

Supporting Information for:

Synthesis of Tetra-substituted 5-Trifluoromethylpyrazoles via Sequential Halogenation/Palladium-Catalyzed C-C and C-N Cross-Coupling

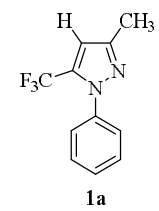
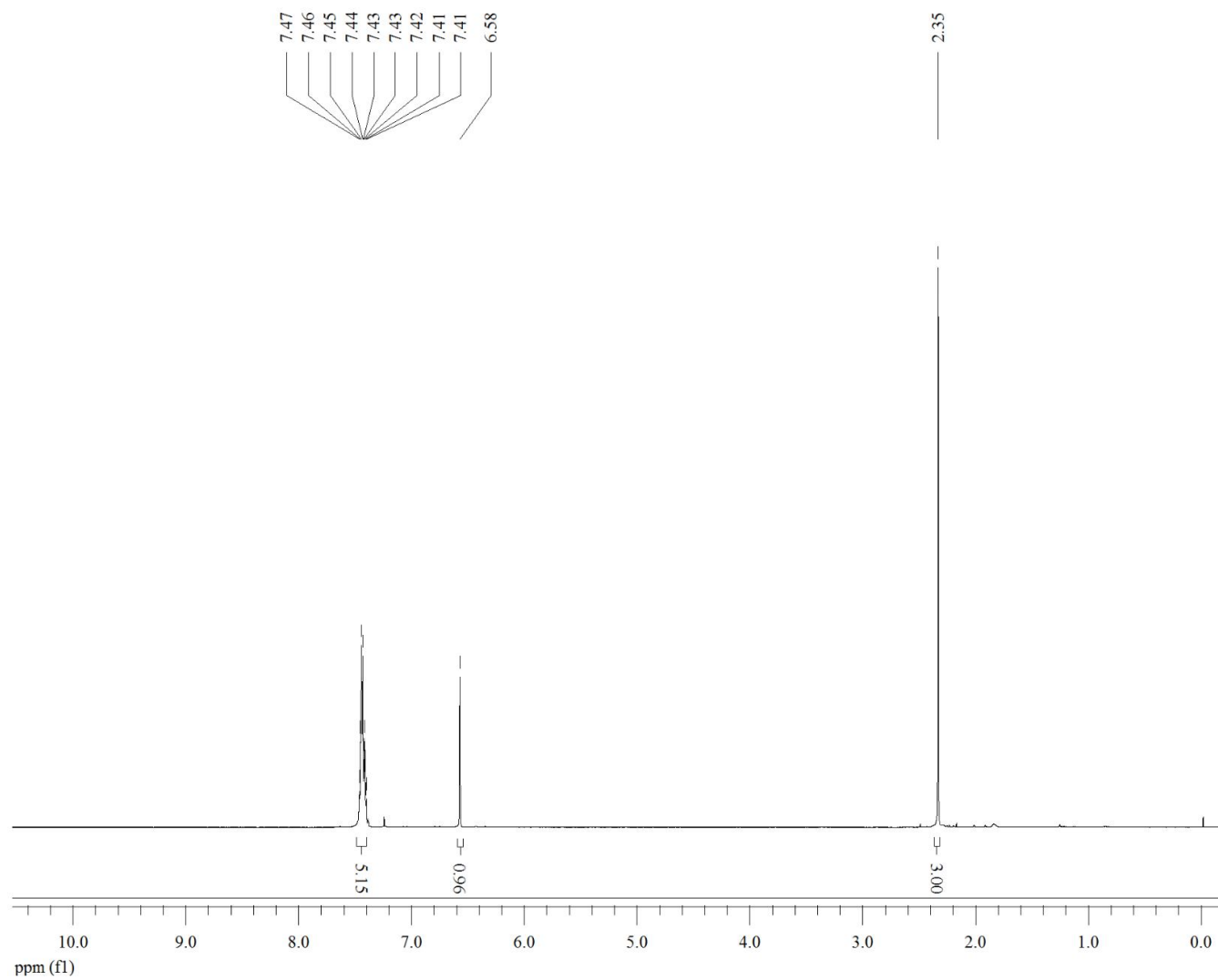
Carson Wiethan,^a Wilian C. Rosa,^a Helio G. Bonacorso,^{a} Mark Stradiotto^{b*}*

^a Departamento de Química, Universidade Federal de Santa Maria, 97105-900 Santa Maria, Brazil

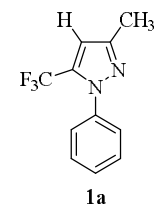
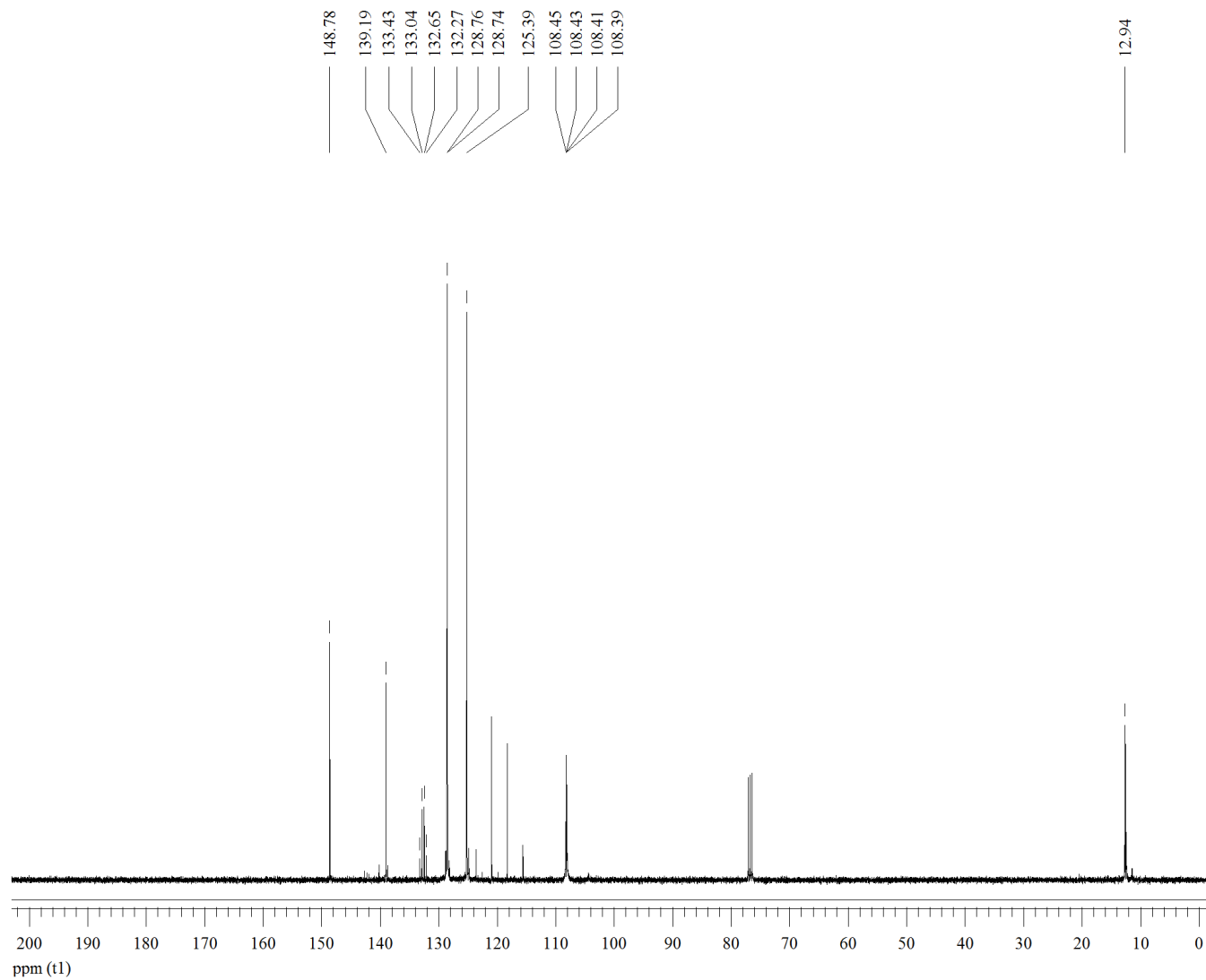
^b Department of Chemistry, Dalhousie University Halifax, NS, B3H 4R2 Canada

Contents: NMR spectral data.

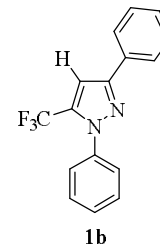
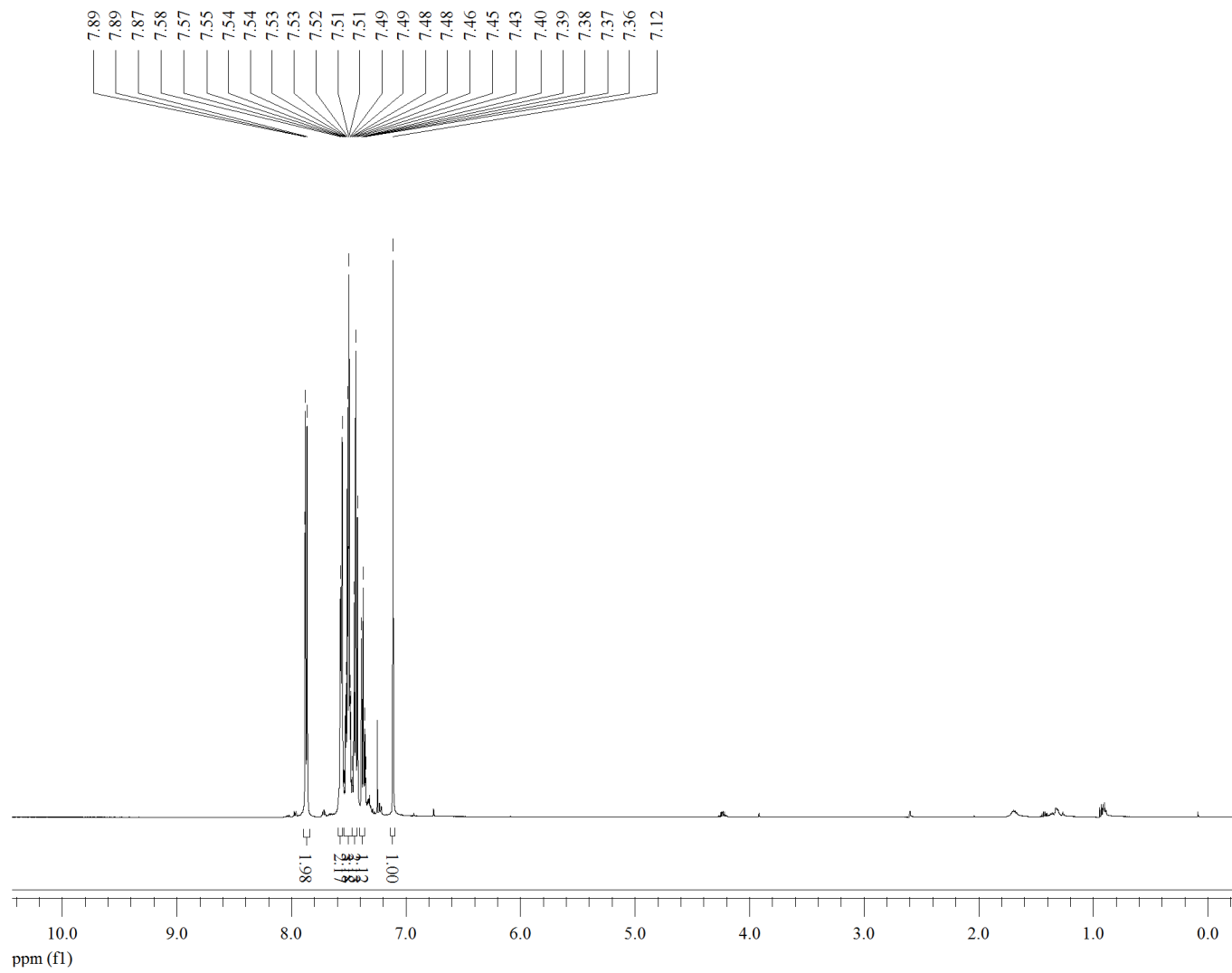
1a - ^1H NMR (400 MHz, CDCl_3 , 25 $^\circ\text{C}$)



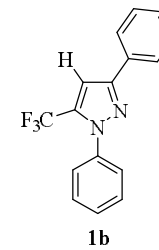
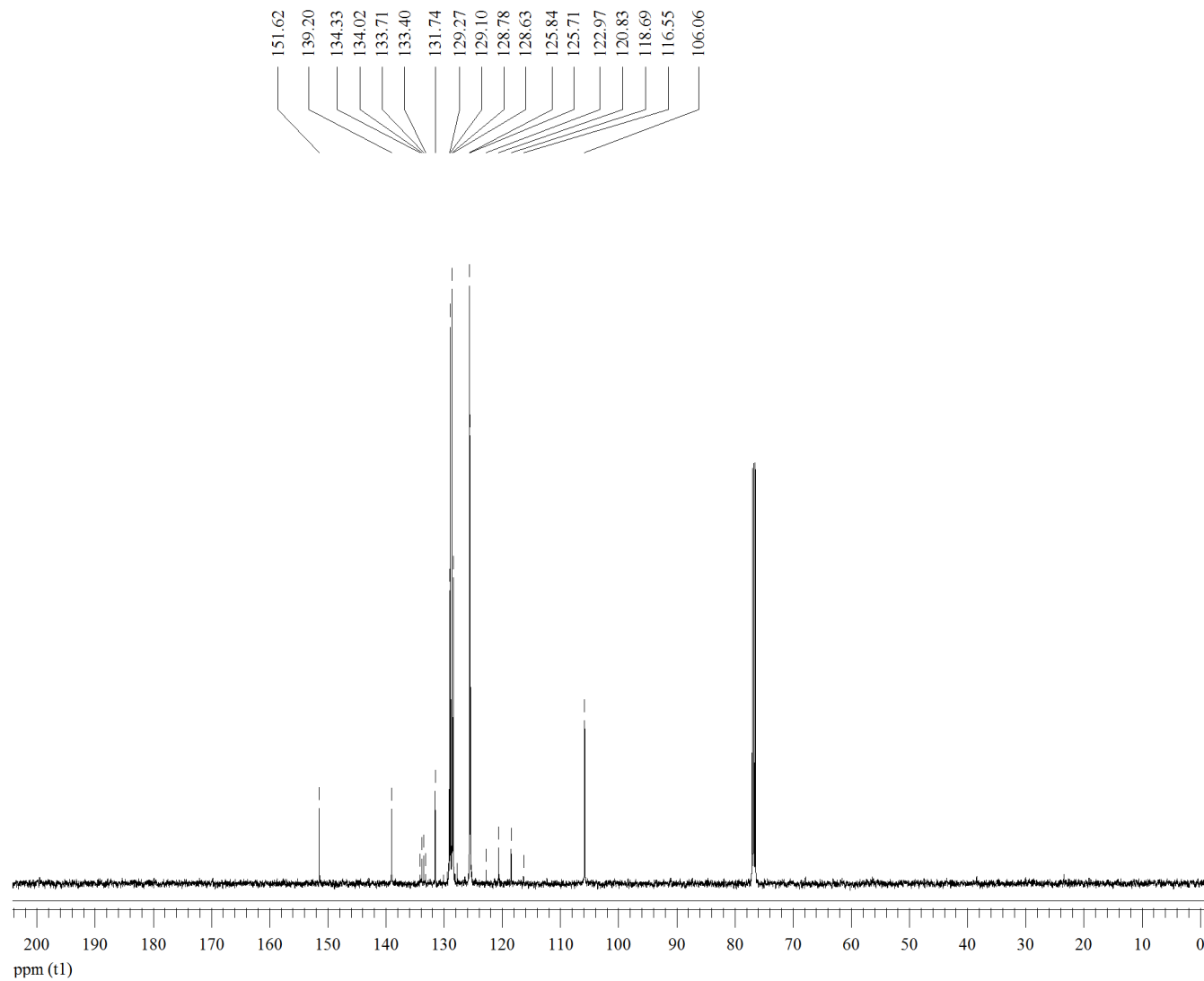
1a - $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3 , 25 °C)



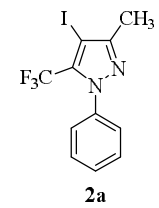
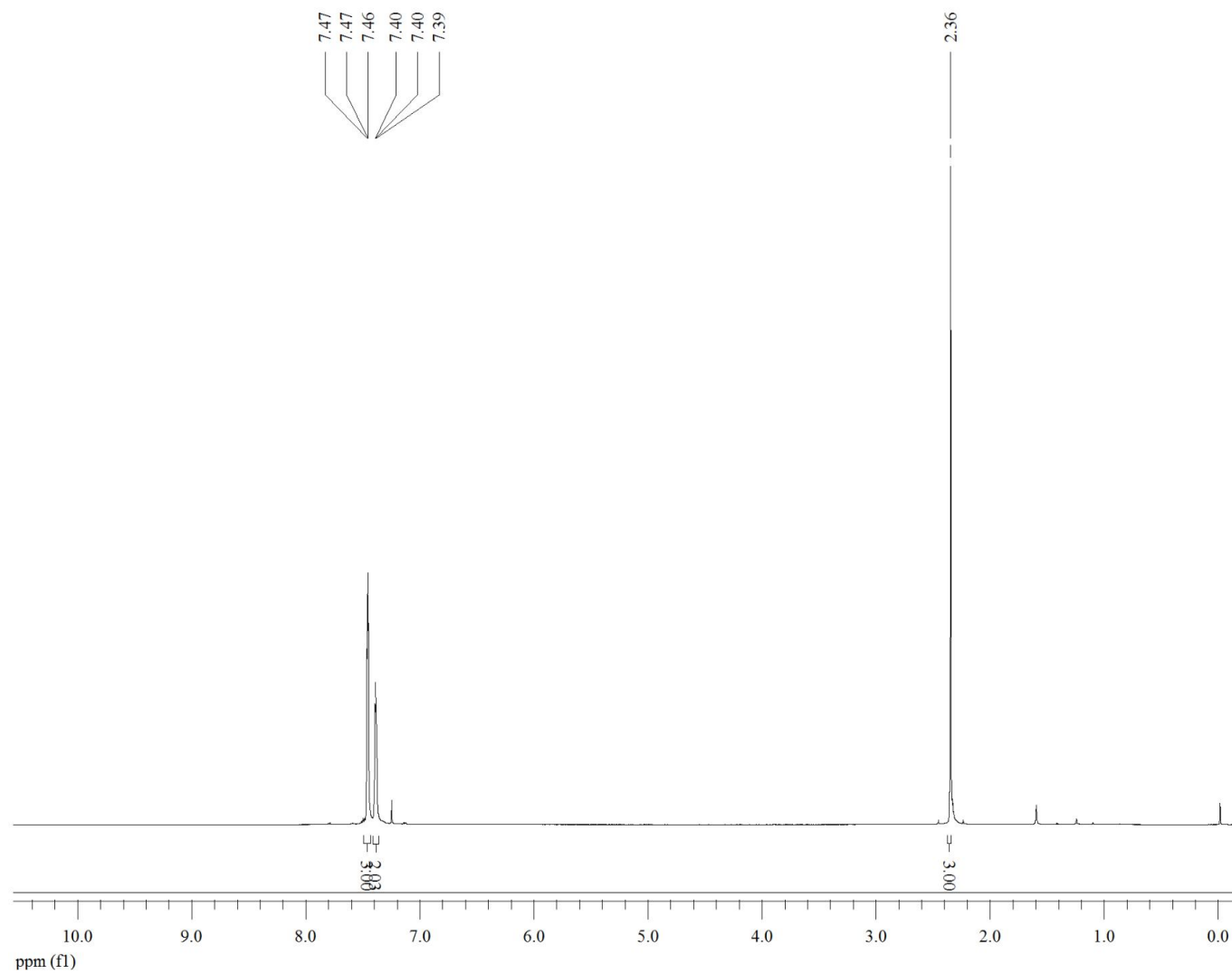
1b - ^1H NMR (500 MHz, CDCl_3 , 25 °C)



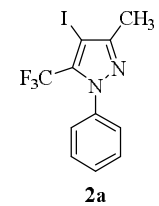
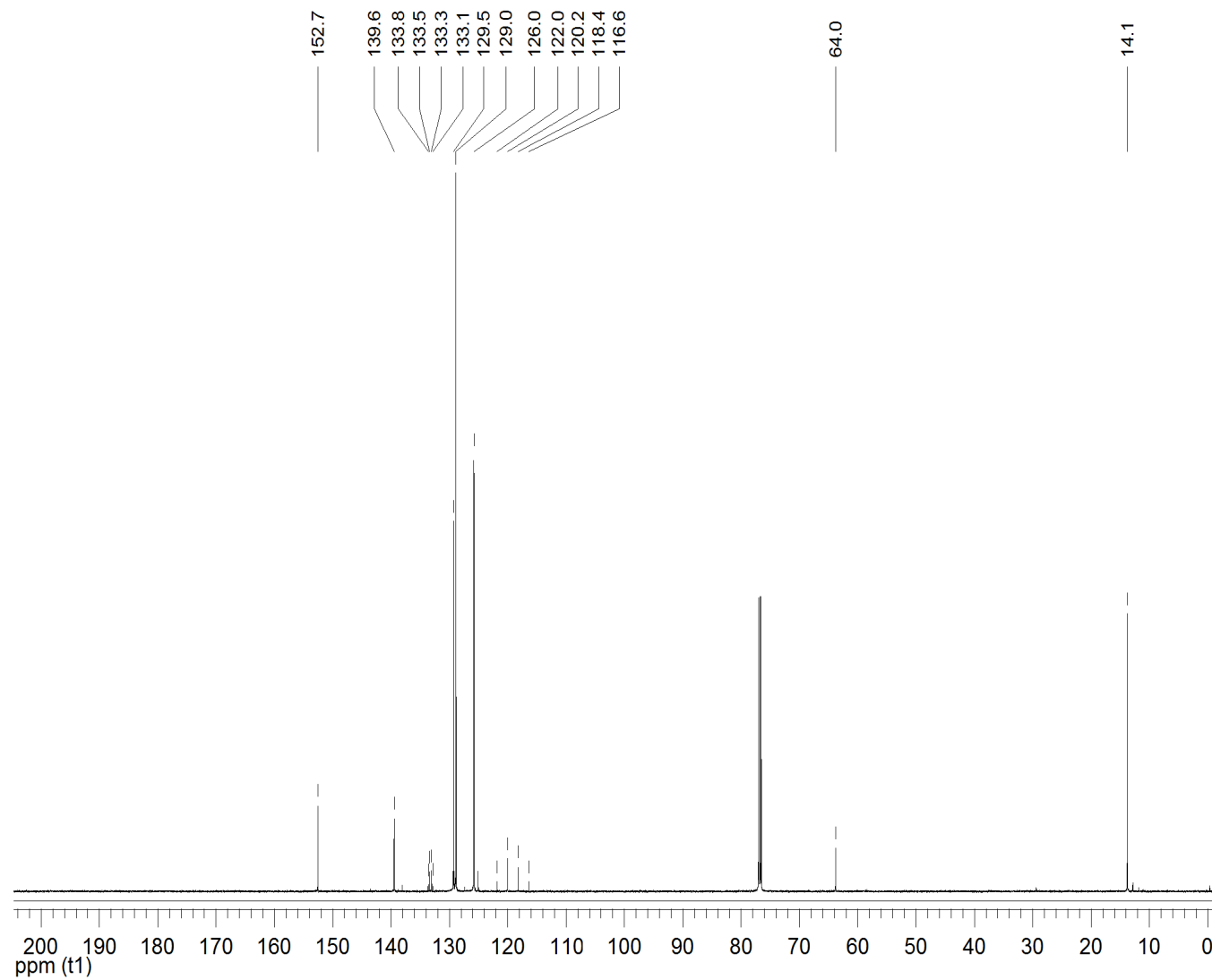
1b - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



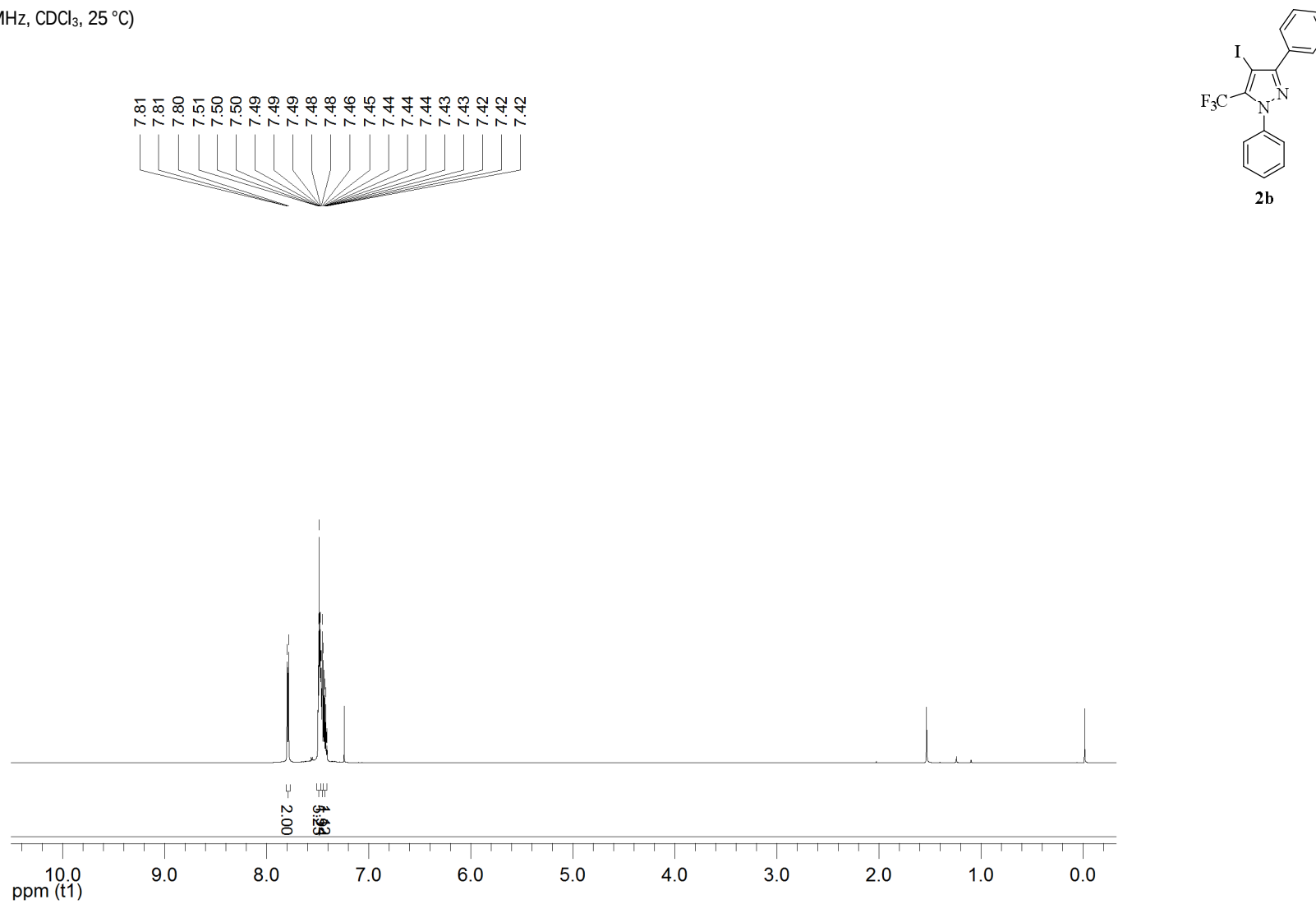
2a - ^1H NMR (600 MHz, CDCl_3 , 25 $^\circ\text{C}$)



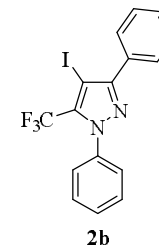
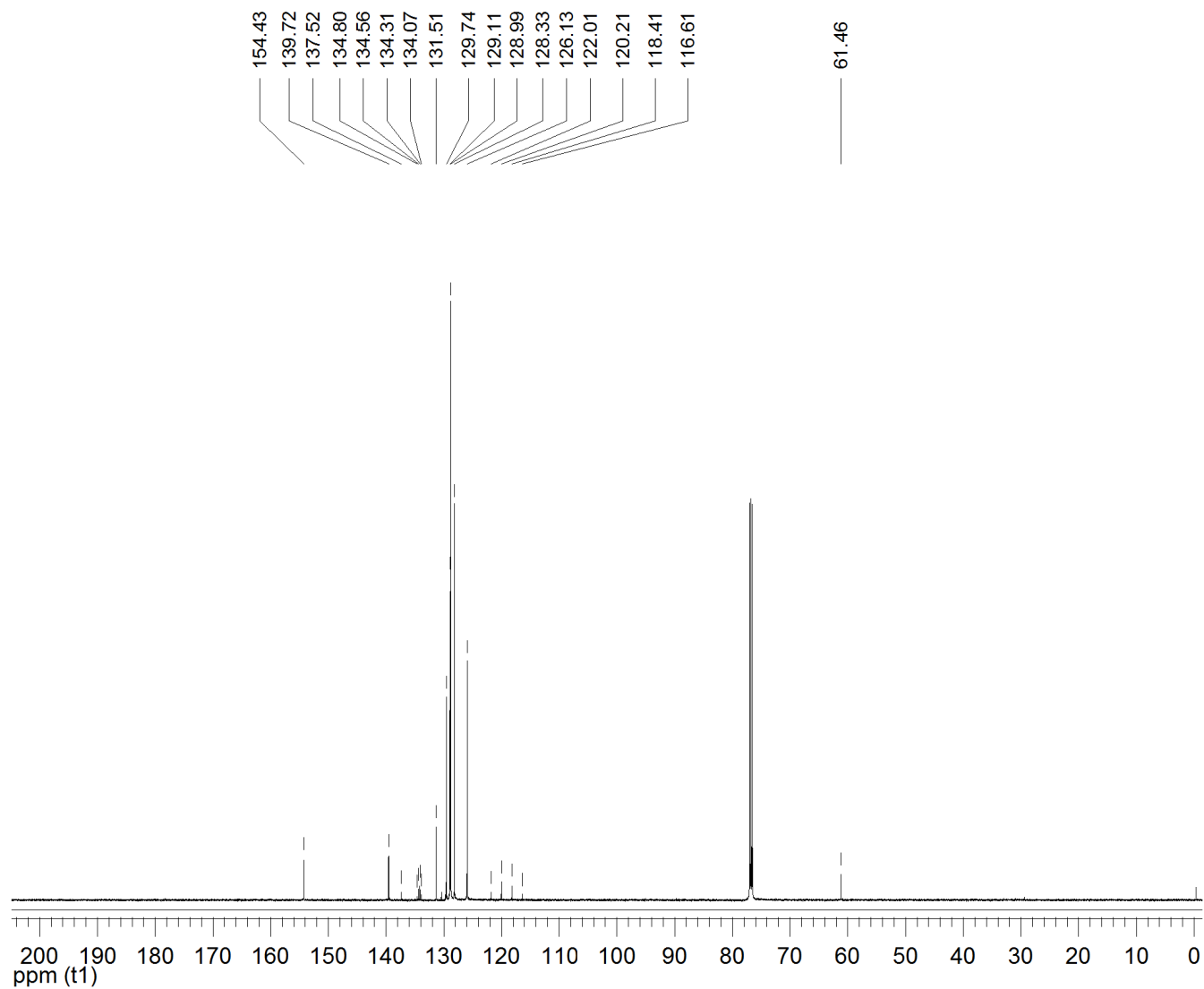
2a - $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CDCl_3 , 25 °C)



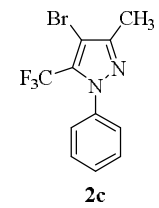
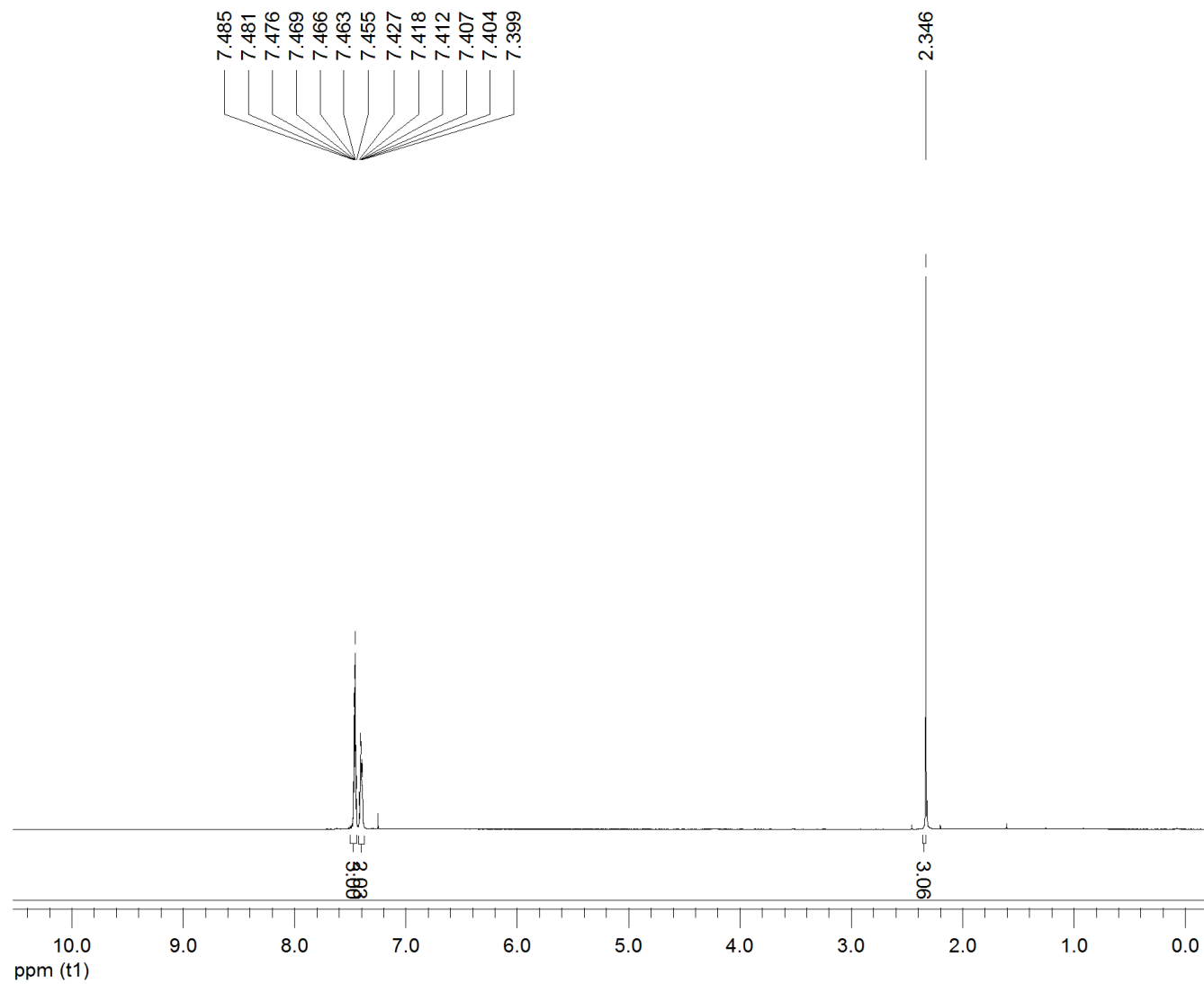
2b - ^1H NMR (600 MHz, CDCl_3 , 25 $^\circ\text{C}$)



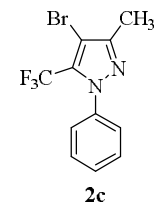
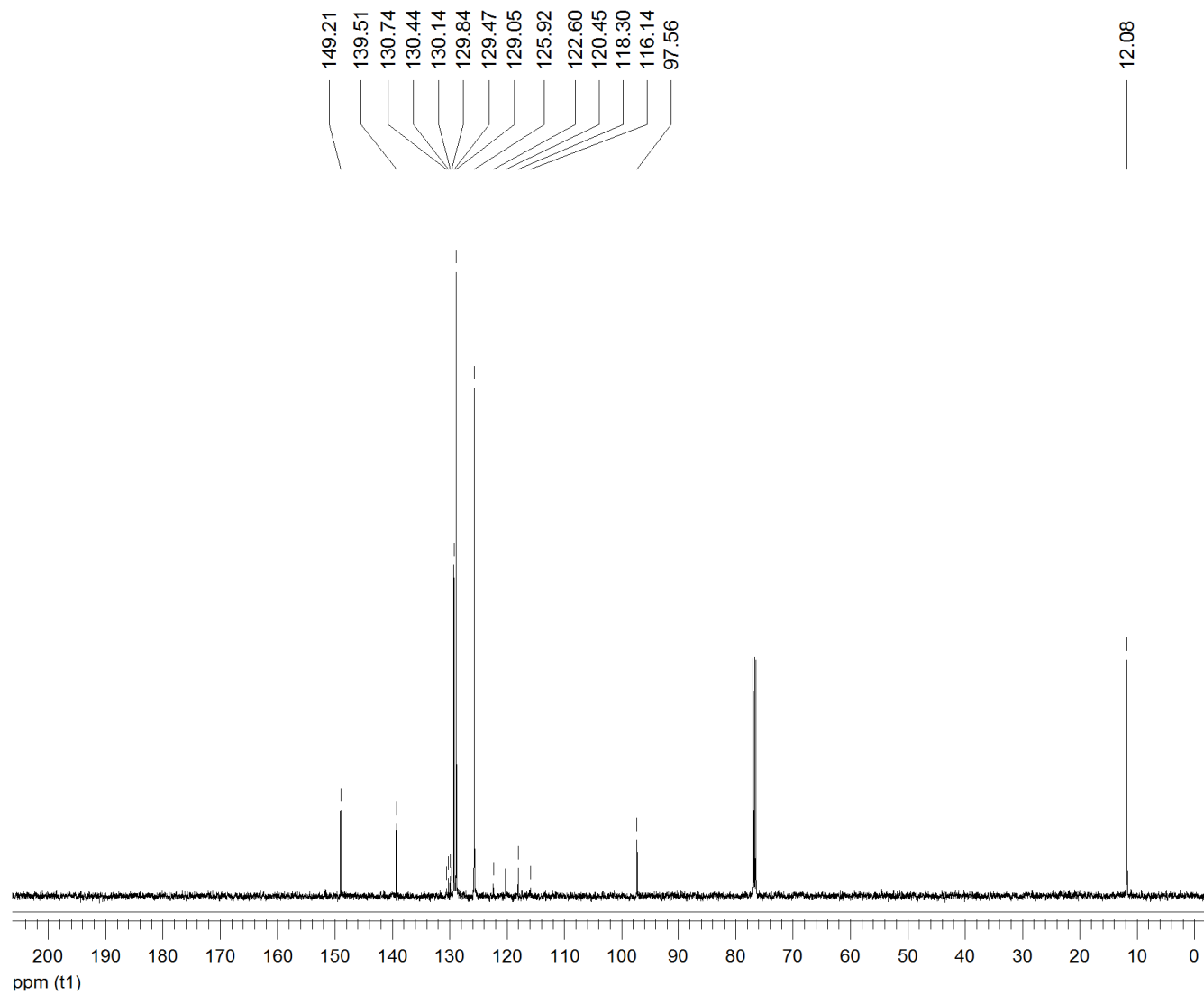
2b - $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CDCl_3 , 25 °C)



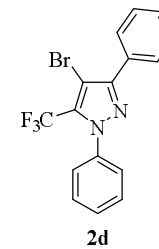
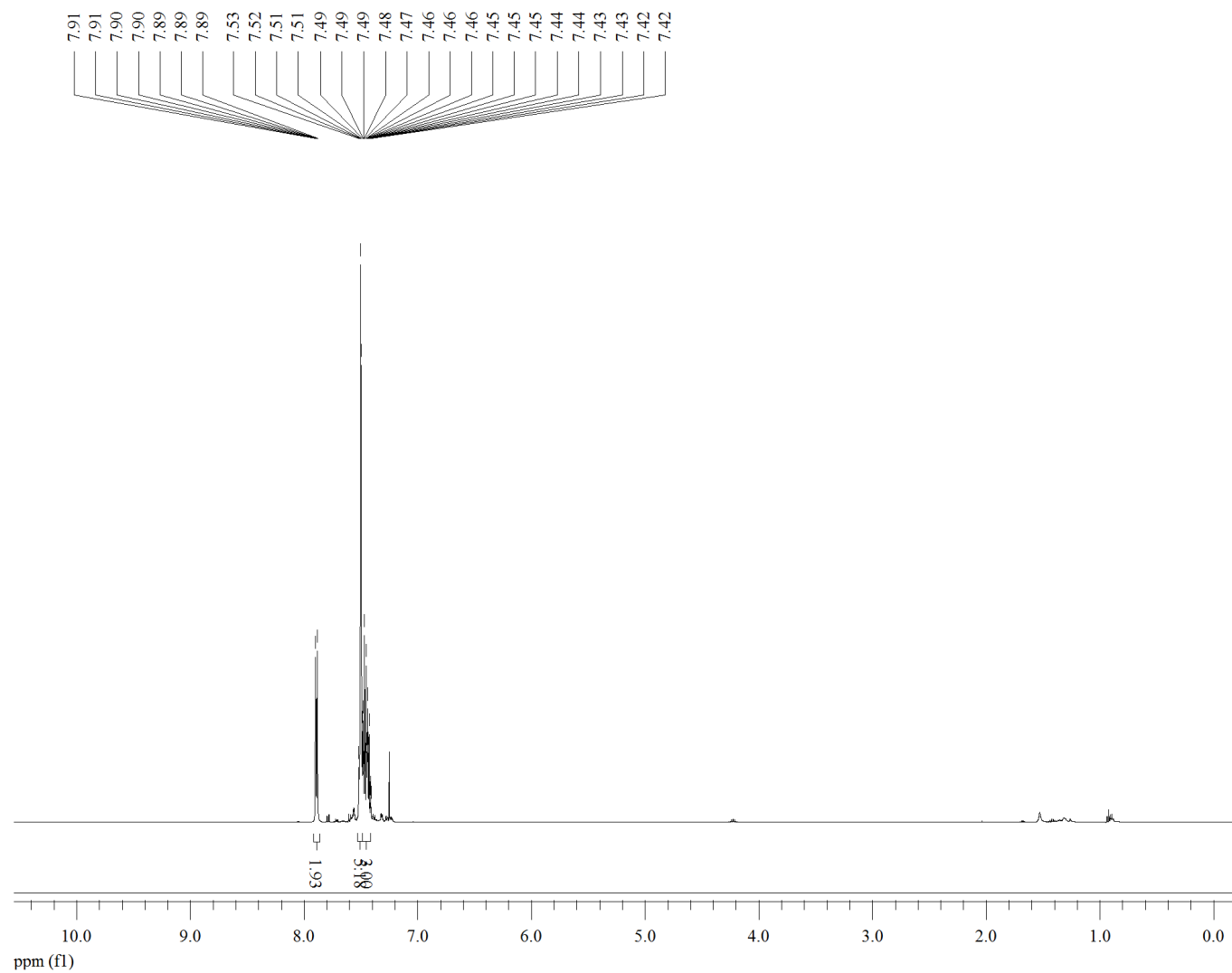
2c - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



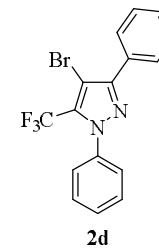
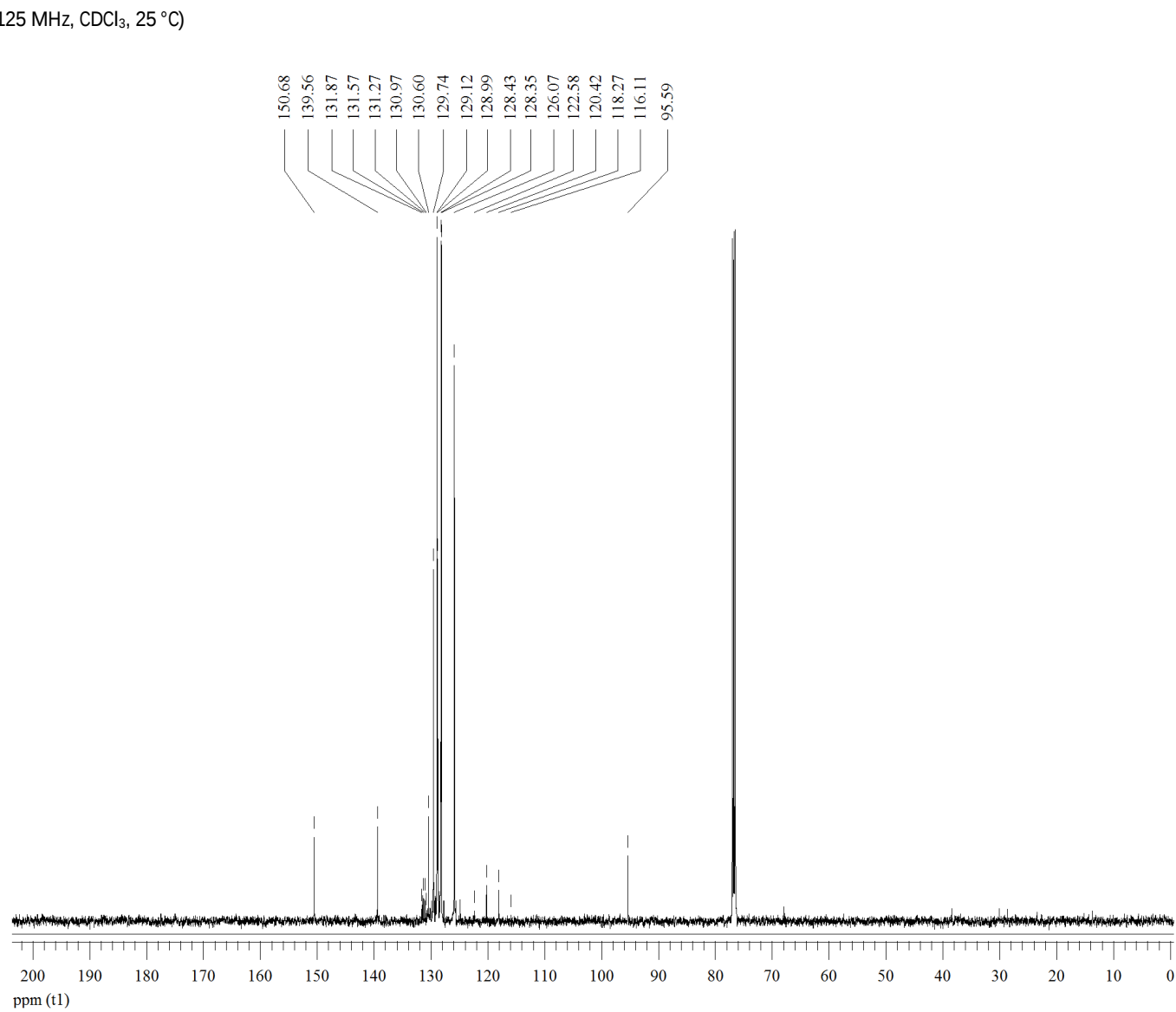
2c - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



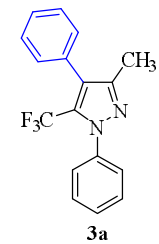
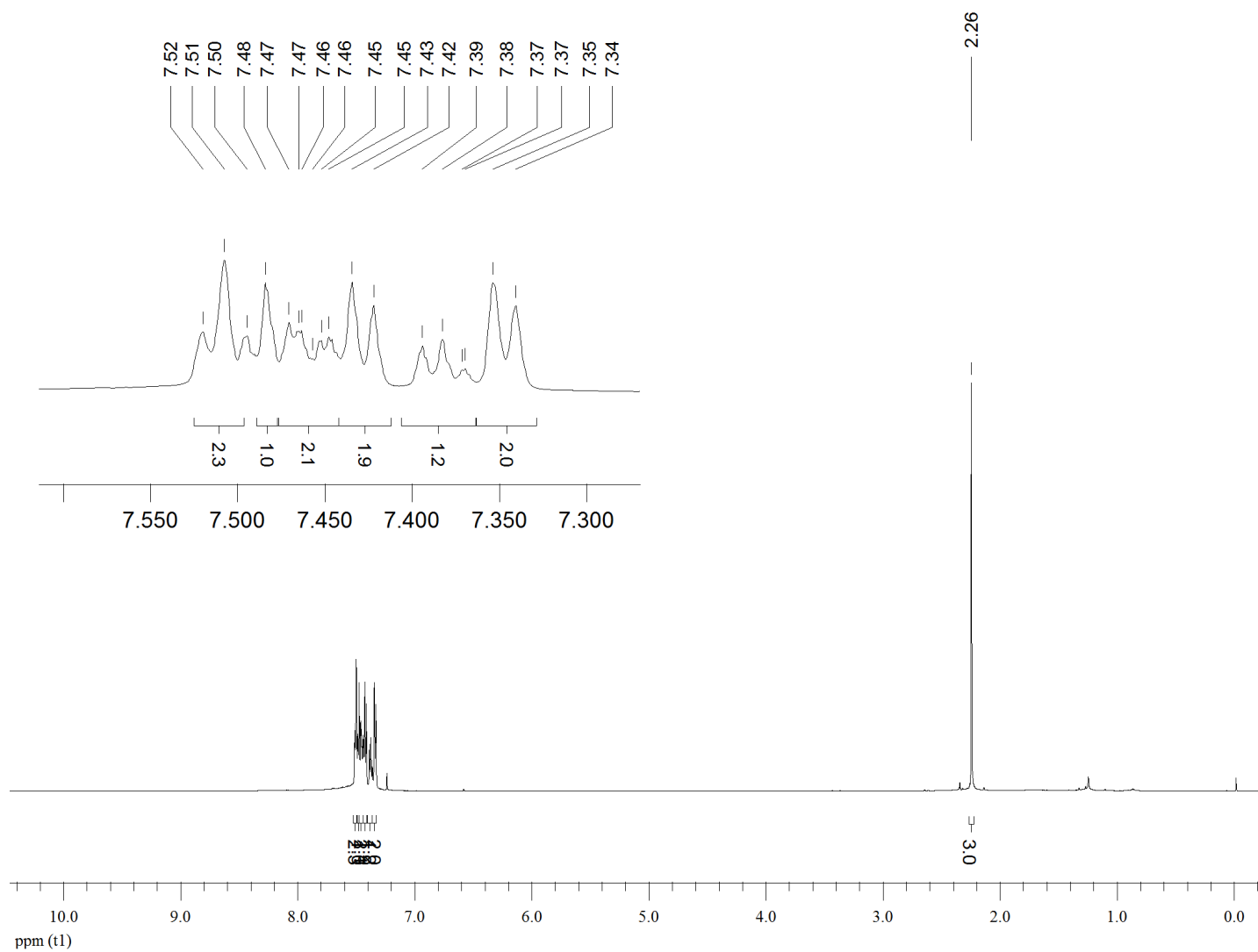
2d - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



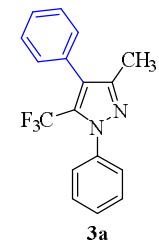
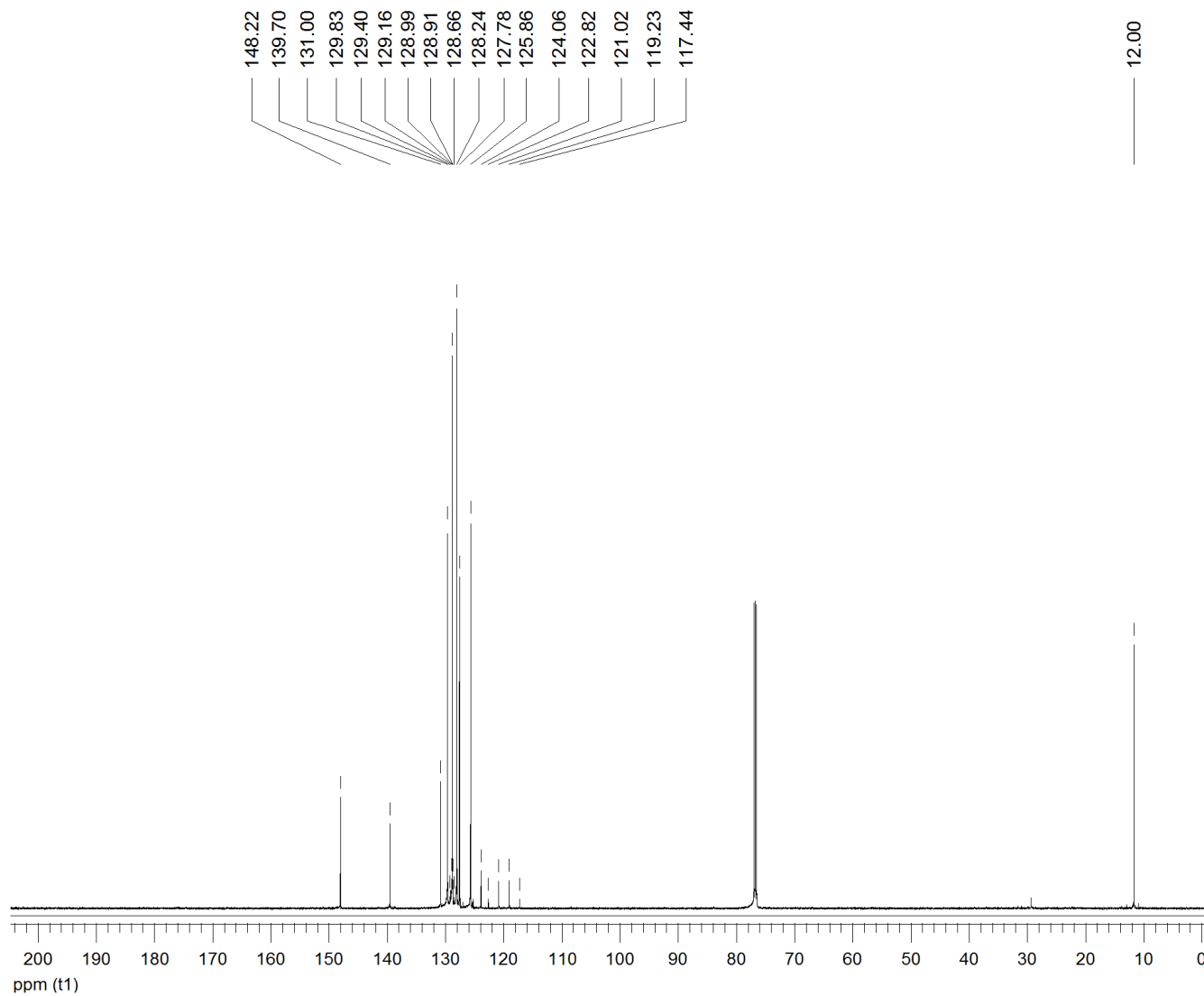
2d – $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



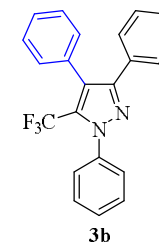
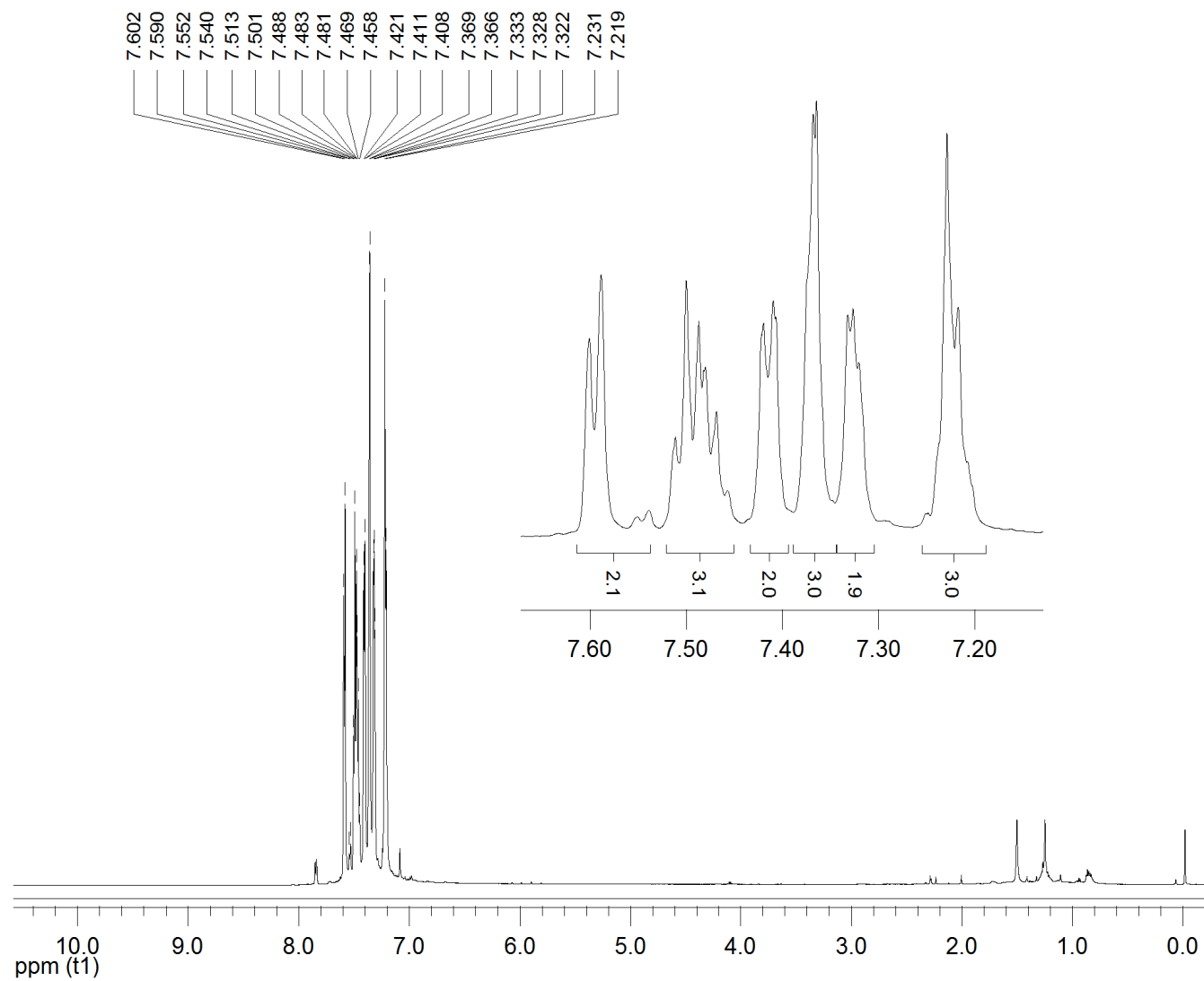
3a - ^1H NMR (600 MHz, CDCl_3 , 25 $^\circ\text{C}$)



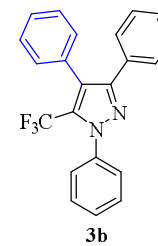
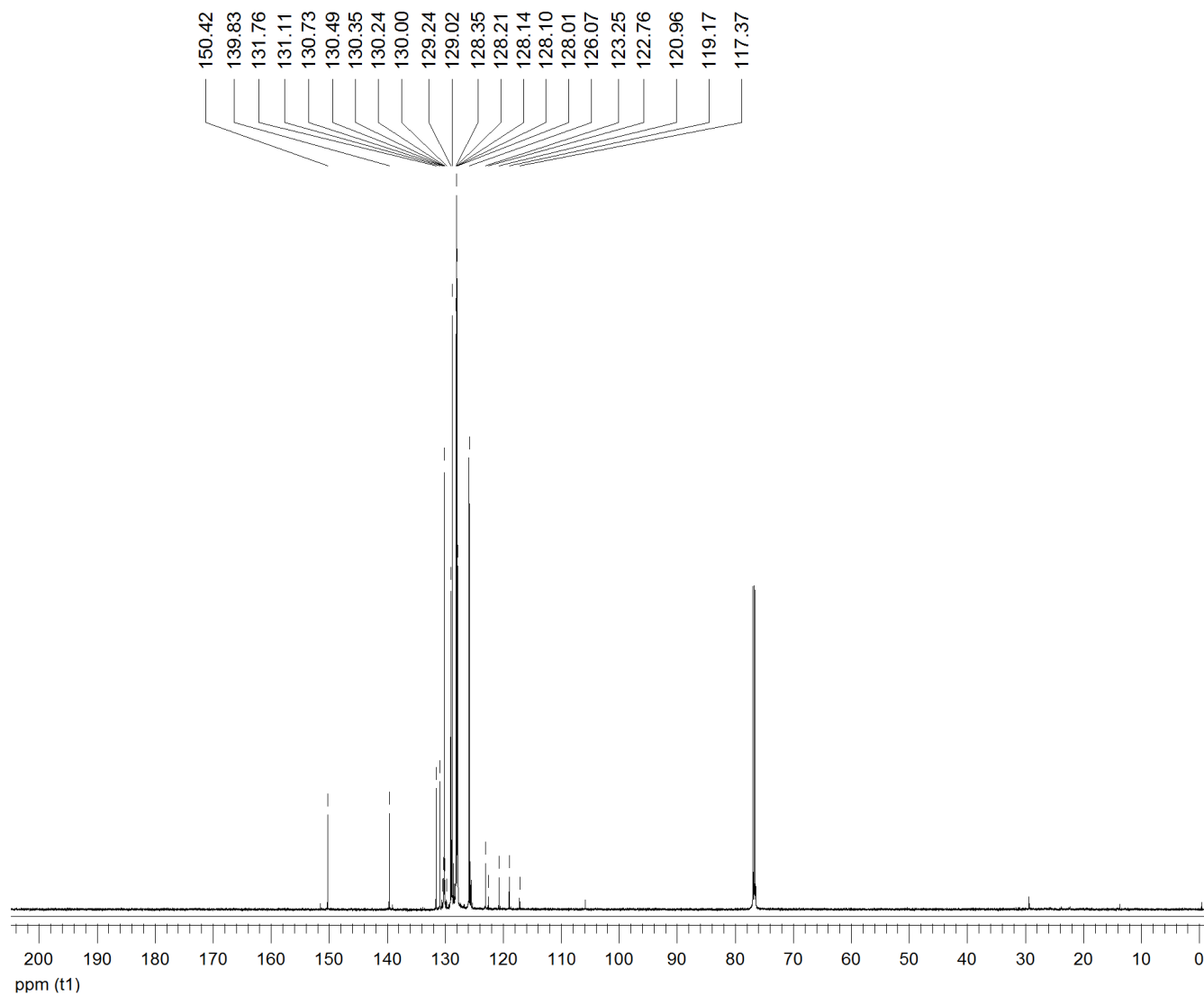
3a - $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CDCl_3 , 25 °C)



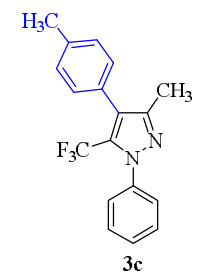
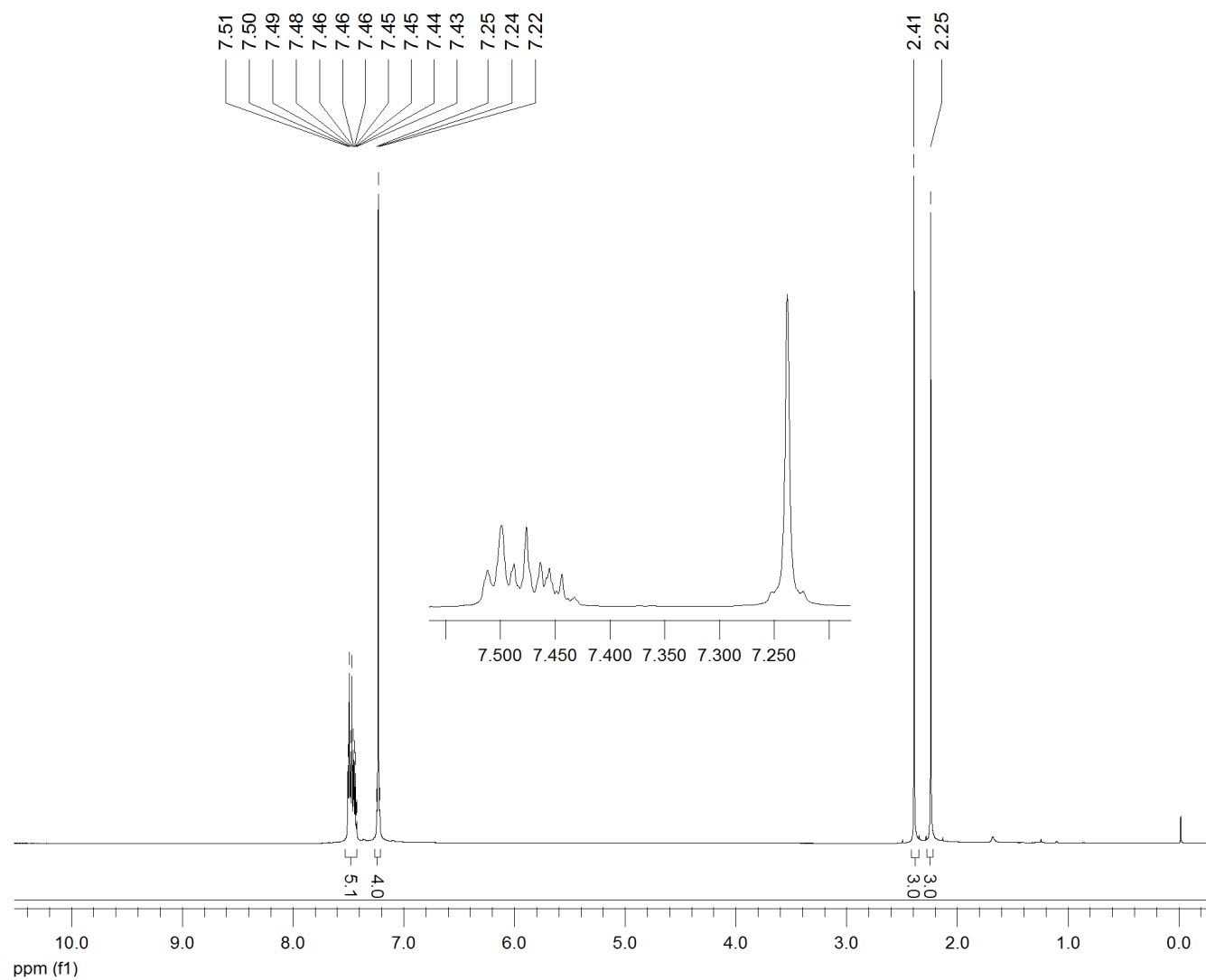
3b - ^1H NMR (600 MHz, CDCl_3 , 25 $^\circ\text{C}$)



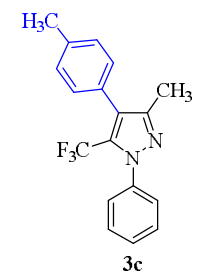
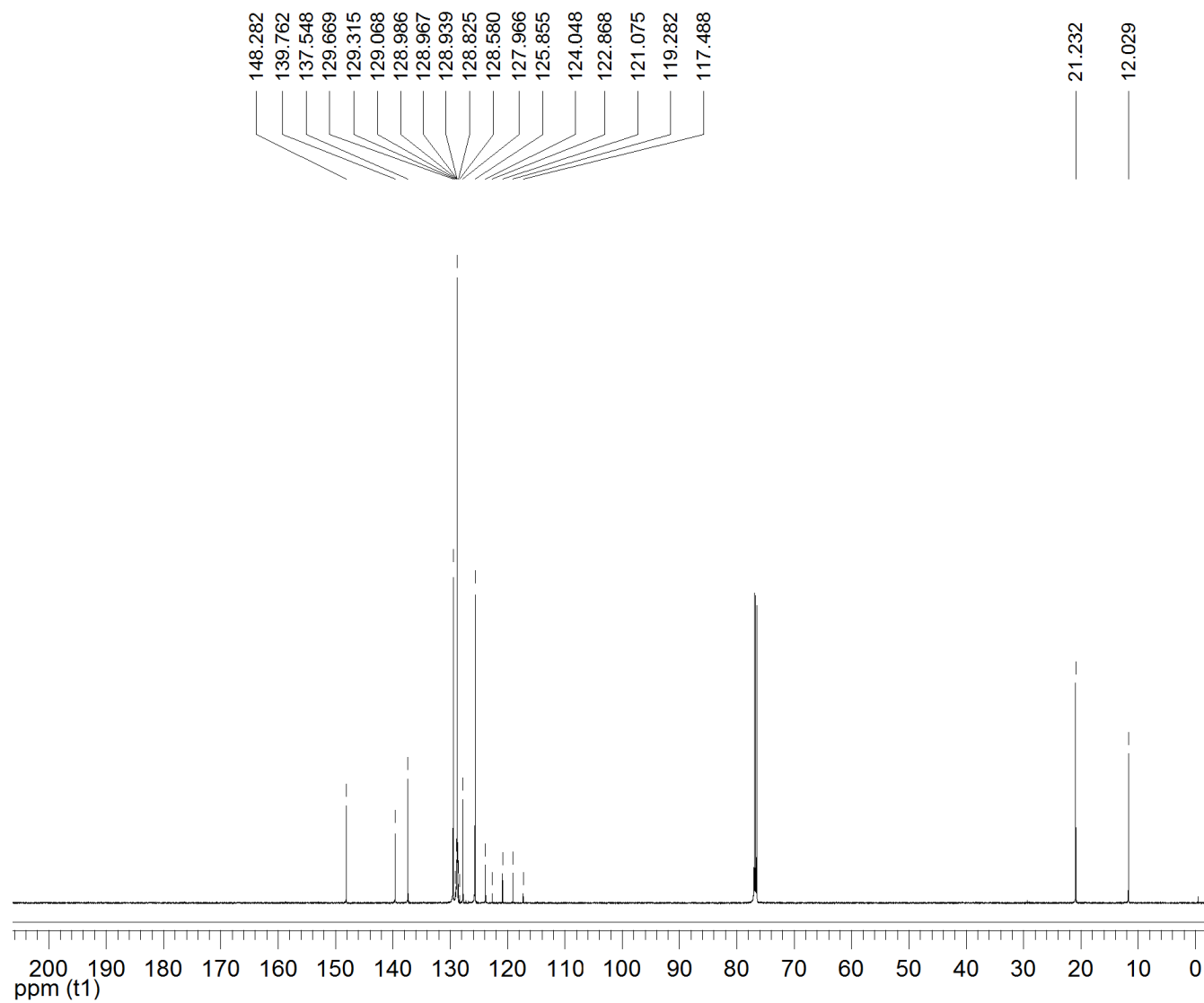
3b - $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CDCl_3 , 25 °C)



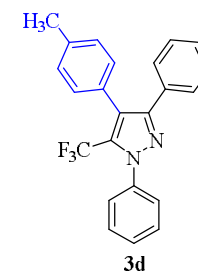
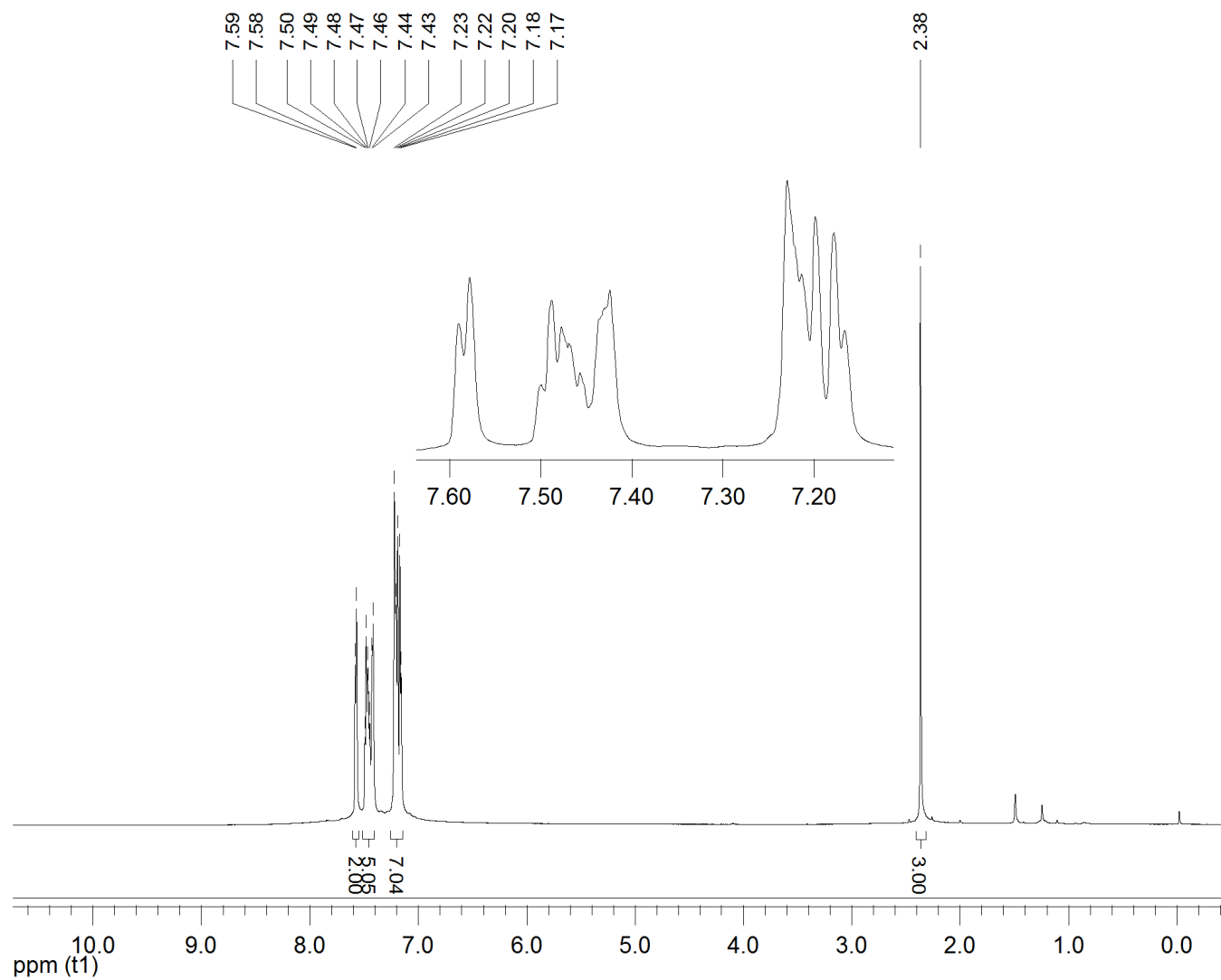
3c - ^1H NMR (600 MHz, CDCl_3 , 25 $^\circ\text{C}$)



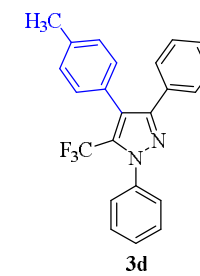
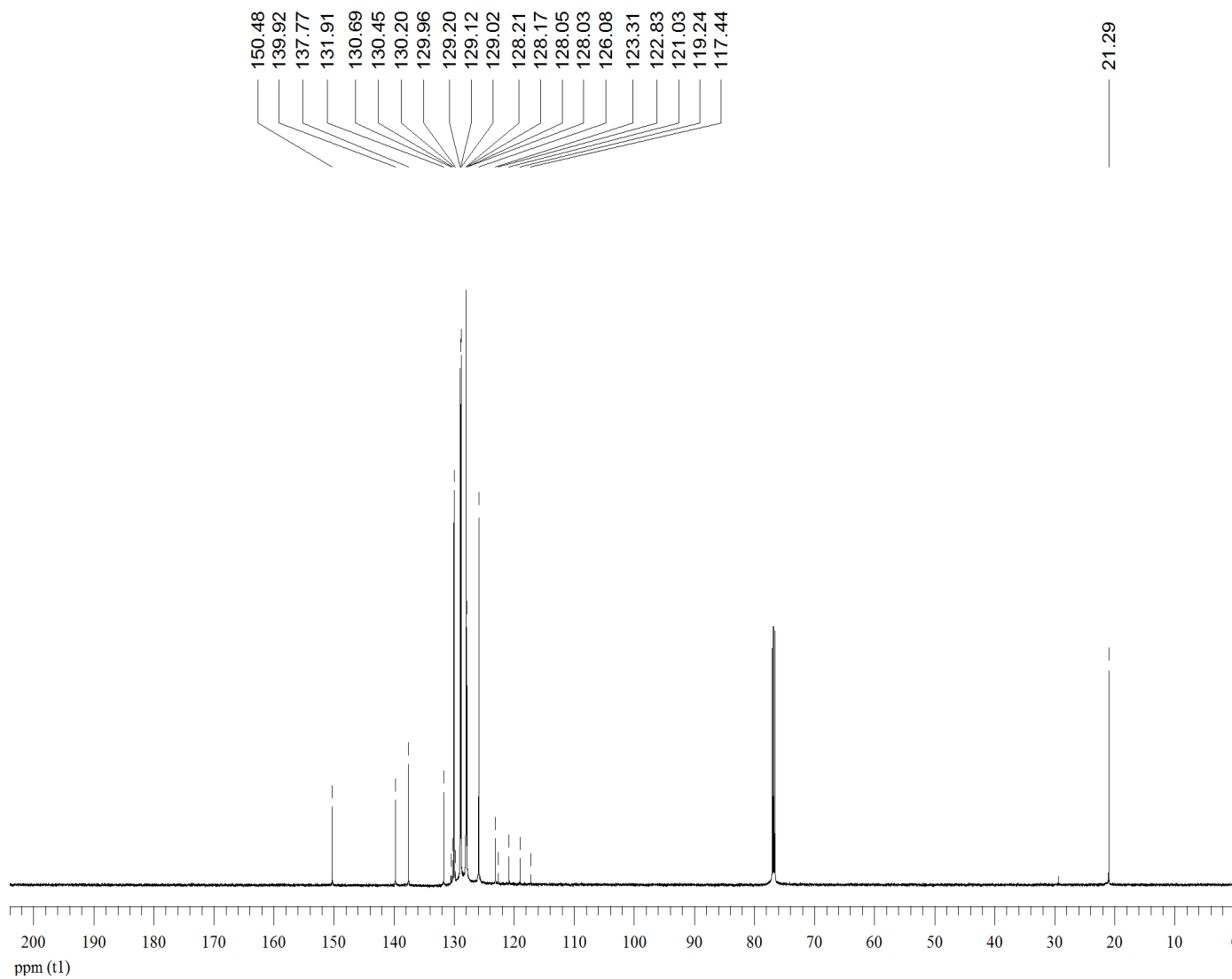
3c - $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CDCl_3 , 25 °C)



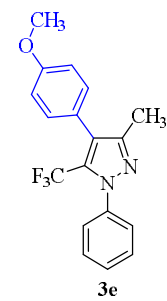
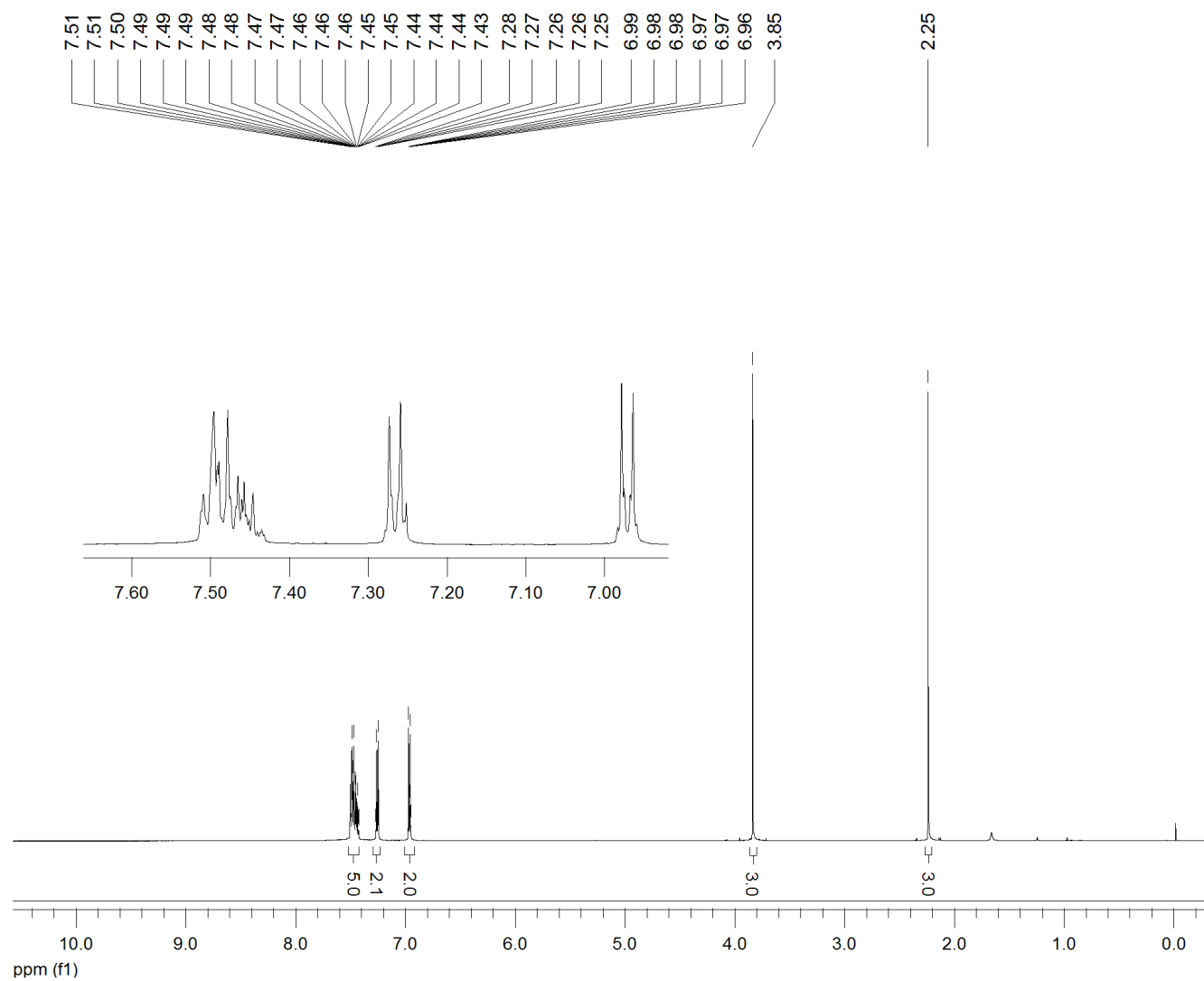
3d - ^1H NMR (600 MHz, CDCl_3 , 25 $^\circ\text{C}$)



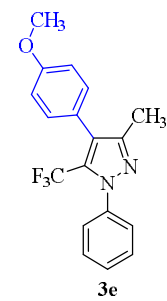
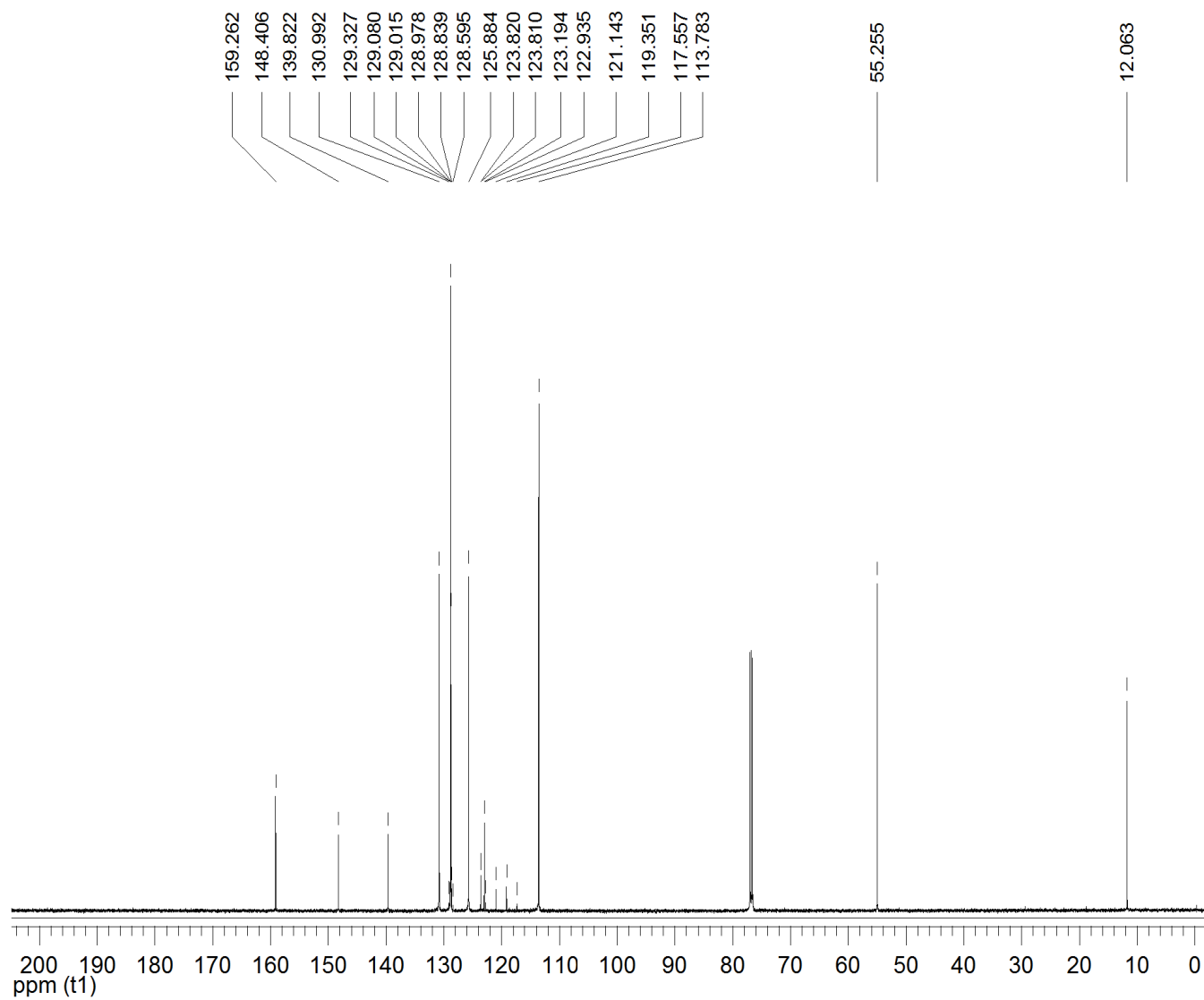
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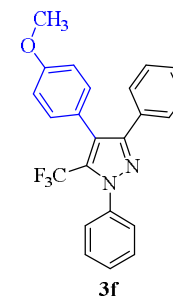
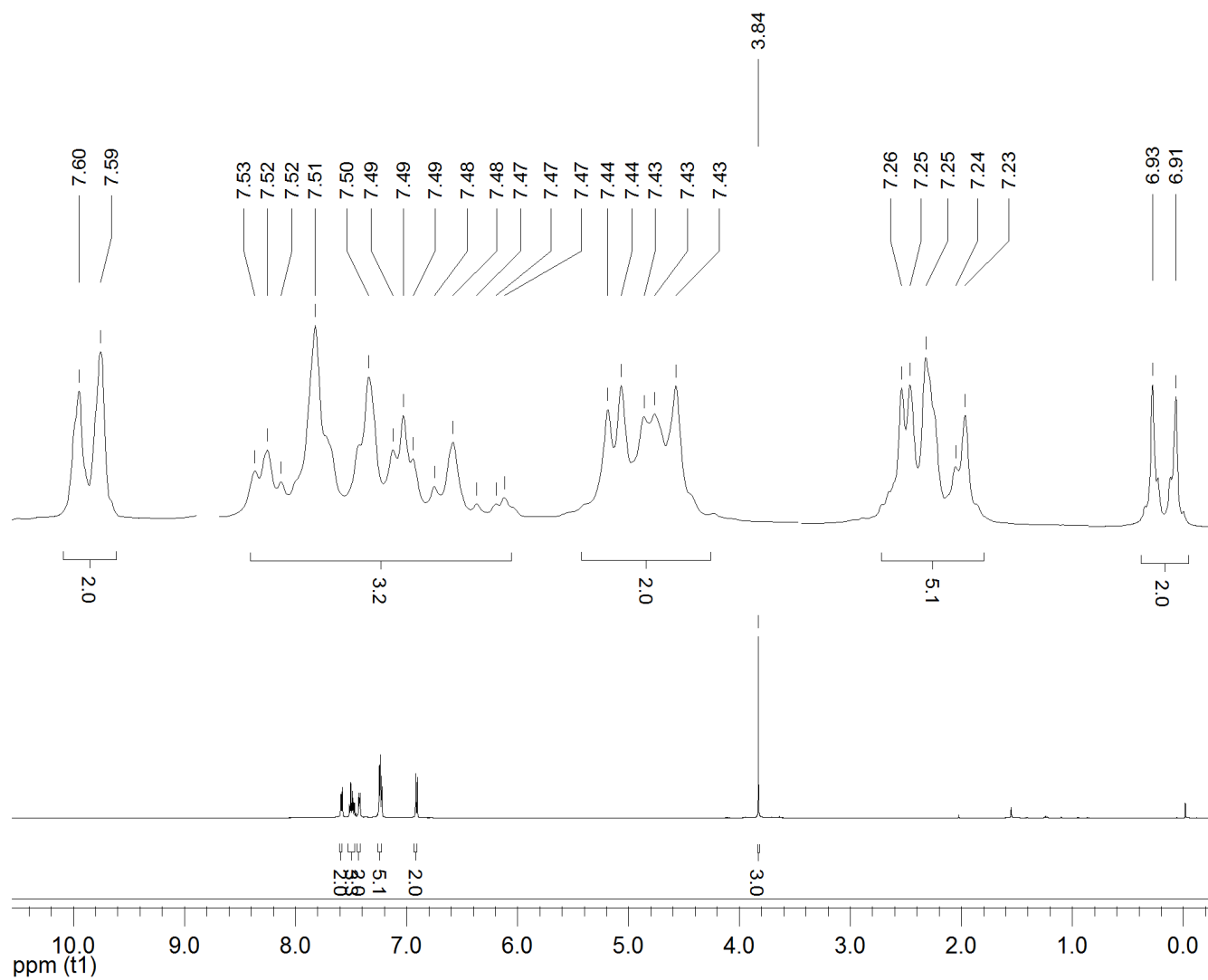
3e - ^1H NMR (600 MHz, CDCl_3 , 25 $^\circ\text{C}$)



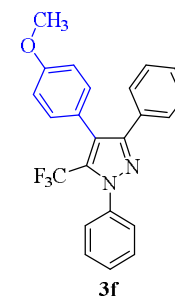
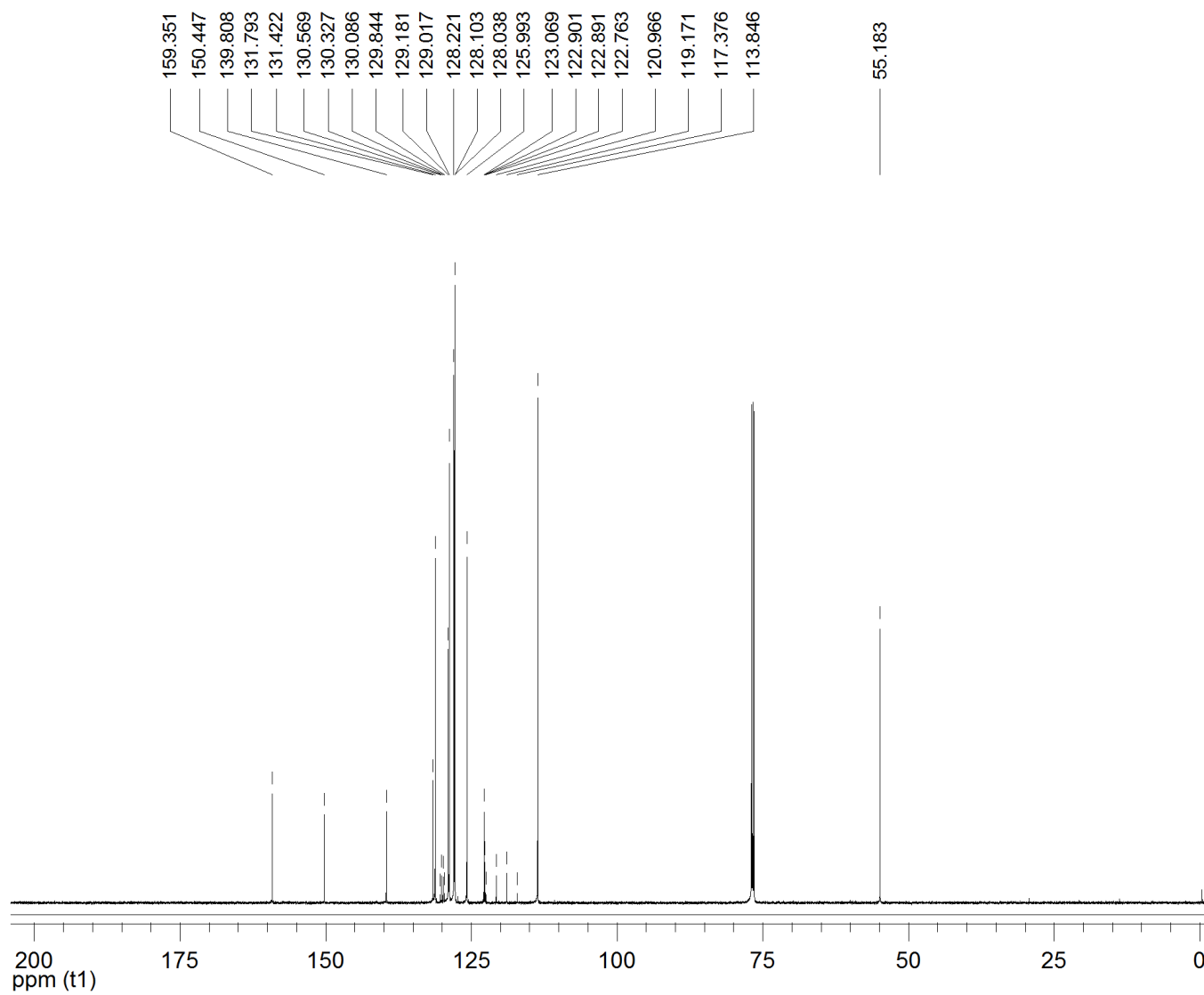
3e – $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CDCl_3 , 25 °C)



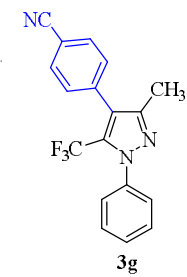
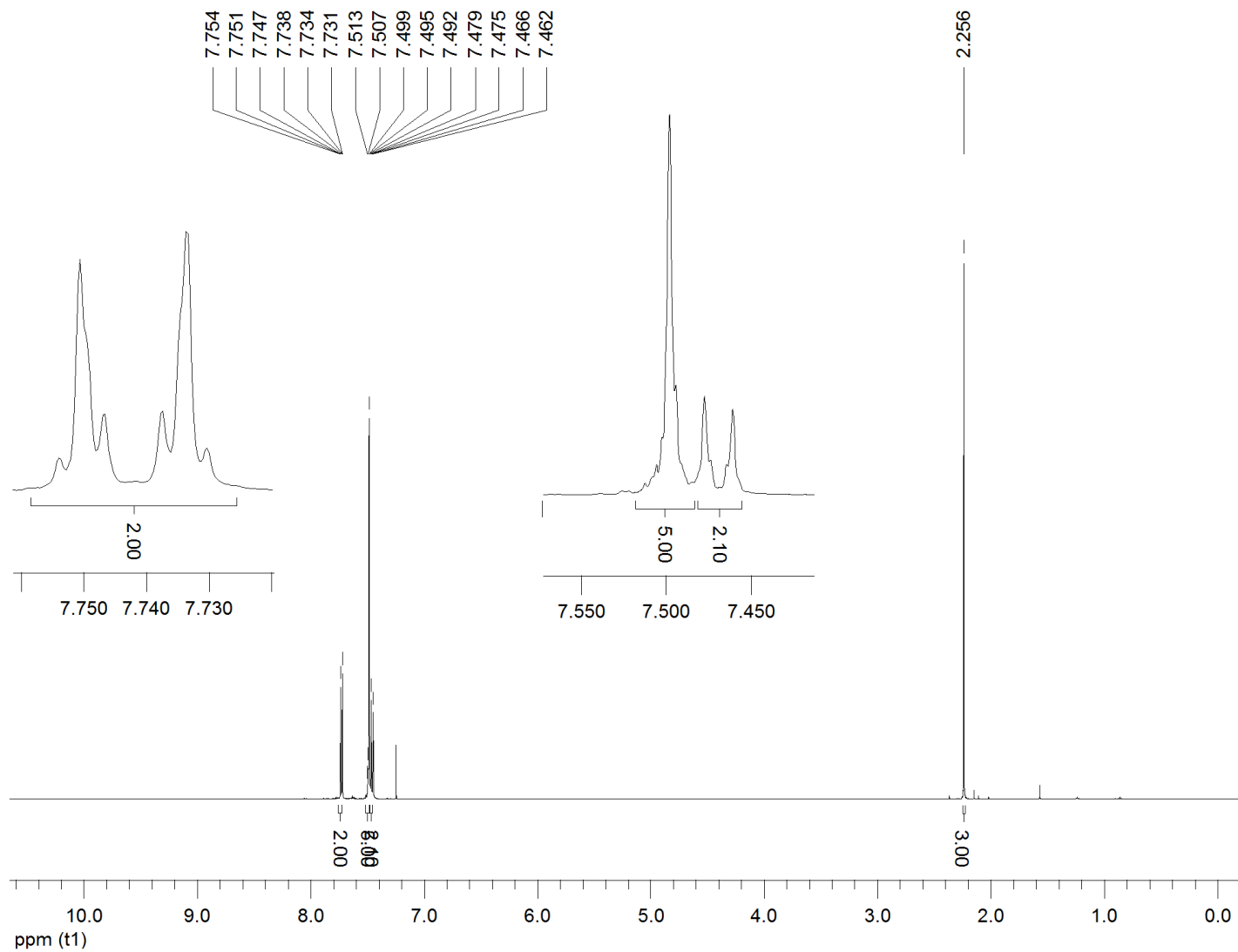
3f - ^1H NMR (600 MHz, CDCl_3 , 25 $^\circ\text{C}$)



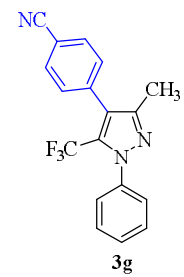
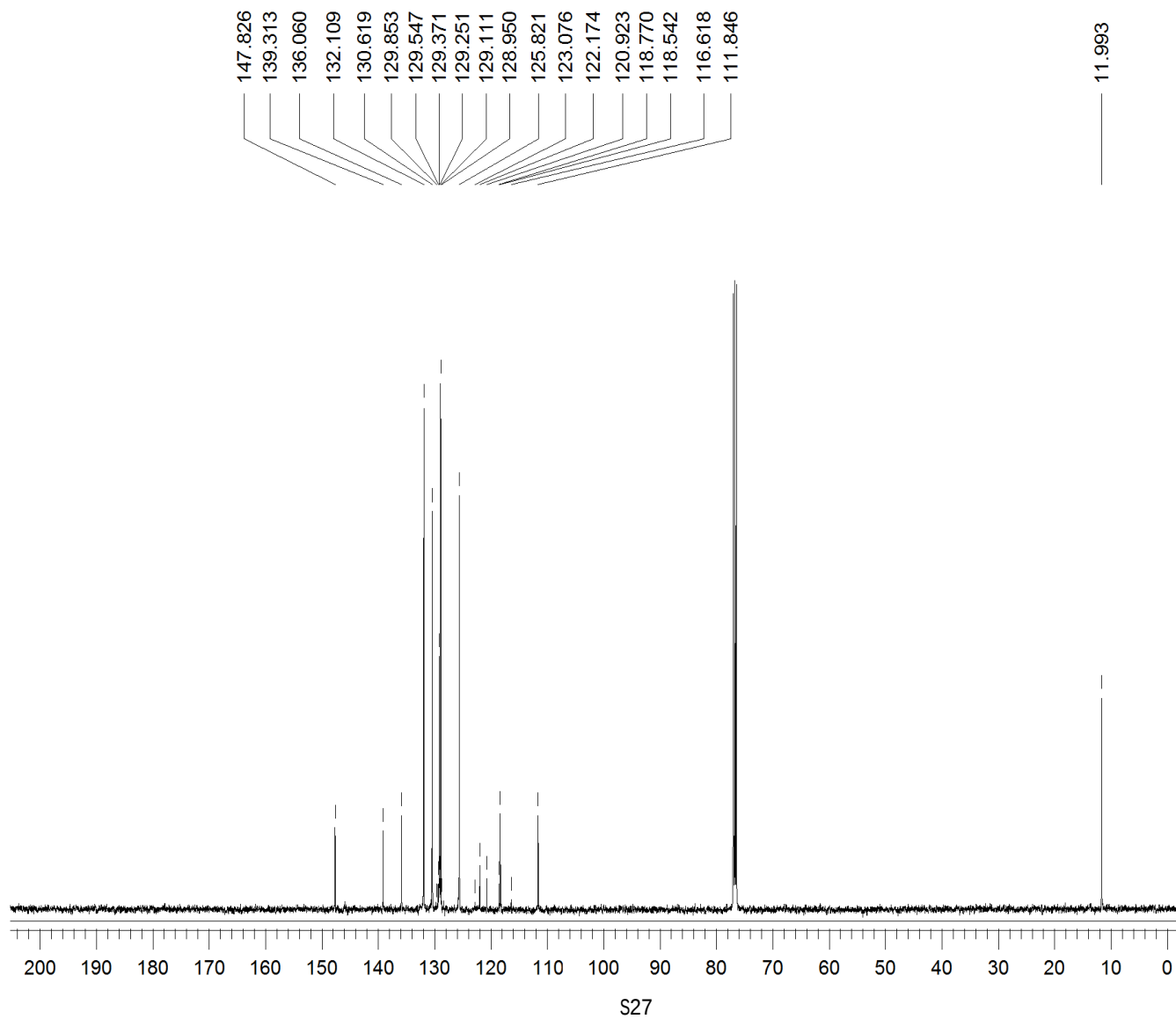
3f – $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, CDCl_3 , 25 °C)



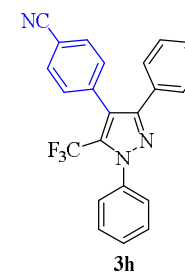
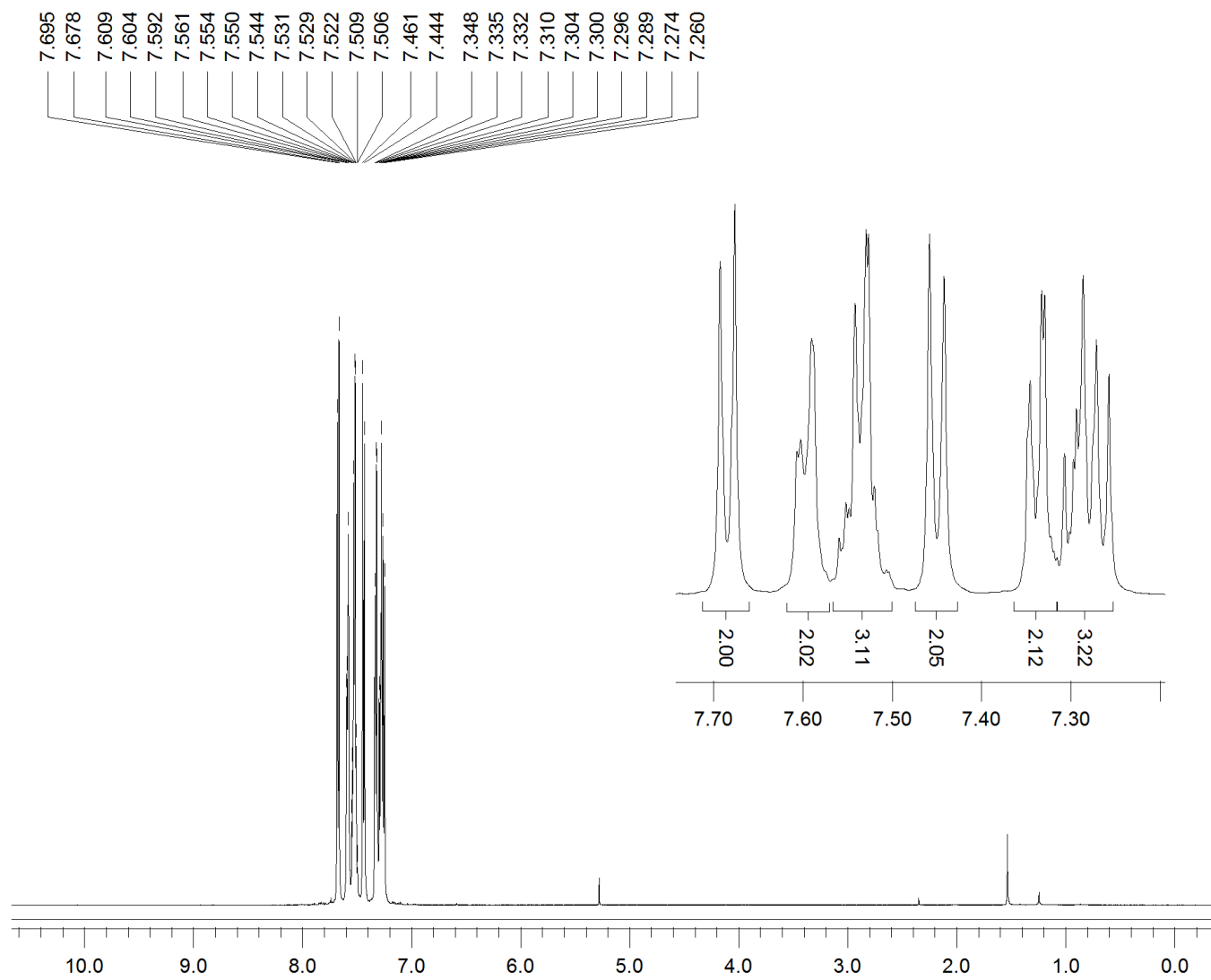
3g - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



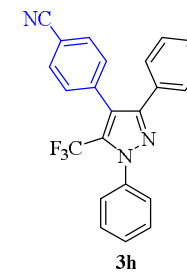
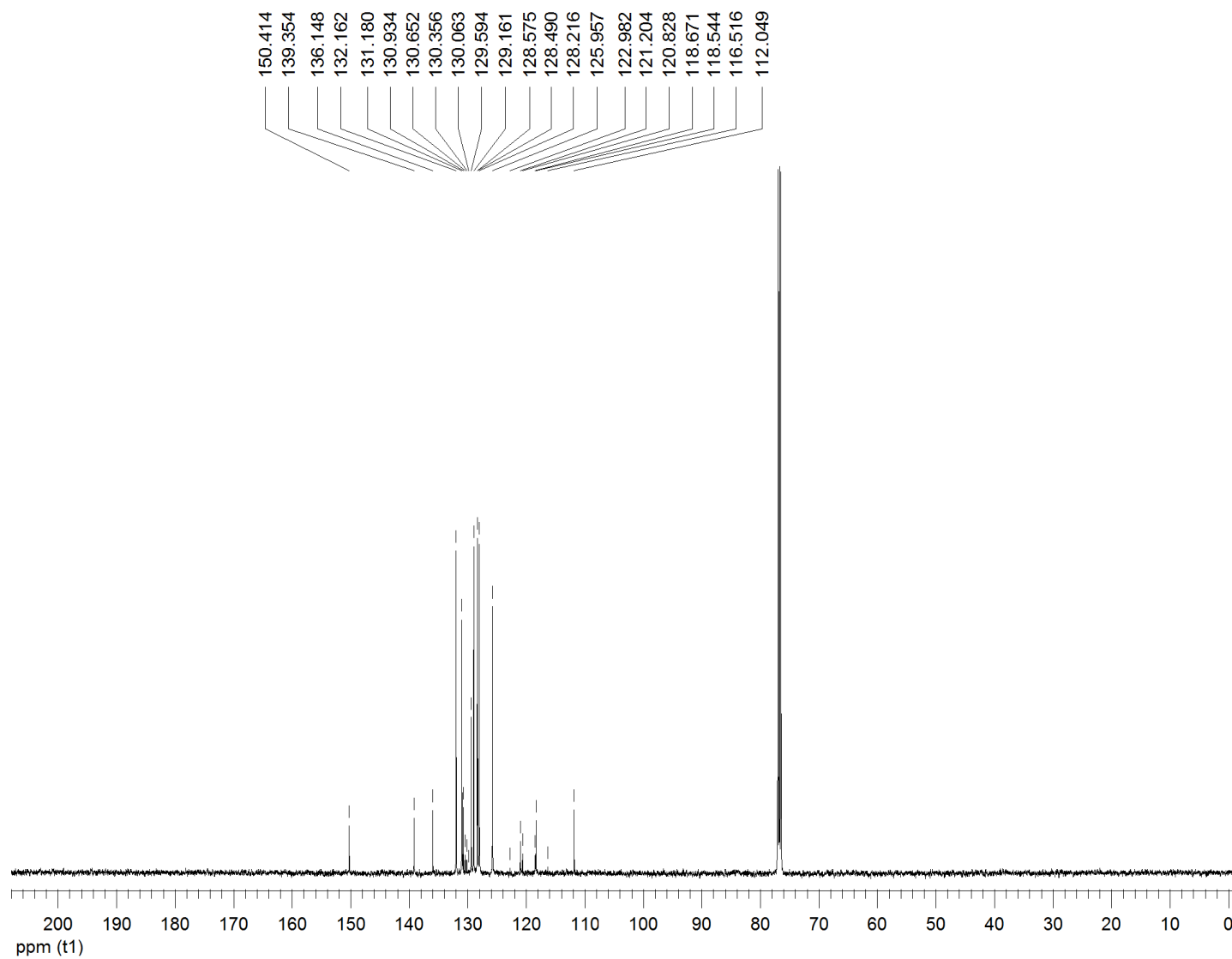
3g - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



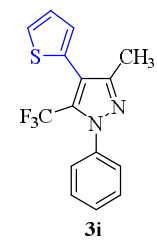
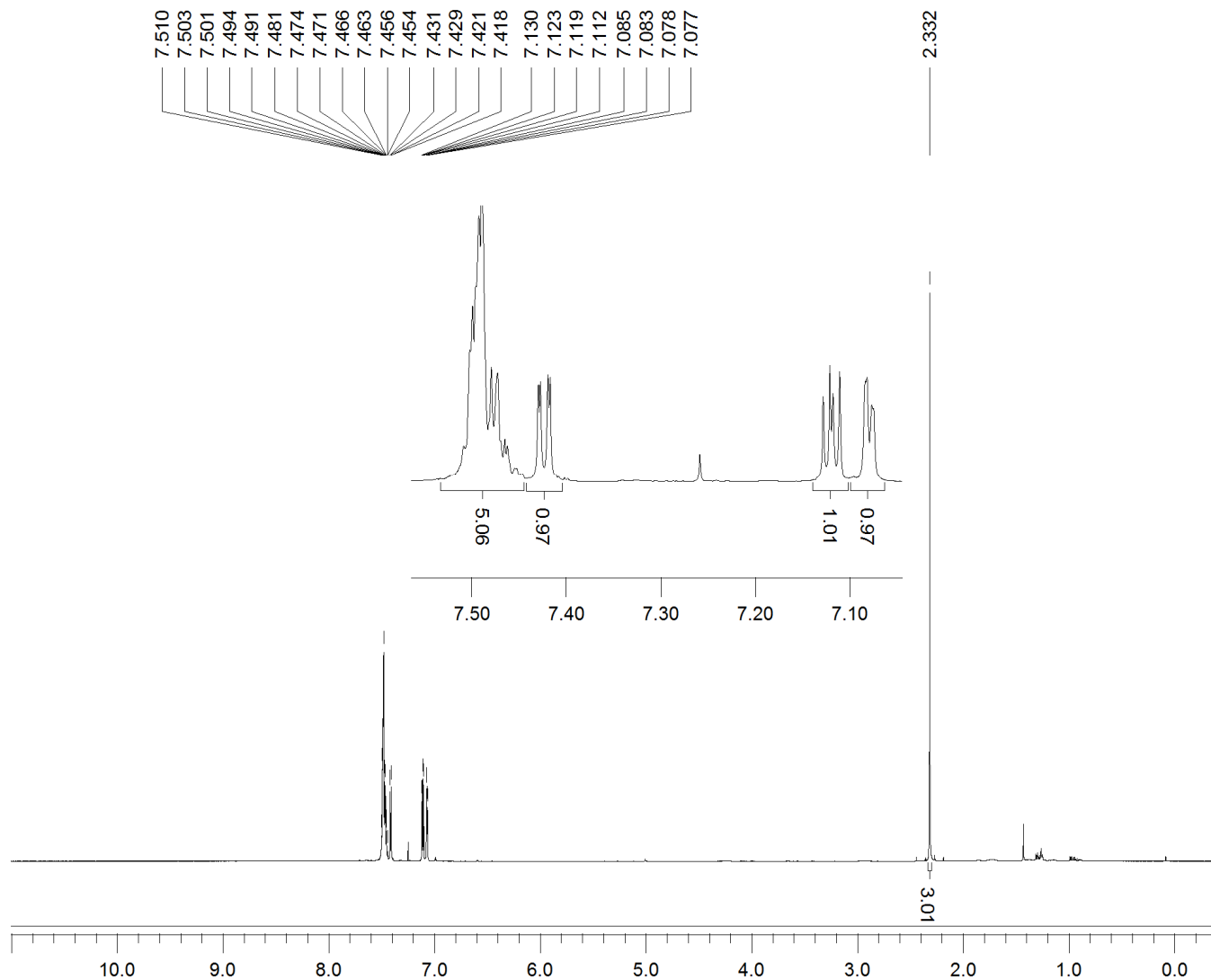
3h - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



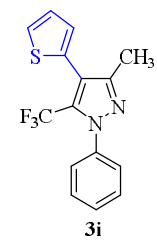
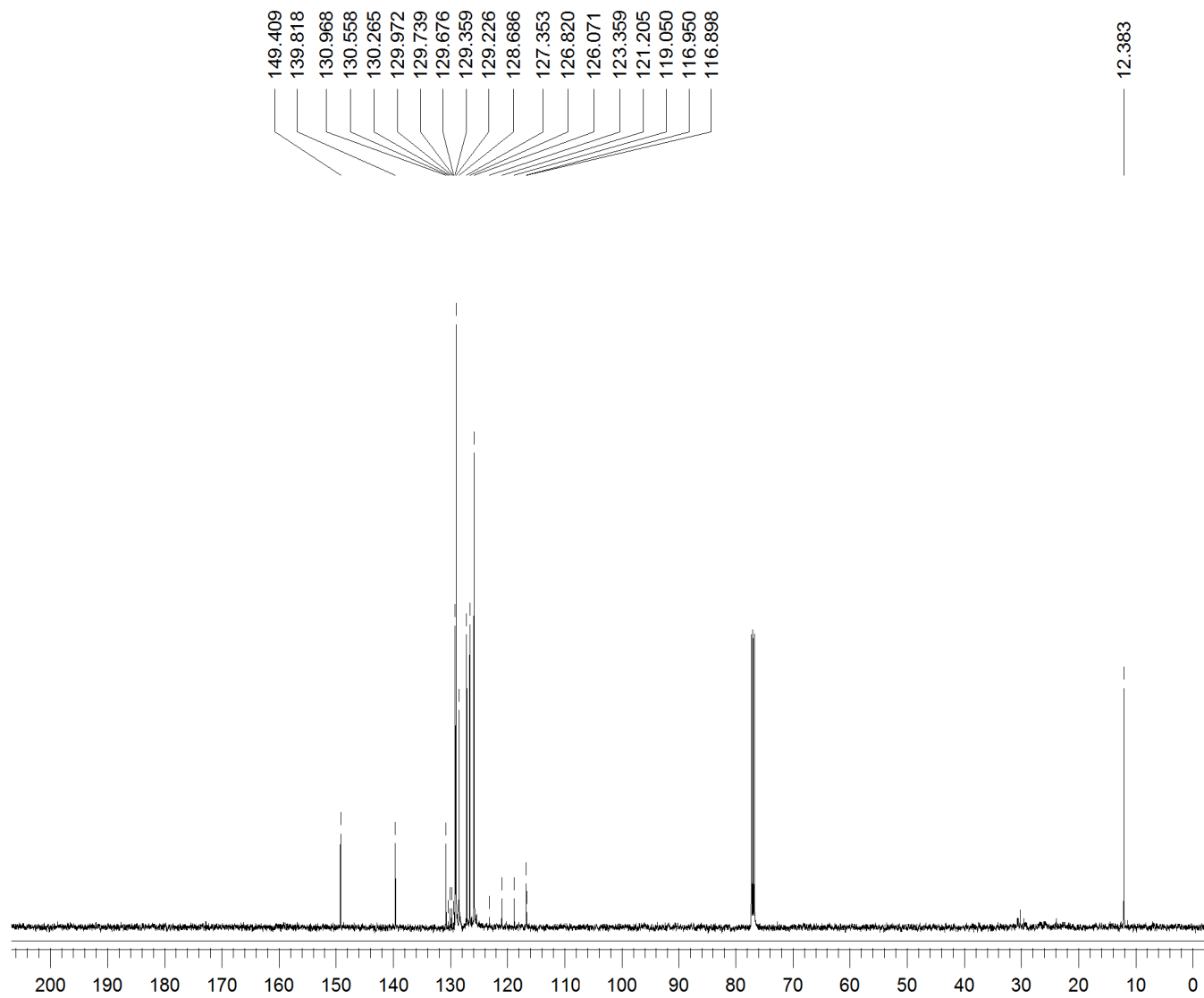
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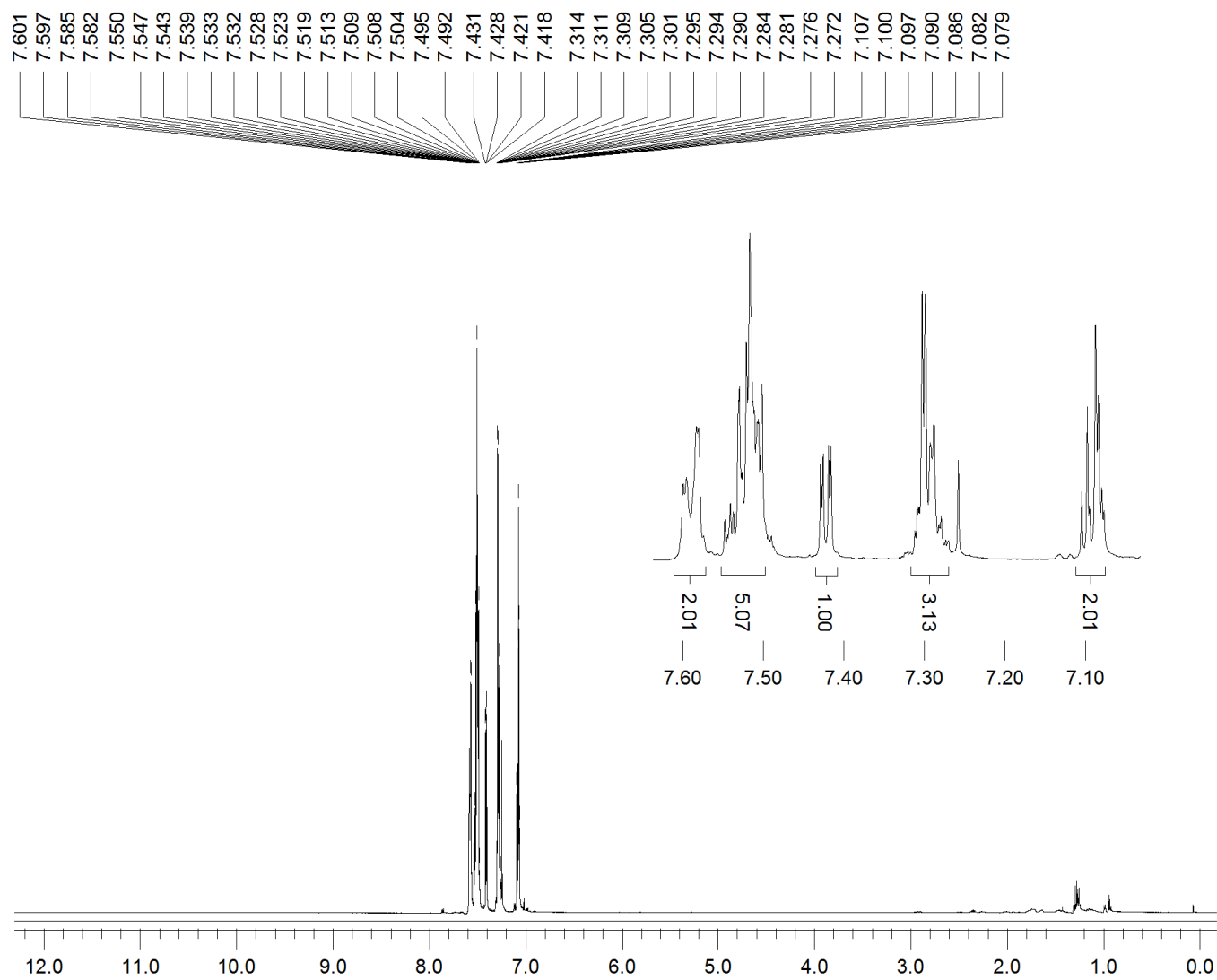
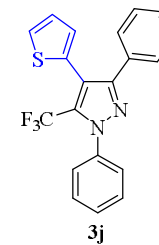
3i - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



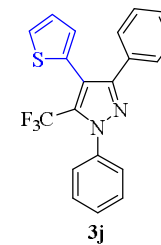
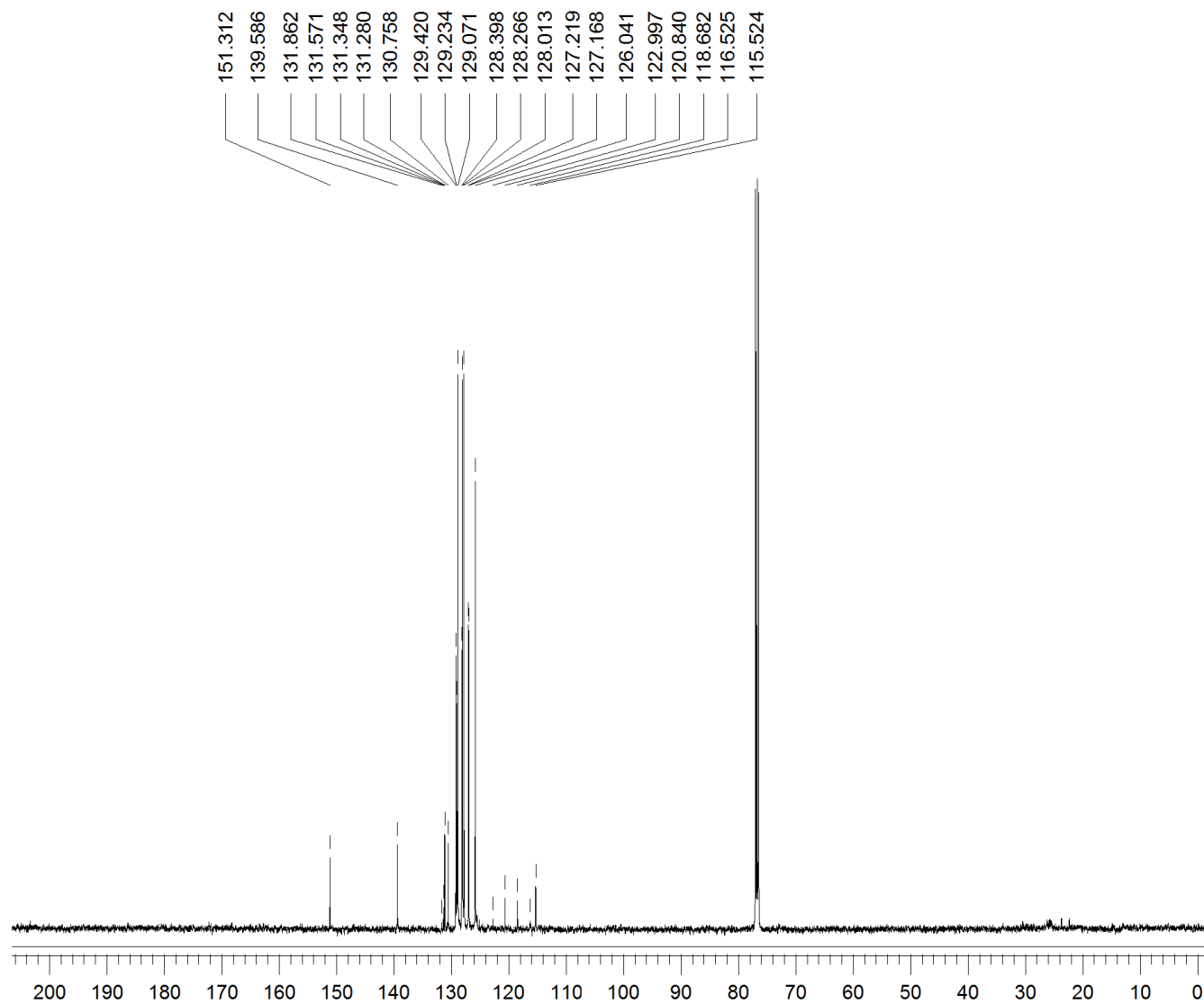
3i - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



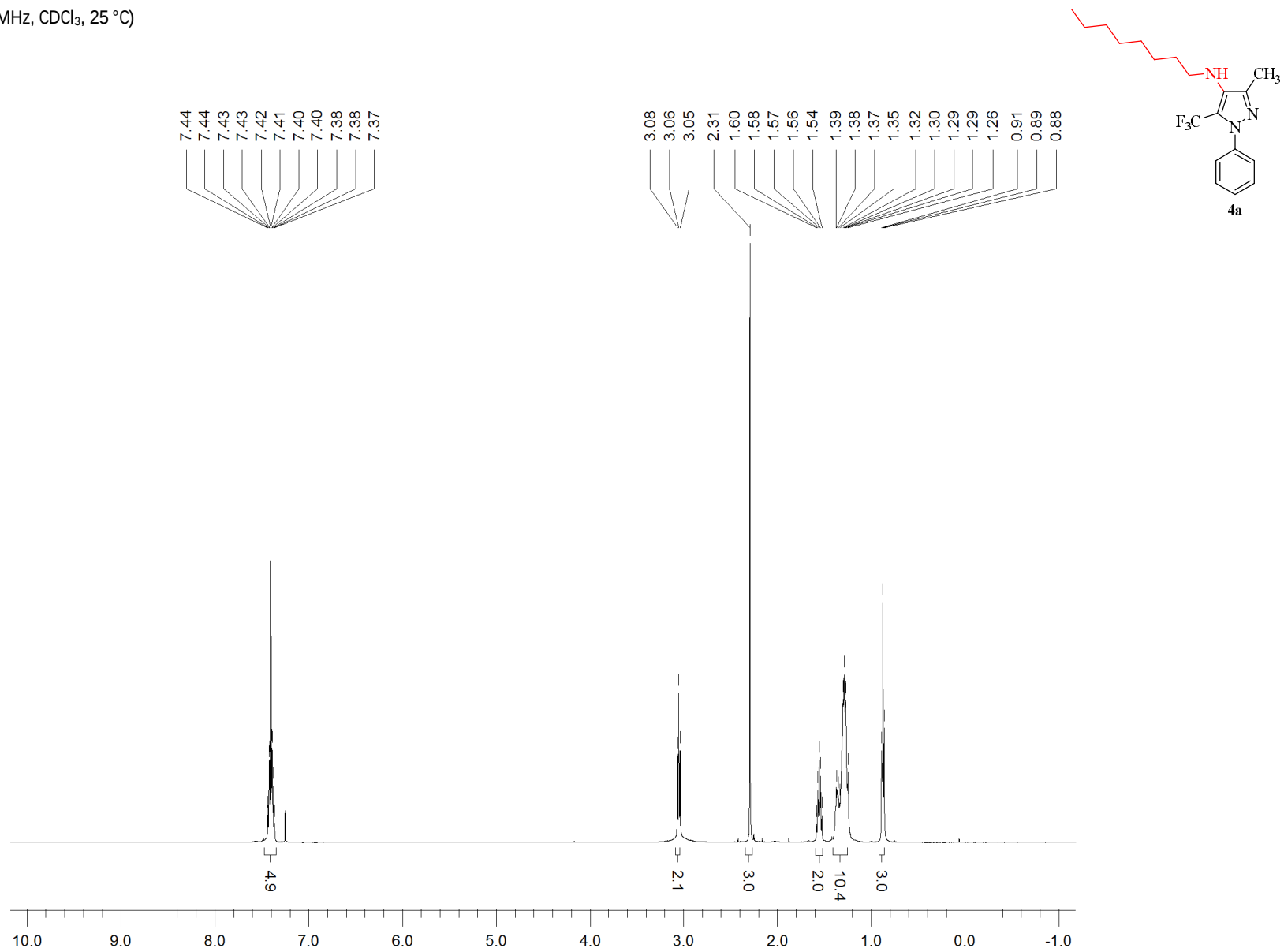
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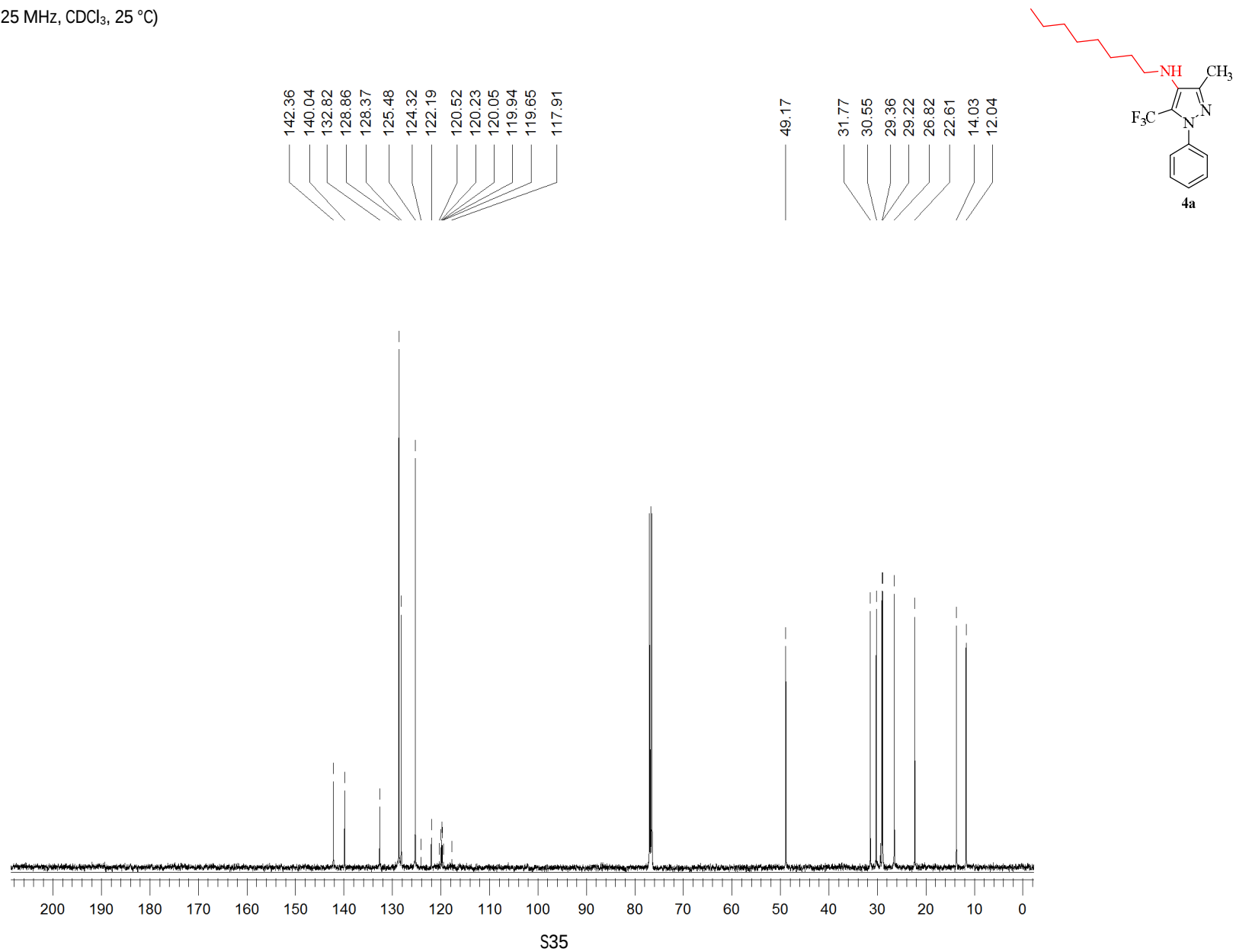
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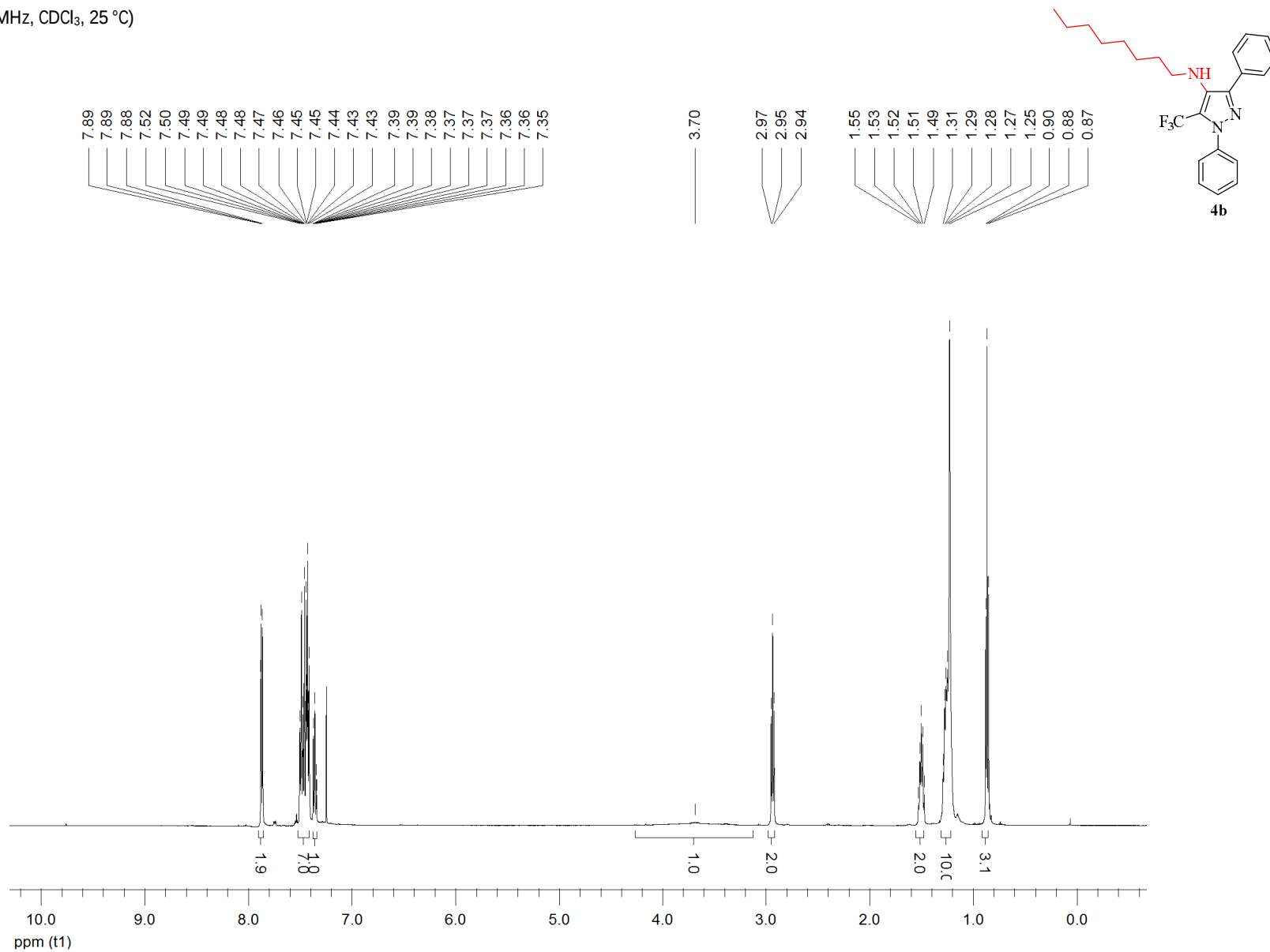
4a - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



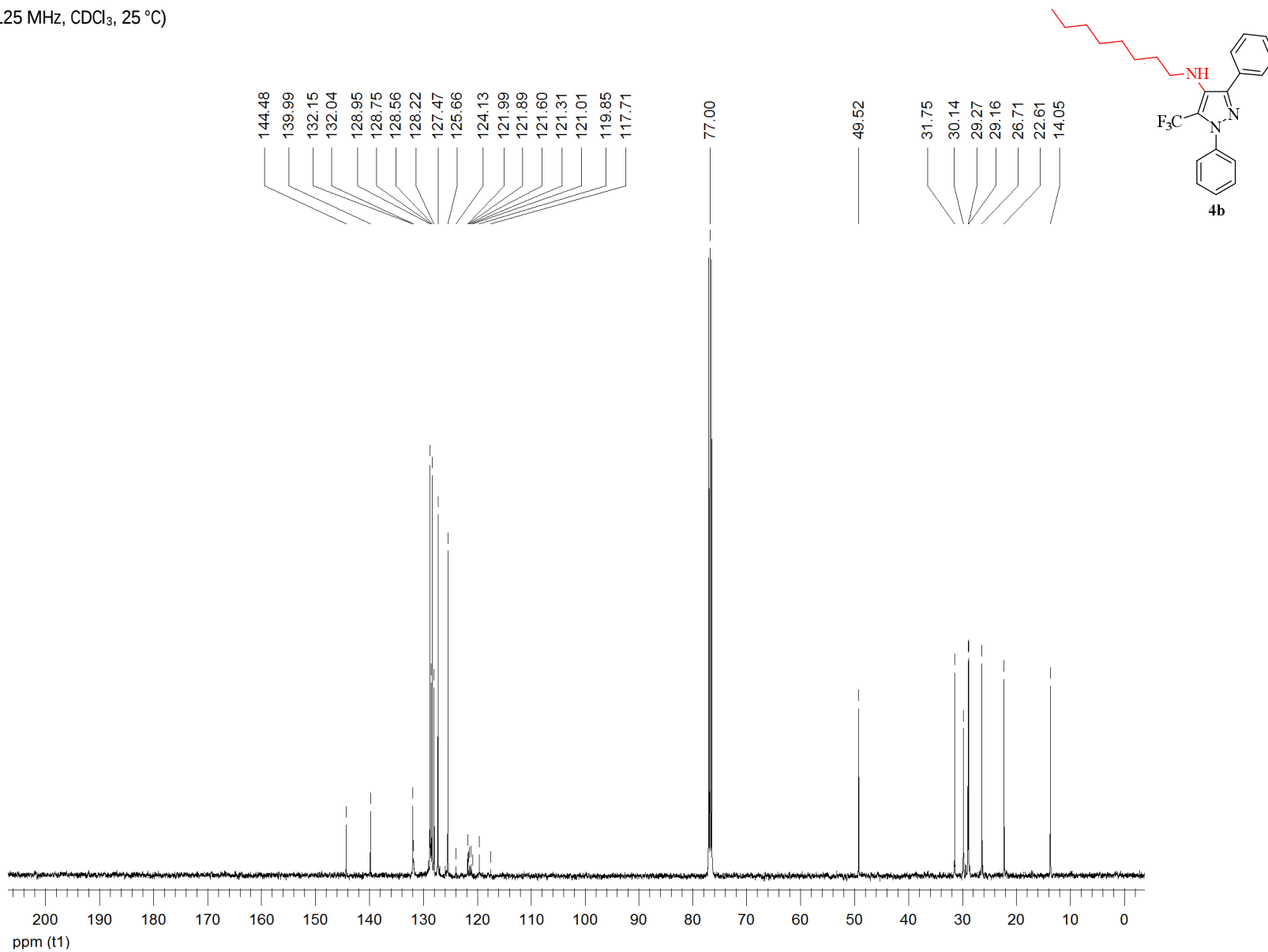
4a - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



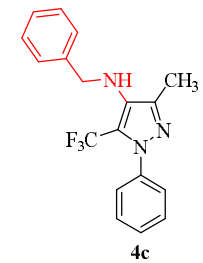
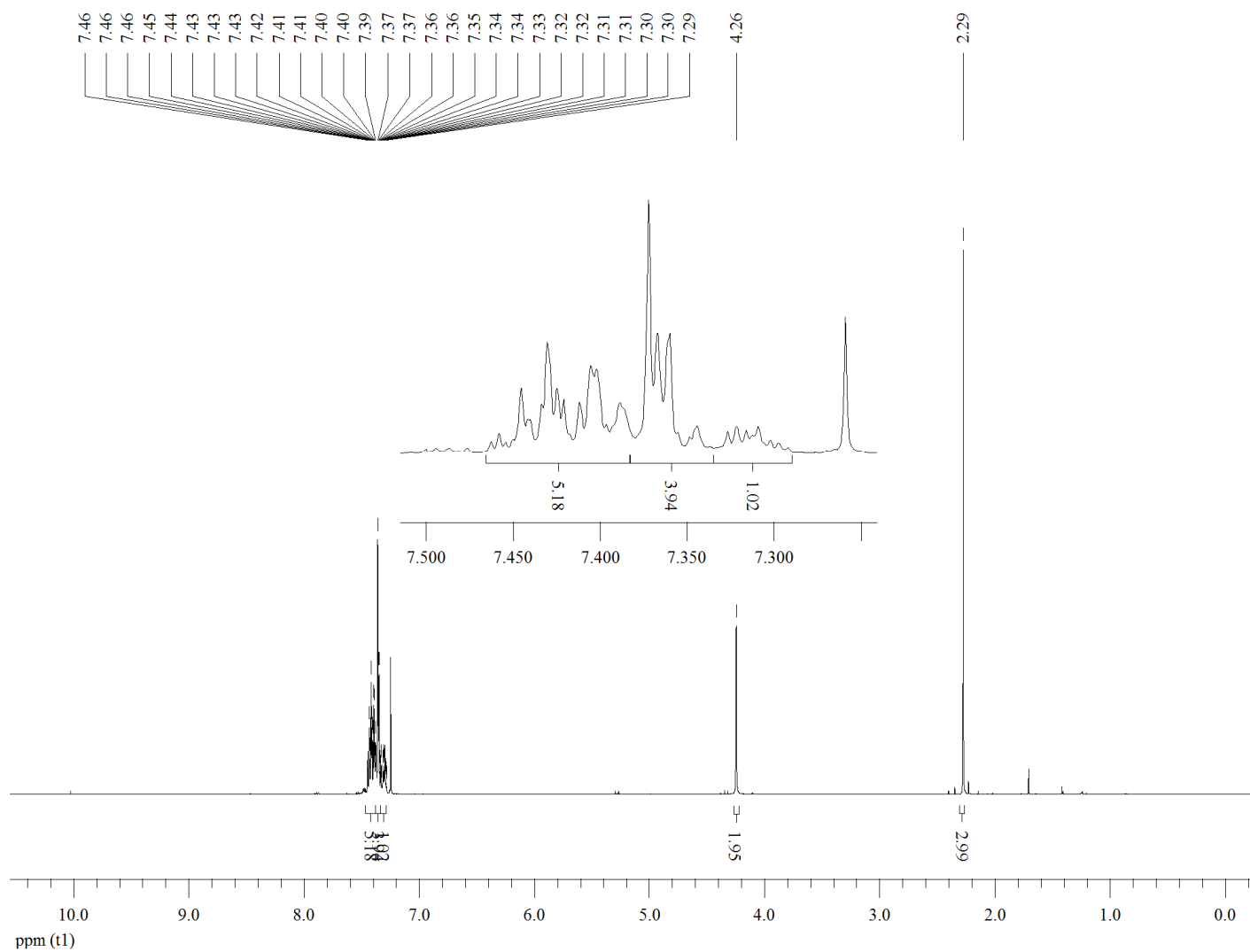
4b - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



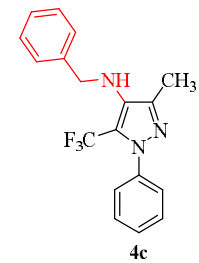
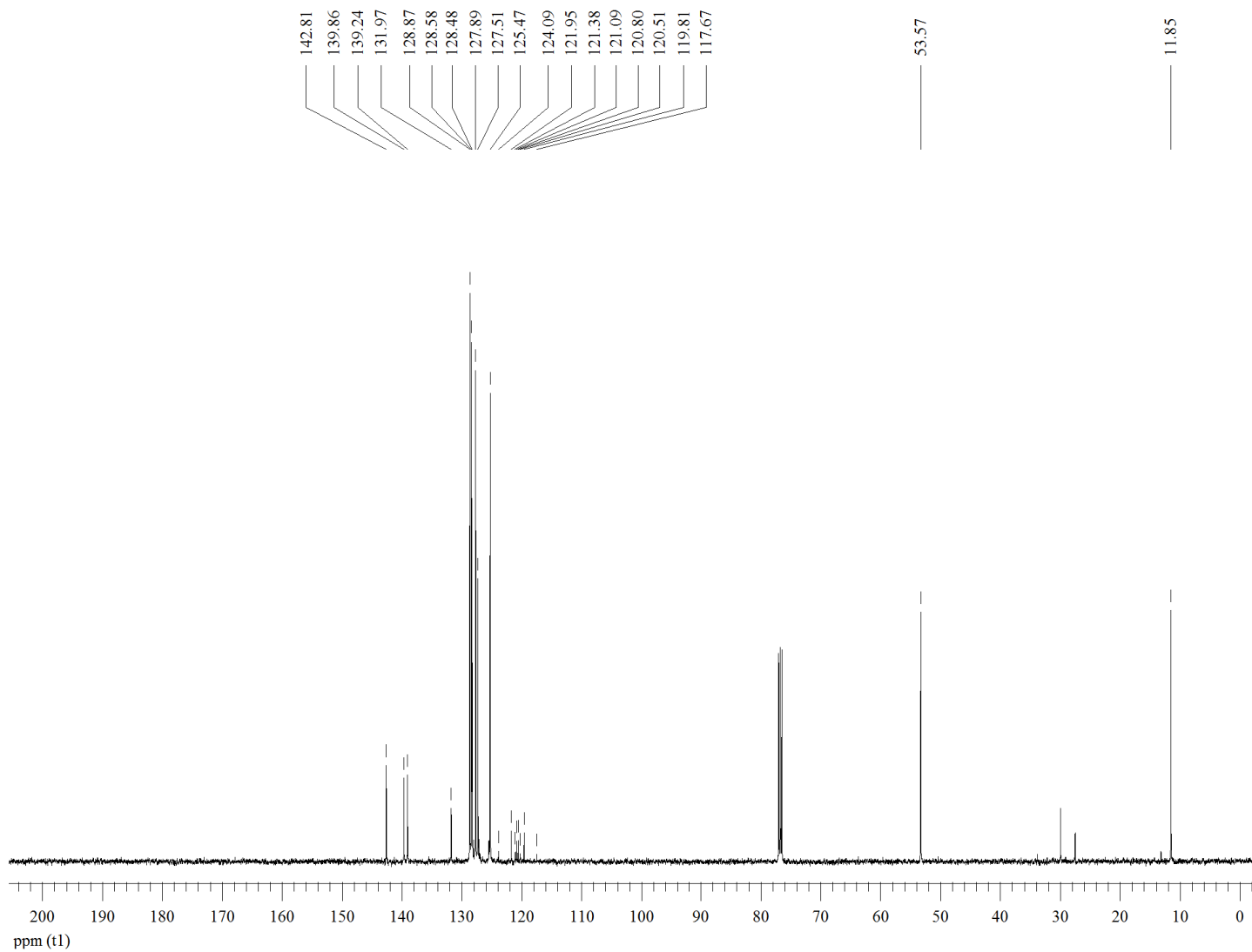
4b - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



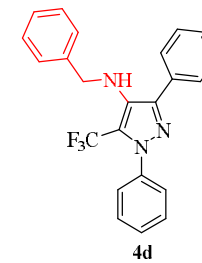
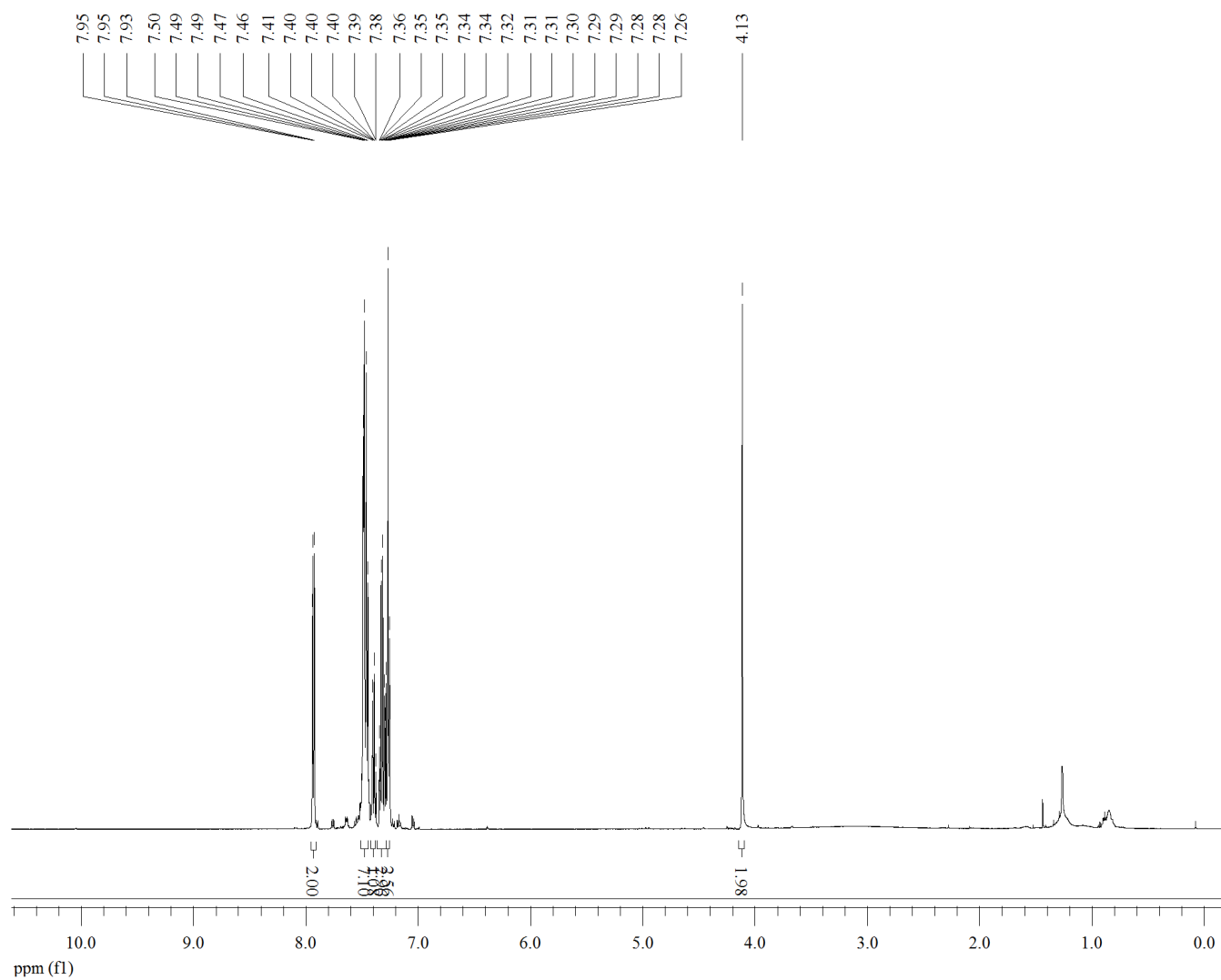
4c - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



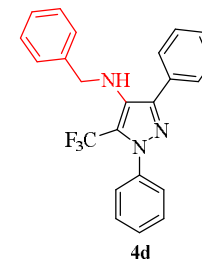
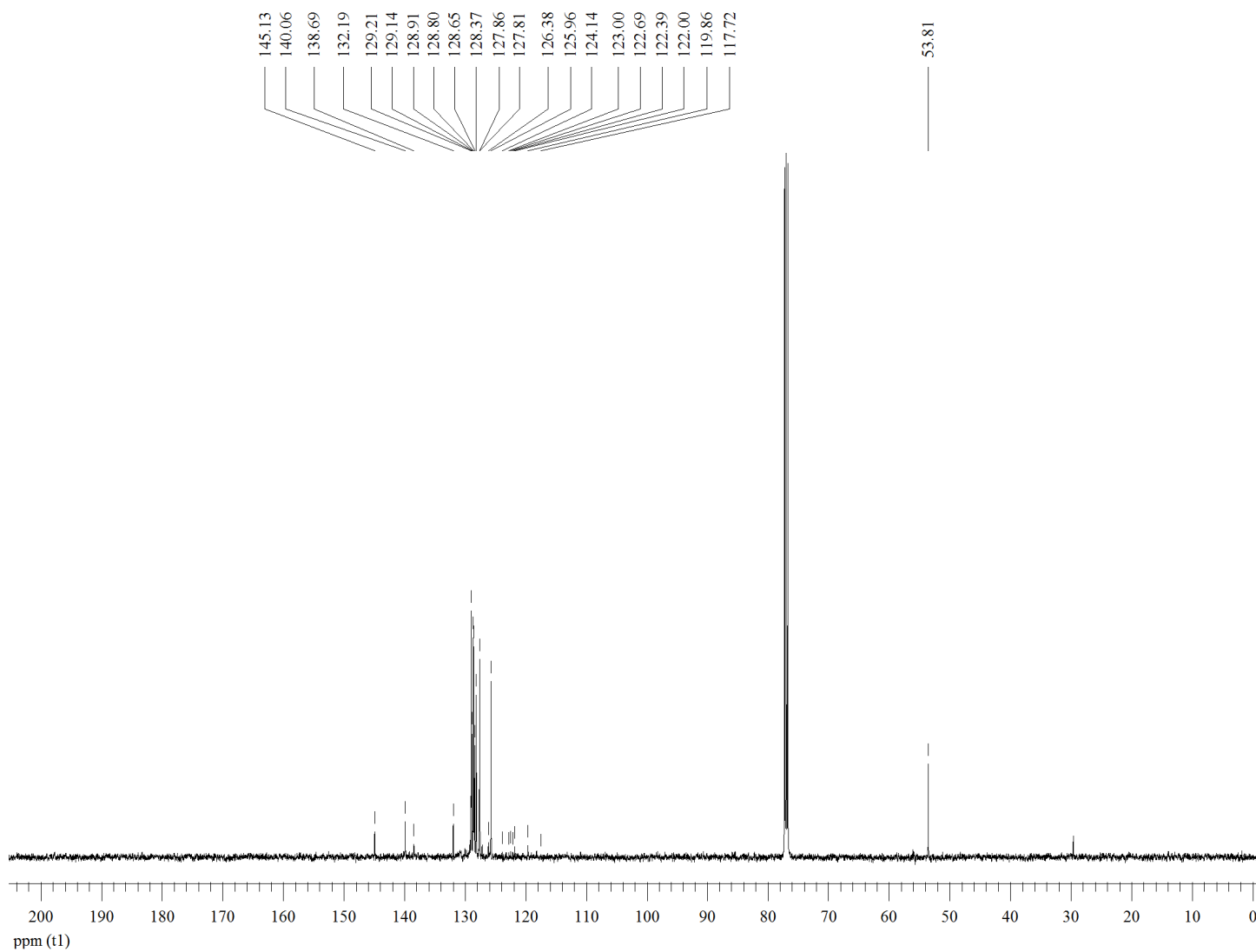
4c - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



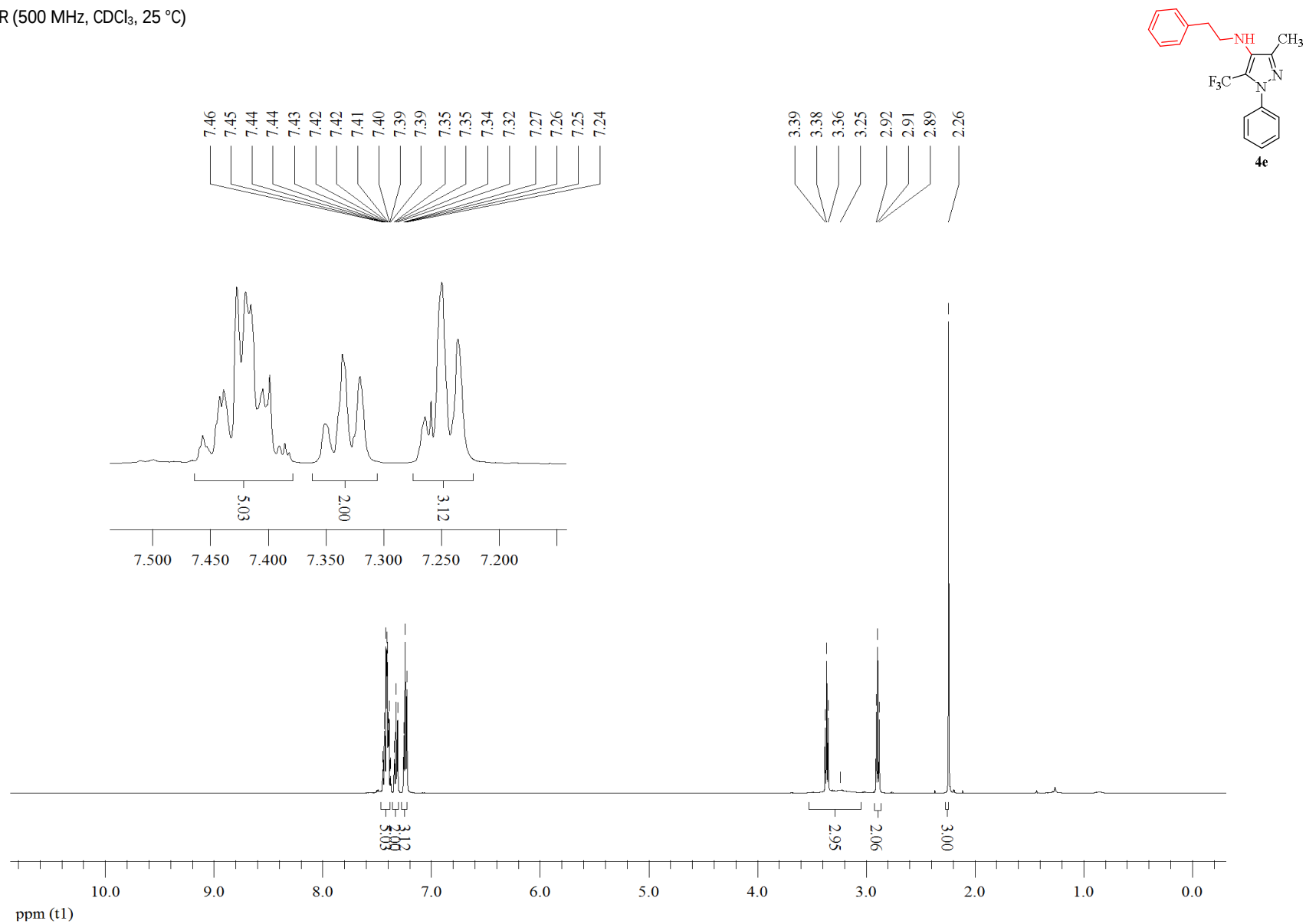
4d - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



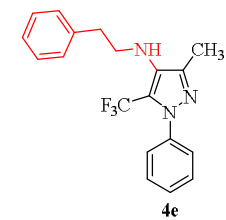
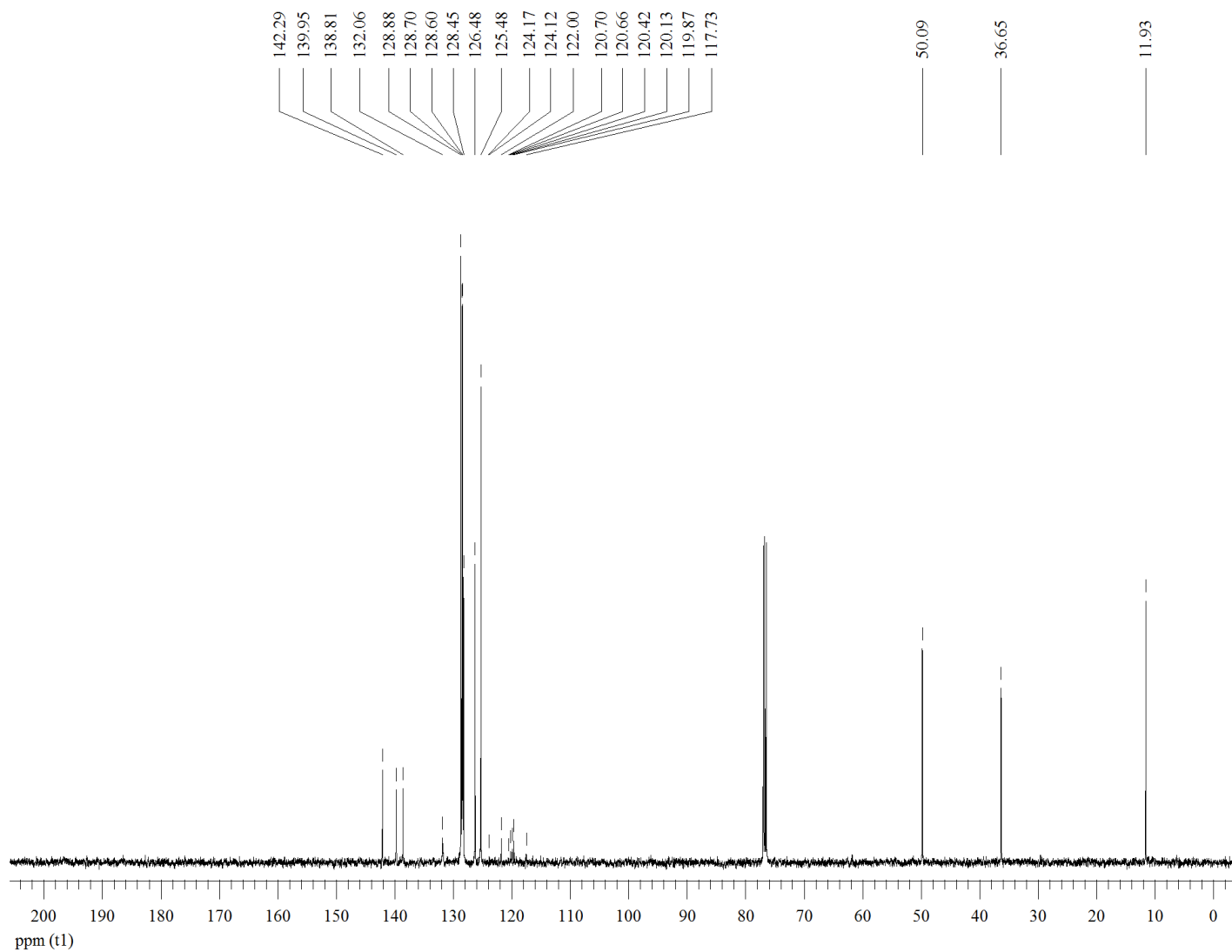
4d - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



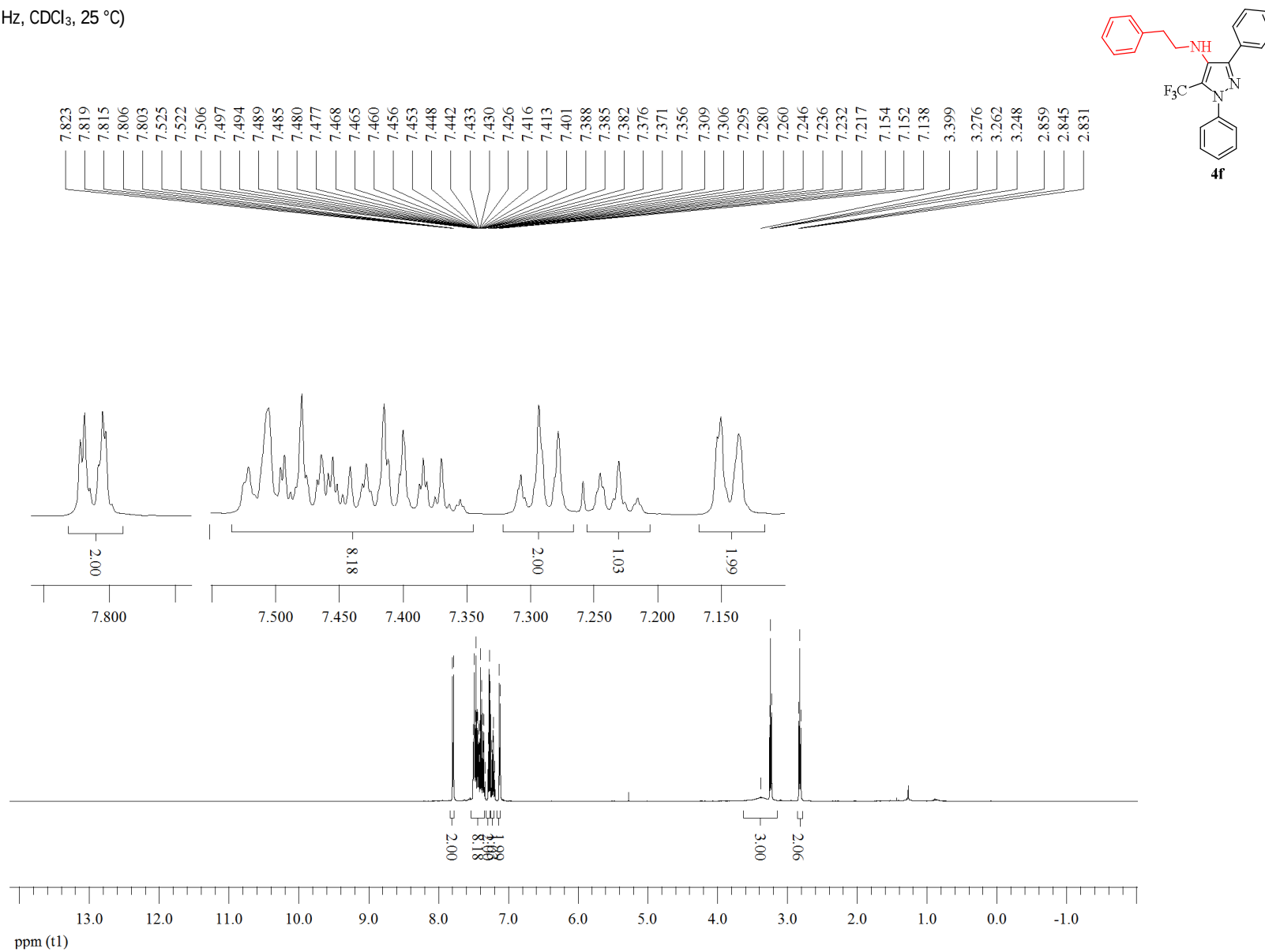
4e - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



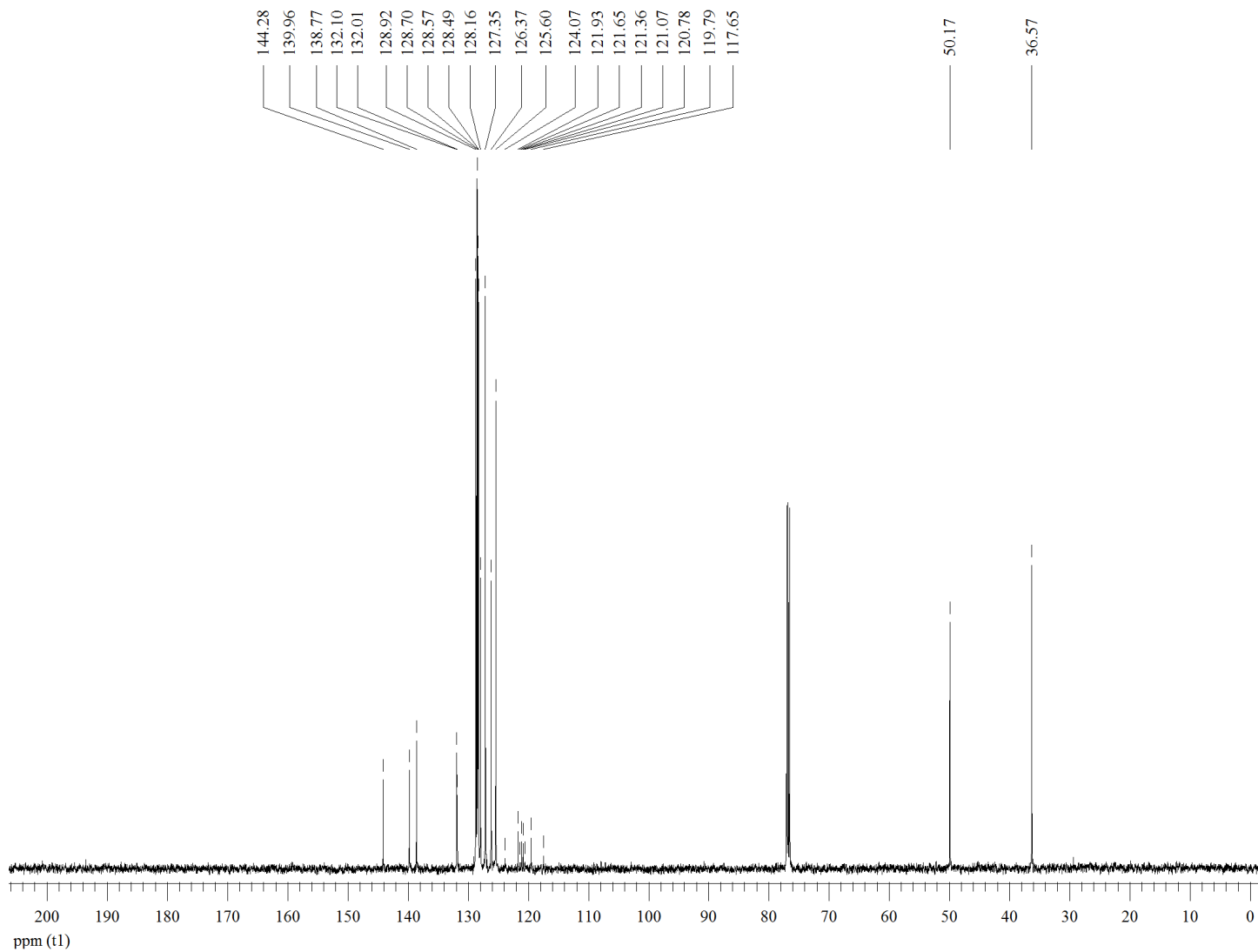
4e - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



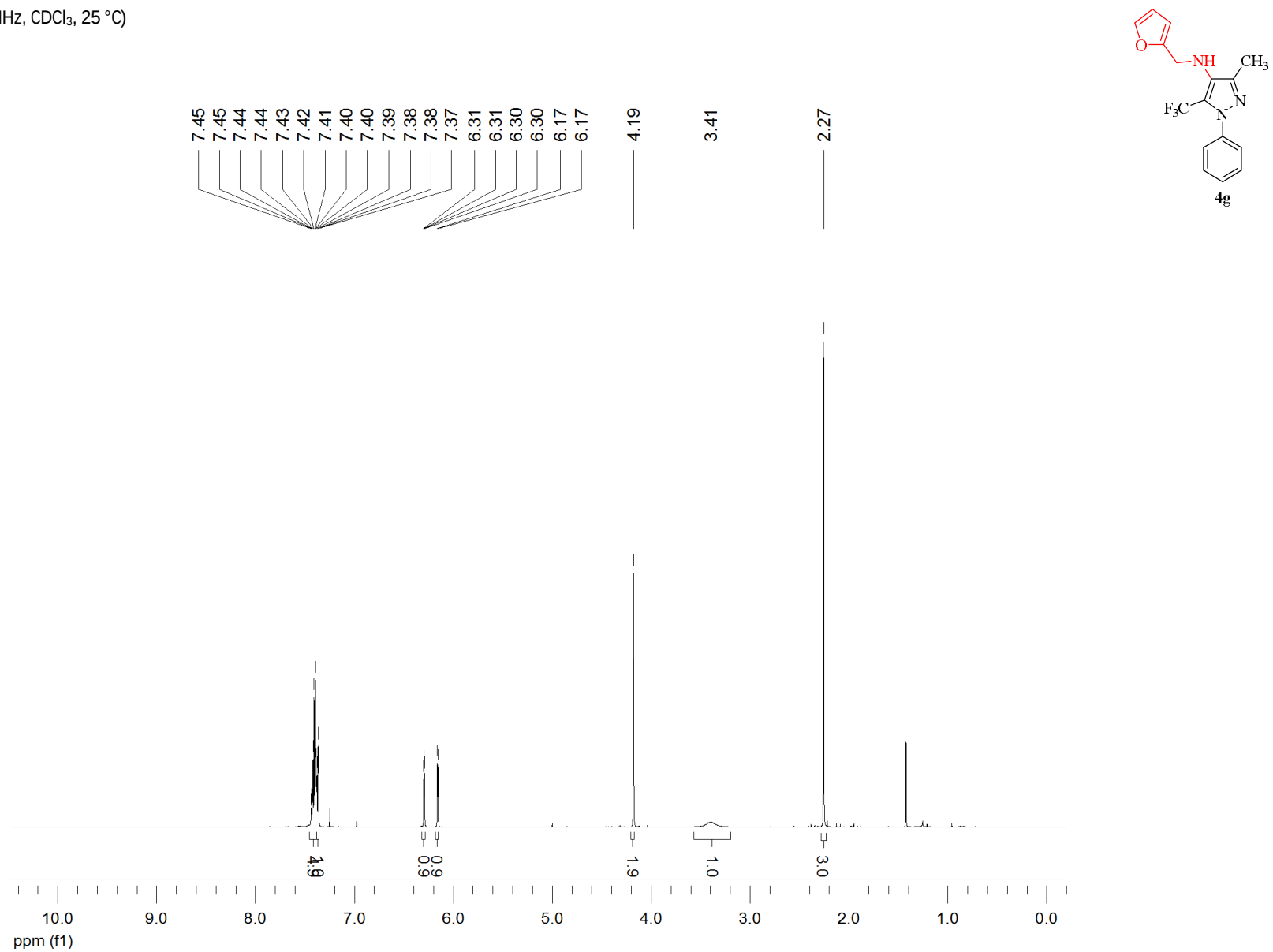
4f - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



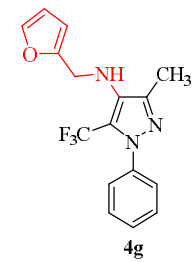
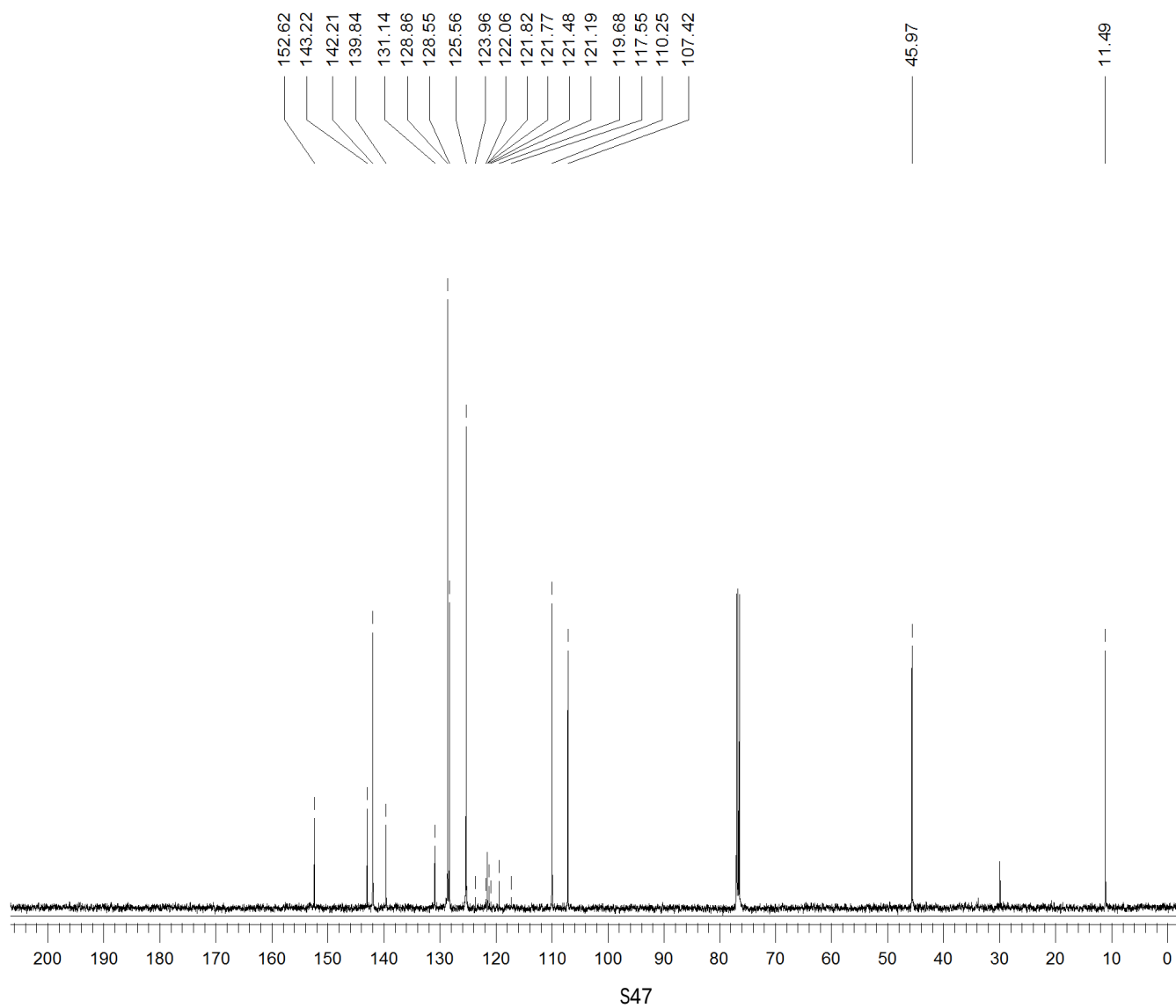
4f - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



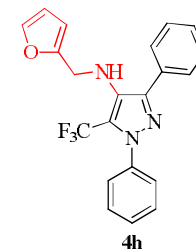
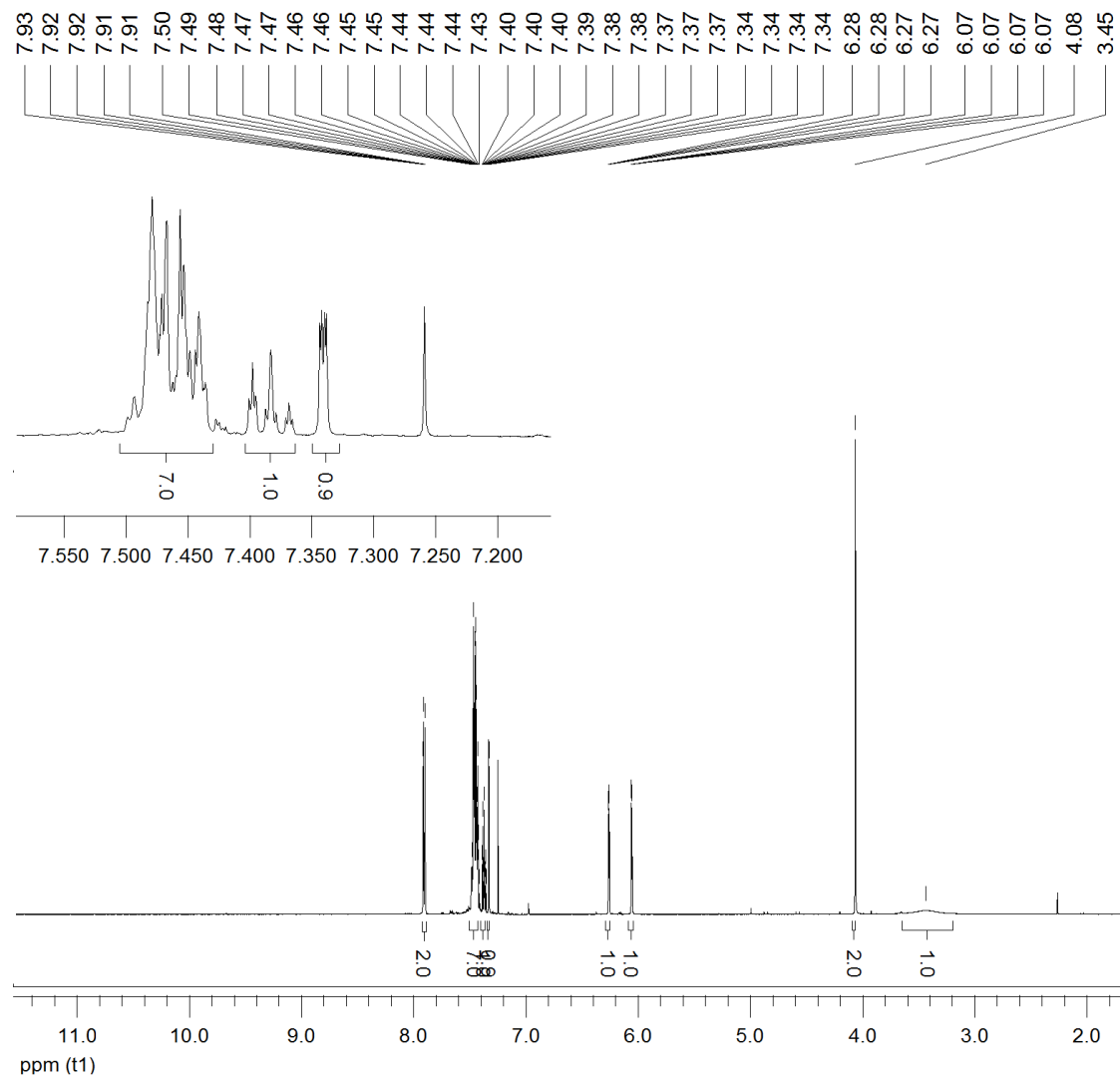
4g - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



4g - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)



4h - ^1H NMR (500 MHz, CDCl_3 , 25 $^\circ\text{C}$)



4h - $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , 25 °C)

