

# Cross-coupling of Mesylated Phenol Derivatives with Potassium Cyclopropyltrifluoroborate

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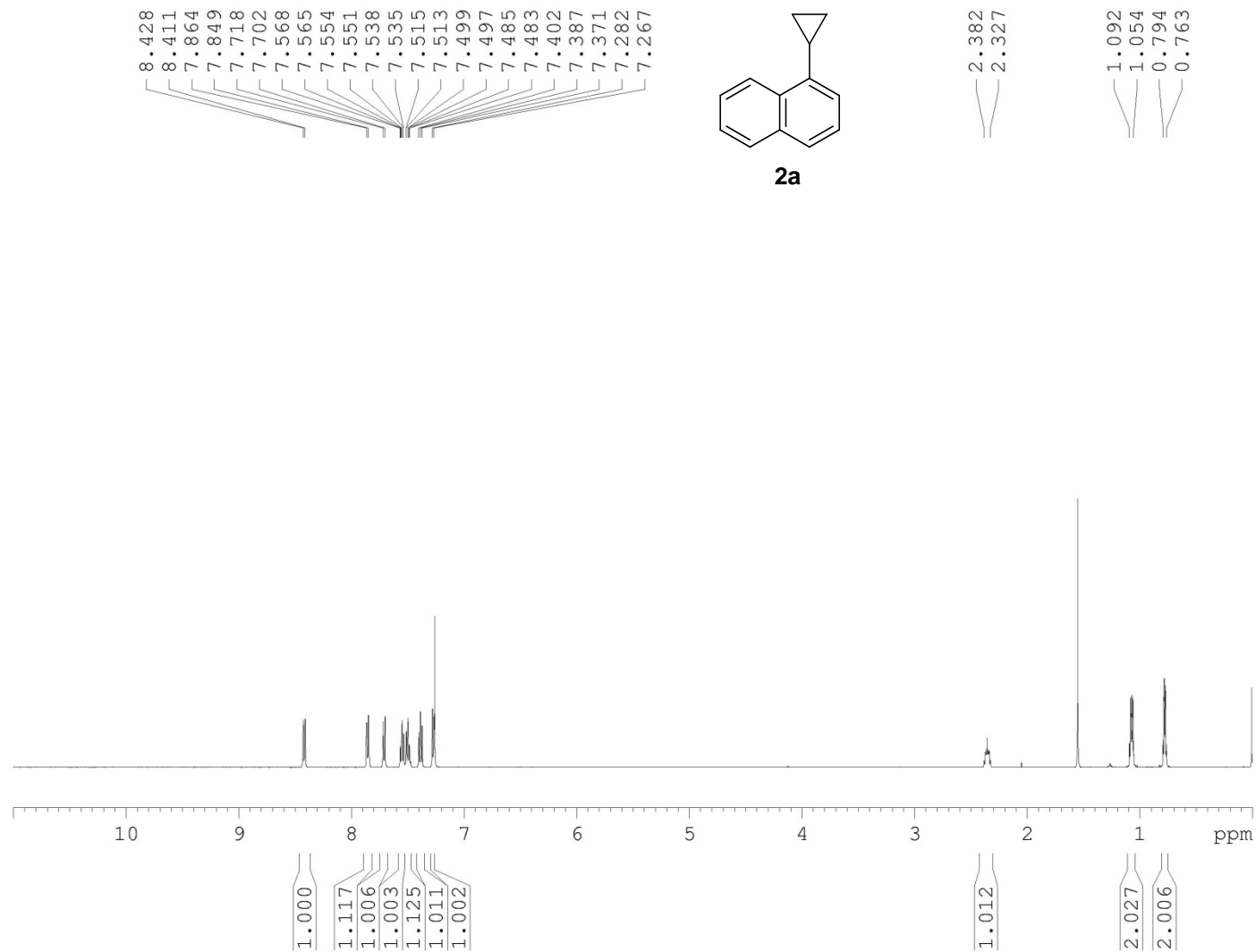
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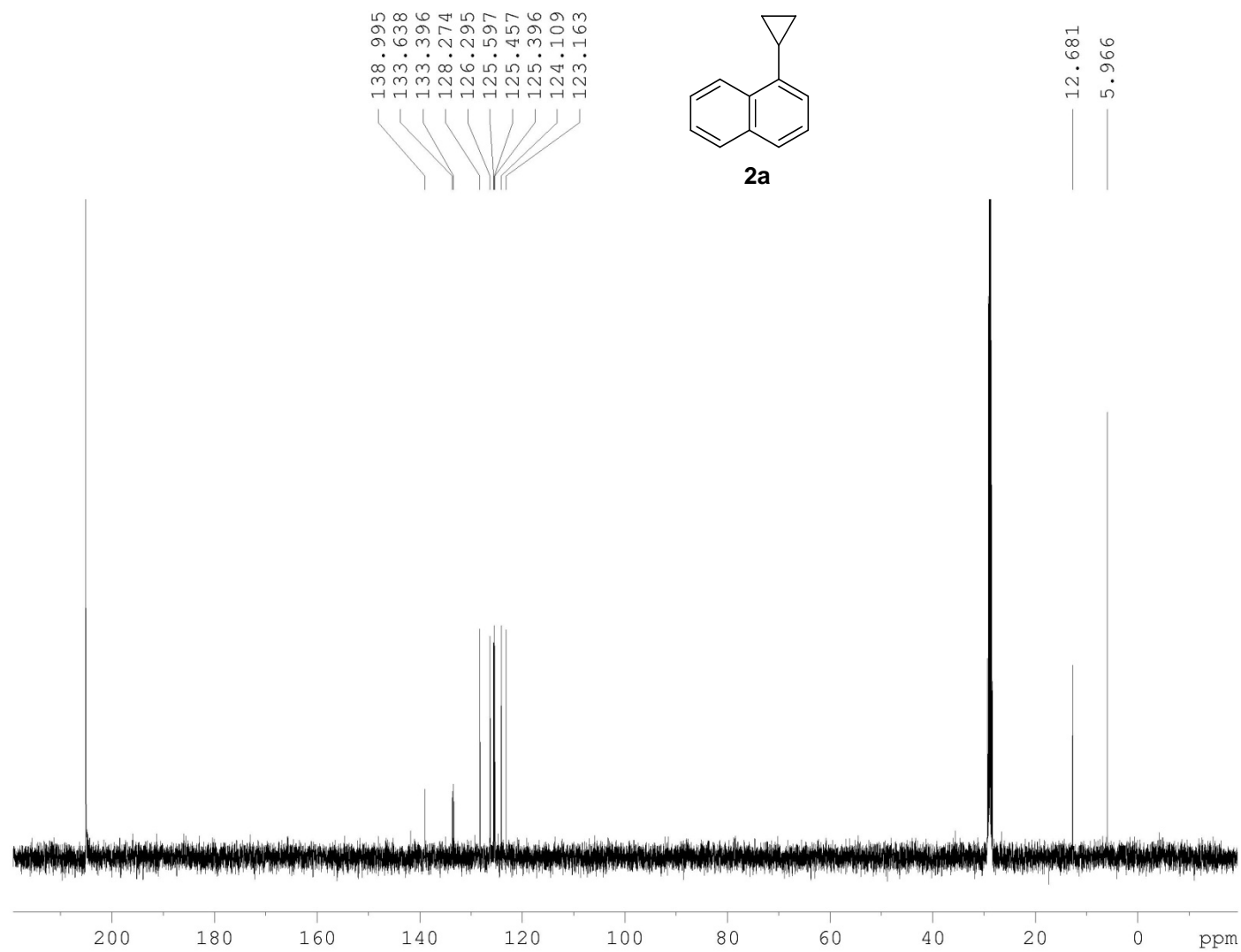
<b>General considerations</b>	<b>S2</b>
<b><sup>1</sup>H/<sup>13</sup>C NMR Spectra of 1-cyclopropyl aryl compounds</b>	<b>S3-S21</b>
<b><sup>1</sup>H/<sup>13</sup>C NMR Spectra of 1-cyclopropyl heteroaryl compounds</b>	<b>S22-S34</b>

## General Considerations

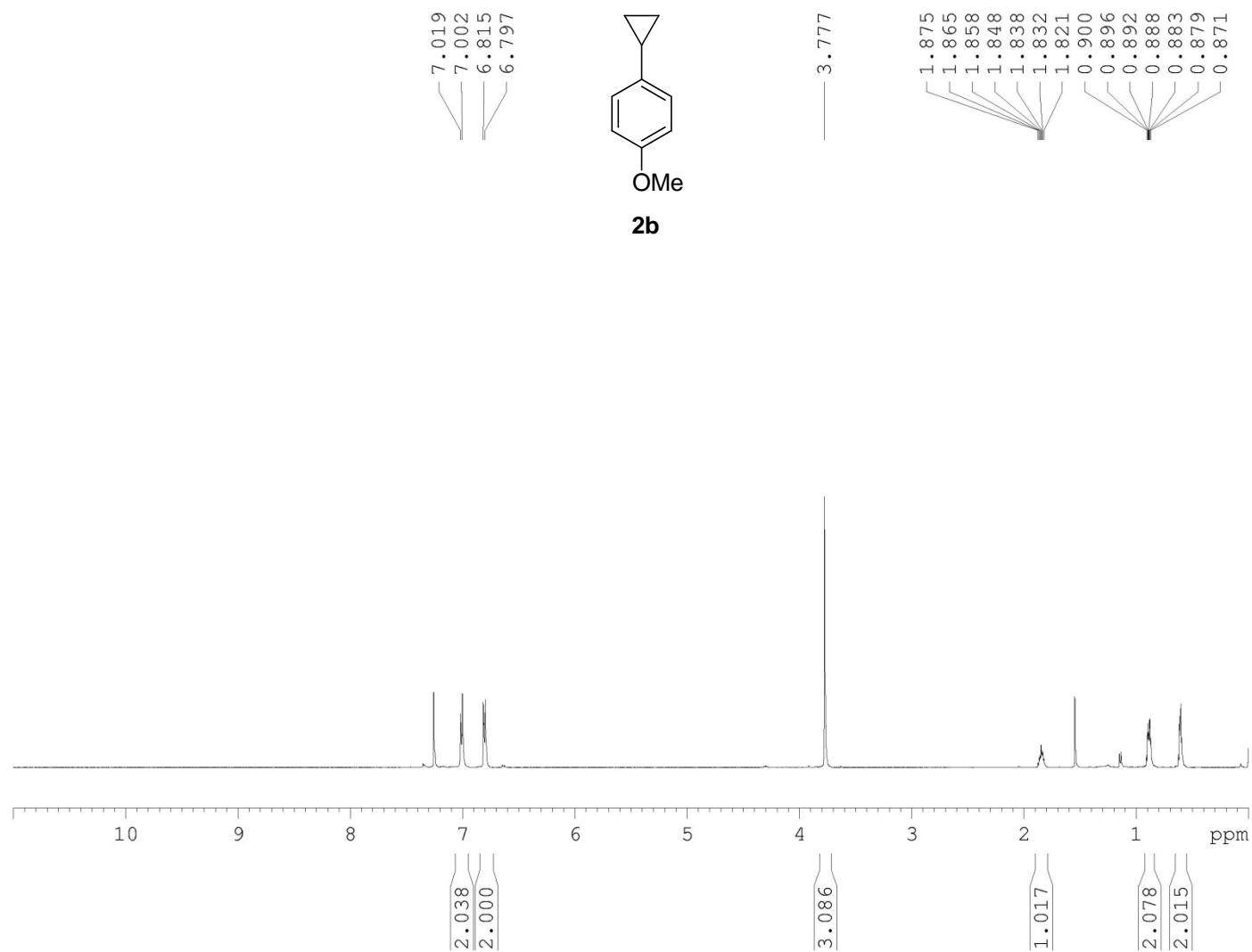
All reactions were carried out under an argon atmosphere. Pd(OAc)<sub>2</sub>, PdCl<sub>2</sub>(COD), RuPhos, potassium cyclopropyltrifluoroborate and K<sub>3</sub>PO<sub>4</sub> were used as received. Both solvents and deionized water were degassed with argon each time prior to use. Standard benchtop techniques were employed for handling air-sensitive reagents. Melting points (°C) are uncorrected. NMR spectra were recorded on a 500, 400, or 360 MHz spectrometer. Data are presented as follows: chemical shift (ppm), multiplicity (*s* = singlet, *d* = doublet, *t* = triplet, *m* = multiplet, *br* = broad), coupling constant *J* (Hz) and integration. Analytical thin-layer chromatography (TLC) was performed on TLC silica or alumina gel plates (0.25 mm) precoated with a fluorescent indicator. Standard flash chromatography procedures were followed using 32–63 μm silica gel. Visualization was effected with ultraviolet light.



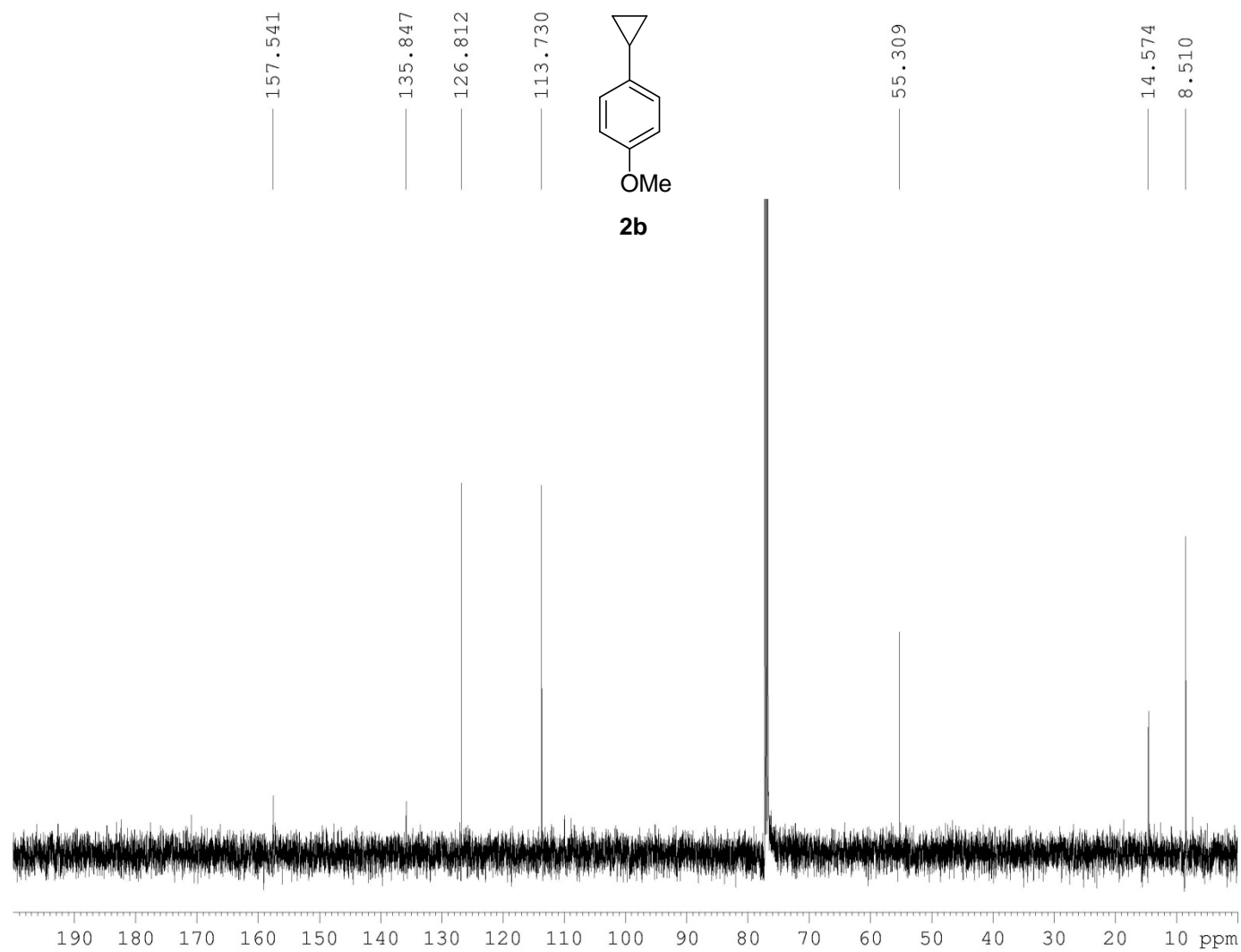
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 1-cyclopropyl-naphthalene **2a** (Table 2, entry 1)



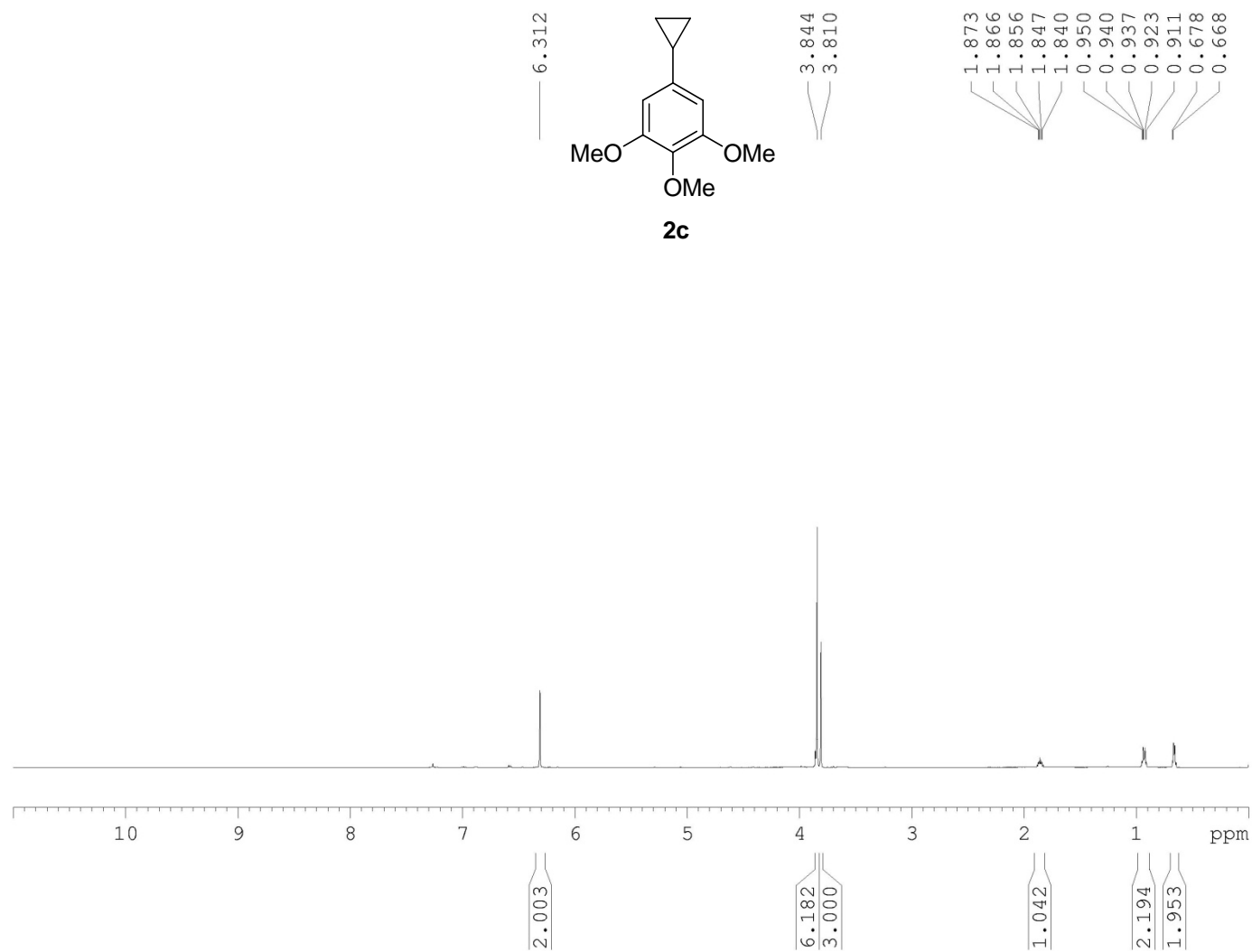
<sup>13</sup>C NMR (125 MHz, acetone-*d*<sub>6</sub>) Spectrum of 1-cyclopropyl-naphthalene **2a** (Table 2, entry 1)



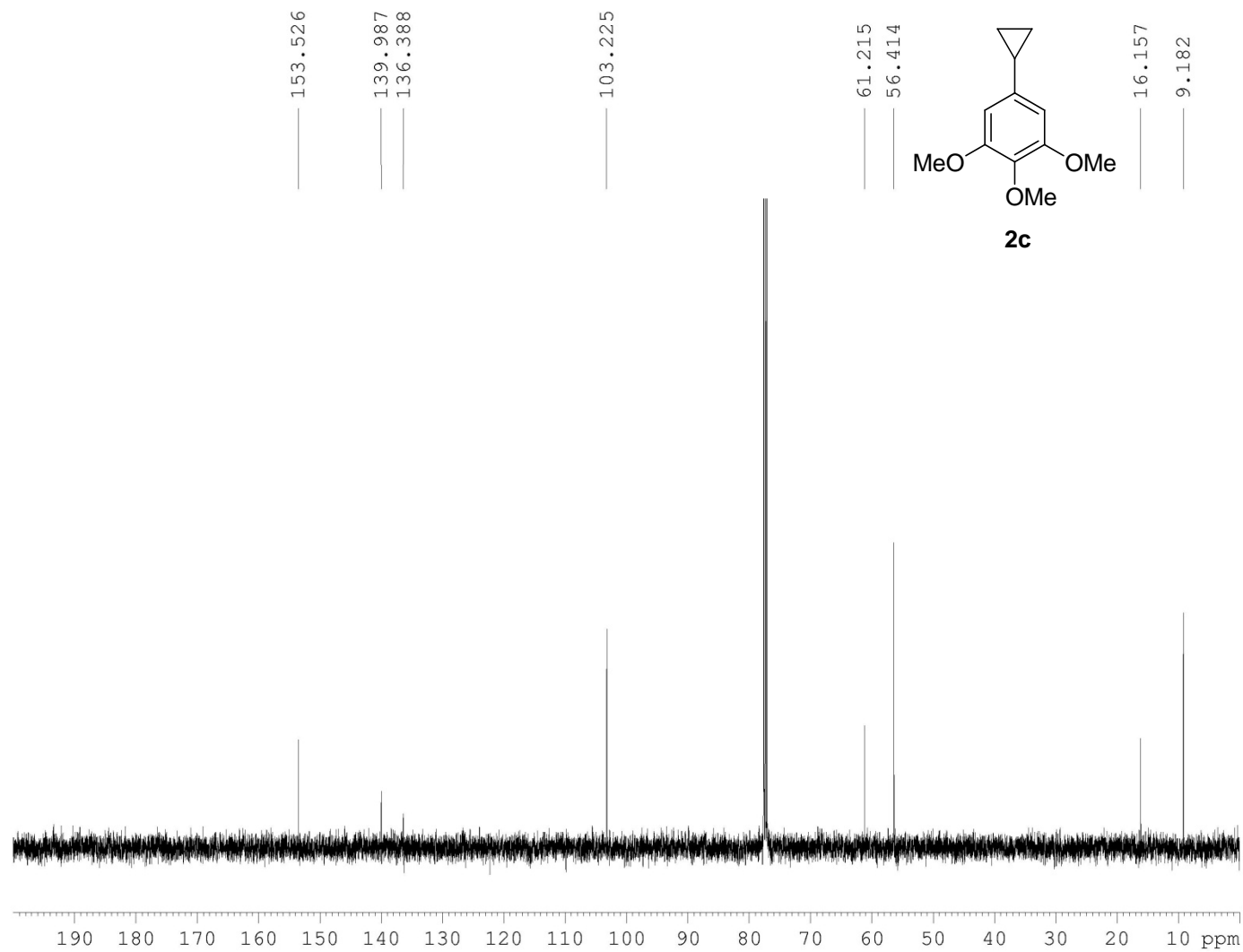
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 1-cyclopropyl-4-methoxybenzene **2b** (Table 2, entry 2)



<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) Spectrum of 1-cyclopropyl-4-methoxybenzene **2b** (Table 2, entry 2)

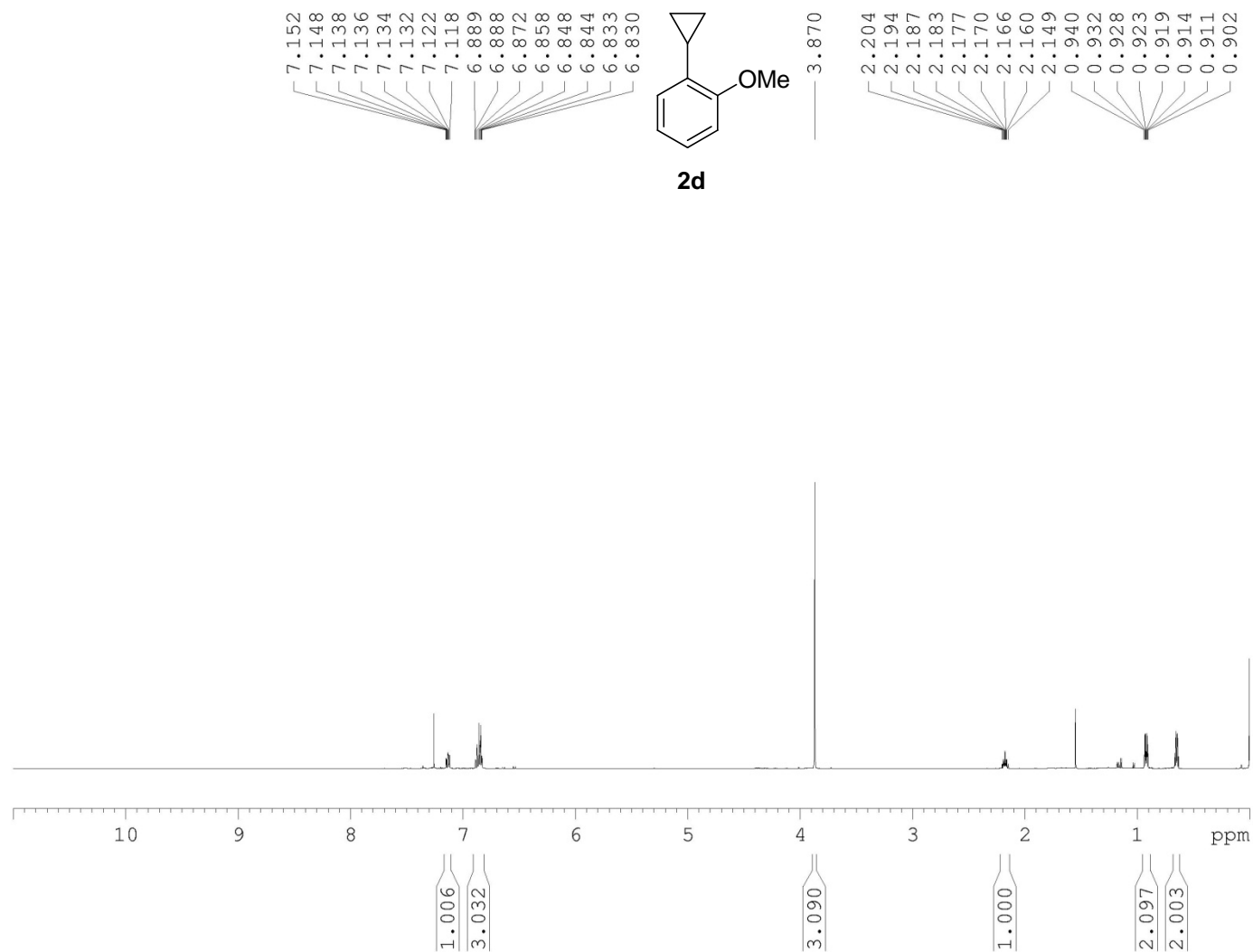


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) Spectrum of 5-cyclopropyl-1,2,3-trimethoxybenzene **2c** (Table 2, entry 3)

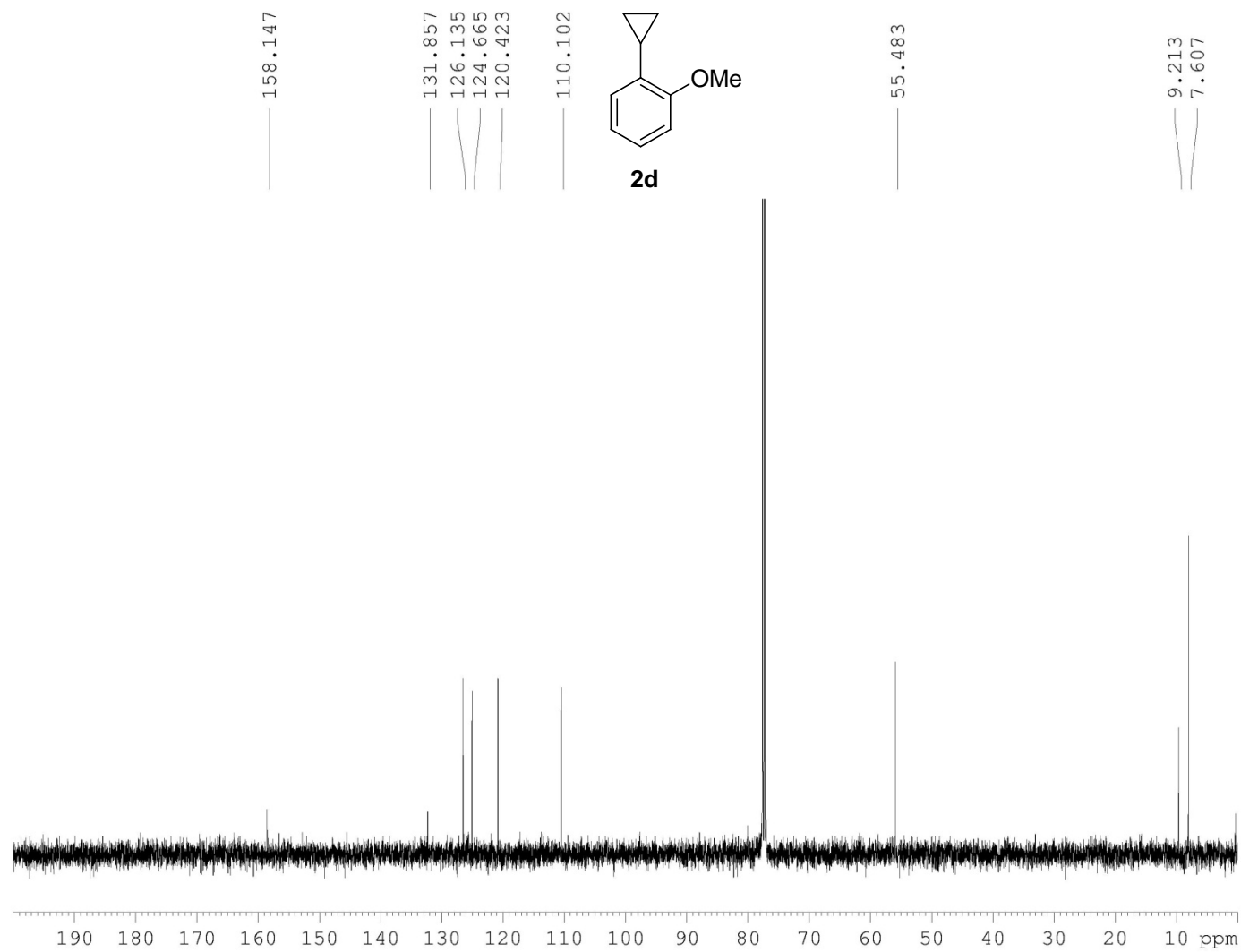


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) Spectrum of 5-cyclopropyl-1,2,3-trimethoxybenzene **2c** (Table 2, entry 3)

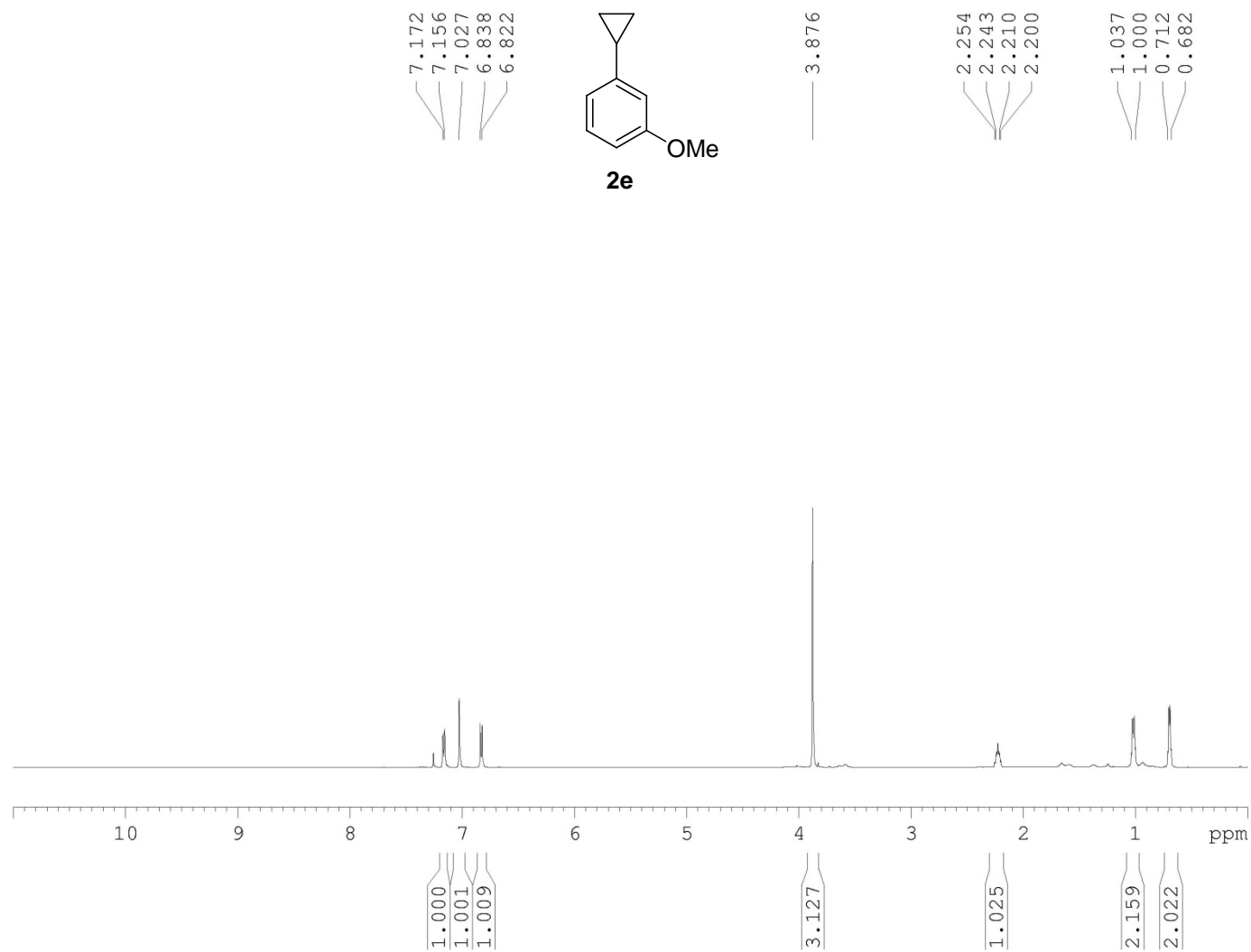




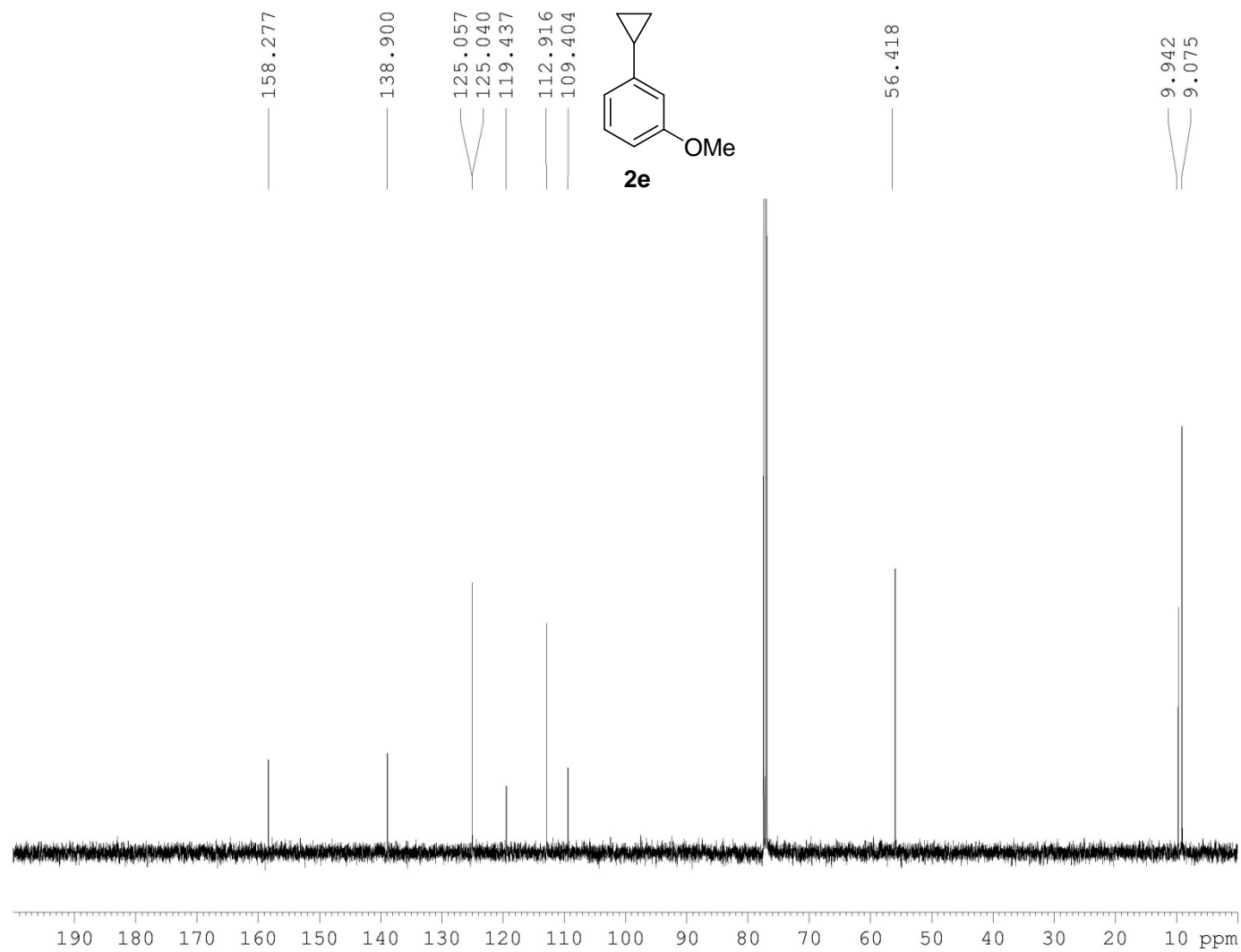
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 1-cyclopropyl-2-methoxybenzene **2d** (Table 2, entry 4)



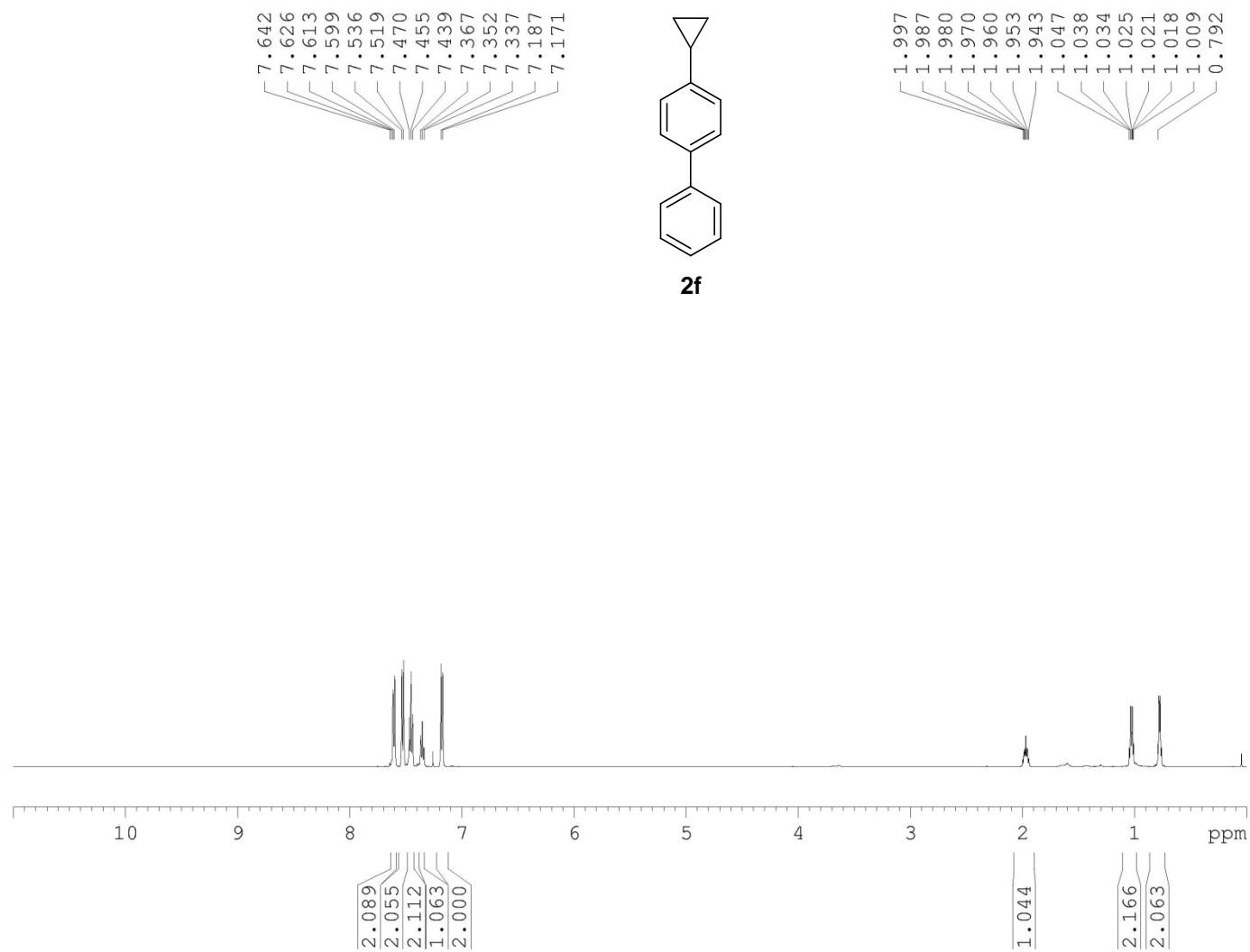
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) Spectrum of 1-cyclopropyl-2-methoxybenzene **2d** (Table 2, entry 4)



<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 4-cyclopropyl-3-methoxybenzonitrile **2e** (Table 2, entry 5)

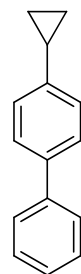


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) Spectrum of 4-cyclopropyl-3-methoxybenzonitrile **2e** (Table 2, entry 5)



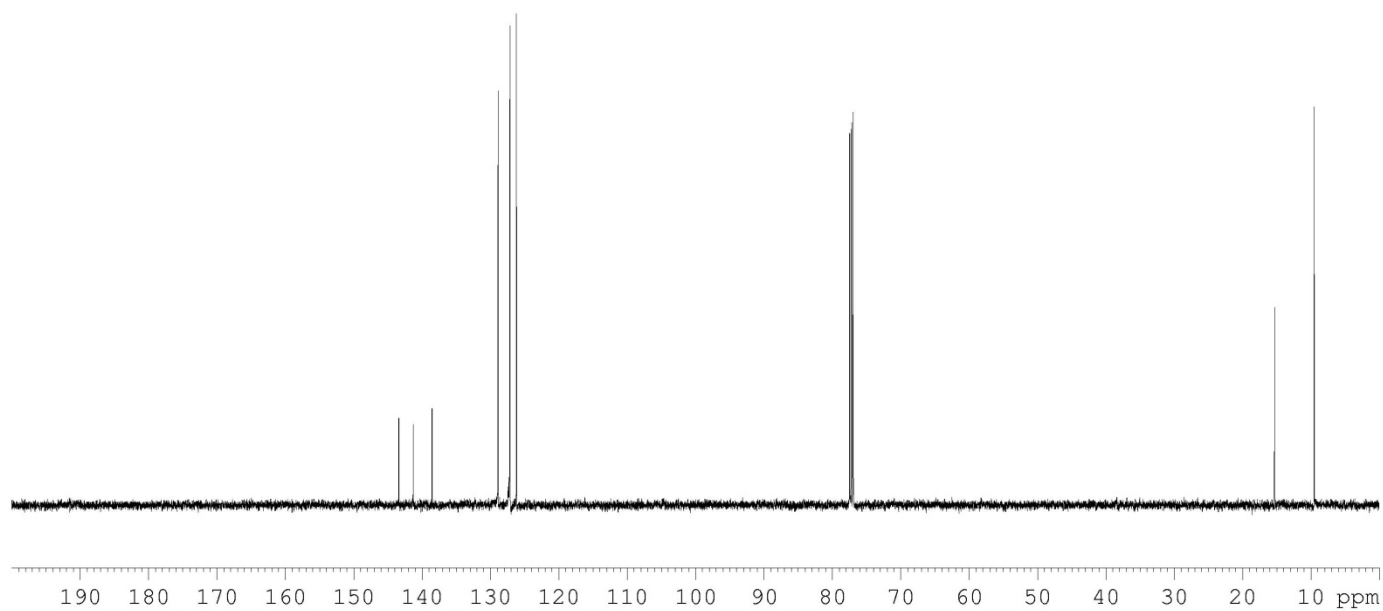
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 4-cyclopropyl-1,1'-biphenyl **2f** (Table 2, entry 6)

143.405  
141.283  
138.527  
128.895  
127.196  
127.108  
126.212

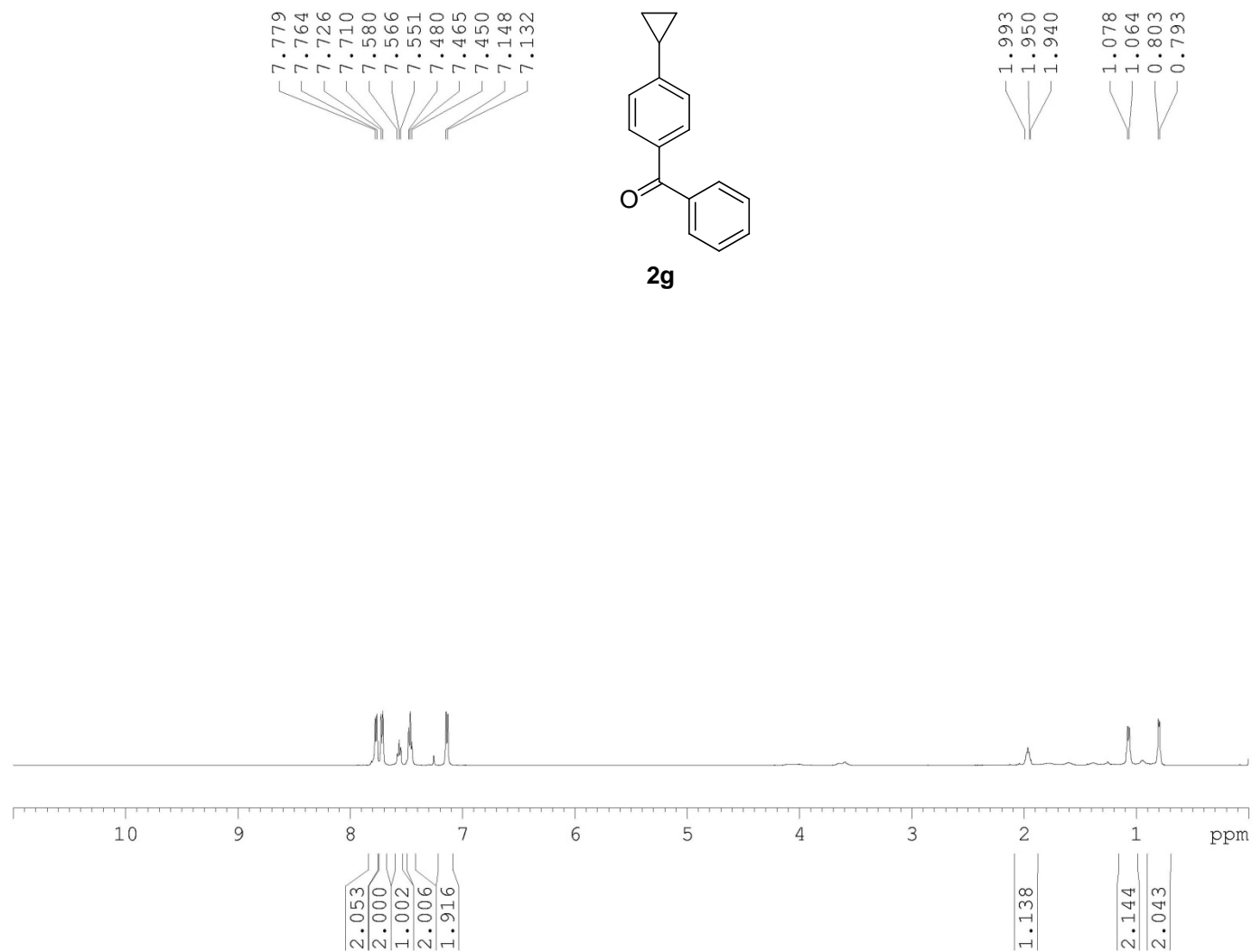


**2f**

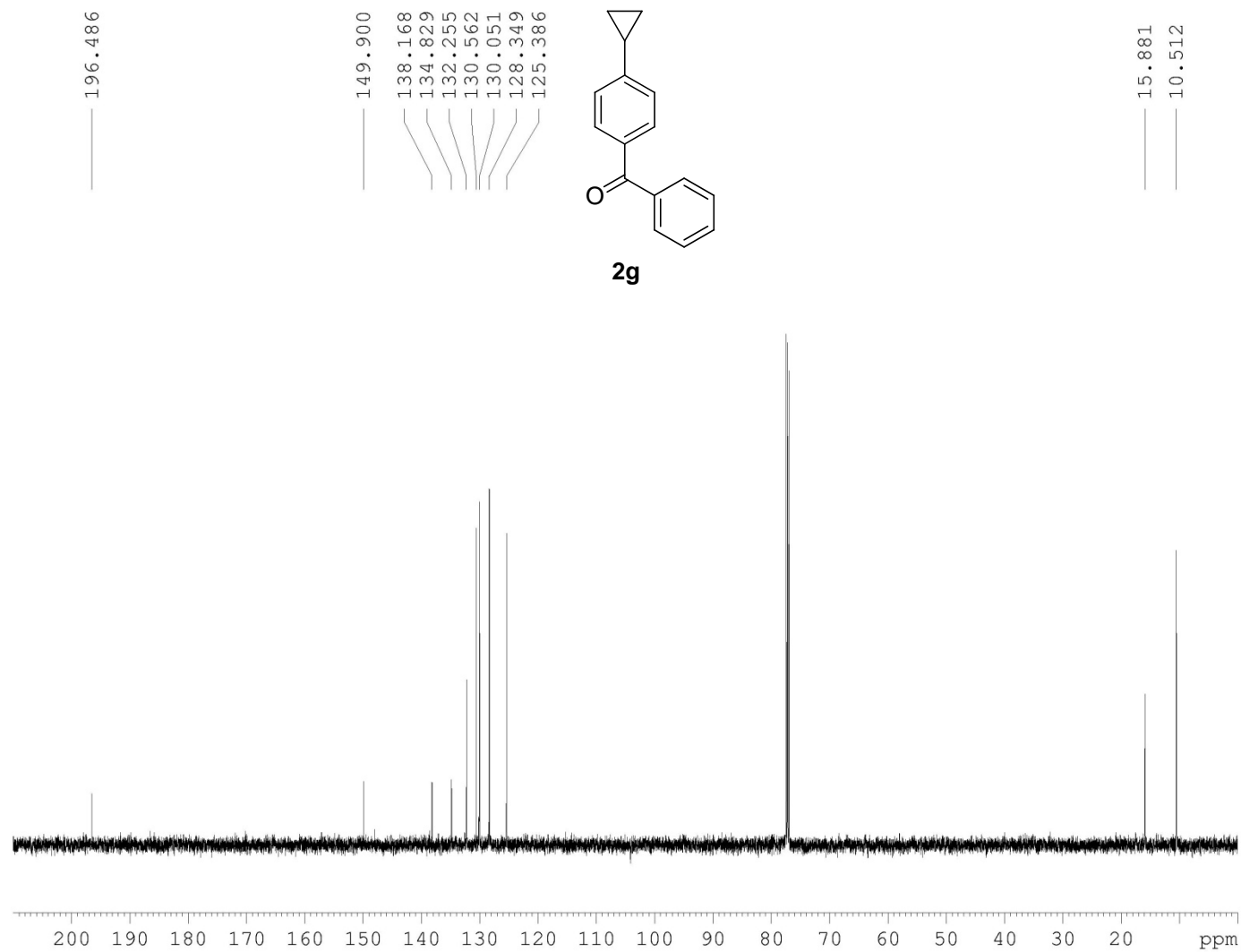
15.318  
9.546



$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) Spectrum of 4-cyclopropyl-1,1'-biphenyl **2f** (Table 2, entry 6)

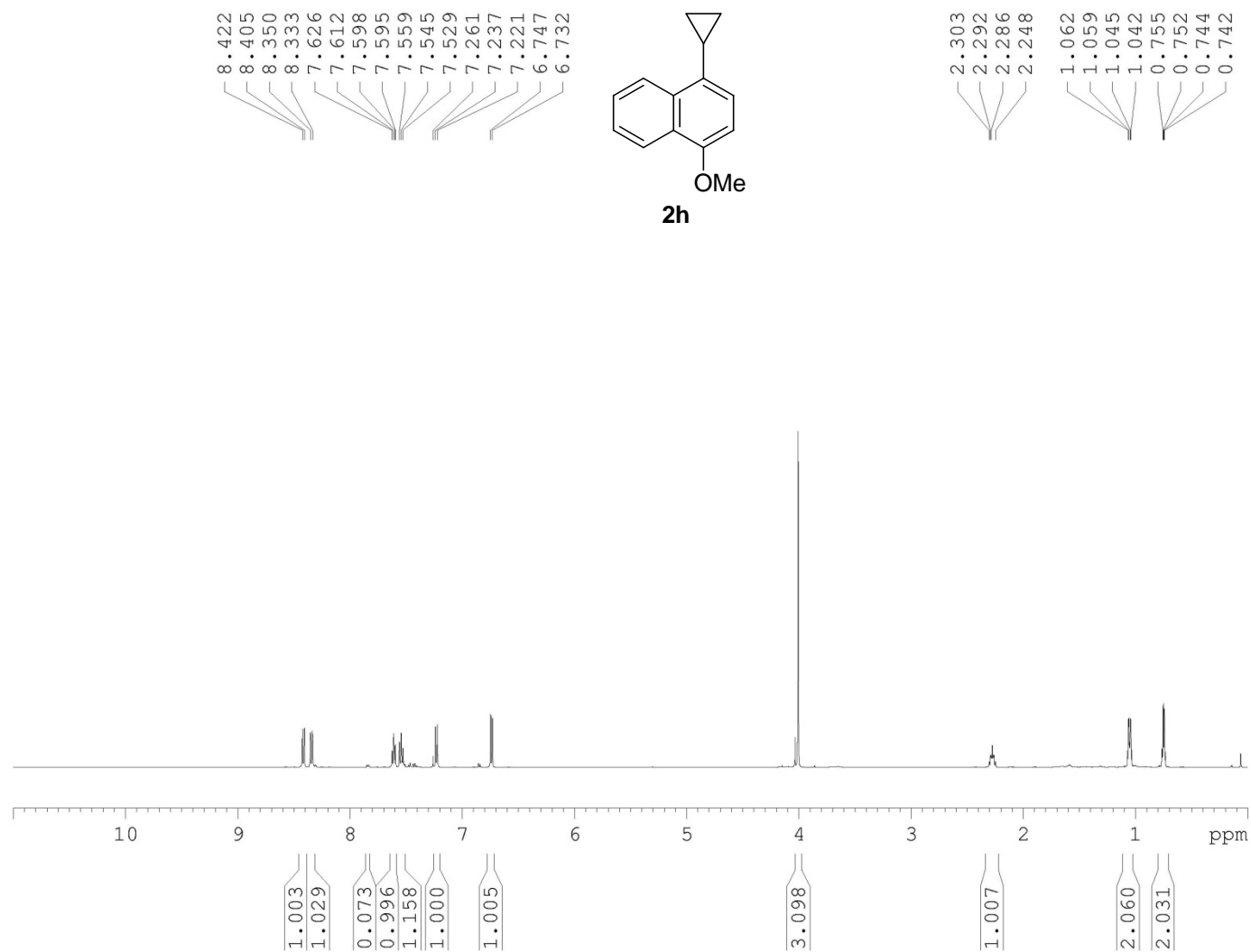


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 4-cyclopropylphenyl(phenyl)methanone **2g** (Table 2, entry 7)

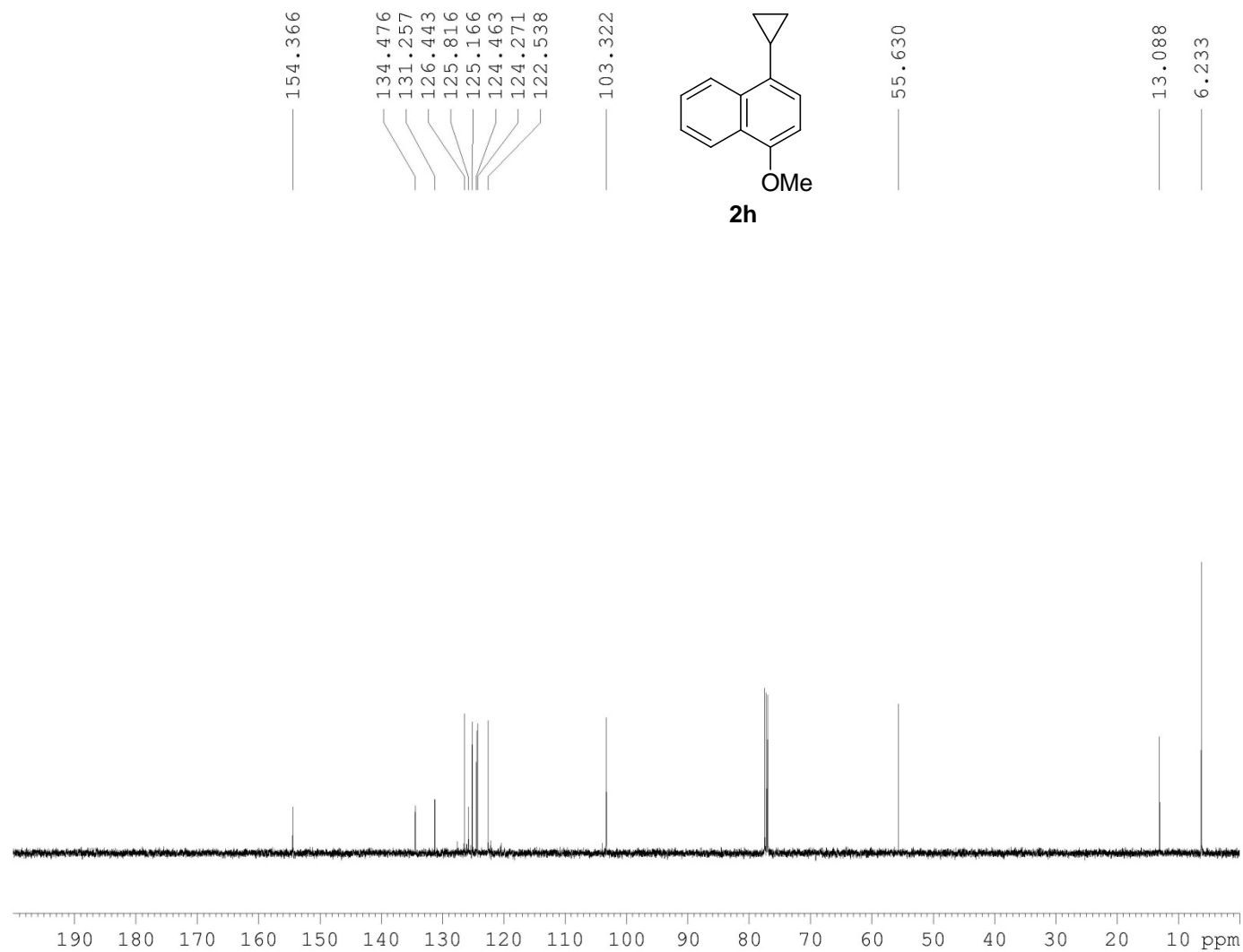


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) Spectrum of 4-cyclopropylphenyl(phenyl)methanone **2g** (Table 2, entry 7)

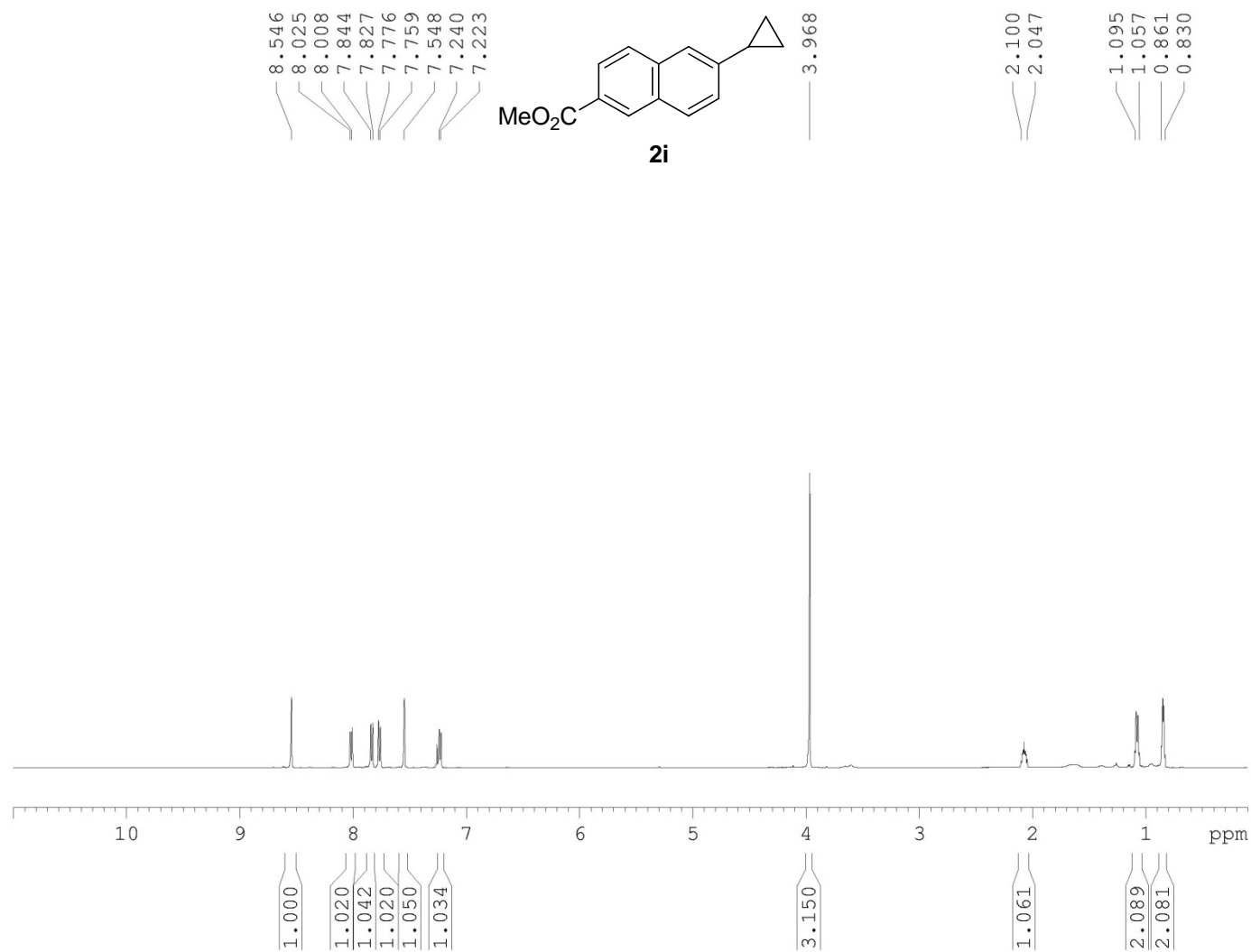




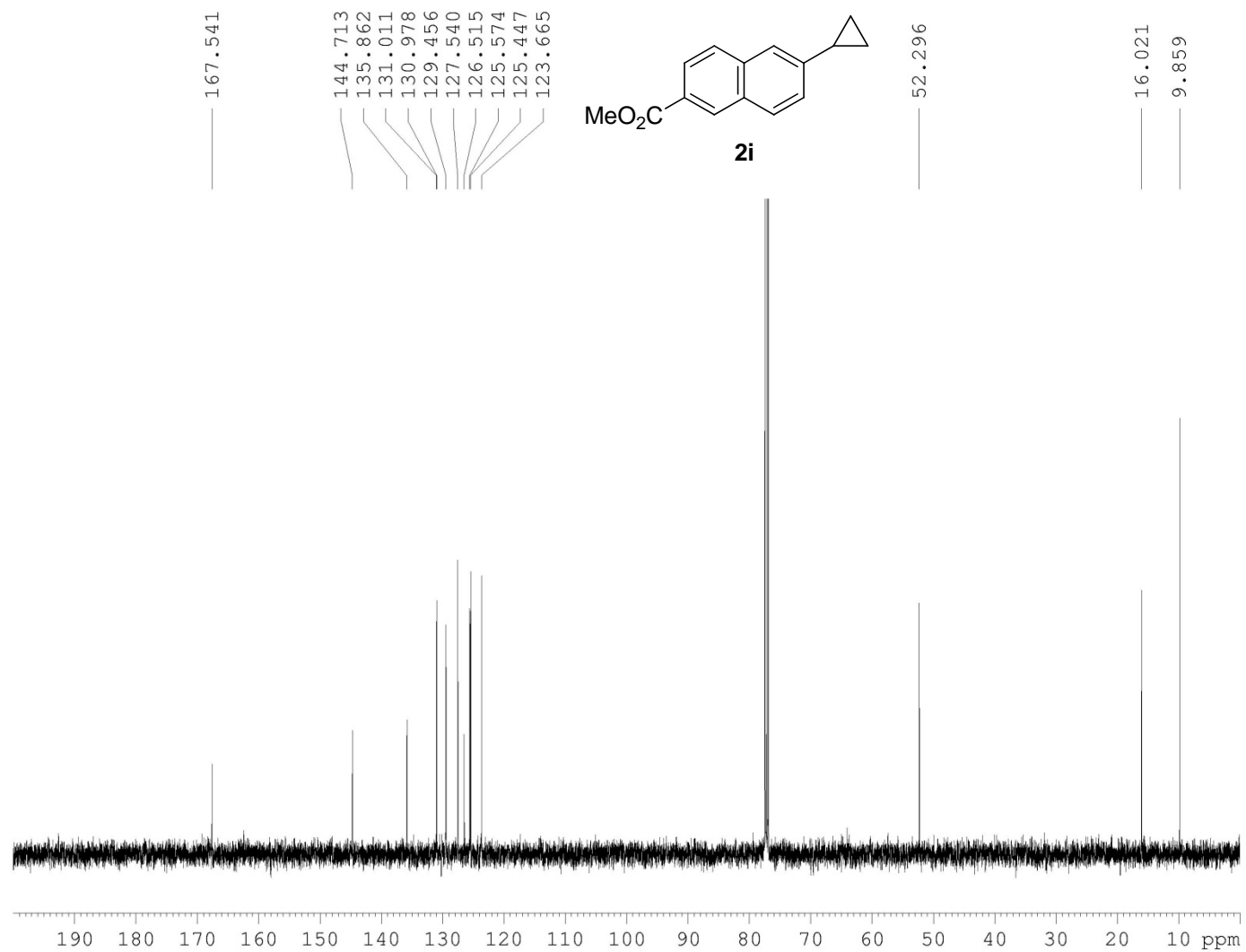
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 1-cyclopropyl-4-methoxynaphthalene **2h** (Table 2, entry 8)



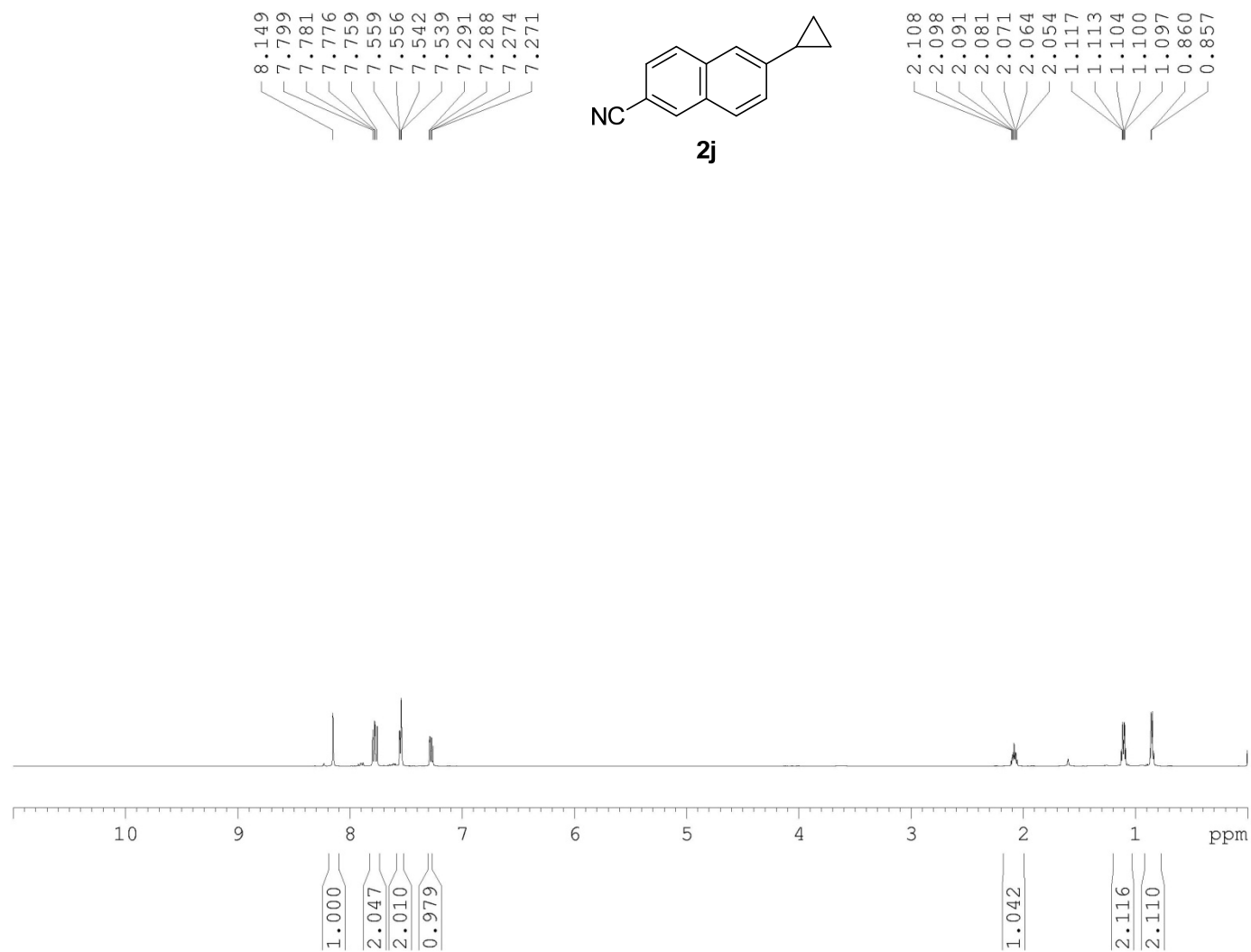
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) Spectrum of 1-cyclopropyl-4-methoxynaphthalene **2h** (Table 2, entry 8)



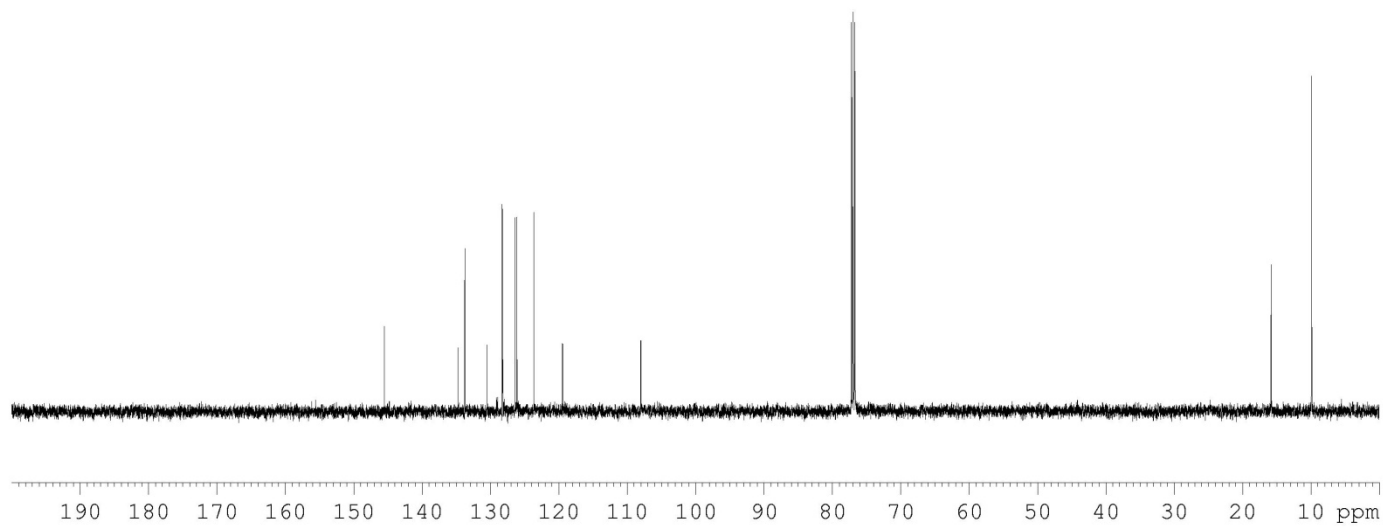
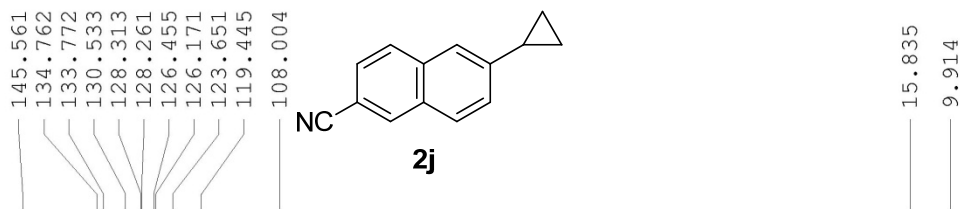
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of methyl 6-cyclopropyl-2-naphthoate **2i** (Table 2, entry 9)



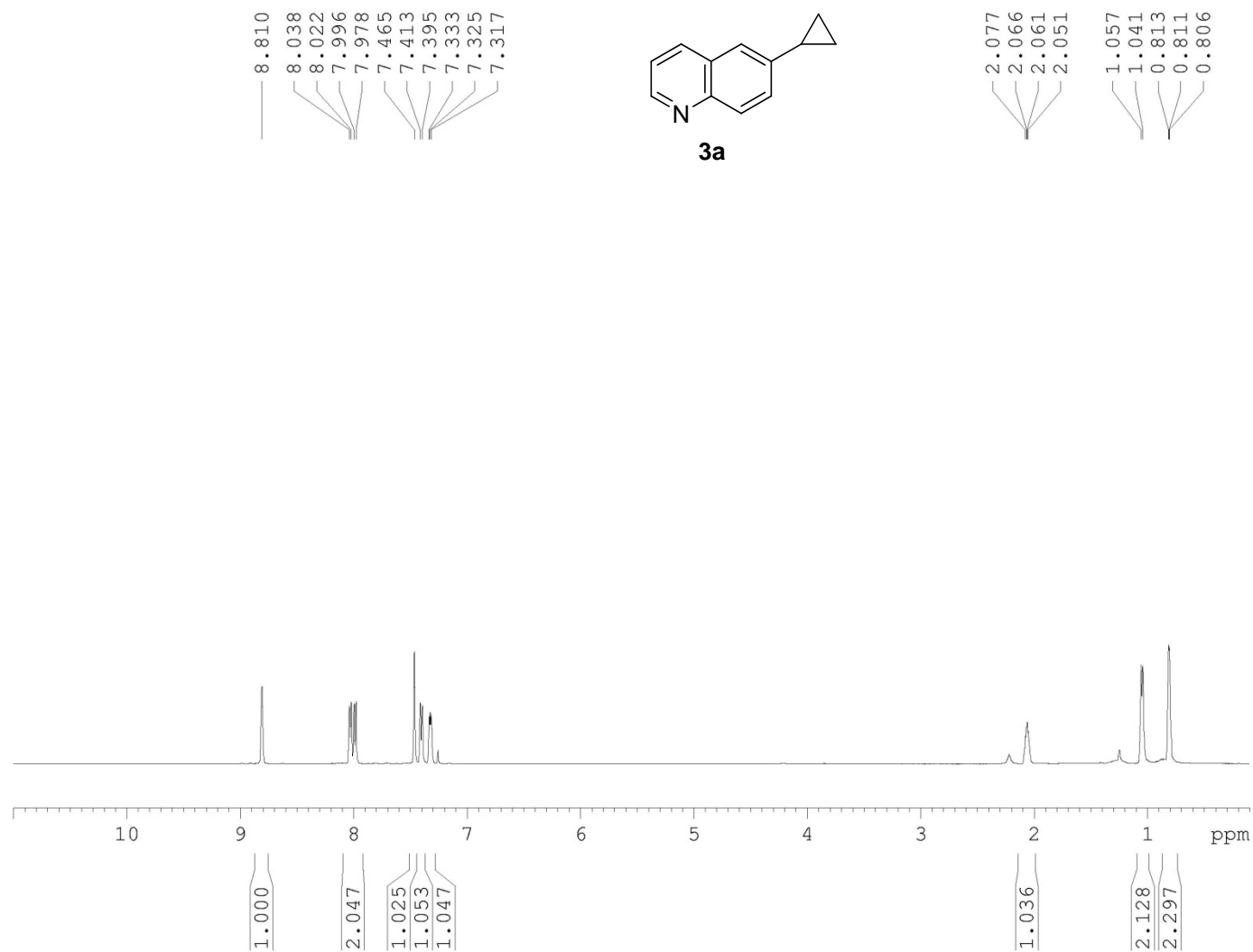
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) Spectrum of methyl 6-cyclopropyl-2-naphthoate **2i** (Table 2, entry 9)



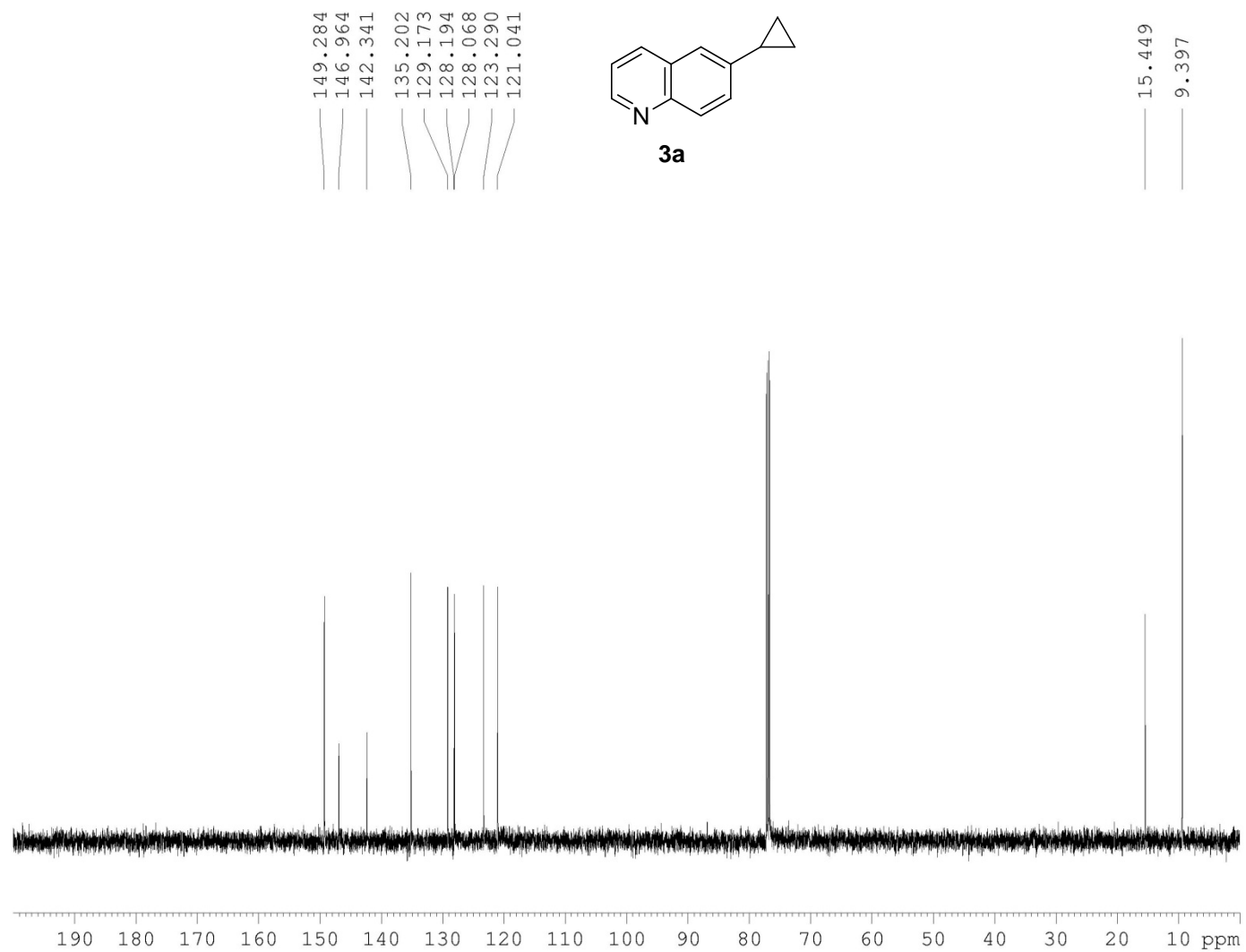
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 6-cyclopropyl-2-naphthonitrile **2j** (Table 2, entry 10)



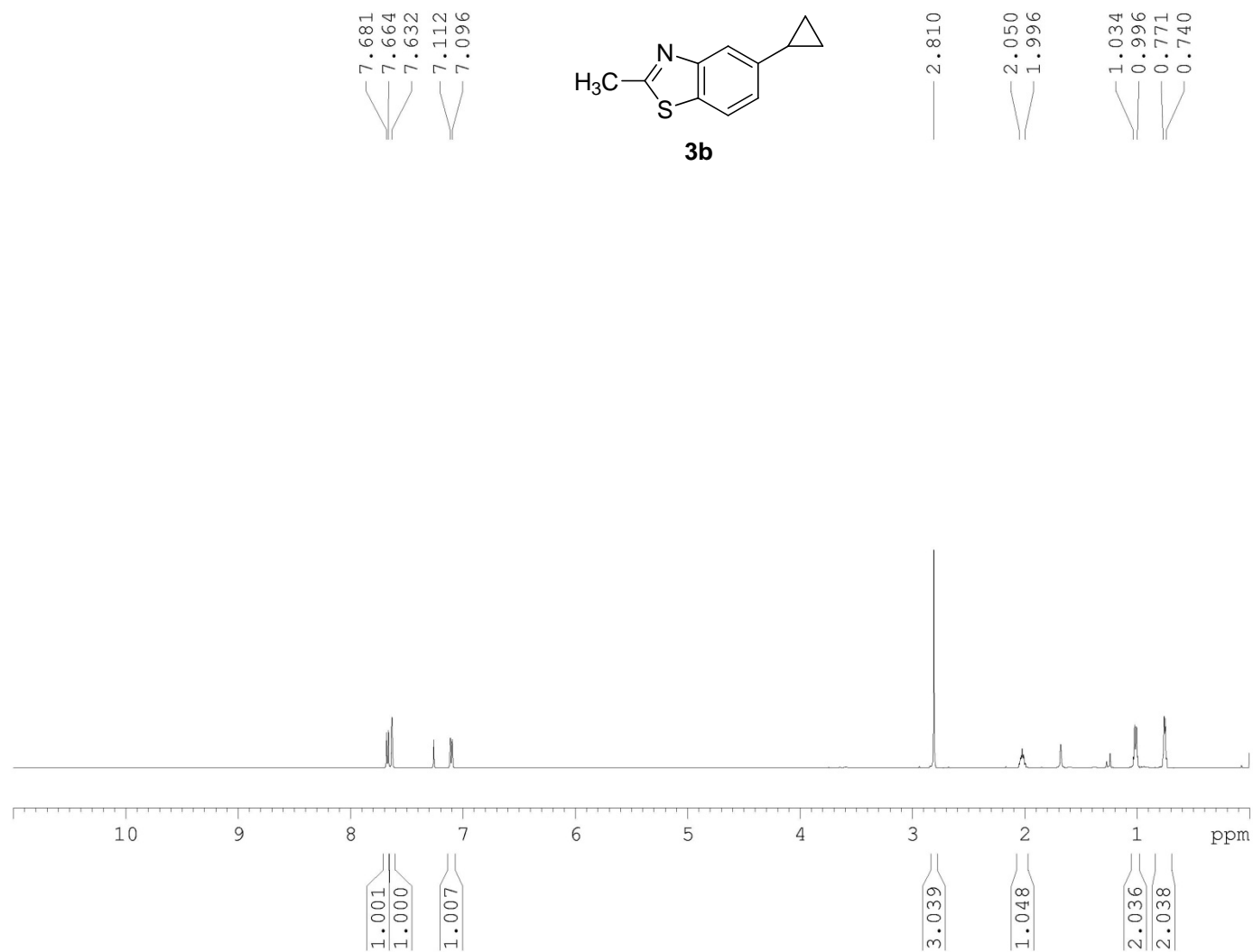
<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) Spectrum of 6-cyclopropyl-2-naphthonitrile **2j** (Table 2, entry 10)



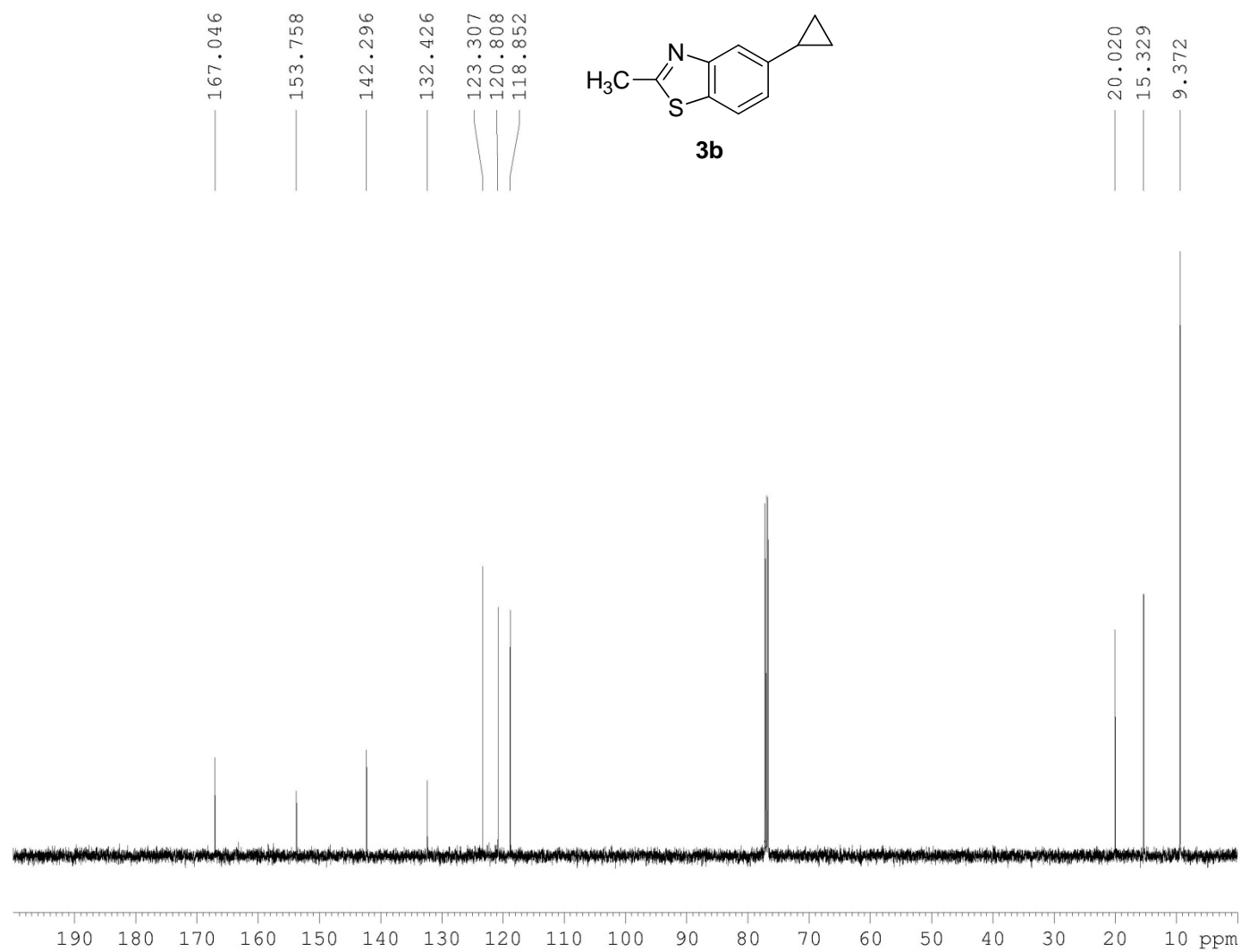
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 6-cyclopropylquinoline **3a** (Table 3, entry 1)



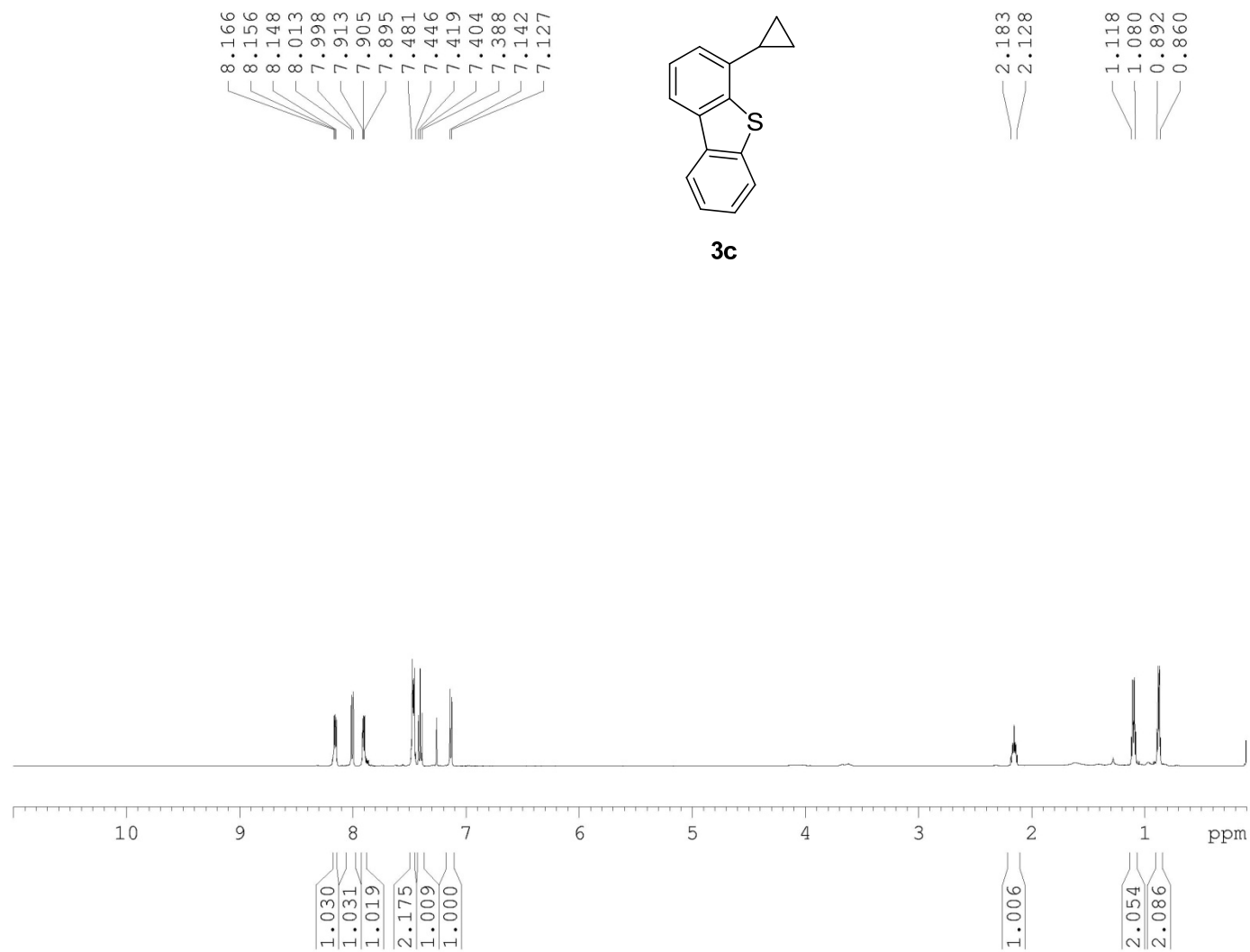




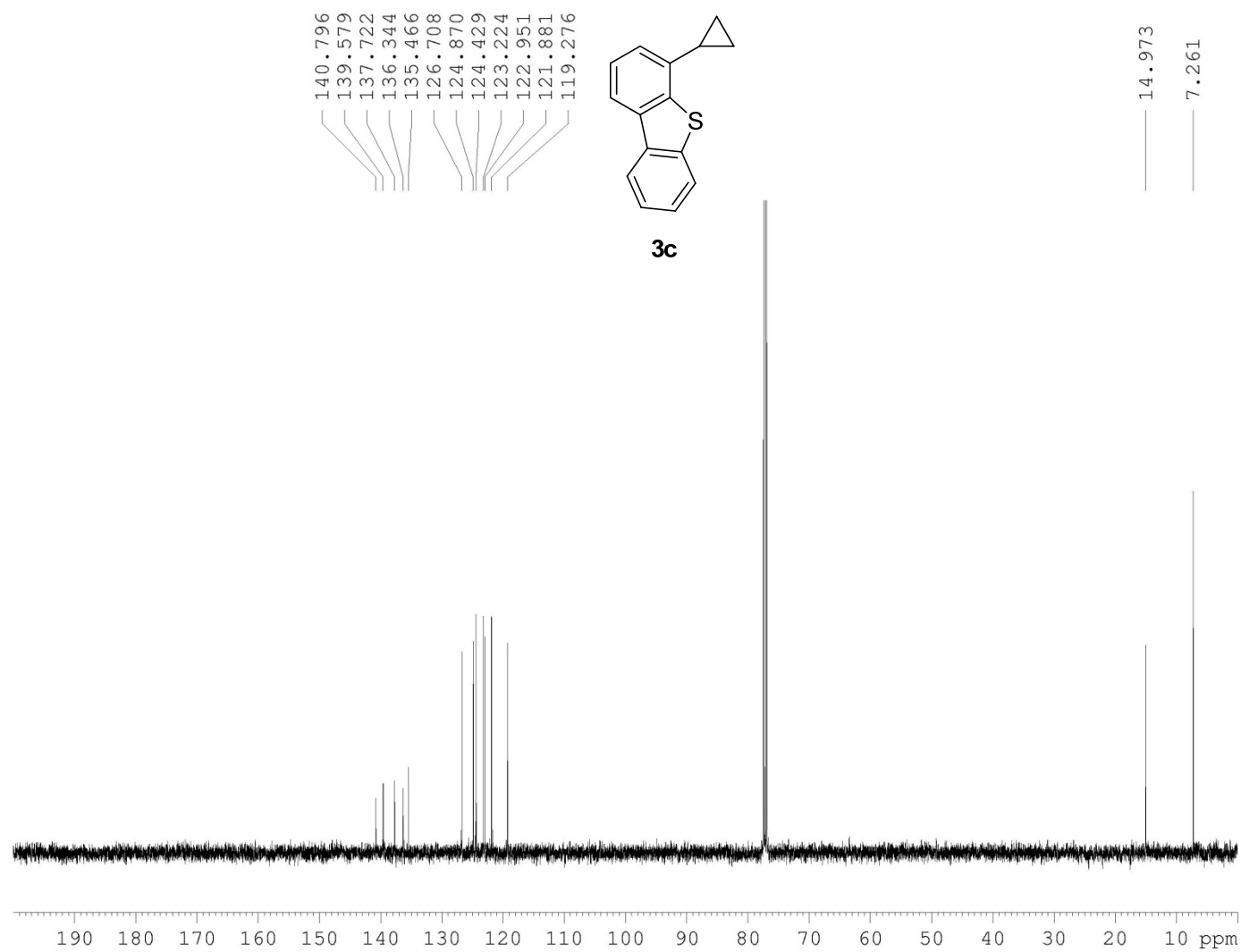
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 5-cyclopropyl-2-methylbenzo[d]thiazole **3b** (Table 3, entry 2)



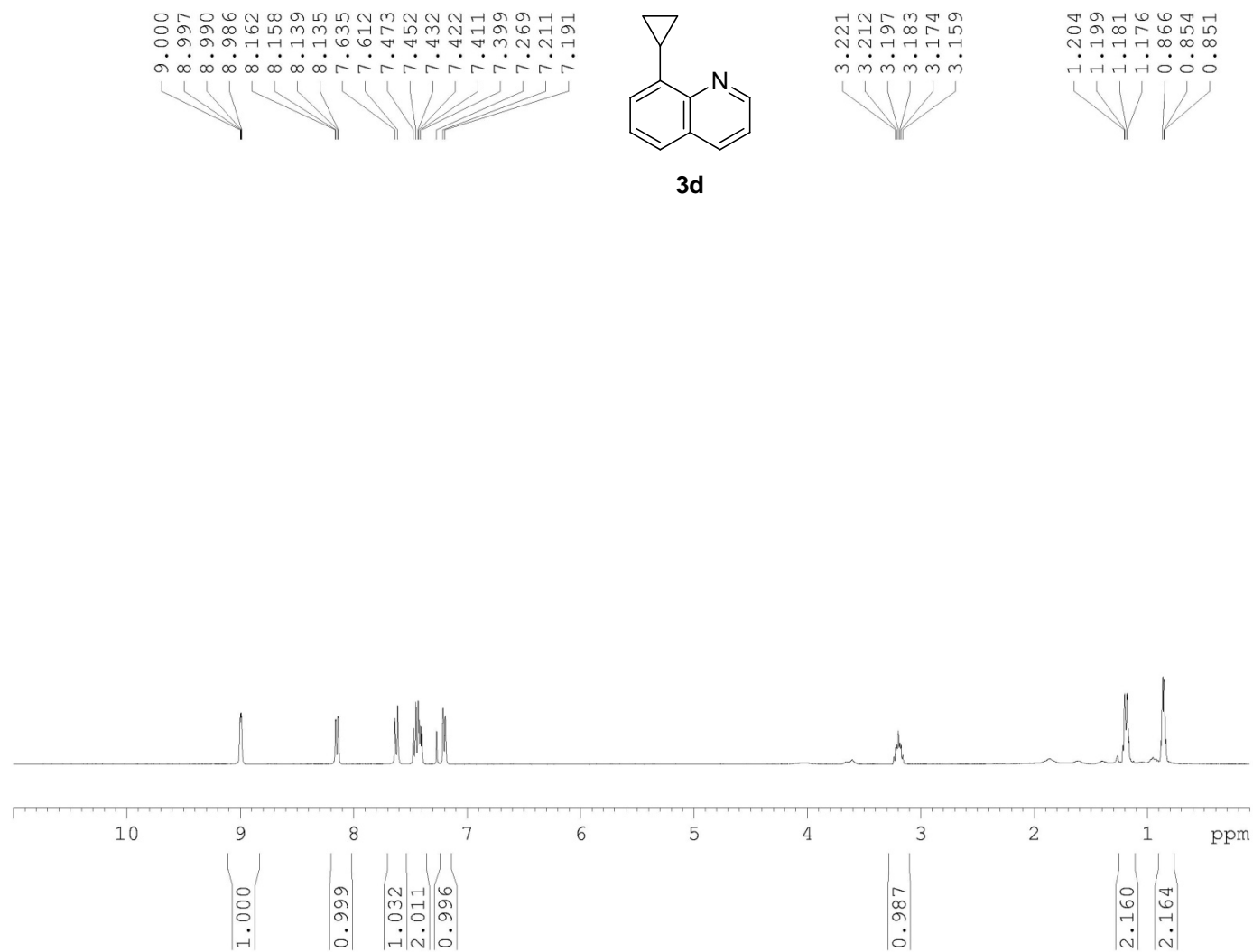
<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) Spectrum of 5-cyclopropyl-2-methylbenzo[d]thiazole **3b** (Table 3, entry 2)



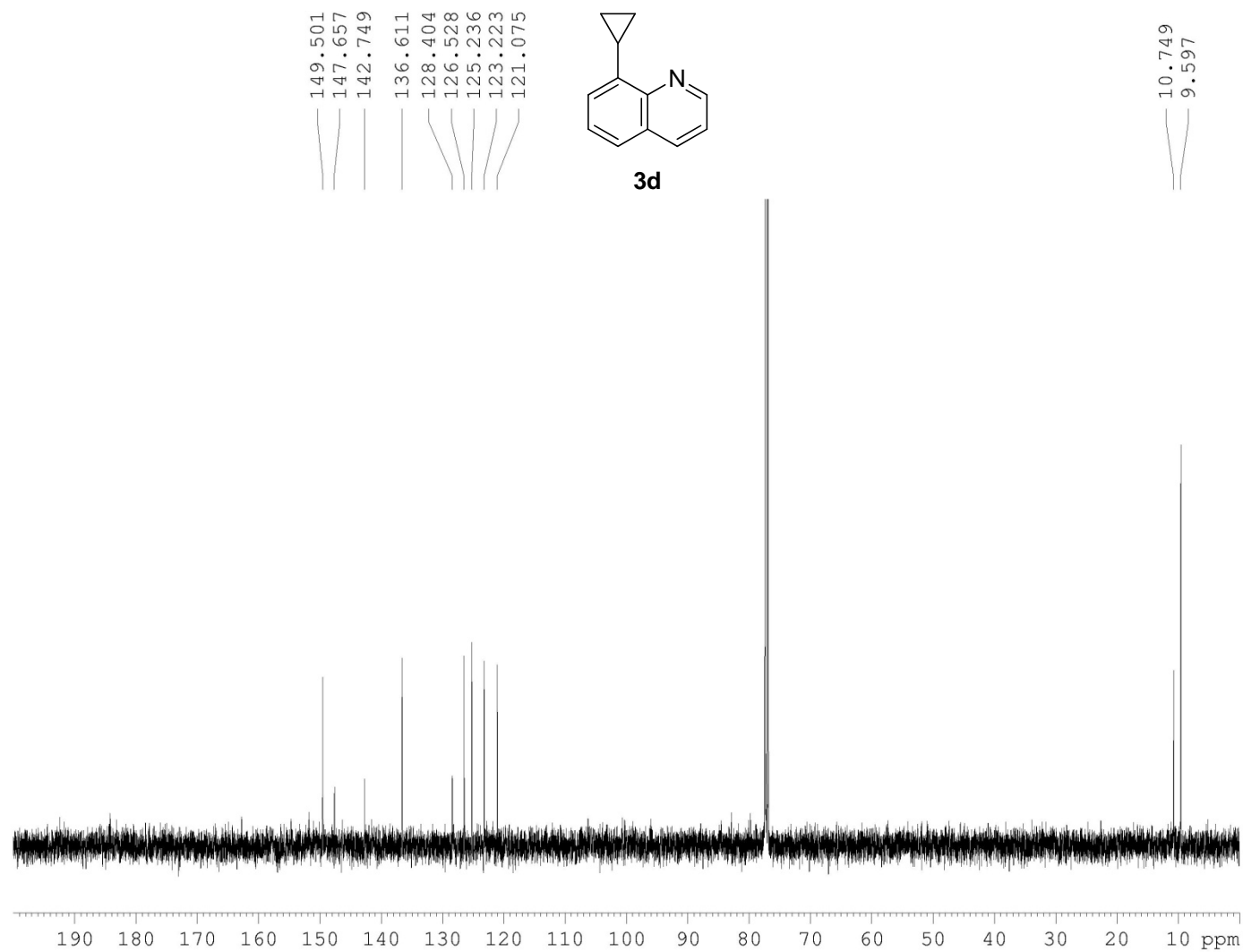
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 4-cyclopropyldibenzo[b,d]thiophene **3c** (Table 3, entry 3)



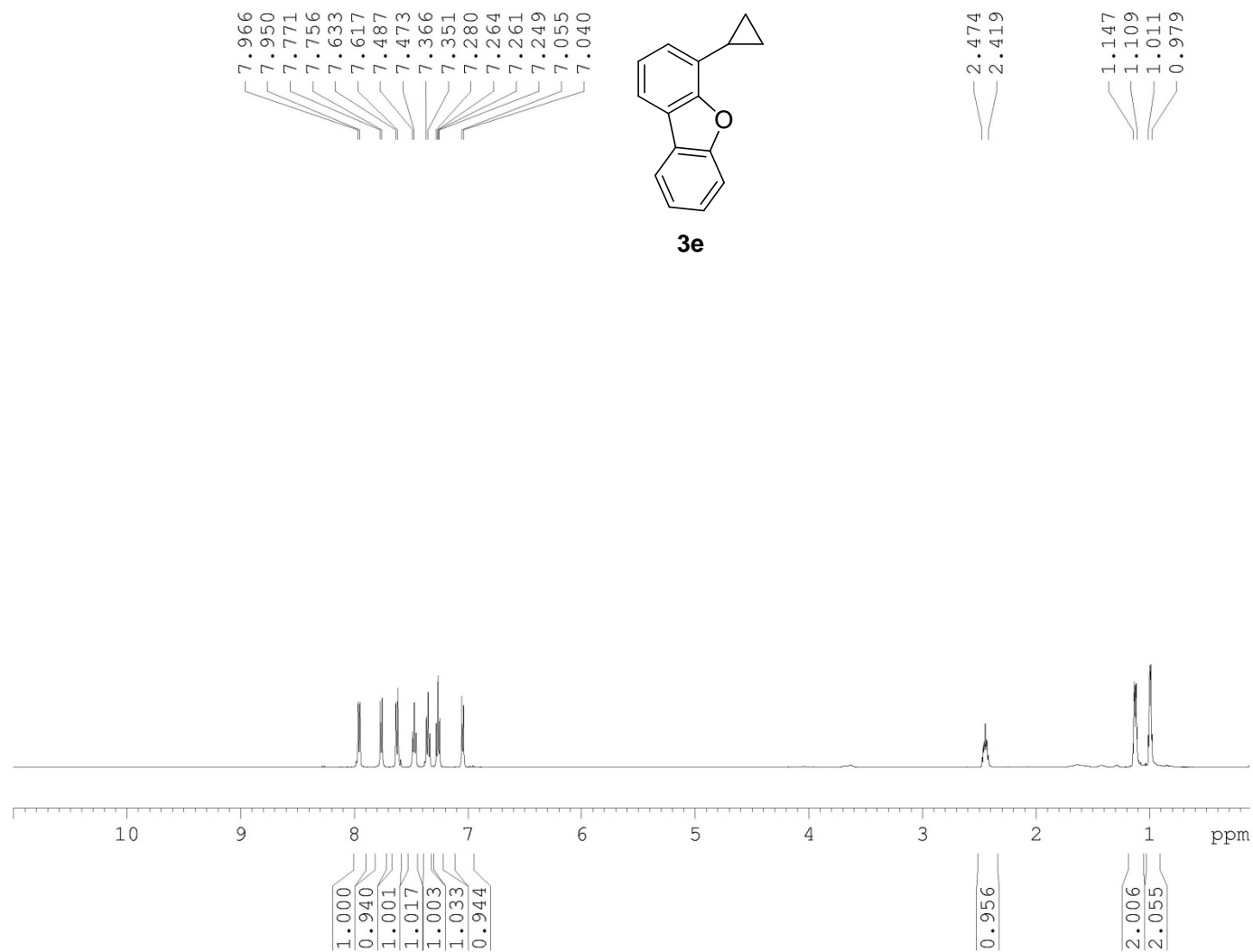
<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) Spectrum of 4-cyclopropyldibenzo[b,d]thiophene **3c** (Table 3, entry 3)



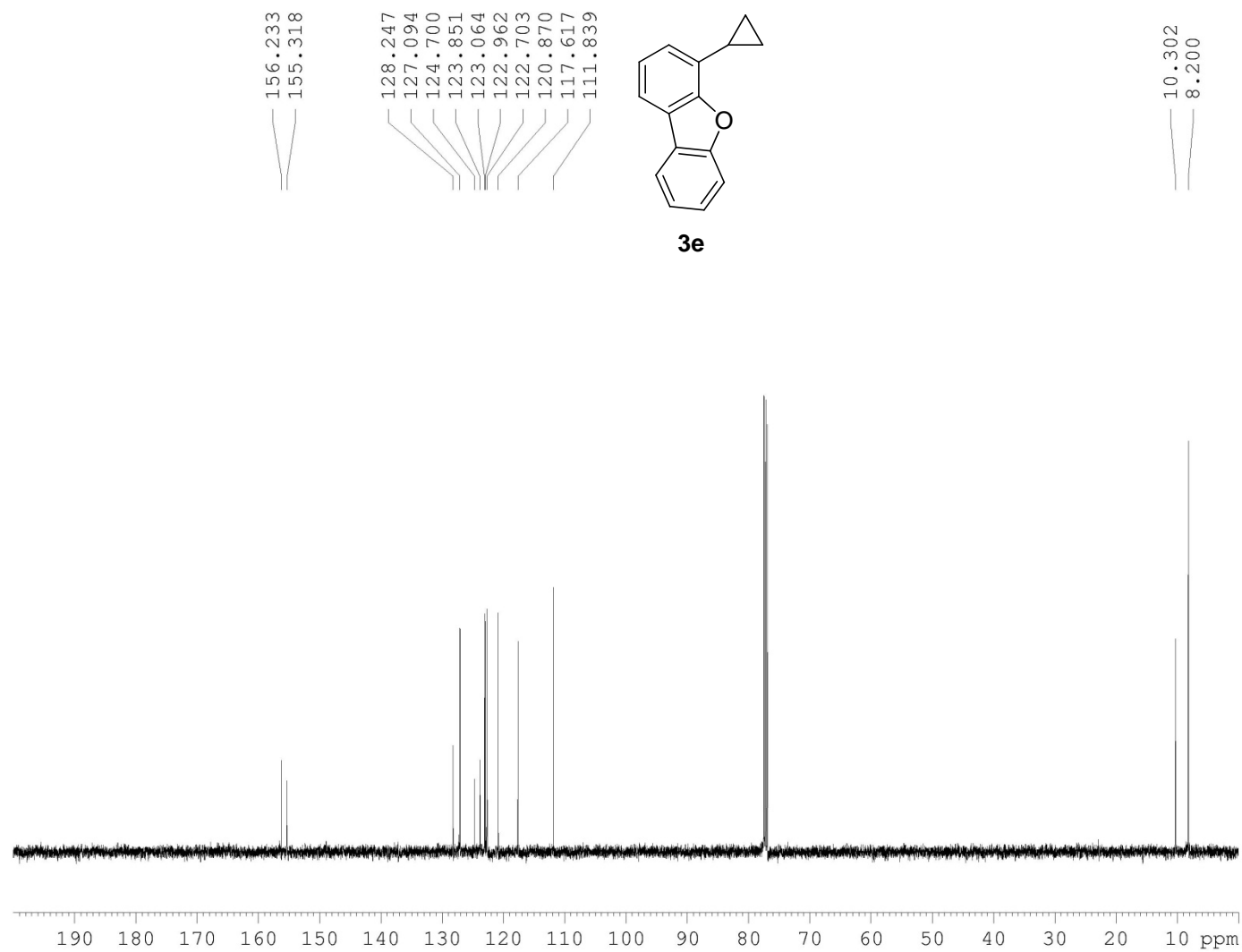
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 8-cyclopropylquinoline **3d** (Table 3, entry 4)



<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) Spectrum of 8-cyclopropylquinoline **3d** (Table 3, entry 4)

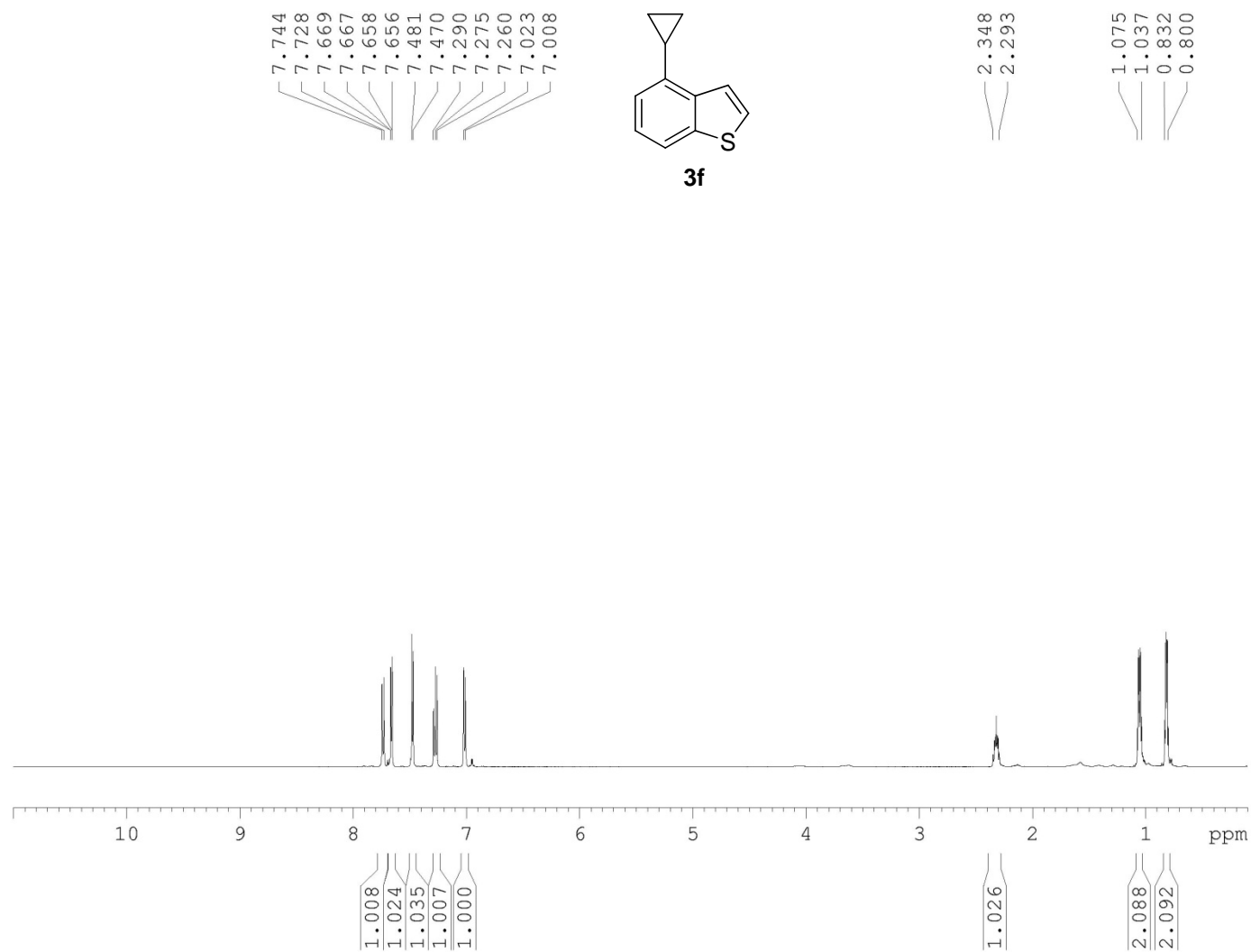


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 4-cyclopropyldibenzo[b,d]furan **3e** (Table 3, entry 5)

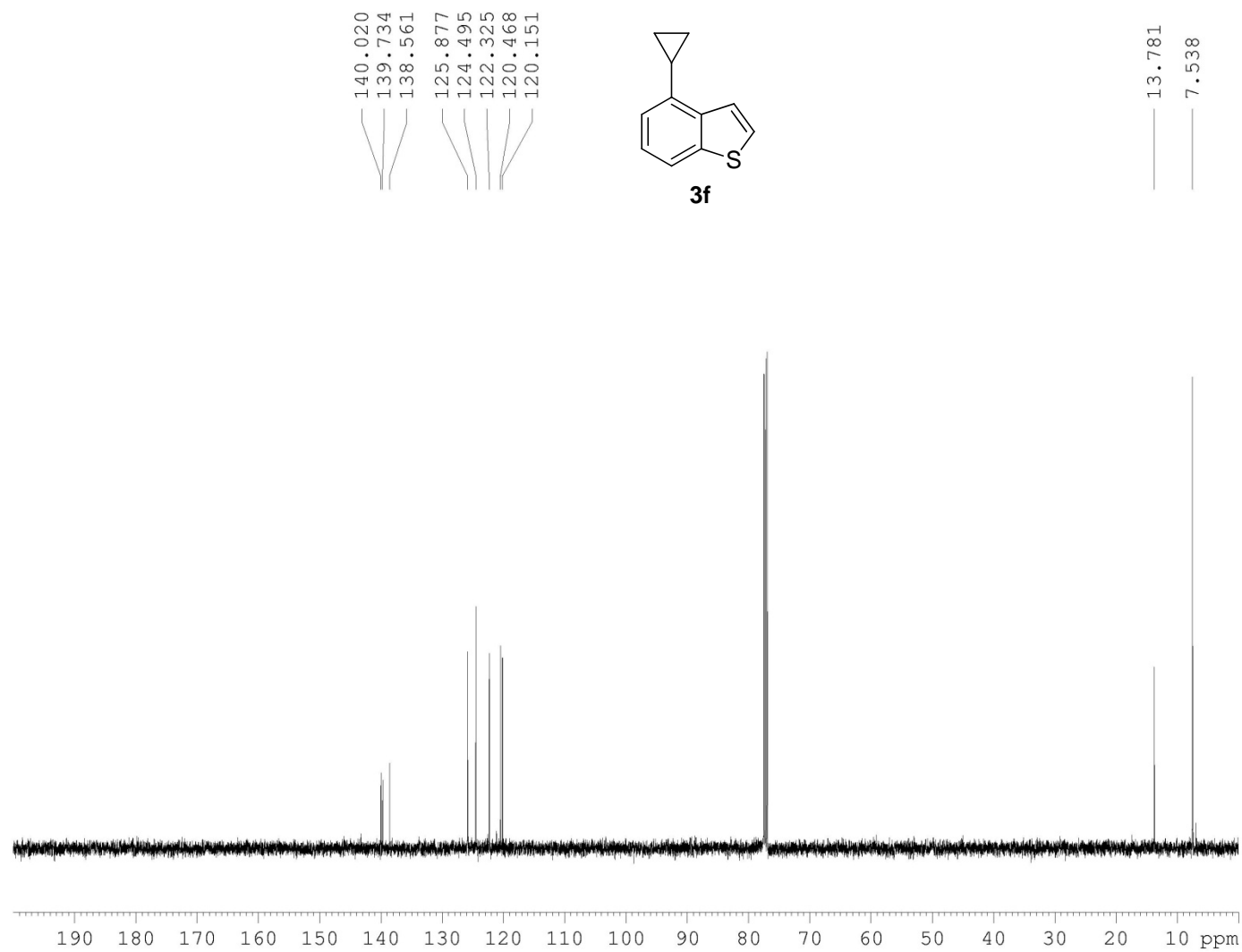


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) Spectrum of 4-cyclopropyldibenzo[b,d]furan **3e** (Table 3, entry 5)





<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Spectrum of 4-cyclopropylbenzo[b]thiophene **3f** (Table 3, entry 6)



<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) Spectrum of 4-cyclopropylbenzo[b]thiophene **3f** (Table 3, entry 6)