

**Supporting Information for:**

**Sequential One-Pot Three-Step Synthesis of Polysubstituted 4-(5-(trifluoromethyl)-1H-pyrazol-4-yl)-1H-1,2,3-triazole Systems**

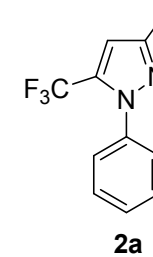
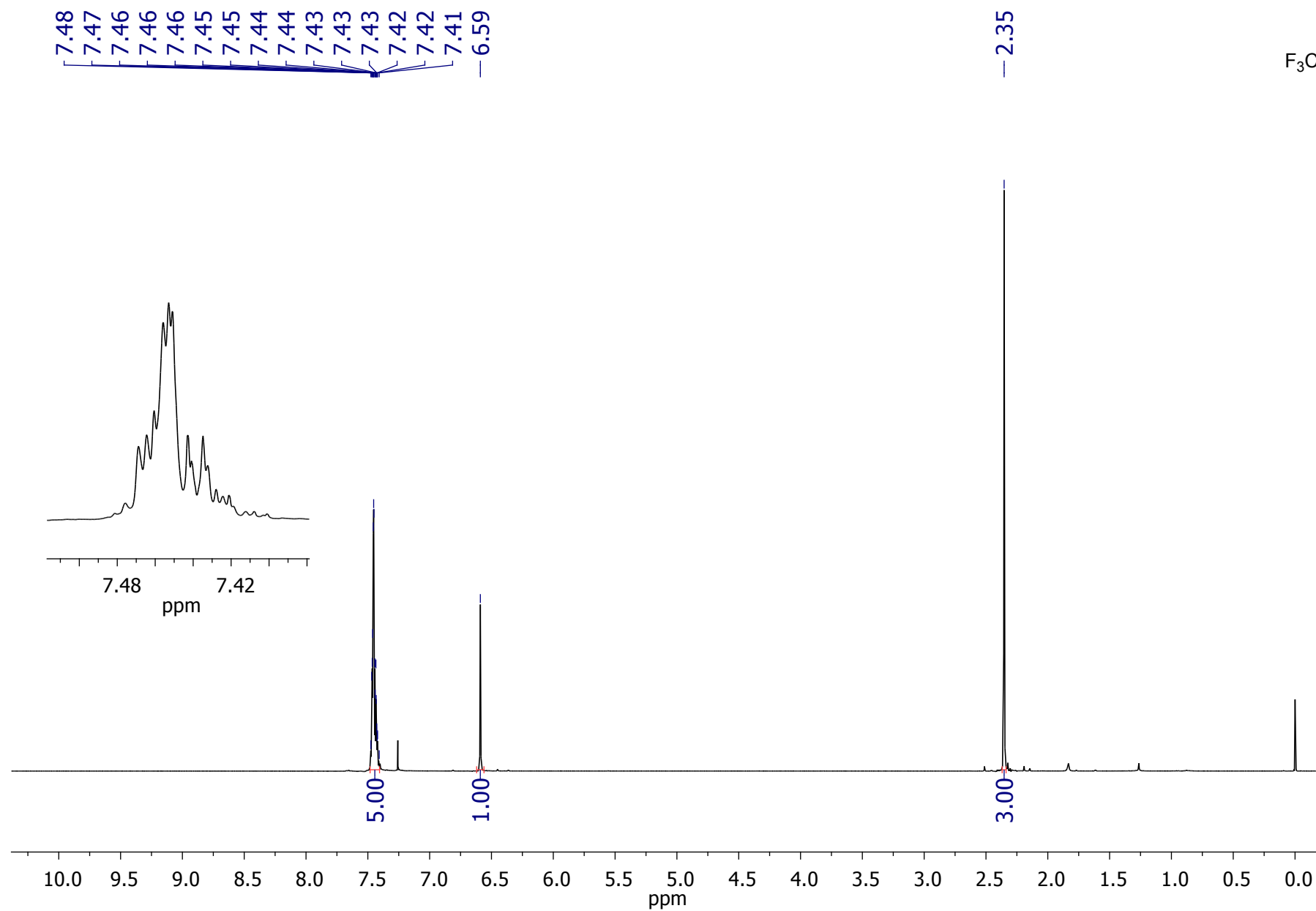
Helio G. Bonacorso,<sup>a\*</sup> Gean M. Dal Forno,<sup>a</sup> Carson Wiethan,<sup>a</sup> Alex Ketzer,<sup>a</sup> Nilo Zanatta,<sup>a</sup>  
Clarissa P. Frizzo,<sup>a</sup> Marcos A. P. Martins<sup>a</sup> and Mark Stradiotto<sup>b</sup>

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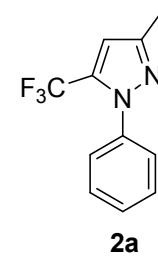
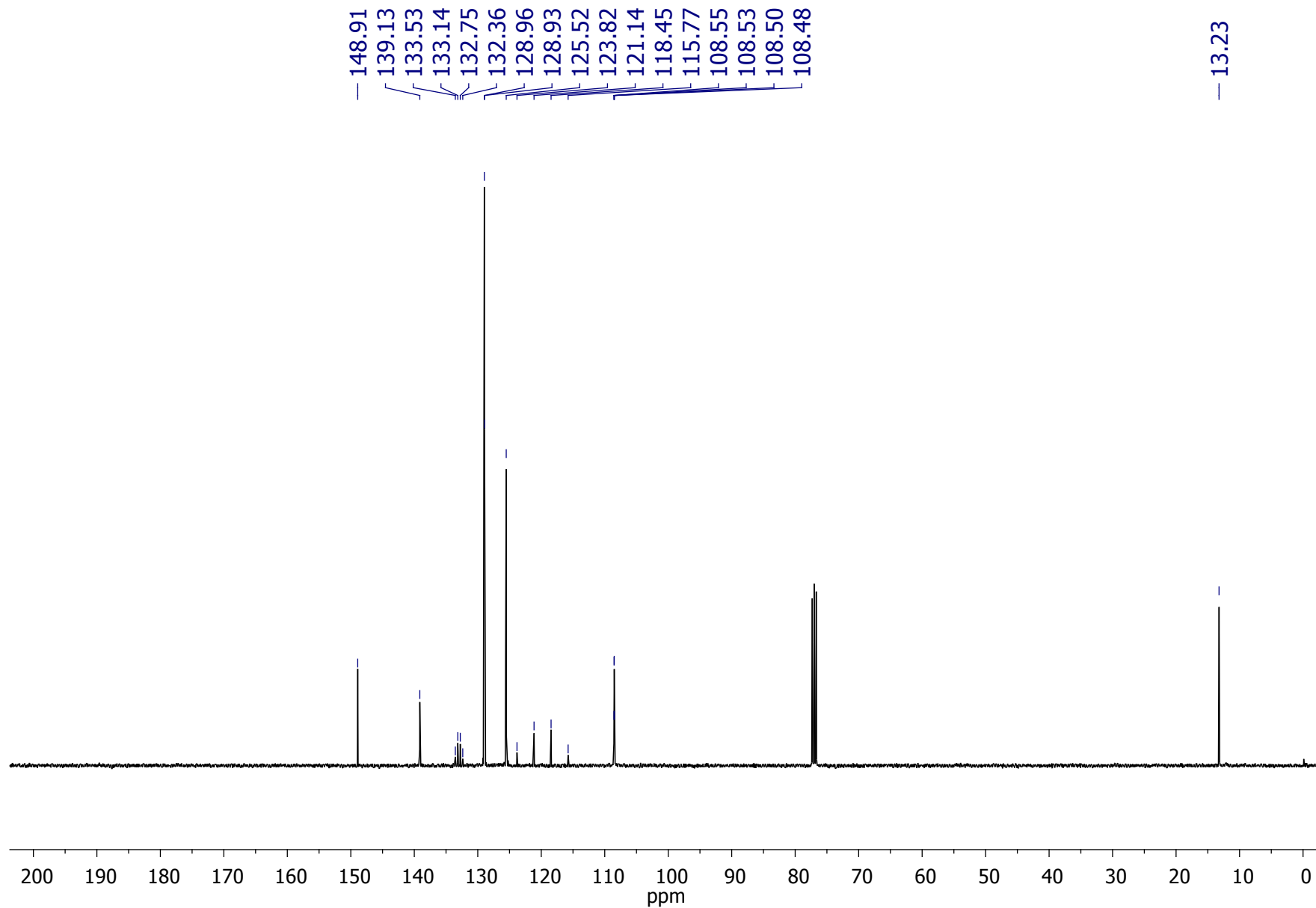
<sup>b</sup>*Department of Chemistry, Dalhousie University, Halifax, NS, B3H 4R2 Canada.*

**Contents:** Copies of <sup>1</sup>H NMR and <sup>13</sup>C NMR

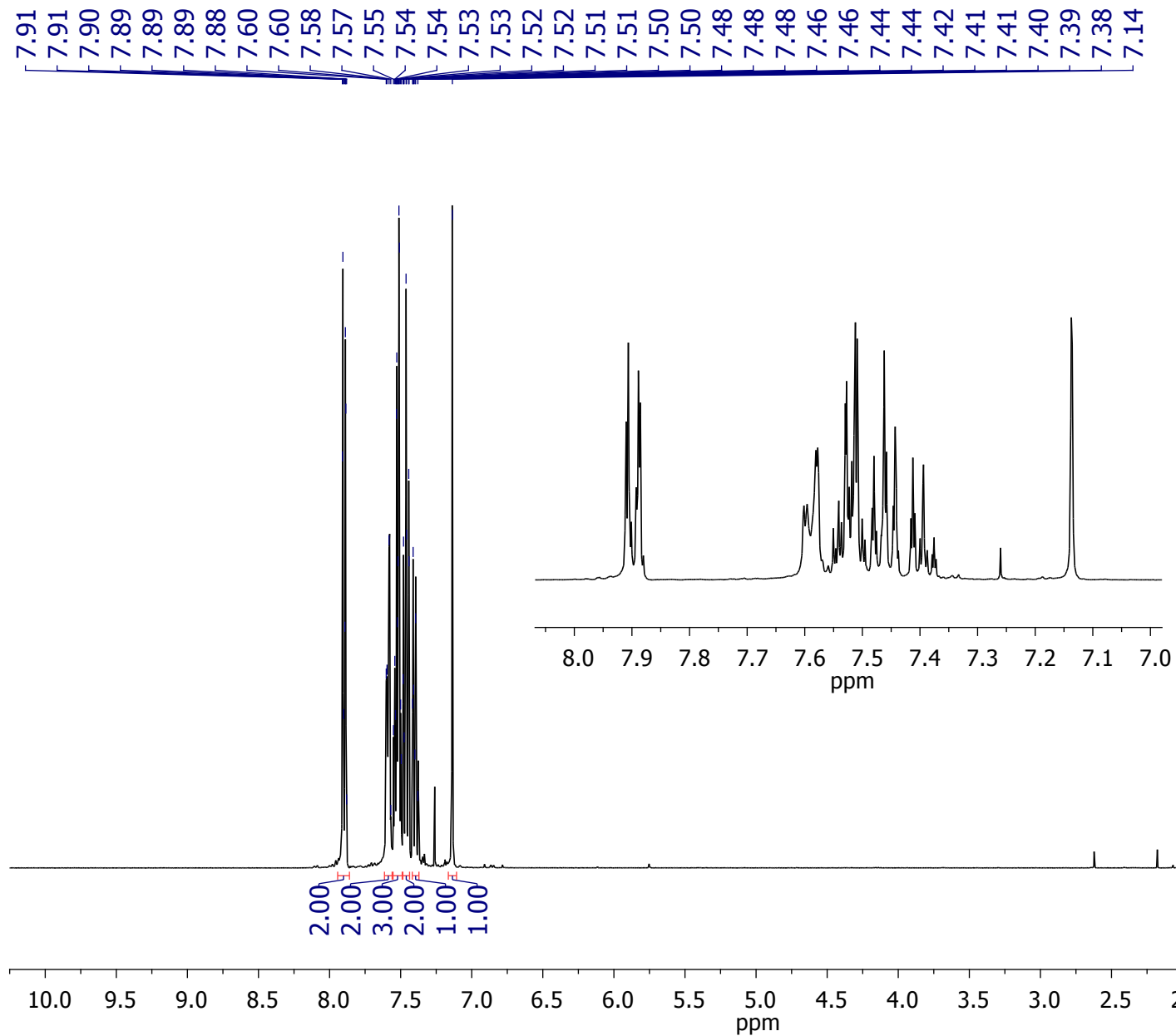
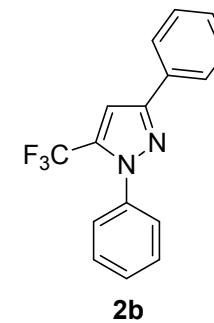
2a -  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ )



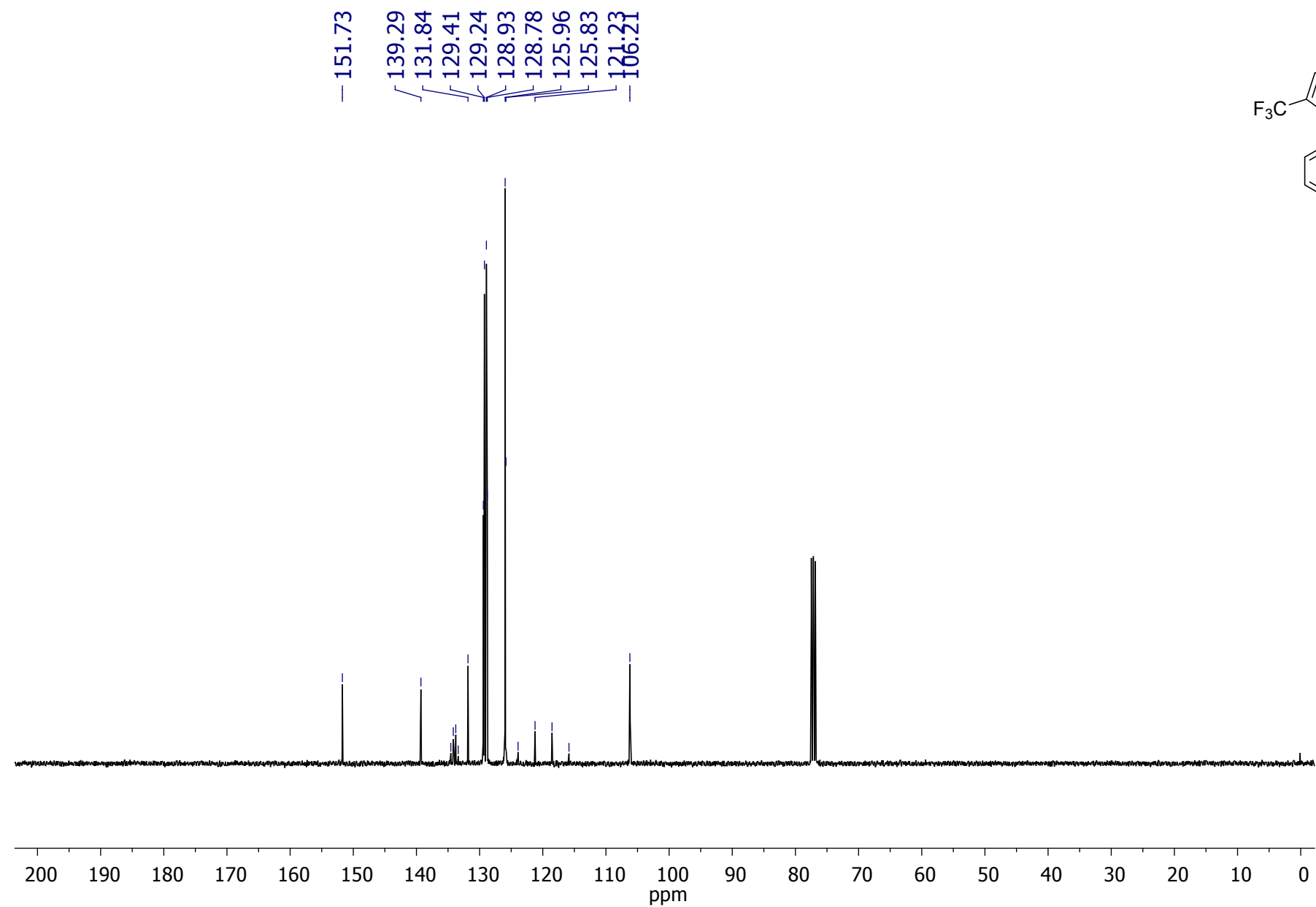
**2a** -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)



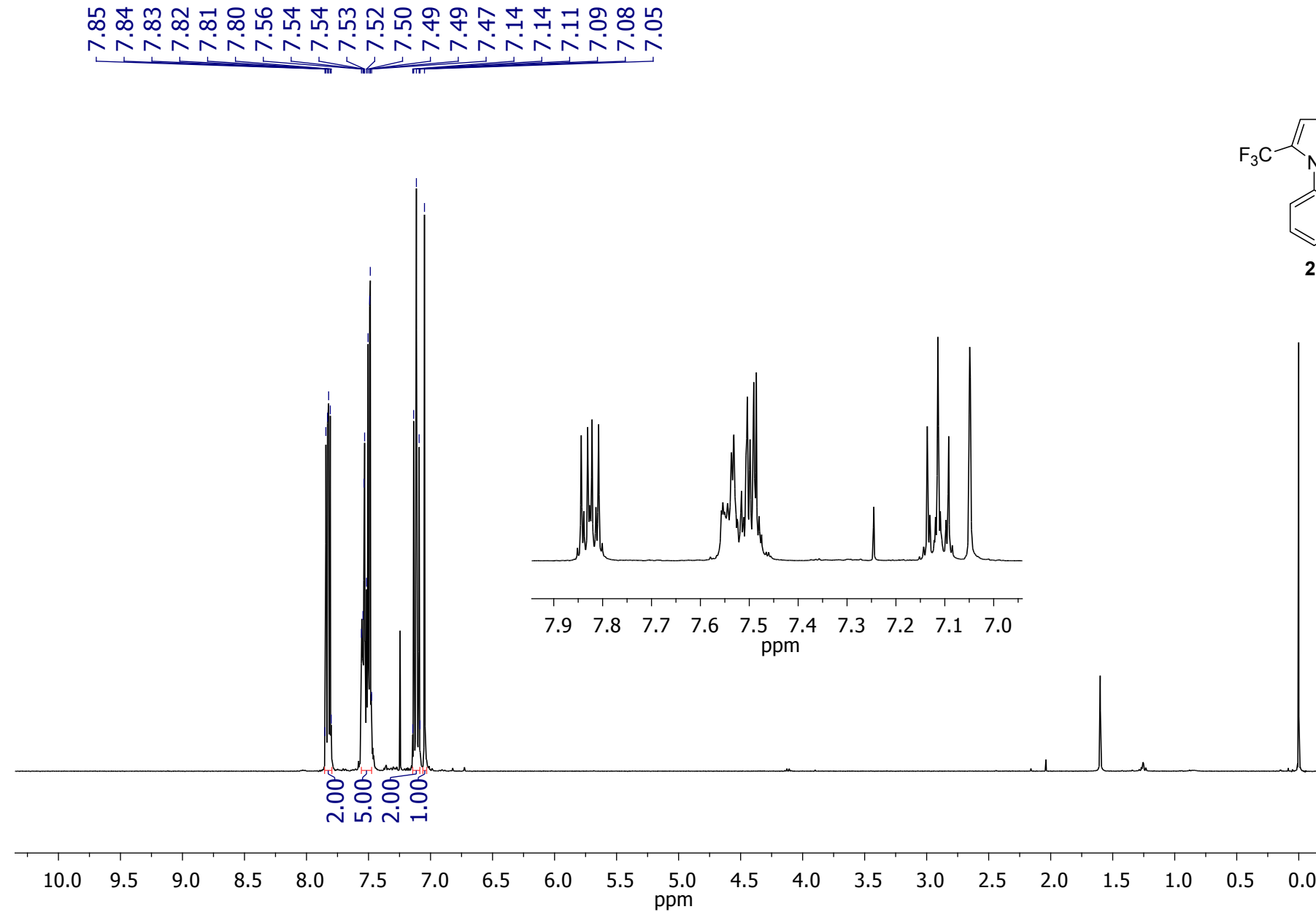
**2b** -  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ )



**2b** -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)

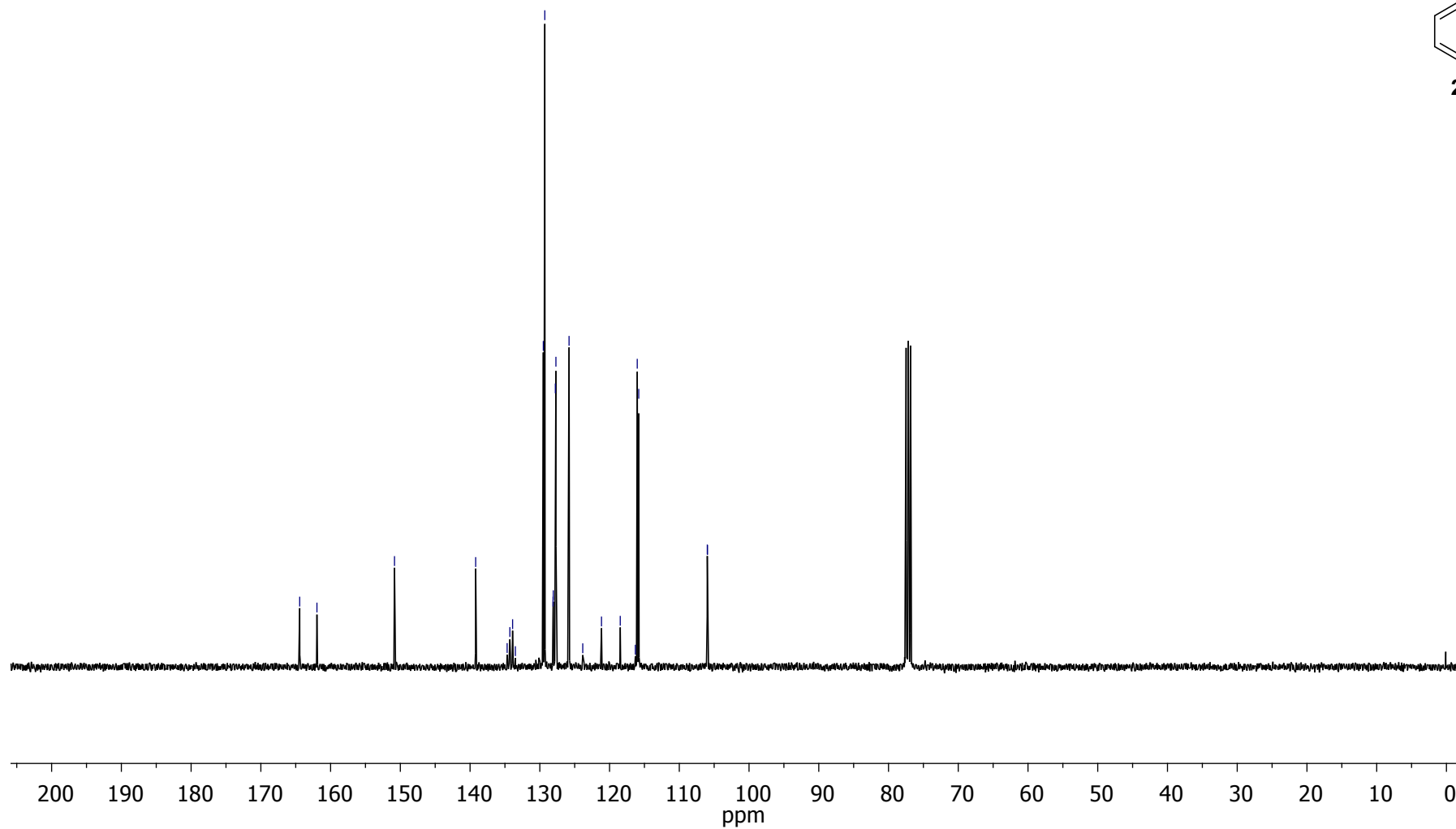
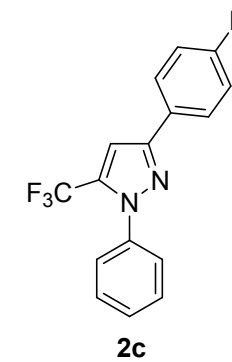


2c - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

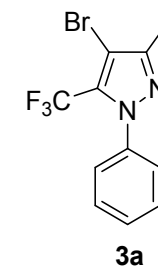
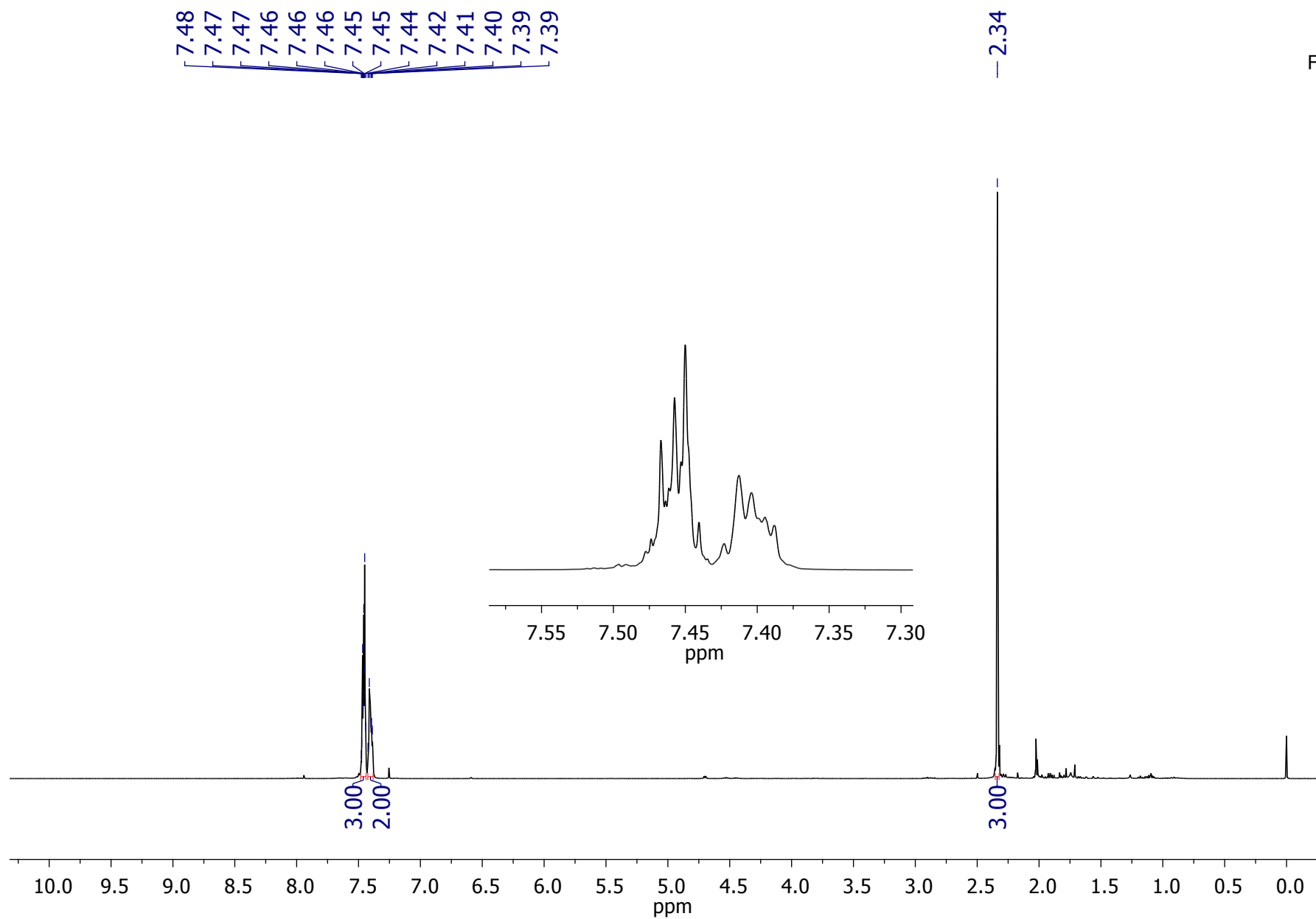


**2c** -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)

~ 164.43  
~ 161.96  
— 150.84  
/ 139.20  
/ 129.50  
/ 129.29  
/ 127.77  
/ 127.69  
/ 125.81  
/ 116.03  
/ 115.81  
/ 105.99  
/ 105.96

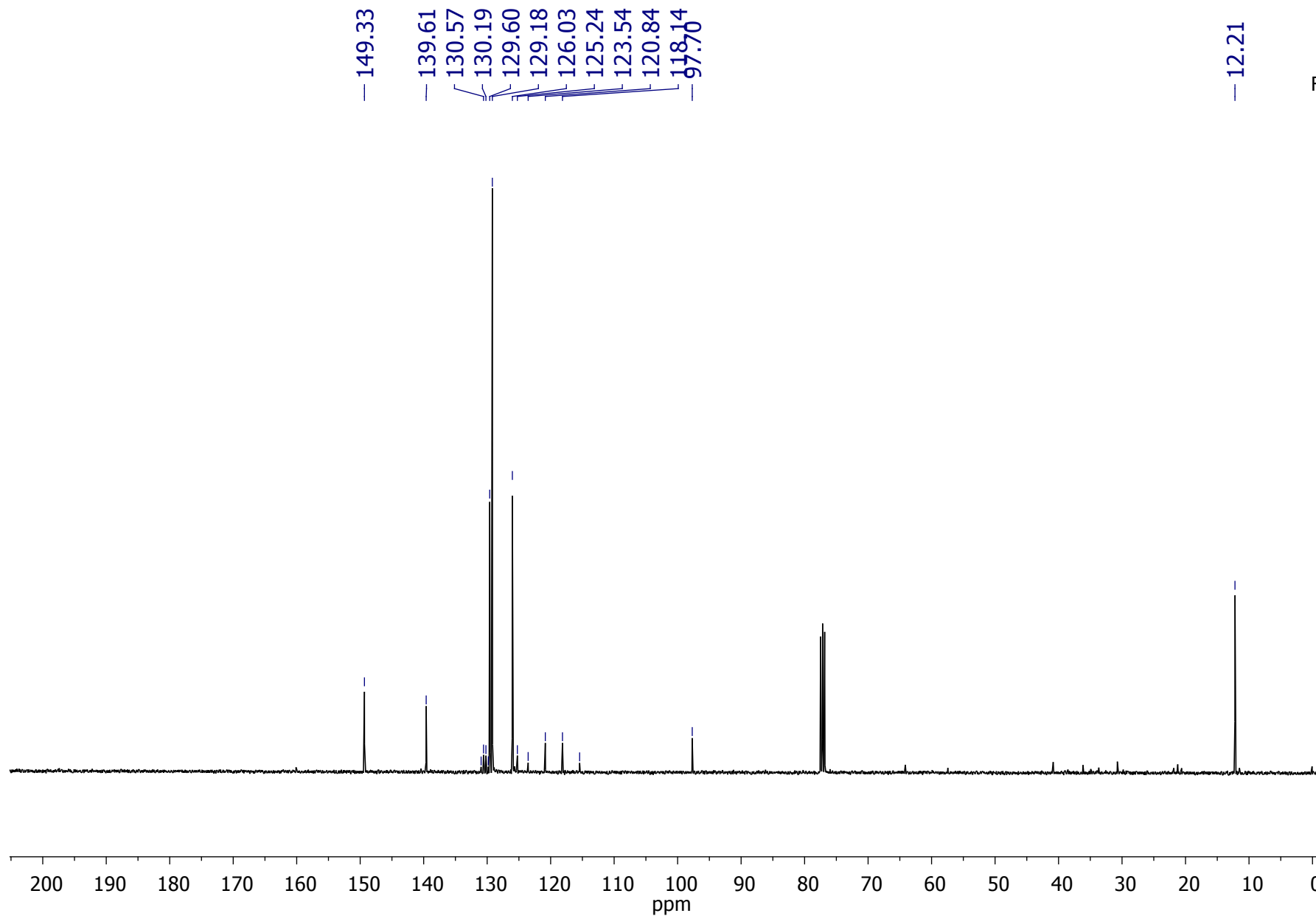


**3a** -  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ )

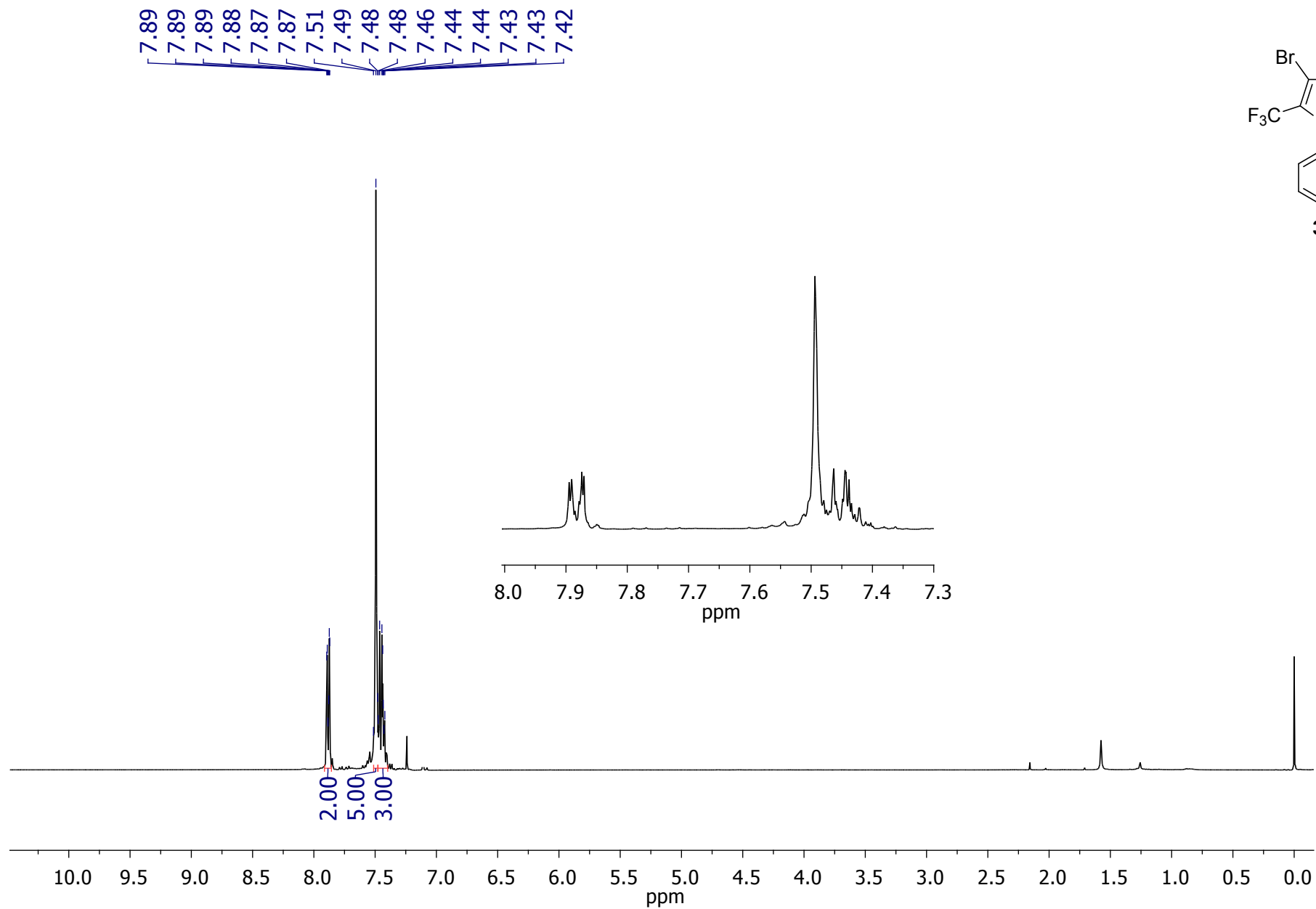
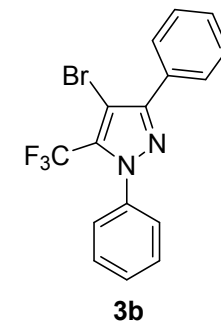




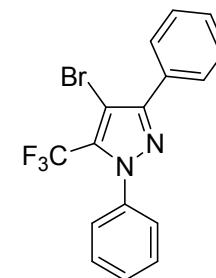
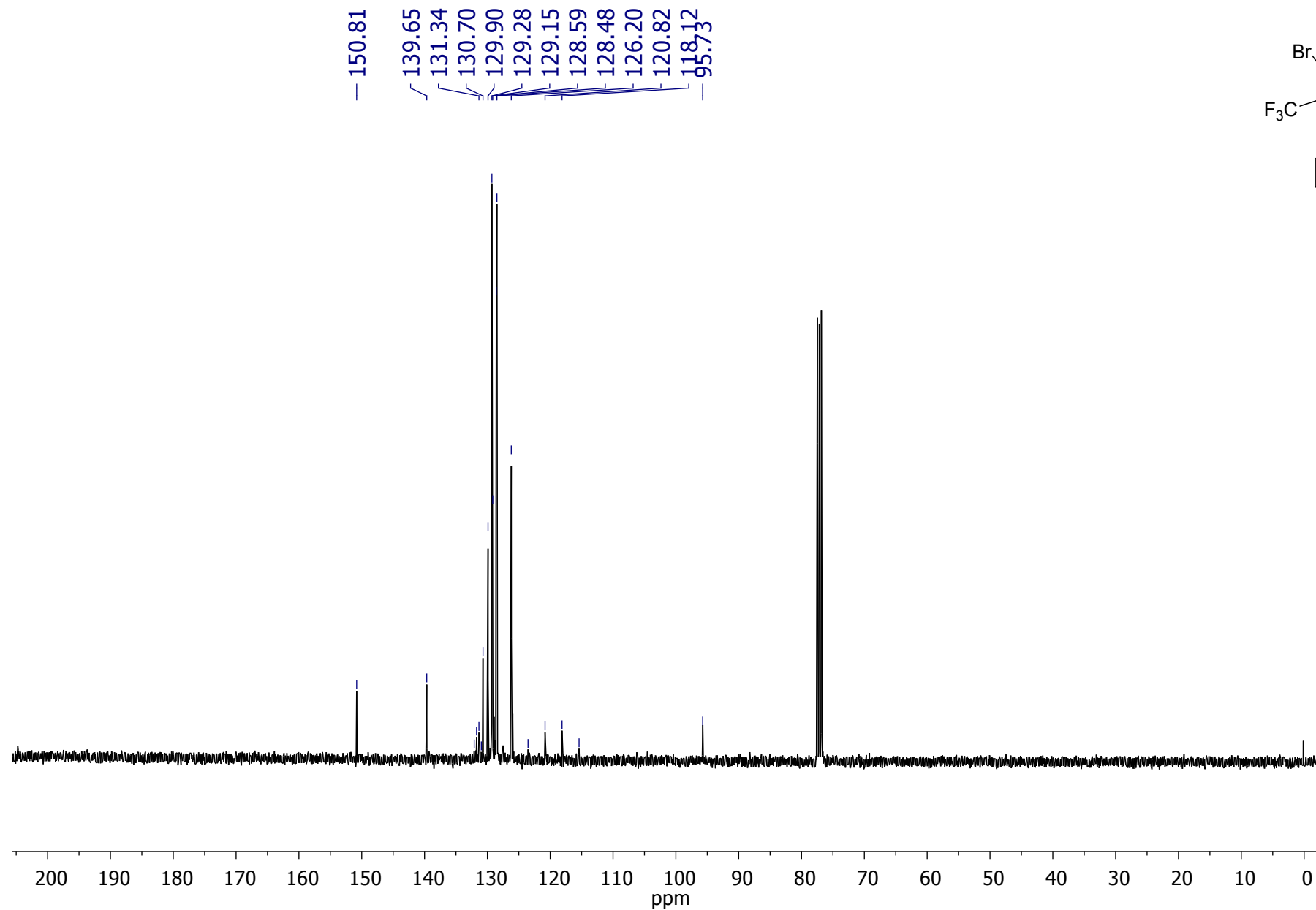
**3a** -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)



**3b** -  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ )

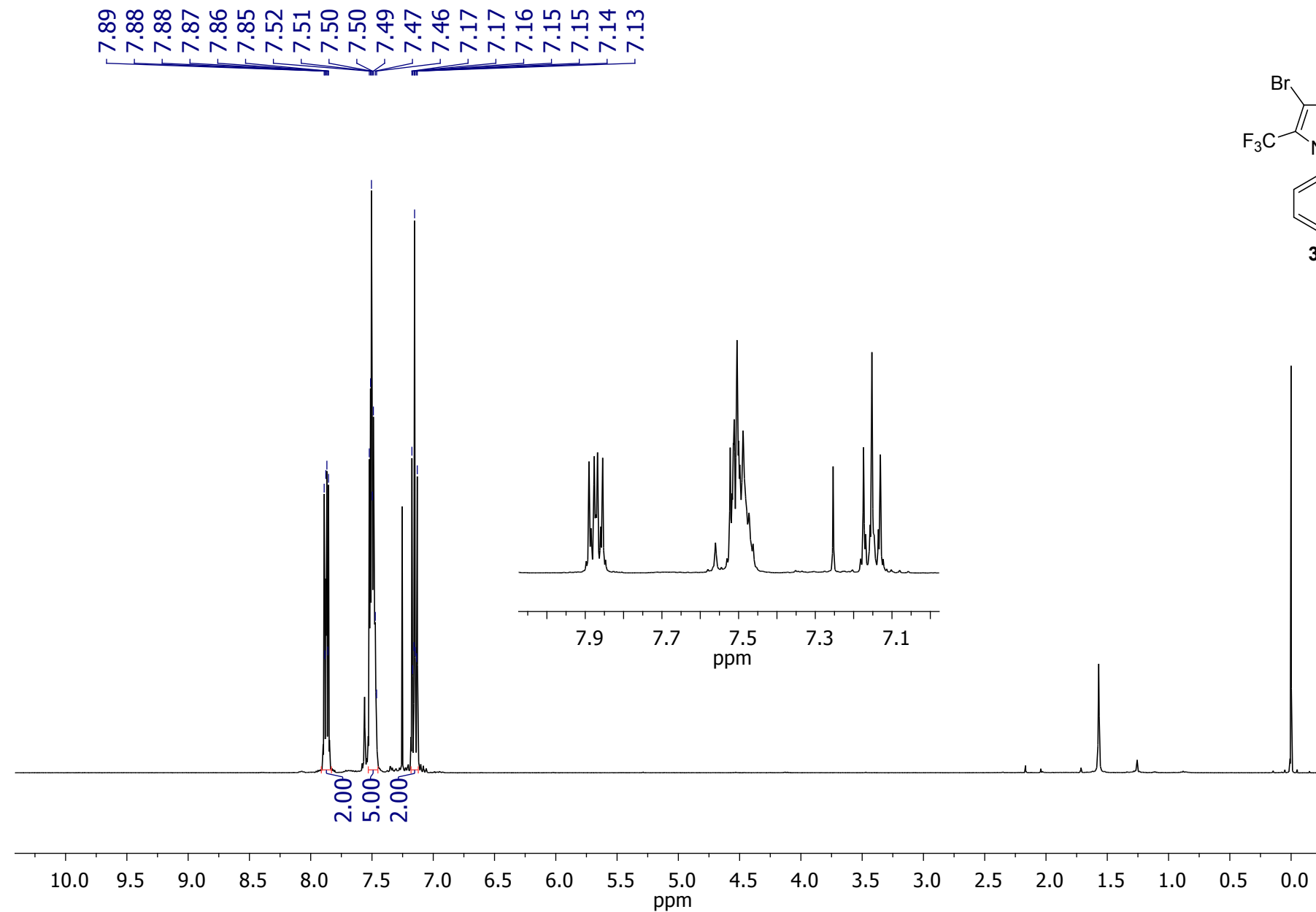


**3b** -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)

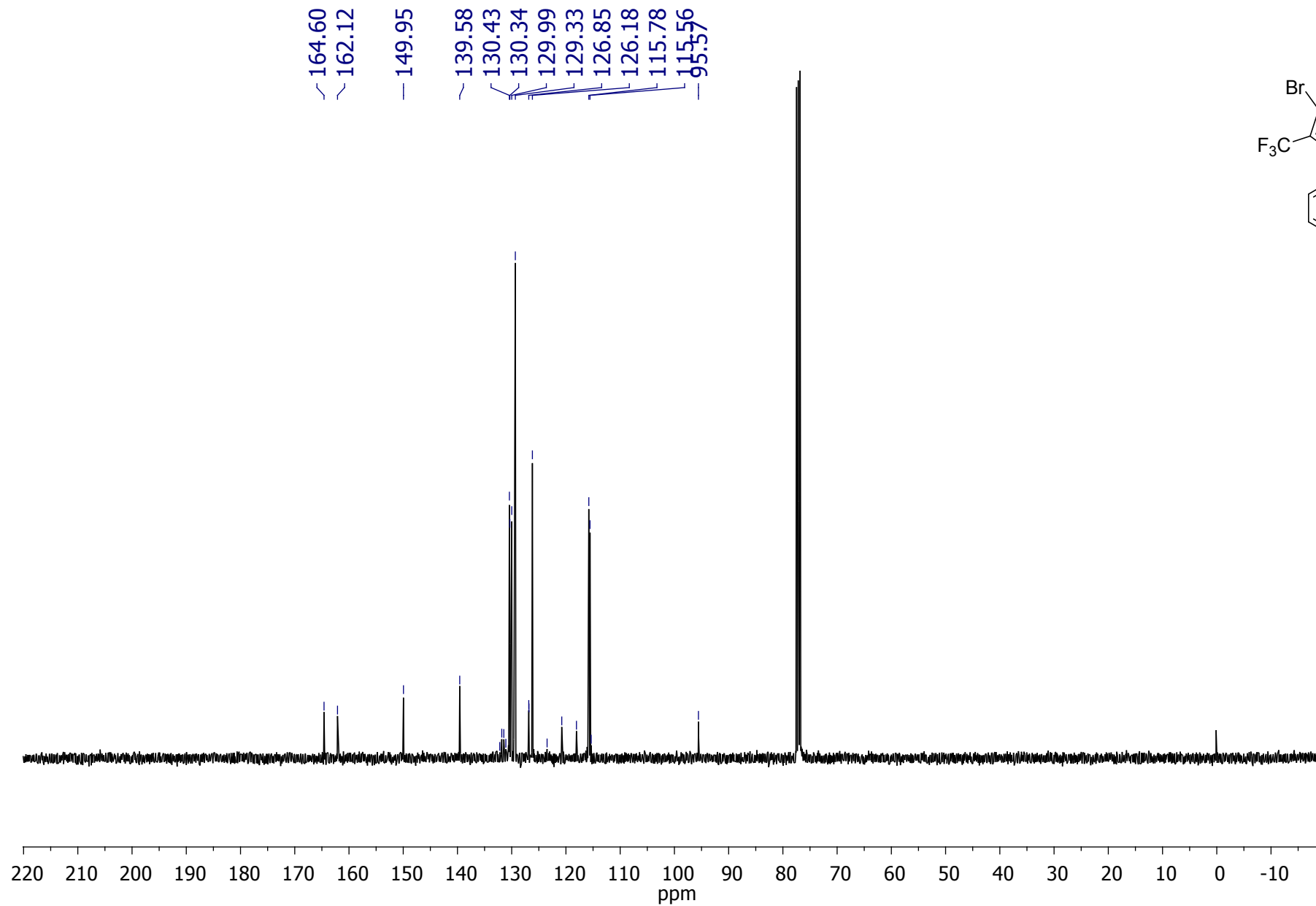


**3b**

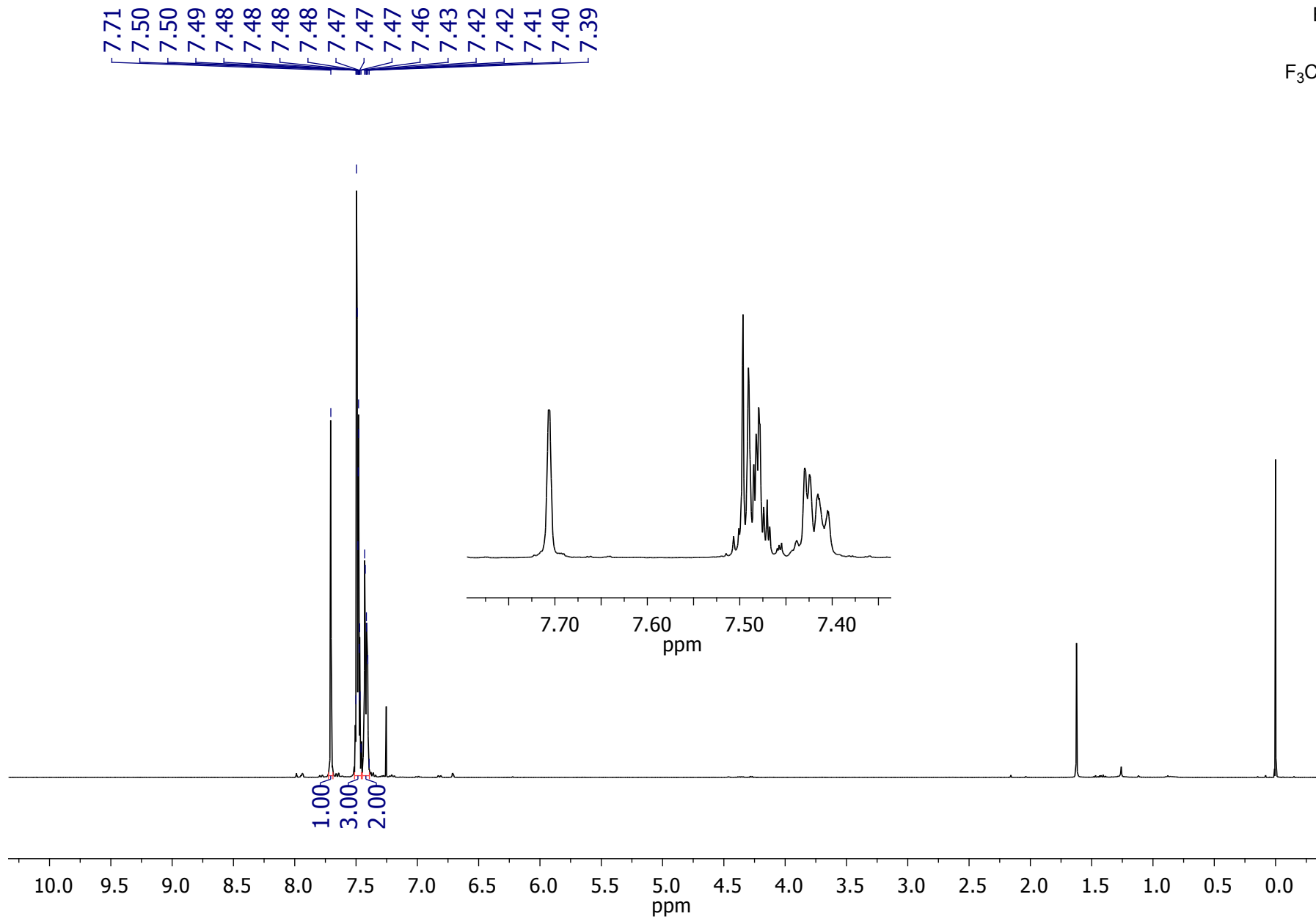
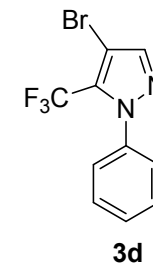
**3c** -  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ )



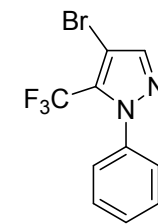
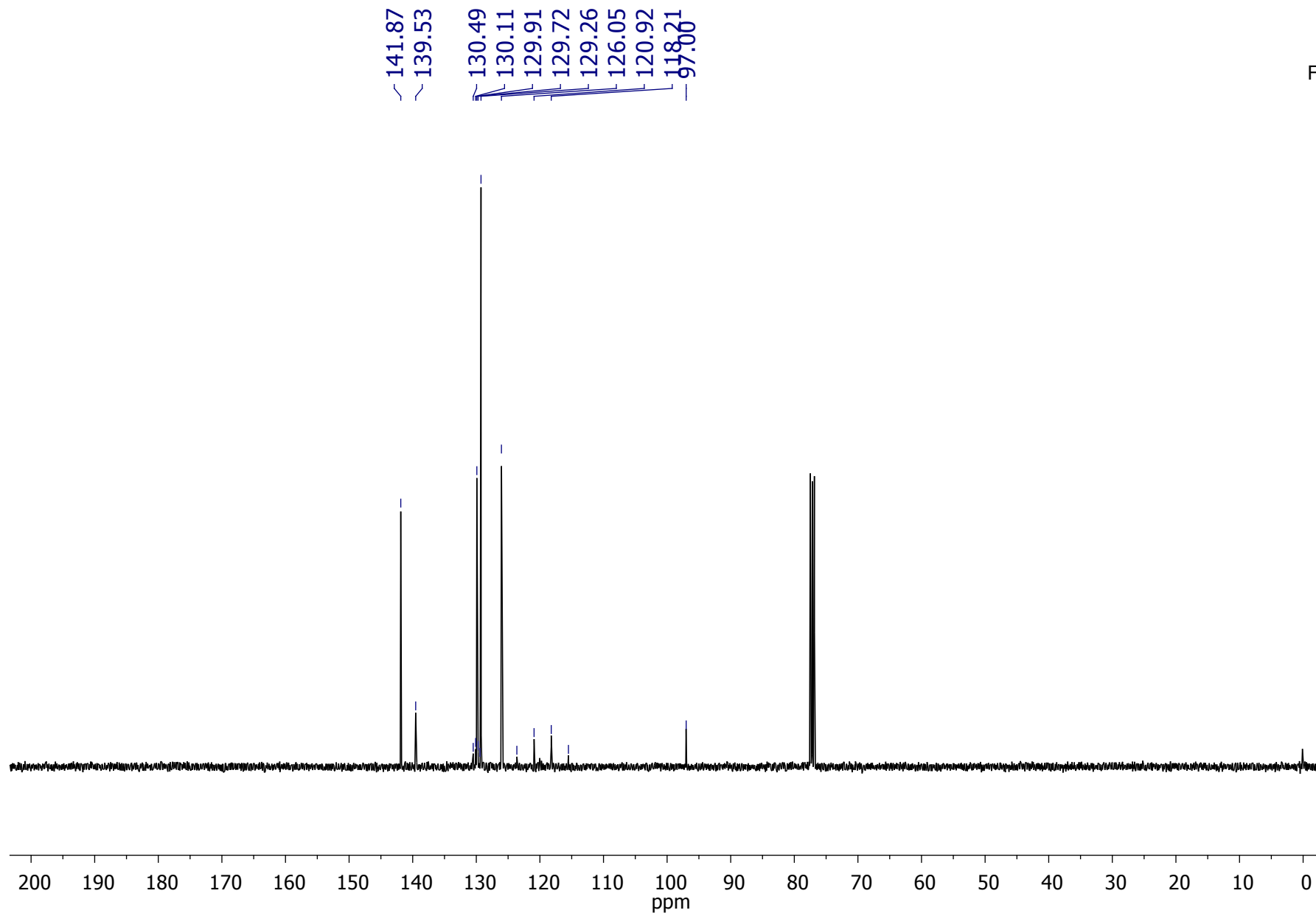
**3c** -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)



**3d** -  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ )

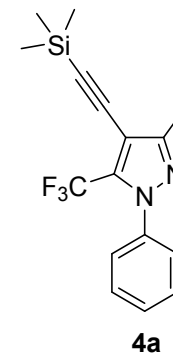
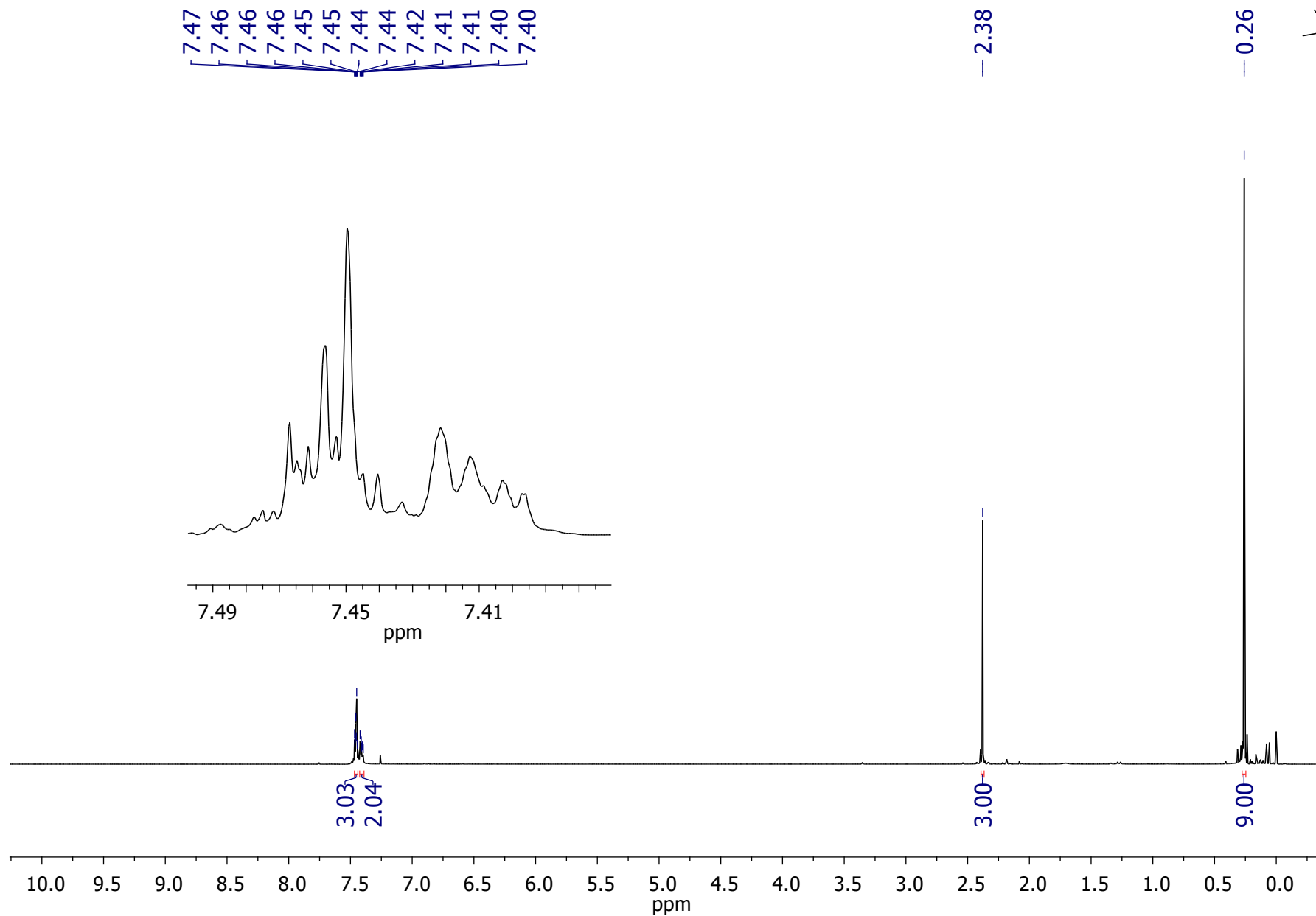


**3d** -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)



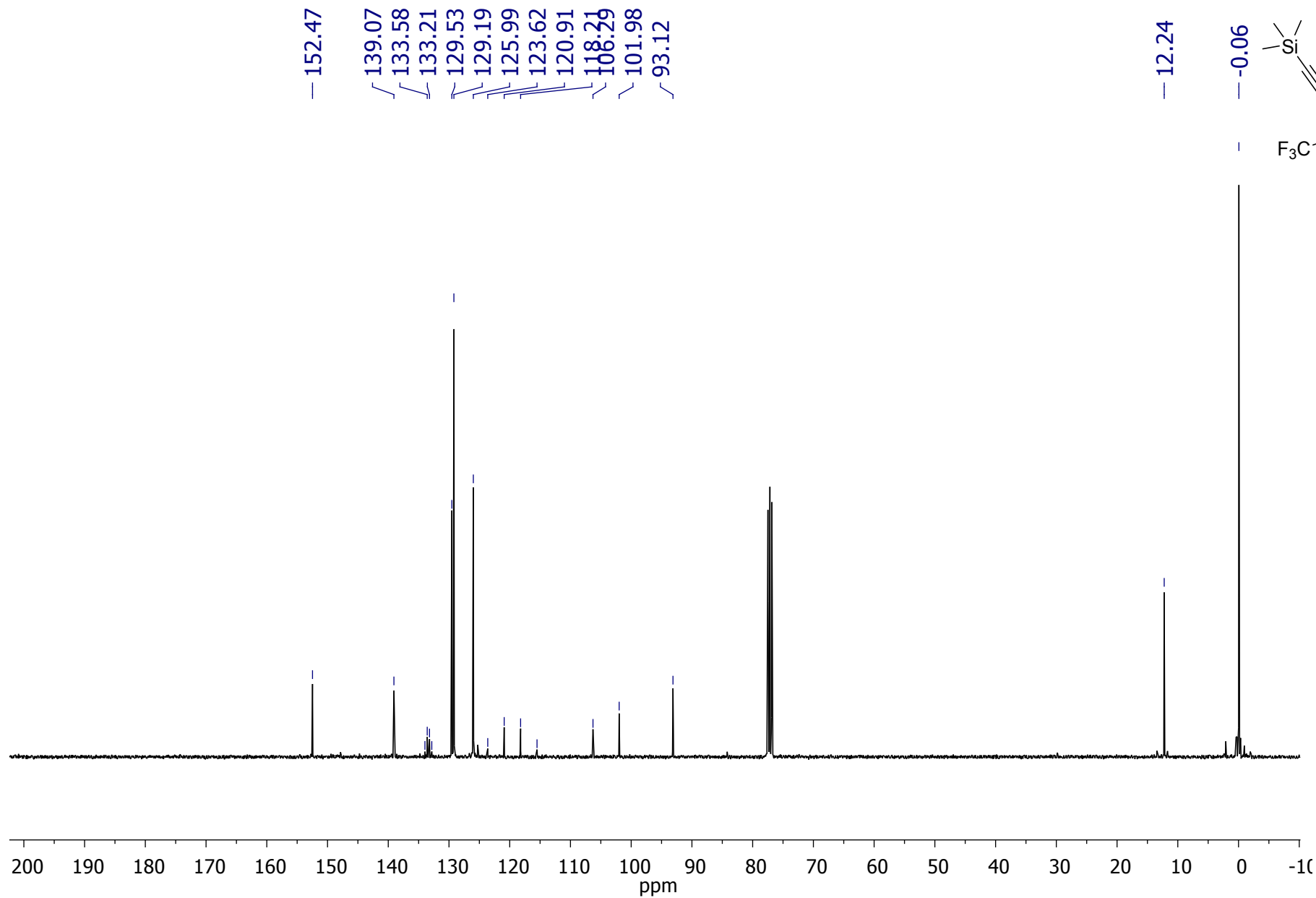
**3d**

4a -  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25  $^\circ\text{C}$ )

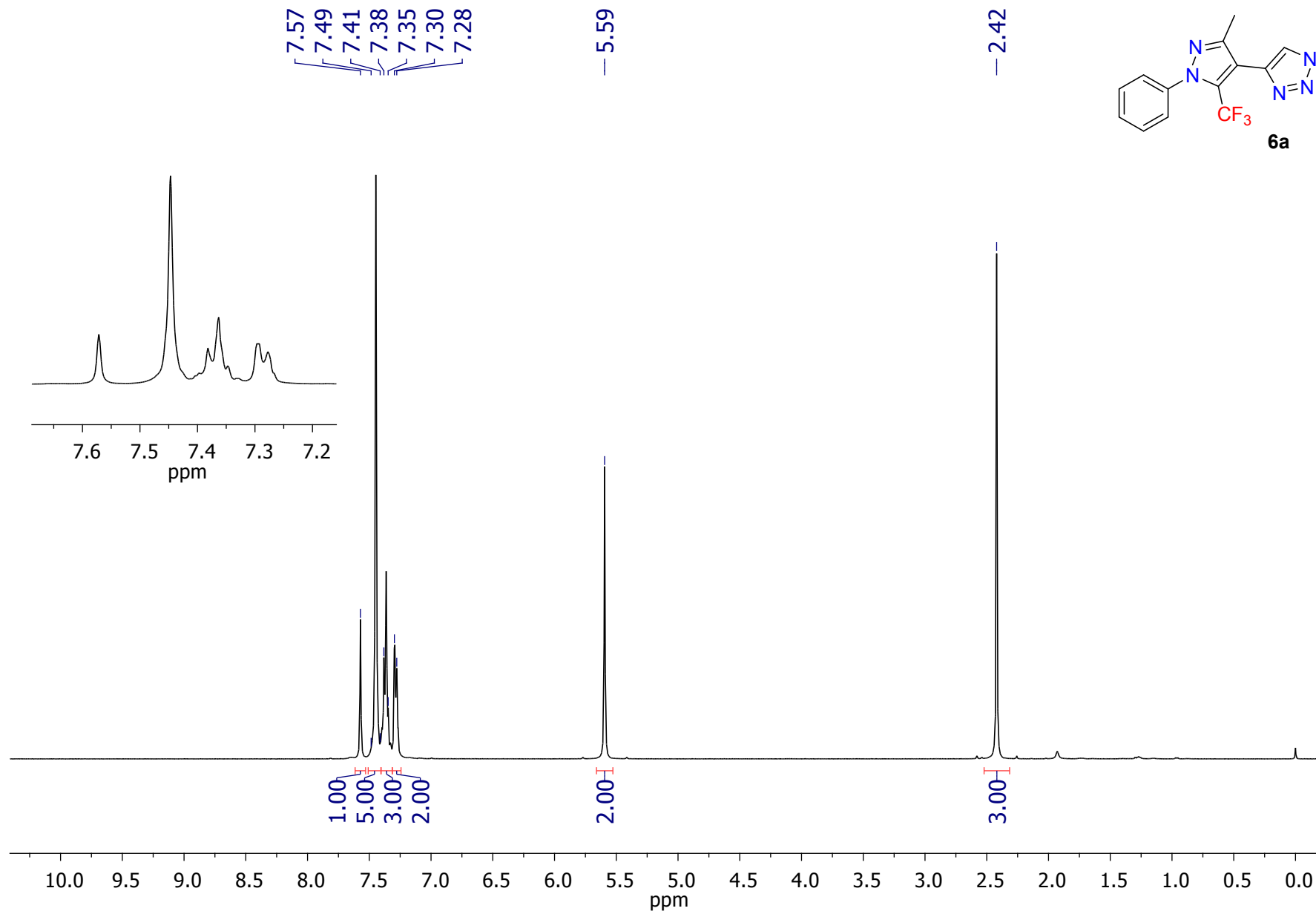




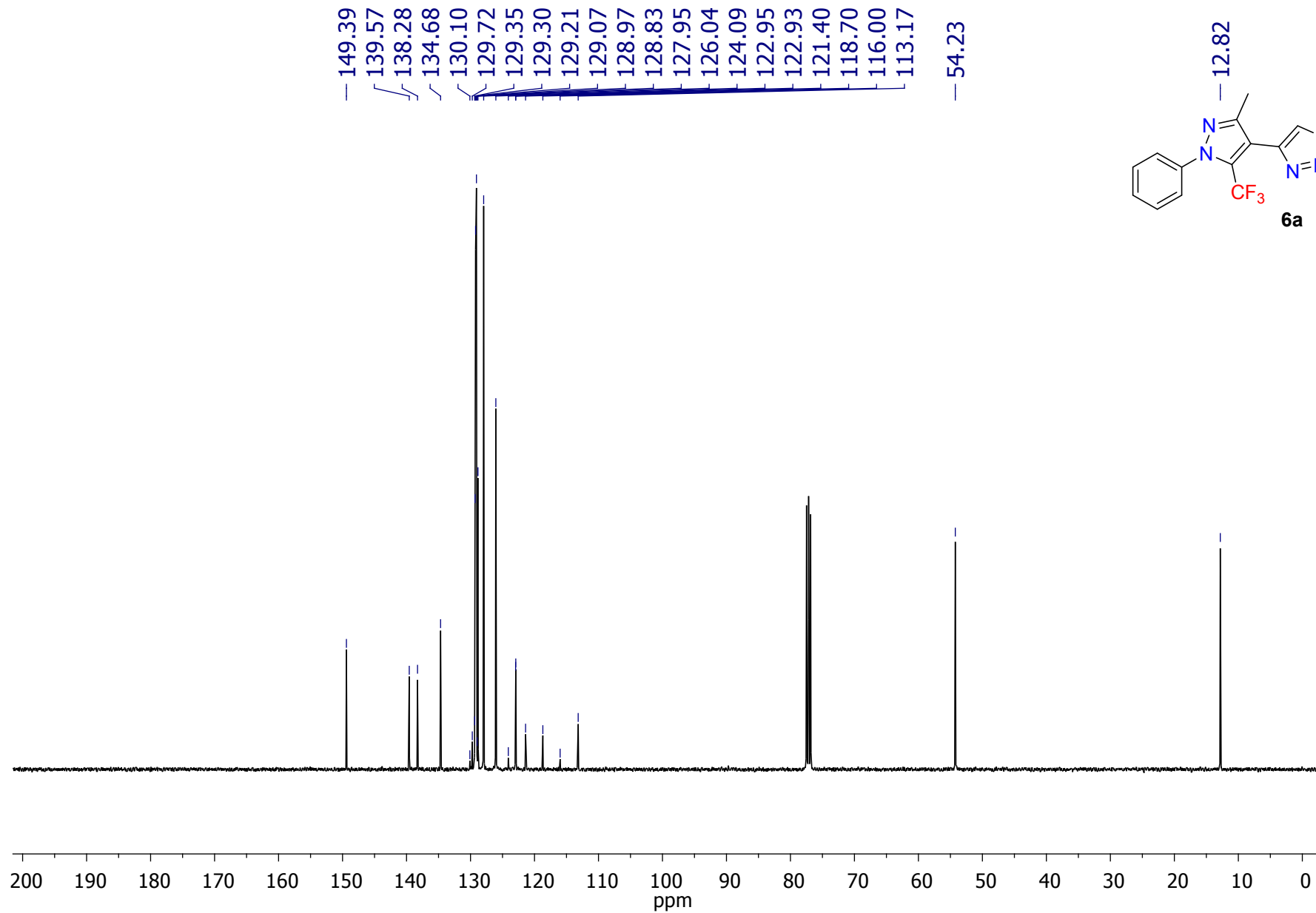
4a -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)



6a - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

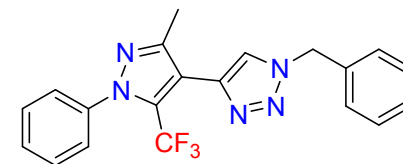


6a -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)

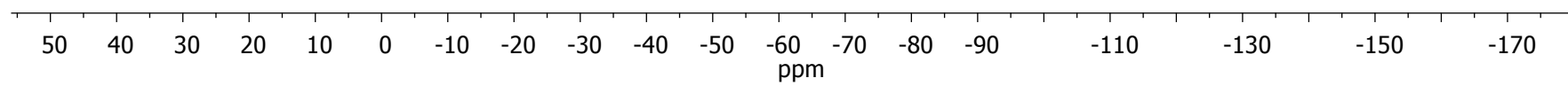


6a -  $^{19}\text{F}$  NMR (565 MHz,  $\text{CDCl}_3$ , 25 °C)

— -55.39



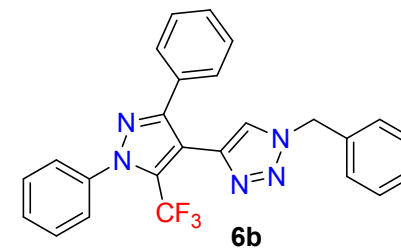
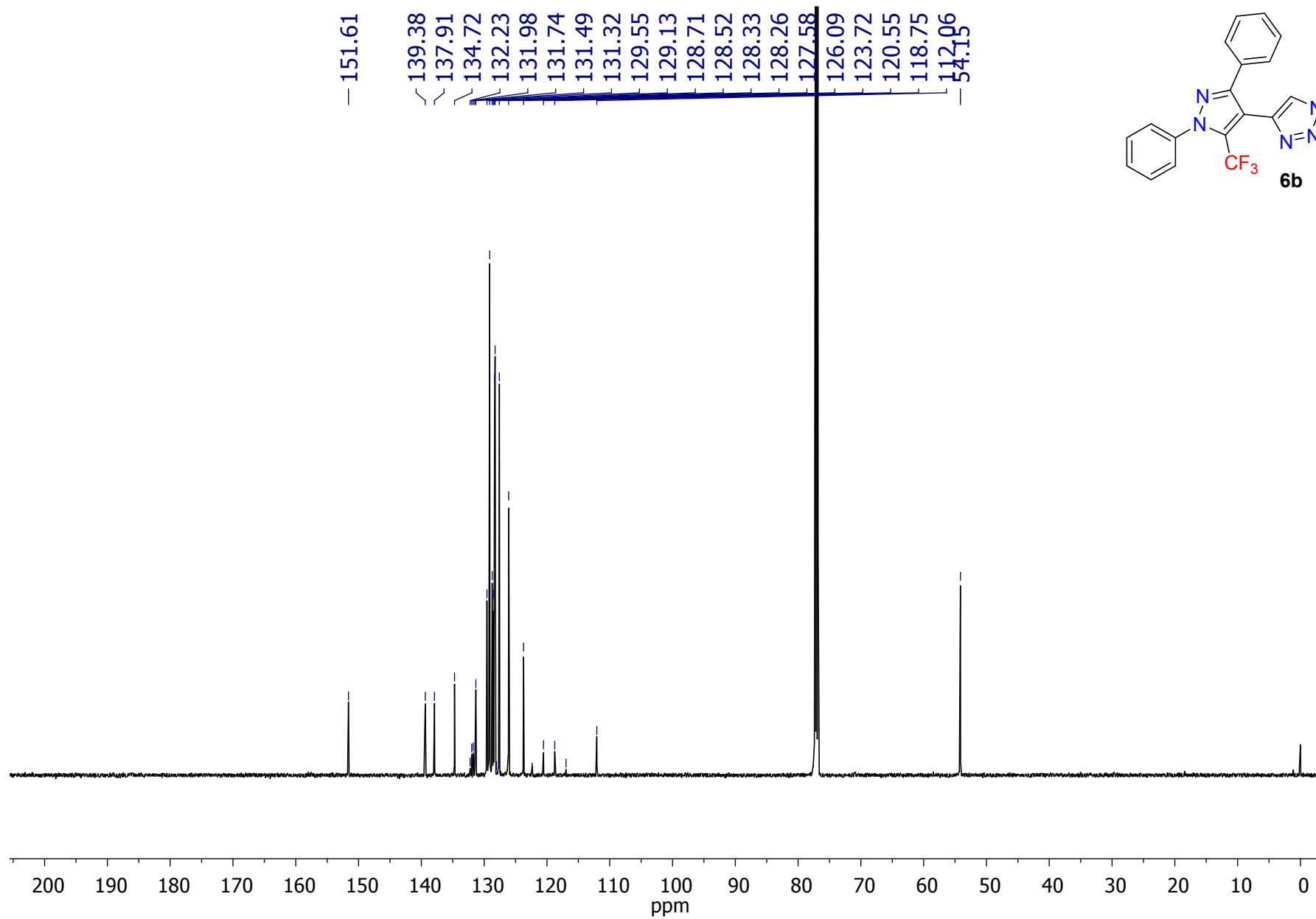
6a



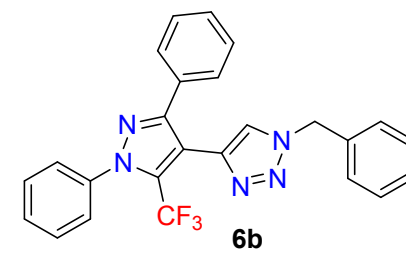
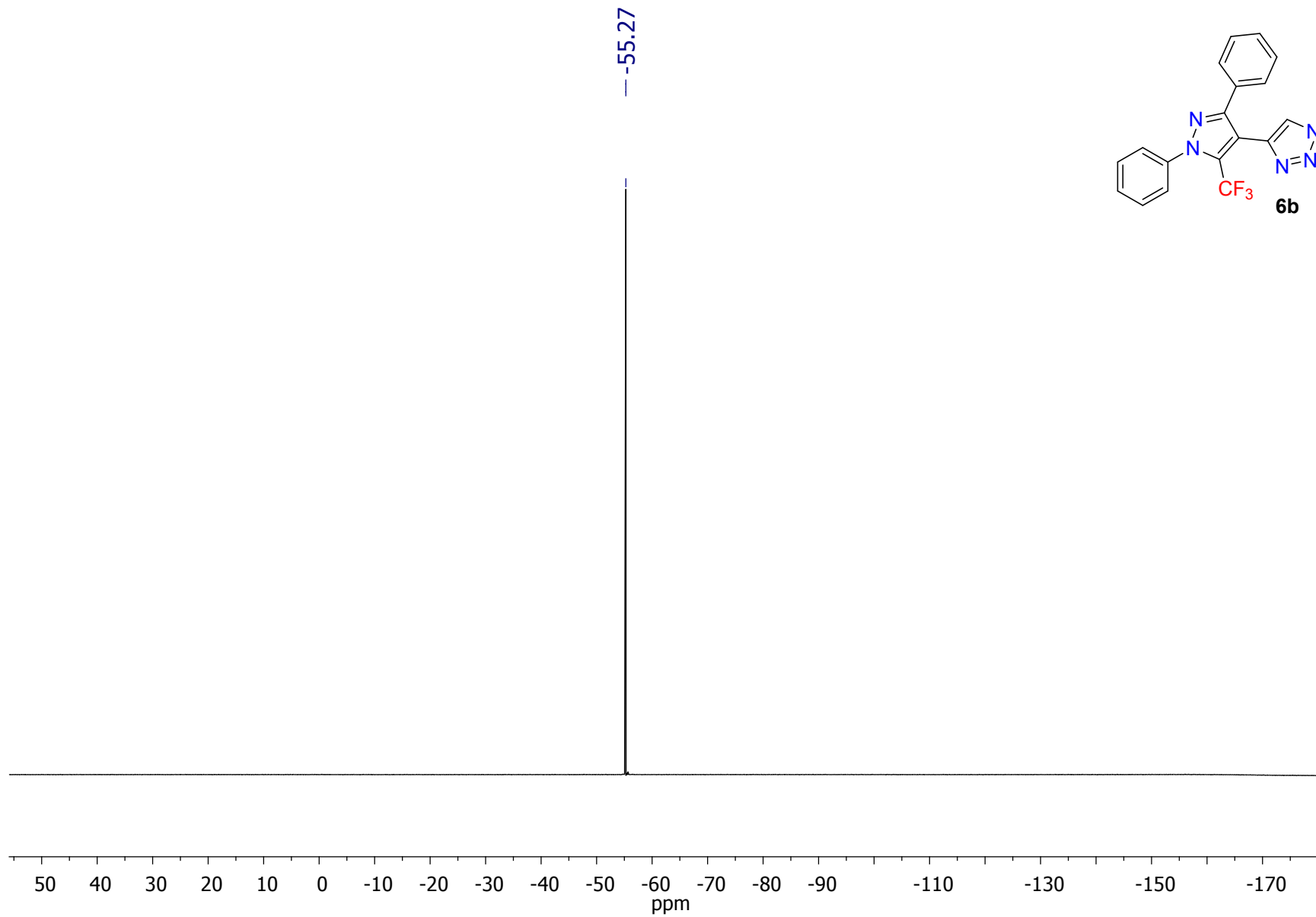
S20



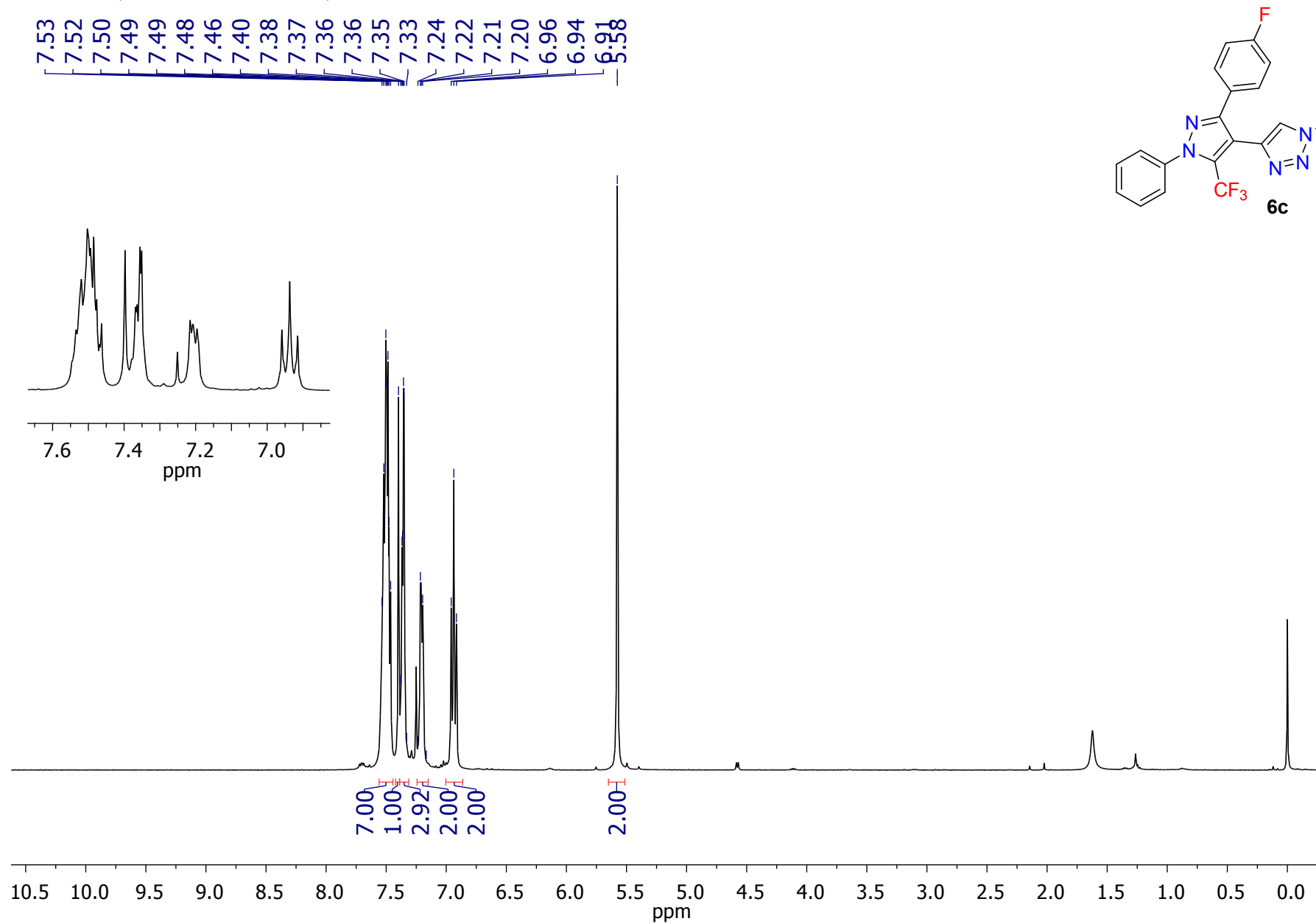
6b -  $^{13}\text{C}\{^1\text{H}\}$  NMR (150 MHz,  $\text{CDCl}_3$ , 25 °C)



**6b** -  $^{19}\text{F}$  NMR (565 MHz,  $\text{CDCl}_3$ , 25 °C)

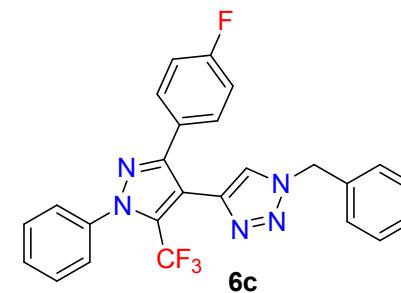
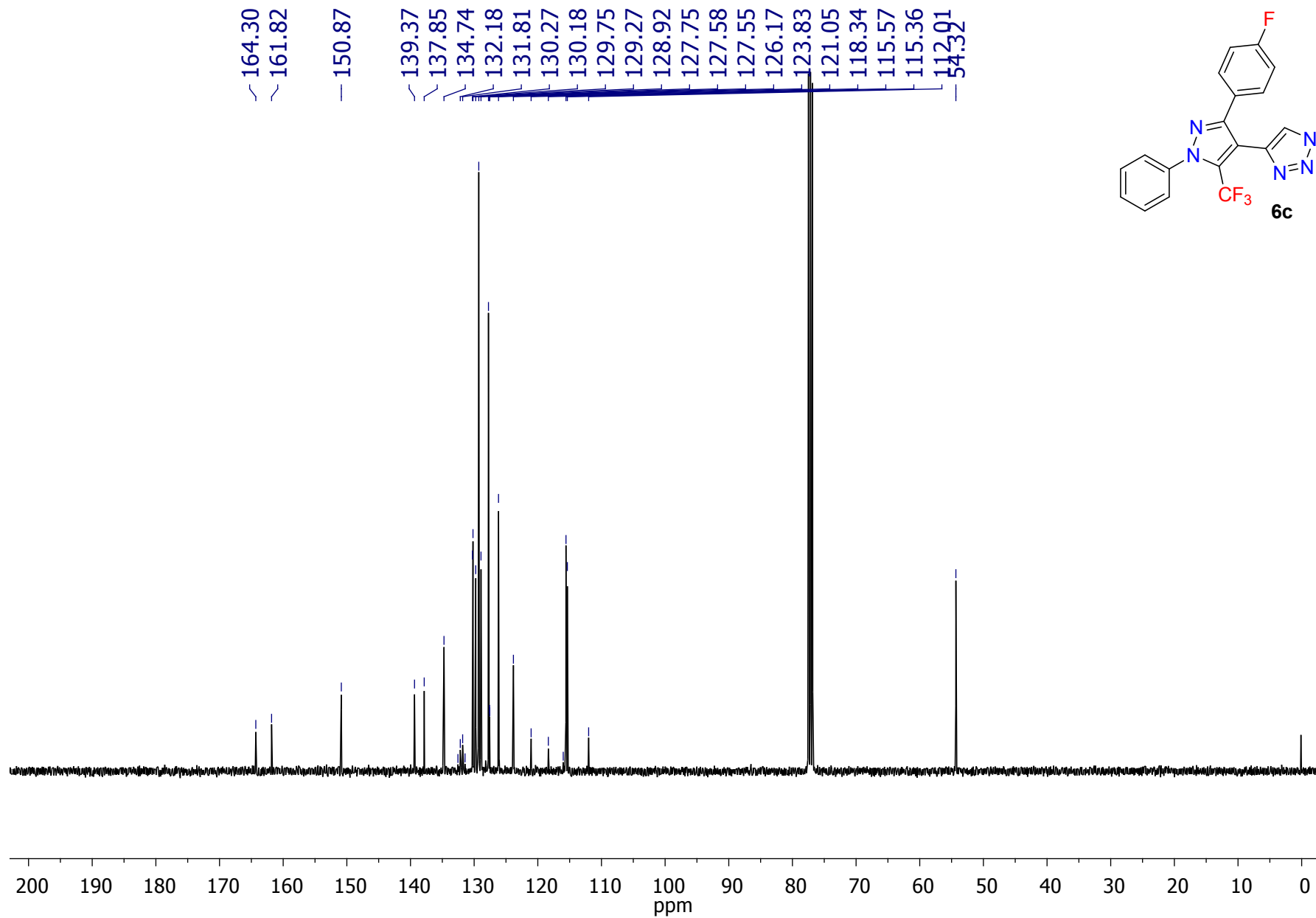


6c - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

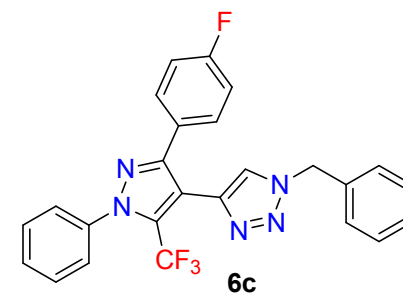
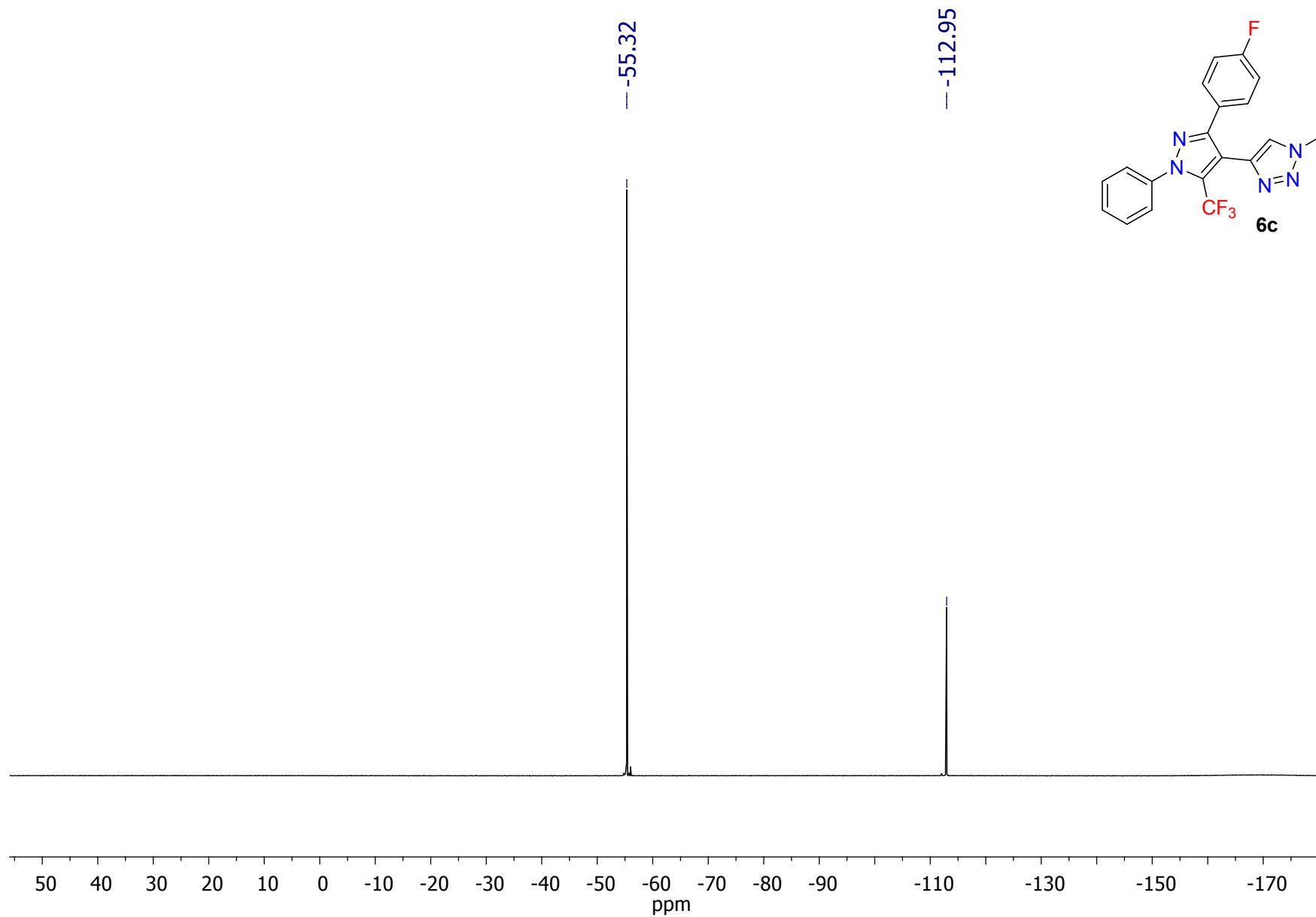




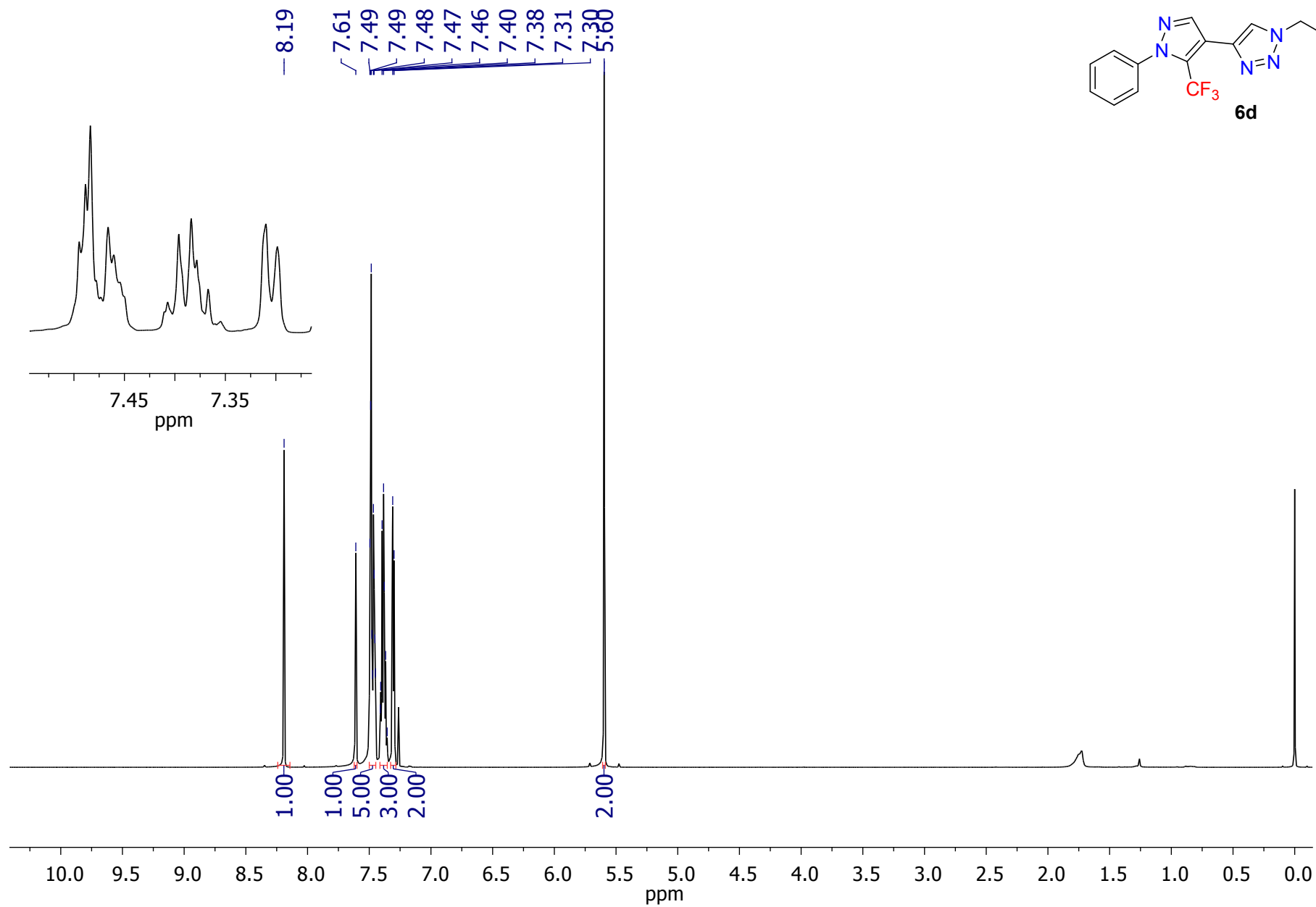
6c -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)



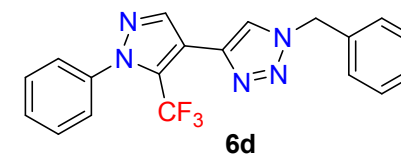
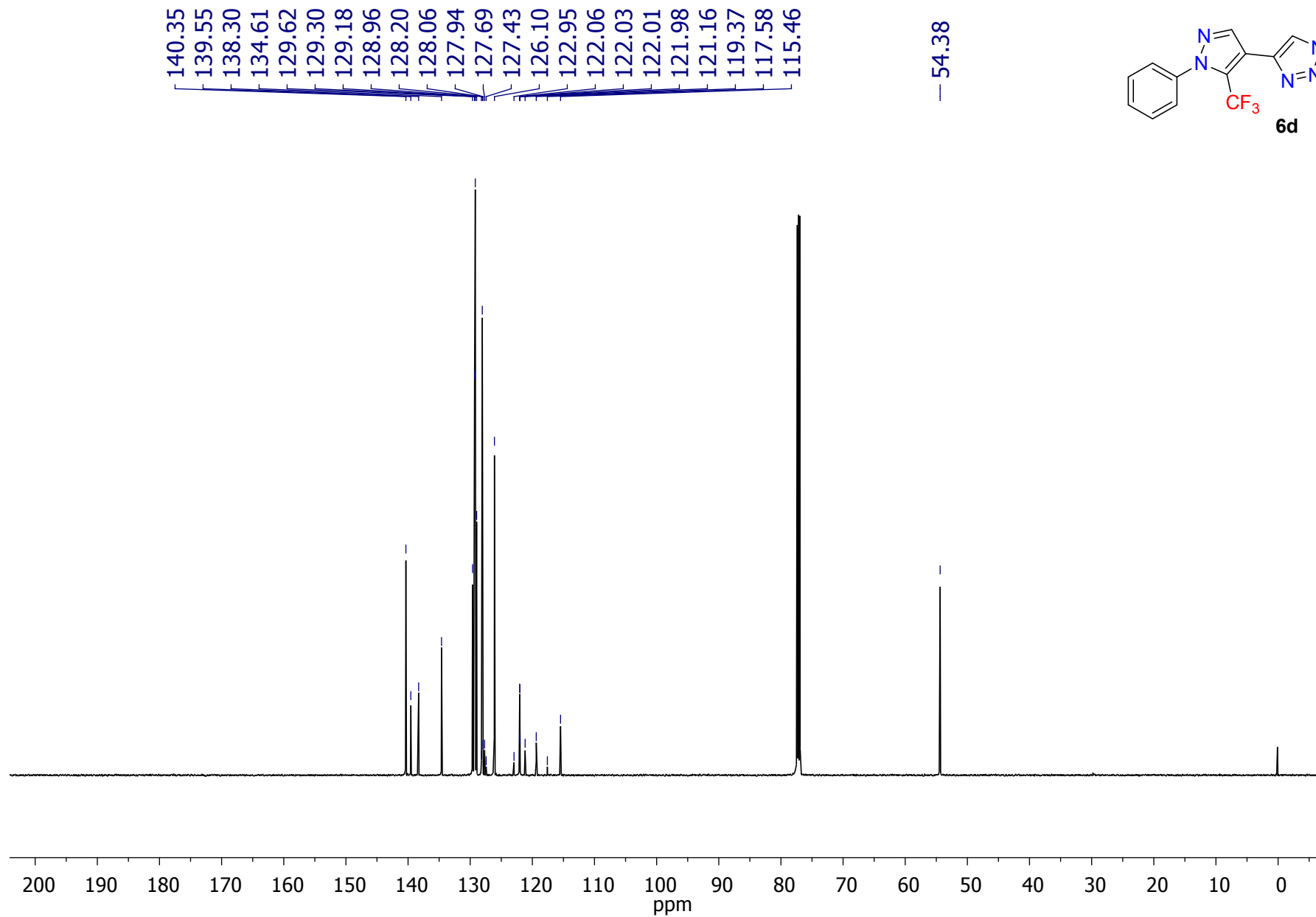
6c -  $^{19}\text{F}$  NMR (565 MHz,  $\text{CDCl}_3$ , 25 °C)



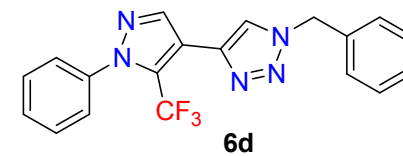
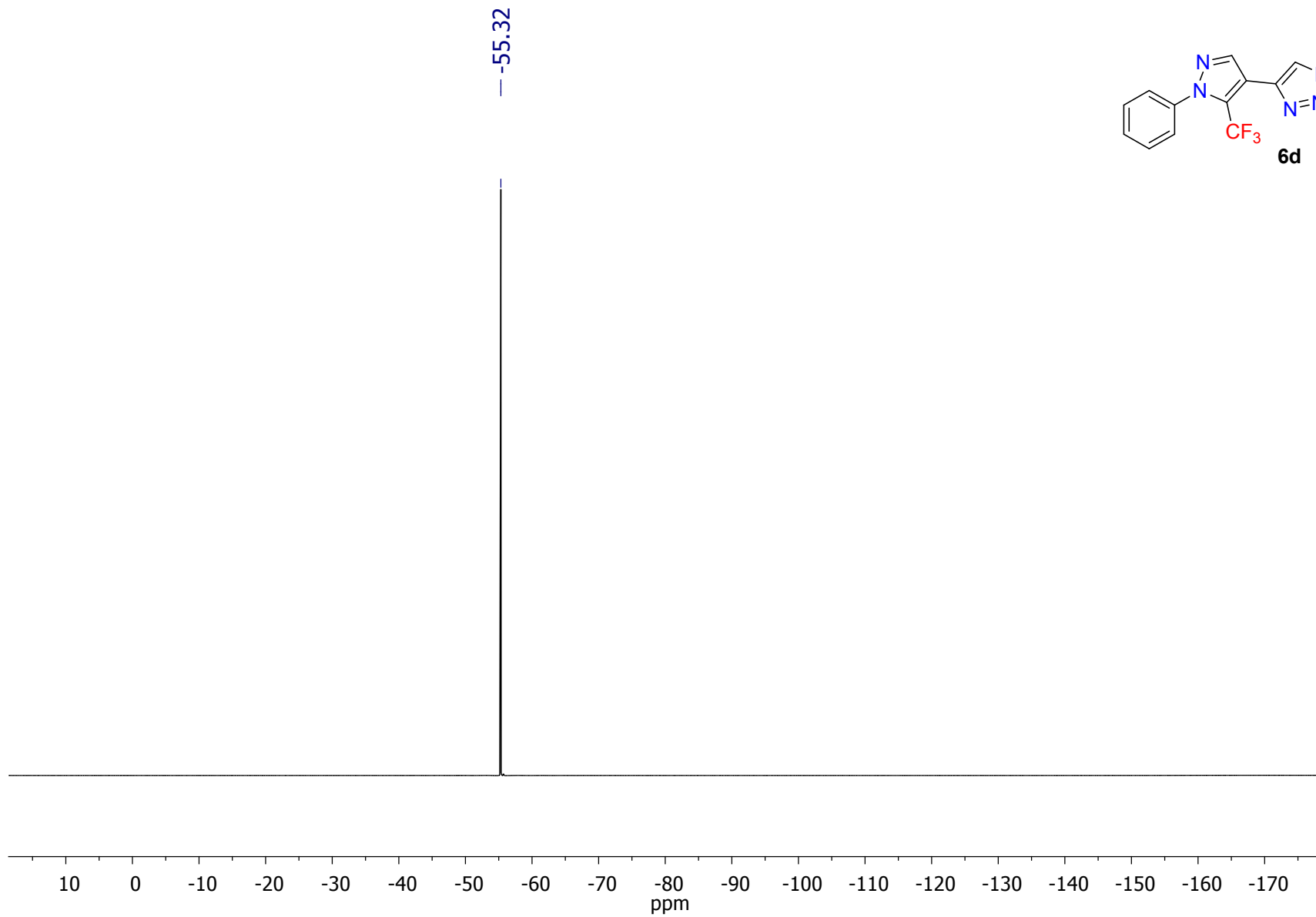
6d - <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>, 25 °C)



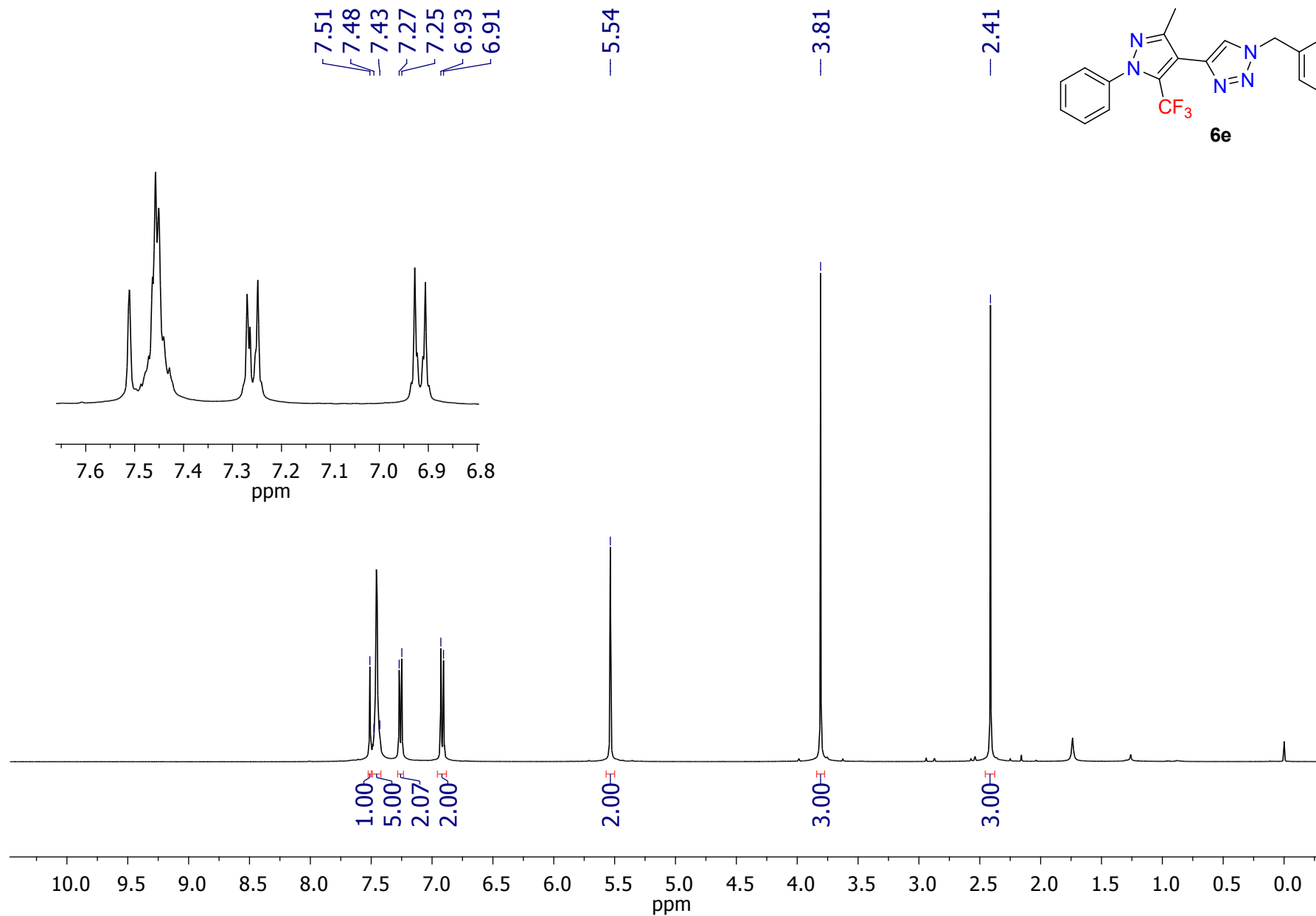
**6d** -  $^{13}\text{C}\{^1\text{H}\}$  NMR (150 MHz,  $\text{CDCl}_3$ , 25 °C)



**6d** -  $^{19}\text{F}$  NMR (565 MHz,  $\text{CDCl}_3$ , 25 °C)

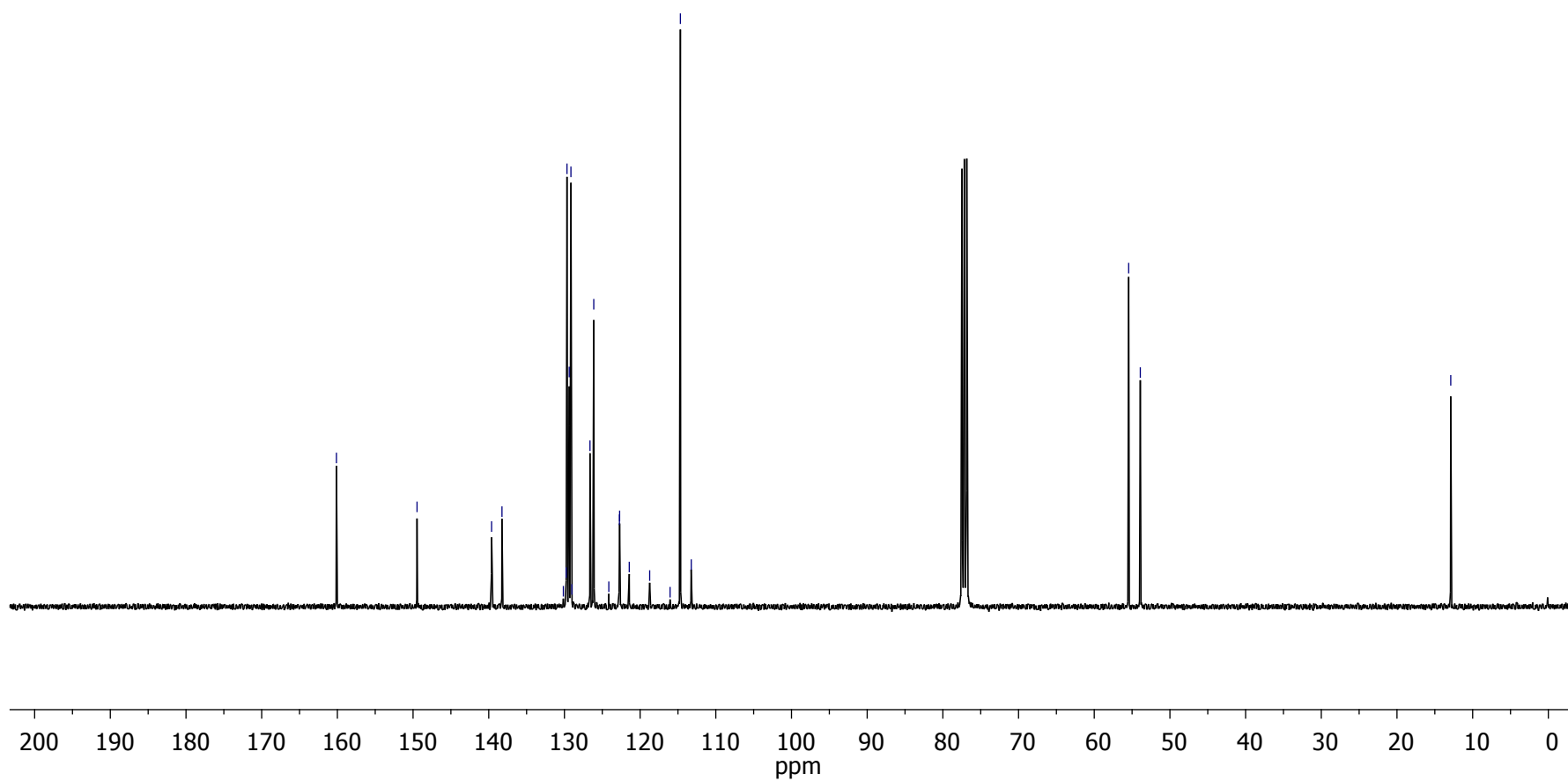
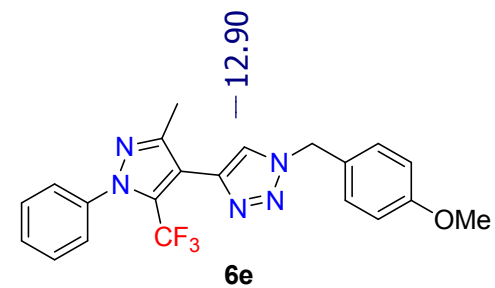


6e - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)



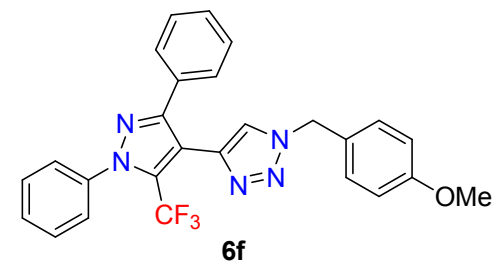
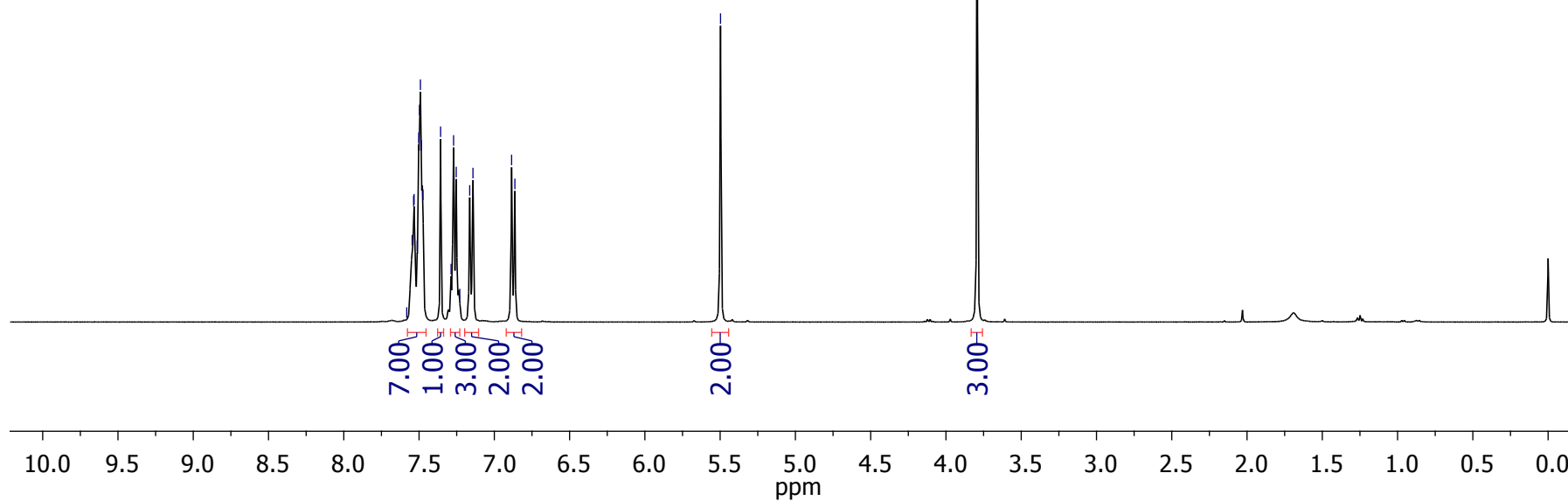
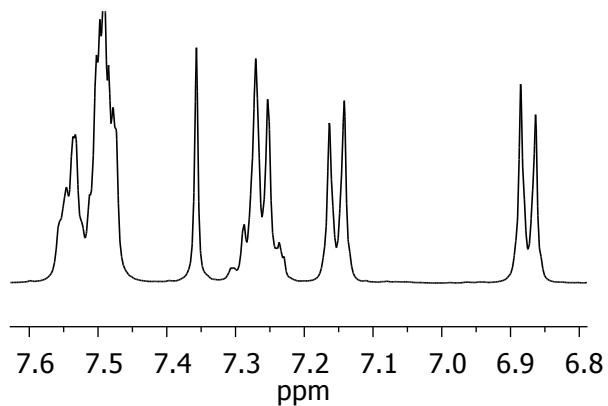
6e -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)

160.12  
149.47  
139.62  
138.25  
130.14  
129.77  
129.66  
129.37  
129.14  
129.02  
126.62  
126.12  
124.14  
122.73  
122.71  
121.44  
118.74  
116.04  
114.68  
113.24  
55.45  
53.91



6f - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

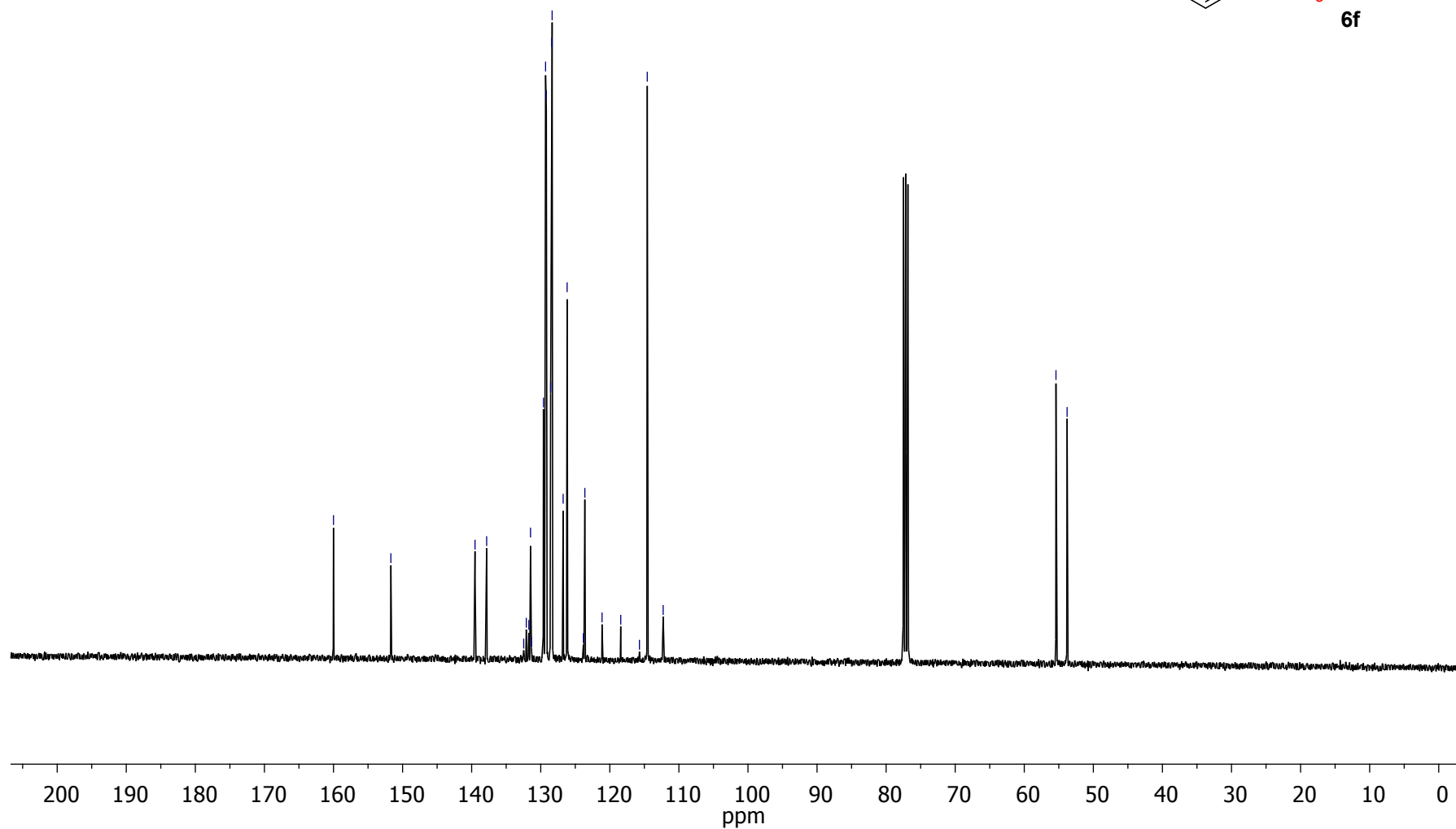
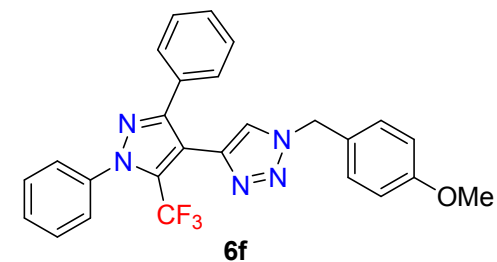
7.58  
7.55  
7.54  
7.53  
7.51  
7.50  
7.50  
7.49  
7.48  
7.47  
7.36  
7.29  
7.27  
7.25  
7.23  
7.16  
7.14  
6.89  
6.86  
— 5.50





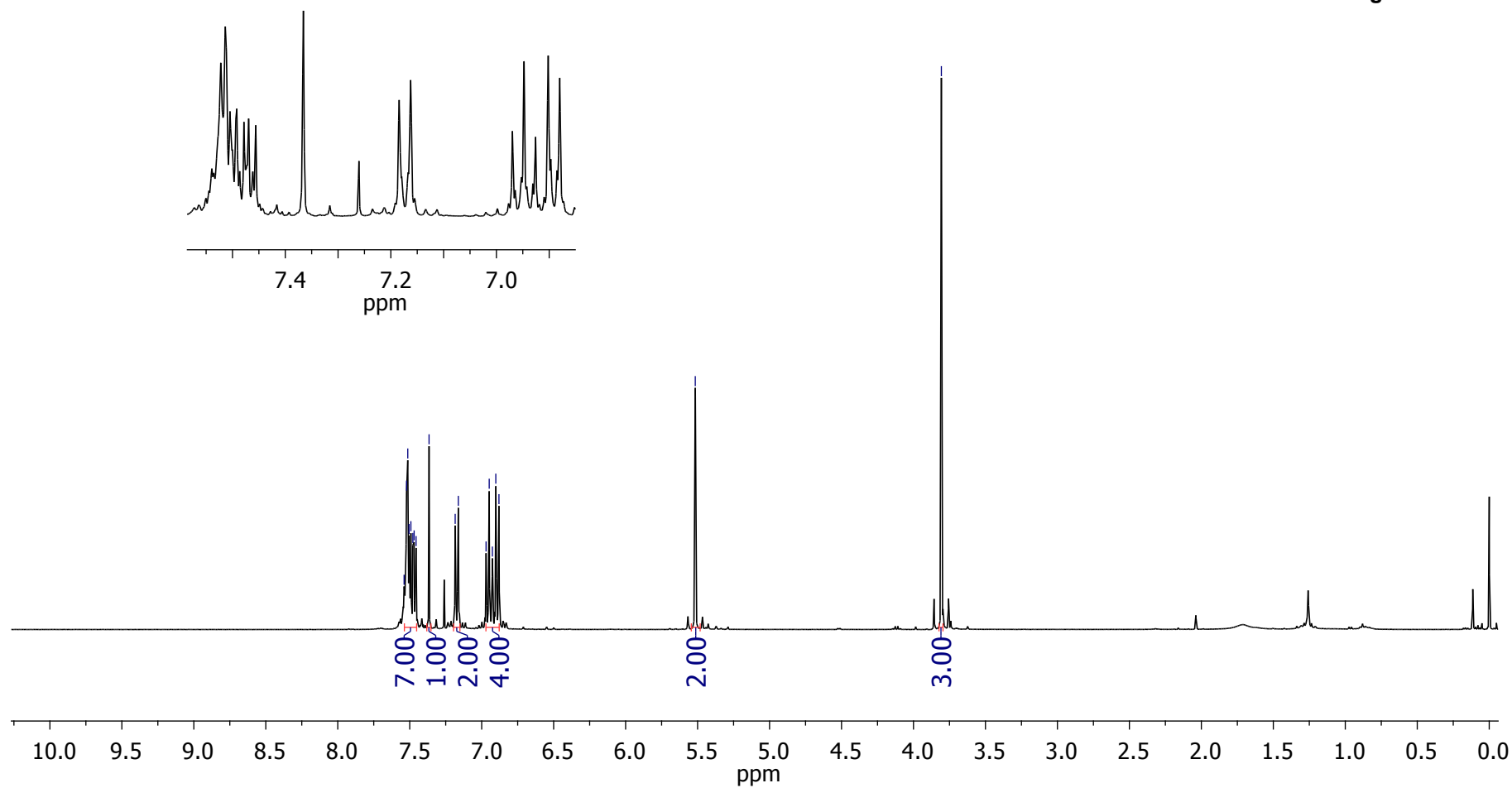
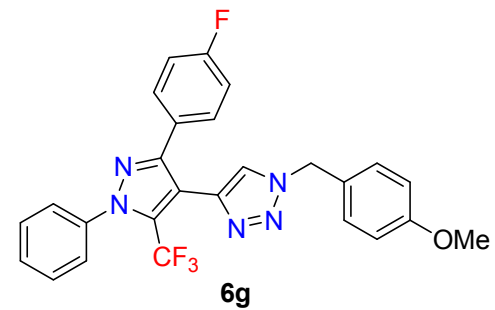
6f -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)

160.00  
151.69  
139.51  
137.83  
132.09  
131.72  
131.48  
131.35  
129.61  
129.30  
129.19  
128.57  
128.39  
128.35  
126.76  
126.18  
123.83  
123.61  
121.12  
118.42  
114.58  
112.28  
55.41  
53.80

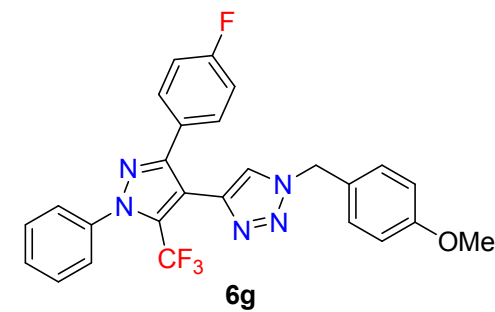
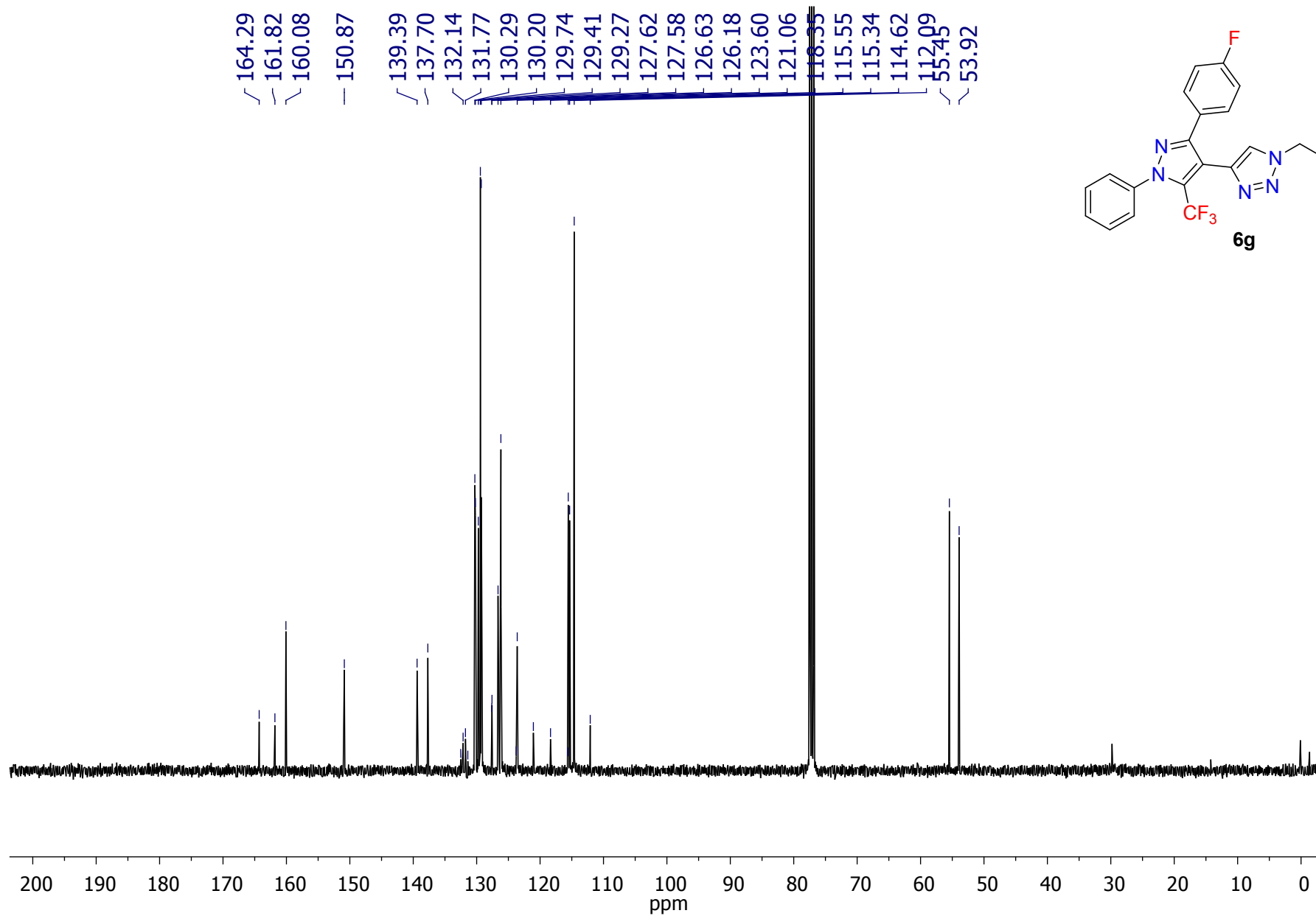


6g - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

7.54  
7.52  
7.51  
7.50  
7.49  
7.48  
7.47  
7.46  
7.37  
7.18  
7.16  
6.97  
6.95  
6.93  
6.90  
6.88  
5.52  
3.81



6g -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)

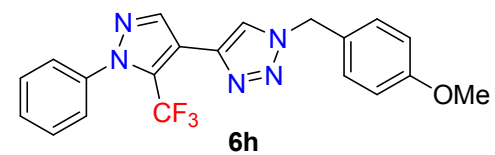


6h - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

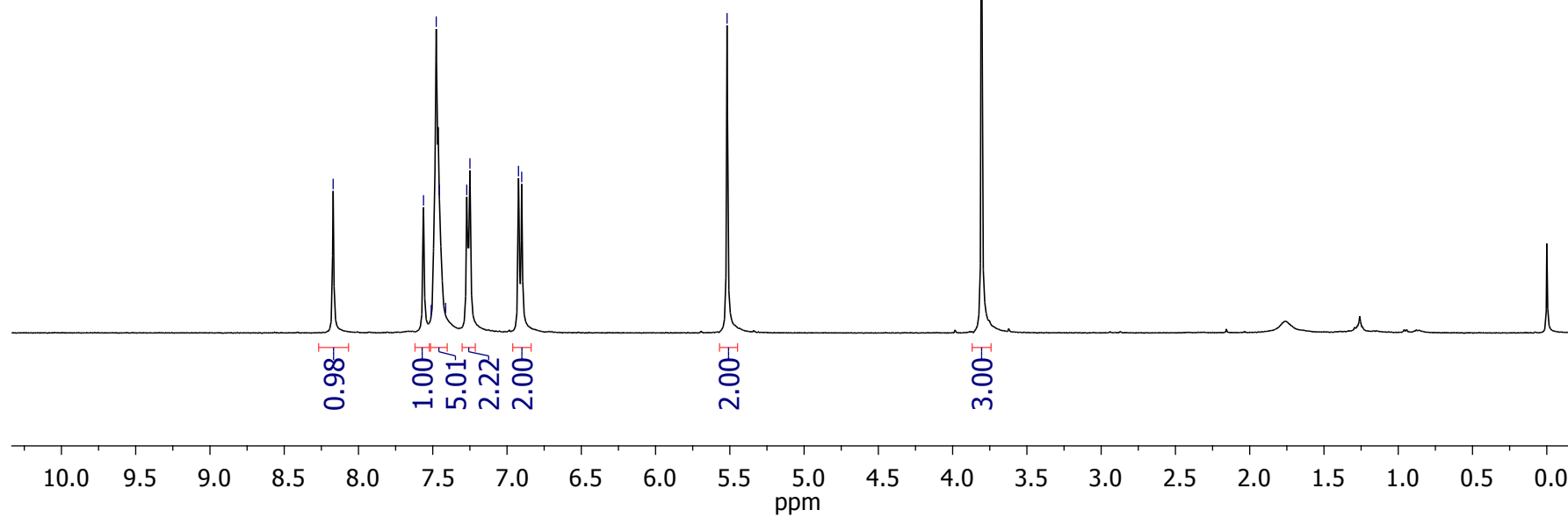
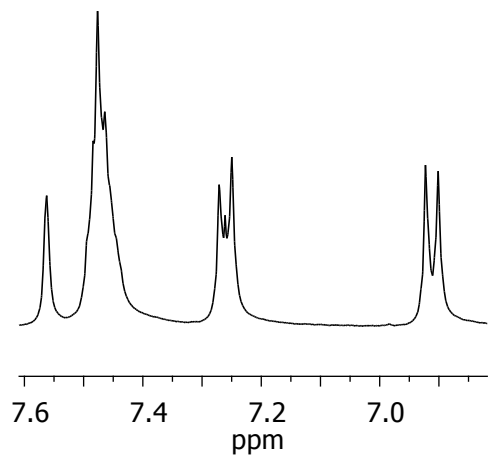
8.17  
7.56  
7.51  
7.48  
7.46  
7.41  
7.27  
7.25  
6.92  
6.90

5.52

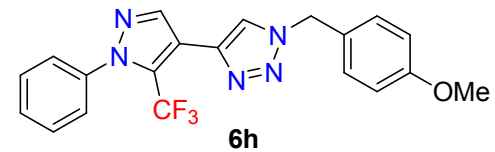
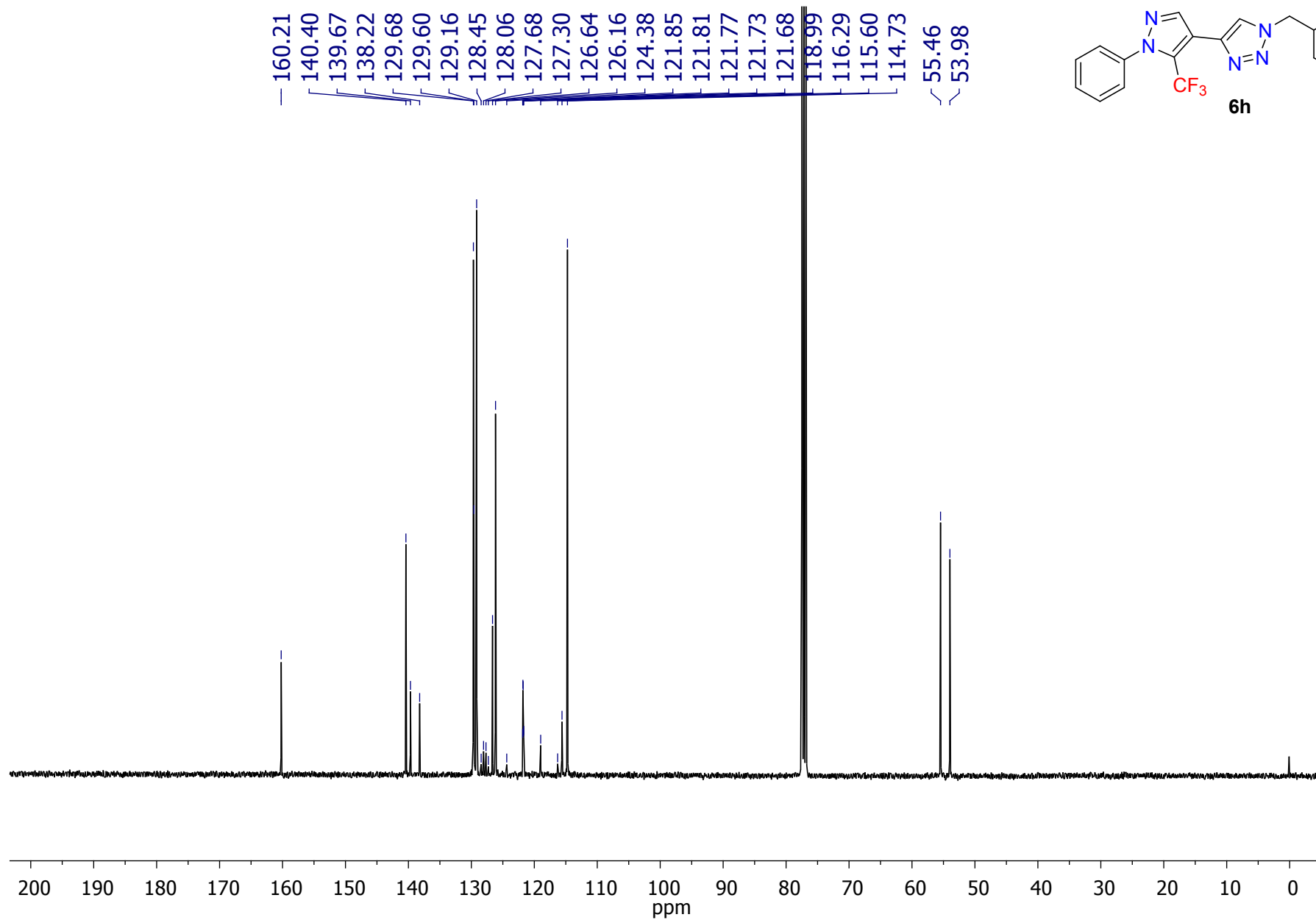
3.81



6h



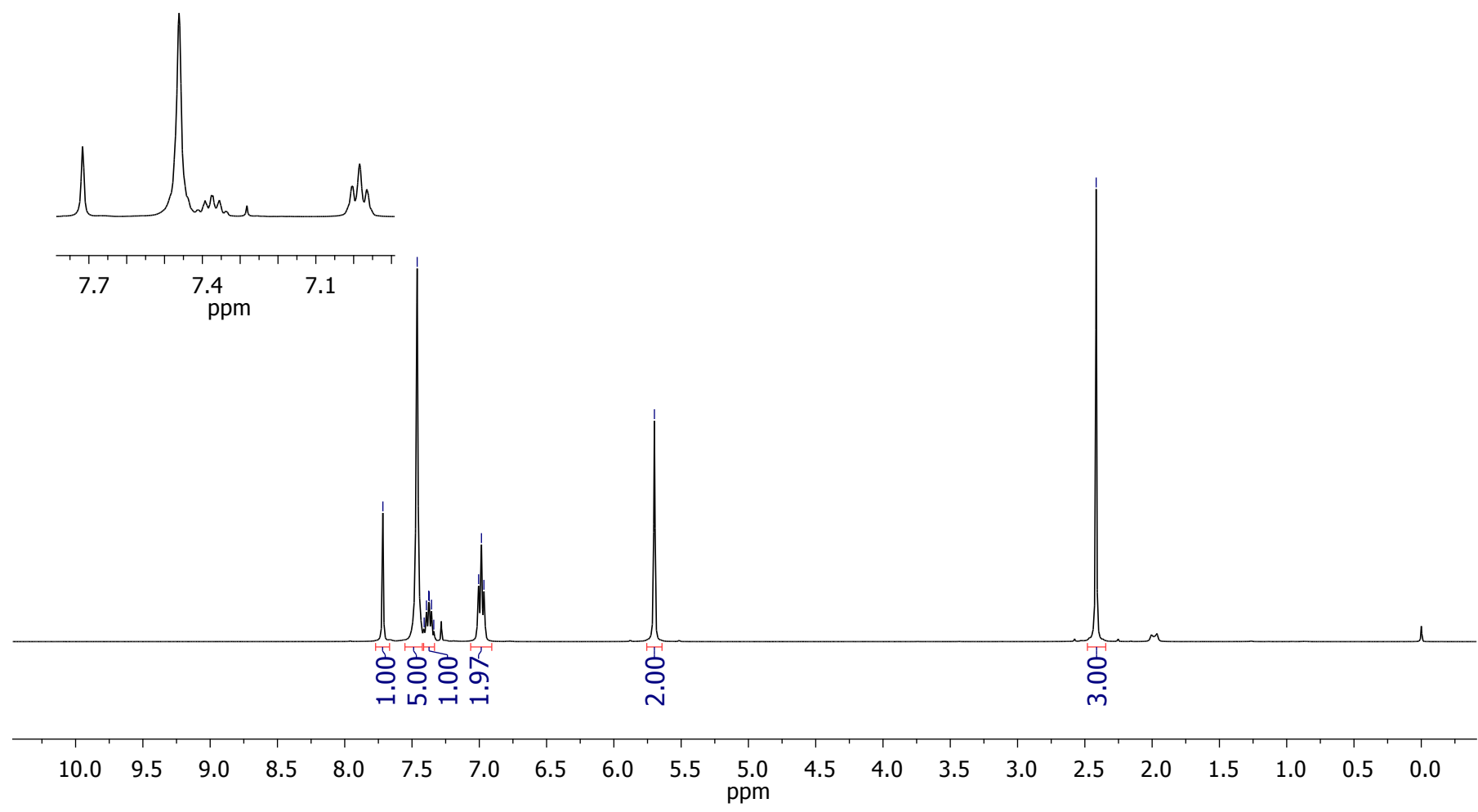
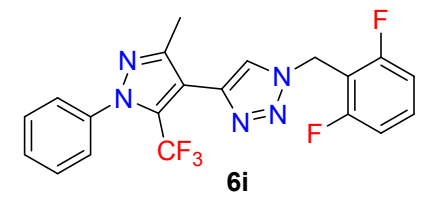
6h -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)



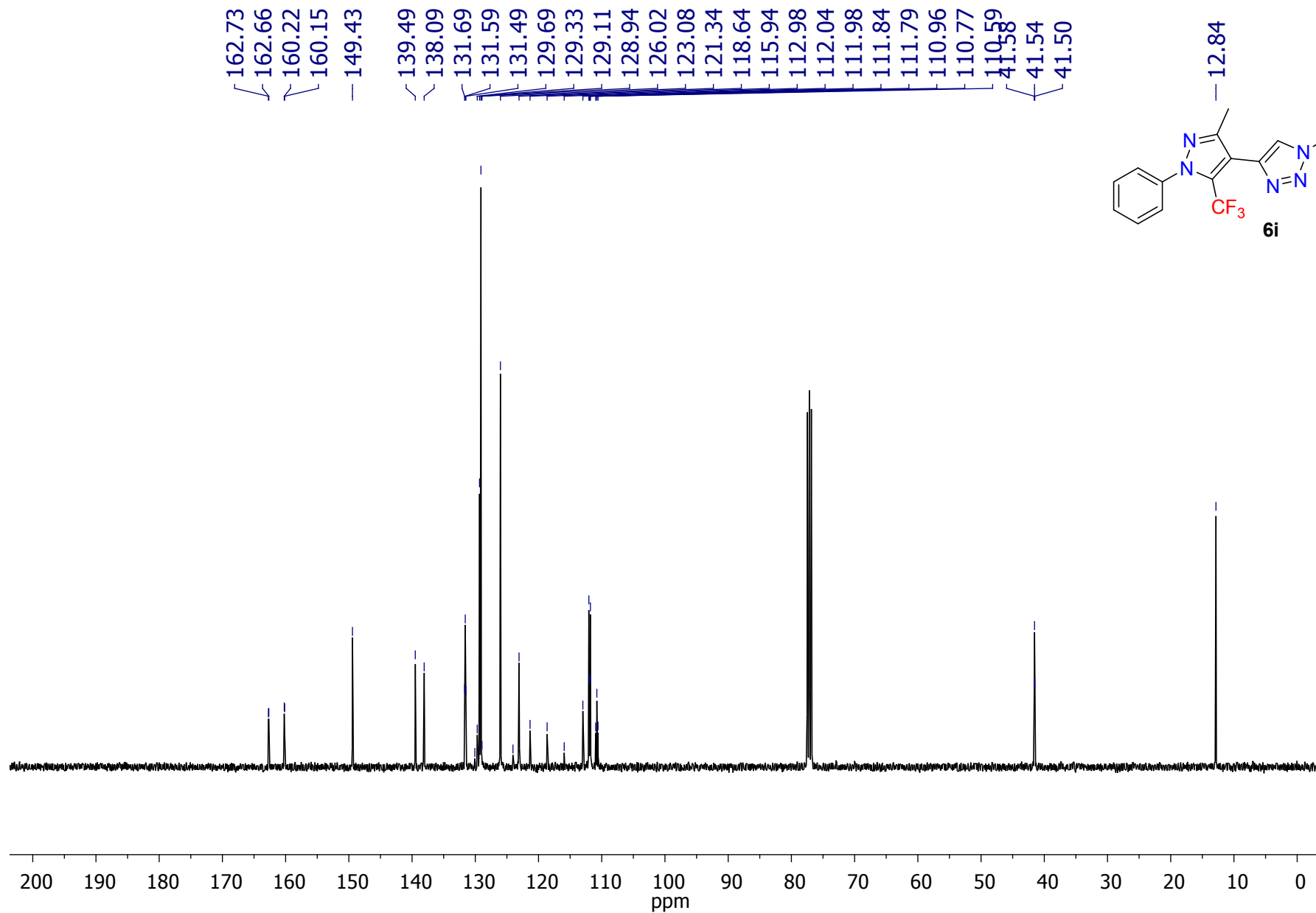
6i - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

7.72  
7.46  
7.41  
7.39  
7.38  
7.37  
7.36  
7.34  
7.01  
6.98  
6.97  
— 5.70

— 2.42



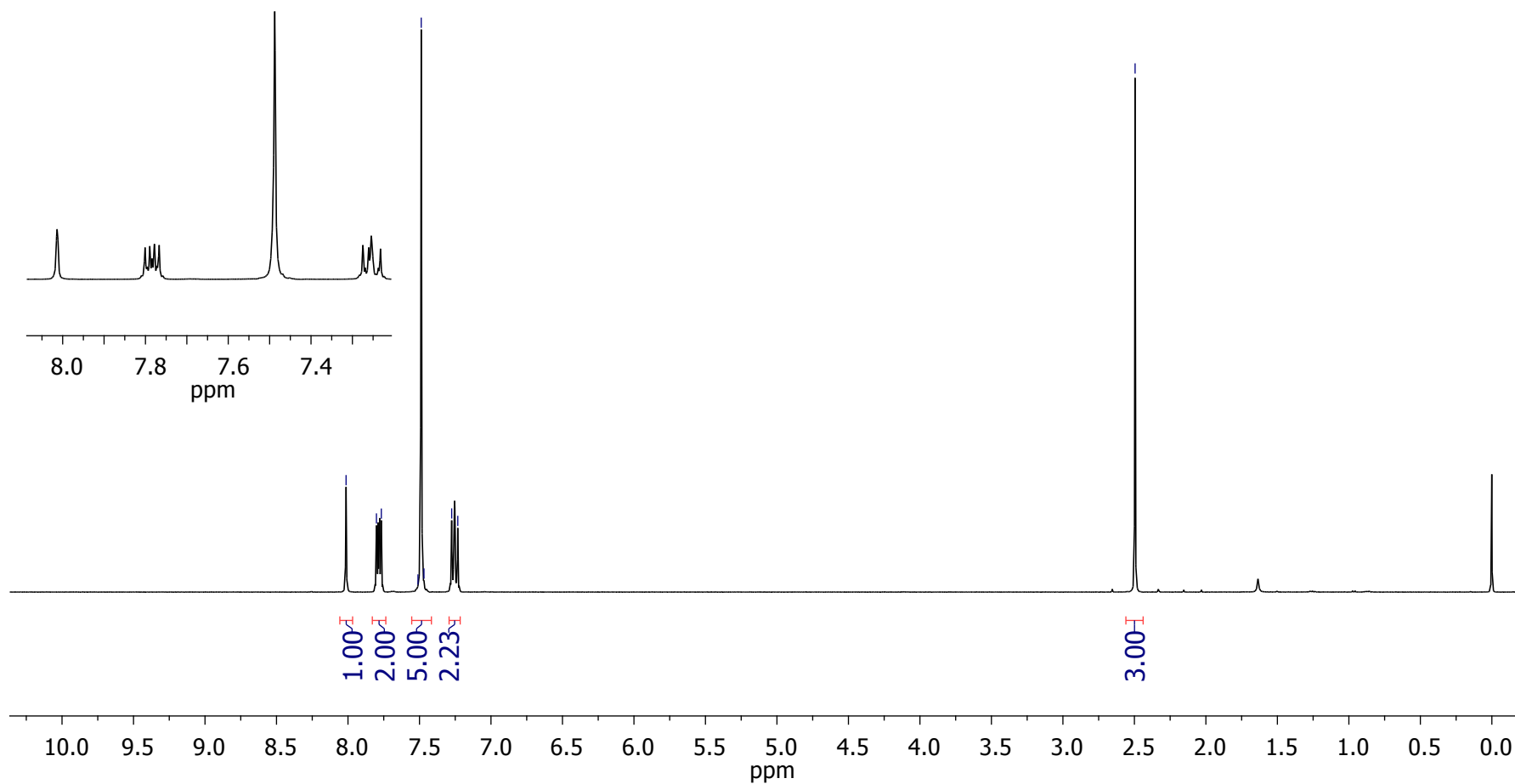
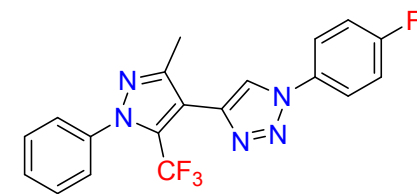
6i -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)



6j - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

8.01  
7.80  
7.77  
7.51  
7.49  
7.47  
7.27  
7.23

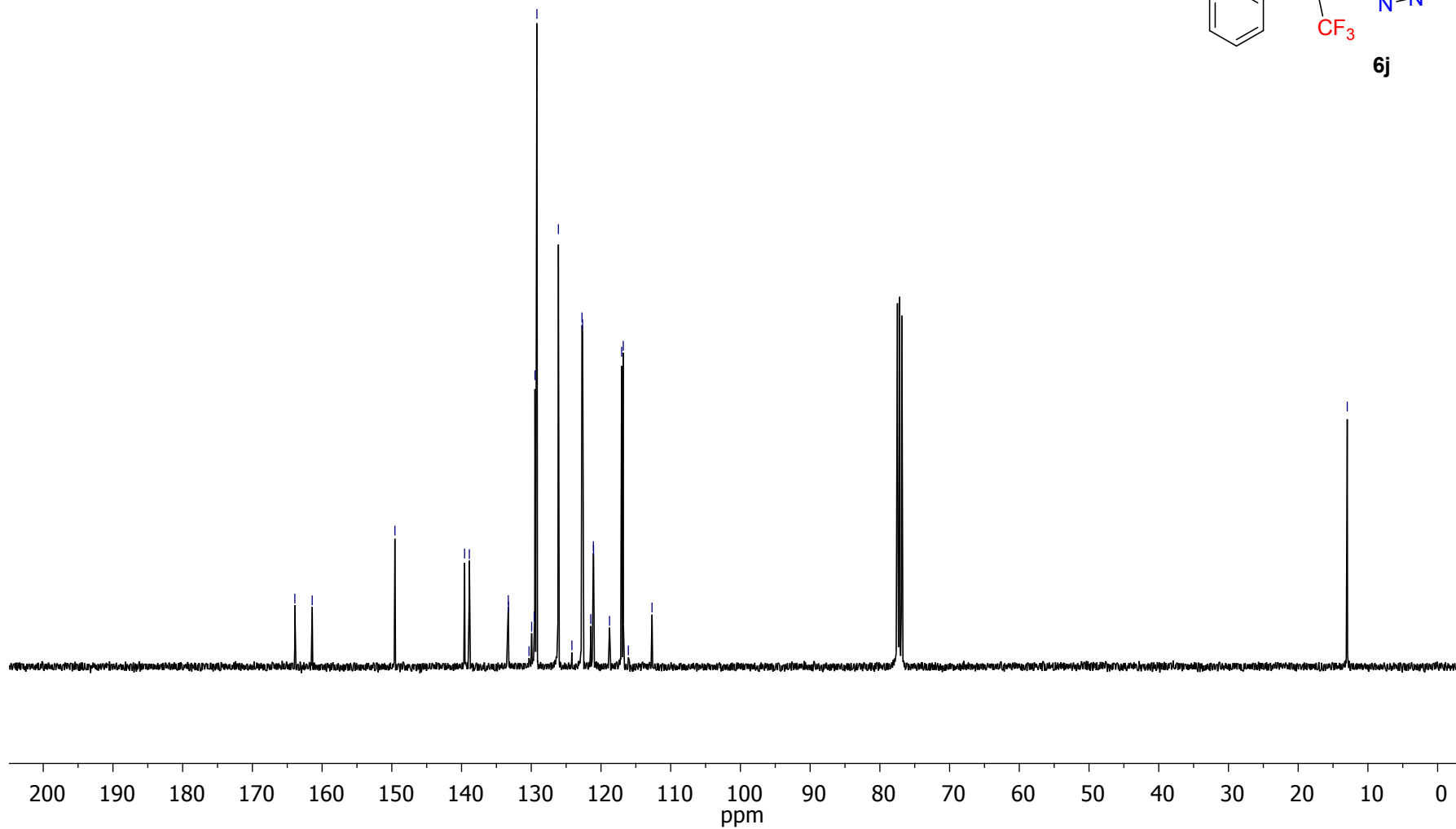
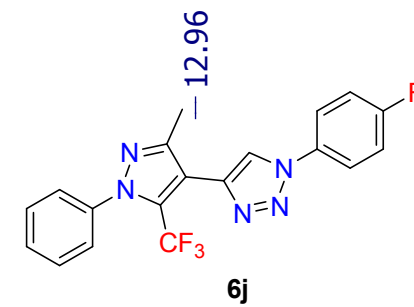
2.50





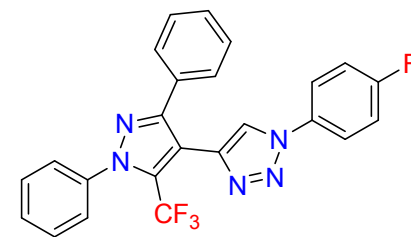
6j -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)

163.91  
161.42  
149.55  
139.57  
138.88  
133.30  
133.27  
130.32  
129.95  
129.57  
129.47  
129.19  
126.11  
124.17  
122.73  
122.64  
121.47  
121.09  
121.07  
118.77  
117.04  
116.80  
116.08  
112.68

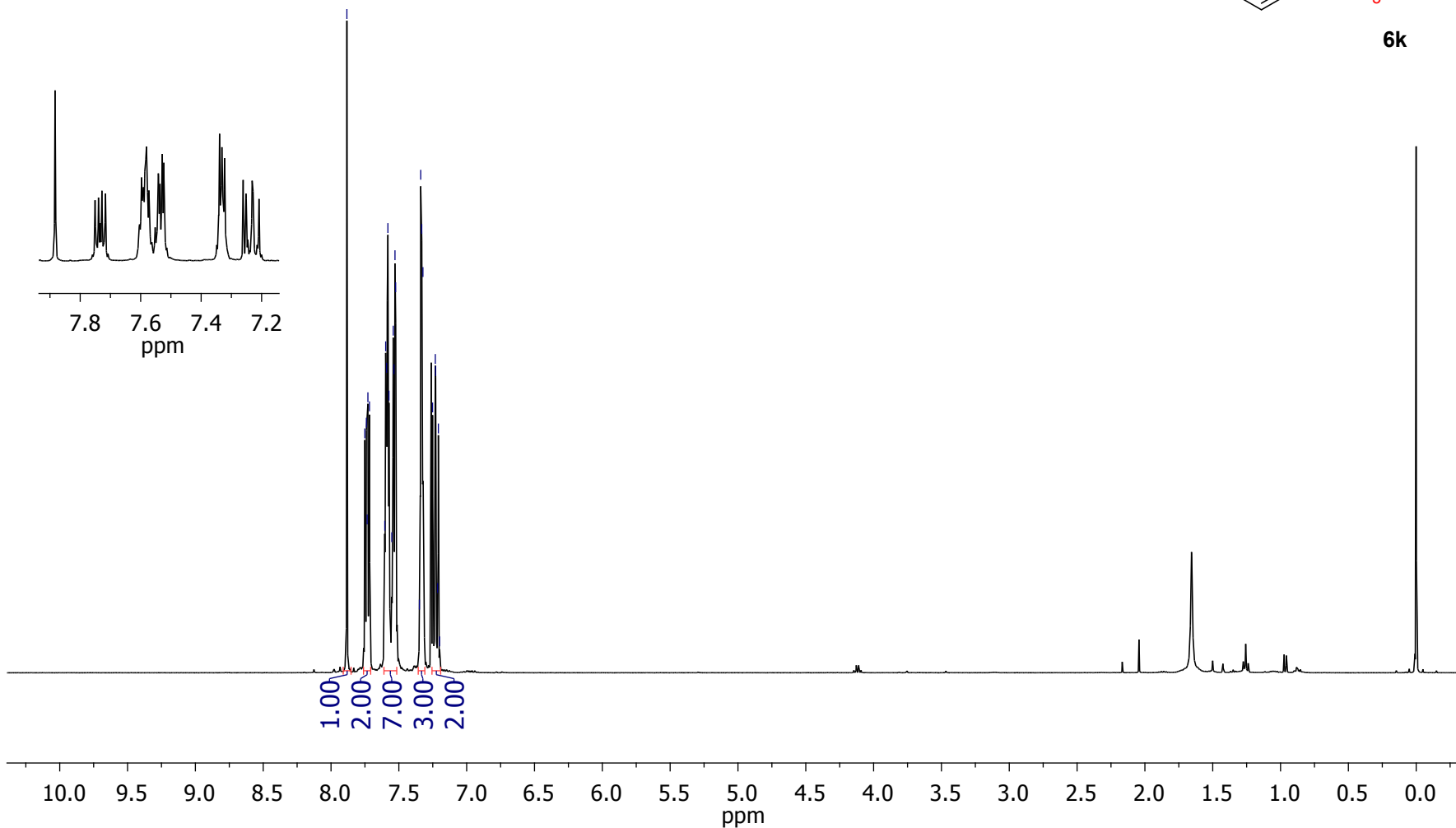


6k - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

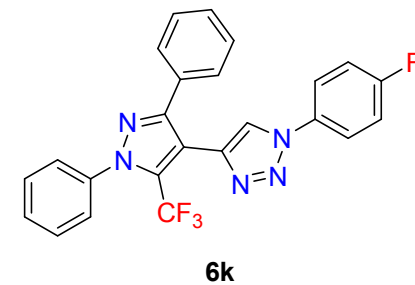
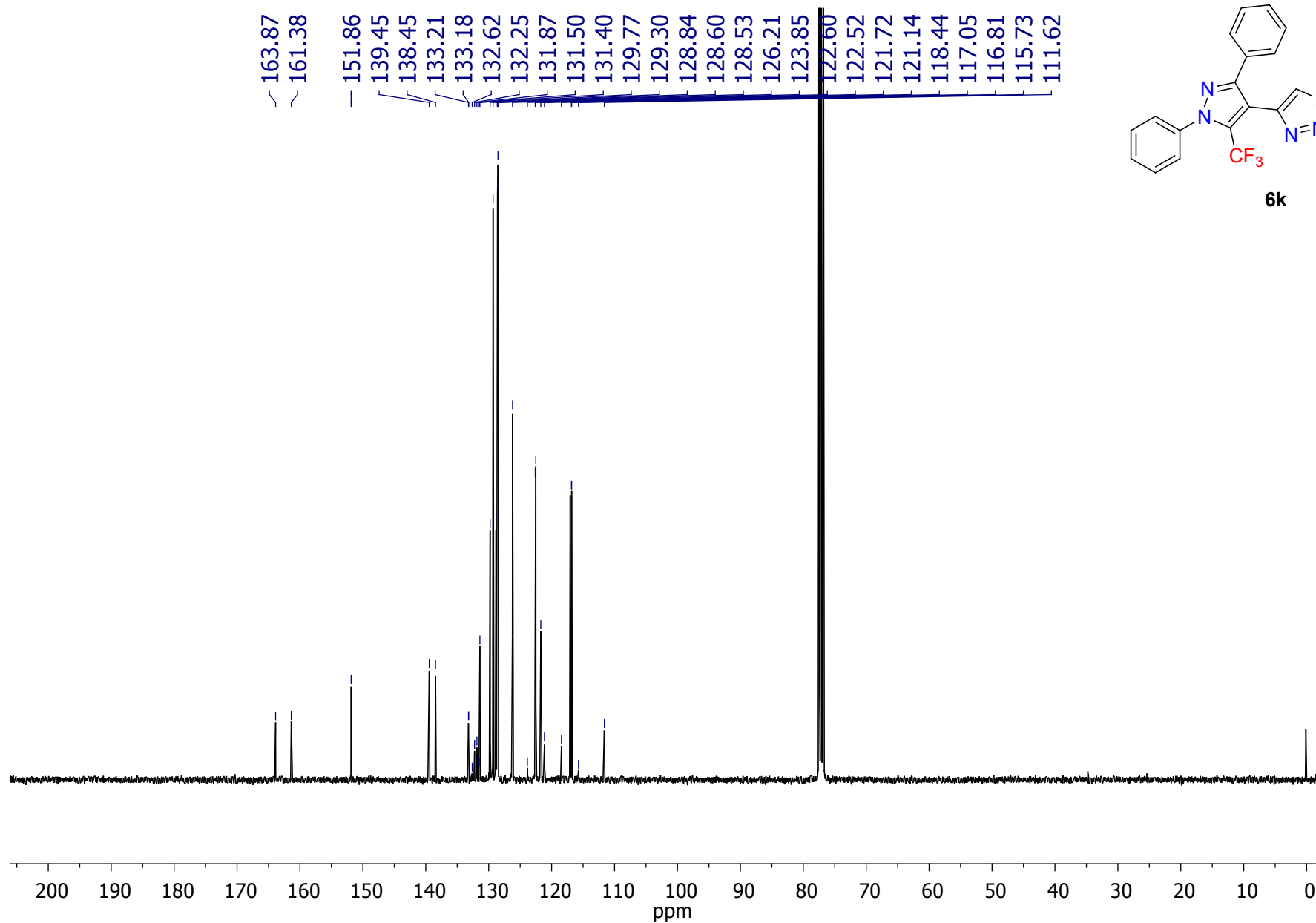
7.88  
7.75  
7.74  
7.73  
7.73  
7.72  
7.60  
7.60  
7.59  
7.58  
7.57  
7.55  
7.54  
7.54  
7.53  
7.52  
7.35  
7.34  
7.33  
7.32  
7.25  
7.23  
7.23  
7.21  
7.21  
7.20



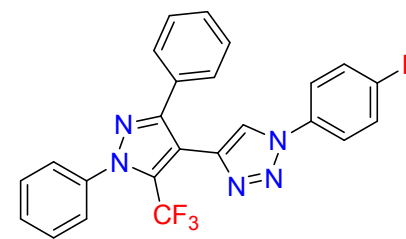
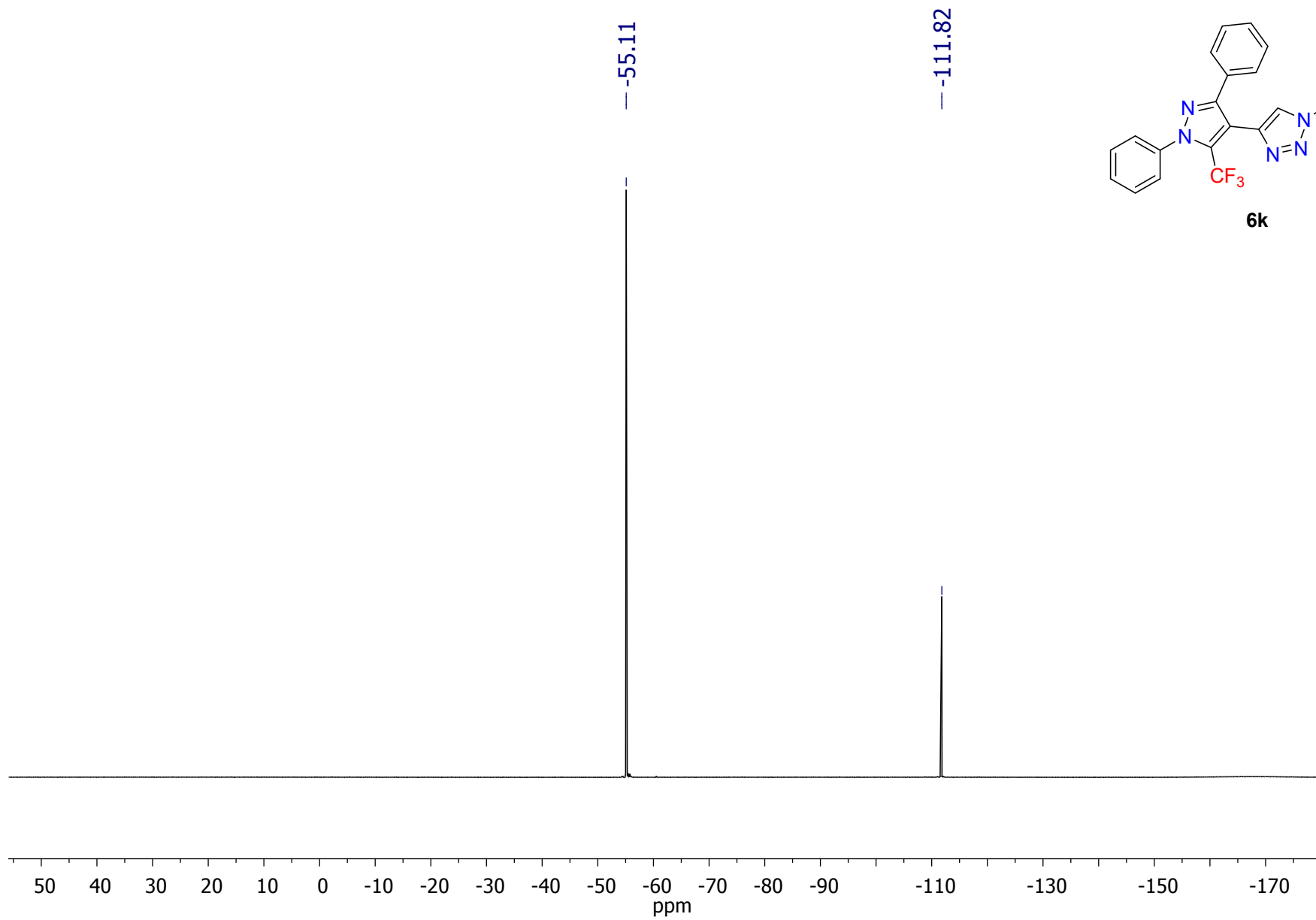
6k



6k -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)

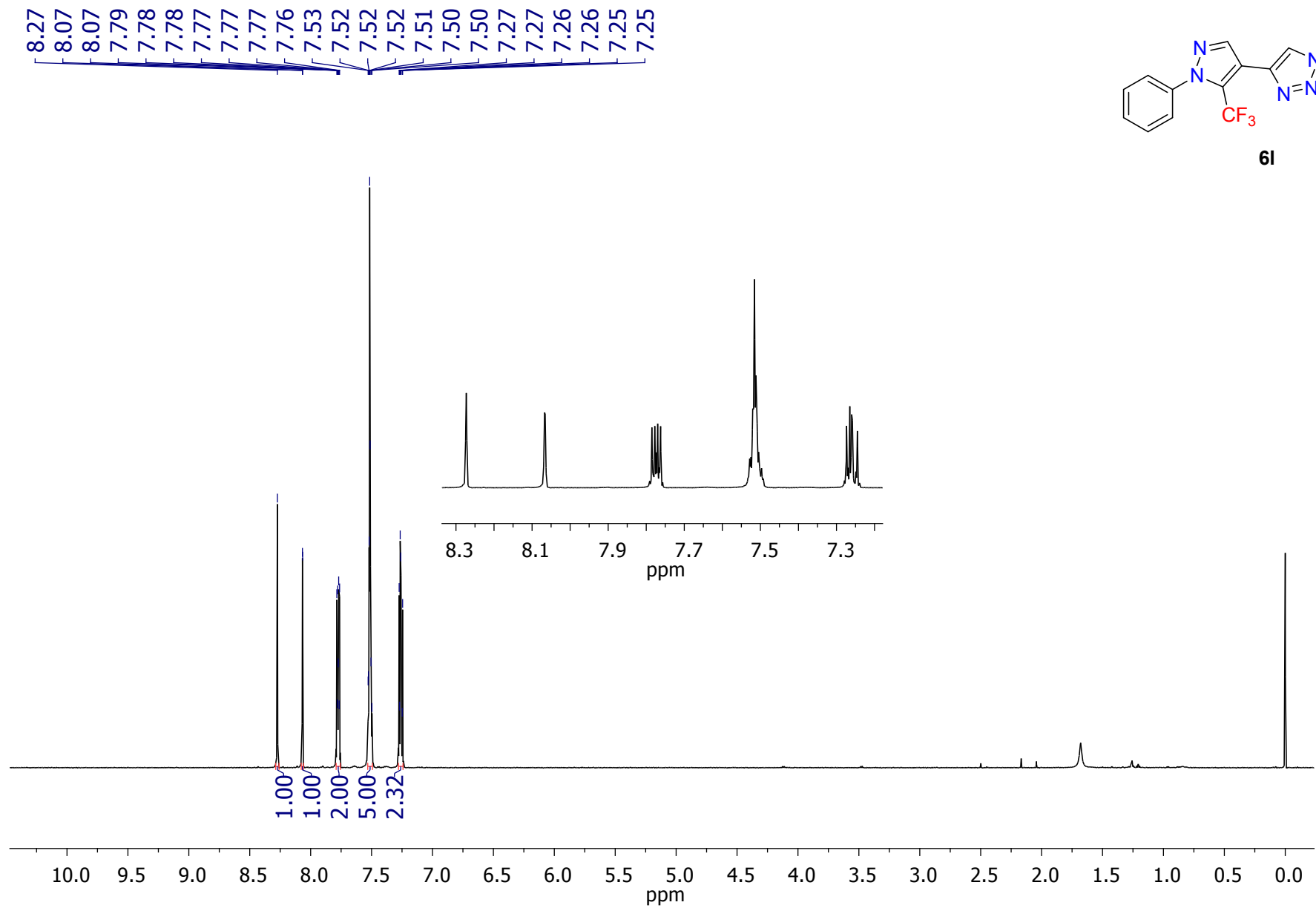
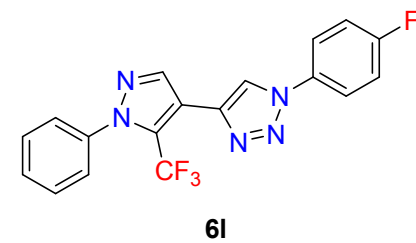


6k -  $^{19}\text{F}$  NMR (565 MHz,  $\text{CDCl}_3$ , 25 °C)

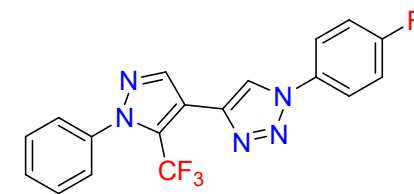
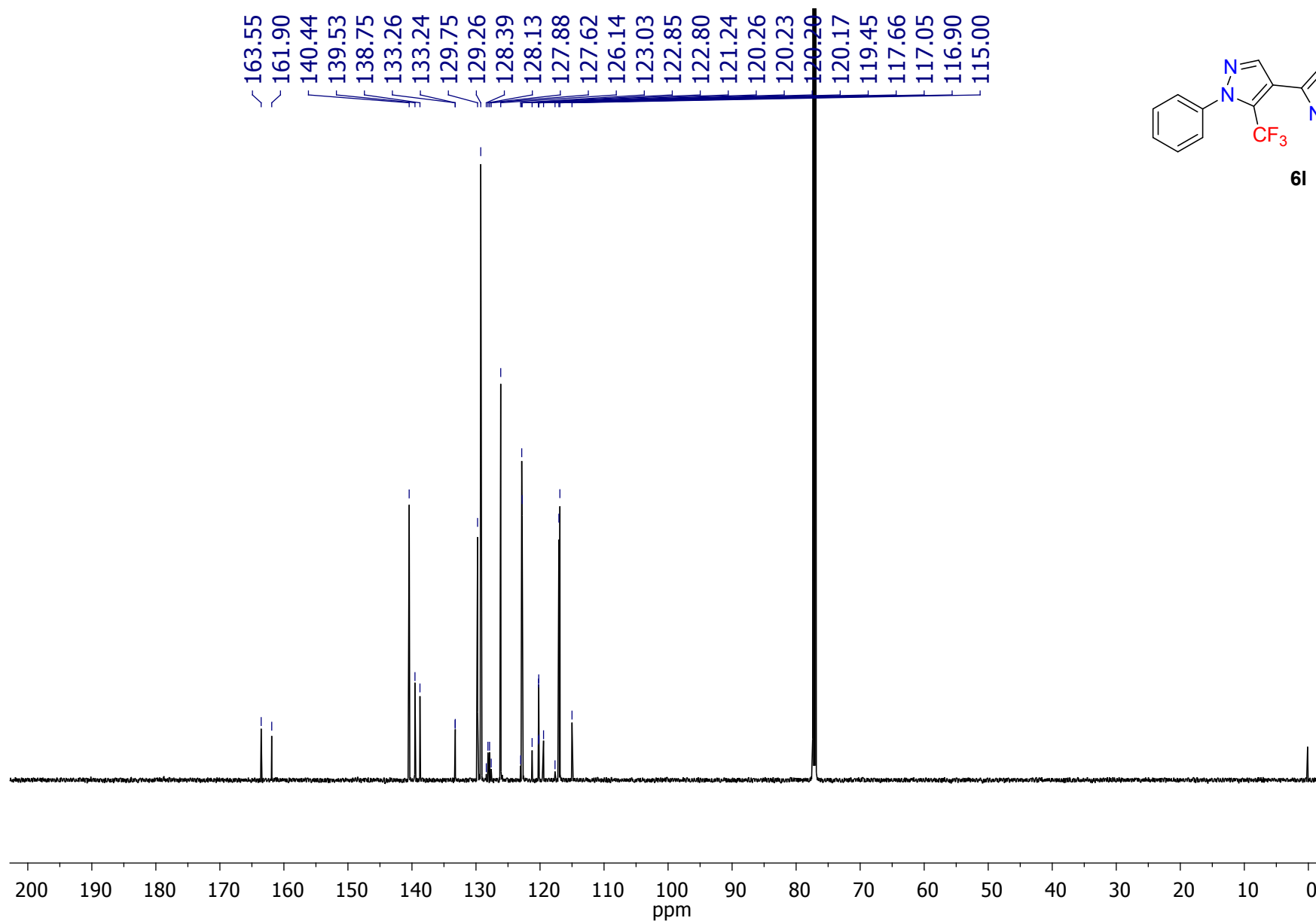


6k

61 - <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>, 25 °C)

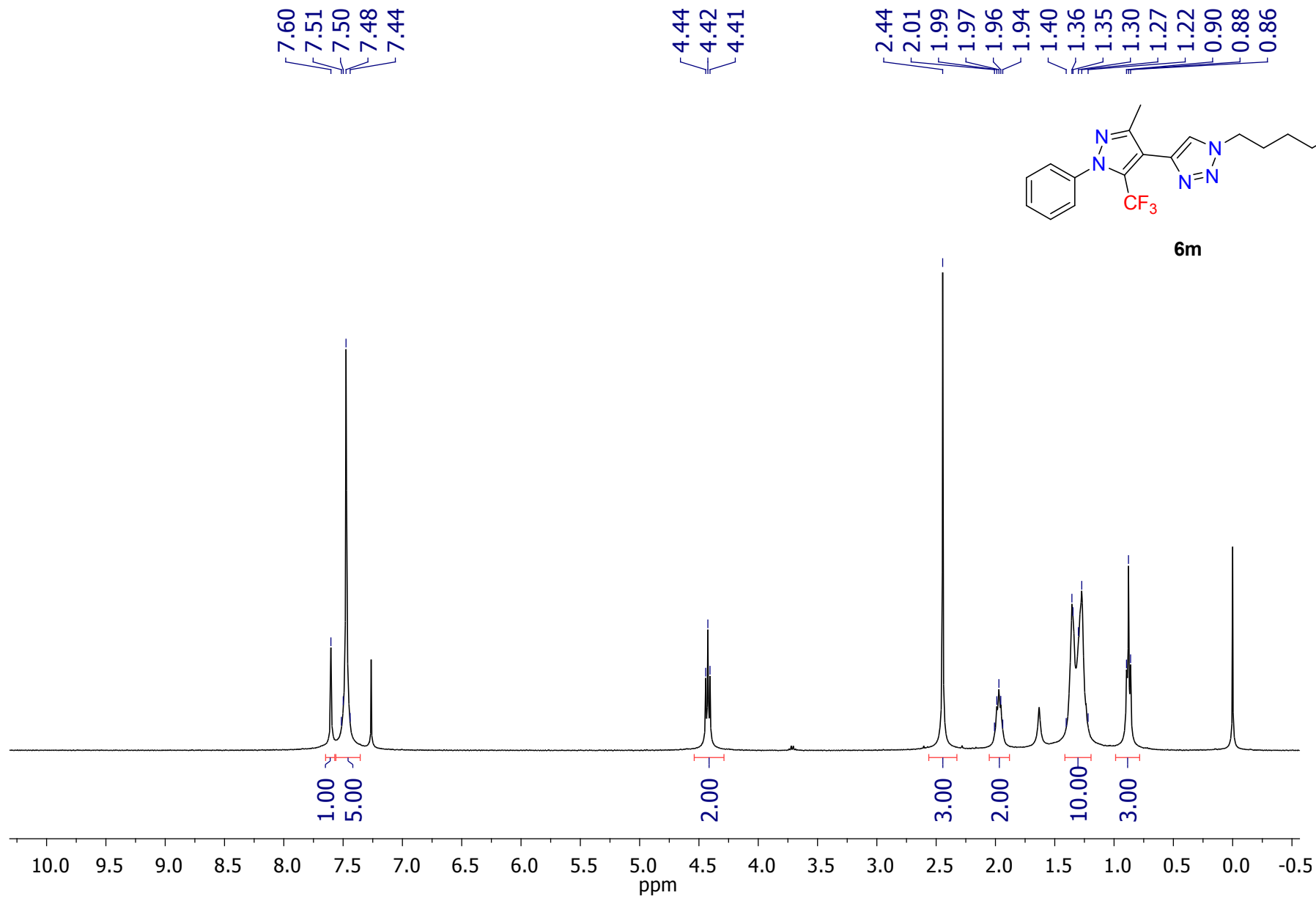


61 -  $^{13}\text{C}\{^1\text{H}\}$  NMR (150 MHz,  $\text{CDCl}_3$ , 25 °C)



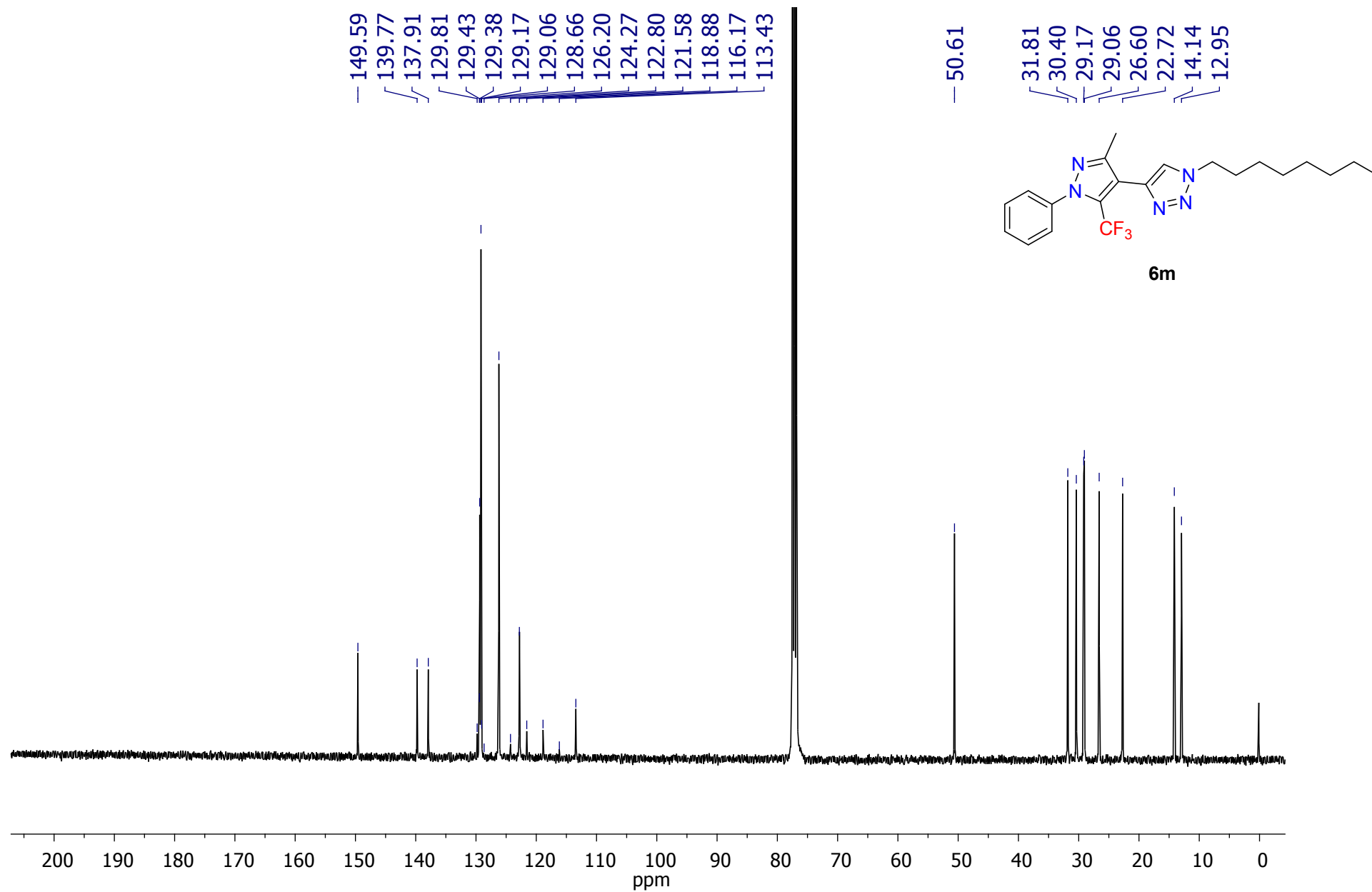
61

6m - <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

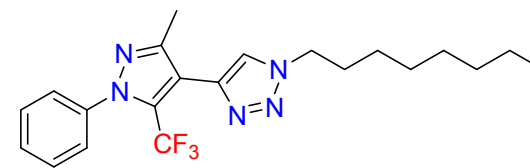


**6m** -  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 25 °C)



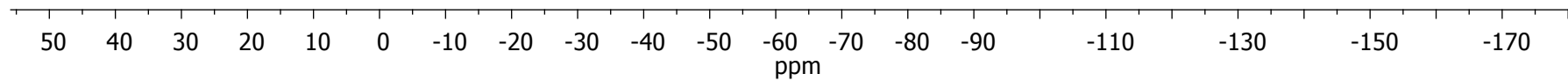
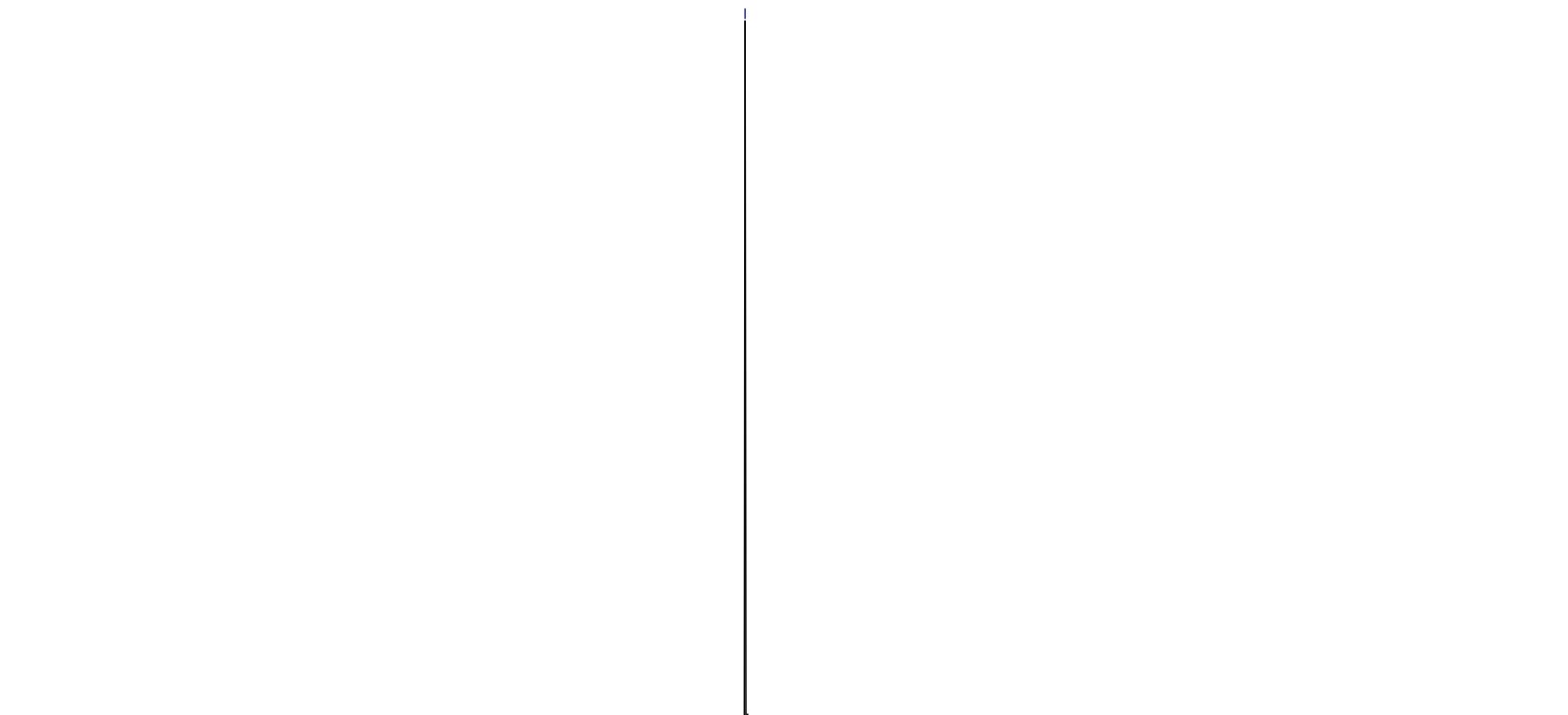


**6m** -  $^{13}\text{C}$  NMR (565 MHz,  $\text{CDCl}_3$ , 25 °C)



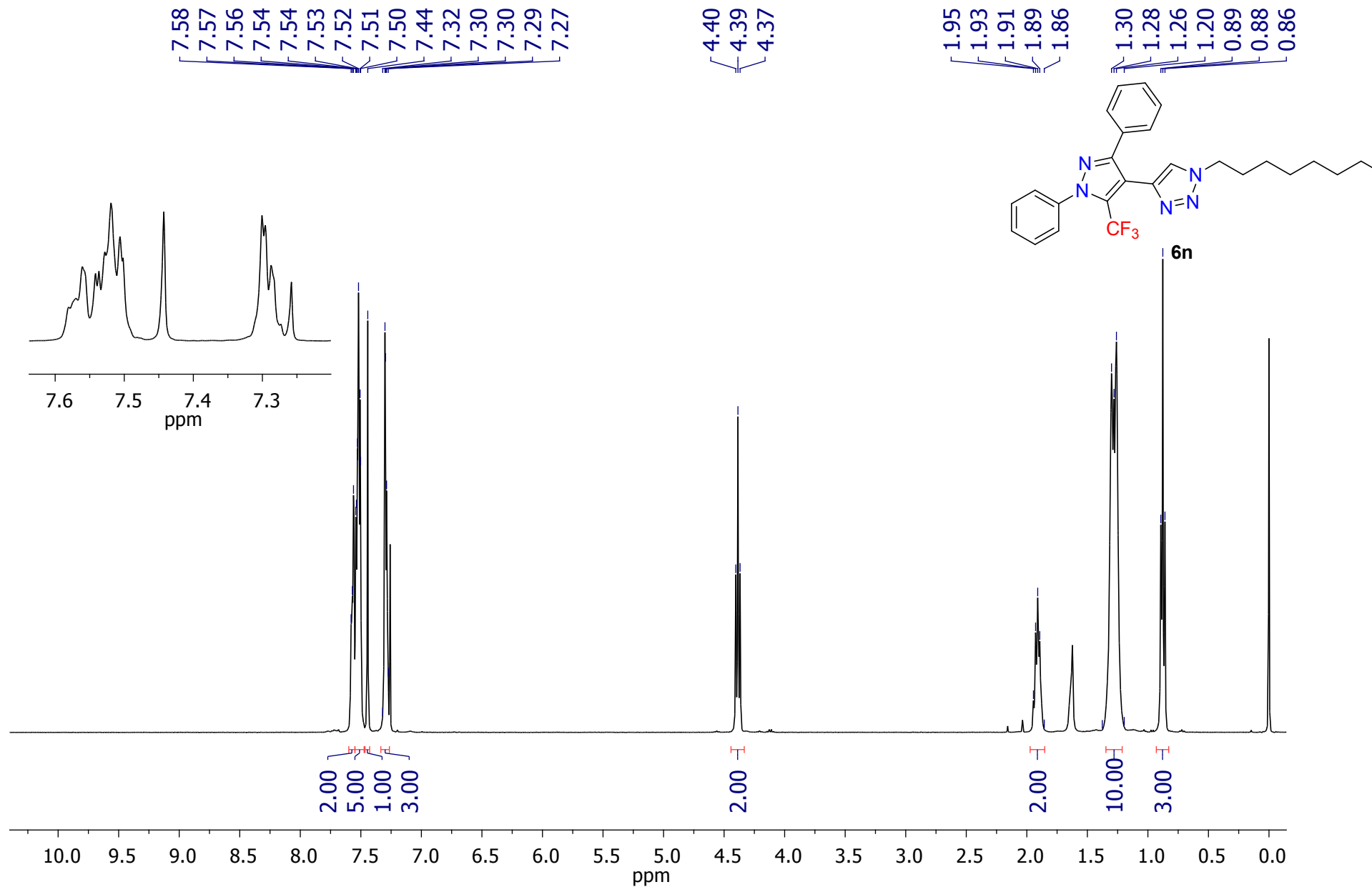
**6m**

--55.36

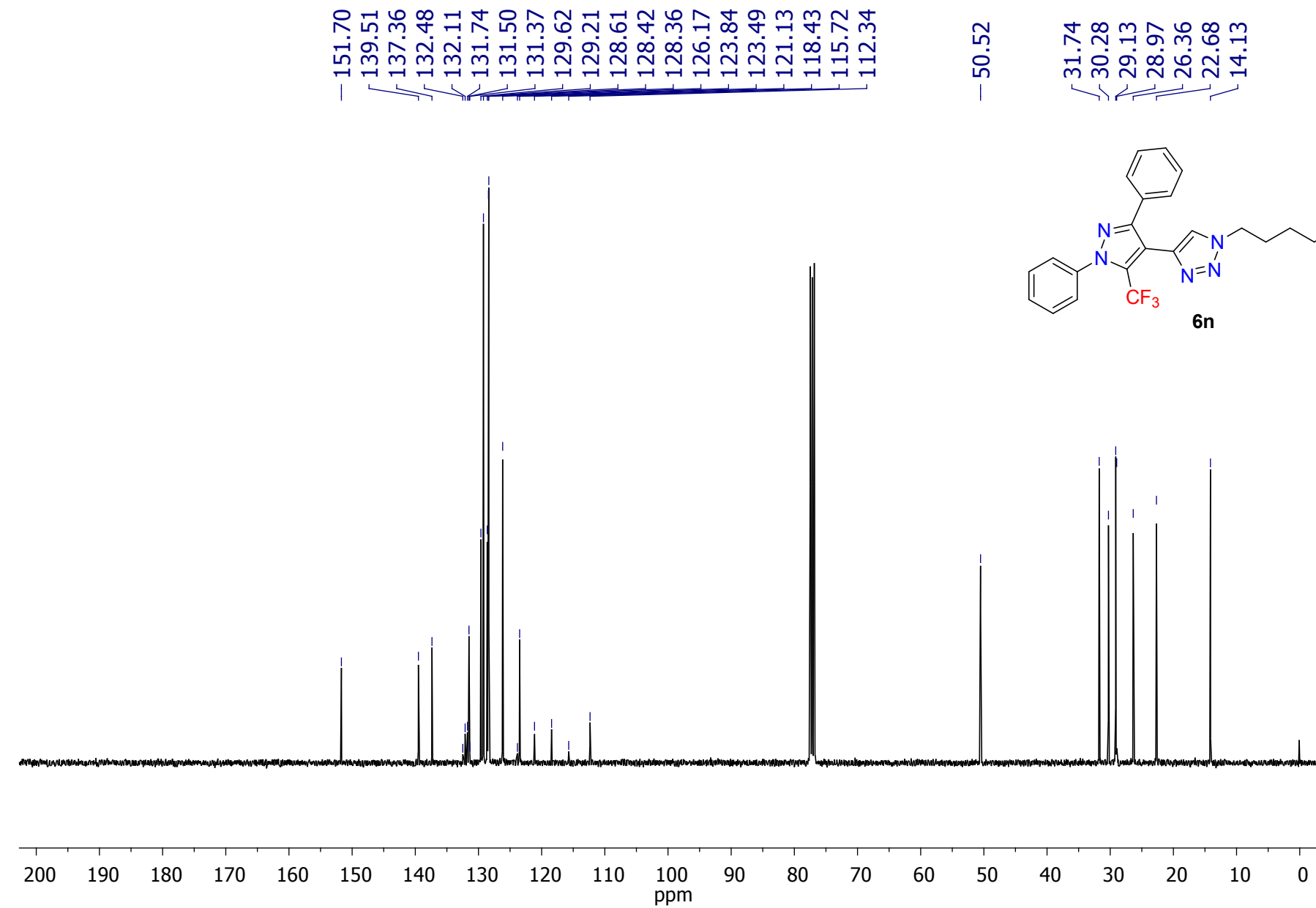


**6n** -  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , 25 °C)

S50



**6n** - <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>, 25 °C)



**6o** - <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>, 25 °C)

