz, 1H), 7.48 – 7.40 (m, 2H), 7.37 – 7.31 (m, 2H), 6.21 (d, *J* = 9.9 Hz, 1H), 3.13 (tt, *J* = 10.3, 3.9 Hz, 1H), 1.77 (d, *J* = 12.4 Hz, 1H), 1.69 – 1.60 (m, 1H), 1.54 (d, *J* = 2.3 Hz, 1H), 1.49 (s, 3H), 1.44 – 1.38 (m, 1H), 1.32 – 1.14 (m, 3H), 1.07 – 0.94 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.3, 145.3, 145.0, 130.2, 129.7, 129.5, 128.0, 127.9, 125.4, 79.8, 76.1, 34.1, 34.1, 31.7, 25.5, 24.9, 24.8; FT-IR (neat) 2950, 2924, 2853, 1669, 1446, 1230, 1079, 927, 757 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{17}H_{20}NaO_2$: 279.1355, found: 279.1358.



3g

1-(allyloxy)-1-methylnaphthalen-2(1*H*)-one (3g). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonum tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and allylic alcohol (1.5 ml) were used and stirred for 8 h. The product was purified by column chromatography on silica gel (1:4 EtOAc:hexanes): 37.4 mg (55%), yellow oil.

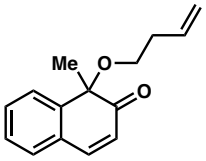
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.7 Hz, 1H), 7.49 – 7.28 (m, 4H), 6.18 (dd, *J* = 9.9, 1.4 Hz, 1H), 5.97 – 5.82 (m, 1H), 5.31 – 5.19 (m, 1H), 5.14 – 5.07 (m, 1H), 3.75 (ddt, *J* = 11.7, 5.7, 1.4 Hz, 1H), 3.50 (ddt, *J* = 11.6, 5.5, 1.4 Hz, 1H), 1.53 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.1, 145.0, 144.1, 134.5, 130.6, 130.4, 129.6, 128.3, 126.3, 125.3, 117.2, 82.3, 67.6, 31.1; FT-IR (neat) 2923, 2360, 1670, 1357, 1231, 1078, 992, 921, 826, 758, 687 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{14}H_{14}NaO_2$: 237.0892, found: 237.0887.



3h

1-methyl-1-((2-methylallyl)oxy)naphthalen-2(1*H*)-one (3h). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and 2-methylprop-2-en-1-ol (1.5 ml) were used and stirred for 8 h. The product was purified by column chromatography on silica gel (1:8 EtOAc:hexanes): 35.0 mg (49%), yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.6 Hz, 1H), 7.48 – 7.40 (m, 2H), 7.35 (dd, *J* = 4.0, 2.3 Hz, 2H), 6.20 (d, *J* = 9.9 Hz, 1H), 5.05 (s, 1H), 4.86 (s, 1H), 3.65 (d, *J* = 11.6 Hz, 1H), 3.37 (d, *J* = 11.6 Hz, 1H), 1.73 (s, 3H), 1.55 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.0, 145.0, 144.2, 142.0, 130.6, 130.5, 129.6, 128.3, 126.4, 125.5, 111.9, 82.0, 69.9, 31.1, 19.9; FT-IR (neat) 2953, 2923, 2853, 2361, 1674, 1449, 1375, 1231, 1079, 1024, 896, 826, 758 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{15}H_{16}NaO_2$: 251.1042, found: 251.1042.

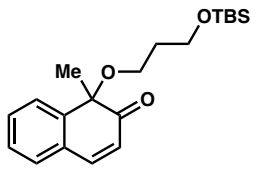


3i

1-(but-3-en-1-yloxy)-1-methylnaphthalen-2(1*H*)-one (3i). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and but-3-en-1-ol (1.5 ml) were used and stirred for 8 h. The product was purified by column chromatography on silica gel (1:8 EtOAc:hexanes: 36.1 mg (50%), yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.8 Hz, 1H), 7.46 (tt, *J* = 5.7, 3.0 Hz, 1H), 7.40 (d, *J* = 9.9 Hz, 1H), 7.34 (dd, *J* = 4.2, 2.0 Hz, 2H), 6.18 (d, *J* = 9.9 Hz, 1H), 5.76 (ddt, *J* = 17.1, 10.3, 6.7 Hz, 1H), 5.08 – 4.90 (m, 2H), 3.24 (dt, *J* = 8.6, 6.8 Hz, 1H), 2.99 (dt, *J* = 8.6, 7.2 Hz, 1H), 2.42 – 2.30 (m, 2H), 1.50 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.3, 145.1, 144.4, 135.0, 130.6, 130.5, 129.6, 128.2, 126.5, 125.4,

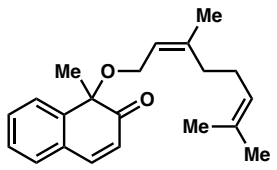
116.6, 82.1, 65.6, 34.6, 31.1; FT-IR (neat) 2953, 2923, 2869, 2358, 1672, 1446, 1232, 1098, 1079, 912, 826, 758 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{15}H_{16}NaO_2$: 251.1042, found: 251.1043.



3j

1-(3-((tert-butyldimethylsilyl)oxy)propoxy)-1-methylnaphthalen-2(1*H*)-one (3j). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and 3-((*tert*-butyldimethylsilyl)oxy)propan-1-ol (1.5 ml) were used and stirred for 6 h. Remained 3-((*tert*-butyldimethylsilyl)oxy)propan-1-ol was evaporated by air blowing. The product was purified by column chromatography on silica gel (1:8 EtOAc:hexanes): 38.3 mg (35%), yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.6 Hz, 1H), 7.44 (dt, *J* = 5.4, 3.8 Hz, 1H), 7.40 (d, *J* = 9.9 Hz, 1H), 7.36 – 7.30 (m, 2H), 6.18 (d, *J* = 9.9 Hz, 1H), 3.72 (dt, *J* = 10.3, 6.4 Hz, 1H), 3.63 (dt, *J* = 10.1, 6.2 Hz, 1H), 3.19 (dt, *J* = 8.6, 6.3 Hz, 1H), 3.09 (dt, *J* = 8.7, 6.8 Hz, 1H), 1.88 – 1.70 (m, *J* = 7.0 Hz, 2H), 1.49 (s, 3H), 0.81 (s, 9H), -0.00 (d, *J* = 5.7 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.4, 145.0, 144.4, 130.6, 130.5, 129.6, 128.1, 126.5, 125.4, 82.0, 63.3, 60.1, 33.5, 31.1, 26.0, 18.3, -5.2; FT-IR (neat) 2953, 2926, 2866, 1676, 1250, 1079, 834, 775, 756 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{20}H_{30}NaO_3Si$: 369.1856, found: 369.1858.

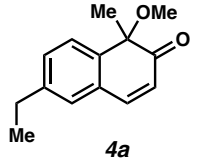


3k

(Z)-1-(3,7-dimethylocta-2,6-dien-1-yl)oxy)-1-methylnaphthalen-2(1*H*)-one (3k). Following the general procedure 2, 1-methyl-1-((1-methylnaphthalen-2-yl)oxy)naphthalen-2(1*H*)-one **2a** (50.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and geraniol (1.5 ml) were used and stirred for 9 h. The product was purified by column chromatography on silica gel (1:8 EtOAc:hexanes): 37.9 mg (39%), yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.6 Hz, 1H), 7.49 – 7.44 (m, 1H), 7.41 (d, *J* = 9.9 Hz, 0H), 7.37 – 7.31 (m, 2H), 6.20 (d, *J* = 9.9 Hz, 1H), 5.42 – 5.31 (m, 1H), 5.10 – 4.99 (m, 1H), 3.75 (dd, *J* = 10.6,

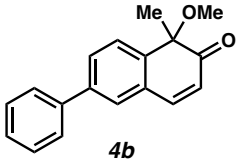
7.0 Hz, 1H), 3.53 (dd, *J* = 10.7, 6.8 Hz, 1H), 2.07 – 2.01 (m, 2H), 2.01 – 1.96 (m, 2H), 1.66 (s, *J* = 1.1 Hz, 3H), 1.57 (s, 3H), 1.52 (s, 3H), 1.49 (s, *J* = 1.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.4, 144.9, 144.5, 140.6, 131.7, 130.6, 130.5, 129.6, 128.2, 126.5, 125.5, 124.1, 120.7, 81.9, 63.3, 39.7, 31.2, 26.4, 25.8, 17.8, 16.6; FT-IR (neat) 2954, 2922, 2853, 1674, 1445, 1232, 1093, 1077, 1014, 827, 757 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{21}H_{26}NaO_2$: 333.1825, found: 333.1826.



4a

6-ethyl-1-methoxy-1-methylnaphthalen-2(1*H*)-one (4a). Following the general procedure 2, 6-ethyl-1-((6-ethyl-1-methylnaphthalen-2-yl)oxy)-1-methylnaphthalen-2(1*H*)-one **2h** (59.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and methanol (1.5 ml) were used and stirred for 5 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 30.1 mg (44%), yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 9.9 Hz, 1H), 7.30 (dd, *J* = 7.9, 2.0 Hz, 1H), 7.17 (d, *J* = 2.0 Hz, 1H), 6.18 (d, *J* = 9.9 Hz, 1H), 3.04 (d, *J* = 2.2 Hz, 3H), 2.68 (q, *J* = 7.6 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.7, 145.5, 144.4, 140.9, 130.6, 130.3, 129.2, 126.5, 125.3, 82.6, 54.0, 31.1, 28.5, 15.5; FT-IR (neat) 2956, 2924, 2870, 1673, 1456, 1378, 1242, 1106, 1064, 837, 693 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{14}H_{16}NaO_2$: 239.1042, found: 239.1043.

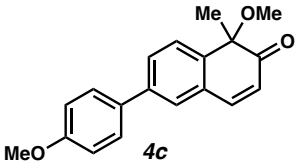


4b

1-methoxy-1-methyl-6-phenylnaphthalen-2(1*H*)-one (4b). Following the general procedure 2, 1-methyl-1-((1-methyl-6-phenylnaphthalen-2-yl)oxy)-6-phenylnaphthalen-2(1*H*)-one **2j** (73.7 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and methanol (1.5 ml) were used and stirred for 9 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 53.3 mg (64%), yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 1.4 Hz, 2H), 7.61 (dd, *J* = 7.2, 2.1 Hz, 2H), 7.56 (s, 1H), 7.50 – 7.44 (m, 3H), 7.42 – 7.37 (m, 1H), 6.25 (d, *J* = 9.9 Hz, 1H), 3.10 (s, 3H), 1.56 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.3, 145.1, 142.4, 141.4, 139.9, 131.1, 129.3, 129.1, 128.3, 128.0, 127.1, 127.0,

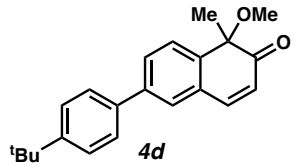
125.8, 82.7, 54.1, 31.1; FT-IR (neat) 2954, 2917, 2850, 1673, 1452, 1373, 1238, 1105, 1080, 824, 759, 695 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{18}H_{16}NaO_2$: 287.1042, found: 287.1045.



4c

1-methoxy-6-(4-methoxyphenyl)-1-methylnaphthalen-2(1*H*)-one (4c). Following the general procedure 2, 6-(4-methoxyphenyl)-1-((6-(4-methoxyphenyl)-1-methylnaphthalen-2-yl)oxy)-1-methylnaphthalen-2(1*H*)-one **2l** (83.2 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and methanol (1.5 ml) were used and stirred for 6 h. The product was purified by column chromatography on silica gel (1:1:4 EtOAc:CH_2Cl_2:hexanes): 49.4 mg (53%), yellow solid.

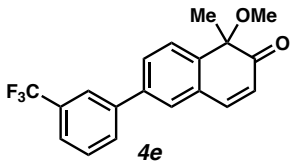
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.62 (m, 2H), 7.58 – 7.53 (m, 2H), 7.51 (d, *J* = 1.7 Hz, 1H), 7.48 (d, *J* = 9.9 Hz, 1H), 7.03 – 6.96 (m, 2H), 6.24 (d, *J* = 9.9 Hz, 1H), 3.87 (s, 3H), 3.09 (s, 3H), 1.55 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.4, 159.7, 145.3, 141.8, 141.1, 132.4, 131.1, 128.9, 128.2, 127.9, 127.0, 125.8, 114.5, 82.7, 55.5, 54.1, 31.1; FT-IR (neat) 2594, 2924, 2869, 1674, 1518, 1460, 1376, 1263, 1249, 1179, 827, 736, 703 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{19}H_{18}NaO_3$: 317.1148, found: 317.1148.



4d

6-(4-(tert-butyl)phenyl)-1-methoxy-1-methylnaphthalen-2(1*H*)-one (4d). Following the general procedure 2, 6-(4-(tert-butyl)phenyl)-1-((6-(4-(tert-butyl)phenyl)-1-methylnaphthalen-2-yl)oxy)-1-methylnaphthalen-2(1*H*)-one **2k** (91.5 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), methanol (1.5 ml) and toluene instead of acetonitrile were used and stirred for 12 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 61.9 mg (61%), yellow solid.

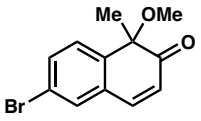
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (t, *J* = 1.1 Hz, 2H), 7.57 – 7.53 (m, 23), 7.52 – 7.46 (m, 3H), 6.24 (dd, *J* = 9.9, 1.0 Hz, 1H), 3.09 (d, *J* = 1.1 Hz, 3H), 1.56 (d, *J* = 0.7 Hz, 3H), 1.37 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.3, 151.0, 145.2, 142.0, 141.2, 136.9, 131.0, 129.1, 128.2, 126.9, 126.8, 126.7, 126.0, 125.9, 125.7, 82.6, 54.0, 34.7, 31.4, 31.0; FT-IR (neat) 2956, 2925, 2868, 1674, 1460, 1371, 1239, 1106, 826, 725 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{22}H_{24}NaO_2$: 343.1669, found: 233.1668.



4e

1-methoxy-1-methyl-6-(3-(trifluoromethyl)phenyl)naphthalen-2(1*H*)-one (4e). Following the general procedure 2, 1-methyl-1-((1-methyl-6-(3-(trifluoromethyl)phenyl)naphthalen-2-yl)oxy)-6-(3-(trifluoromethyl)phenyl)naphthalen-2(1*H*)-one **2m** (95.2 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and methanol (1.5 ml) were used and stirred for 7 h. The product was purified by column chromatography on silica gel (1:1:4 EtOAc:CH_2Cl_2:hexanes): 76.6 mg (73%), brown oil.

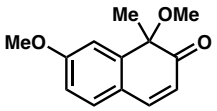
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.81 – 7.75 (m, 1H), 7.75 – 7.67 (m, 2H), 7.67 – 7.56 (m, 3H), 7.50 (d, *J* = 10.0 Hz, 1H), 6.27 (d, *J* = 9.9 Hz, 1H), 3.10 (d, *J* = 2.7 Hz, 3H), 1.56 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.02, 144.66, 143.33, 140.75, 139.98, 131.50 (q, *J* = 32.1 Hz), 131.39, 130.44, 129.62, 129.28, 128.32, 127.19, 126.15, 124.66 (d, *J* = 3.7 Hz), 123.97 (d, *J* = 4.0 Hz), 121.15 (q, *J* = 272.5 Hz), 82.68, 54.16, 31.04; ^{19}F NMR (377 MHz, $CDCl_3$) δ –62.59; FT-IR (neat) 2953, 2923, 2854, 1675, 1454, 1375, 1335, 1126, 736, 699; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{19}H_{15}F_3NaO_2$: 355.0916, found: 355.0918.



4f

6-bromo-1-((6-bromo-1-methylnaphthalen-2-yl)oxy)-1methylnaphthalen-2(1*H*)-one (4f). Following the general procedure 2, 6-bromo-1-((6-bromo-1-methylnaphthalen-2-yl)oxy)-1-methylnaphthalen-2(1*H*)-one **2i** (74.6 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and methanol (1.5 ml) were used and stirred for 9 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 41.4 mg (49%), yellow stick oil..

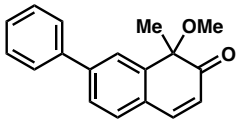
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.51 – 7.46 (m, 2H), 7.33 (d, *J* = 10.0 Hz, 1H), 6.22 (d, *J* = 10.0 Hz, 1H), 3.02 (s, 3H), 1.47 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.6, 143.6, 142.6, 133.5, 132.6, 132.3, 128.2, 126.7, 122.2, 82.6, 54.2, 31.0; FT-IR (neat) 2953, 2925, 1673, 1450, 1231, 1104, 1078, 826, 684 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{12}H_{11}BrNaO_2$: 288.9834, found: 288.9836.



4g

1,7-dimethoxy-1-methylnaphthalen-2(1*H*)-one (4g). Following the general procedure 2, 7-methoxy-1-((7-methoxy-1-methylnaphthalen-2-yl)oxy)-1-methylnaphthalen-2(1*H*)-one **2n** (59.1 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and methanol (1.5 ml) were used and stirred for 6 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 21.2 mg (30%), yellow solid.

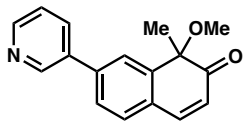
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 9.9 Hz, 1H), 7.27 (d, *J* = 8.3 Hz, 1H), 7.18 (d, *J* = 2.7 Hz, 1H), 6.86 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.07 (d, *J* = 9.8 Hz, 1H), 3.87 (s, 3H), 3.08 (d, *J* = 0.9 Hz, 3H), 1.51 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.3, 162.1, 146.3, 145.1, 131.4, 123.8, 122.8, 113.8, 112.1, 82.9, 55.7, 54.1, 31.5; FT-IR (neat) 2955, 2918, 2850, 2360, 1669, 1601, 1557, 1463, 1282, 1106, 1032, 837, 738 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{13}H_{14}NaO_3$: 241.0835, found: 241.0836.



4h

1-methoxy-1-methyl-7-phenylnaphthalen-2(1*H*)-one (4h). Following the general procedure 2, 1-methyl-1-((1-methyl-7-phenylnaphthalen-2-yl)oxy)-7-phenylnaphthalen-2(1*H*)-one **2o** (73.7 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and methanol (1.5 ml) were used and stirred for 9 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 43.1 mg (52%), purple solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 2.1 Hz, 1H), 7.70 – 7.64 (m, 2H), 7.60 (dd, *J* = 7.8, 2.0 Hz, 1H), 7.53 – 7.38 (m, 5H), 6.23 (d, *J* = 9.9 Hz, 1H), 3.12 (s, 3H), 1.58 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.3, 144.8, 144.3, 143.5, 139.9, 130.3, 129.7, 129.1, 129.3, 127.3, 126.8, 125.3, 125.0, 83.0, 54.2, 31.4; FT-IR (neat) 2954, 2918, 2850, 1713, 1675, 1605, 1457, 1377, 1219, 1105, 847, 757, 697 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{18}H_{16}NaO_2$: 287.1042, found: 287.1045.

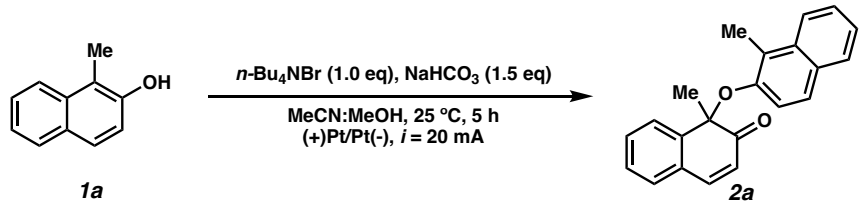


4i

1-methoxy-1-methyl-7-(pyridin-3-yl)naphthalen-2(1*H*)-one (4i). Following the general procedure 2, 1-methyl-1-((1-methyl-7-(pyridin-3-yl)naphthalen-2-yl)oxy)-7-(pyridin-3-yl)naphthalen-2(1*H*)-one **2p** (74.0 mg, 0.158 mmol), tetrabutylammonium tetrafluoroborate (52.4 mg, 0.158 mmol), sodium phosphate dibasic (22.6 mg, 0.158 mmol), and methanol (1.5 ml) were used and stirred for 9 h. The product was purified by MPLC on C-18 silica gel (5–100% acetonitrile/water): 35.7 mg (43%), yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (d, *J* = 2.4 Hz, 1H), 8.72 – 8.59 (m, 1H), 8.05 (d, *J* = 7.6 Hz, 1H), 7.88 (d, *J* = 2.1 Hz, 1H), 7.61 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.56 – 7.45 (m, 3H), 6.27 (d, *J* = 9.9 Hz, 1H), 3.12 (s, 3H), 1.58 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.9, 149.1, 148.1, 144.8, 144.4, 139.9, 135.7, 134.8, 130.6, 130.5, 126.9, 125.9, 125.0, 124.0, 83.0, 54.3, 31.3; FT-IR (neat) 3032, 2954, 2921, 2850, 1710, 1674, 1456, 1360, 1222, 1105, 1085, 850, 804, 712 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{17}H_{15}NaNO_2$: 288.0995, found: 288.0997.

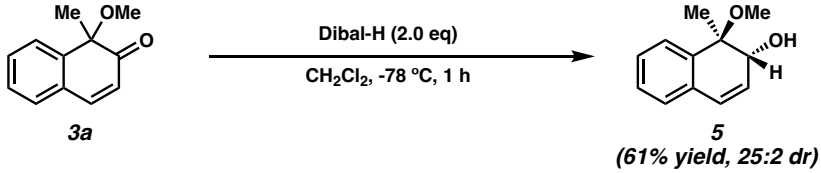
Gram scale and diversification



1a ***(1.0 g, 6.3 mmol)*** ***2a*** ***(0.75 g, 75% yield)***

A gram scale experiment was performed using a Ivium Vertex.One potentiostat instead of IKA electrasyn 2.0. To a 100 ml beaker with magnetic stir bar, tetrabutylammonium bromide (6.32 mmol, 1.00 equiv), sodium hydrogen carbonate (9.48 mmol, 1.50 equiv), 1-methylnaphthalen-2-ol (6.32 mmol, 1.00 equiv) were added. The mixture was dissolved in MeCN:MeOH (1:1, 0.105 M). The cell was sealed using cap carrying a platinum sheet (10.0 mm x 25.0 mm x 2.0 mm) as working electrode and a platinum mesh (10.0 mm x 25.0 mm x 2.0 mm) as counter electrode. The reaction mixture was stirred at 25 °C for 5 h with constant current of 20 mA. After the completion of reaction, the mixture was concentrated under reduced pressure and diluted with H_2O. The aqueous phase was extracted with CH_2Cl_2. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residues was purified by flash column chromatography on silica gel (1:8 EtOAc:hexanes): 745 mg(75%), yellow solid.

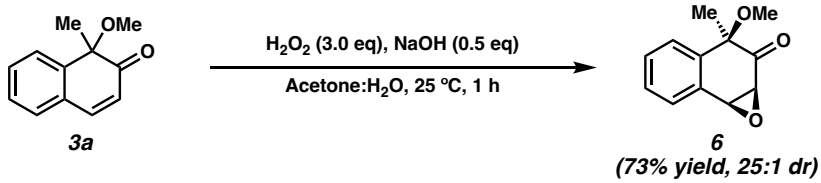
The faradaic efficiency (FE) was calculated based on the total amount of product formed with respect to the total charge passed during electrolysis. For the formation **2a** in gram scale, an FE of 64% was obtained, as determined by isolation yield.



3a *5* ***(61% yield, 25:2 dr)***

(1*R*,2*R*)-1-methoxy-1-methyl-1,2-dihydronaphthalen-2-ol (5). To a solution of **3a** (56.0 mg, 0.300 mmol) in CH_2Cl_2 (2.00 ml), Dibal-H (1.00 M solution in toluene, 0.600 mmol) was added dropwise -78°C under N_2 atmosphere. After stirring for 2 h, saturated NH_4Cl aqueous solution or 1M NaOH in aqueous solution (2.00 ml) was added. The aqueous layer was extracted with CH_2Cl_2. The organic layer was washed with brine, dried over Na_2SO_4, filtered and then concentrated. The residue was purified by silica gel column chromatography on silica gel (1:8 EtOAc:hexanes): 34.9 mg (61%), colorless oil

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 (dd, *J* = 7.1, 2.0 Hz, 1H), 7.29 – 7.20 (m, 2H), 7.07 (dd, *J* = 6.6, 2.3 Hz, 1H), 6.33 (dd, *J* = 9.8, 2.6 Hz, 1H), 5.99 (dd, *J* = 9.8, 2.4 Hz, 1H), 4.96 (t, *J* = 2.6 Hz, 1H), 3.30 (s, 3H), 1.88 (s, 1H), 1.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.3, 133.5, 131.4, 128.2, 128.0, 127.2, 126.9, 125.1, 82.9, 69.6, 51.2, 21.0; FT-IR (neat) 3433, 2935, 1707, 14520, 1365, 1230, 1061, 904, 789, 731, 643 cm^{-1}; HRMS (ESI) *m/z* ([M+Na]$^+$) calcd for $C_{12}H_{14}NaO_2$: 213.0886, found: 213.0887.

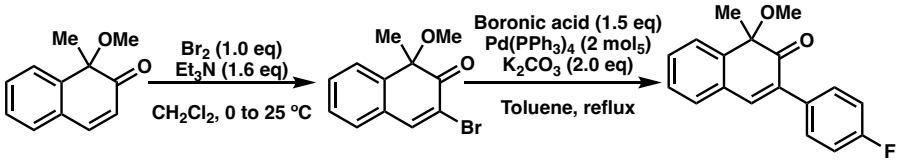


3a *6* ***(73% yield, 25:1 dr)***

(1*R*,2*R*)-1-methoxy-1-methylnaphthalen-2(1*H*)-one (6). To a solution of **3a** (56.0 mg, 0.300 mmol), in acetone/H_2O (0.5 mL/0.5 mL) were added 35% H_2O_2 (90.0 µL, 0.900 mmol) and 1M NaOH in aqueous solution (150 µL, 0.150 mmol) at room temperature. After stirring for 1 h, the mixture was quenched with aqueous NH_4Cl and the organic material was extracted with EtOAc. The organic layer was dried over Na_2SO_4. After filtraton, the filtrate was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (1:8 EtOAc:hexanes): 44.7 mg (73%), purple oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.46 (m, 3H), 7.42 – 7.34 (m, 1H), 4.24 (d, *J* = 3.9 Hz, 1H), 3.83 – 3.74 (m, 1H), 3.00 (s, 3H), 1.68 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 206.6, 140.7, 131.3, 130.2, 129.5,

128.2, 127.3, 82.6, 58.9, 54.1, 53.7, 31.4; FT-IR (neat) 2979, 2360, 1720, 1451, 1361, 1230, 1109, 1008, 871, 761, 664 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{12}H_{12}NaO_2$: 227.0678, found: 227.0679.



3a ***7*** ***(76% yield)*** ***8*** ***(89% yield)***

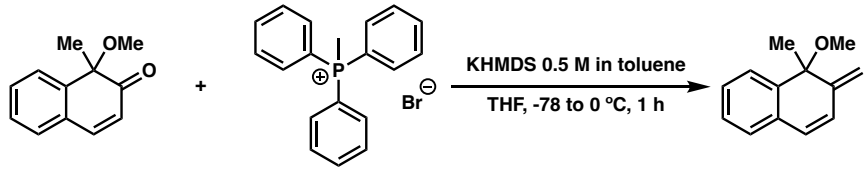
3-bromo-1-methoxy-1-methylnaphthalen-2(1*H*)-one (7). To a solution of **3a** (56.0 mg, 0.300 mmol) in CH_2Cl_2 (1.50 mL) were added Br_2 (15.0 µL, 0.300 mmol) and Et_3N (66.0 µL, 0.480 mmol) at 0 °C. After stirring overnight, the reaction was warmed to 40 °C and was stirred for 1 h. The reaction was quenched with aqueous Na_2SO_3. The organic material was extracted with CH_2Cl_2 and washed with brine. The organic layer was dried over Na_2SO_4. After concentration, the residue was purified by column chromatography on silica gel (1:8 EtOAc:hexanes): 61.0 mg (76%), yellow solid.

^1H NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.64 – 7.57 (m, 1H), 7.50 (td, *J* = 7.5, 1.6 Hz, 1H), 7.38 (td, *J* = 7.4, 1.4 Hz, 1H), 7.34 – 7.30 (m, 1H), 3.07 (s, 3H), 1.55 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.2, 146.7, 143.0, 131.0, 130.3, 129.4, 128.7, 126.6, 121.5, 84.4, 54.3, 31.5; FT-IR (neat) 3039, 2391, 2830, 1681, 1438, 1346, 1225, 1101, 968, 852, 764, 700, 637 cm^{-1}; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{12}H_{11}BrNaO_2$: 288.9832, found: 288.9836.

3-(4-fluorophenyl)-1-methoxy-1-methylnaphthalen-2(1*H*)-one (8). To a flame-dried vial containing solution of **7** (27.0 mg, 0.100 mmol) in toluene (1.00 mL), (4-fluorophenyl)boronic acid (21.0 mg, 0.150 mmol) was added. To this mixture potassium carbonate (28.0 mg, 0.200 mmol) and $Pd(PPh_3)_4$ (2.30 mg, 0.002 mmol) were sequentially added under N_2 atmosphere at room temperature. The mixture was refluxed for 12 h then cooled to room temperature, filtered through a pad of celite and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (1:8 EtOAc:hexanes): 25.0 mg (89%), yellow solid.

^1H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.1 Hz, 1H), 7.56 – 7.44 (m, 4H), 7.39 (dd, *J* = 8.2, 1.6 Hz, 2H), 7.17 – 7.05 (m, 2H), 3.13 (s, 3H), 1.61 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.0, 163.0 (d, *J* = 248.3 Hz), 143.1, 141.7, 134.8, 131.2 (d, *J* = 3.3 Hz), 130.8, 130.5, 130.4 (d, *J* = 4.0 Hz), 129.9, 128.5, 126.2, 115.5 (d, *J* = 21.3 Hz), 83.8, 54.2, 31.1; ^{19}F NMR (377 MHz, $CDCl_3$) δ –113.2; FT-IR (neat) 2981,

2826, 1675, 1600, 1506, 1225, 1104, 832, 758, 728, 618 cm^{-1} ; HRMS (ESI) *m/z* ($[M+Na]^+$) calcd for $C_{18}H_{15}FNaO_2$: 305.0948, found: 305.0949.



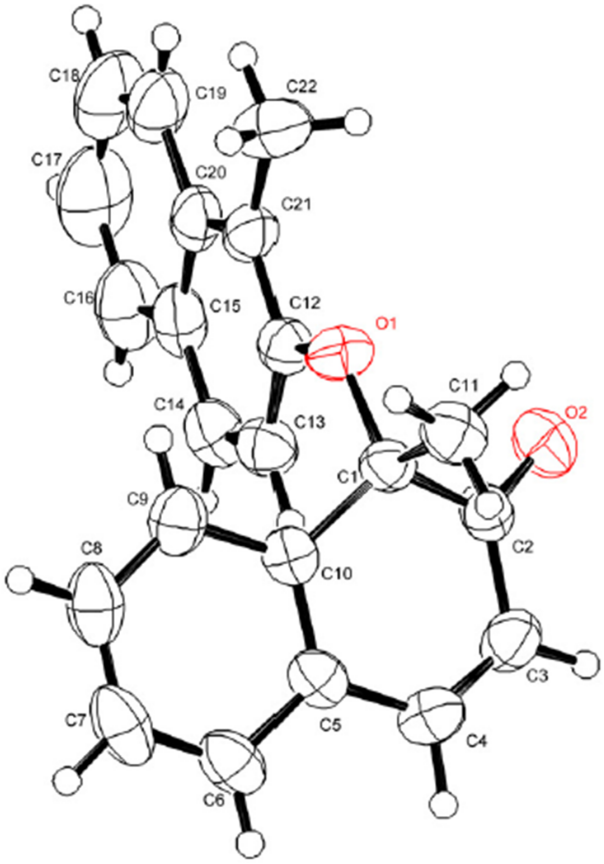
3a ***9 (78% yield)***

1-methoxy-1-methyl-2-methylene-1,2-dihydronaphthalene (9)

KHMDS 0.5 M in toluene (1.01 ml, 0.551 mmol) and methyltriphenylphosphonium bromide (522 mg, 1.46 mmol) were dissolved in THF at -78 °C. The solution was stirred at -78 °C for 30 min. To a mixture, **3a** (50.0 mg, 0.266 mmol) was added at -78 °C. The reaction mixture was stirred at 0 °C for 1 h. After the completion of reaction, the mixture was concentrated under reduced pressure and diluted with aqueous $NaHCO_3$. The aqueous phase was extracted with EtOAc. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residues was purified by flash column chromatography on silica gel (1:4 EtOAc:hexanes): 38.7 mg (78%), yellow oil.

^1H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.4 Hz, 1H), 7.27 (d, *J* = 6.6 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 1H), 6.43 – 6.34 (m, 2H), 5.47 (s, 1H), 5.34 (s, 1H), 2.95 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8, 146.5, 139.8, 133.4, 128.6, 127.9, 127.5, 127.0, 126.1, 125.9, 116.0, 52.3, 37.0; FT-IR (neat) ; HRMS (ESI) *m/z* ($[M+H]^+$) calcd for $C_{13}H_{15}O_2$: 187.1123, found: 188.0828.

8. The X-ray single-crystal diffraction analysis of 2a



EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{22}H_{18}O_2$
Formula Weight	314.38
Crystal Color, Habit	yellow, block
Crystal Dimensions	0.400 X 0.300 X 0.200 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 8.8617(7) Å

	b = 6.9703(4) Å c = 27.1759(17) Å b = 100.016(3) ° V = 1653.04(19) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.263 g/cm^3
F_{000}	664.00
m(MoKa)	0.796 cm^{-1}

B. Intensity Measurements

Diffractometer	R-AXIS RAPID
Radiation	MoKa (l = 0.71075 Å) graphite monochromated
Voltage, Current	50kV, 30mA
Temperature	23.0°C
Detector Aperture	460.0 x 256.0 mm
Data Images	44 exposures
w oscillation Range (c=45.0, f=0.0)	130.0 - 190.0°
Exposure Rate	60.0 sec./°
w oscillation Range (c=45.0, f=180.0)	0.0 - 160.0°
Exposure Rate	60.0 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2q_{max}$	54.9°

No. of Reflections Measured	Total: 15637 Unique: 3778 (R_{int} = 0.0367)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.791 - 0.984)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR2008)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$S\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\ s^2(Fo^2) + (0.1014 \cdot P)^2 + 0.0000 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2q_{max}$ cutoff	54.9^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	3778
No. Variables	225
Reflection/Parameter Ratio	16.79
Residuals: R1 (I>2.00s(I))	0.0471
Residuals: R (All reflections)	0.0911
Residuals: wR2 (All reflections)	0.1729
Goodness of Fit Indicator	1.034
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.29 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.27 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
O1	0.81324(15)	0.52042(16)	0.41564(5)	3.74(3)
O2	0.97251(15)	0.2023(2)	0.45603(6)	4.81(3)
C1	0.7395(2)	0.3844(2)	0.44296(6)	3.13(3)
C2	0.8343(2)	0.2000(3)	0.45376(7)	3.46(3)
C3	0.7509(2)	0.0285(3)	0.46429(8)	4.13(4)
C4	0.5985(2)	0.0206(3)	0.45185(8)	4.00(4)
C5	0.5044(2)	0.1768(3)	0.42809(6)	3.41(3)
C6	0.3466(2)	0.1536(3)	0.41167(7)	4.32(4)
C7	0.2614(2)	0.2995(4)	0.38658(8)	5.03(5)
C8	0.3319(3)	0.4682(3)	0.37704(8)	4.88(5)
C9	0.4859(2)	0.4953(3)	0.39373(7)	4.06(4)
C10	0.5738(2)	0.3510(2)	0.41979(6)	3.13(3)
C11	0.7446(3)	0.4781(3)	0.49452(7)	4.19(4)
C12	0.8445(2)	0.4732(2)	0.36909(7)	3.23(3)
C13	0.7975(2)	0.2991(3)	0.34478(7)	3.76(4)
C14	0.8350(2)	0.2590(3)	0.29961(7)	4.23(4)
C15	0.9204(2)	0.3882(3)	0.27598(7)	4.28(4)
C16	0.9625(3)	0.3450(4)	0.22908(8)	5.99(6)
C17	1.0445(3)	0.4714(5)	0.20672(10)	7.47(8)
C18	1.0895(3)	0.6481(5)	0.22995(10)	7.19(7)
C19	1.0507(3)	0.6956(4)	0.27487(9)	5.59(5)
C20	0.9658(2)	0.5659(3)	0.29988(7)	4.07(4)
C21	0.9264(2)	0.6075(3)	0.34750(7)	3.57(4)
C22	0.9740(3)	0.7908(3)	0.37495(9)	5.26(5)

$B_{eq} = 8/3\ p^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H6	0.29935	0.03898	0.41776	5.184
H7	0.15644	0.28430	0.37609	6.038
H8	0.27457	0.56504	0.35909	5.859
H9	0.53158	0.61086	0.38753	4.876
H11A	0.69085	0.59826	0.49059	5.025
H11B	0.84929	0.49997	0.50977	5.025
H11C	0.69687	0.39465	0.51536	5.025
H13	0.74058	0.21155	0.35978	4.517
H14	0.80351	0.14351	0.28399	5.081
H16	0.93336	0.22855	0.21360	7.191
H17	1.07125	0.44173	0.17600	8.959
H18	1.14653	0.73378	0.21441	8.624
H19	1.08013	0.81390	0.28926	6.713

H22A	1.03729	0.76173	0.40646	6.309
H22B	0.88456	0.85929	0.38058	6.309
H22C	1.03061	0.86854	0.35536	6.309
H3	0.817(3)	-0.078(3)	0.4782(8)	5.4(5)
H4	0.539(2)	-0.098(3)	0.4567(7)	4.5(4)

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	0.0541(8)	0.0426(7)	0.0490(7)	-0.0079(5)	0.0188(6)	-0.0026(6)
O2	0.0362(8)	0.0727(10)	0.0720(10)	0.0026(6)	0.0038(7)	0.0060(8)
C1	0.0382(10)	0.0422(9)	0.0398(10)	-0.0043(7)	0.0100(8)	0.0011(8)
C2	0.0351(10)	0.0520(10)	0.0430(10)	0.0008(8)	0.0036(8)	0.0016(8)
C3	0.0507(12)	0.0458(11)	0.0612(13)	0.0066(9)	0.0117(10)	0.0121(10)
C4	0.0531(12)	0.0442(10)	0.0577(12)	-0.0028(9)	0.0181(10)	0.0040(9)
C5	0.0373(10)	0.0534(11)	0.0401(9)	-0.0022(8)	0.0102(8)	-0.0053(8)
C6	0.0392(11)	0.0773(14)	0.0491(11)	-0.0073(10)	0.0119(9)	-0.0082(10)
C7	0.0336(11)	0.1020(17)	0.0543(12)	0.0081(11)	0.0040(9)	-0.0099(12)
C8	0.0481(12)	0.0838(15)	0.0524(12)	0.0234(11)	0.0052(10)	0.0037(11)
C9	0.0498(12)	0.0571(11)	0.0483(11)	0.0107(9)	0.0106(9)	0.0040(9)
C10	0.0372(10)	0.0450(9)	0.0375(9)	0.0033(7)	0.0083(7)	-0.0022(8)
C11	0.0538(12)	0.0590(12)	0.0469(11)	-0.0056(9)	0.0104(9)	-0.0087(9)
C12	0.0343(9)	0.0454(9)	0.0427(10)	0.0029(7)	0.0061(8)	0.0022(8)
C13	0.0417(11)	0.0537(11)	0.0476(10)	-0.0033(8)	0.0077(8)	0.0024(9)
C14	0.0486(12)	0.0640(12)	0.0469(11)	-0.0001(10)	0.0042(9)	-0.0052(10)
C15	0.0438(11)	0.0777(14)	0.0403(10)	0.0081(10)	0.0047(9)	0.0077(10)
C16	0.0700(16)	0.1124(19)	0.0470(13)	0.0132(14)	0.0149(12)	0.0051(13)
C17	0.088(2)	0.147(3)	0.0545(15)	0.017(2)	0.0302(15)	0.0209(18)
C18	0.0770(19)	0.132(2)	0.0701(17)	0.0079(17)	0.0309(15)	0.0472(18)
C19	0.0565(14)	0.0926(17)	0.0647(14)	0.0025(12)	0.0139(11)	0.0319(13)
C20	0.0353(10)	0.0688(13)	0.0500(11)	0.0068(9)	0.0060(9)	0.0201(10)
C21	0.0364(10)	0.0466(10)	0.0524(11)	0.0036(8)	0.0075(8)	0.0117(9)
C22	0.0691(15)	0.0481(11)	0.0866(17)	-0.0074(10)	0.0246(13)	0.0036(11)

The general temperature factor expression: $\exp(-2p^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O1	C1	1.430(2)	O1	C12	1.381(2)
O2	C2	1.215(2)	C1	C2	1.536(2)
C1	C10	1.512(2)	C1	C11	1.540(3)
C2	C3	1.460(3)	C3	C4	1.335(3)
C4	C5	1.453(3)	C5	C6	1.401(3)
C5	C10	1.397(3)	C6	C7	1.375(3)

C7	C8	1.377(3)	C8	C9	1.375(3)
C9	C10	1.388(2)	C12	C13	1.409(3)
C12	C21	1.376(3)	C13	C14	1.356(3)
C14	C15	1.402(3)	C15	C16	1.421(3)
C15	C20	1.423(3)	C16	C17	1.351(4)
C17	C18	1.410(5)	C18	C19	1.365(4)
C19	C20	1.423(3)	C20	C21	1.428(3)
C21	C22	1.503(3)			

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C3	H3	0.98(2)	C4	H4	1.00(2)
C6	H6	0.930	C7	H7	0.930
C8	H8	0.930	C9	H9	0.930
C11	H11A	0.960	C11	H11B	0.960
C11	H11C	0.960	C13	H13	0.930
C14	H14	0.930	C16	H16	0.930
C17	H17	0.930	C18	H18	0.930
C19	H19	0.930	C22	H22A	0.960
C22	H22B	0.960	C22	H22C	0.960

Table 6. Bond angles (º)

atom	atom	atom	angle	atom	atom	atom	angle
C1	O1	C12	120.00(13)	O1	C1	C2	111.70(15)
O1	C1	C10	112.60(13)	O1	C1	C11	104.32(14)
C2	C1	C10	114.22(14)	C2	C1	C11	104.64(14)
C10	C1	C11	108.49(15)	O2	C2	C1	120.76(17)
O2	C2	C3	122.74(17)	C1	C2	C3	116.37(16)
C2	C3	C4	120.55(17)	C3	C4	C5	123.99(18)
C4	C5	C6	121.27(18)	C4	C5	C10	119.23(16)
C6	C5	C10	119.45(17)	C5	C6	C7	120.3(2)
C6	C7	C8	119.79(19)	C7	C8	C9	120.8(2)
C8	C9	C10	120.37(19)	C1	C10	C5	119.31(14)
C1	C10	C9	121.24(16)	C5	C10	C9	119.25(16)
O1	C12	C13	122.99(16)	O1	C12	C21	115.65(15)
C13	C12	C21	121.36(18)	C12	C13	C14	120.20(18)
C13	C14	C15	121.28(18)	C14	C15	C16	121.4(2)
C14	C15	C20	118.82(18)	C16	C15	C20	119.7(2)
C15	C16	C17	120.7(3)	C16	C17	C18	120.0(3)
C17	C18	C19	121.1(3)	C18	C19	C20	120.6(2)
C15	C20	C19	117.77(19)	C15	C20	C21	119.74(18)
C19	C20	C21	122.48(19)	C12	C21	C20	118.58(17)
C12	C21	C22	119.35(18)	C20	C21	C22	122.06(18)

Table 7. Bond angles involving hydrogens (º)

atom	atom	atom	angle	atom	atom	atom	angle
C2	C3	H3	113.8(14)	C4	C3	H3	125.4(13)
C3	C4	H4	122.3(12)	C5	C4	H4	113.7(11)
C5	C6	H6	119.9	C7	C6	H6	119.9
C6	C7	H7	120.1	C8	C7	H7	120.1
C7	C8	H8	119.6	C9	C8	H8	119.6
C8	C9	H9	119.8	C10	C9	H9	119.8
C1	C11	H11A	109.5	C1	C11	H11B	109.5
C1	C11	H11C	109.5	H11A	C11	H11B	109.5
H11A	C11	H11C	109.5	H11B	C11	H11C	109.5
C12	C13	H13	119.9	C14	C13	H13	119.9
C13	C14	H14	119.4	C15	C14	H14	119.4
C15	C16	H16	119.7	C17	C16	H16	119.6
C16	C17	H17	120.0	C18	C17	H17	120.0
C17	C18	H18	119.4	C19	C18	H18	119.4
C18	C19	H19	119.7	C20	C19	H19	119.7
C21	C22	H22A	109.5	C21	C22	H22B	109.5
C21	C22	H22C	109.5	H22A	C22	H22B	109.5
H22A	C22	H22C	109.5	H22B	C22	H22C	109.5

Table 8. Torsion Angles(º)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C1	O1	C12	C13	4.6(2)	C1	O1	C12	C21	-175.07(12)
C12	O1	C1	C2	60.21(17)	C12	O1	C1	C10	-69.88(18)
C12	O1	C1	C11	172.69(12)	O1	C1	C2	O2	25.8(2)
O1	C1	C2	C3	-158.20(13)	O1	C1	C10	C5	154.31(13)
O1	C1	C10	C9	-30.8(2)	C2	C1	C10	C5	25.5(2)
C2	C1	C10	C9	-159.56(14)	C10	C1	C2	O2	155.04(15)
C10	C1	C2	C3	-29.0(2)	C11	C1	C2	O2	-86.5(2)
C11	C1	C2	C3	89.52(17)	C11	C1	C10	C5	-90.75(17)
C11	C1	C10	C9	84.17(18)	O2	C2	C3	C4	-166.50(18)
C1	C2	C3	C4	17.6(3)	C2	C3	C4	C5	-0.7(3)
C3	C4	C5	C6	173.89(18)	C3	C4	C5	C10	-3.7(3)
C4	C5	C6	C7	-176.06(16)	C4	C5	C10	C1	-9.8(2)
C4	C5	C10	C9	175.16(15)	C6	C5	C10	C1	172.59(15)
C6	C5	C10	C9	-2.4(2)	C10	C5	C6	C7	1.5(3)
C5	C6	C7	C8	0.8(3)	C6	C7	C8	C9	-2.1(3)
C7	C8	C9	C10	1.2(3)	C8	C9	C10	C1	-173.79(17)
C8	C9	C10	C5	1.1(3)	O1	C12	C13	C14	-178.37(13)
O1	C12	C21	C20	178.54(12)	O1	C12	C21	C22	-0.3(2)
C13	C12	C21	C20	-1.1(2)	C13	C12	C21	C22	-179.94(14)
C21	C12	C13	C14	1.3(3)	C12	C13	C14	C15	-0.2(3)
C13	C14	C15	C16	178.76(16)	C13	C14	C15	C20	-1.0(3)
C14	C15	C16	C17	179.80(18)	C14	C15	C20	C19	-179.23(15)
C14	C15	C20	C21	1.2(3)	C16	C15	C20	C19	1.0(3)
C16	C15	C20	C21	-178.65(17)	C20	C15	C16	C17	-0.4(3)

C15	C16	C17	C18	0.1(4)	C16	C17	C18	C19	-0.5(4)
C17	C18	C19	C20	1.1(4)	C18	C19	C20	C15	-1.3(3)
C18	C19	C20	C21	178.29(19)	C15	C20	C21	C12	-0.1(2)
C15	C20	C21	C22	178.69(14)	C19	C20	C21	C12	-179.69(16)
C19	C20	C21	C22	-0.9(3)					

Table 9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	O2	2.7521(18)	O1	C9	2.863(2)
O1	C22	2.712(3)	O2	C4	3.532(3)
O2	C11	3.099(3)	O2	C12	3.082(2)
O2	C13	3.220(2)	C1	C4	2.856(3)
C1	C13	2.866(3)	C2	C5	2.890(3)
C2	C12	3.000(3)	C2	C13	3.003(3)
C3	C10	2.885(3)	C3	C11	3.243(3)
C4	C11	3.560(3)	C5	C8	2.766(3)
C5	C11	3.297(3)	C6	C9	2.765(3)
C7	C10	2.782(3)	C9	C11	3.254(3)
C9	C12	3.363(3)	C9	C13	3.541(3)
C10	C12	3.087(3)	C10	C13	3.102(3)
C12	C15	2.792(3)	C13	C20	2.793(3)
C14	C21	2.808(3)	C15	C18	2.783(4)
C16	C19	2.792(4)	C17	C20	2.818(4)
C19	C22	2.990(4)			

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H9	2.559	O1	H11A	2.527
O1	H11B	2.526	O1	H11C	3.186
O1	H13	2.648	O1	H22A	2.647
O1	H22B	2.664	O2	H11B	2.861
O2	H11C	3.425	O2	H13	3.033
O2	H3	2.52(2)	C1	H9	2.681
C1	H13	2.563	C1	H3	3.40(2)
C2	H11A	3.281	C2	H11B	2.576
C2	H11C	2.615	C2	H13	2.546
C2	H4	3.35(2)	C3	H11B	3.566
C3	H11C	2.984	C3	H13	3.101
C4	H6	2.655	C4	H11C	3.164
C4	H13	3.273	C5	H7	3.248
C5	H9	3.244	C5	H11C	3.071
C5	H13	3.039	C5	H3	3.37(2)
C6	H8	3.218	C6	H4	2.60(2)
C7	H9	3.228	C8	H6	3.220
C9	H7	3.230	C9	H11A	3.013
C9	H11C	3.572	C9	H13	3.252

C10	H6	3.256	C10	H8	3.233
C10	H11A	2.656	C10	H11B	3.308
C10	H11C	2.654	C10	H13	2.575
C10	H4	3.31(2)	C11	H9	3.311
C12	H9	3.057	C12	H14	3.236
C12	H22A	2.719	C12	H22B	2.725
C12	H22C	3.266	C13	H9	3.546
C14	H16	2.641	C15	H13	3.241
C15	H17	3.251	C15	H19	3.280
C16	H14	2.630	C16	H18	3.223
C17	H19	3.253	C18	H16	3.233
C19	H17	3.249	C19	H22C	2.531
C20	H14	3.272	C20	H16	3.298
C20	H18	3.259	C20	H22A	3.165
C20	H22B	3.172	C20	H22C	2.599
C21	H13	3.260	C21	H19	2.680
C22	H19	2.664	H6	H7	2.305
H6	H4	2.399	H7	H8	2.304
H8	H9	2.297	H9	H11A	2.910
H9	H13	3.497	H13	H14	2.275
H14	H16	2.470	H16	H17	2.276
H17	H18	2.332	H18	H19	2.283
H19	H22A	3.293	H19	H22B	3.280
H19	H22C	1.959	H3	H4	2.44(3)

Table 11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O2	C3[1]	3.382(2)	O2	C7[2]	3.501(3)
O2	C11[3]	3.447(2)	C3	O2[1]	3.382(2)
C4	C4[4]	3.401(3)	C7	O2[5]	3.501(3)
C7	C11[6]	3.592(3)	C11	O2[3]	3.447(2)
C11	C7[6]	3.592(3)			

Symmetry Operators:

(1) -X+2,-Y,-Z+1	(2) X+1,Y,Z
(3) -X+2,-Y+1,-Z+1	(4) -X+1,-Y,-Z+1
(5) X-1,Y,Z	(6) -X+1,-Y+1,-Z+1

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H11B[1]	3.311	O1	H3[2]	3.27(2)
O2	H6[3]	3.437	O2	H7[3]	2.989
O2	H11A[1]	3.381	O2	H11B[1]	2.674
O2	H22A[4]	3.442	O2	H22B[4]	3.158

O2	H3[5]	2.50(2)	C2	H11B[1]	3.500
C2	H22B[4]	3.178	C2	H3[5]	3.42(2)
C3	H6[6]	3.345	C3	H11A[4]	3.149
C3	H22B[4]	2.984	C4	H6[6]	3.526
C4	H9[4]	3.347	C4	H11A[4]	3.185
C4	H17[7]	3.580	C4	H4[6]	3.00(2)
C5	H11A[8]	3.416	C5	H17[7]	3.237
C5	H4[6]	3.27(2)	C6	H11A[8]	3.235
C6	H17[7]	2.998	C6	H18[7]	3.483
C6	H22C[9]	3.555	C6	H3[6]	3.59(2)
C6	H4[6]	3.56(2)	C7	H11A[8]	3.367
C7	H11B[8]	3.437	C7	H11C[8]	3.382
C7	H17[7]	3.491	C7	H18[7]	3.031
C8	H11C[8]	3.129	C8	H18[7]	3.008
C8	H22A[10]	3.516	C9	H11C[8]	3.272
C9	H16[11]	3.520	C9	H18[7]	3.484
C9	H4[2]	3.31(2)	C11	H22A[1]	3.459
C11	H3[2]	3.21(2)	C11	H4[2]	3.53(2)
C12	H7[3]	3.037	C12	H16[11]	3.515
C13	H7[3]	3.148	C13	H22B[4]	3.268
C14	H7[3]	3.225	C14	H14[11]	3.589
C14	H22B[4]	3.530	C14	H22C[4]	3.434
C15	H7[3]	3.213	C15	H14[11]	2.939
C16	H9[7]	3.573	C16	H14[11]	3.118
C17	H9[7]	3.568	C17	H13[11]	3.296
C17	H14[11]	3.359	C17	H18[12]	3.577
C17	H19[12]	3.486	C18	H13[11]	3.495
C18	H14[11]	3.437	C19	H8[3]	2.902
C19	H14[11]	3.286	C20	H7[3]	3.127
C20	H8[3]	2.923	C20	H14[11]	3.048
C21	H7[3]	3.047	C21	H8[3]	3.061
C21	H16[11]	3.434	C22	H6[13]	3.390
C22	H8[3]	3.187	C22	H13[2]	3.571
C22	H3[2]	3.46(2)	H6	O2[10]	3.437
H6	C3[6]	3.345	H6	C4[6]	3.526
H6	C22[9]	3.390	H6	H11A[8]	3.540
H6	H11C[6]	3.524	H6	H17[7]	3.047
H6	H22A[9]	2.996	H6	H22C[9]	2.925
H6	H3[6]	3.187	H6	H4[6]	3.486
H7	O2[10]	2.989	H7	C12[10]	3.037
H7	C13[10]	3.148	H7	C14[10]	3.225
H7	C15[10]	3.213	H7	C20[10]	3.127
H7	C21[10]	3.047	H7	H11B[8]	3.455
H7	H18[7]	3.273	H7	H22C[9]	3.121
H8	C19[10]	2.902	H8	C20[10]	2.923
H8	C21[10]	3.061	H8	C22[10]	3.187
H8	H11C[8]	3.389	H8	H17[11]	3.182
H8	H18[7]	3.209	H8	H19[10]	2.905

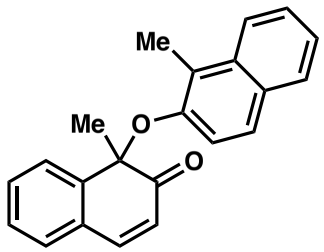
H8	H22A[10]	2.983	H8	H22C[10]	3.014
H9	C4[2]	3.347	H9	C16[11]	3.573
H9	C17[11]	3.568	H9	H11C[8]	3.595
H9	H16[11]	2.936	H9	H17[11]	2.930
H9	H4[2]	2.762	H11A	O2[1]	3.381
H11A	C3[2]	3.149	H11A	C4[2]	3.185
H11A	C5[8]	3.416	H11A	C6[8]	3.235
H11A	C7[8]	3.367	H11A	H6[8]	3.540
H11A	H11C[8]	3.412	H11A	H3[2]	2.569
H11A	H4[2]	2.592	H11B	O1[1]	3.311
H11B	O2[1]	2.674	H11B	C2[1]	3.500
H11B	C7[8]	3.437	H11B	H7[8]	3.455
H11B	H11B[1]	2.812	H11B	H22A[1]	2.954
H11B	H3[2]	3.066	H11C	C7[8]	3.382
H11C	C8[8]	3.129	H11C	C9[8]	3.272
H11C	H6[6]	3.524	H11C	H8[8]	3.389
H11C	H9[8]	3.595	H11C	H11A[8]	3.412
H11C	H22A[1]	3.084	H11C	H4[6]	3.128
H13	C17[7]	3.296	H13	C18[7]	3.495
H13	C22[4]	3.571	H13	H17[7]	3.344
H13	H22B[4]	2.779	H13	H22C[4]	3.528
H14	C14[7]	3.589	H14	C15[7]	2.939
H14	C16[7]	3.118	H14	C17[7]	3.359
H14	C18[7]	3.437	H14	C19[7]	3.286
H14	C20[7]	3.048	H14	H16[7]	3.581
H14	H19[4]	3.345	H14	H22B[4]	3.267
H14	H22C[4]	3.182	H16	C9[7]	3.520
H16	C12[7]	3.515	H16	C21[7]	3.434
H16	H9[7]	2.936	H16	H14[11]	3.581
H16	H22B[7]	3.579	H17	C4[11]	3.580
H17	C5[11]	3.237	H17	C6[11]	2.998
H17	C7[11]	3.491	H17	H6[11]	3.047
H17	H8[7]	3.182	H17	H9[7]	2.930
H17	H13[11]	3.344	H17	H19[12]	3.196
H17	H4[11]	3.580	H18	C6[11]	3.483
H18	C7[11]	3.031	H18	C8[11]	3.008
H18	C9[11]	3.484	H18	C17[14]	3.577
H18	H7[11]	3.273	H18	H8[11]	3.209
H19	C17[14]	3.486	H19	H8[3]	2.905
H19	H14[2]	3.345	H19	H17[14]	3.196
H22A	O2[2]	3.442	H22A	C8[3]	3.516
H22A	C11[1]	3.459	H22A	H6[13]	2.996
H22A	H8[3]	2.983	H22A	H11B[1]	2.954
H22A	H11C[1]	3.084	H22A	H3[2]	3.190
H22B	O2[2]	3.158	H22B	C2[2]	3.178
H22B	C3[2]	2.984	H22B	C13[2]	3.268
H22B	C14[2]	3.530	H22B	H13[2]	2.779
H22B	H14[2]	3.267	H22B	H16[11]	3.579

H22B	H3[2]	2.852	H22C	C6[13]	3.555
H22C	C14[2]	3.434	H22C	H6[13]	2.925
H22C	H7[13]	3.121	H22C	H8[3]	3.014
H22C	H13[2]	3.528	H22C	H14[2]	3.182
H3	O1[4]	3.27(2)	H3	O2[5]	2.50(2)
H3	C2[5]	3.42(2)	H3	C6[6]	3.59(2)
H3	C11[4]	3.21(2)	H3	C22[4]	3.46(2)
H3	H6[6]	3.187	H3	H11A[4]	2.569
H3	H11B[4]	3.066	H3	H22A[4]	3.190
H3	H22B[4]	2.852	H3	H3[5]	3.43(3)
H4	C4[6]	3.00(2)	H4	C5[6]	3.27(2)
H4	C6[6]	3.56(2)	H4	C9[4]	3.31(2)
H4	C11[4]	3.53(2)	H4	H6[6]	3.486
H4	H9[4]	2.762	H4	H11A[4]	2.592
H4	H11C[6]	3.128	H4	H17[7]	3.580
H4	H4[6]	2.90(3)			

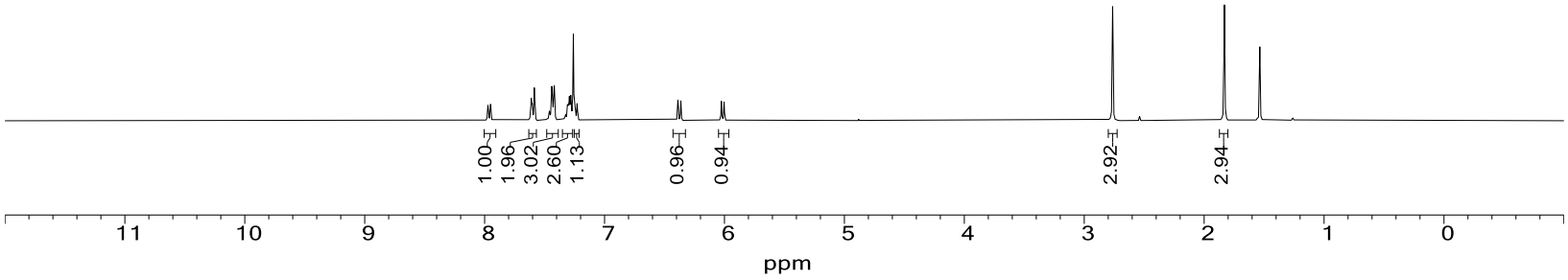
Symmetry Operators:

(1) -X+2,-Y+1,-Z+1
(2) X,Y+1,Z
(3) X+1,Y,Z
(4) X,Y-1,Z
(5) -X+2,-Y,-Z+1
(6) -X+1,-Y,-Z+1
(7) -X+1/2+1,Y+1/2-1,-Z+1/2
(8) -X+1,-Y+1,-Z+1
(9) X-1,Y-1,Z
(10) X-1,Y,Z
(11) -X+1/2+1,Y+1/2,-Z+1/2
(12) -X+1/2+2,Y+1/2-1,-Z+1/2
(13) X+1,Y+1,Z
(14) -X+1/2+2,Y+1/2,-Z+1/2

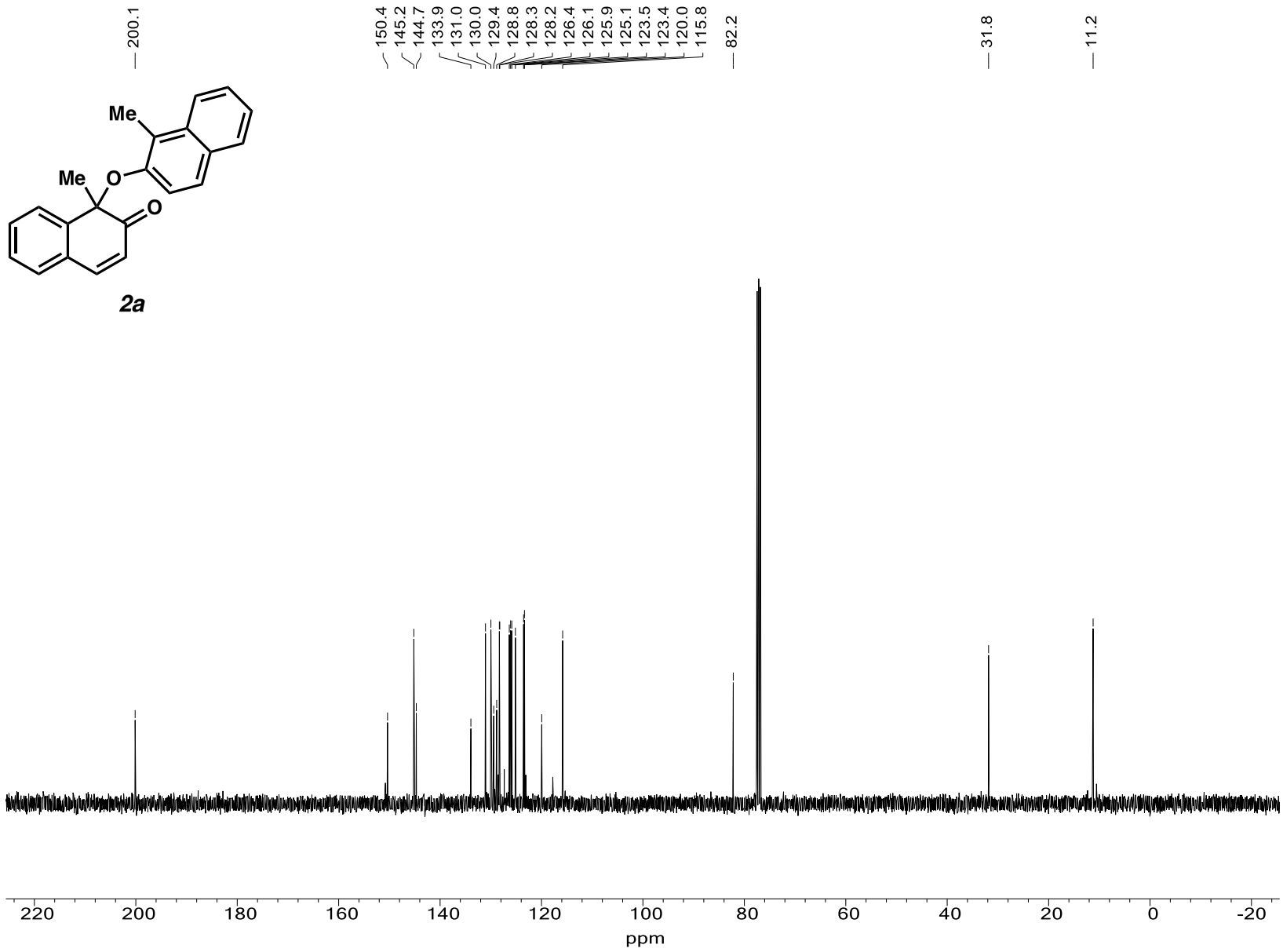
9. NMR Spectra (^{1}H NMR, ^{13}C NMR)



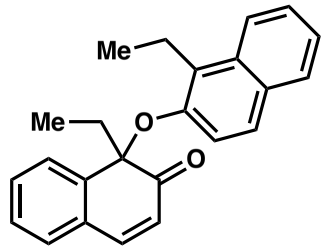
2a



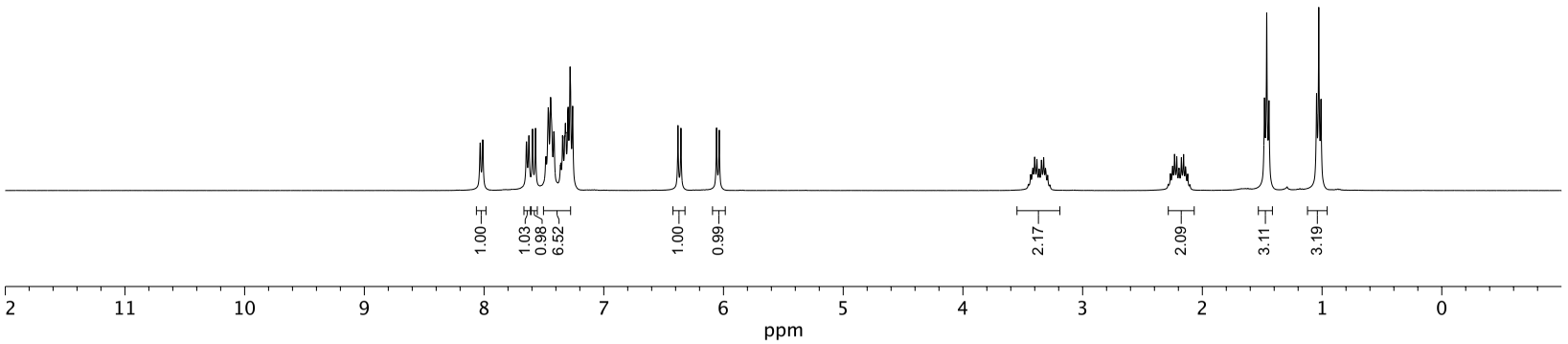
^{1} HNMR (400 MHz, $CDCl_3$) of compound **2a**.



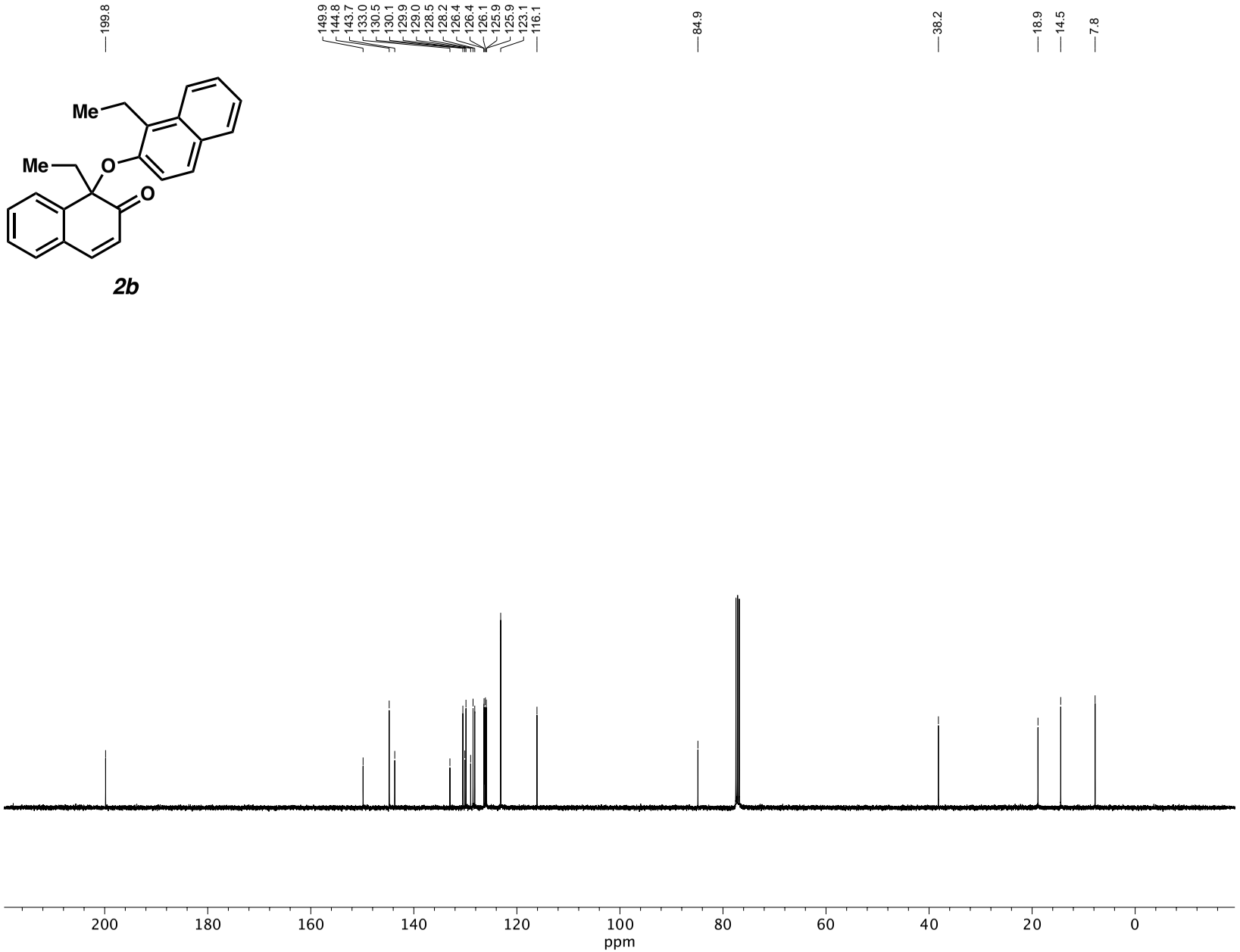
^{13}C NMR (101 MHz, $CDCl_3$) of compound **2a.**



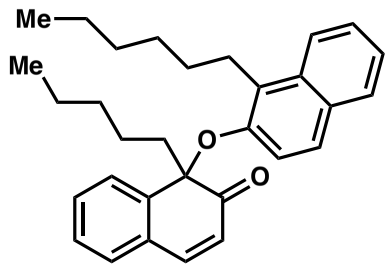
2b



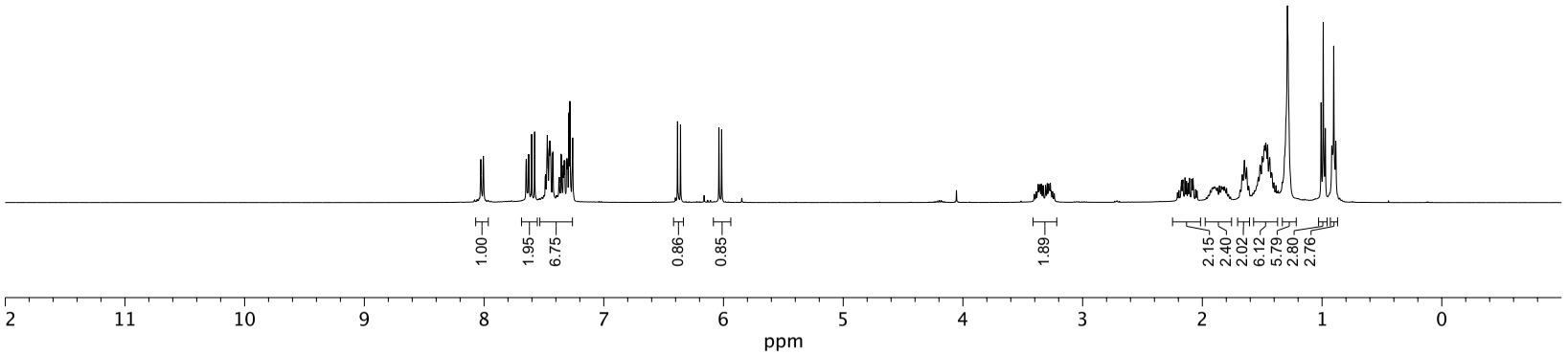
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2b**.



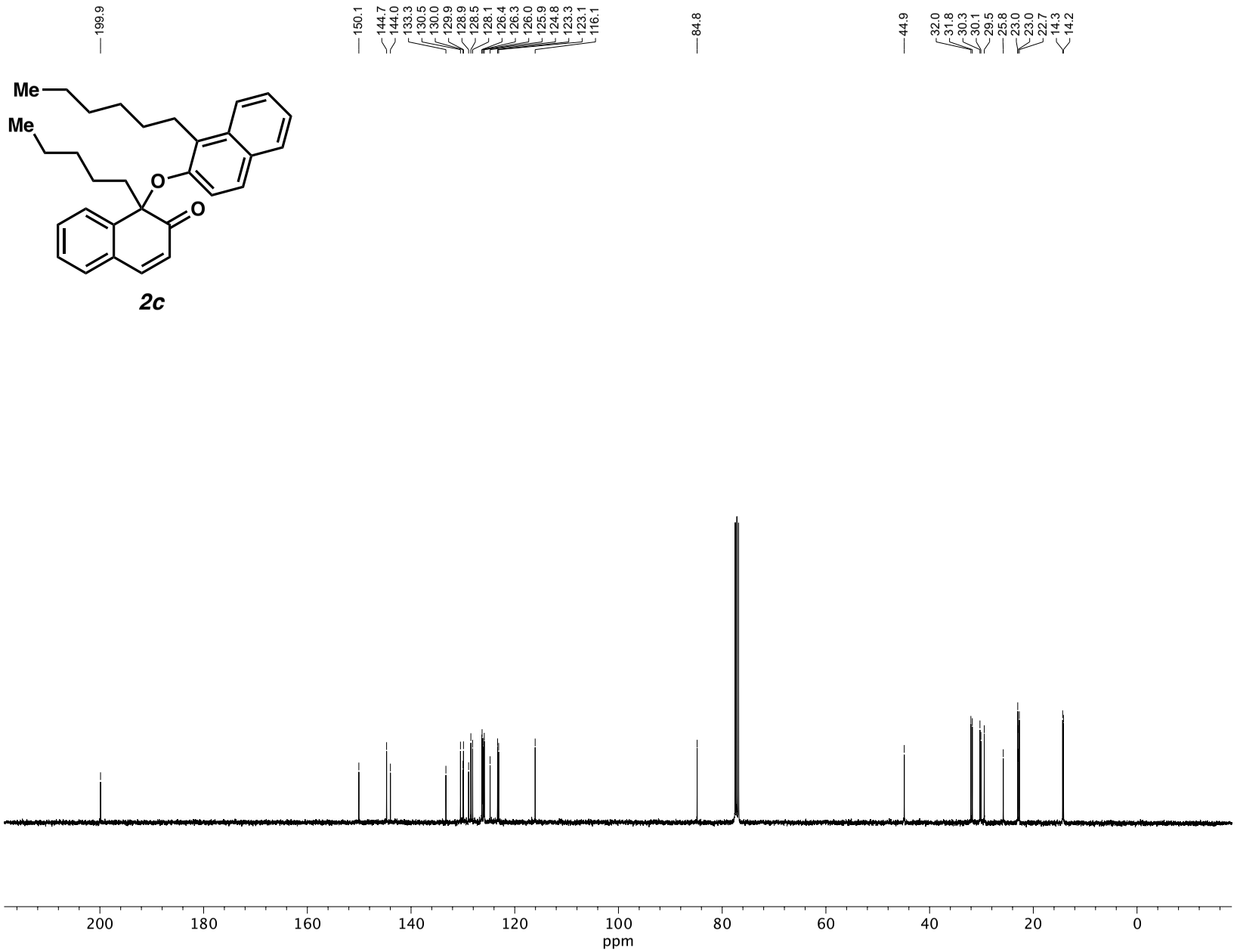
^{13}C NMR (101 MHz, $CDCl_3$) of compound **2b**.



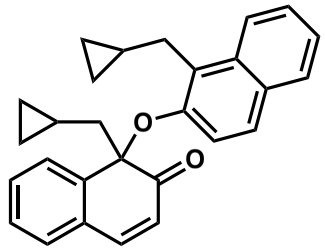
2c



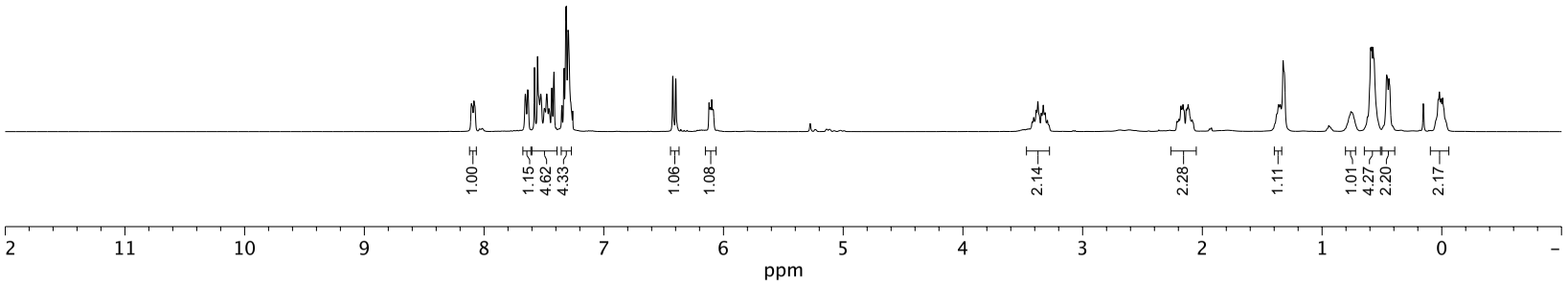
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2c**.



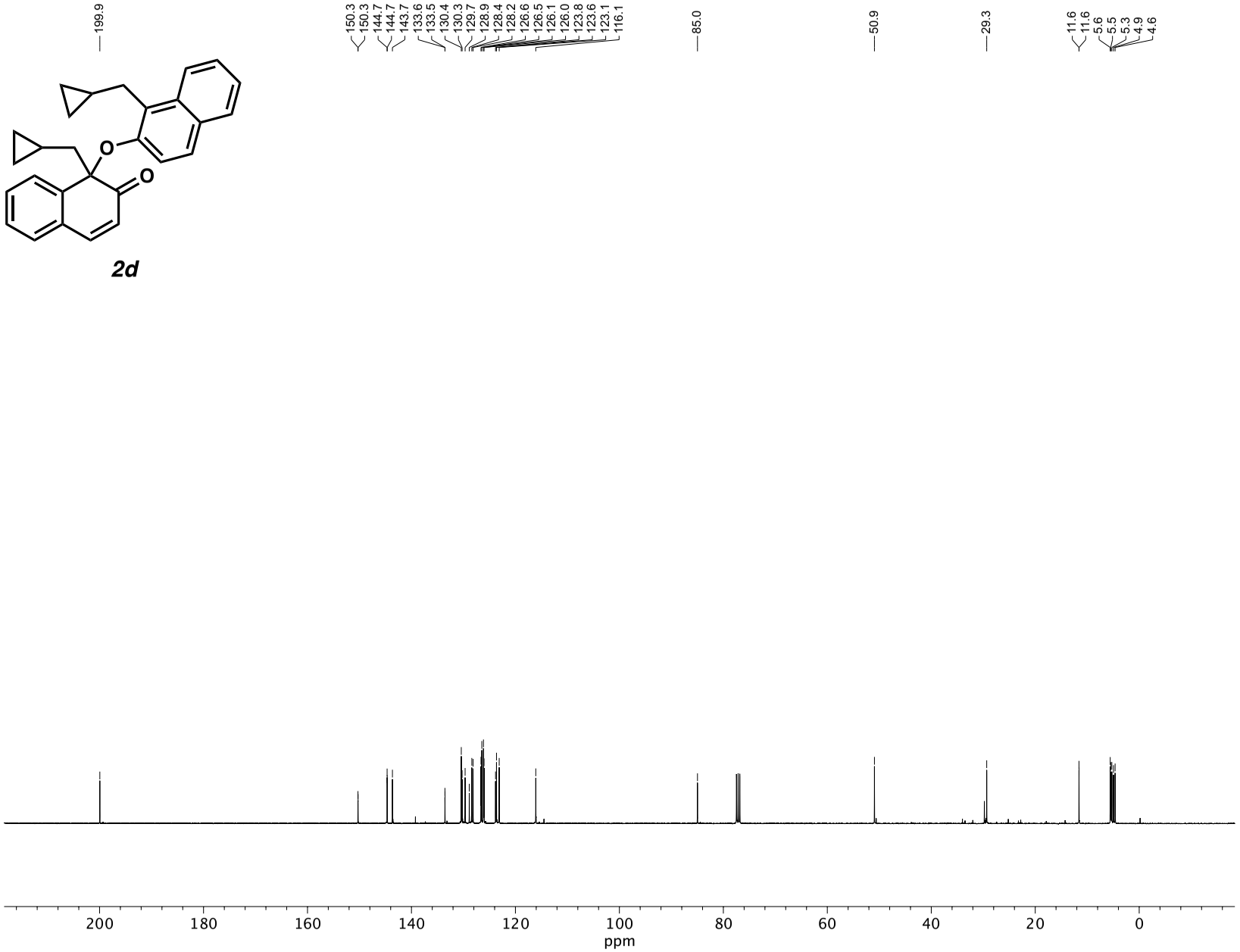
^{13}C NMR (101 MHz, $CDCl_3$) of compound **2c.**



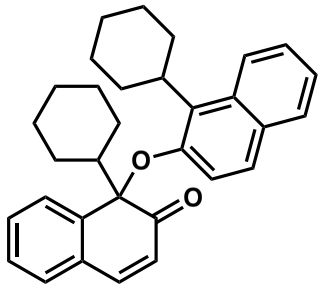
2d



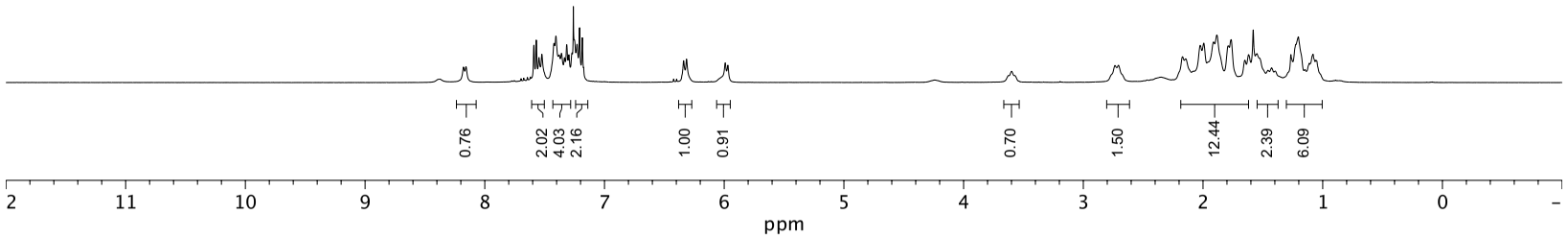
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2d**.



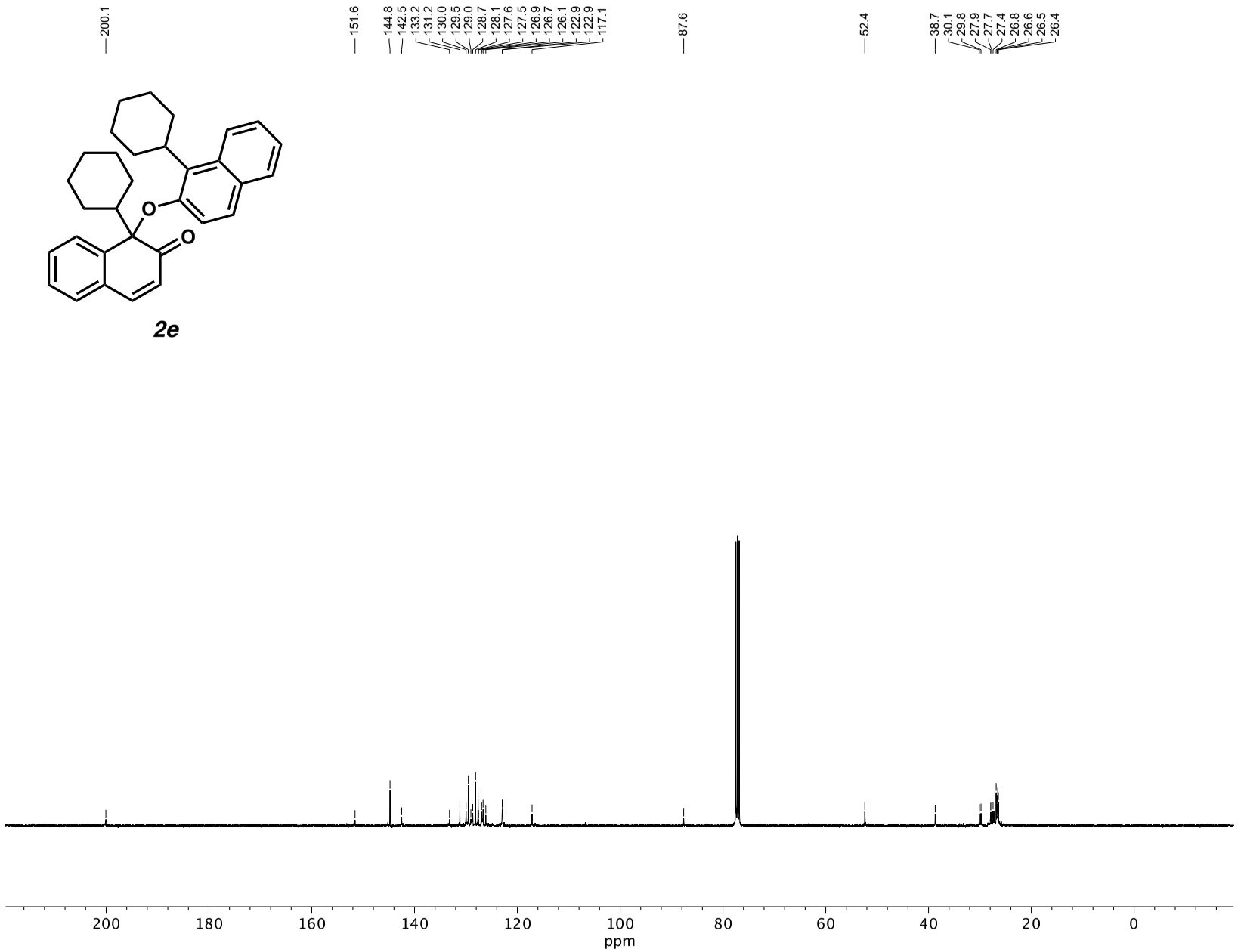
^{13}C NMR (101 MHz, $CDCl_3$) of compound **2d.**



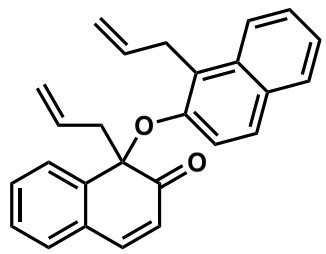
2e



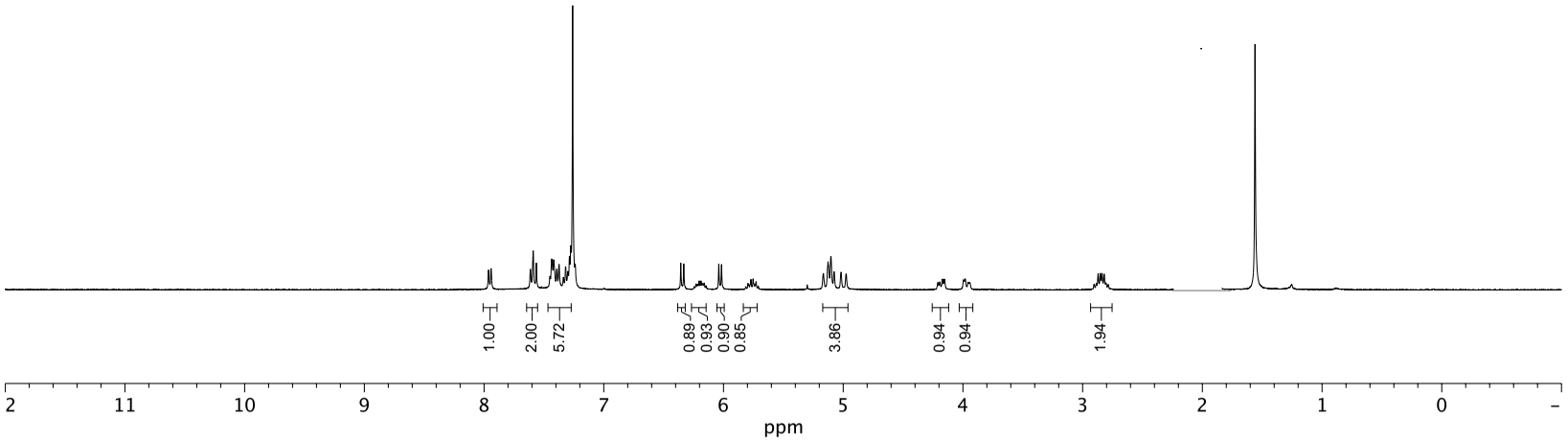
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2e**.



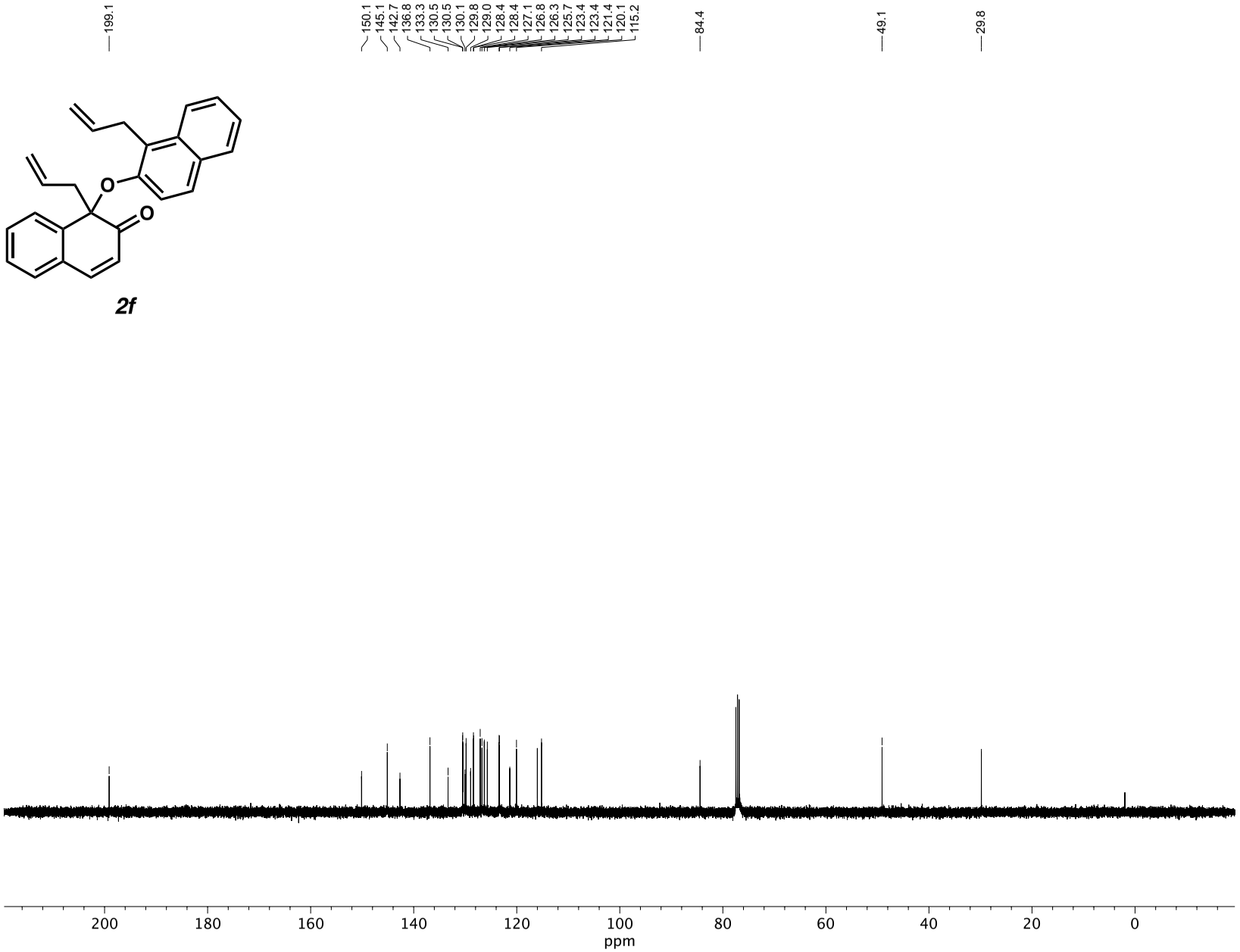
^{13}C NMR (101 MHz,$CDCl_3$) of compound **2e.**



2f

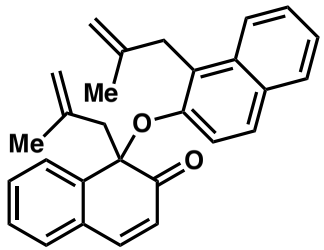


^{1}H NMR (400 MHz, $CDCl_3$) of compound **2f**.

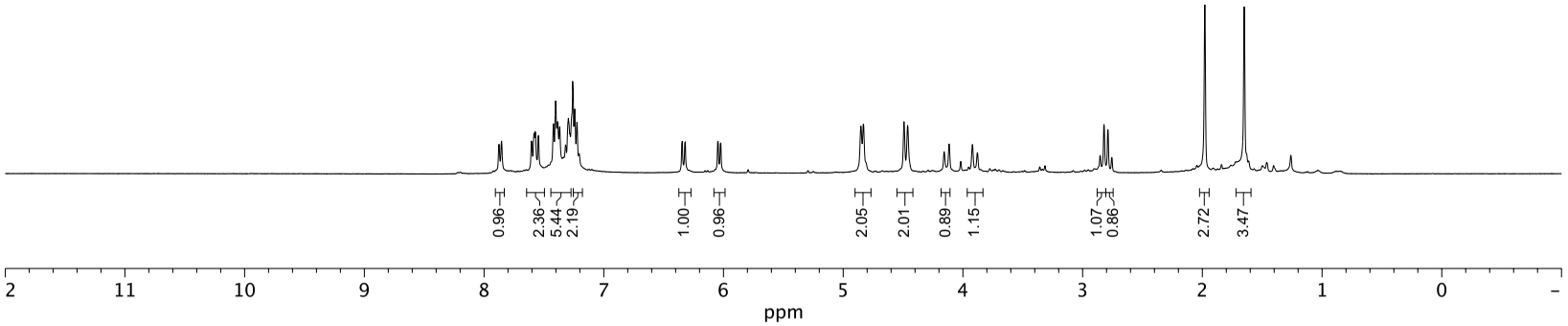


^{13}C NMR (101 MHz,$CDCl_3$) of compound **2f.**

^{1}H NMR (400 MHz, $CDCl_3$) of compound **2g**.

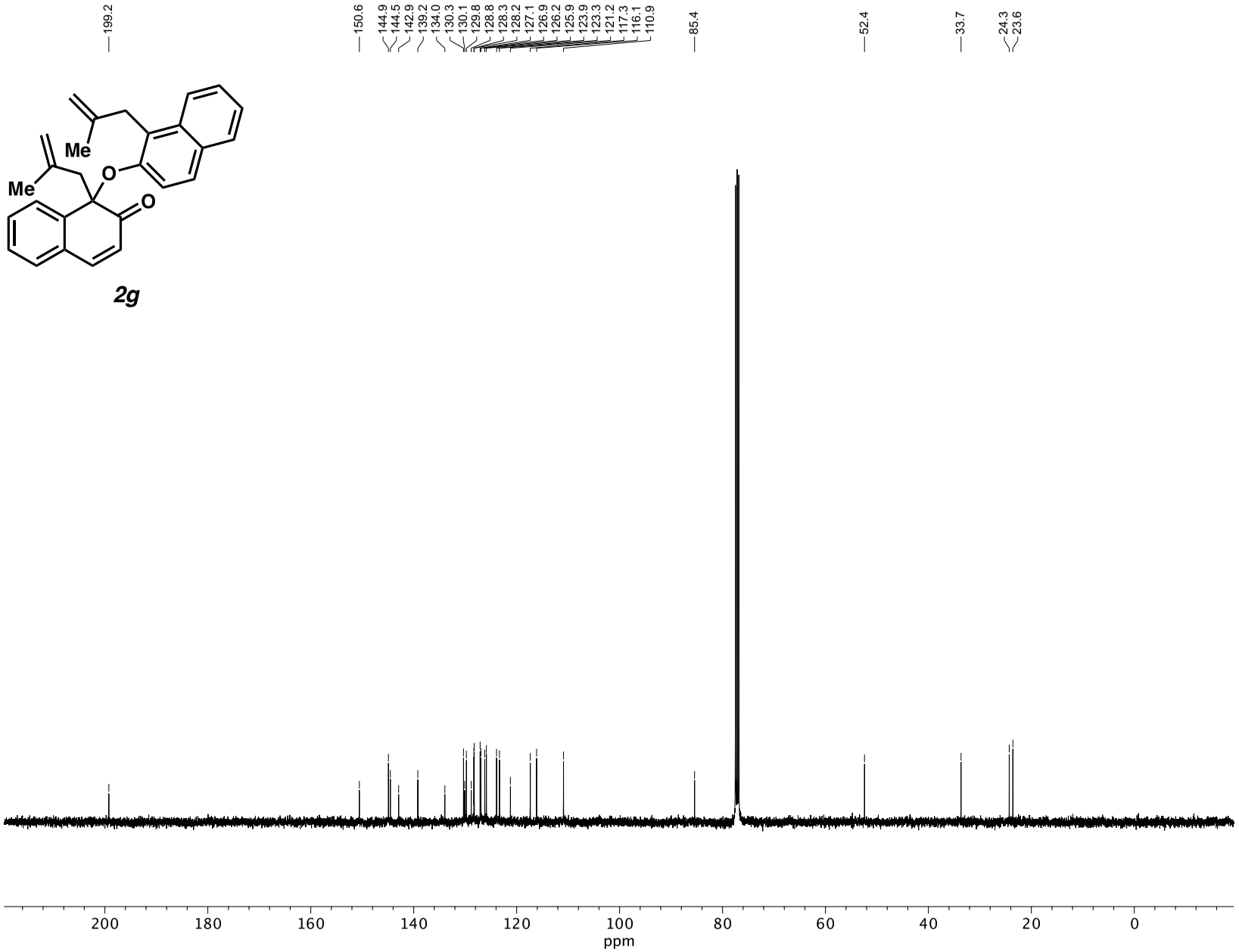


2g

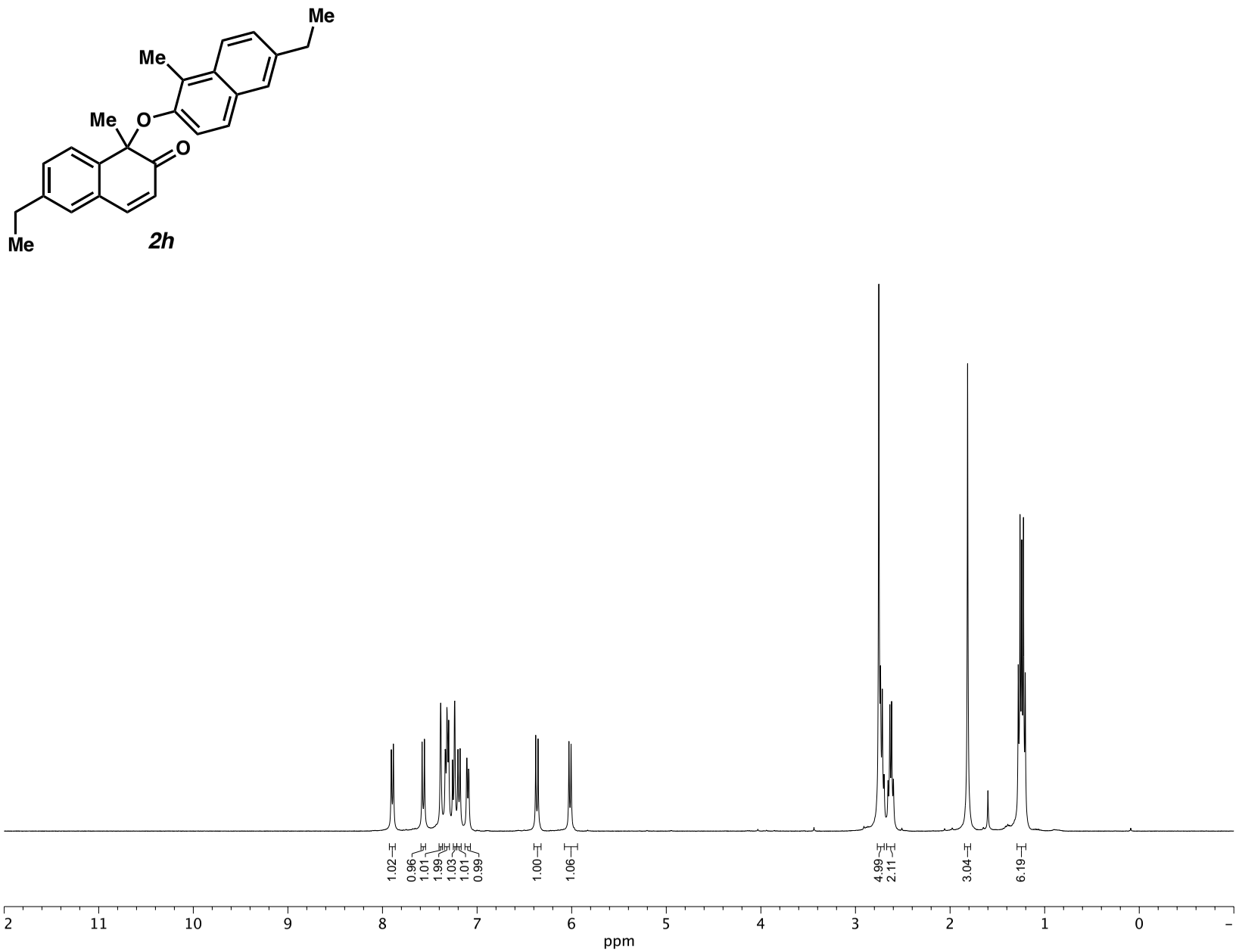


^{1}H NMR (400 MHz, $CDCl_3$) of compound **2g**.

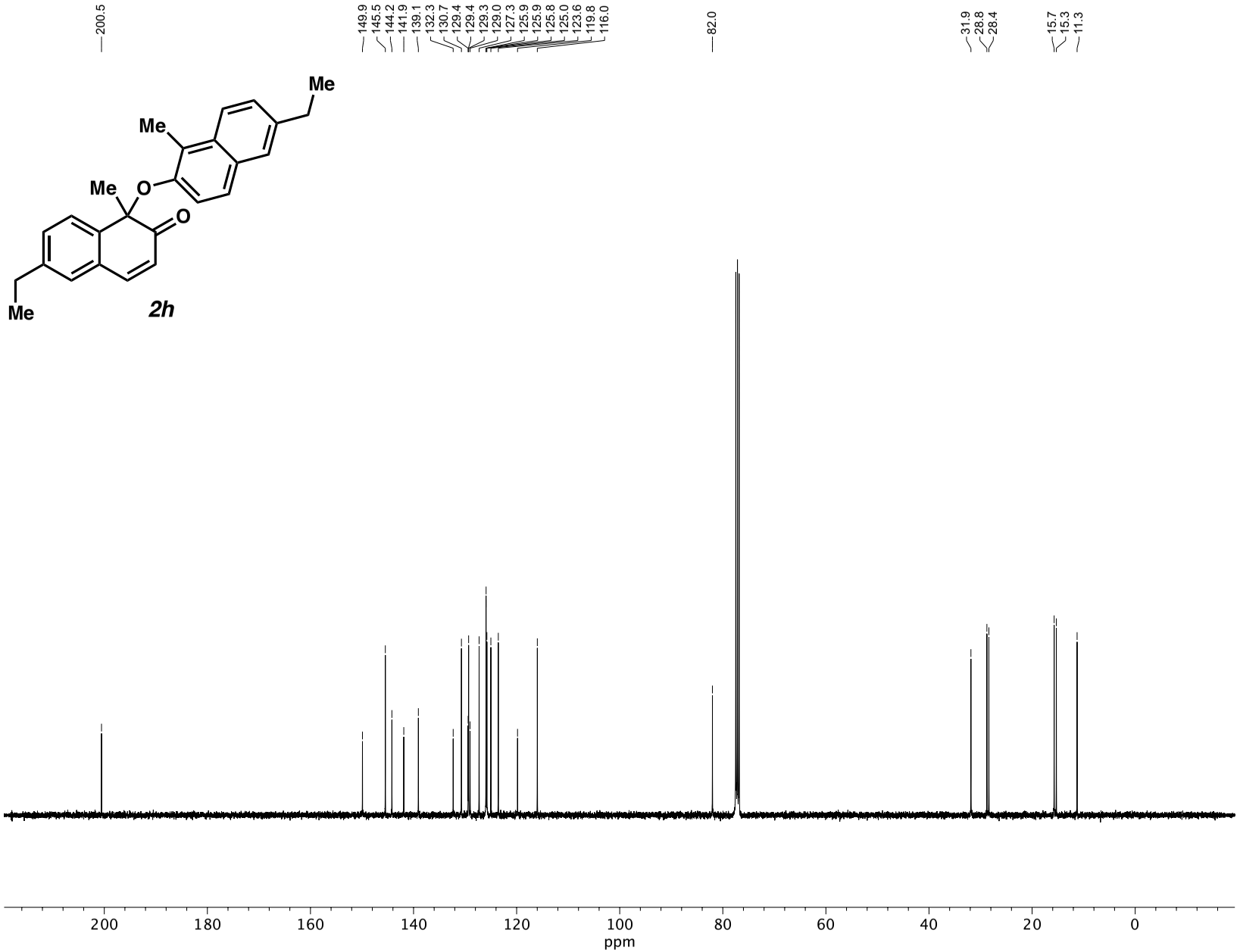
^{13}C NMR (101 MHz,$CDCl_3$) of compound **2g.**



^{13}C NMR (101 MHz,$CDCl_3$) of compound **2g.**

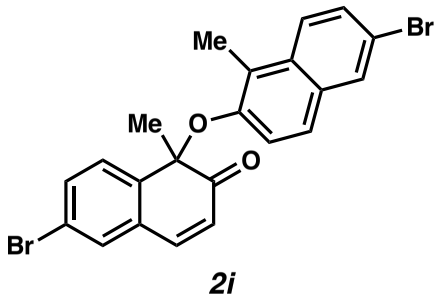


^{1}H NMR (400 MHz, $CDCl_3$) of compound **2h**.

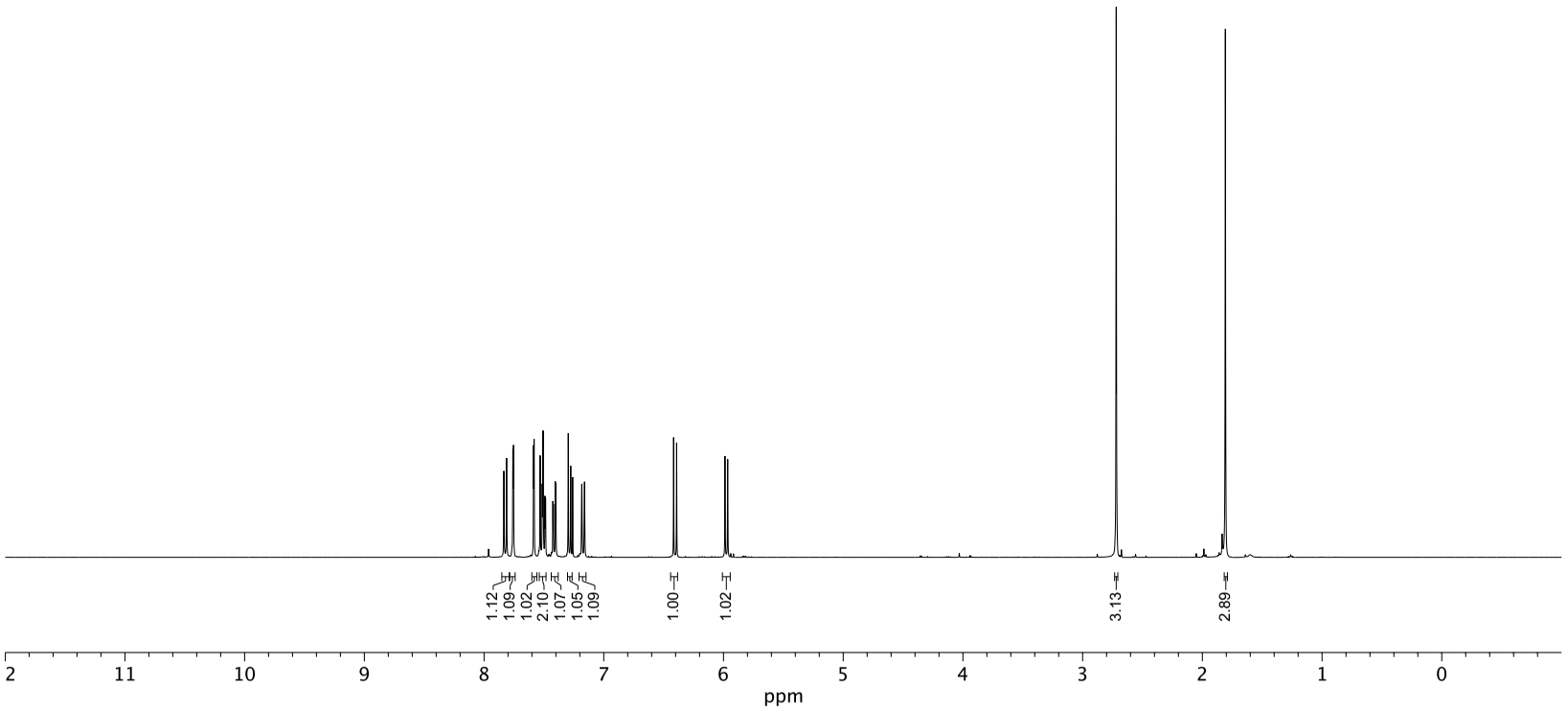


^{13}C NMR (101 MHz,$CDCl_3$) of compound **2h.**

^{1}H NMR (400 MHz, $CDCl_3$) of compound **2i**.

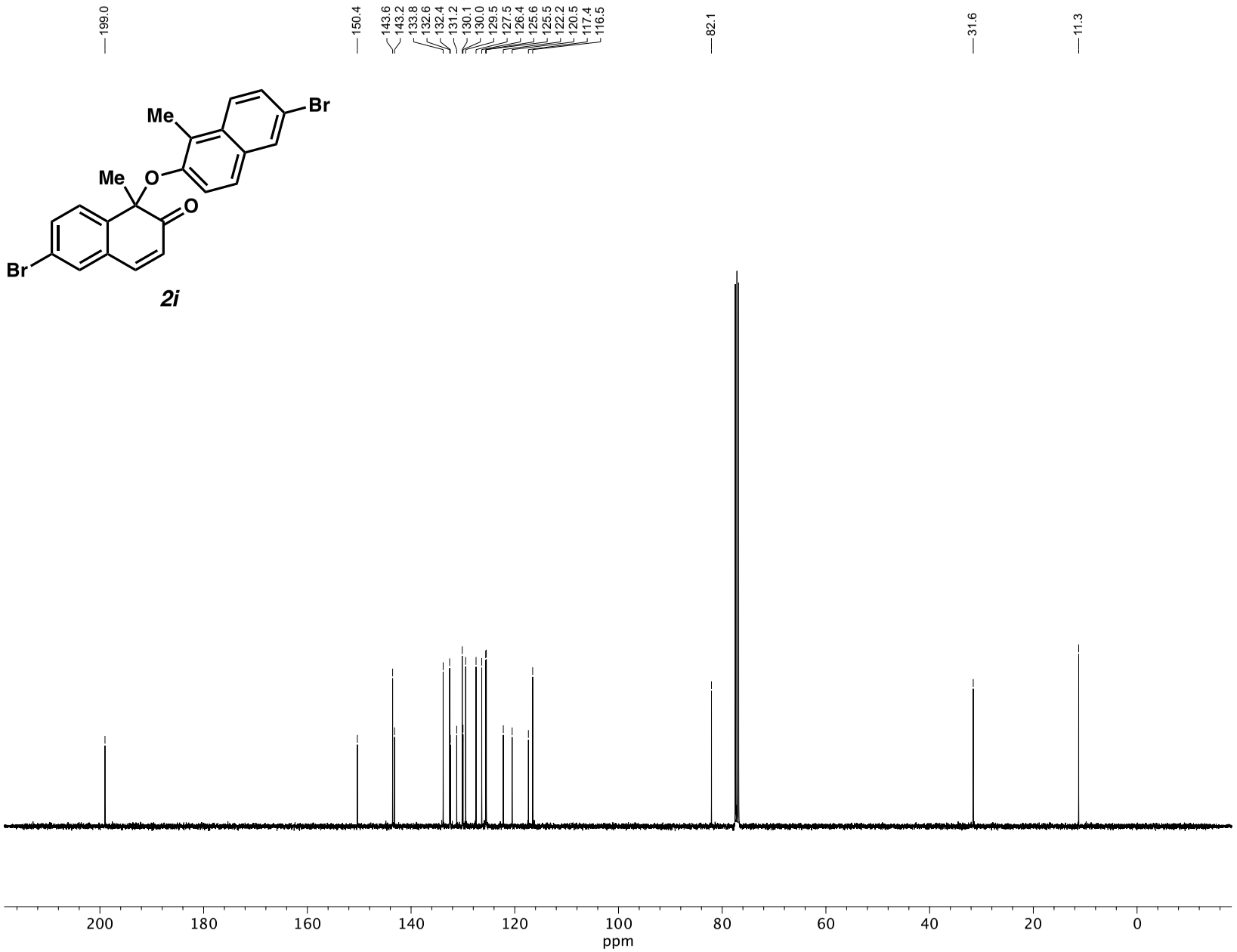


2i

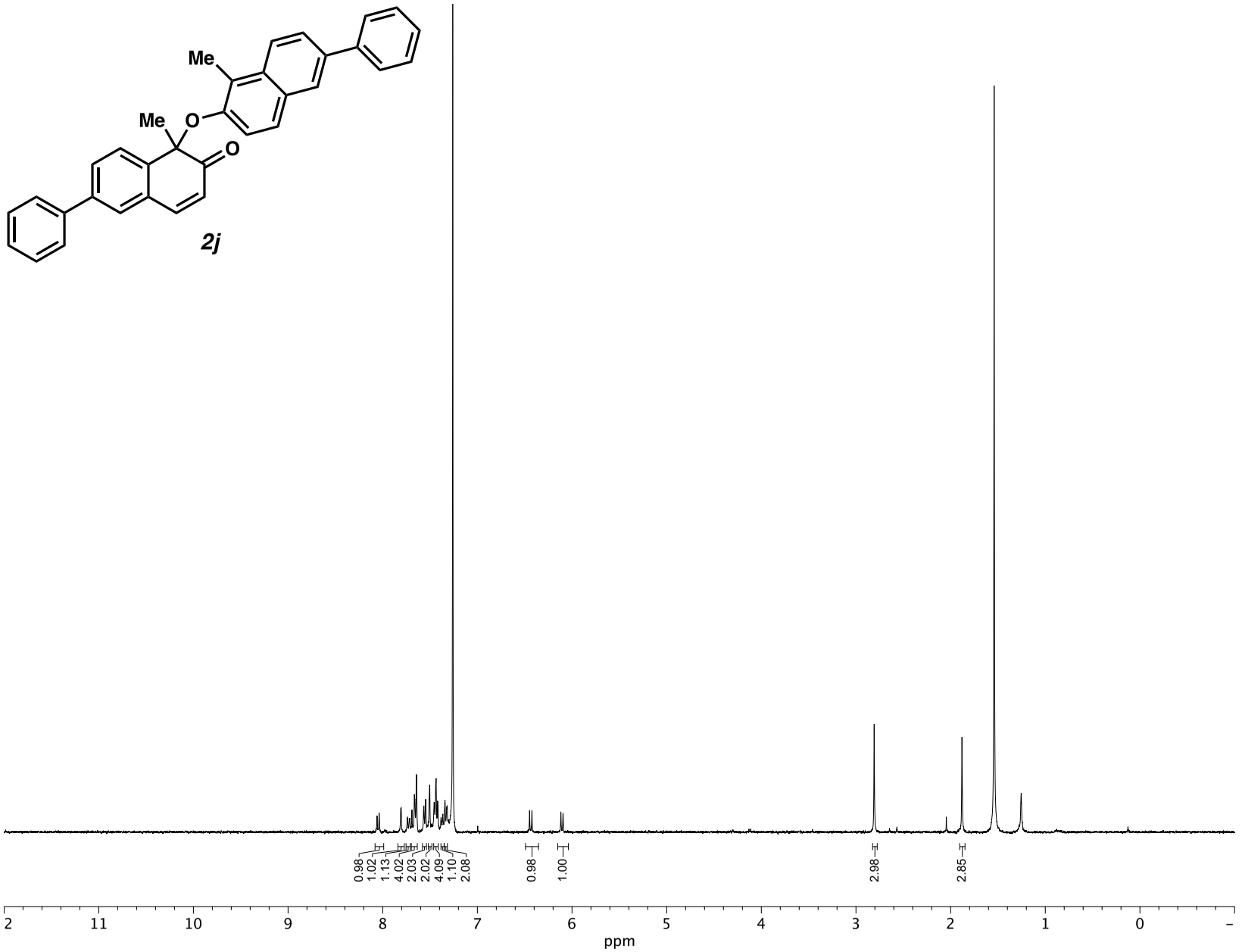


^{1}H NMR (400 MHz, $CDCl_3$) of compound **2i**.

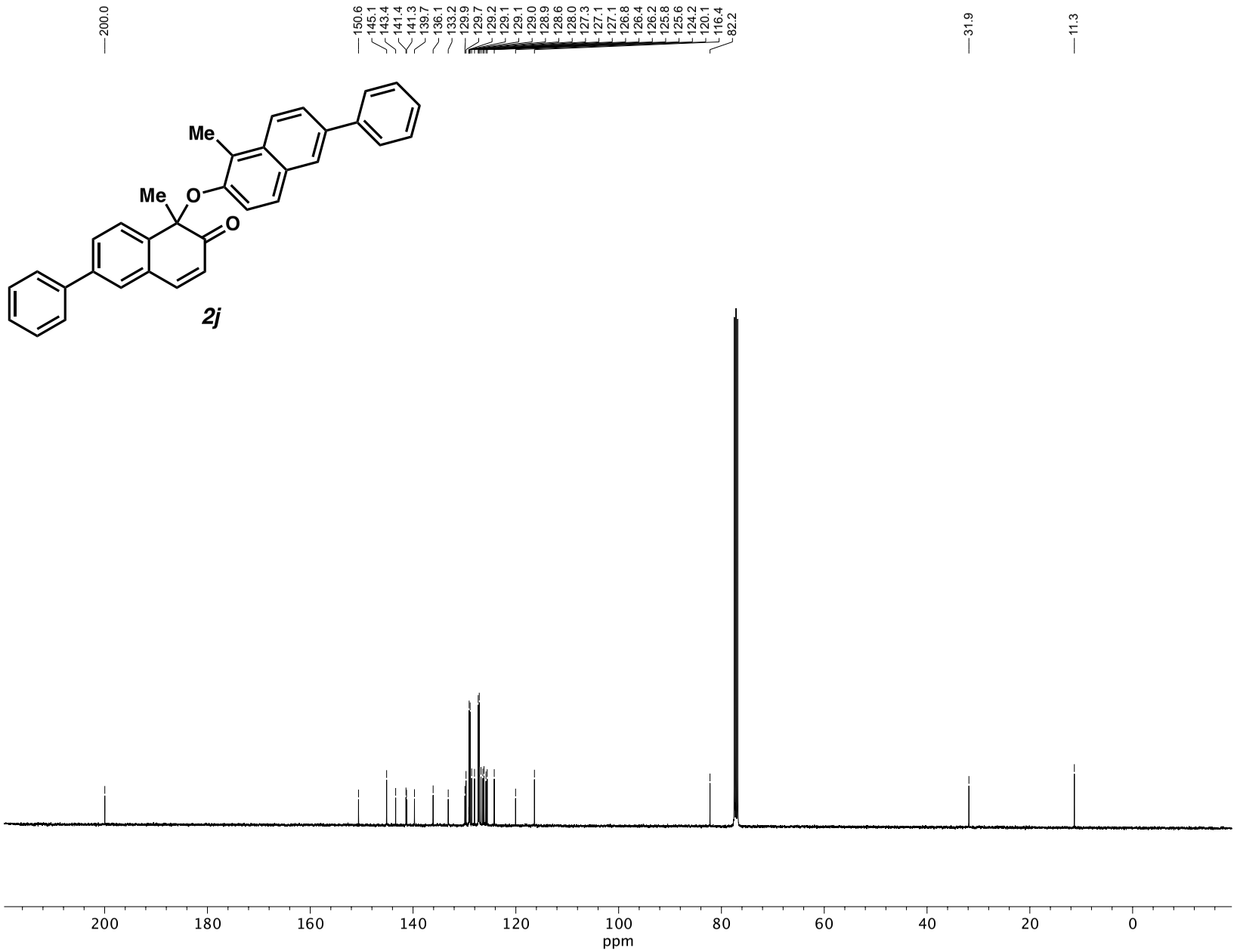
^{13}C NMR (101 MHz,$CDCl_3$) of compound **2i.**



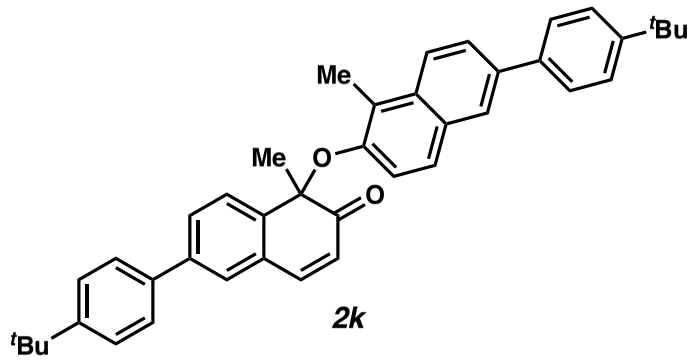
^{13}C NMR (101 MHz,$CDCl_3$) of compound **2i.**



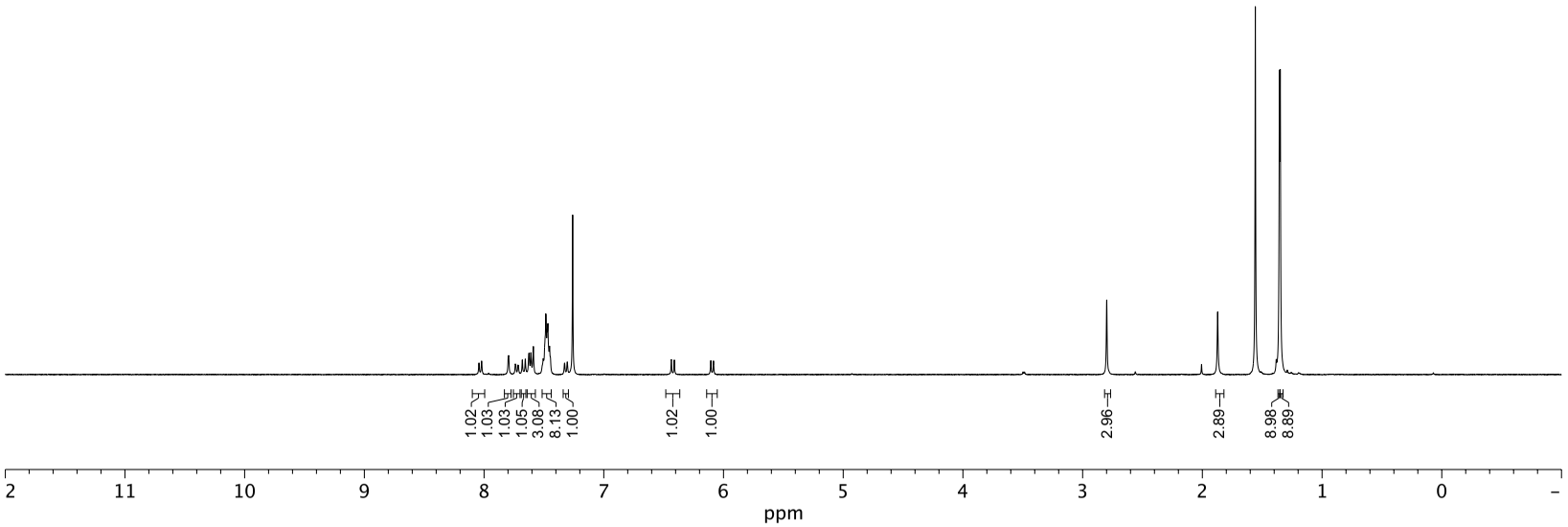
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2j**.



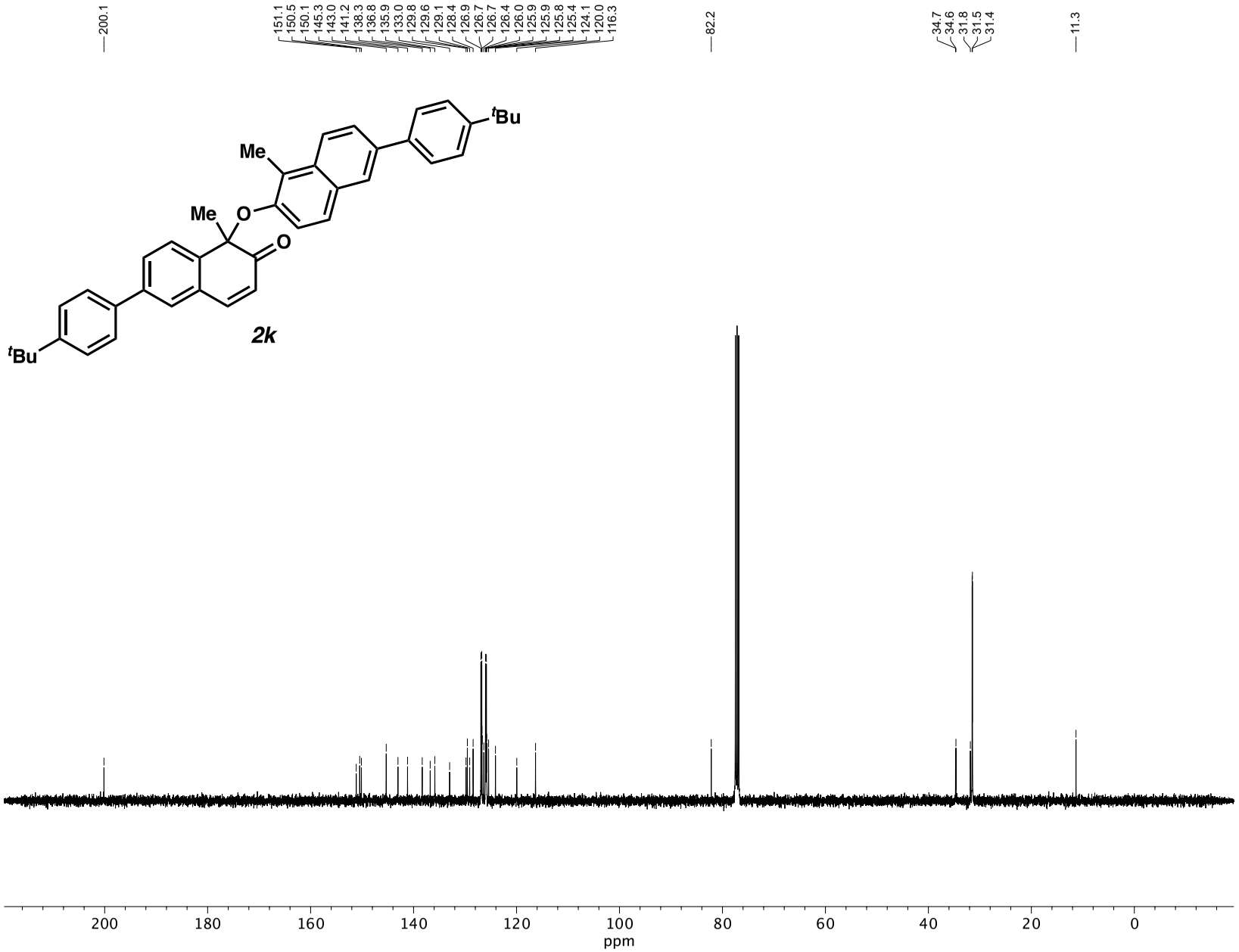
^{13}C NMR (101 MHz,$CDCl_3$) of compound **2j.**



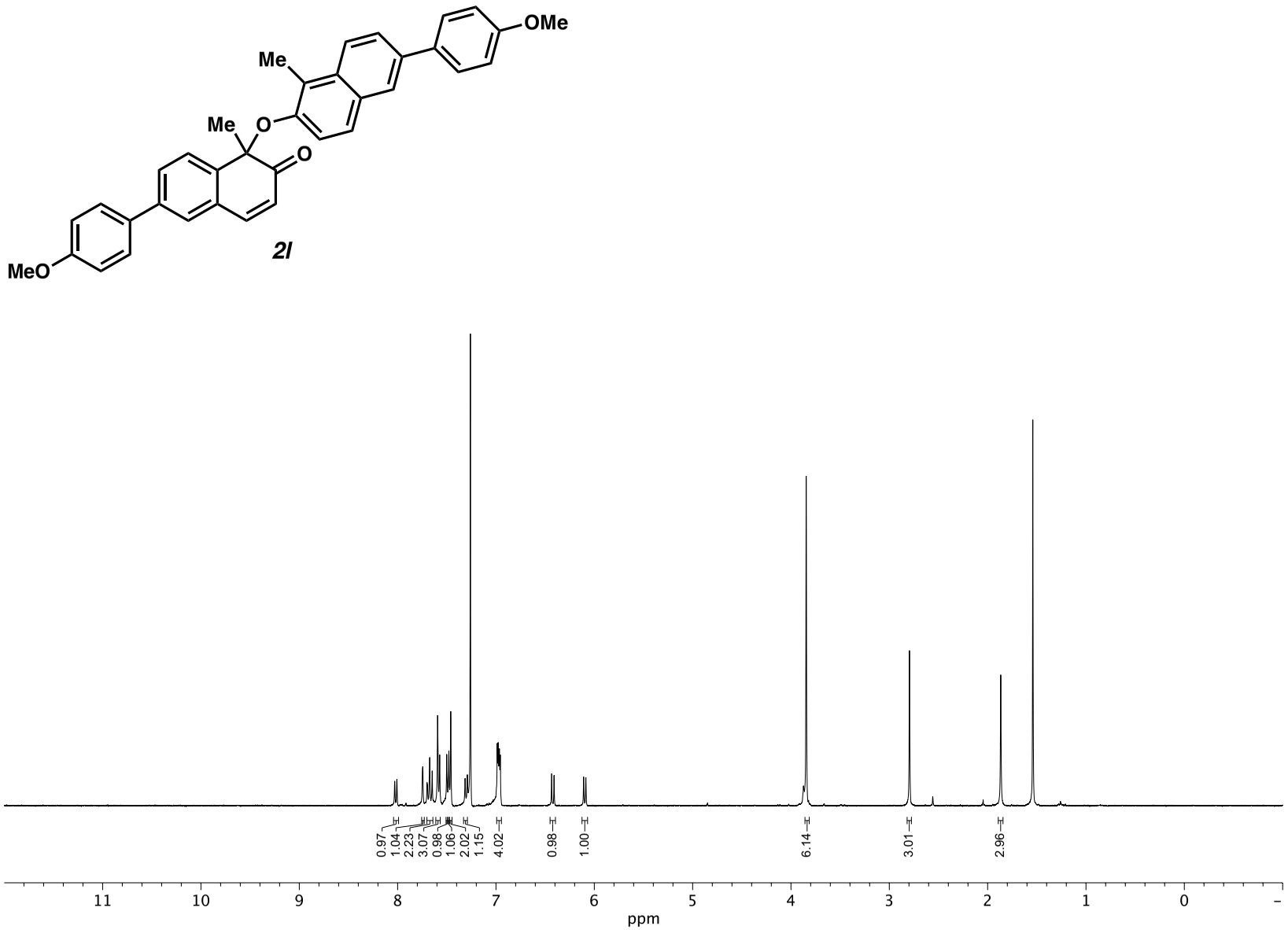
2k



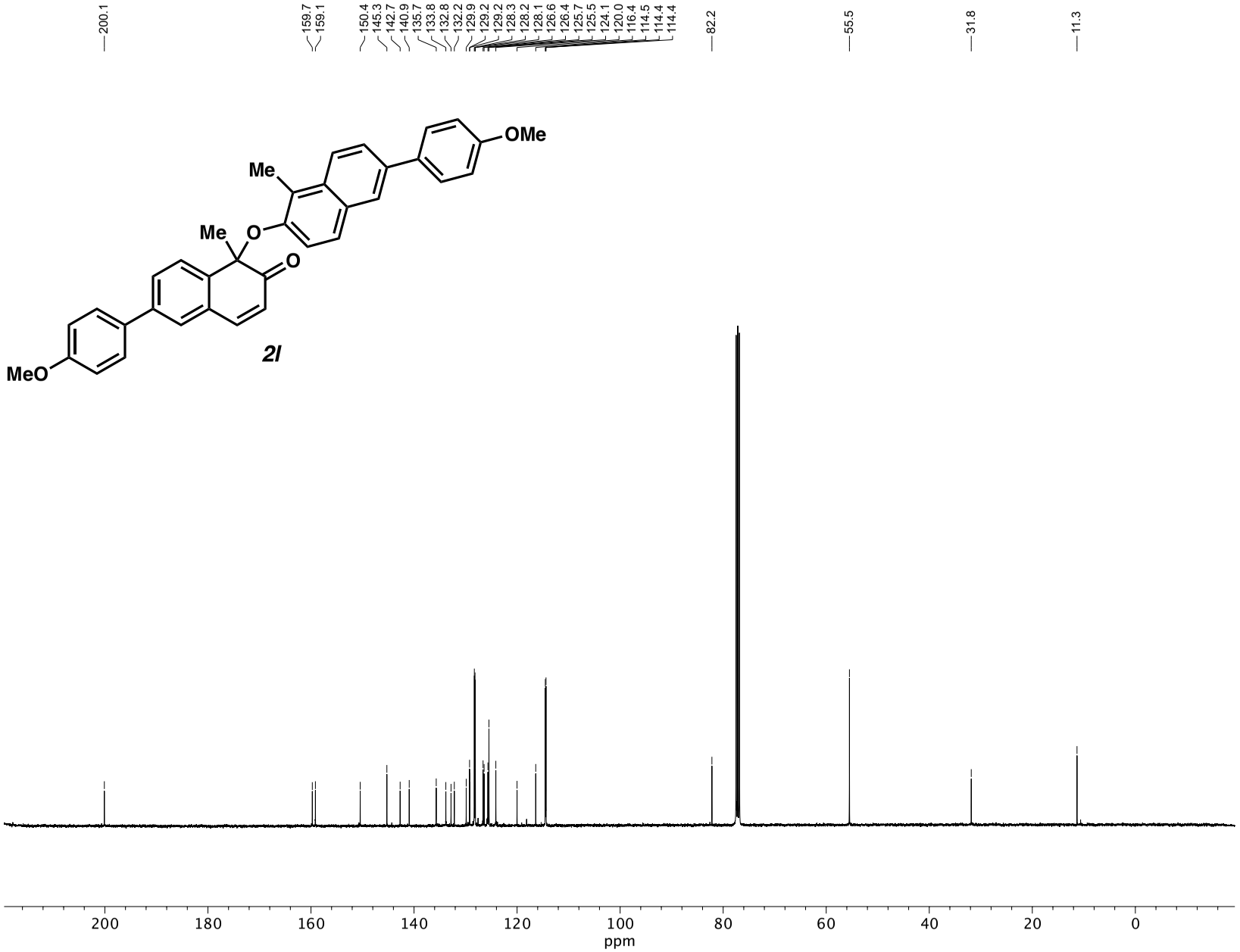
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2k**.



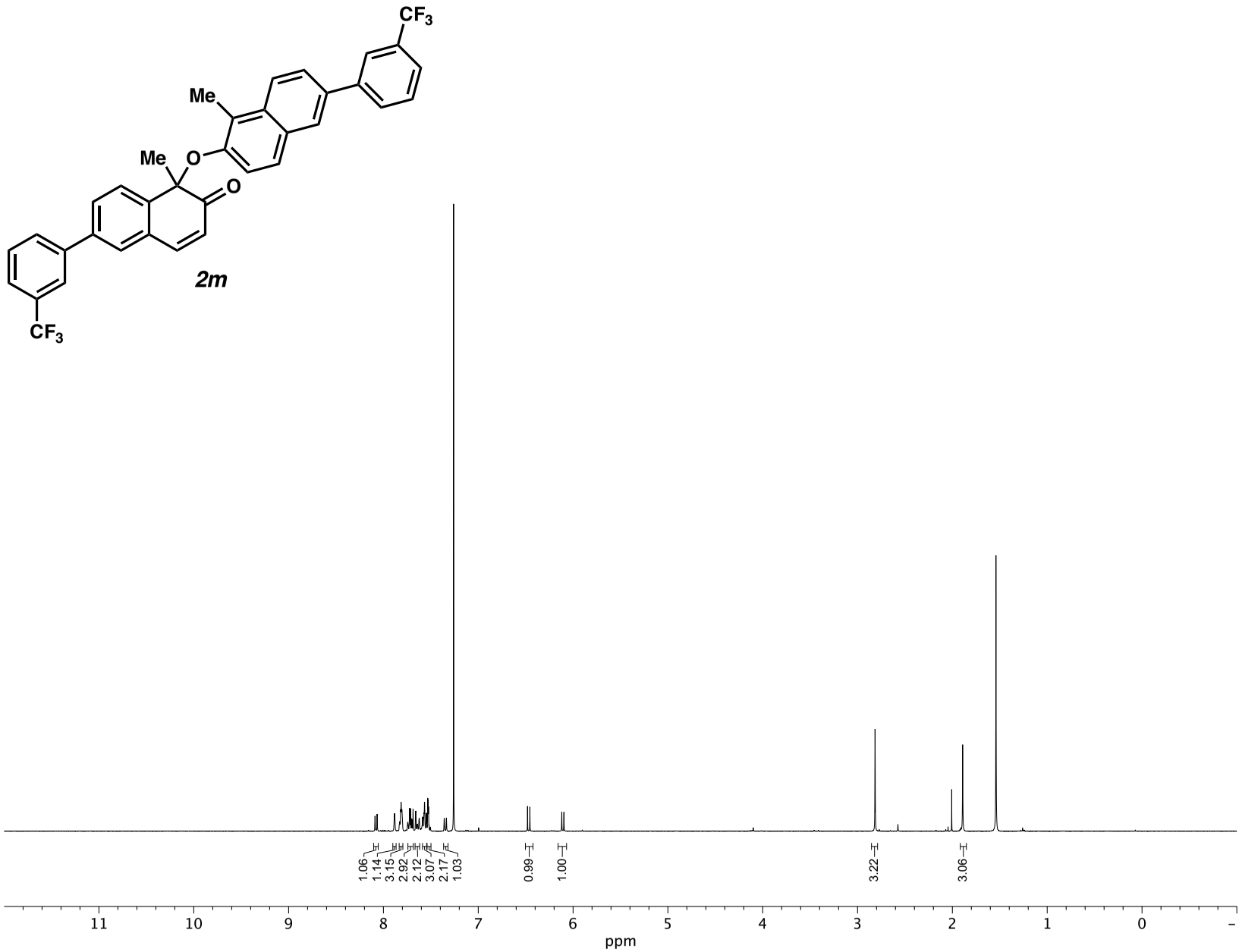
^{13}C NMR (101 MHz,$CDCl_3$) of compound **2k.**



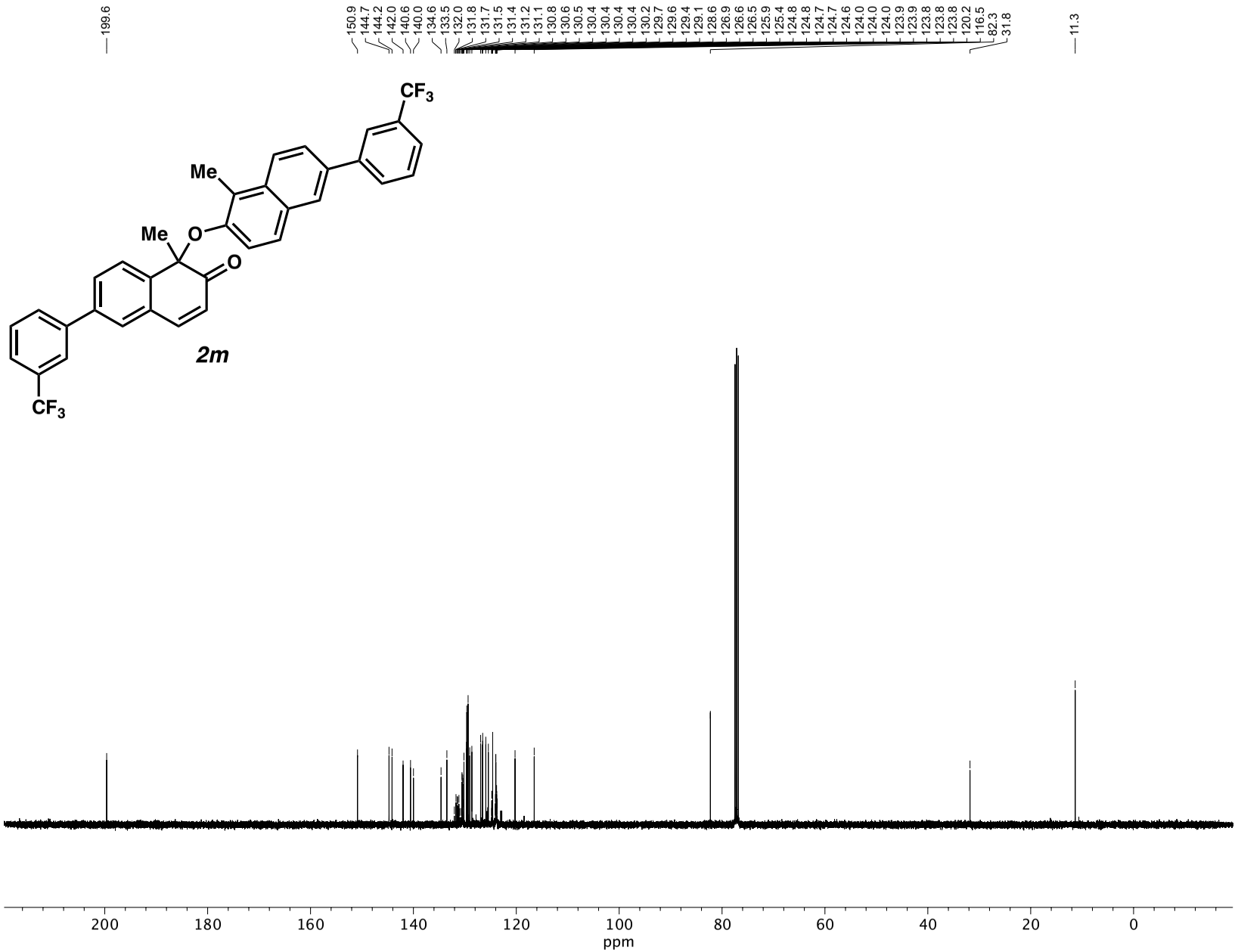
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2l**.



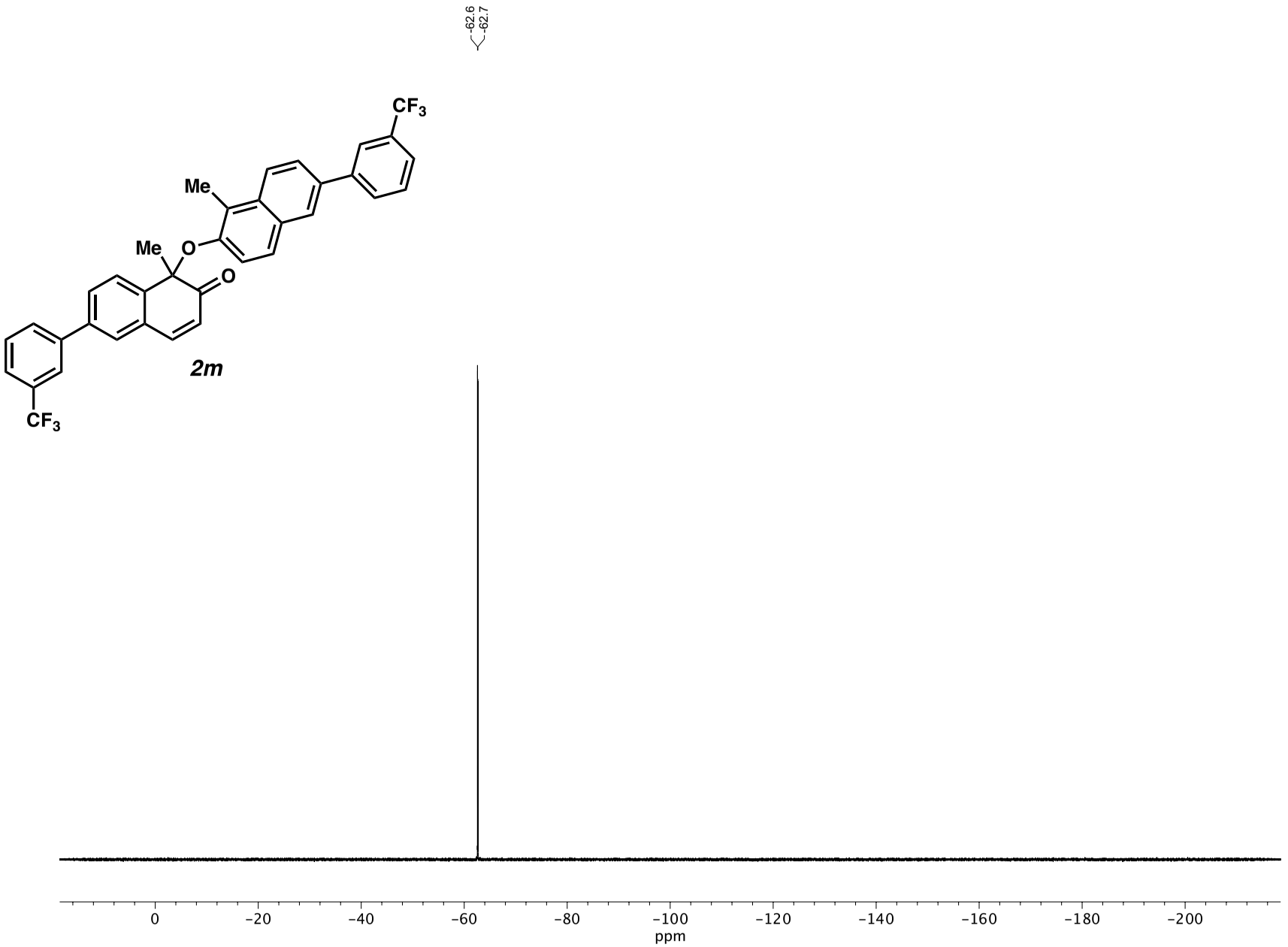
^{13}C NMR (101 MHz,$CDCl_3$) of compound **2l.**



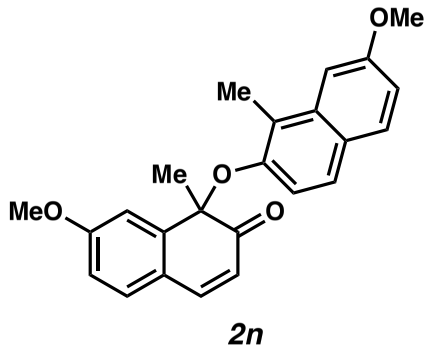
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2m**.



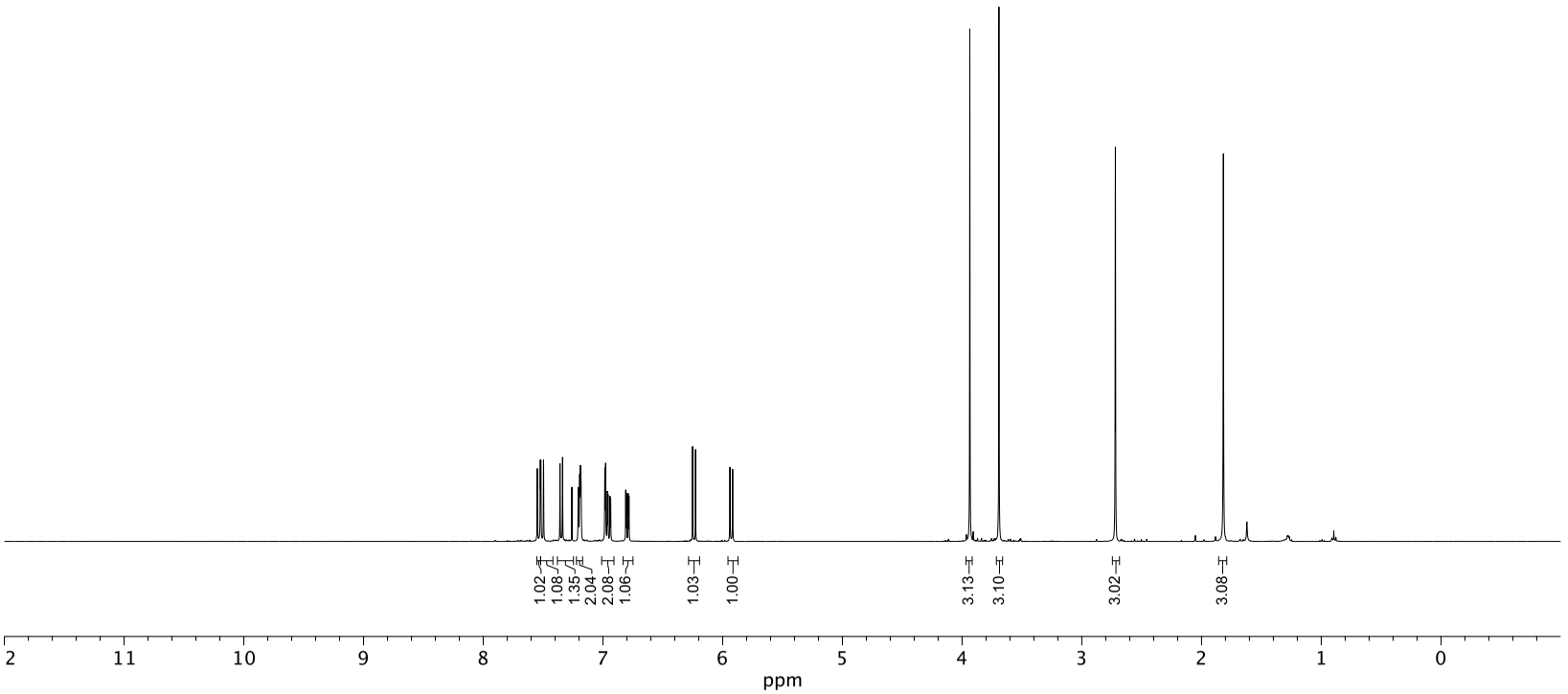
^{13}C NMR (101 MHz,$CDCl_3$) of compound **2m.**



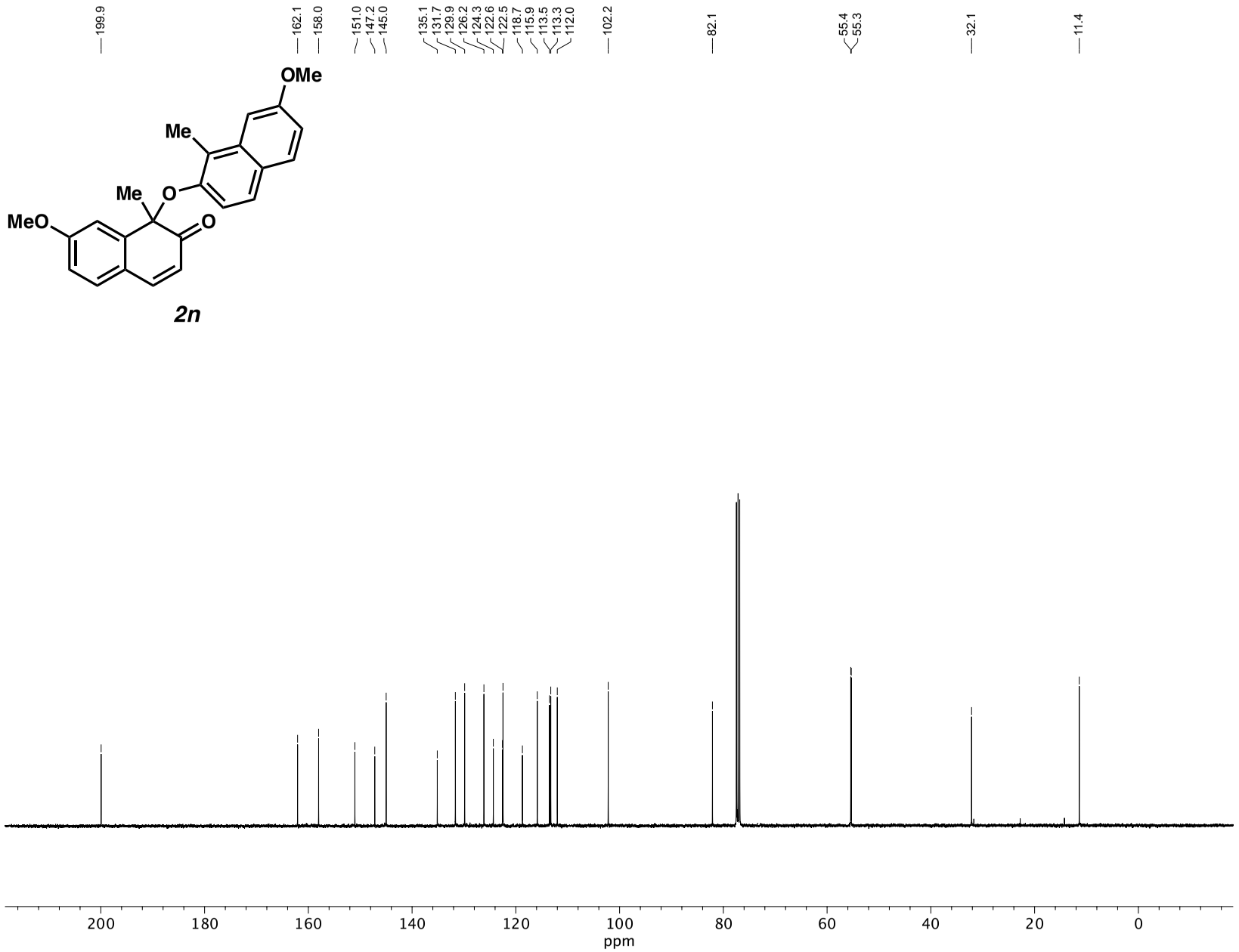
^{19}F NMR (377 MHz,$CDCl_3$) of compound **2m.**



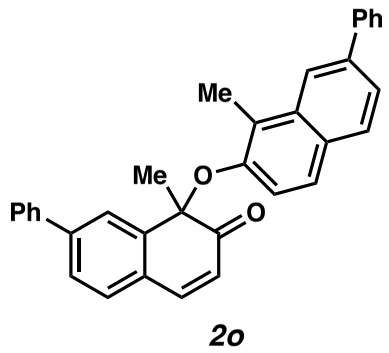
2n



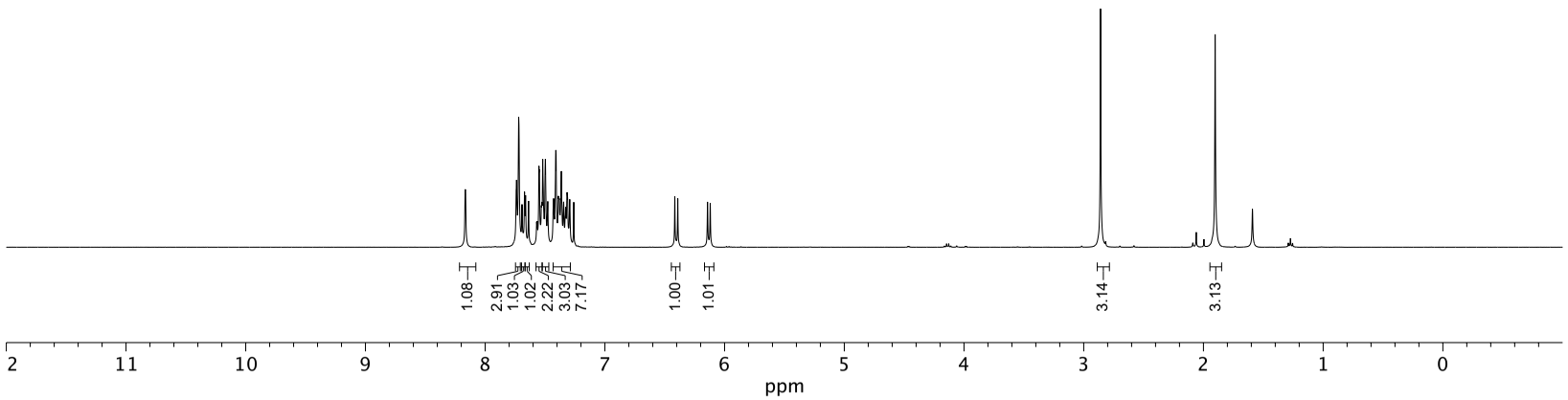
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2n**.



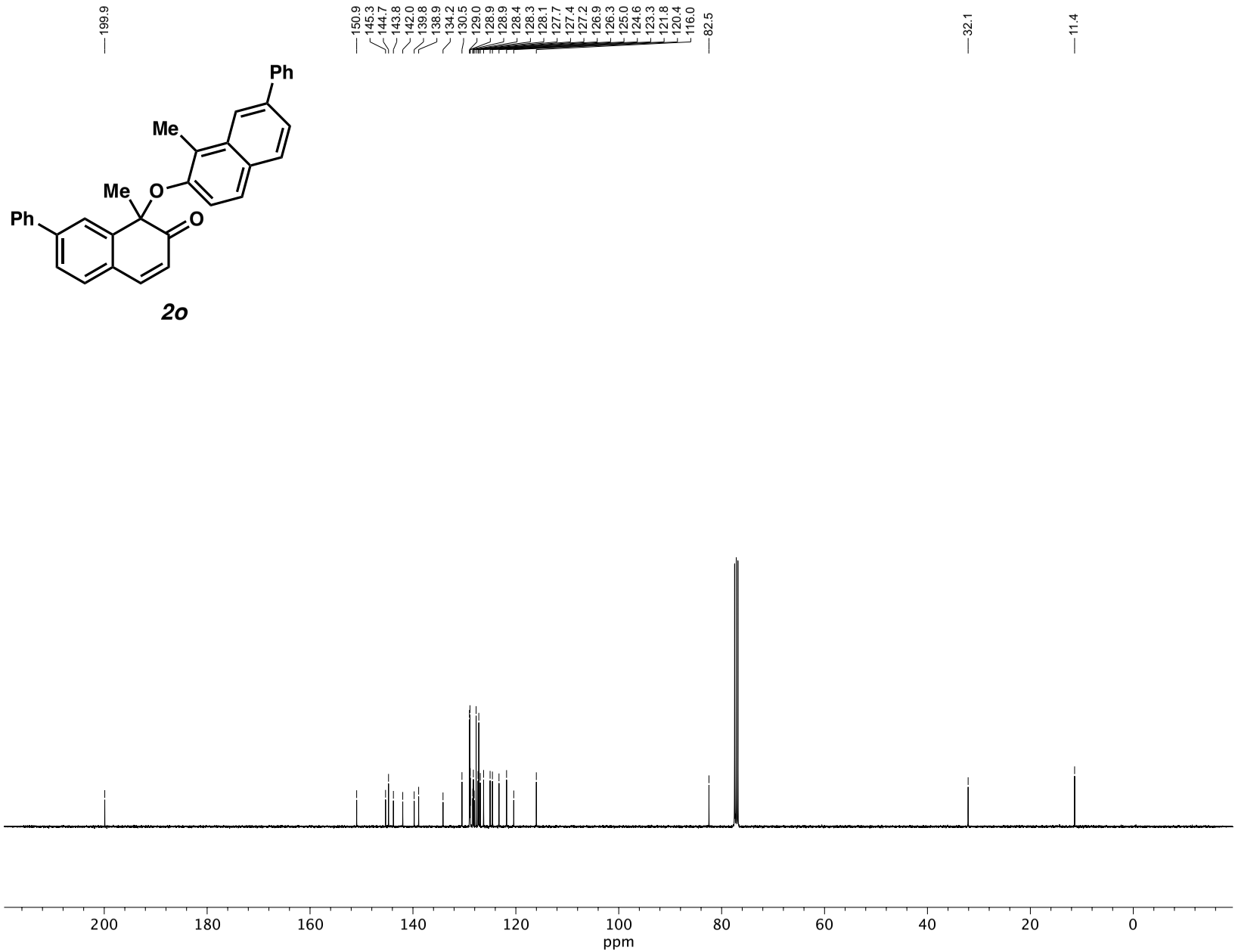
^{13}C NMR (101 MHz,$CDCl_3$) of compound **2n.**



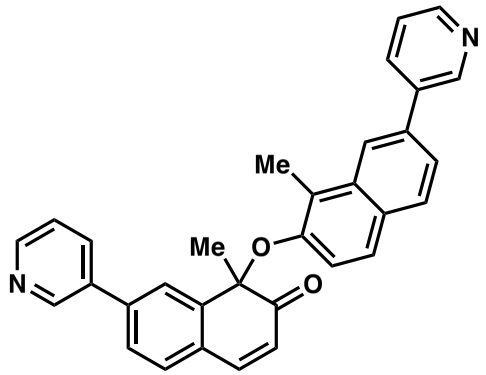
2o



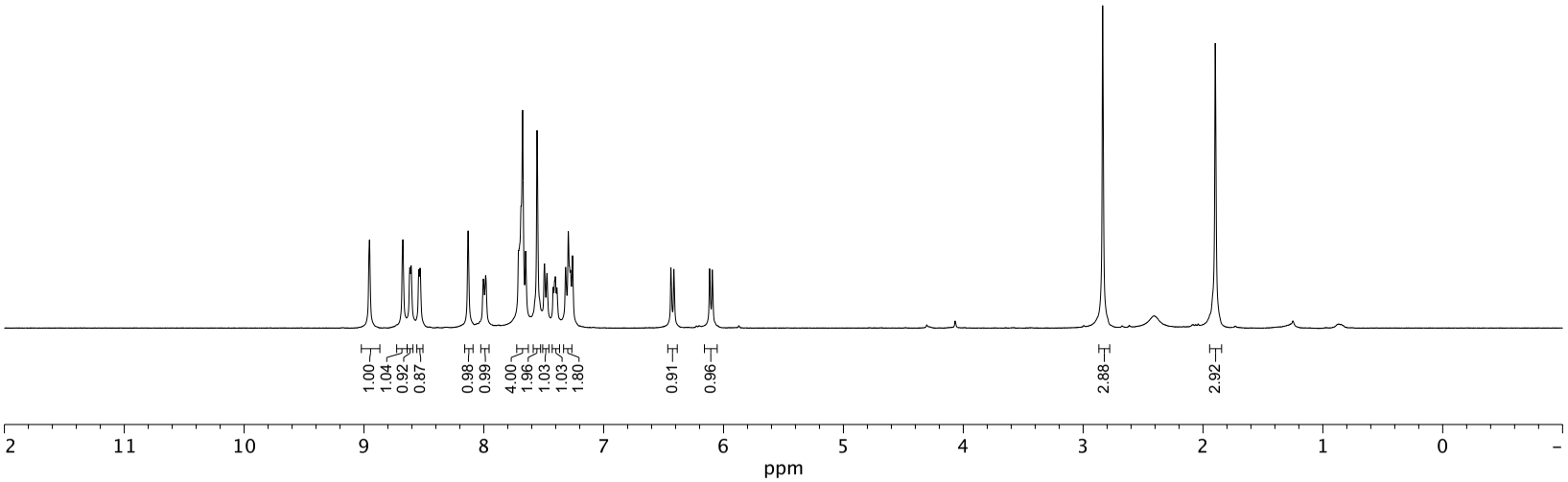
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2o**.



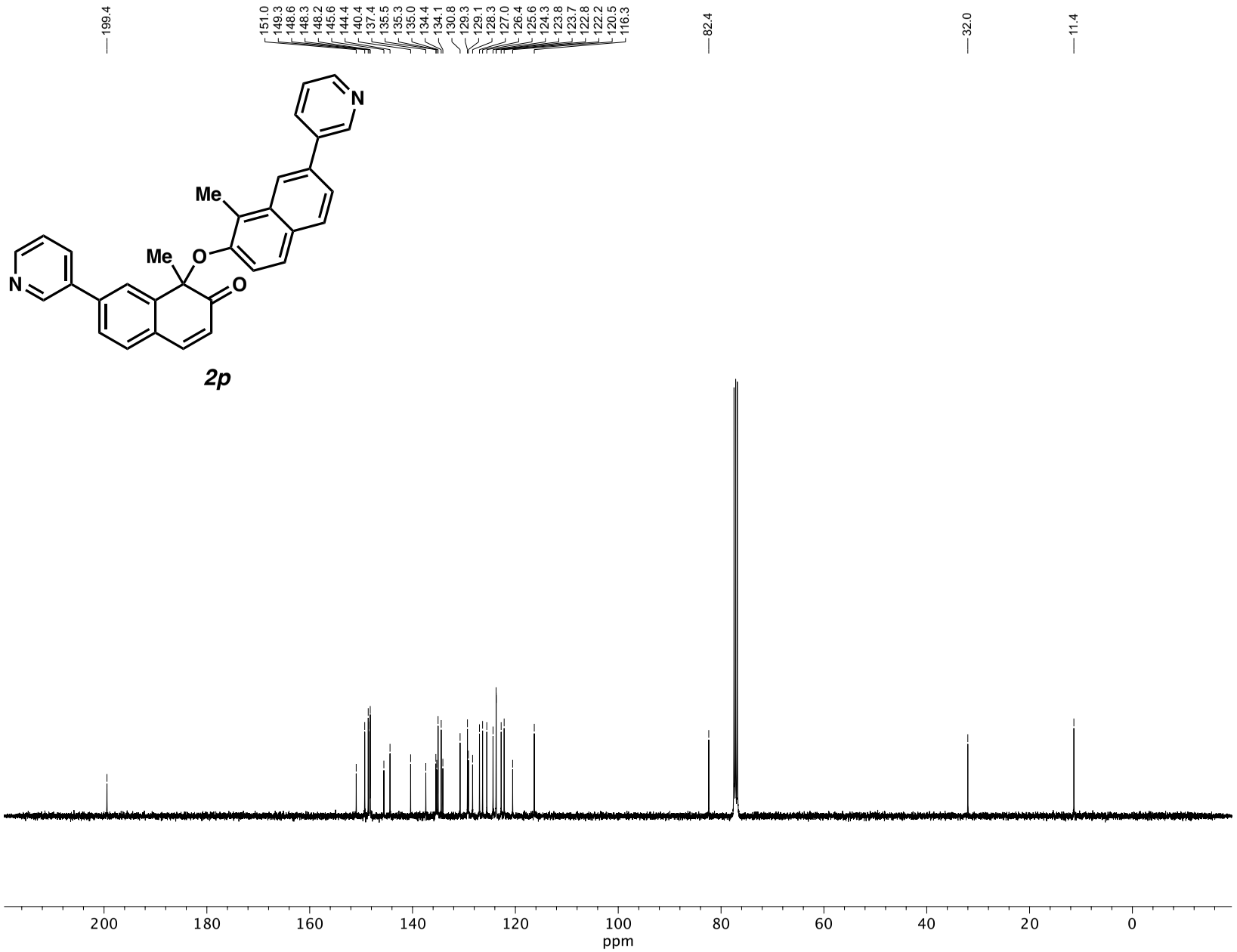
^{13}C NMR (101 MHz,$CDCl_3$) of compound **2o.**



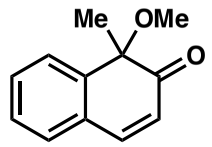
2p



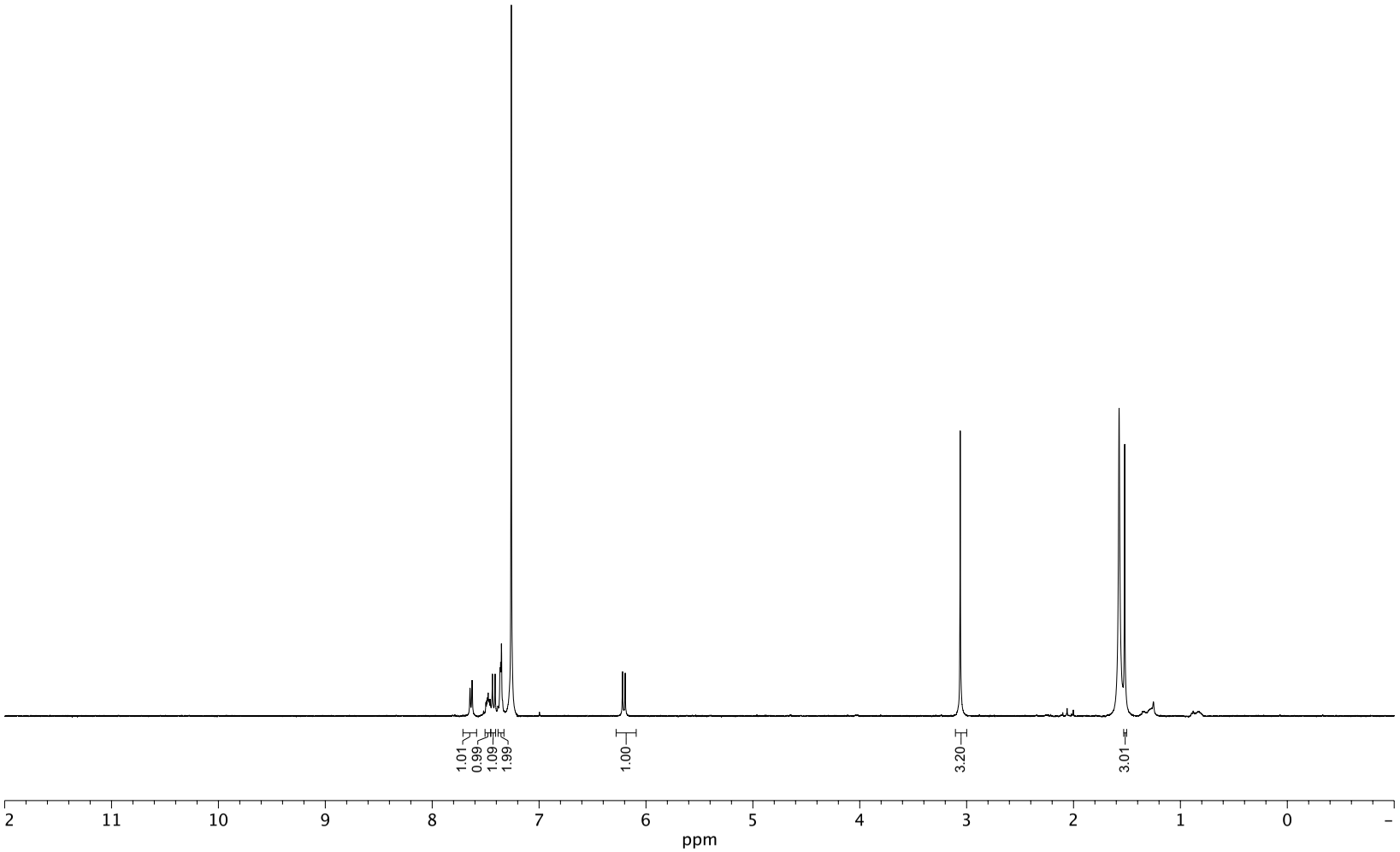
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2p**.



^{13}C NMR (101 MHz,$CDCl_3$) of compound **2p.**

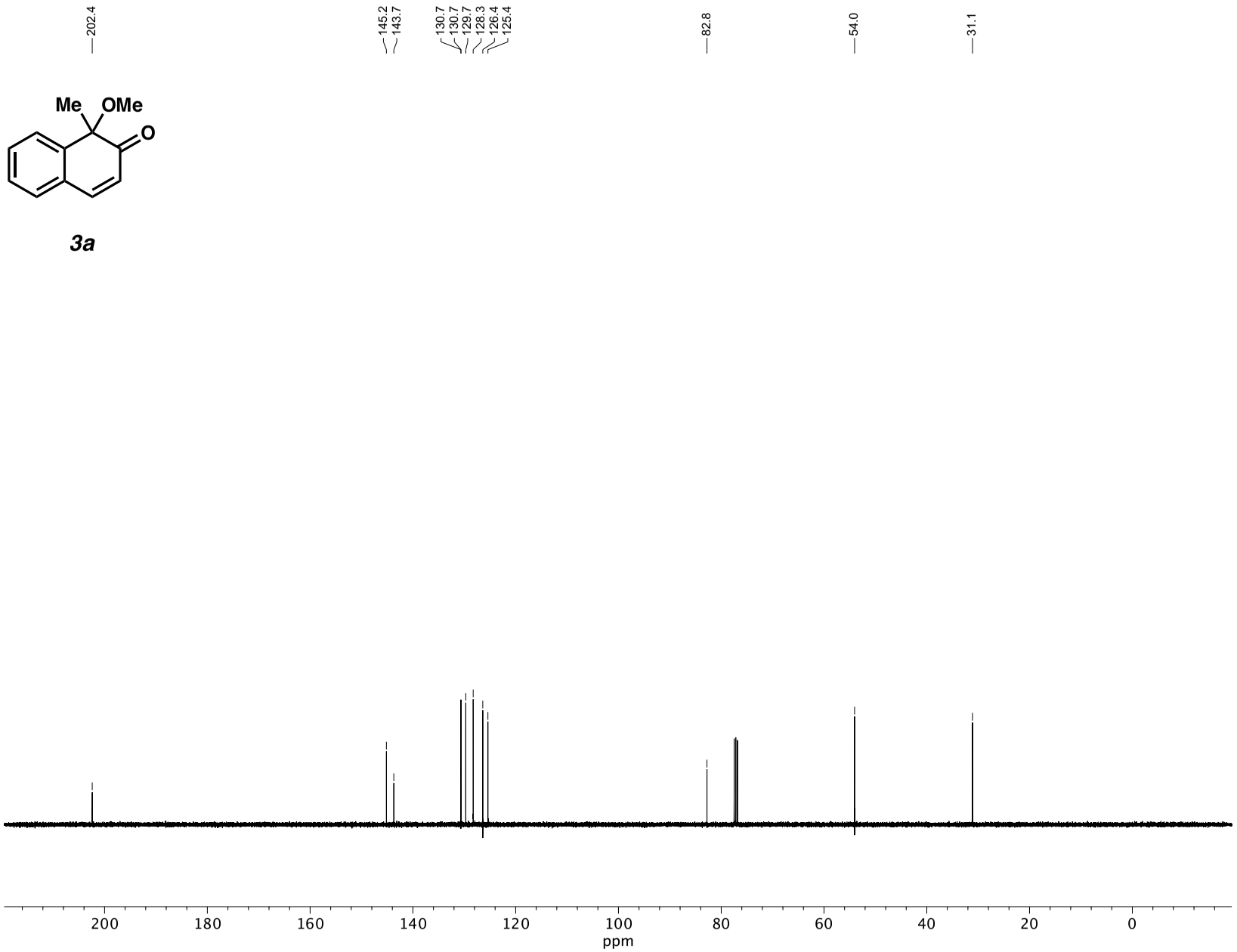


3a



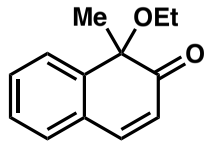
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3a**.

^{13}C NMR (101 MHz,$CDCl_3$) of compound **3a**.

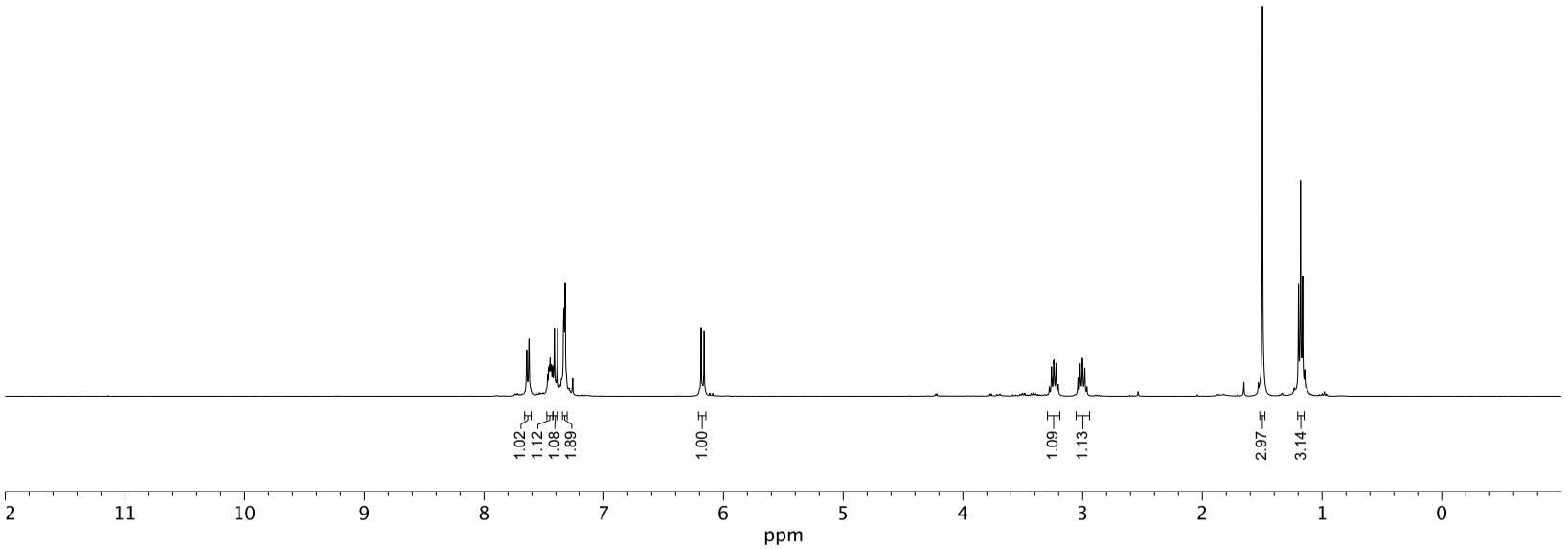


3a

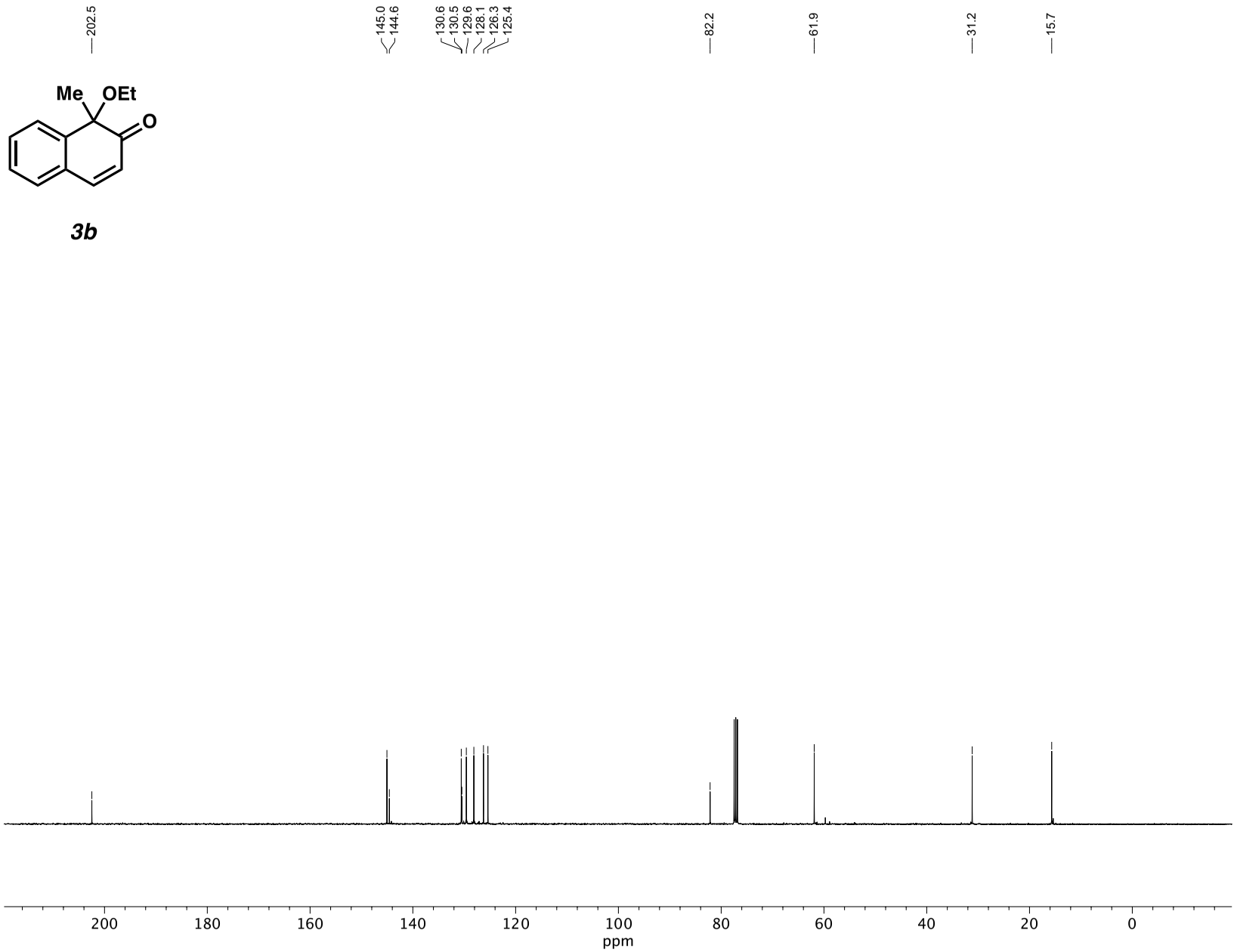
^{13}C NMR (101 MHz,$CDCl_3$) of compound **3a**.



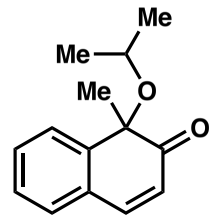
3b



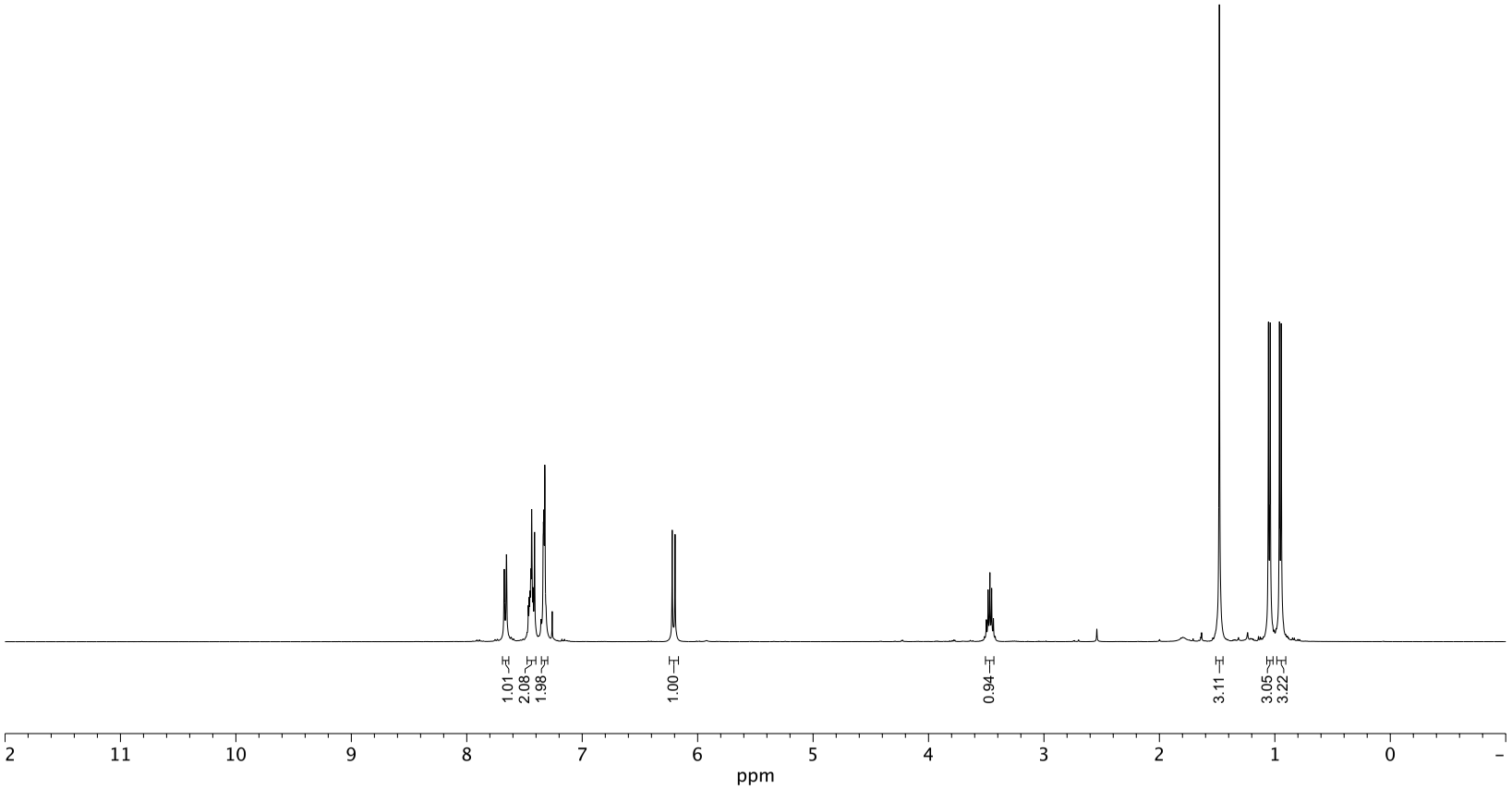
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3b**.



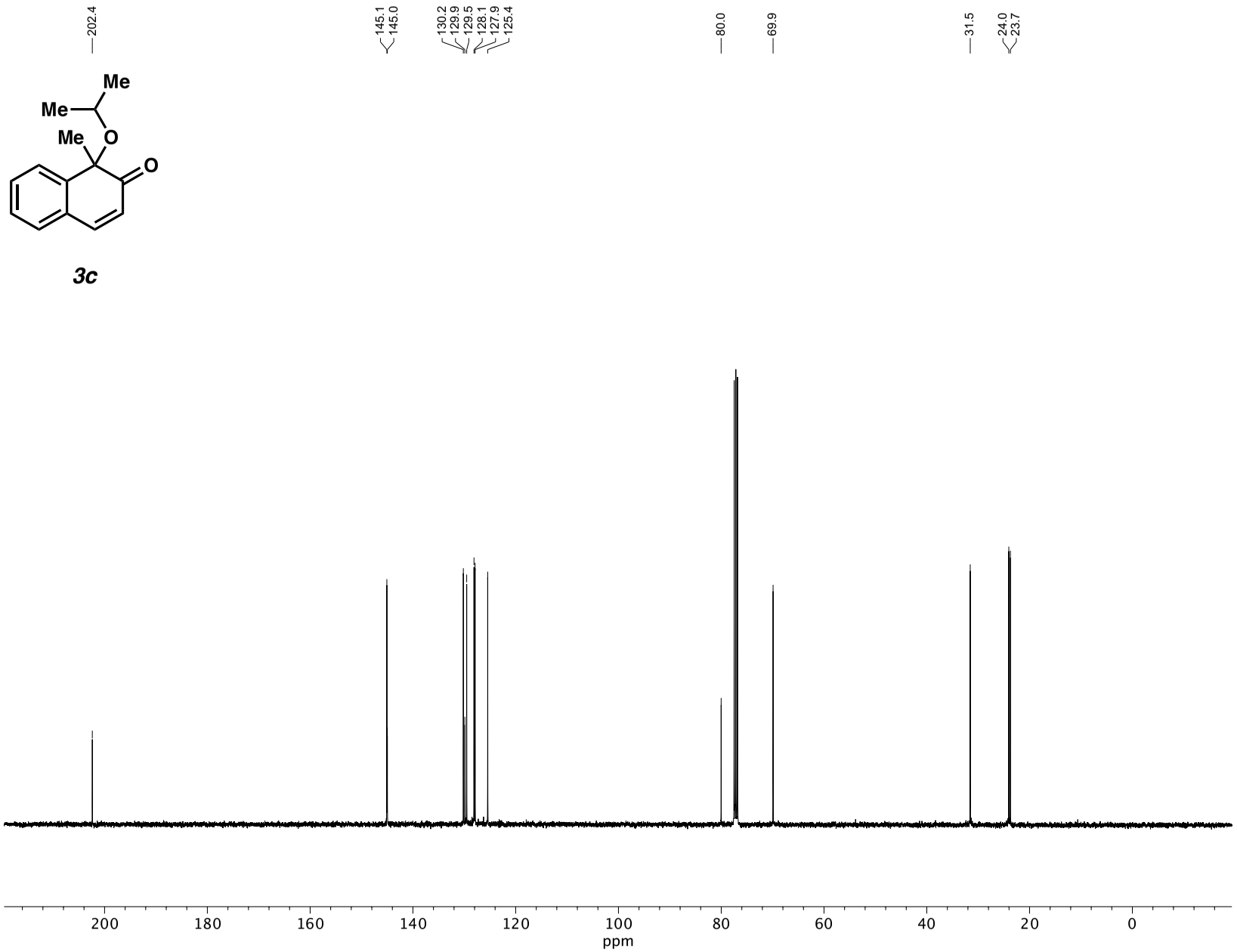
^{13}C NMR (101 MHz,$CDCl_3$) of compound **3b**.



3c

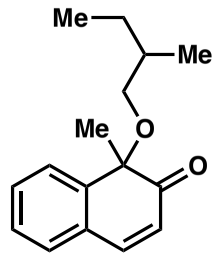


^{1}H NMR (400 MHz, $CDCl_3$) of compound **3c**.

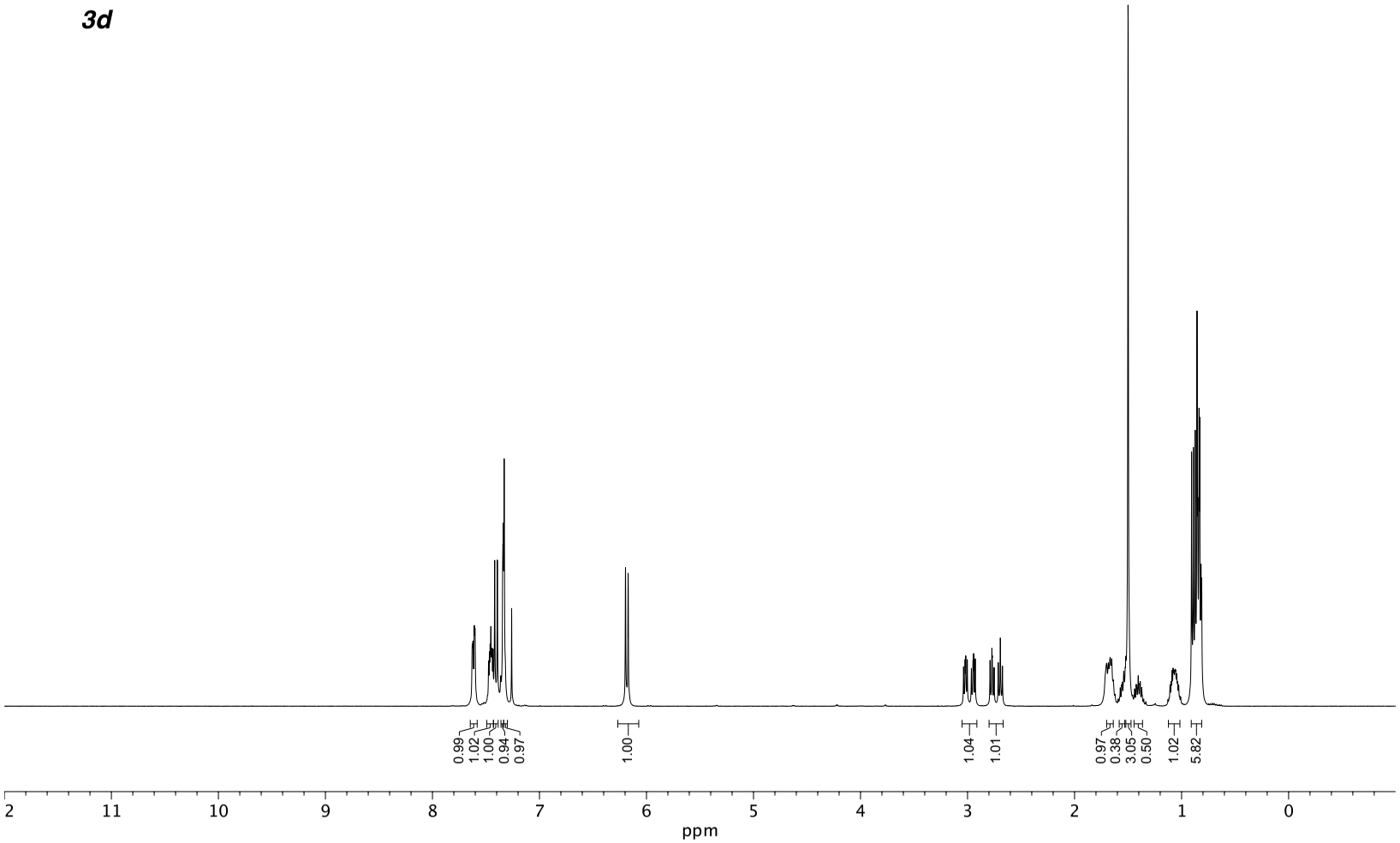


3c

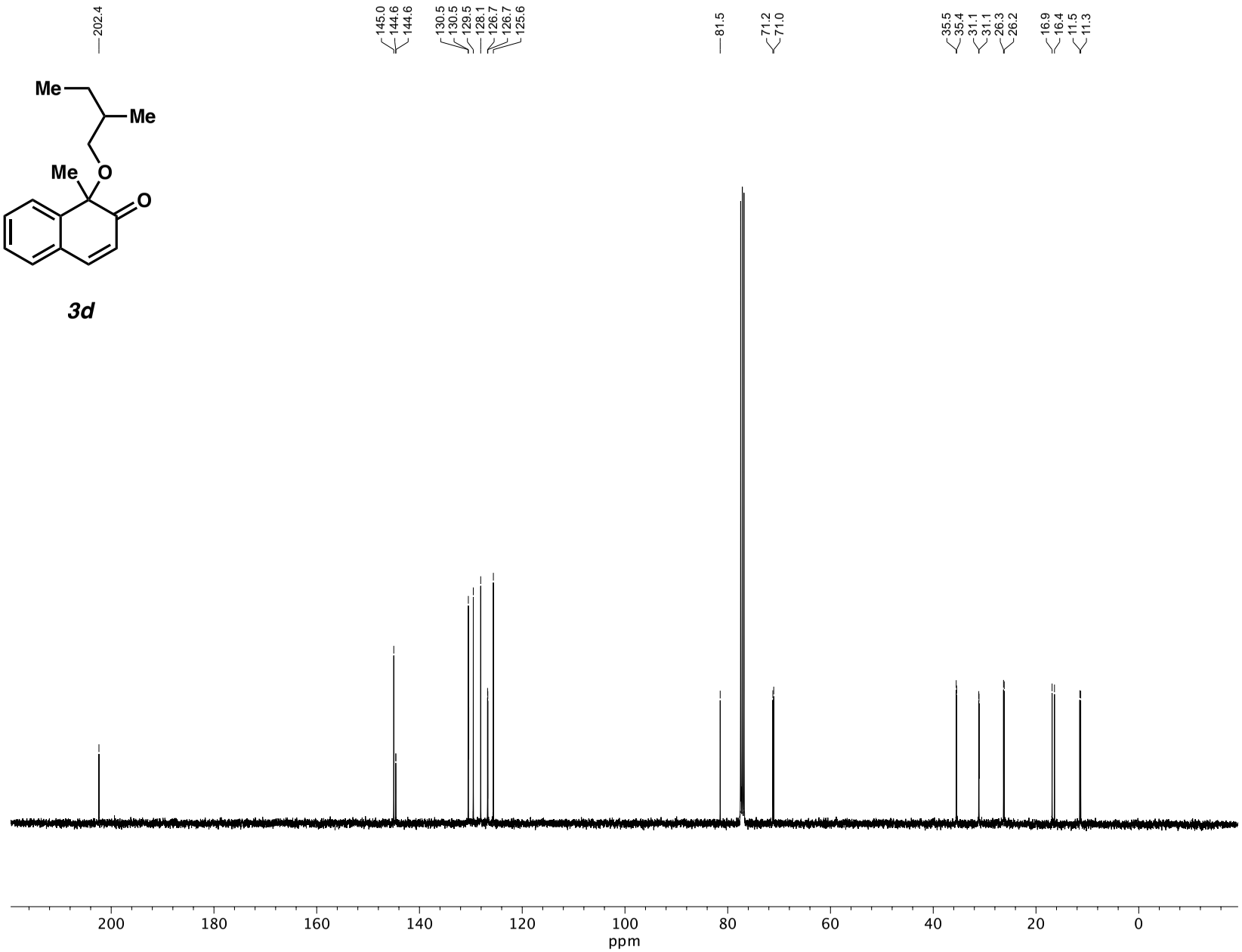
^{13}C NMR (101 MHz,$CDCl_3$) of compound **3c**.



3d

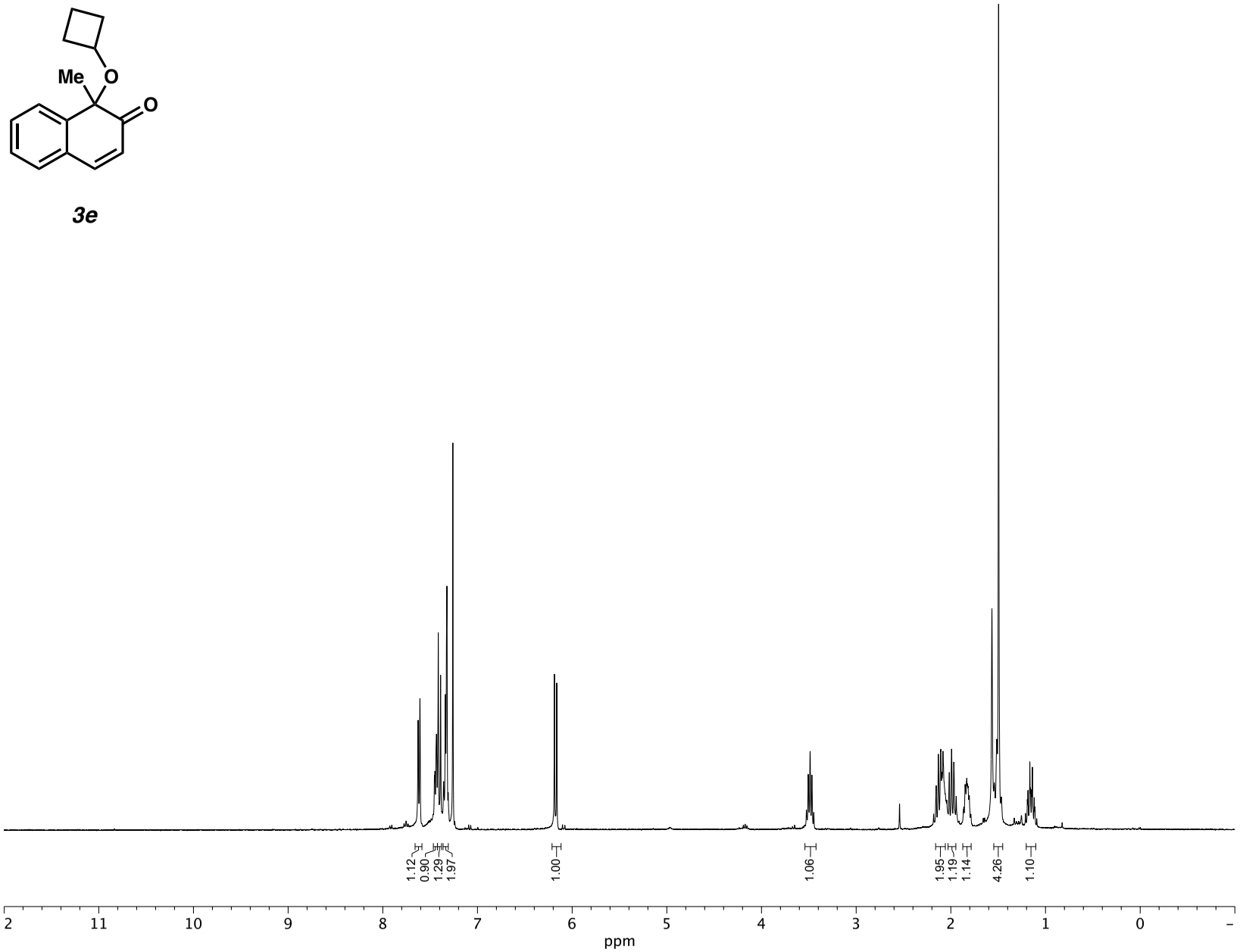


^{1}H NMR (400 MHz, $CDCl_3$) of compound **3d**.

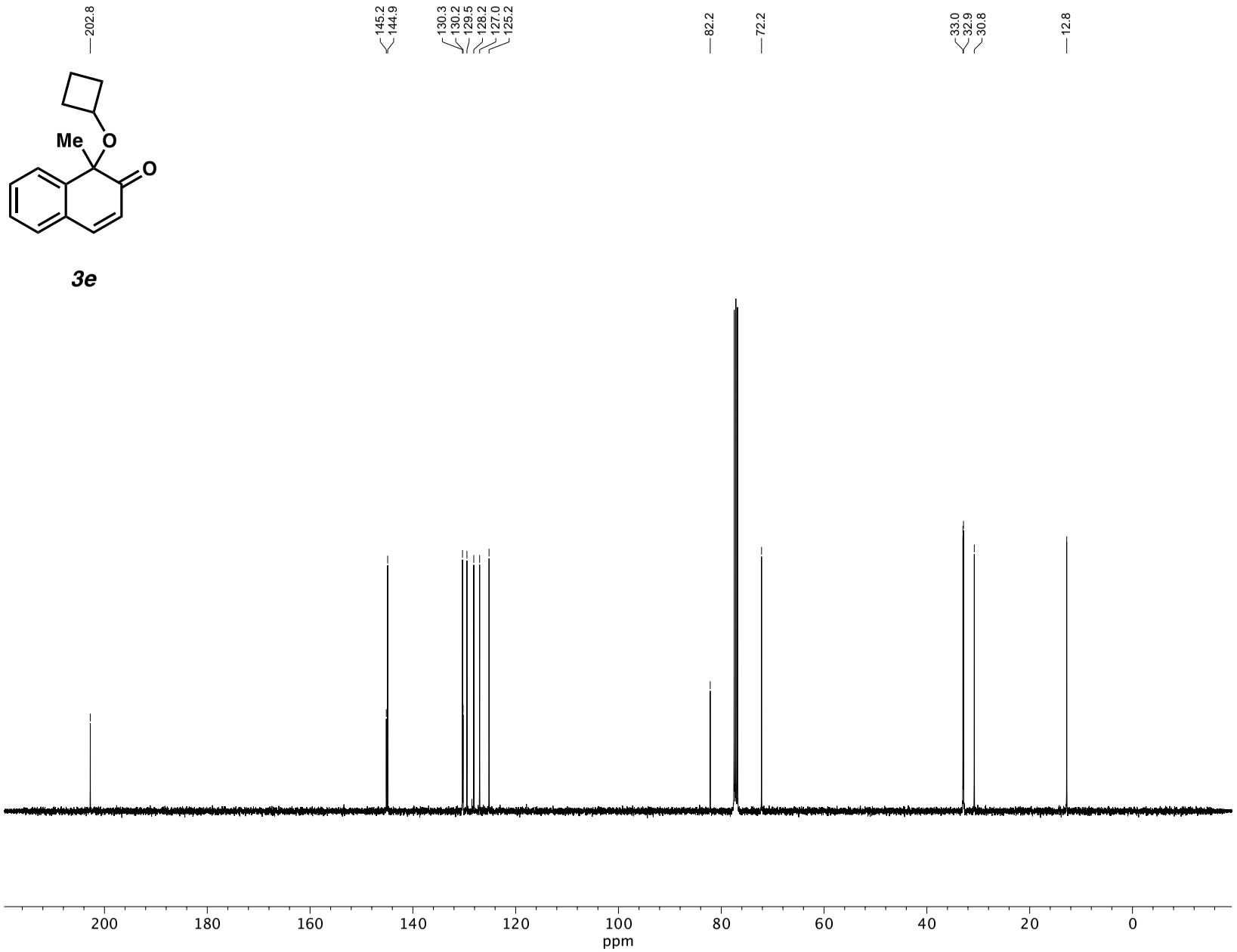


^{13}C NMR (101 MHz,$CDCl_3$) of compound **3d**.

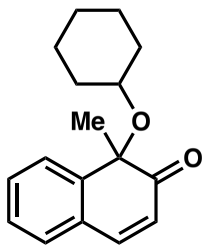
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3e**.



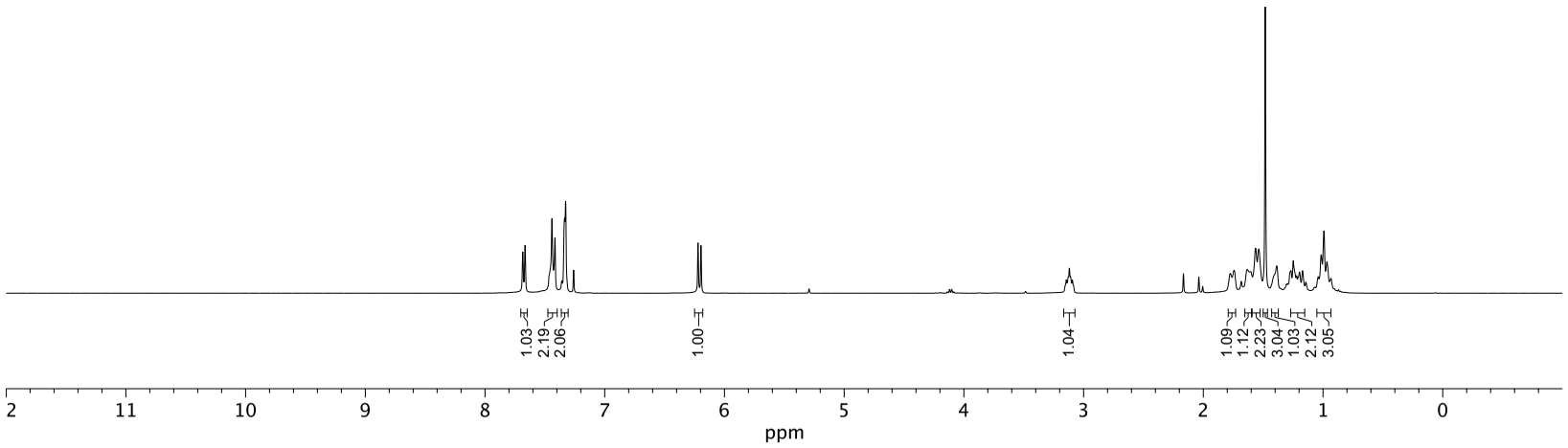
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3e**.



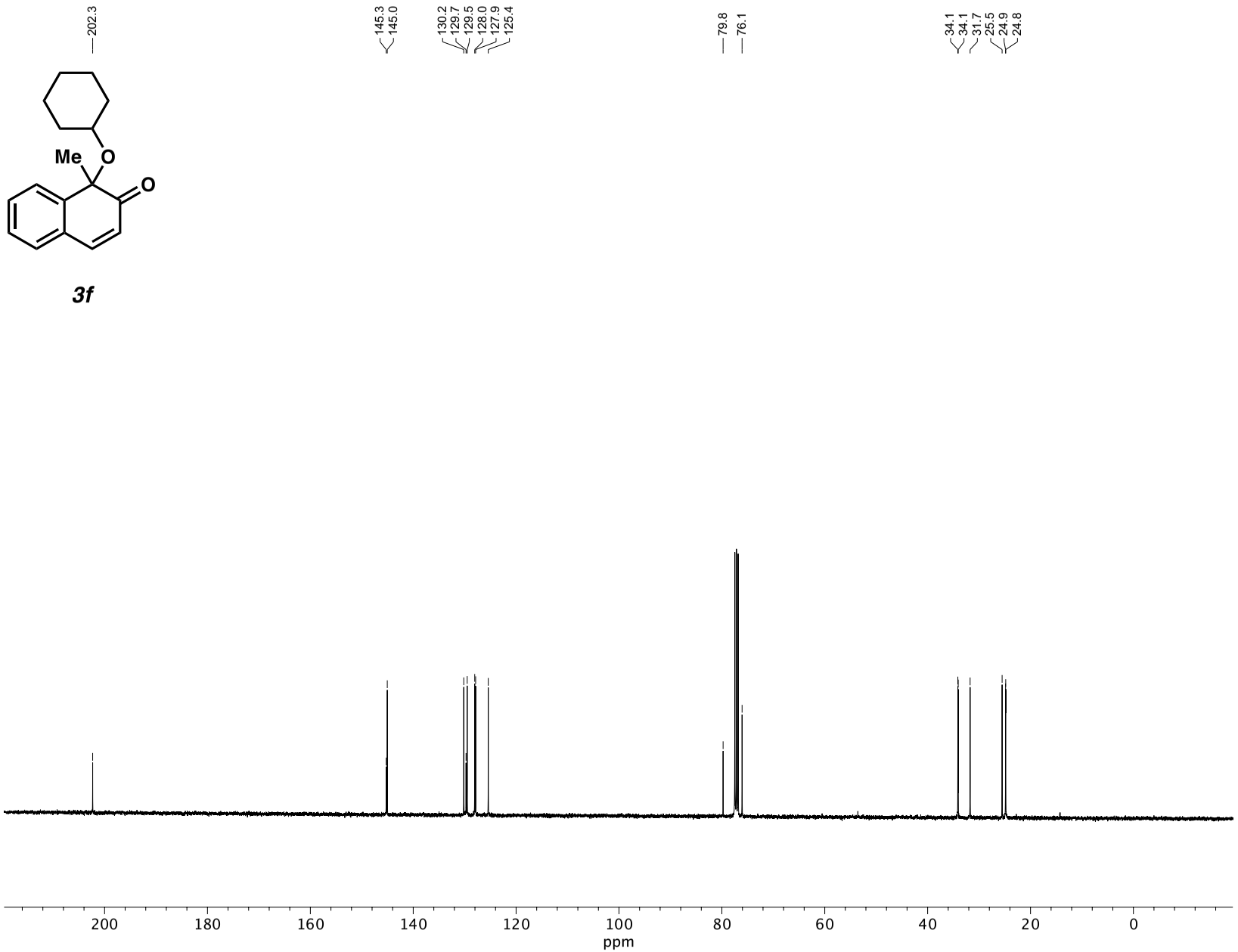
^{13}C NMR (101 MHz,$CDCl_3$) of compound **3e**.



3f

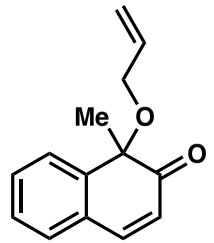


^{1}H NMR (400 MHz, $CDCl_3$) of compound **3f**.

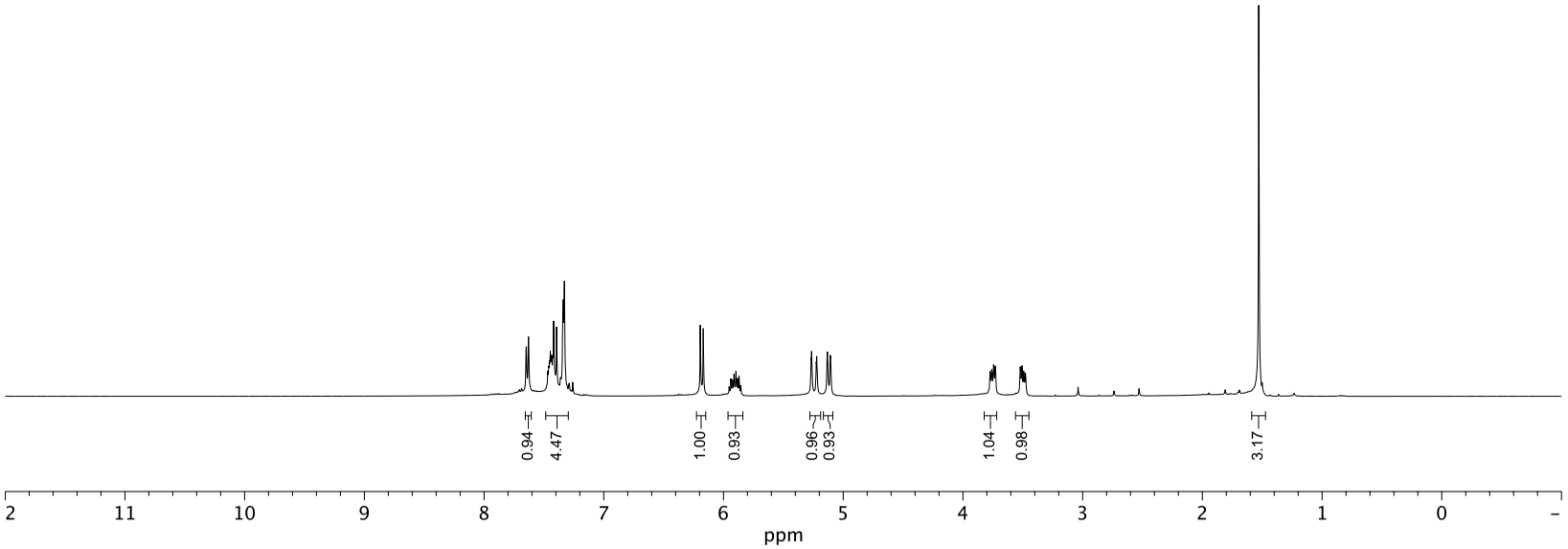


3f

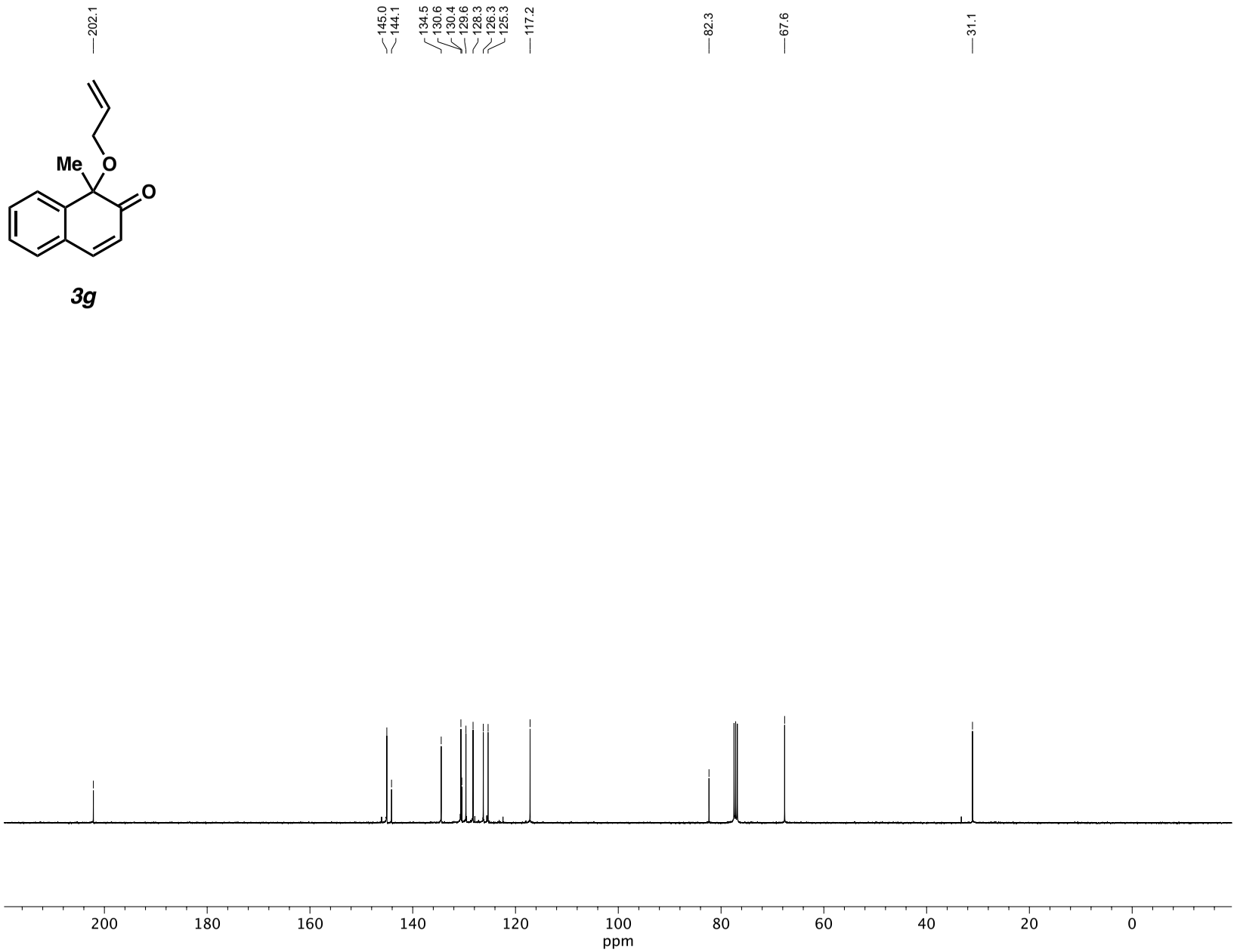
^{13}C NMR (101 MHz,$CDCl_3$) of compound **3f**.



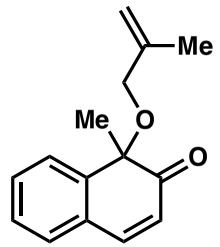
3g



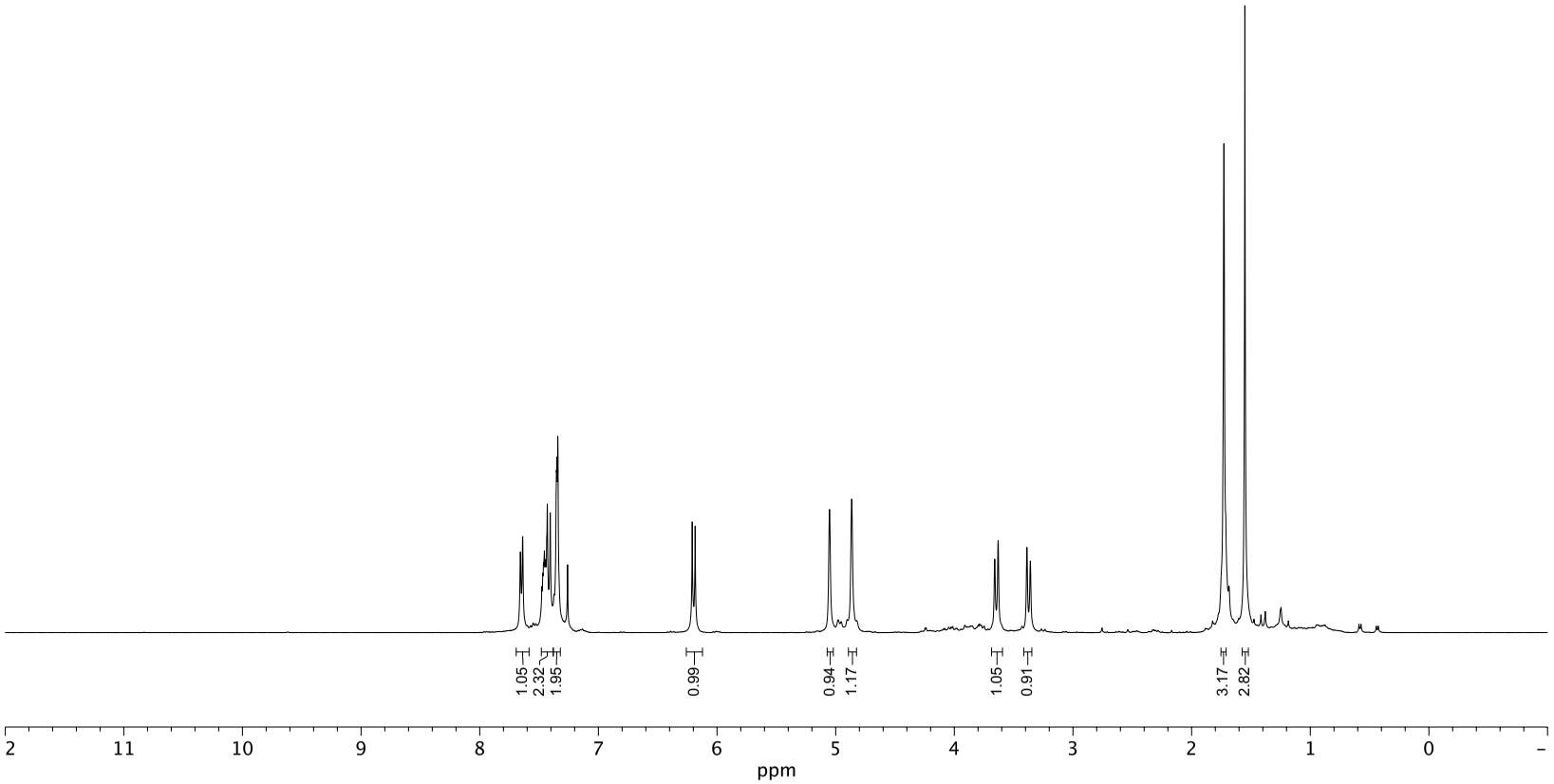
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3g**.



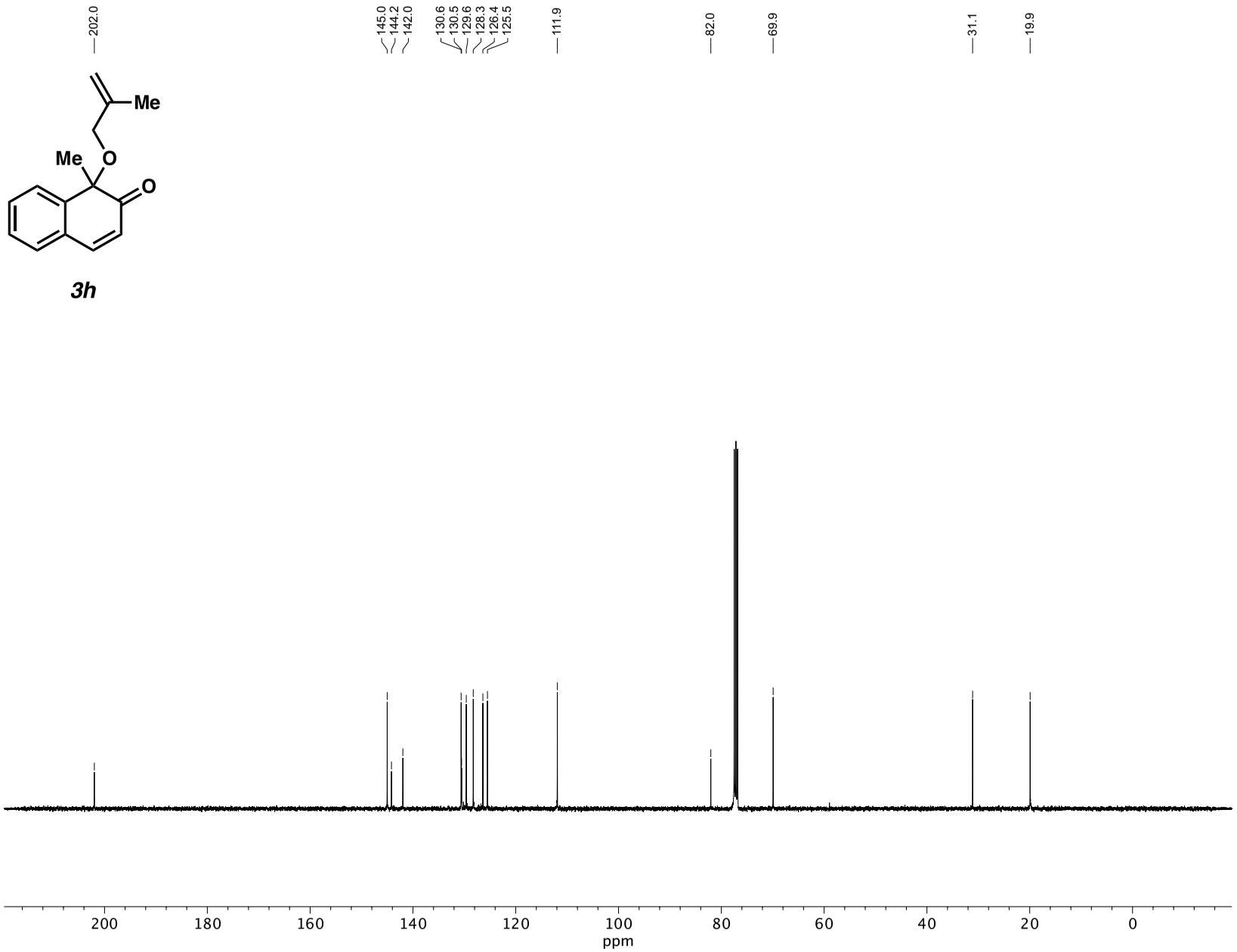
^{13}C NMR (101 MHz,$CDCl_3$) of compound **3g**.



3h

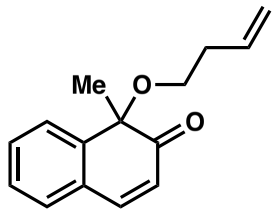


^{1}H NMR (400 MHz, $CDCl_3$) of compound **3h**.

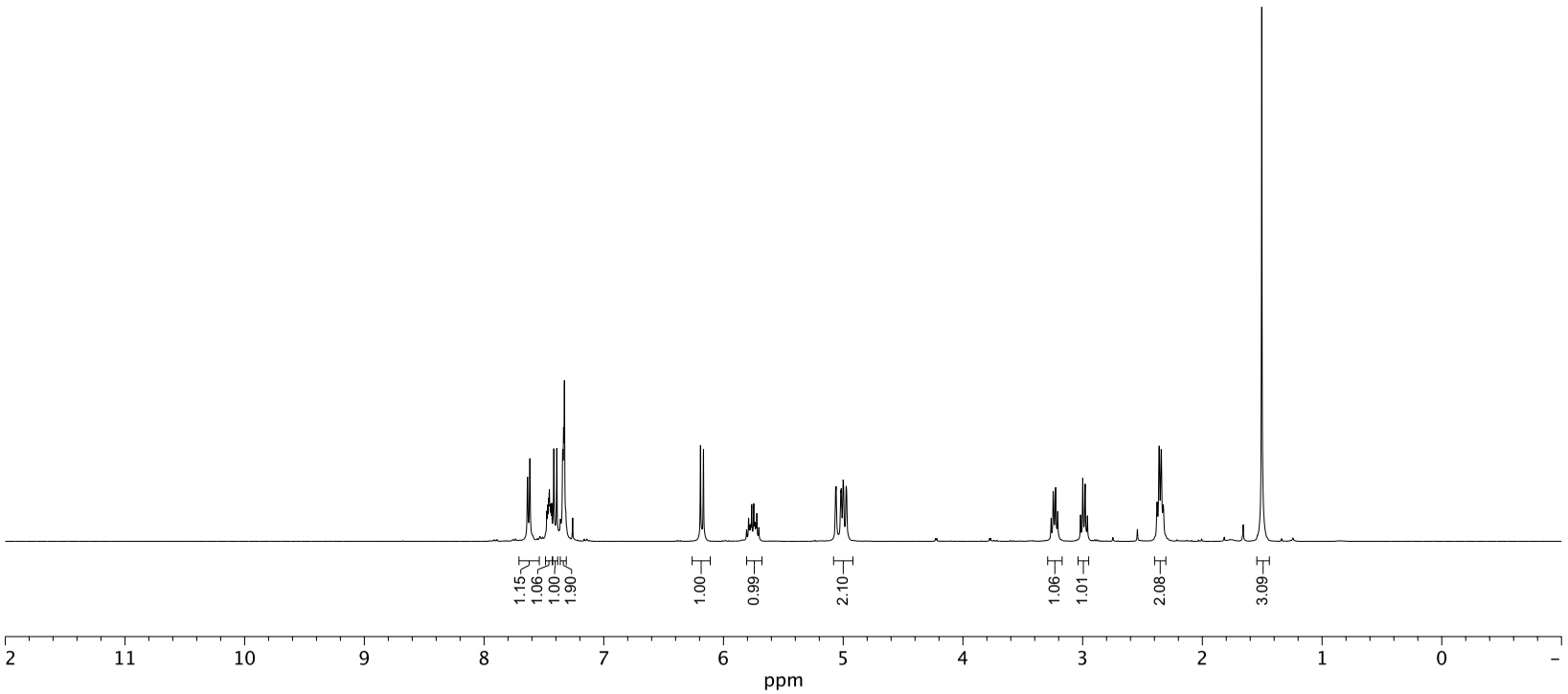


3h

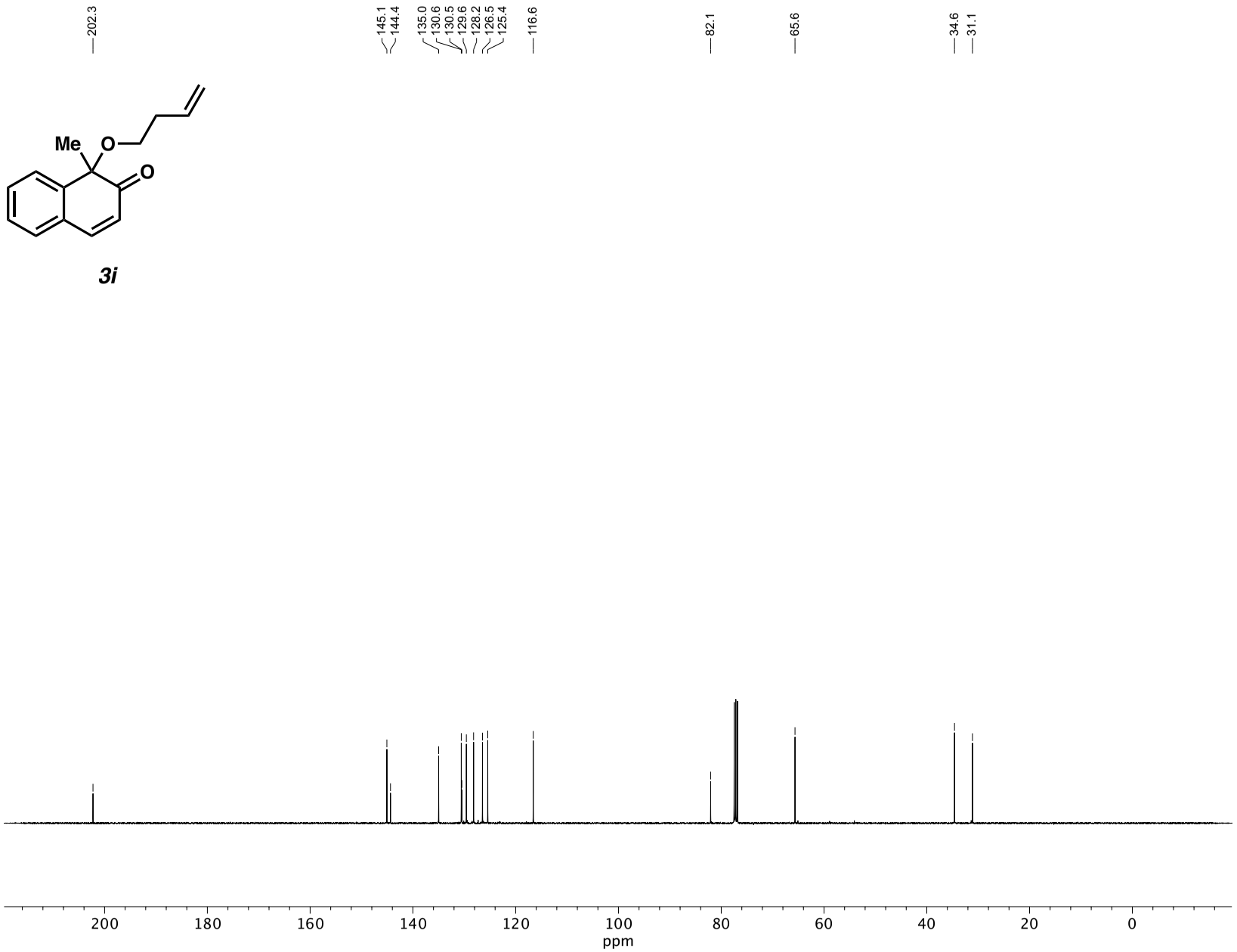
^{13}C NMR (101 MHz,$CDCl_3$) of compound **3h**.



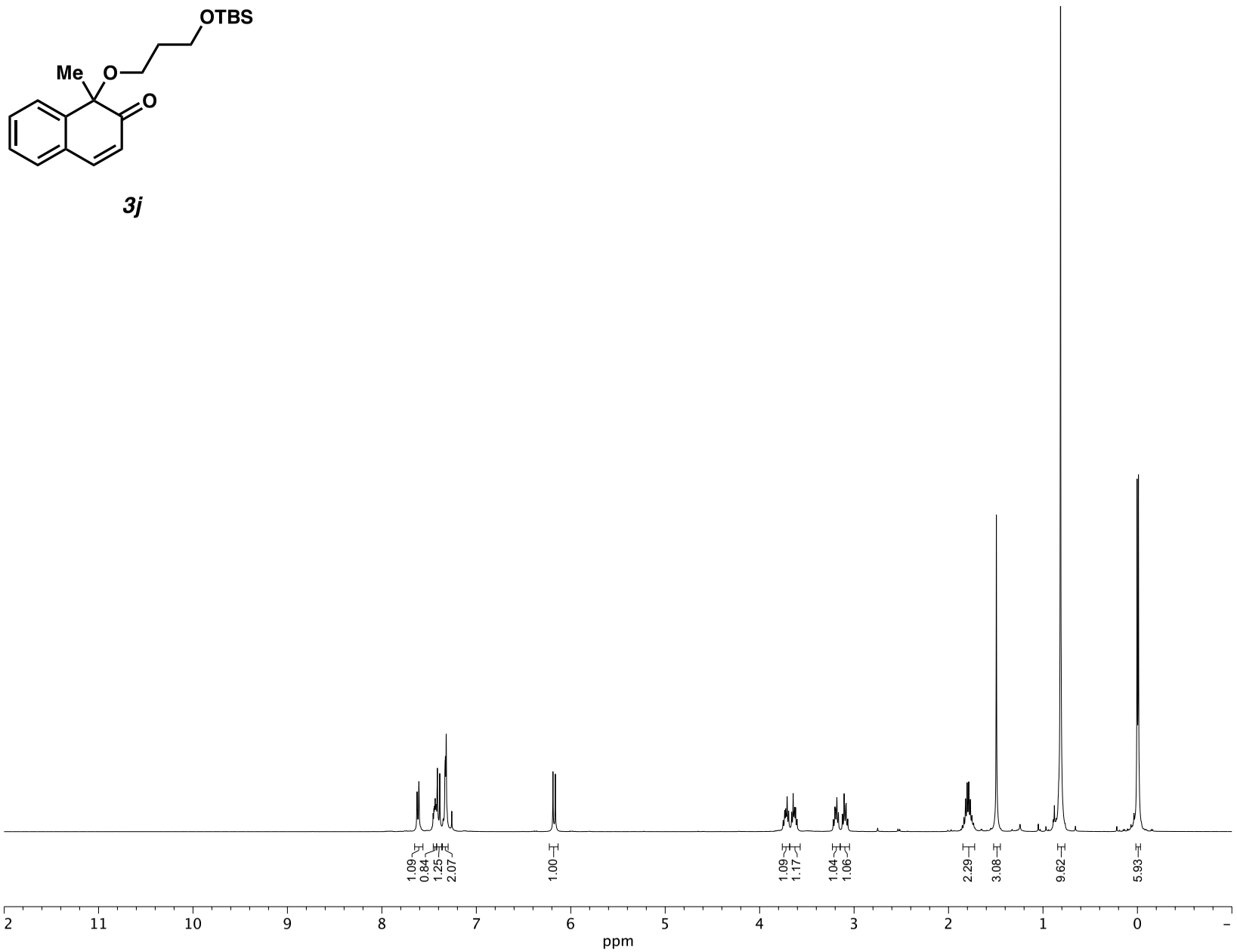
3i



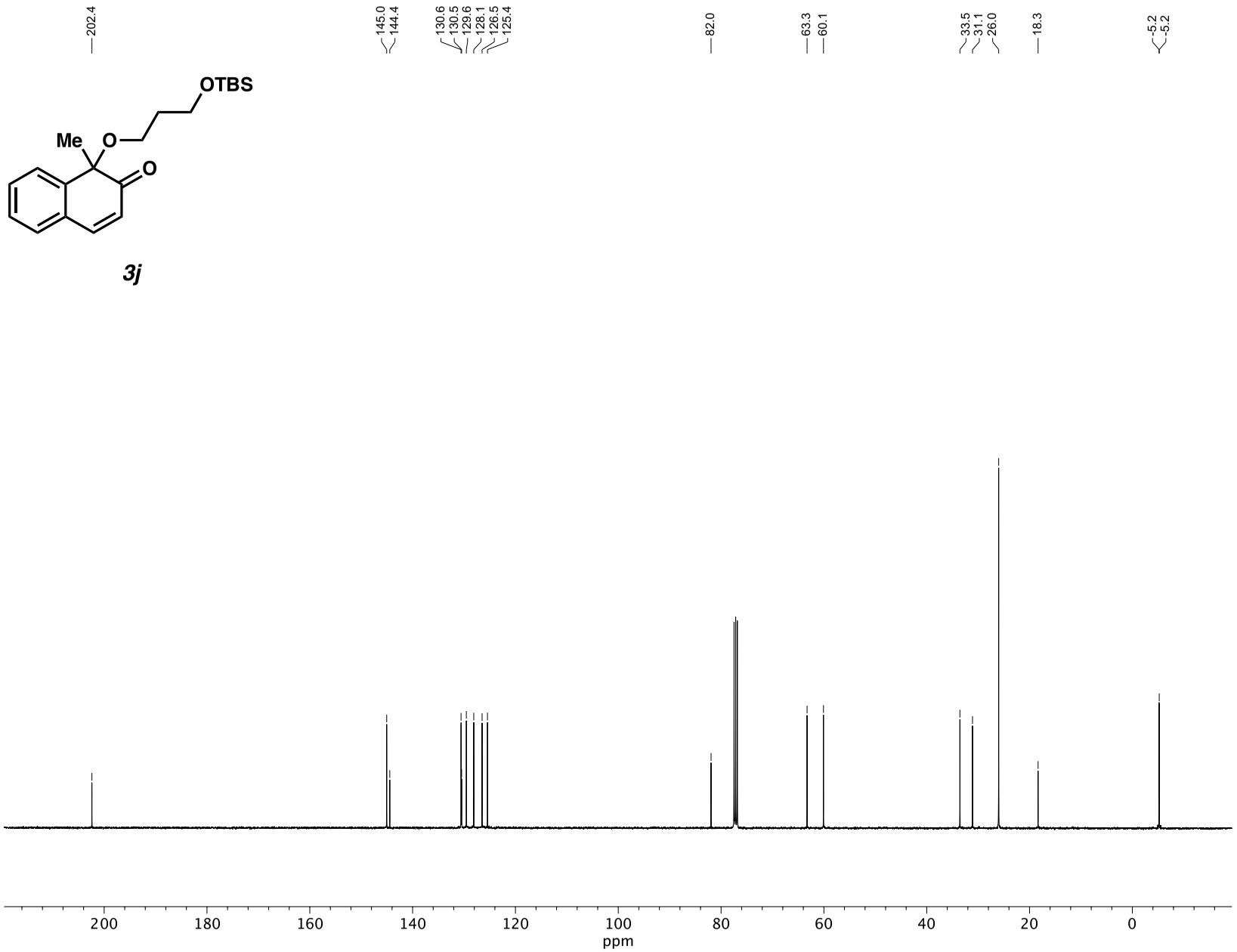
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3i**.



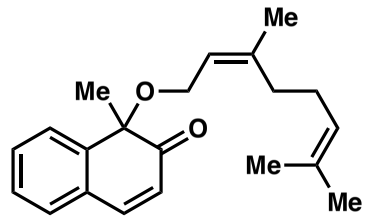
^{13}C NMR (101 MHz,$CDCl_3$) of compound **3i**.



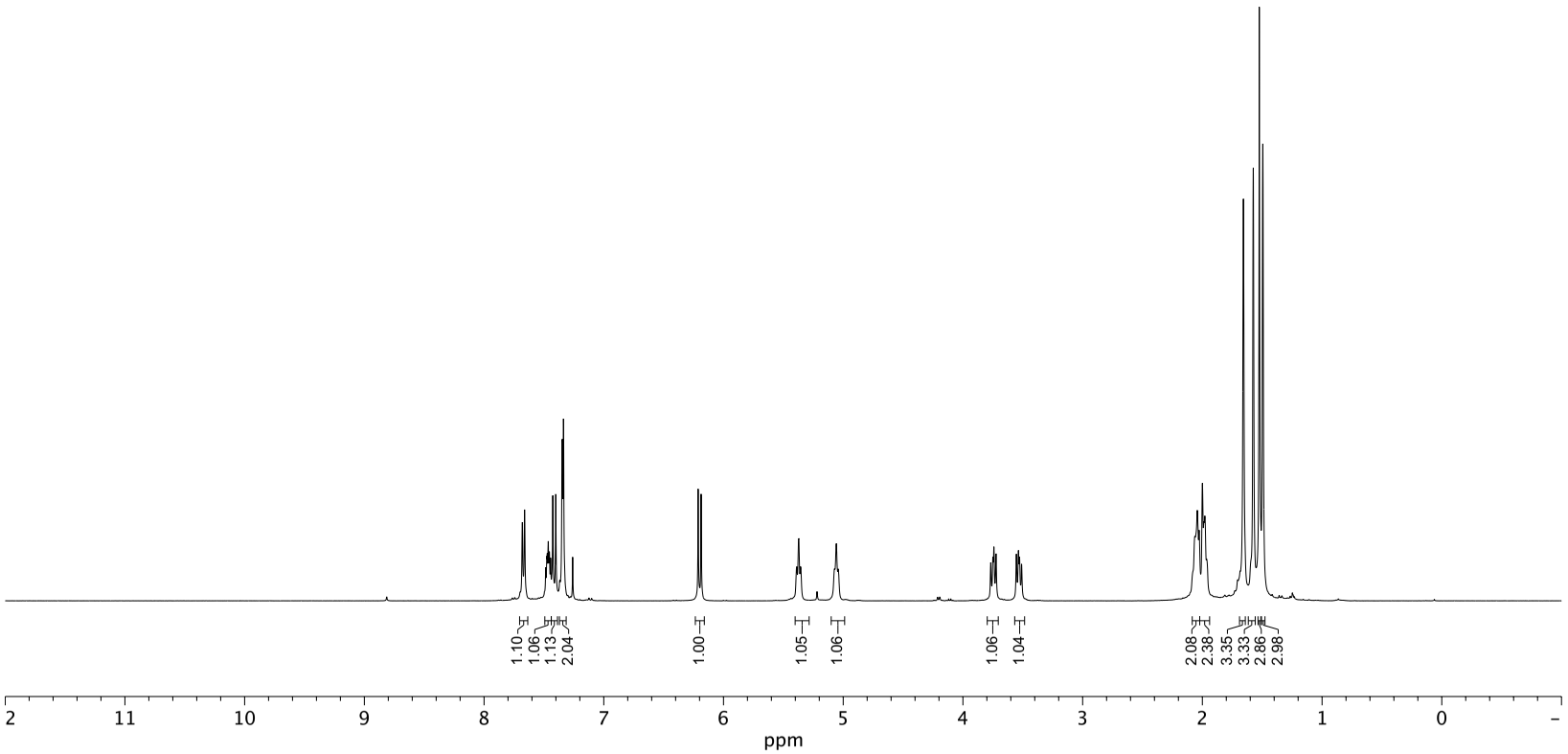
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3j**.



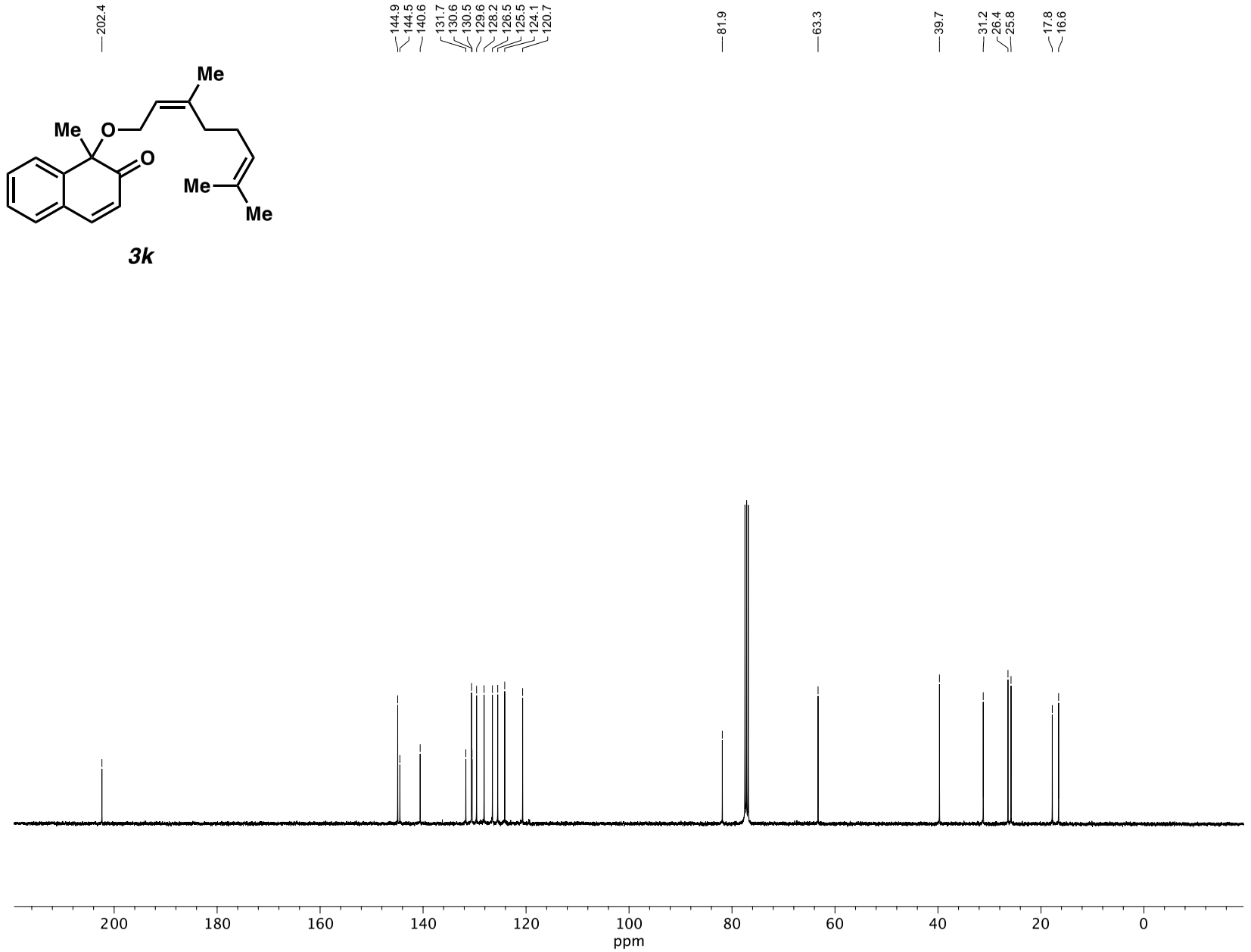
^{13}C NMR (101 MHz,$CDCl_3$) of compound **3j**.



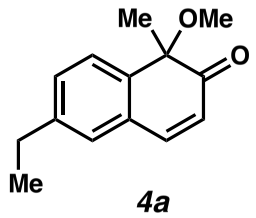
3k



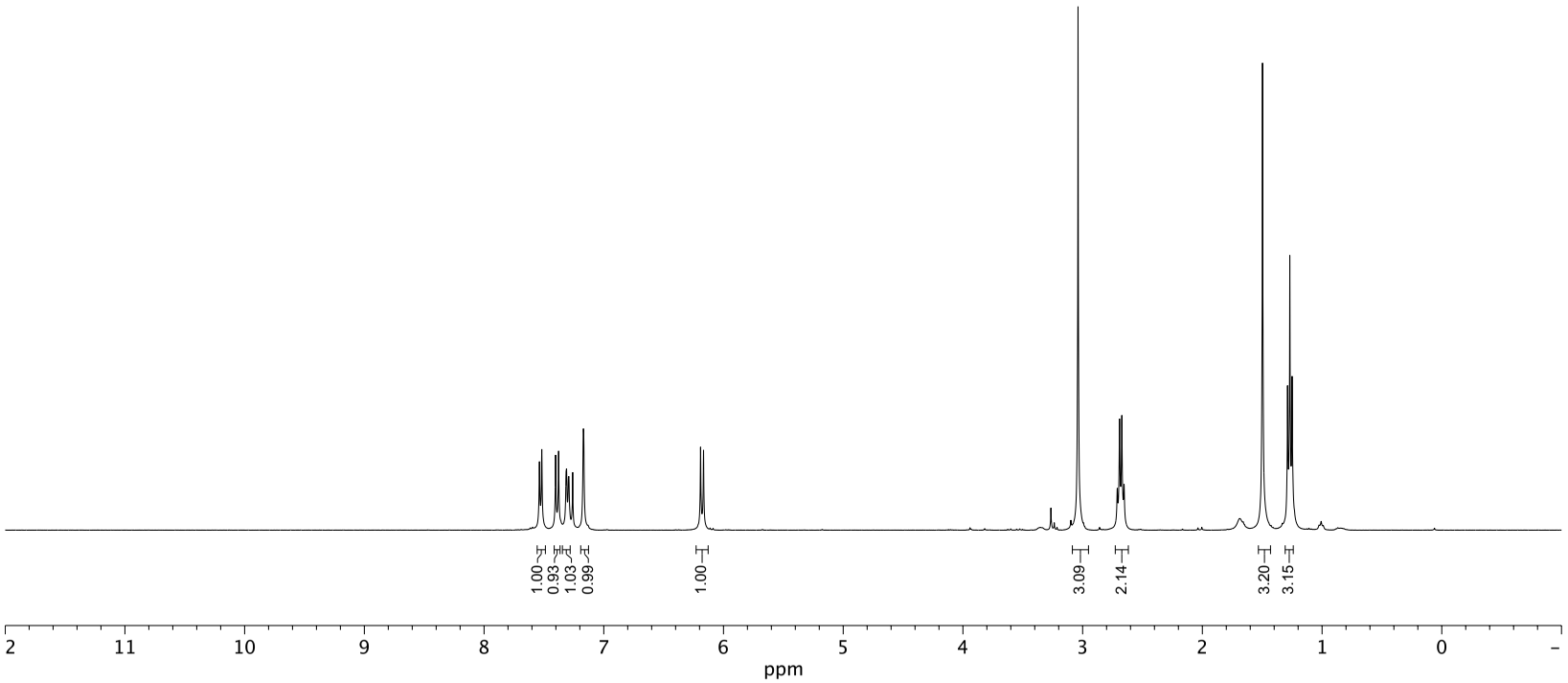
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3k**.



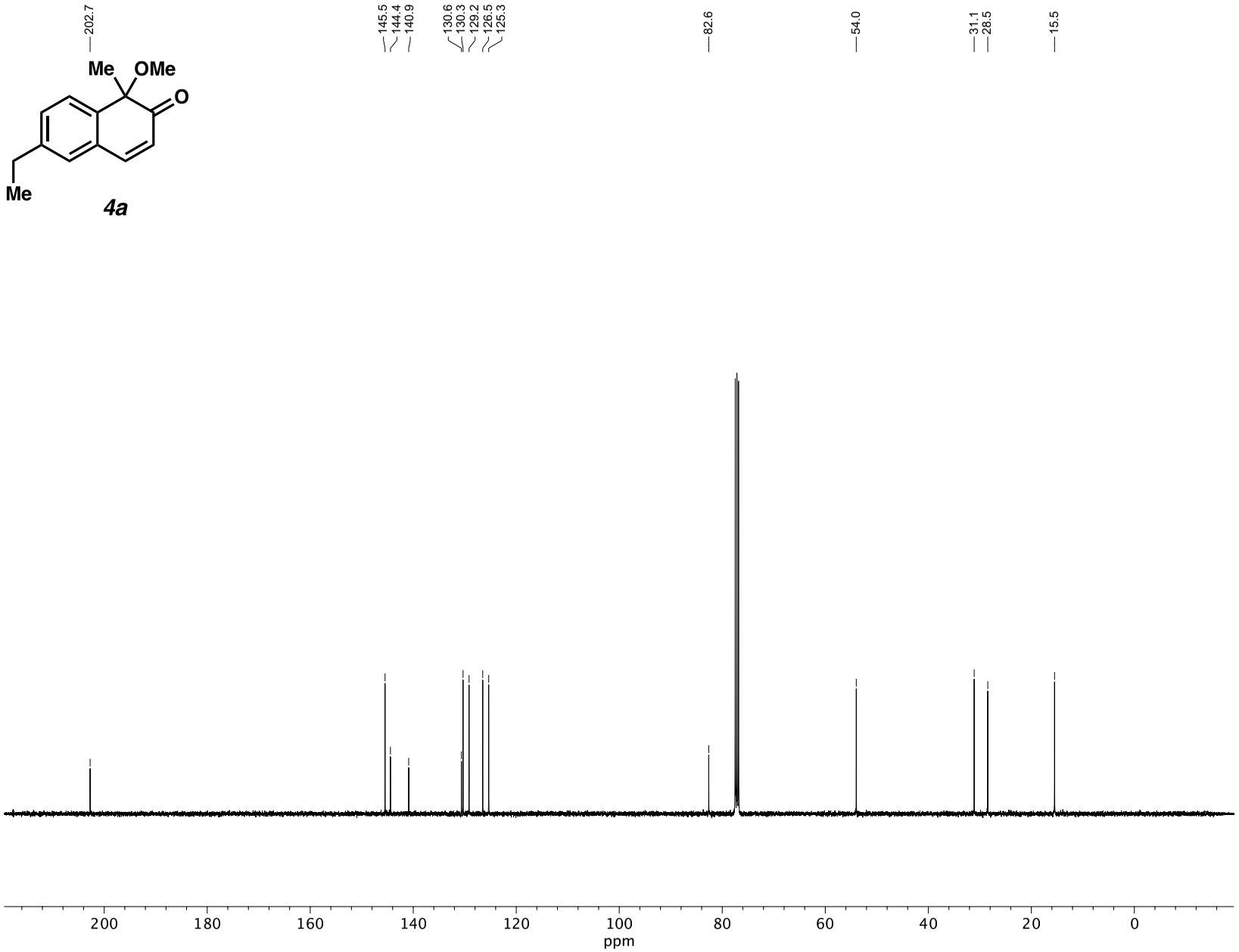
^{13}C NMR (101 MHz,$CDCl_3$) of compound **3k**.



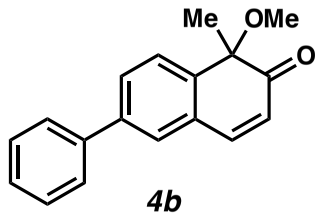
4a



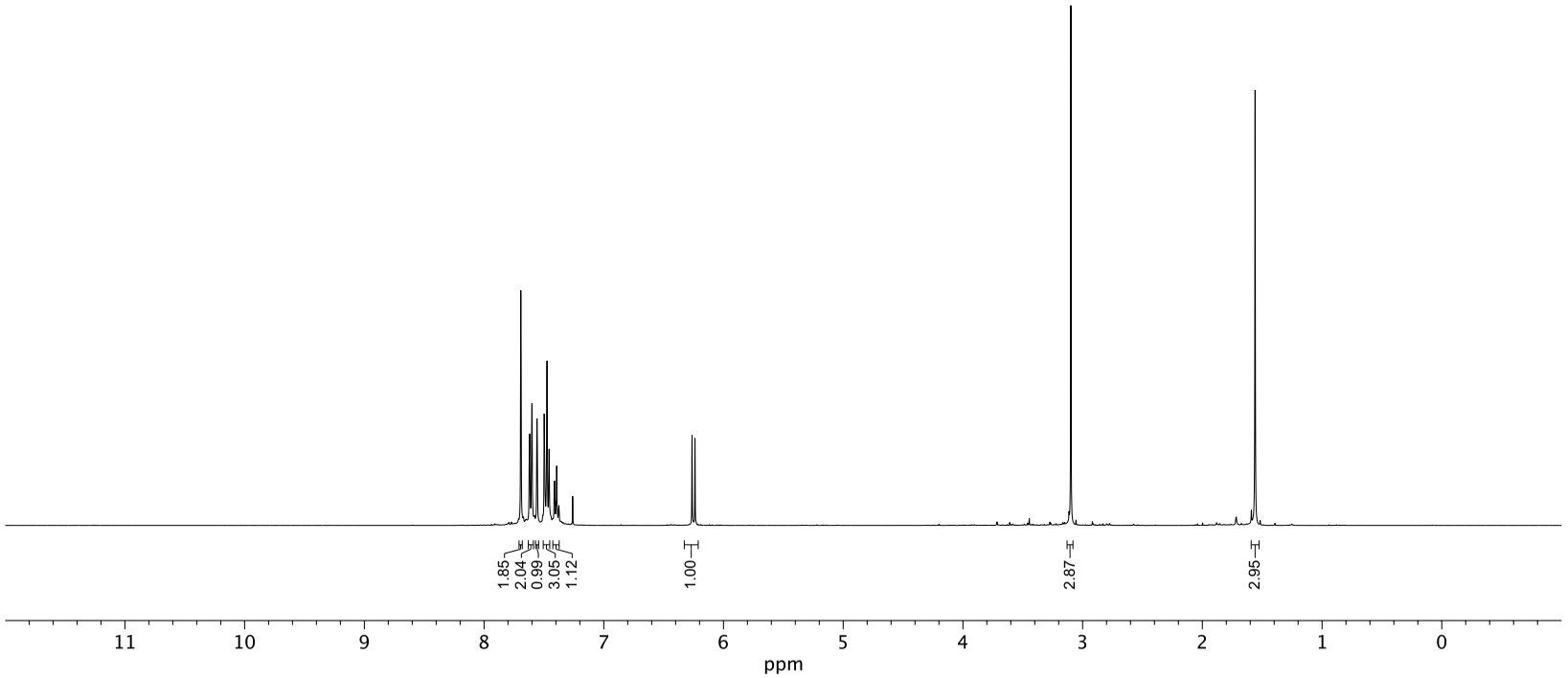
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4a**.



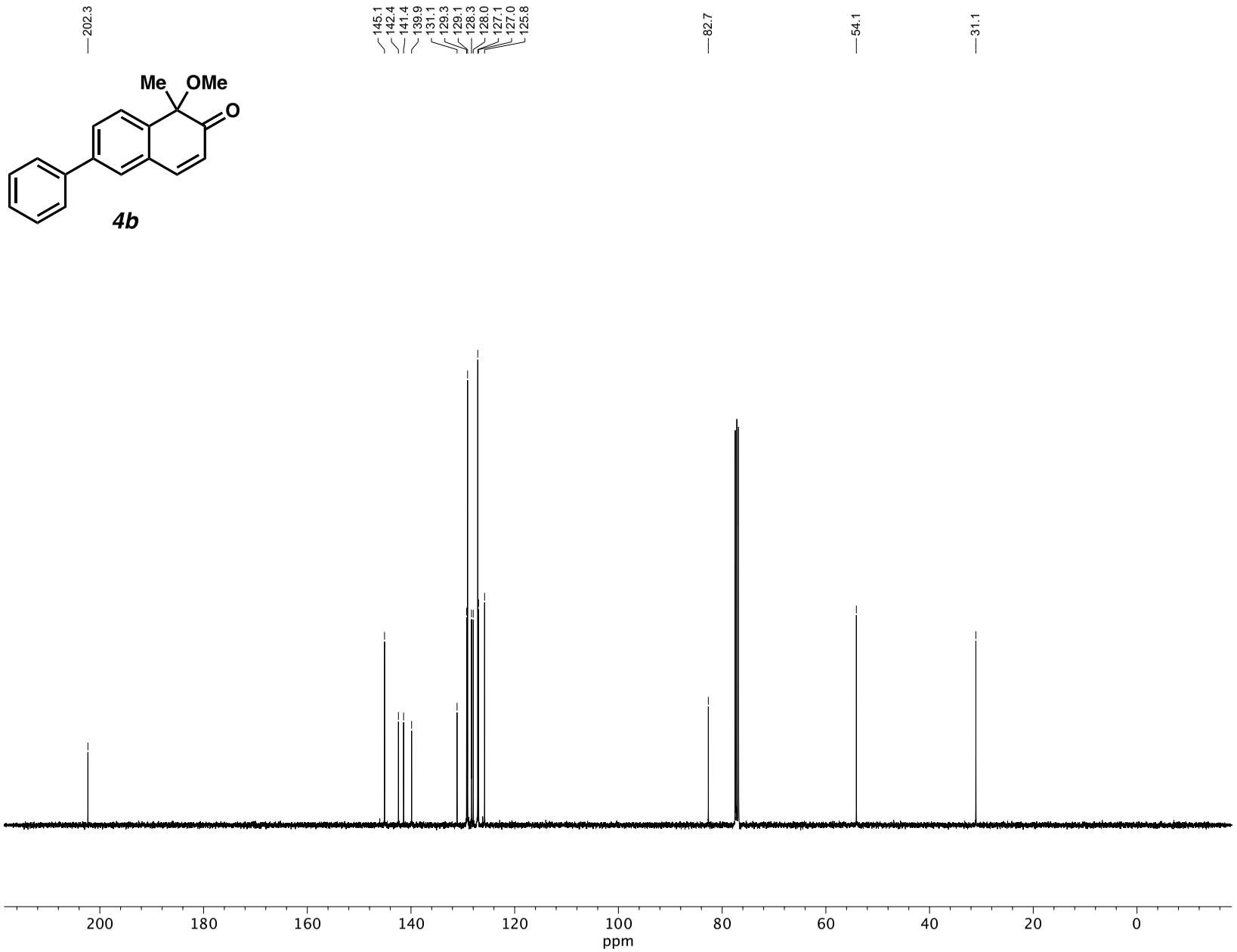
^{13}C NMR (101 MHz,$CDCl_3$) of compound **4a**.



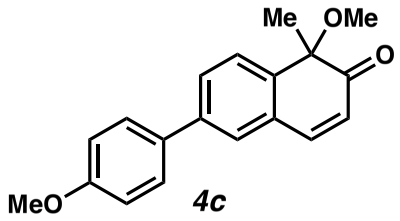
4b



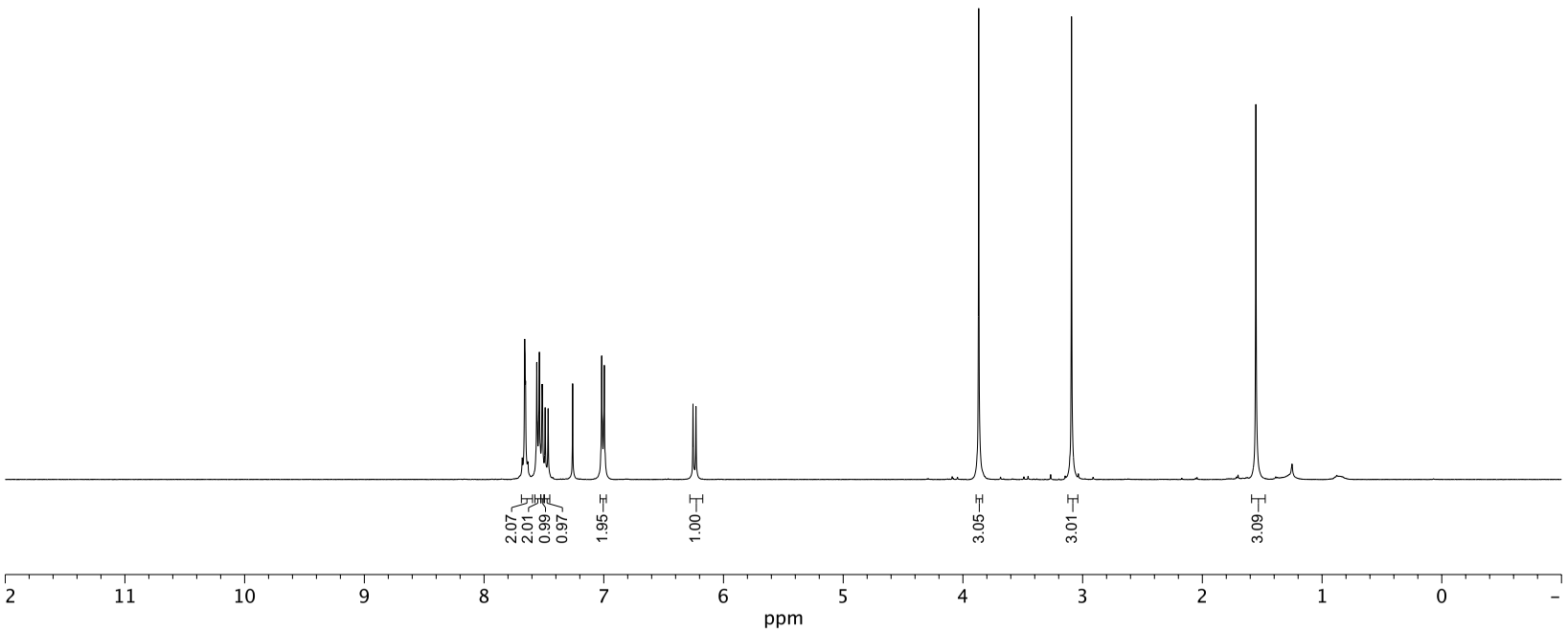
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4b**.



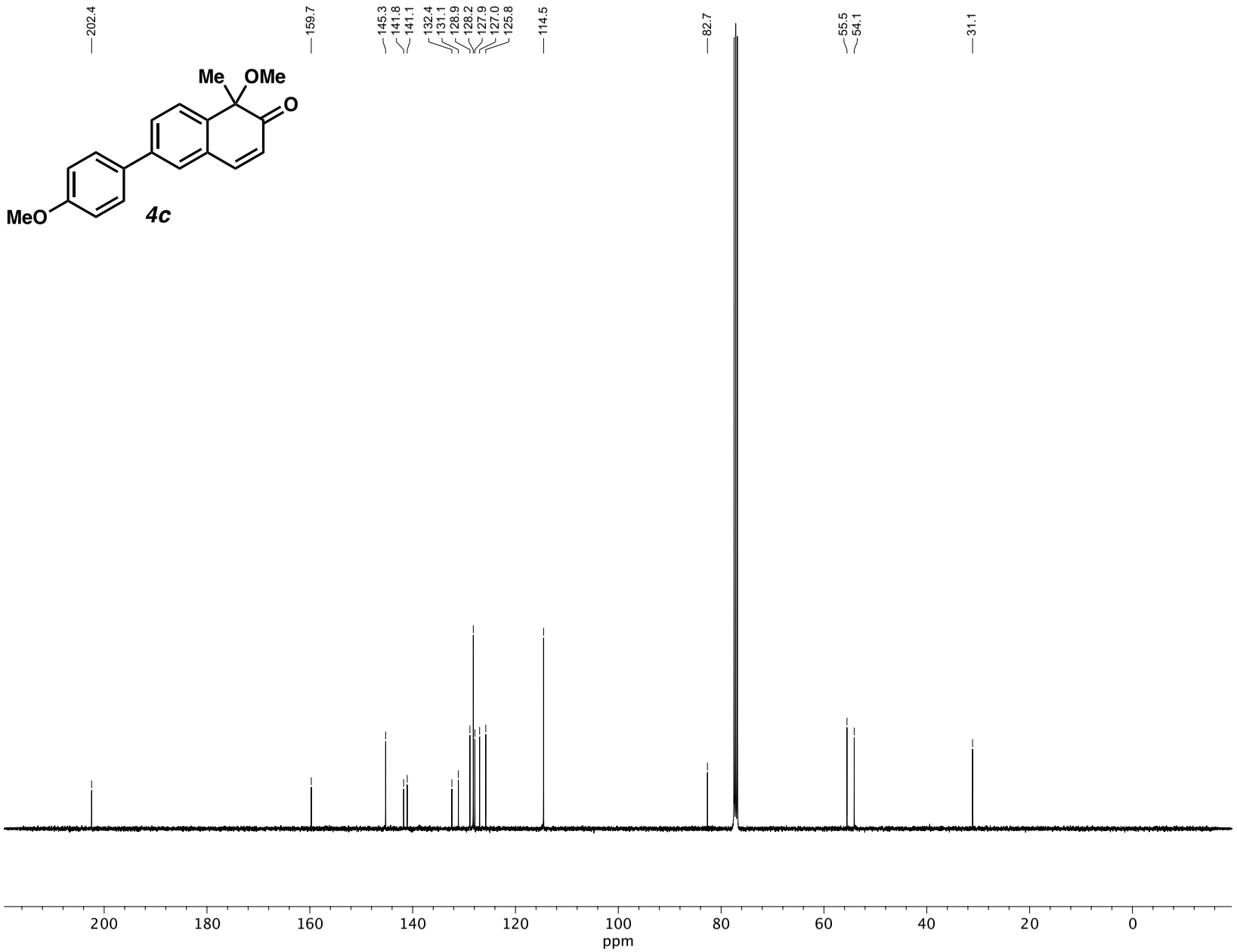
^{13}C NMR (101 MHz,$CDCl_3$) of compound **4b**.



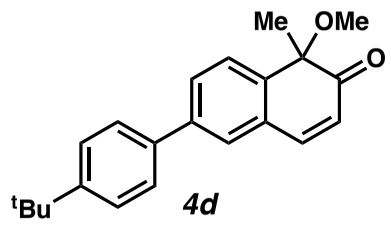
4c



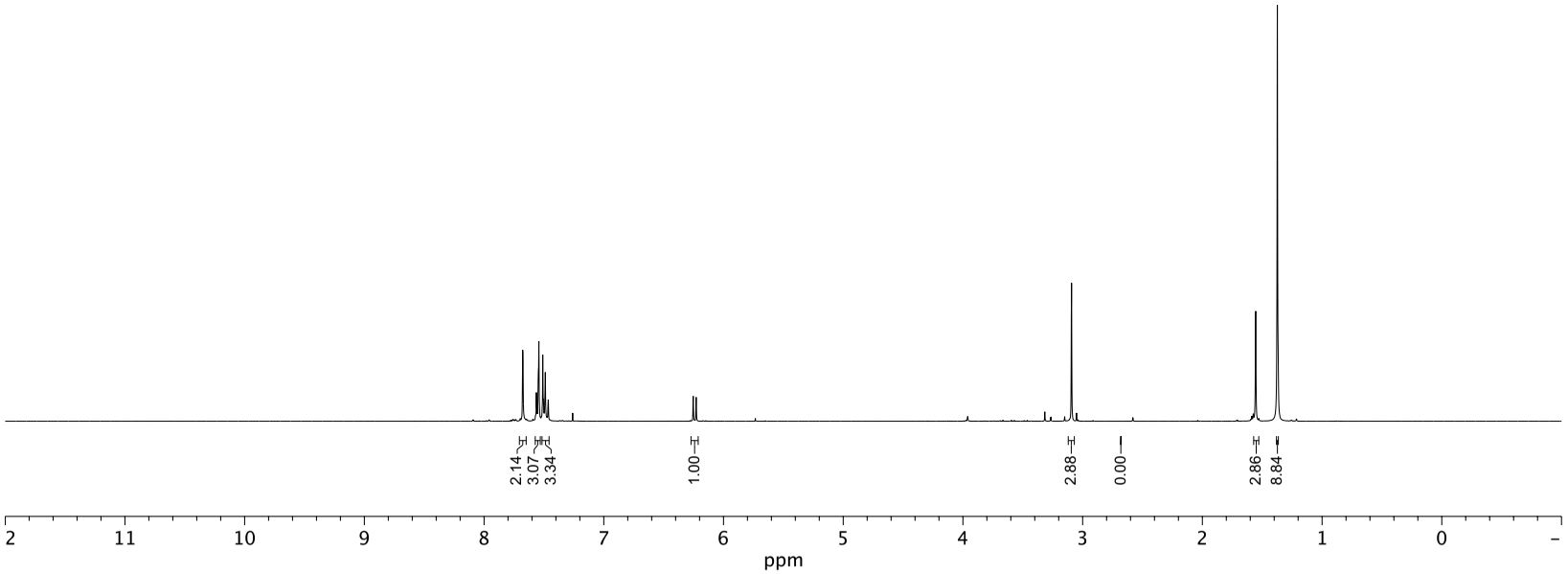
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4c**.



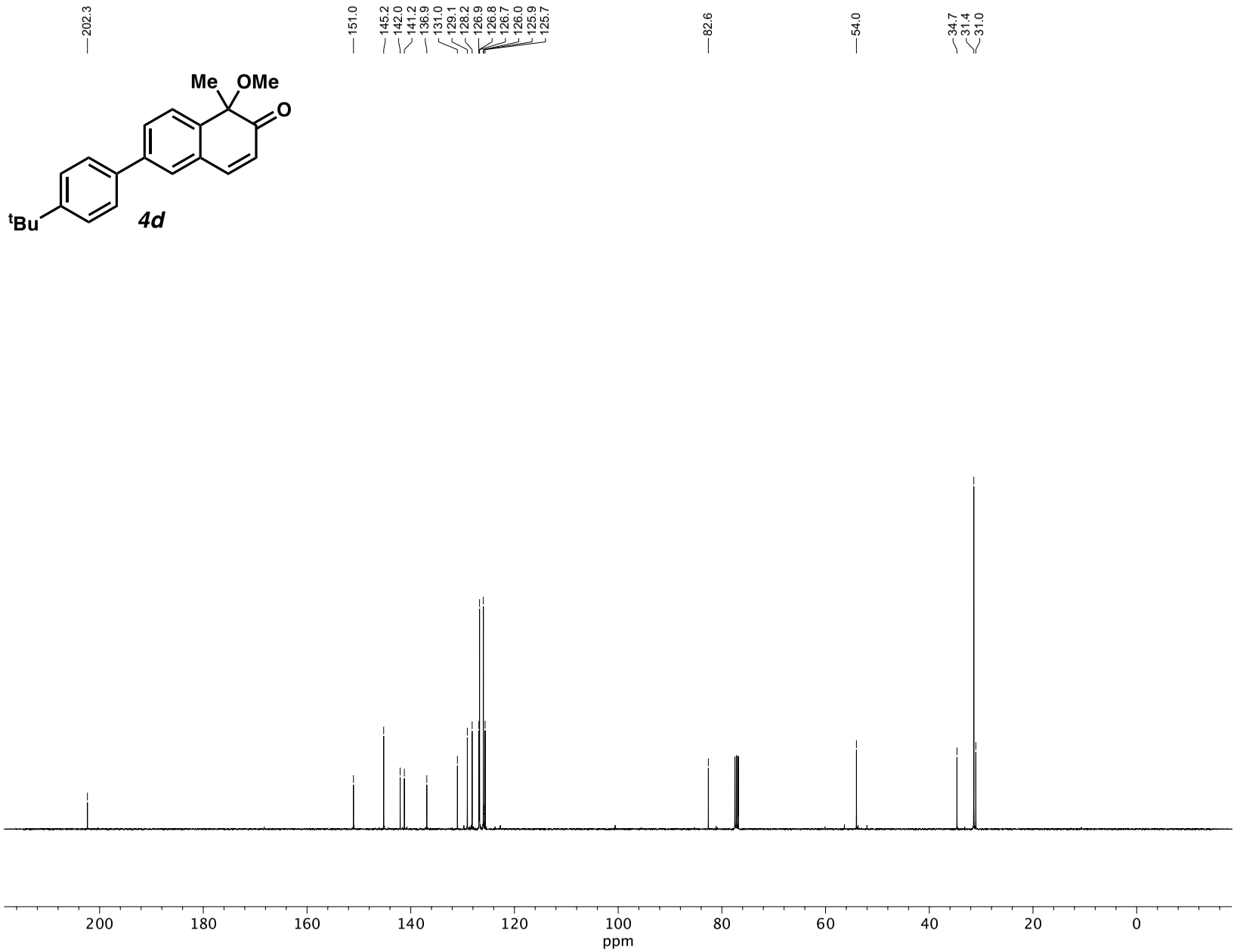
^{13}C NMR (101 MHz,$CDCl_3$) of compound **4c**.



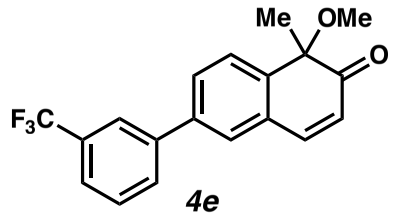
4d



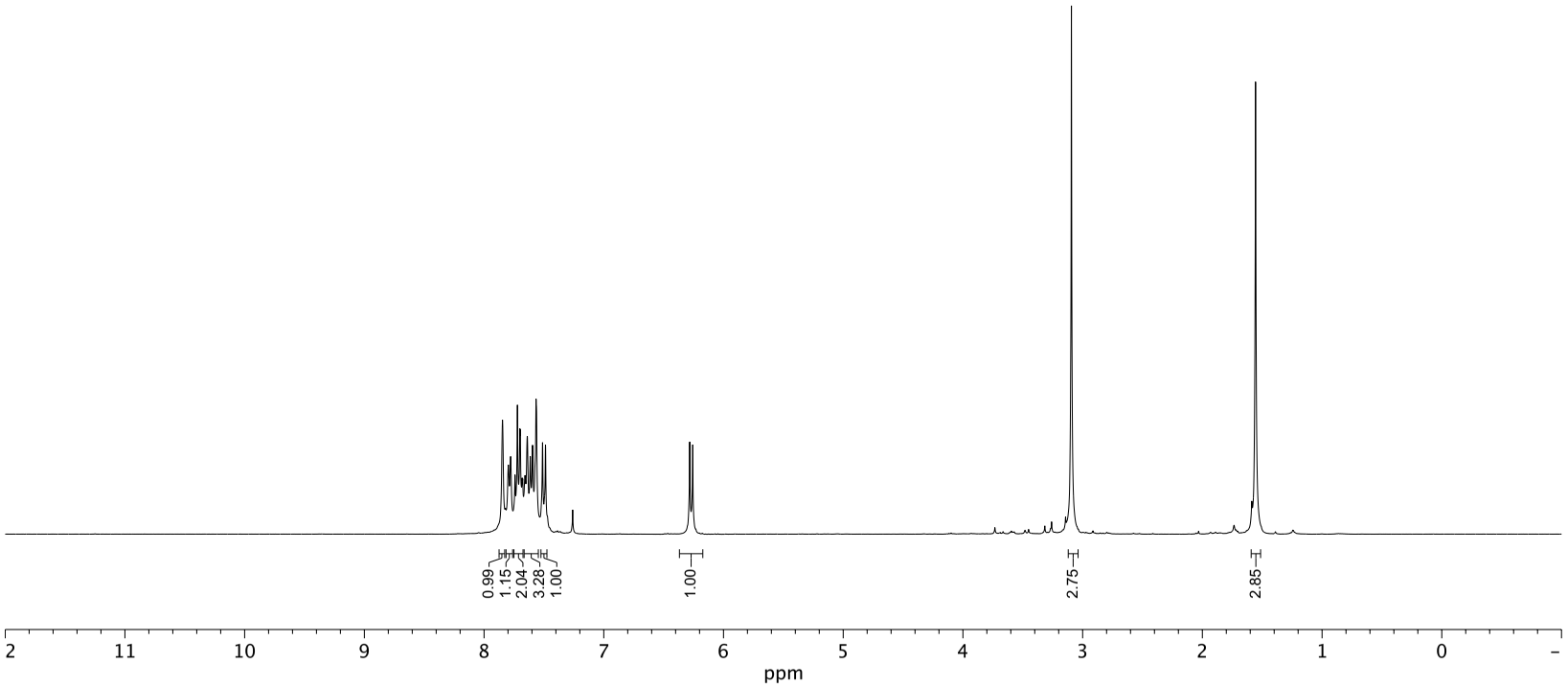
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4d**.



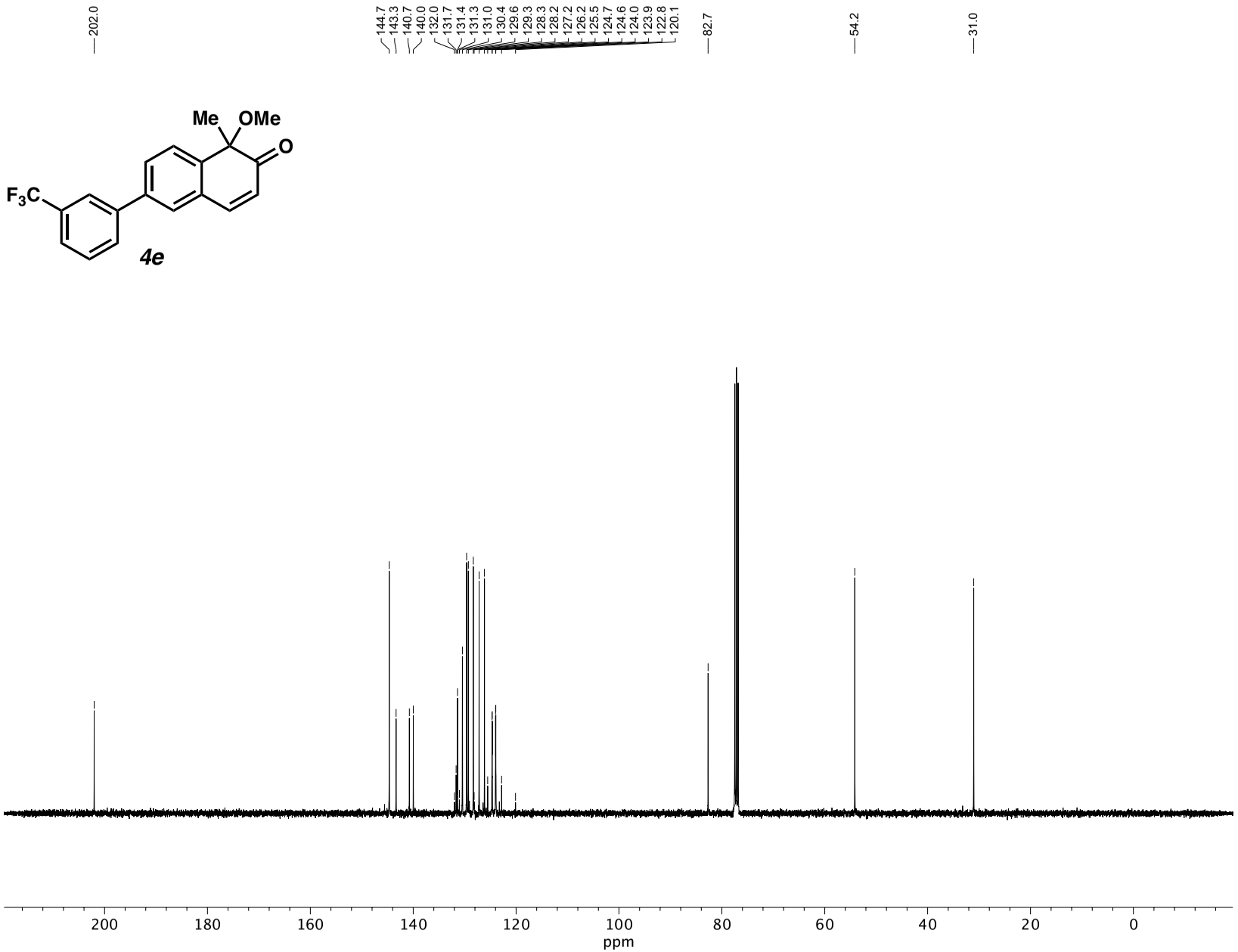
^{13}C NMR (101 MHz,$CDCl_3$) of compound **4d**.



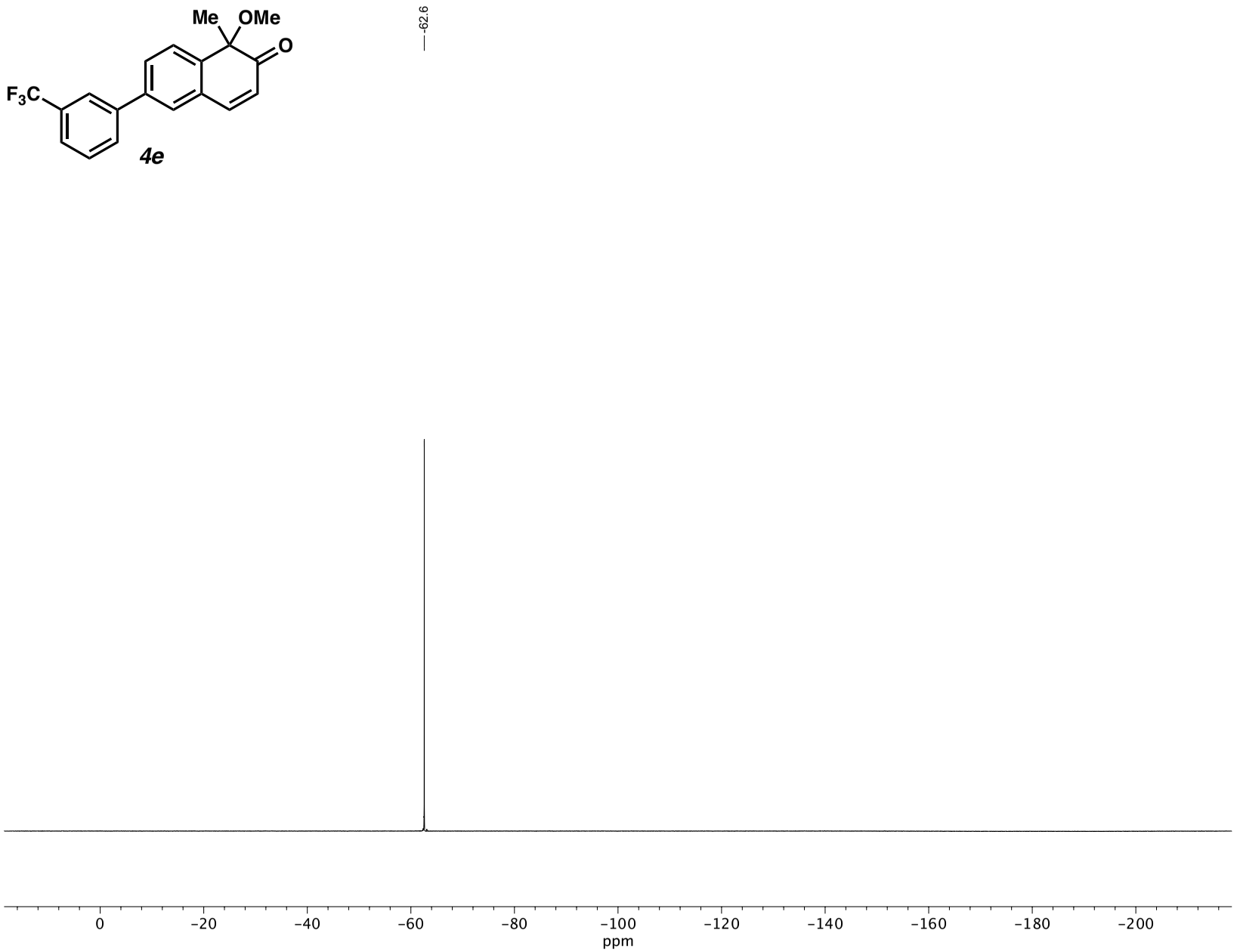
4e



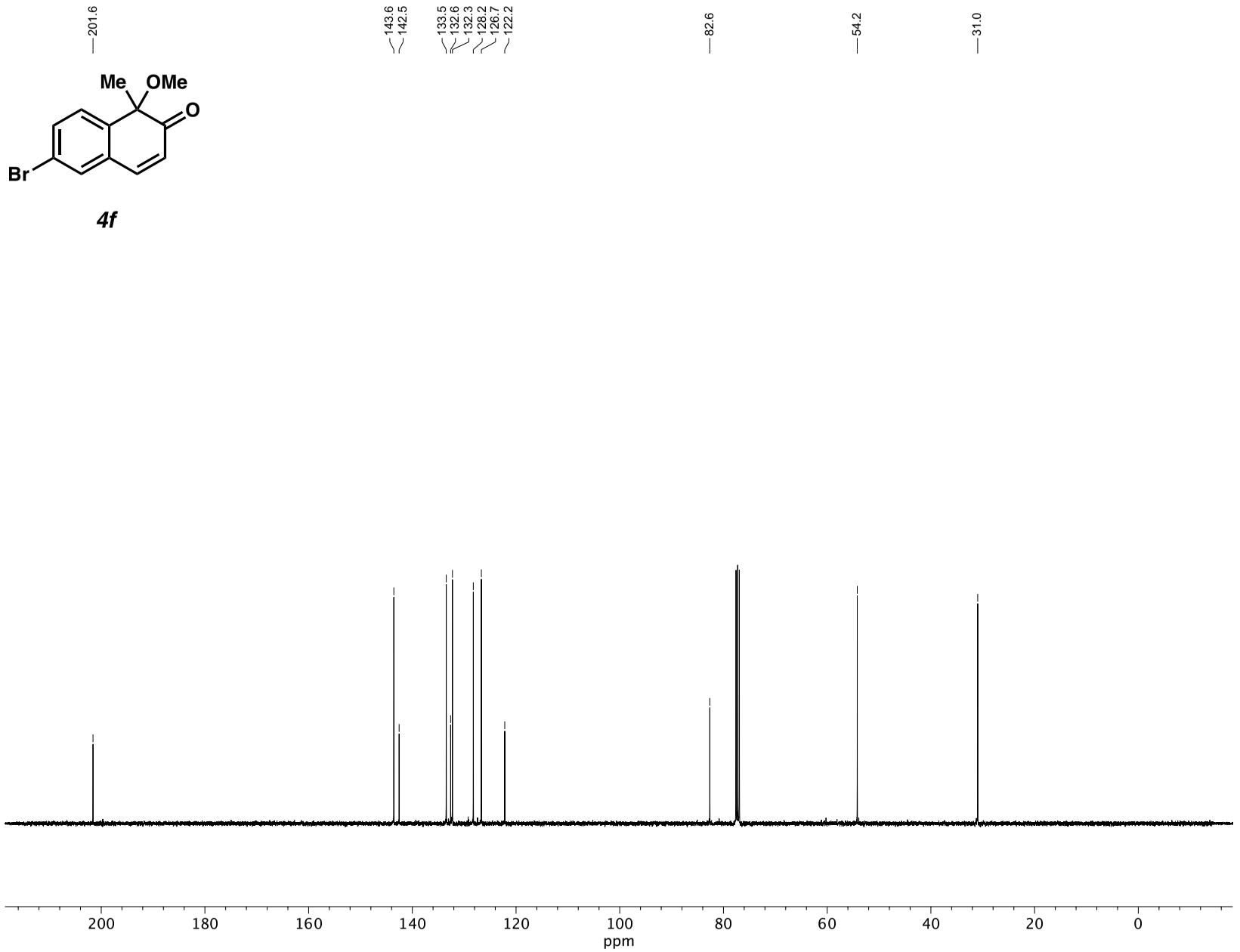
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4e**.



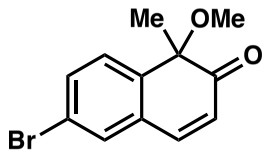
^{13}C NMR (101 MHz,$CDCl_3$) of compound **4e**.



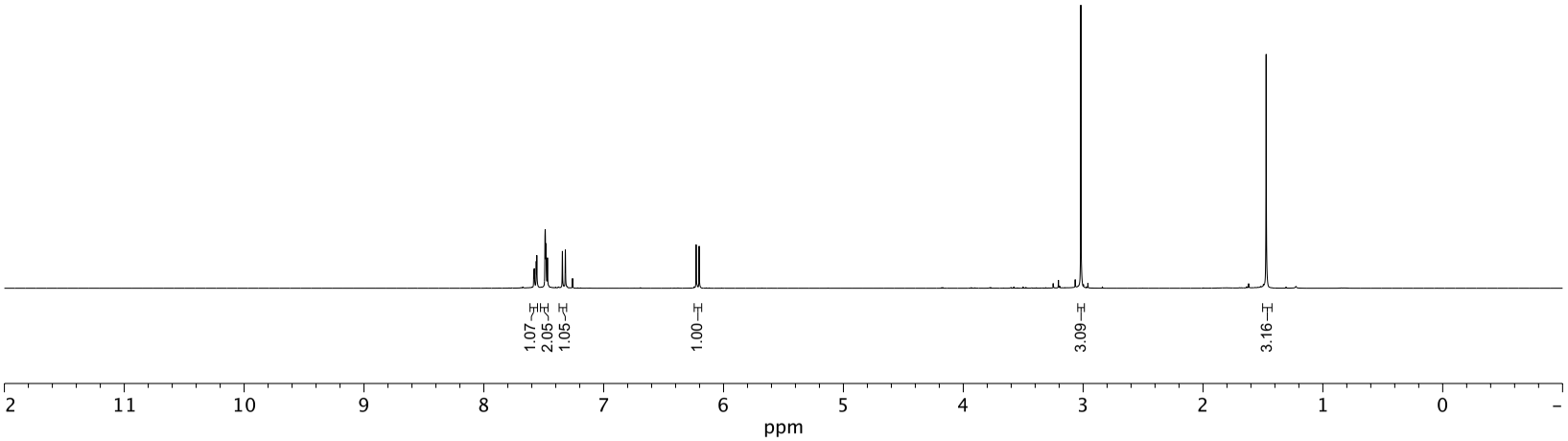
^{19}F NMR (400 MHz, $CDCl_3$) of compound **4e**.



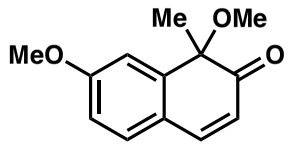
^{13}C NMR (101 MHz,$CDCl_3$) of compound **4f**.



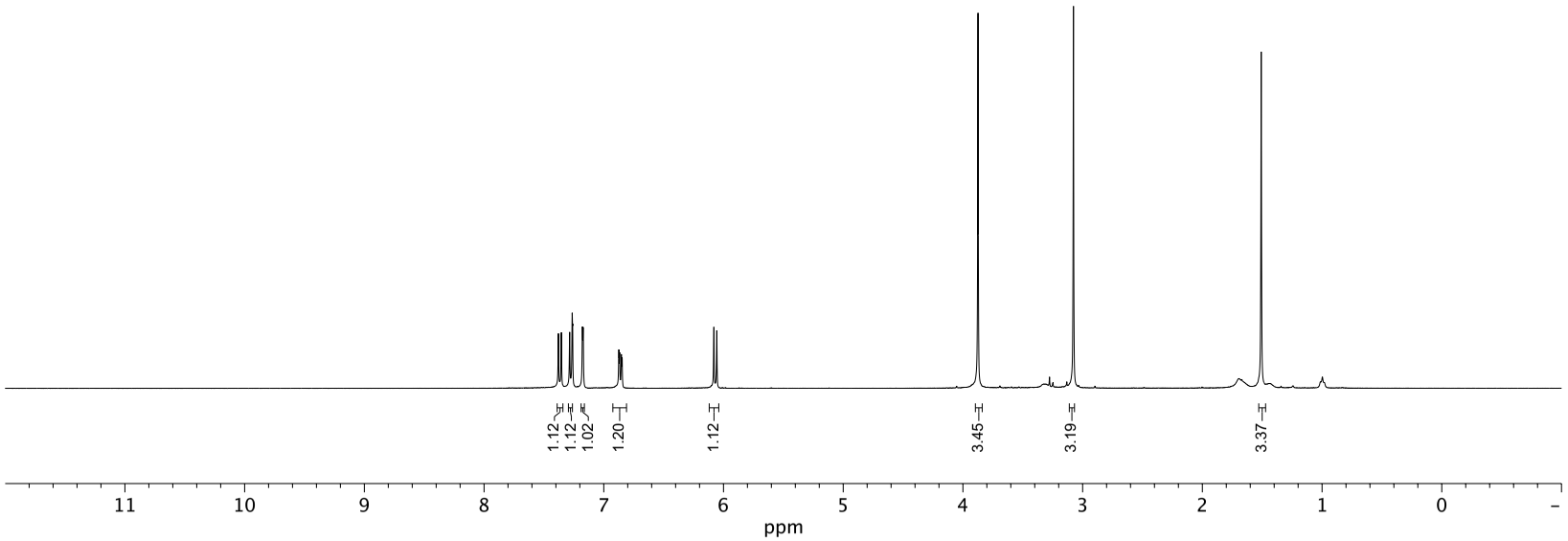
4f



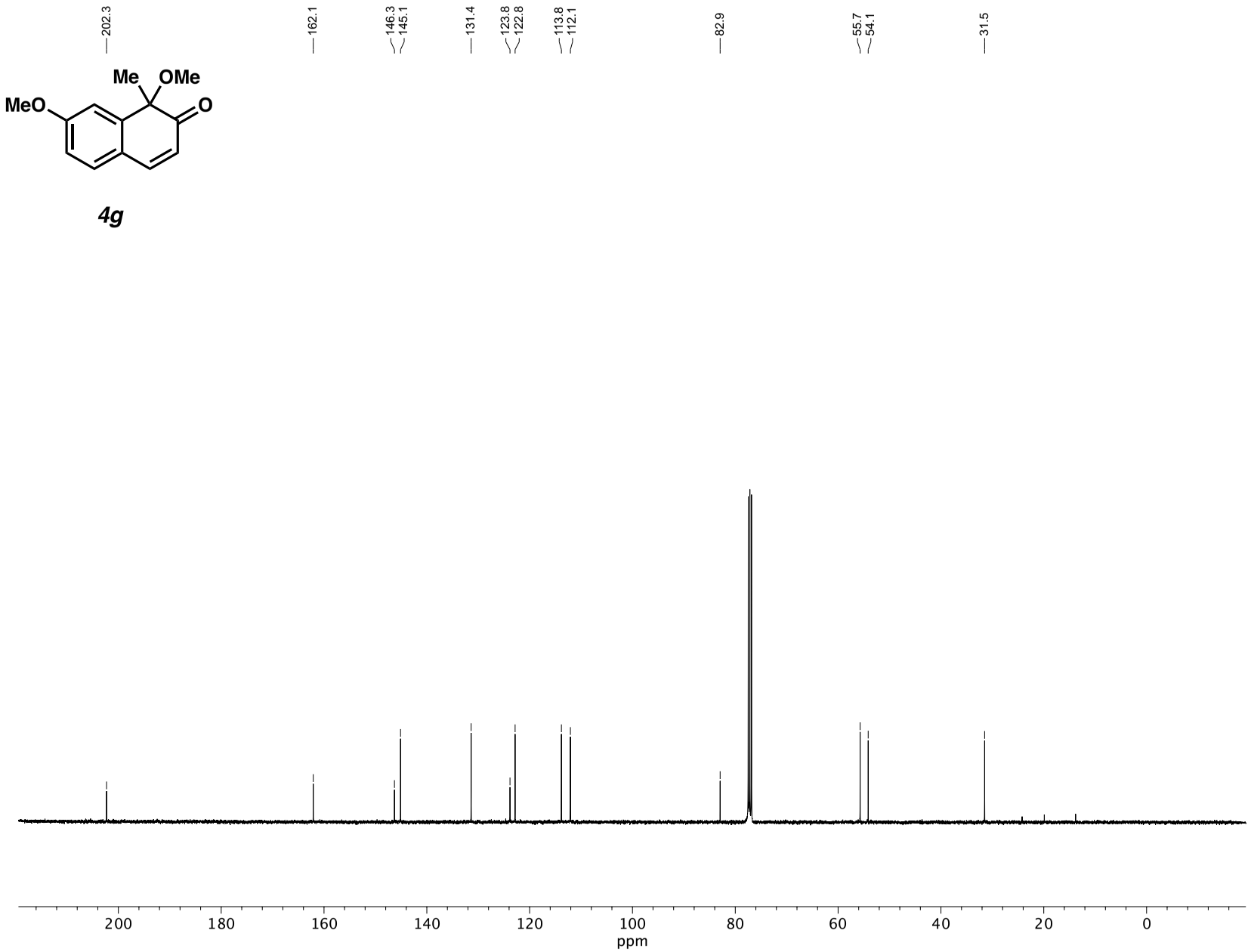
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4f**.



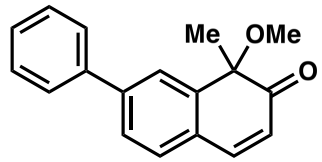
4g



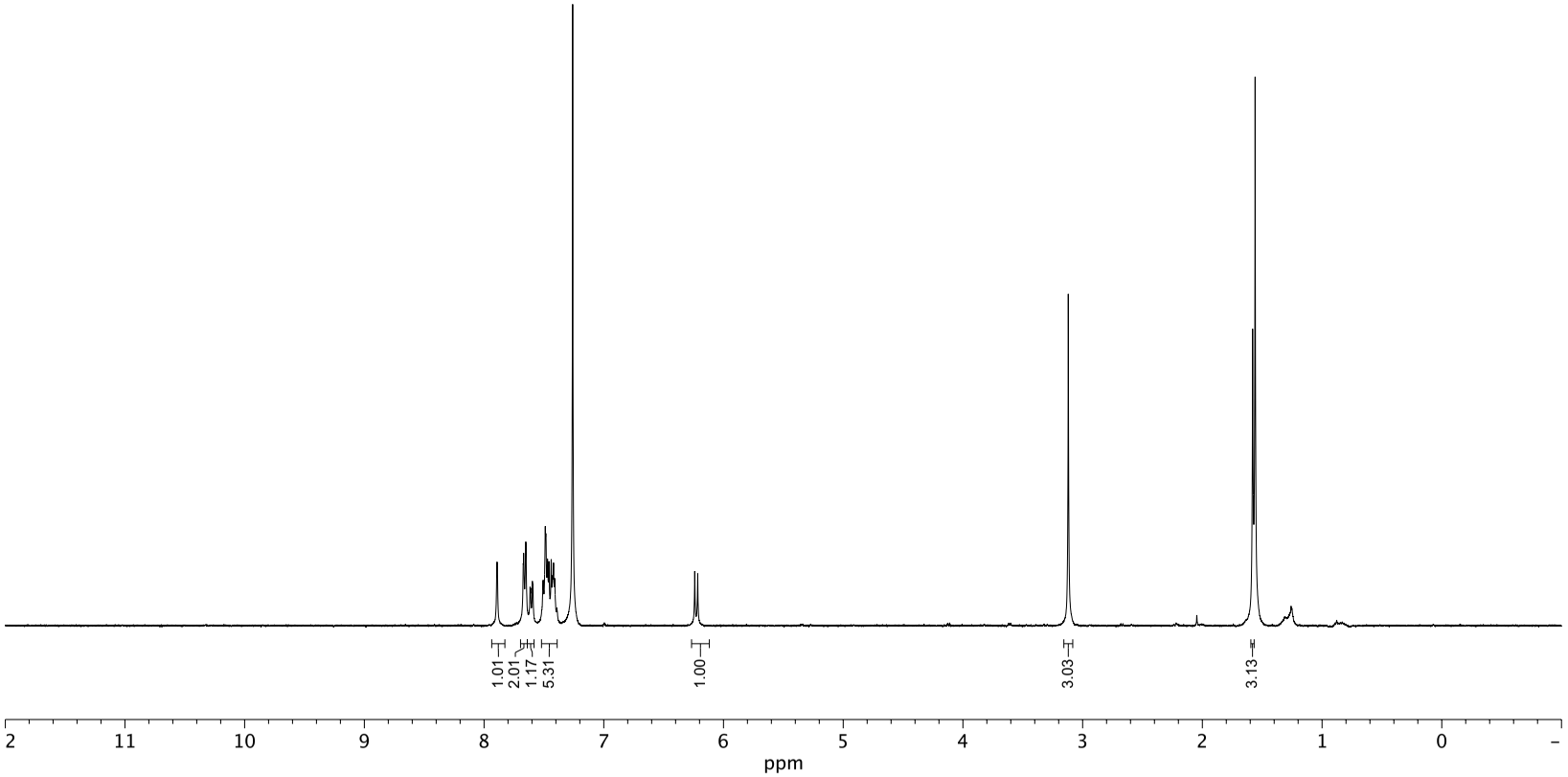
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4g**.



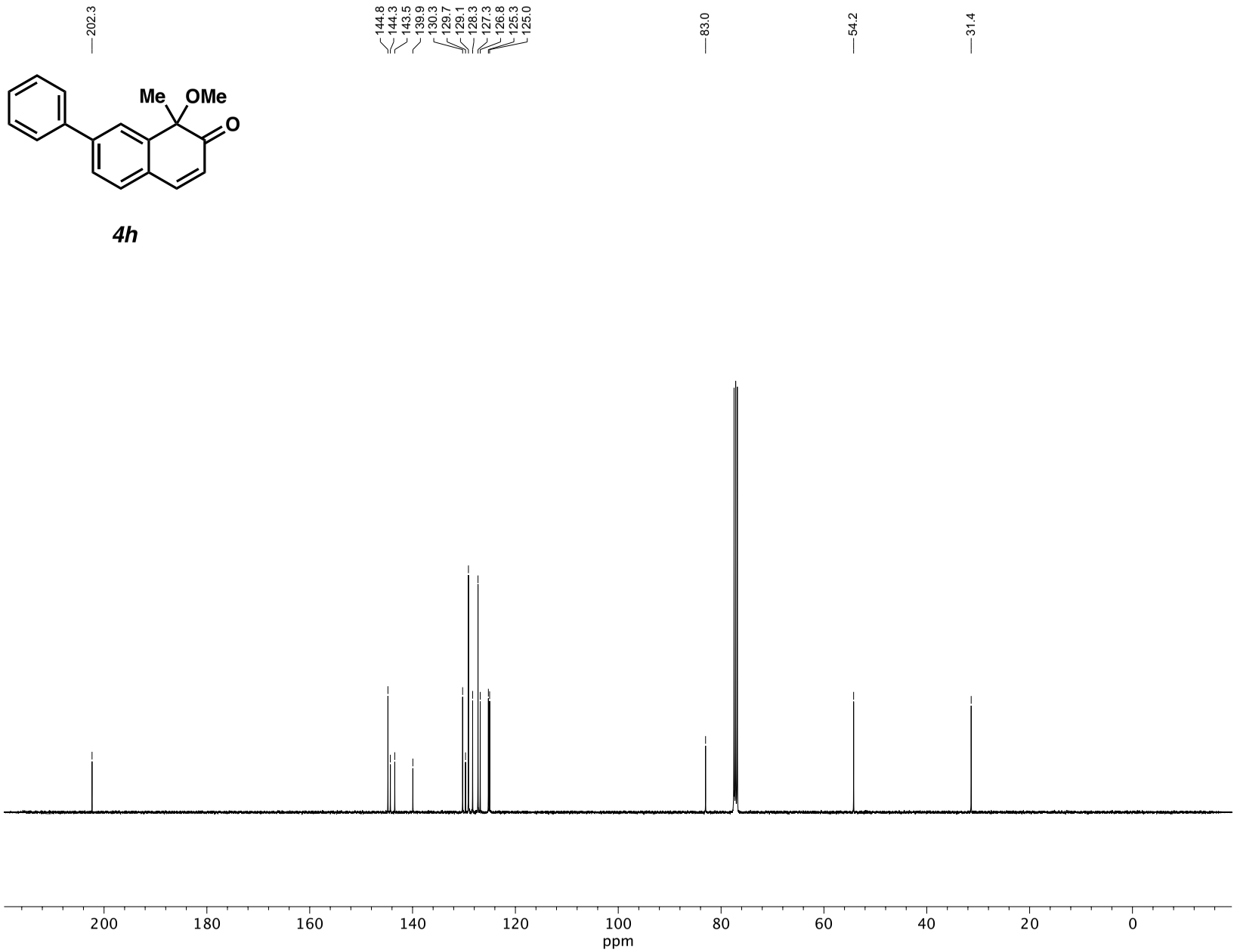
^{13}C NMR (101 MHz,$CDCl_3$) of compound **4g**.



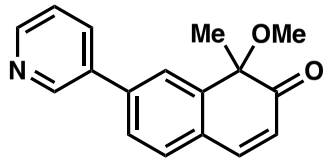
4h



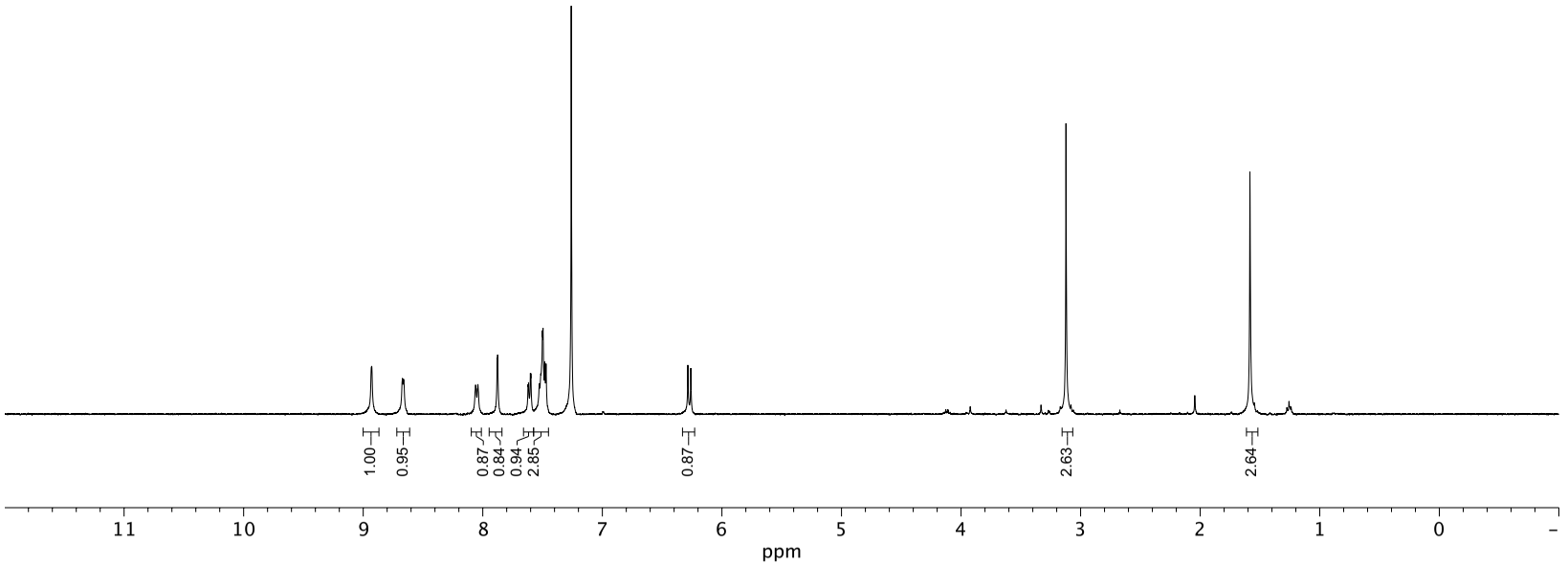
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4h**.



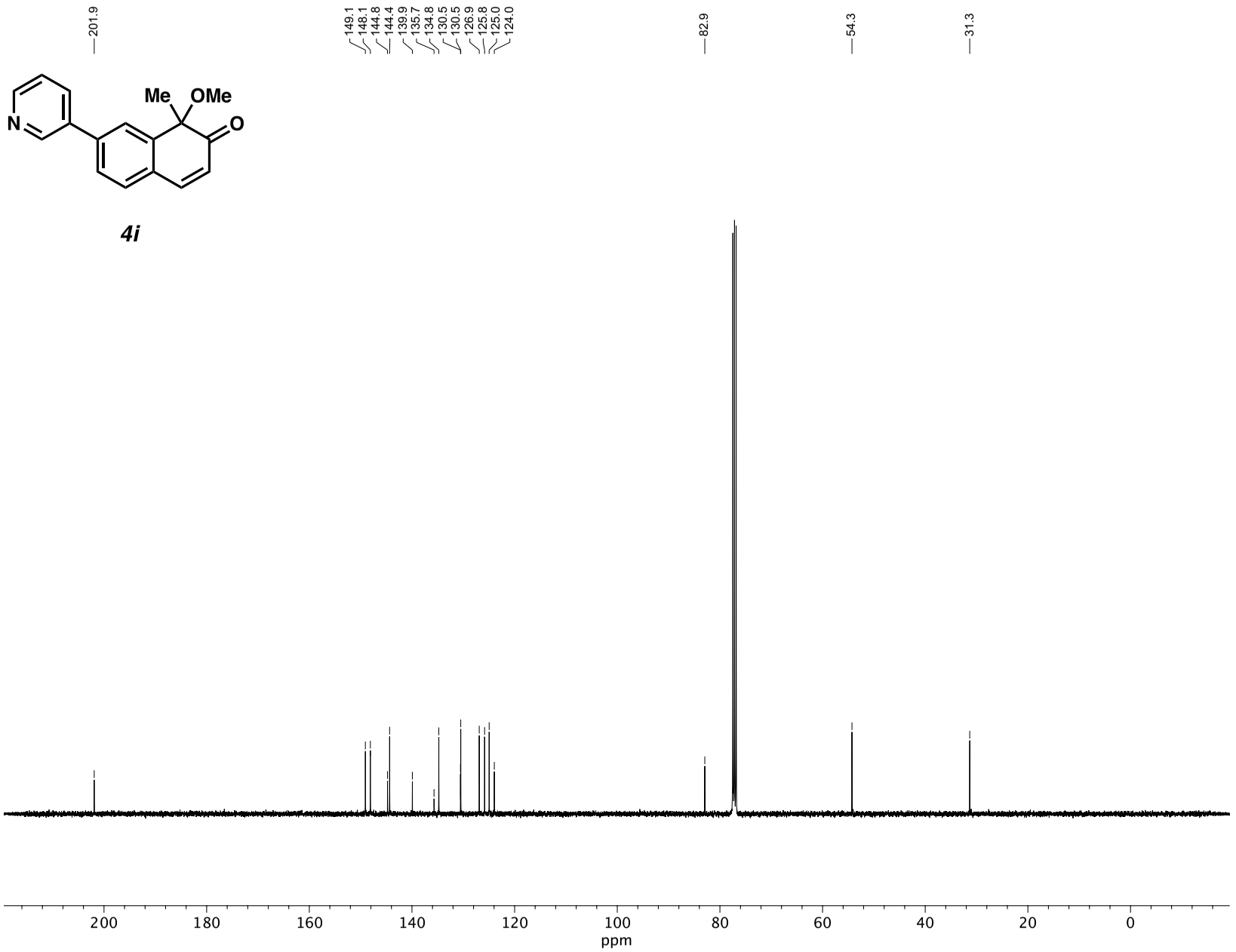
^{13}C NMR (101 MHz,$CDCl_3$) of compound **4h**.



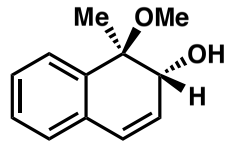
4i



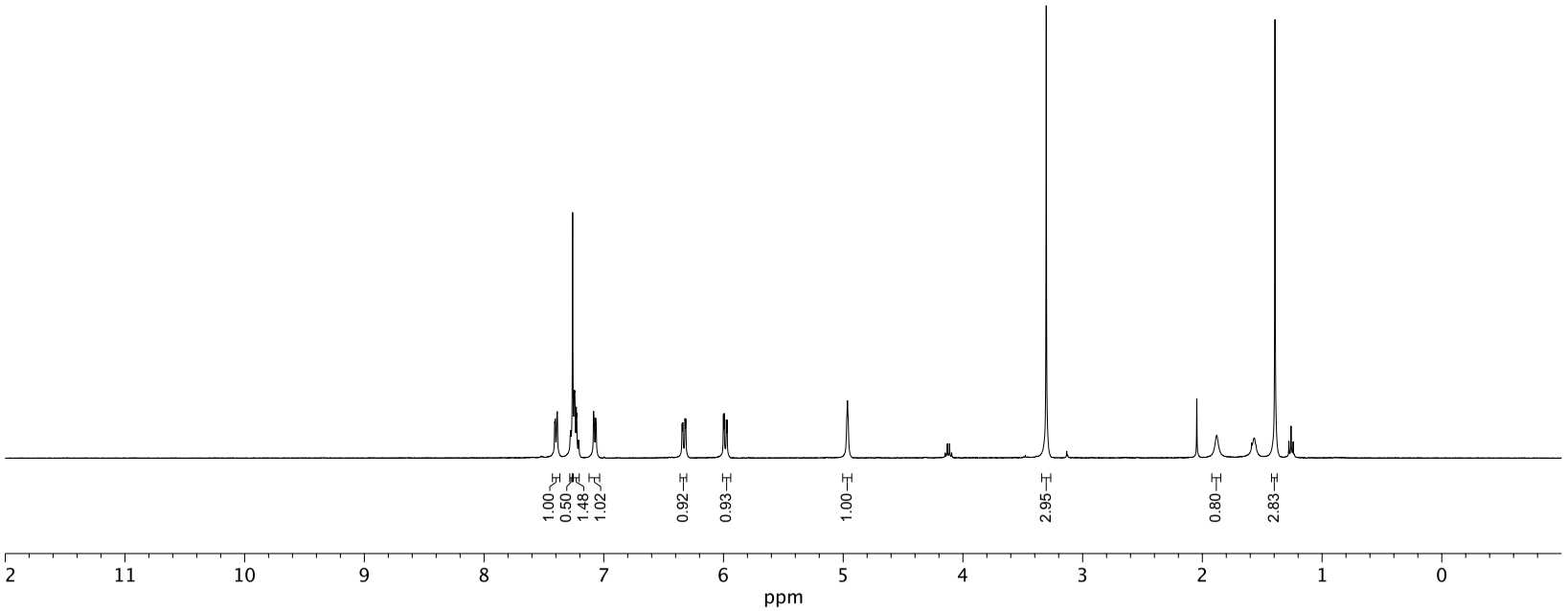
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4i**.



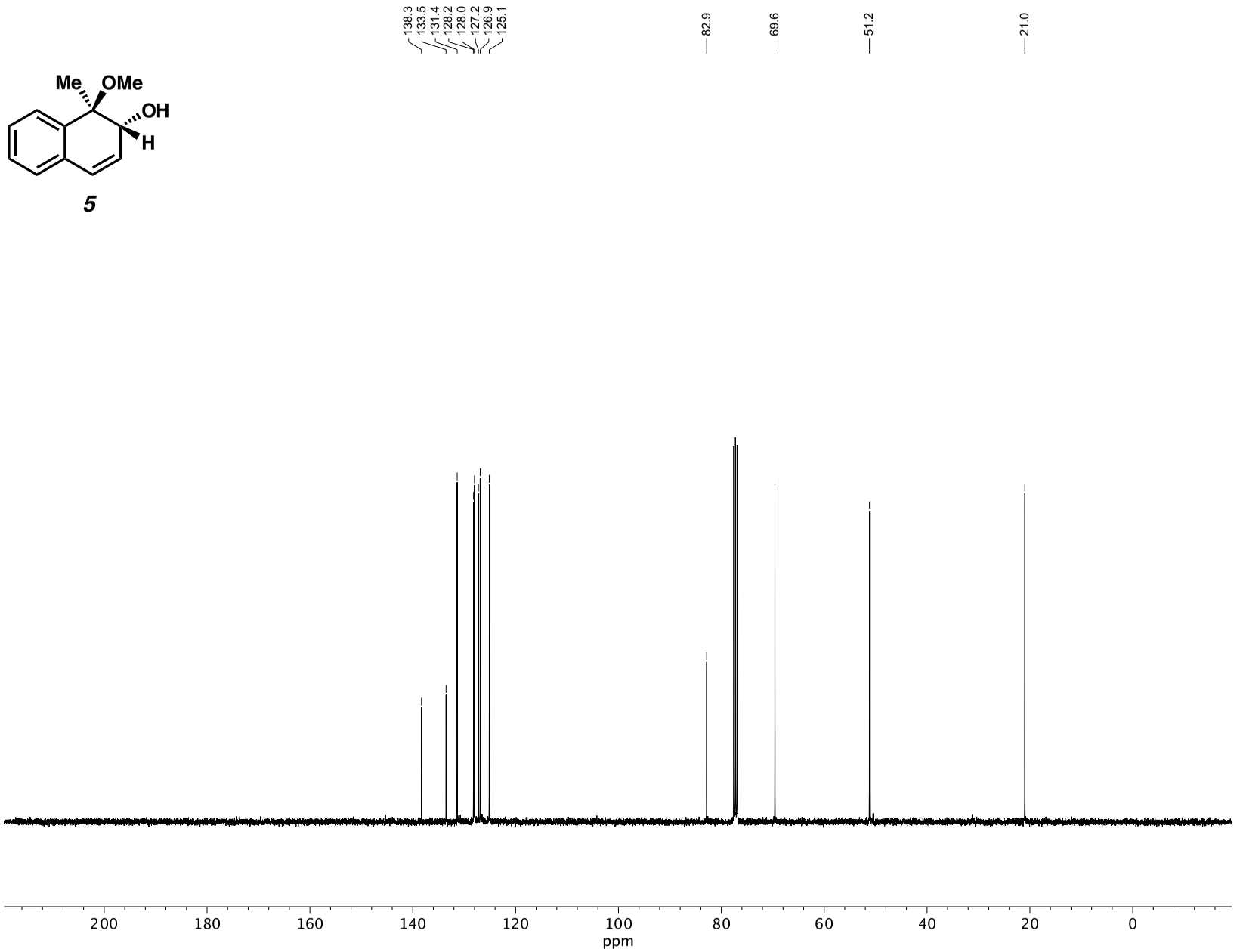
^{13}C NMR (101 MHz,$CDCl_3$) of compound **4i**.



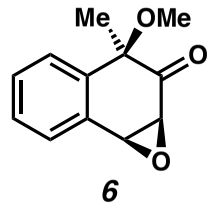
5



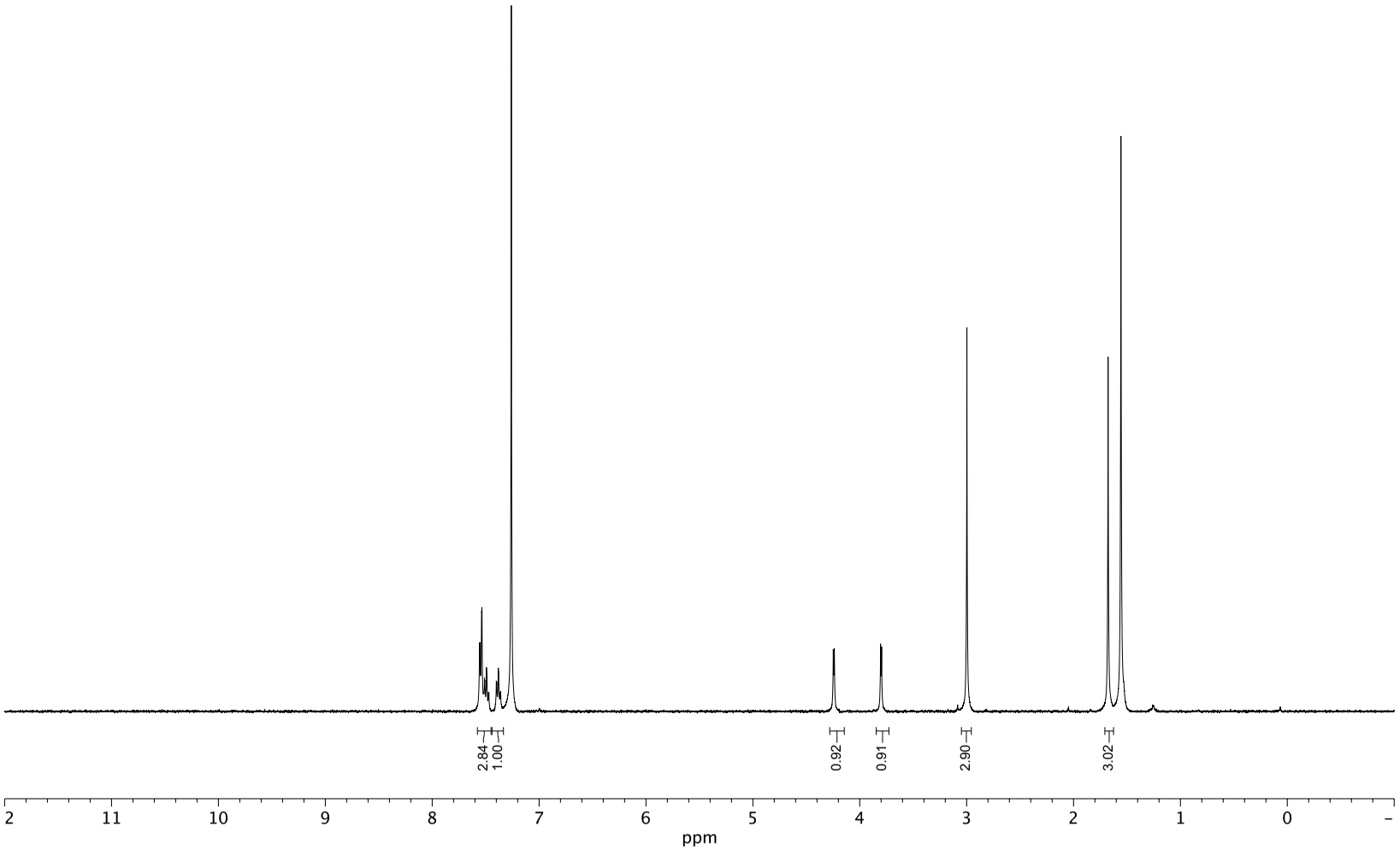
^{1}H NMR (400 MHz, $CDCl_3$) of compound **5**.



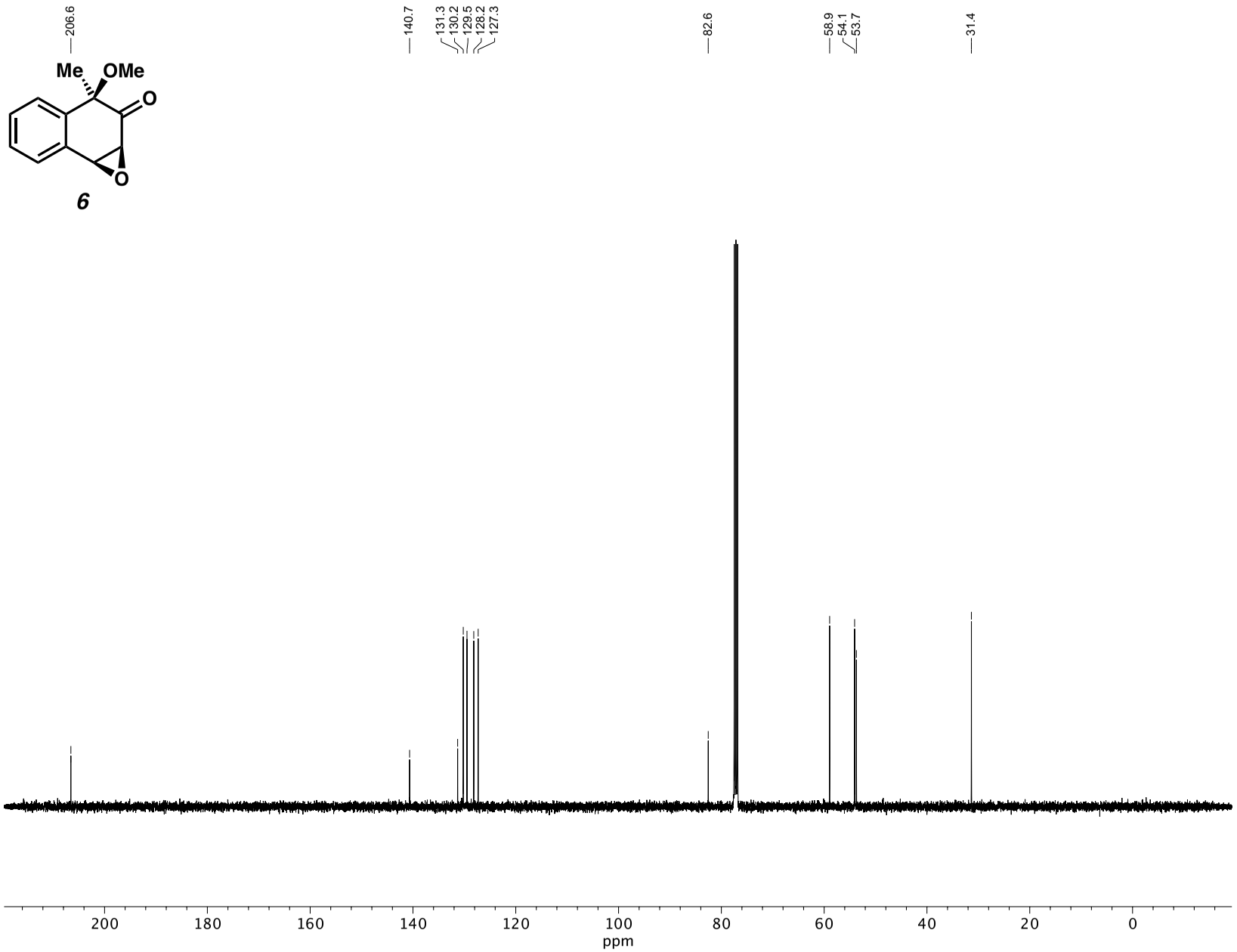
^{13}C NMR (101 MHz,$CDCl_3$) of compound **5**.



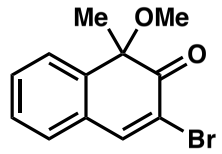
6



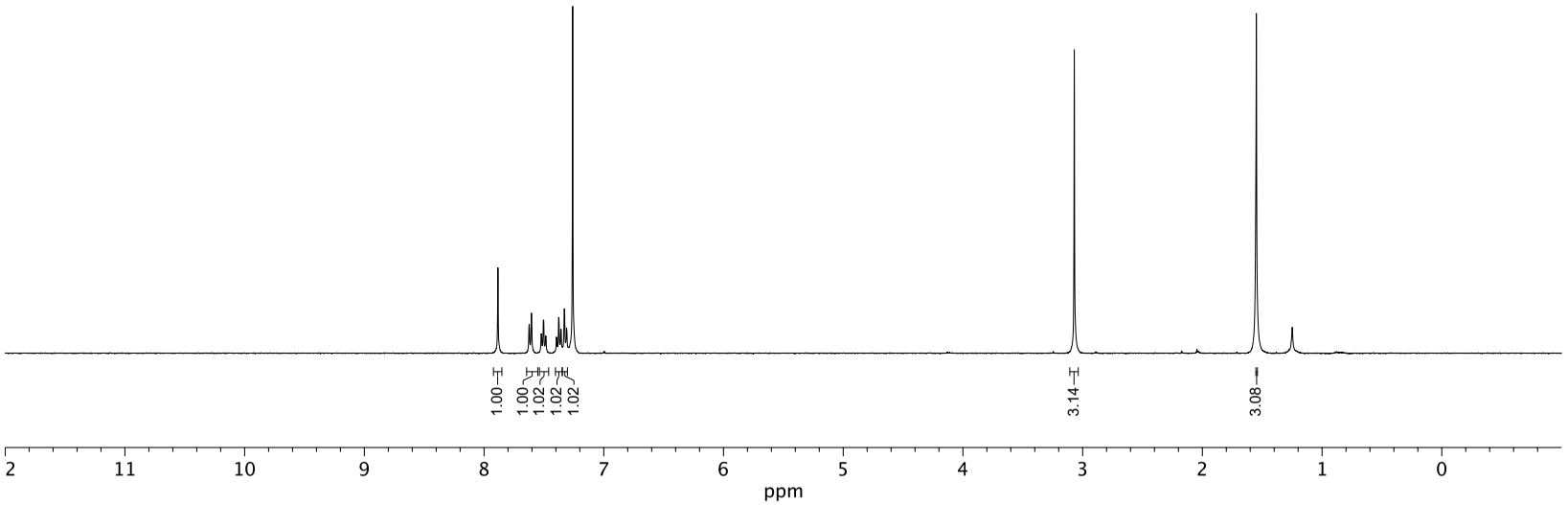
^{1}H NMR (400 MHz, $CDCl_3$) of compound **6**.



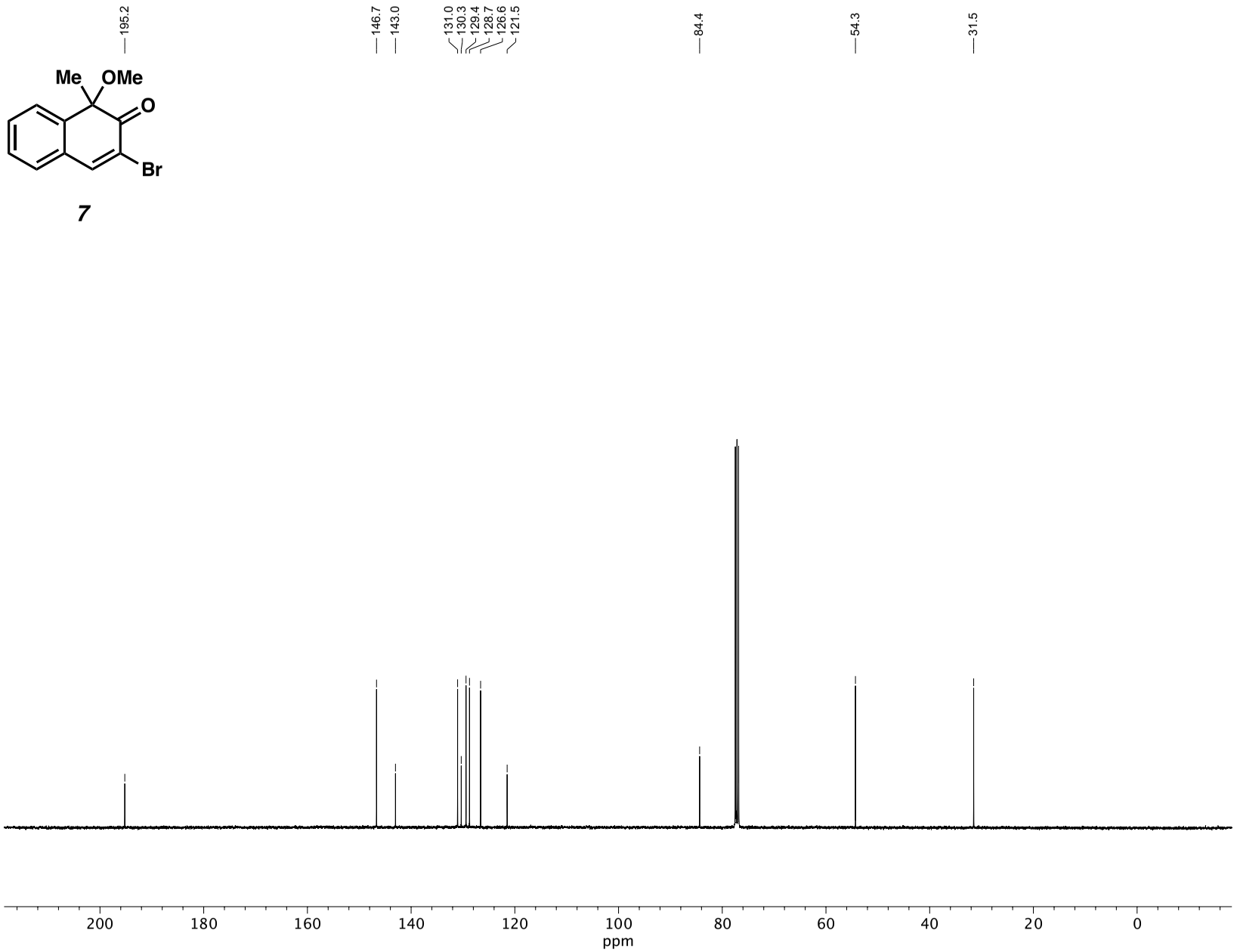
^{13}C NMR (101 MHz,$CDCl_3$) of compound **6**.



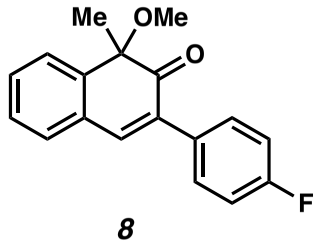
7



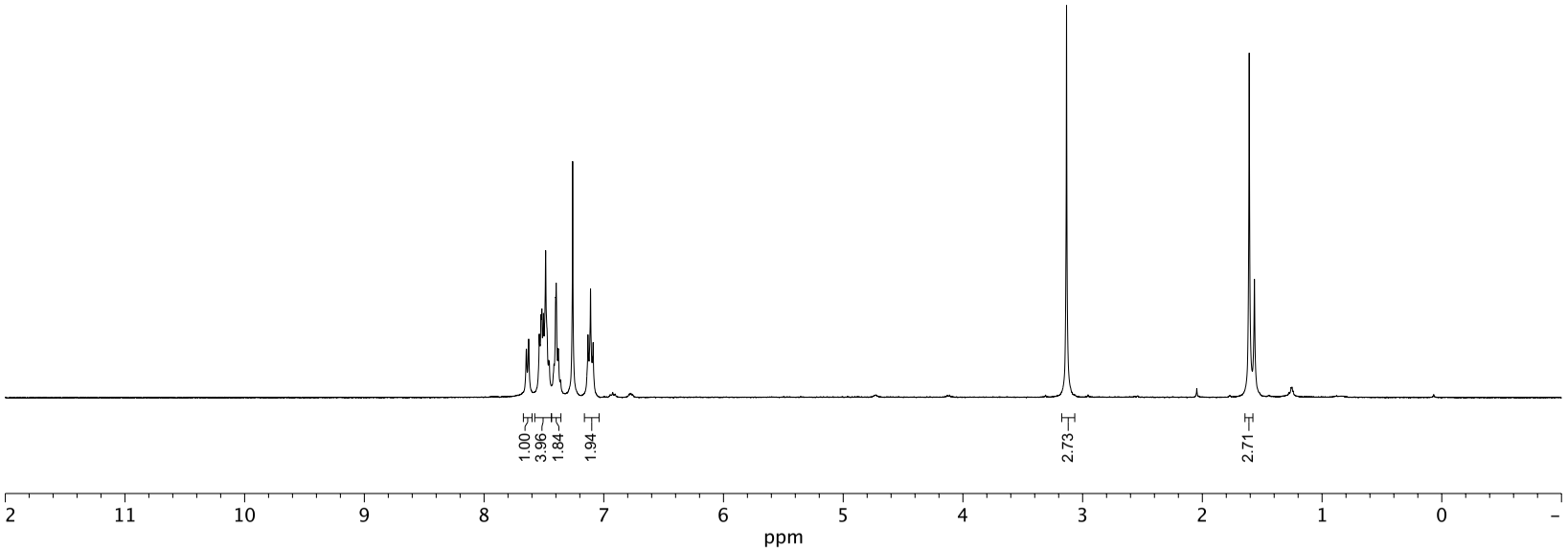
^{1}H NMR (400 MHz, $CDCl_3$) of compound **7**.



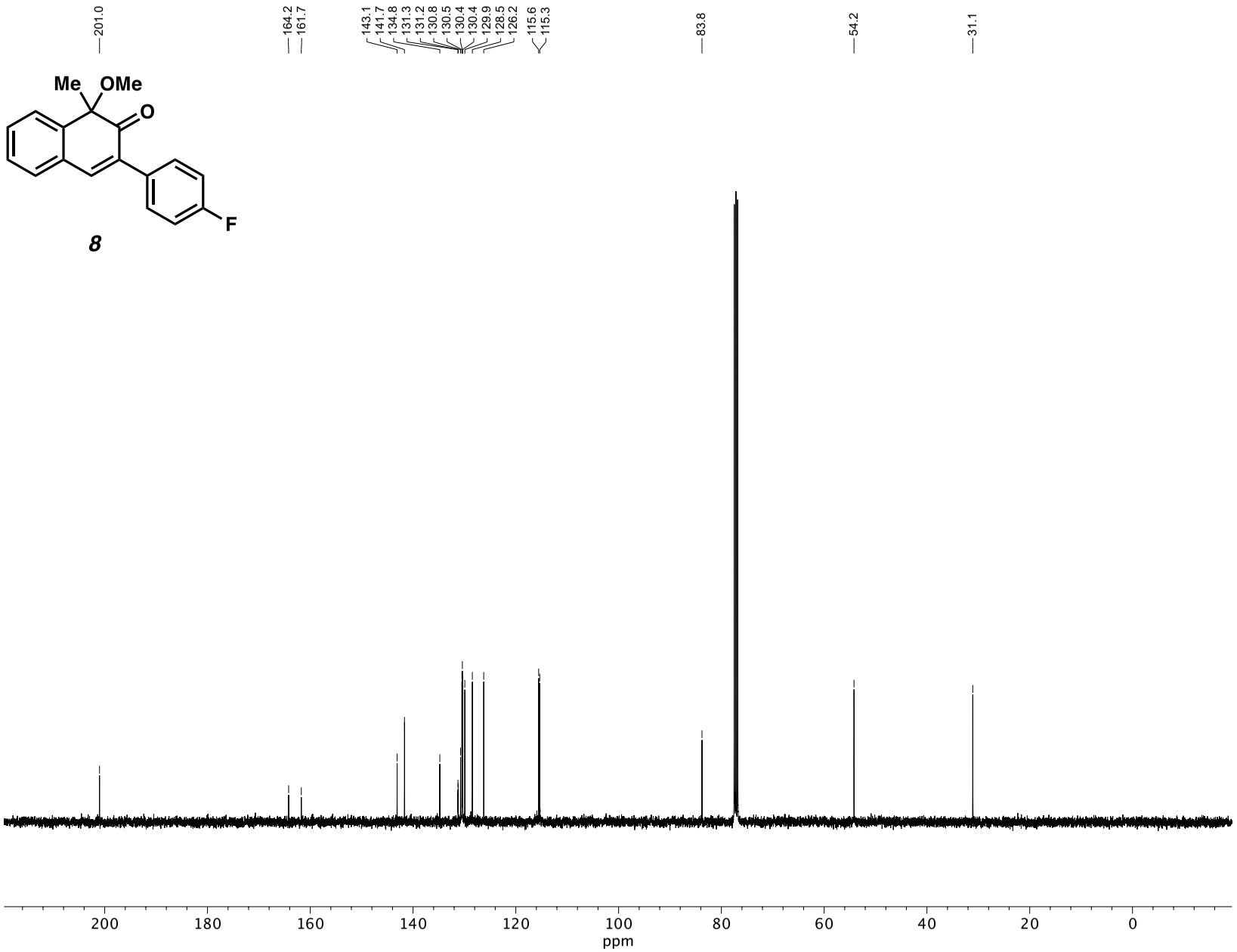
^{13}C NMR (101 MHz,$CDCl_3$) of compound **7**.



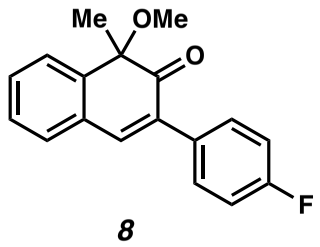
8



^{1}H NMR (400 MHz, $CDCl_3$) of compound **8**.

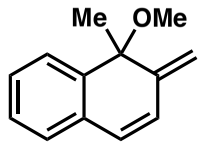


^{13}C NMR (101 MHz,$CDCl_3$) of compound **8**.

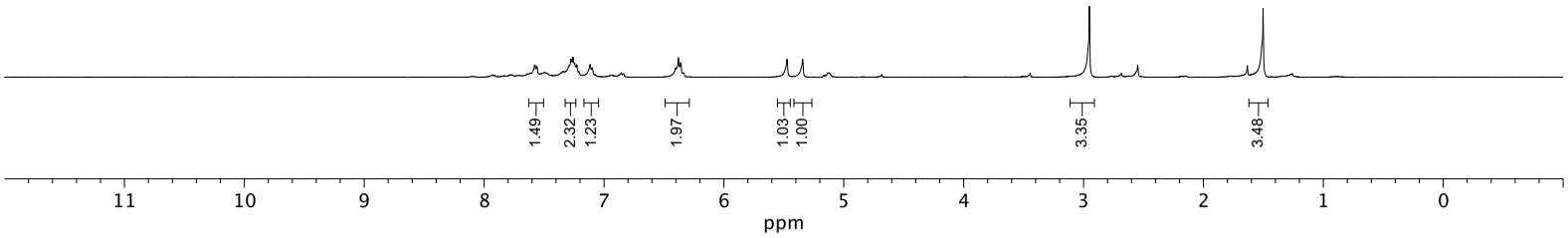


8

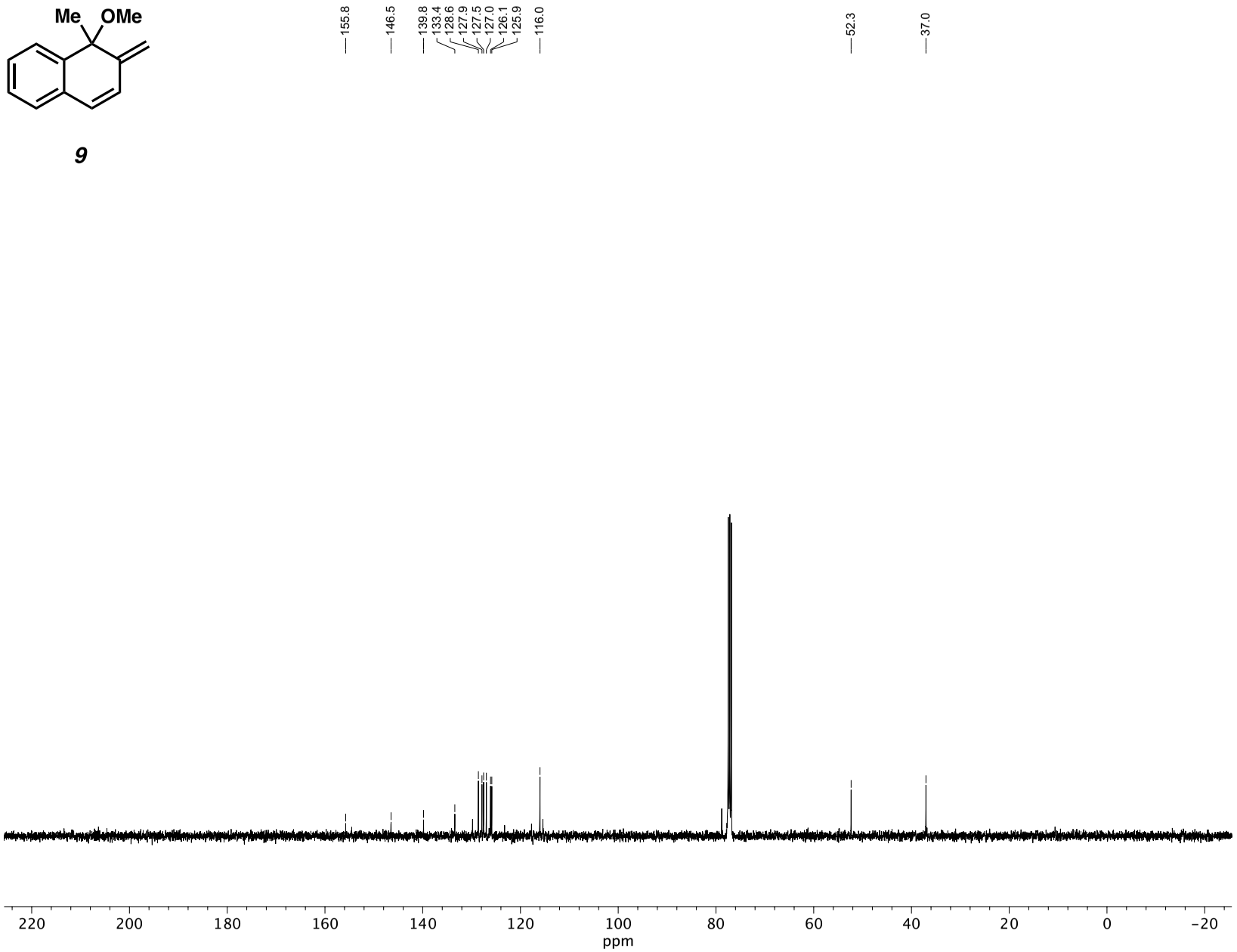
^{19}F NMR (377 MHz,$CDCl_3$) of compound **8**.



9



^{1} HNMR (400 MHz, $CDCl_3$) of compound **9**.



$^{1}{}_{3}$ C NMR (101 MHz,$CDCl_3$) of compound **9**.

10. References

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