

## Supplementary Information

### Potential Antileishmanial Activity of 4-*N*-Acylhydrazone Pyrazolo[3,4-*d*]pyridazin-7-ones: Synthesis, *in vitro* Biological Evaluations and Computational Studies

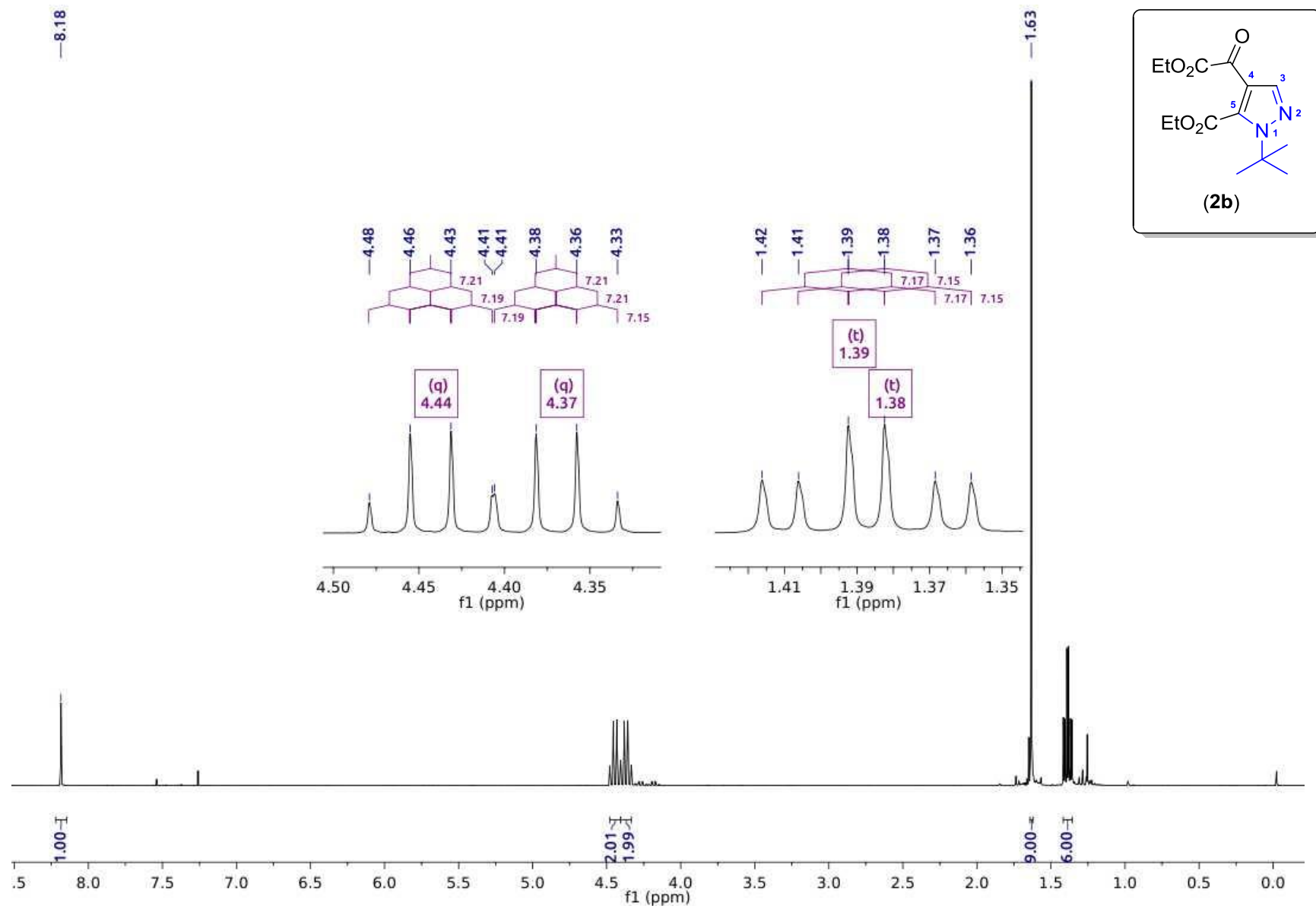
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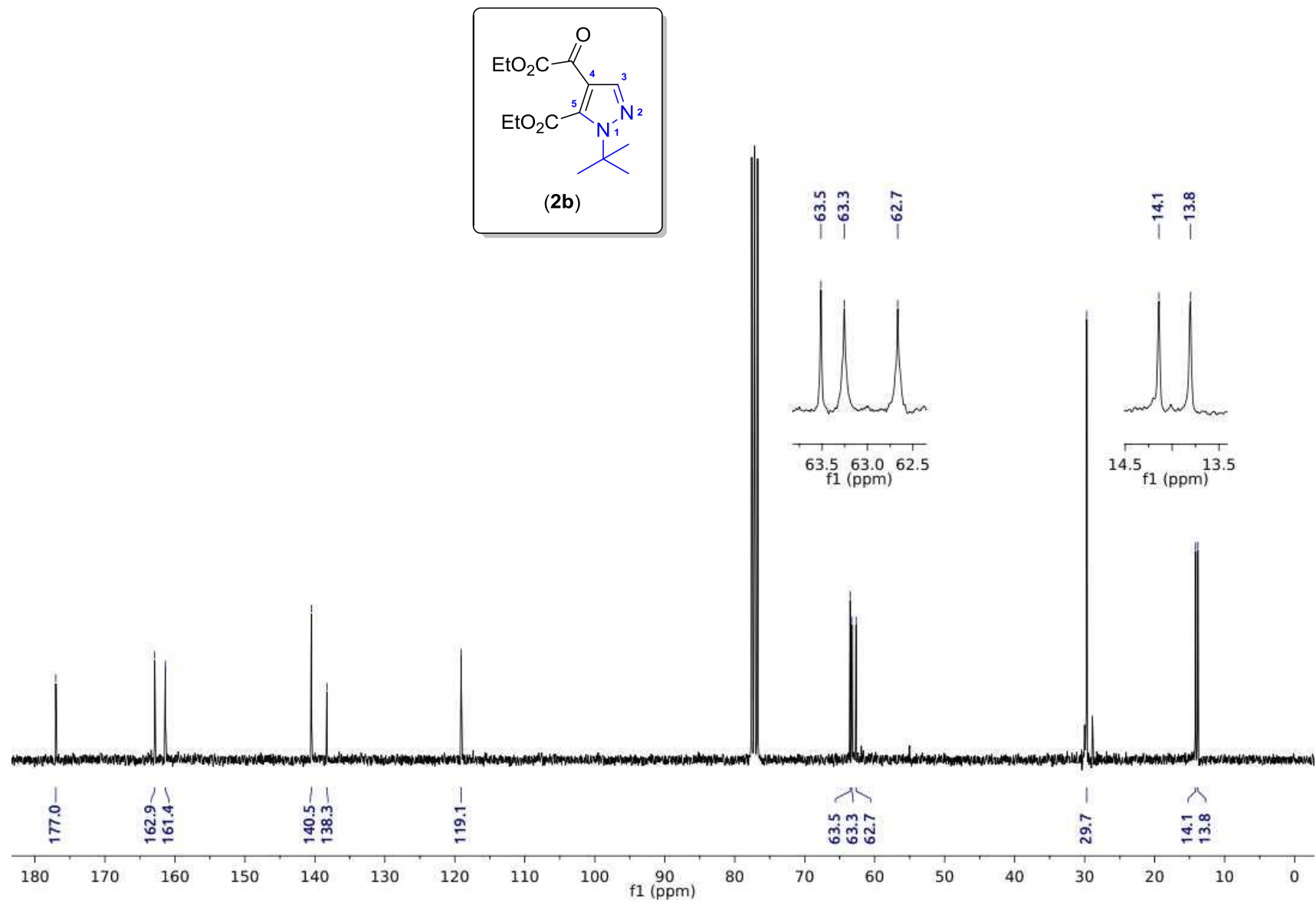
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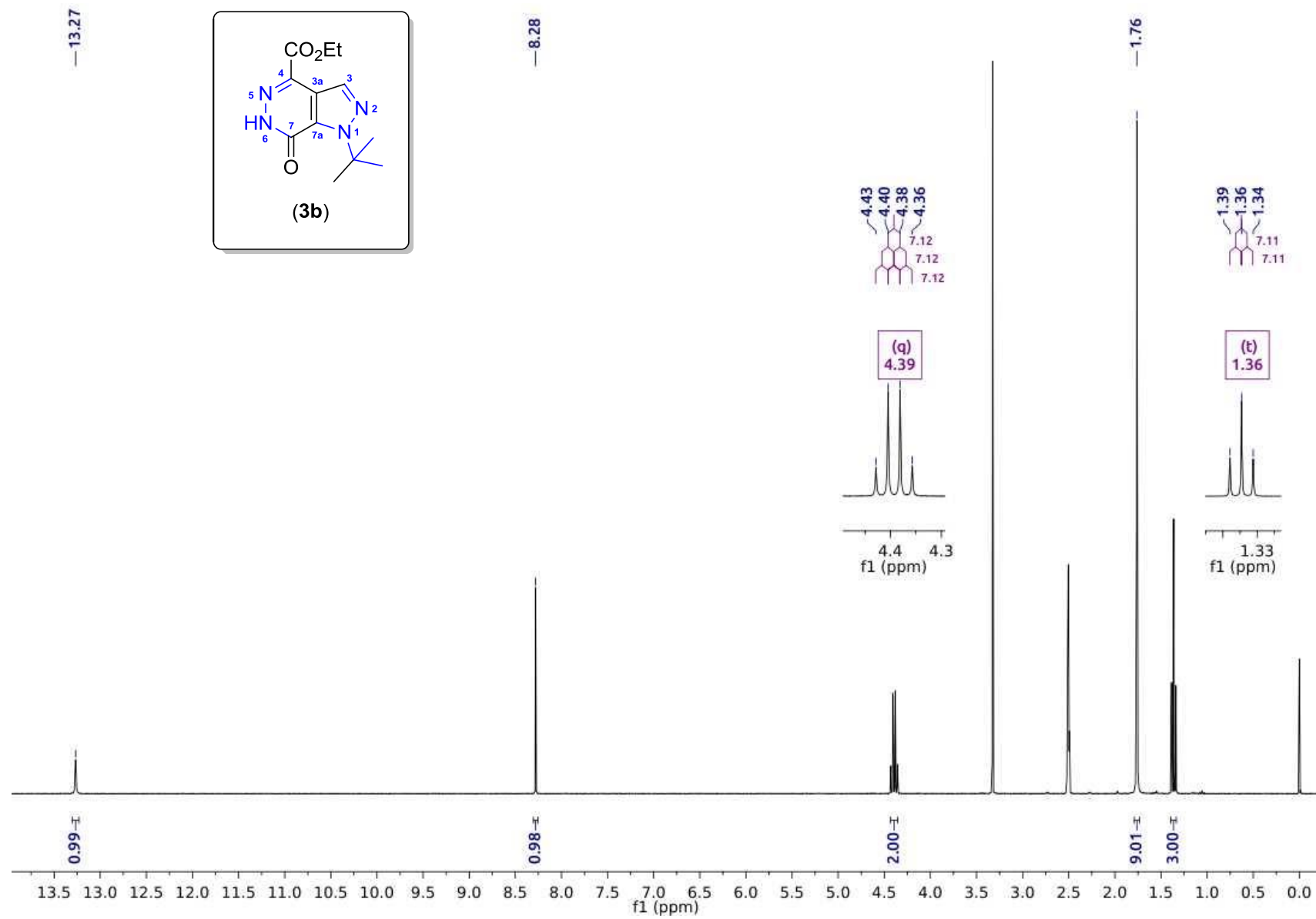
<sup>1</sup>H and <sup>13</sup>C NMR spectra



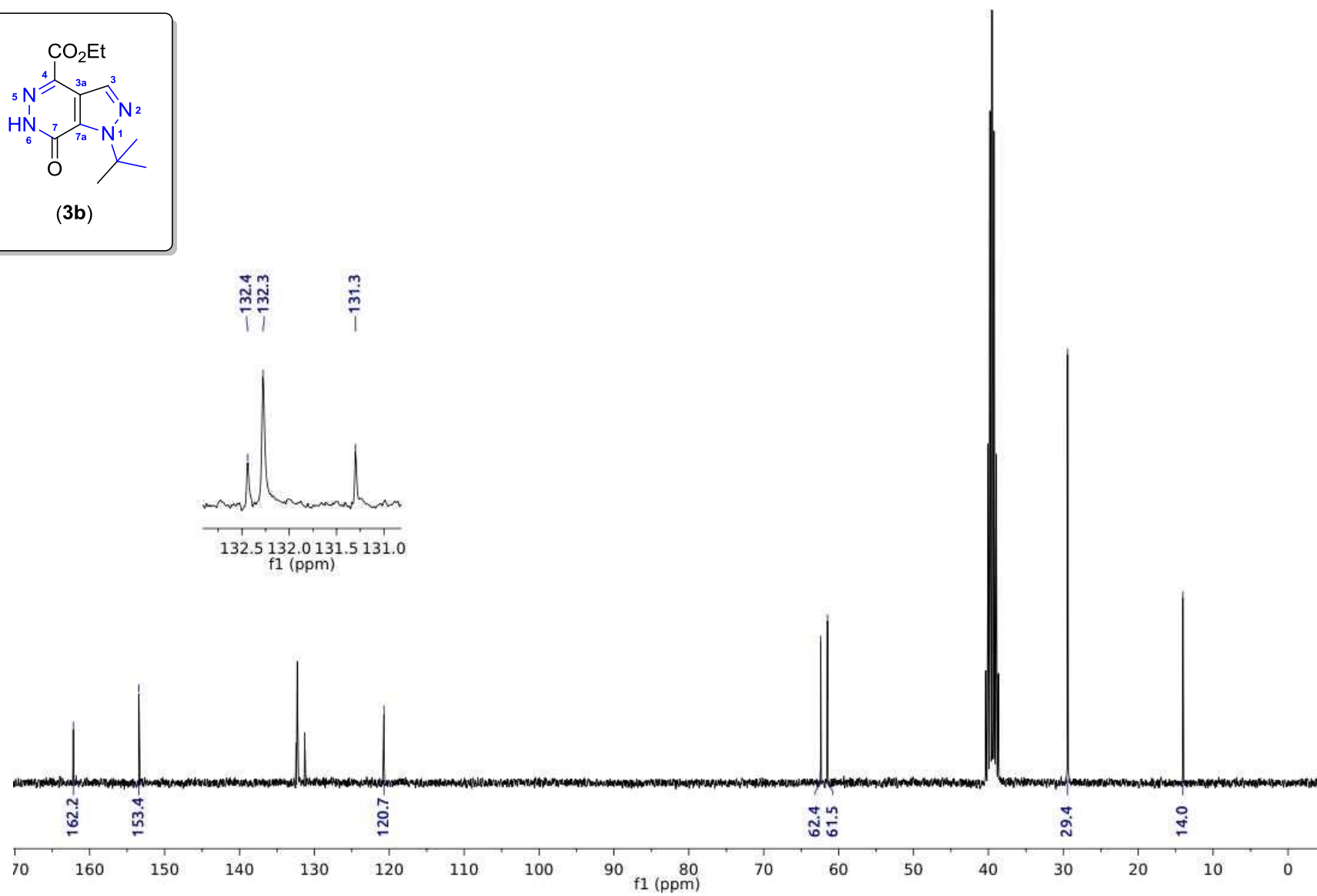
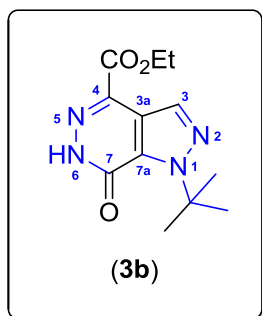
**Figure S1.** <sup>1</sup>H NMR spectrum (300.06 MHz, CDCl<sub>3</sub>) of **2b**.



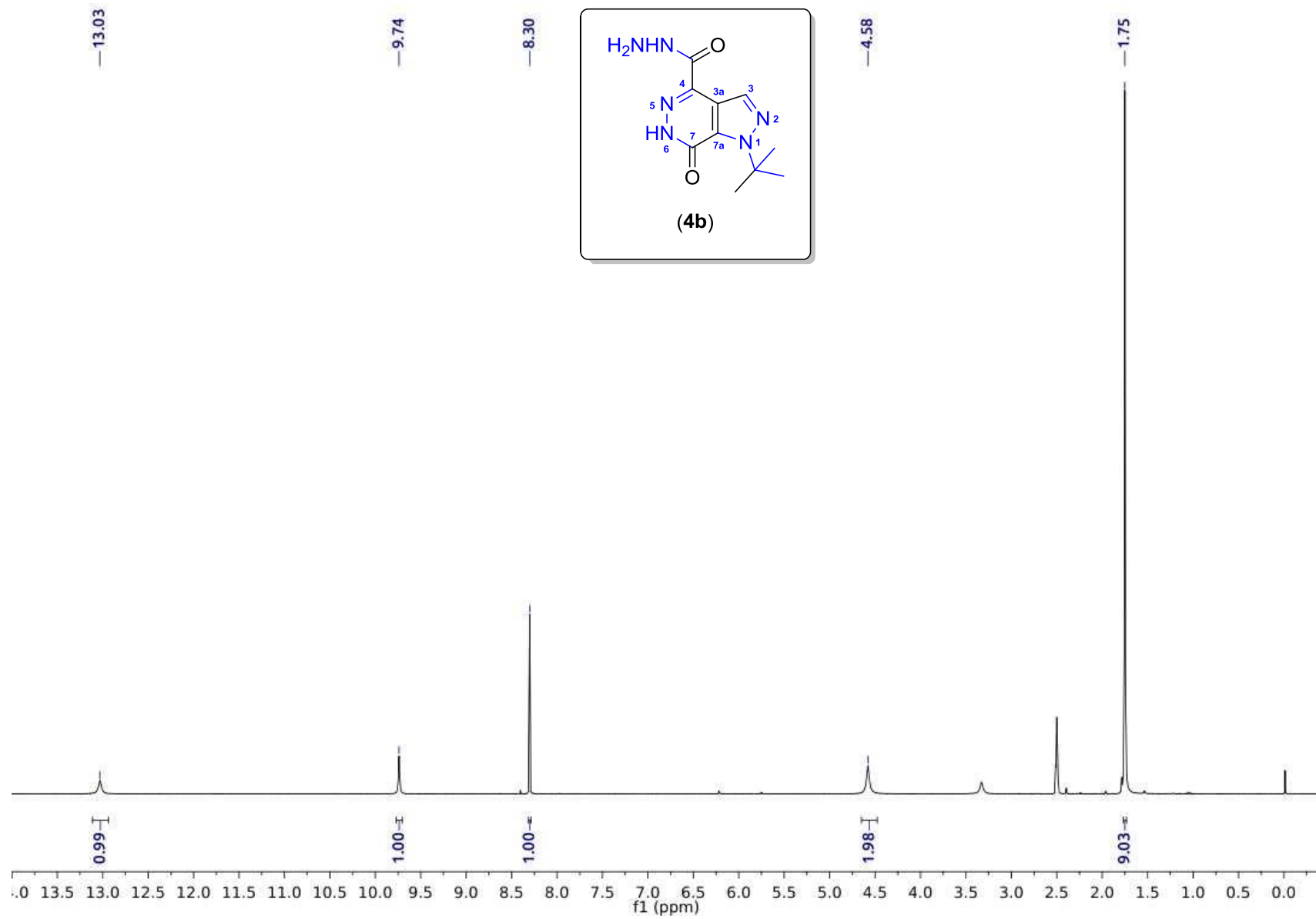
**Figure S2.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{CDCl}_3$ ) of **2b**.



**Figure S3.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **3b**.



**Figure S4.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **3b**.



**Figure S5.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **4b**.

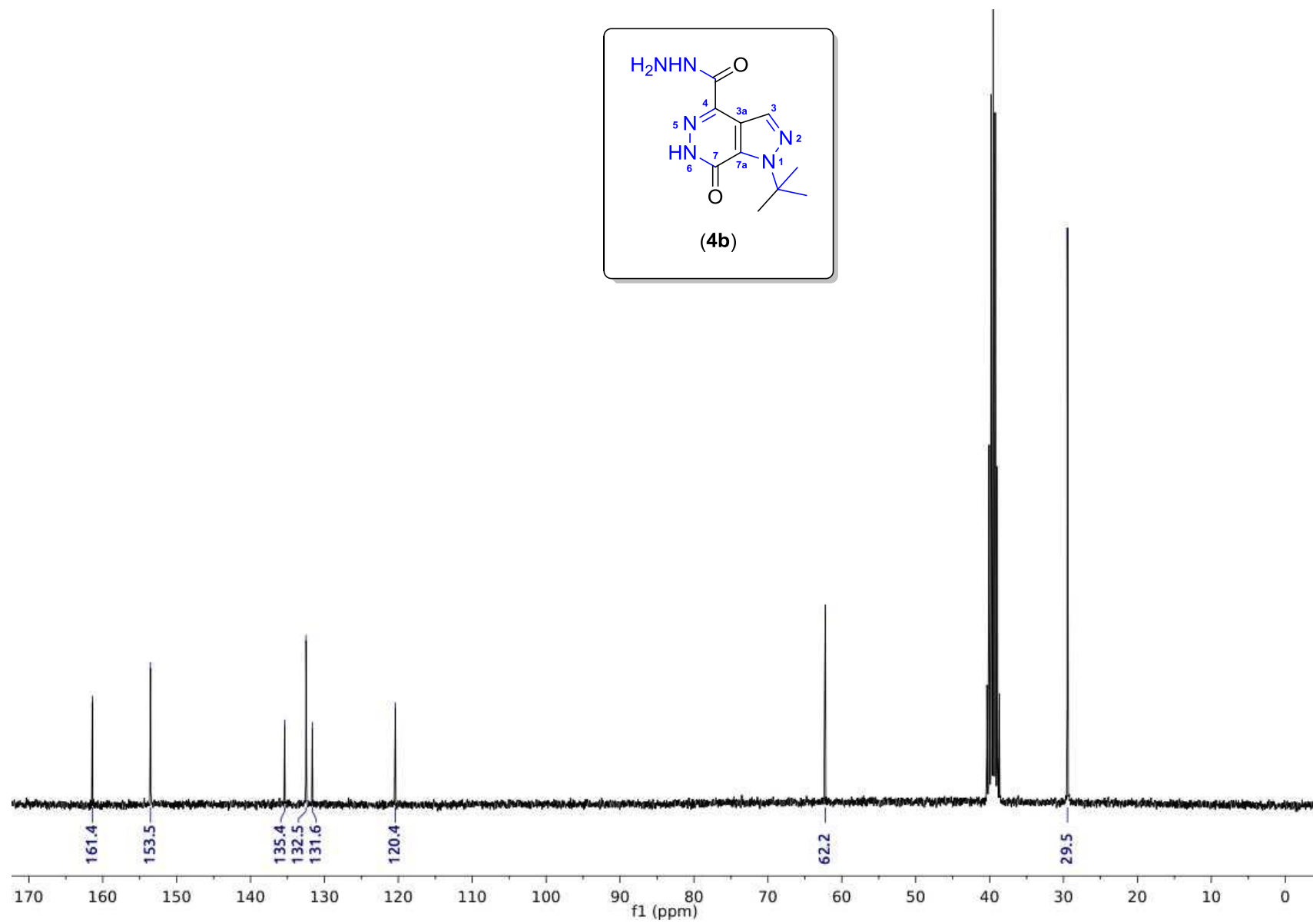
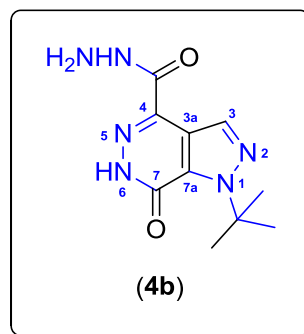
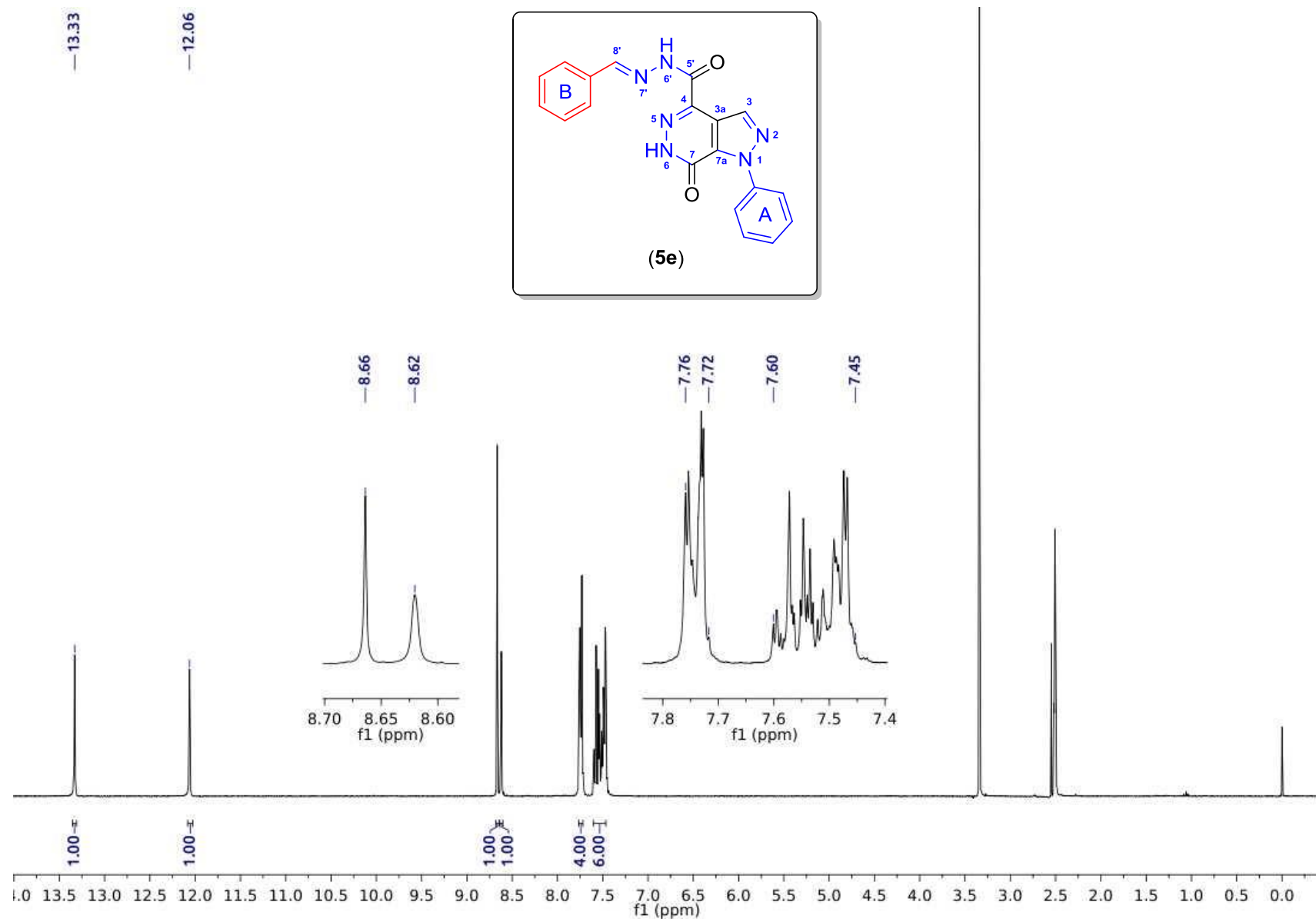
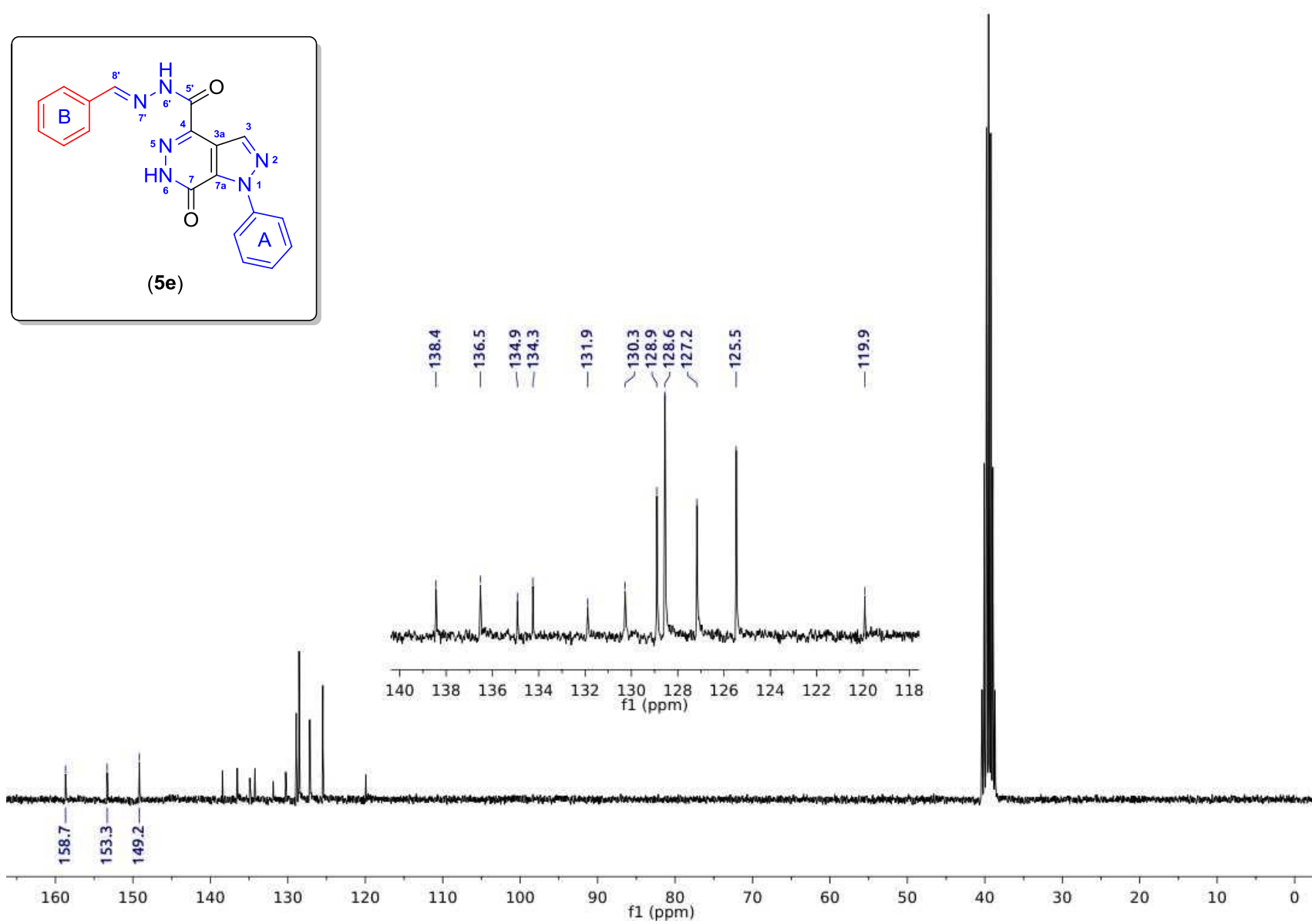


Figure S6. <sup>13</sup>C NMR spectrum (75.46 MHz, DMSO-*d*<sub>6</sub>) of **4b**.

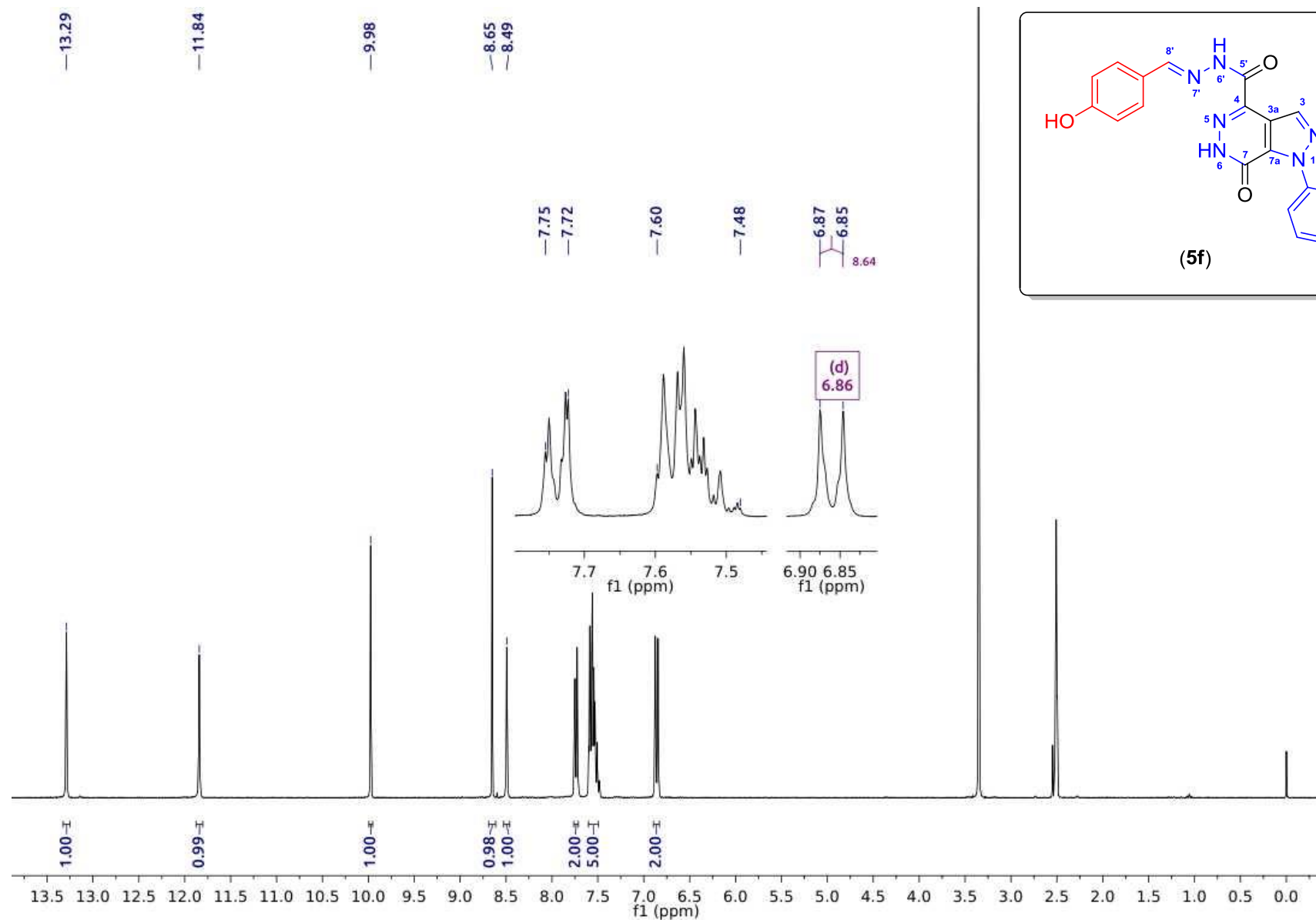


**Figure S7.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **5e**.

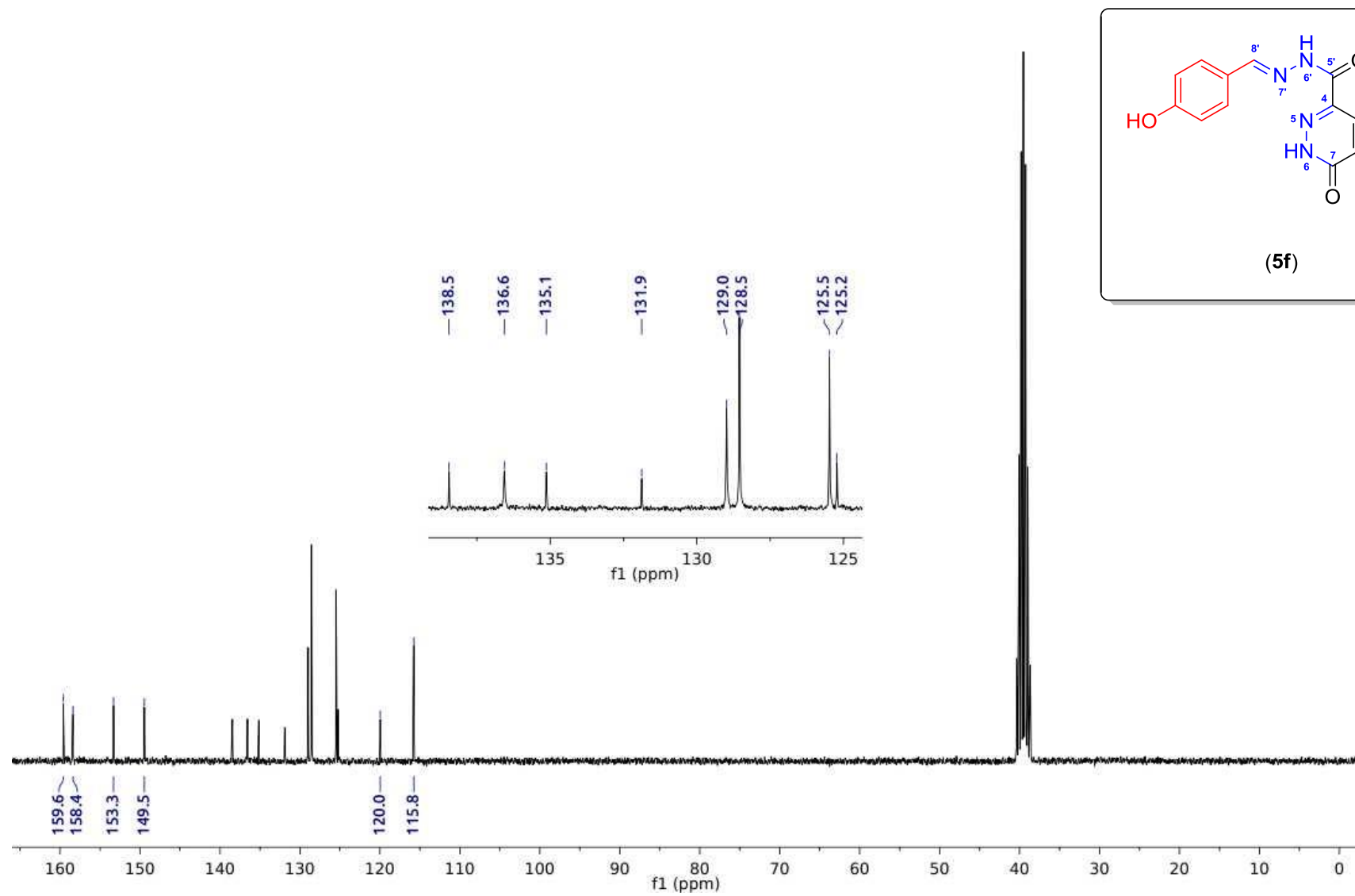




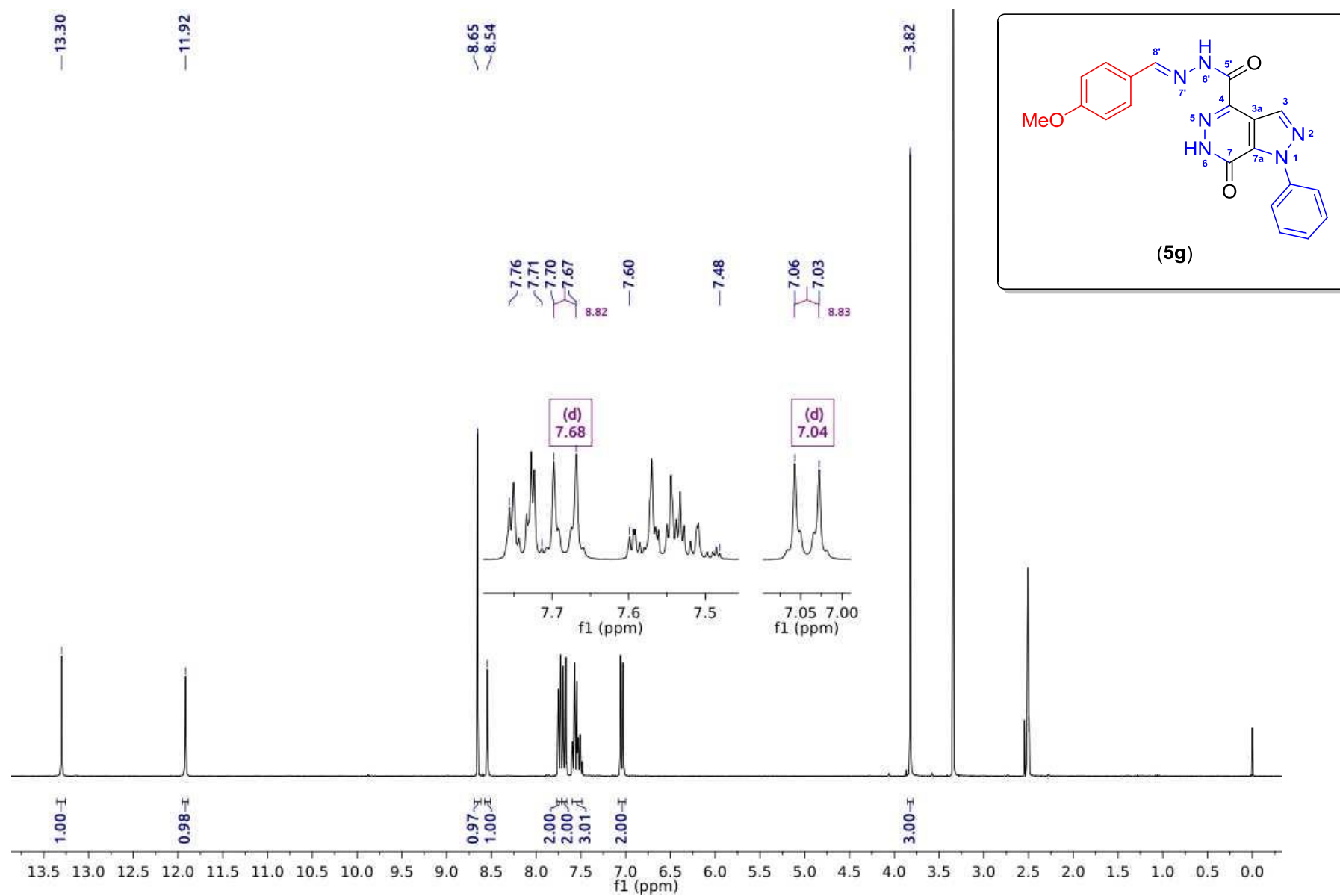
**Figure S8.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **5e**.



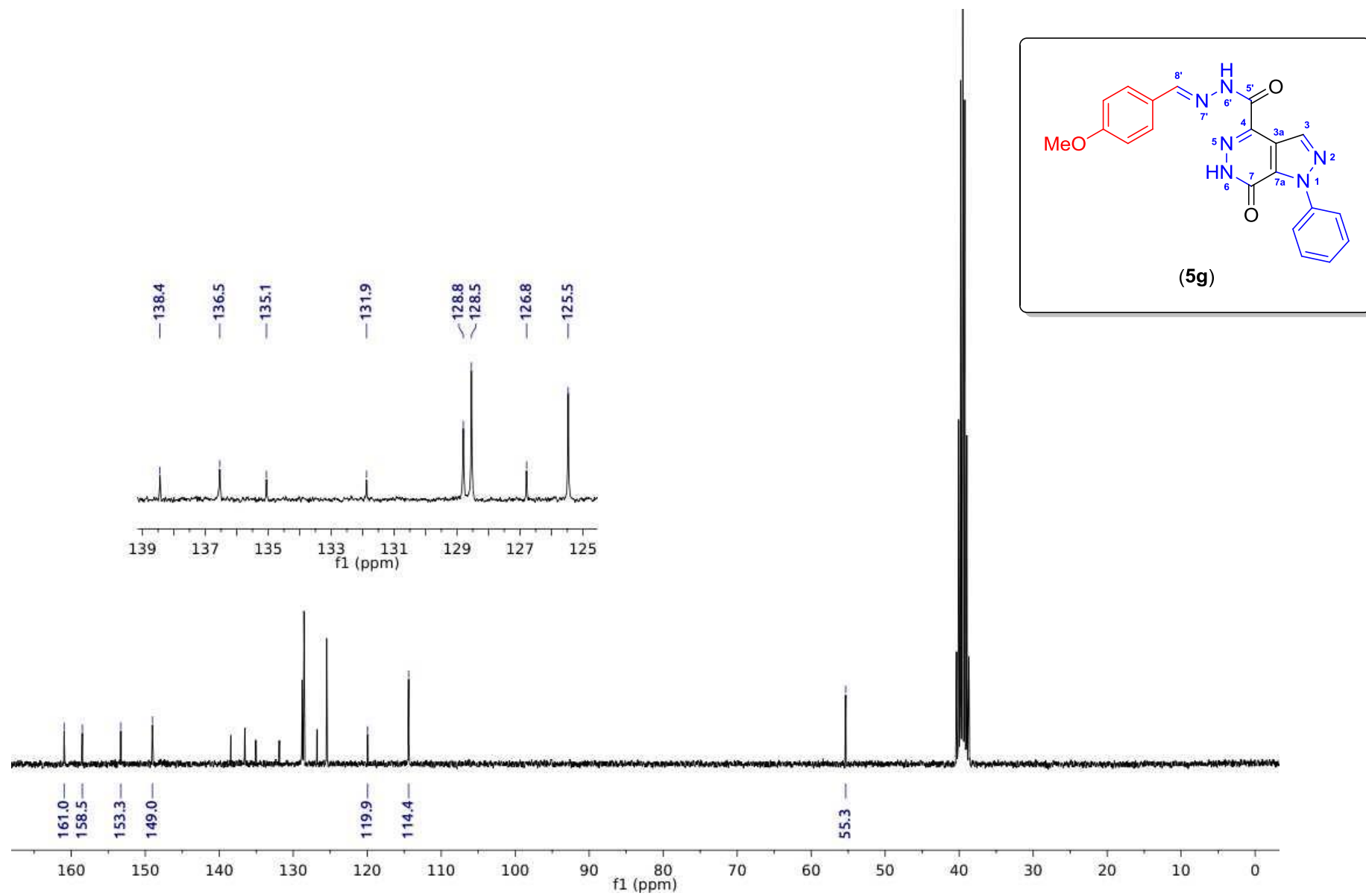
**Figure S9.**  $^1\text{H NMR}$  spectrum (300.06 MHz,  $\text{DMSO-}d_6$ ) of **5f**.



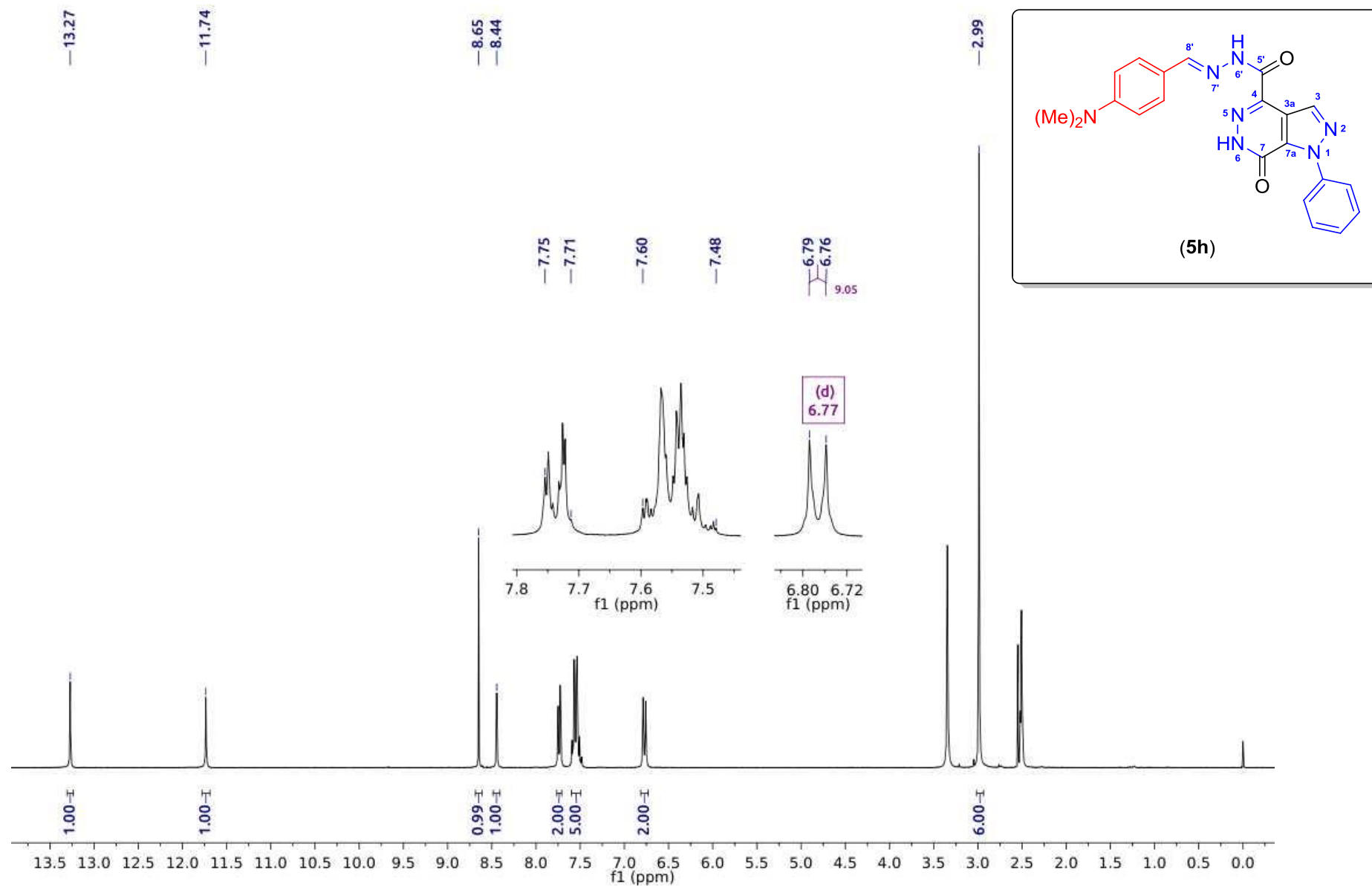
**Figure S10.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **5f**.



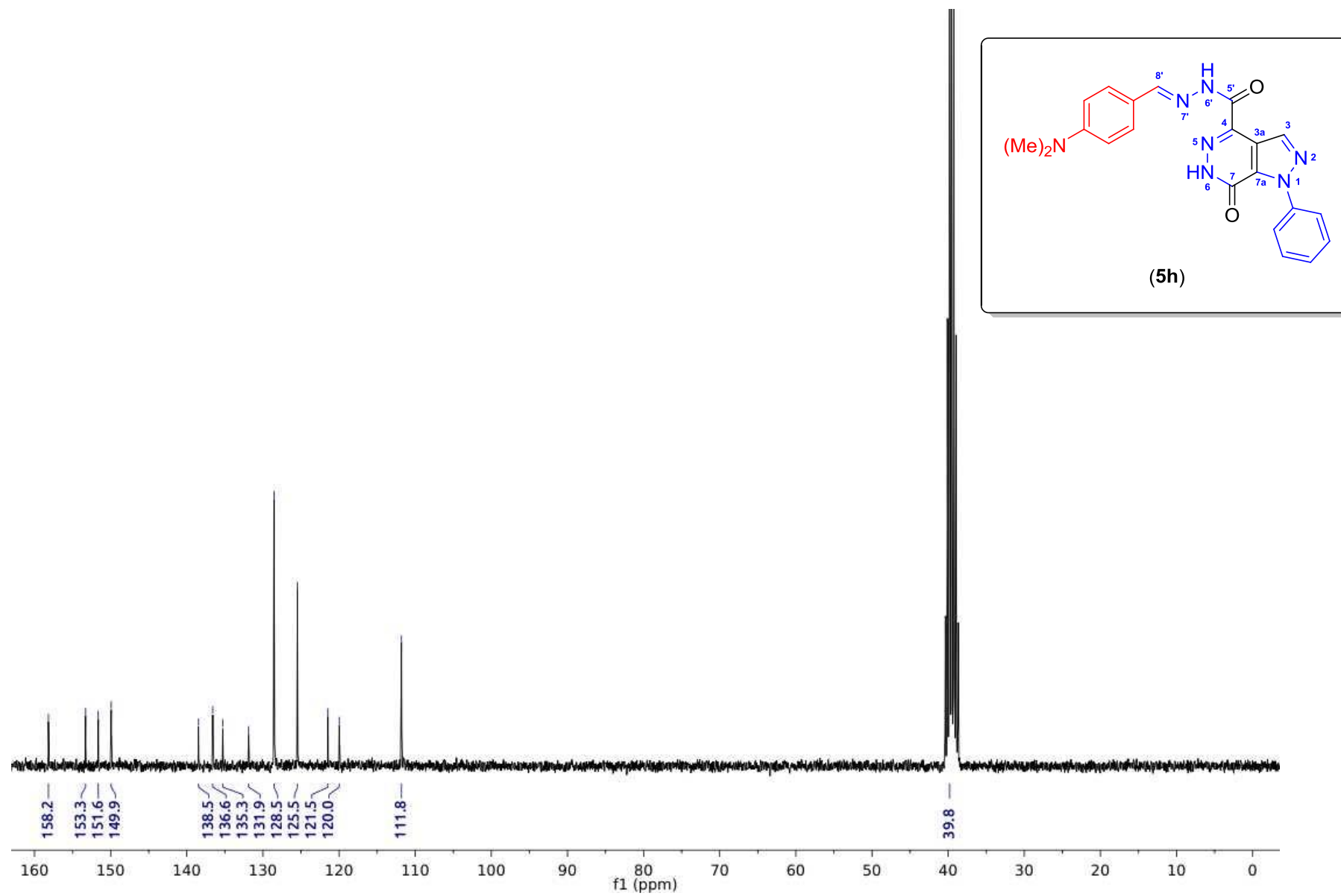
**Figure S11.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **5g**.



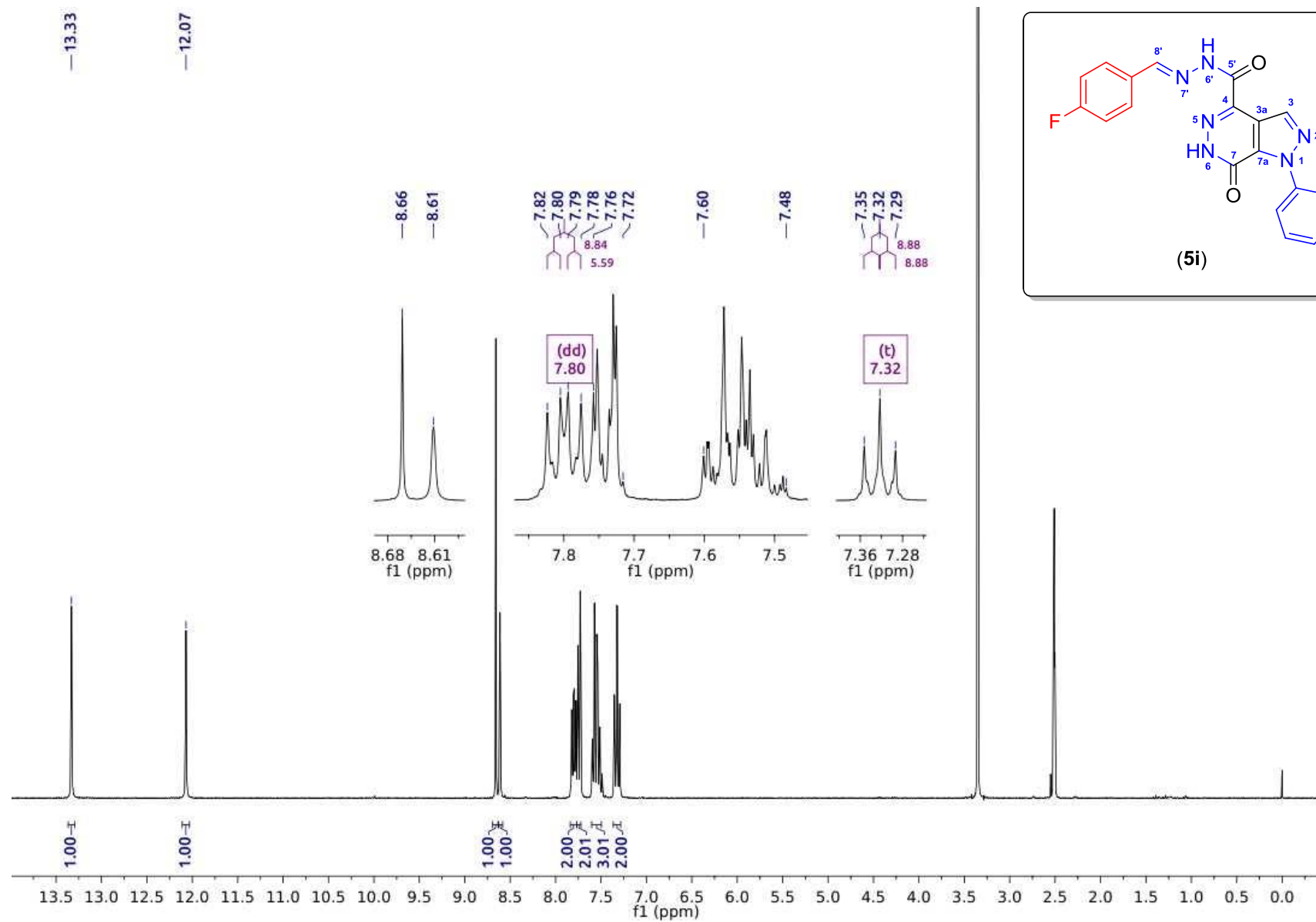
**Figure S12.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **5g**.



**Figure S13.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **5h**.

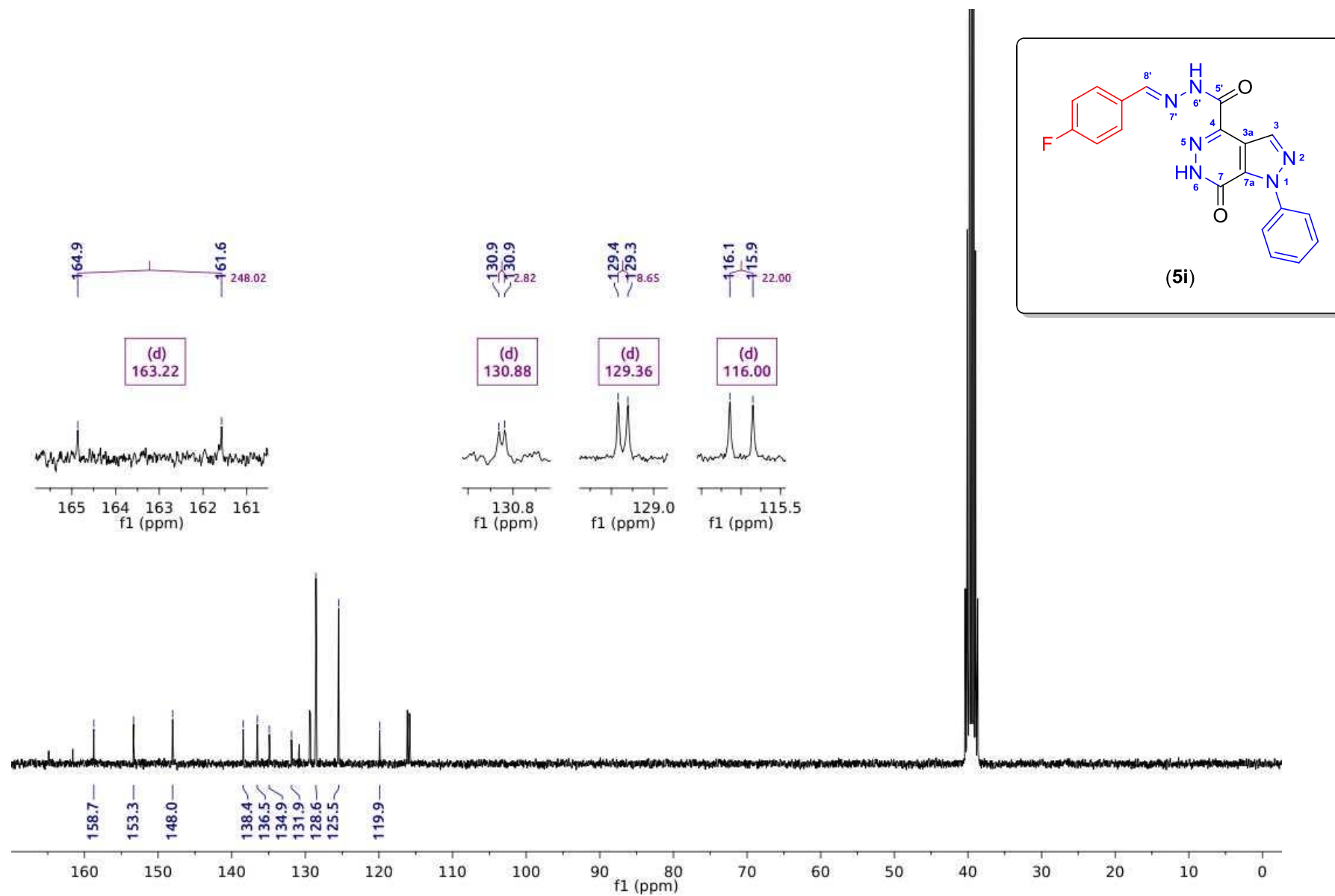


**Figure S14.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **5h**.

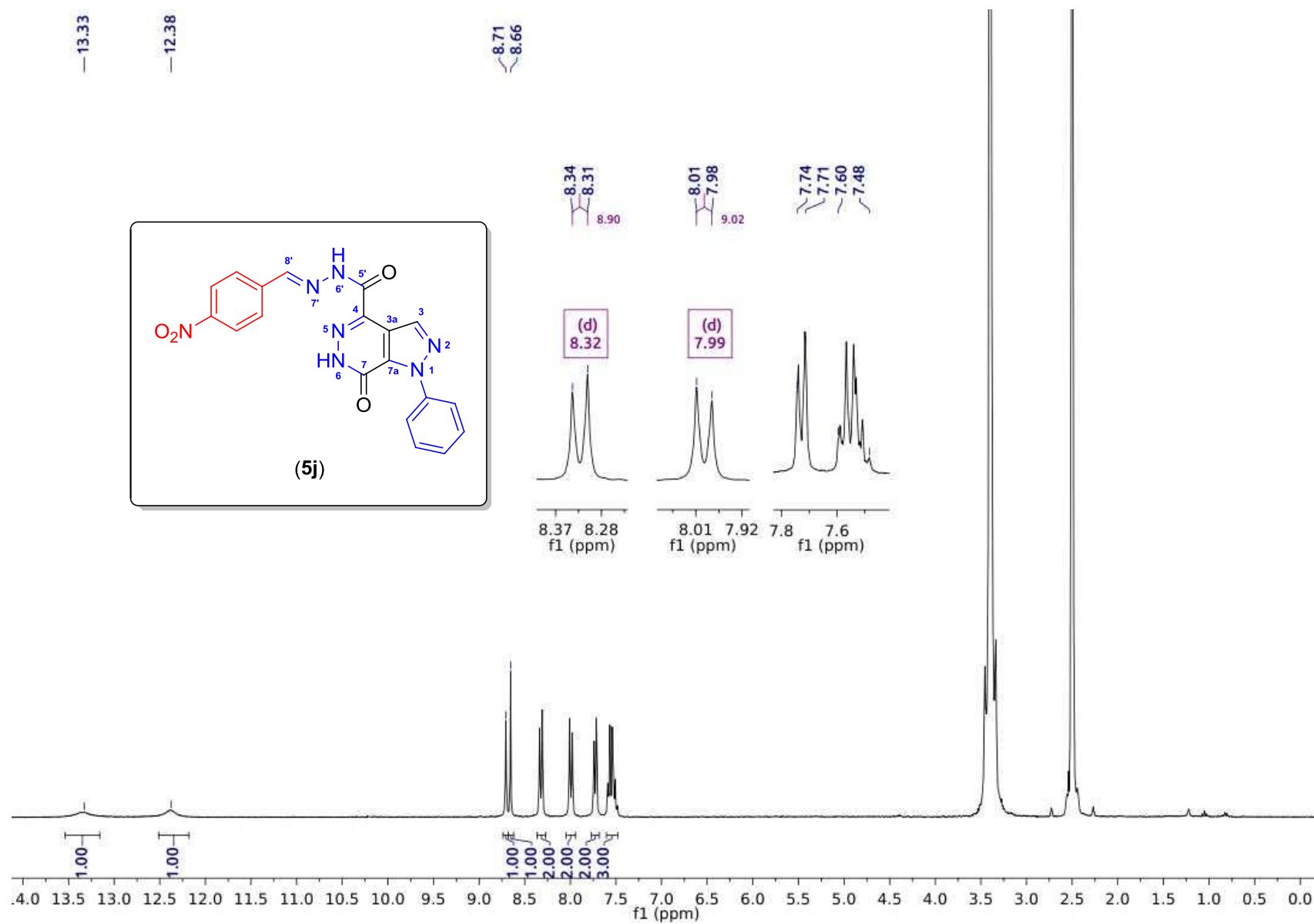


**Figure S15.**  $^1\text{H}$  NMR spectrum (300.06 MHz,  $\text{DMSO-}d_6$ ) of **5i**.

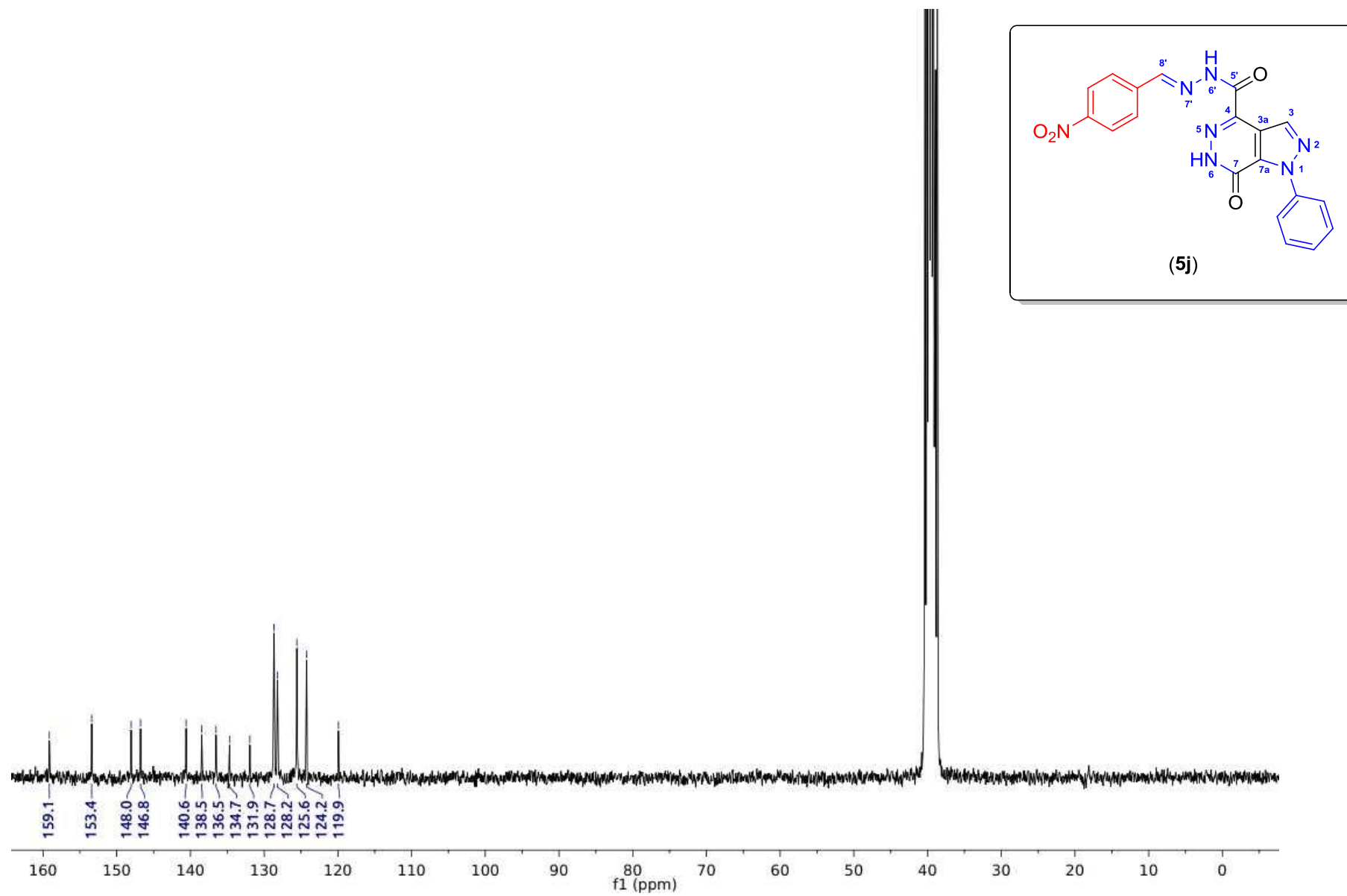




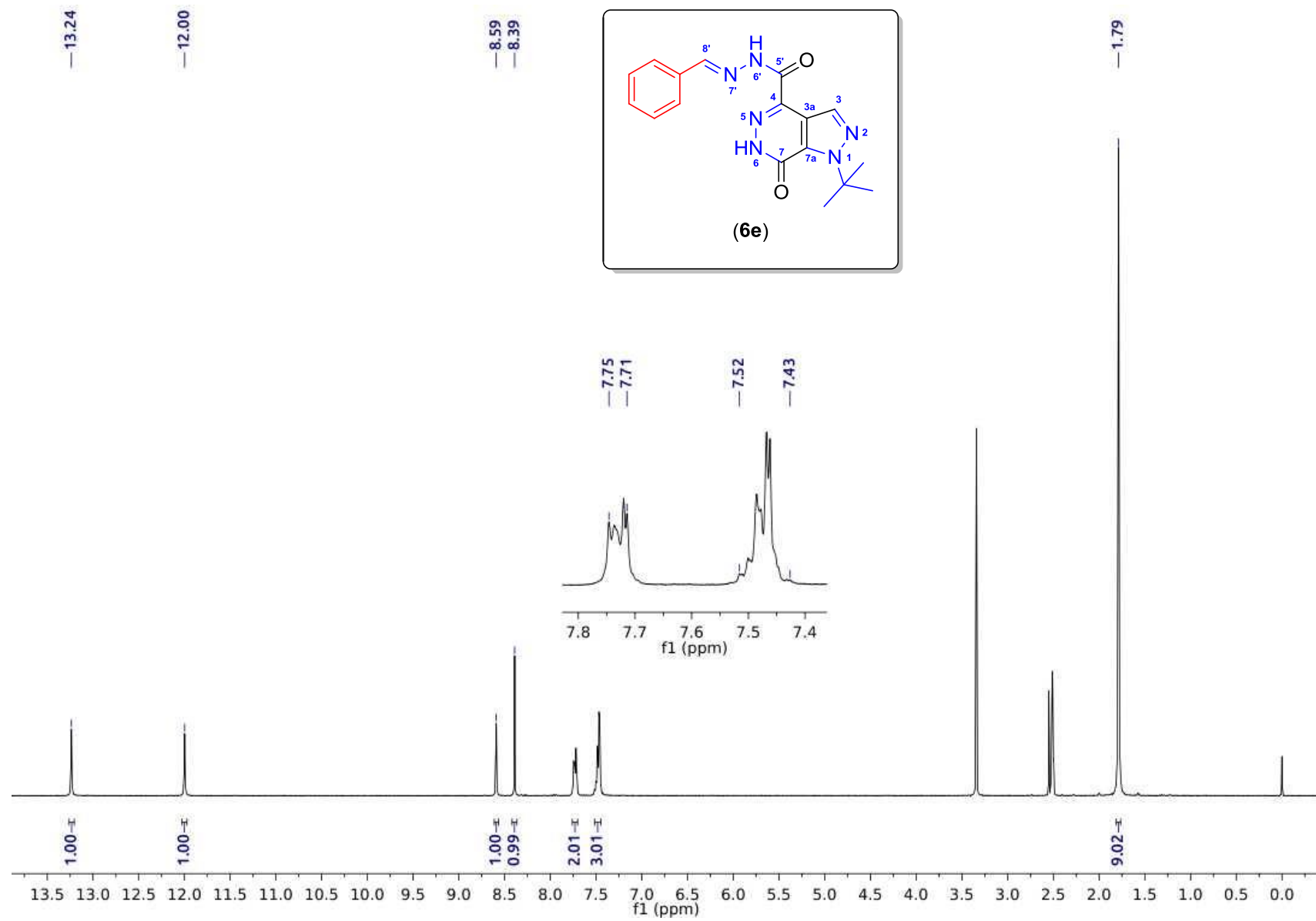
**Figure S16.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **5i**.



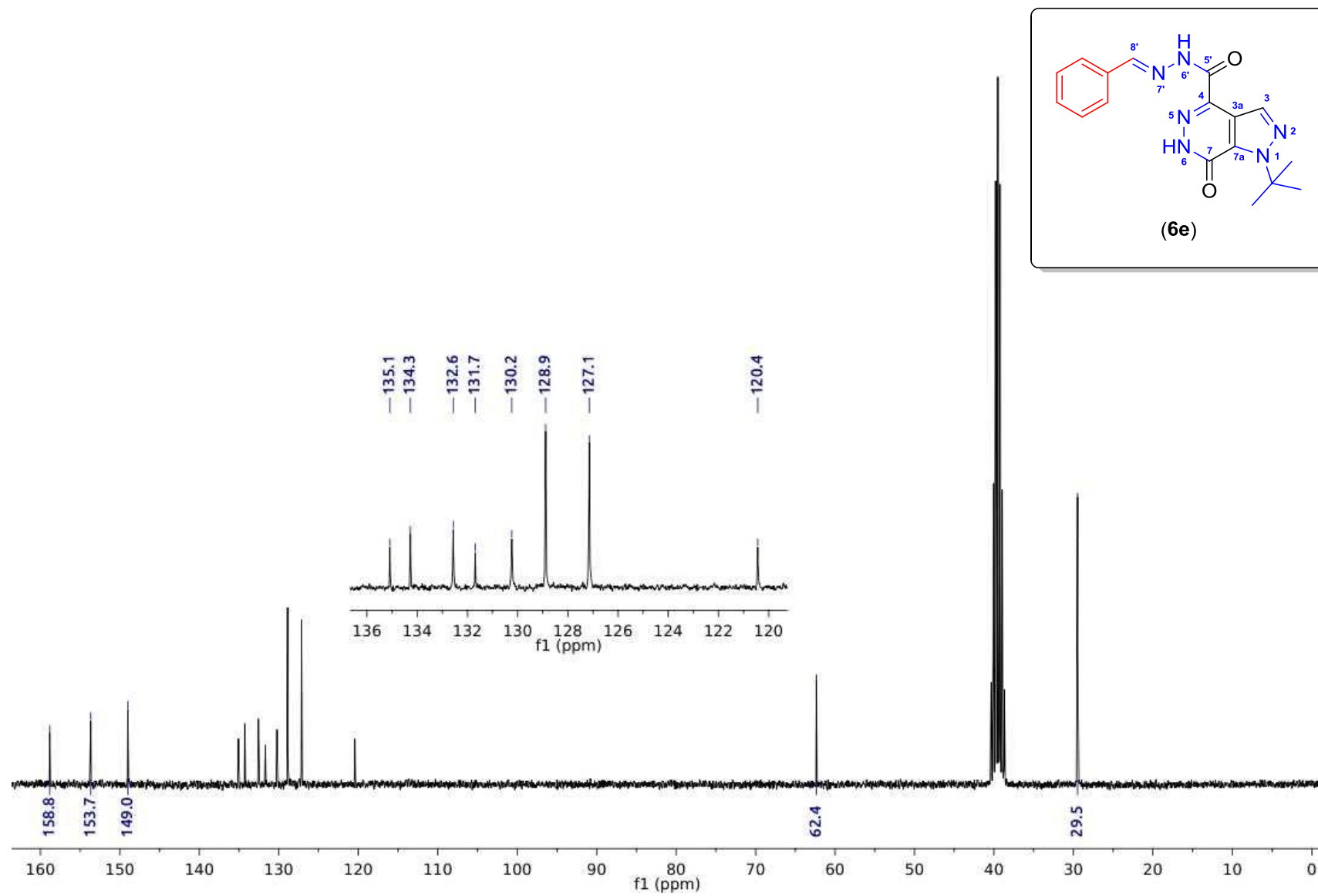
**Figure S17.**  $^1\text{H}$  NMR spectrum (300.06 MHz,  $\text{DMSO-}d_6$ ) of **5j**.



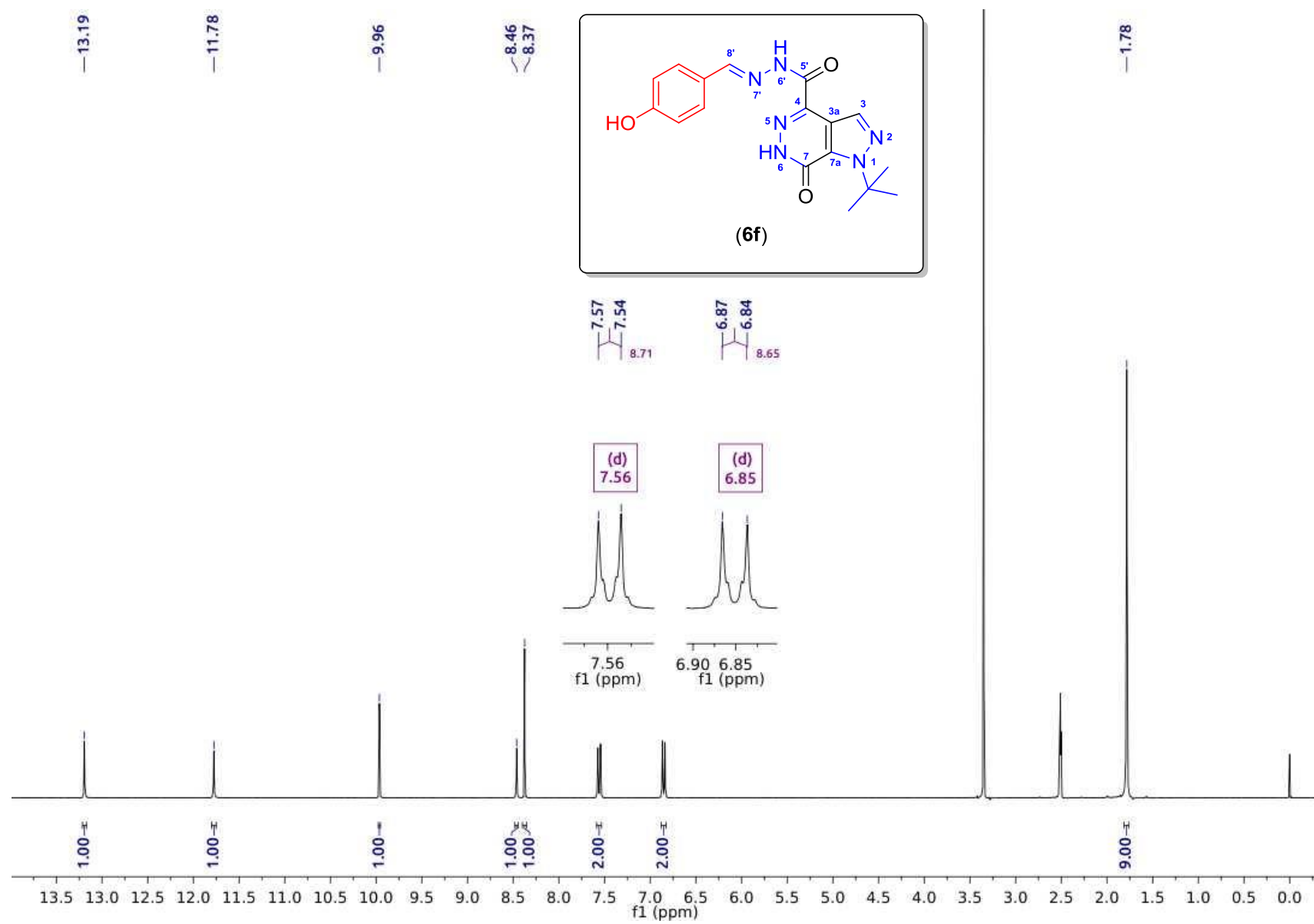
**Figure S18.** <sup>13</sup>C NMR spectrum (75.46 MHz, DMSO-*d*<sub>6</sub>) of **5j**.



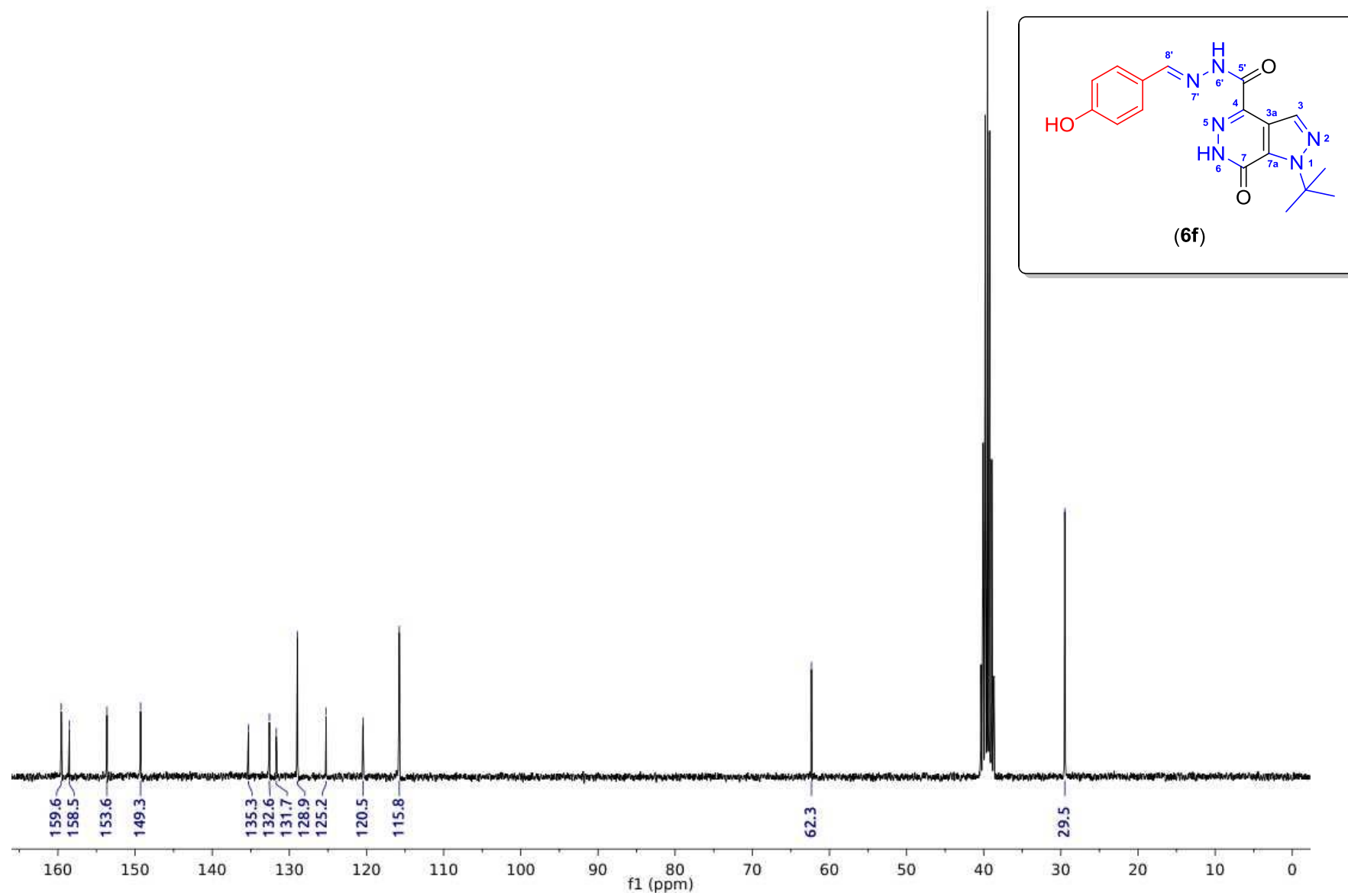
**Figure S19.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **6e**.



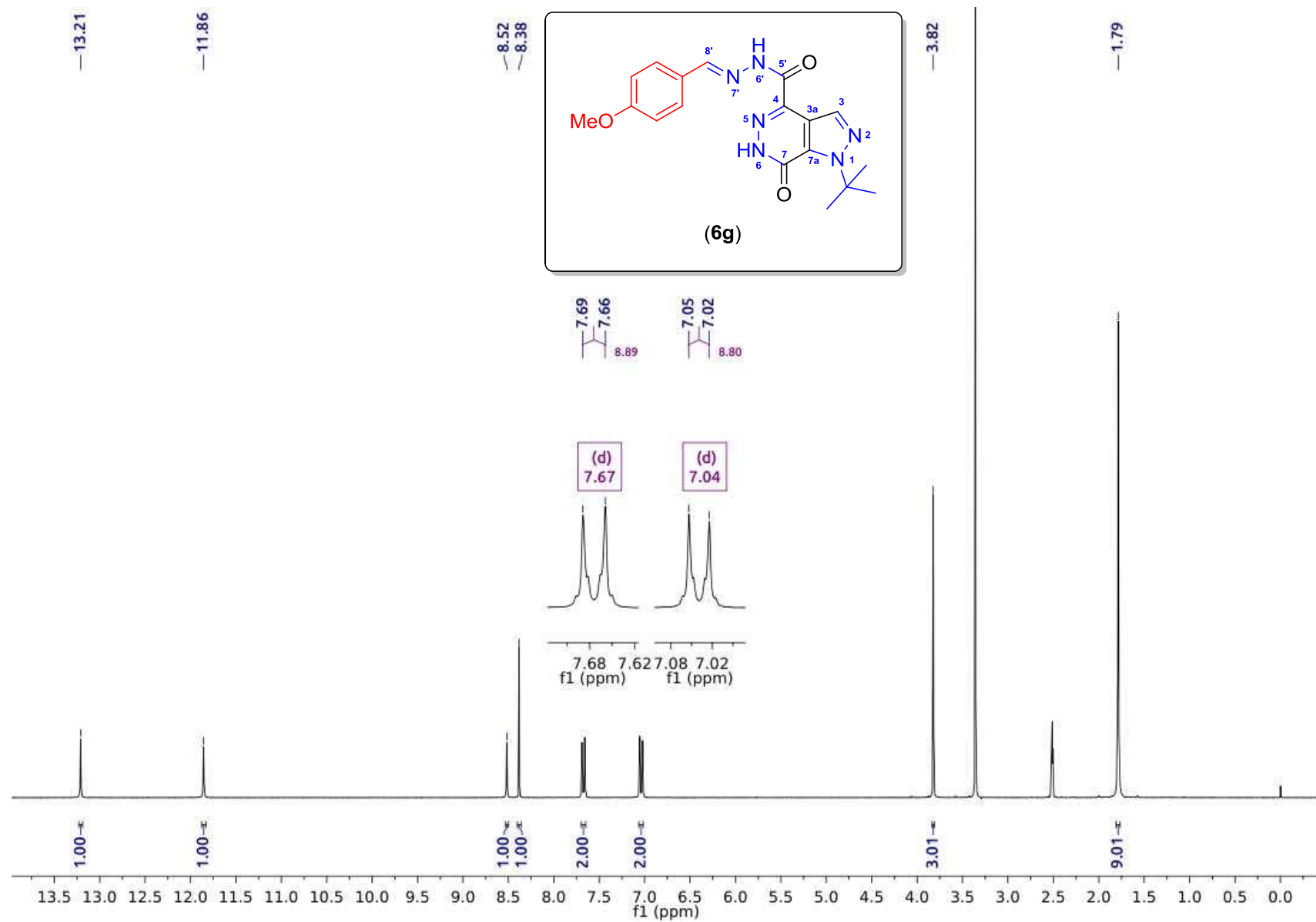
**Figure S20.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **6e**.



**Figure S21.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **6f**.

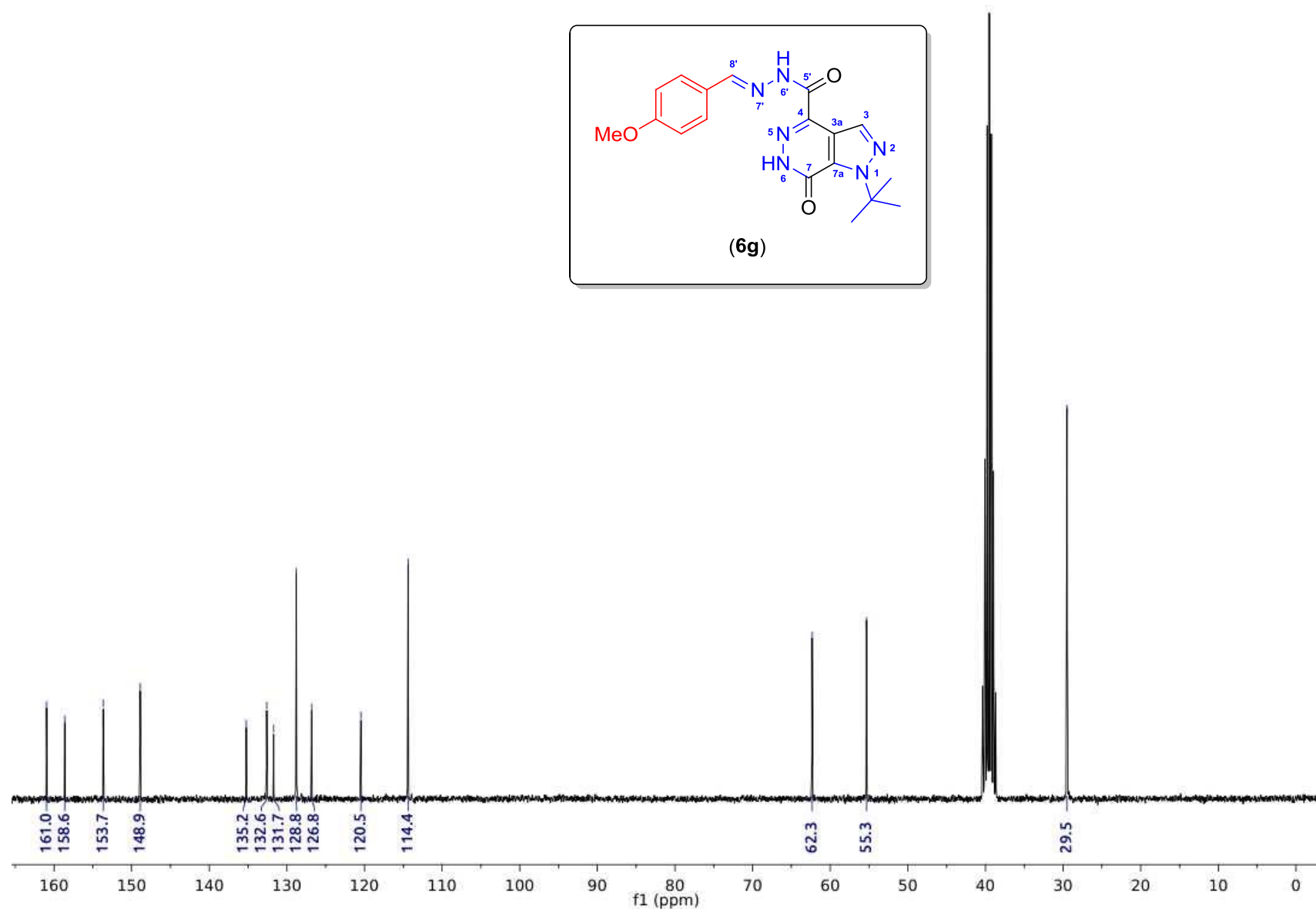
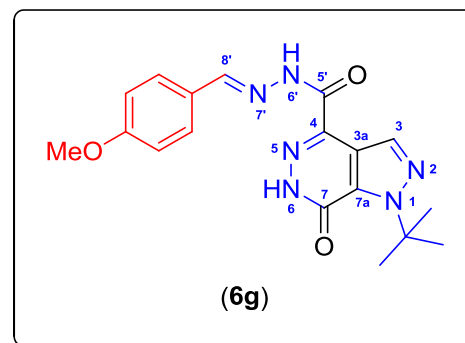


**Figure S22.** <sup>13</sup>C NMR spectrum (75.46 MHz, DMSO-*d*<sub>6</sub>) of **6f**.

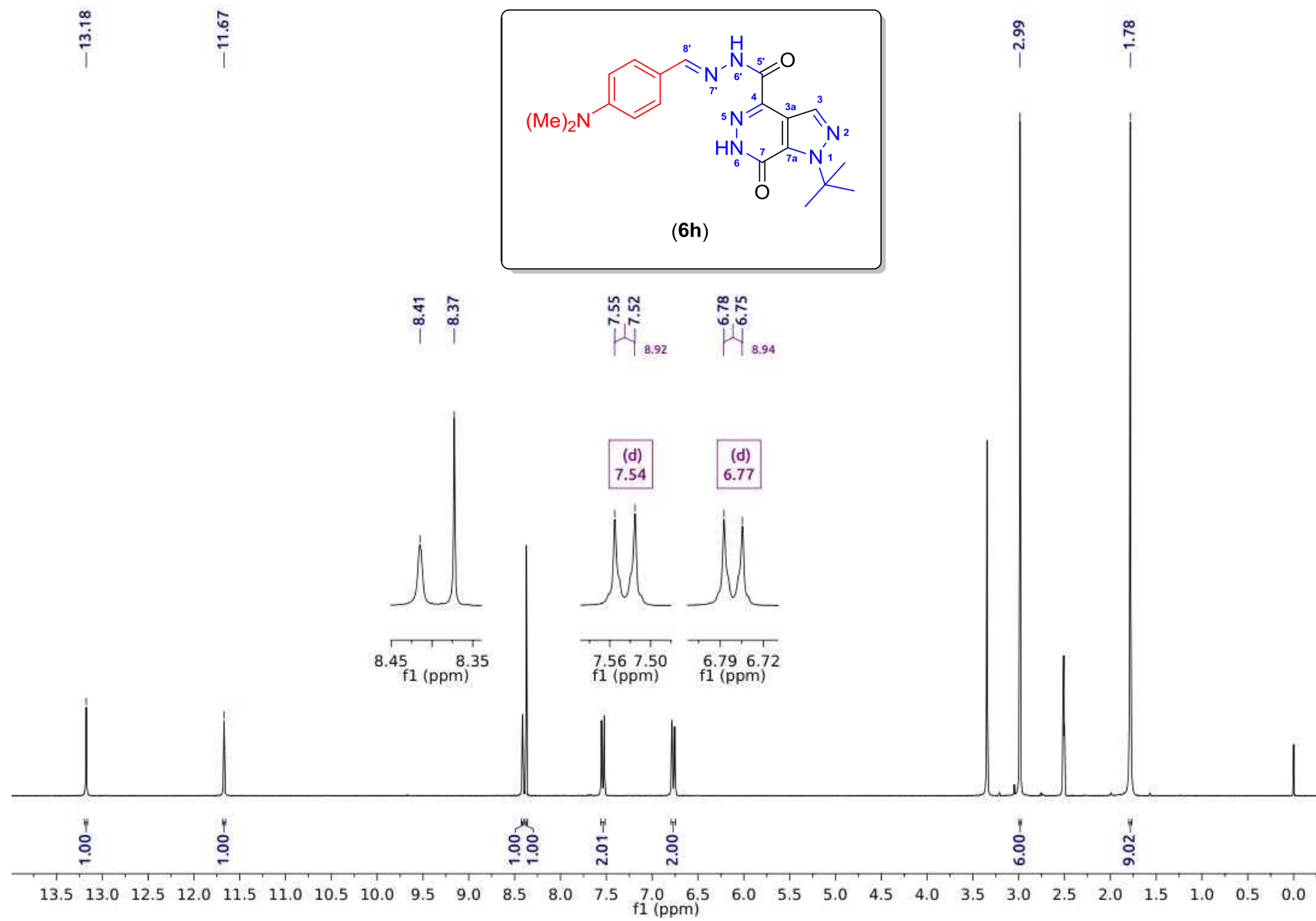


**Figure S23.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **6g**.

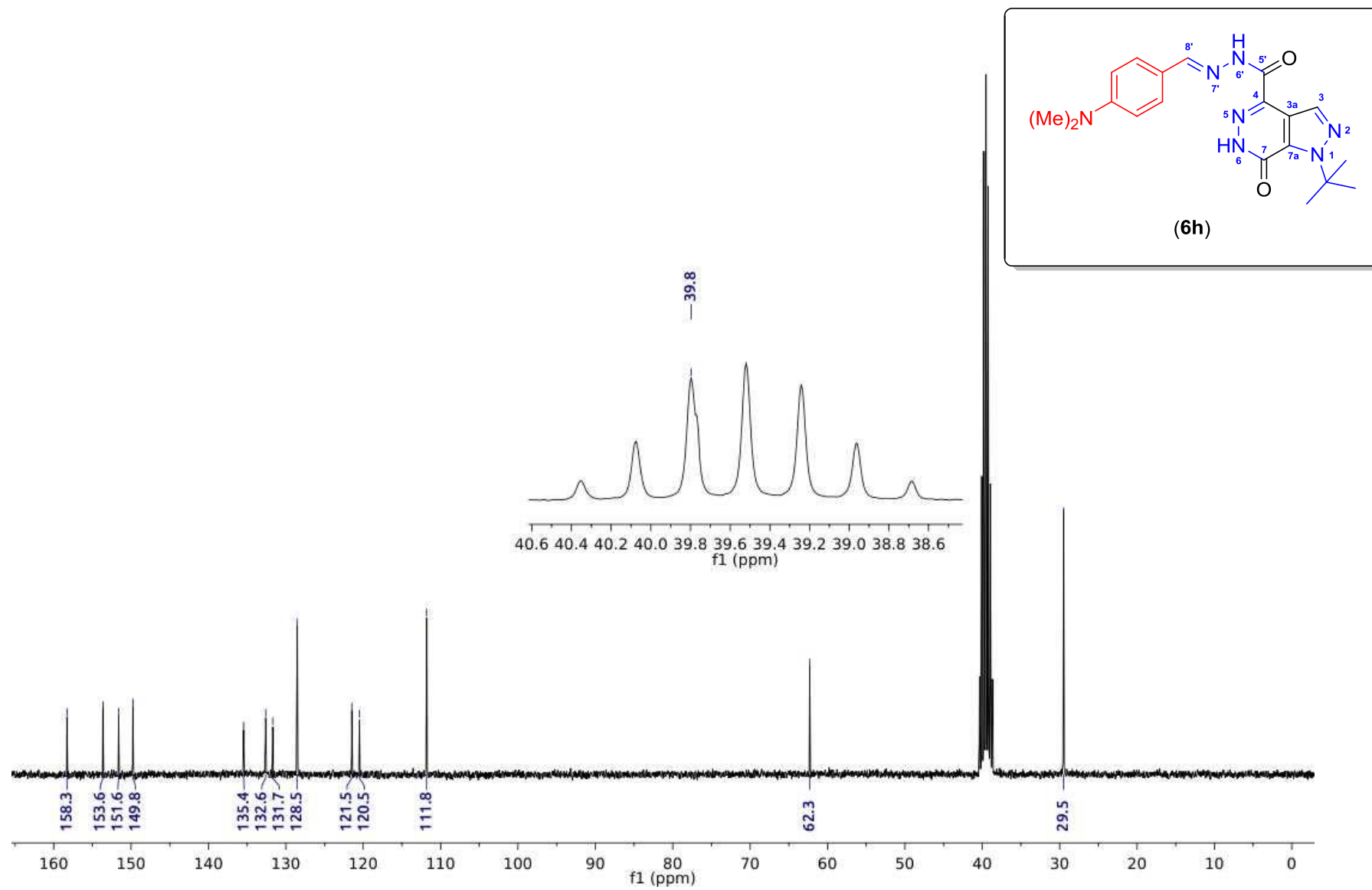




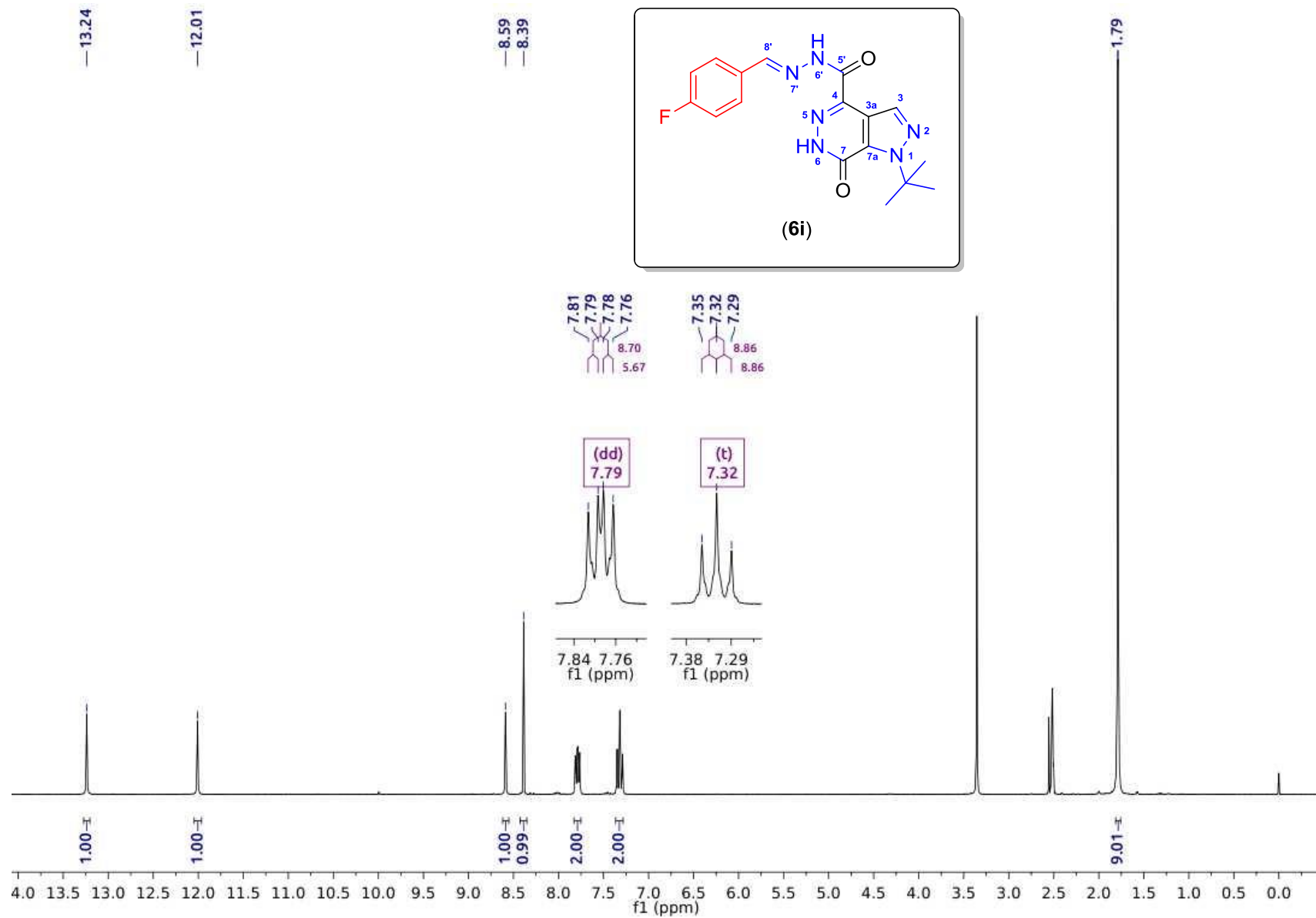
**Figure S24.** <sup>13</sup>C NMR spectrum (75.46 MHz, DMSO-*d*<sub>6</sub>) of **6g**.



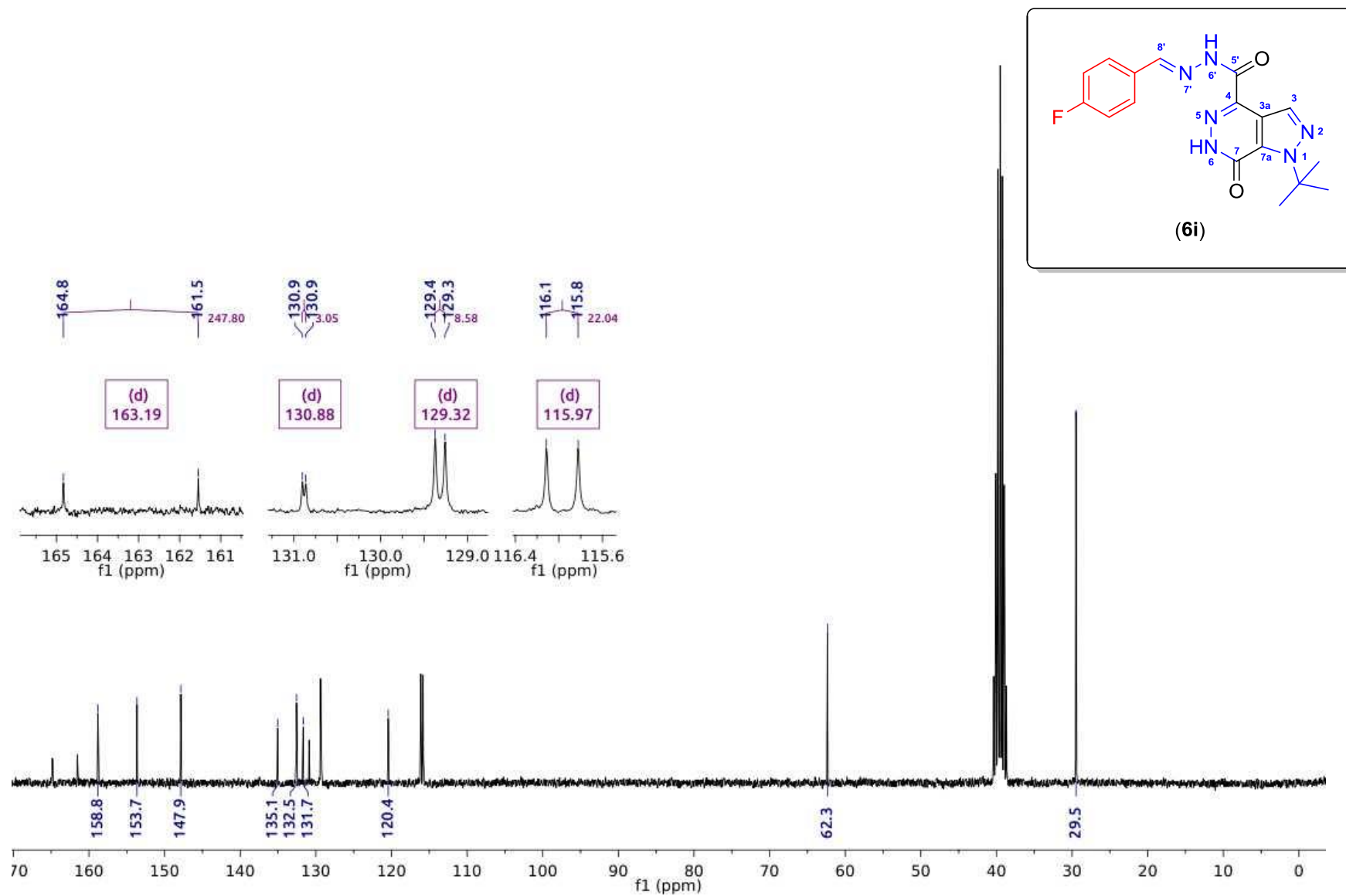
**Figure S25.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **6h**.



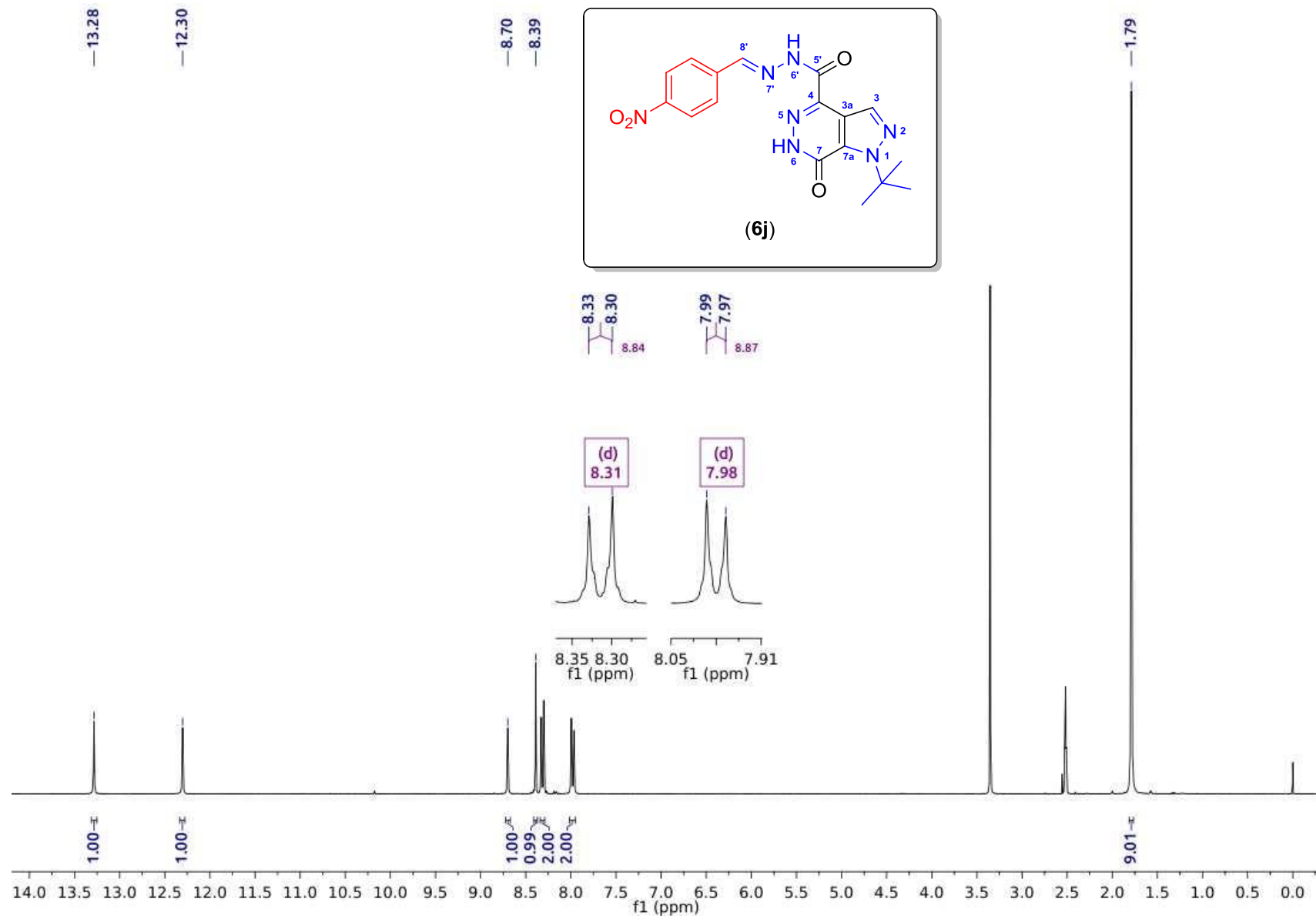
**Figure S26.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **6h**.



**Figure S27.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **6i**.



**Figure S28.** <sup>13</sup>C NMR spectrum (75.46 MHz, DMSO-*d*<sub>6</sub>) of **6i**.



**Figure S29.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **6j**.

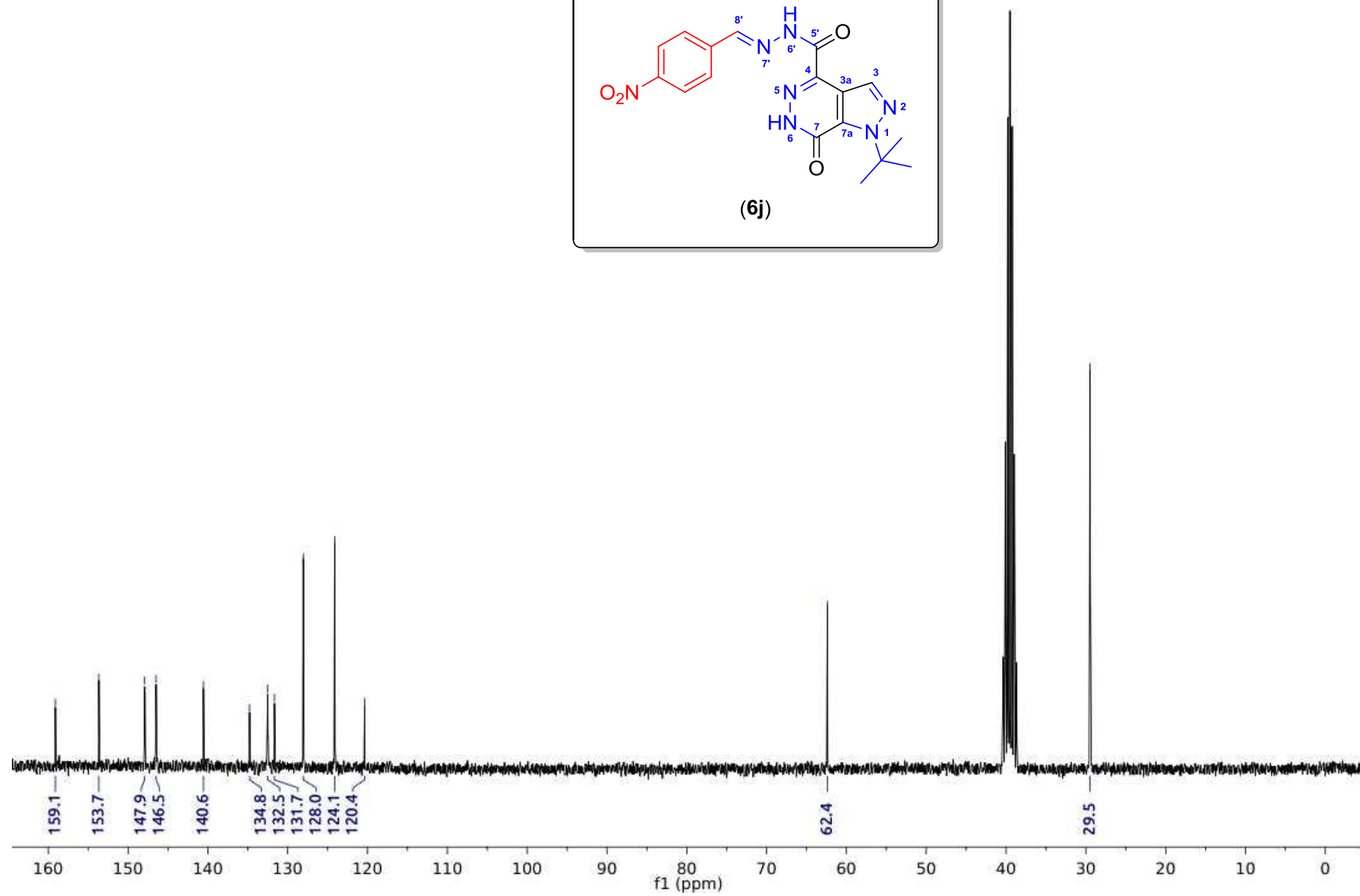
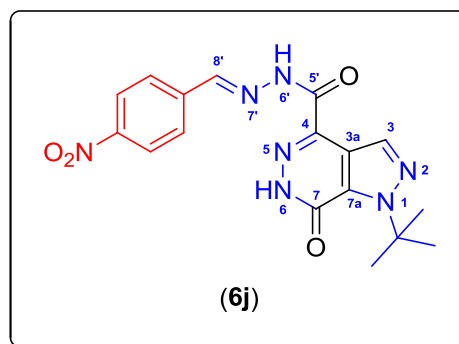
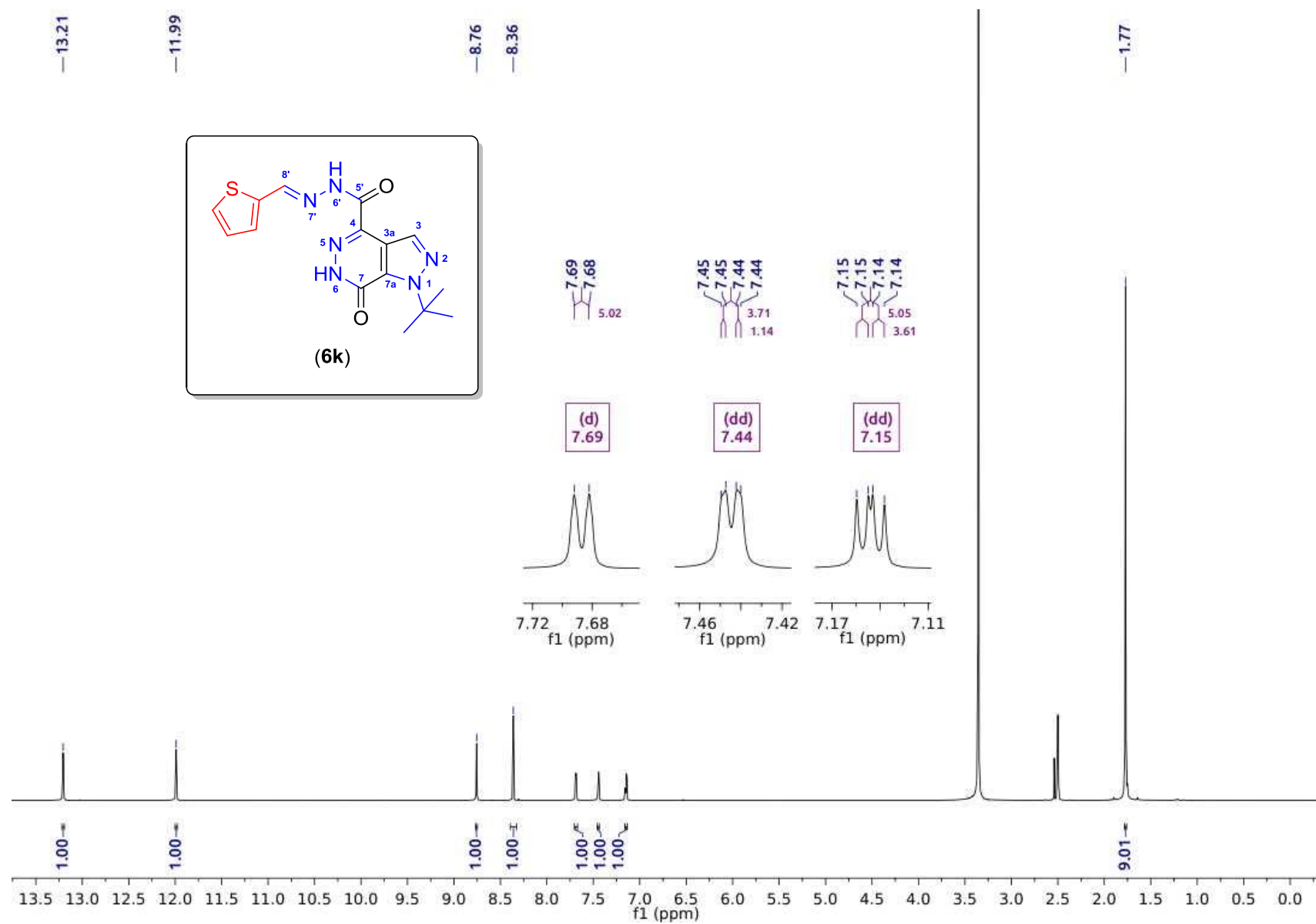


Figure S30.  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **6j**.



**Figure S31.**  $^1\text{H}$  NMR spectrum (500.13 MHz,  $\text{DMSO-}d_6$ ) of **(6k)**.



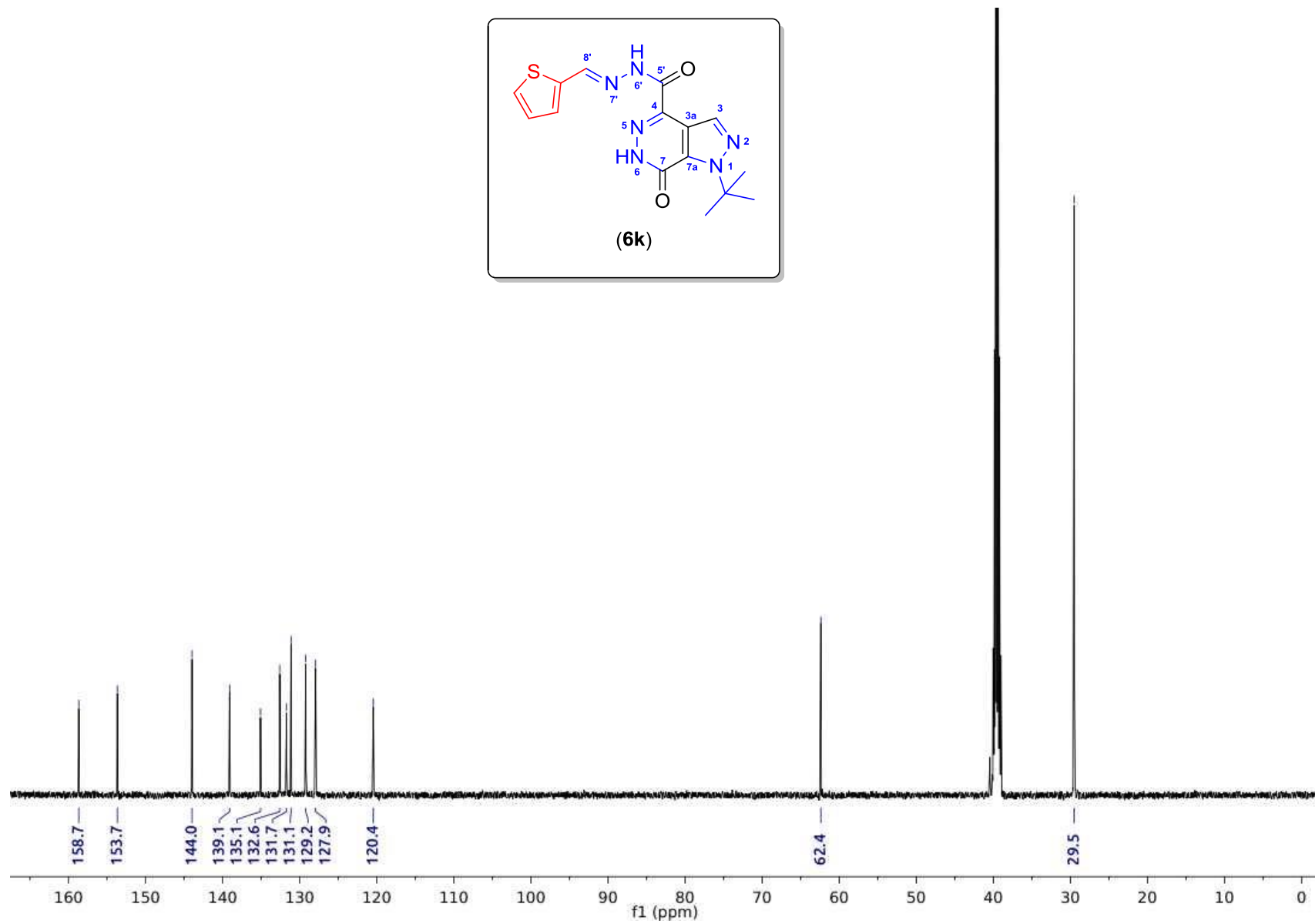
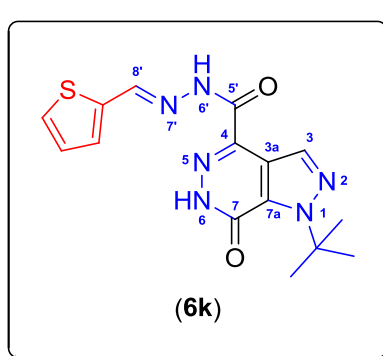
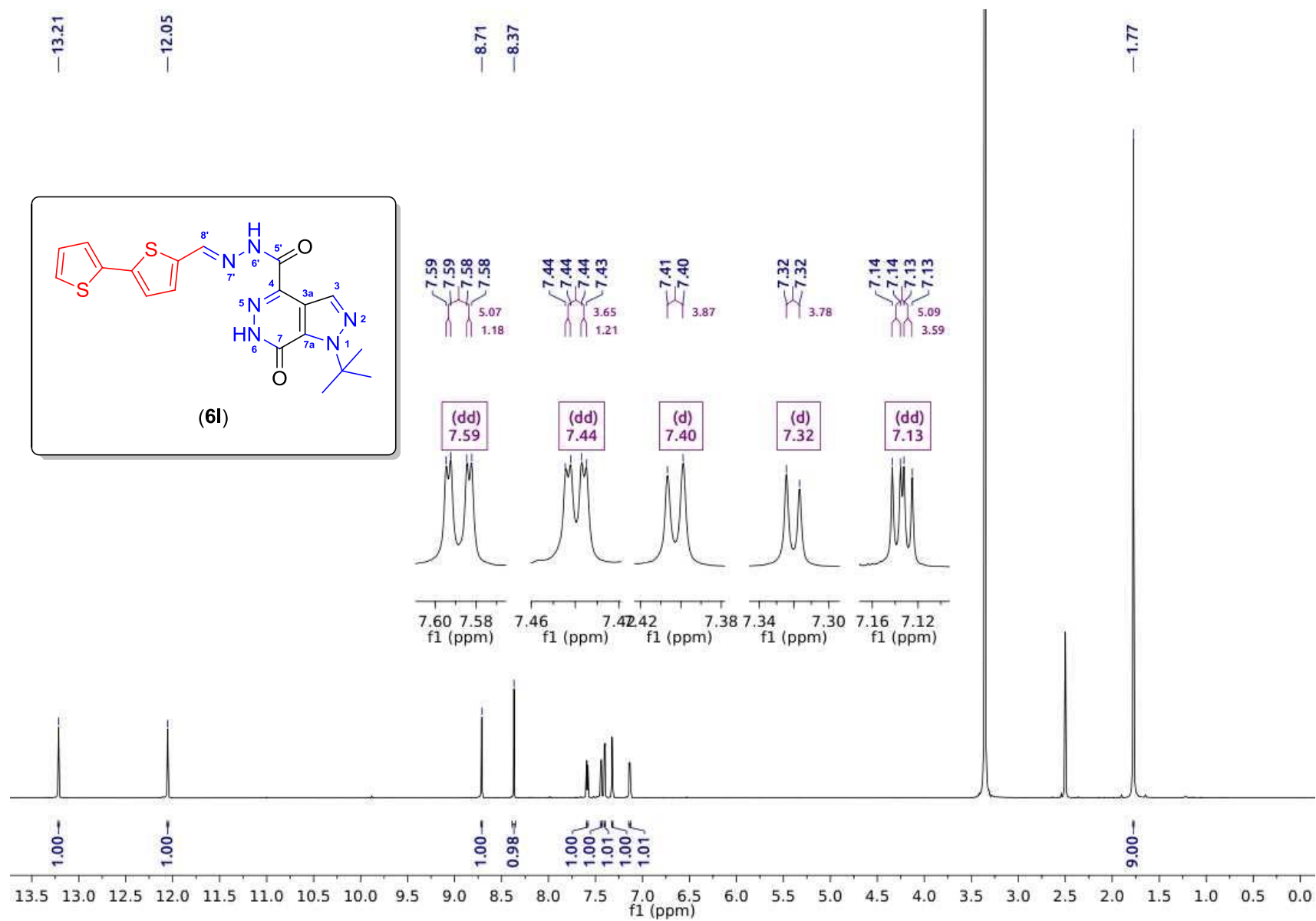


Figure S32.  $^{13}\text{C}$  NMR spectrum (125.77 MHz,  $\text{DMSO-}d_6$ ) of **6k**.



**Figure S33.** <sup>1</sup>H NMR spectrum (500.13 MHz, DMSO-*d*<sub>6</sub>) of **6l**.

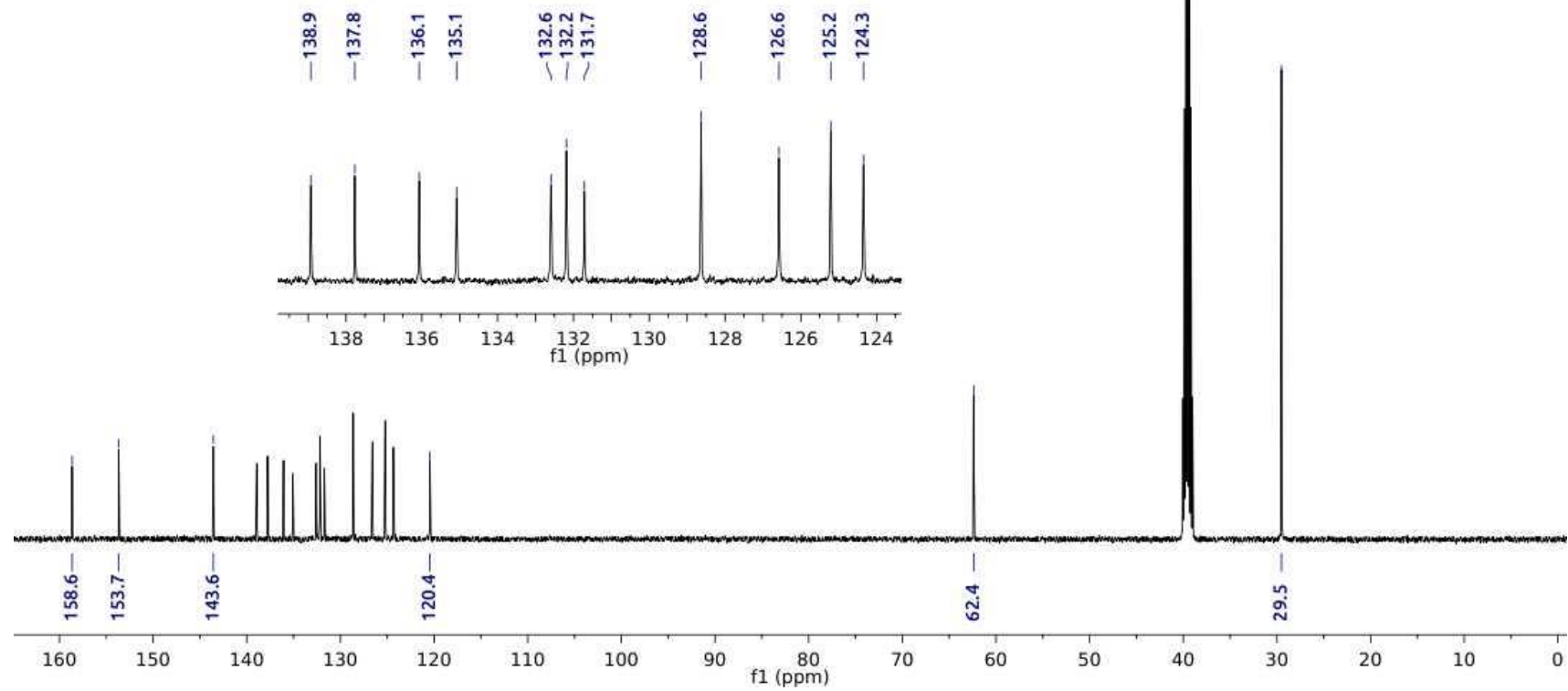
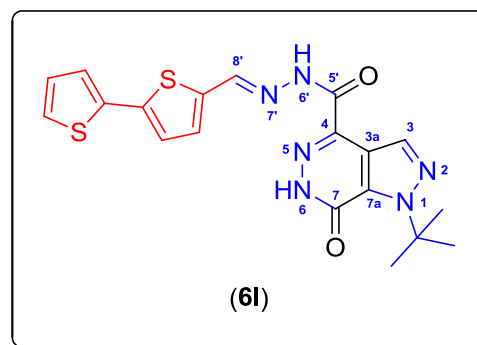
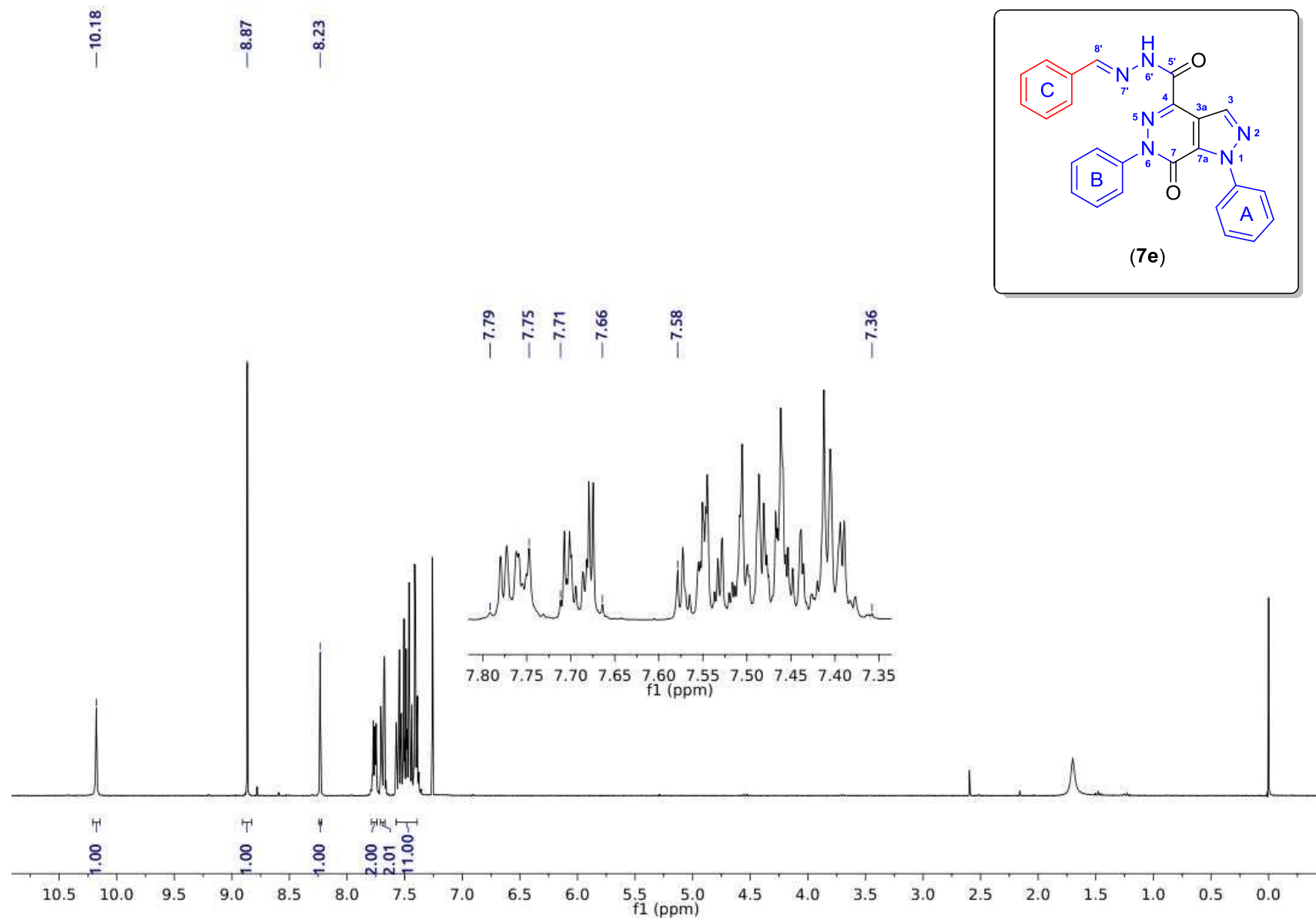
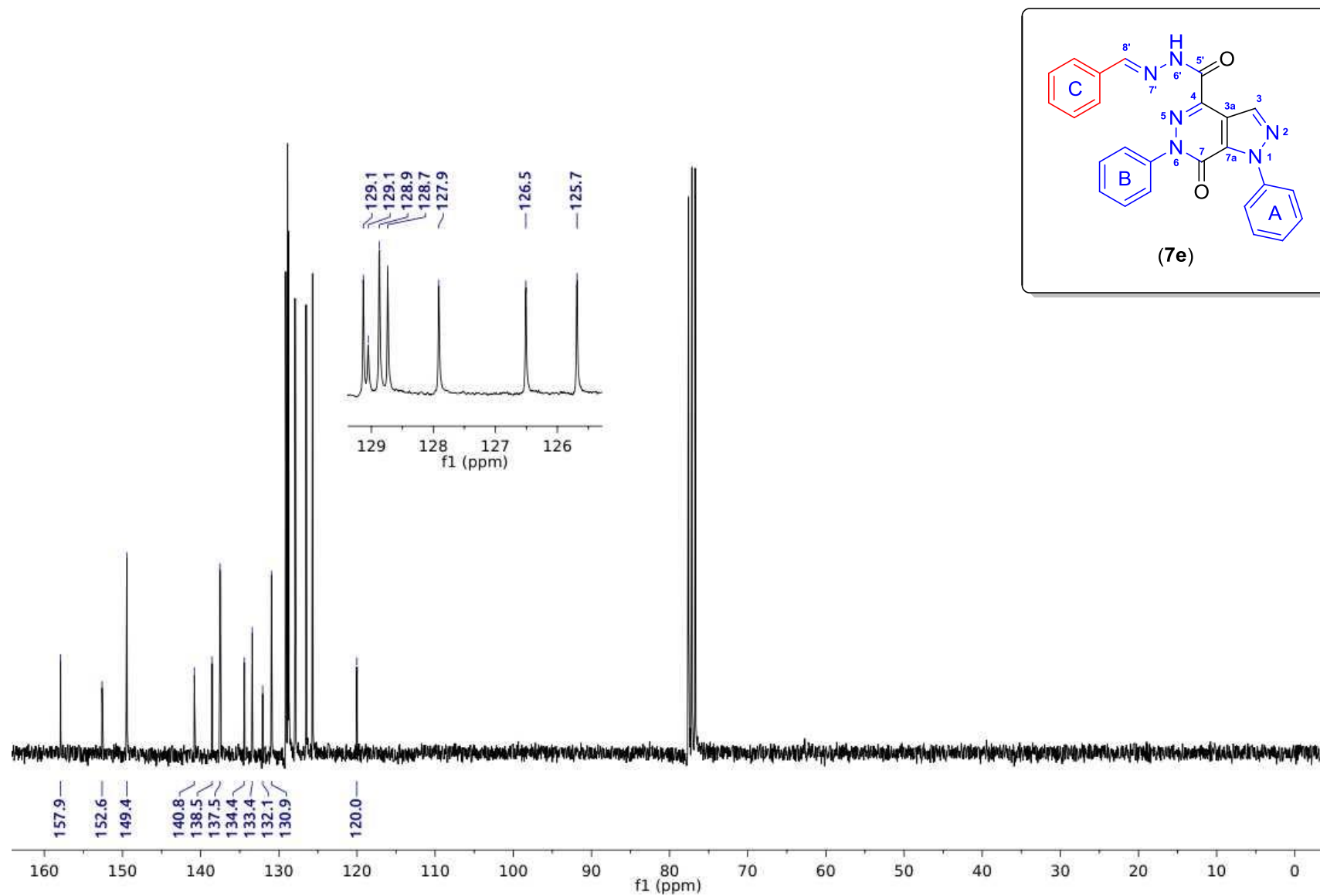


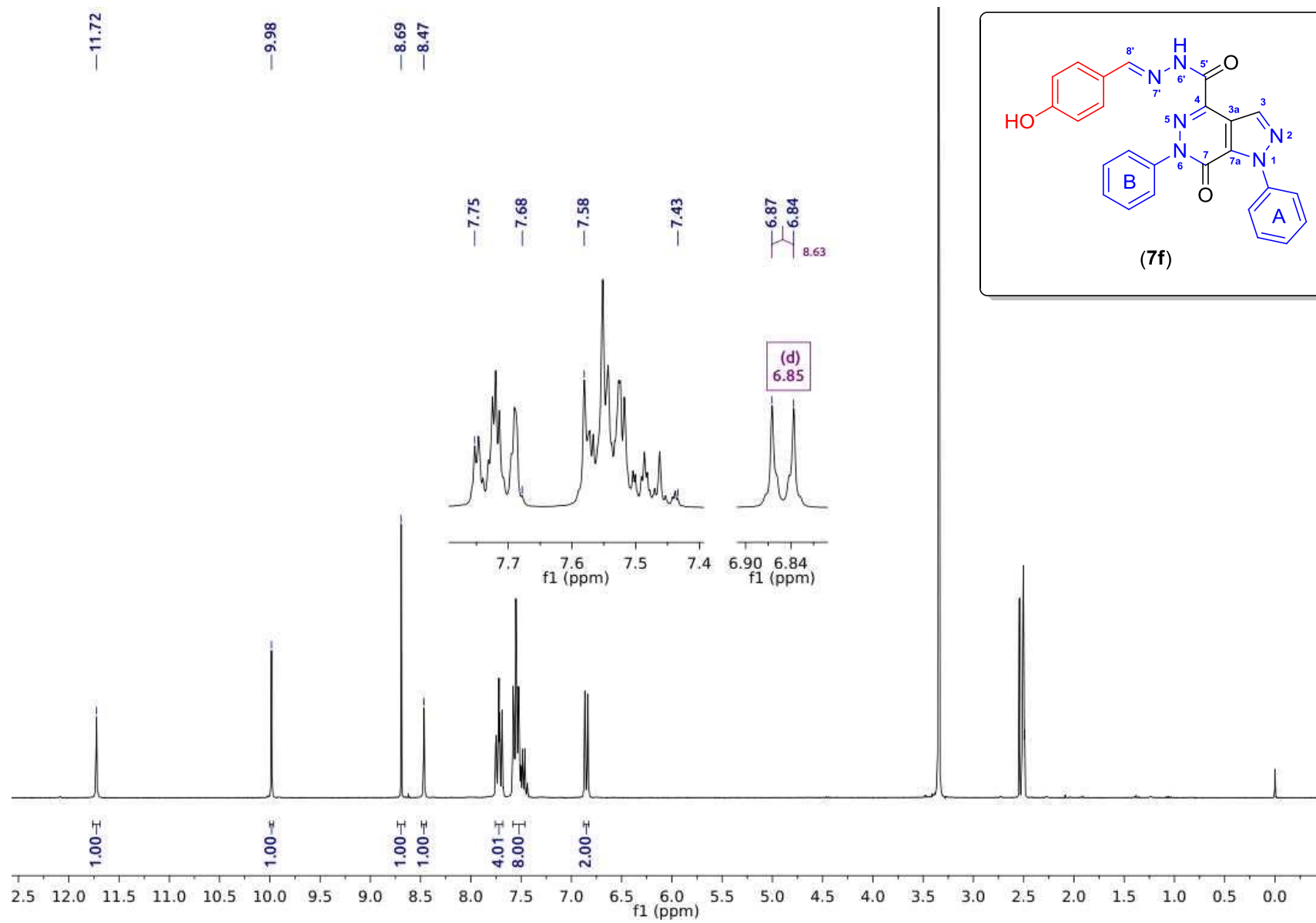
Figure S34.  $^{13}\text{C}$  NMR spectrum (125.77 MHz,  $\text{DMSO-}d_6$ ) of **6l**.



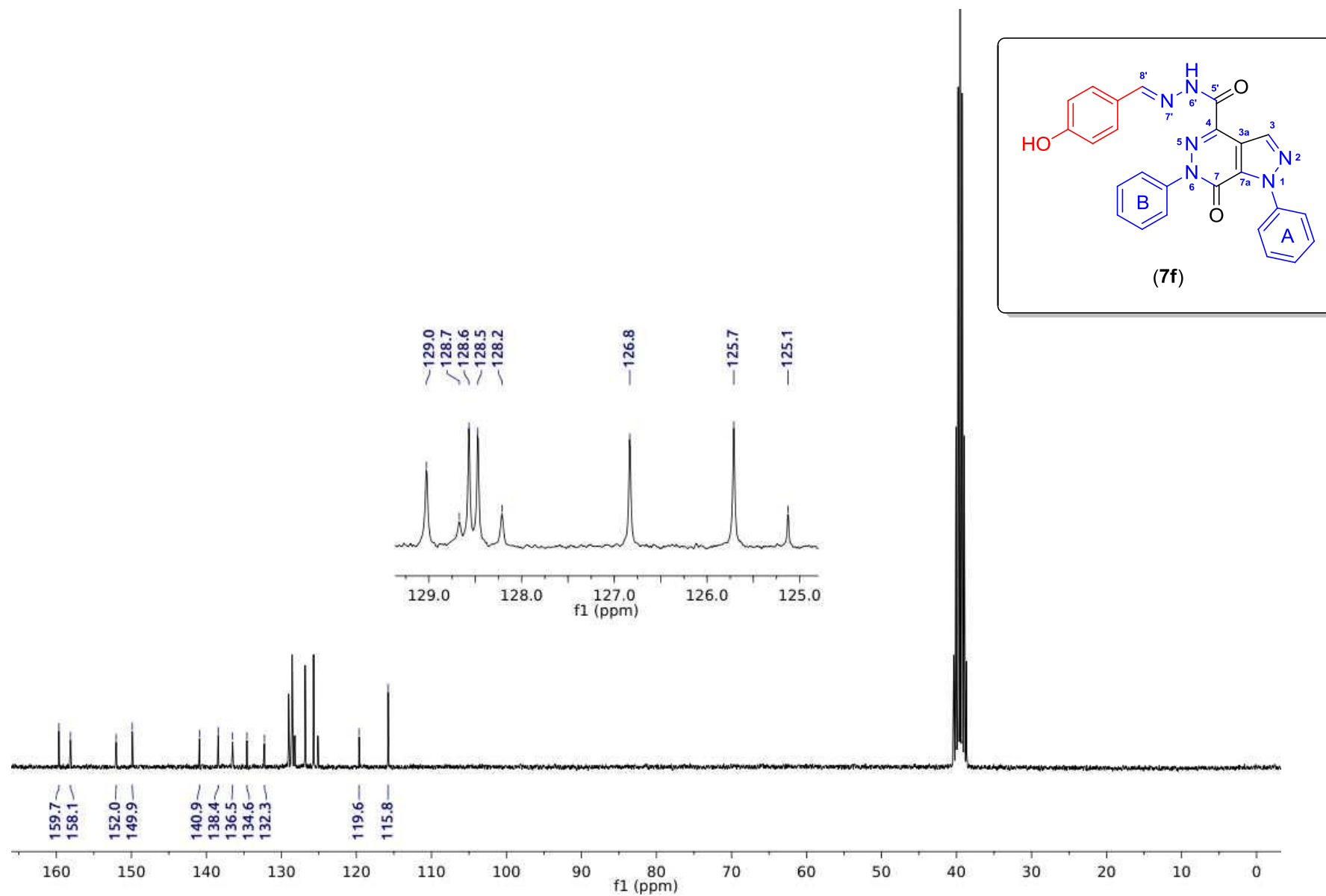
**Figure S35.**  $^1\text{H}$  NMR spectrum (300.06 MHz,  $\text{CDCl}_3$ ) of **7e**.



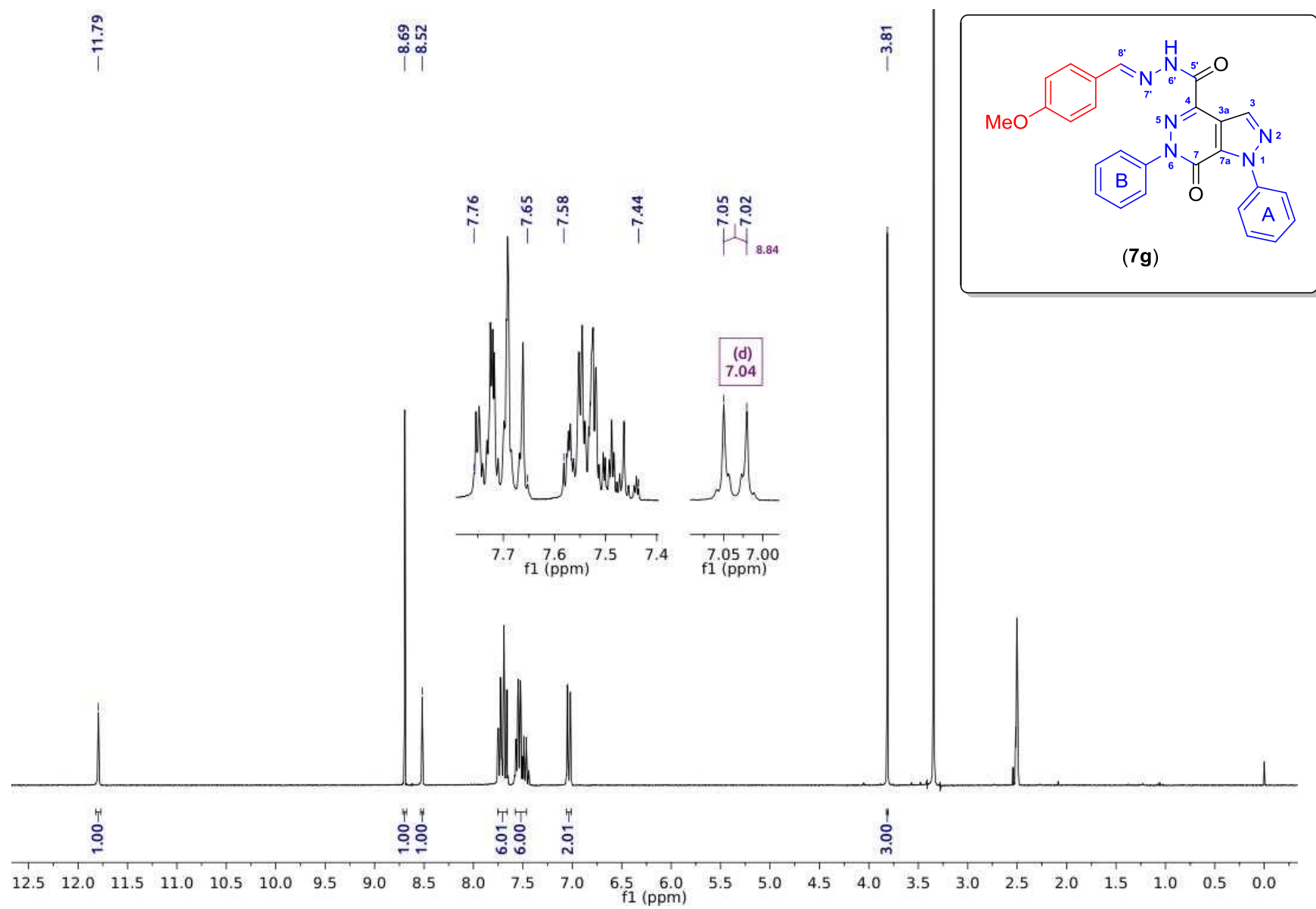
**Figure S36.** <sup>13</sup>C NMR spectrum (75.46 MHz, CDCl<sub>3</sub>) of **7e**.



**Figure S37.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **7f**.

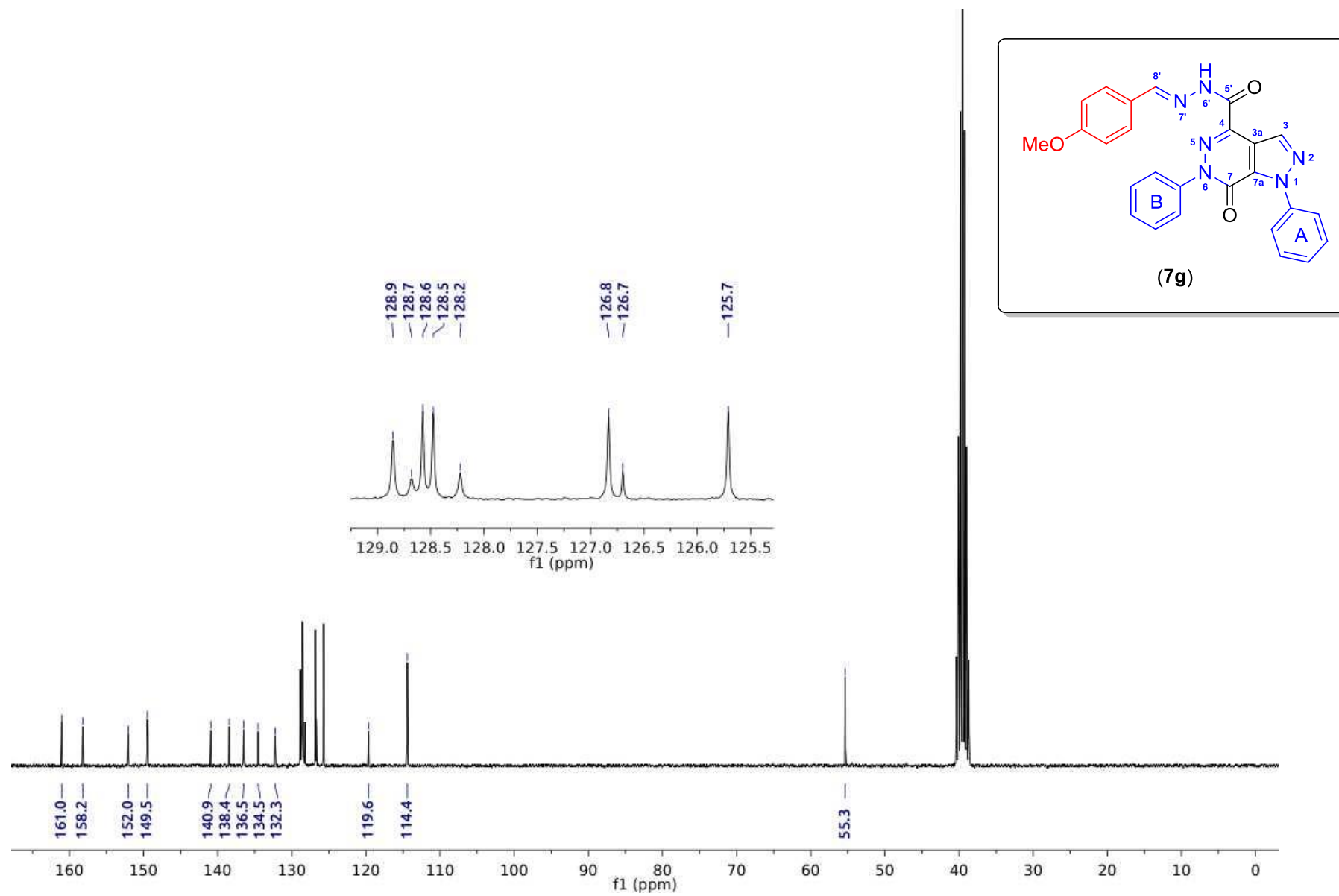


**Figure S38.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **7f**.

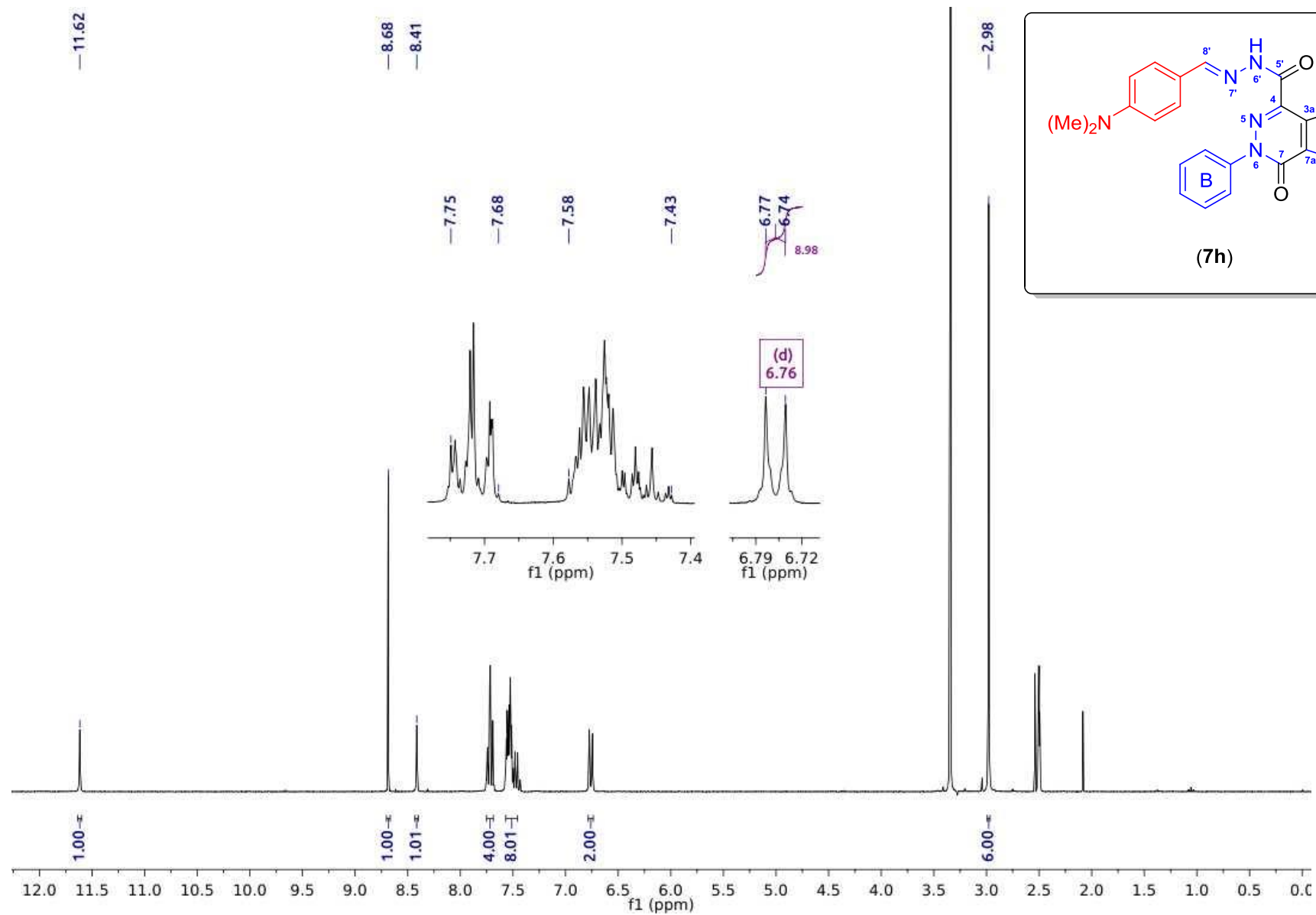


**Figure S39.**  $^1\text{H}$  NMR spectrum (300.06 MHz,  $\text{DMSO-}d_6$ ) of **7g**.

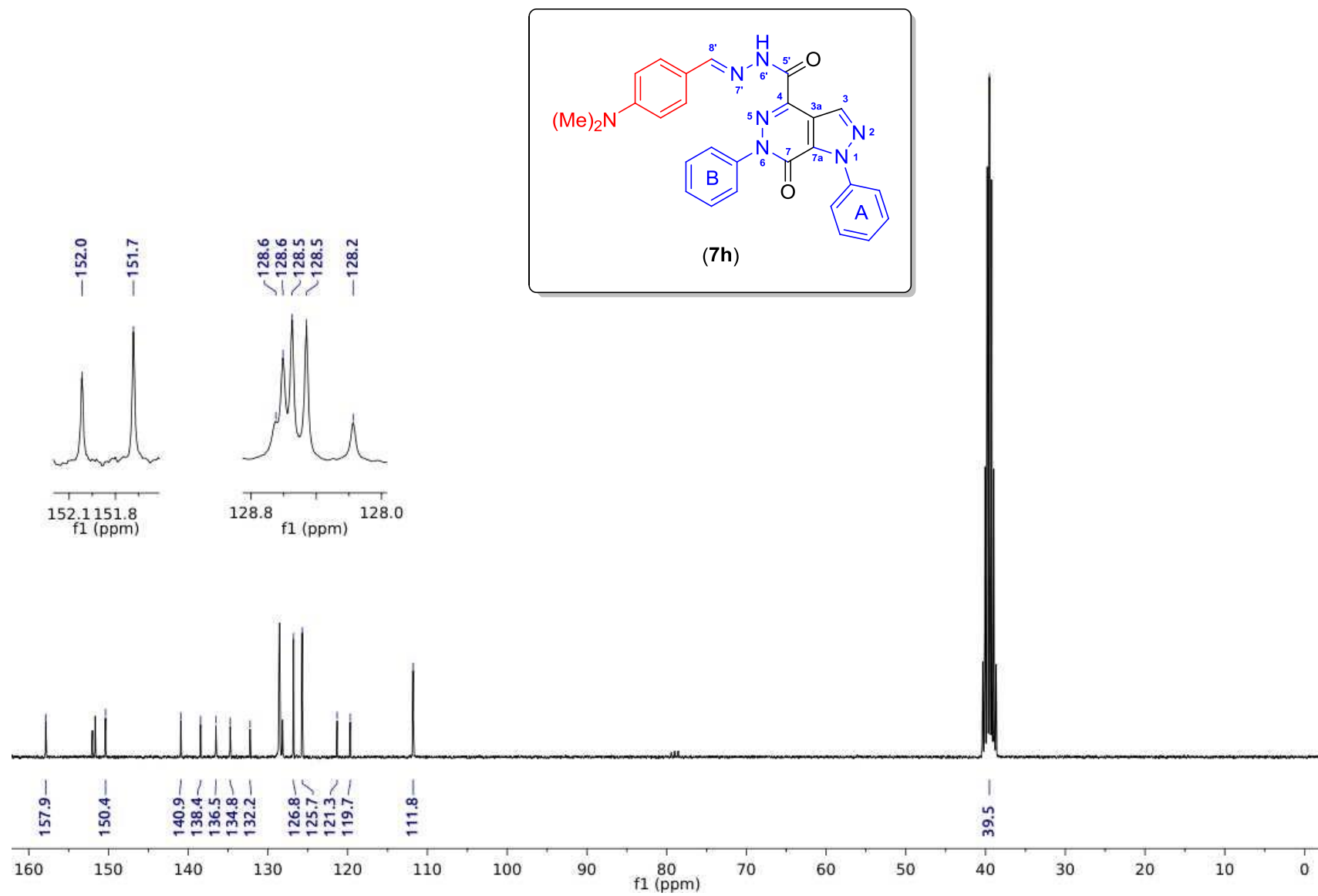




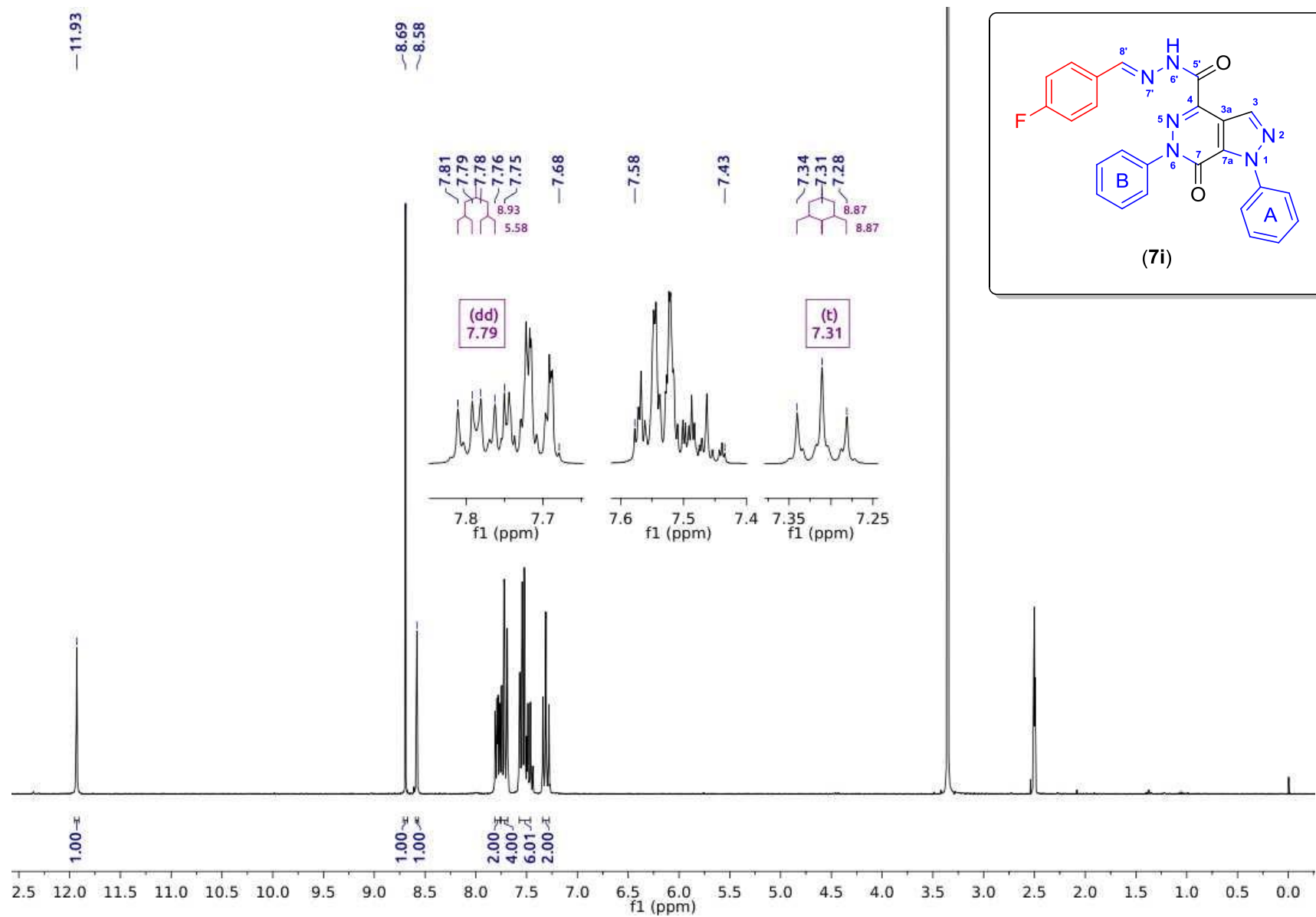
**Figure S40.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **7g**.



**Figure S41.**  $^1\text{H}$  NMR spectrum (300.06 MHz,  $\text{DMSO-}d_6$ ) of **7h**.



**Figure S42.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **7h**.



**Figure S43.**  $^1\text{H}$  NMR spectrum (300.06 MHz,  $\text{DMSO-}d_6$ ) of **7i**.

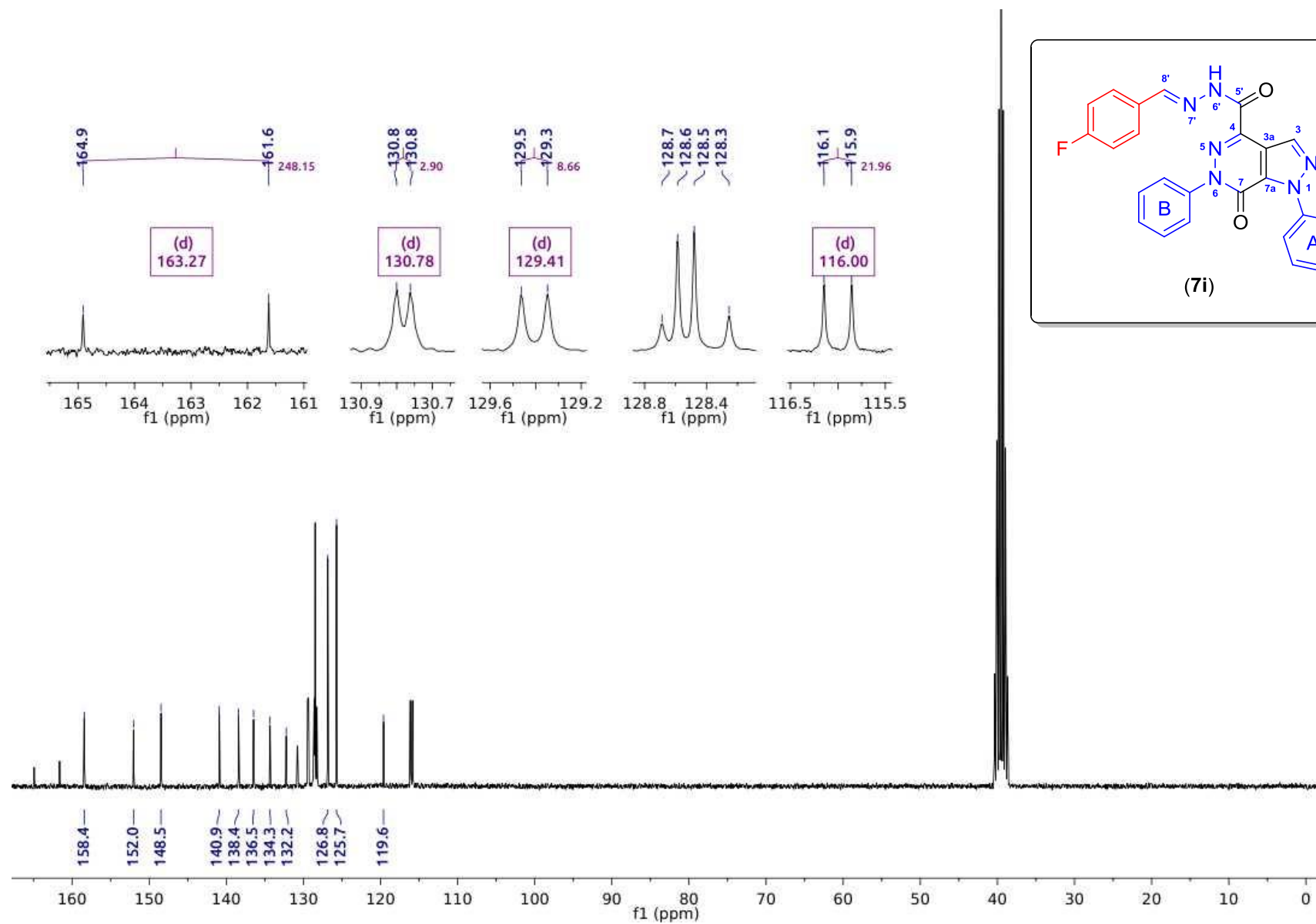
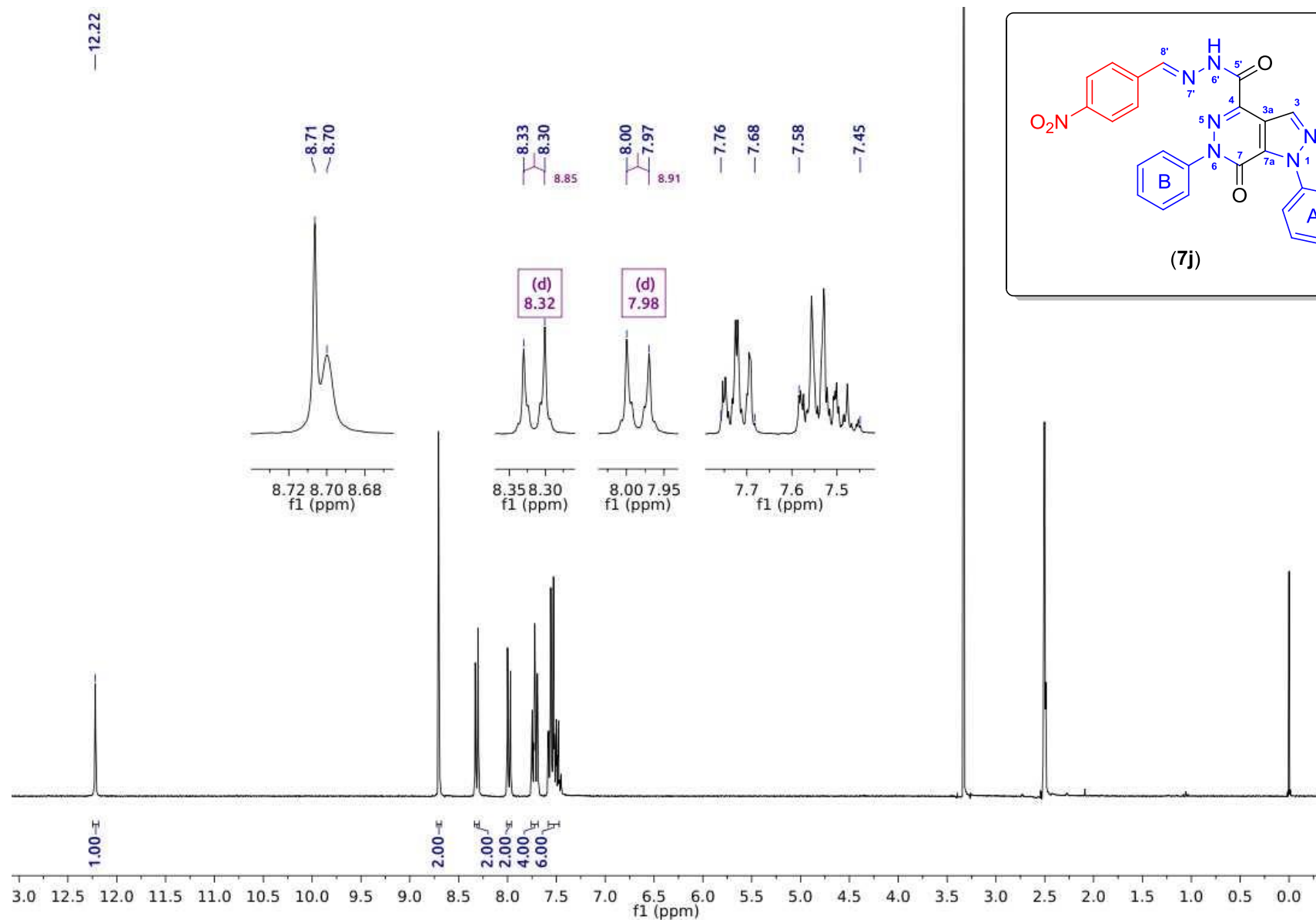


Figure S44.  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO}-d_6$ ) of **7i**.



**Figure S45.** <sup>1</sup>H NMR spectrum (300.06 MHz, DMSO-*d*<sub>6</sub>) of **7j**.

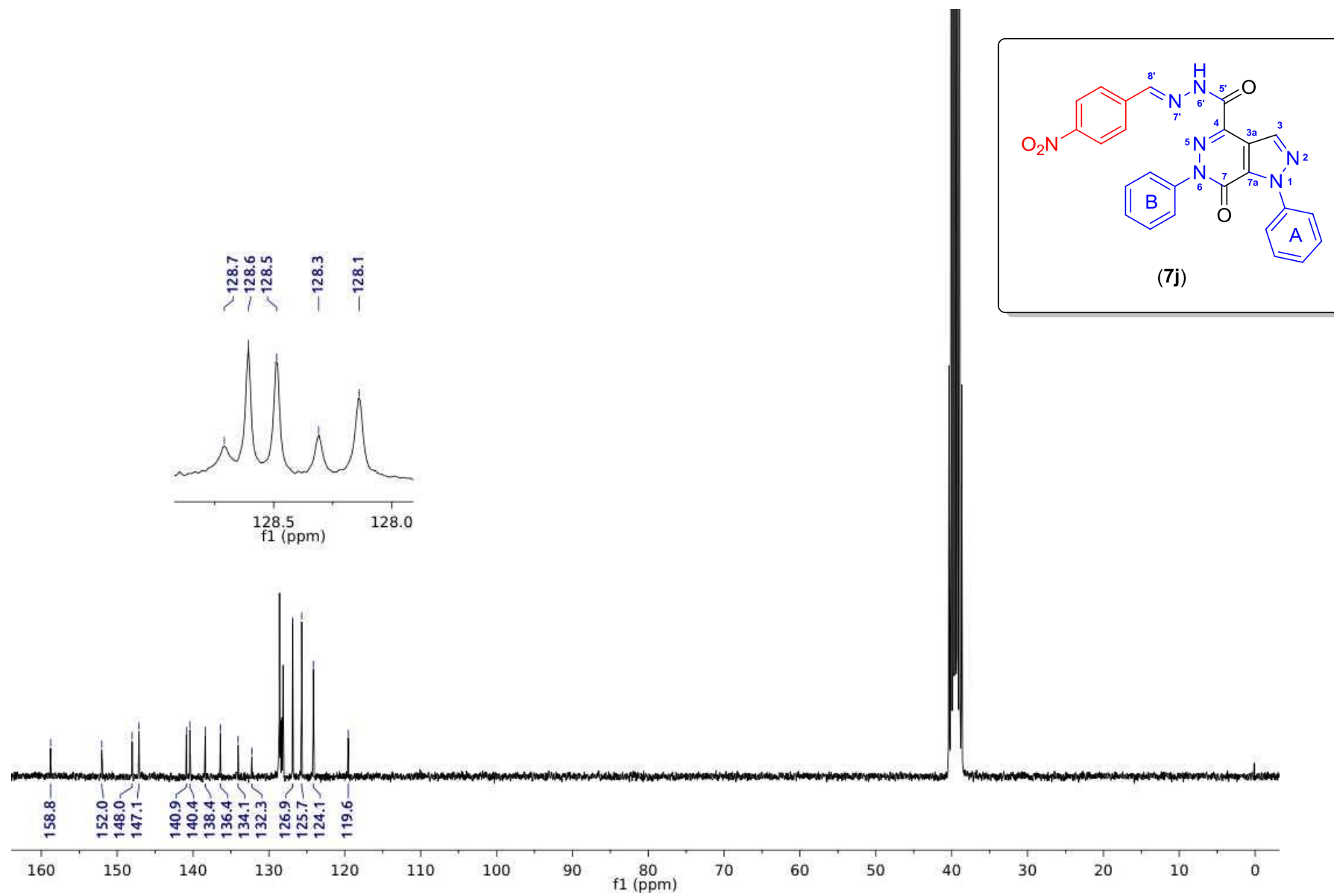
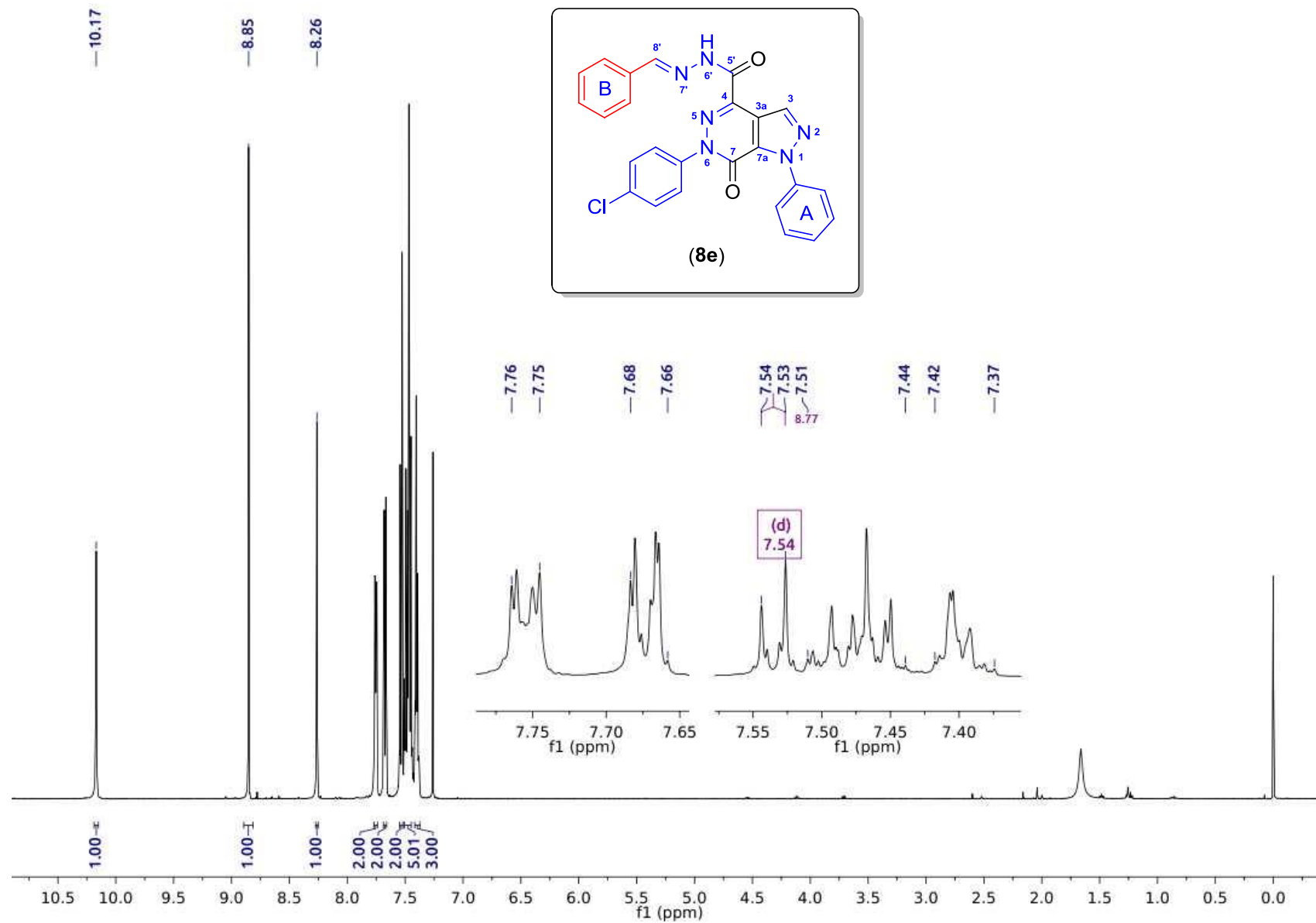


Figure S46.  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **7j**.



**Figure S47.** <sup>1</sup>H NMR spectrum (500.13 MHz, CDCl<sub>3</sub>) of **8e**.



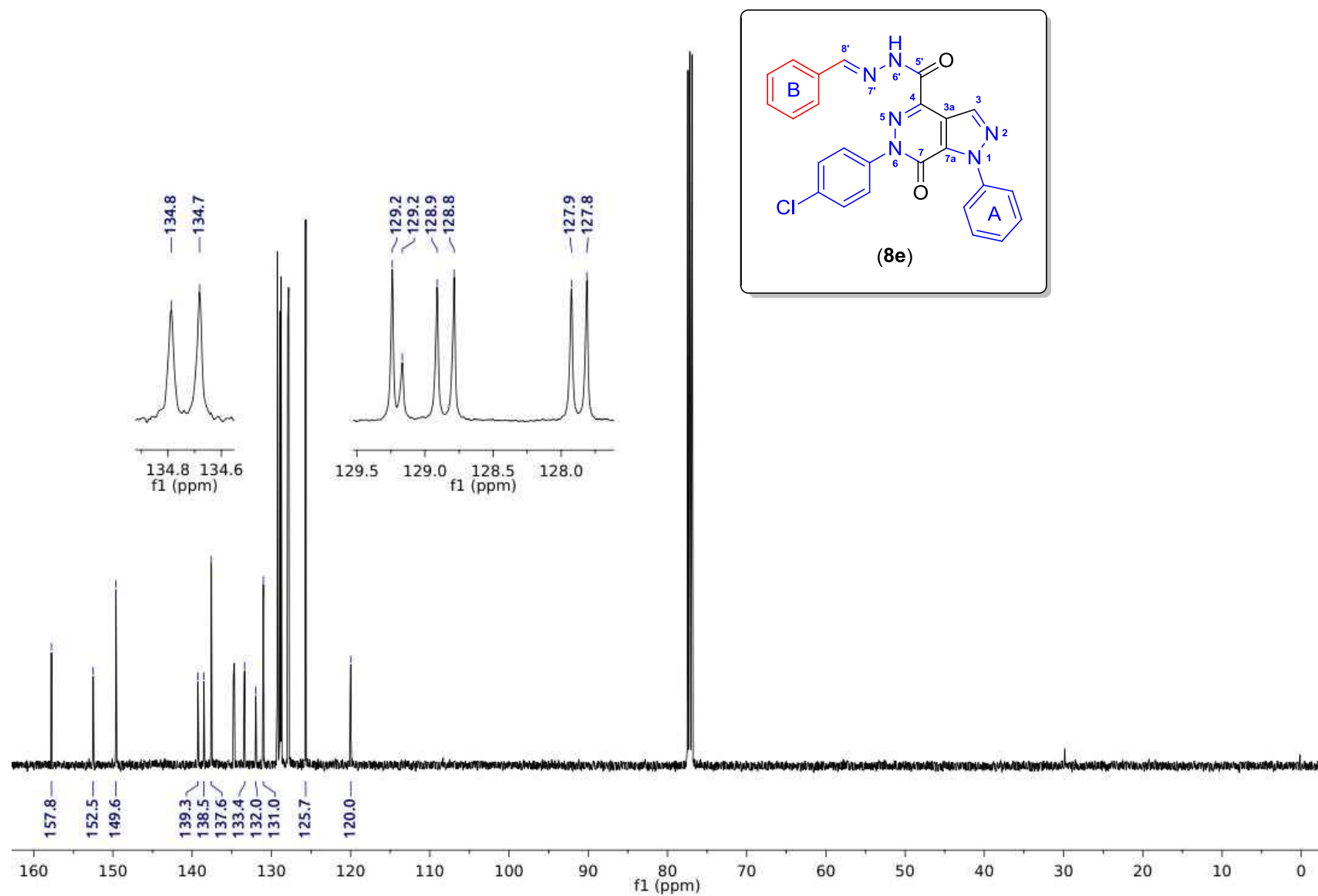
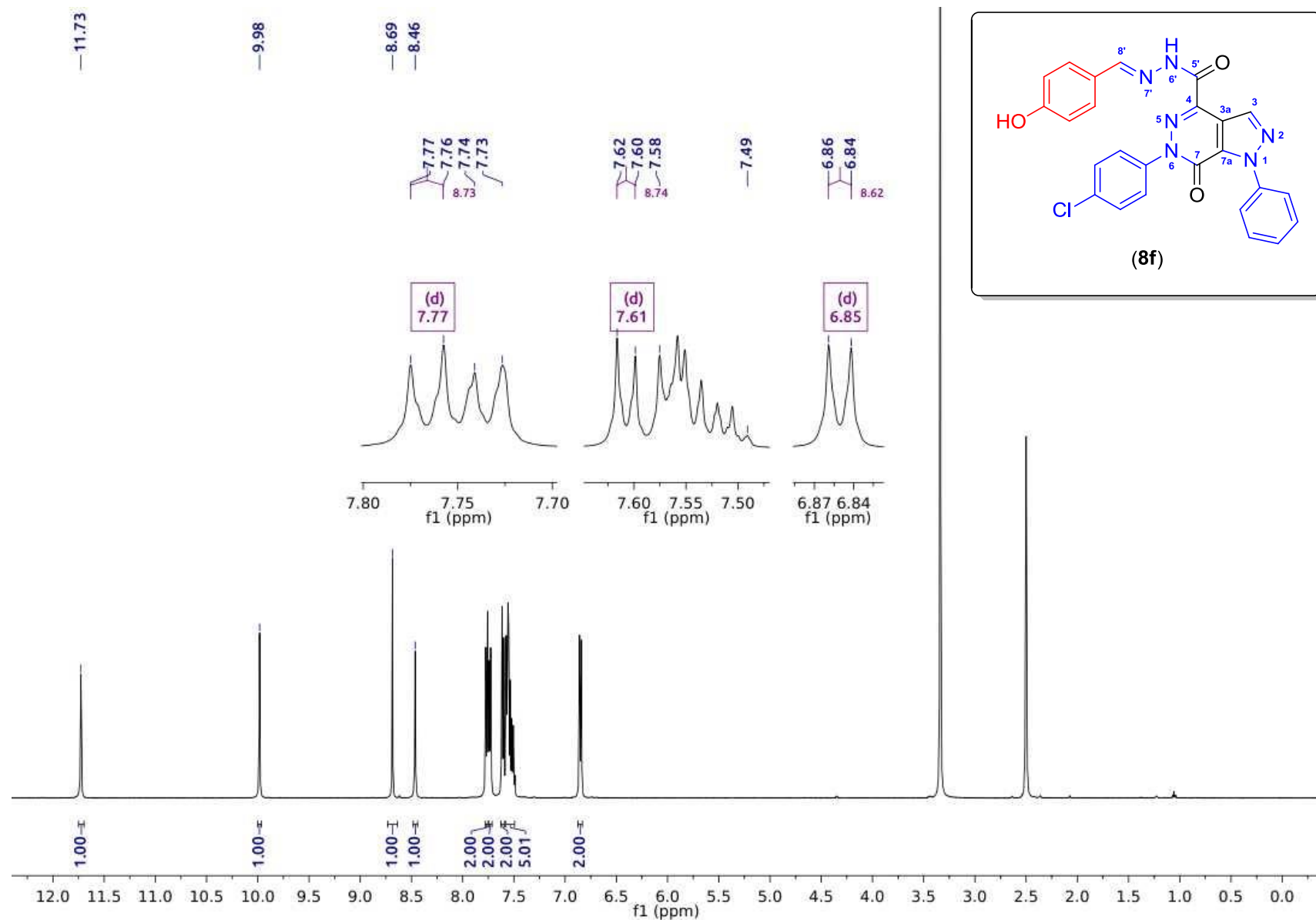
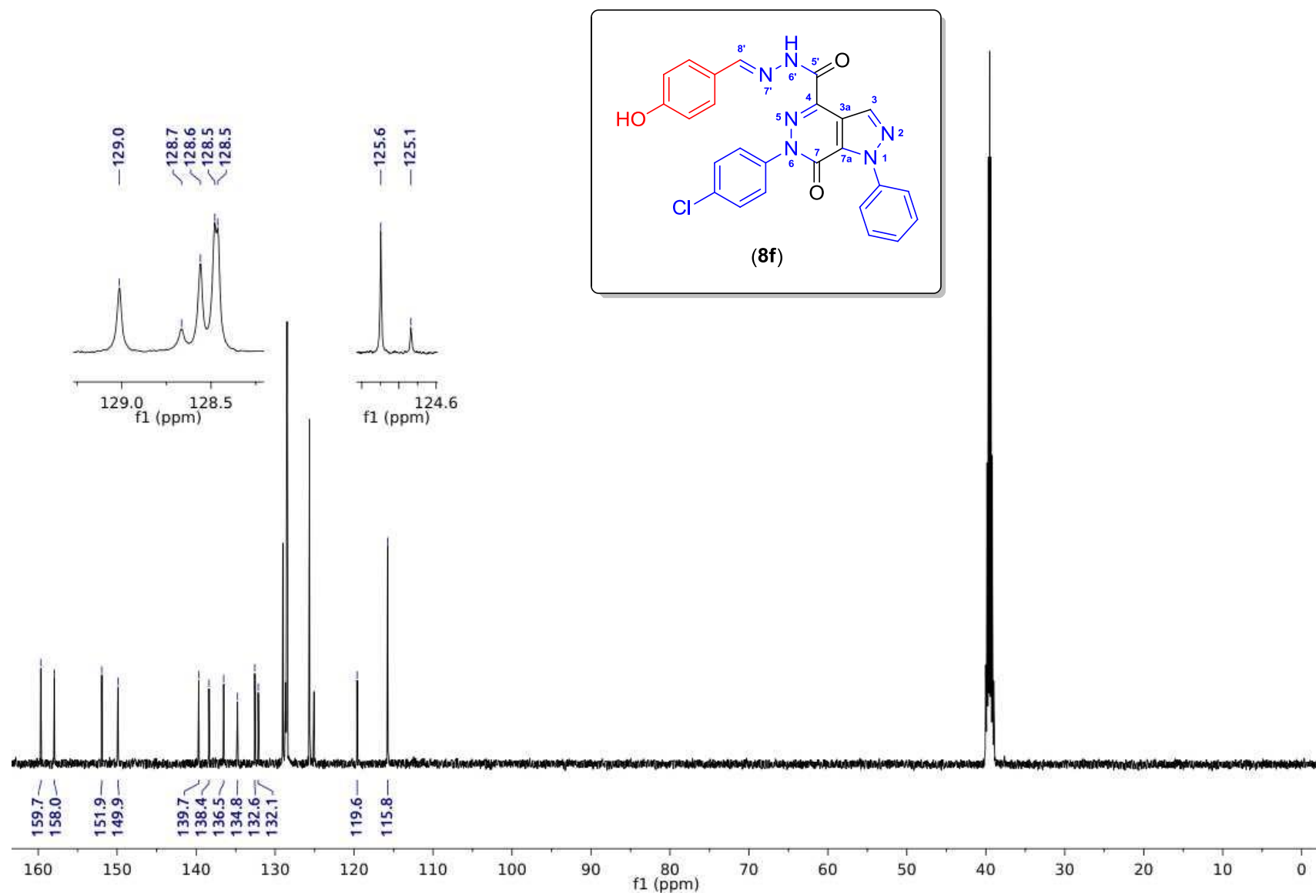


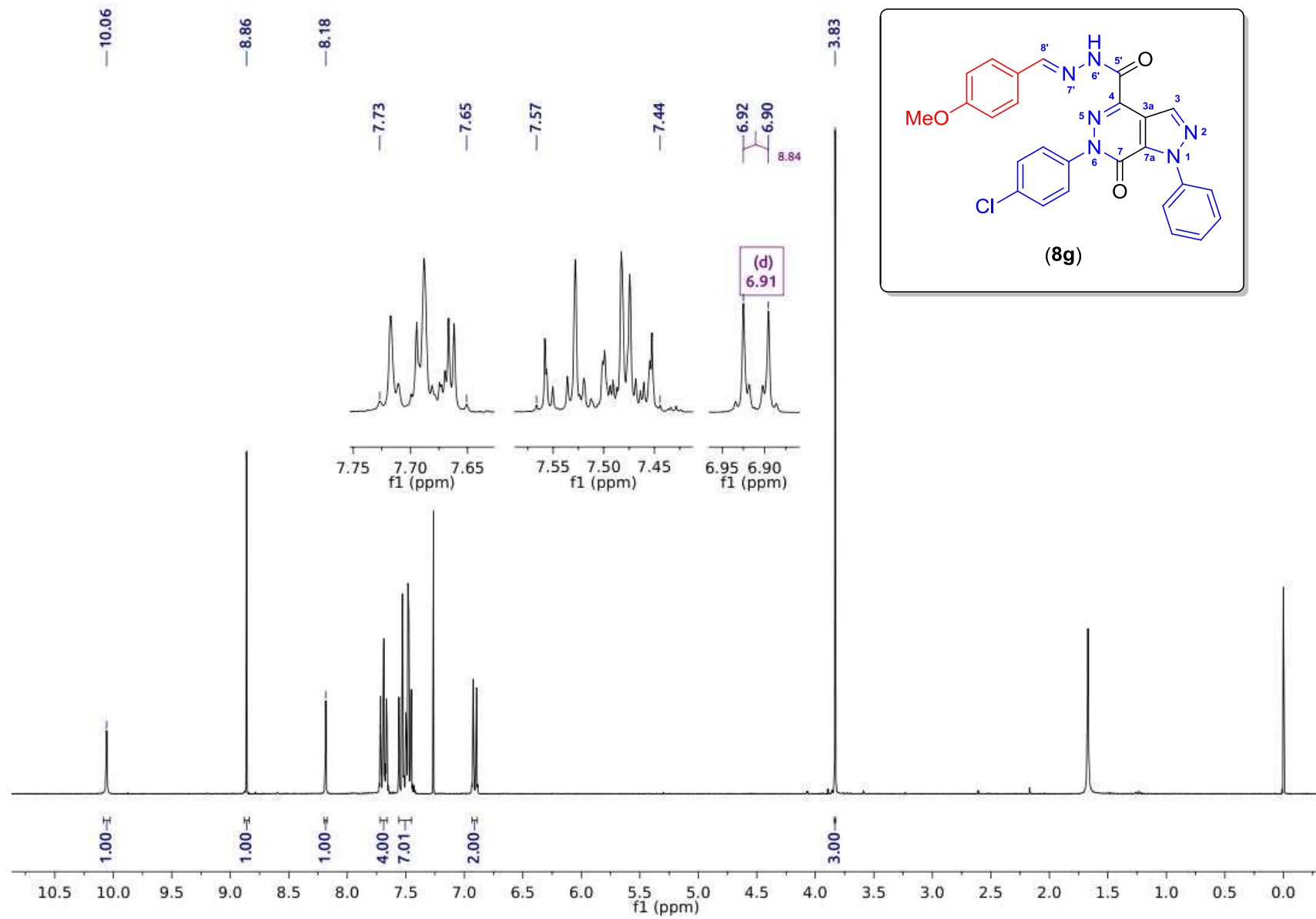
Figure S48.  $^{13}\text{C}$  NMR spectrum (125.77 MHz,  $\text{CDCl}_3$ ) of **8e**.



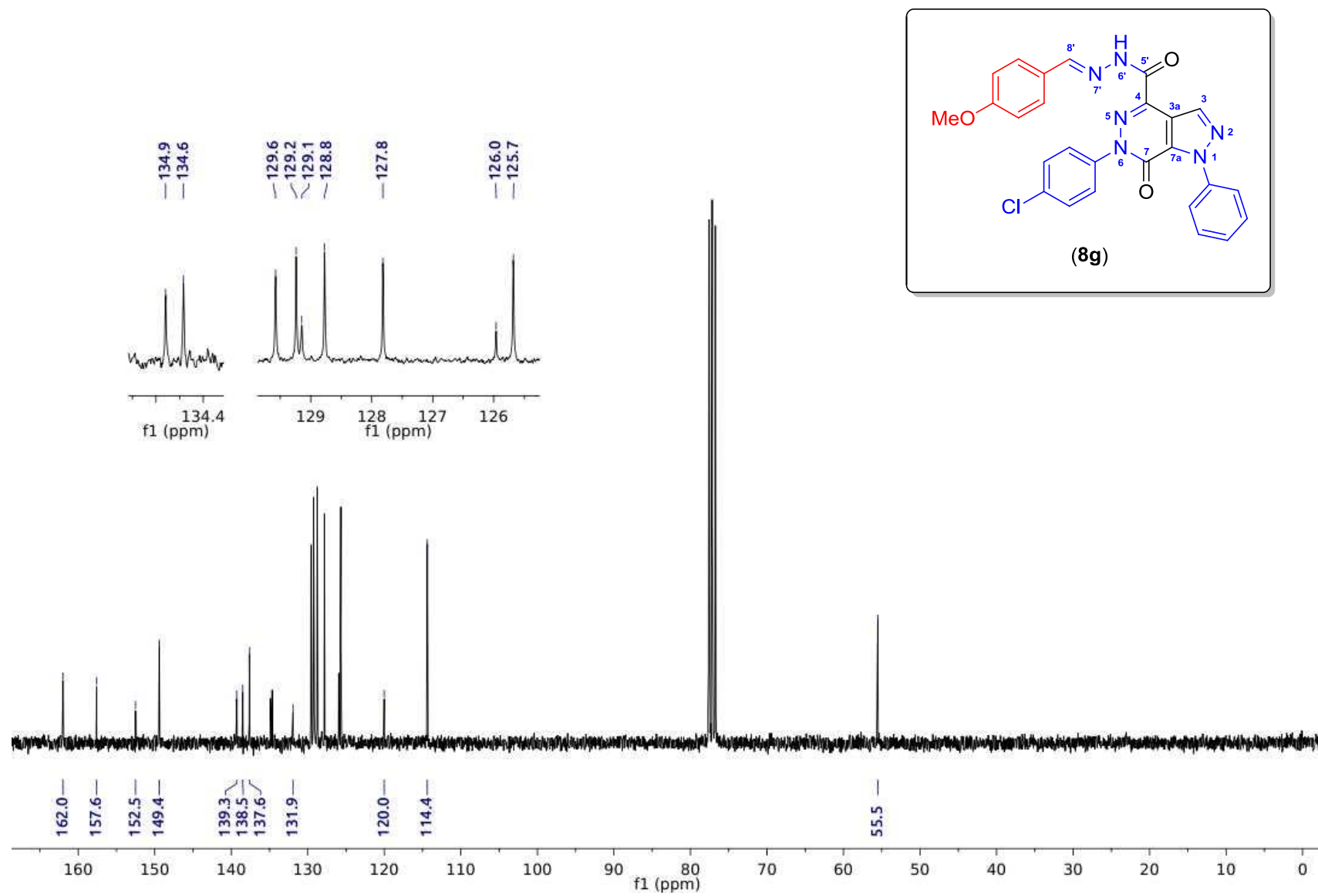
**Figure S49.**  $^1\text{H}$  NMR spectrum (500.13 MHz,  $\text{DMSO-}d_6$ ) of **8f**.



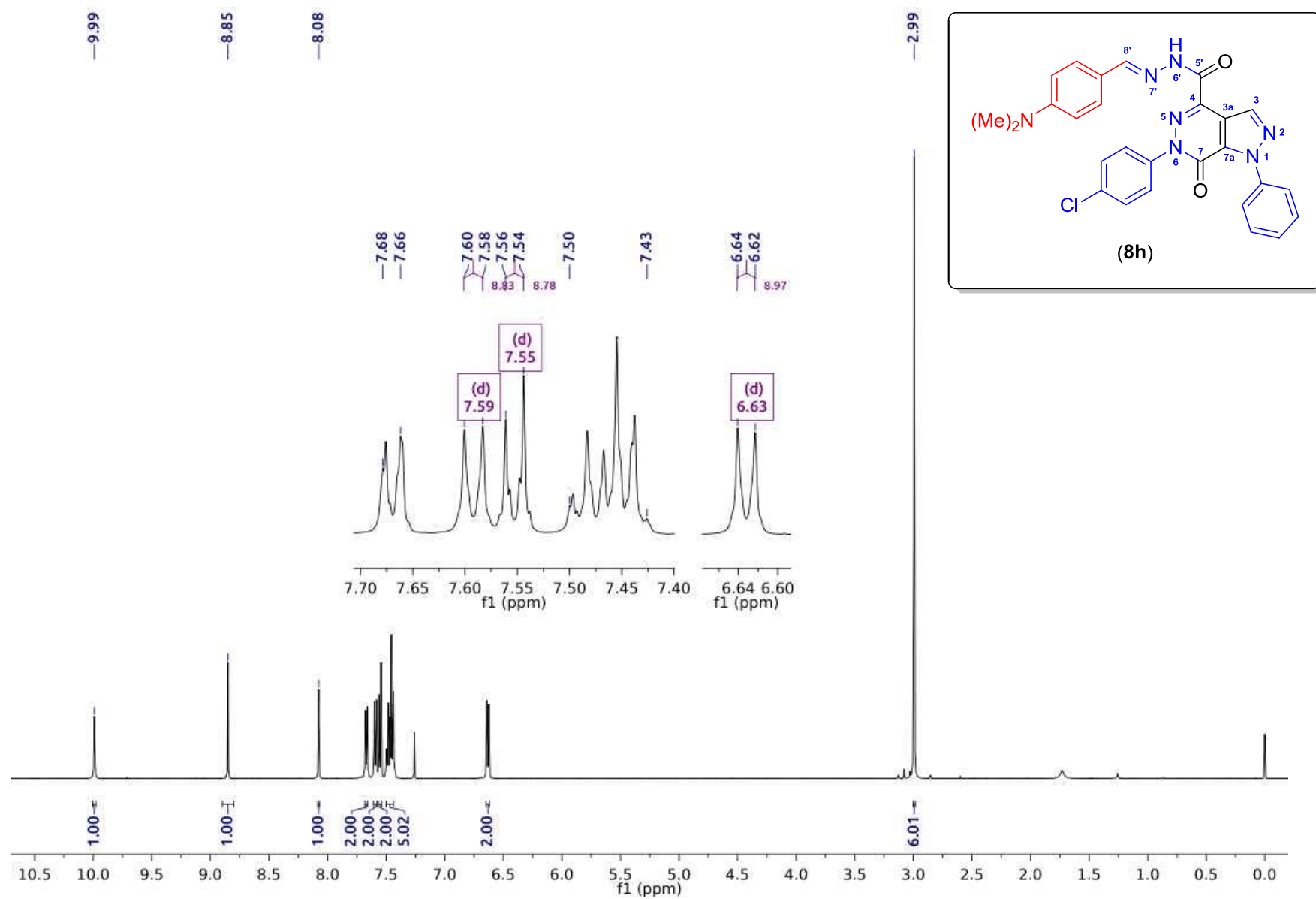
**Figure S50.**  $^{13}\text{C}$  NMR spectrum (125.77 MHz,  $\text{DMSO-}d_6$ ) of **8f**.



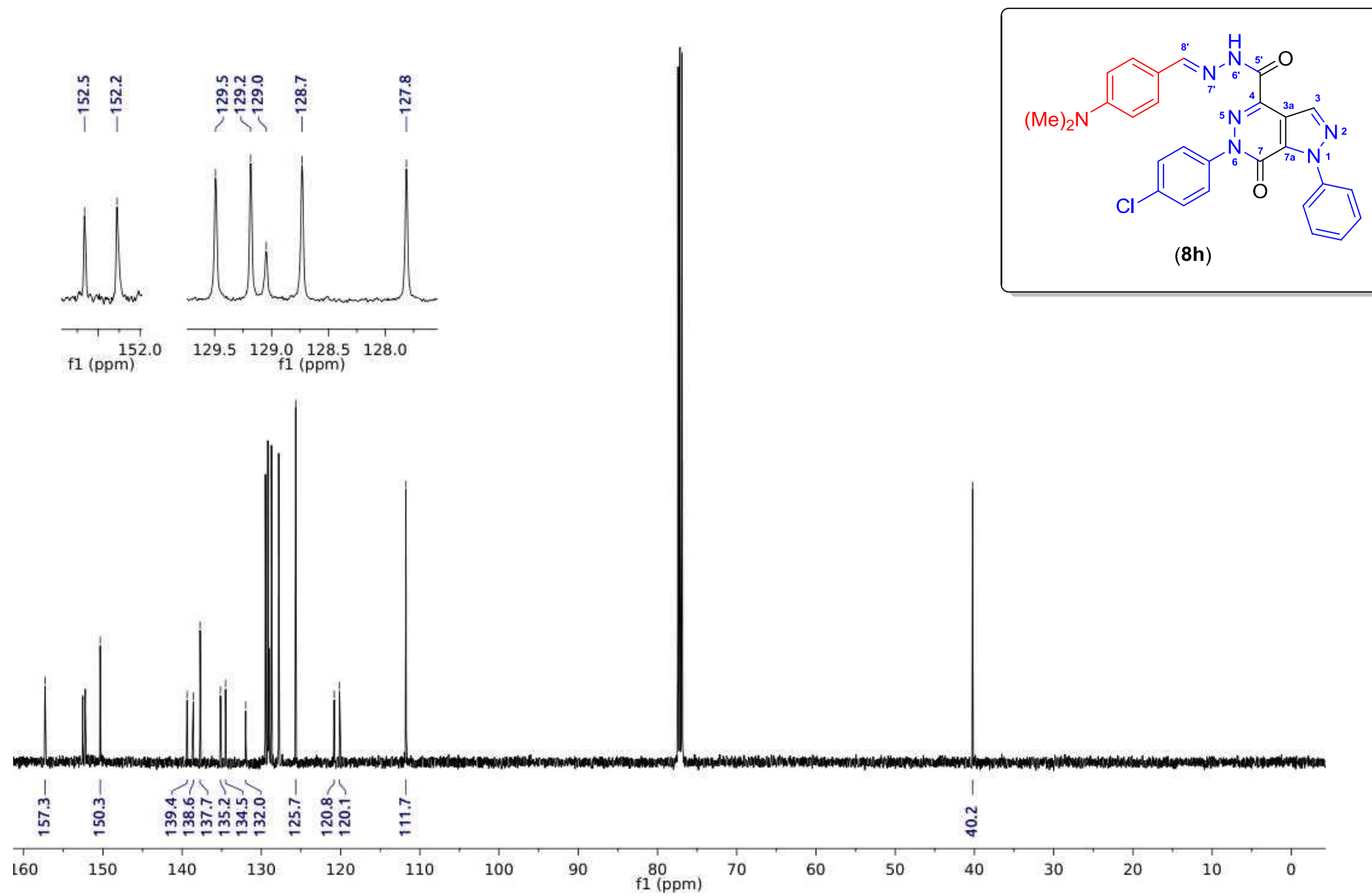
**Figure S51.** <sup>1</sup>H NMR spectrum (300.06 MHz, CDCl<sub>3</sub>) of **8g**.



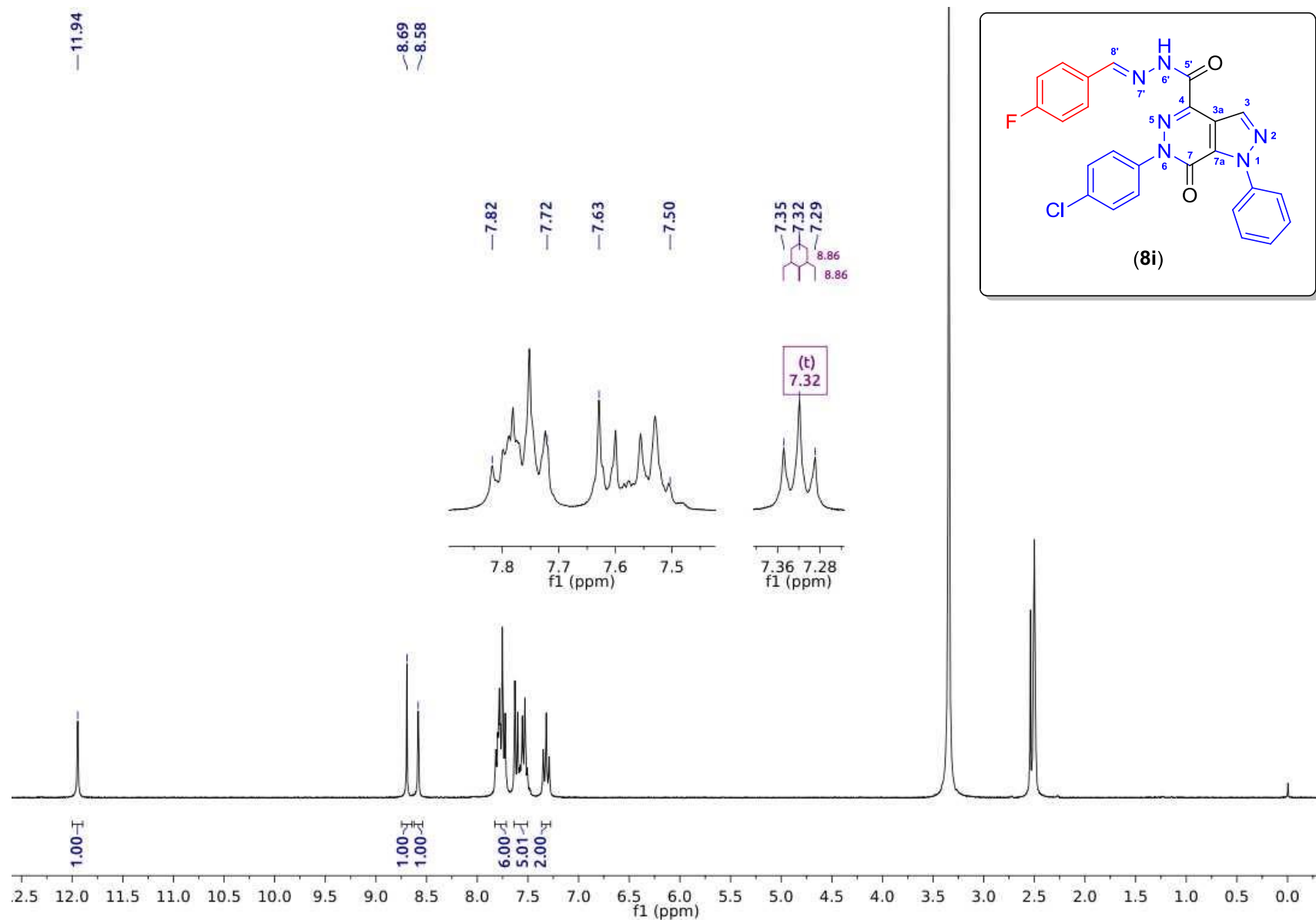
**Figure S52.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{CDCl}_3$ ) of **8g**.



**Figure S53.** <sup>1</sup>H NMR spectrum (500.13 MHz, CDCl<sub>3</sub>) of **8h**.

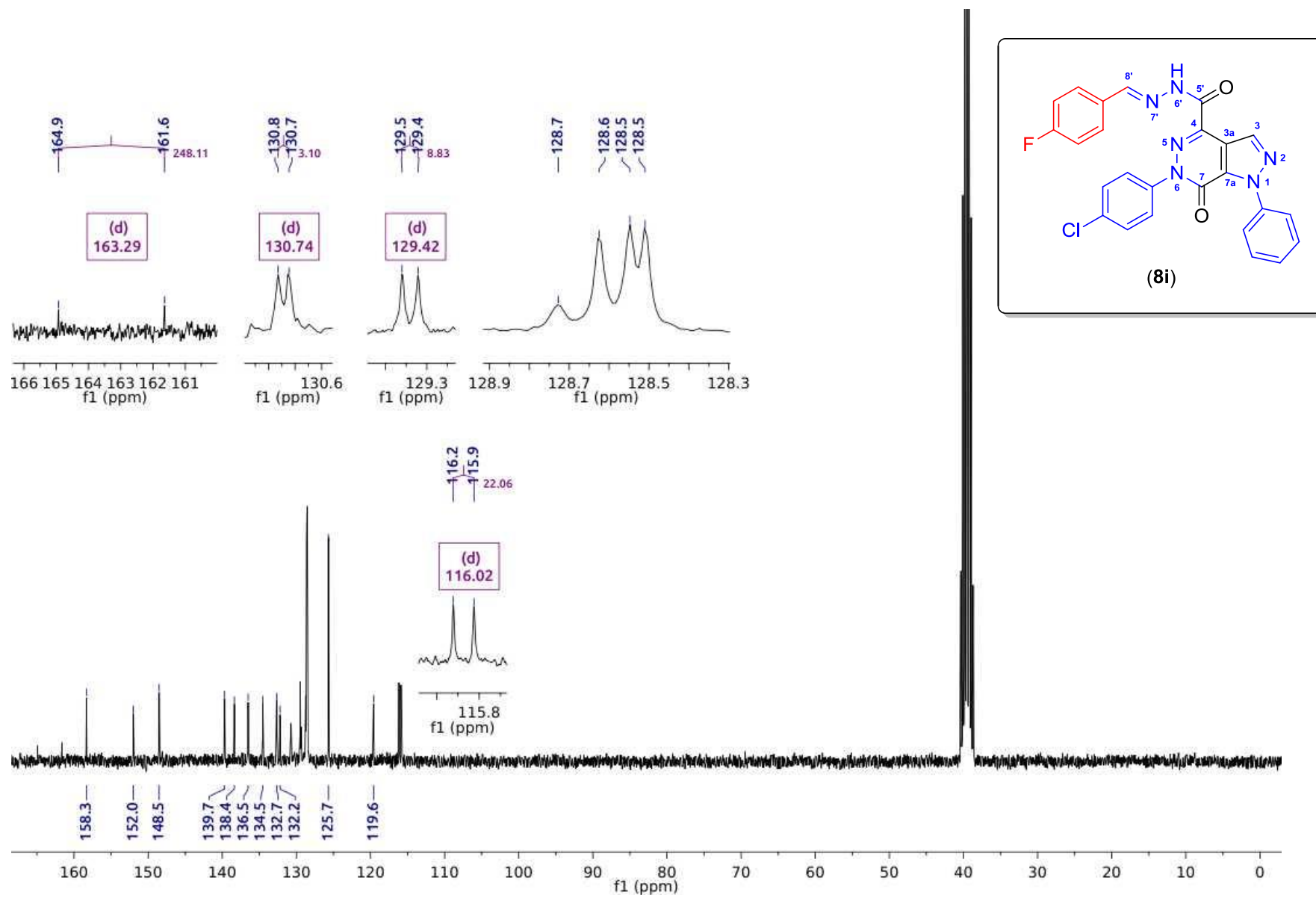


**Figure S54.**  $^{13}\text{C}$  NMR spectrum (125.77 MHz,  $\text{CDCl}_3$ ) of **8h**.

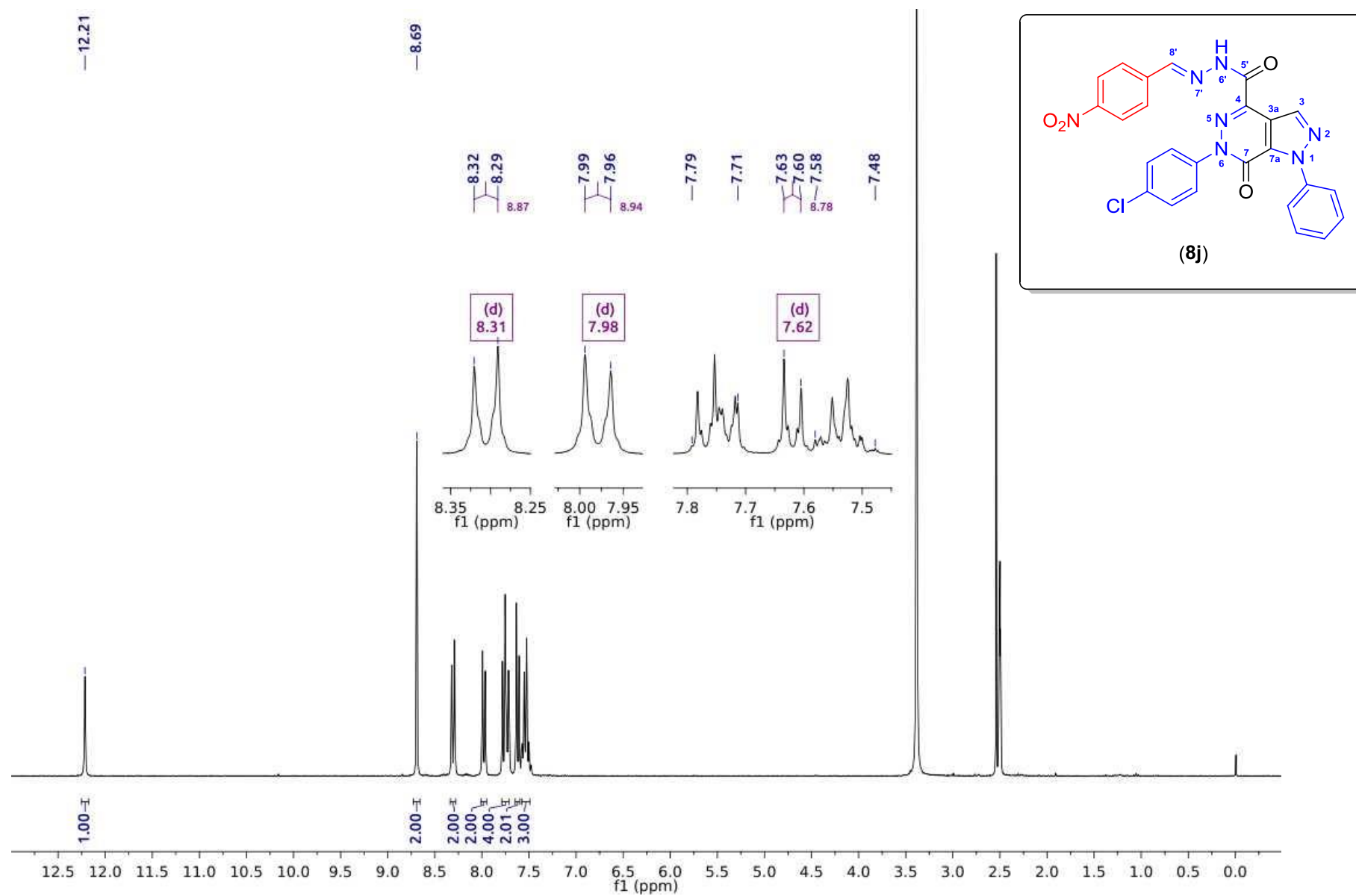


**Figure S55.**  $^1\text{H NMR}$  spectrum (300.06 MHz,  $\text{DMSO-}d_6$ ) of **8i**.





**Figure S56.**  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO-}d_6$ ) of **8i**.



**Figure S57.**  $^1\text{H}$  NMR spectrum (300.06 MHz,  $\text{DMSO-}d_6$ ) of **8j**.

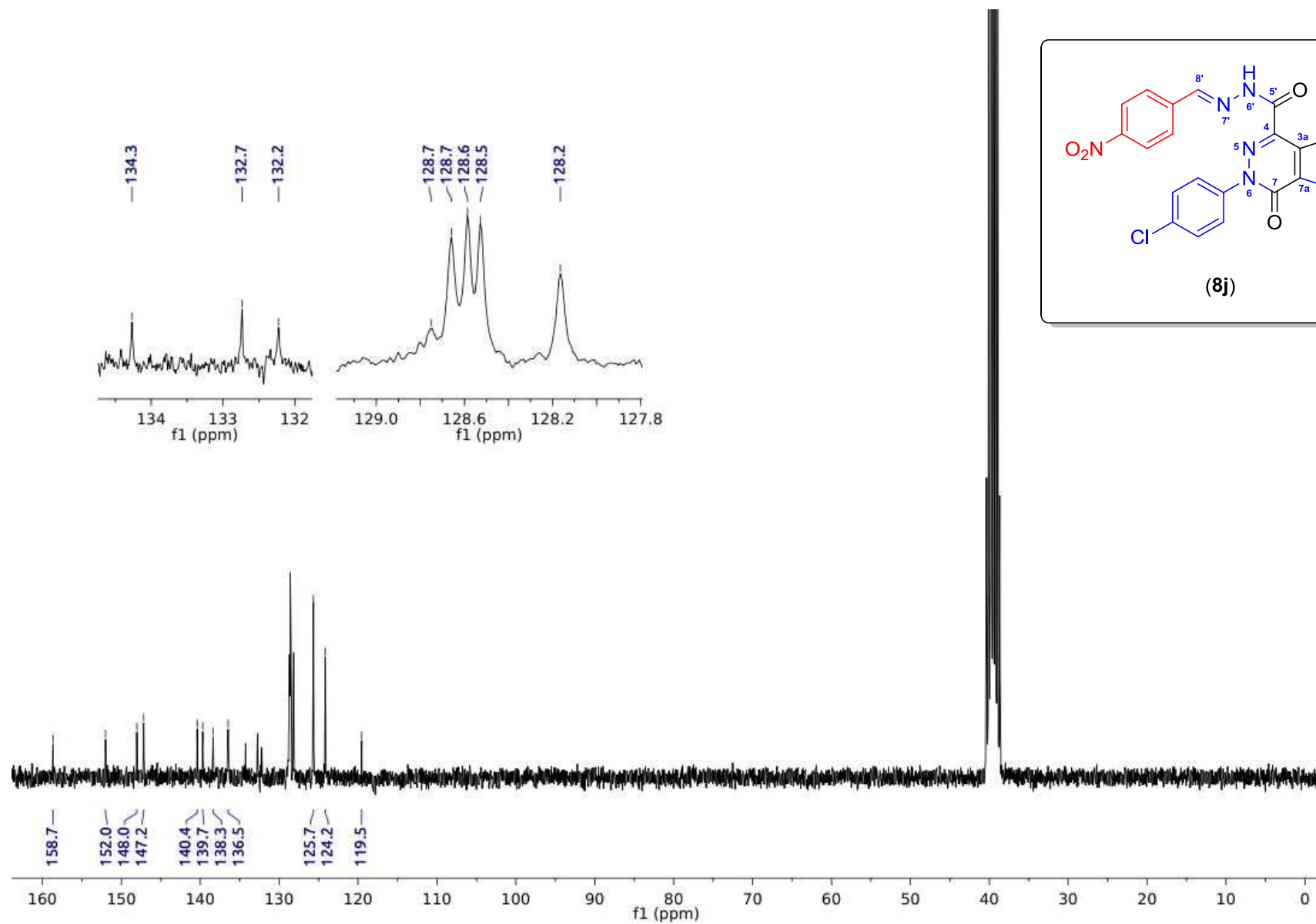


Figure S58.  $^{13}\text{C}$  NMR spectrum (75.46 MHz,  $\text{DMSO}-d_6$ ) of **8j**.