

Supporting Information

Bi(III)-catalyzed synthesis of furocoumarins *via* a three component reaction of arylglyoxal monohydrates, coumarins and *N*-substituted anilines

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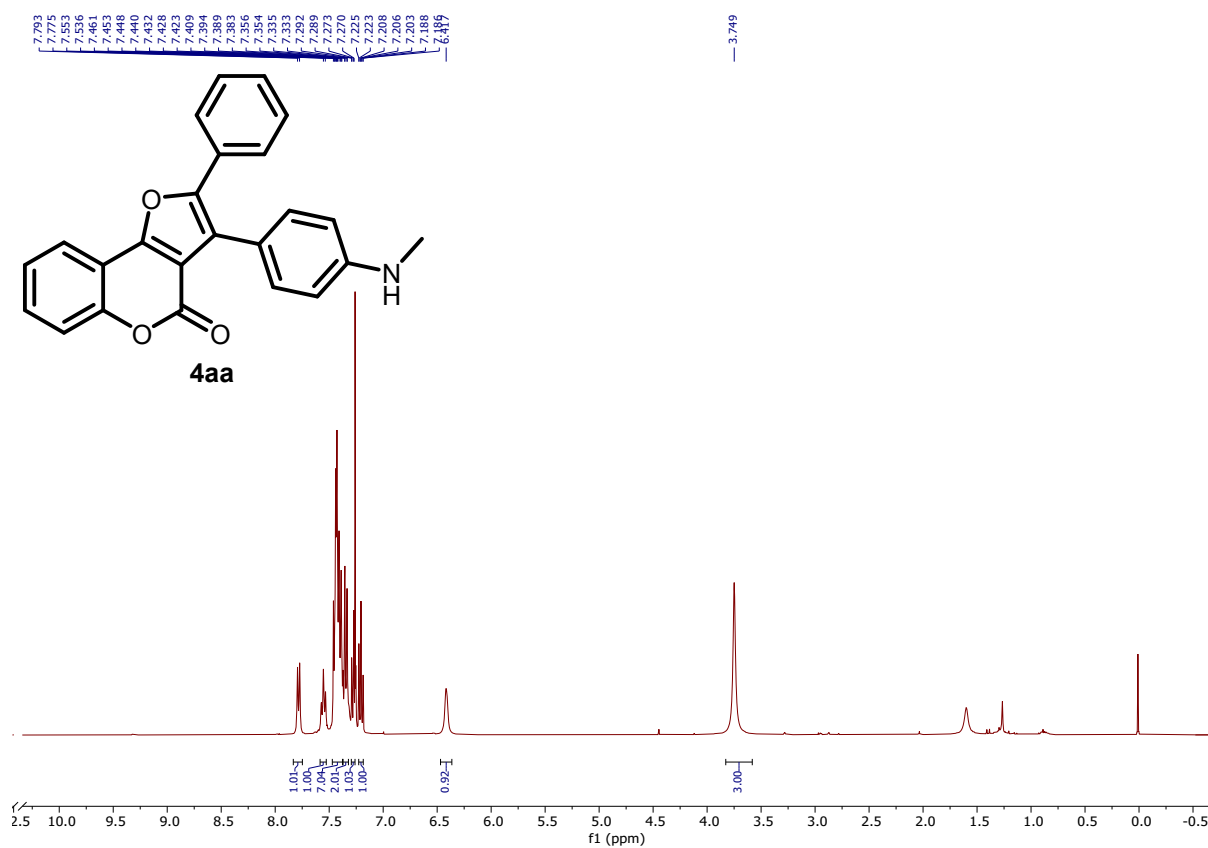
Table S1 Reaction optimization studies to form **7** & **8**^{a,b}

1a + 2a + 6a $\xrightarrow[\text{Solvent, Temp}^r]{\text{Lewis Acid}}$ 7aaa + 8aaa (0 %)

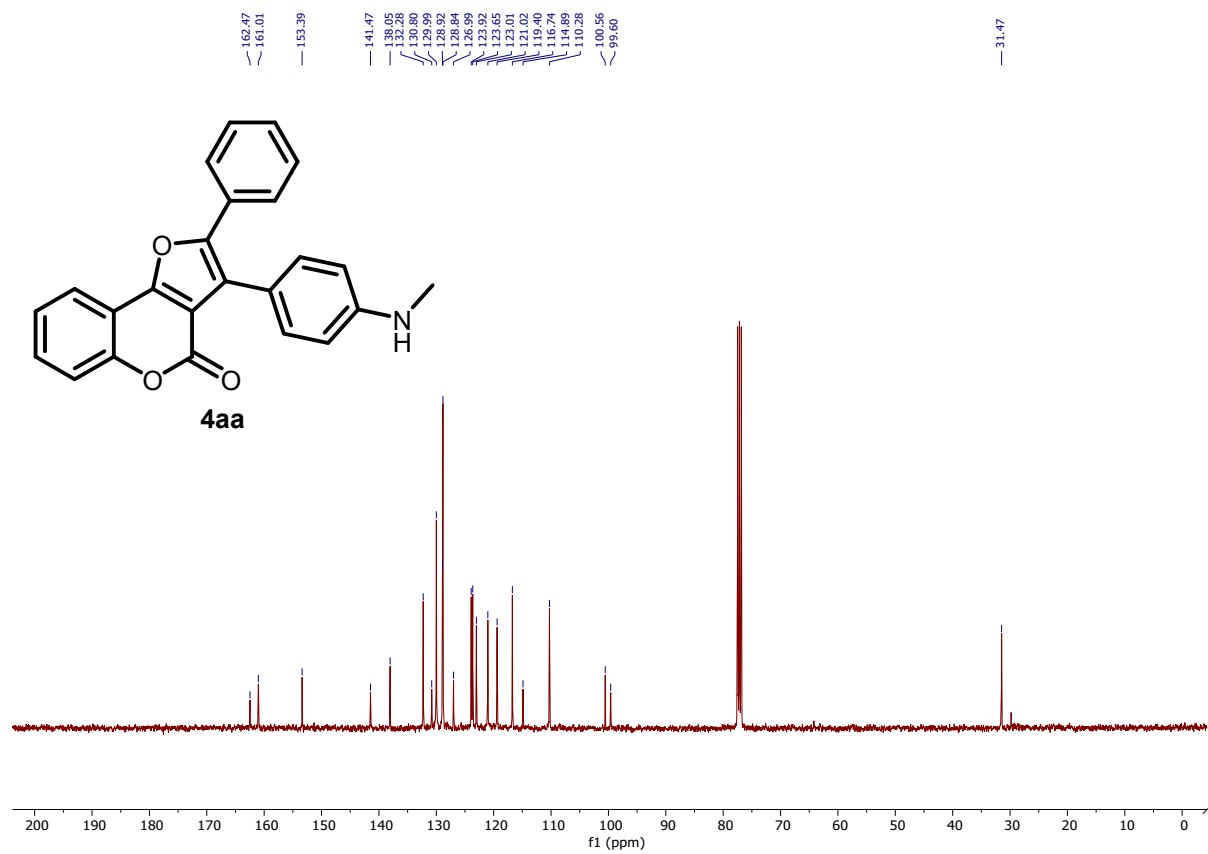
Entry	Lewis acid (20 mol%)	Solvent	Temp (°C)	Yield of 7aaa (%) ^b
1	--	DCE	r.t.	24
2	--	DCE	90	28
3	--	DCE	120	28
4	Bi(OTf) ₃	DCE	r.t.	29
5	Bi(OTf) ₃	DCE	90	44
6	Bi(OTf) ₃	DCE	120	44
7	AlCl ₃	DCE	90	35
8	BiCl ₃	DCE	90	38
9	FeCl ₃	DCE	90	28
10	BF ₃ .OEt ₂	DCE	90	c.r.m. ^c
11	BF ₃ .OEt ₂	Toluene	90	c.r.m. ^c

^aReaction conditions: A mixture of **1a** (0.5 mmol), **2a** (0.5 mmol) and **6** (0.6 mmol) in the presence of Lewis acid was stirred as mentioned above in the table. ^bIsolated yields after column chromatography. ^cc.r.m. = complex reaction mixture.

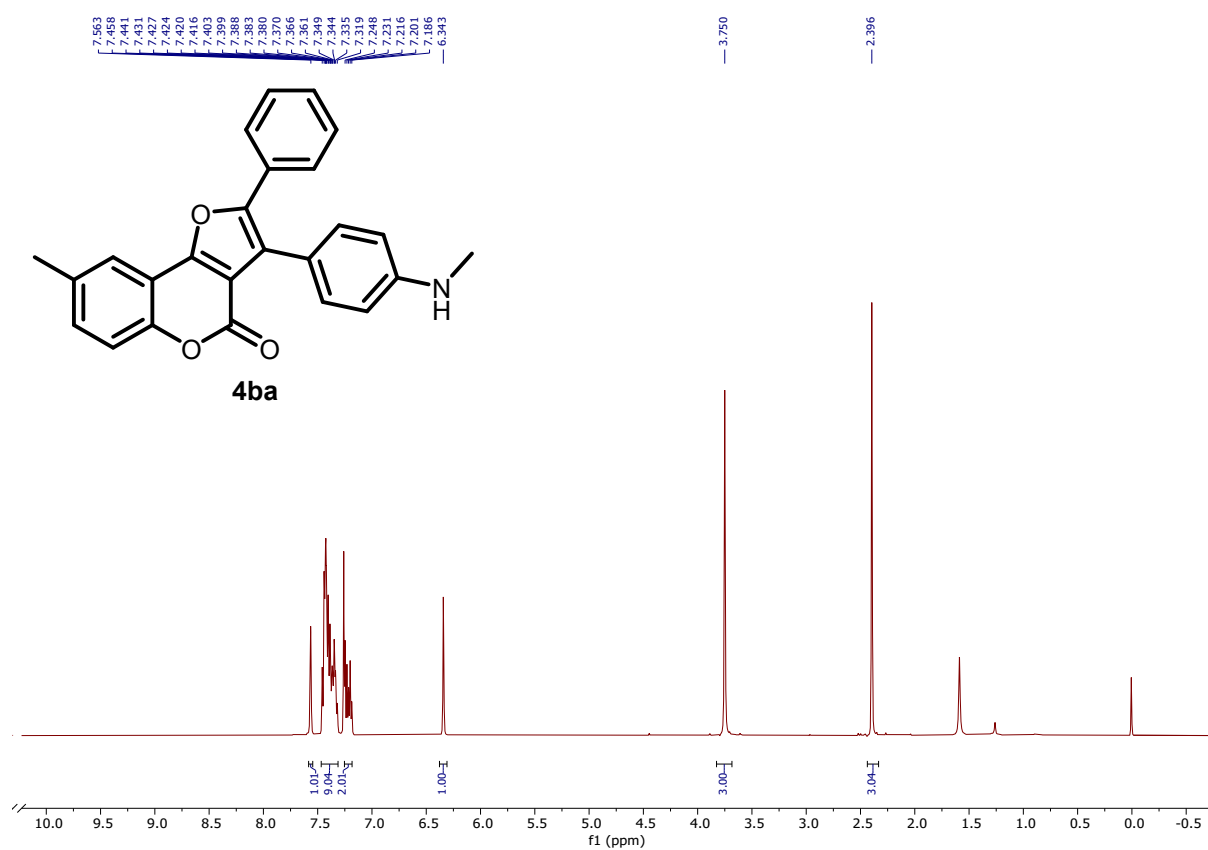
¹H-NMR (400 MHz, CDCl₃)



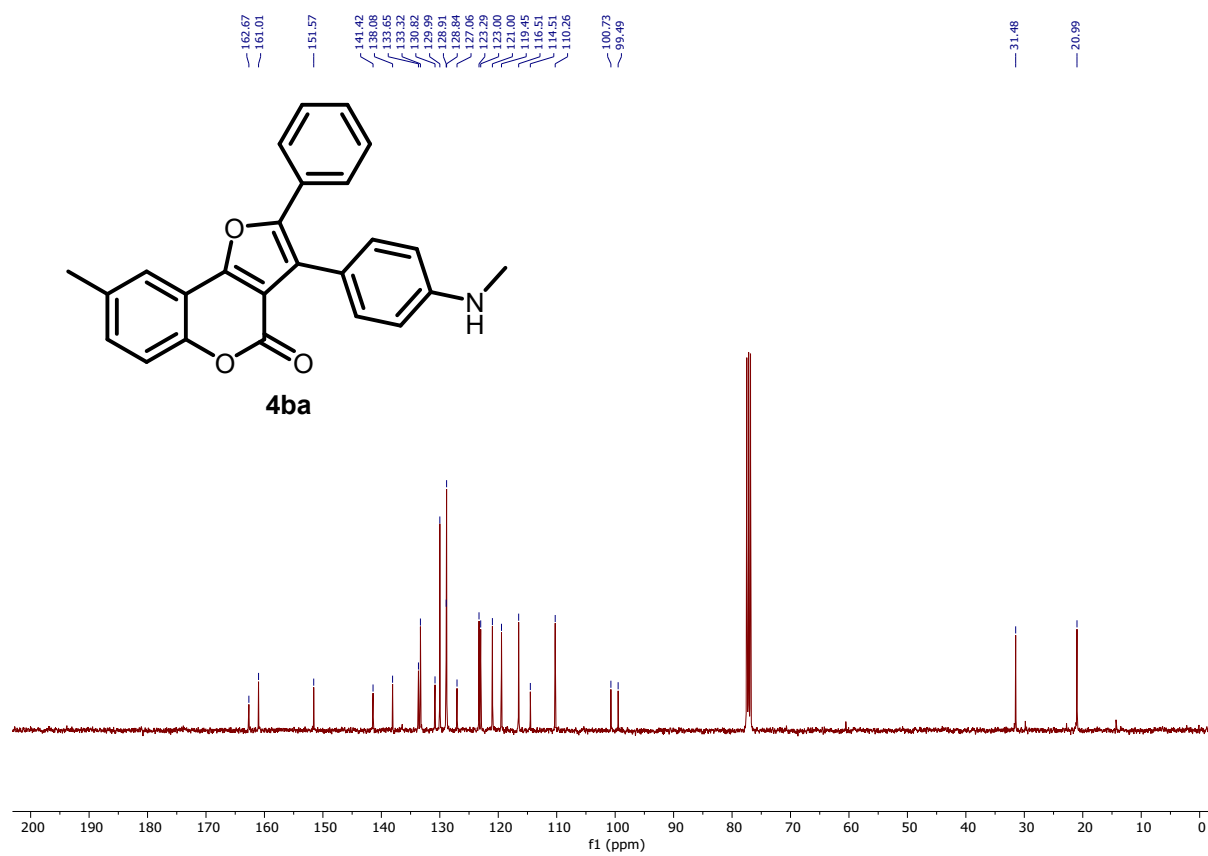
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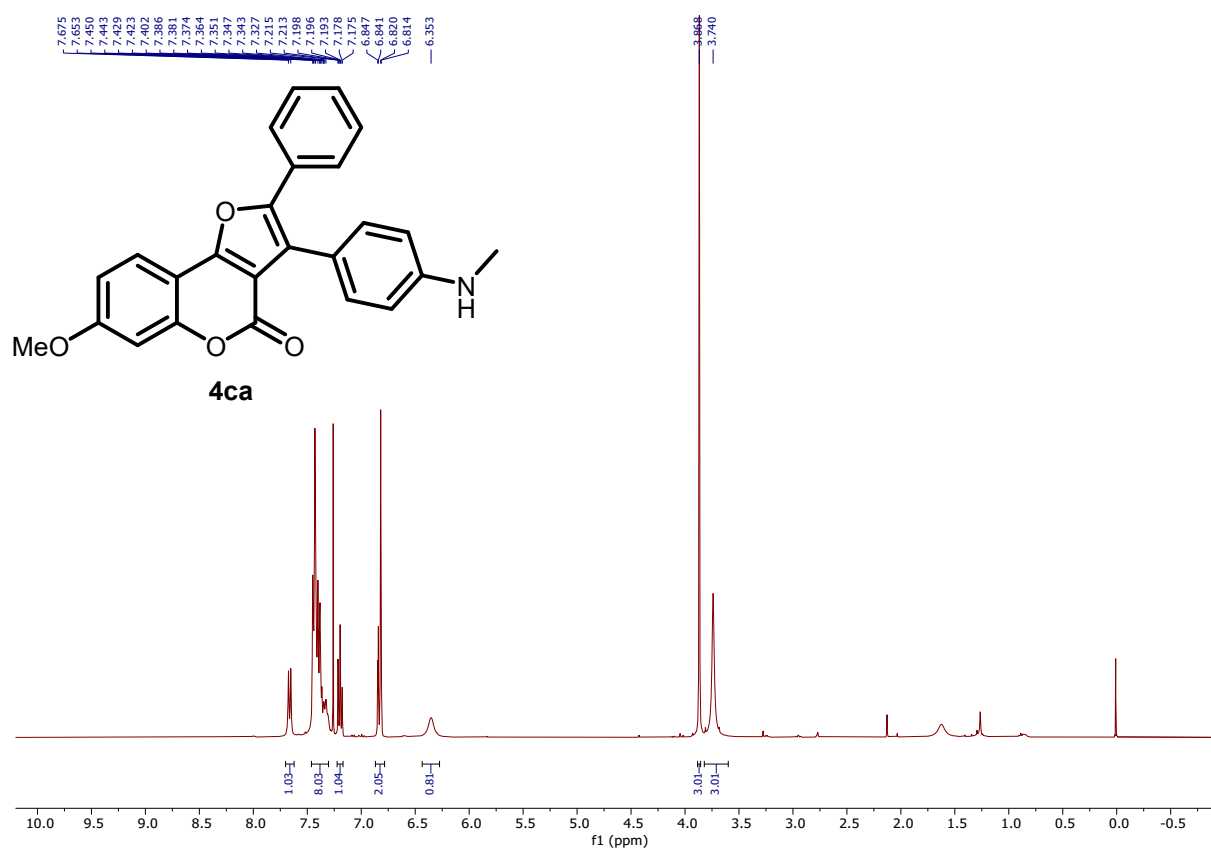
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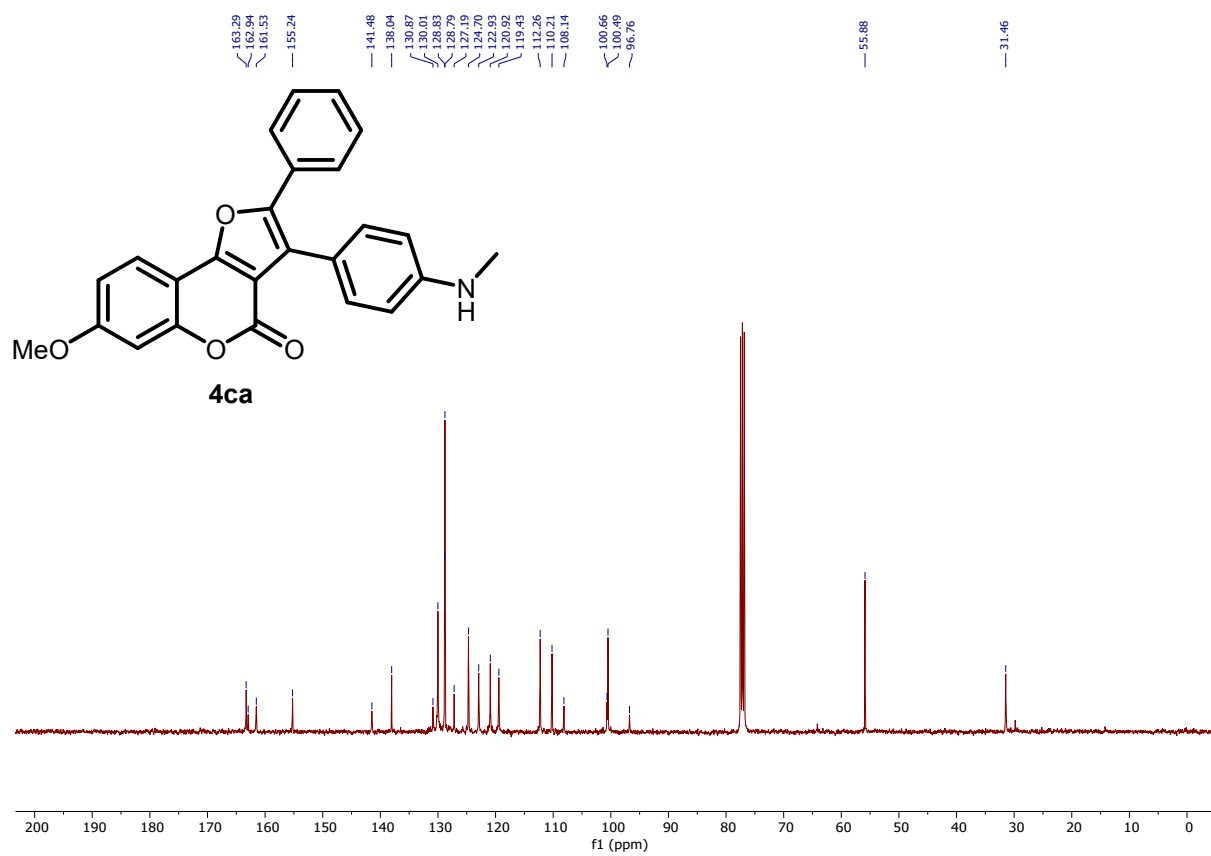
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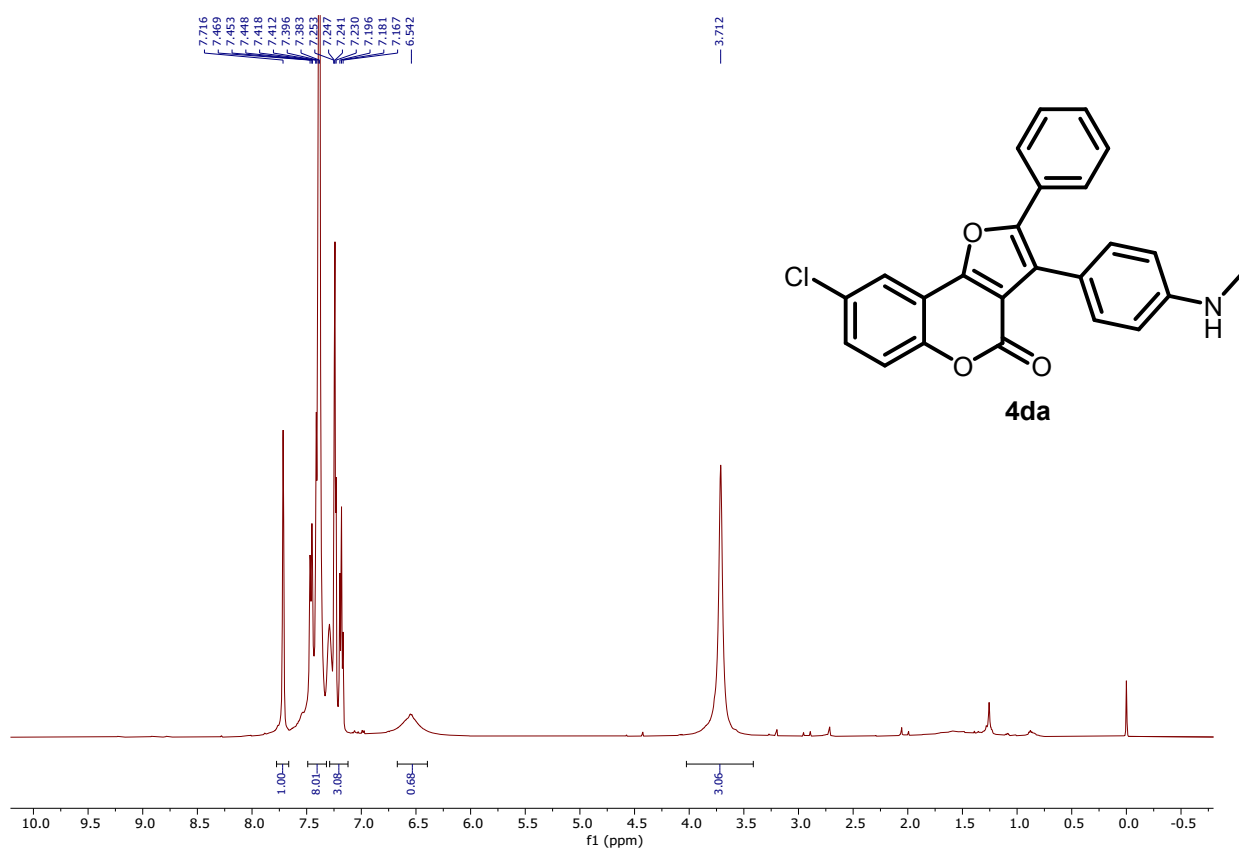
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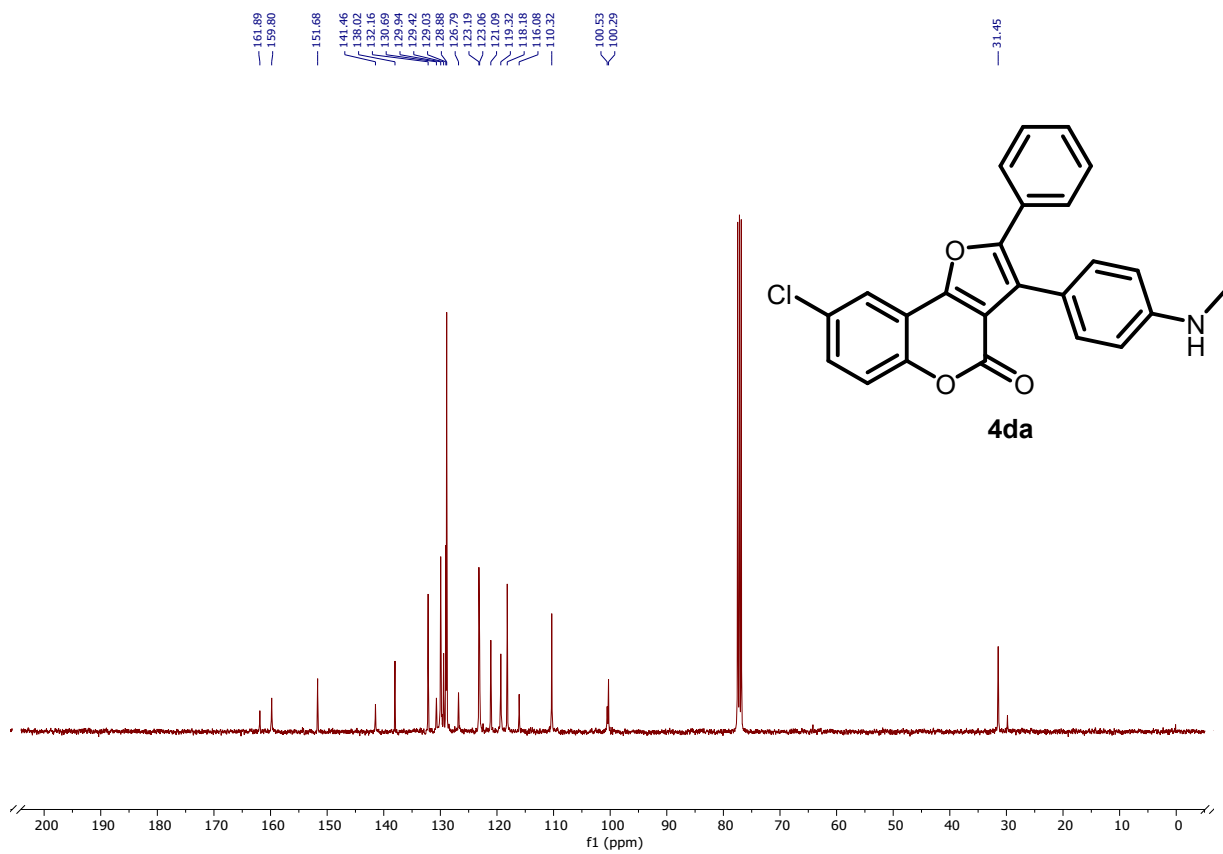
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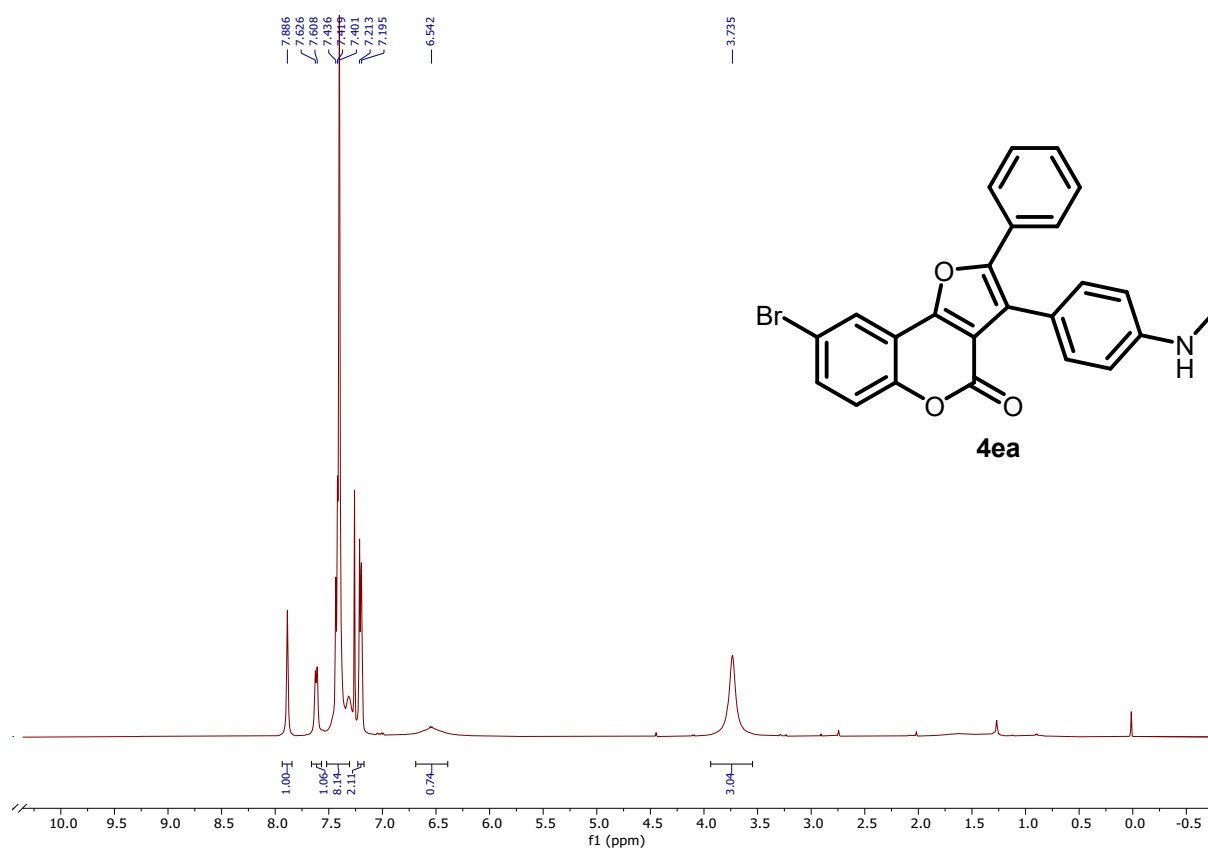
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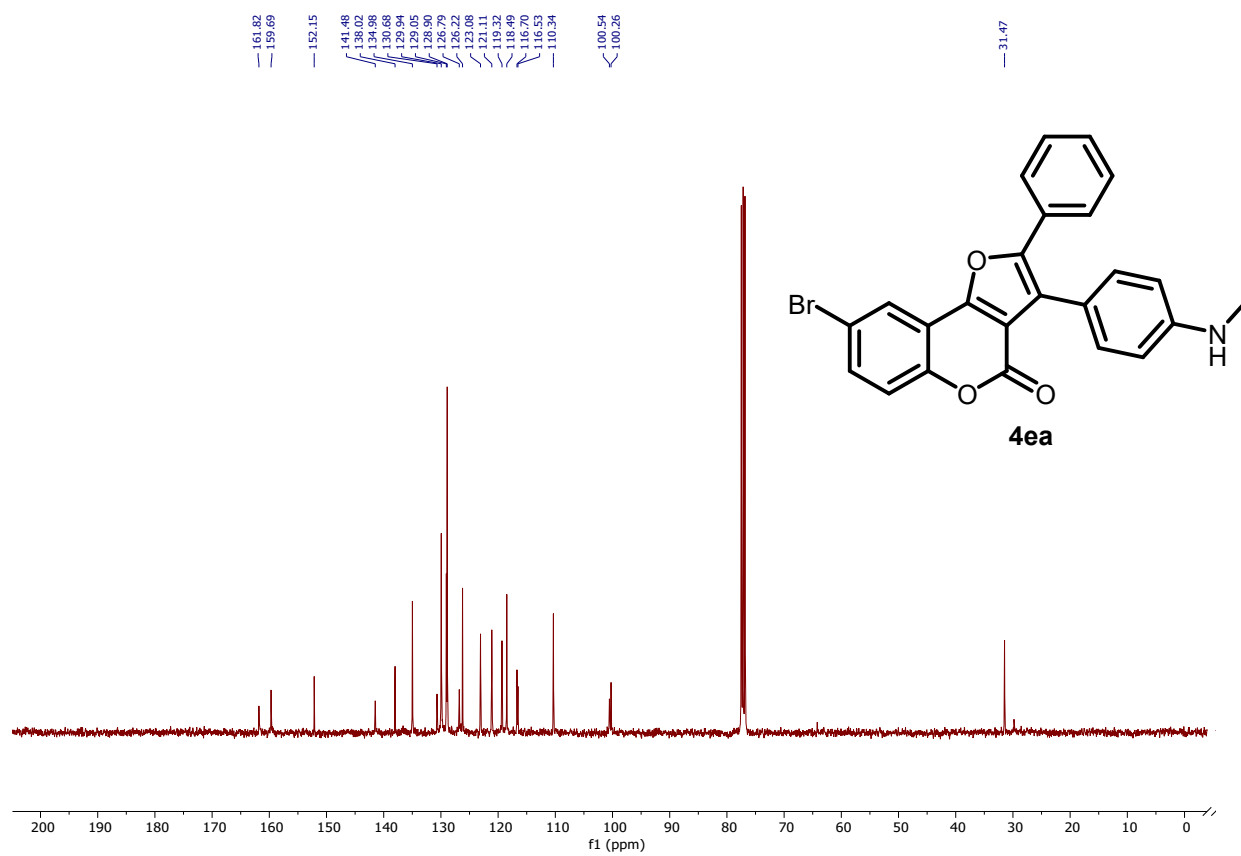
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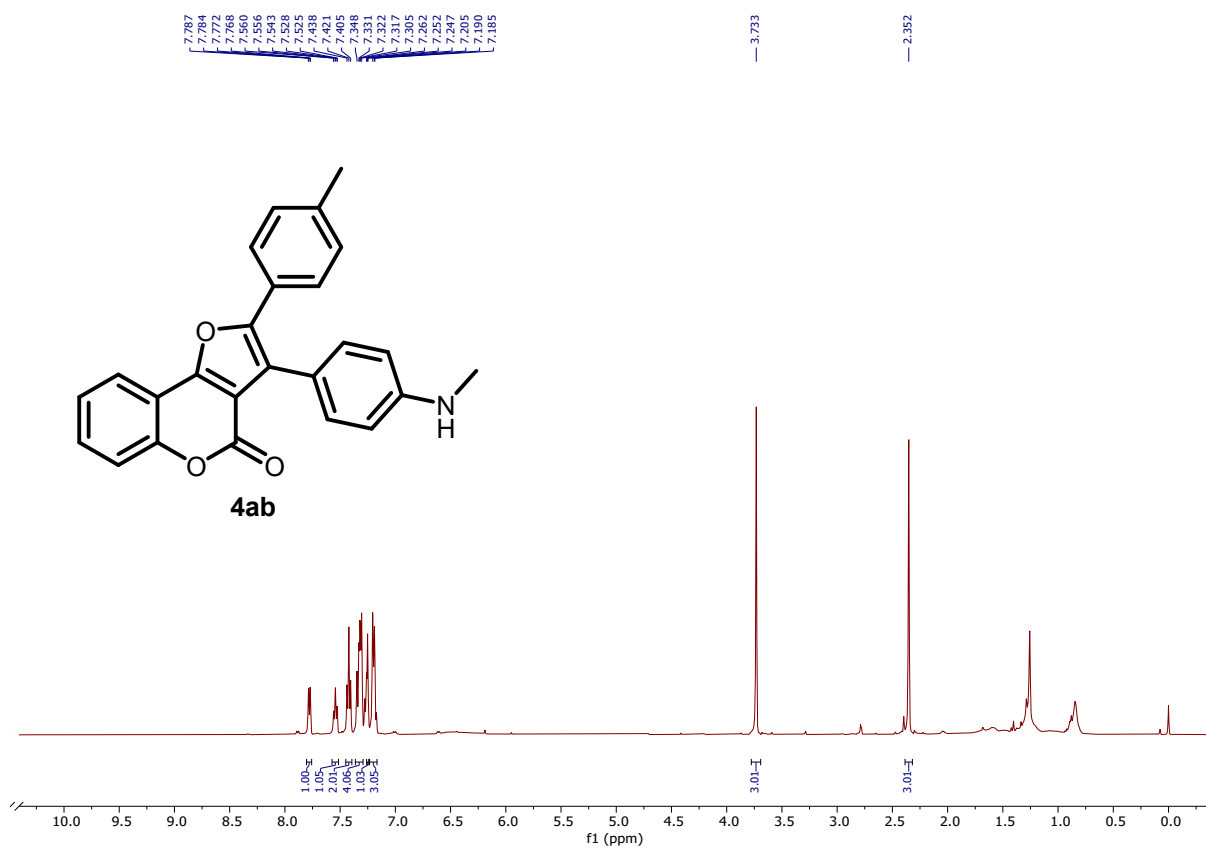
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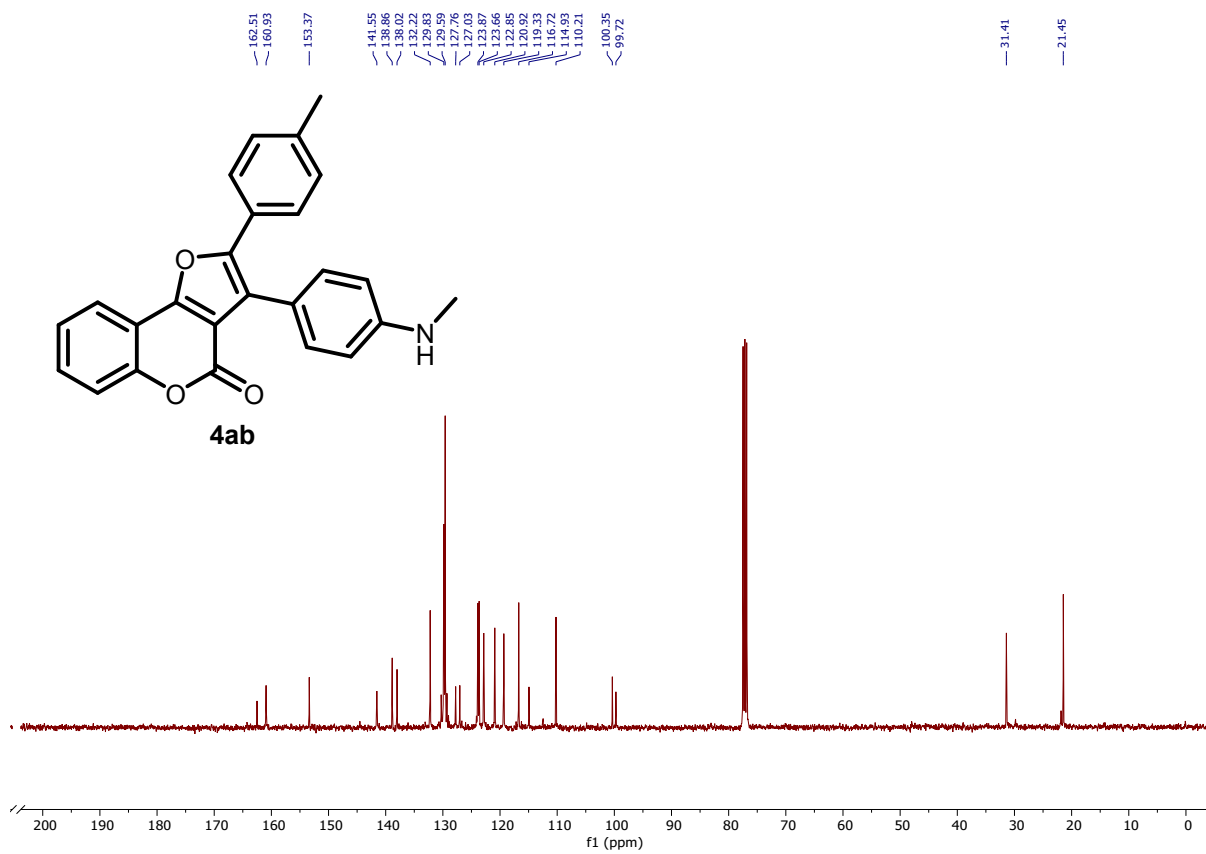
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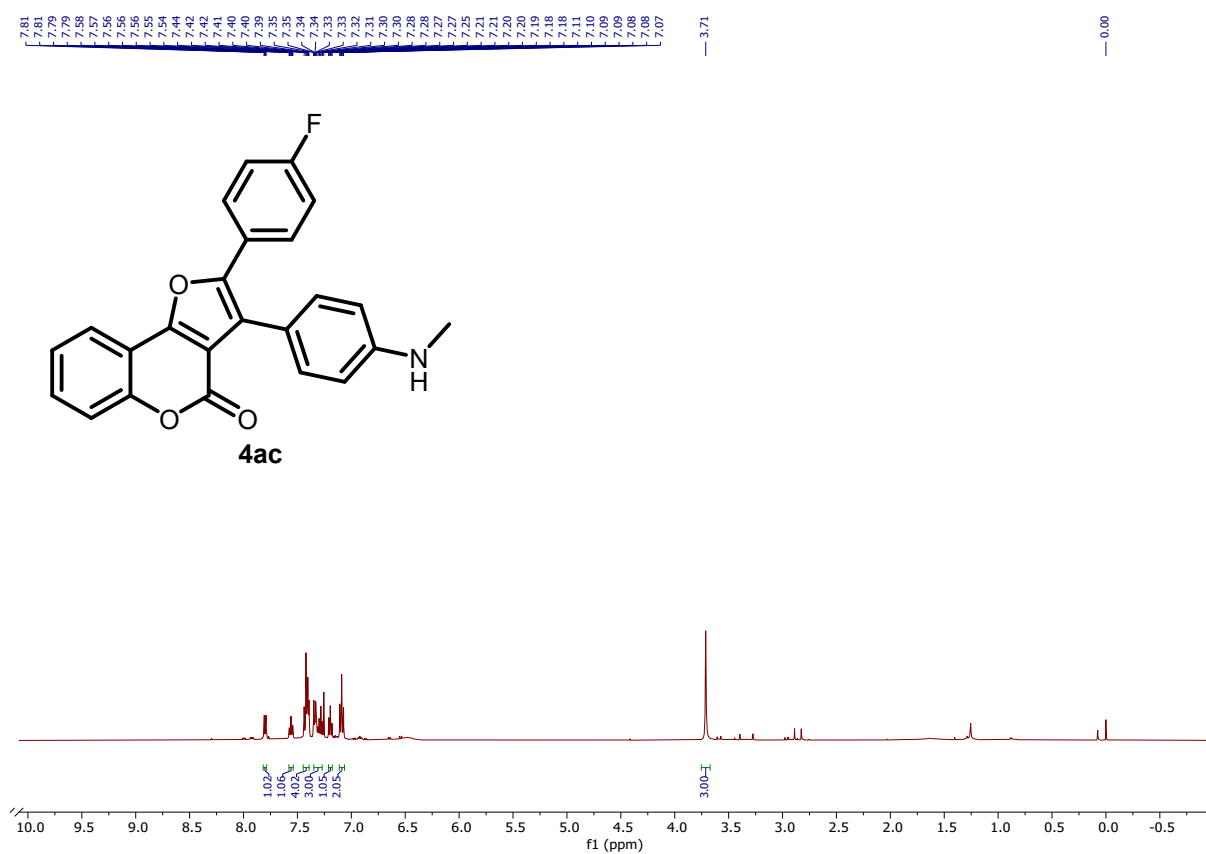
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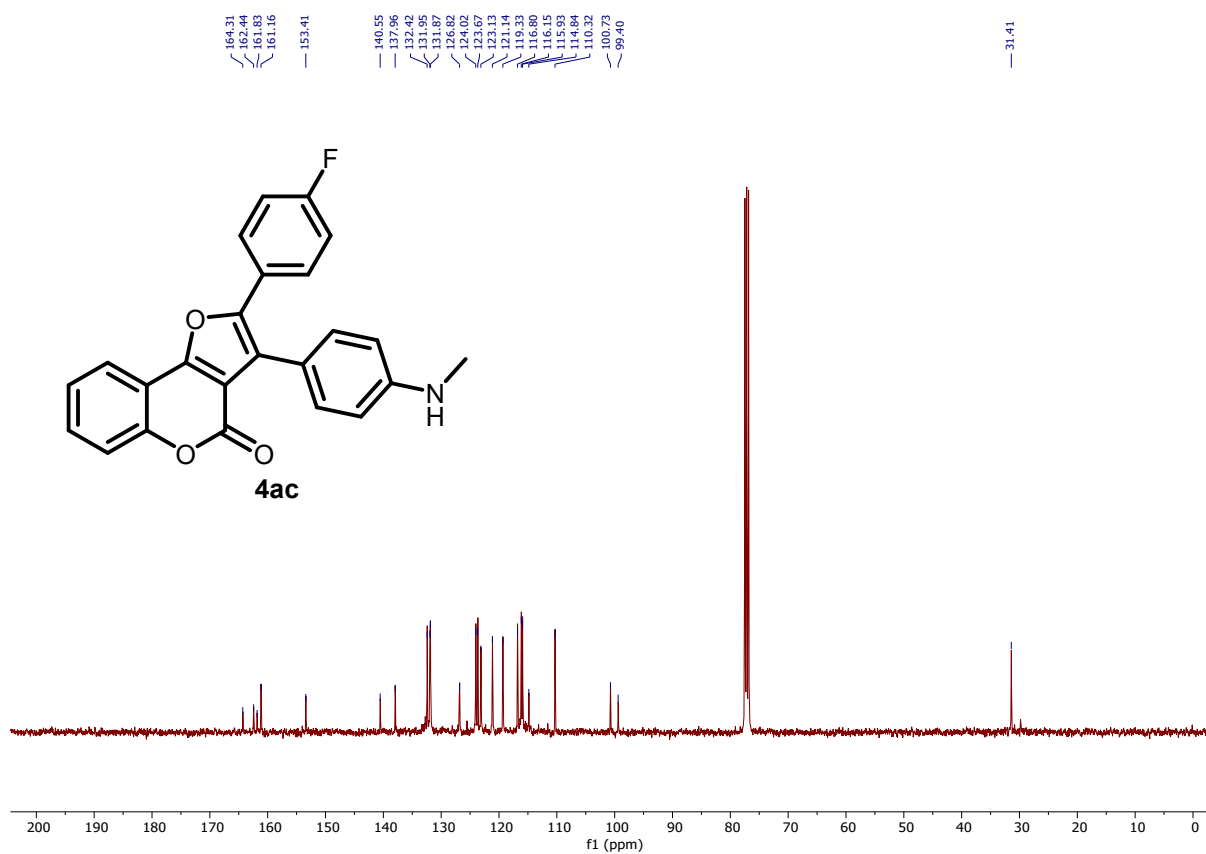
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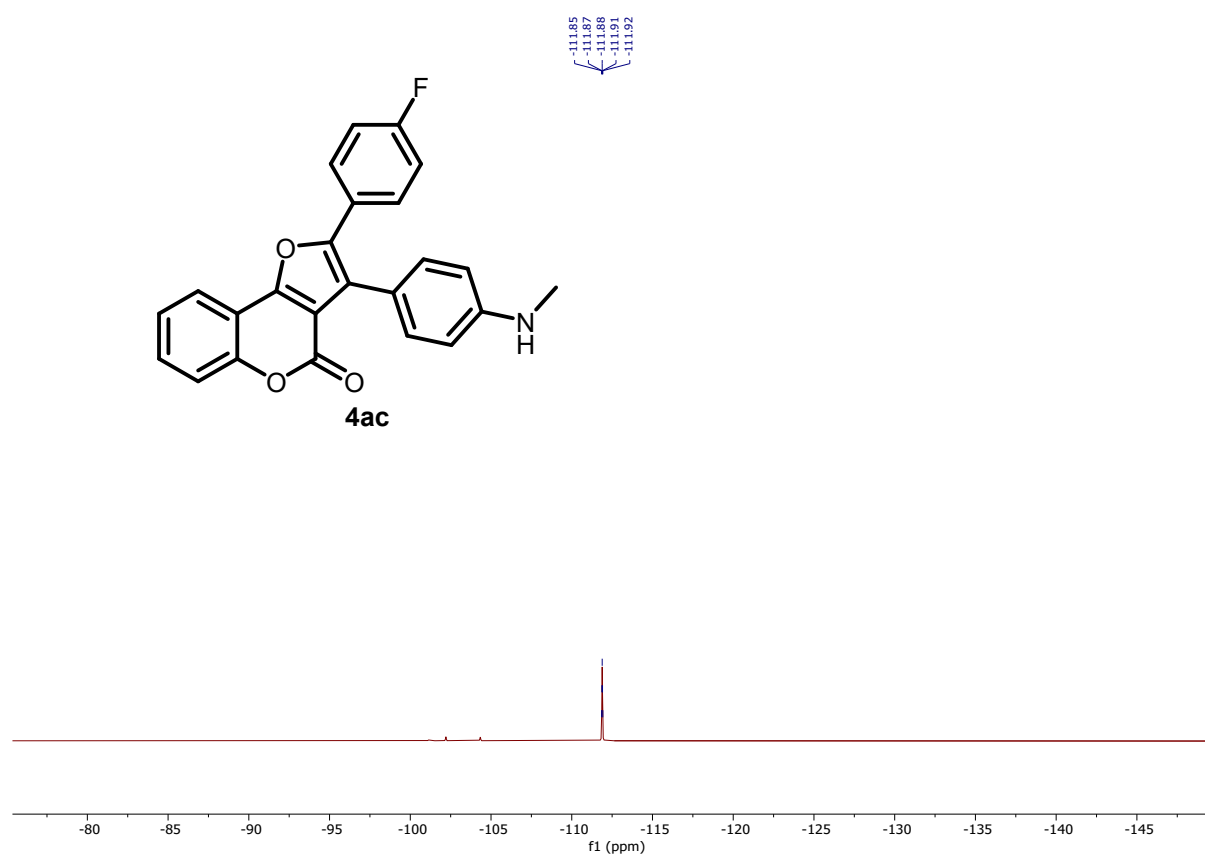
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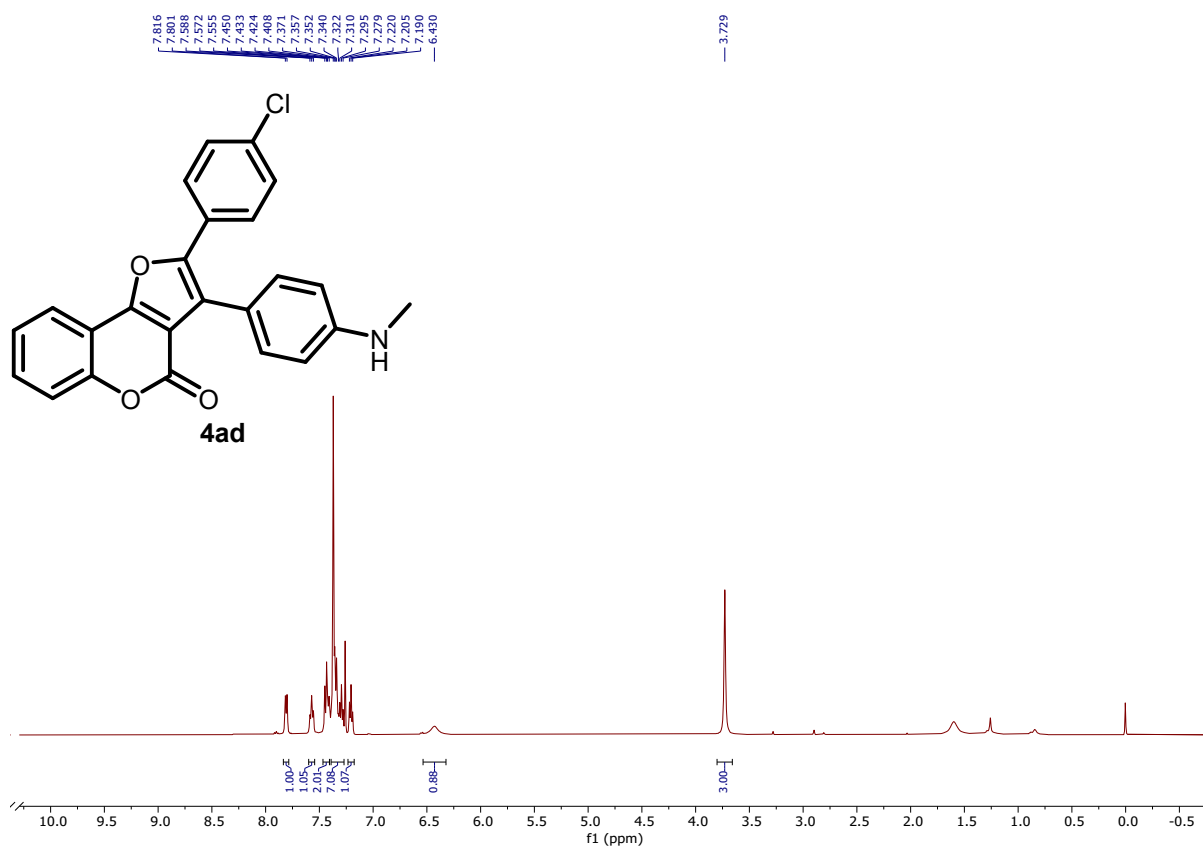
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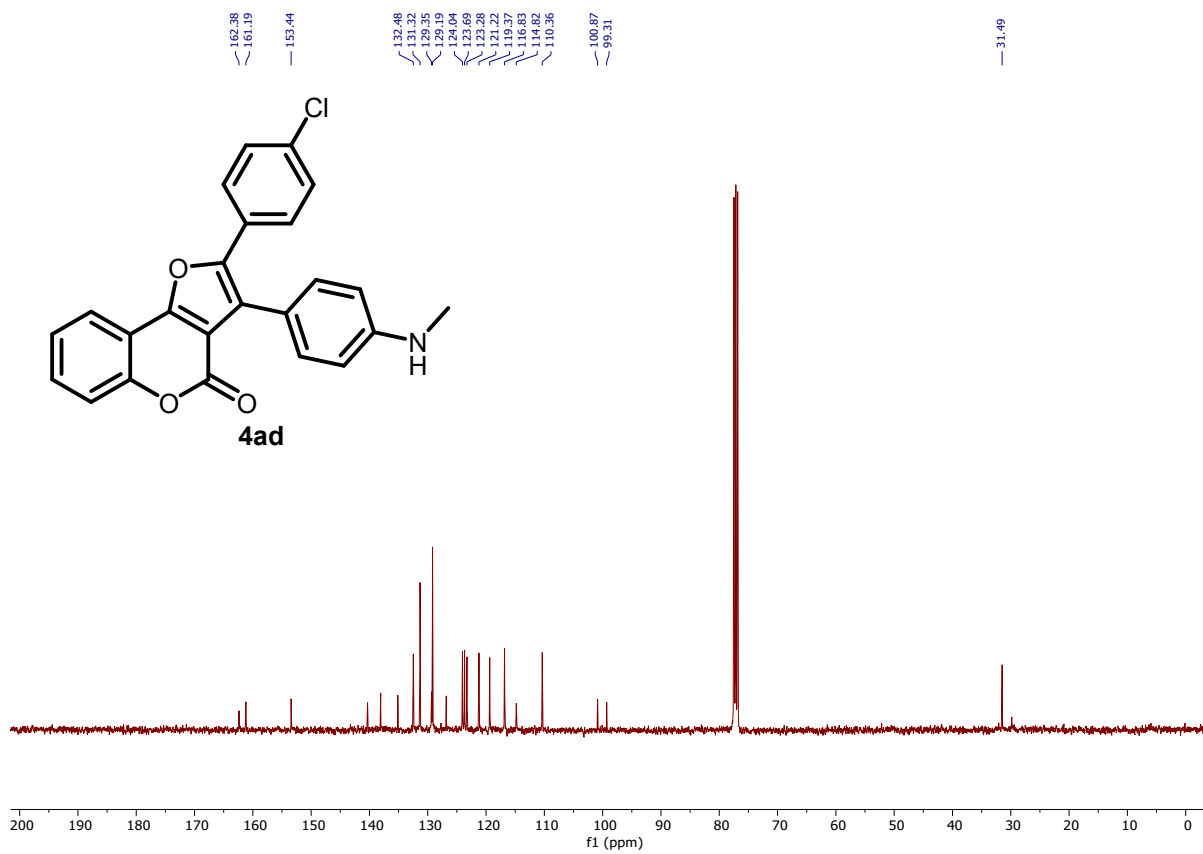
^{19}F NMR (376 MHz, CDCl_3)



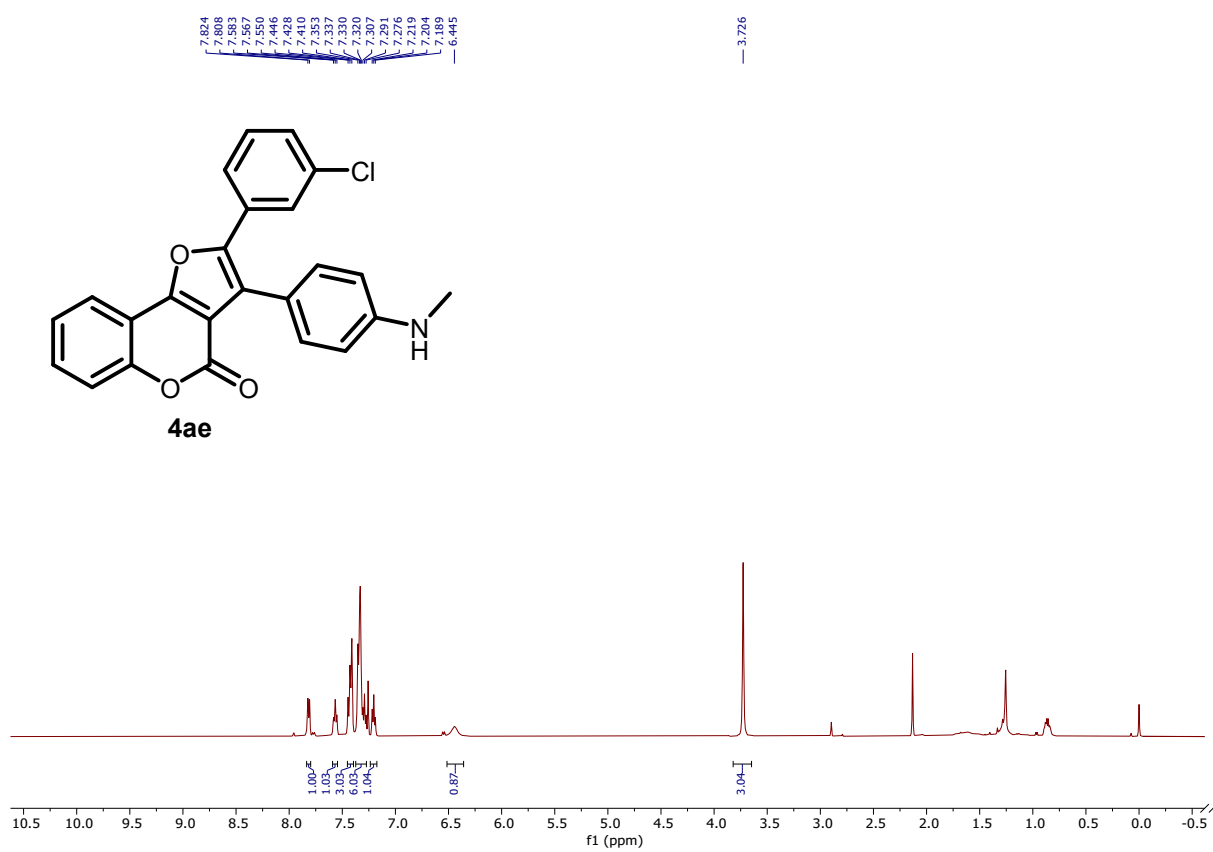
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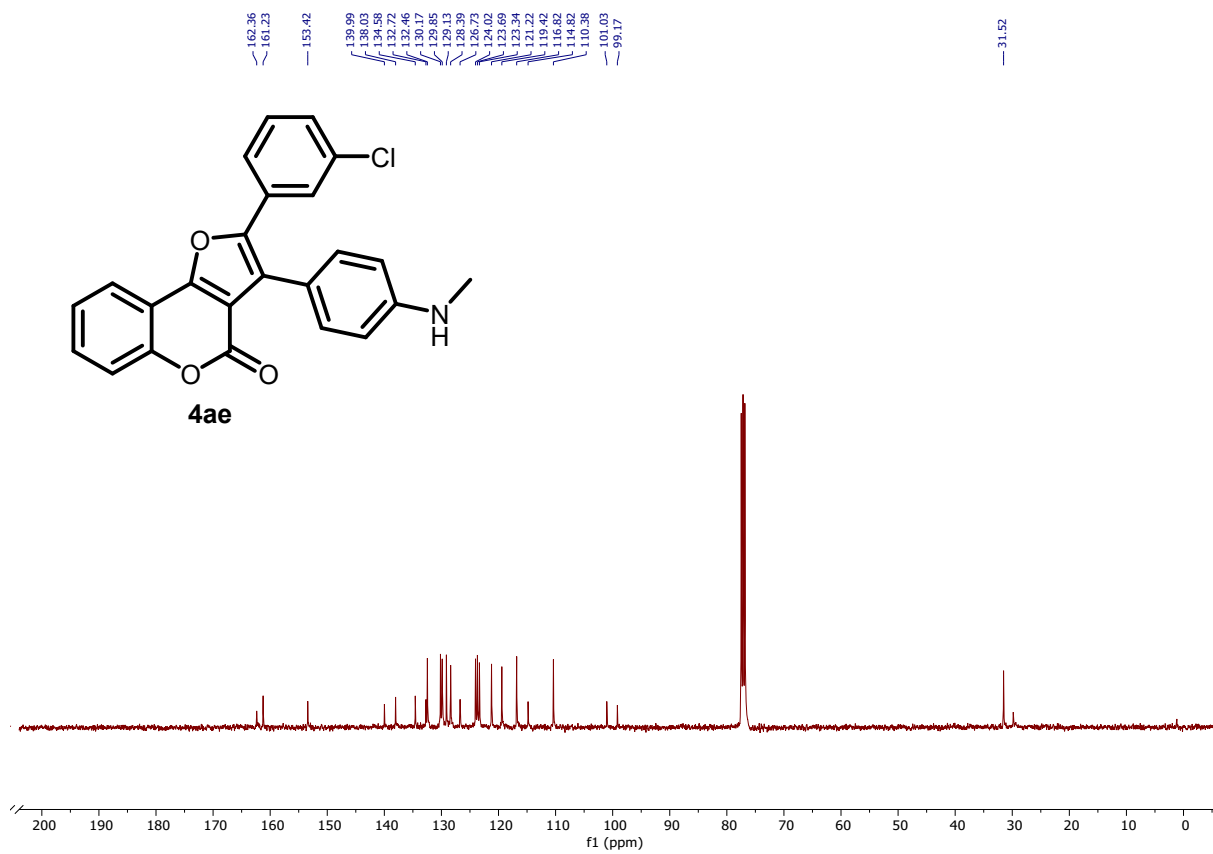
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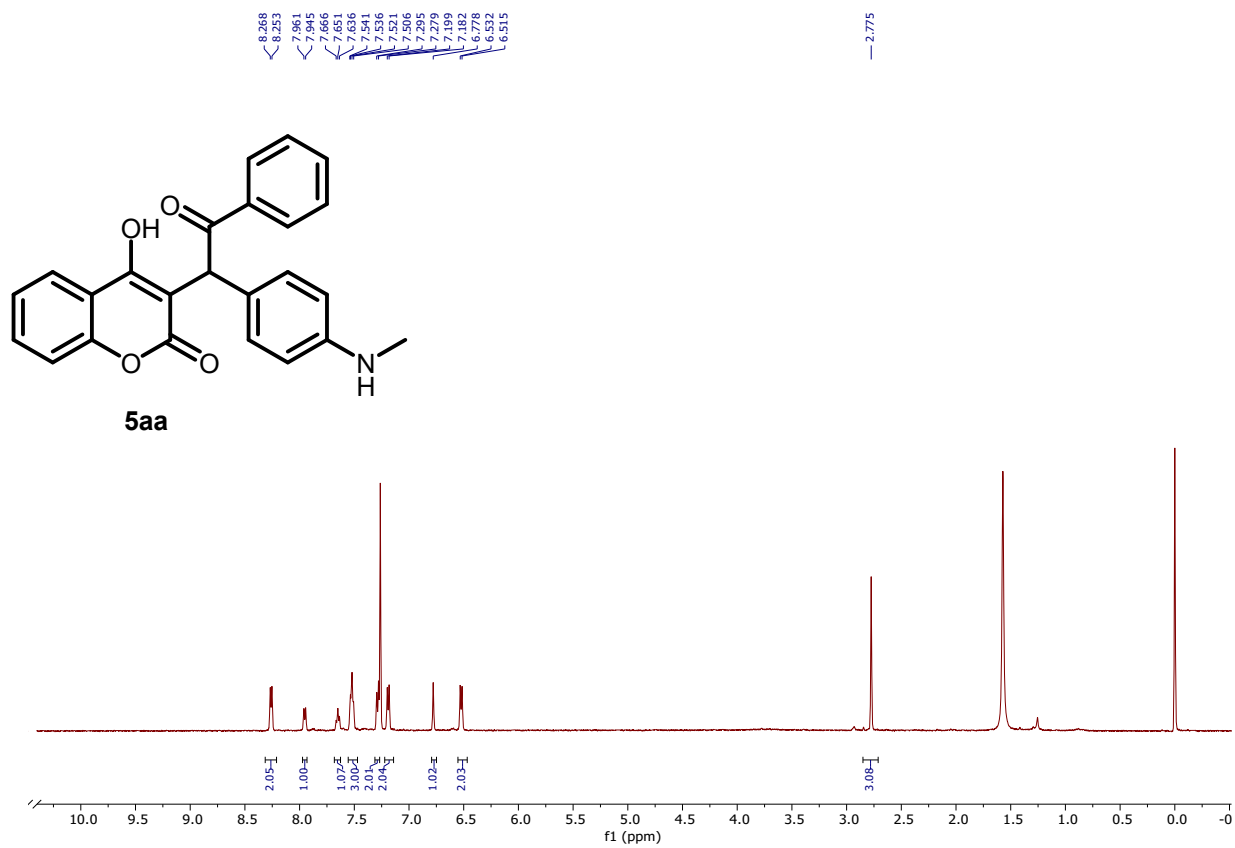
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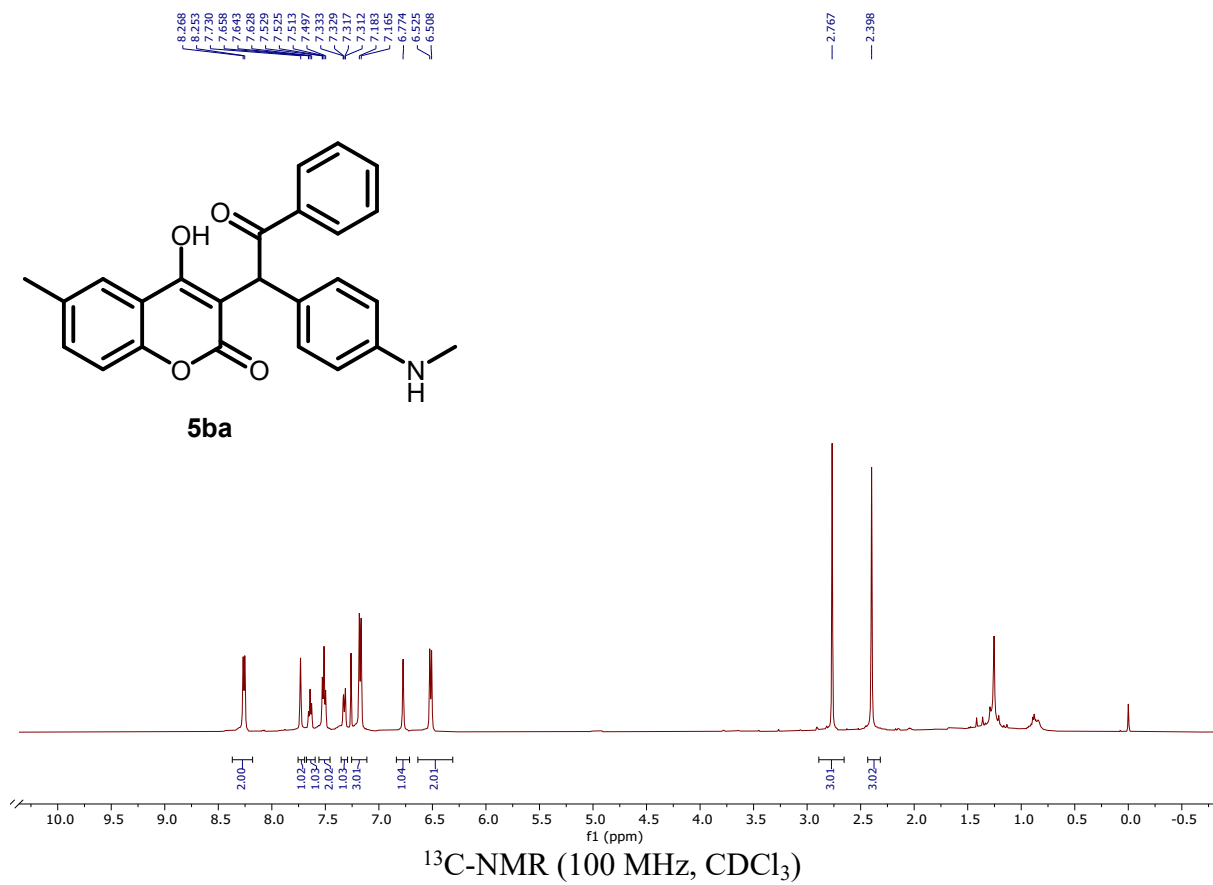
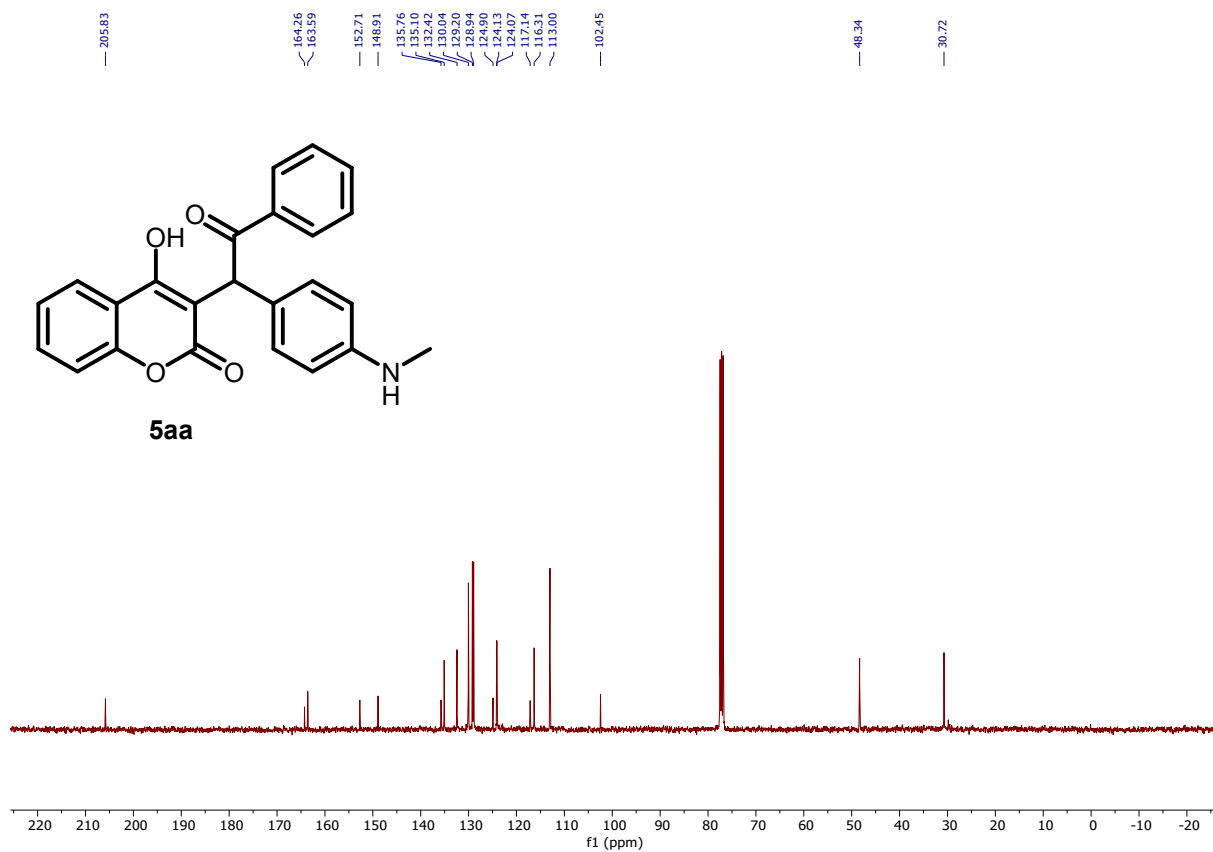
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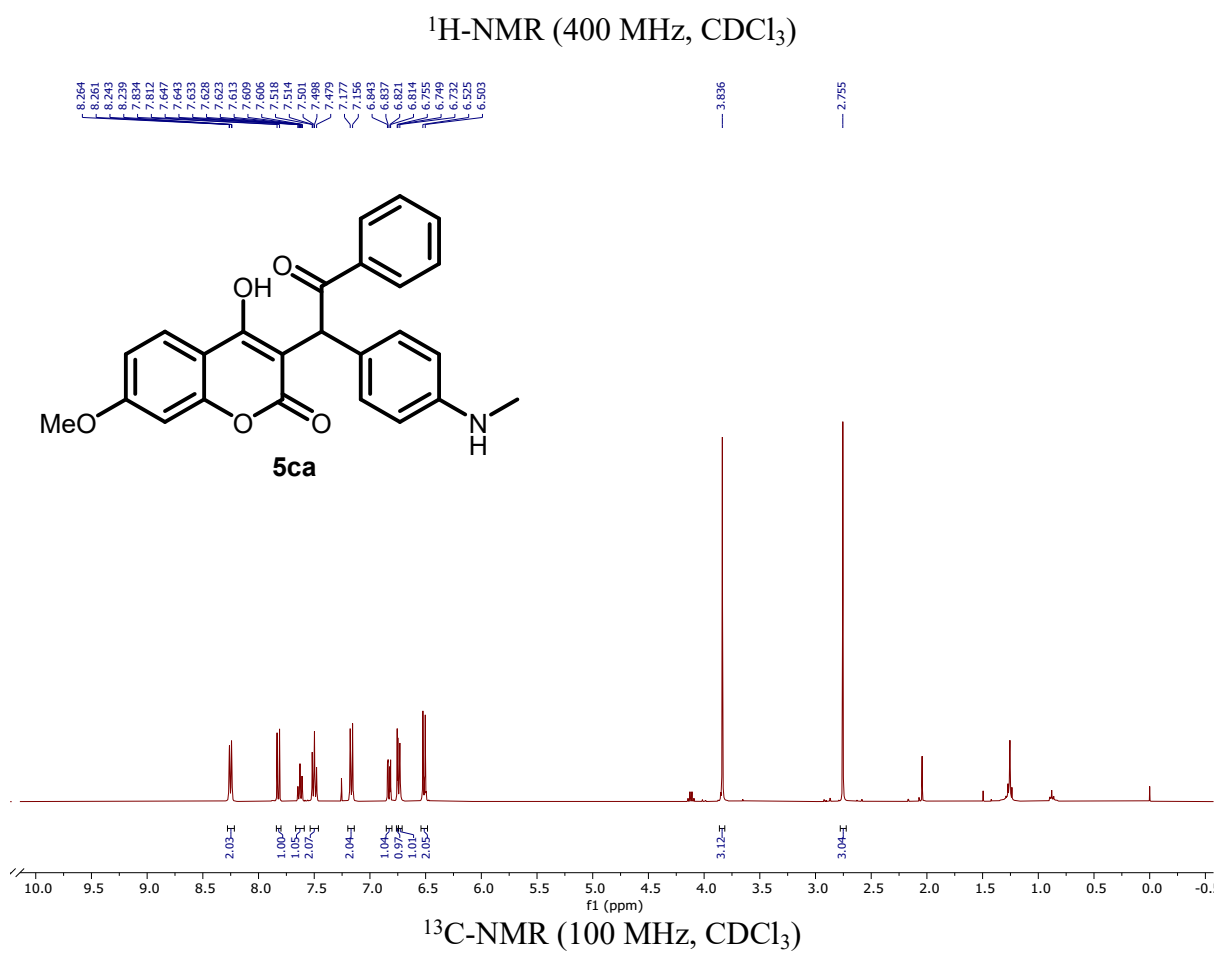
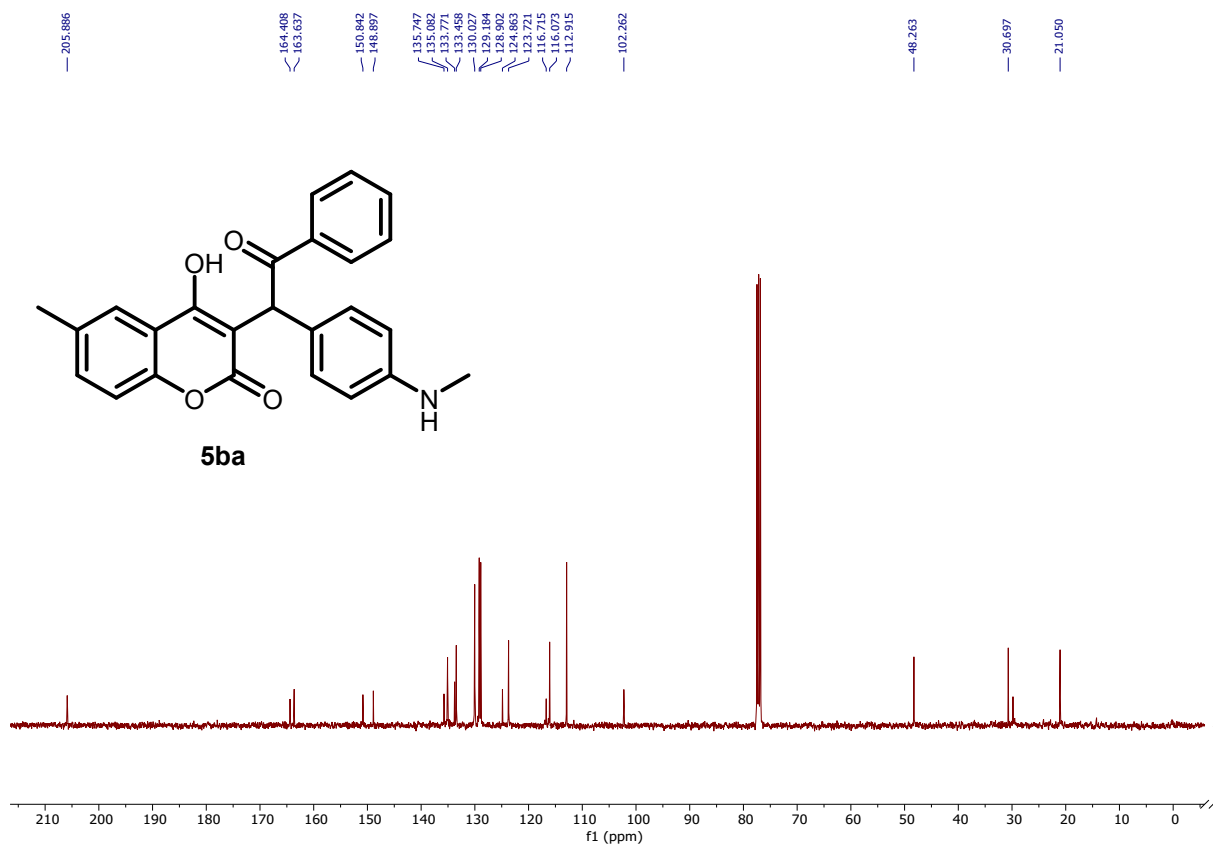


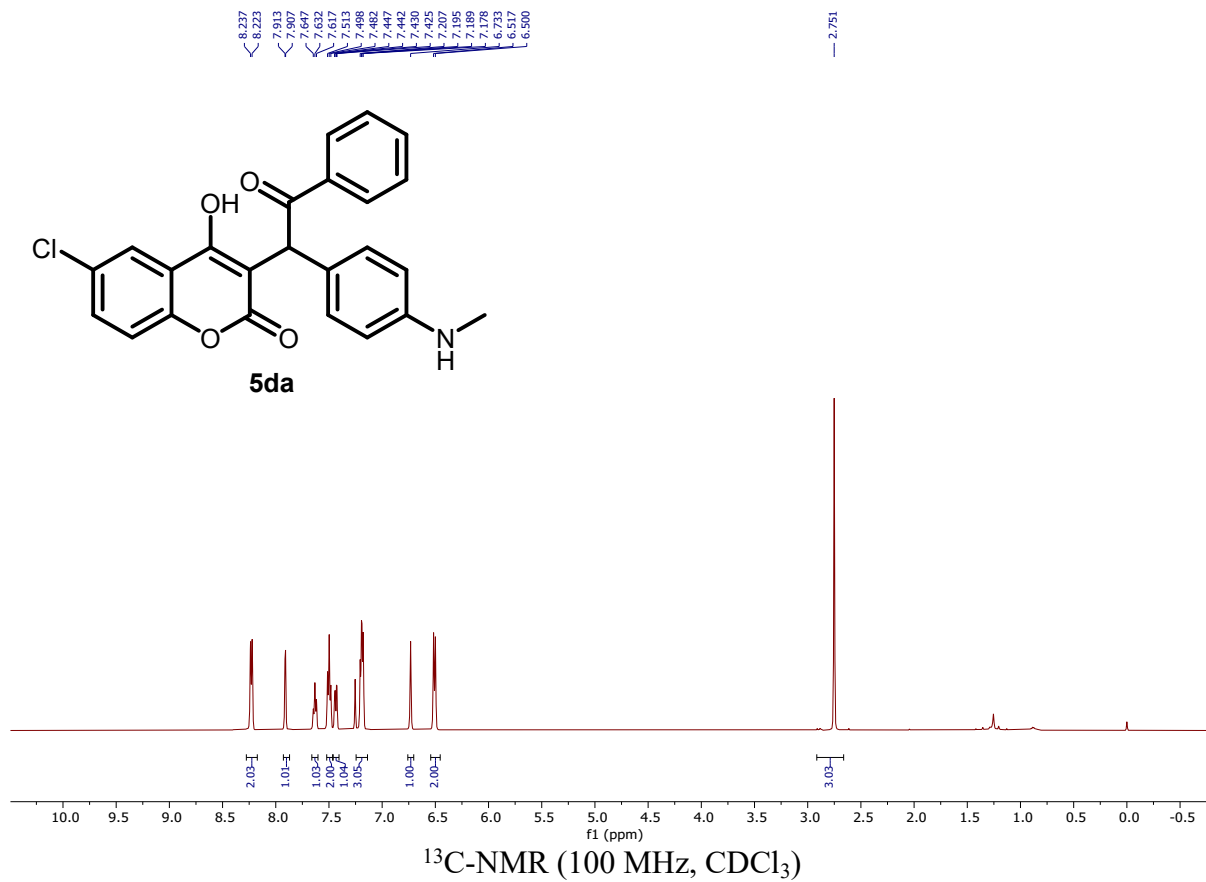
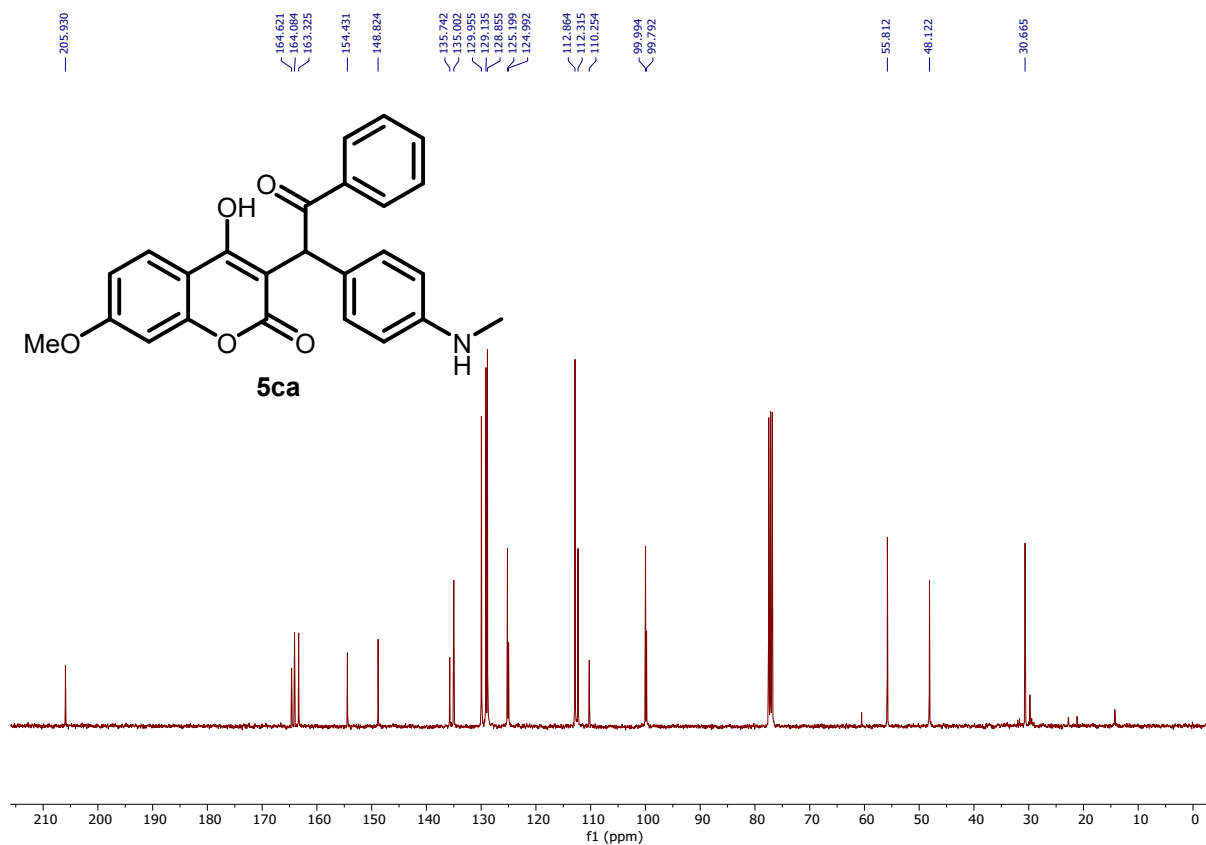
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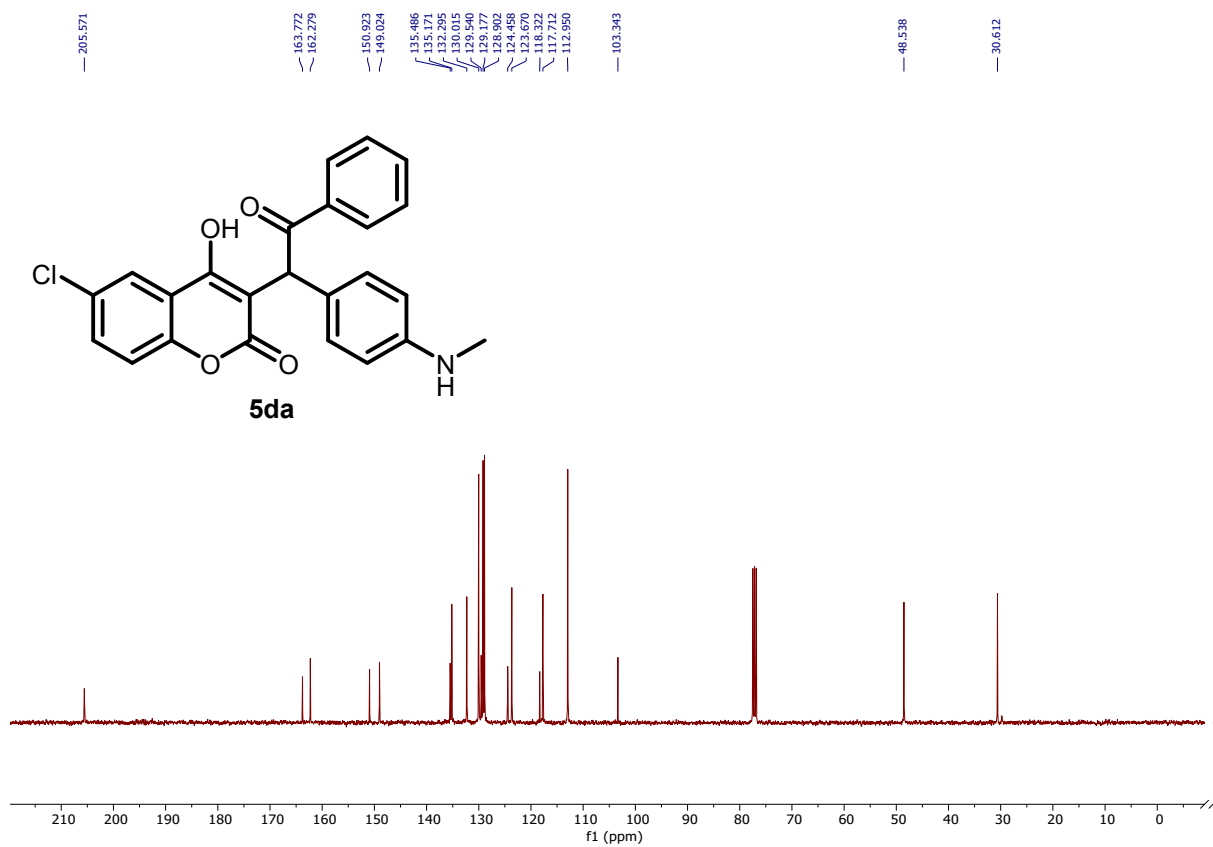


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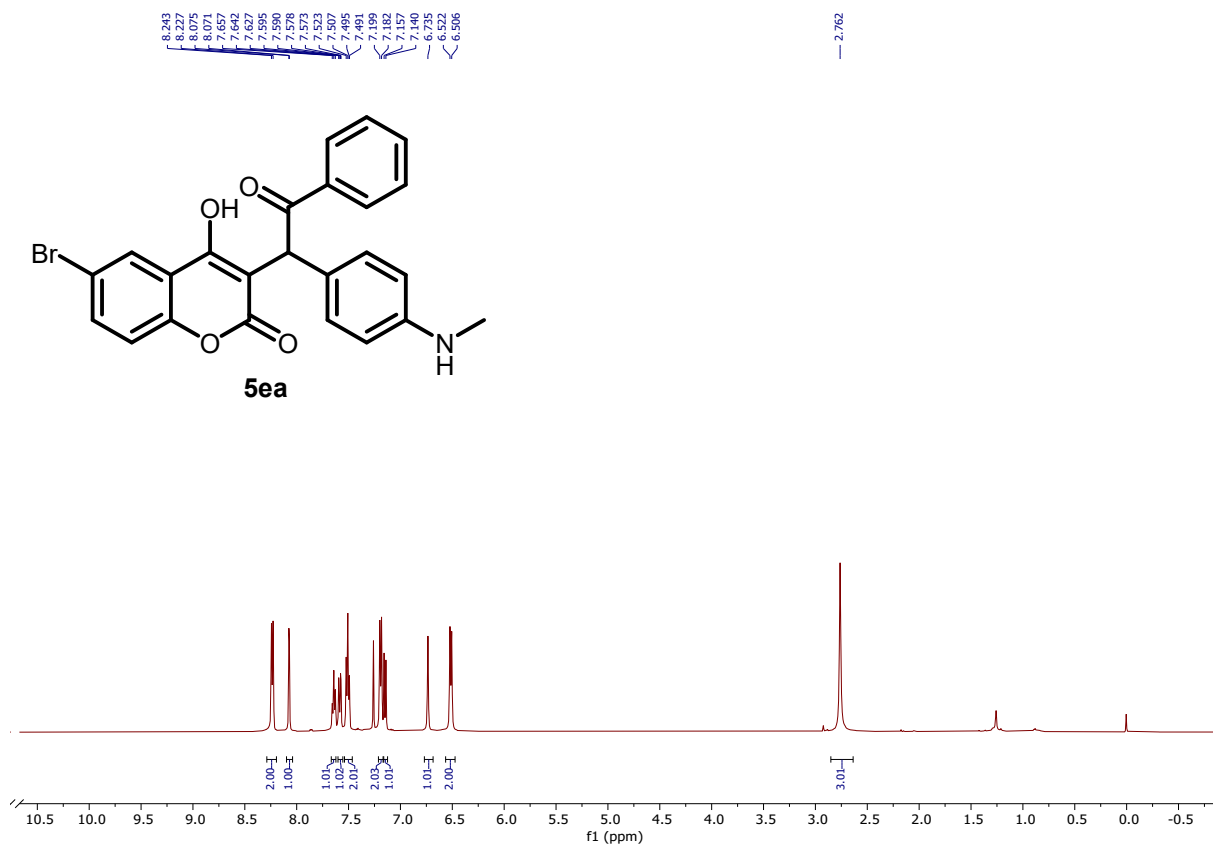




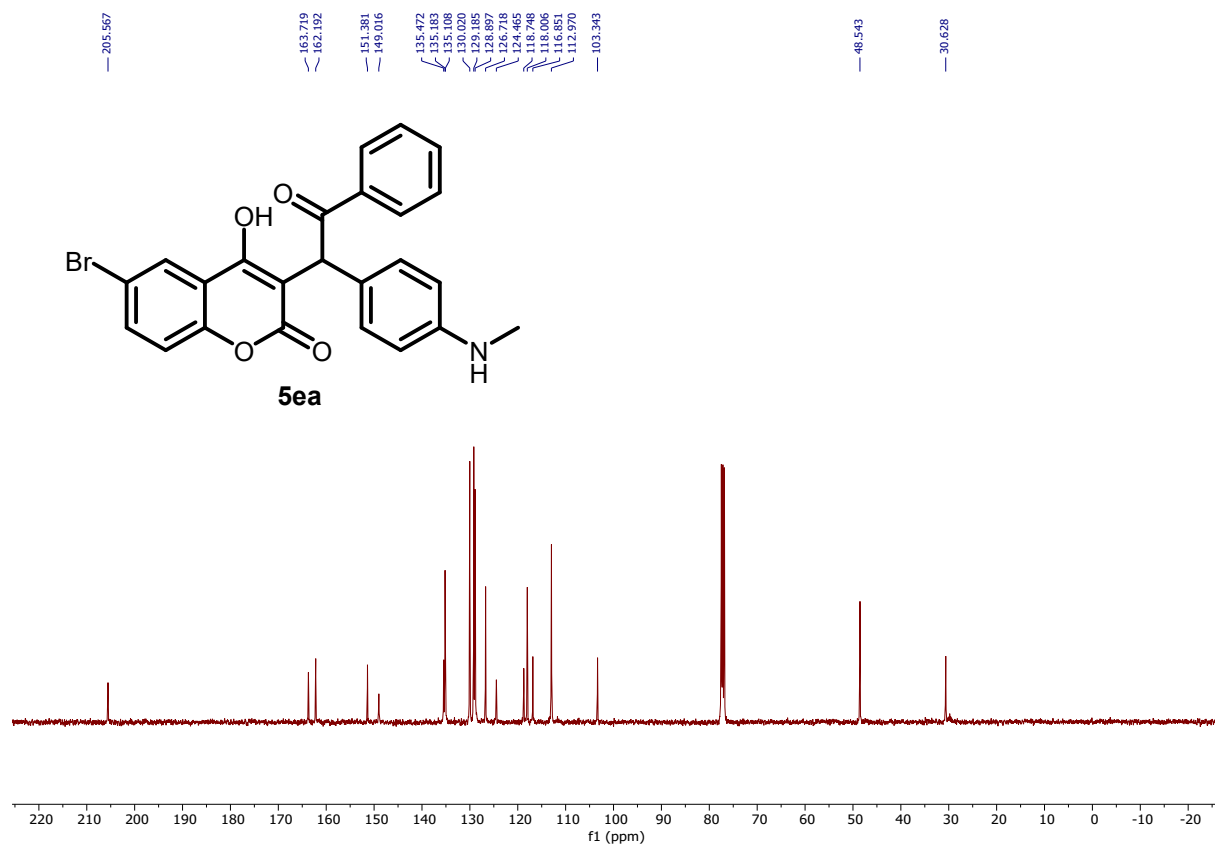




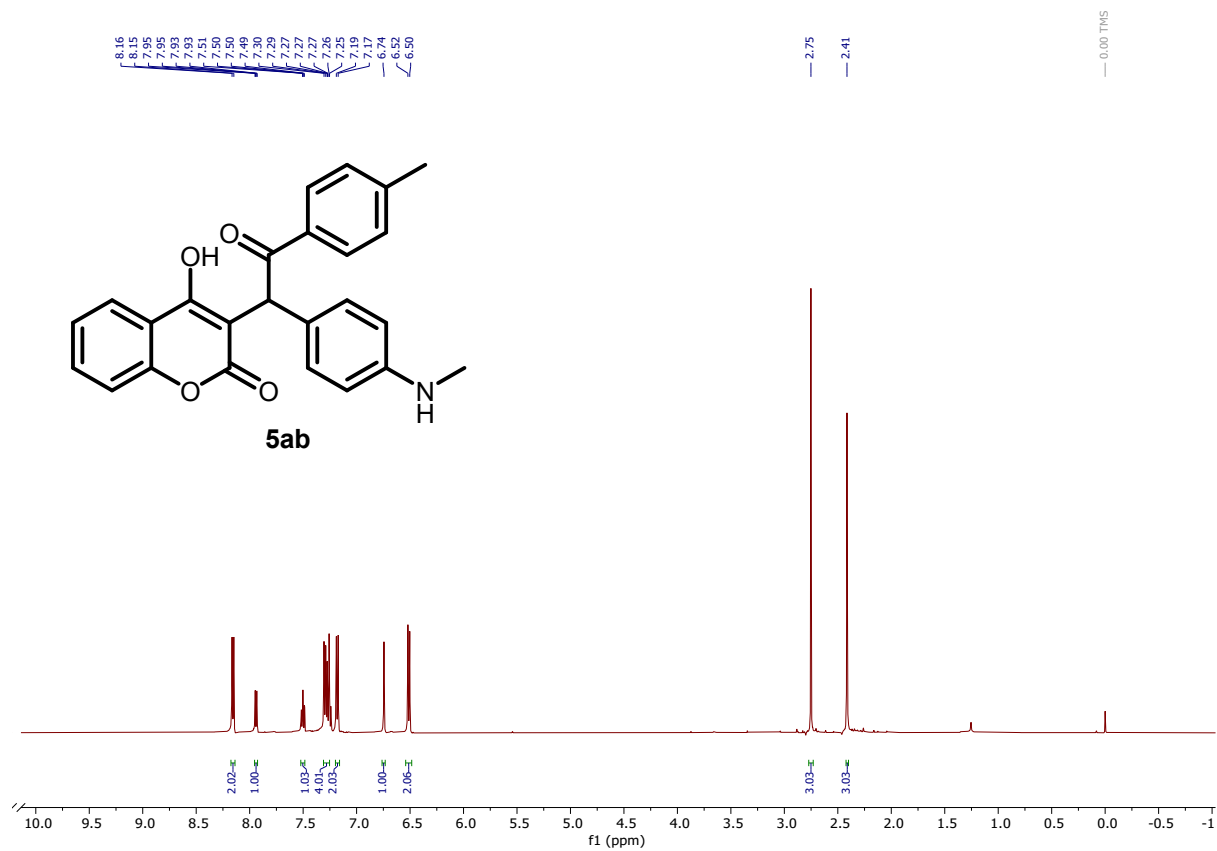
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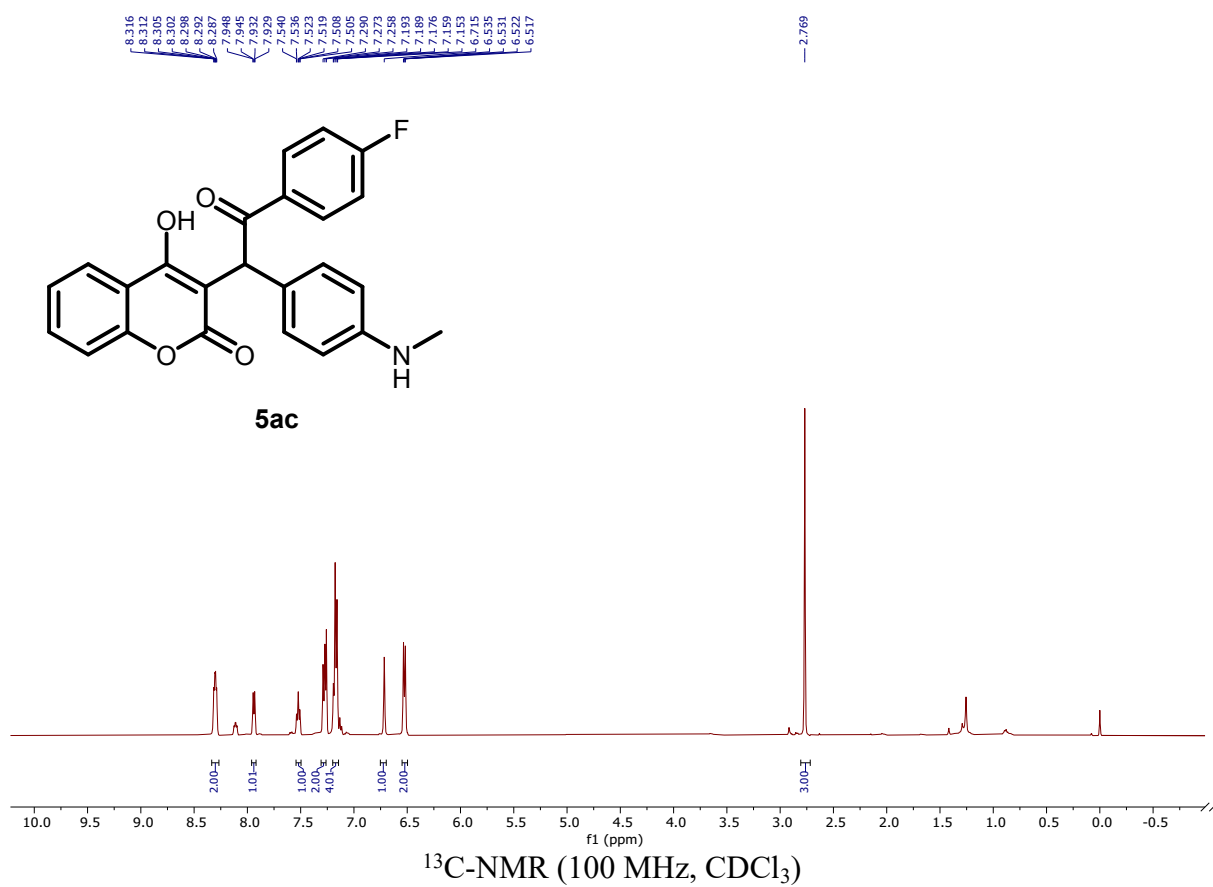
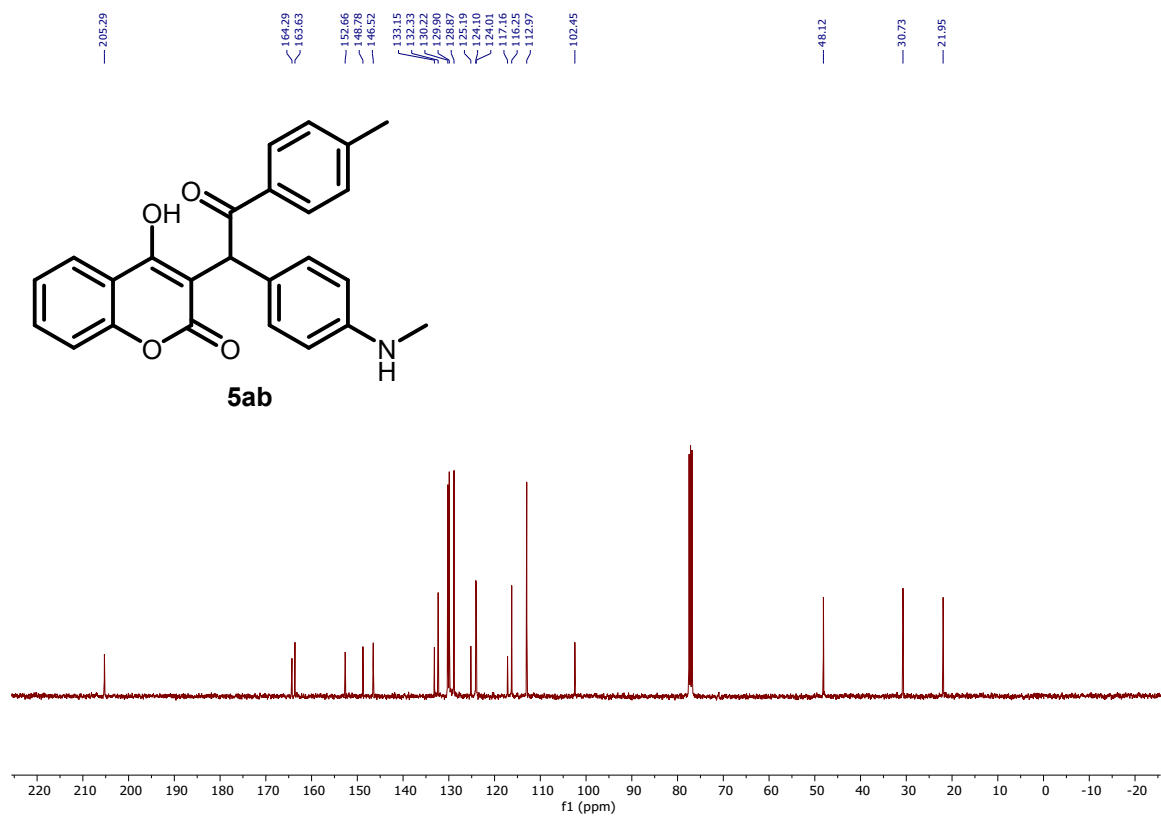
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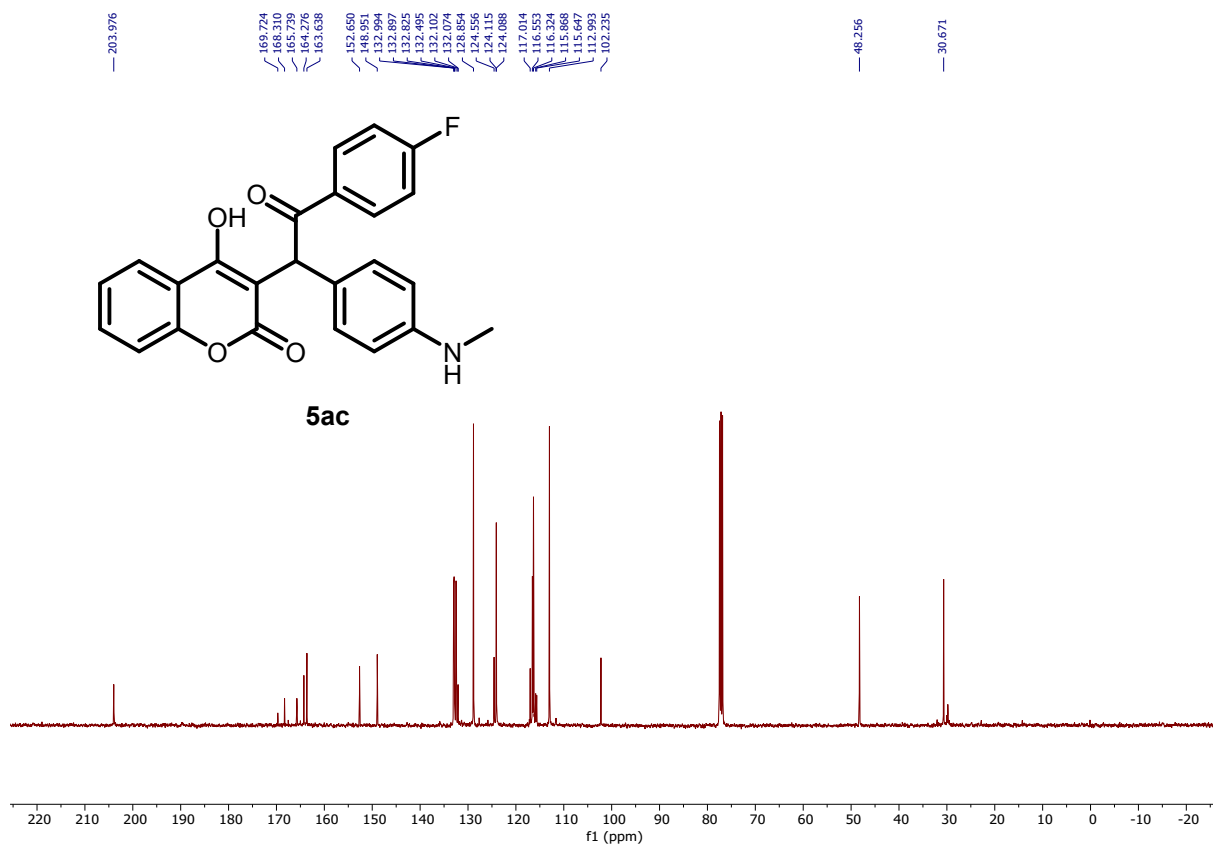


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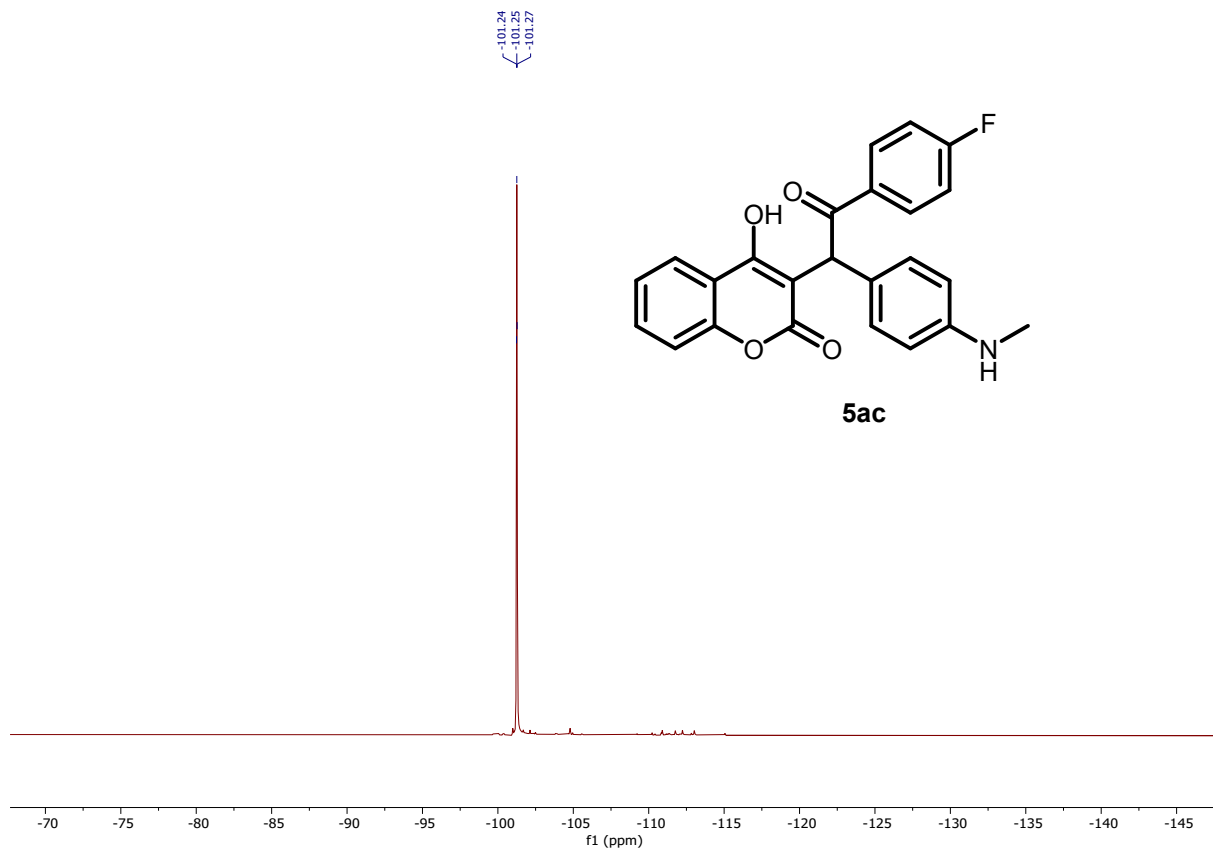


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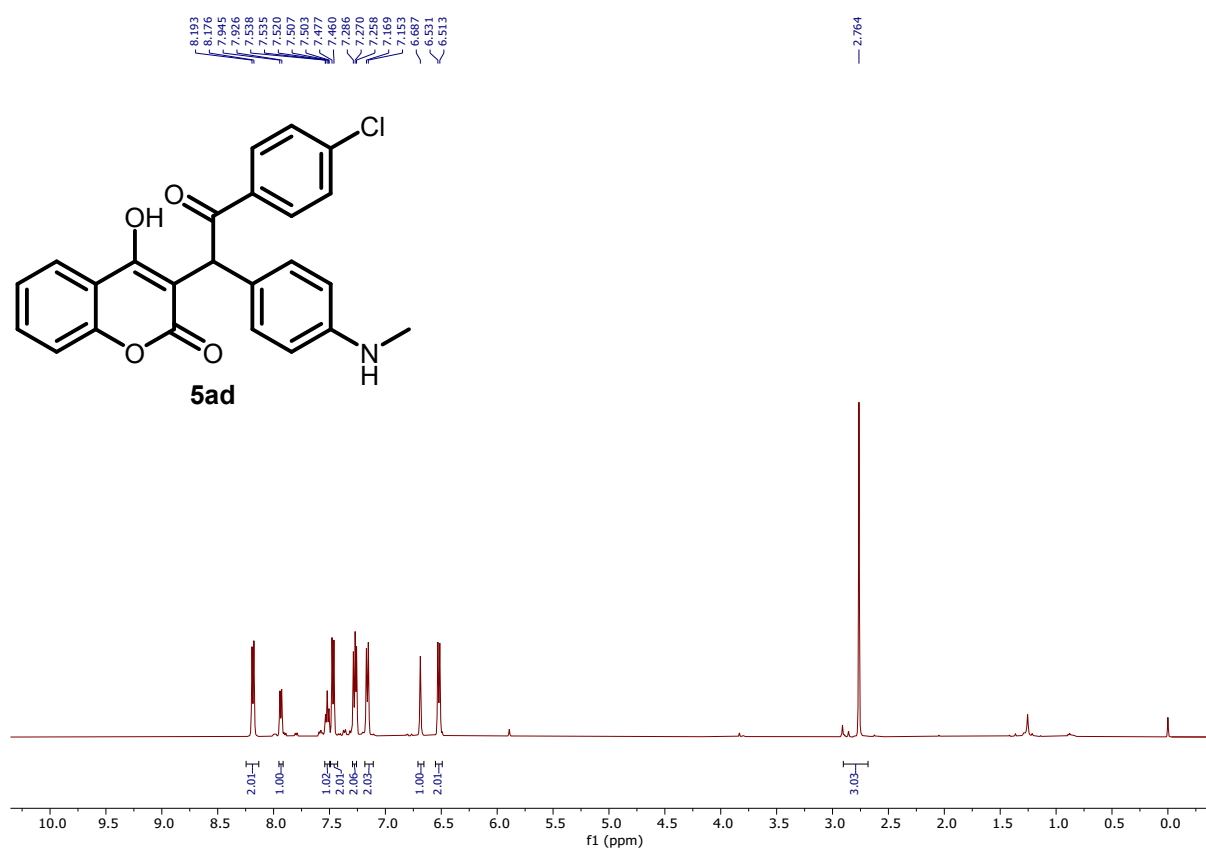




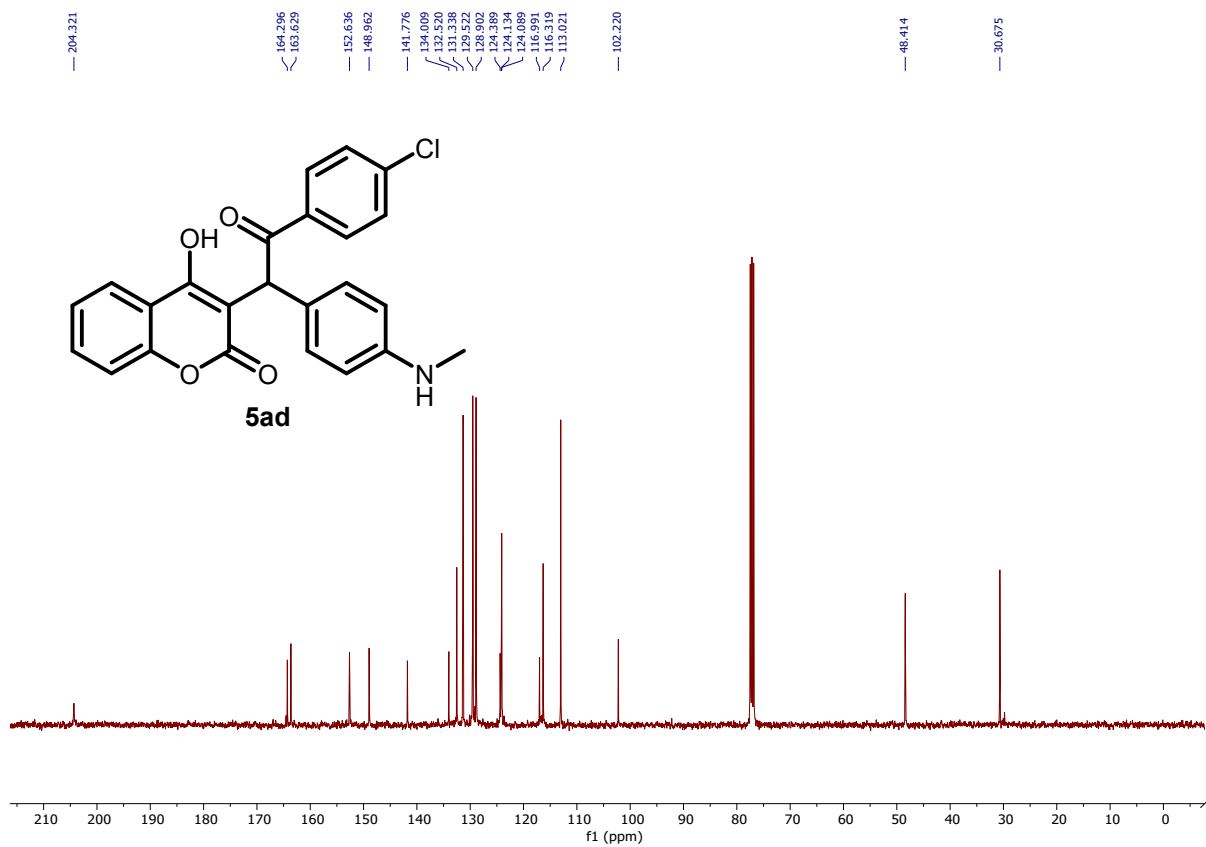
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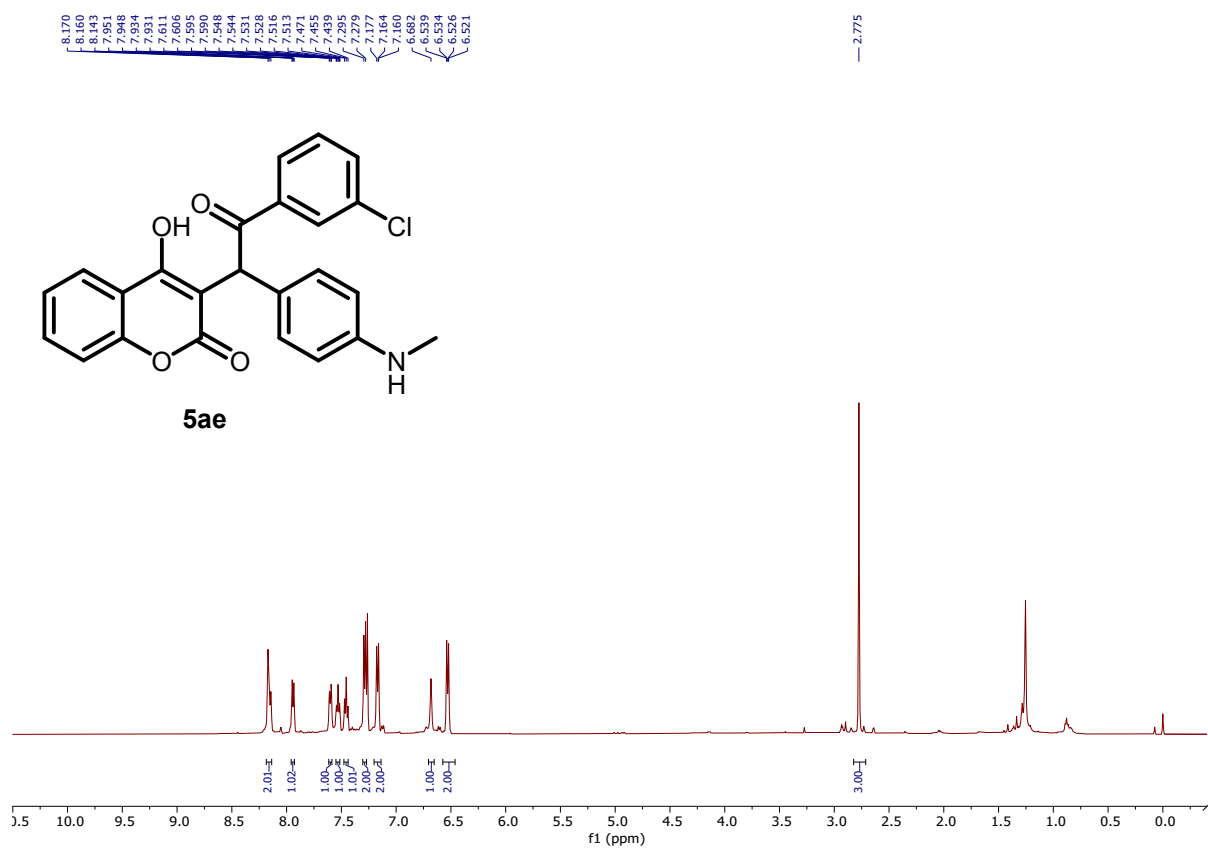
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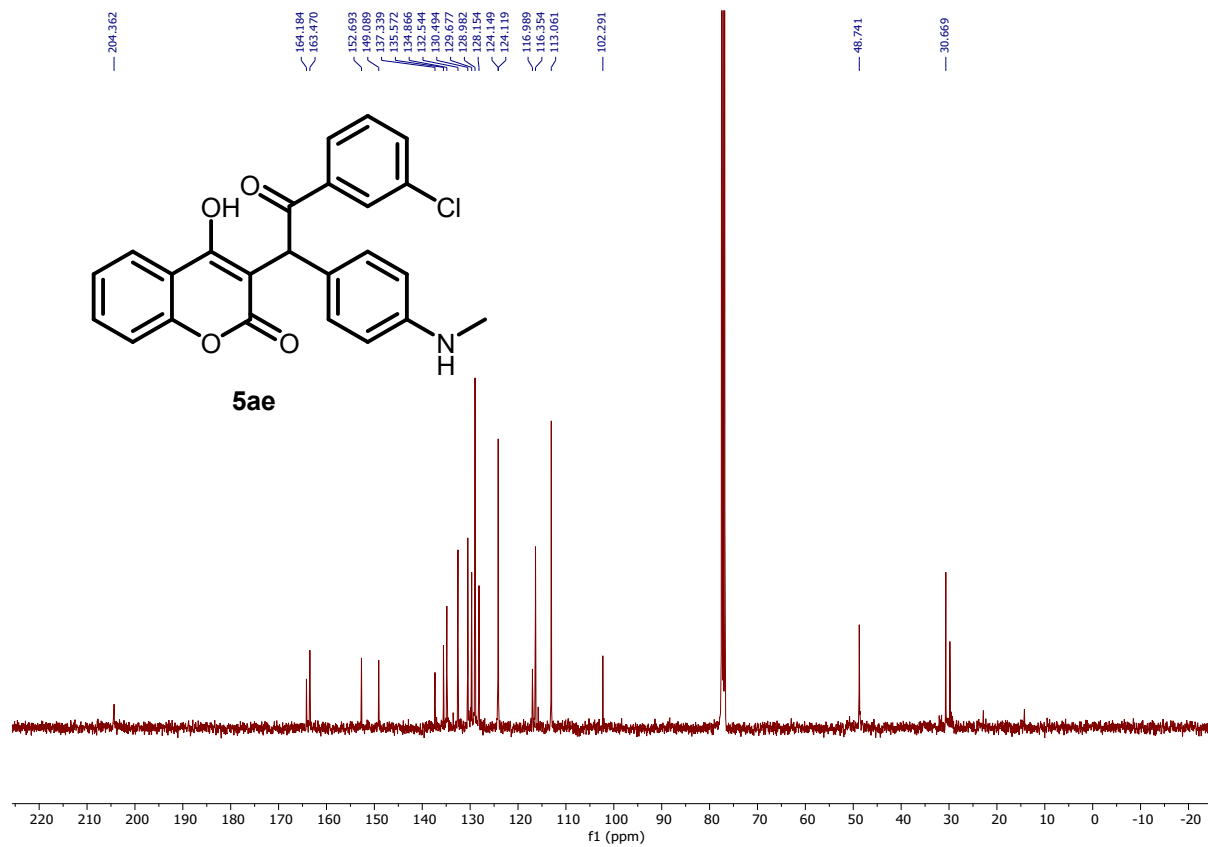
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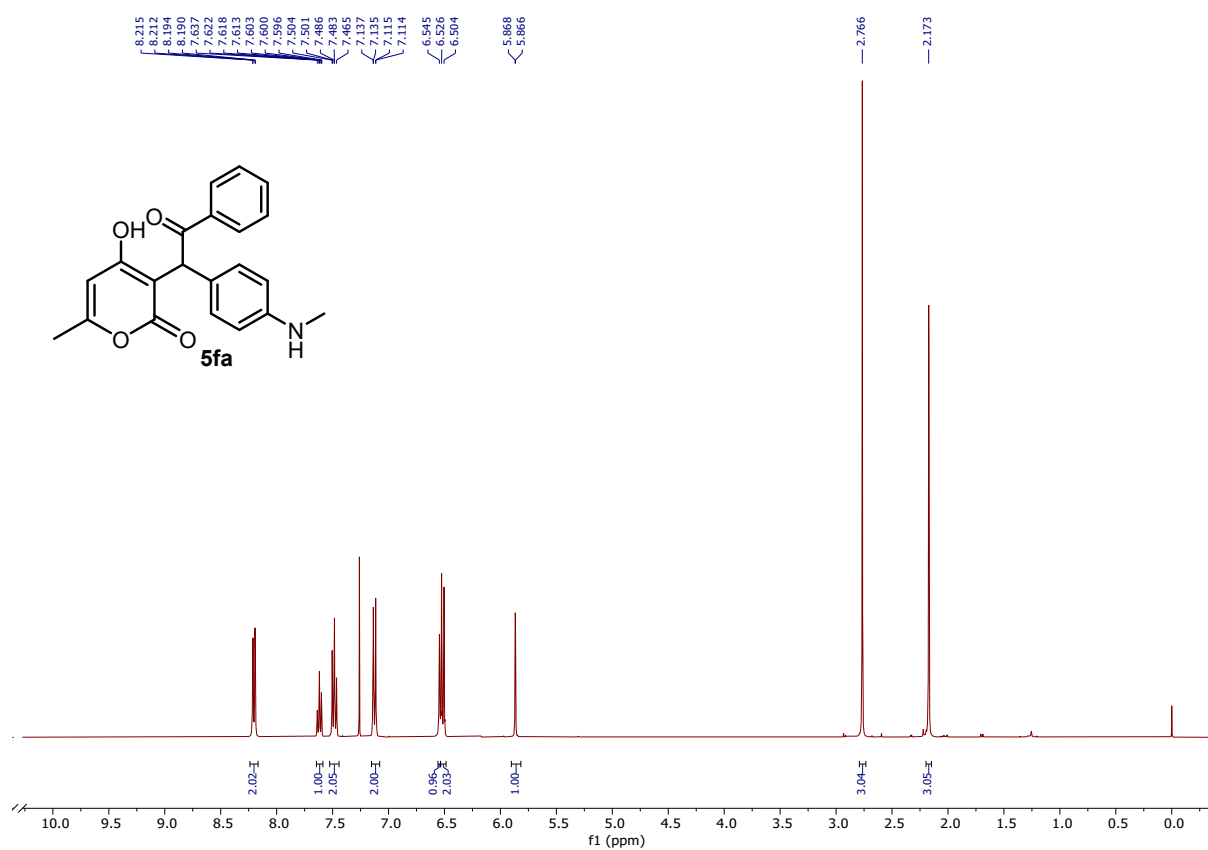
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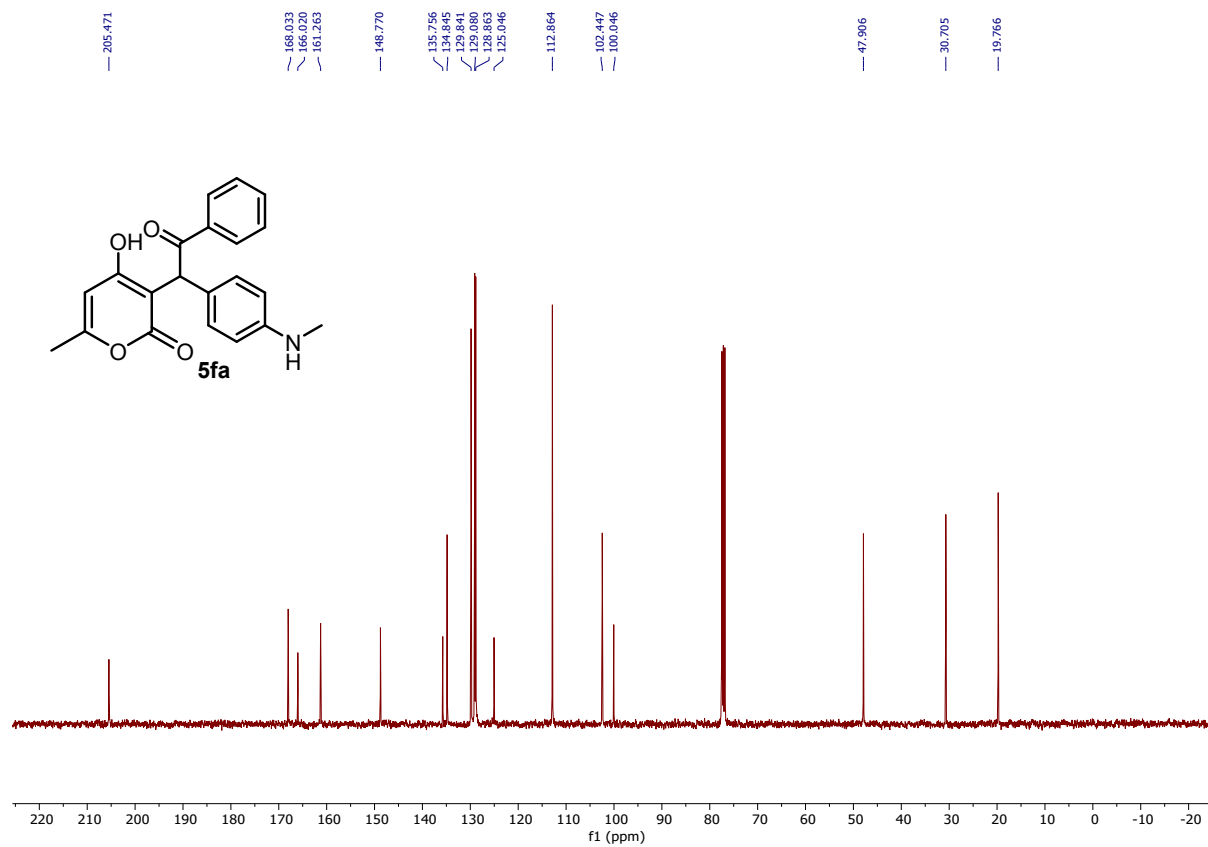
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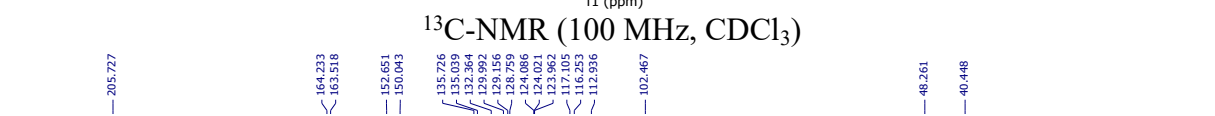
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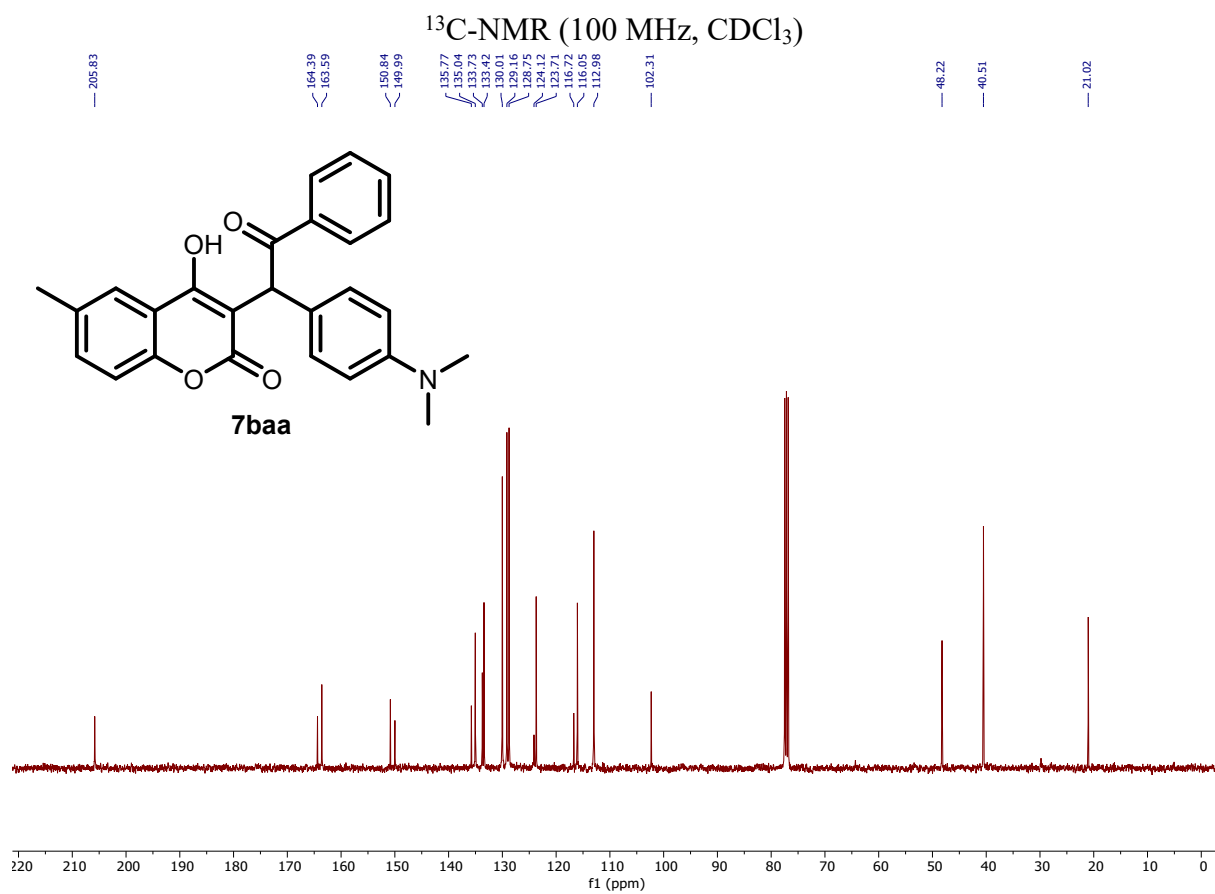
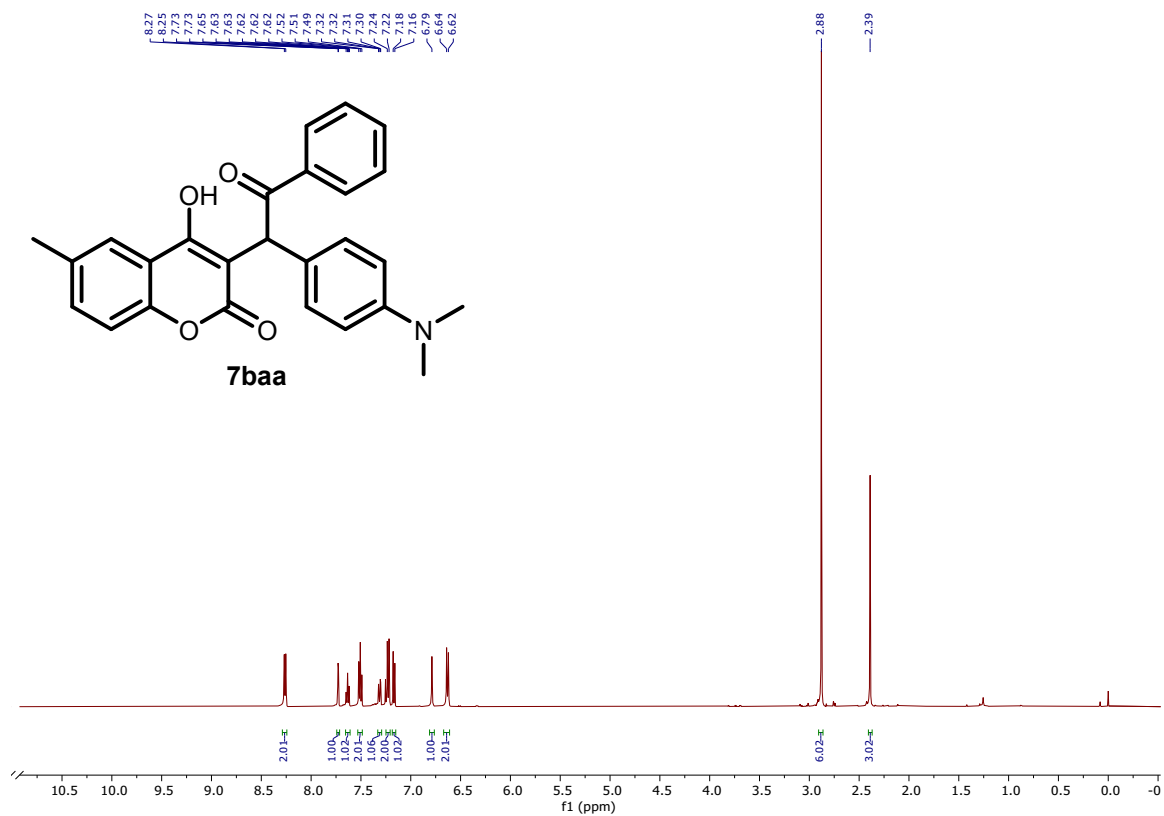


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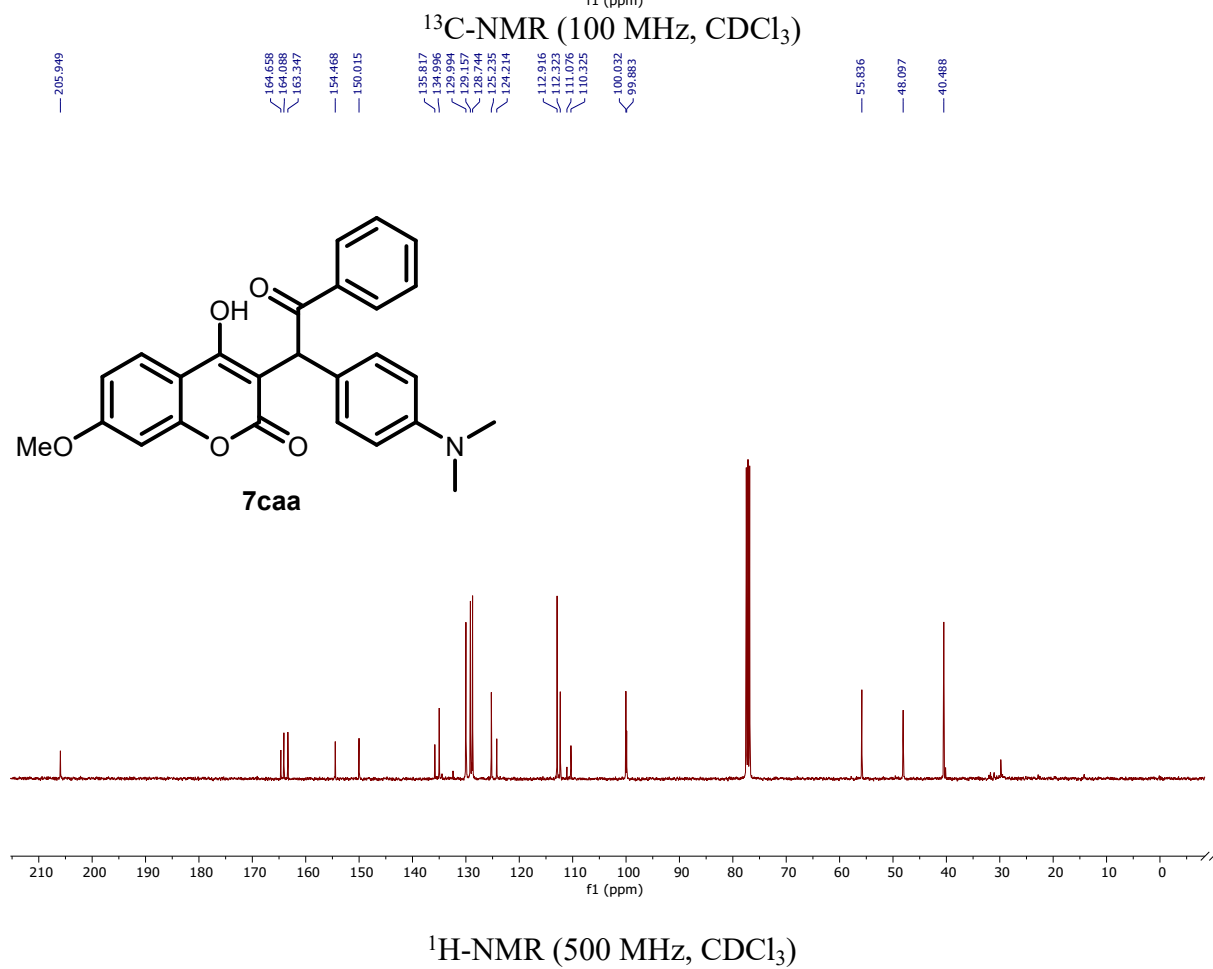
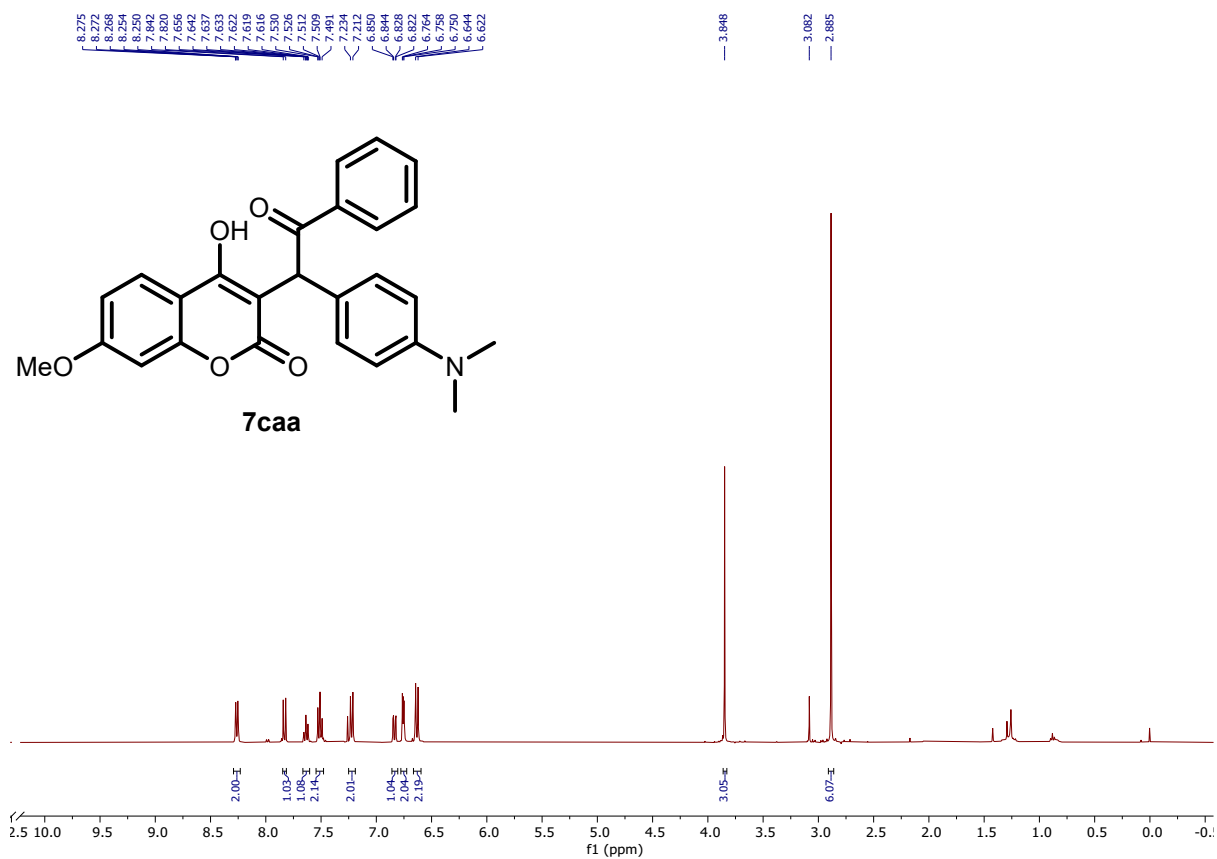


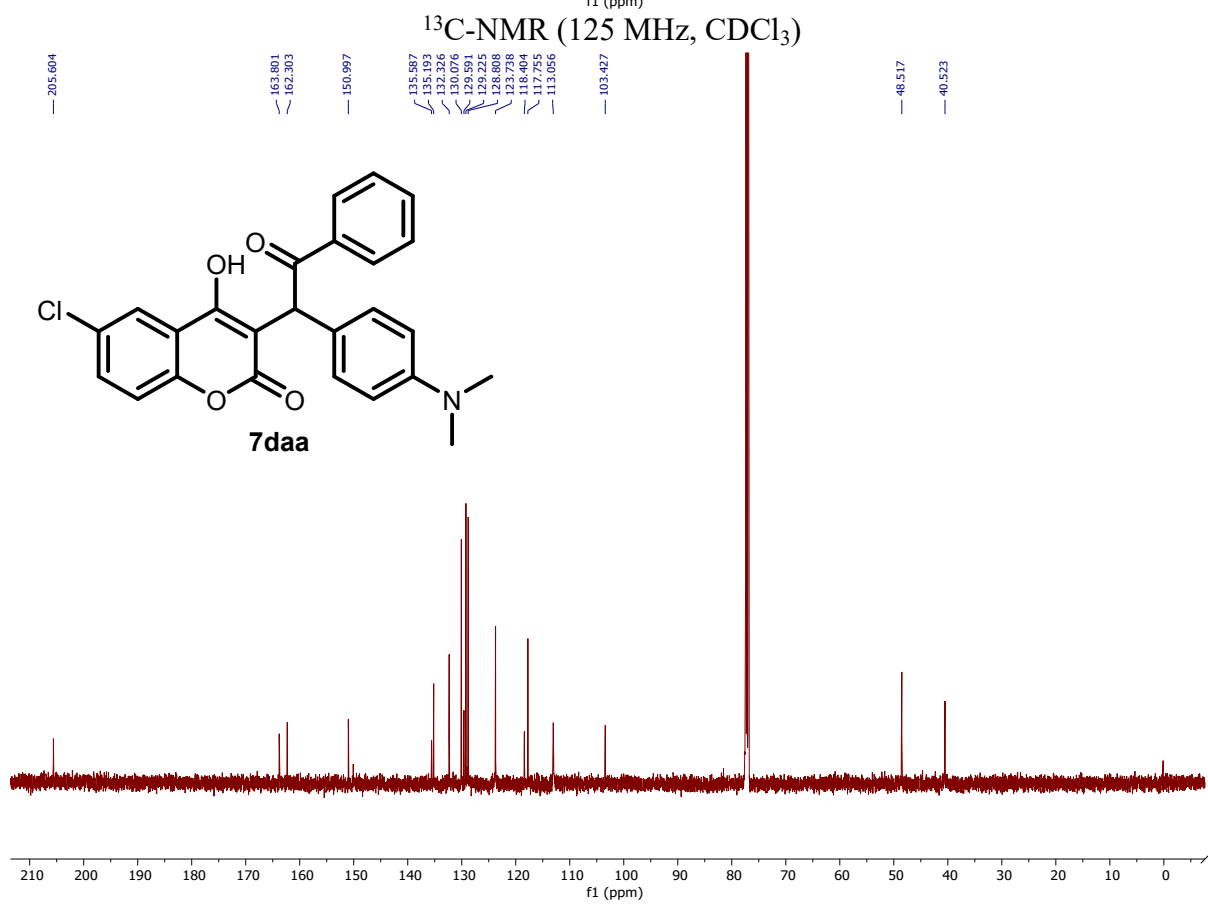
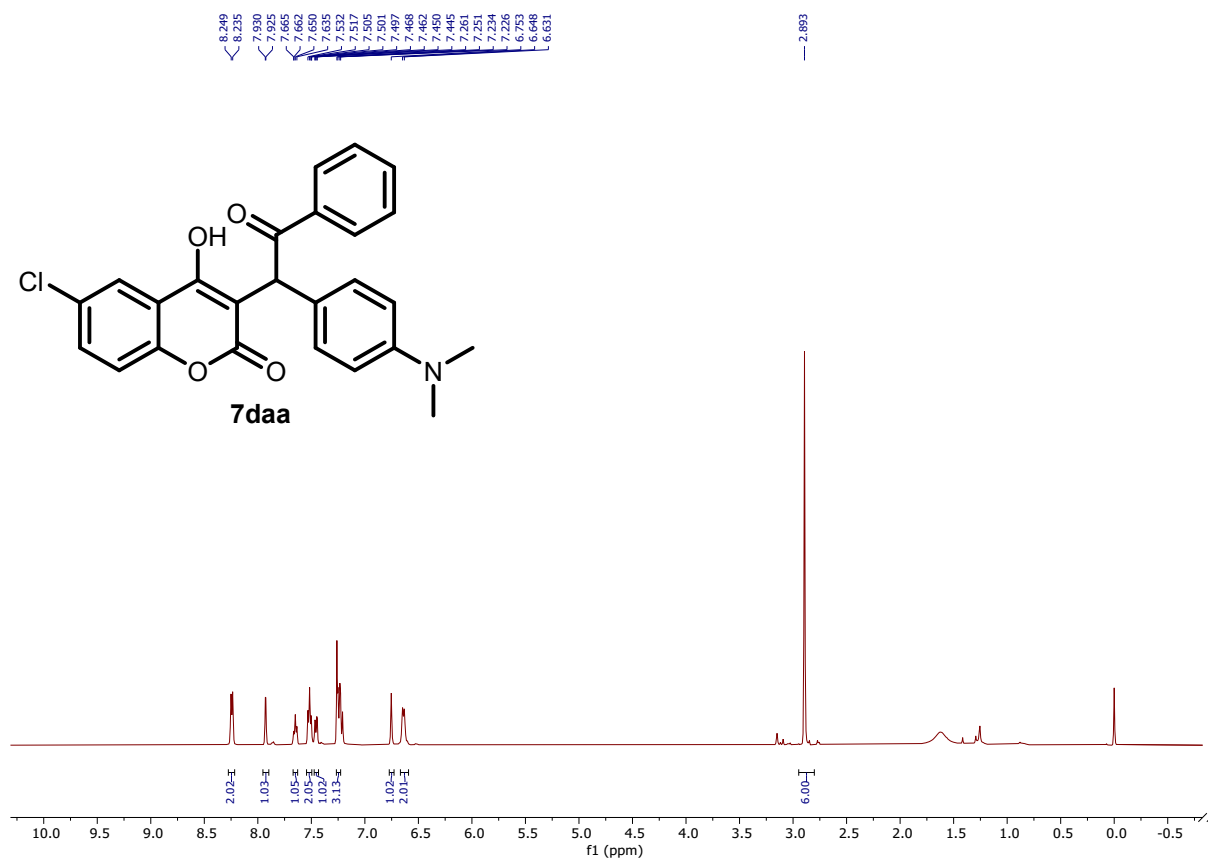
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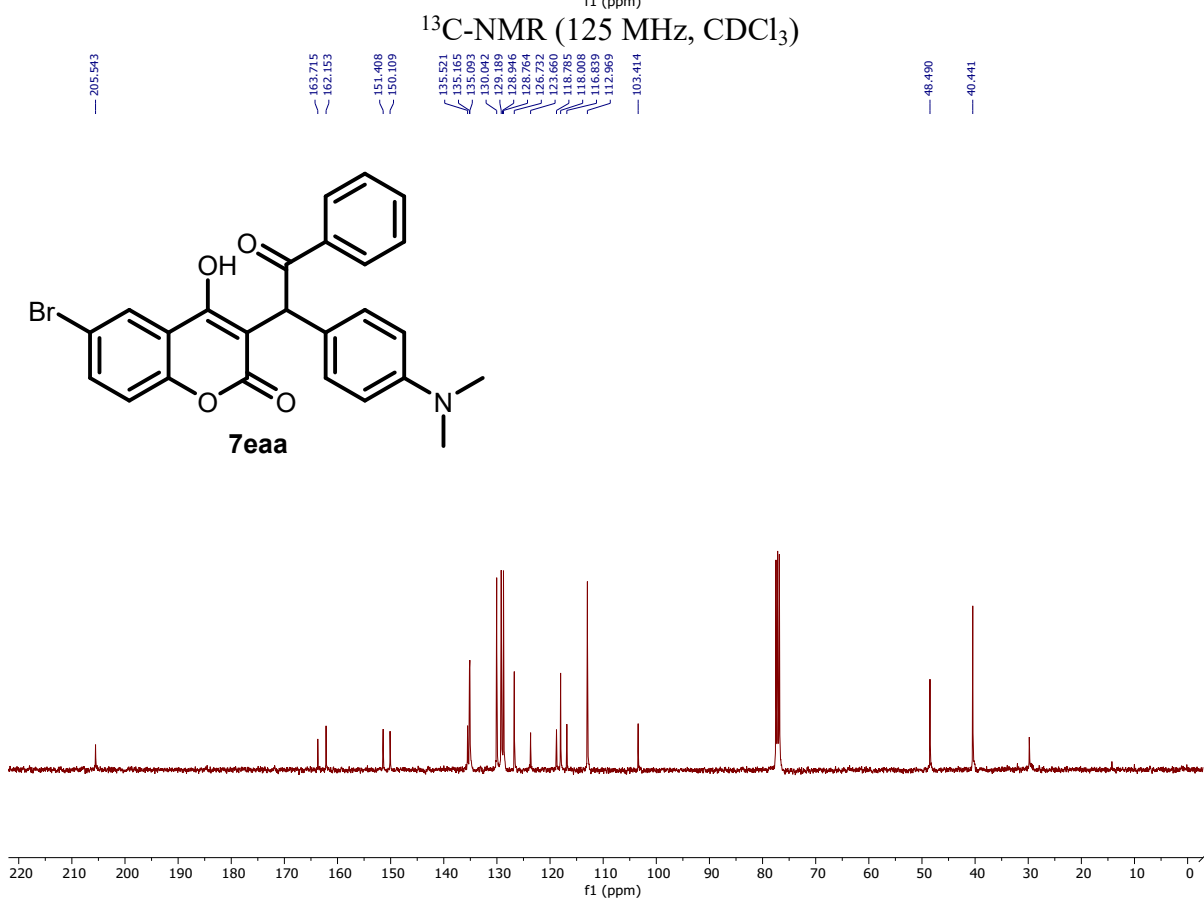
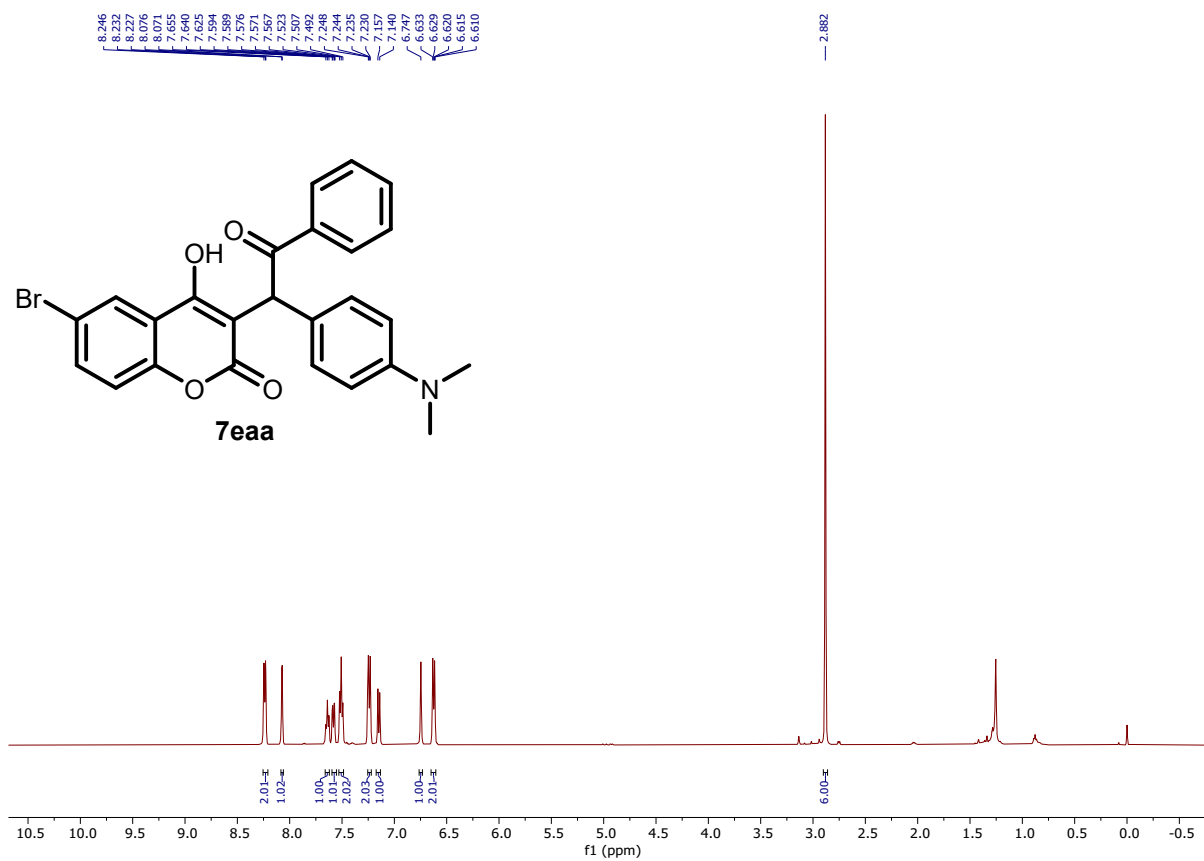


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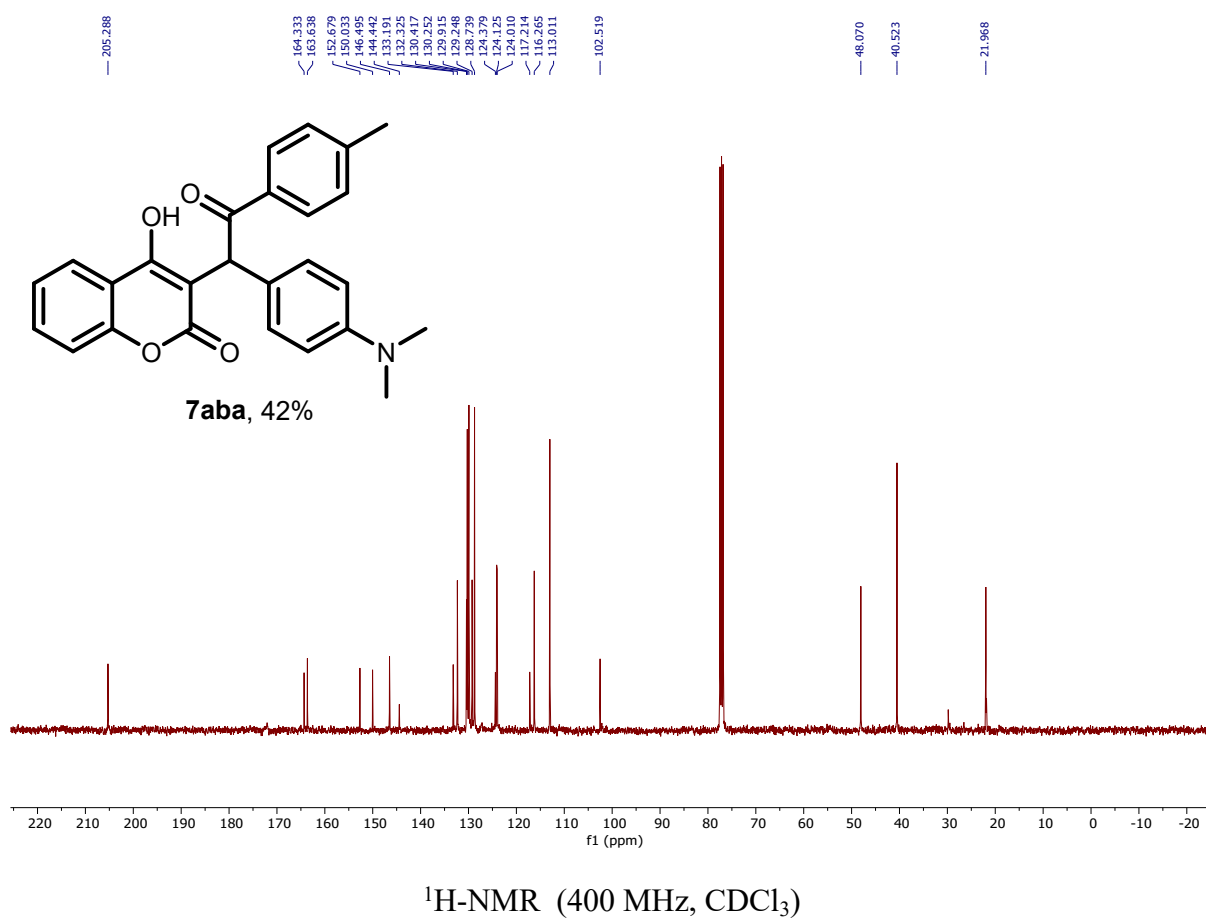
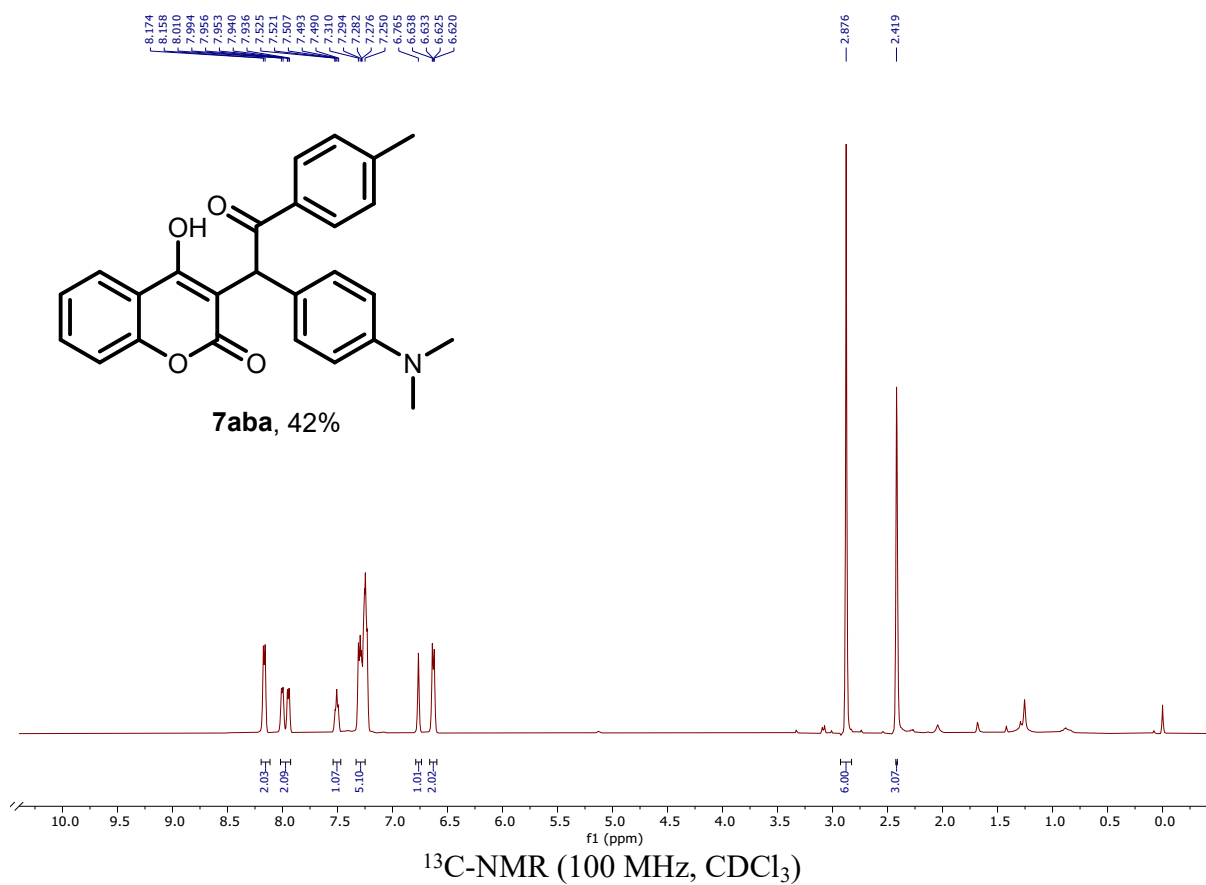


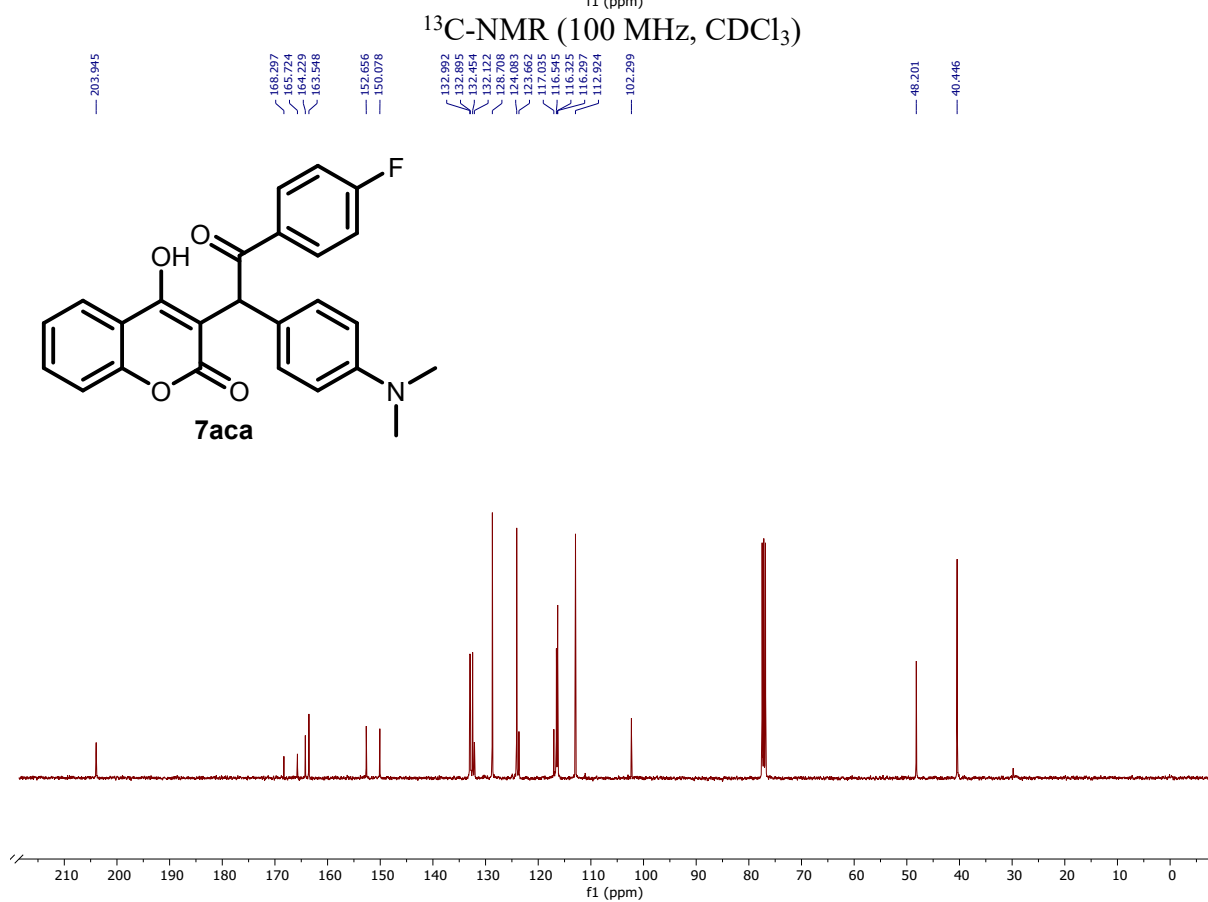
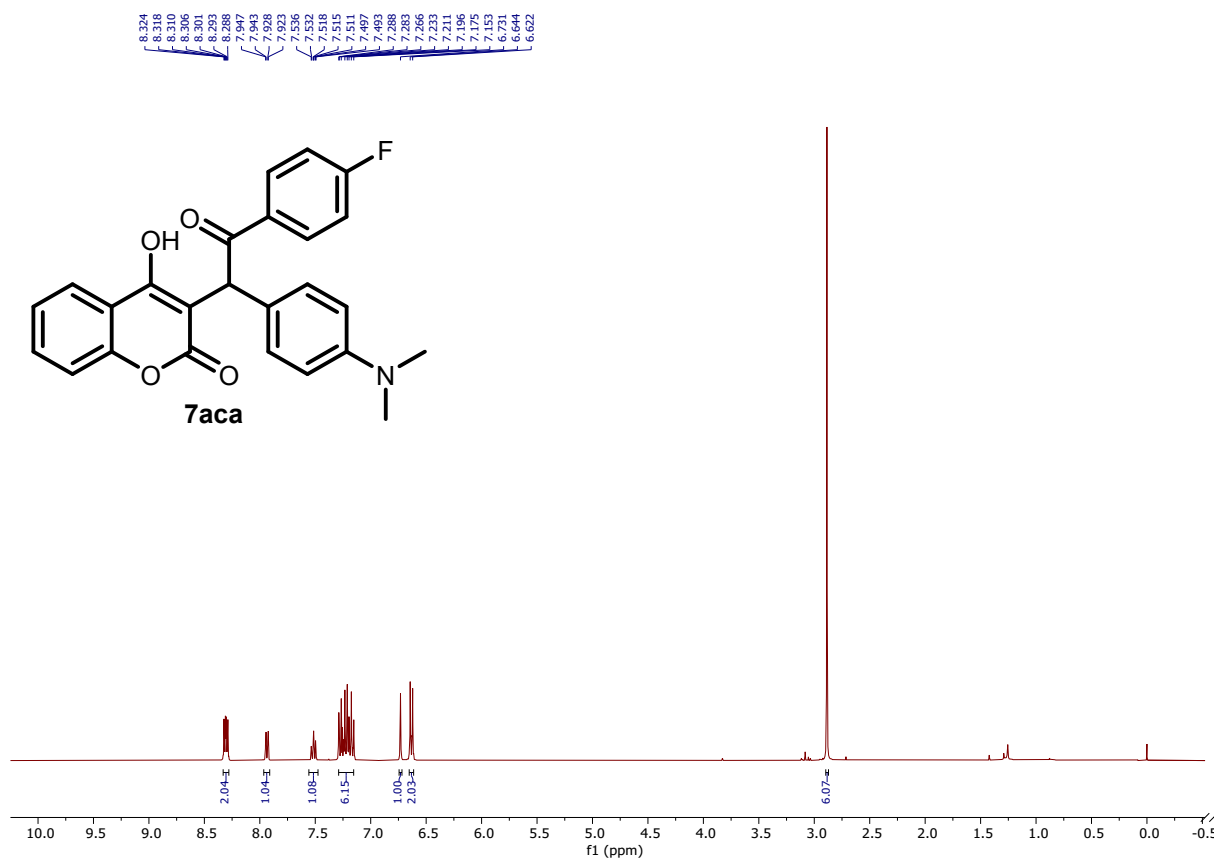


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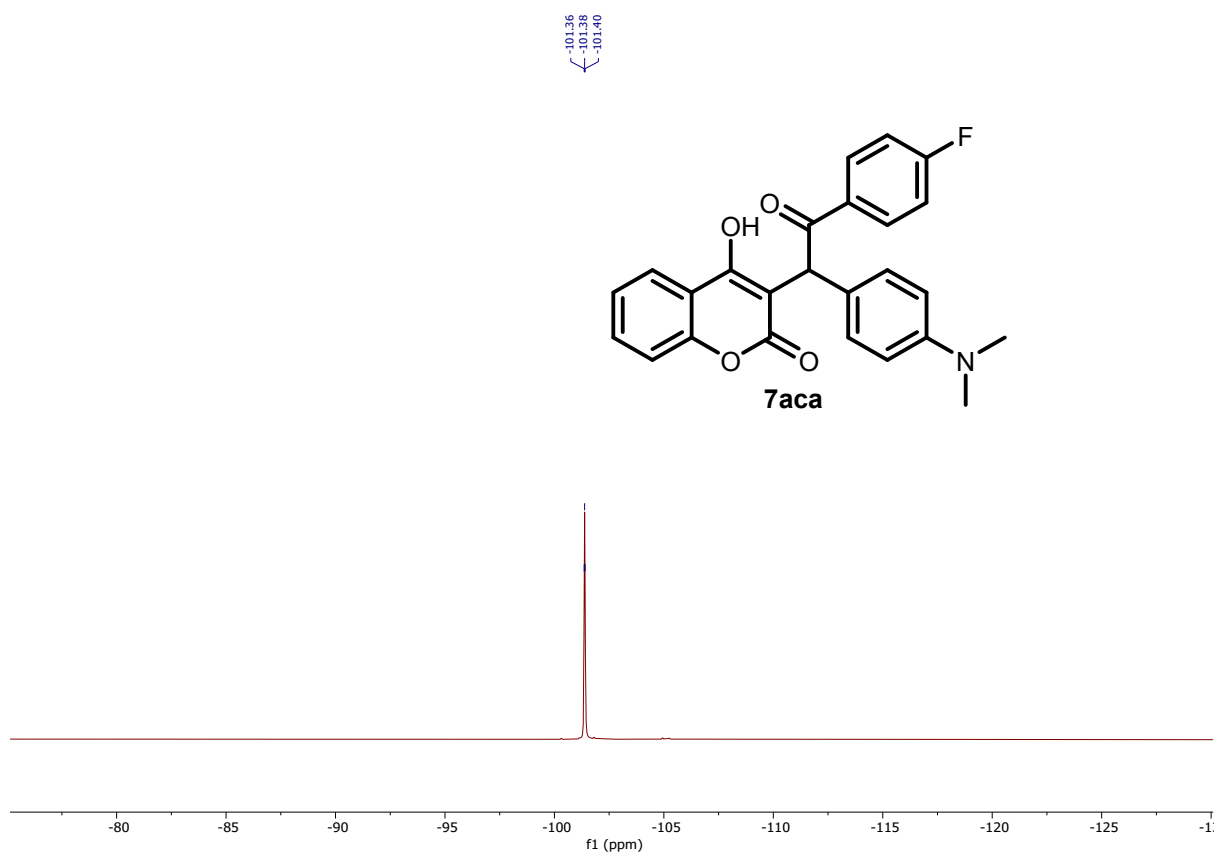


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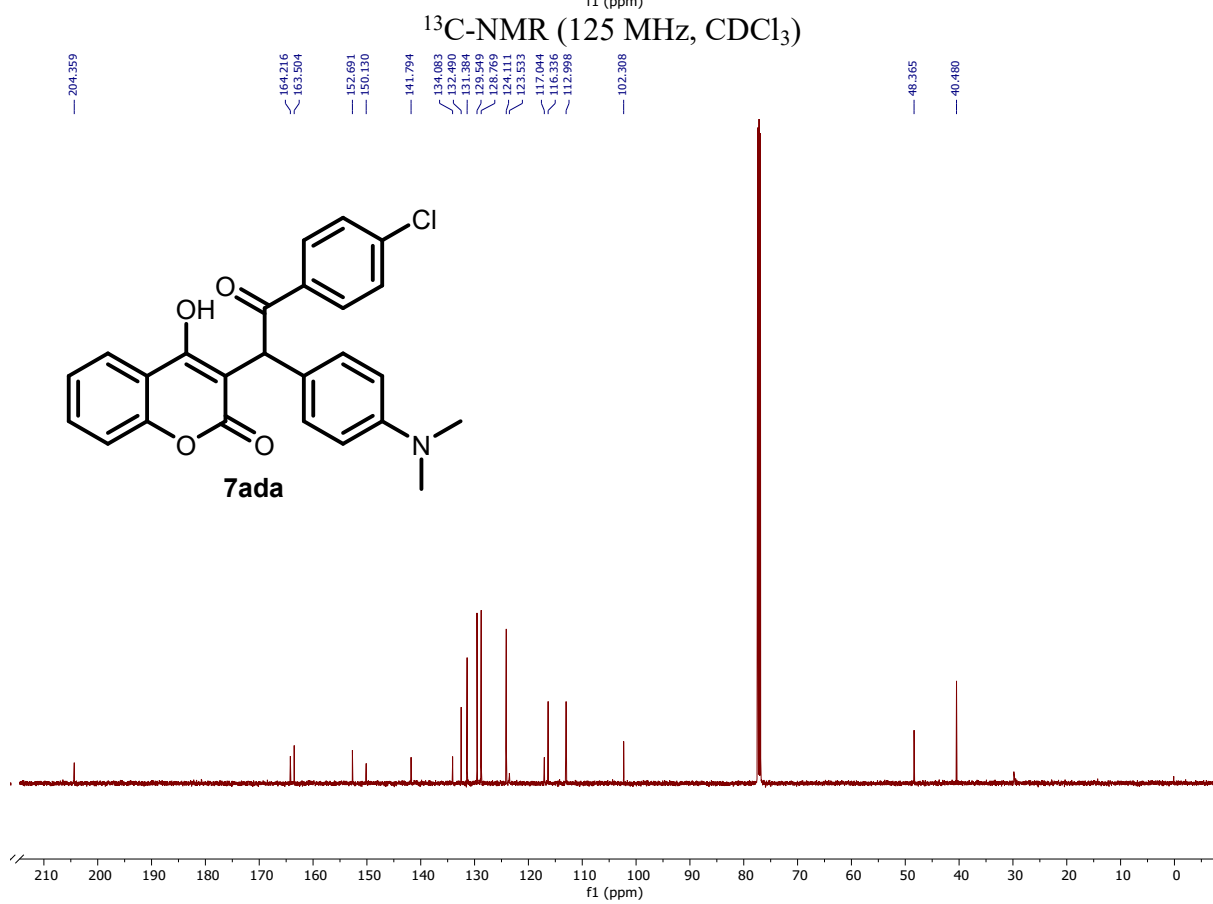
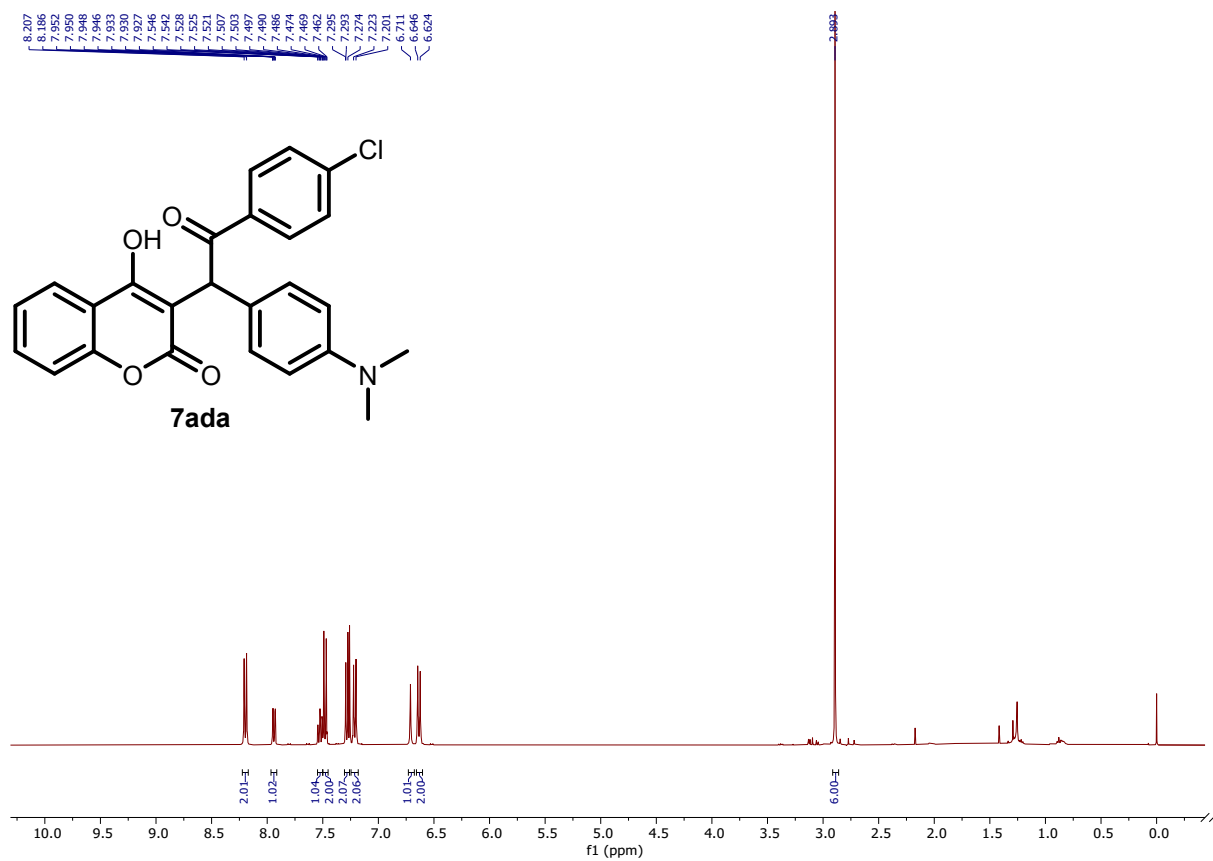




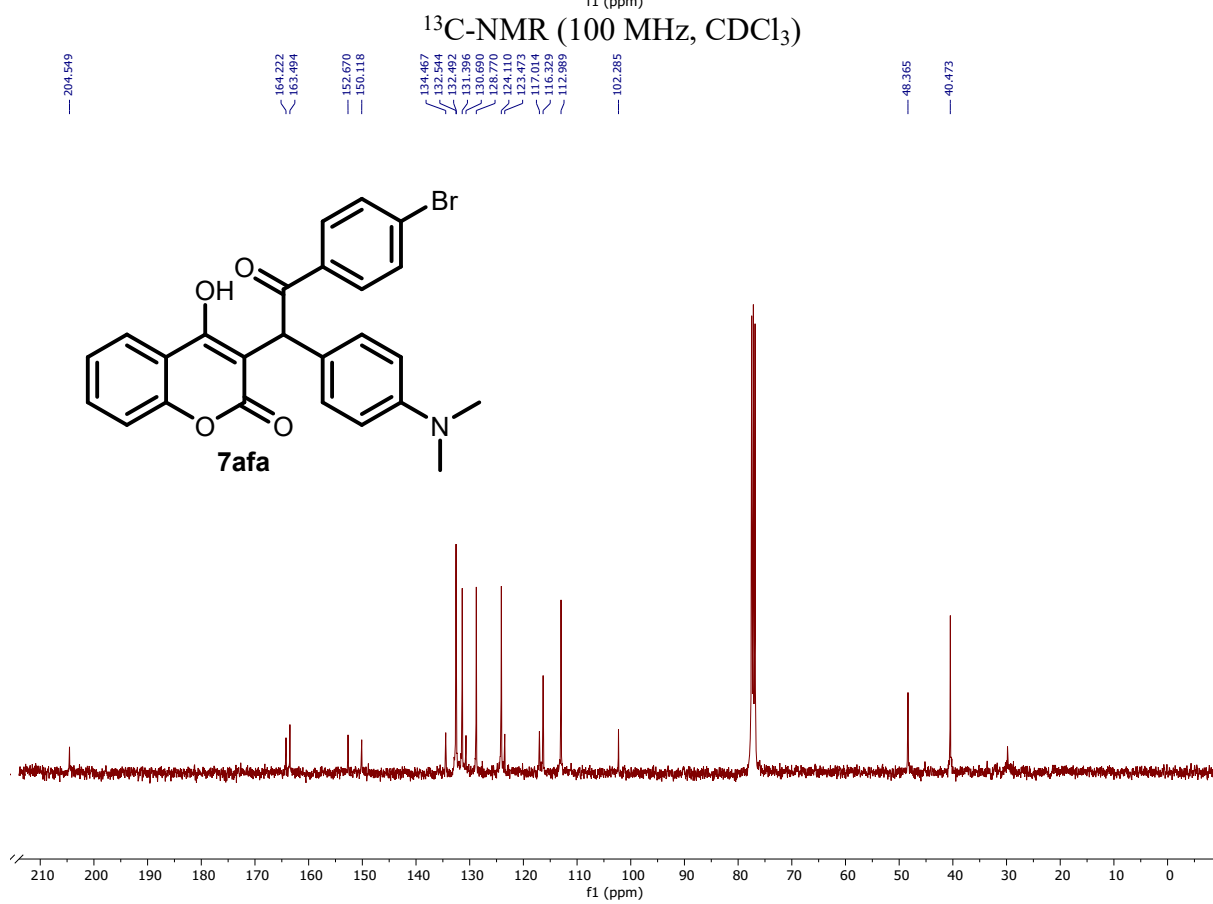
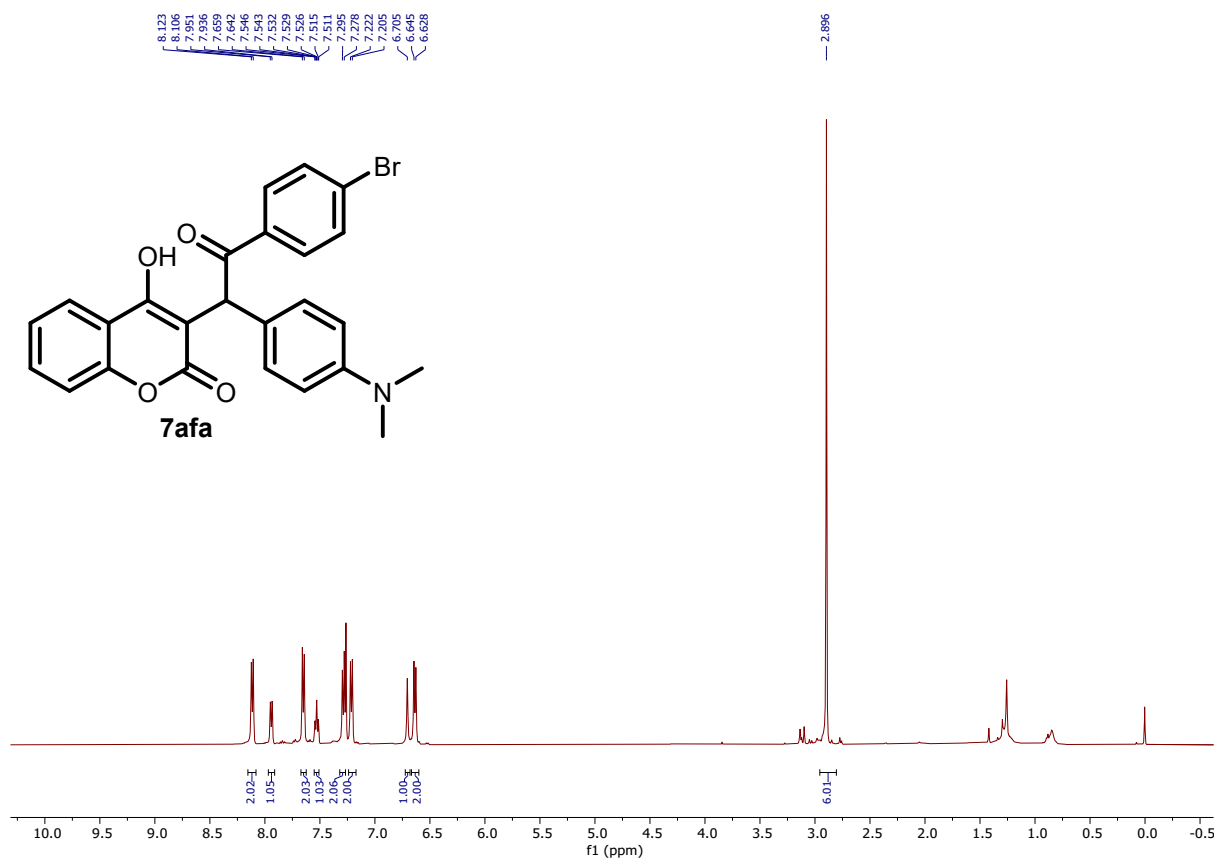
¹⁹F NMR (376 MHz, CDCl₃)



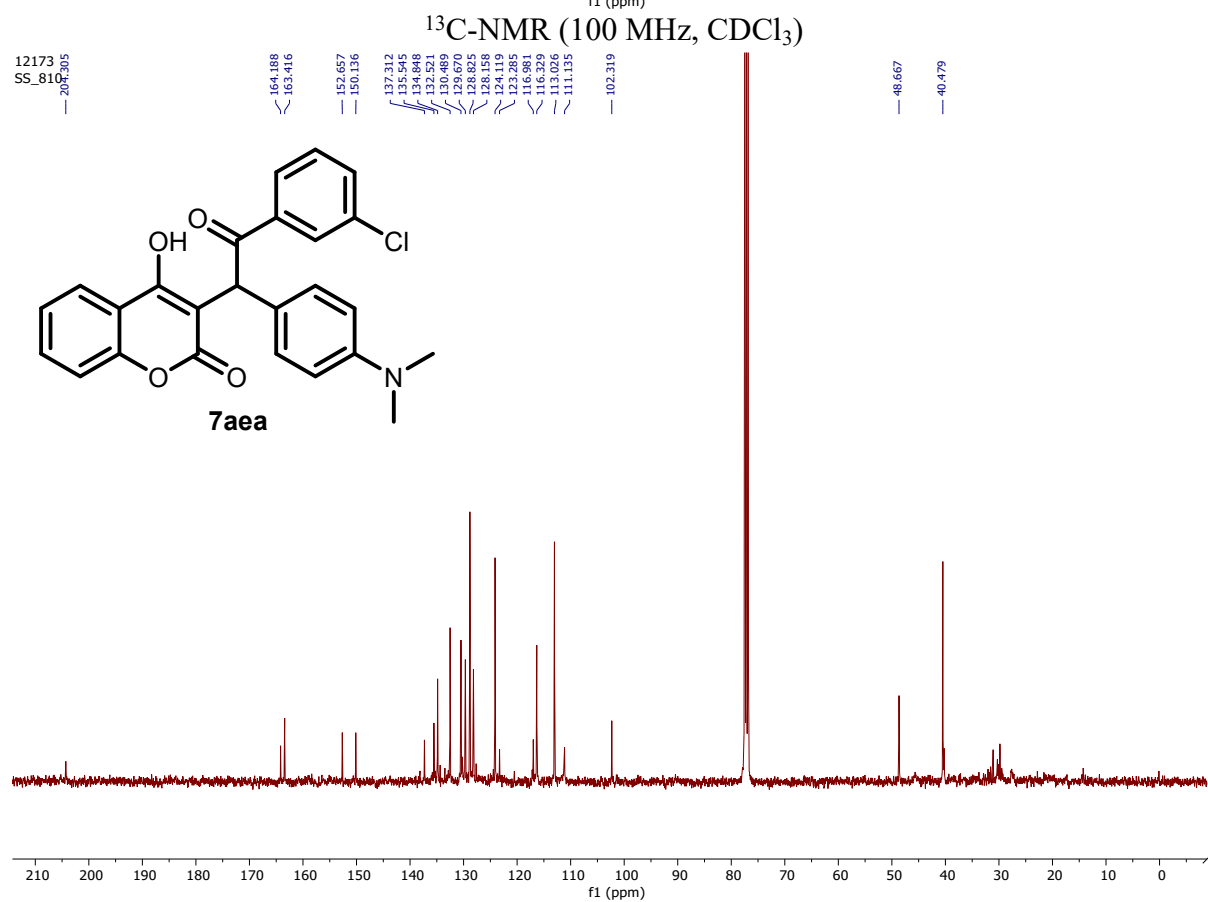
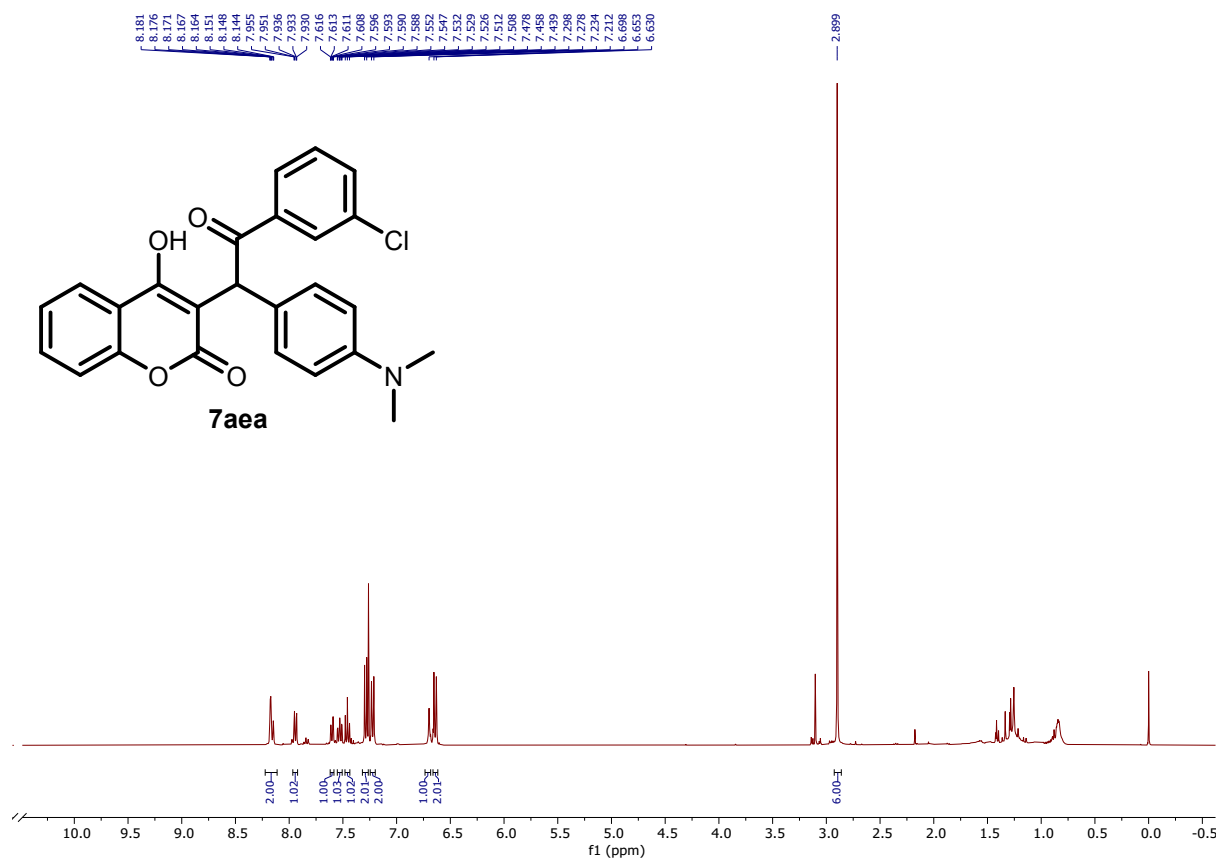
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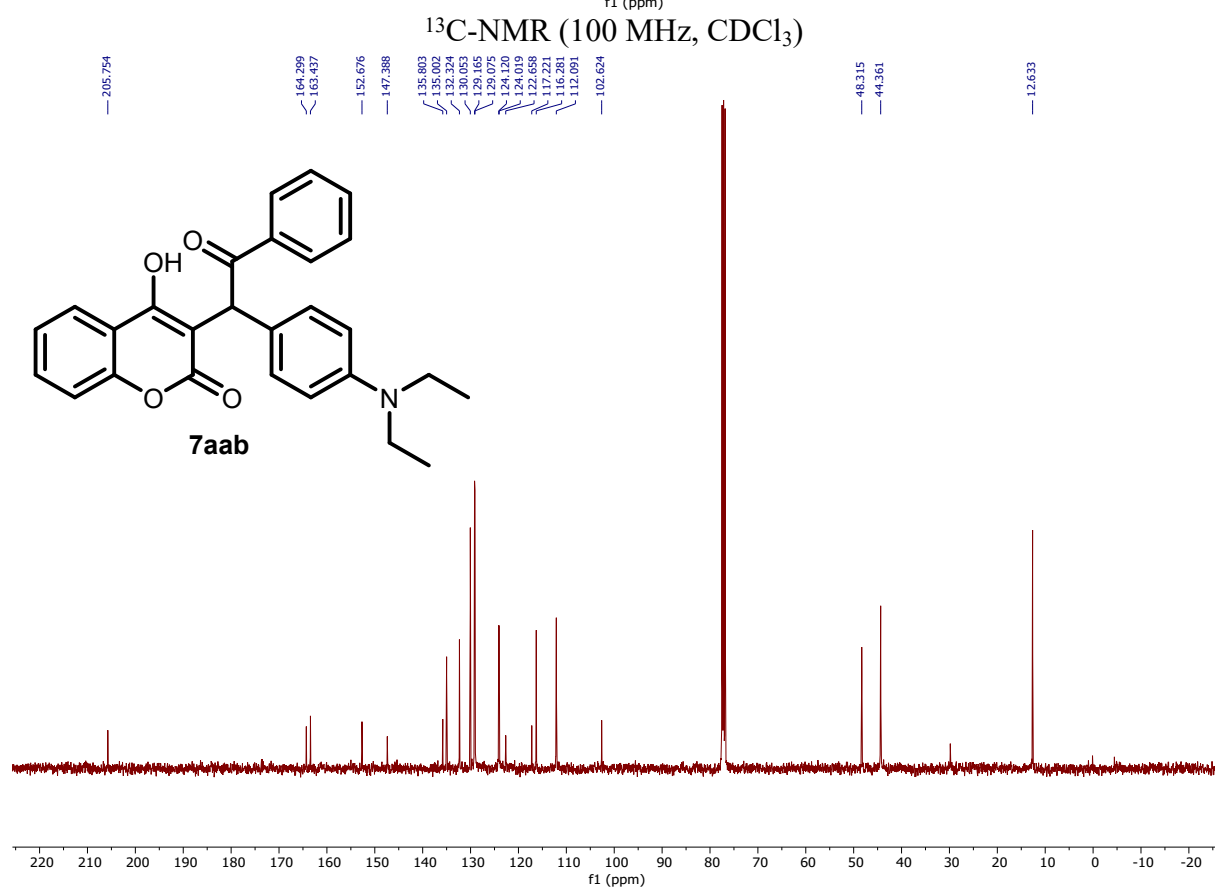
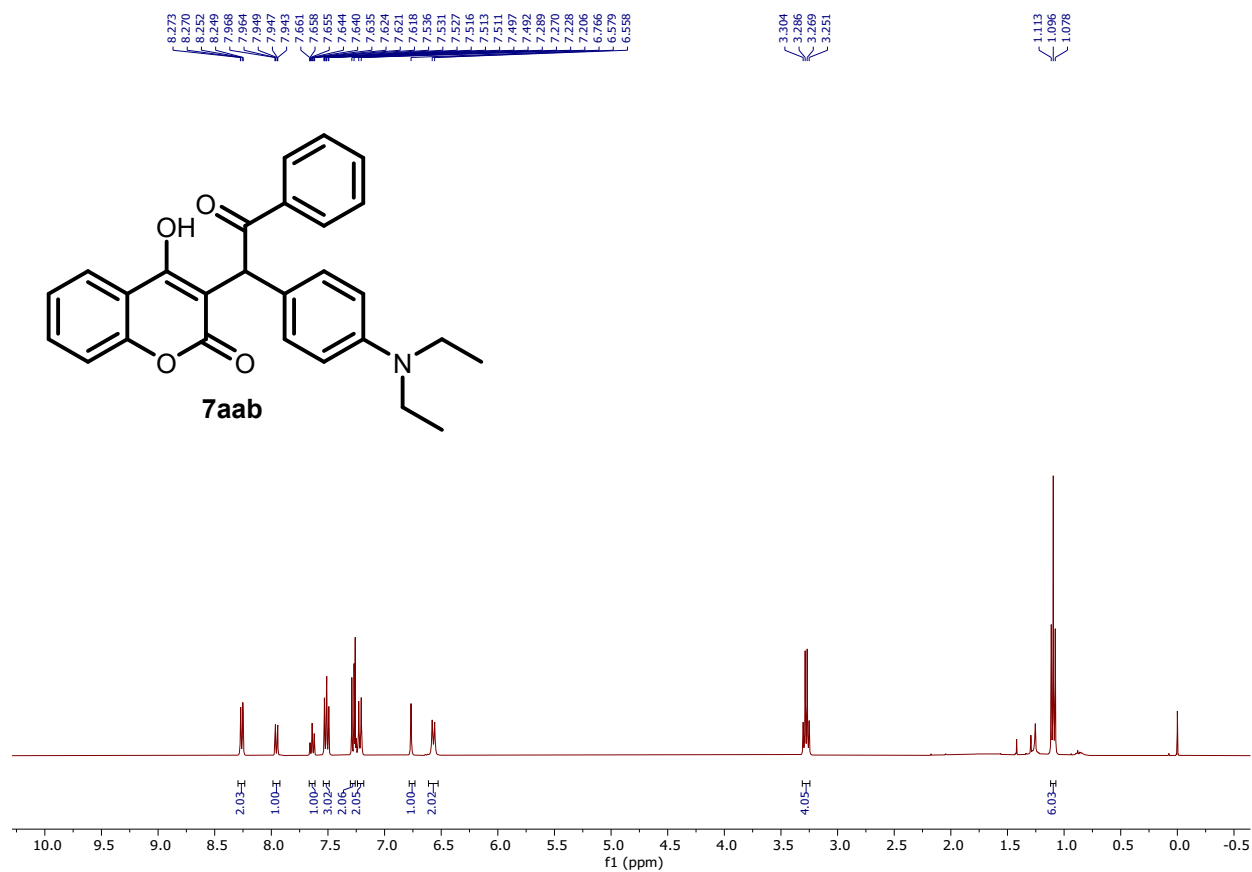
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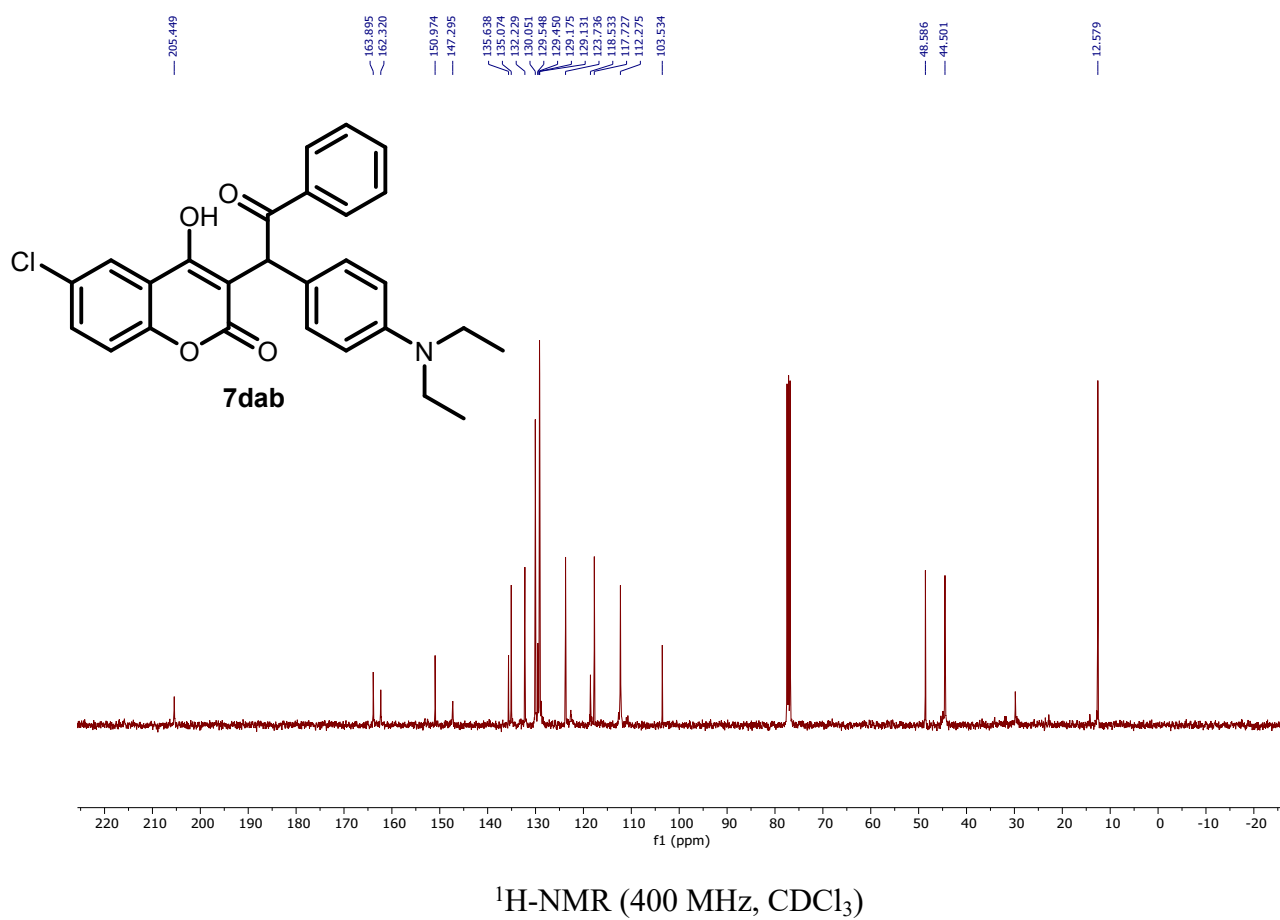
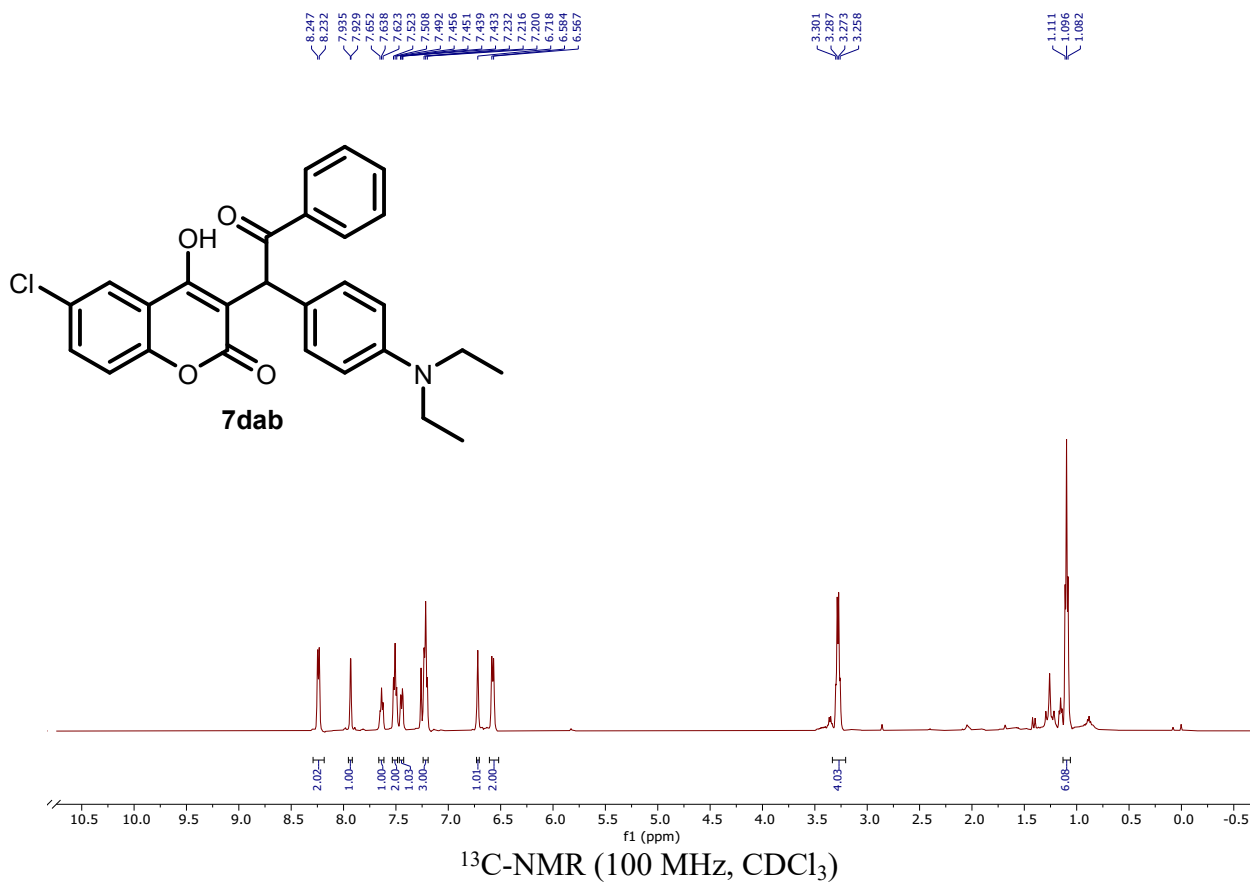
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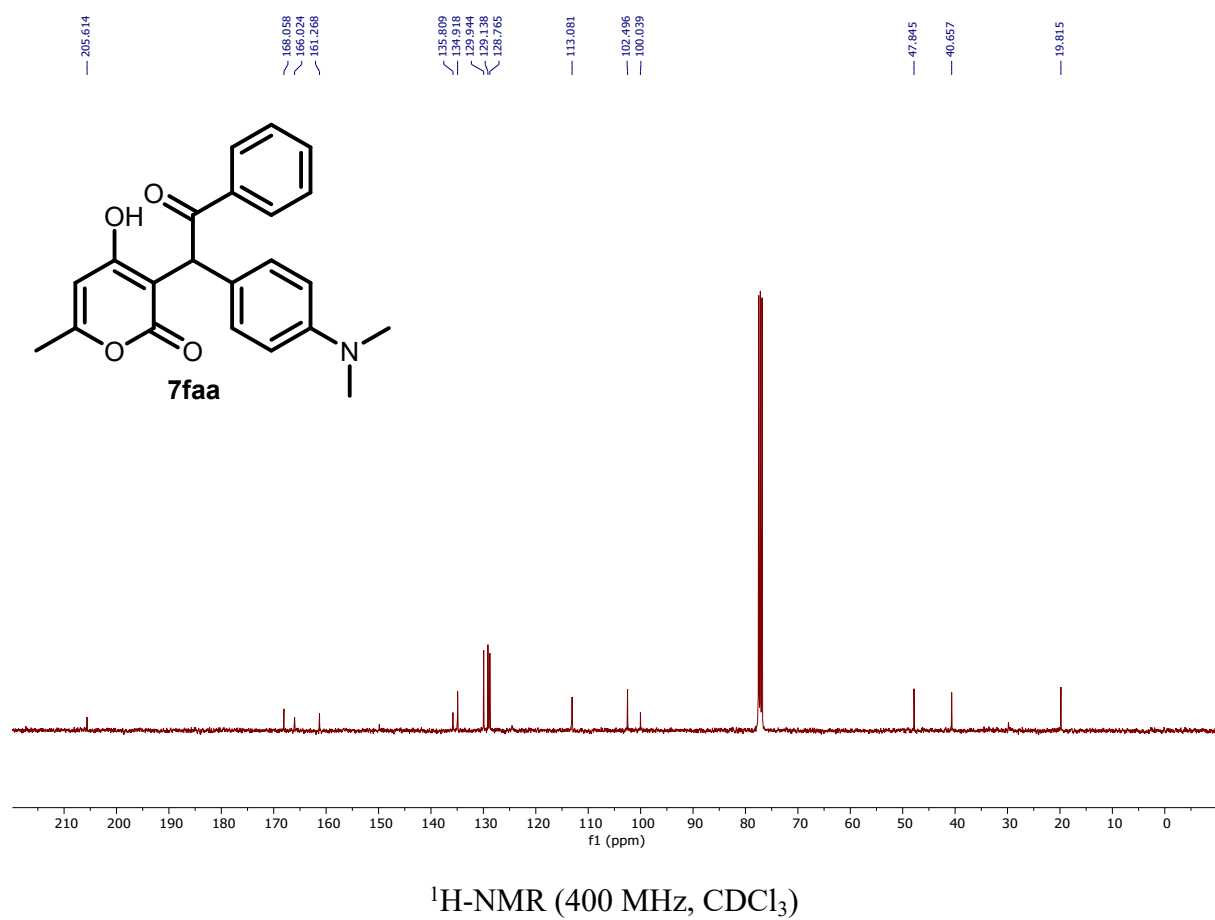
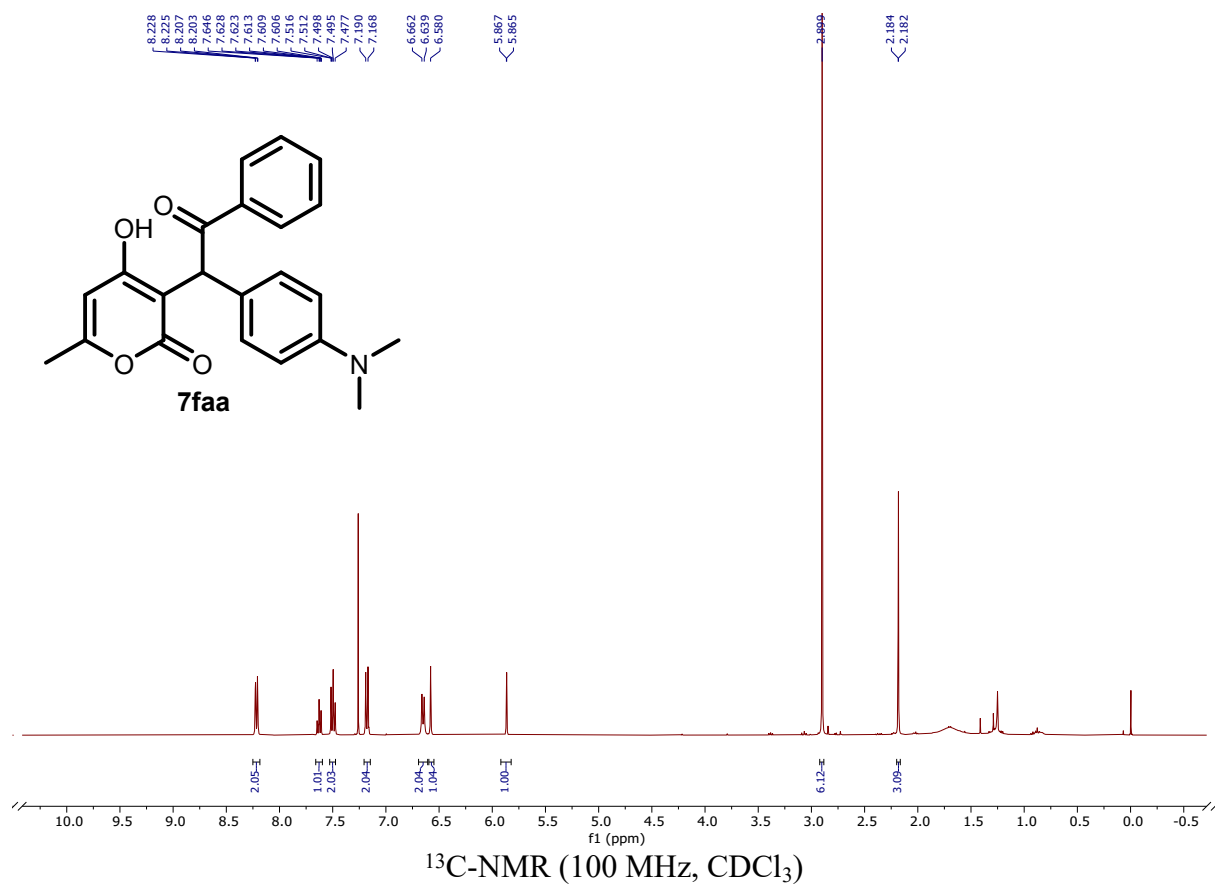


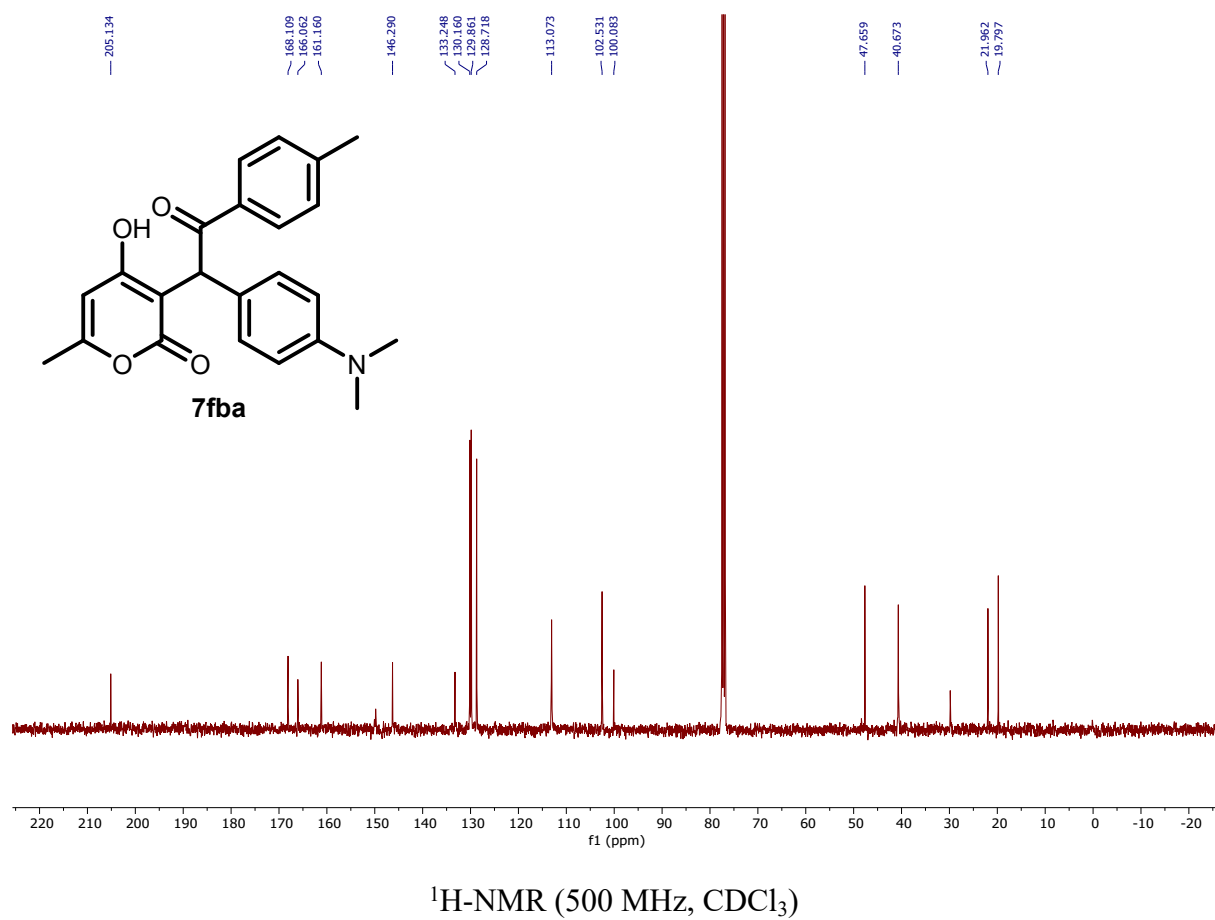
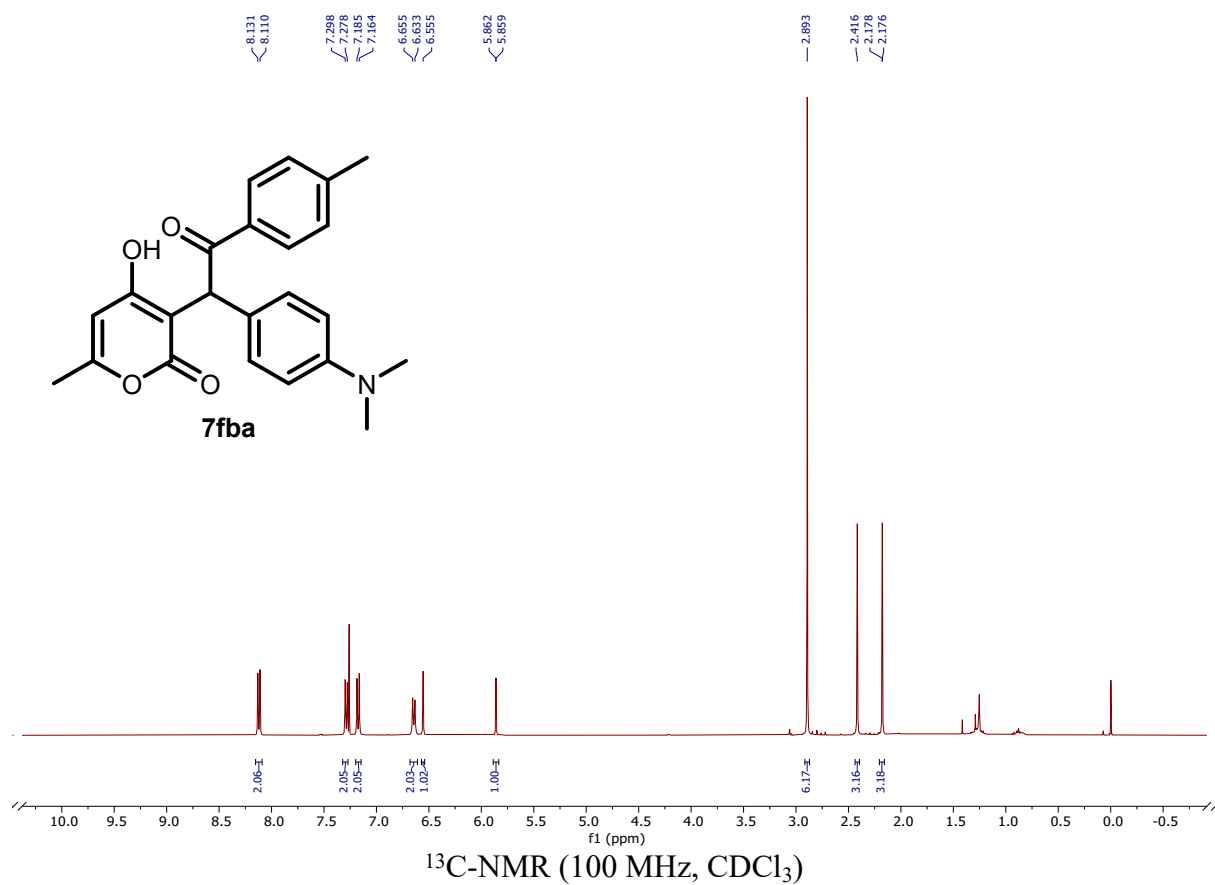
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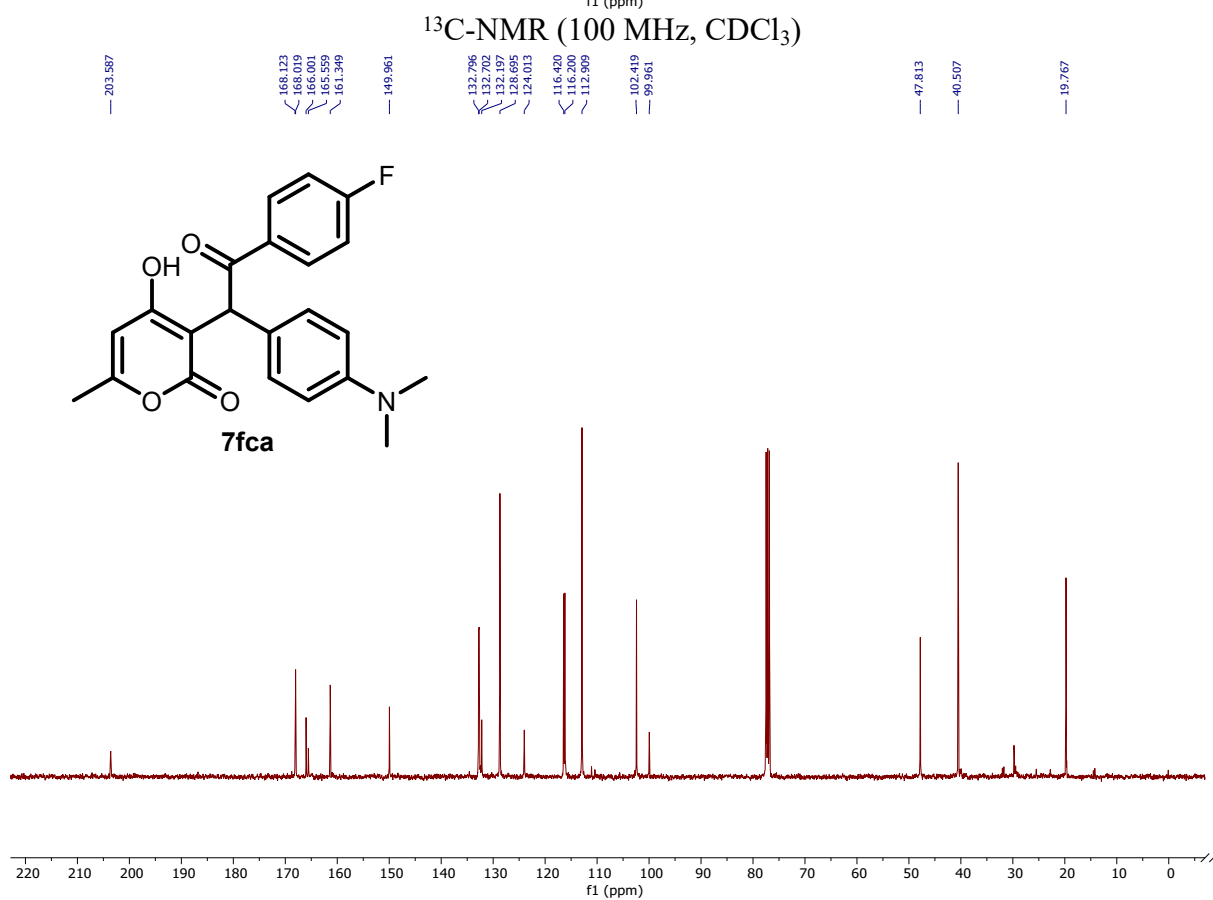
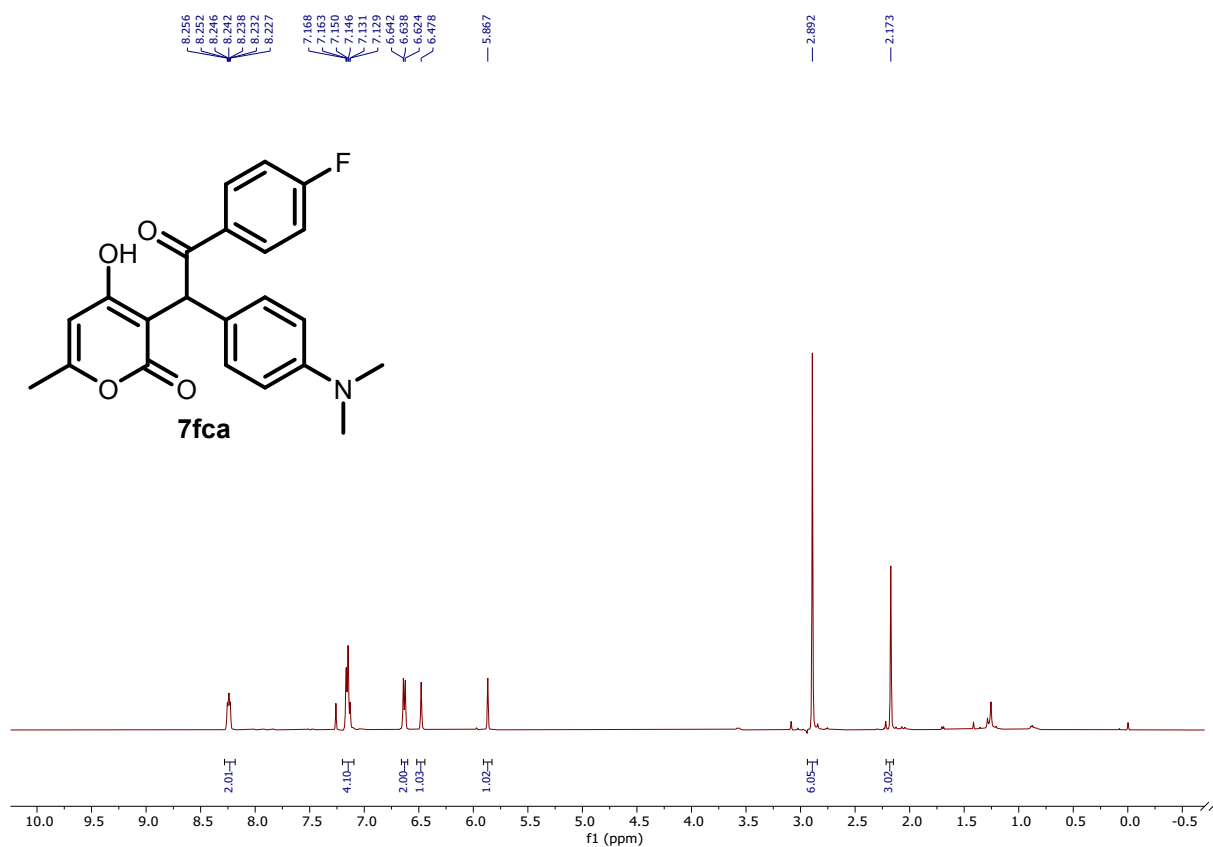


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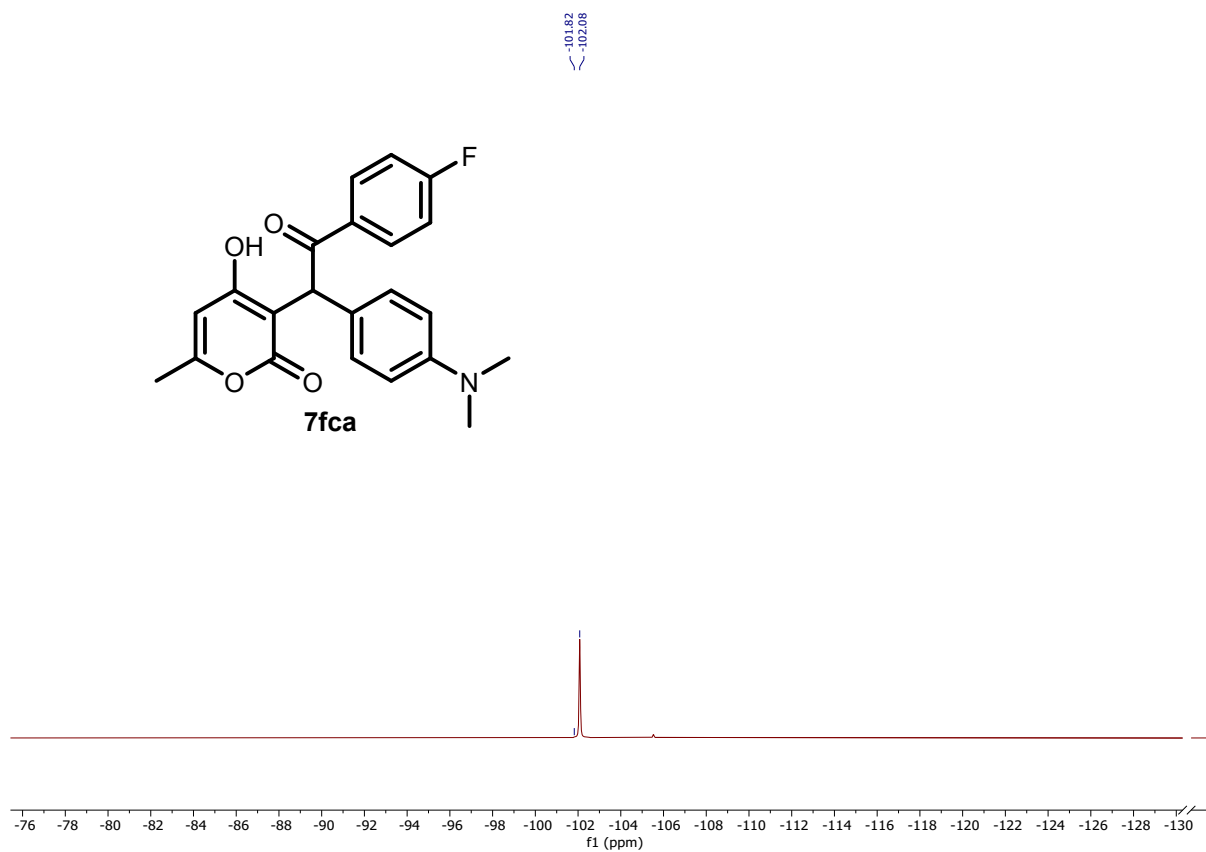




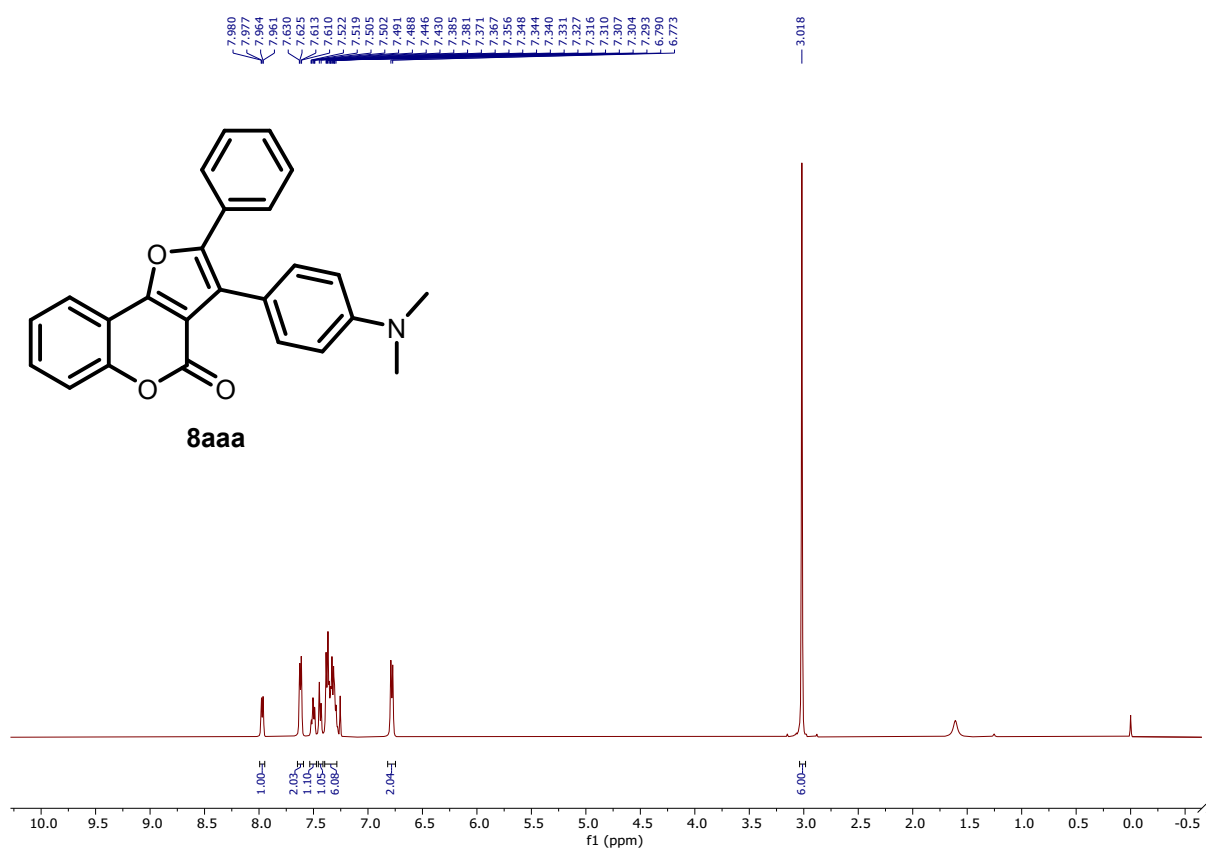




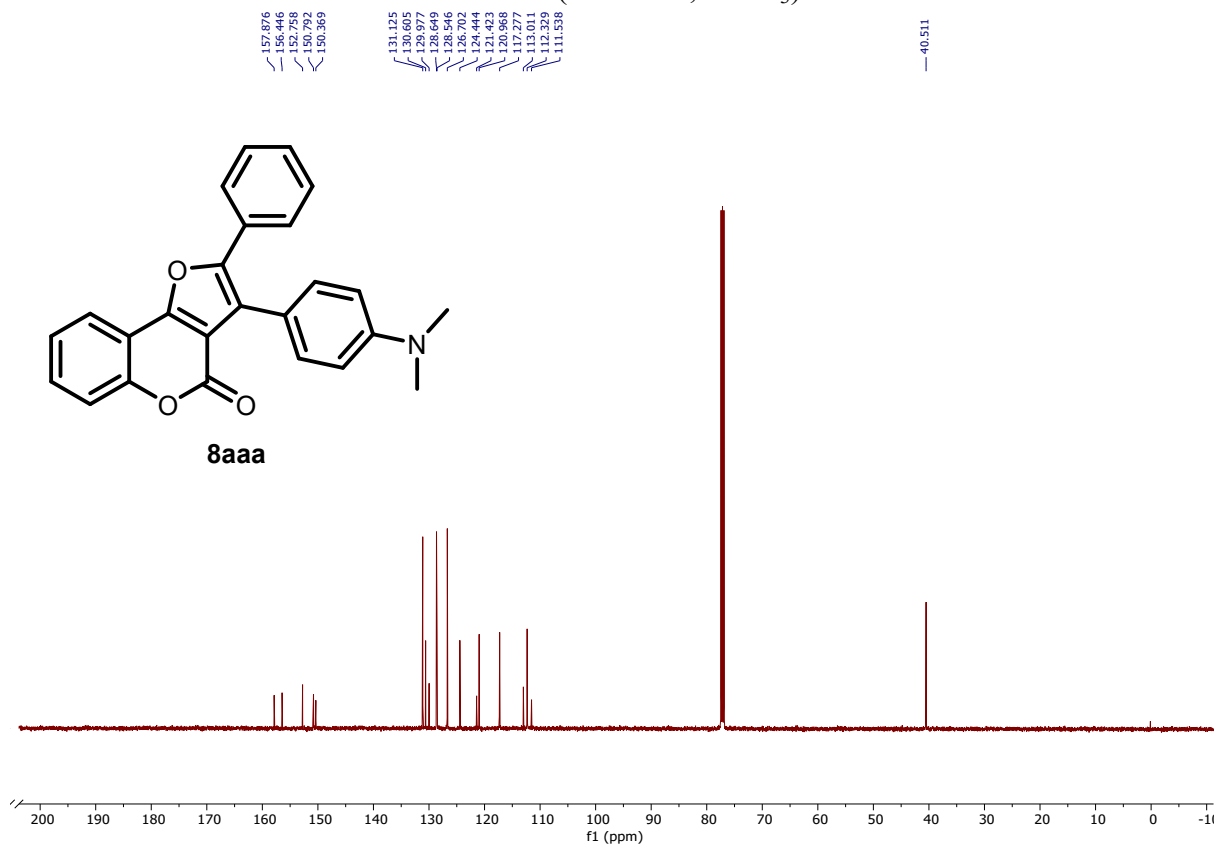
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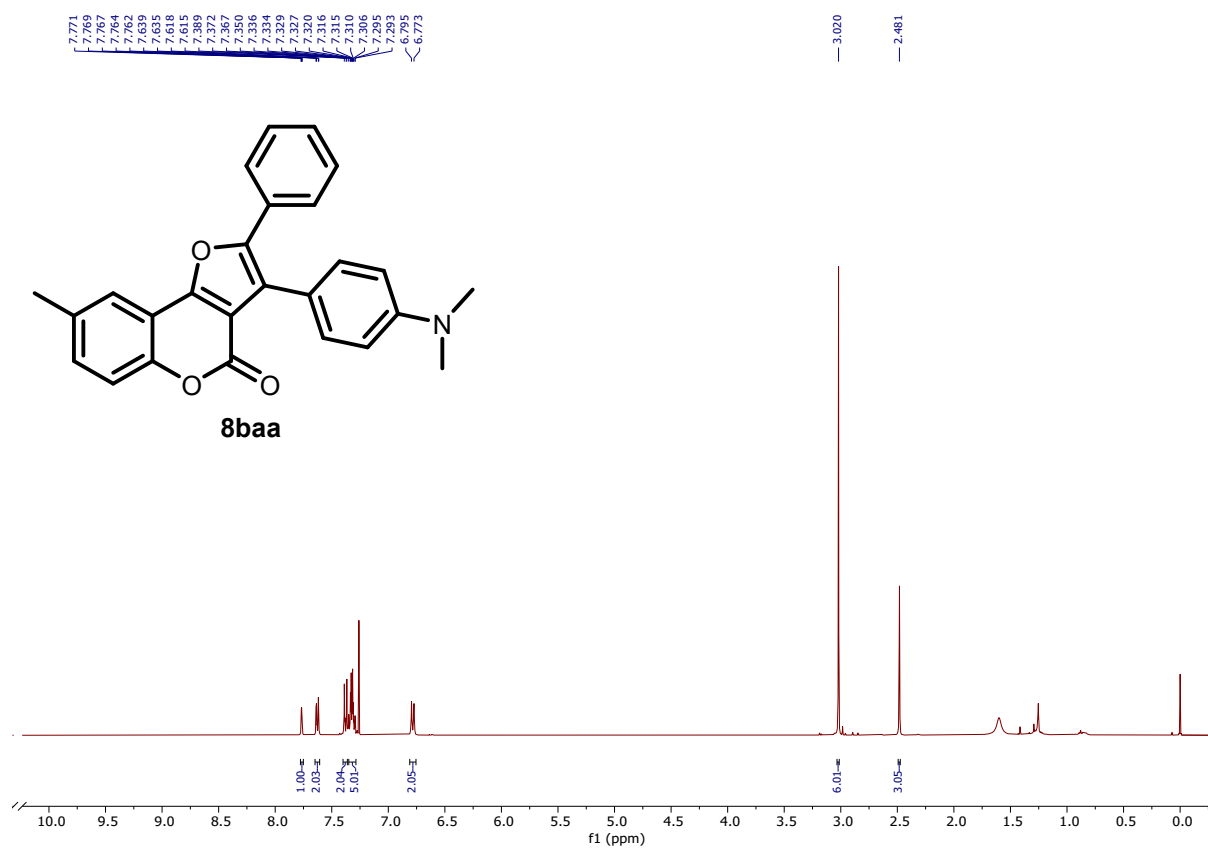
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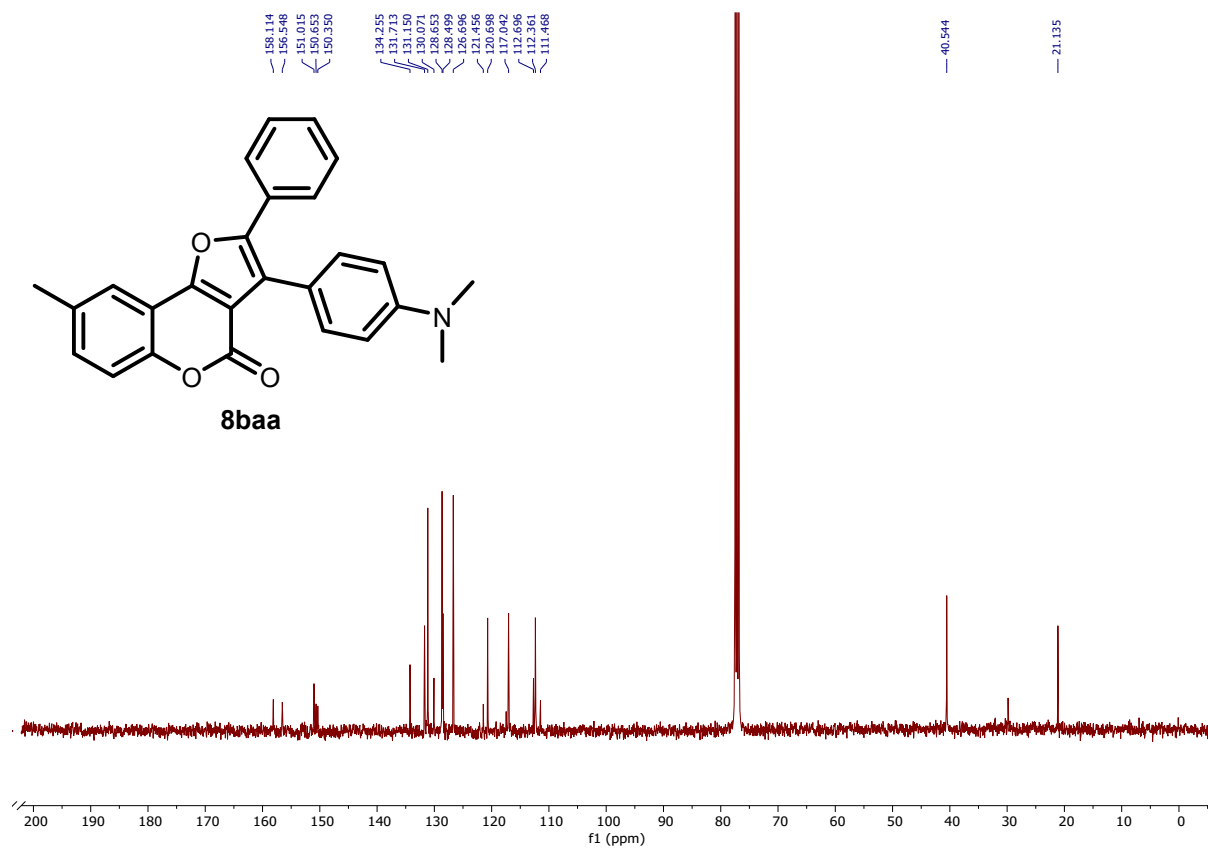
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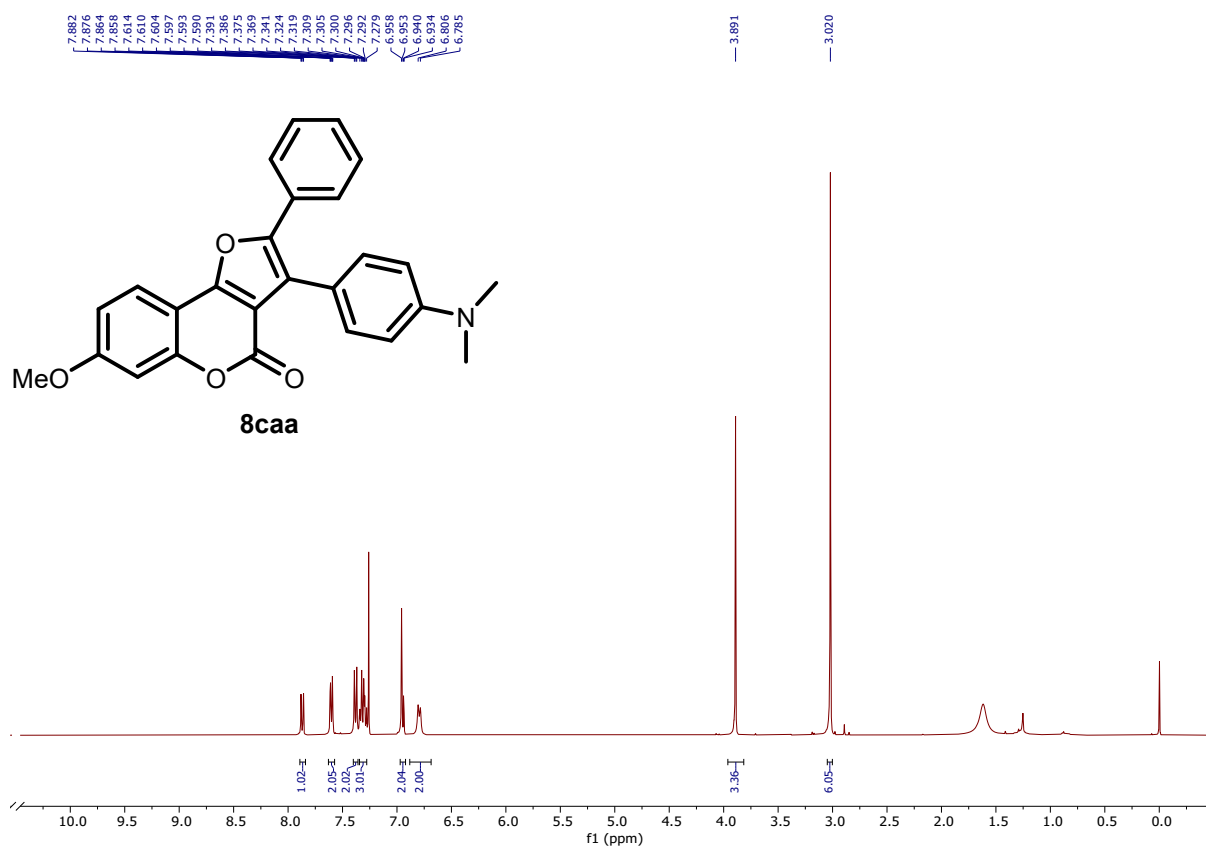
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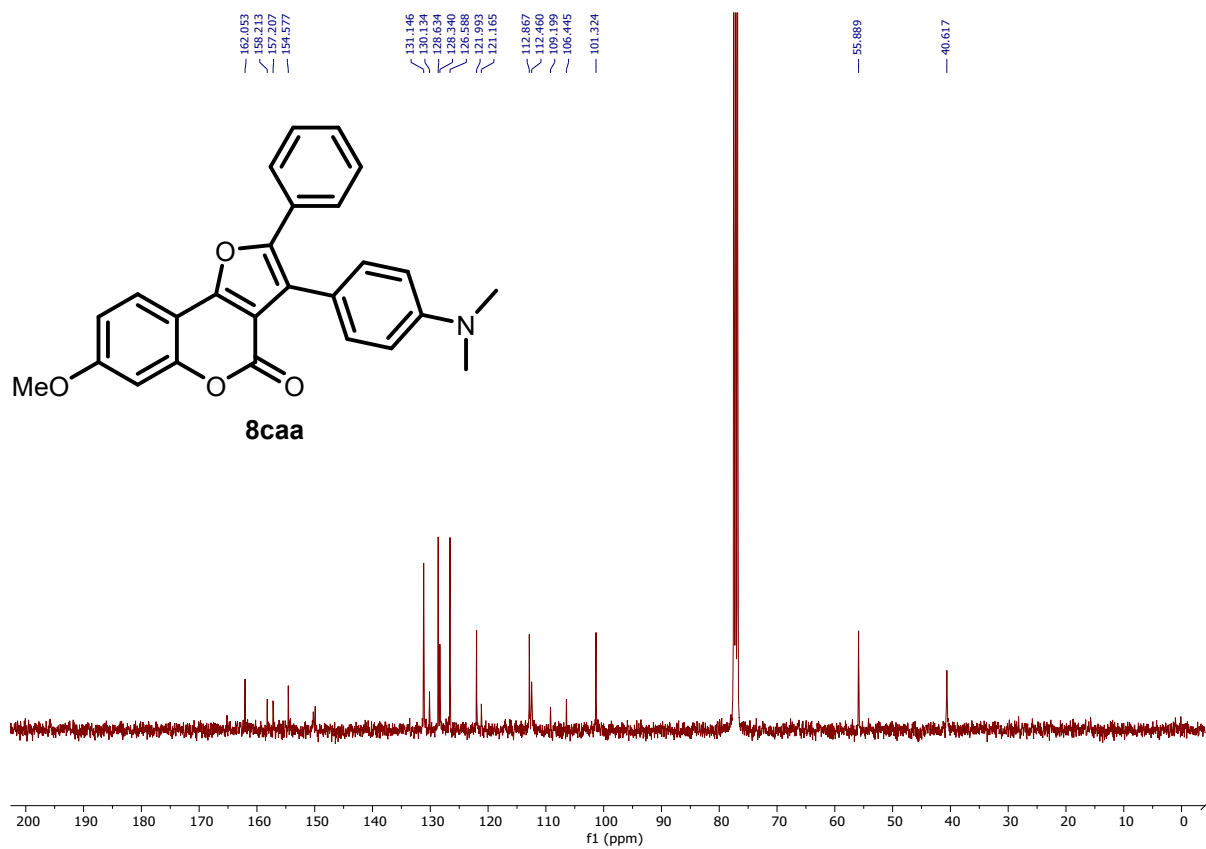
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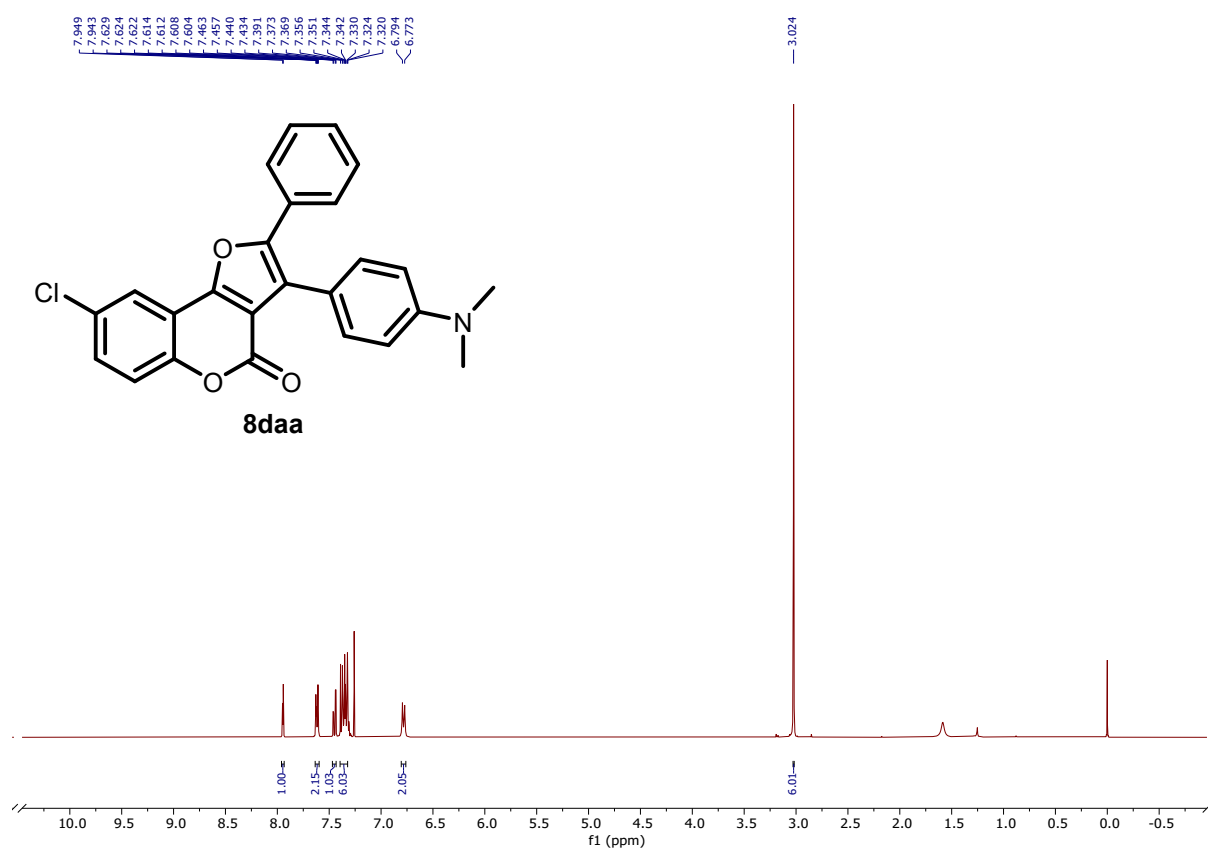
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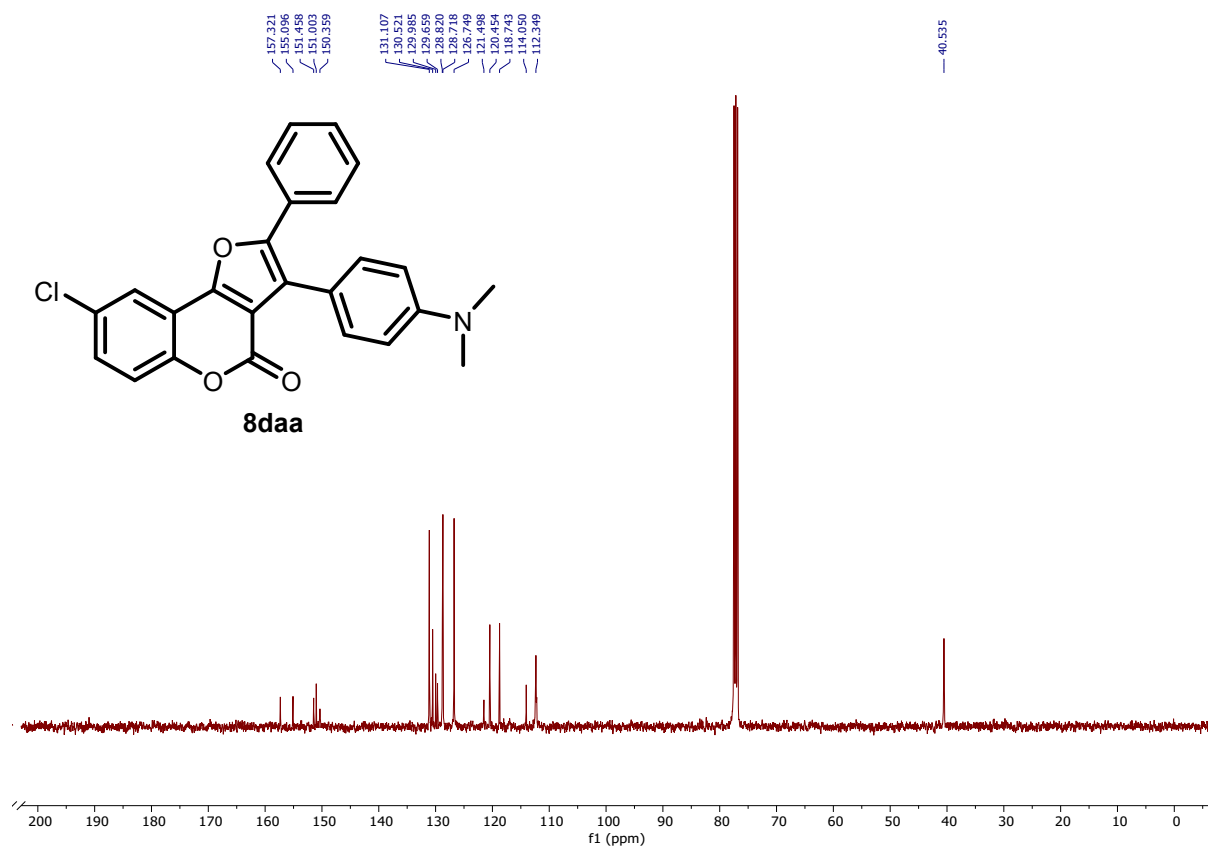
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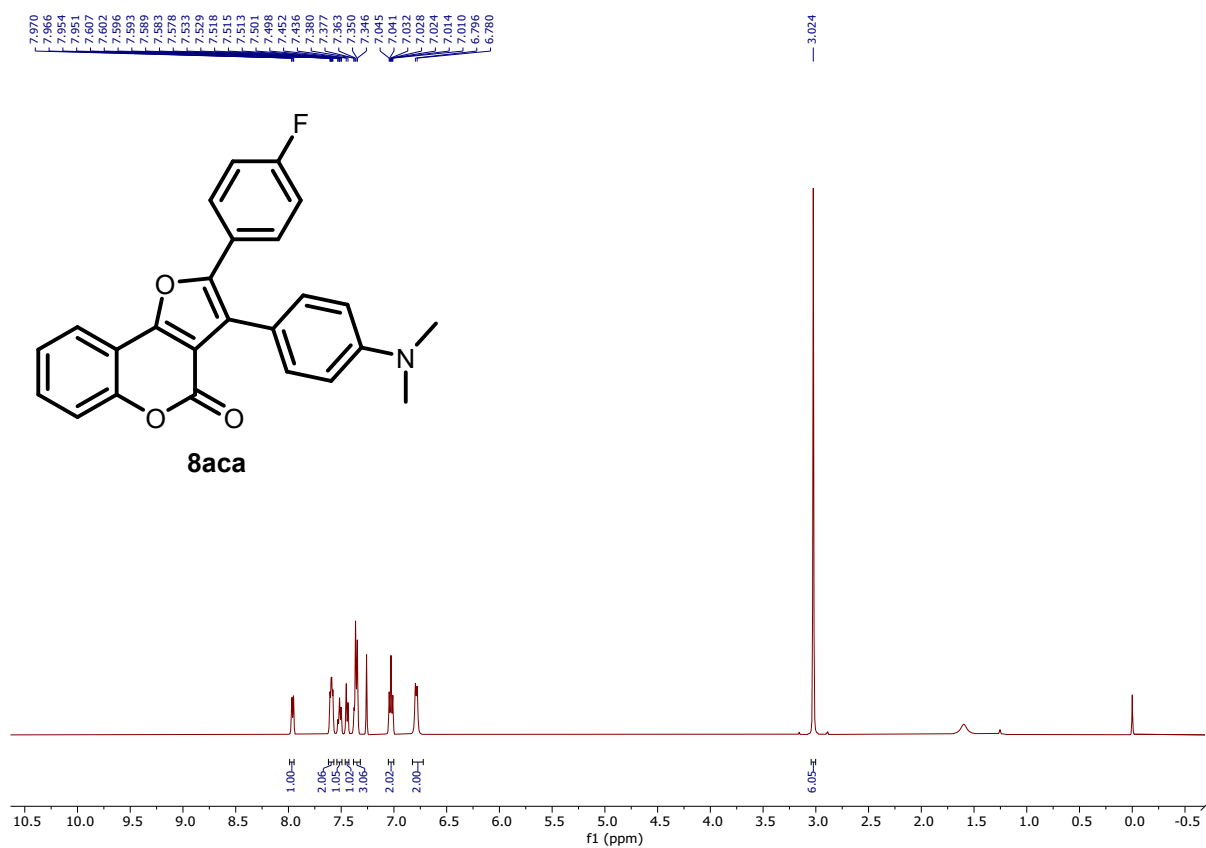
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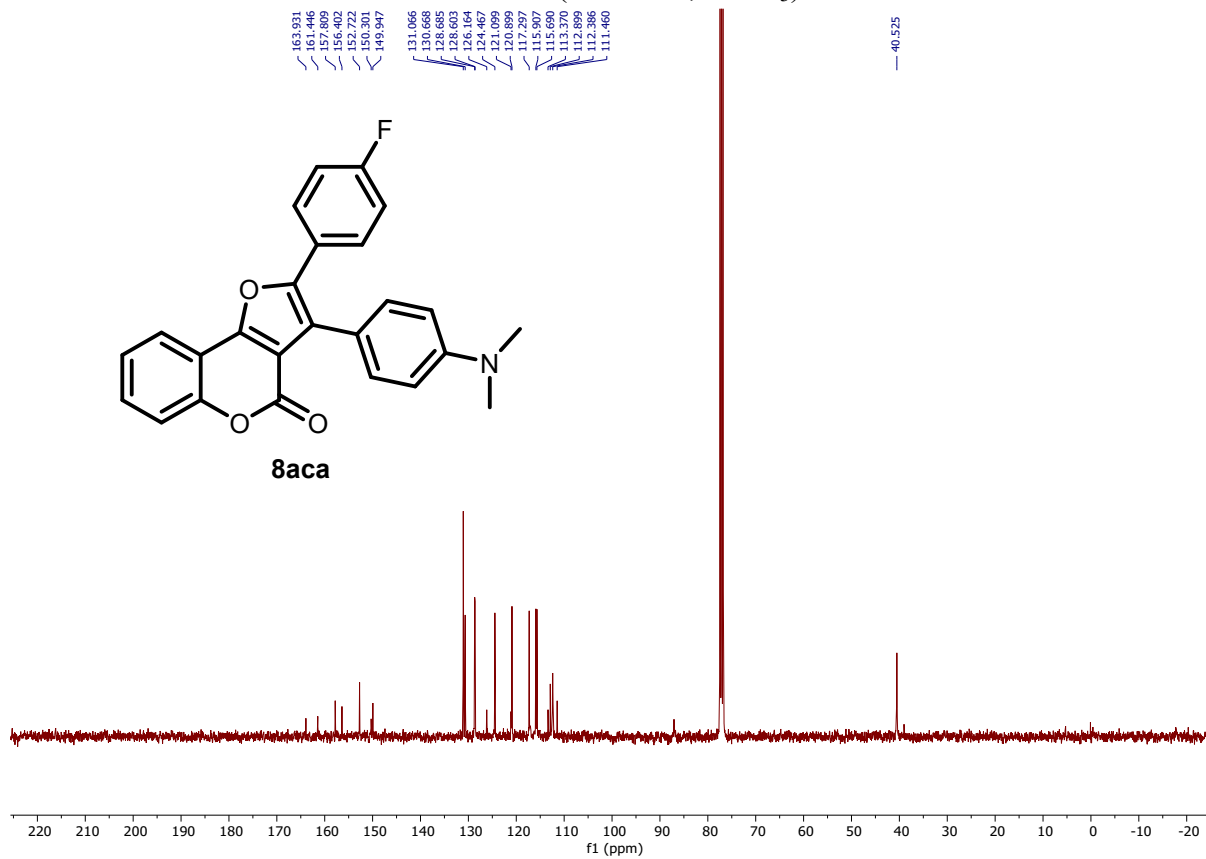
¹³C-NMR (100 MHz, CDCl₃)



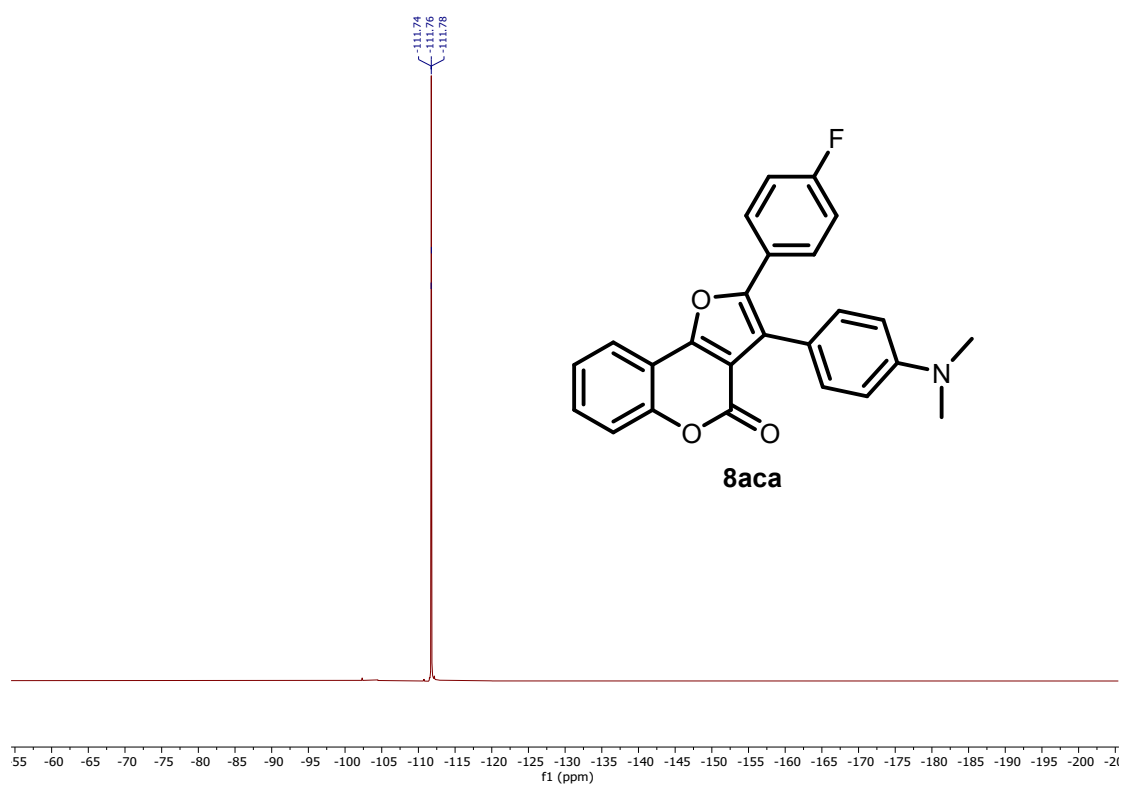
¹H-NMR (500 MHz, CDCl₃)



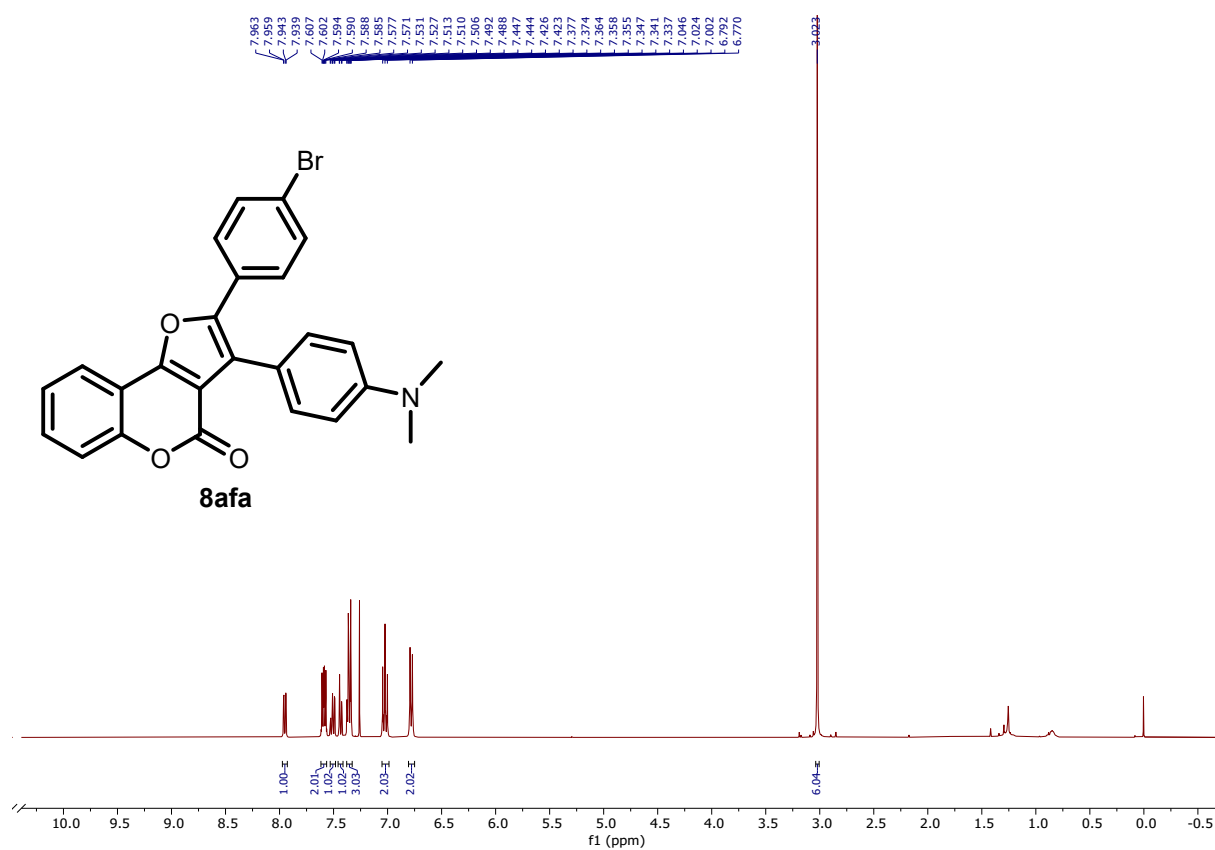
¹³C-NMR (100 MHz, CDCl₃)



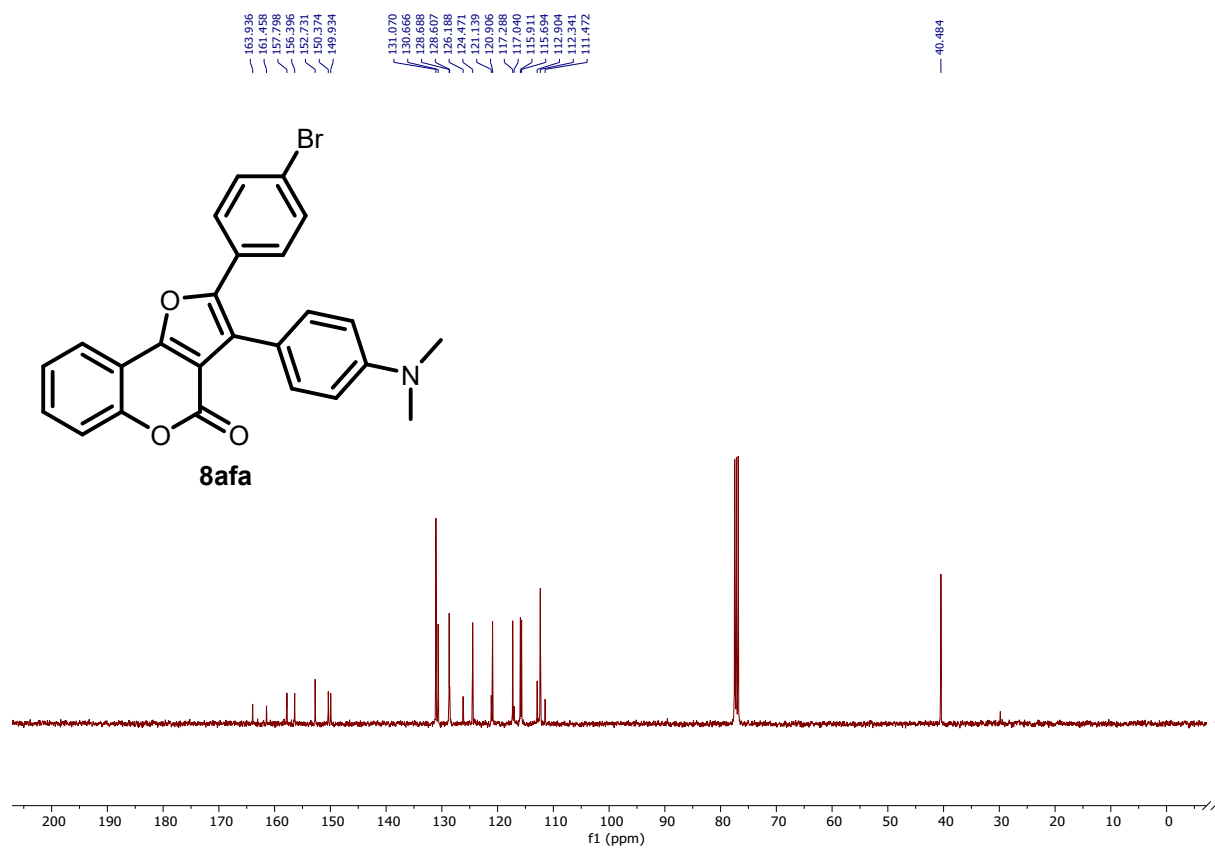
^{19}F NMR (376 MHz, CDCl_3)

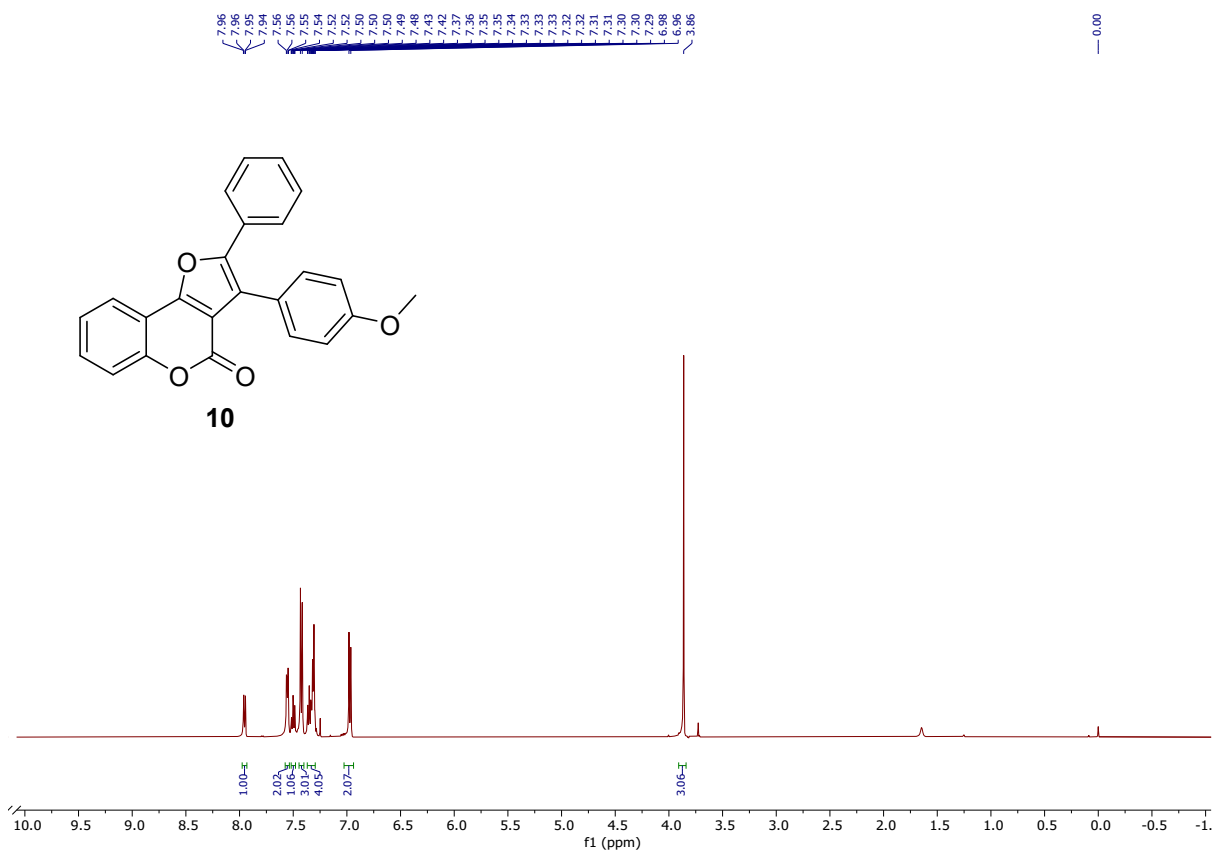
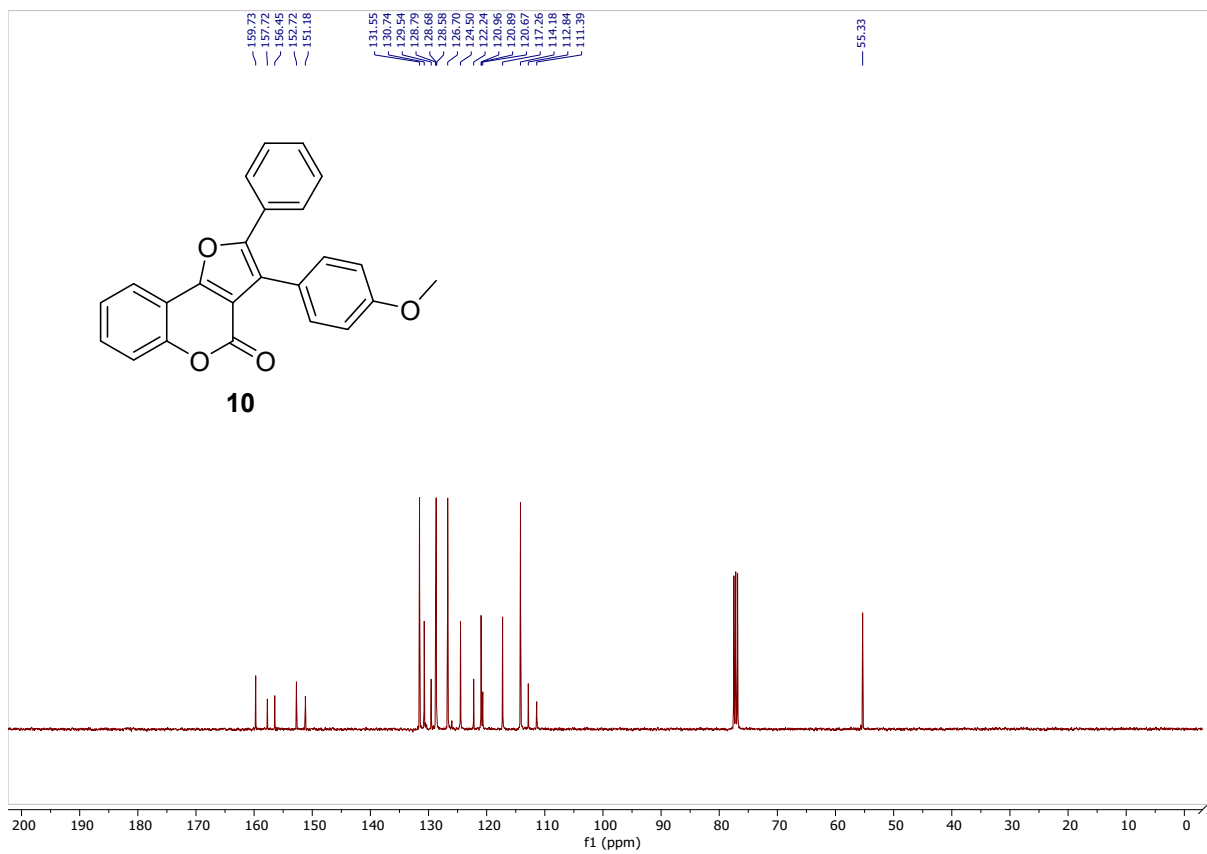


¹H-NMR (400 MHz, CDCl₃)

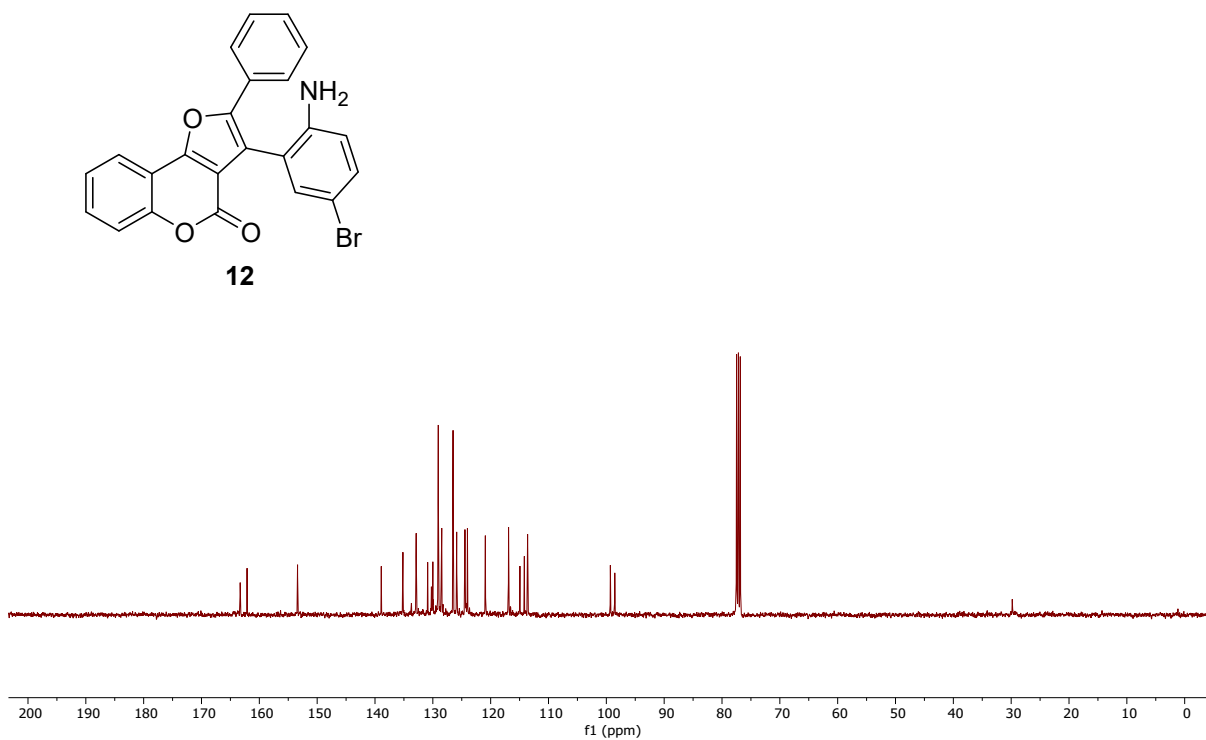
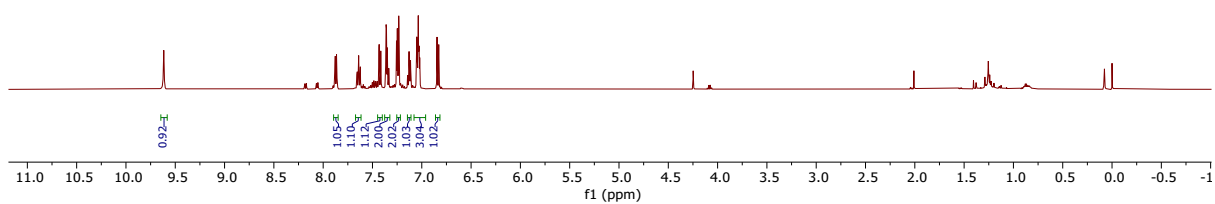
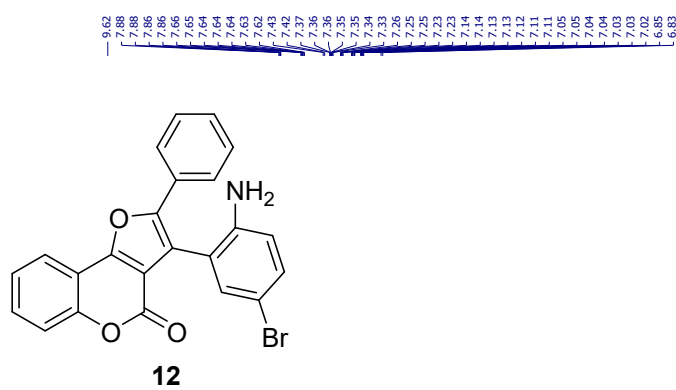


¹³C-NMR (100 MHz, CDCl₃)

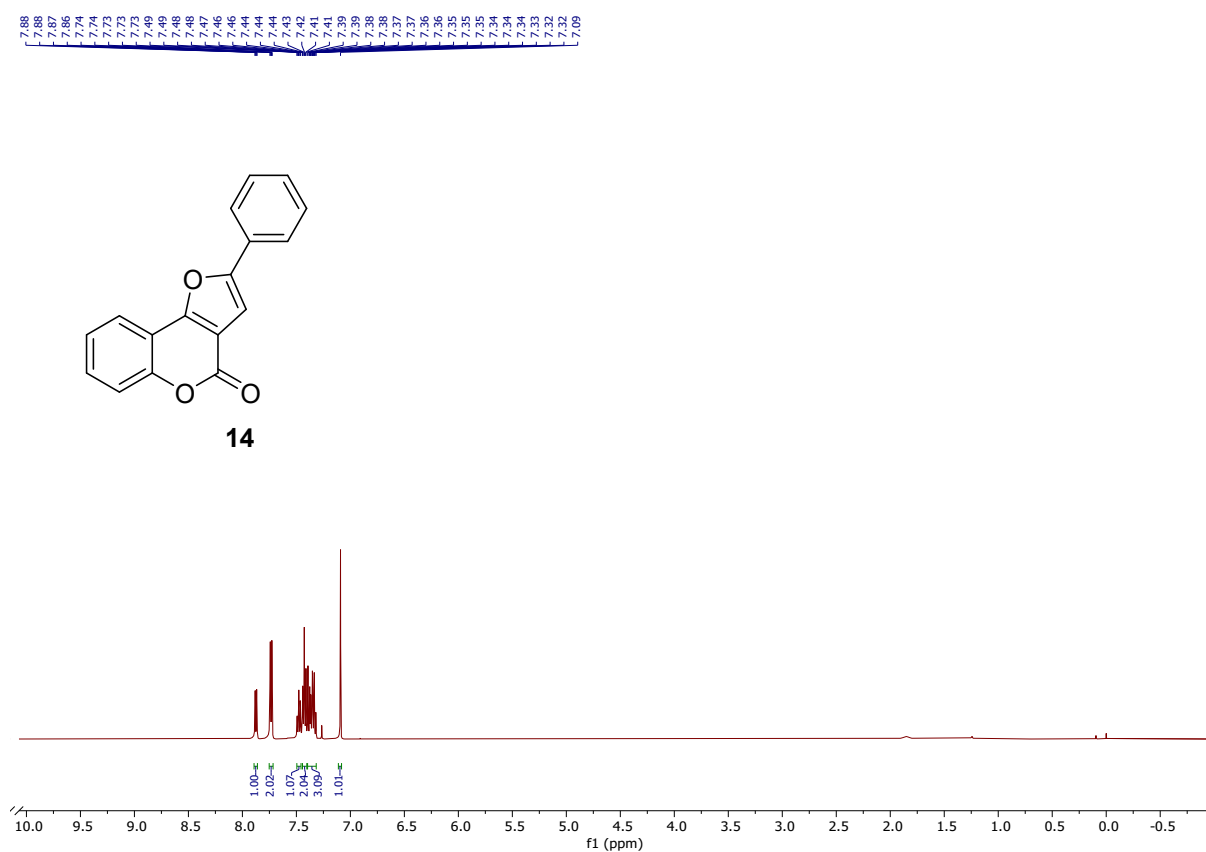


¹H-NMR (500 MHz, CDCl₃) ^{13}C -NMR (100 MHz, CDCl_3)

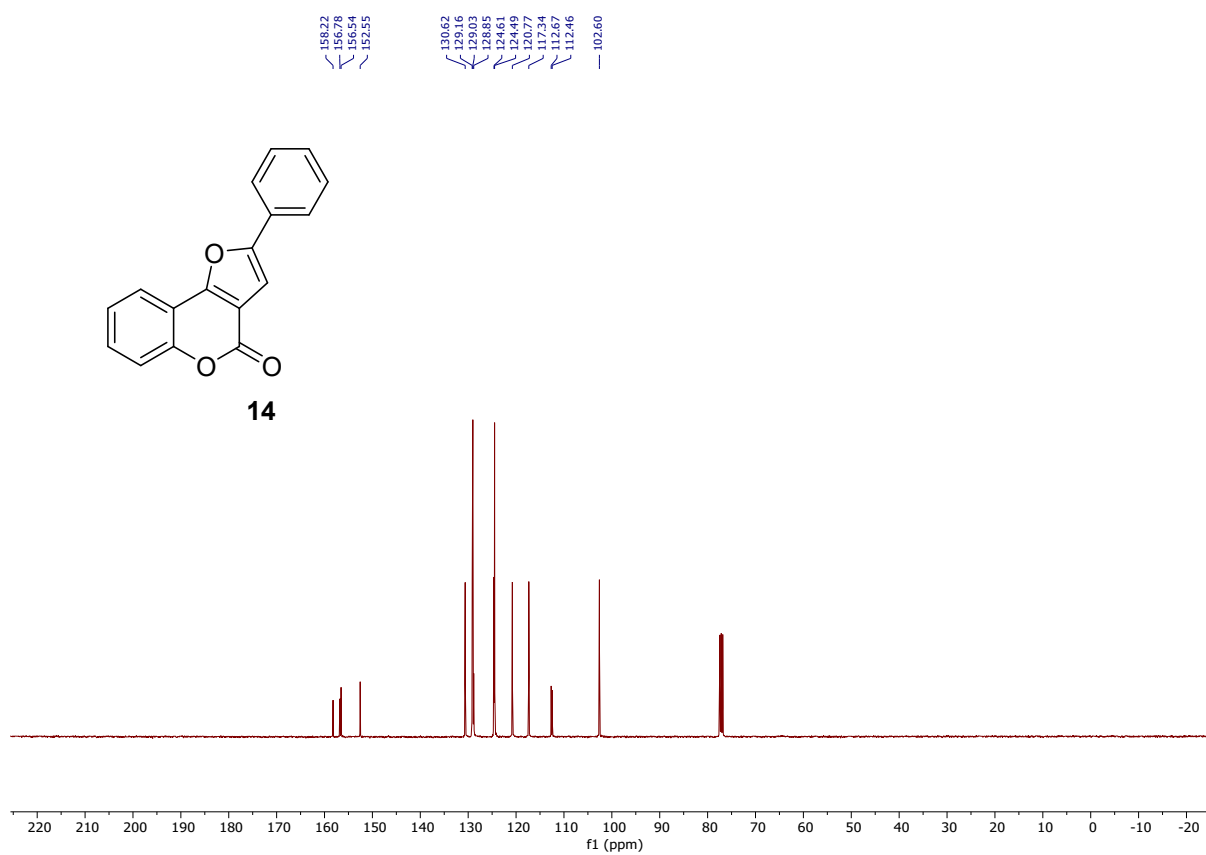
¹H-NMR (500 MHz, CDCl₃)



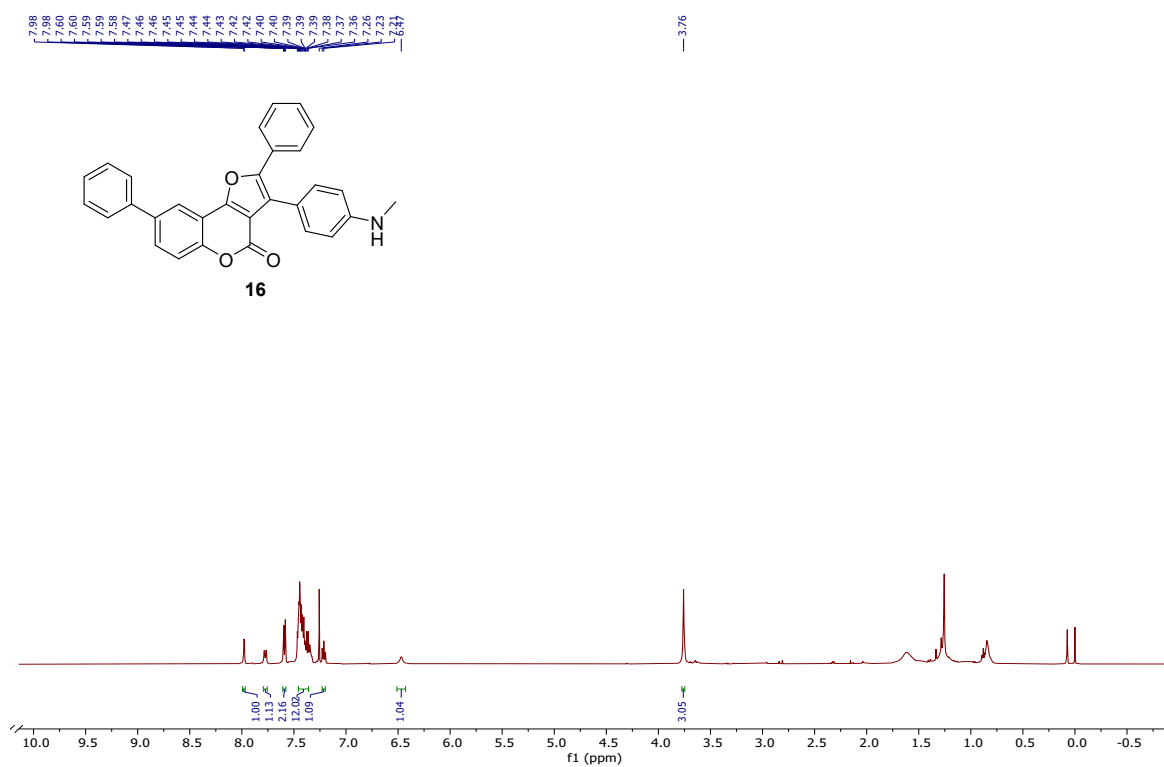
¹H-NMR (500 MHz, CDCl₃)



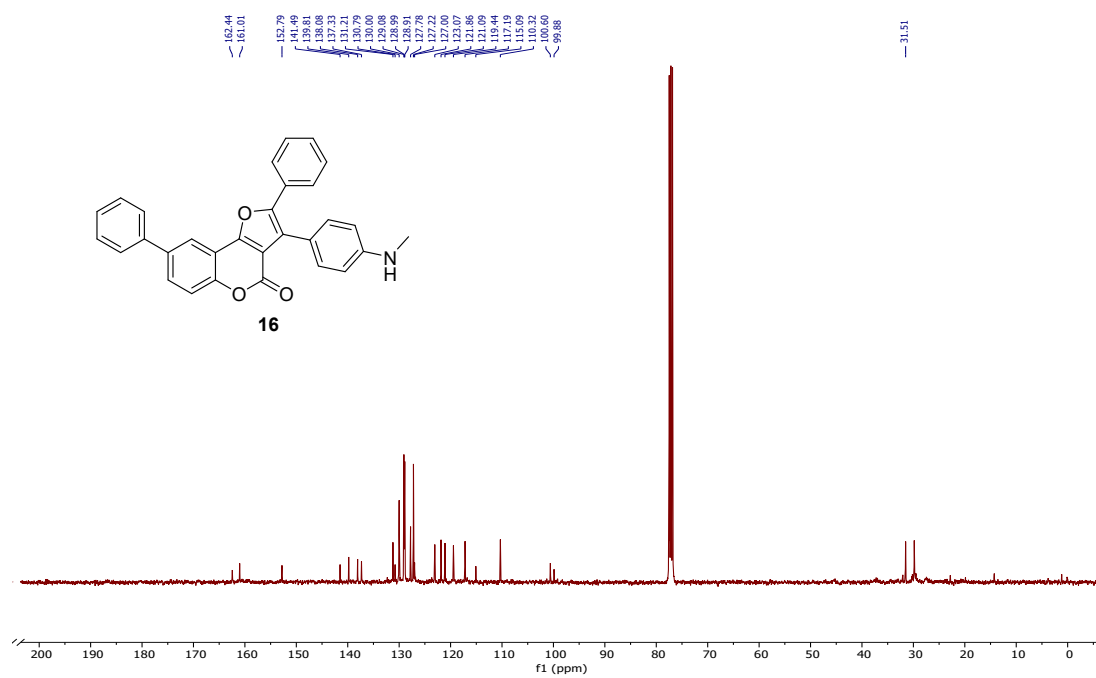
¹³C-NMR (100 MHz, CDCl₃)



¹H-NMR (500 MHz, CDCl₃)



¹³C-NMR (100 MHz, CDCl₃)



HRMS Data

