

Synthesis of Conjugation-ready Zwitterionic Oligosaccharides by Chemoselective Thioglycoside Activation

Supporting Information: Spectral Characterization

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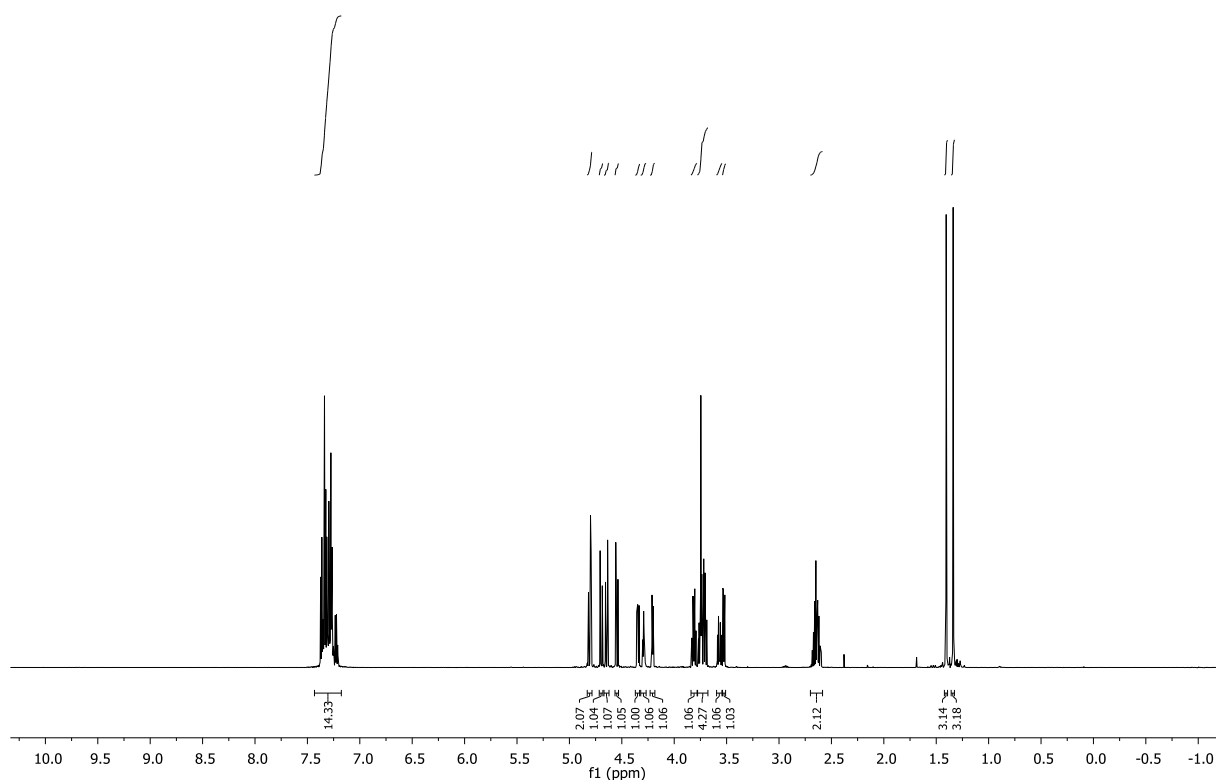
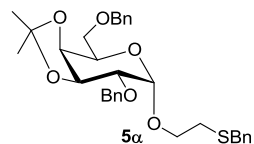
^cPresent address: National Center for Advancing Translational Sciences,
National Institutes of Health, 9800 Medical Center Drive, Rockville, MD 20850,
USA

*e-Mail addresses:

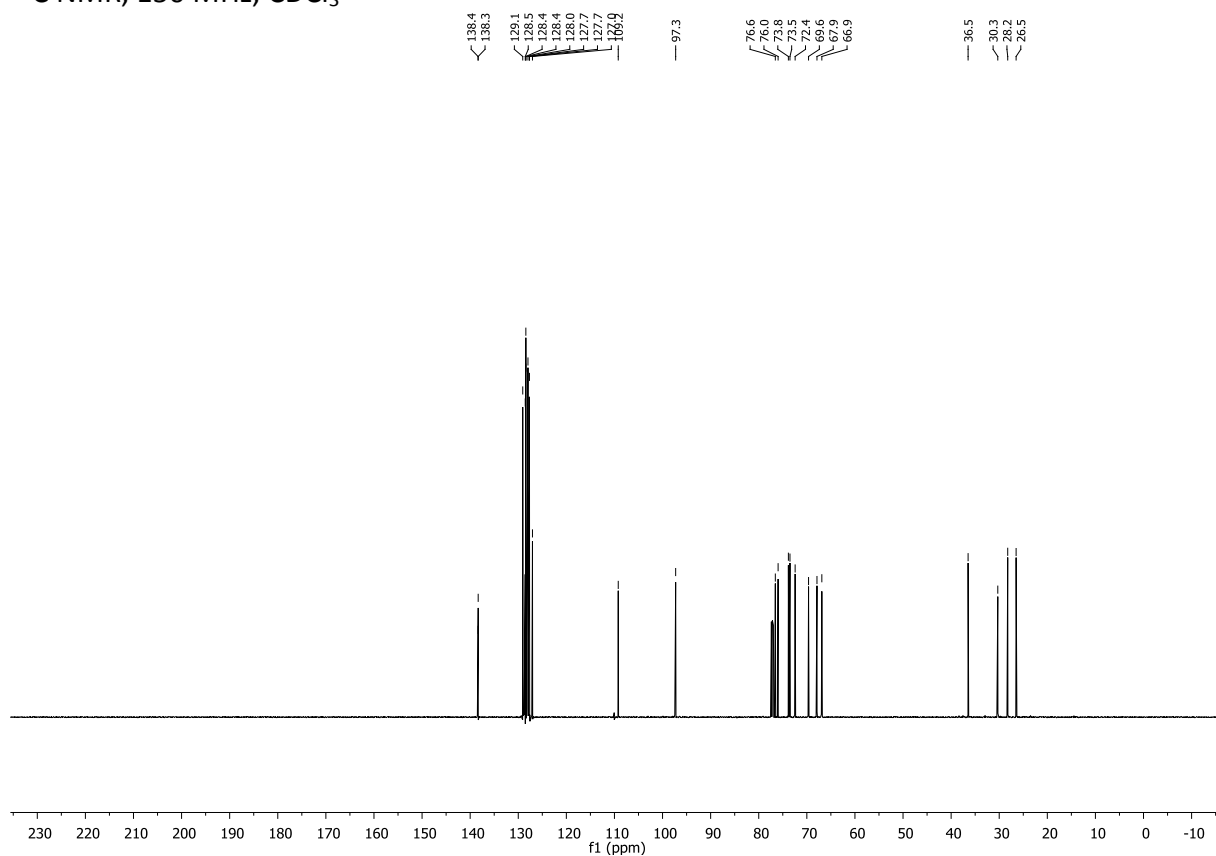
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clanylebev.pereira@mpikg.mpg.de

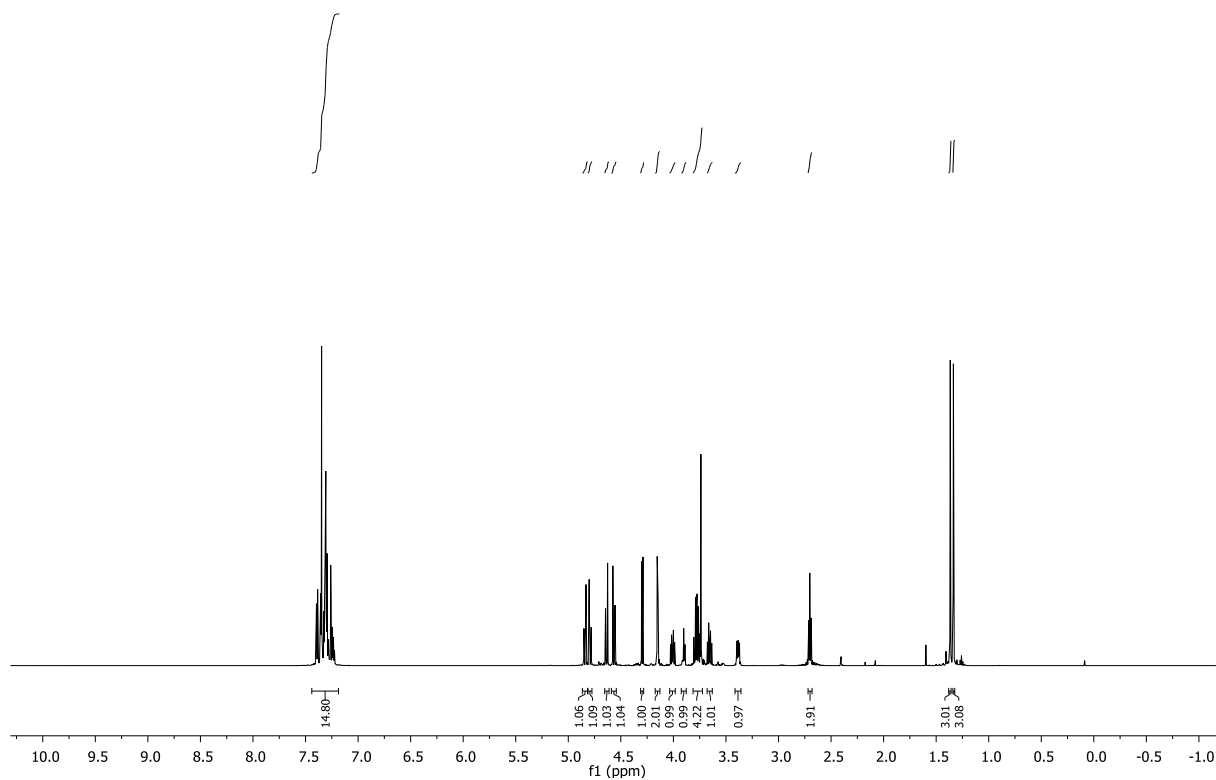
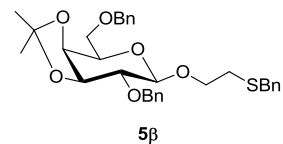
^1H NMR, 600 MHz, CDCl_3



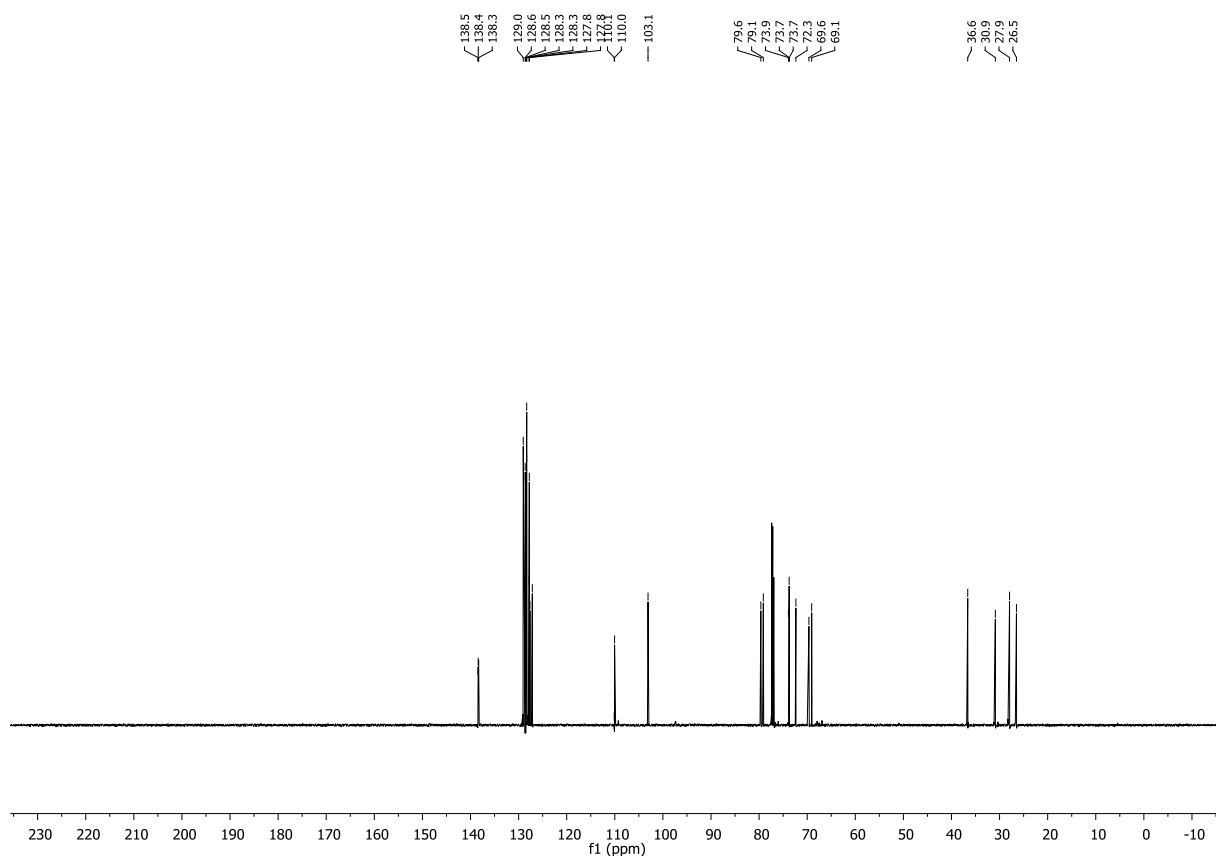
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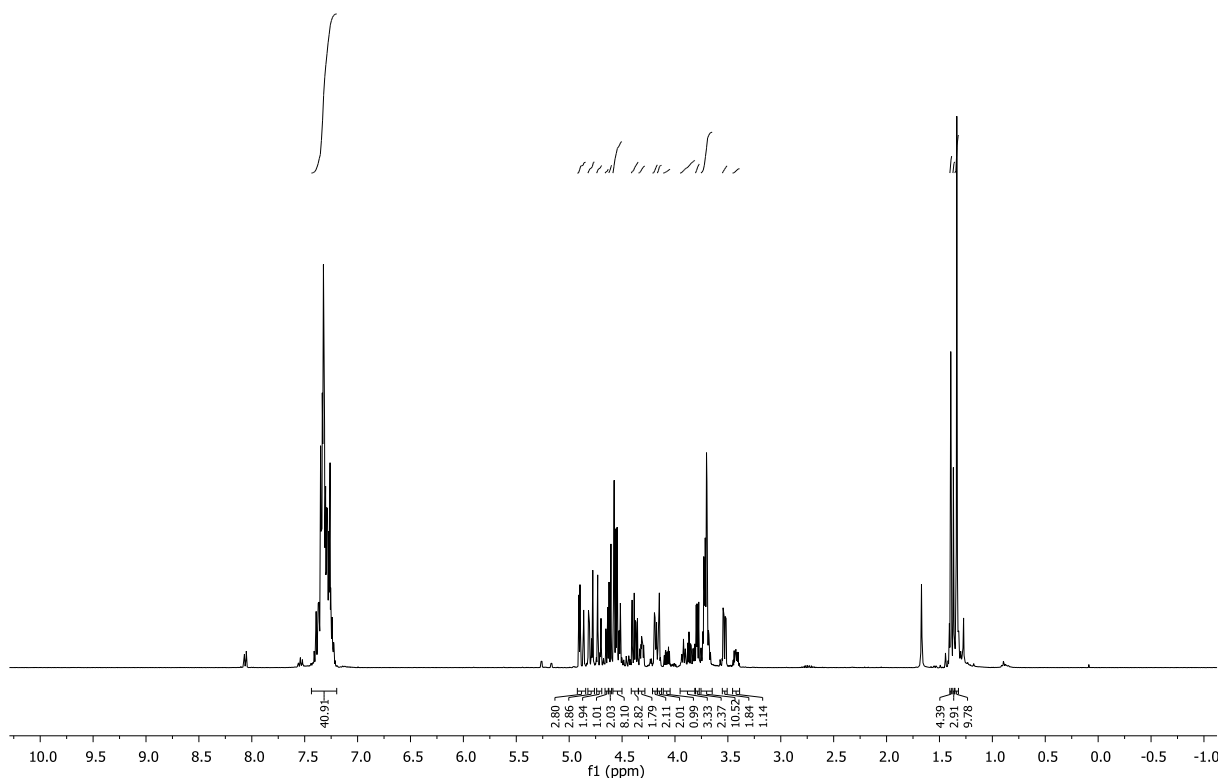
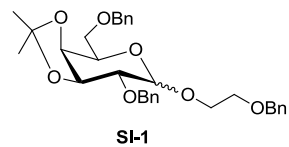
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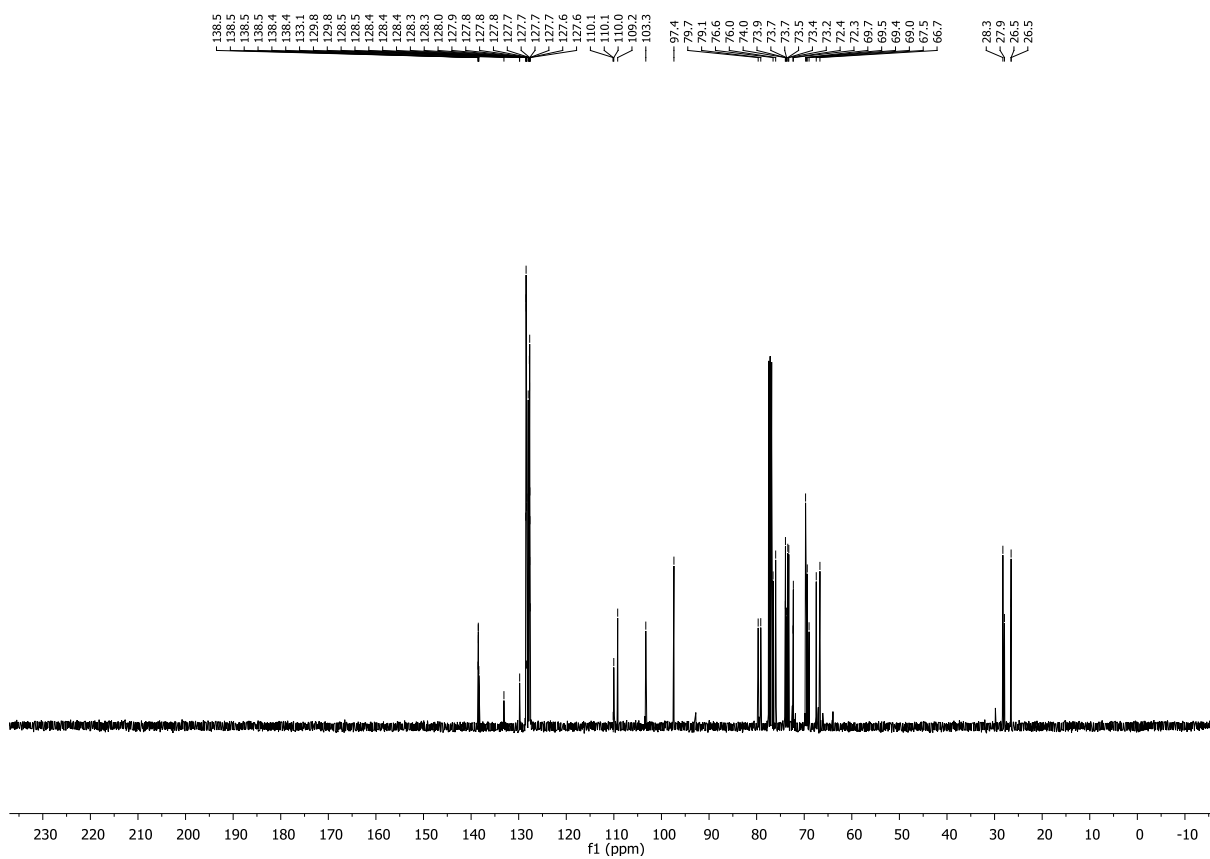
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^1H NMR, 400 MHz, CDCl_3

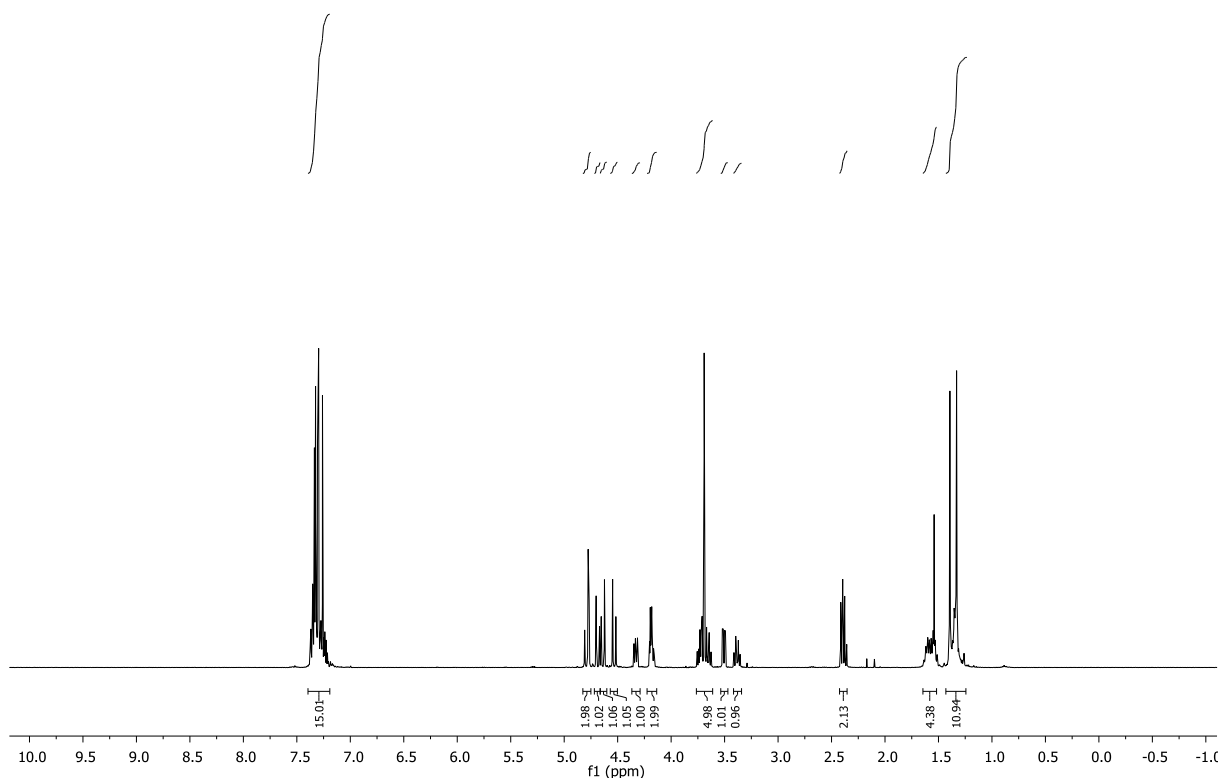
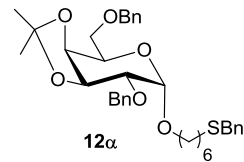


^{13}C NMR, 100 MHz, CDCl_3

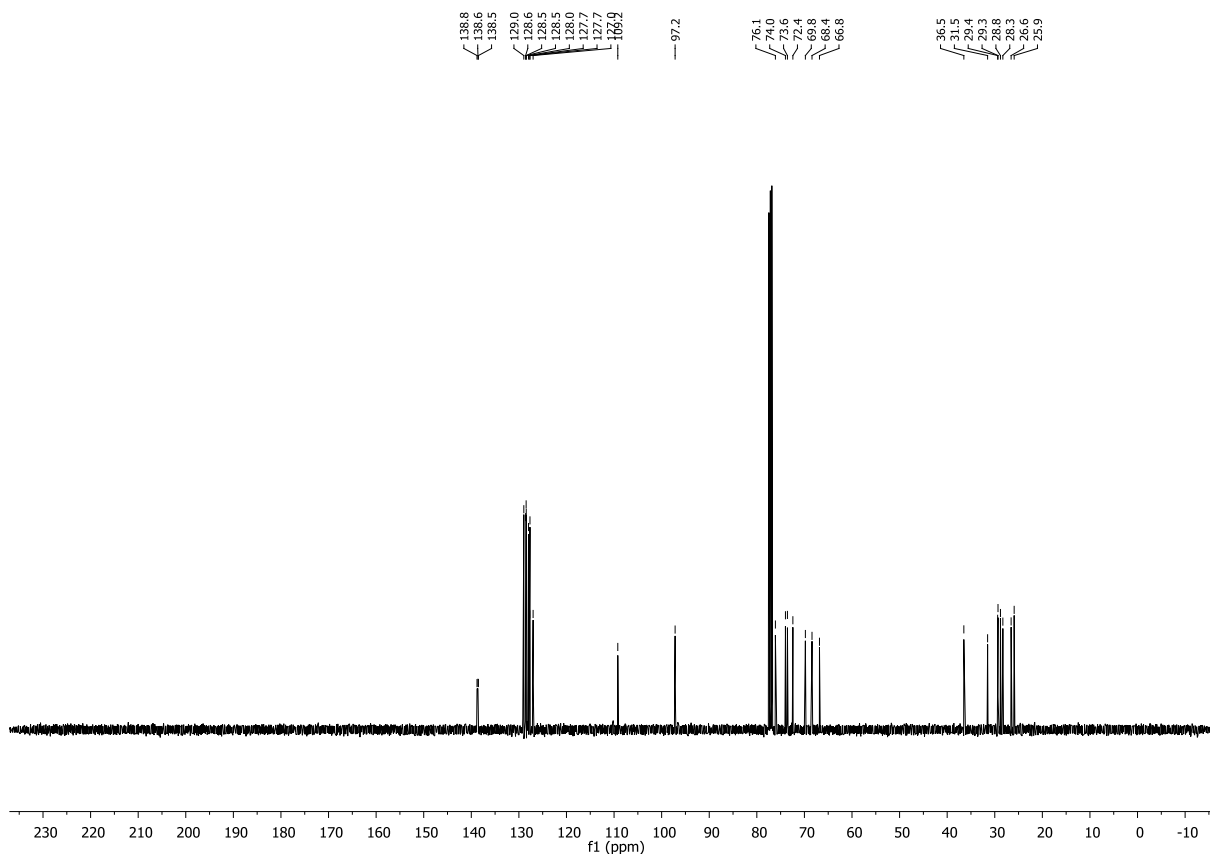


SI-4

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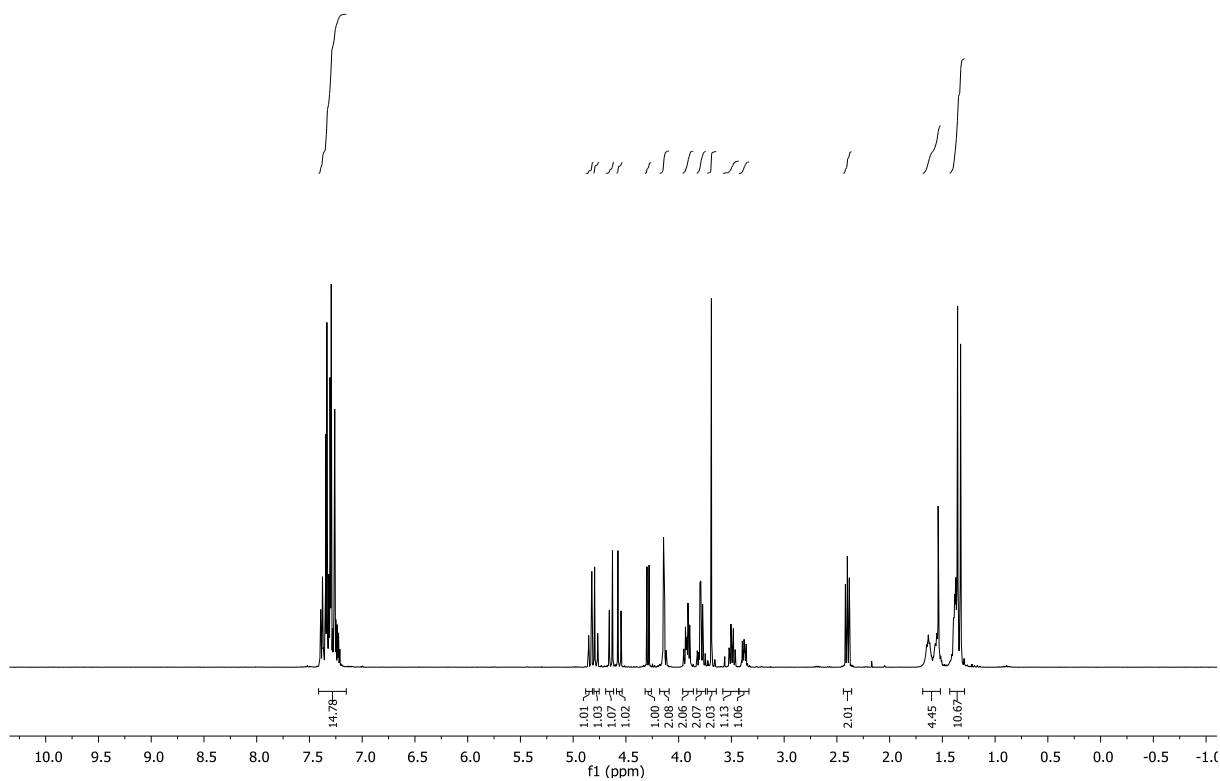
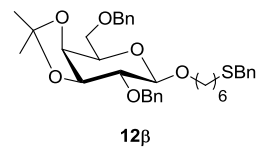


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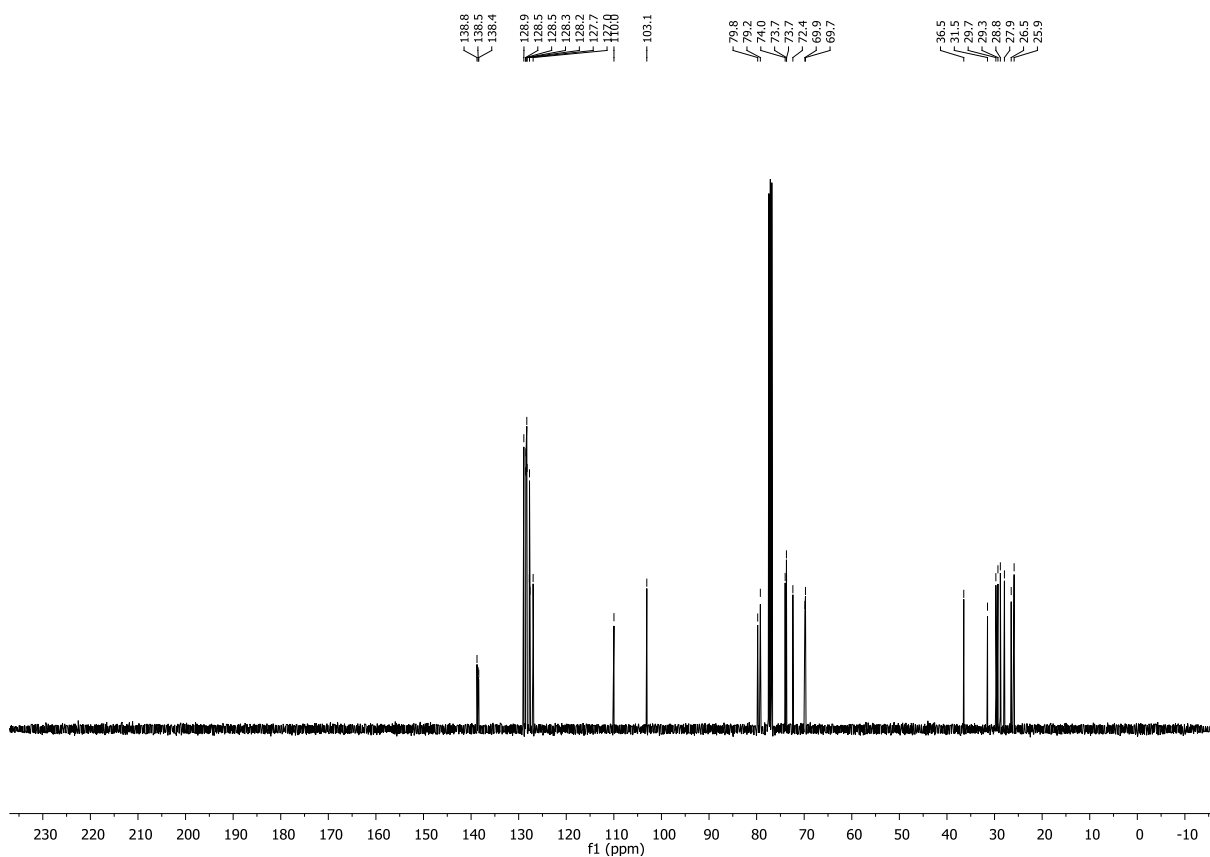


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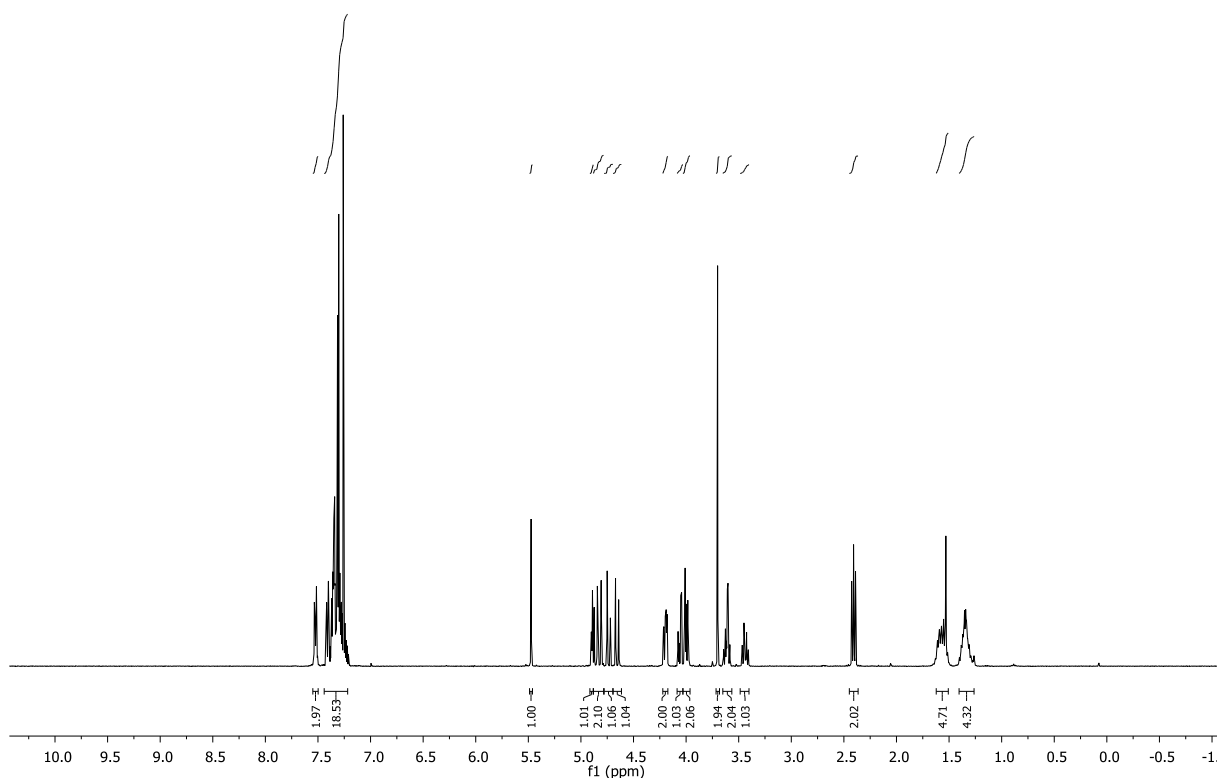
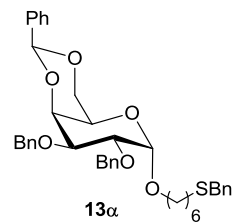
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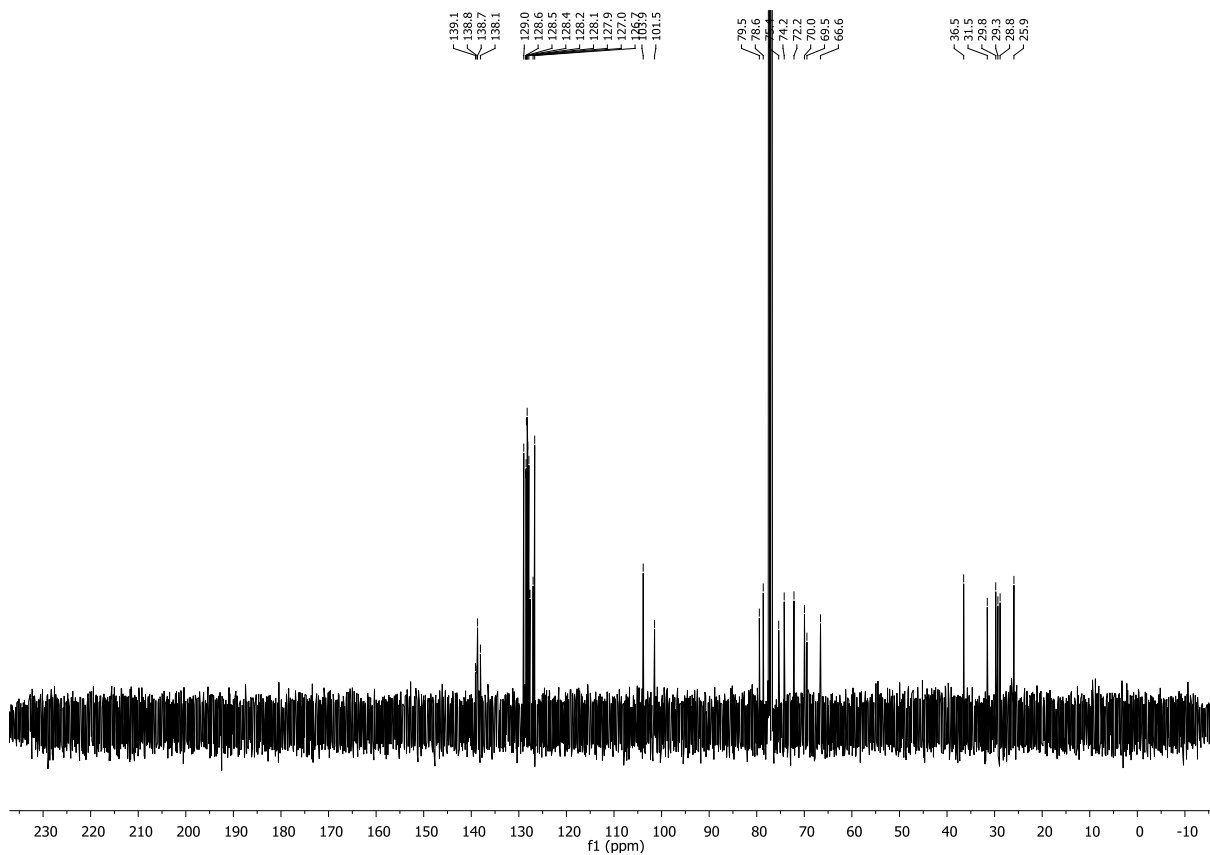
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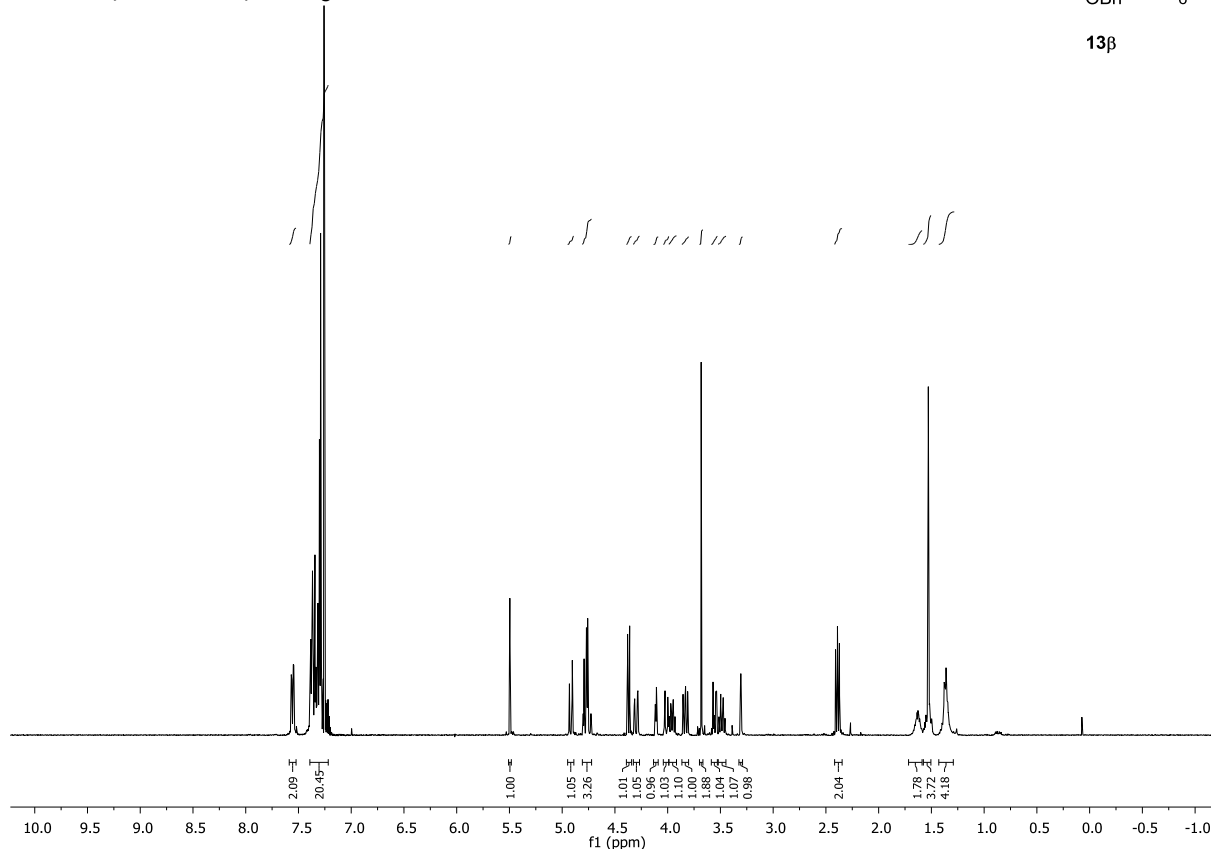
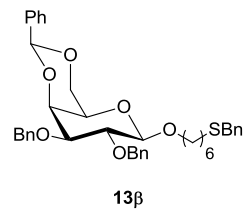
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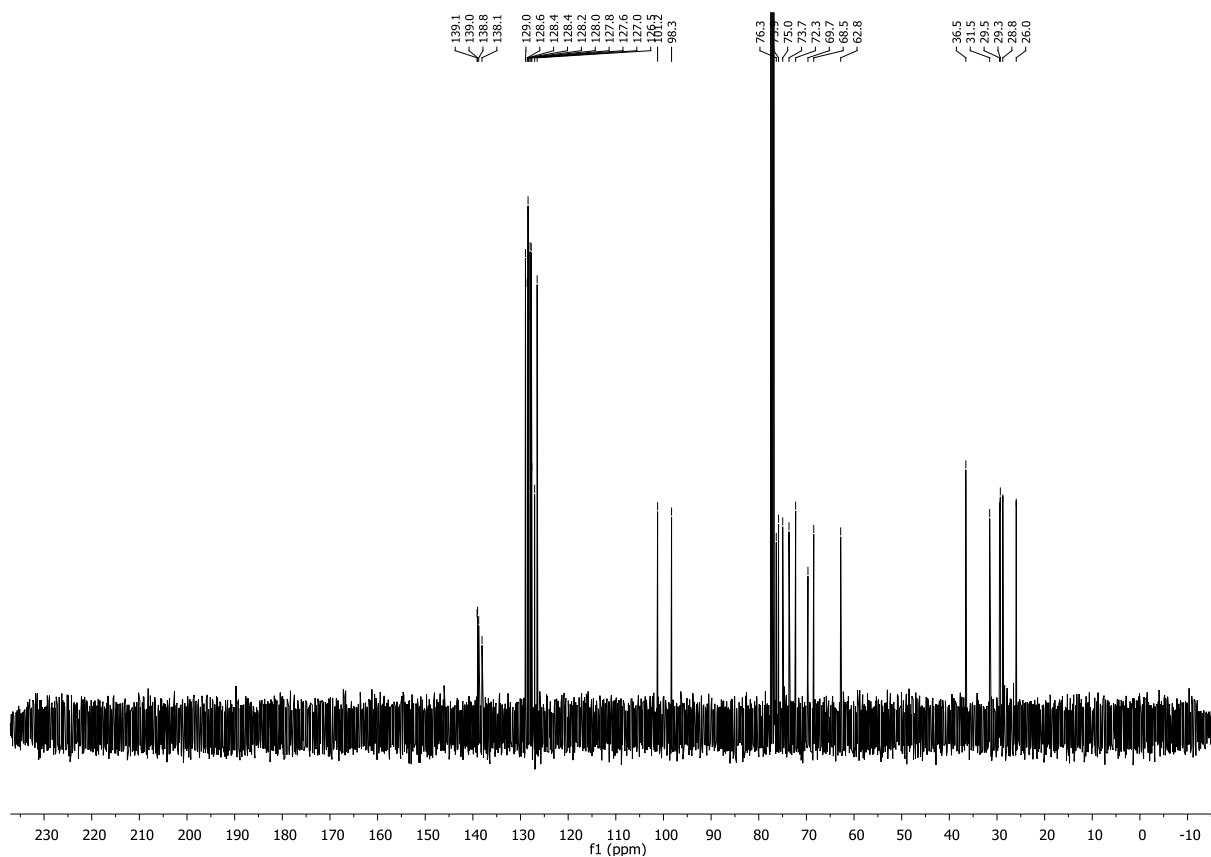
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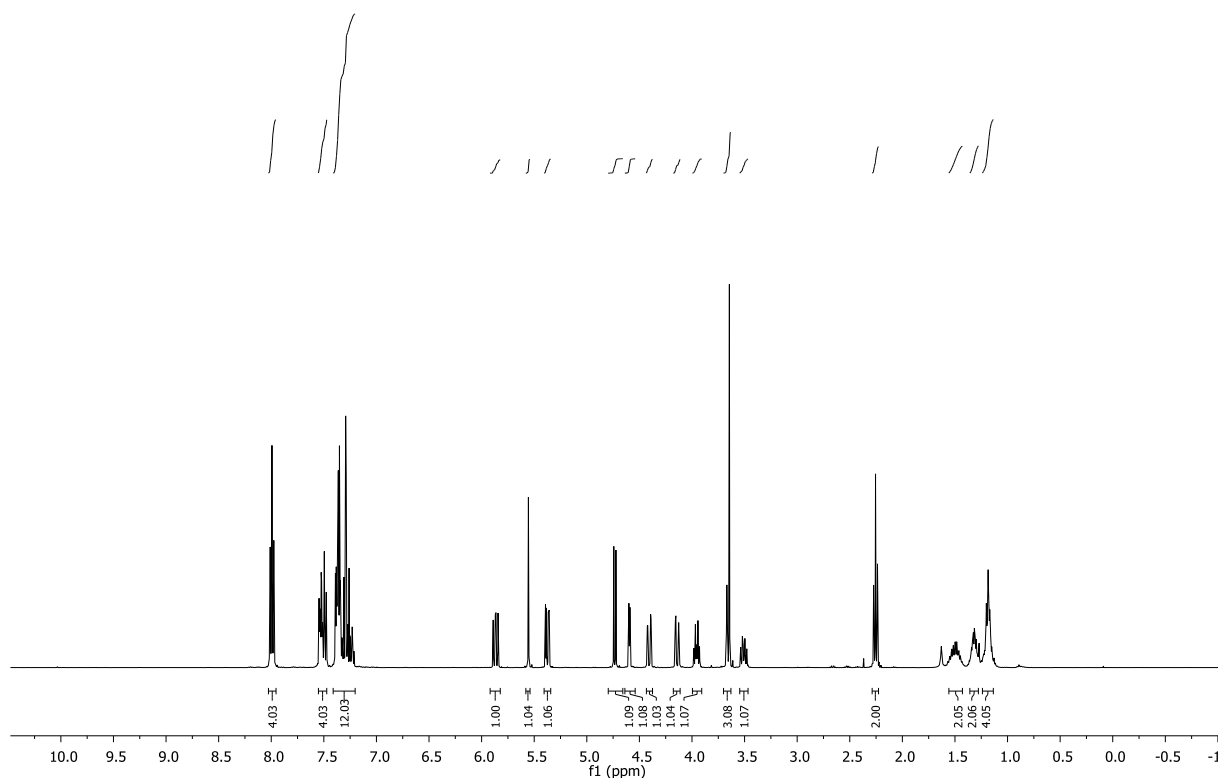
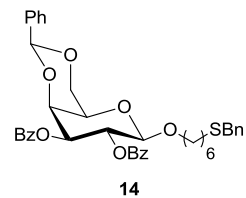
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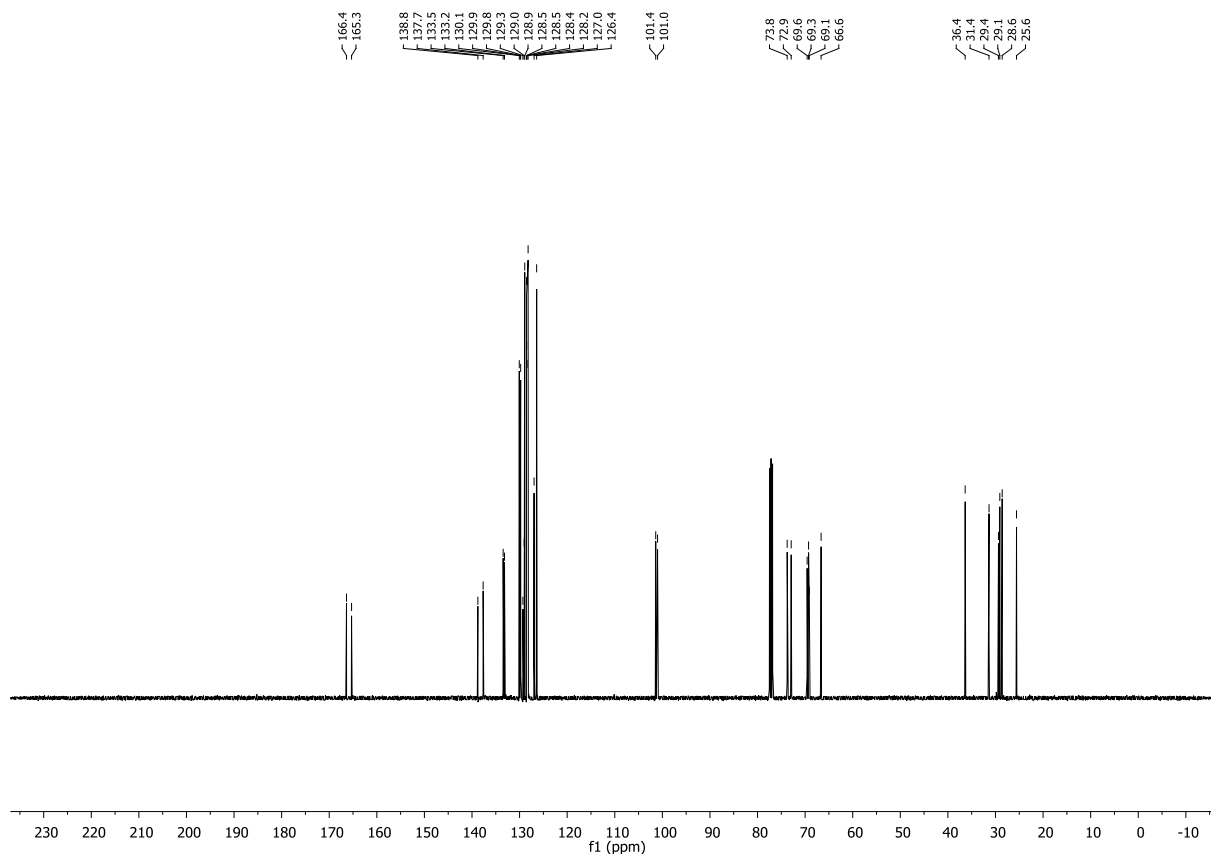
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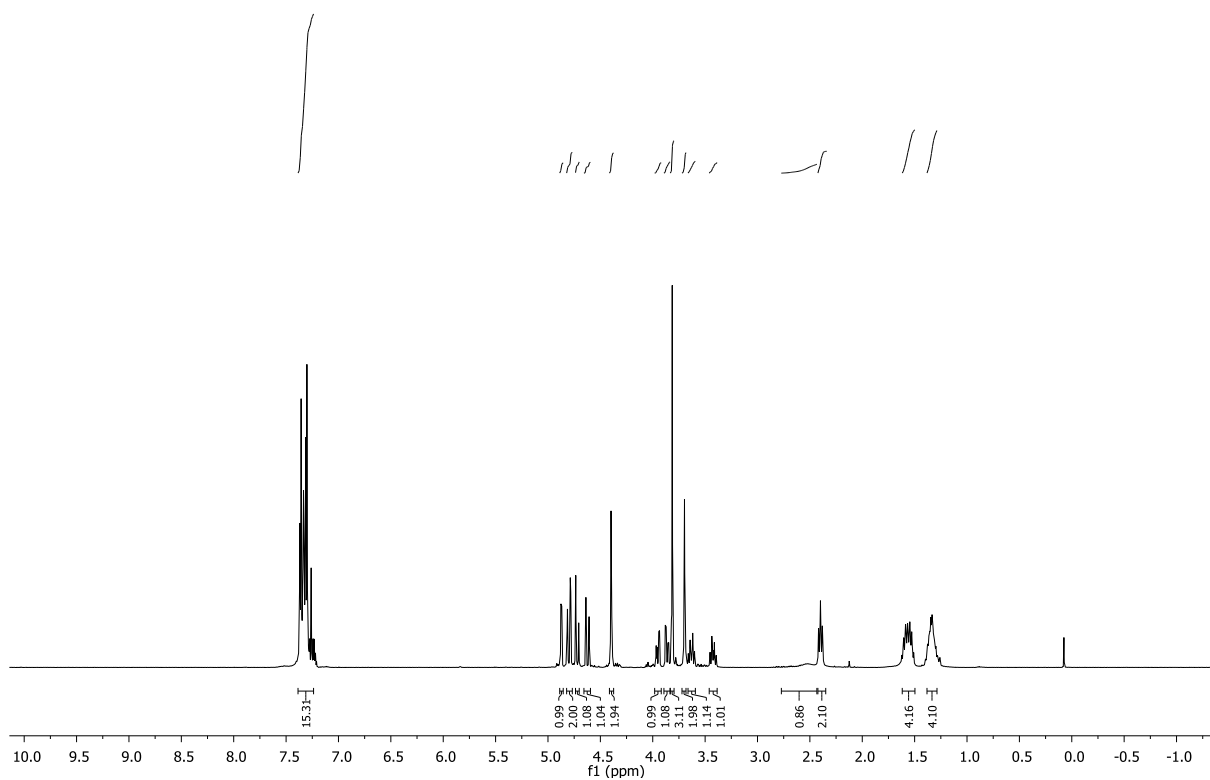
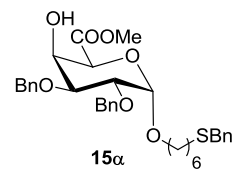
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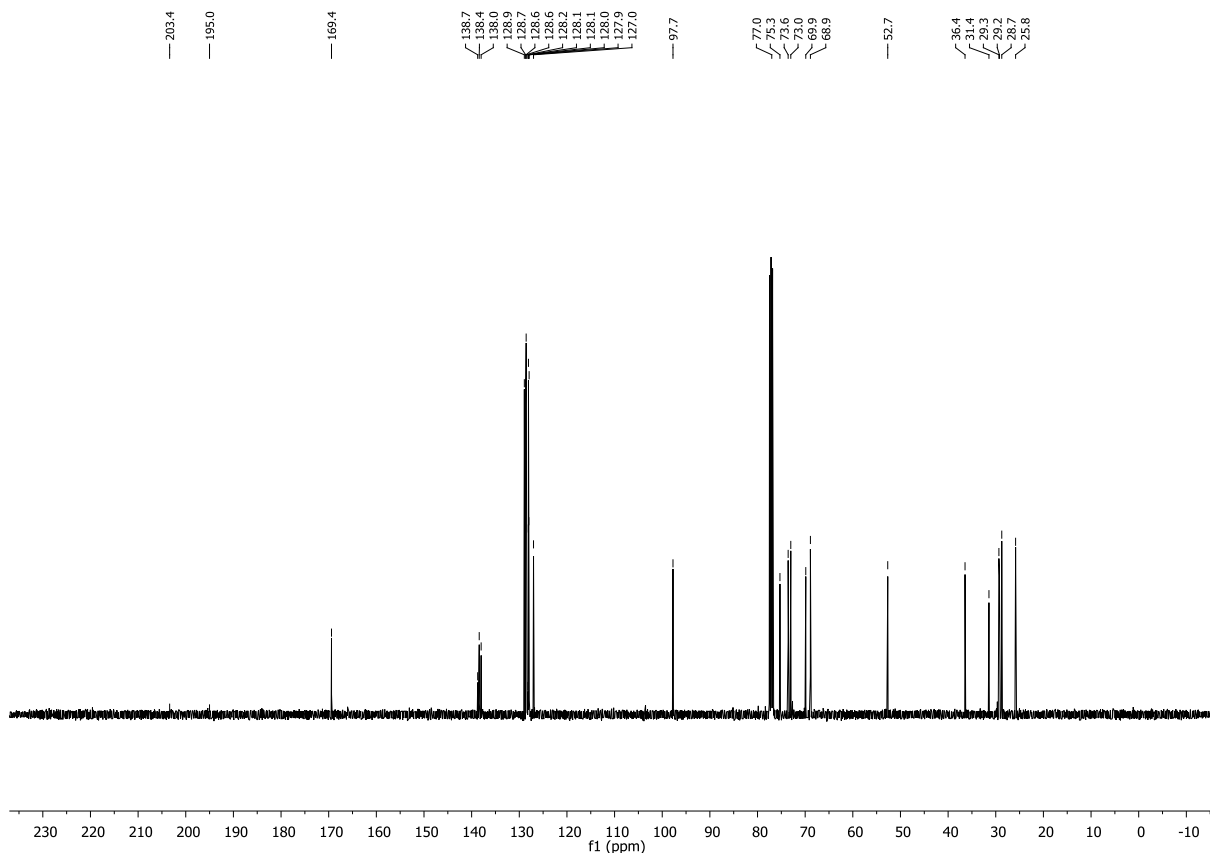
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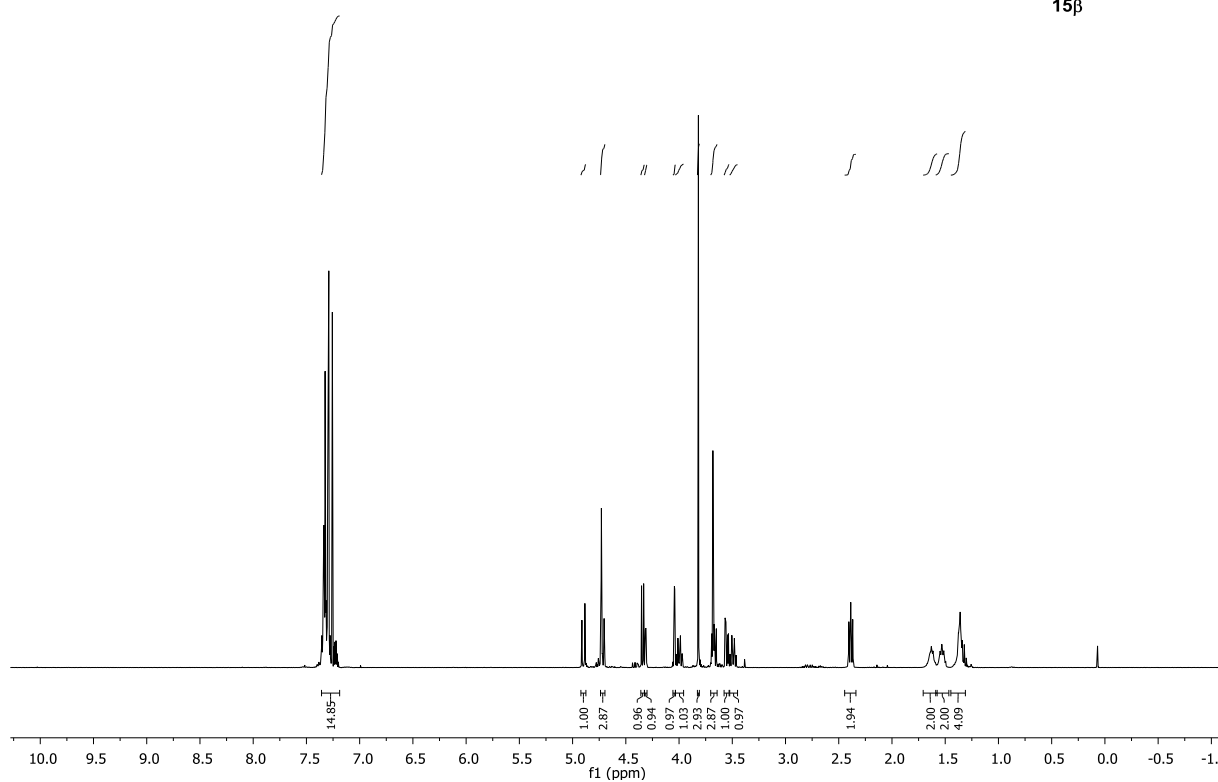
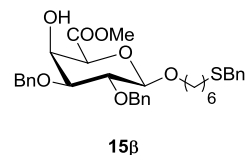
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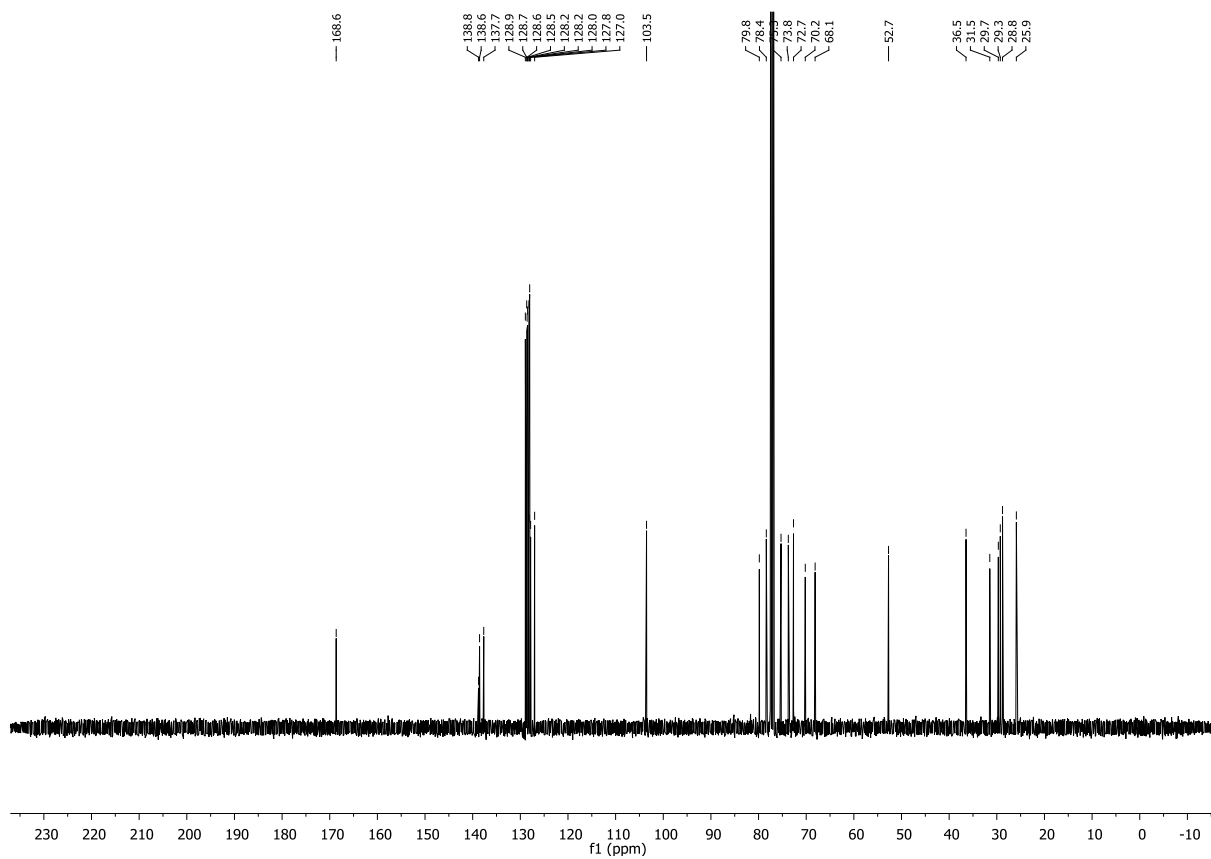
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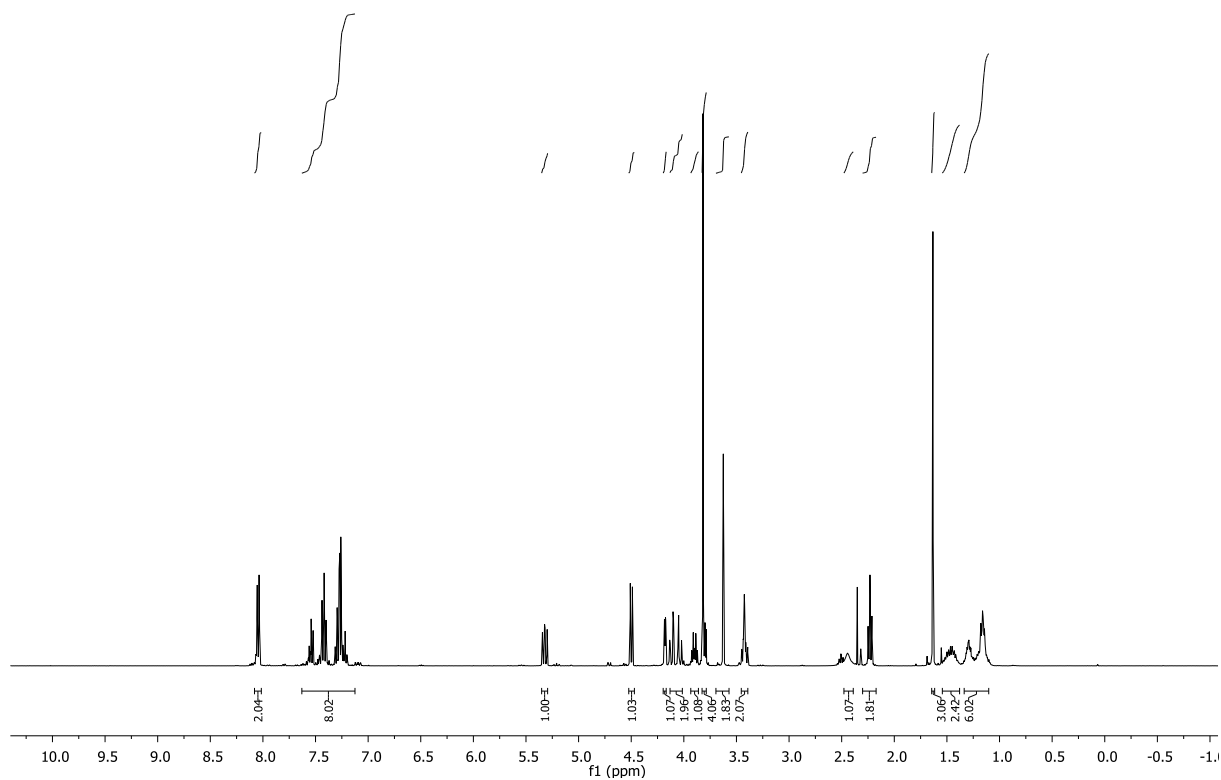
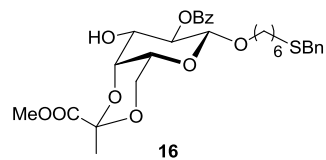
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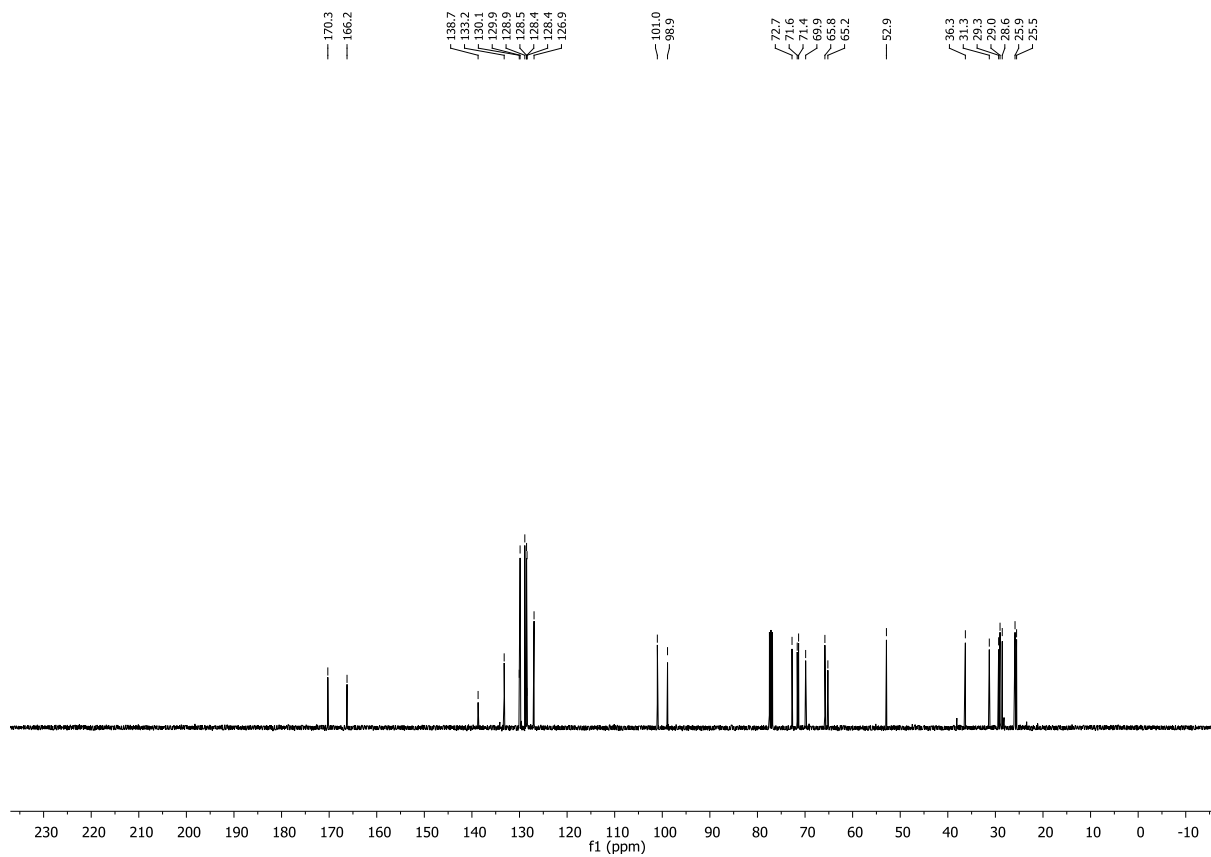
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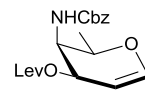


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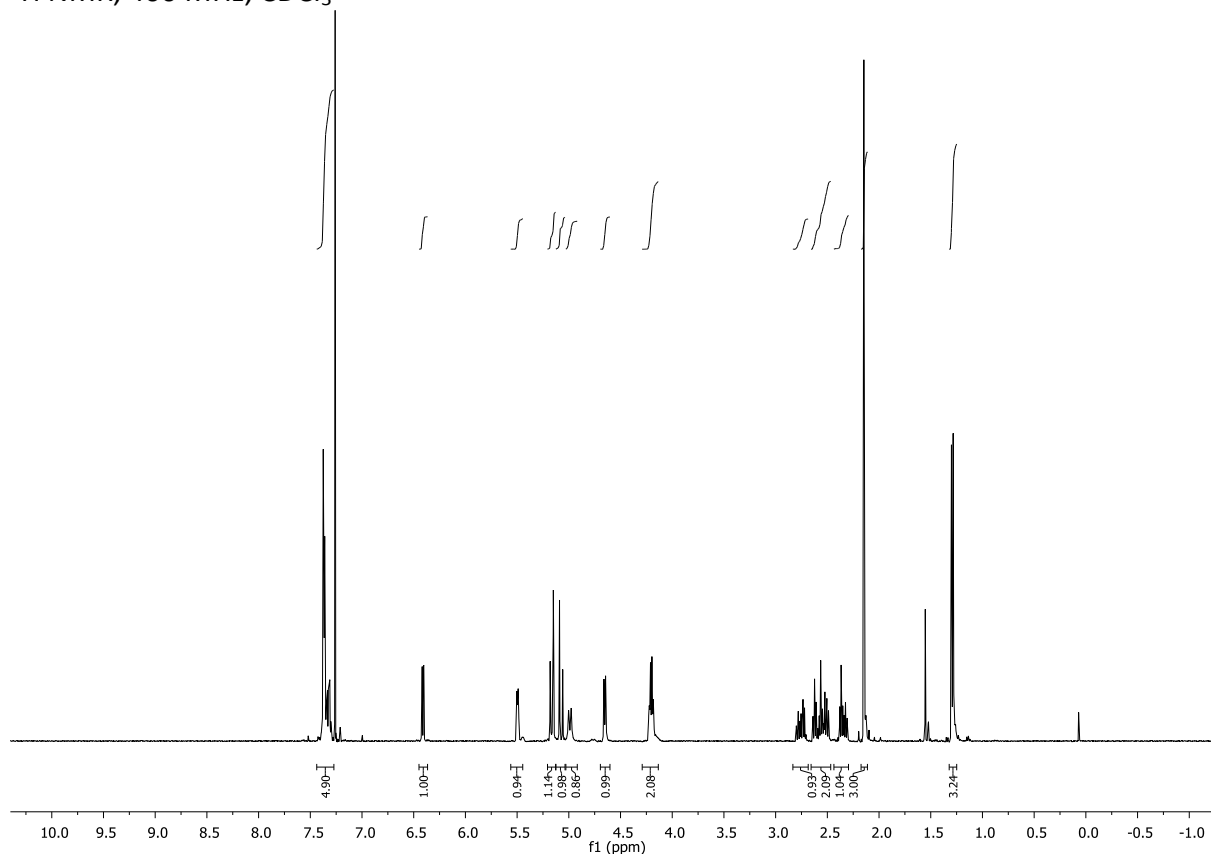
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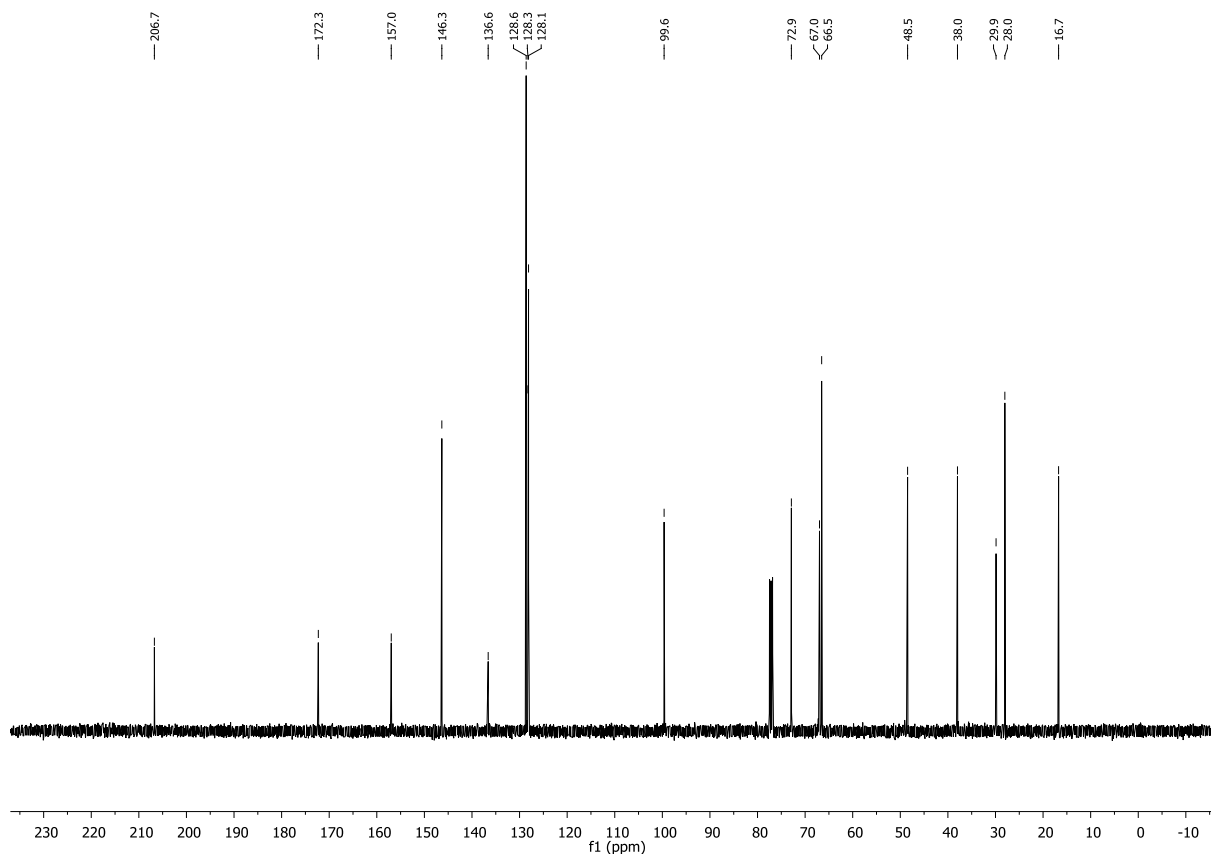


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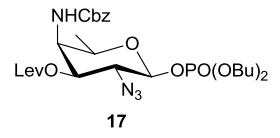
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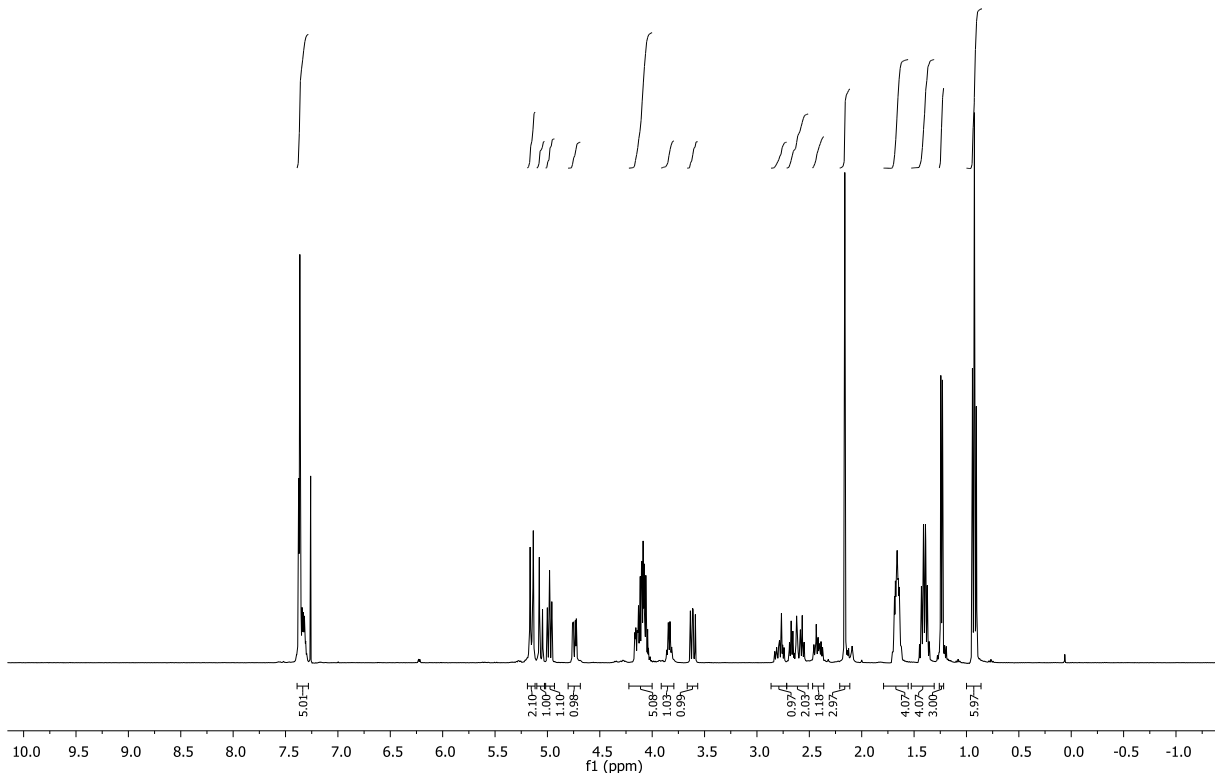
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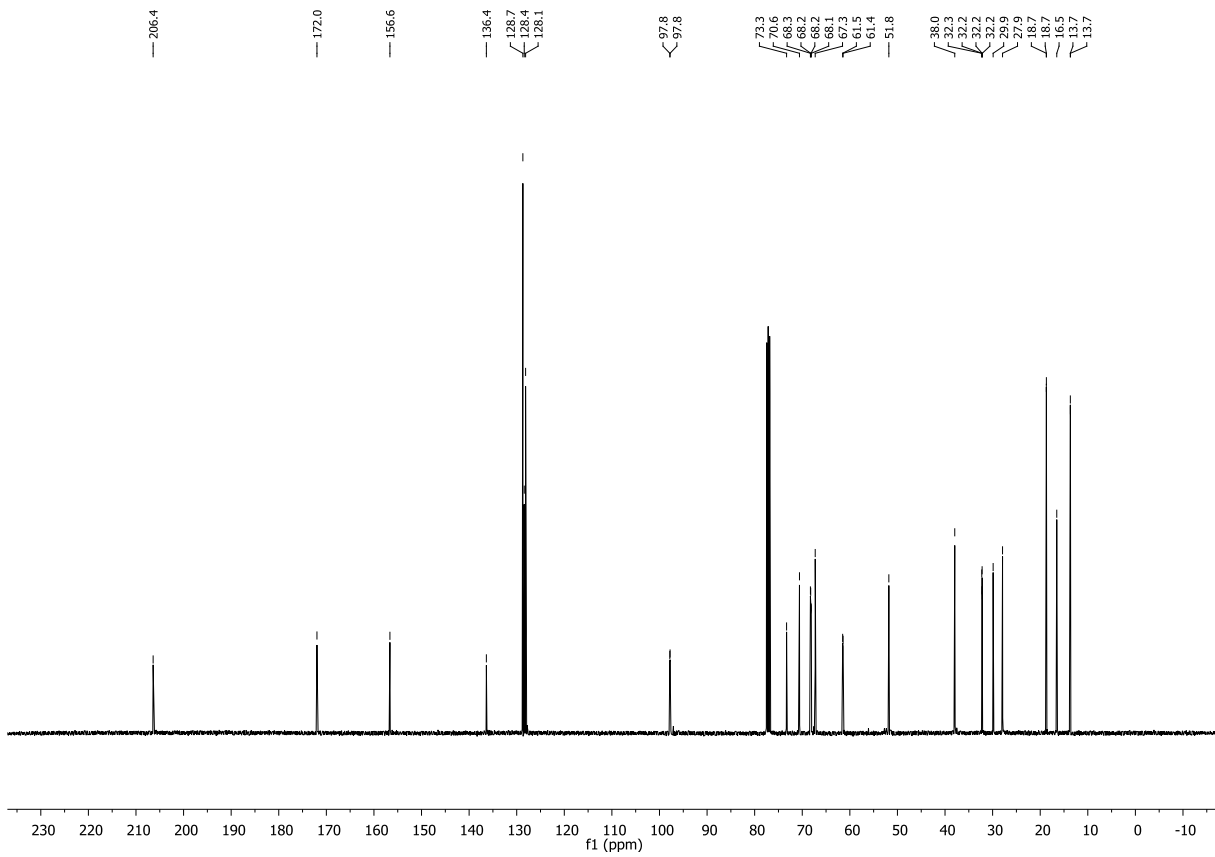
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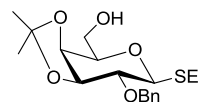


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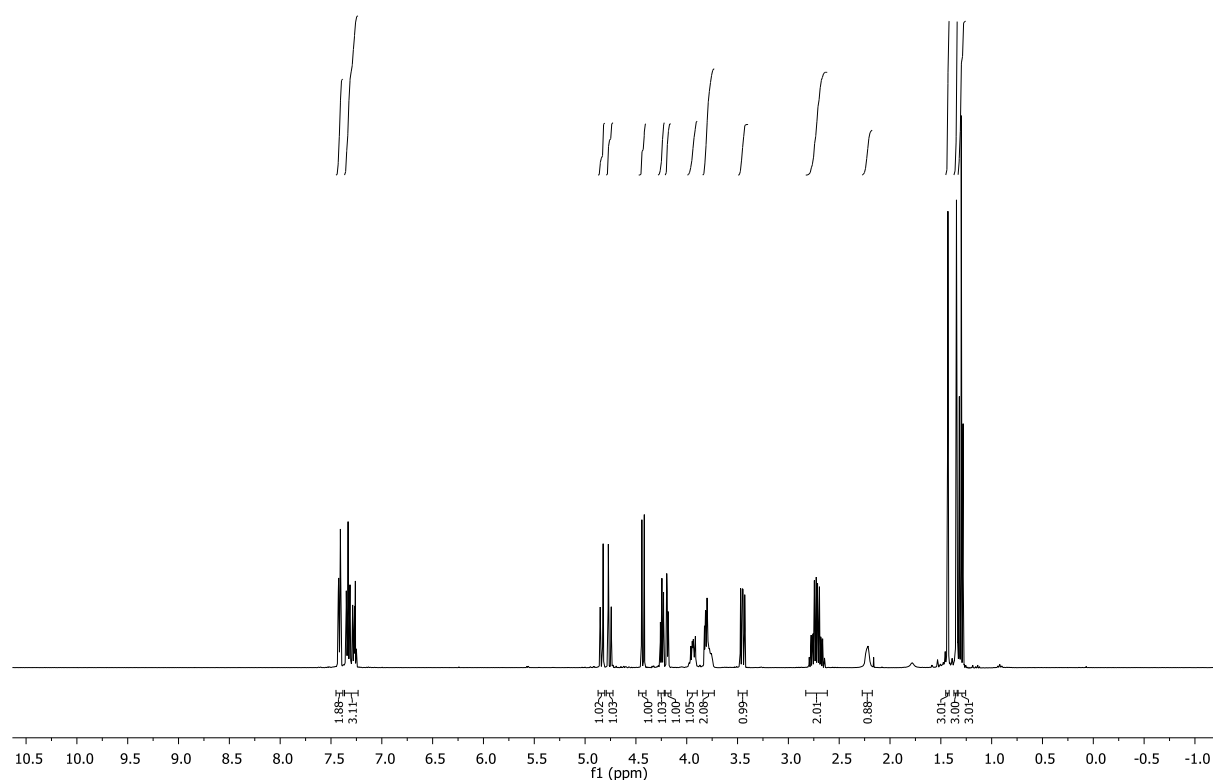
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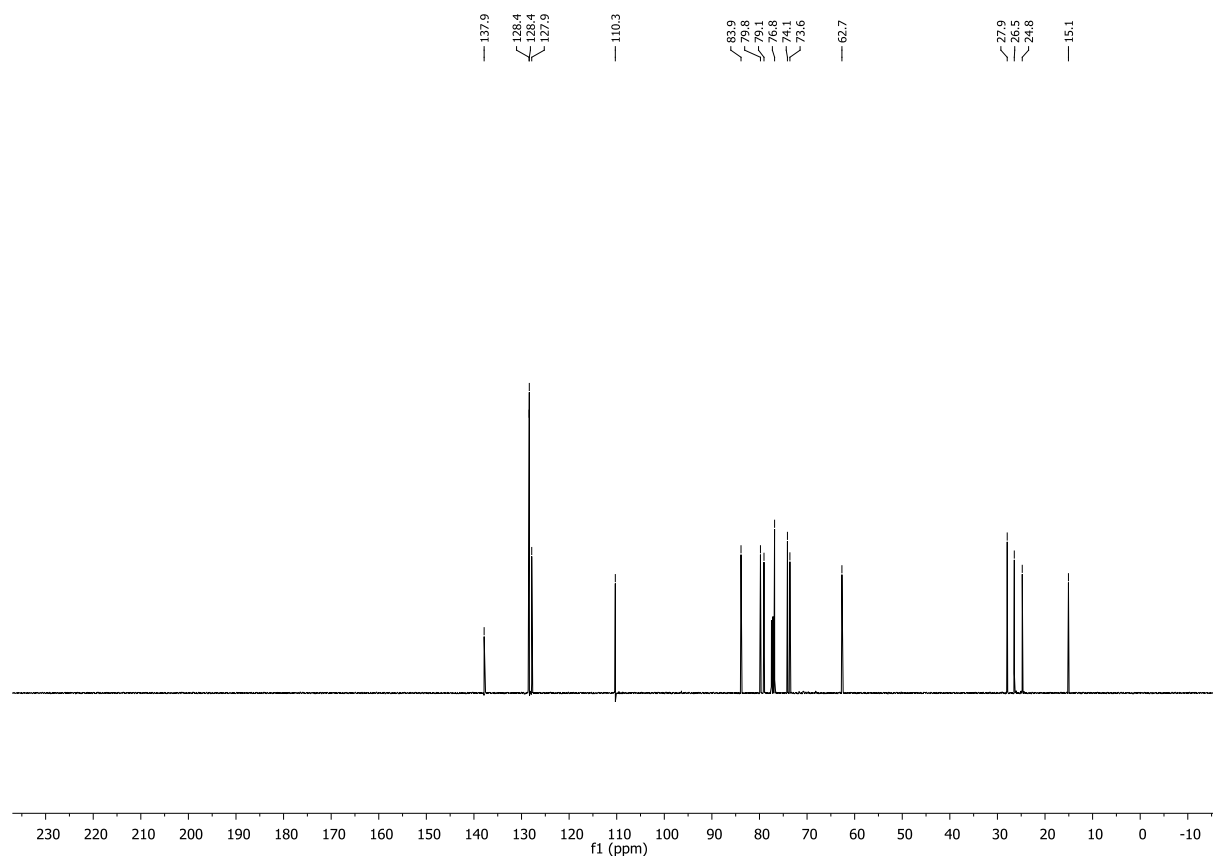


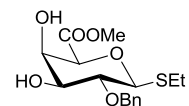
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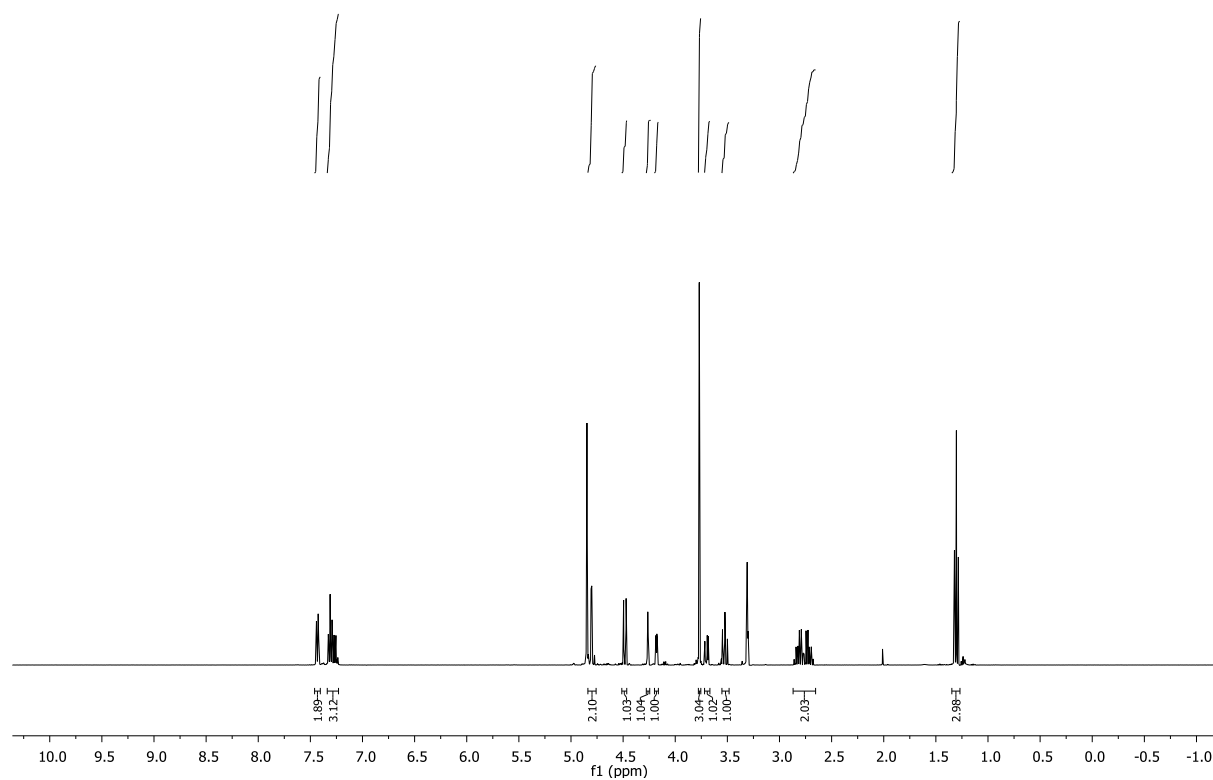
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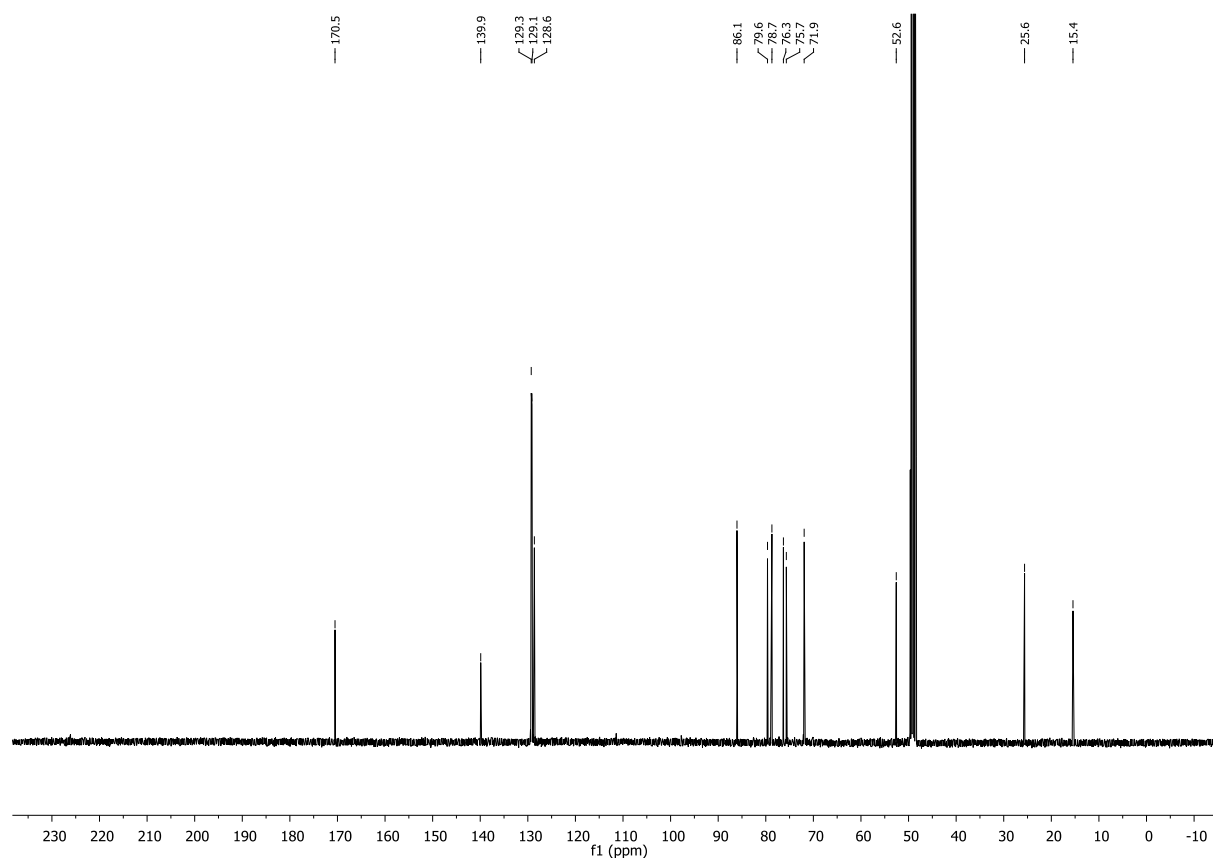


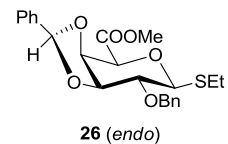
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^1H NMR, 400 MHz, CD_3OD

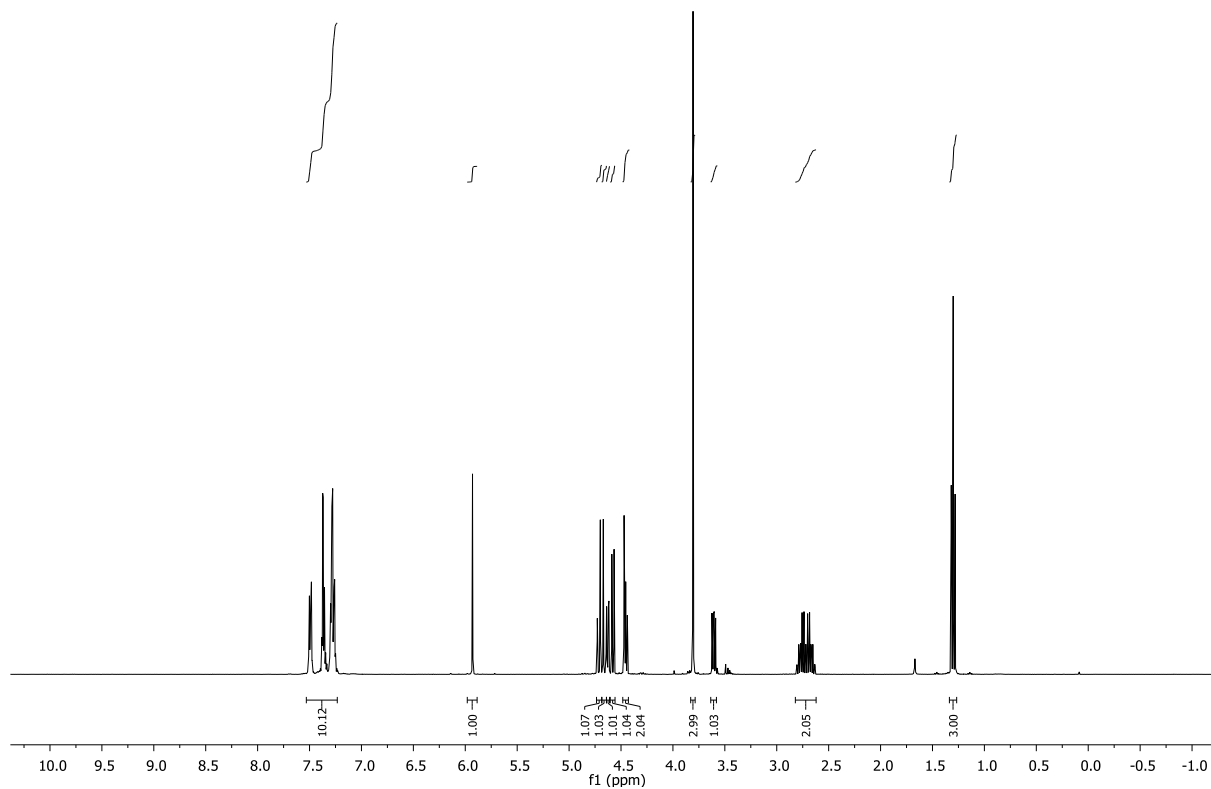


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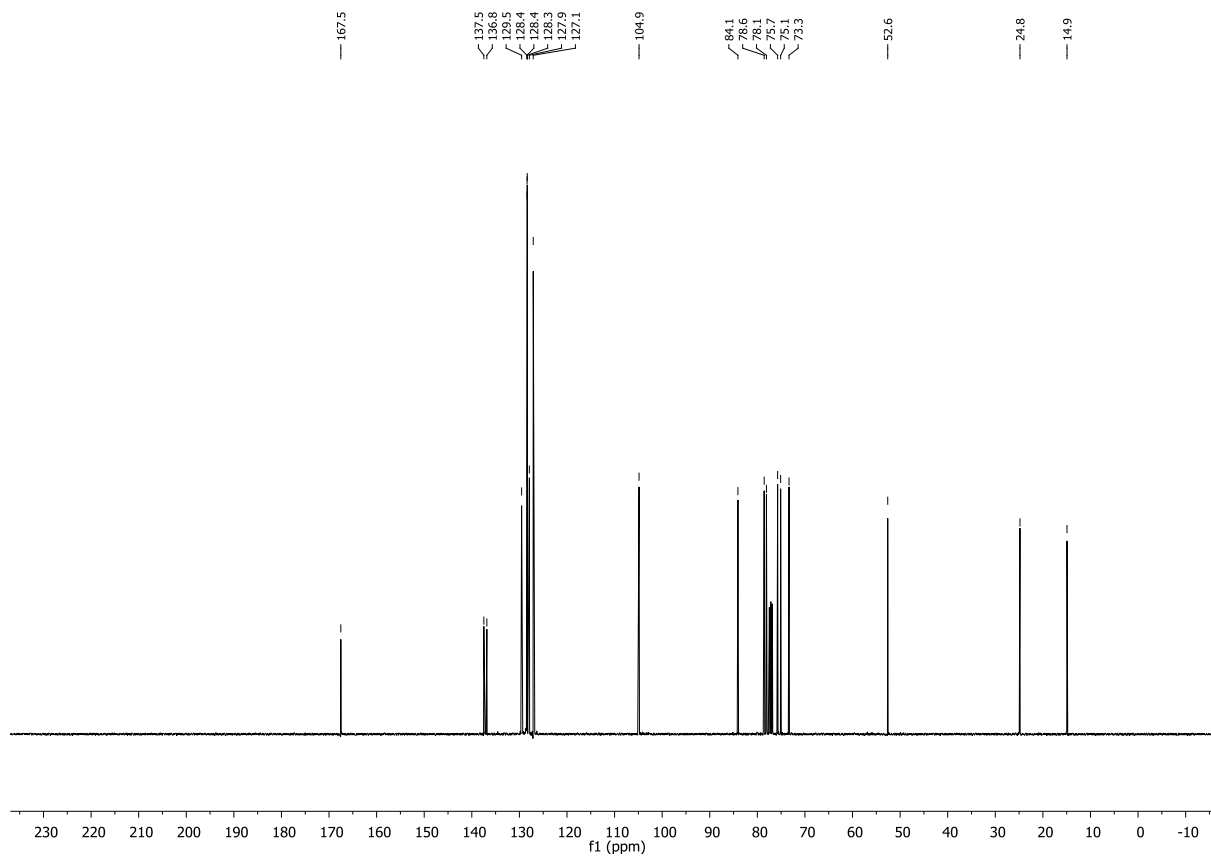


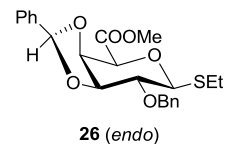


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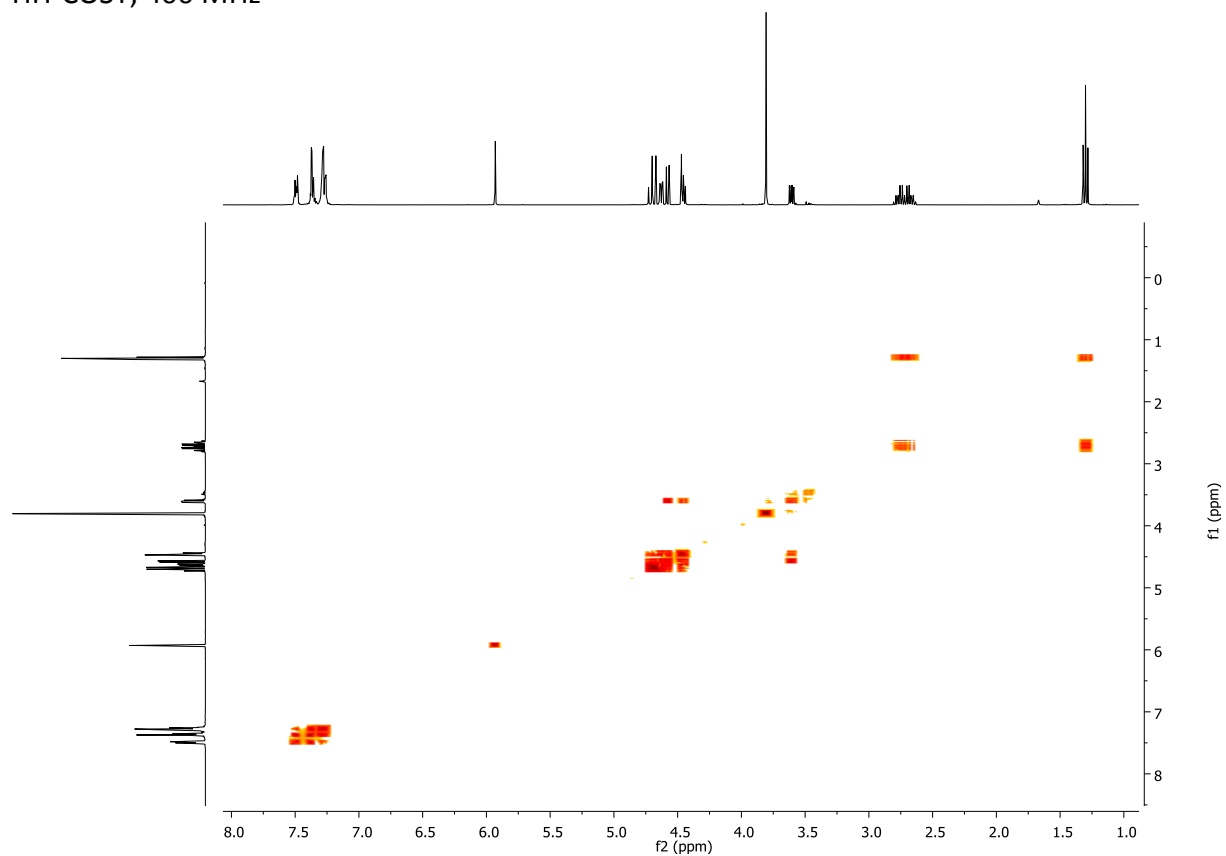


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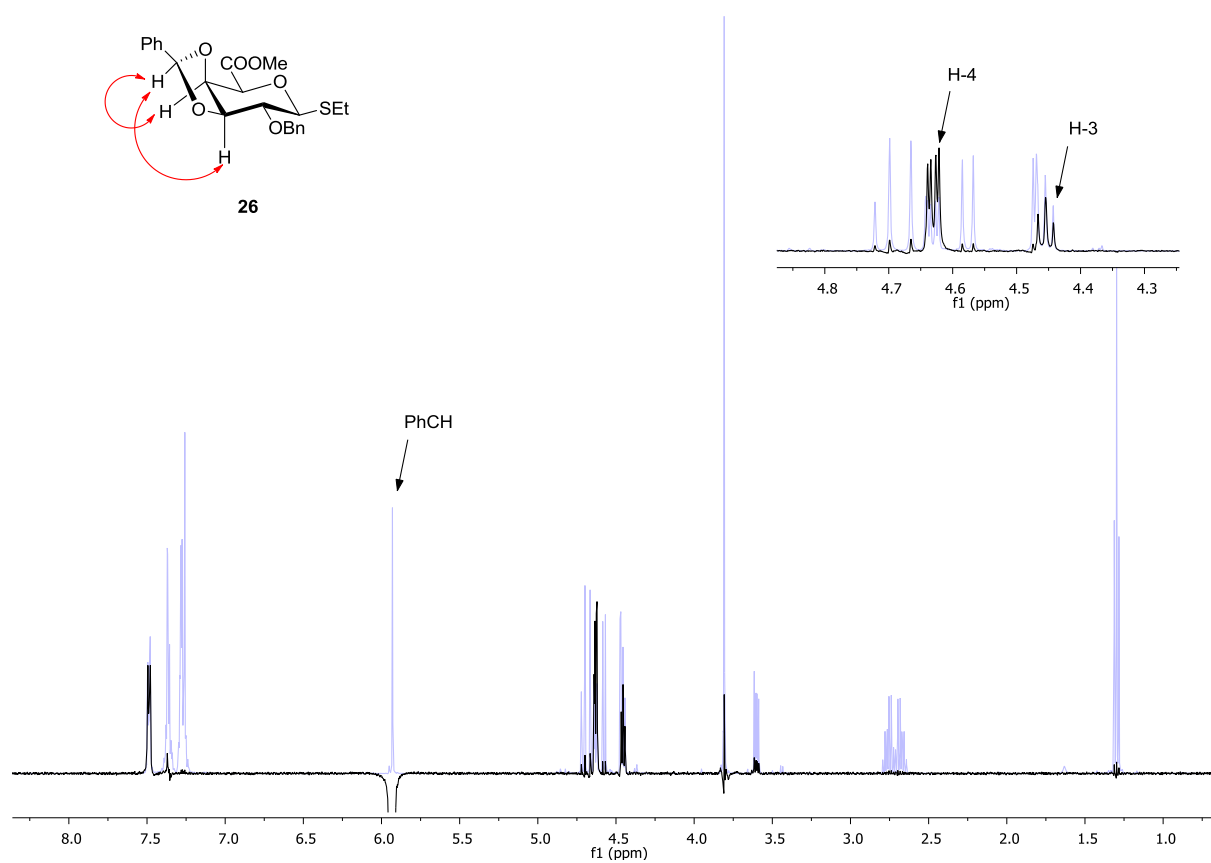


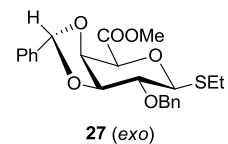


HH-COSY, 400 MHz

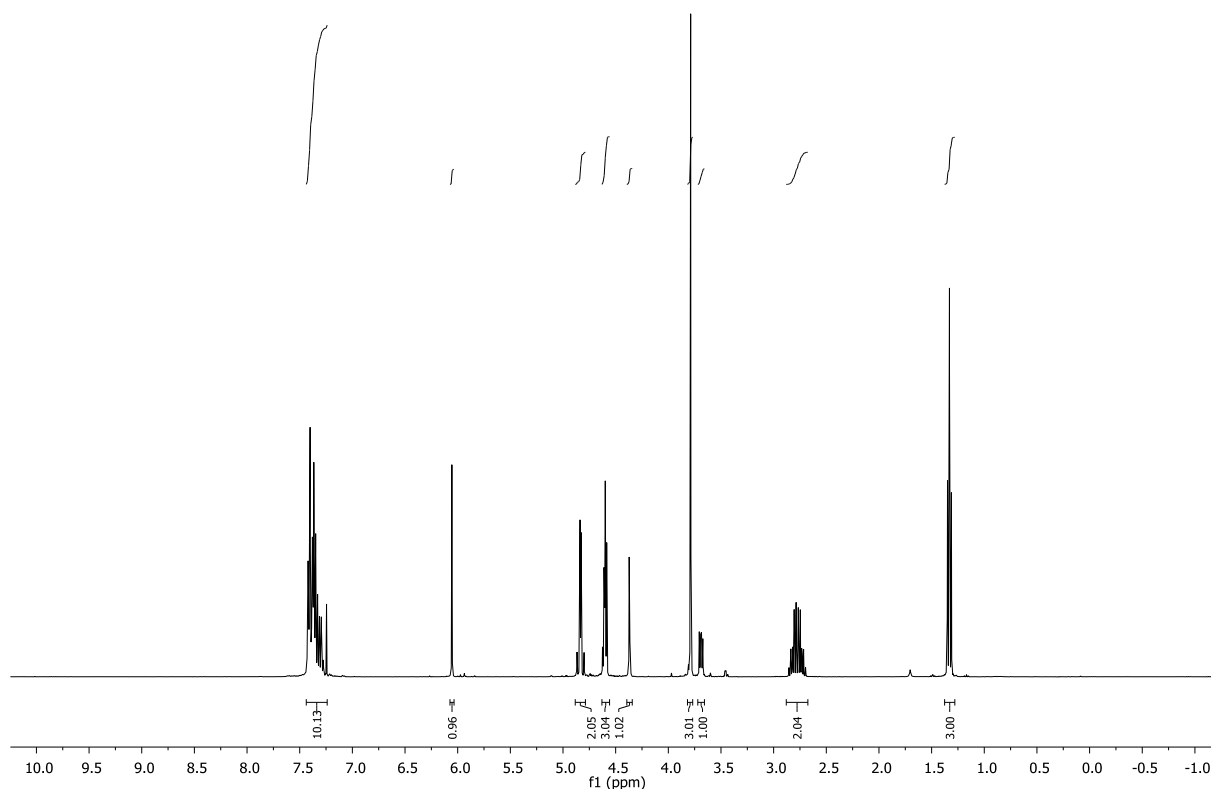


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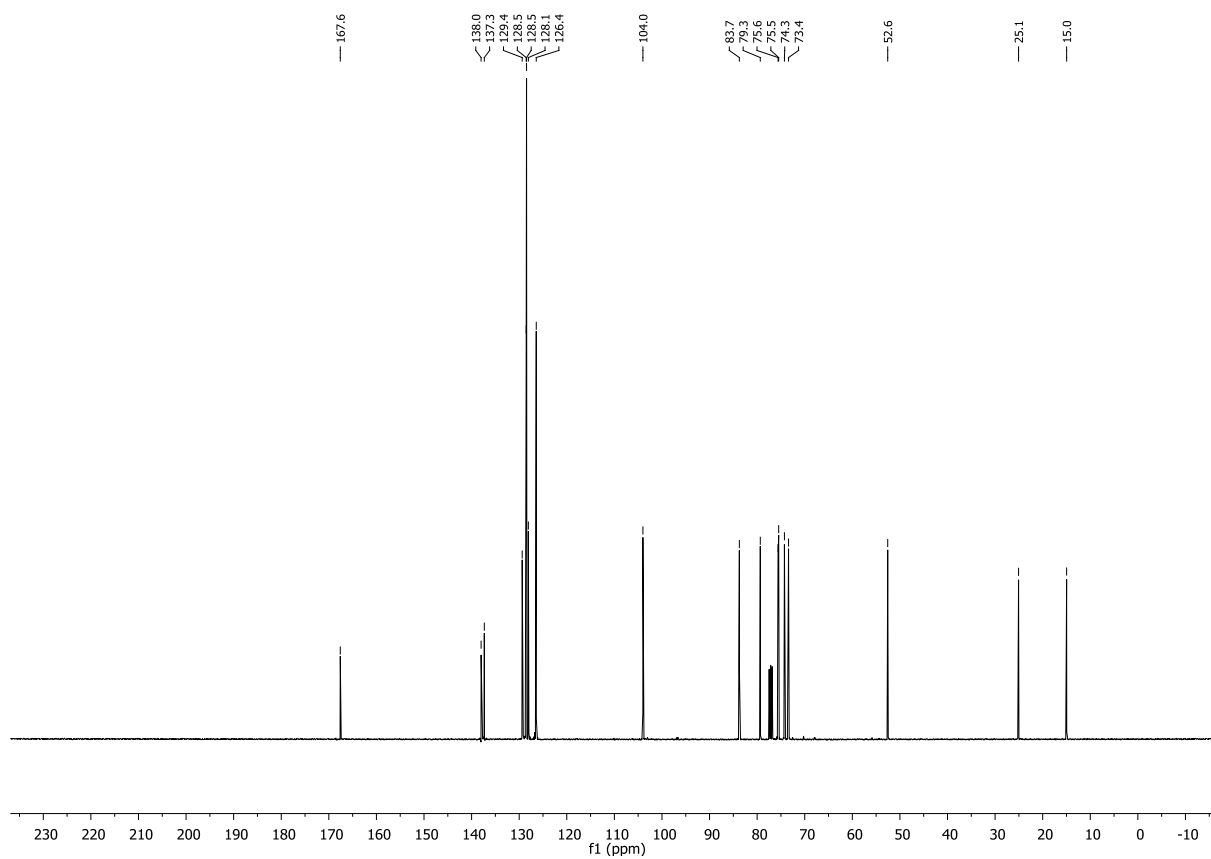


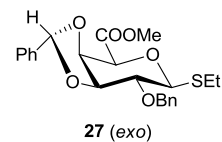


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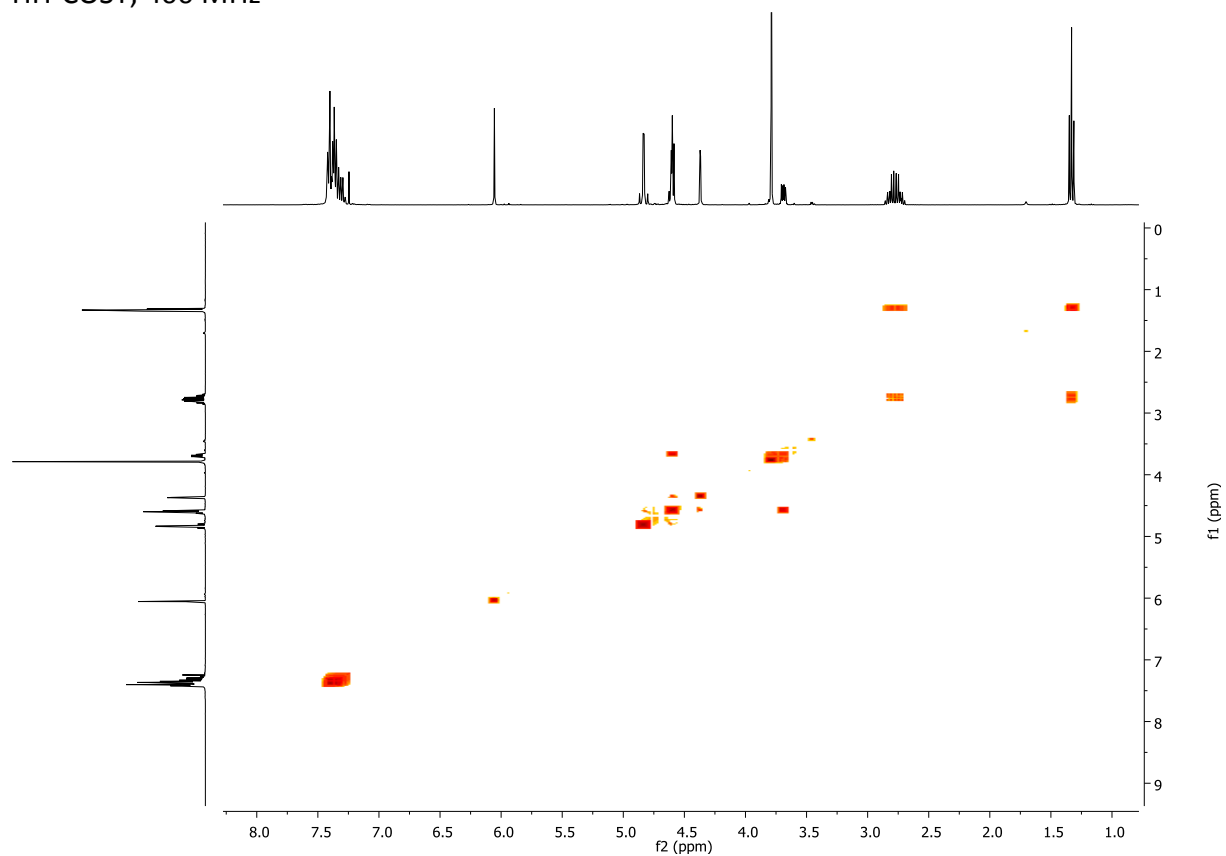


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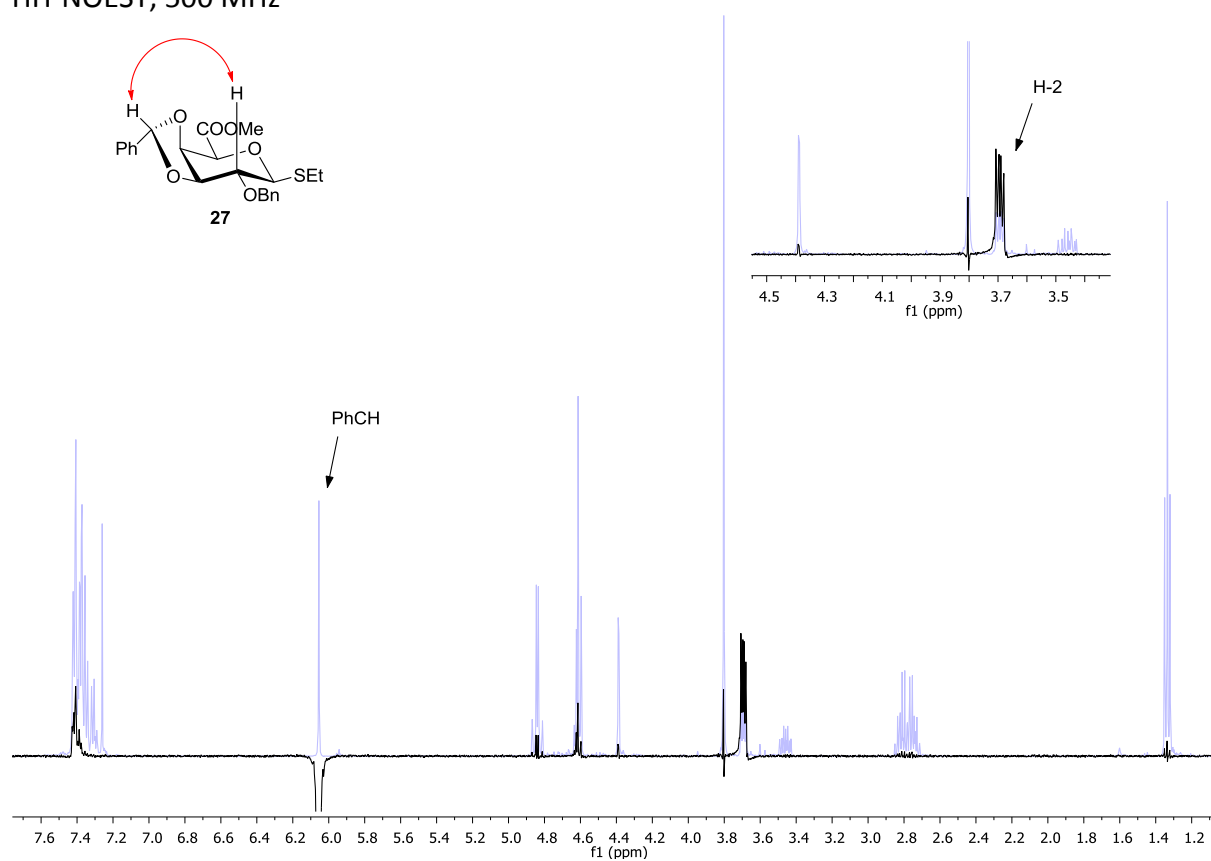


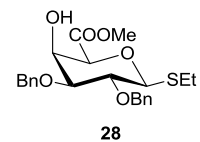


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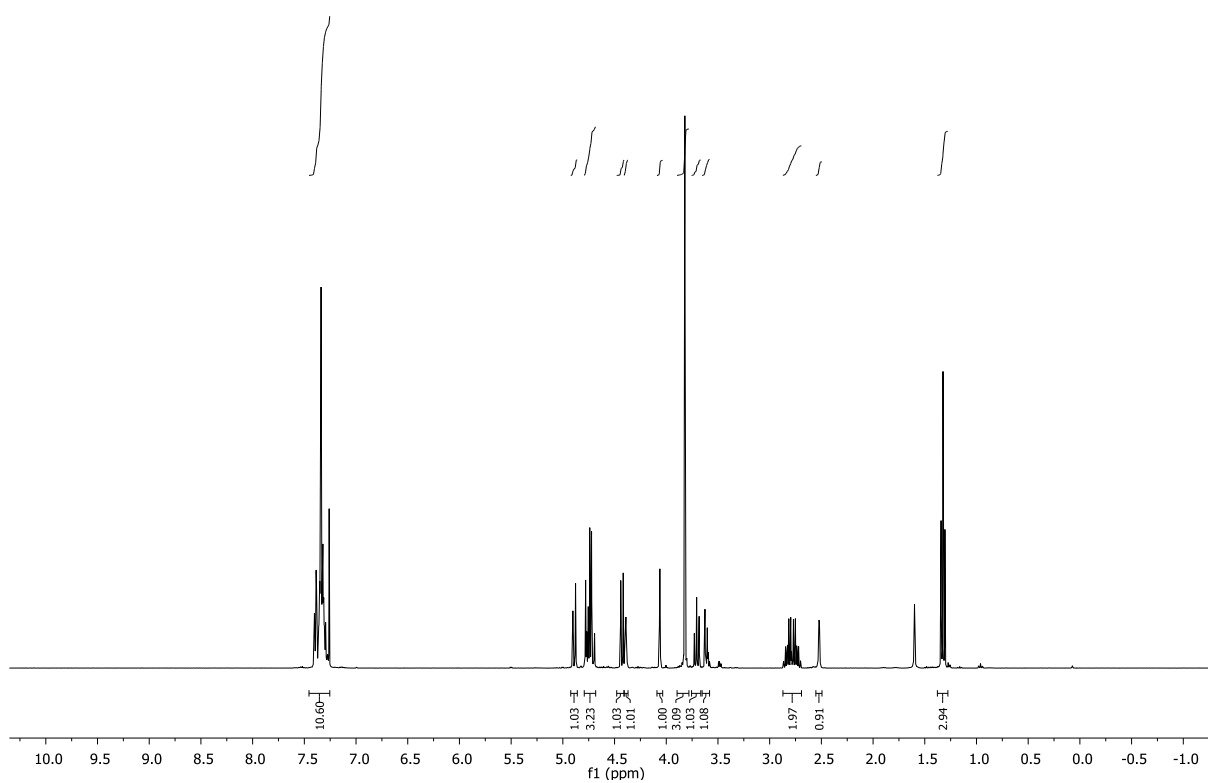


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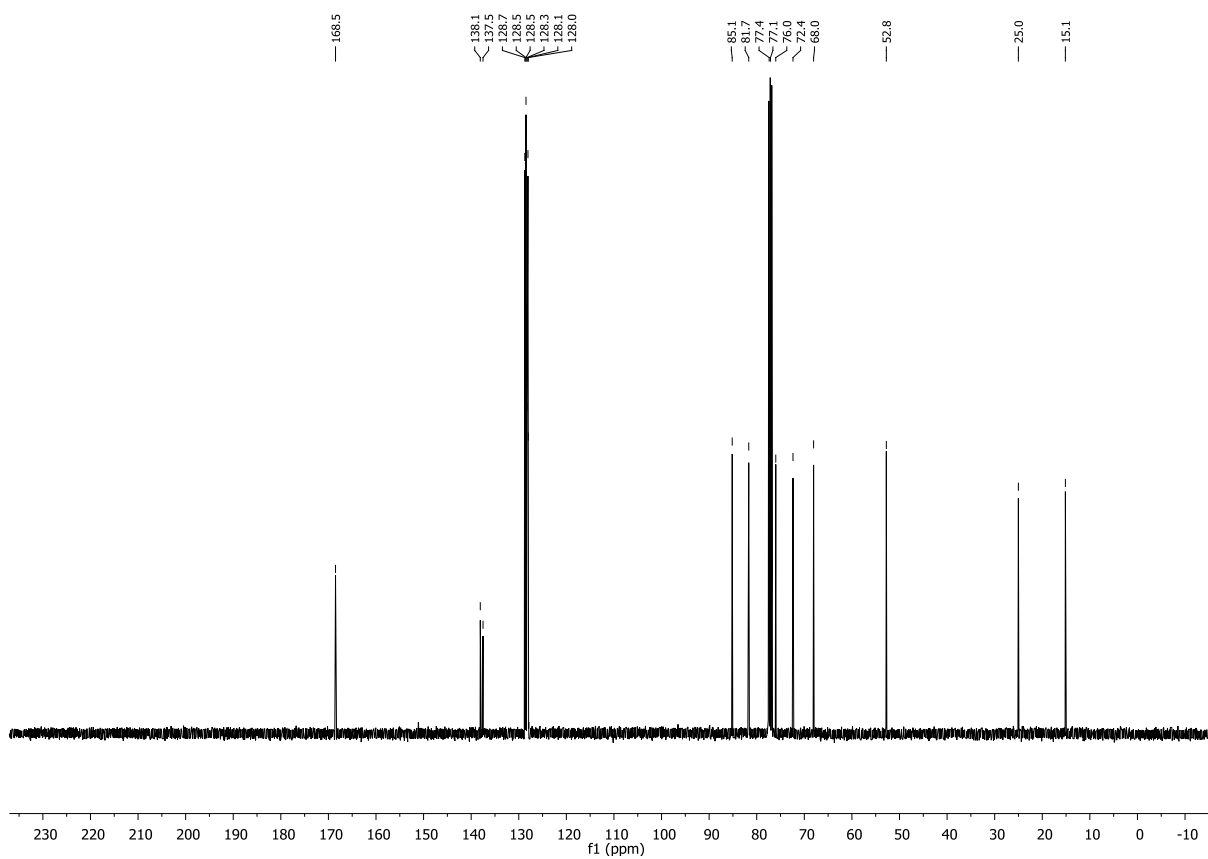


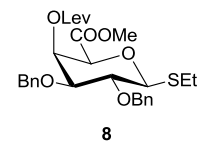


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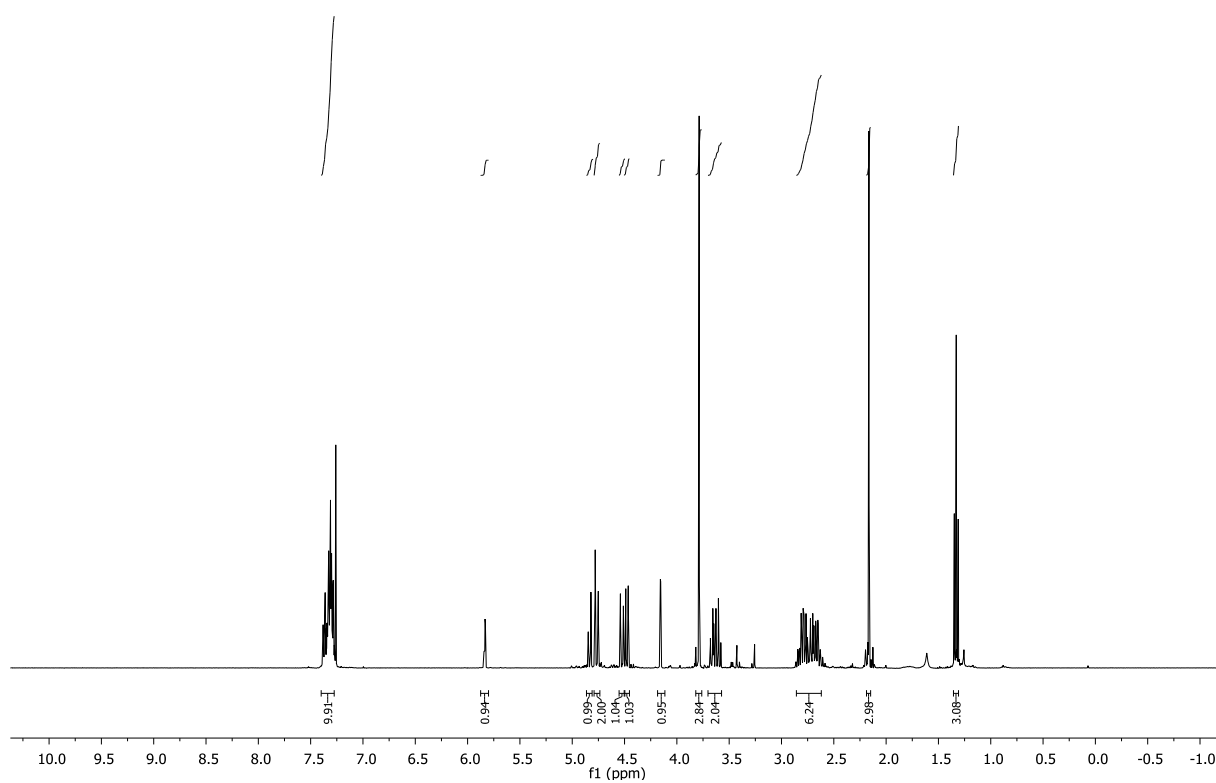


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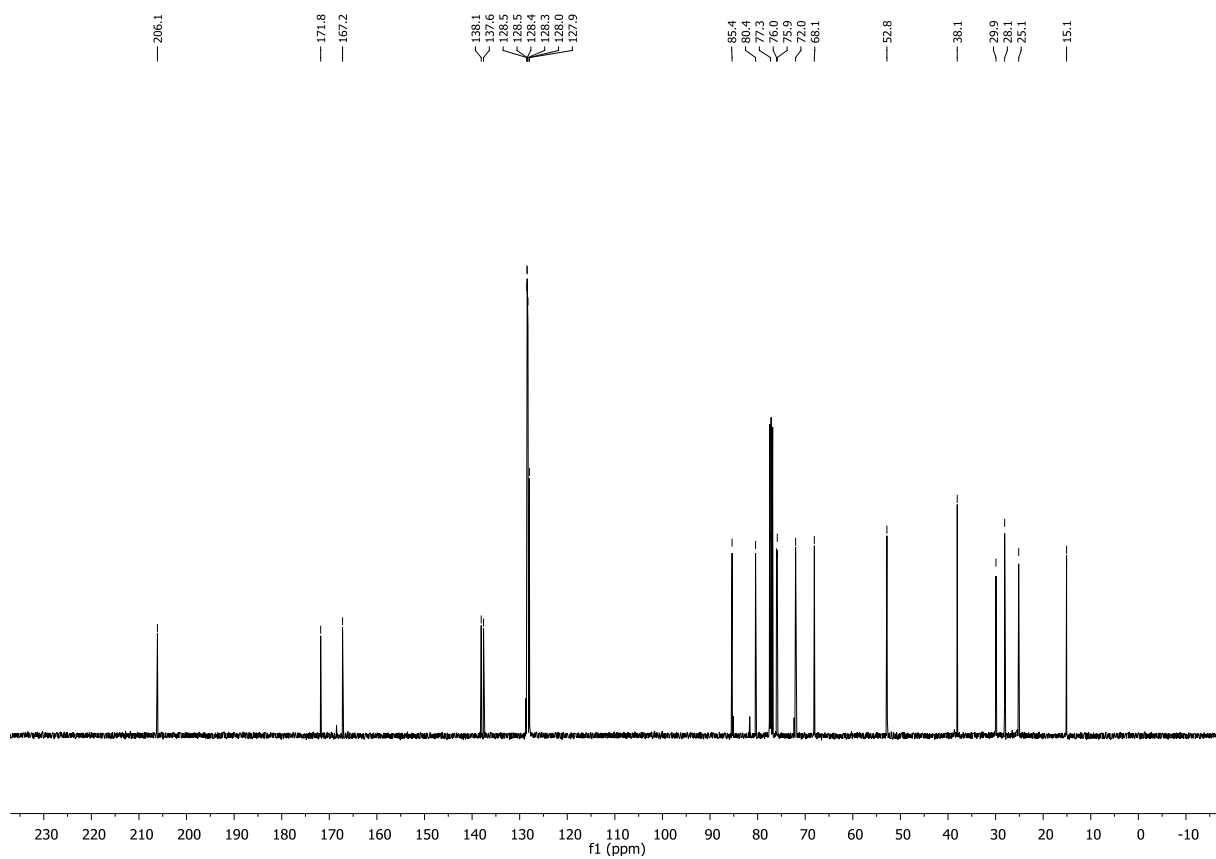


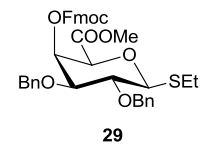


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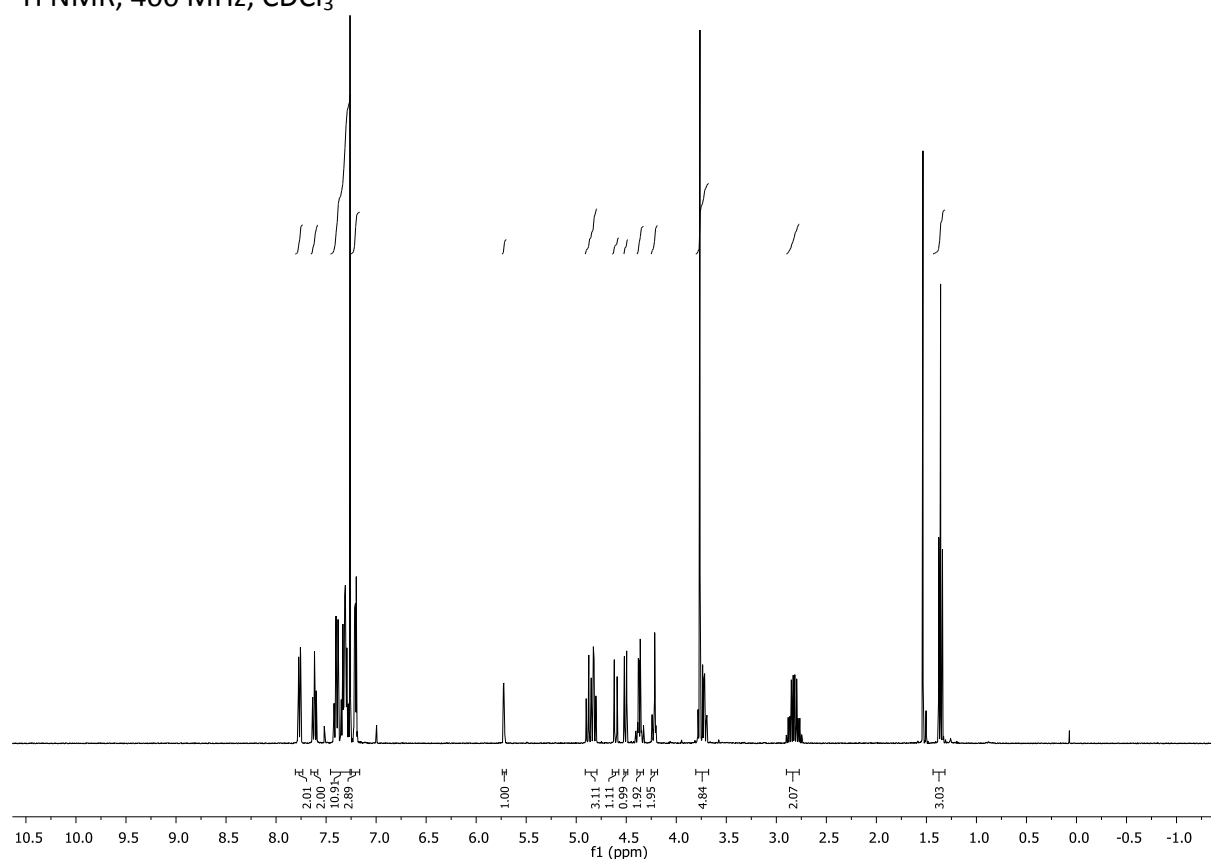


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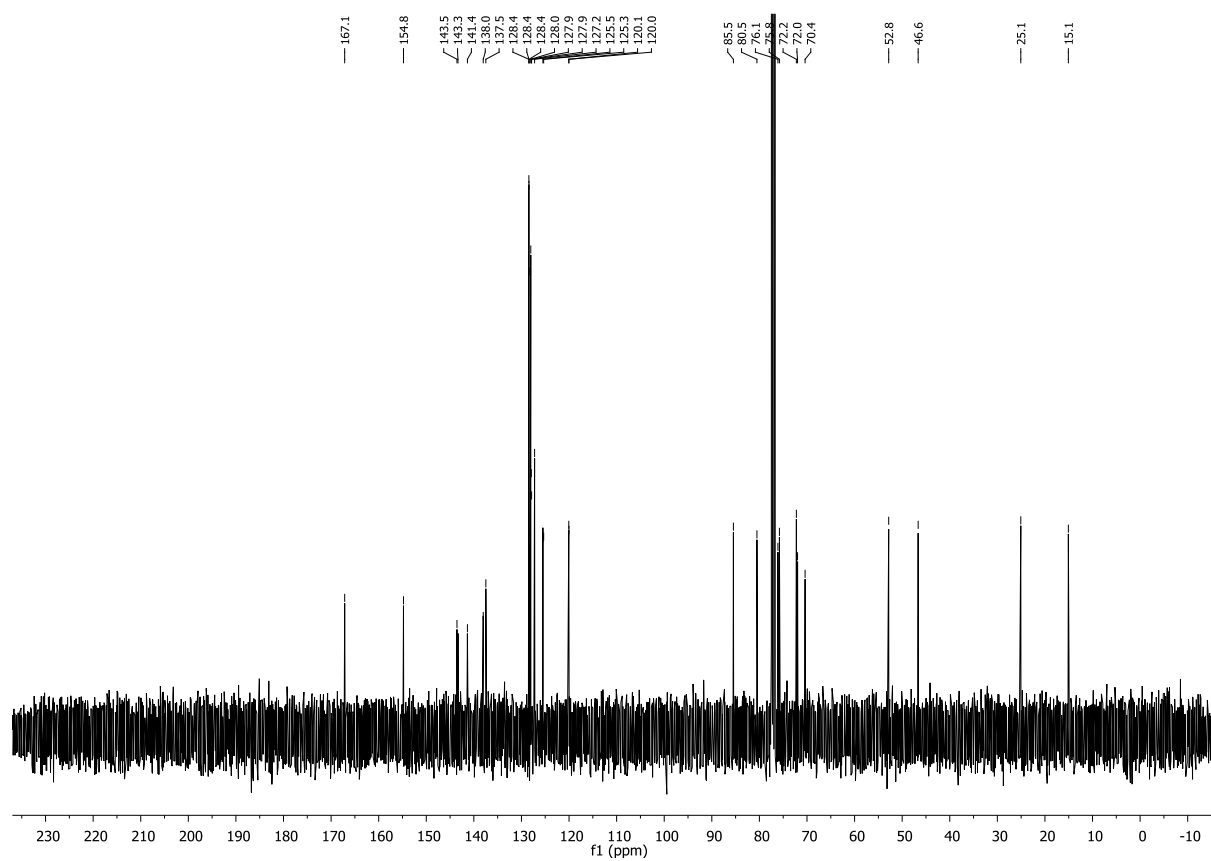




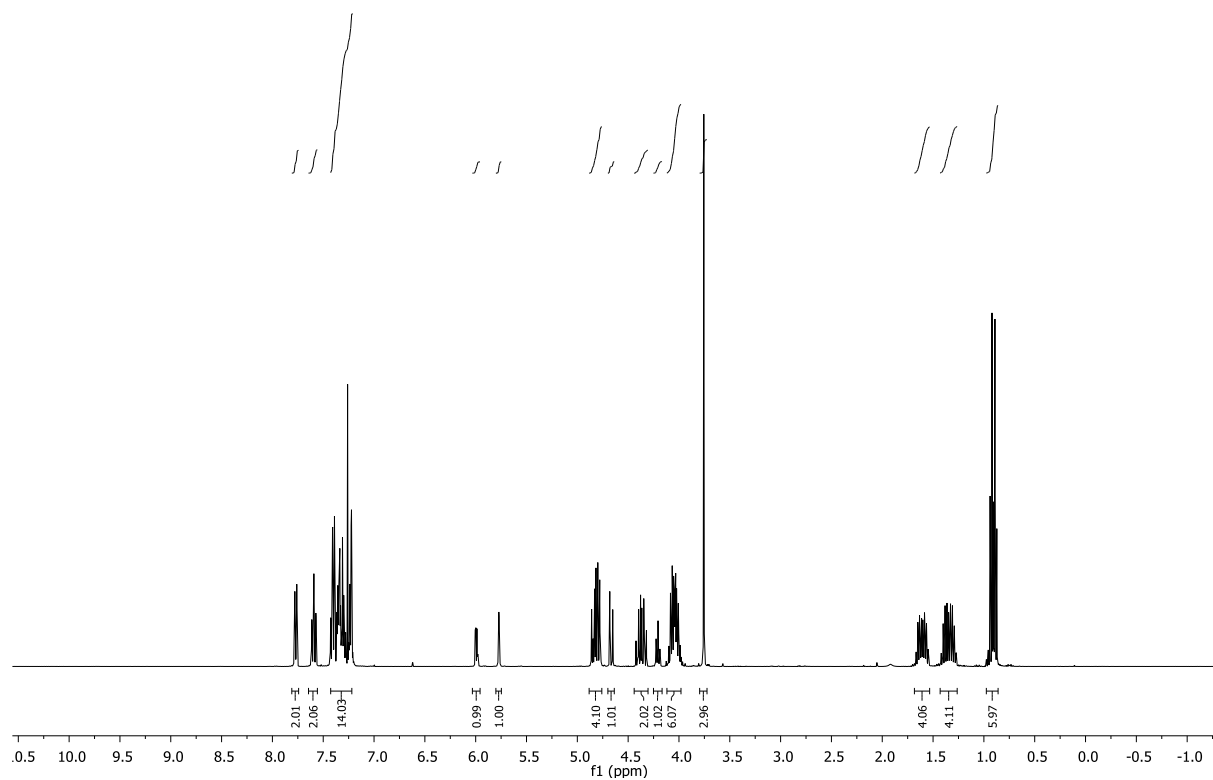
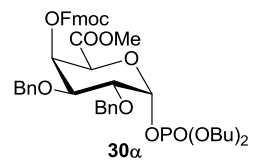
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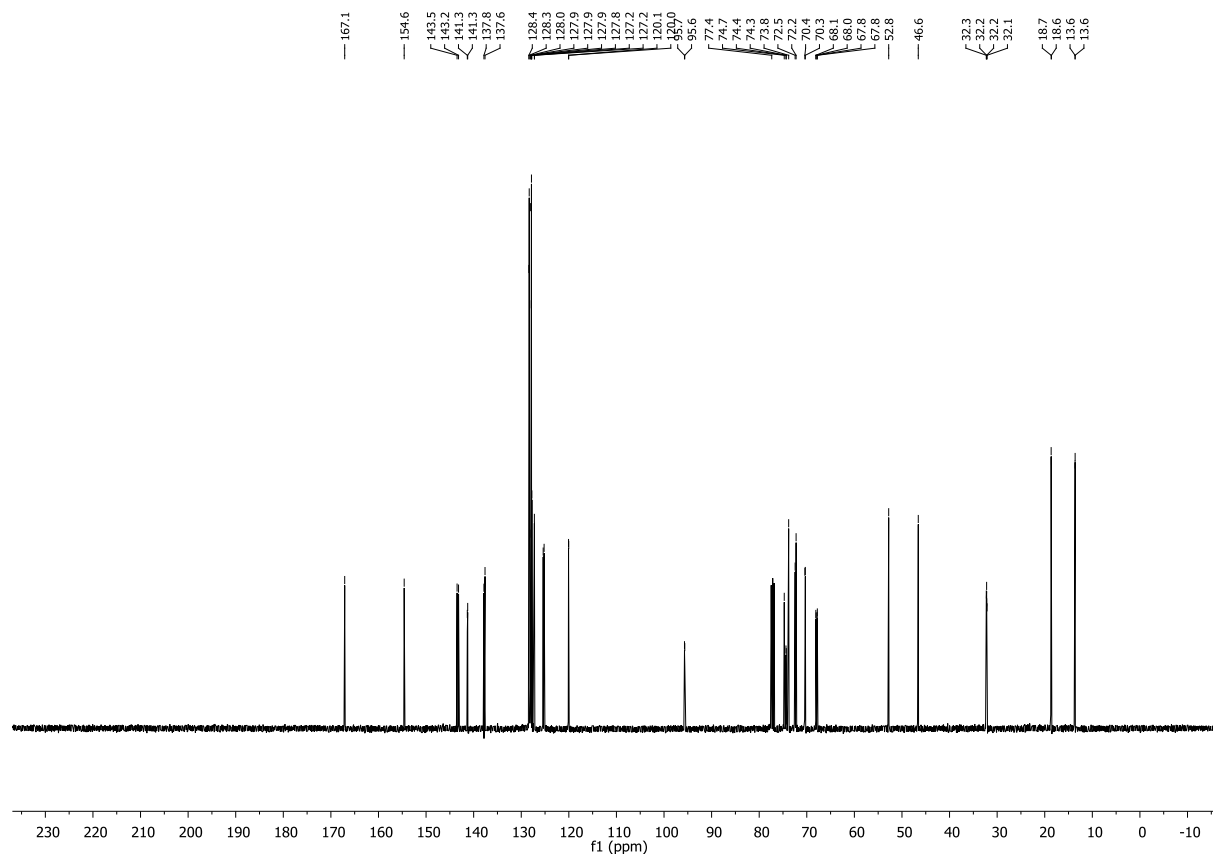
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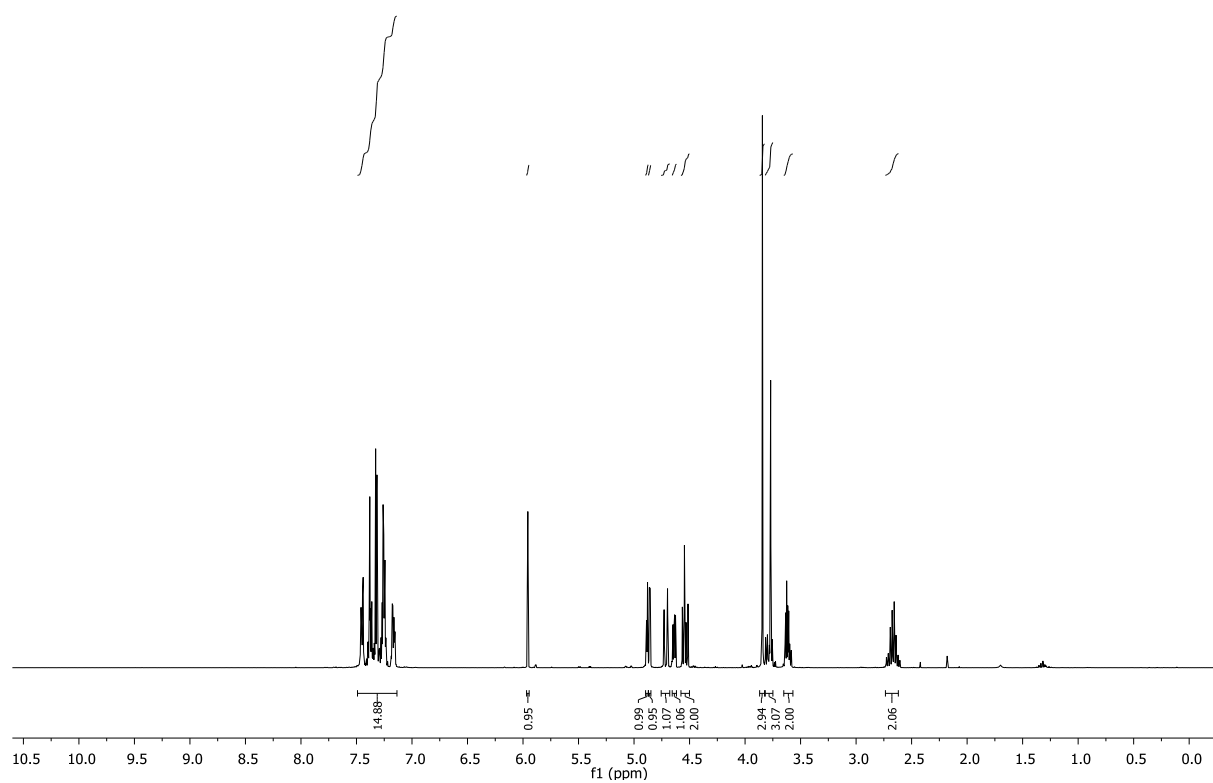
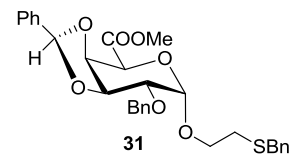
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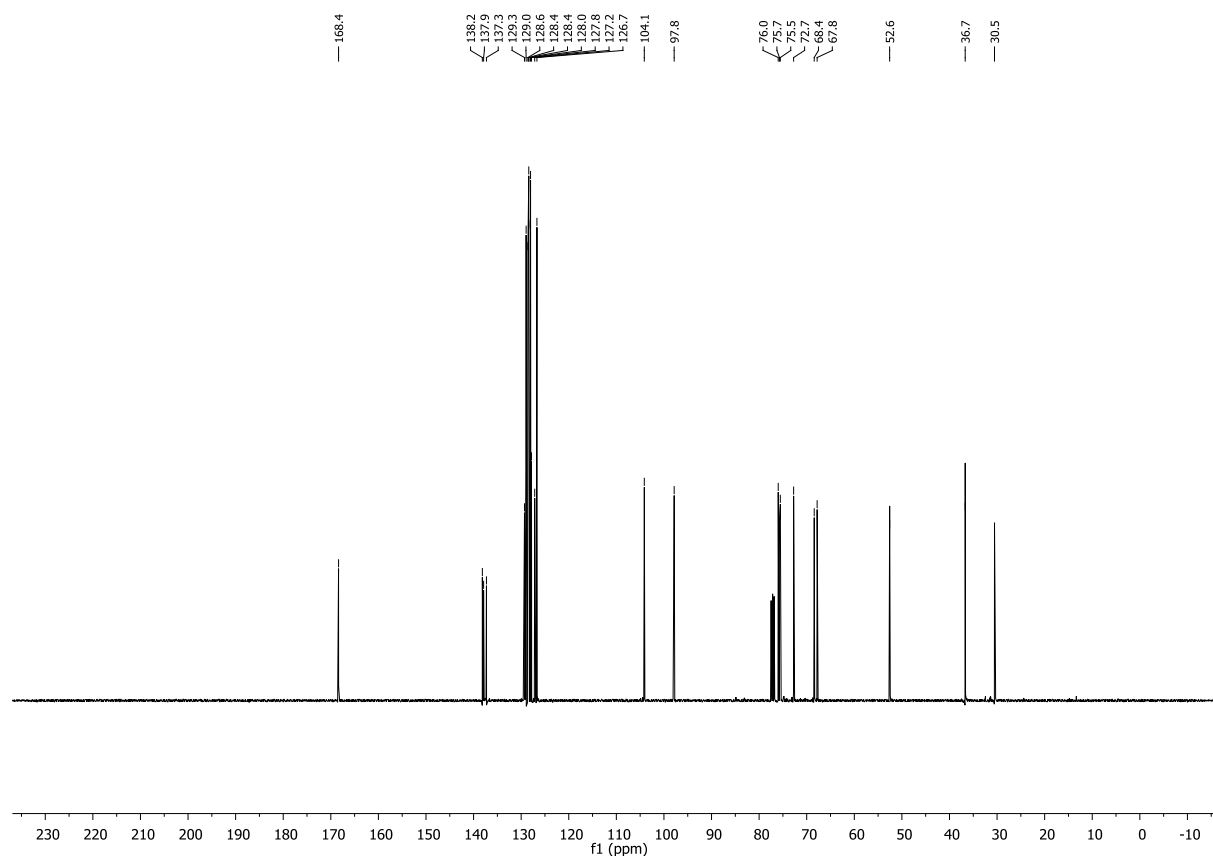
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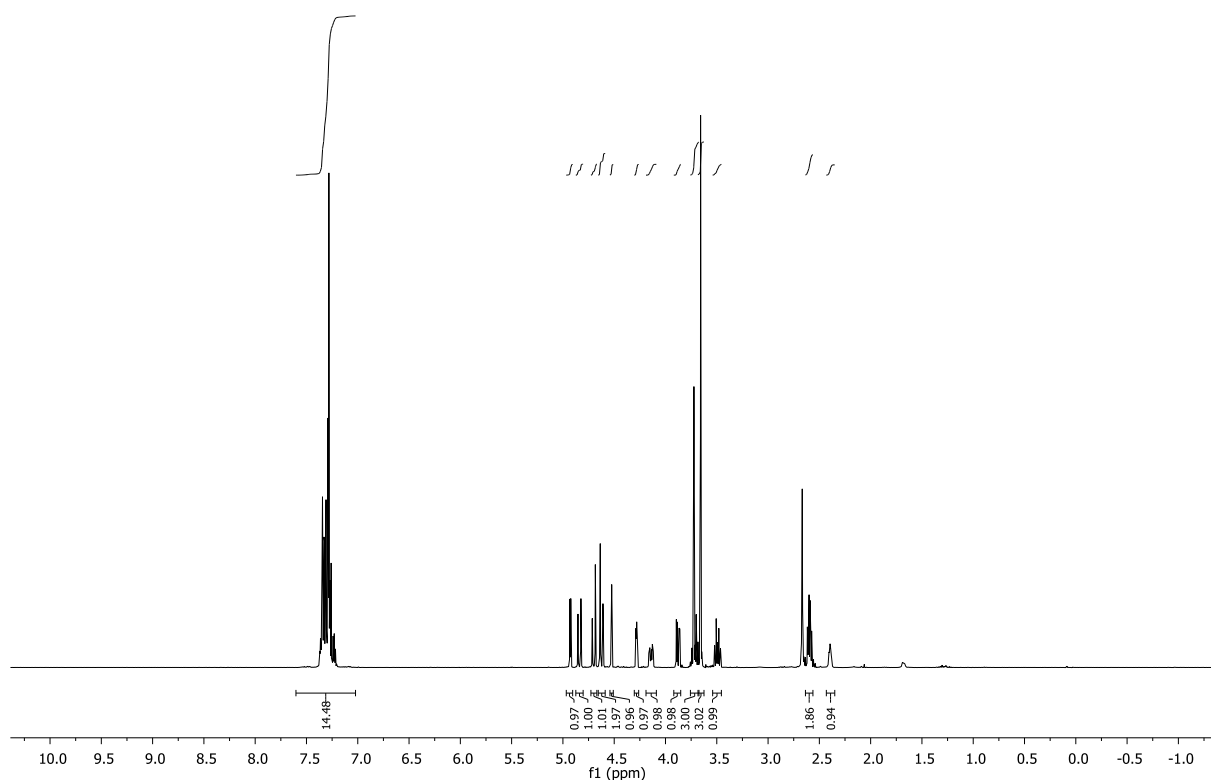
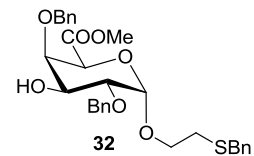
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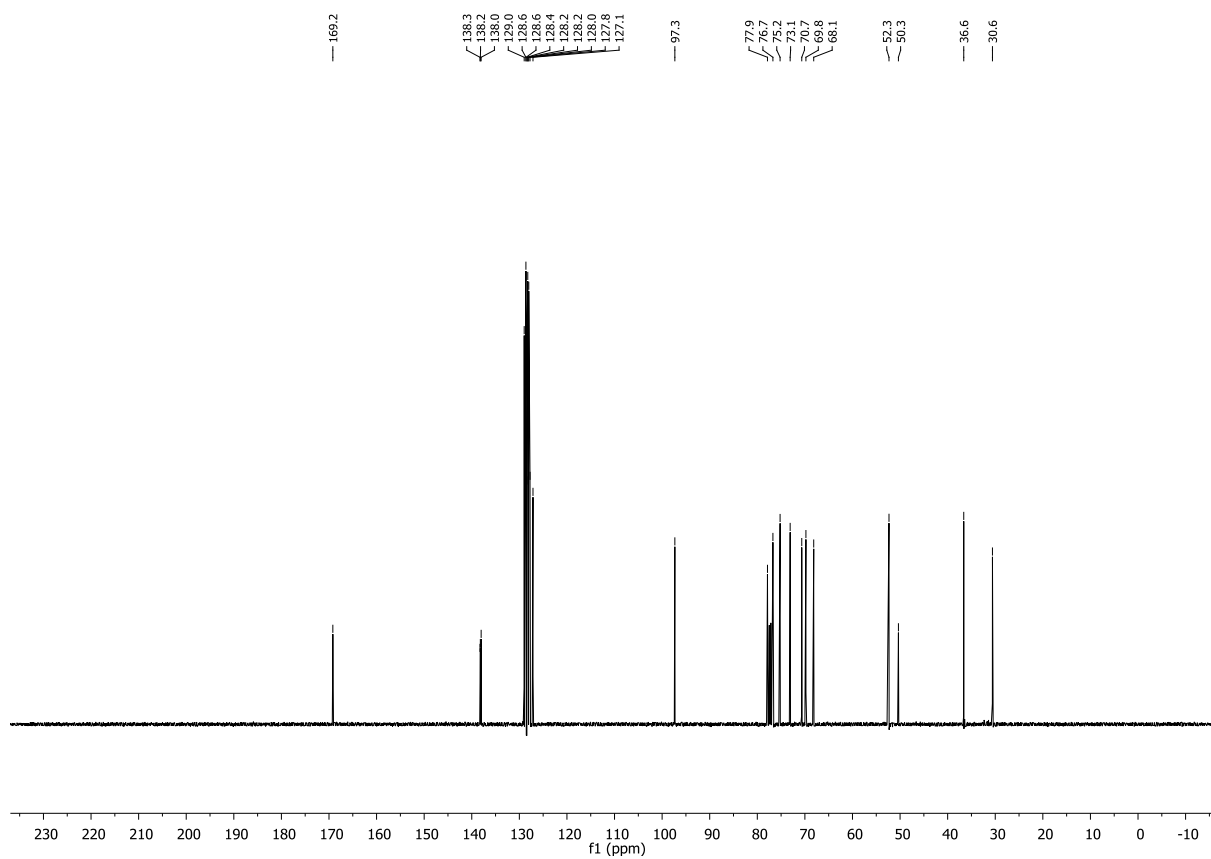
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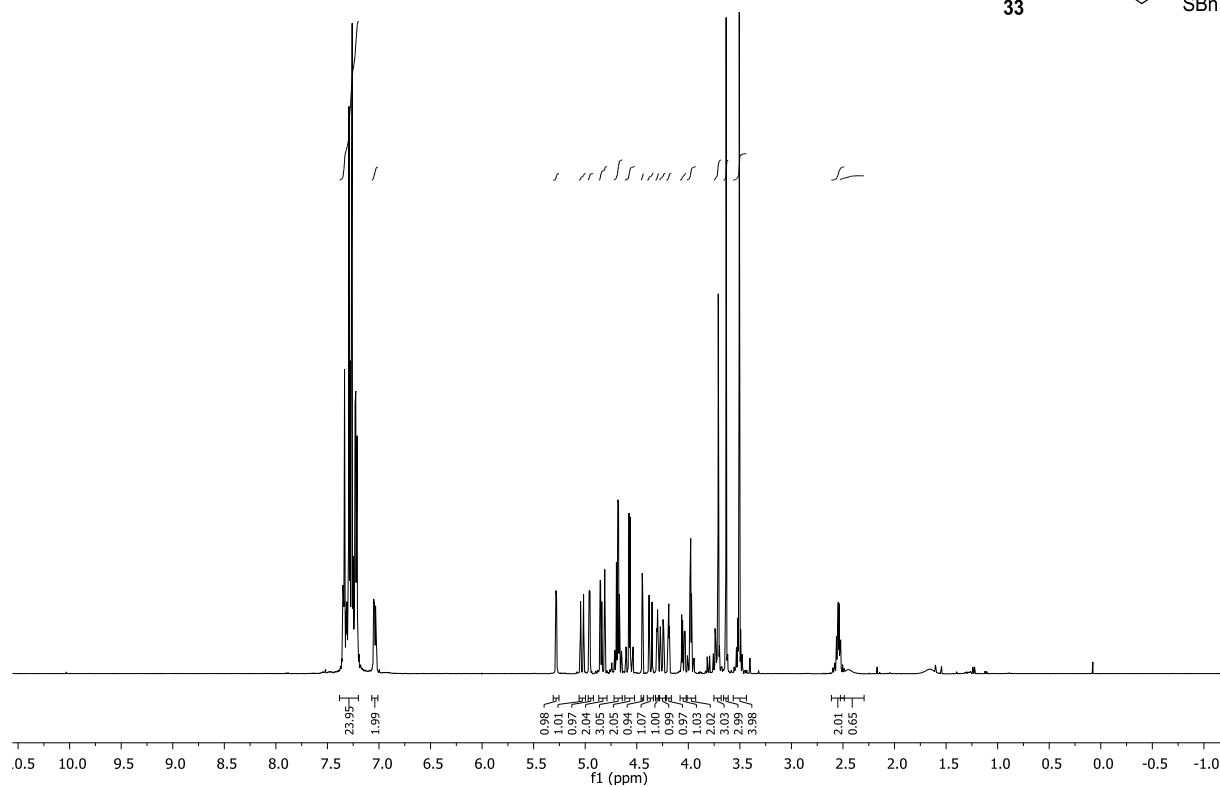
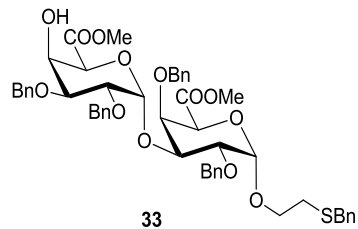
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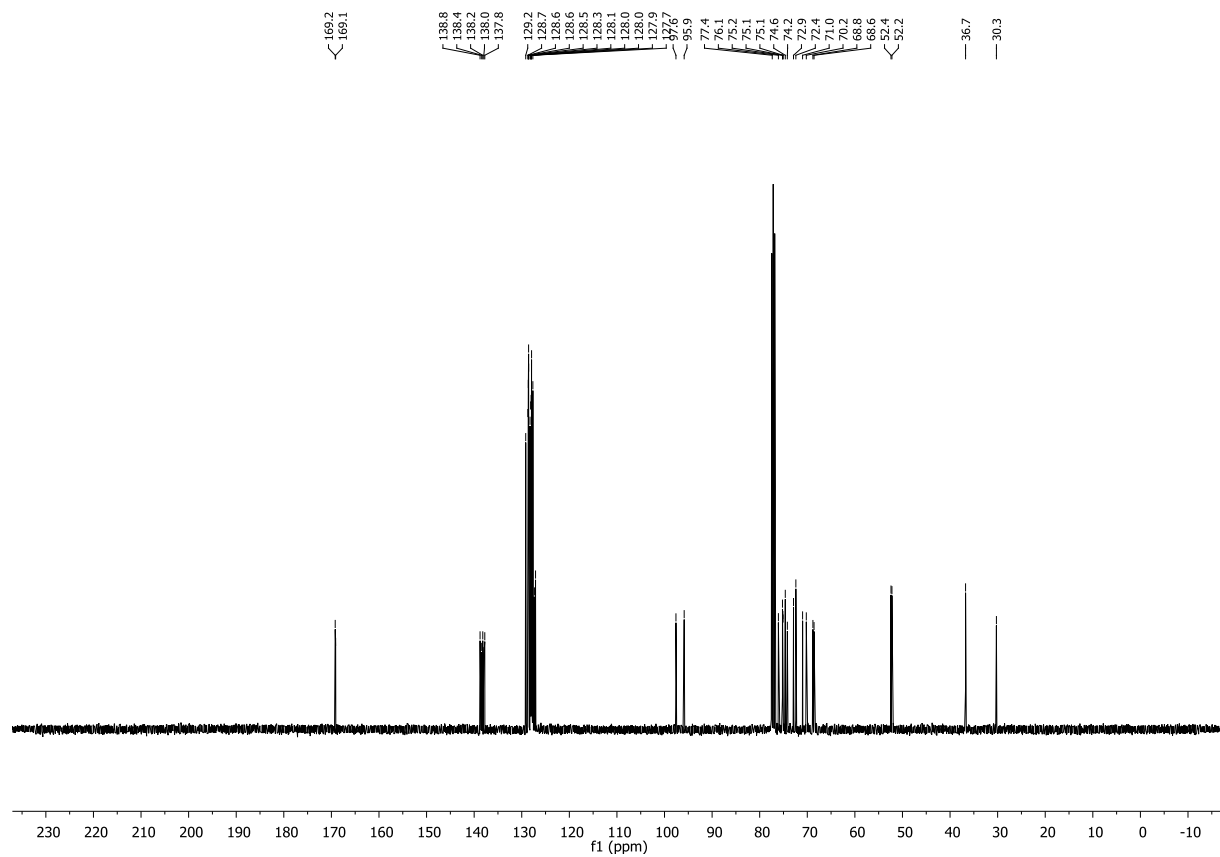
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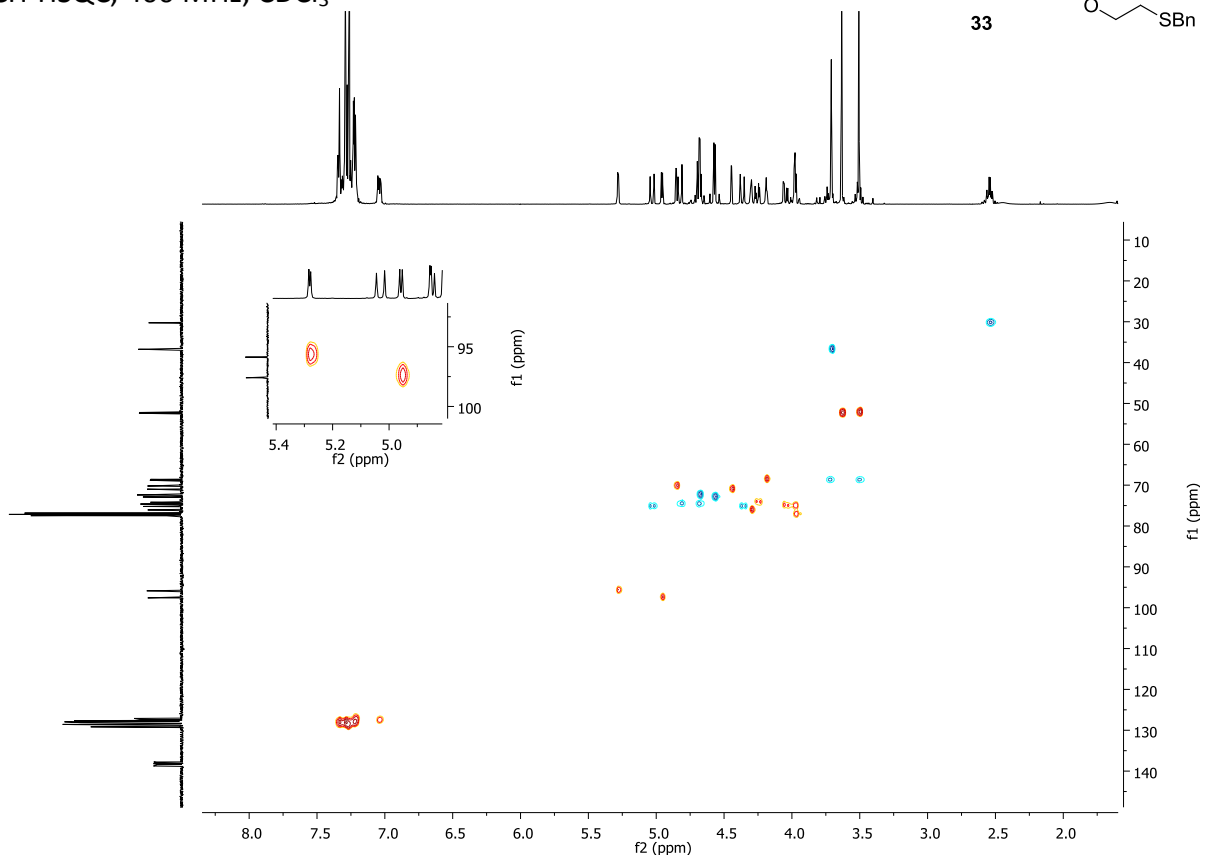
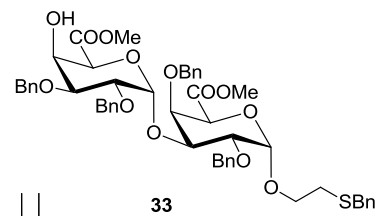
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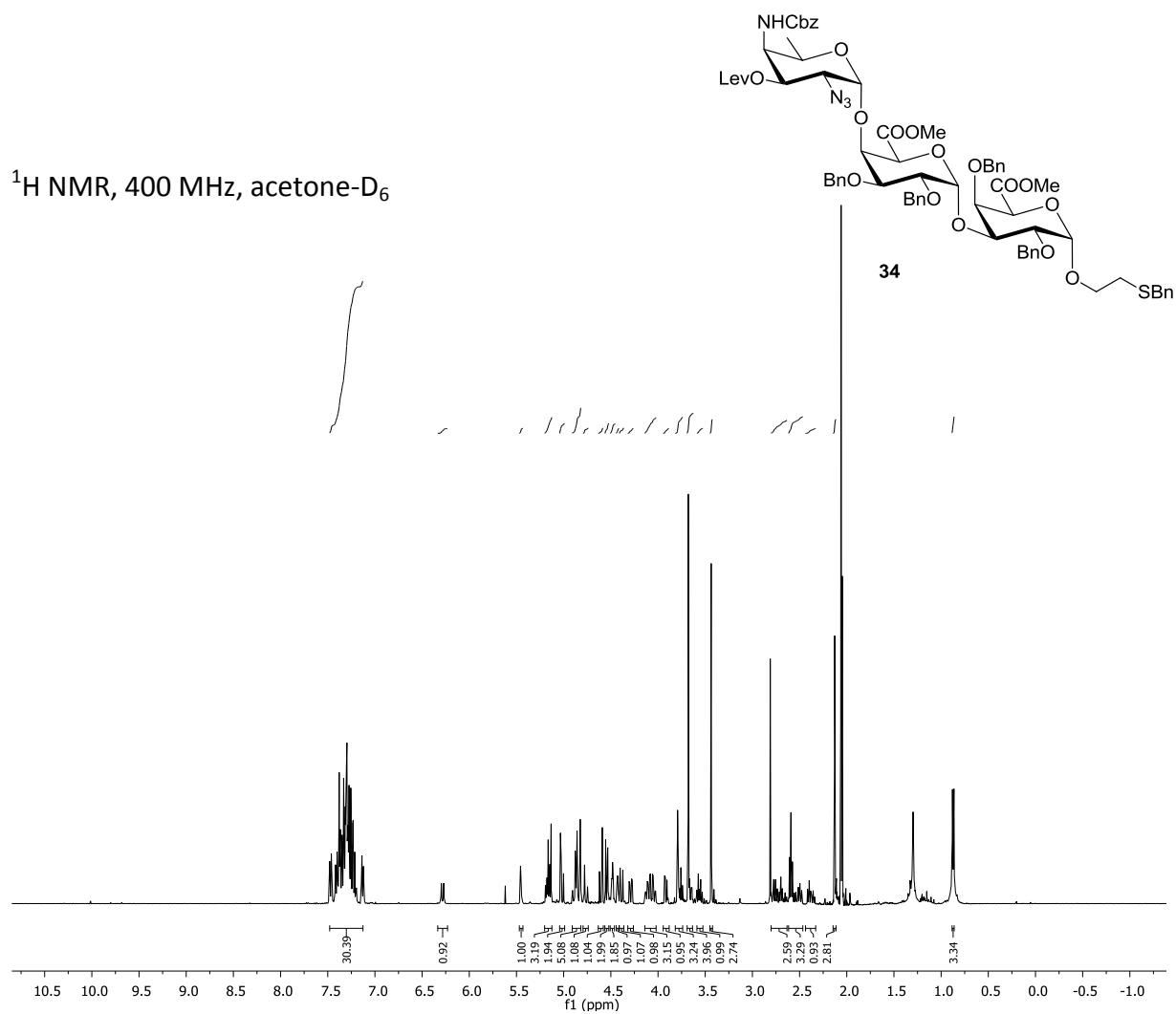
^{13}C NMR, 100 MHz, CDCl_3



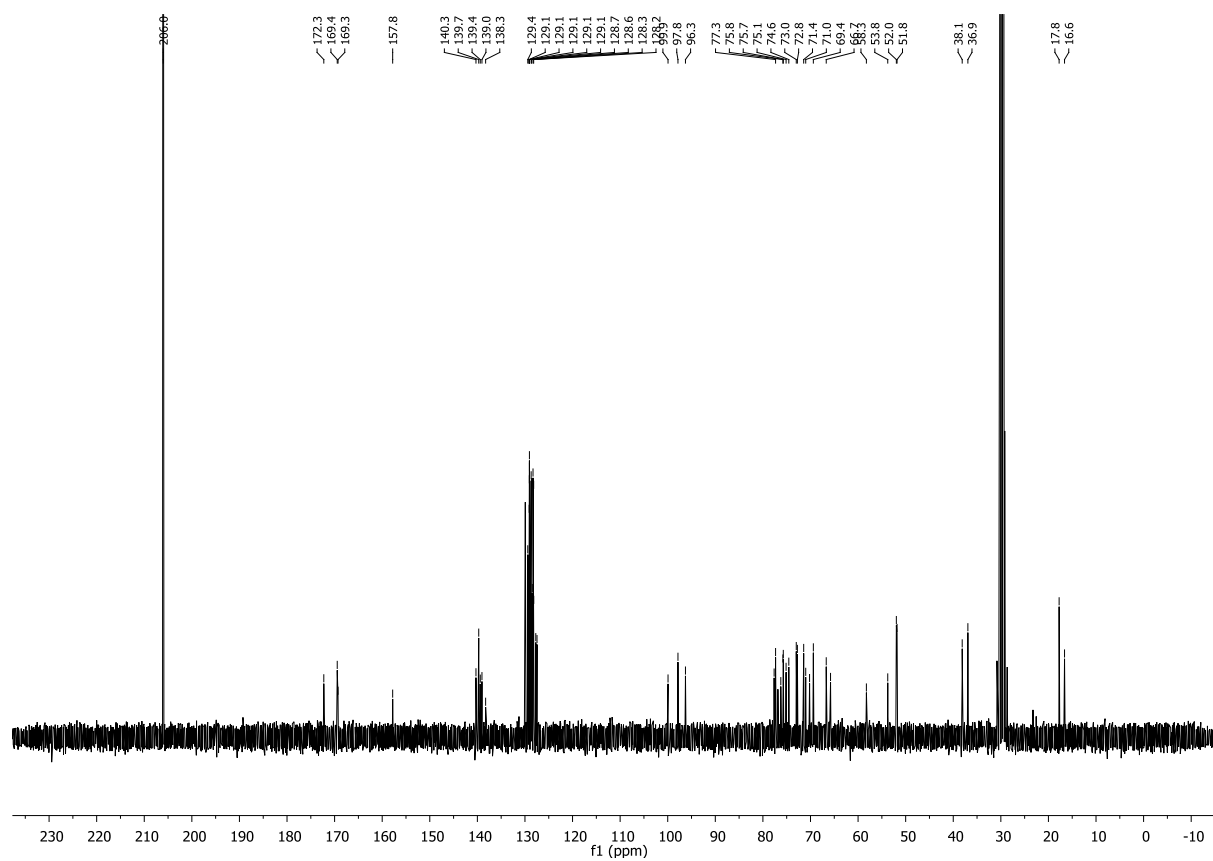
CH-HSQC, 400 MHz, CDCl₃



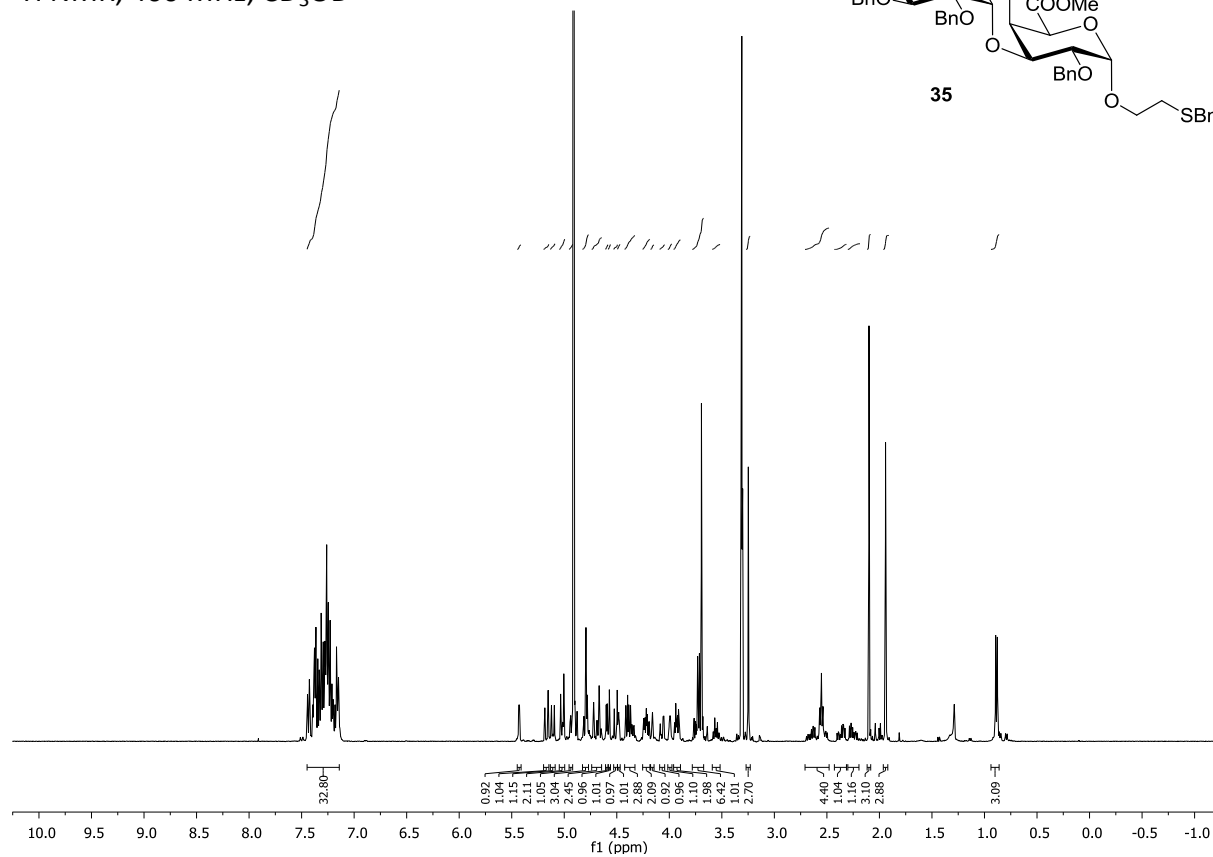
¹H NMR, 400 MHz, acetone-D₆



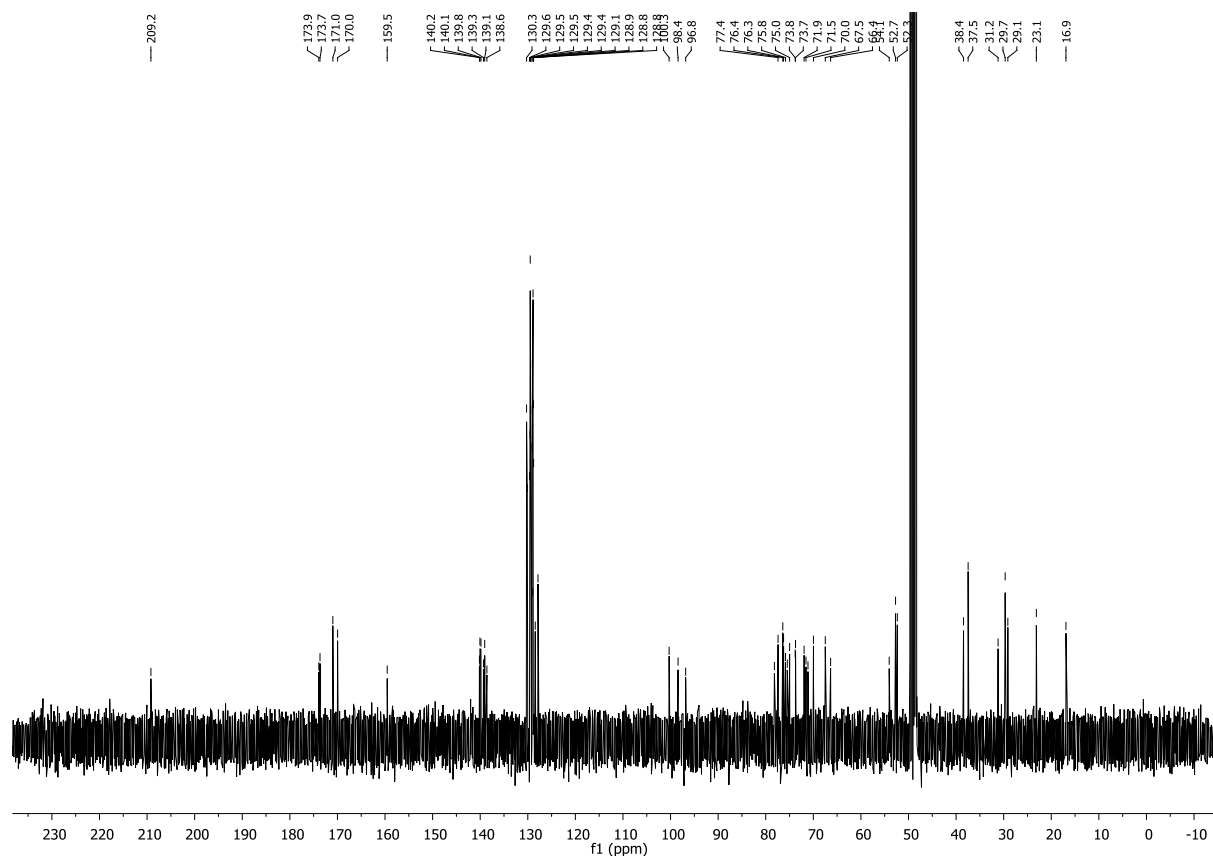
¹³C NMR, 100 MHz, acetone-D₆



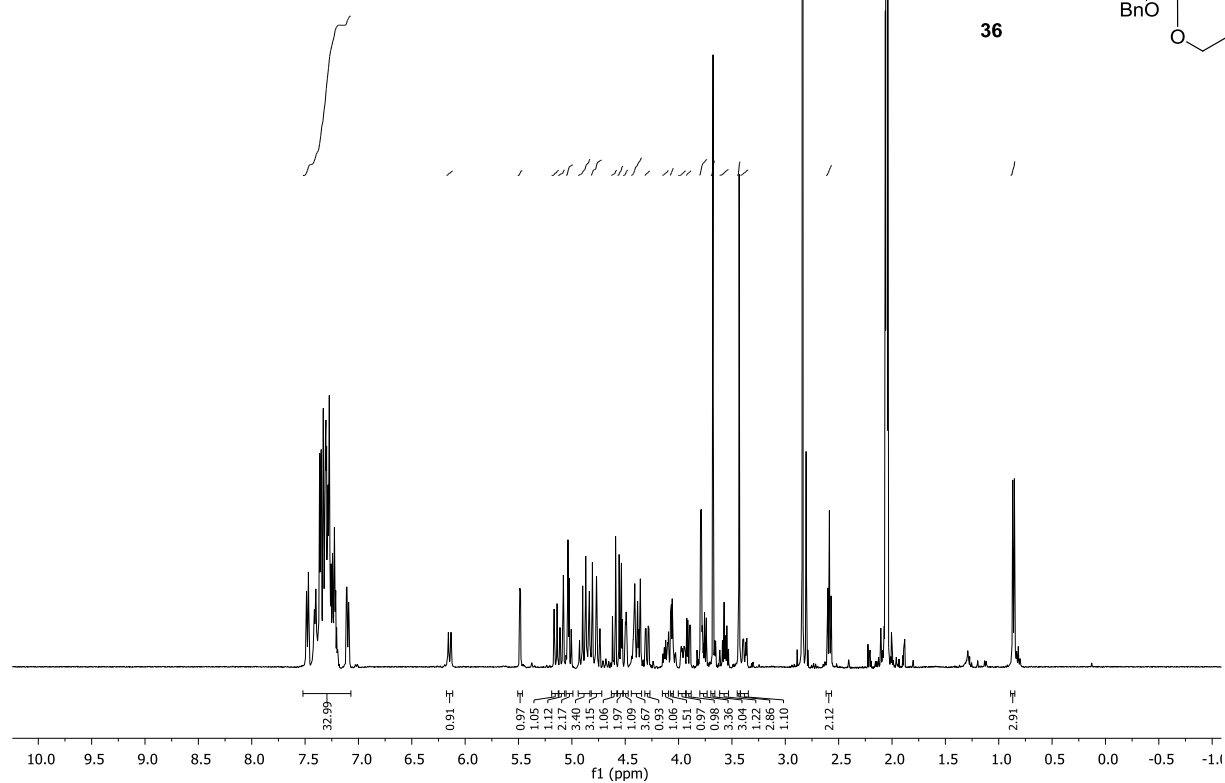
^1H NMR, 400 MHz, CD_3OD



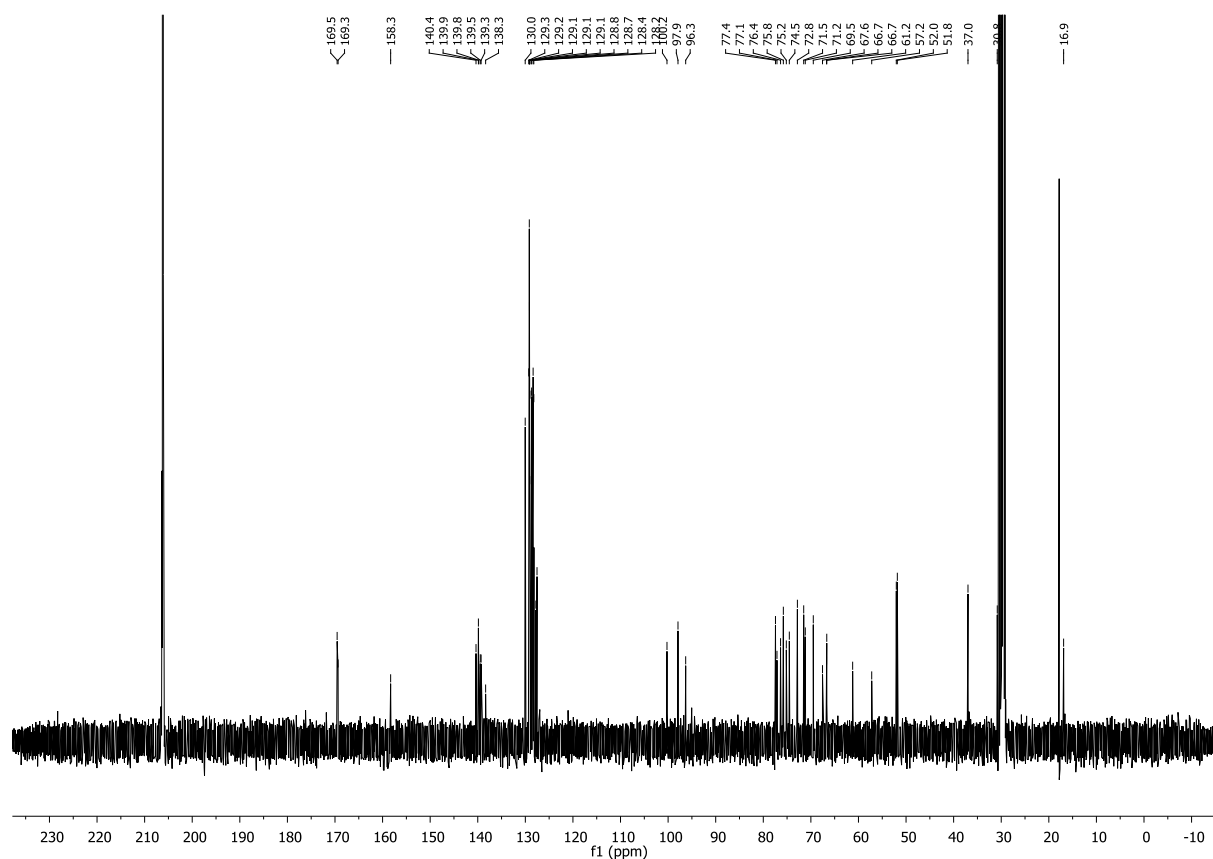
^{13}C NMR, 100 MHz, CD_3OD



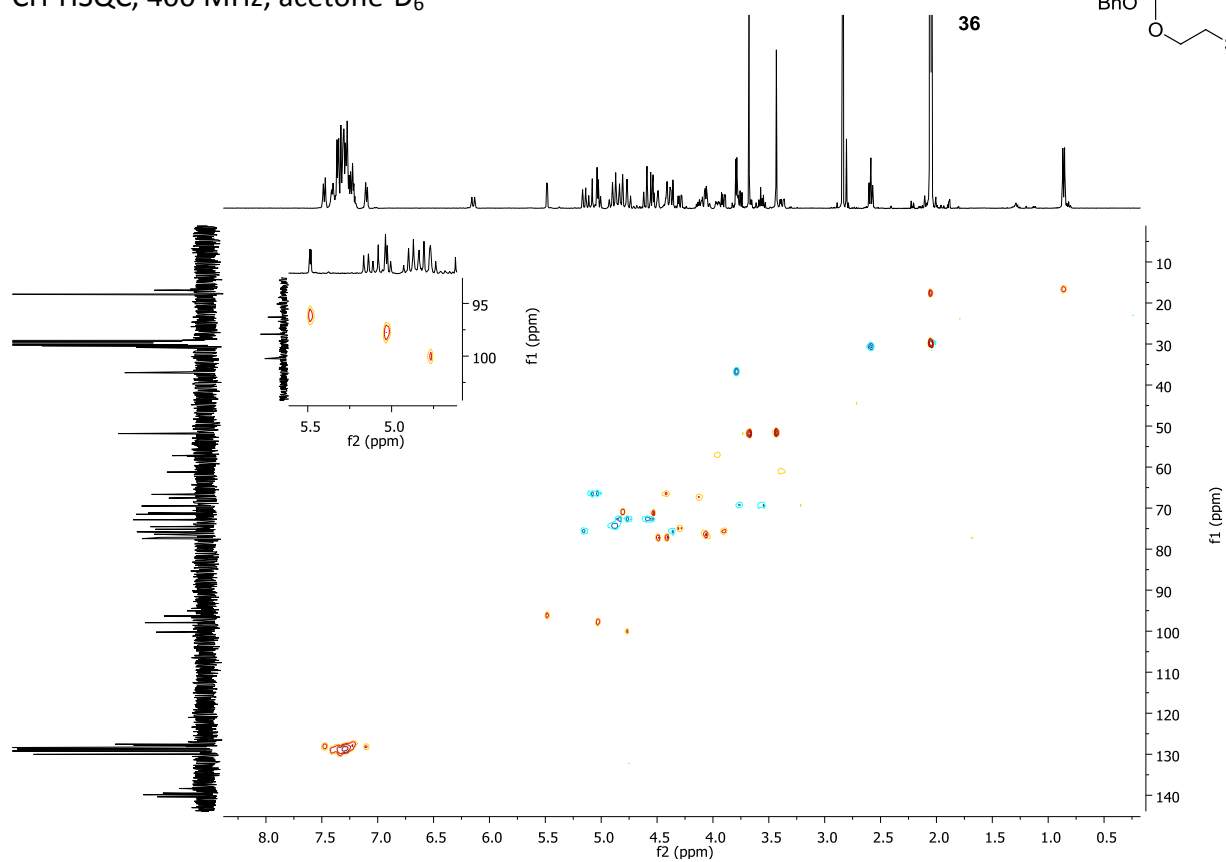
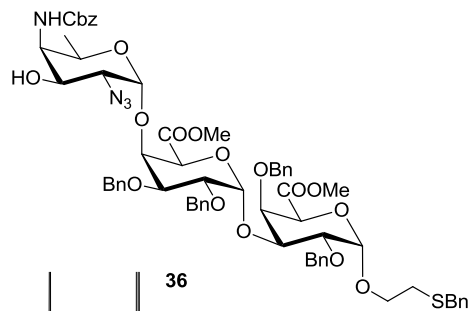
^1H NMR, 400 MHz, acetone- D_6

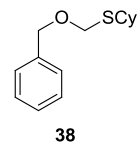


^{13}C NMR, 100 MHz, acetone- D_6

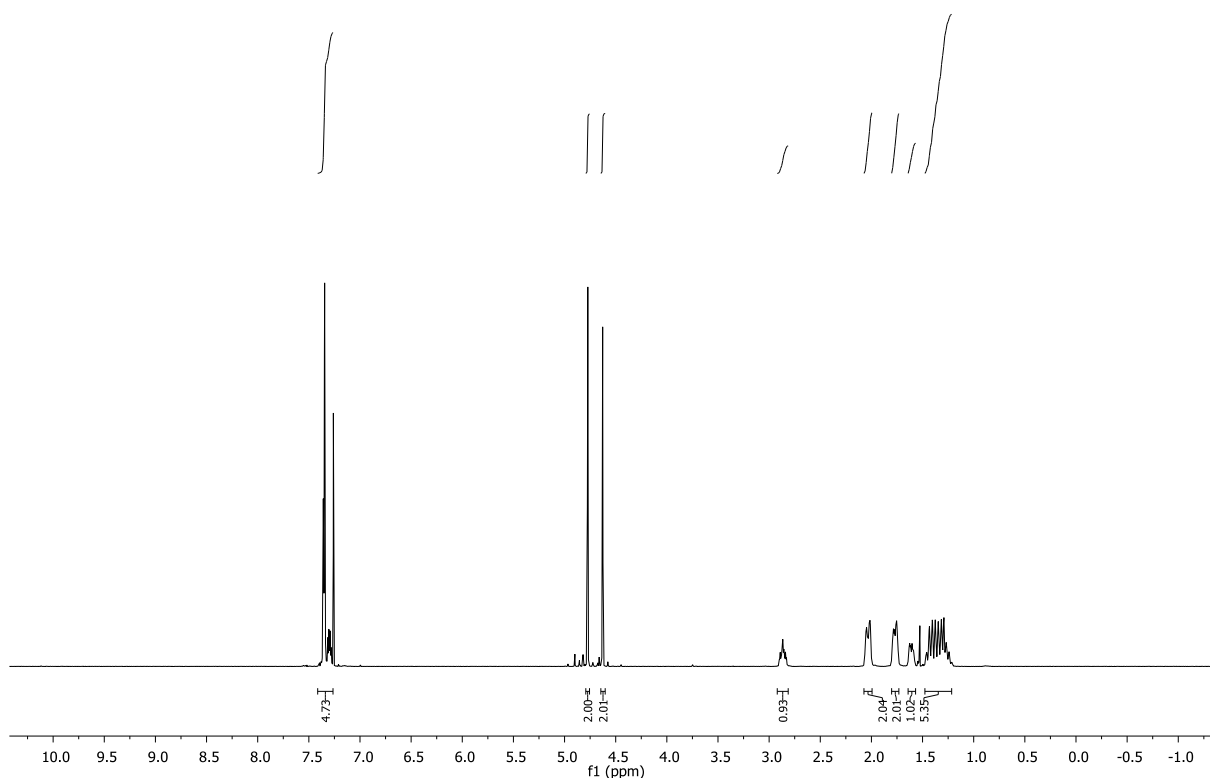


CH-HSQC, 400 MHz, acetone-D₆

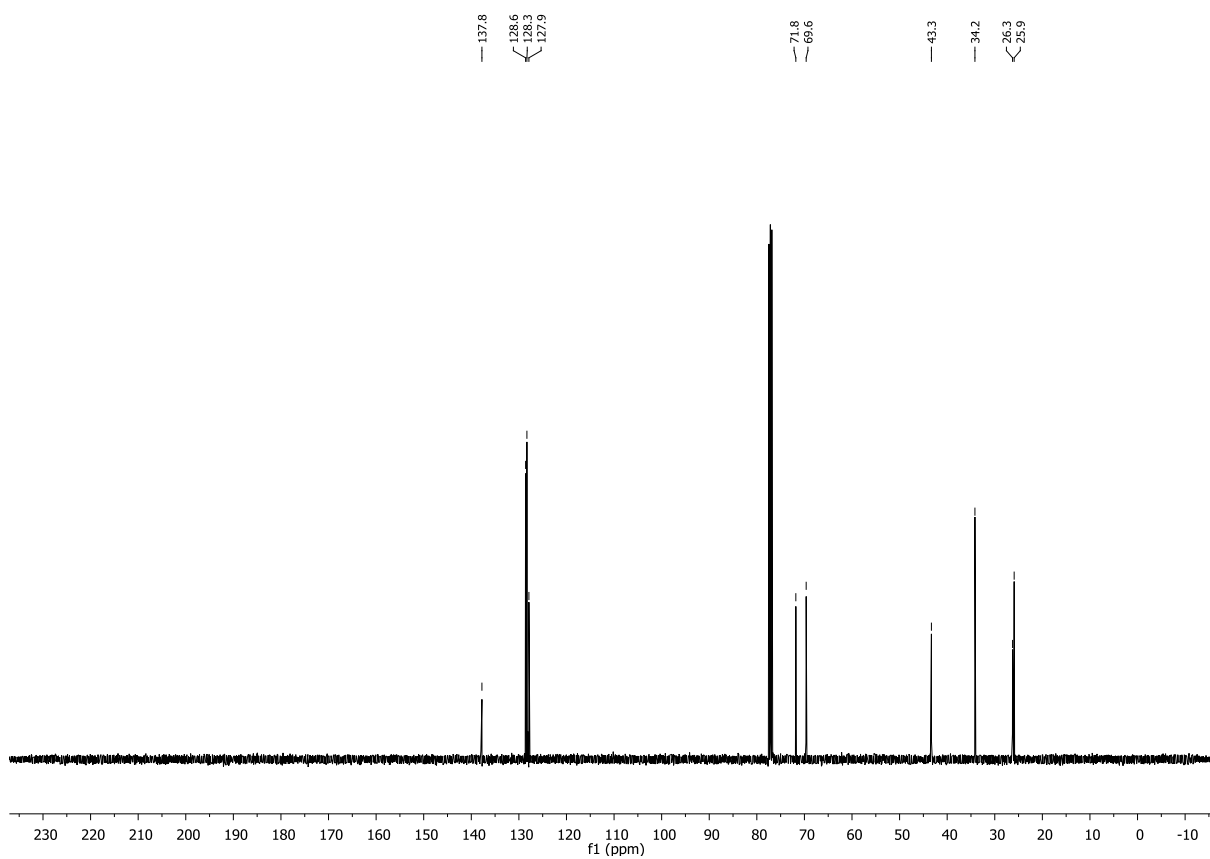




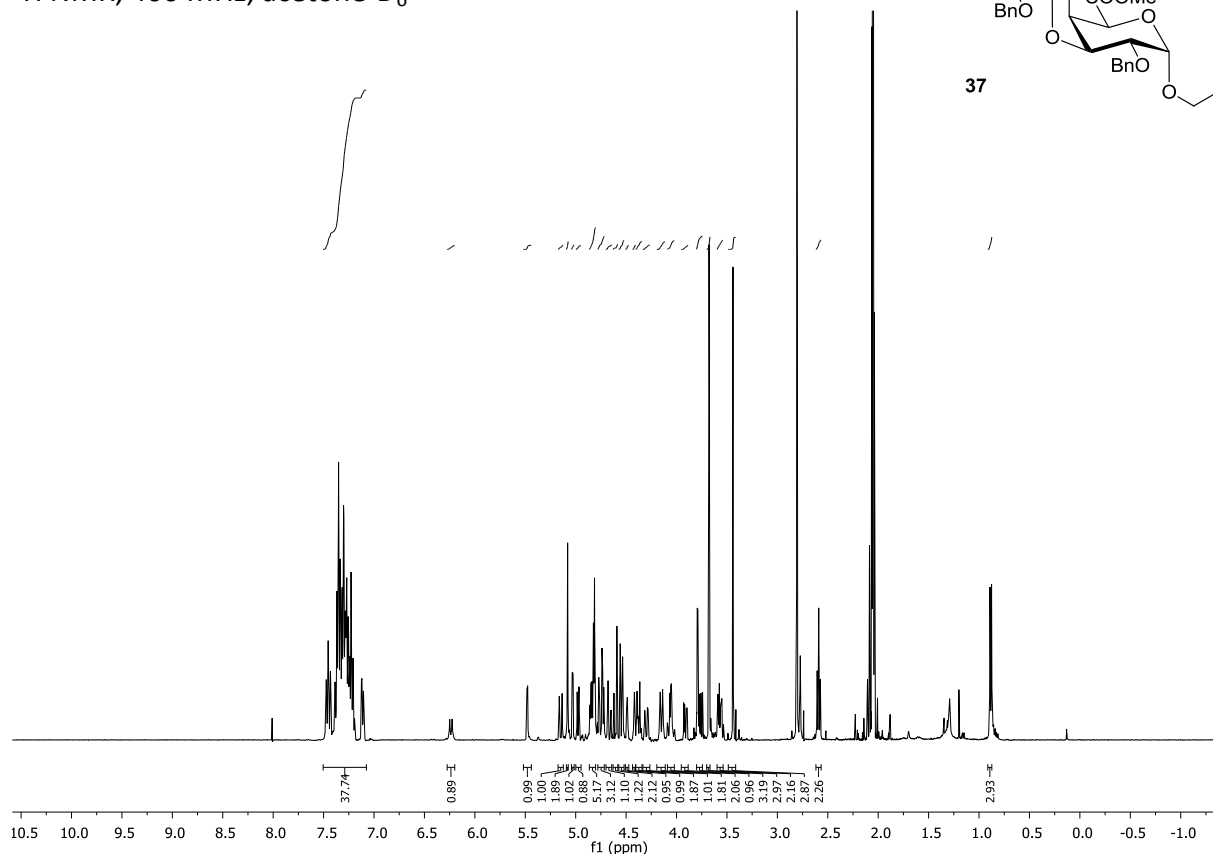
^1H NMR, 400 MHz, acetone- D_6



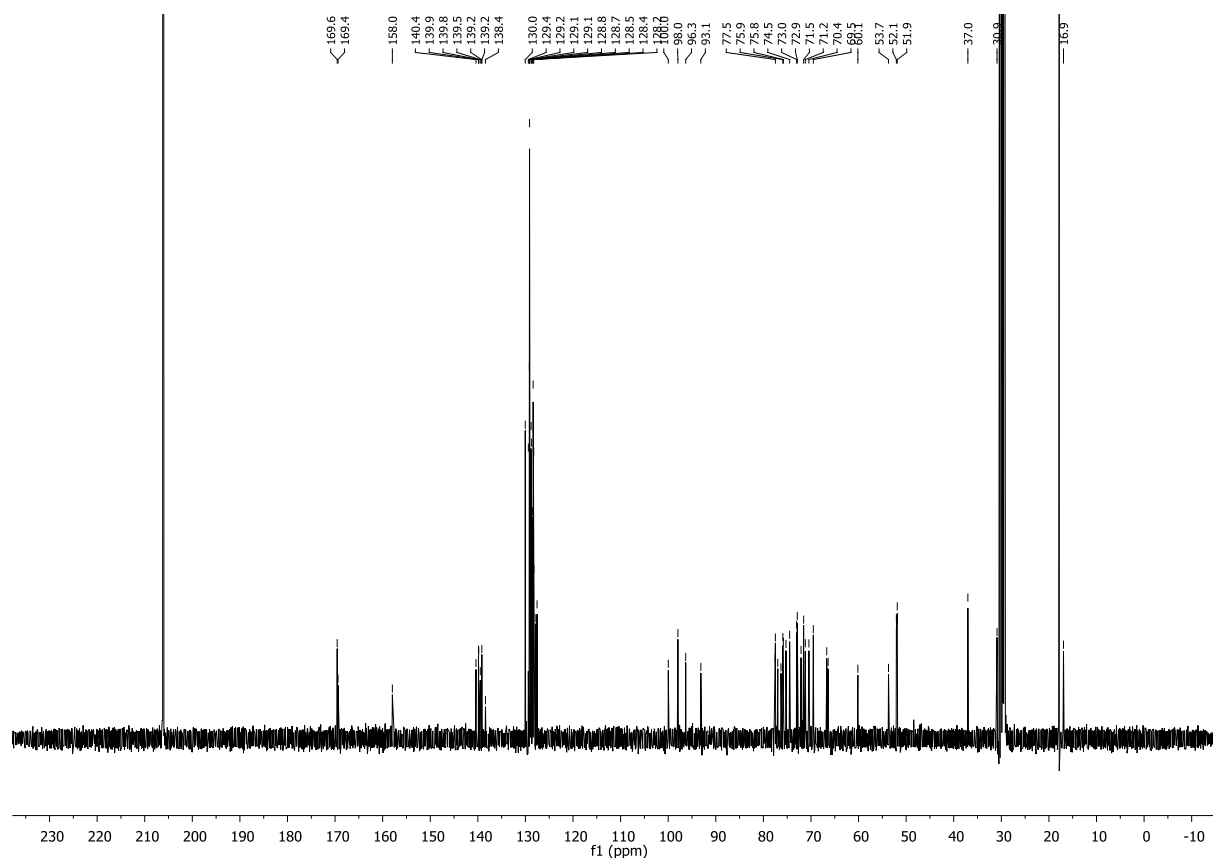
^{13}C NMR, 100 MHz, acetone- D_6

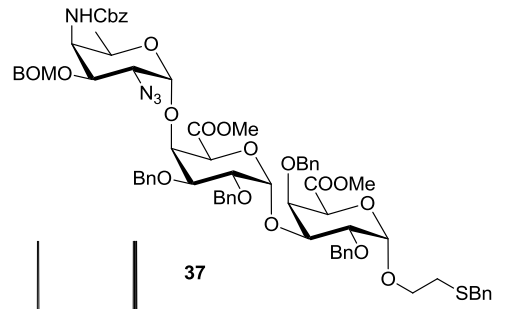


¹H NMR, 400 MHz, acetone-D₆

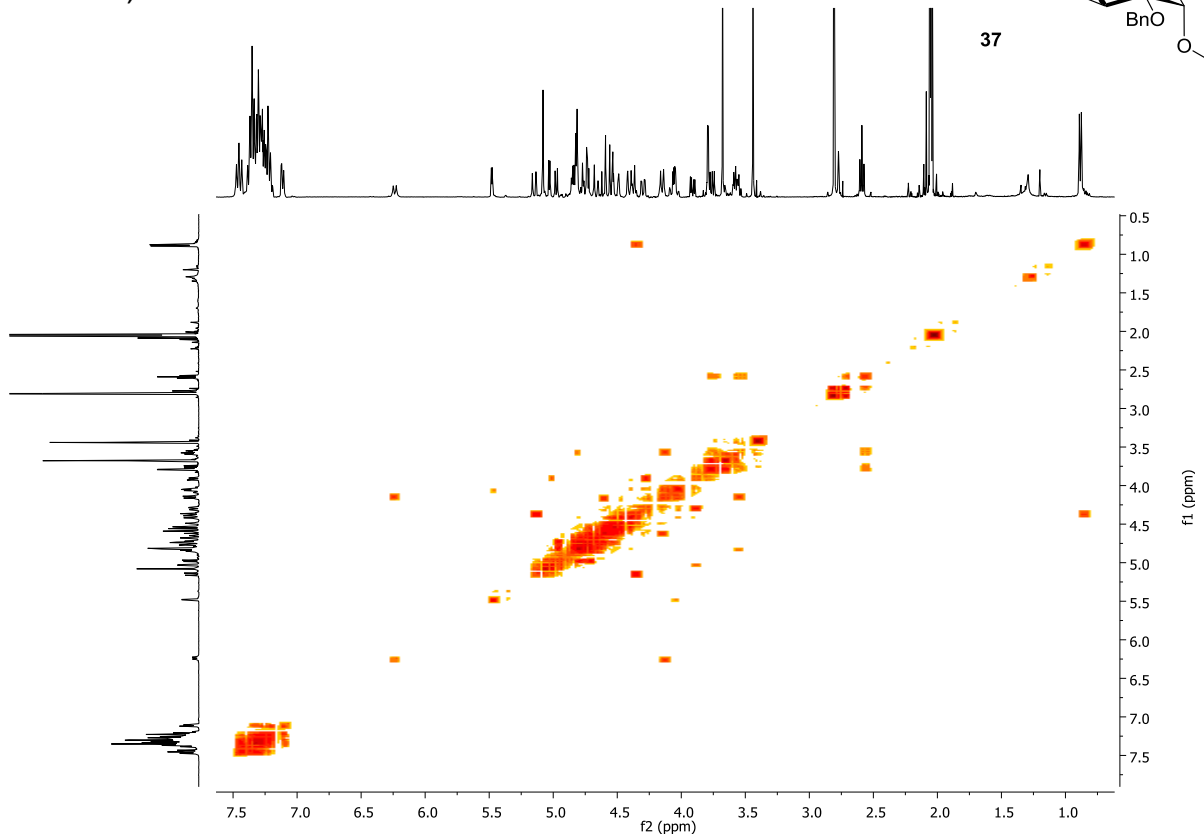


¹³C NMR, 100 MHz, acetone-D₆

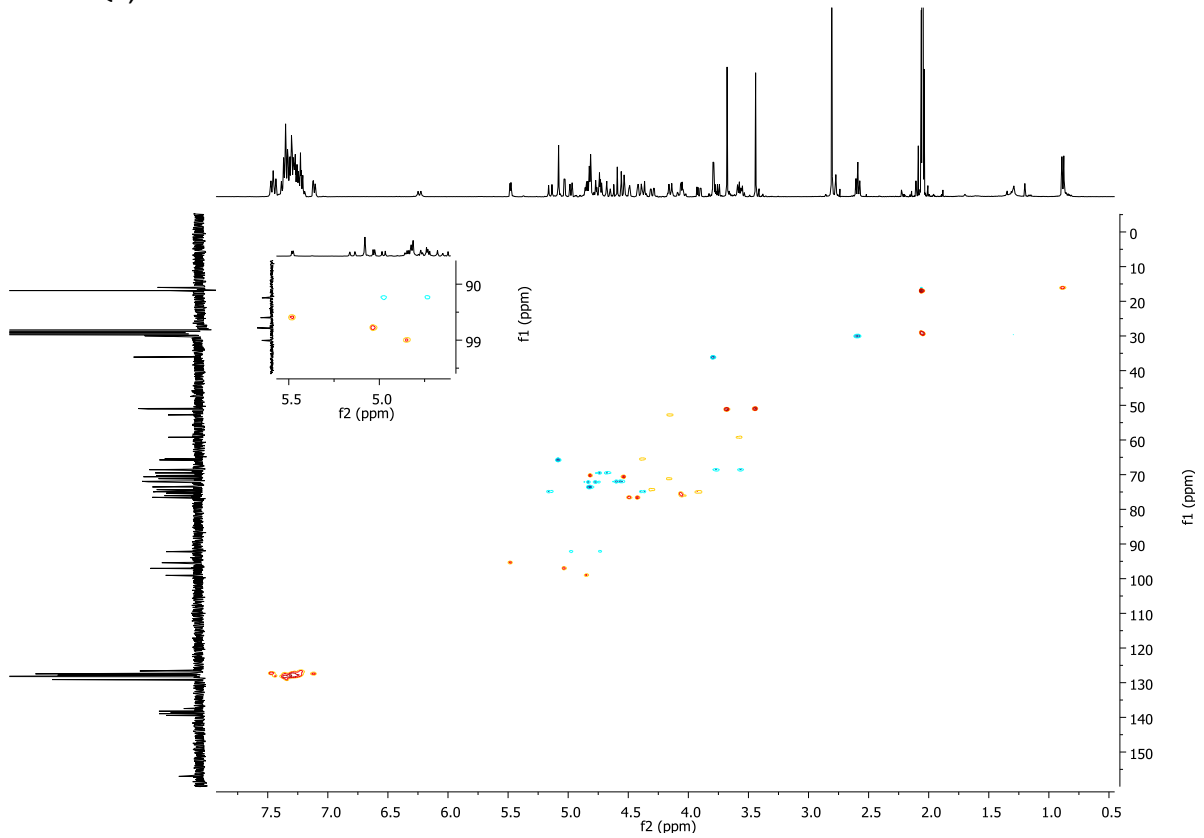




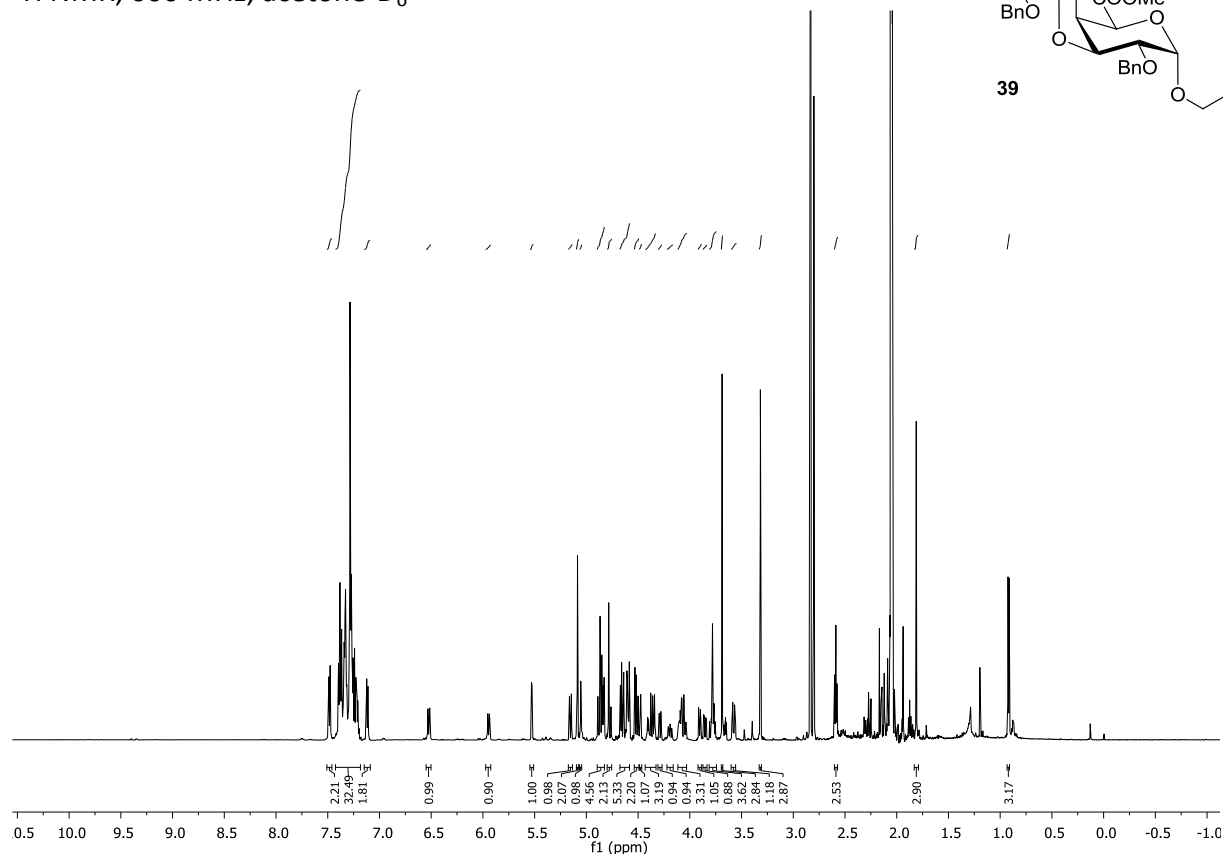
HH-COSY, 400 MHz



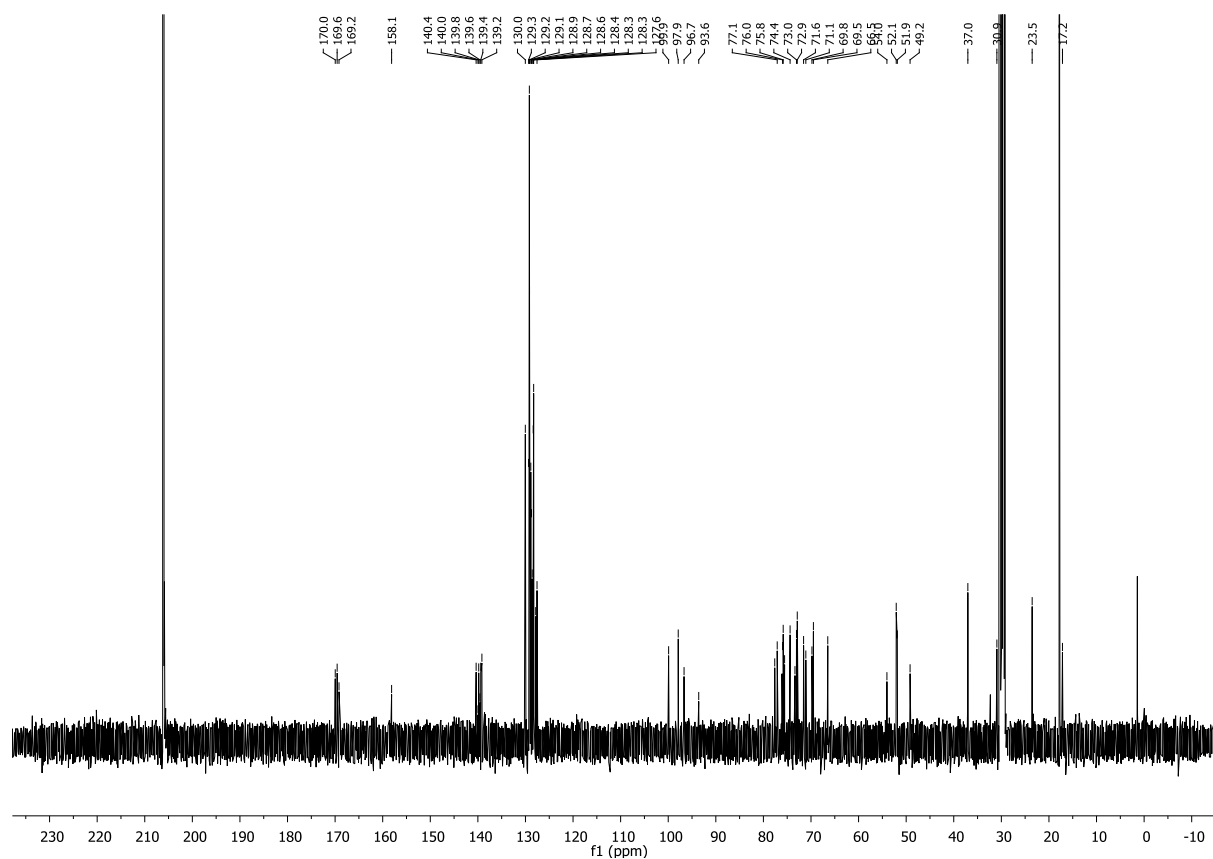
CH-HSQC, 400 MHz



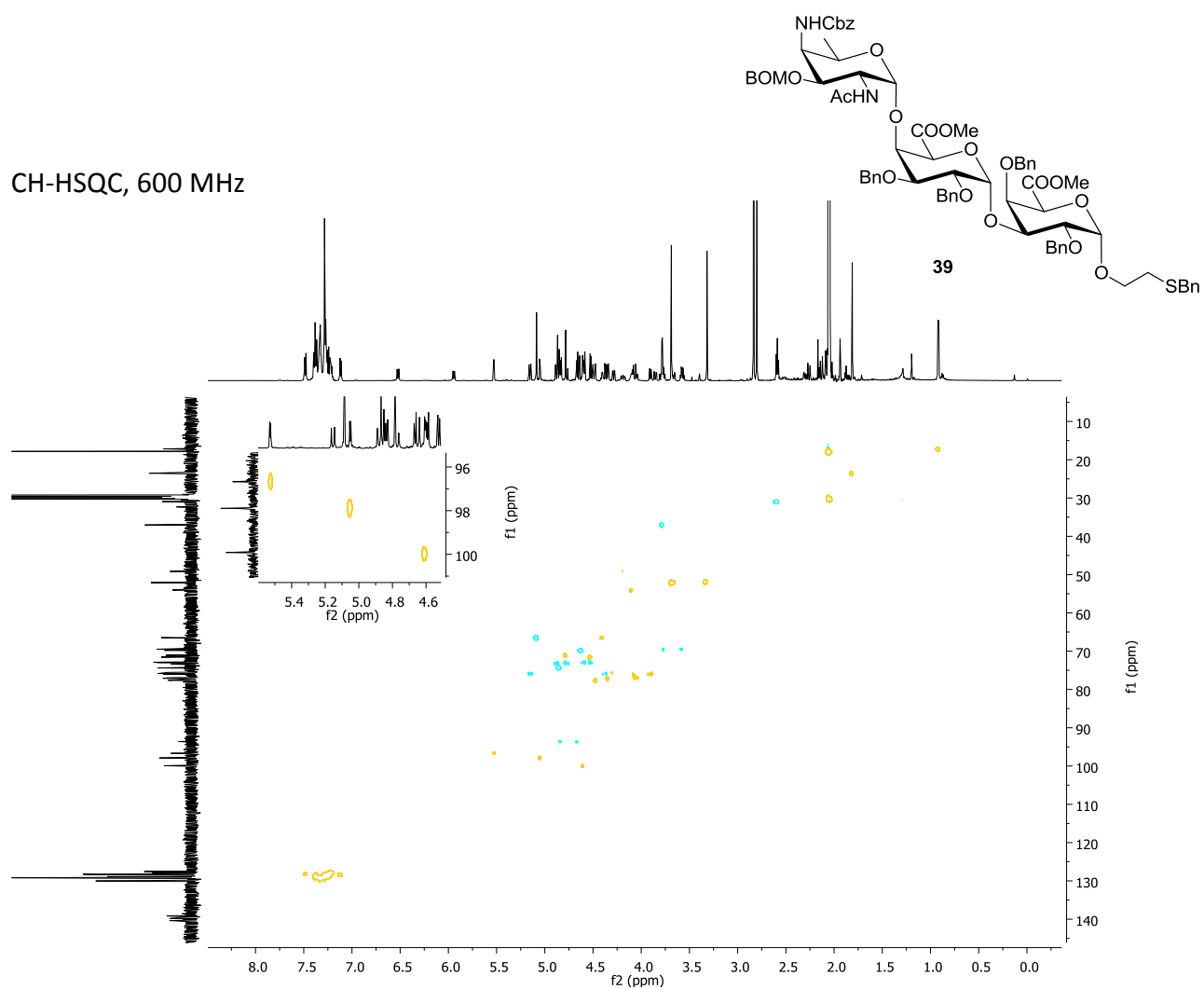
^1H NMR, 600 MHz, acetone- D_6



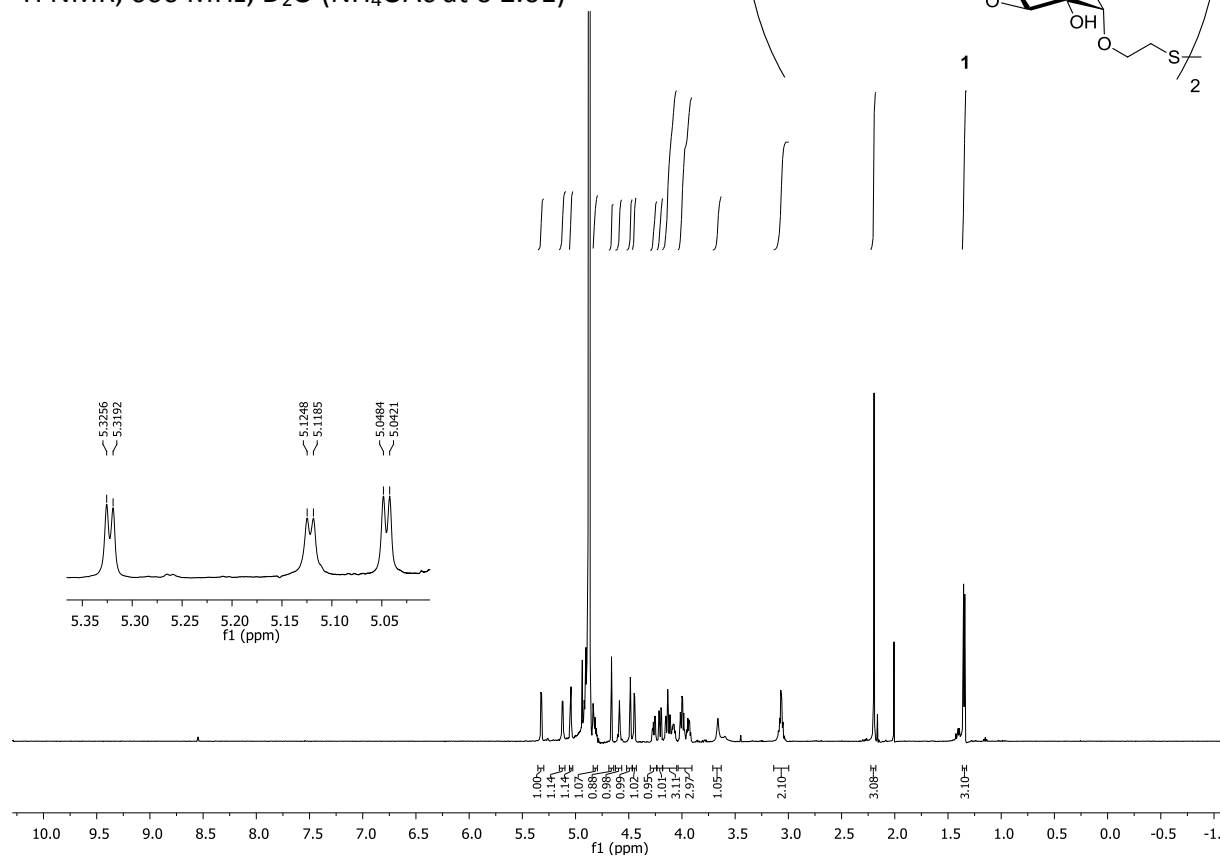
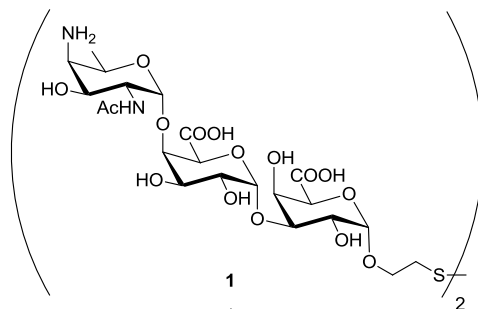
^{13}C NMR, 100 MHz, acetone- D_6



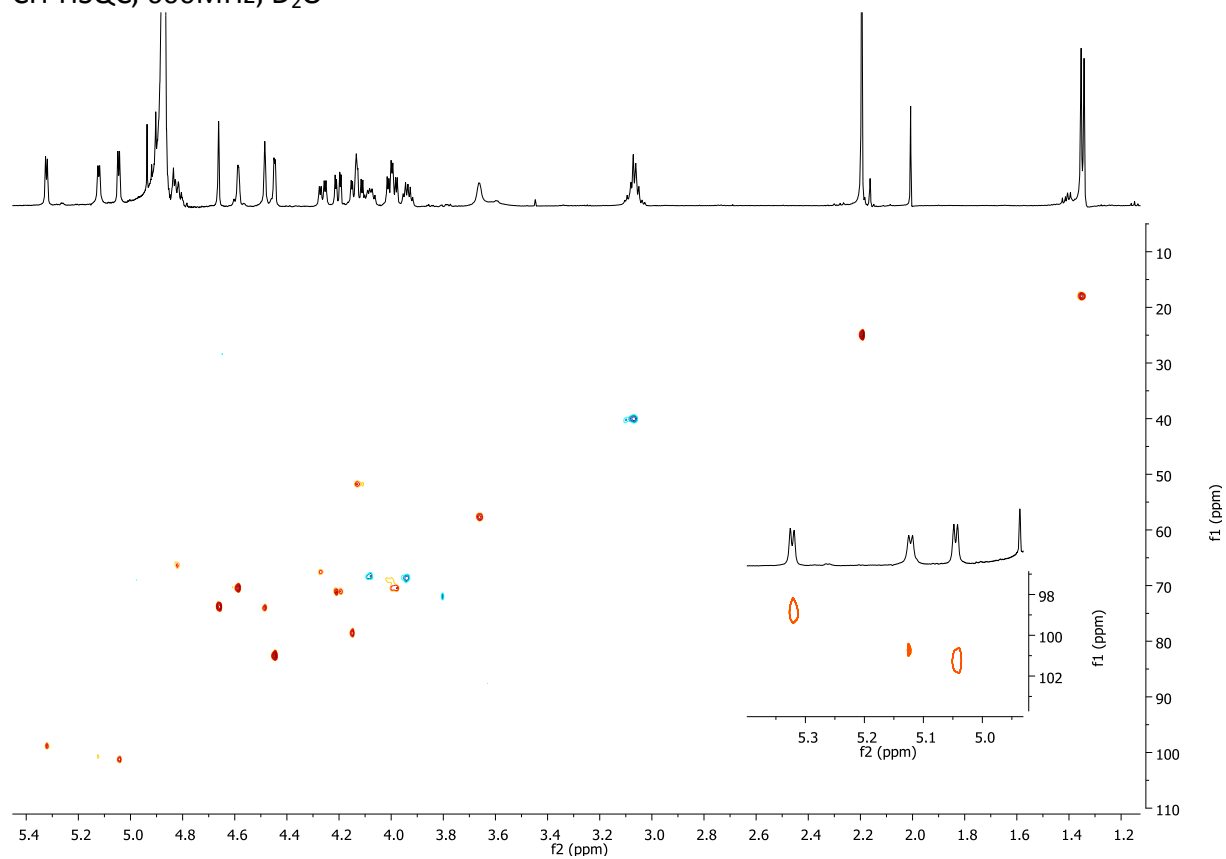
CH-HSQC, 600 MHz



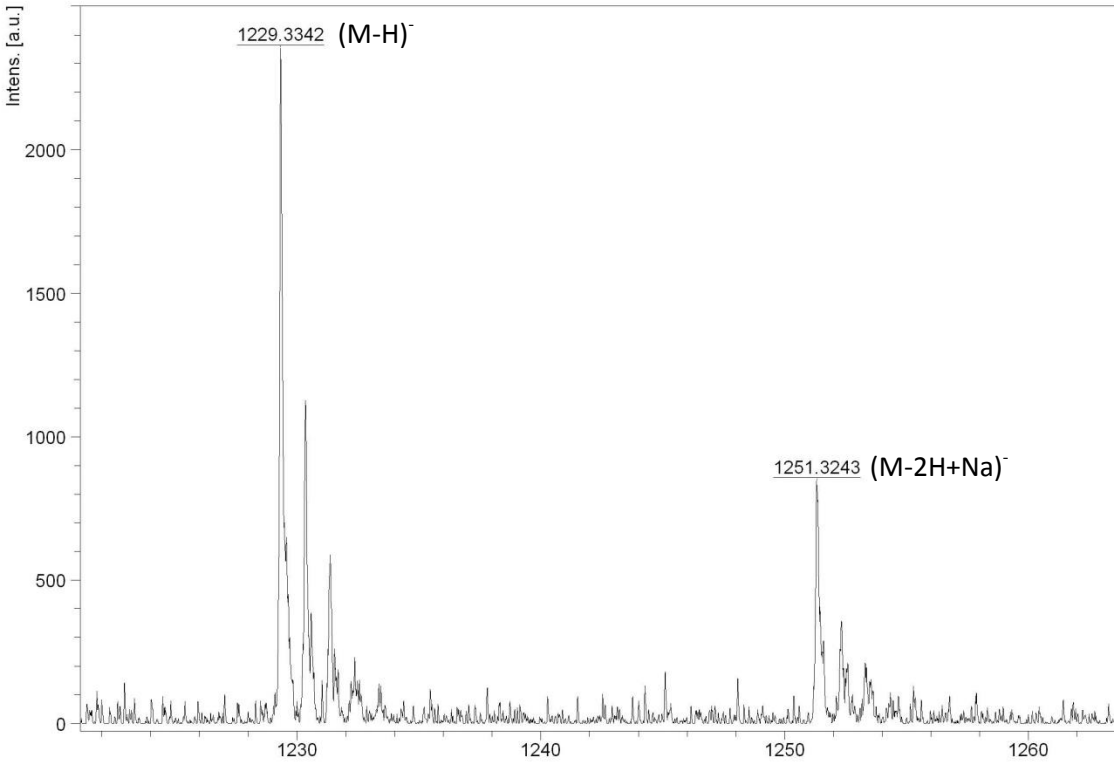
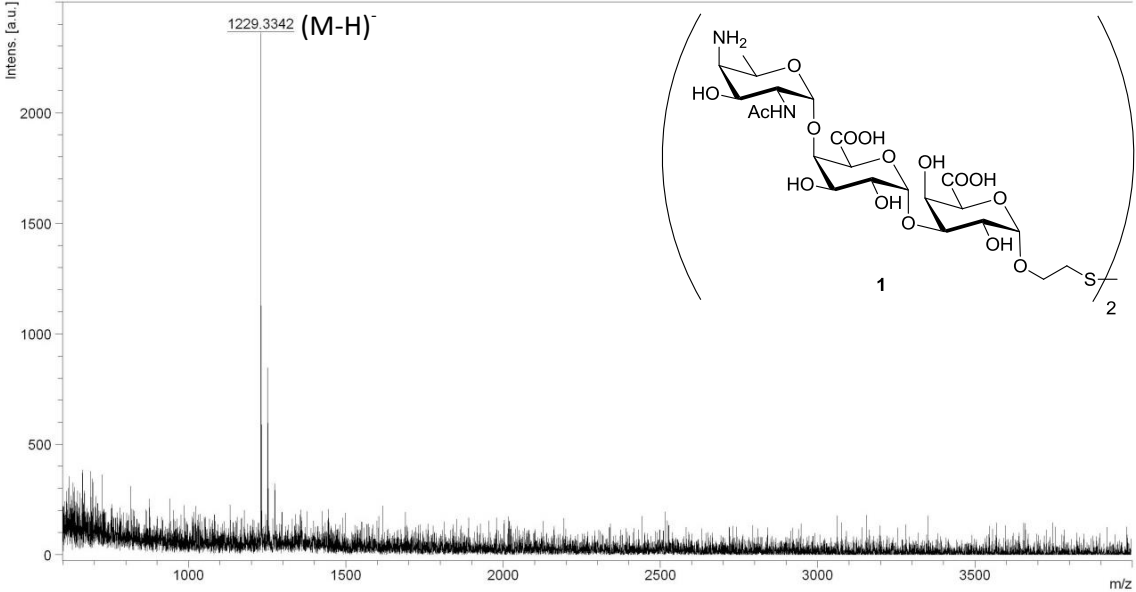
^1H NMR, 600 MHz, D_2O (NH_4OAc at δ 2.01)



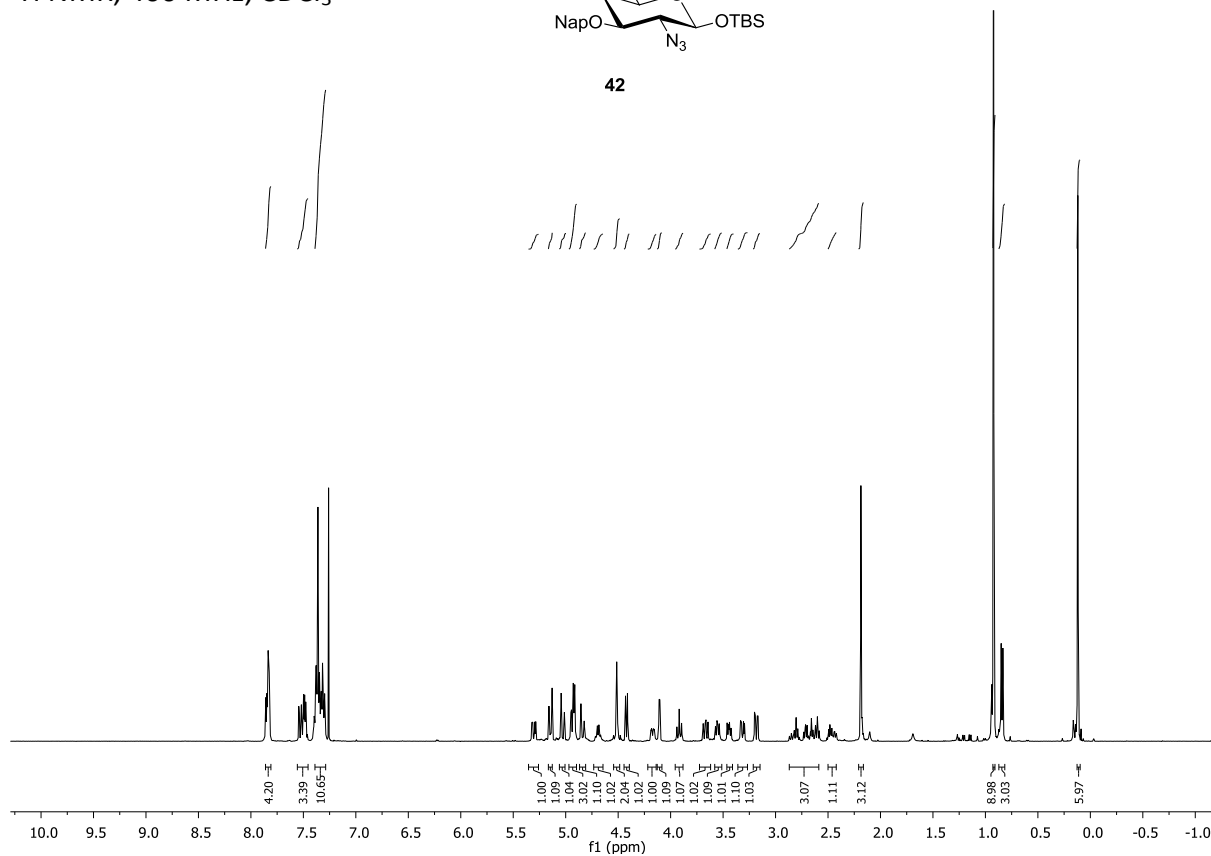
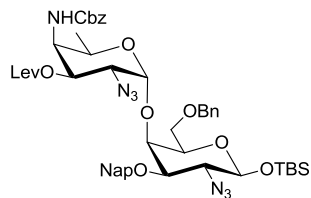
CH-HSQC, 600MHz, D_2O



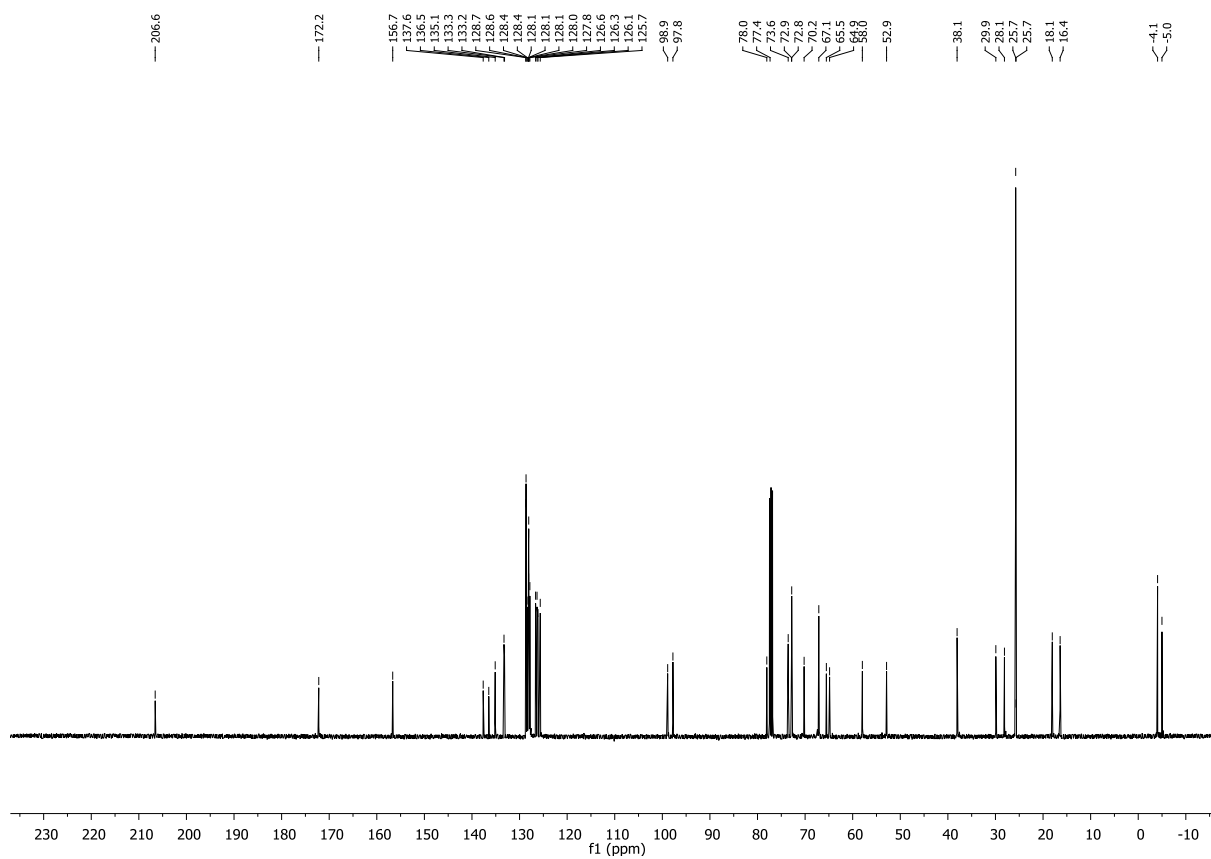
MALDI-MS (negative mode, matrix 2',4',6'-trihydroxyacetophenone)



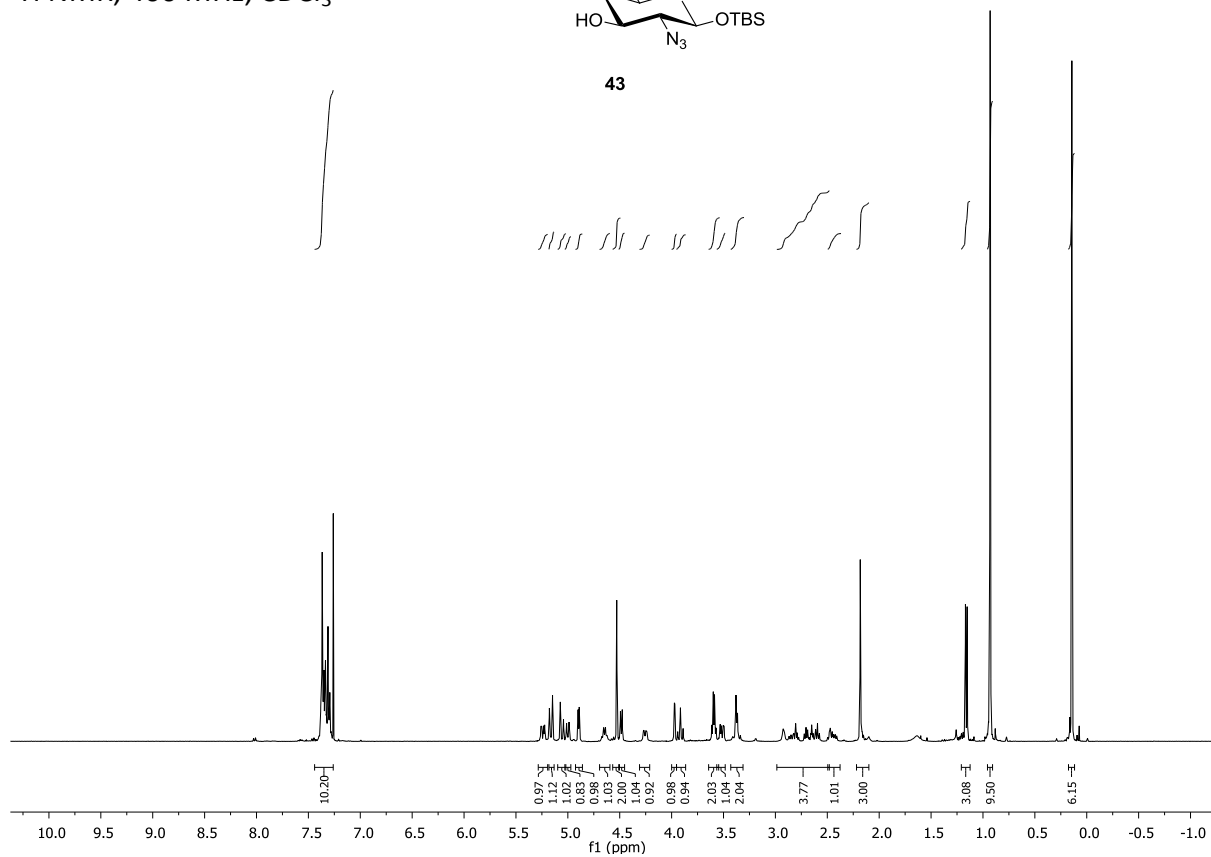
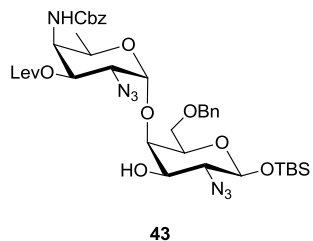
^1H NMR, 400 MHz, CDCl_3



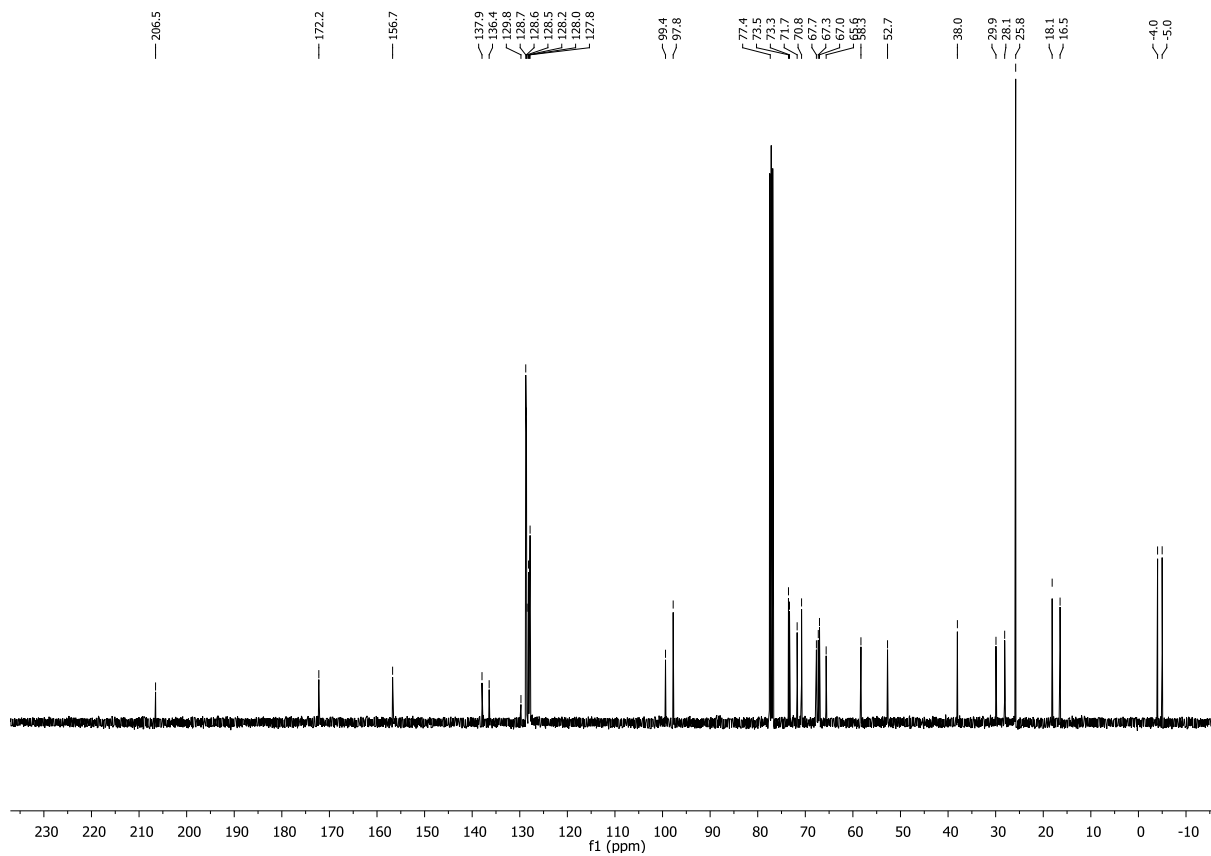
^{13}C NMR, 100 MHz, CDCl_3



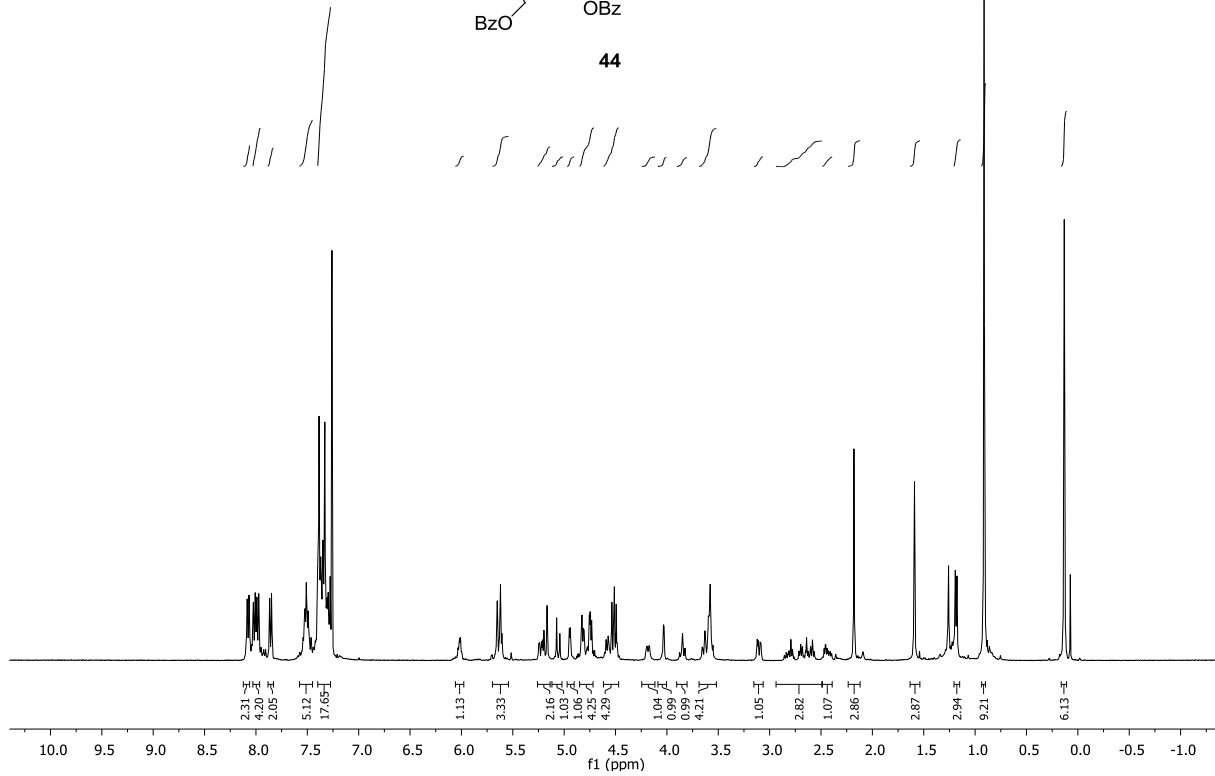
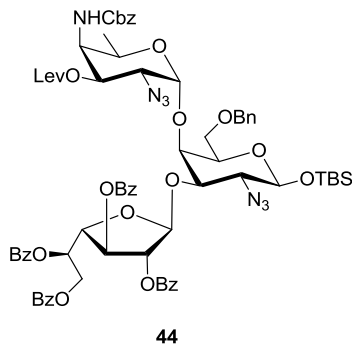
^1H NMR, 400 MHz, CDCl_3



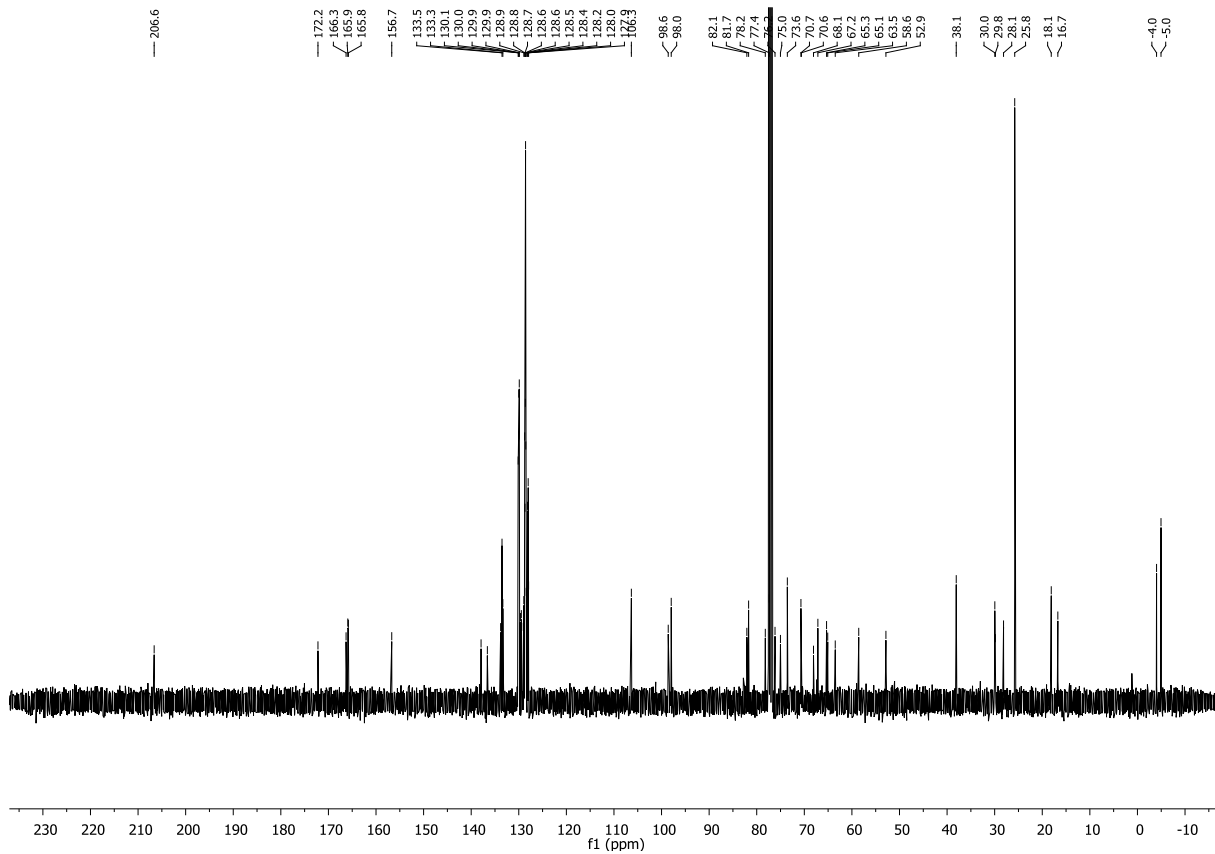
^{13}C NMR, 100 MHz, CDCl_3



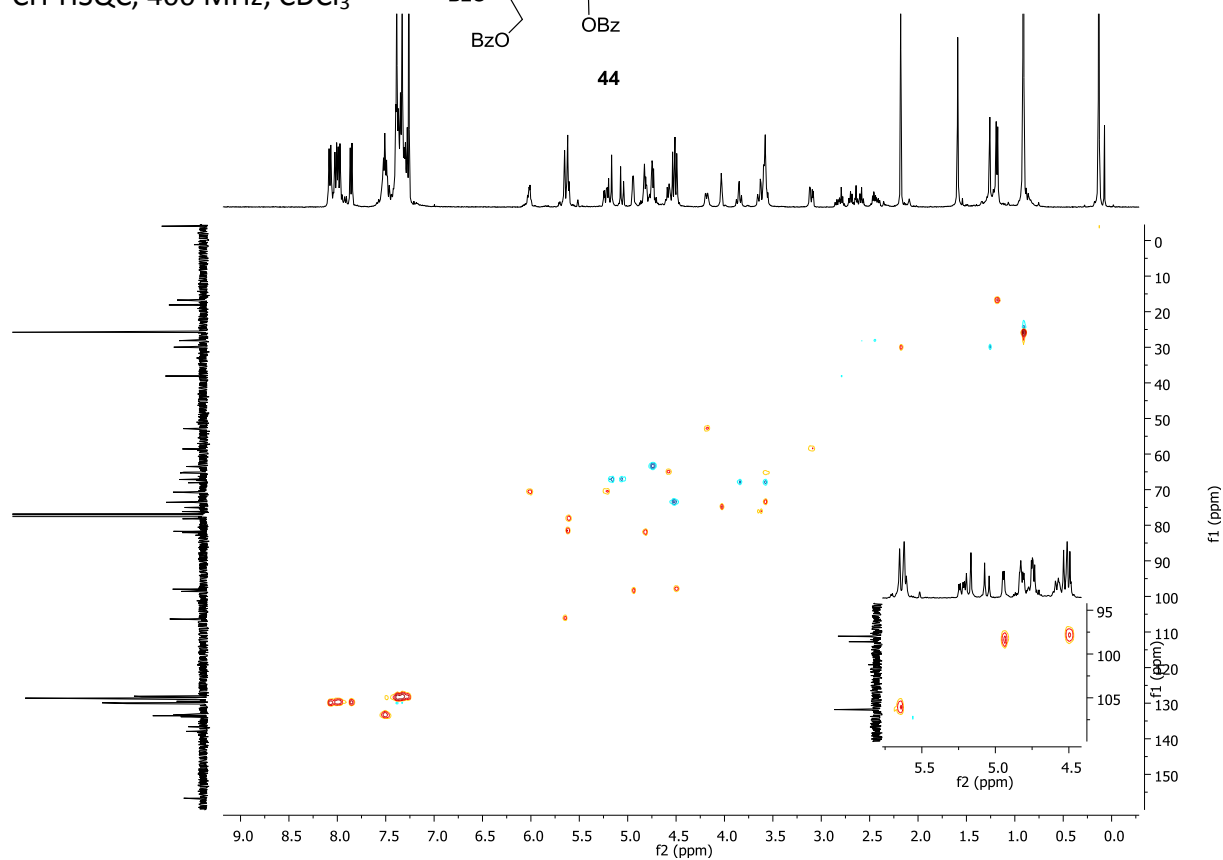
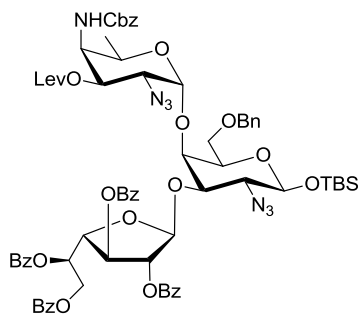
¹H NMR, 400 MHz, CDCl₃



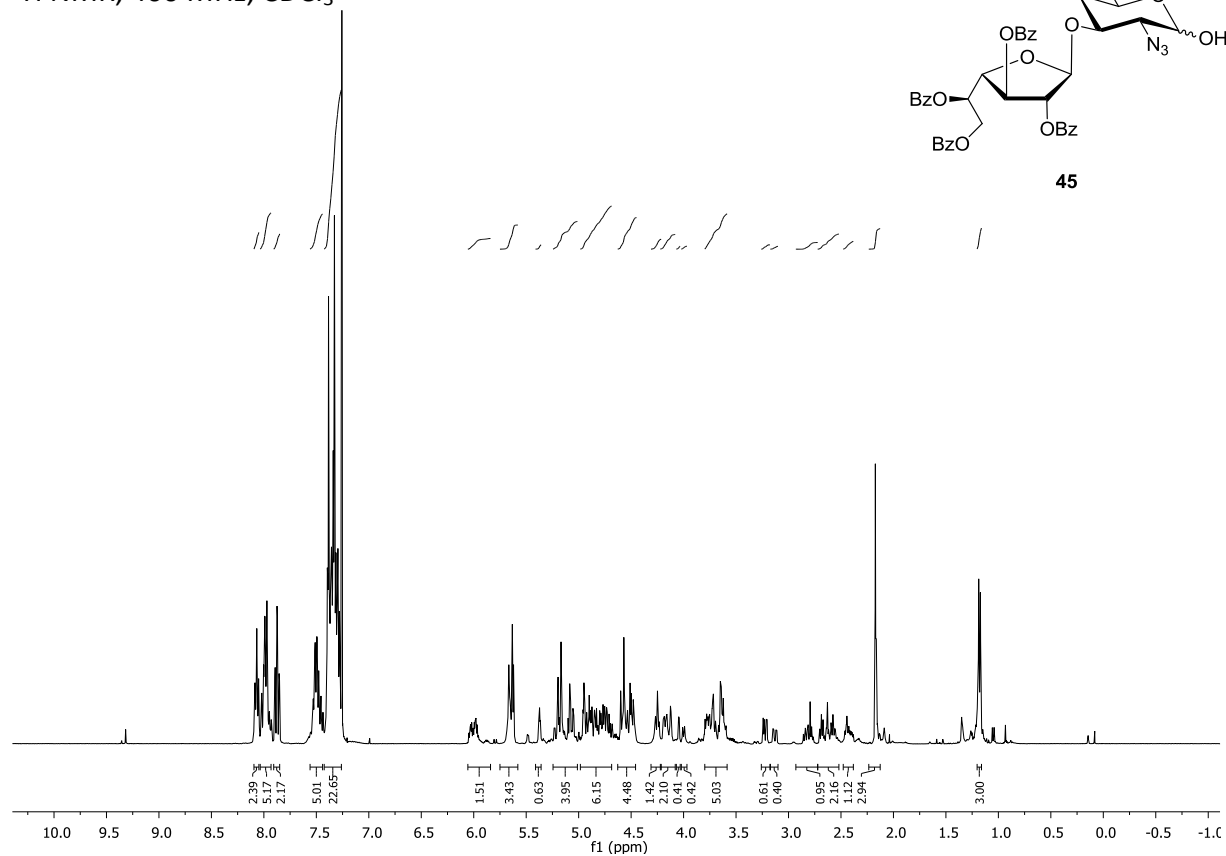
¹³C NMR, 100 MHz, CDCl₃



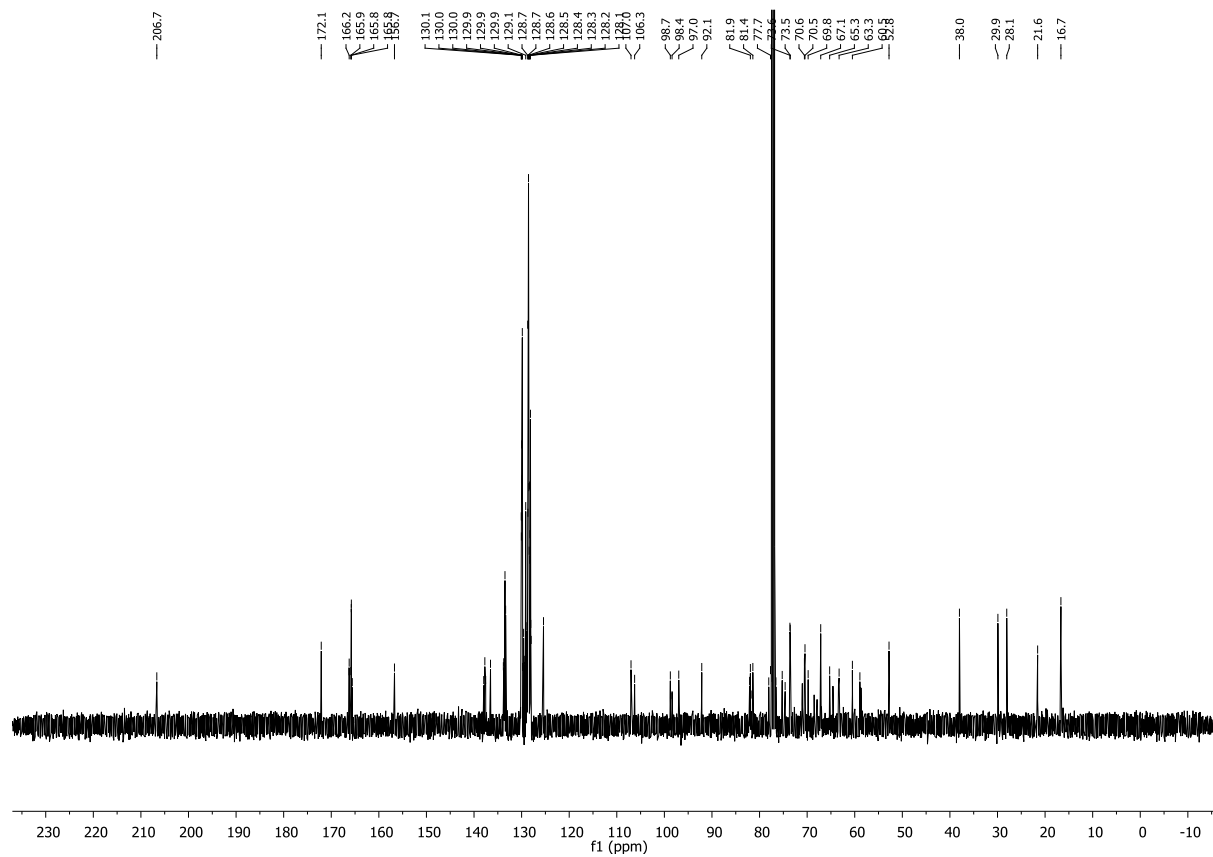
CH-HSQC, 400 MHz, CDCl₃



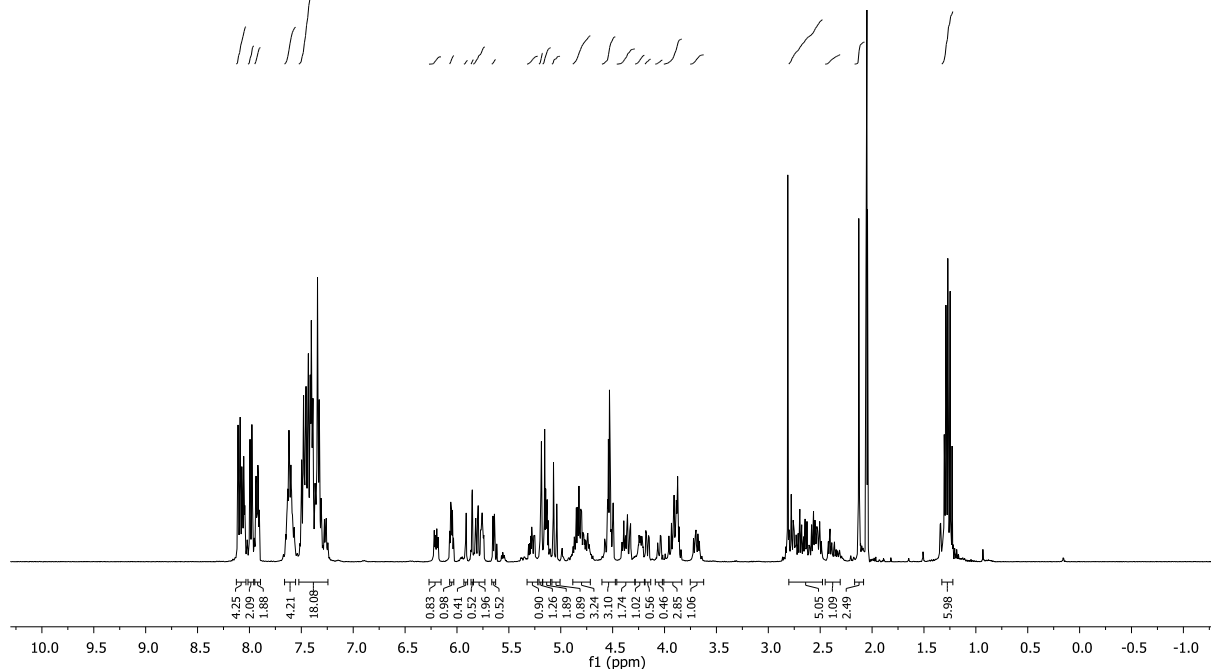
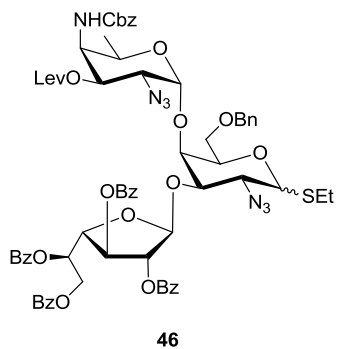
^1H NMR, 400 MHz, CDCl_3



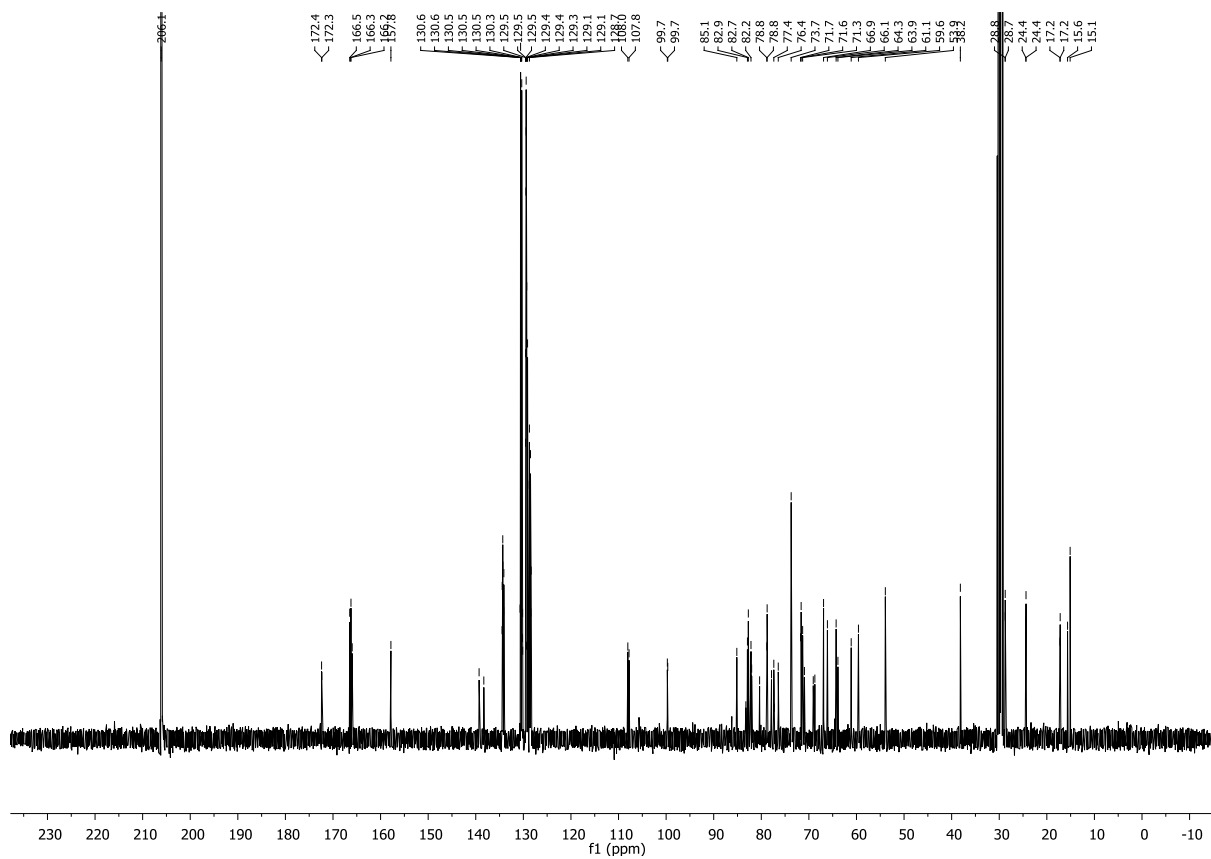
^{13}C NMR, 100 MHz, CDCl_3



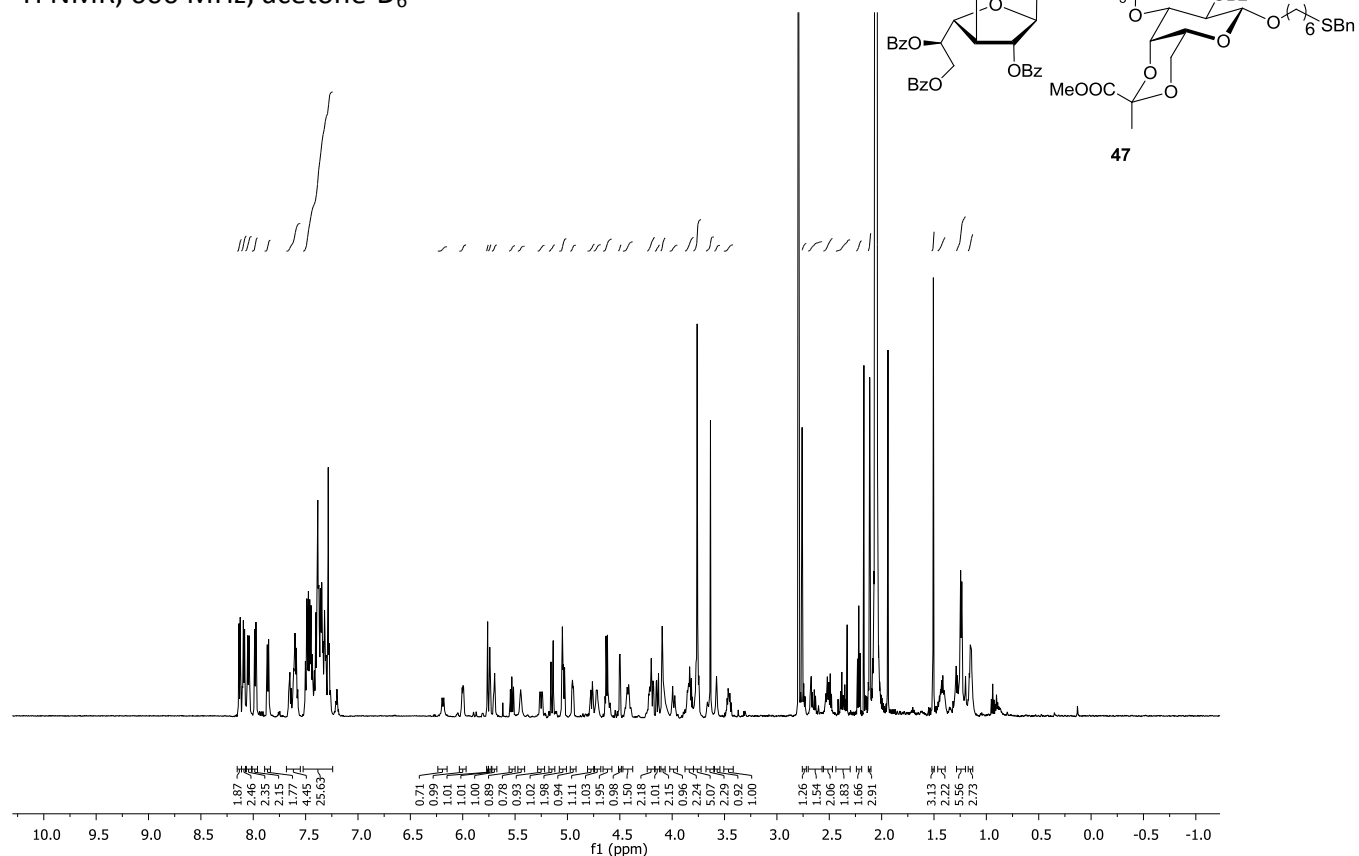
^1H NMR, 400 MHz, acetone- D_6



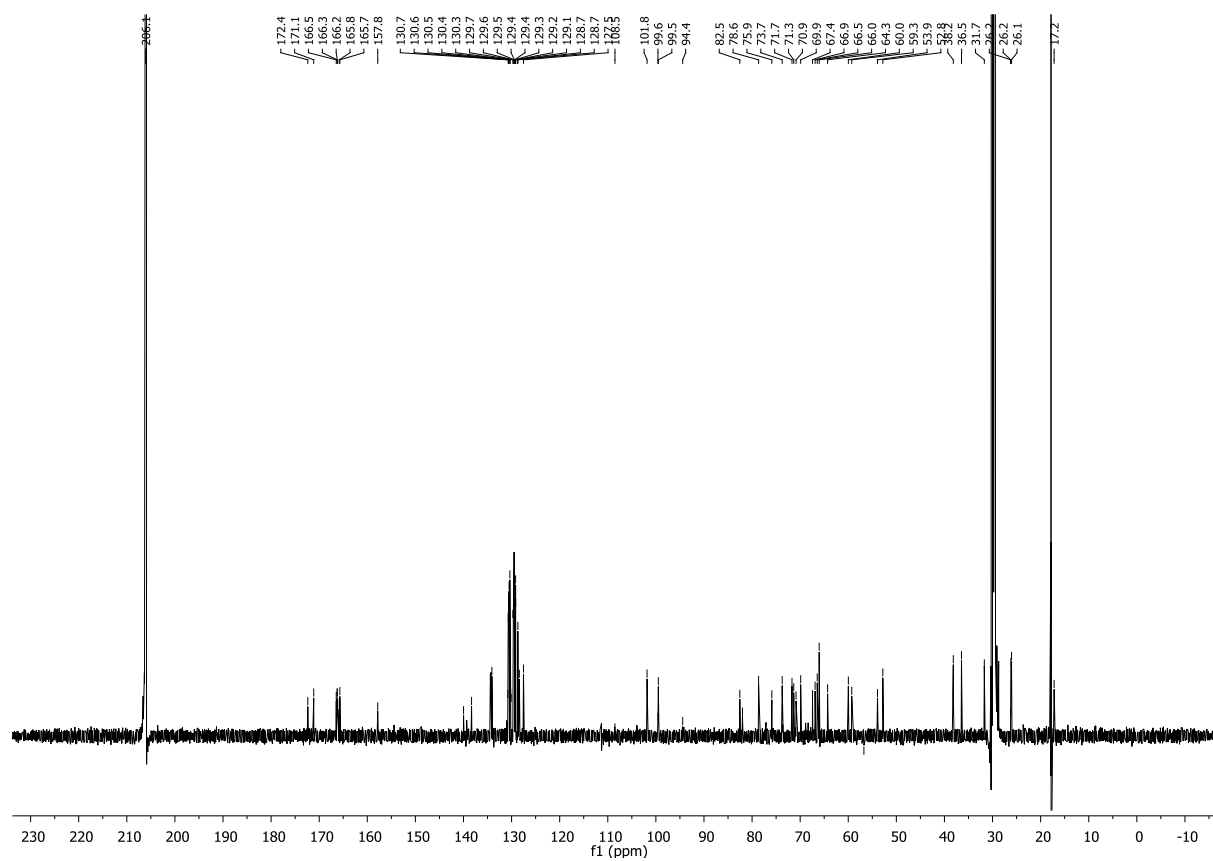
^{13}C NMR, 100 MHz, acetone- D_6



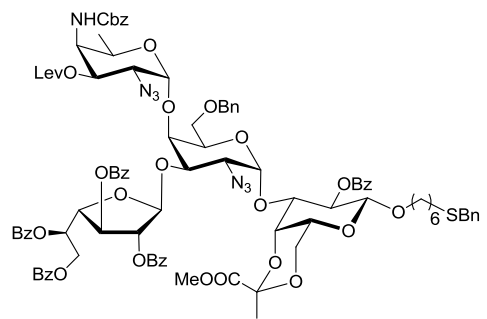
^1H NMR, 600 MHz, acetone- D_6



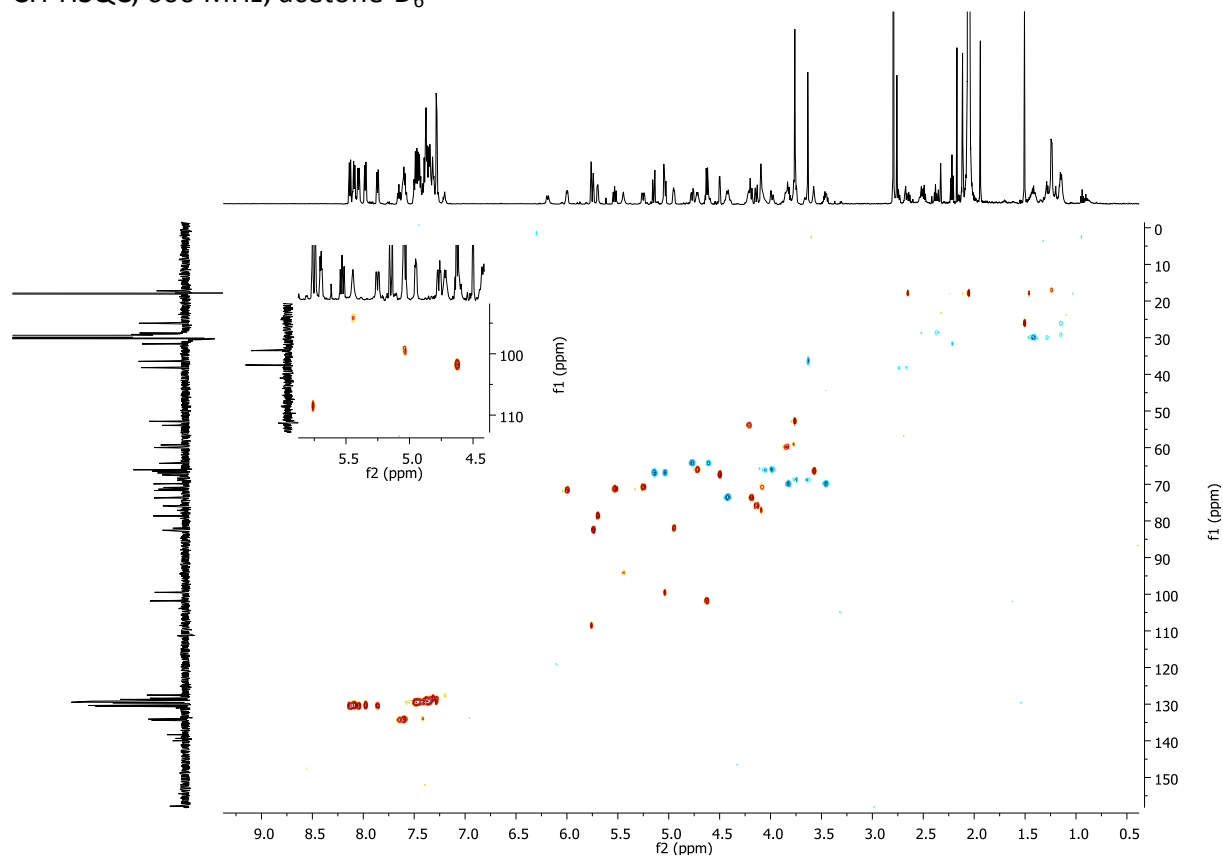
^{13}C NMR, 150 MHz, acetone- D_6



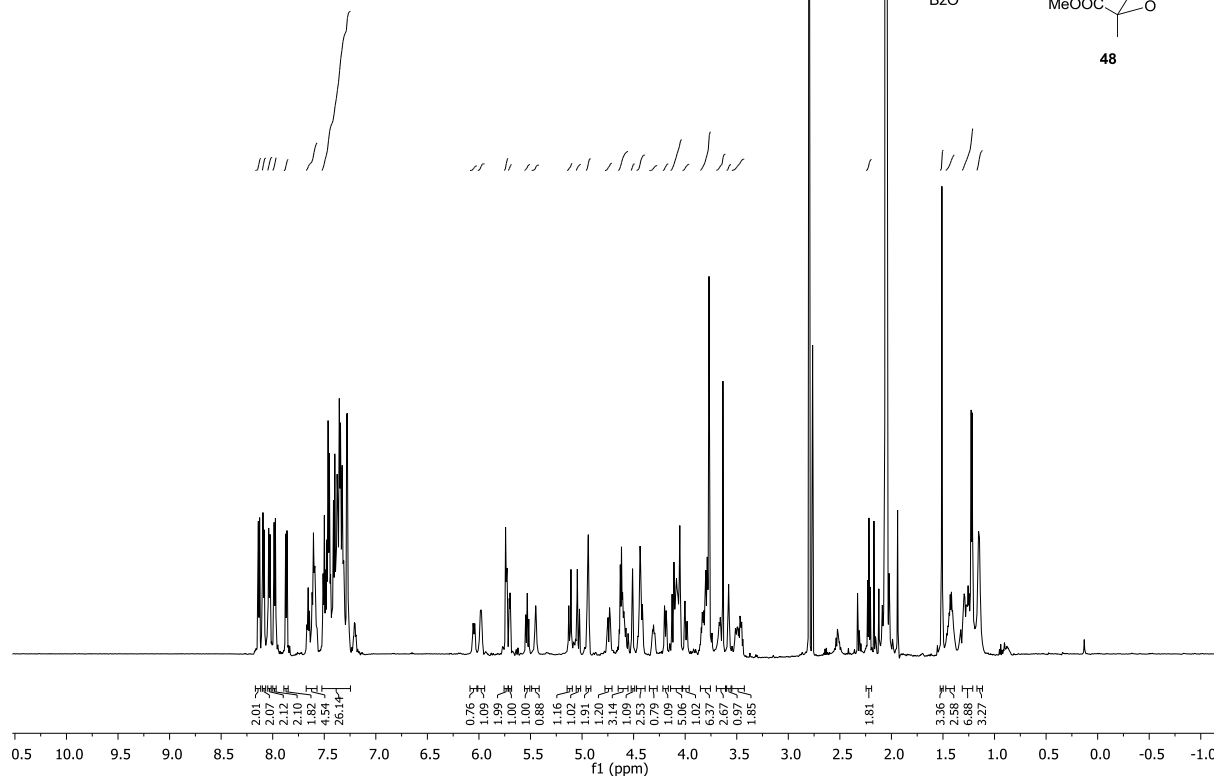
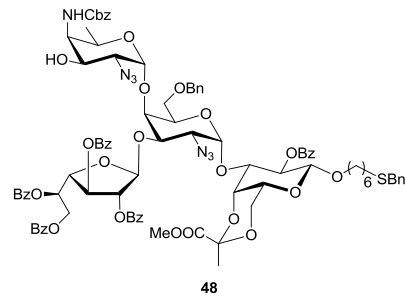
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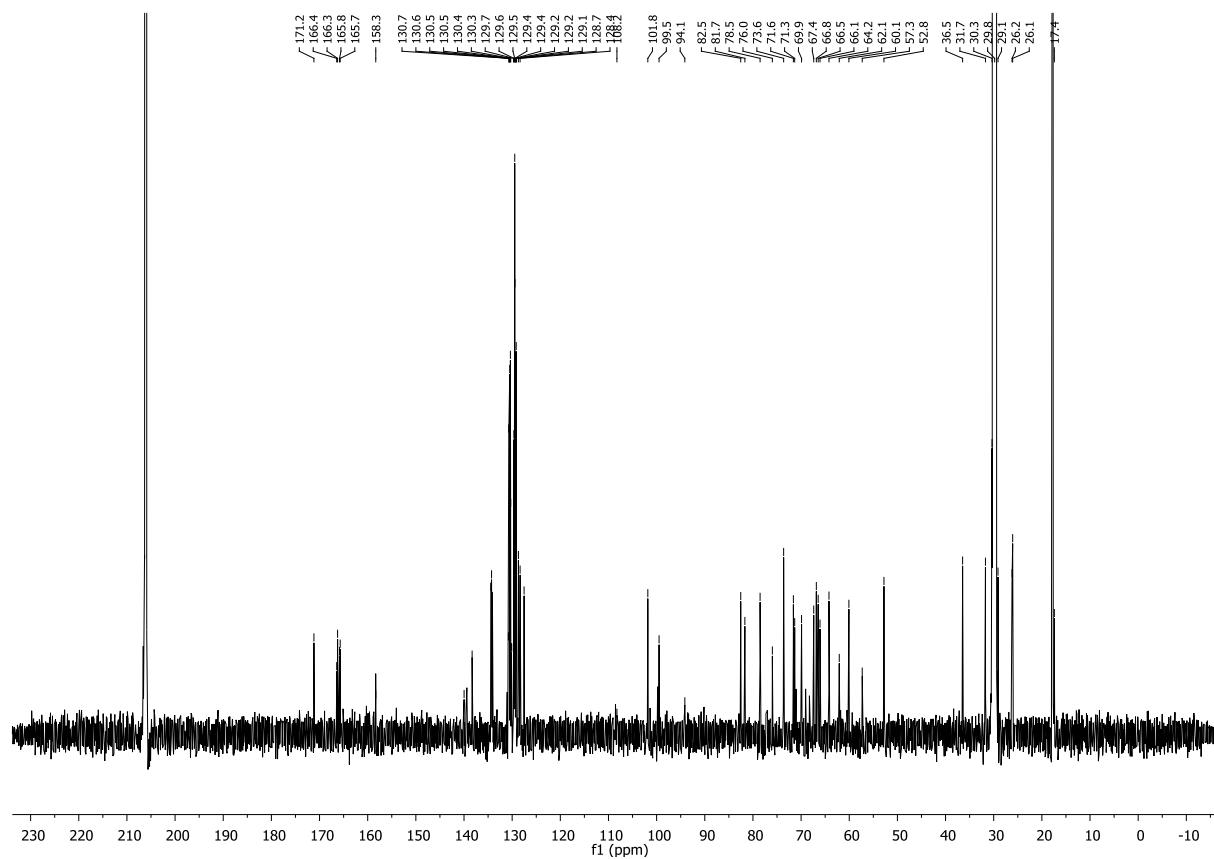
CH-HSQC, 600 MHz, acetone-D₆

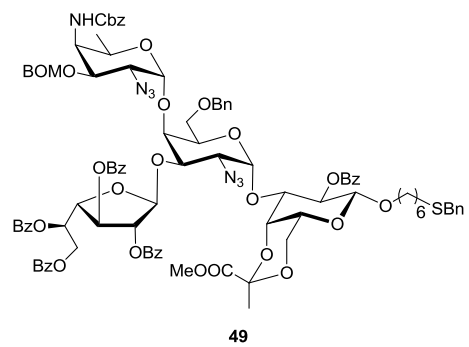


¹H NMR, 600 MHz, acetone-D₆

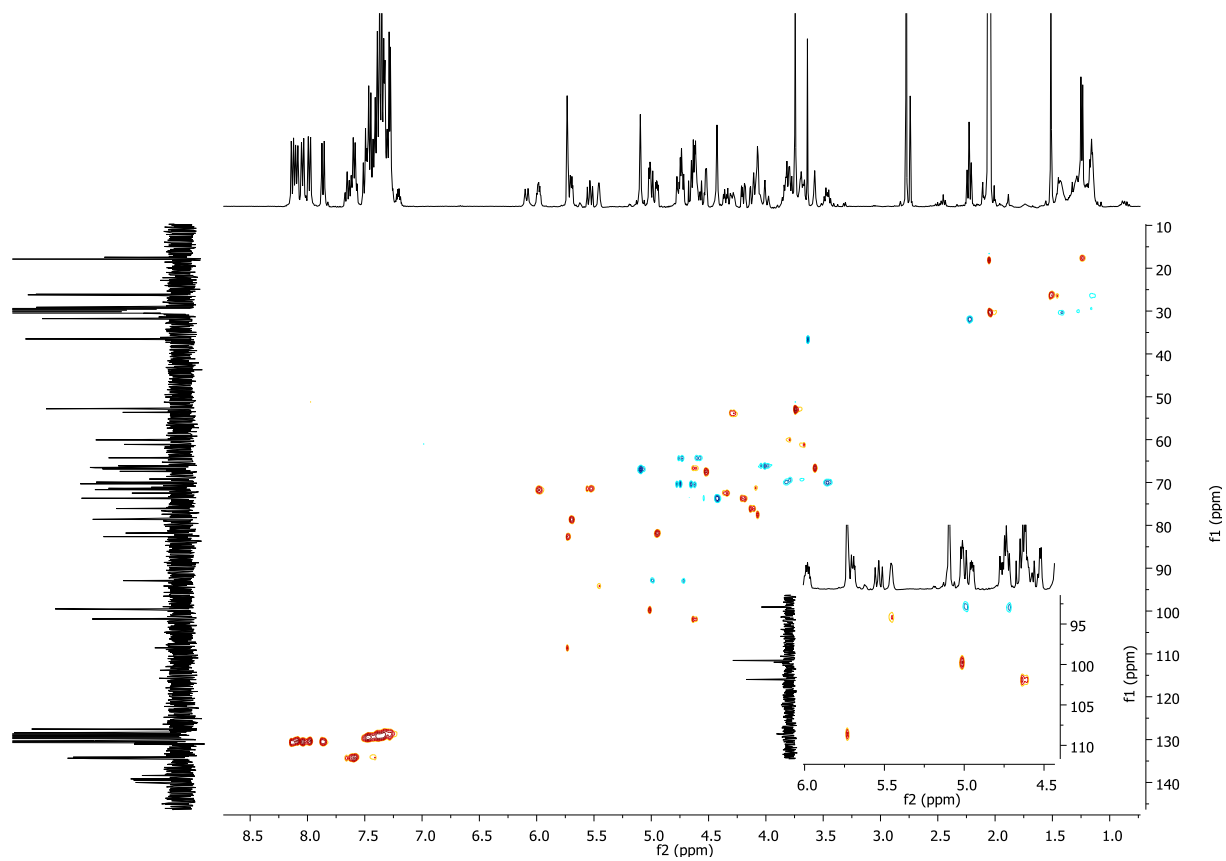


¹³C NMR, 150 MHz, acetone-D₆

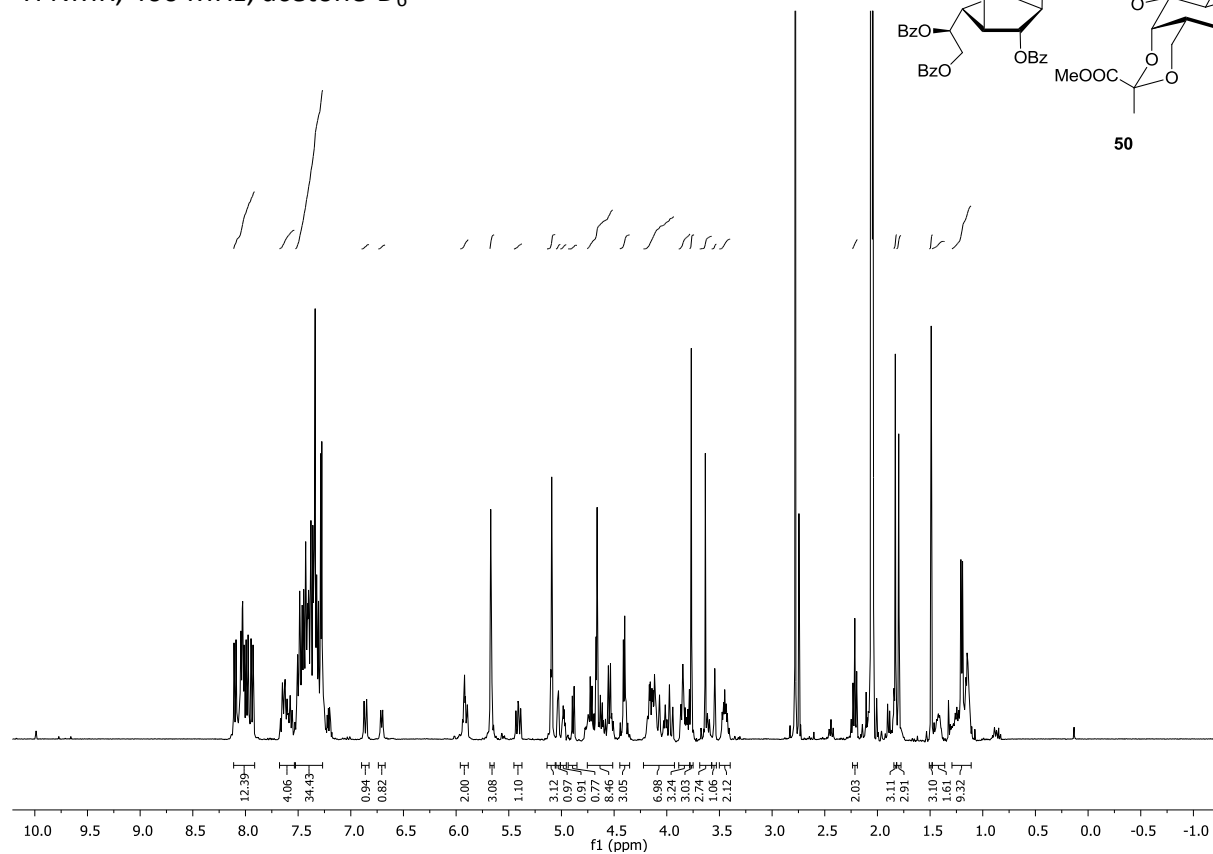




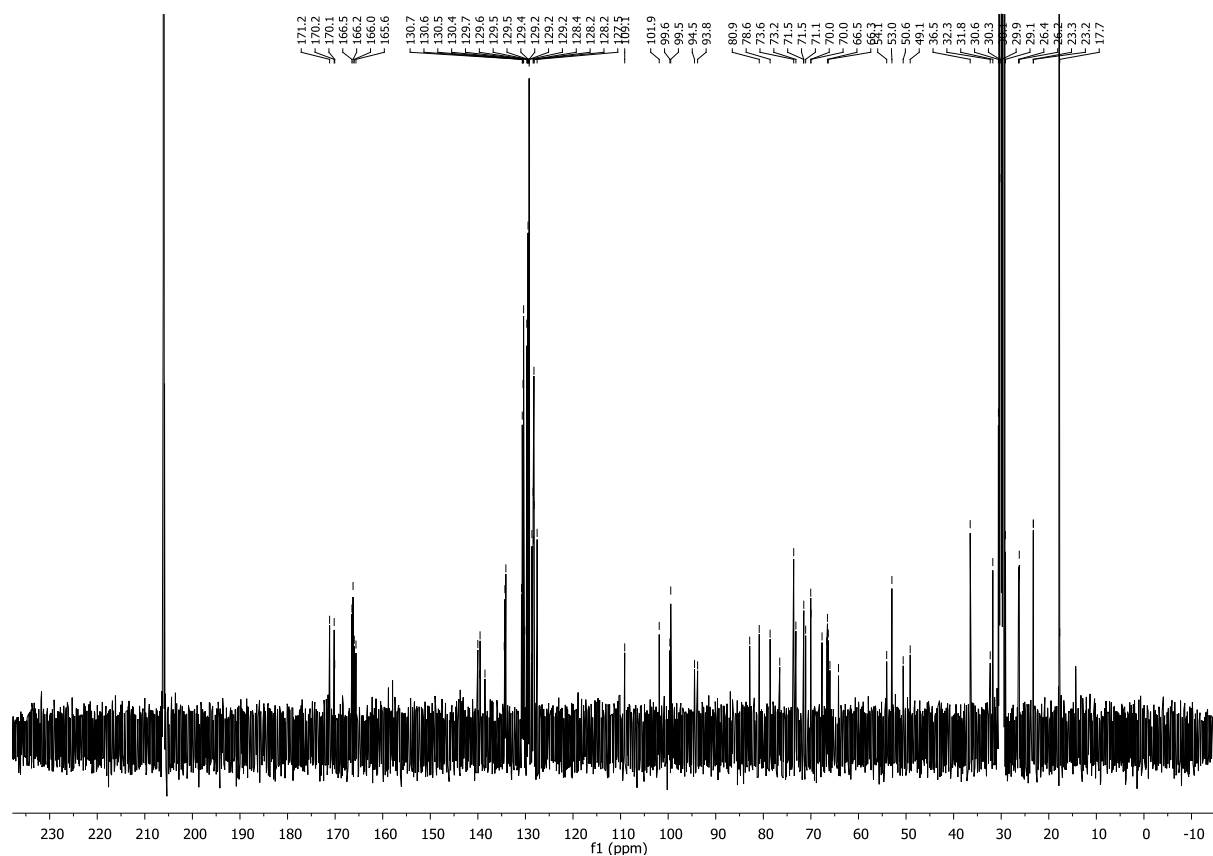
CH-HSQC, 400 MHz, acetone-D₆

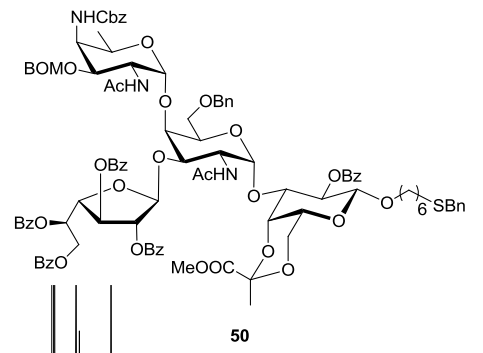


¹H NMR, 400 MHz, acetone-D₆

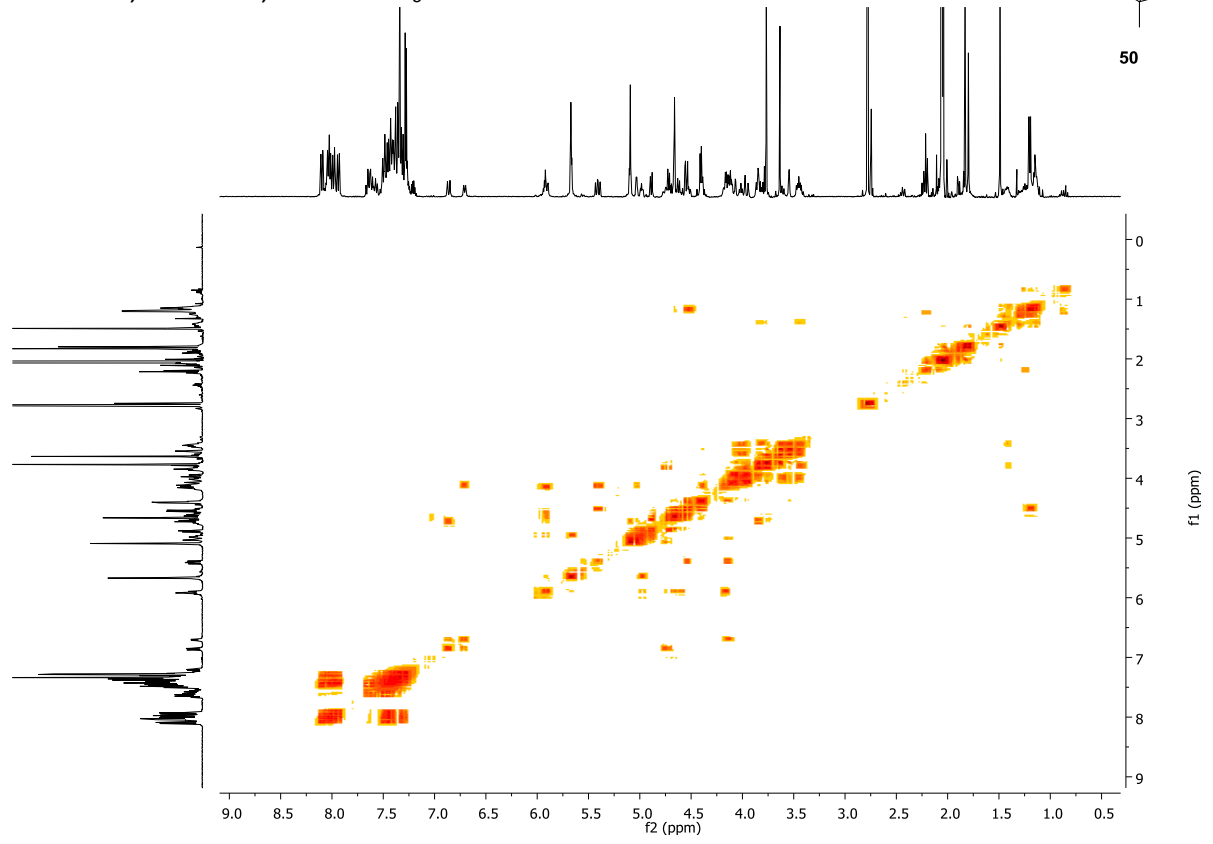


¹³C NMR, 100 MHz, acetone-D₆

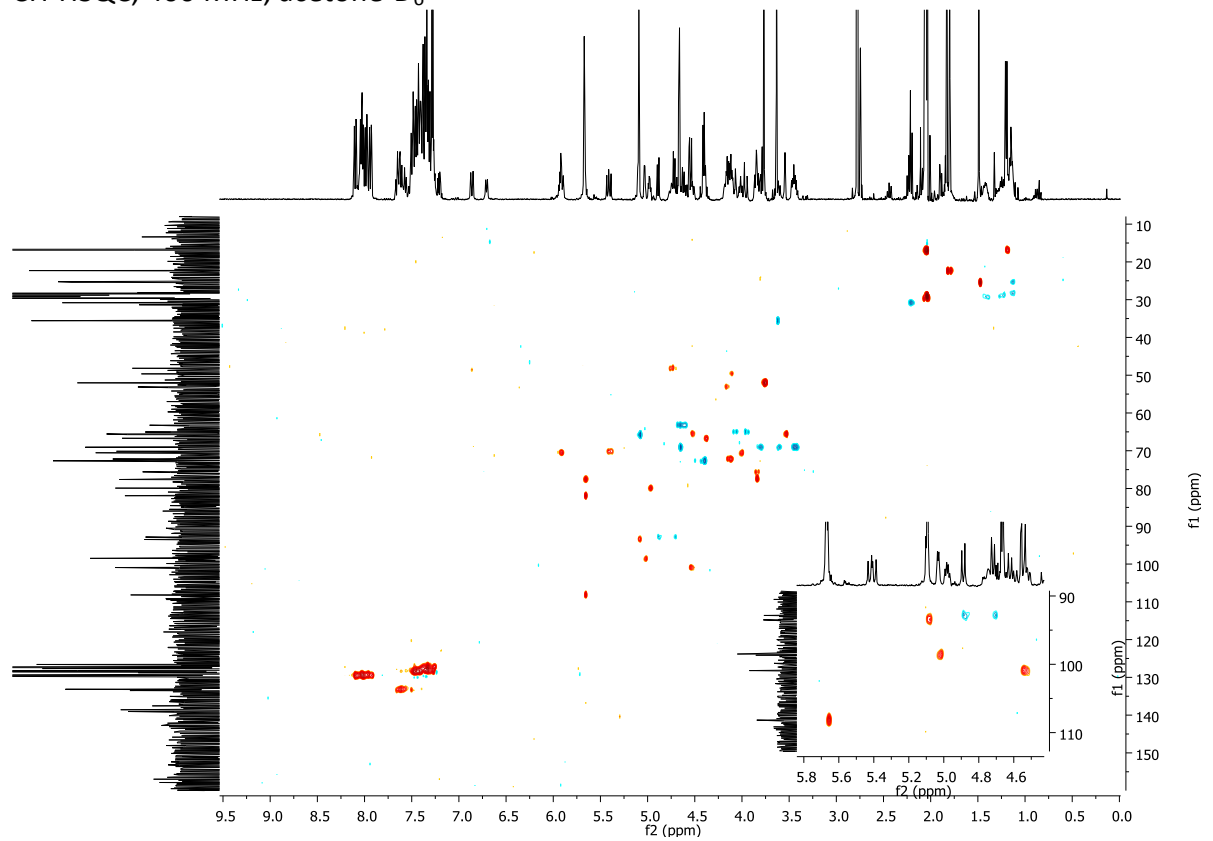




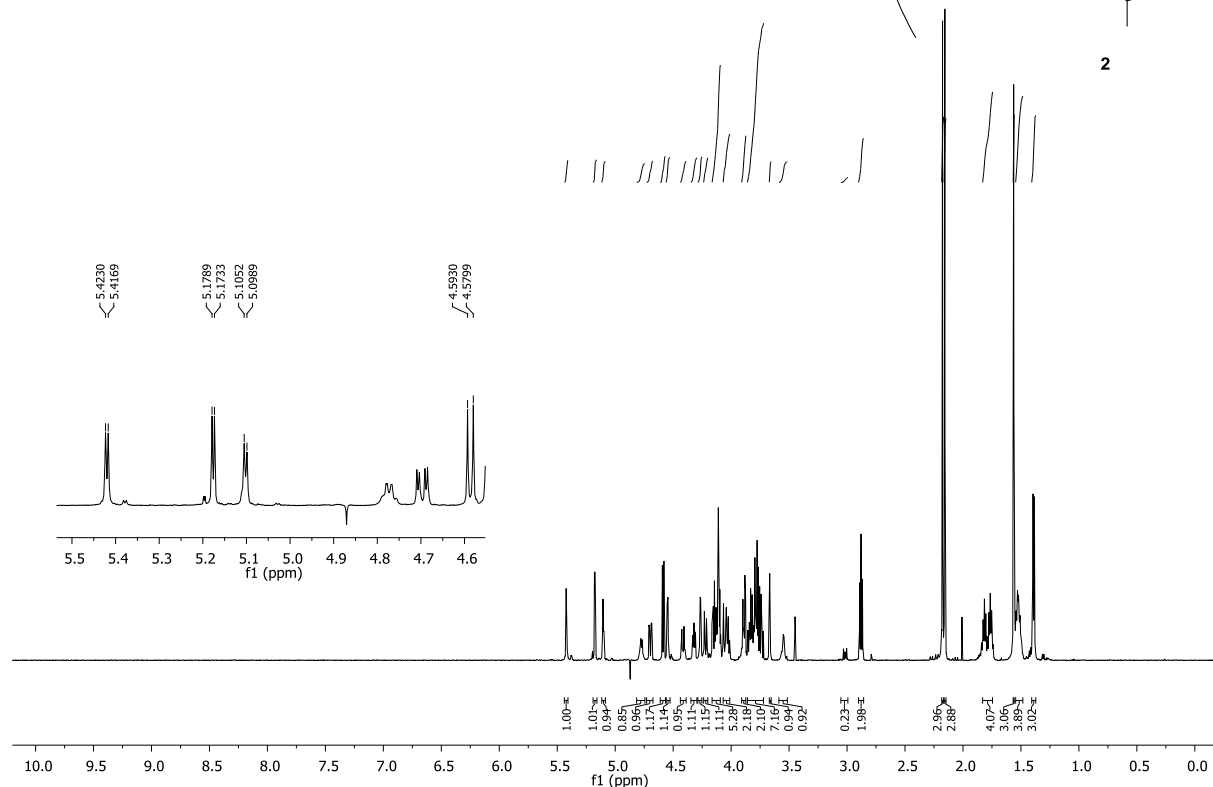
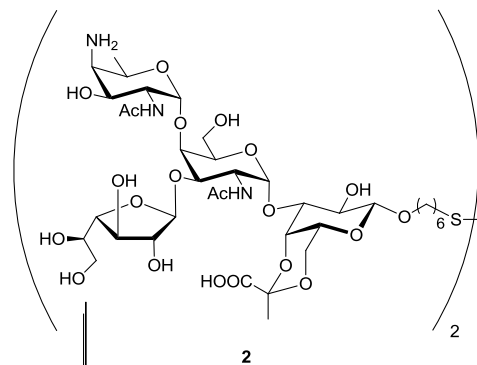
HH-COSY, 400 MHz, acetone-D₆



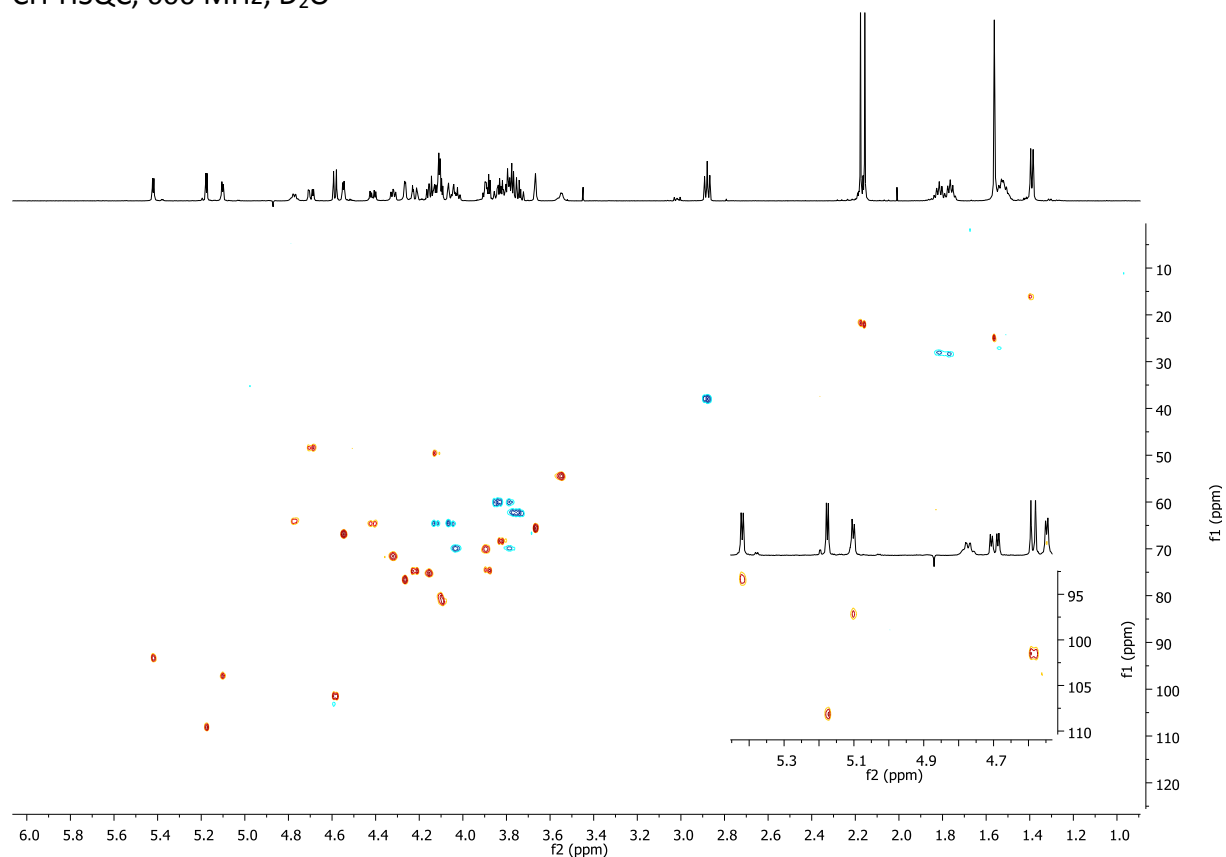
CH-HSQC, 400 MHz, acetone-D₆



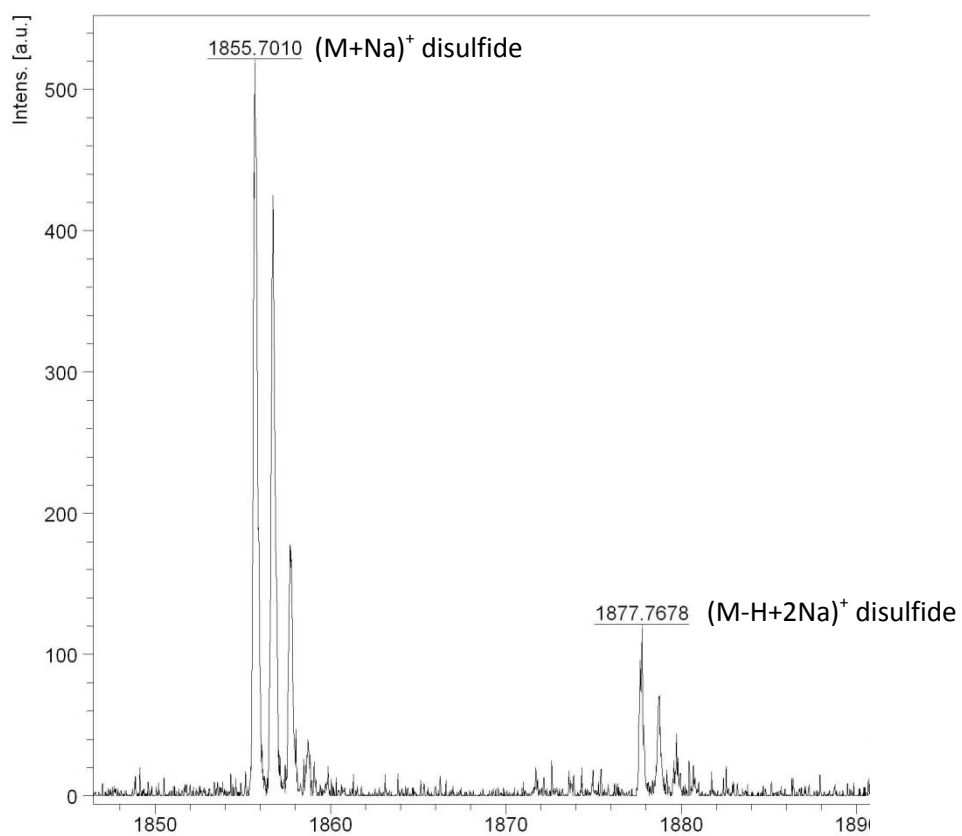
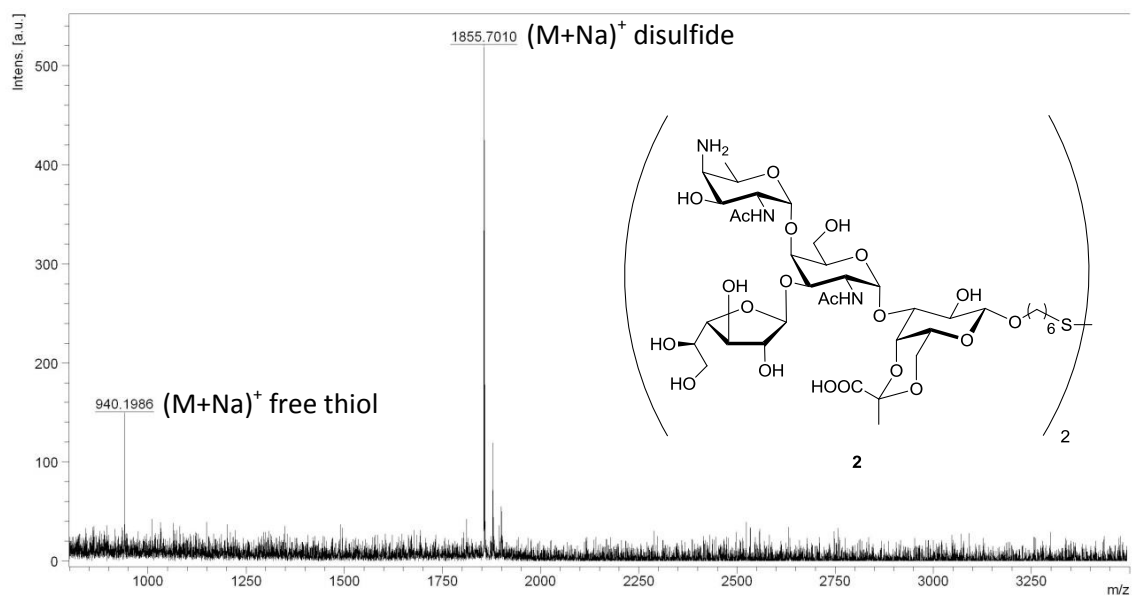
^1H NMR, 600 MHz, D_2O (water suppression; NH_4OAc at δ 2.01)



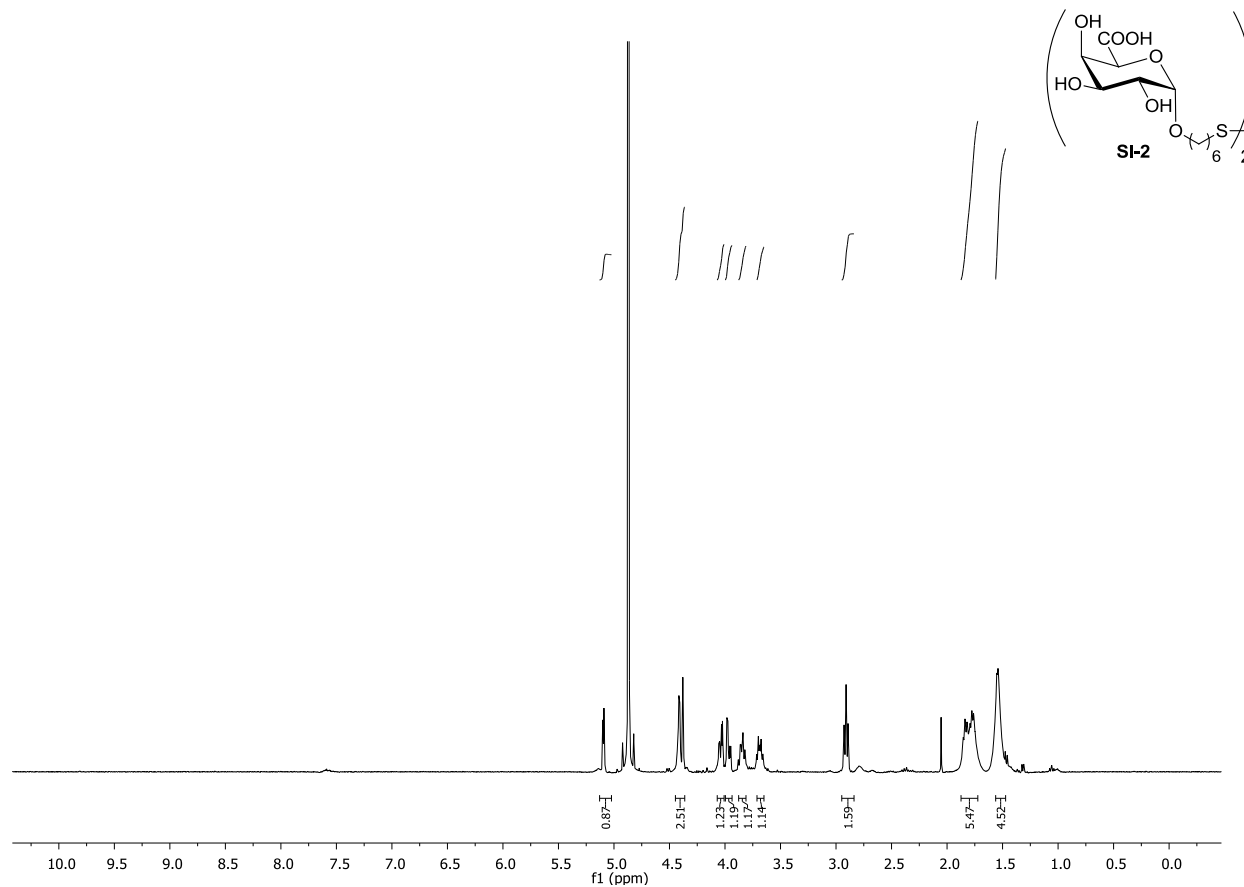
CH-HSQC, 600 MHz, D_2O



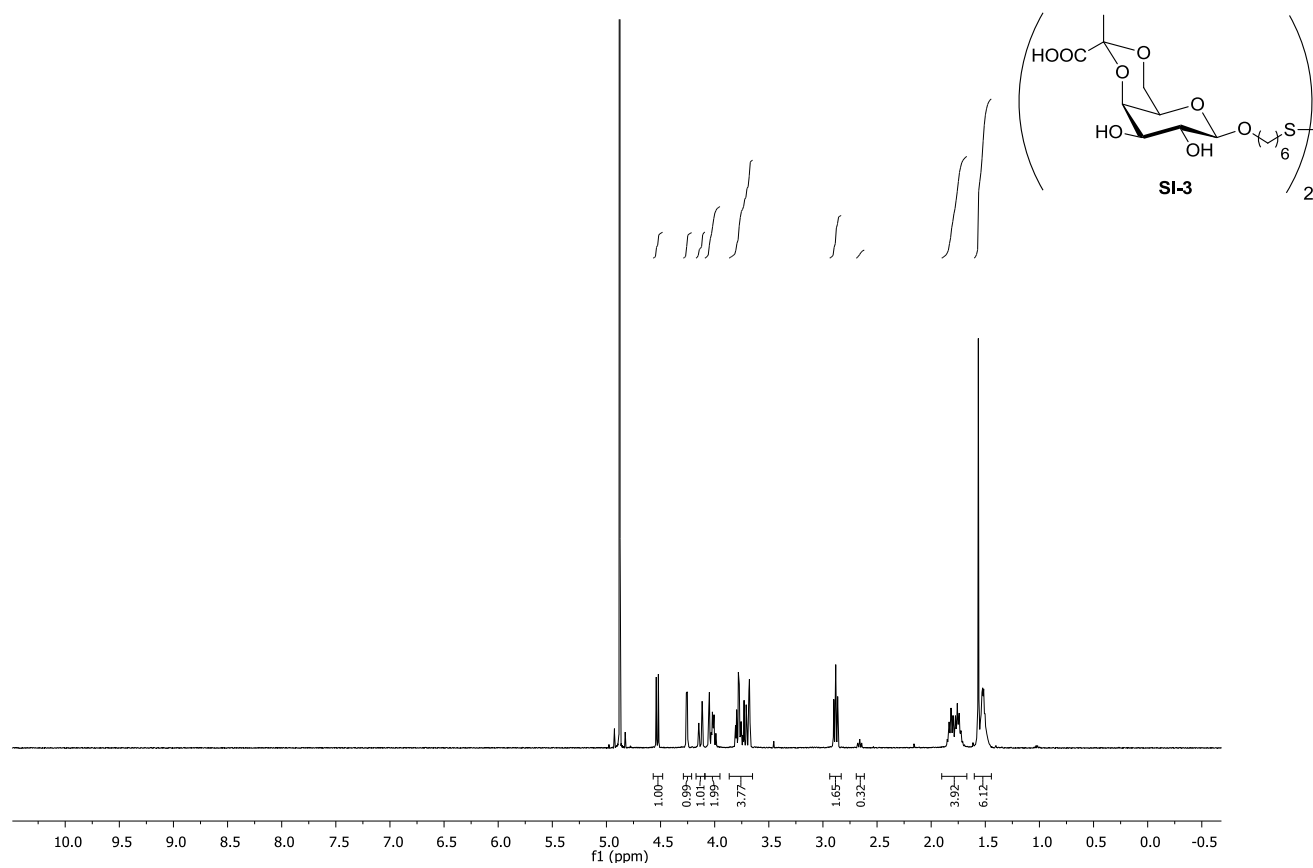
MALDI-MS (positive mode, matrix 2',4',6'-trihydroxyacetophenone)



^1H NMR, 400 MHz, D_2O



^1H NMR, 400 MHz, D_2O



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