

Supplementary Data for

**IDENTIFICATION OF NEW ALKYL PYRAZINES  
OFF FLAVORS IN OAK WOOD**

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Table 1S. Validation parameters for the quantitative analysis of 2,5-dialkylpyrazines by SPME-GC-MS in oak wood macerate.

Compounds (odoriferous zone)	Spiked concentrations for linear regression (mg/L)	R <sup>2</sup>	LOD (µg/L) <sup>a</sup>	LOQ (µg/L) <sup>b</sup>
2,5-diisopropylpyrazine ( <b>1</b> )	0, 0.1, 0.2, 0.4, 0.8, 1, 2, 5	0.996	0.6	1.9
2-( <i>sec</i> -butyl)-5-isopropylpyrazine ( <b>2</b> )	0, 0.1, 0.2, 0.4, 0.8, 1, 5, 10	0.996	1.2	3.0
2-isobutyl-5-isopropylpyrazine ( <b>3</b> )	0, 0.1, 0.2, 0.4, 0.8, 1, 5, 10	0.998	1.6	3.2
2,5-di- <i>sec</i> -butylpyrazine ( <b>4</b> )	0, 0.1, 0.2, 0.4, 0.8, 1, 5, 10	0.999	1.7	3.0
2-( <i>sec</i> -butyl)-5-isobutylpyrazine ( <b>5</b> )	0, 0.1, 0.2, 0.4, 0.8, 1, 5, 10	0.999	0.8	2.0
2,5-diisobutylpyrazine ( <b>6</b> )	0, 0.1, 0.2, 0.4, 0.8, 1, 2, 5	0.997	0.5	1.9

<sup>a</sup> Limit of detection (signal to noise ratio of 3).

<sup>b</sup> Limit of quantitation (signal to noise ratio of 10).

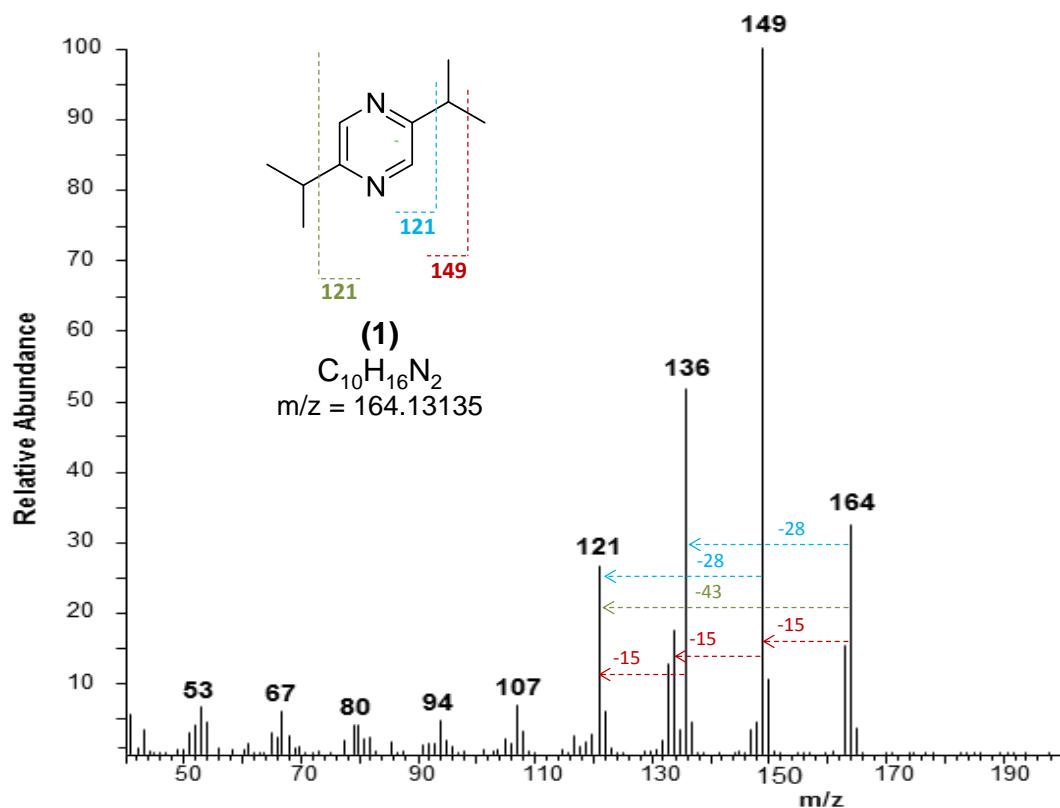


Figure 1S. Mass spectrum and attributed chemical structure of 2,5-diisopropylpyrazine (1).

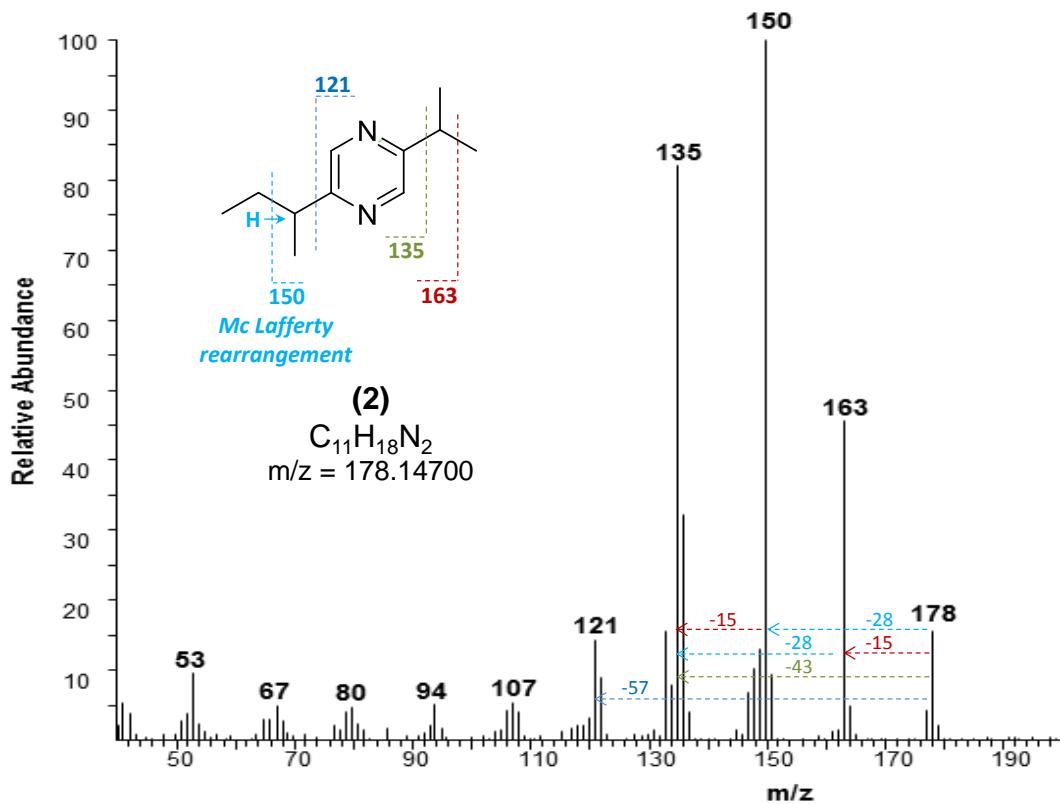


Figure 2S. Mass spectrum and attributed chemical structure of 2-(sec-butyl)-5-isopropylpyrazine (2).

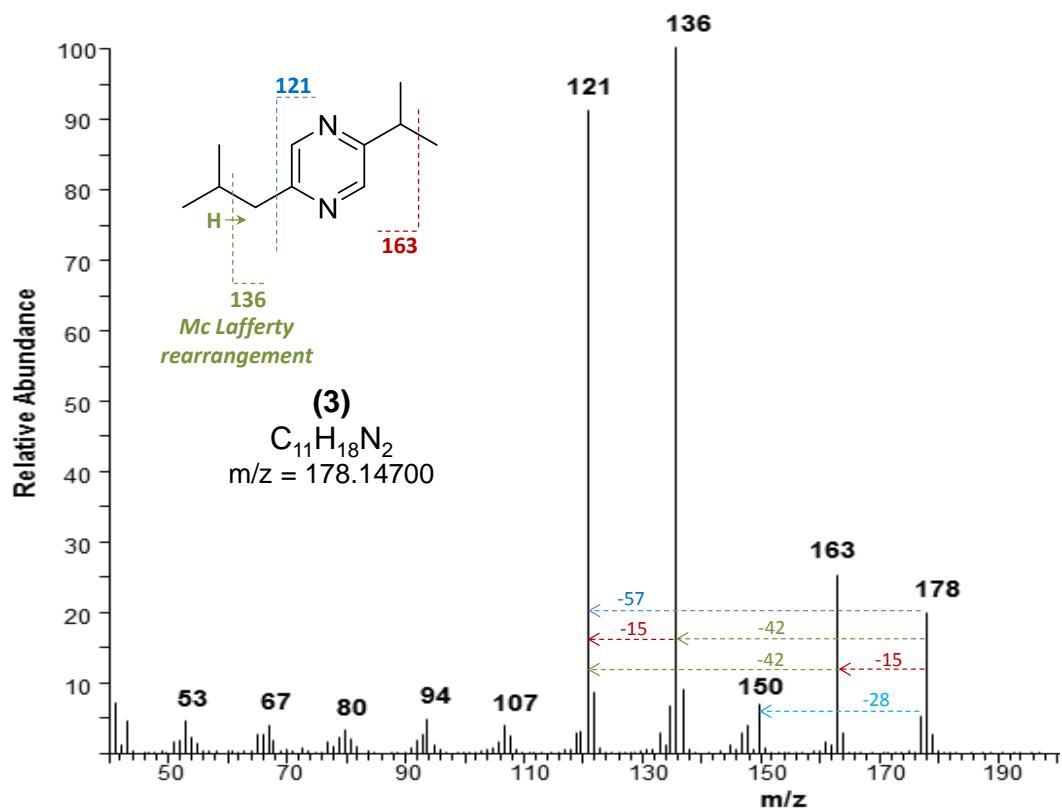


Figure 3S. Mass spectrum and attributed chemical structure of 2-isobutyl-5-isopropylpyrazine (3).

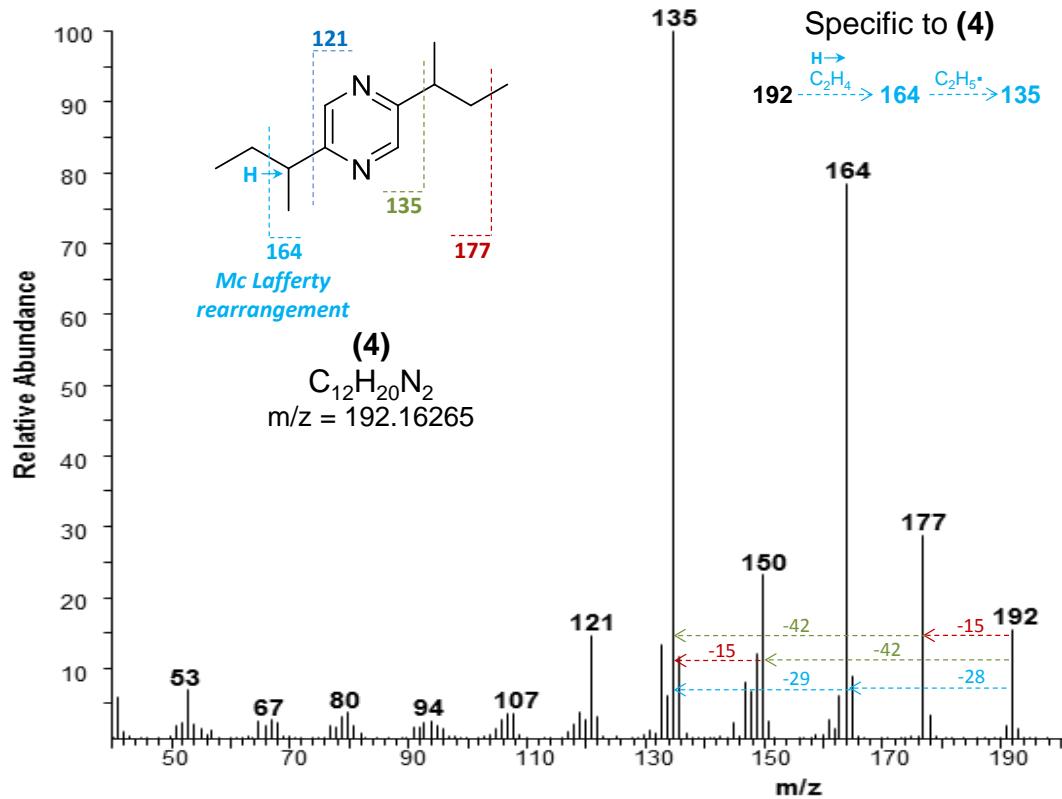


Figure 4S. Mass spectrum and attributed chemical structure of 2,5-di-sec-butylpyrazine (4).

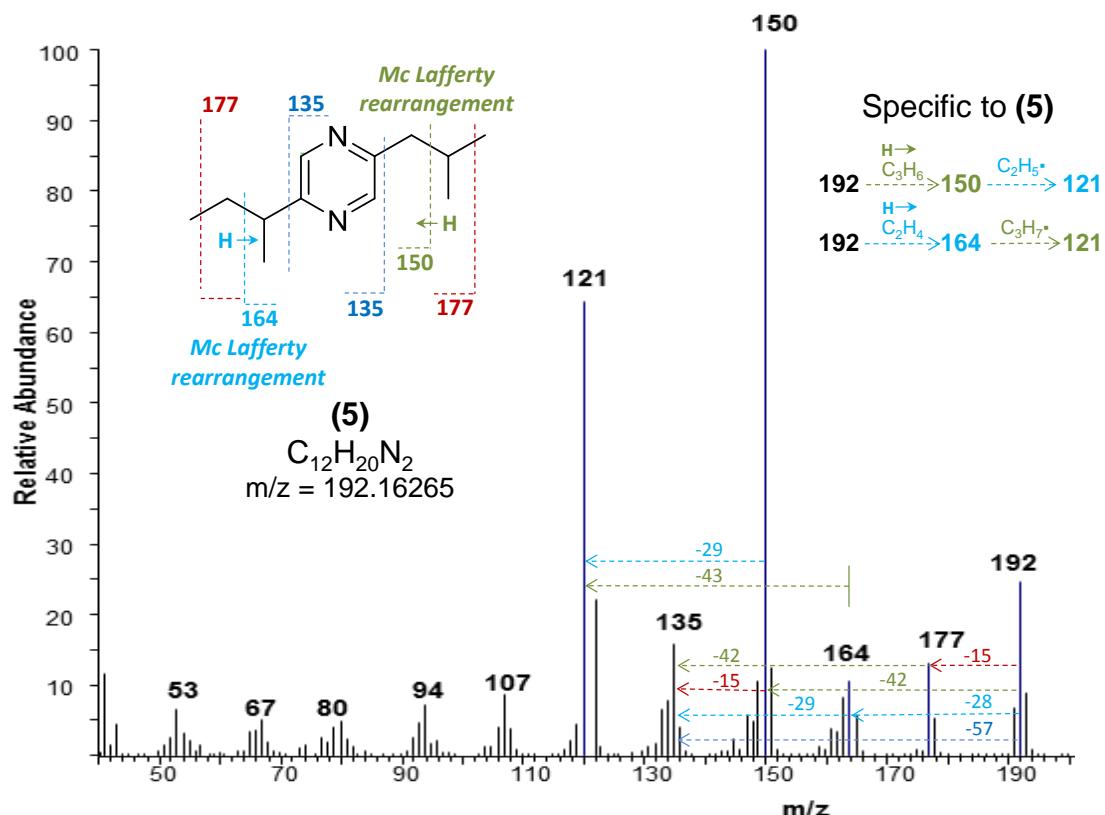


Figure 5S. Mass spectrum and attributed chemical structure of 2-(sec-butyl)-5-isobutylpyrazine (5).

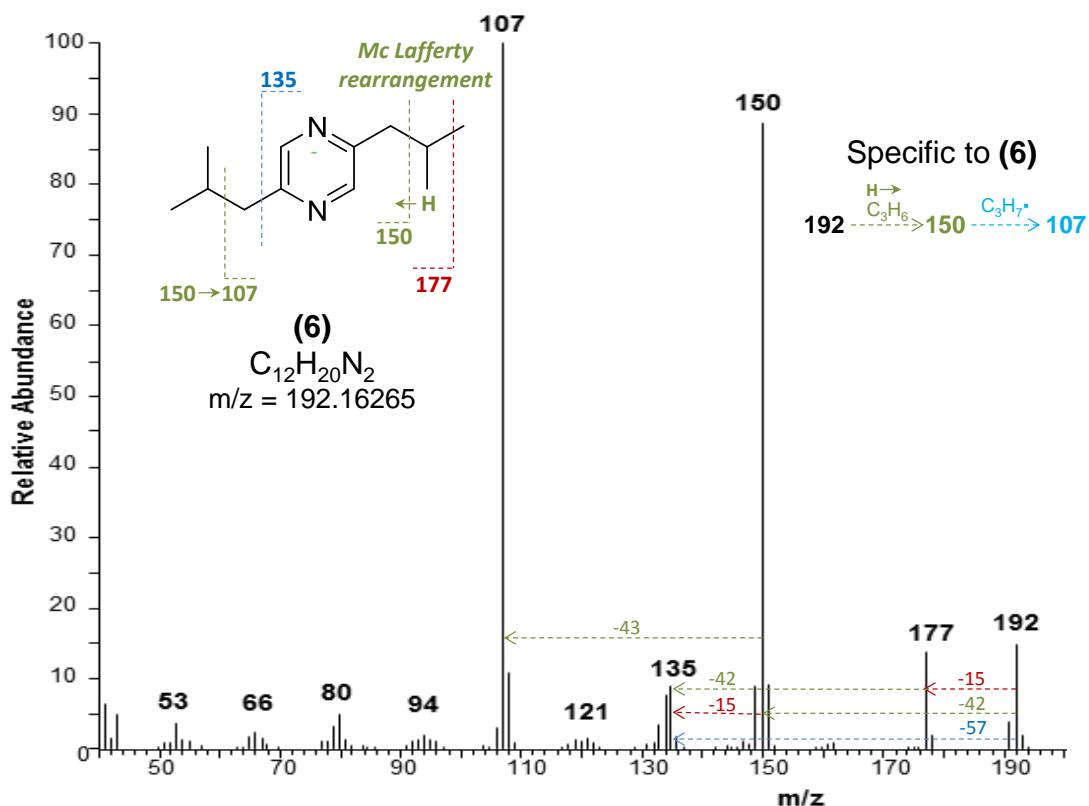


Figure 6S. Mass spectrum and attributed chemical structure of 2,5-diisobutylpyrazine (6).

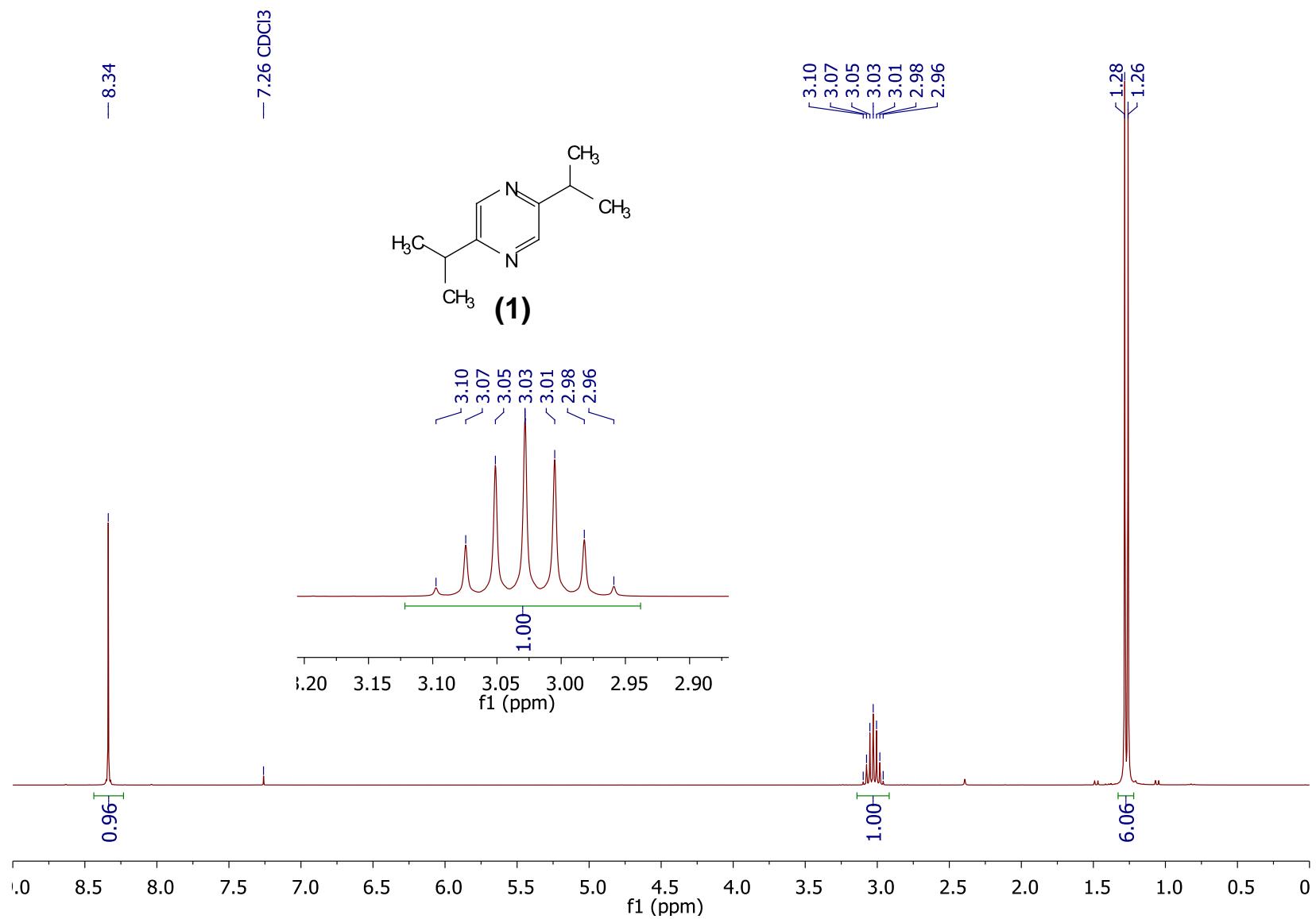


Figure 7S. <sup>1</sup>H NMR spectrum of 2,5-diisopropylpyrazine (**1**) in CDCl<sub>3</sub>.

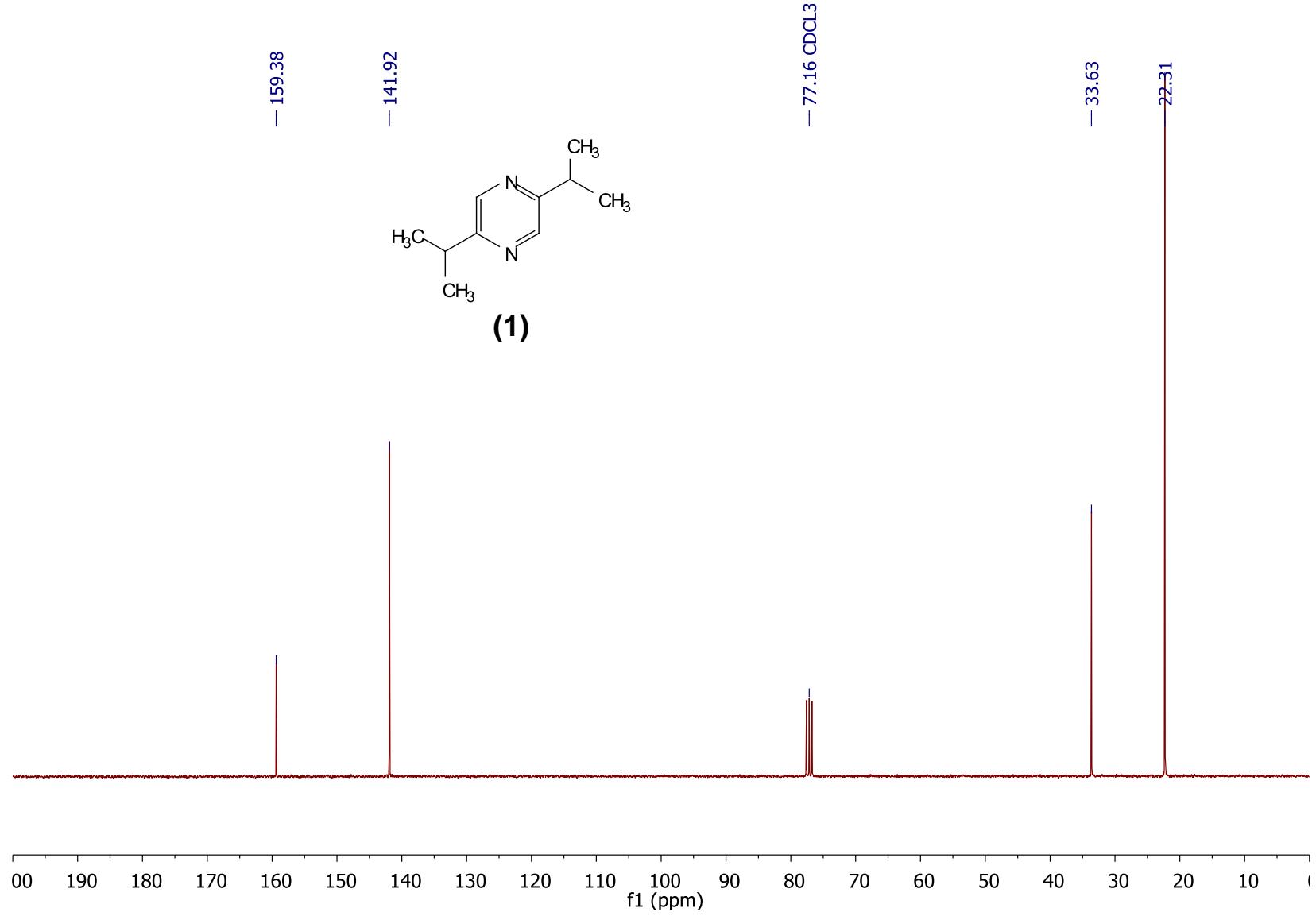


Figure 8S.  $^{13}\text{C}$  NMR spectrum of 2,5-diisopropylpyrazine (**1**) in CDCl<sub>3</sub>.

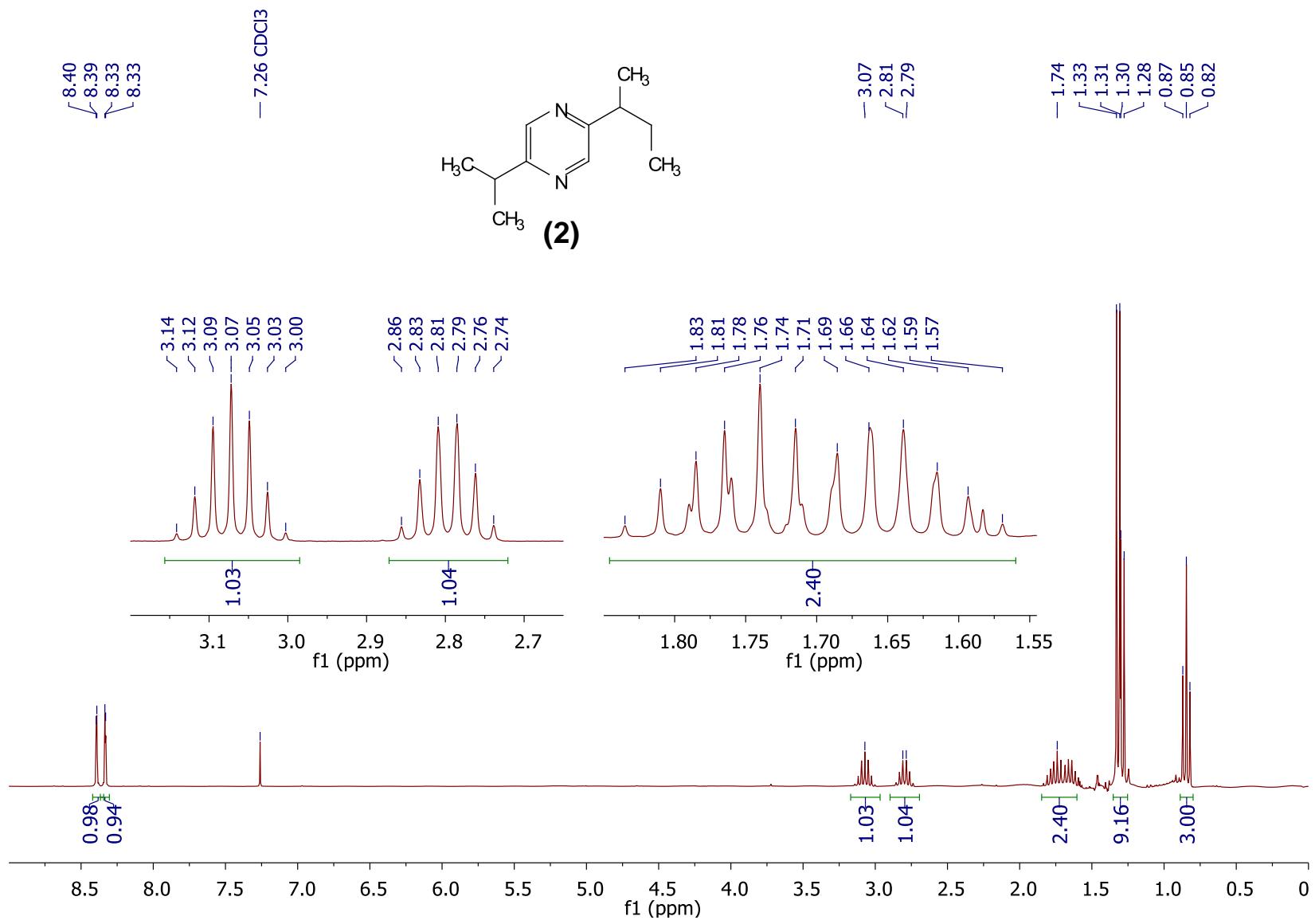


Figure 9S. <sup>1</sup>H NMR spectrum of 2-(*sec*-butyl)-5-isopropylpyrazine (2) in CDCl<sub>3</sub>.

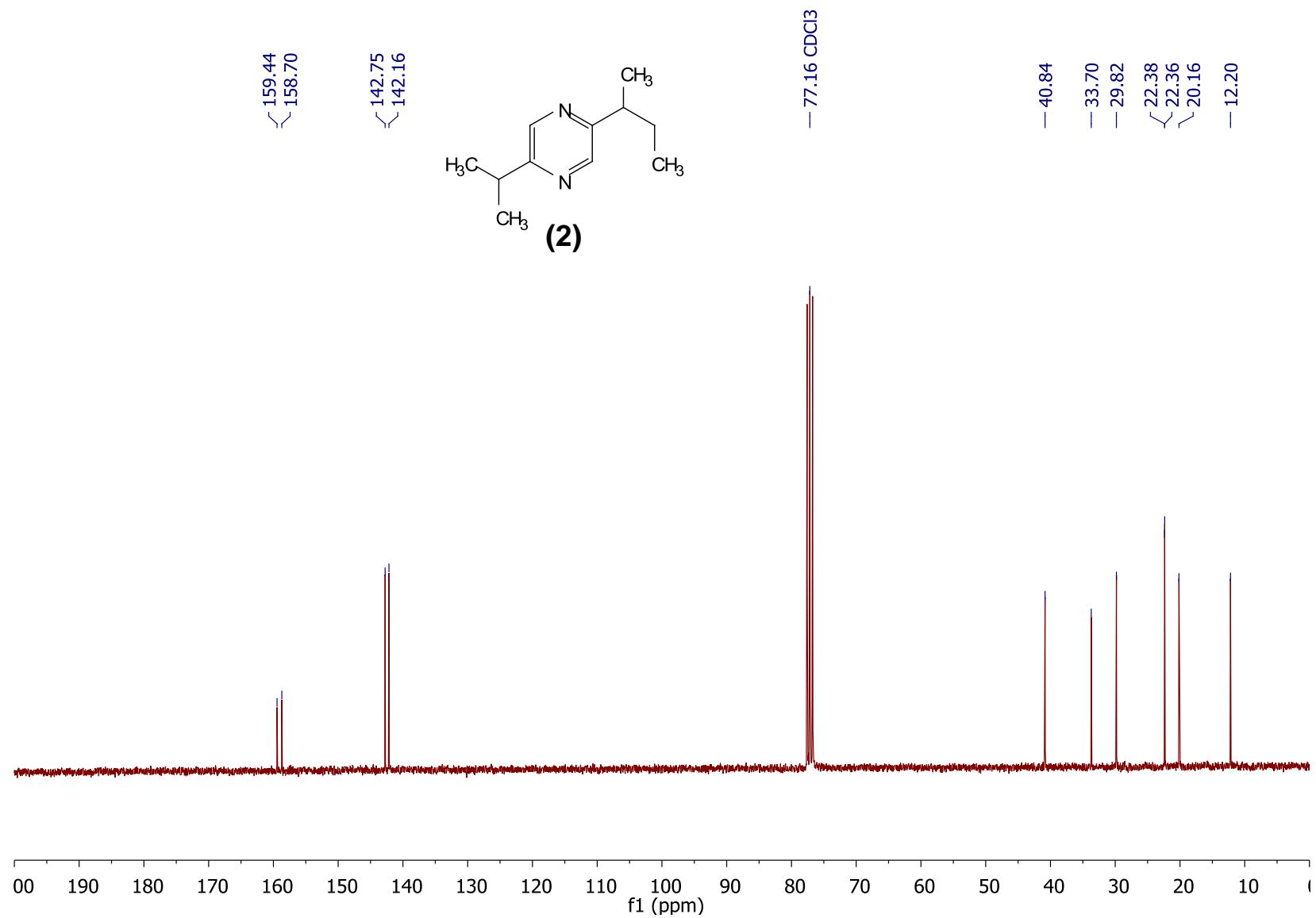


Figure 10S. <sup>13</sup>C NMR spectrum of 2-(*sec*-butyl)-5-isopropylpyrazine (**2**) in CDCl<sub>3</sub>.

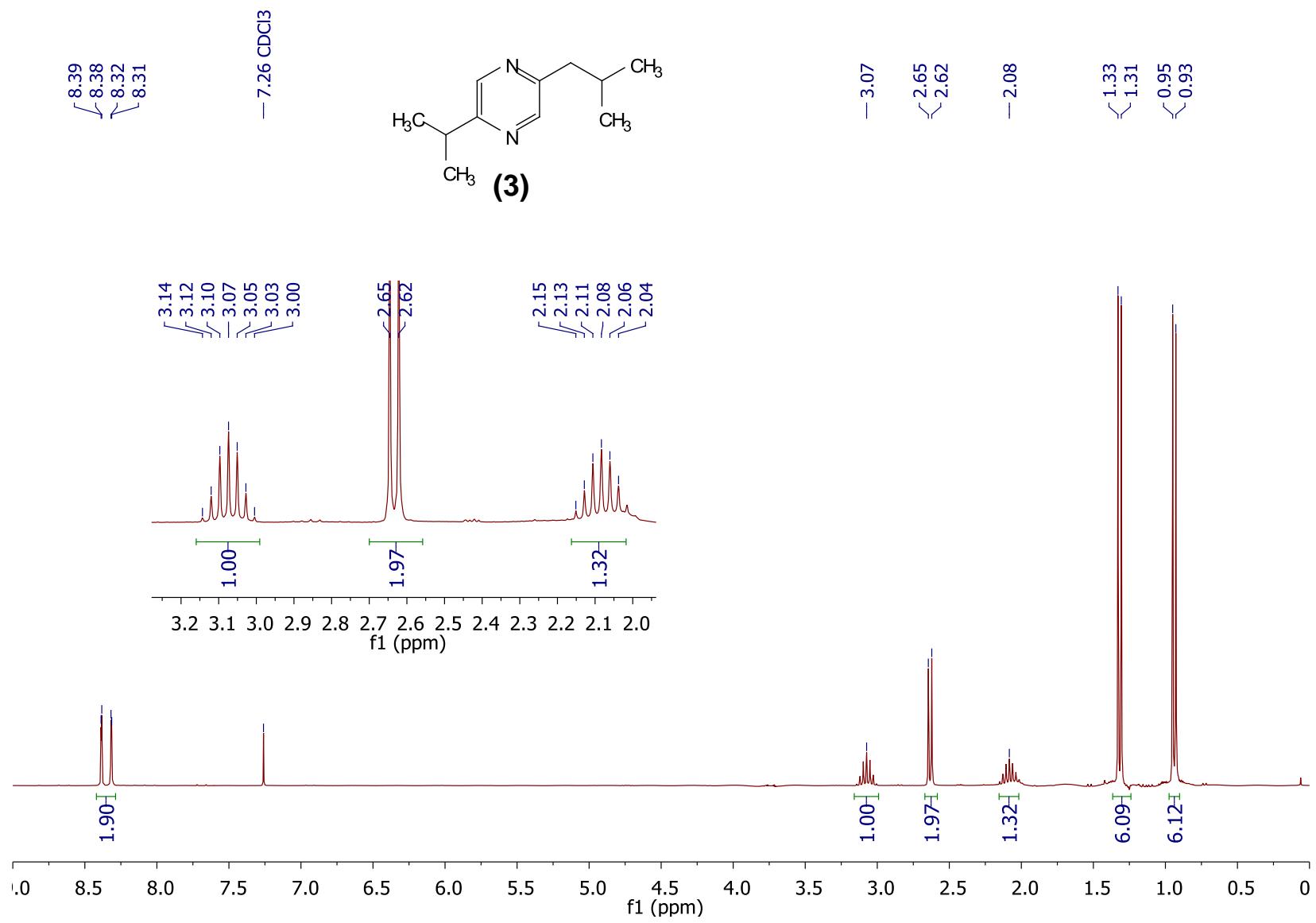


Figure 11S.  $^1\text{H}$  NMR spectrum of 2-isobutyl-5-isopropylpyrazine (**3**) in  $\text{CDCl}_3$ .

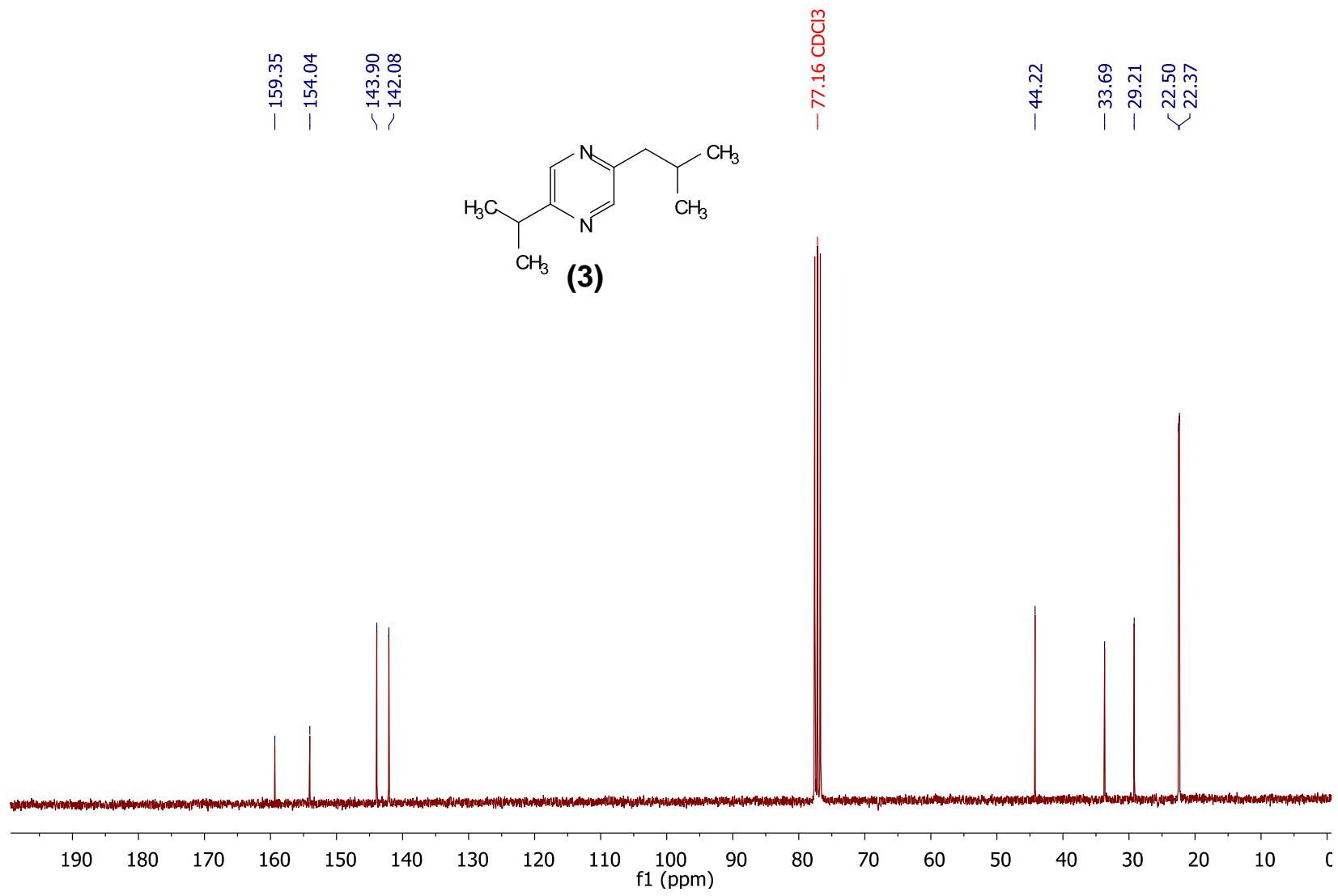


Figure 12S. <sup>13</sup>C NMR spectrum of 2-isobutyl-5-isopropylpyrazine (**3**) in CDCl<sub>3</sub>.

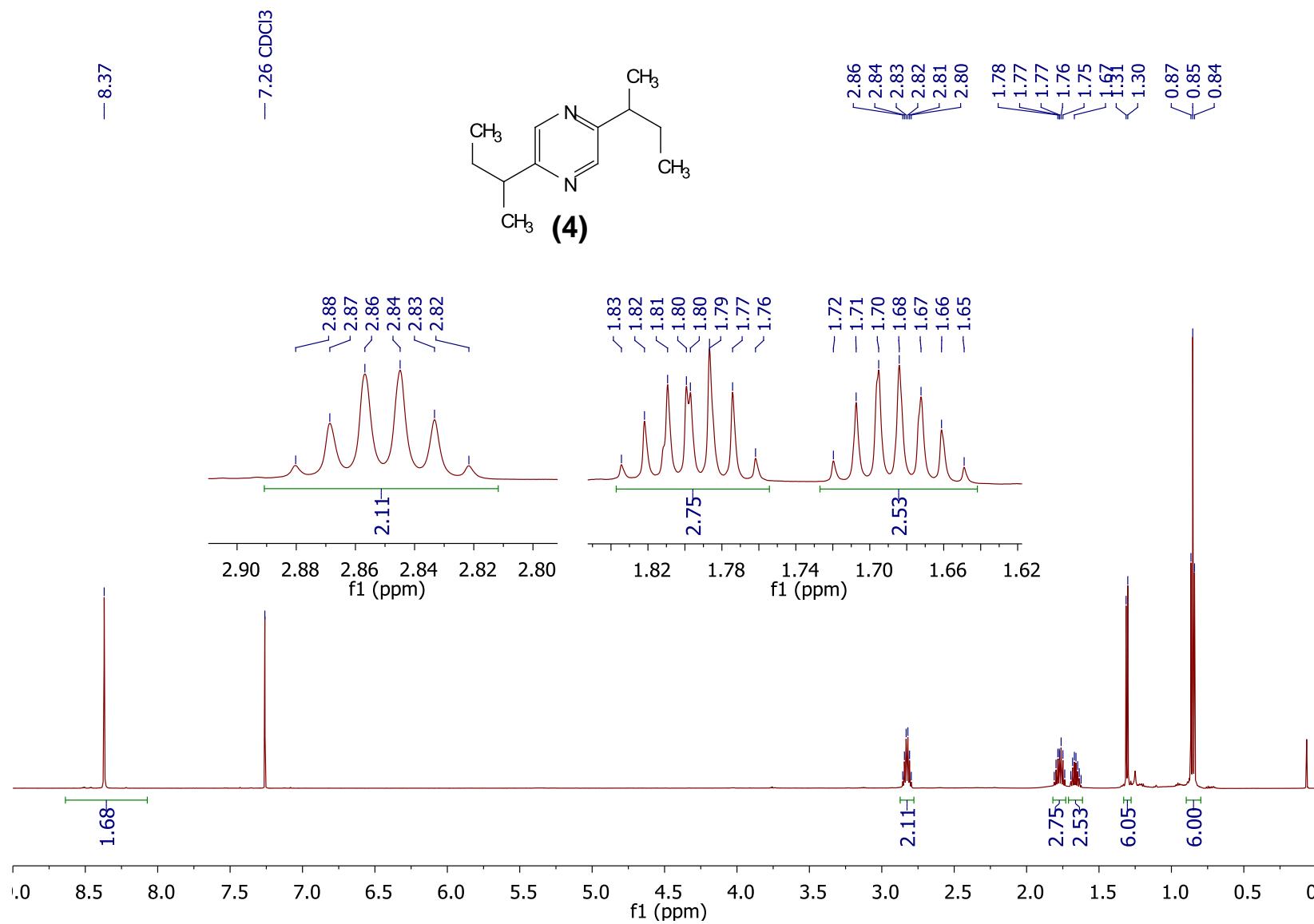


Figure 13S.  $^1\text{H}$  NMR spectrum of 2,5-di-*sec*-butylpyrazine (**4**) in  $\text{CDCl}_3$ .

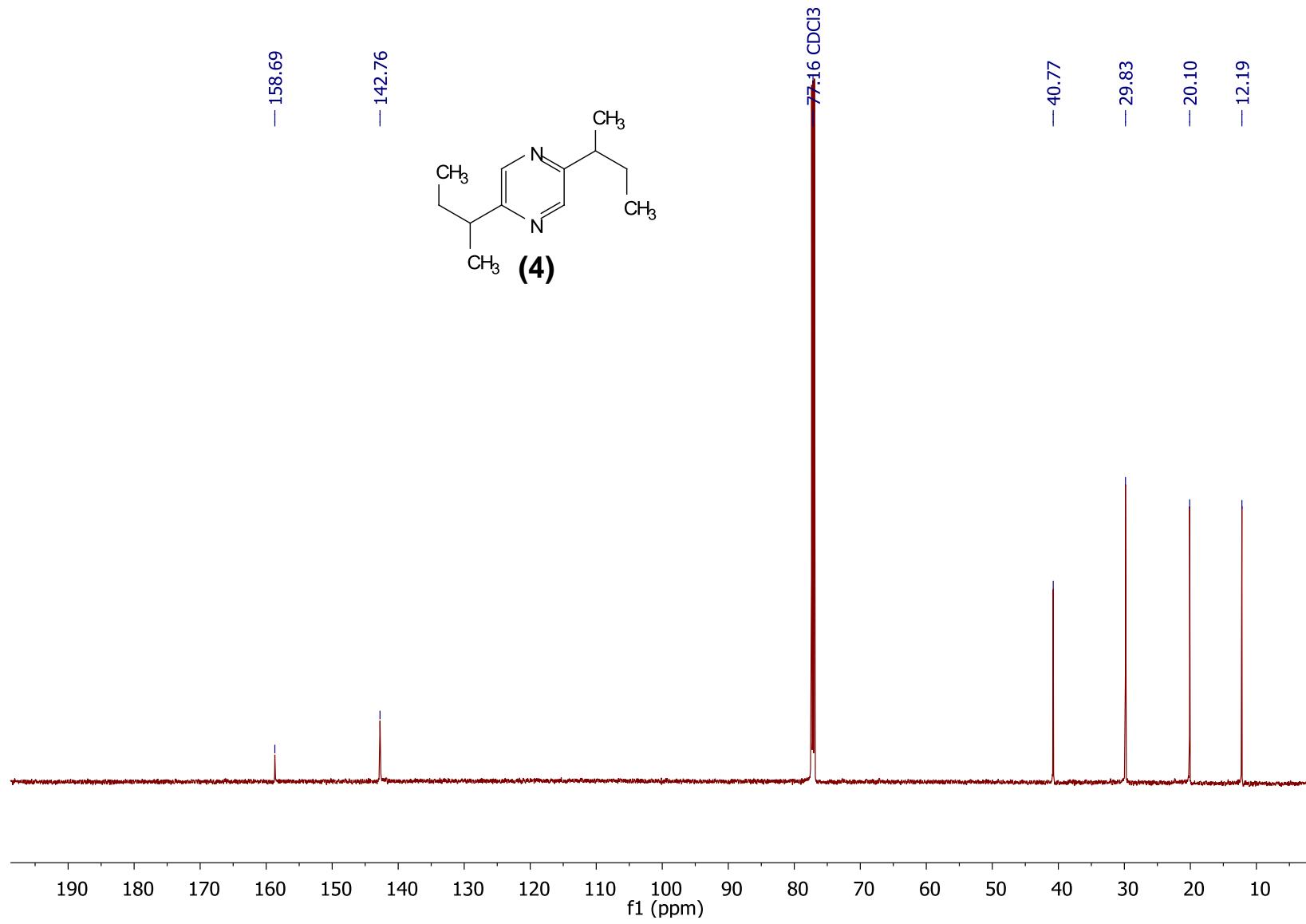


Figure 14S.  $^{13}\text{C}$  NMR spectrum of 2,5-di-*sec*-butylpyrazine (4) in  $\text{CDCl}_3$ .

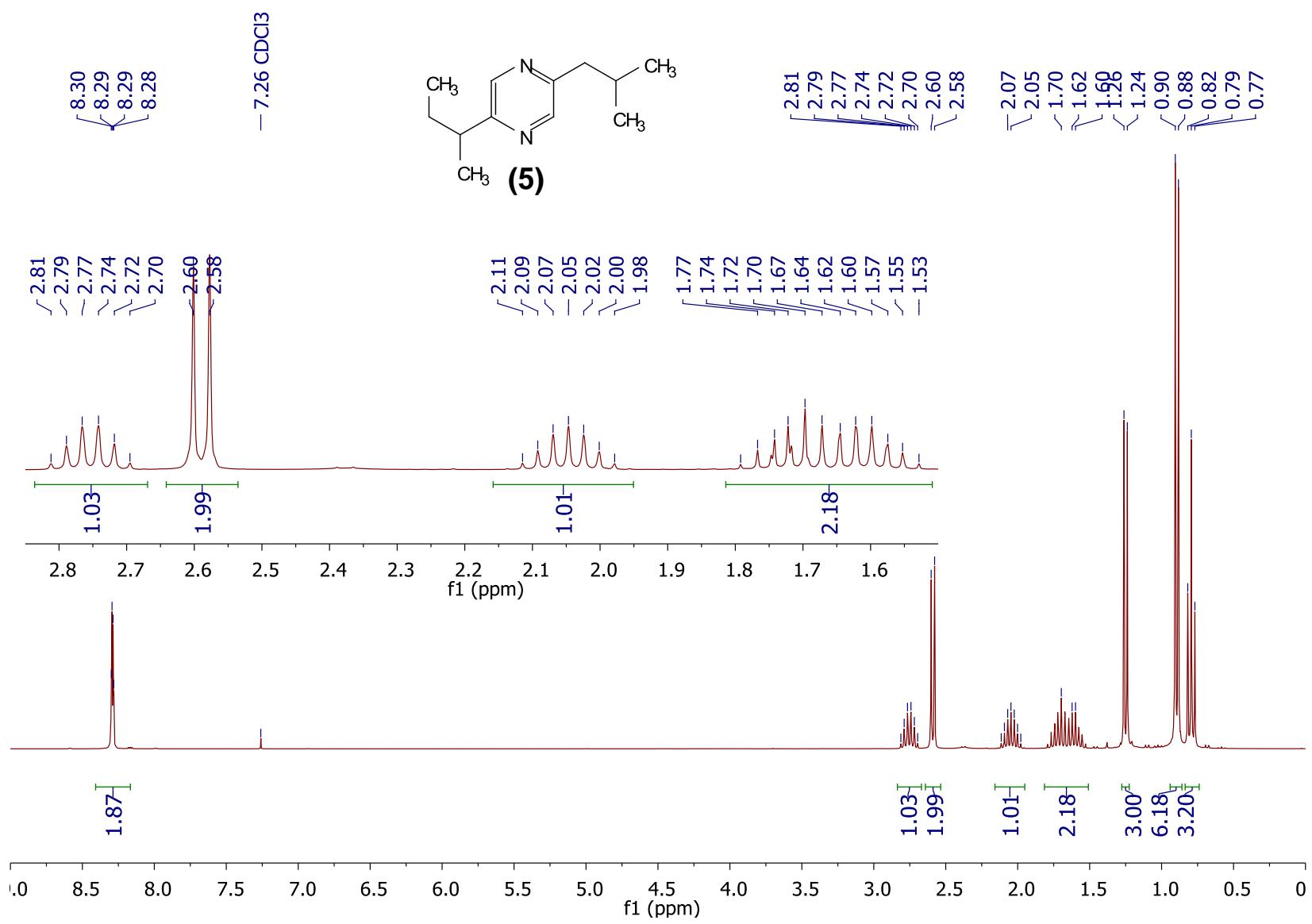


Figure 15S.  $^1\text{H}$  NMR spectrum of 2-(*sec*-butyl)-5-isobutylpyrazine (**5**) in  $\text{CDCl}_3$ .

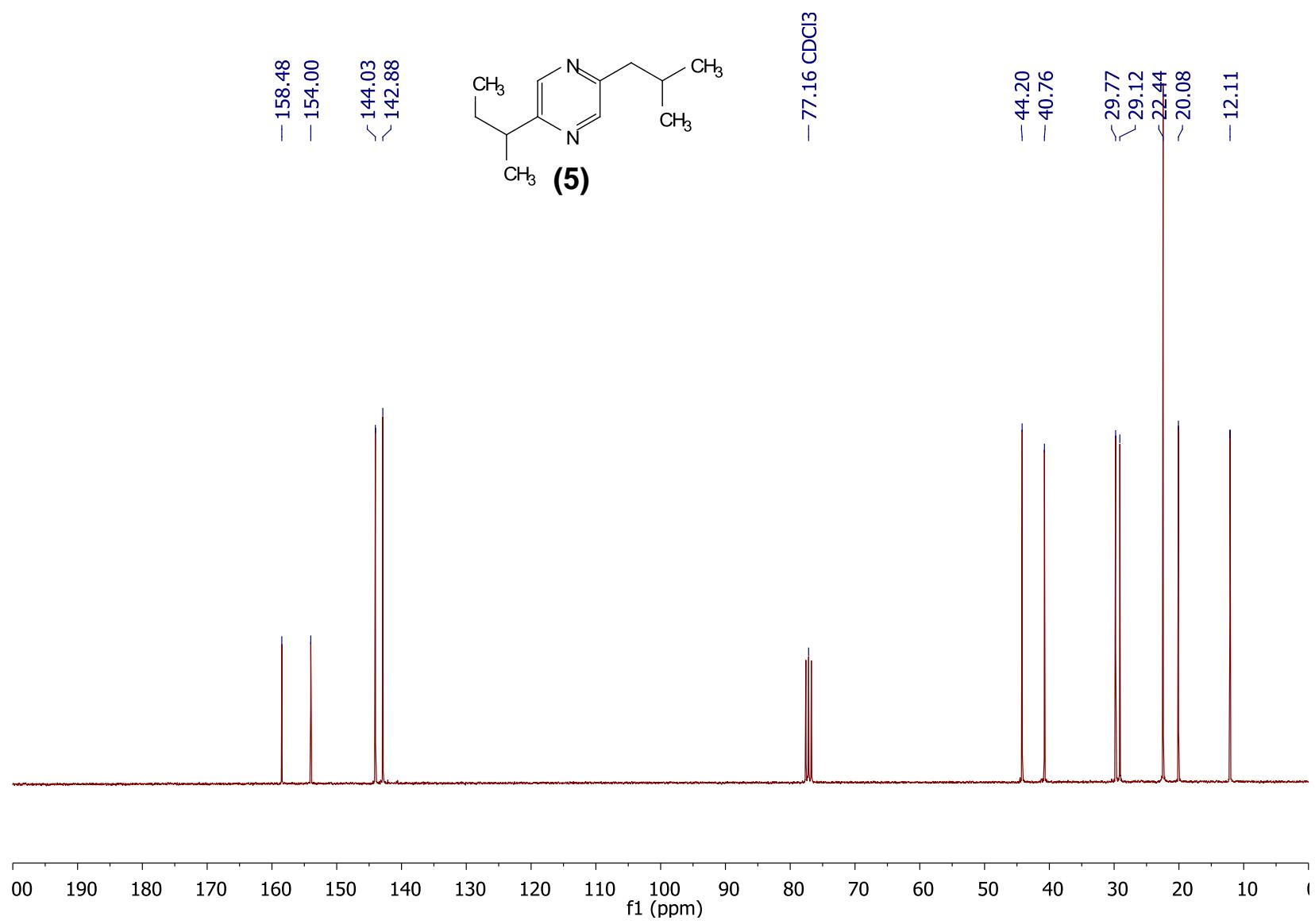


Figure 16S.  $^{13}\text{C}$  NMR spectrum of 2-(*sec*-butyl)-5-isobutylpyrazine (5) in  $\text{CDCl}_3$ .

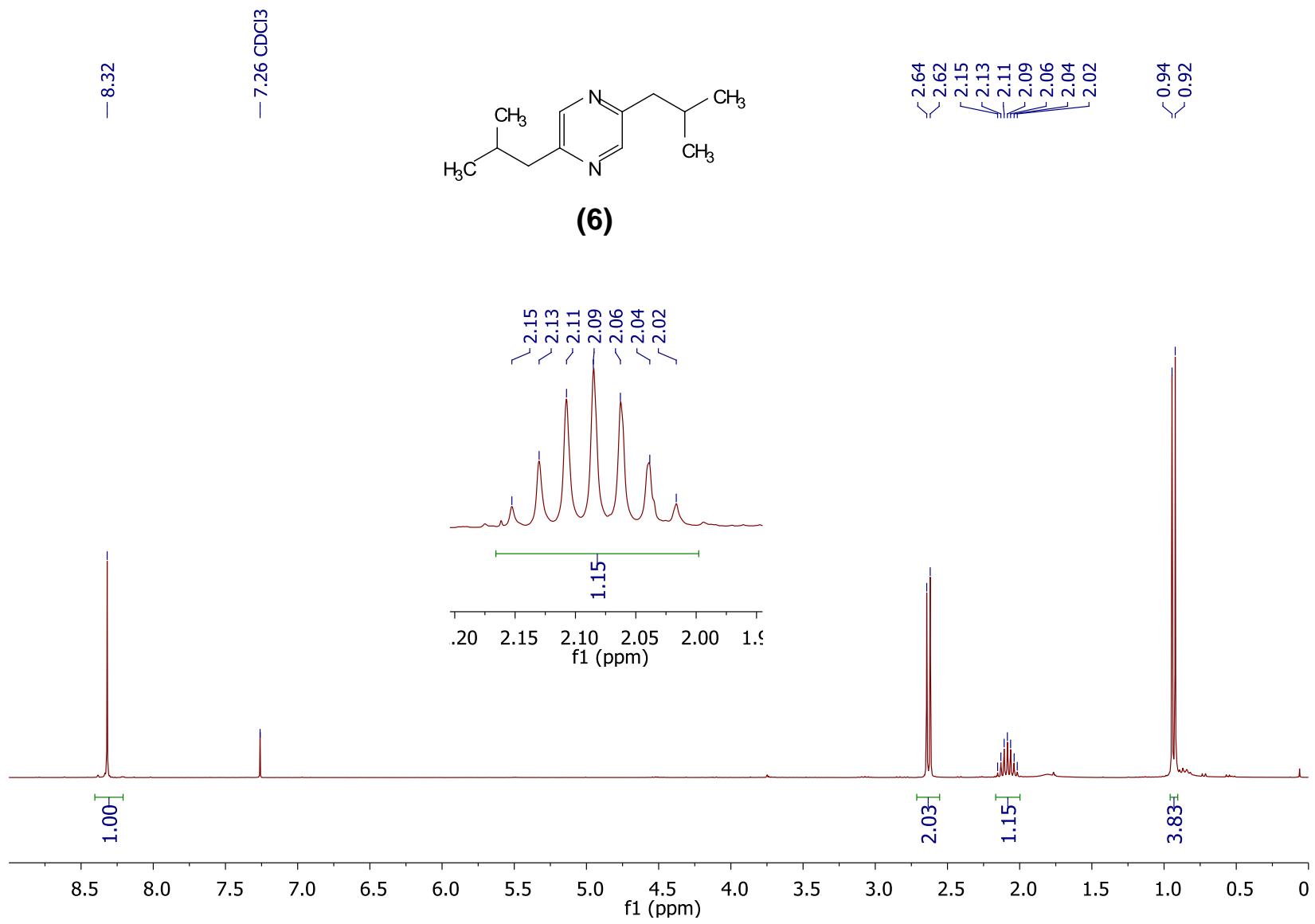


Figure 17S. <sup>1</sup>H NMR spectrum of 2,5-diisobutylpyrazine (**6**) in CDCl<sub>3</sub>.

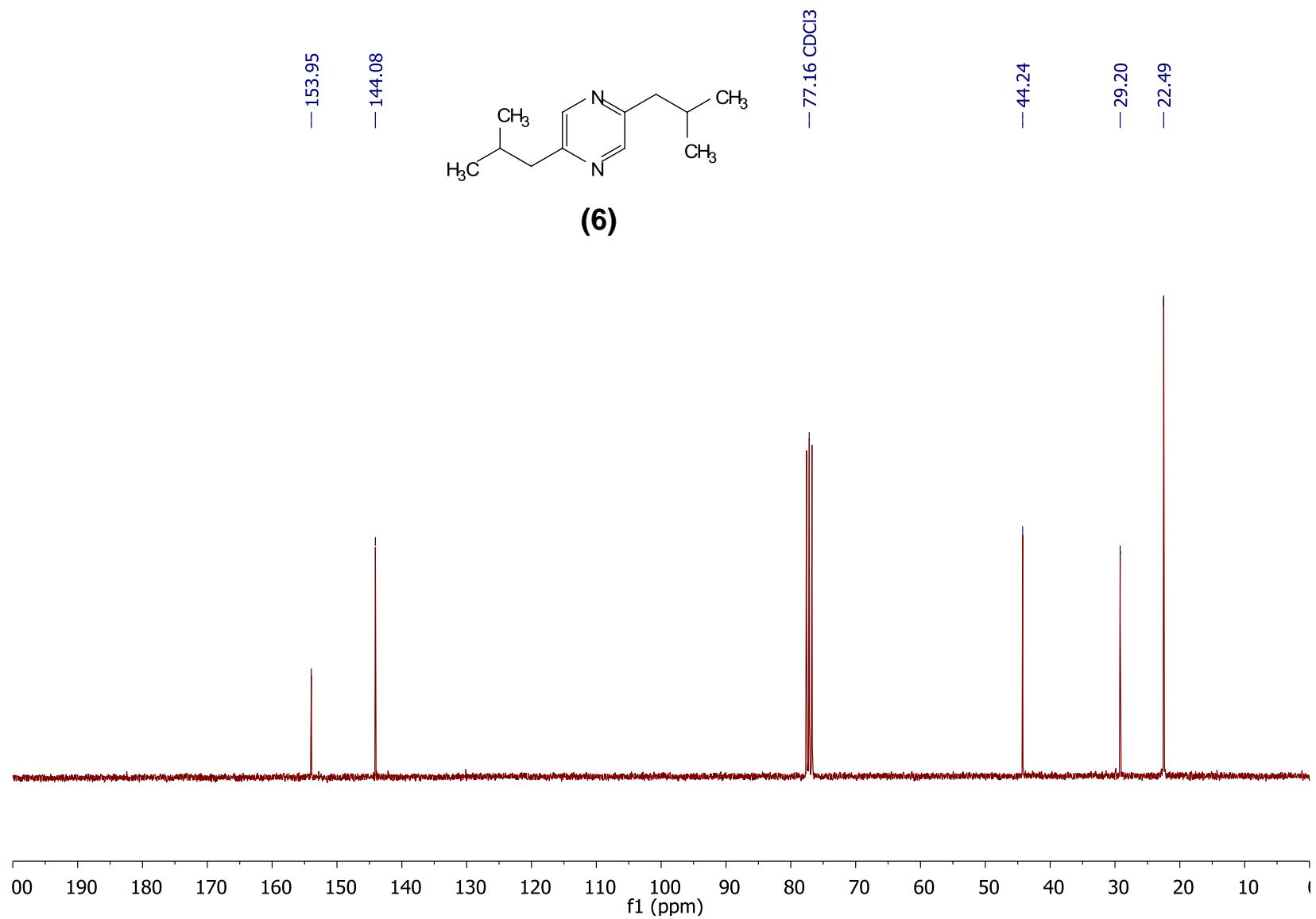


Figure 18S.  $^{13}\text{C}$  NMR spectrum of 2,5-diisobutylpyrazine (**6**) in CDCl<sub>3</sub>.