

Supporting Information

**Iron(III)/Quinoxaline-Derived *N*, *N*-Ligand Catalyzed Oxygen Transfer Reaction of *N*-Vinyl Nitrones through Selective 4 $\pi$ -Electrocyclization and N-O Bond Cleavage**

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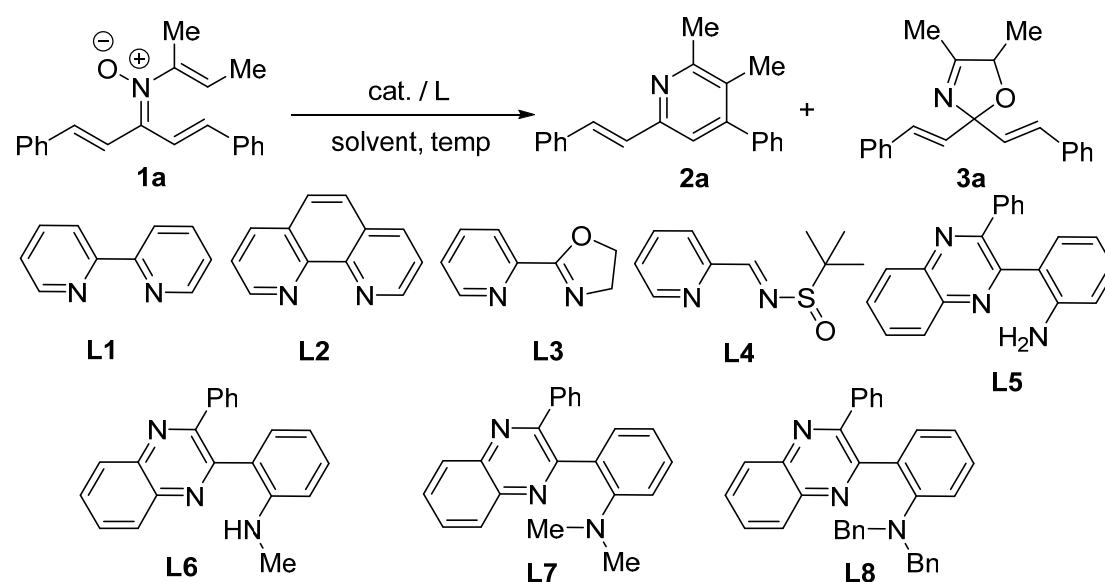
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## 1. General experimental information

$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and  $^{19}\text{F}$  NMR spectra were recorded at ambient temperature using 400, 500 or 600 MHz spectrometers. The data are reported as follows: chemical shift in ppm from internal tetramethylsilane on the  $\delta$  scale, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), and integration. High resolution mass spectra were acquired on an LTQ FT spectrometer, and were obtained by peak matching. Melting points are reported uncorrected. Analytical thin layer chromatography was performed on 0.25 mm extra hard silica gel plates with UV254 fluorescent indicator. Chromatography was performed using with 300-400 mesh silica gel ( $\text{SiO}_2$ ). Unless otherwise noted, all reagents and solvents were obtained from commercial sources and, where appropriate, purified prior to use. Ligands **L1-L4** were purchased from Energy Chemical. *N*-Vinyl nitrones **1a-1w**<sup>[1,2]</sup>, **1z**,<sup>[3]</sup> **1aa**,<sup>[4]</sup> **1ab**<sup>[5]</sup> were prepared according to literature methods and their spectral data matched literature values.

## 2. Optimization conditions (Table S1)

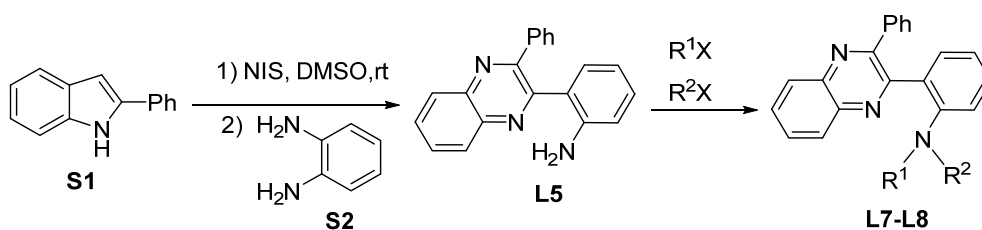


entry	Cat./L	solvent/temp	2a%/3a% <sup>b</sup>
1	FeCl <sub>3</sub>	dioxane/80 °C	21/16
2	FeCl <sub>3</sub>	Et <sub>2</sub> O/80 °C	39/36
3	FeCl <sub>3</sub>	<i>n</i> -Bu <sub>2</sub> O/80 °C	34/17

4	FeCl <sub>3</sub>	TBME/80 °C	29/21
5	FeCl <sub>3</sub>	Et <sub>2</sub> O/40 °C	44/18
6	FeCl <sub>3</sub> /L1	Et <sub>2</sub> O/40 °C	70/-
7	FeCl <sub>3</sub> /L2	Et <sub>2</sub> O/40 °C	77/-
8	FeCl <sub>3</sub> /L3	Et <sub>2</sub> O/40 °C	60/<5
9	FeCl <sub>3</sub> /L4	Et <sub>2</sub> O/40 °C	38/6
10	FeCl <sub>3</sub> /L5	Et <sub>2</sub> O/40 °C	<5/48
11	FeCl <sub>3</sub> /L6	Et <sub>2</sub> O/40 °C	<5/52
12	FeCl <sub>3</sub> /L7	Et <sub>2</sub> O/40 °C	<5/65
13	FeCl <sub>3</sub> /L8	Et <sub>2</sub> O/40 °C	<5/58
14	FeCl <sub>2</sub> /L7	Et <sub>2</sub> O/40 °C	<5/38
15	FeBr <sub>3</sub> /L7	Et <sub>2</sub> O/40 °C	<5/59
16	Fe(OTf) <sub>3</sub> /L7	Et <sub>2</sub> O/40 °C	<5/62
17	FeF <sub>3</sub> /L7	Et <sub>2</sub> O/40 °C	-
18	CuSO <sub>4</sub> /L7	Et <sub>2</sub> O/40 °C	<5/<5
19	Pd(OAc) <sub>2</sub> /L7	Et <sub>2</sub> O/40 °C	<5/<5
20	FeCl <sub>3</sub> /L7	Et <sub>2</sub> O/40 °C	<5/60 <sup>c</sup>
21	-/L7	Et <sub>2</sub> O/40 °C	-

<sup>a</sup> Reaction conditions: **1a** (0.2 mmol), cat (20 mol%), ligand (24 mol%), solvent (2.0 mL), 16-48 h; <sup>b</sup> isolated yield. <sup>c</sup> 4A MS.

### 3. Synthesis of ligands L5-L8

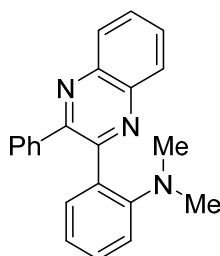


Ligands **L5-L6** were prepared according to literature method<sup>[6]</sup>, and their spectral data matched literature values.

**General Procedure A:** *N*-Iodosuccinimide (NIS) (0.22 g, 1 mmol) was added to a solution of 2-arylidoles **S1** (0.193 g, 1 mmol) in DMSO (10 mL) under an air atmosphere. The mixture was stirred at room temperature for 2 hours (complete consumption of 2-arylidole indicated by TLC). Then, 1,2-aminobenzenes **S2** (0.108

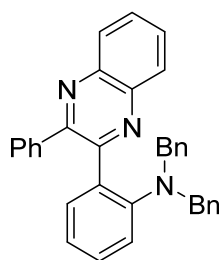
g, 1 mmol) was added into the solution, the reaction for another 4-6 hours at room temperature. The reaction mixture was poured into 30 mL saturated aqueous NaCl solutions, and extracted with ethyl acetate (2 × 15 mL). The combined organic phase was dried with anhydrous Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (1/10, ethyl acetate/petroleum ether) to afford ligand **L5**.

In a 25 mL reaction flask was charged with **L5** (0.149 g, 0.5 mmol), NaH (0.1 g, 2.5 mmol, 5.0 equiv.) and DMF (5.0 mL) under N<sub>2</sub> atmosphere. The reaction mixture was stirred vigorously at room temperature for 0.5 h and CH<sub>3</sub>I or BnBr (3.0 equiv.) was added. The reaction mixture was stirred vigorously at room temperature for 12 h until the substrate **L5** disappeared (monitored by TLC). At this time, the reaction was quenched by H<sub>2</sub>O (10 mL) and extracted with DCM (3 × 10 mL). Then, the combined organic layers were washed with brine (10 mL), dried over Na<sub>2</sub>SO<sub>4</sub>, and filtered. The solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (1/20, ethyl acetate/petroleum ether) to afford ligands **L7-L8**.



**L7**

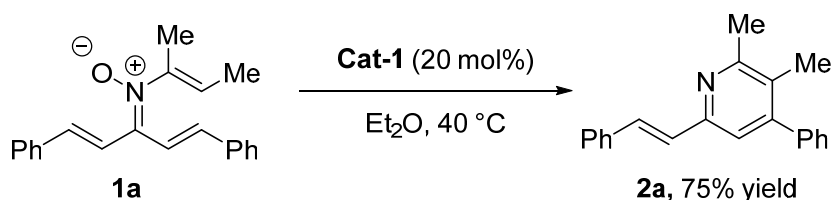
**N,N-dimethyl-2-(3-phenylquinoxalin-2-yl)aniline (L7):** **L5** (0.149 g, 0.5 mmol) ran for 12 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **L7**. A yellow solid (0.122 g, 75% yield); Mp: 51–52 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.12-8.10 (m, 2H), 7.69-7.67 (m, 2H), 7.62 (d, *J* = 6.8 Hz, 1H), 7.29-7.25 (m, 3H), 7.17-7.10 (m, 4H), 6.71-6.69 (d, *J* = 8.0 Hz, 1H), 1.97 (s, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 154.9, 154.8, 151.5, 141.3, 141.0, 139.7, 133.1, 131.4, 130.1, 129.5, 129.3, 129.2, 128.9, 128.1, 128.0, 127.4, 122.7, 118.7, 43.0; HRMS (ESI) *m/z* calcd for C<sub>22</sub>H<sub>20</sub>N<sub>3</sub>[M + H]<sup>+</sup>: 326.1652, found 326.1654.



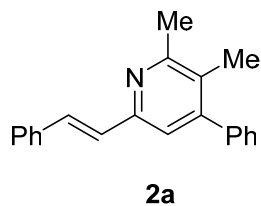
**L8**

**N,N-dibenzyl-2-(3-phenylquinoxalin-2-yl)aniline (L8):** **L5** (0.149 g, 0.5 mmol) ran for 12 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **L8**. A yellow solid (0.138 g, 58% yield); Mp: 154–155 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.10 (d, *J* = 8.0 Hz, 1H), 8.02 (d, *J* = 8 Hz, 1H), 7.69–7.63 (m, 2H), 7.44 (d, *J* = 7.6 Hz, 2H), 7.36 (d, *J* = 7.2 Hz, 1H), 7.23–7.15 (m, 2H), 7.10–7.08 (m, 3H), 7.01–7.00 (m, 6H), 6.82 (d, *J* = 7.2 Hz, 1H), 6.72–6.71 (m, 4H), 3.71 (m, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 154.4, 153.4, 149.8, 141.3, 140.9, 138.4, 137.2, 134.6, 131.8, 129.7, 129.6, 129.5, 129.4, 129.3, 129.0, 128.9, 128.8, 128.6, 127.9, 126.8, 123.3, 122.5, 56.2; HRMS (ESI) *m/z* calcd for C<sub>34</sub>H<sub>28</sub>N<sub>3</sub>[M + H]<sup>+</sup>: 478.2278, found 478.2274.

#### 4. Synthesis of compound 2a

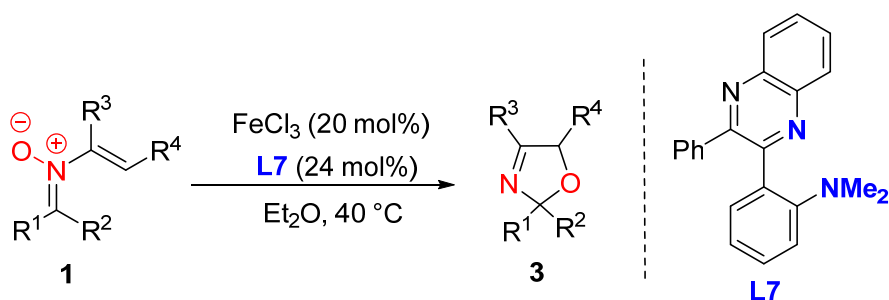


A 10 mL reaction flask was charged with N-vinyl nitrones **1a** (0.20 mmol) and **Cat-1** (0.04 mmol, 20 mol%) under N<sub>2</sub> atmosphere. Et<sub>2</sub>O (2 mL) was then added via syringe and the reaction vessel was sealed with a Teflon cap. The reaction mixture was stirred vigorously at 40 °C in an oil bath for 20 h until **1a** was consumed completely (monitored by TLC). At this time, the solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (1/30, ethyl acetate/petroleum ether) to afford compound **2a**.

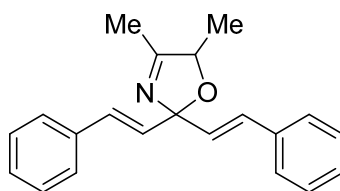


**(E)-2,3-dimethyl-4-phenyl-6-styrylpyridine (2a)**<sup>[1]</sup>: **1a** (0.061 g, 0.20 mmol) ran for 20 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **2a**. A light yellow solid (0.043 g, 75% yield); Mp: 101–102 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.57-7.53(m, 3H), 7.48-7.41 (m, 3H), 7.37-7.26 (m, 5H), 7.20-7.17 (m, 2H), 2.63 (s, 3H), 2.20 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 157.6, 151.9, 150.0, 140.0, 136.9, 131.6, 128.7, 128.6, 128.3, 128.2, 128.0, 127.7, 127.6, 127.0, 120.4, 23.6, 16.2; HRMS (ESI) *m/z* calcd for C<sub>21</sub>H<sub>20</sub>N [M + H]<sup>+</sup>: 286.1590, found 286.1583.

### 5. Synthesis of compounds 3

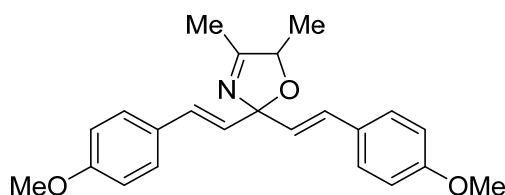


**General procedure B:** A 10 mL reaction flask was charged with *N*-vinyl nitrones **1** (0.20 mmol), FeCl<sub>3</sub> (6.4 mg, 20 mol%) and **L7** (15.6 mg, 24 mol%) under N<sub>2</sub> atmosphere. Et<sub>2</sub>O (2 mL) was then added via syringe and the reaction vessel was sealed with a Teflon cap. The reaction mixture was stirred vigorously at 40 °C in an oil bath for 16-29 h until **1** was consumed completely (monitored by TLC). At this time, the solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (1/20 to 1/10, ethyl acetate/petroleum ether) to afford compounds **3**.



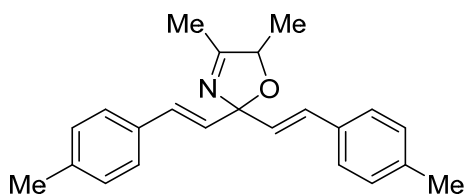
**3a**

**4,5-dimethyl-2,2-di((E)-styryl)-2,5-dihydrooxazole (3a):** **1a** (0.061 g, 0.20 mmol) ran for 20 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3a**. A yellow solid (0.039 g, 65% yield); Mp: 79–80 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.42–7.40 (m, 4H), 7.36–7.27 (m, 4H), 7.25–7.21 (m, 2H), 6.81–6.75 (m, 2H), 6.47–6.38 (m, 2H), 4.86 (q,  $J = 6.4$  Hz, 1H), 2.07 (s, 3H), 1.45 (d,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  172.4, 137.1, 132.6, 131.4, 129.9, 129.6, 129.4, 129.1, 128.8, 128.7, 127.6, 127.5, 109.1, 83.5, 19.8, 15.9; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{21}\text{H}_{22}\text{NO}$   $[\text{M} + \text{H}]^+$ : 304.1696, found 304.1695.



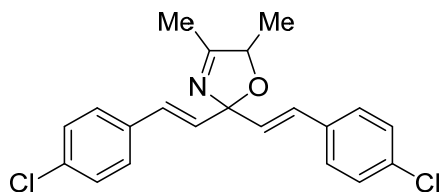
**3b**

**2,2-bis((E)-4-methoxystyryl)-4,5-dimethyl-2,5-dihydrooxazole (3b):** **1b** (0.073 g, 0.20 mmol) ran for 20 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/10) afforded **3b**. A yellow solid (0.035 g, 48% yield); Mp: 58–59 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.35 (d,  $J = 7.2$  Hz, 4H), 6.85 (d,  $J = 8.8$  Hz, 4H), 6.74–6.67 (m, 2H), 6.32–6.23 (m, 2H), 4.84 (q,  $J = 6.4$  Hz, 1H), 3.80 (s, 6H), 2.07 (s, 3H), 1.44 (d,  $J = 6.4$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  171.4, 159.3, 129.4, 129.3, 129.1, 128.9, 128.6, 128.0, 127.9, 127.6, 113.9, 113.8, 108.7, 83.0, 55.3, 19.1, 15.5; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{26}\text{NO}_3$   $[\text{M} + \text{H}]^+$ : 364.1907, found 364.1909.



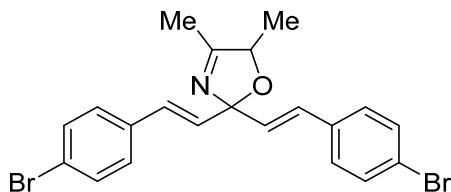
**3c**

**4,5-dimethyl-2,2-bis((E)-4-methylstyryl)-2,5-dihydrooxazole (3c):** **1c** (0.066 g, 0.20 mmol) ran for 22 h. Purification using medium pressure chromatography (eluents with a mixed ethyl acetate/petroleum ether = 1/10) afforded **3c**. A yellow solid (0.040 g, 61% yield); Mp: 63–64 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.31 (d, *J* = 6.4 Hz, 4H), 7.12 (d, *J* = 7.6 Hz, 4H), 6.77-6.70 (m, 2H), 6.41-6.32 (m, 2H), 4.85 (q, *J* = 6.4 Hz, 1H), 2.33 (s, 6H), 2.07 (s, 3H), 1.44 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 171.6, 137.6, 133.8, 133.7, 129.9, 129.6, 129.2, 129.1, 128.7, 126.7, 126.6, 108.7, 83.1, 21.2, 19.1, 15.5; HRMS (ESI) *m/z* calcd for C<sub>23</sub>H<sub>26</sub>NO [M + H]<sup>+</sup>: 332.2009, found 332.1999.



**3d**

**2,2-bis((E)-4-chlorostyryl)-4,5-dimethyl-2,5-dihydrooxazole (3d):** **1d** (0.074 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluents with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3d**. A yellow solid (0.050 g, 68% yield); Mp: 88–89 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.35-7.32 (m, 4H), 7.28 (d, *J* = 8.8 Hz, 4H), 6.75-6.68 (m, 2H), 6.43-6.33 (m, 2H), 4.86 (q, *J* = 6.8 Hz, 1H), 2.08 (s, 3H), 1.44 (d, *J* = 6.4 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 172.1, 135.0, 134.9, 133.5, 131.3, 130.1, 128.7, 128.6, 128.5, 128.2, 128.0, 108.4, 83.3, 29.7, 19.0, 15.5; HRMS (ESI) *m/z* calcd for C<sub>21</sub>H<sub>20</sub>Cl<sub>2</sub>NO [M + H]<sup>+</sup>: 372.0916, found 372.0911.

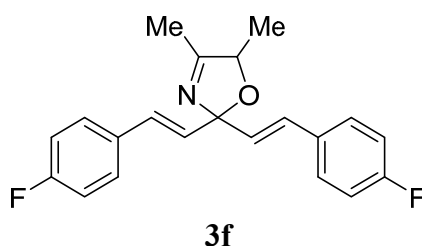


**3e**

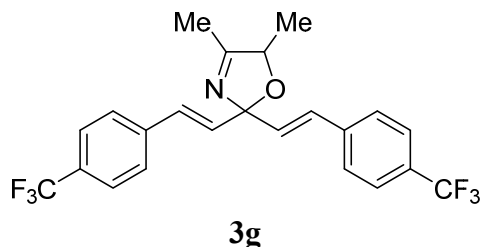
**2,2-bis((E)-4-bromostyryl)-4,5-dimethyl-2,5-dihydrooxazole (3e):** **1e** (0.092 g, 0.20



mmol) ran for 20 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/10) afforded **3e**. A yellow solid (0.058 g, 63% yield); Mp: 97–98 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.44 (d, *J* = 8.4 Hz, 4H), 7.28–7.25 (m, 4H), 6.74–6.67 (m, 2H), 6.44–6.34 (m, 2H), 4.85 (q, *J* = 6.4 Hz, 1H), 2.07 (s, 3H), 1.44 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 172.1, 135.4, 135.3, 131.7, 131.6, 131.4, 130.2, 128.7, 128.3, 121.7, 108.4, 83.3, 19.0, 15.5; HRMS (ESI) *m/z* calcd for C<sub>21</sub>H<sub>20</sub>Br<sub>2</sub>NO [M + H]<sup>+</sup>: 459.9906, found 459.9899.

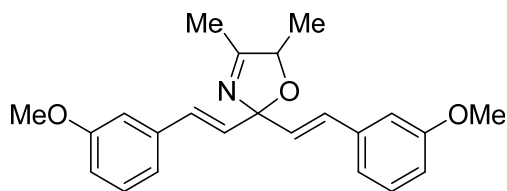


**2,2-bis((E)-4-fluorostyryl)-4,5-dimethyl-2,5-dihydrooxazole (3f):** **1f** (0.068 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/10) afforded **3f**. A yellow solid (0.041 g, 61% yield); Mp: 74–75 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.39–7.35 (m, 4H), 7.02–6.97 (m, 4H), 6.76–6.70 (m, 2H), 6.37–6.28 (m, 2H), 4.86 (q, *J* = 6.8 Hz, 1H), 2.08 (s, 3H), 1.45 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 171.9, 163.7 (d, *J* = 245.8 Hz), 132.6 (d, *J* = 2.9 Hz), 132.5 (d, *J* = 2.9 Hz), 130.5, 129.3, 128.6, 128.3 (d, *J* = 1.5 Hz), 128.2 (d, *J* = 1.4 Hz), 128.1, 115.6 (d, *J* = 3.6 Hz), 115.4 (d, *J* = 2.9 Hz), 108.4, 83.2, 19.0, 15.5; <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -114.0, -114.1; HRMS (ESI) *m/z* calcd for C<sub>21</sub>H<sub>20</sub>F<sub>2</sub>NO [M + H]<sup>+</sup>: 340.1507, found 340.1519.



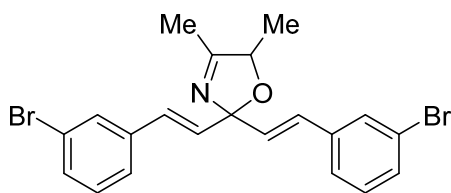
**4,5-dimethyl-2,2-bis((E)-4-(trifluoromethyl)styryl)-2,5-dihydrooxazole (3g):** **1g** (0.088 g, 0.20 mmol) ran for 29 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/10) afforded **3g**. A yellow solid (0.060 g, 68% yield); Mp: 94–95 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.58 (d, *J* = 8.4

Hz, 4H), 7.51-7.49 (m, 4H), 6.84-6.78 (m, 2H), 6.55-6.45 (m, 2H), 4.88 (q,  $J = 6.4$  Hz, 1H), 2.09 (s, 3H), 1.46 (d,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  172.4, 139.9 (q,  $J = 6.6$  Hz), 133.1, 131.9, 130.2 (q,  $J = 32$  Hz), 128.6, 128.3, 126.9, 125.5 (q,  $J = 274.8$  Hz), 108.2, 19.0, 15.5;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.5; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{20}\text{F}_6\text{NO}$   $[\text{M} + \text{H}]^+$ : 440.1444, found 440.1457.



**3h**

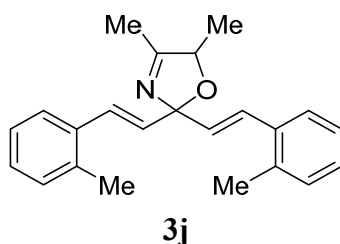
**2,2-bis((E)-3-methoxystyryl)-4,5-dimethyl-2,5-dihydrooxazole (3h):** **1h** (0.073 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/10) afforded **3h**. A yellow solid (0.040 g, 56% yield); Mp: 71–72 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.25-7.21 (m, 2H), 7.04 (s, 4H), 6.82 (d,  $J = 8.4$  Hz, 2H), 6.67-6.61 (m, 2H), 6.55-6.46 (m, 2H), 4.84 (q,  $J = 6.4$  Hz, 1H), 3.76 (s, 6H), 2.01 (s, 3H), 1.34 (d,  $J = 6.4$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ ):  $\delta$  172.4, 160.5, 160.4, 138.6, 138.5, 132.8, 131.7, 130.6, 129.4, 129.1, 120.1, 114.9, 114.8, 112.4, 112.3, 109.1, 83.5, 56.0, 19.8, 15.9; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{26}\text{NO}_3$   $[\text{M} + \text{H}]^+$ : 364.1907, found 364.1909.



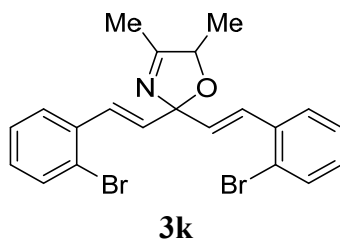
**3i**

**2,2-bis((E)-3-bromostyryl)-4,5-dimethyl-2,5-dihydrooxazole (3i):** **1i** (0.092 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3i**. A yellow solid (0.032 g, 60% yield); Mp: 75–76 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.56 (s, 2H), 7.37-7.30 (m, 4H), 7.19-7.15 (m, 2H), 6.73-6.66 (m, 2H), 6.45-6.35 (m, 2H), 4.85 (q,  $J = 6.4$  Hz, 1H), 2.07 (s, 3H), 1.44 (d,  $J = 6.4$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  172.1, 138.6, 138.6, 132.1, 130.1, 130.0, 129.9, 128.5, 128.1, 125.4, 122.7, 108.3, 83.4, 19.0, 15.4; HRMS

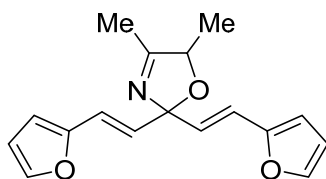
(ESI)  $m/z$  calcd for  $C_{21}H_{19}Br_2NO$   $[M + H]^+$ : 459.9906, found 459.9900.



**4,5-dimethyl-2,2-bis((E)-2-methylstyryl)-2,5-dihydrooxazole (3j):** **1j** (0.066 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3j**. A yellow solid (0.039 g, 60% yield); Mp: 111–112 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.48 (d,  $J$  = 4.0 Hz, 2H), 7.17 (d,  $J$  = 9.2 Hz, 6H), 7.06 (m, 2H), 6.37–6.27 (m, 2H), 4.88 (q,  $J$  = 6.4 Hz, 1H), 2.36 (s, 6H), 2.08 (s, 3H), 1.47 (d,  $J$  = 6.4 Hz, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  171.5, 135.9, 135.8, 135.7, 135.6, 132.4, 131.1, 130.2, 130.1, 127.7, 127.6, 127.3, 126.0, 125.9, 125.8, 109.0, 83.2, 19.9, 19.8, 19.1, 15.4; HRMS (ESI)  $m/z$  calcd for  $C_{23}H_{26}NO$   $[M + H]^+$ : 332.2009, found 332.2002.

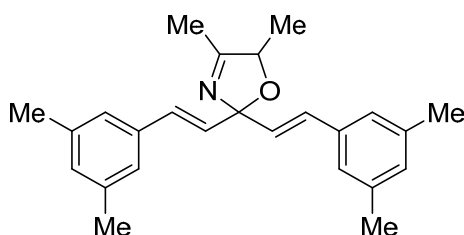


**2,2-bis((E)-2-bromostyryl)-4,5-dimethyl-2,5-dihydrooxazole (3k):** **1k** (0.092 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3k**. A yellow solid (0.056 g, 62% yield); Mp: 96–97 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.55–7.53 (m, 4H), 7.28–7.24 (m, 2H), 7.21 (s, 1H), 7.17 (d,  $J$  = 5.2 Hz, 1H), 7.12–7.08 (m, 2H), 6.44–6.33 (m, 2H), 4.92 (q,  $J$  = 6.8 Hz, 1H), 2.09 (s, 3H), 1.49 (d,  $J$  = 6.4 Hz, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  172.0, 136.6, 136.5, 133.5, 132.9, 132.8, 132.3, 129.0, 128.6, 127.4, 127.3, 127.2, 124.1, 124.0, 108.5, 83.6, 19.1, 15.4; HRMS (ESI)  $m/z$  calcd for  $C_{21}H_{20}Br_2NO$   $[M + H]^+$ : 459.9906, found 459.9907.



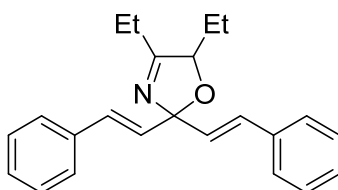
**3l**

**2,2-bis((E)-2-(furan-2-yl)vinyl)-4,5-dimethyl-2,5-dihydrooxazole (3l):** **1l** (0.057 g, 0.20 mmol) ran for 22 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3l**. A yellow solid (0.028 g, 48% yield); Mp: 80–81 °C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 7.63 (s, 2H), 6.53–6.47 (m, 6H), 6.26–6.16 (m, 2H), 4.81 (q, *J* = 6.4 Hz, 1H), 1.99 (s, 3H), 1.31 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 172.8, 152.5, 144.0, 130.4, 129.2, 118.3, 118.1, 112.7, 110.5, 110.4, 108.5, 83.6, 19.8, 15.8; HRMS (ESI) *m/z* calcd for C<sub>17</sub>H<sub>18</sub>NO<sub>3</sub> [M + H]<sup>+</sup>: 284.1281, found 284.1286.



**3m**

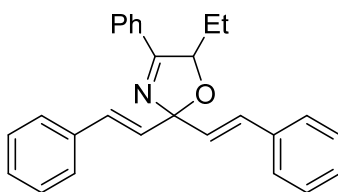
**2,2-bis((E)-3,5-dimethylstyryl)-4,5-dimethyl-2,5-dihydrooxazole (3m):** **1m** (0.072 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3m**. A yellow solid (0.043 g, 60% yield); Mp: 92–93 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.04 (s, 4H), 6.88 (s, 2H), 6.74–6.67 (m, 2H), 6.43–6.33 (m, 2H), 4.83 (q, *J* = 6.4 Hz, 1H), 2.29 (s, 12H), 2.06 (s, 3H), 1.43 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 171.5, 137.9, 137.8, 136.5, 136.4, 130.6, 129.9, 129.4, 129.3, 124.7, 124.6, 108.7, 83.0, 21.2, 19.1, 15.4; HRMS (ESI) *m/z* calcd for C<sub>25</sub>H<sub>30</sub>NO [M + H]<sup>+</sup>: 360.2322, found 360.2316.



**3n**

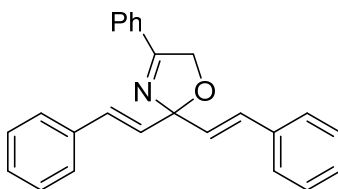
**4,5-diethyl-2,2-di((E)-styryl)-2,5-dihydrooxazole (3n):** **1n** (0.066 g, 0.20 mmol) ran

for 17 h. Purification using medium pressure chromatography (eluents with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3n**. A yellow solid (0.044 g, 66% yield); Mp: 85–86 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.43 (d, *J* = 7.2 Hz, 5H), 7.33-7.29 (m, 4H), 7.26-7.21 (m, 1H), 6.81-6.74 (m, 2H), 6.48-6.41 (m, 2H), 4.78-4.75 (m, 1H), 2.38-2.29 (m, 2H), 1.92-1.89 (m, 1H), 1.87-1.84 (m, 2H), 1.04 (t, *J* = 7.2 Hz, 3H), 0.88-0.86 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 175.2, 143.3, 136.7, 136.6, 134.8, 130.7, 130.0, 129.8, 129.2, 129.0, 128.5, 128.4, 127.7, 126.8, 125.4, 108.5, 87.4, 25.6, 22.9, 10.1, 9.6; HRMS (ESI) *m/z* calcd for C<sub>23</sub>H<sub>26</sub>NO [M + H]<sup>+</sup>: 332.2009, found 332.2002.



**3o**

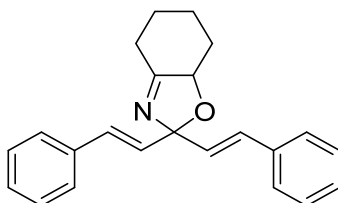
**5-ethyl-4-phenyl-2,2-di((E)-styryl)-2,5-dihydrooxazole (3o): 1o** (0.076 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluents with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3o**. A yellow oli (0.052 g, 68% yield); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.81 (d, *J* = 6.8 Hz, 2H), 7.48-7.45 (m, 5H), 7.42-7.38 (m, 2H), 7.35-7.29 (m, 3H), 7.27-7.19 (m, 3H) 6.92-6.82 (m, 2H), 6.59-6.49 (m, 2H), 5.46-5.44 (m, 1H), 2.01-1.95 (m, 1H), 1.78-1.71 (m, 1H), 1.02 (t, *J* = 7.6 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 170.5, 136.3, 136.2, 130.4, 130.1, 129.7, 128.9, 128.6, 128.5, 128.0, 127.9, 126.8, 126.7, 110.8, 80.3, 73.6, 68.3, 32.2; HRMS (ESI) *m/z* calcd for C<sub>27</sub>H<sub>26</sub>NO [M + H]<sup>+</sup>: 380.2009, found 380.1993.



**3p**

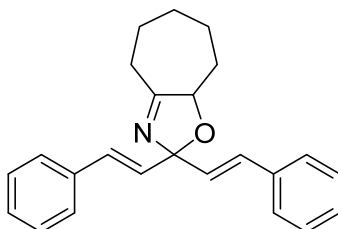
**4-phenyl-2,2-di((E)-styryl)-2,5-dihydrooxazole (3p): 1p** (0.070 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluents with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3p**. A yellow solid (0.041 g, 58% yield); Mp: 140–141 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.84 (d, *J* = 7.2 Hz, 2H), 7.53-7.43 (m,

7H), 7.33-7.29 (m, 4H), 7.25-7.22 (m, 2H), 6.88 (d,  $J = 16.4$  Hz, 2H), 6.54 (d,  $J = 16.0$  Hz, 2H), 5.17 (s, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  167.2, 136.4, 131.7, 130.9, 130.1, 129.3, 128.8, 128.5, 127.9, 127.8, 126.8, 111.3, 73.8; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{25}\text{H}_{22}\text{NO}$   $[\text{M} + \text{H}]^+$ : 352.1696, found 352.1684.



**3q**

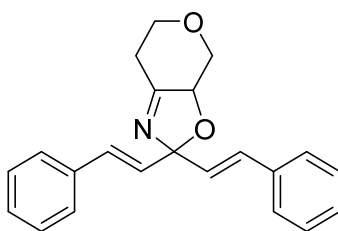
**2,2-di((E)-styryl)-2,4,5,6,7,7a-hexahydrobenzo[d]oxazole (3q):** **1q** (0.066 g, 0.20 mmol) ran for 20 h. Purification using medium pressure chromatography (eluents with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3q**. A yellow solid (0.041 g, 62% yield); Mp: 139–140 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.46-7.39 (m, 4H), 7.34-7.29 (m, 4H), 7.28-7.21 (m, 2H), 6.84-6.73 (m, 2H), 6.51-6.39 (m, 2H), 4.65 (t,  $J = 6.8$  Hz, 1H), 2.82-2.78 (m, 1H), 2.47-2.43 (m, 1H), 2.33-2.25 (m, 1H), 2.04-2.01 (m, 1H), 1.89-1.87 (m, 1H), 1.60-1.59 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  173.8, 136.6, 130.8, 129.9, 129.5, 129.2, 128.5, 128.4, 127.8, 126.8, 126.7, 109.3, 83.9, 35.1, 30.2, 26.4, 22.7; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{24}\text{NO}$   $[\text{M} + \text{H}]^+$ : 330.1852, found 330.1850.



**3r**

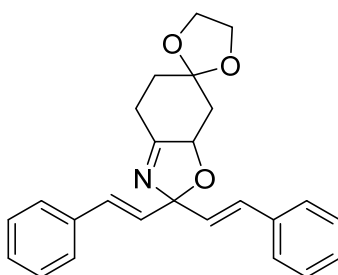
**2,2-di((E)-styryl)-4,5,6,7,8,8a-hexahydro-2H-cyclohepta[d]oxazole (3r):** **1r** (0.069 g, 0.20 mmol) ran for 21 h. Purification using medium pressure chromatography (eluents with a mixed ethyl acetate/petroleum ether = 1/10) afforded **3r**. A yellow solid (0.041 g, 60% yield); Mp: 72–73 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.42 (d,  $J = 4.8$  Hz, 4H), 7.32-7.29 (m, 4H), 7.25-7.21 (m, 2H), 6.82–6.75 (m, 2H), 6.47-6.39 (m, 2H), 4.90-4.87 (m, 1H), 2.64 (d,  $J = 5.2$  Hz, 2H), 2.10-2.06 (m, 1H), 1.84-1.61 (m, 5H), 1.57-1.46 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  176.2, 136.6, 136.5, 130.6, 129.8, 129.5, 129.2, 128.5, 128.4, 127.7, 126.8, 126.7, 108.6, 87.6, 33.5, 30.6, 30.2, 26.0, 25.3;

HRMS (ESI)  $m/z$  calcd for  $C_{24}H_{26}NO$   $[M + H]^+$ : 344.2009, found 344.2011.



**3s**

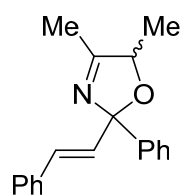
**2,2-di((E)-styryl)-3a,4,6,7-tetrahydro-2H-pyrano[4,3-d]oxazole (3s):** **1s** (0.066 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/10) afforded **3s**. A yellow solid (0.033 g, 50% yield); Mp: 92–93 °C;  $^1H$  NMR (600 MHz,  $CDCl_3$ ):  $\delta$  7.44–7.41 (m, 3H), 7.33–7.31 (m, 3H), 7.27–7.24 (m, 4H), 6.82–6.73 (m, 2H), 6.47–6.39 (m, 2H), 4.73–4.70 (m, 1H), 4.48–4.46 (m, 1H), 4.30–4.26 (m, 1H), 3.44–3.40 (m, 1H), 3.25 (t,  $J = 6.8$  Hz, 1H), 2.78–2.70 (m, 2H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ ):  $\delta$  170.5, 136.3, 136.2, 130.4, 130.1, 129.7, 128.9, 128.6, 128.5, 128.0, 127.9, 126.8, 126.7, 110.8, 80.3, 73.6, 68.3, 32.2; HRMS (ESI)  $m/z$  calcd for  $C_{22}H_{22}NO_2$   $[M + H]^+$ : 332.1645 found 332.1645.



**3t**

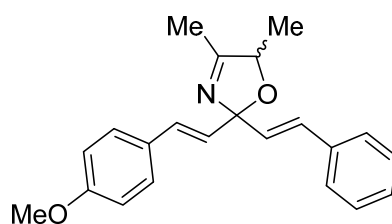
**2,2-di((E)-styryl)-4,5,7,7a-tetrahydro-2H-spiro[benzo[d]oxazole-6,2'-[1,3]dioxolane] (3t):** **1t** (0.077 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3t**. A yellow solid (0.044 g, 56% yield); Mp: 51–52 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.43–7.40 (m, 4H), 7.36–7.29 (m, 4H), 7.24–7.22 (m, 2H), 6.84–6.73 (m, 2H), 6.50–6.37 (m, 2H) 4.90–4.86 (m, 1H), 4.07–3.97 (m, 4H), 2.78–2.73 (m, 1H), 2.64–2.56 (m, 1H), 2.53–2.48 (m, 1H), 2.04–1.99 (m, 1H), 1.86–1.78 (m, 2H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  172.3, 136.4, 136.3, 130.4, 130.2, 129.4, 129.0, 128.6, 128.5, 127.9, 127.8, 126.8, 126.7, 110.5, 108.1, 82.0, 64.8, 64.6, 42.6, 34.3, 25.5; HRMS (ESI)  $m/z$  calcd

for C<sub>25</sub>H<sub>26</sub>NO<sub>3</sub> [M + H]<sup>+</sup>: 388.1907 found 388.1900.



**3u**, dr = 4:1

**(E)-4,5-dimethyl-2-phenyl-2-styryl-2,5-dihydrooxazole (3u, dr = 4:1):** **1u** (0.055 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3u**. A yellow solid (0.036 g, 66% yield); Mp: 61–62 °C; *Major isomer*: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.59 (d, *J* = 7.6 Hz, 2H), 7.39–7.33 (m, 4H), 7.29–7.26 (m, 3H), 7.24–7.19 (m, 1H), 6.74 (d, *J* = 16.0 Hz, 1H), 6.58 (d, *J* = 16.0 Hz, 1H), 4.83 (q, *J* = 6.8 Hz, 1H), 2.06 (s, 3H), 1.47 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 171.4, 142.8, 136.5, 132.7, 131.2, 129.0, 128.4, 128.2, 127.6, 126.8, 125.8, 109.8, 83.3, 19.0, 15.3; *Minor isomer*: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.61 (d, *J* = 7.6 Hz, 2H), 7.39–7.33 (m, 4H), 7.29–7.26 (m, 3H), 7.24–7.19 (m, 1H), 6.74 (d, *J* = 16.0 Hz, 1H), 6.52 (d, *J* = 16.0 Hz, 1H), 4.90 (q, *J* = 6.4 Hz, 1H), 2.06 (s, 3H), 1.40 (d, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 171.5, 143.2, 136.4, 132.7, 131.2, 129.2, 128.6, 128.2, 127.7, 126.8, 125.8, 109.6, 83.3, 18.7, 15.3; HRMS (ESI) *m/z* calcd for C<sub>19</sub>H<sub>20</sub>NO [M + H]<sup>+</sup>: 278.1539 found 278.1542.

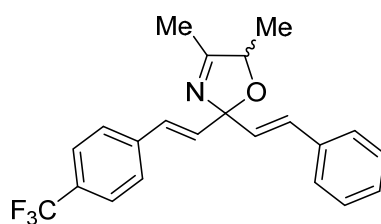


**3v**, dr = 1:1

**2-((E)-4-methoxystyryl)-4,5-dimethyl-2-((E)-styryl)-2,5-dihydrooxazole (3v):** **1v** (0.067 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluent with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3v**. A yellow solid (0.034 g, 51% yield); Mp: 83–84 °C; *One isomer*: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.42 (d, *J* = 7.2 Hz, 2H), 7.36–7.29 (m, 4H), 7.25–7.21 (m, 1H), 6.86 (d, *J* = 8.4 Hz, 2H), 6.81–6.69 (m, 2H), 6.48–6.38 (m, 1H), 6.33–6.24 (m, 1H), 4.86 (q, *J* = 6.4 Hz, 1H), 3.80 (s, 3H), 2.07 (s, 3H), 1.45 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 171.6,

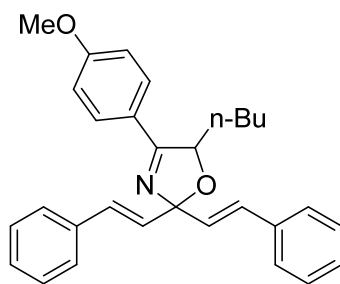


159.3, 136.6, 131.1, 129.8, 129.6, 129.3, 129.2, 129.1, 128.8, 128.7, 128.5, 128.0, 127.7, 127.5, 126.7, 113.9, 108.7, 83.1, 55.2, 19.1, 15.4; *Another isomer*:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.42 (d,  $J = 7.2$  Hz, 2H), 7.36-7.29 (m, 4H), 7.25-7.21 (m, 1H), 6.86 (d,  $J = 8.4$  Hz, 2H), 6.81-6.69 (m, 2H), 6.48-6.38 (m, 1H), 6.33-6.24 (m, 1H), 4.86 (q,  $J = 6.4$  Hz, 1H), 3.80 (s, 3H), 2.07 (s, 3H), 1.45 (d,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  171.5, 159.3, 136.5, 131.1, 129.8, 129.6, 129.3, 129.2, 129.1, 128.8, 128.7, 128.5, 128.0, 127.7, 127.5, 126.7, 113.9, 108.7, 83.0, 55.2, 19.1, 15.4; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{24}\text{NO}_2$   $[\text{M} + \text{H}]^+$ : 334.1802 found 334.1795.



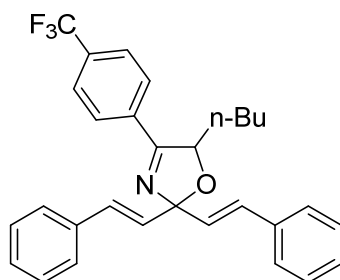
**3w**,  $dr = 1:1$

**4,5-dimethyl-2-((E)-styryl)-2-((E)-4-(trifluoromethyl)styryl)-2,5-dihydrooxazole (3w)**: **1w** (0.074 g, 0.20 mmol) ran for 16 h. Purification using medium pressure chromatography (eluents with a mixed ethyl acetate/petroleum ether = 1/20) afforded **3w**. A yellow solid (0.045 g, 61% yield); Mp: 74–75 °C; *One isomer*:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (d,  $J = 8.4$  Hz, 2H), 7.51-7.49 (m, 2H), 7.42 (d,  $J = 8.4$  Hz, 2H), 7.33-7.30 (m, 2H), 7.26-7.23 (m, 1H), 6.84-6.75 (m, 2H), 6.56-6.37 (m, 2H), 4.87 (q,  $J = 6.4$  Hz, 1H), 2.09 (s, 3H), 1.46 (d,  $J = 6.4$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  172.1, 140.1, 136.4, 133.5, 130.4, 129.6 (q,  $J = 5.1$  Hz), 129.4 (q,  $J = 32.1$  Hz), 129.1, 128.6 (q,  $J = 2.7$  Hz), 128.4, 128.0, 127.8, 126.9, 125.5 (q,  $J = 269.1$  Hz), 108.5, 83.4, 19.1, 15.5;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.5; *Another isomer*:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (d,  $J = 8.4$  Hz, 2H), 7.51-7.49 (m, 2H), 7.42 (d,  $J = 8.4$  Hz, 2H), 7.33-7.30 (m, 2H), 7.26-7.23 (m, 1H), 6.84-6.75 (m, 2H), 6.56-6.37 (m, 2H), 4.87 (q,  $J = 6.4$  Hz, 1H), 2.09 (s, 3H), 1.46 (d,  $J = 6.4$  Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  172.1, 140.0, 136.3, 132.4, 130.0, 129.6 (q,  $J = 5.1$  Hz), 129.3 (q,  $J = 32.1$  Hz), 129.1, 128.6 (q,  $J = 2.7$  Hz), 128.4, 127.9, 127.8, 126.8, 125.4 (q,  $J = 269.1$  Hz), 108.3, 83.3, 19.0, 15.5;  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.5; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{22}\text{H}_{21}\text{F}_3\text{NO}$   $[\text{M} + \text{H}]^+$ : 372.1570 found 372.1563.



**3x**

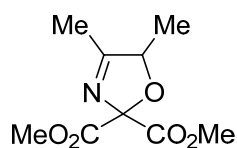
**5-butyl-4-(4-methoxyphenyl)-2,2-di((E)-styryl)-2,5-dihydrooxazole (3x).** A colorless oli, 0.040 g, 46% yield;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 8.5$  Hz, 2H), 7.45 (d,  $J = 7.5$  Hz, 2H), 7.42 (d,  $J = 7.5$  Hz, 2H), 7.35-7.27 (m, 5H), 7.25-7.20 (m, 1H), 6.97 (d,  $J = 8.5$  Hz, 2H), 6.88-6.80 (m, 2H), 6.58-6.47 (m, 2H), 5.43 (t,  $J = 6.0$  Hz, 1H), 3.86 (s, 3H), 1.92-1.86 (m, 1H), 1.71-1.64 (m, 1H), 1.55-1.47 (m, 2H), 1.43-1.33 (m, 2H), 0.89 (t,  $J = 7.0$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  169.2, 161.9, 136.7, 136.6, 131.0, 130.4, 129.9, 129.8, 129.6, 128.5, 128.4, 127.7, 127.6, 126.8, 126.7, 124.0, 114.0, 109.1, 85.2, 55.4, 33.9, 28.0, 22.5, 14.0; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{30}\text{H}_{32}\text{NO}_2$   $[\text{M} + \text{H}]^+$ : 438.2428, found 438.2404.



**3y**

**5-butyl-2,2-di((E)-styryl)-4-(4-(trifluoromethyl)phenyl)-2,5-dihydrooxazole (3y).** A colorless oli, 0.059 g, 62% yield;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.93 (d,  $J = 8.0$  Hz, 2H), 7.73 (d,  $J = 8.0$  Hz, 2H), 7.46 (d,  $J = 7.5$  Hz, 2H), 7.42 (d,  $J = 7.5$  Hz, 2H), 7.36-7.26 (m, 5H), 7.25-7.22 (m, 1H), 6.90-6.81 (m, 2H), 6.57-6.47 (m, 2H), 5.48-5.46 (m, 1H), 1.91-1.84 (m, 1H), 1.71-1.64 (m, 1H), 1.52-1.44 (m, 1H), 1.43-1.28 (m, 3H), 0.90 (t,  $J = 7.5$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  168.8, 136.5, 136.3, 134.8, 132.9 (d,  $J = 32.0$  Hz), 130.3, 130.2, 129.9, 129.7, 128.6, 128.5, 128.4, 127.9 (q,  $J = 5.6$  Hz), 126.8, 125.7 (q,  $J = 3.1$  Hz), 124.8 (q,  $J = 270.4$  Hz), 109.6, 85.3, 33.5, 27.9, 22.4, 13.9;  $^{19}\text{F}$  NMR (470 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.9; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{30}\text{H}_{29}\text{F}_3\text{NO}$   $[\text{M} +$

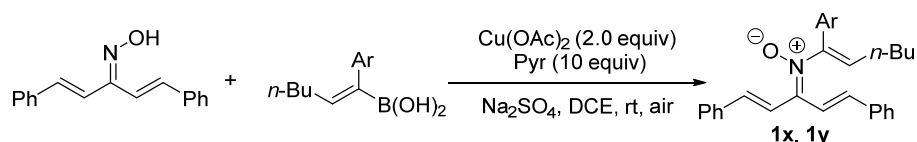
$[H]^+$ : 476.2196, found 476.2176.



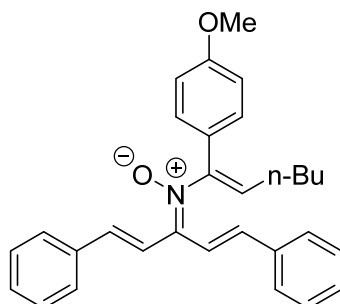
**3z**

**dimethyl 4,5-dimethyloxazole-2,2(5H)-dicarboxylate (3z).** A colorless oli, 0.009 g, 22% yield;  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  3.84 (s, 3H), 3.81 (s, 3H), 3.21 (q,  $J = 7.2$  Hz, 1H), 1.53 (s, 3H), 1.10 (d,  $J = 7.8$  Hz, 3H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  171.1, 169.7, 169.2, 106.7, 53.5, 53.4, 51.1, 22.5, 10.3; HRMS (ESI)  $m/z$  calcd for  $C_9H_{14}NO_5$   $[M + H]^+$ : 216.0866, found 216.0860.

## 6. Synthesis of *N*-vinyl nitrones **1x** and **1y**



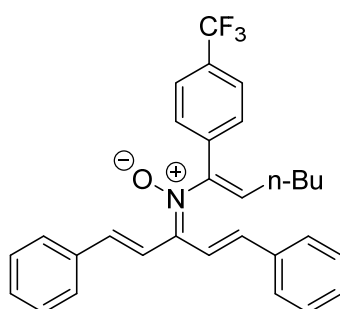
**General procedure B:** A scintillation vial was charged with oxime (1.0 mmol, 1.0 equiv), alkenyl boronic acid (3.0 mmol, 3.0 equiv),  $Cu(OAc)_2$  (2.0 equiv), and anhydrous  $Na_2SO_4$  (8.0 equiv). These solids were diluted with DCE to form a 0.1 M solution of oxime. Pyridine (10.0 equiv) was added to the resulting slurry via syringe. The scintillation vial was then capped with a septum pierced with a ventilation needle and the reaction mixture was stirred at 25 °C for 12 h. DCE and pyridine were removed under reduced pressure and the crude reaction mixture was purified by medium pressure chromatography (1/6 to 1/1, ethyl acetate/petroleum ether) to give nitrones **1x** and **1y**.



**1x**

**(1E,4E)-N-((E)-1-(4-methoxyphenyl)hex-1-en-1-yl)-1,5-diphenylpenta-1,4-dien-3-imine oxide (1x).** A yellow oli, 0.184 g, 42% yield;  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.62-

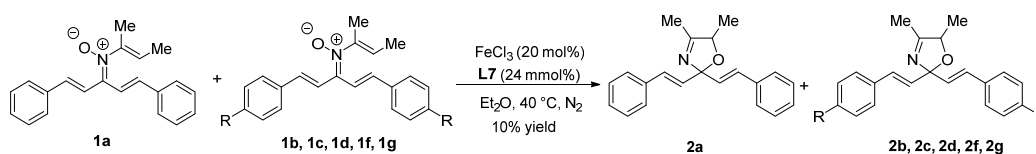
7.58 (m, 4H), 7.46 (d,  $J = 8.5$  Hz, 2H), 7.42-7.39 (m, 3H), 7.37-7.36 (m, 3H), 7.34-7.31 (m, 2H), 7.11 (d,  $J = 16.0$  Hz, 1H), 6.97-6.92 (m, 3H), 5.95 (t,  $J = 7.5$  Hz, 1H), 3.79 (s, 3H), 2.38-2.33 (m, 2H), 1.47-1.42 (m, 2H), 1.36-1.30 (m, 2H), 0.84 (t,  $J = 7.5$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  159.7, 146.2, 143.8, 139.8, 136.3, 136.0, 134.8, 130.0, 129.7, 129.1, 128.9, 128.8, 128.7, 127.4, 126.7, 125.3, 120.3, 118.7, 113.9, 55.1, 31.4, 27.7, 22.3, 13.7; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{30}\text{H}_{32}\text{NO}_2$  [ $\text{M} + \text{H}$ ] $^+$ : 438.2428, found 438.2411.



**1y**

**(1E,4E)-1,5-diphenyl-N-((E)-1-(4-(trifluoromethyl)phenyl)hex-1-en-1-yl)penta-1,4-dien-3-imine oxide (1y).** A yellow oli, 0.399 g, 84% yield;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69-7.64 (m, 5H), 7.61 (d,  $J = 7.0$  Hz, 2H), 7.57 (d,  $J = 16.5$  Hz, 1H), 7.42-7.37 (m, 6H), 7.35-7.33 (m, 2H), 7.09 (d,  $J = 16.0$  Hz, 1H), 6.99 (d,  $J = 16.5$  Hz, 1H), 6.12 (t,  $J = 7.5$  Hz, 1H), 2.39-2.34 (m, 2H), 1.51-1.46 (m, 2H), 1.37-1.31 (m, 2H), 0.86 (t,  $J = 7.5$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  146.1, 142.9, 139.9, 136.6, 136.3, 135.9, 134.9, 132.4, 131.0 (q,  $J = 32.6$  Hz), 129.2, 129.0, 128.9, 128.8, 128.7, 127.4, 127.0 (q,  $J = 270.9$  Hz), 126.7, 125.5 (q,  $J = 3.6$  Hz), 120.0, 118.6, 31.3, 27.7, 22.3, 13.7;  $^{19}\text{F}$  NMR (470 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.7; HRMS (ESI)  $m/z$  calcd for  $\text{C}_{30}\text{H}_{29}\text{F}_3\text{NO}$  [ $\text{M} + \text{H}$ ] $^+$ : 476.2196, found 476.2179.

## 7. Description of Hammett study experiments

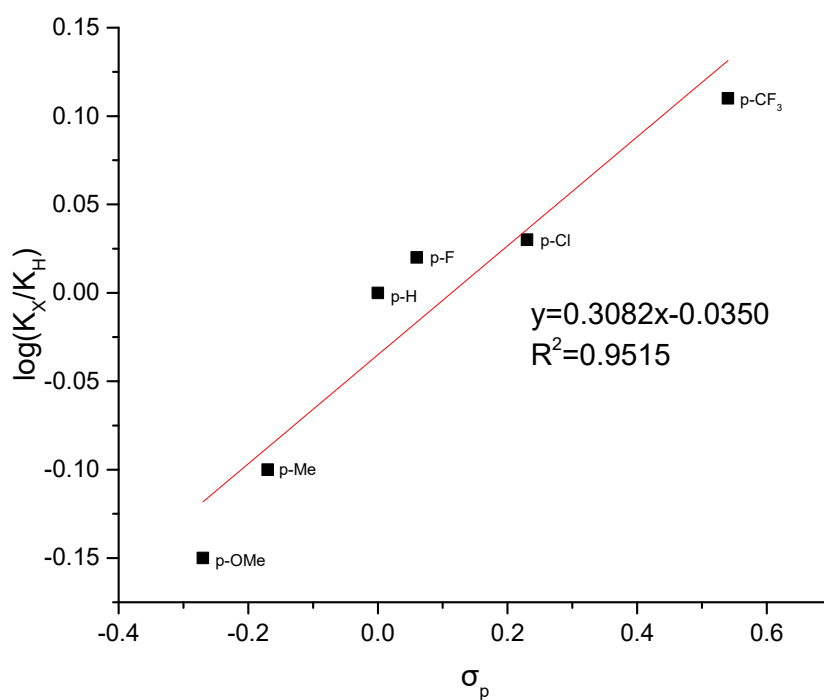


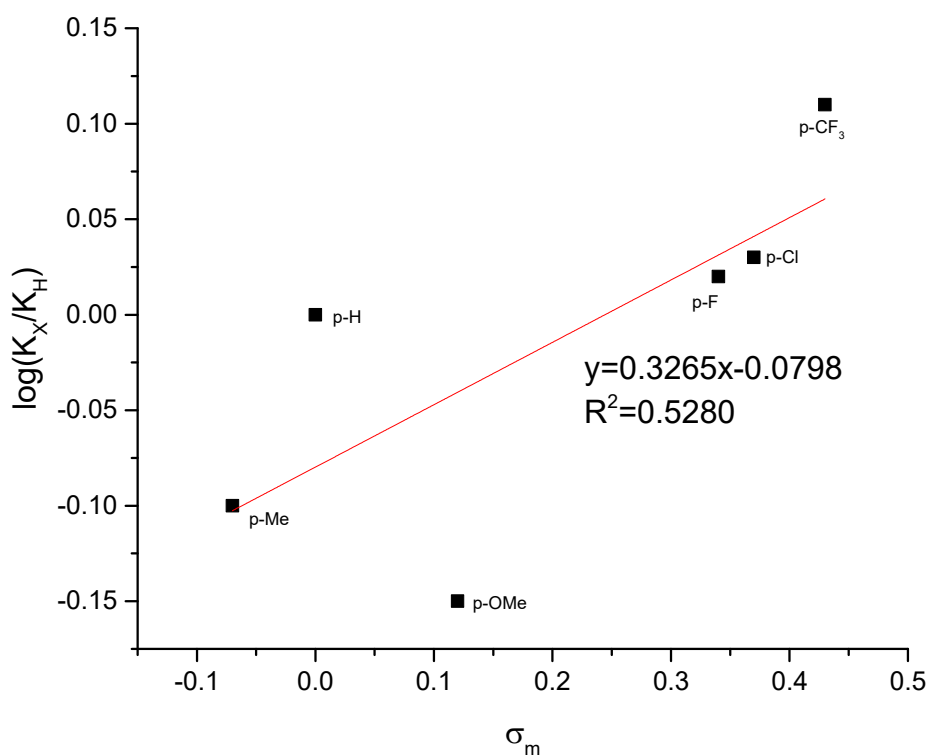
Competition experiments were set up using general procedure **B** but substituting **1**

equiv. of **1** for a 1:1 mixture of 0.5 equiv. of **1a** and 0.5 equiv. of **1b**, **1c**, **1d**, **1f**, or **1g**. Then conversion reaction was carried out for 1h. At this time, the ratio of the 2,5-dihydrooxazole resonances was recorded as in indication of the relative initial rates of the two substrates. The results were then plotted against Hammett parameters as illustrated in **Table S2**<sup>[7]</sup>

**Table S2.** Hammett parameters of substituents

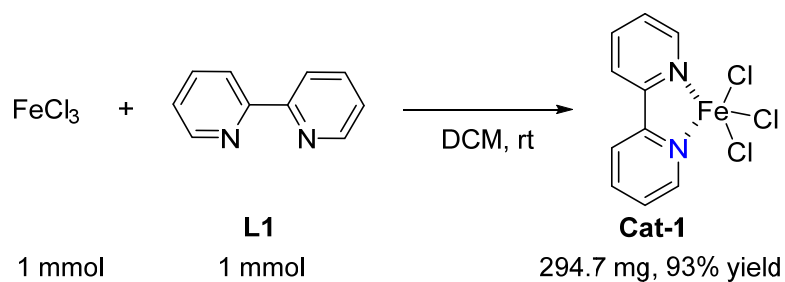
$\sigma_p$	$\sigma_m$	$K_X/K_H$	$\log(K_X/K_H)$
-0.27	0.12	0.70	-0.15
-0.17	-0.07	0.79	-0.10
0	0	0	0
0.06	0.34	1.05	0.02
0.23	0.37	1.08	0.03
0.54	0.43	1.29	0.11



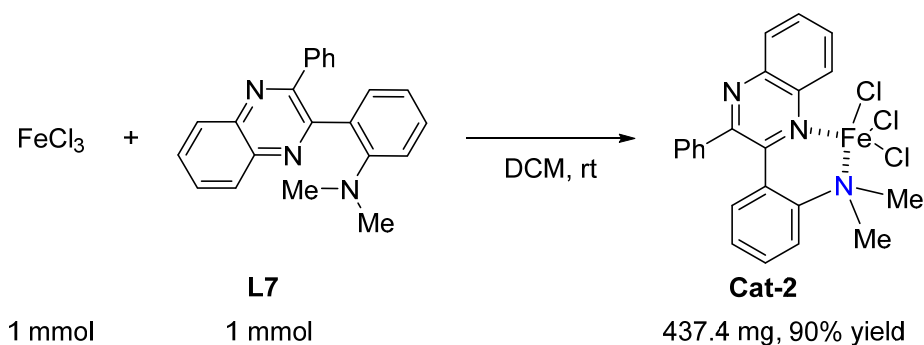
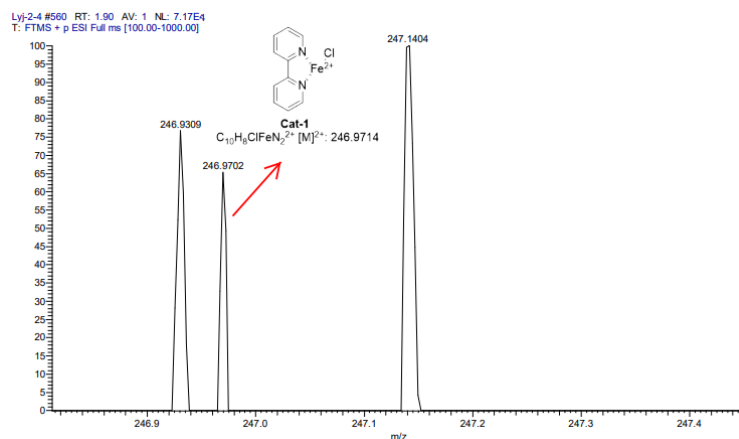


## 8. Studies of mechanism by HRMS (ESI)

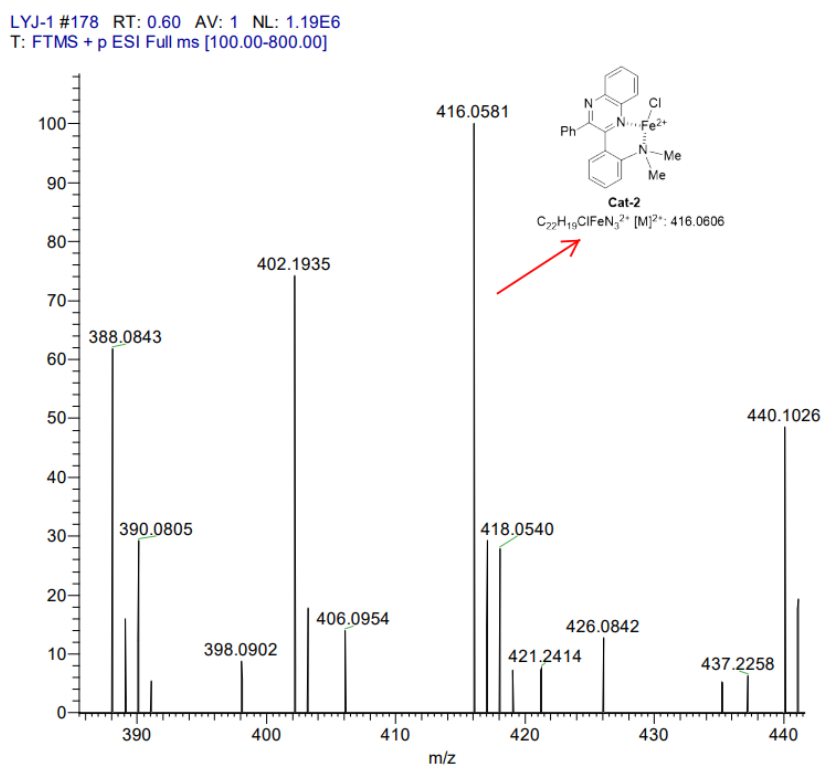
### 8.1 Synthesis of Cat-1. and Cat-2.



A solution of bipyridine **L1** (156 mg, 1.0 mmol) in DCM (20 mL) was added to a solution of  $\text{FeCl}_3$  (161 mg, 1.0 mmol) in DCM (20 mL) at rt for 1 h. After stirring for 1 h, the resulting mixture was filtered off, washed with hexane (3×3 mL), and dried in vacuo to afford  $\text{FeCl}_3 \cdot \text{L1}$  as a yellow solid 294.7 mg (93%) yield.

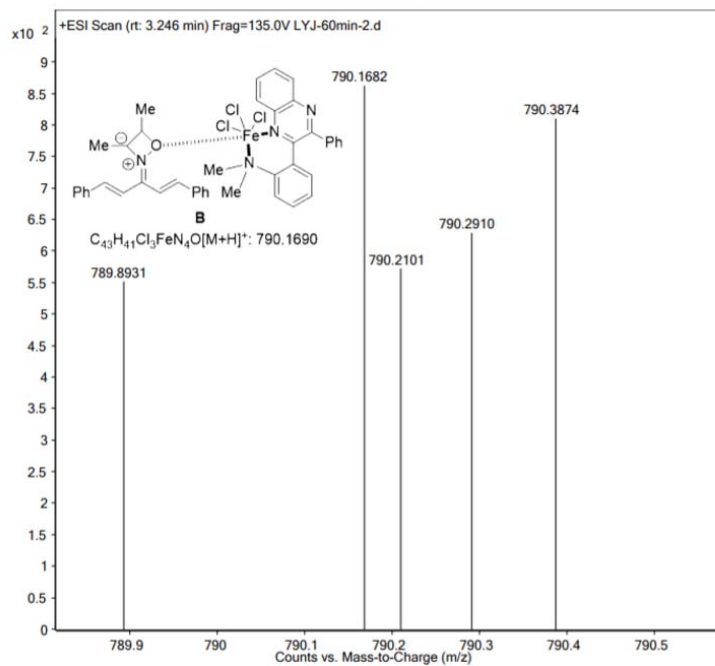
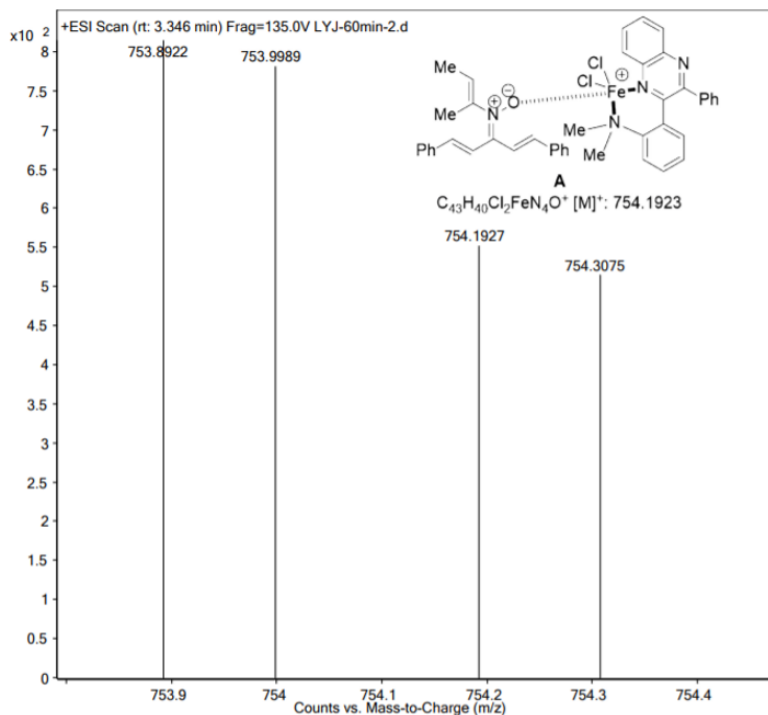


A solution of **L7** (325 mg, 1.0 mmol) in DCM (20 mL) was added to a solution of  $\text{FeCl}_3$  (161 mg, 1.0 mmol) in DCM (20 mL) at rt for 1 h. After stirring for 1 h, the resulting mixture was filtered off, washed with hexane (3×3 mL), and dried in vacuo to afford  $\text{FeCl}_3 \cdot \text{L7}$  as a black solid 437.4 mg (90%) yield.

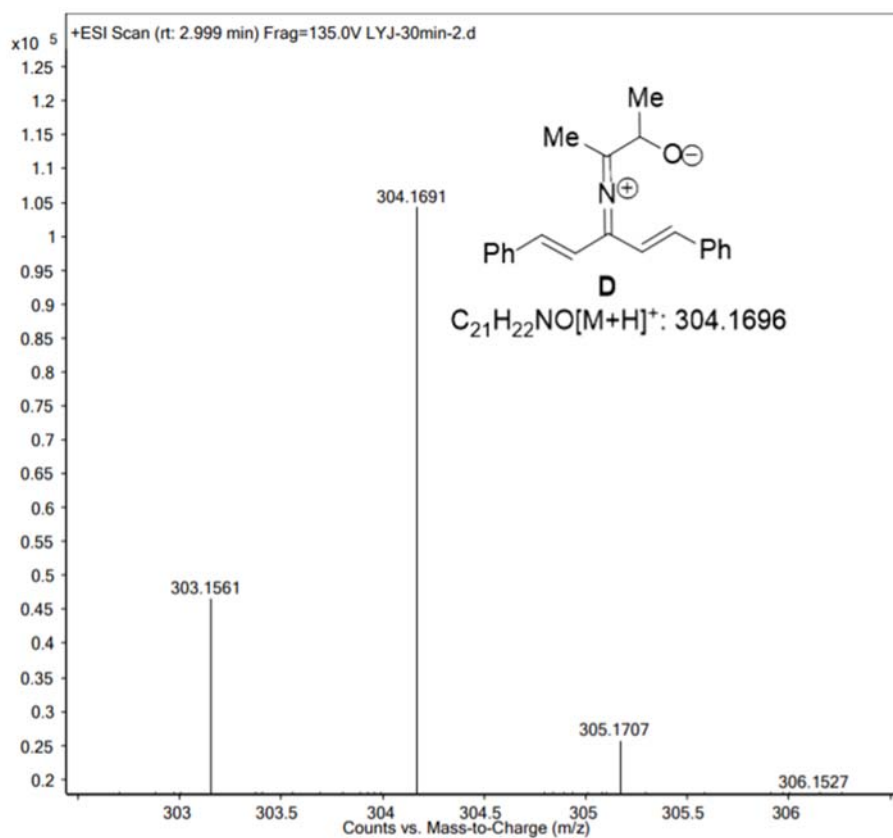
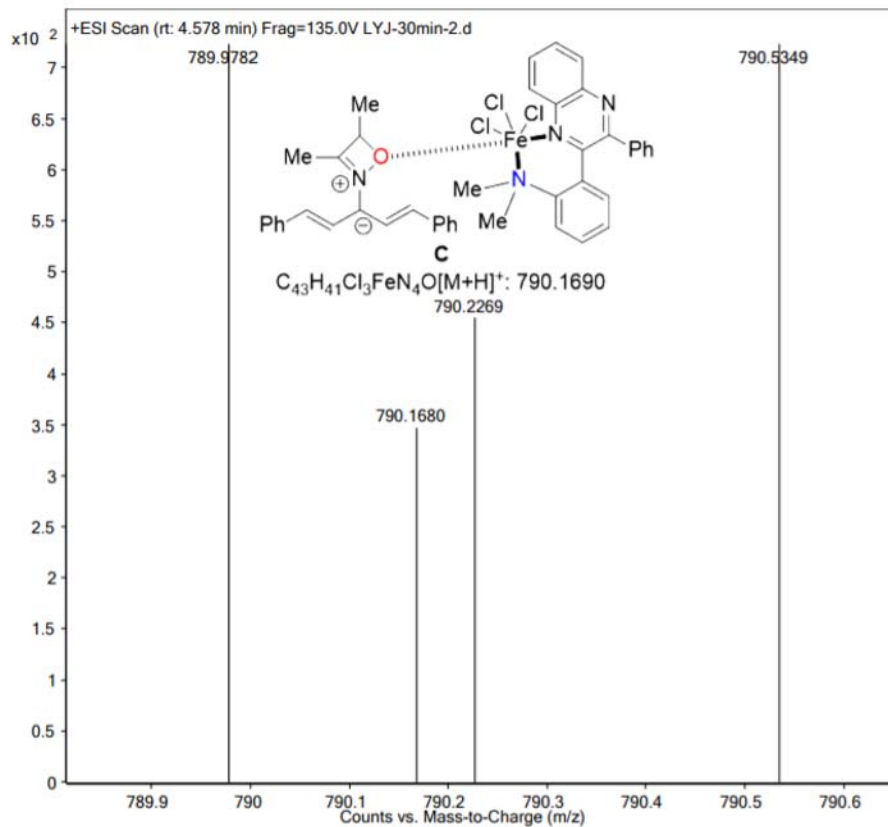


## 8.2 Intermediates detected by HRMS(ESI)

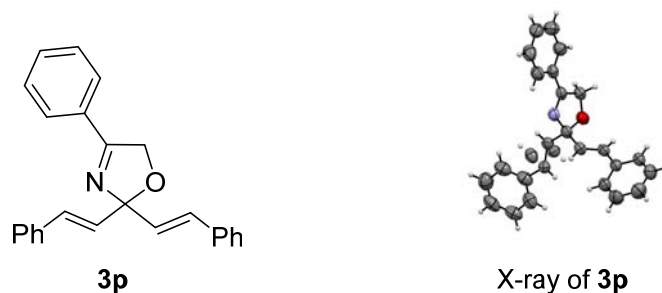
Nitron **1a** was carried out under the standard conditions for 30 min, then, the reaction mixture was directly detected by HRMS (ESI). The details of intermediates peaks are as follows:







## 9. X-ray structure for compound 3p



**Figure S1:** ORTEP diagram of **3p** at 50% ellipsoid probability

The preparation of crystal of **3p**: compound **3p** (15 mg) was dissolved in DCM (2 mL) at room temperature. n-Hexane (1.0 mL) was dropped carefully to the mixture. Then, the flask was capped with thin film. Finally, a needle crystal was obtained for 2 days.

**Table S3.** Crystal data and structure refinement details for compound **3p**

Empirical formula	C <sub>25</sub> H <sub>21</sub> NO
Formula weight ( <i>M</i> )	351.43
Crystal system	triclinic
Space group	(2)
<i>a</i> /Å	10.0700(5)
<i>b</i> /Å	10.0719(4)
<i>c</i> /Å	10.4742(5)
$\alpha$ /°	83.935(4)
$\beta$ /°	79.110(4)
$\gamma$ /°	66.858(4)
<i>V</i> / Å <sup>3</sup>	958.68(8)
<i>Z</i>	2
<i>D<sub>c</sub></i> (Mg cm <sup>-3</sup> )	1.217
<i>F</i> (000)	372
2 $\theta$ range for data collection (°)	8.60 to 151.41
Reflections collected	12109
Independent reflections	3755 [R(int) = 0.0504, R(sigma) =

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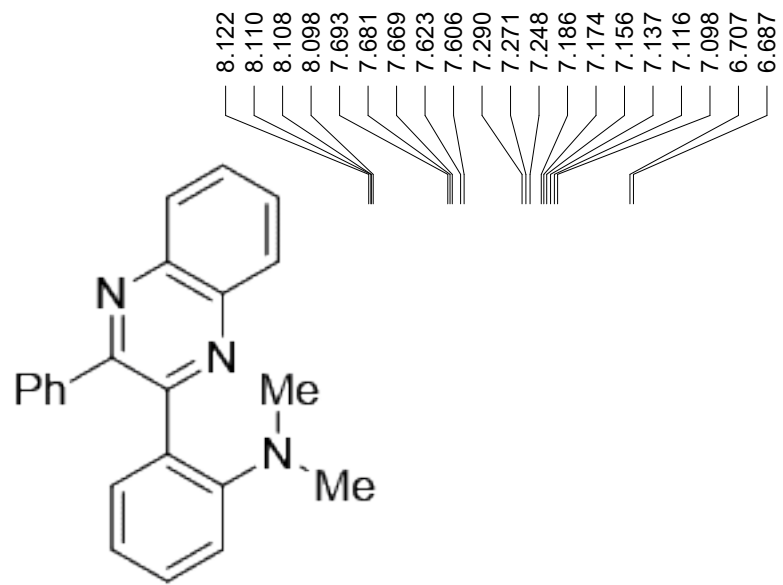
	0.0487]
Goodness-of-fit on F <sup>2</sup>	1.087
Final R indices [I>2sigma(I)]	R <sub>1</sub> = 0.0630, ωR <sub>2</sub> = 0.1787
R indices (all data)	R <sub>1</sub> = 0.0742, ωR <sub>2</sub> = 0.1873

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## 10. References

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- [6] Chen, H.; Wei, C.; Pang, G.-L.; Liang, C.; Mo, D.-L.; Ma, X.-P. *Org. Lett.* **2022**, *24*, 6013.
- [7] Hansch, C.; Leo, A.; Taft, R. W. *Chem. Rev.* **1991**, *91*, 165.

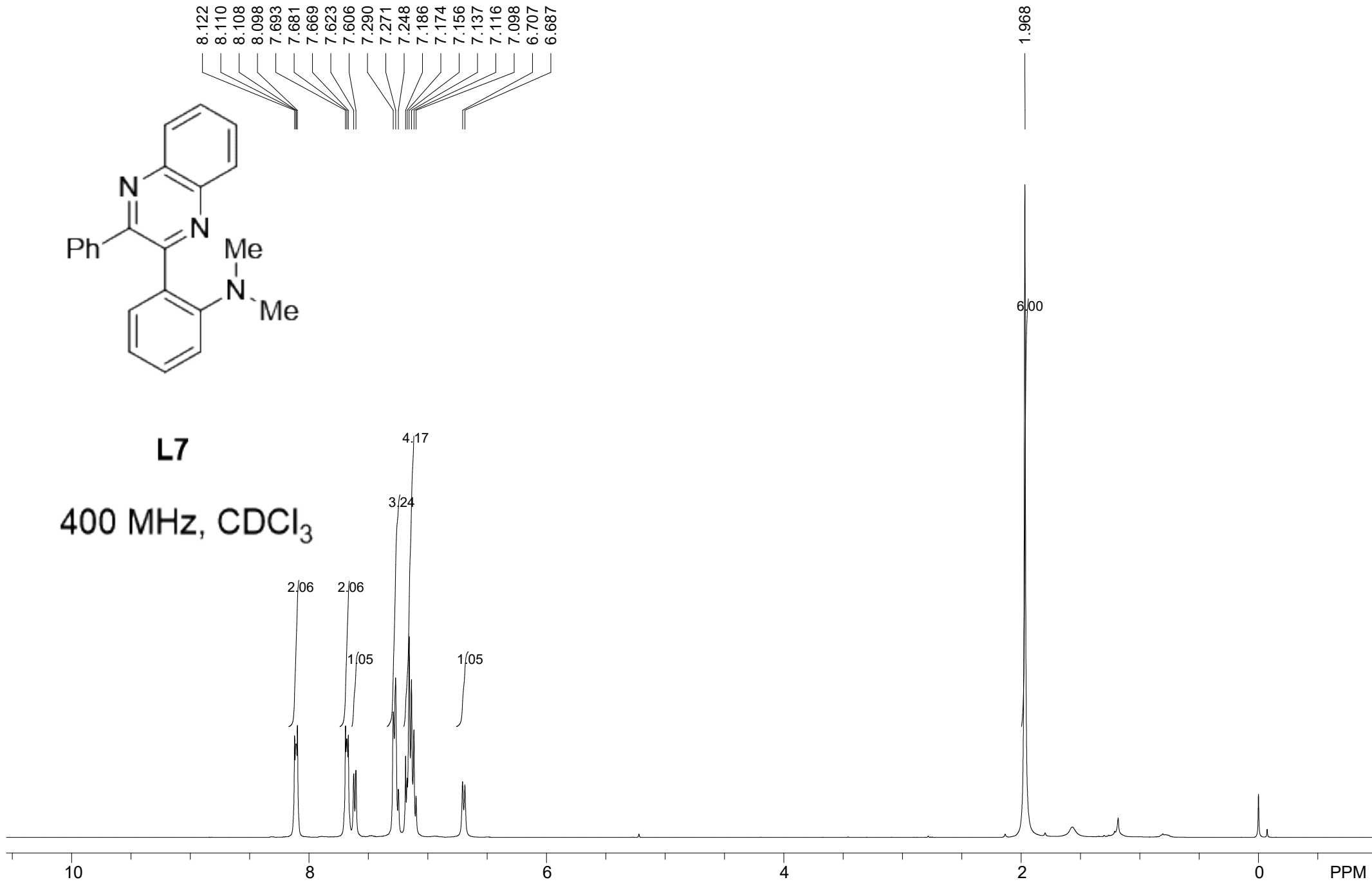
## 11. NMR spectra for compounds L7, L8, 1x-1y, 2a, and 3

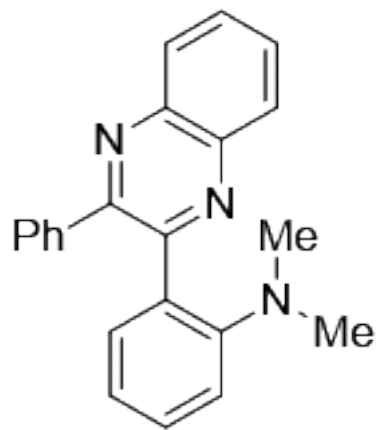


8.122  
8.110  
8.108  
8.098  
7.693  
7.681  
7.669  
7.623  
7.606  
7.290  
7.271  
7.248  
7.186  
7.174  
7.156  
7.137  
7.116  
7.098  
6.707  
6.687

**L7**

400 MHz, CDCl<sub>3</sub>

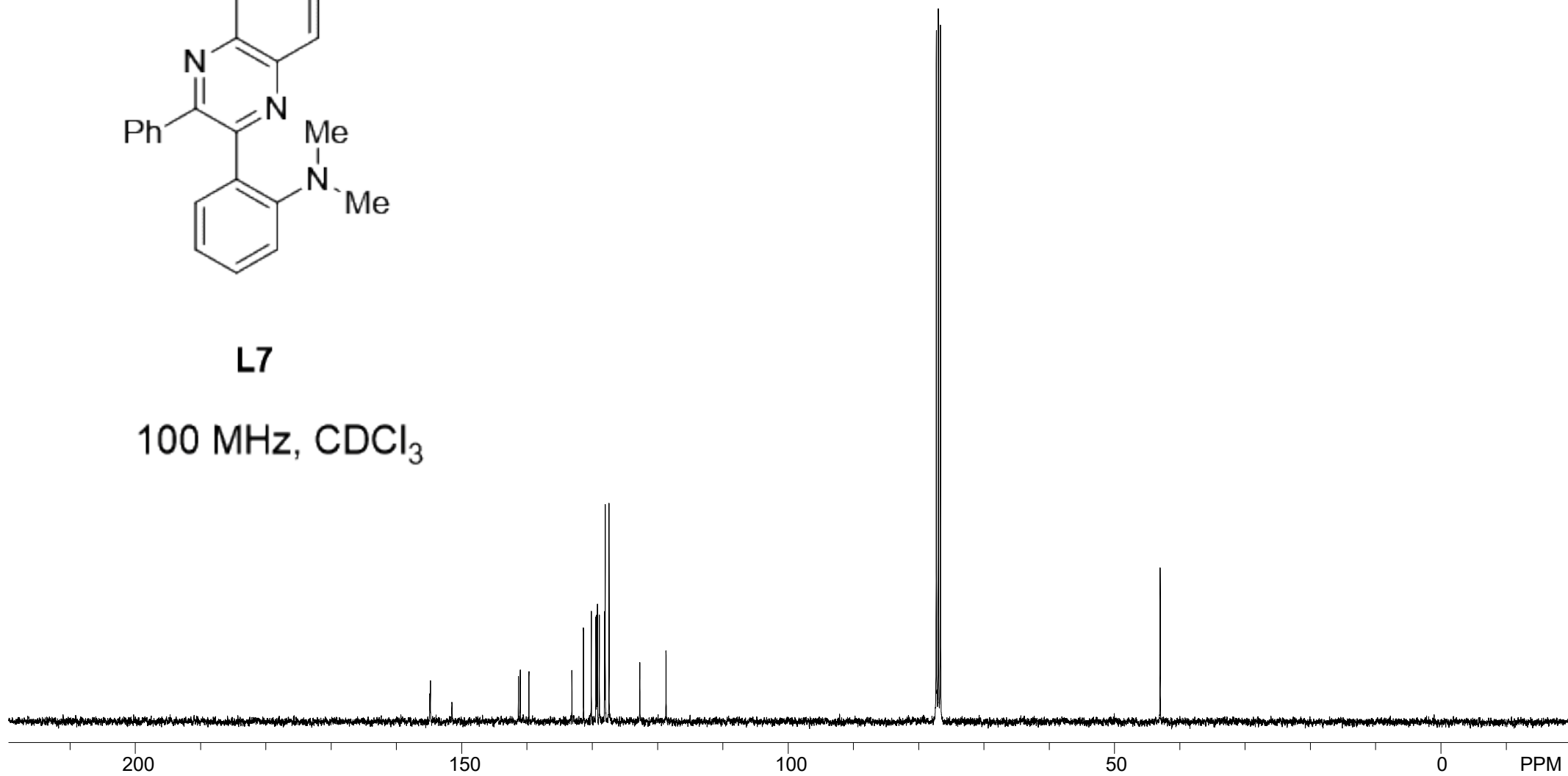




L7

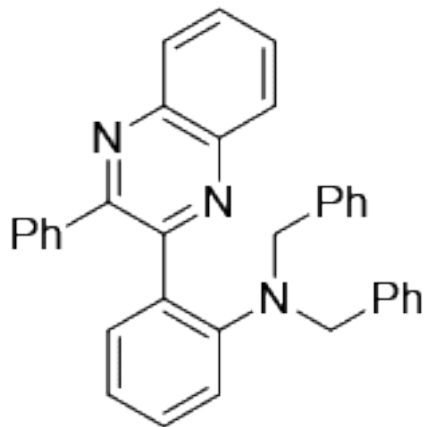
100 MHz, CDCl<sub>3</sub>

154.888  
154.800  
151.512  
141.318  
141.049  
139.714  
133.130  
131.365  
130.162  
129.455  
129.346  
129.229  
128.937  
128.128  
128.033  
127.443  
122.732  
118.715  
77.314  
77.000  
76.679  
42.992



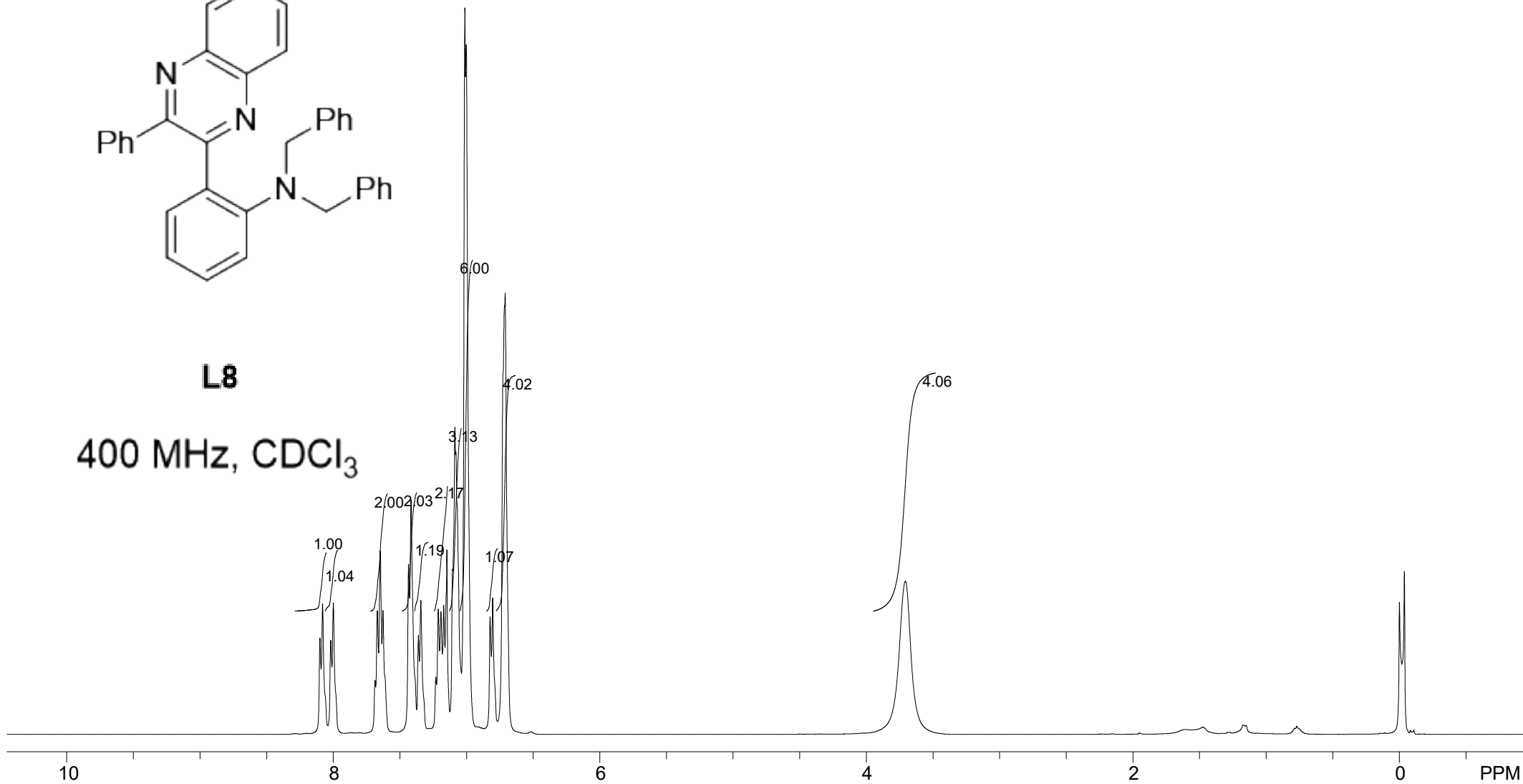
8.100  
8.080  
8.019  
7.999  
7.687  
7.670  
7.649  
7.627  
7.435  
7.416  
7.361  
7.343  
7.231  
7.212  
7.192  
7.172  
7.147  
7.105  
7.088  
7.080  
7.013  
7.002  
6.823  
6.805  
6.715  
6.710

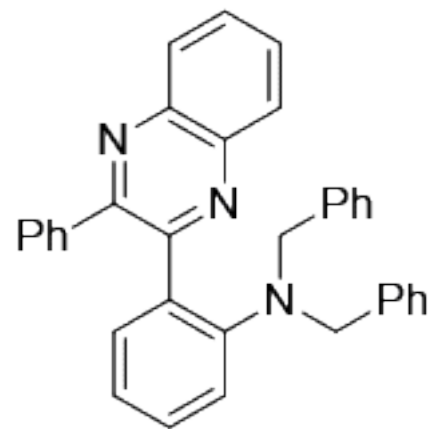
3.707



**L8**

400 MHz, CDCl<sub>3</sub>





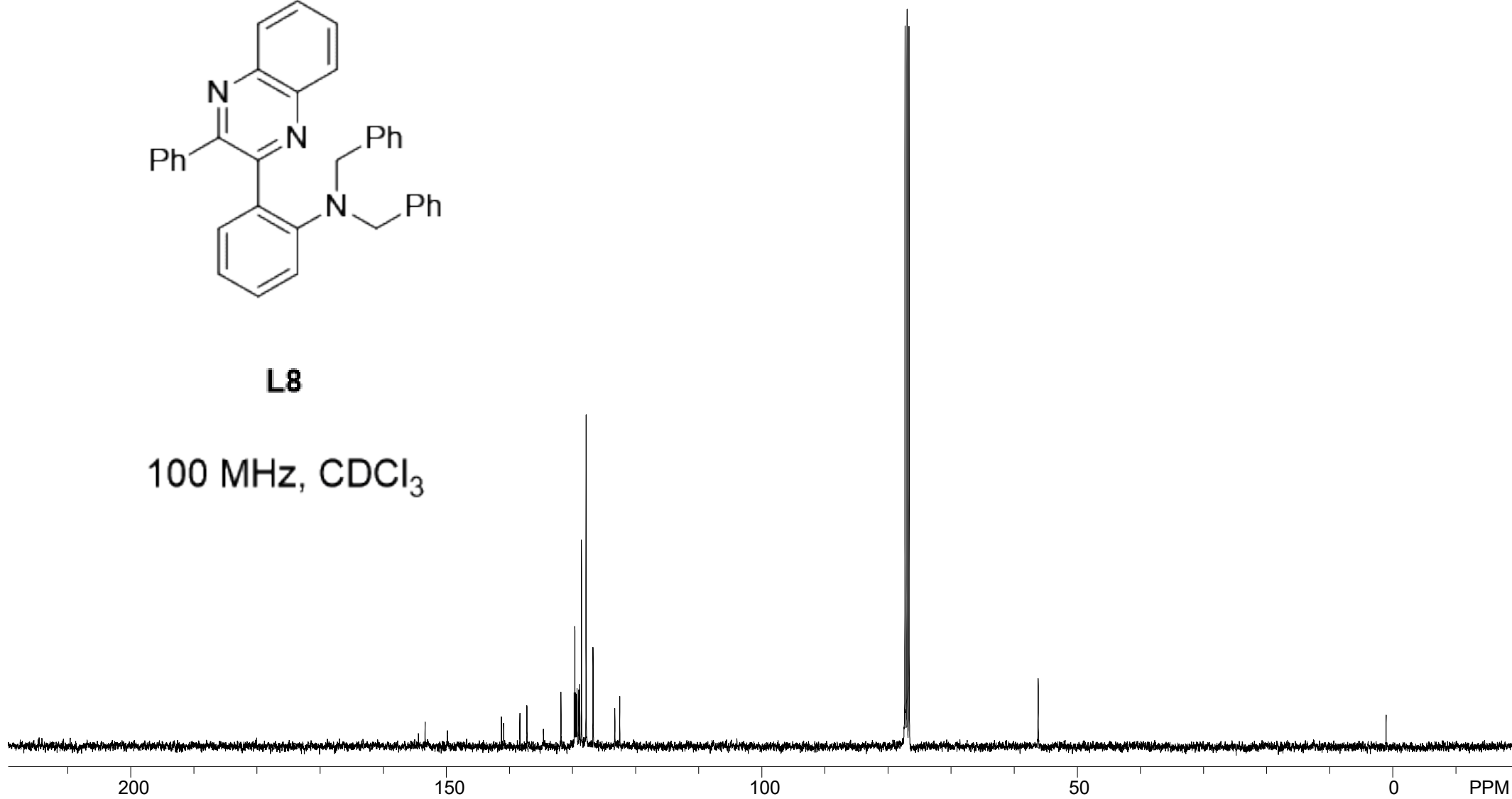
**L8**

100 MHz, CDCl<sub>3</sub>

154.428  
153.364  
149.835  
141.275  
140.917  
138.351  
137.242  
134.617  
131.847  
129.747  
129.637  
129.521  
129.404  
129.280  
129.010  
128.945  
128.872  
128.595  
127.858  
126.757  
123.308  
122.521

77.321  
77.000  
76.686

56.197

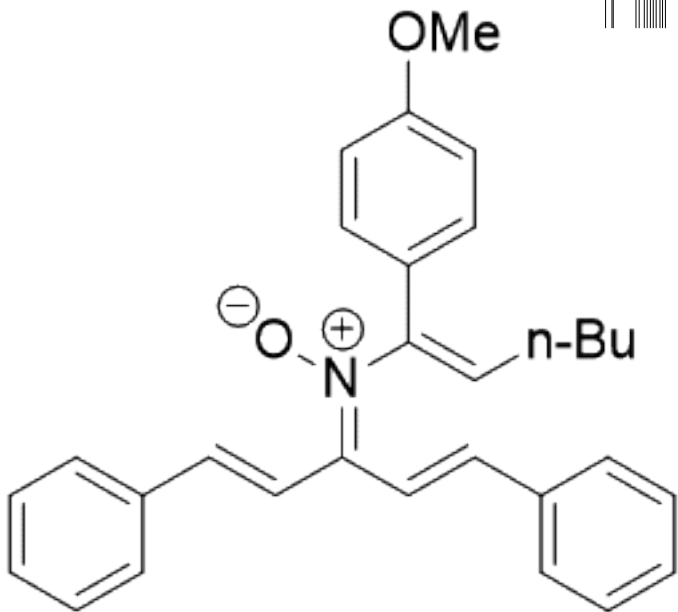


7.618  
7.585  
7.578  
7.460  
7.443  
7.416  
7.401  
7.385  
7.371  
7.355  
7.335  
7.321  
7.307  
7.108  
7.076  
6.973  
6.940  
6.932  
6.915  
5.954  
5.939  
5.923

3.793

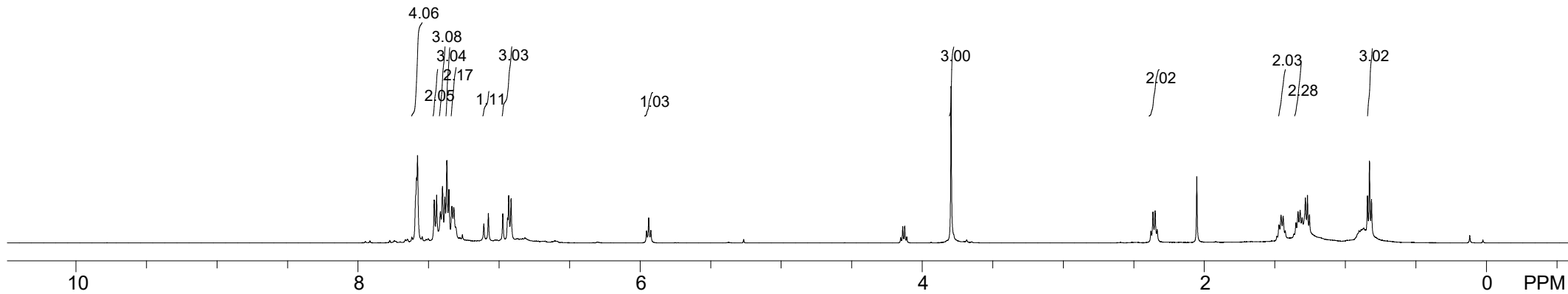
2.376  
2.361  
2.346  
2.332

1.468  
1.453  
1.438  
1.423  
1.362  
1.347  
1.332  
1.317  
1.303  
0.840  
0.825  
0.811

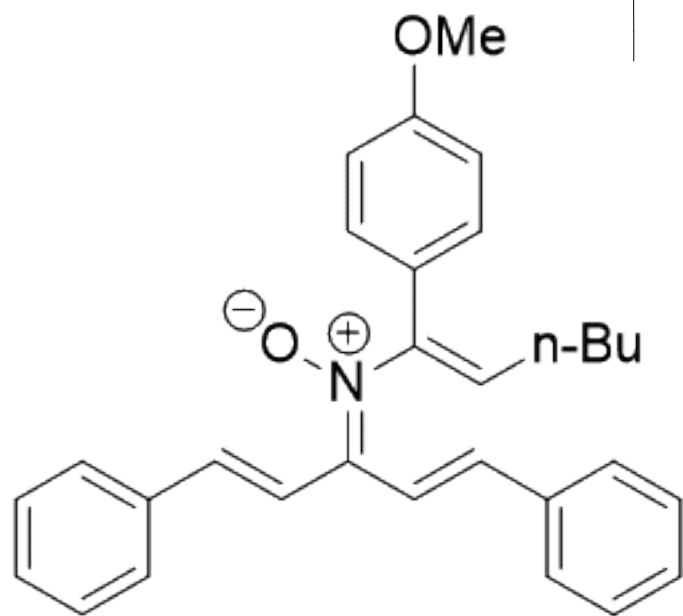


**1x**

500 MHz, CDCl<sub>3</sub>

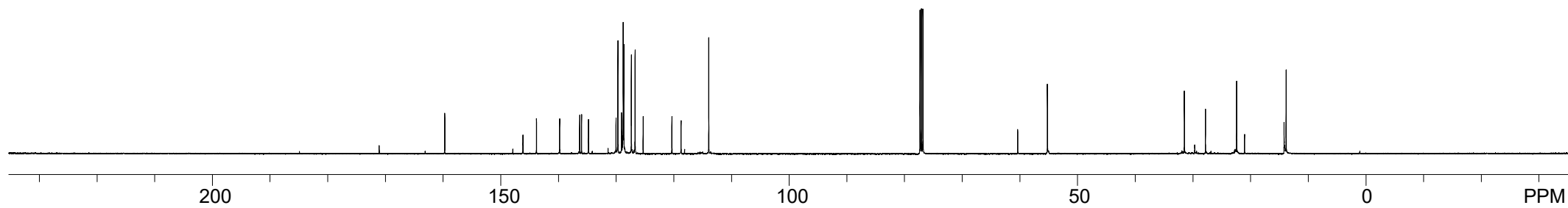
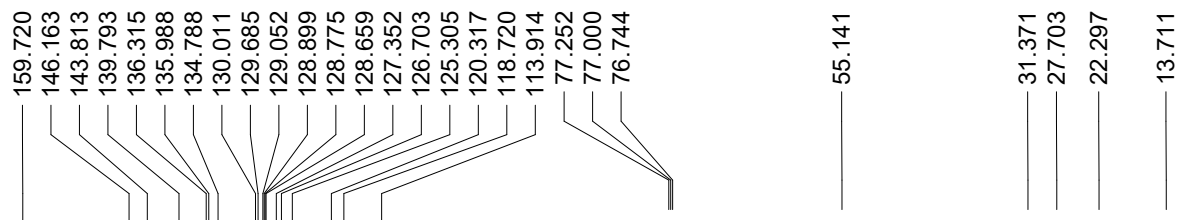


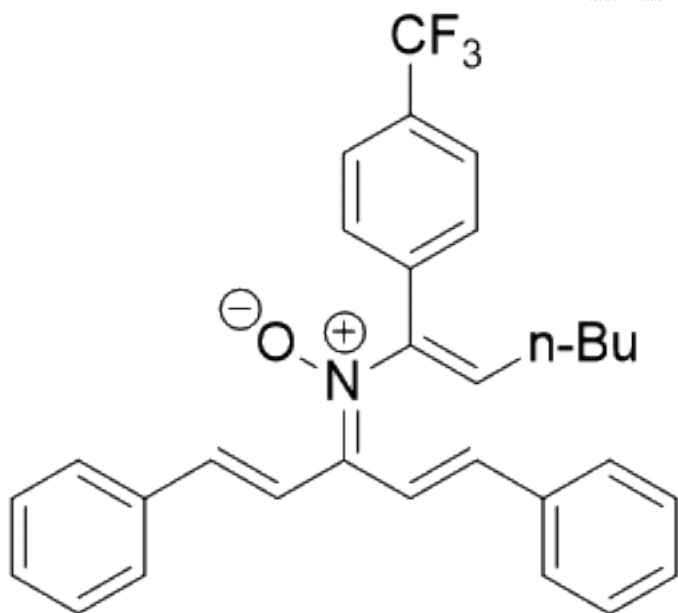




**1x**

125 MHz, CDCl<sub>3</sub>



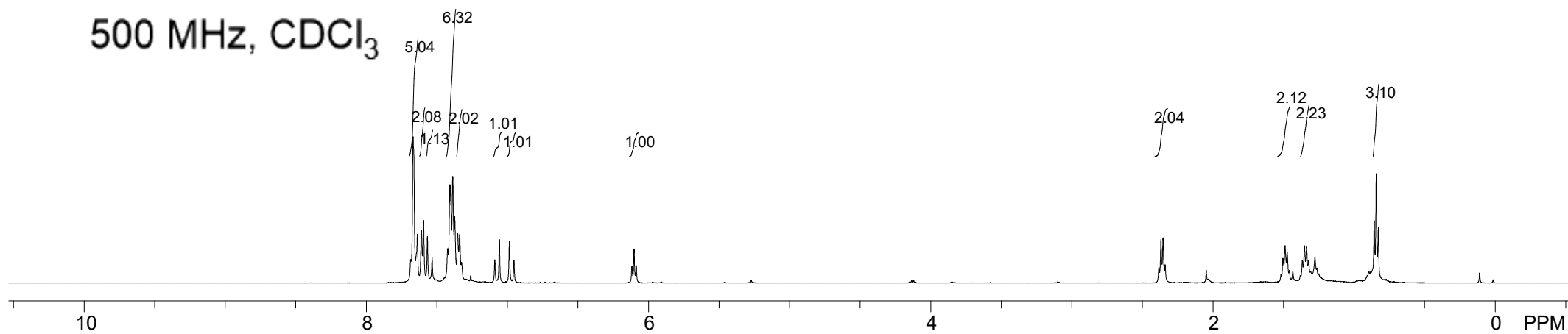


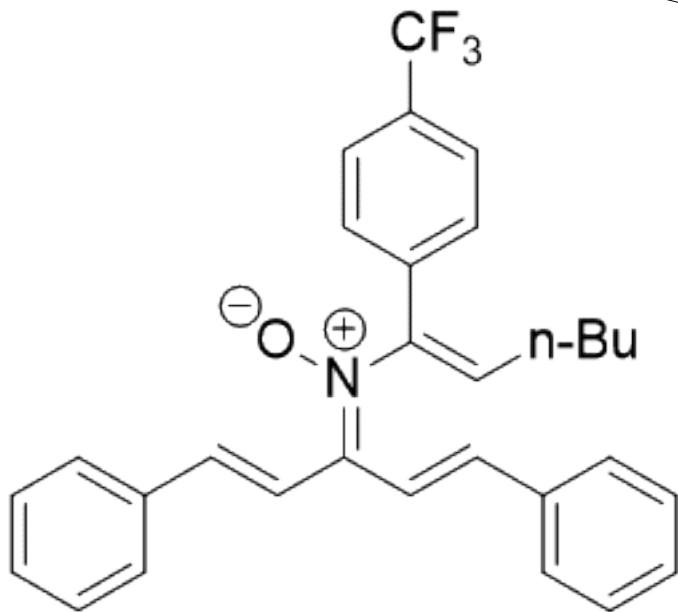
**1y**

500 MHz, CDCl<sub>3</sub>

7.685  
7.668  
7.665  
7.638  
7.609  
7.595  
7.567  
7.534  
7.423  
7.407  
7.387  
7.374  
7.352  
7.338  
7.325  
7.089  
7.057  
6.986  
6.953  
6.118  
6.103  
6.087

2.385  
2.370  
2.356  
2.341  
1.506  
1.491  
1.476  
1.461  
1.369  
1.353  
1.338  
1.324  
1.309  
0.860  
0.845  
0.831

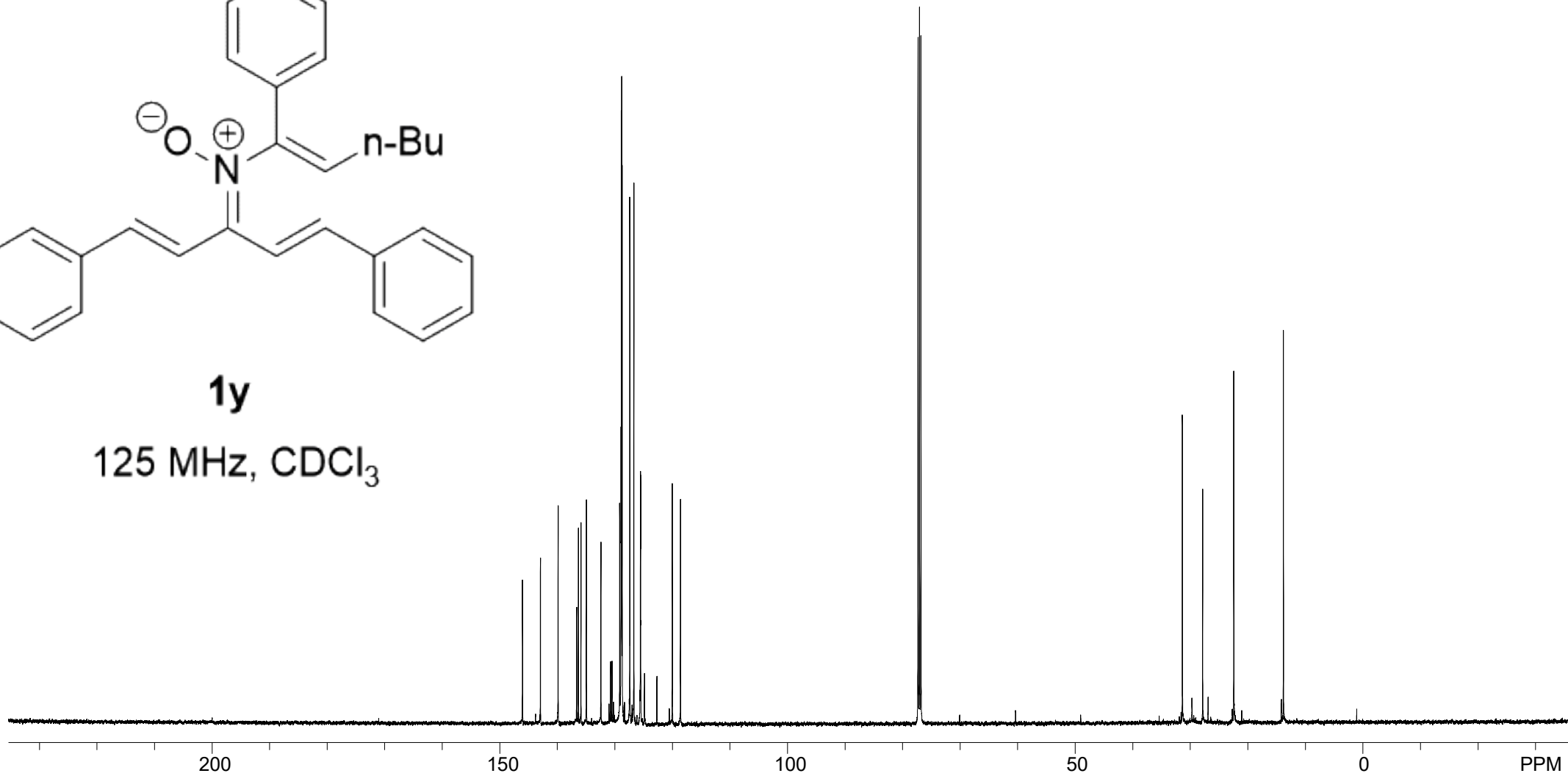


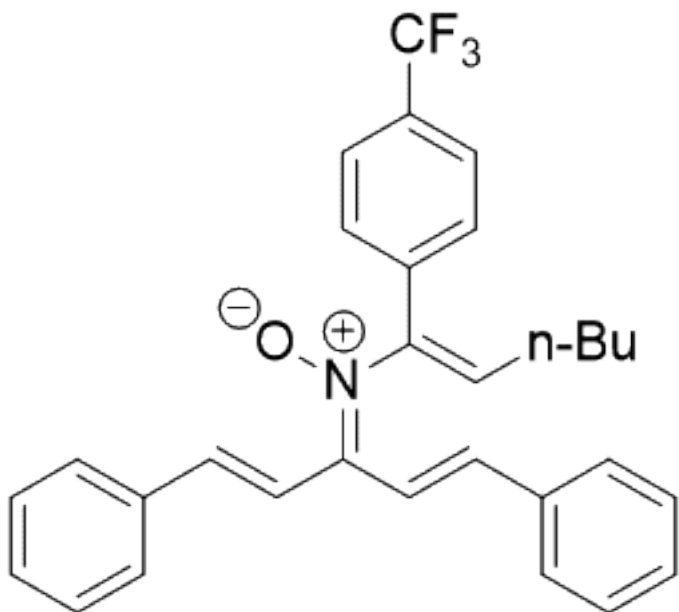


**1y**

125 MHz, CDCl<sub>3</sub>

146.059  
142.936  
139.863  
136.629  
136.335  
135.885  
134.946  
132.414  
131.000  
130.739  
130.483  
130.222  
129.151  
128.919  
128.870  
128.816  
128.717  
127.389  
127.009  
126.682  
125.536  
125.507  
125.478  
124.845  
122.678  
120.515  
119.990  
118.571  
77.256  
77.000  
76.748  
31.268  
27.736  
22.318  
13.686

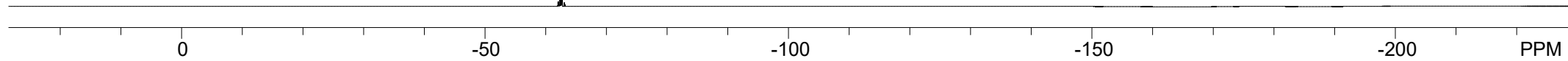




**1y**

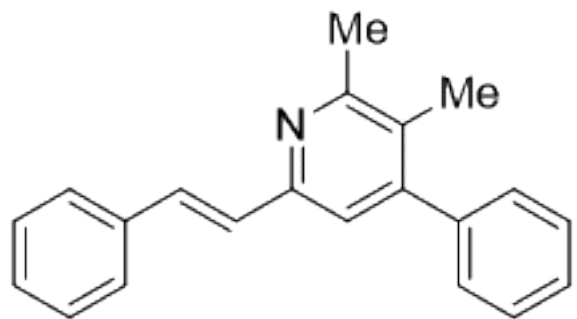
470 MHz, CDCl<sub>3</sub>

62.698



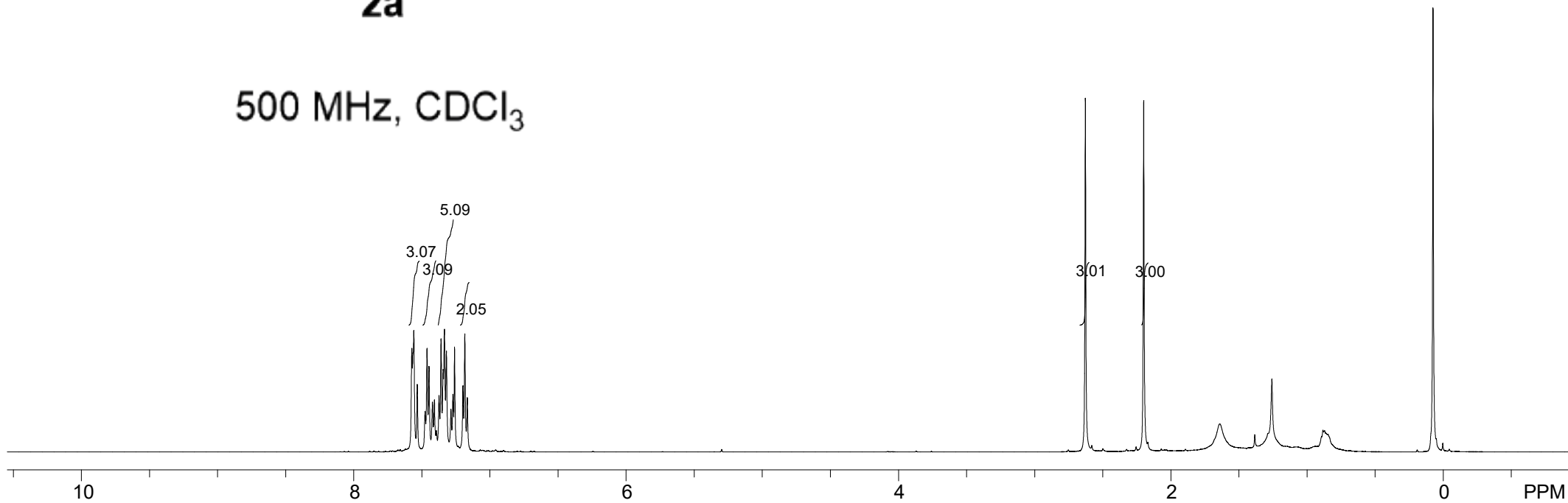
7.573  
7.565  
7.559  
7.533  
7.476  
7.462  
7.447  
7.422  
7.408  
7.374  
7.359  
7.343  
7.334  
7.319  
7.287  
7.272  
7.260  
7.198  
7.184  
7.166

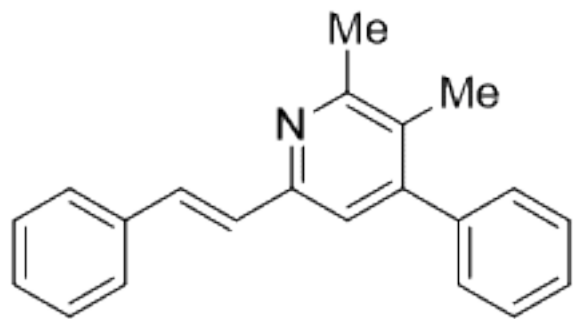
2.627  
2.198



**2a**

500 MHz, CDCl<sub>3</sub>





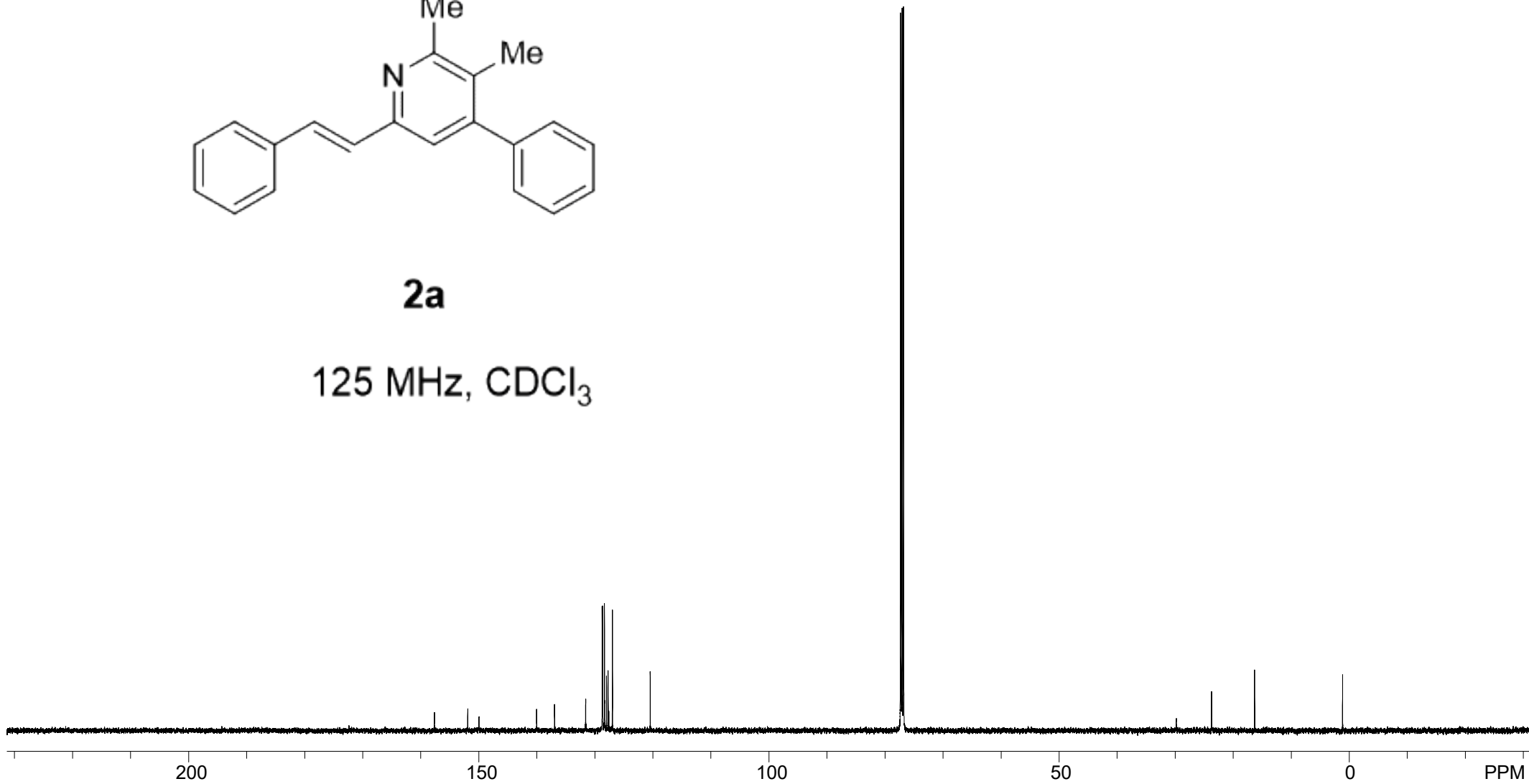
**2a**

125 MHz, CDCl<sub>3</sub>

157.643  
151.911  
149.979  
140.038  
136.943  
131.572  
128.730  
128.646  
128.329  
128.281  
127.976  
127.700  
127.579  
126.950  
120.436

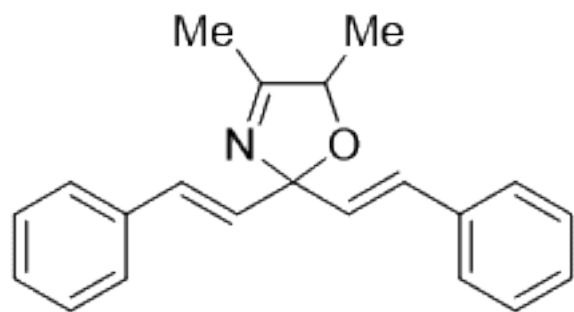
77.257  
77.000  
76.747

23.603  
16.179



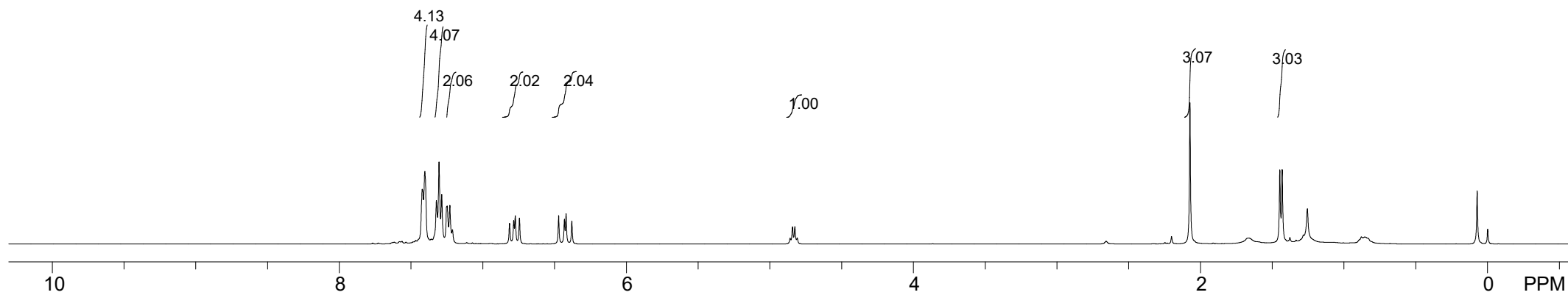
7.422  
7.404  
7.360  
7.323  
7.305  
7.286  
7.253  
7.248  
7.230  
7.212  
6.814  
6.785  
6.774  
6.745  
6.472  
6.432  
6.420  
6.380  
4.859  
4.843  
4.826  
4.810

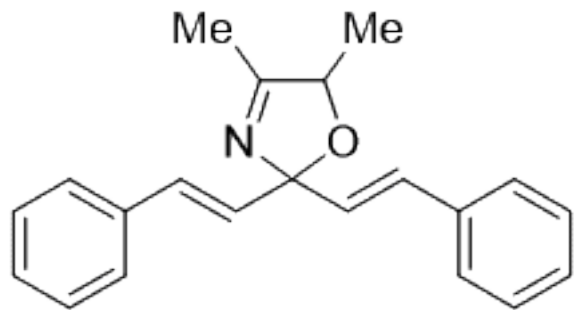
2.074  
1.448  
1.431



**3a**

400 MHz, CDCl<sub>3</sub>





**3a**

100 MHz, DMSO-*d*<sub>6</sub>

172.382

132.593

131.382

137.084

129.939

129.581

129.436

129.100

128.765

128.736

127.591

127.576

109.107

83.506

41.077

40.873

40.661

40.450

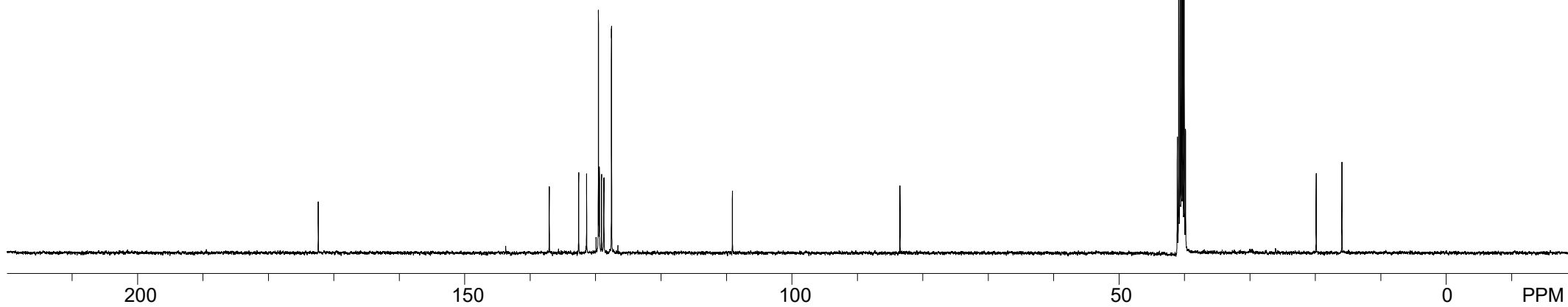
40.246

40.034

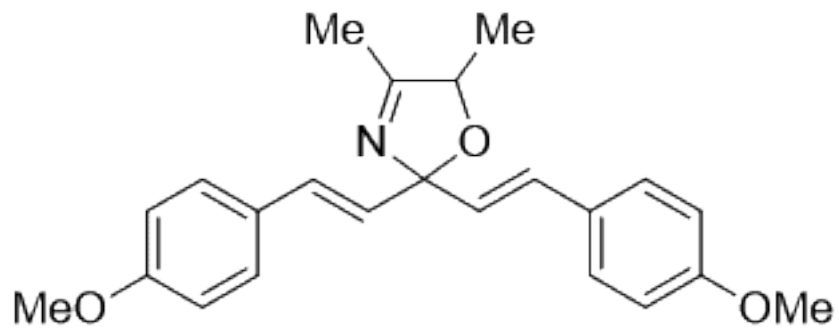
39.830

19.837

15.900







**3b**

400 MHz, CDCl<sub>3</sub>

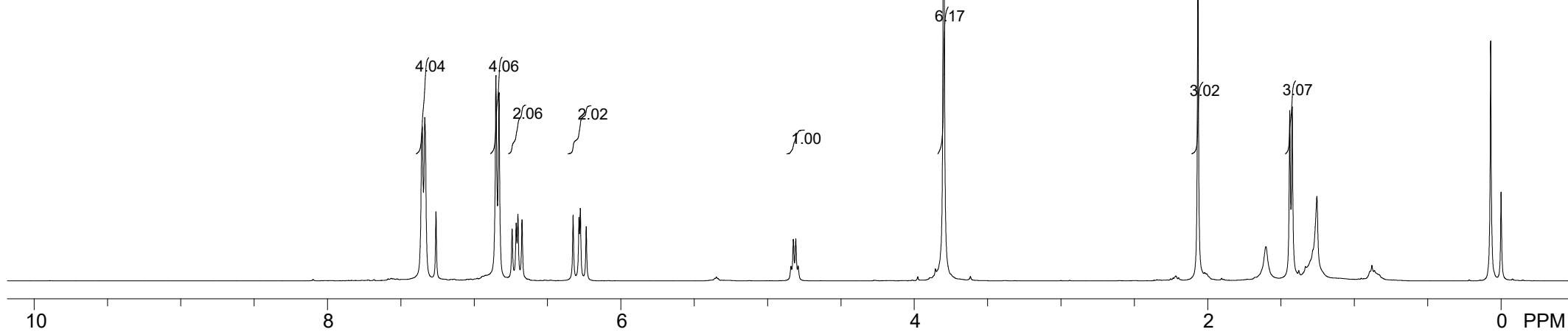
7.354  
7.336  
6.852  
6.830  
6.742  
6.714  
6.701  
6.674  
6.326  
6.285  
6.276  
6.236

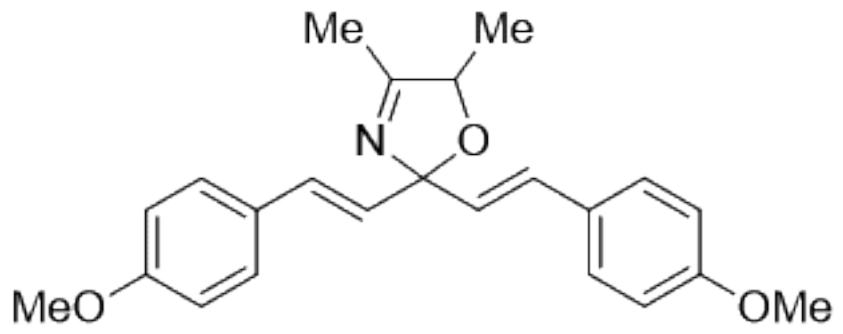
4.840  
4.824  
4.807  
4.792

3.799

2.066

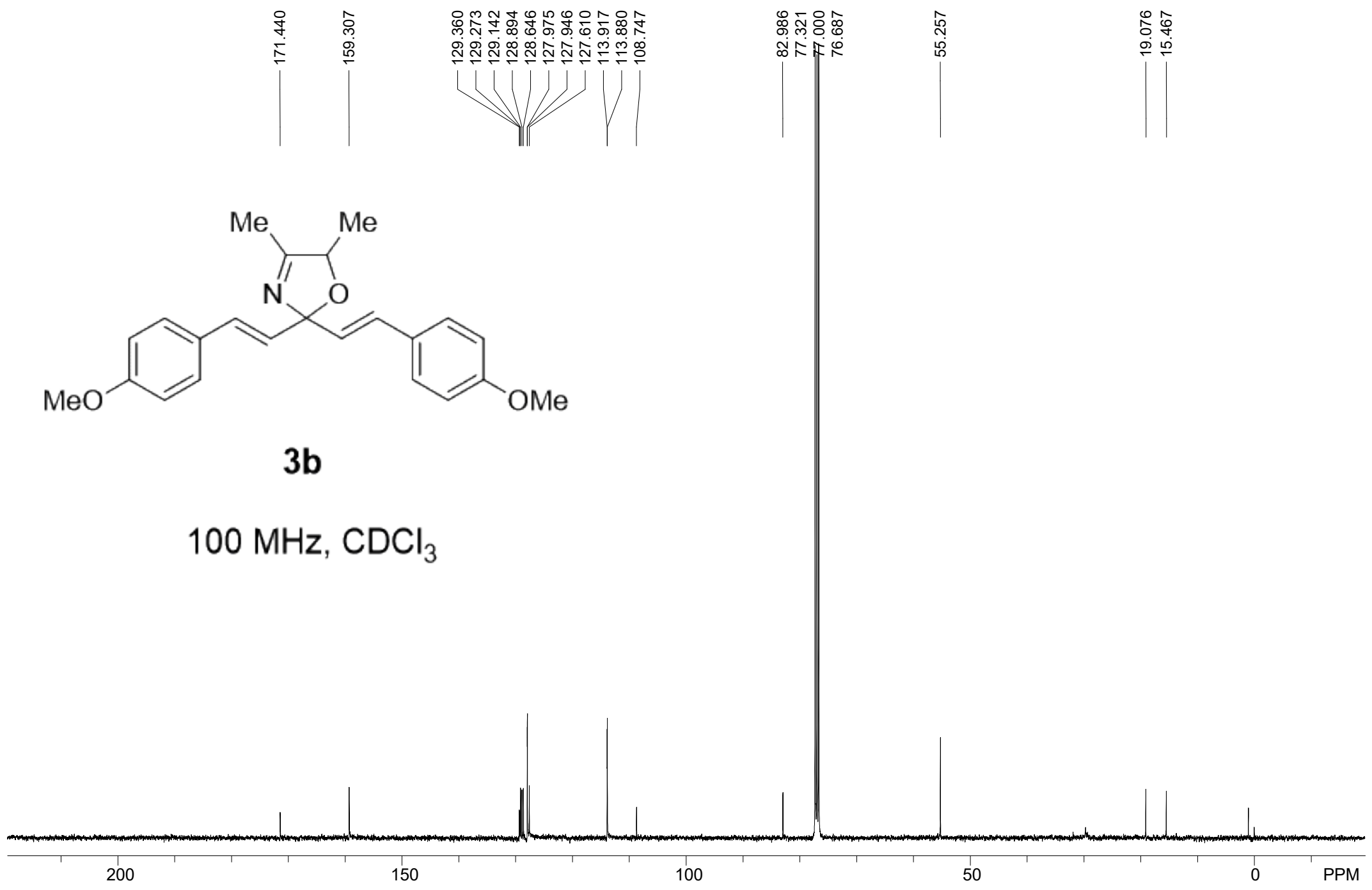
1.440  
1.424

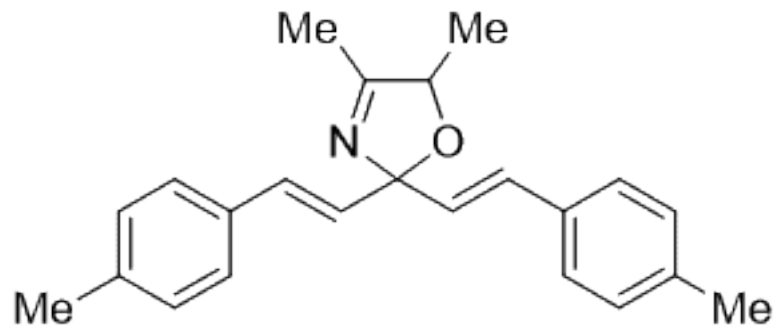




**3b**

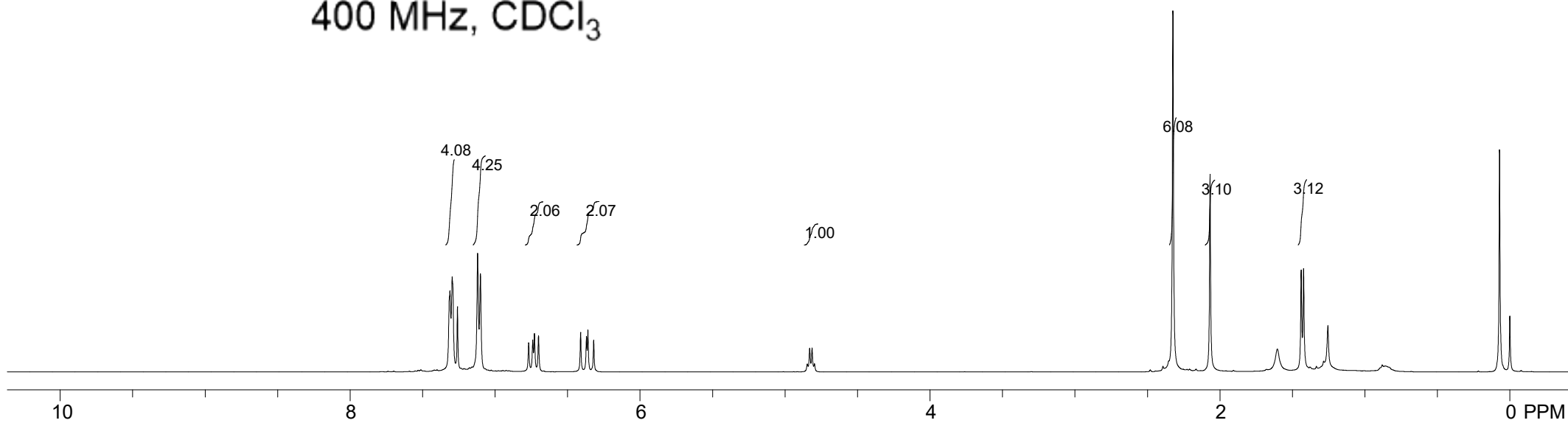
100 MHz, CDCl<sub>3</sub>

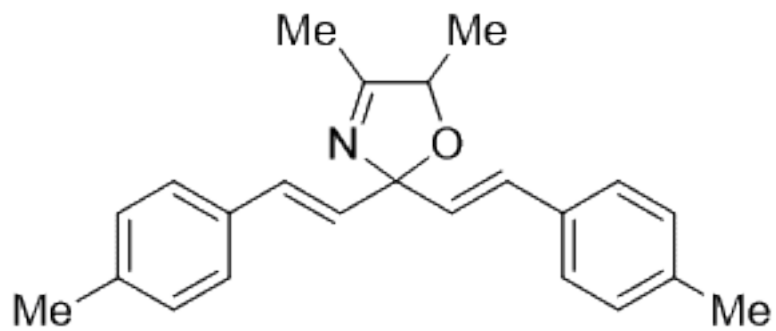




**3c**

400 MHz, CDCl<sub>3</sub>





**3c**

100 MHz, CDCl<sub>3</sub>

171.556

133.794

137.585

133.713

129.944

129.623

129.215

129.178

129.156

128.682

126.684

126.662

108.696

83.052

77.321

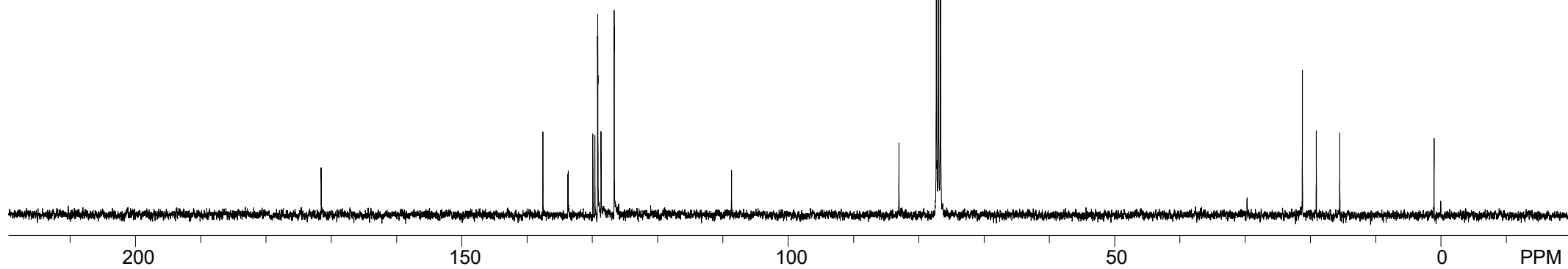
77.000

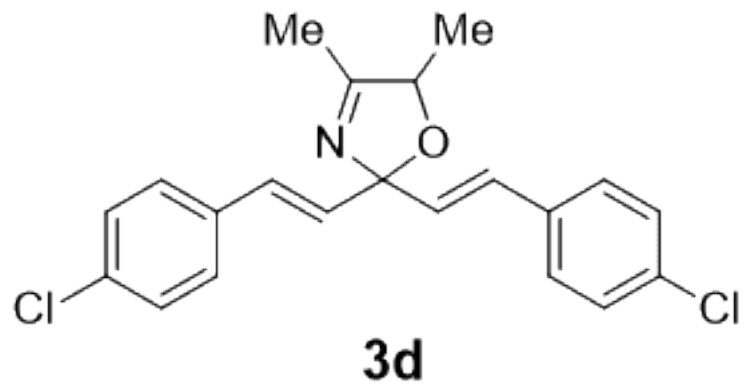
76.687

21.198

19.062

15.460





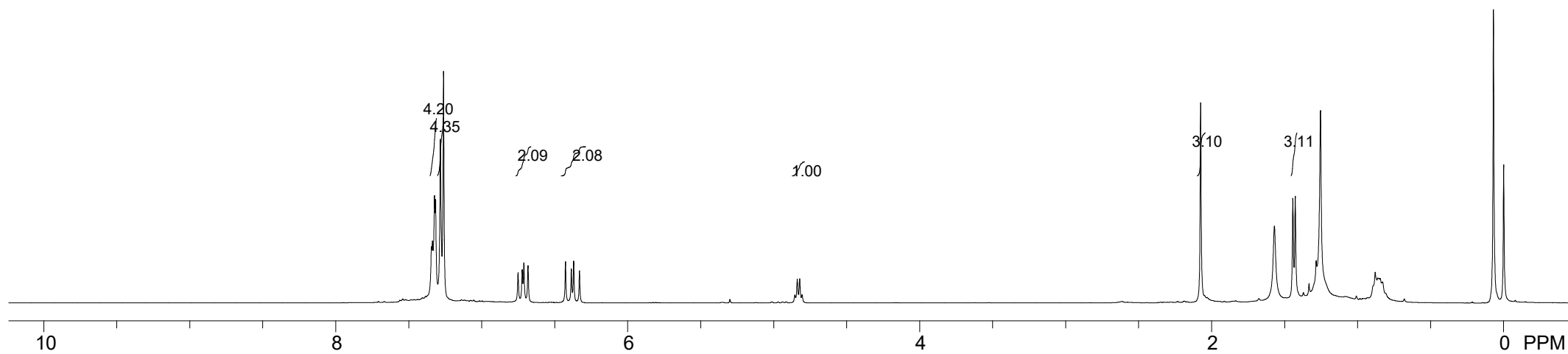
400 MHz, CDCl<sub>3</sub>

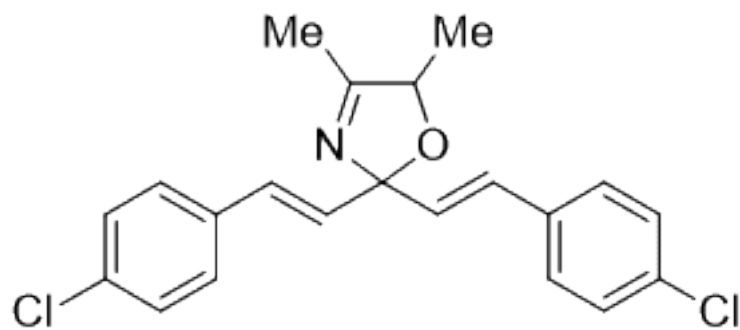
7.345  
7.338  
7.324  
7.317  
7.284  
7.262  
6.751  
6.723  
6.712  
6.683  
6.426  
6.387  
6.371  
6.330

4.856  
4.839  
4.822  
4.805

2.076

1.444  
1.428





**3d**

100 MHz, CDCl<sub>3</sub>

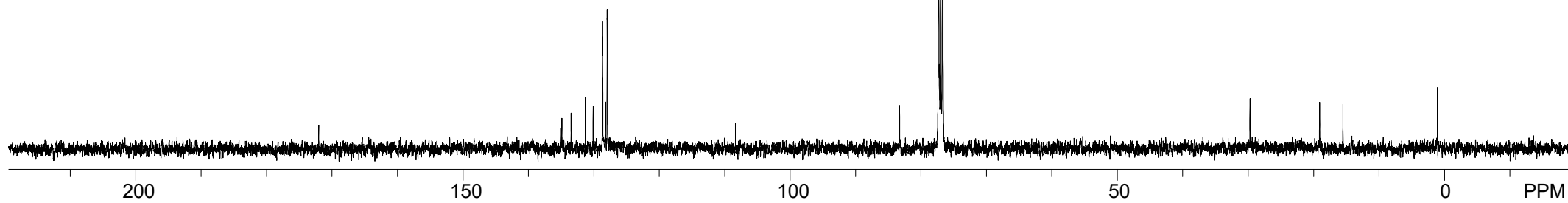
172.052

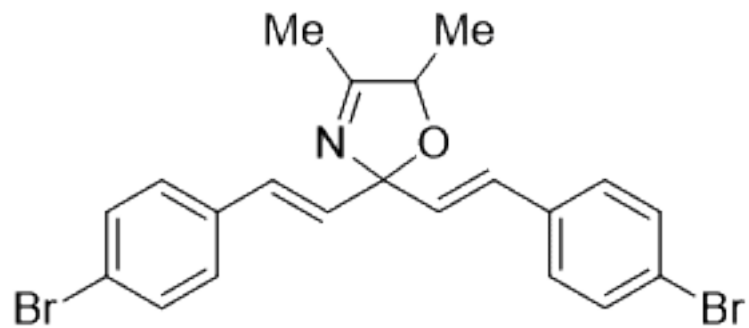
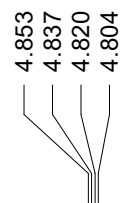
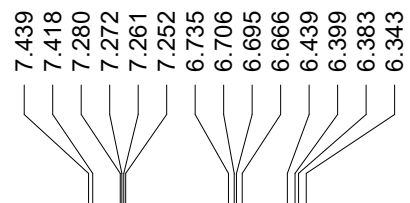
134.975  
134.902  
133.487  
131.314  
130.119  
128.719  
128.690  
128.646  
128.237  
127.968  
108.368

83.293  
77.321  
77.000  
76.687

29.686

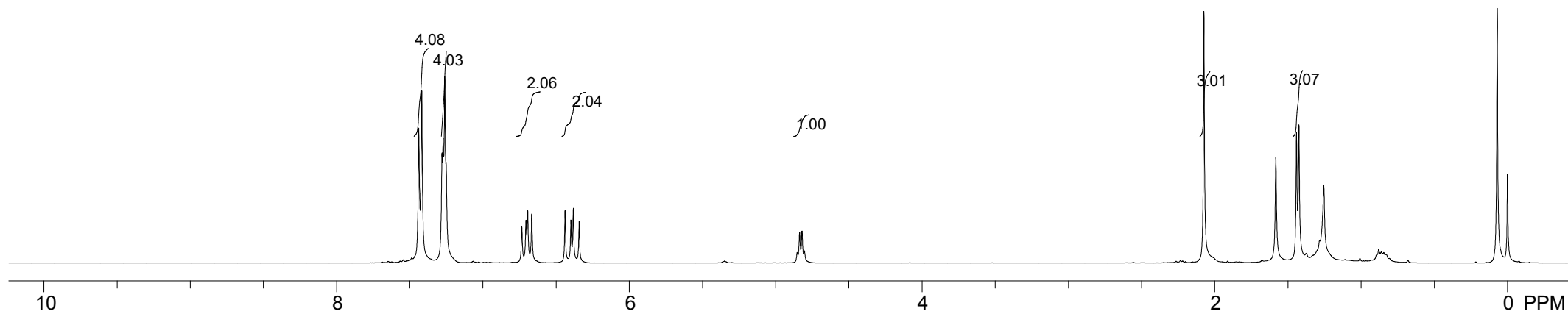
19.033  
15.467

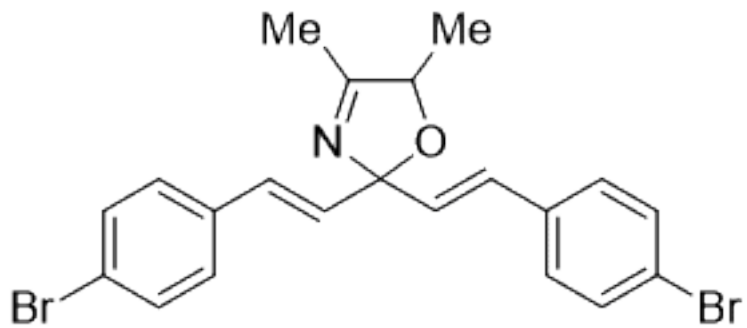




**3e**

400 MHz, CDCl<sub>3</sub>





**3e**

100 MHz, CDCl<sub>3</sub>

172.089

135.405

135.332

131.657

131.635

131.395

130.199

128.711

128.296

121.668

108.361

83.307

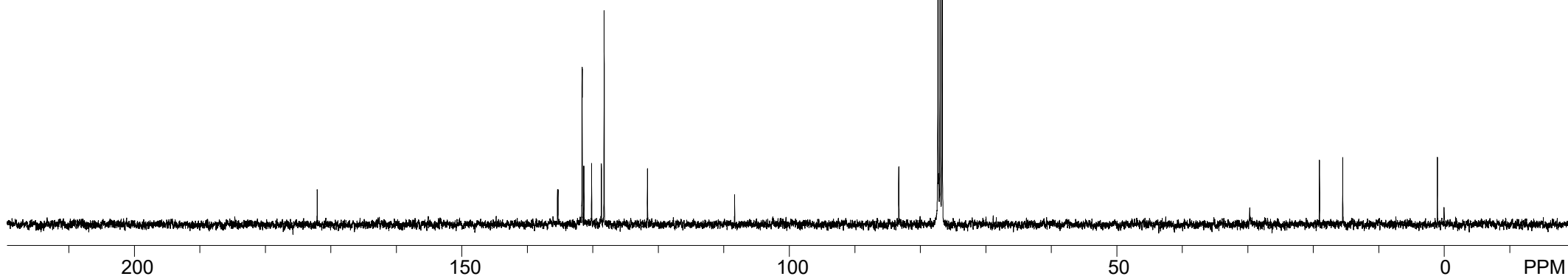
77.321

77.000

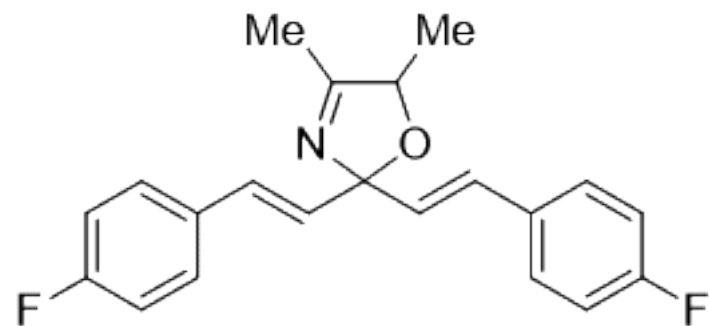
76.687

19.025

15.460

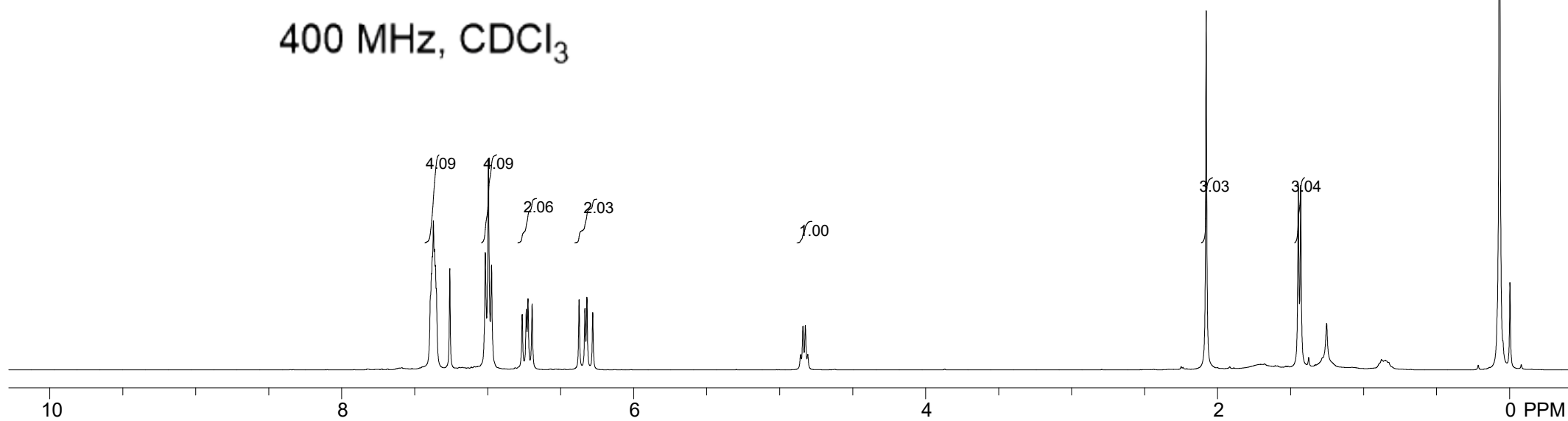
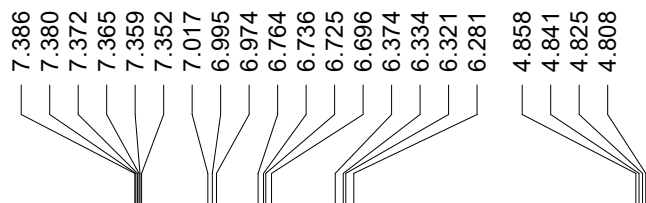


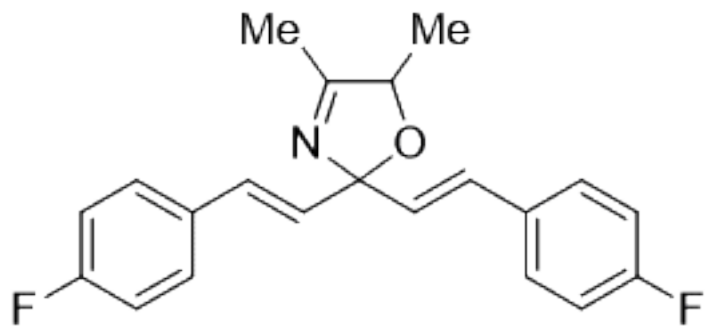




**3f**

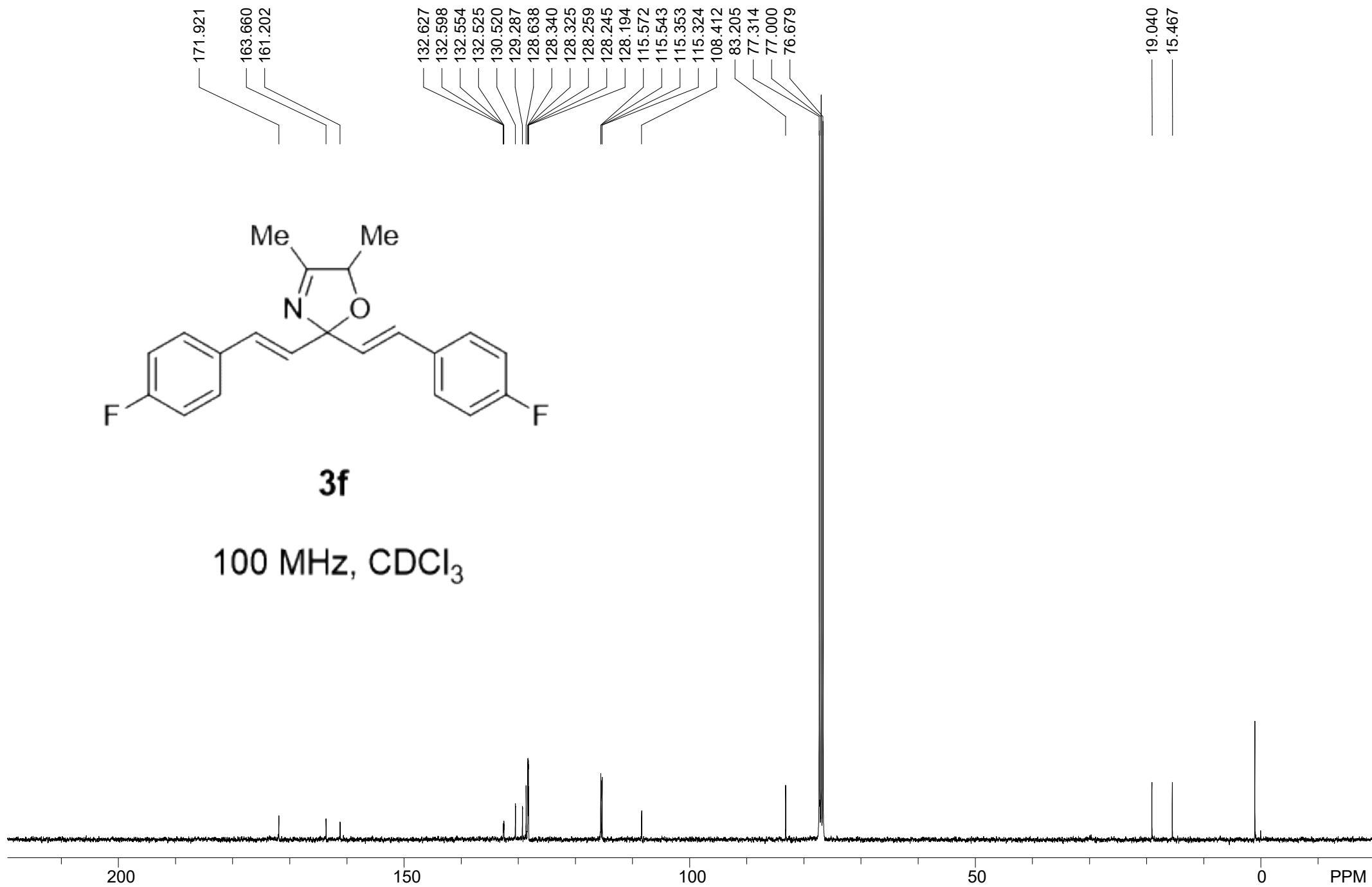
400 MHz, CDCl<sub>3</sub>

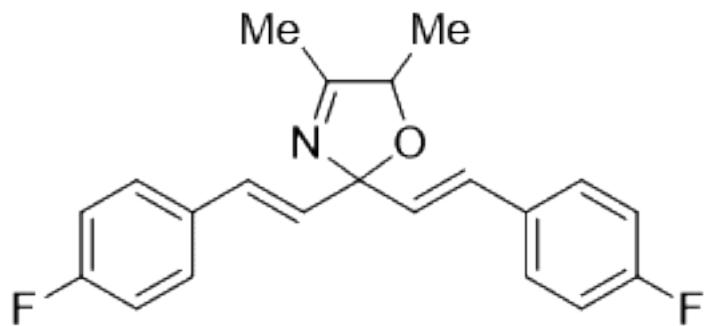




**3f**

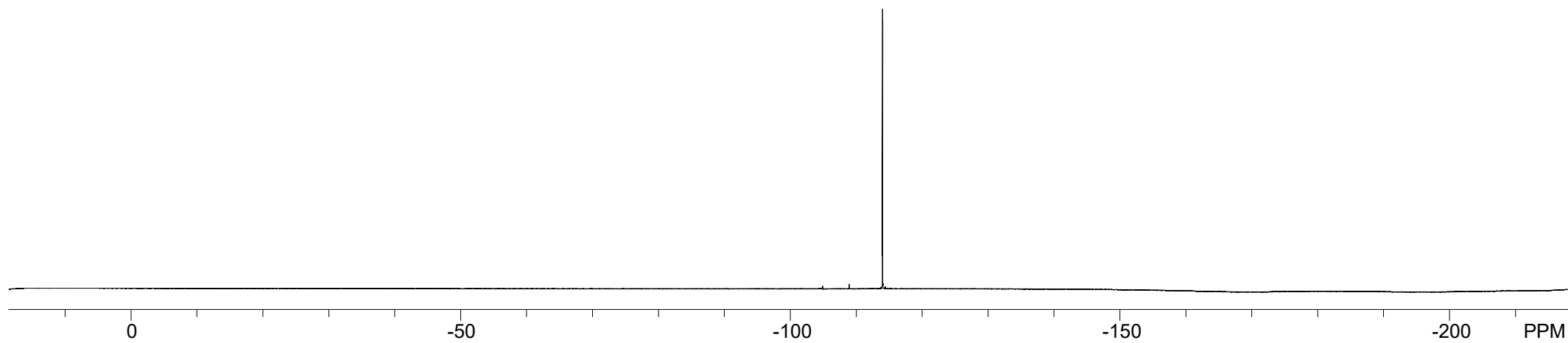
100 MHz, CDCl<sub>3</sub>

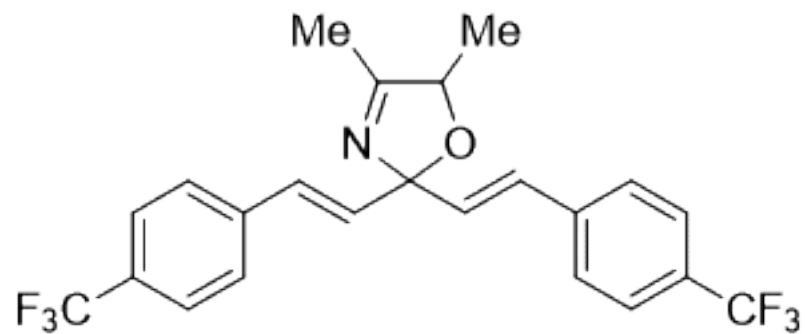




**3f**

376 MHz, CDCl<sub>3</sub>





**3g**

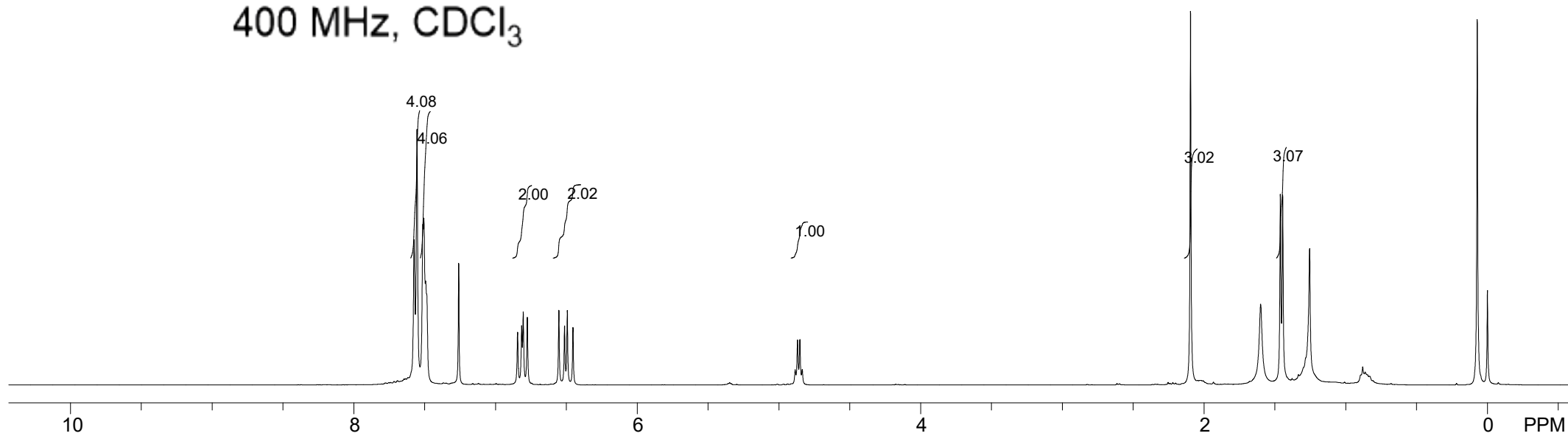
400 MHz, CDCl<sub>3</sub>

7.575  
7.554  
7.512  
7.506  
7.493  
6.844  
6.816  
6.804  
6.776  
6.553  
6.513  
6.493  
6.453

4.884  
4.868  
4.851  
4.835

2.094

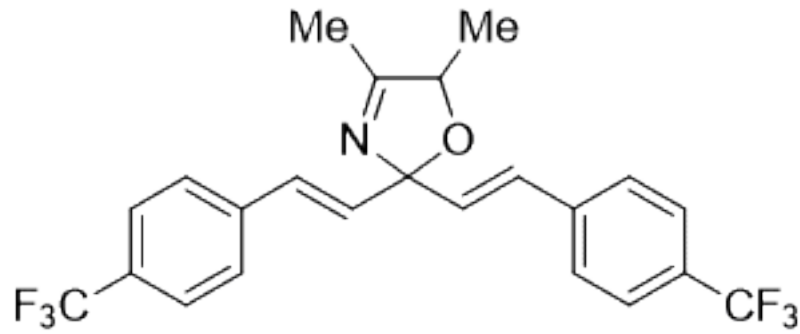
1.460  
1.443



172.439  
139.904  
139.831  
133.072  
131.920  
130.162  
129.842  
129.521  
129.200  
128.638  
128.267  
126.932  
125.510  
125.314  
122.754  
108.222

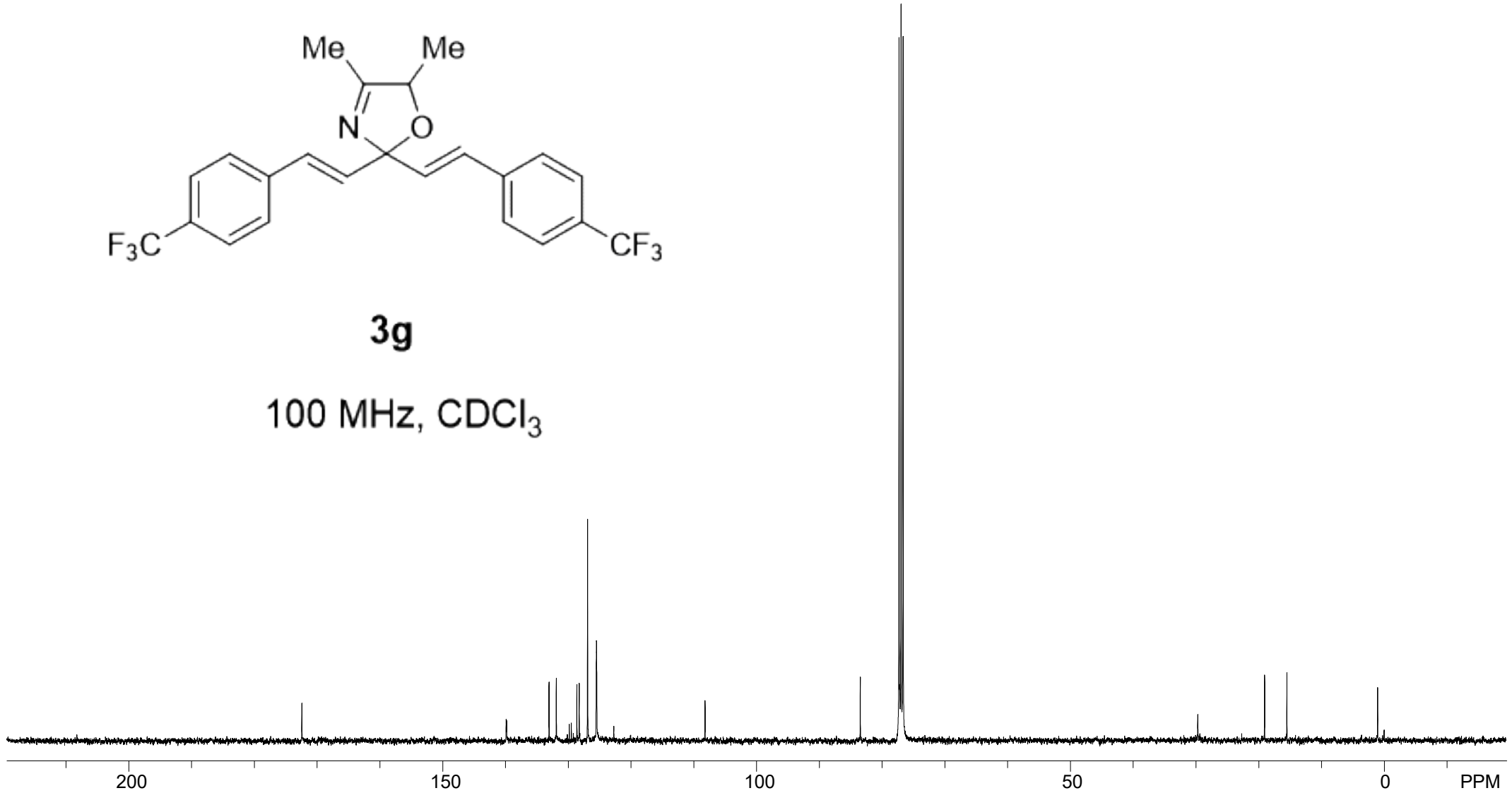
83.497  
77.321  
77.000  
76.679

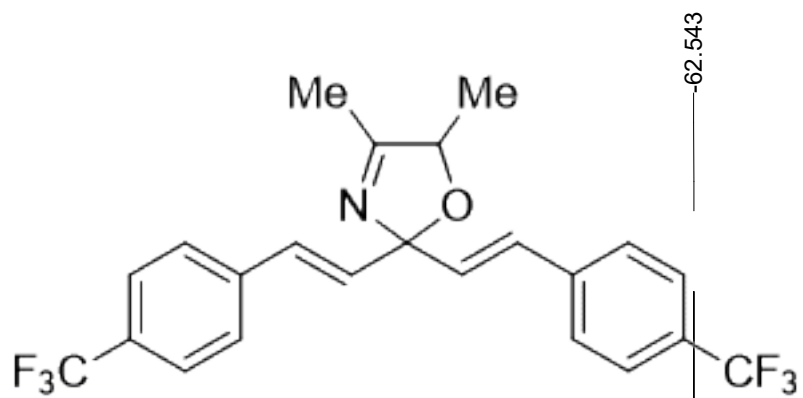
19.025  
15.474



**3g**

100 MHz, CDCl<sub>3</sub>

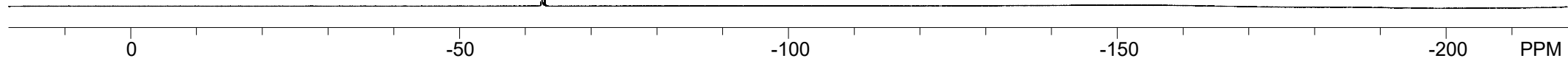


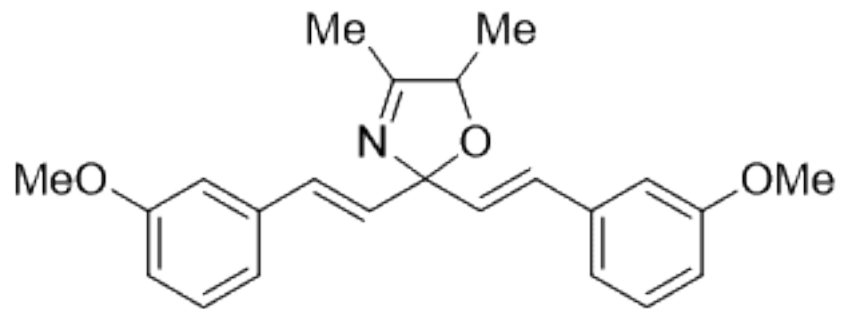


**3g**

376 MHz, CDCl<sub>3</sub>

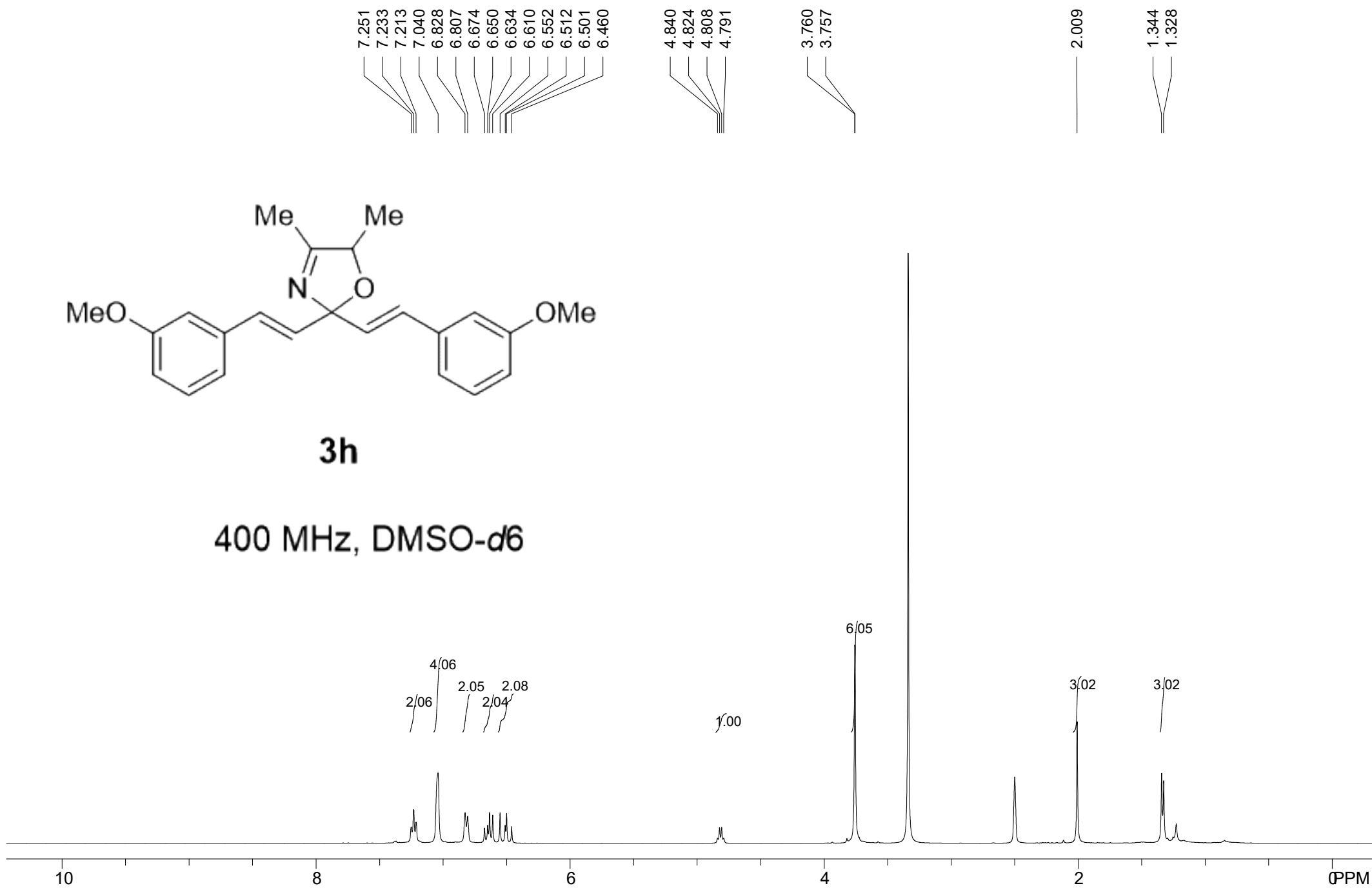
62.543

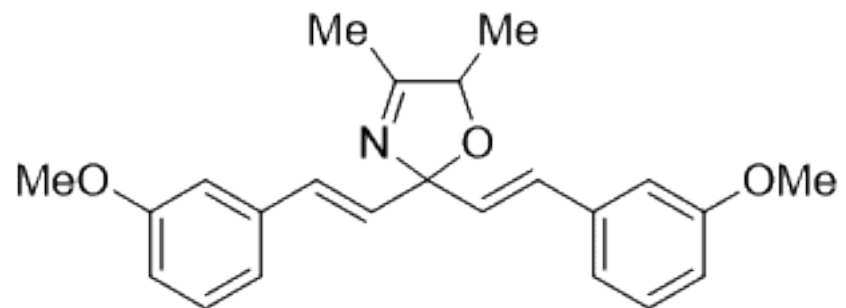




**3h**

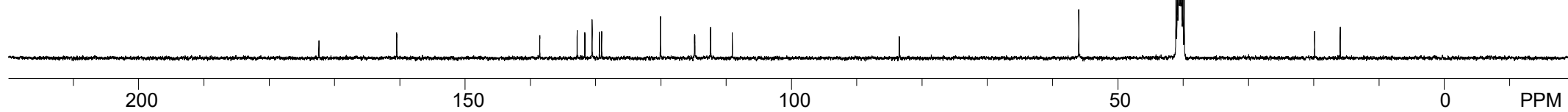
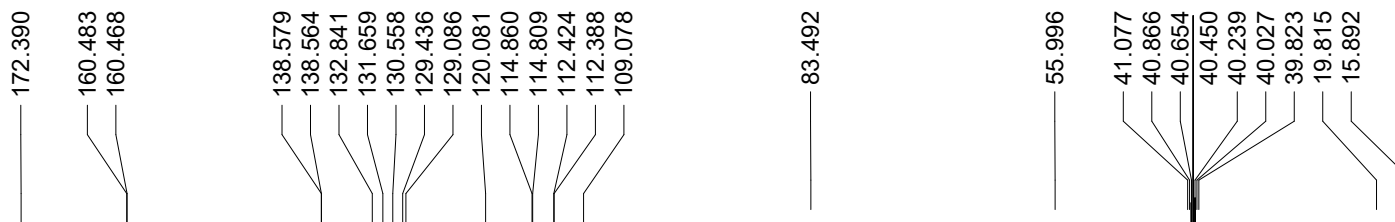
400 MHz, DMSO-*d*<sub>6</sub>



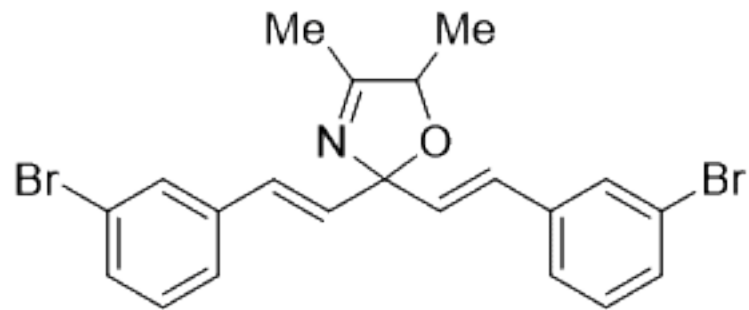


**3h**

100 MHz, DMSO-*d*<sub>6</sub>







**3i**

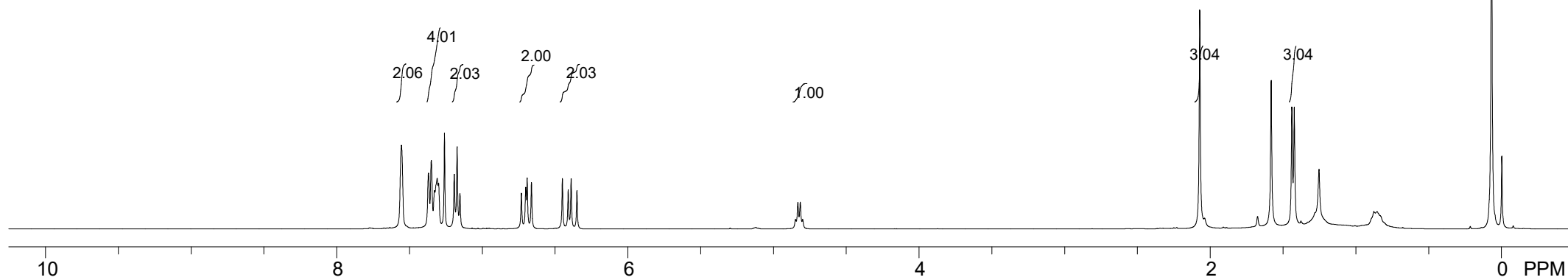
400 MHz, CDCl<sub>3</sub>

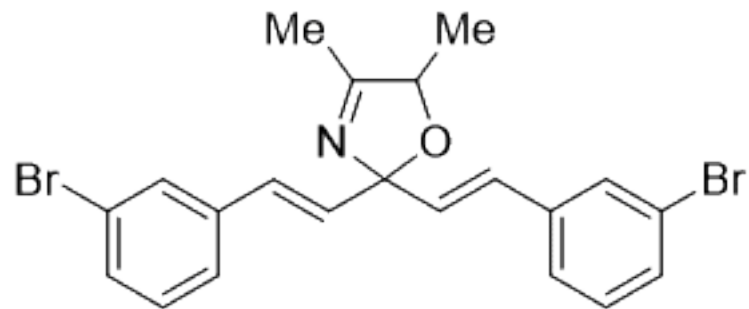
7.555  
7.370  
7.350  
7.328  
7.310  
7.300  
7.193  
7.173  
7.154  
6.732  
6.702  
6.692  
6.662  
6.450  
6.410  
6.390  
6.350

4.849  
4.833  
4.817  
4.800

2.073

1.441  
1.424





**3i**

100 MHz, CDCl<sub>3</sub>

172.176

138.635

138.562

132.124

130.957

130.695

130.024

129.659

128.515

128.135

125.386

122.703

108.251

83.351

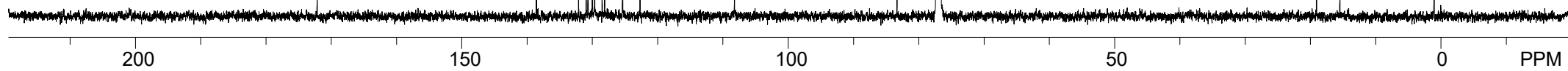
77.314

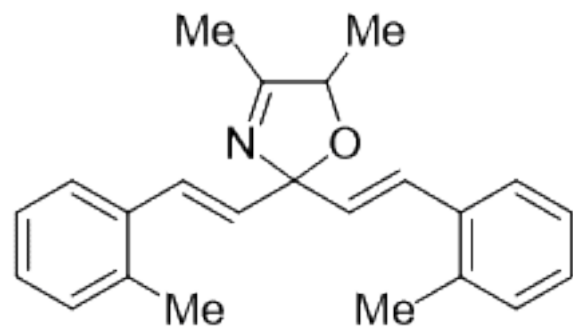
77.000

76.679

19.033

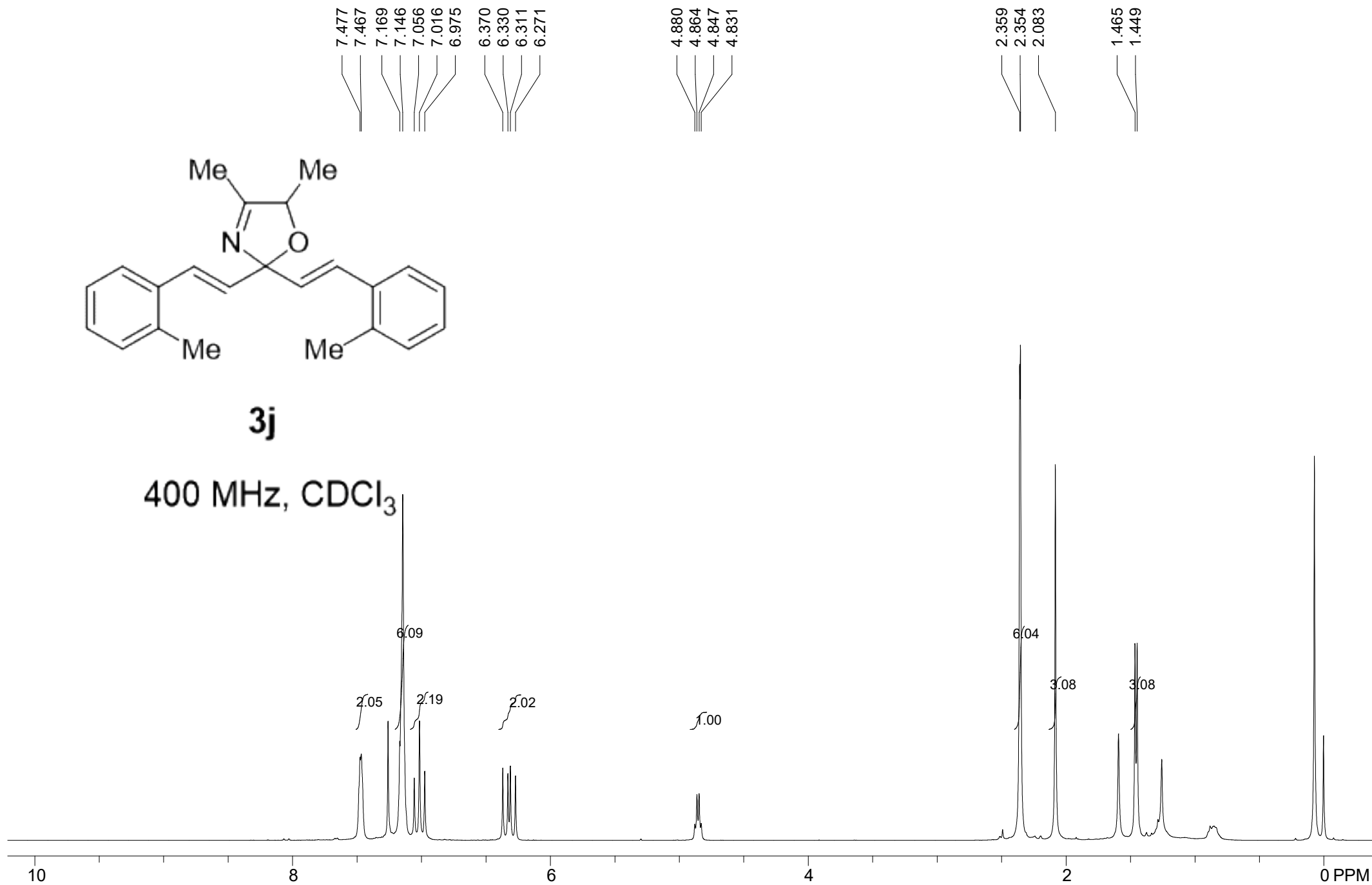
15.453

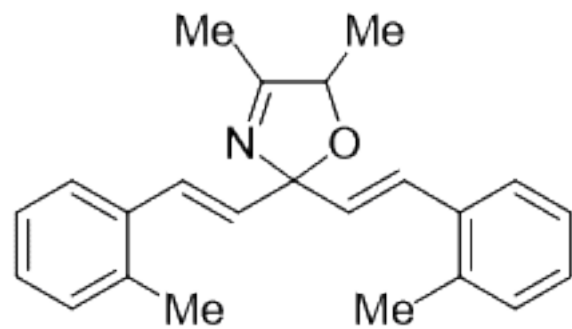




**3j**

400 MHz, CDCl<sub>3</sub>





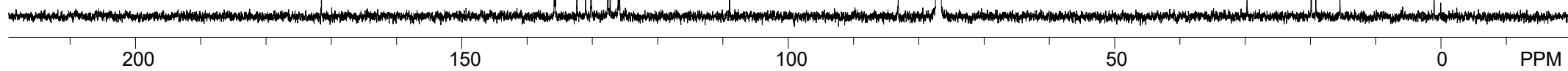
**3j**

100 MHz, CDCl<sub>3</sub>

171.520  
135.857  
135.821  
135.755  
135.667  
132.386  
131.074  
130.228  
130.199  
127.705  
127.625  
127.282  
126.043  
125.853  
125.839  
108.988

83.176  
77.321  
77.000  
76.687

19.878  
19.827  
19.135  
15.445

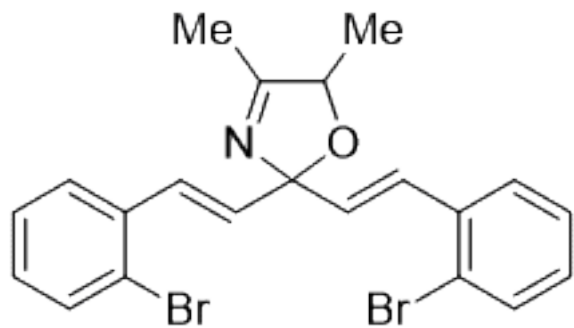


7.550  
7.539  
7.531  
7.279  
7.260  
7.242  
7.216  
7.177  
7.164  
7.124  
7.119  
7.097  
7.079  
6.437  
6.397  
6.367  
6.327

4.921  
4.904  
4.888  
4.871

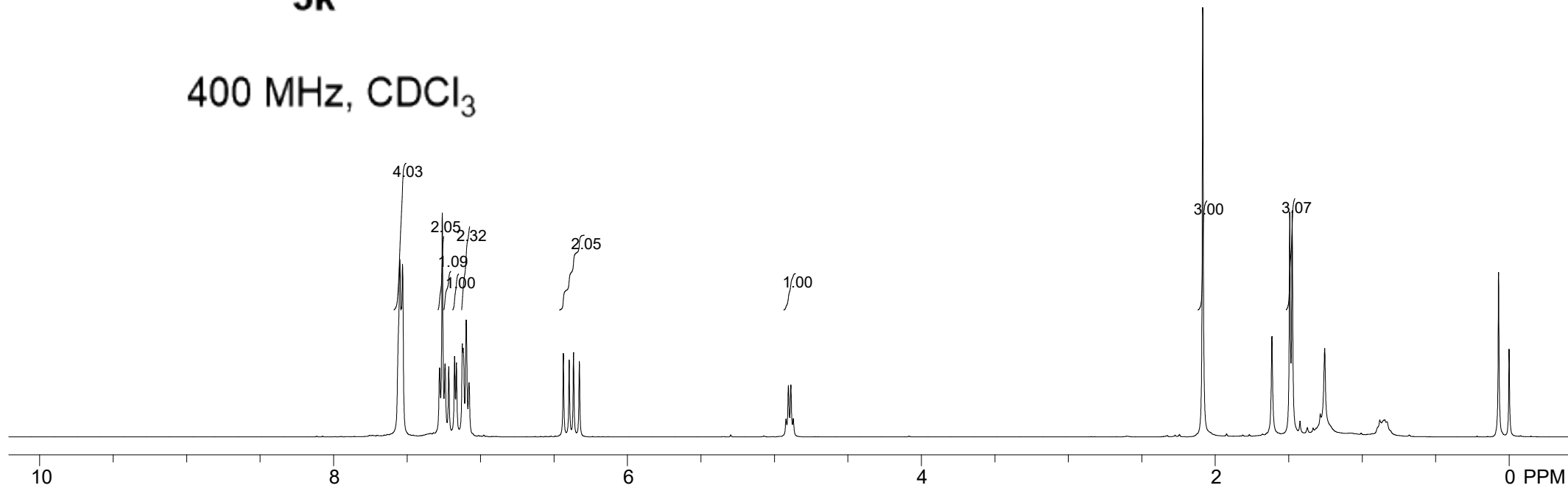
2.085

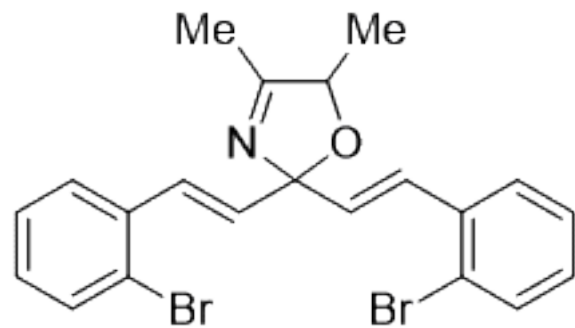
1.492  
1.476



**3k**

400 MHz, CDCl<sub>3</sub>





**3k**

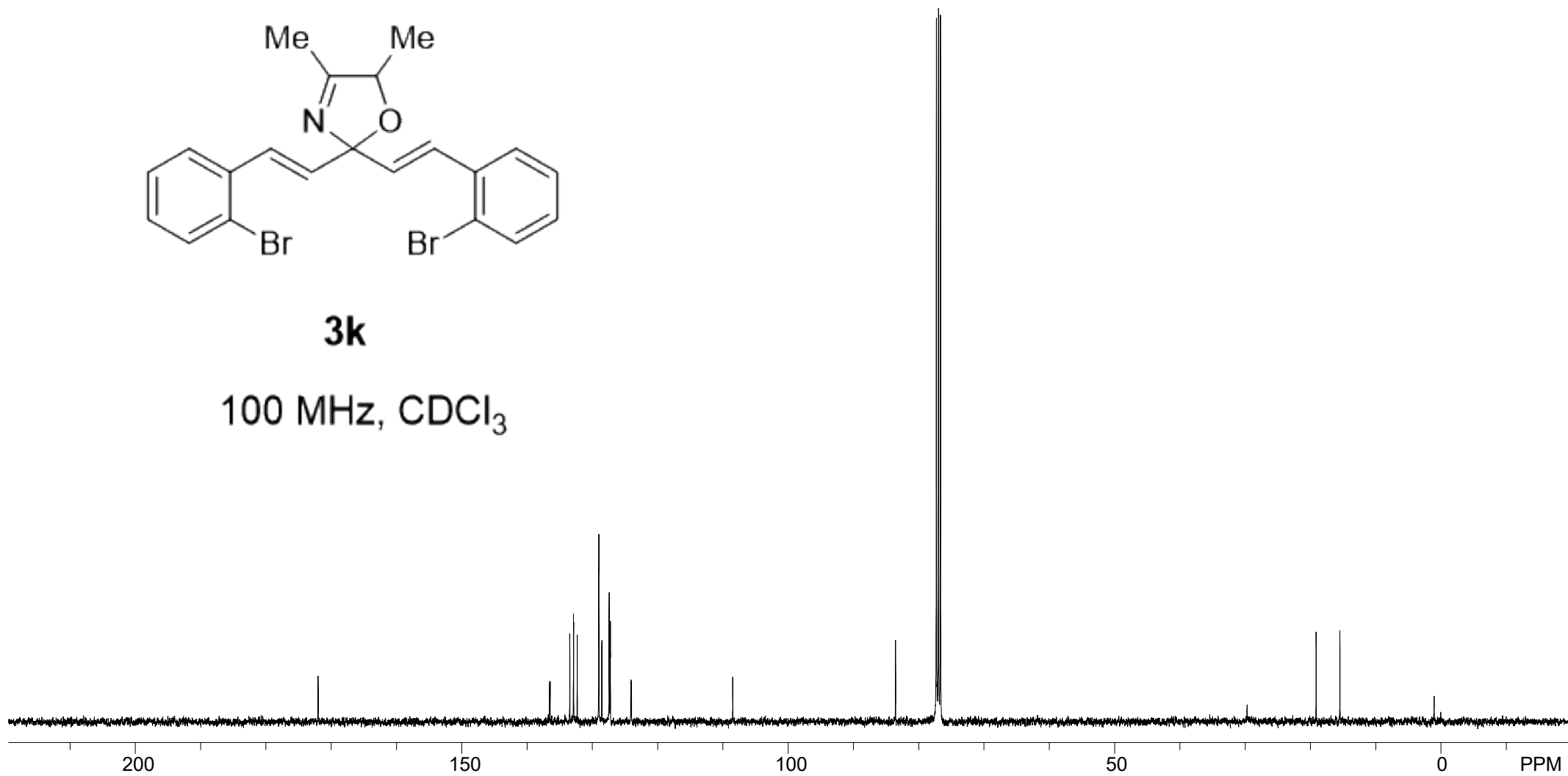
100 MHz, CDCl<sub>3</sub>

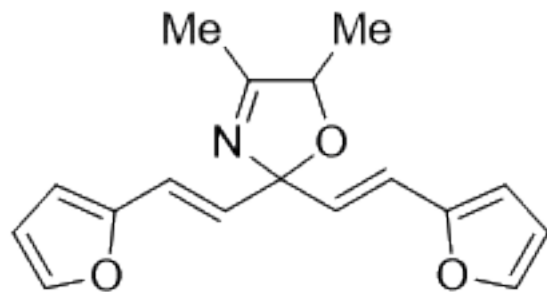
172.008

136.550  
136.469  
133.458  
132.897  
132.867  
132.321  
129.010  
128.551  
127.435  
127.268  
127.238  
124.110  
124.023  
108.499

83.570  
77.314  
77.000  
76.679

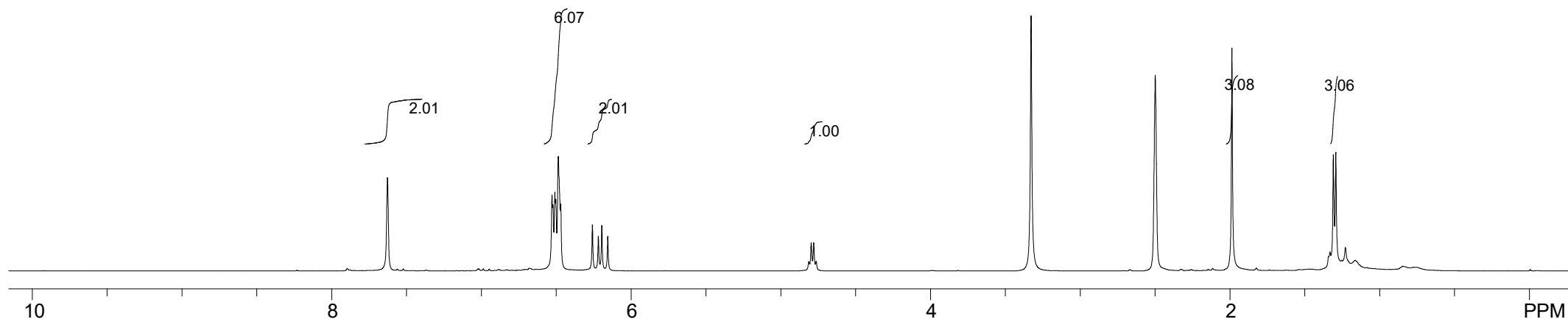
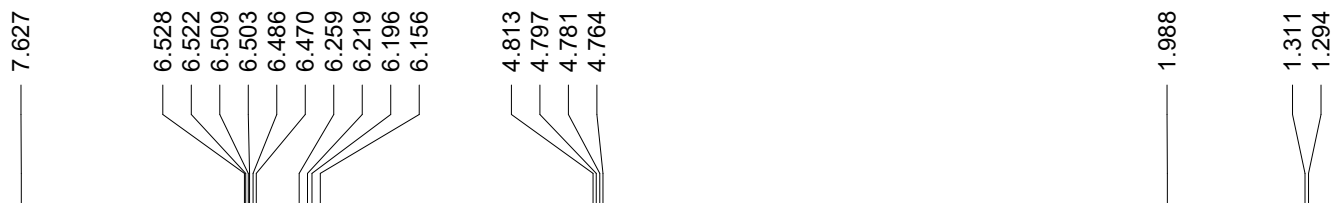
19.084  
15.438

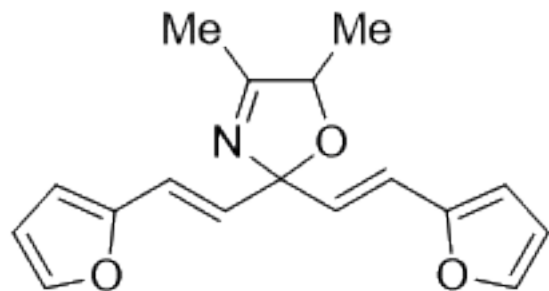




**31**

100 MHz, DMSO-*d*6





**31**

100 MHz, DMSO-*d*6

172.798

152.462

143.975

130.362

129.217

118.331

118.119

112.665

110.478

110.434

108.451

83.608

41.077

40.873

40.661

40.450

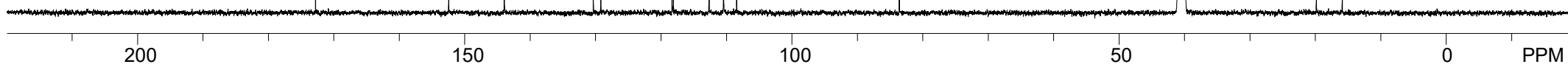
40.246

40.034

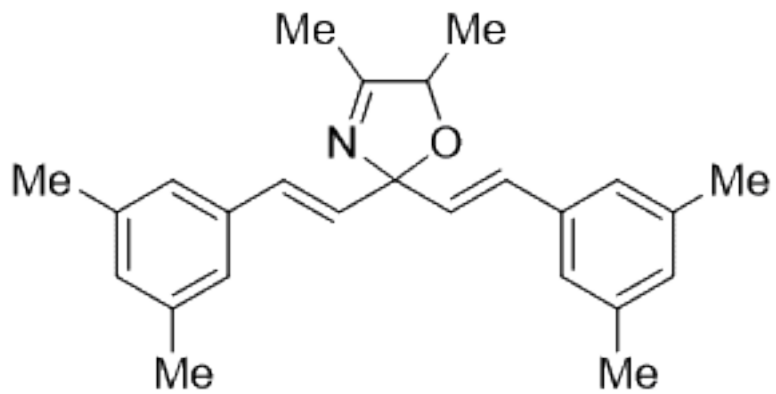
39.830

19.822

15.848

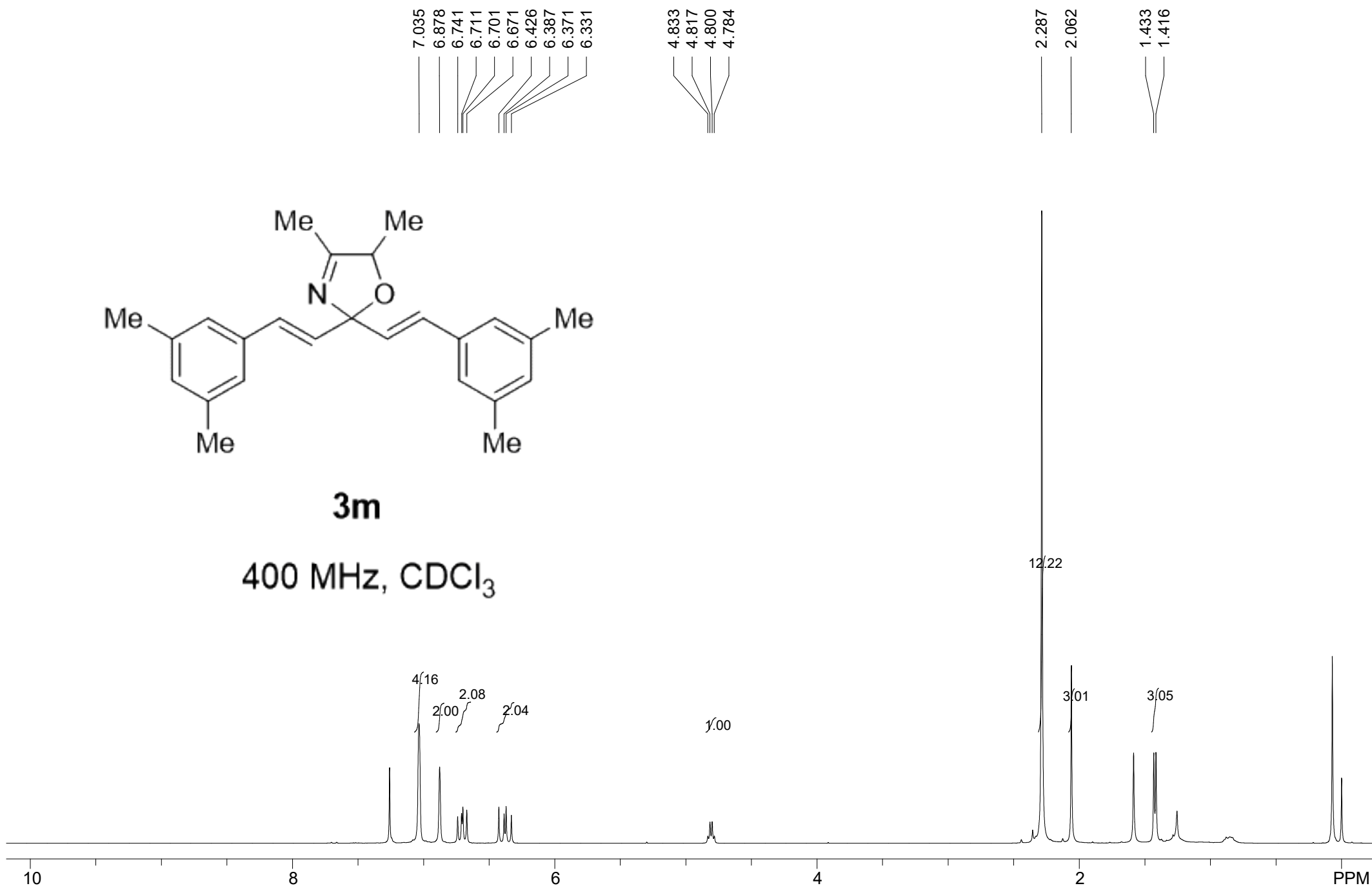


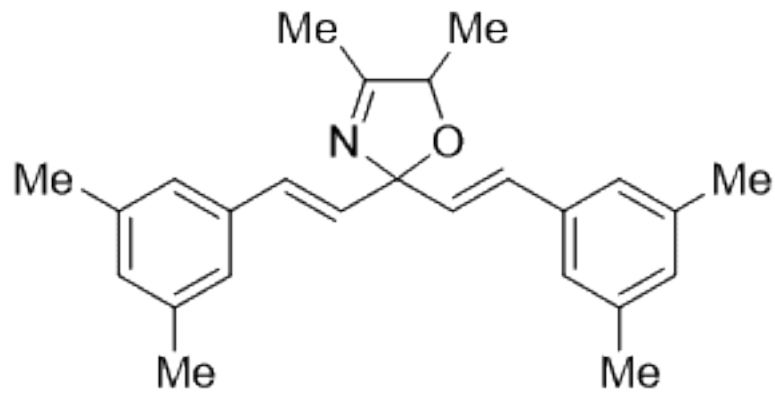




**3m**

400 MHz, CDCl<sub>3</sub>





**3m**

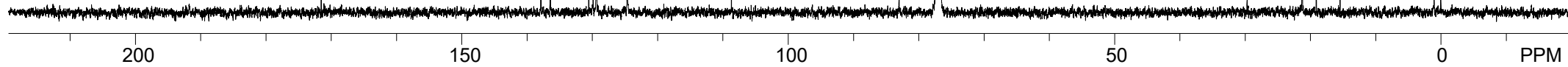
100 MHz, CDCl<sub>3</sub>

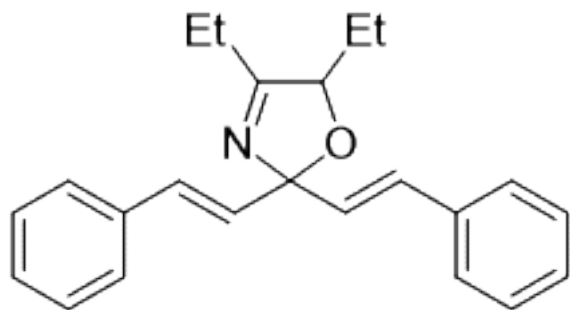
171.549

137.913  
137.891  
136.499  
136.419  
130.571  
129.900  
129.448  
129.338  
124.672  
124.657  
108.711

83.037  
77.321  
77.204  
77.000  
76.679

21.220  
19.069  
15.431





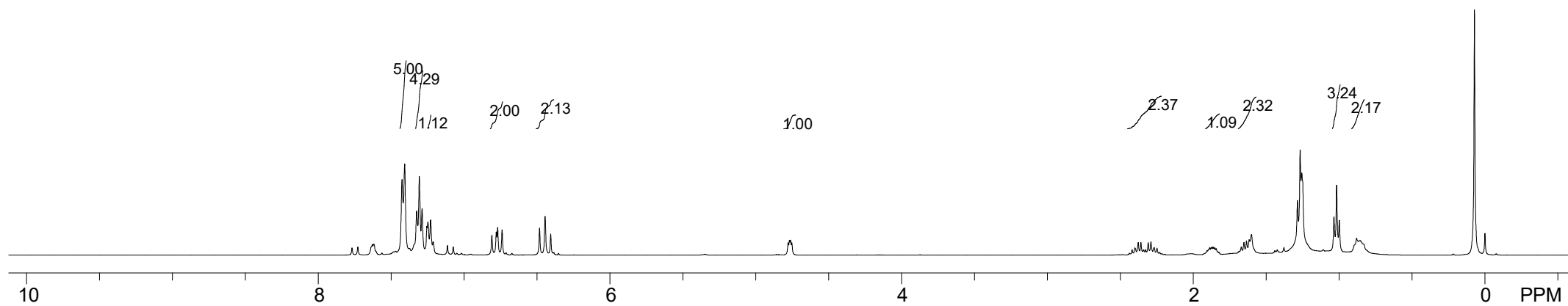
**3n**

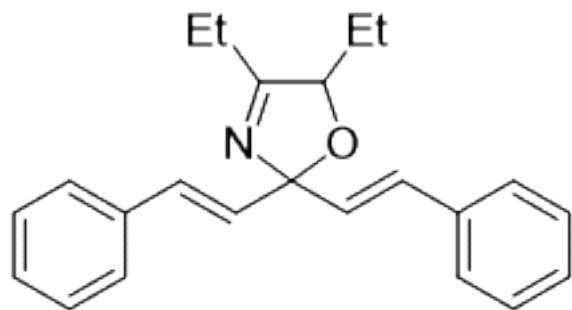
400 MHz, CDCl<sub>3</sub>

7.426  
7.408  
7.325  
7.307  
7.289  
7.256  
7.248  
7.230  
7.212  
6.810  
6.780  
6.770  
6.740  
6.482  
6.445  
6.406

4.779  
4.769  
4.762  
4.753

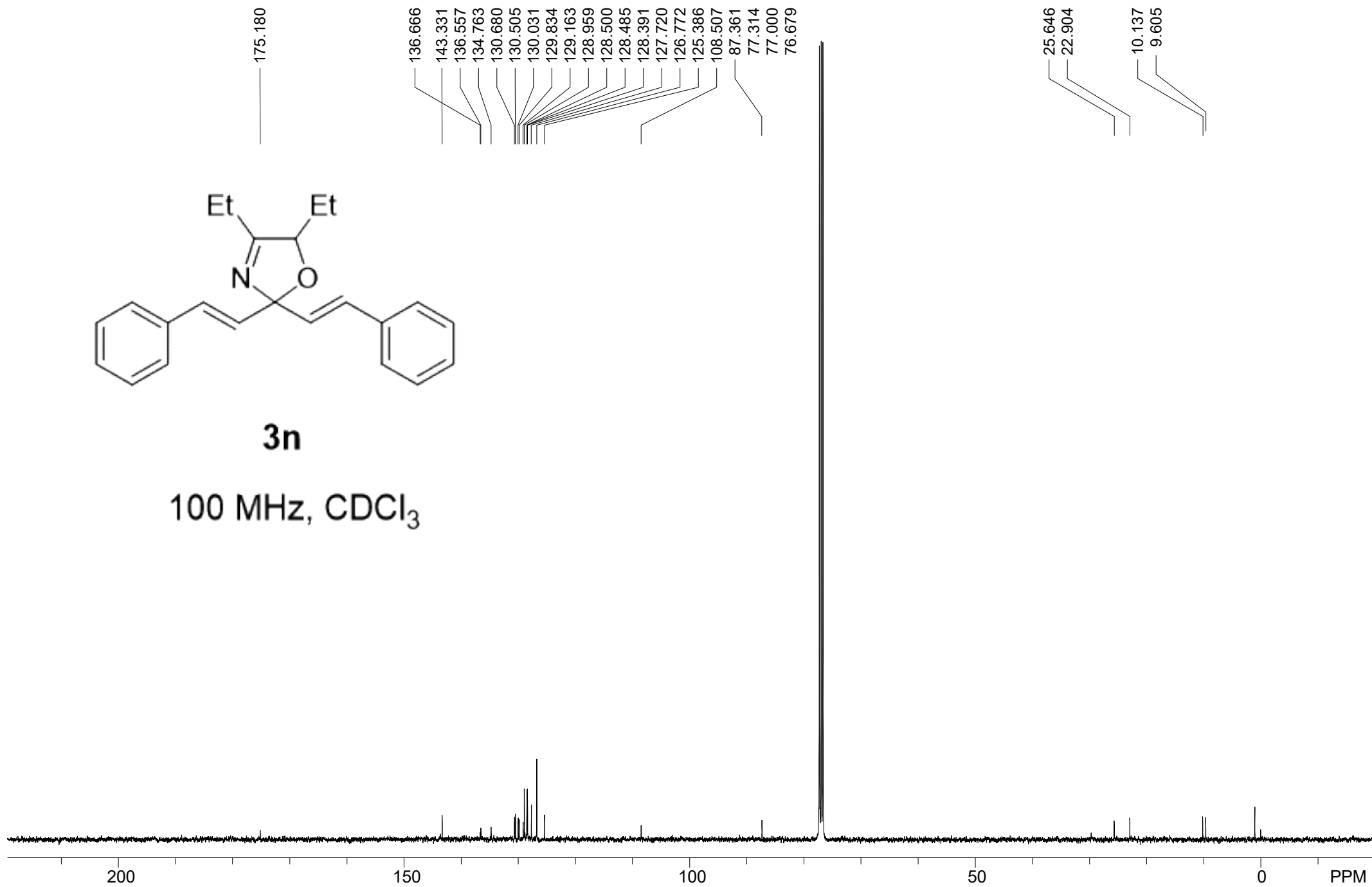
2.377  
2.359  
2.309  
2.291  
1.924  
1.906  
1.888  
1.870  
1.861  
1.843  
1.843  
1.653  
1.635  
1.617  
1.601  
1.035  
1.017  
0.999  
0.881  
0.856





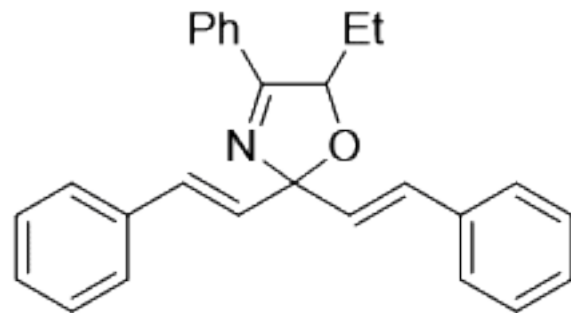
**3n**

100 MHz, CDCl<sub>3</sub>



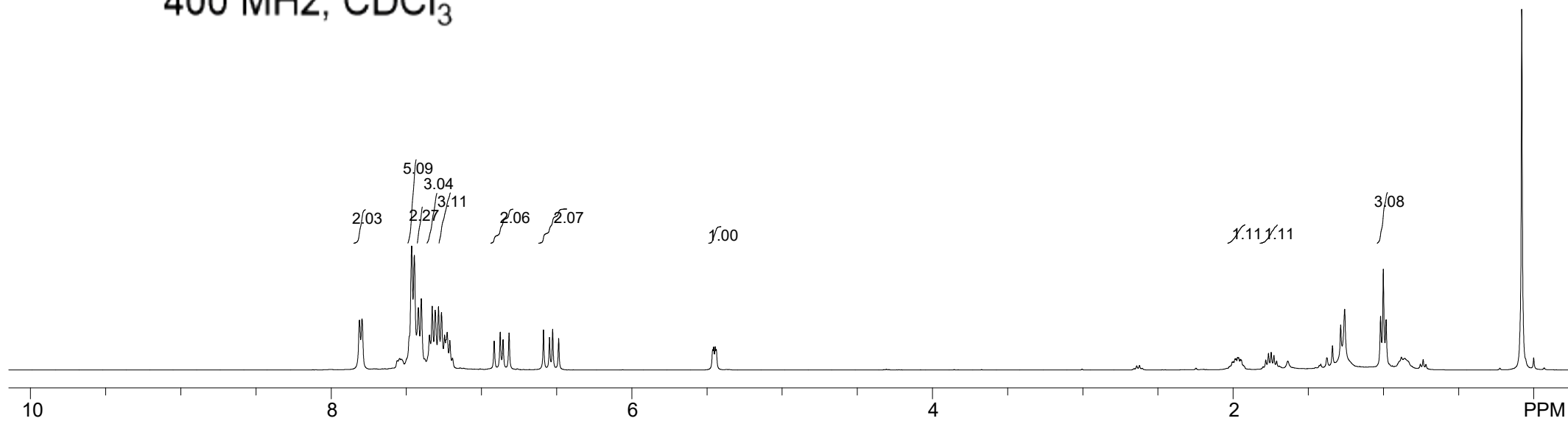
7.812  
7.795  
7.480  
7.465  
7.447  
7.420  
7.400  
7.377  
7.346  
7.328  
7.308  
7.286  
7.266  
7.245  
7.236  
7.229  
7.210  
7.193  
6.916  
6.875  
6.856  
6.817  
6.588  
6.547  
6.526  
6.487  
5.462  
5.456  
5.445  
5.438

2.006  
1.999  
1.988  
1.981  
1.970  
1.963  
1.952  
1.945  
1.783  
1.764  
1.747  
1.728  
1.711  
1.019  
1.000  
0.982

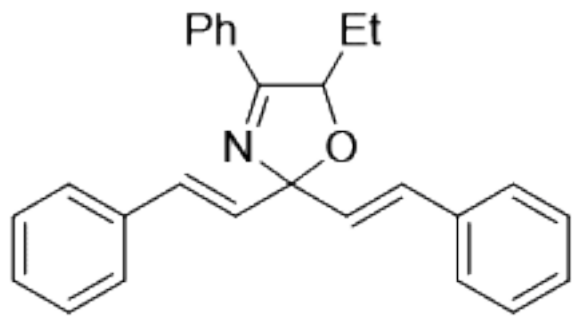


**3o**

400 MHz, CDCl<sub>3</sub>

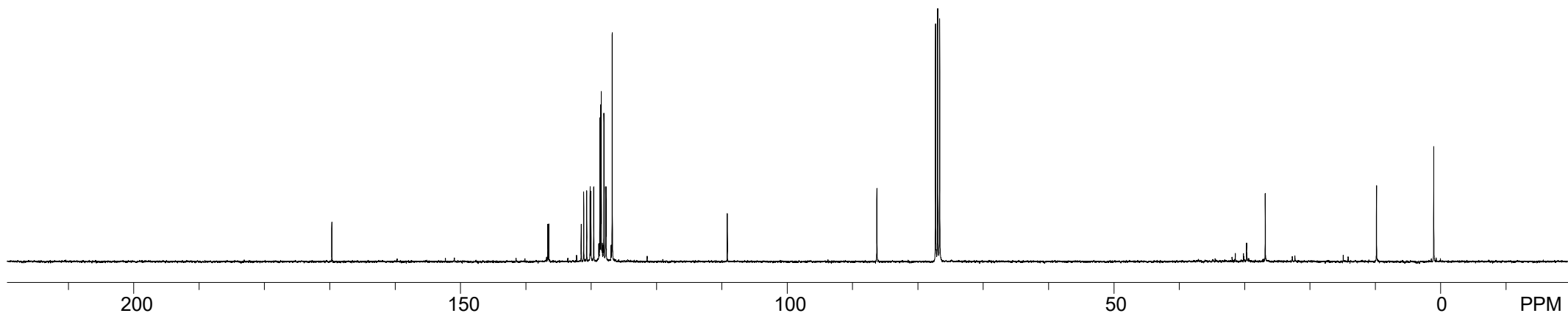


169.697  
 136.637  
 136.499  
 131.533  
 131.154  
 130.702  
 130.170  
 130.053  
 129.616  
 128.843  
 128.675  
 128.529  
 128.463  
 128.369  
 128.310  
 128.157  
 128.055  
 127.800  
 127.742  
 126.961  
 126.786  
 109.185  
 86.289  
 77.321  
 77.000  
 76.679  
 26.813  
 9.772

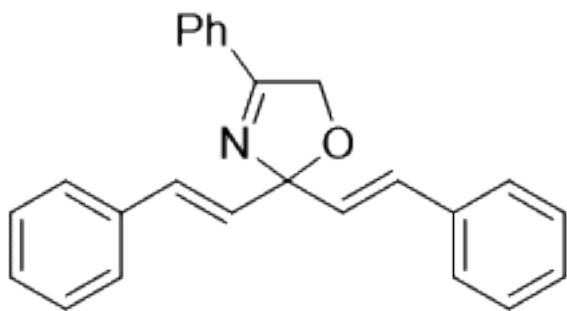


**30**

100 MHz, CDCl<sub>3</sub>

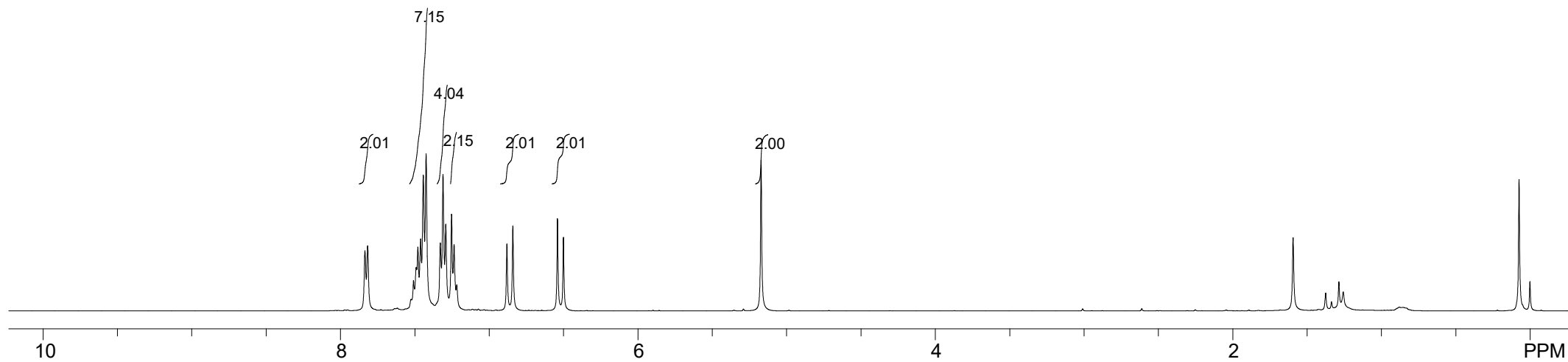


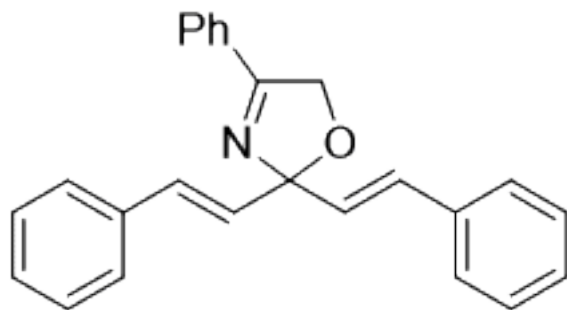
7.836  
7.818  
7.526  
7.509  
7.491  
7.480  
7.462  
7.443  
7.425  
7.329  
7.311  
7.292  
7.253  
7.237  
7.218  
6.882  
6.841  
6.541  
6.501  
5.172



**3p**

400 MHz, CDCl<sub>3</sub>





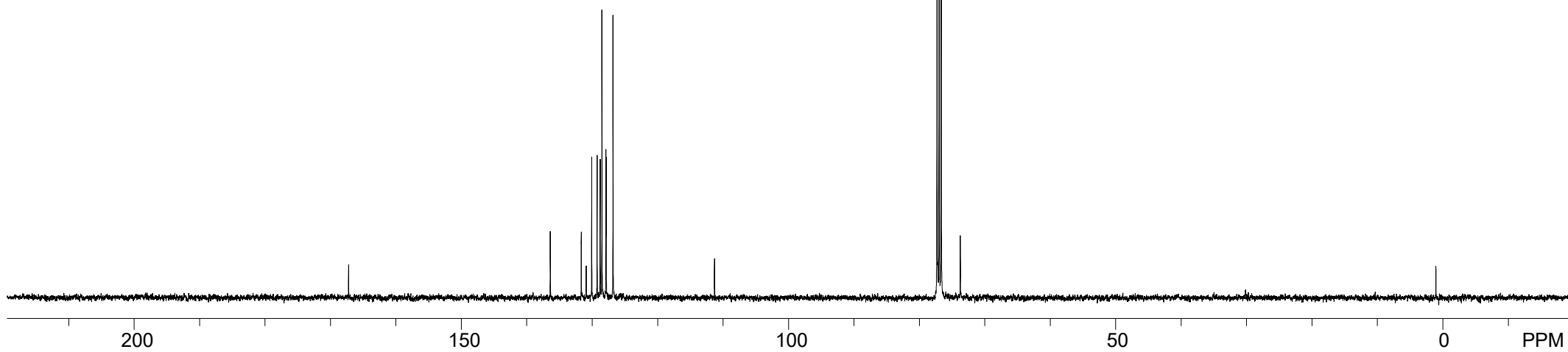
**3p**

100 MHz, CDCl<sub>3</sub>

167.232

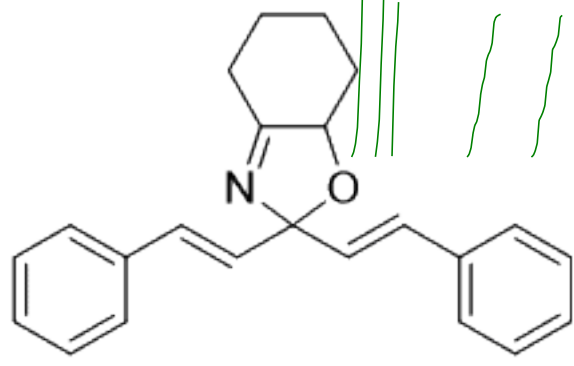
131.679  
136.419  
130.921  
130.089  
129.258  
128.792  
128.522  
127.917  
127.873  
126.830  
111.321

77.321  
77.000  
76.687  
73.763



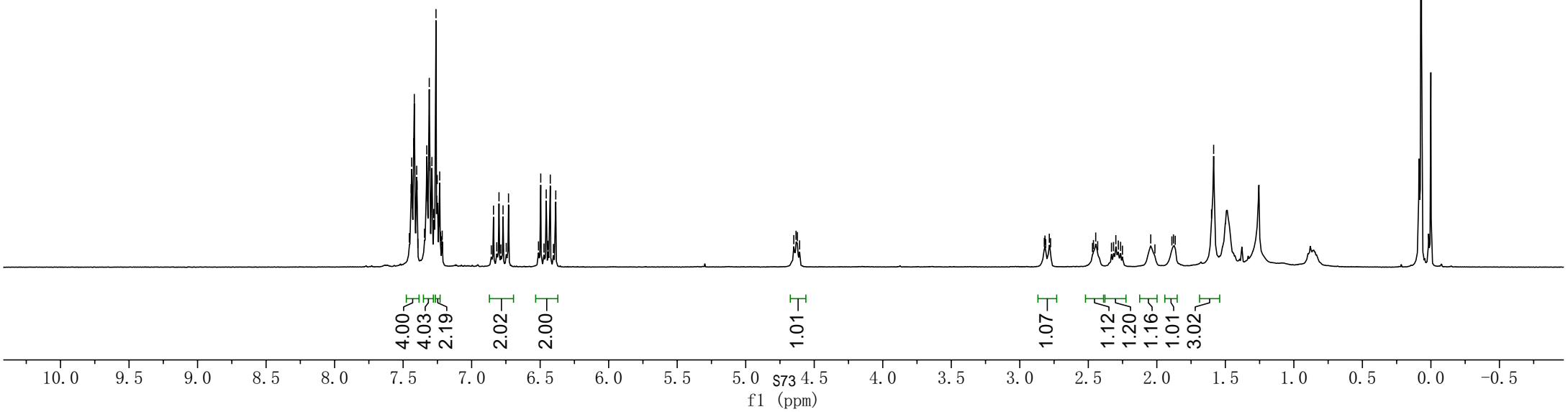


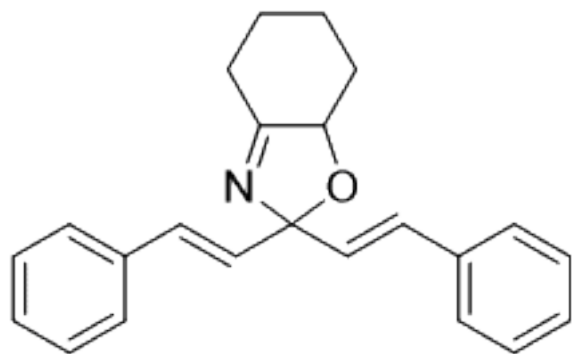
7.455  
7.454  
7.441  
7.437  
7.432  
7.423  
7.418  
7.404  
7.401  
7.398  
7.393  
7.344  
7.327  
7.322  
7.309  
7.305  
7.293  
7.290  
7.277  
7.260  
7.255  
7.251  
7.247  
7.239  
7.233  
7.227  
7.218  
7.215  
7.211  
6.840  
6.800  
6.771  
6.731  
6.512  
6.496  
6.456  
6.443  
6.426  
6.386  
4.649  
4.633  
4.623  
4.607  
2.821  
2.816  
2.811  
2.785  
2.776  
2.462  
2.446  
2.432  
2.299  
2.281  
2.264  
2.044  
1.890  
1.879  
1.866  
1.601  
1.585



**3q**

400 MHz, CDCl<sub>3</sub>





**3q**

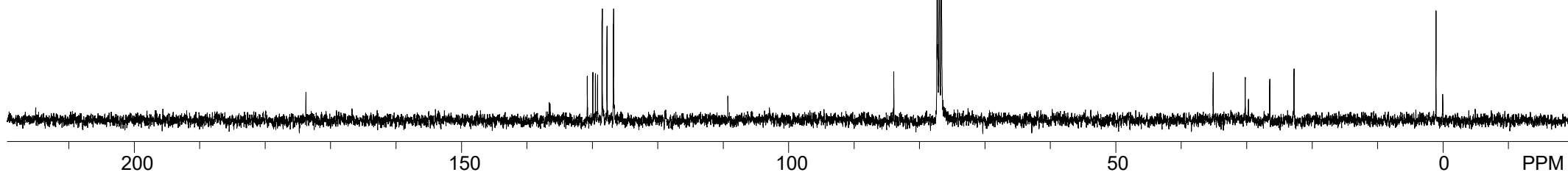
100 MHz, CDCl<sub>3</sub>

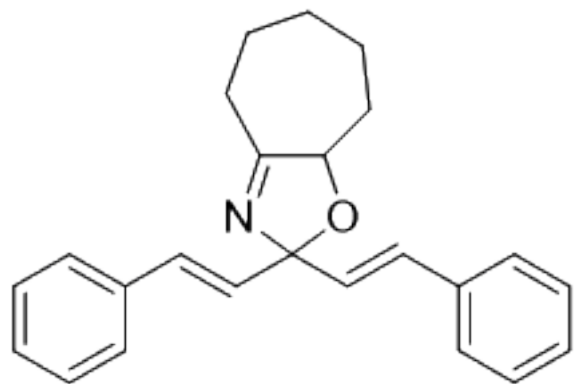
173.780

130.789  
136.579  
129.936  
129.543  
129.215  
128.529  
128.493  
127.778  
126.808  
126.765  
109.309

83.942  
77.321  
77.000  
76.679

35.096  
30.203  
26.448  
22.737





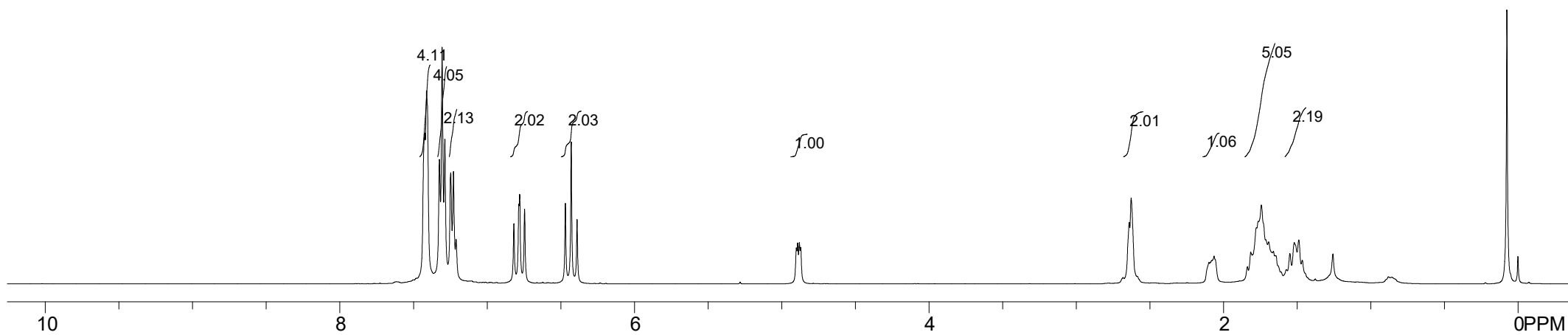
**3r**

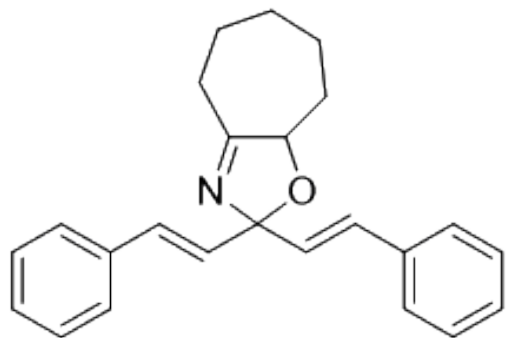
400 MHz, CDCl<sub>3</sub>

7.423  
7.411  
7.324  
7.306  
7.287  
7.248  
7.229  
7.211  
6.819  
6.785  
6.779  
6.746  
6.469  
6.429  
6.390

4.900  
4.892  
4.879  
4.871

2.640  
2.627  
2.099  
2.088  
2.080  
2.063  
1.837  
1.815  
1.801  
1.776  
1.764  
1.742  
1.712  
1.693  
1.670  
1.660  
1.649  
1.643  
1.629  
1.609  
1.572  
1.549  
1.519  
1.488  
1.464





**3r**

100 MHz, CDCl<sub>3</sub>

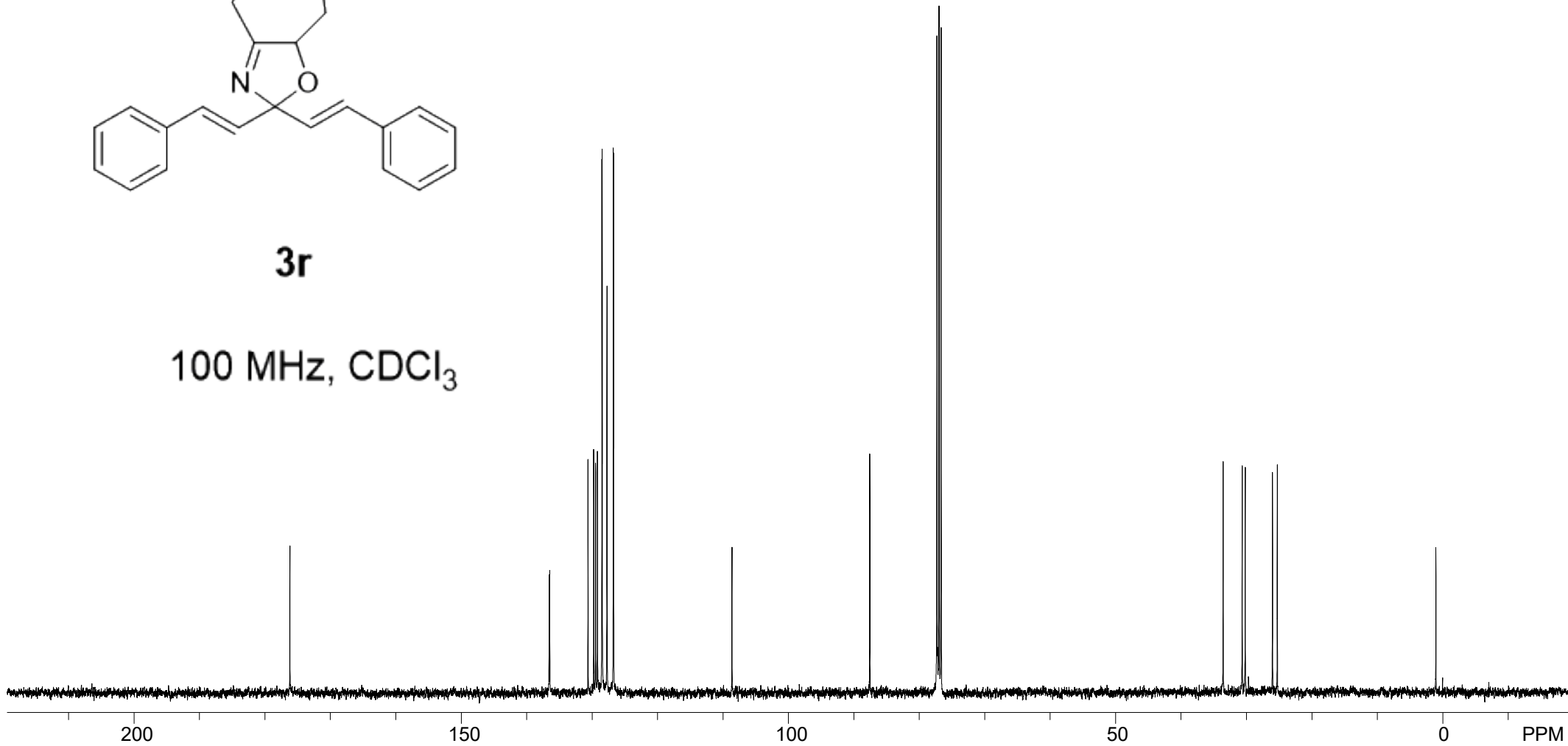
176.194

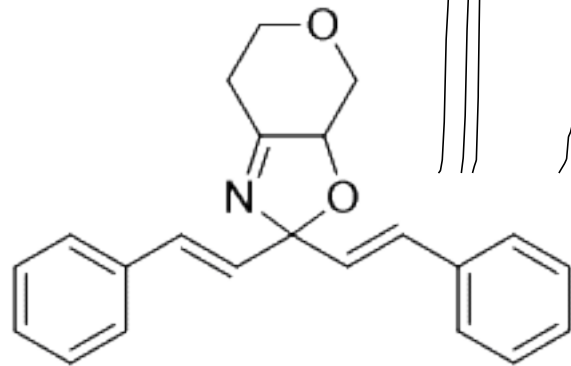
136.586  
136.477  
130.636  
129.761  
129.477  
129.185  
128.507  
128.463  
127.734  
126.772  
126.728  
108.645

87.573

77.314  
77.000  
76.679

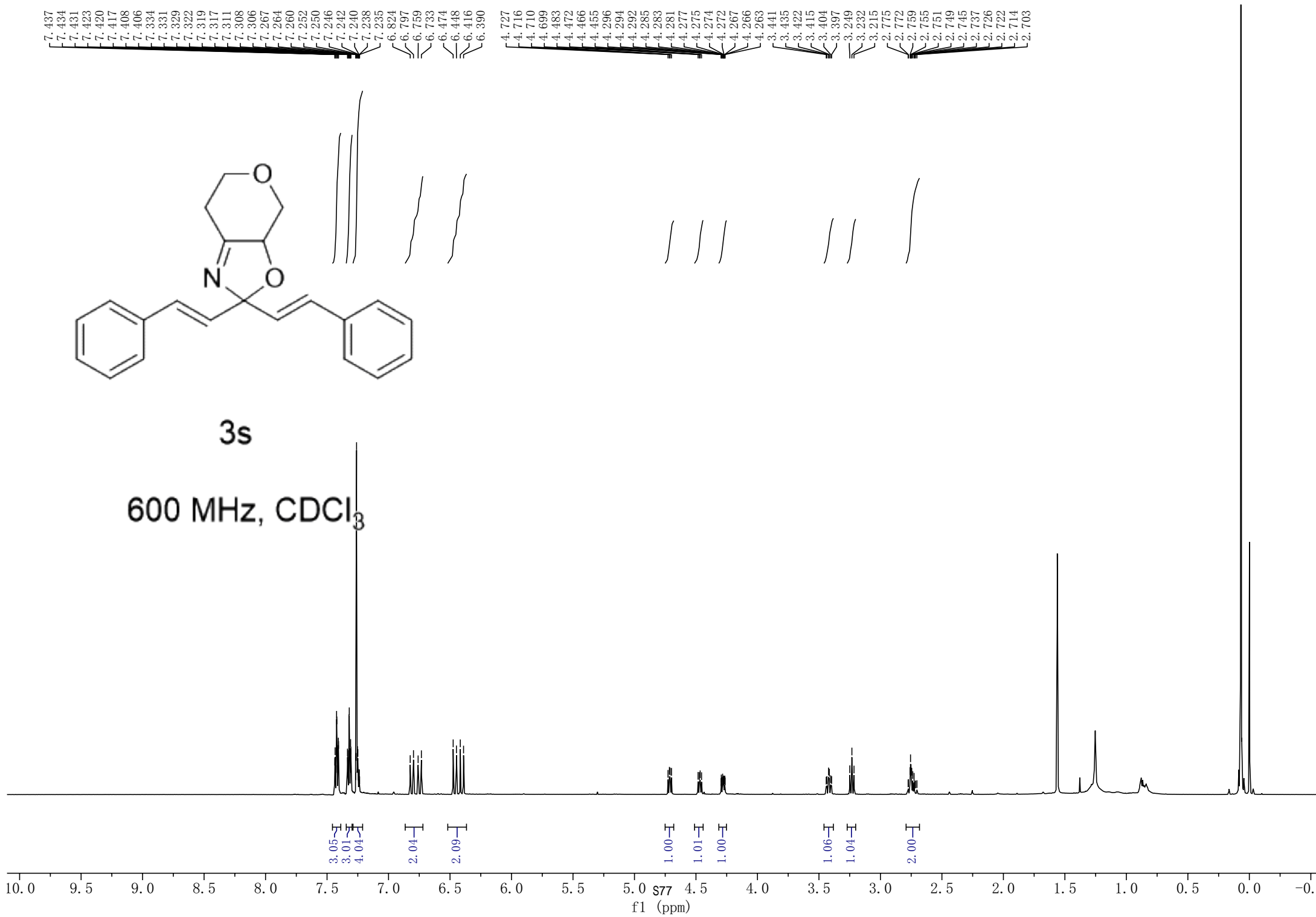
33.543  
30.626  
30.167  
25.996  
25.252

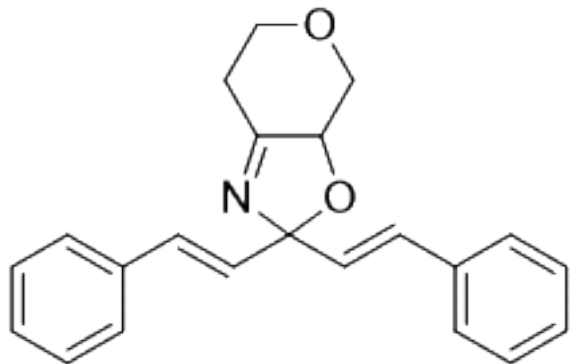




3s

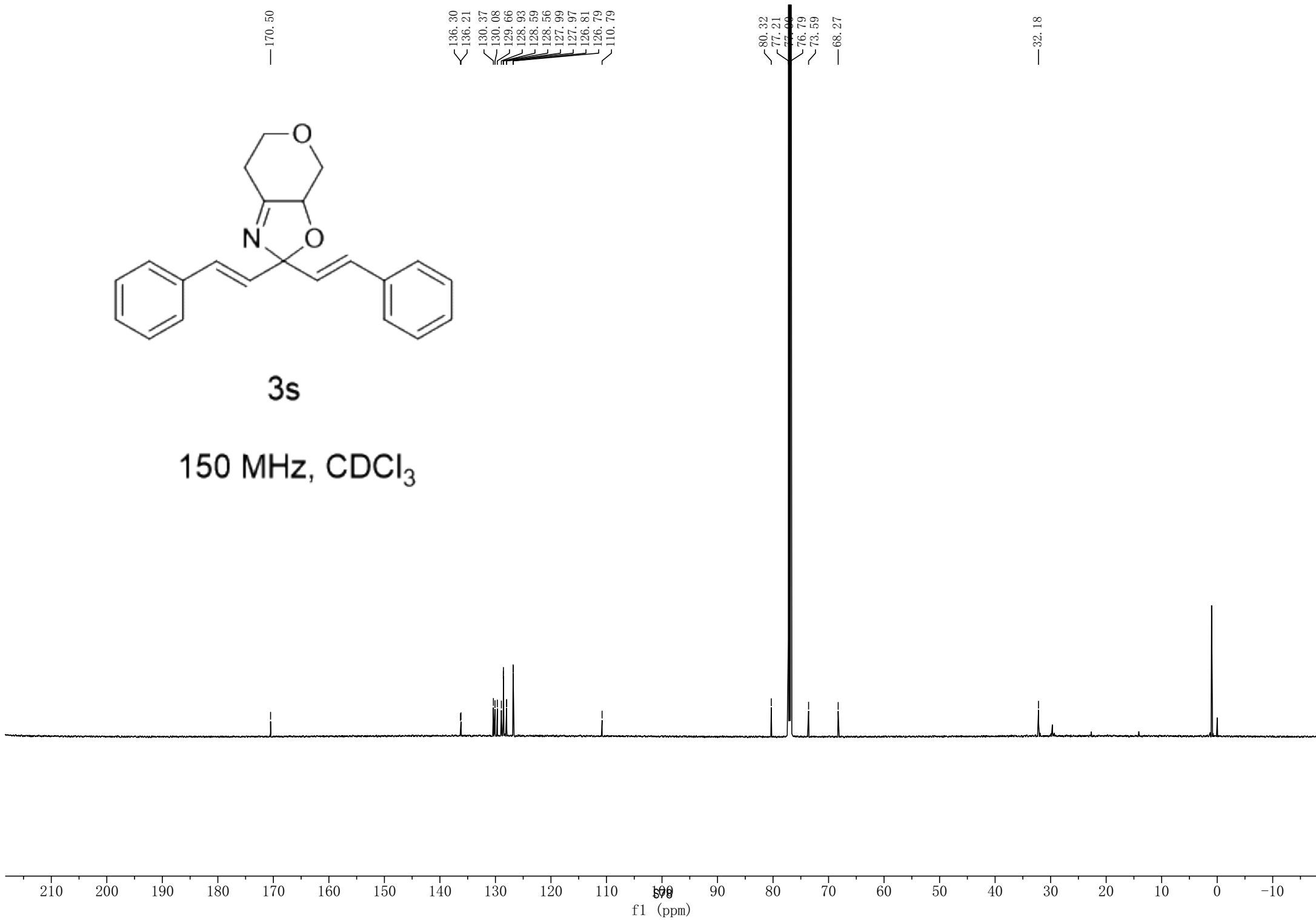
600 MHz, CDCl<sub>3</sub>

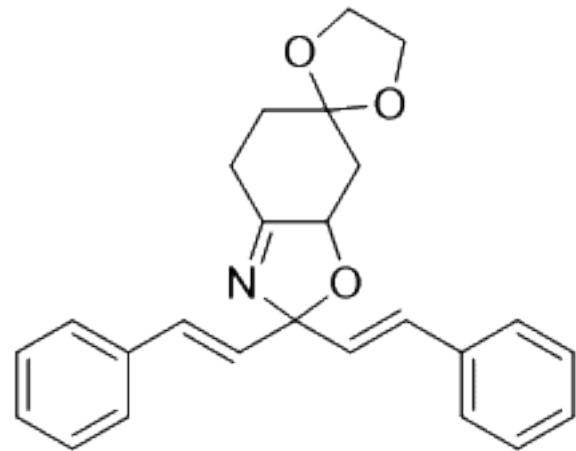




3s

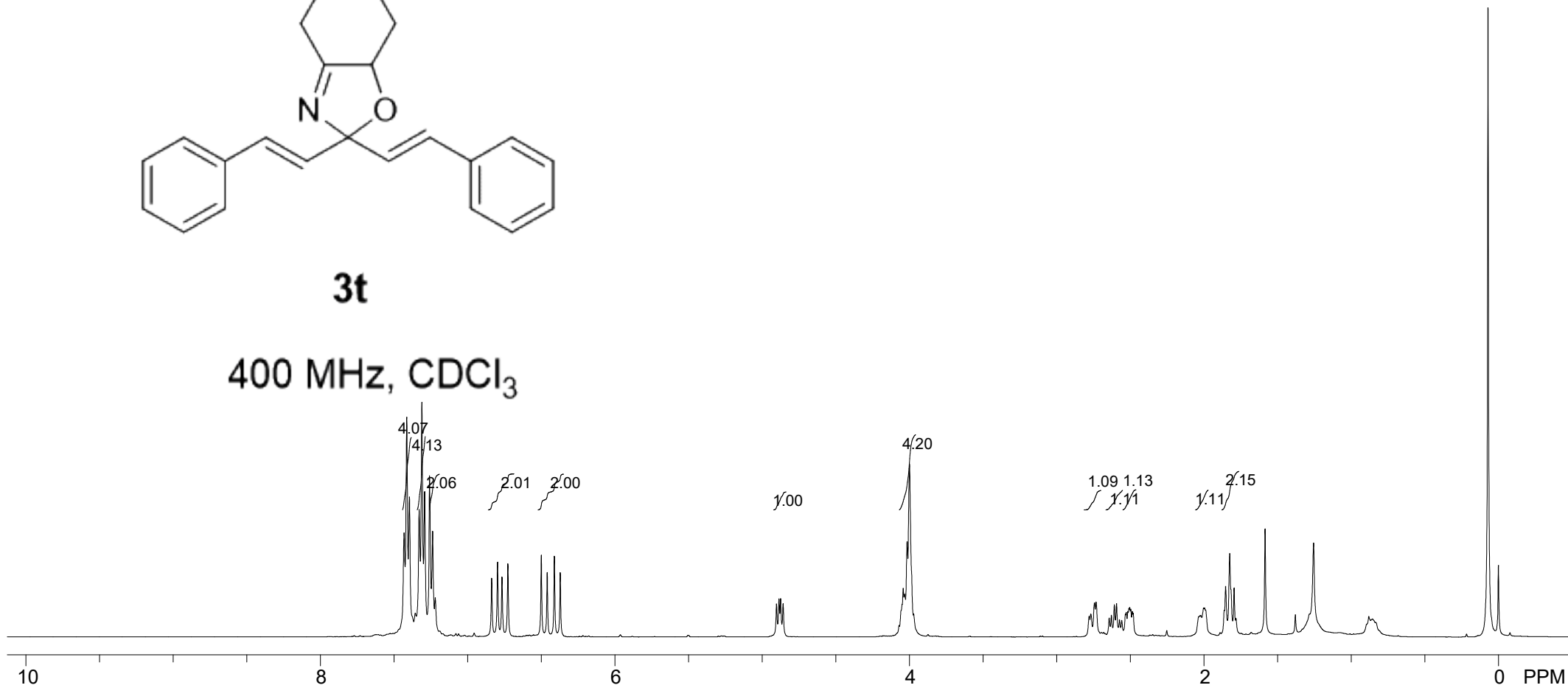
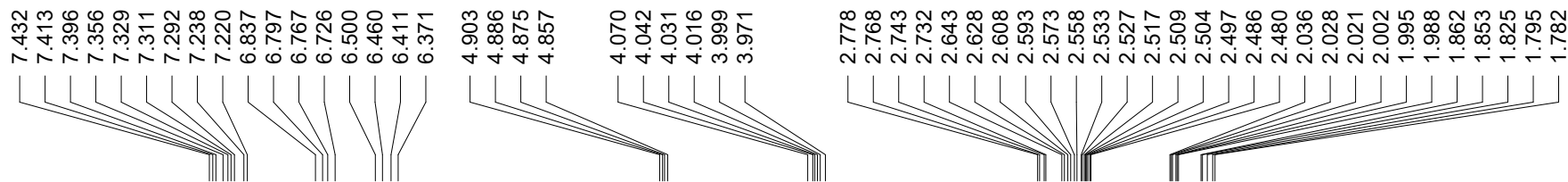
150 MHz, CDCl<sub>3</sub>

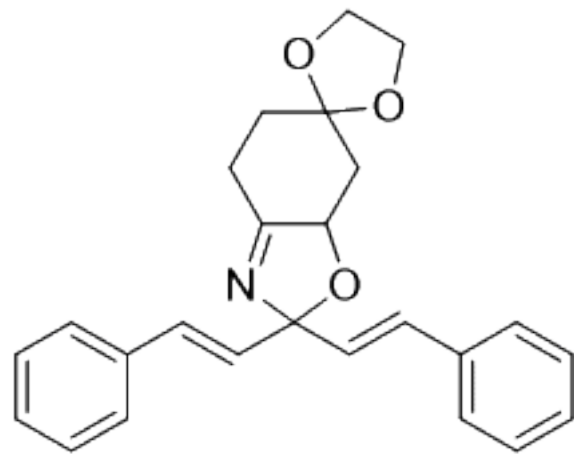




**3t**

400 MHz, CDCl<sub>3</sub>



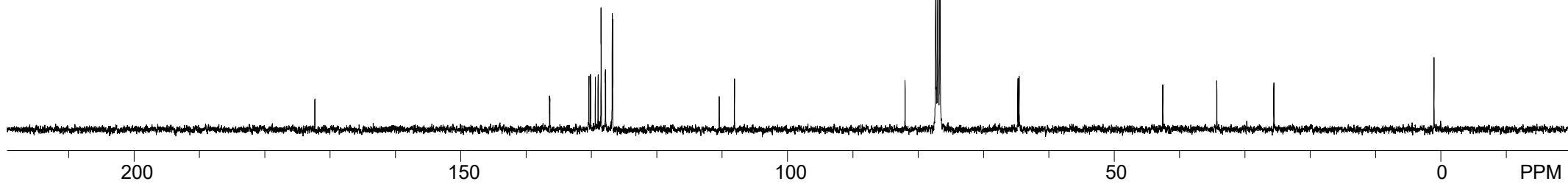


**3t**

100 MHz, CDCl<sub>3</sub>

172.329  
136.419  
136.375  
130.396  
130.155  
129.419  
128.996  
128.544  
128.507  
127.873  
127.844  
126.830  
126.779  
110.461  
108.127

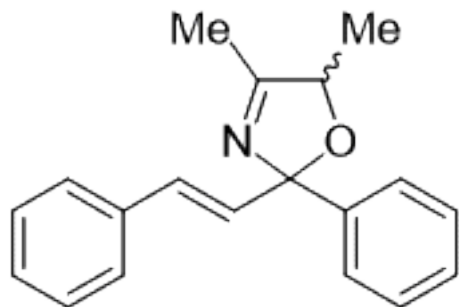
82.024  
77.321  
77.000  
76.687  
64.750  
64.561  
42.555  
34.279  
25.537





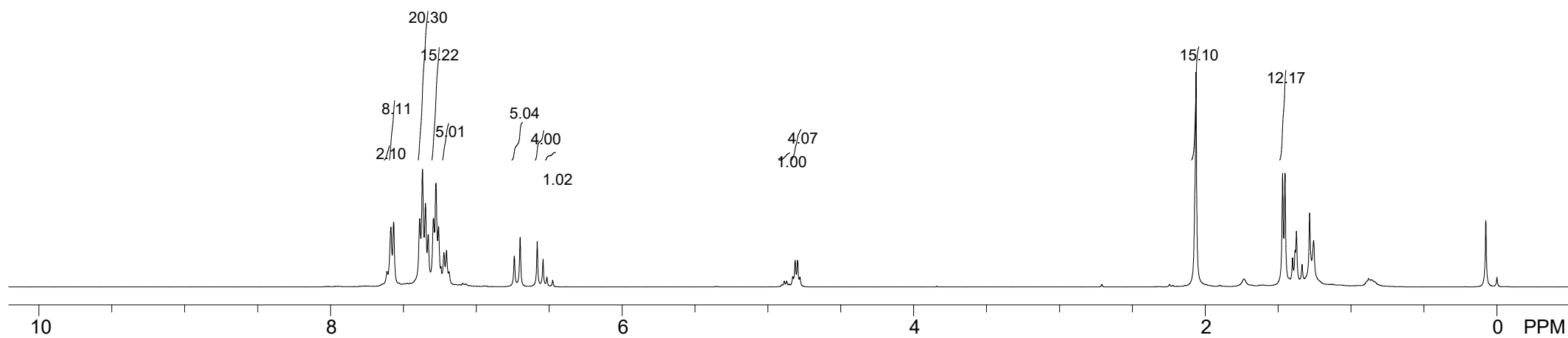
7.612  
7.586  
7.567  
7.388  
7.369  
7.349  
7.330  
7.294  
7.278  
7.259  
7.242  
7.223  
7.204  
7.187  
6.739  
6.699  
6.582  
6.542  
6.516  
6.476  
4.904  
4.888  
4.871  
4.830  
4.813  
4.797  
4.780

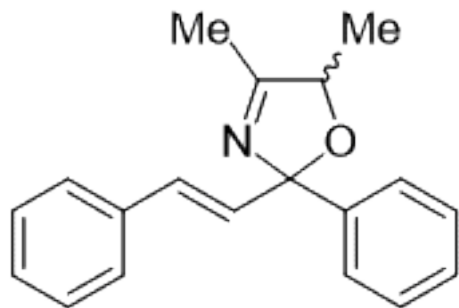
2.064  
1.470  
1.453  
1.402  
1.384



**3u** dr = 4:1

400 MHz, CDCl<sub>3</sub>





**3u** dr = 4:1

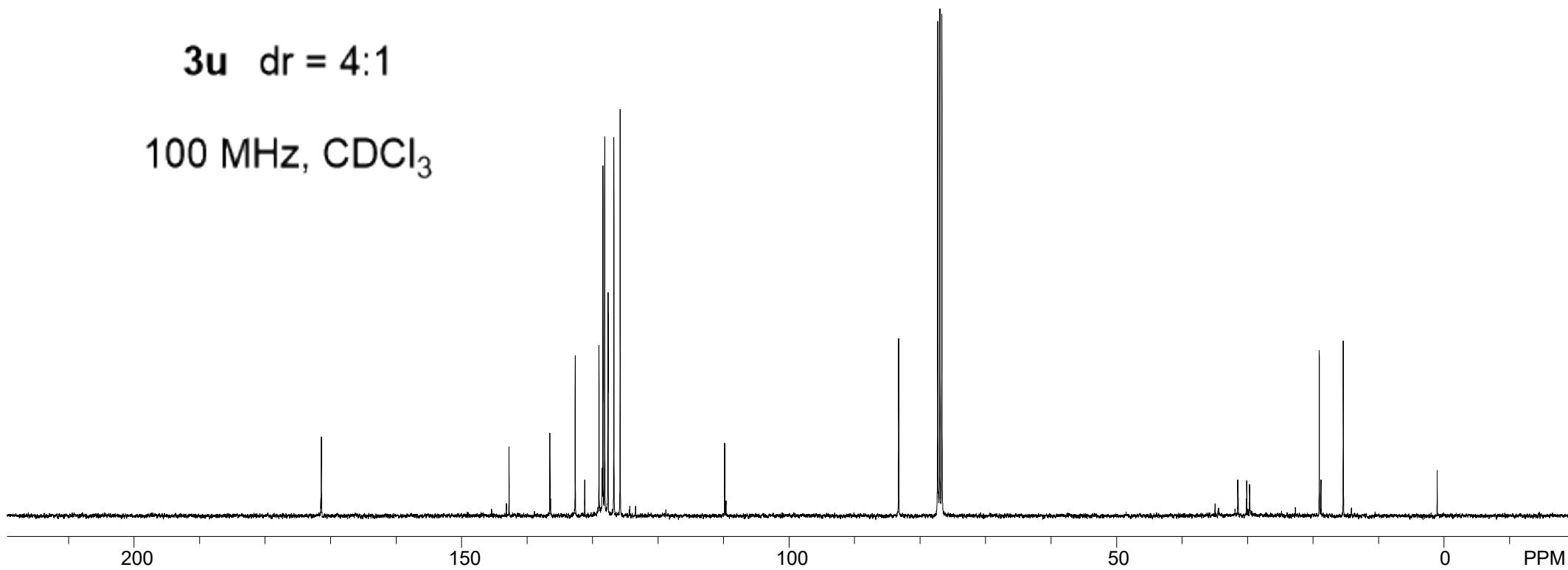
100 MHz, CDCl<sub>3</sub>

171.491  
171.418

143.163  
142.762  
136.528  
136.426  
132.656  
131.205  
129.185  
129.025  
128.551  
128.456  
128.420  
128.157  
127.669  
127.632  
126.757  
125.802  
109.841  
109.637

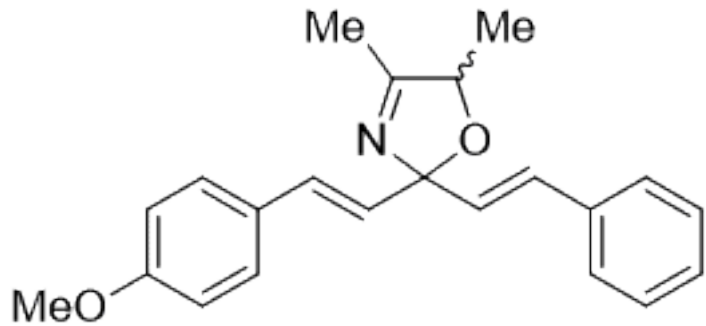
83.285  
77.314  
77.000  
76.679

19.011  
18.748  
15.336



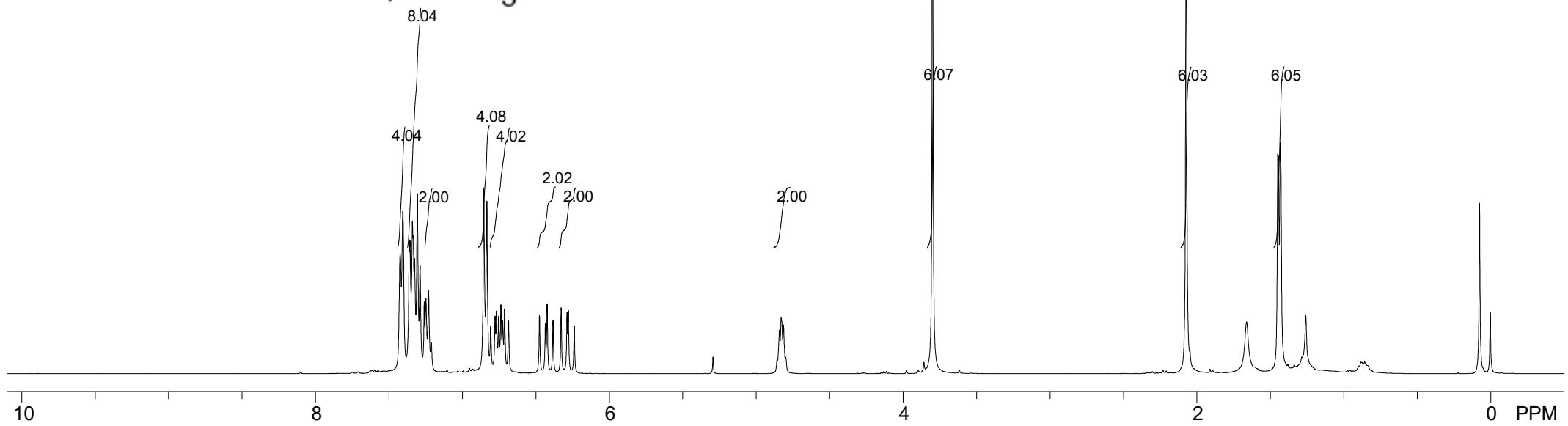
7.424  
7.406  
7.362  
7.357  
7.341  
7.335  
7.326  
7.307  
7.288  
7.260  
7.248  
7.231  
7.212  
6.855  
6.834  
6.808  
6.778  
6.768  
6.753  
6.738  
6.726  
6.713  
6.686  
6.476  
6.436  
6.423  
6.384  
6.328  
6.288  
6.279  
6.239  
4.858  
4.842  
4.830  
4.814  
4.798  
3.799

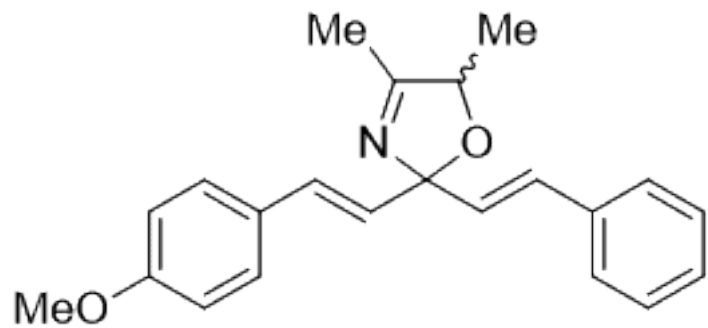
2.073  
1.449  
1.445  
1.432  
1.428



**3v** dr = 1:1

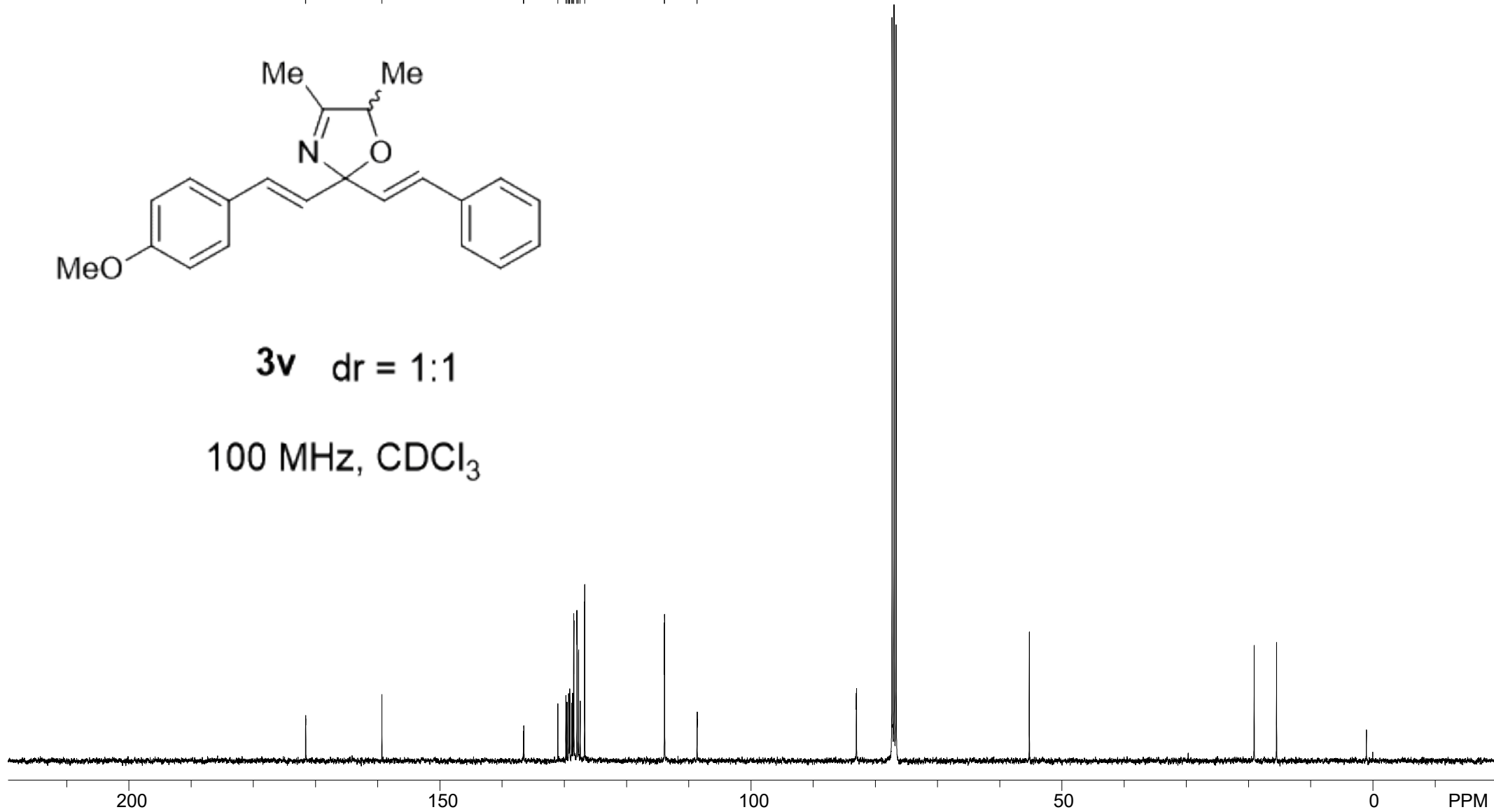
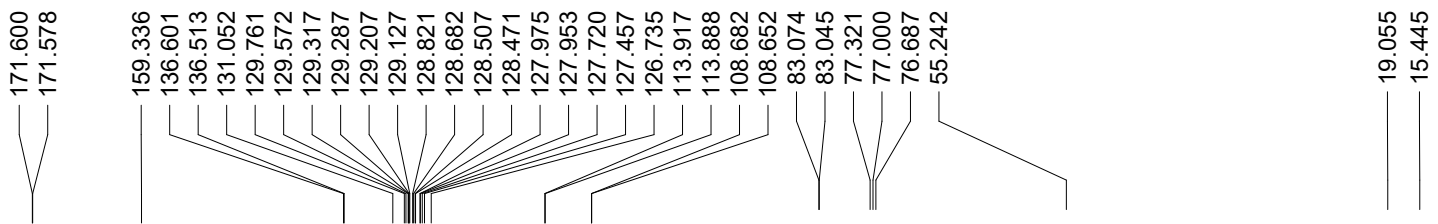
400 MHz, CDCl<sub>3</sub>

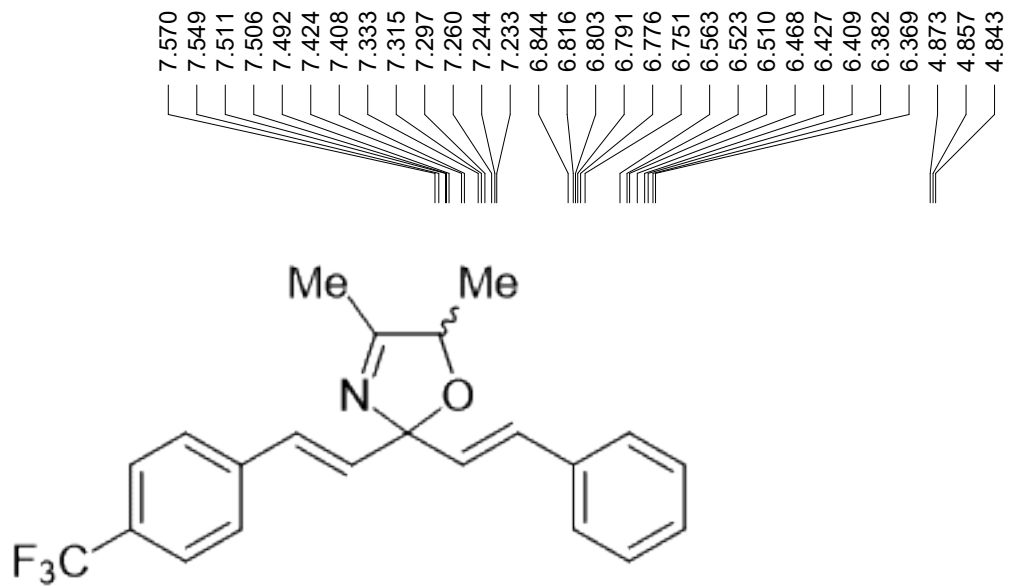




**3v** dr = 1:1

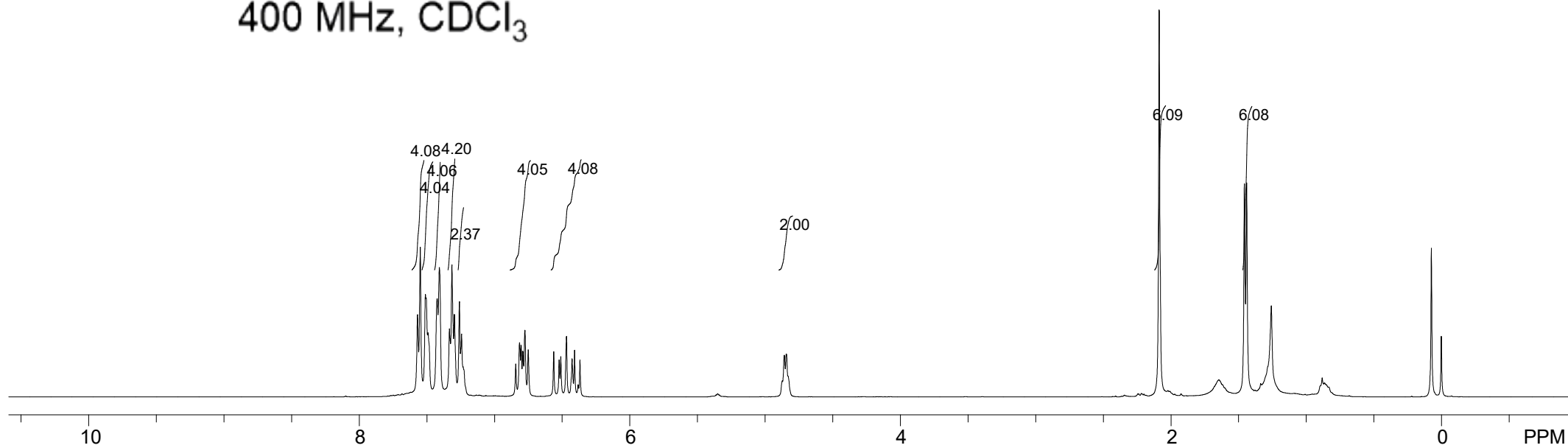
100 MHz, CDCl<sub>3</sub>

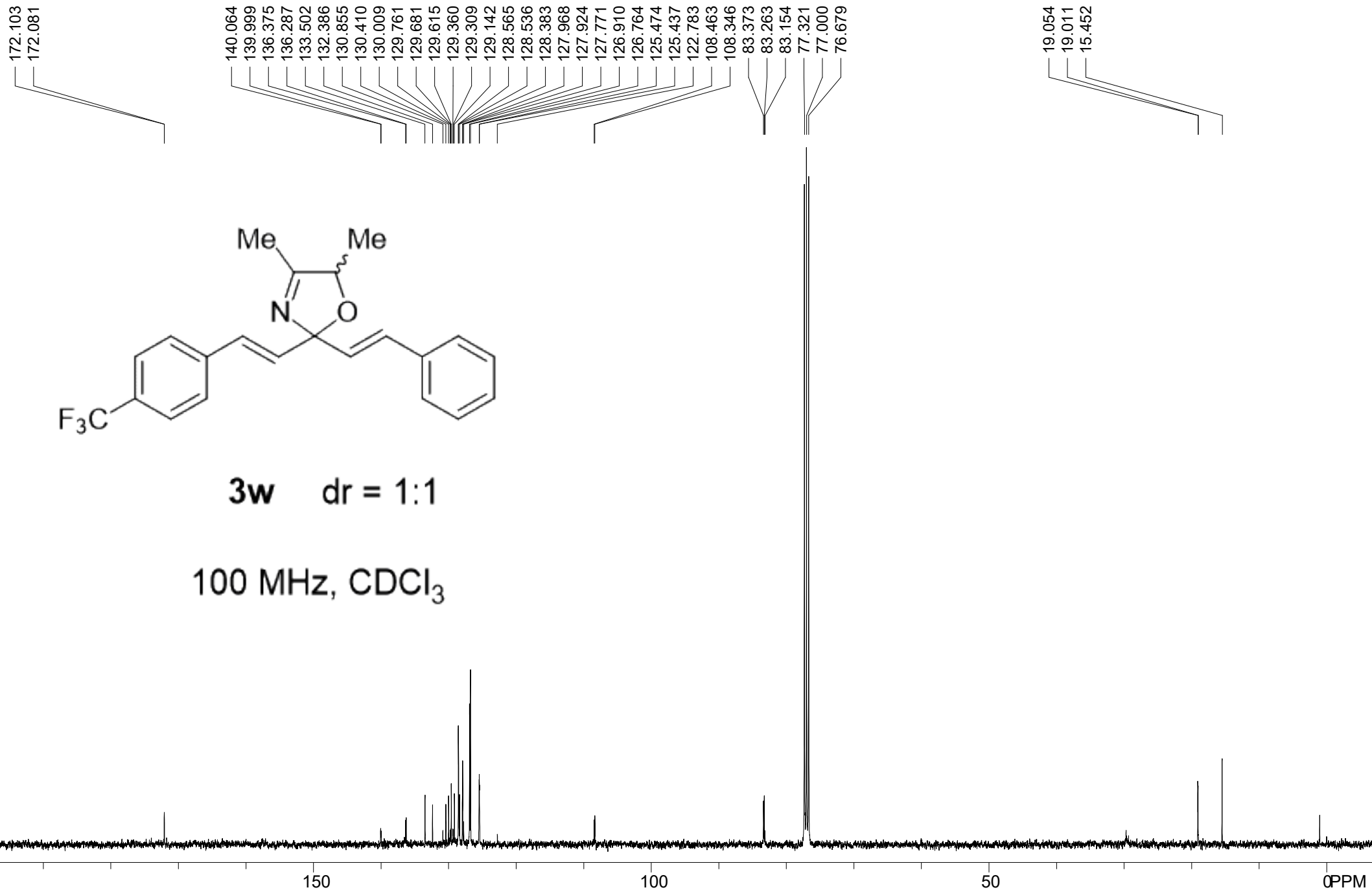


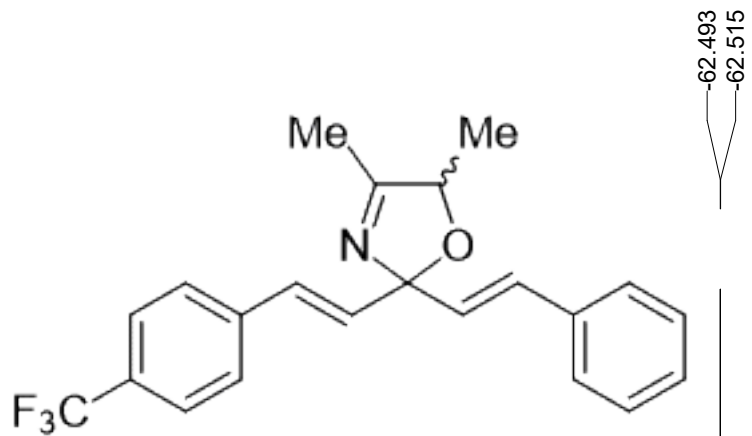


**3w** dr = 1:1

400 MHz, CDCl<sub>3</sub>

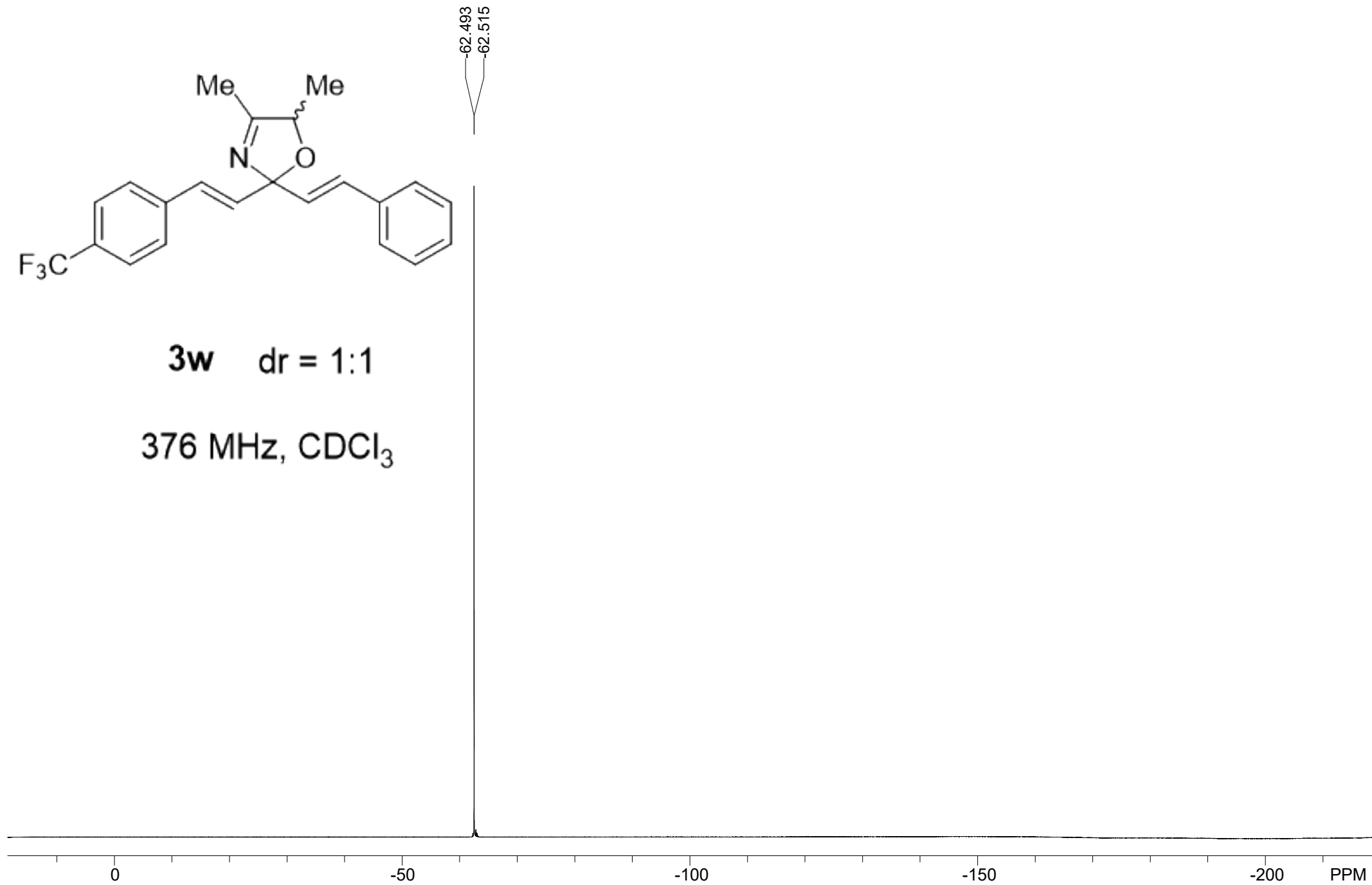


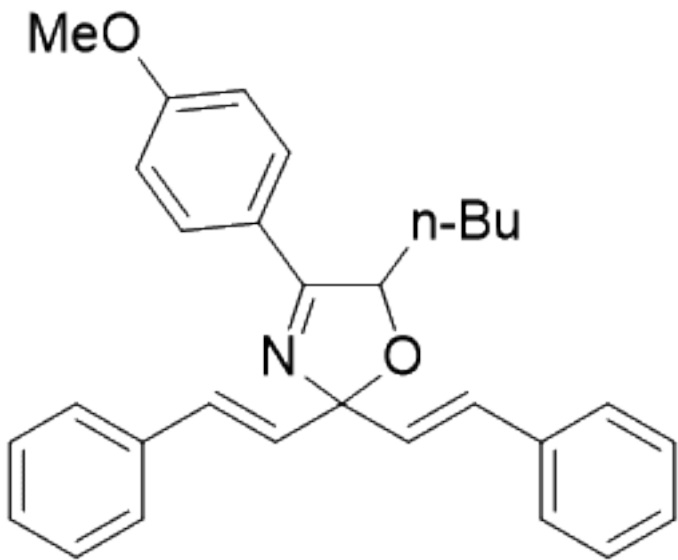




**3w** dr = 1:1

376 MHz, CDCl<sub>3</sub>



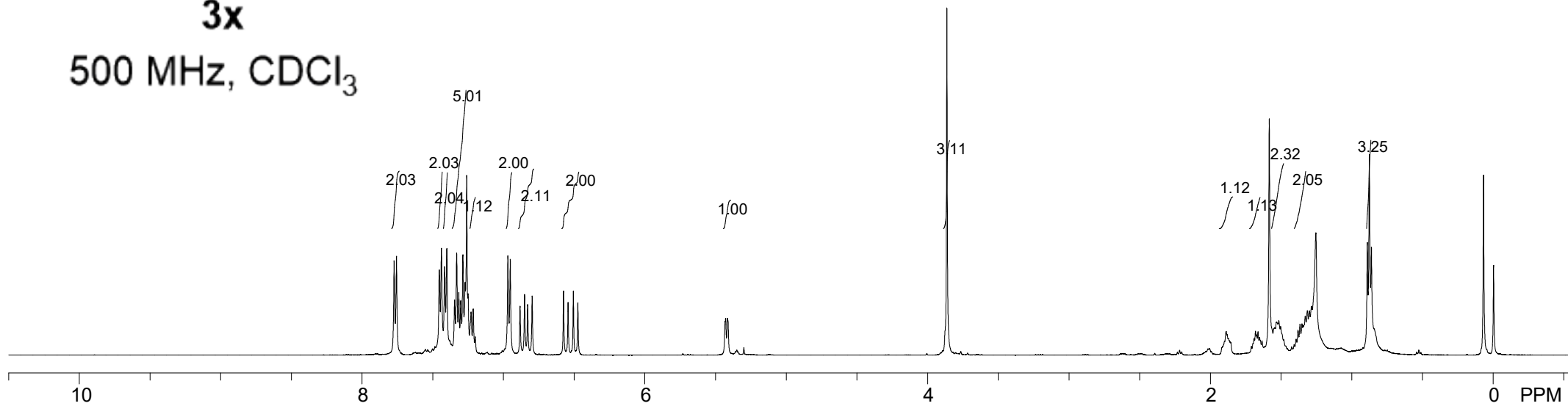


**3x**

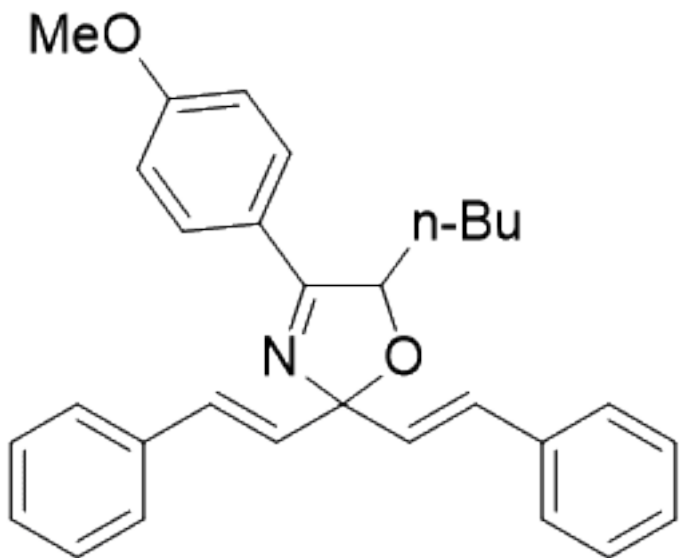
500 MHz, CDCl<sub>3</sub>

7.774  
7.757  
7.454  
7.439  
7.416  
7.401  
7.346  
7.331  
7.316  
7.302  
7.287  
7.272  
7.251  
7.229  
7.214  
7.200  
6.969  
6.952  
6.882  
6.850  
6.829  
6.797  
6.575  
6.543  
6.505  
6.474  
5.428  
5.416  
5.412  
3.863

1.915  
1.901  
1.889  
1.882  
1.873  
1.867  
1.860  
1.711  
1.700  
1.692  
1.682  
1.674  
1.664  
1.654  
1.636  
1.548  
1.543  
1.535  
1.531  
1.525  
1.517  
1.504  
1.483  
1.468  
1.426  
1.409  
1.395  
1.382  
1.368  
1.353  
1.345

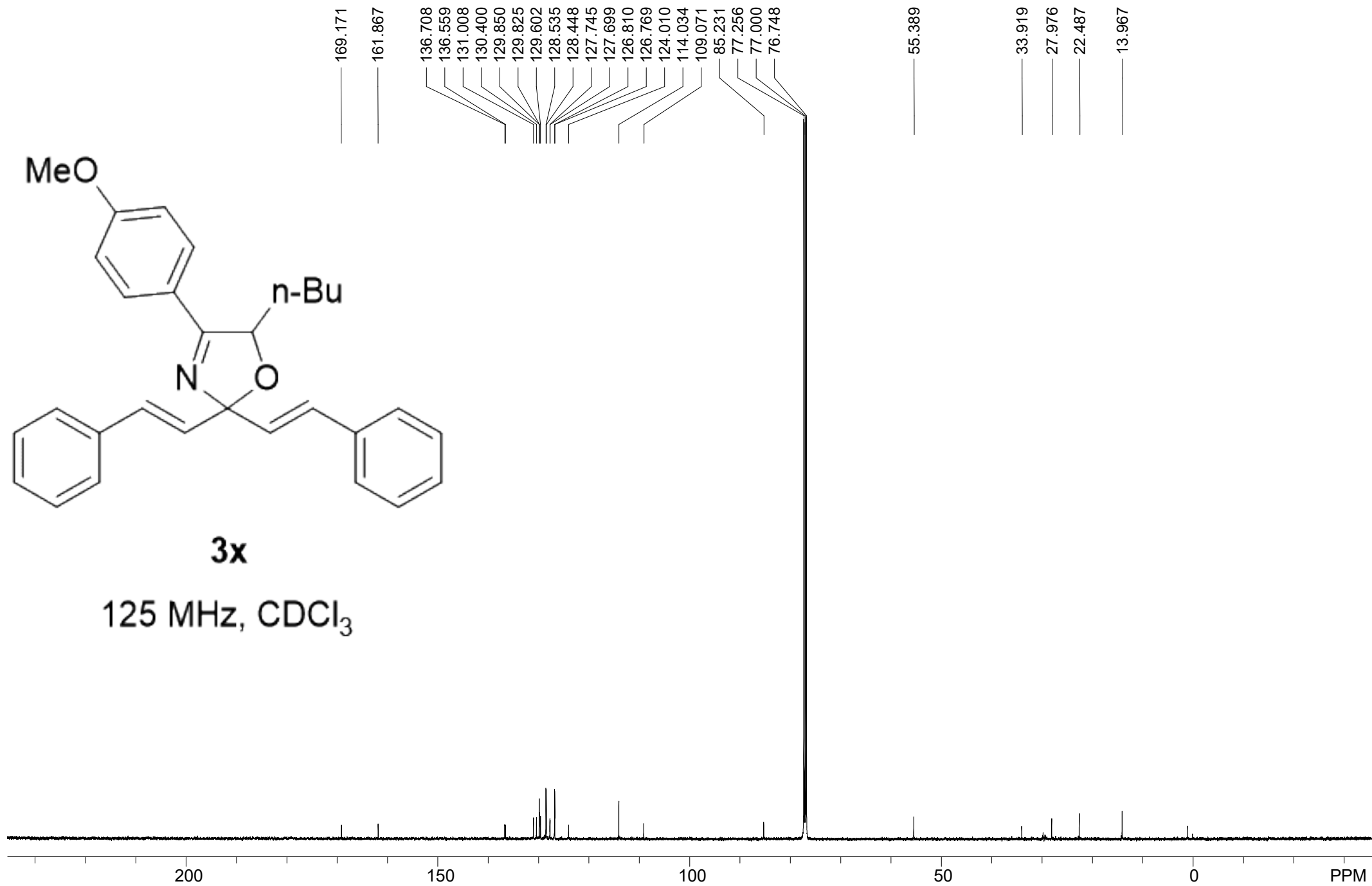


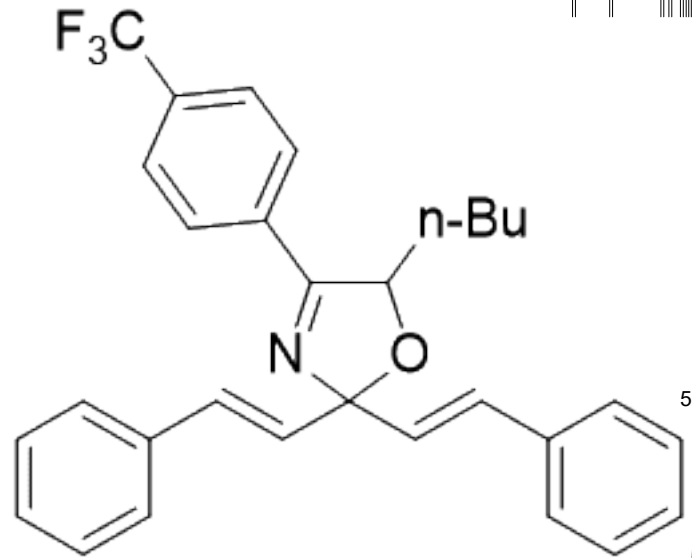
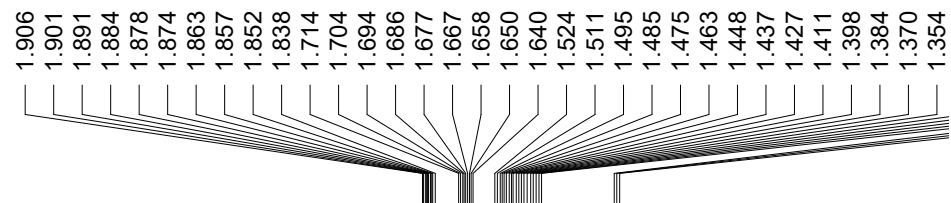
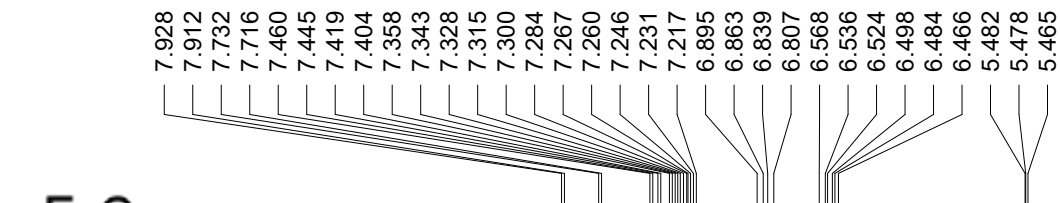




**3x**

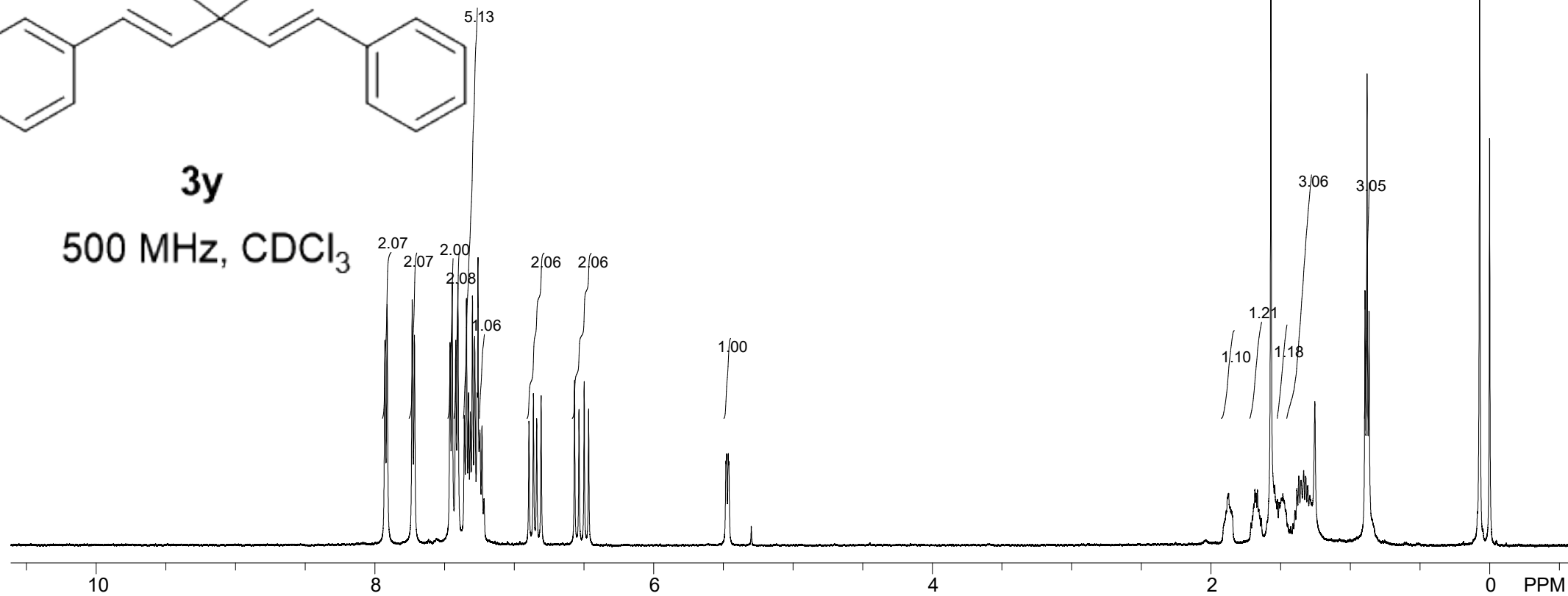
125 MHz, CDCl<sub>3</sub>

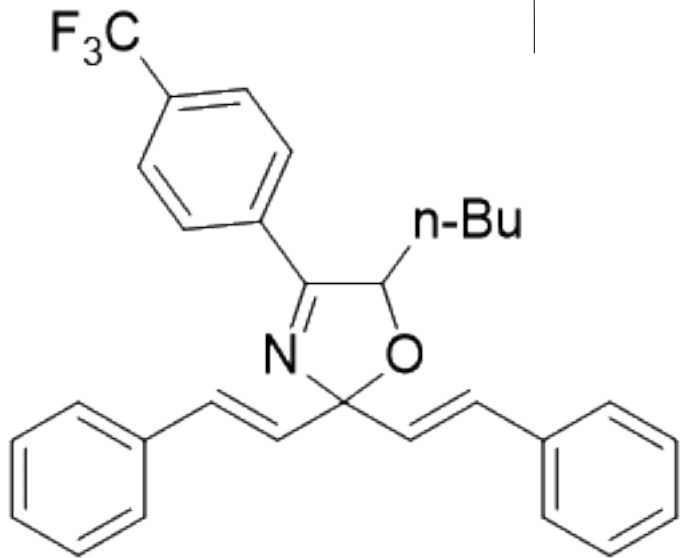




**3y**

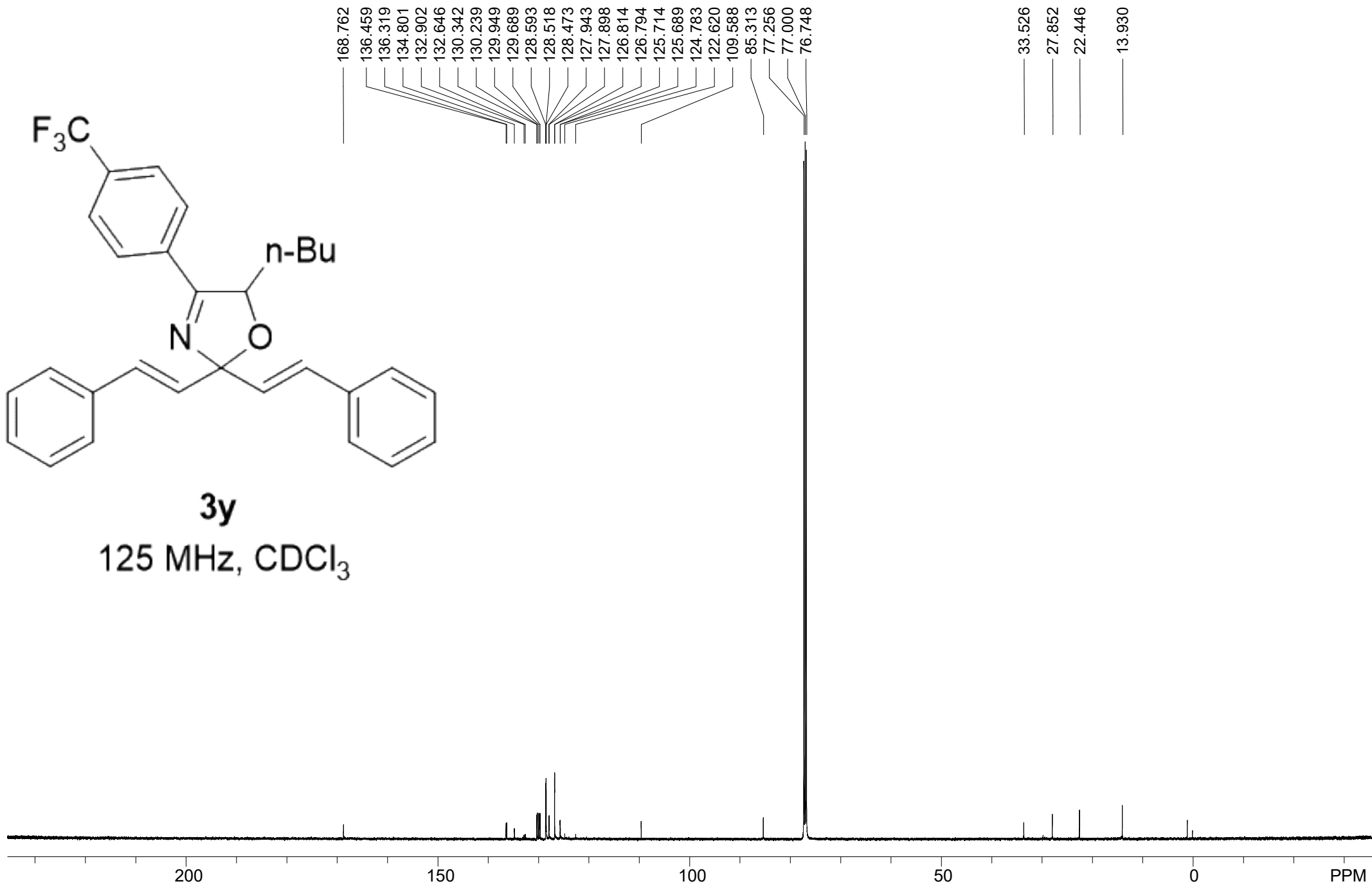
500 MHz, CDCl<sub>3</sub>

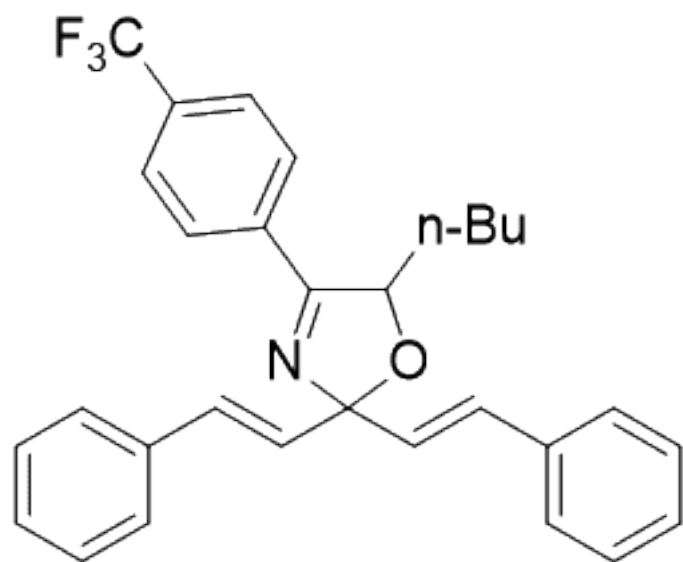




**3y**

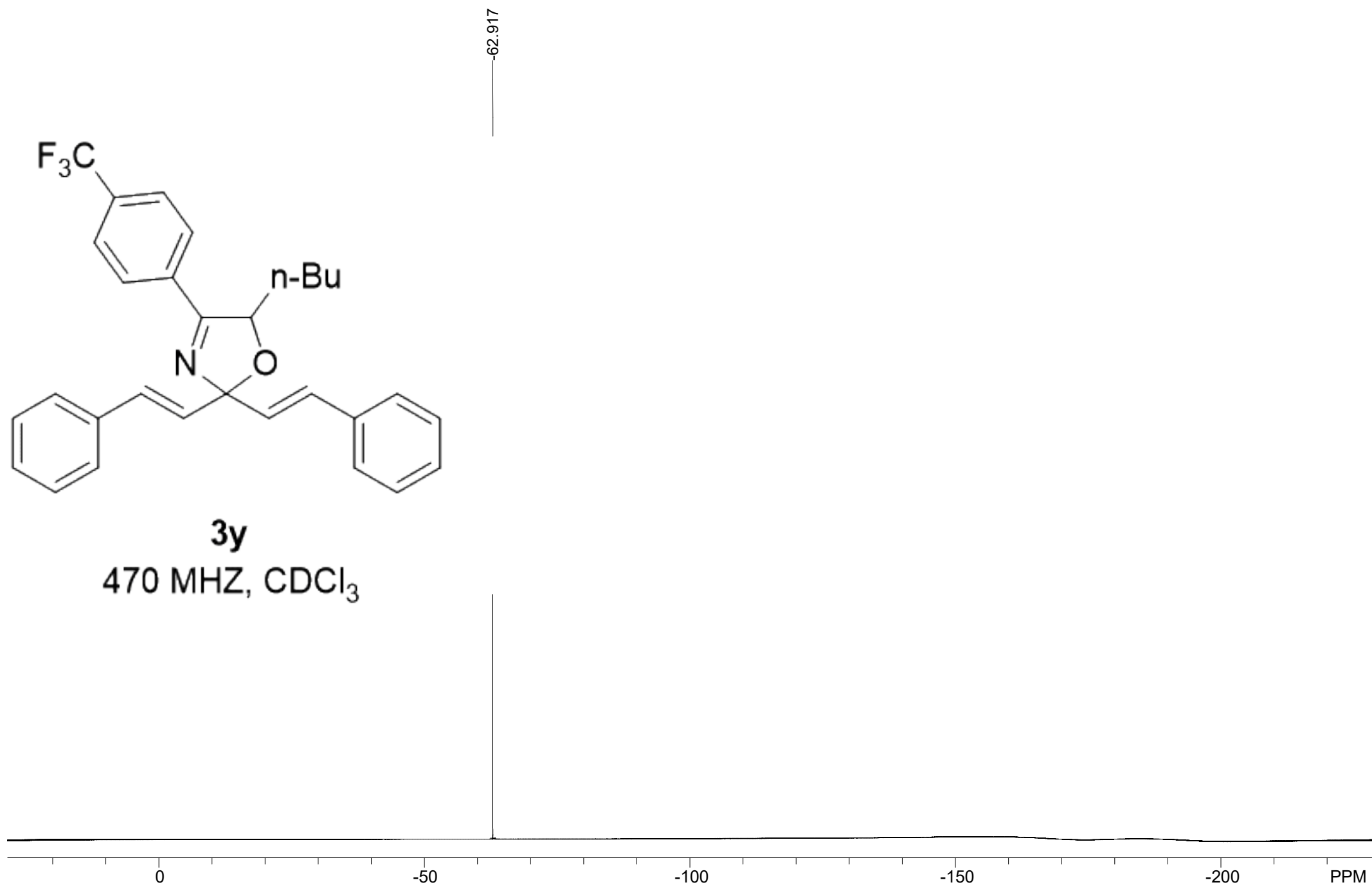
125 MHz, CDCl<sub>3</sub>

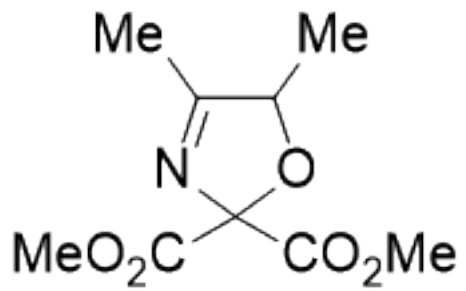




**3y**

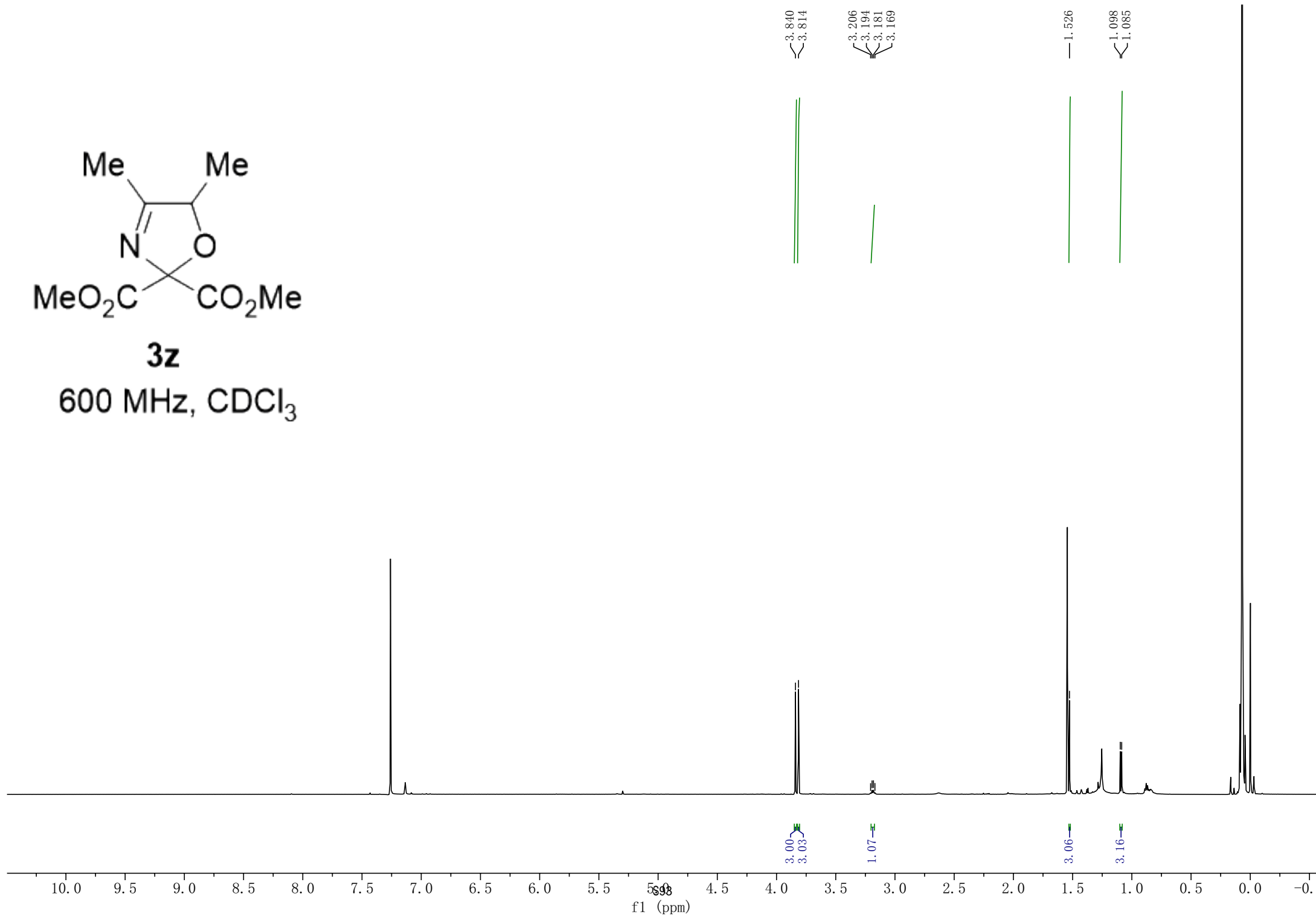
470 MHz, CDCl<sub>3</sub>

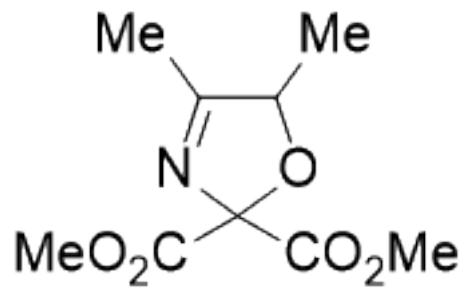




**3z**

600 MHz, CDCl<sub>3</sub>





**3z**

150 MHz, CDCl<sub>3</sub>

171.14  
169.73  
169.23

106.68

77.21  
77.00  
76.79

53.53  
53.41  
51.10

22.51

10.25

