

Supporting Information

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¹H NMR and ¹³C NMR Spectra

Stereoselective Decarboxylative Alkylation of Titanium(IV) Enolates with Diacyl Peroxides

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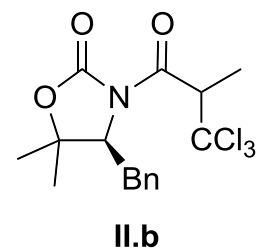
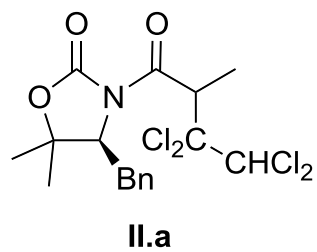
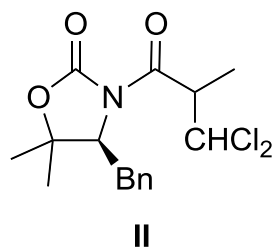
[◇] Departamento de Química Orgánica I, Universidad del País Vasco, UPV/EHU, Apdo. 1072, 20080 San Sebastián, Spain

[#] Unitat de Difracció de RX. CCiTUB. Universitat de Barcelona. Carrer Solé i Sabarís 1-3, 08028 Barcelona, Catalonia, Spain

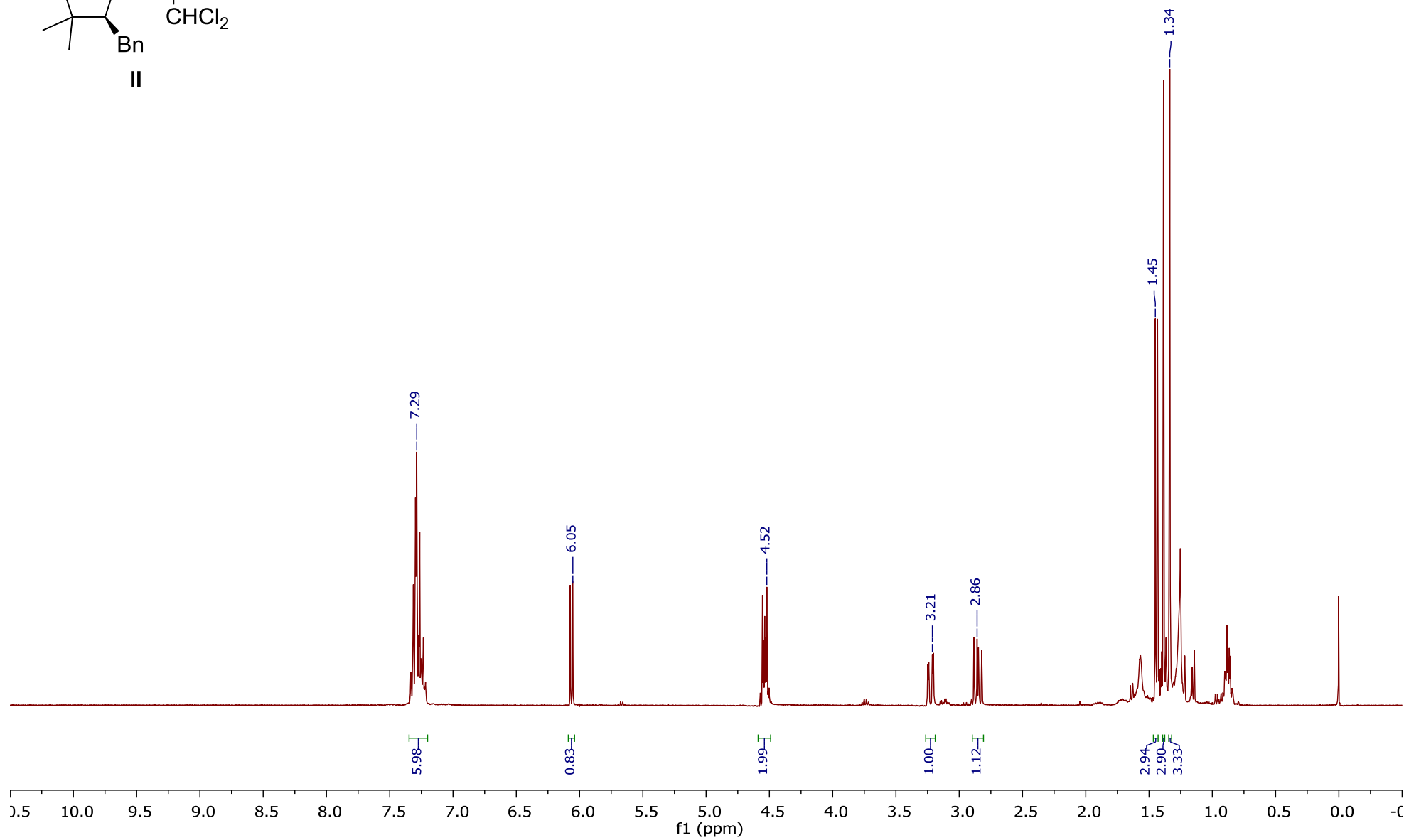
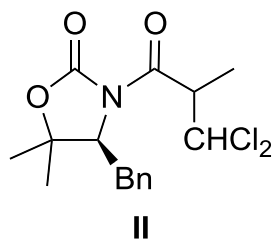
Contents

1. Chloroalkylated Derivatives.....	S'1
2. <i>N</i> -Acyl Oxazolidinones	S'8
3. Diacyl Peroxides.....	S'33
4. Alkylation Products (table 1)	S'55
5. Alkylation Products (table 2)	S'84
6. Arundic Acid Synthesis.....	S'115

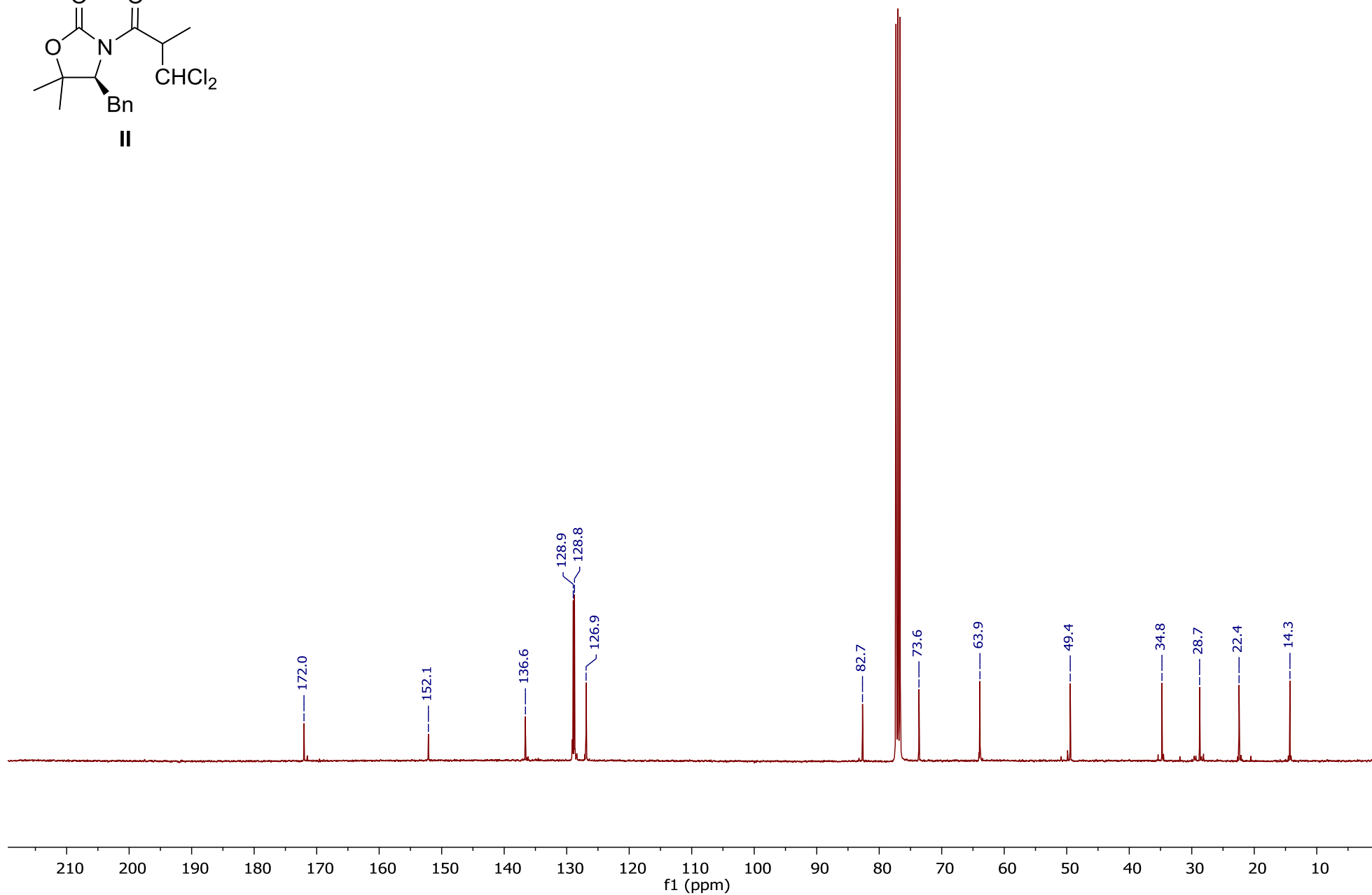
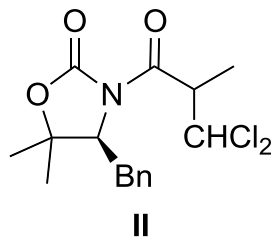
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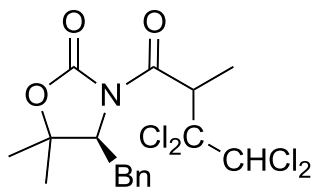
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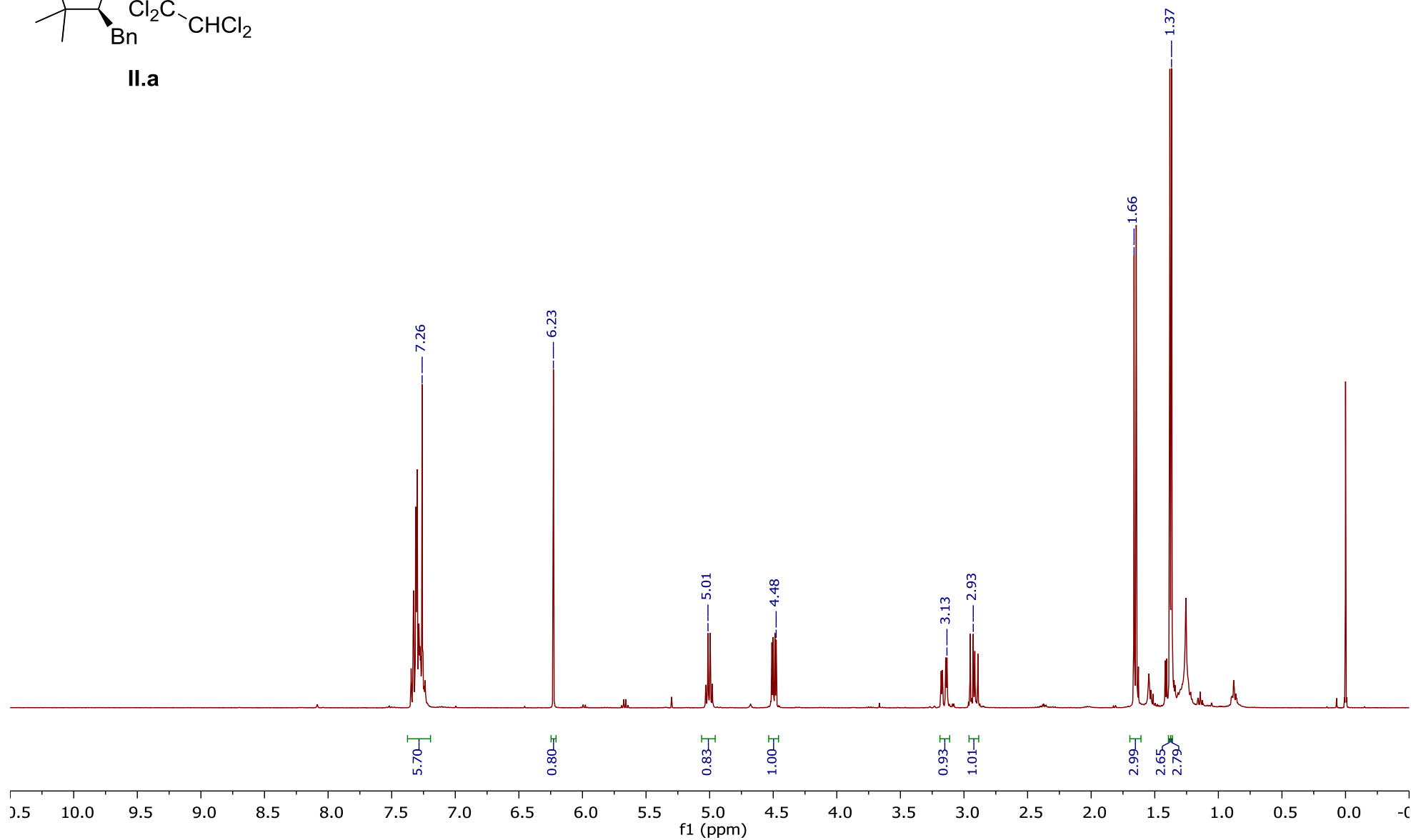
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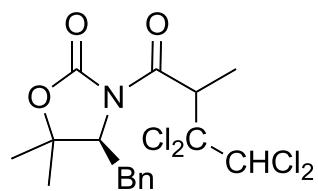
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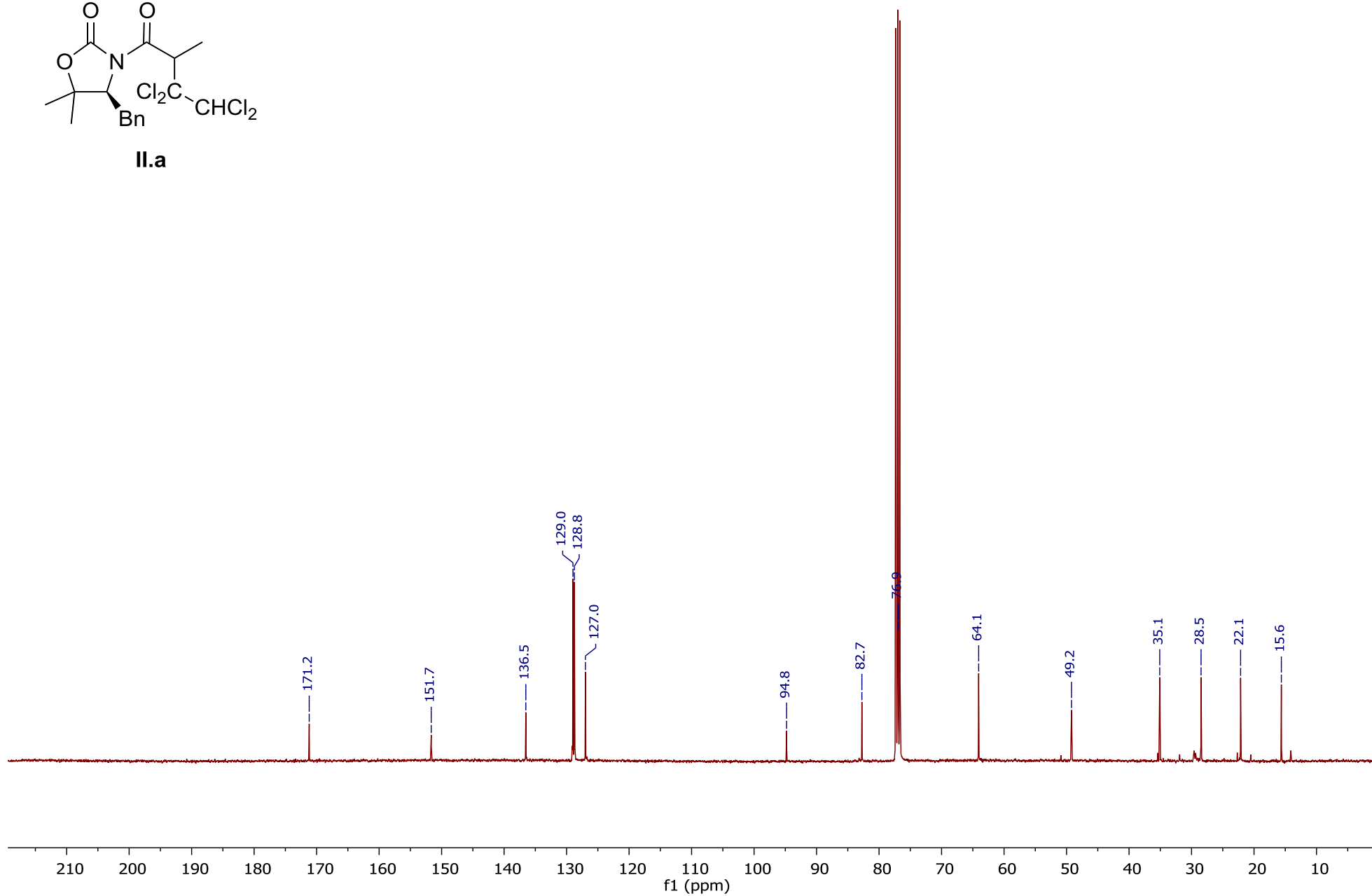
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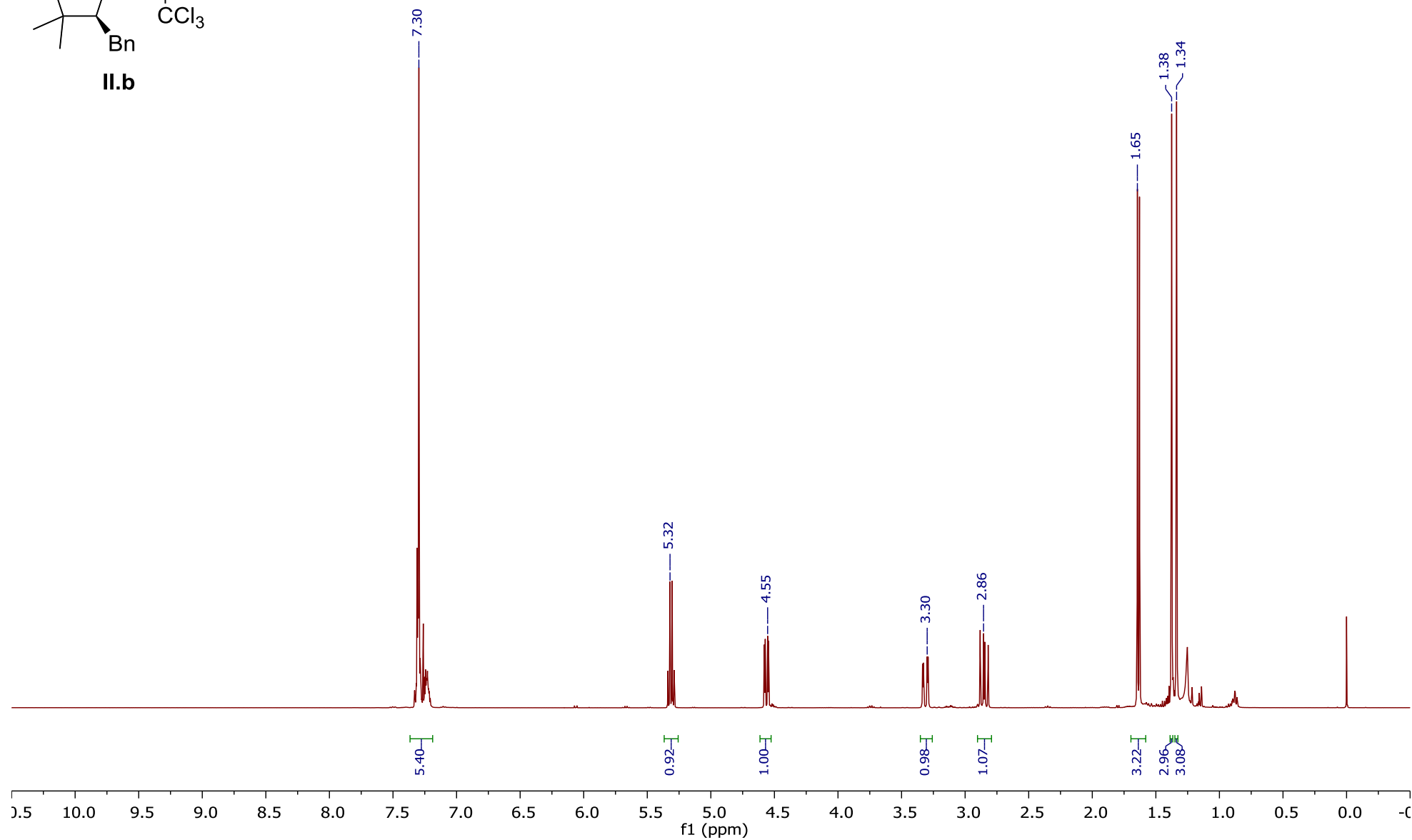
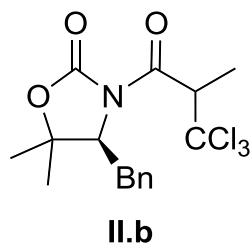
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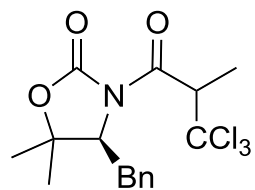
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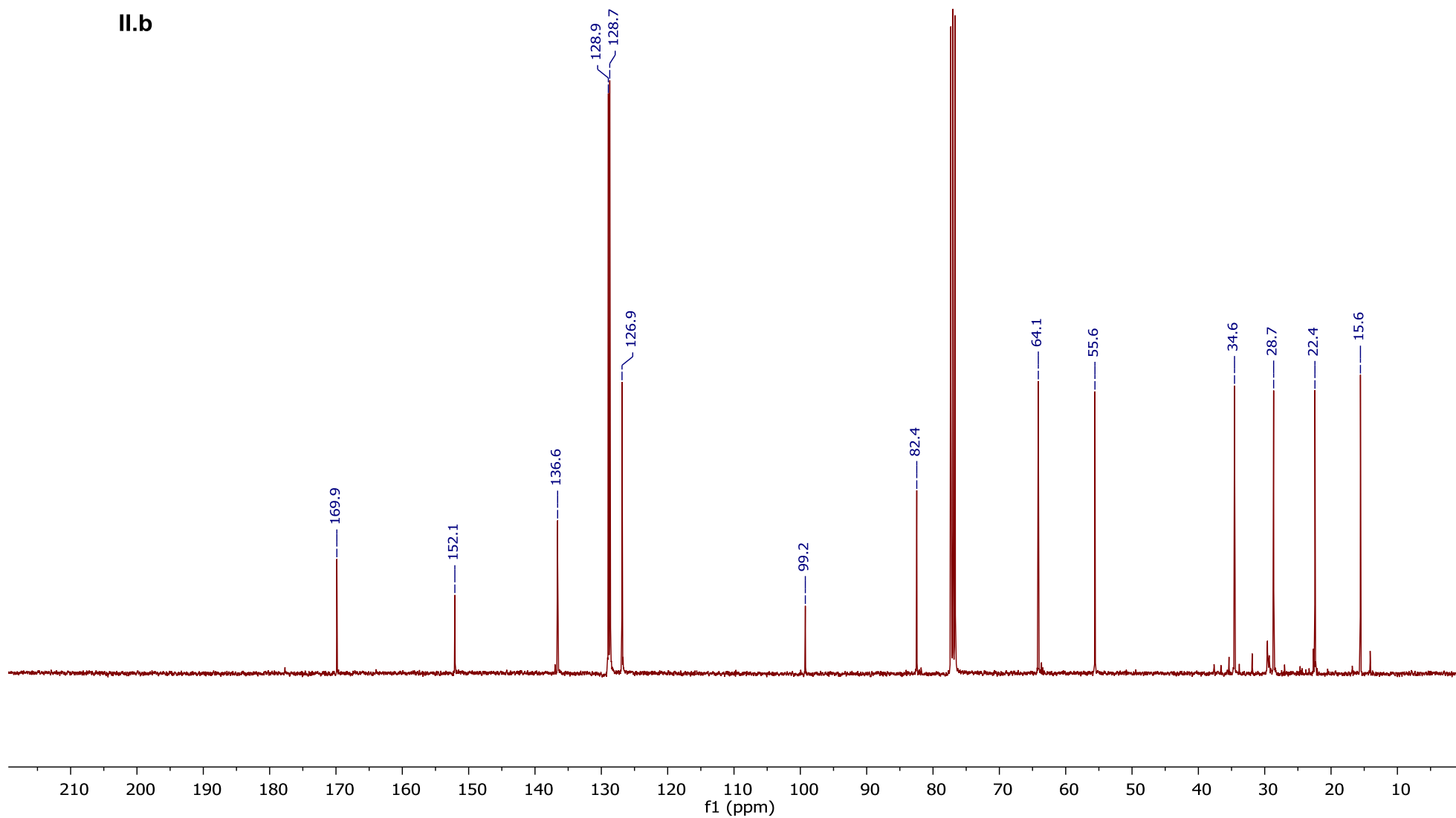
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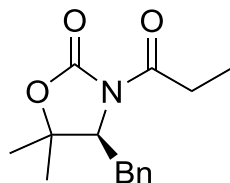
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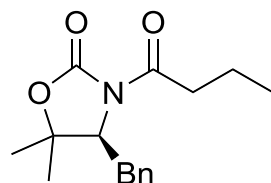
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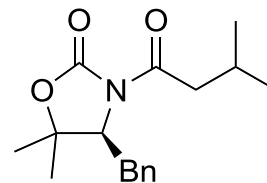
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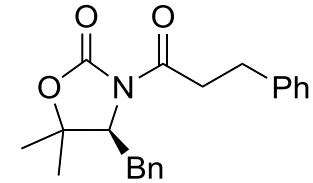
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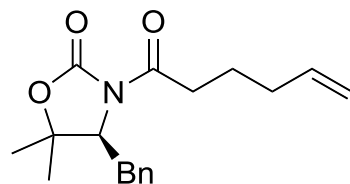
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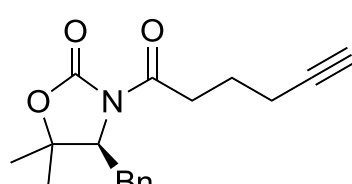
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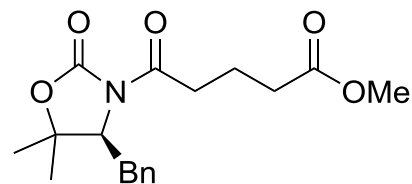
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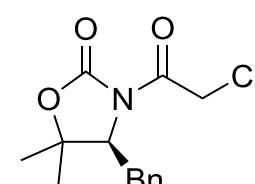
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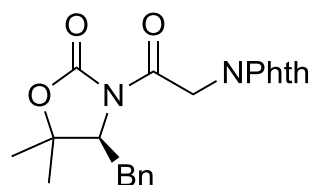
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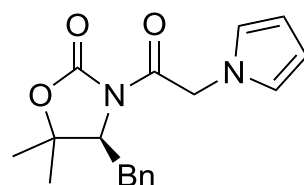
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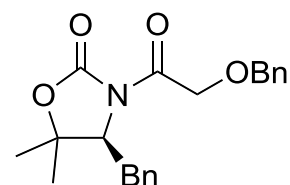
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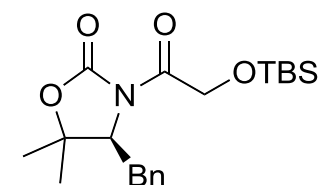
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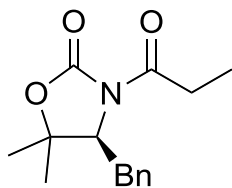


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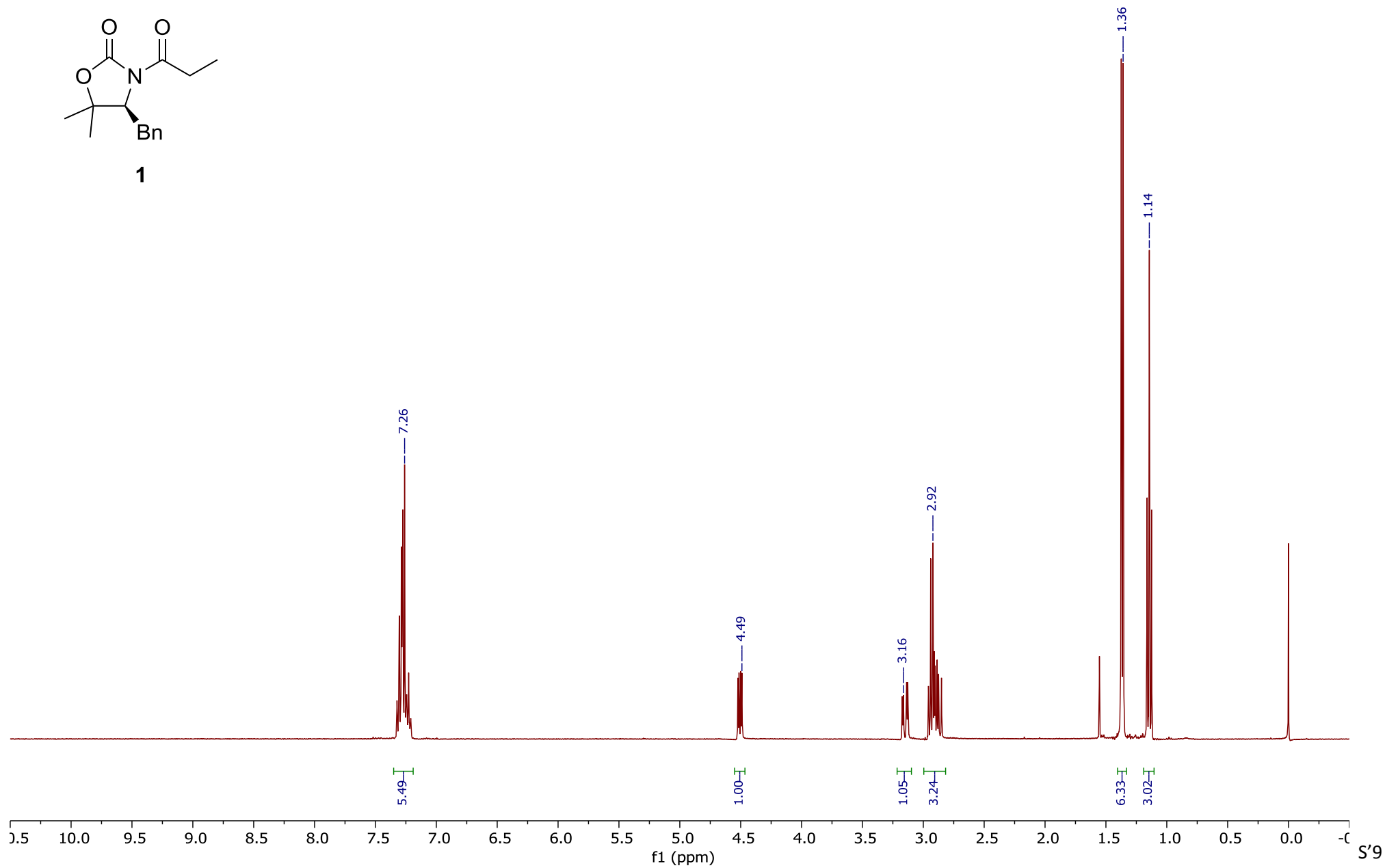


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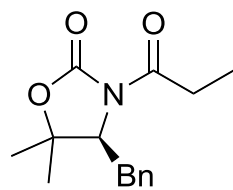
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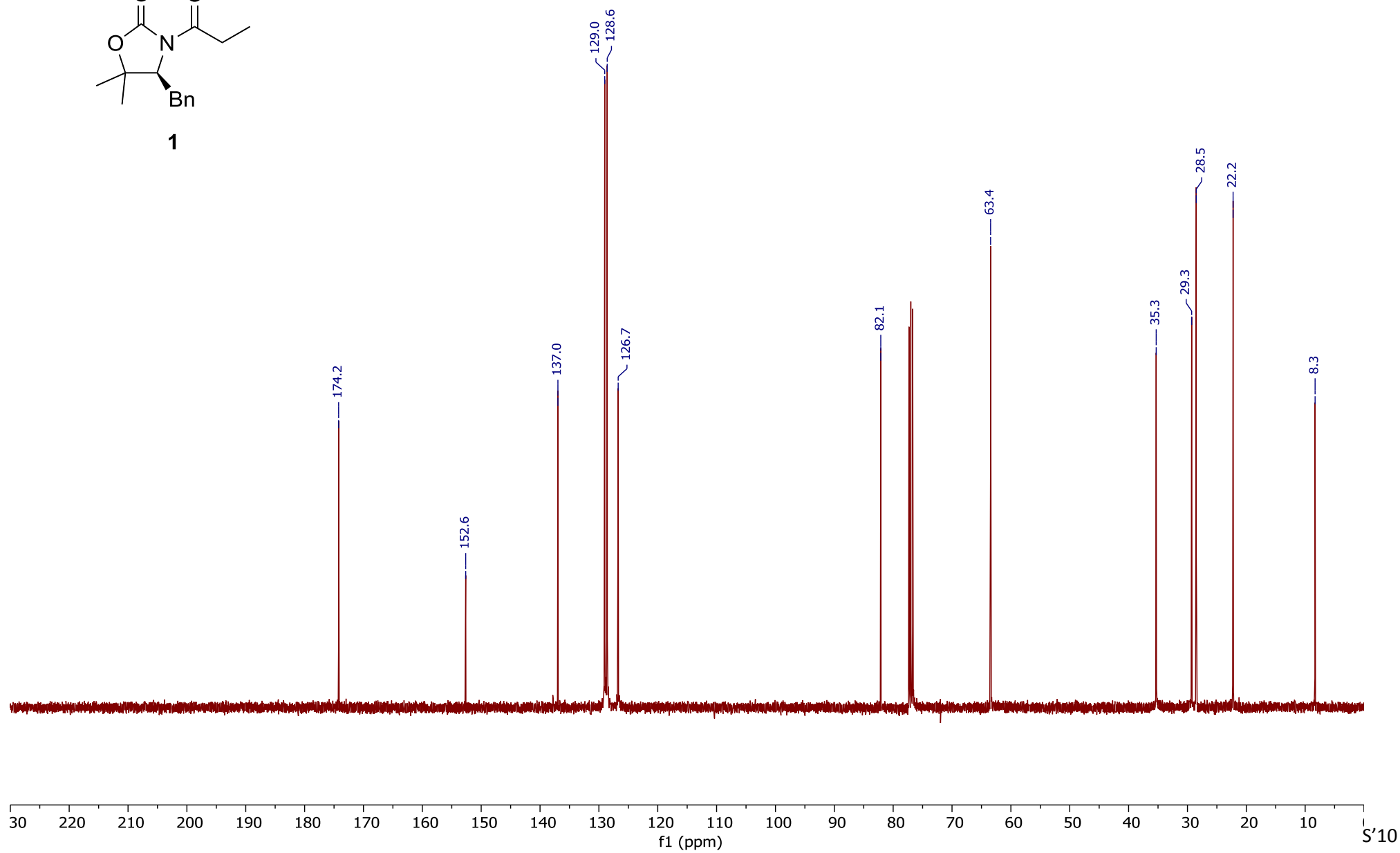
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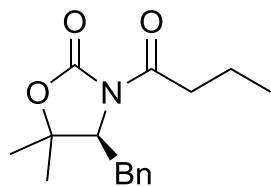
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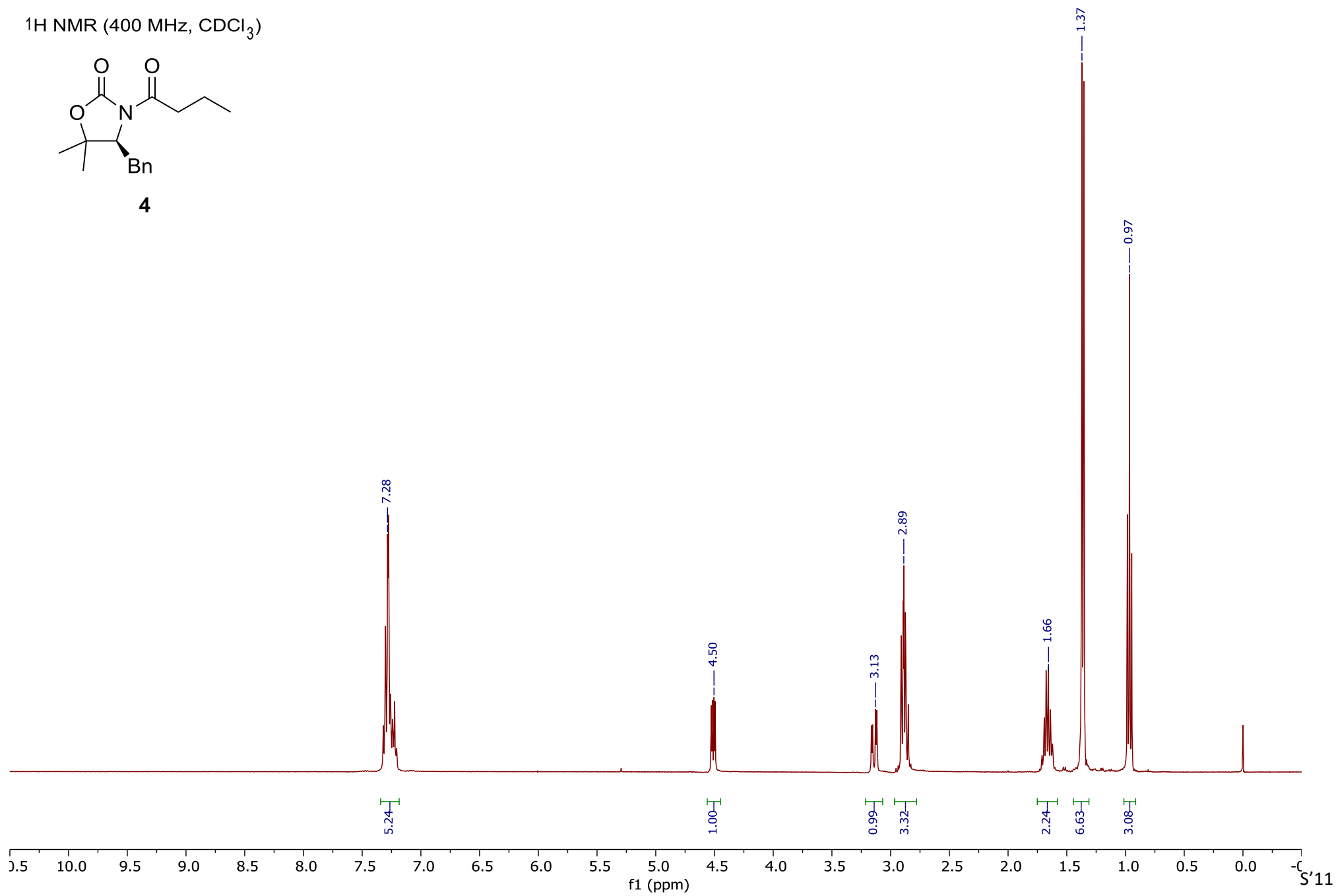
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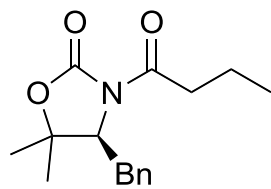
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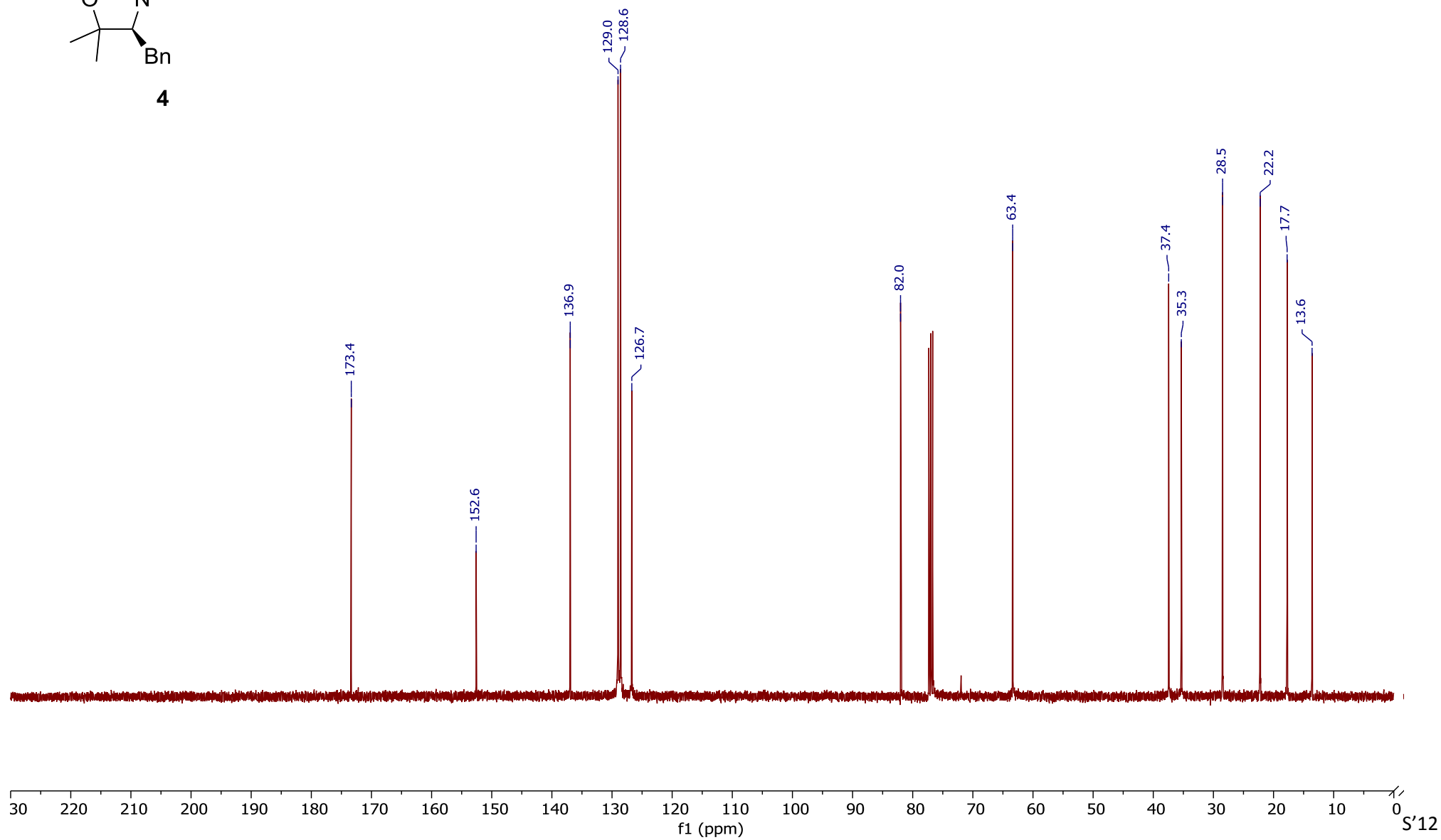
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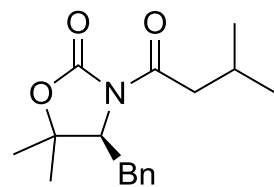
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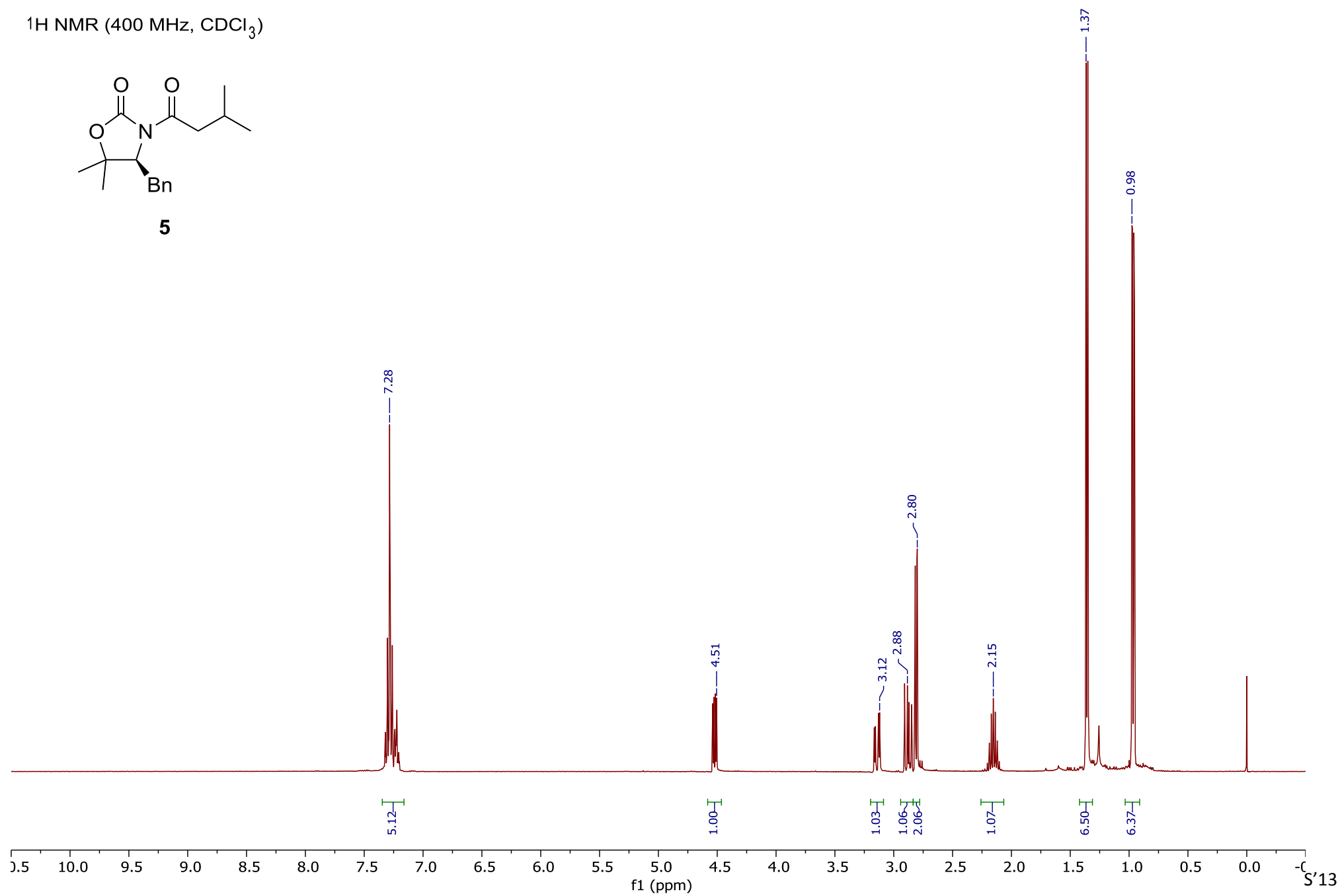
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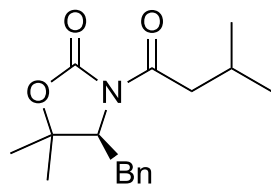
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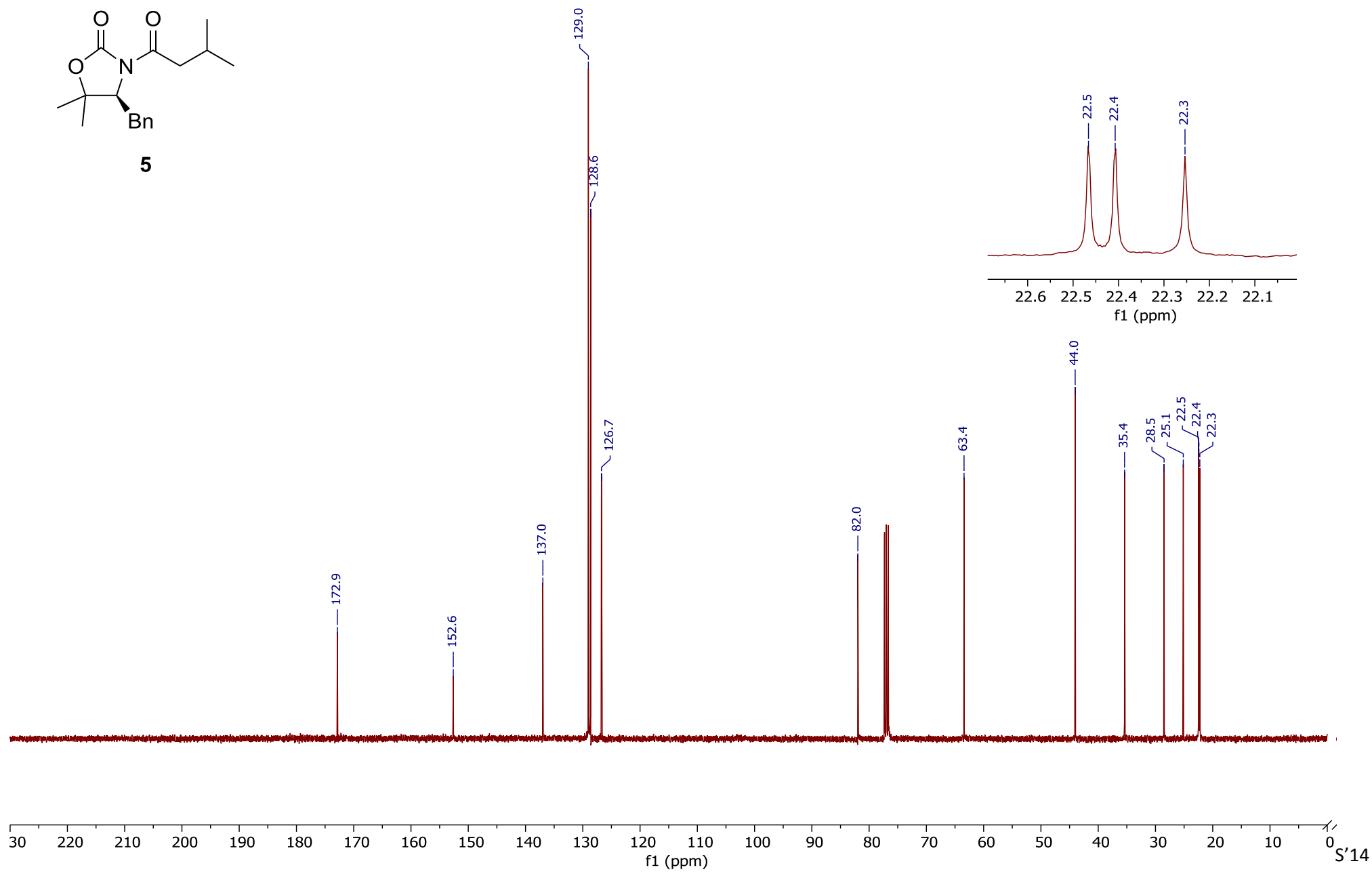
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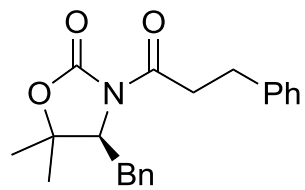
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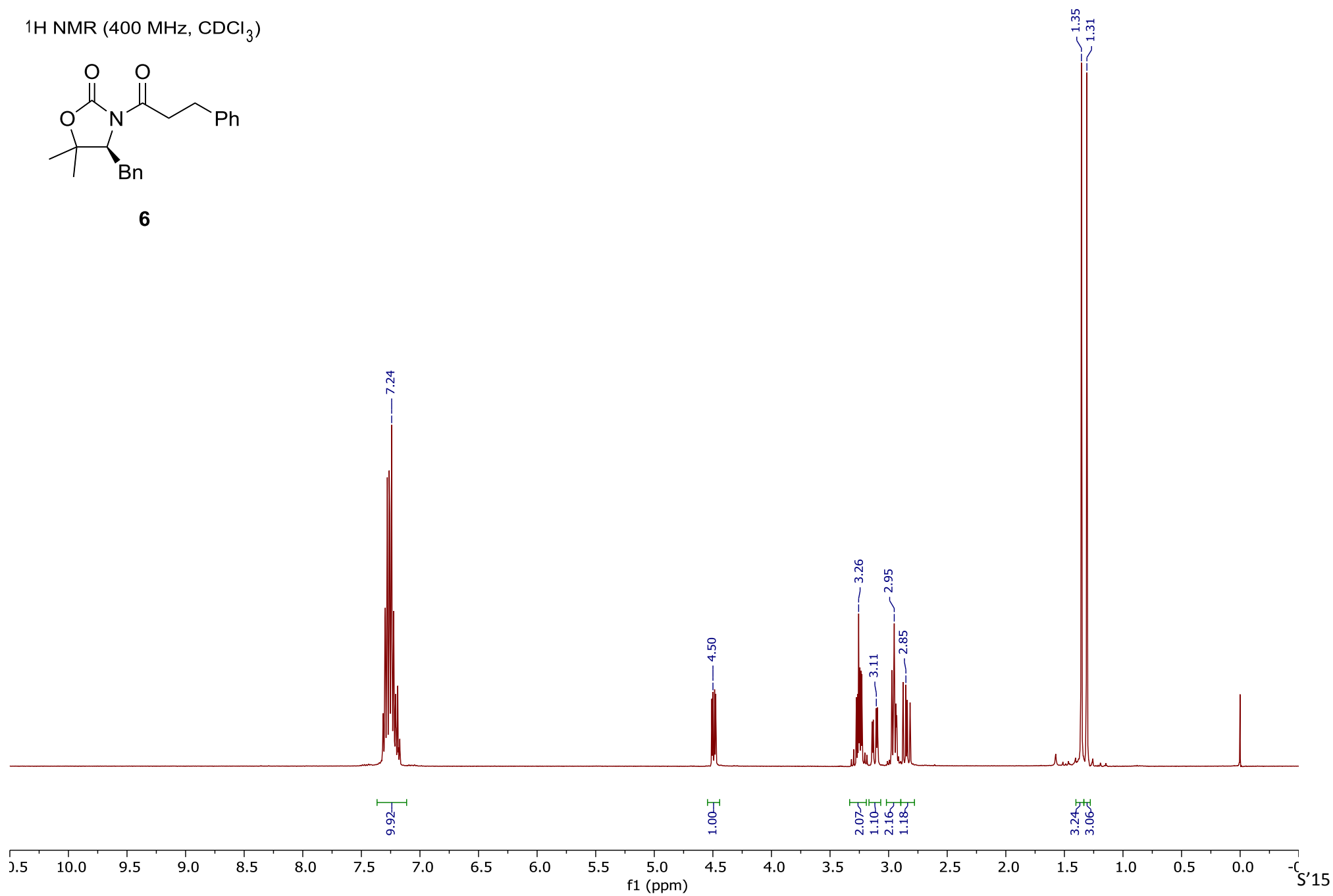
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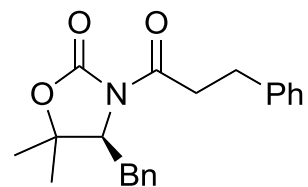
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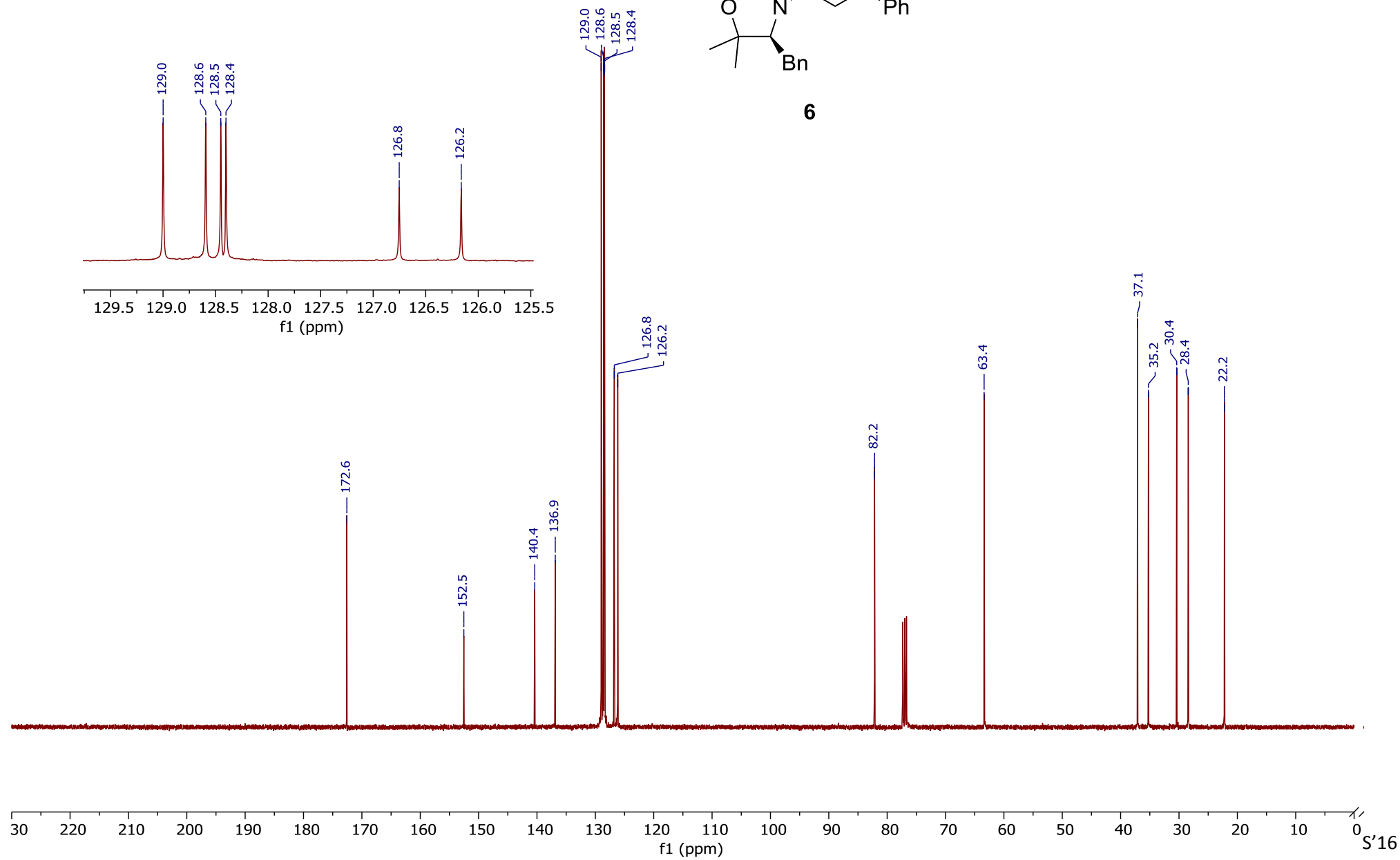
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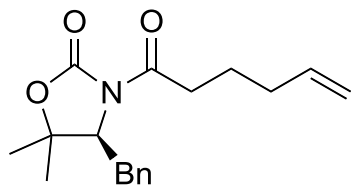
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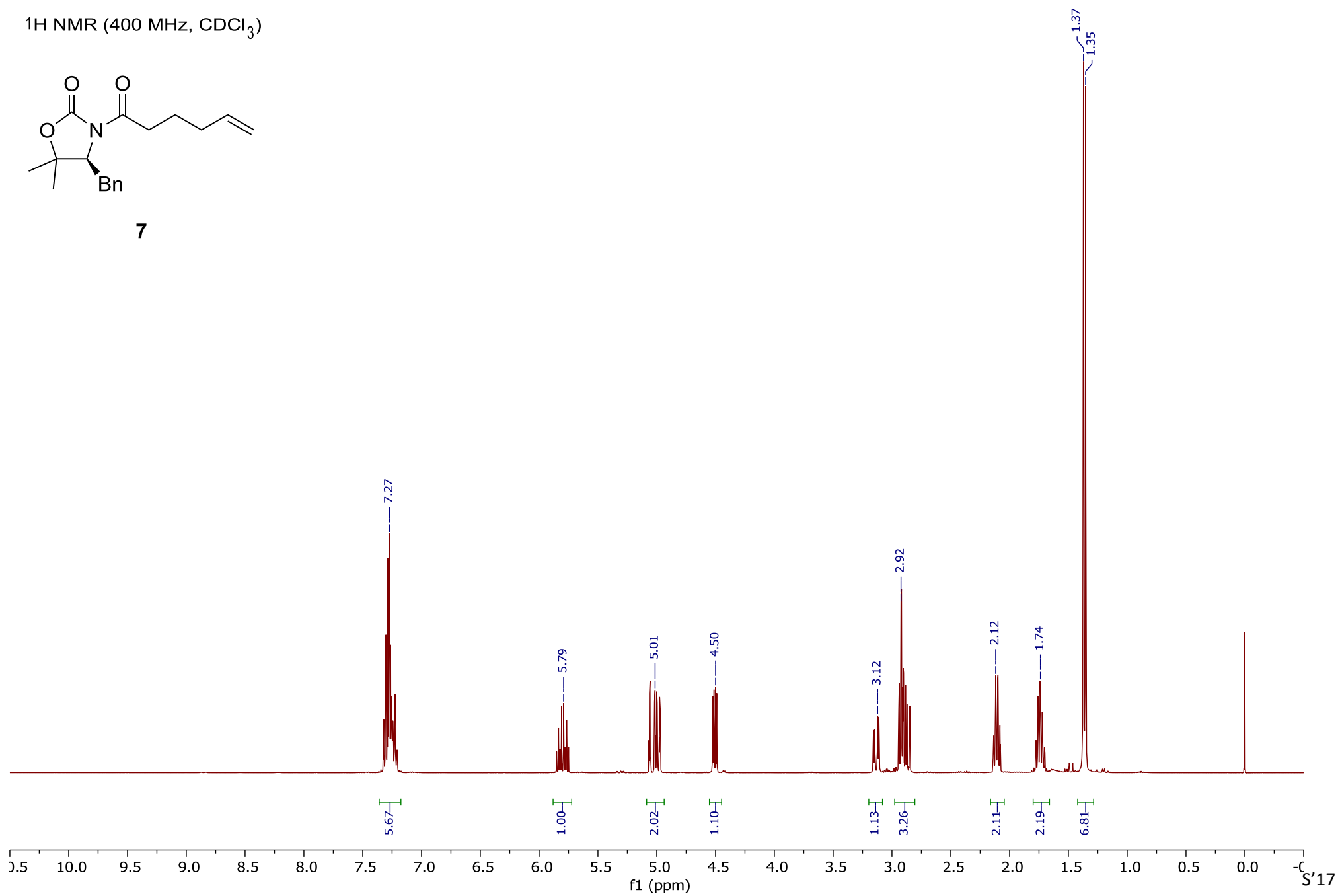
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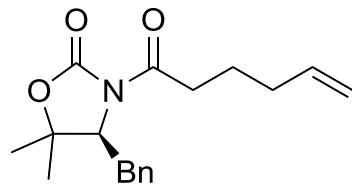
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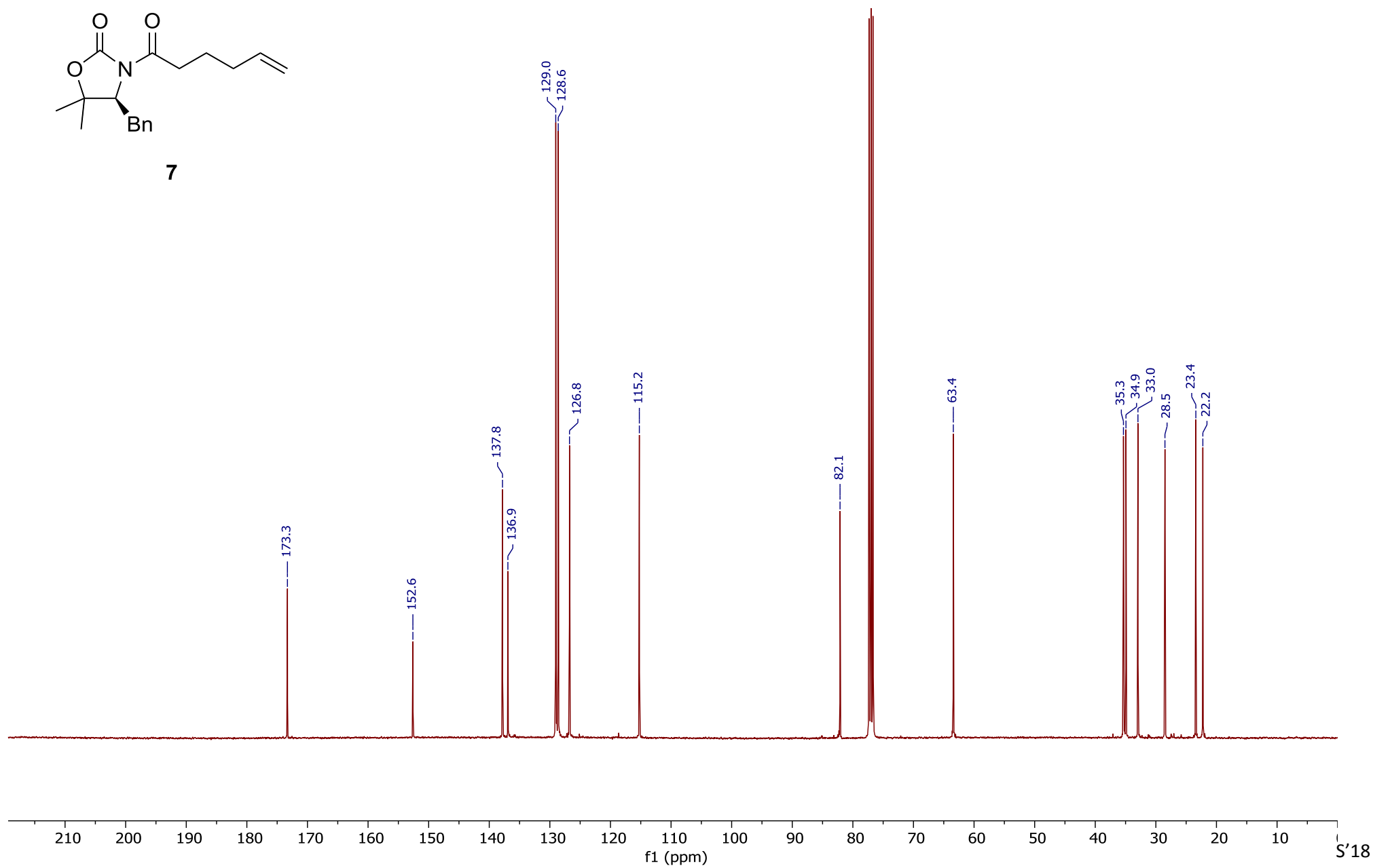
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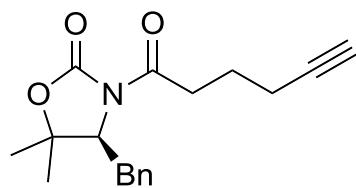
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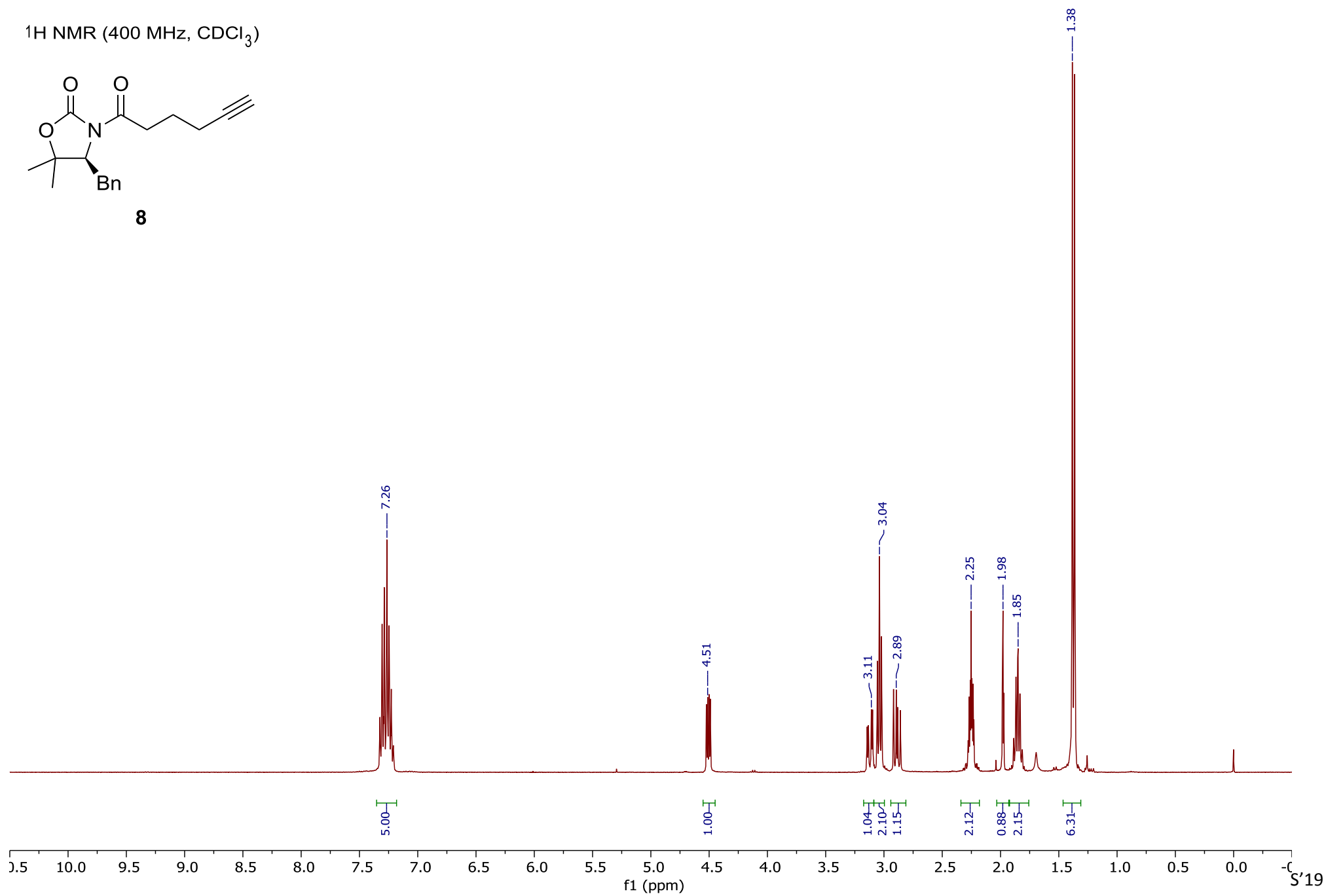
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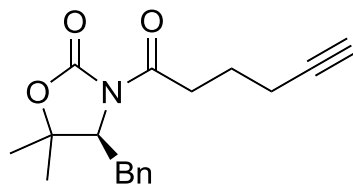
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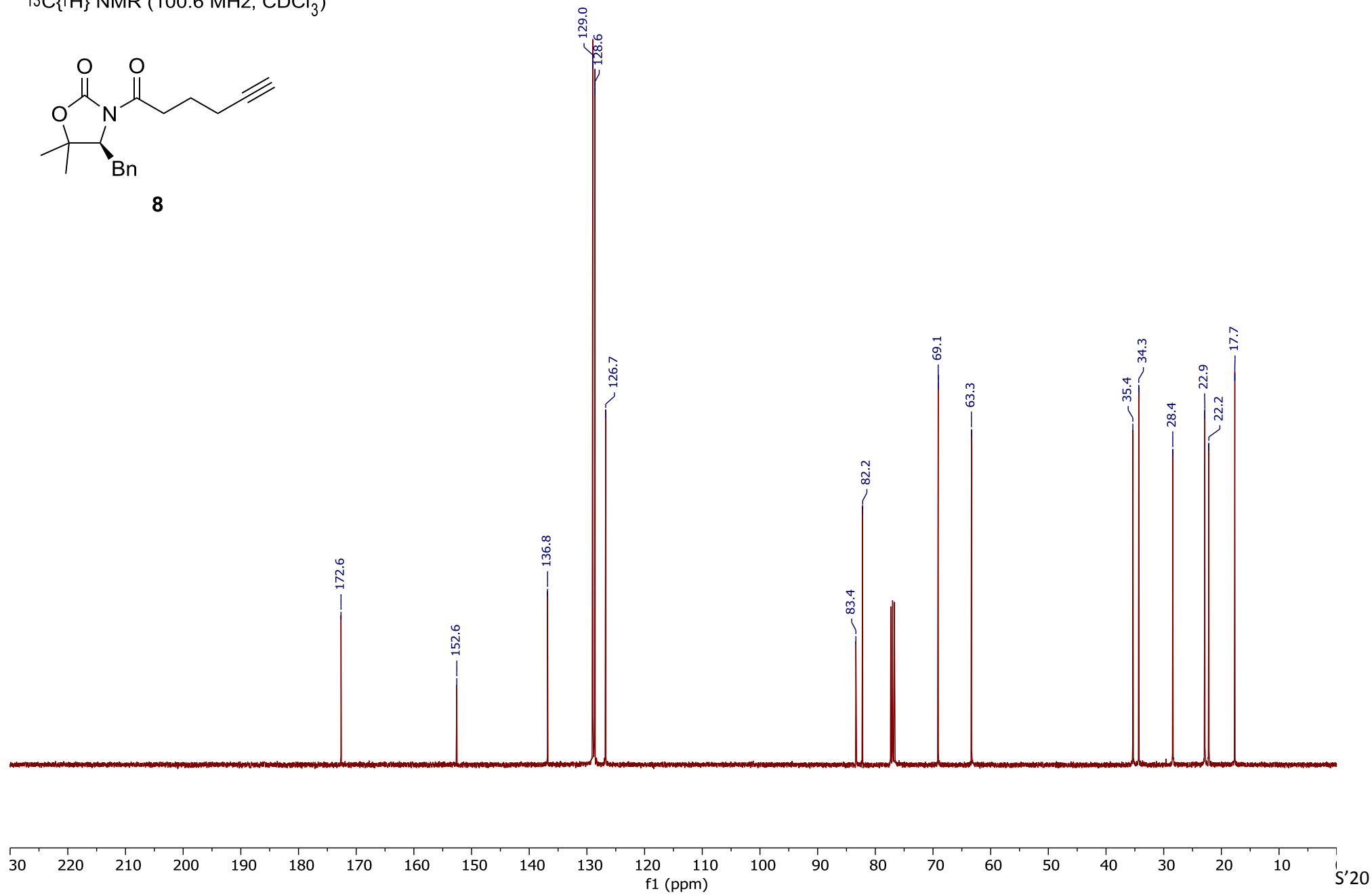
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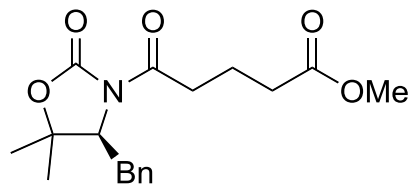
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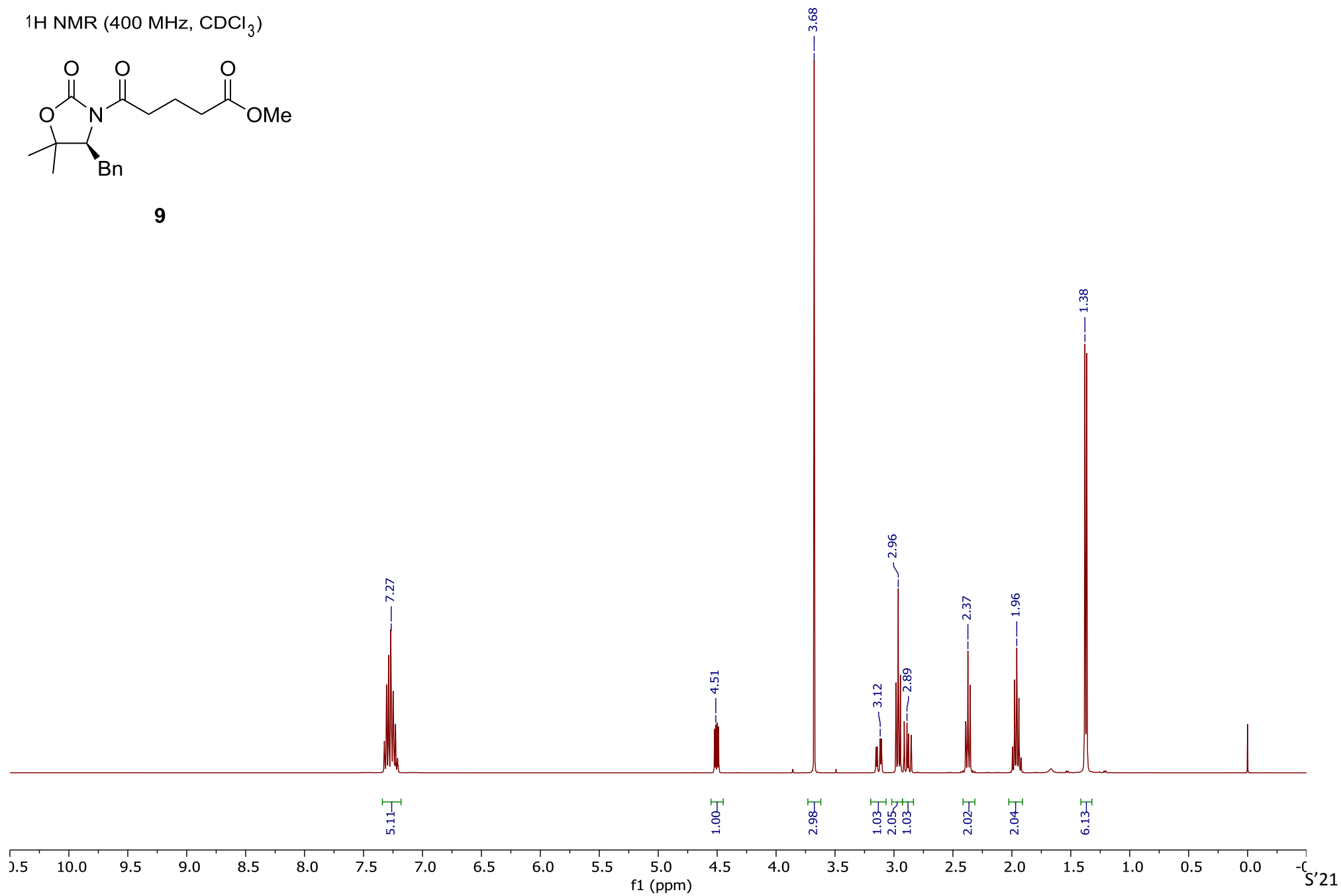
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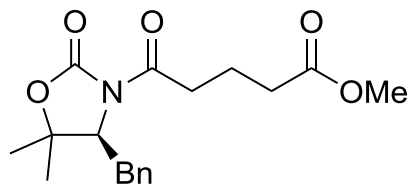
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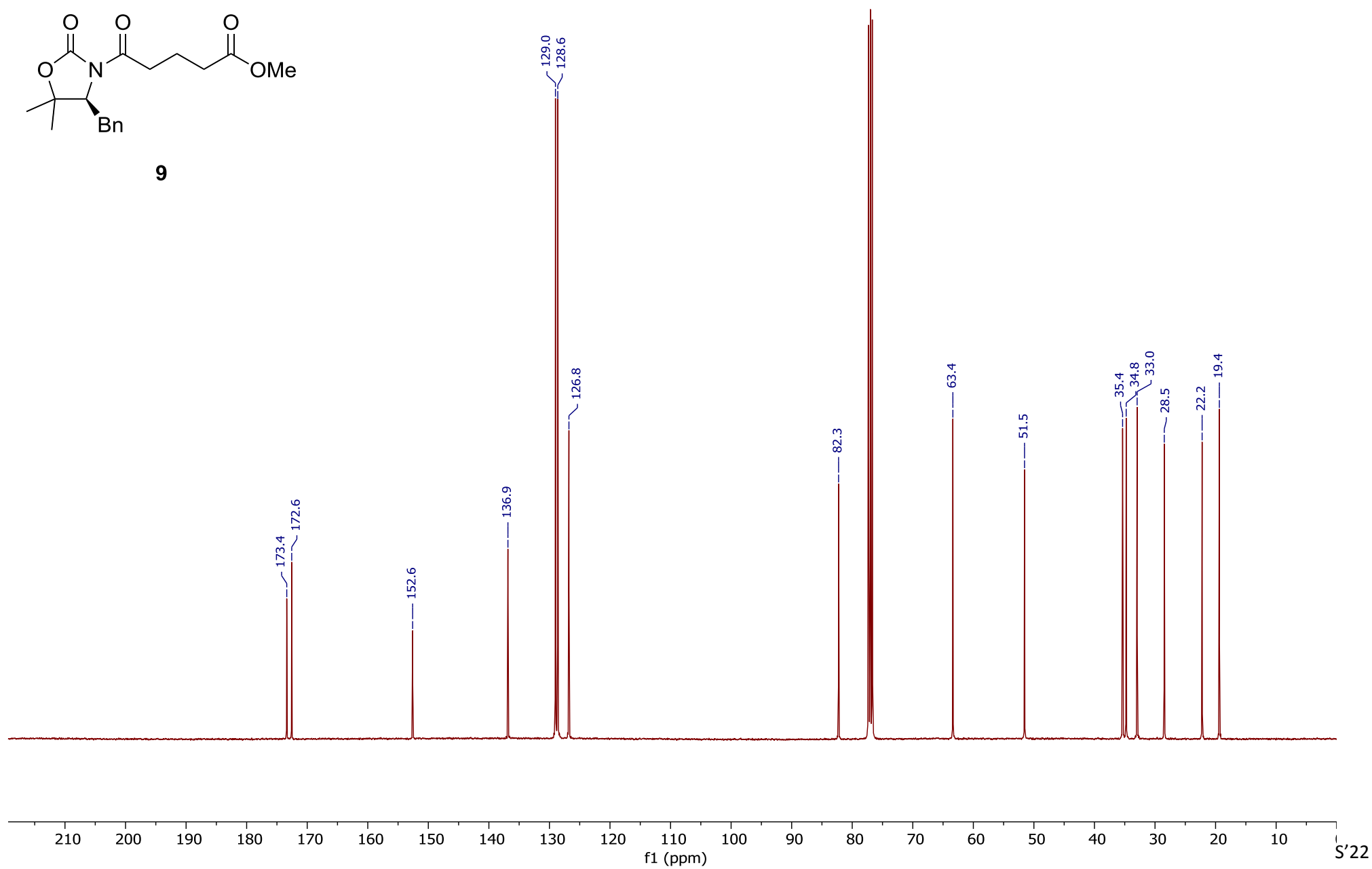
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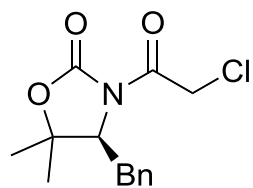


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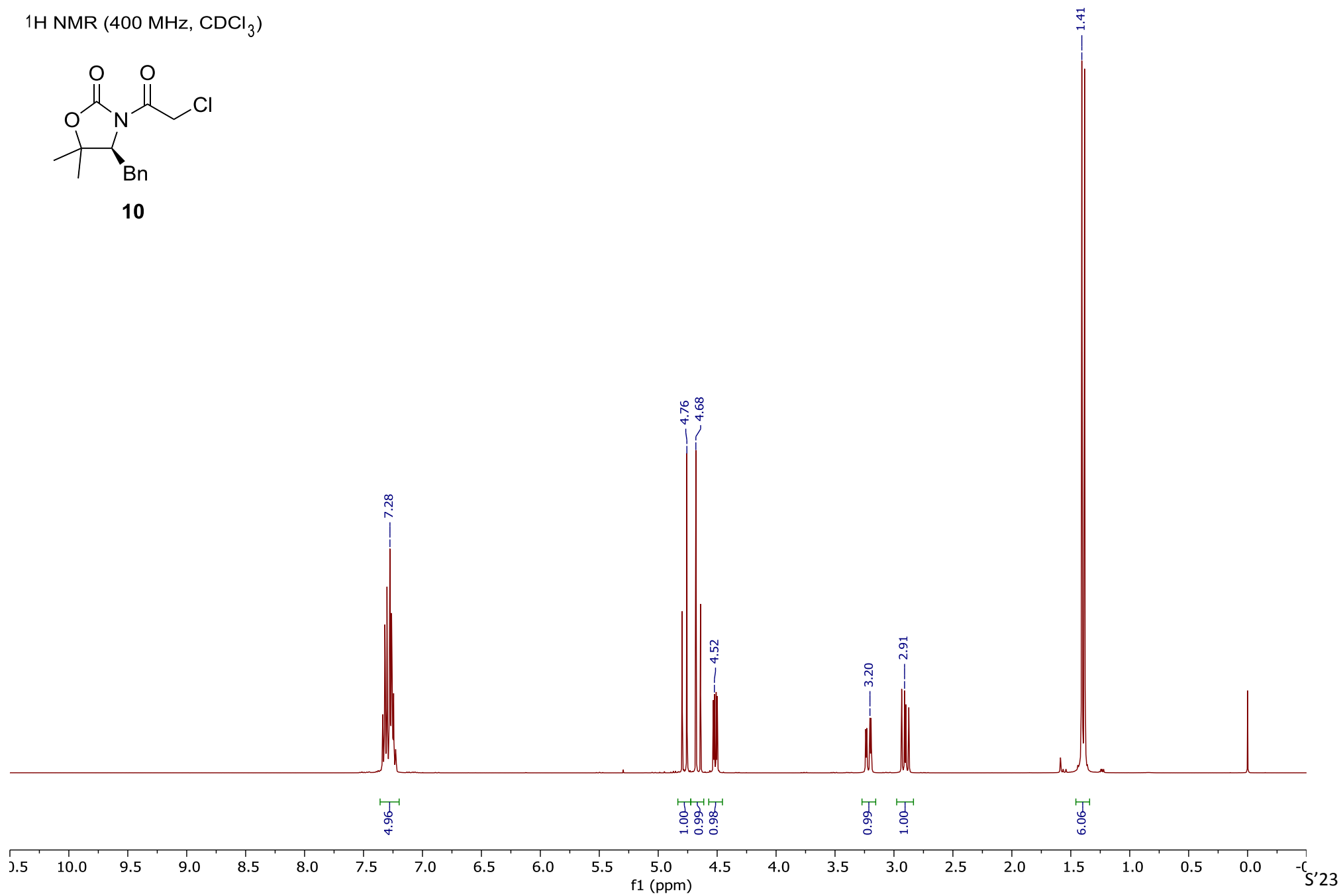


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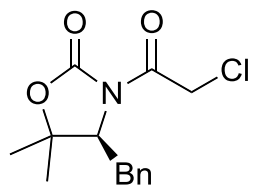
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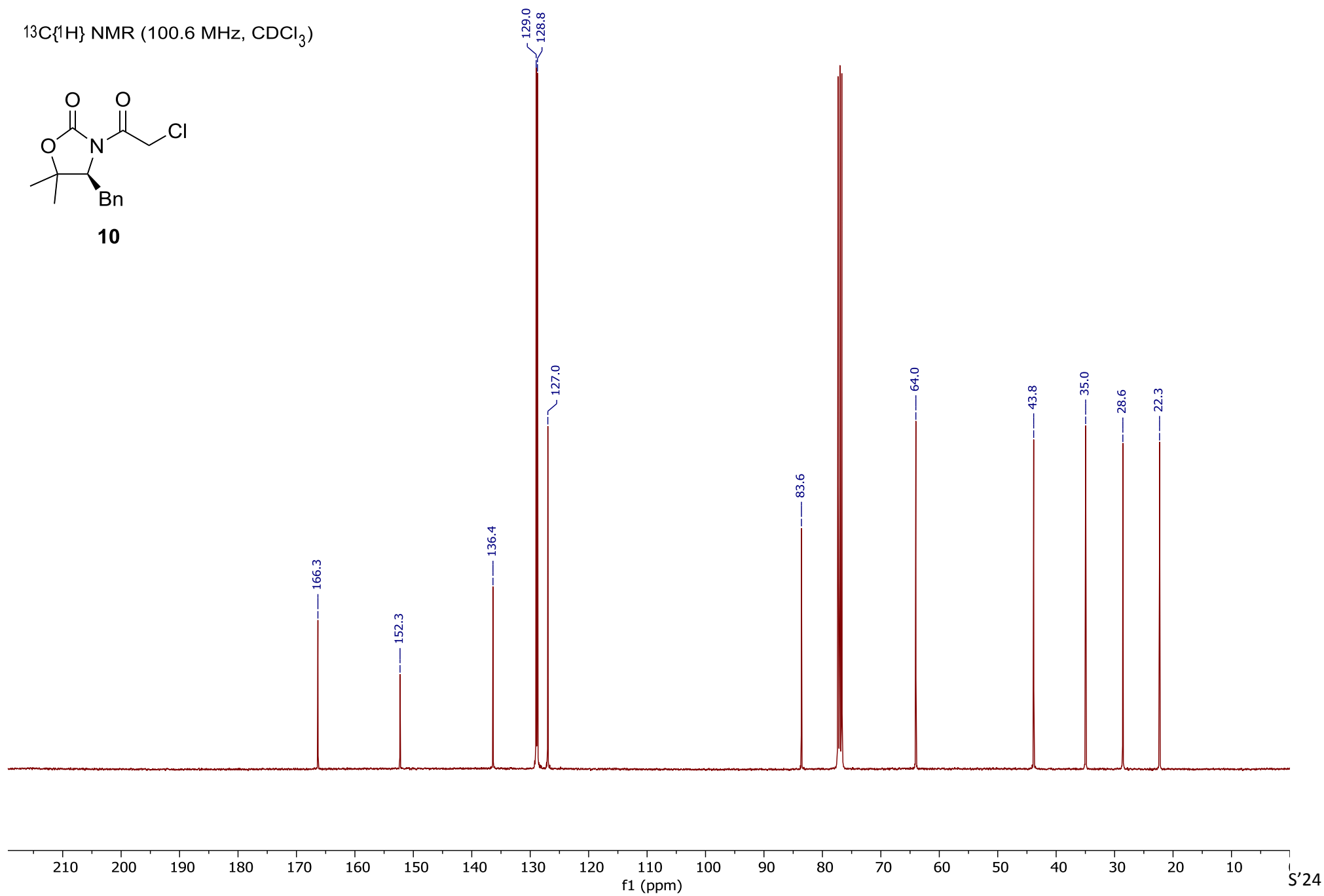
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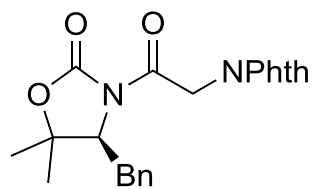
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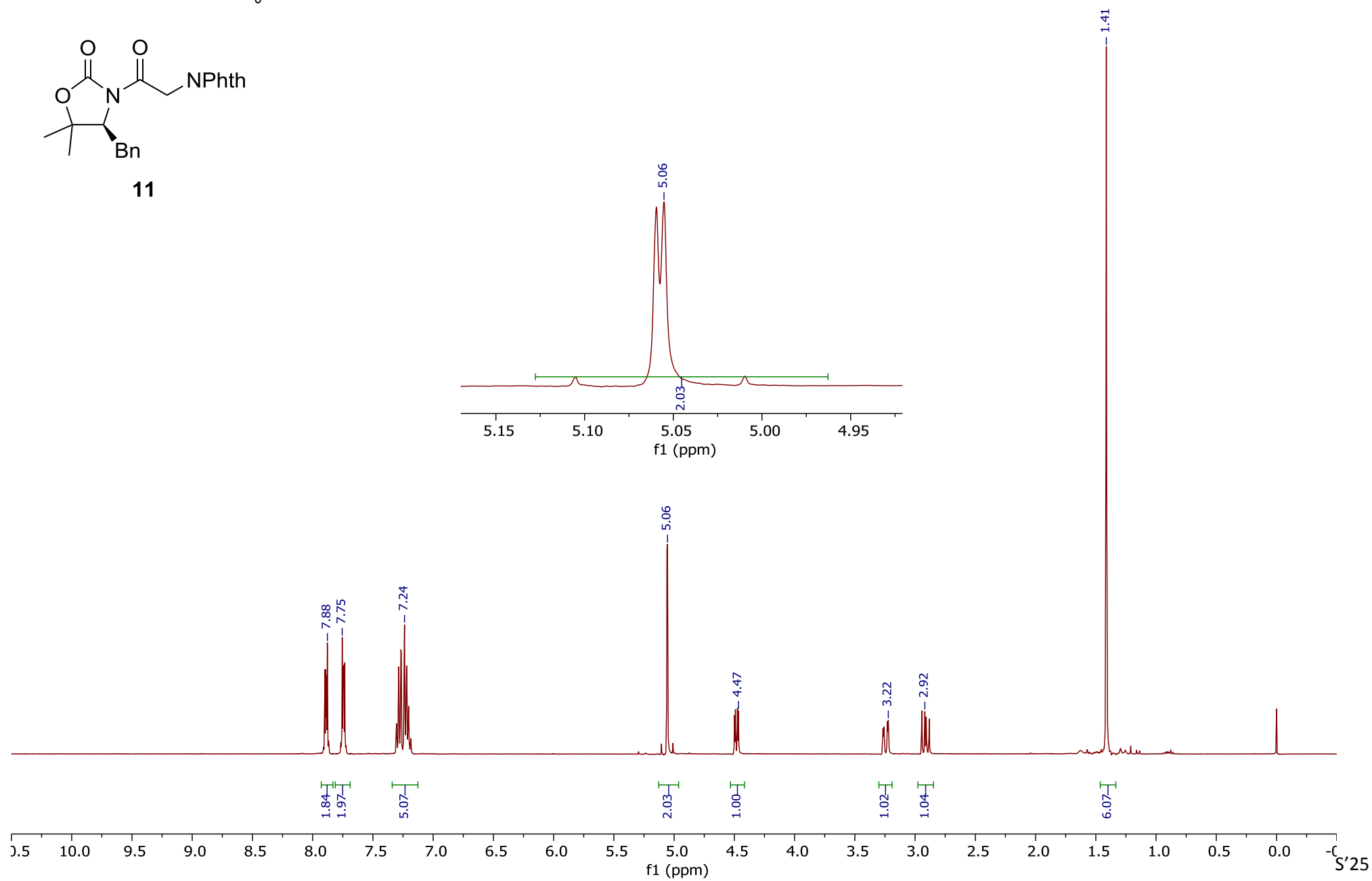
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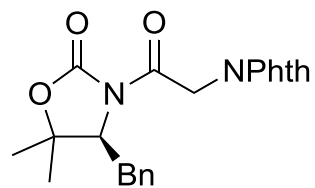
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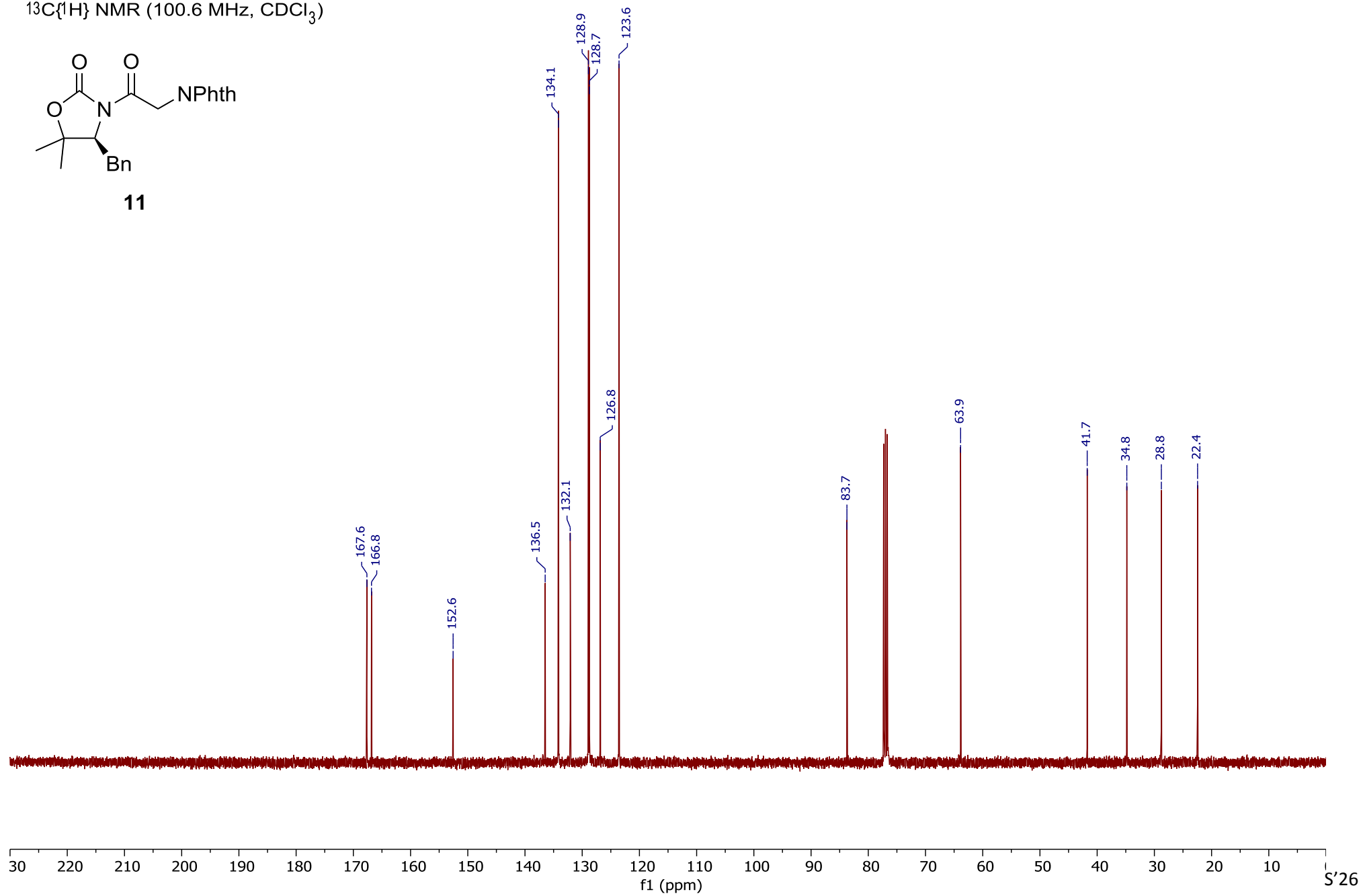
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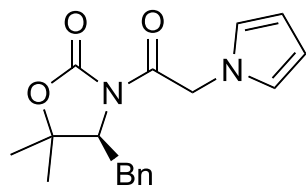
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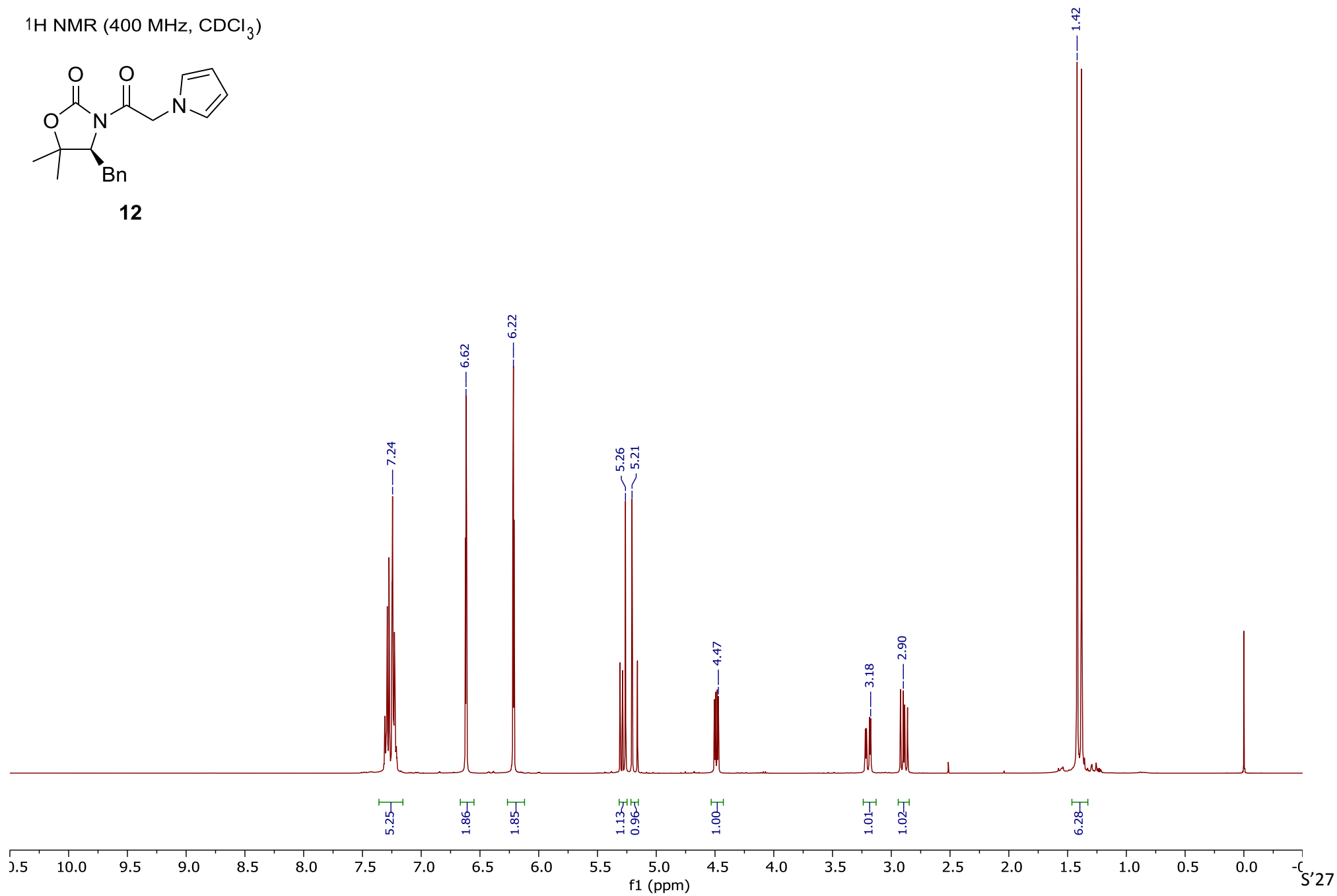
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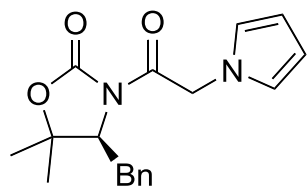
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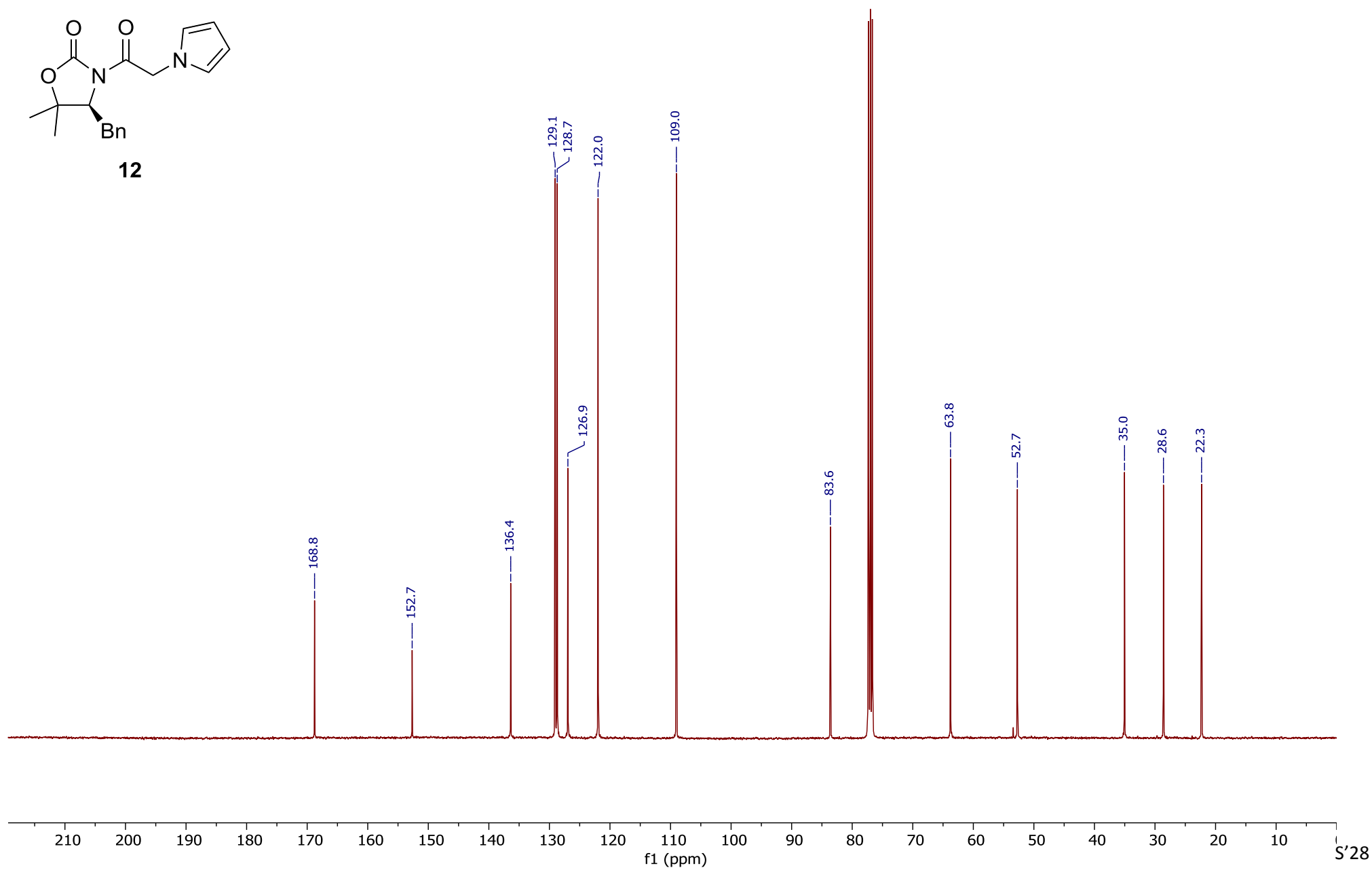
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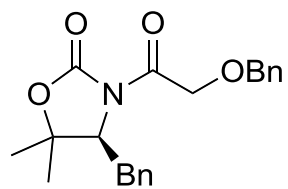
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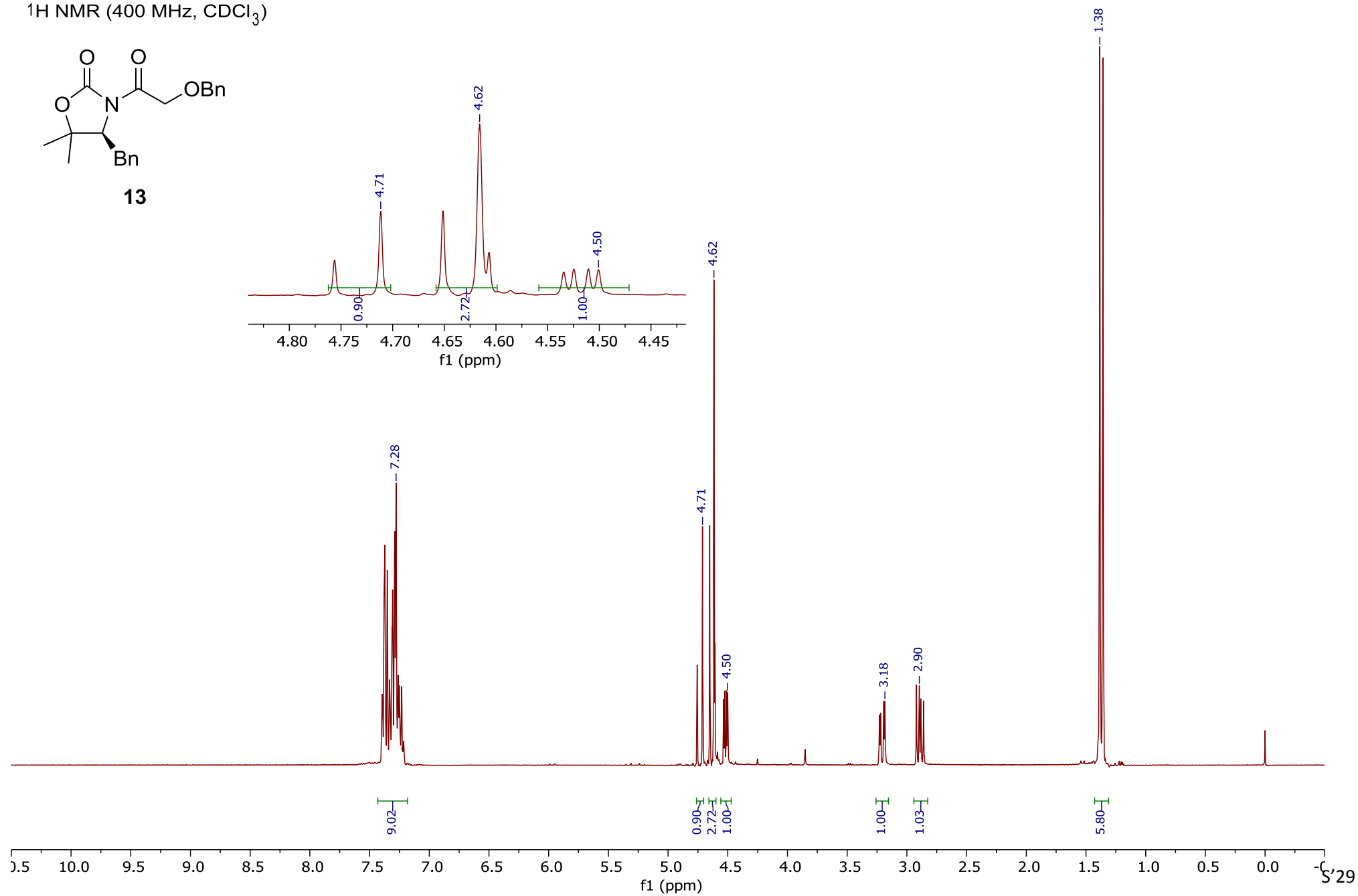
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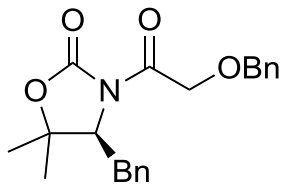
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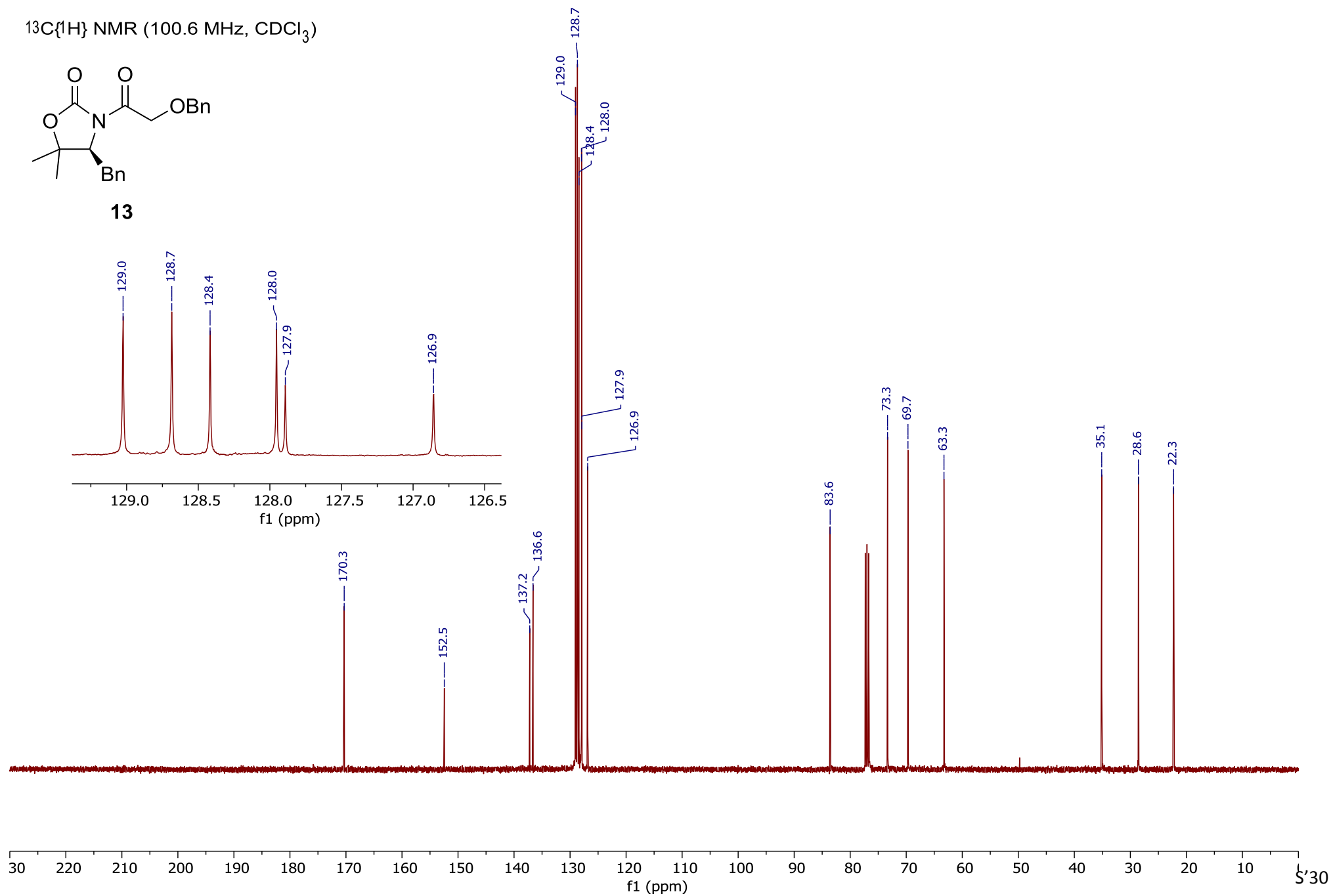
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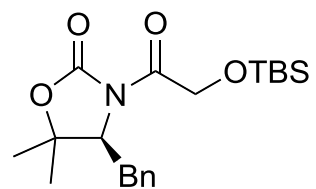
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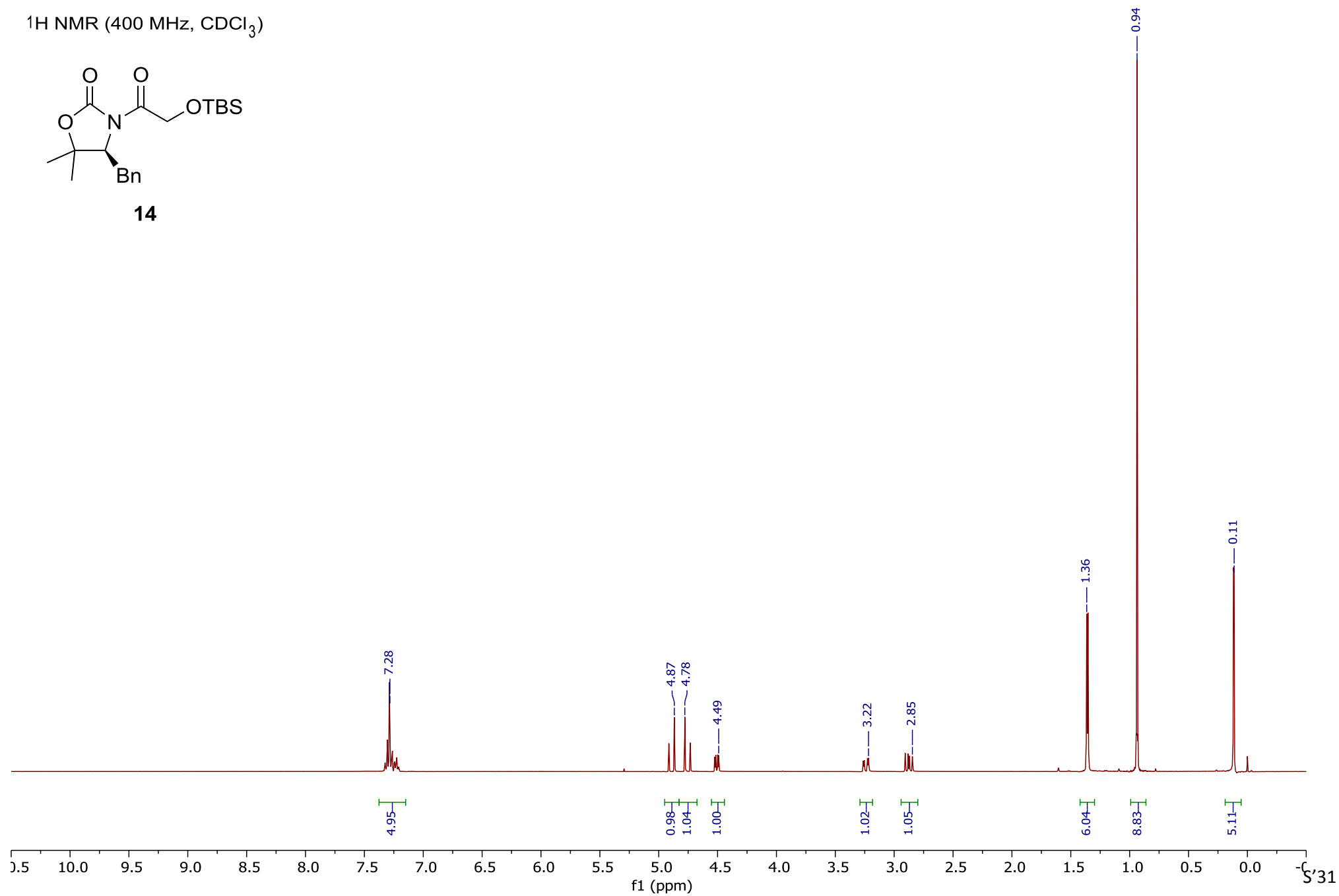
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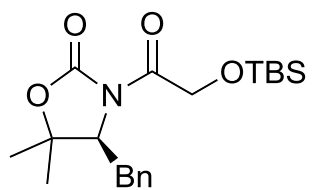
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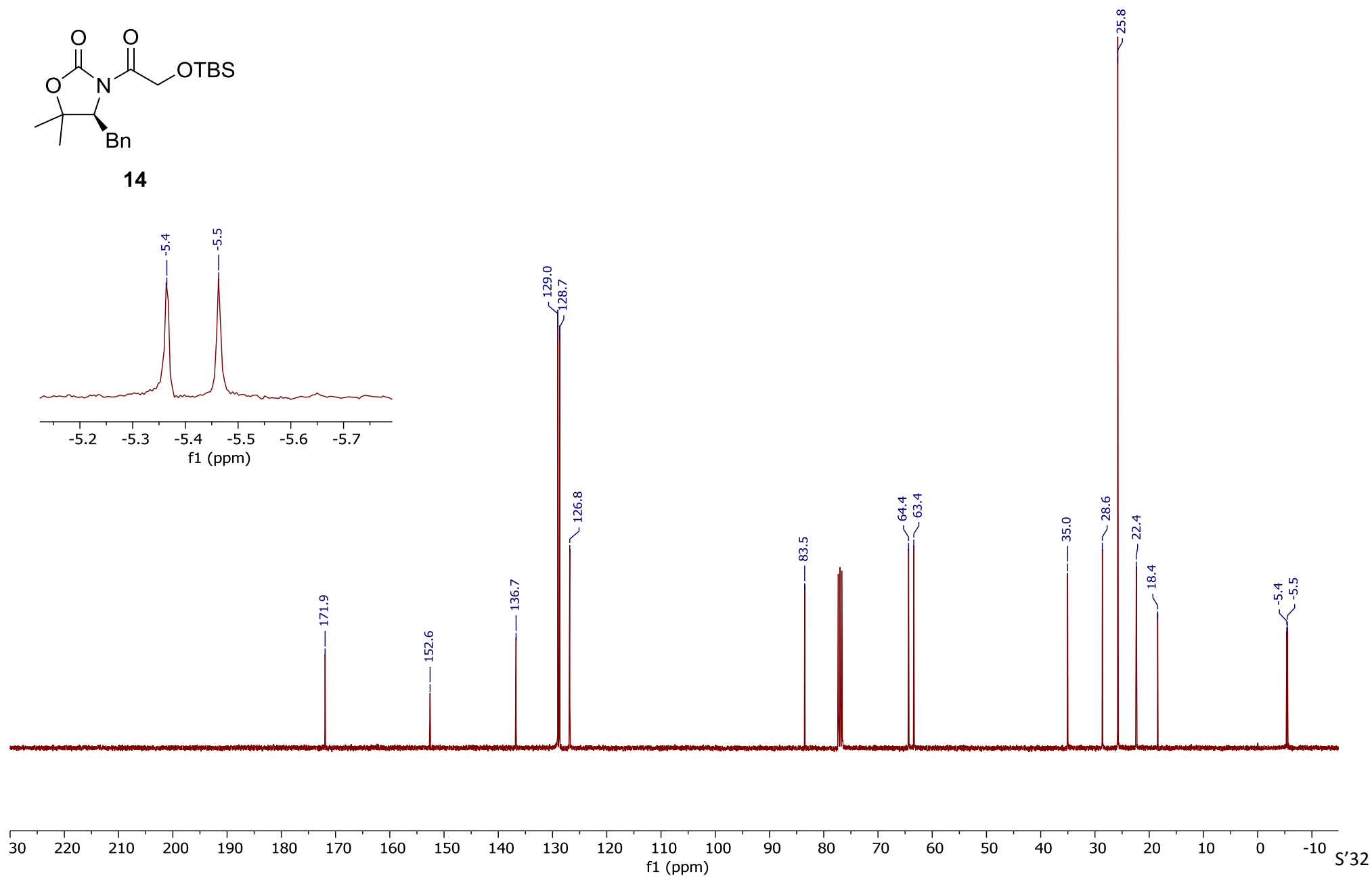
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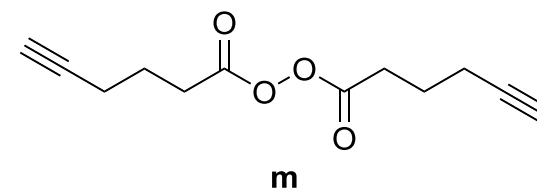
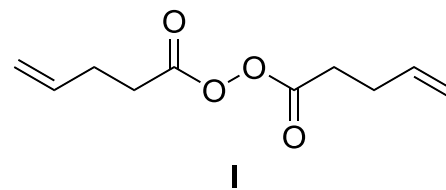
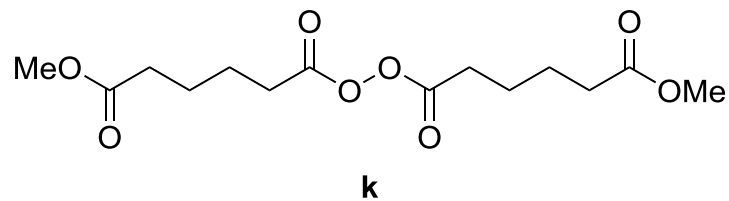
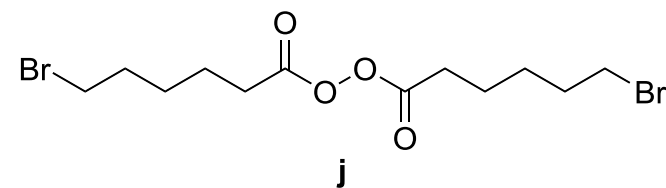
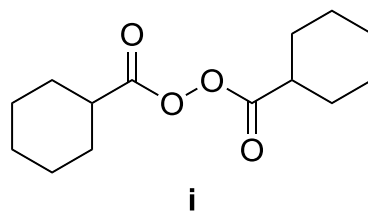
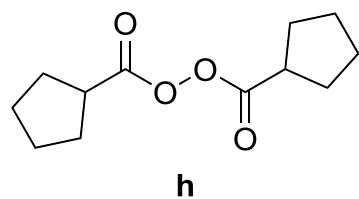
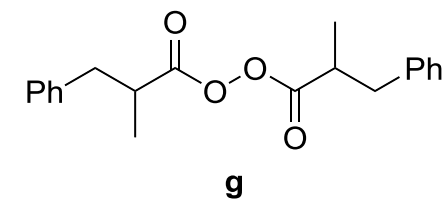
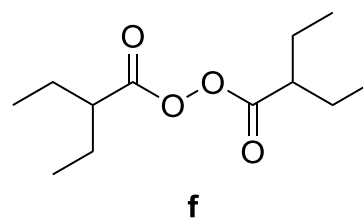
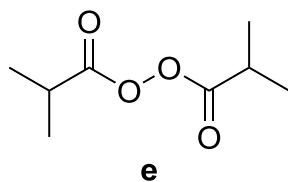
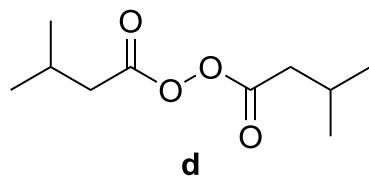
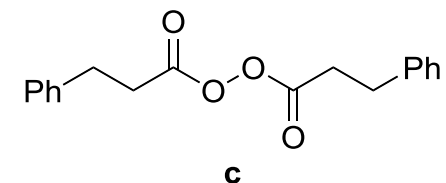
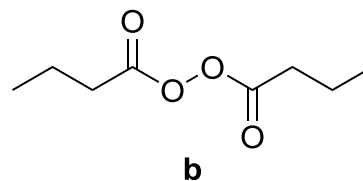
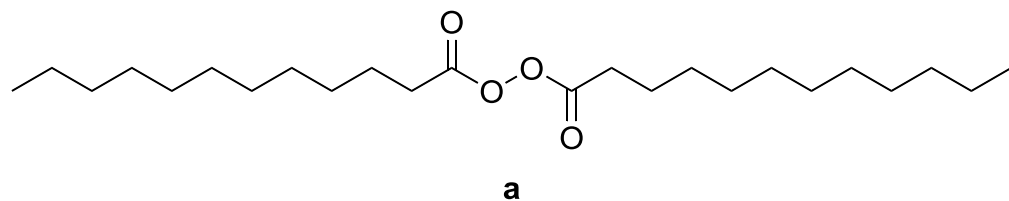
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



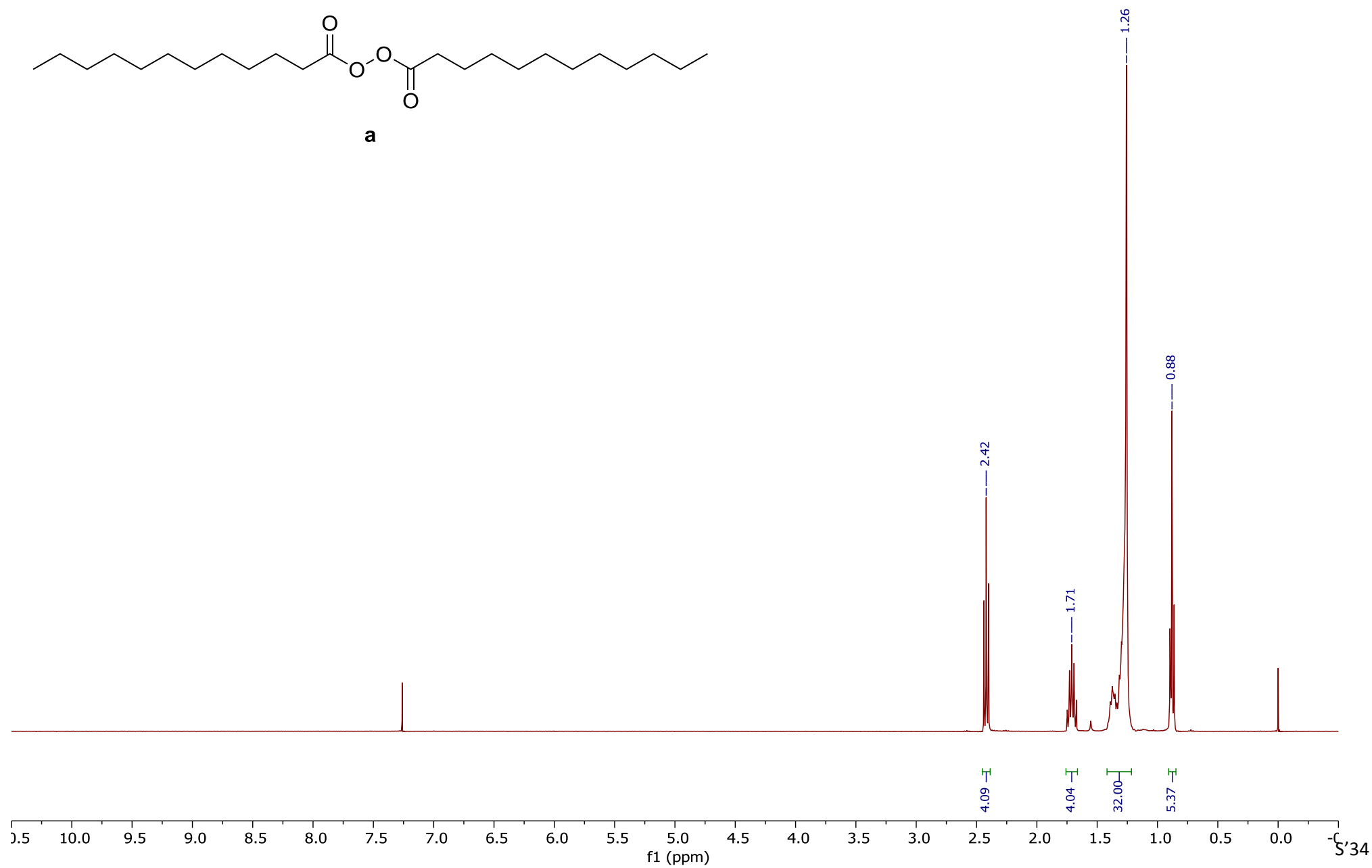
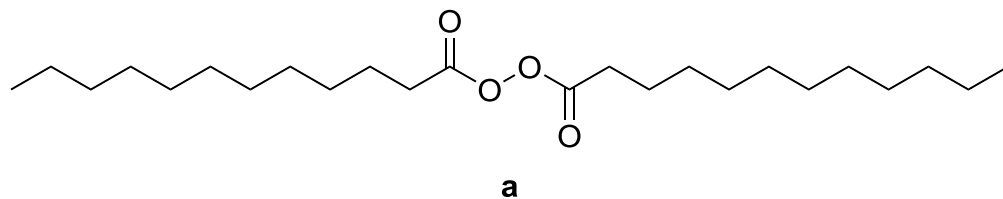
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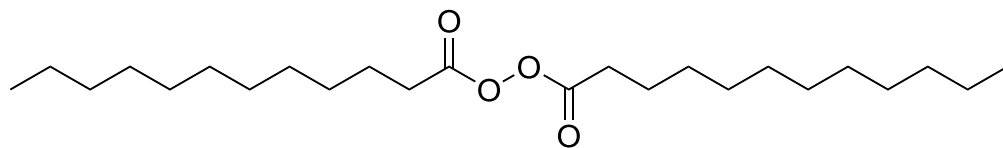
3. DIACYL PEROXIDES



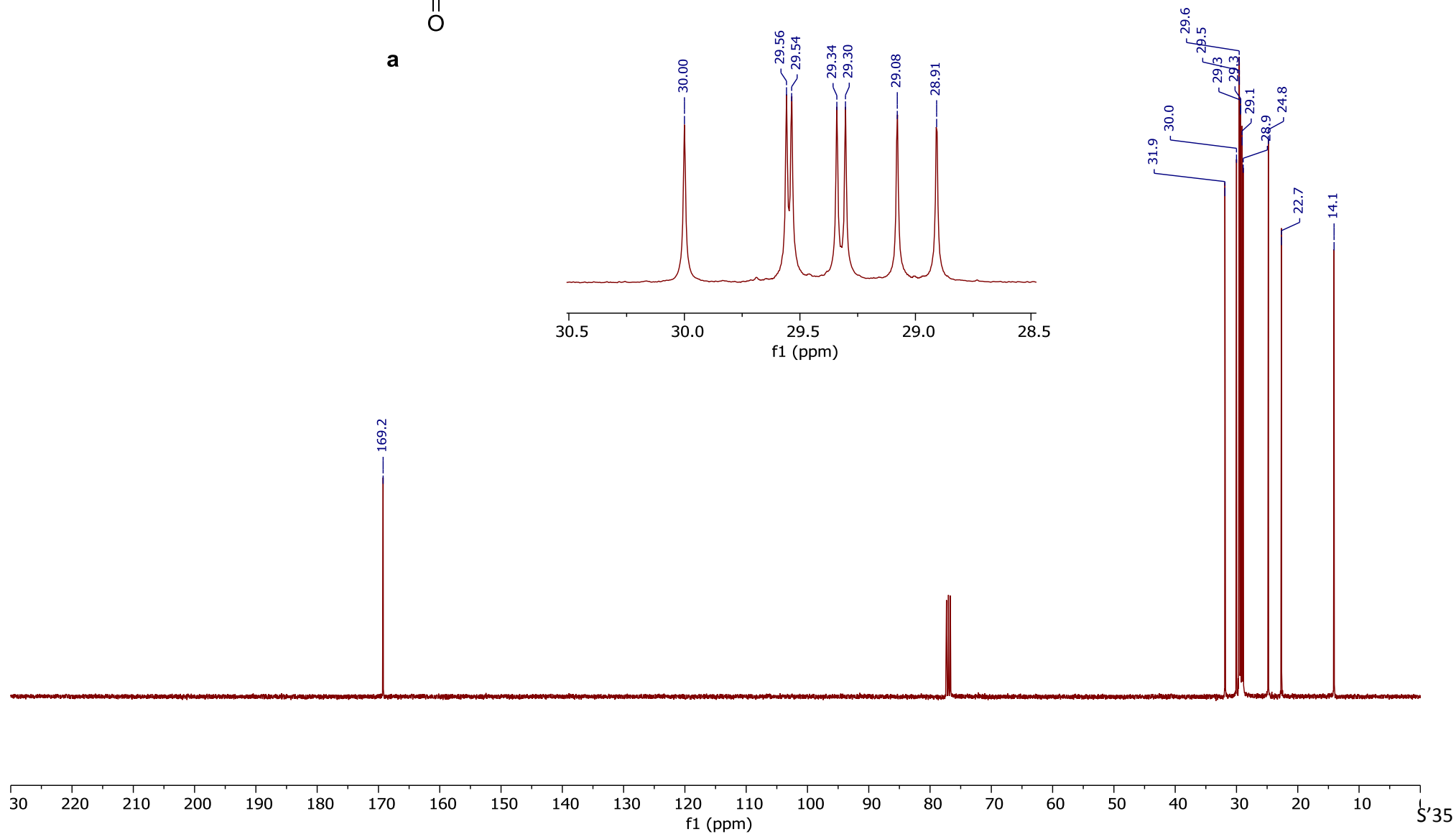
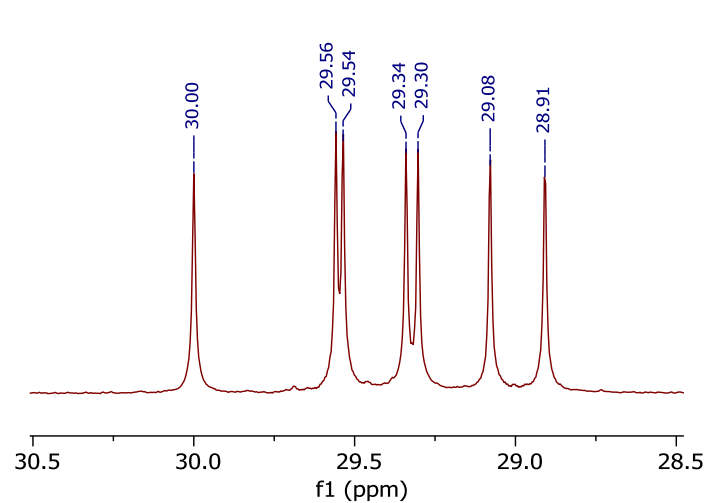
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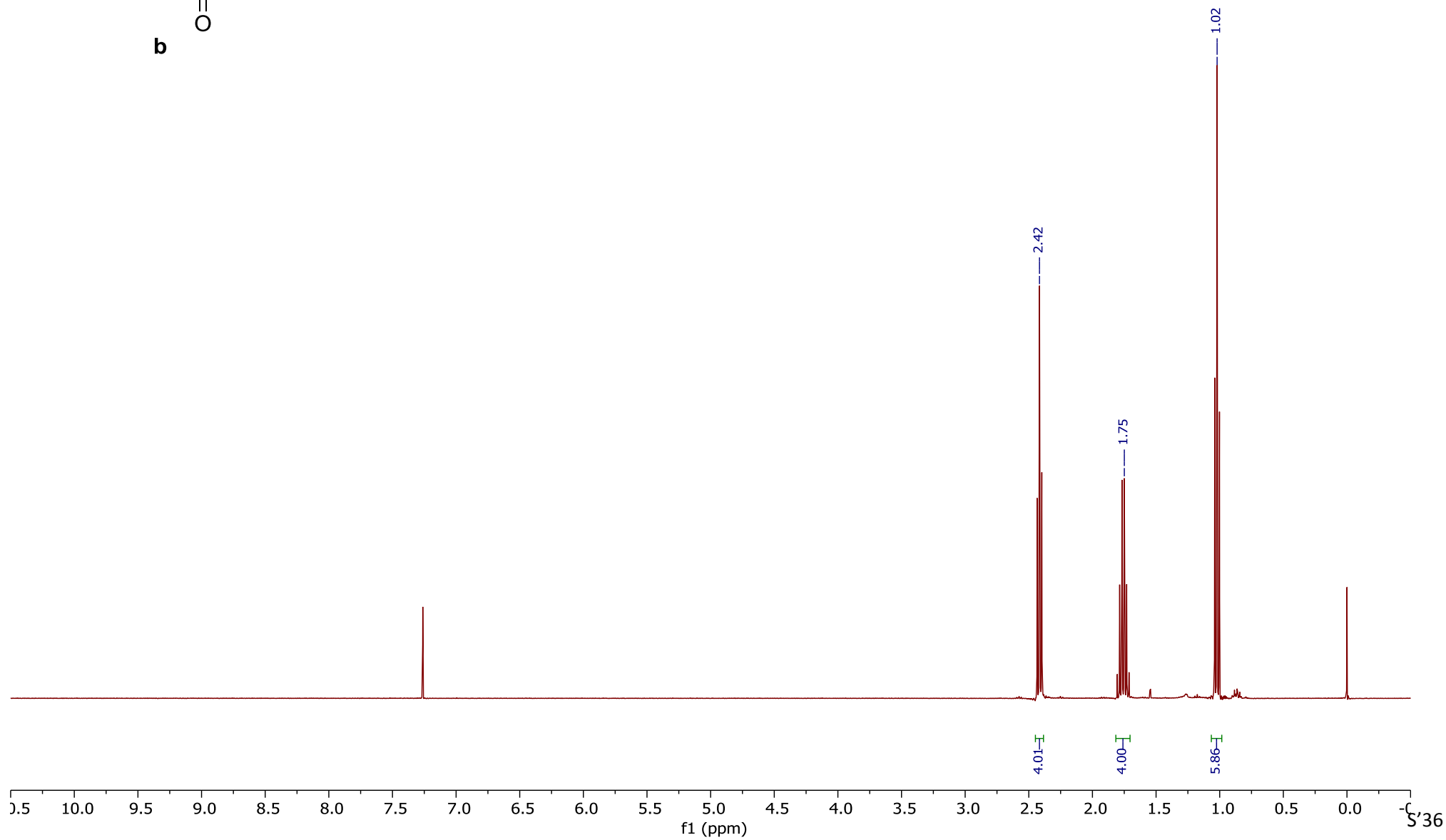
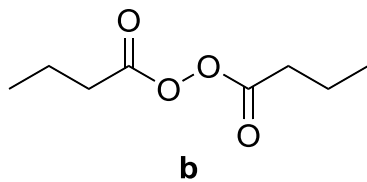
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



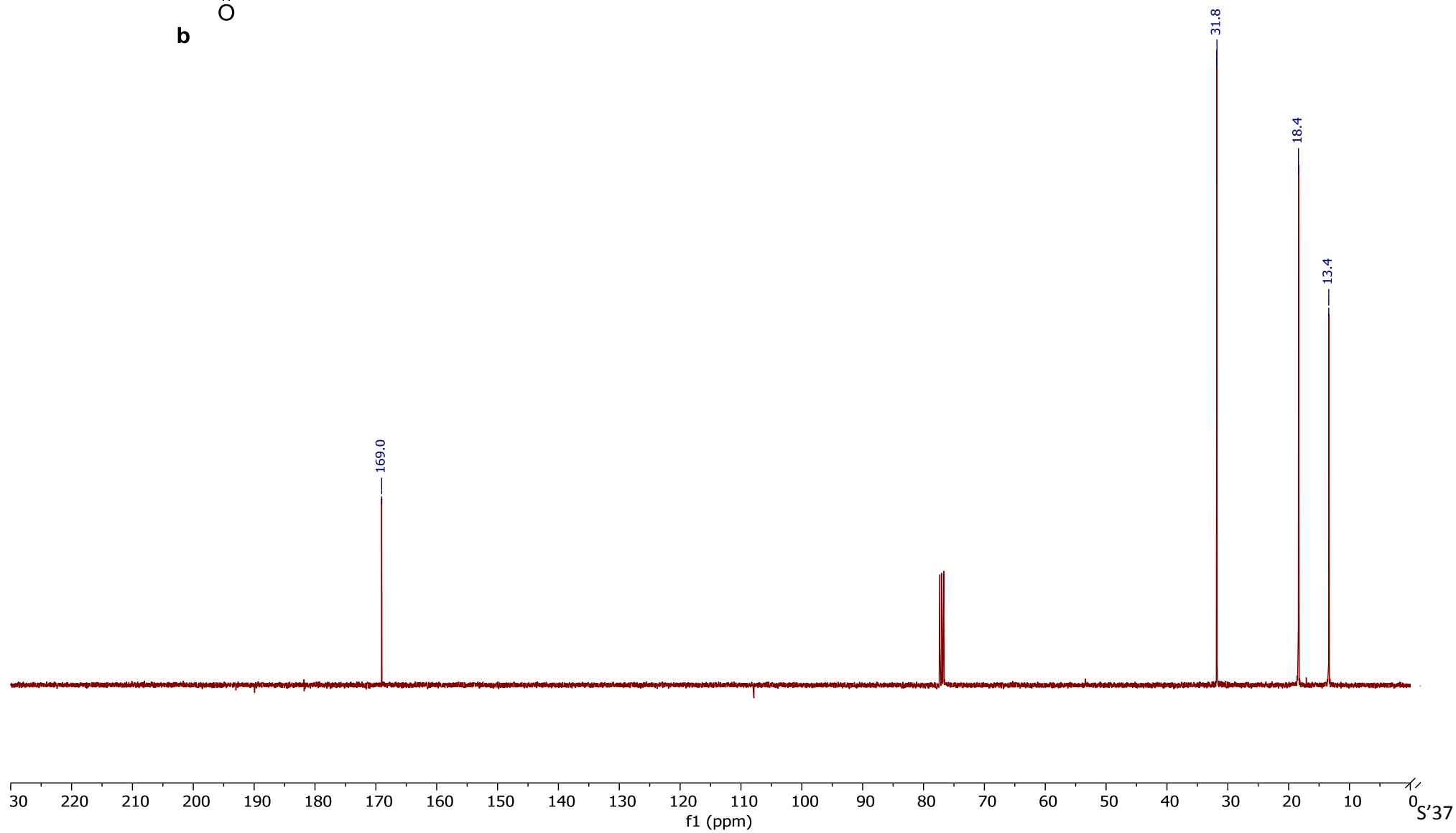
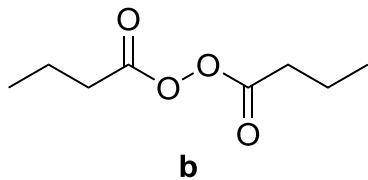
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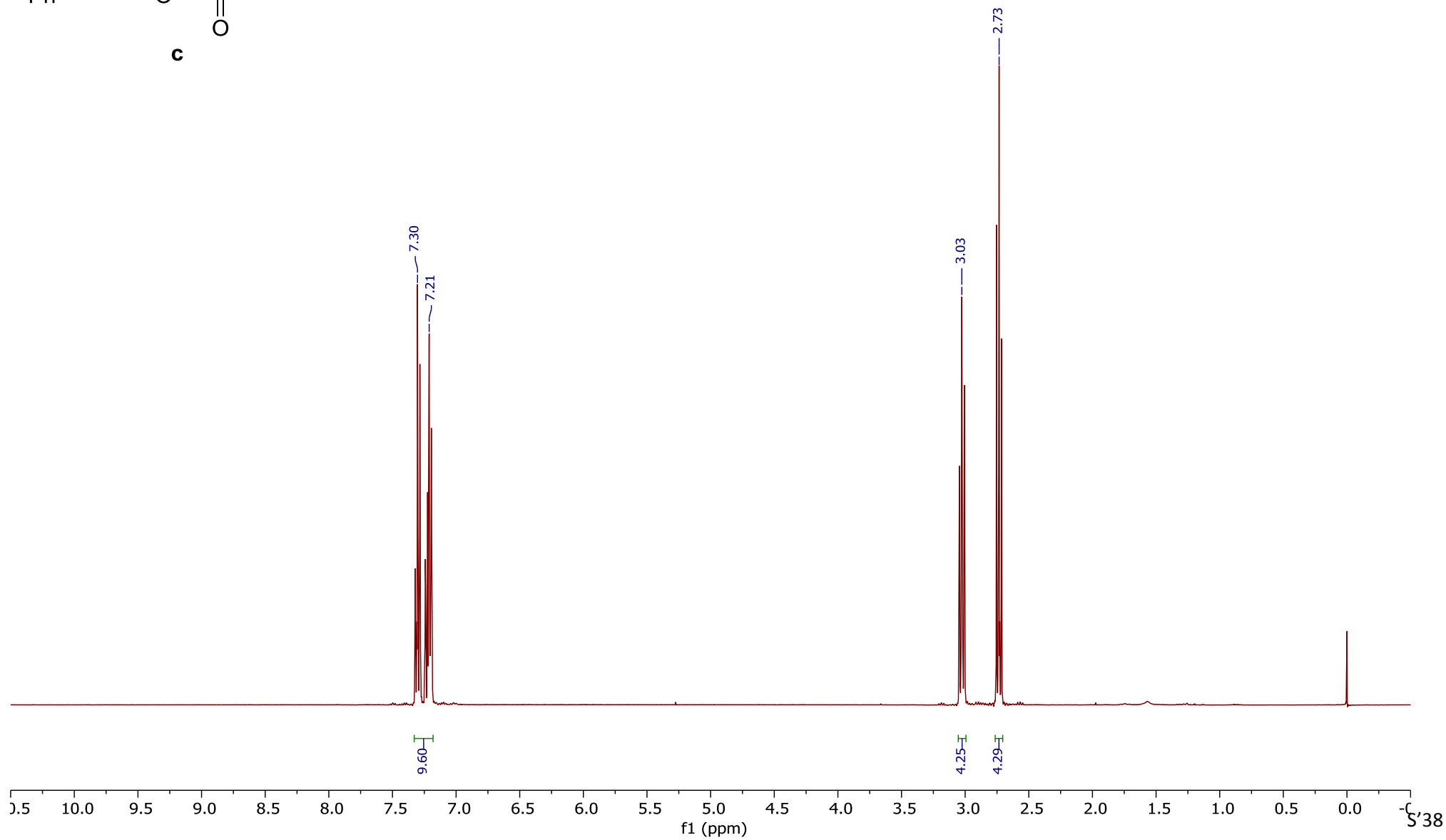
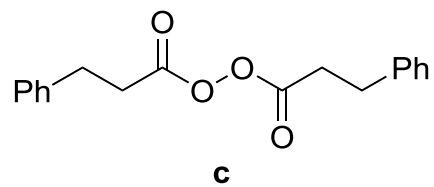
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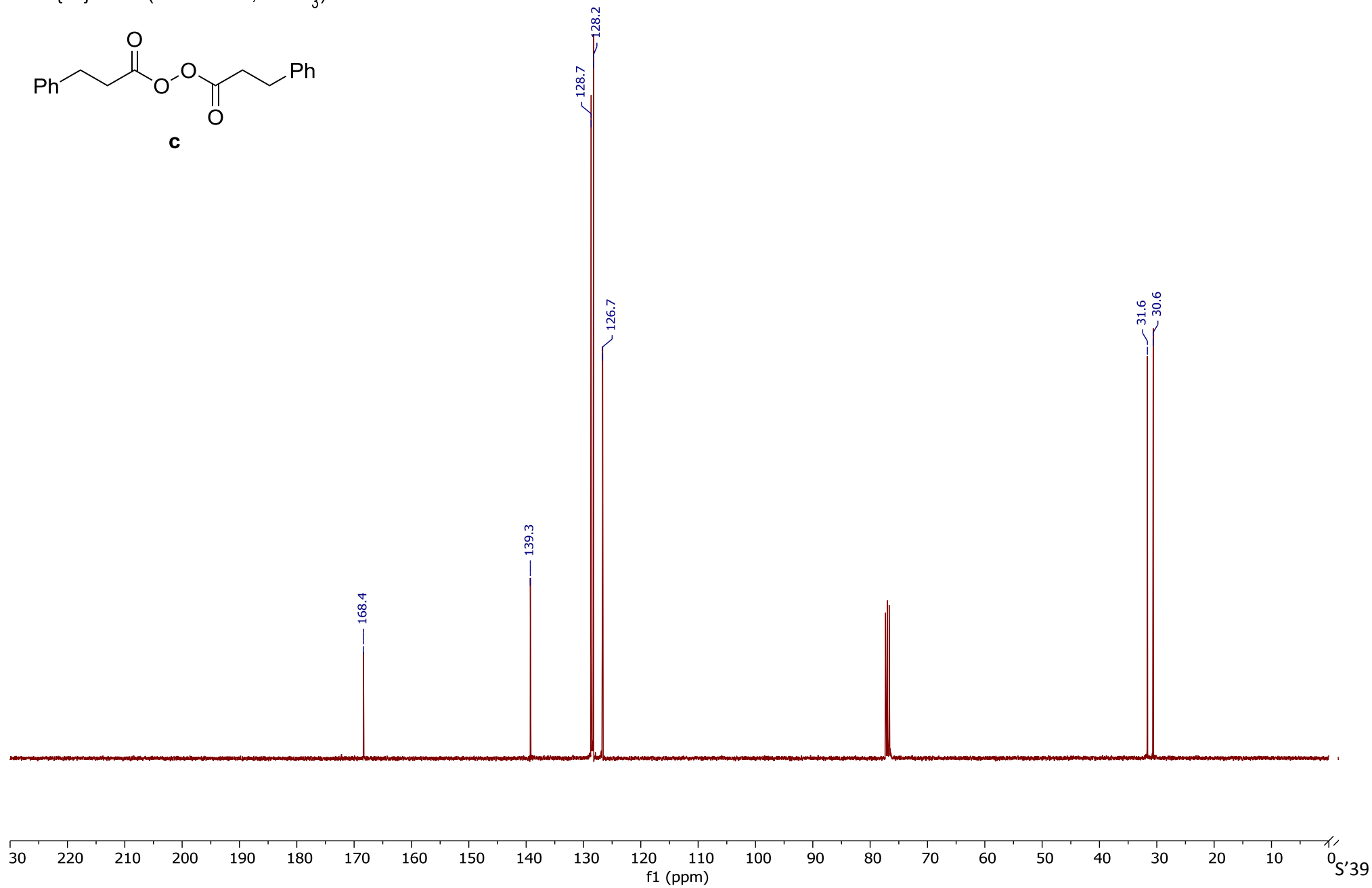
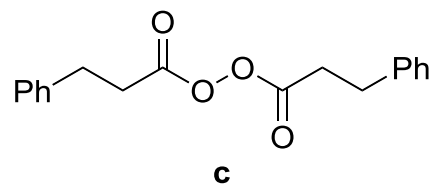
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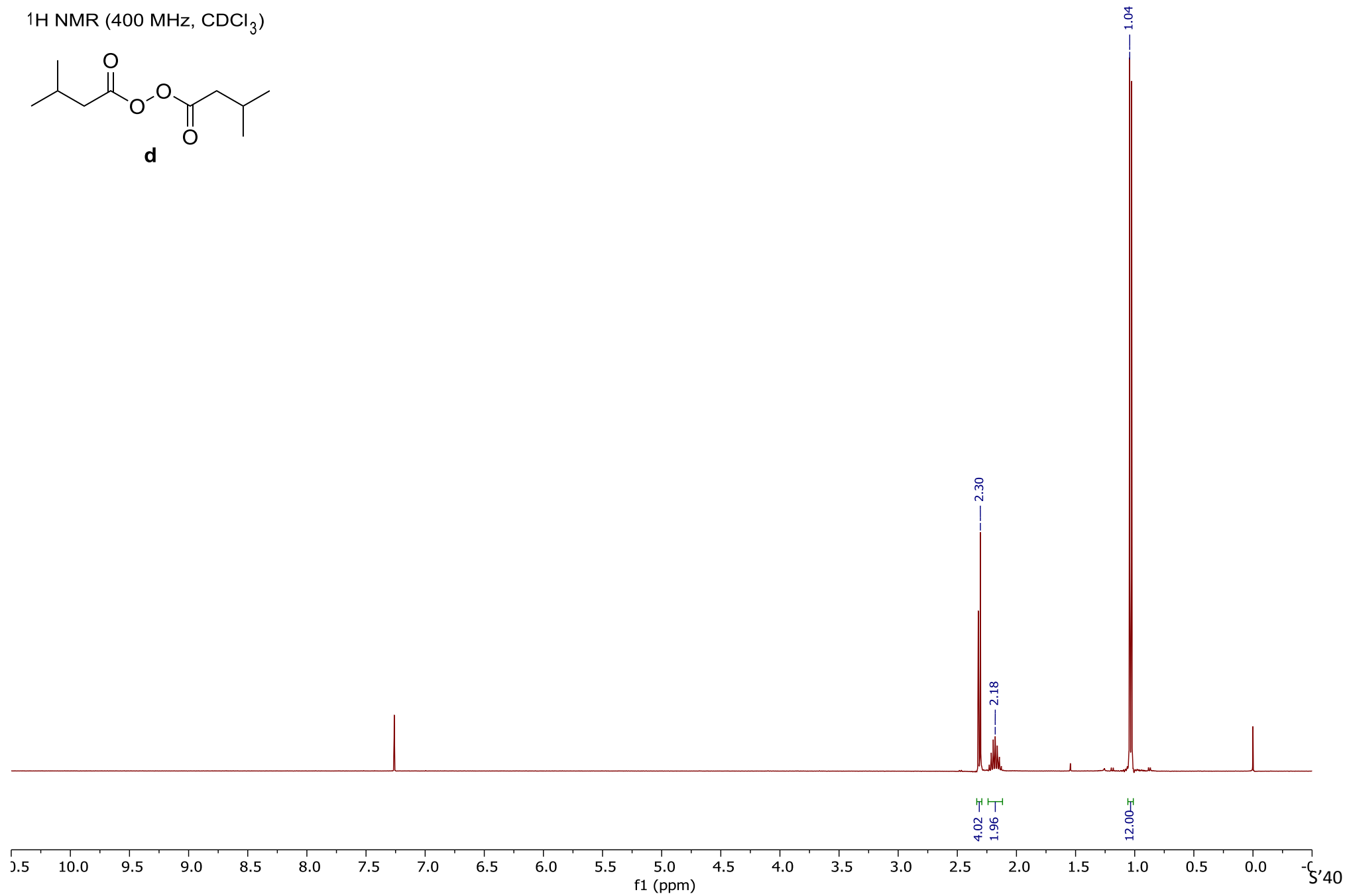
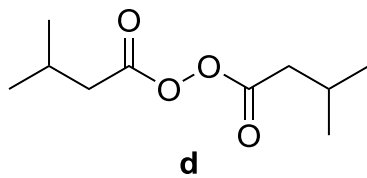
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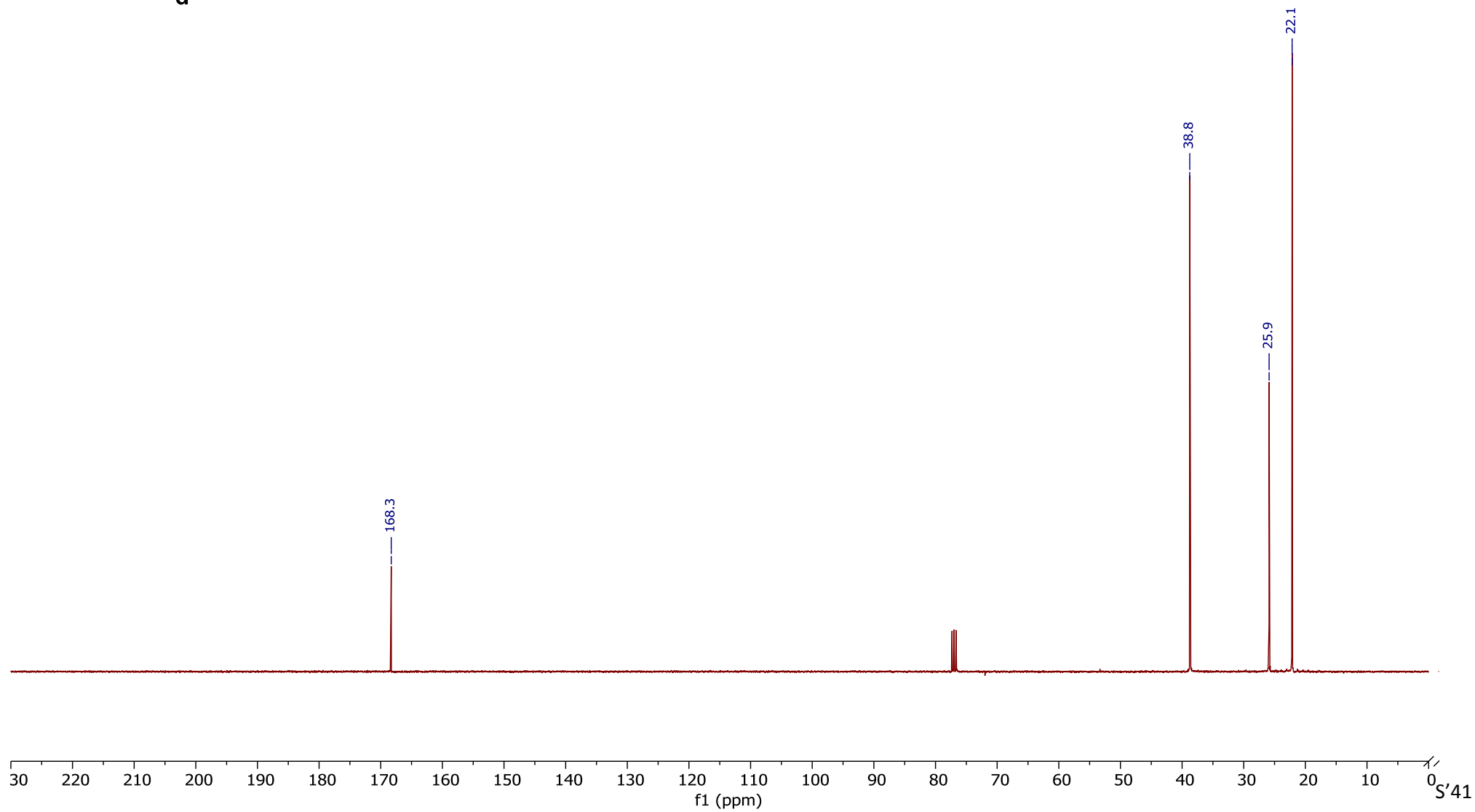
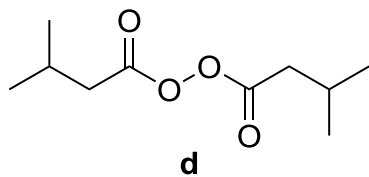
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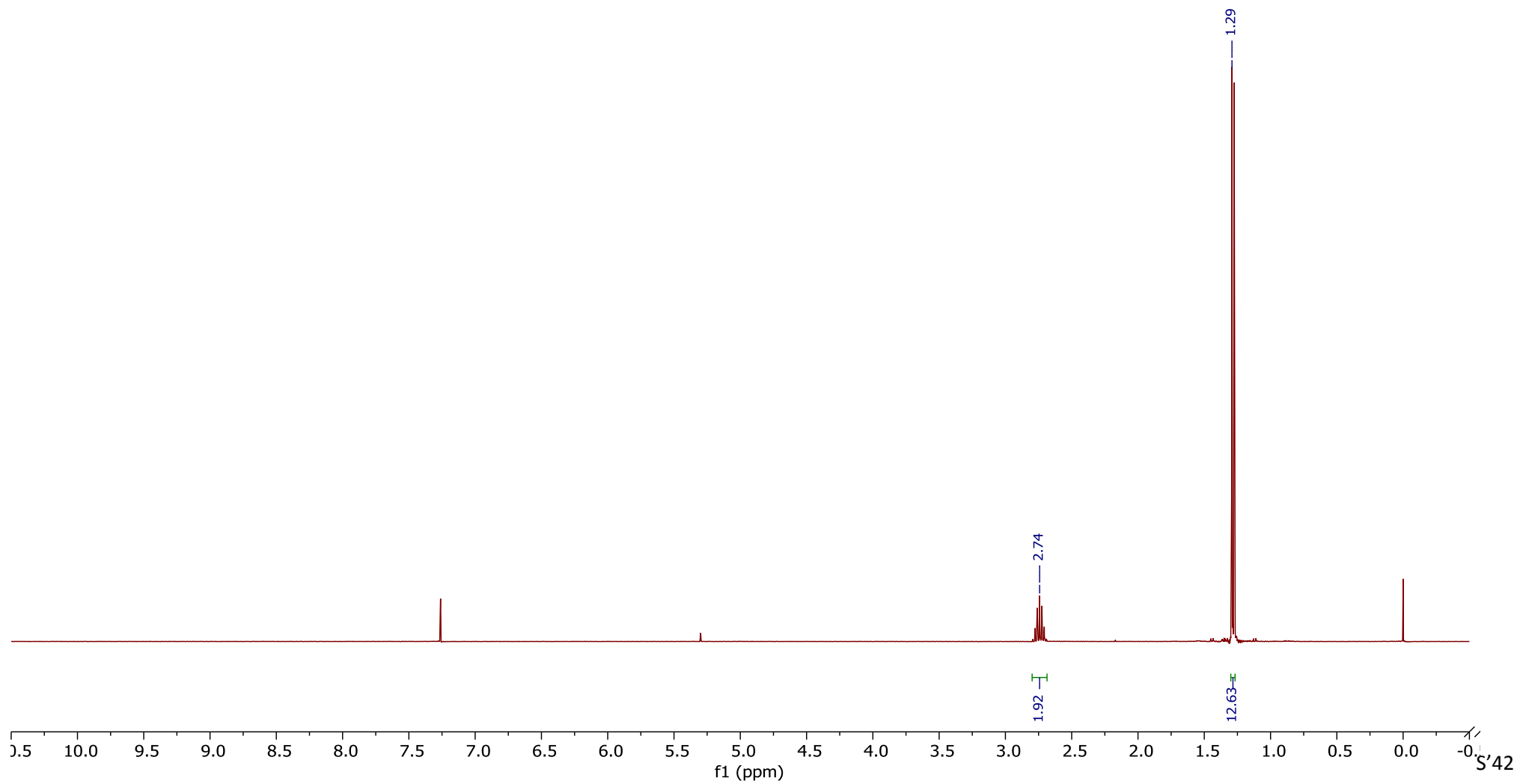
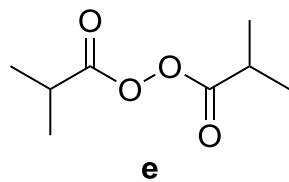
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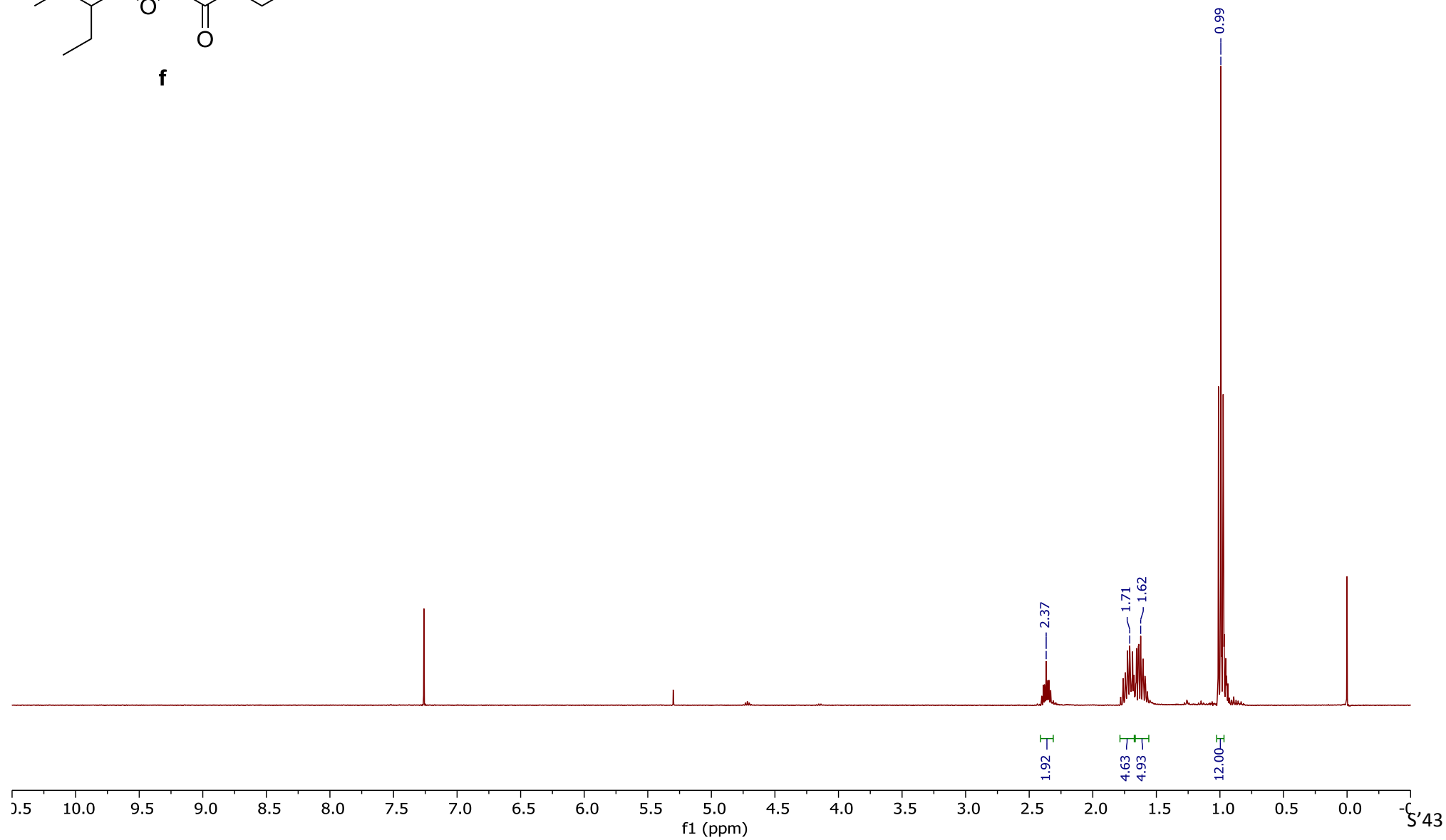
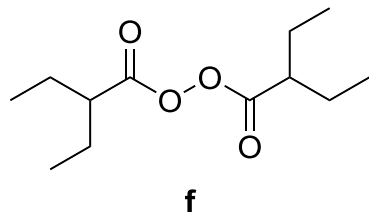
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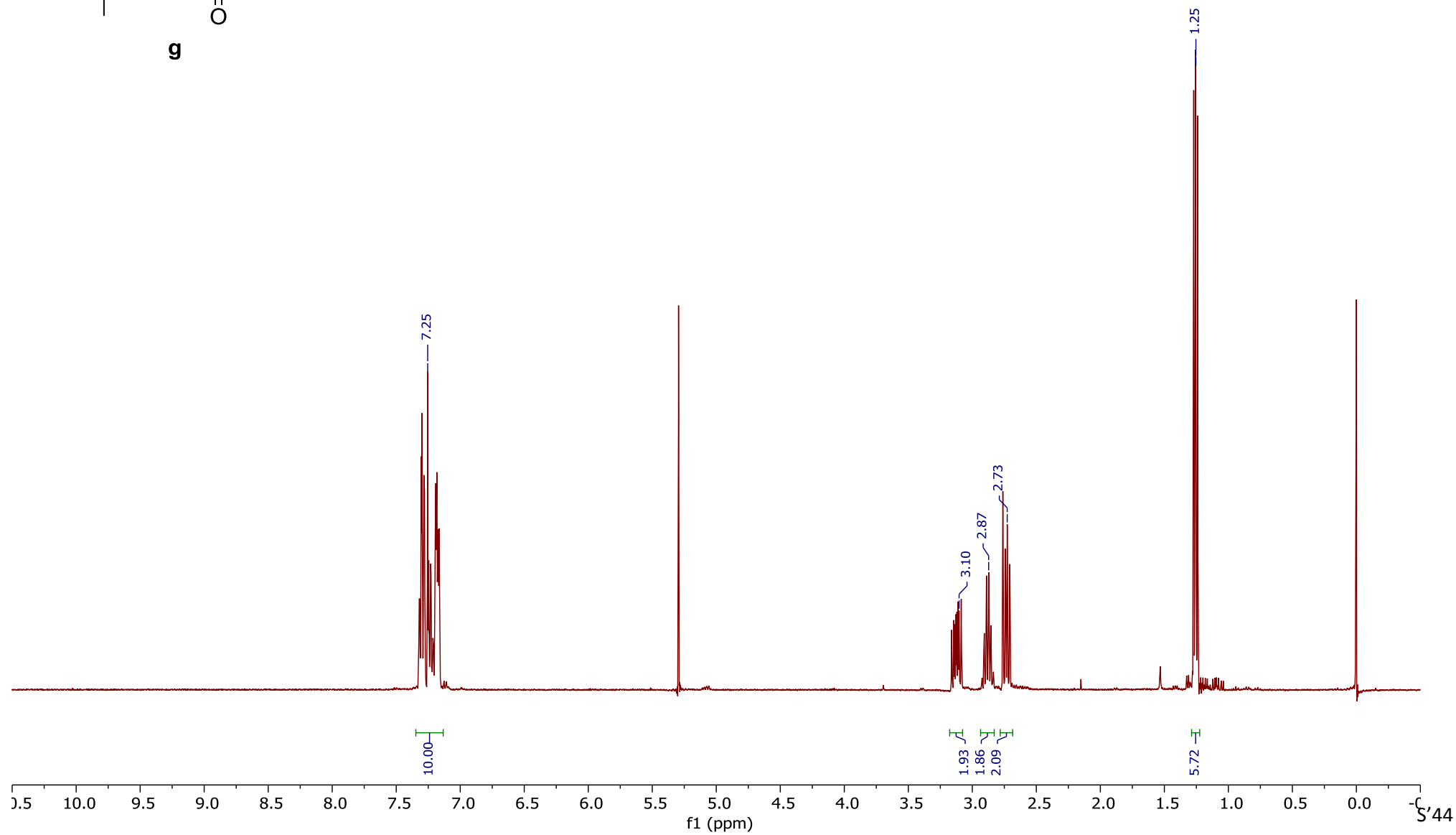
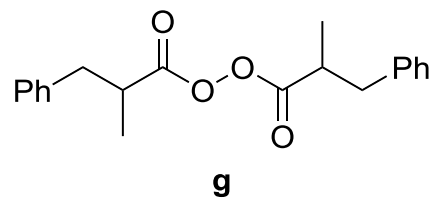
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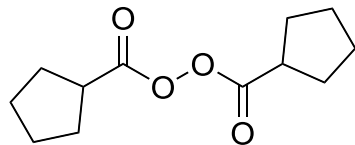
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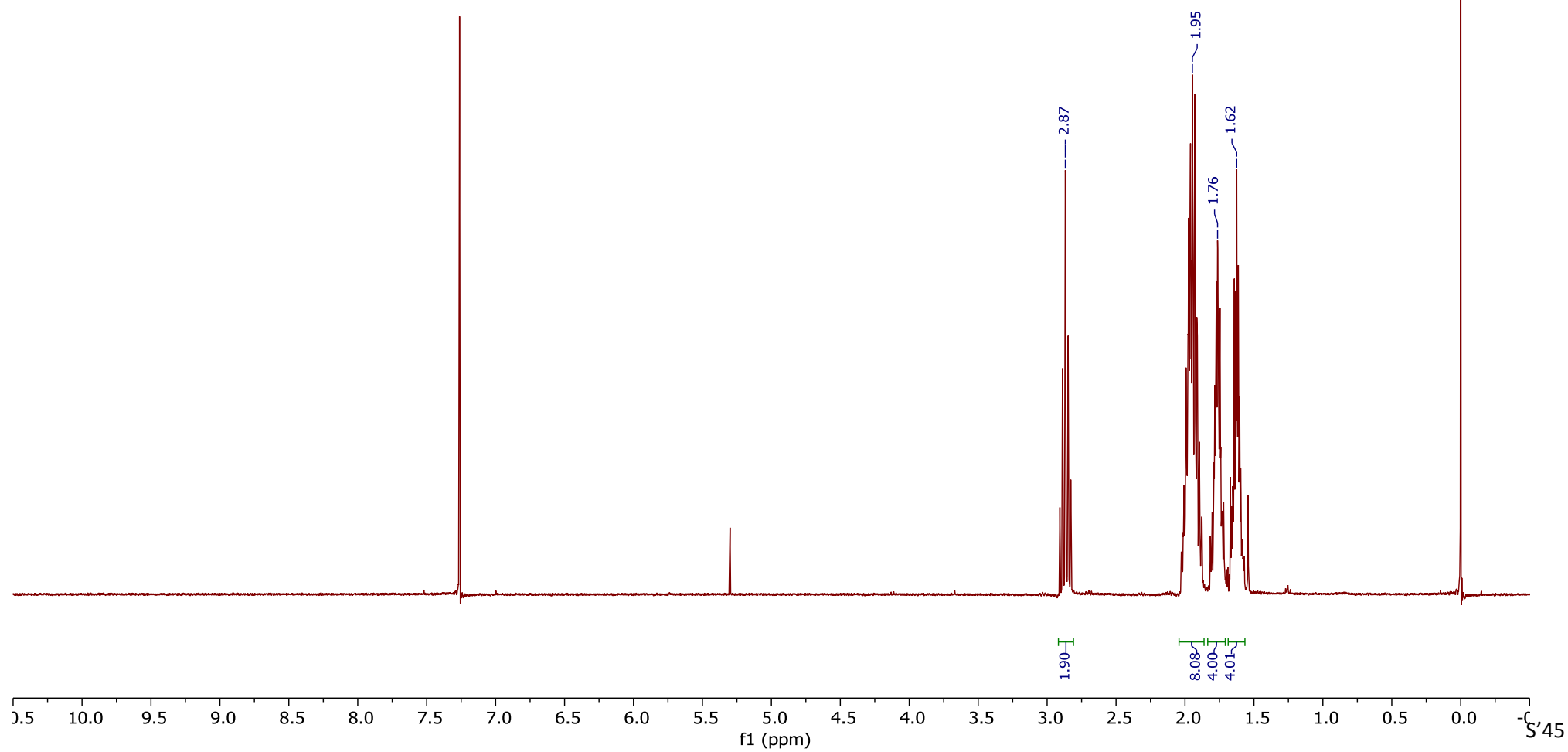
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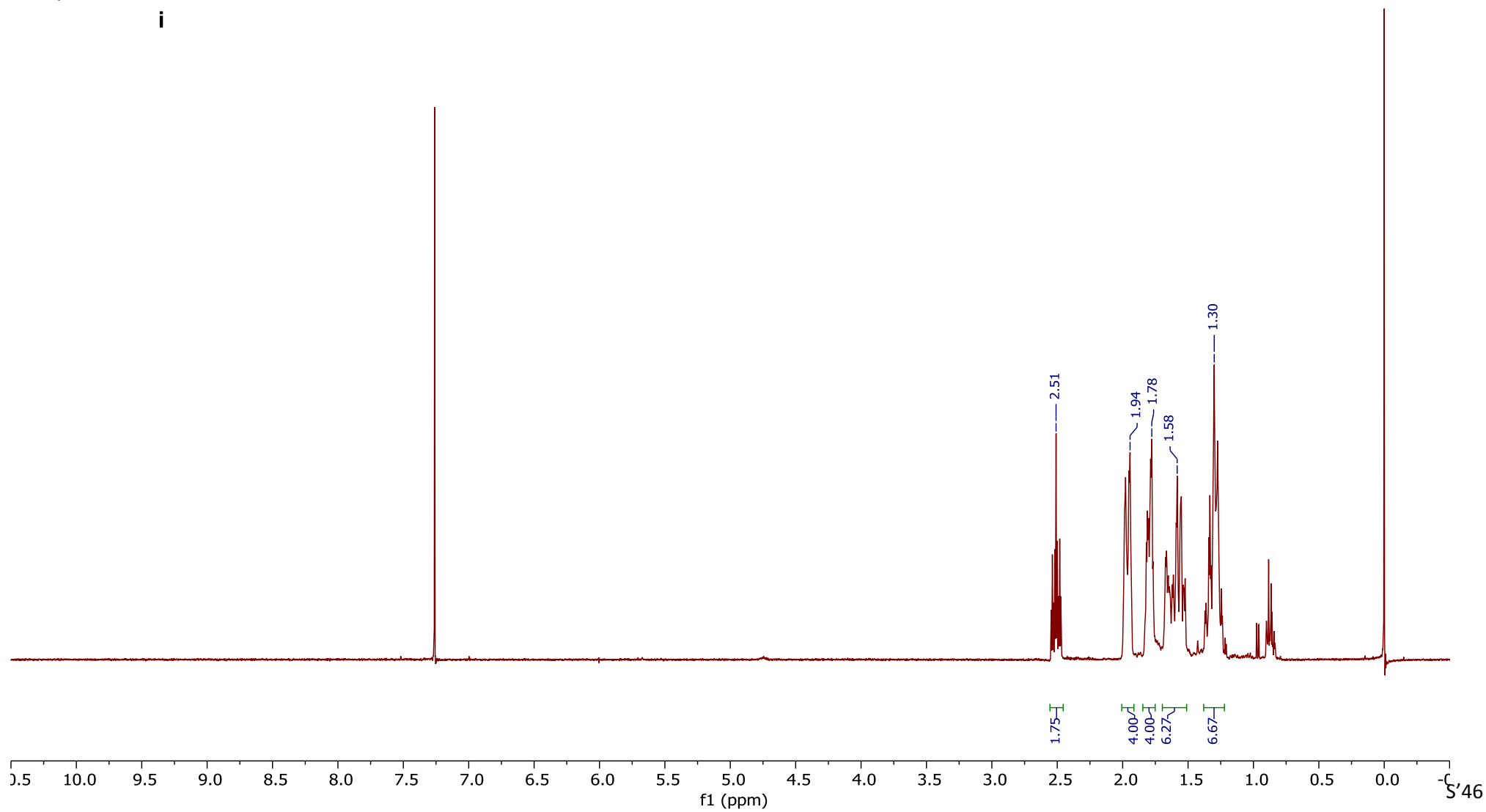
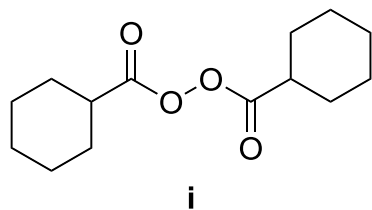
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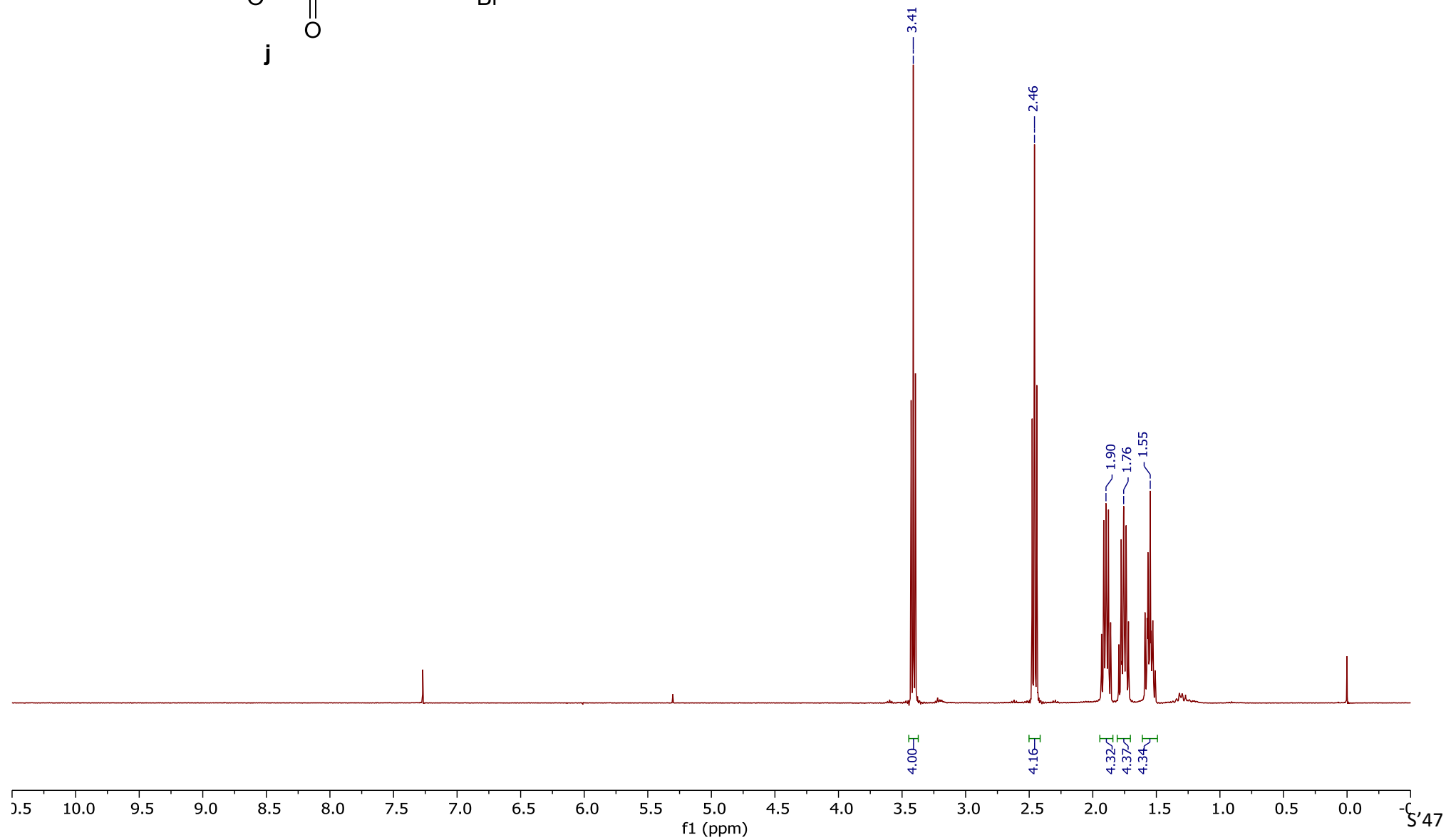
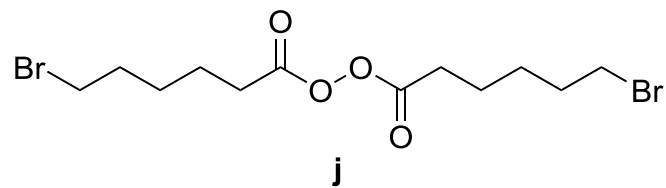
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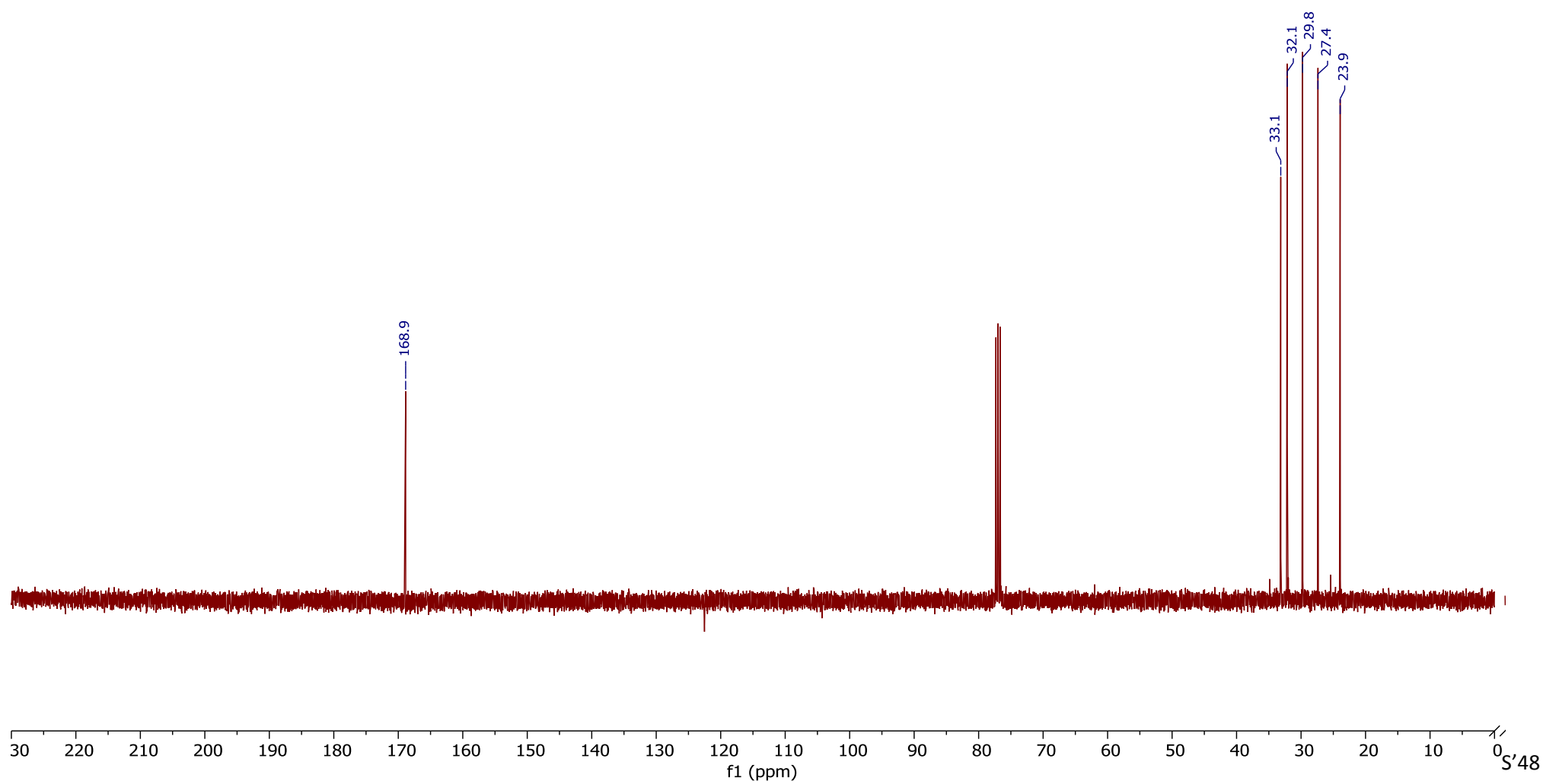
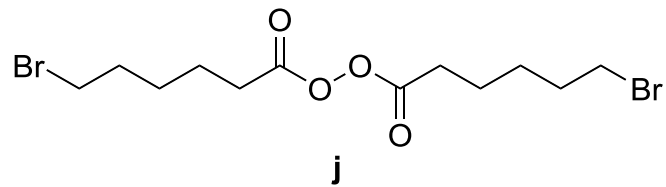
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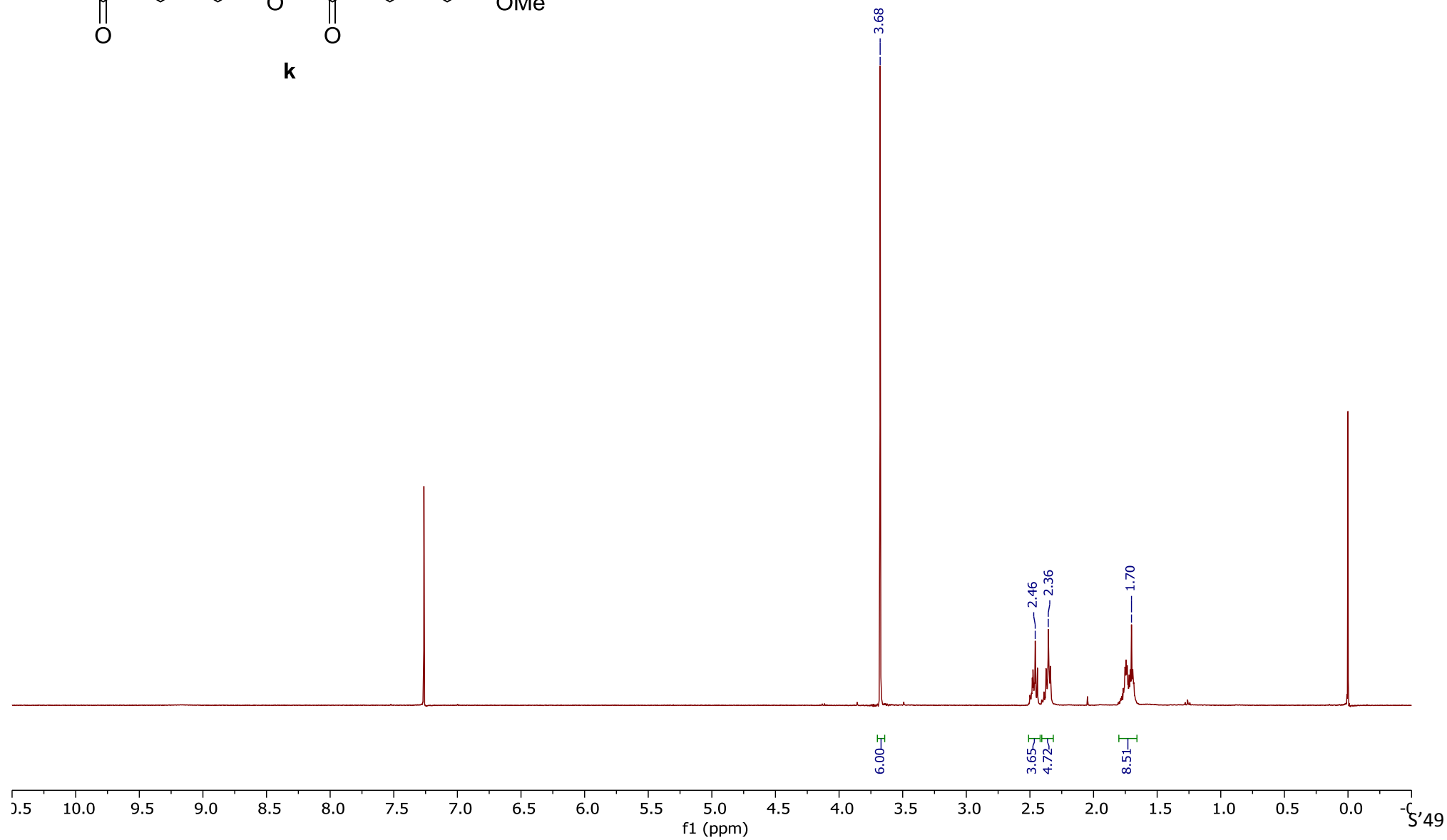
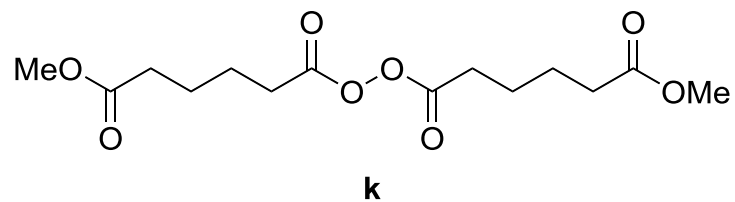
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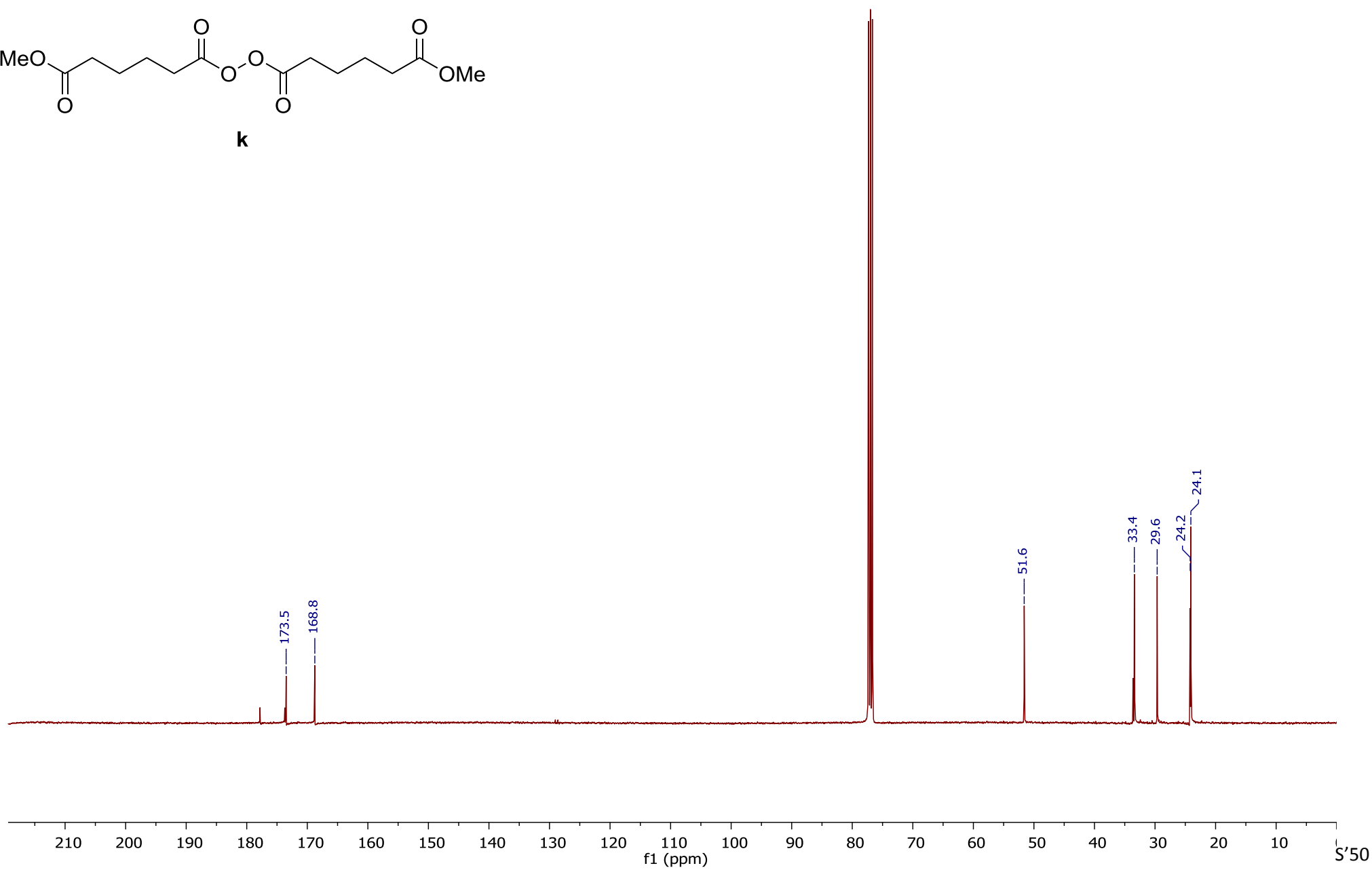
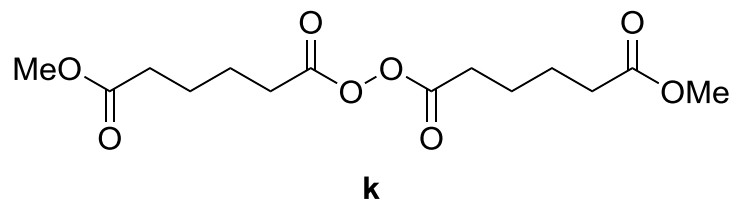
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



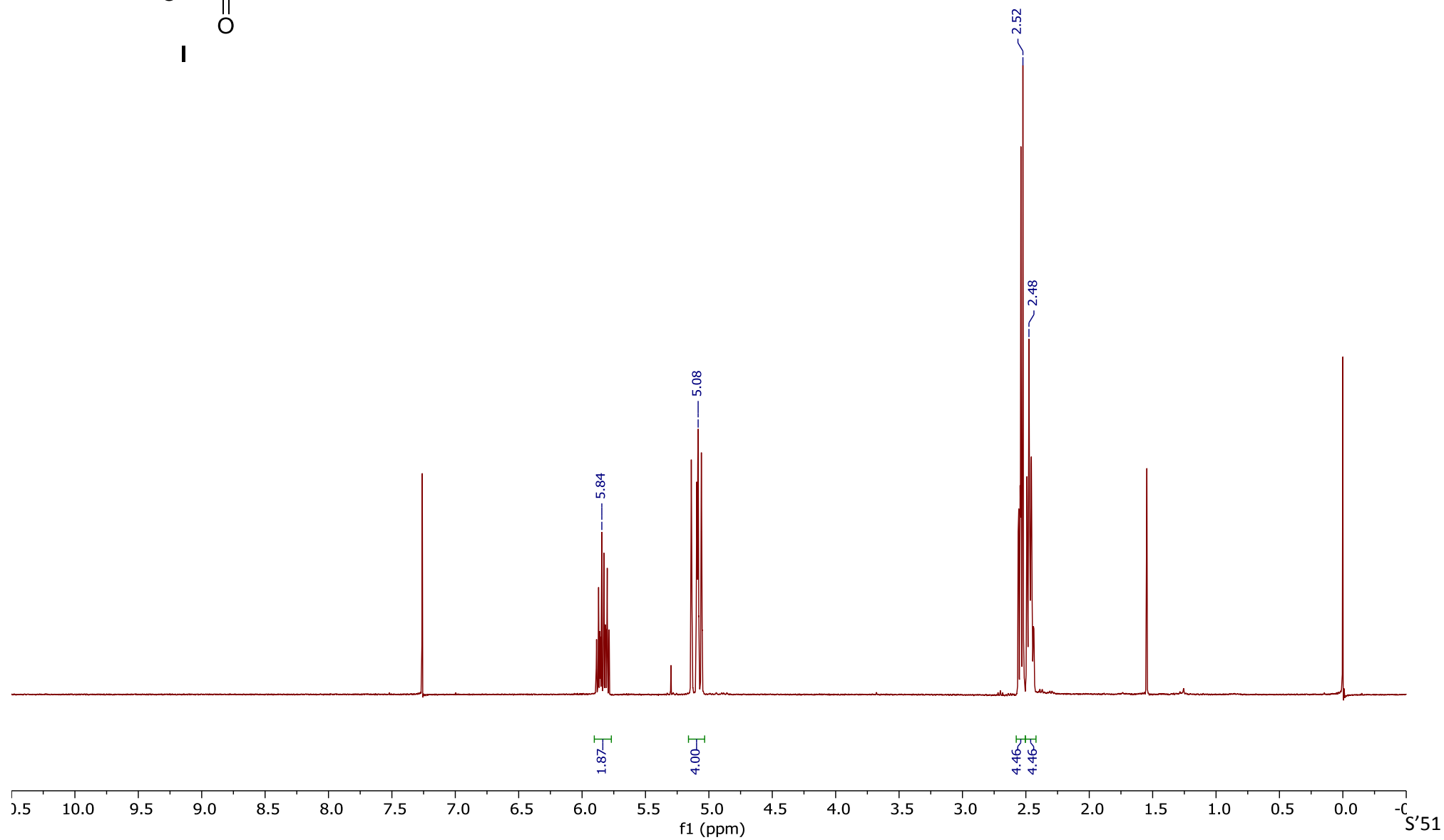
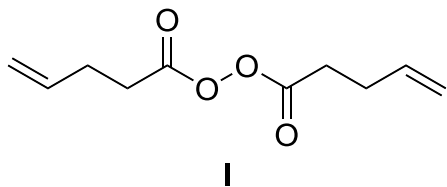
¹H NMR (400 MHz, CDCl₃)



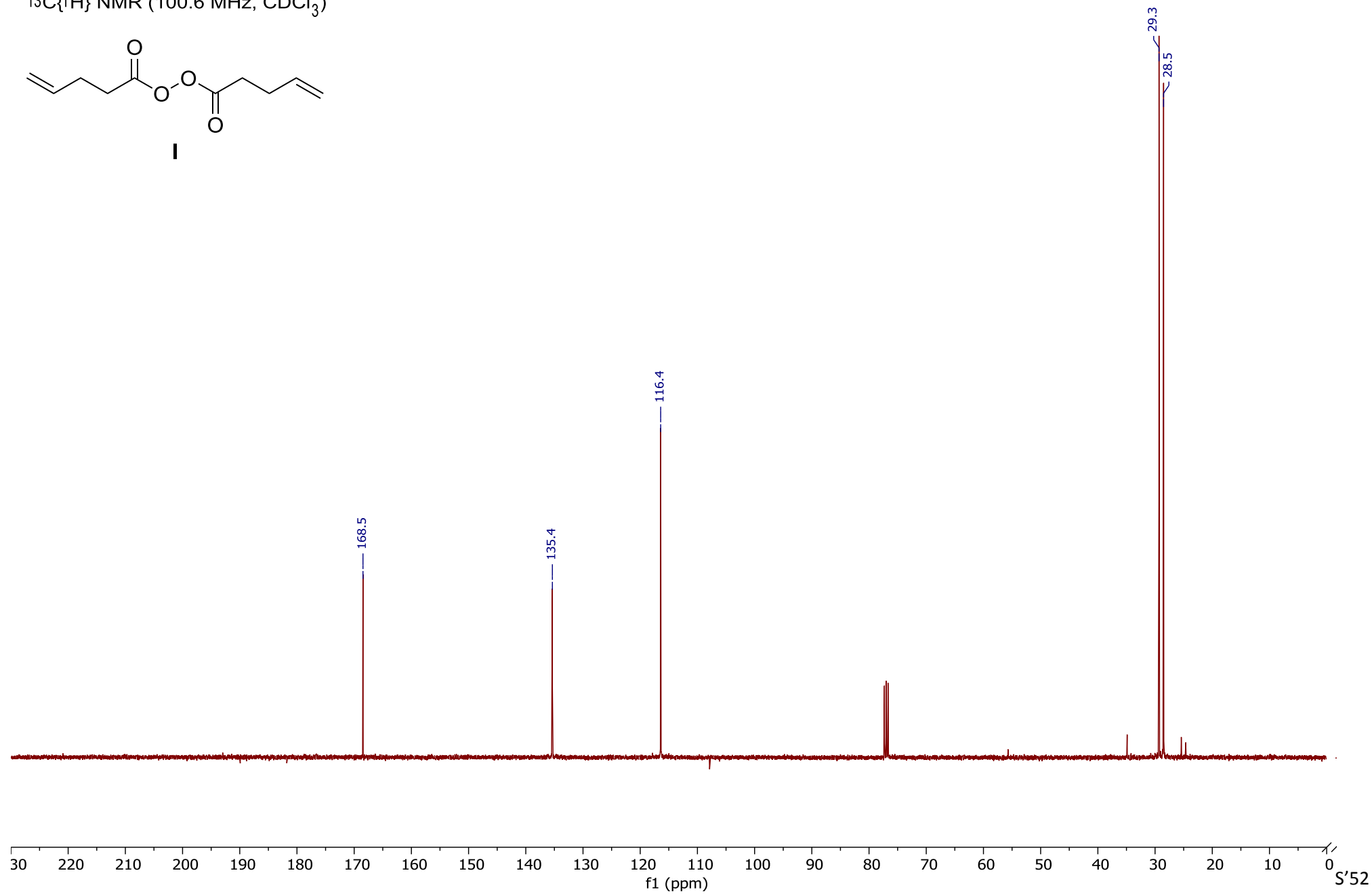
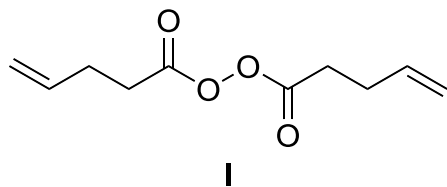
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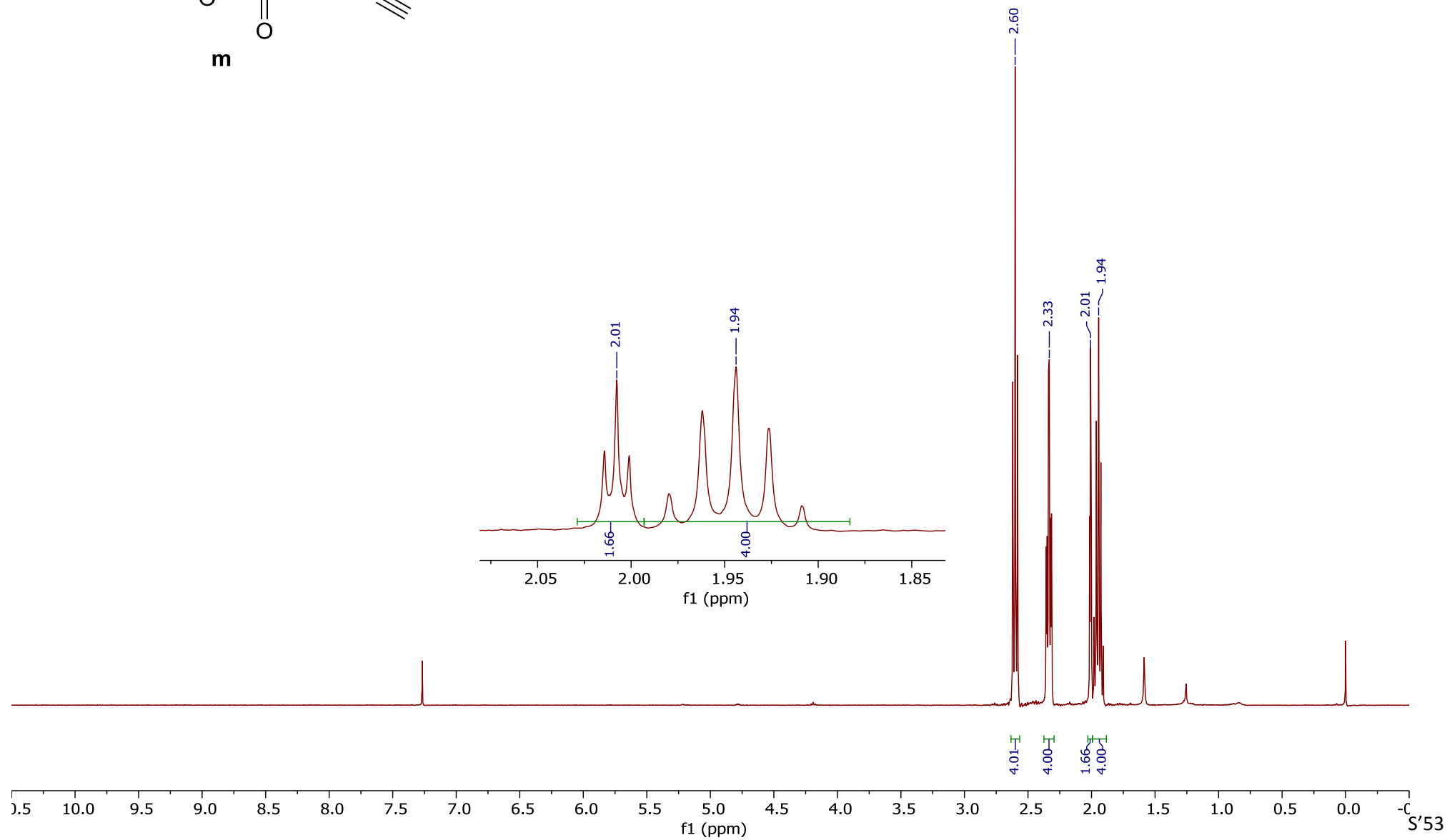
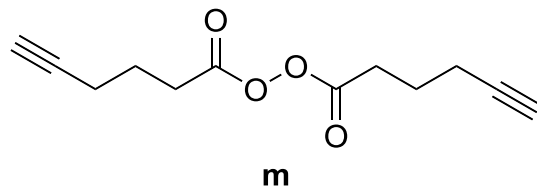
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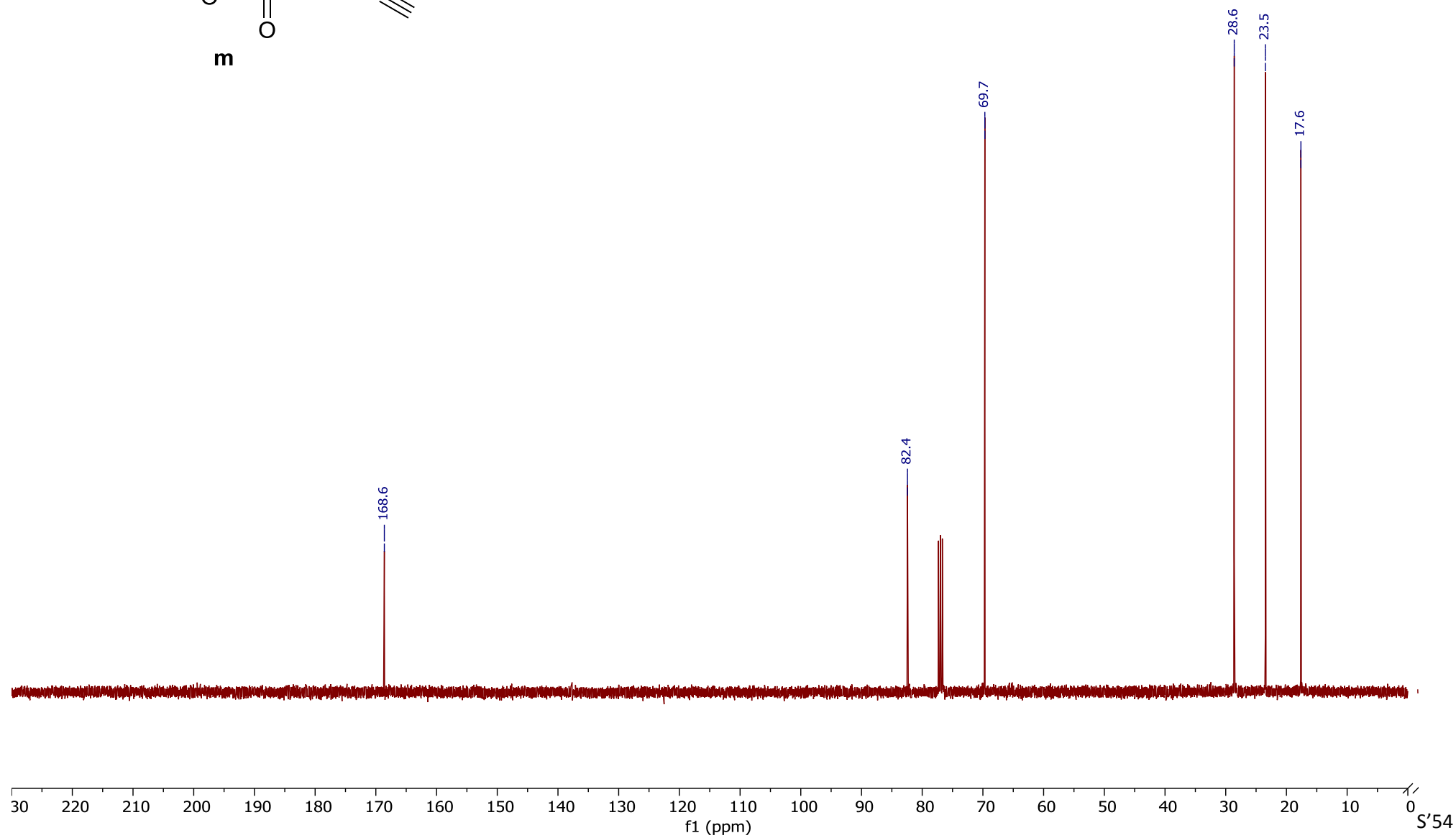
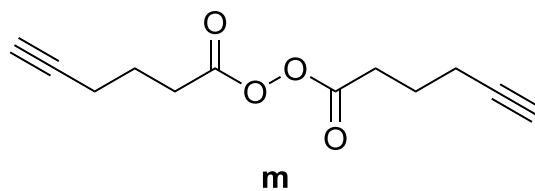
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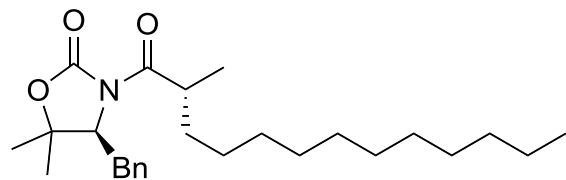
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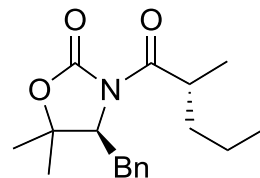
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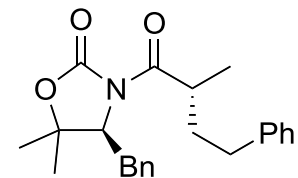
4. ALKYLATION PRODUCTS (TABLE 1)



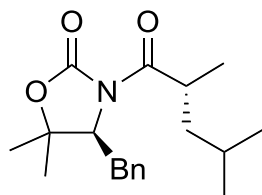
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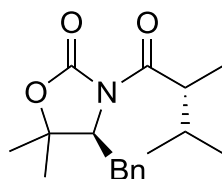
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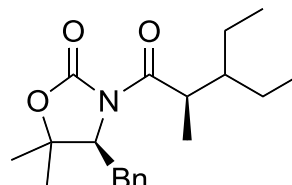
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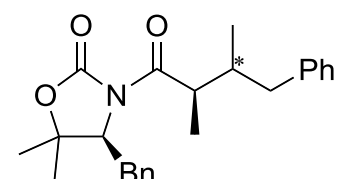
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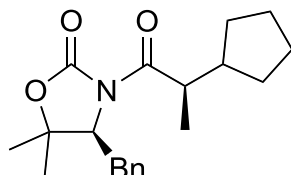
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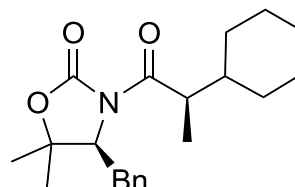
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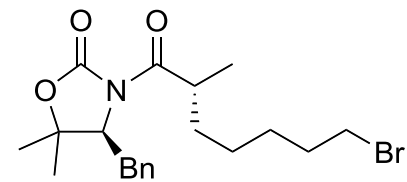
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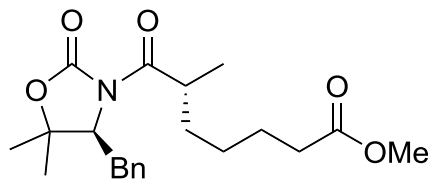
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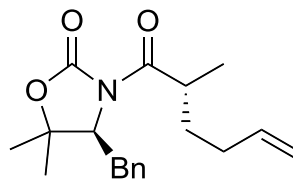
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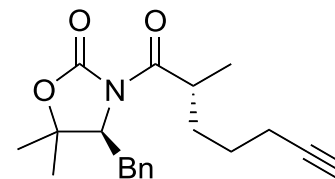
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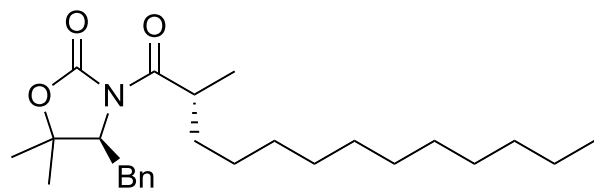


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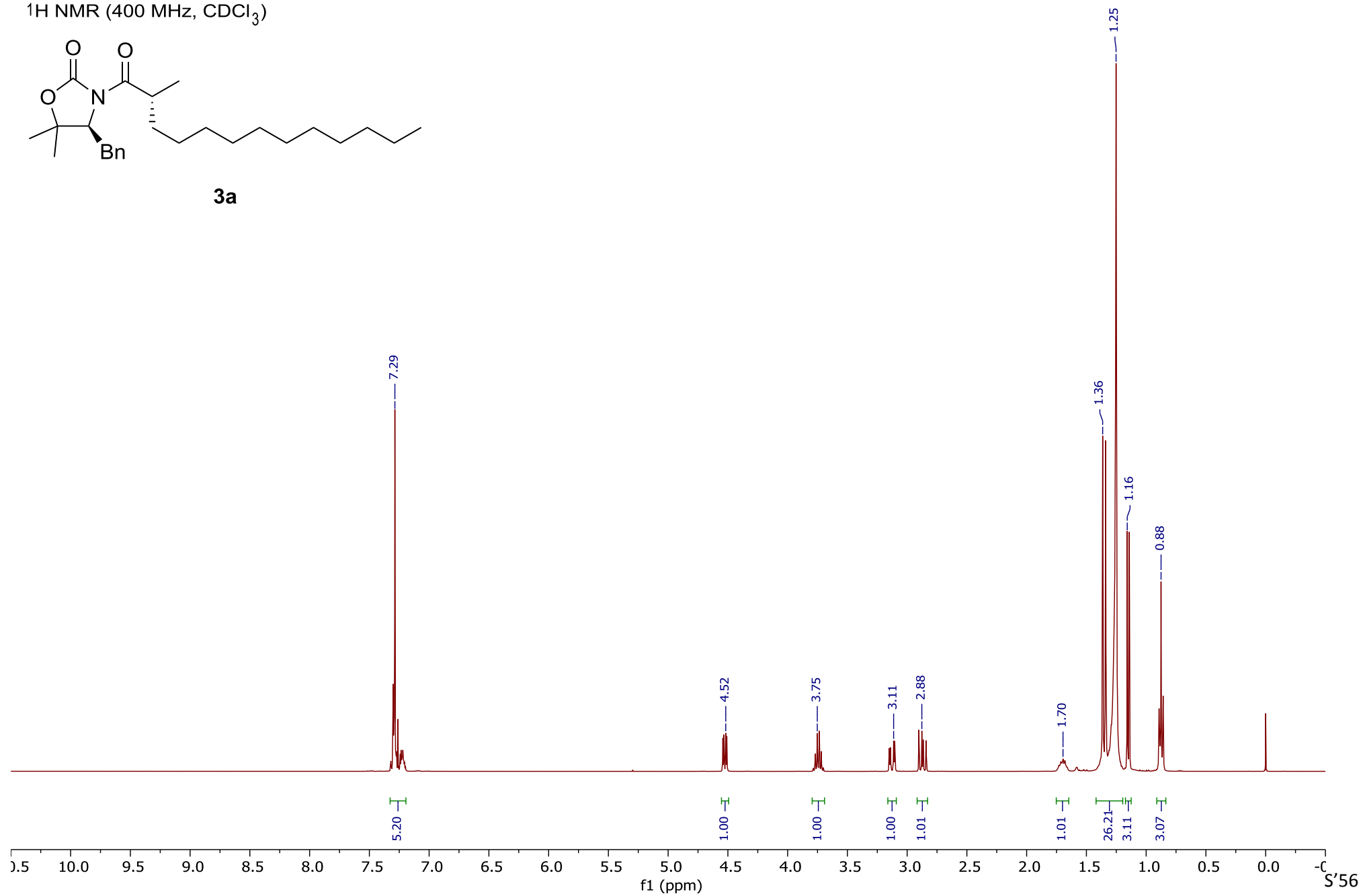


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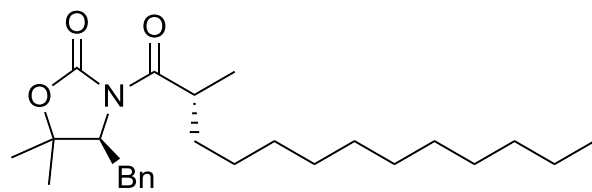
¹H NMR (400 MHz, CDCl₃)



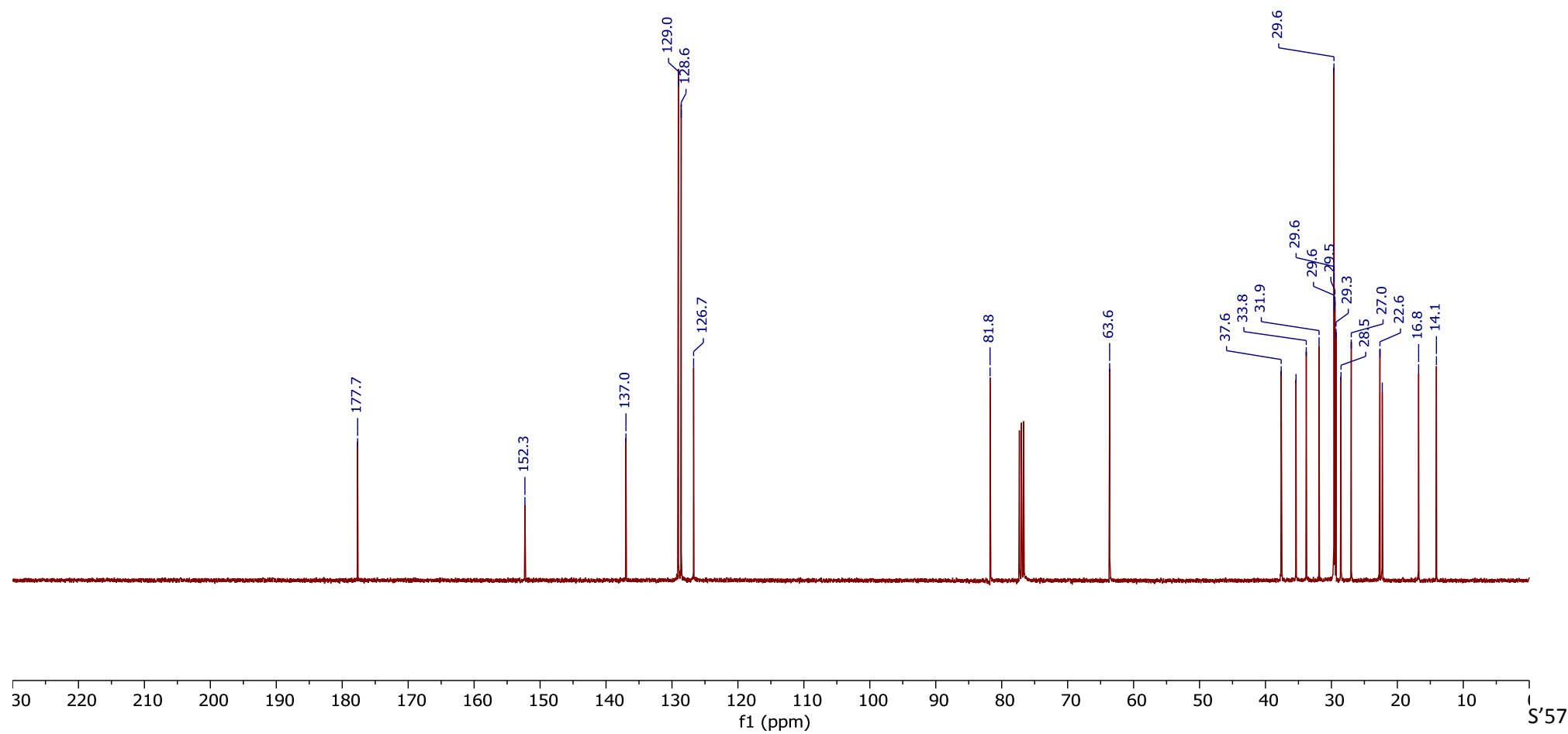
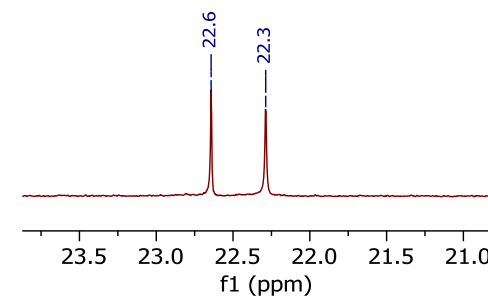
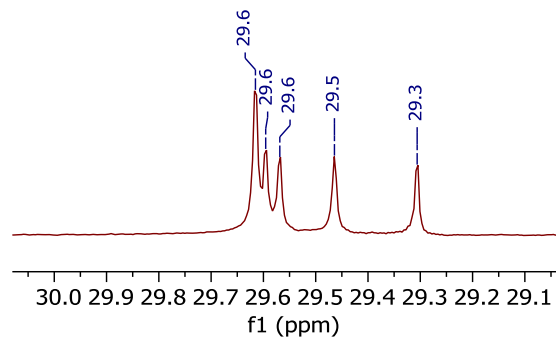
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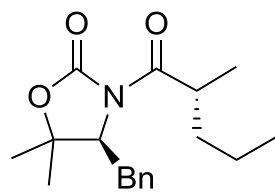
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



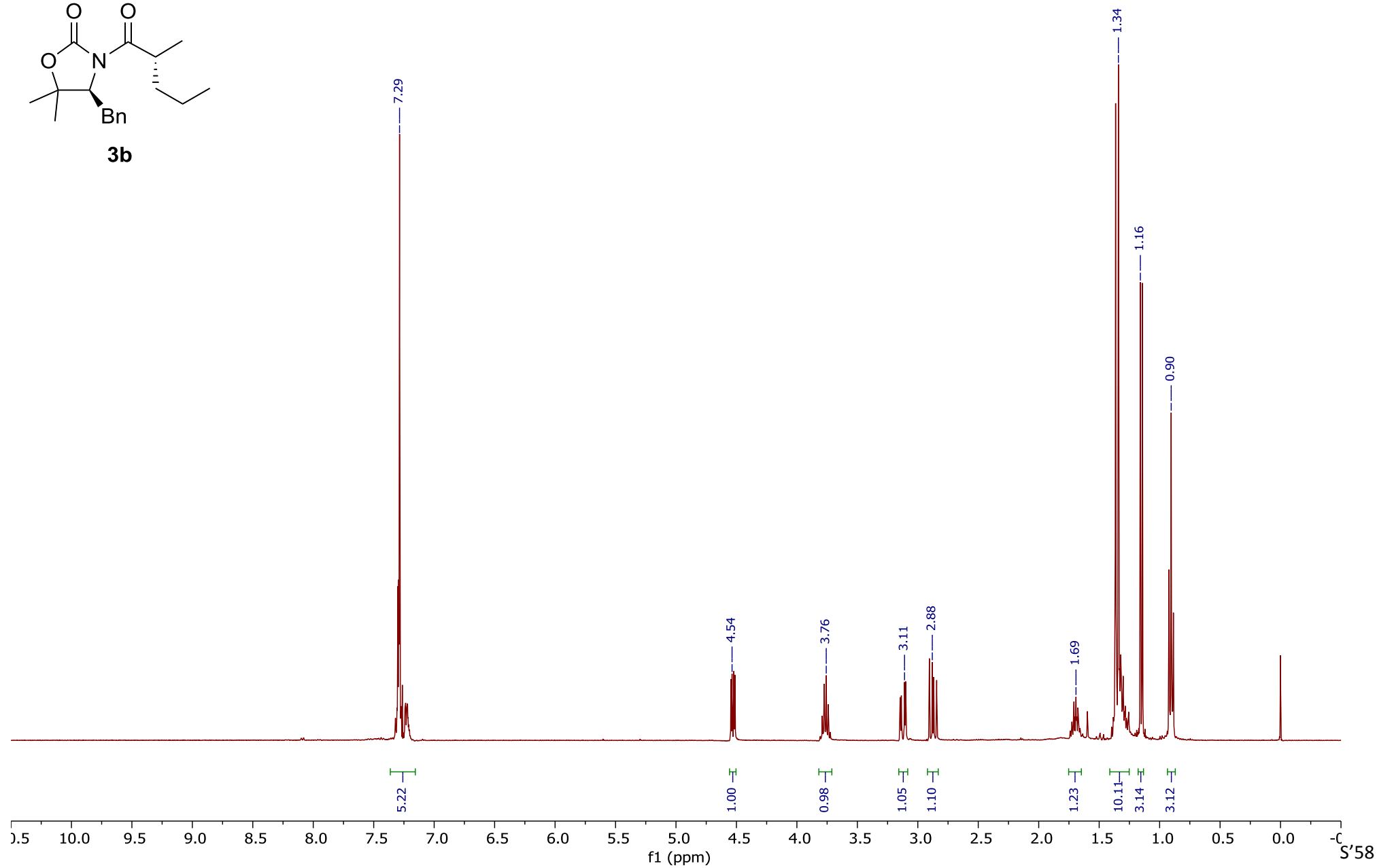
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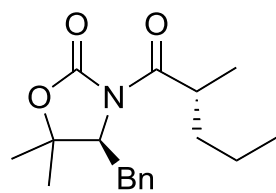
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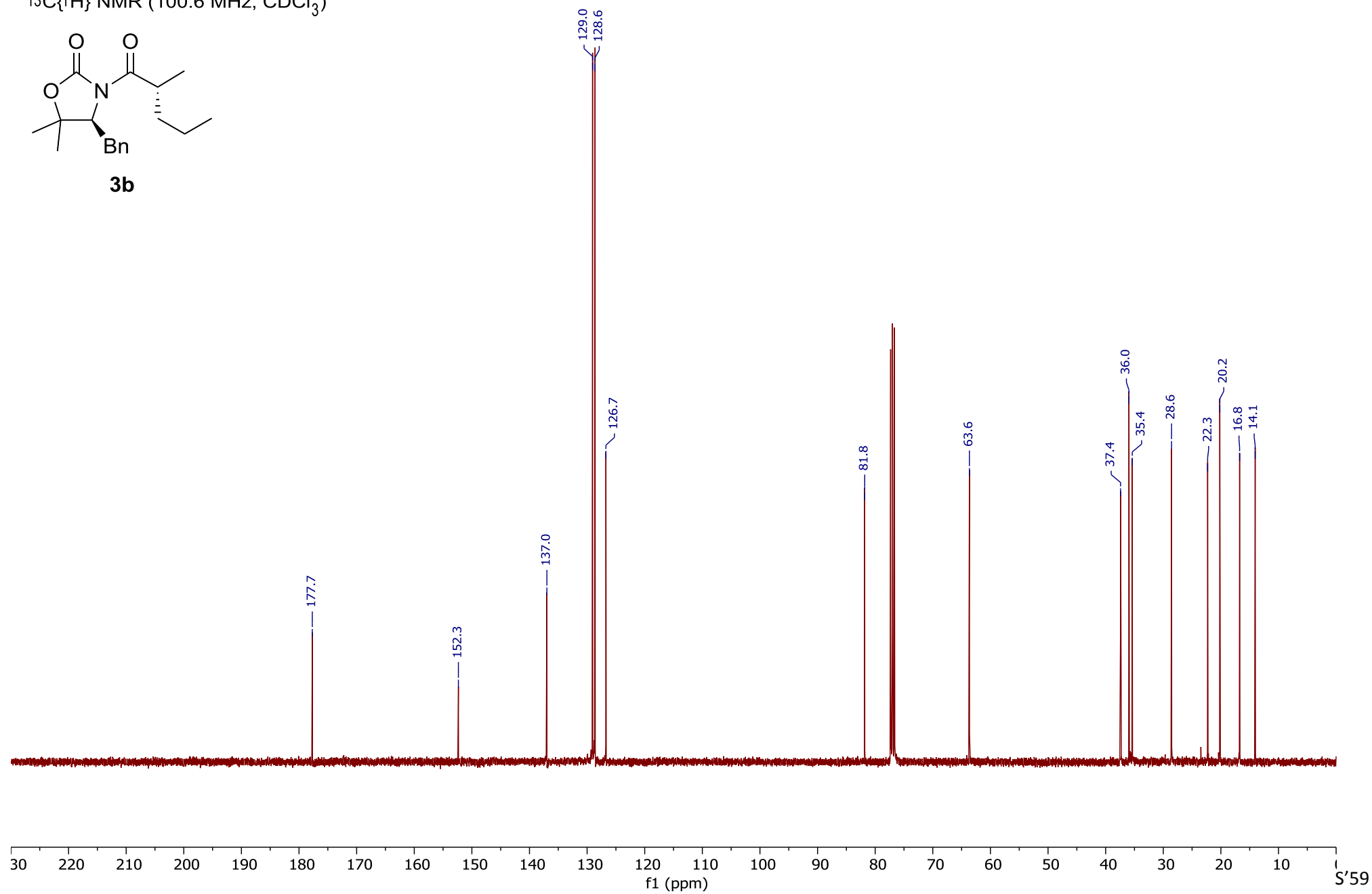
3b



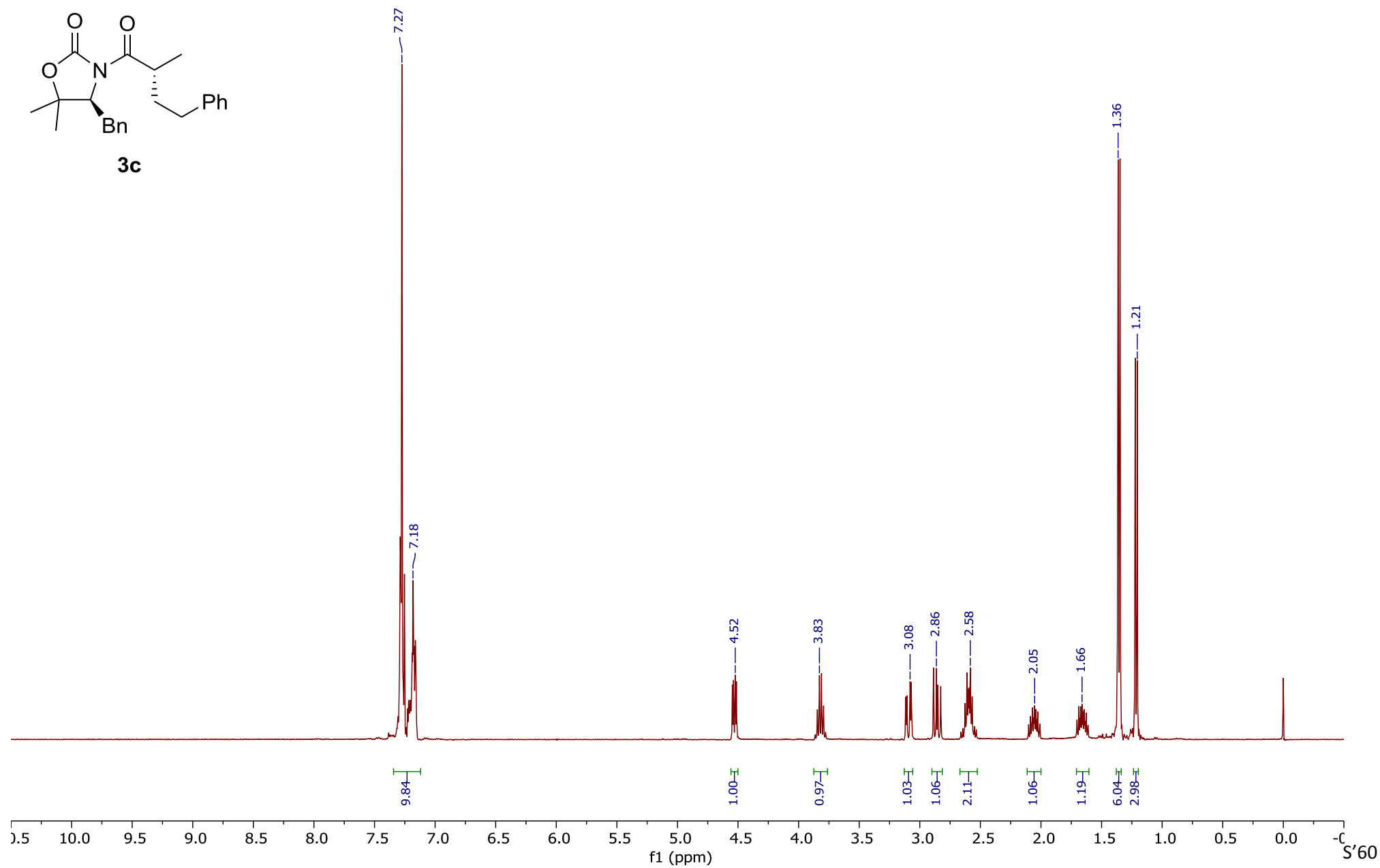
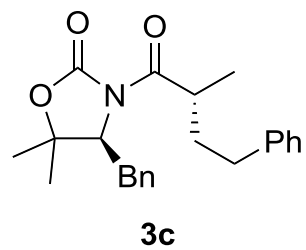
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



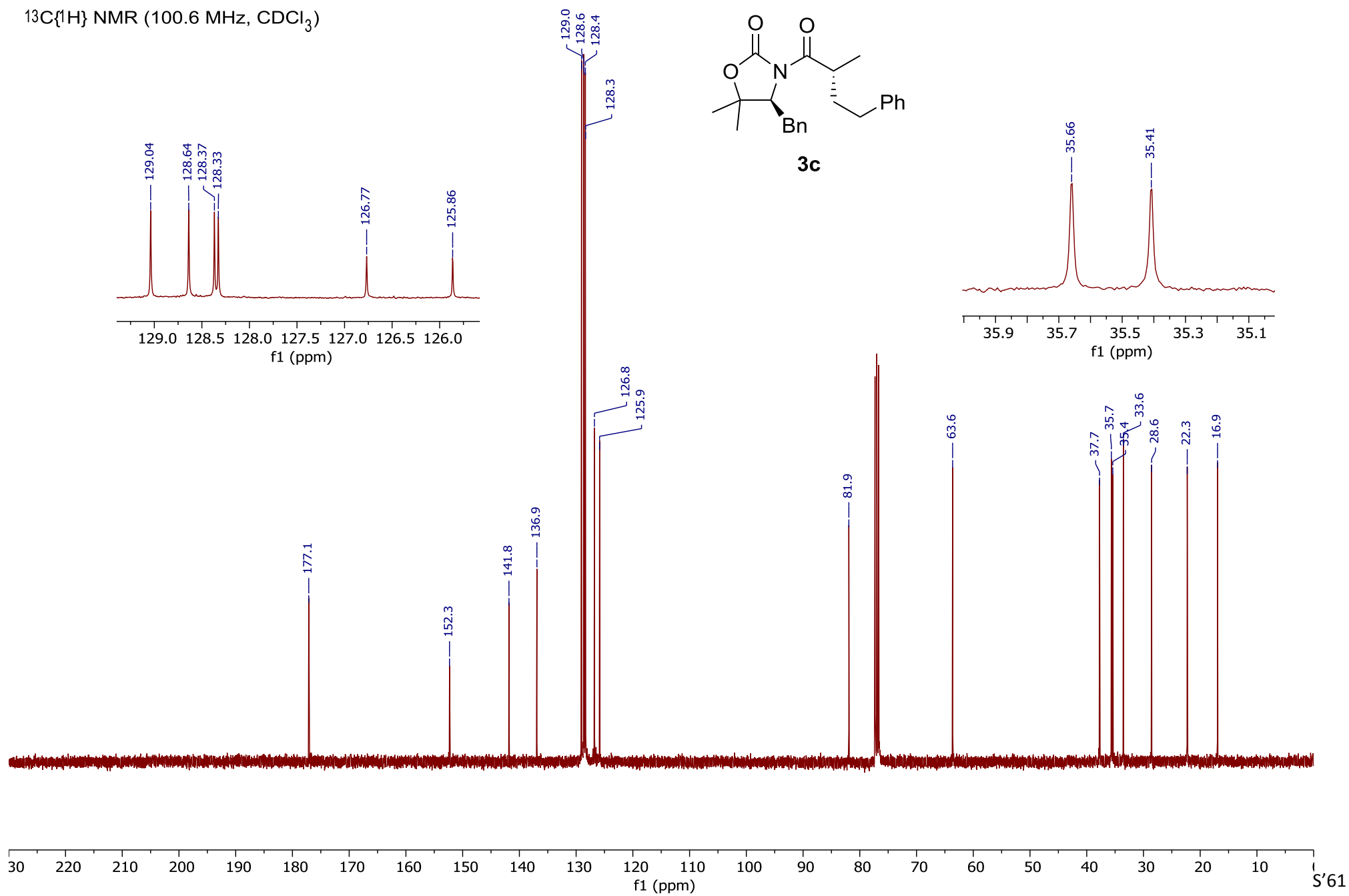
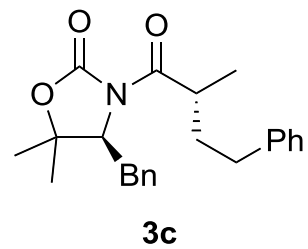
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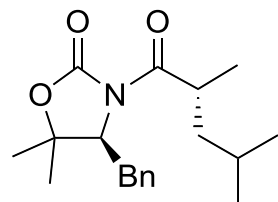
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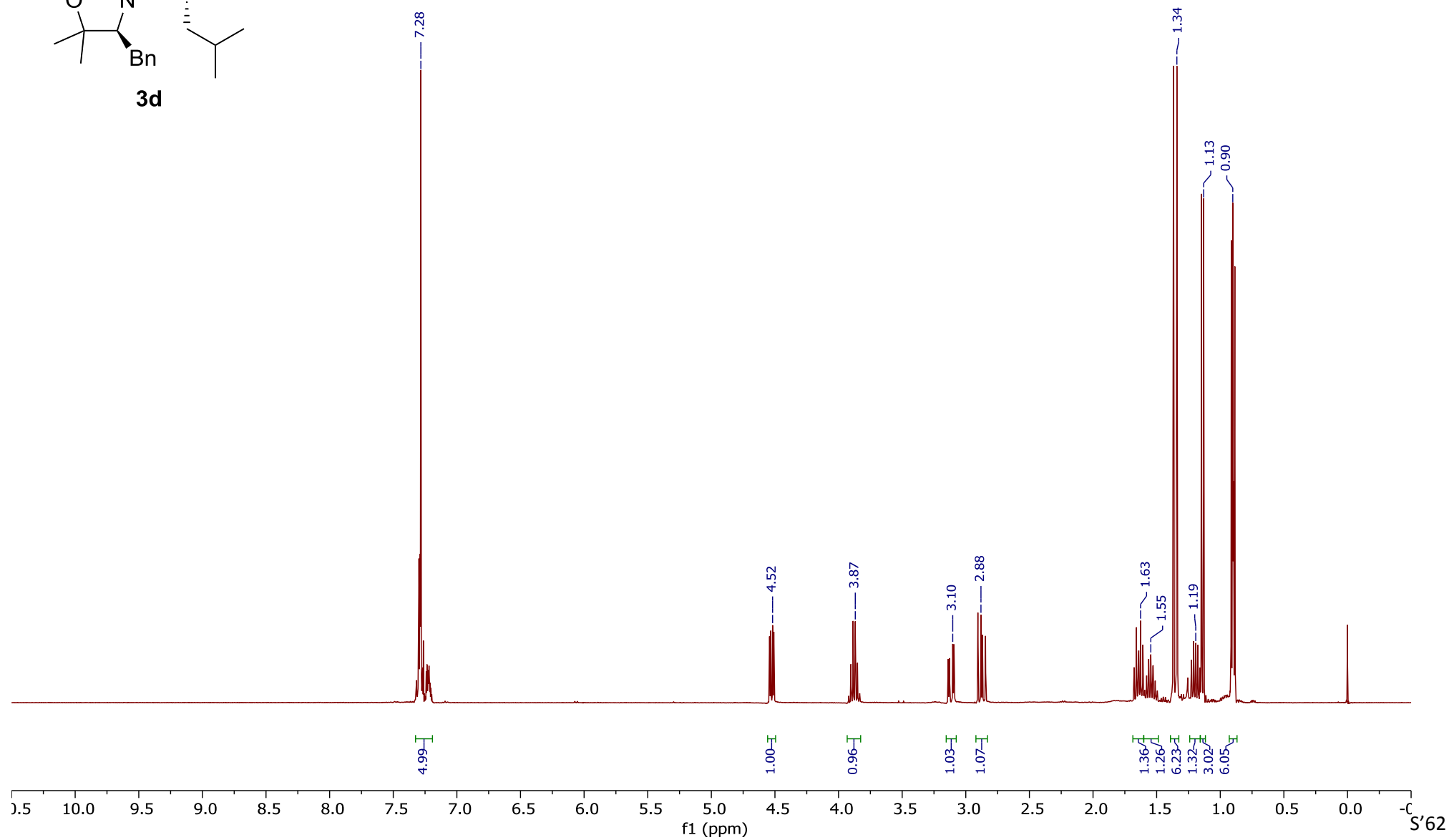
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



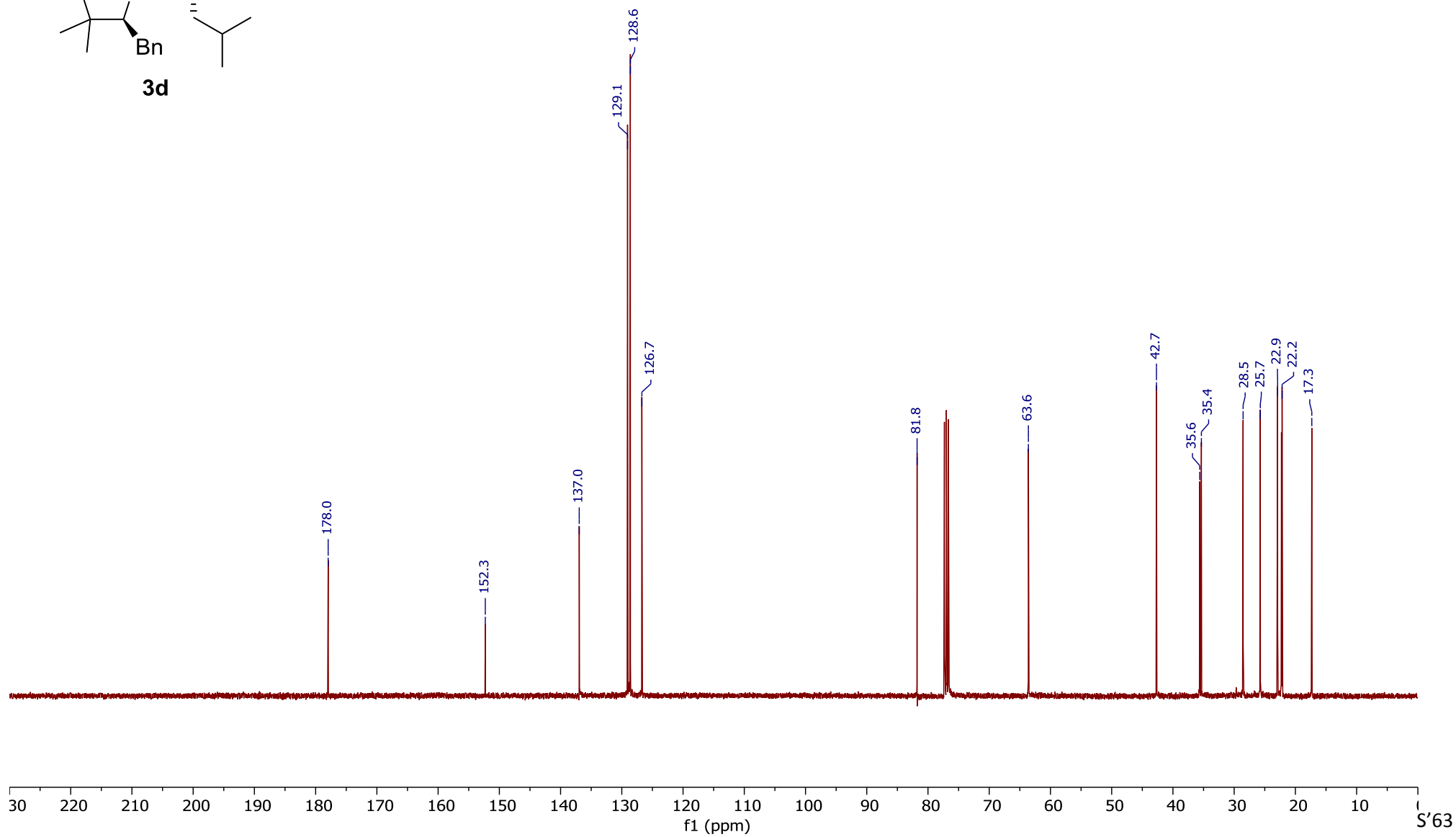
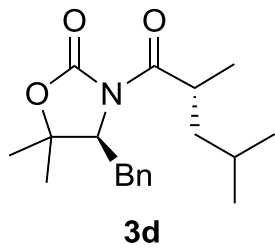
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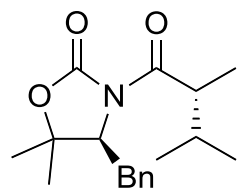
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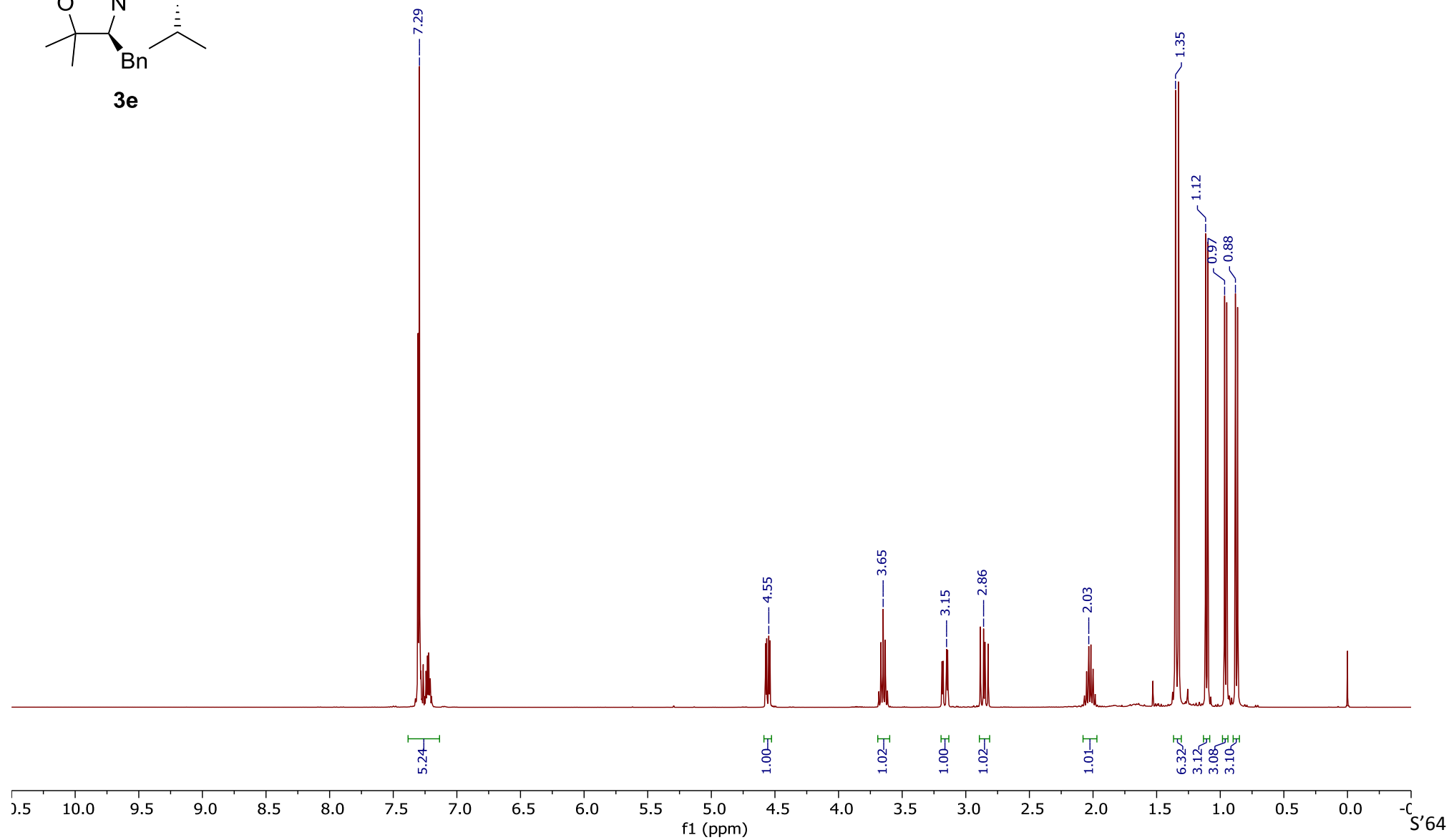
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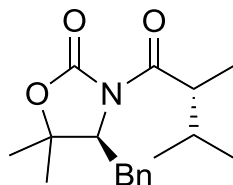
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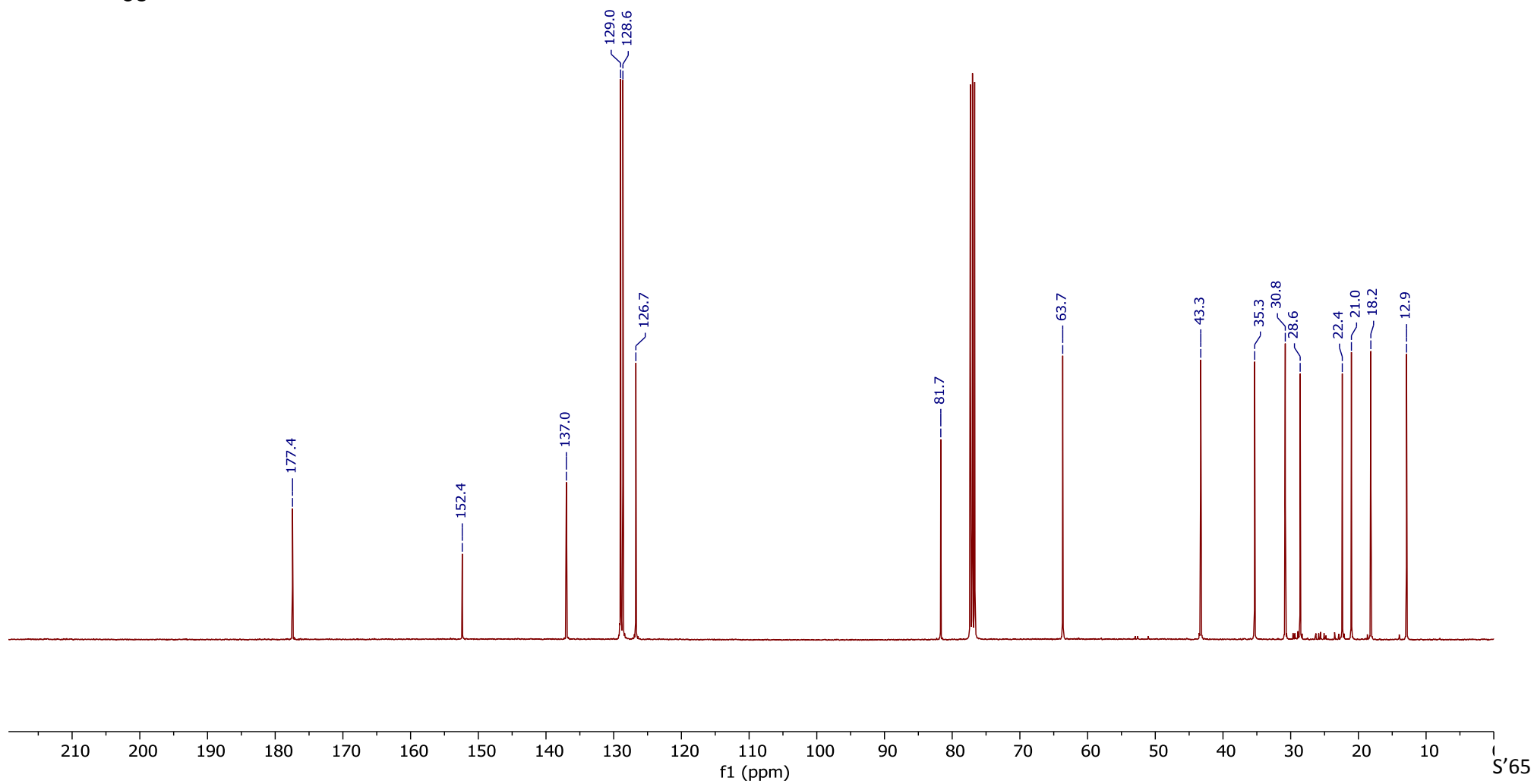
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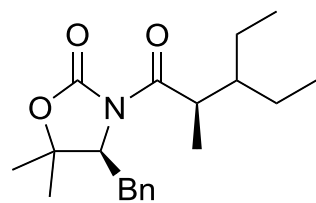
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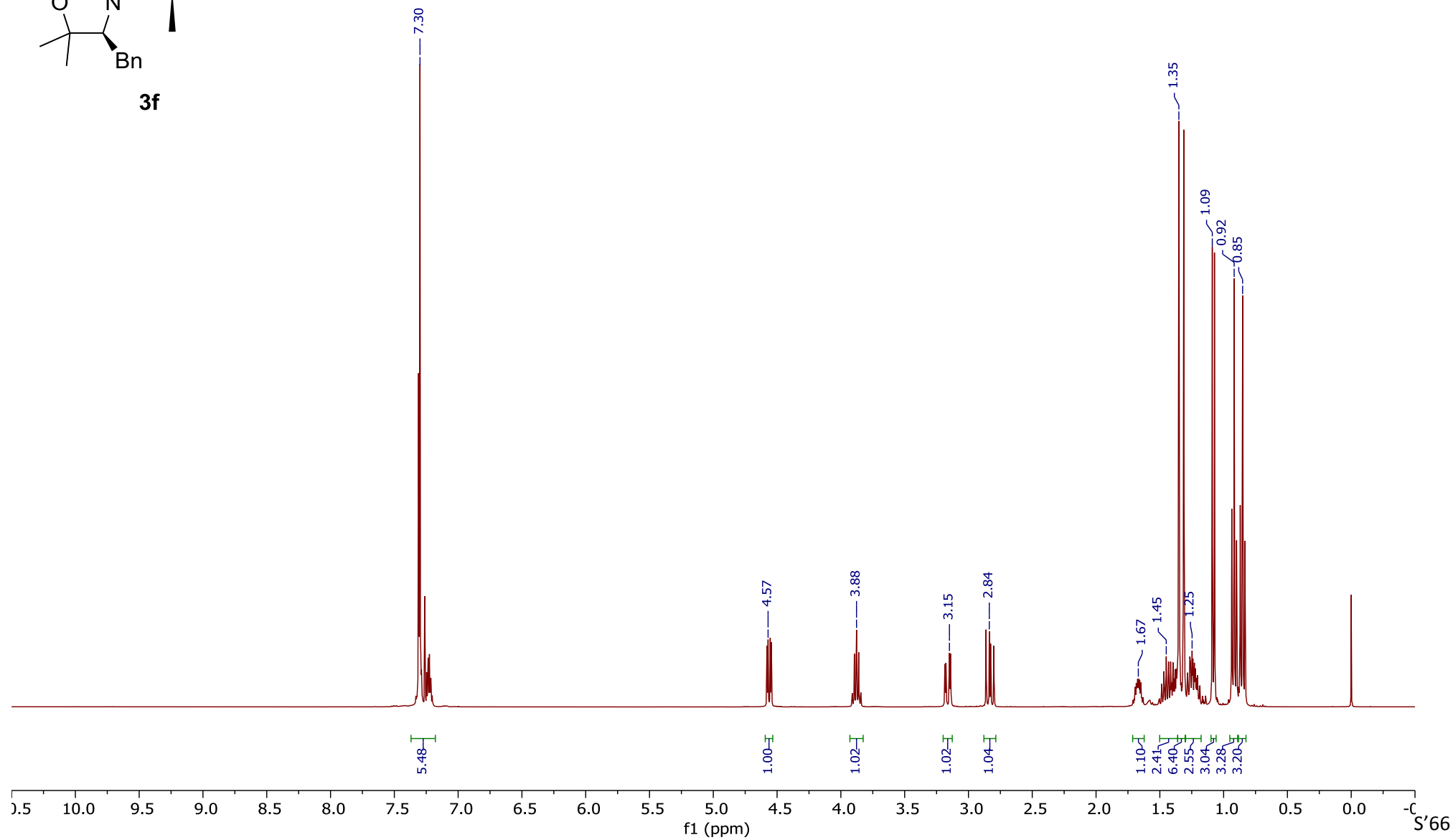
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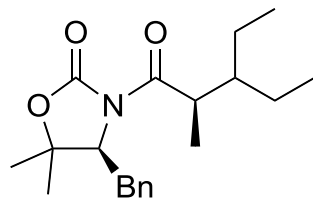
¹H NMR (400 MHz, CDCl₃)



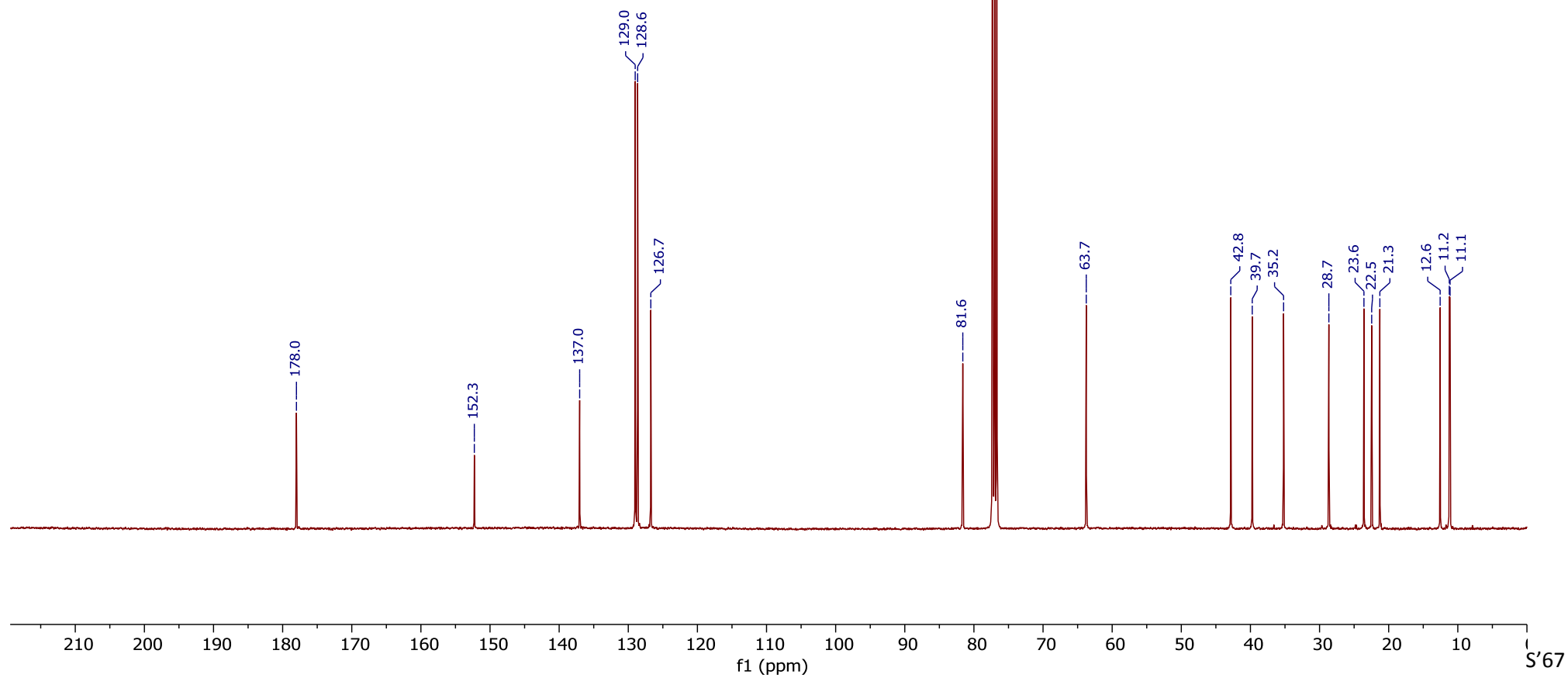
3f



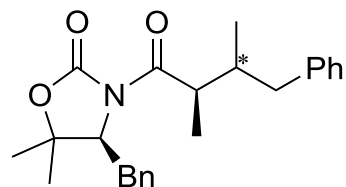
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



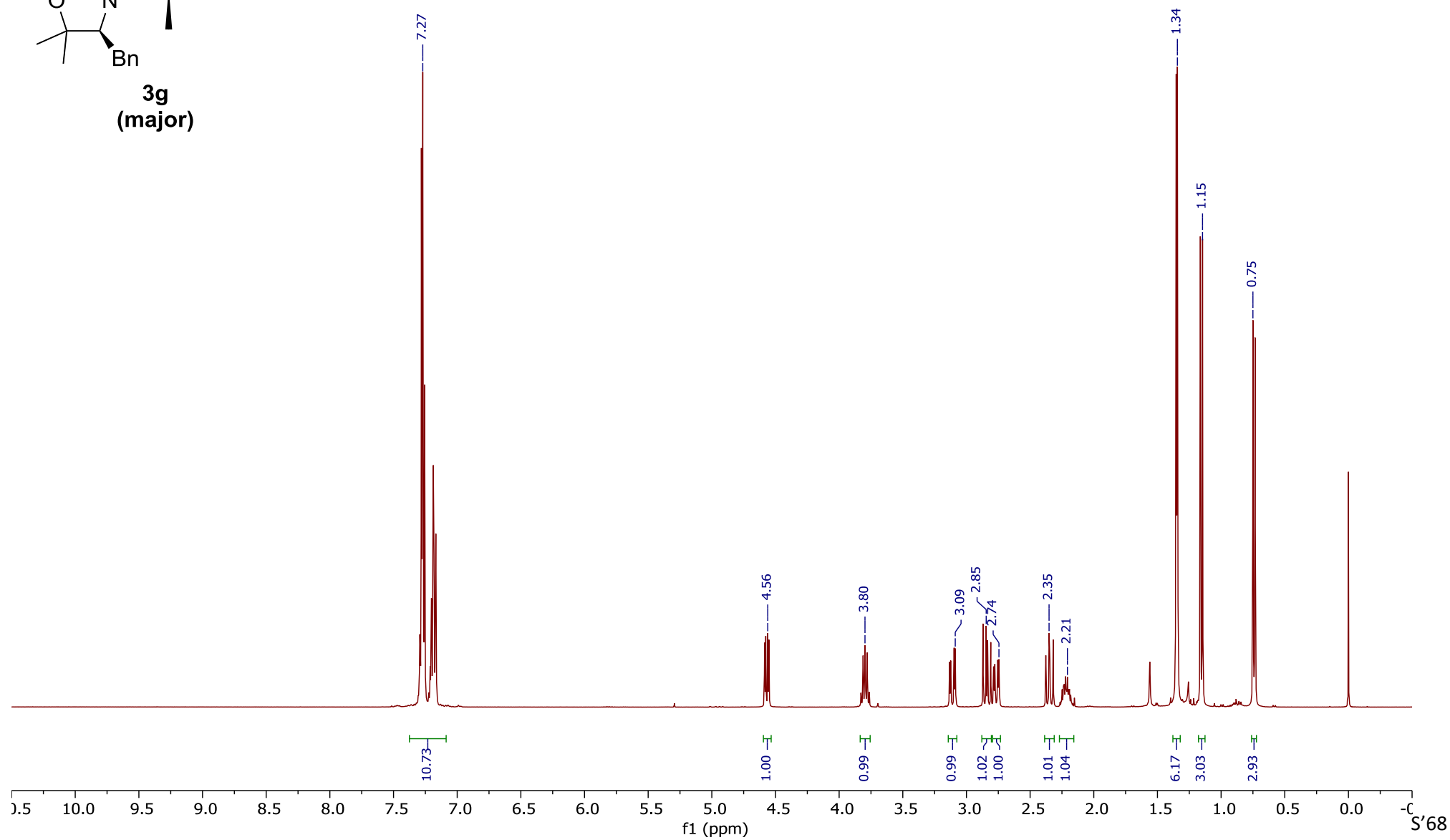
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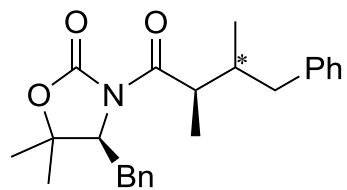
¹H NMR (400 MHz, CDCl₃)



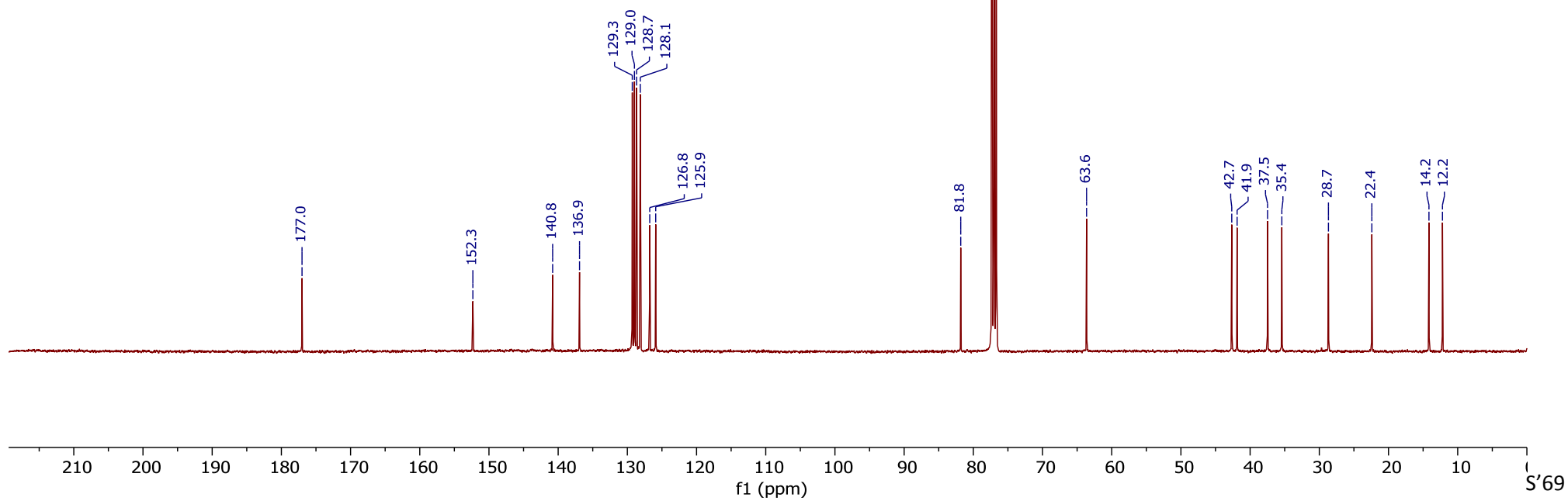
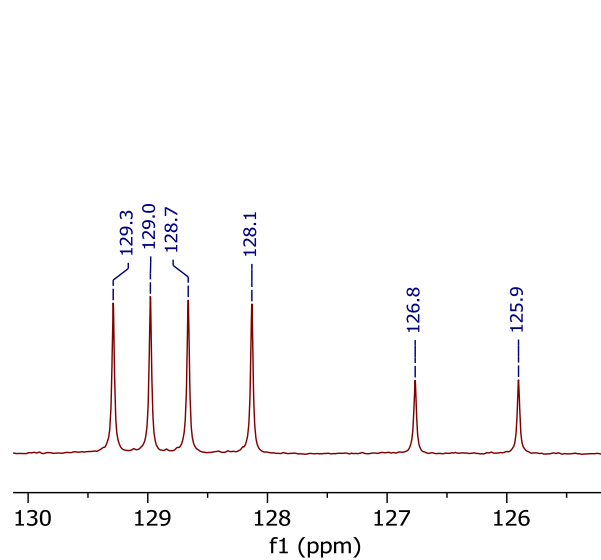
3g
(major)



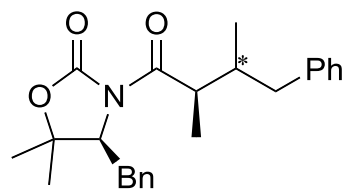
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



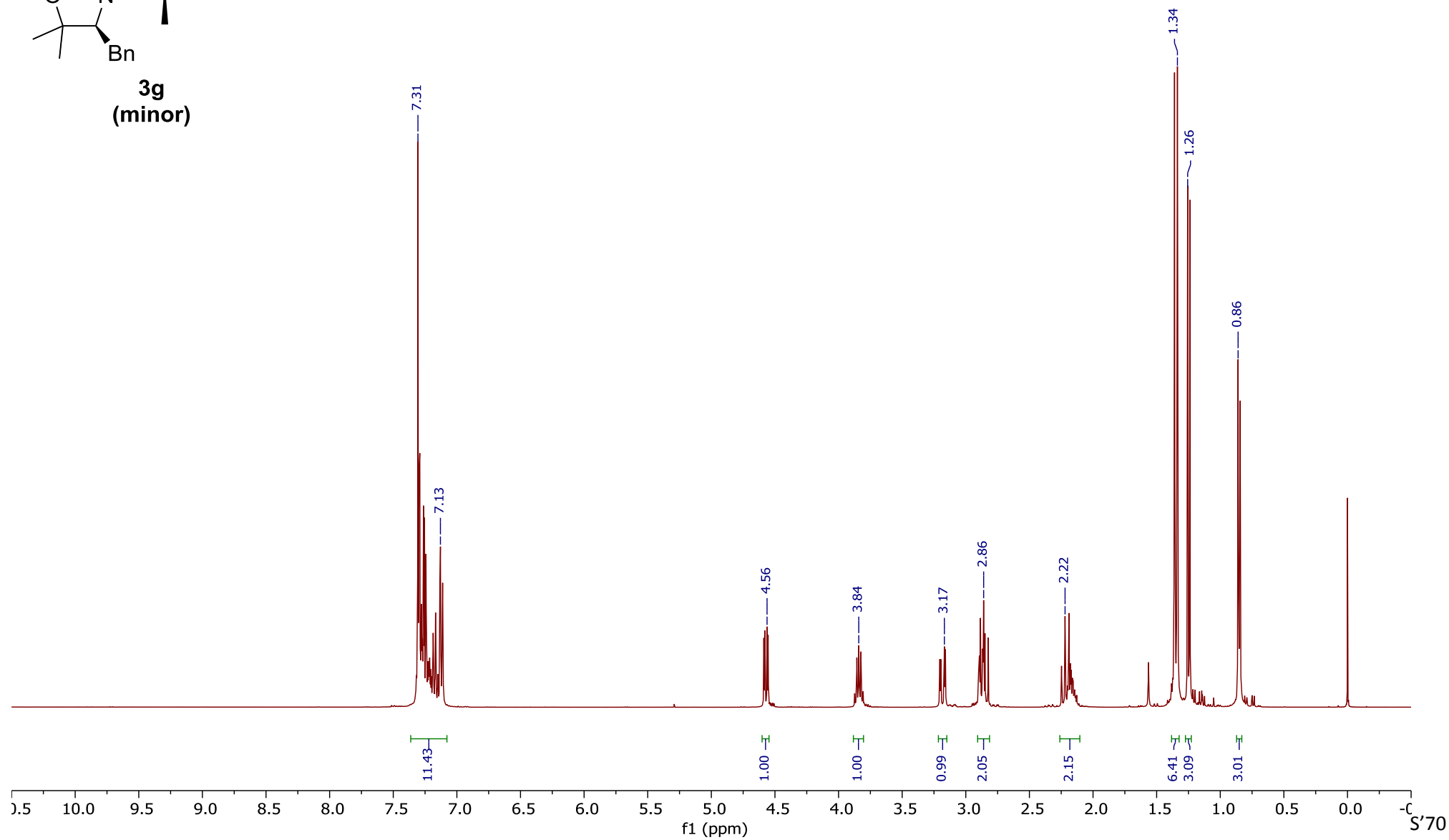
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(major)



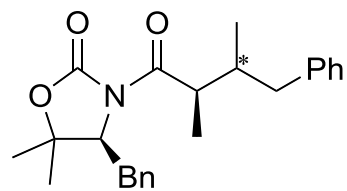
¹H NMR (400 MHz, CDCl₃)



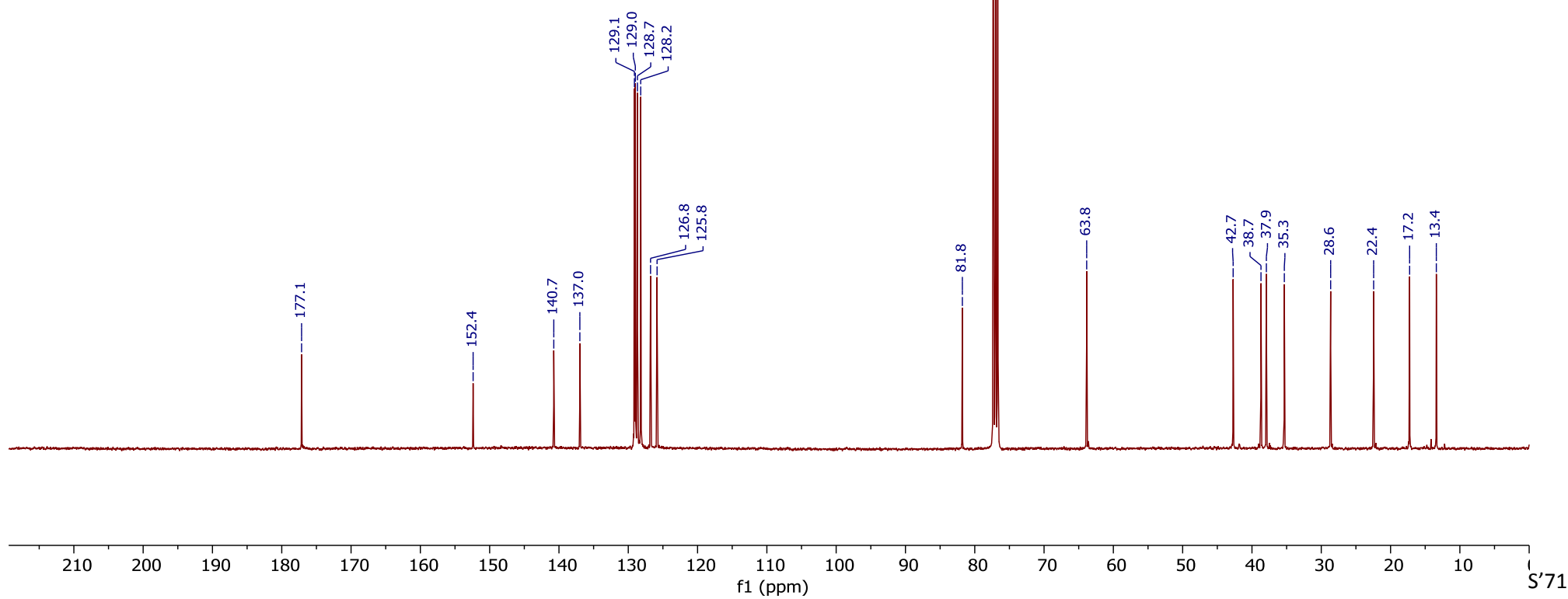
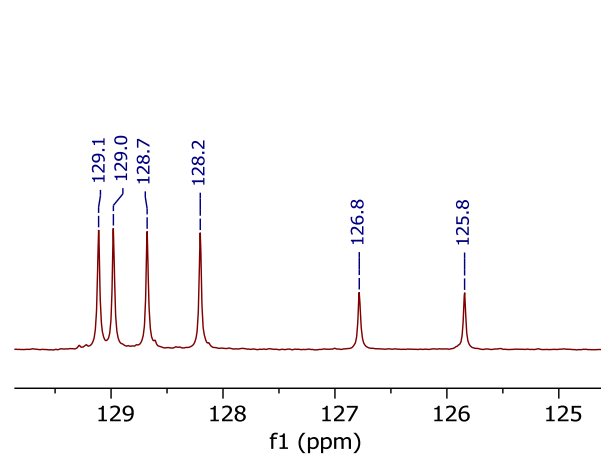
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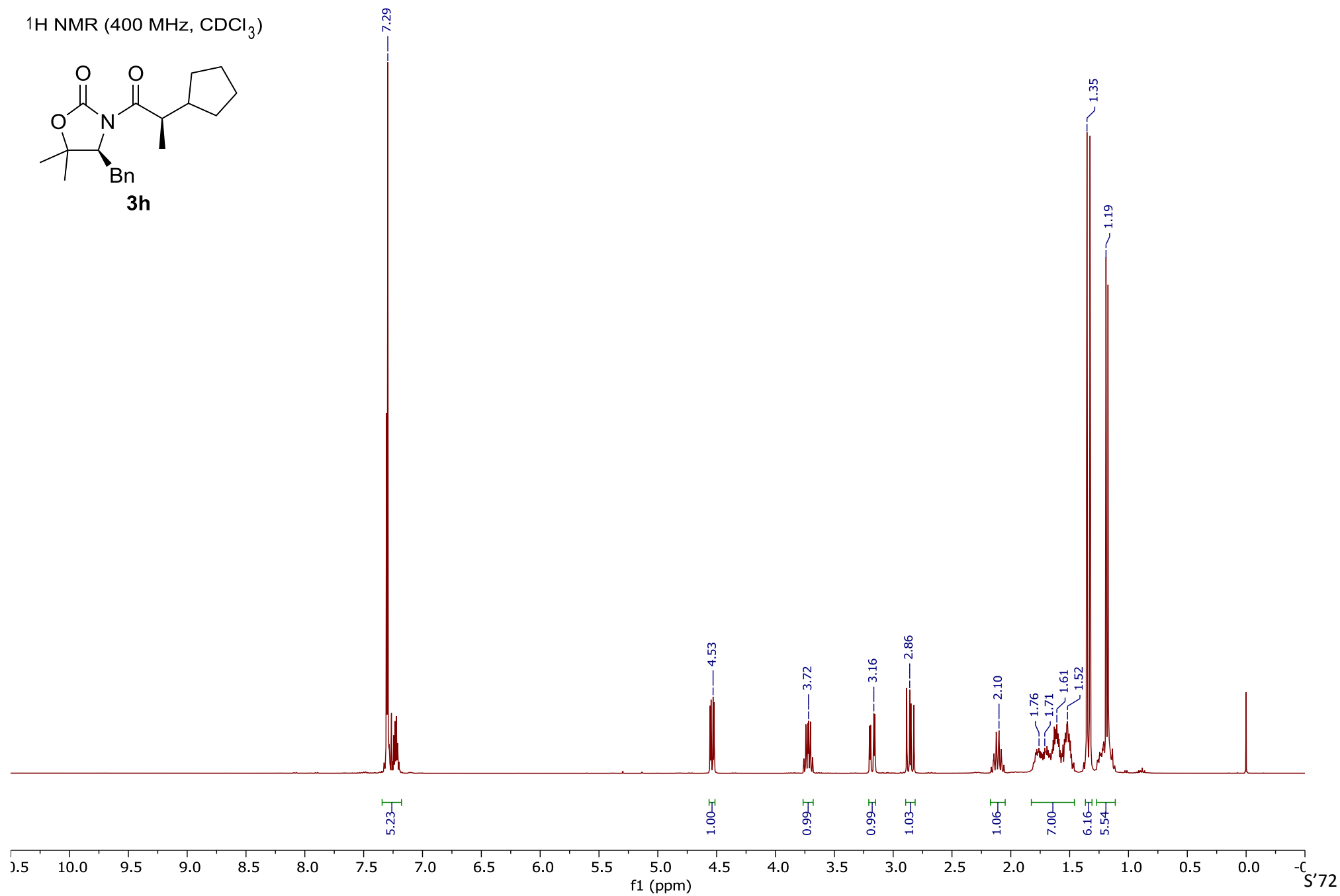
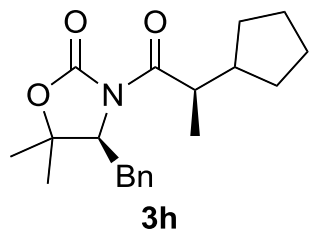
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



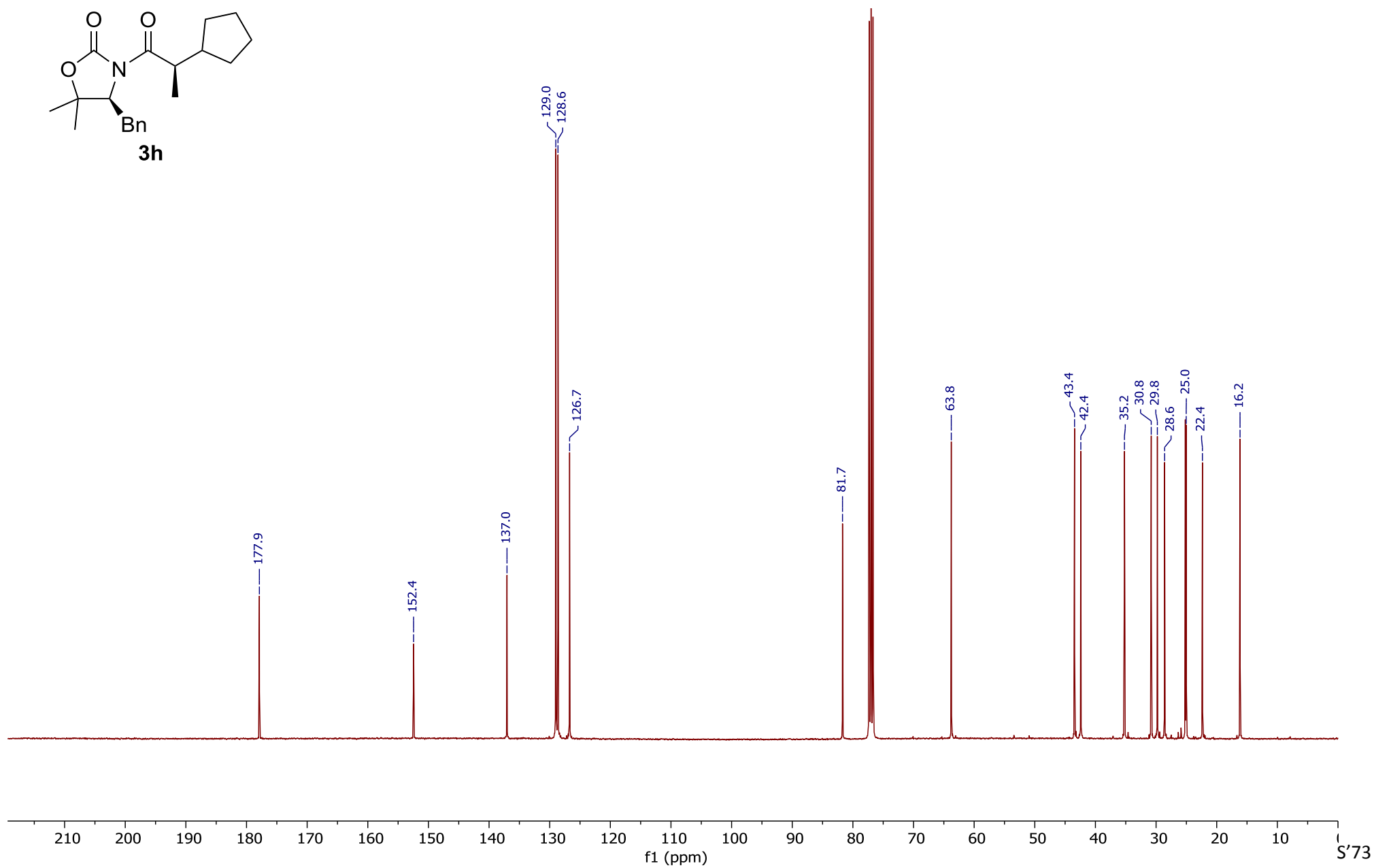
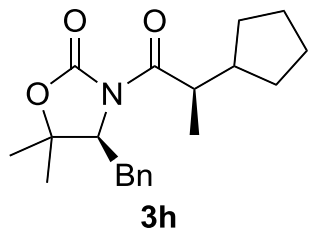
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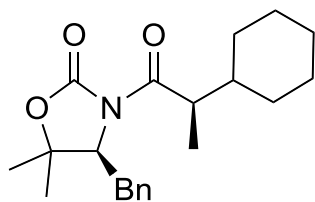
¹H NMR (400 MHz, CDCl₃)



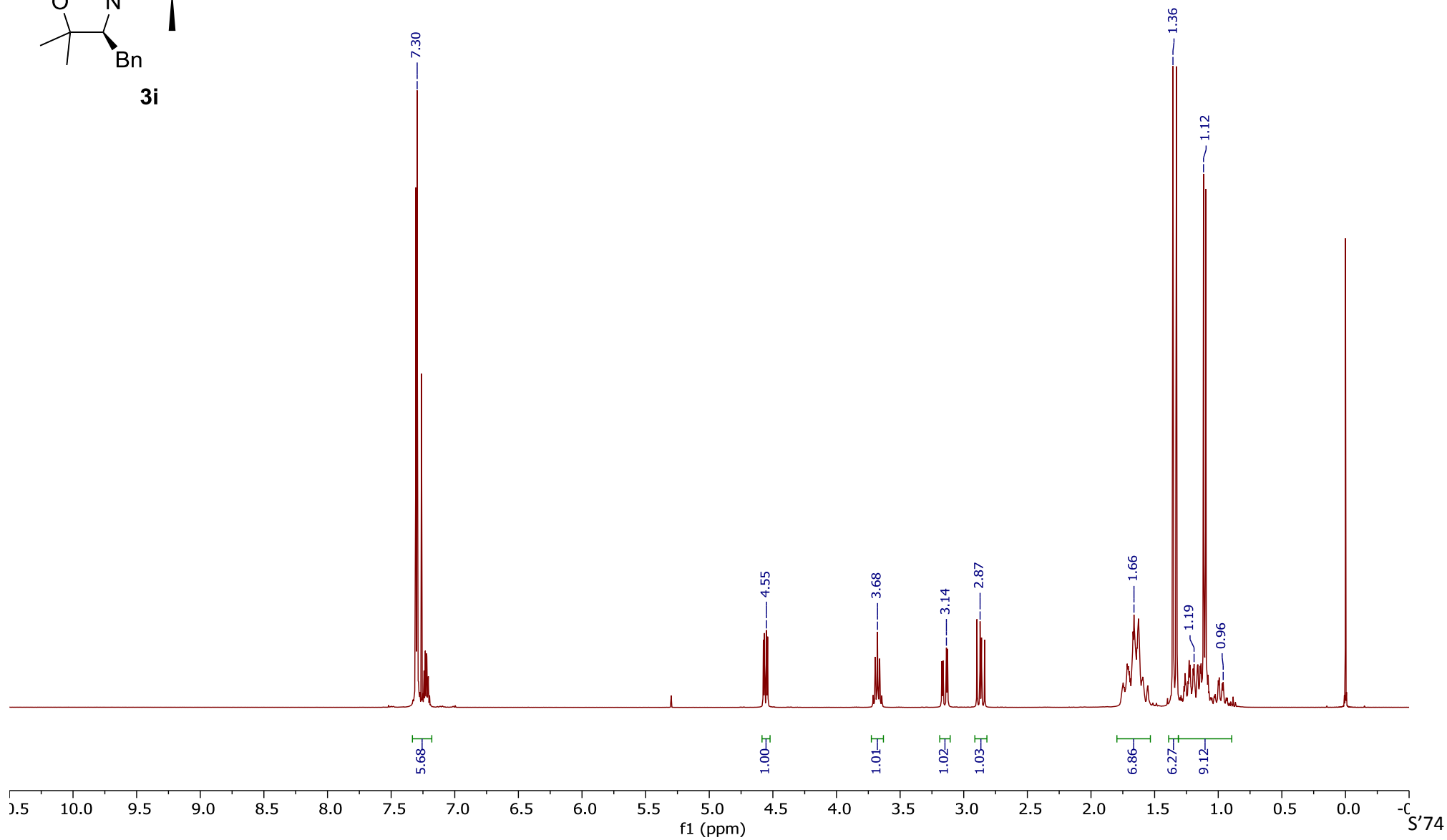
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



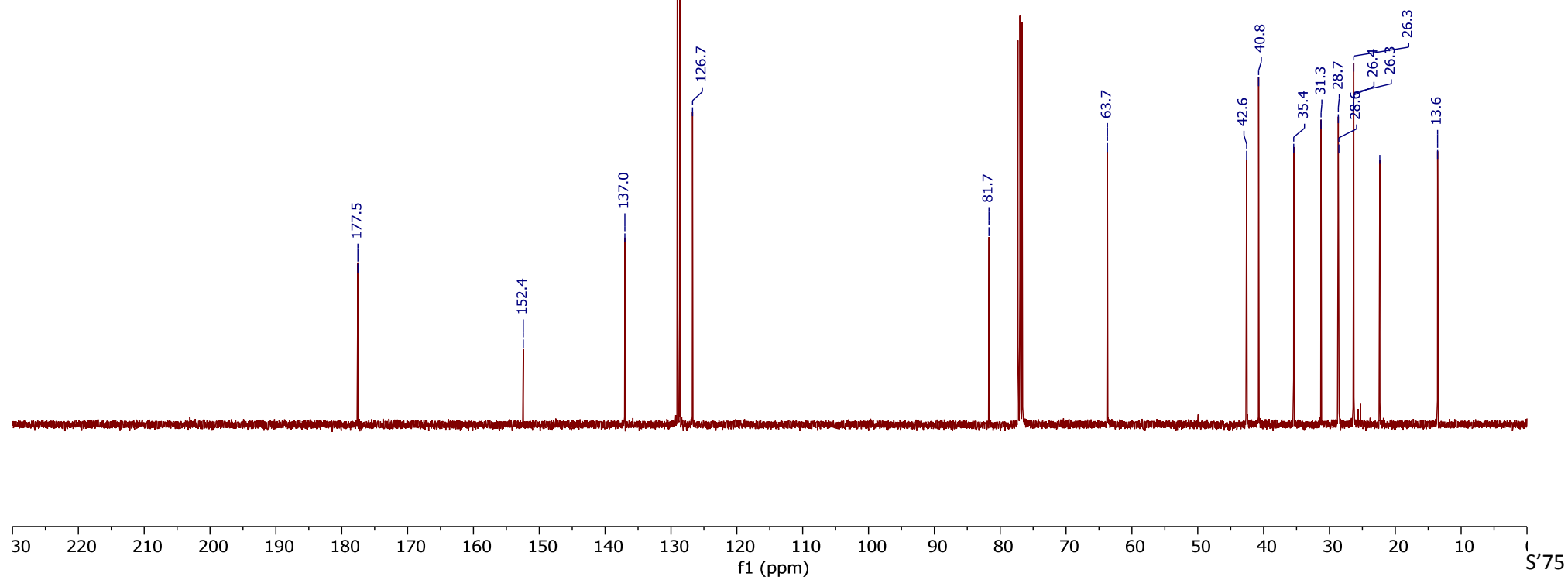
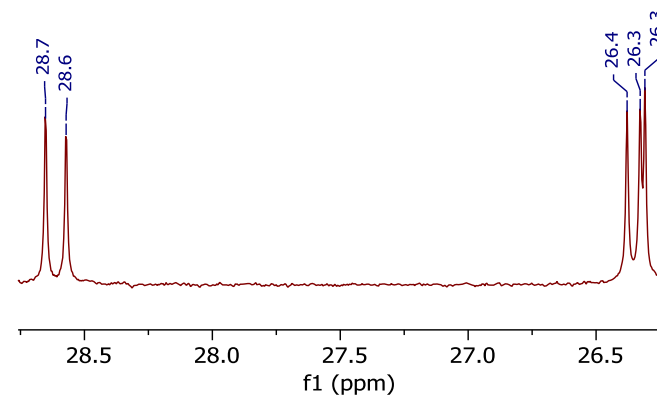
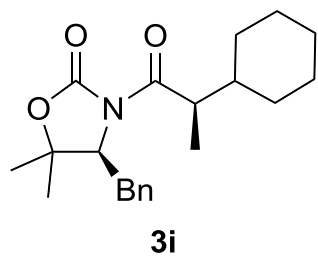
¹H NMR (400 MHz, CDCl₃)



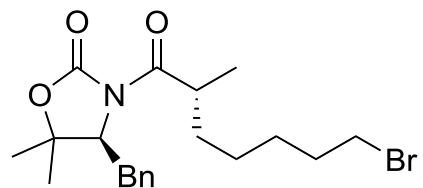
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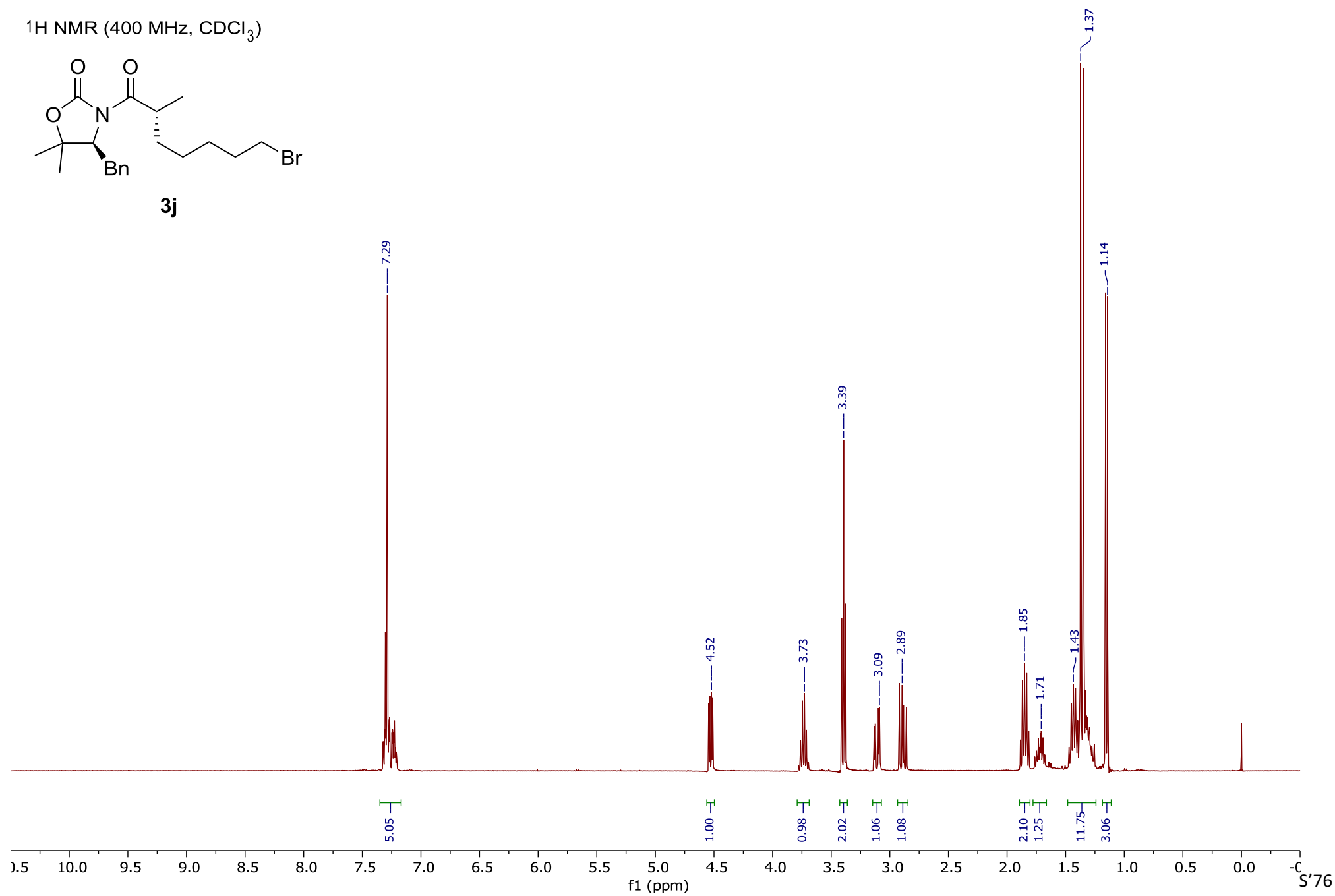
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



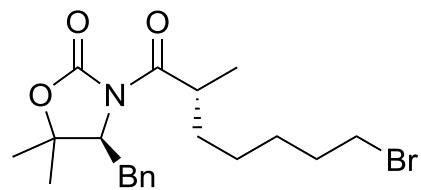
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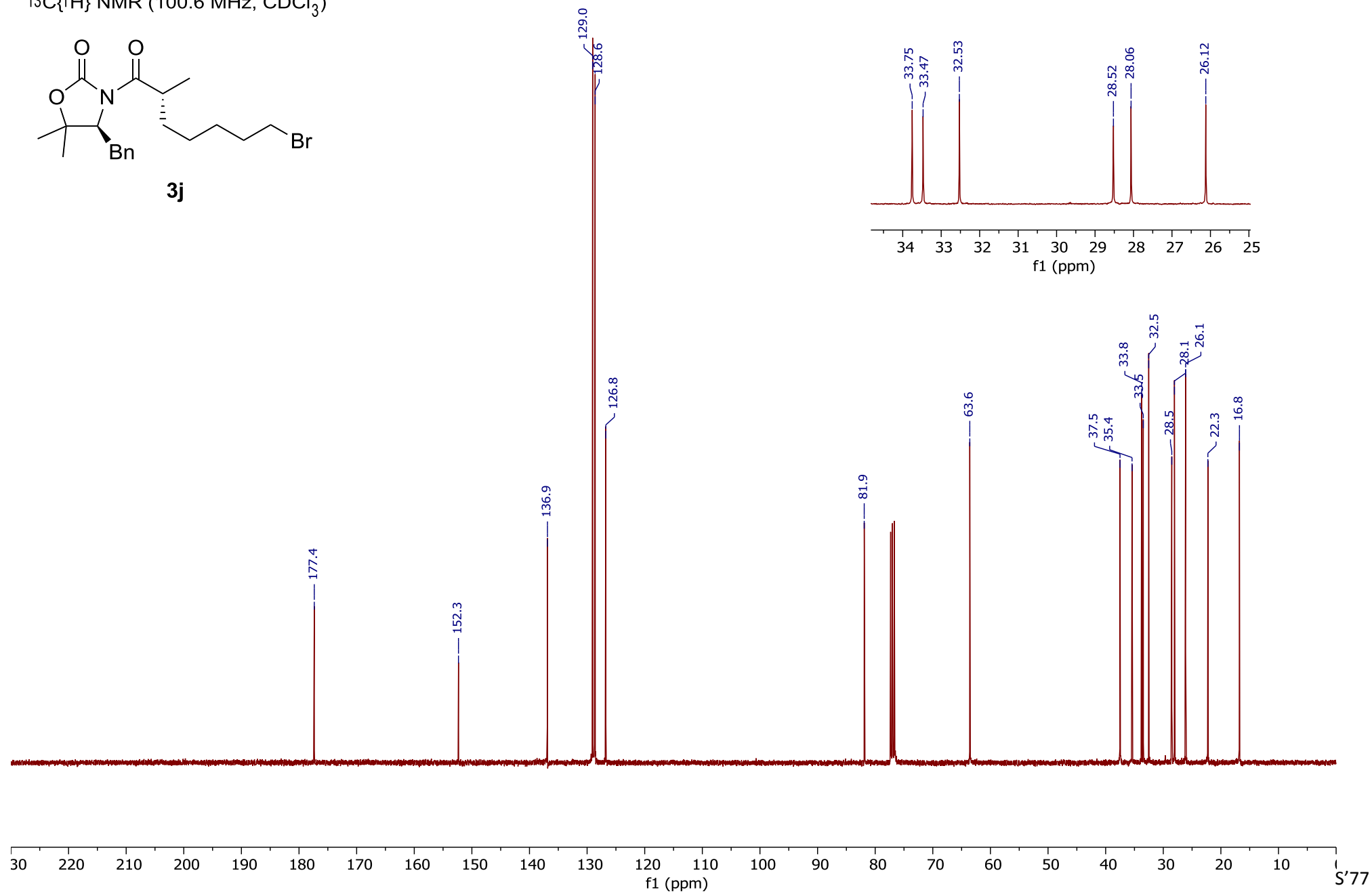
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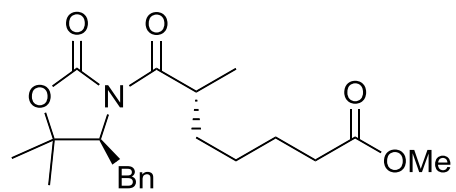
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



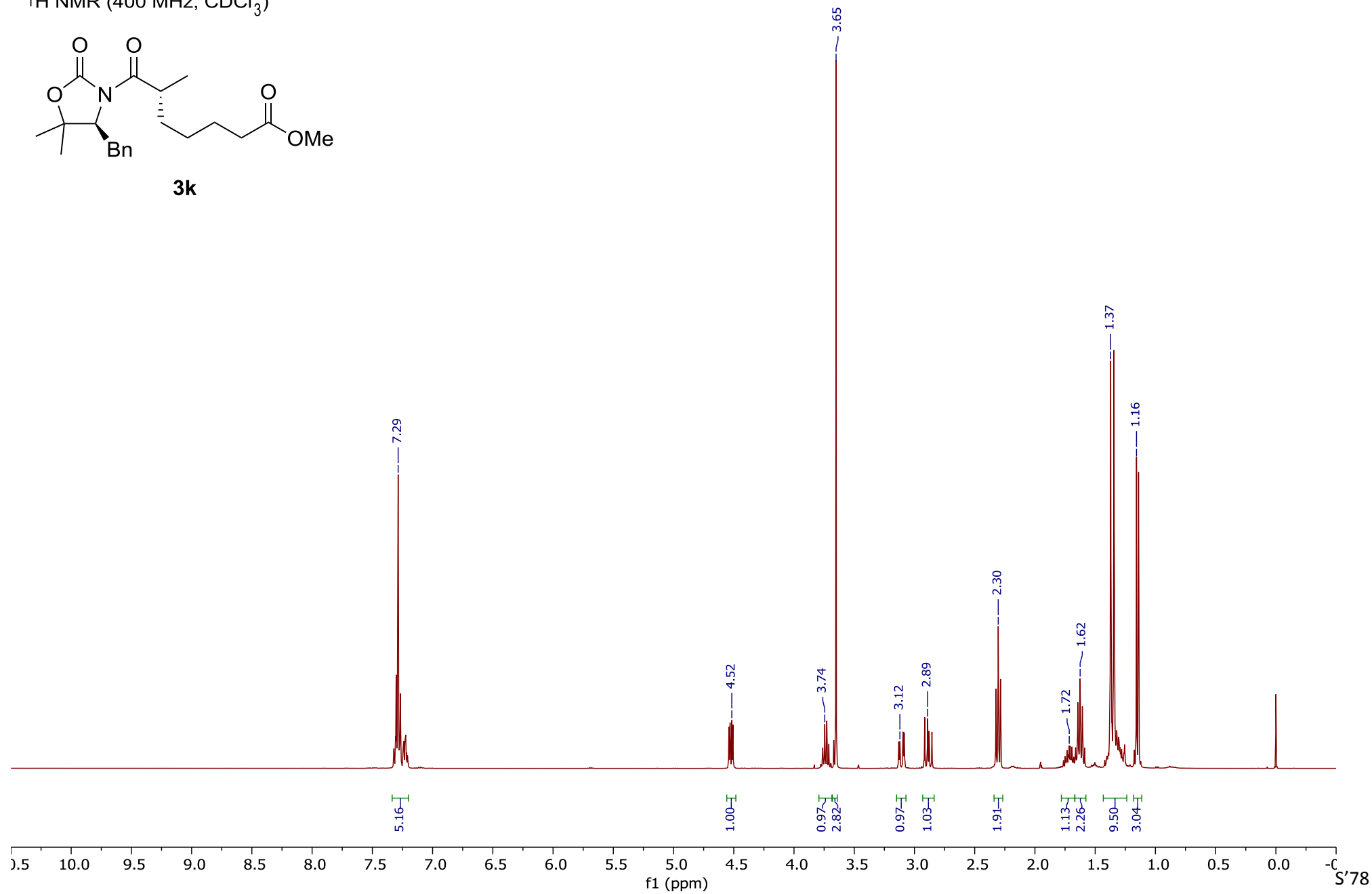
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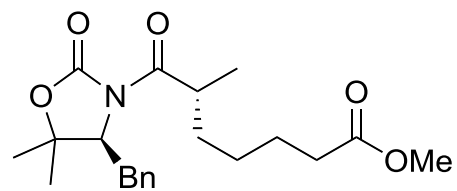
¹H NMR (400 MHz, CDCl₃)



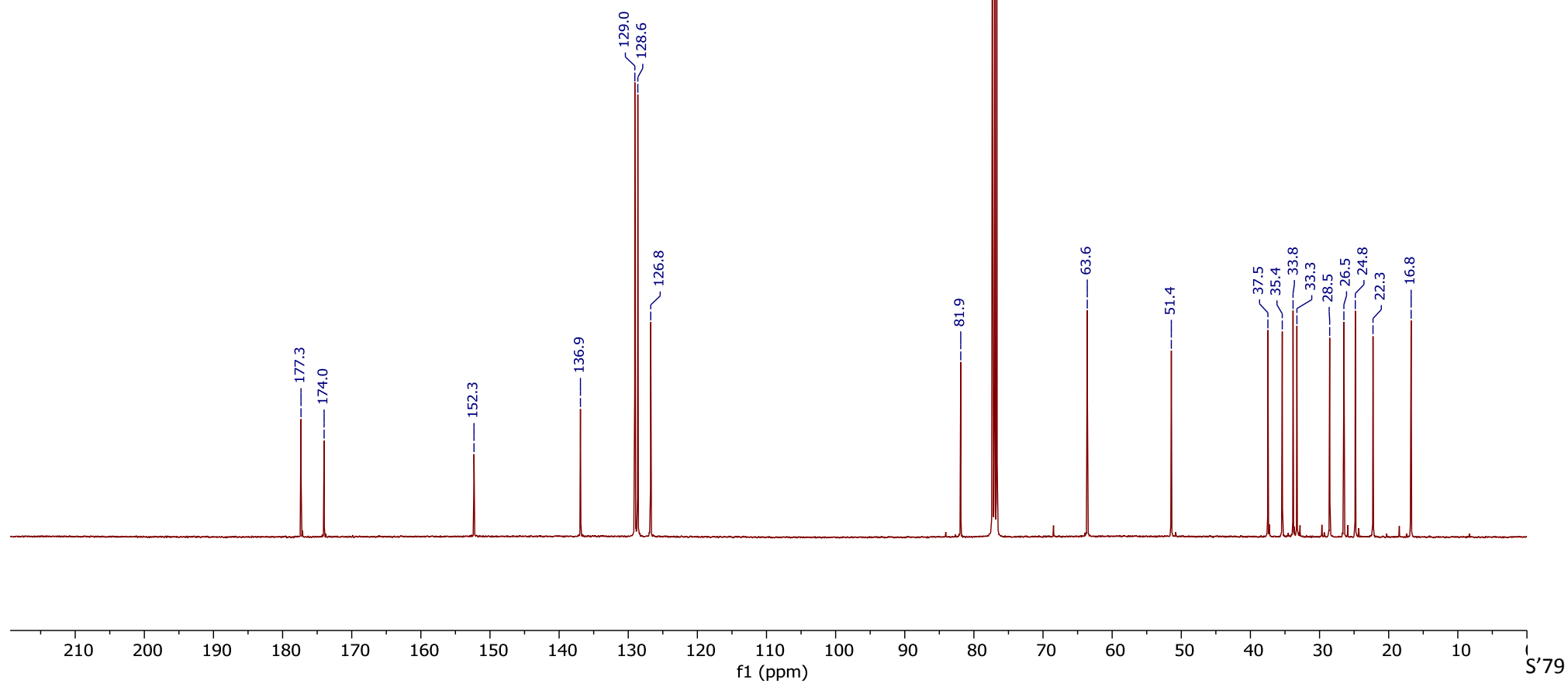
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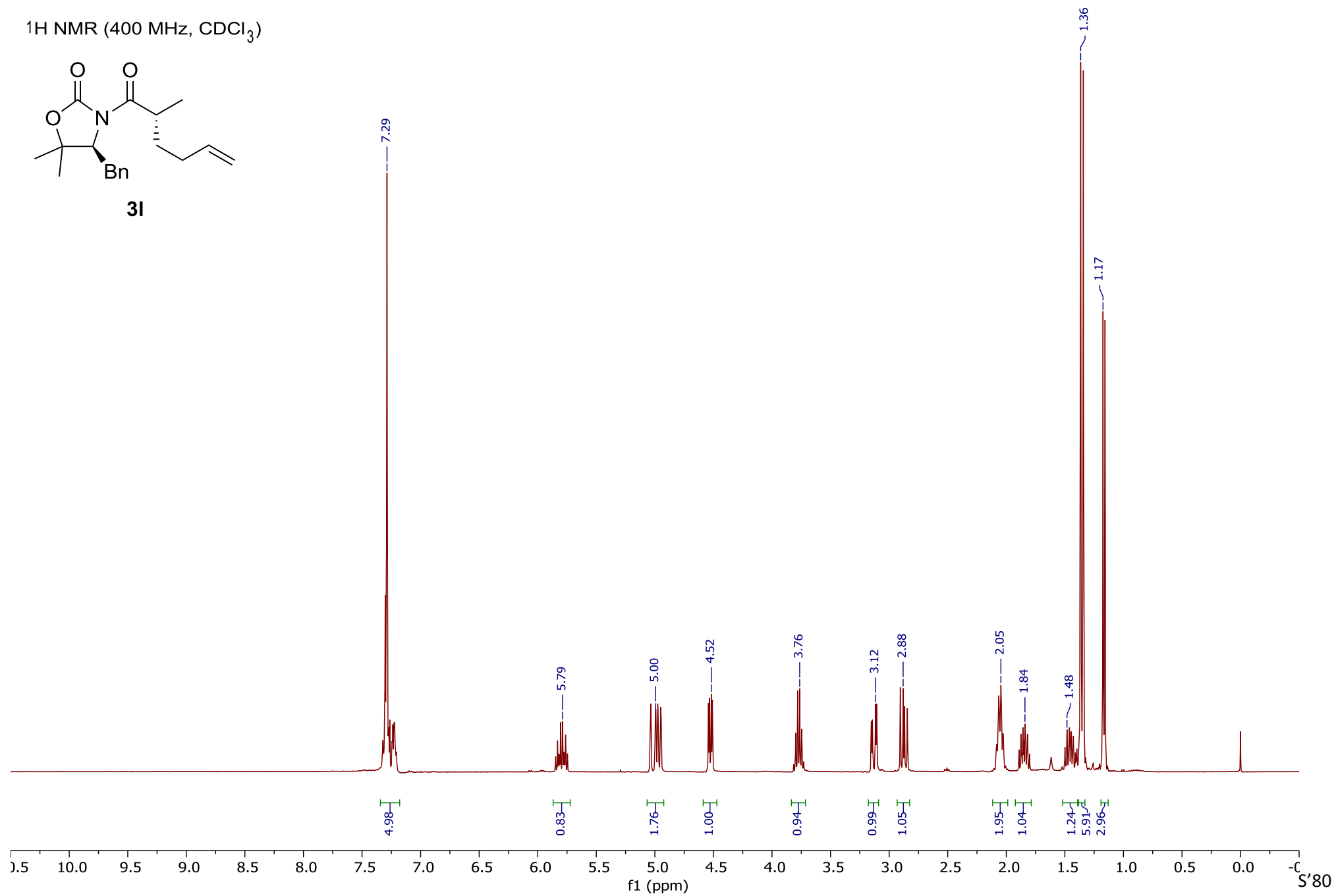
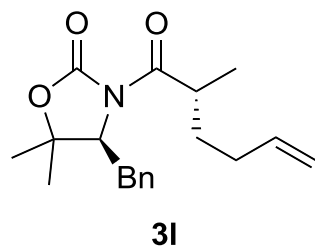
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



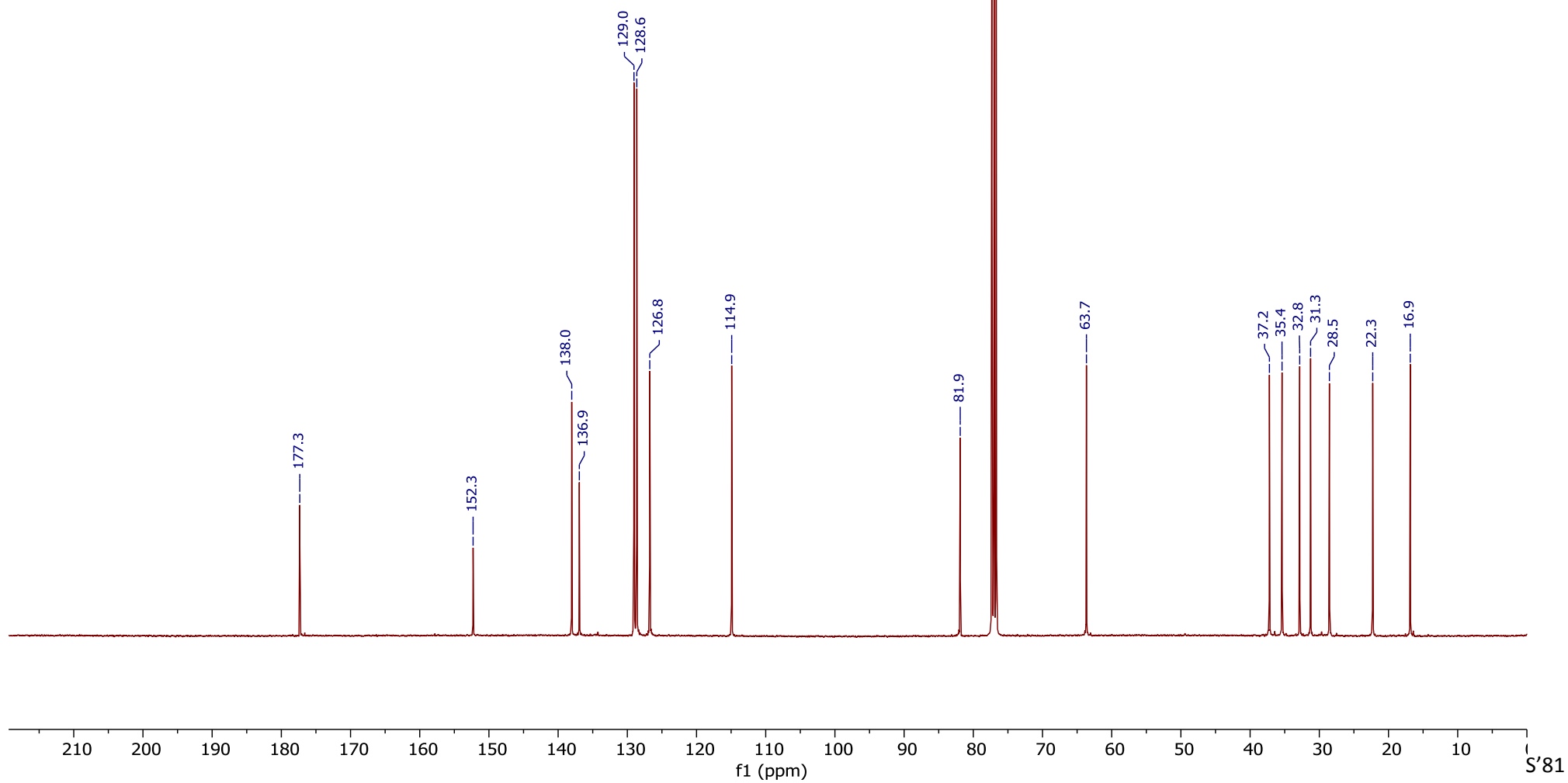
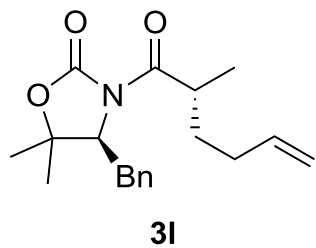
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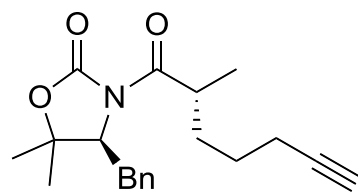
¹H NMR (400 MHz, CDCl₃)



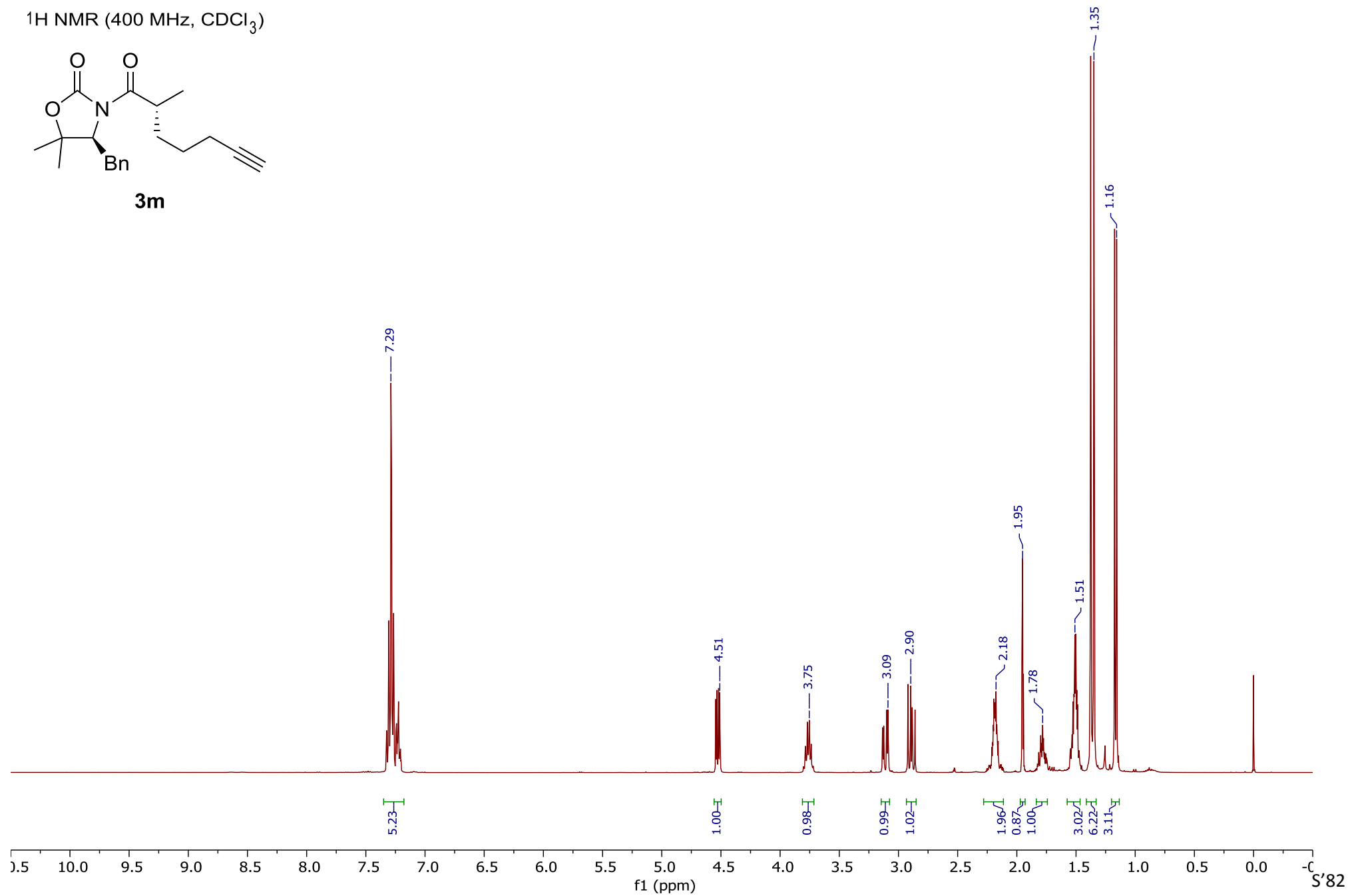
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



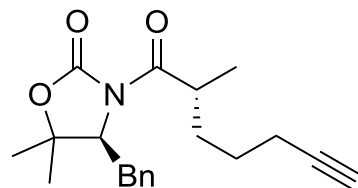
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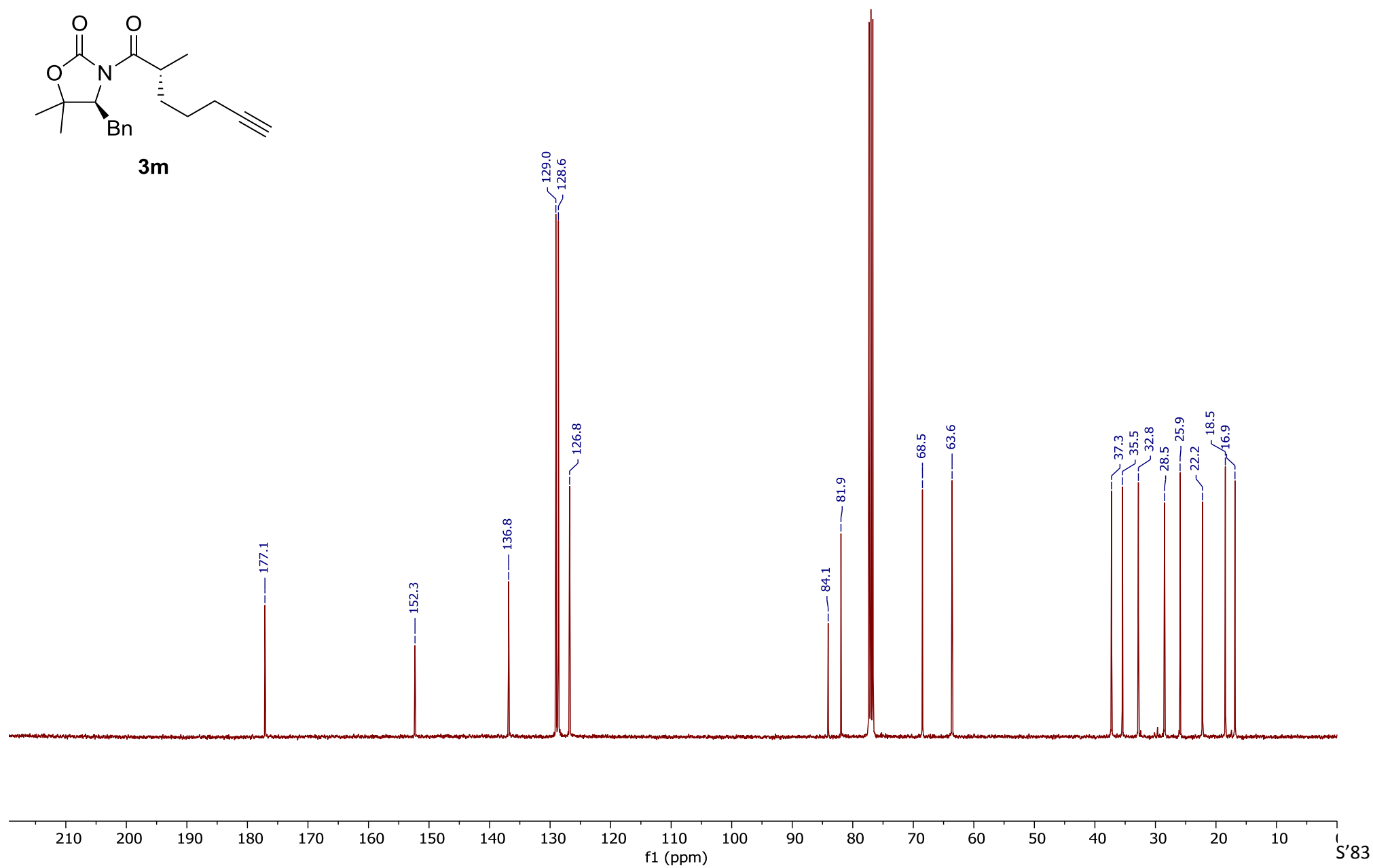
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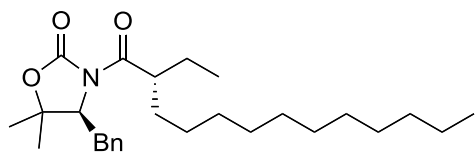
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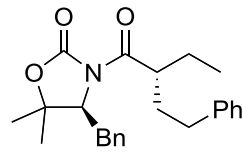
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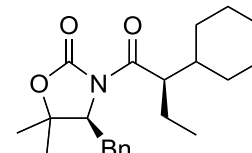
5. ALKYLATION PRODUCTS (TABLE 2)



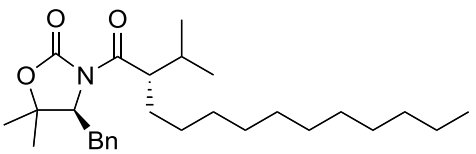
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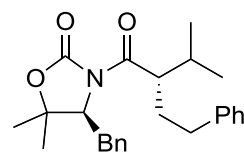
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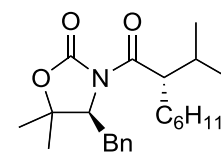
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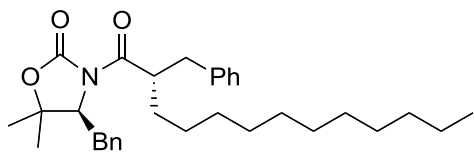
16a



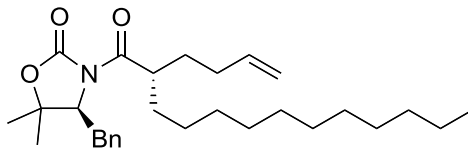
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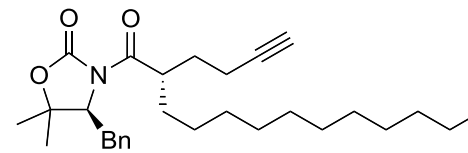
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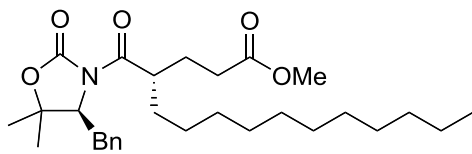
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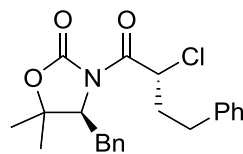
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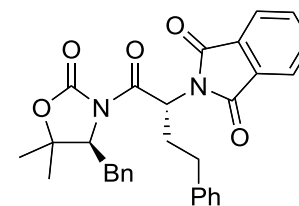
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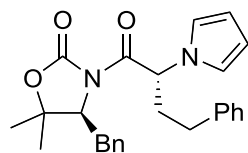
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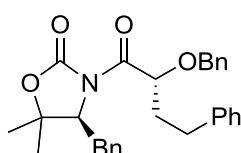
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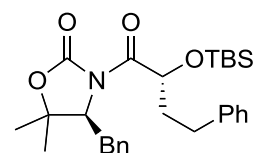
22c



23c

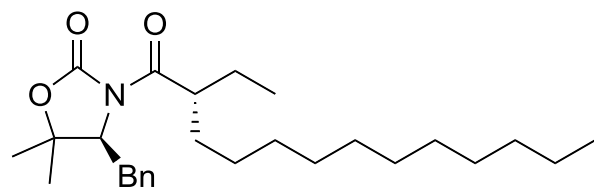


24c

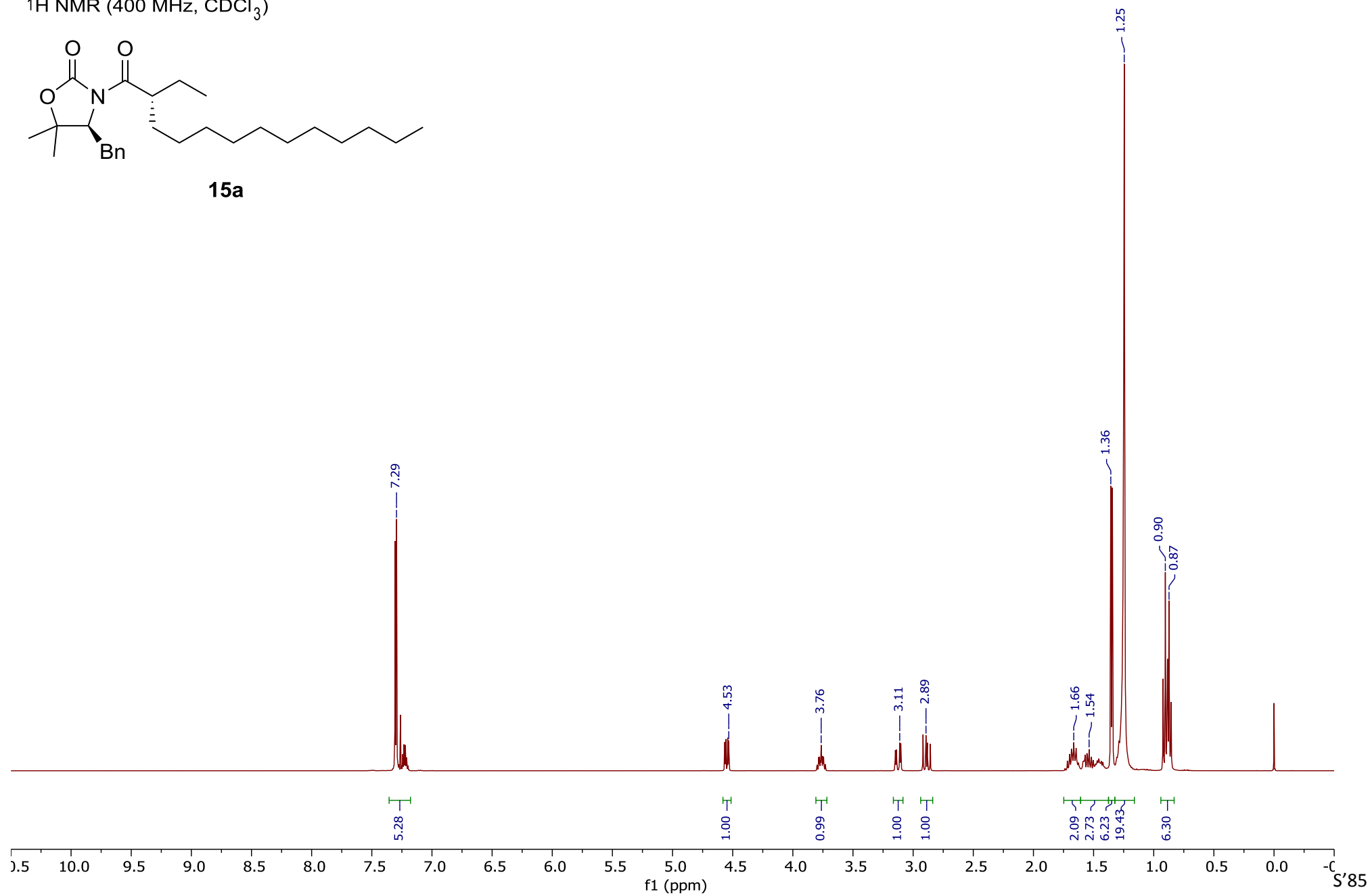


25c

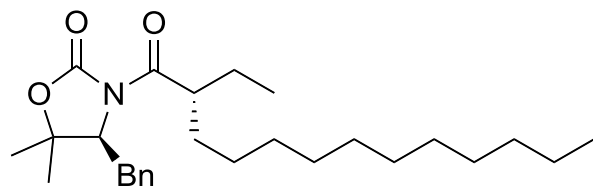
^1H NMR (400 MHz, CDCl_3)



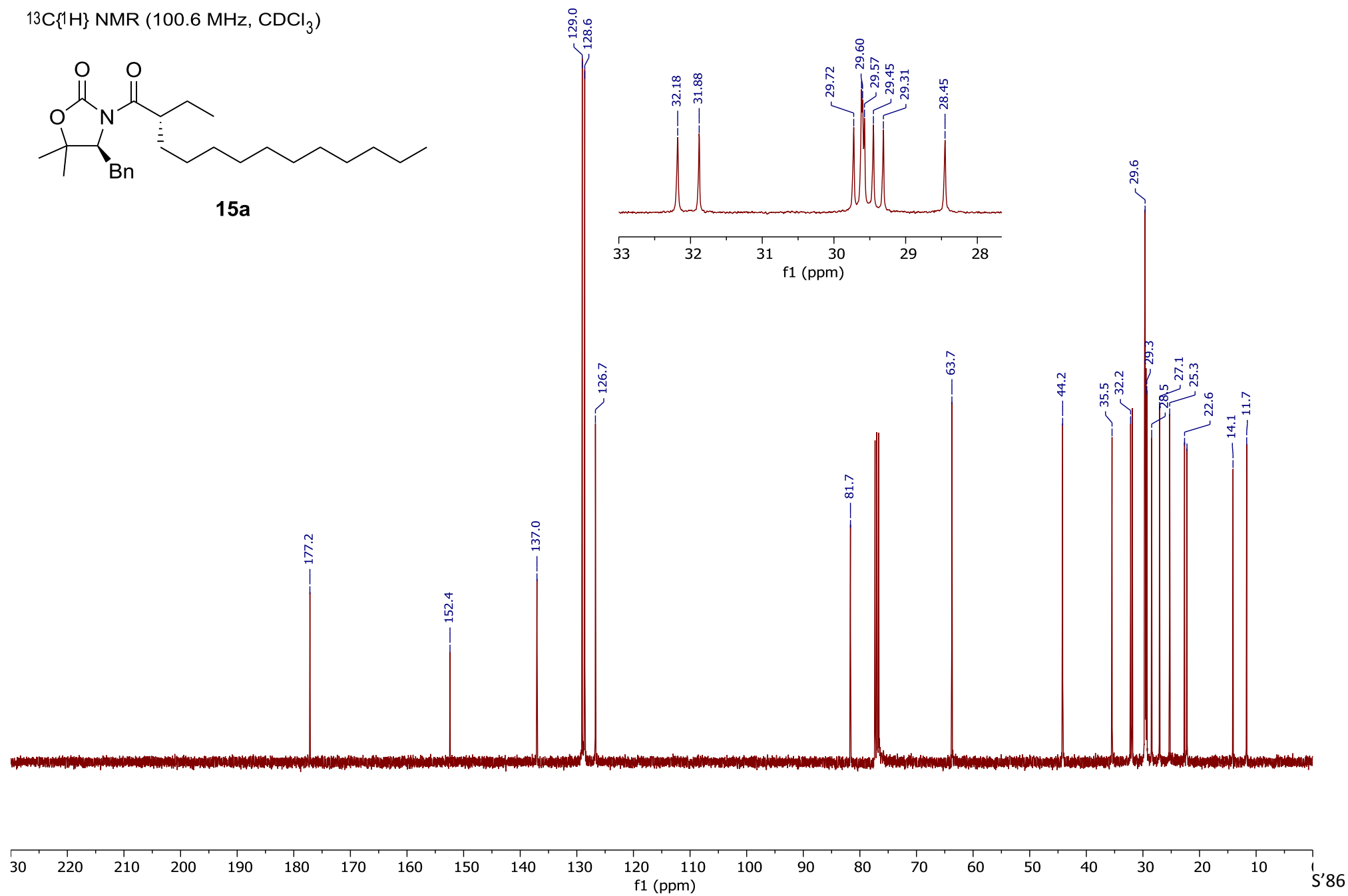
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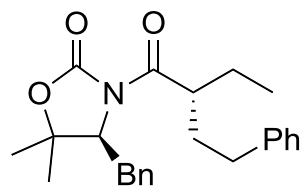
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



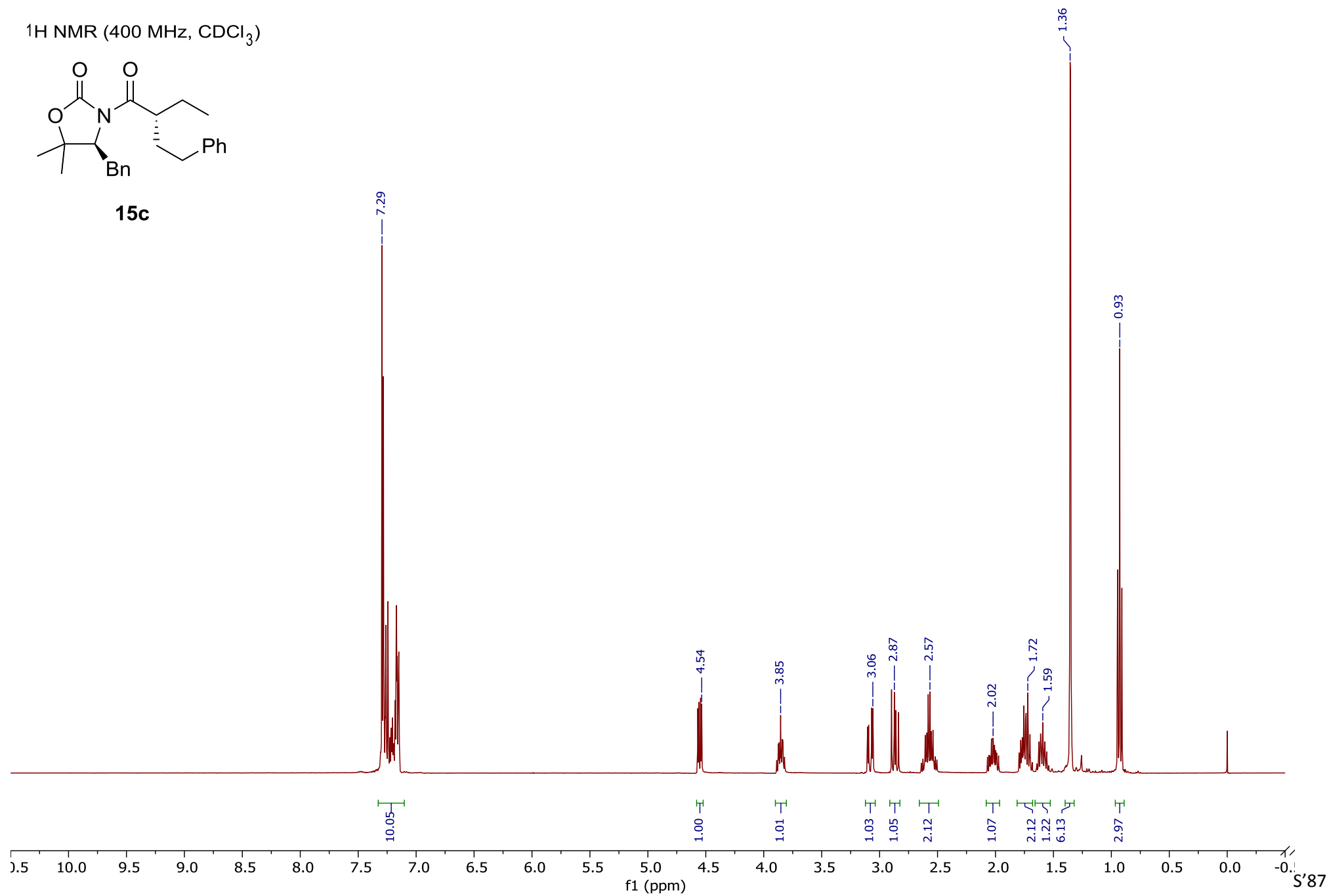
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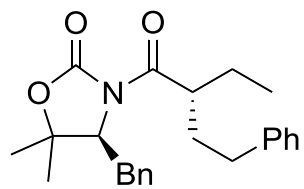
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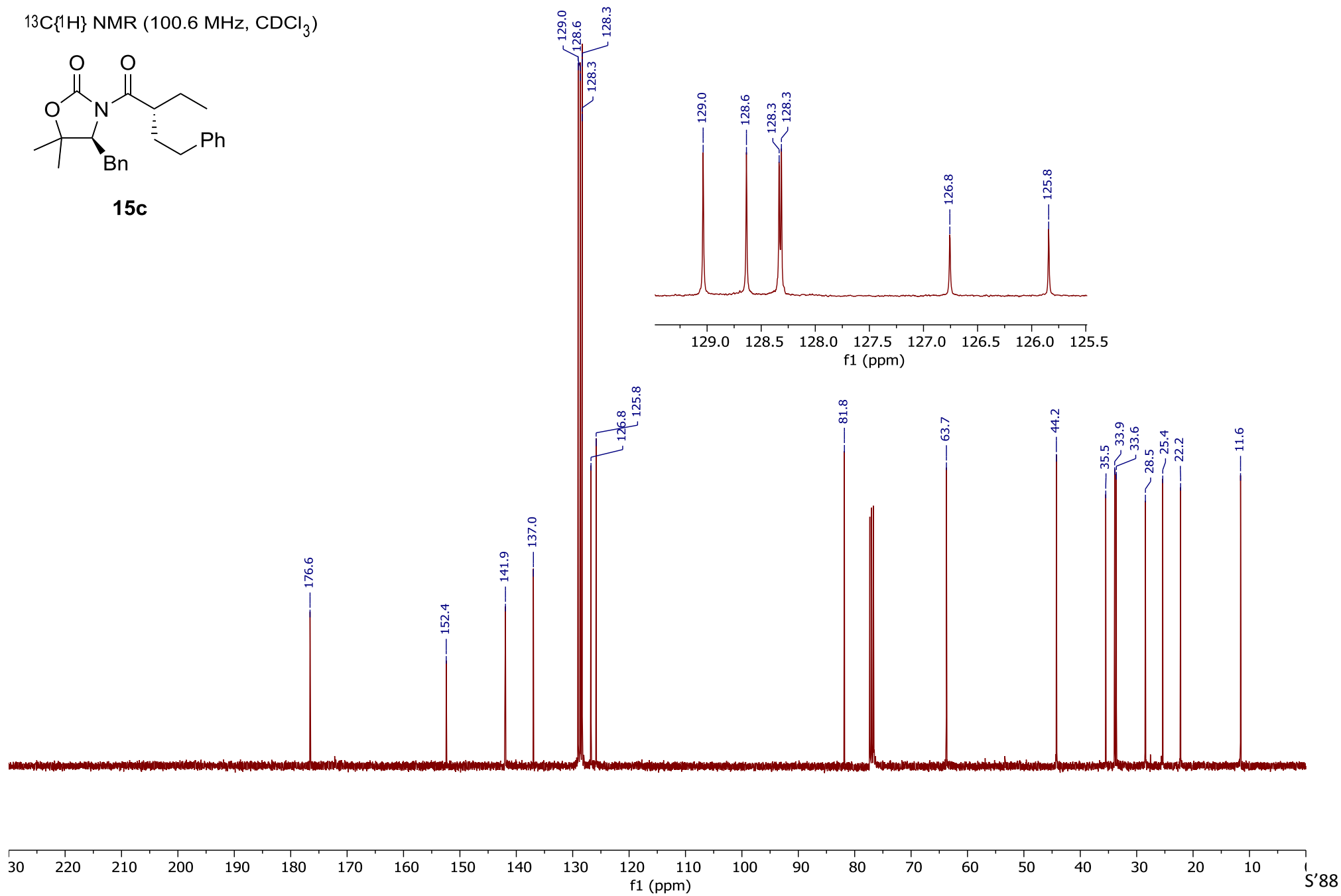
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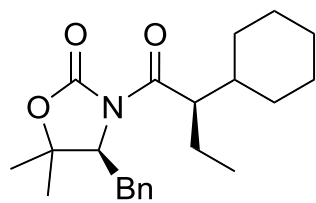
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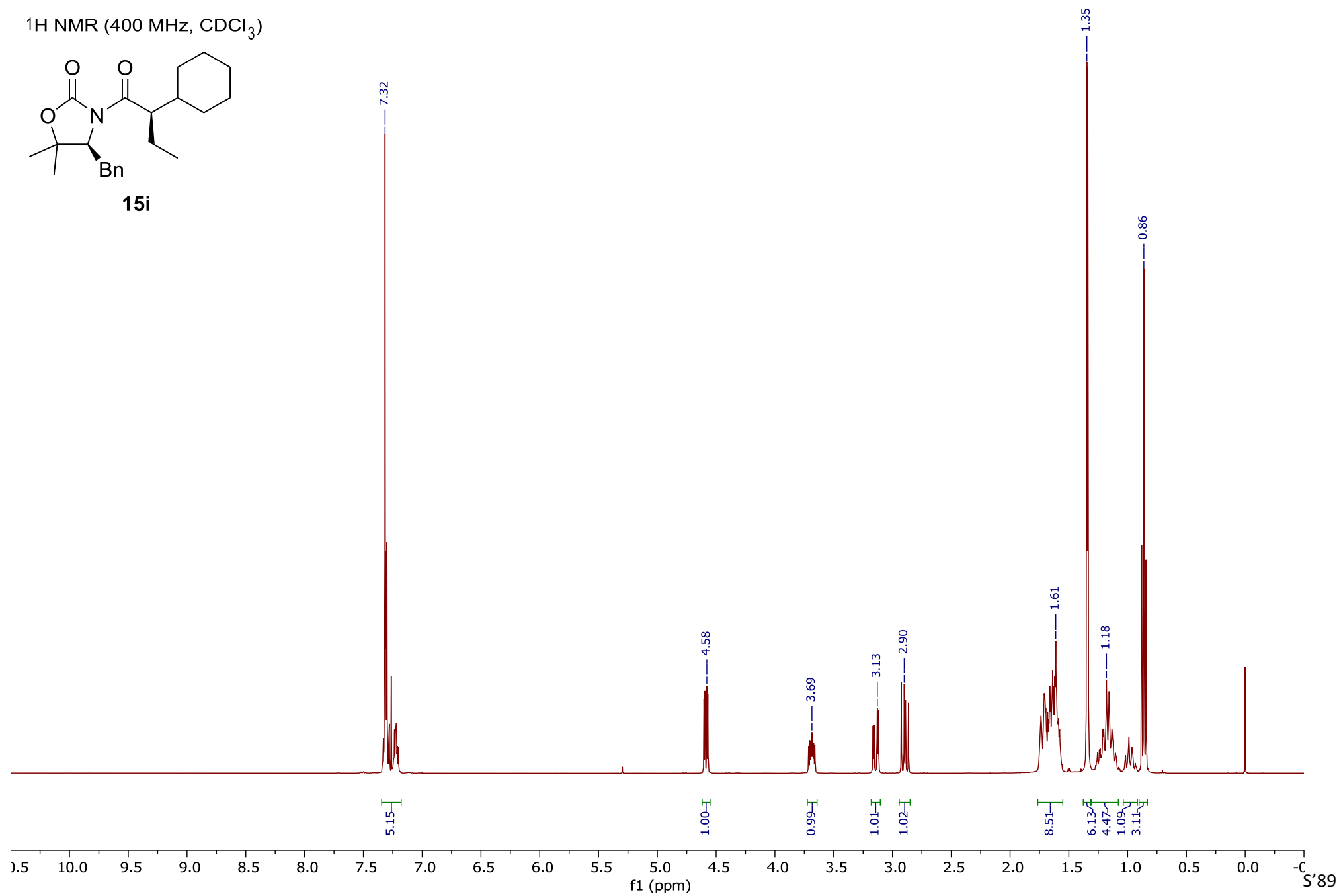
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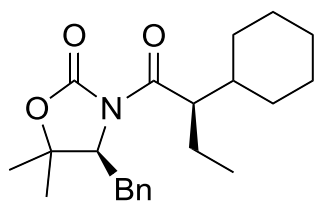


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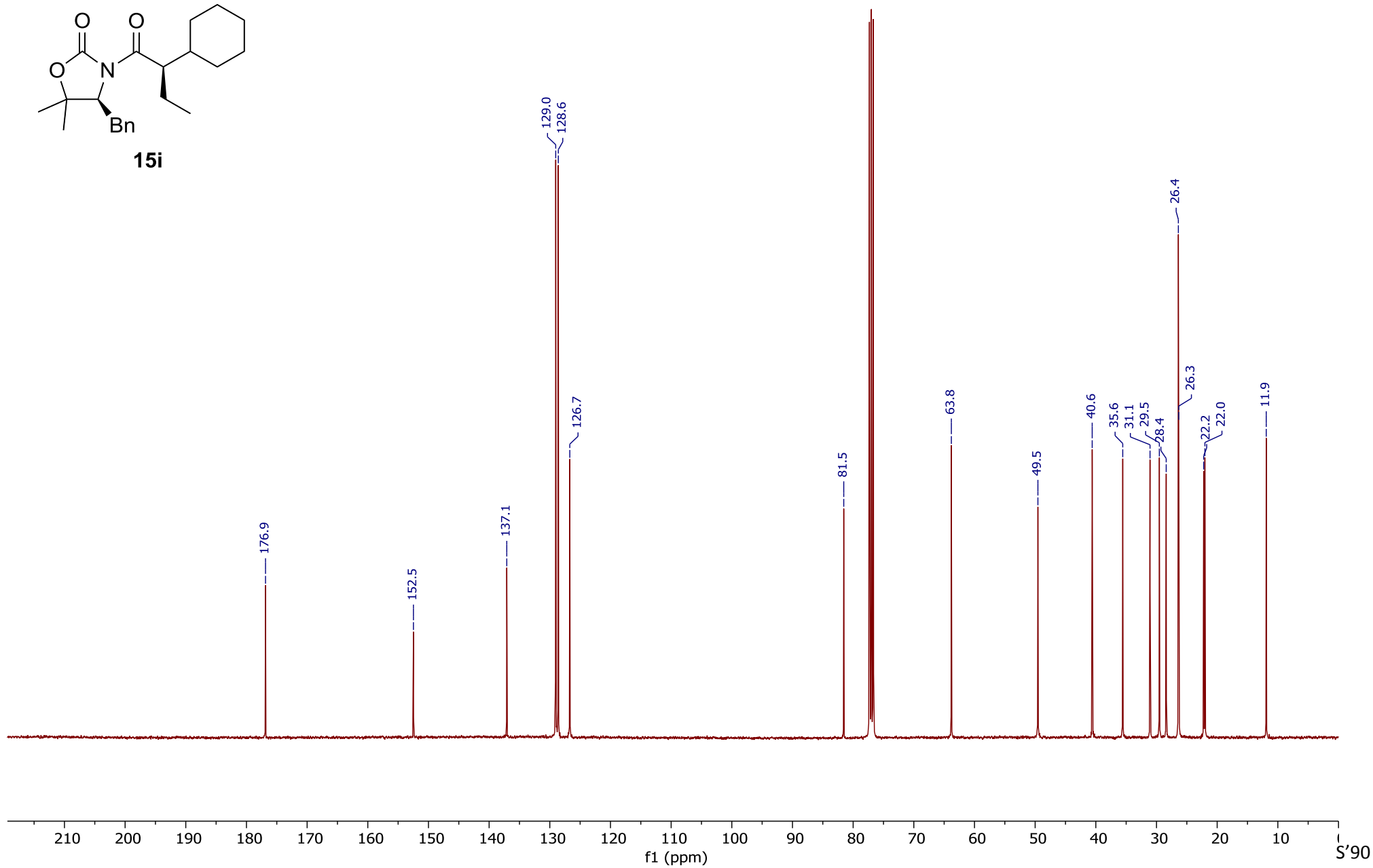


15i

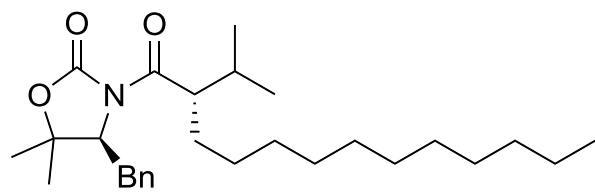




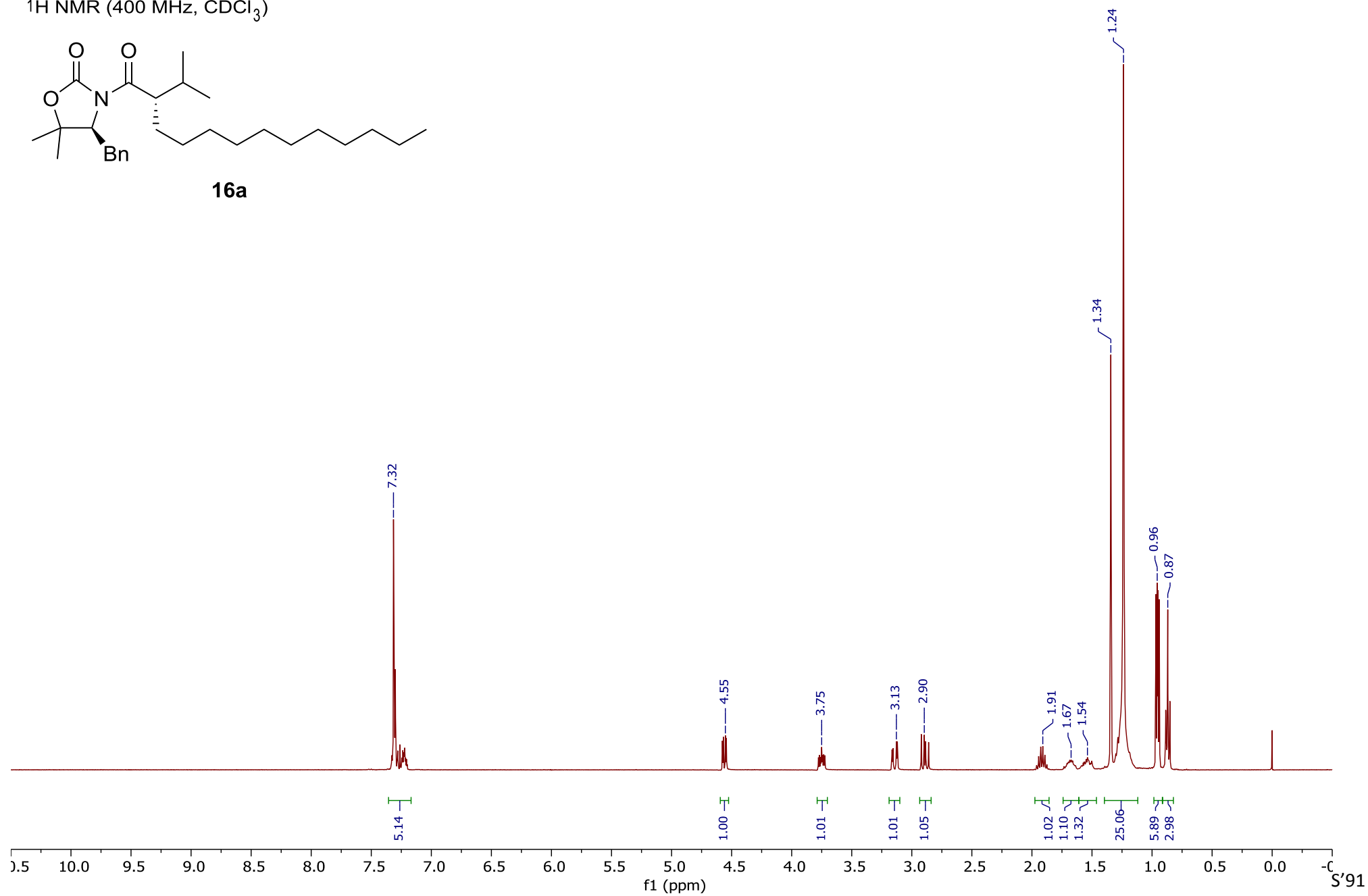
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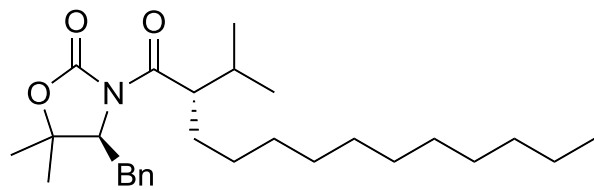
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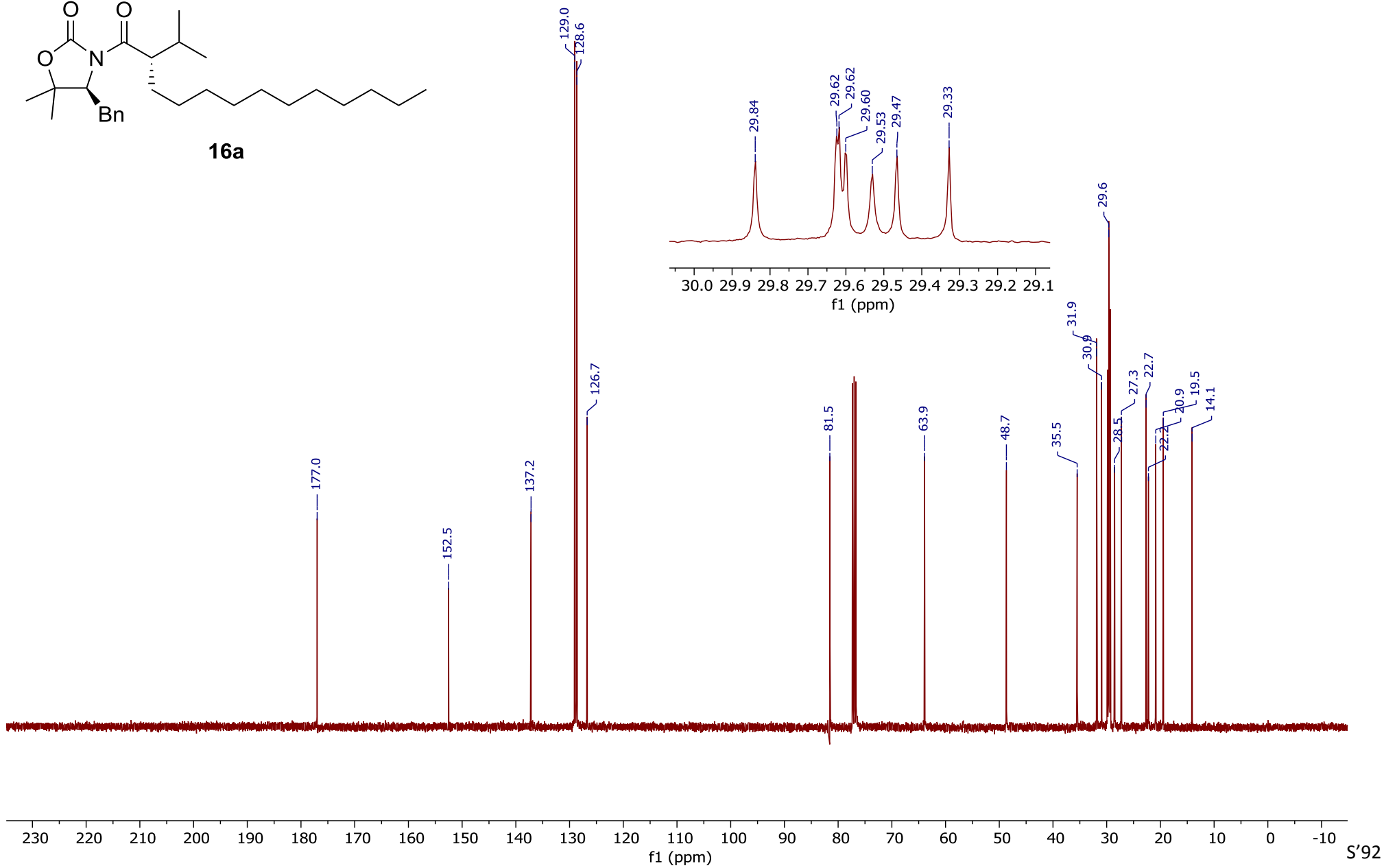
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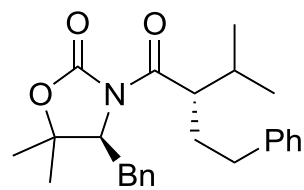
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



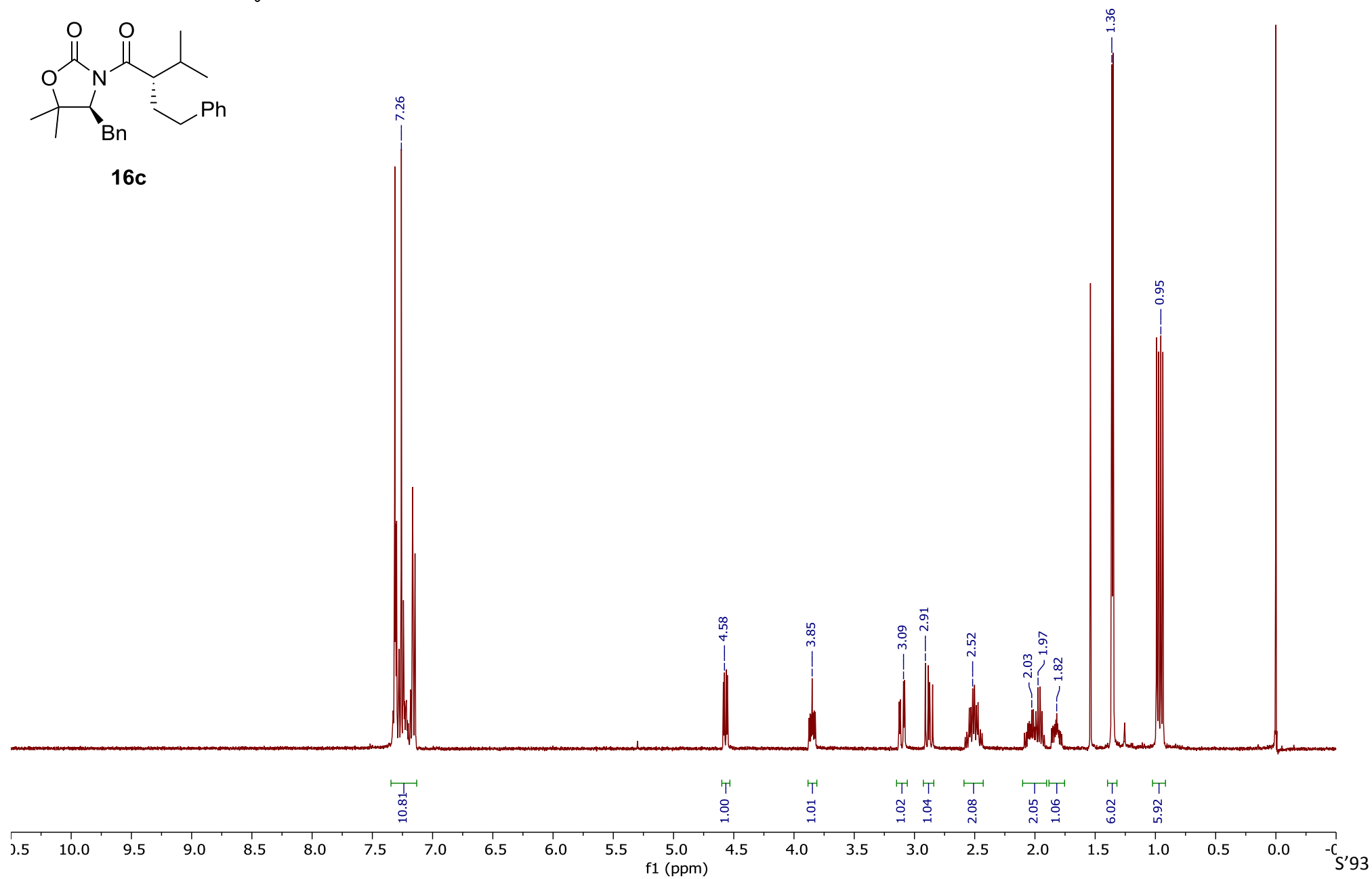
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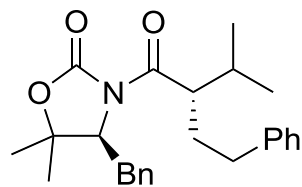
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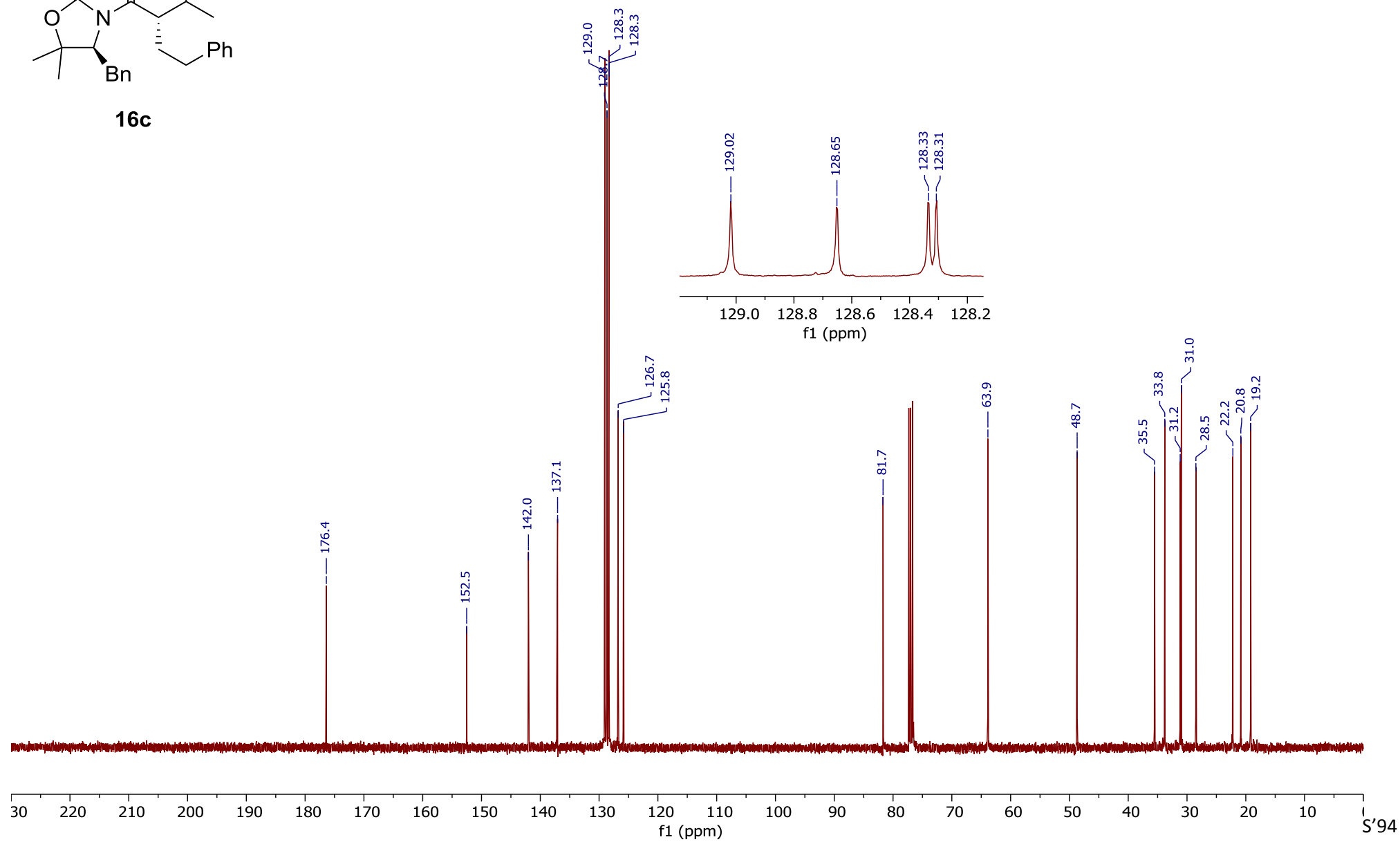
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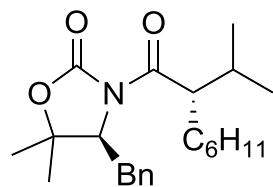
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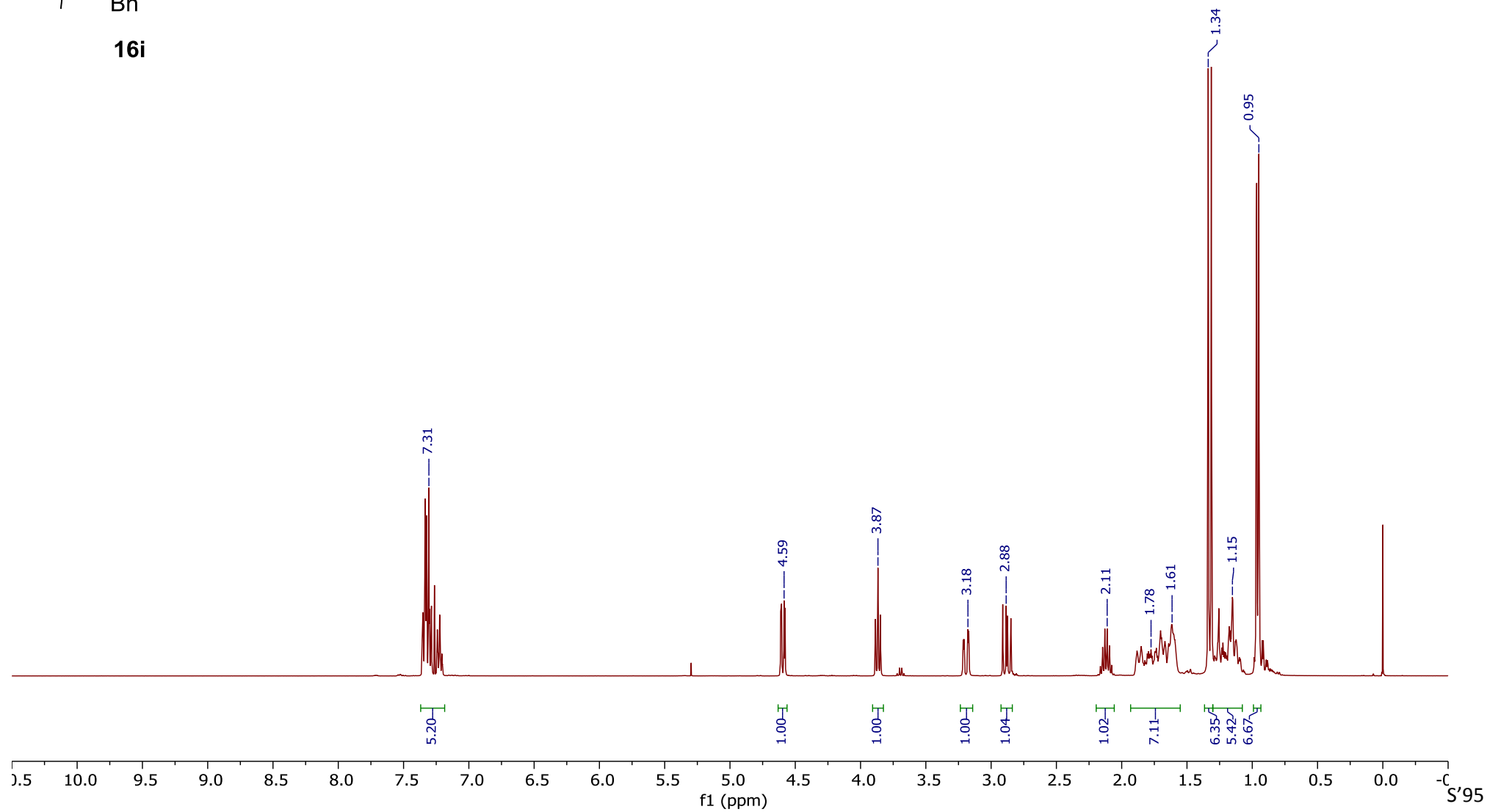
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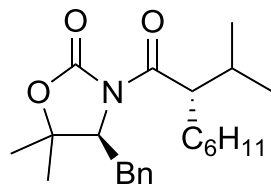
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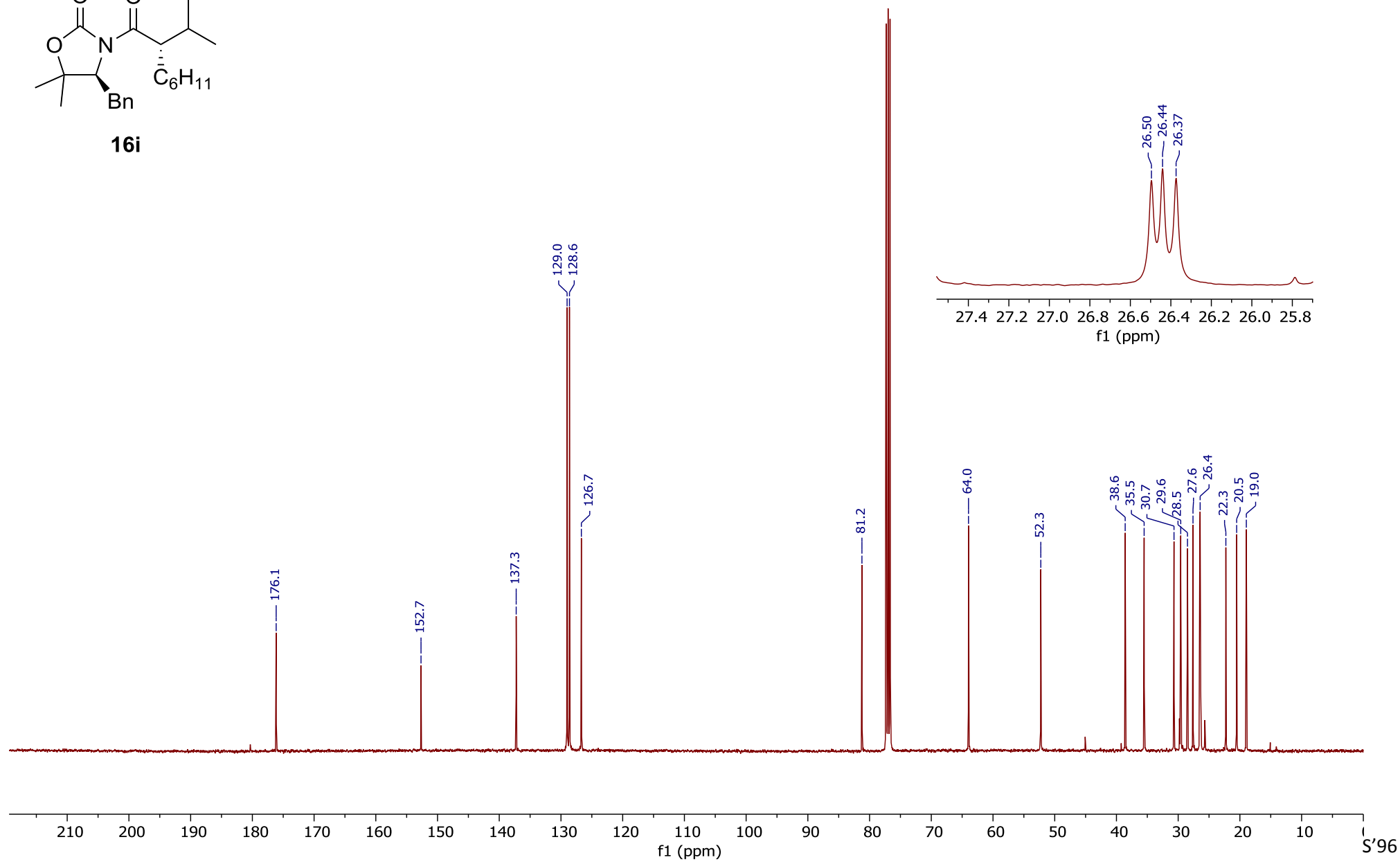
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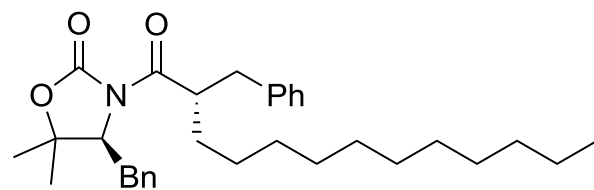
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



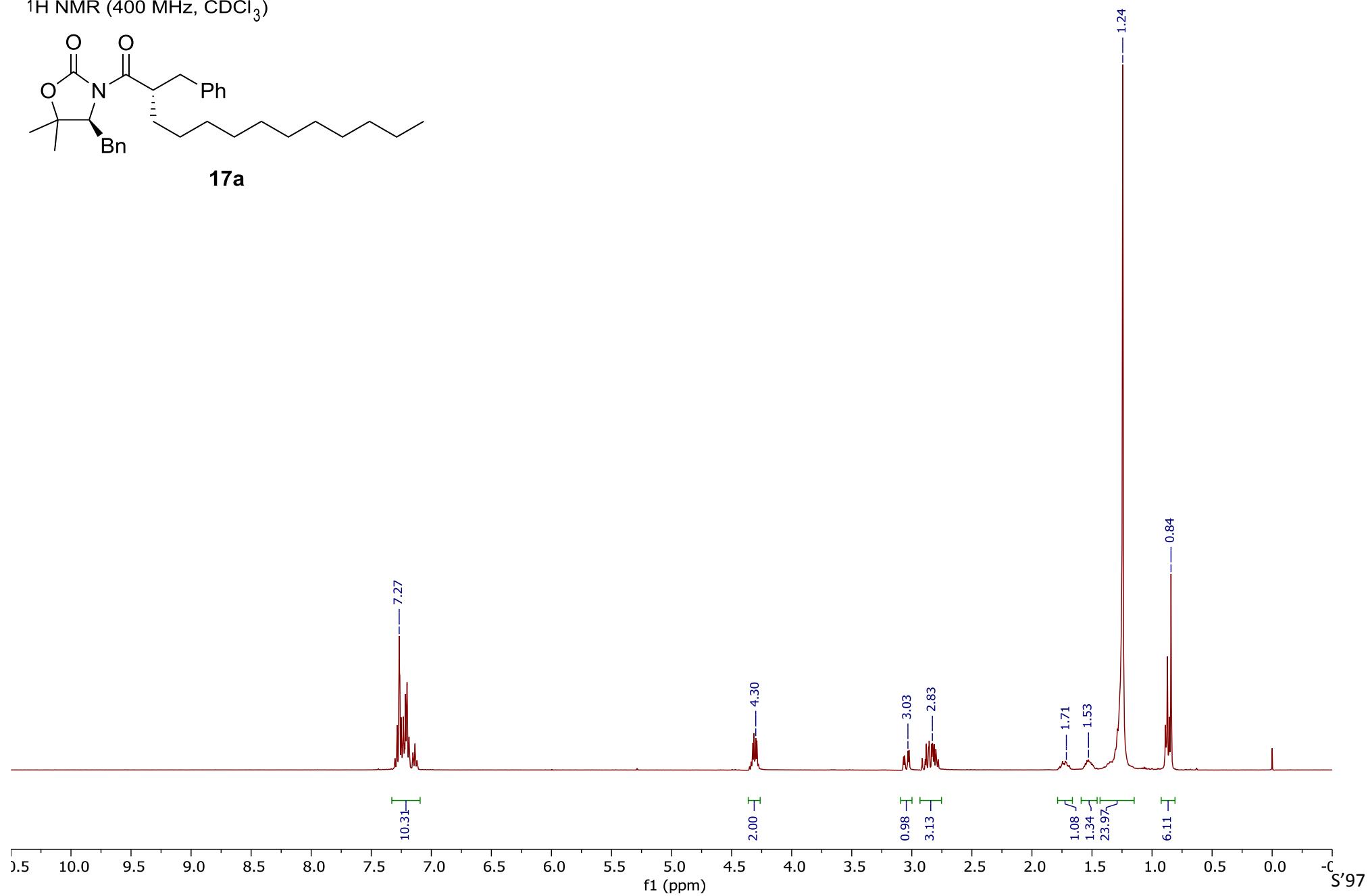
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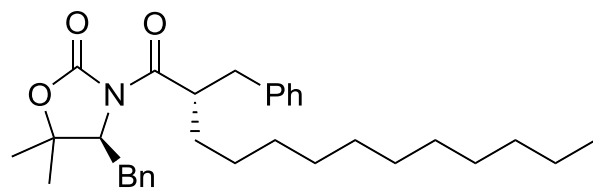
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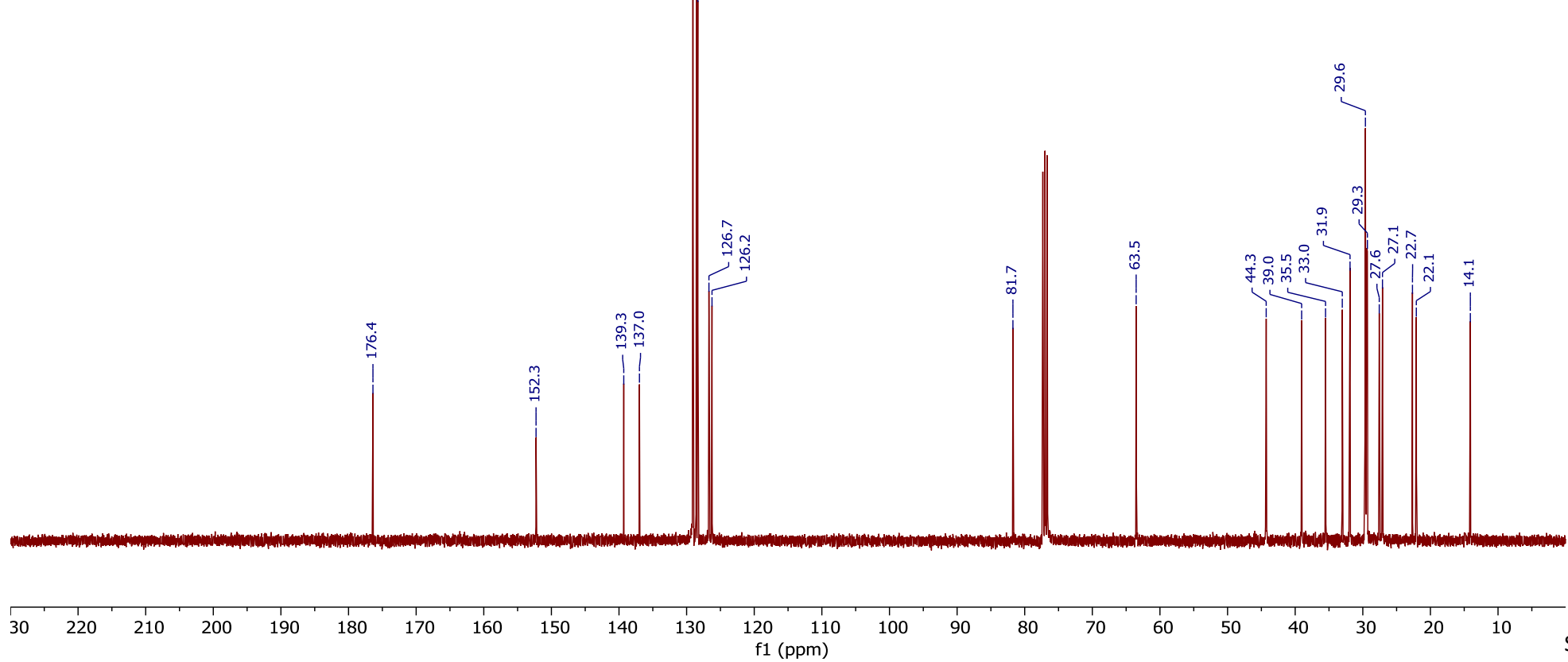
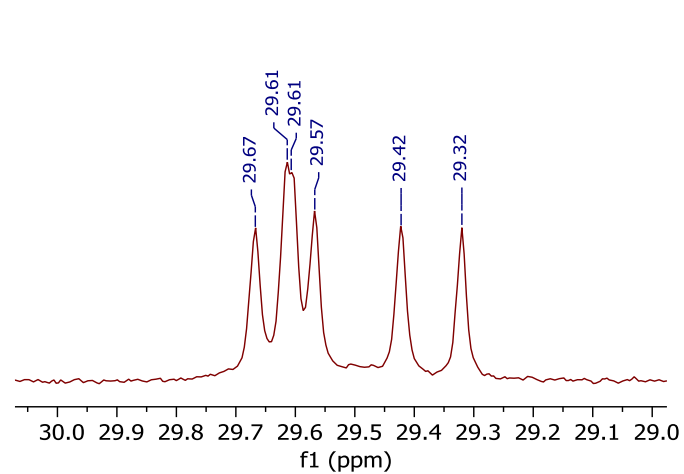
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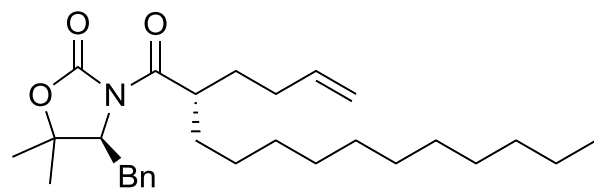
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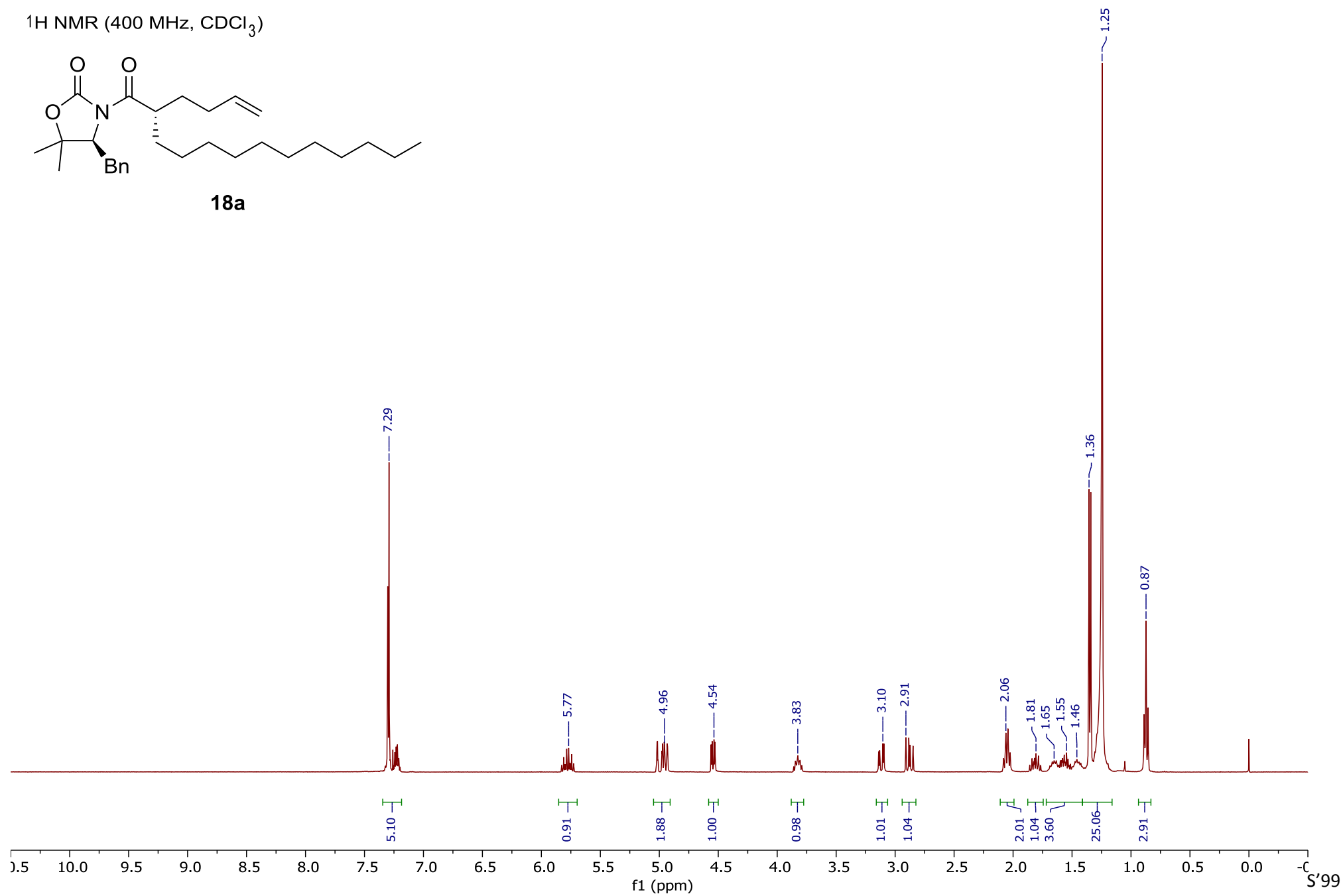
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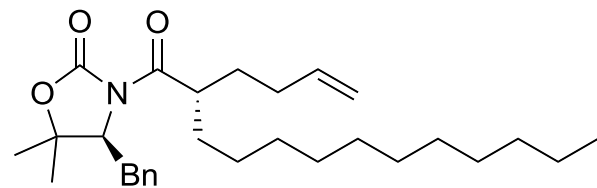
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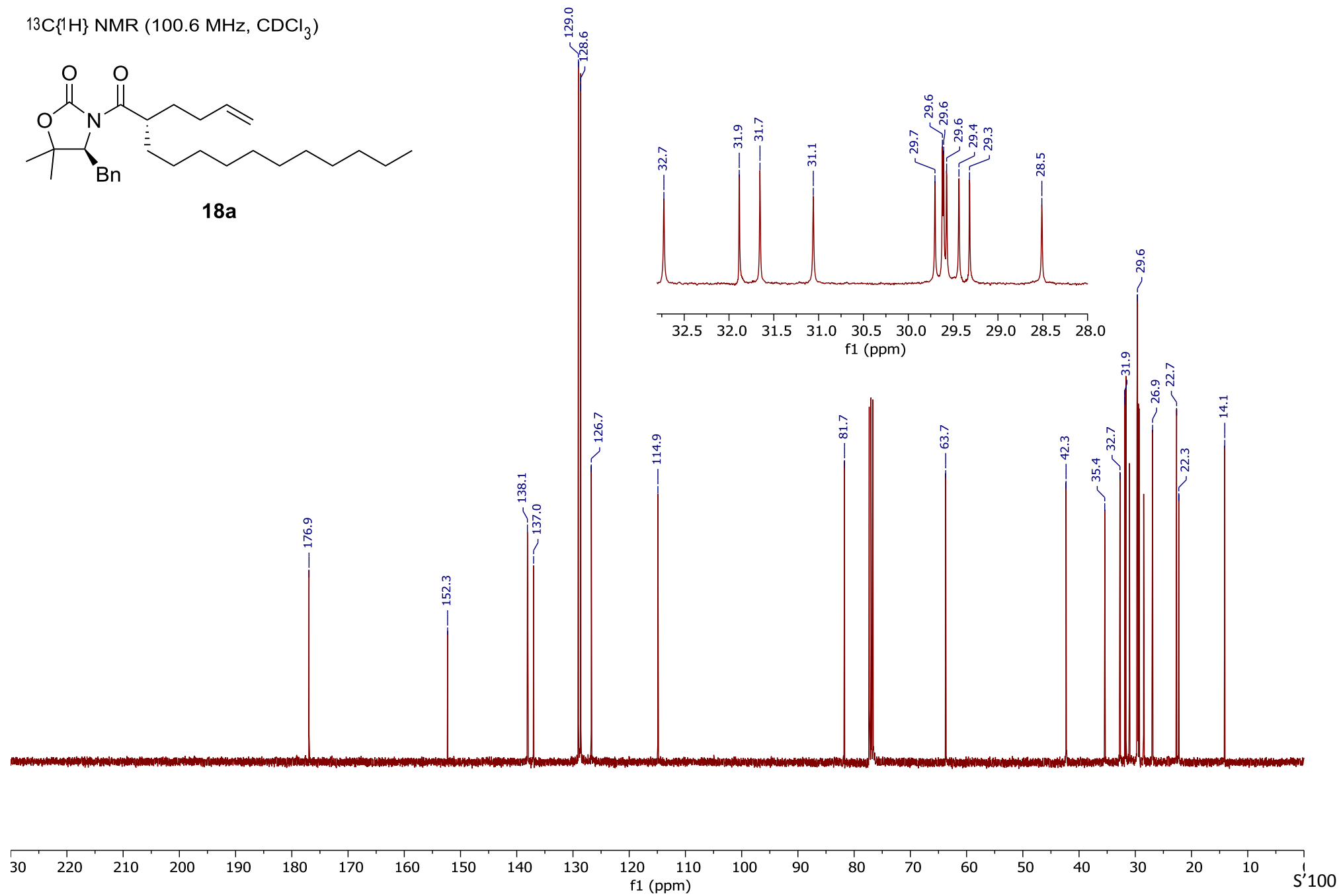
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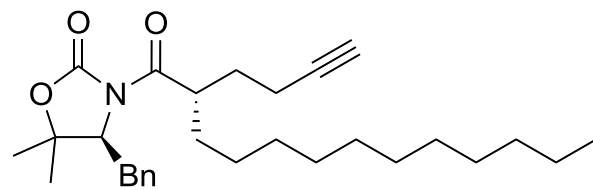
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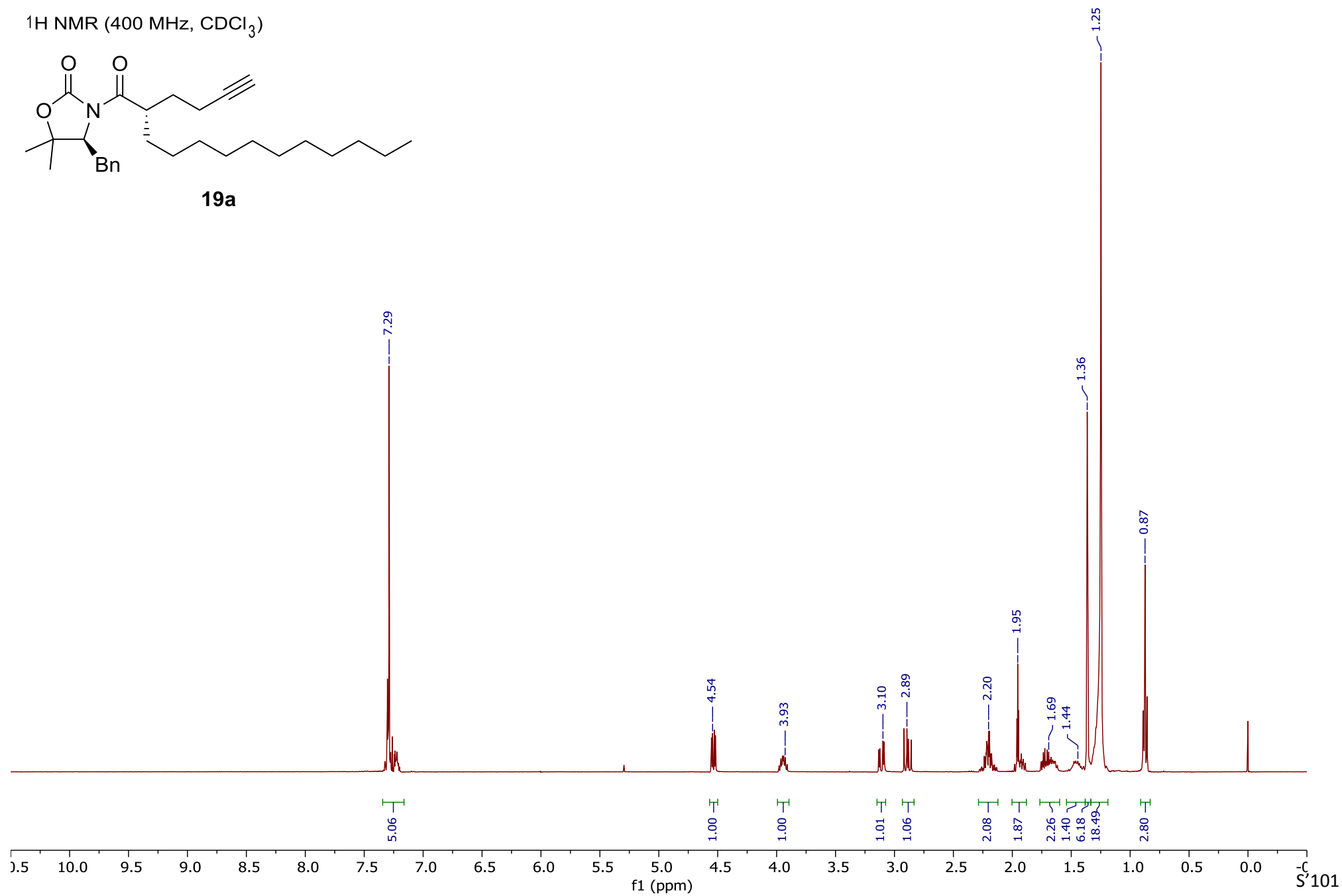
18a



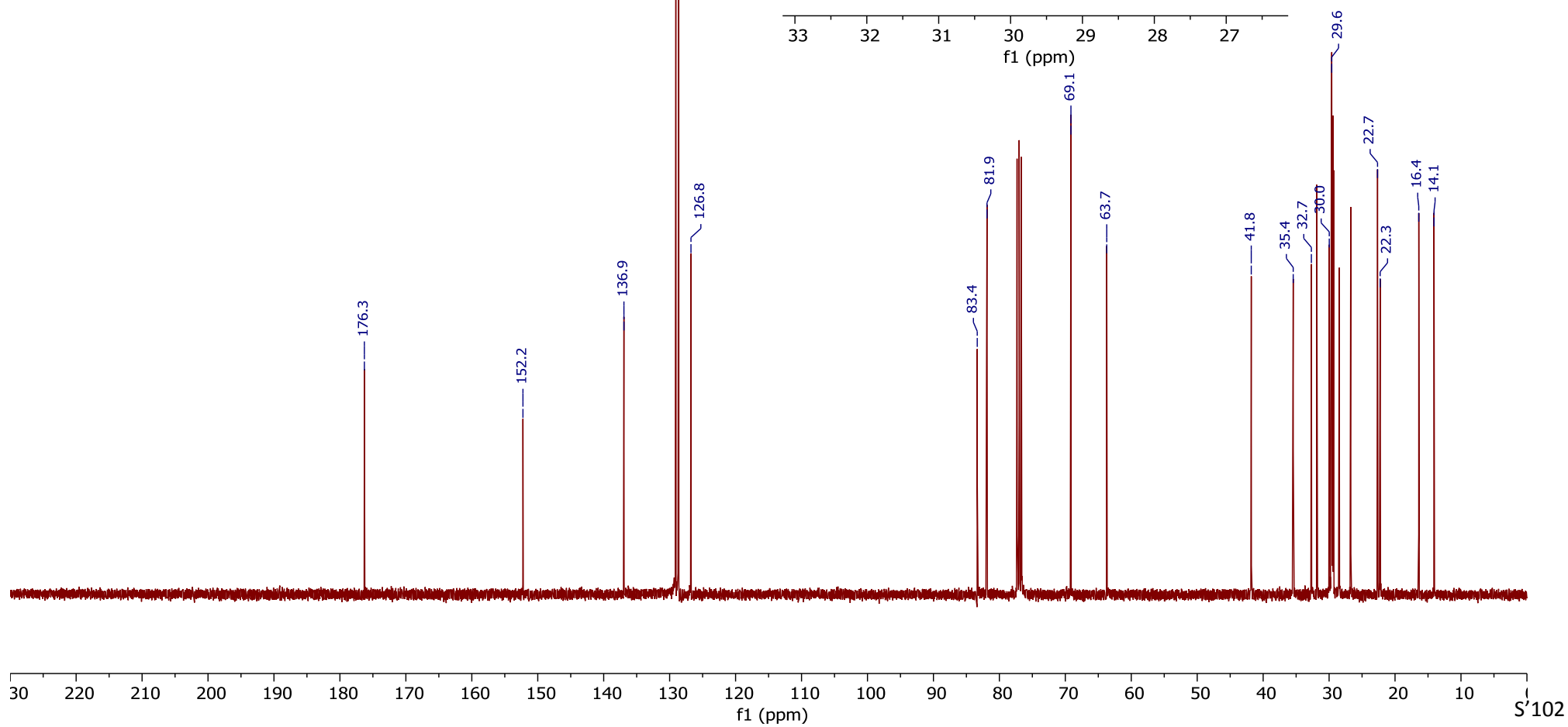
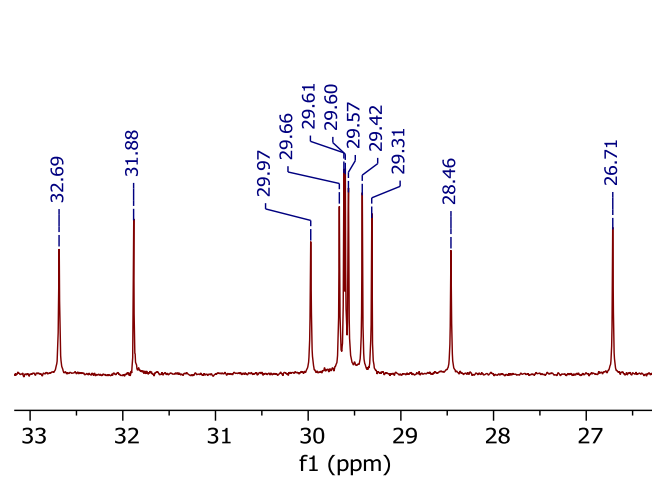
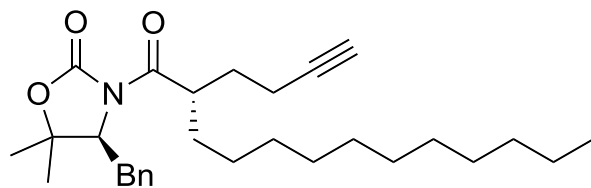
¹H NMR (400 MHz, CDCl₃)



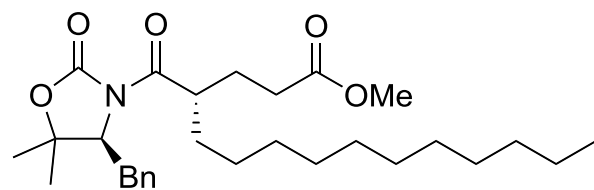
19a



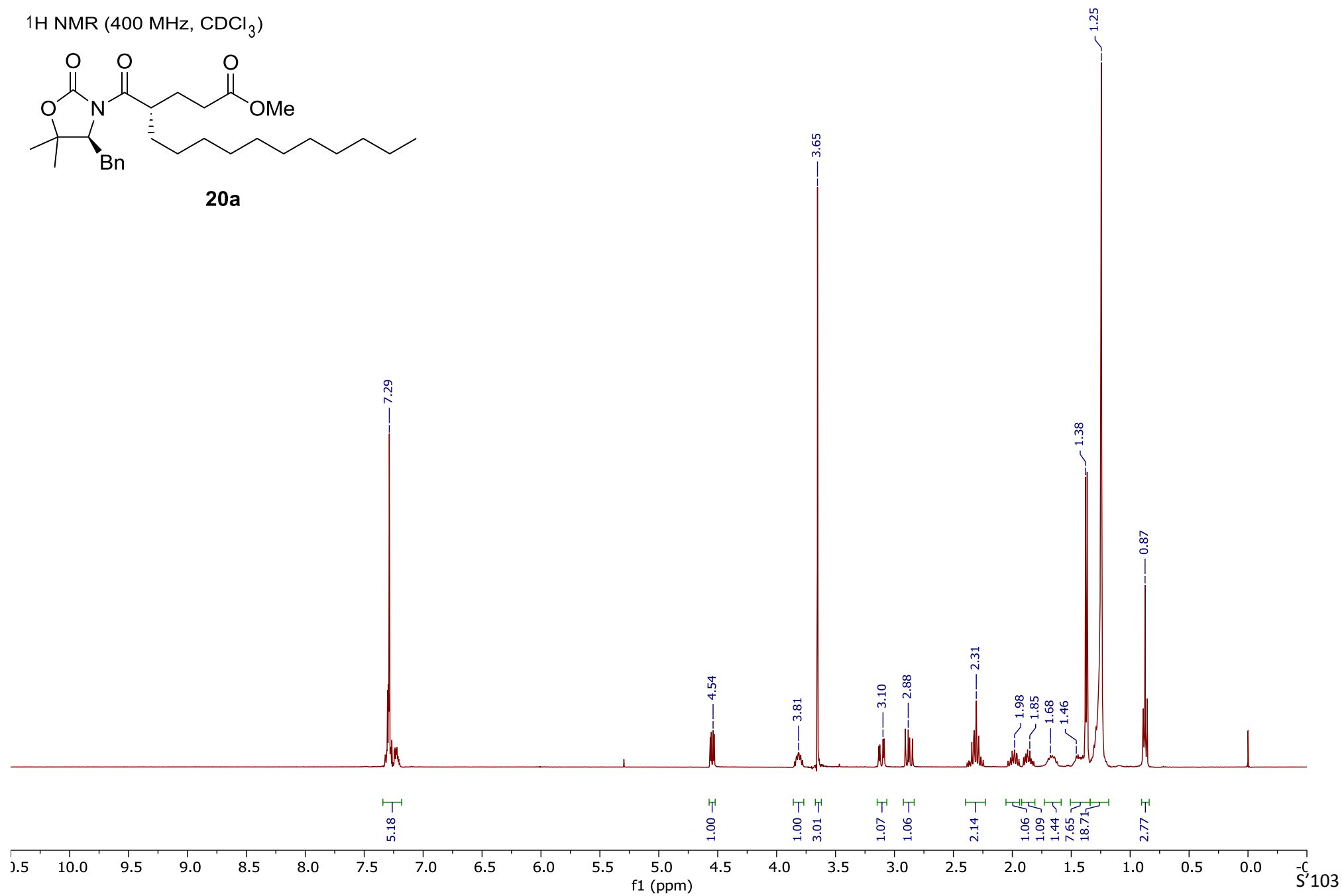
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



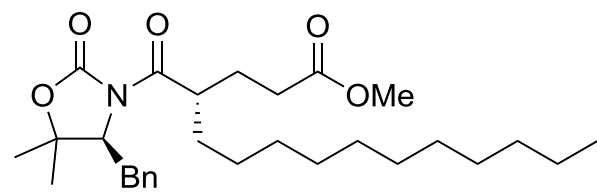
¹H NMR (400 MHz, CDCl₃)



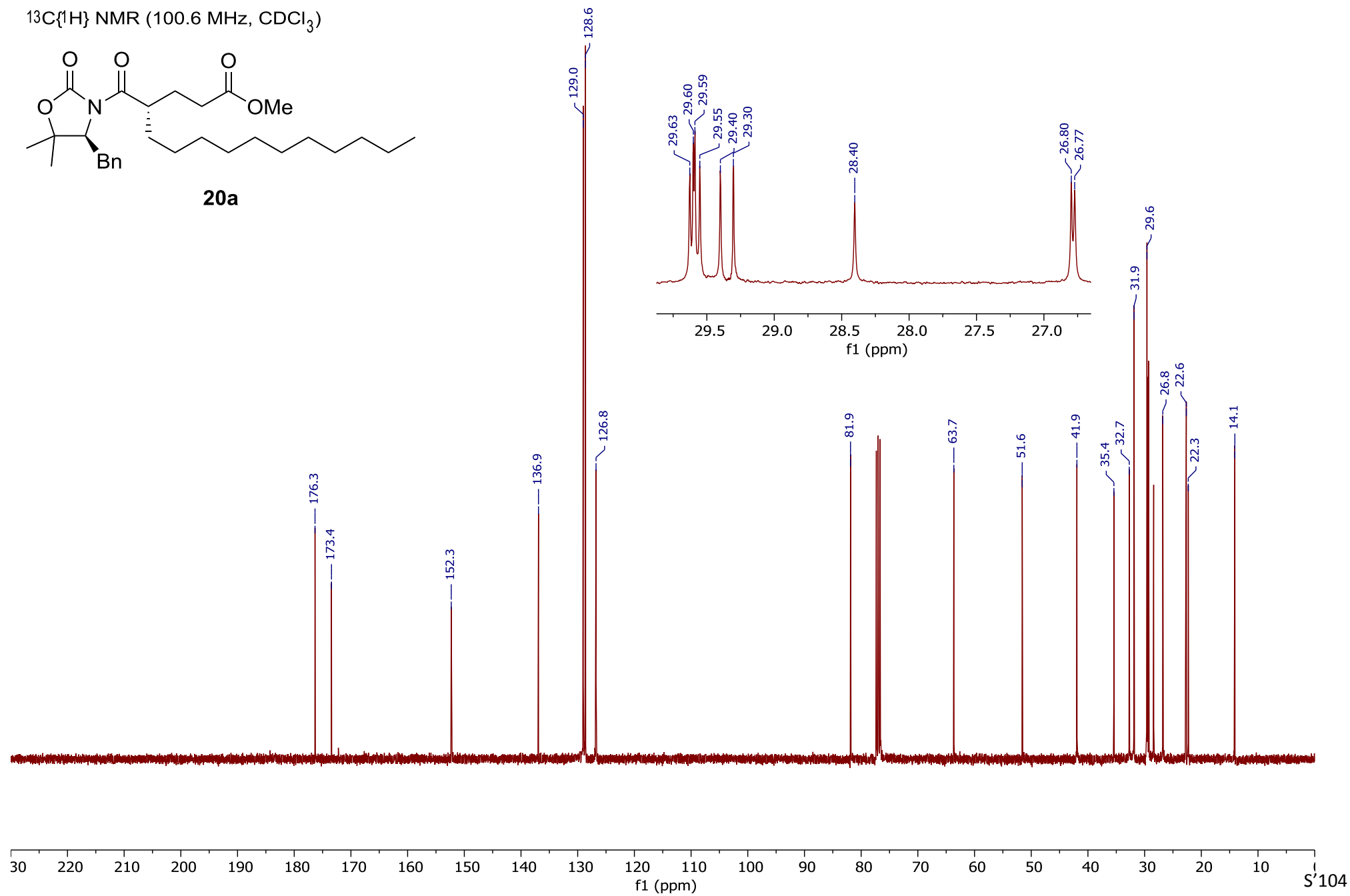
20a



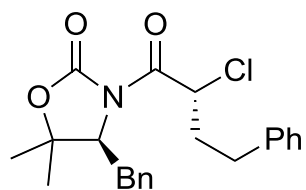
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



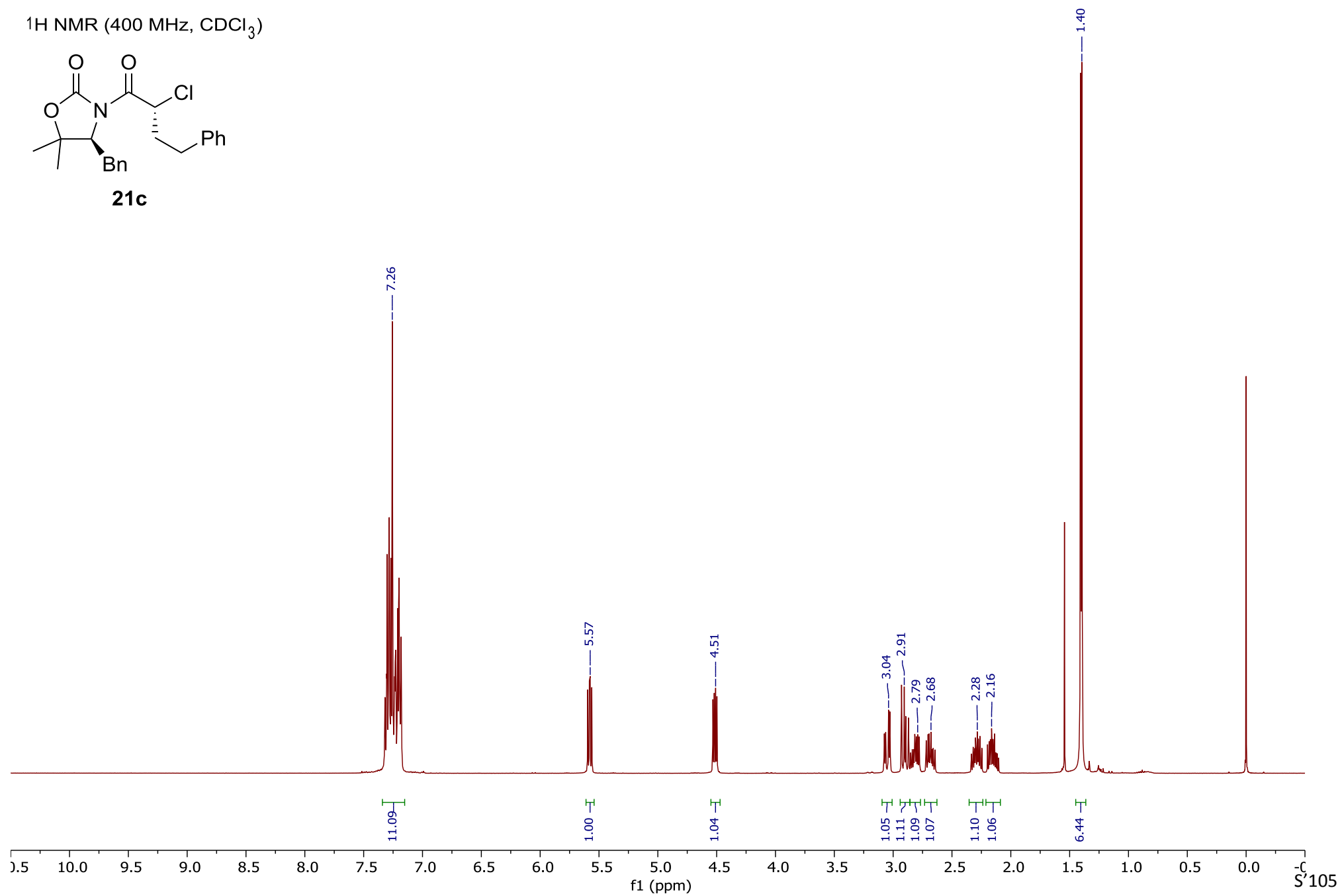
20a



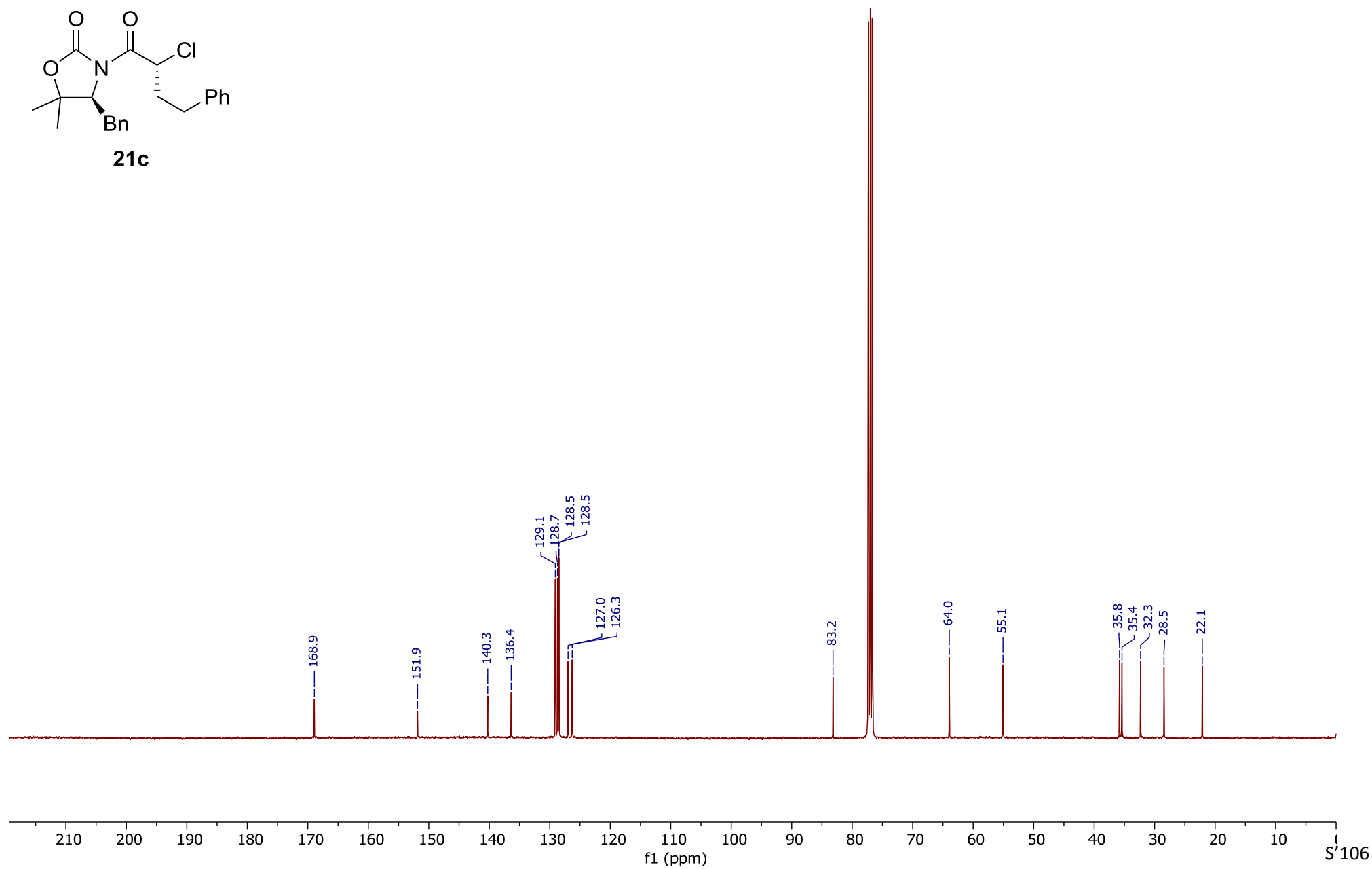
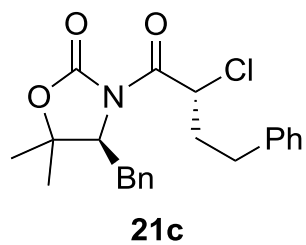
¹H NMR (400 MHz, CDCl₃)



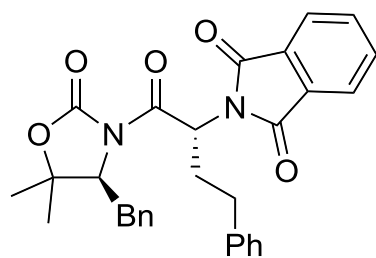
21c



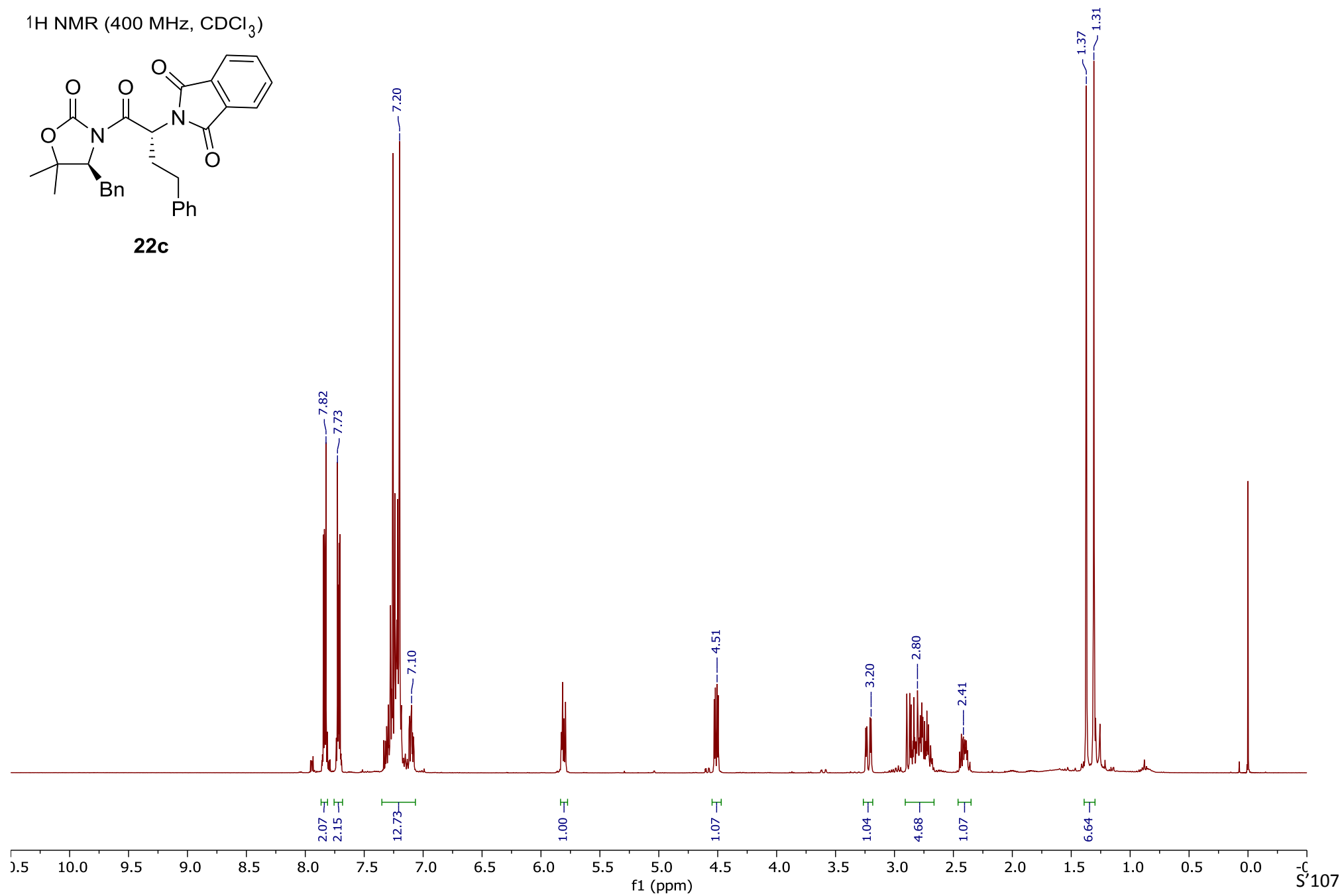
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



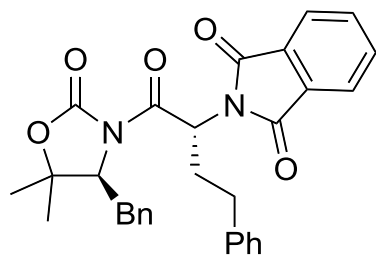
¹H NMR (400 MHz, CDCl₃)



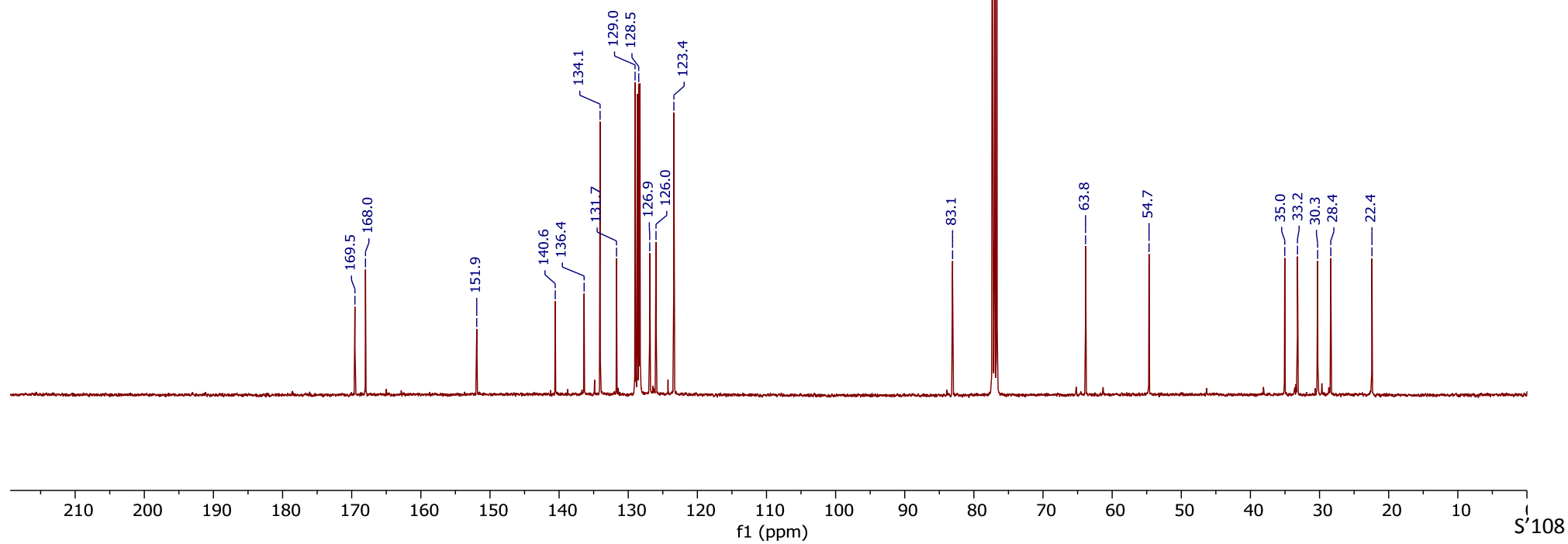
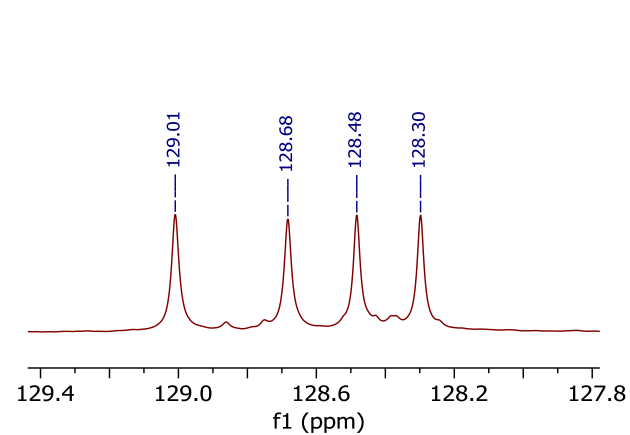
22c



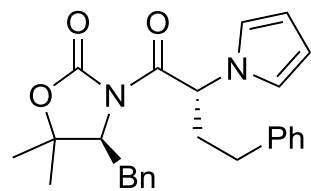
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



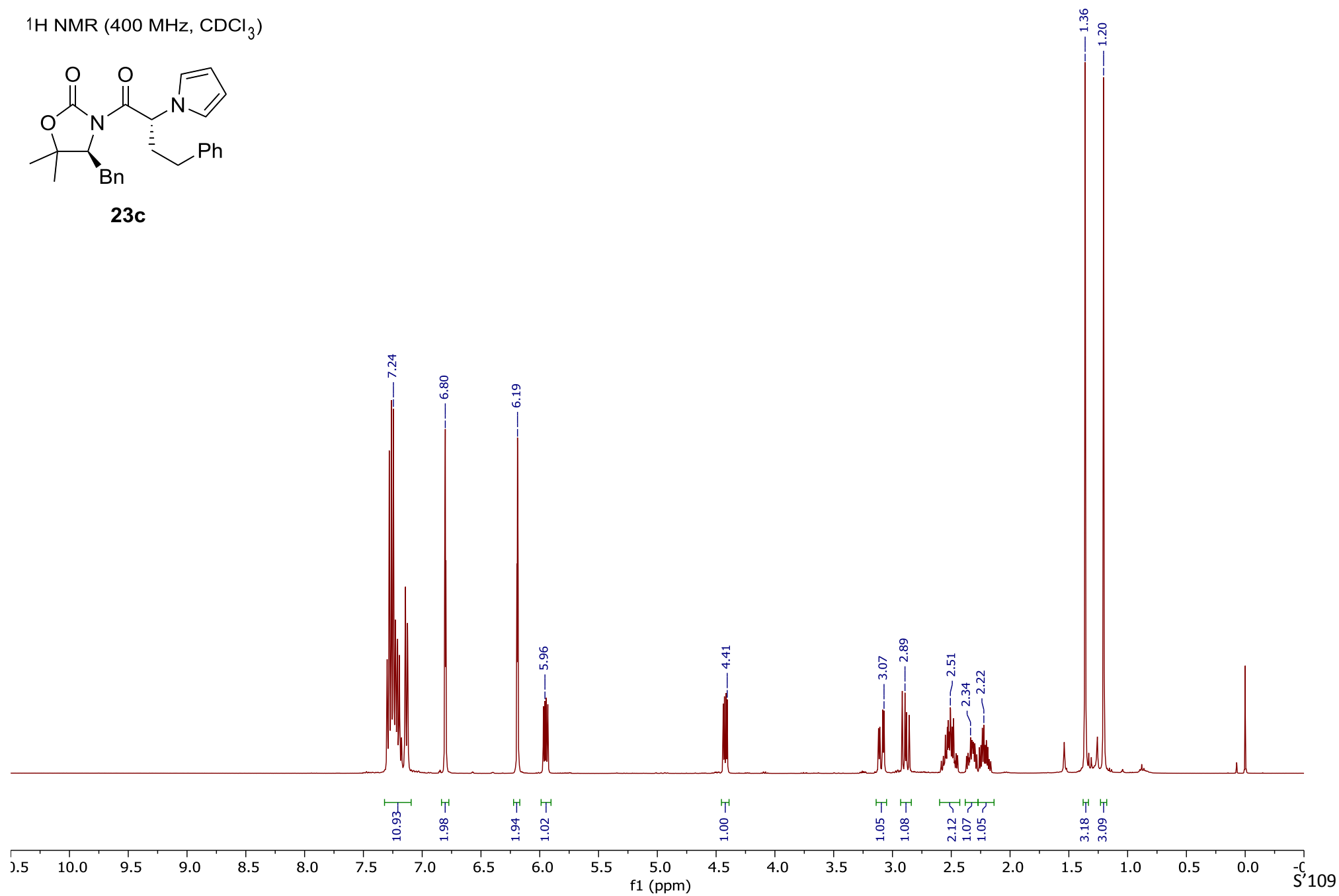
22c



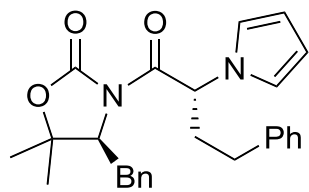
^1H NMR (400 MHz, CDCl_3)



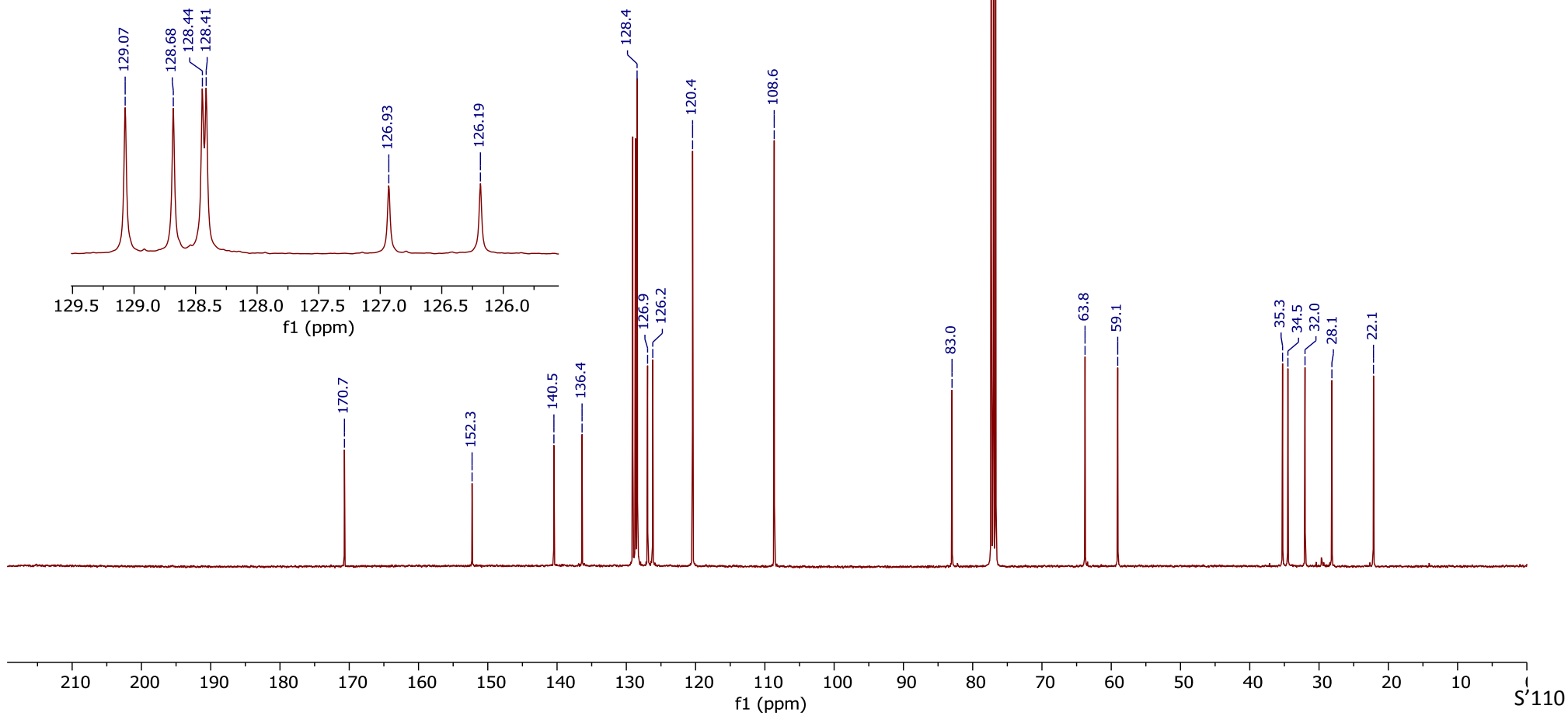
23c



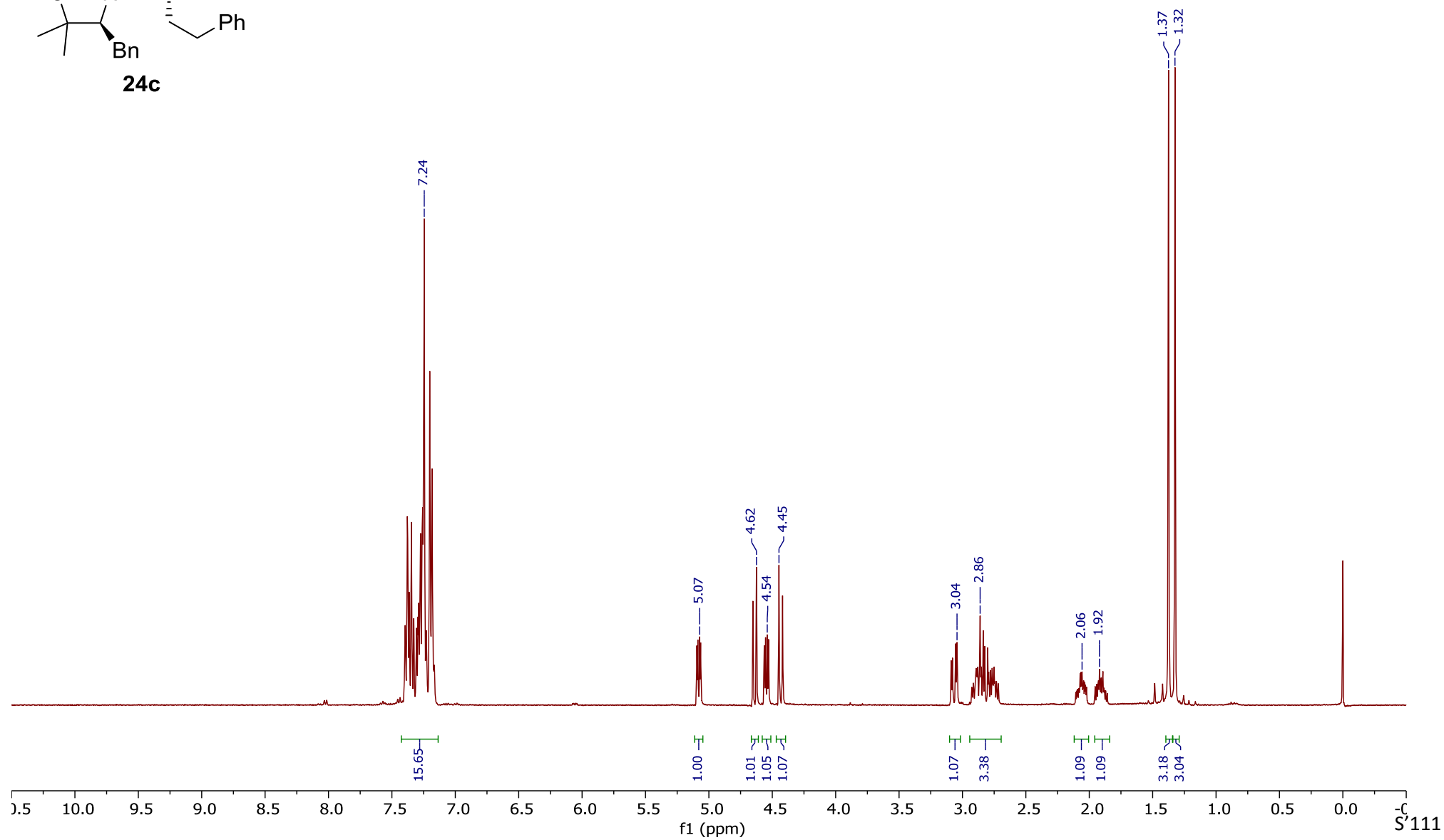
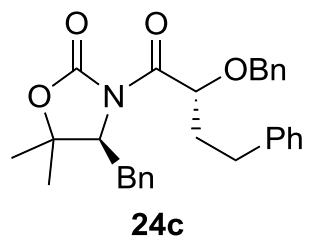
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



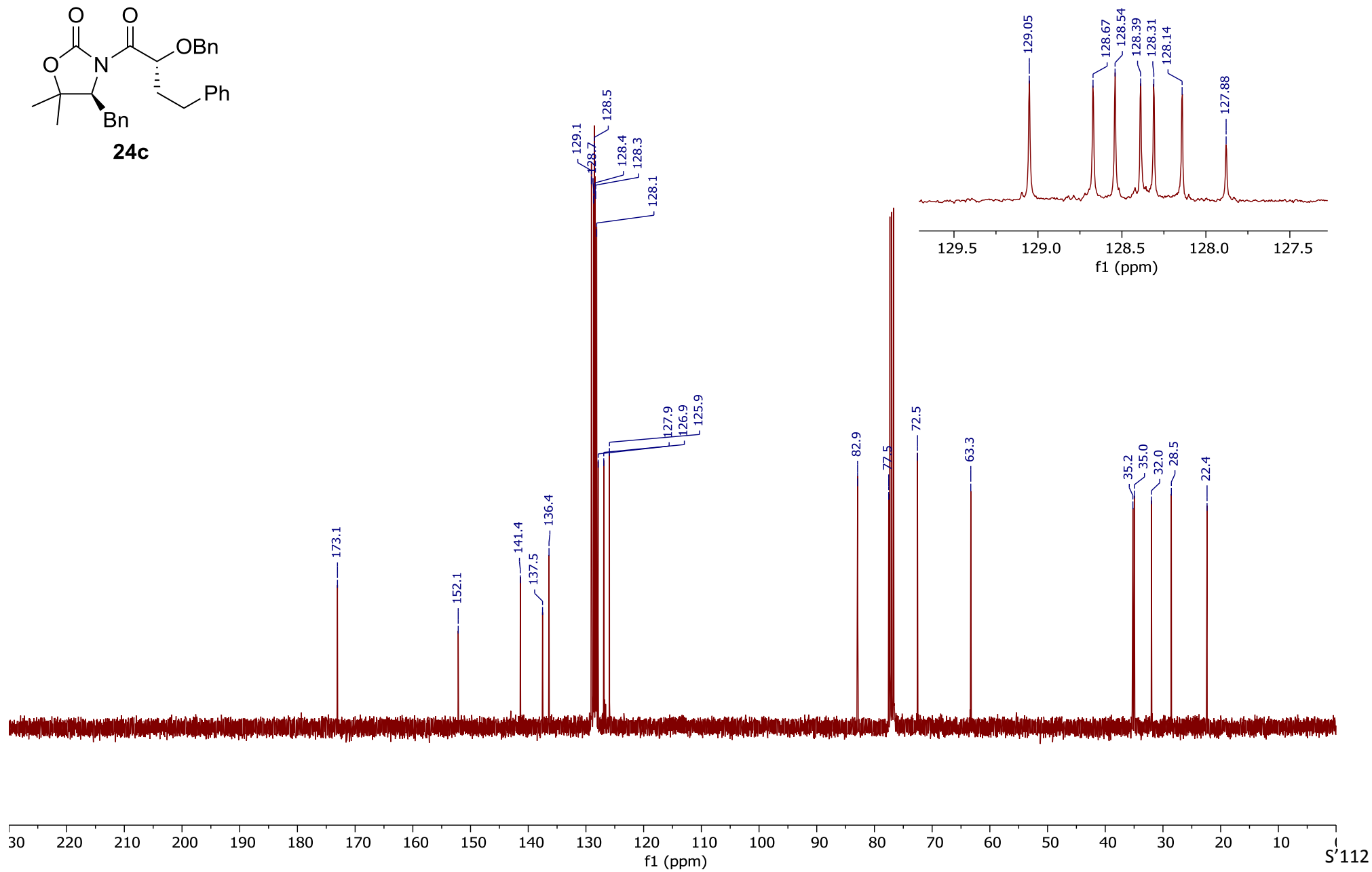
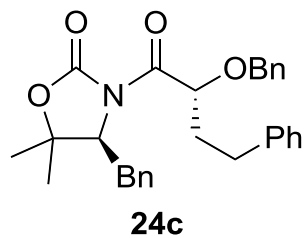
23c



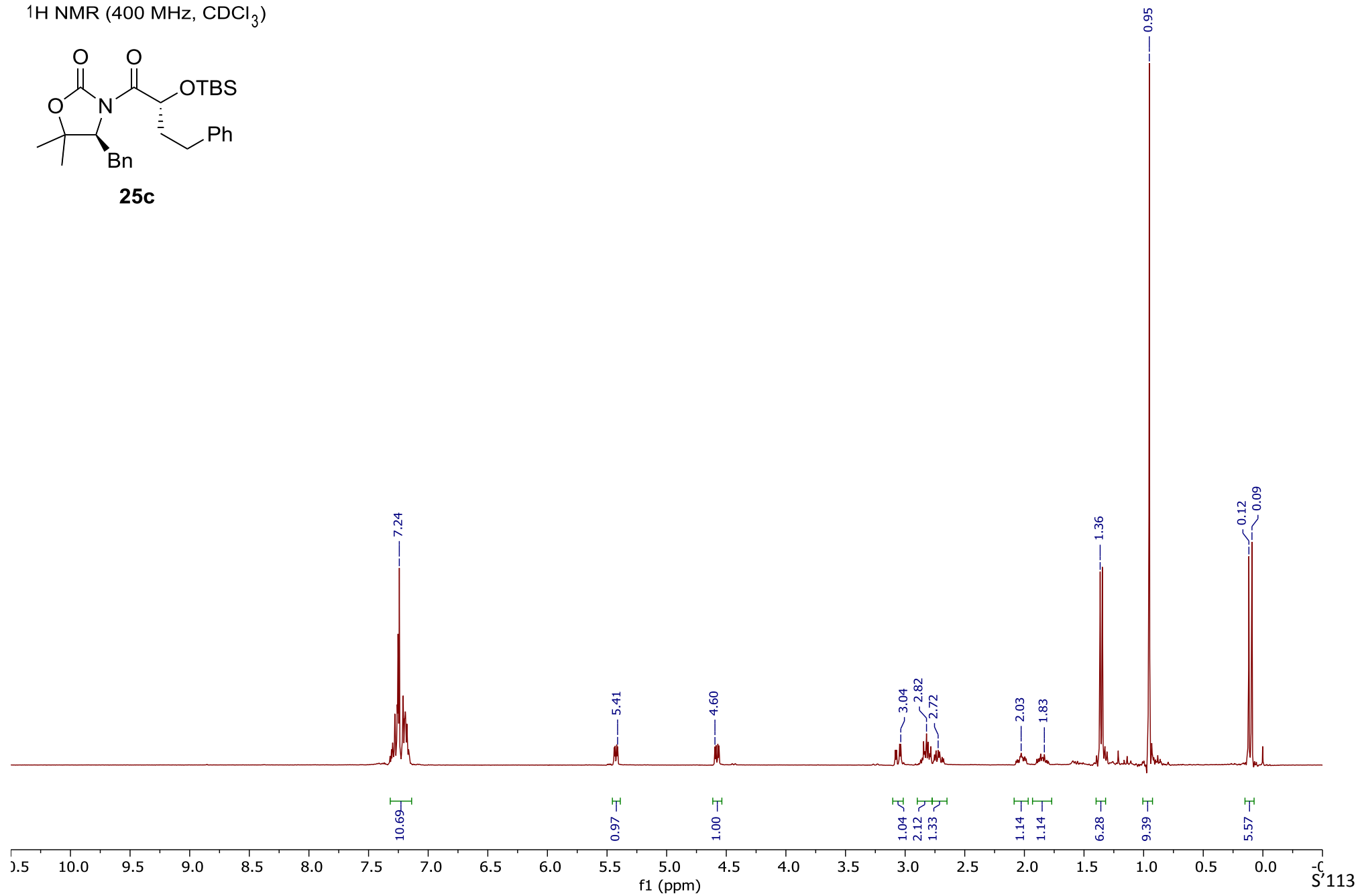
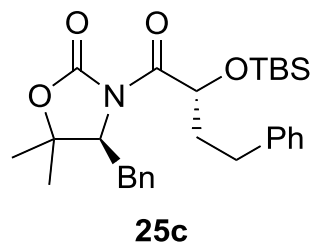
^1H NMR (400 MHz, CDCl_3)



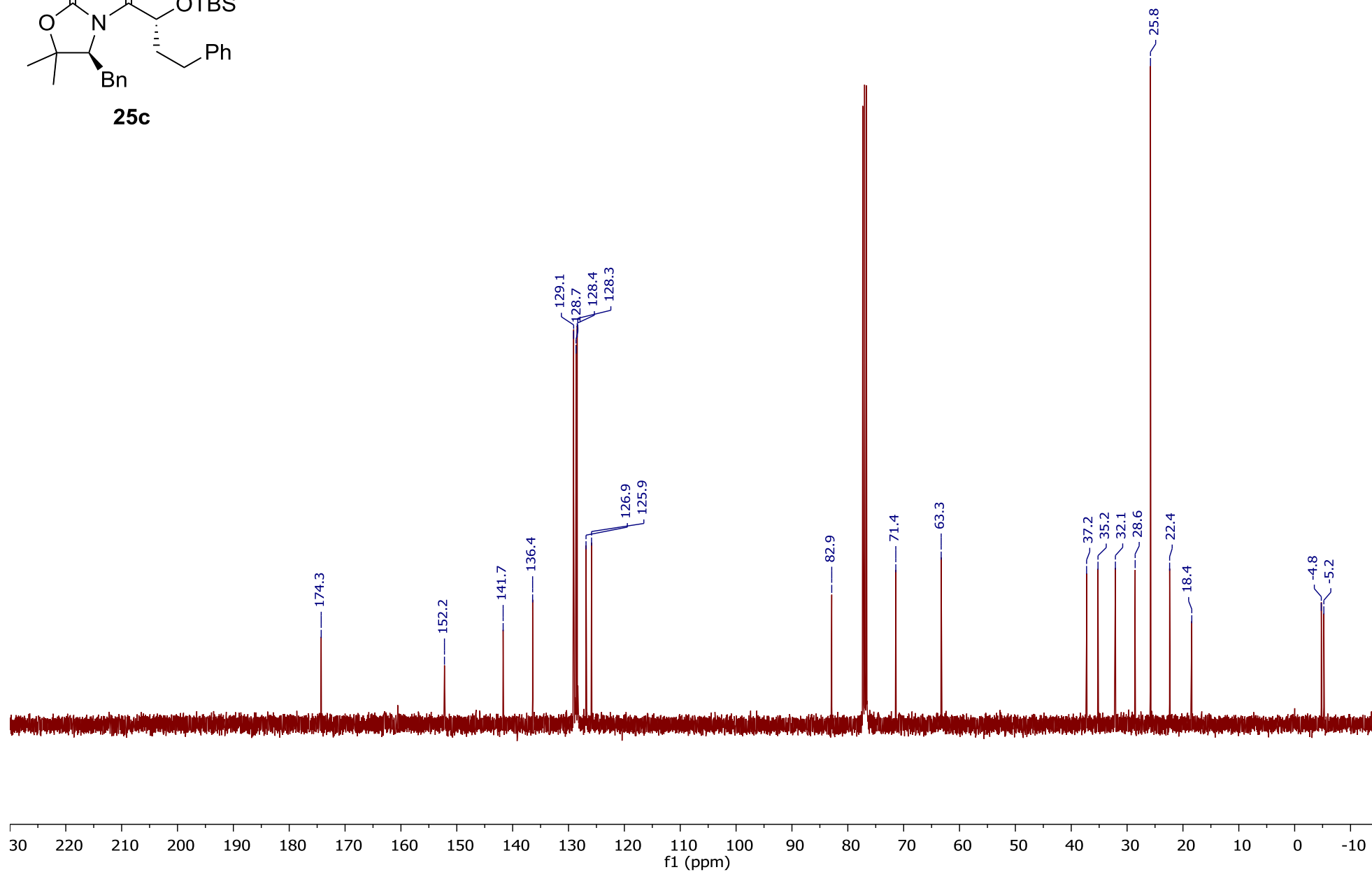
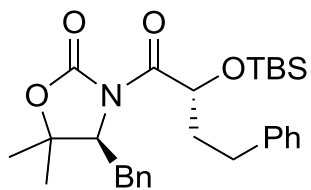
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



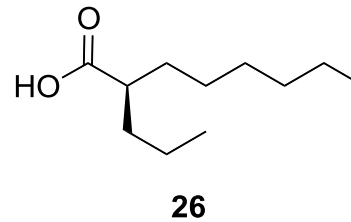
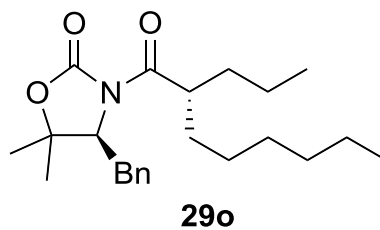
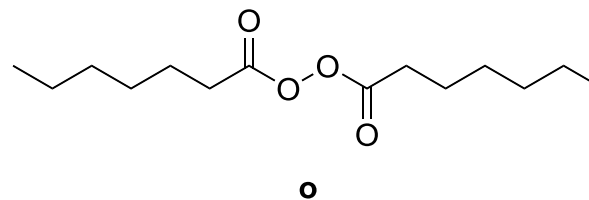
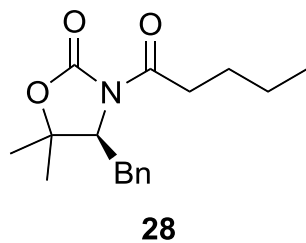
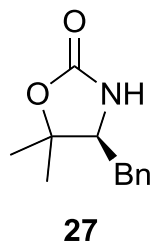
¹H NMR (400 MHz, CDCl₃)



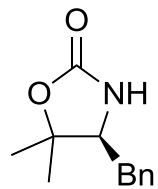
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



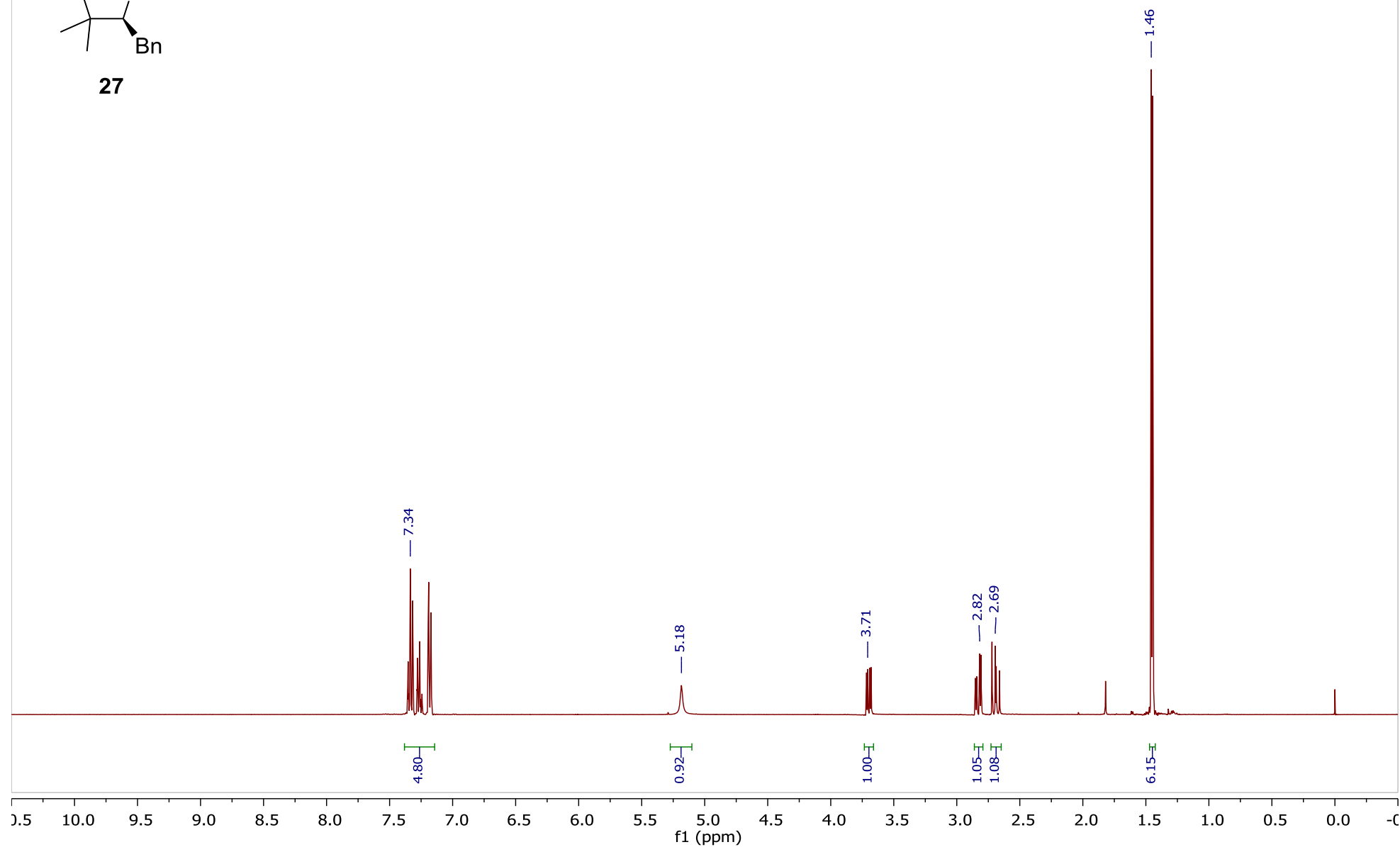
6. ARUNDIC ACID SYNTHESIS



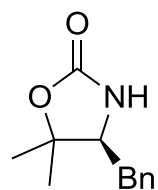
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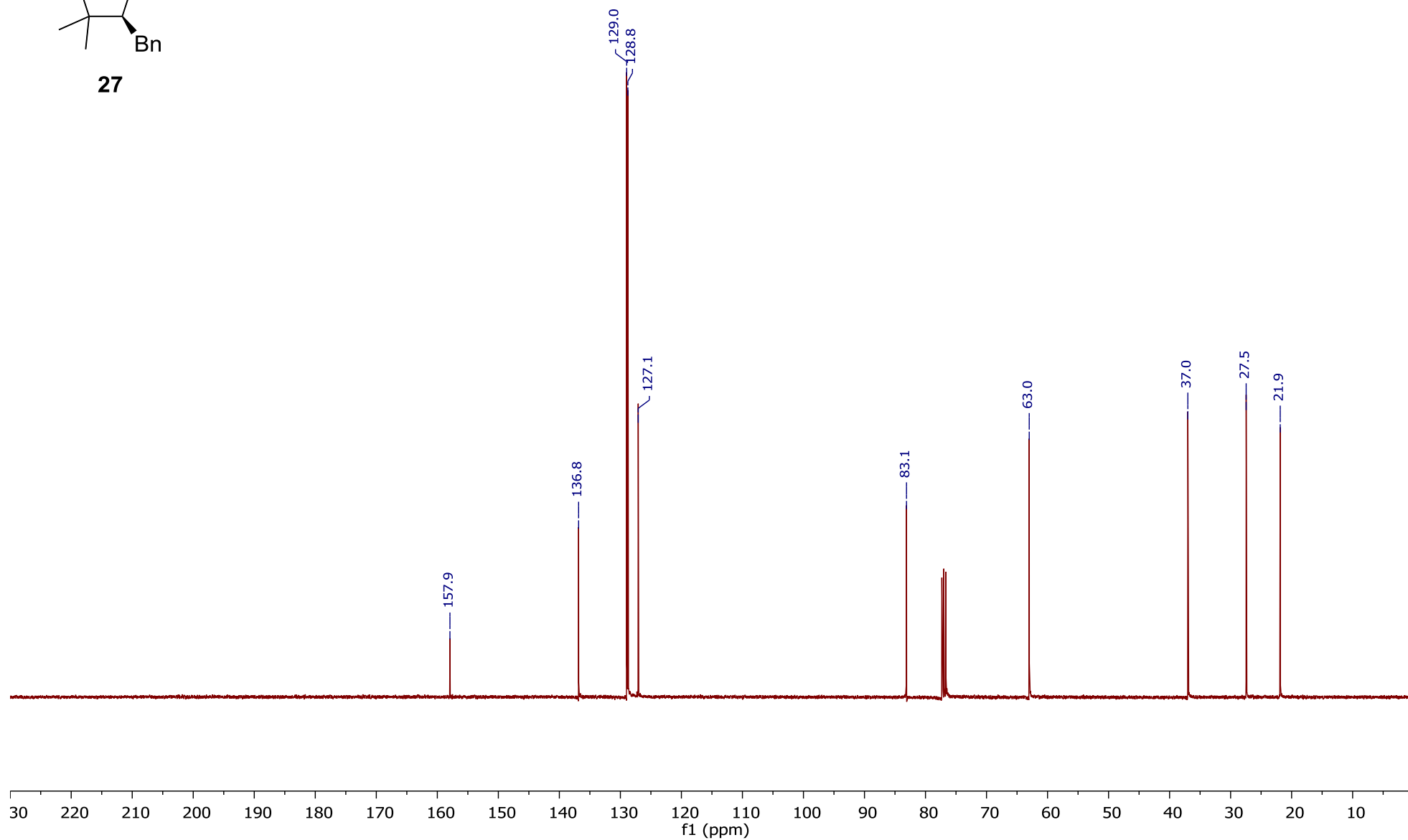
27



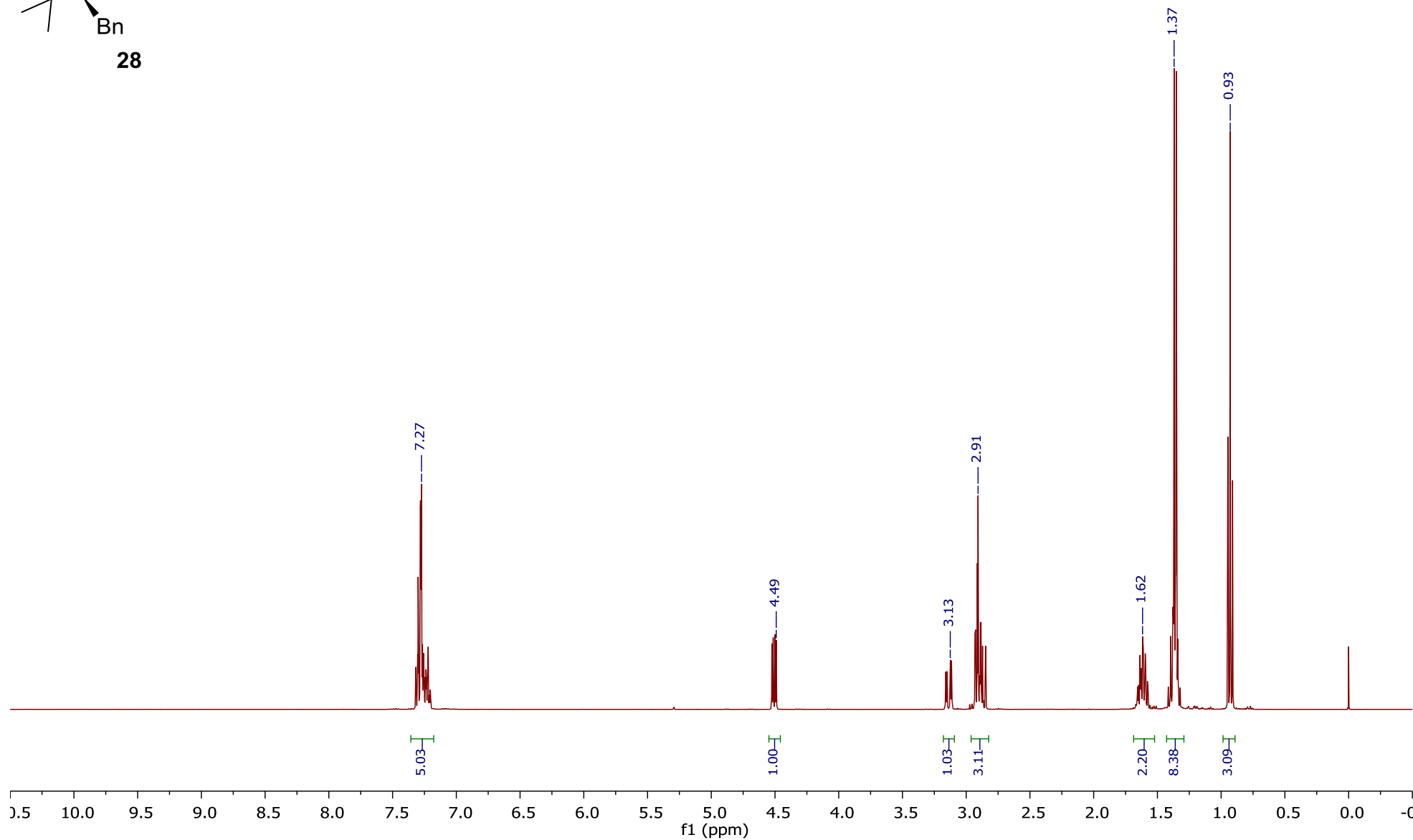
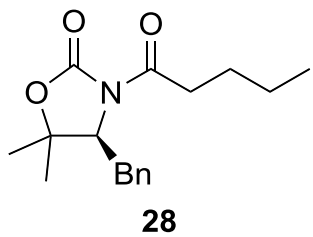
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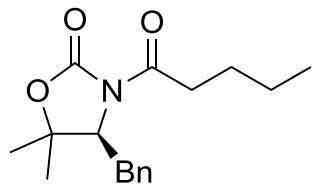
27



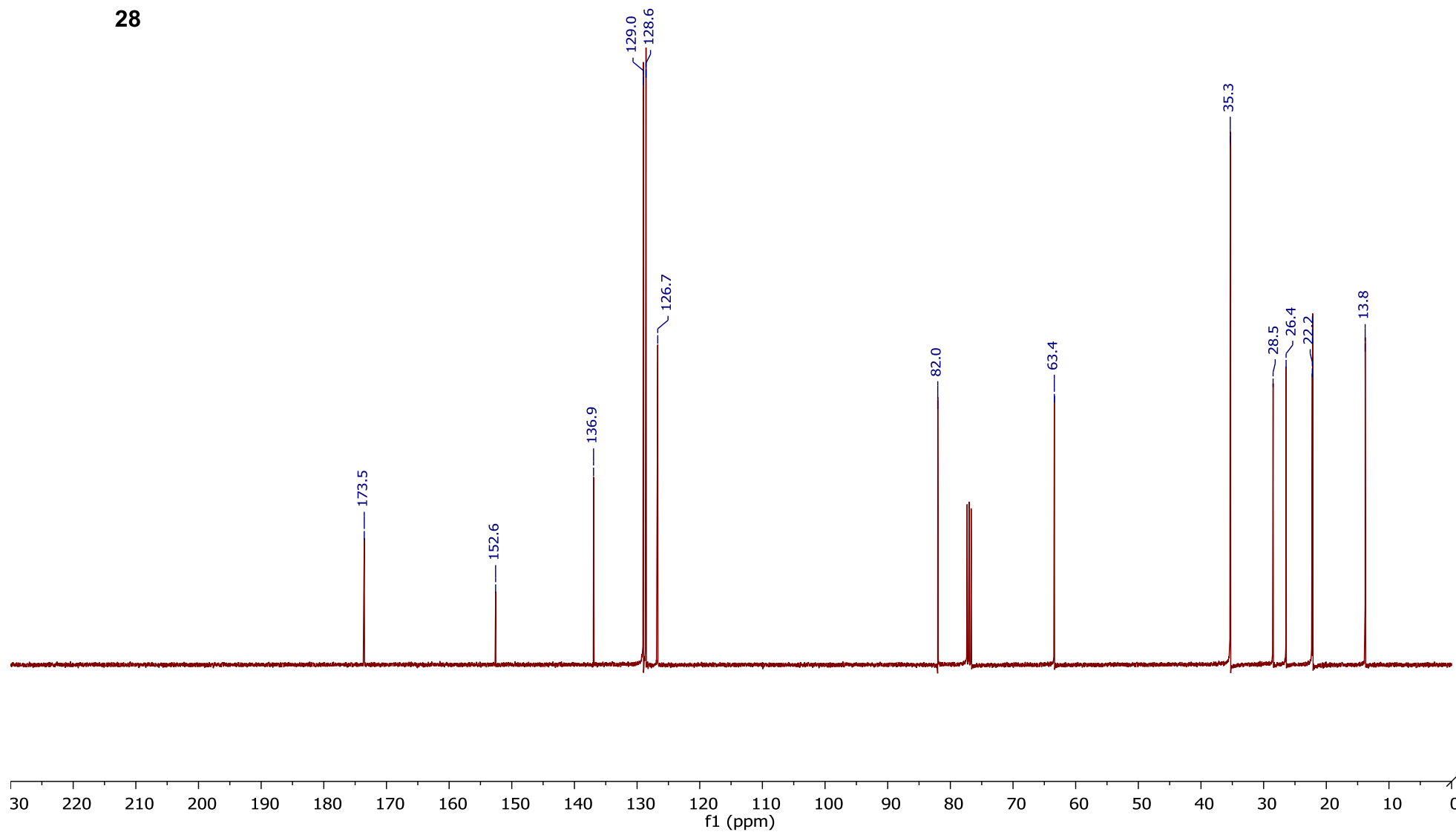
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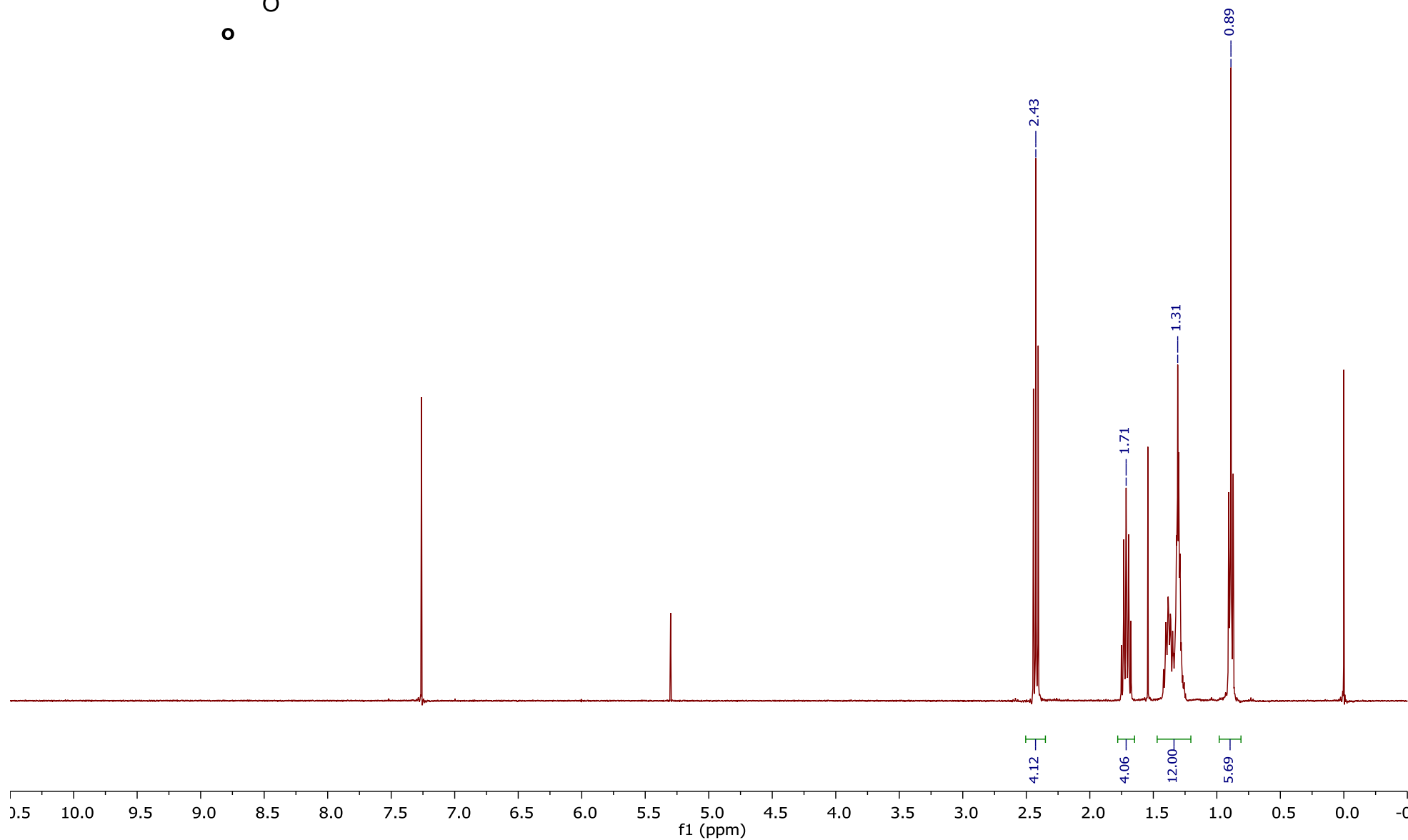
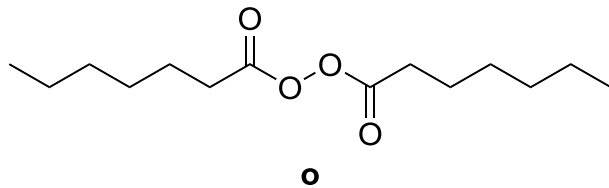
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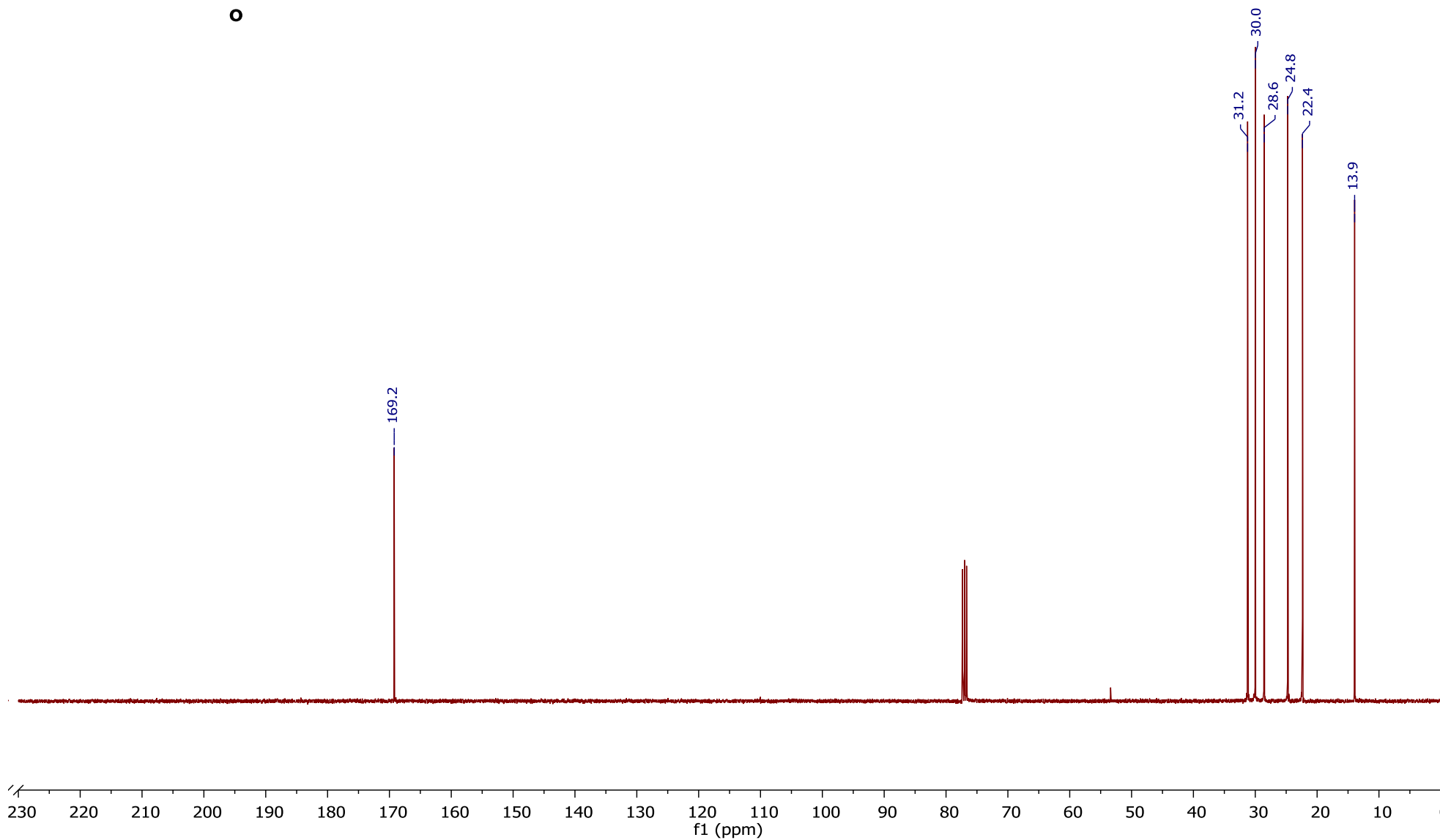
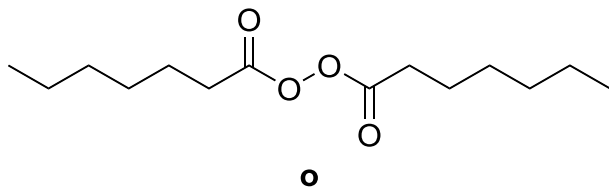
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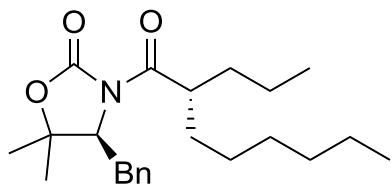
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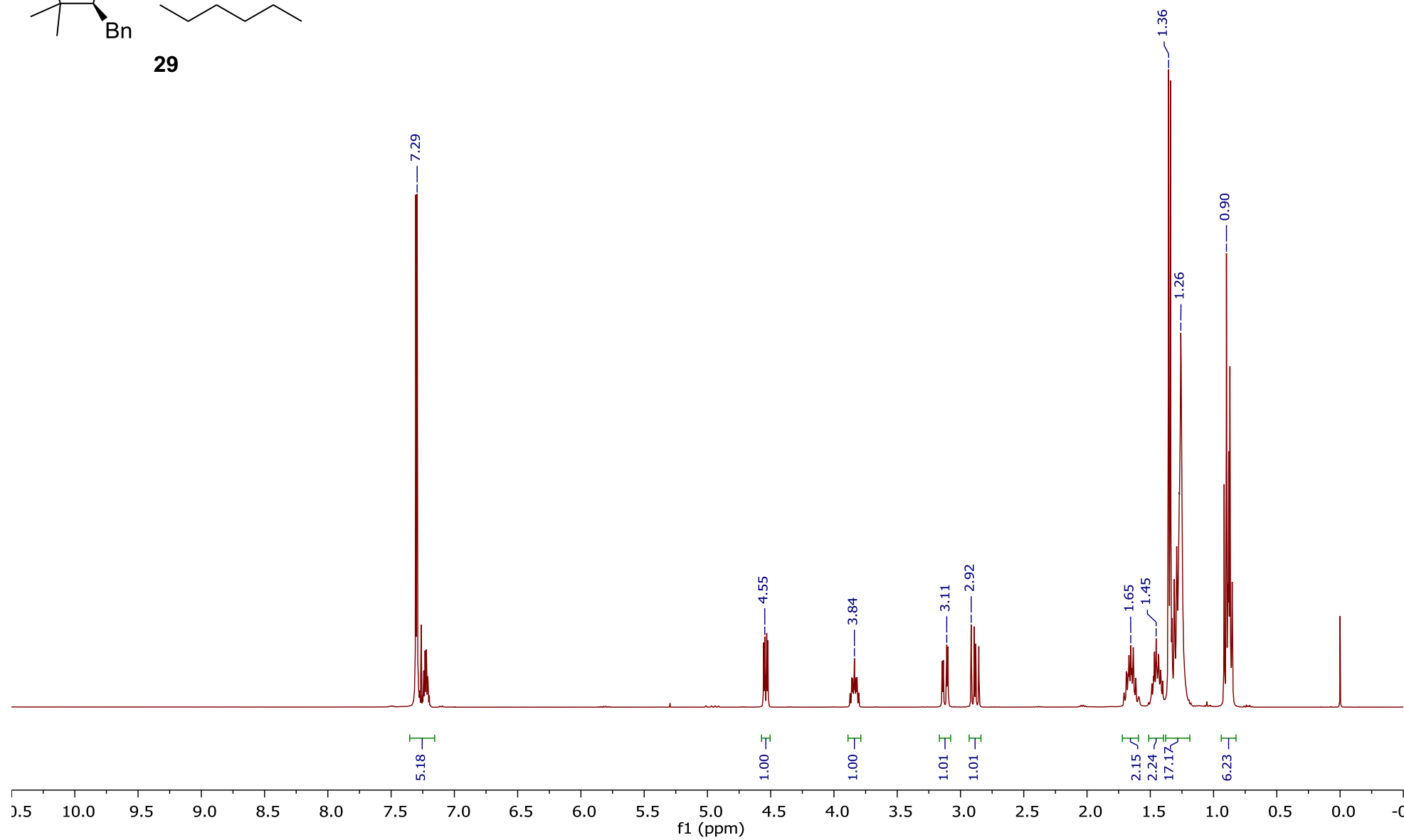
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



¹H NMR (400 MHz, CDCl₃)

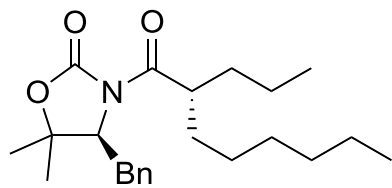


29

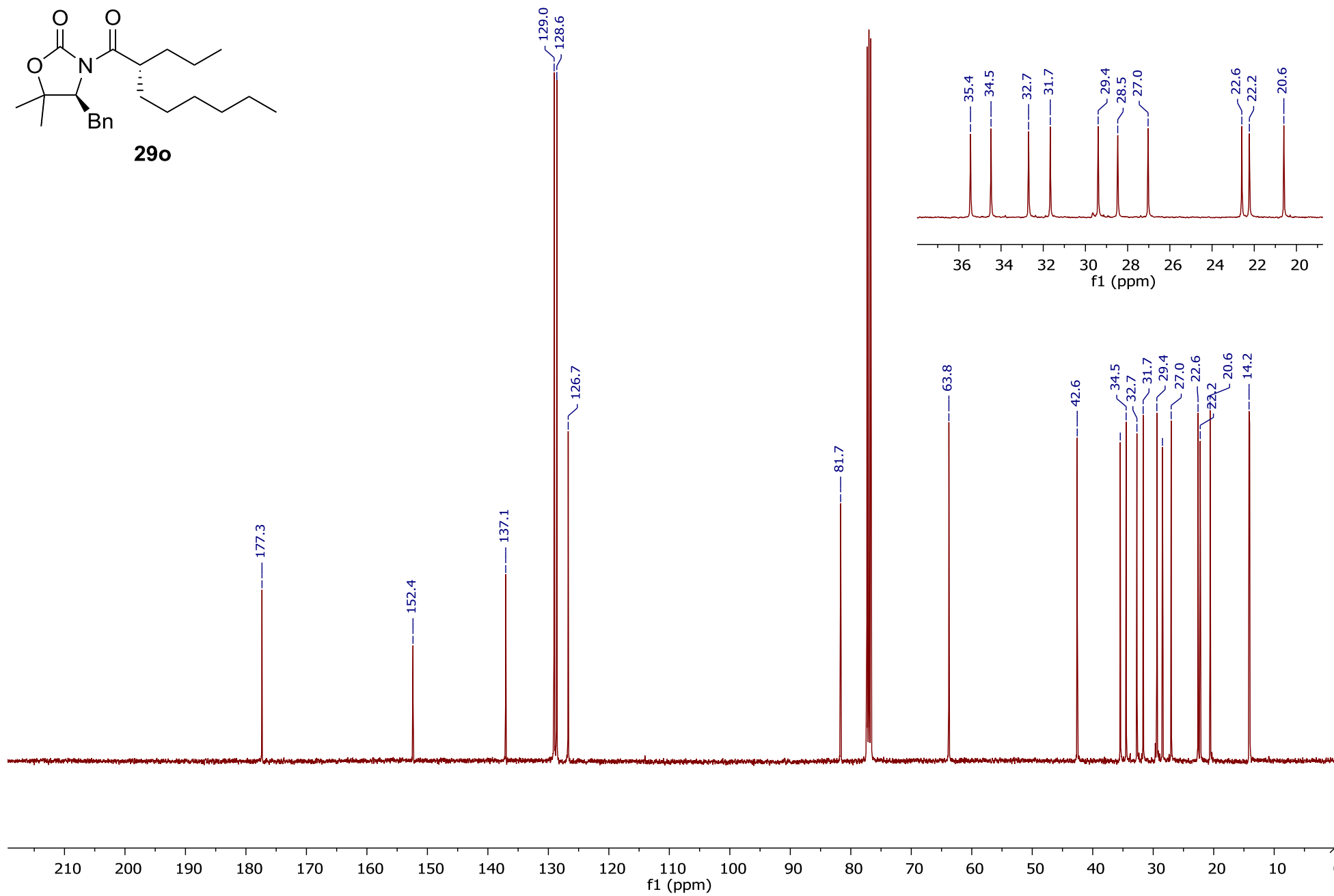


S'122

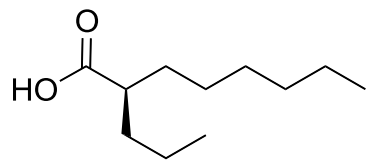
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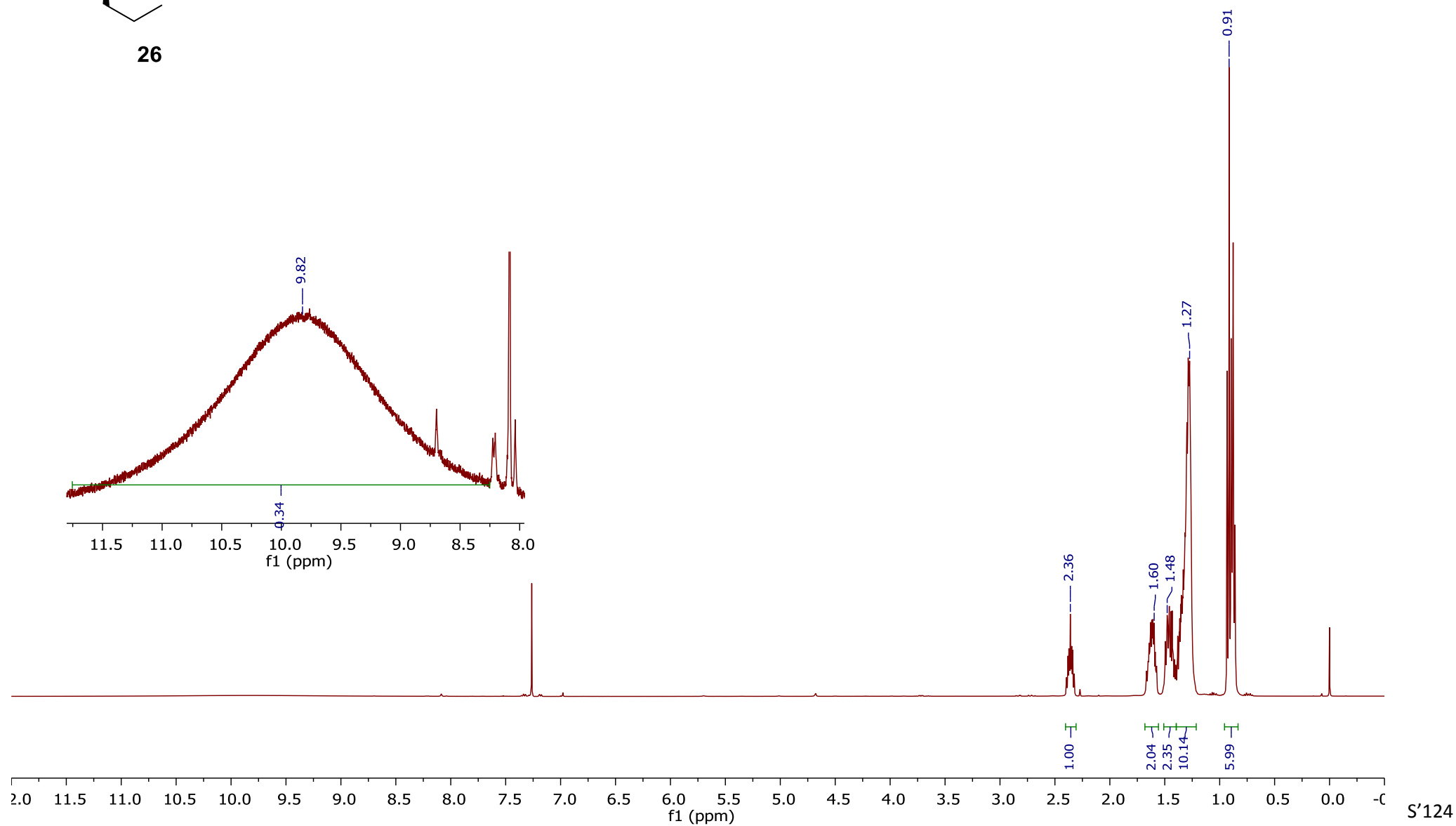
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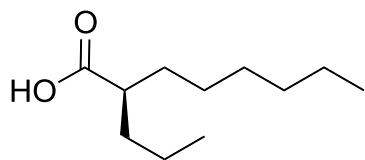
^1H NMR (400 MHz, CDCl_3)



26



$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



26

