

## Supporting Information for

### Synthesis of *N*-glycosyl amides. Conformational analysis and evaluation as inhibitors of the $\beta$ -galactosidase from *E. coli*.

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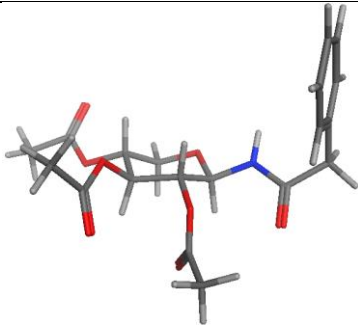
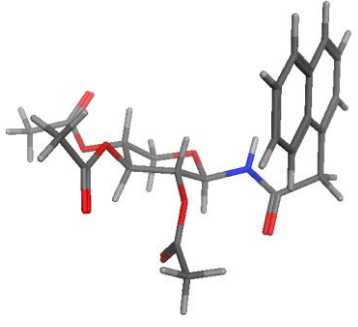
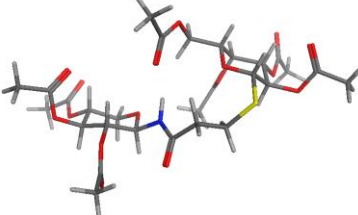
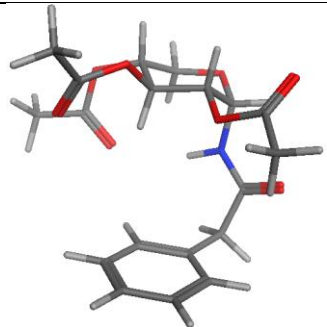
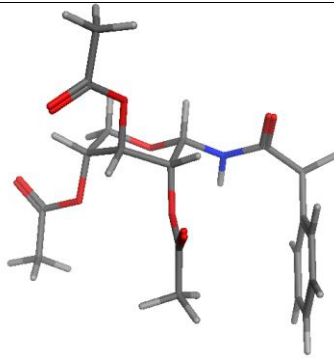
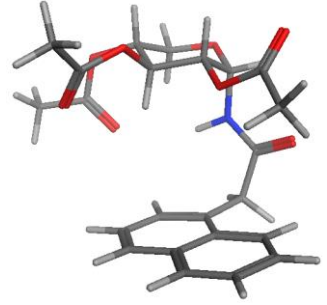
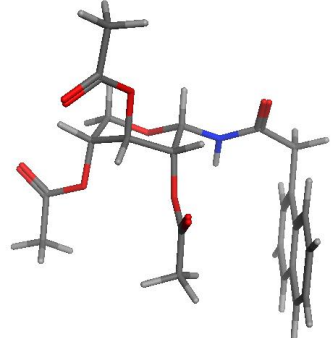
<sup>d</sup>Centro de Investigación en Hidratos de Carbono (CIHIDECAR), Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), UBA, Argentina

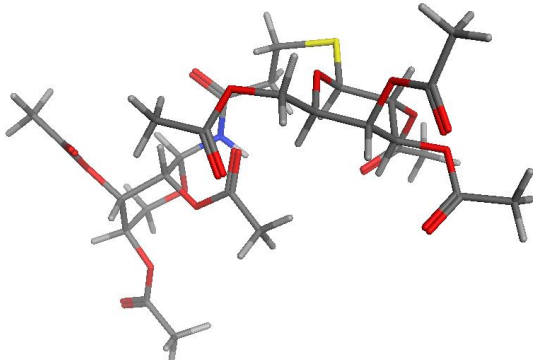
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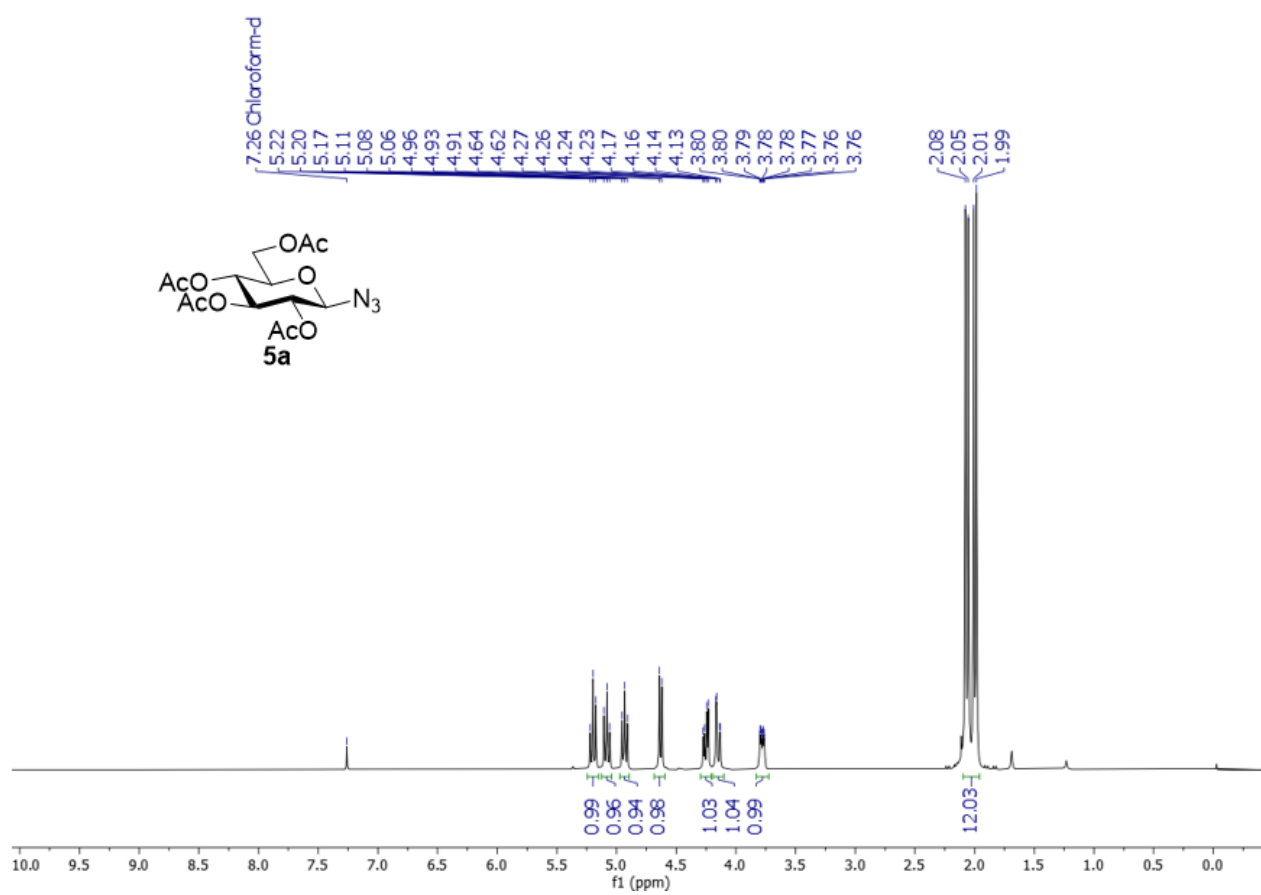
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Table 1. Chair conformations  ${}^4C_1$  and  ${}^1C_4$  and energies obtained for the *xylo* derivatives by conformational search employing MMFF94.

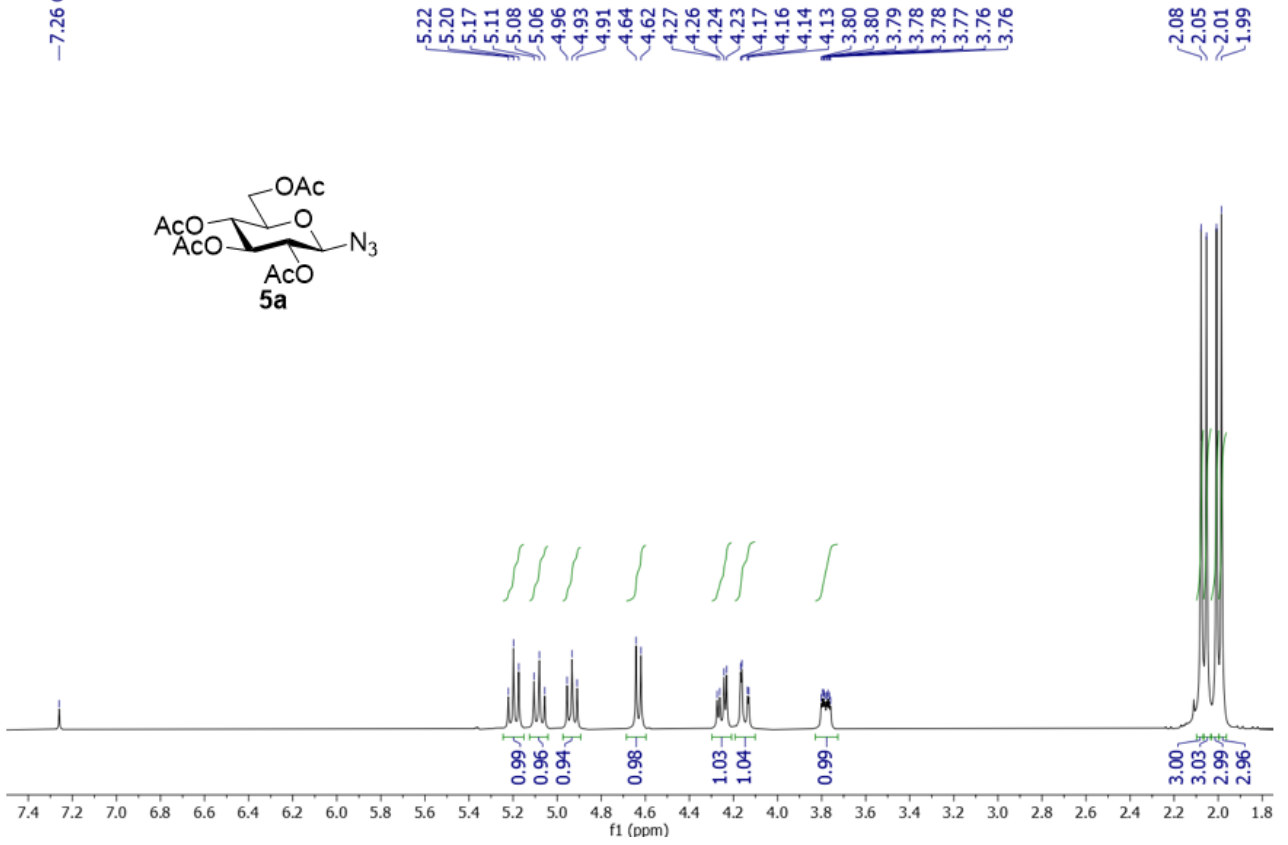
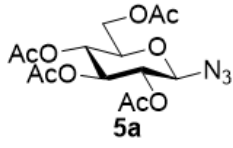
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1	14c $\beta$	 <p>18.47 kcal/mol</p>	Not found
2	15c $\beta$	 <p>34.85 kcal/mol</p>	Not found
3	16c $\beta$	 <p>5.82 kcal/mol</p>	Not found
4	14c $\alpha$	 <p>19.71 kcal/mol</p>	 <p>18.25 kcal/mol</p>
5	15c $\alpha$	 <p>36.54 kcal/mol</p>	

6	16c $\alpha$	Not found	<p style="text-align: center;">33.99 kcal/mol</p>  <p style="text-align: center;">6.50 kcal/mol</p>
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$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of glycosyl azides **5a-c**.



-7.26 CDCl3



170.7  
170.2  
169.4  
169.3

-88.0

77.2 CDCl3

74.2

72.7

70.8

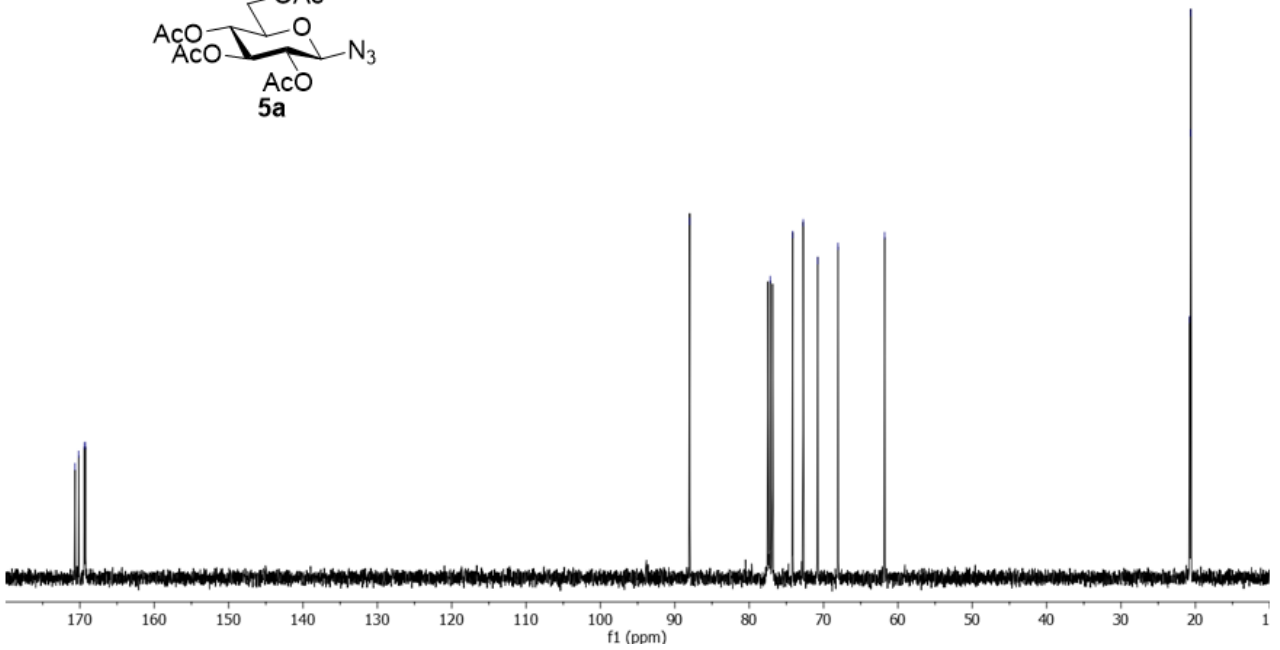
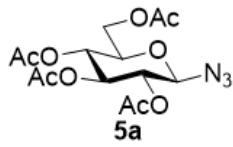
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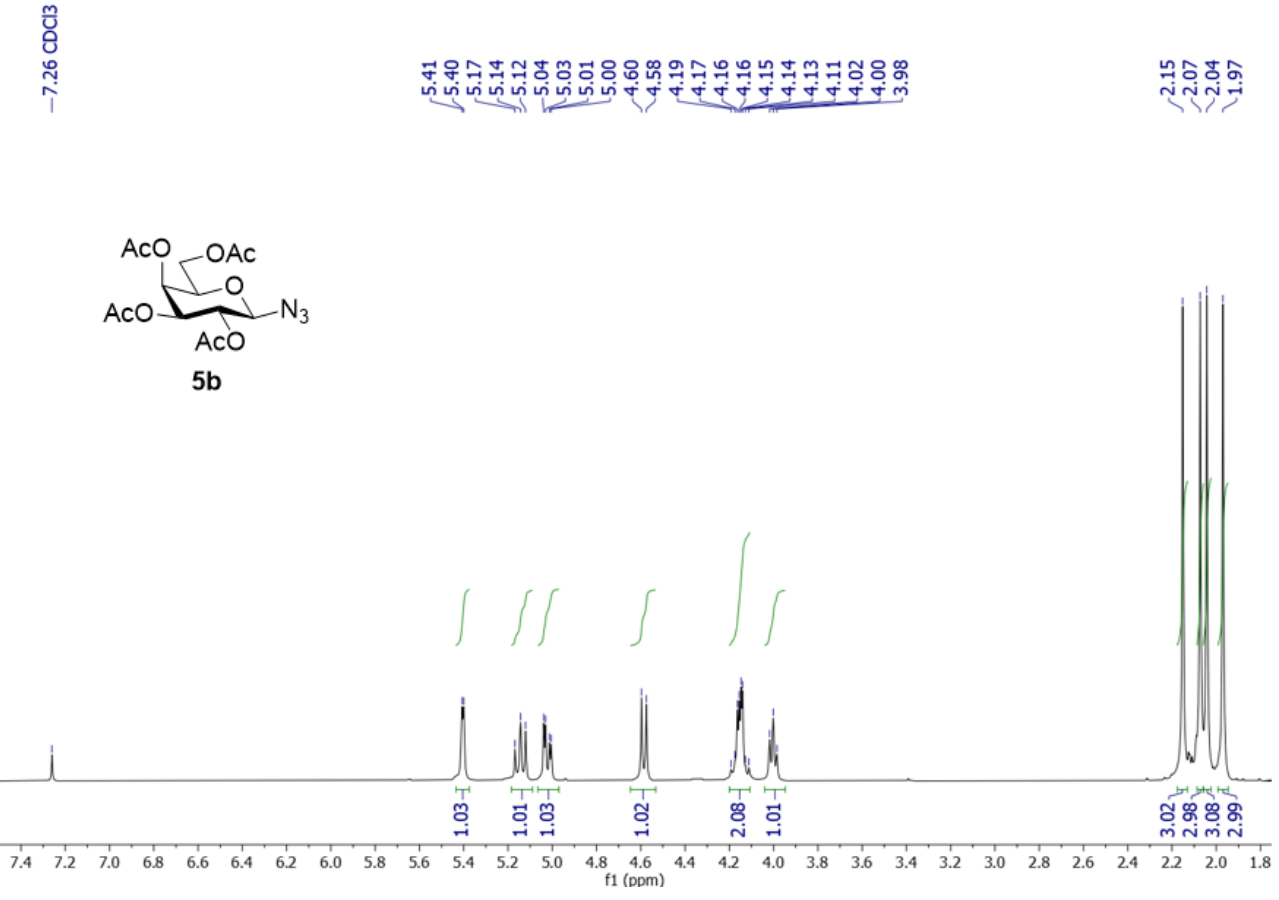
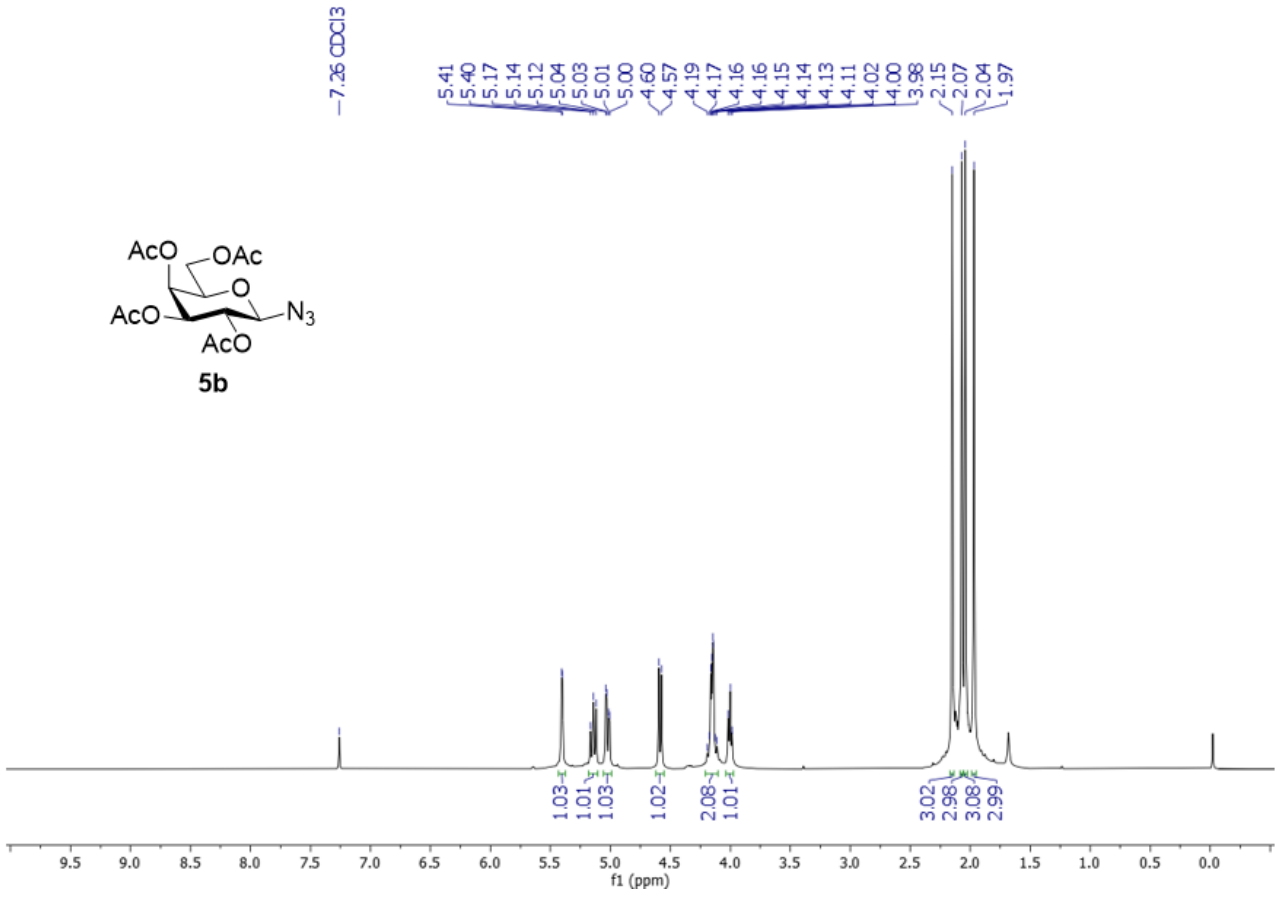
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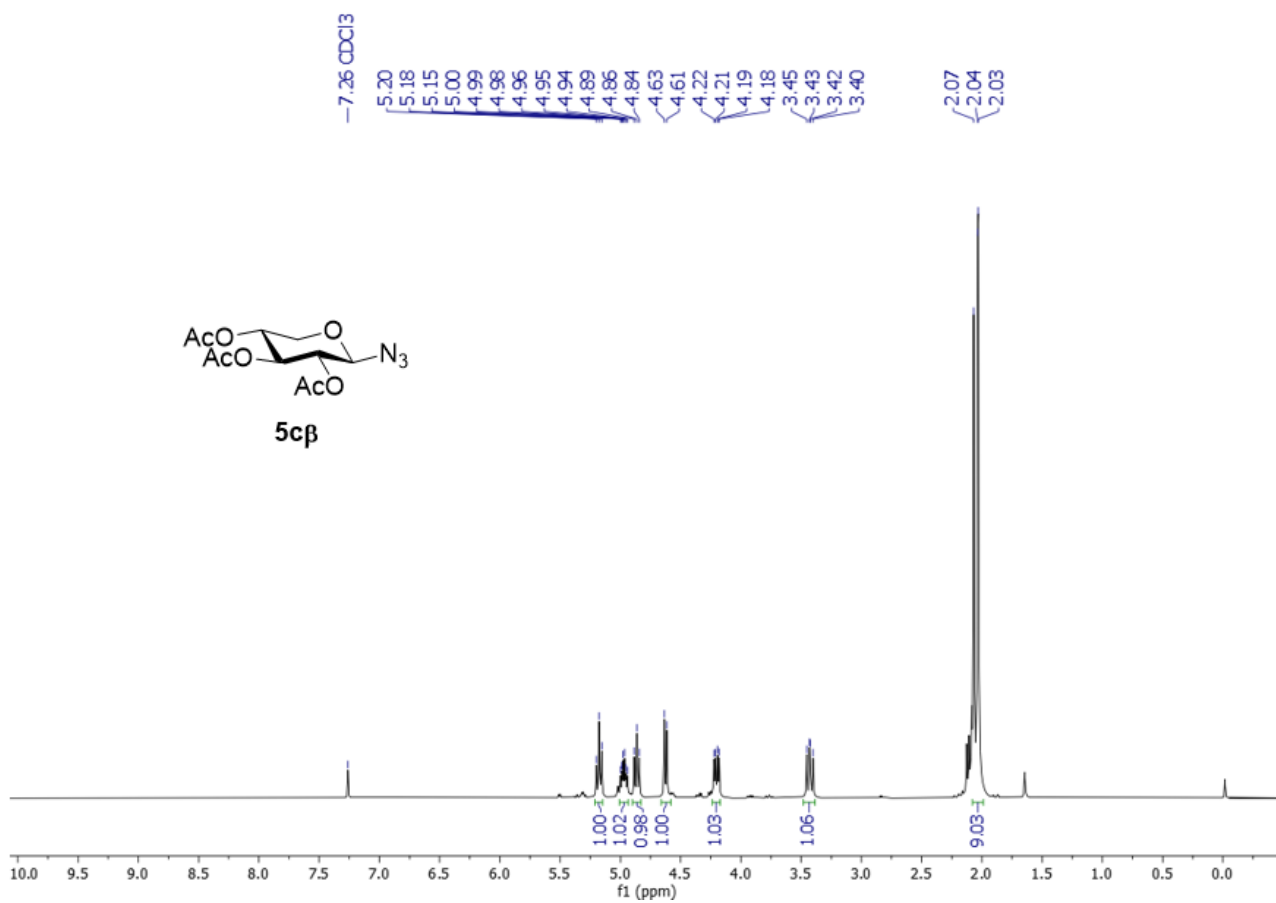
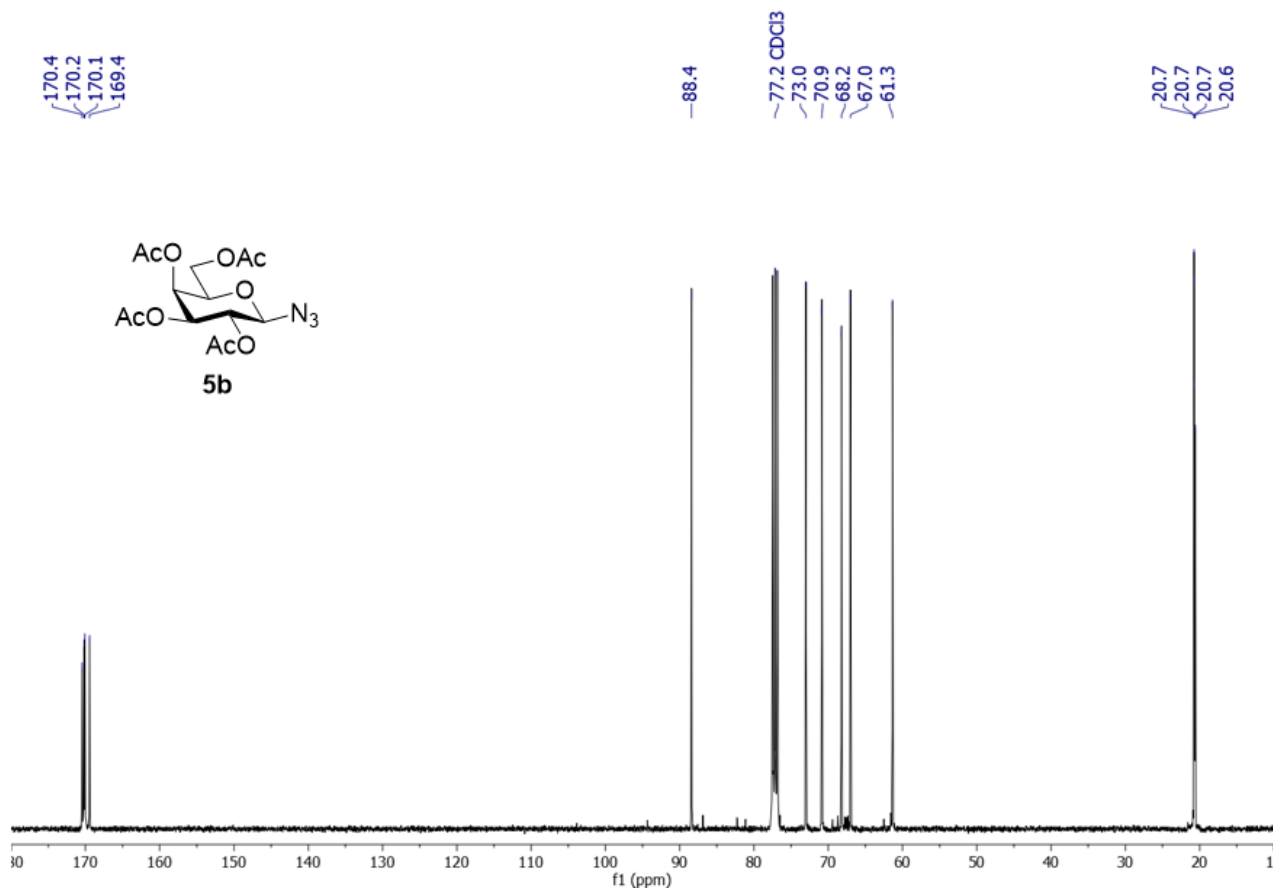
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20.6

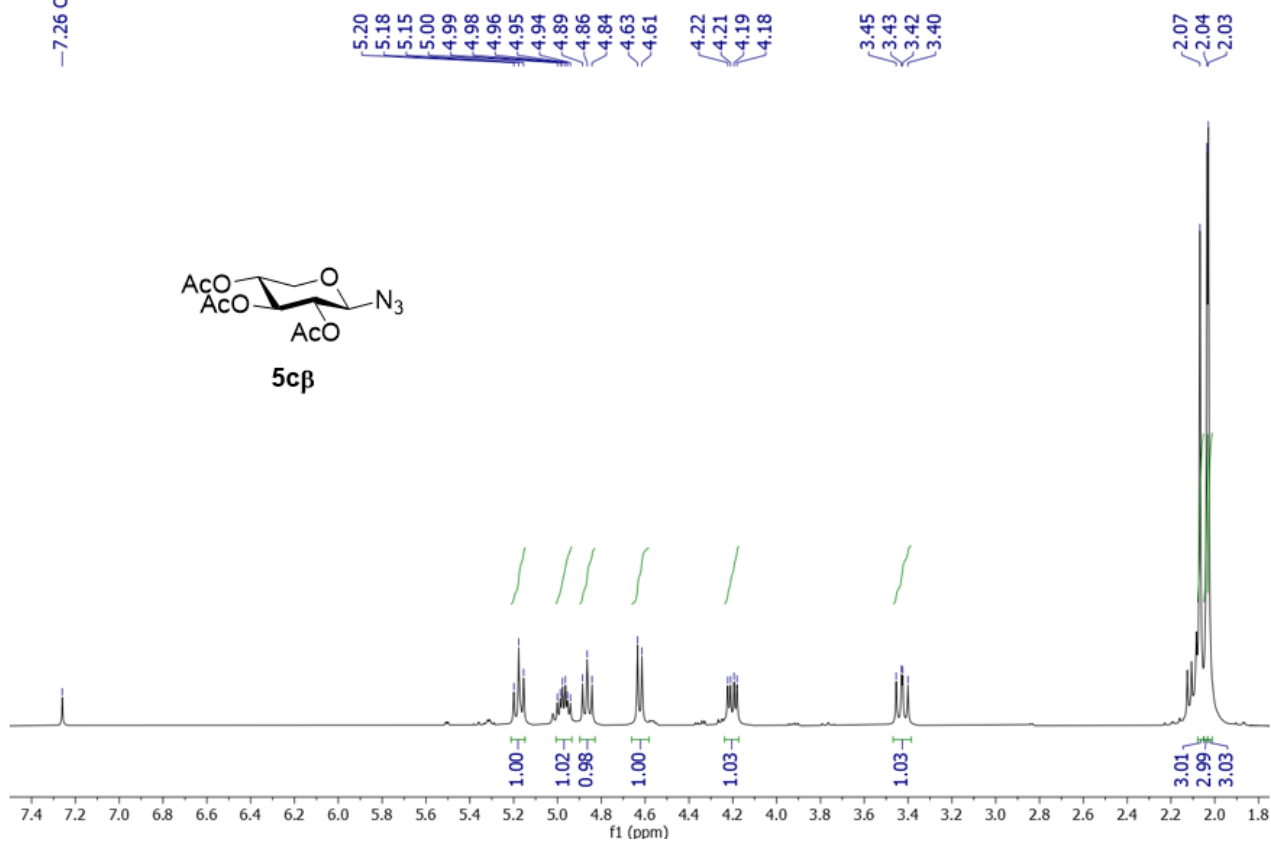
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-7.26 CDCl<sub>3</sub>



170.1  
169.8  
169.4

-88.4

77.2 CDCl<sub>3</sub>

71.6

70.5

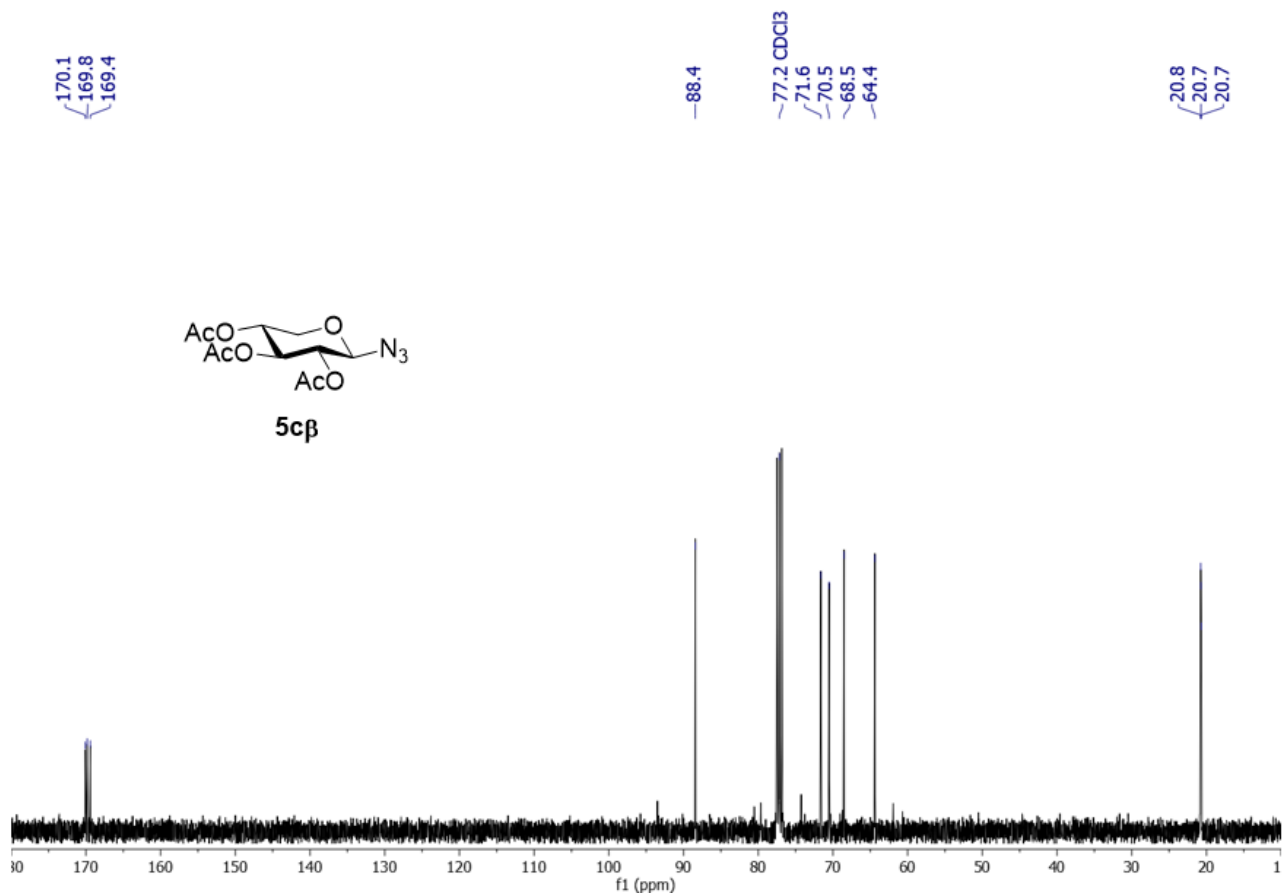
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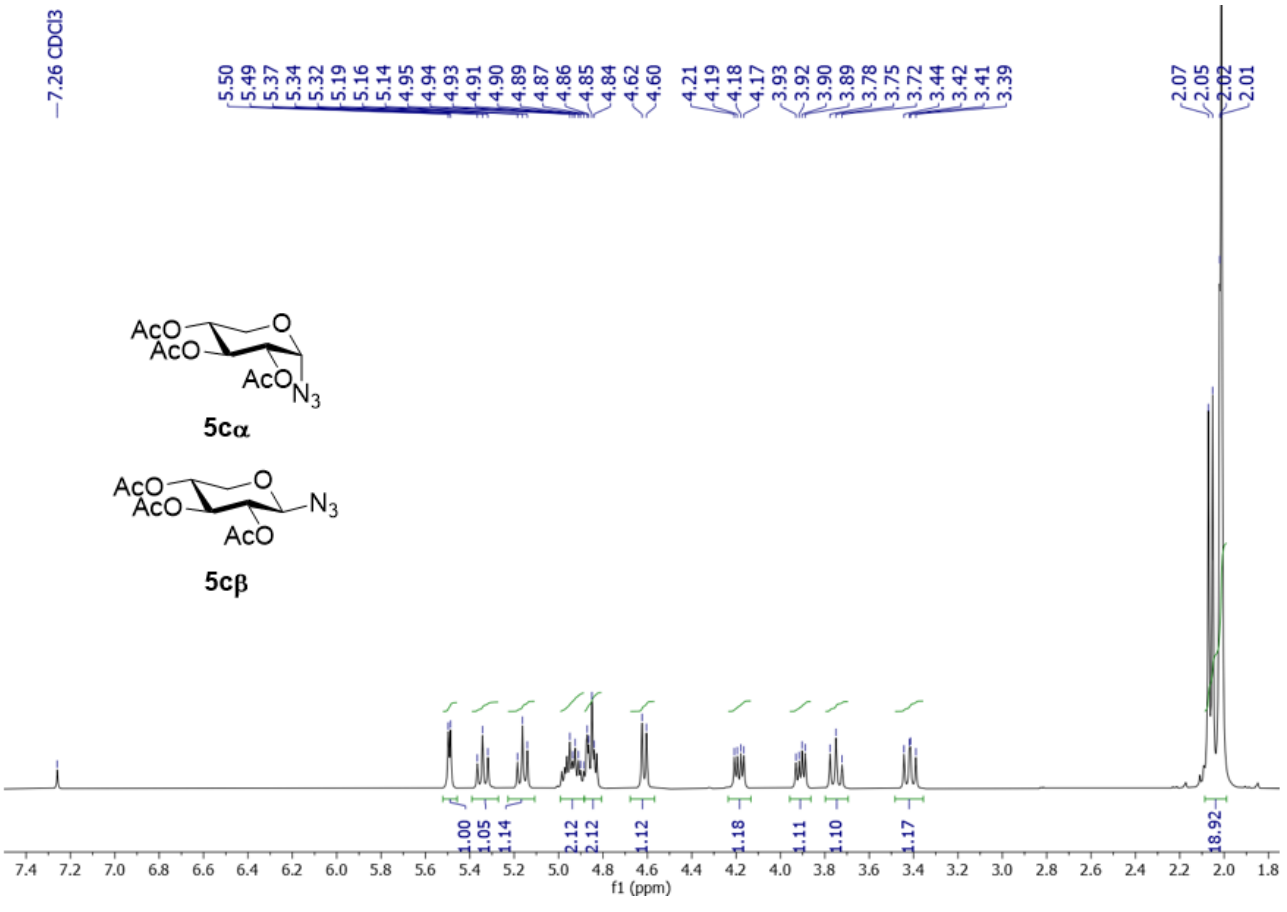
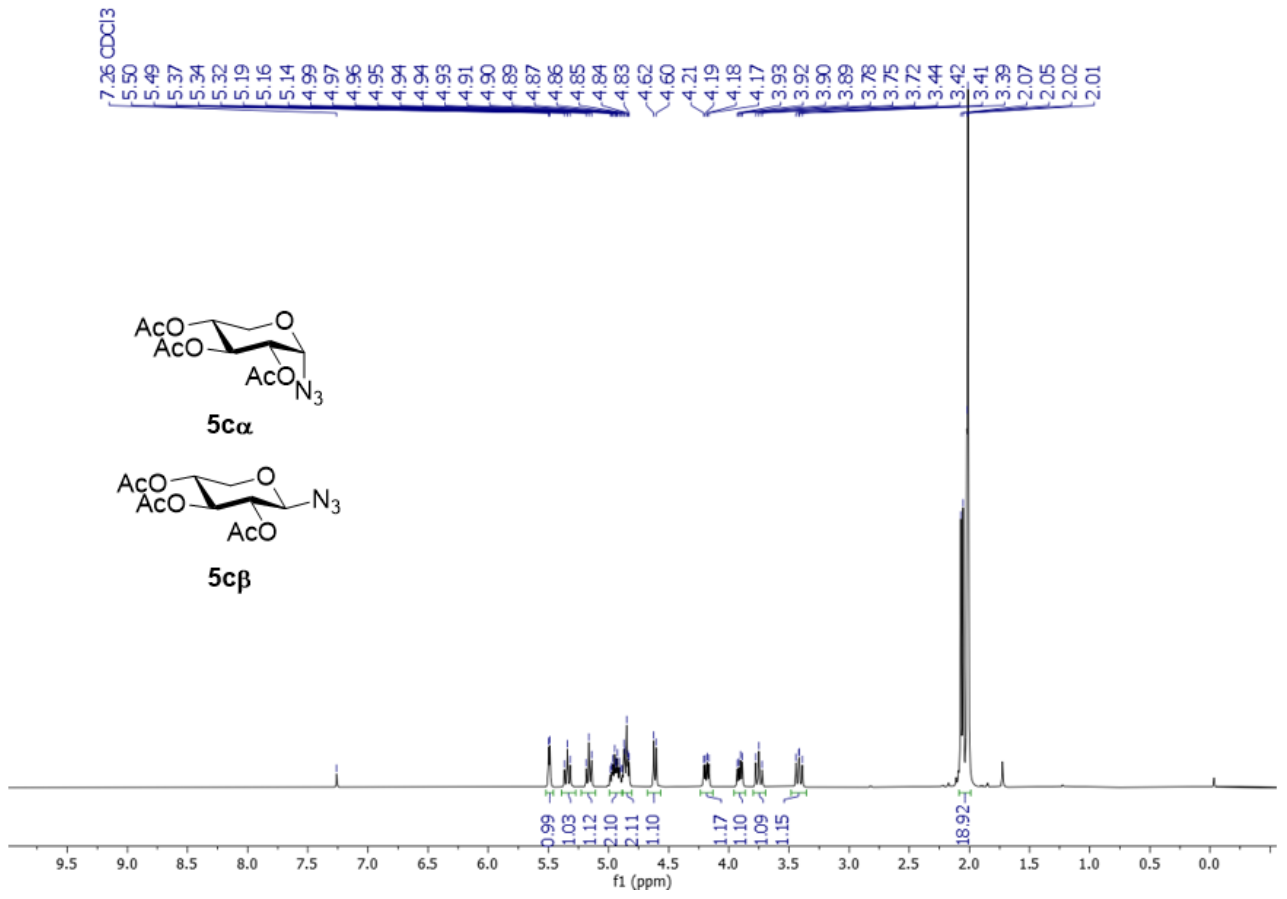
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20.8

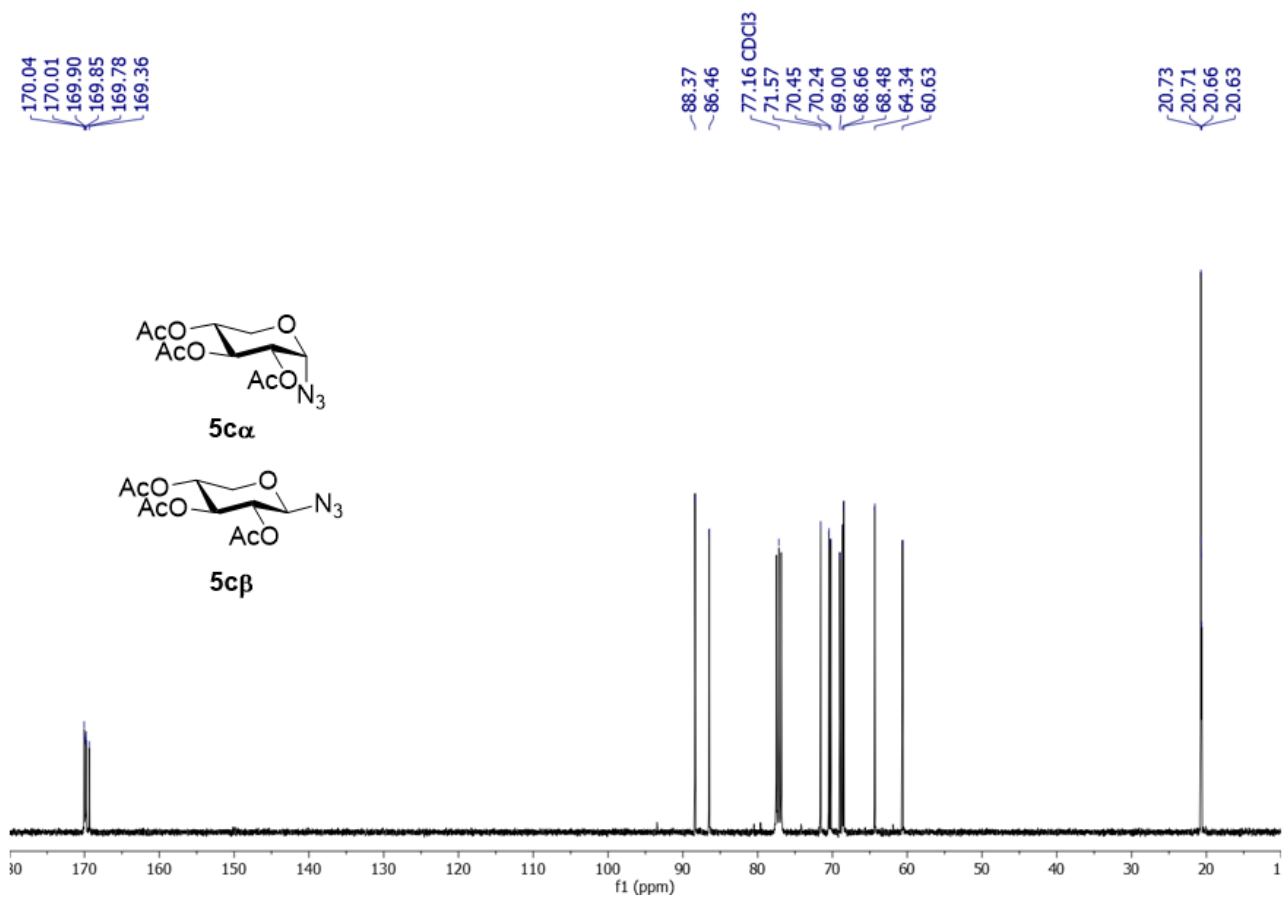
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20.7

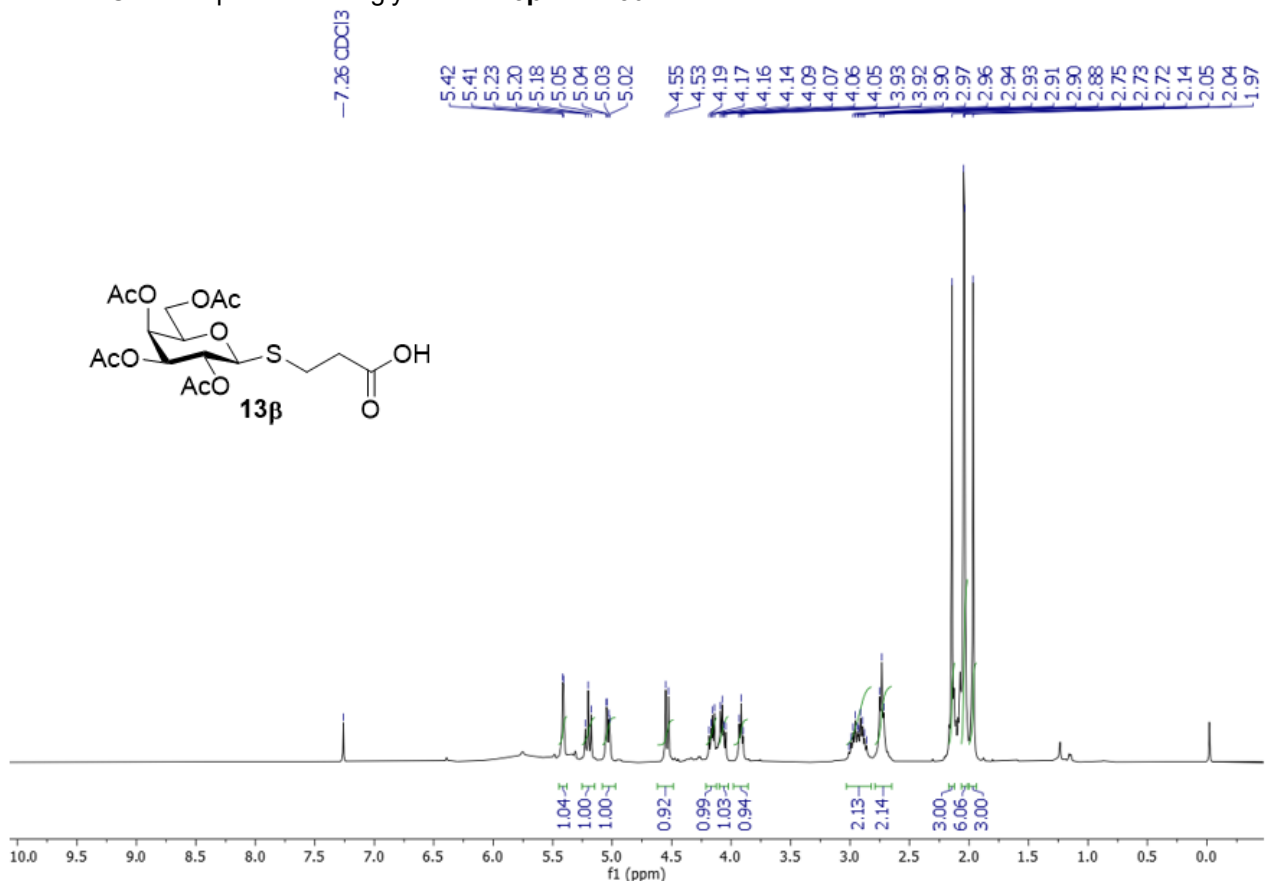




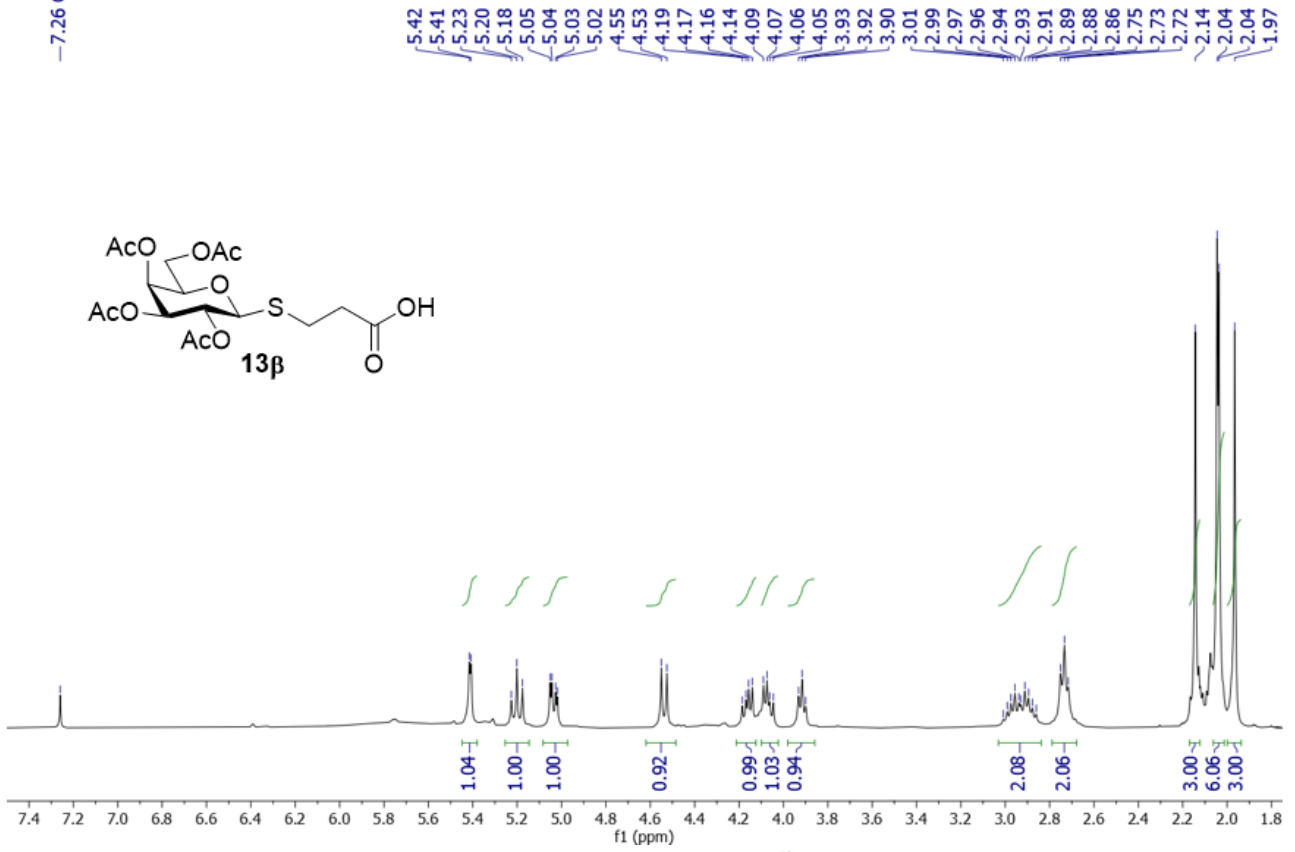
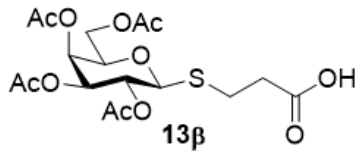




<sup>1</sup>H and <sup>13</sup>C NMR spectra of thioglyco acid **13 $\beta$**  and **13 $\alpha$** .



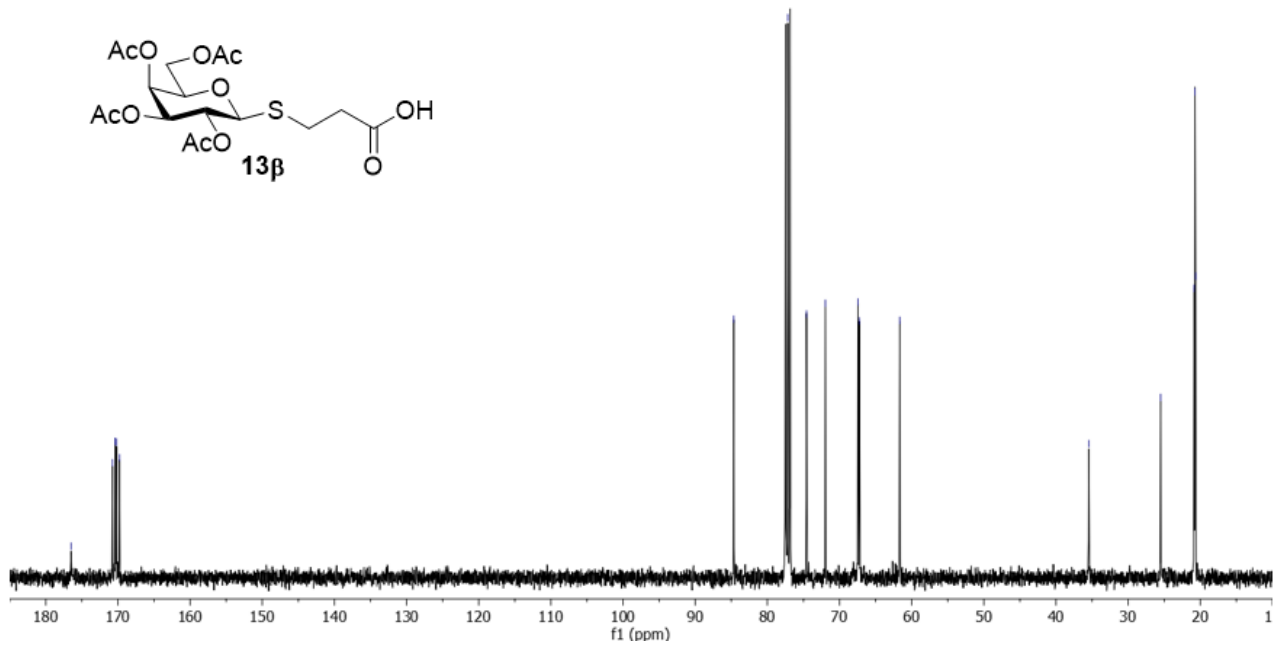
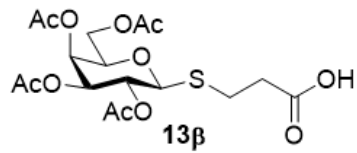
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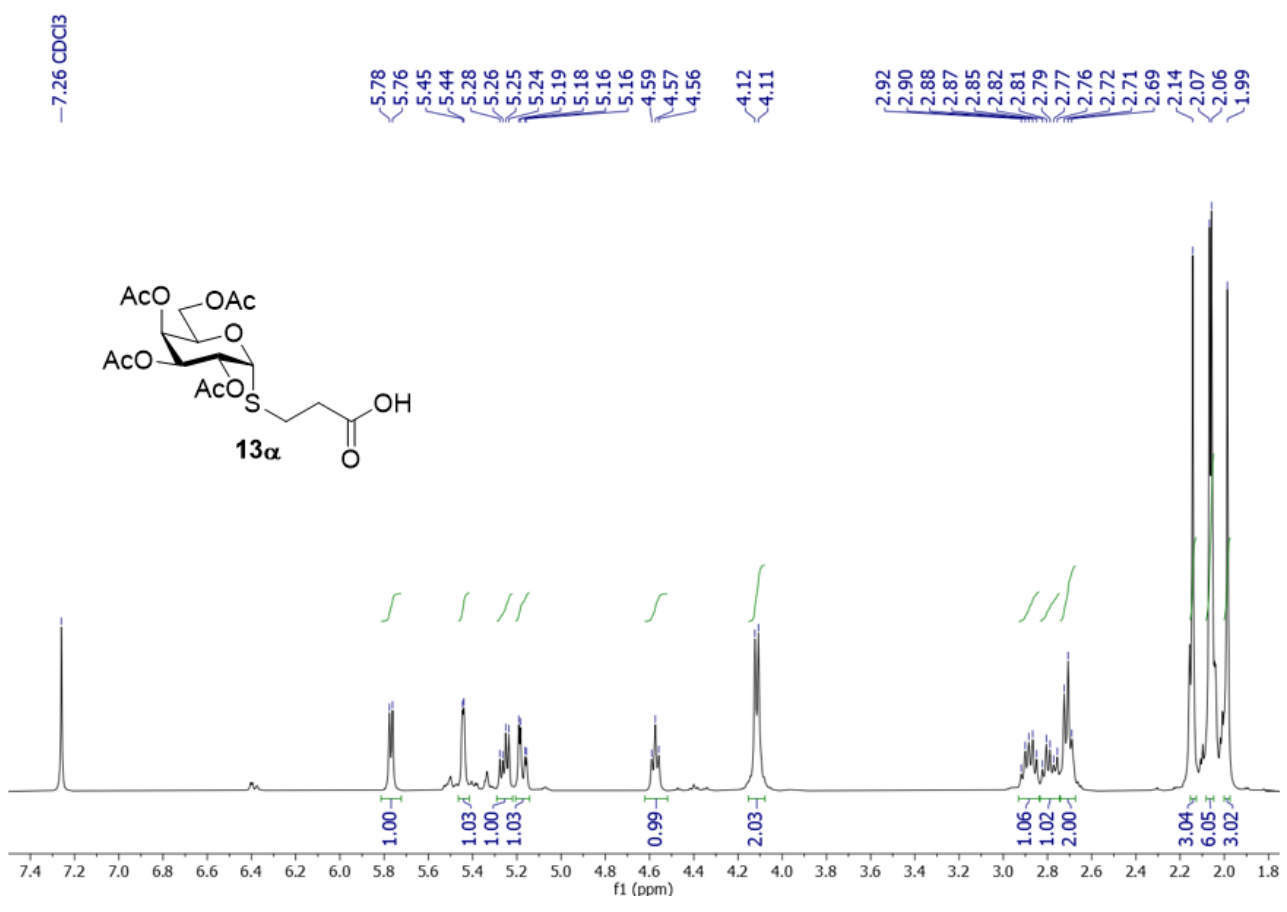
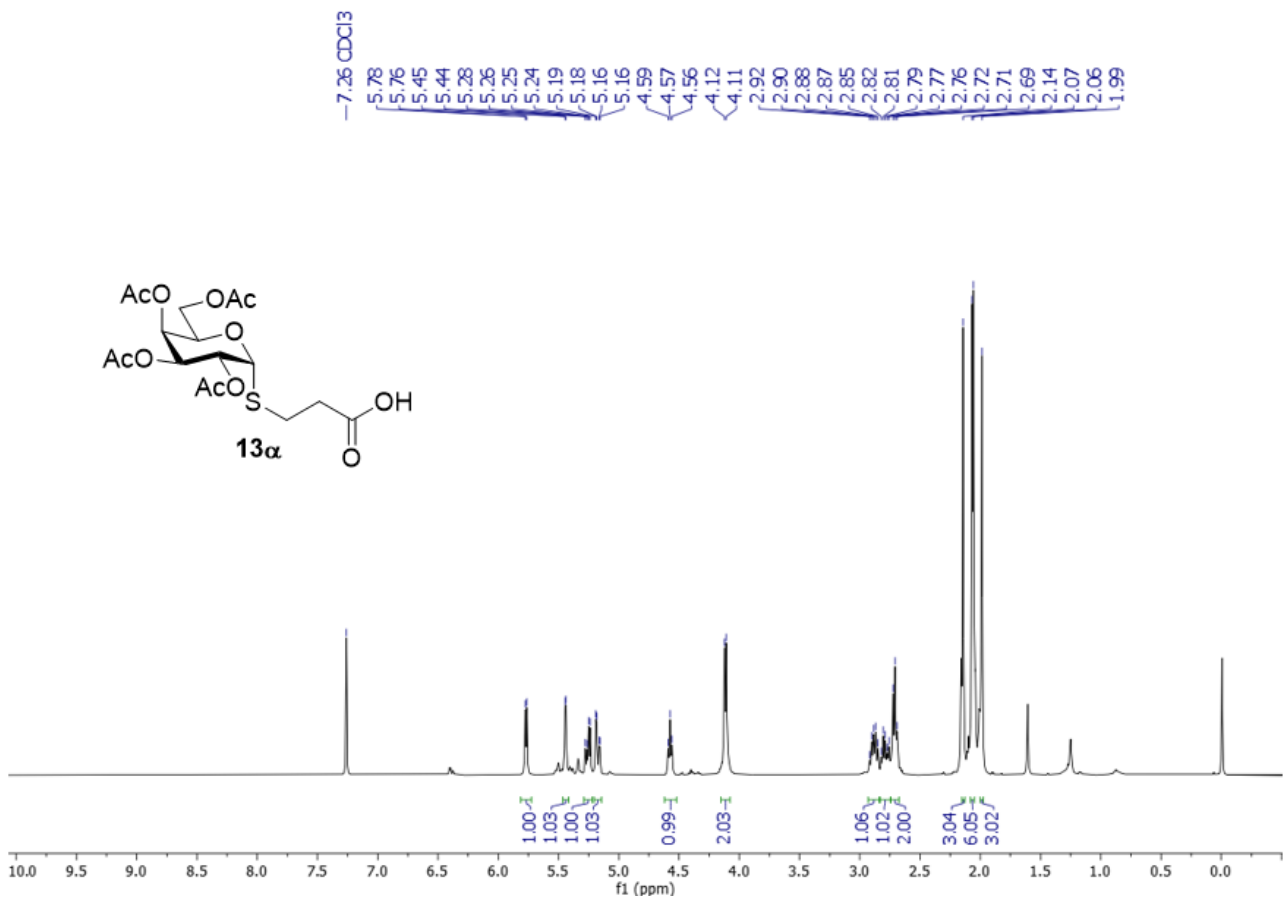


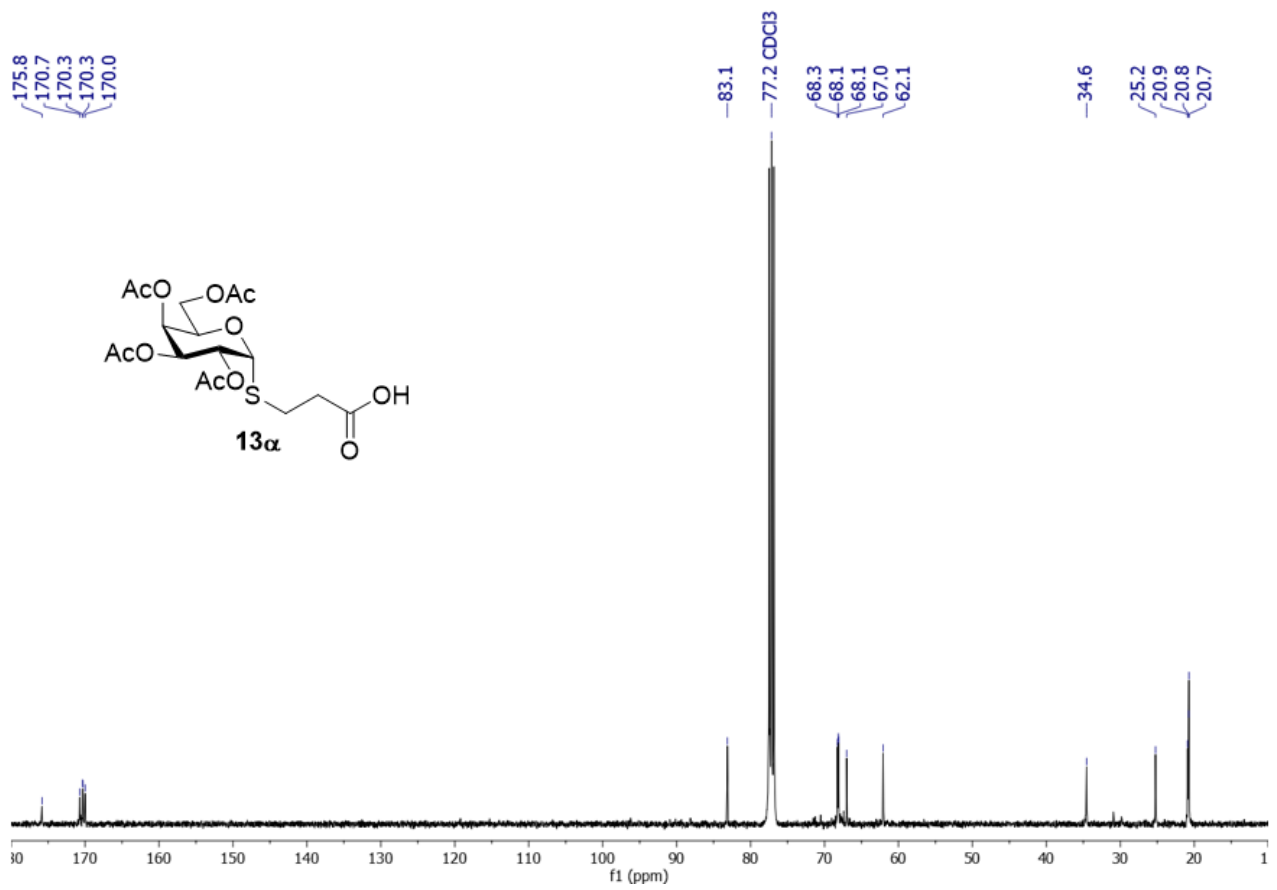
176.5  
170.7  
170.4  
170.2  
169.8

-84.7  
-77.2 CDCl<sub>3</sub>  
-74.6  
-72.0  
-67.4  
-67.3  
-61.7

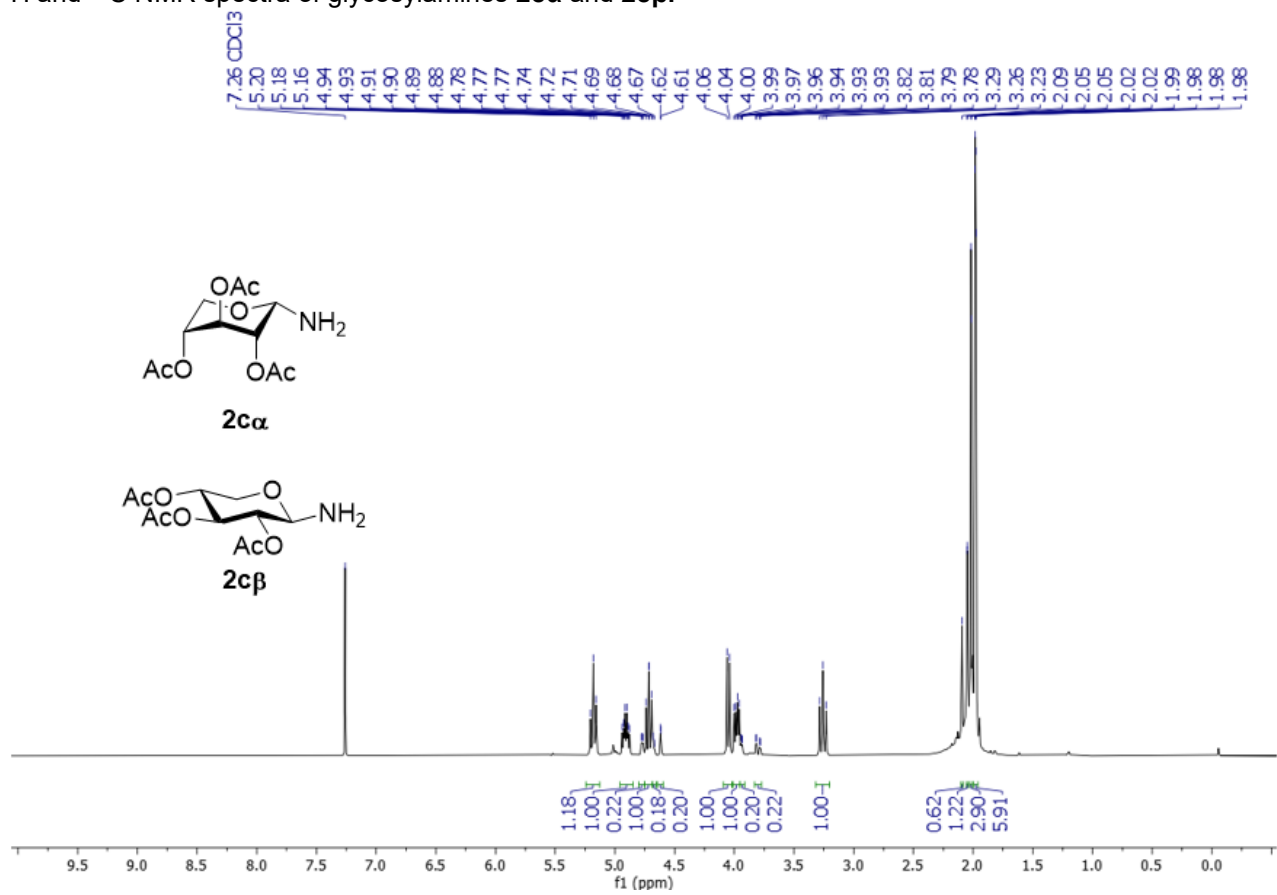
-35.4  
25.5  
20.9  
20.7  
20.7





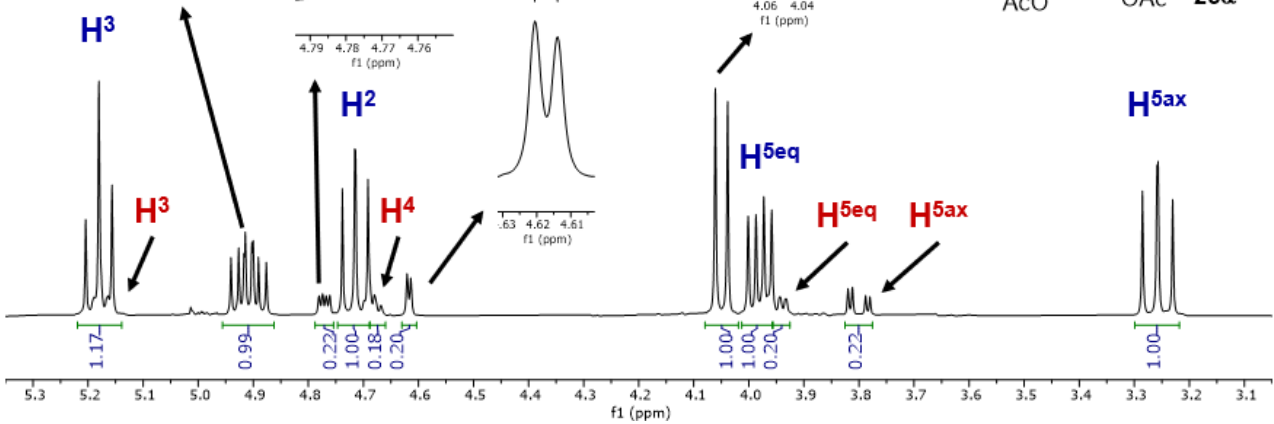
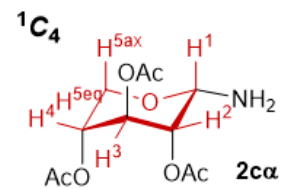
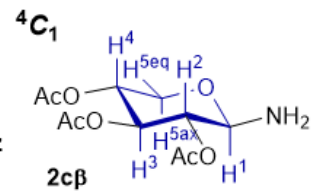
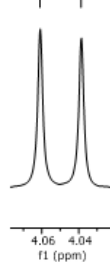
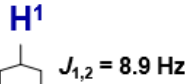
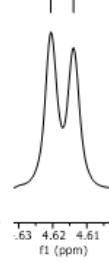
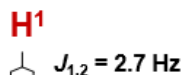
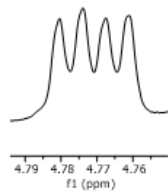
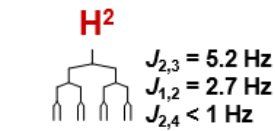
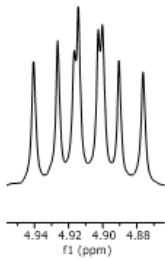
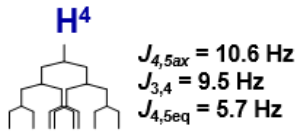
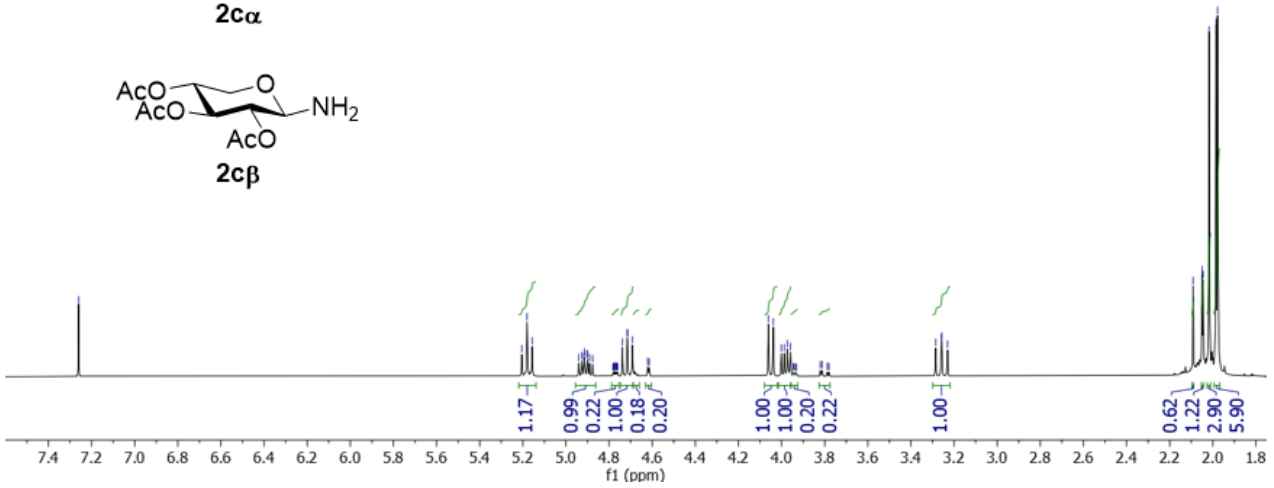
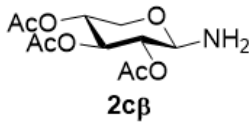
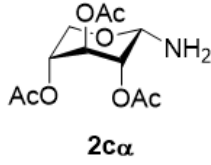


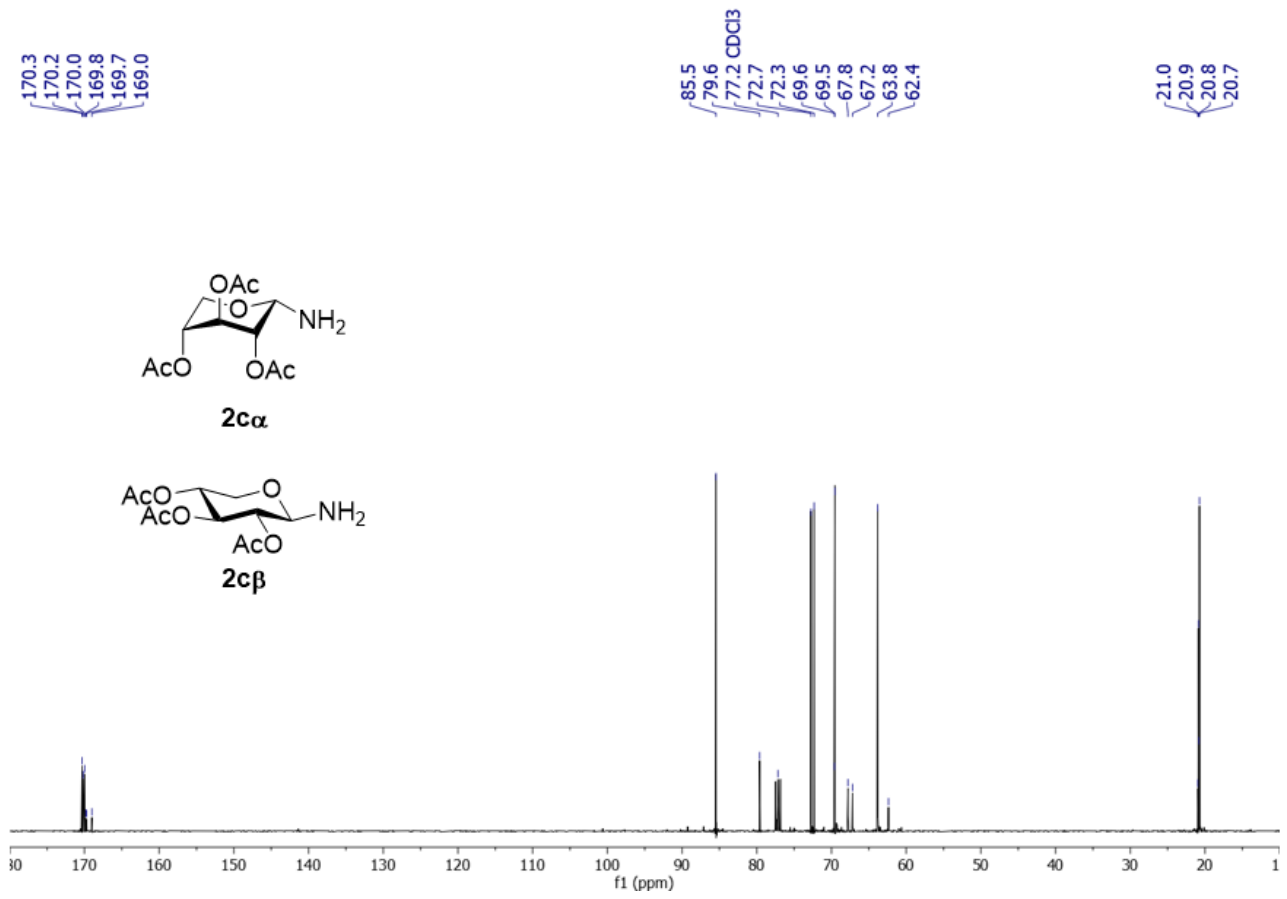
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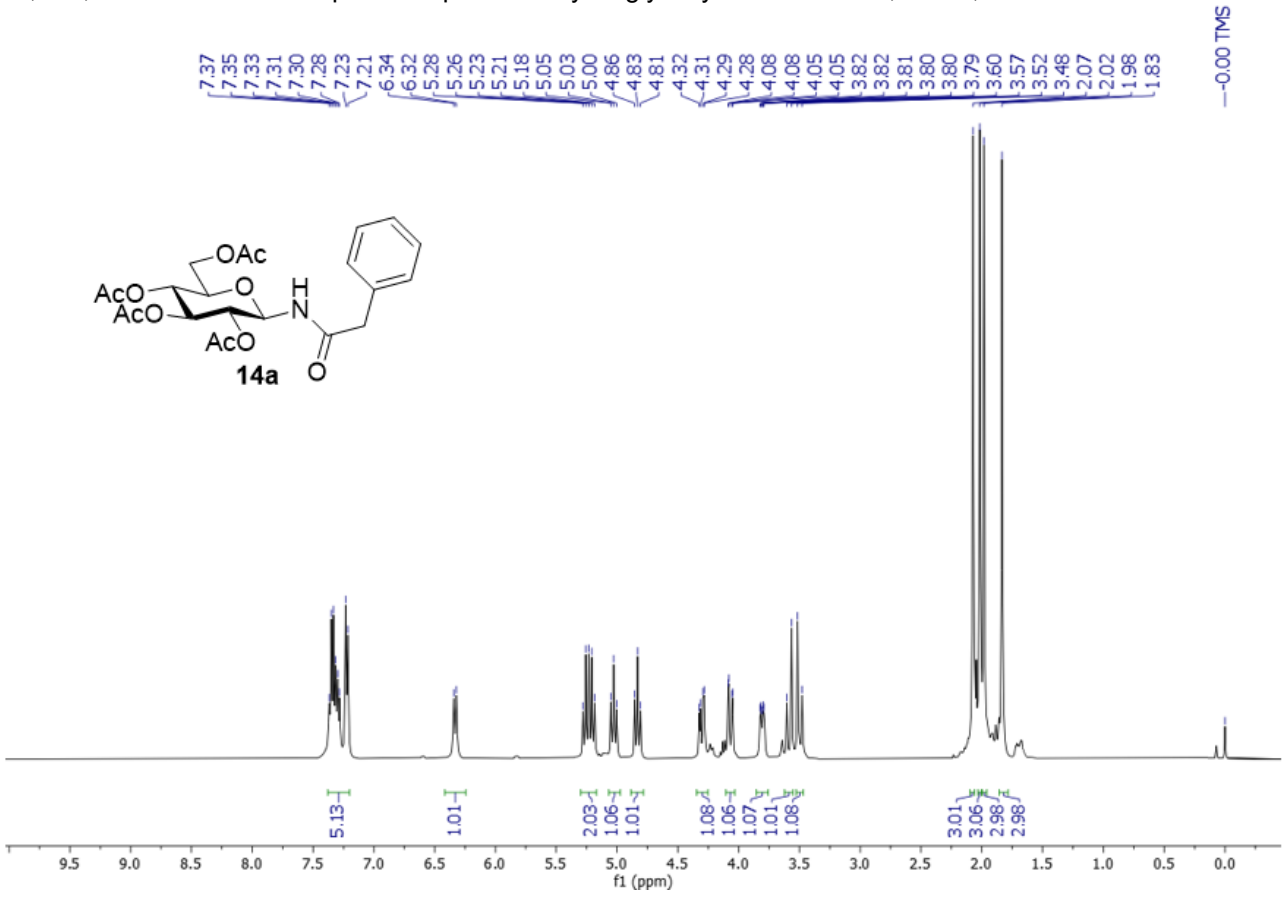
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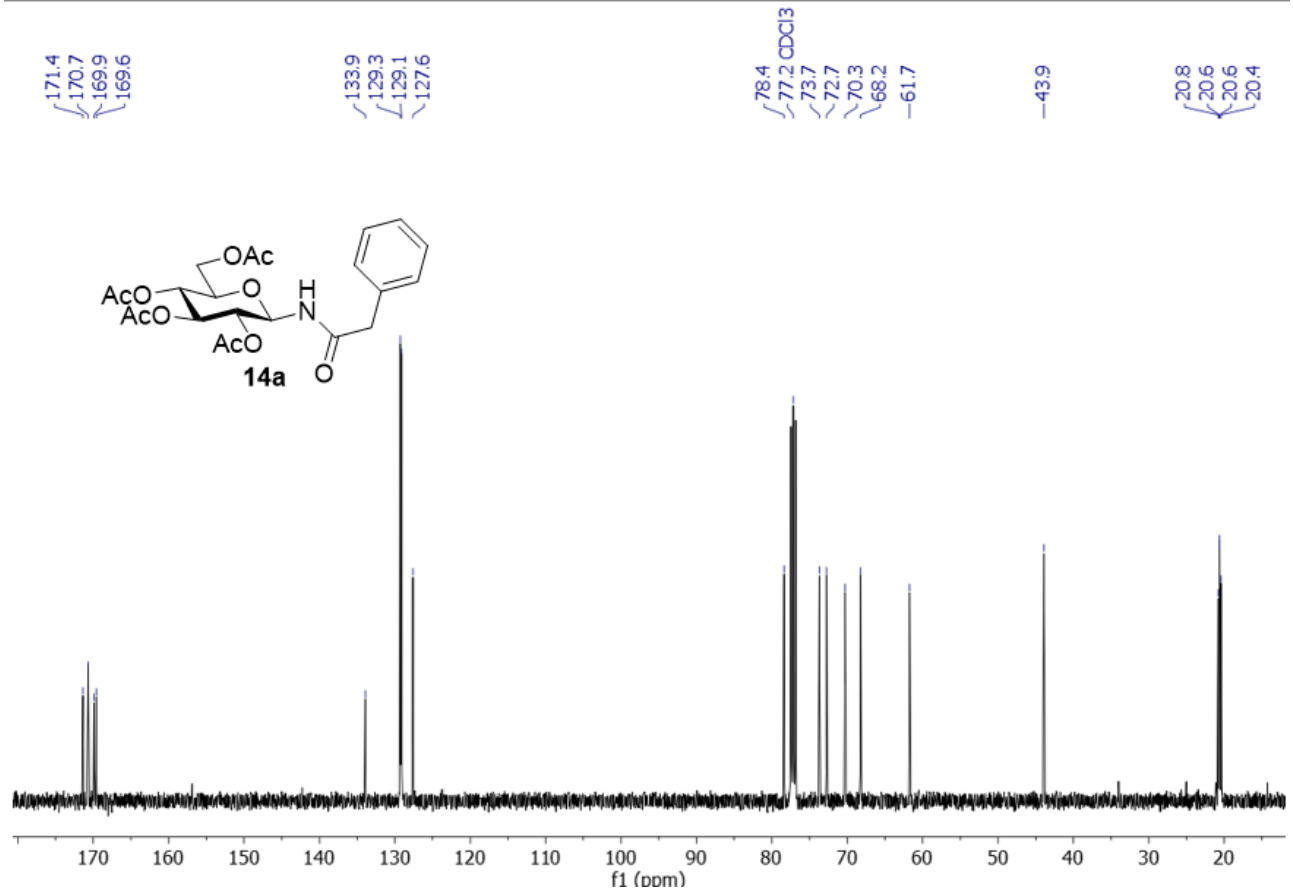
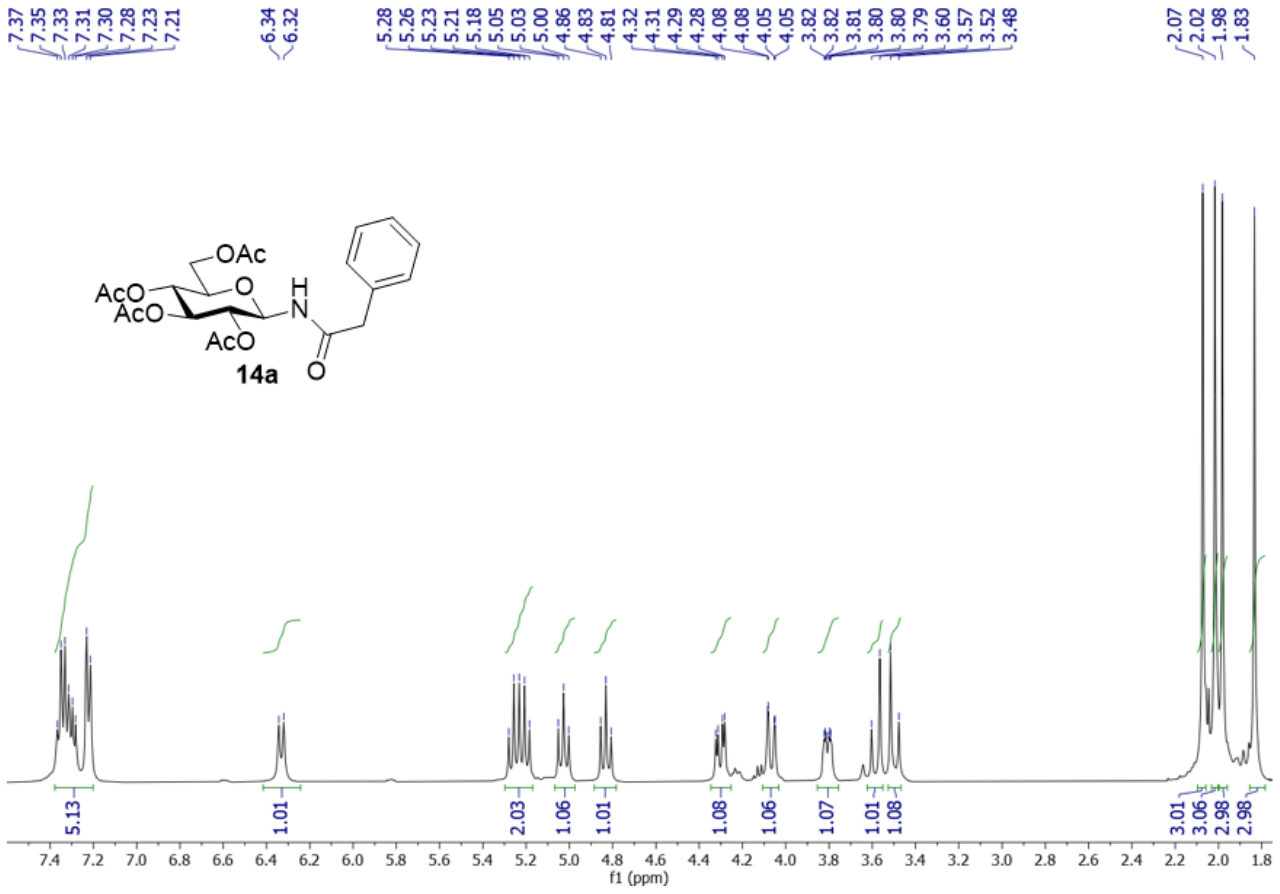
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5.16  
4.94  
4.93  
4.92  
4.91  
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4.89  
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4.78  
4.78  
4.77  
4.77  
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3.97  
3.96  
3.95  
3.94  
3.93  
3.82  
3.81  
3.79  
3.78  
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1.98

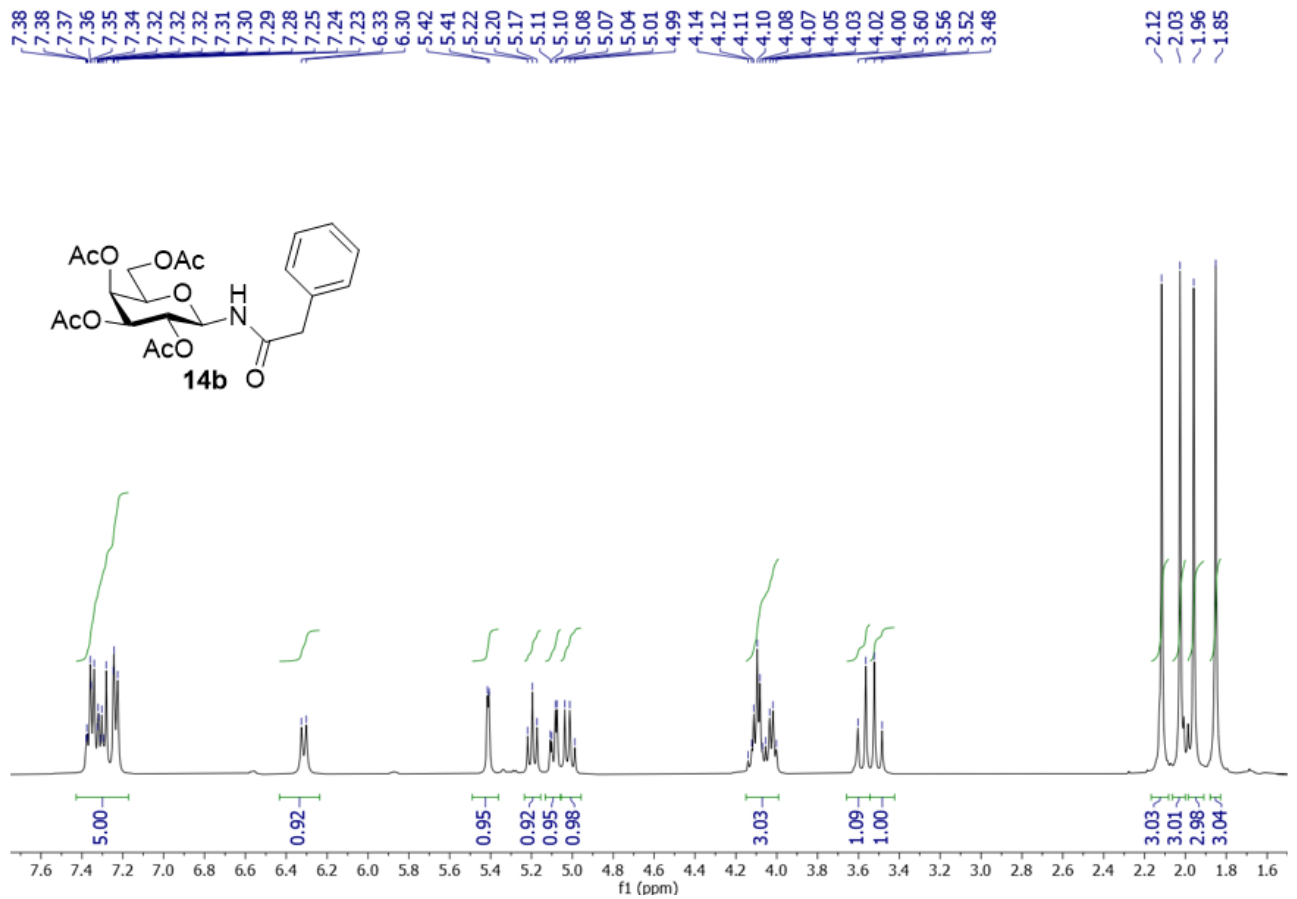
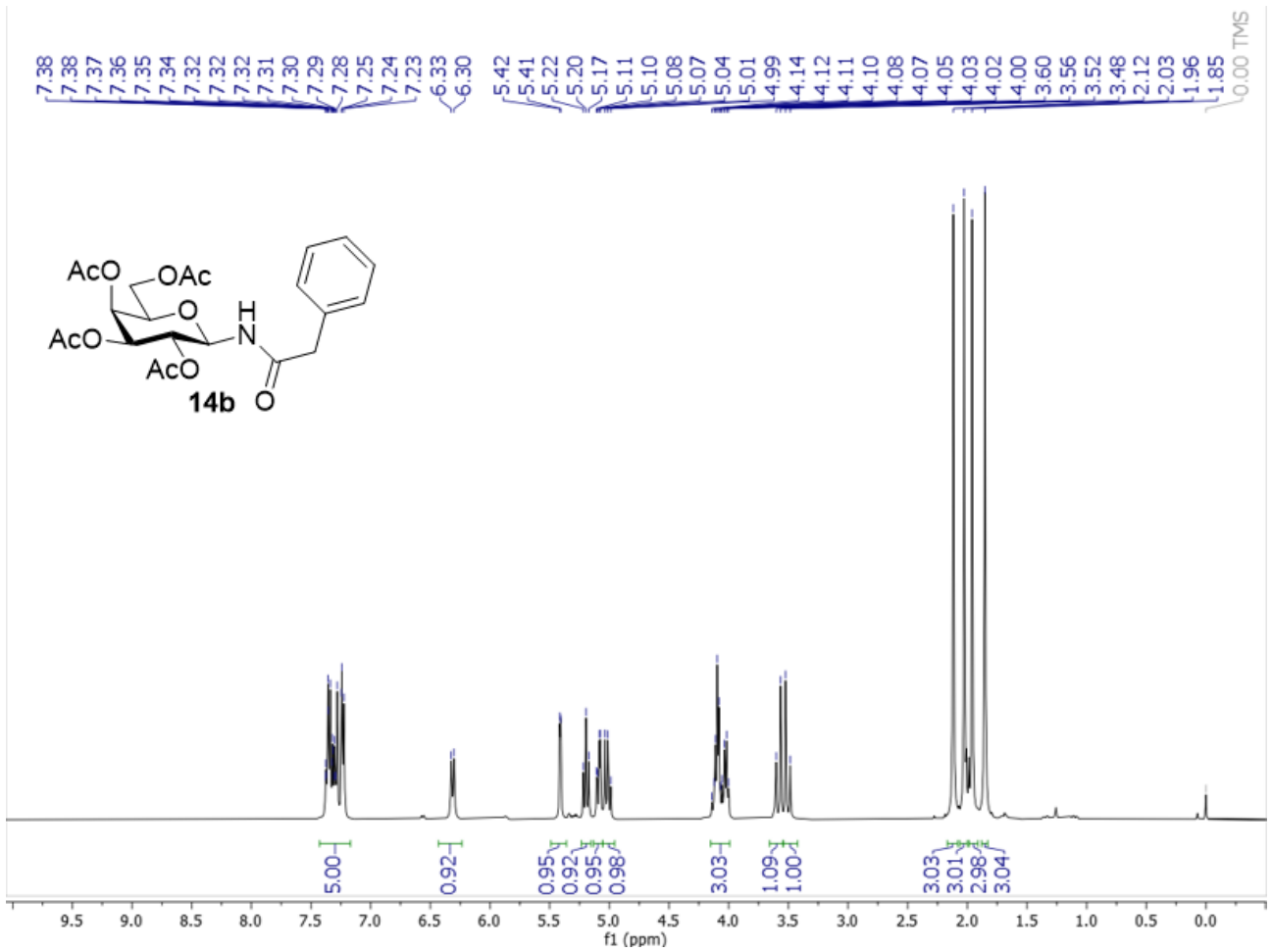




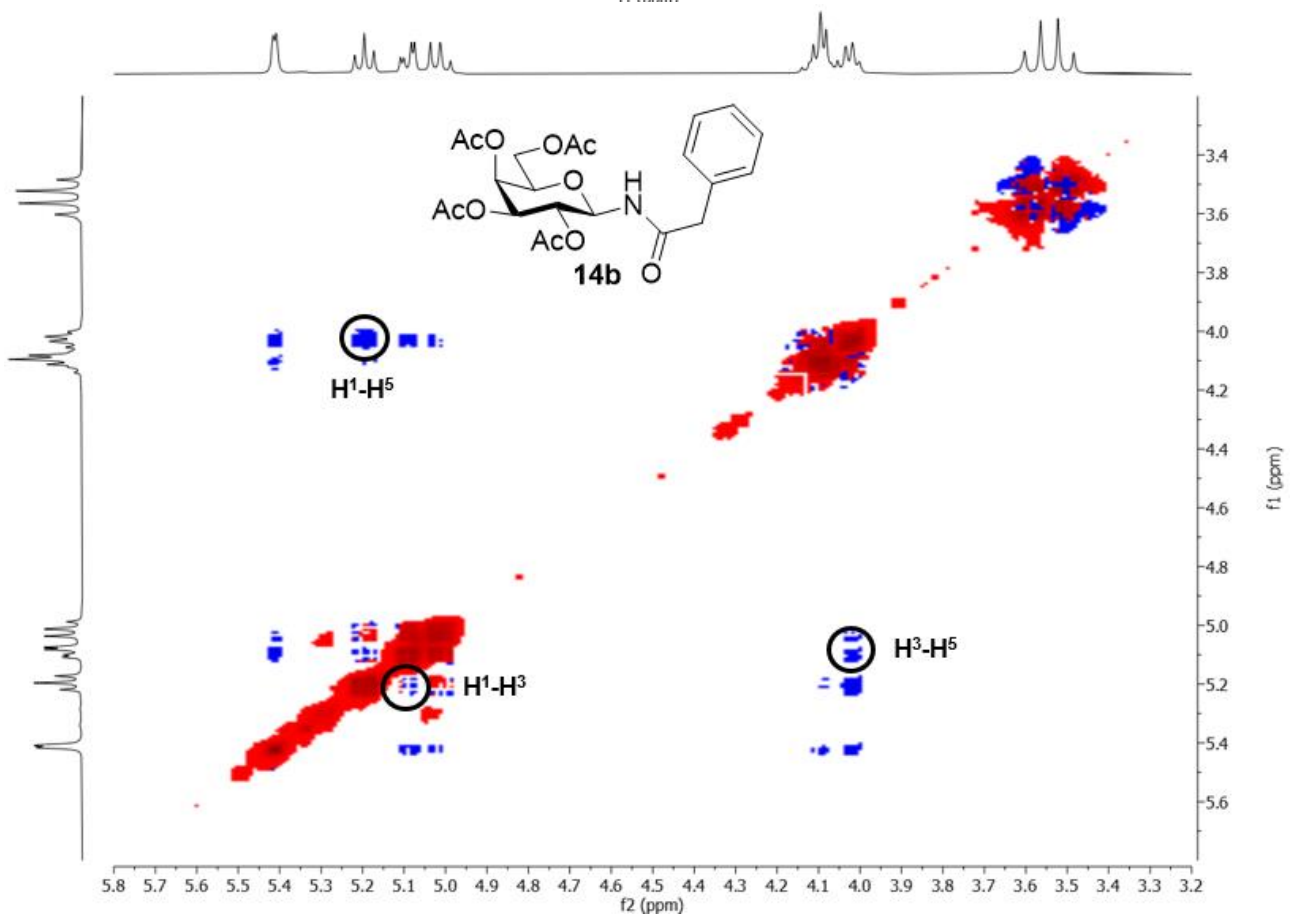
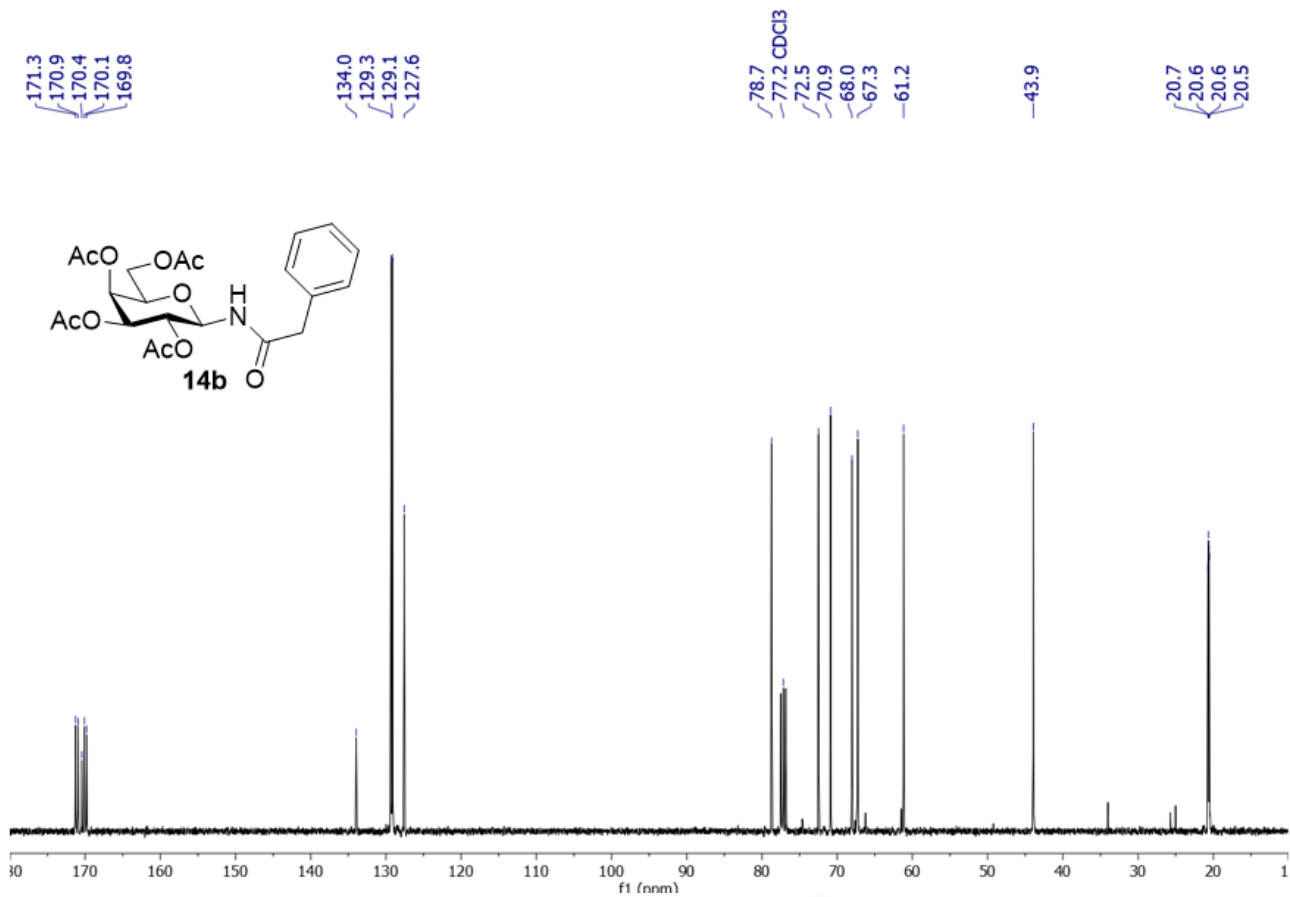
<sup>1</sup>H, <sup>13</sup>C, and NOESY NMR spectra of per-O-acetyl N-glycosyl amides **14a-c**, **15a-c**, and **16a-c**.

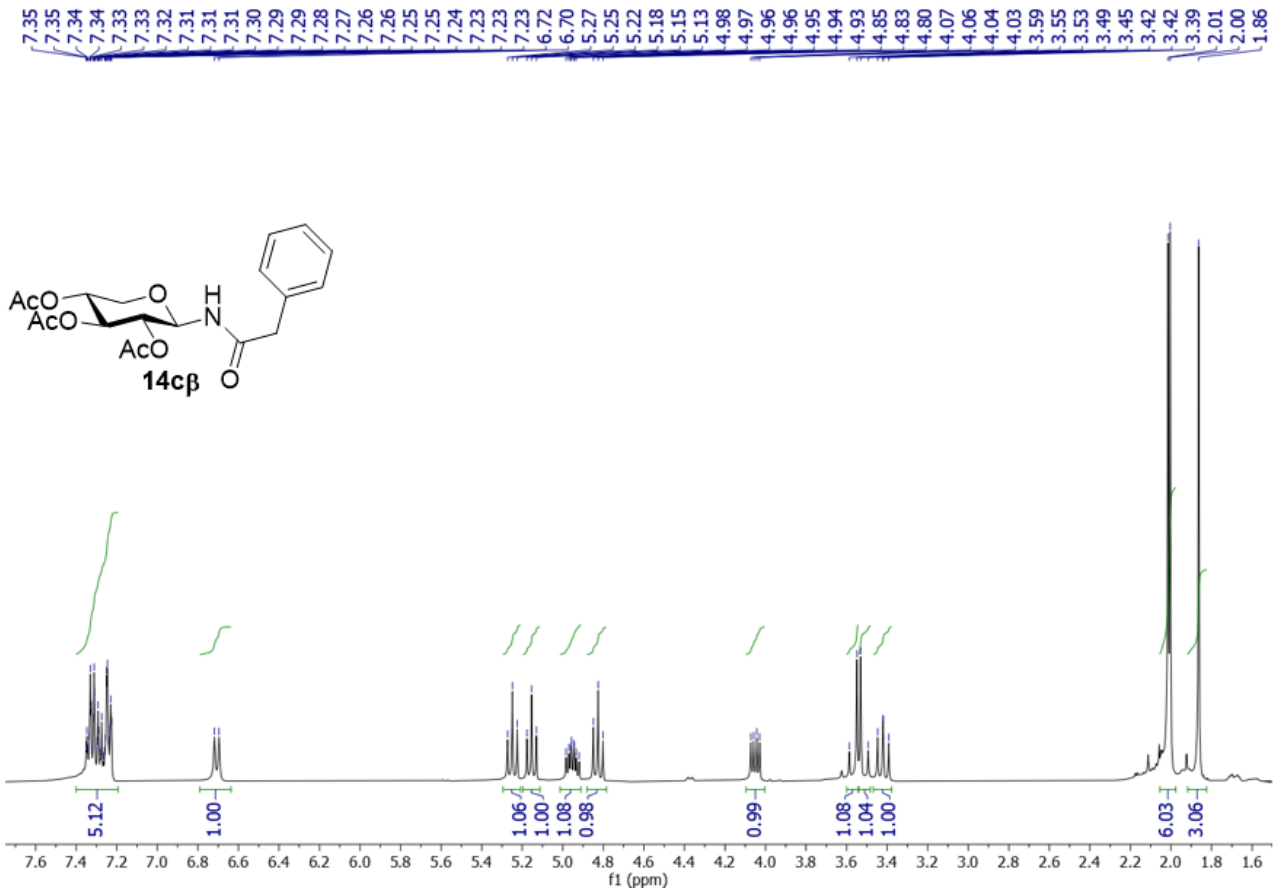
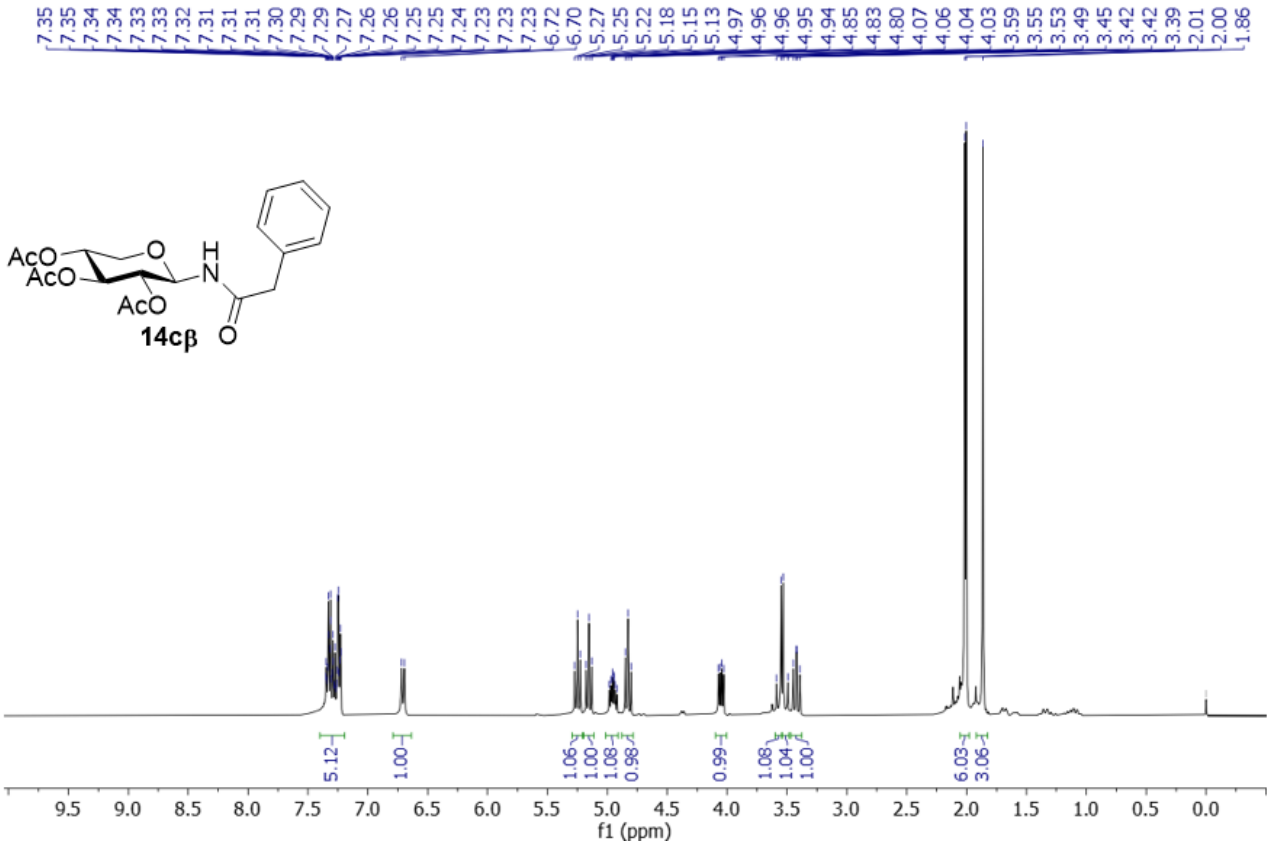


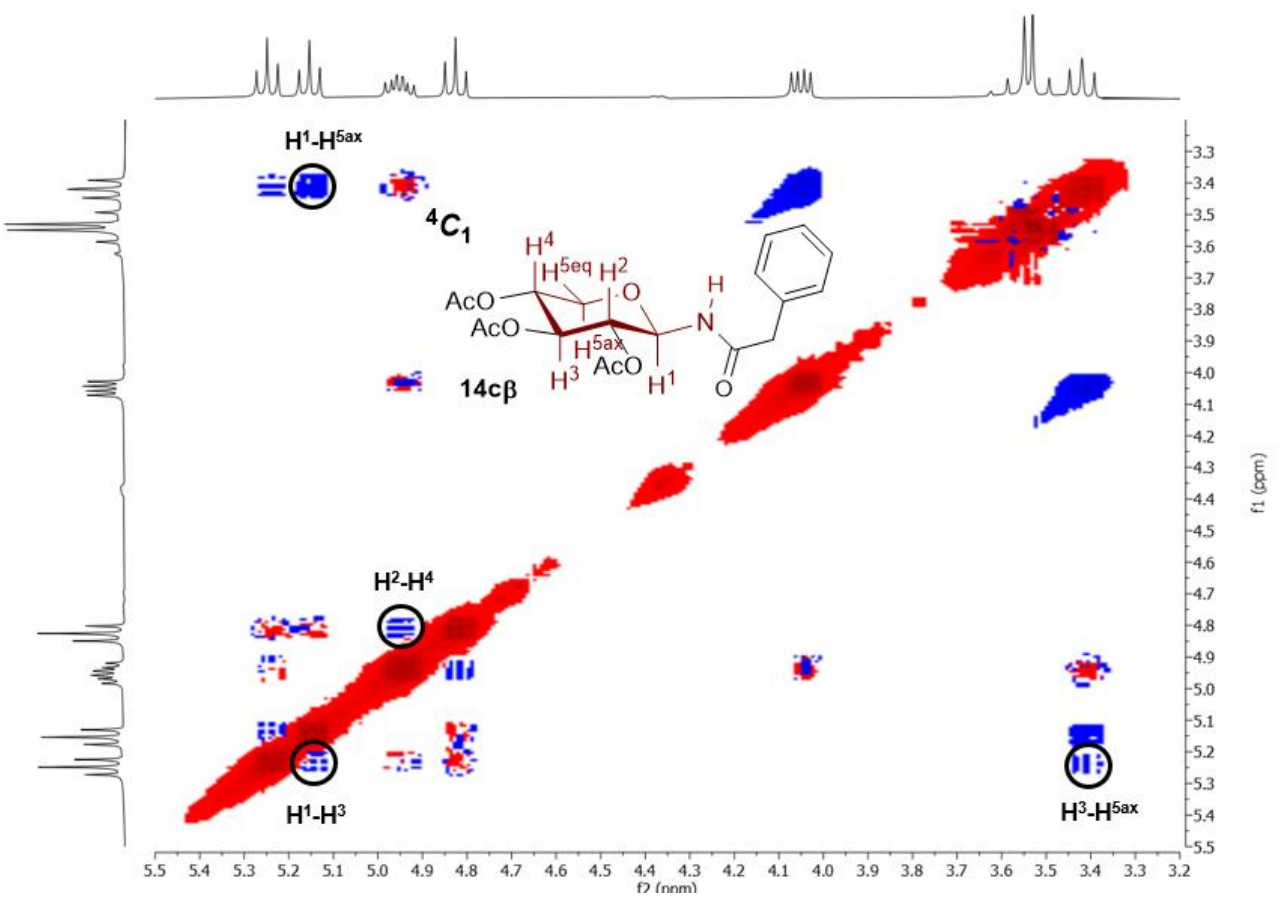
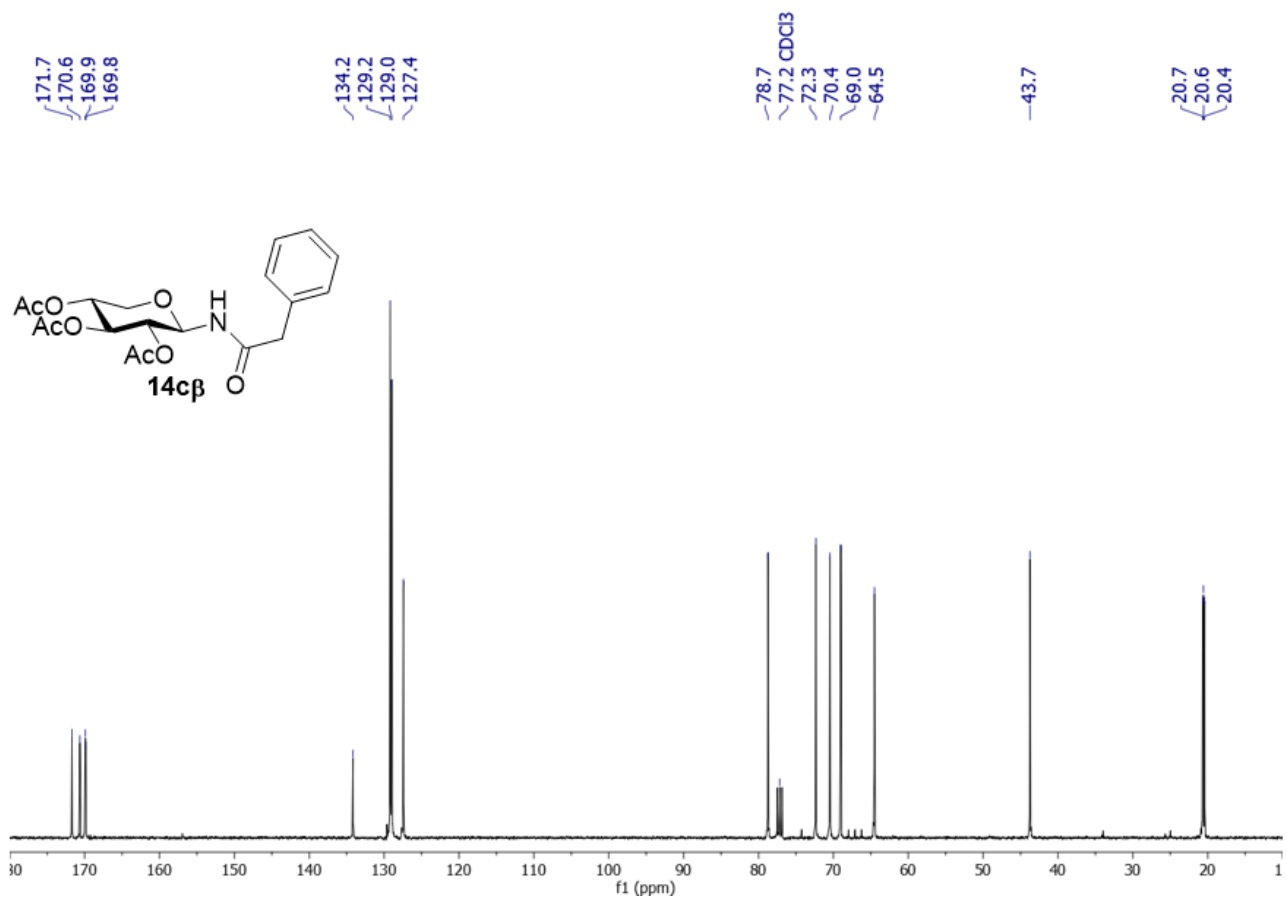


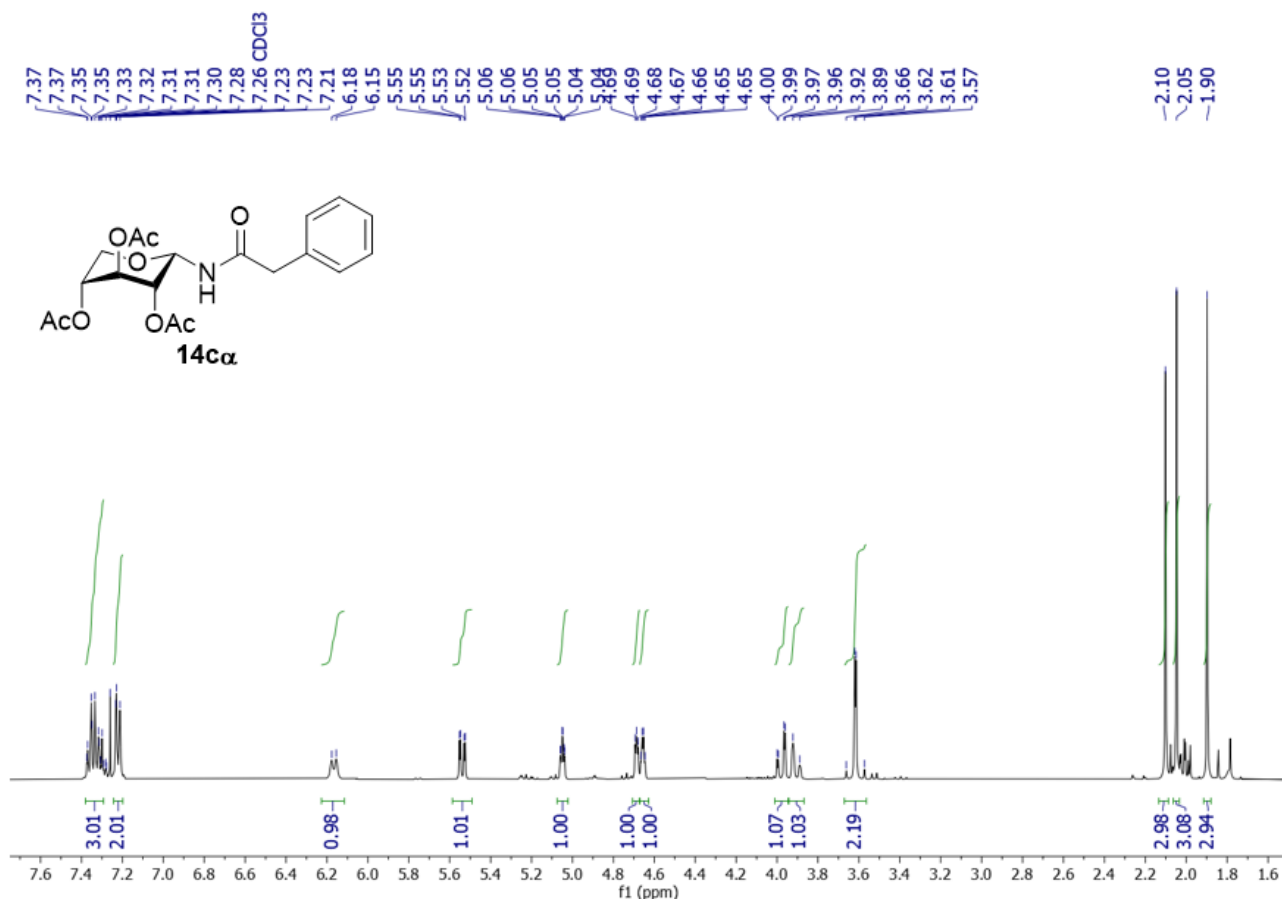
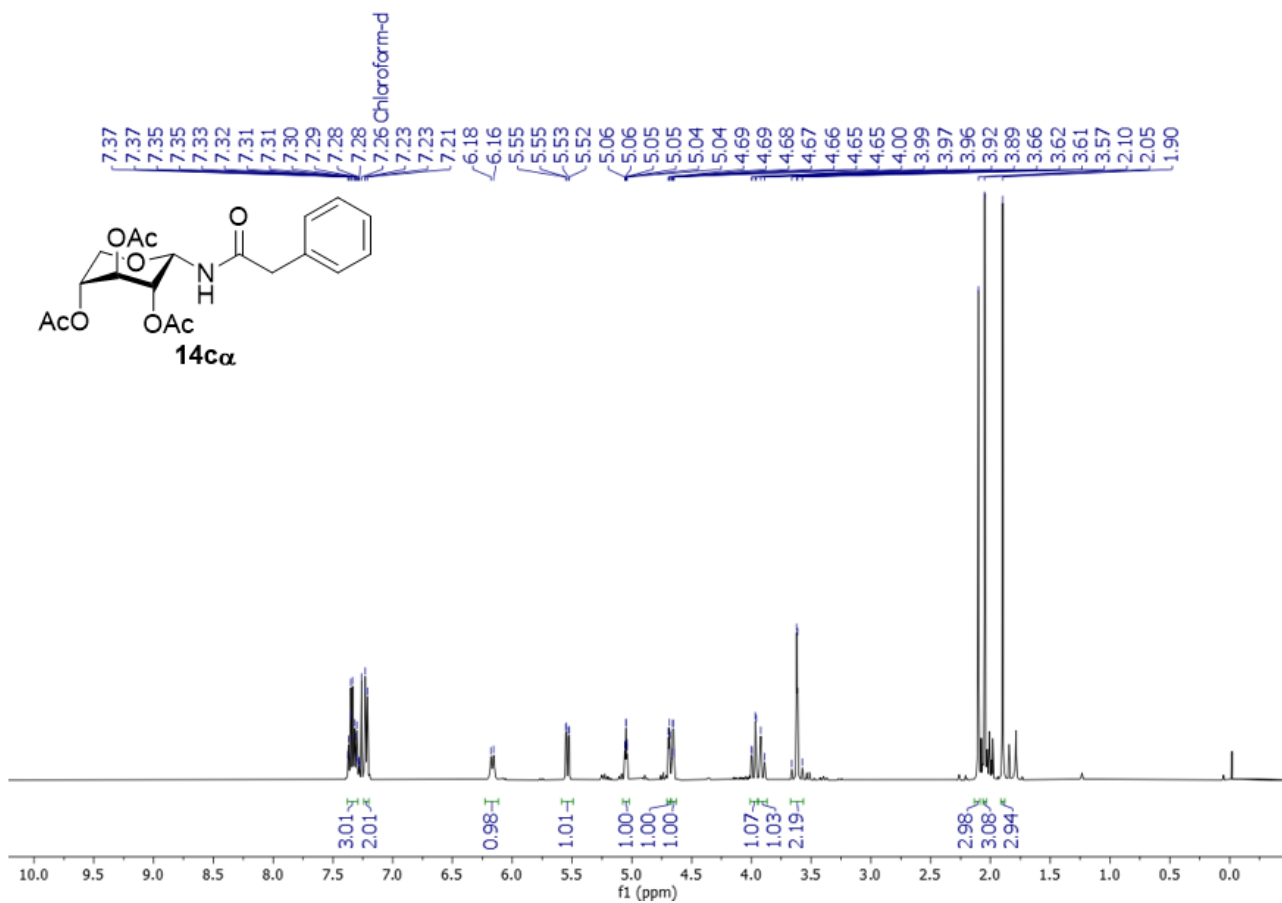


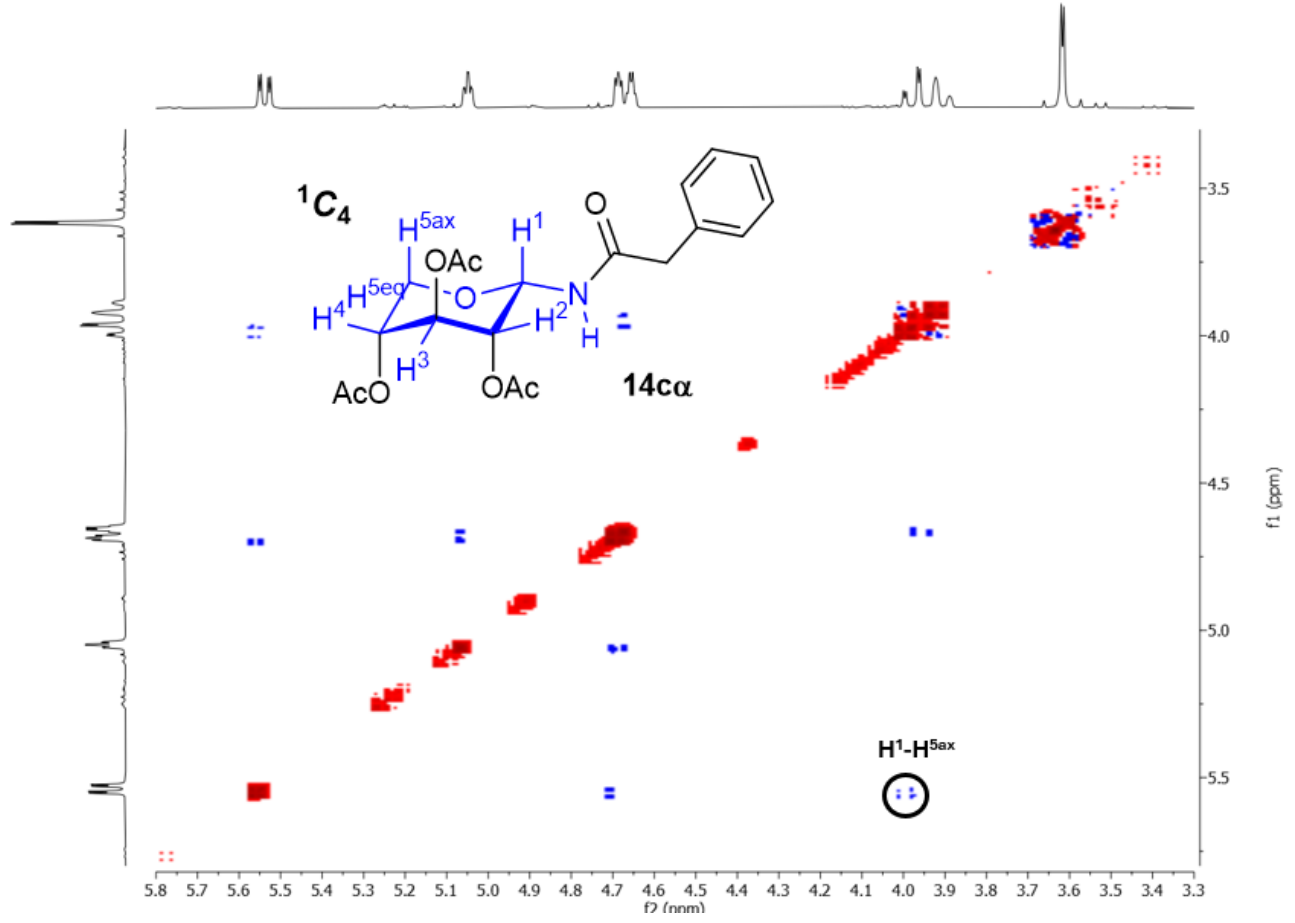
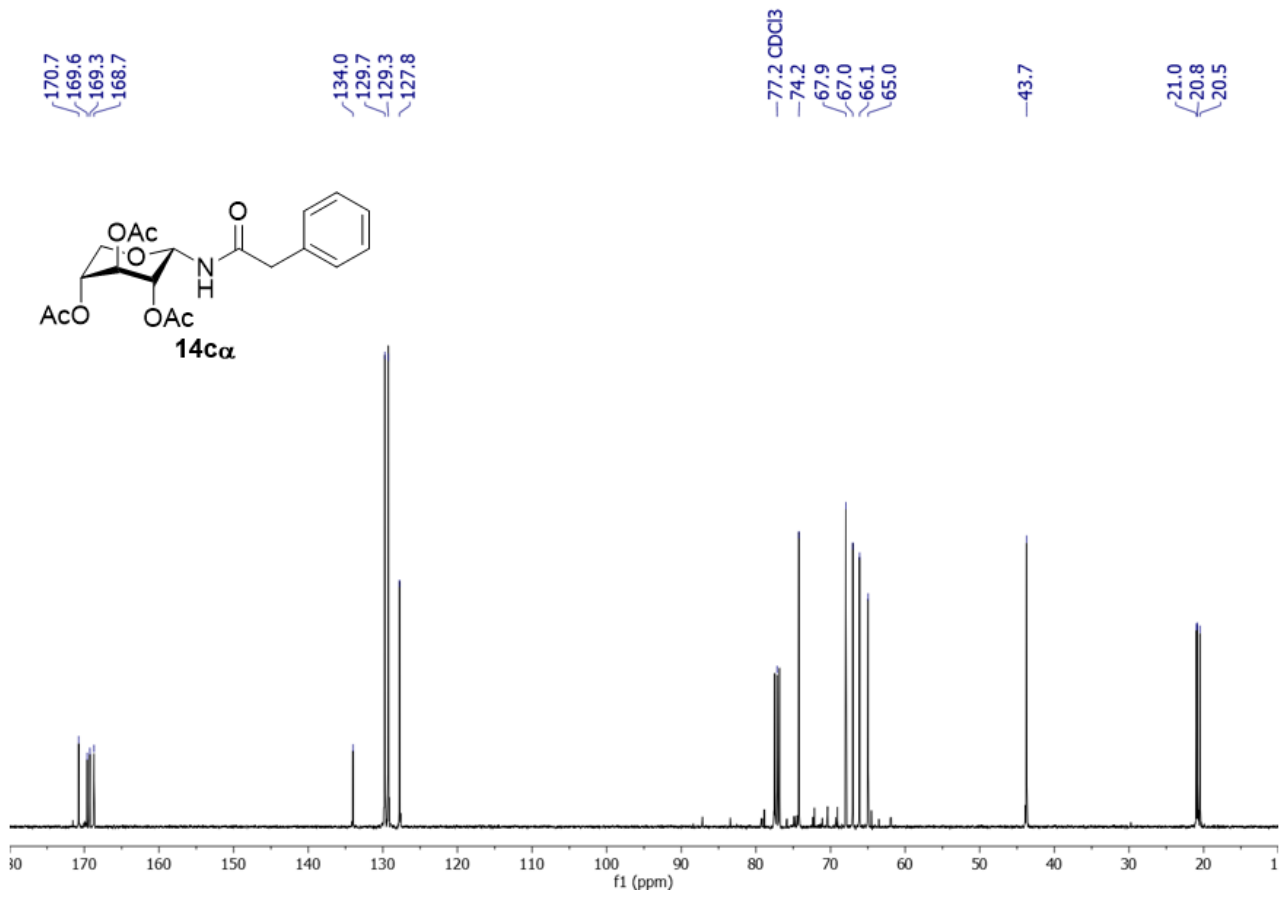


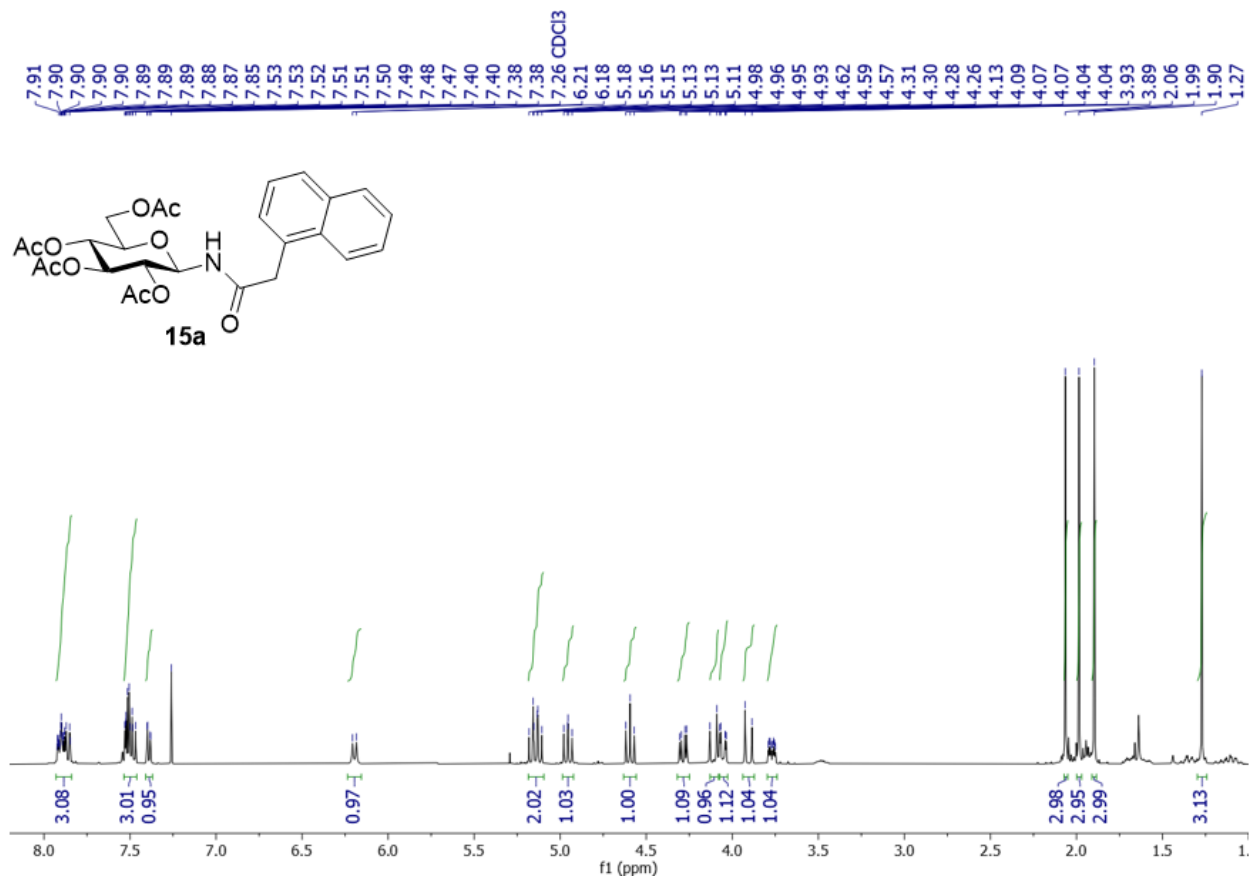
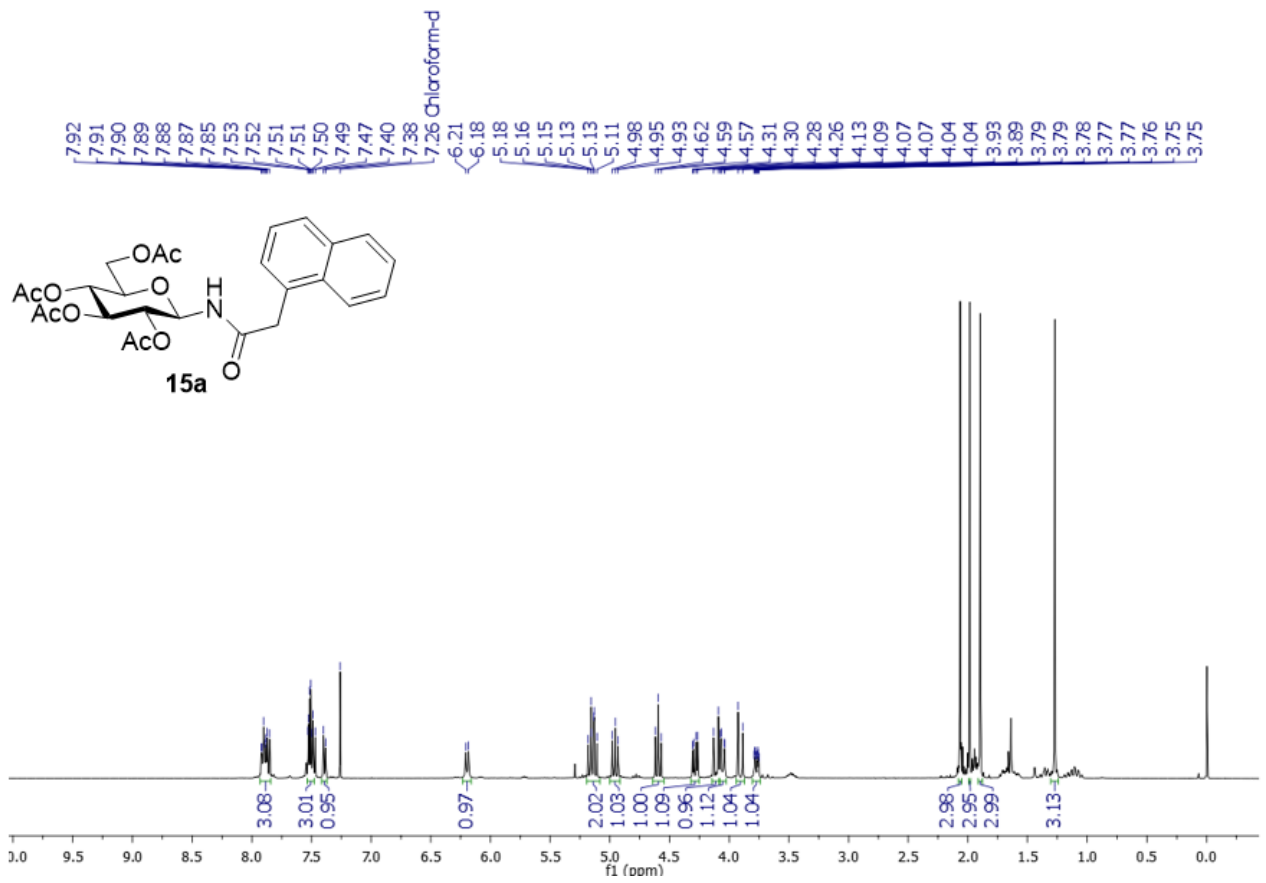


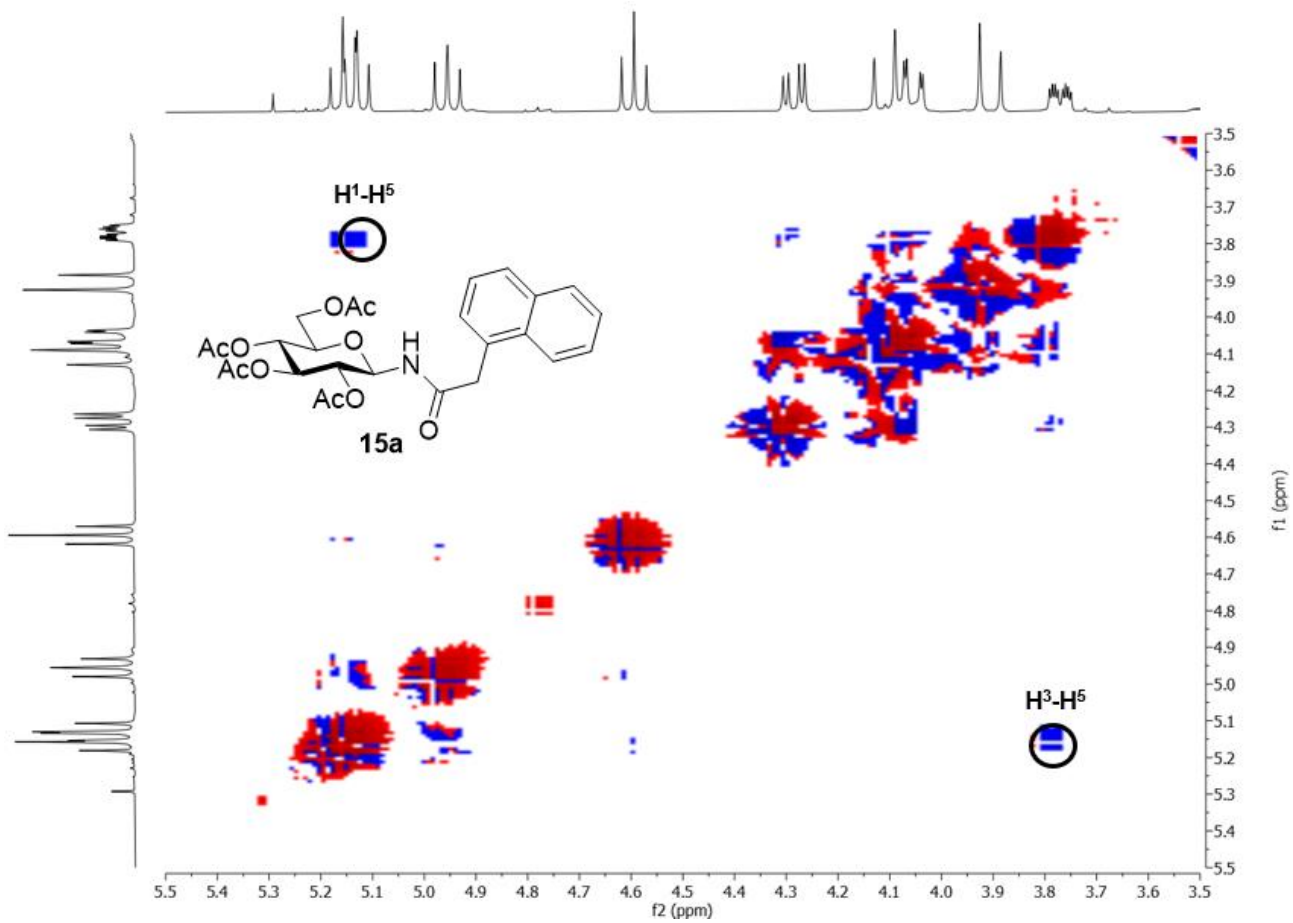
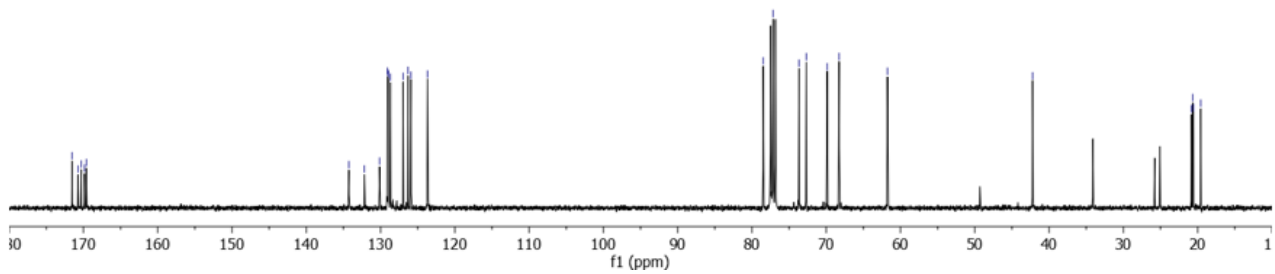


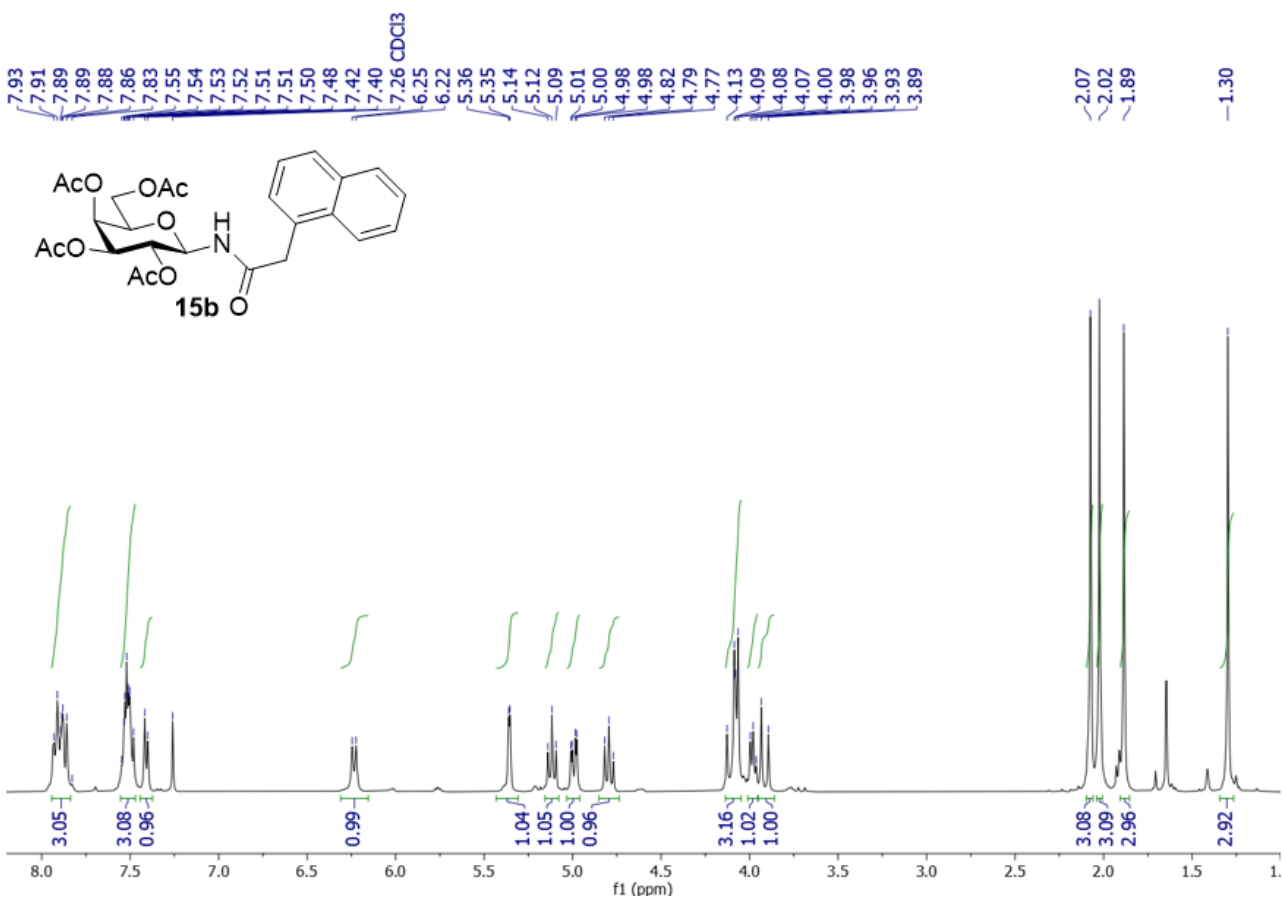
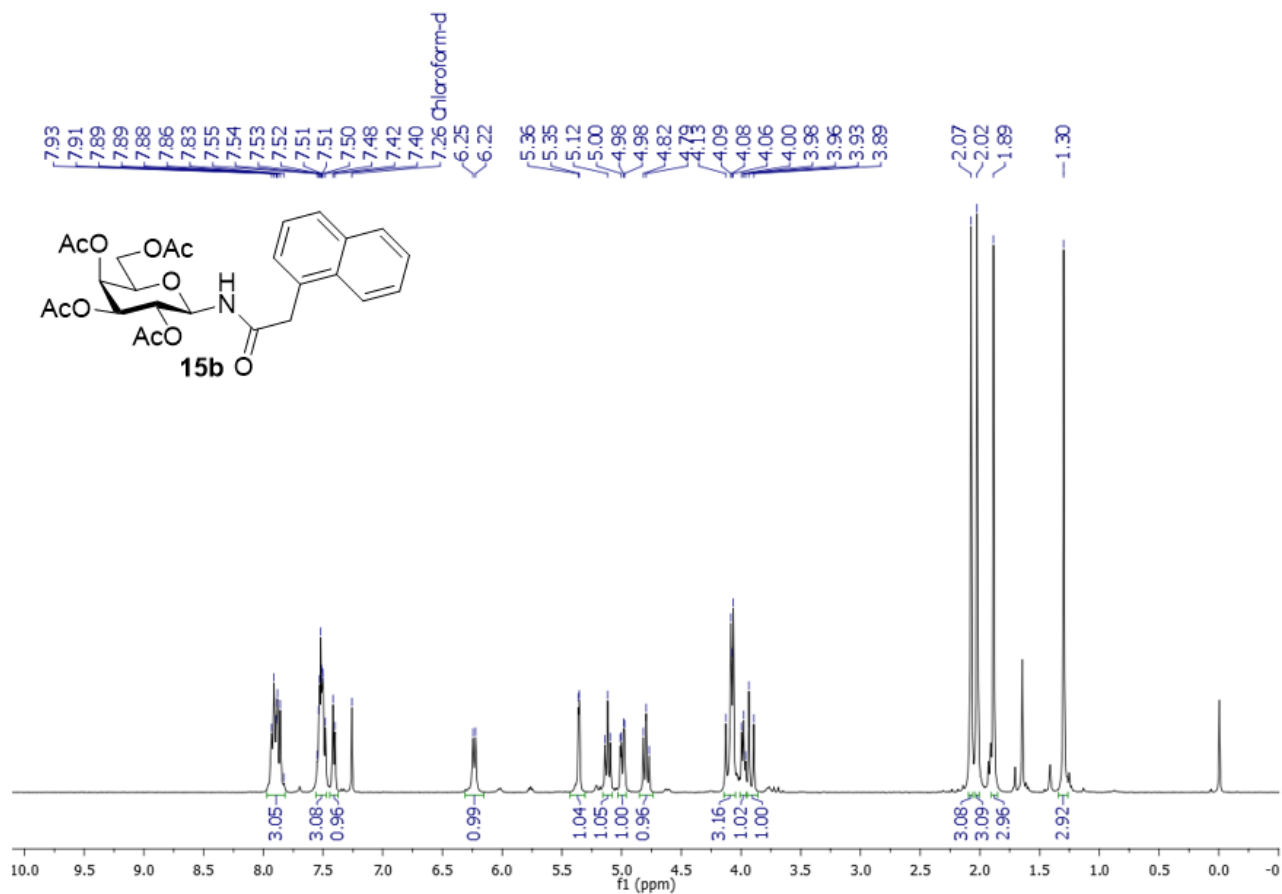




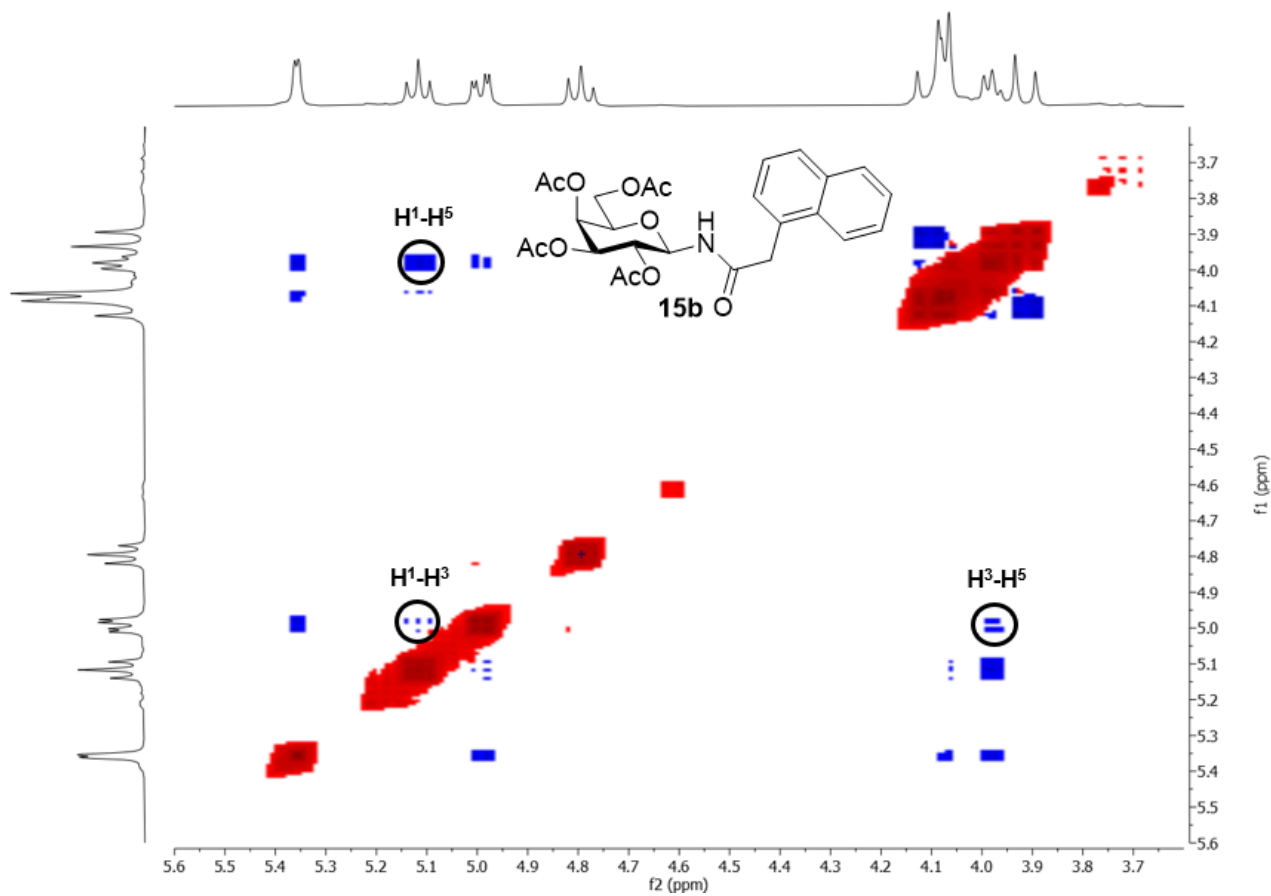
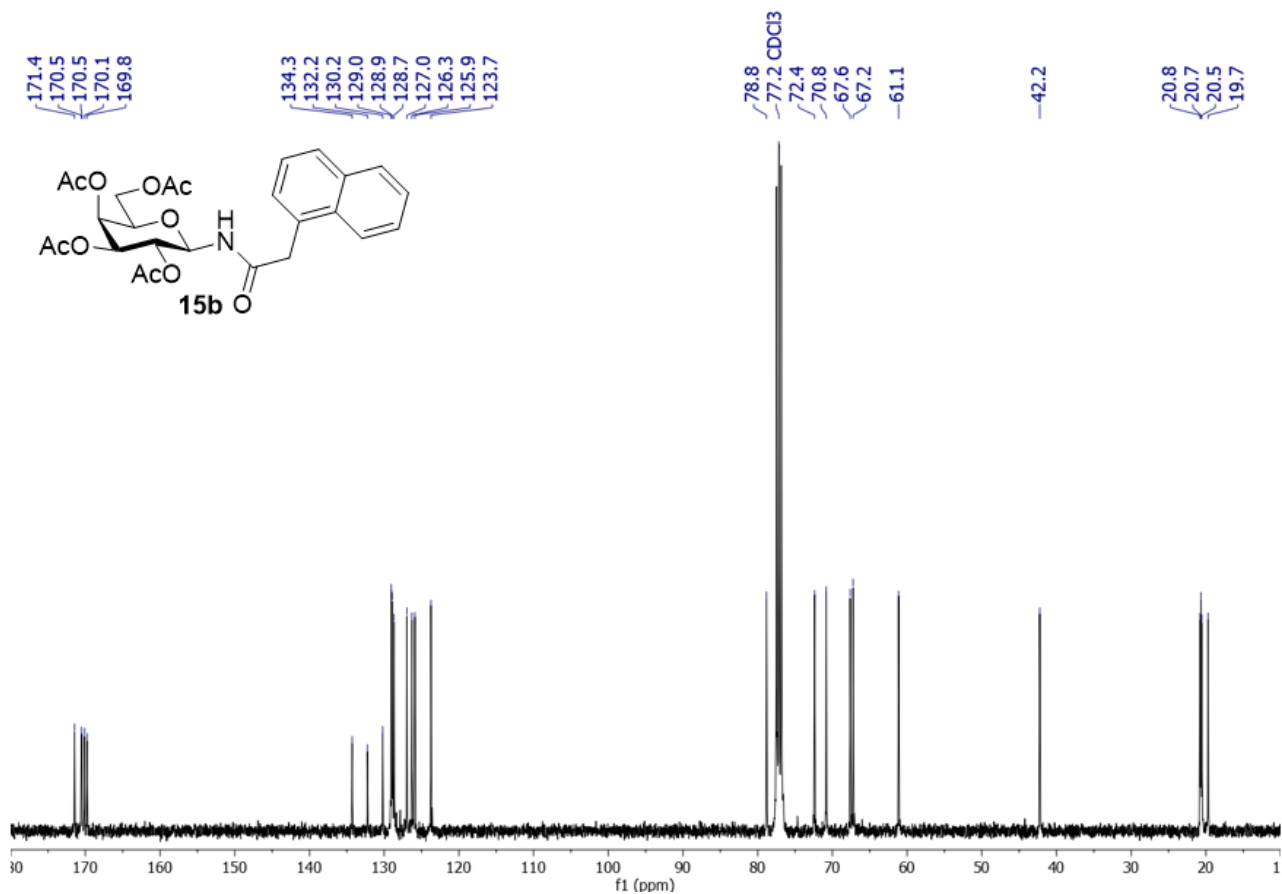


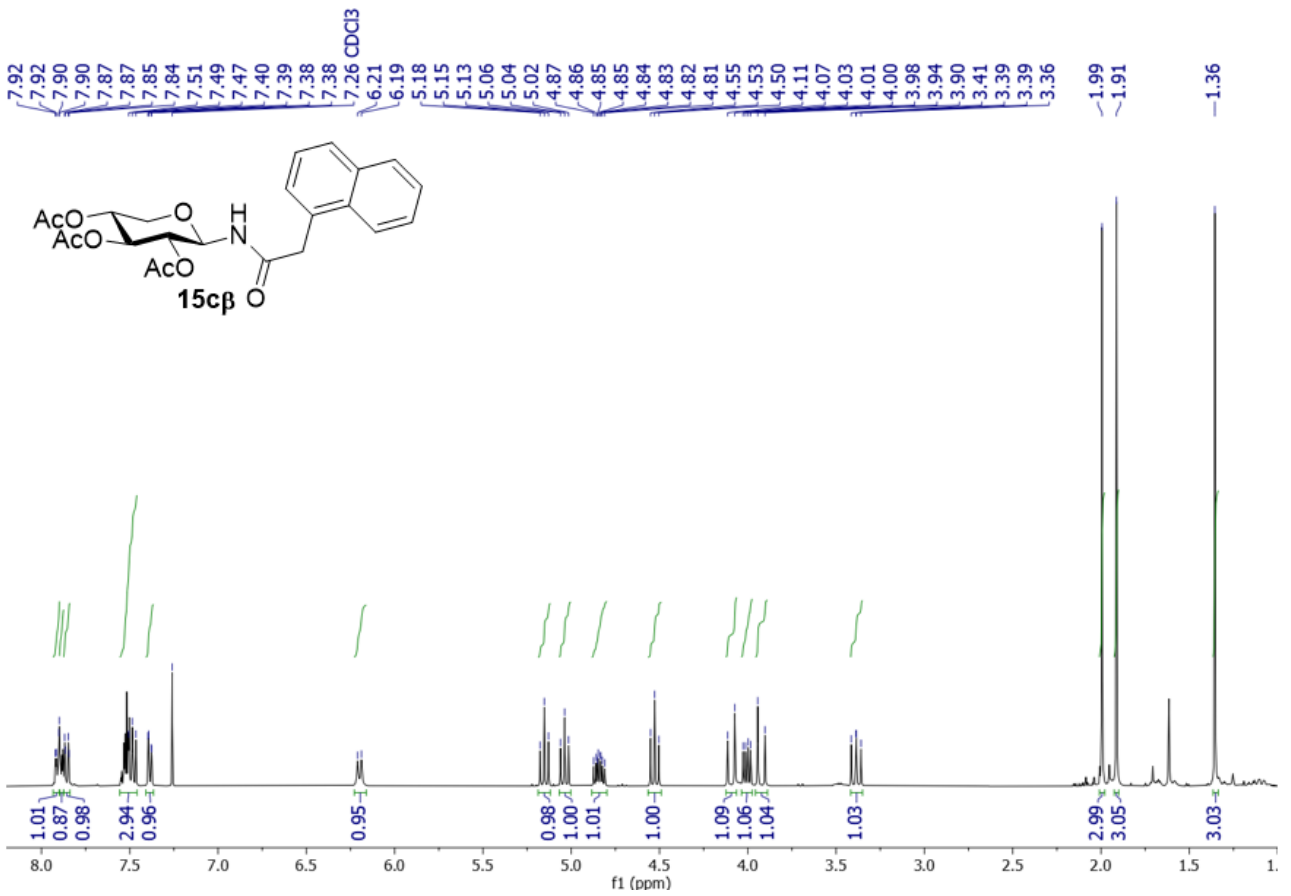
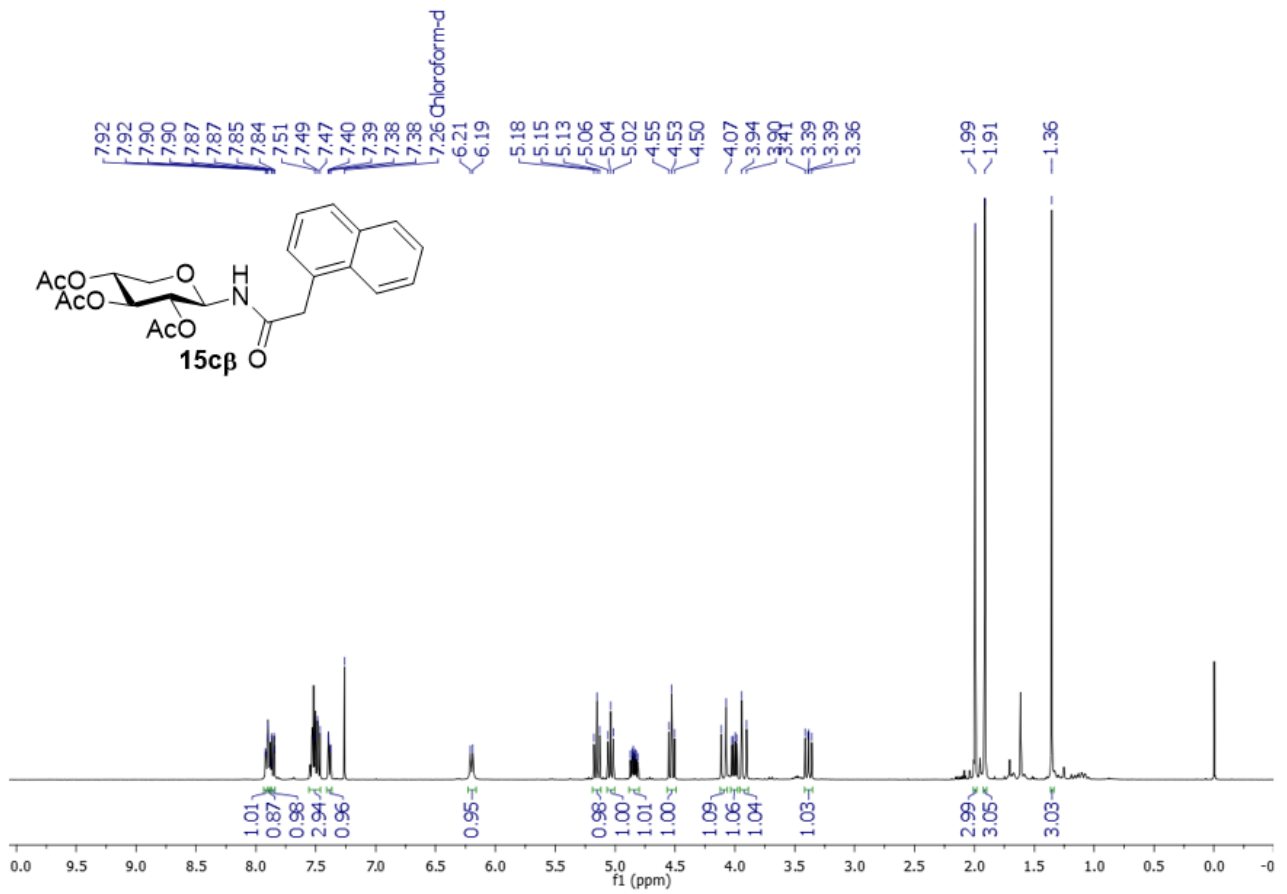


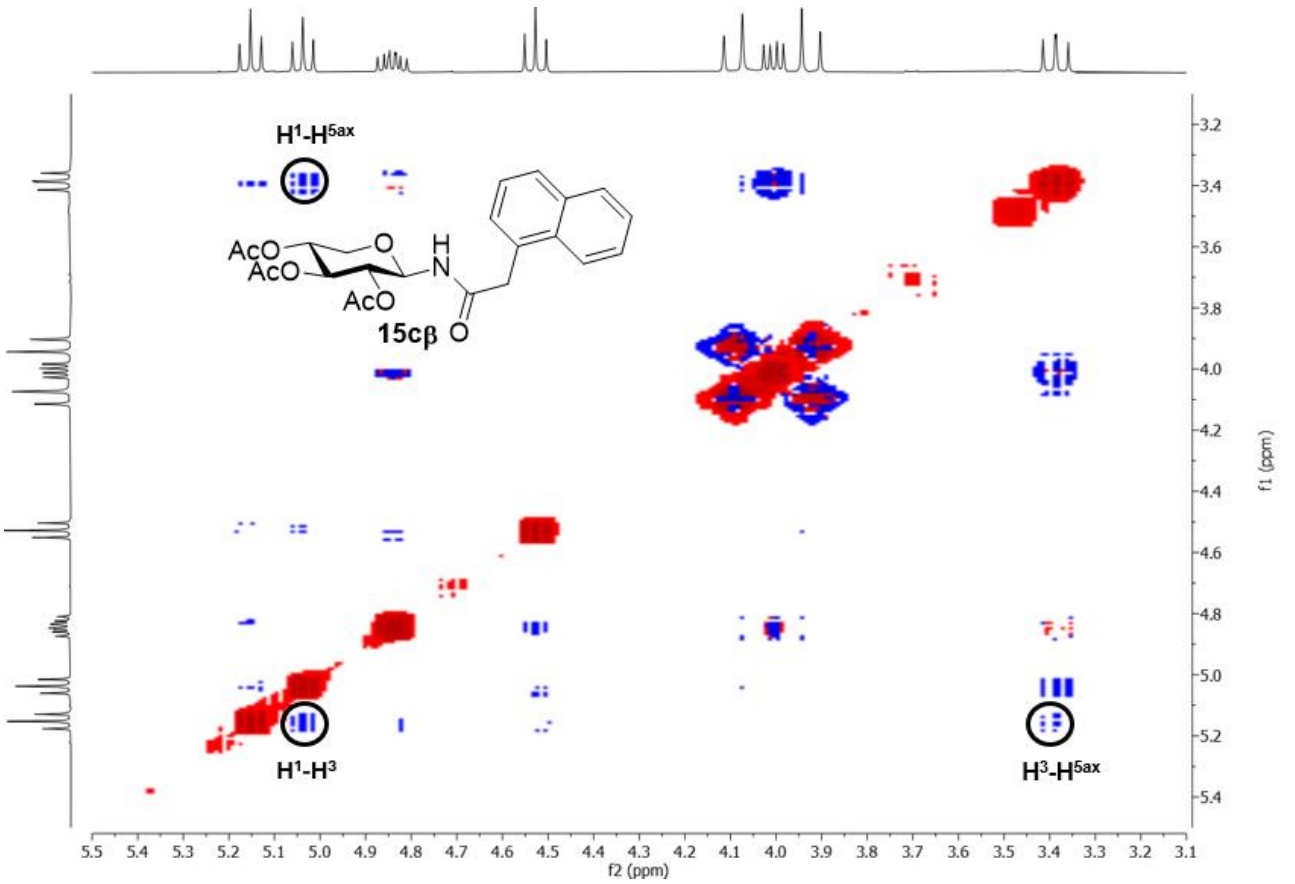
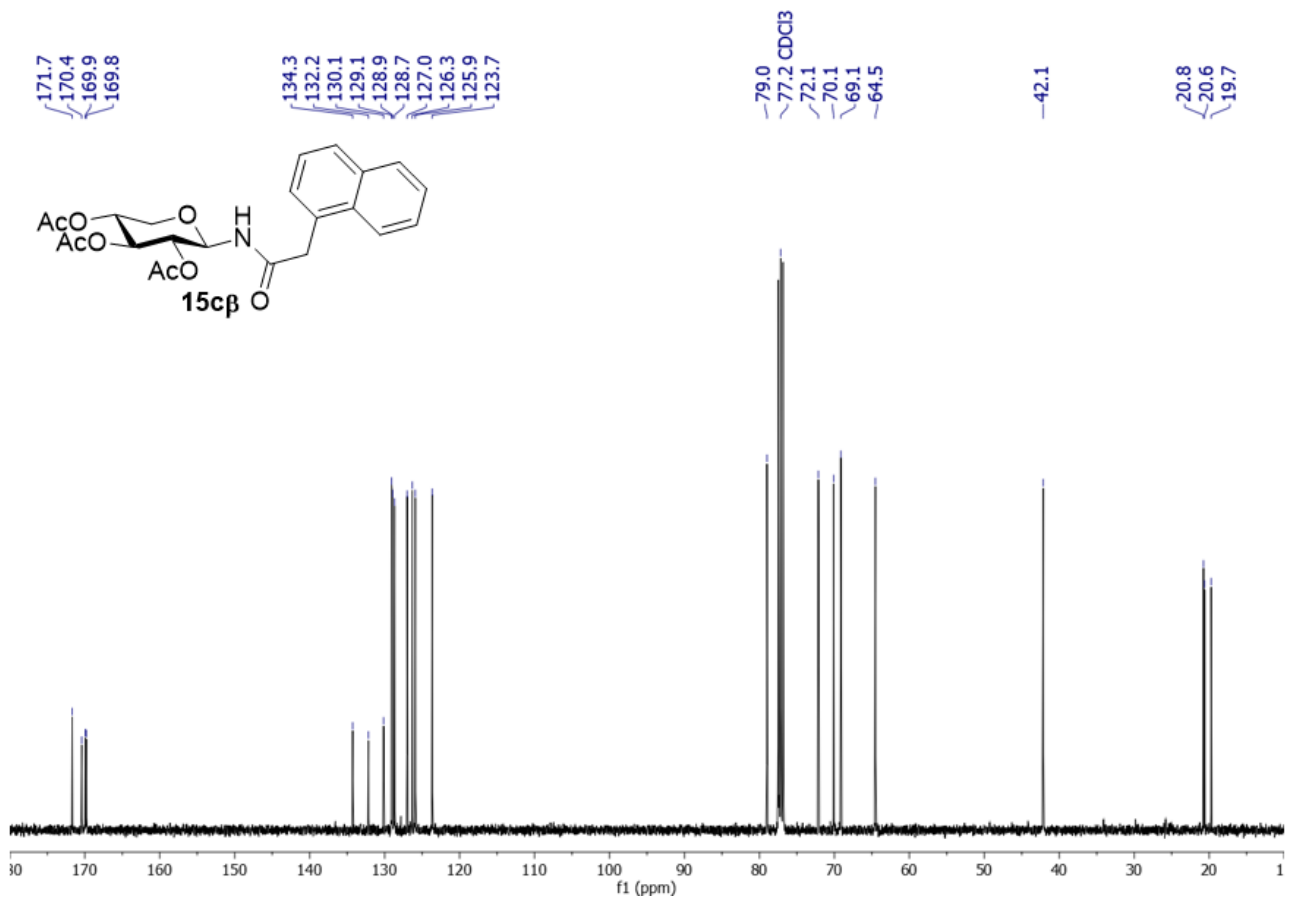


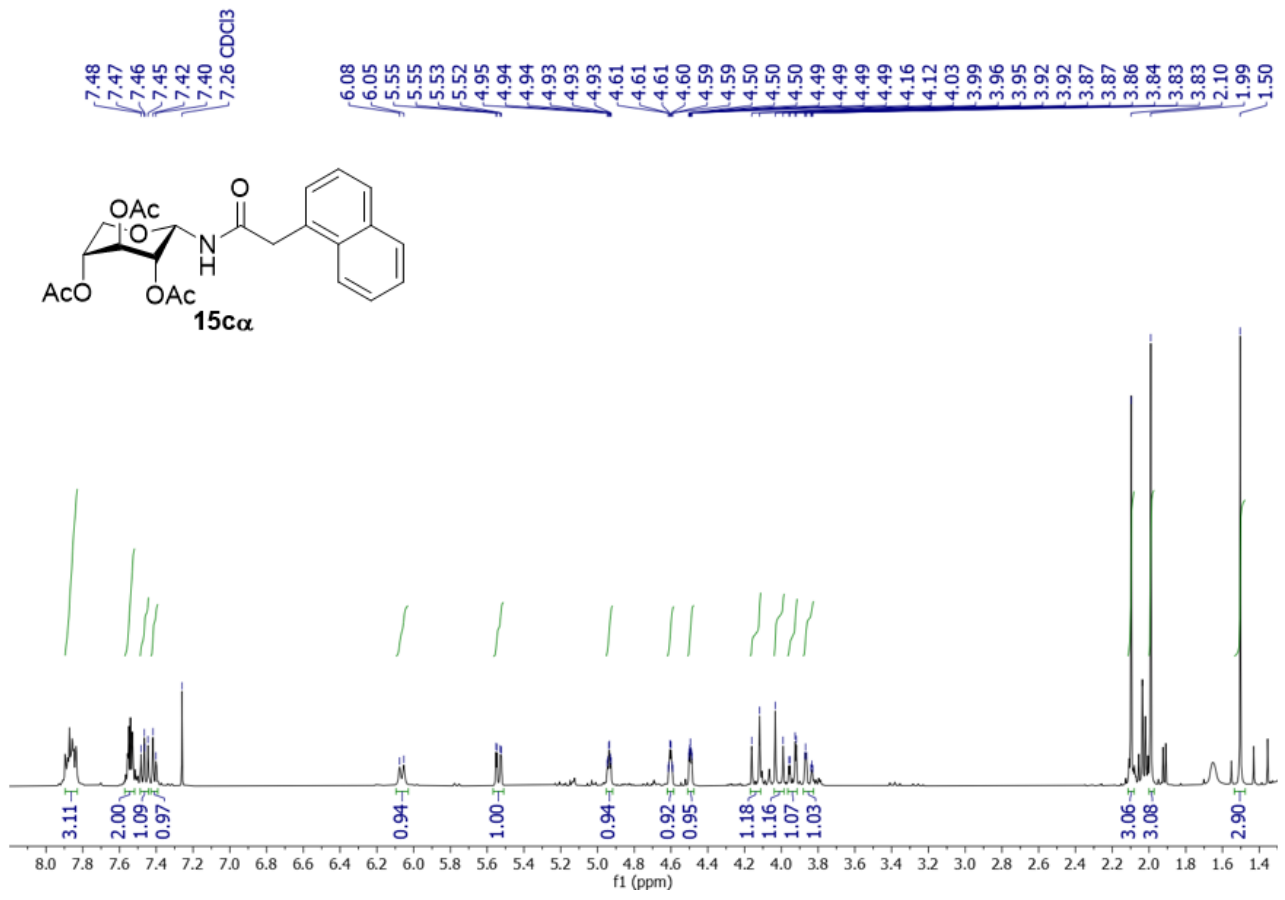
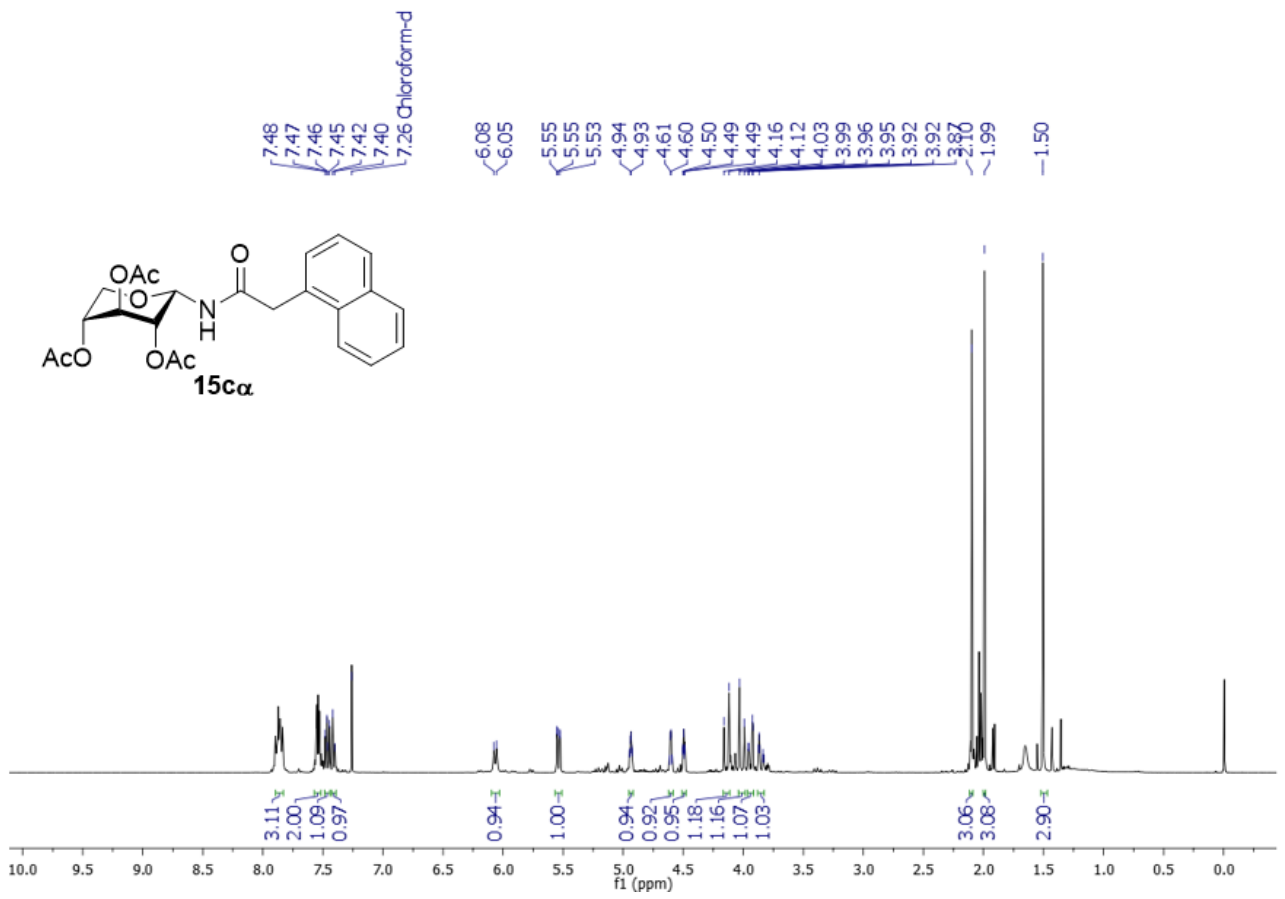












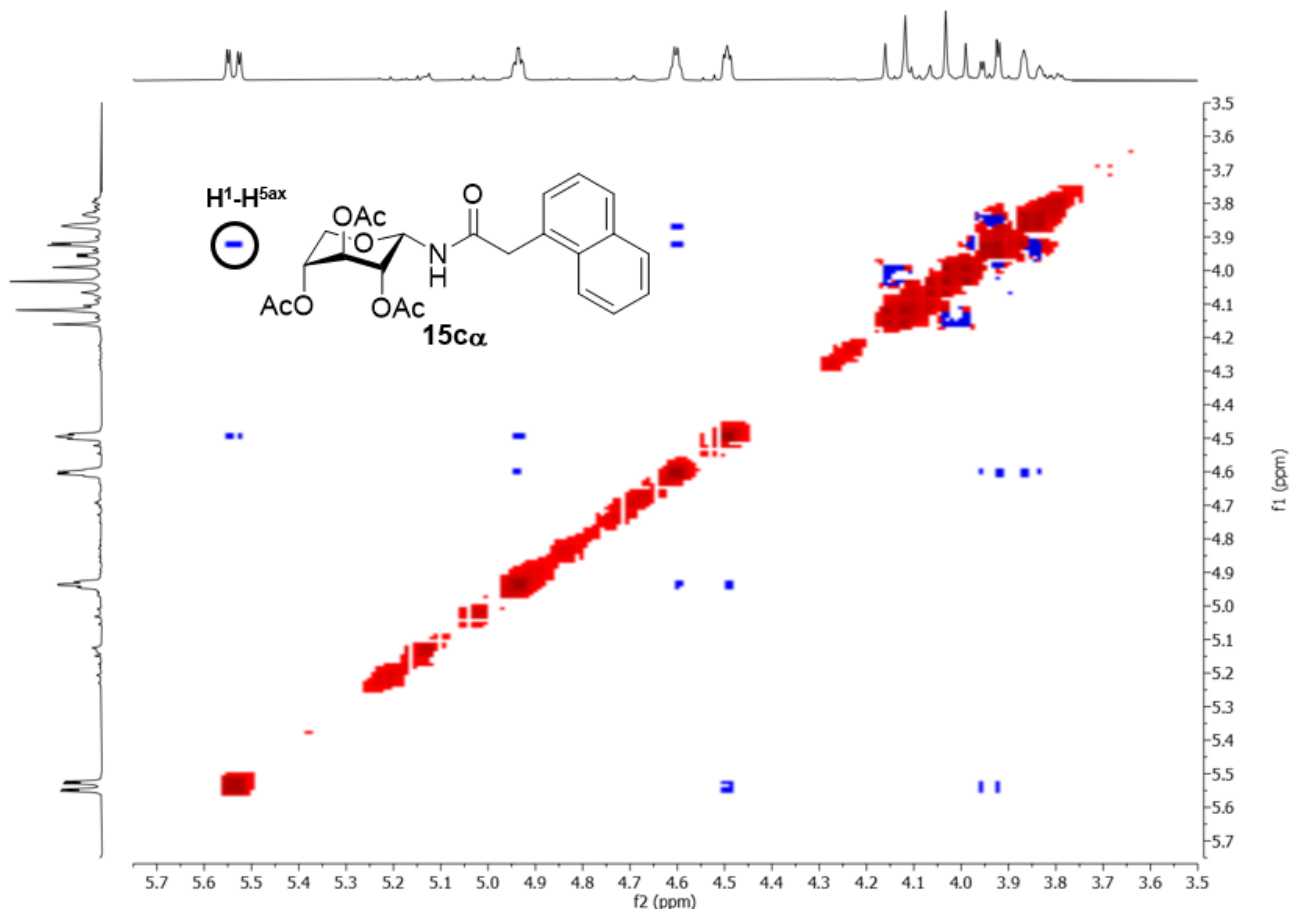
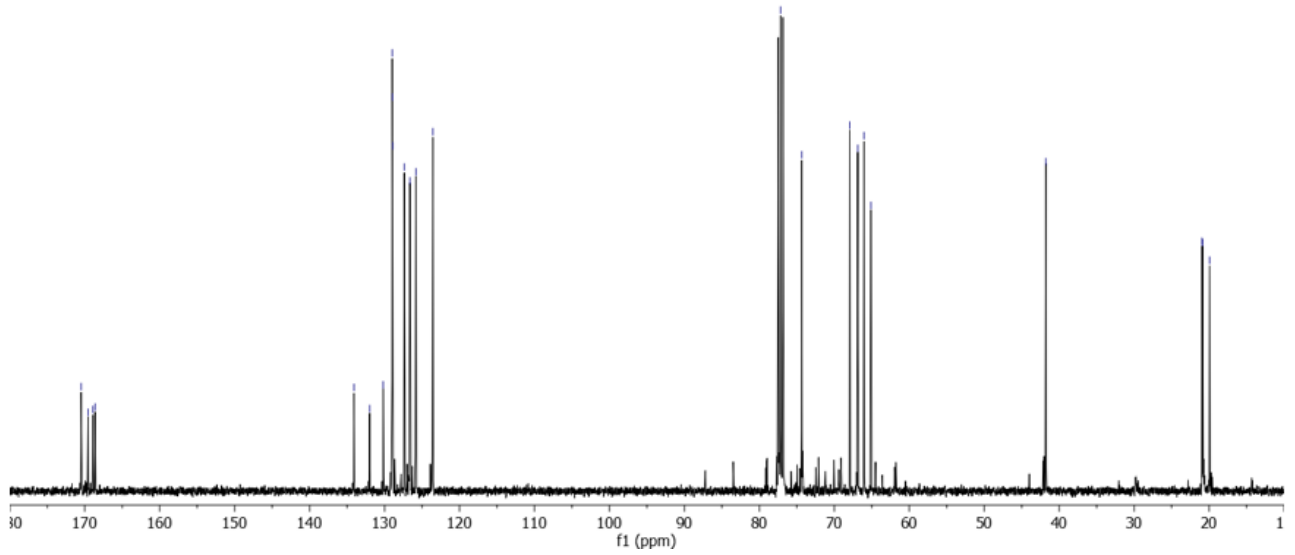
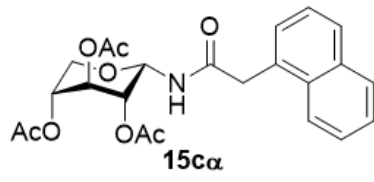
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168.6

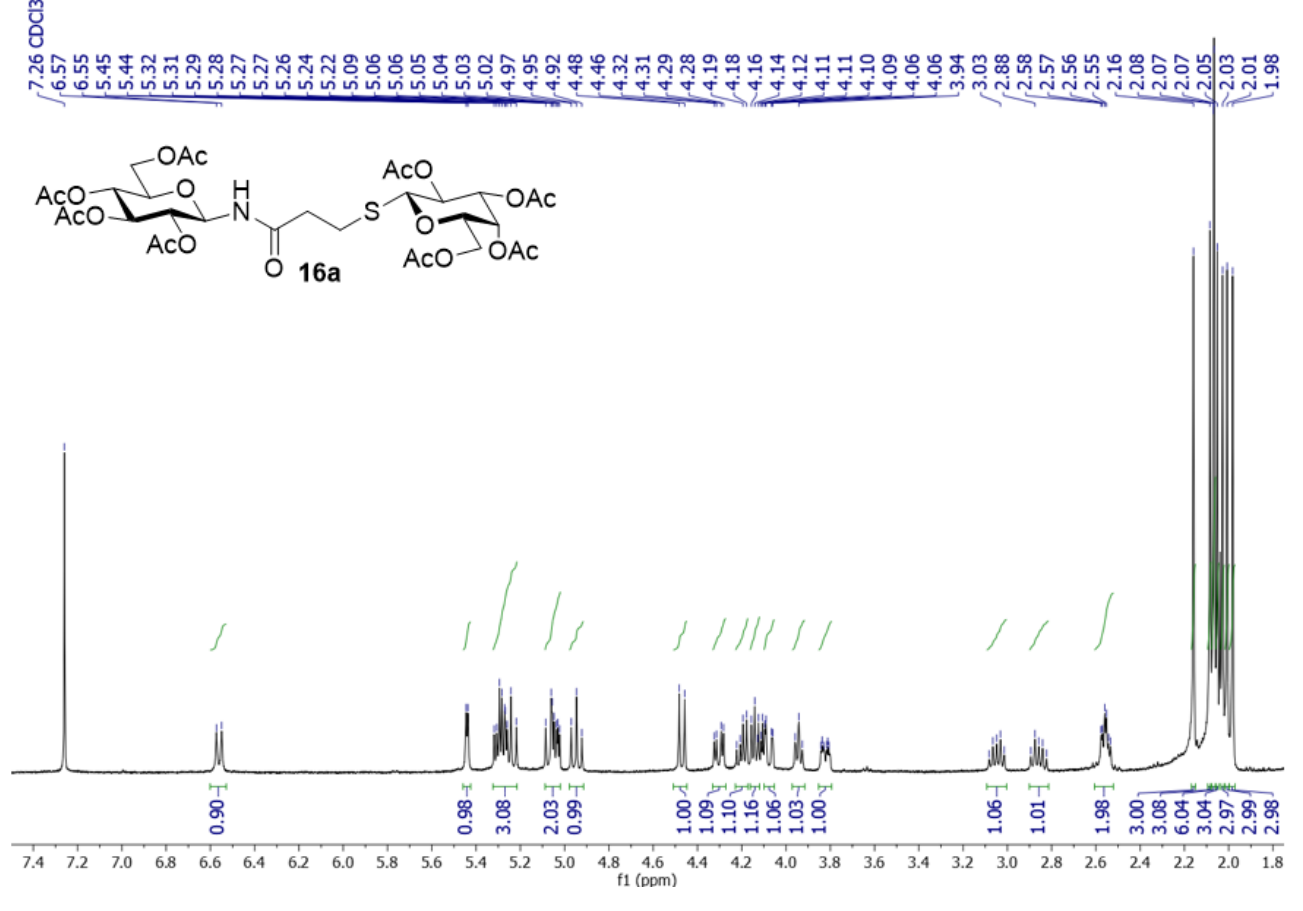
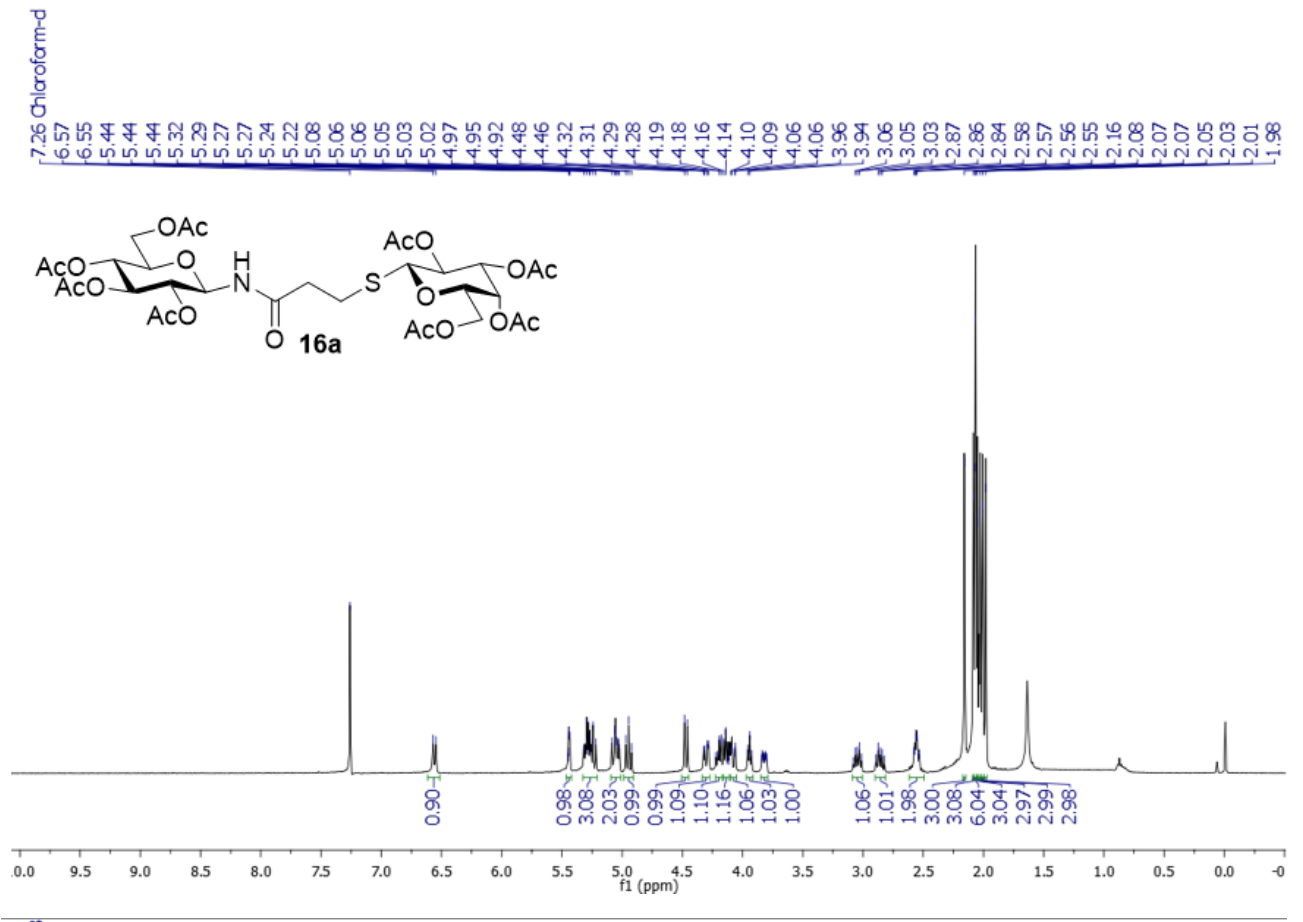
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129.0  
129.0  
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127.4  
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125.8  
123.5

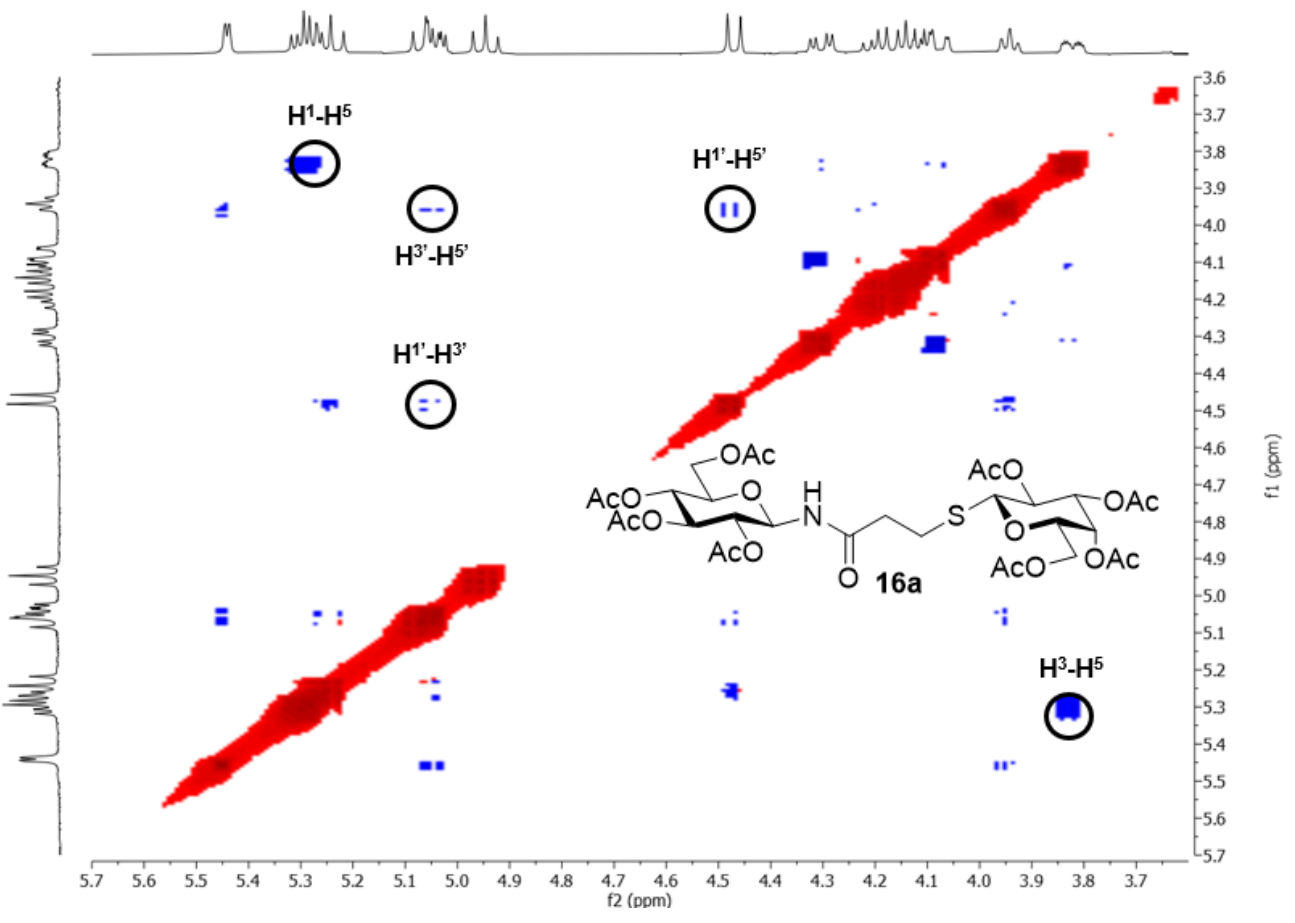
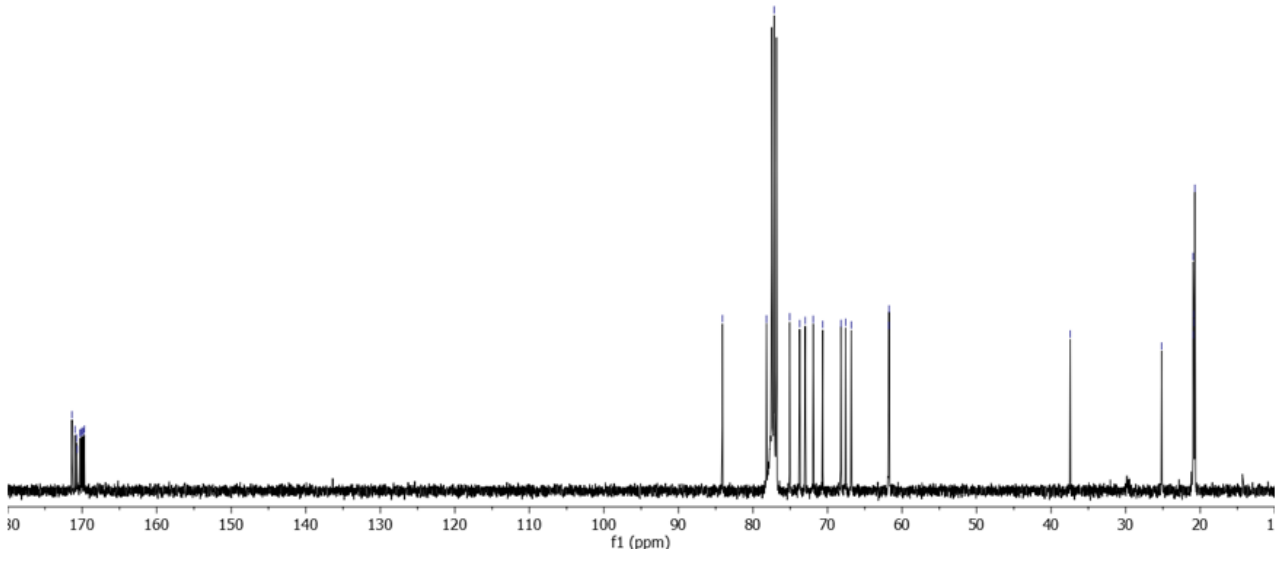
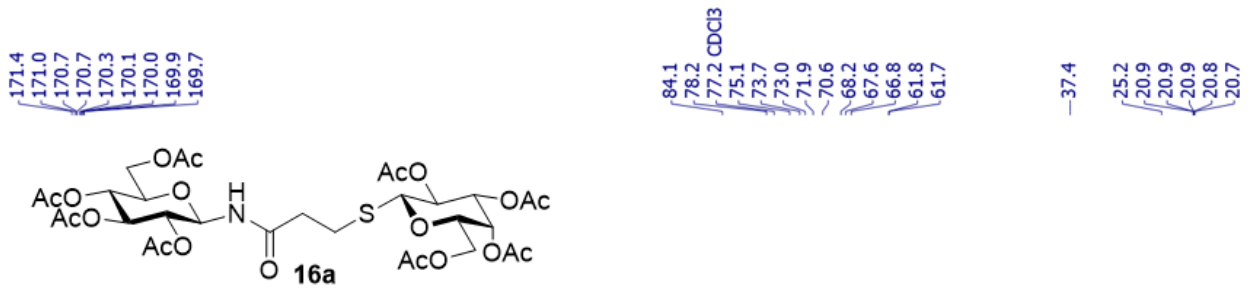
-77.2 CDCl3  
-74.3  
-67.9  
-66.9  
-66.0  
-65.1

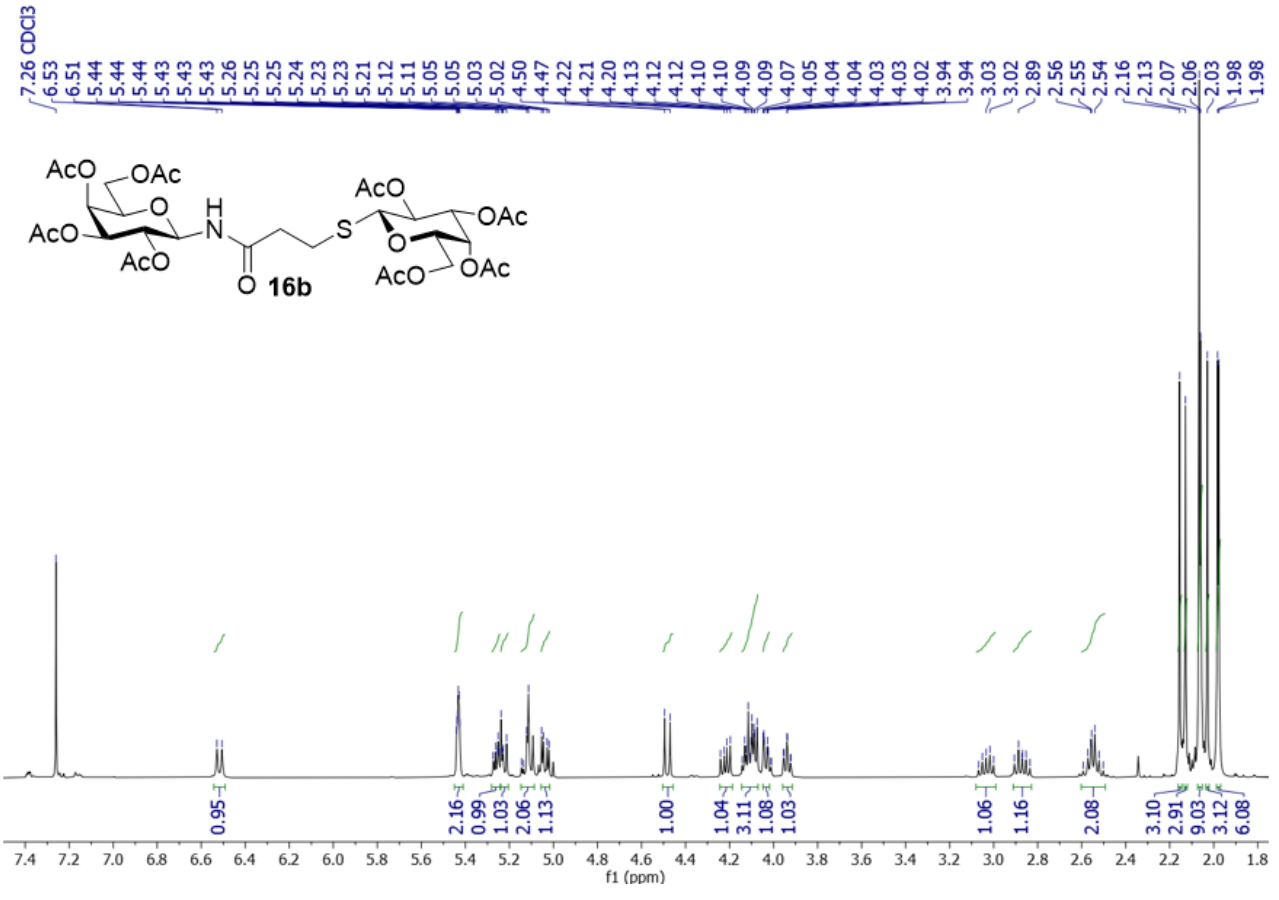
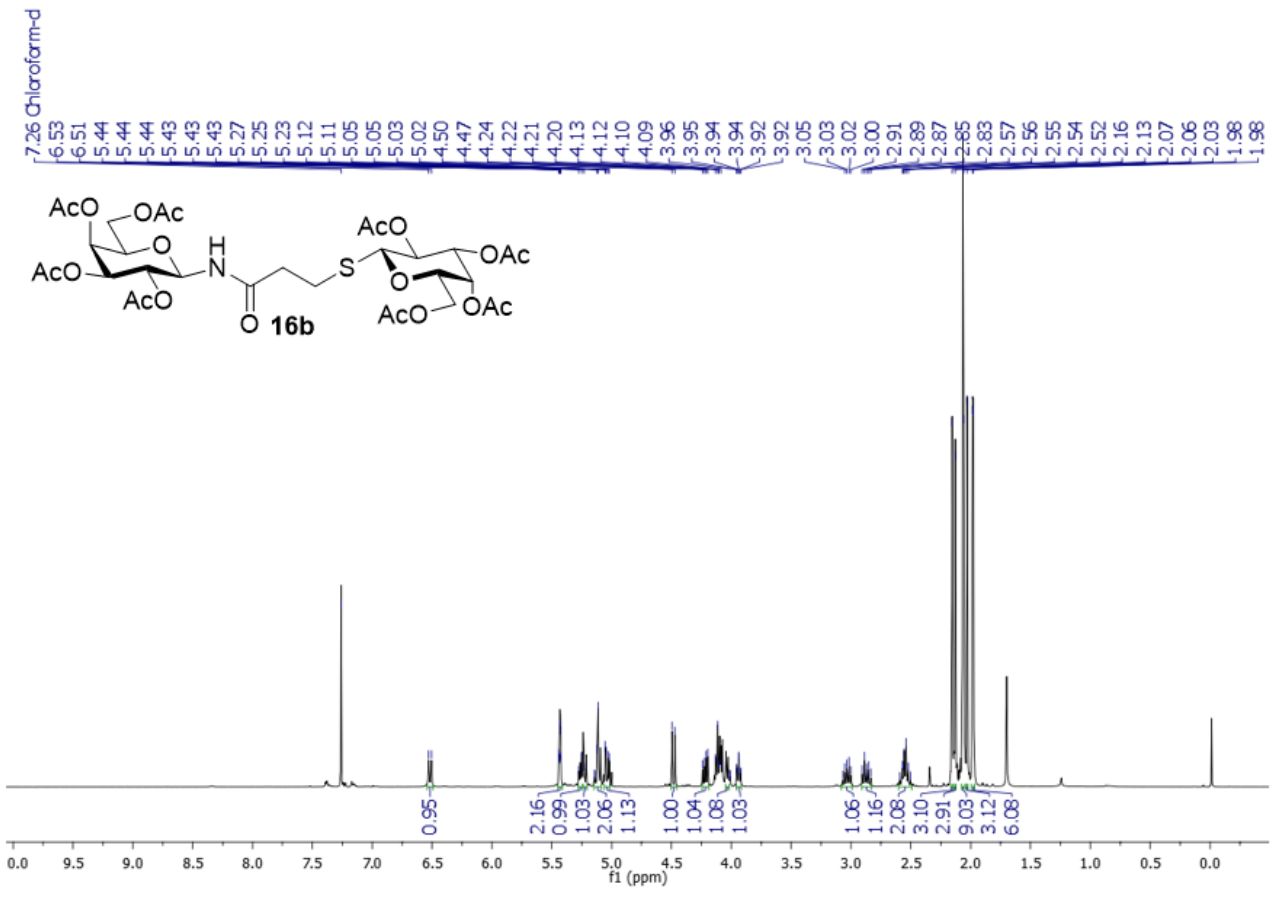
-41.8

21.0  
20.9  
19.9







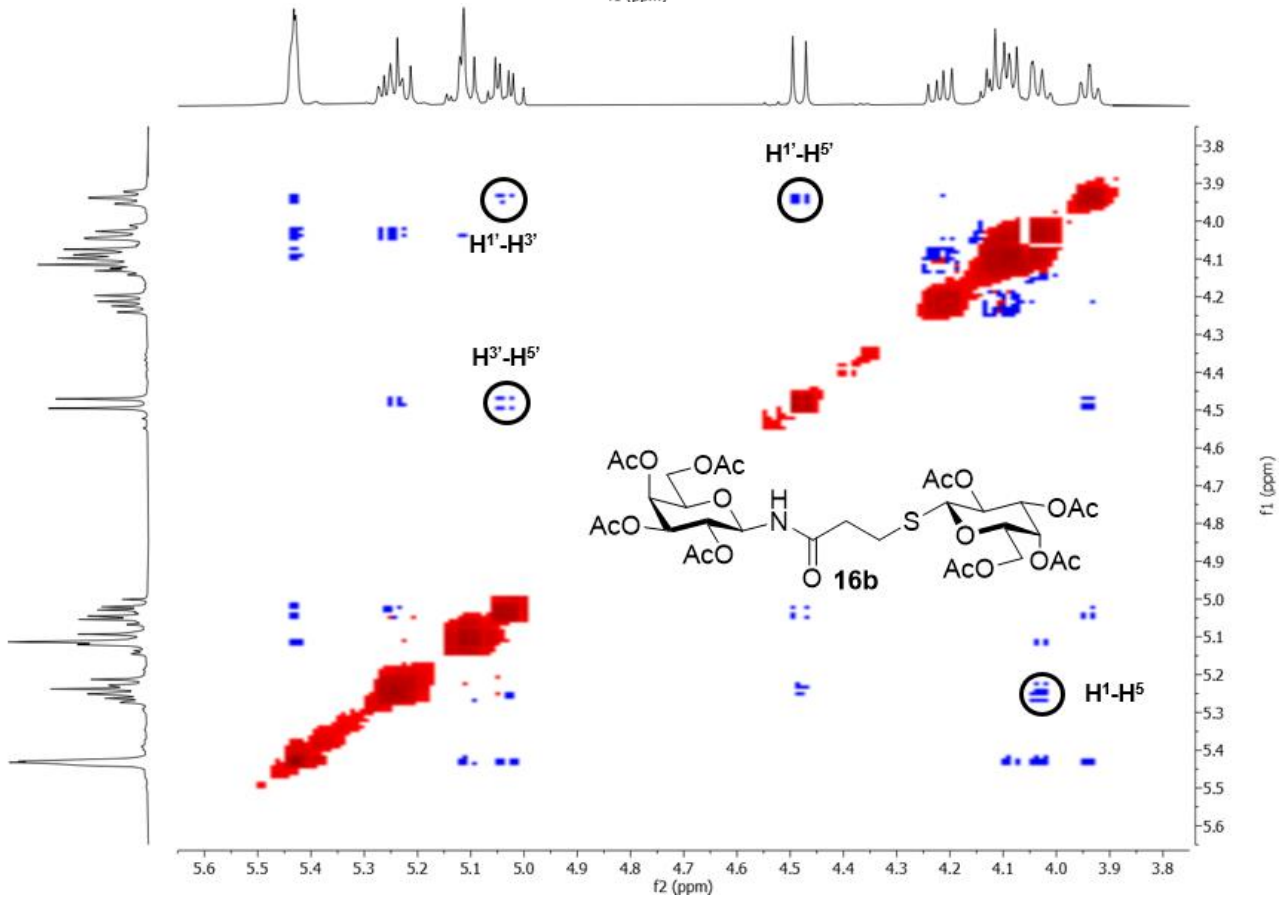
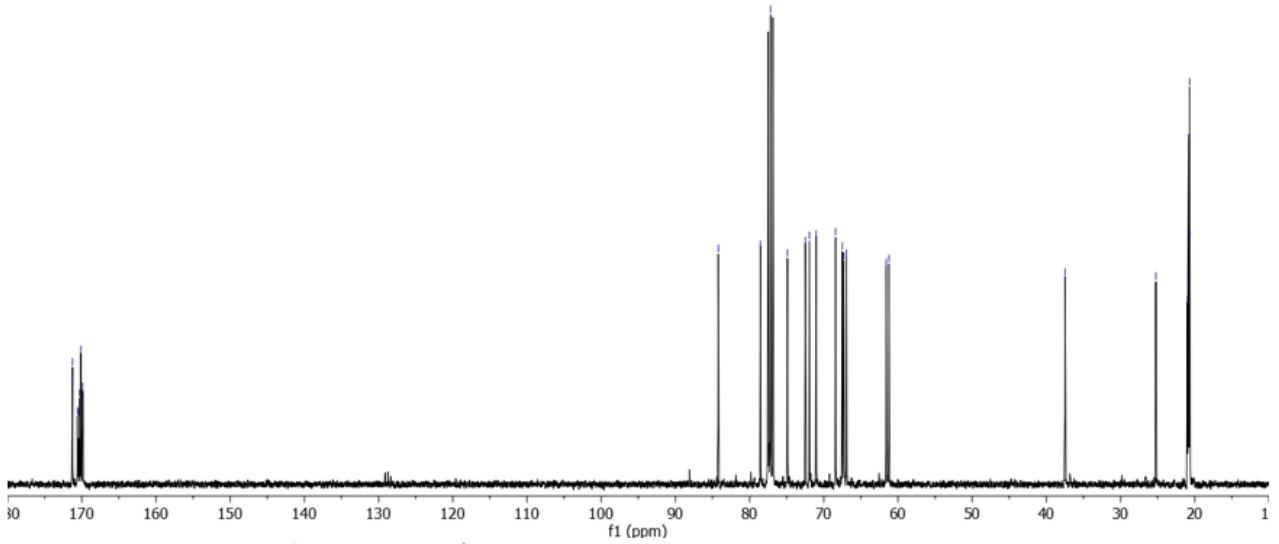
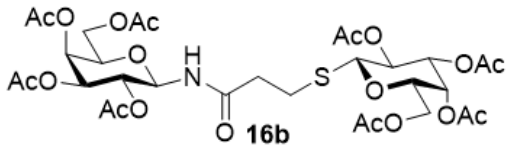


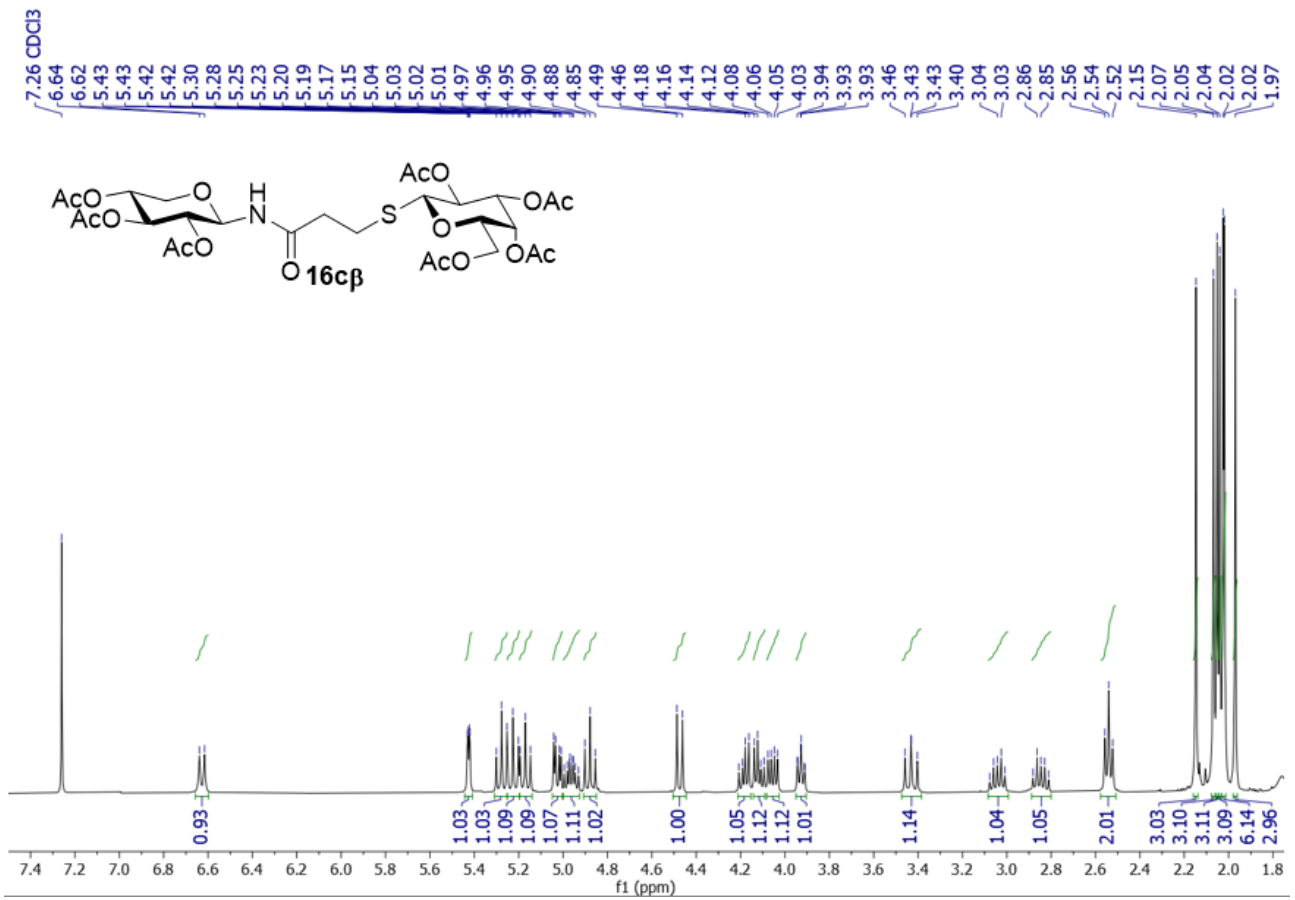
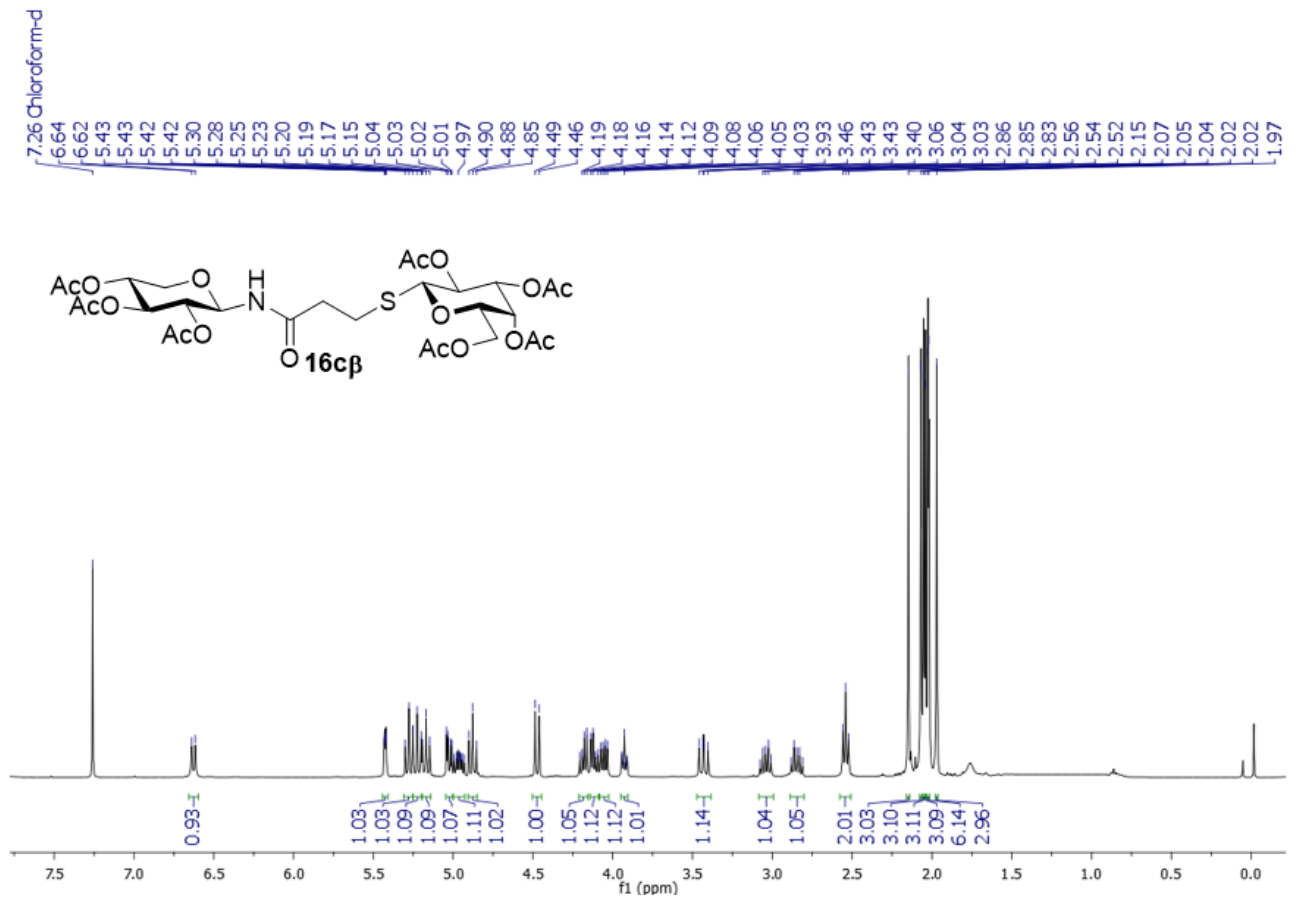


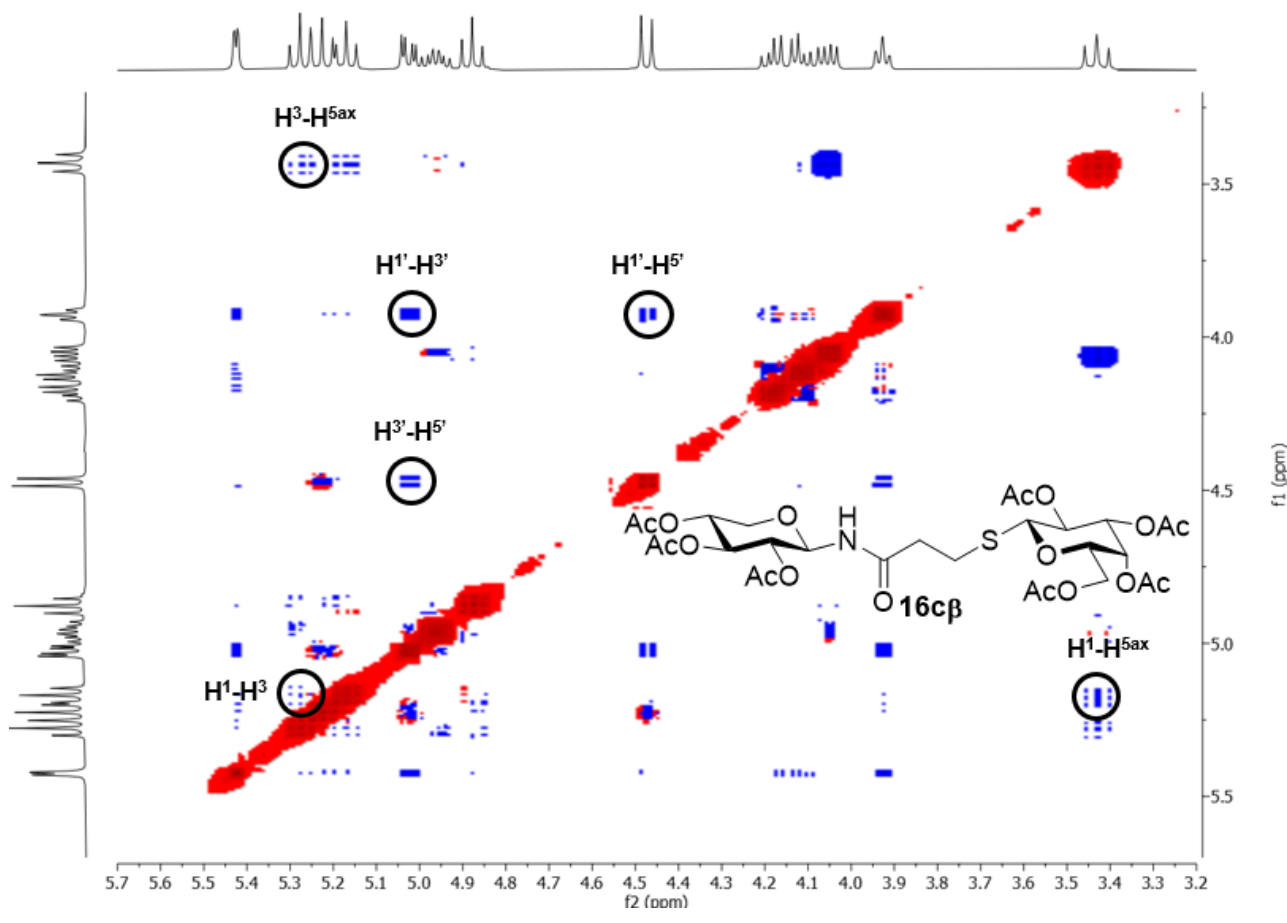
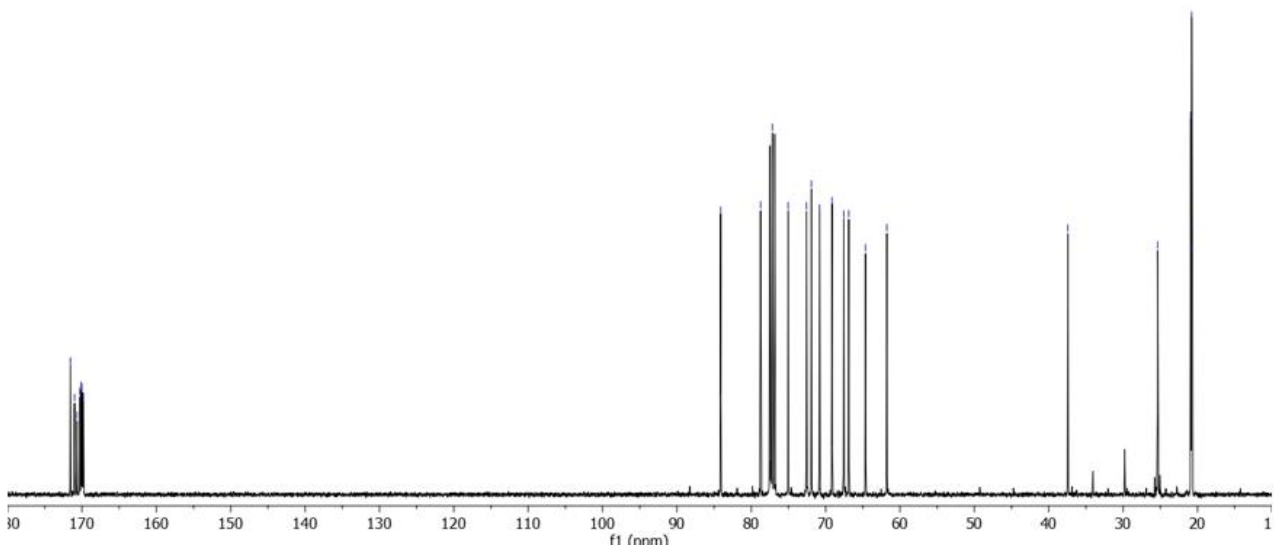
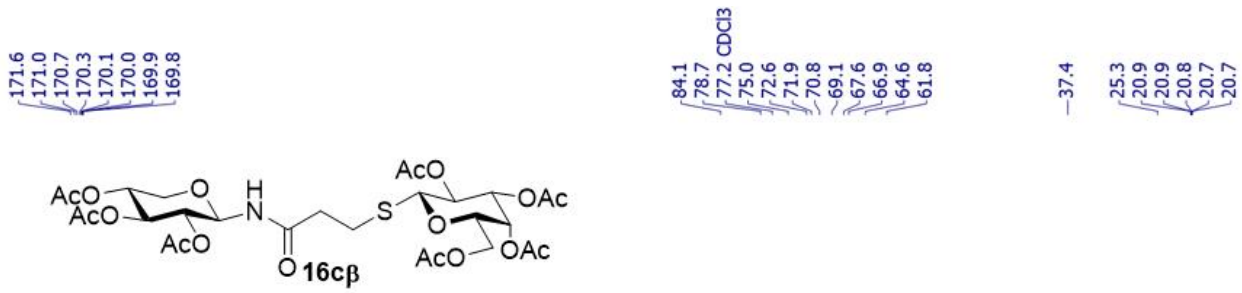
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170.3  
170.1  
169.9  
169.8

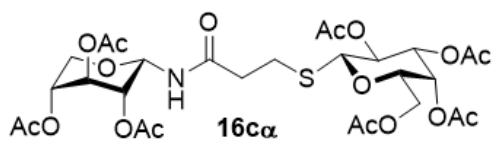
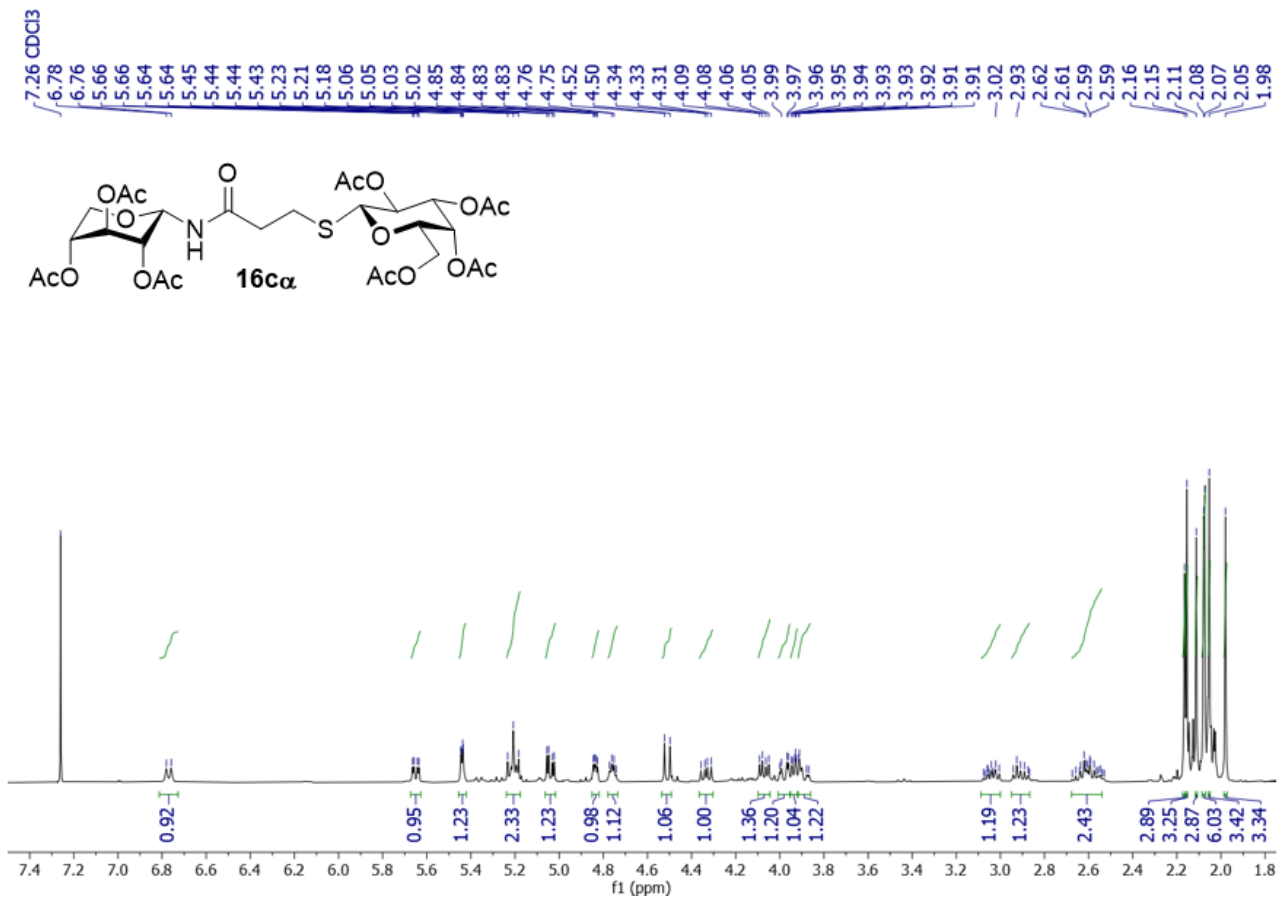
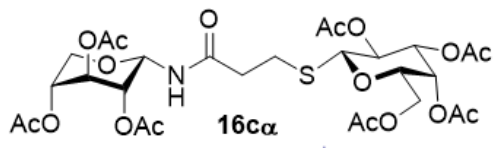
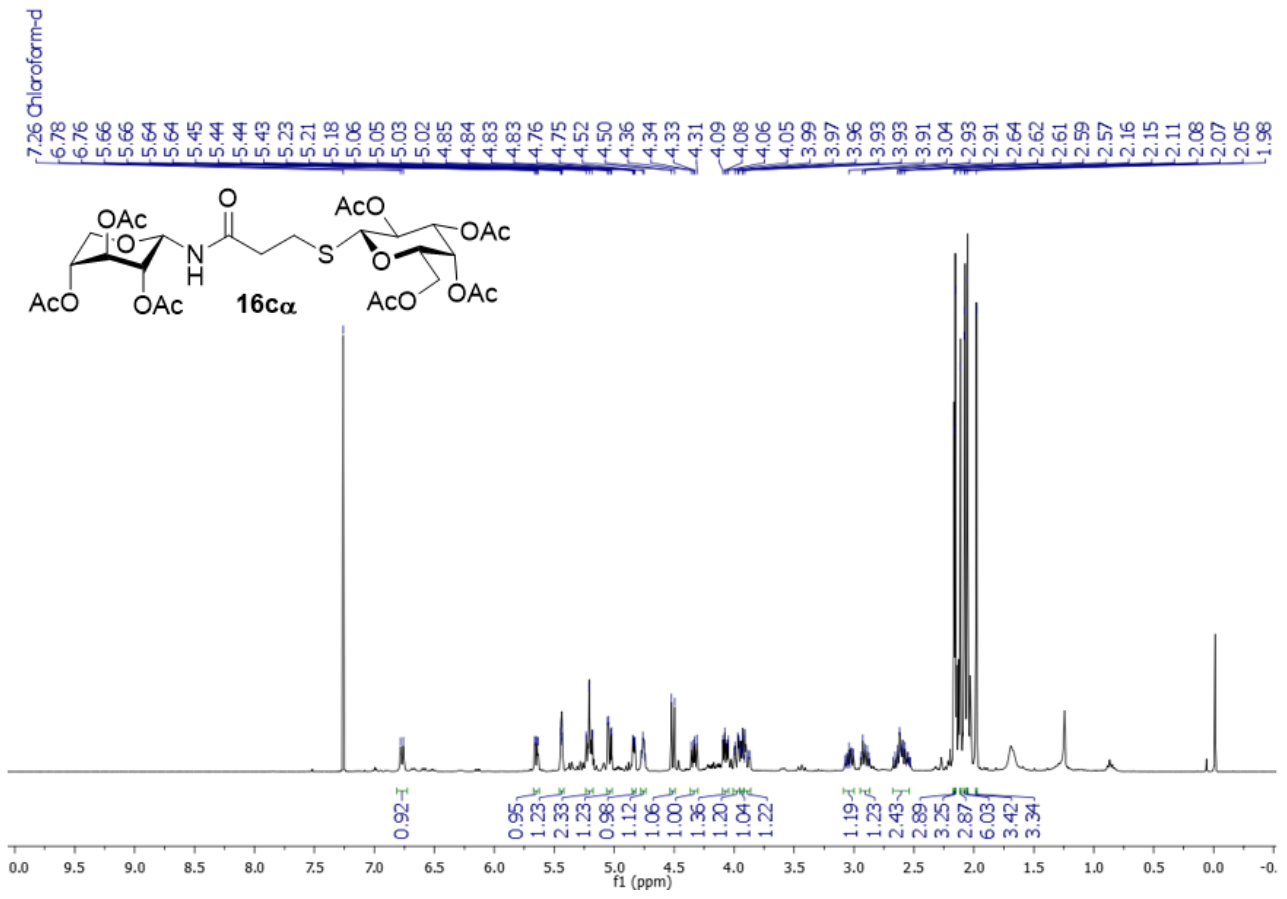
84.2  
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74.9  
72.5  
71.9  
71.0  
68.4  
67.5  
67.3  
66.9  
61.6  
61.2

37.5  
25.2  
21.0  
20.9  
20.8  
20.8  
20.7





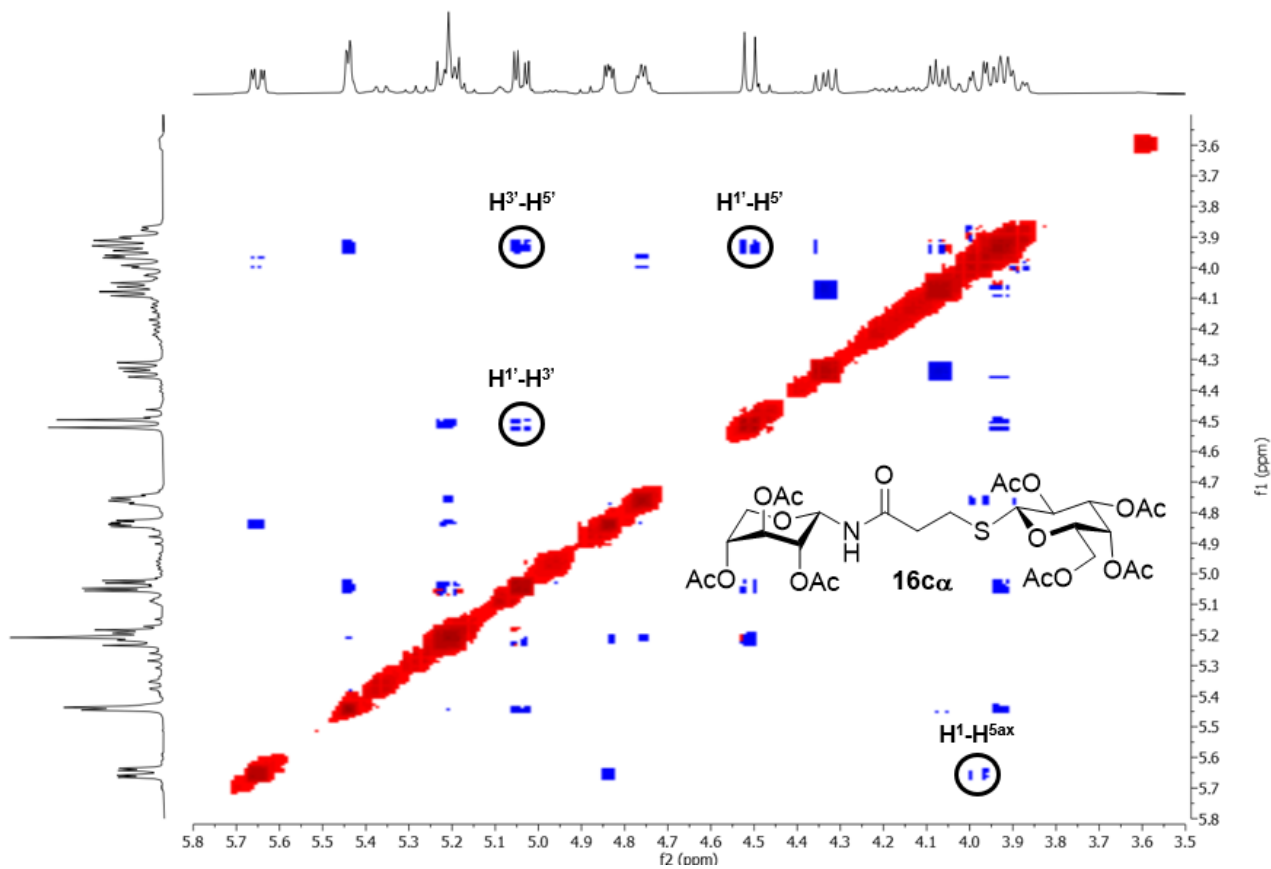
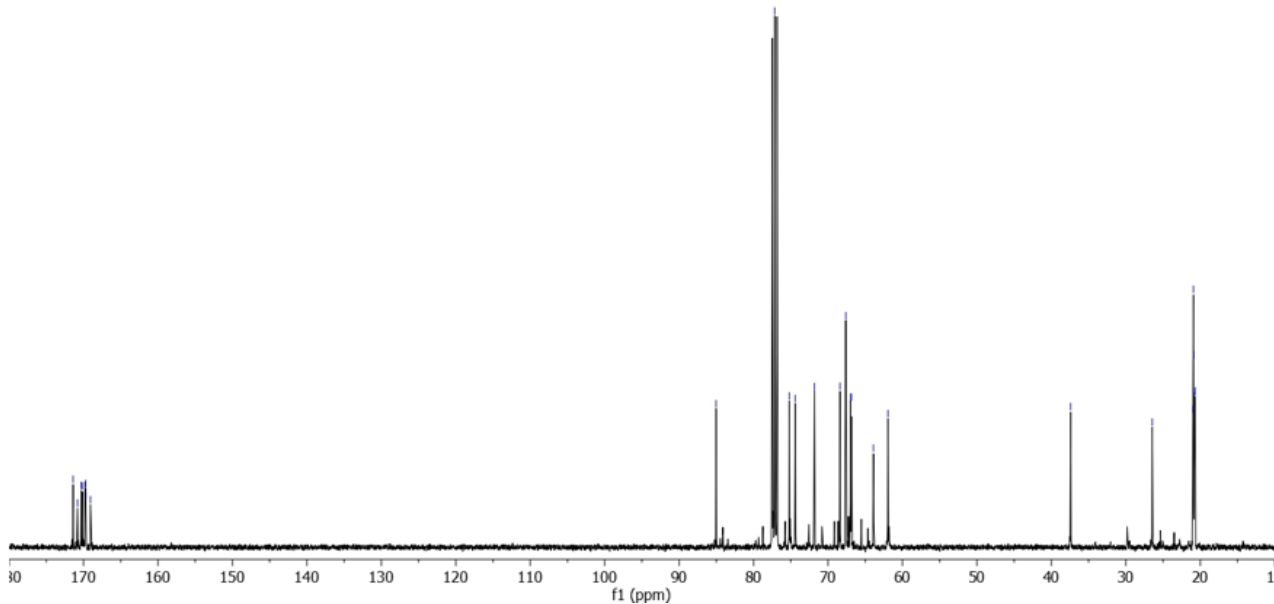
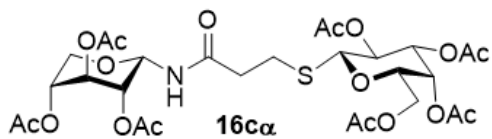




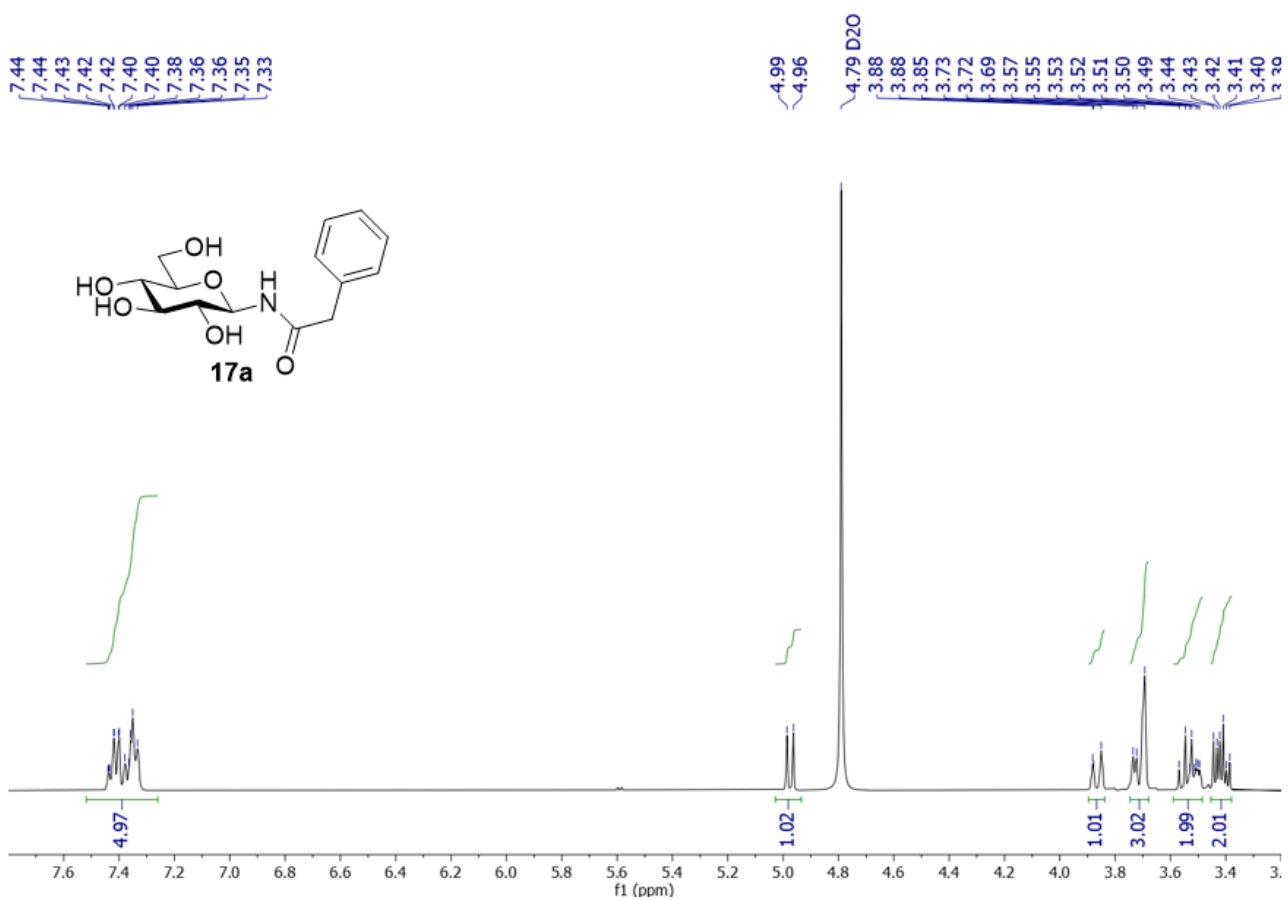
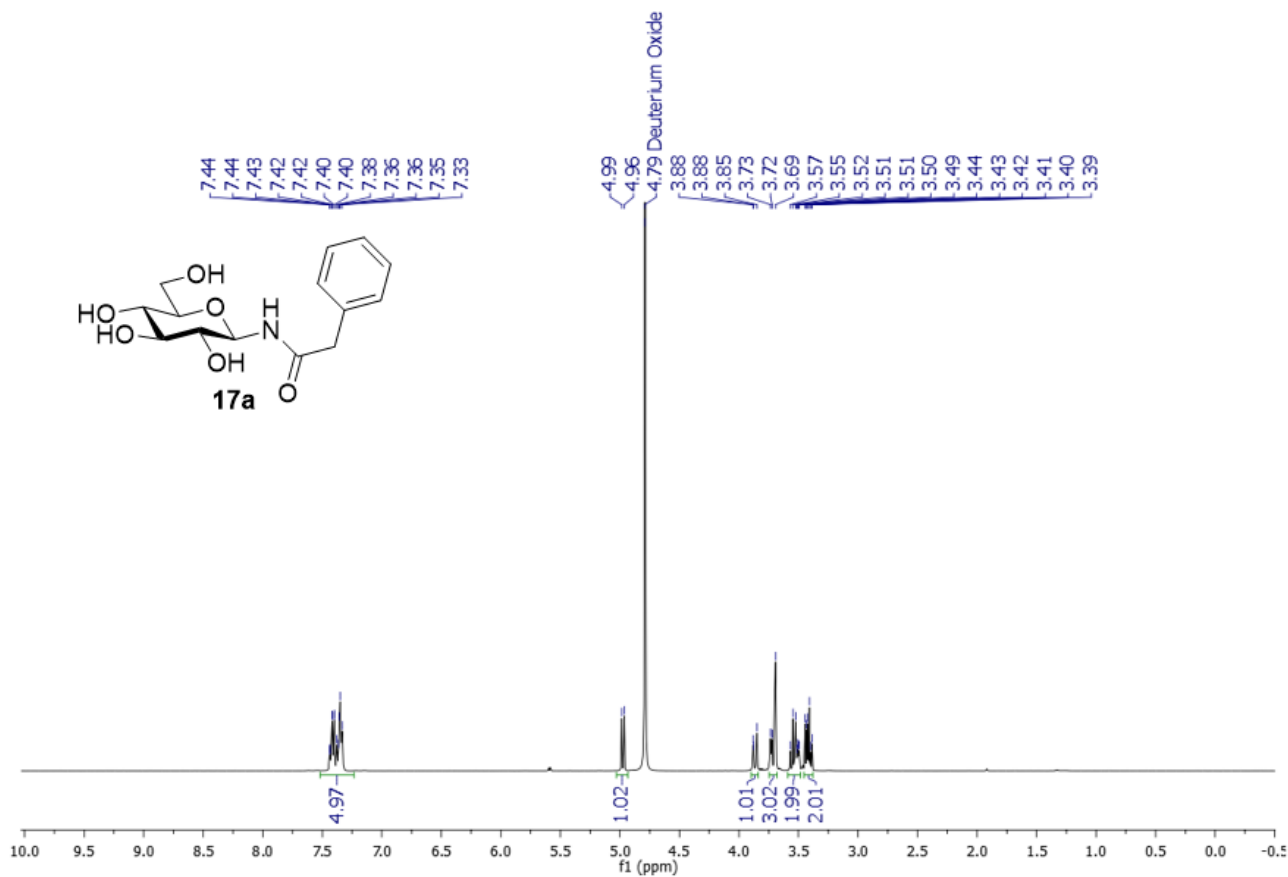
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170.3  
170.1  
169.8  
169.7  
169.1

85.0  
77.2 CDCl<sub>3</sub>  
75.2  
74.4  
71.8  
68.4  
67.6  
67.0  
66.9  
63.9  
62.0

37.4  
26.4  
21.0  
20.9  
20.9  
20.8  
20.7



$^1\text{H}$ ,  $^{13}\text{C}$ , and NOESY NMR spectra of free *N*-glycosyl amides **17a-c $\beta$** , **18a-c $\beta$** , and **19a-c $\beta$** .



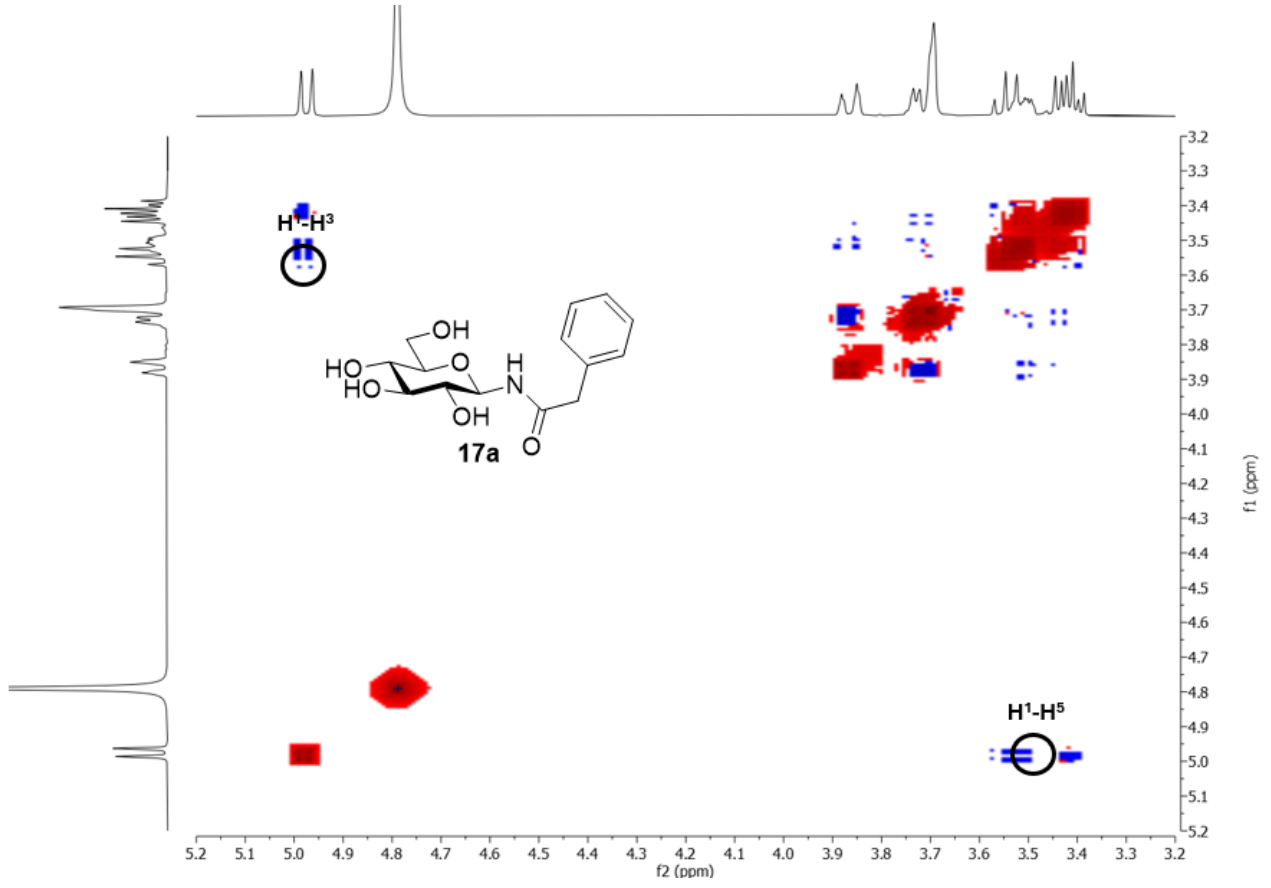
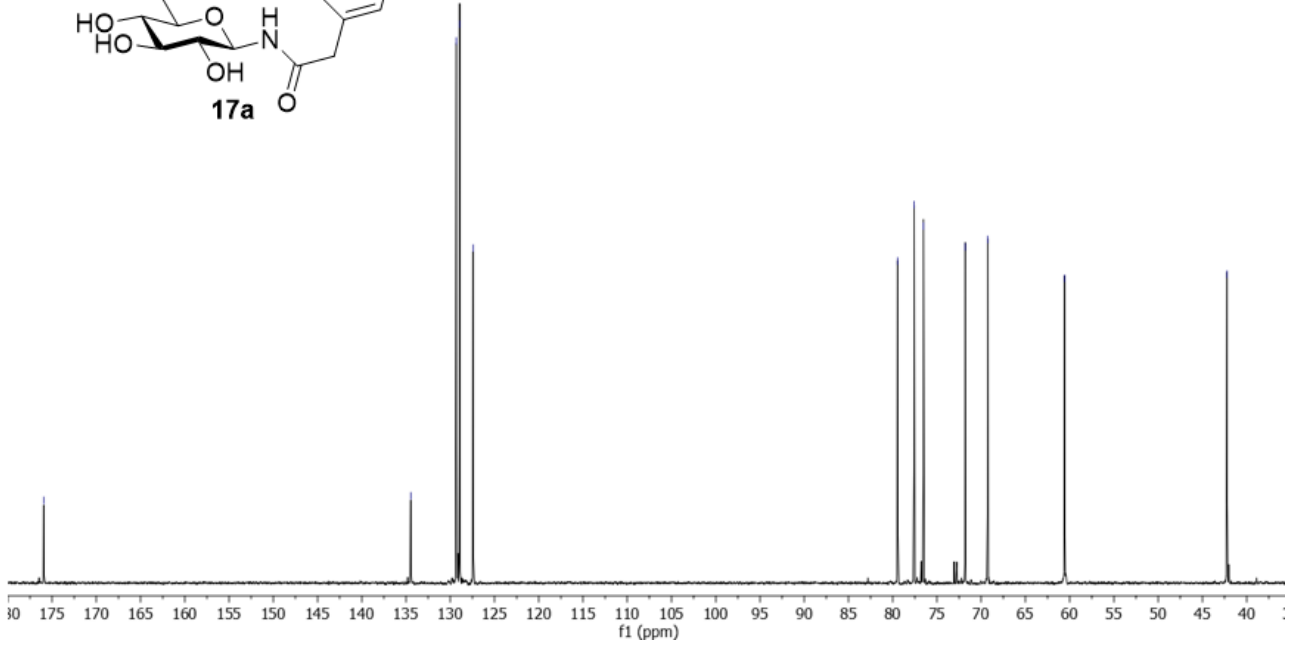
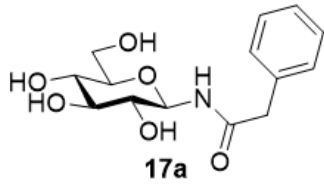
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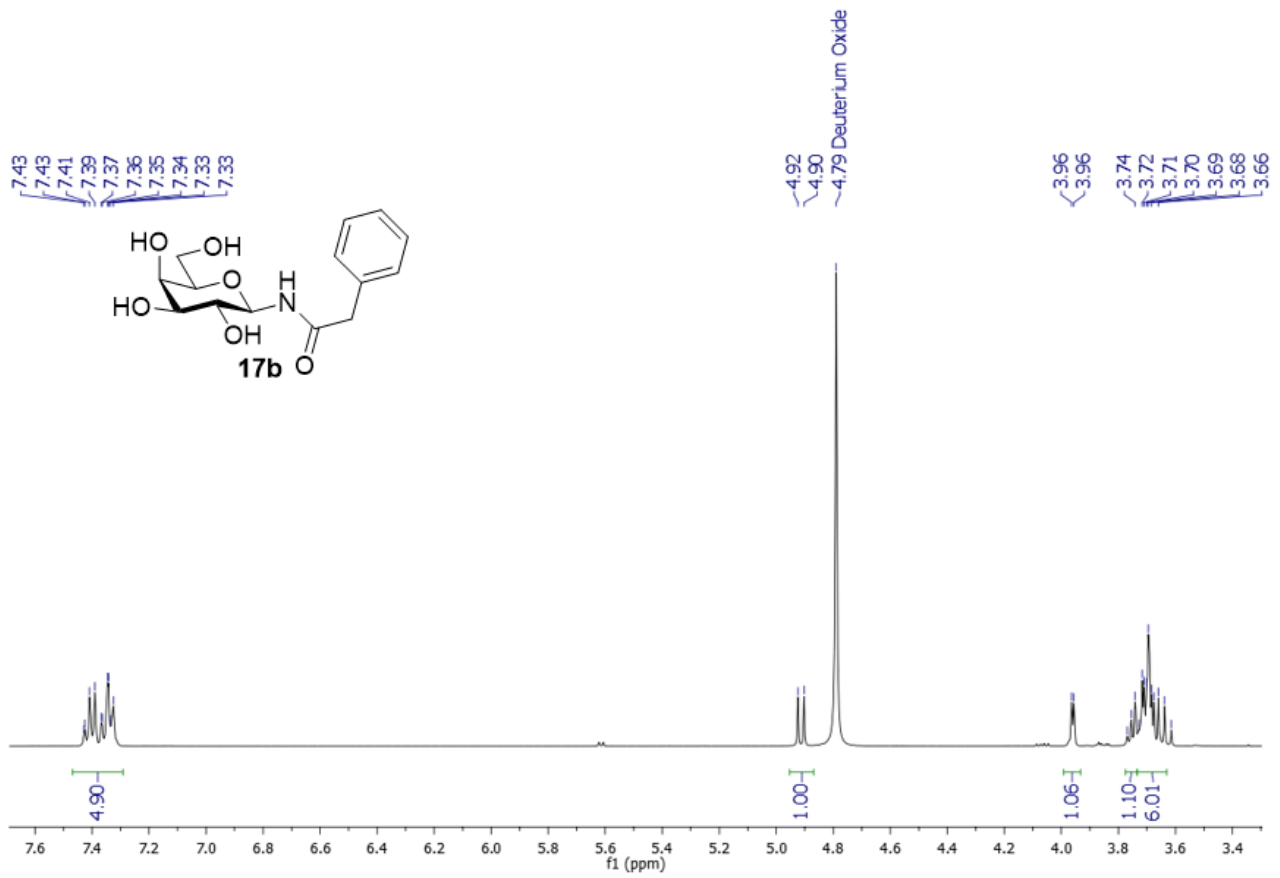
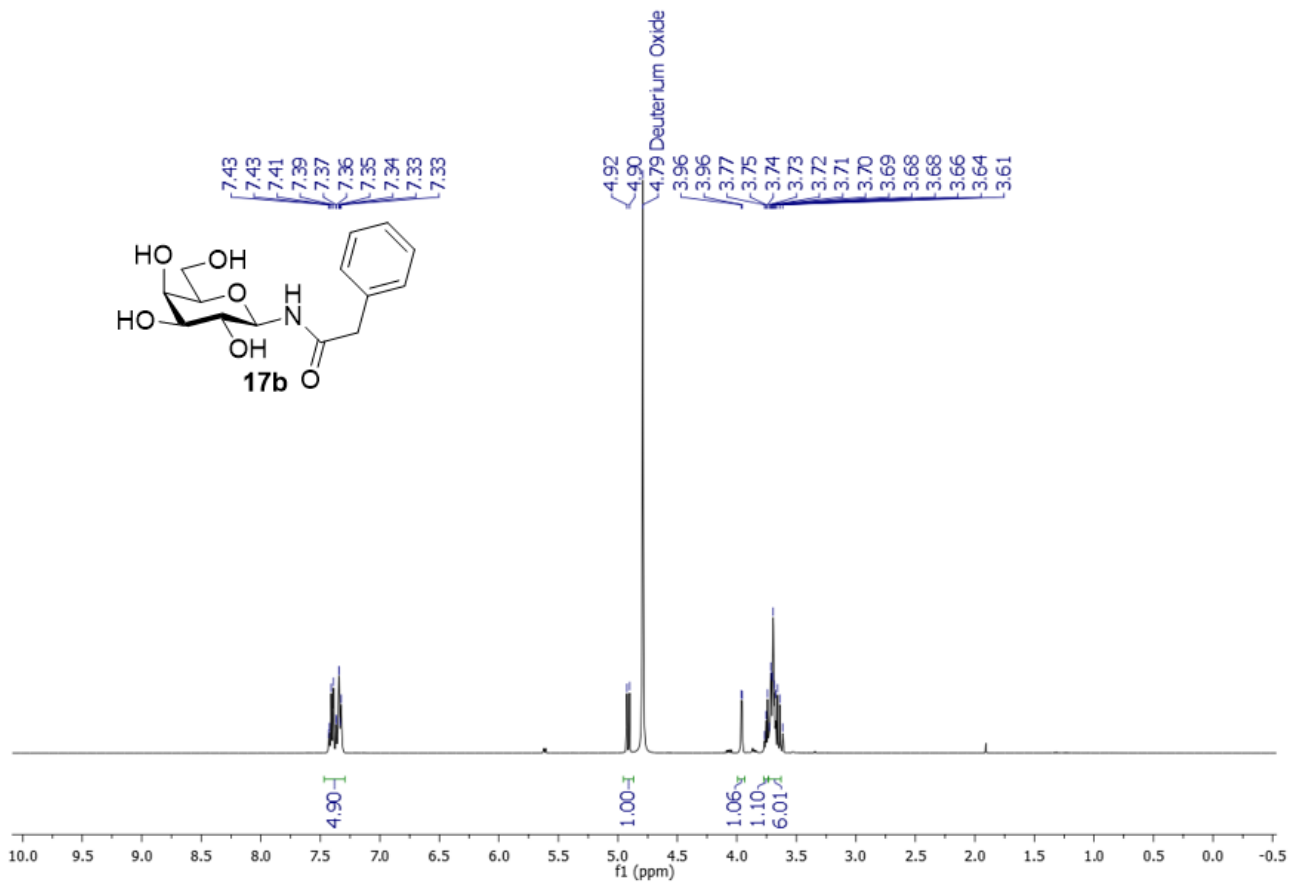
-134.5  
-129.3  
-128.9  
-127.4

-79.4  
-77.6  
-76.5  
-71.8  
-69.3

-60.6

-42.2







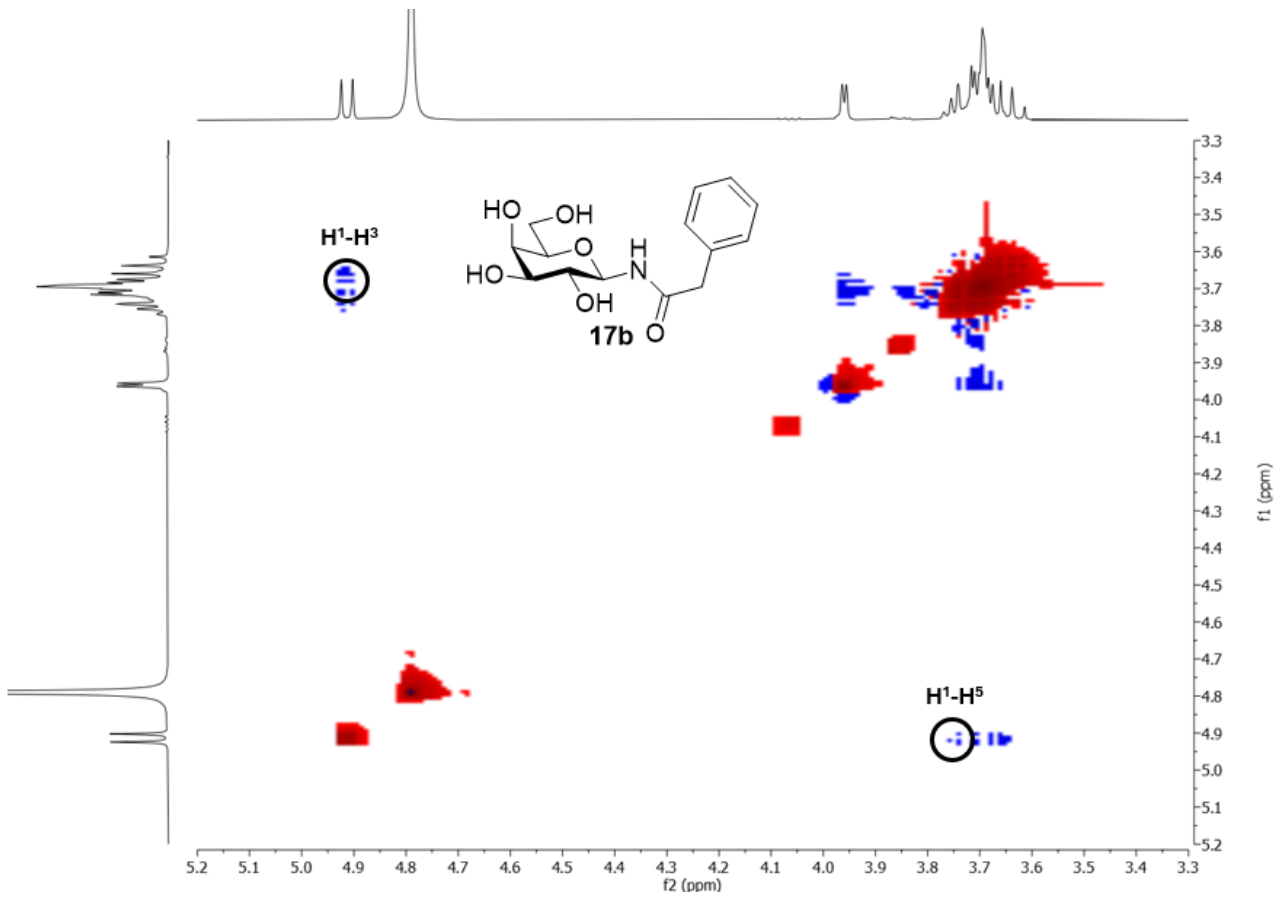
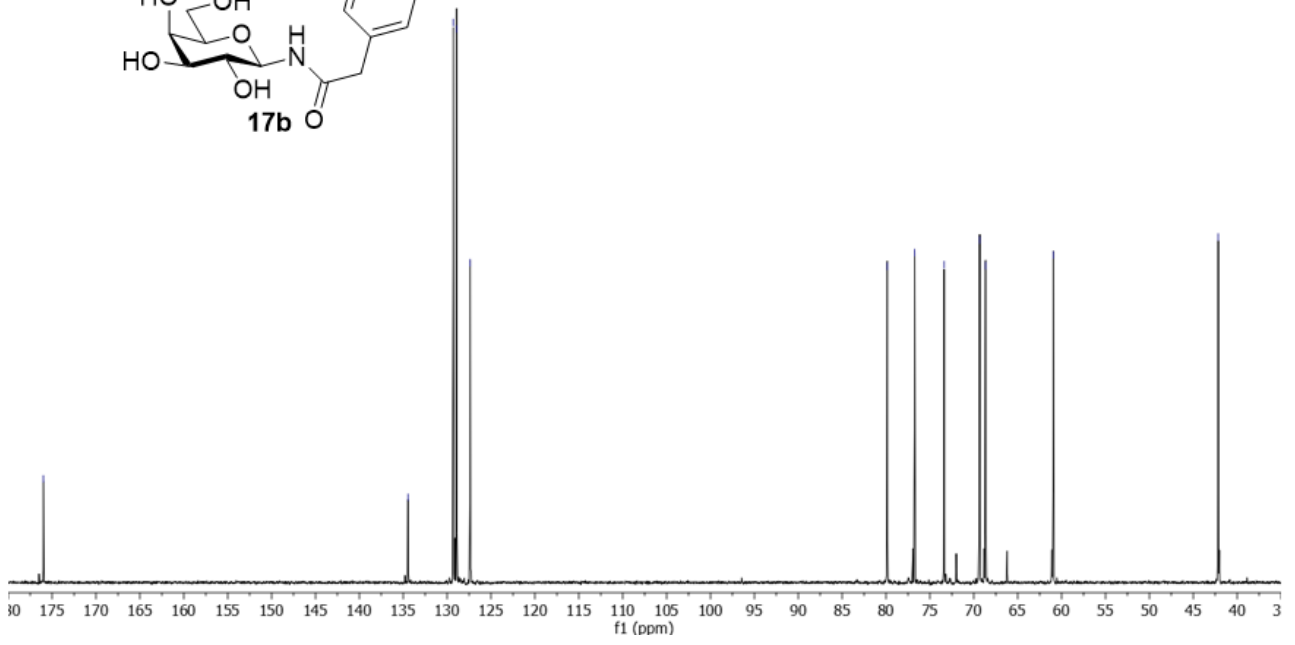
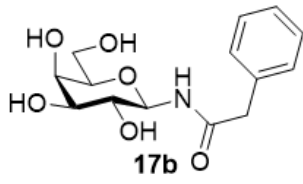
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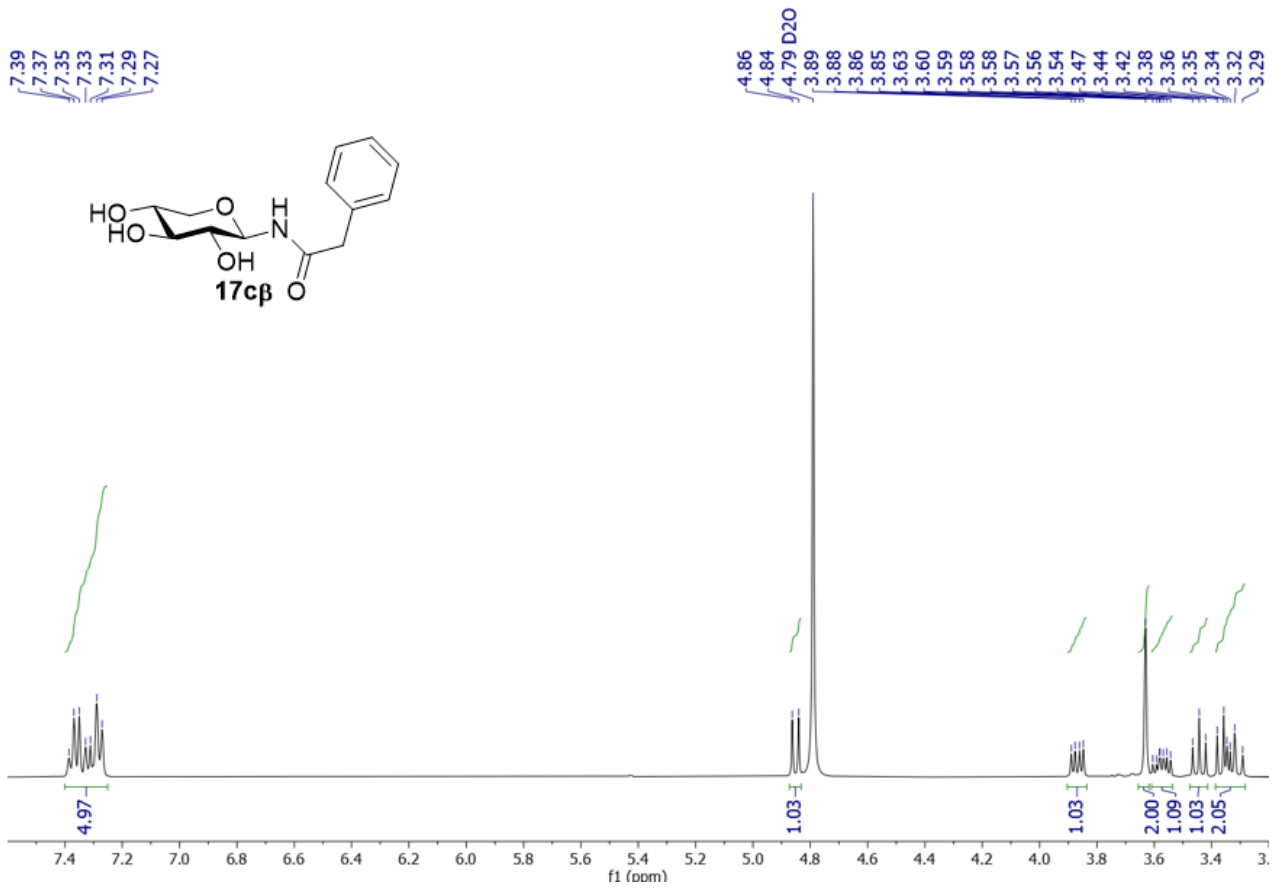
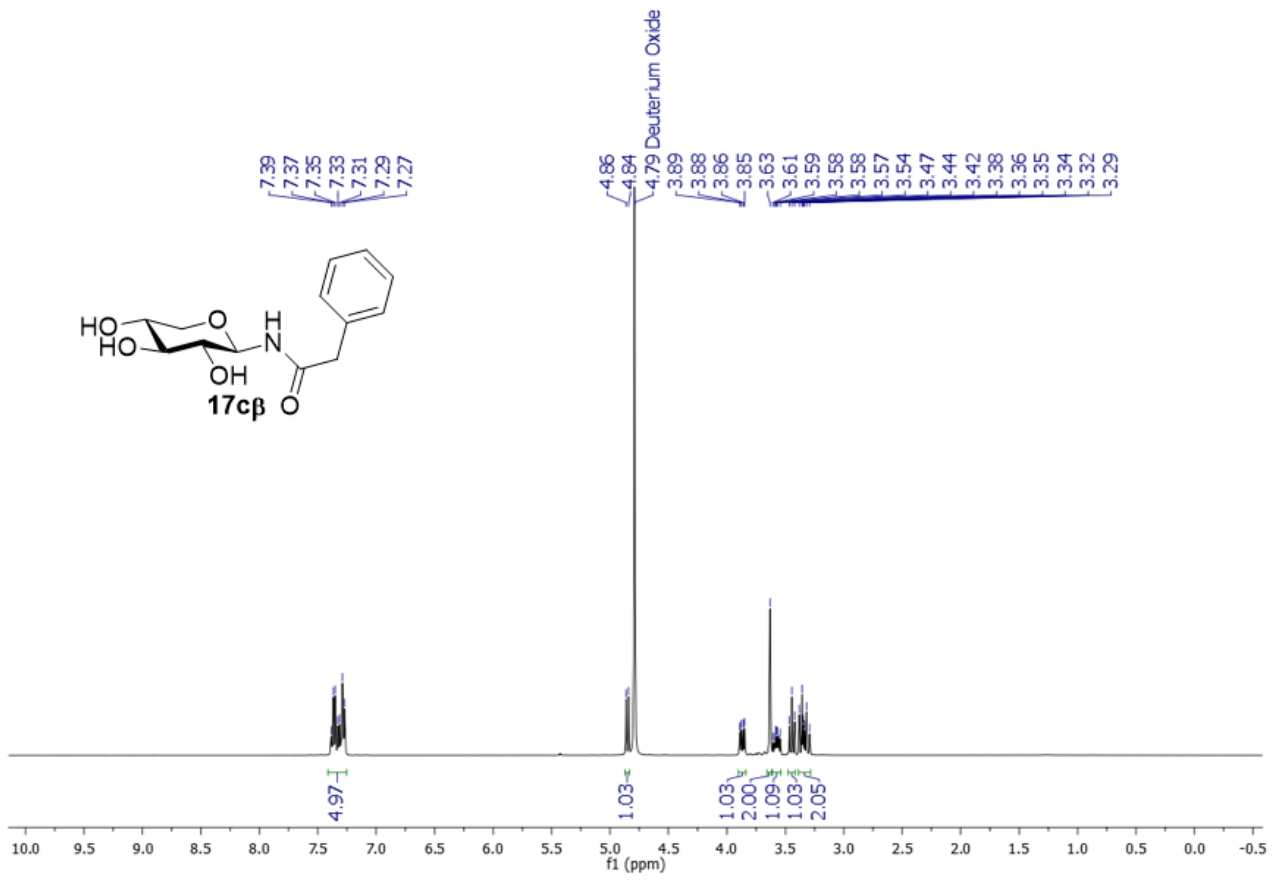
-134.5  
-129.3  
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-127.4

-79.9  
-76.7  
-73.4  
-69.3  
-68.7

-60.9

-42.2



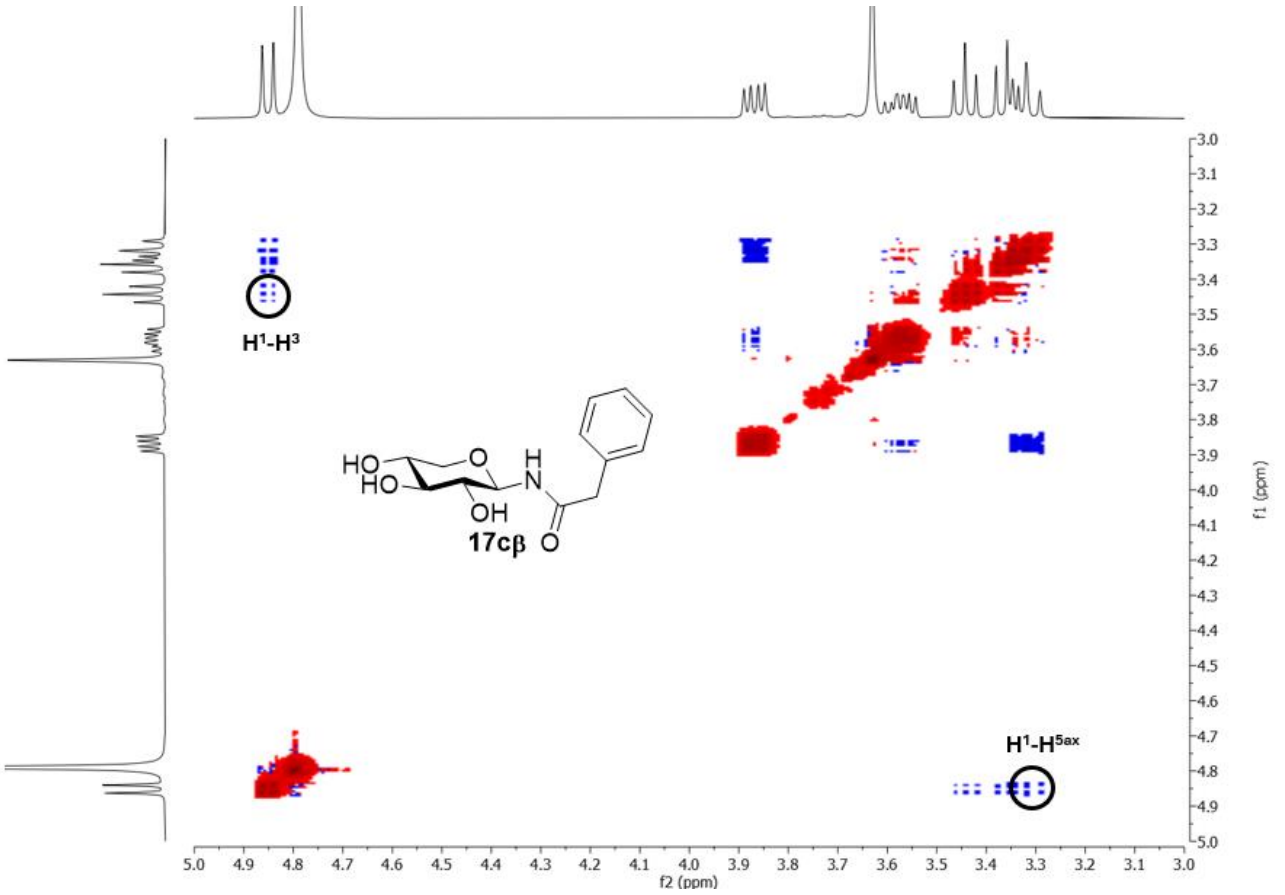
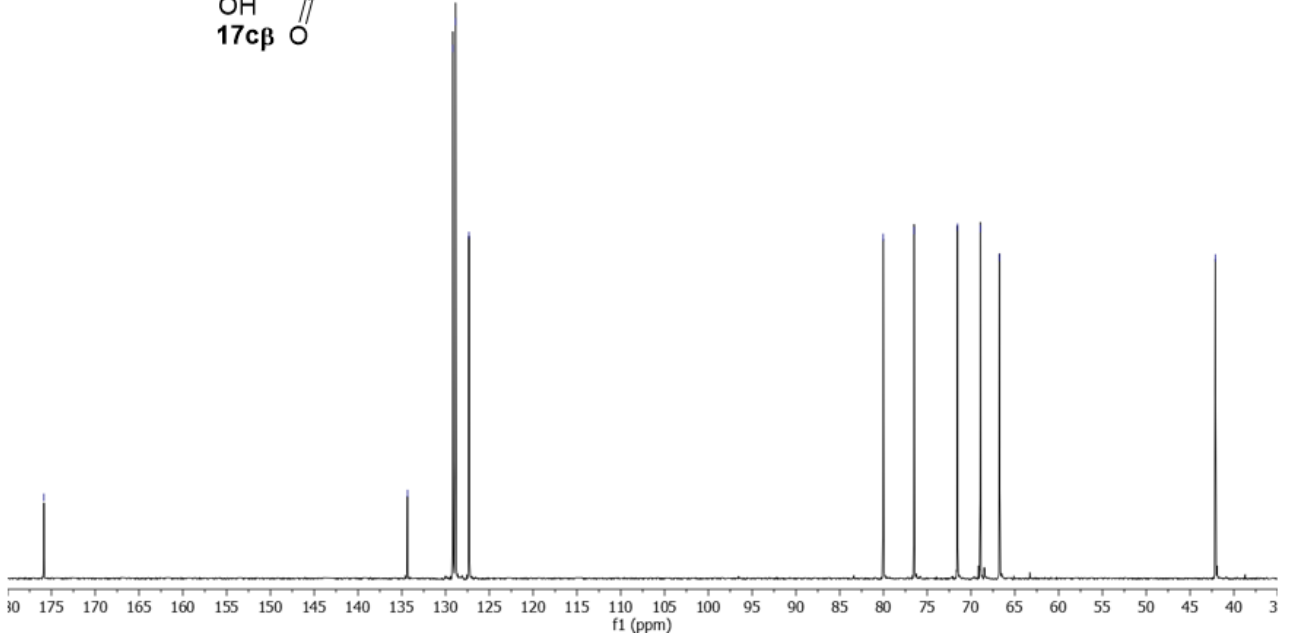
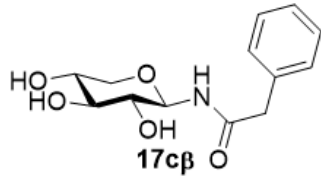


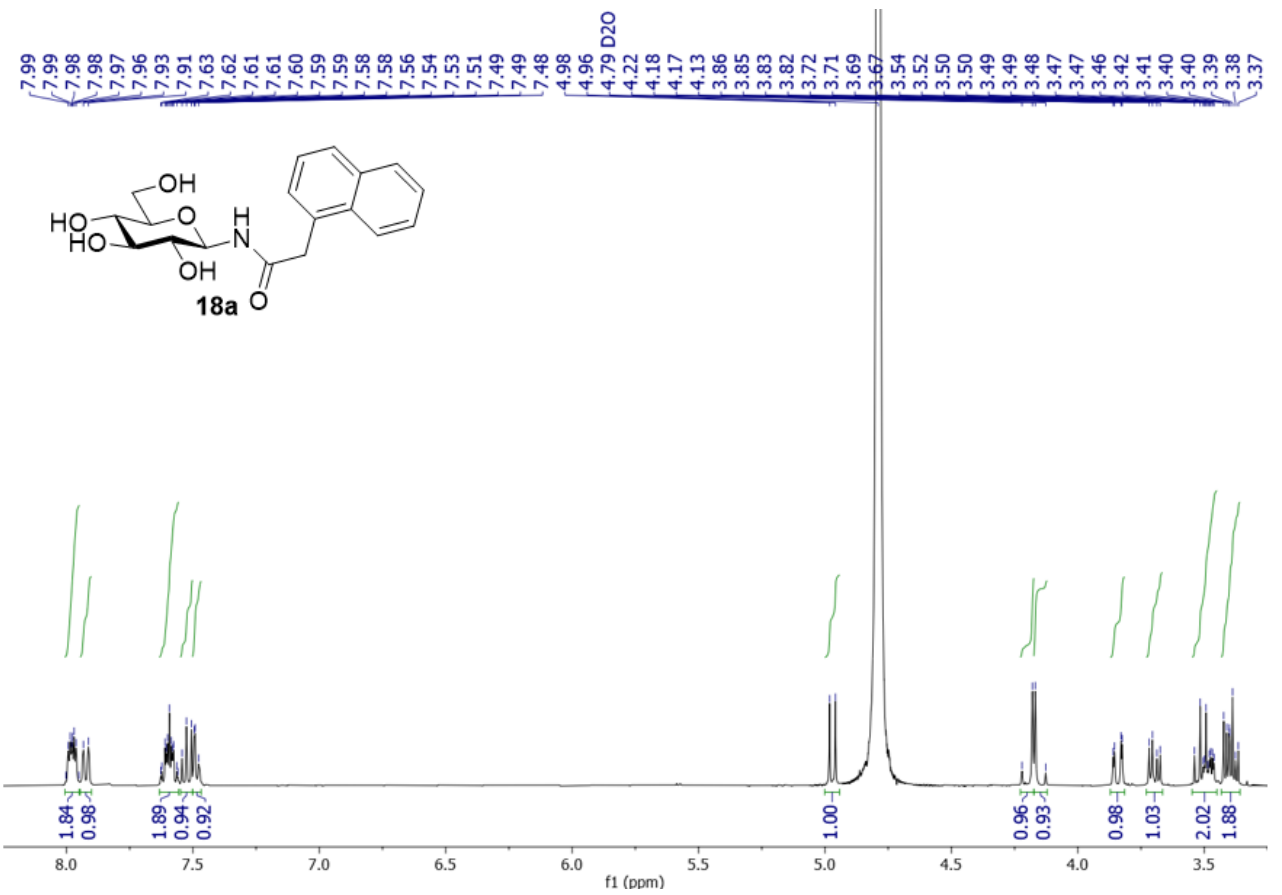
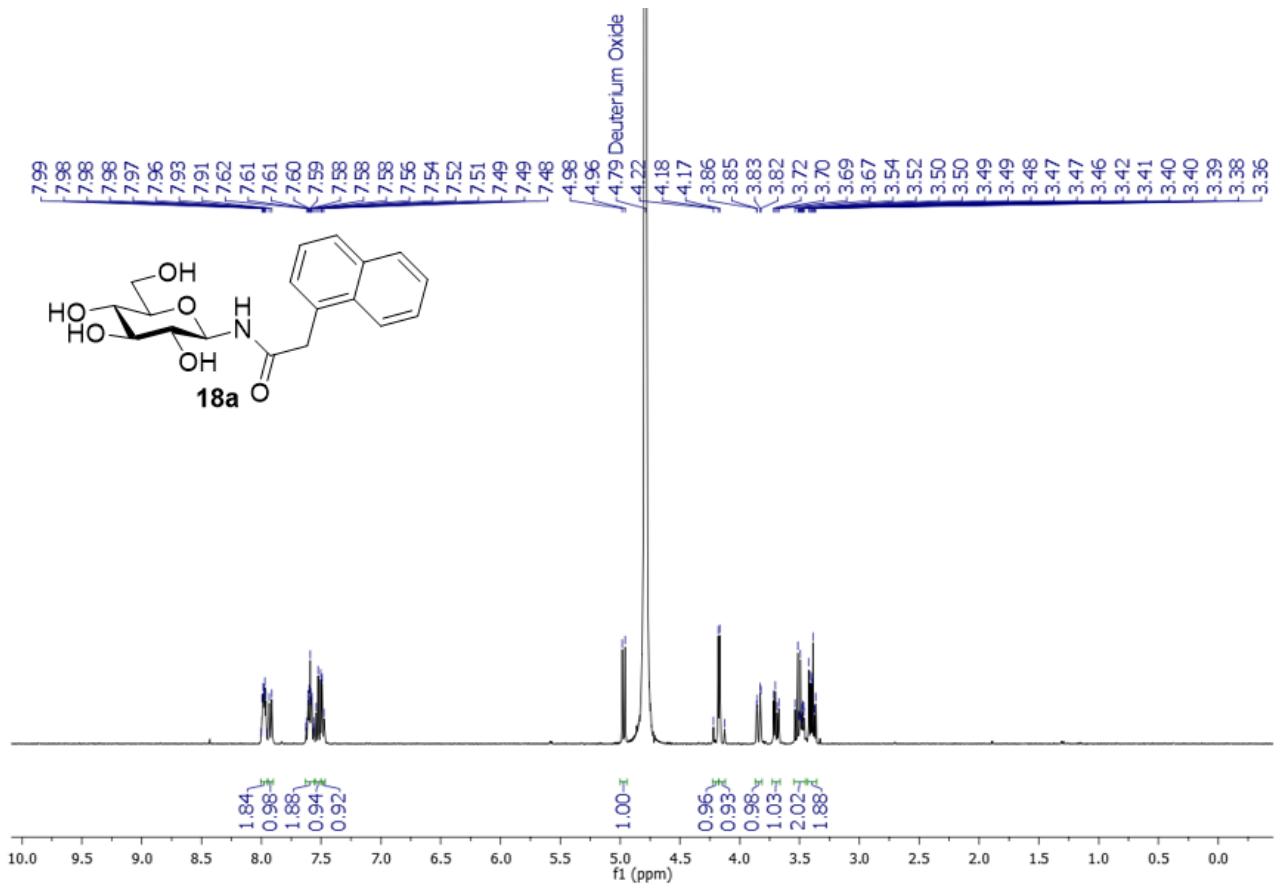
-175.9

-134.3  
-129.2  
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-127.3

-80.0  
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-71.6  
-68.9  
-66.7

-42.1





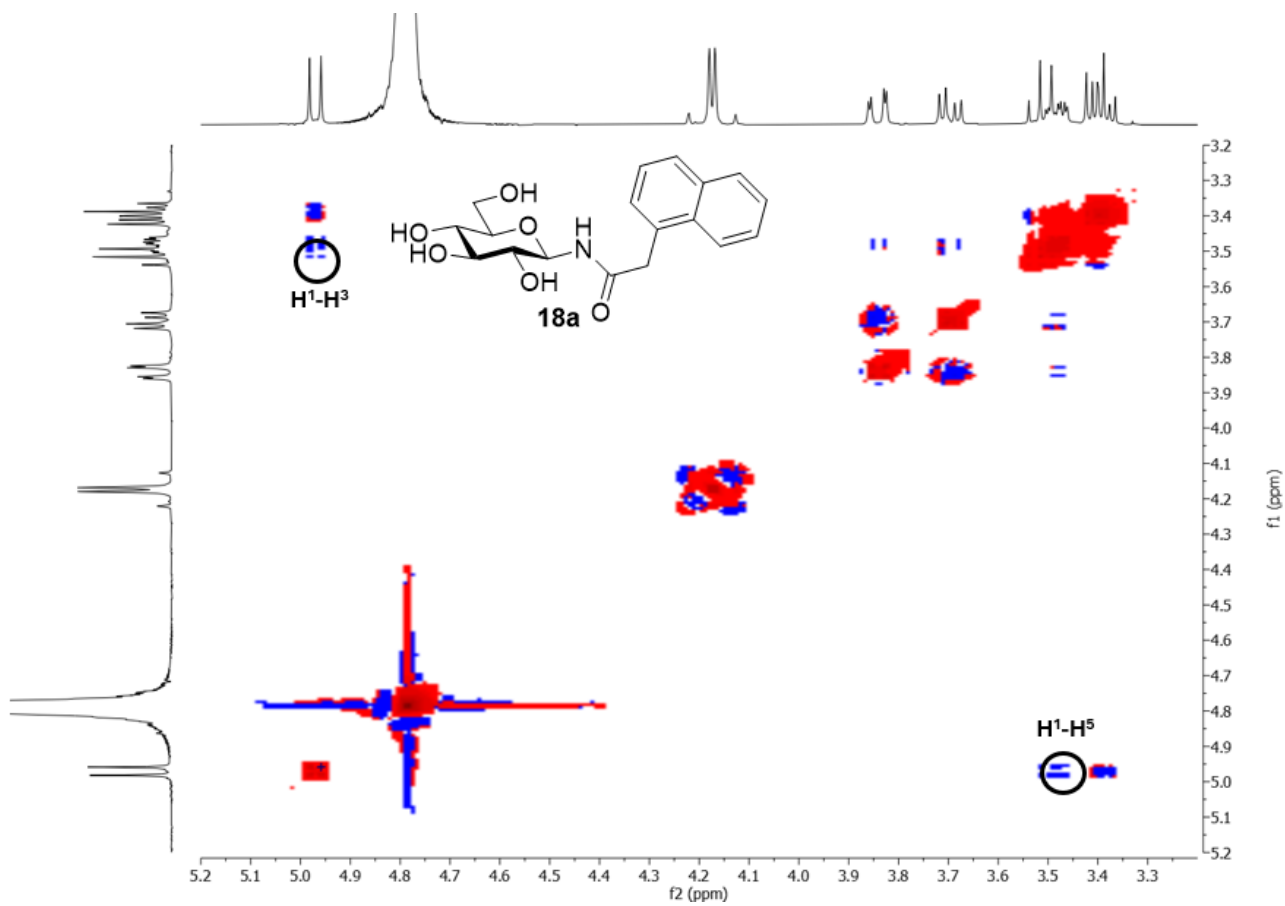
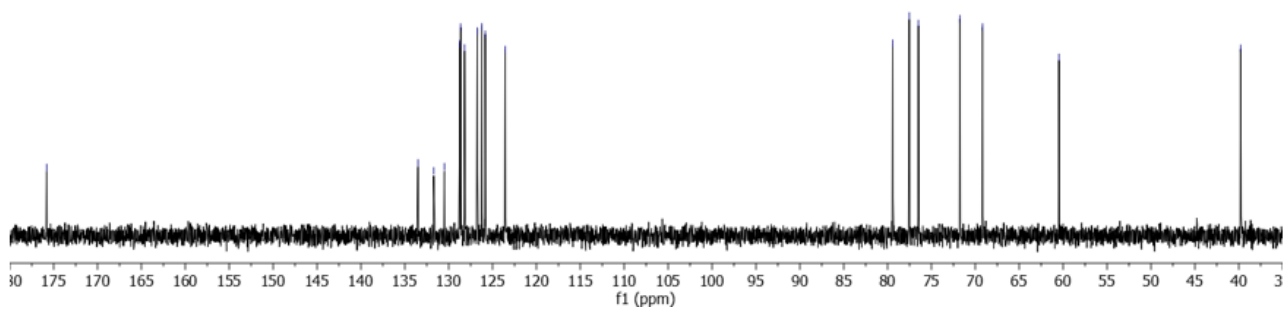
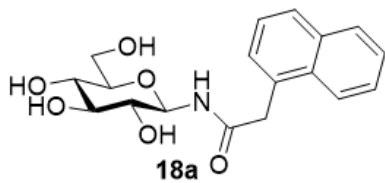
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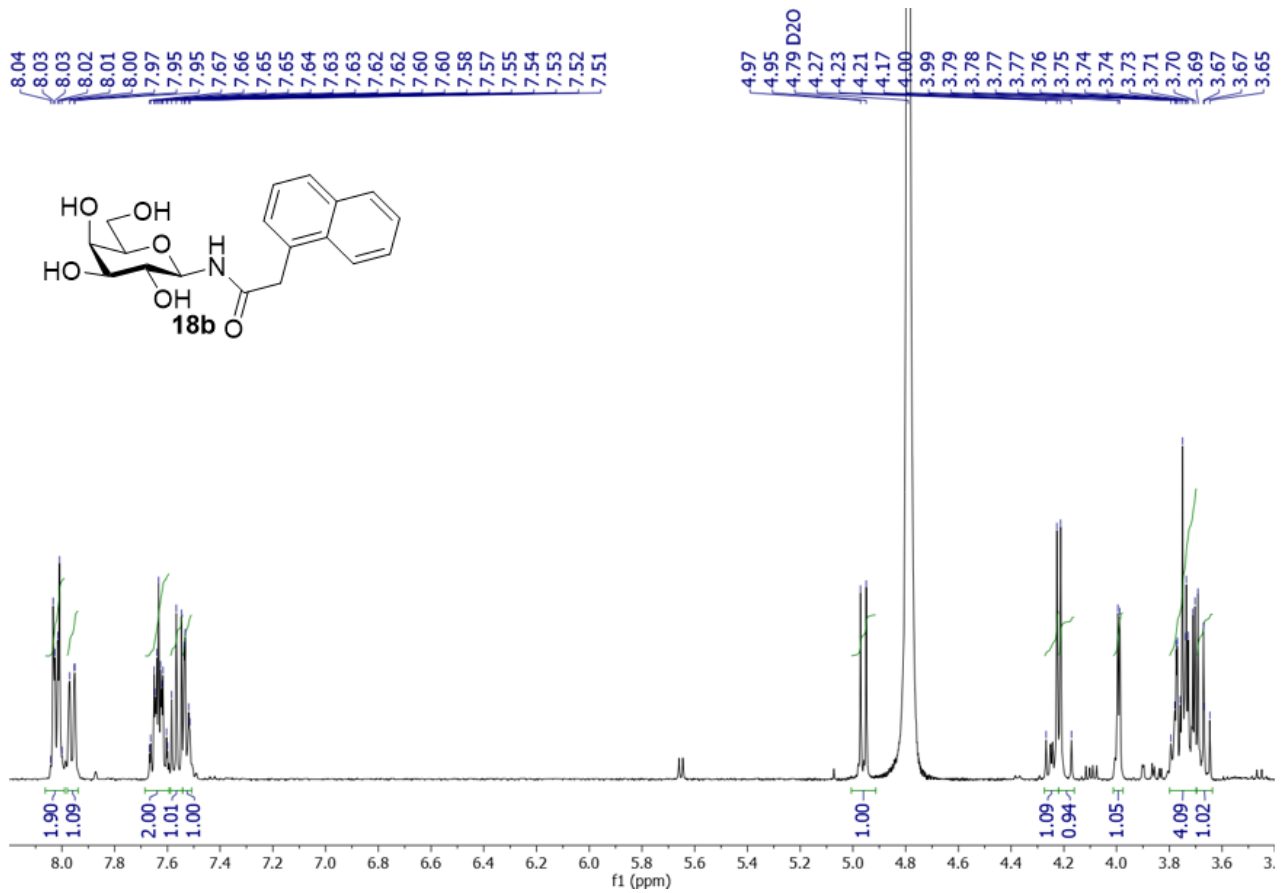
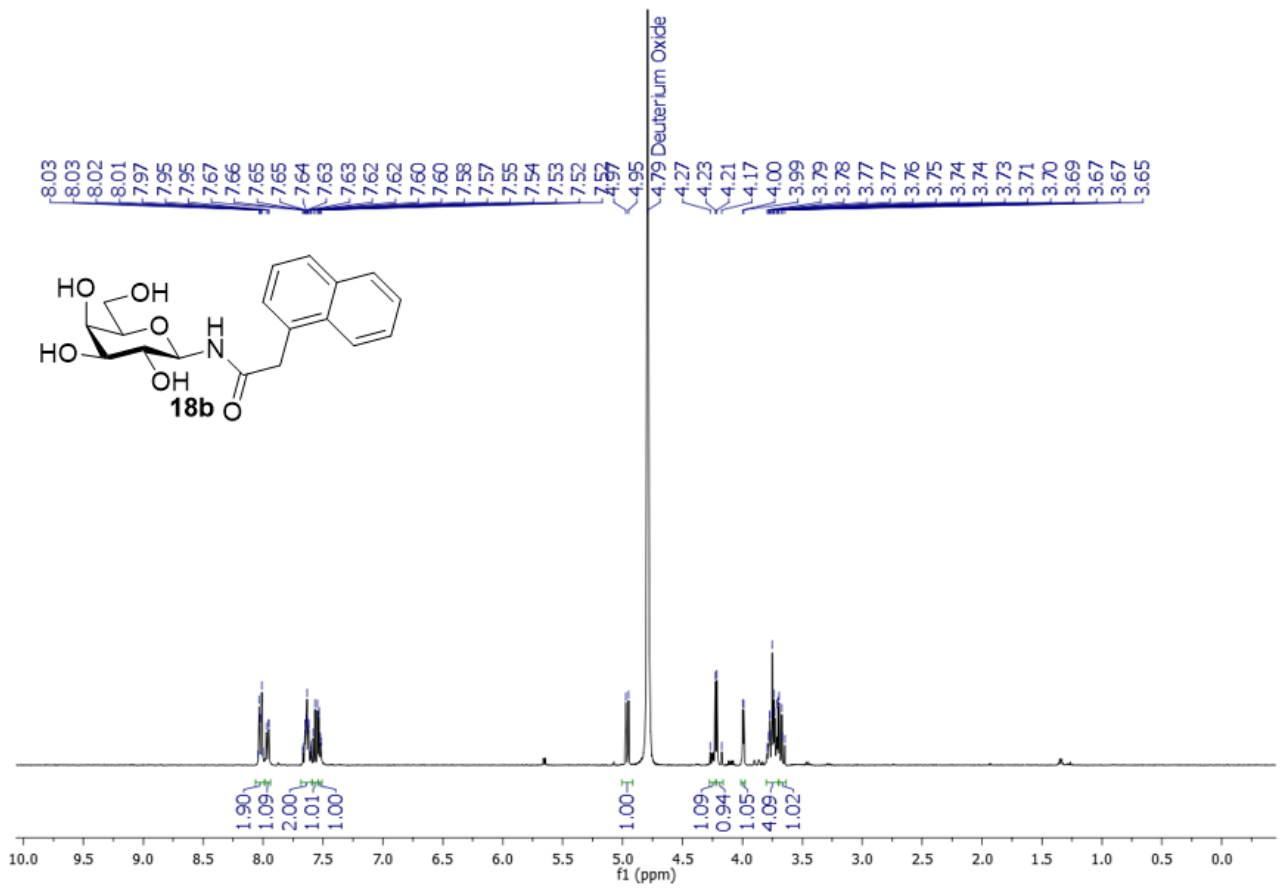
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128.6  
128.2  
126.7  
126.2  
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123.6

-79.4  
-77.5  
-76.5  
-71.8  
-69.2

-60.5

-39.8





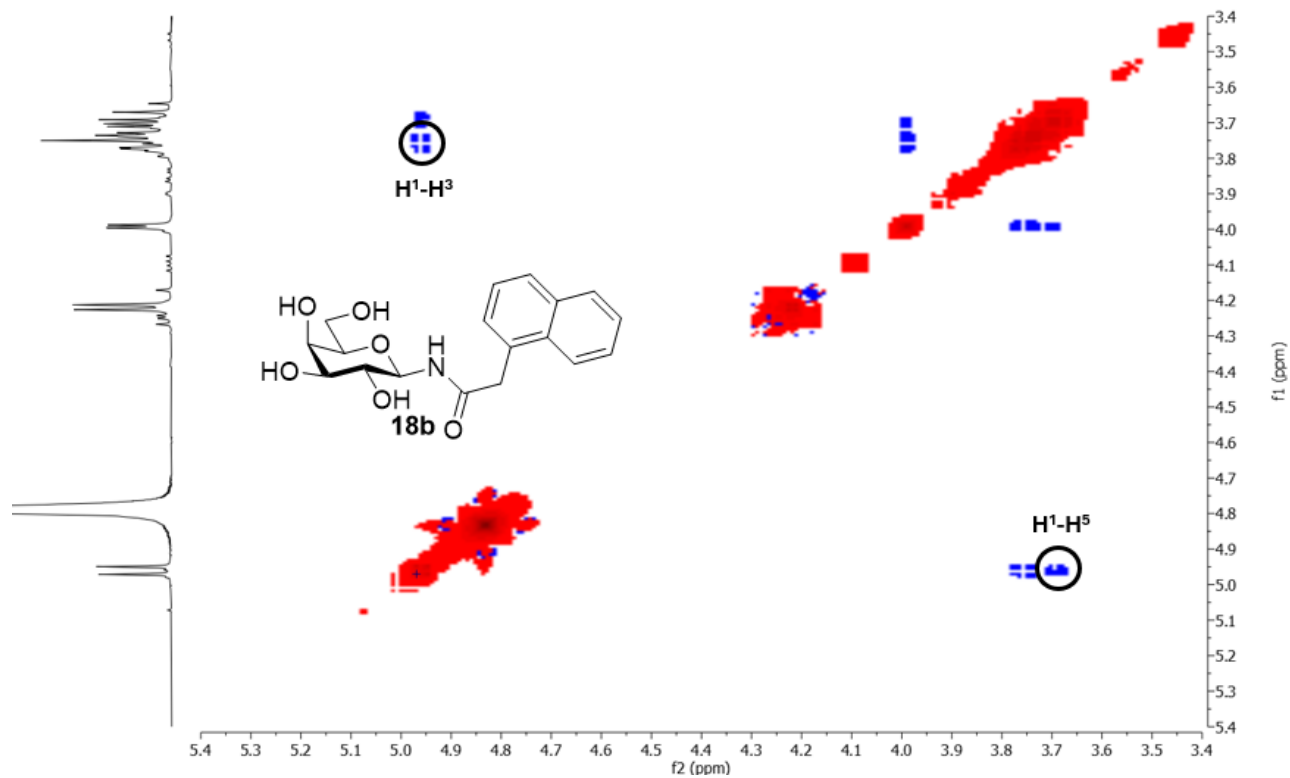
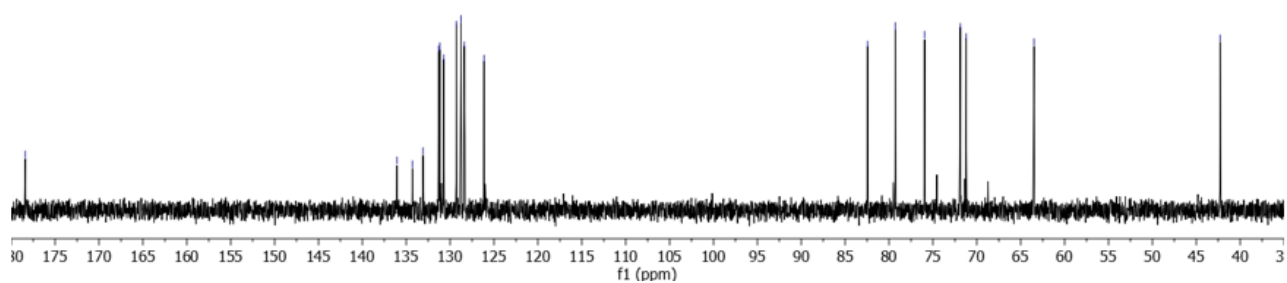
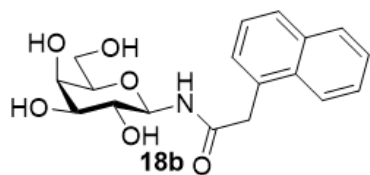
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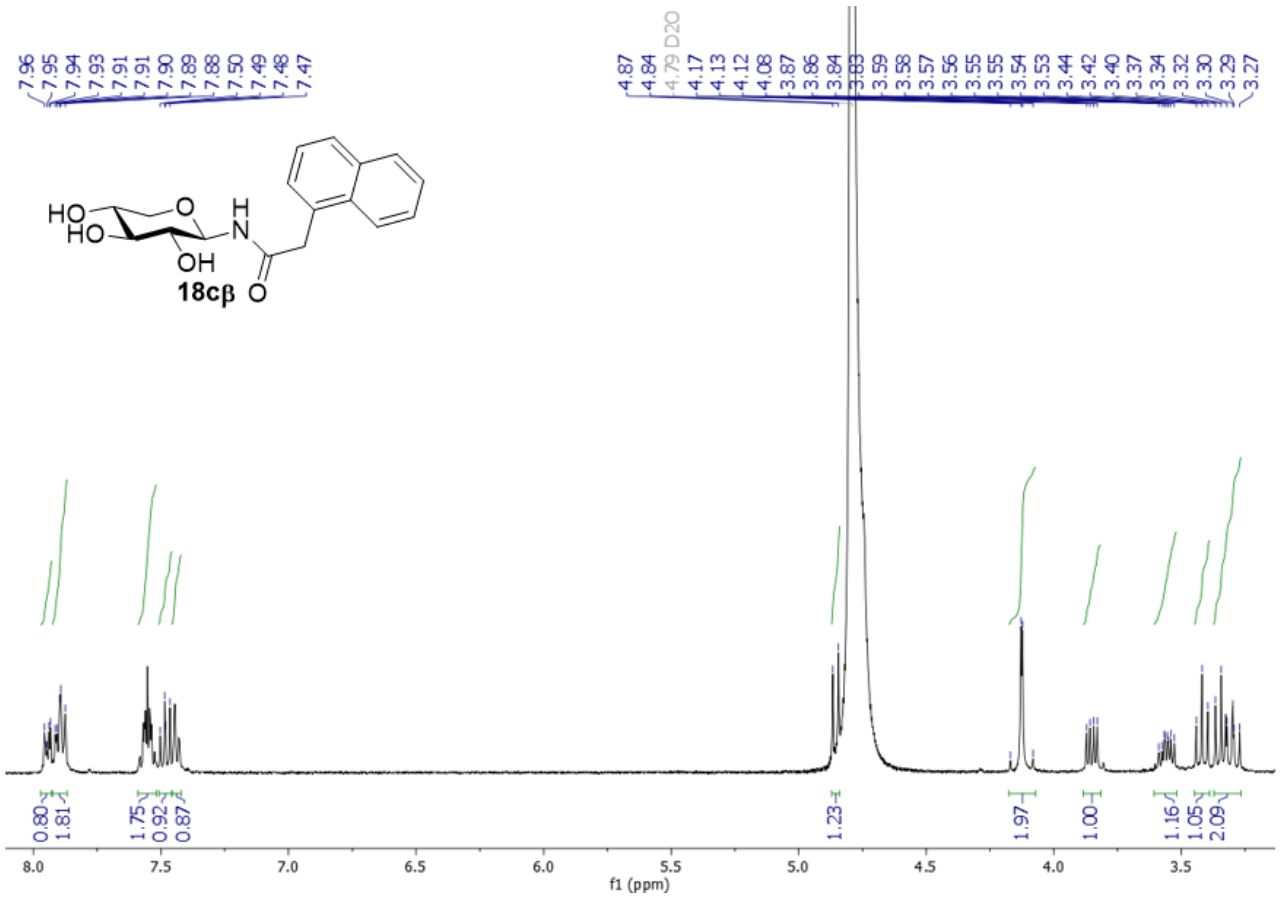
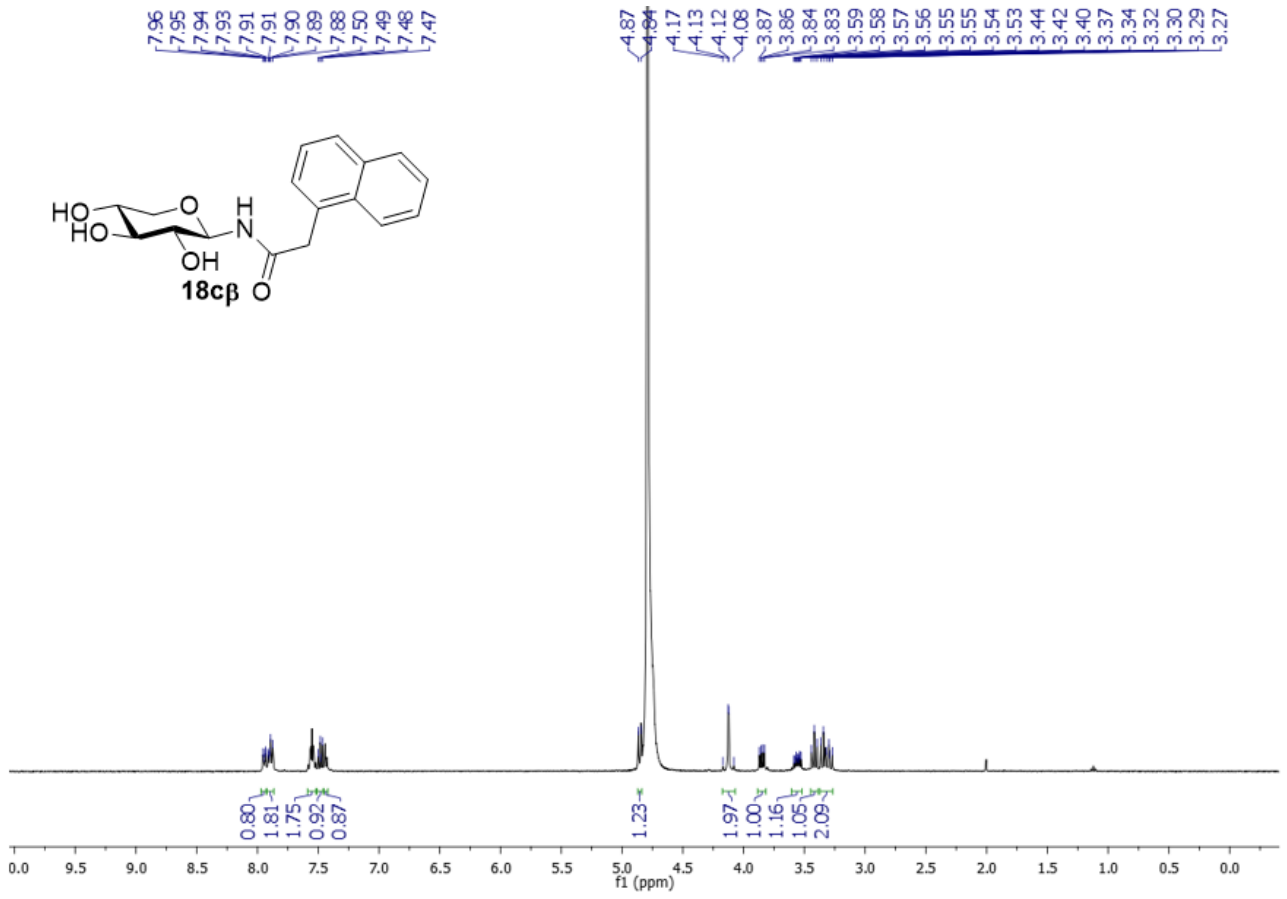
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134.3  
133.1  
131.3  
131.2  
130.7  
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126.1

82.4  
79.3  
75.9  
71.9  
71.2

63.5

42.3





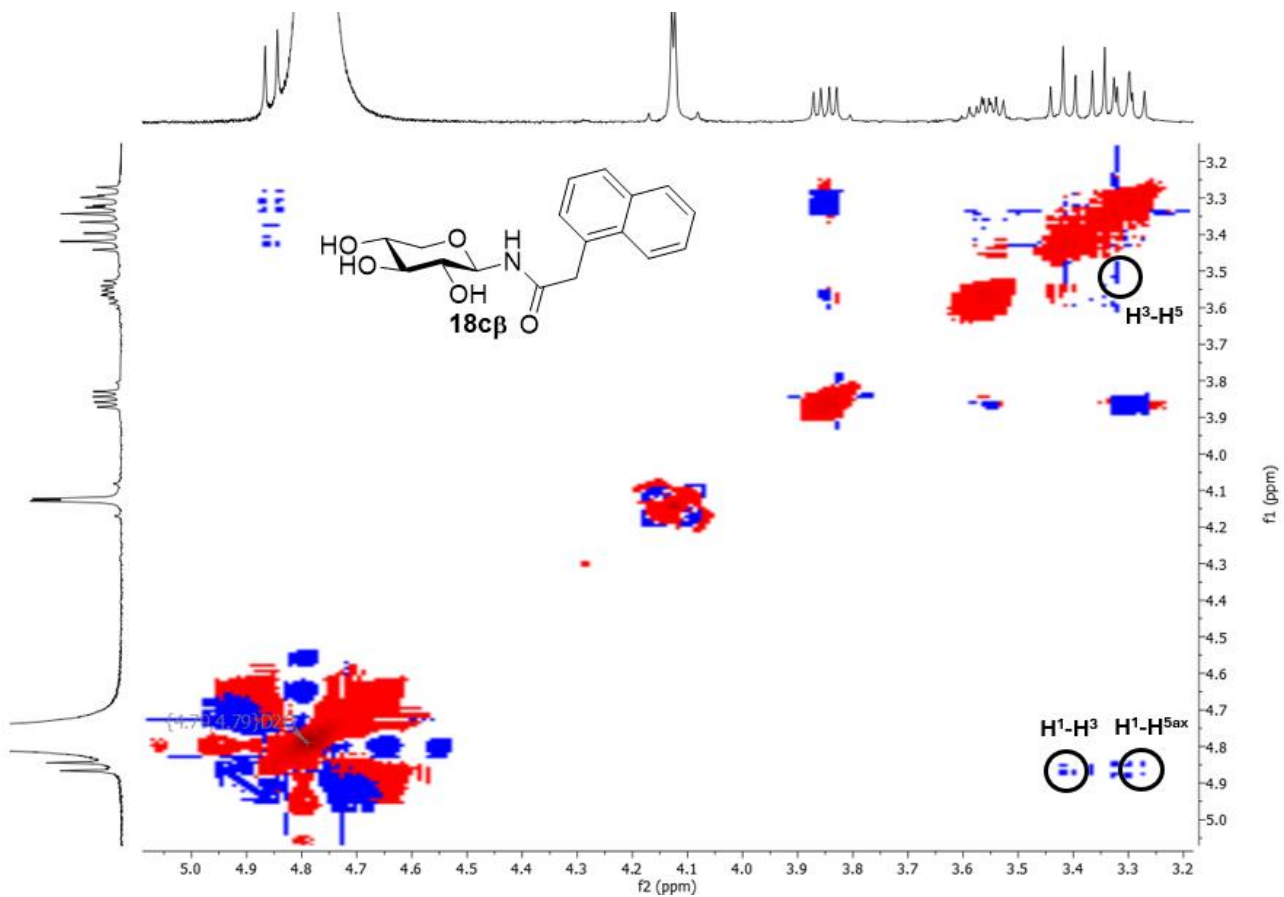
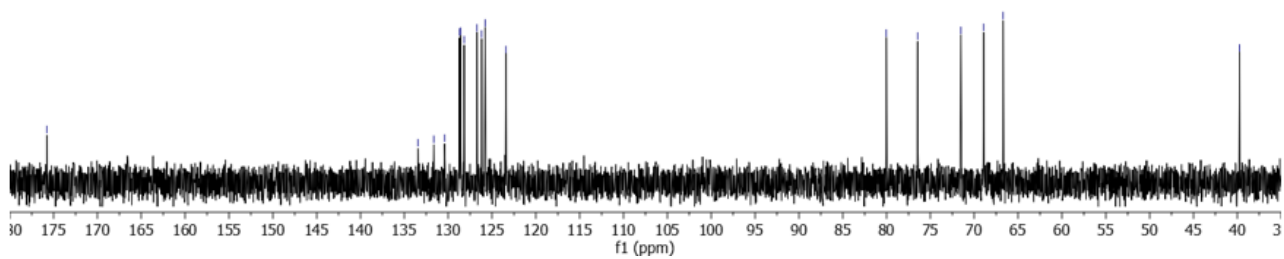
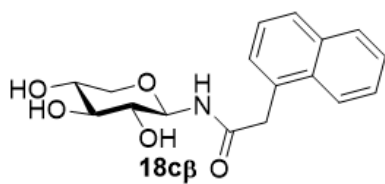


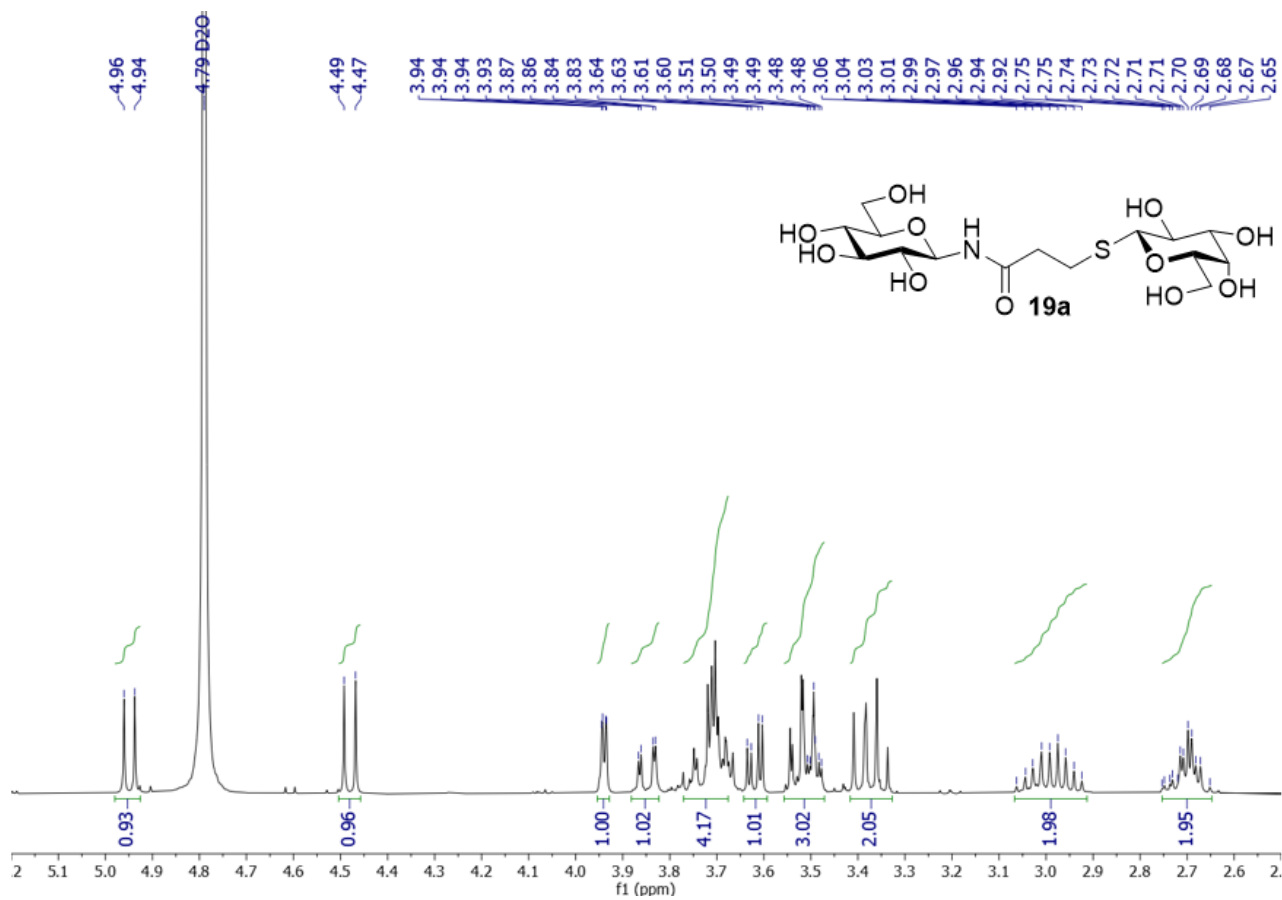
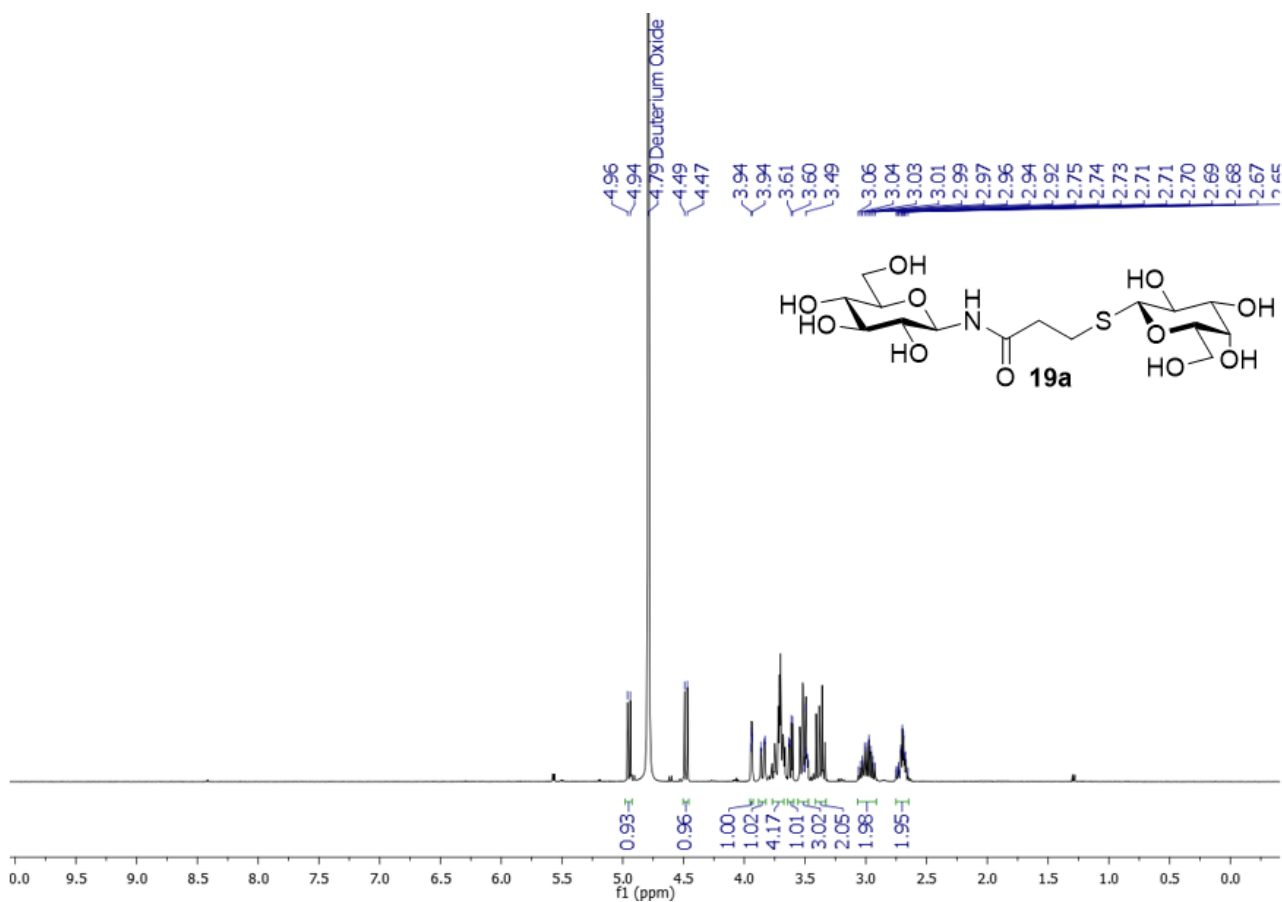
-175.8

133.4  
131.6  
130.4  
128.7  
128.6  
128.2  
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125.8  
123.4

80.0  
76.5  
71.5  
68.9  
66.7

-39.7



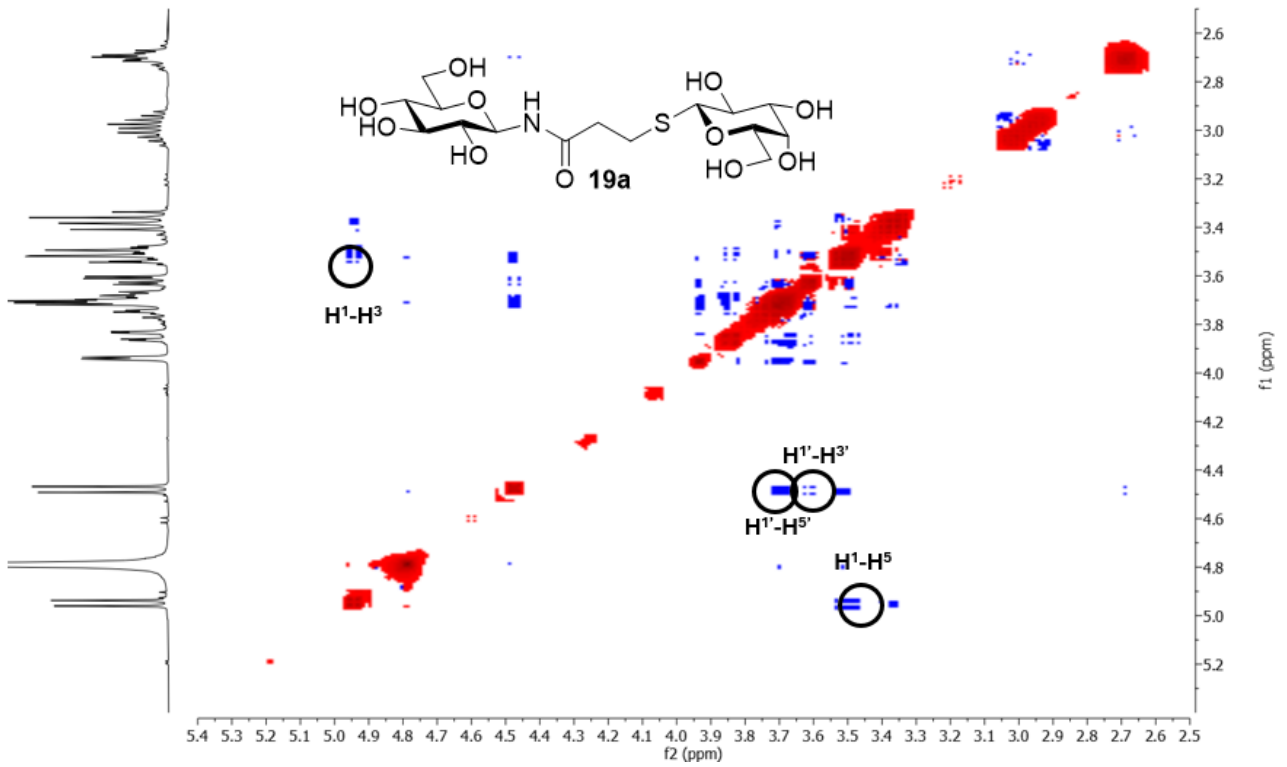
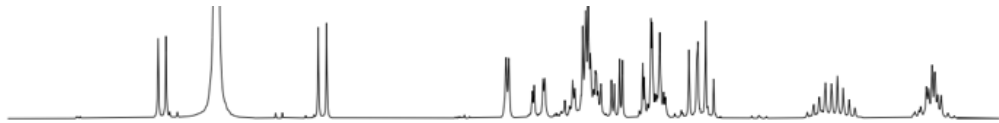
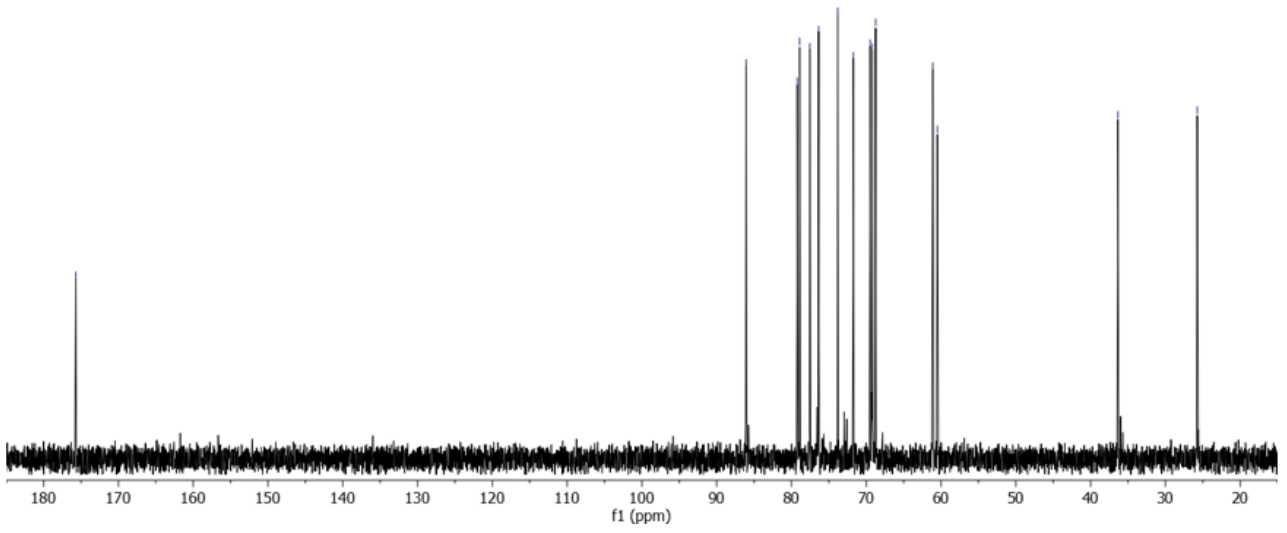
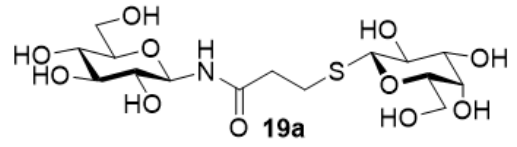


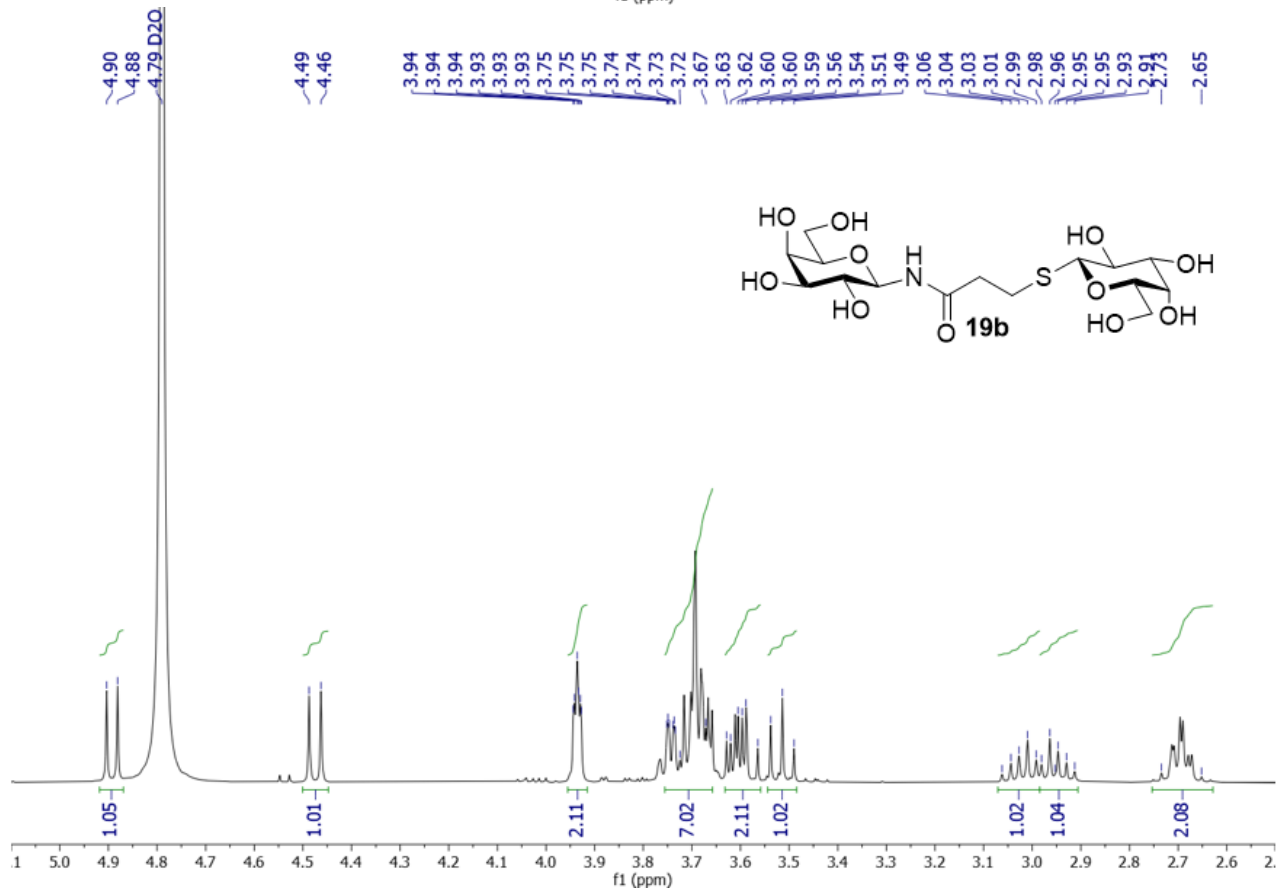
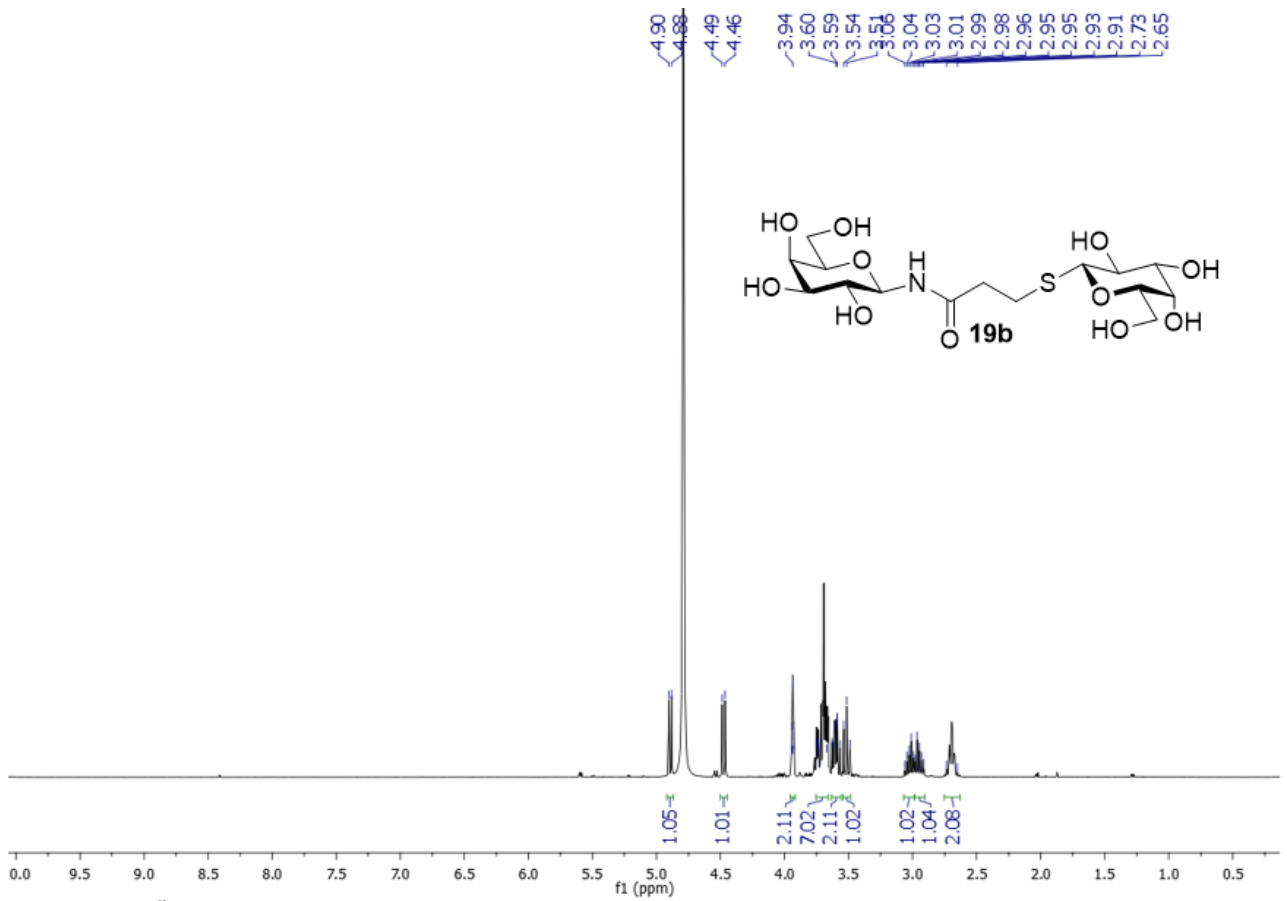
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61.1  
60.5

-36.4

-25.7



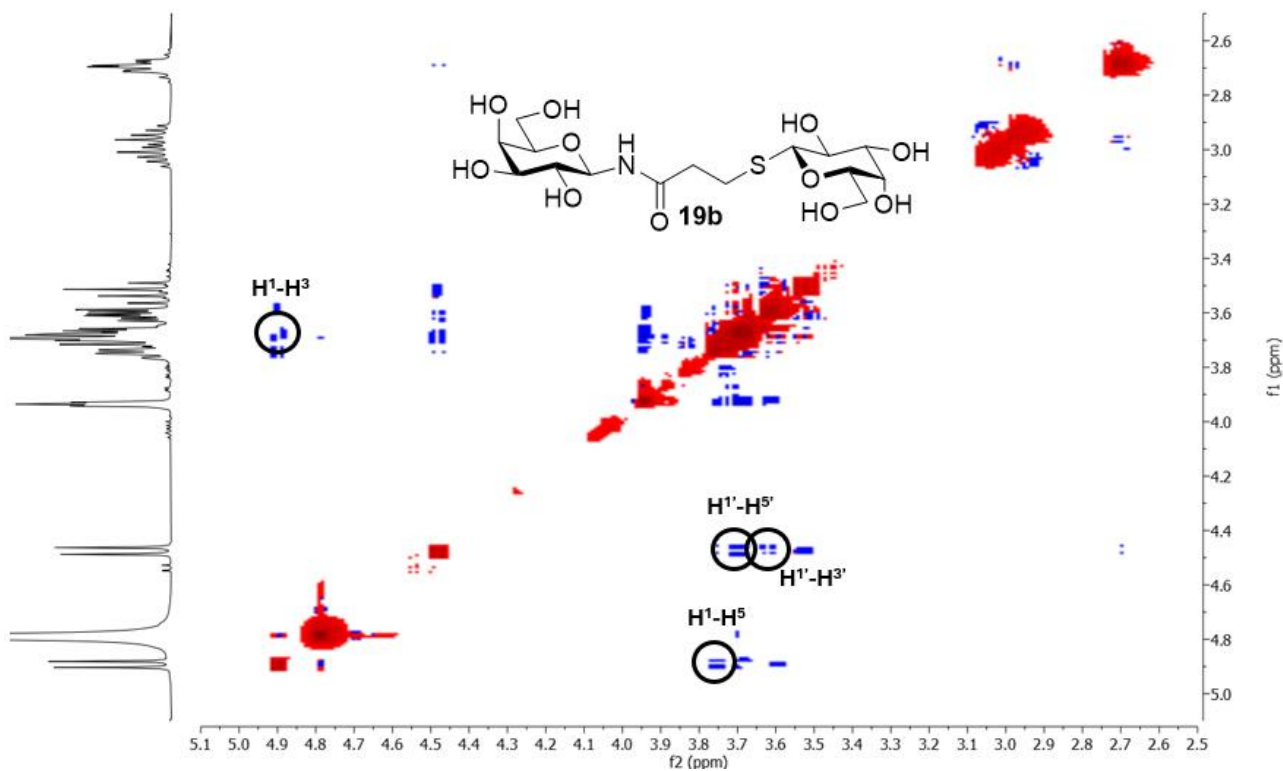
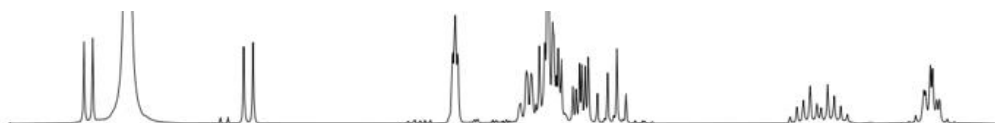
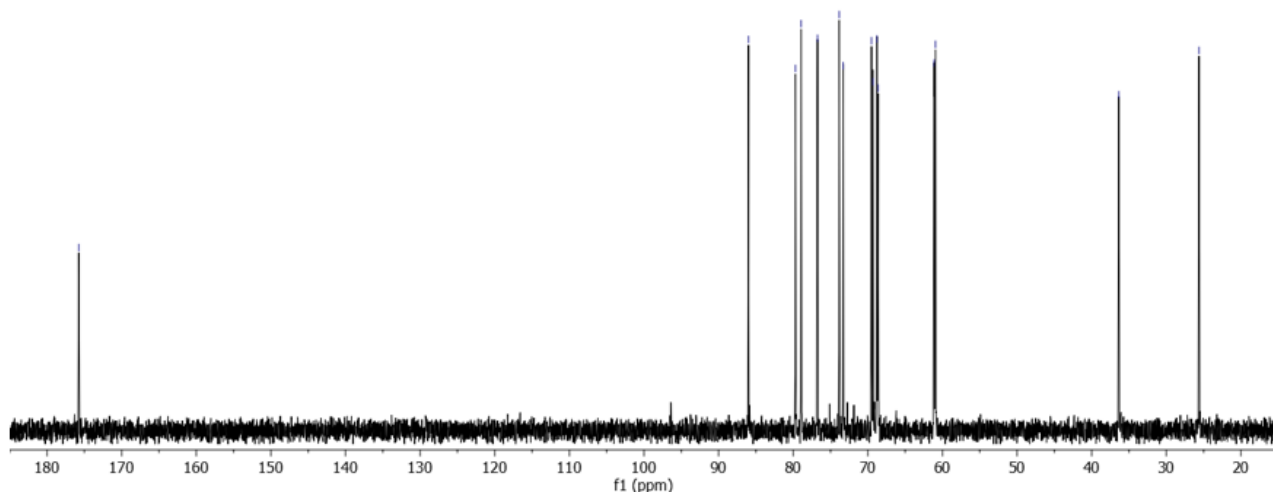
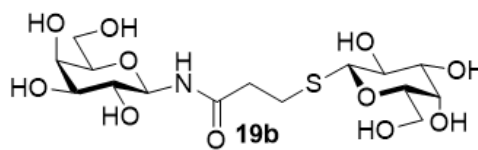


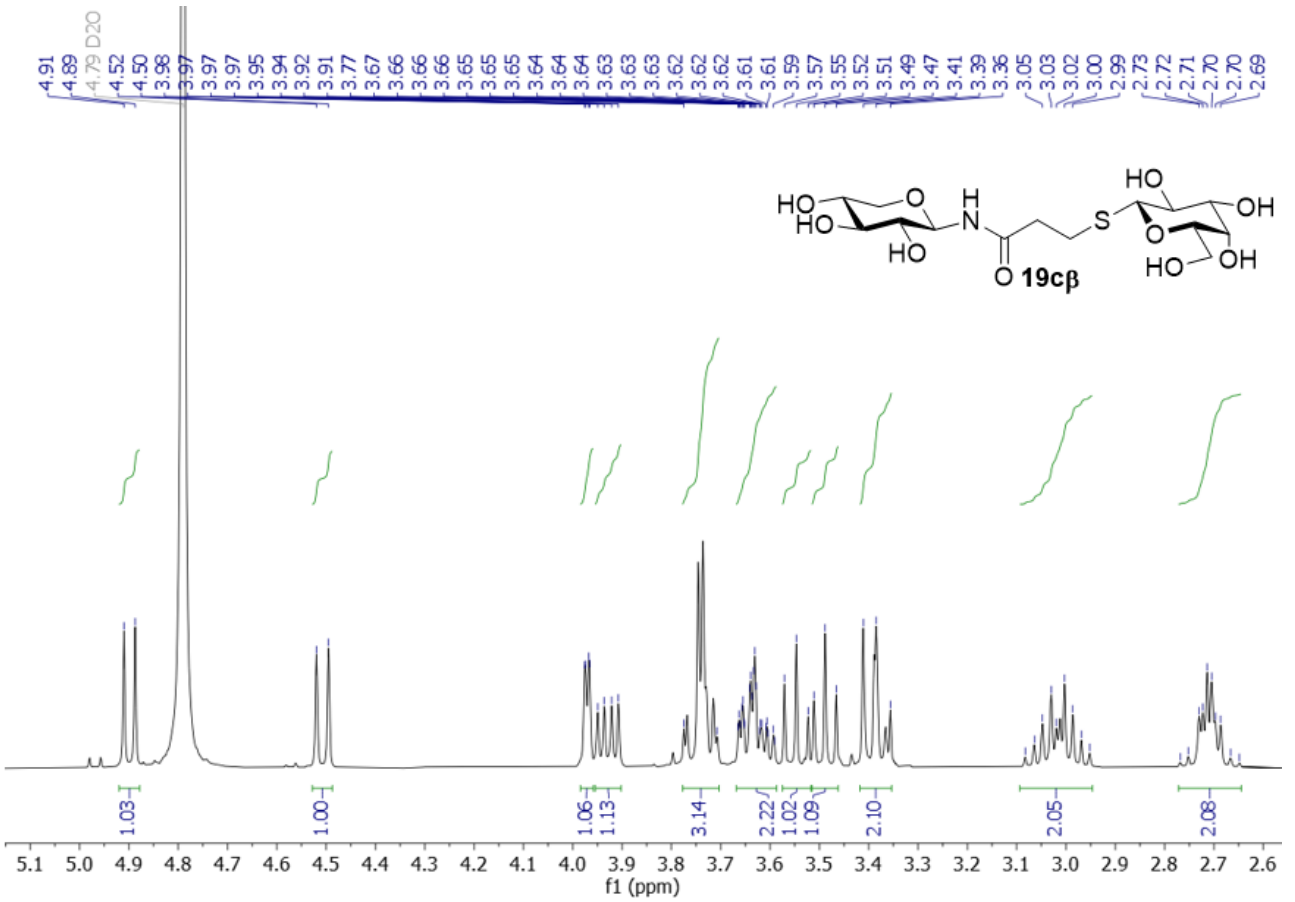
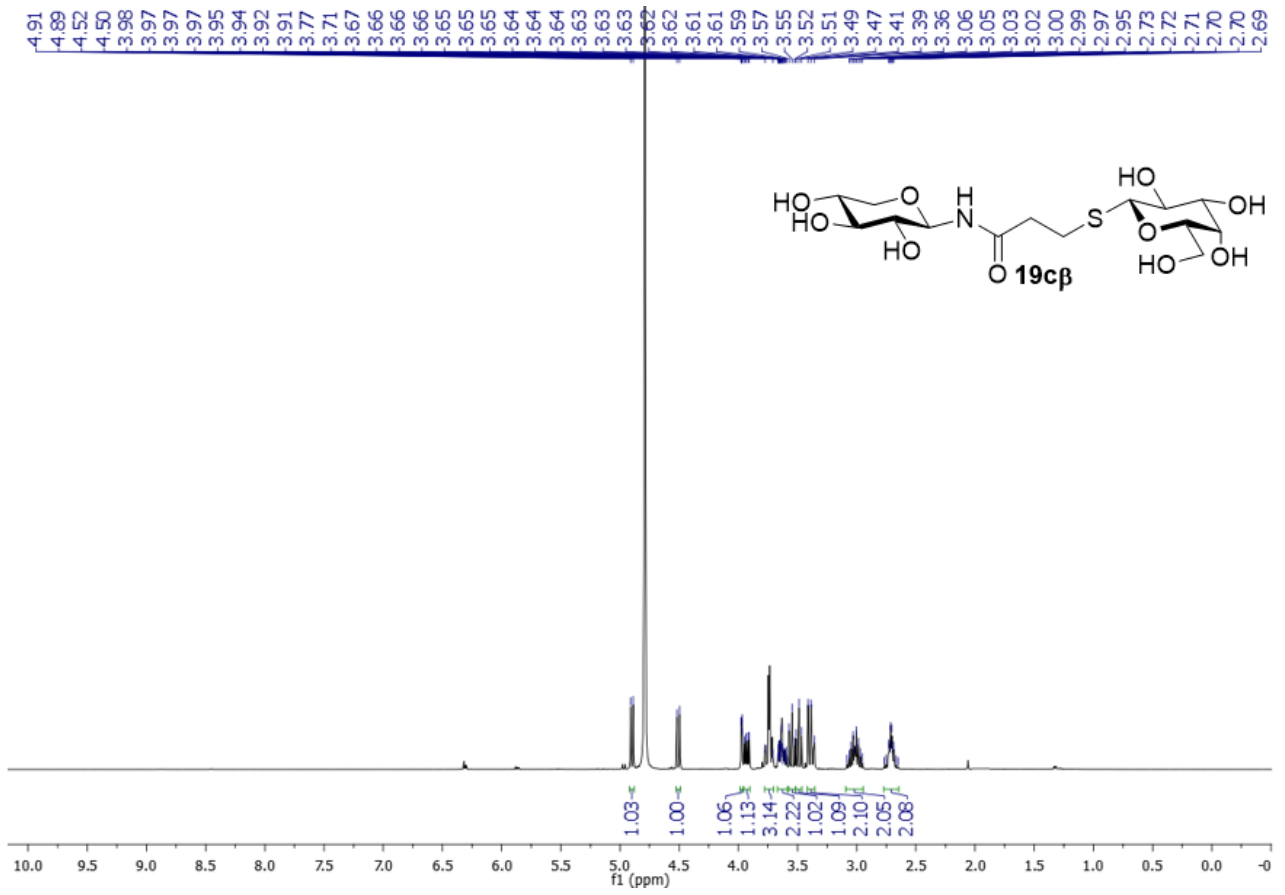
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73.3  
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69.3  
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68.6  
61.1  
60.9

-36.4

-25.6





-175.8

-86.2  
-80.0  
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-36.4

-25.9

