

Supporting Information

Convenient Synthesis of Benziodazolone: New Reagents for Direct Esterification of Alcohols and Amidation of Amines

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1. X-Ray crystallography data of **5a**

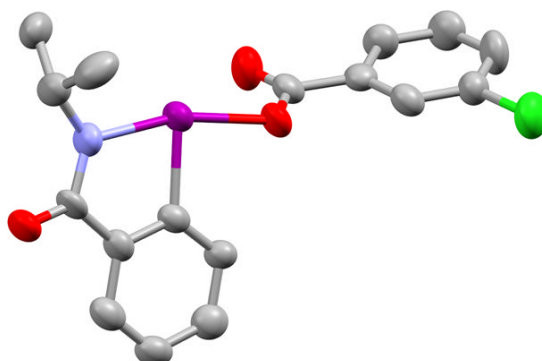
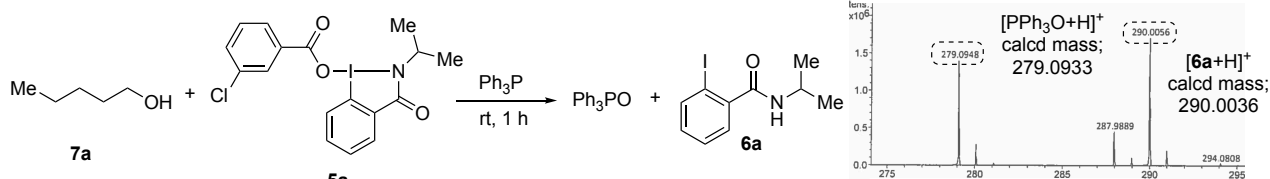


Figure S1. X-Ray crystal structure of **5a**.

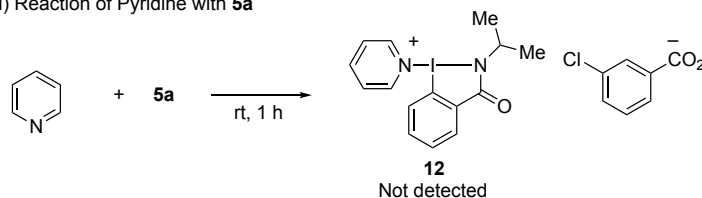
Single crystals of product **5a** suitable for X-ray crystallographic analysis were obtained by slow crystallization from the acetonitrile solution. X-ray diffraction data for **5a** were collected on Rigaku RAPID II Image Plate system using graphite-monochromated CuK α radiation ($\lambda = 1.54187 \text{ \AA}$) at 173 K. The structure was solved by Sir 2011 and refined on F² using ShelXle. Crystal data for **5a** C₁₇H₁₅ClINO₃: monoclinic, space group P2₁/c, $a = 12.6913(3)$, $b = 14.8285(4)$, $c = 18.3997(13) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 104.695(7)^\circ$, $\gamma = 90^\circ$, $V = 3349.4(3) \text{ \AA}^3$, $Z = 8$, 22784 reflections measured, 5815 unique ($4560 I > 2\sigma(I)$); $R_{\text{int}} = 0.0780$, $R_{\text{sigma}} = 0.0834$, $R_1 (I > 2\sigma(I)) = 0.0595$, $R_1 = 0.0696$, $wR2_{\text{all}} = 0.1700$. $S = 1.086$; Please see the cif for more detailed information: CCDC- 2122170.

2. Mass study

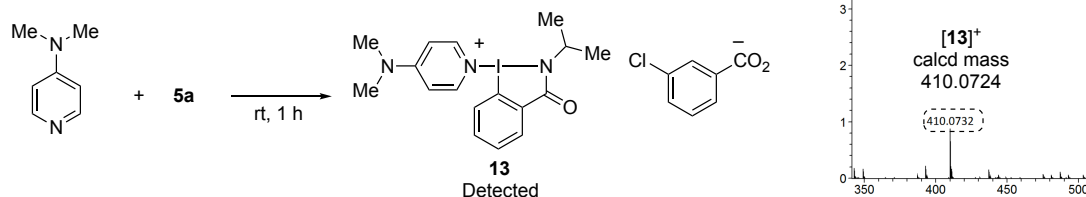
i) Reaction of **7a** with **5a** and Ph₃P



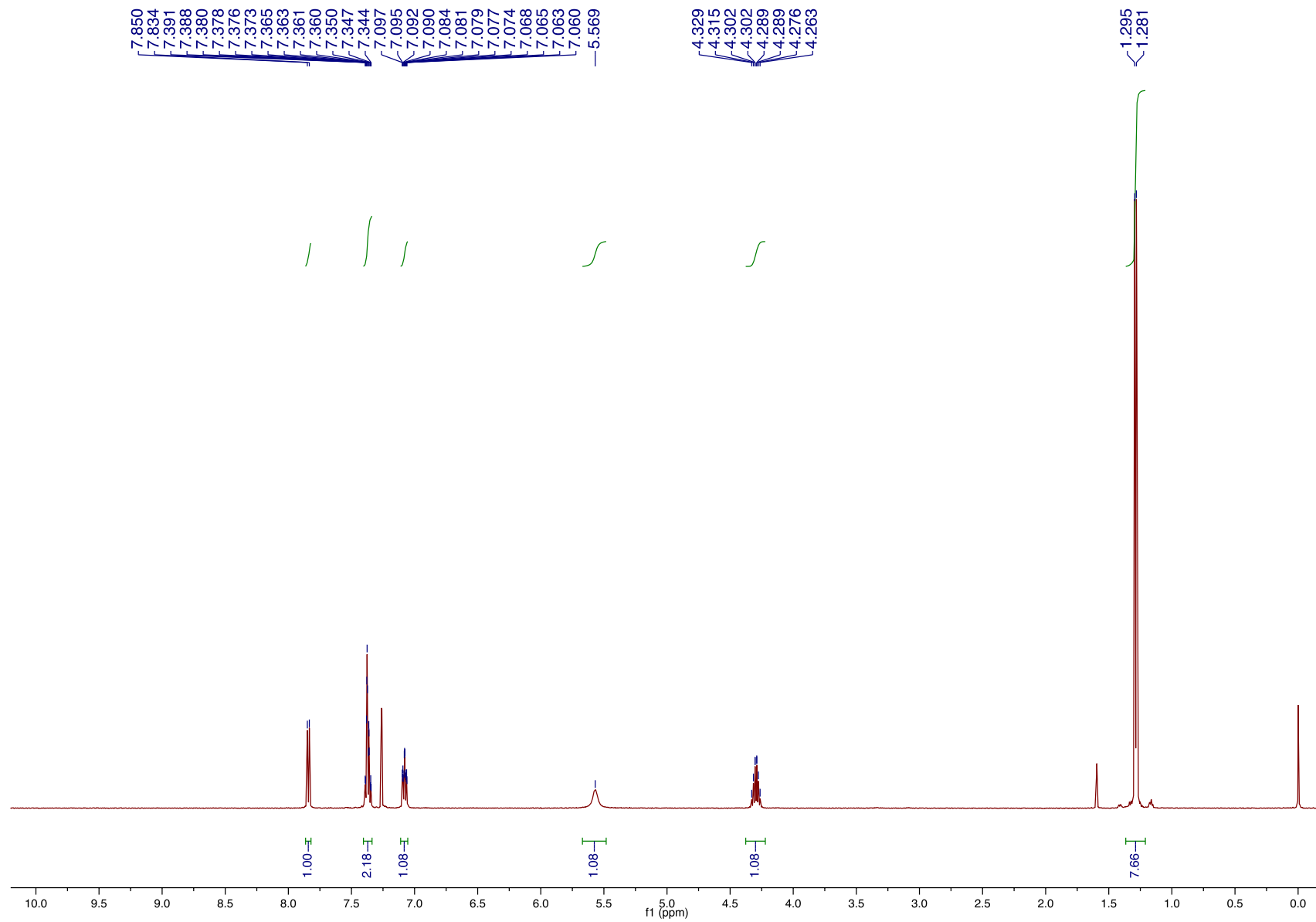
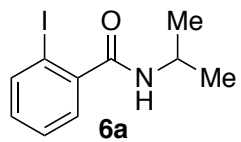
ii) Reaction of Pyridine with **5a**



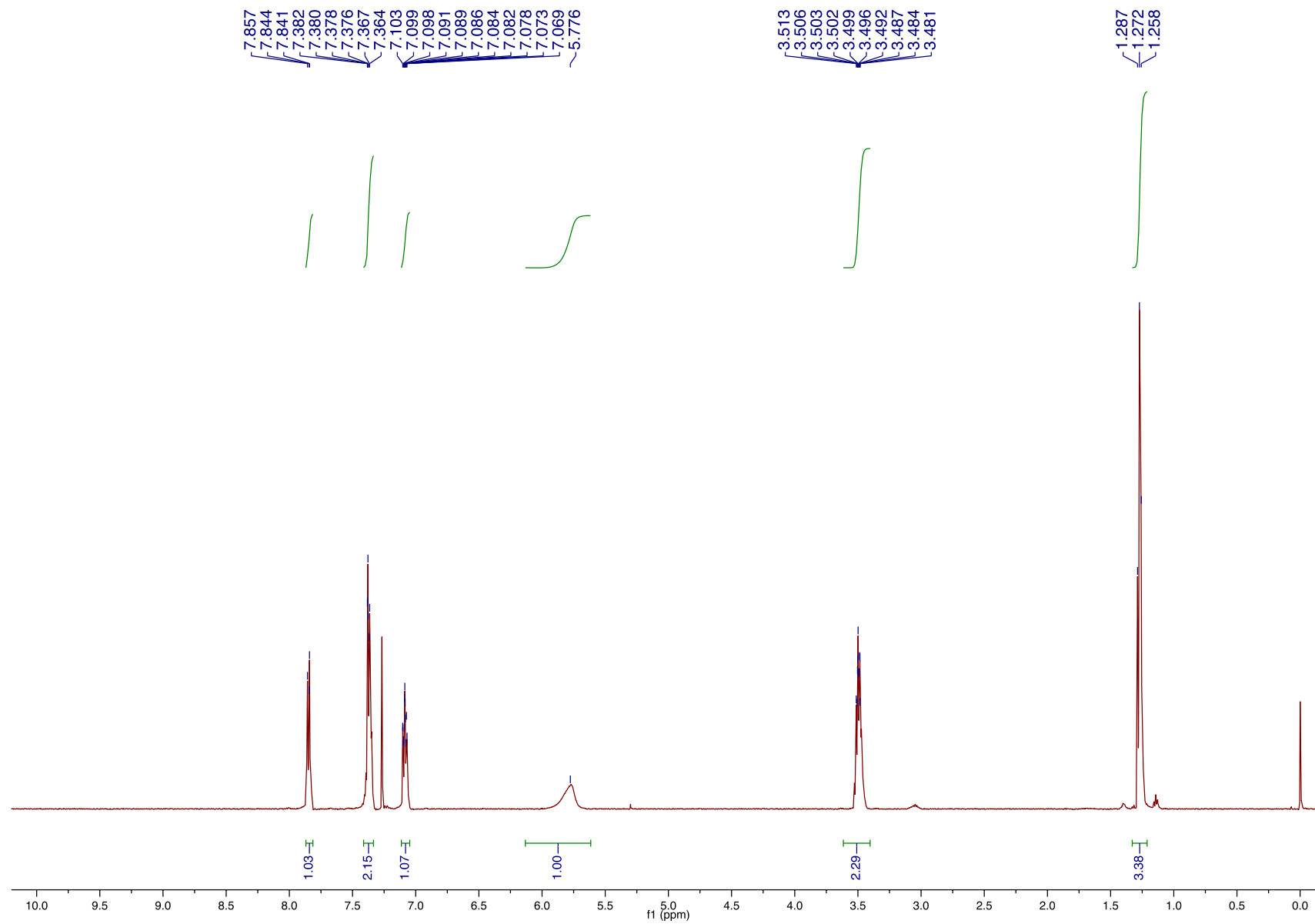
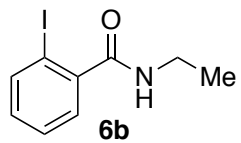
iii) Reaction of DMAP with **5a**



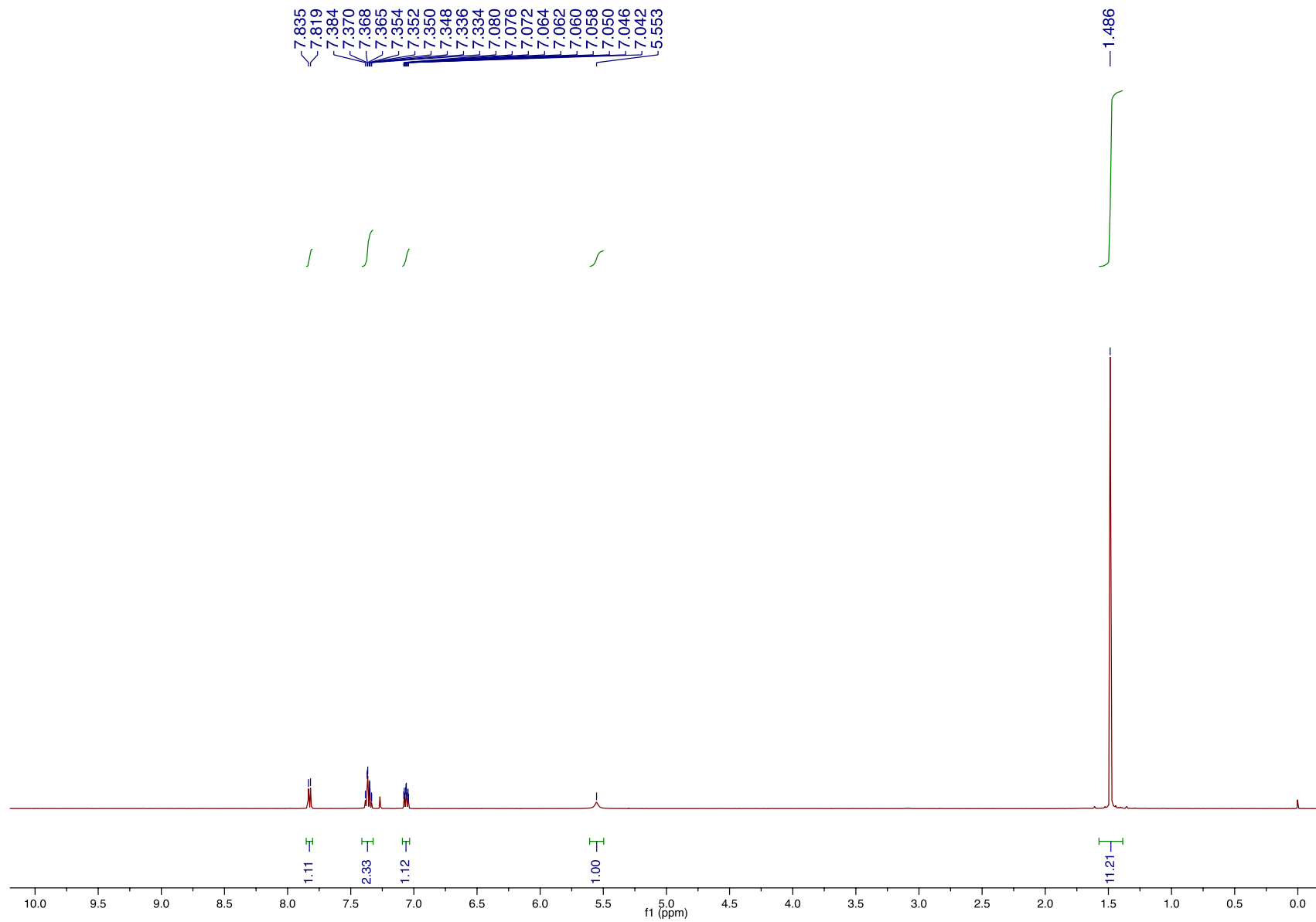
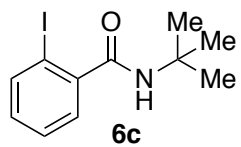
^1H NMR (500 MHz, CDCl_3);



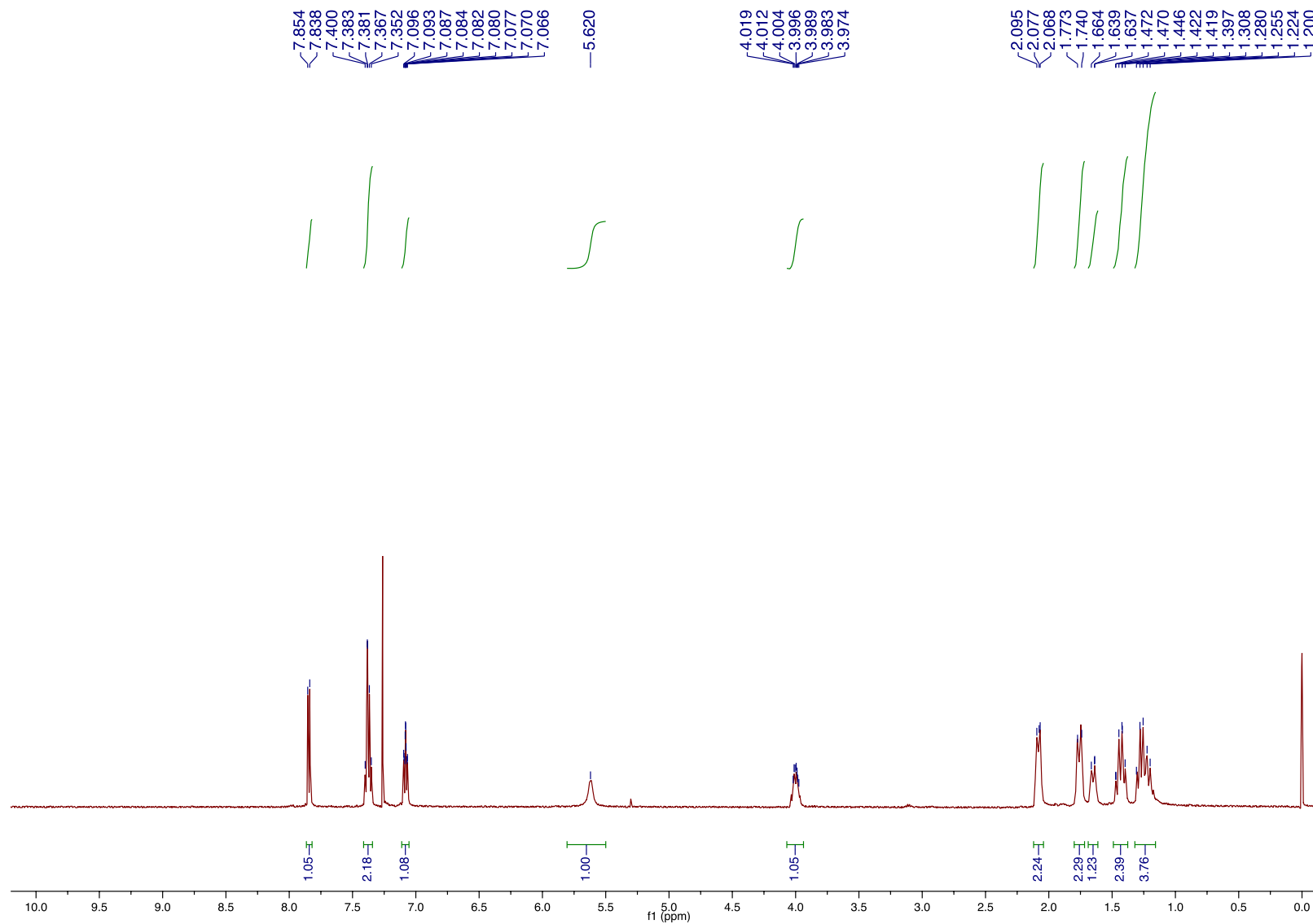
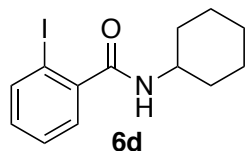
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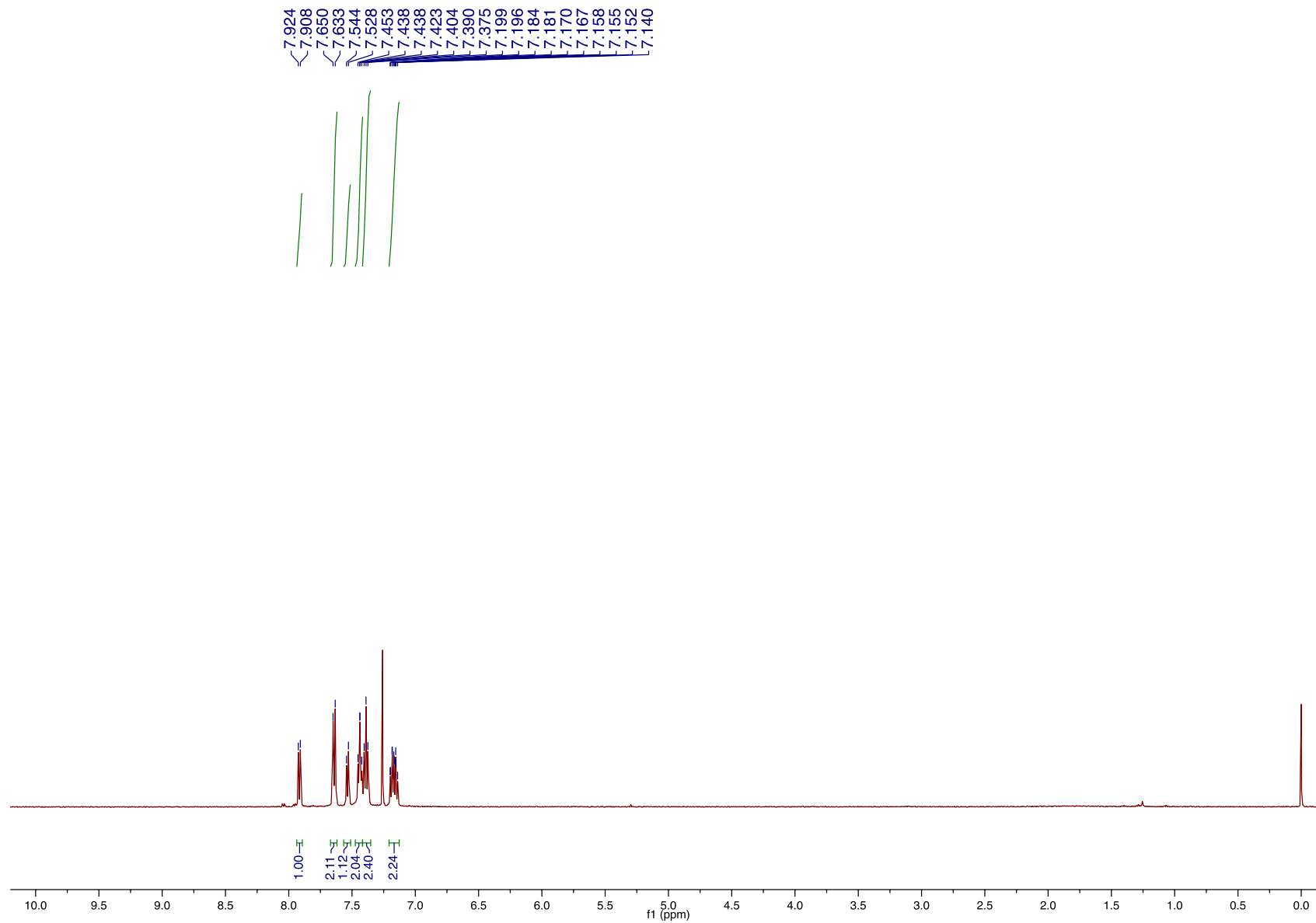
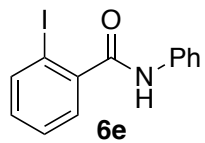
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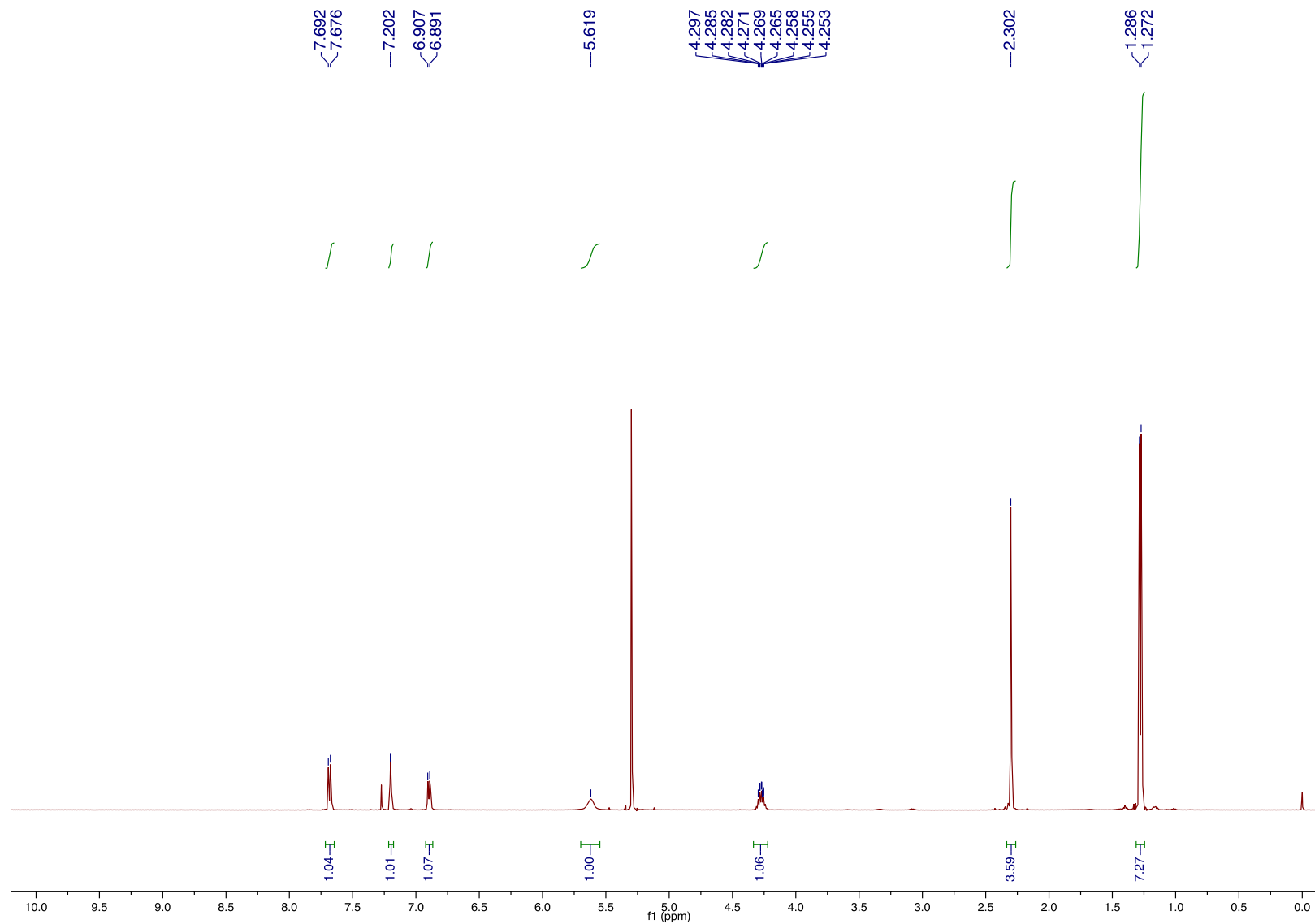
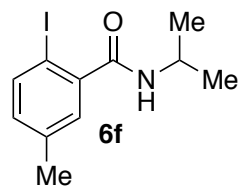
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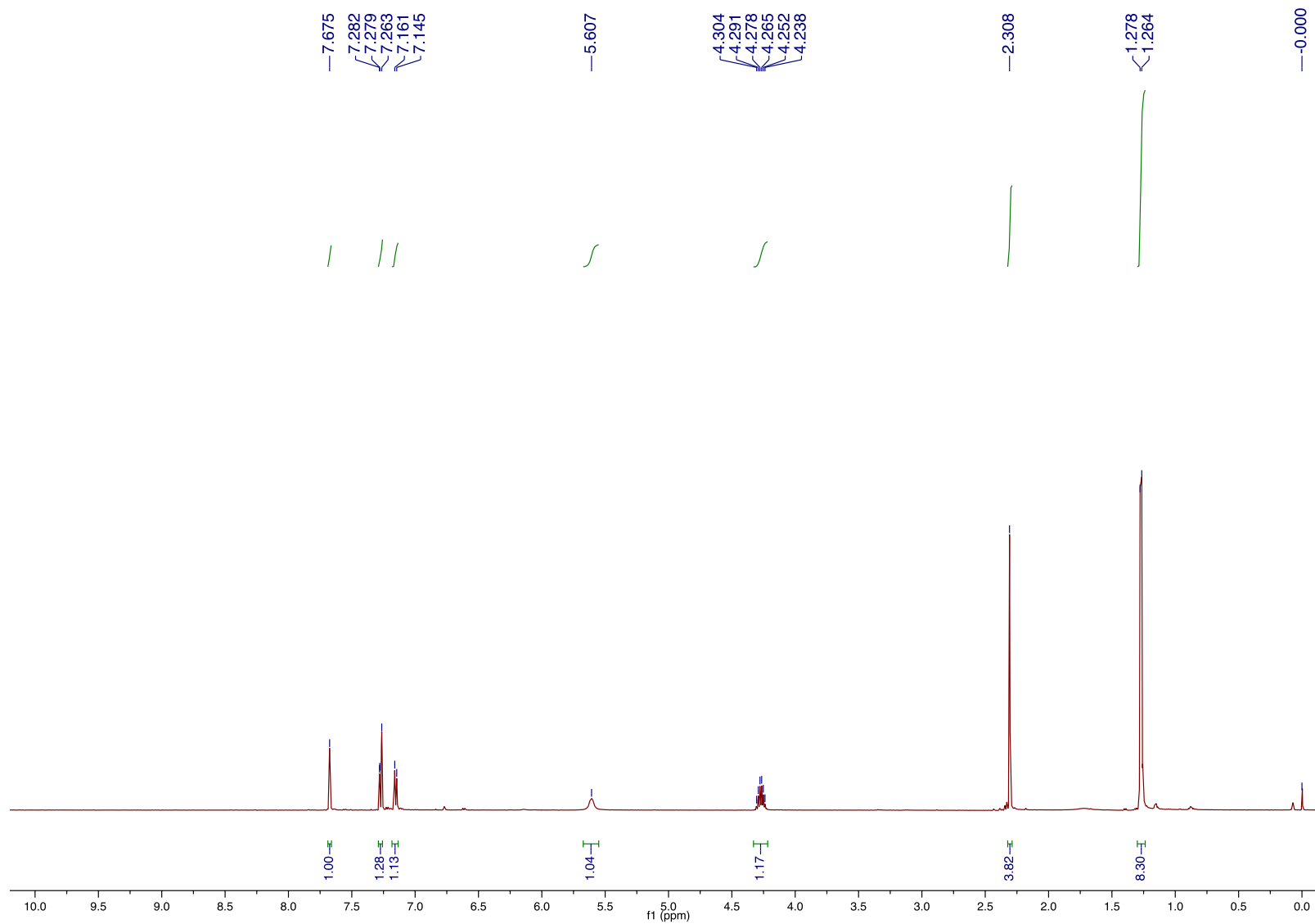
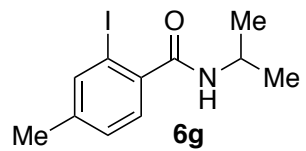
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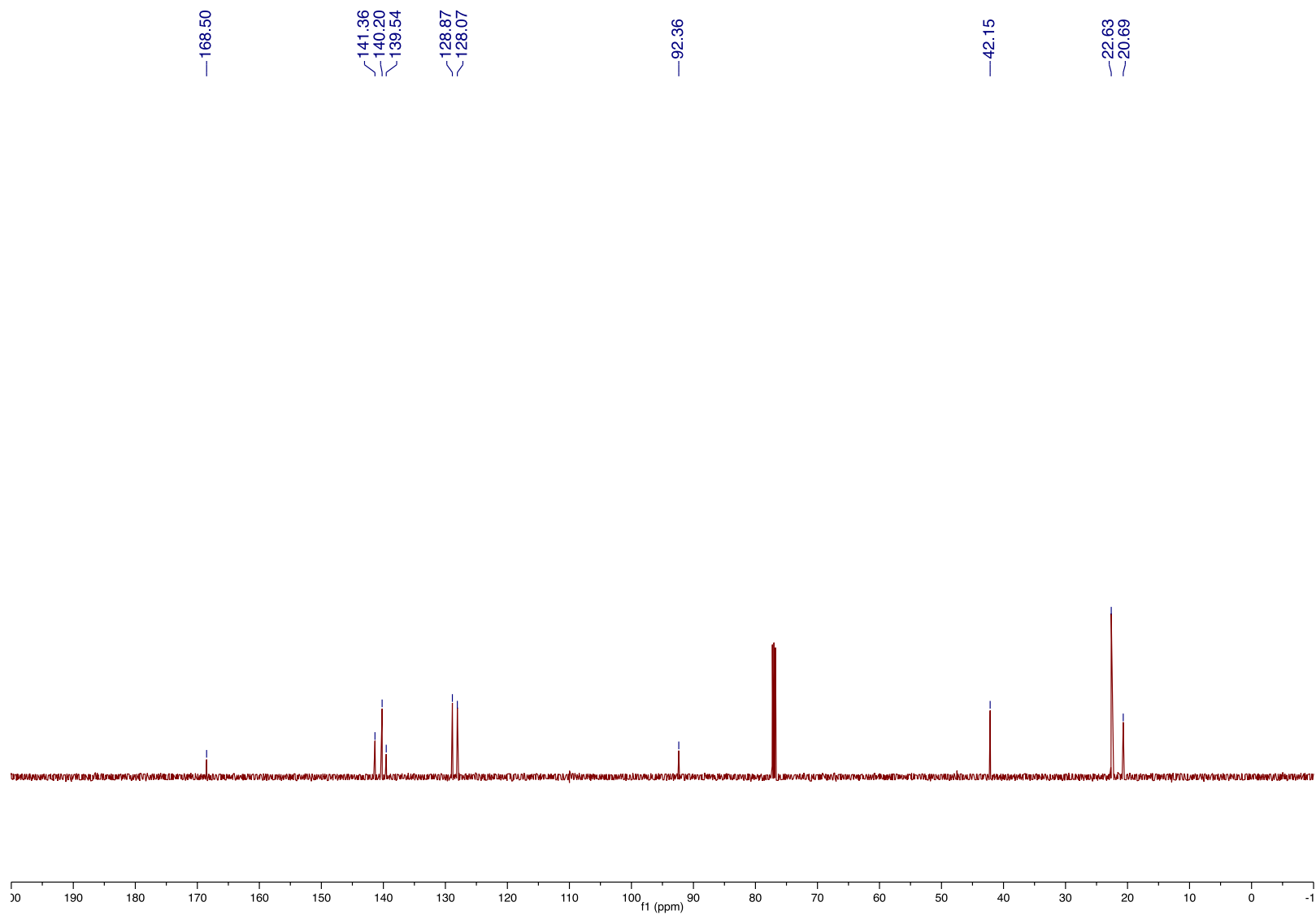
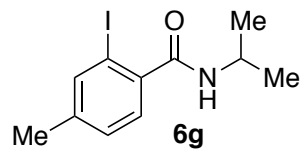
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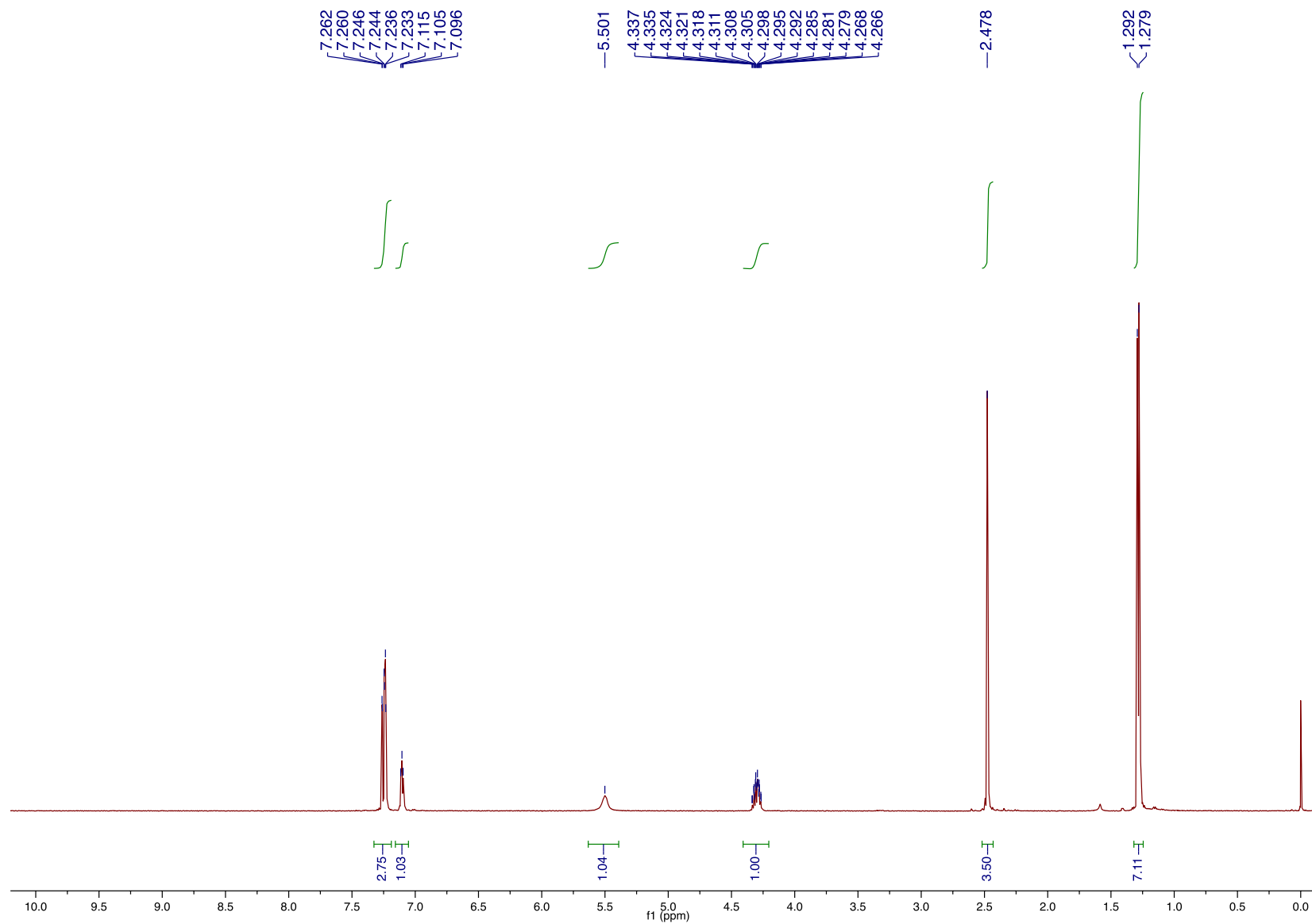
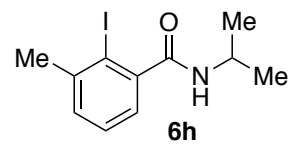
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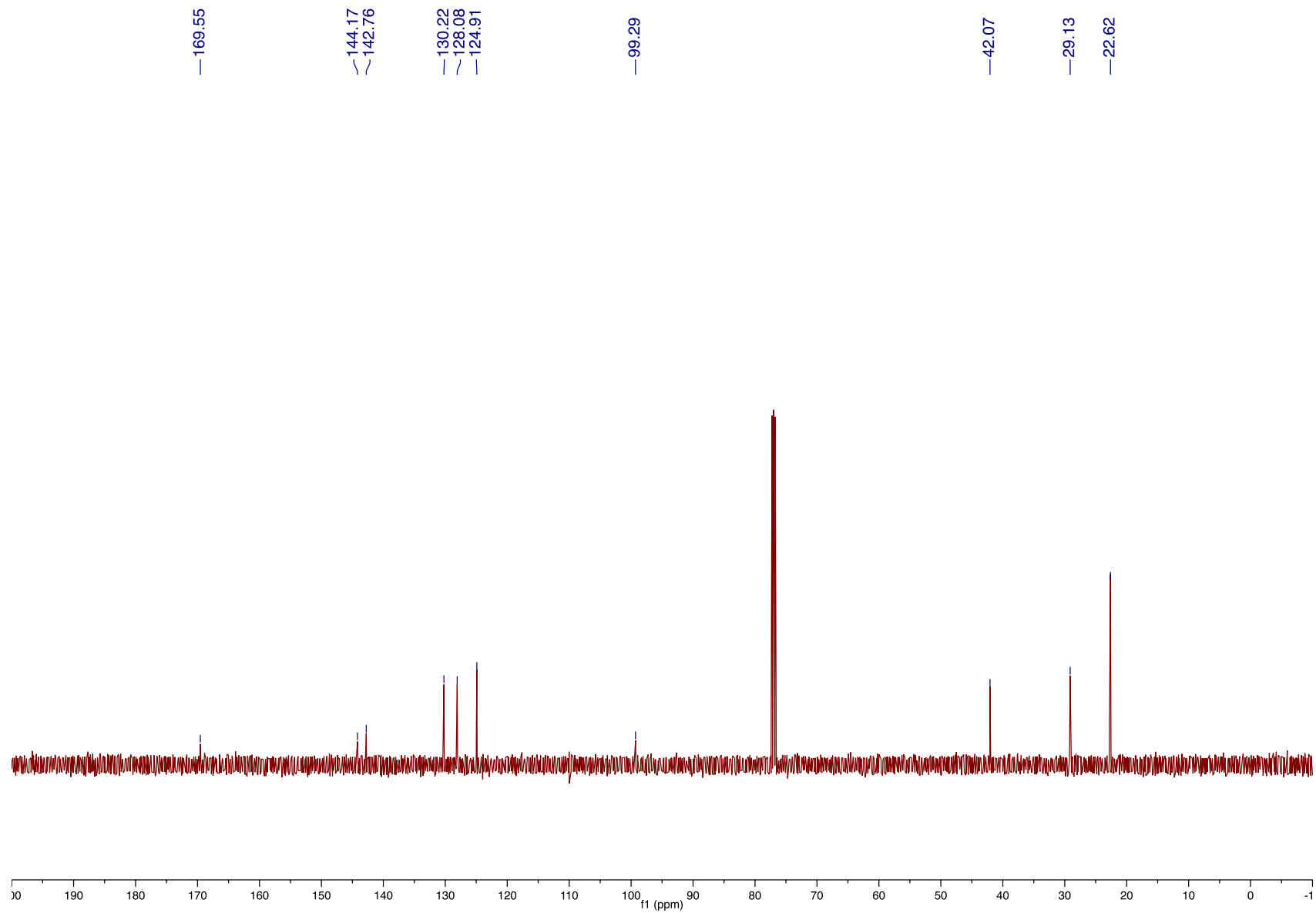
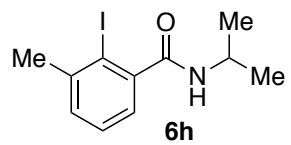
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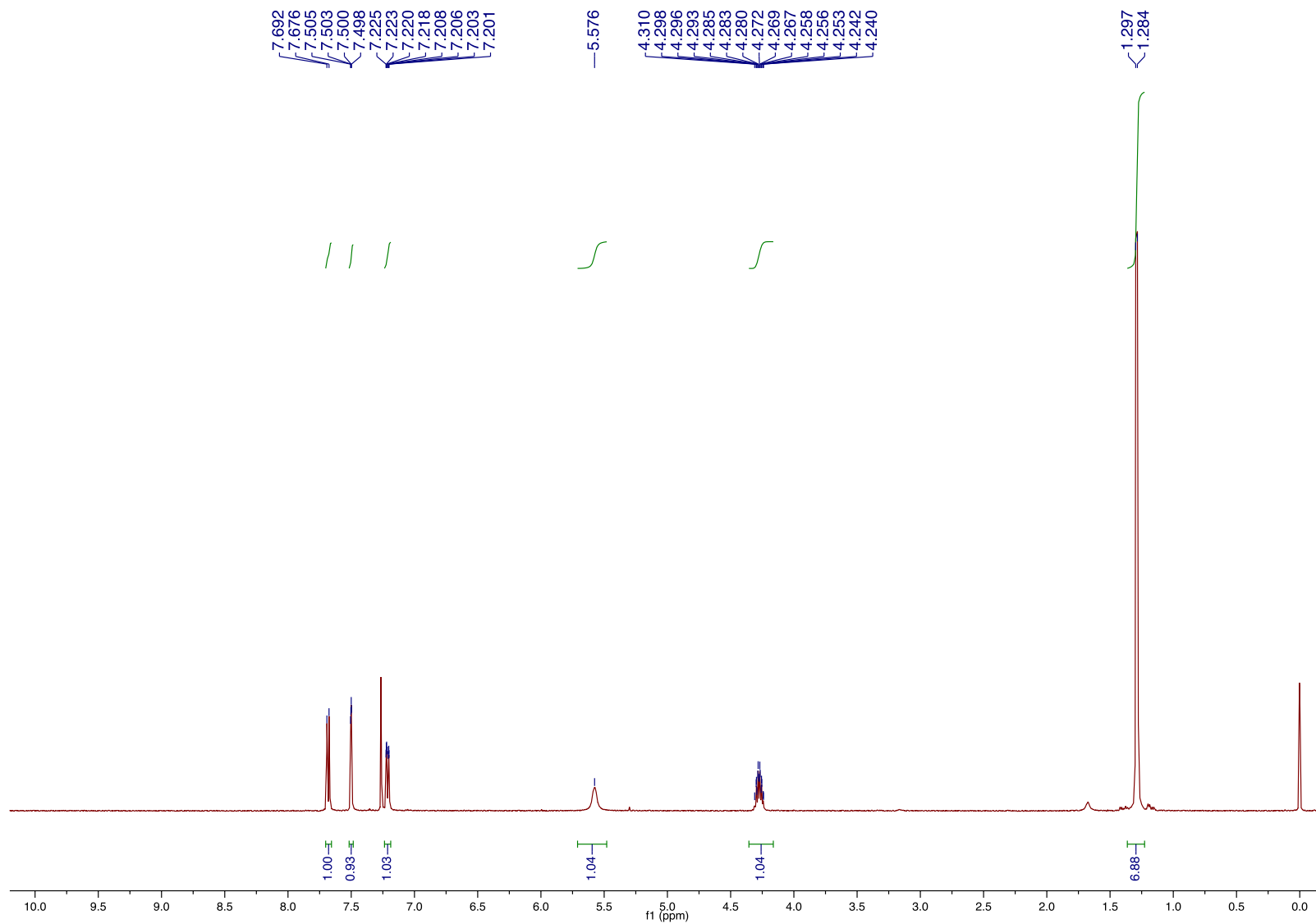
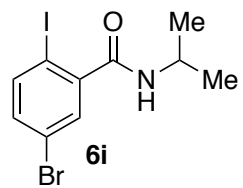
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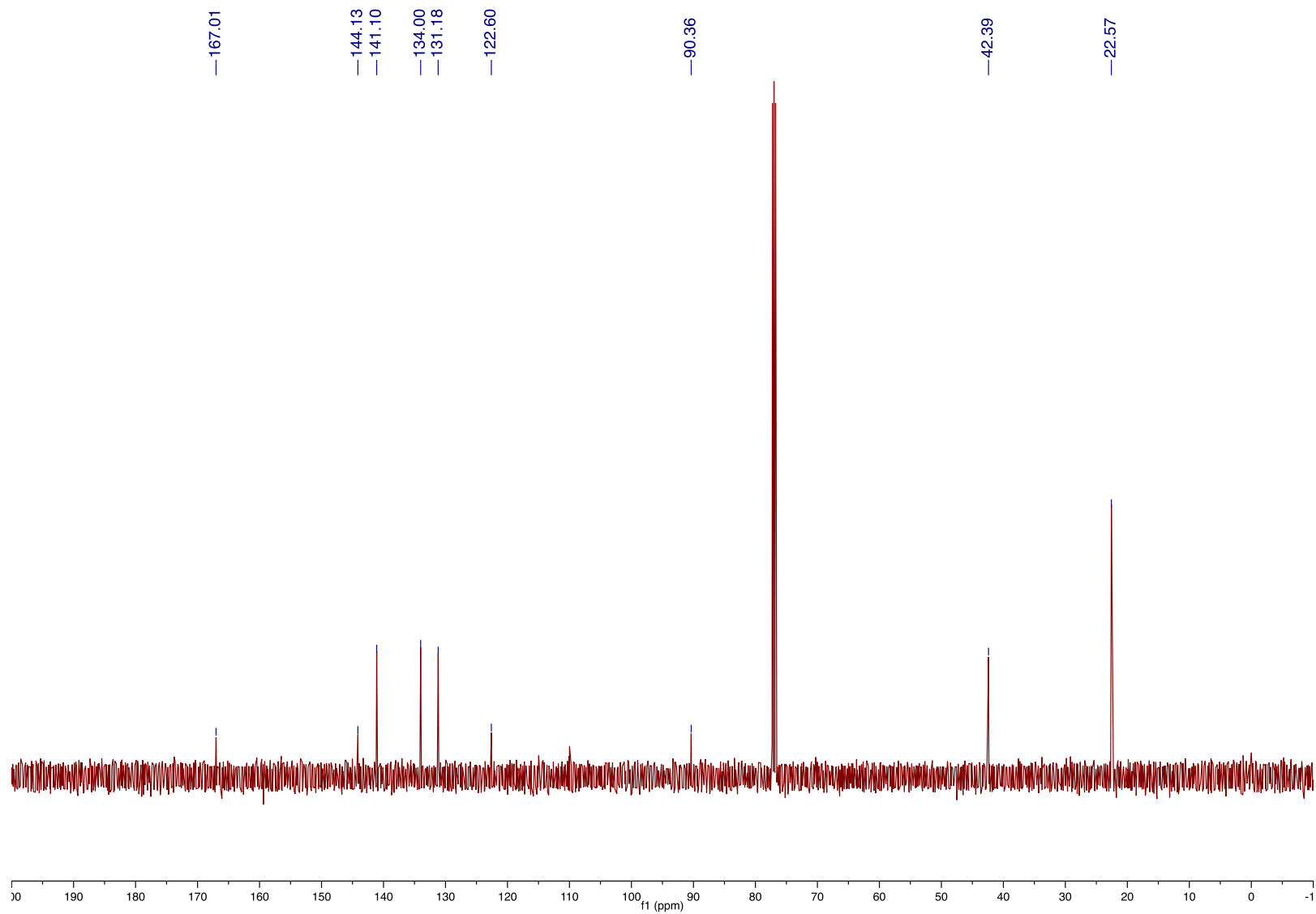
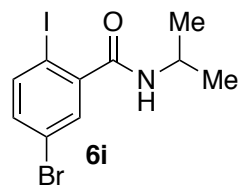
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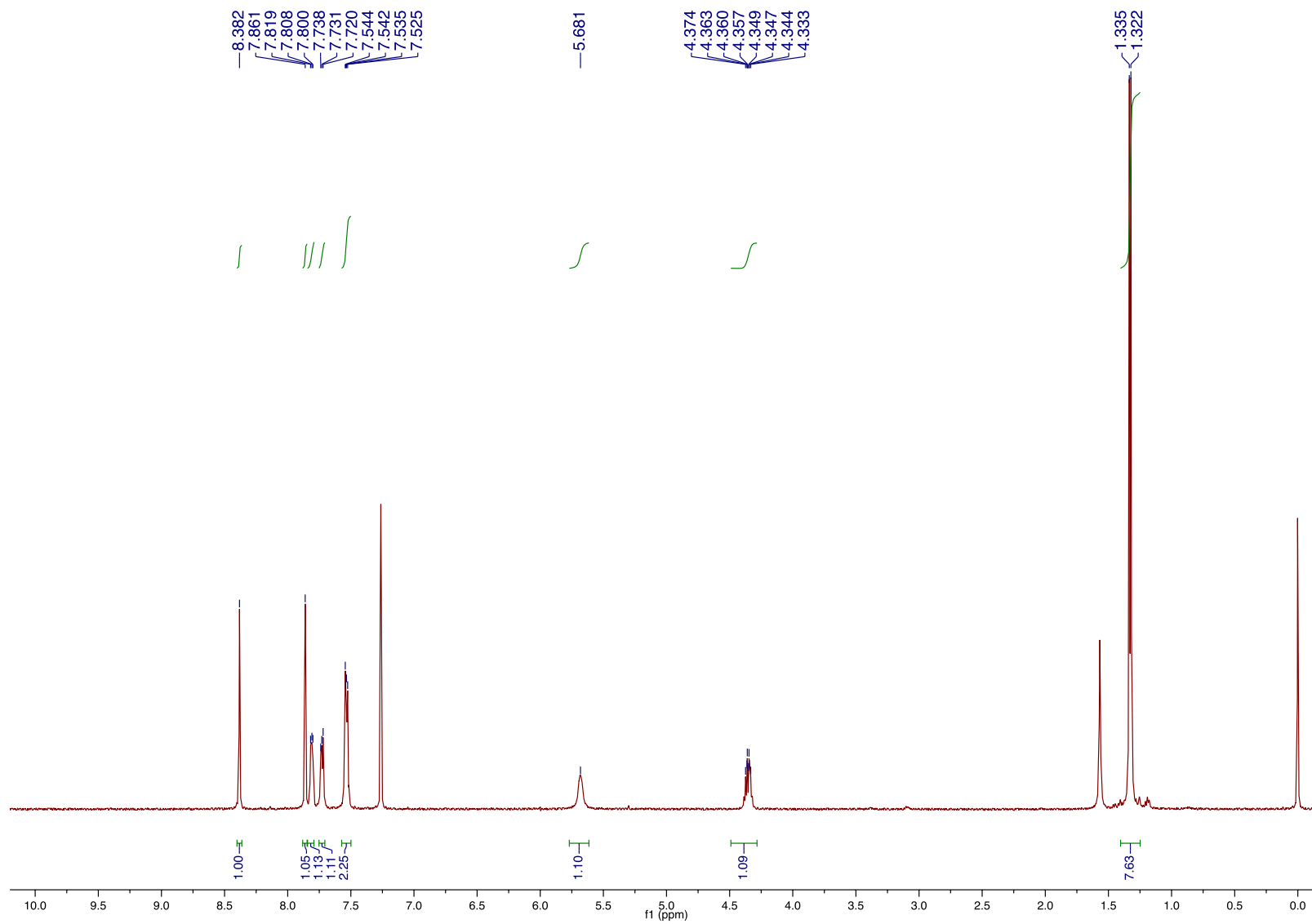
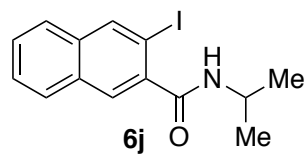
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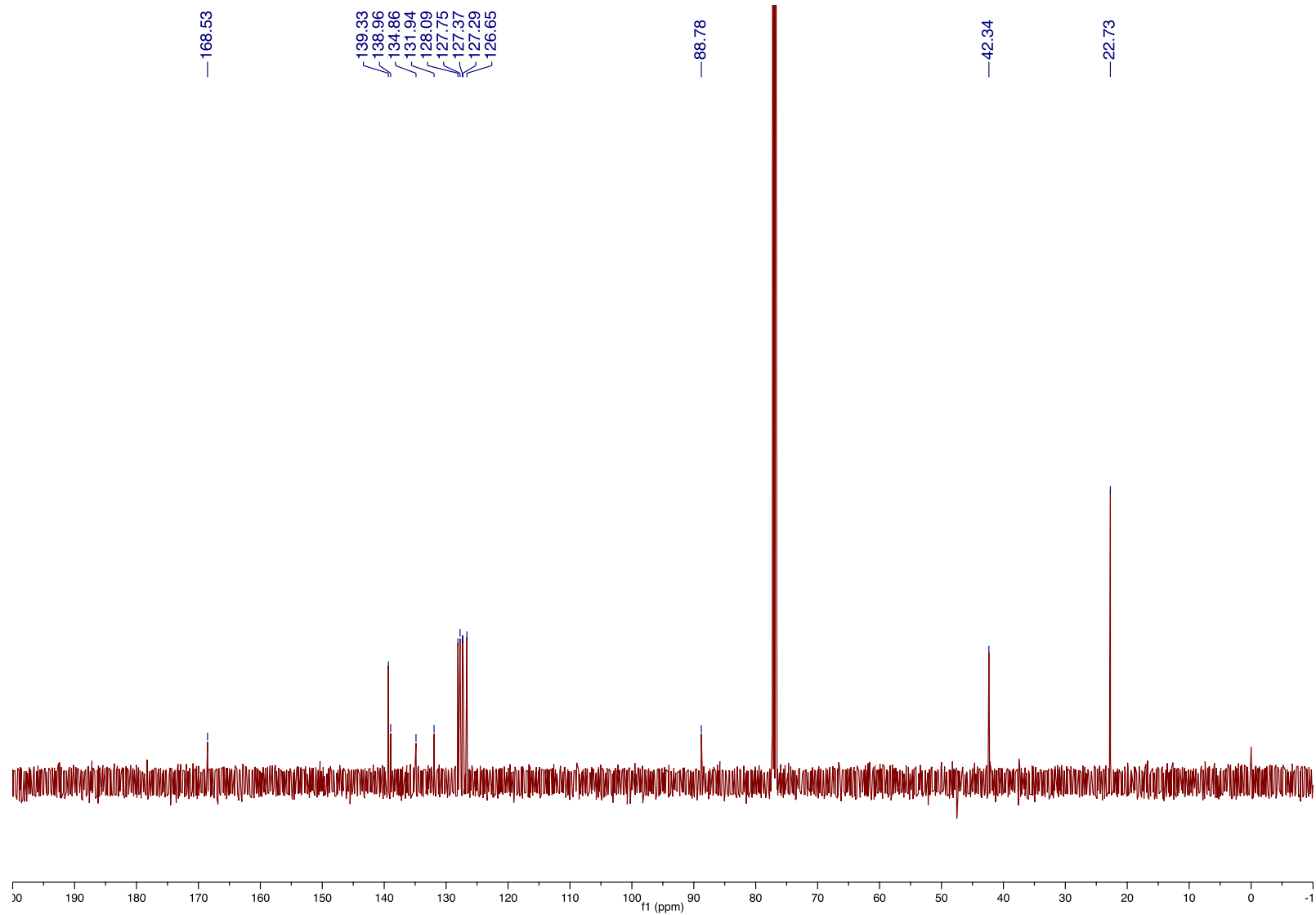
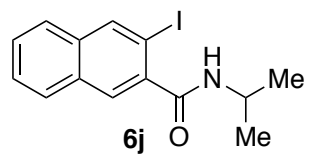
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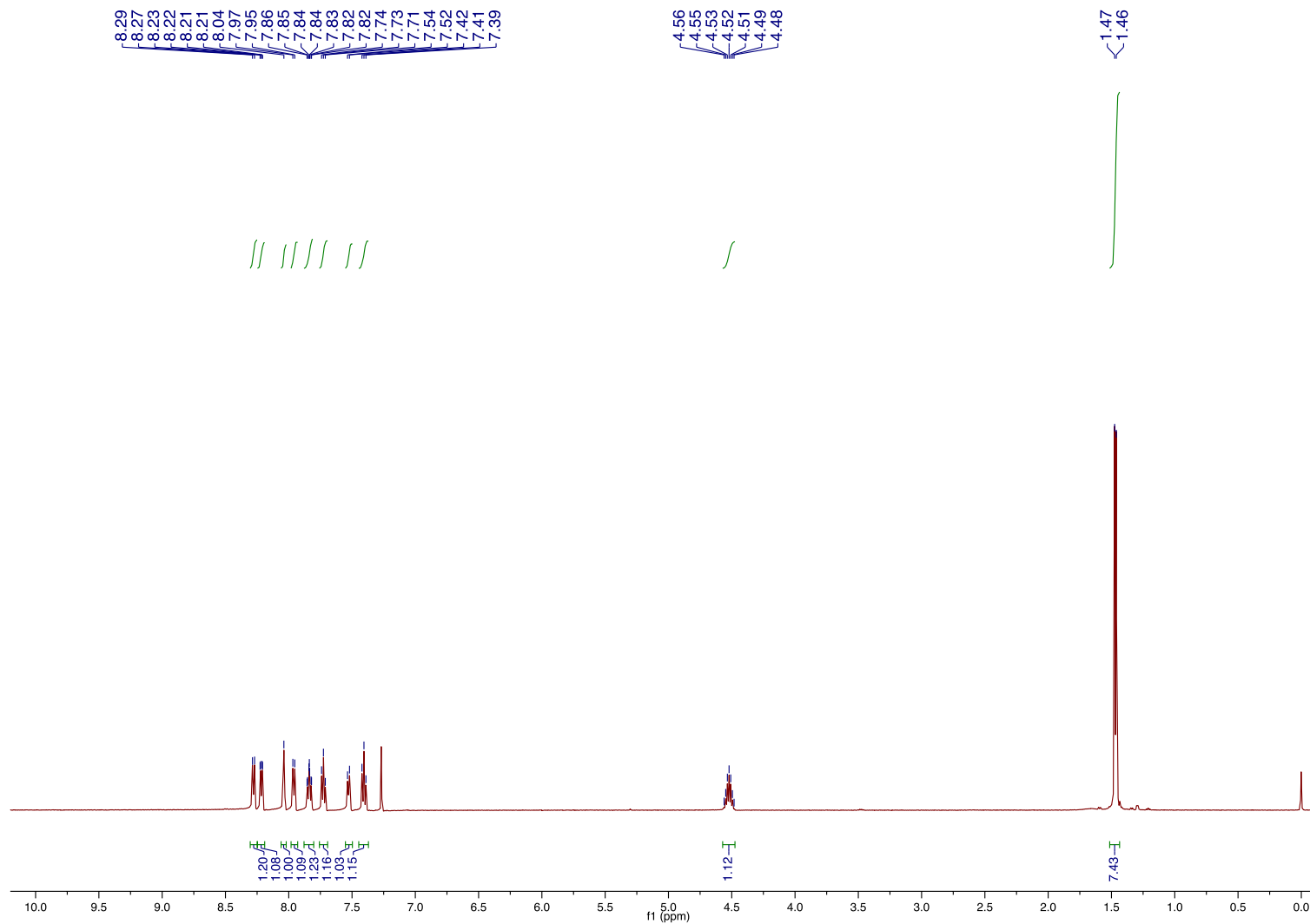
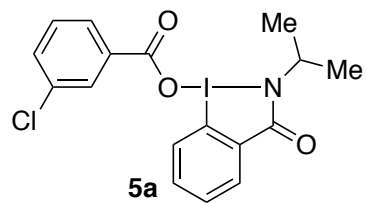
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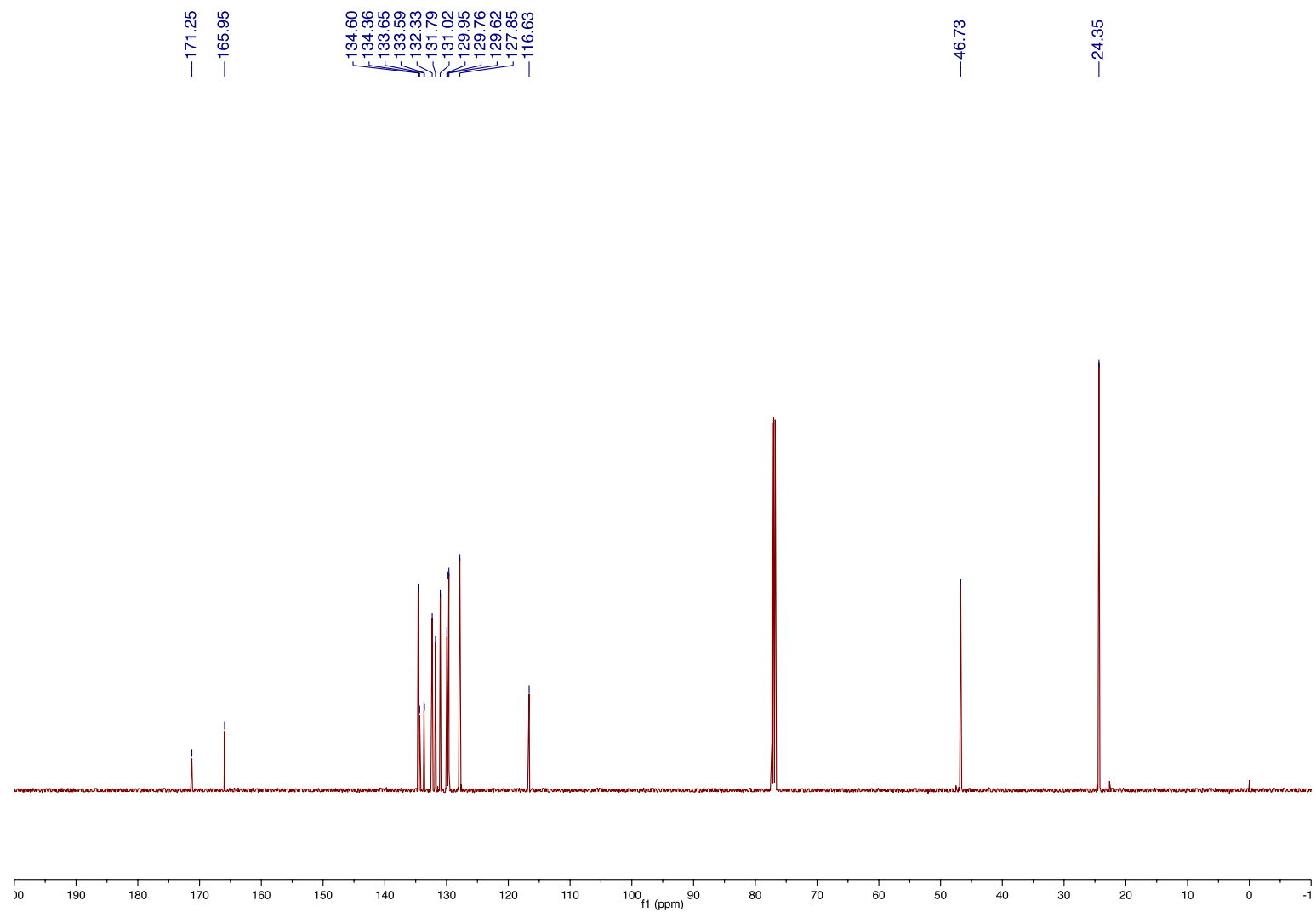
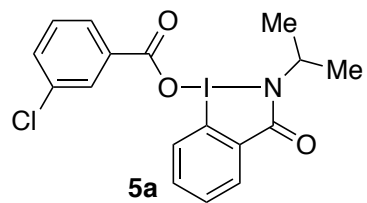
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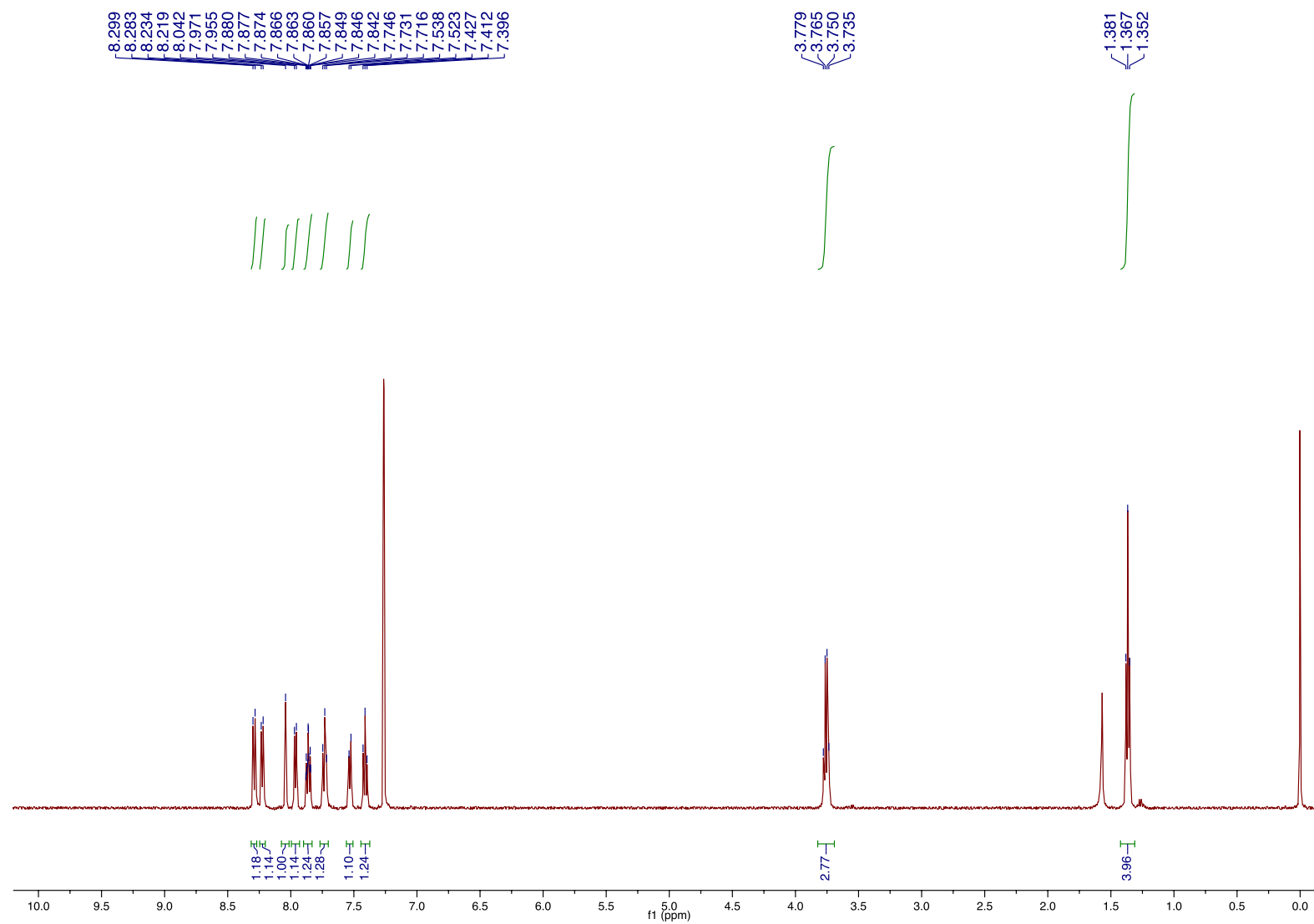
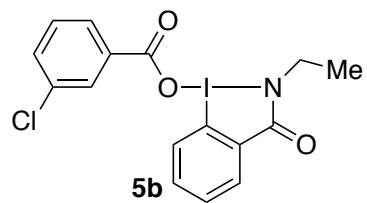
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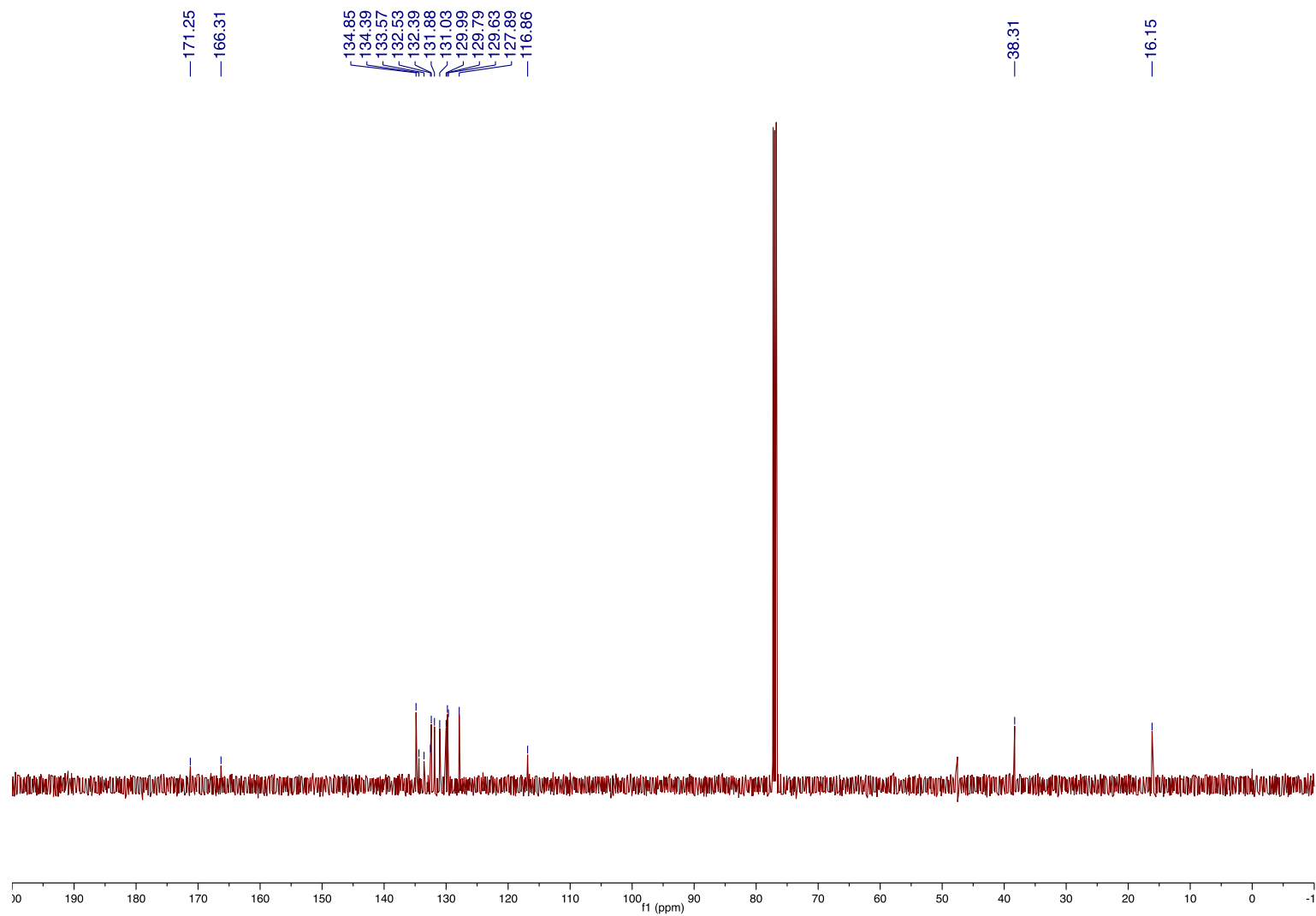
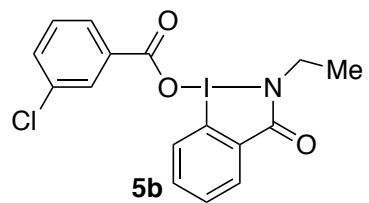
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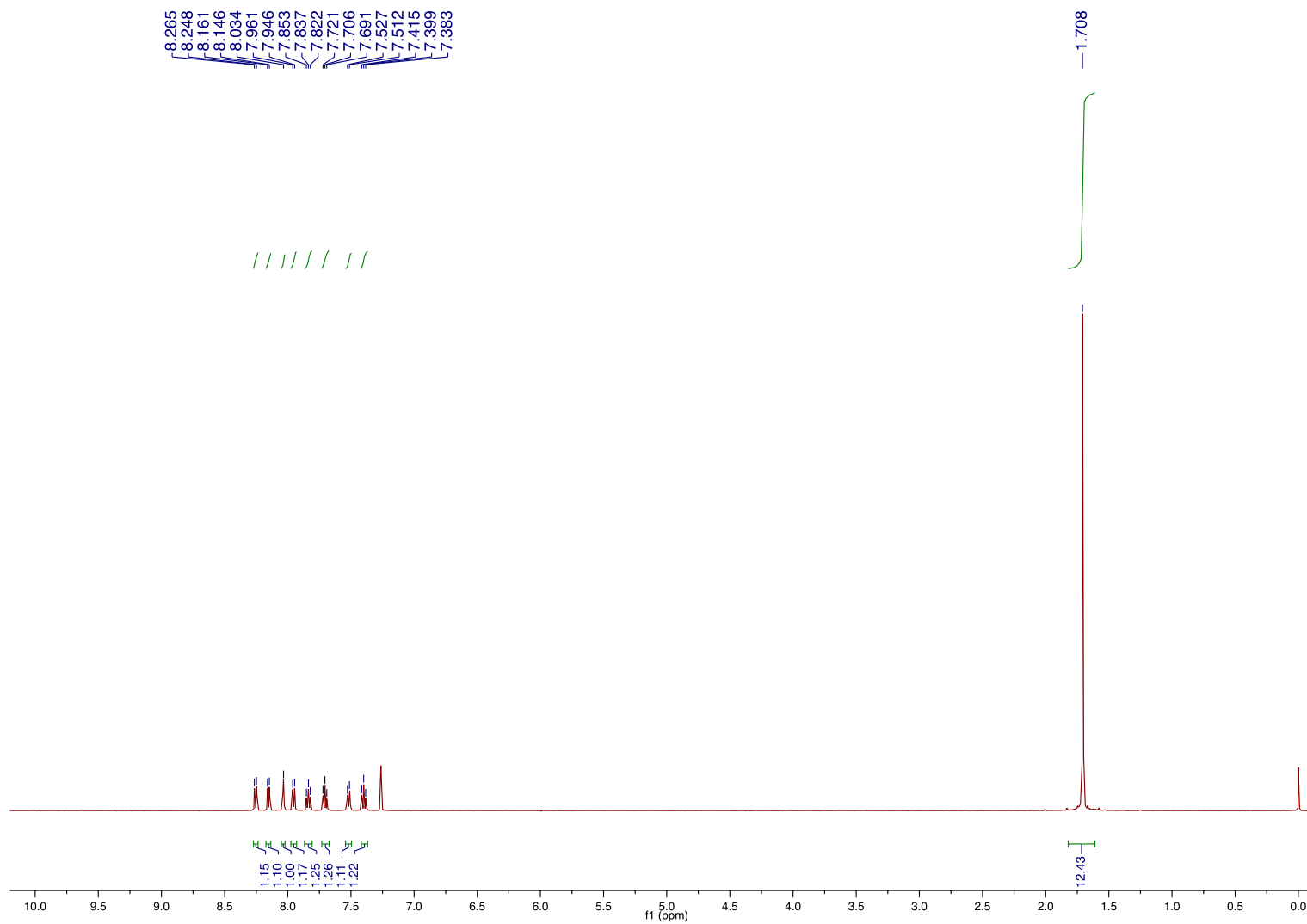
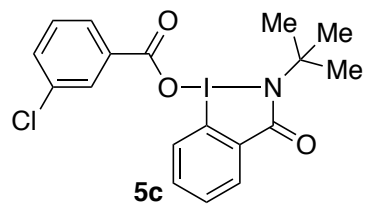
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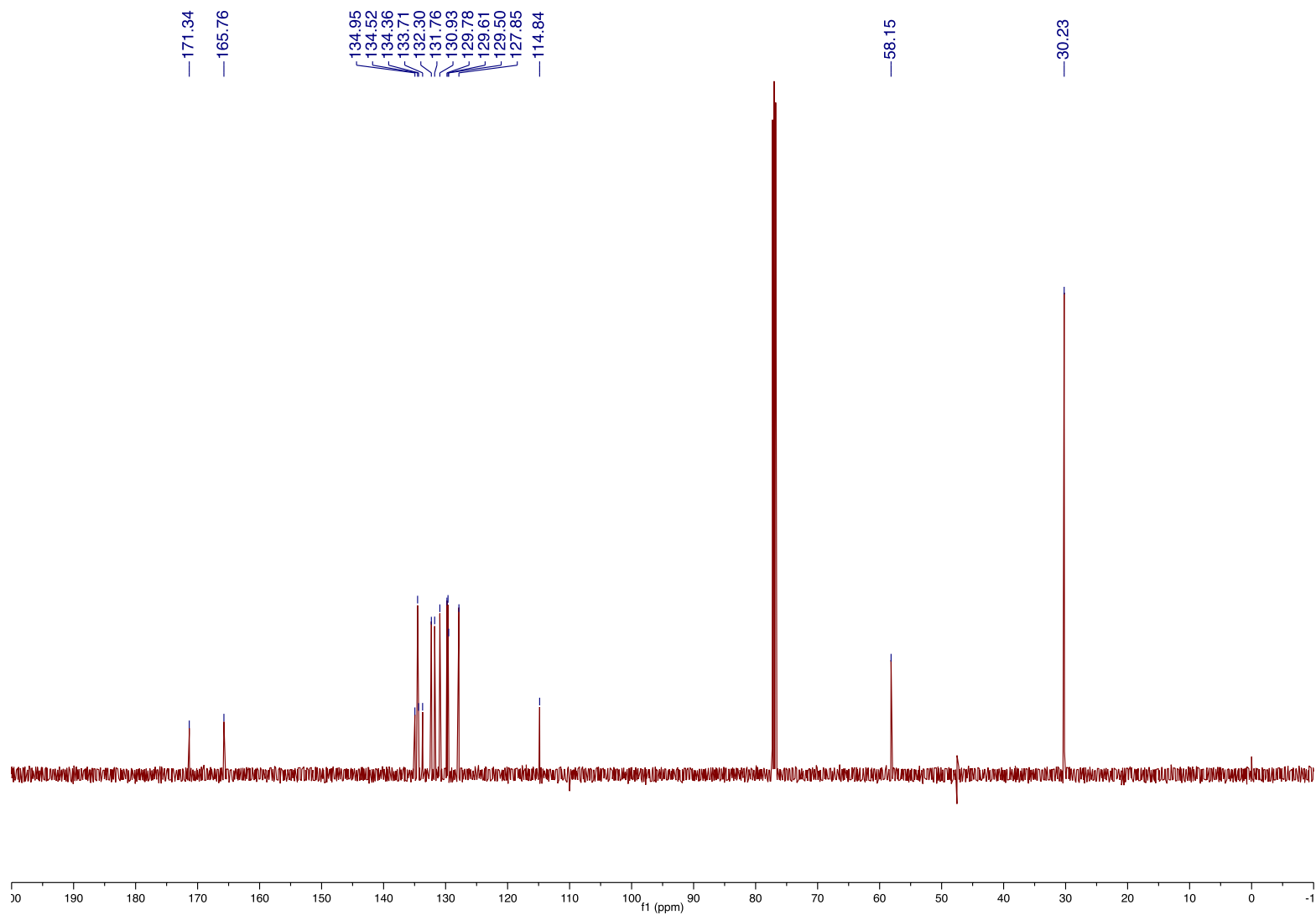
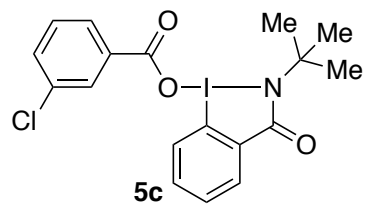
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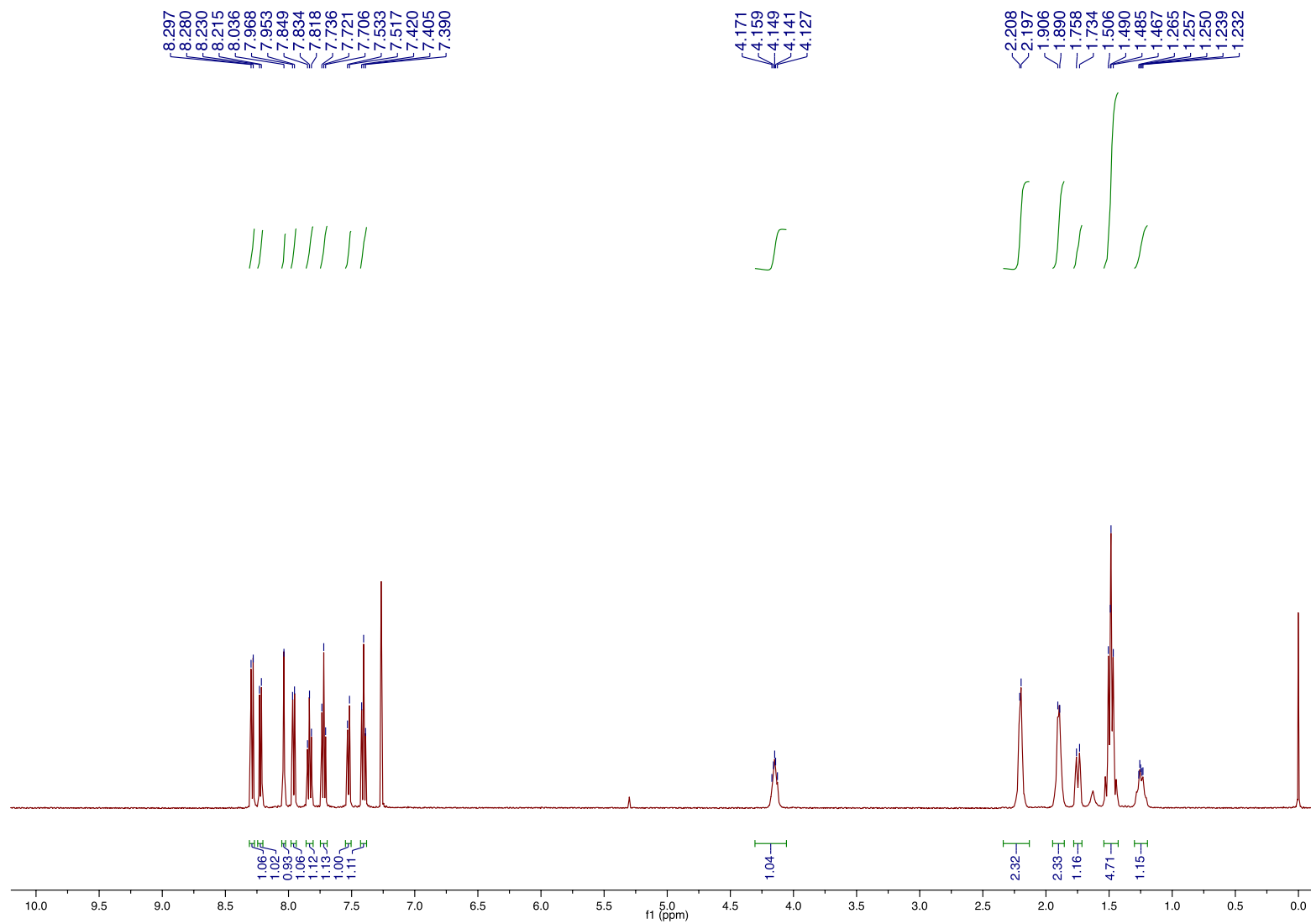
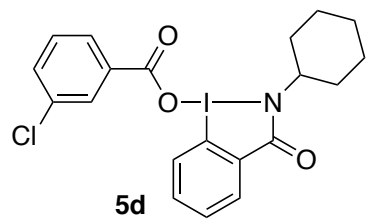
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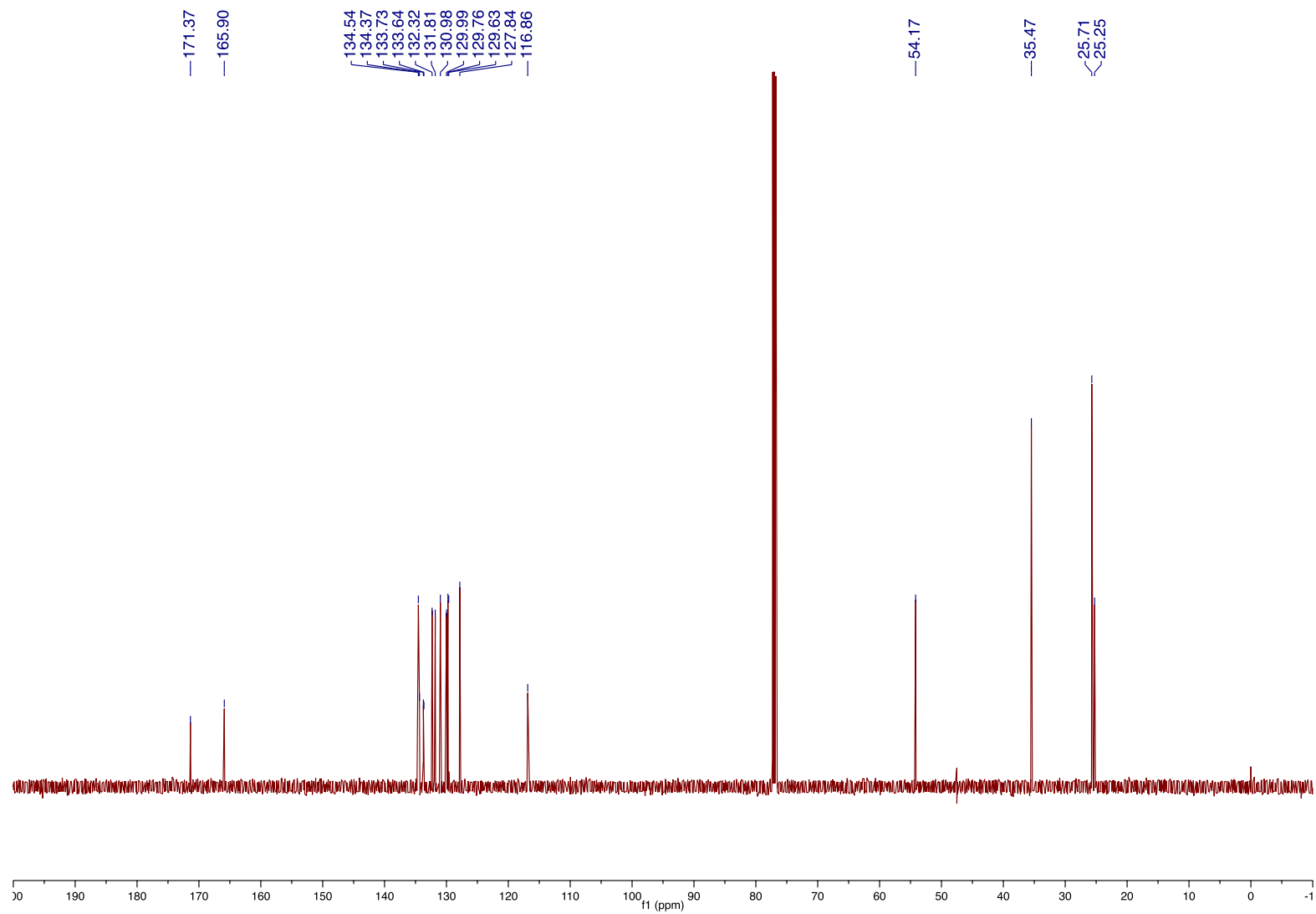
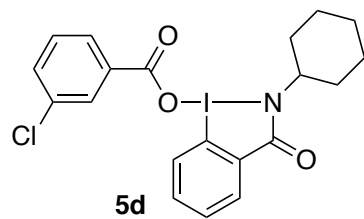
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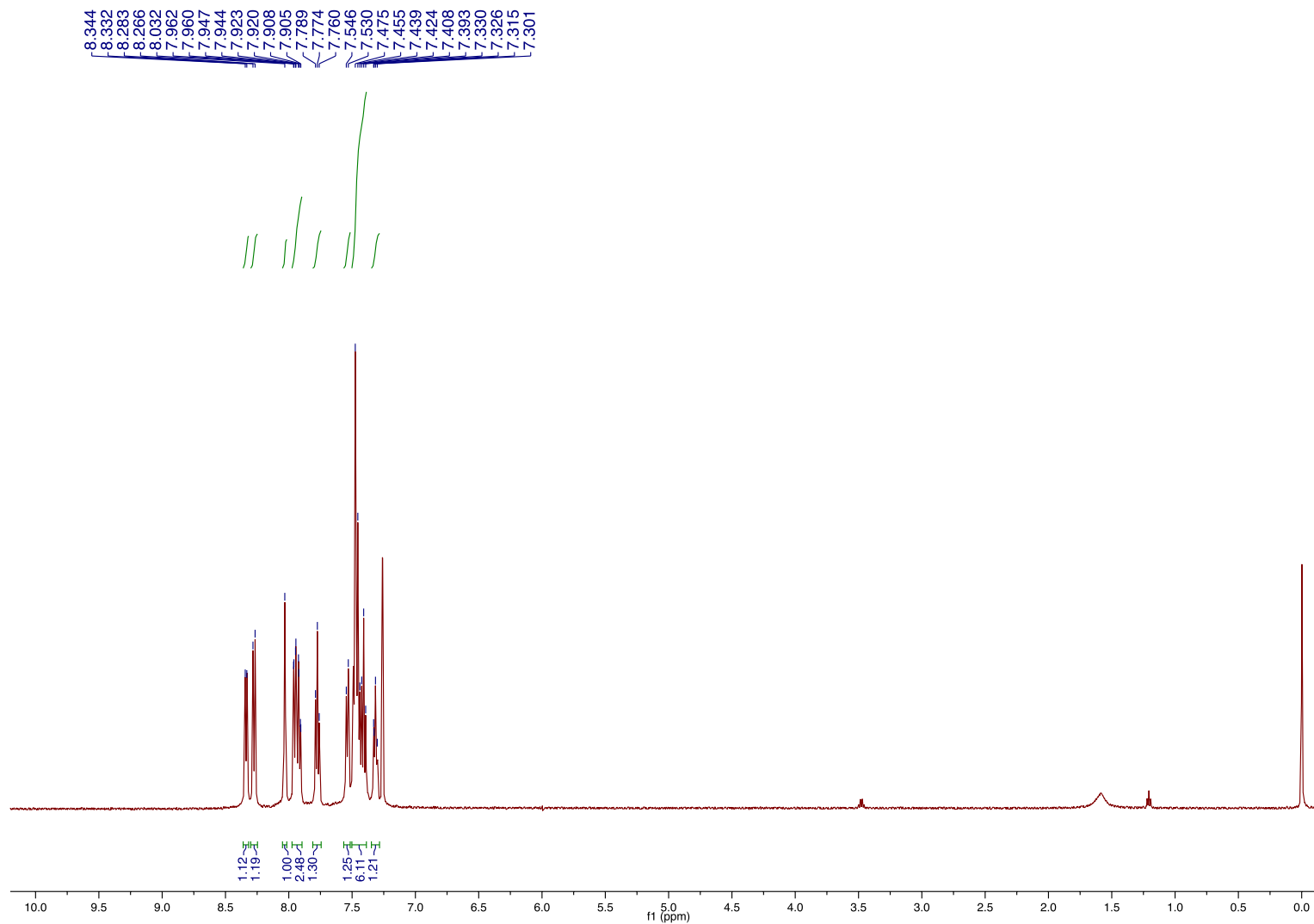
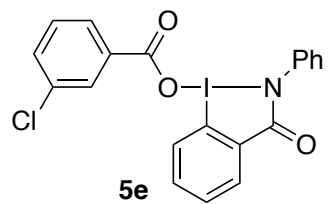
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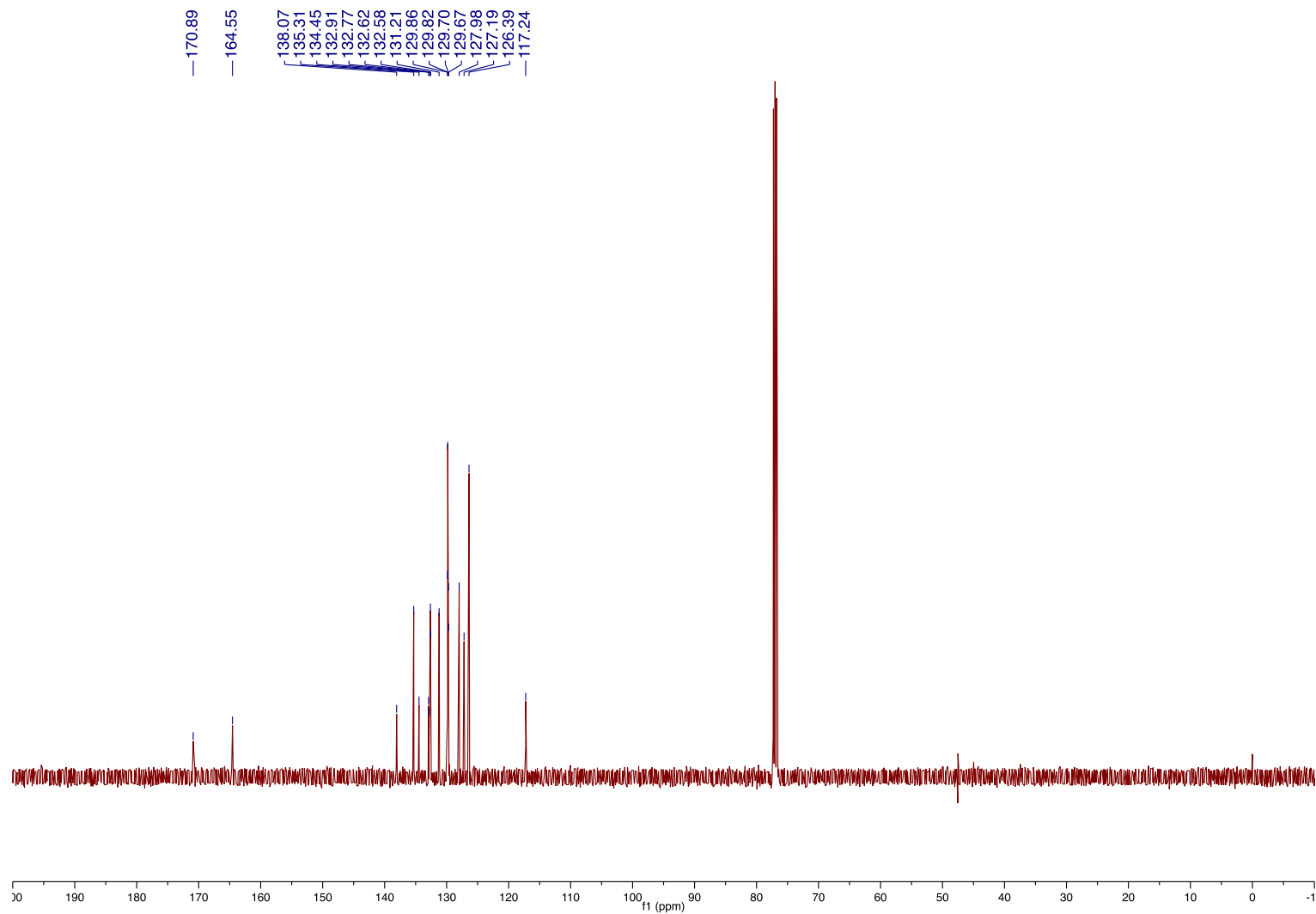
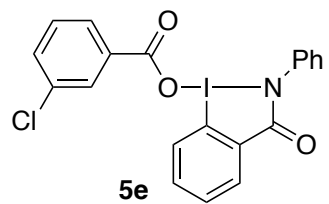
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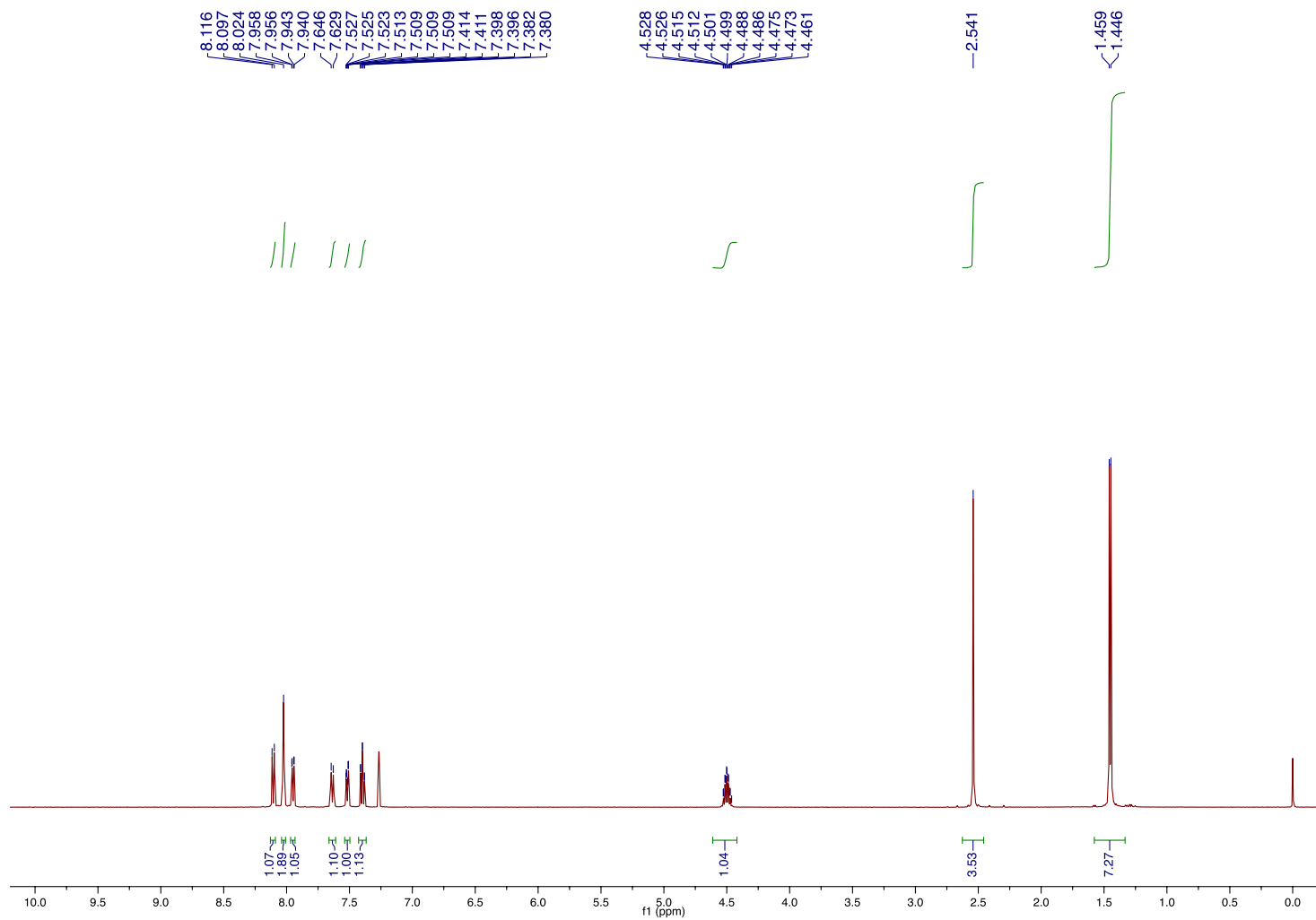
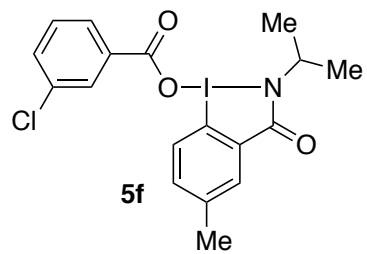
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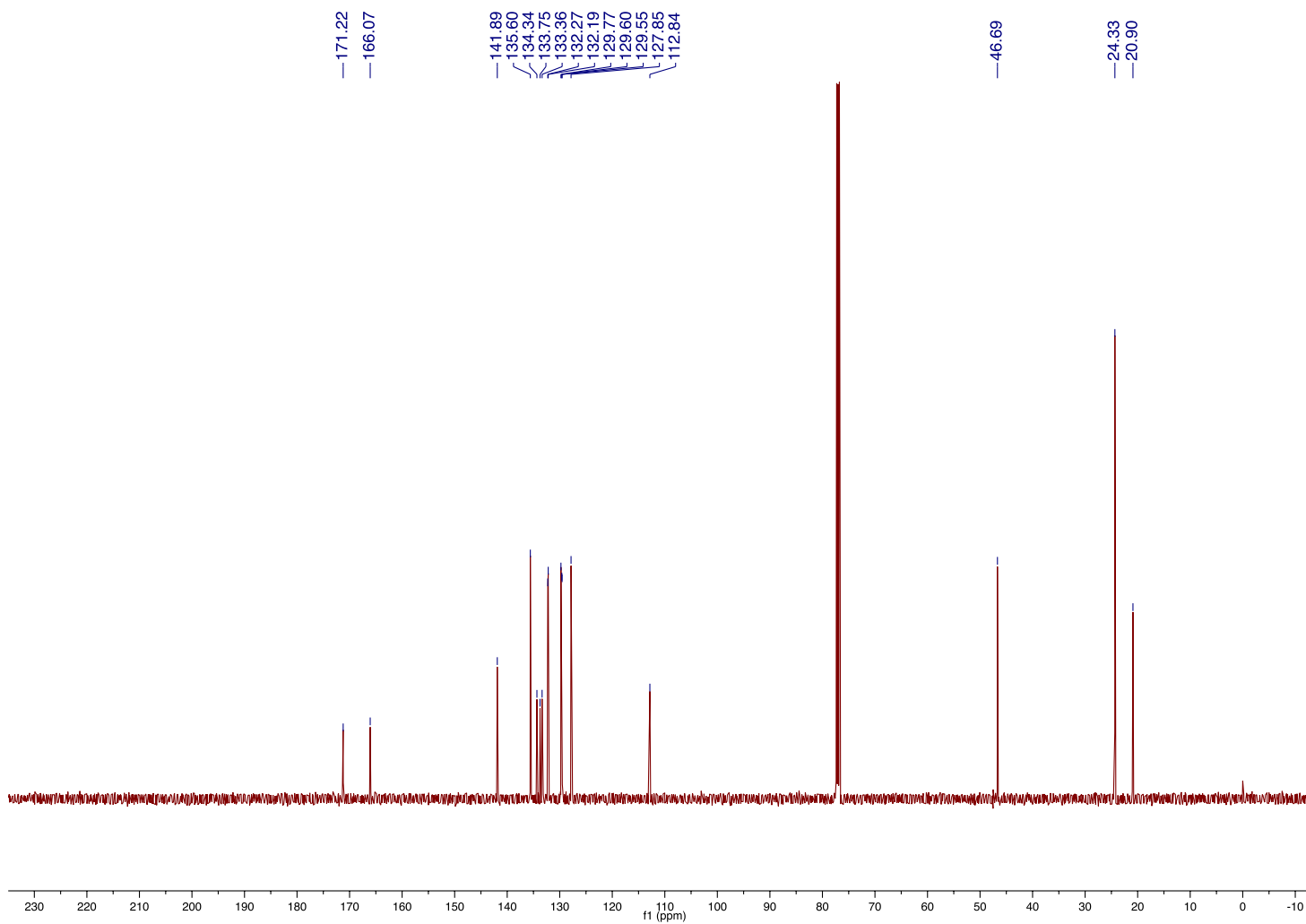
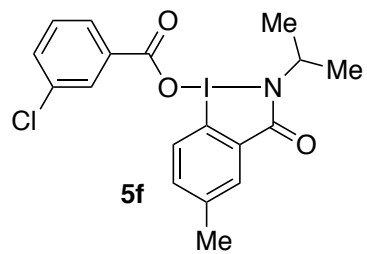
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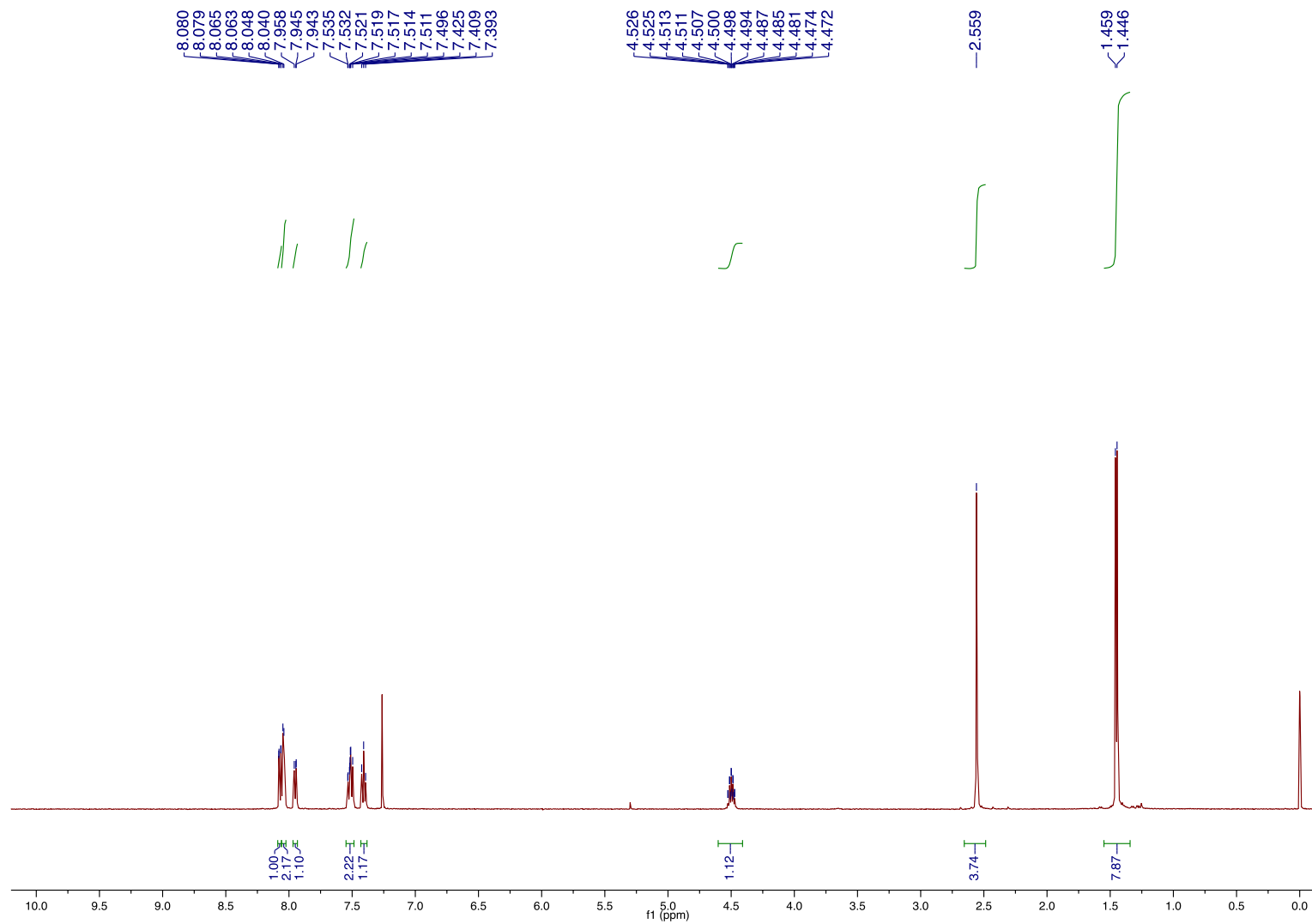
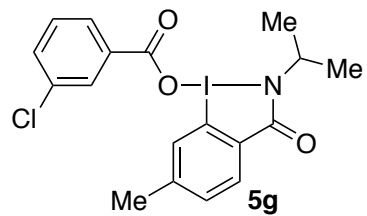
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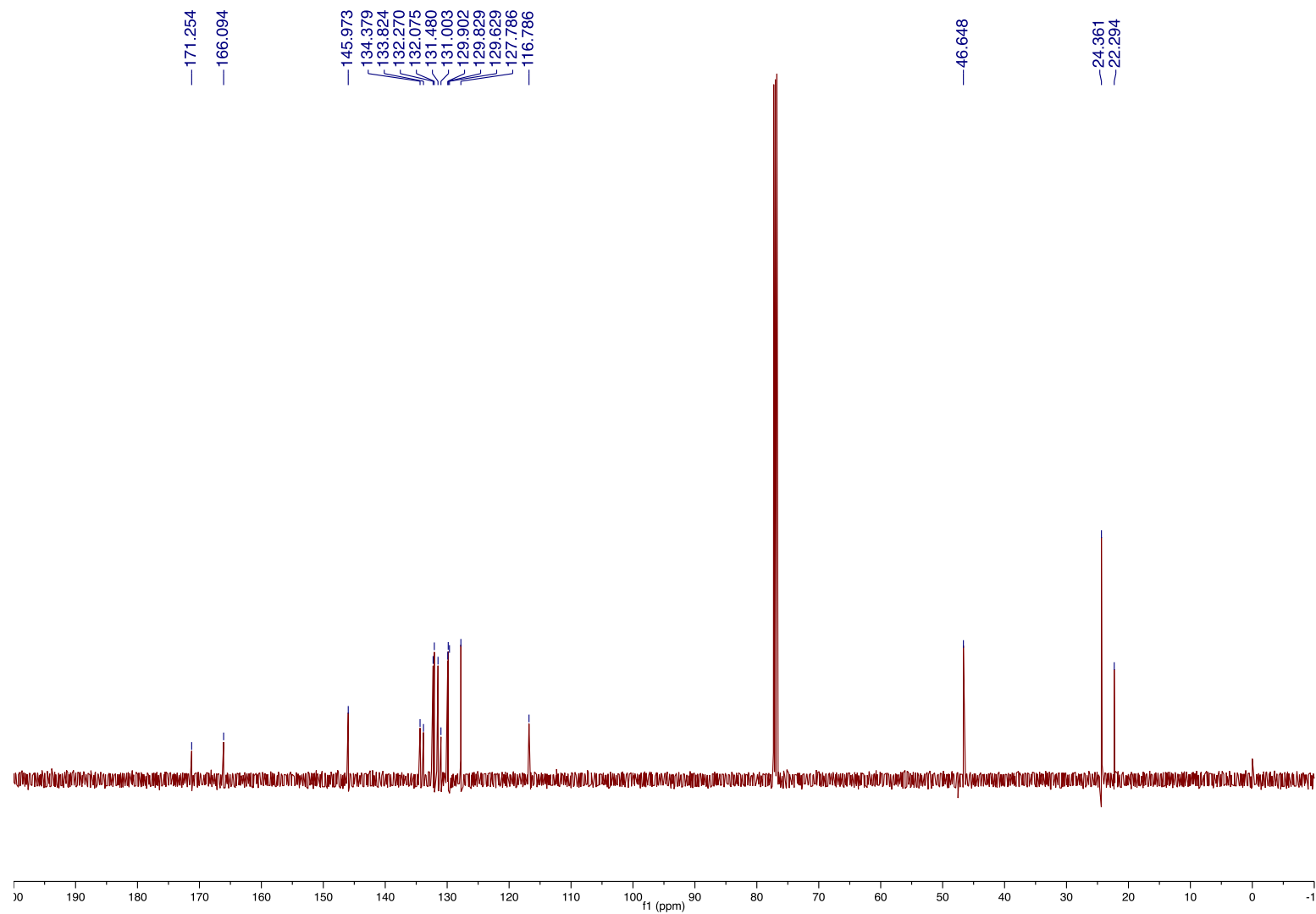
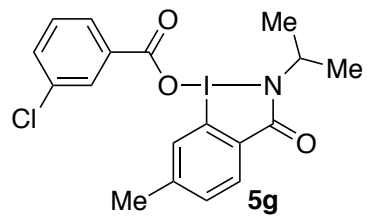
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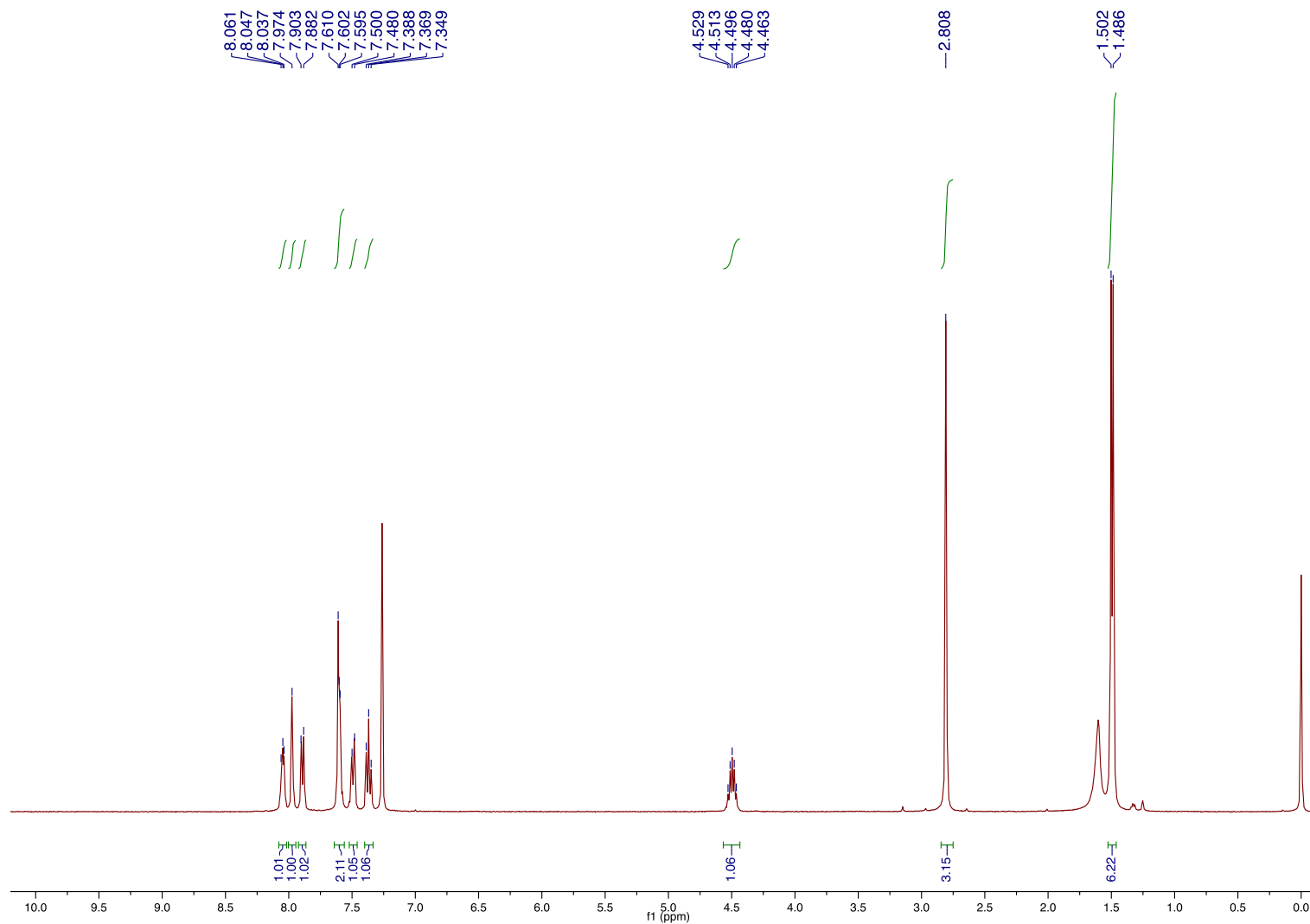
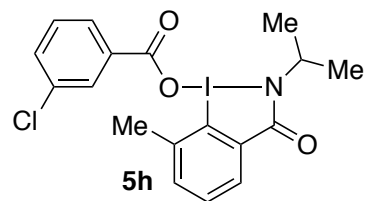
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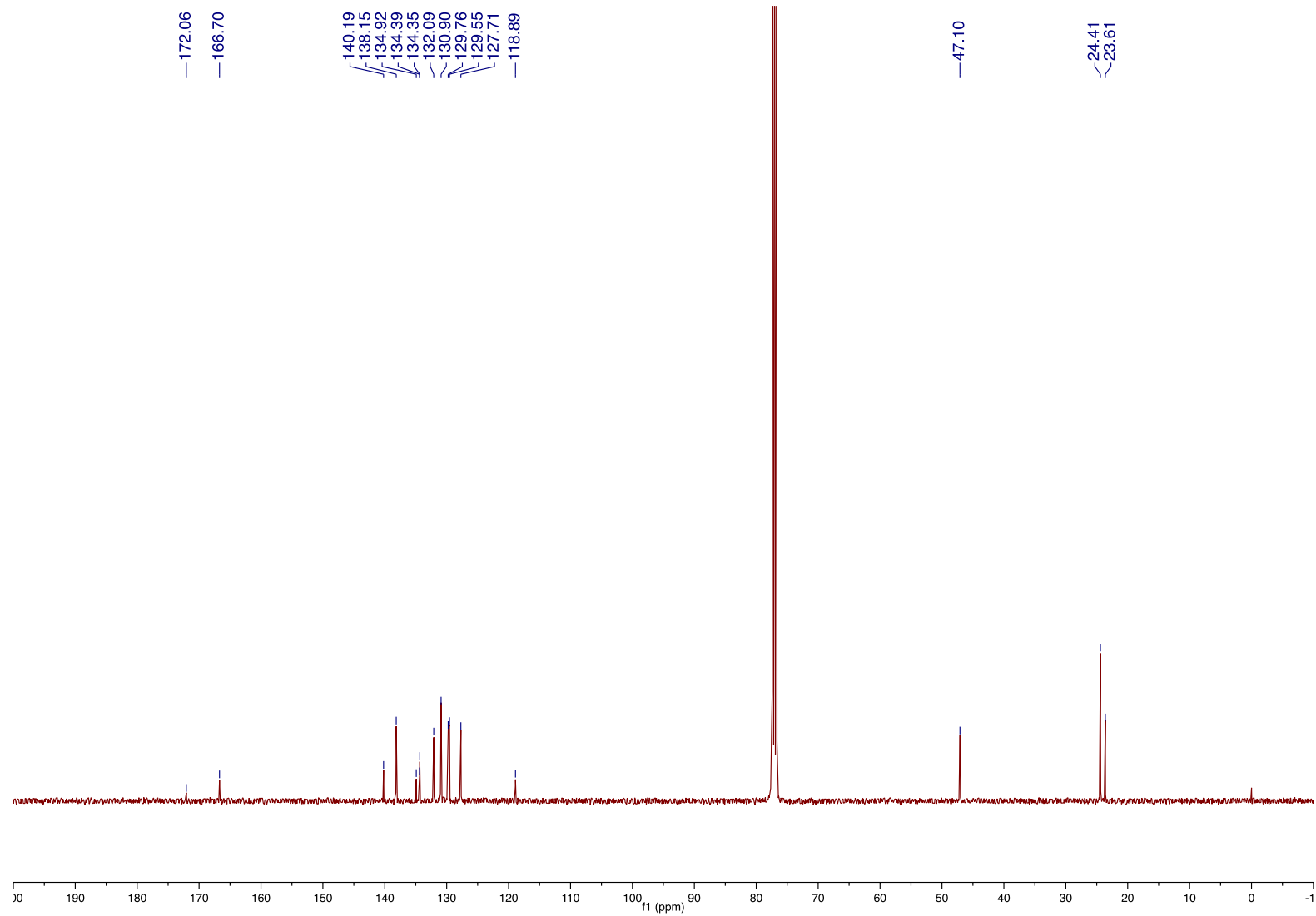
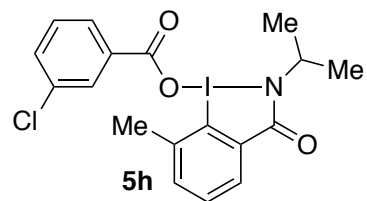
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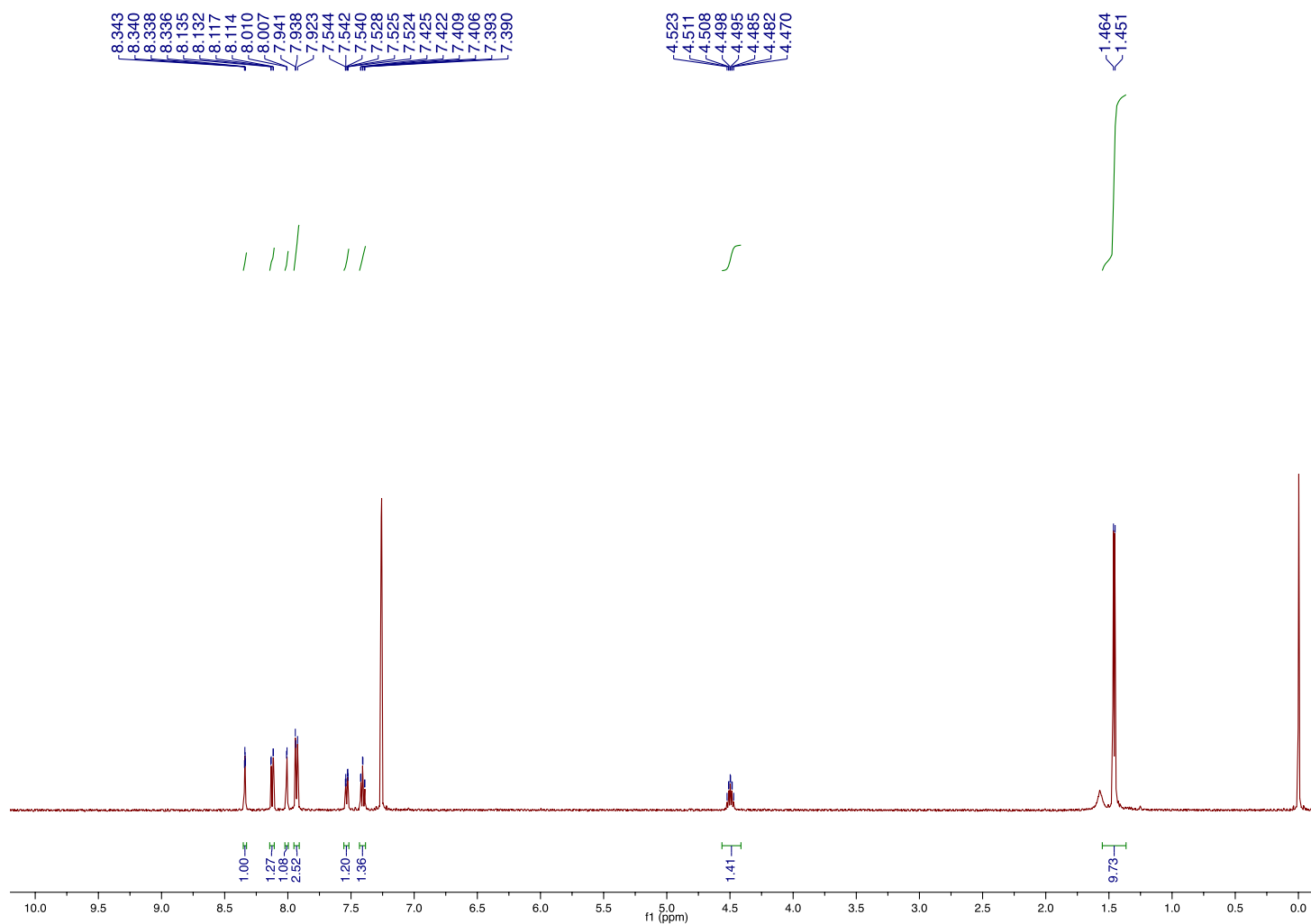
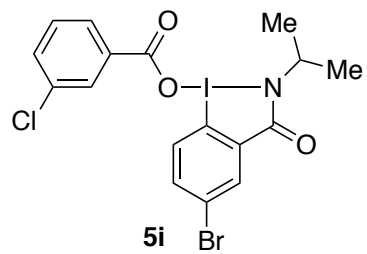
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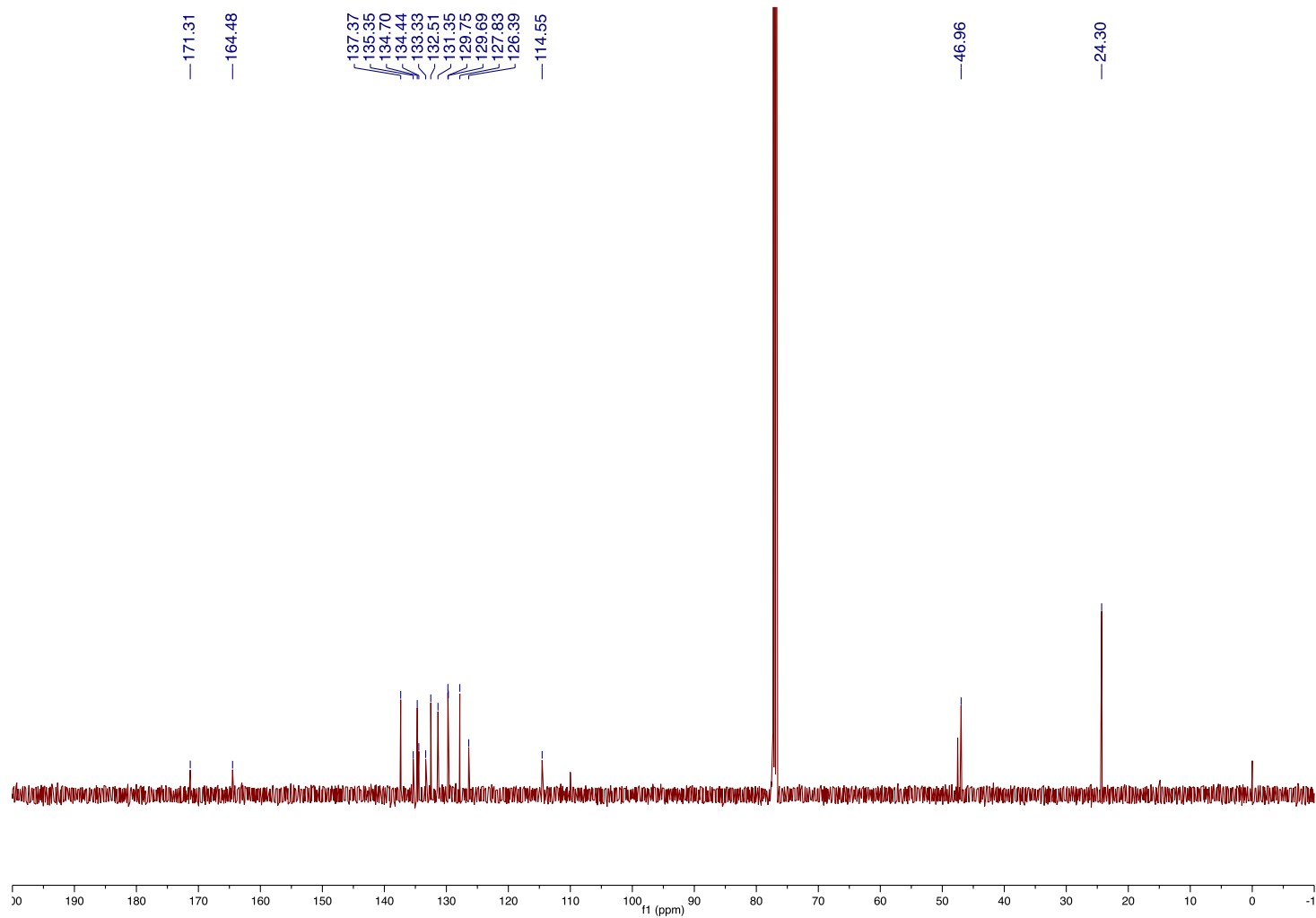
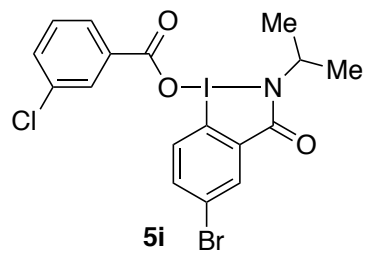
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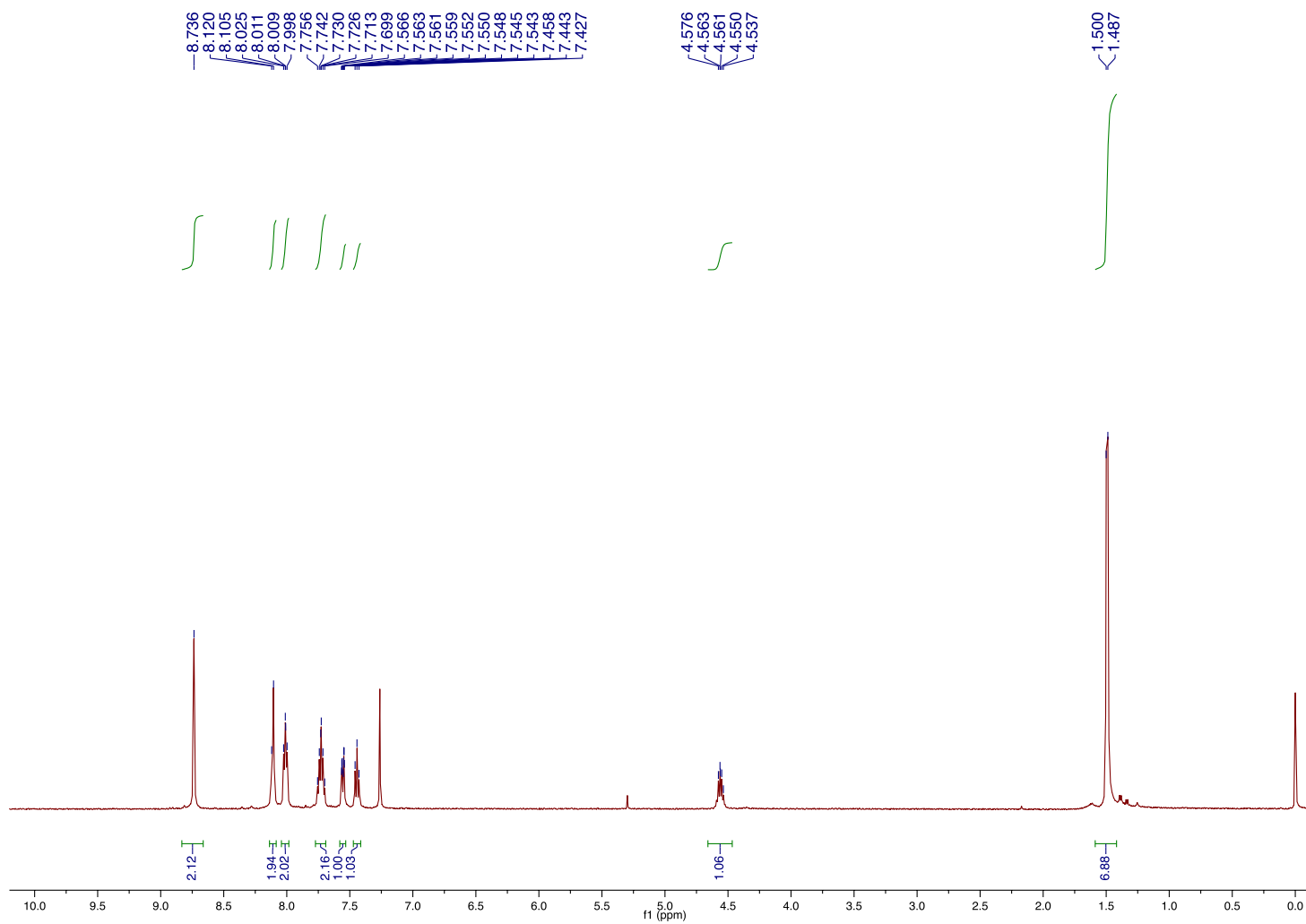
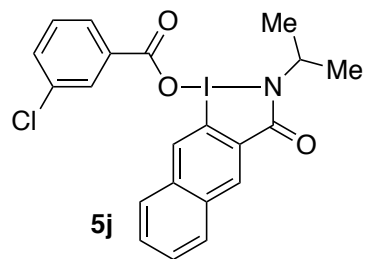
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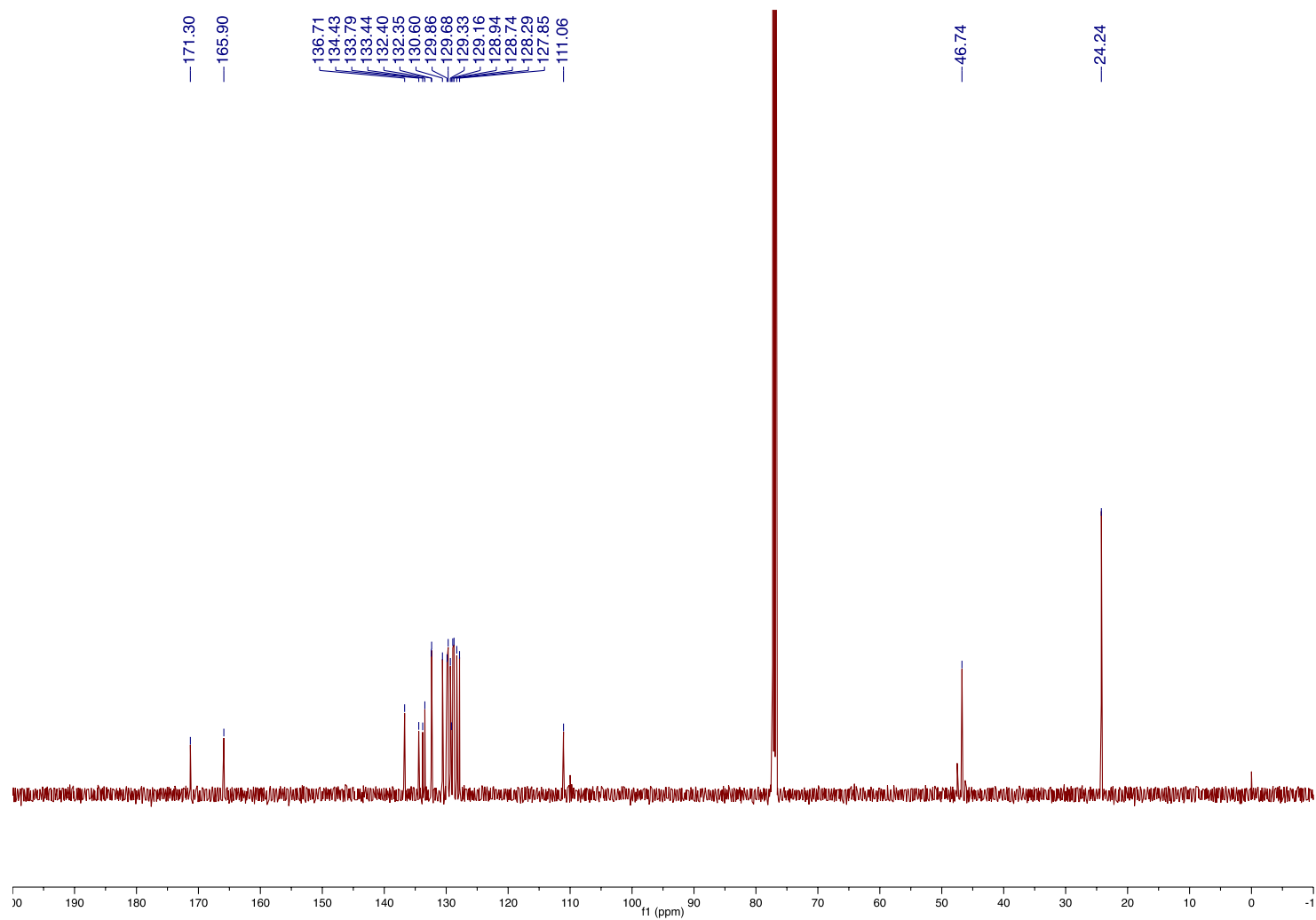
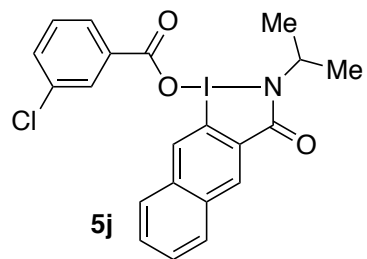
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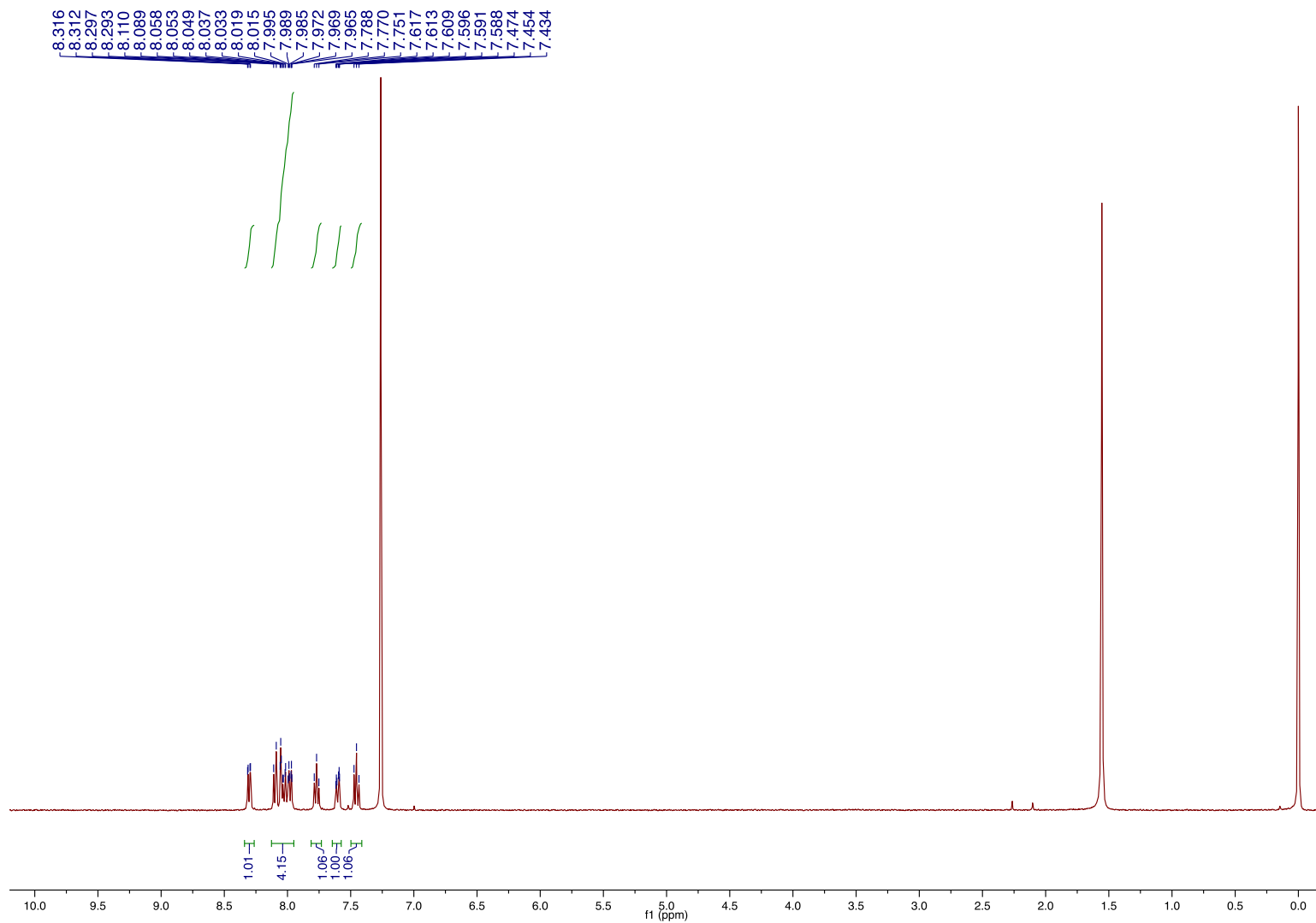
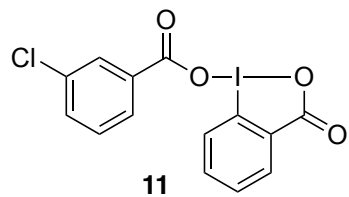
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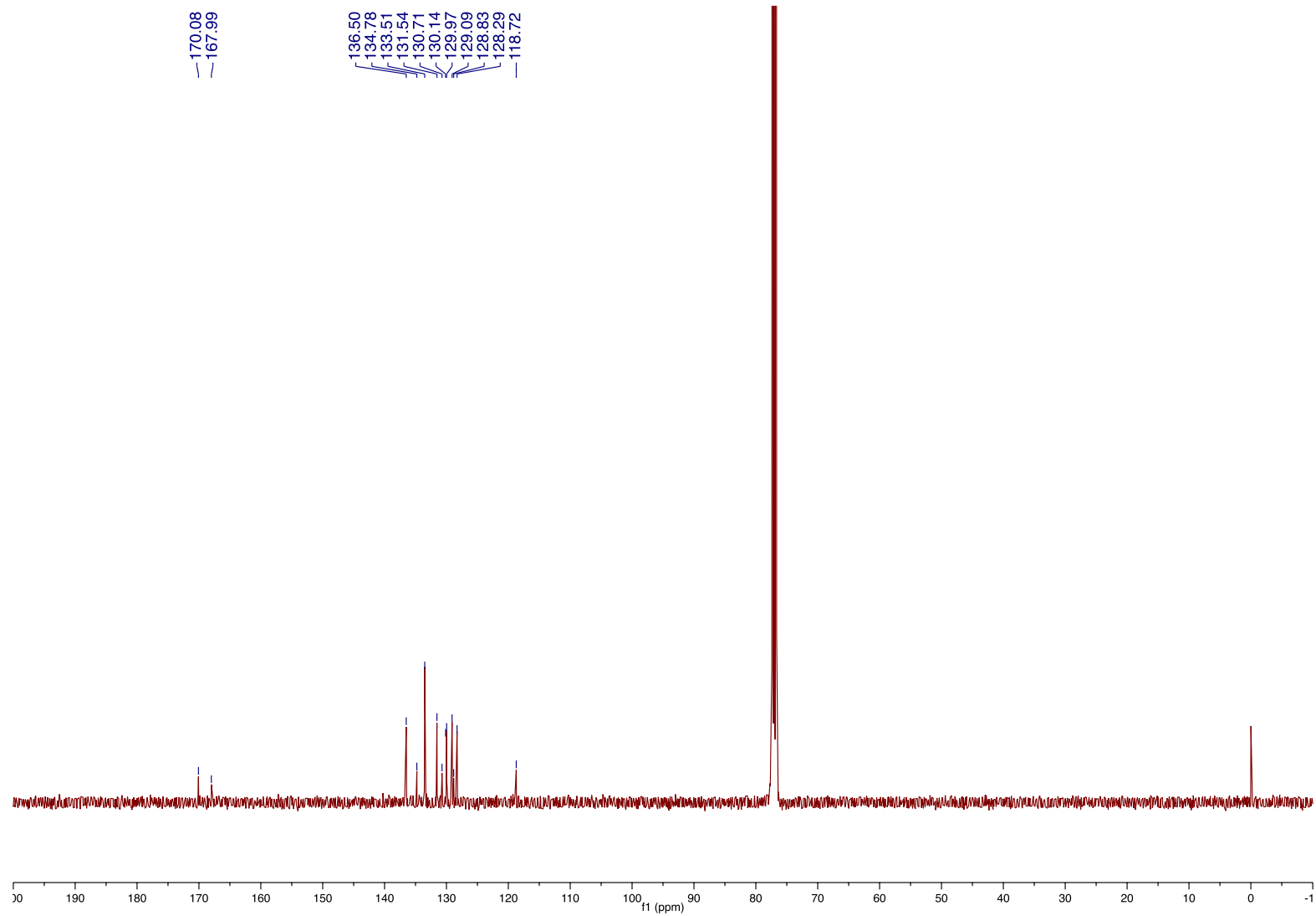
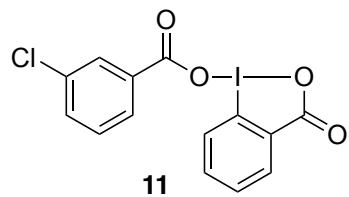
^{13}C NMR (125 MHz, CDCl_3)



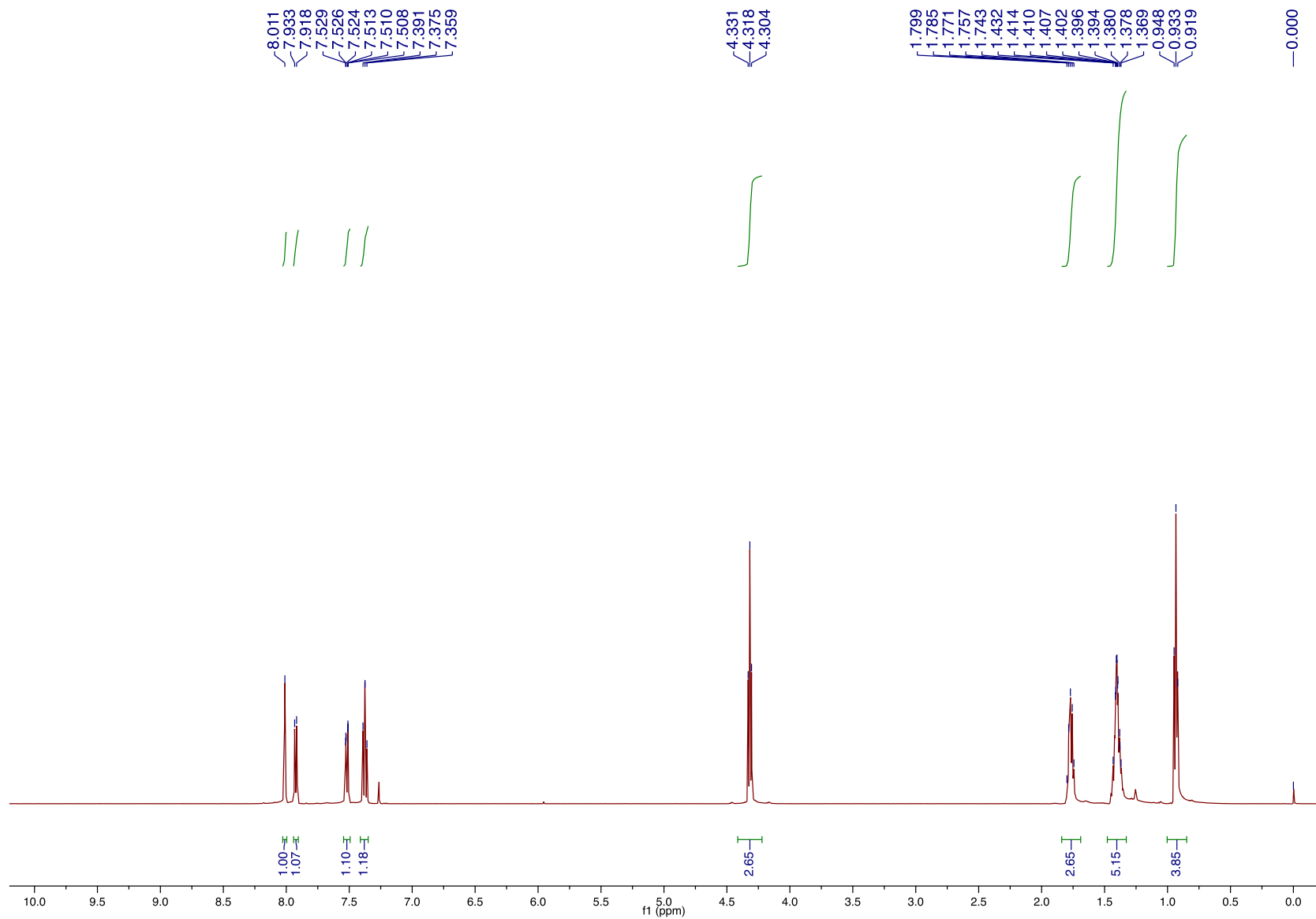
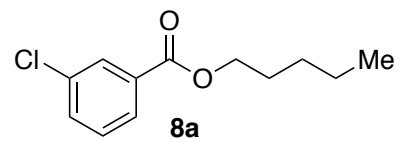
^1H NMR (400 MHz, CDCl_3)



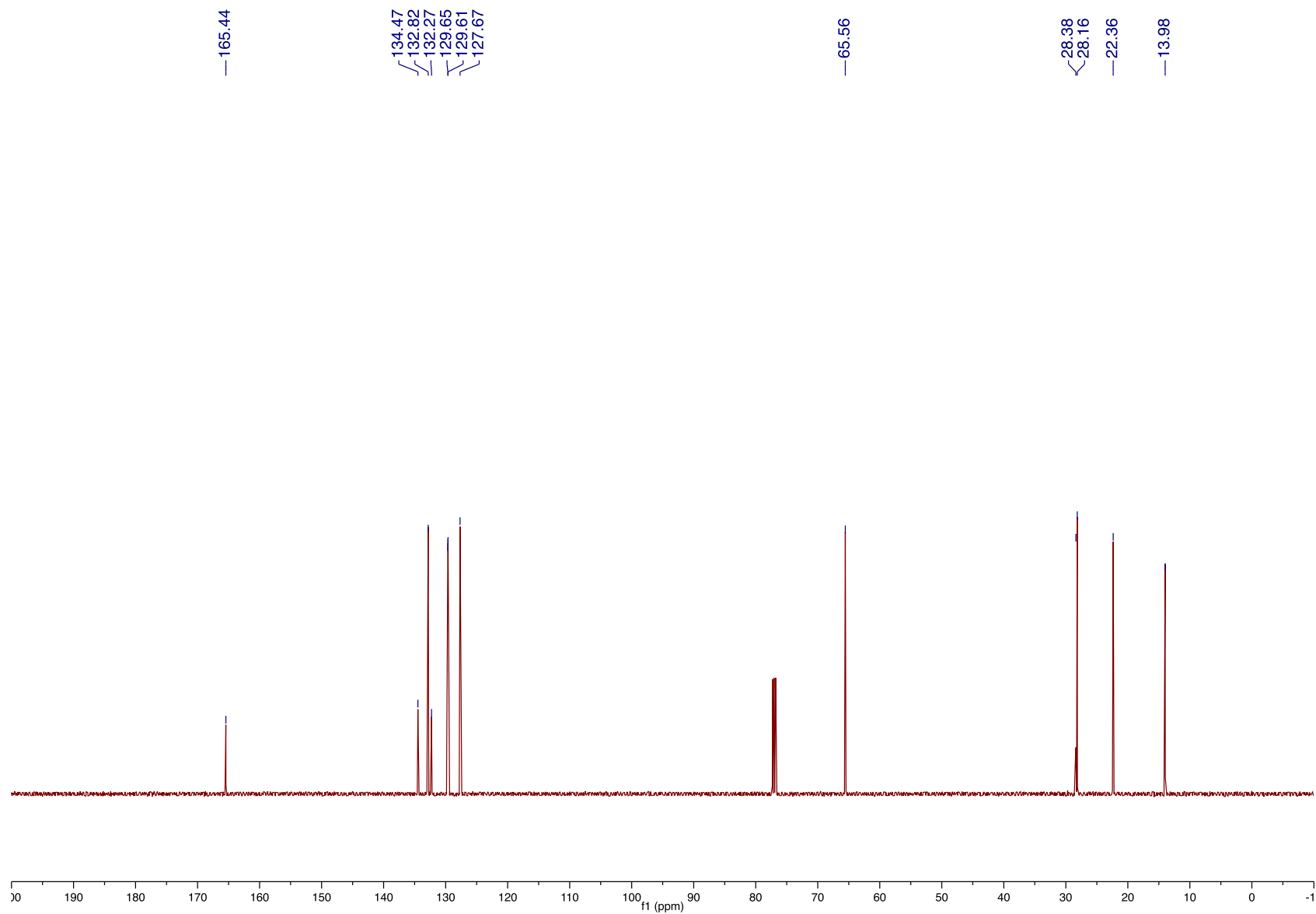
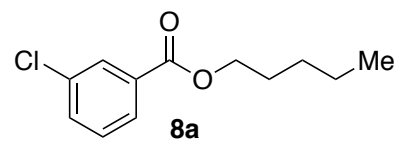
^{13}C NMR (100 MHz, CDCl_3)



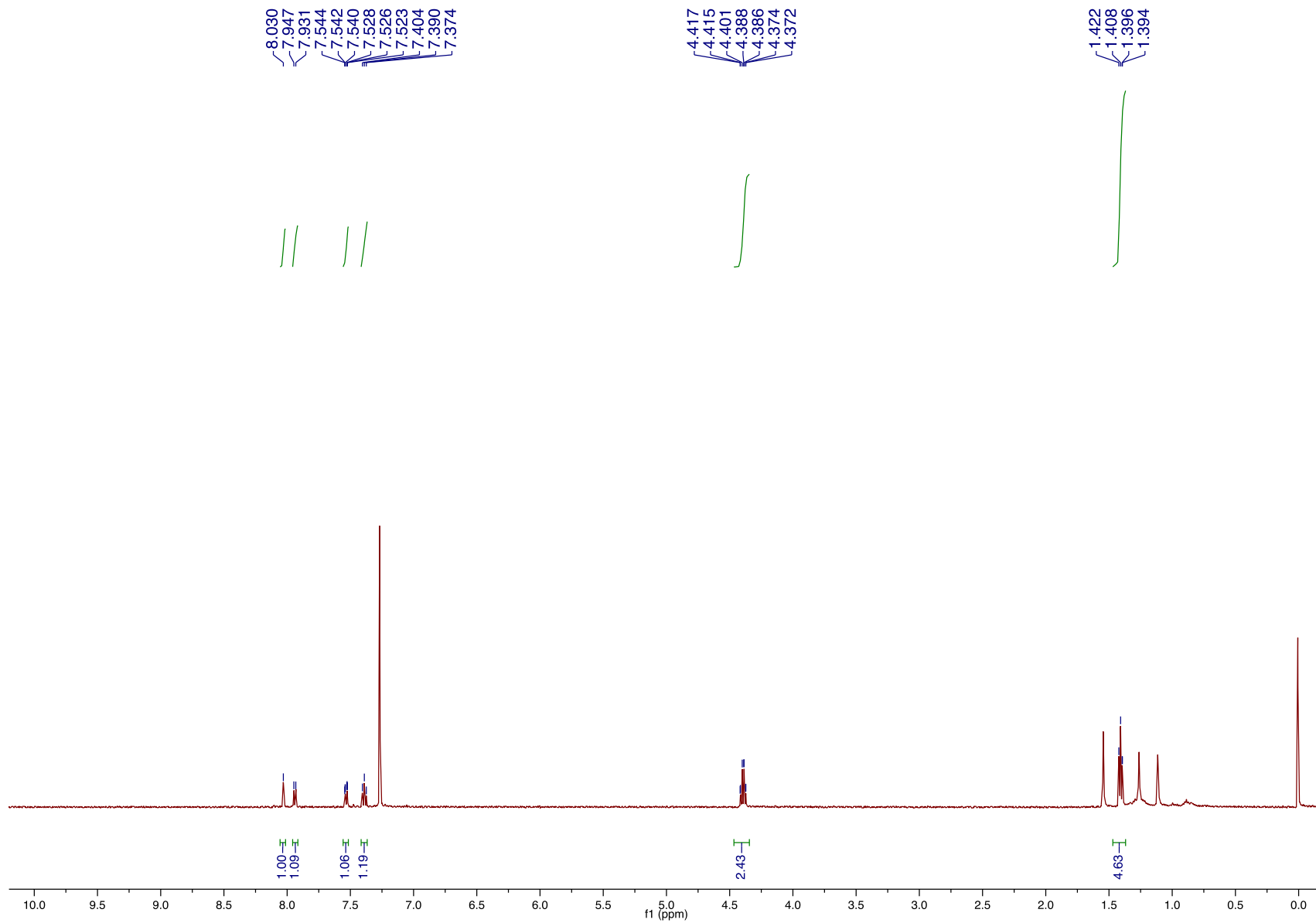
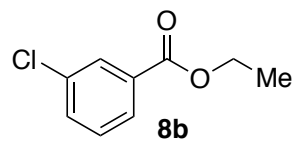
^1H NMR (500 MHz, CDCl_3)



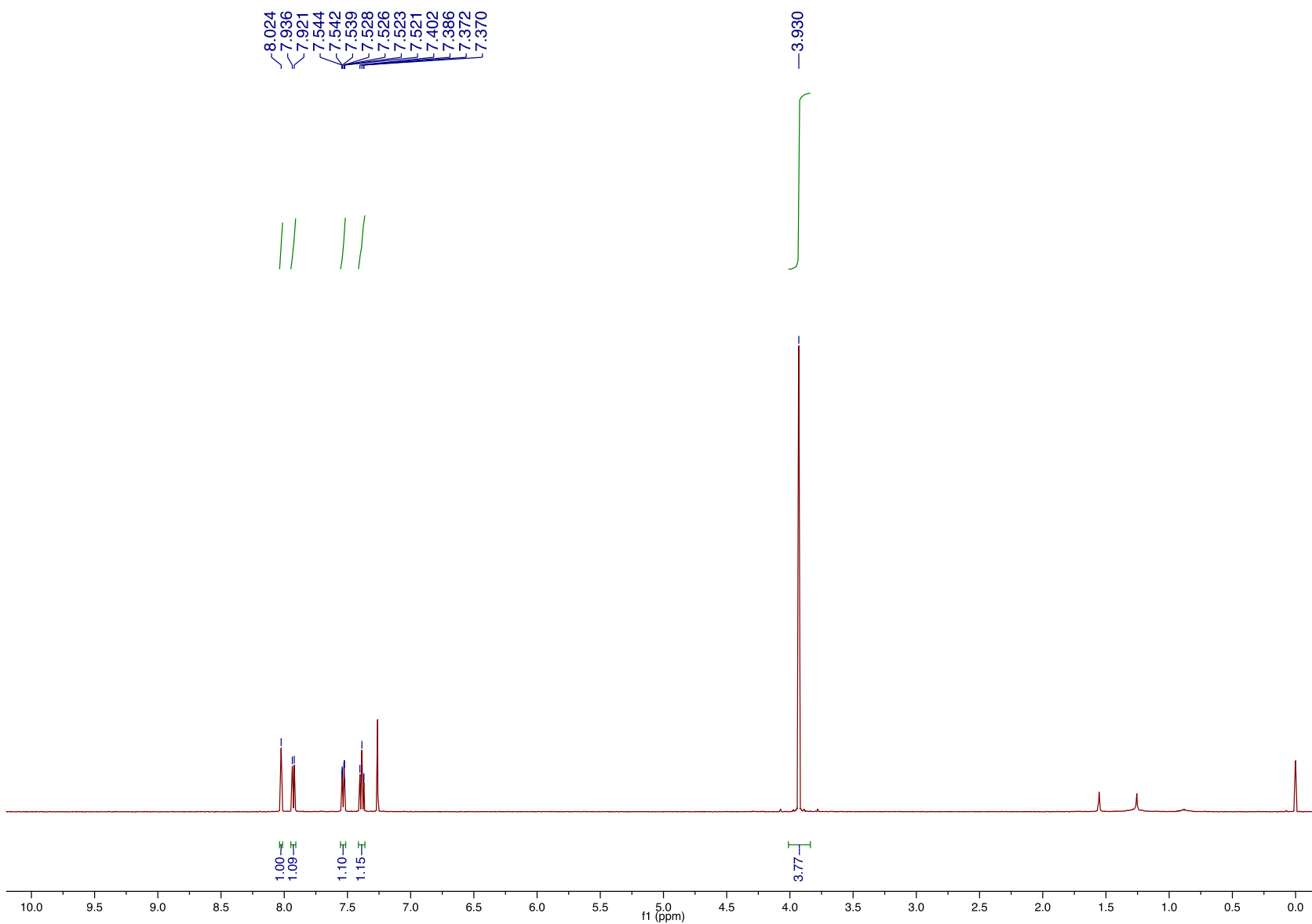
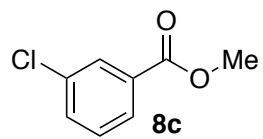
^{13}C NMR (125 MHz, CDCl_3)



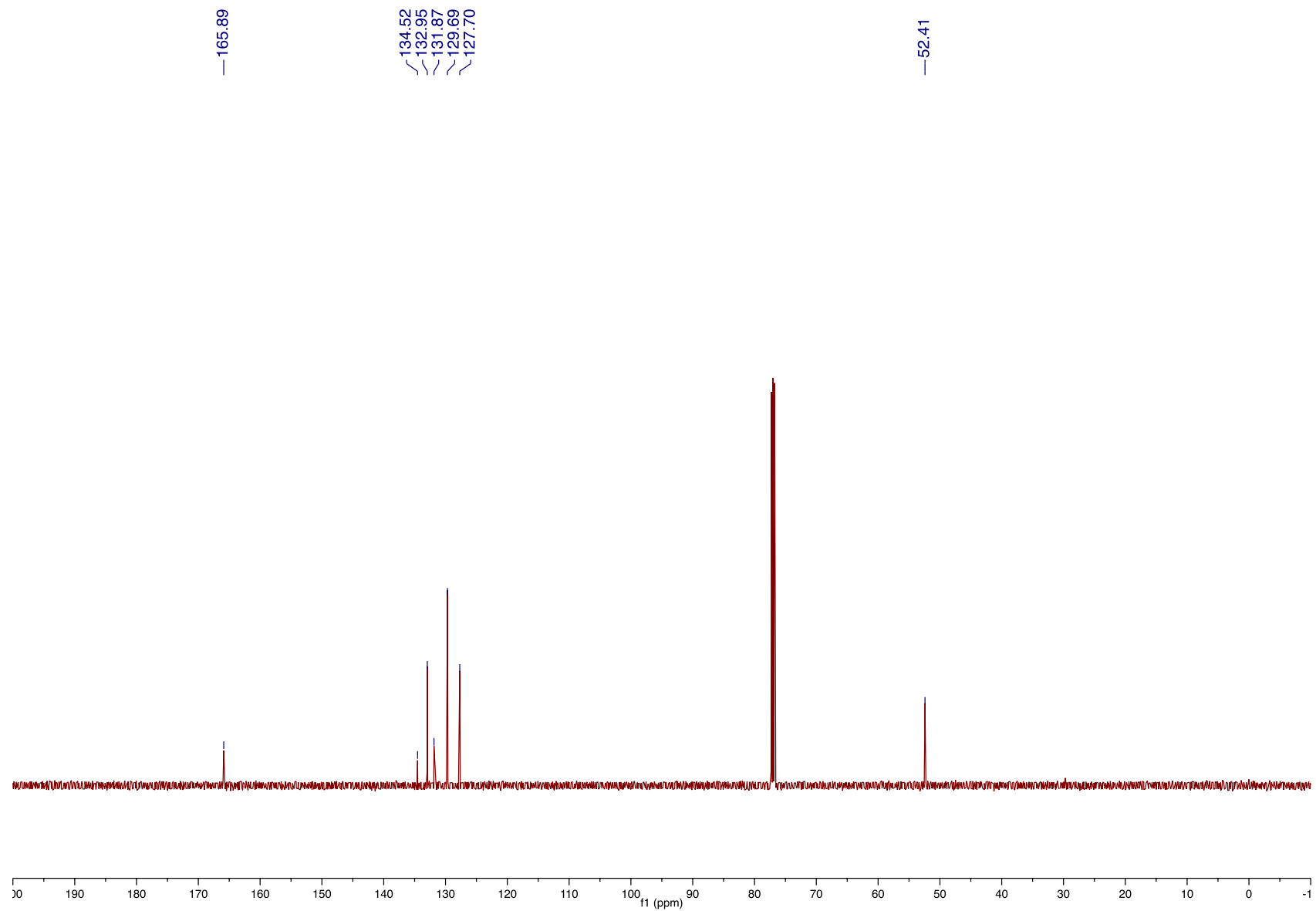
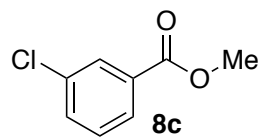
^1H NMR (500 MHz, CDCl_3)



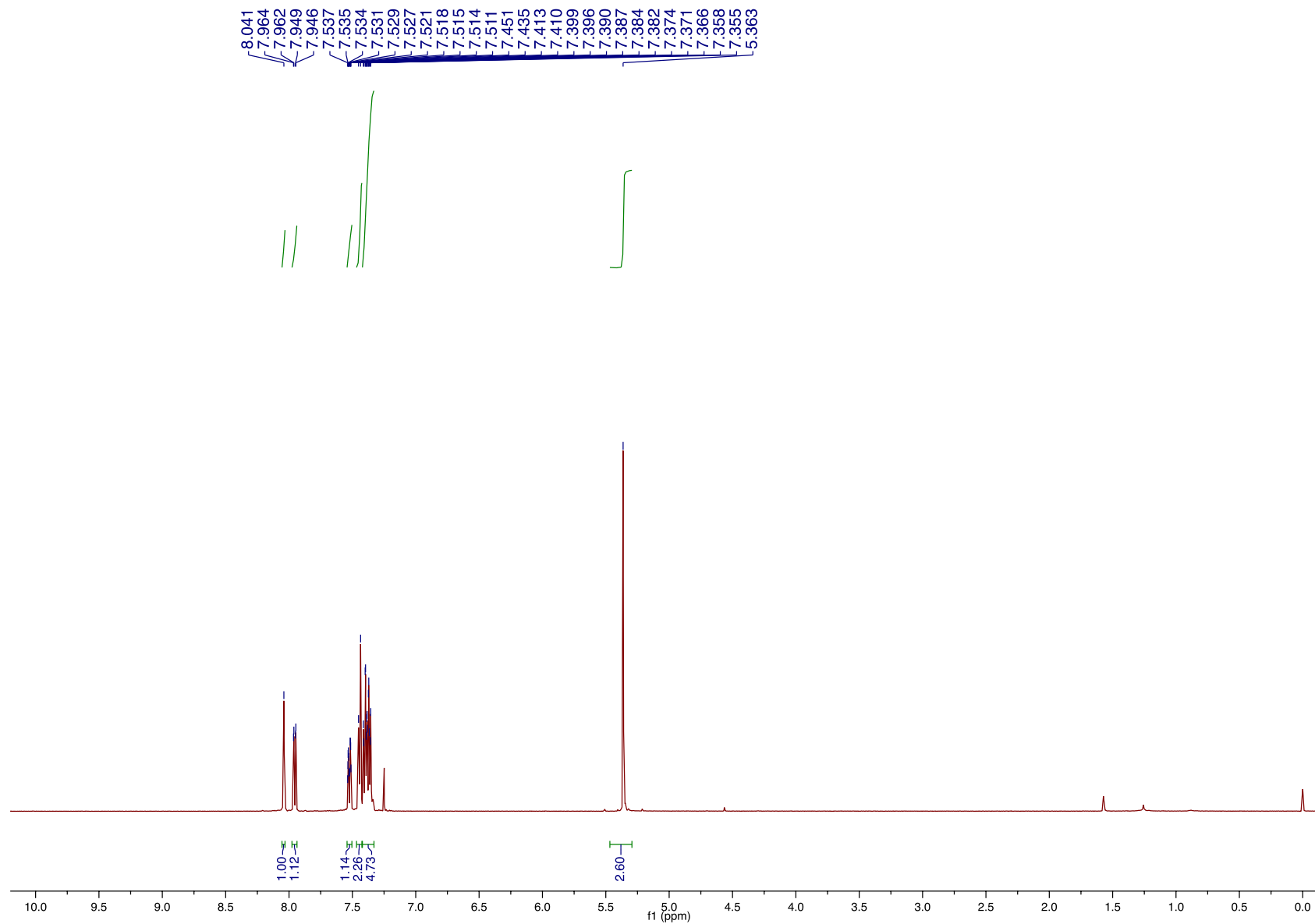
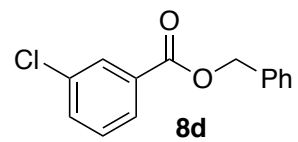
^1H NMR (500 MHz, CDCl_3)



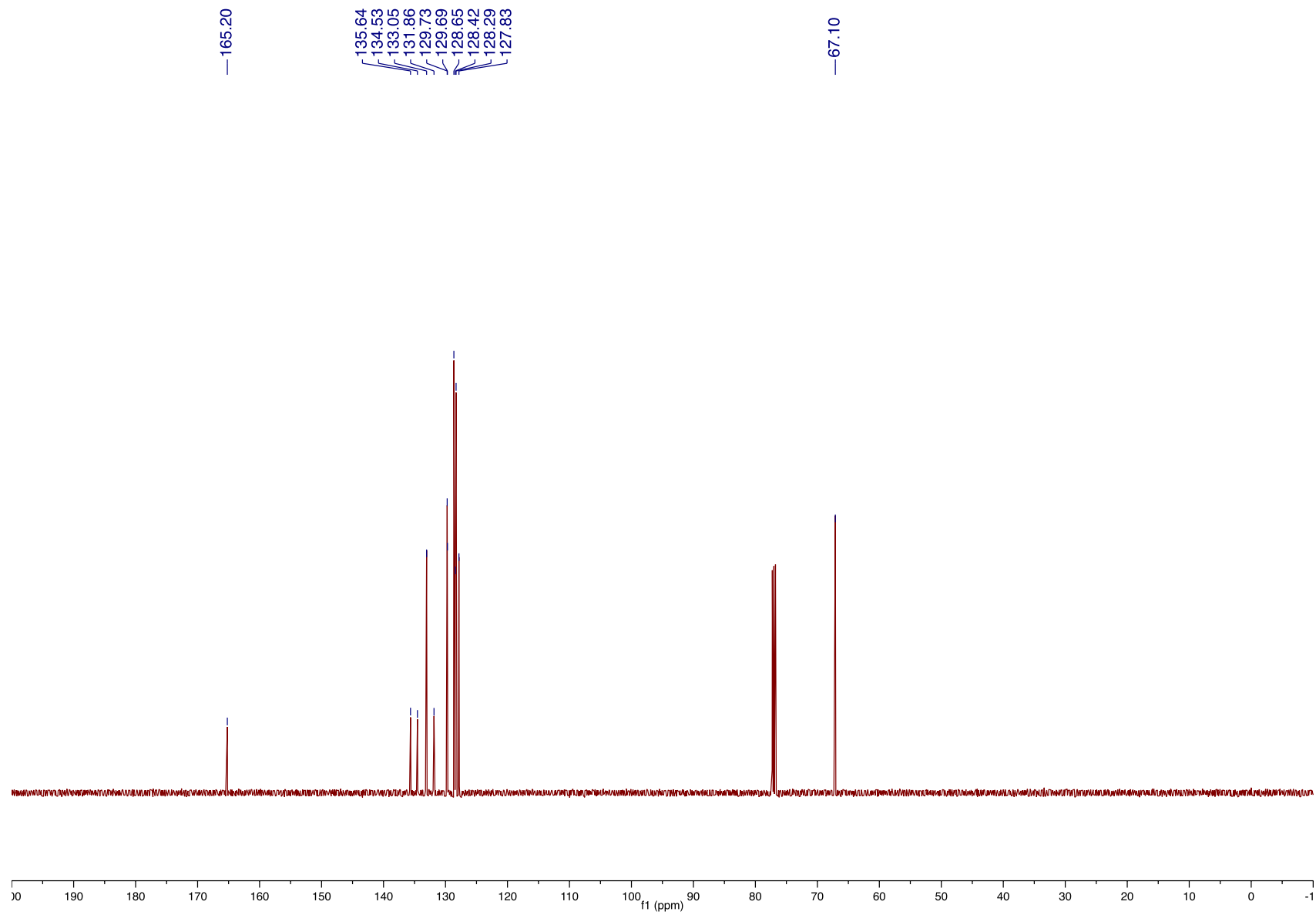
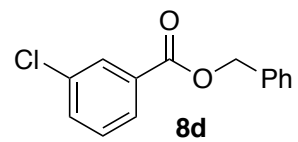
^{13}C NMR (125 MHz, CDCl_3)



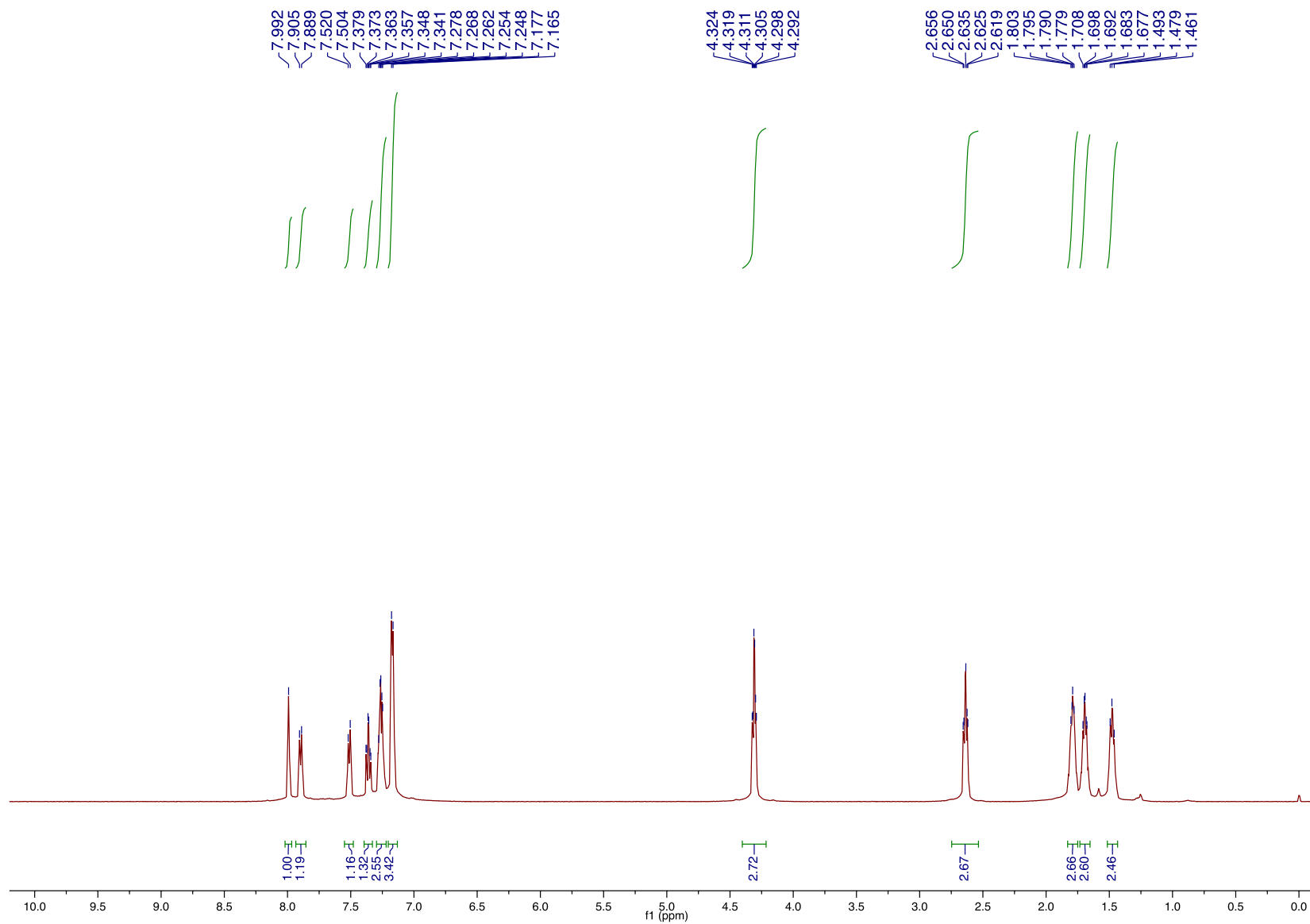
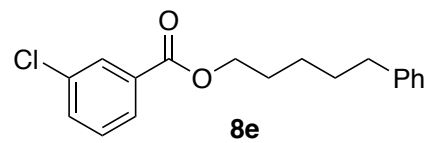
^1H NMR (500 MHz, CDCl_3)



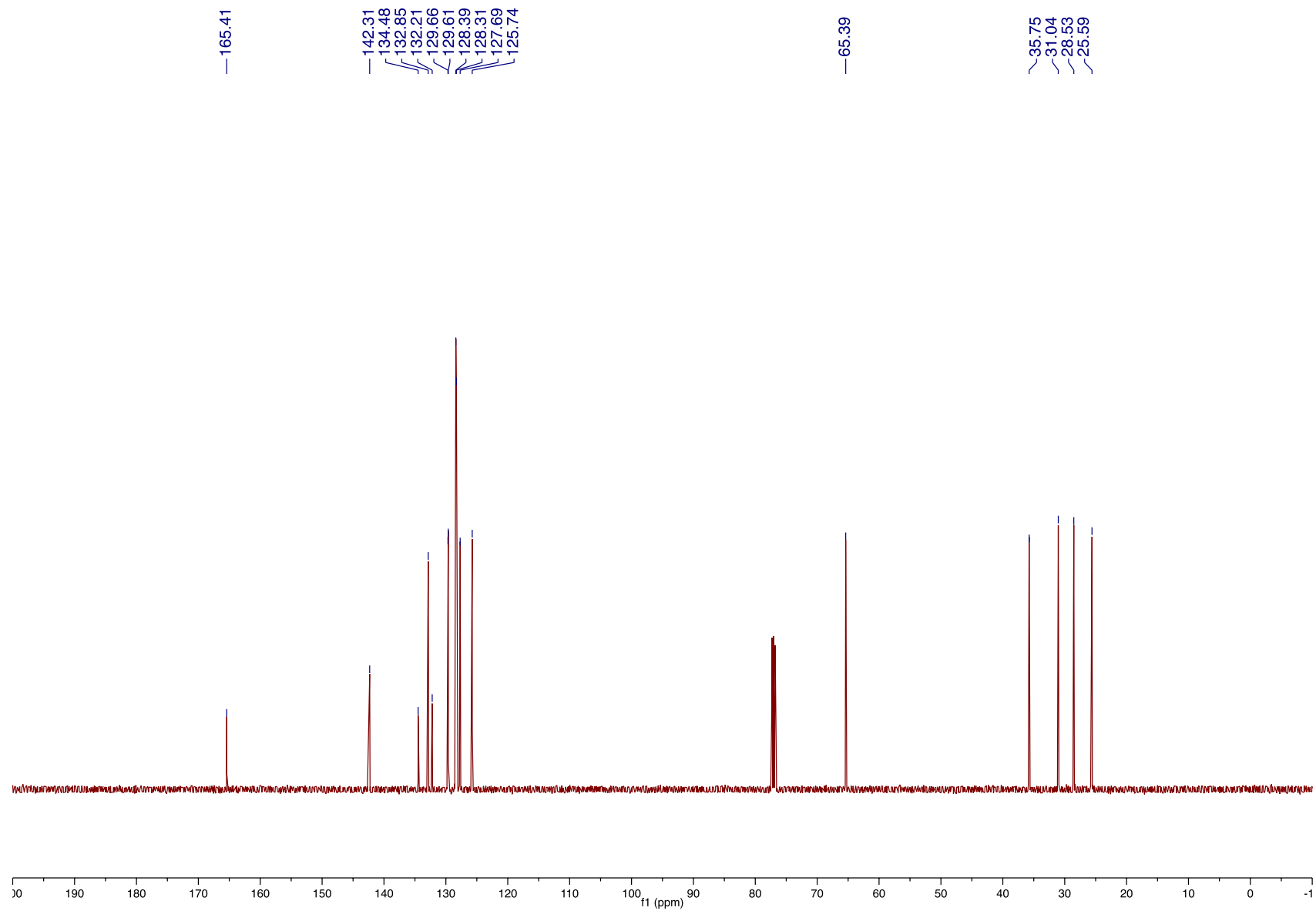
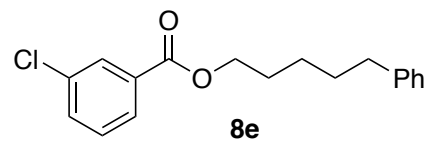
^{13}C NMR (125 MHz, CDCl_3)



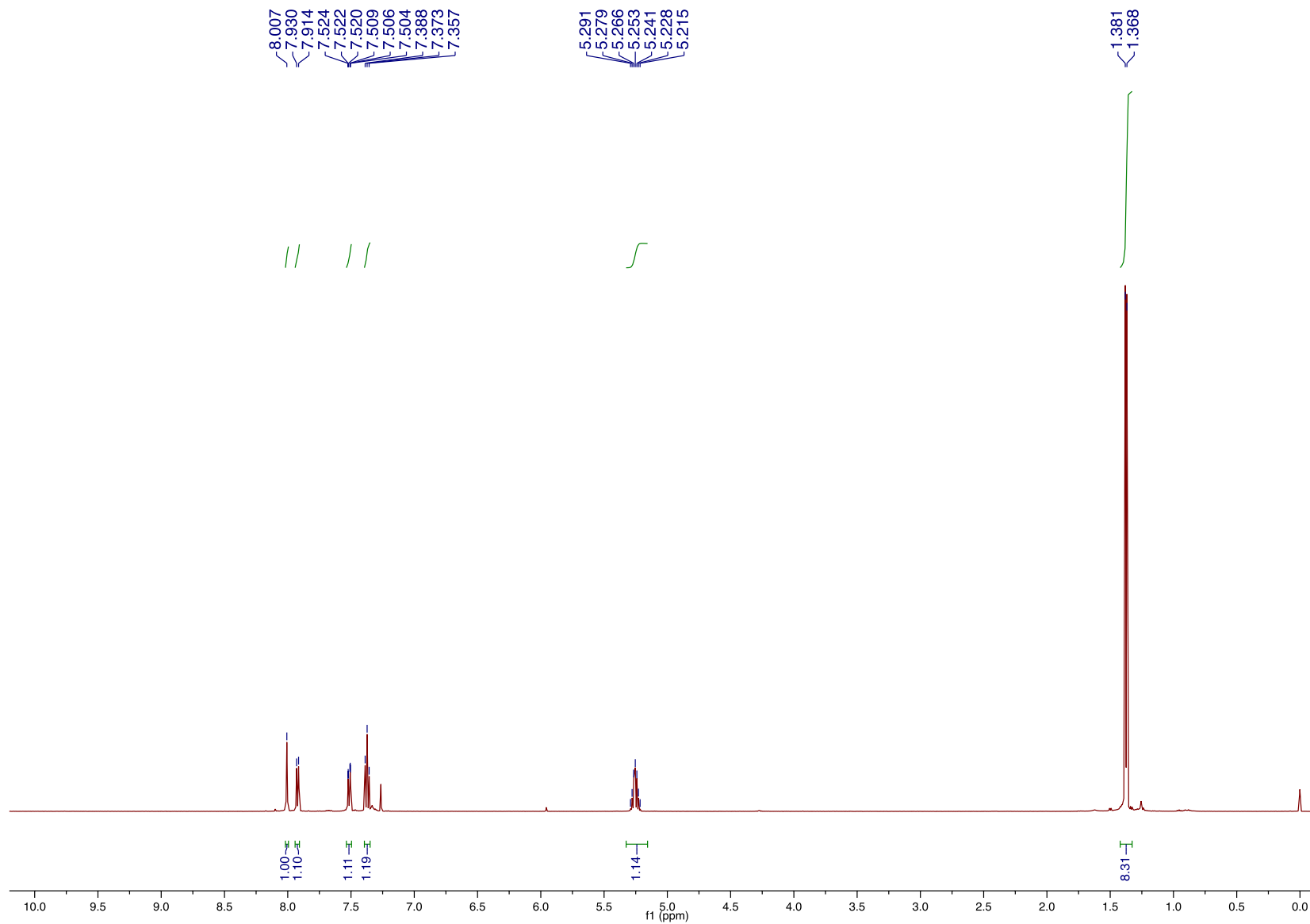
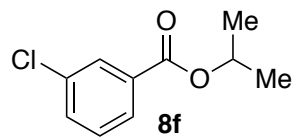
^1H NMR (500 MHz, CDCl_3)



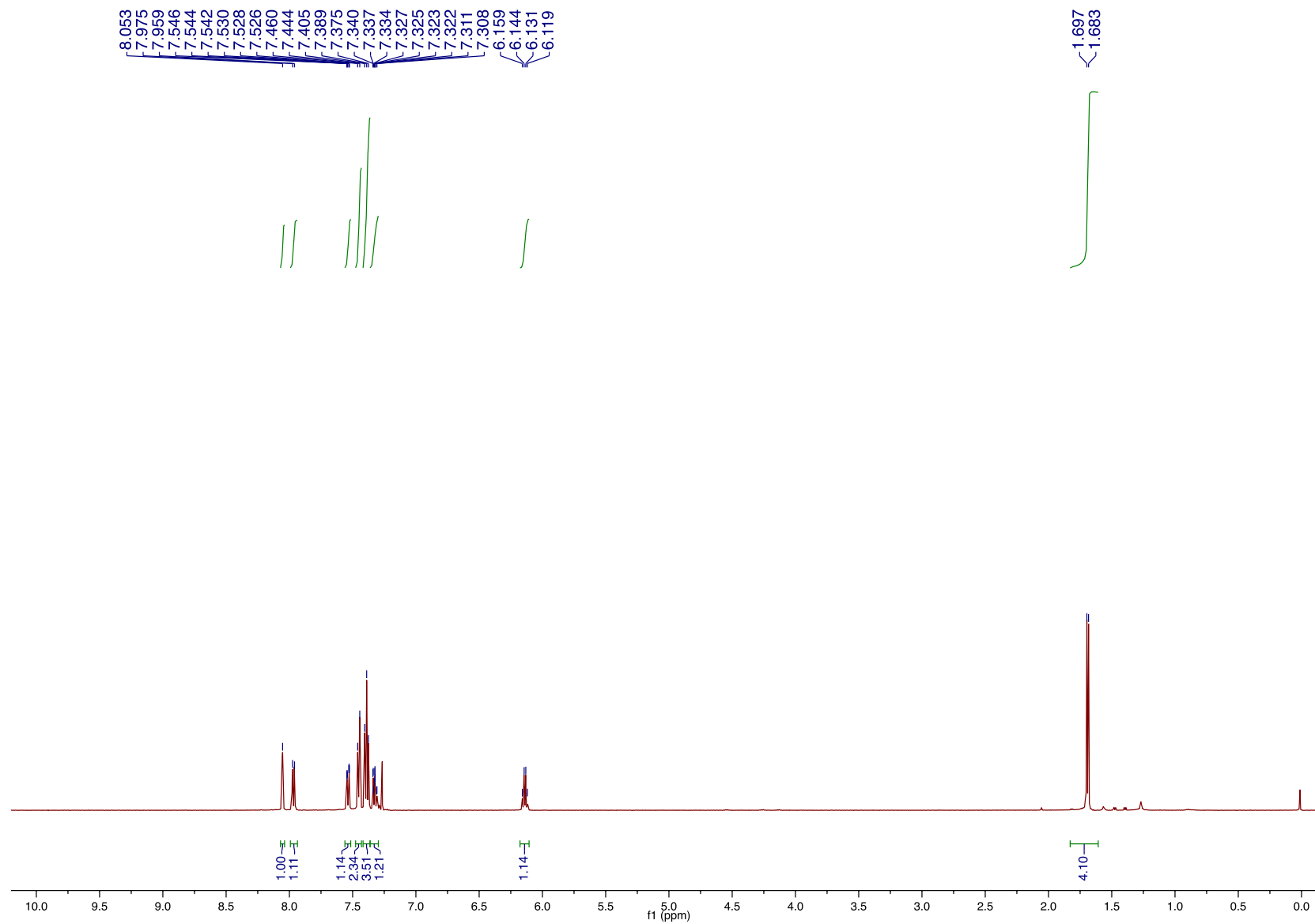
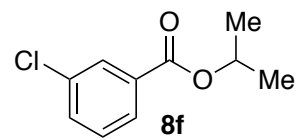
^{13}C NMR (125 MHz, CDCl_3)



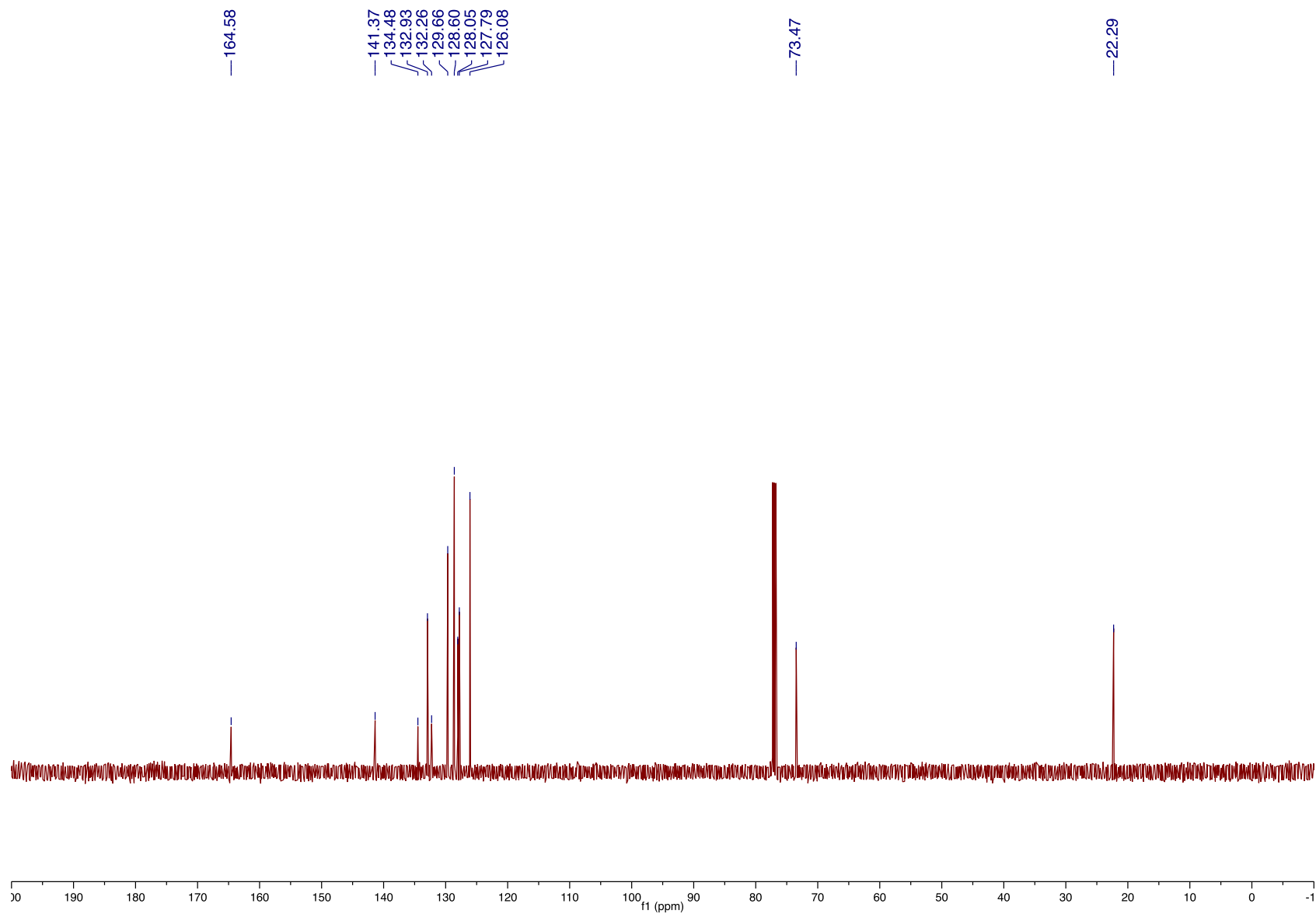
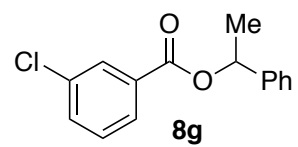
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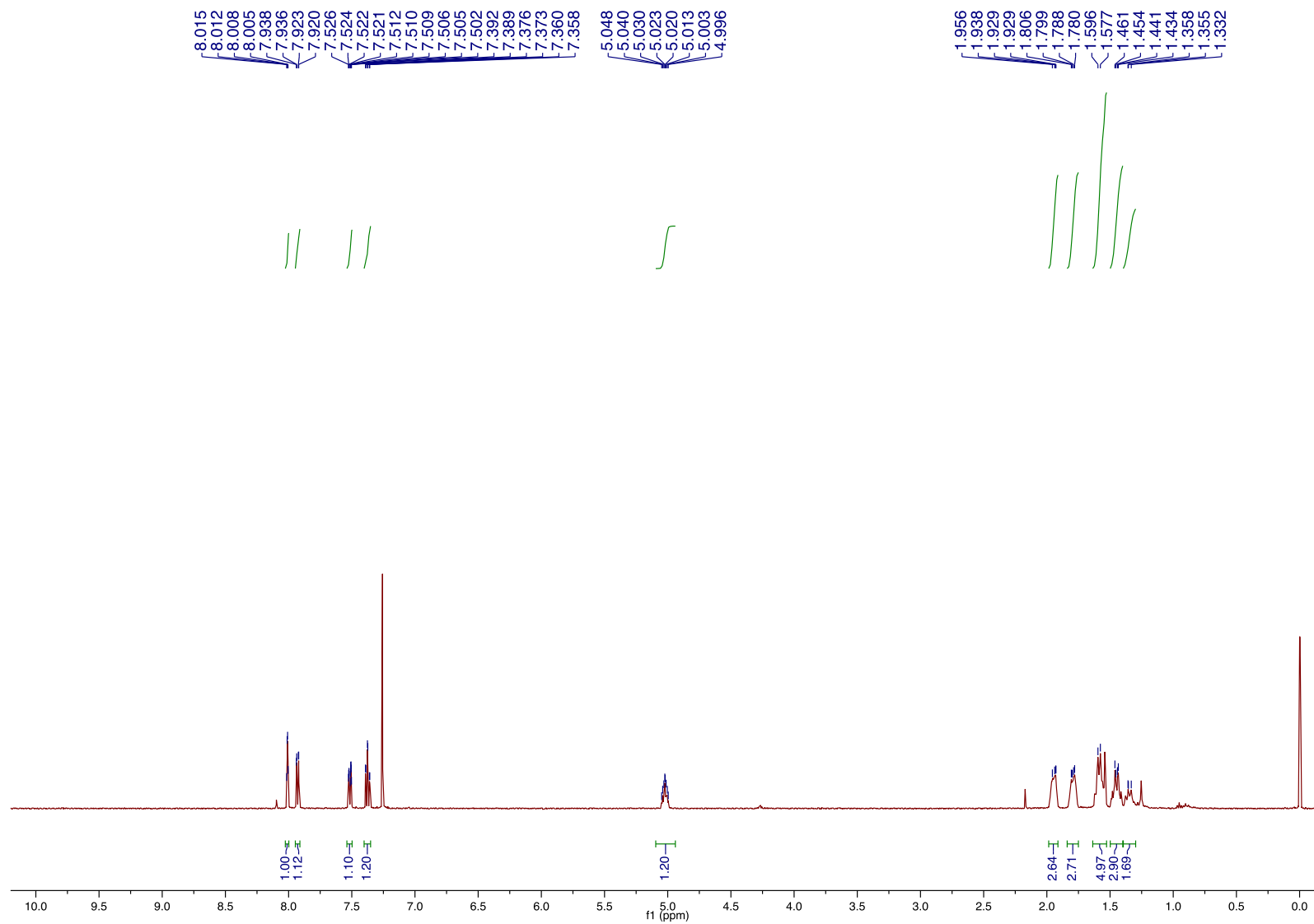
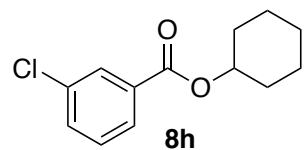
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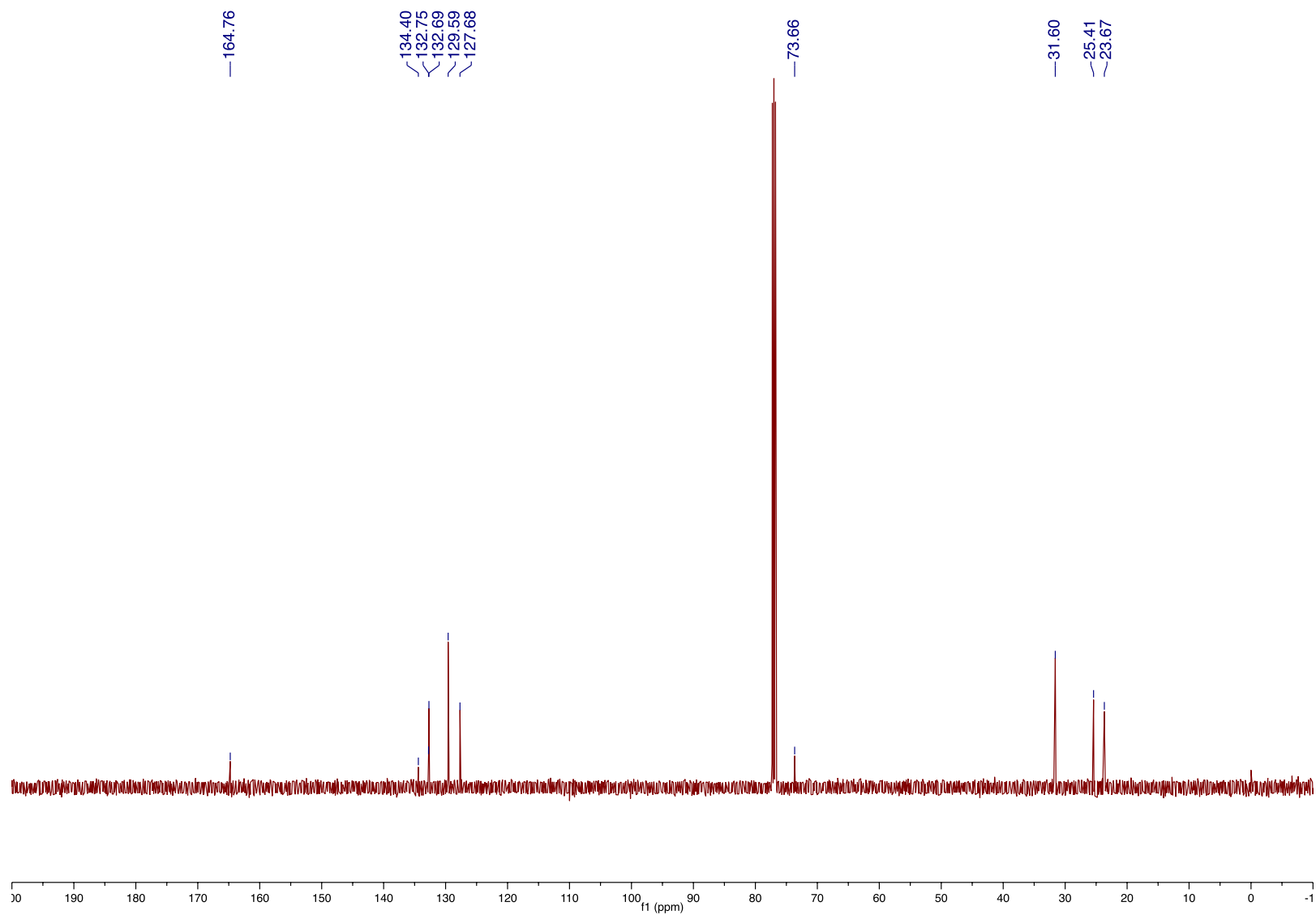
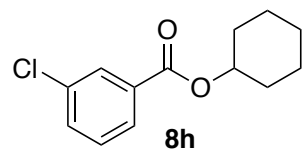
^{13}C NMR (125 MHz, CDCl_3)



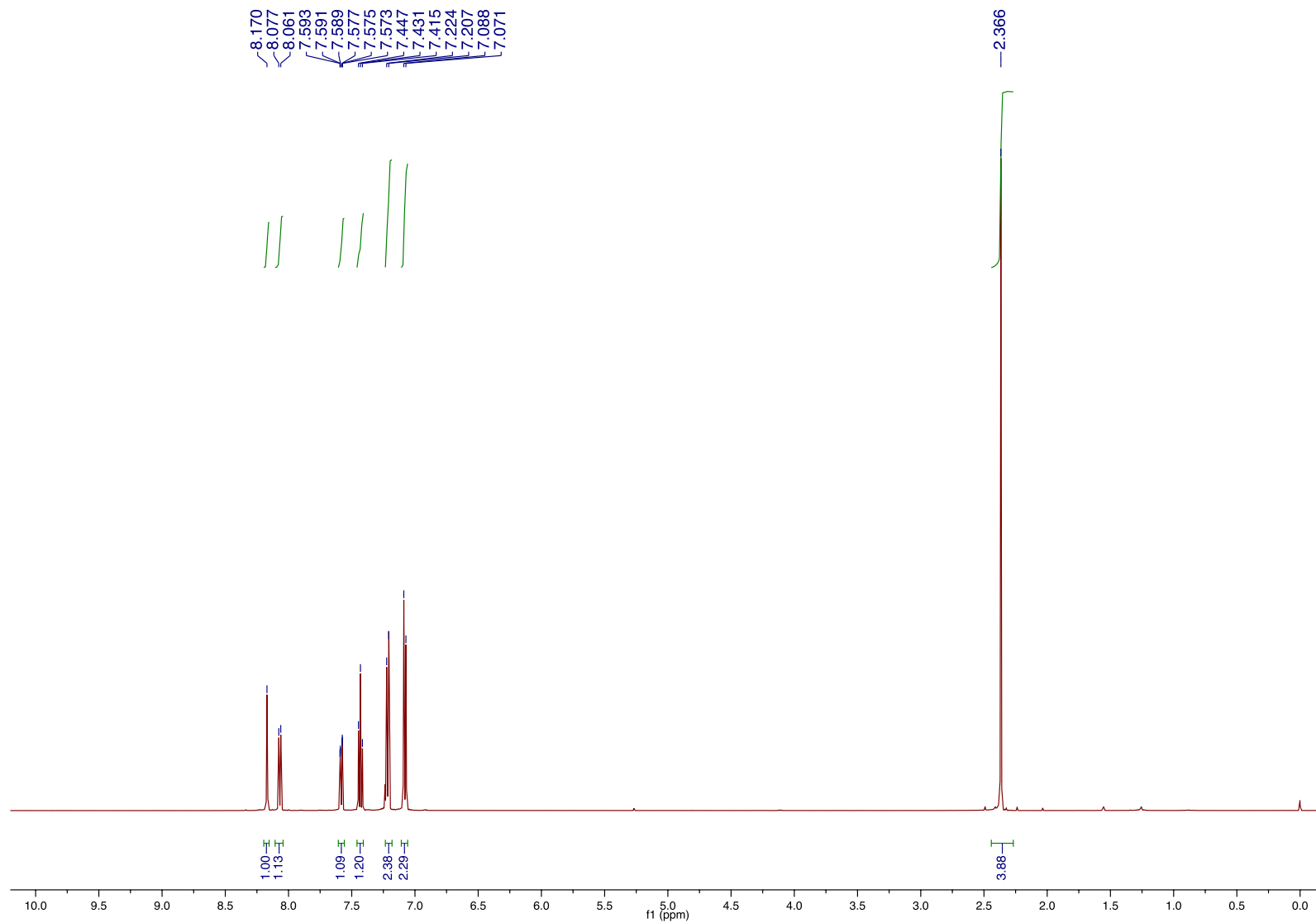
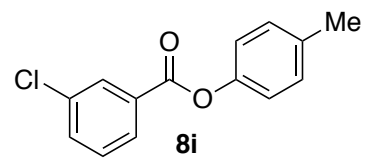
^1H NMR (500 MHz, CDCl_3)



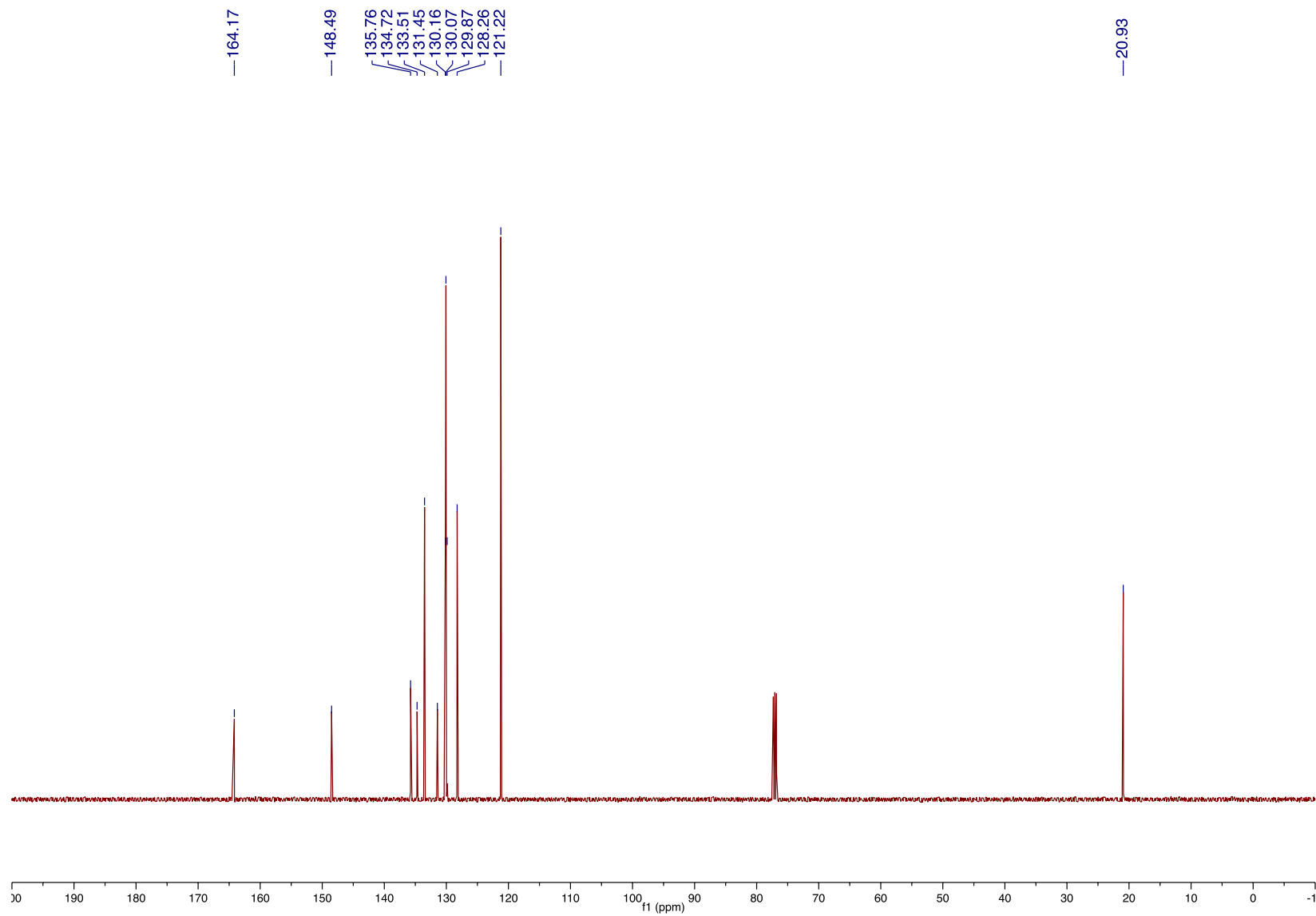
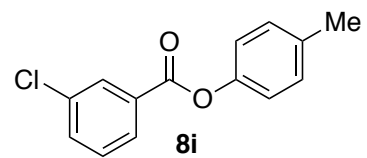
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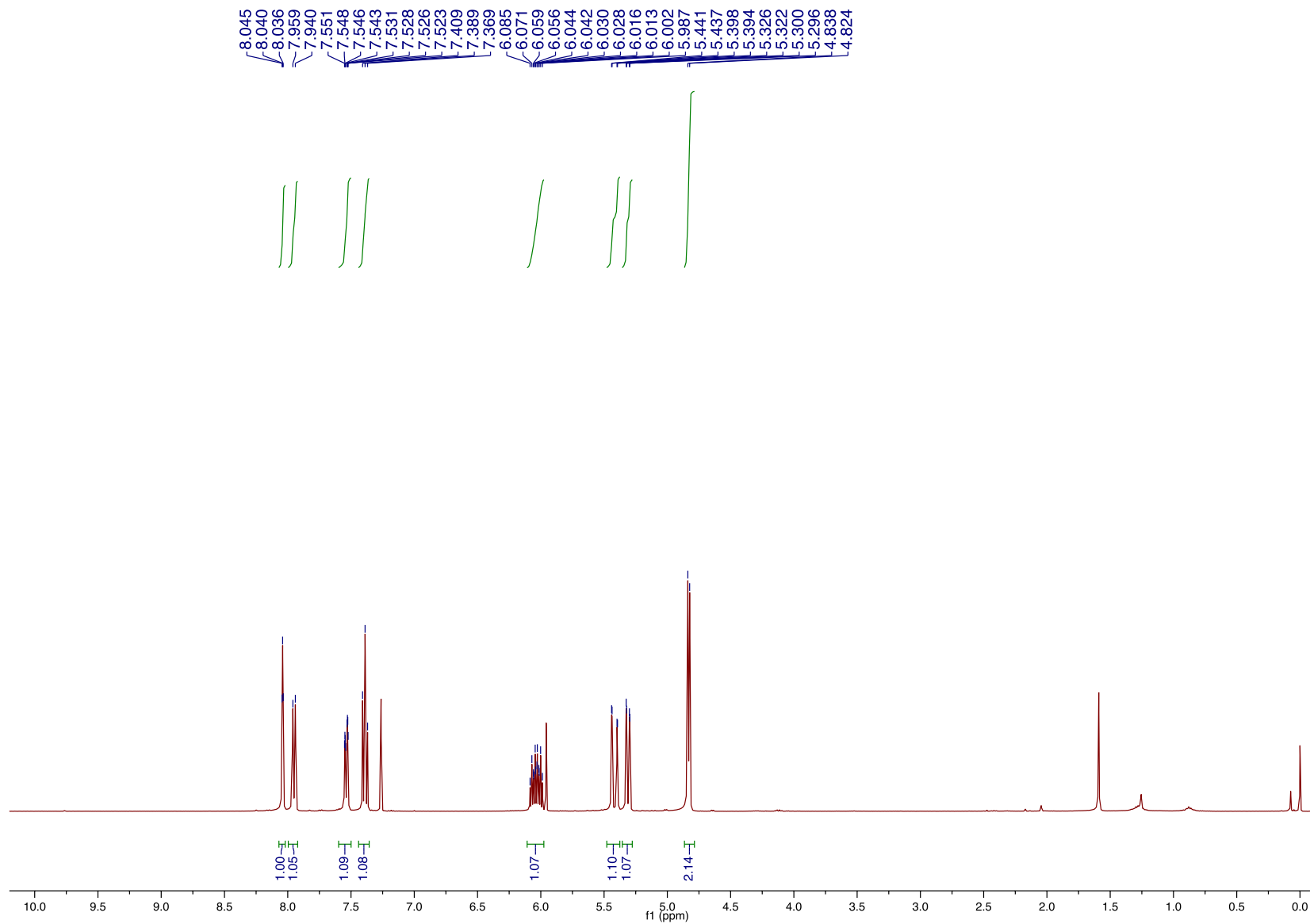
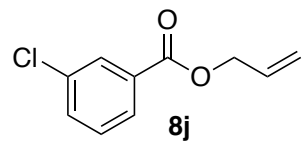
^1H NMR (500 MHz, CDCl_3)



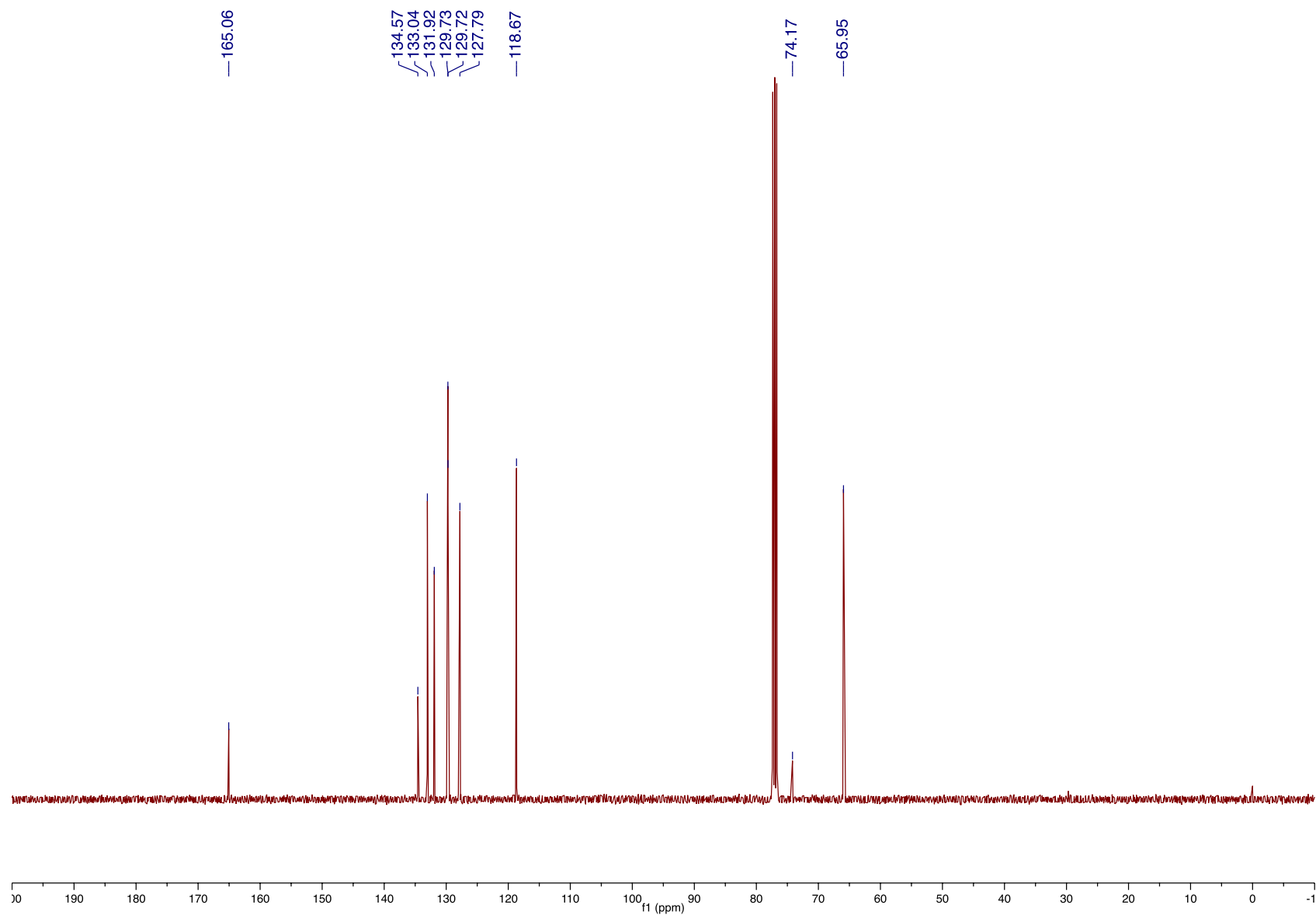
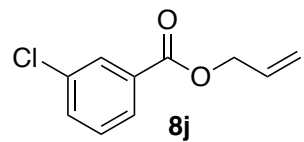
^{13}C NMR (125 MHz, CDCl_3)



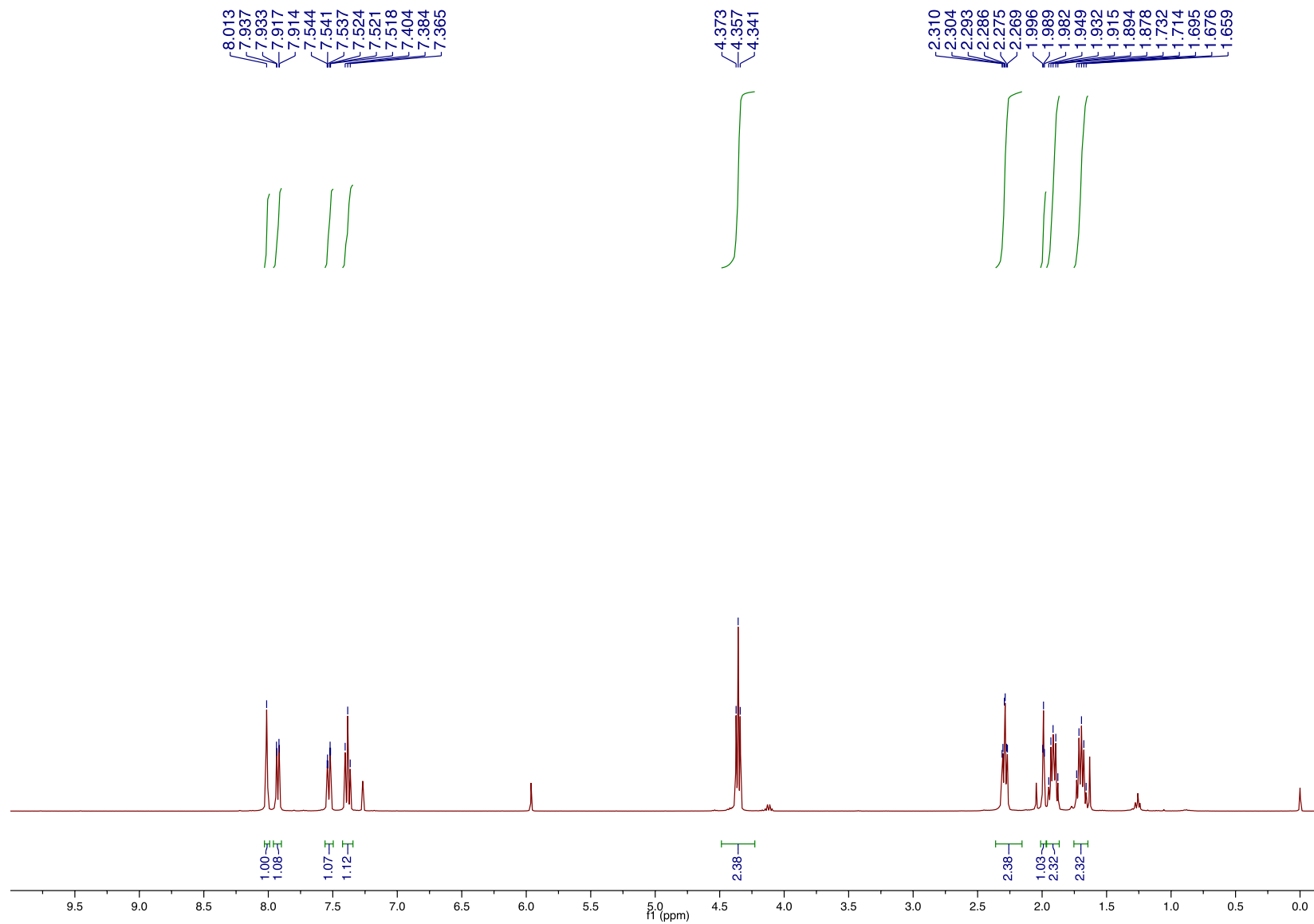
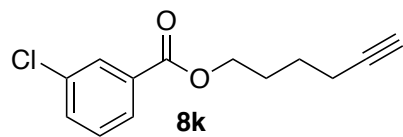
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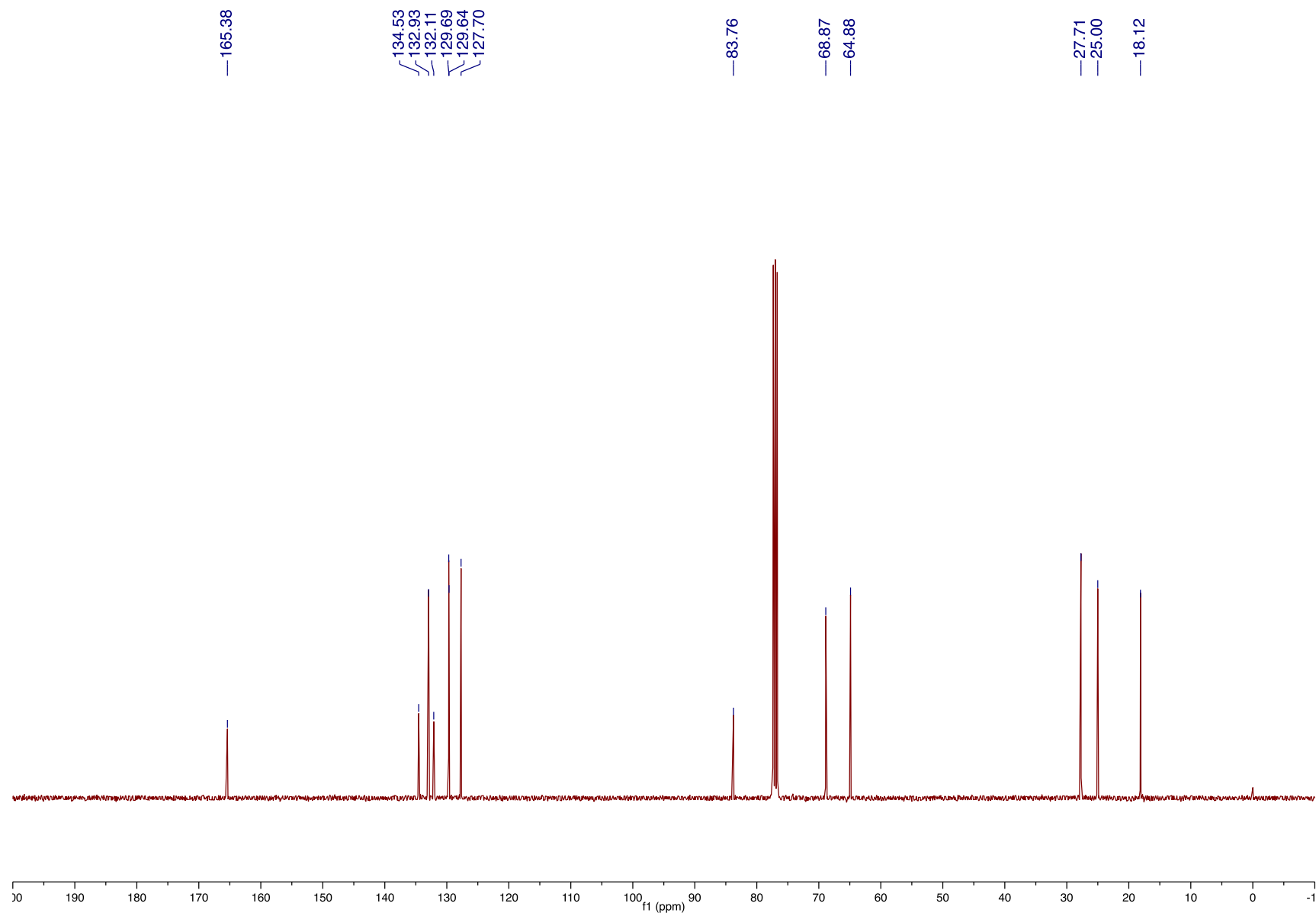
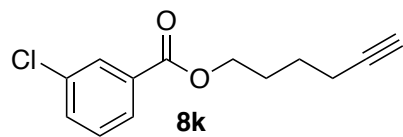
^{13}C NMR (100 MHz, CDCl_3)



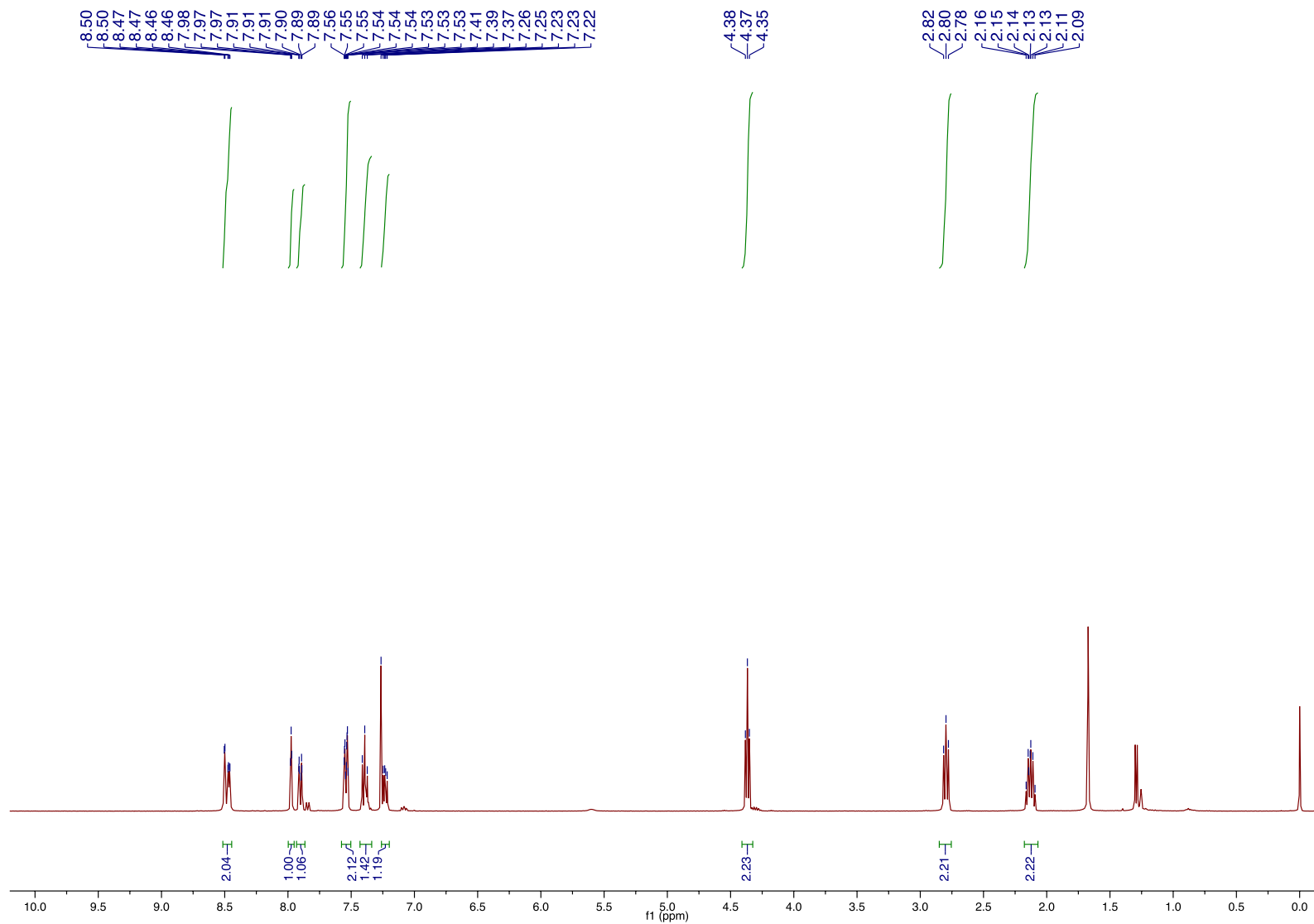
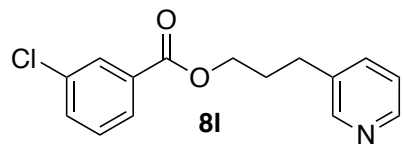
^1H NMR (400 MHz, CDCl_3)



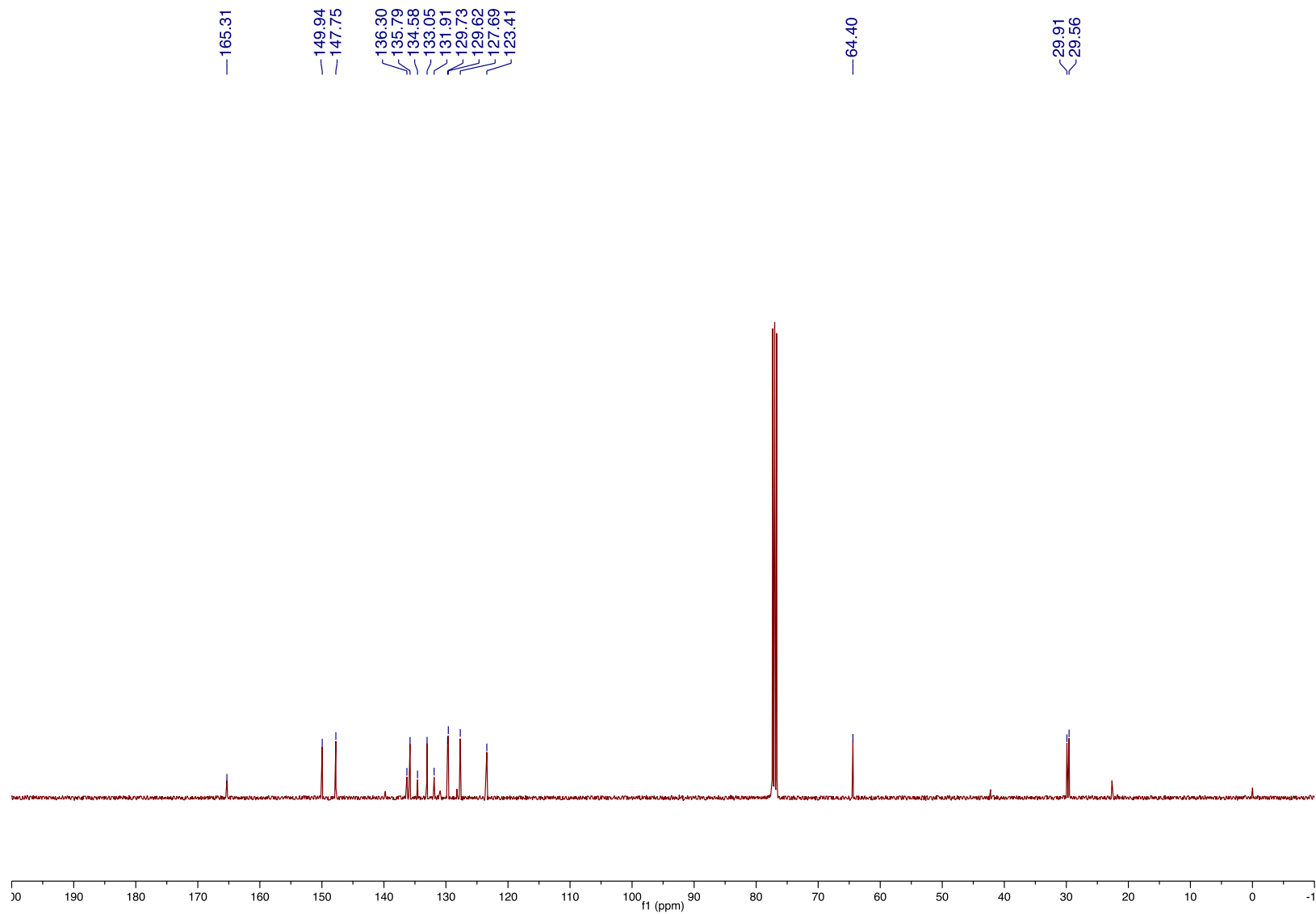
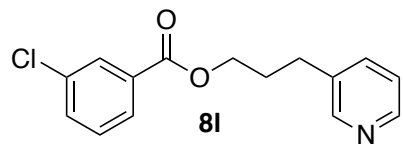
^{13}C NMR (100 MHz, CDCl_3)



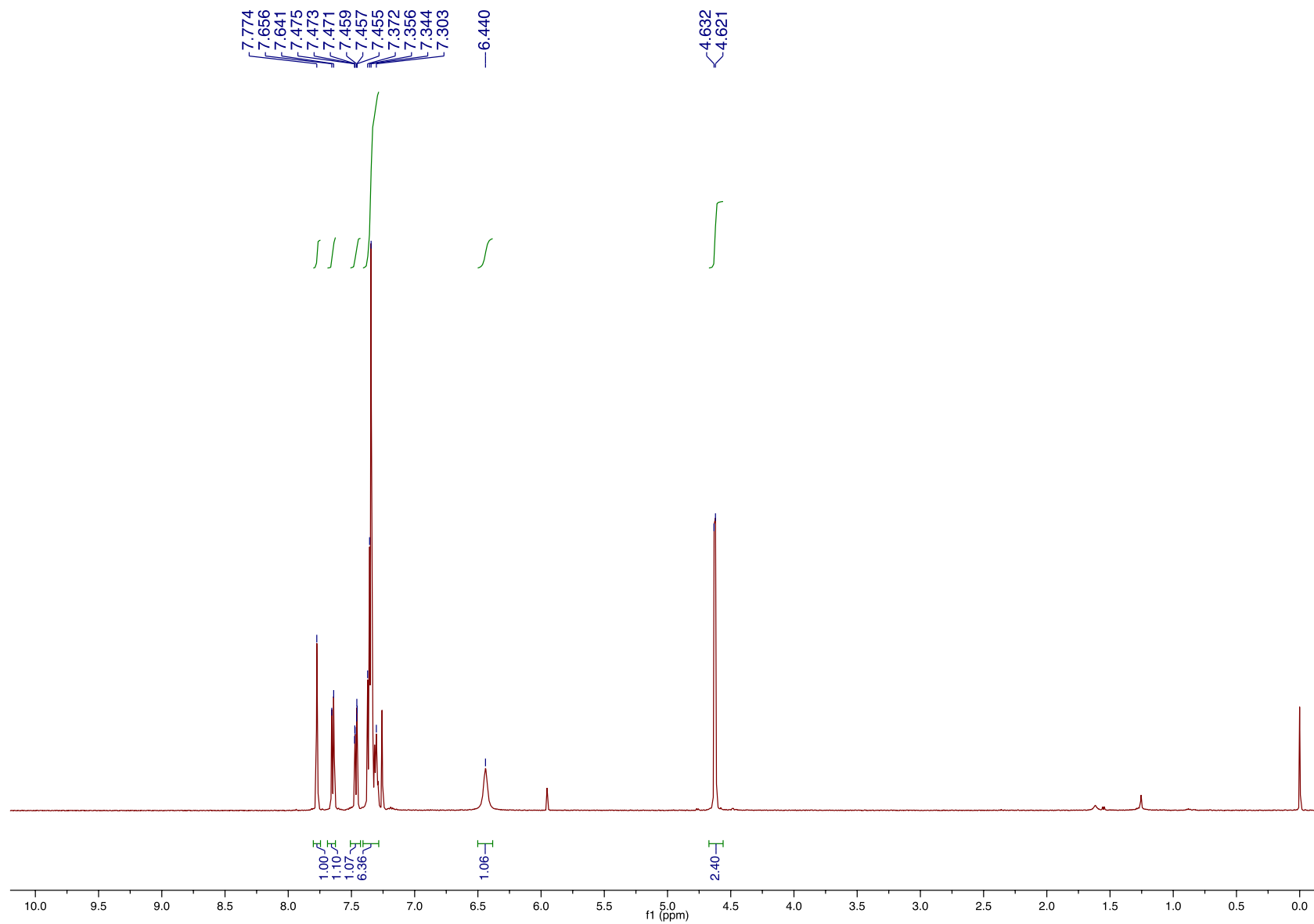
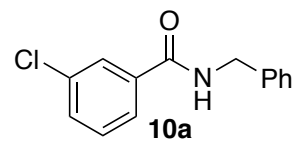
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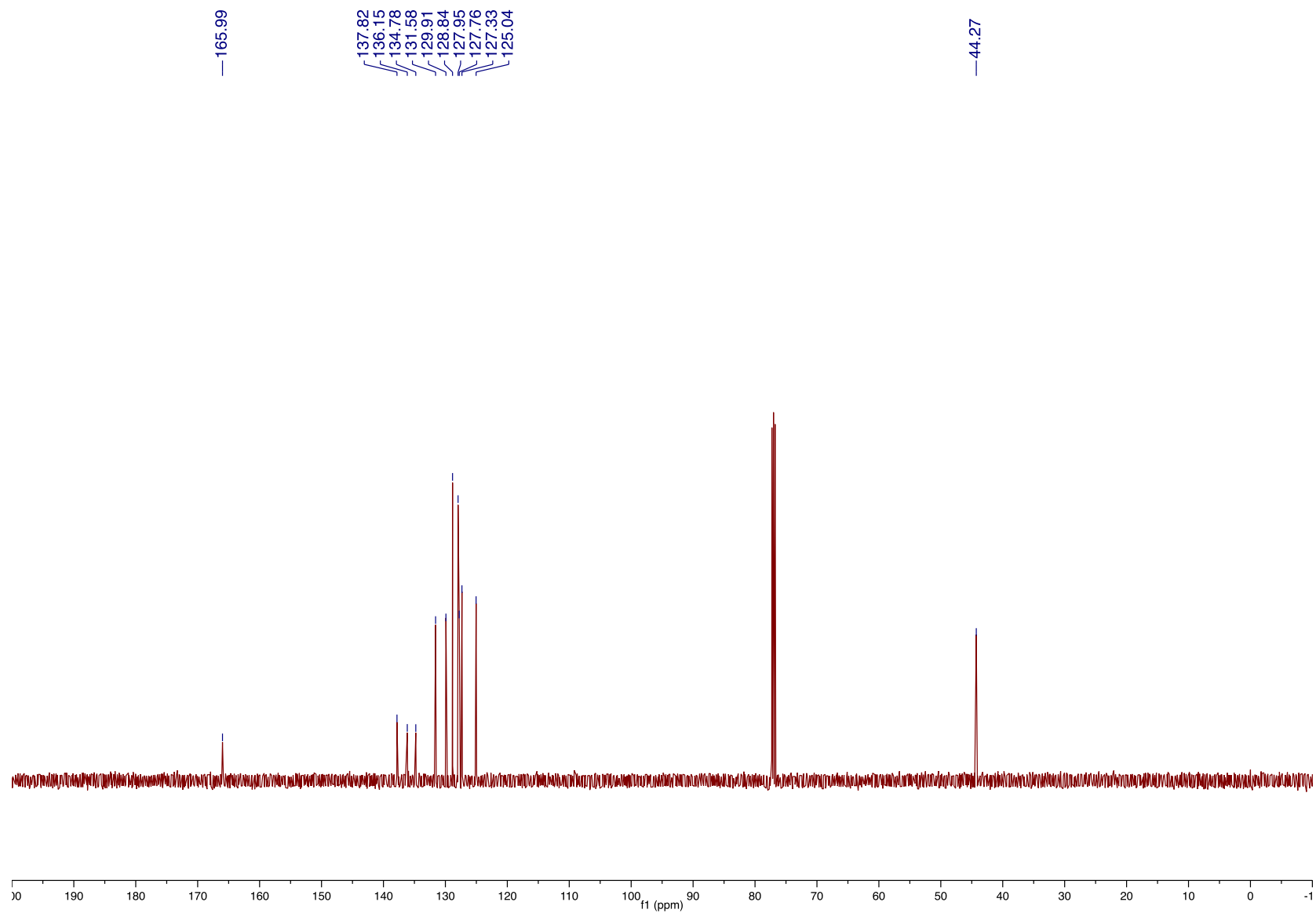
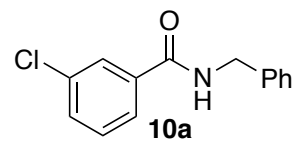
^{13}C NMR (100 MHz, CDCl_3)



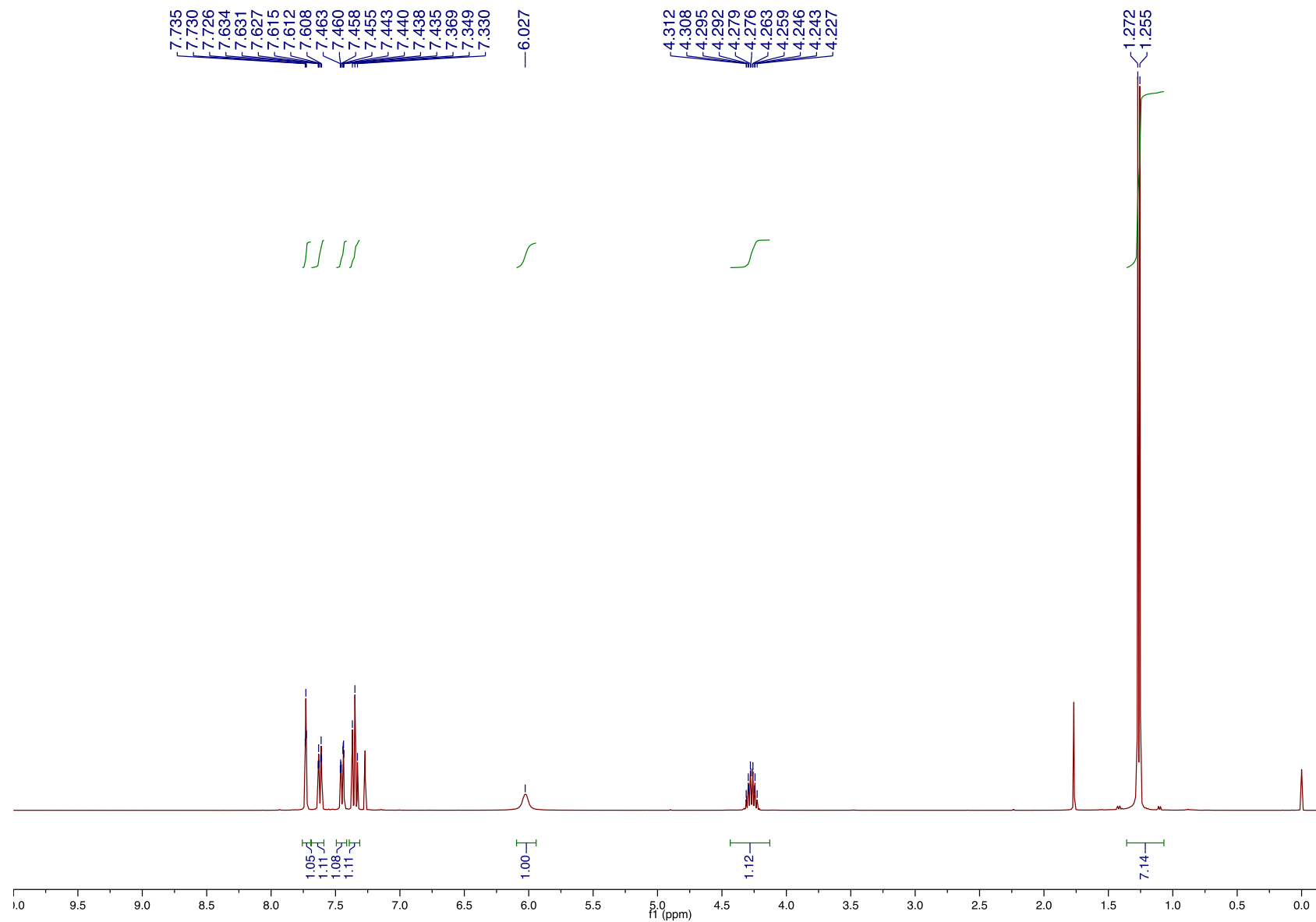
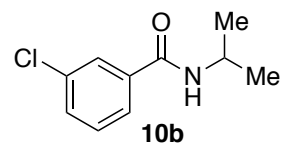
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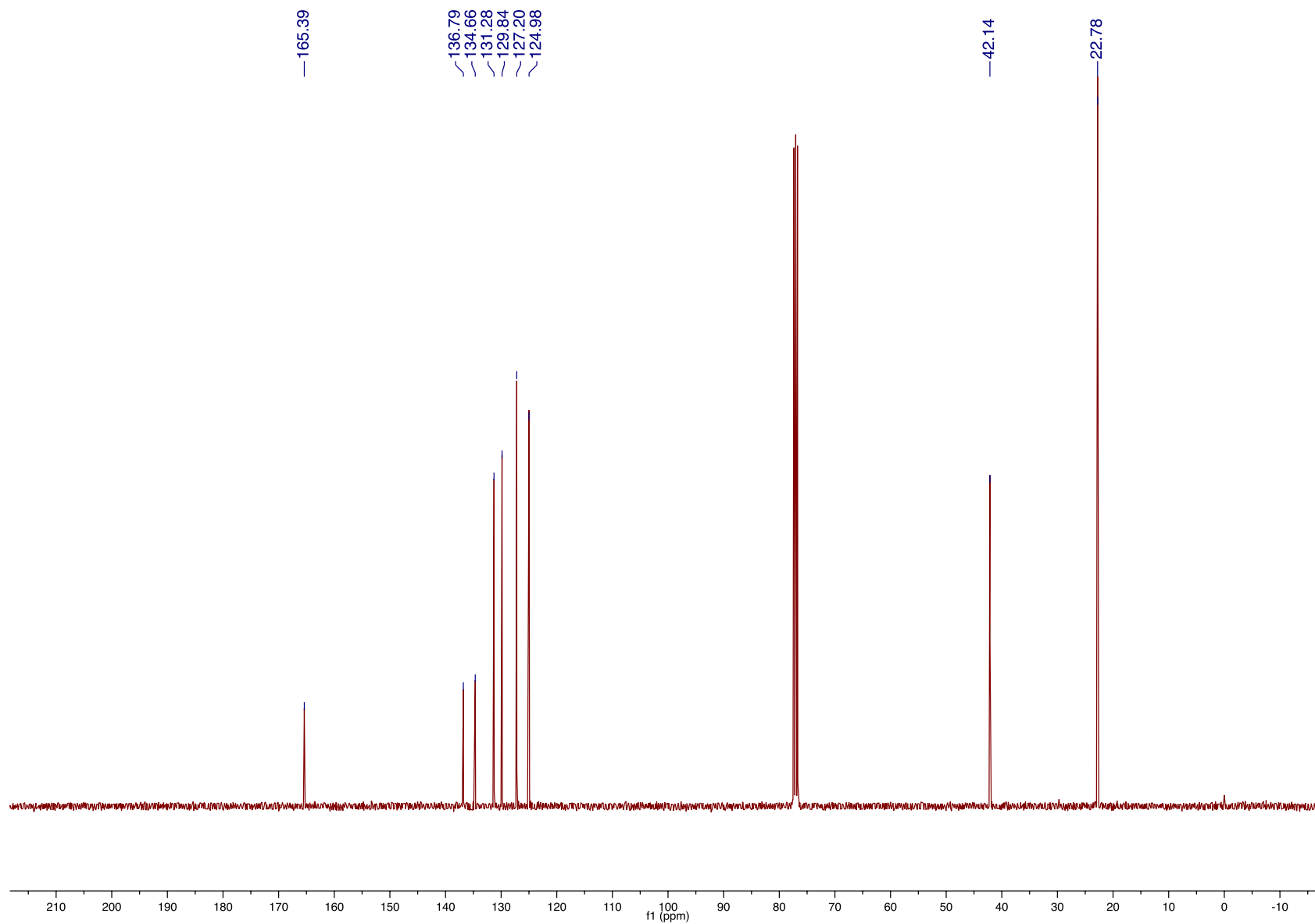
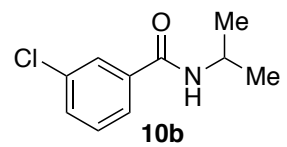
^{13}C NMR (125 MHz, CDCl_3)



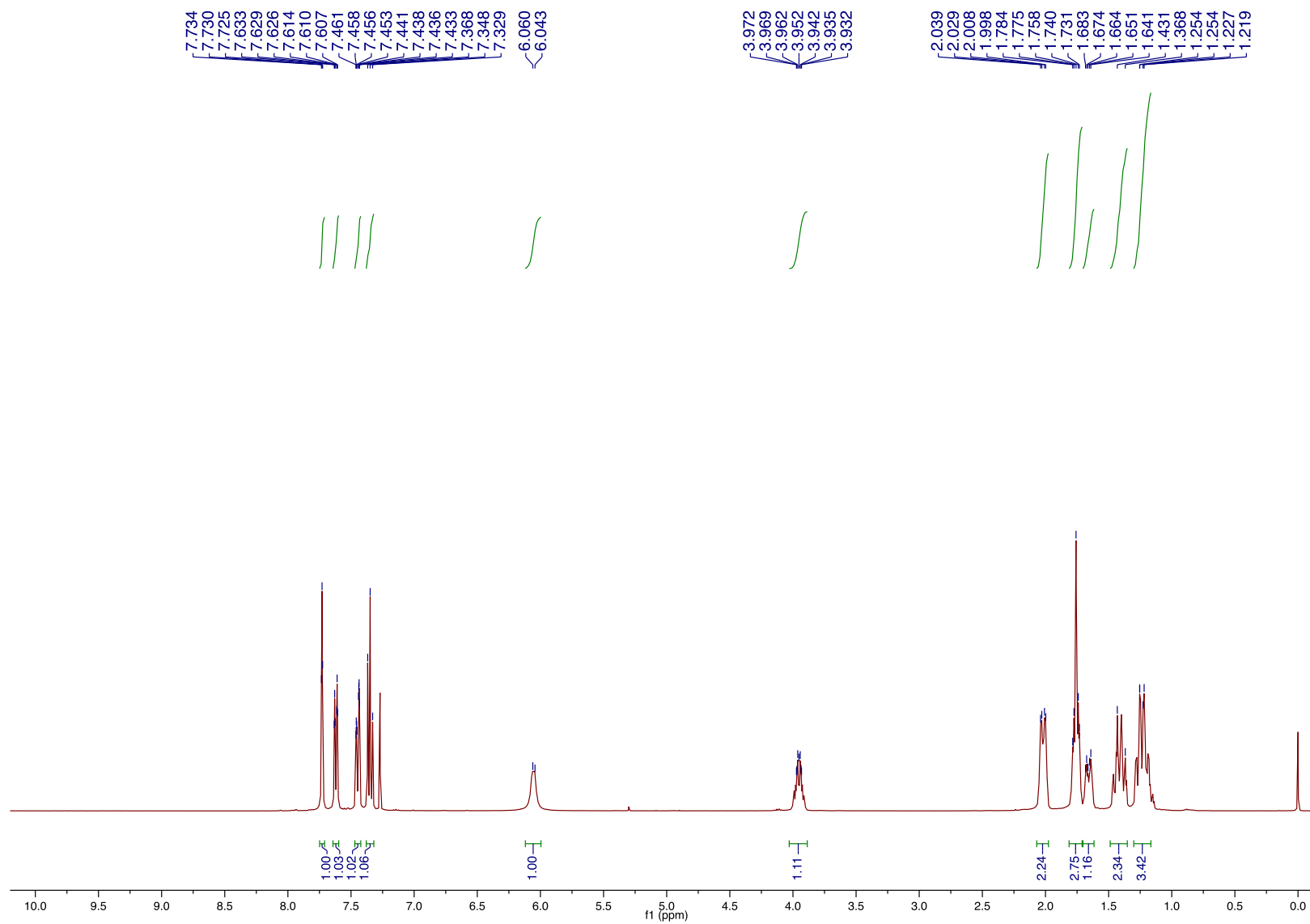
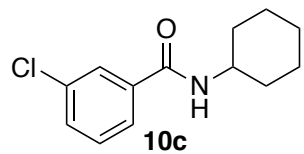
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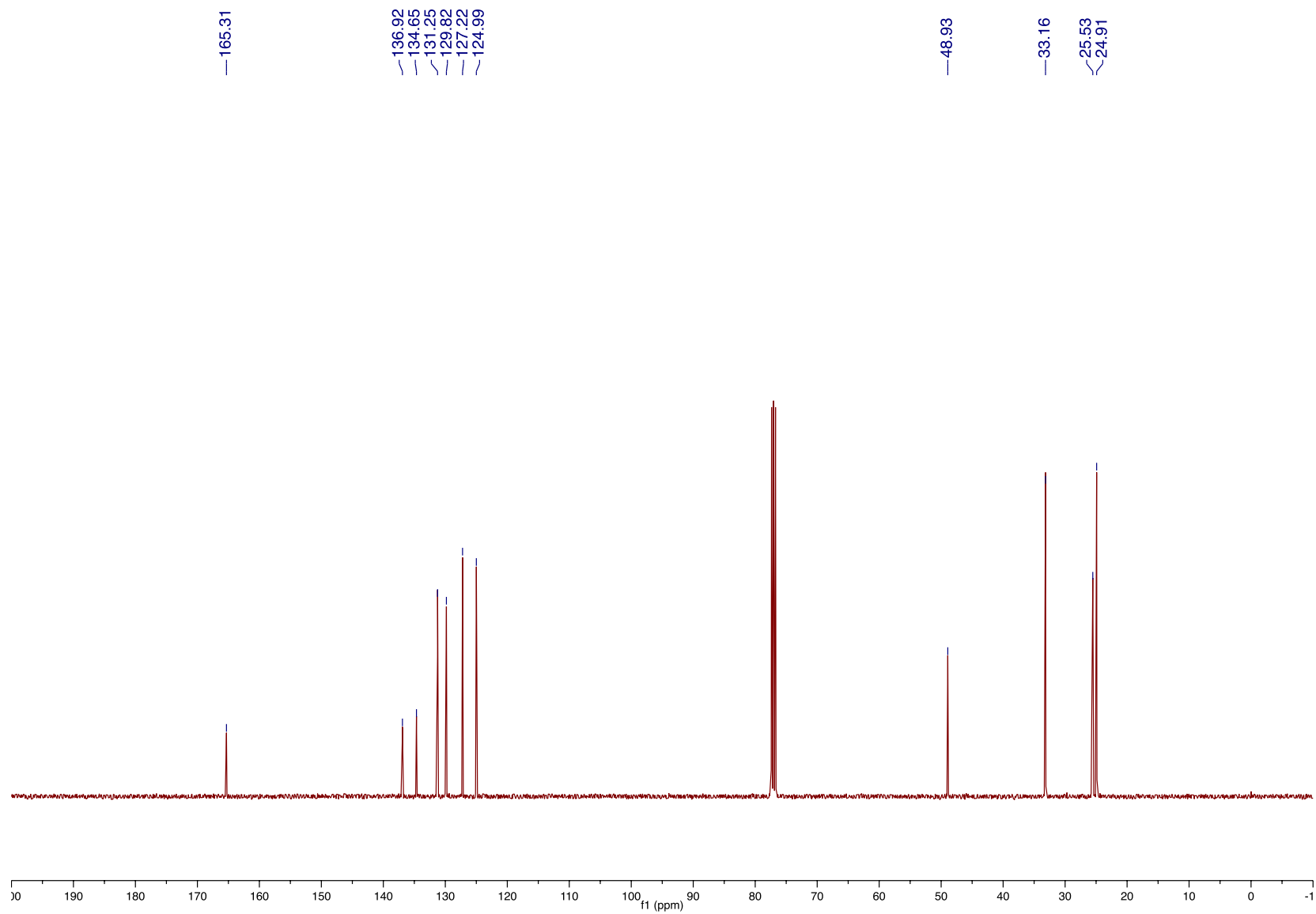
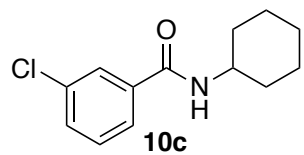
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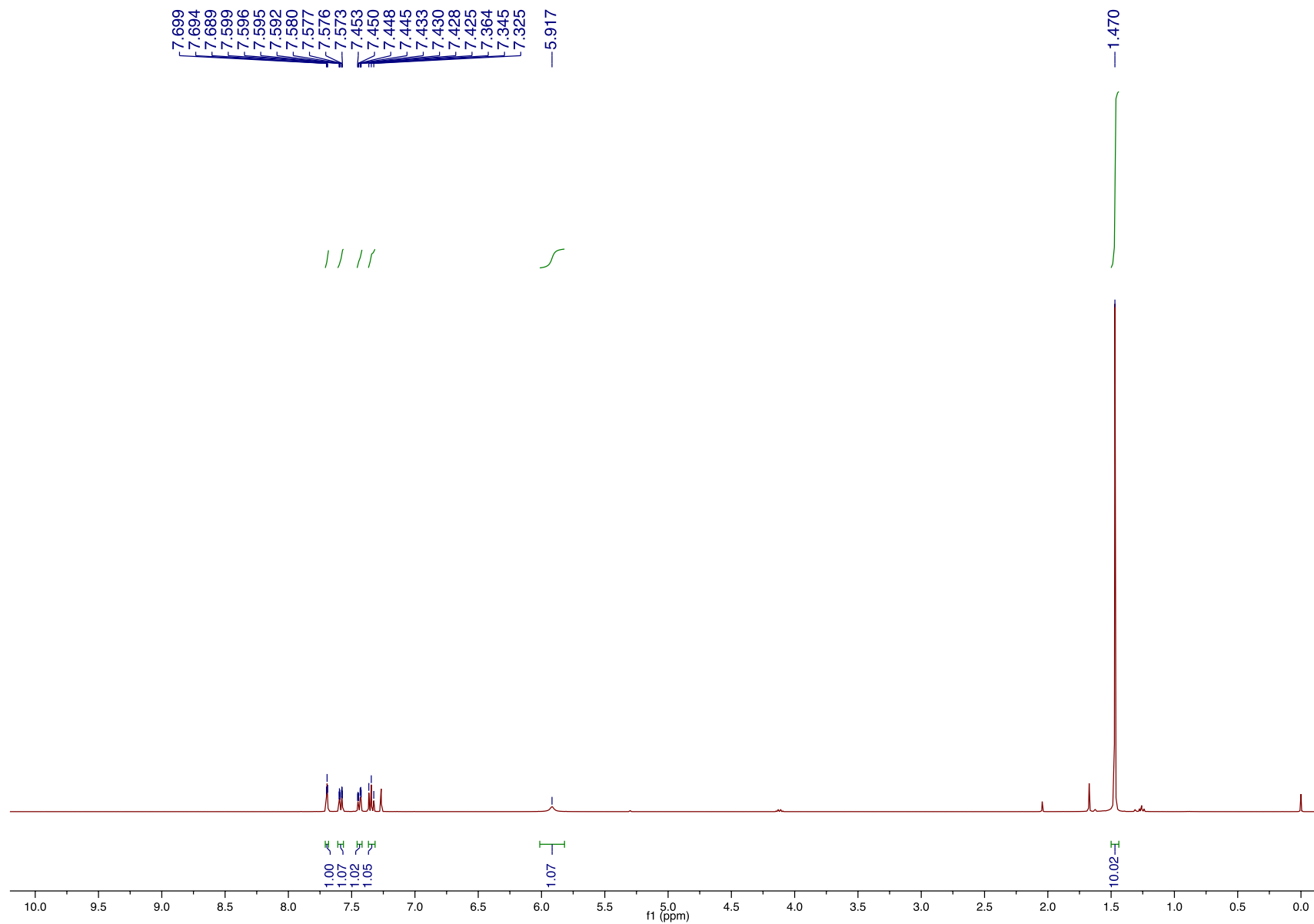
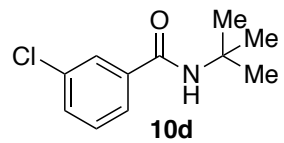
^1H NMR (400 MHz, CDCl_3)



^{13}C NMR (100 MHz, CDCl_3)



^1H NMR (400 MHz, CDCl_3)



^{13}C NMR (100 MHz, CDCl_3)

