

# Benzothiazole and Chromone Derivatives as Potential ATR Kinase Inhibitors and Anticancer Agents

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<sup>5</sup> School of Pharmacy, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece; anthi.petrou.thessaloniki1@gmail.com

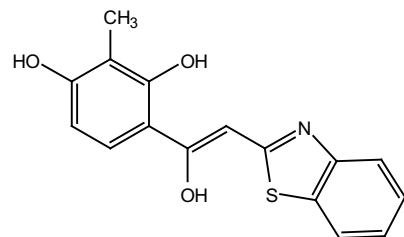
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\* Correspondence: priyak@iitgn.ac.in (S.K.); geronik@pharm.auth.gr (A.G.); domenico.spinelli@unibo.it (D.S.)

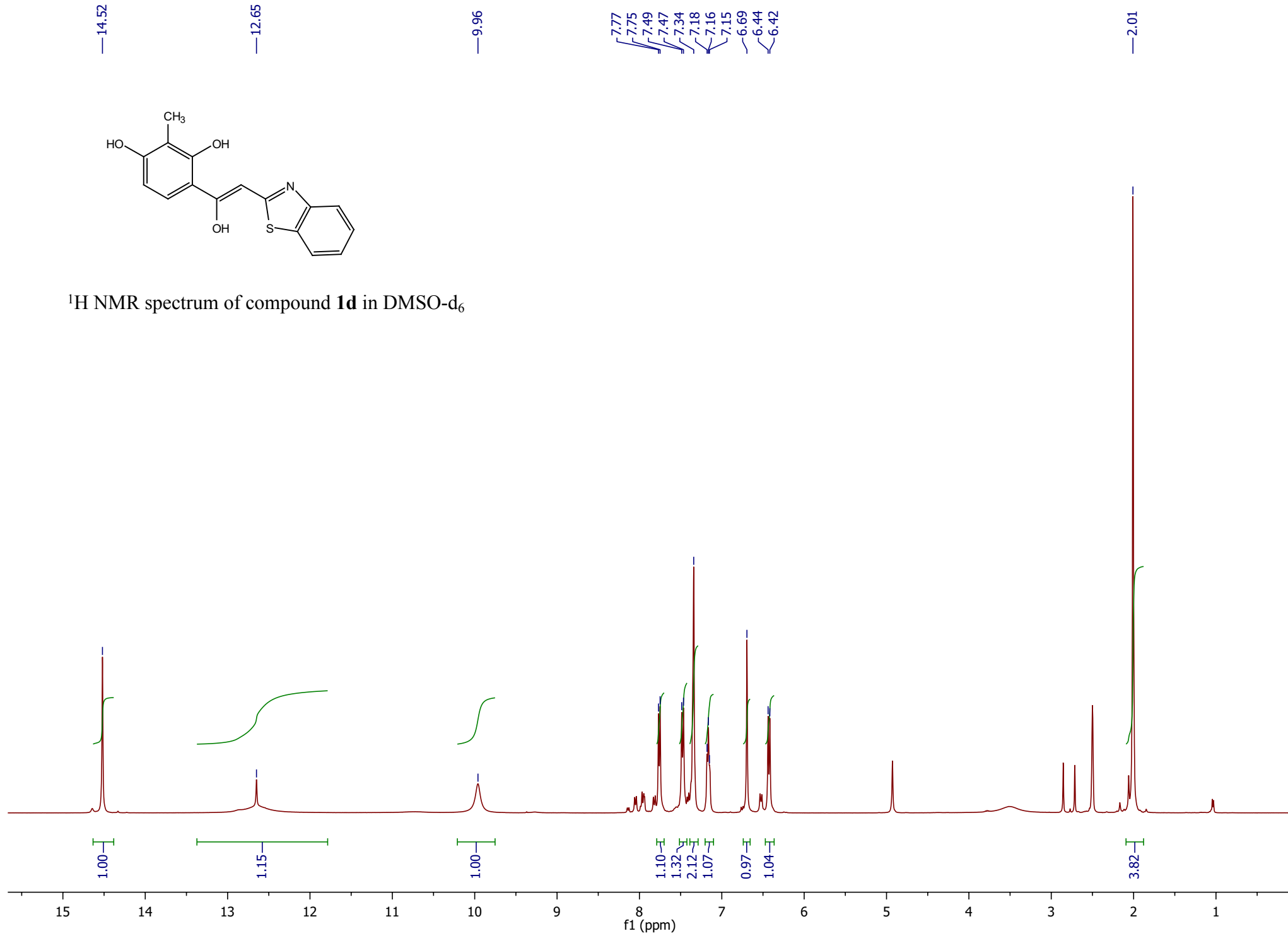
† These authors contributed equally to this work.

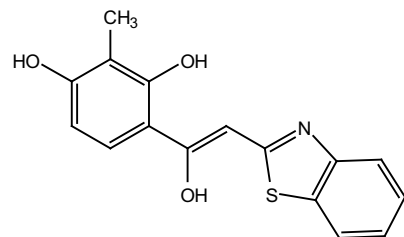
‡ These authors contributed equally to this work.

## Supplementary Material

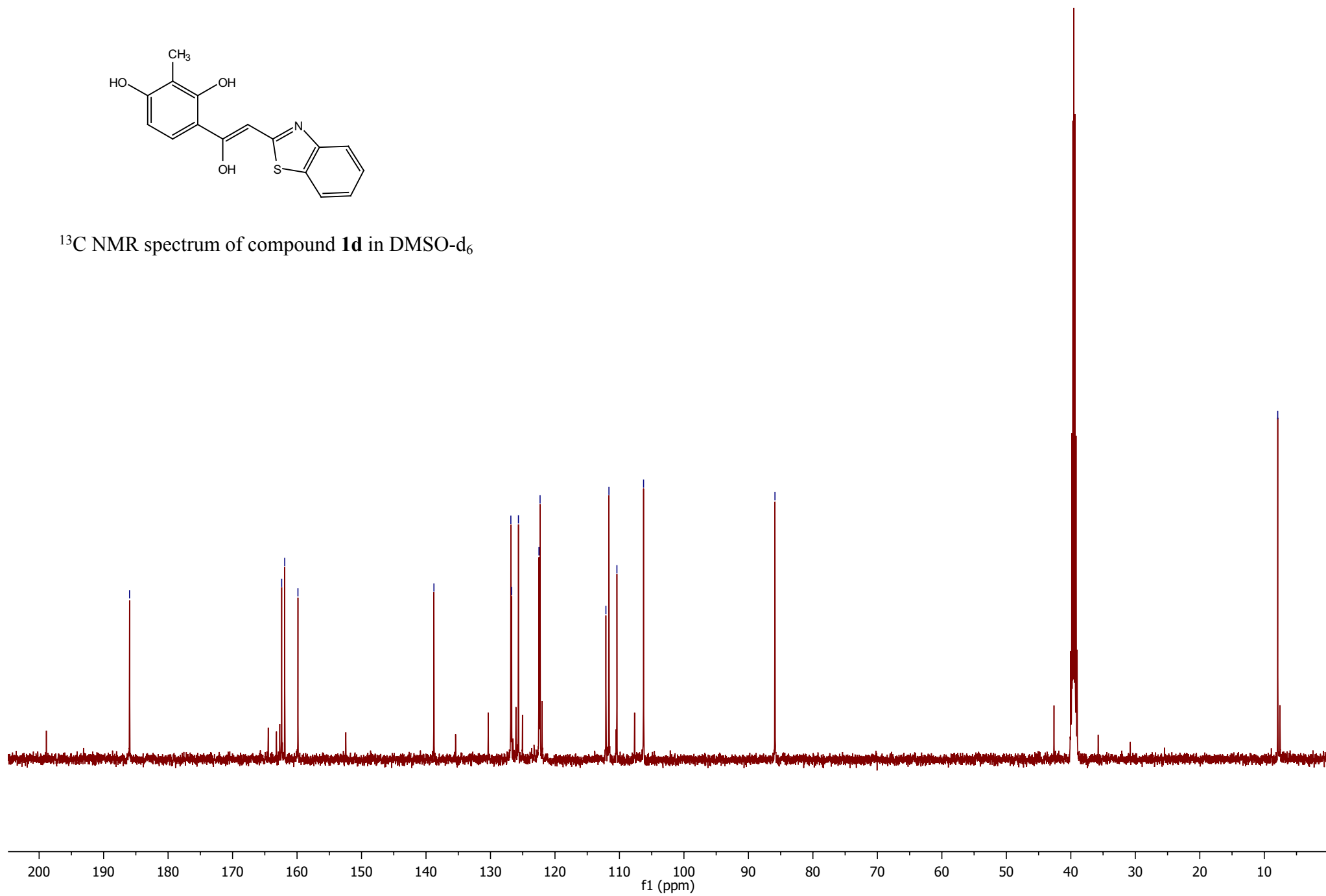


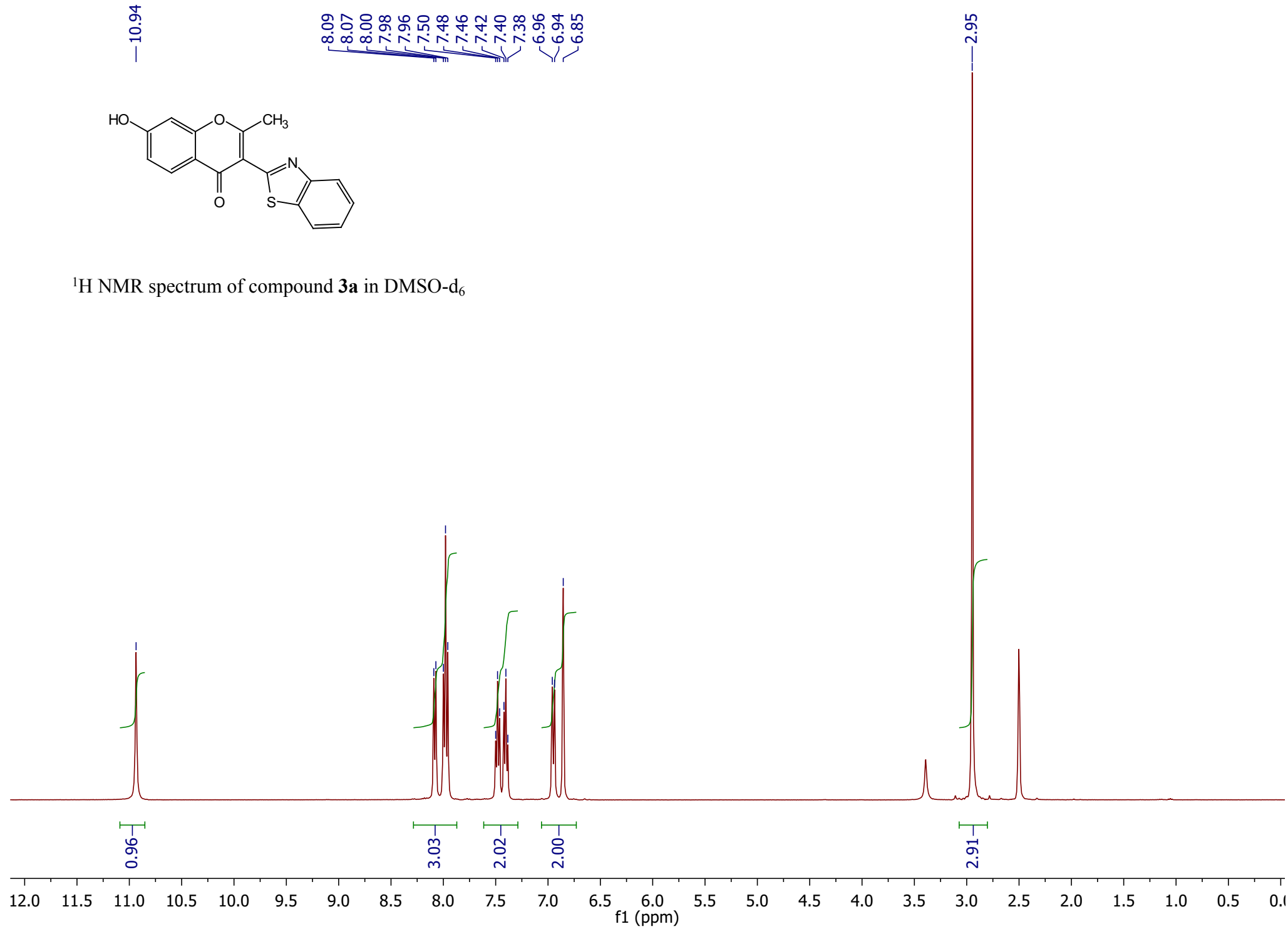
$^1\text{H}$  NMR spectrum of compound **1d** in  $\text{DMSO-d}_6$

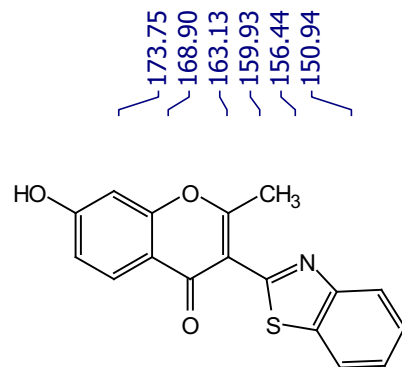




$^{13}\text{C}$  NMR spectrum of compound **1d** in DMSO- $\text{d}_6$



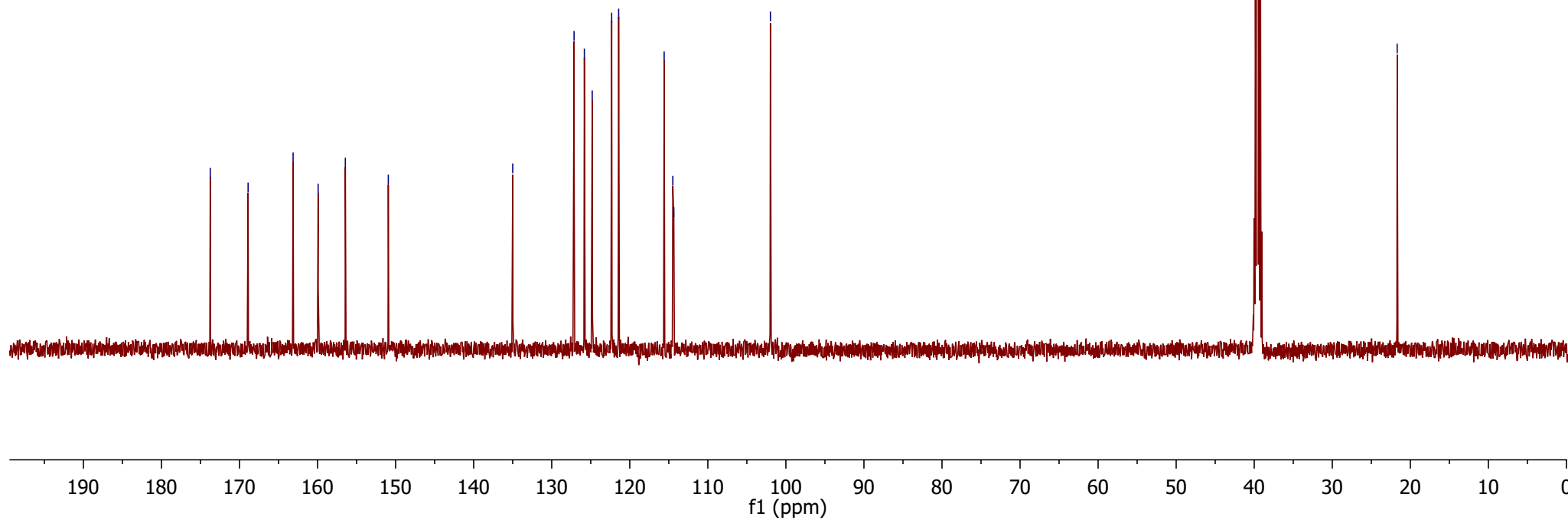


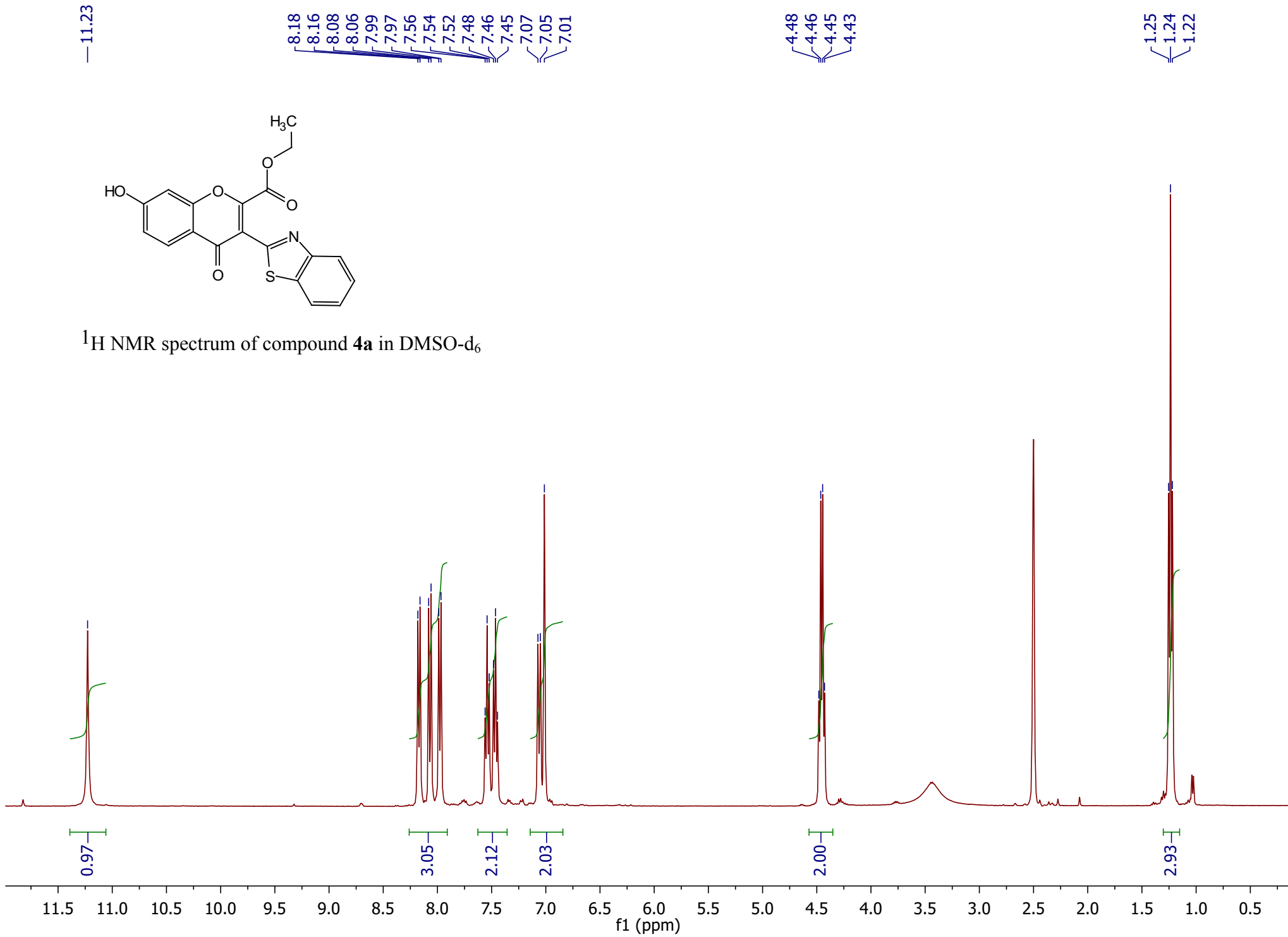


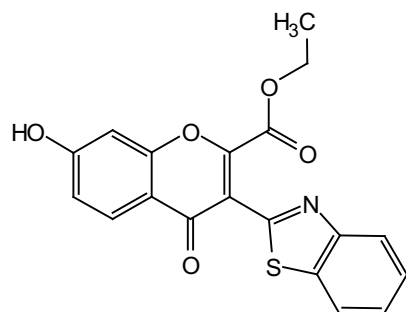
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135.00  
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114.36  
101.98

21.68

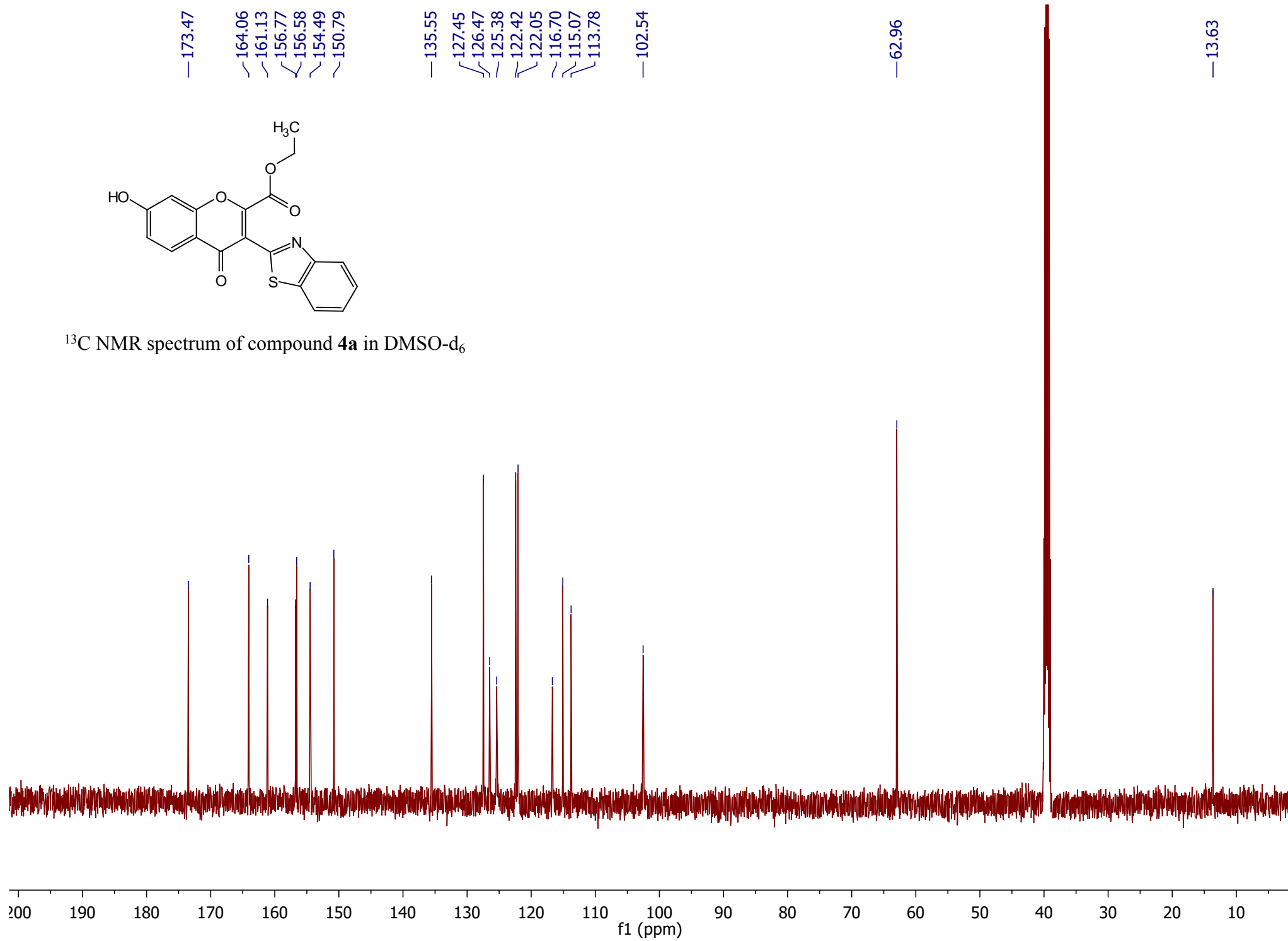
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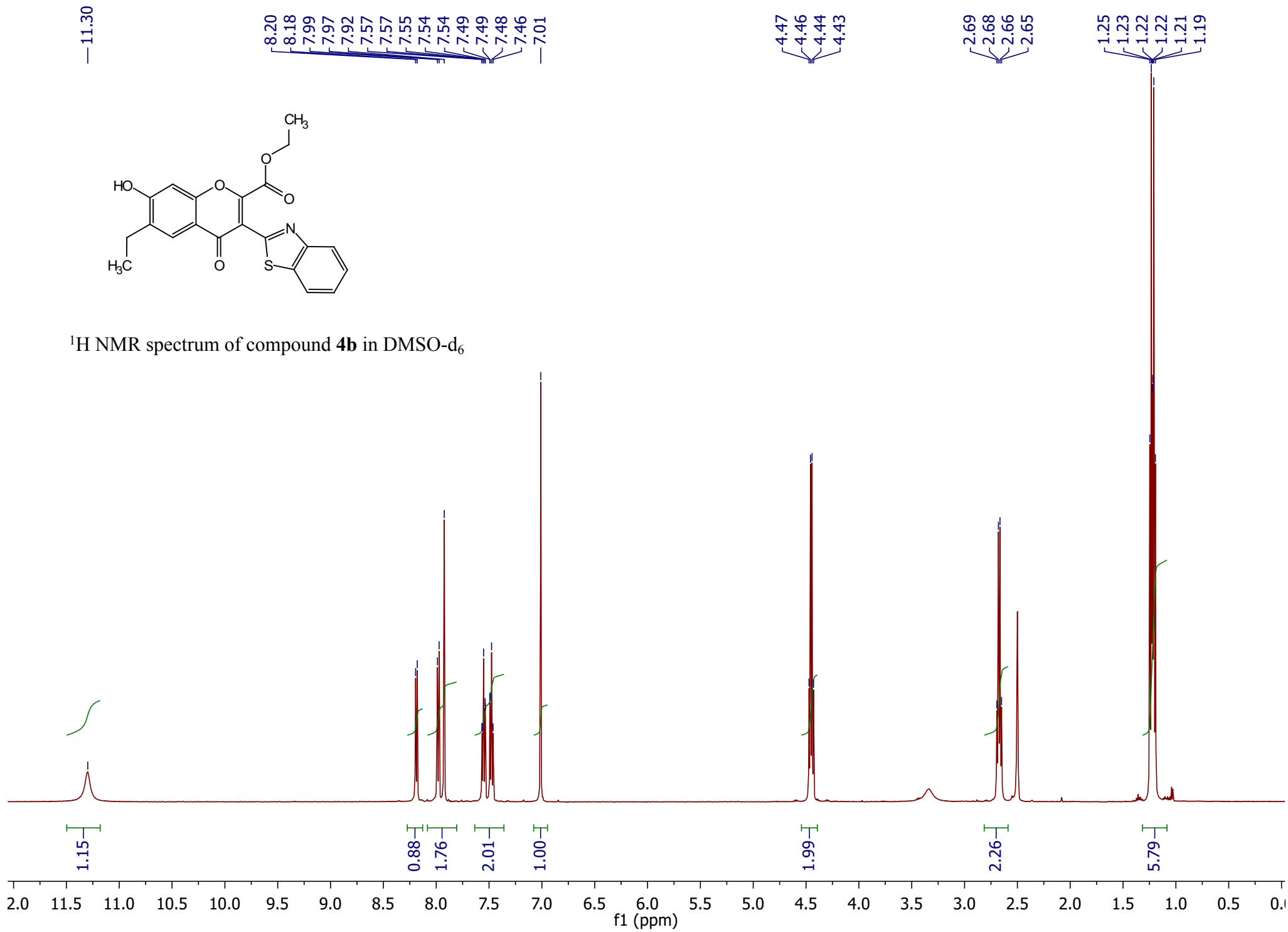




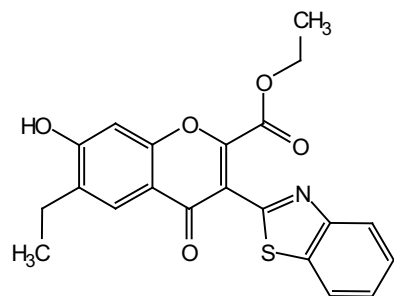


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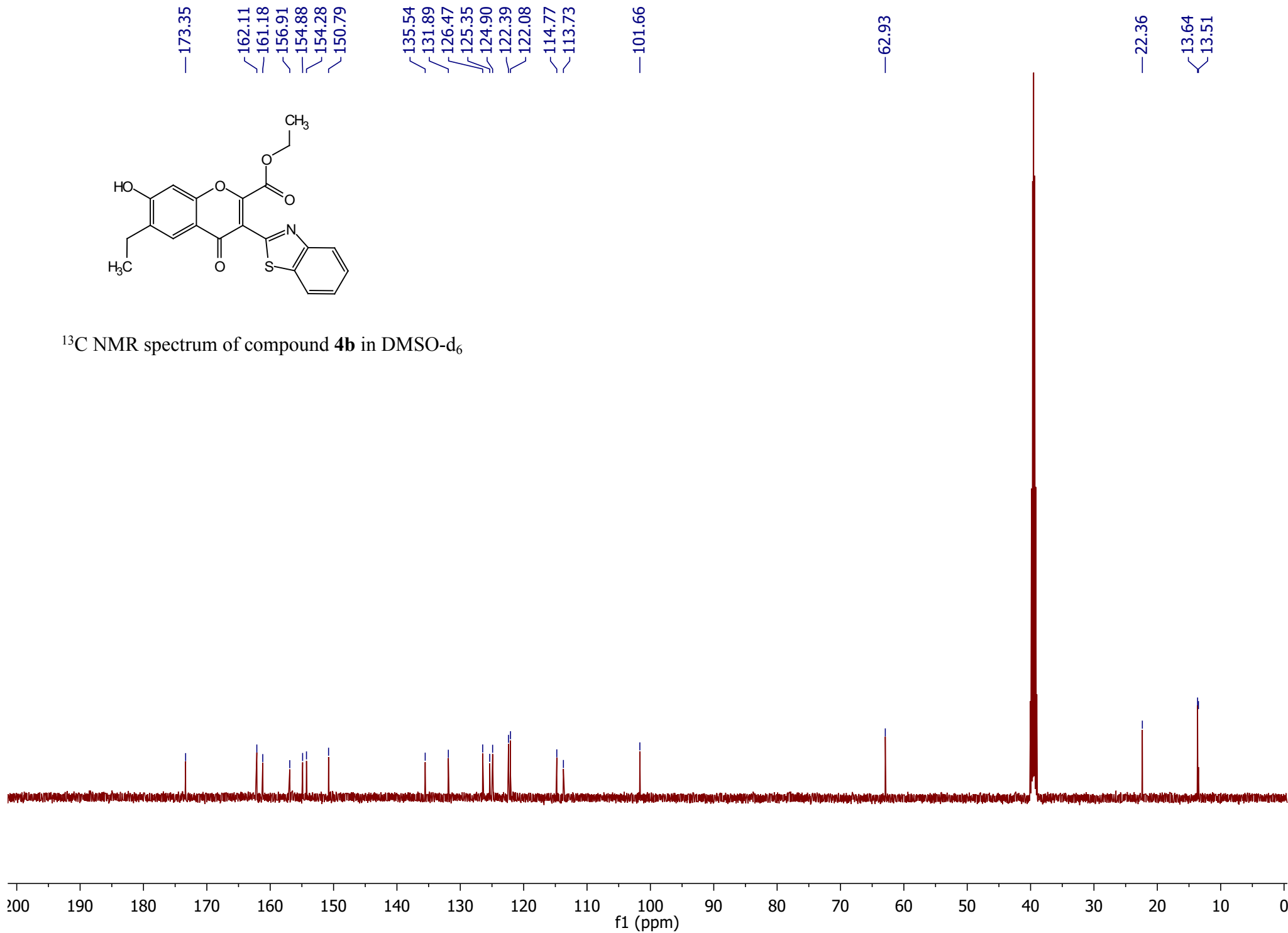








$^{13}\text{C}$  NMR spectrum of compound **4b** in  $\text{DMSO-d}_6$



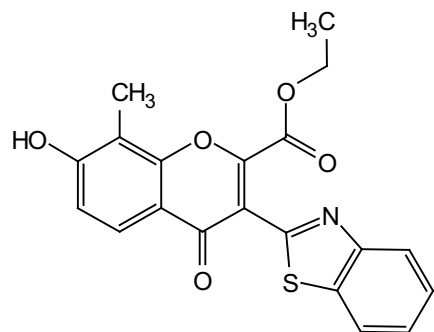
— 11.07

8.17  
8.15  
7.99  
7.97  
7.94  
7.91  
7.56  
7.54  
7.52  
7.48  
7.46  
7.44  
7.12  
7.10

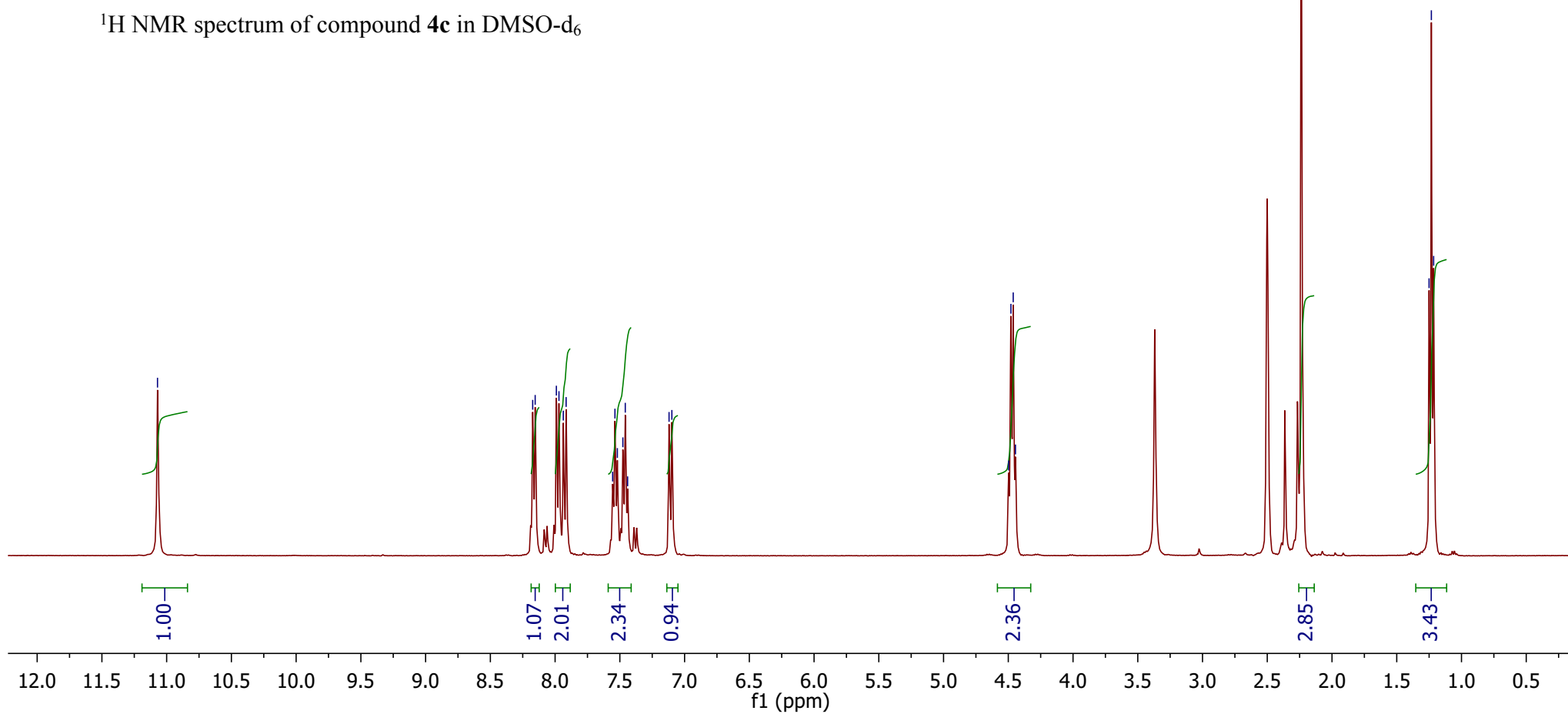
4.50  
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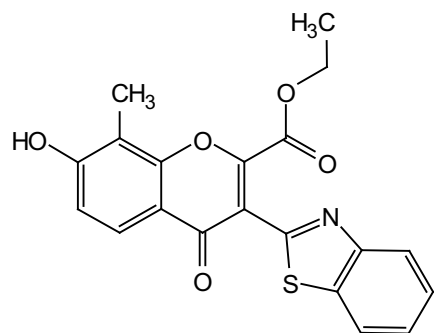
— 2.24

1.25  
1.23  
1.22

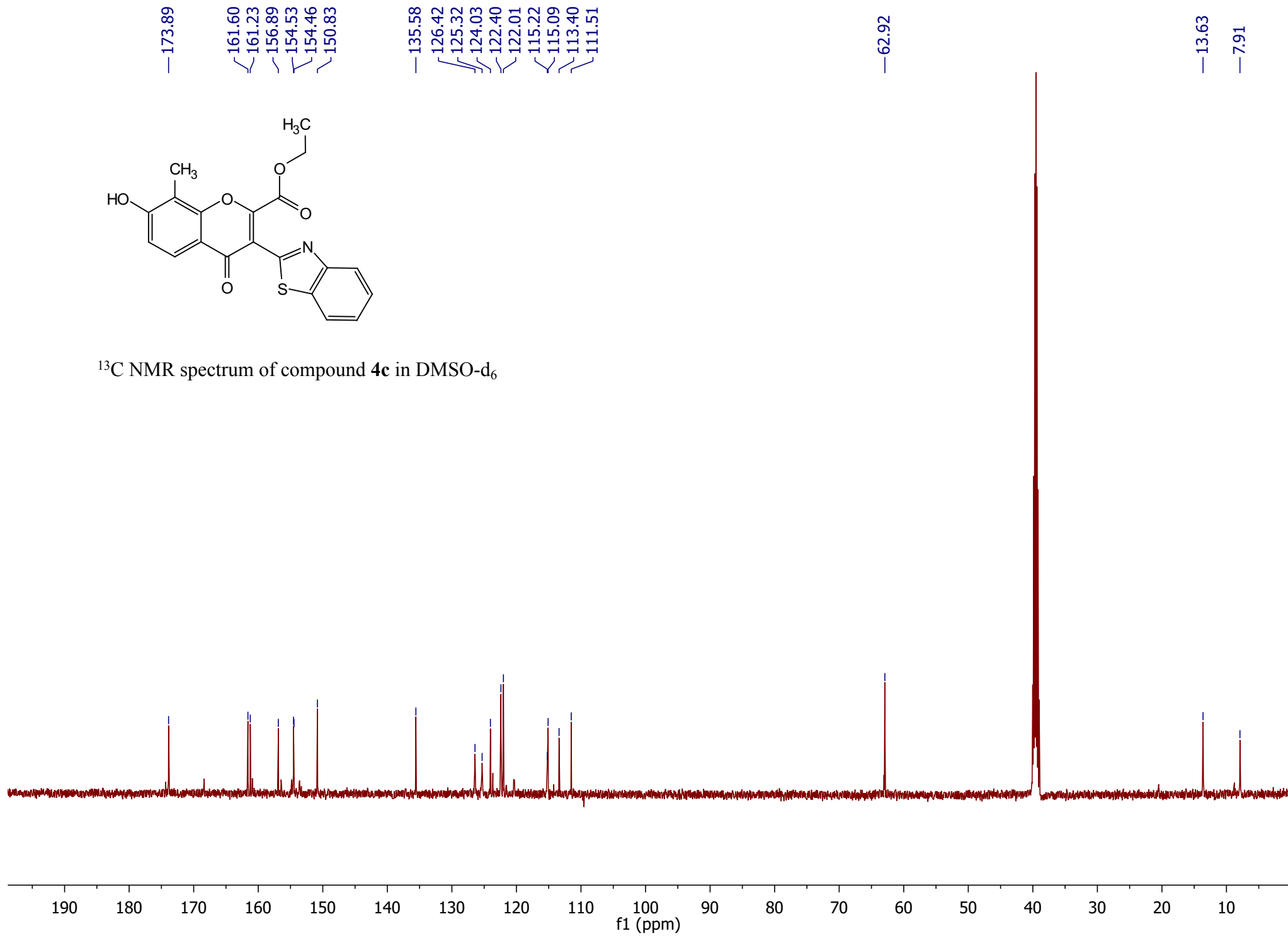


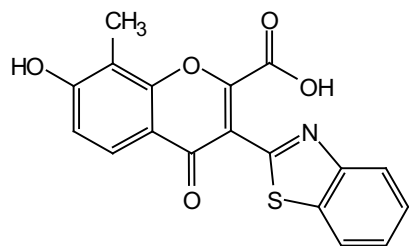
$^1\text{H}$  NMR spectrum of compound **4c** in DMSO- $\text{d}_6$



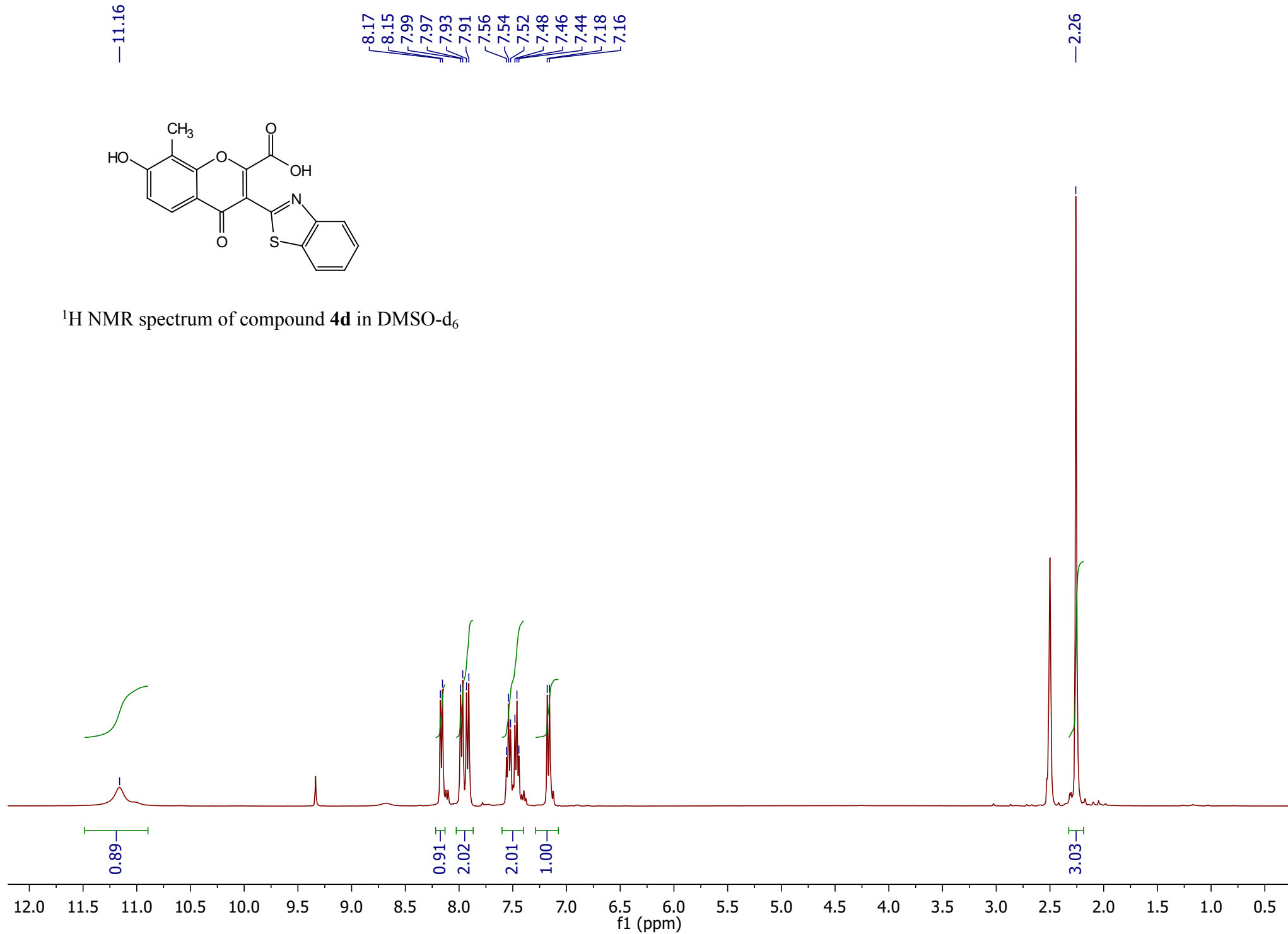


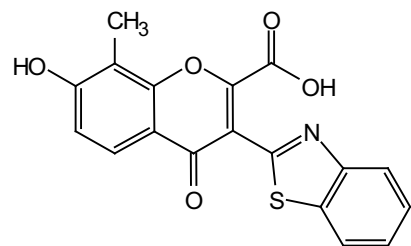
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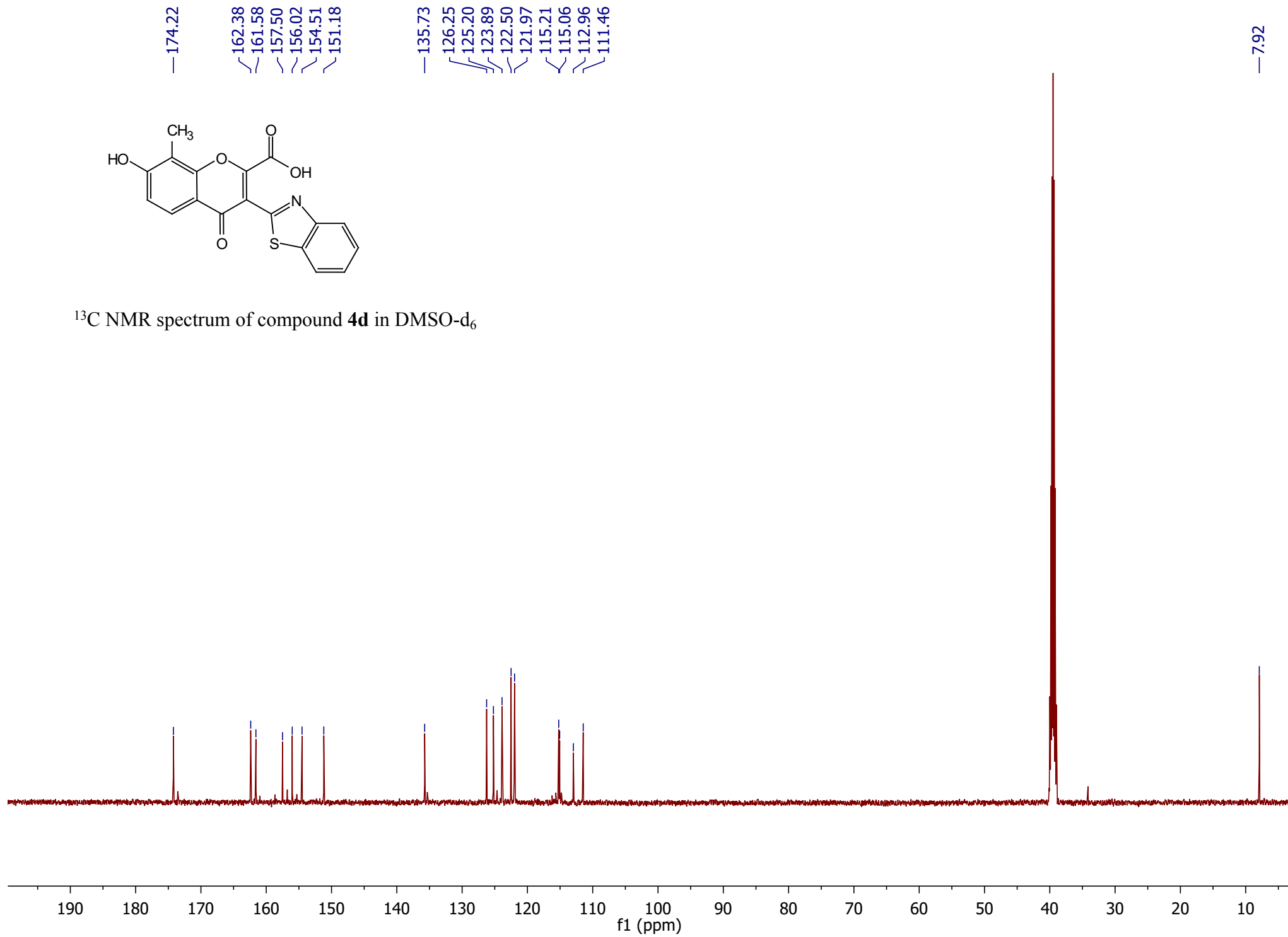


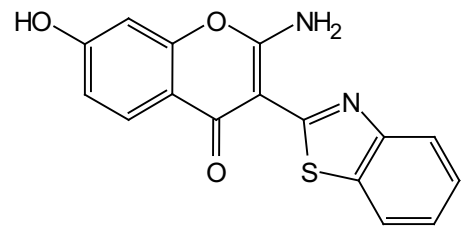
<sup>1</sup>H NMR spectrum of compound **4d** in DMSO-d<sub>6</sub>



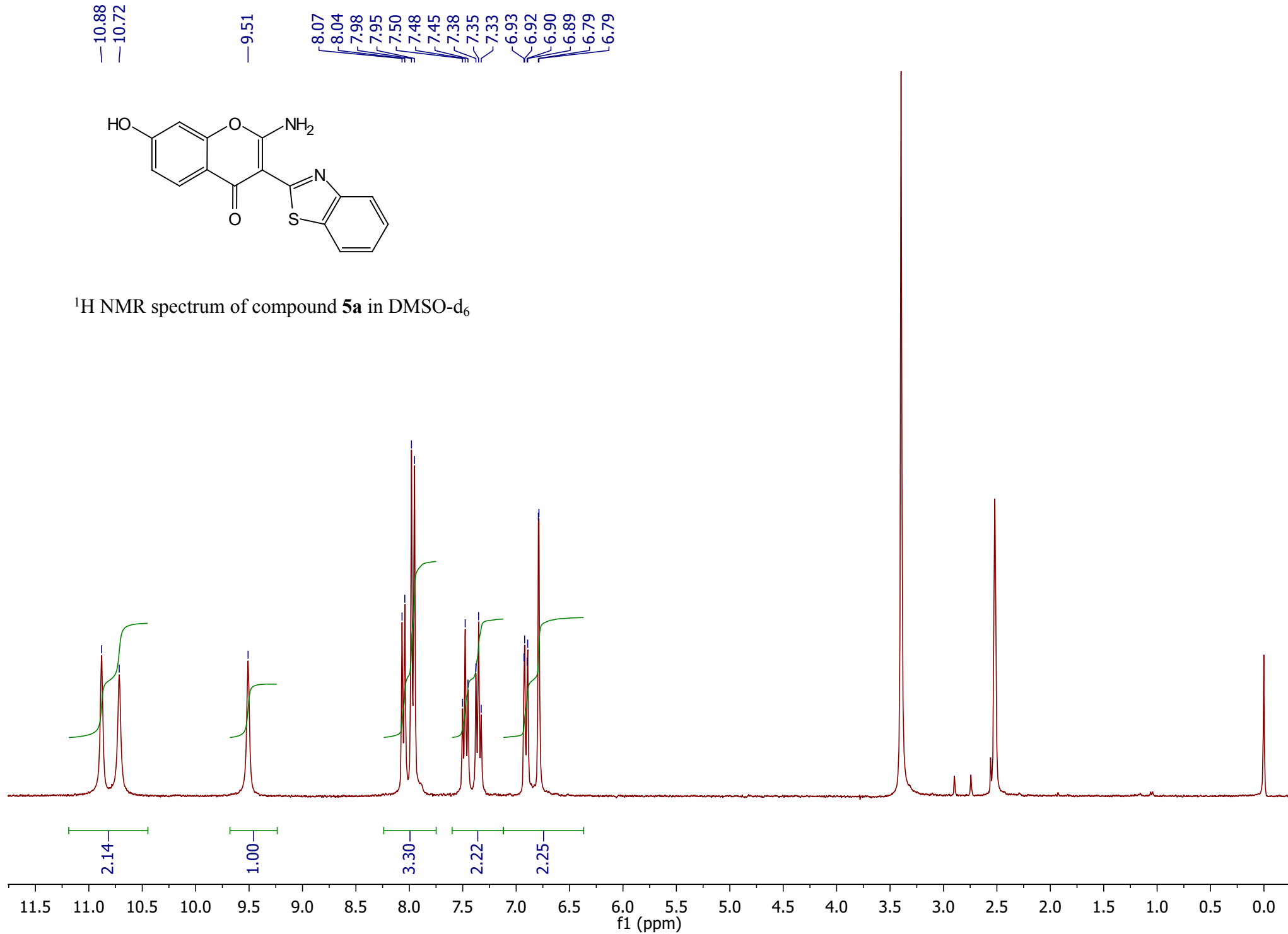


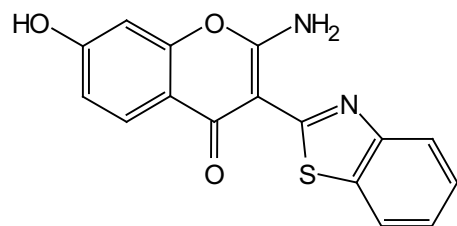
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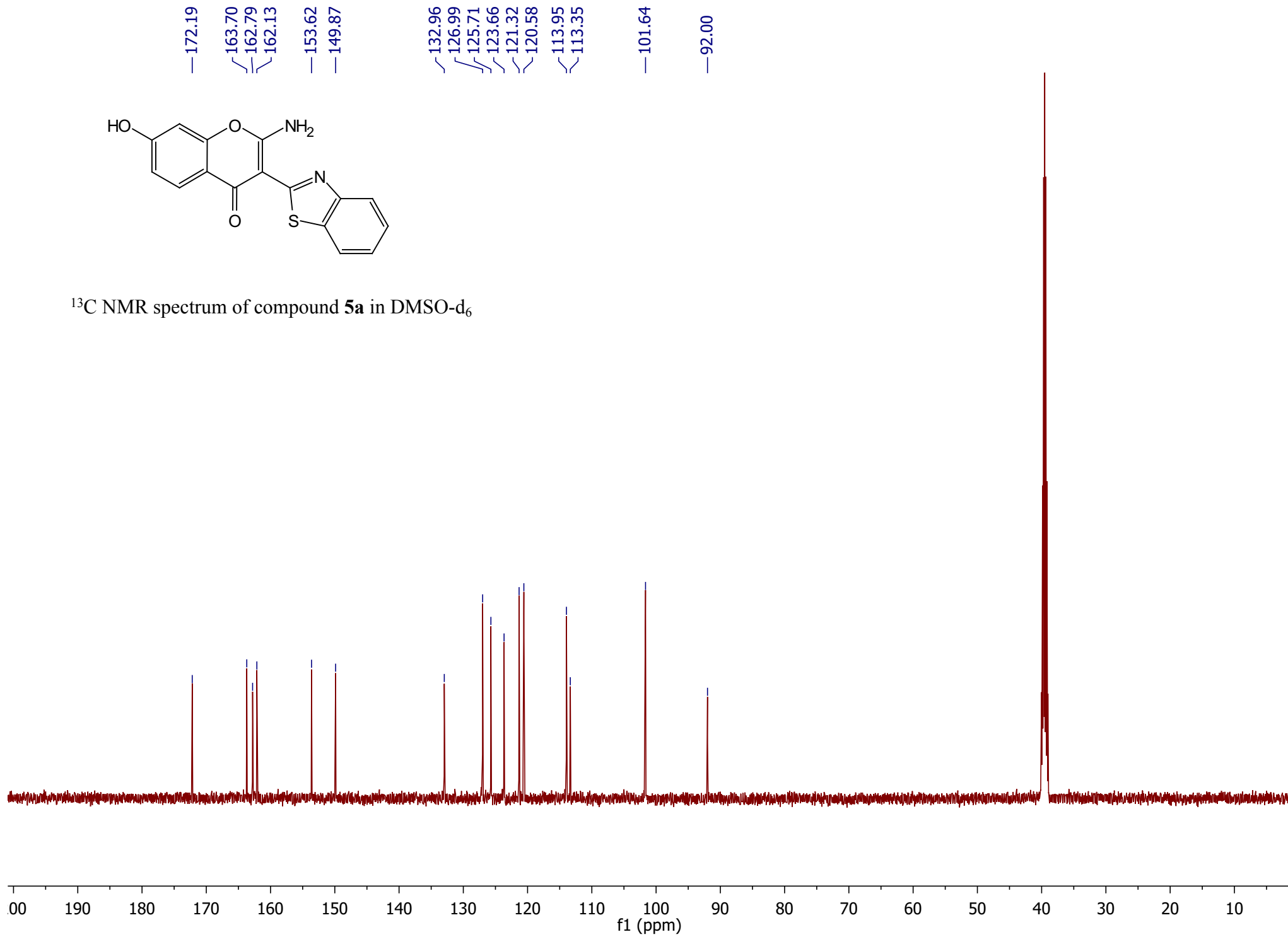


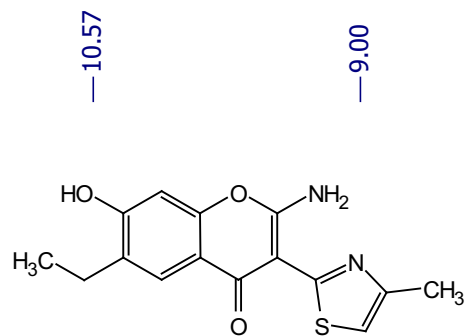
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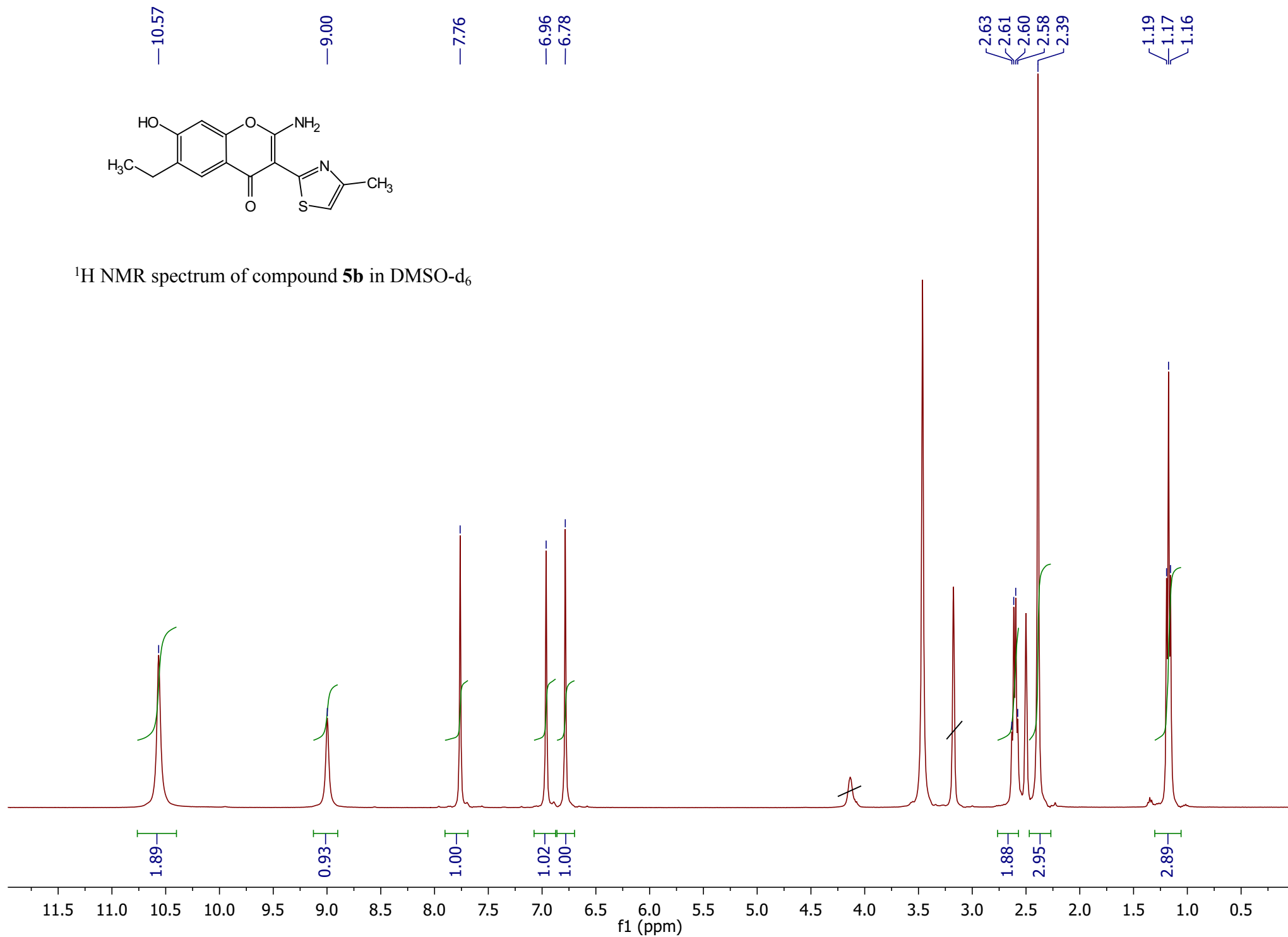


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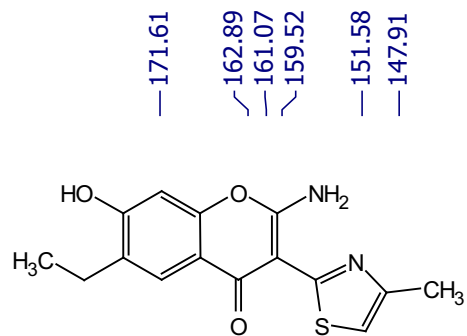




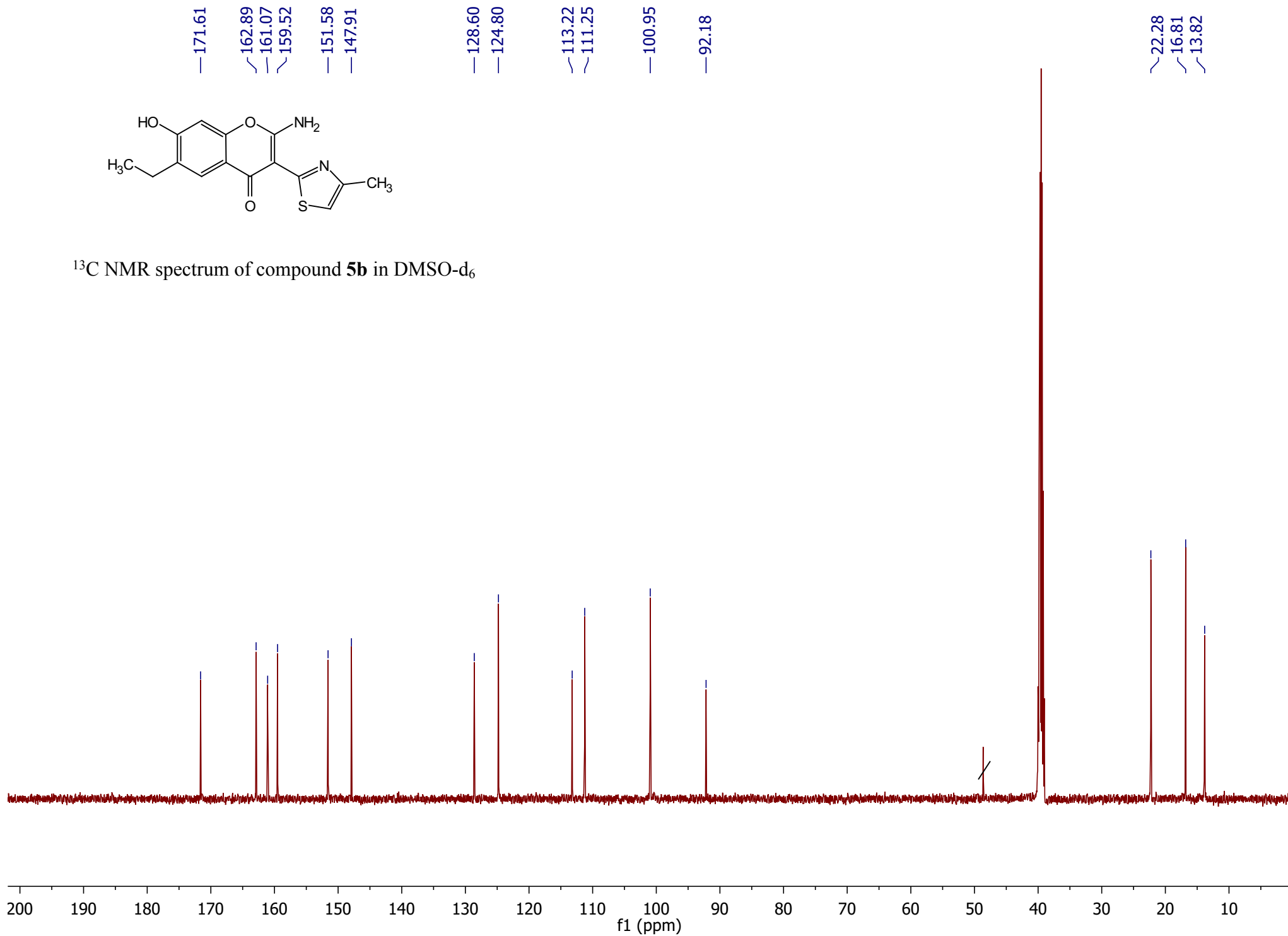
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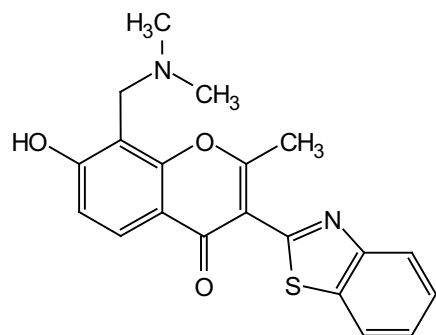




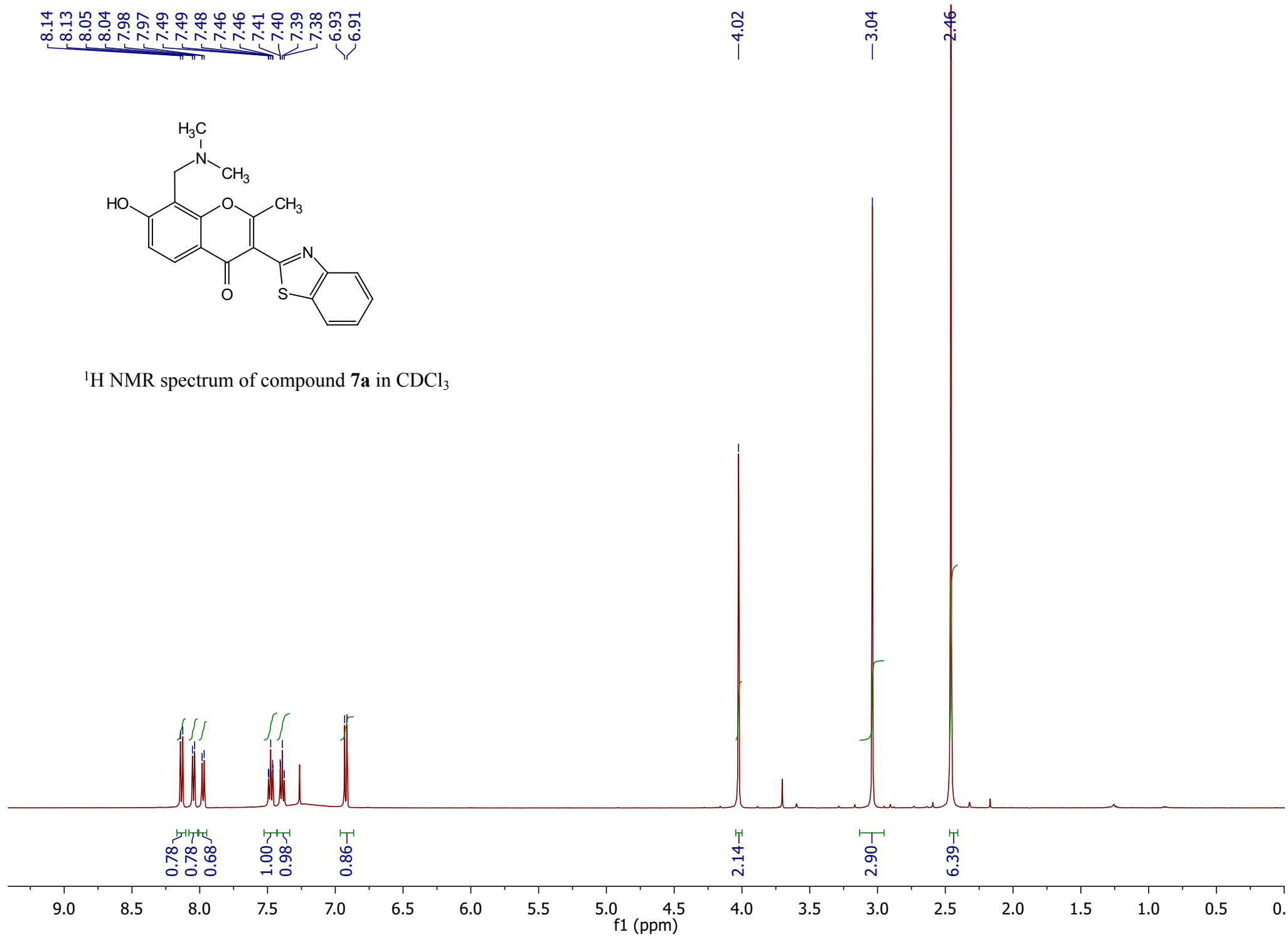


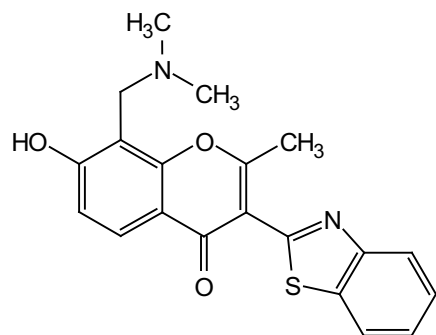
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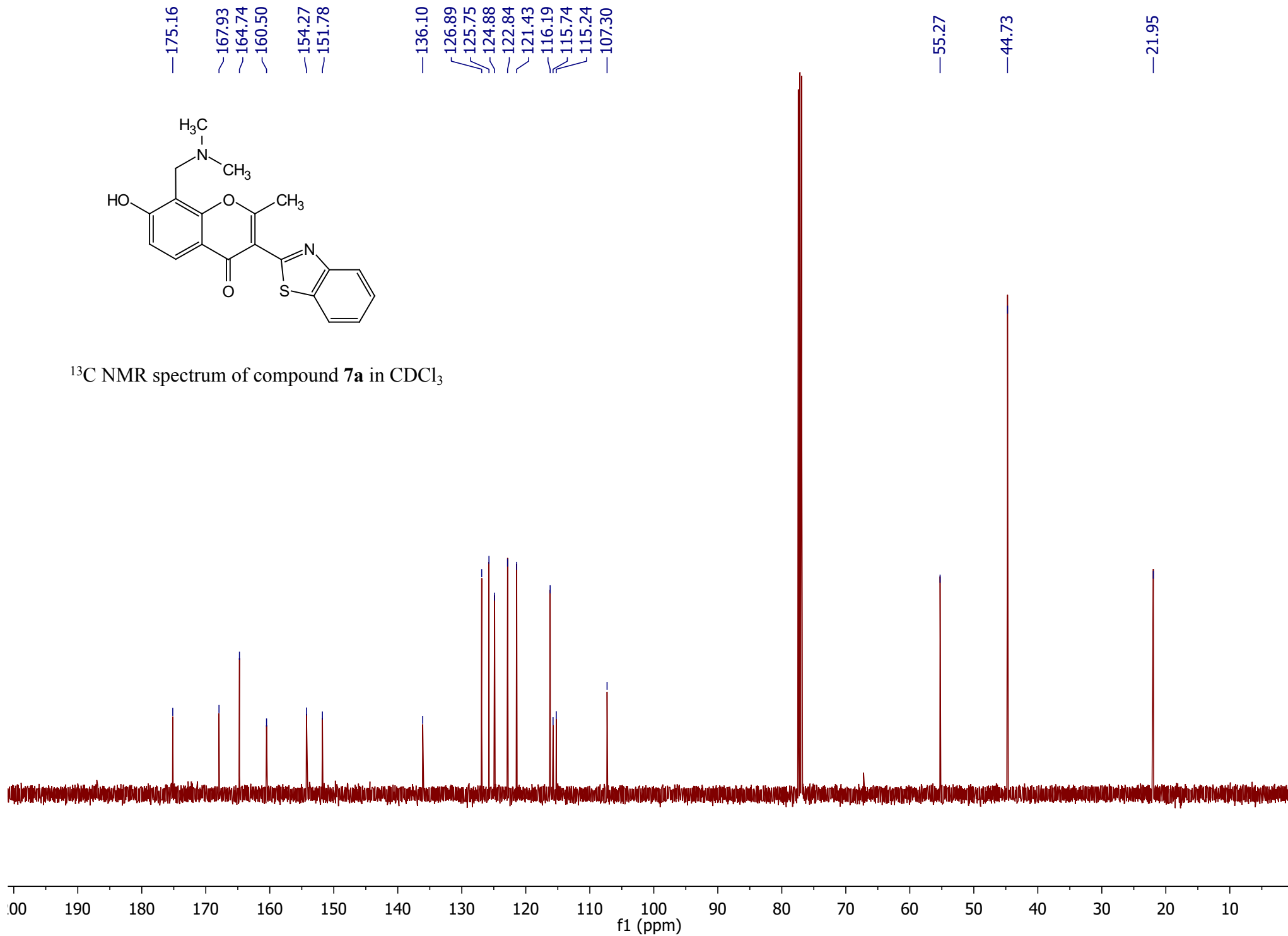


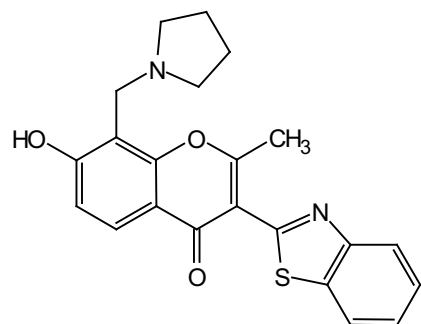
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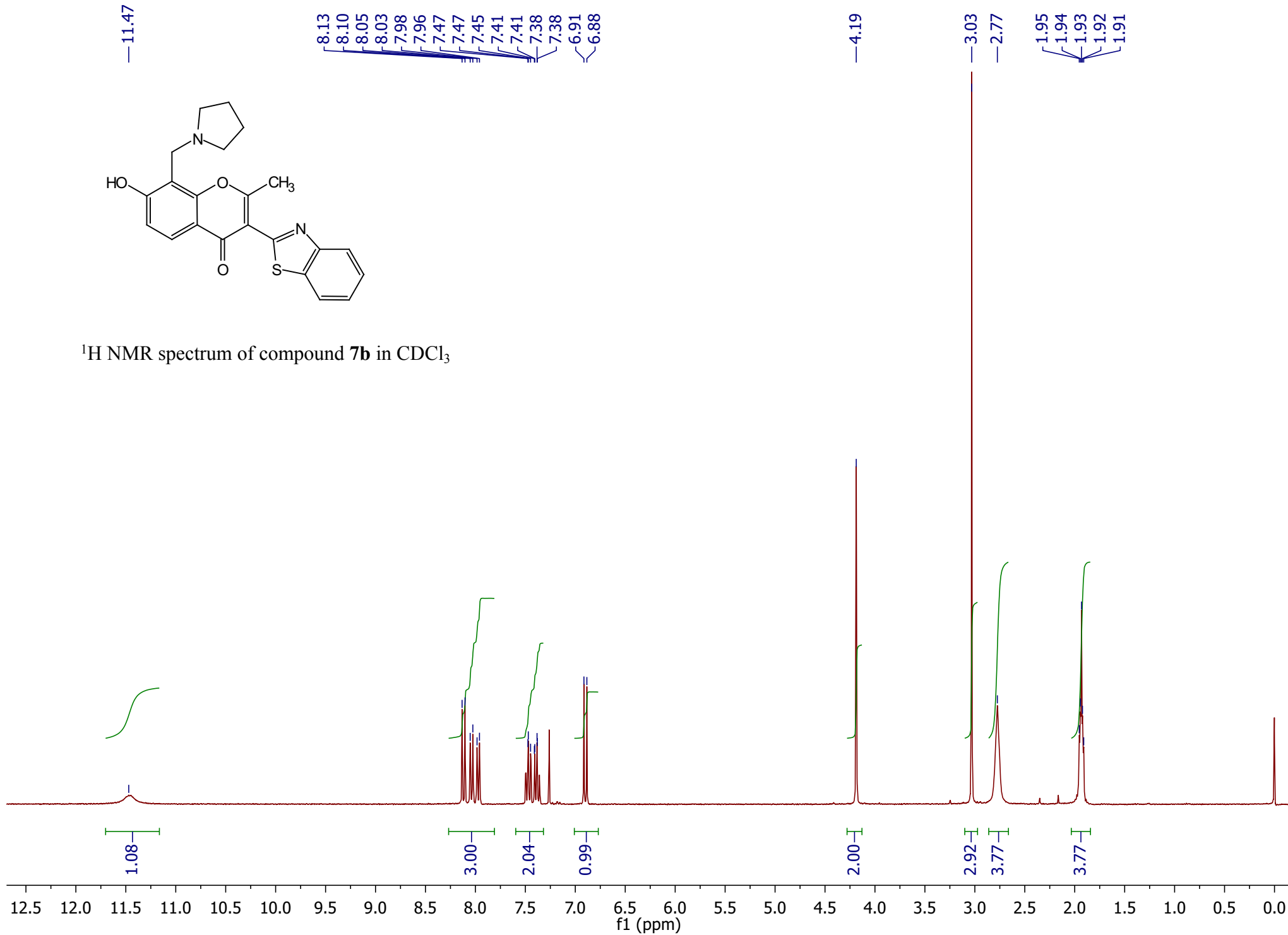


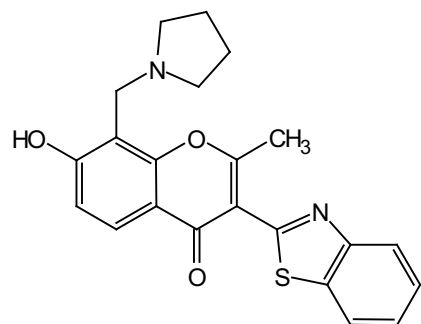
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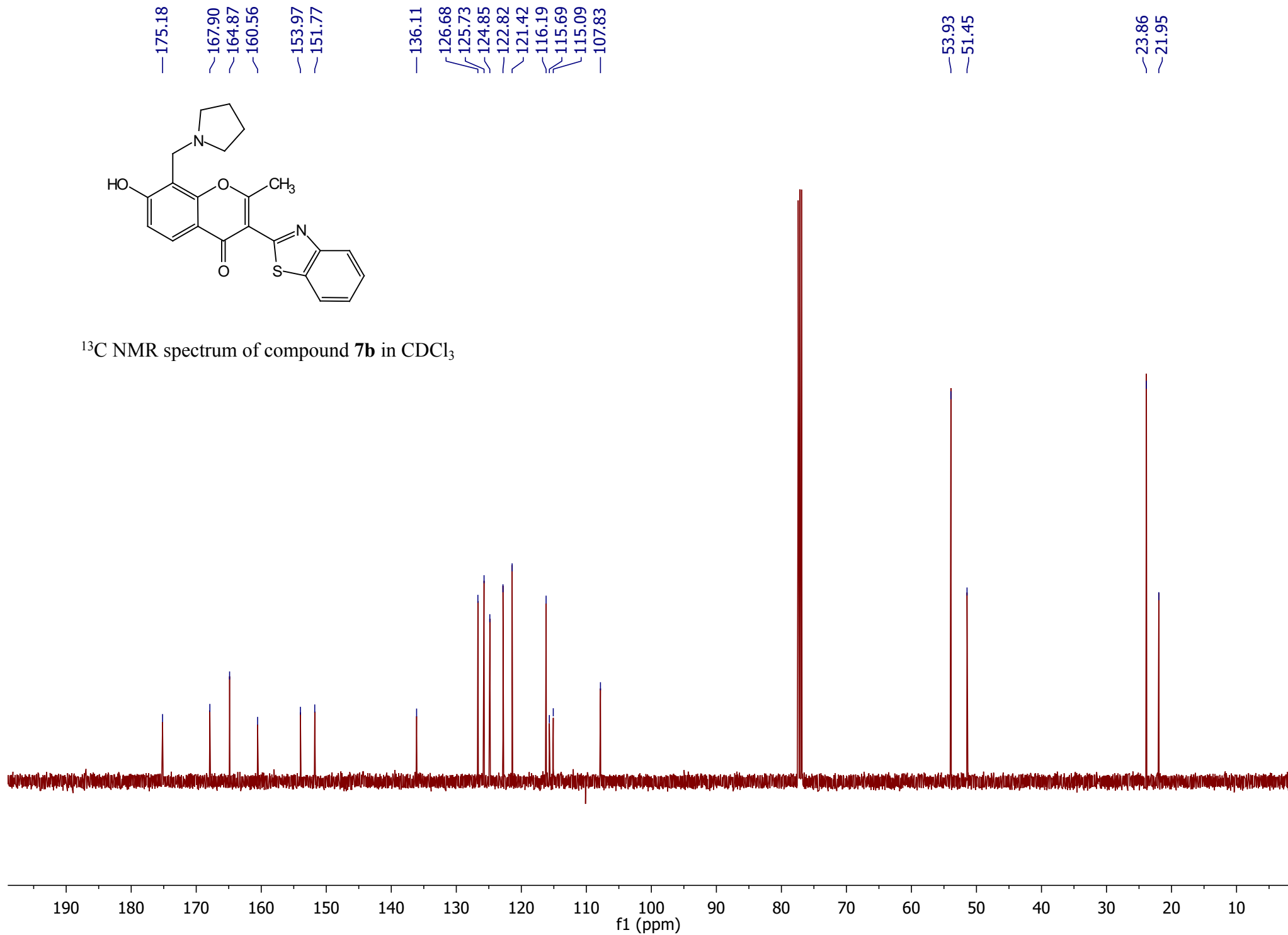


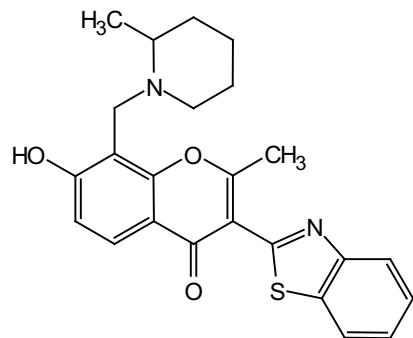
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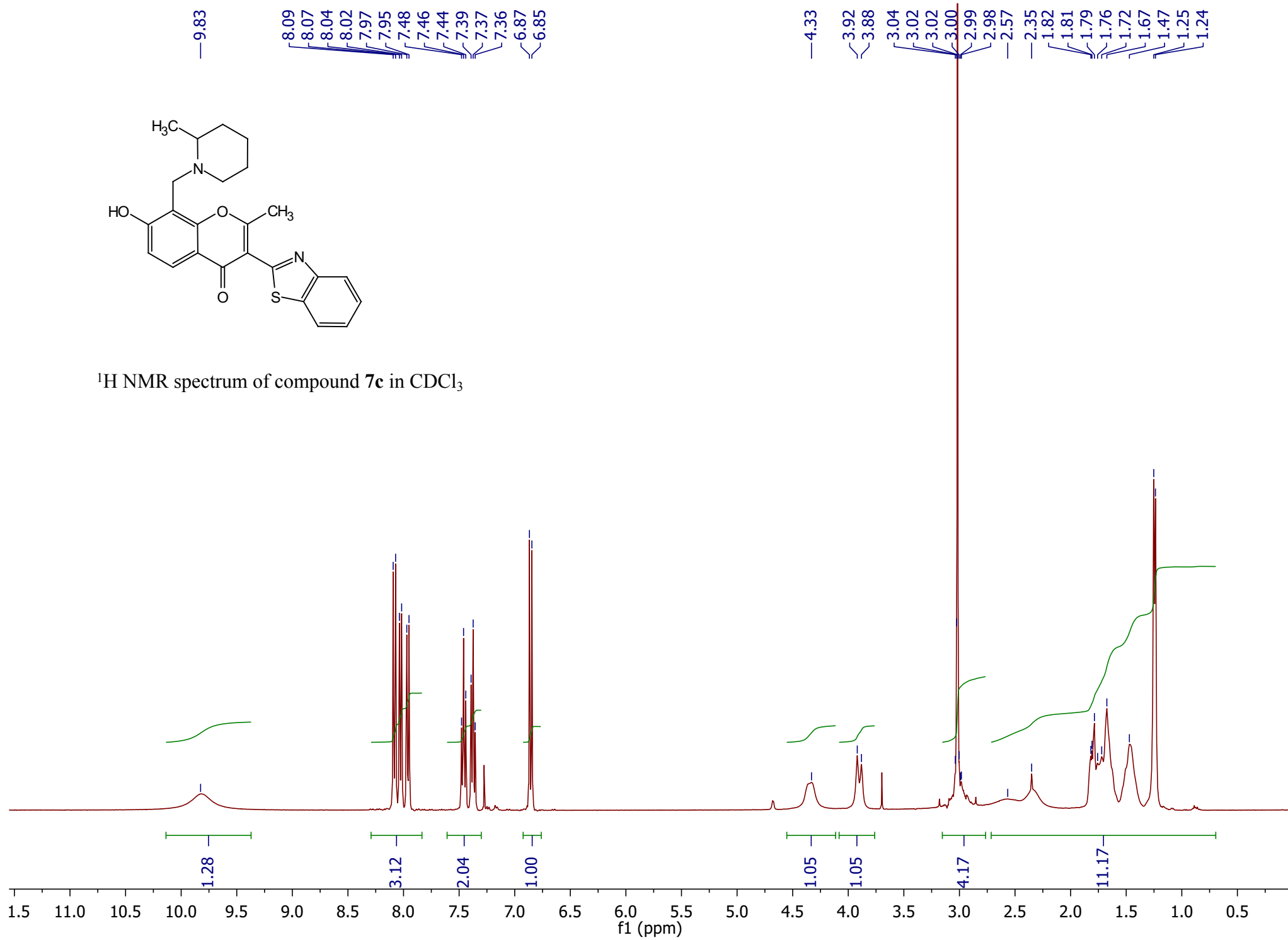


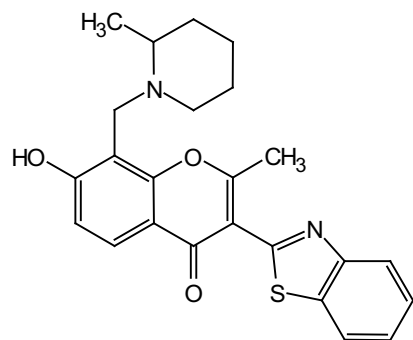
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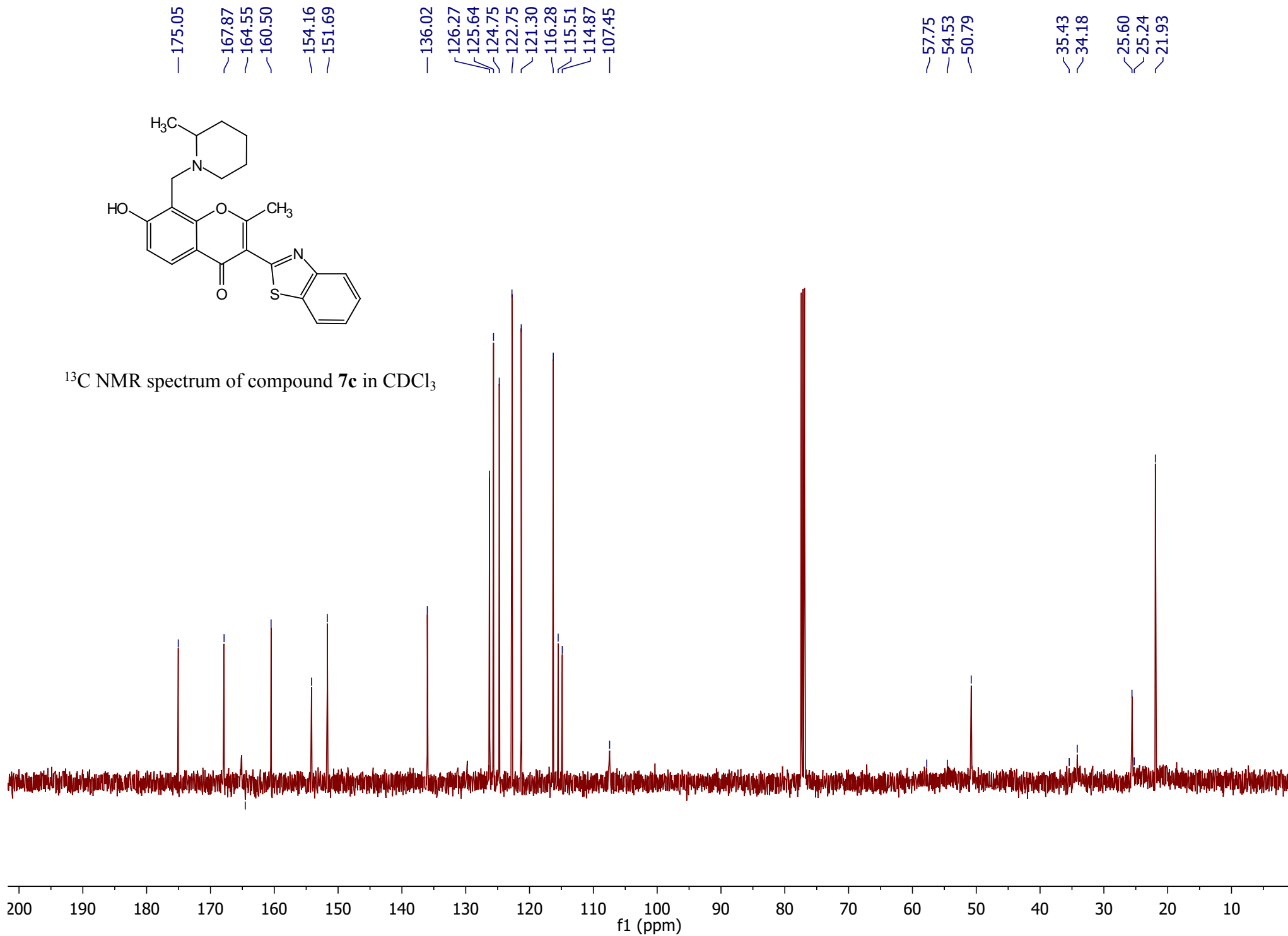


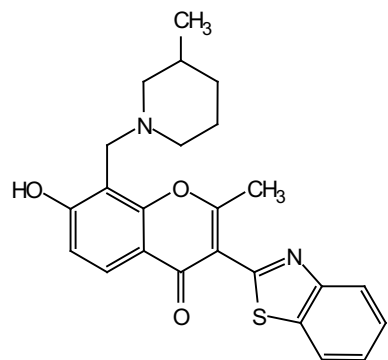
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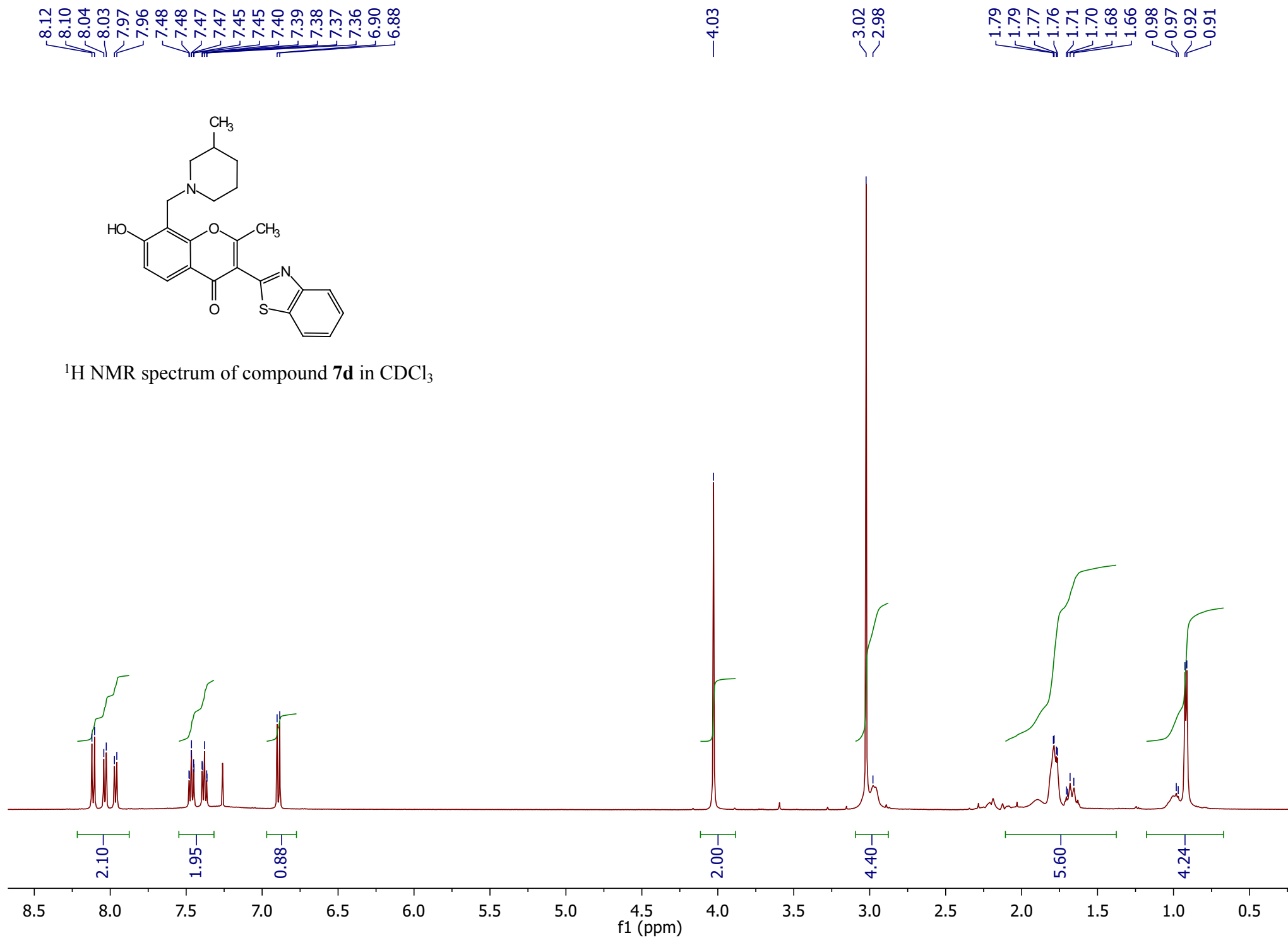


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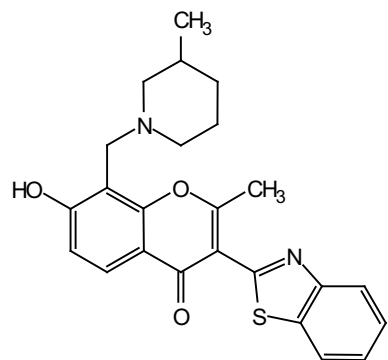




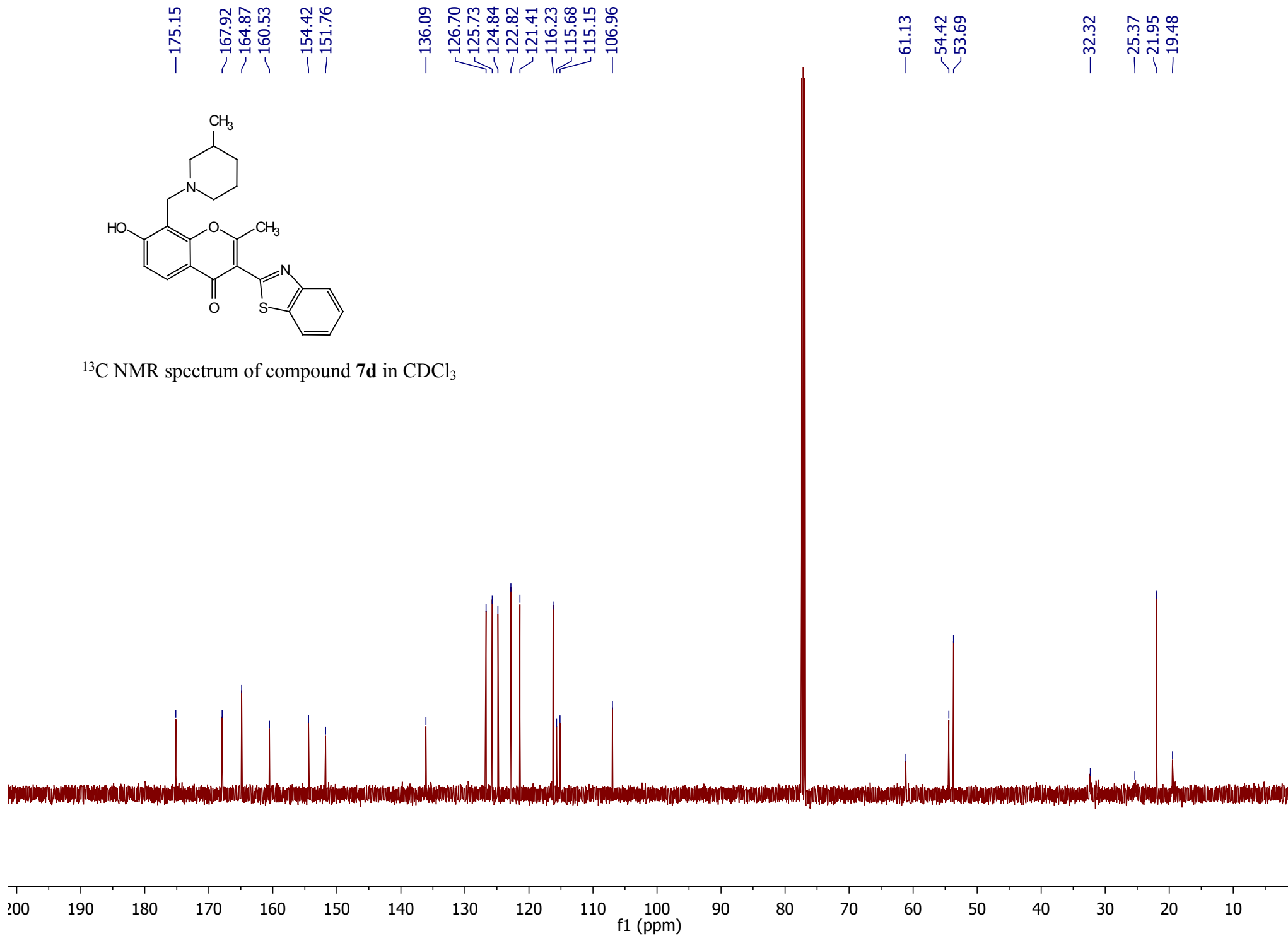
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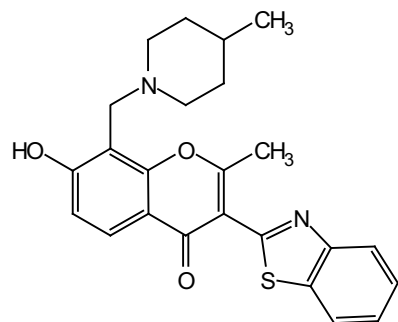




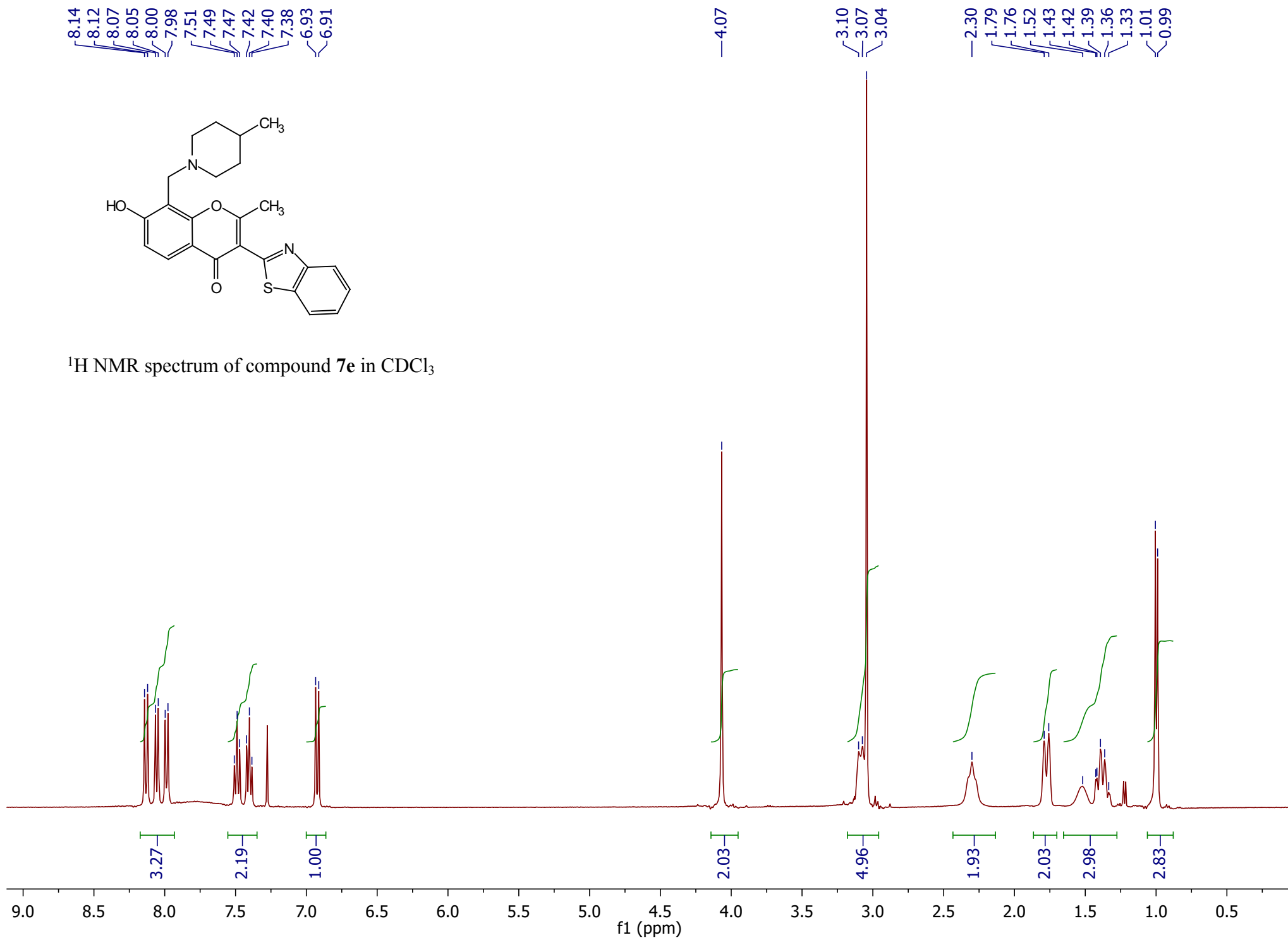


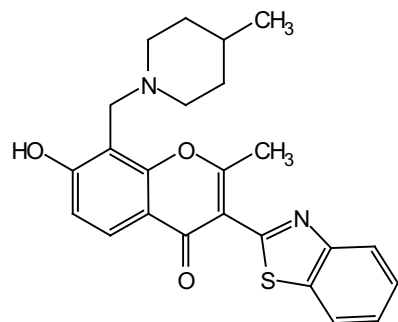
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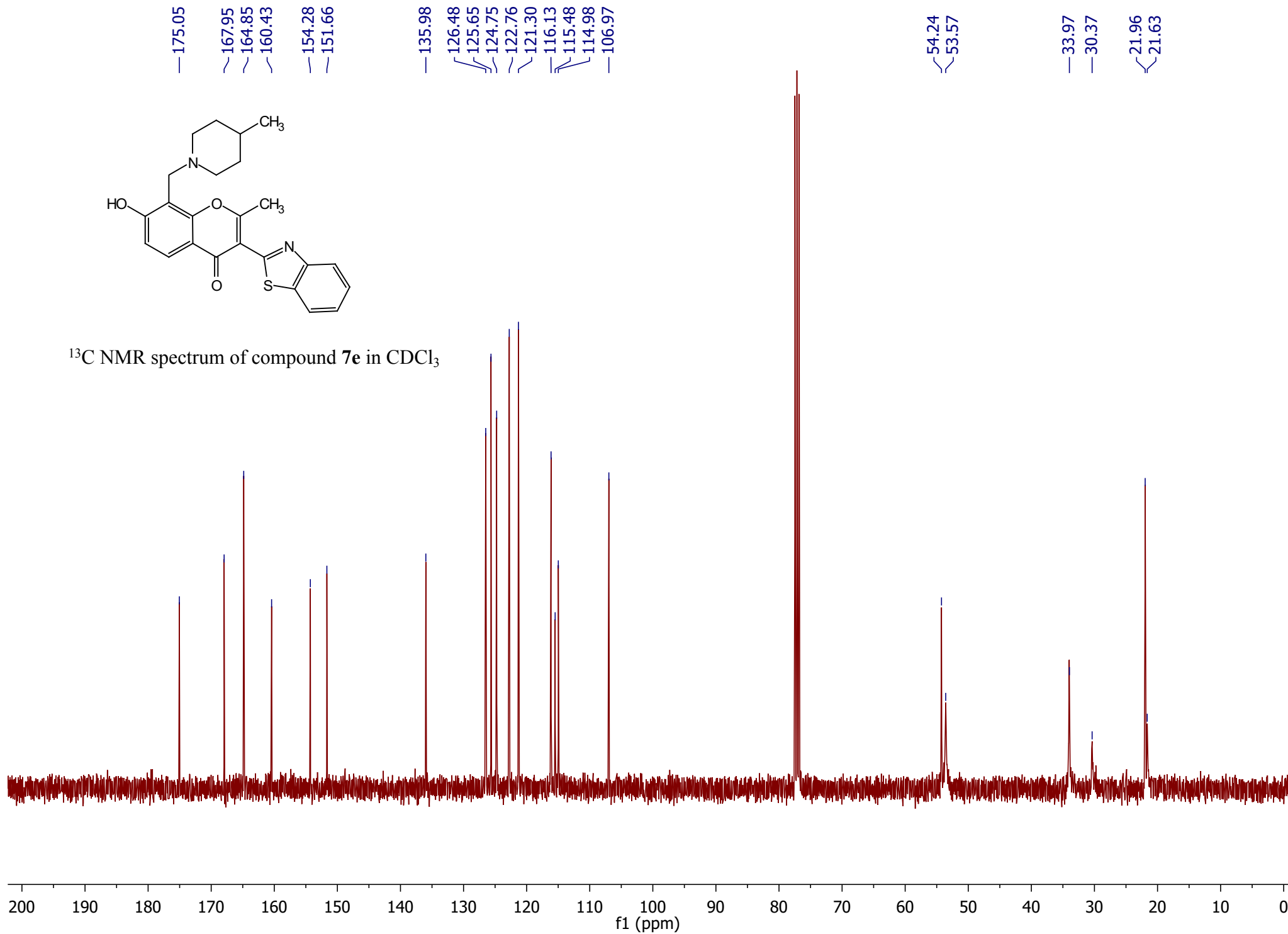


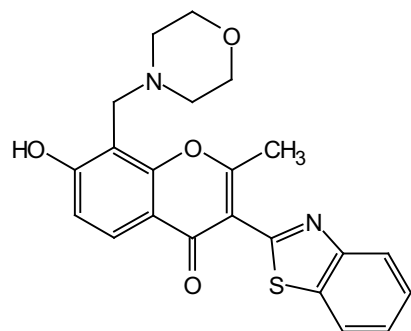
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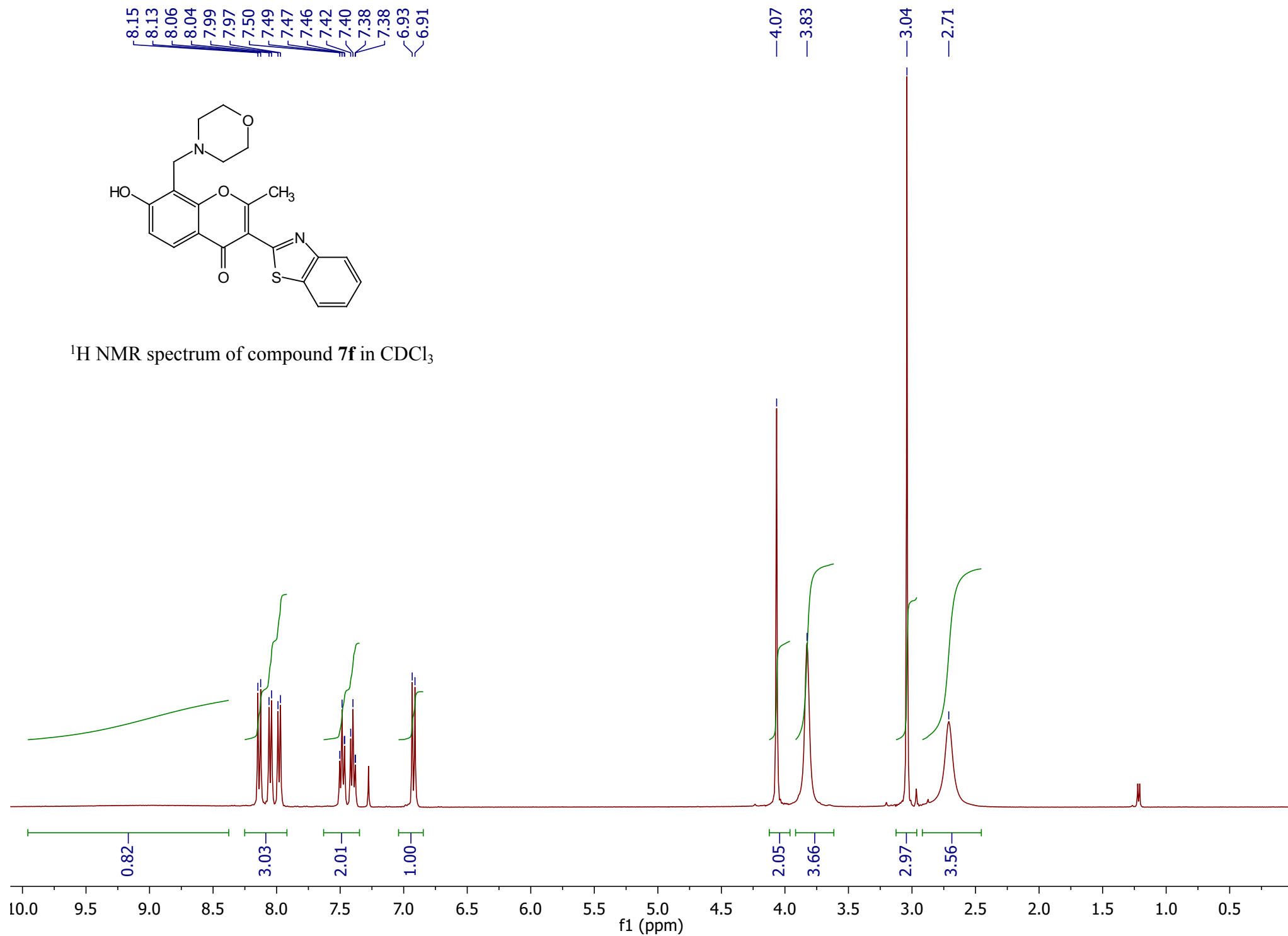


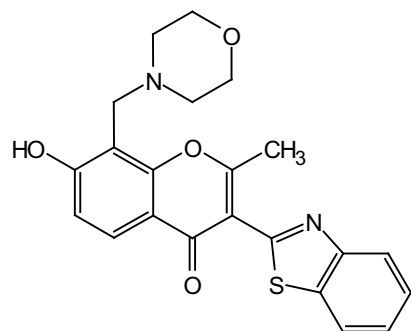
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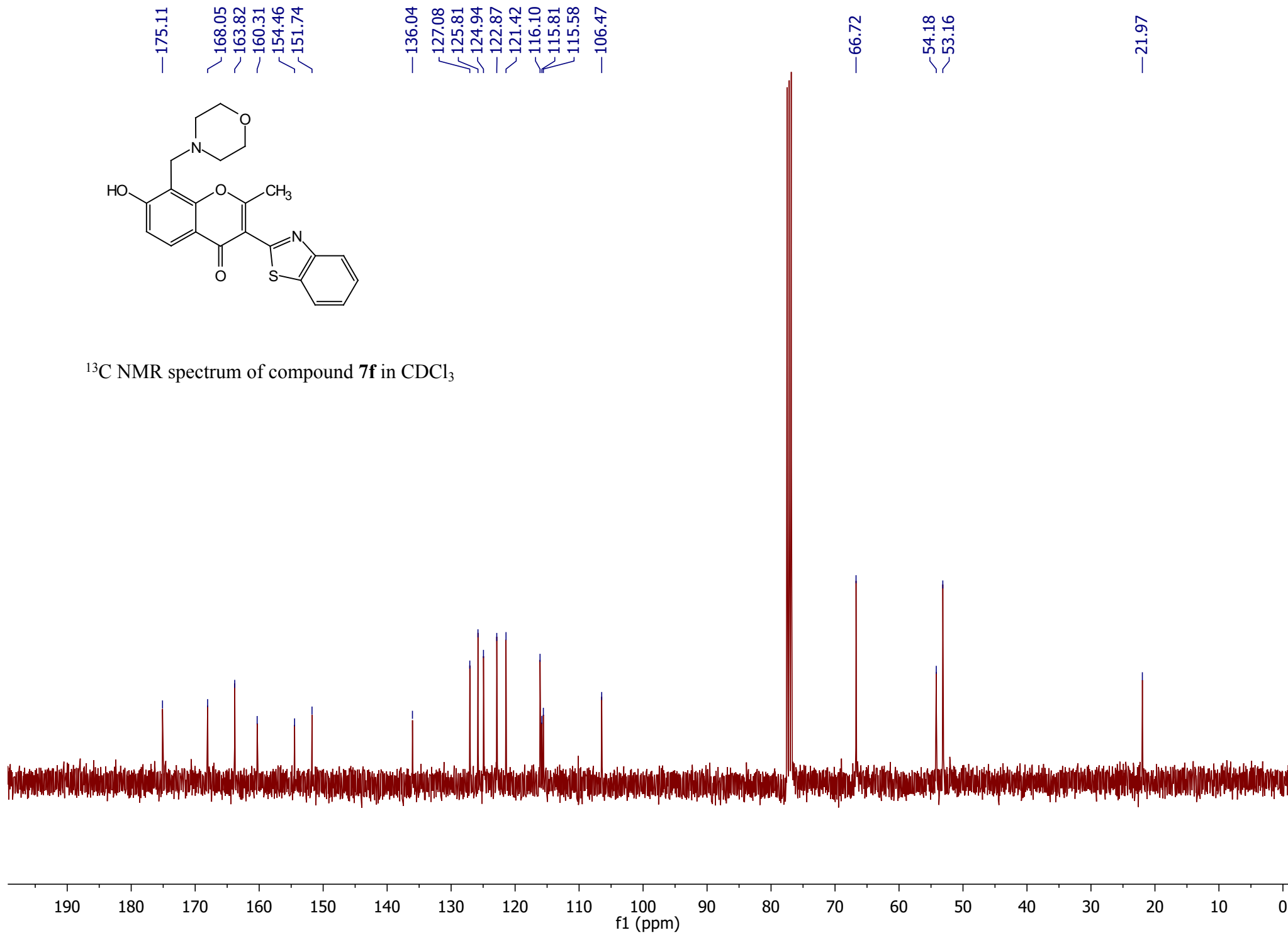


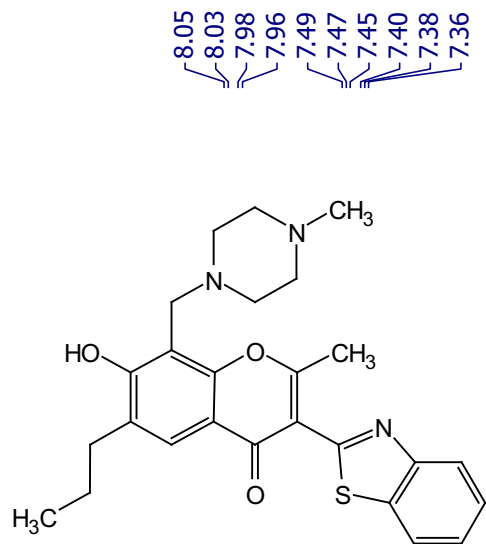
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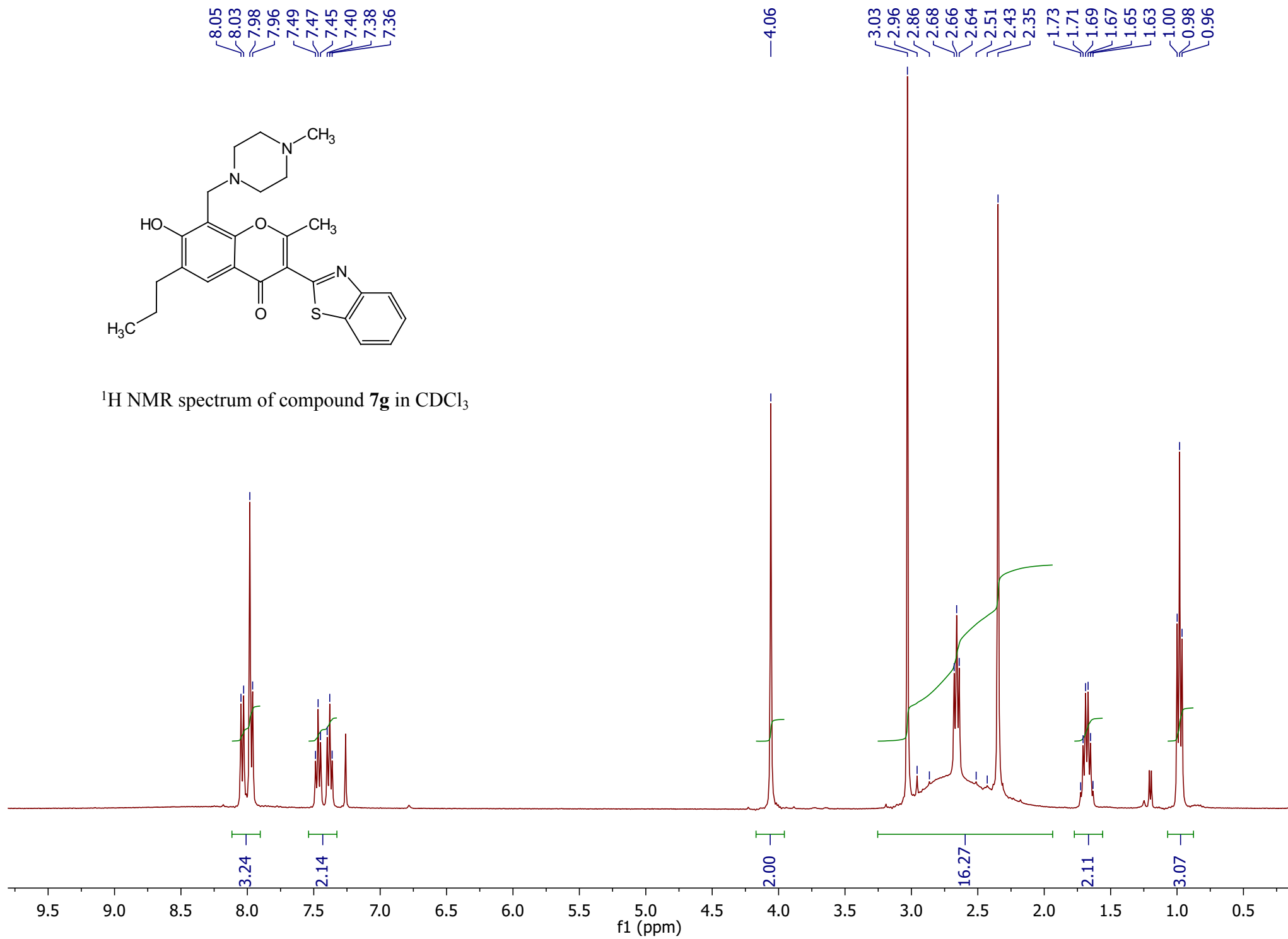


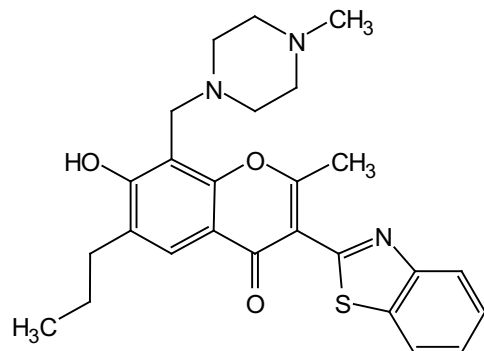
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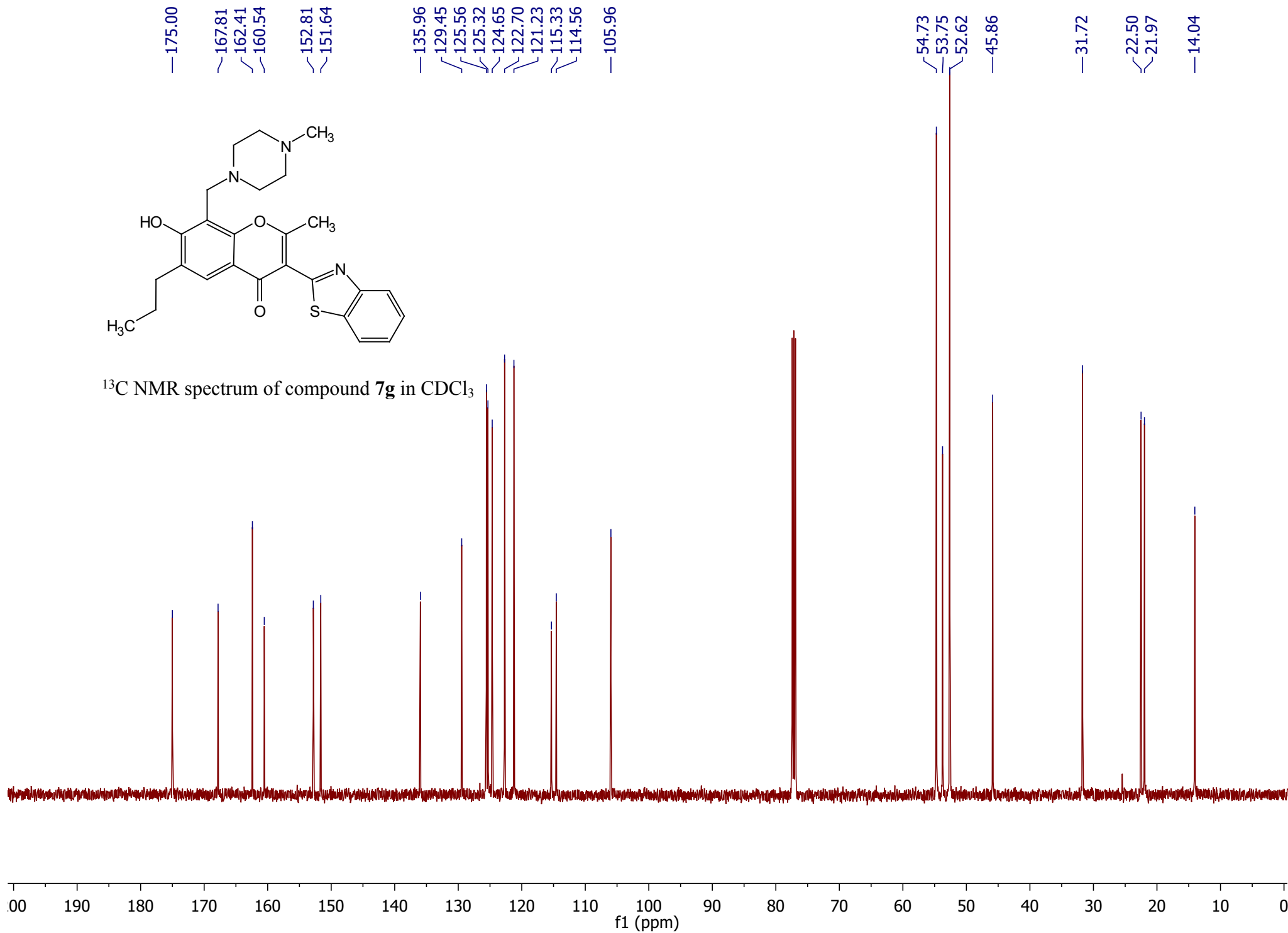


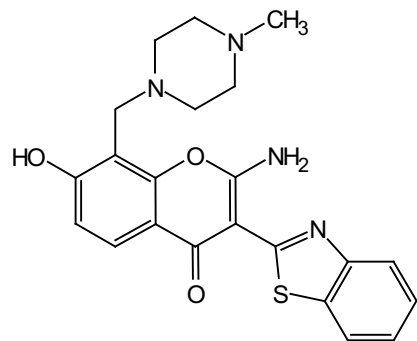
<sup>1</sup>H NMR spectrum of compound **7g** in CDCl<sub>3</sub>



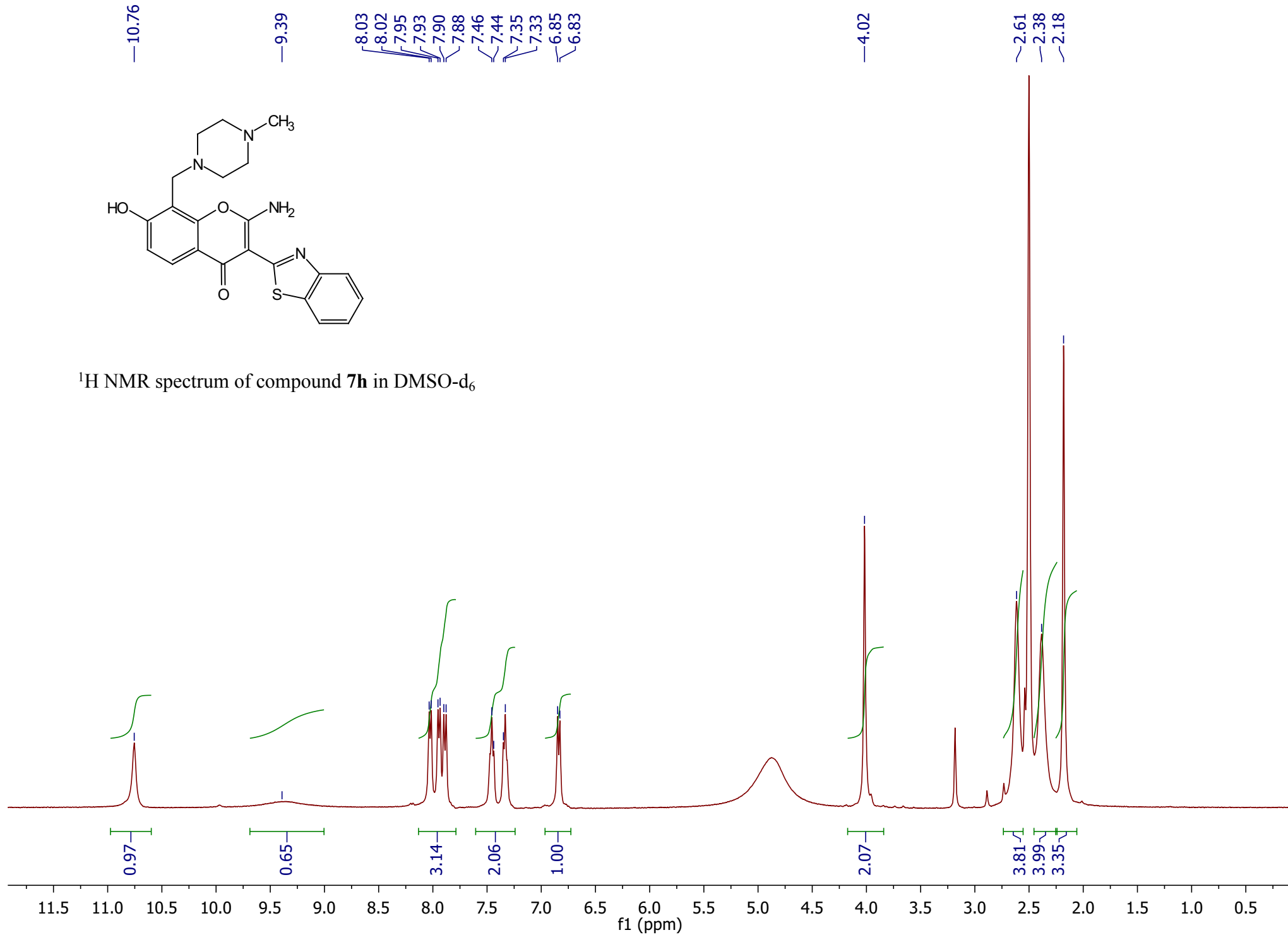


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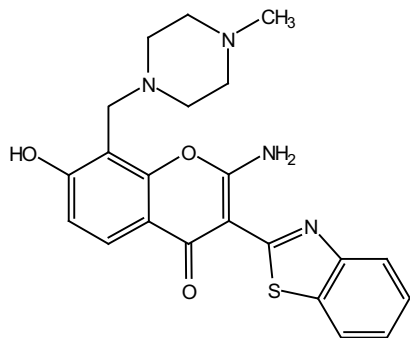




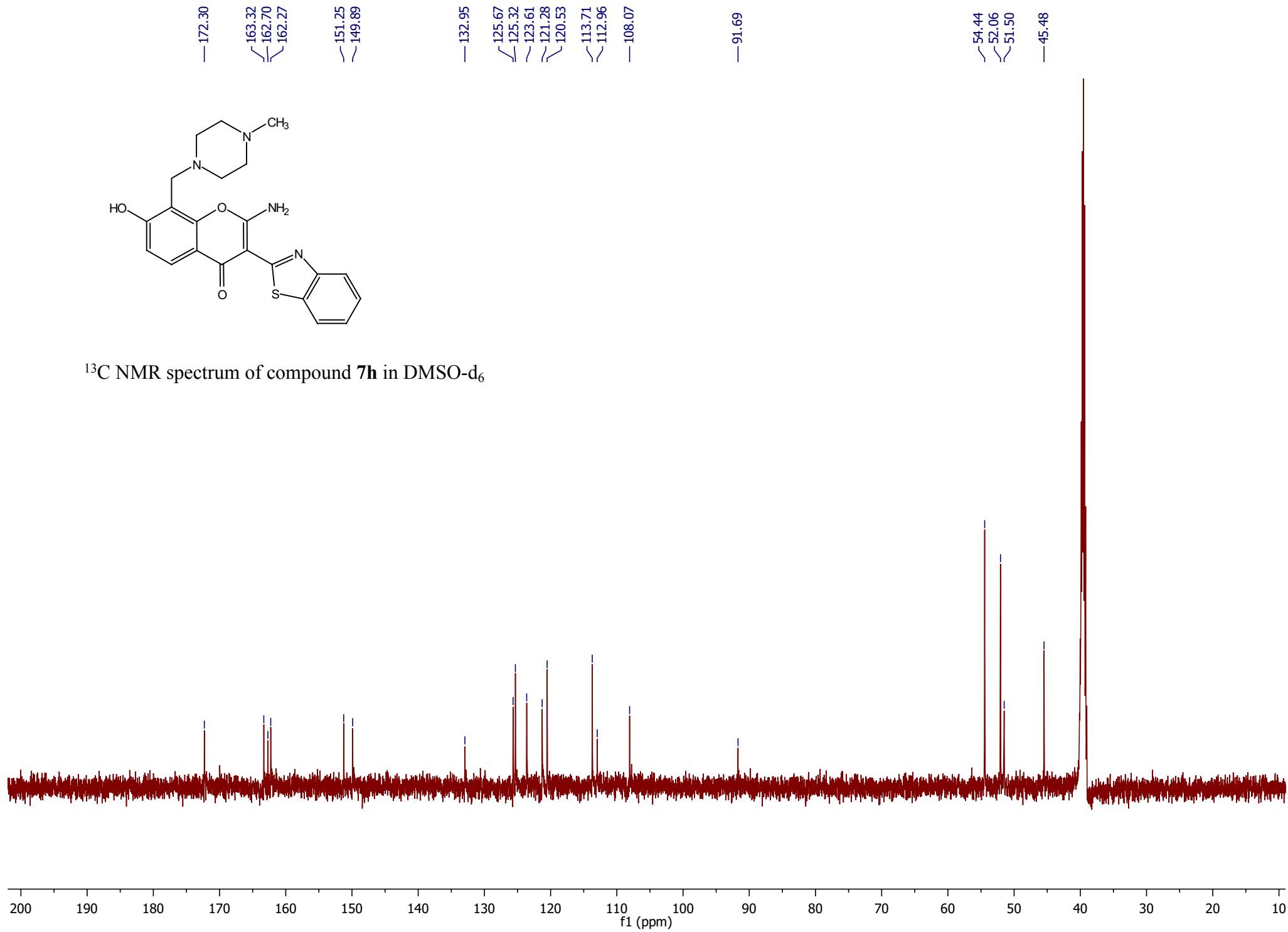
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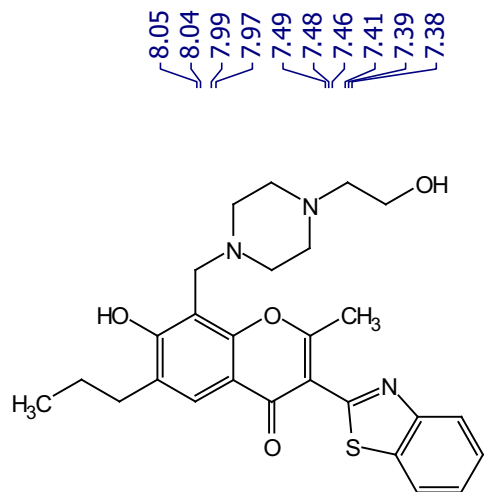




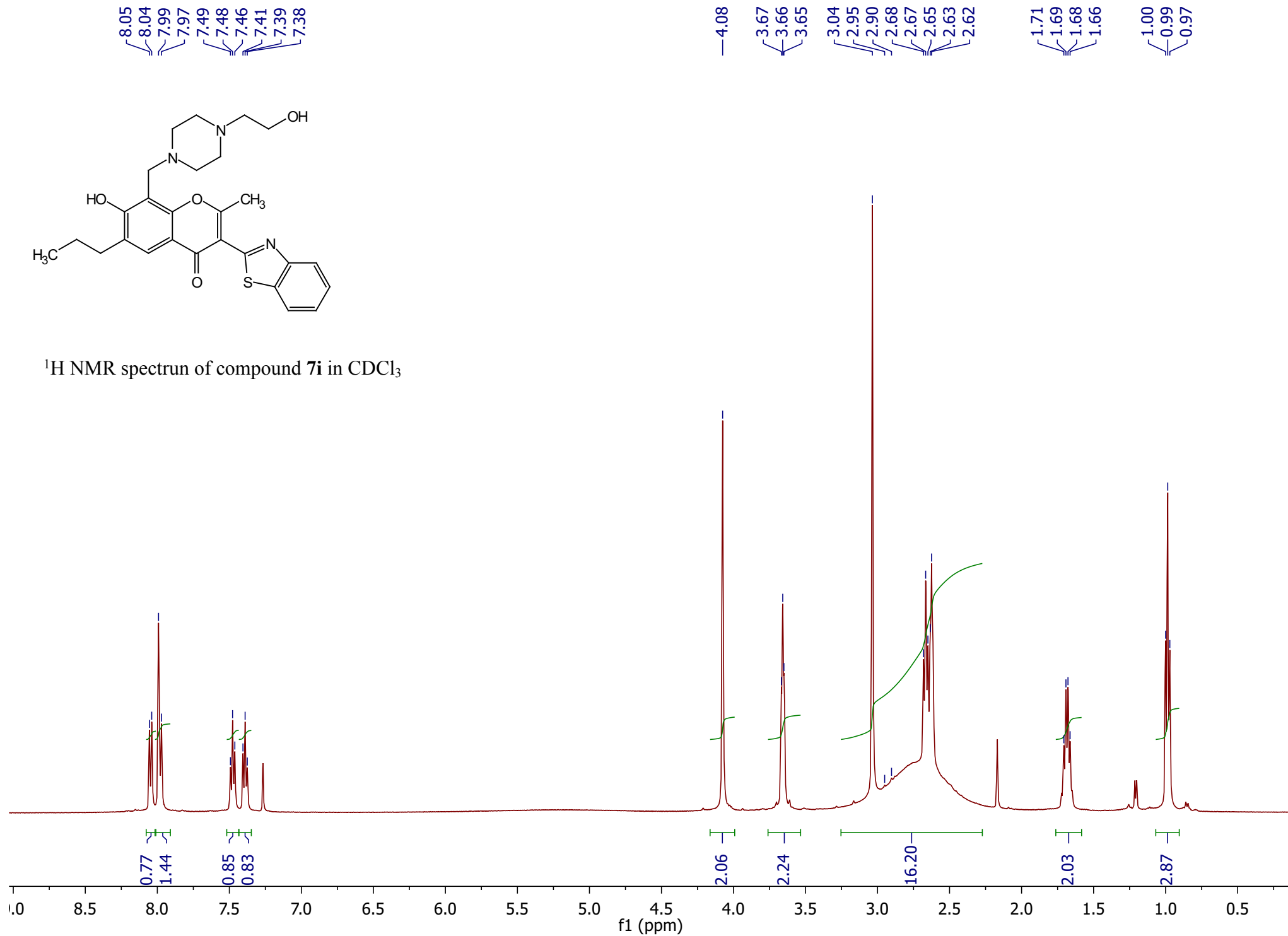


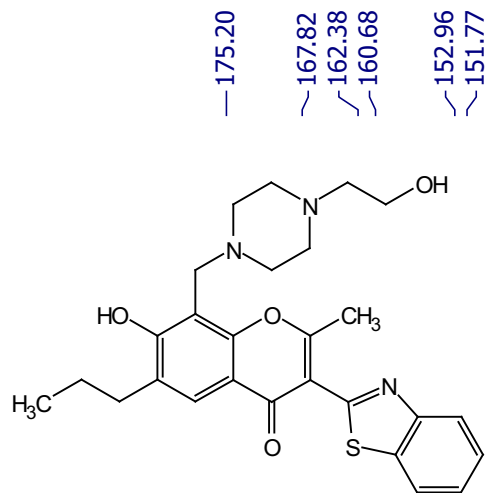
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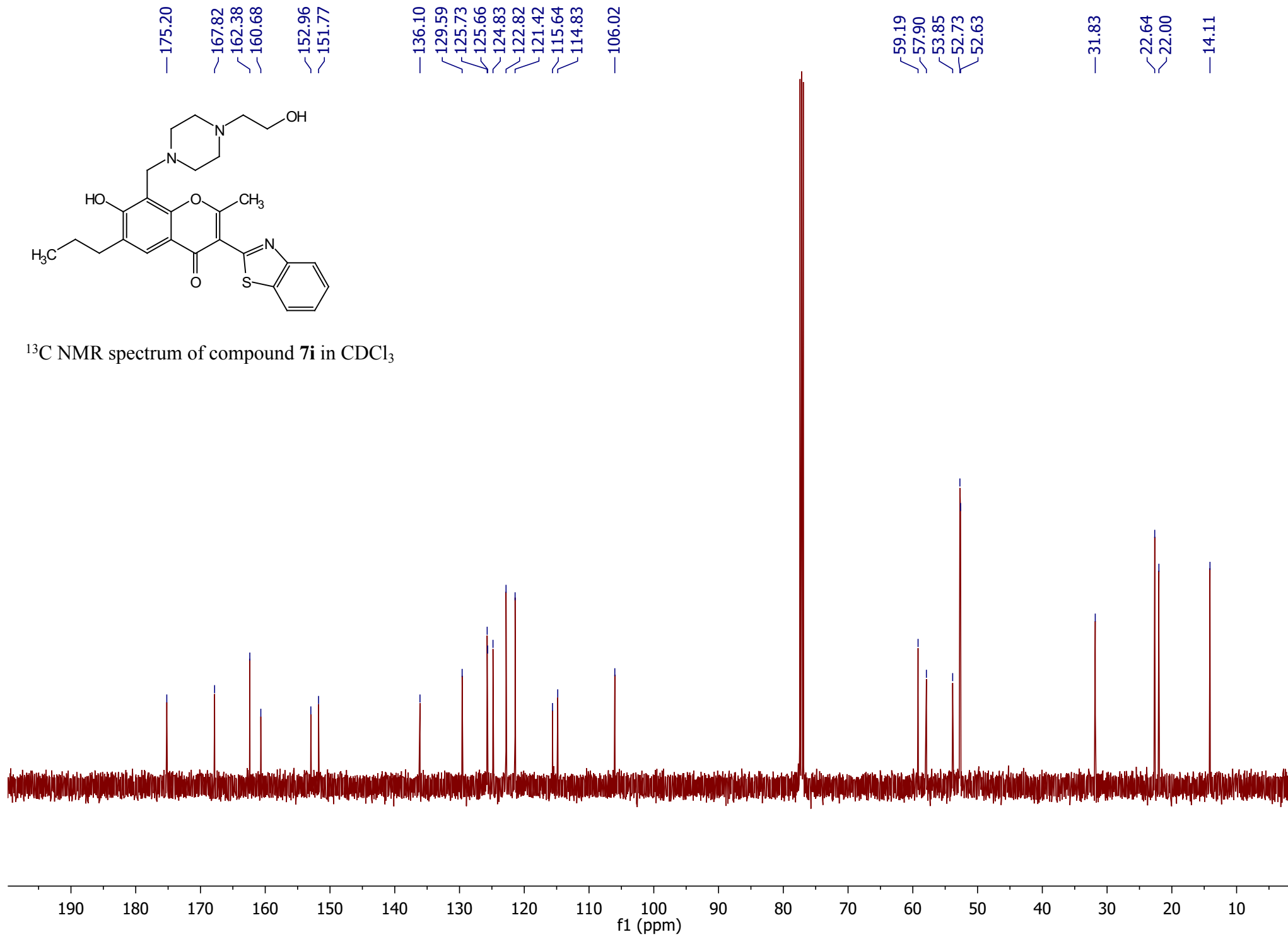


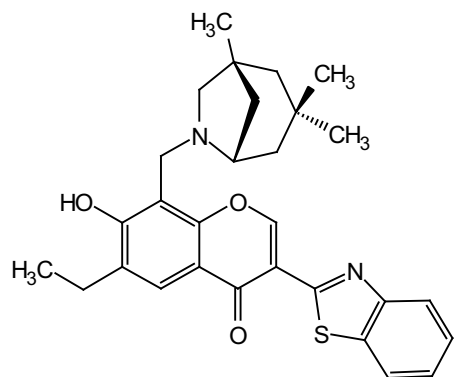
$^1\text{H}$  NMR spectrum of compound **7i** in  $\text{CDCl}_3$



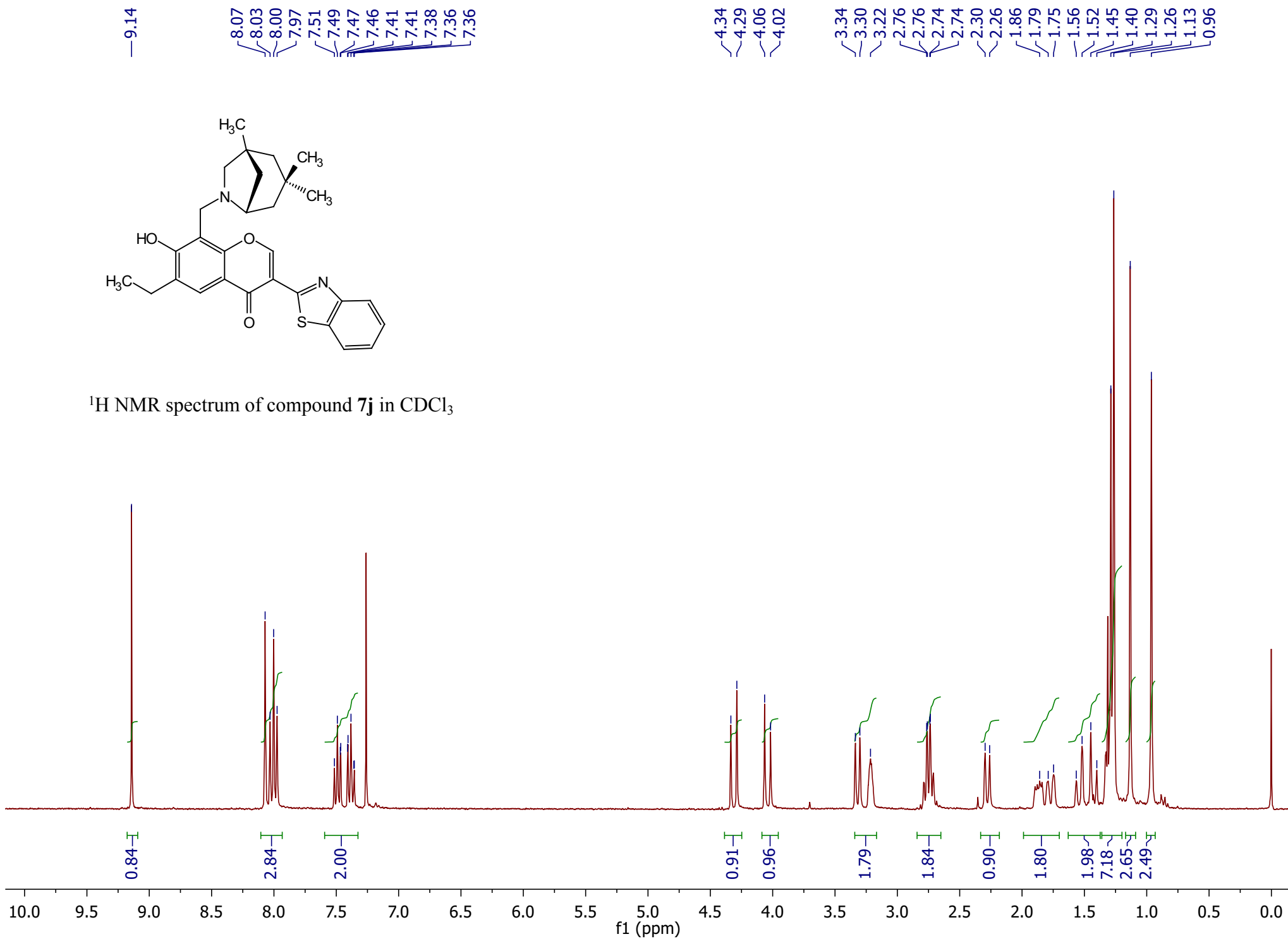


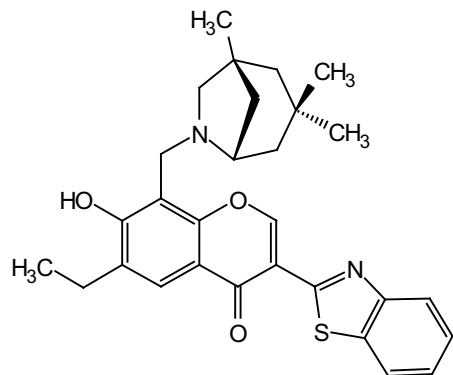
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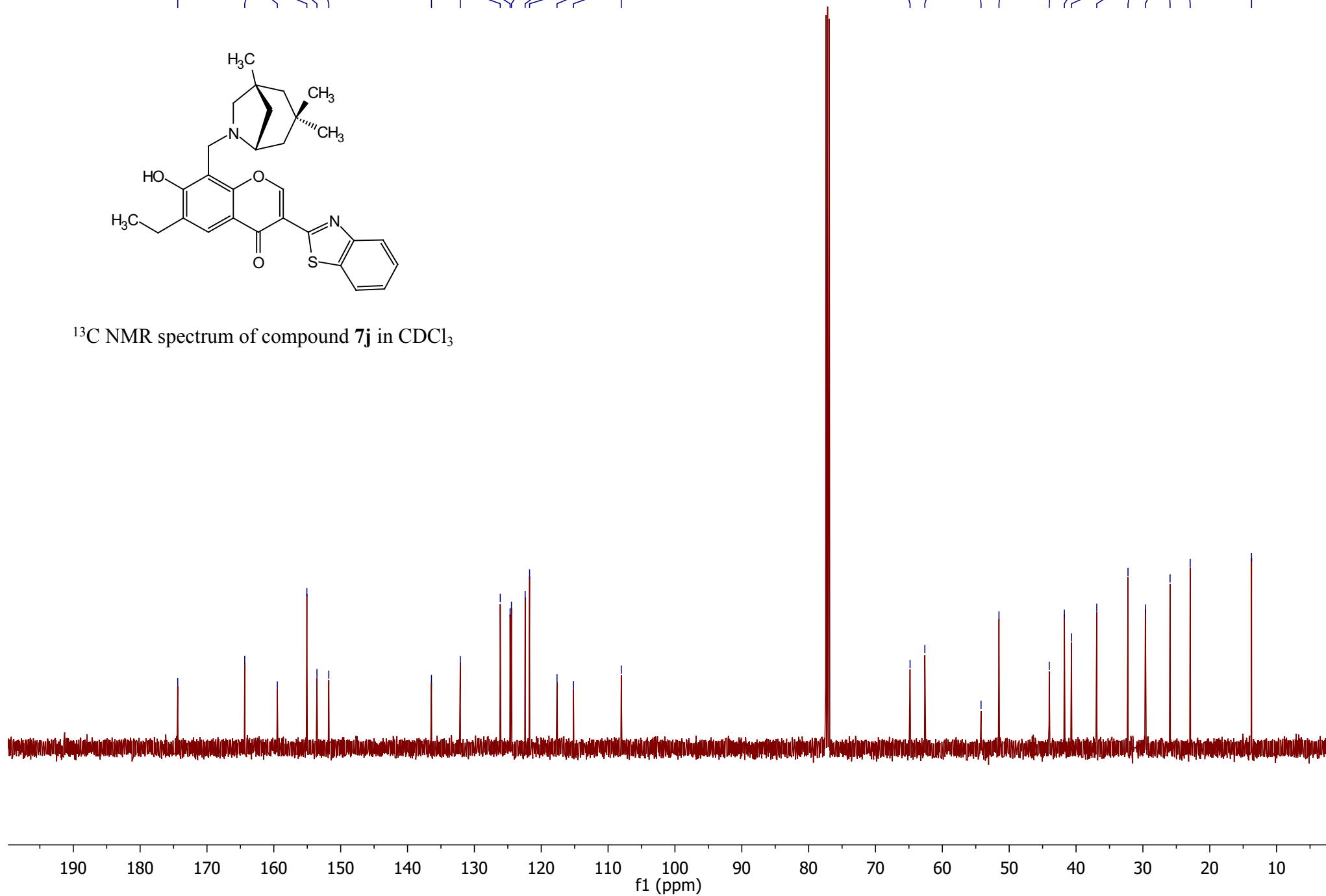


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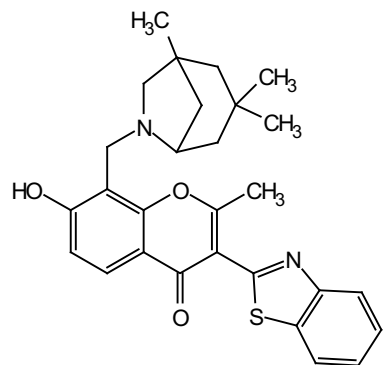




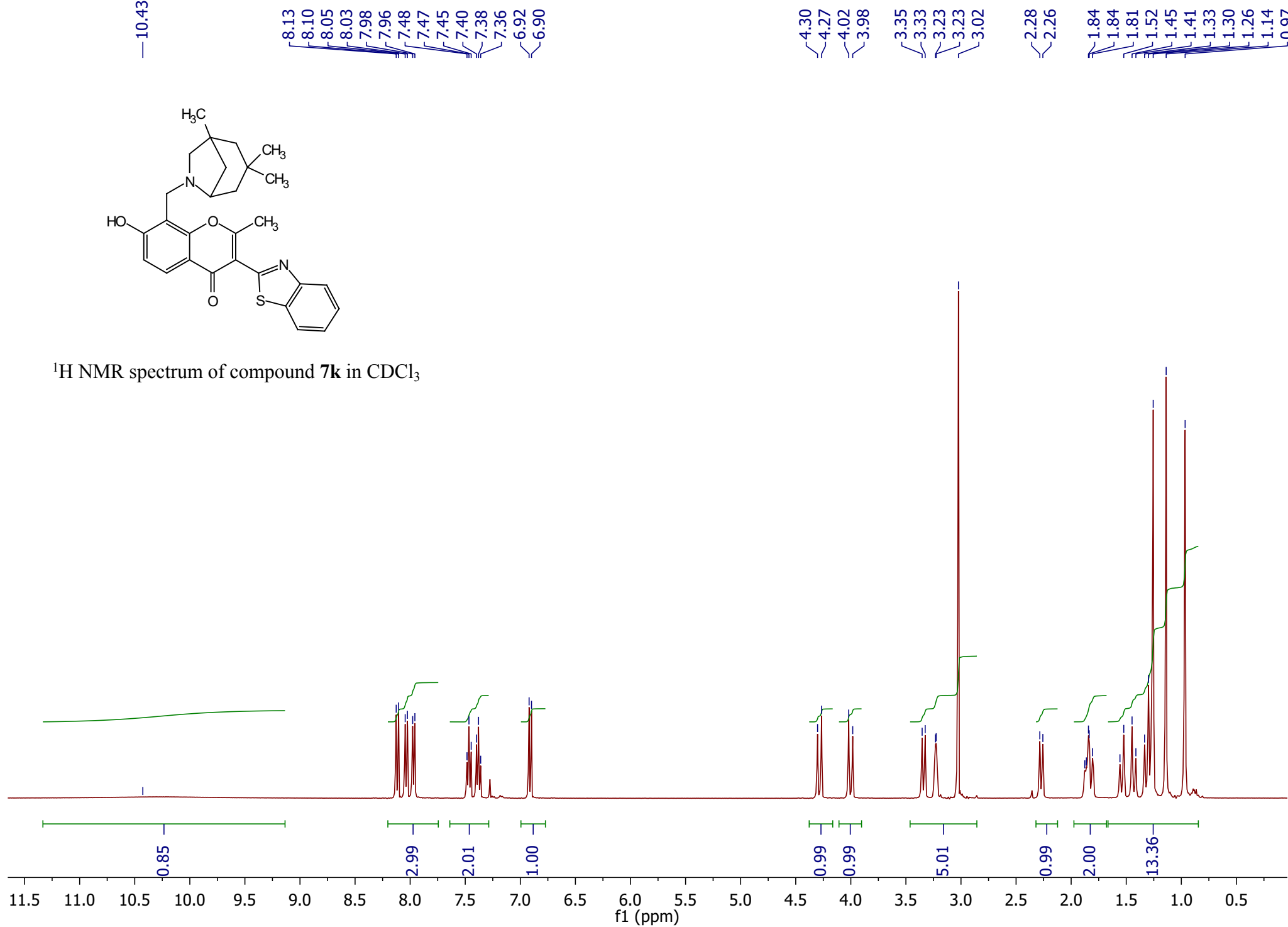
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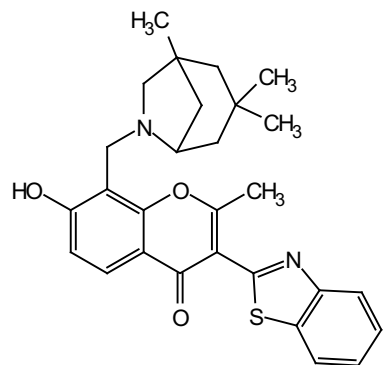


—10.43

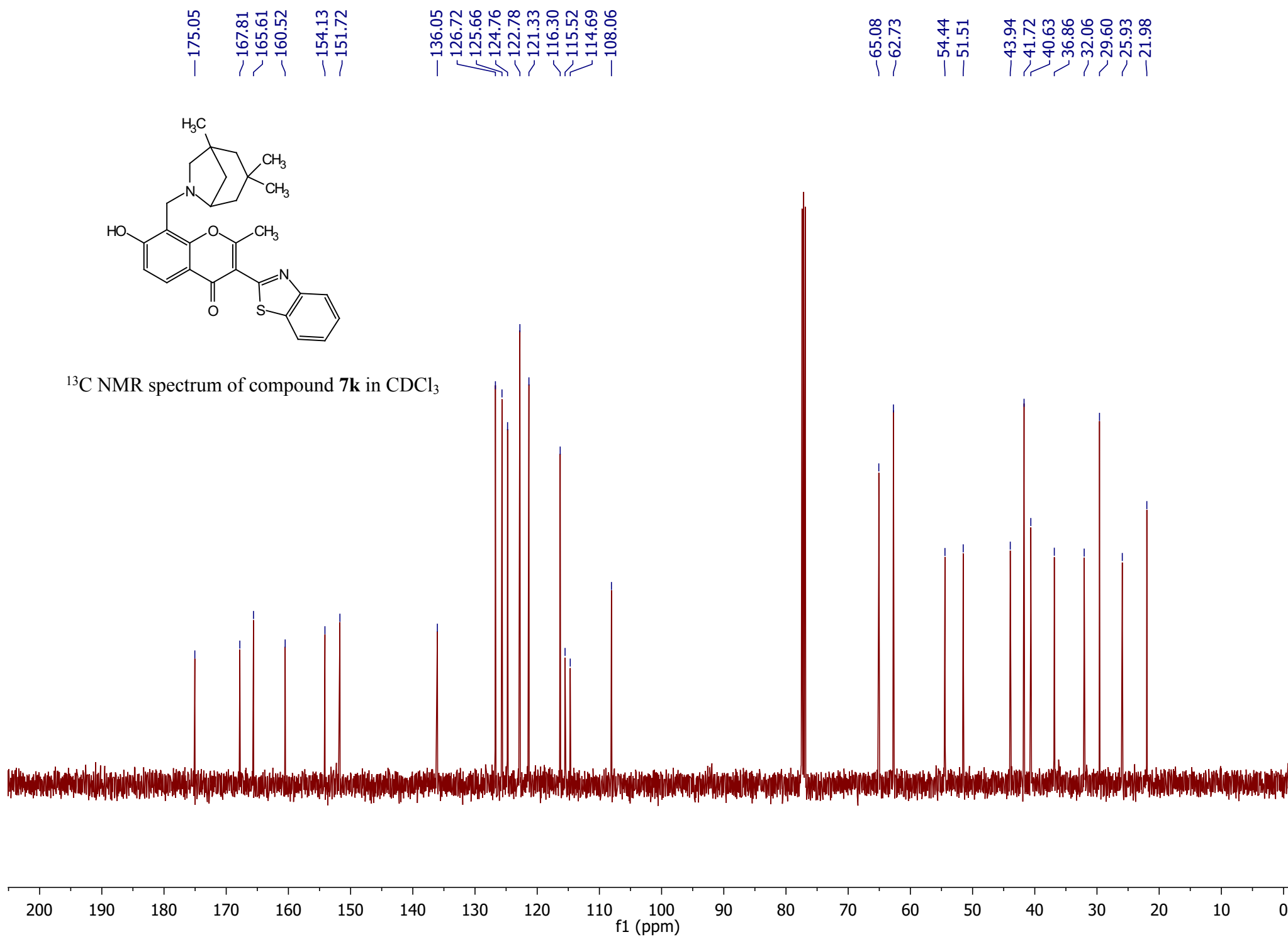


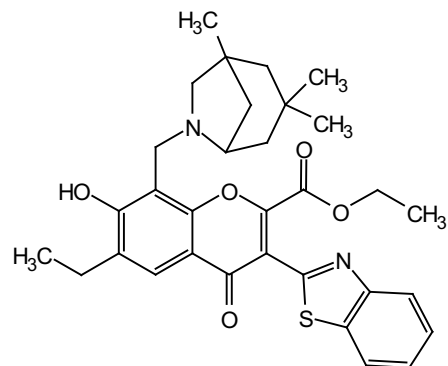
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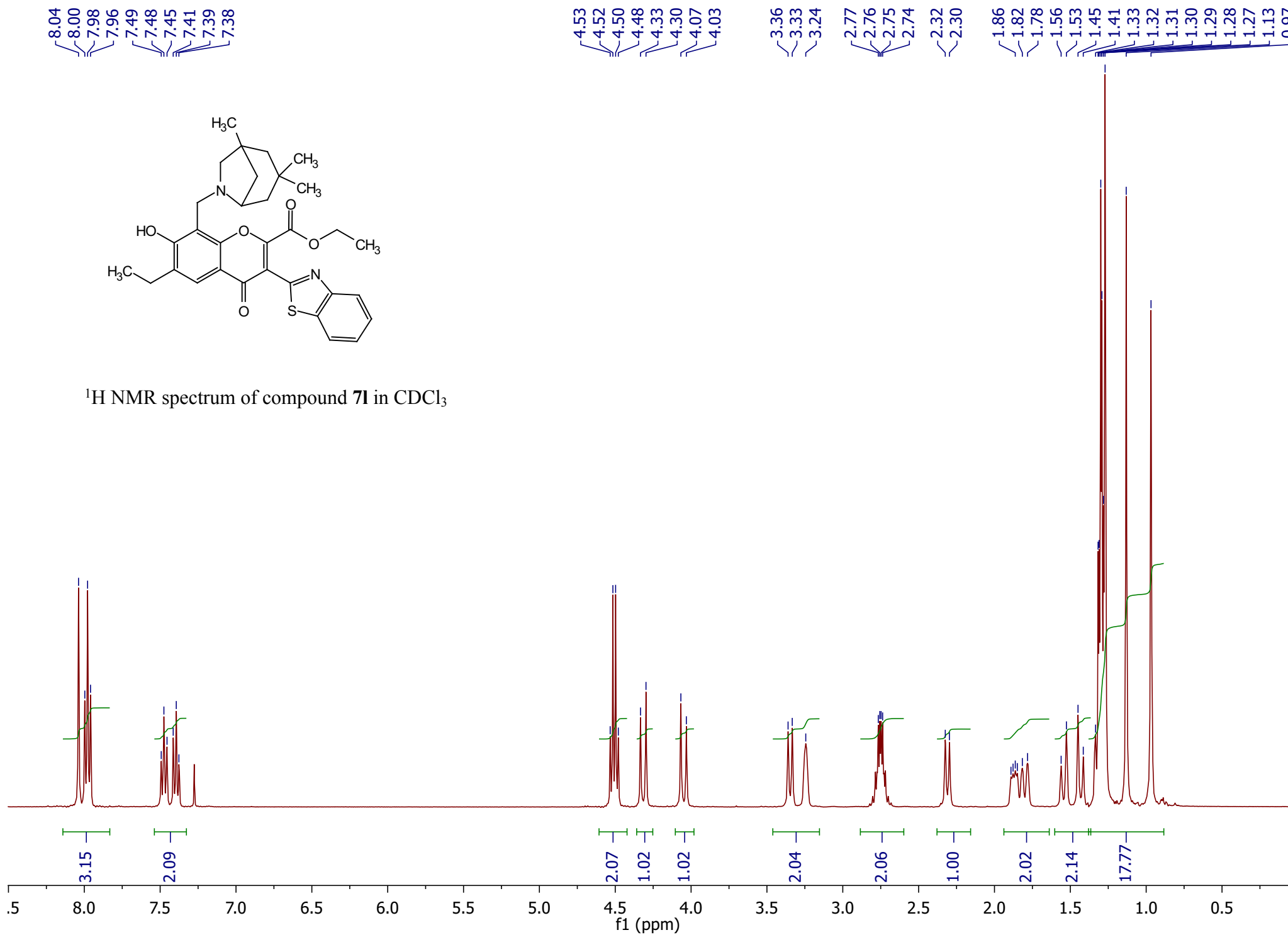


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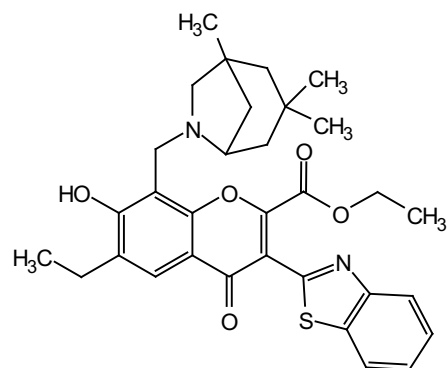




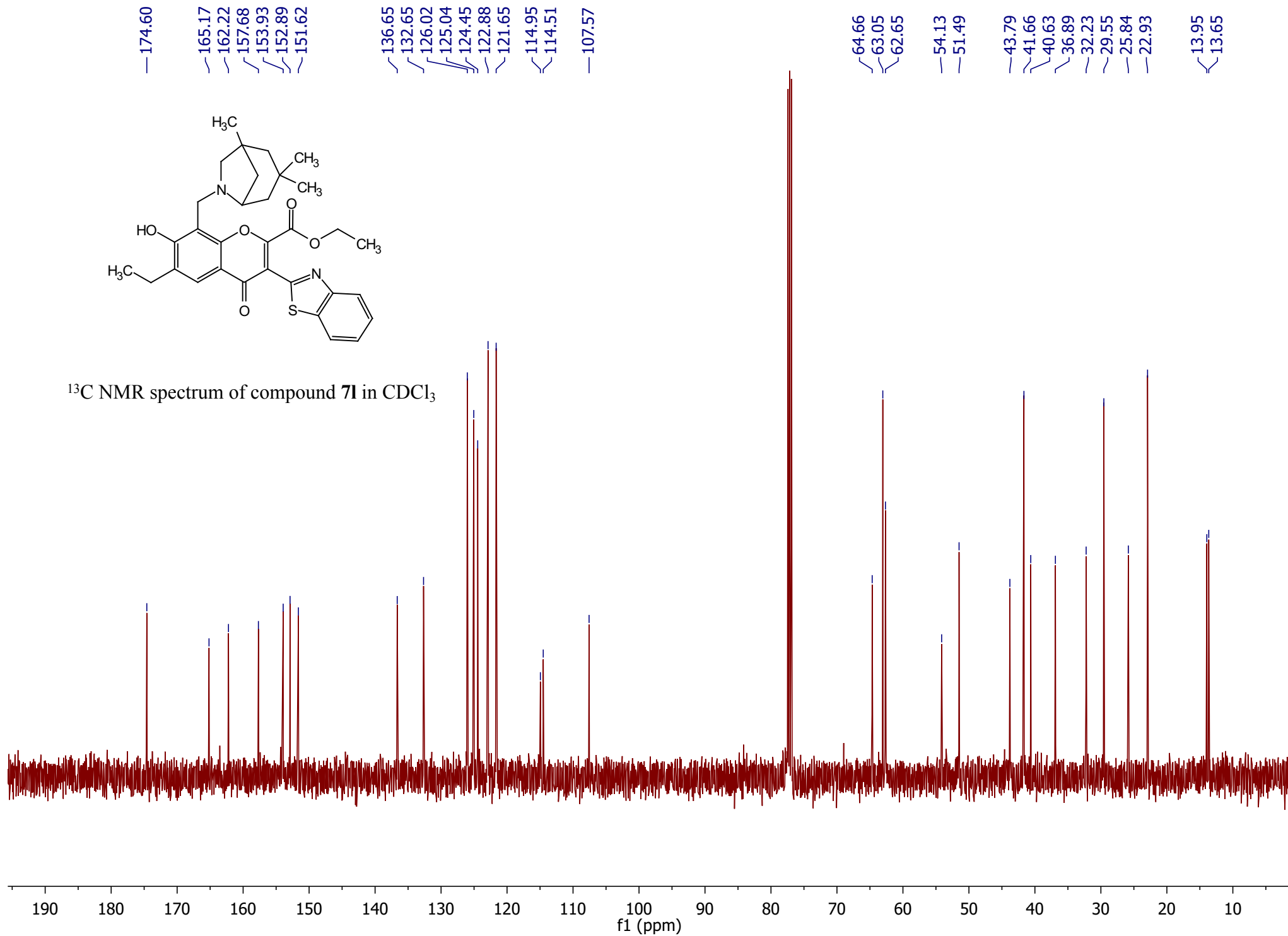
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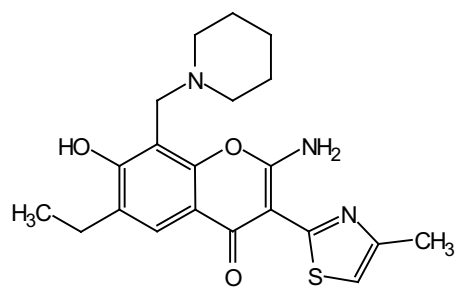




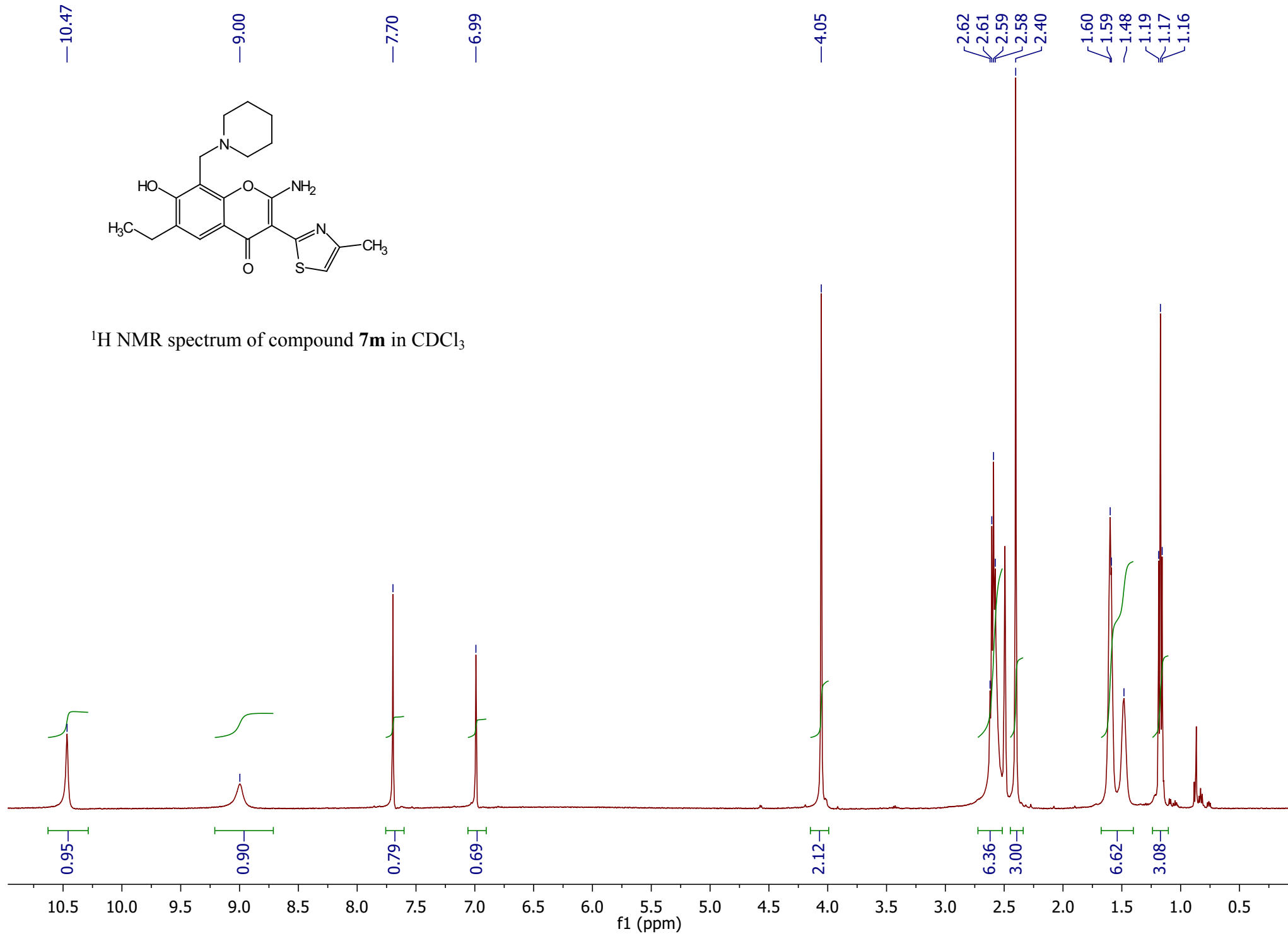


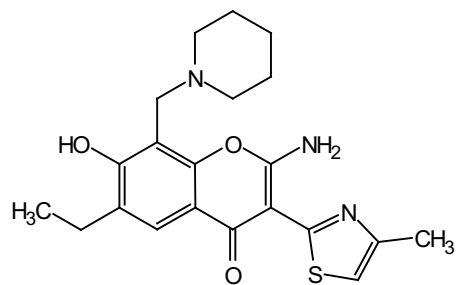
$^{13}\text{C}$  NMR spectrum of compound **7l** in  $\text{CDCl}_3$



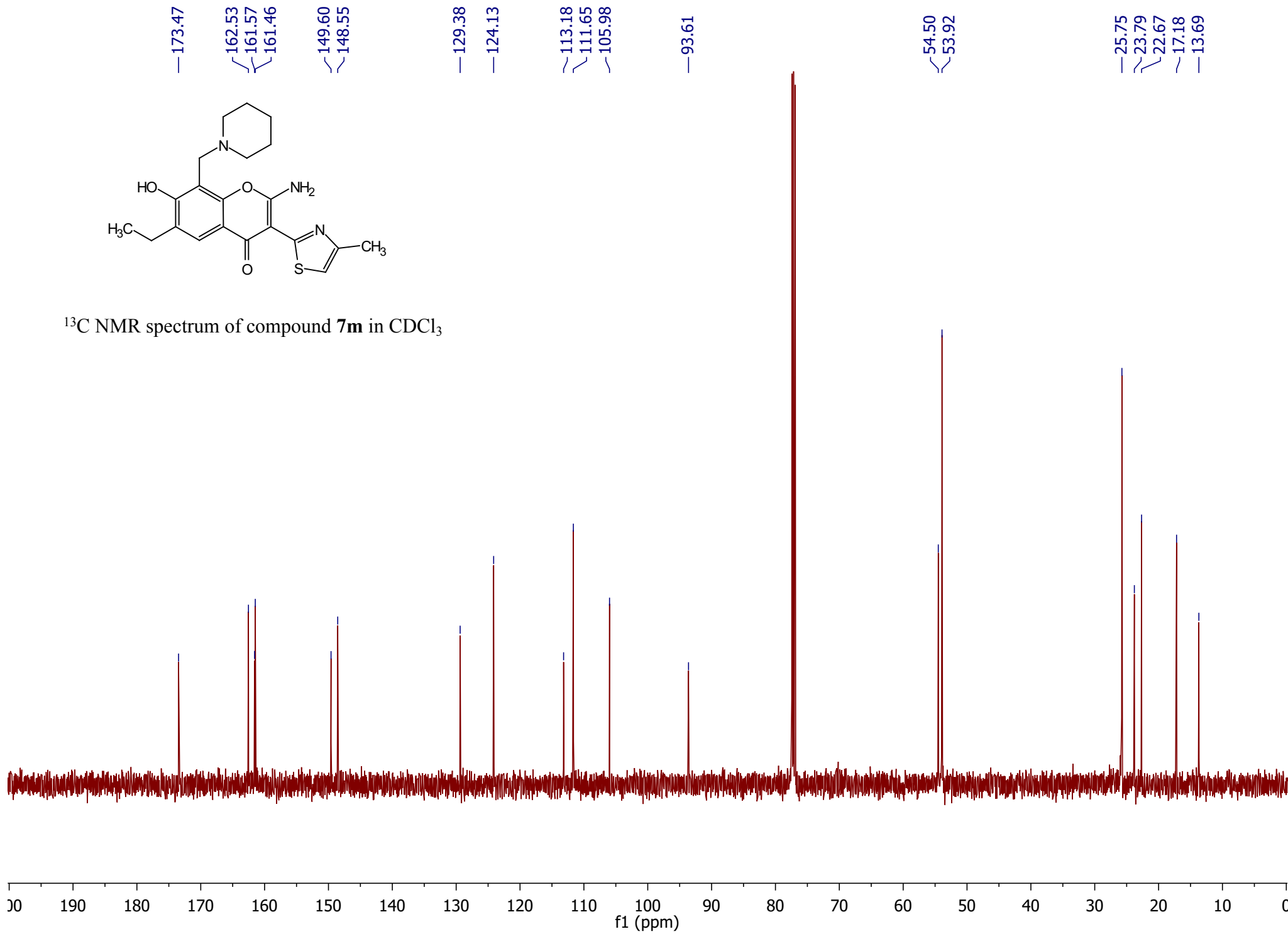


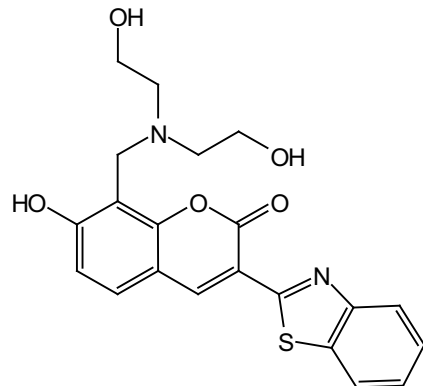
$^1\text{H}$  NMR spectrum of compound **7m** in  $\text{CDCl}_3$



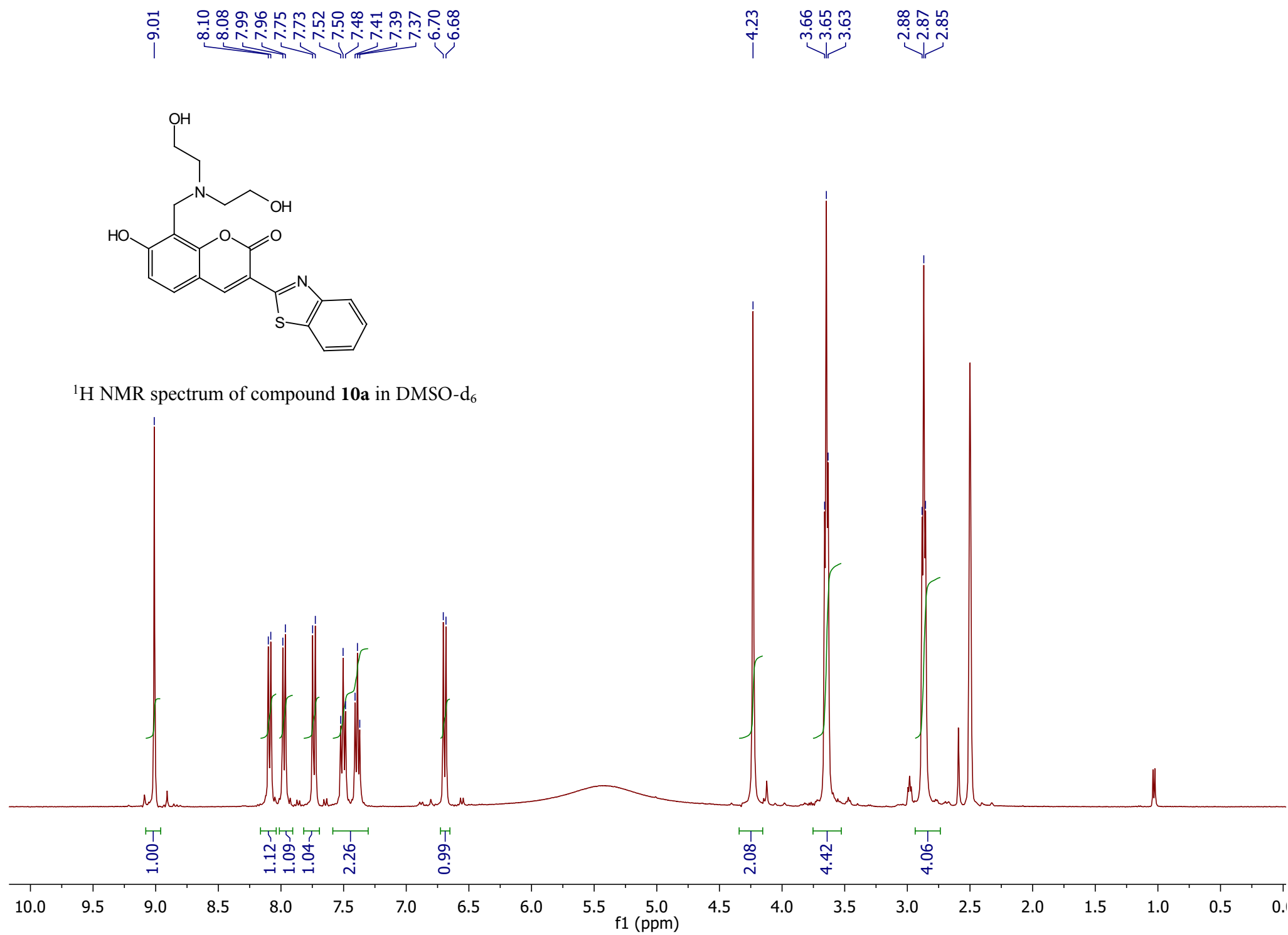


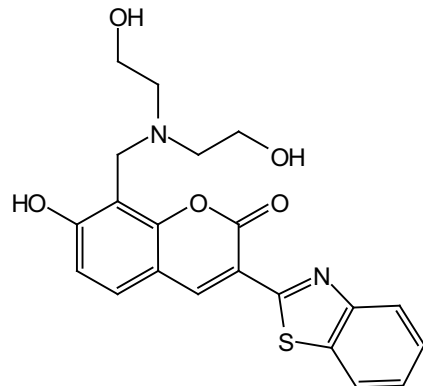
$^{13}\text{C}$  NMR spectrum of compound **7m** in  $\text{CDCl}_3$



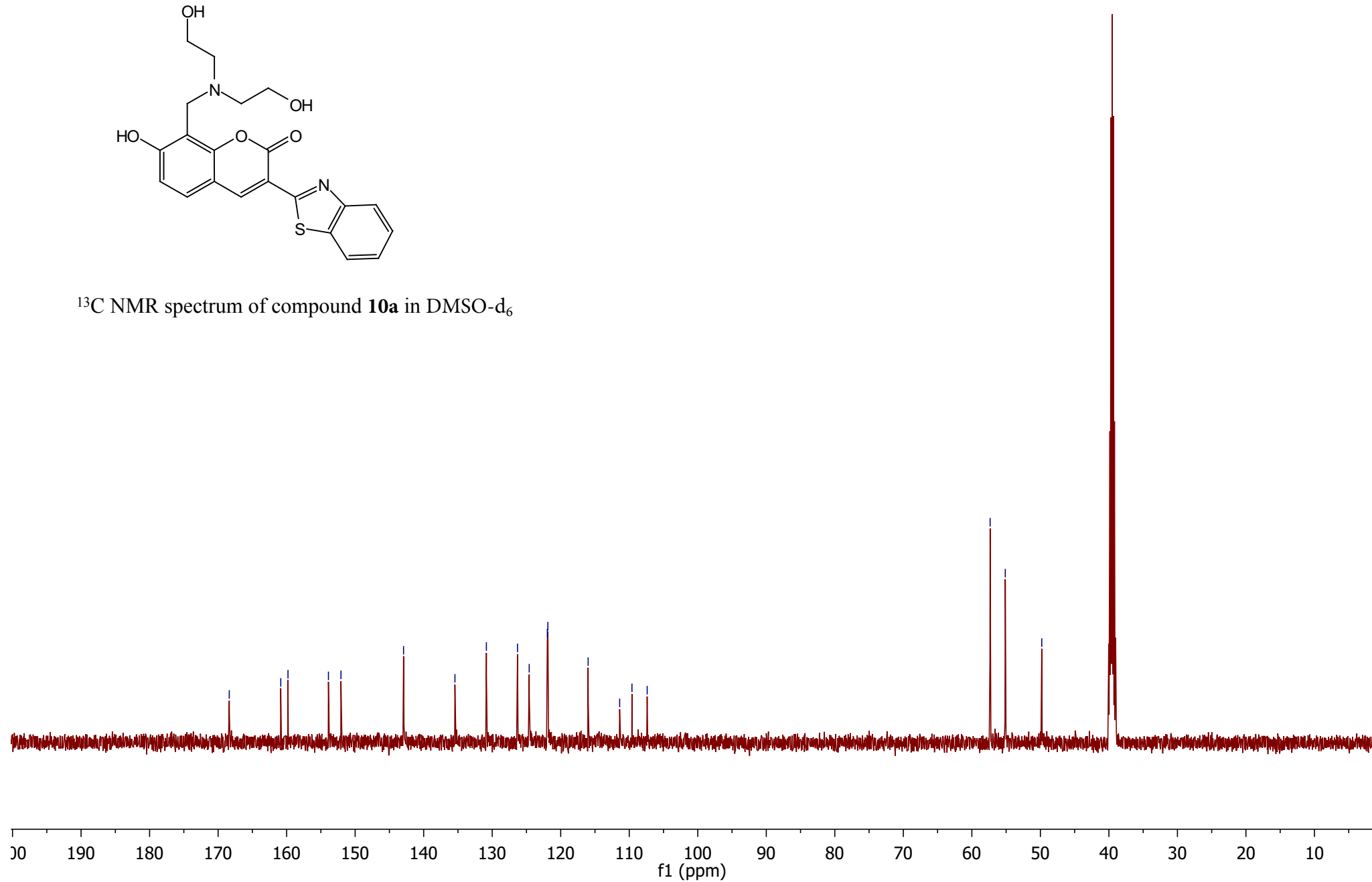


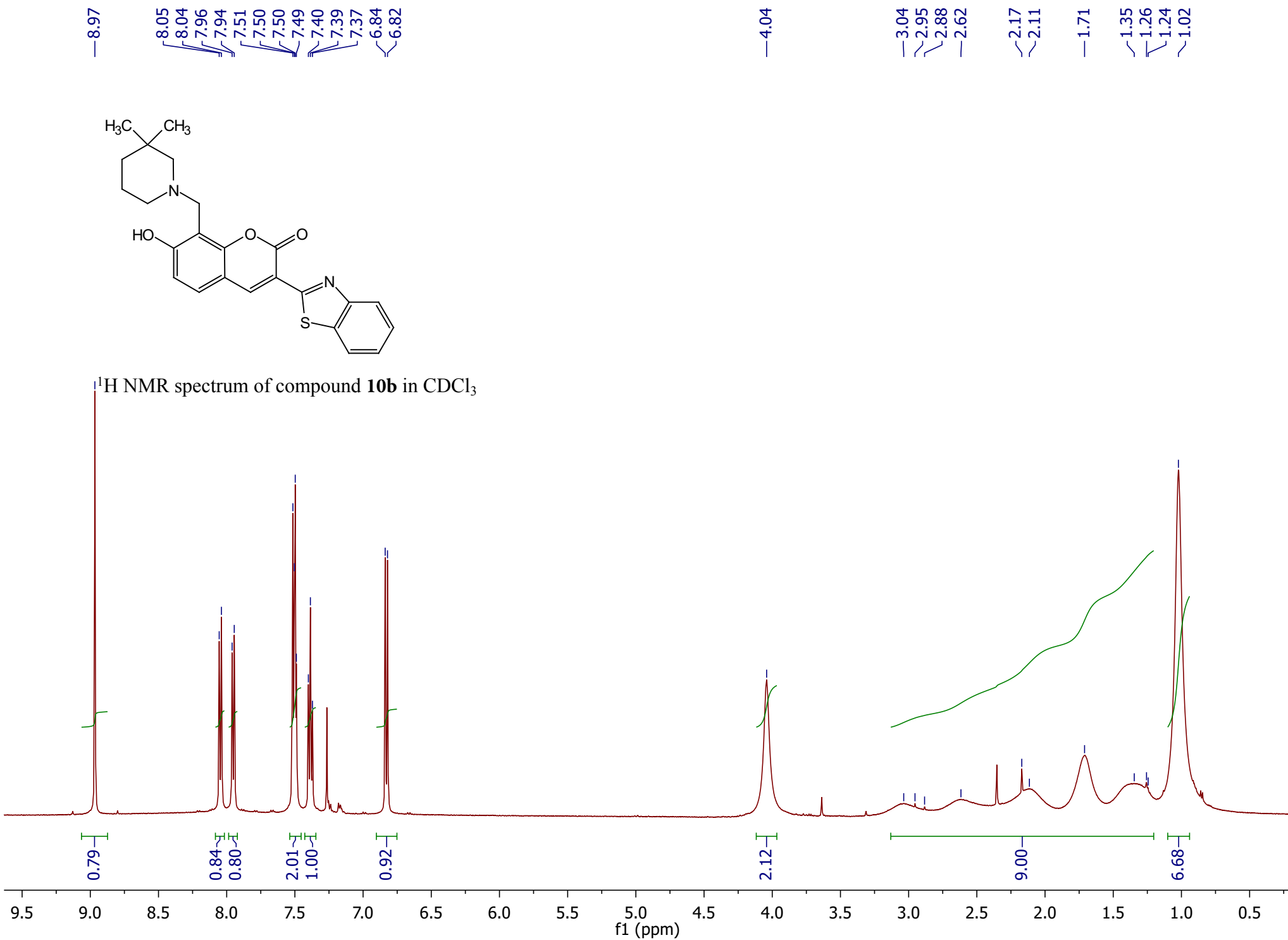
$^1\text{H}$  NMR spectrum of compound **10a** in  $\text{DMSO-d}_6$

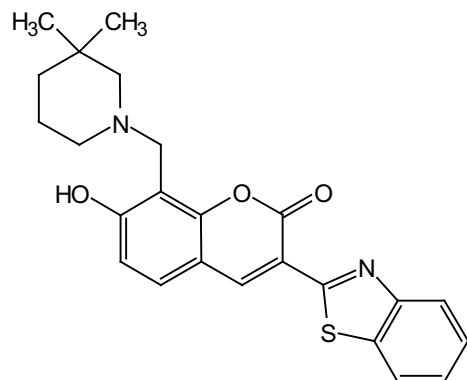




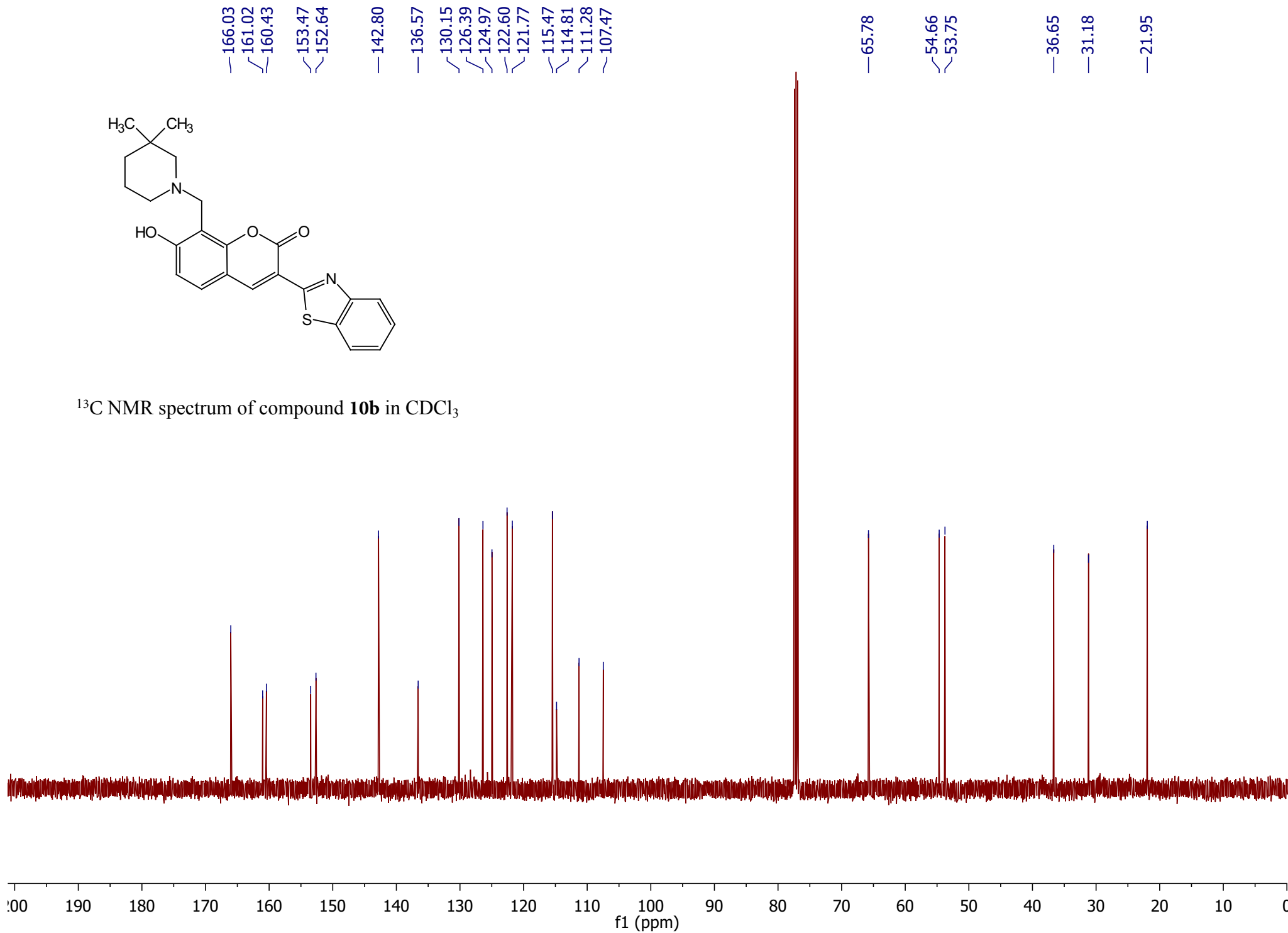
$^{13}\text{C}$  NMR spectrum of compound **10a** in  $\text{DMSO-d}_6$

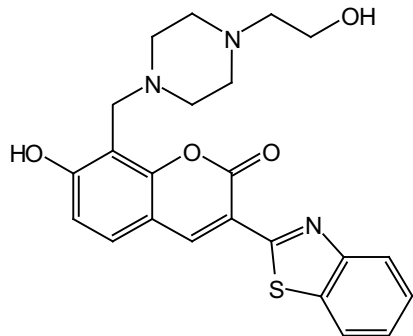




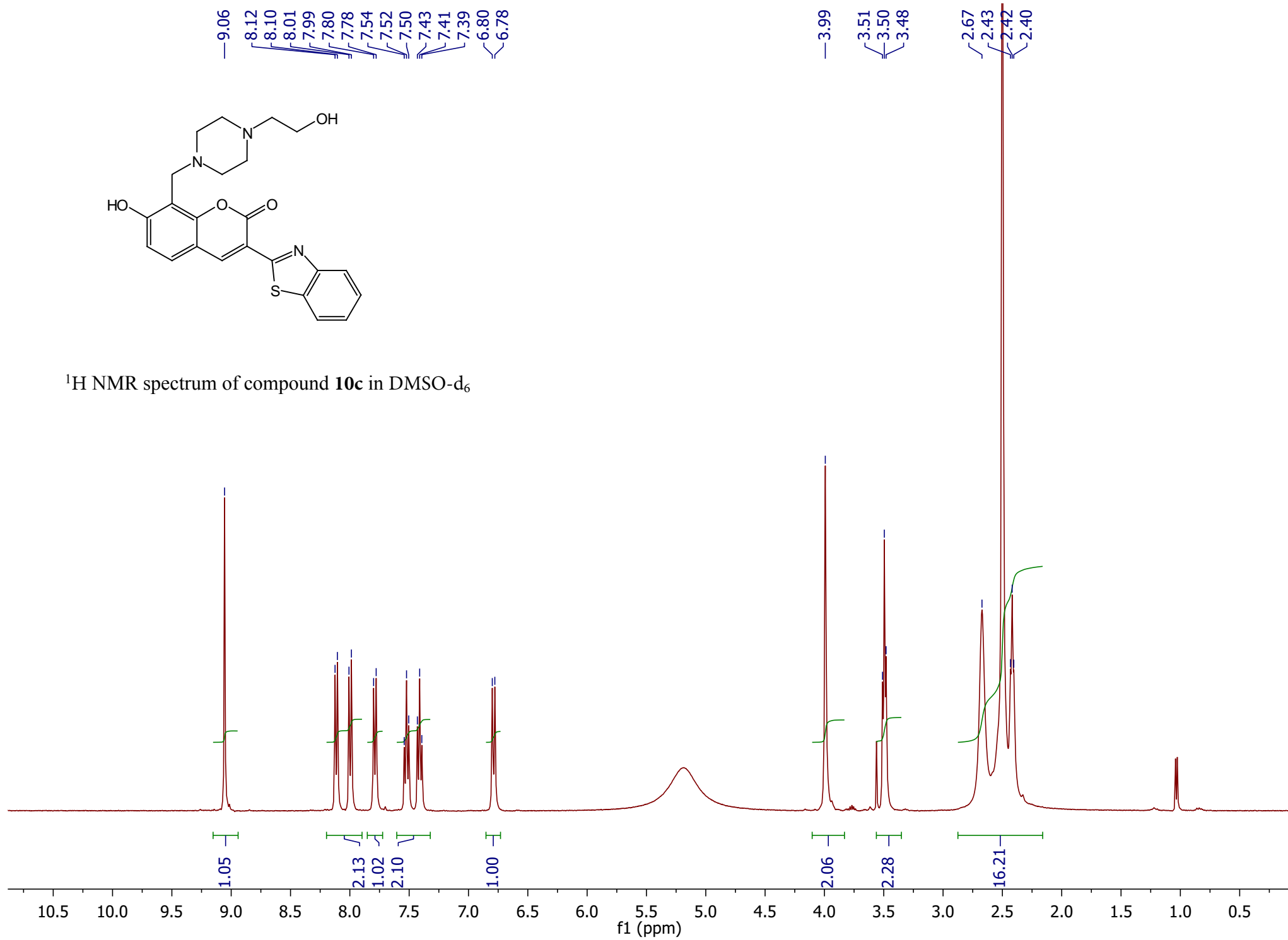


$^{13}\text{C}$  NMR spectrum of compound **10b** in  $\text{CDCl}_3$

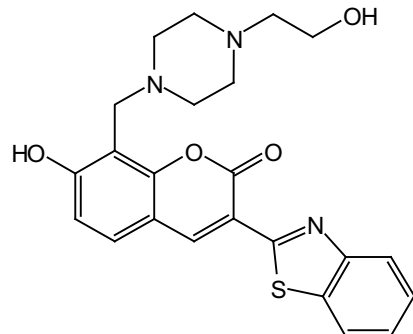




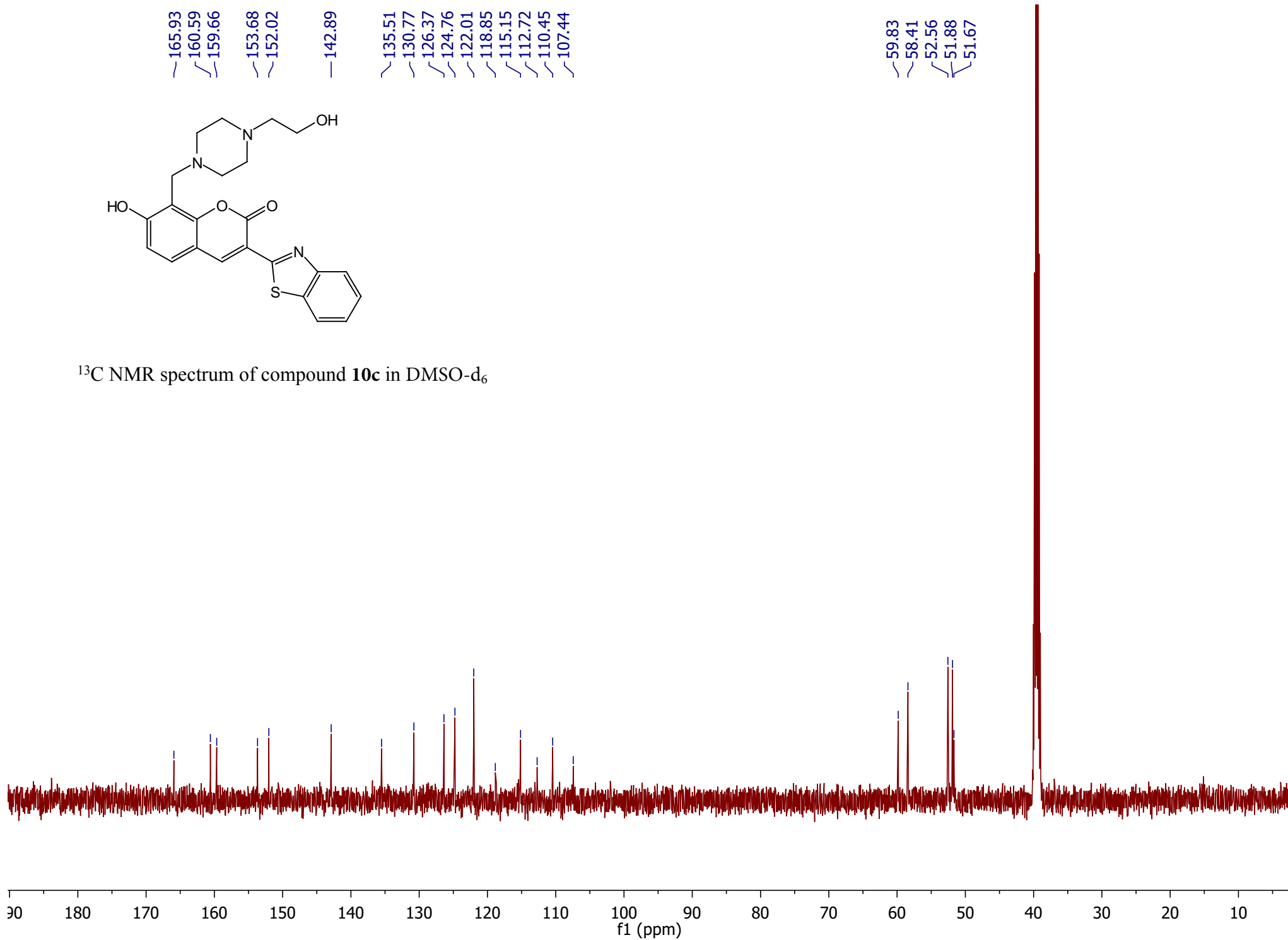
$^1\text{H}$  NMR spectrum of compound **10c** in  $\text{DMSO-d}_6$

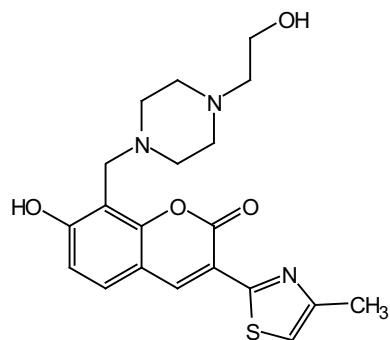




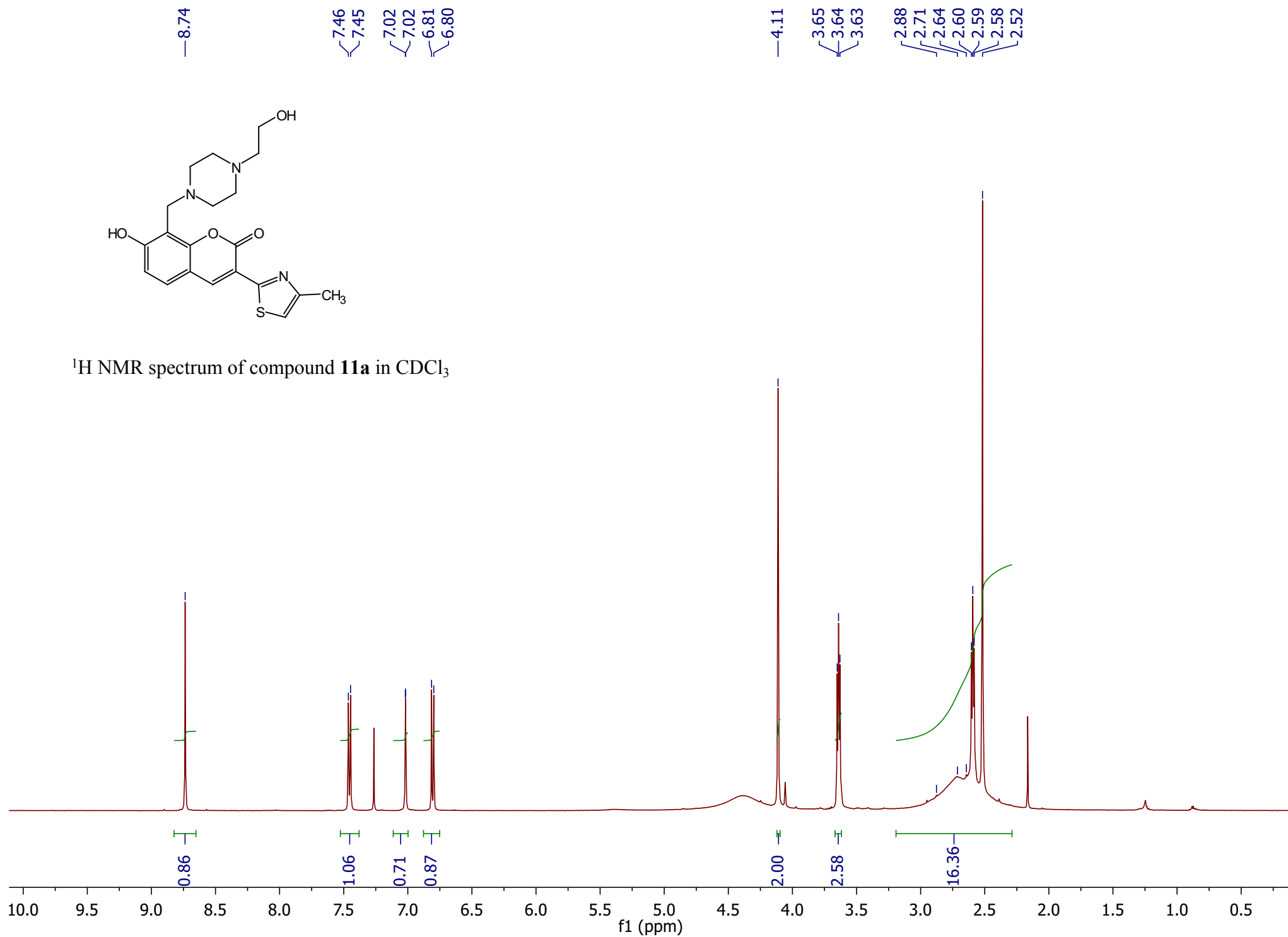


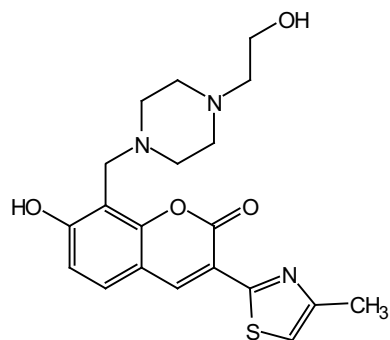
$^{13}\text{C}$  NMR spectrum of compound **10c** in DMSO- $\text{d}_6$



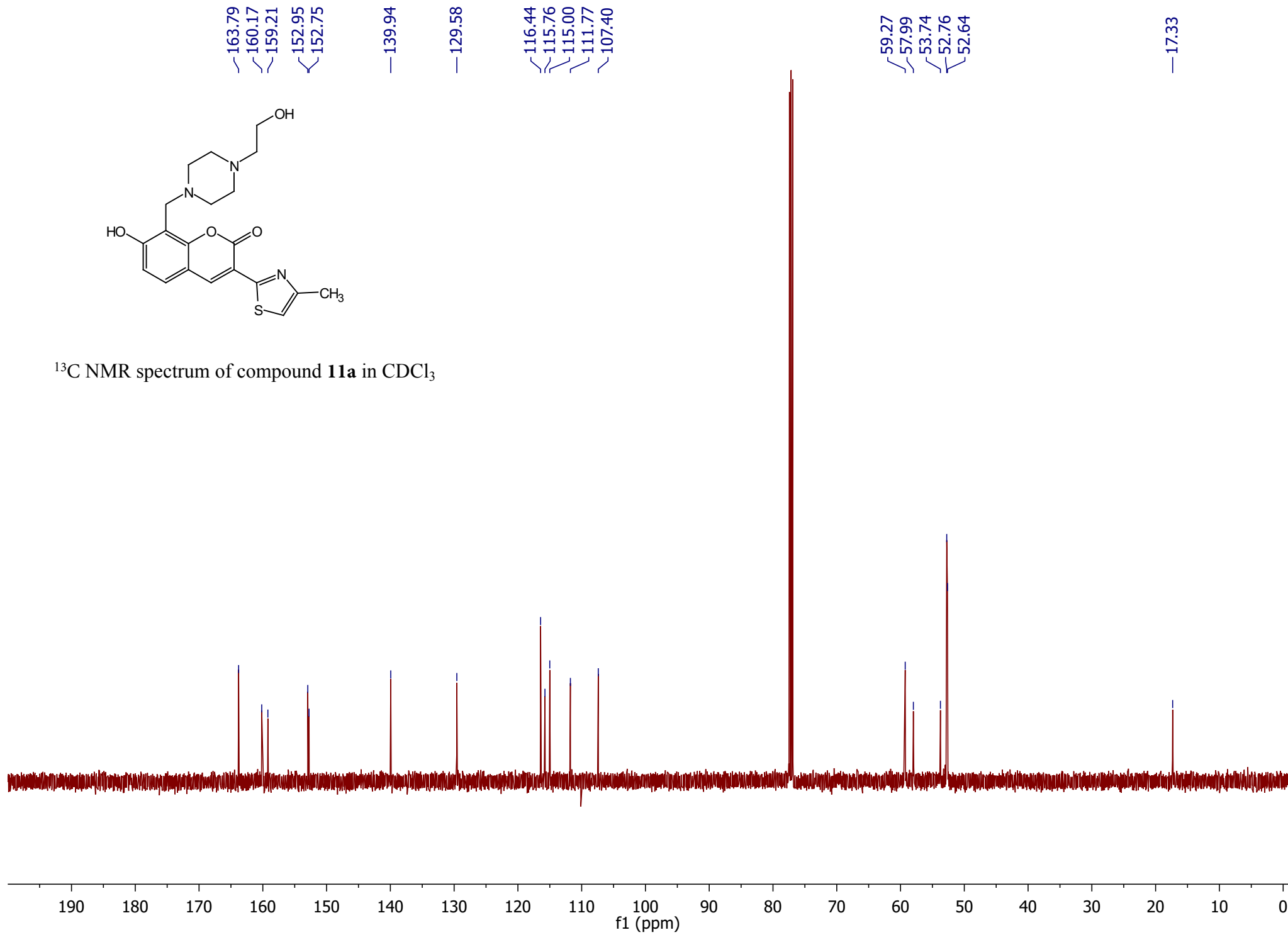


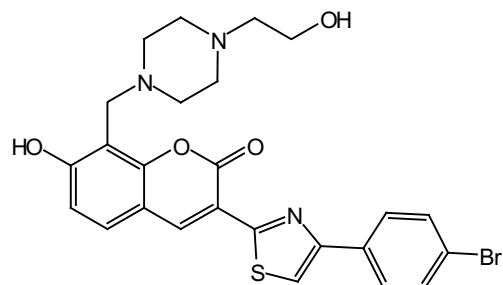
$^1\text{H}$  NMR spectrum of compound **11a** in  $\text{CDCl}_3$



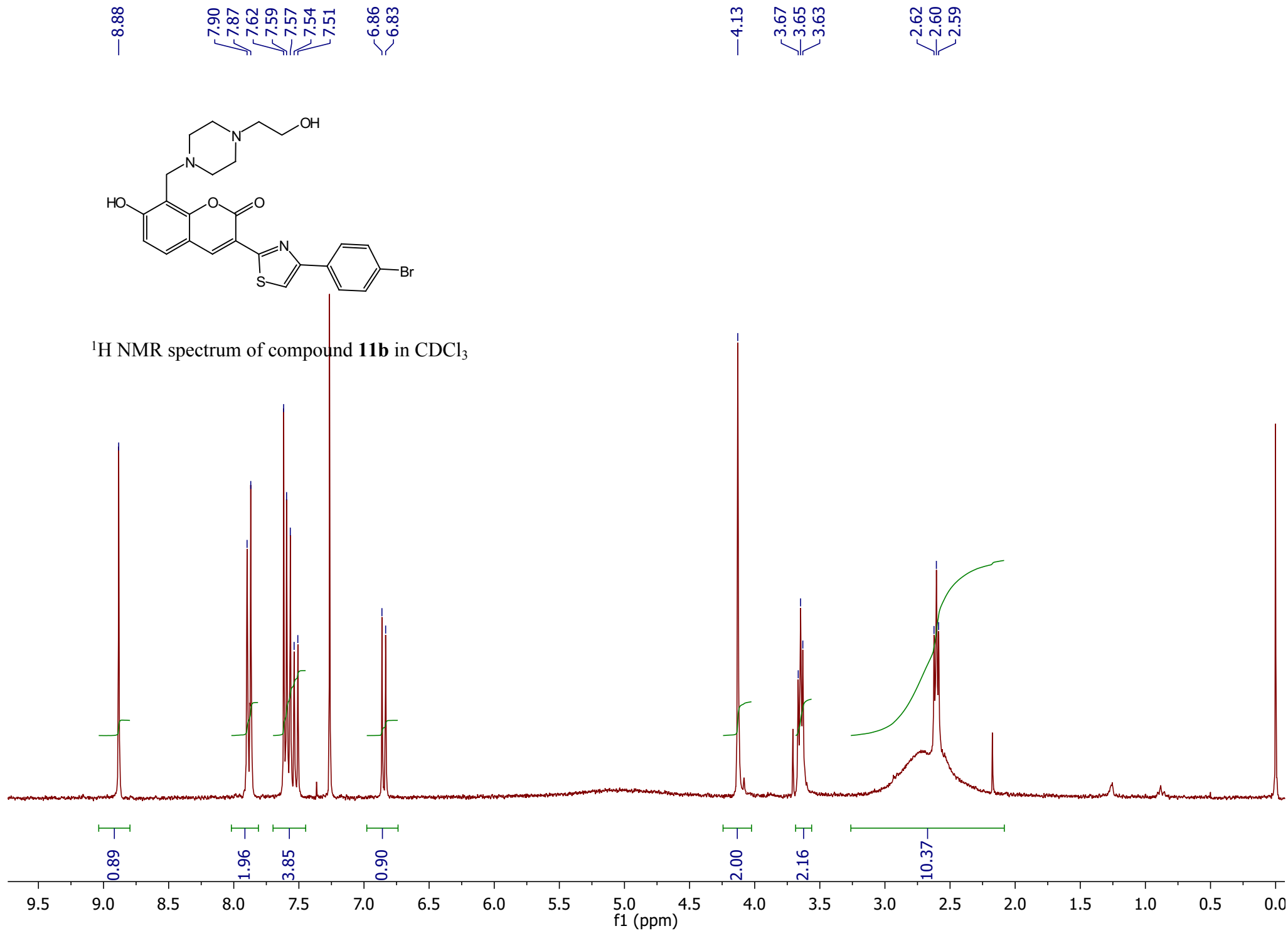


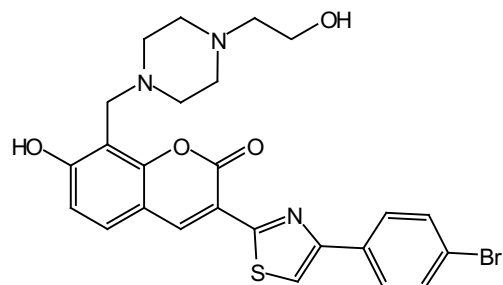
$^{13}\text{C}$  NMR spectrum of compound **11a** in  $\text{CDCl}_3$



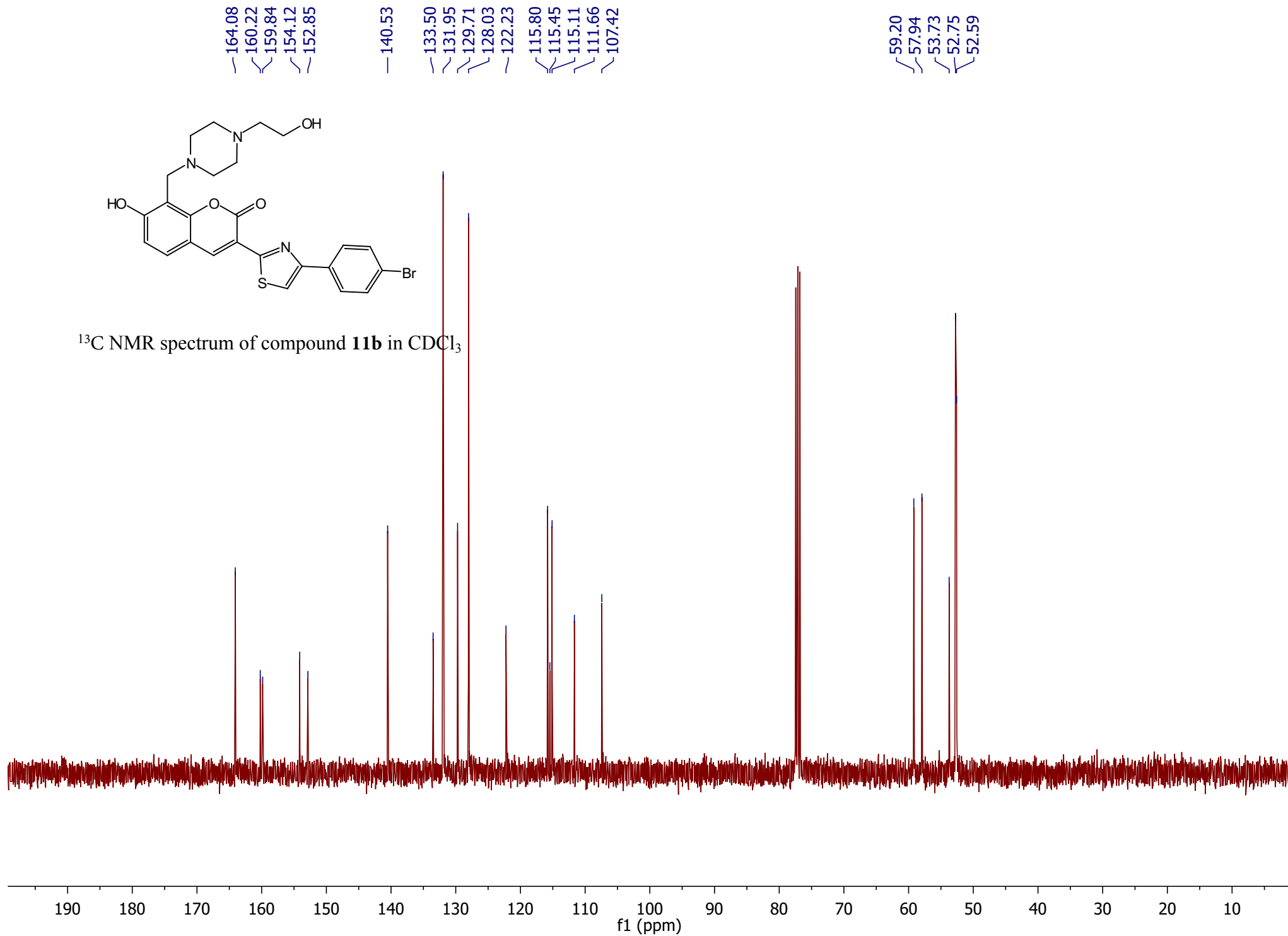


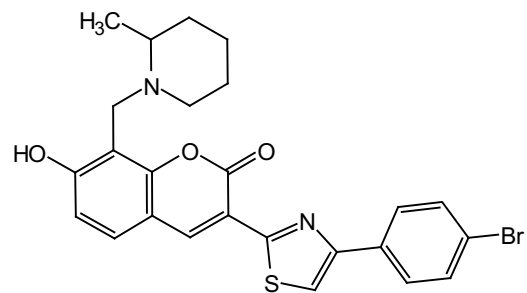
$^1\text{H}$  NMR spectrum of compound **11b** in  $\text{CDCl}_3$



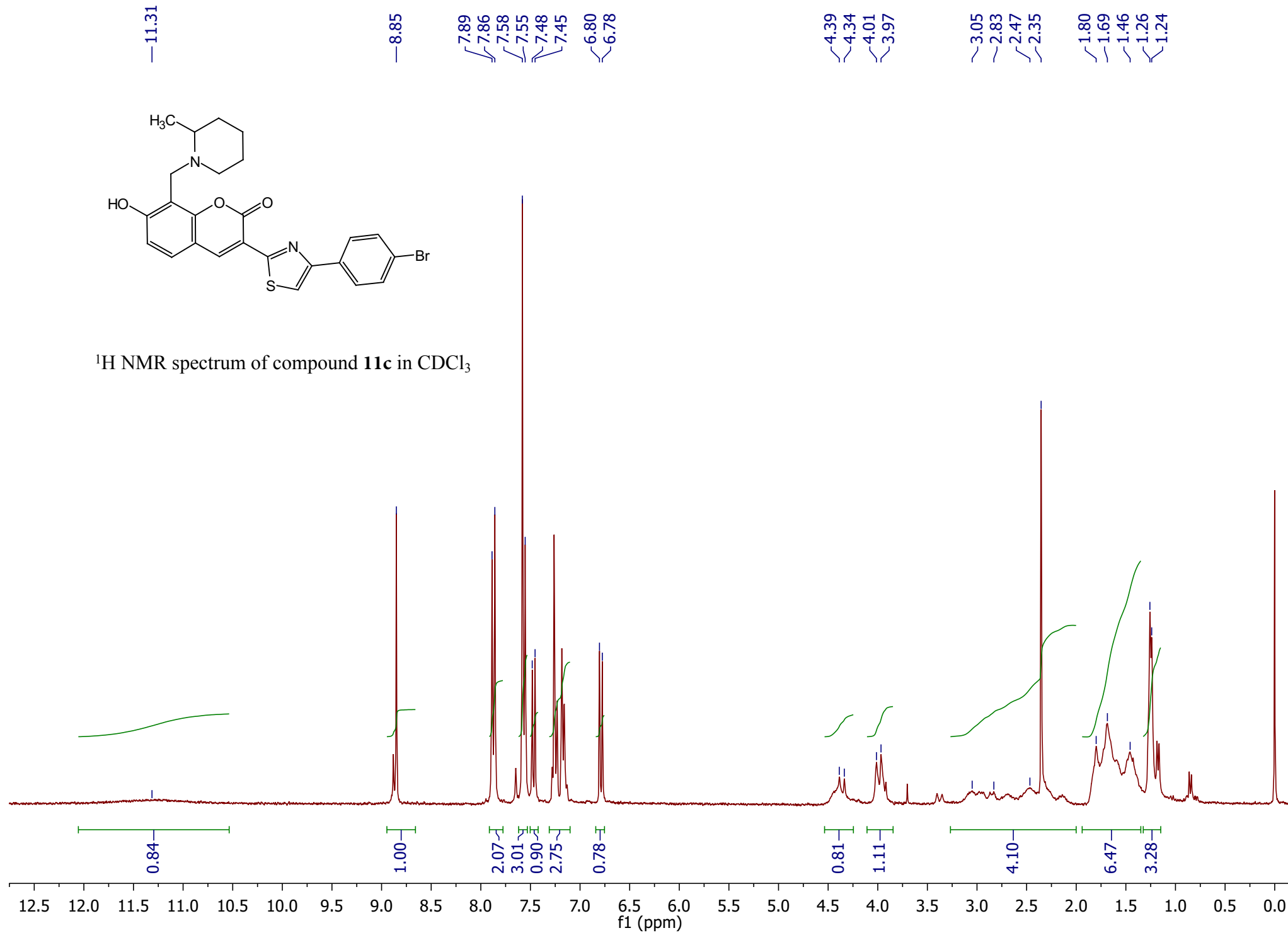


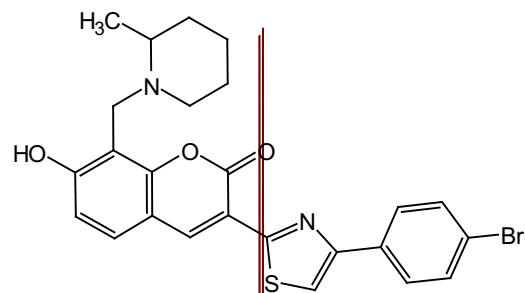
$^{13}\text{C}$  NMR spectrum of compound **11b** in  $\text{CDCl}_3$



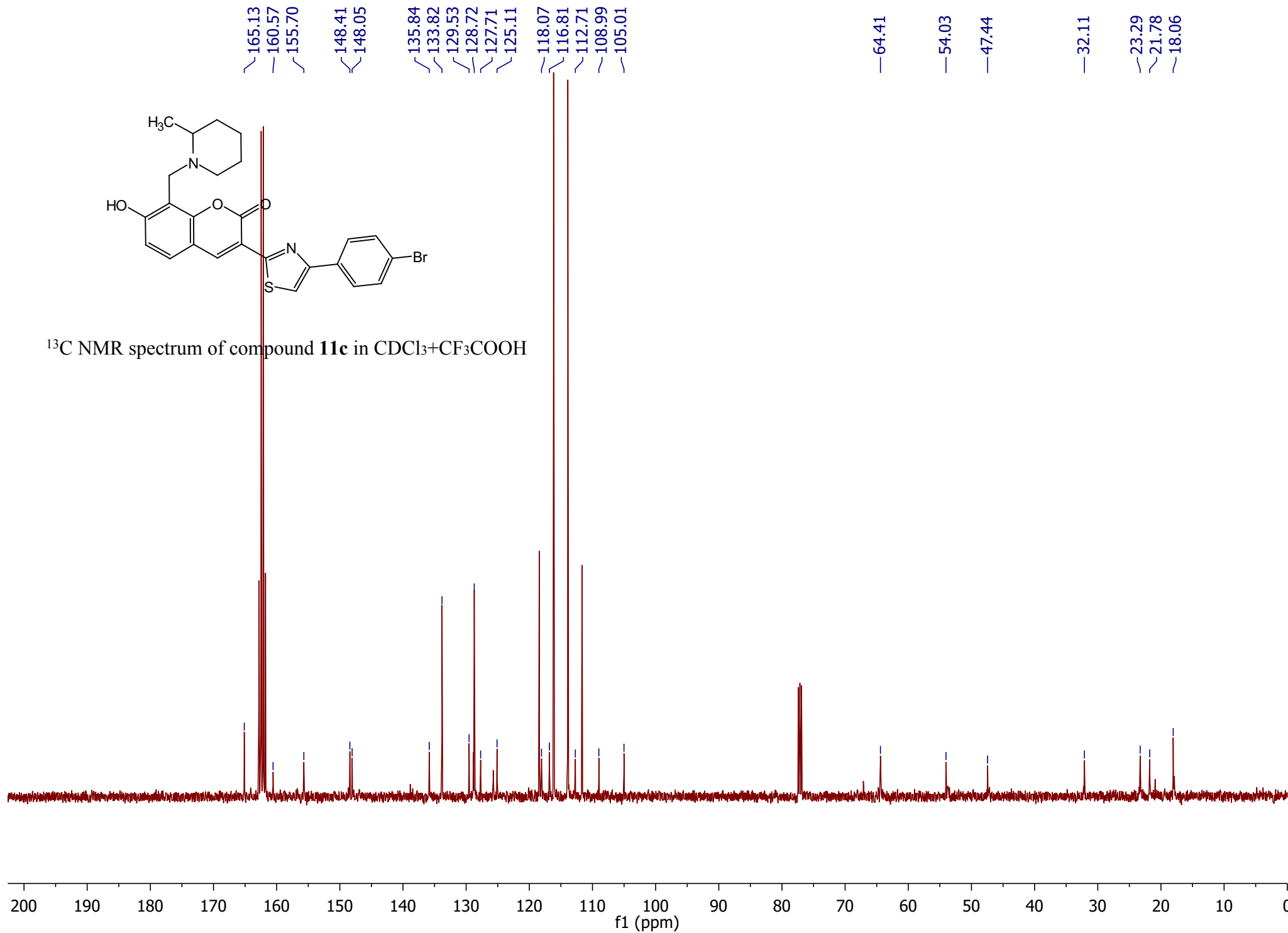


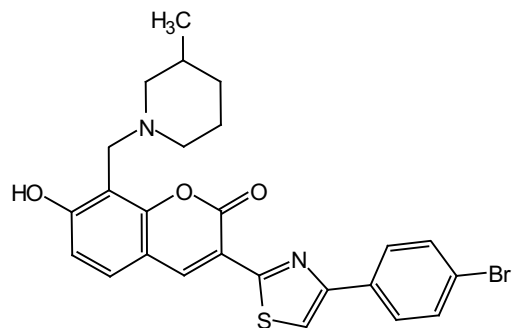
$^1\text{H}$  NMR spectrum of compound **11c** in  $\text{CDCl}_3$



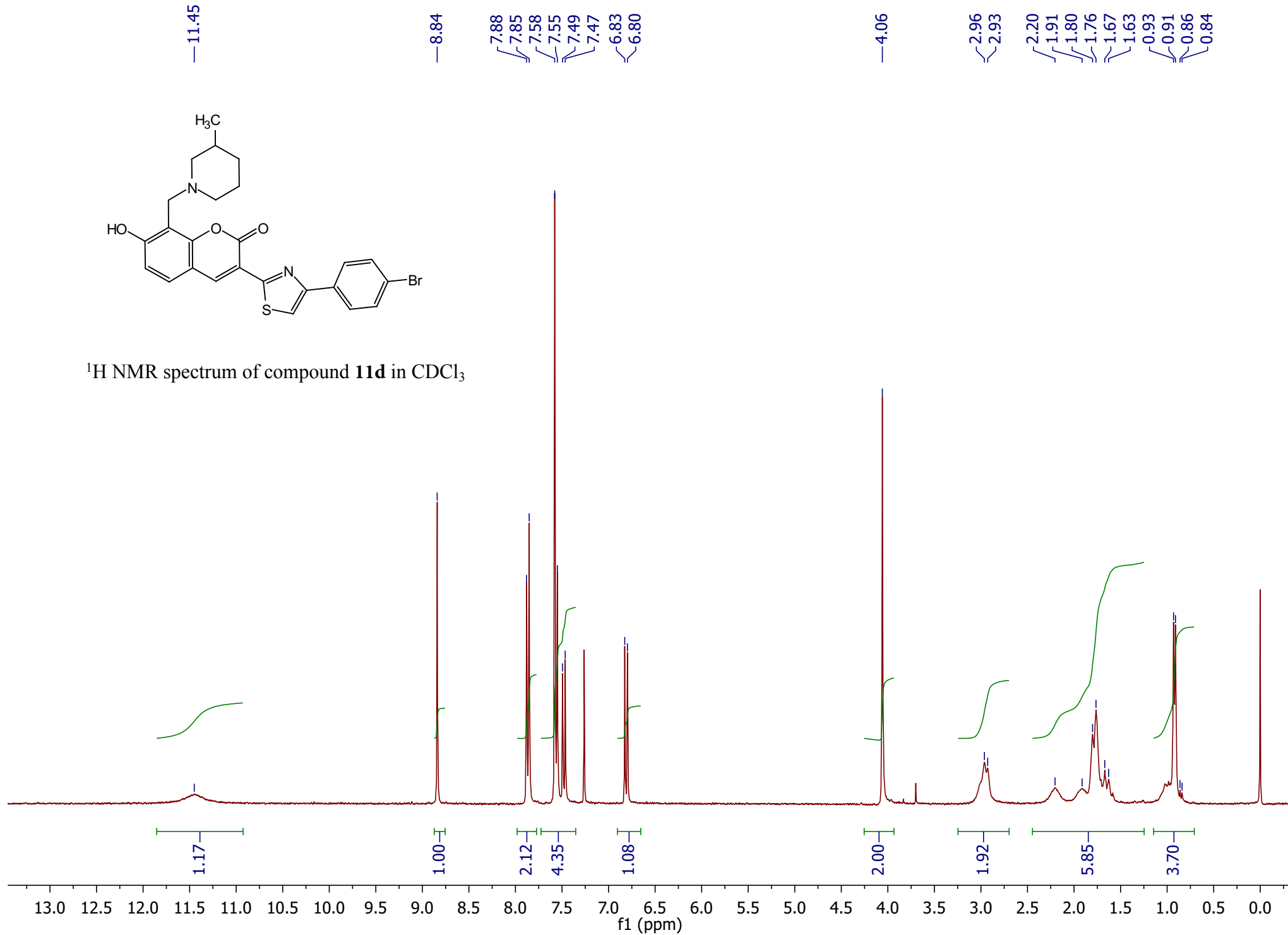


$^{13}\text{C}$  NMR spectrum of compound **11c** in  $\text{CDCl}_3 + \text{CF}_3\text{COOH}$

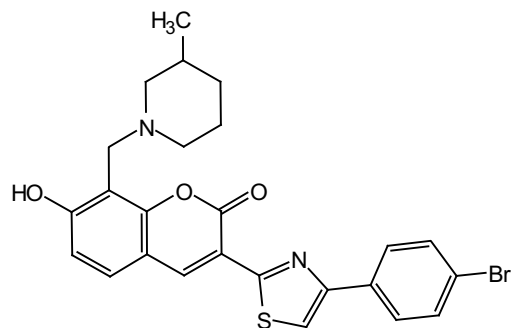




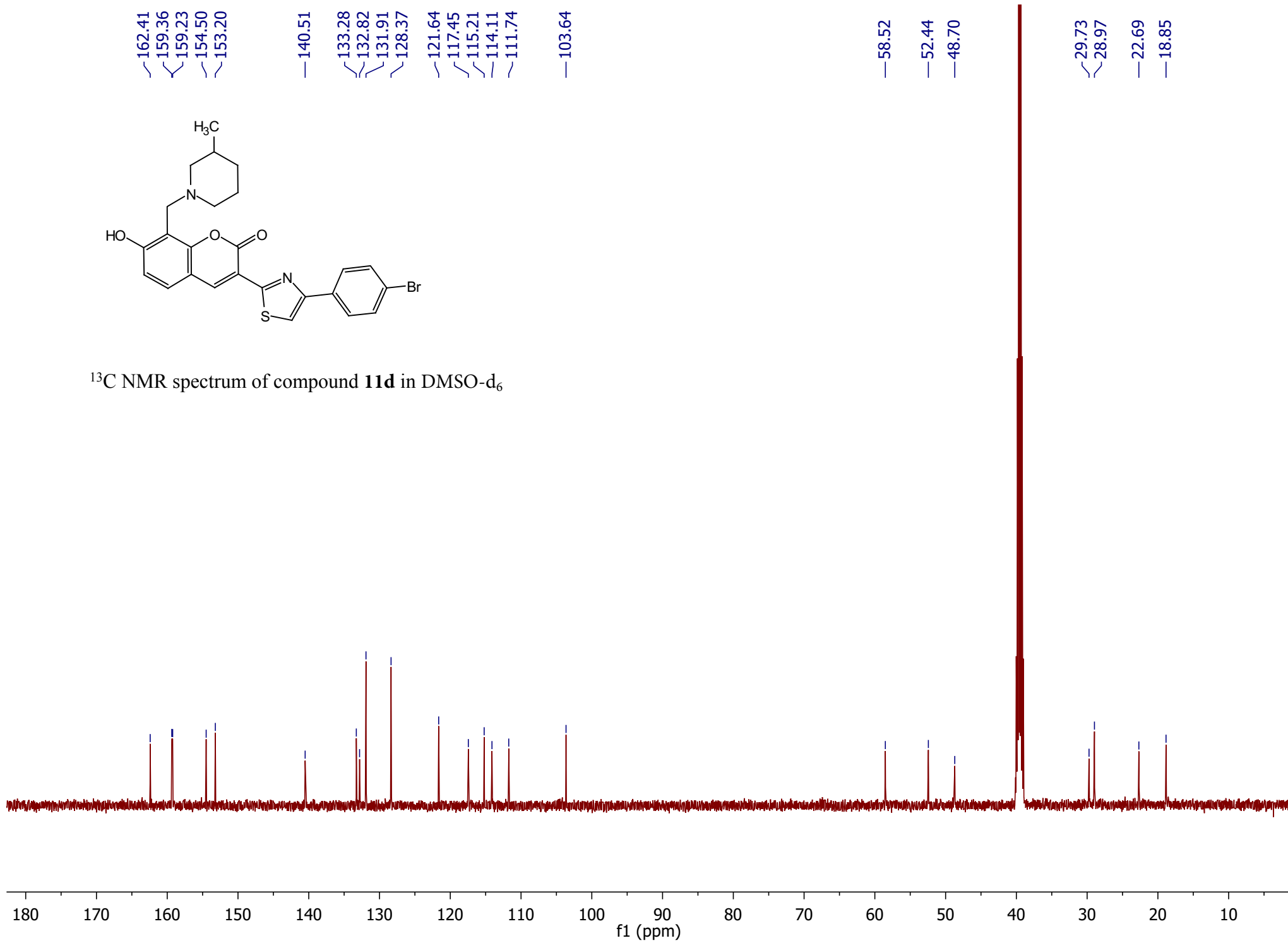
$^1\text{H}$  NMR spectrum of compound **11d** in  $\text{CDCl}_3$

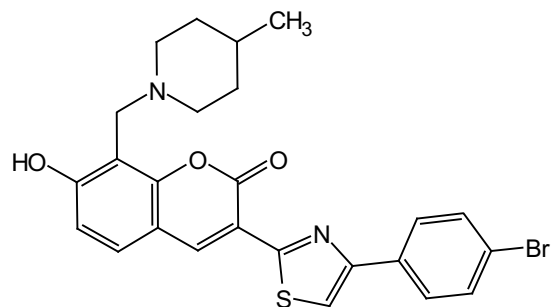




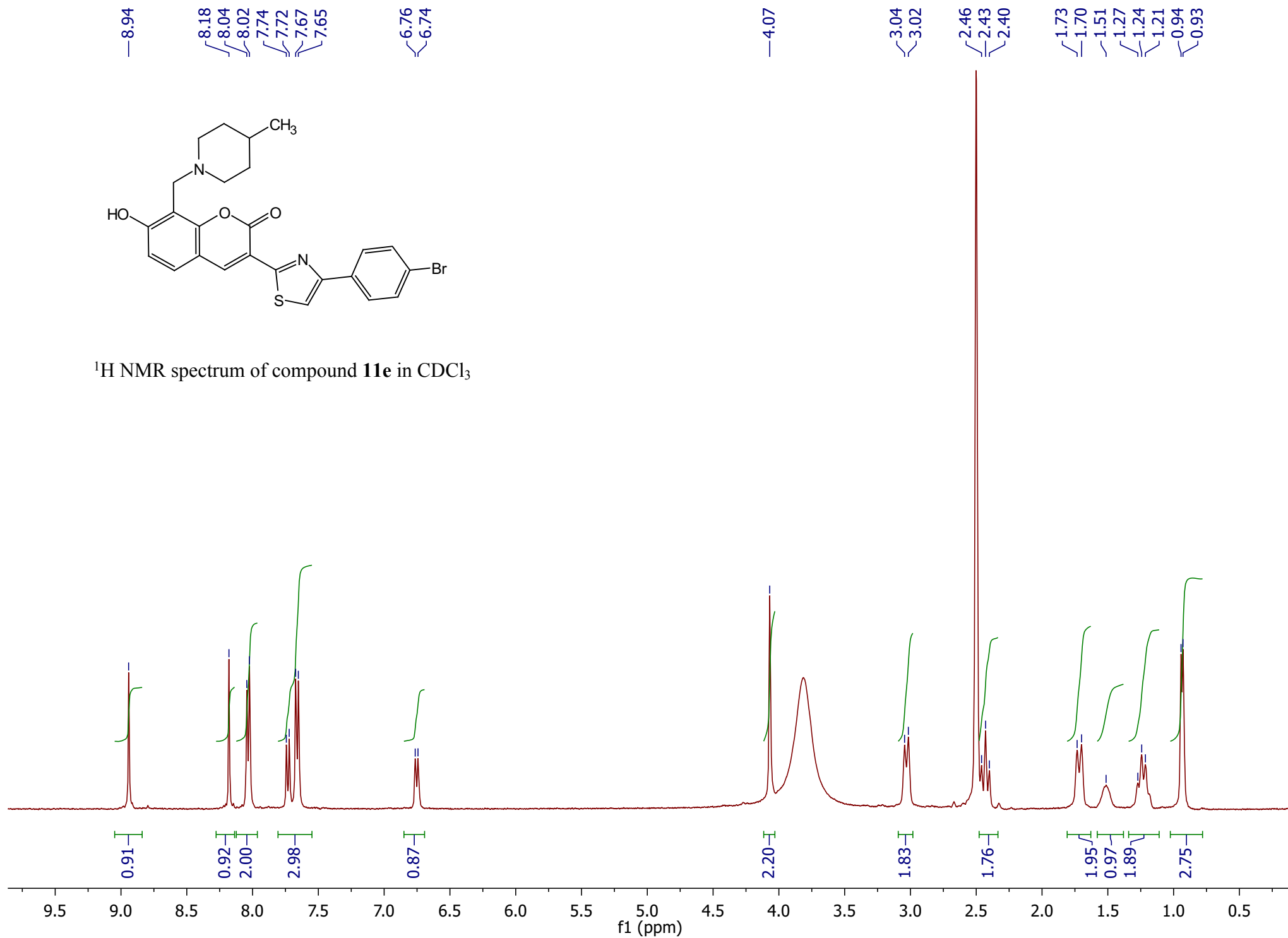


$^{13}\text{C}$  NMR spectrum of compound **11d** in  $\text{DMSO-d}_6$

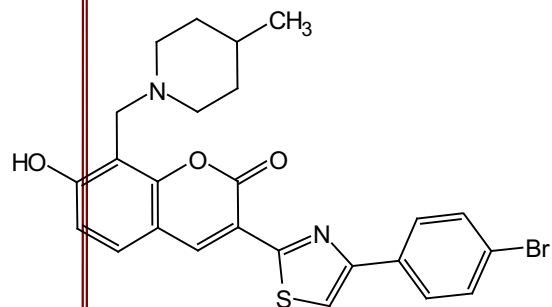




$^1\text{H}$  NMR spectrum of compound **11e** in  $\text{CDCl}_3$



165.34  
164.93  
160.58  
155.65  
148.35  
148.05  
135.83  
133.77  
128.69  
127.69  
125.02  
117.98  
116.83  
112.52  
108.81  
104.49

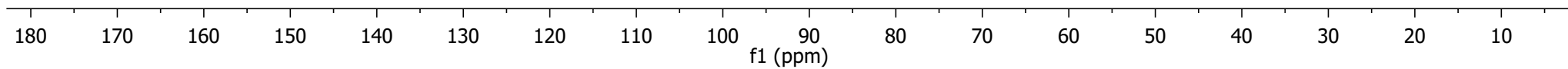


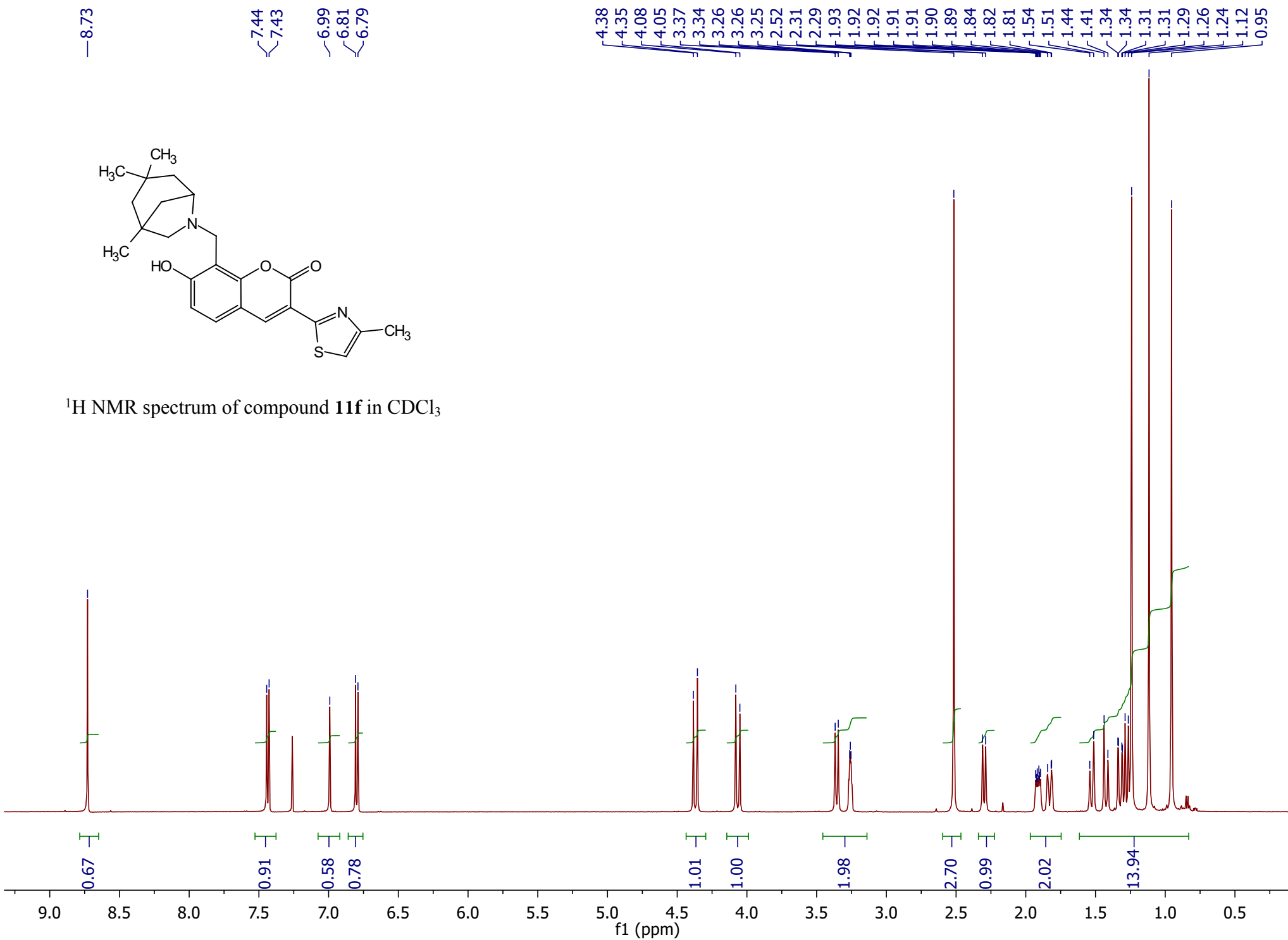
$^{13}\text{C}$  NMR spectrum of compound **11e** in  $\text{CDCl}_3 + \text{CF}_3\text{COOH}$

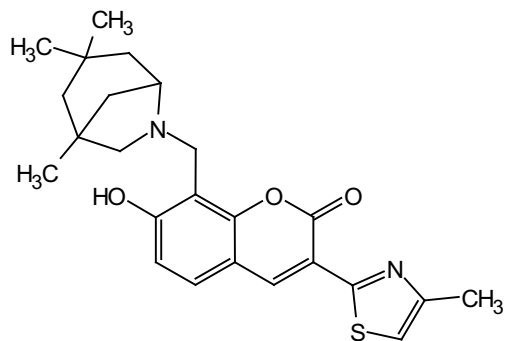
55.27  
50.27

31.63  
29.01

20.29







$^{13}\text{C}$  NMR spectrum of compound **11f** in  $\text{CDCl}_3$

