

**Supporting Information to:**

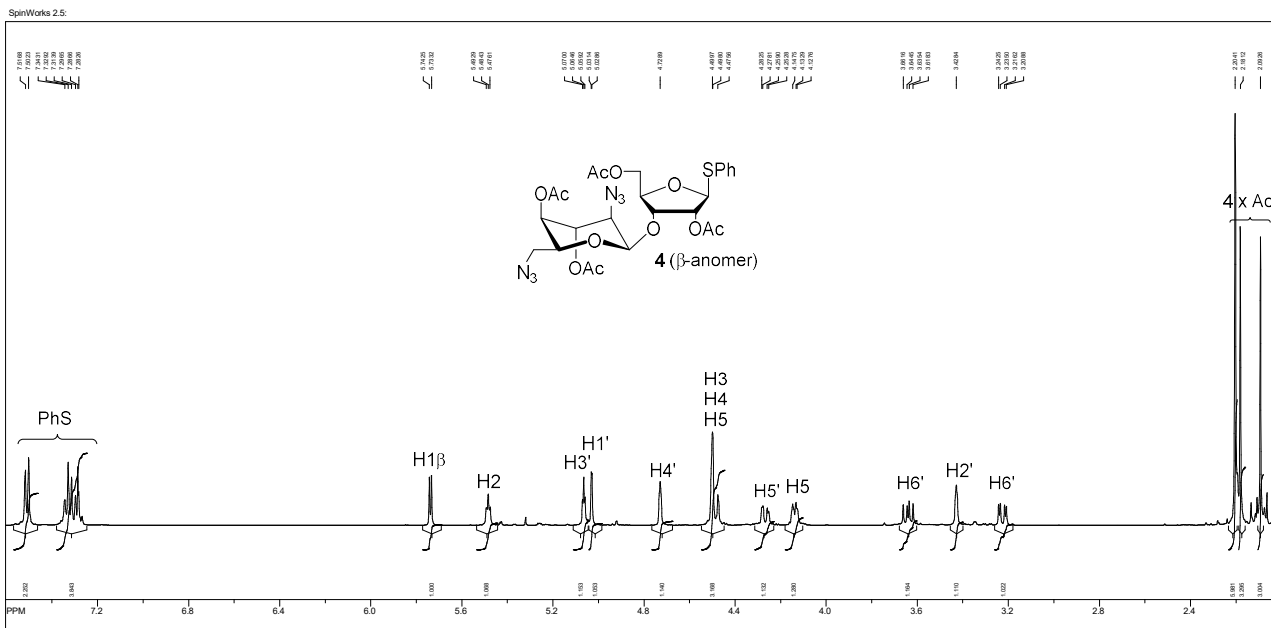
# **Synthesis of glycosidic (1''→3',4' and 6) site-isomers of neomycin B and their effect on RNA- and DNA-triplex stability**

Lotta Granqvist, Ville Tähtinen and Pasi Virta\*

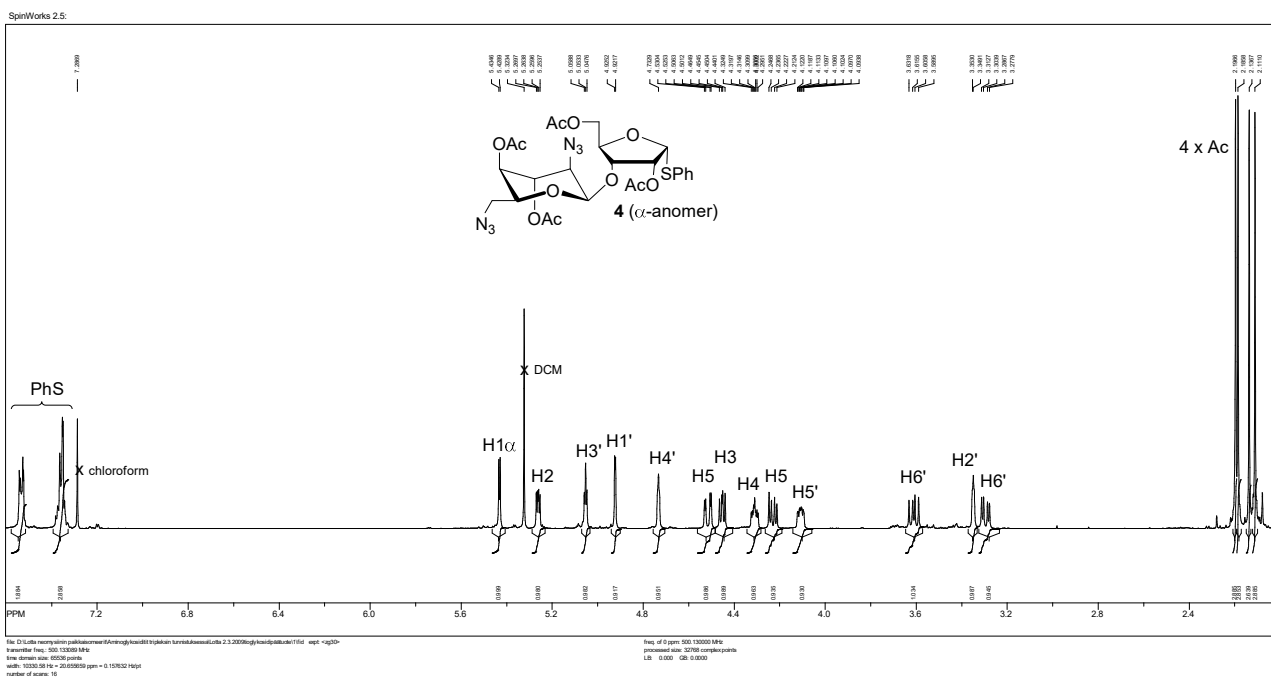
*Department of Chemistry, University of Turku, 20014 Turku, Finland*

## **Contents**

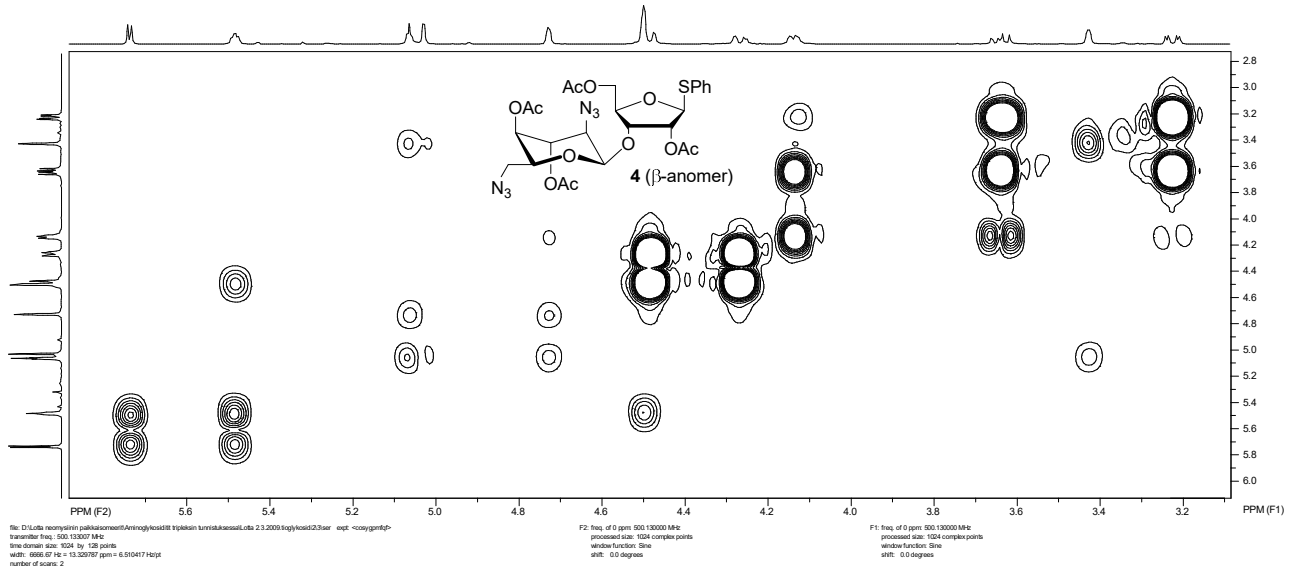
NMR spectra of <b>4</b>	<b>S2-S5</b>
NMR spectra of <b>6</b>	<b>S6-S7</b>
NMR spectra of <b>8</b>	<b>S8-S9</b>
NMR spectra of <b>9+10</b>	<b>S10-S12</b>
NMR spectra of <b>11</b>	<b>S13-S14</b>
NMR spectra of <b>12</b>	<b>S15-S16</b>
NMR spectra of <b>13</b>	<b>S17-S18</b>
NMR spectra of <b>14</b>	<b>S19-S20</b>
NMR spectra of <b>15</b>	<b>S21-S22</b>
NMR spectra of <b>16</b>	<b>S23-S24</b>
NMR spectra of <b>20</b>	<b>S25-S26</b>
NMR spectra of <b>21</b>	<b>S27-S28</b>
NMR spectra of <b>22</b>	<b>S29-S30</b>
NMR spectra of <b>23</b>	<b>S31-S32</b>
NMR spectra of <b>24</b>	<b>S33-S34</b>
NMR spectra of <b>25</b>	<b>S35-S36</b>



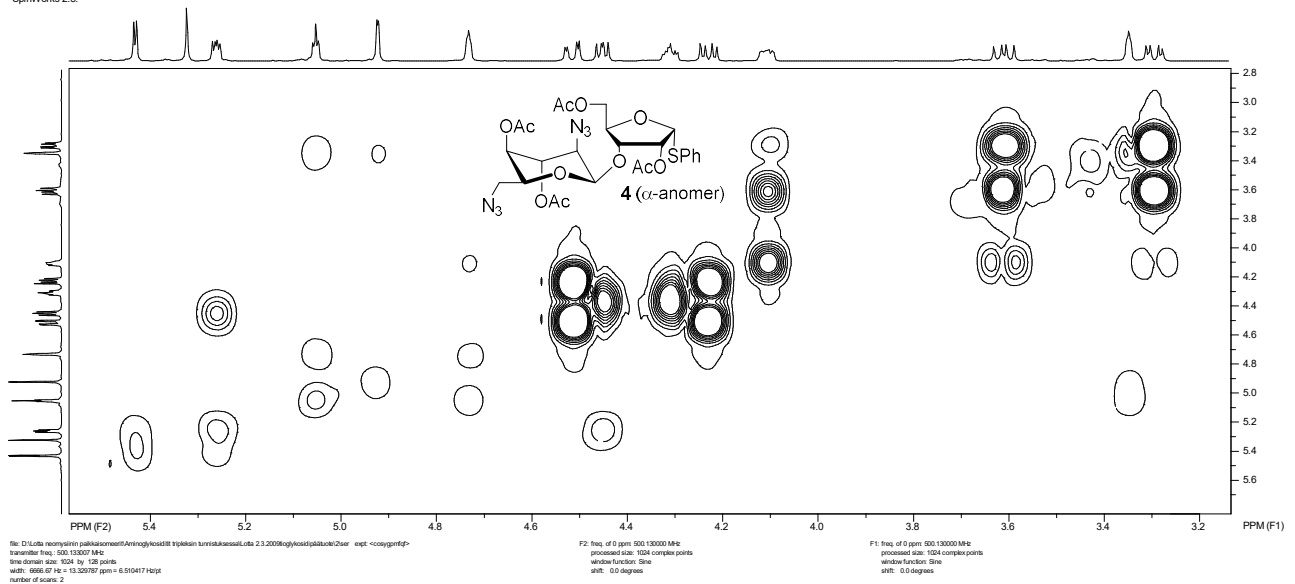
**Figure S1.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of 4 ( $\beta$ -anomer).



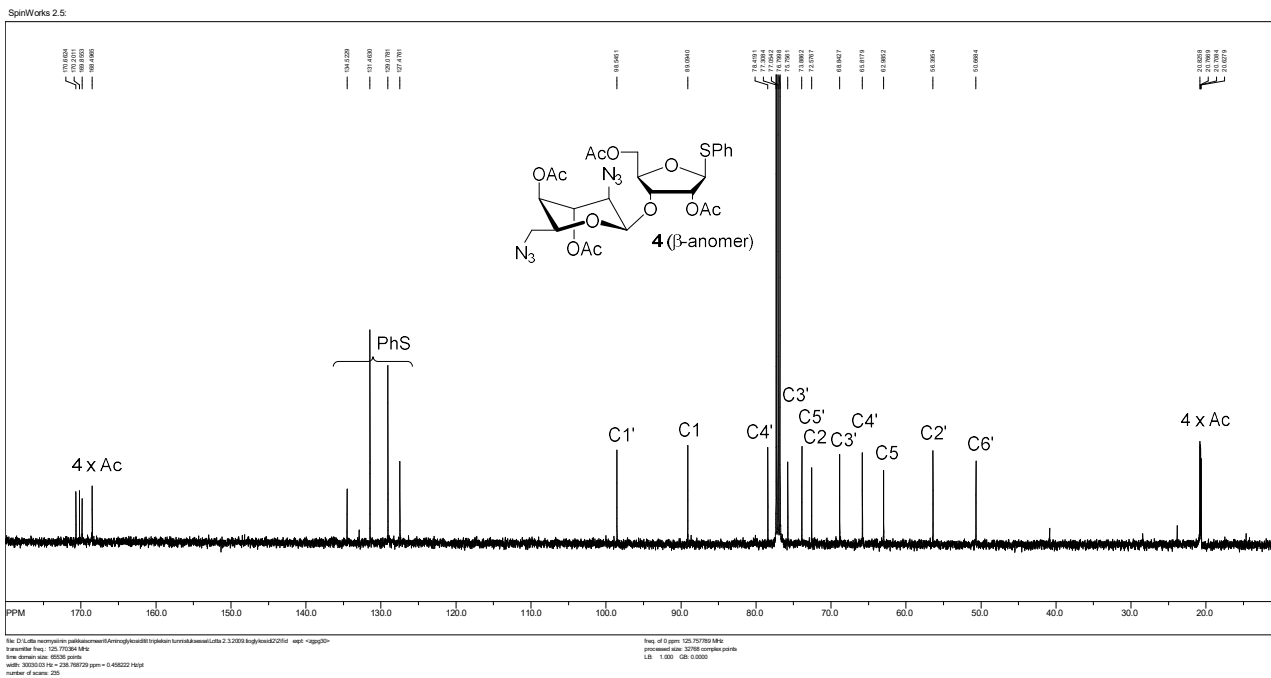
**Figure S2.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of 4 ( $\alpha$ -anomer).



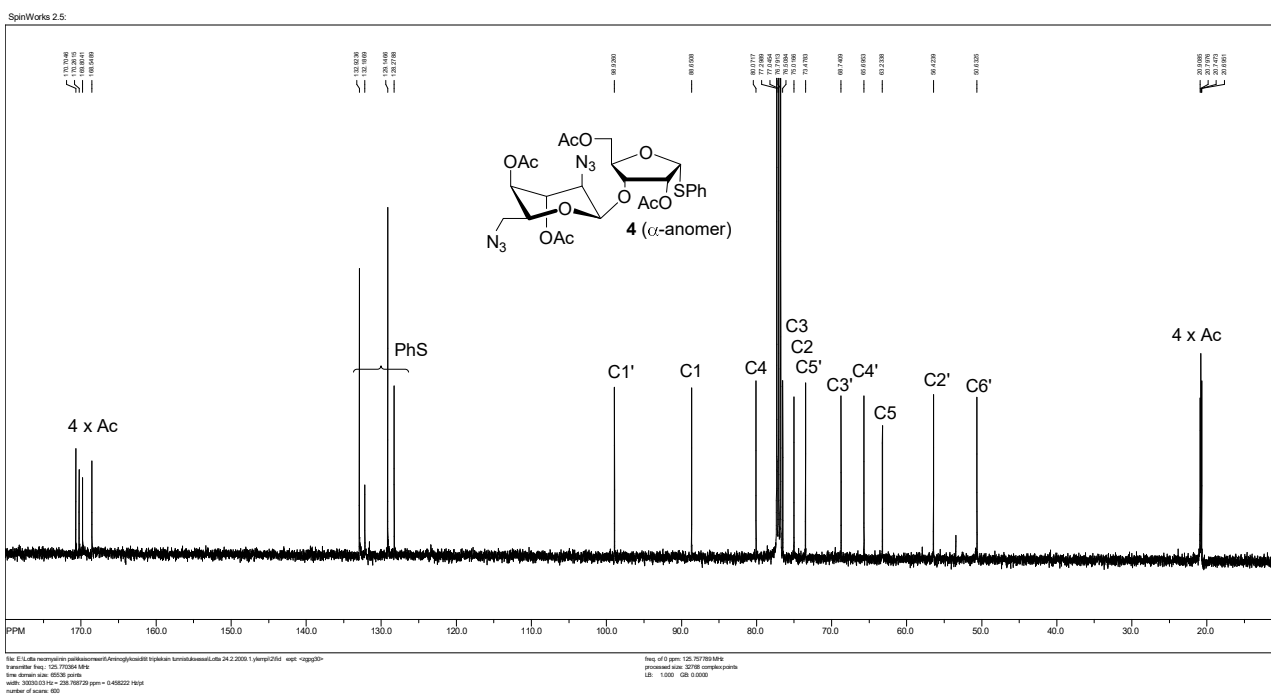
**Figure S3.** COSY spectrum of **4** ( $\beta$ -anomer).



**Figure S4.** COSY spectrum of **4** ( $\alpha$ -anomer).

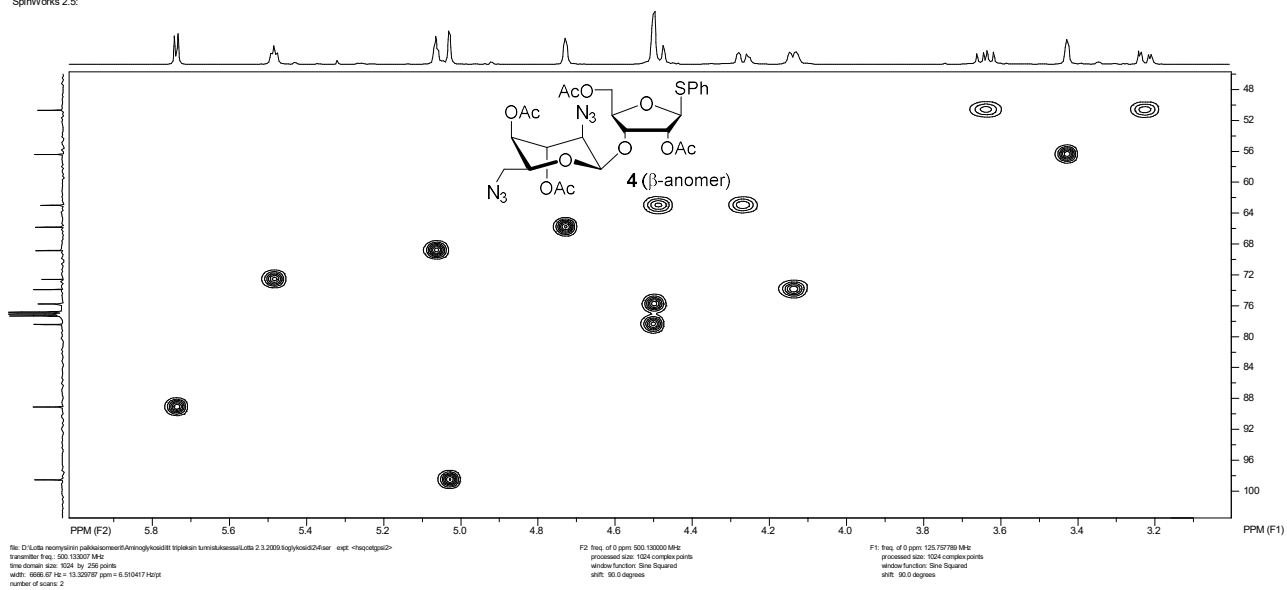


**Figure S5.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of **4** ( $\beta$ -anomer).



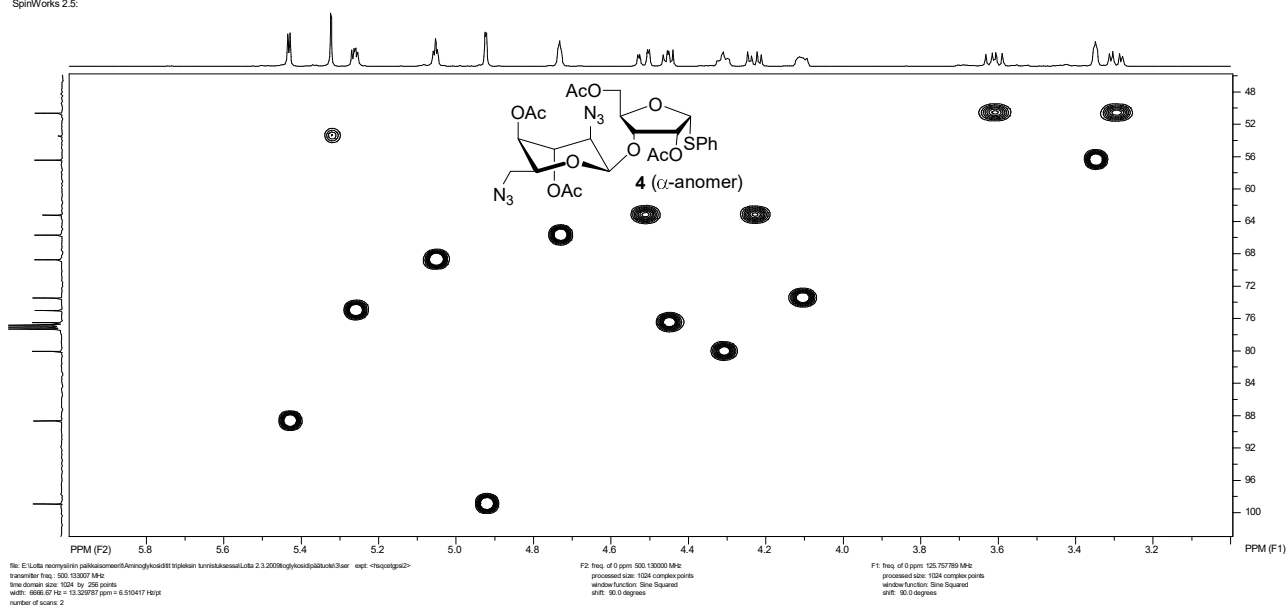
**Figure S6.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of **4** ( $\alpha$ -anomer).

SpinWorks 2.5:



**Figure S7.** HSQC spectrum of 4 (β-anomer).

SpinWorks 2.5:



**Figure S8.** HSQC spectrum of 4 (α-anomer).

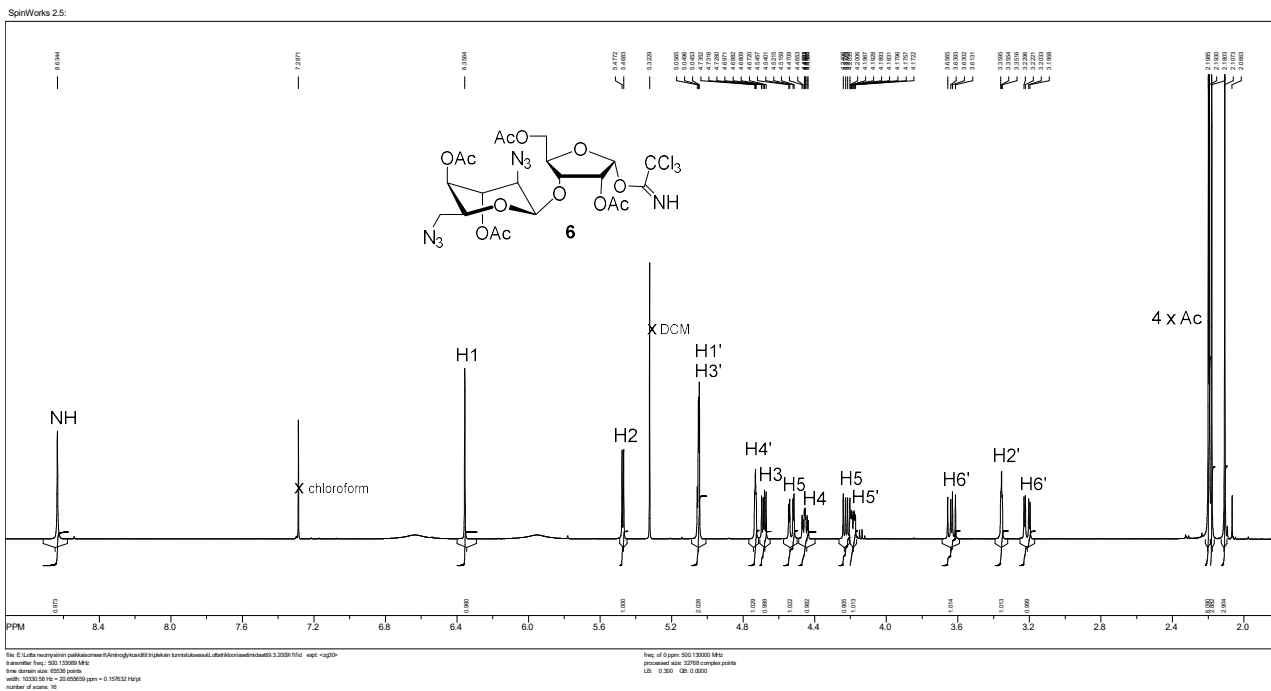


Figure S9. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of 6.

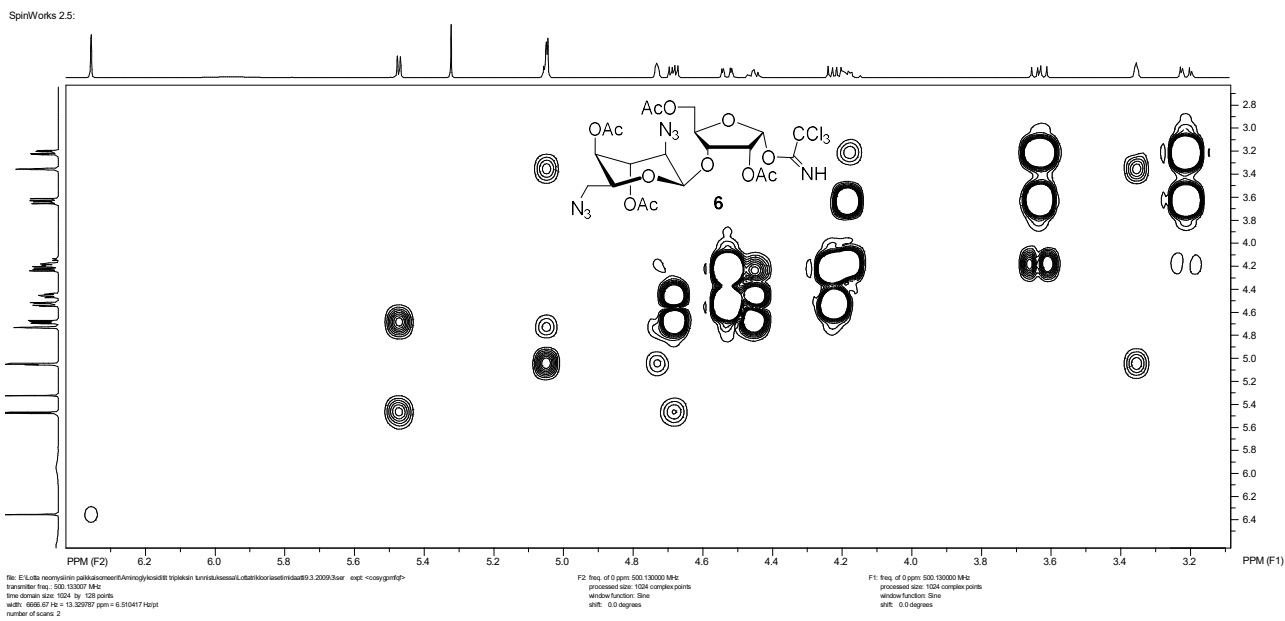
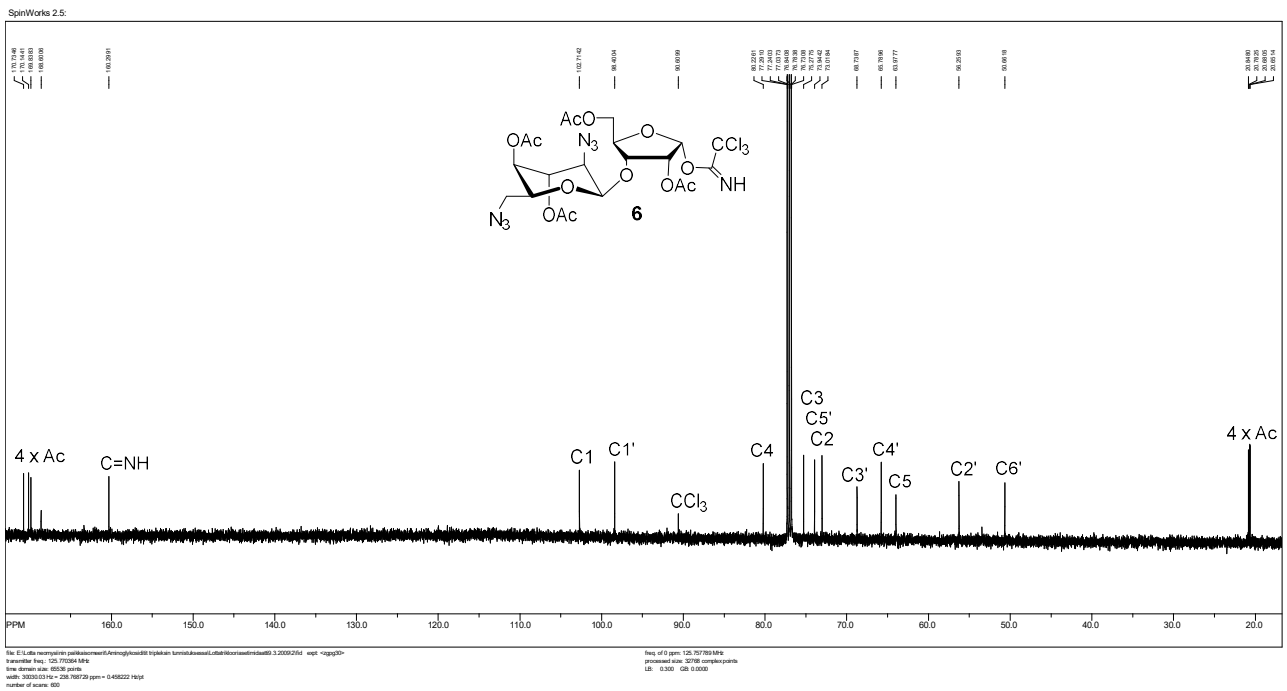
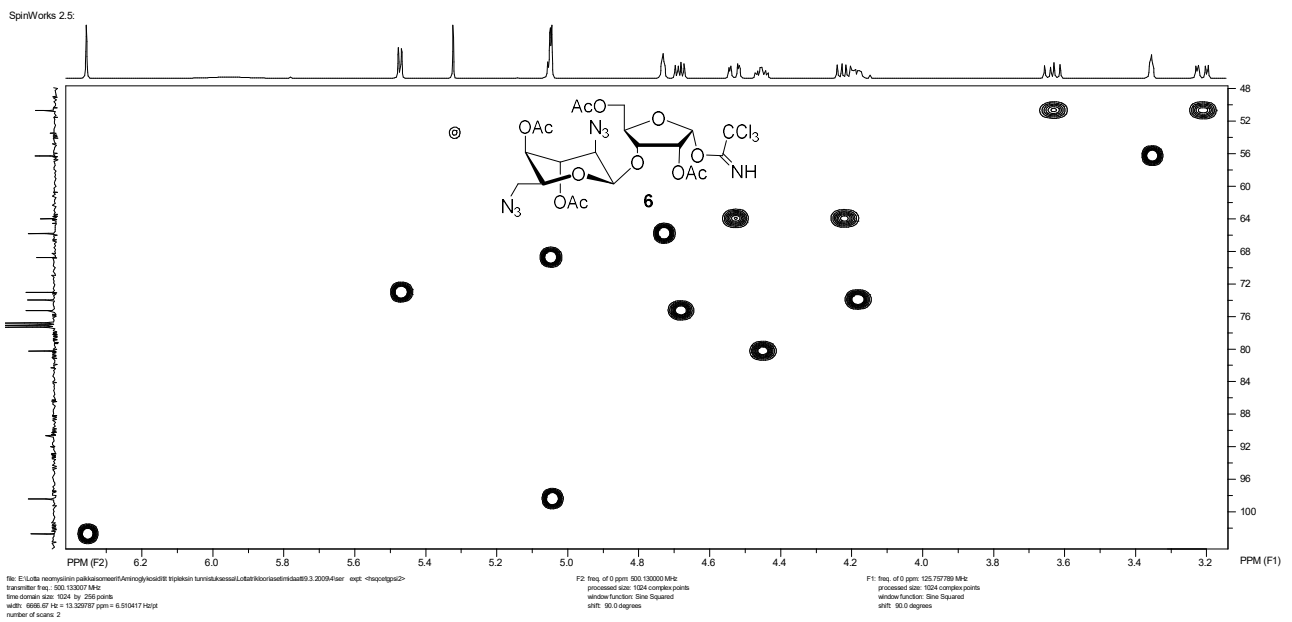


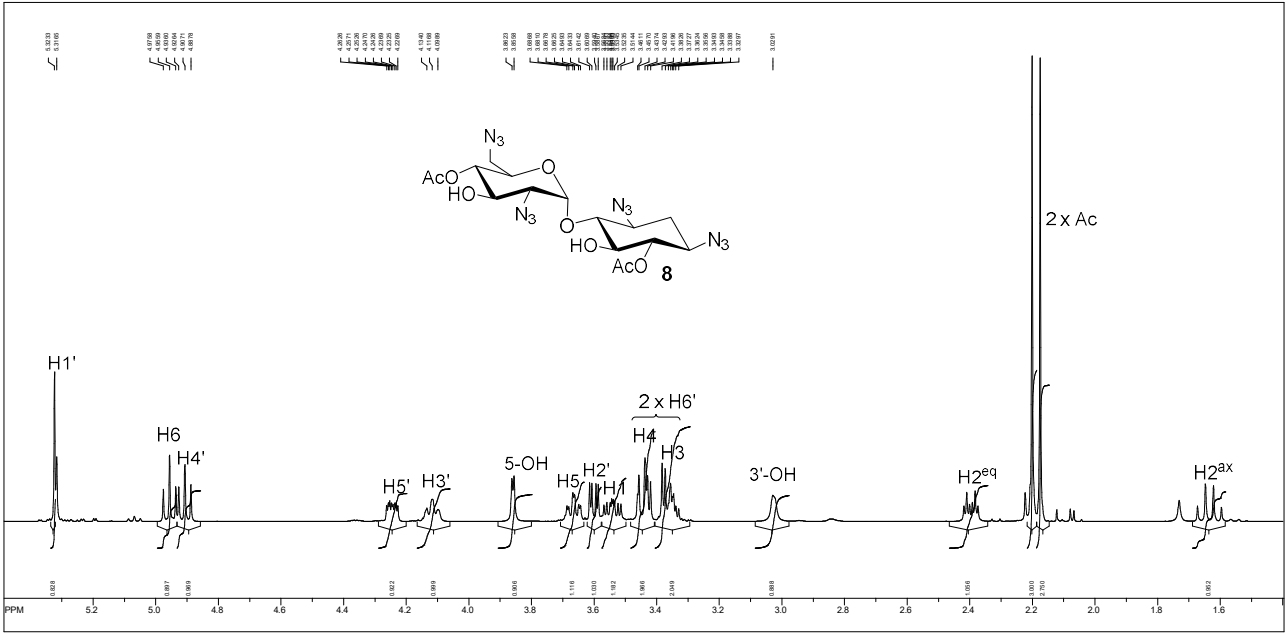
Figure S10. COSY-spectrum of 6.



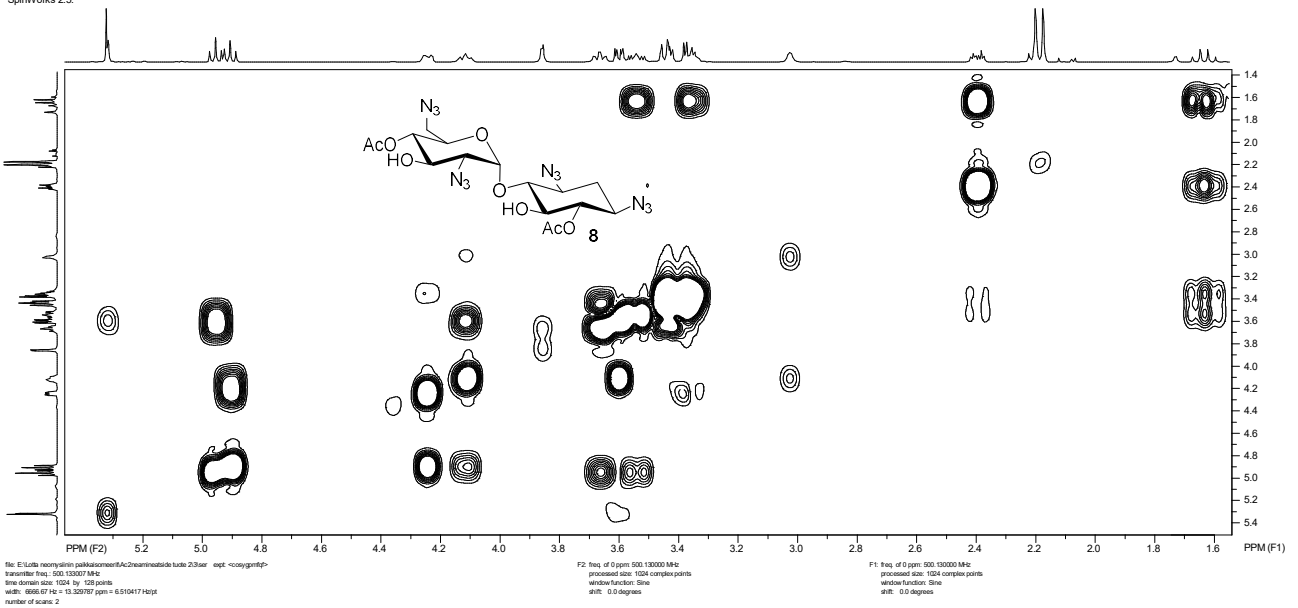
**Figure S11.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of **6**.



**Figure S12.** HSQC spectrum of **6**.



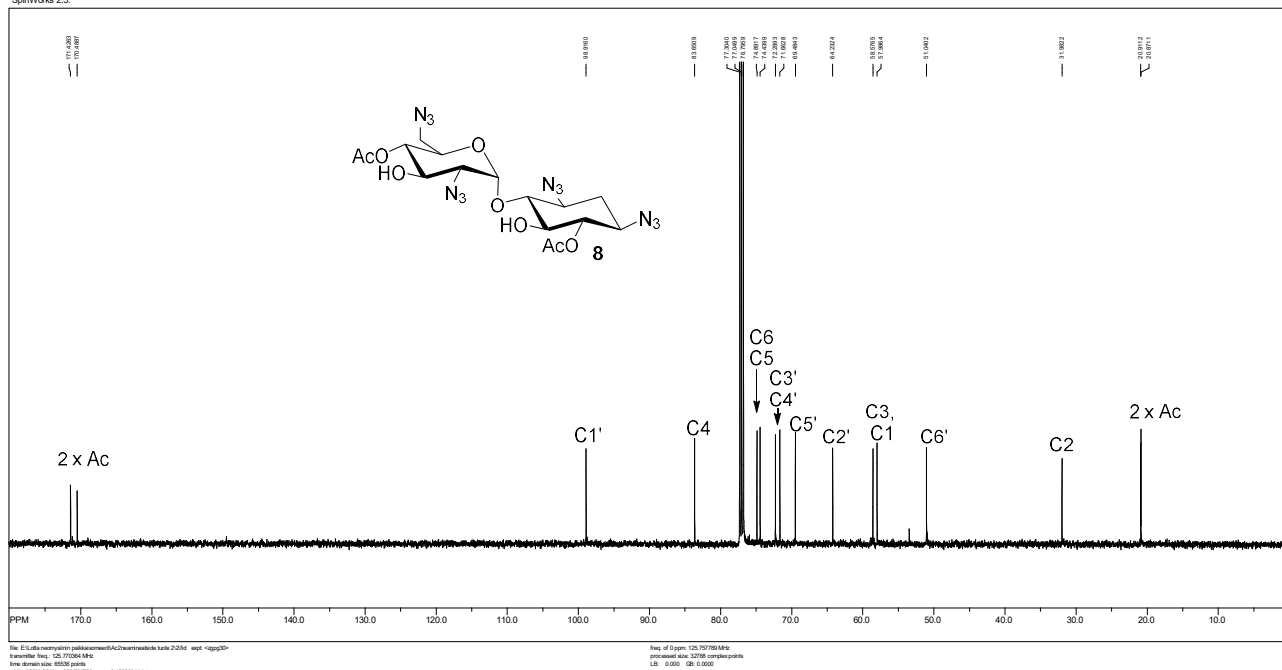
**Figure S13.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **8**.



**Figure S14.** COSY spectrum of **8**.

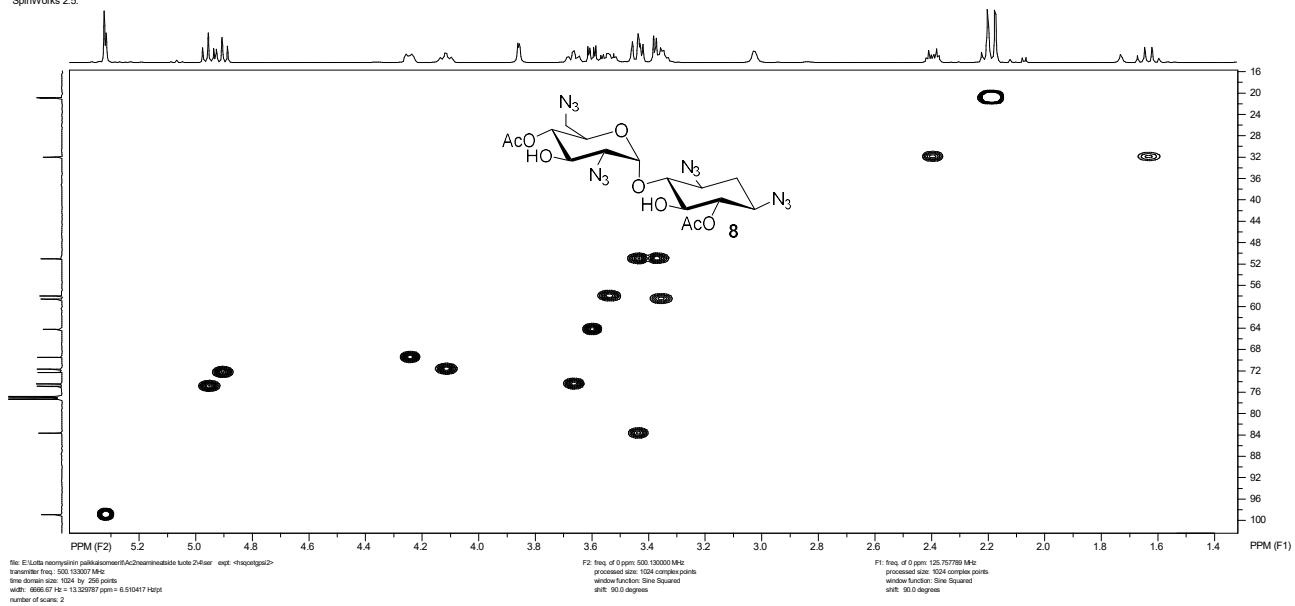


SpinWorks 2.5.

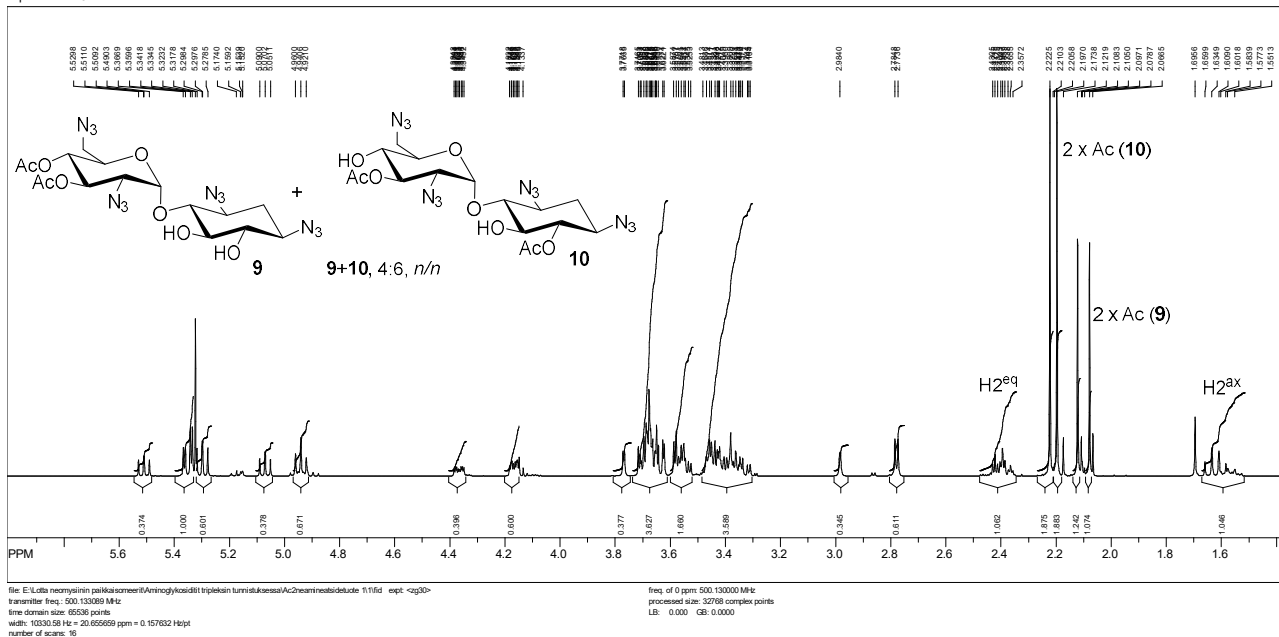
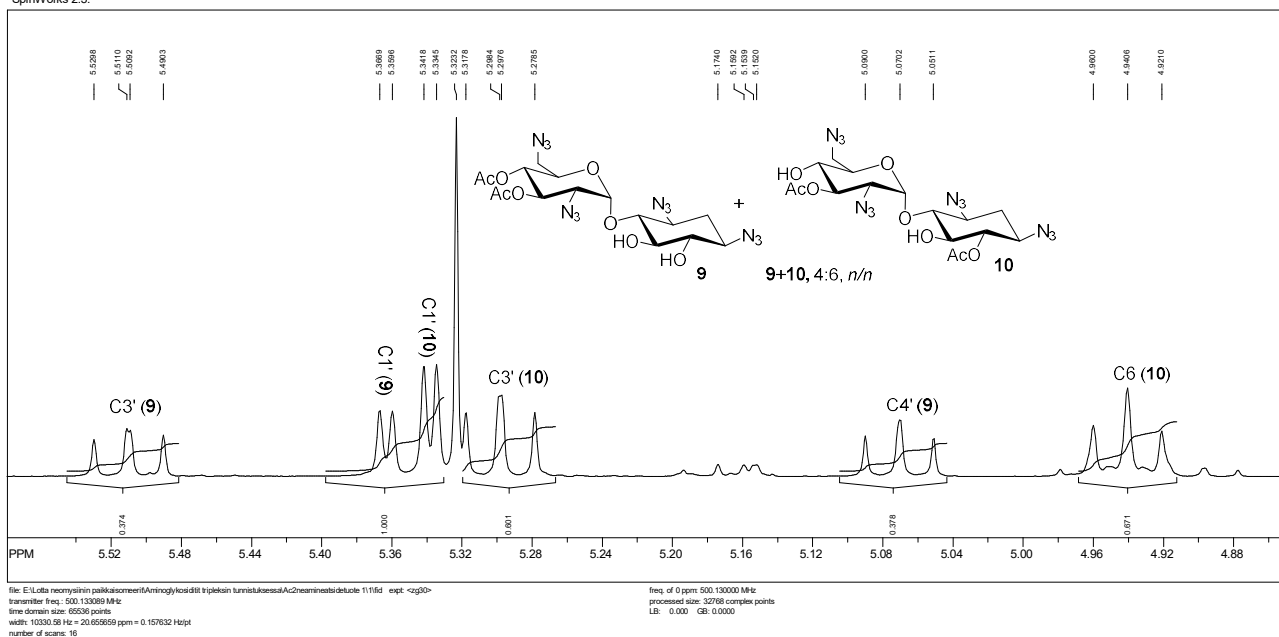


**Figure S15.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of **8**.

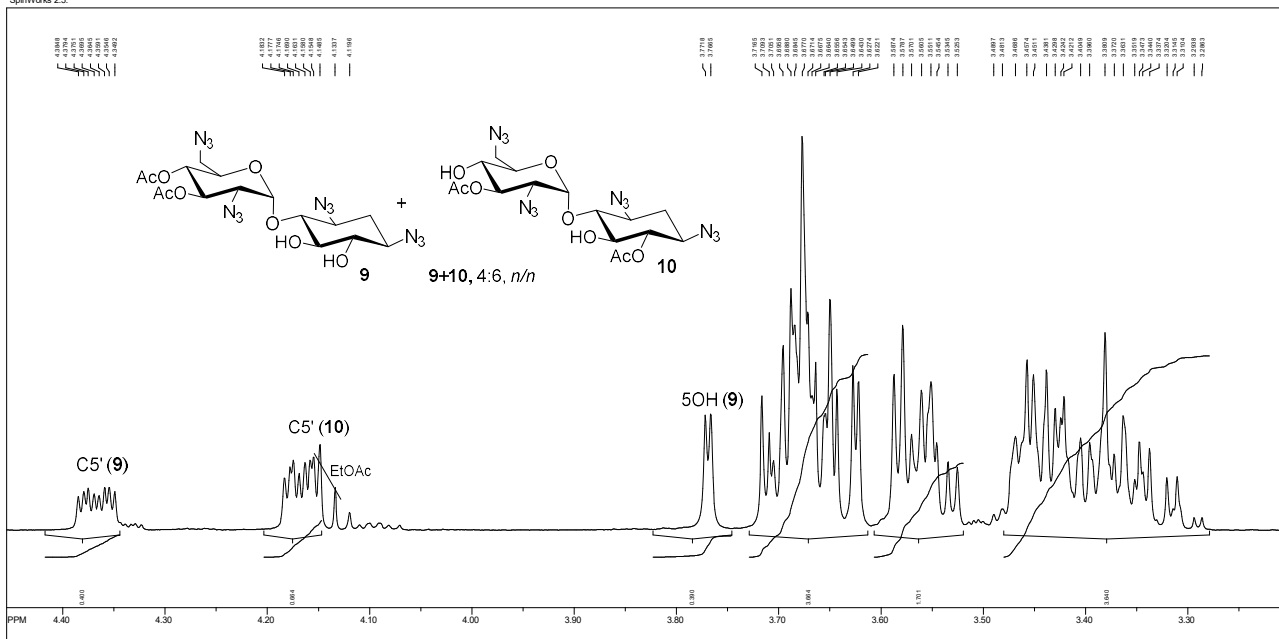
SpinWorks 2.5.



**Figure S16.** HSQC spectrum of **8**.

Figure S17.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **9** + **10**.Figure S18.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **9** + **10**.

SpinWorks 2.5.

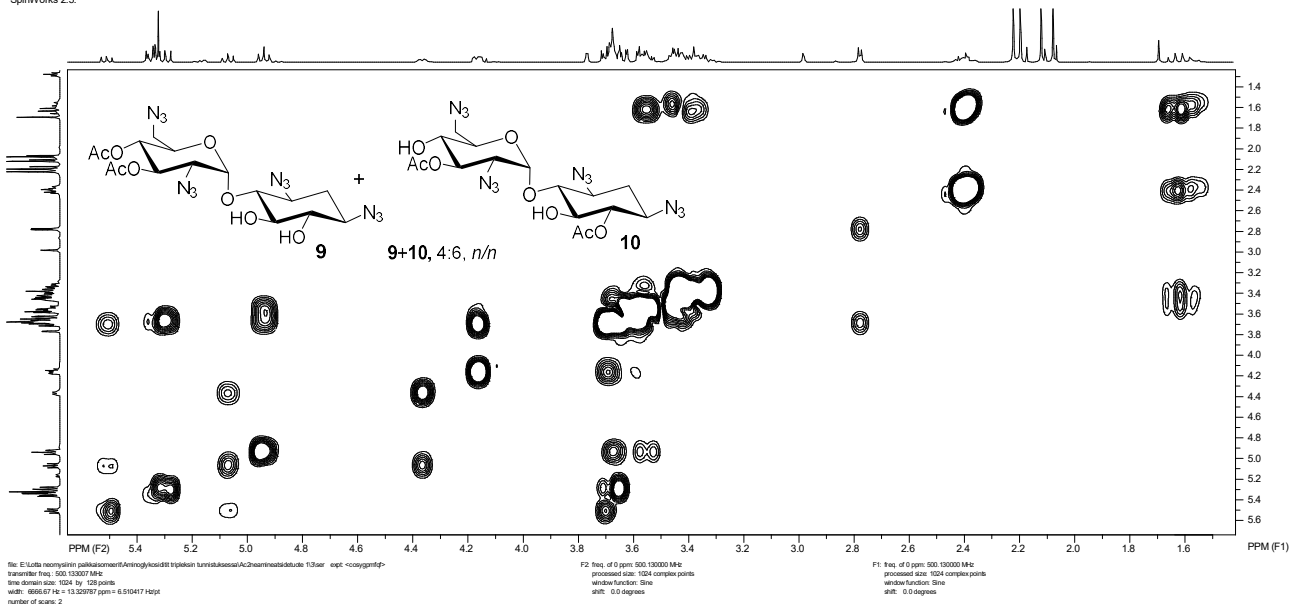


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 time domain size: 65536 points  
 width: 13330.58 Hz = 26.661159 ppm = 0.167632 Hz/pt  
 number of scans: 32

freq of 0 ppm: 500.130000 MHz  
 processed size: 32768 complex points  
 LR: 0.0000 GB 0.00000

**Figure S19.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **9** + **10**.

SpinWorks 2.5.



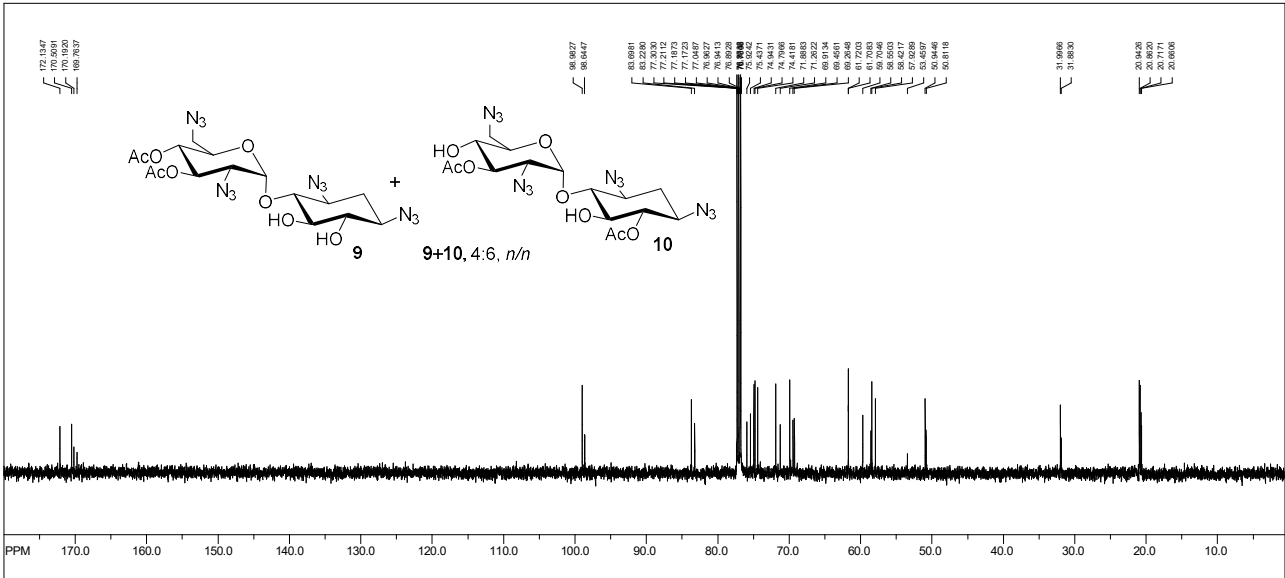
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 transmitter freq: 500.130000 MHz  
 time domain size: 1024 by 128 points  
 width: 8666.87 Hz = 17.333757 ppm = 0.151417 Hz/pt  
 number of scans: 2

F2: freq of 0 ppm: 500.130000 MHz  
 processed size: 1024 complex points  
 window function: Sine  
 shift: 0.0 degrees

F1: freq of 0 ppm: 500.130000 MHz  
 processed size: 1024 complex points  
 window function: Sine  
 shift: 0.0 degrees

**Figure S20.** COSY spectrum of **9** + **10**.

SpinWorks 2.5:

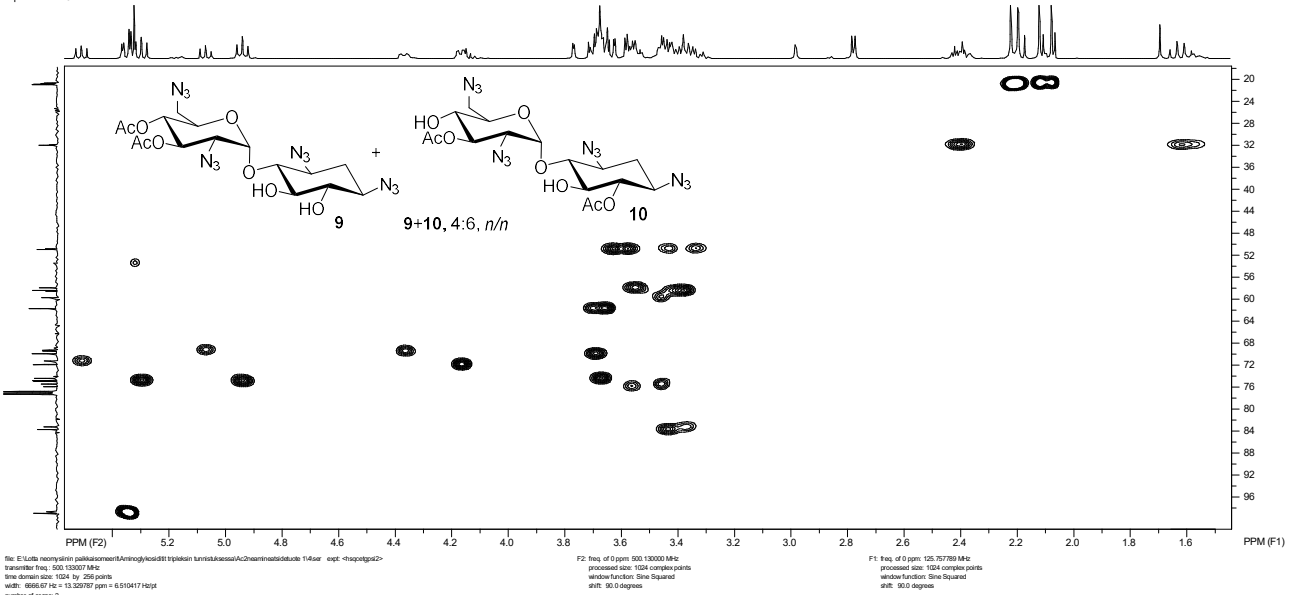


file: E:\Lotta neomycinin palikkaosmitti\Amnoglykosidit\triplekin tunnistuksessa\Ac2neaminestadiidit\126fd exp: <agg3D>  
 transmitter freq: 125.757364 MHz  
 time domain size: 65536 points  
 width: 30030.03 Hz = 238.768729 ppm = 0.458222 Hz/pt  
 number of scans: 163

freq: 0 ppm: 125.757789 MHz  
 processed size: 32768 complex points  
 LS: 0.000 GB: 0.0000

Figure S21.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of 9 + 10.

SpinWorks 2.5:

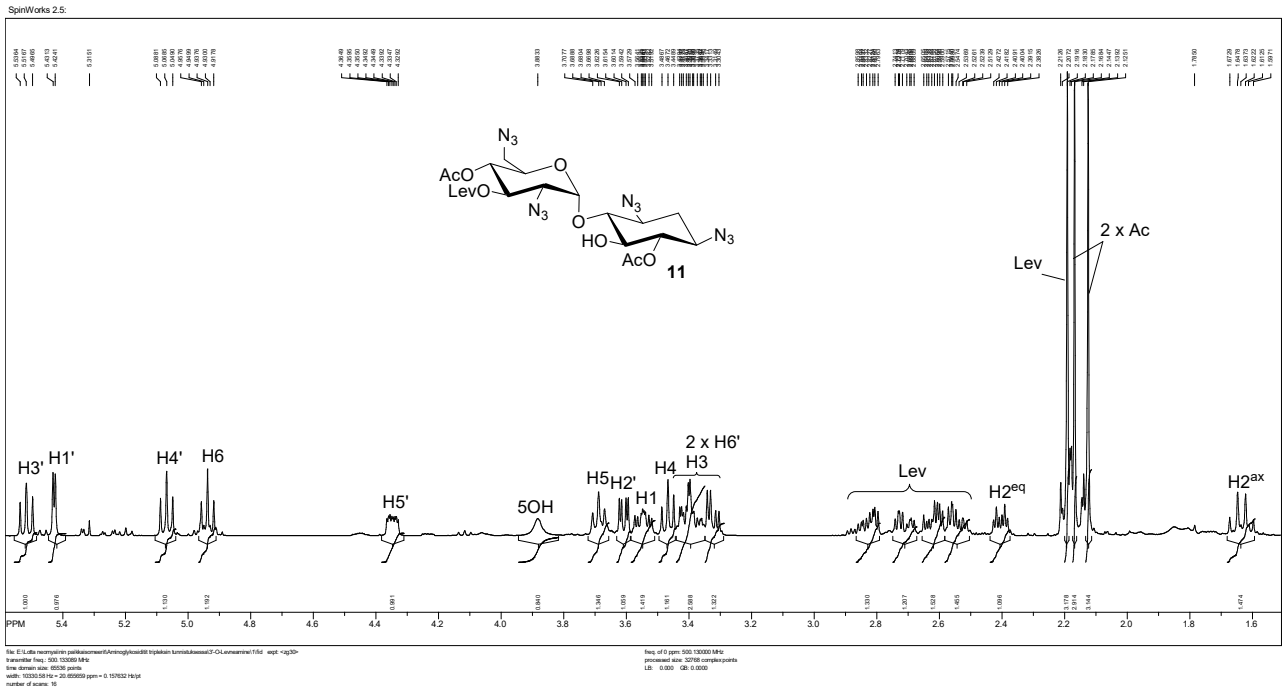


file: E:\Lotta neomycinin palikkaosmitti\Amnoglykosidit\triplekin tunnistuksessa\Ac2neaminestadiidit\148or exp: <hsqptgs2>  
 transmitter freq: 500.133073 MHz  
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 width: 99957 Hz = 79.529787 ppm = 6.510417 Hz/pt  
 number of scans: 2

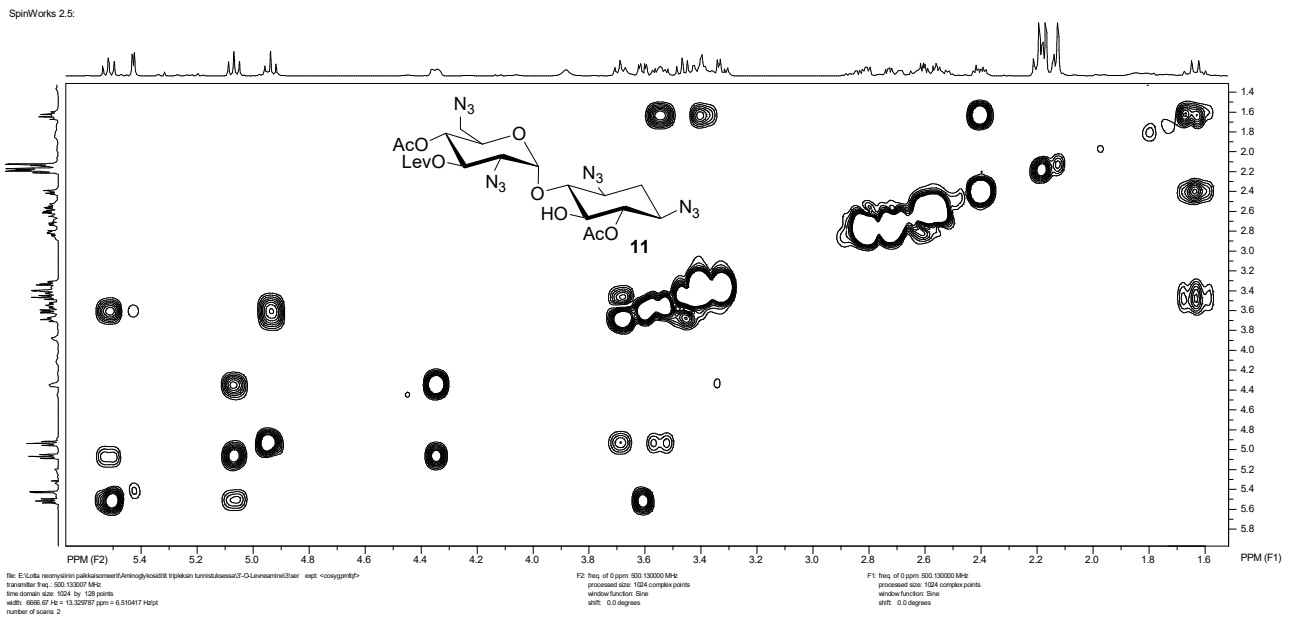
F2: freq: 0 ppm: 500.130000 MHz  
 processed size: 1024 complex points  
 window function: Sine Squared  
 shift: 90.0 degrees

F1: freq: 0 ppm: 125.757789 MHz  
 processed size: 1024 complex points  
 window function: Sine Squared  
 shift: 90.0 degrees

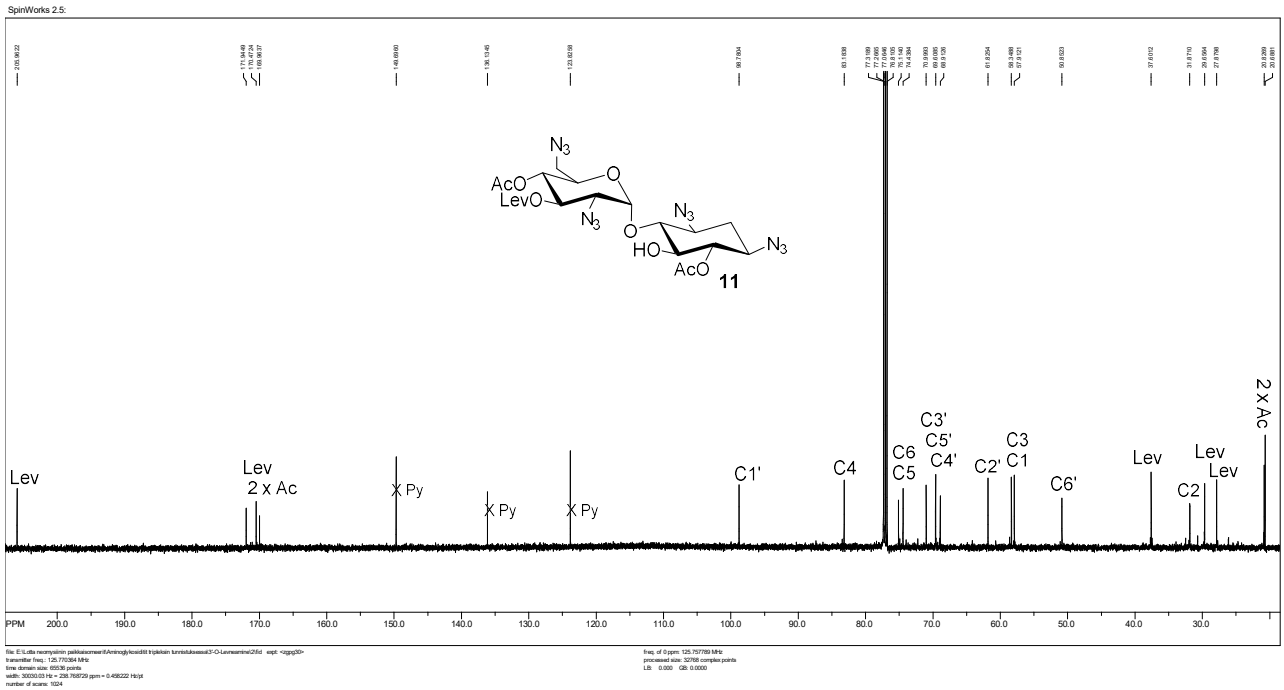
Figure S22. HSQC spectrum of 9 + 10.



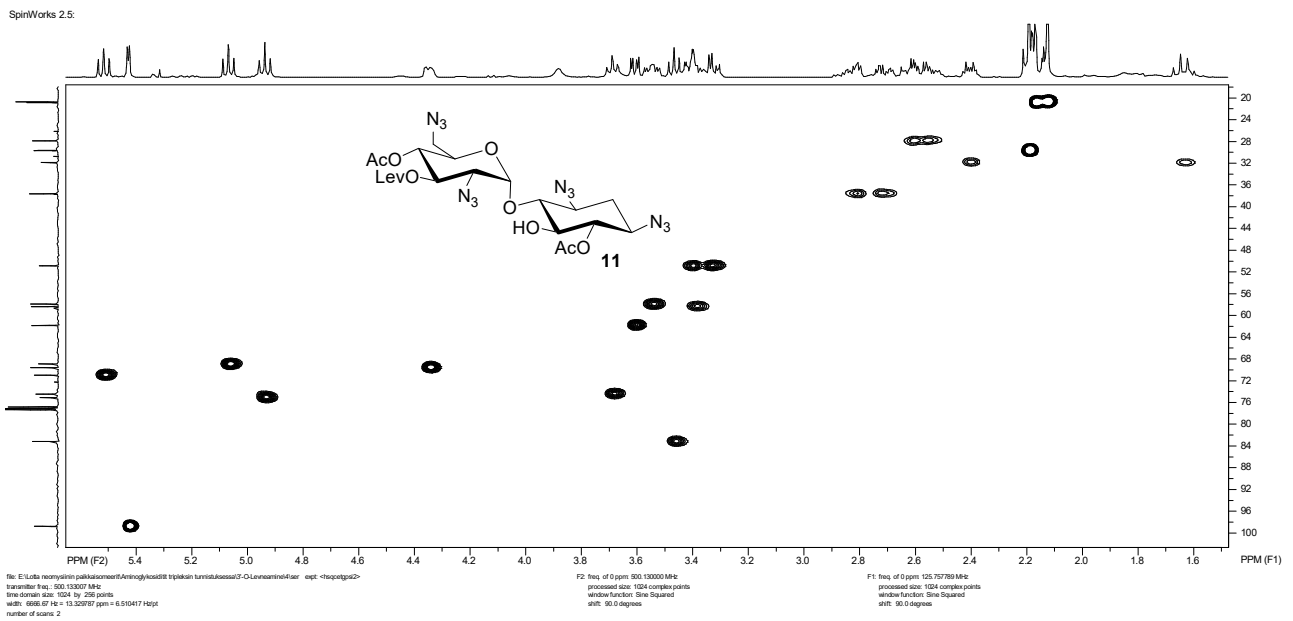
**Figure S23.**  $^1H$  NMR (500 MHz,  $CDCl_3$ ) spectrum of **11**.



**Figure S24.** COSY pectrum of **11**.

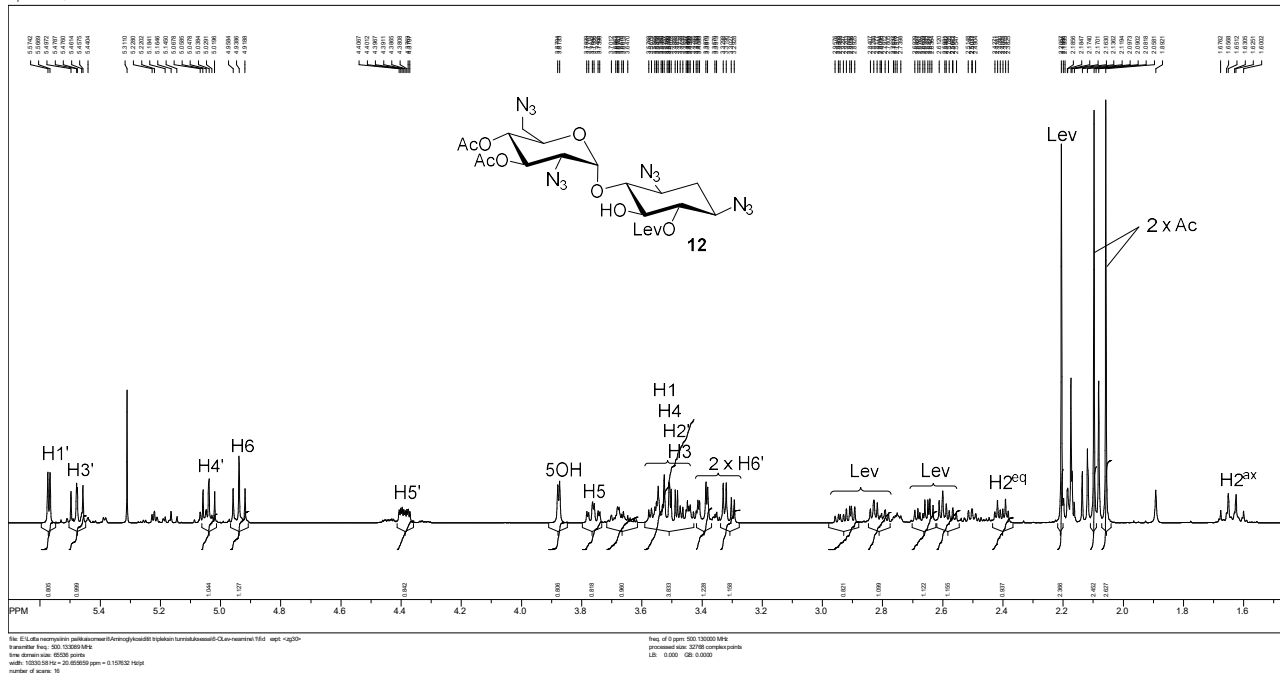


**Figure S25.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of **11**.

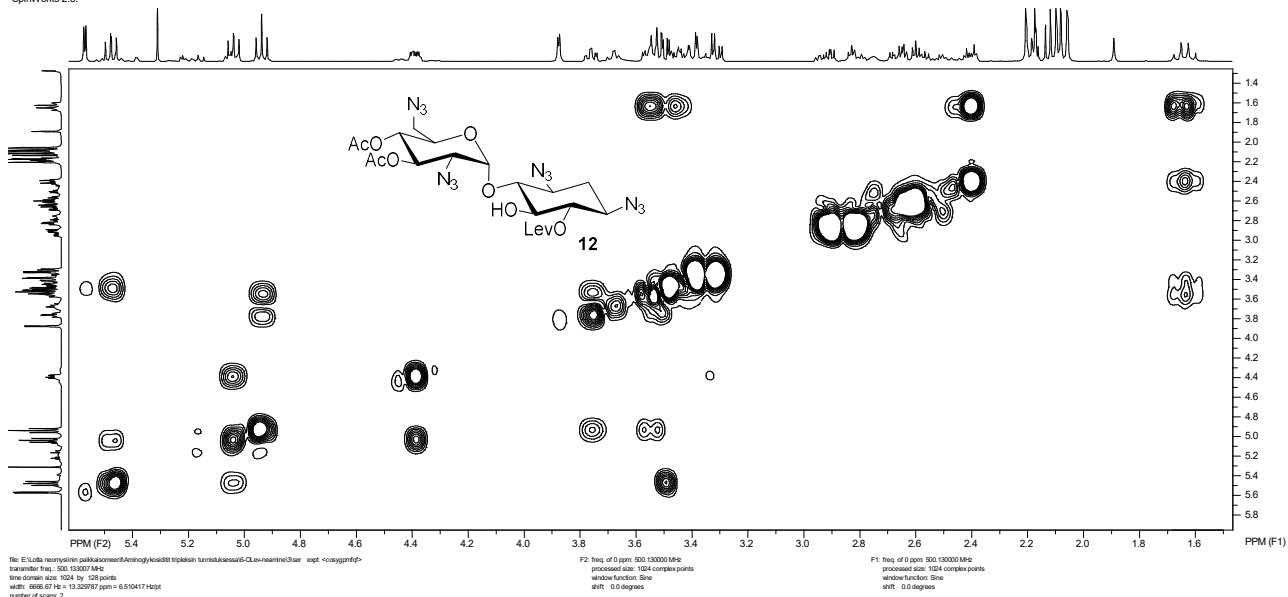


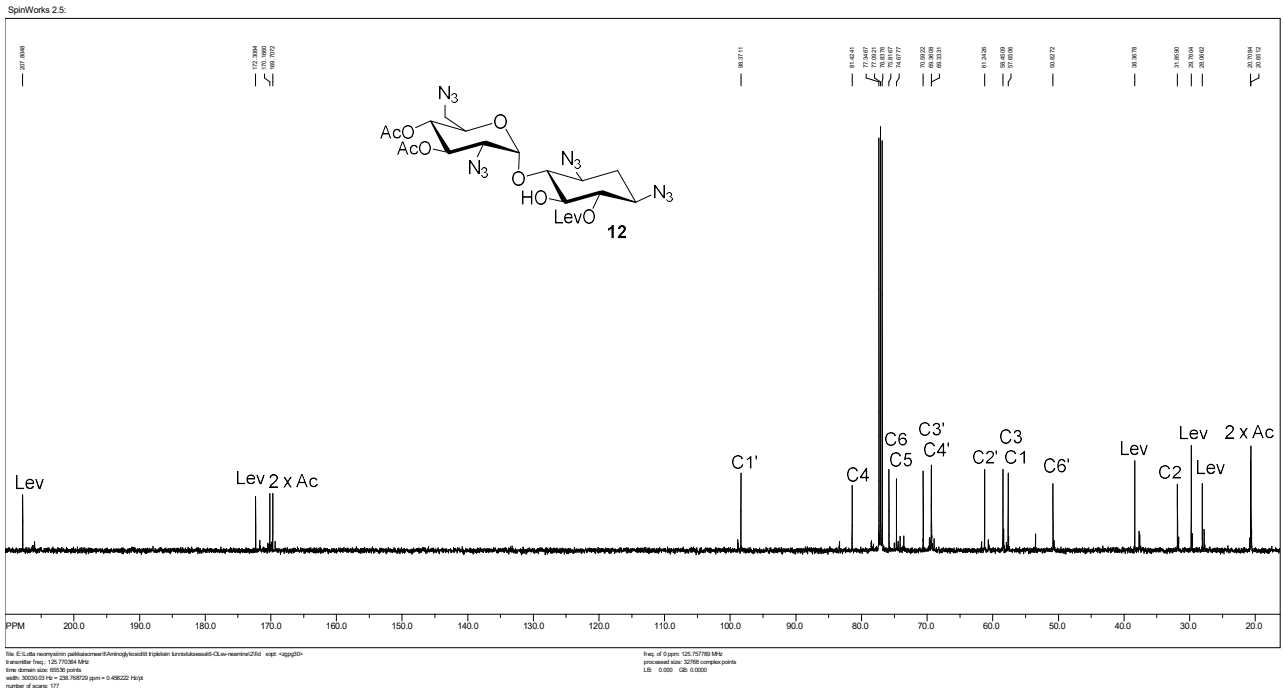
**Figure S26.** HSQC spectrum of **11**.

SpinWorks 2.5:

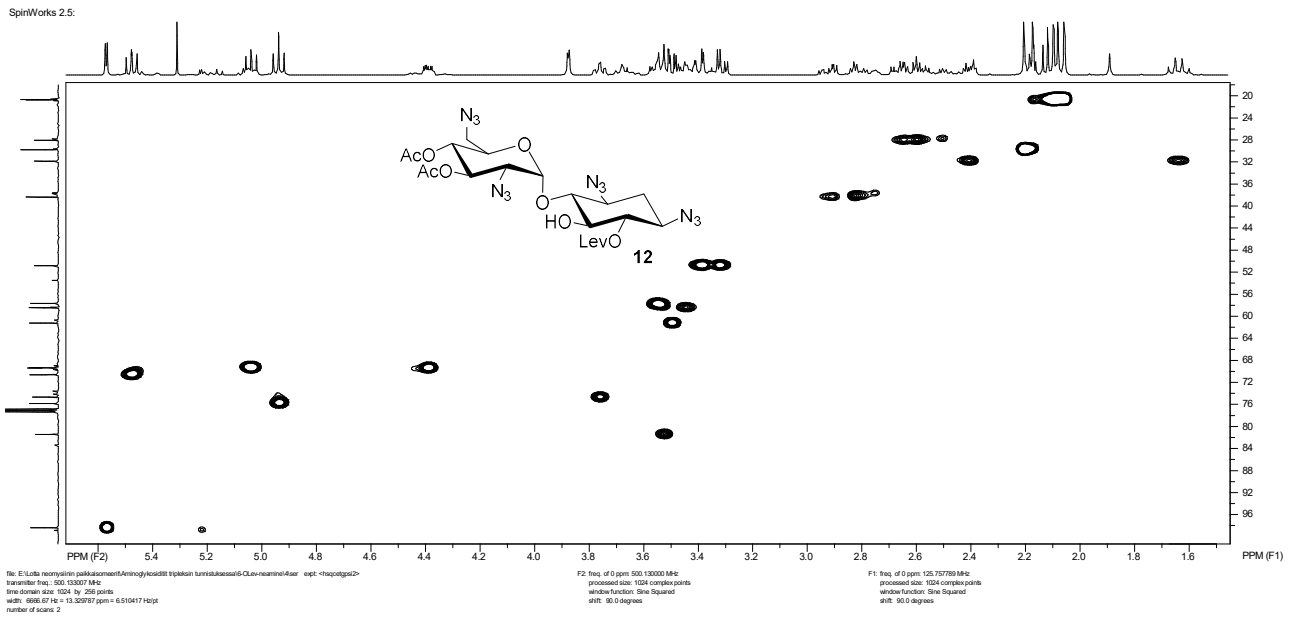
Figure S27.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **12**.

SpinWorks 2.5:

Figure S28. COSY spectrum of **12**.



**Figure S29.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of **12**.



**Figure S30.** HSQC spectrum of **12**.



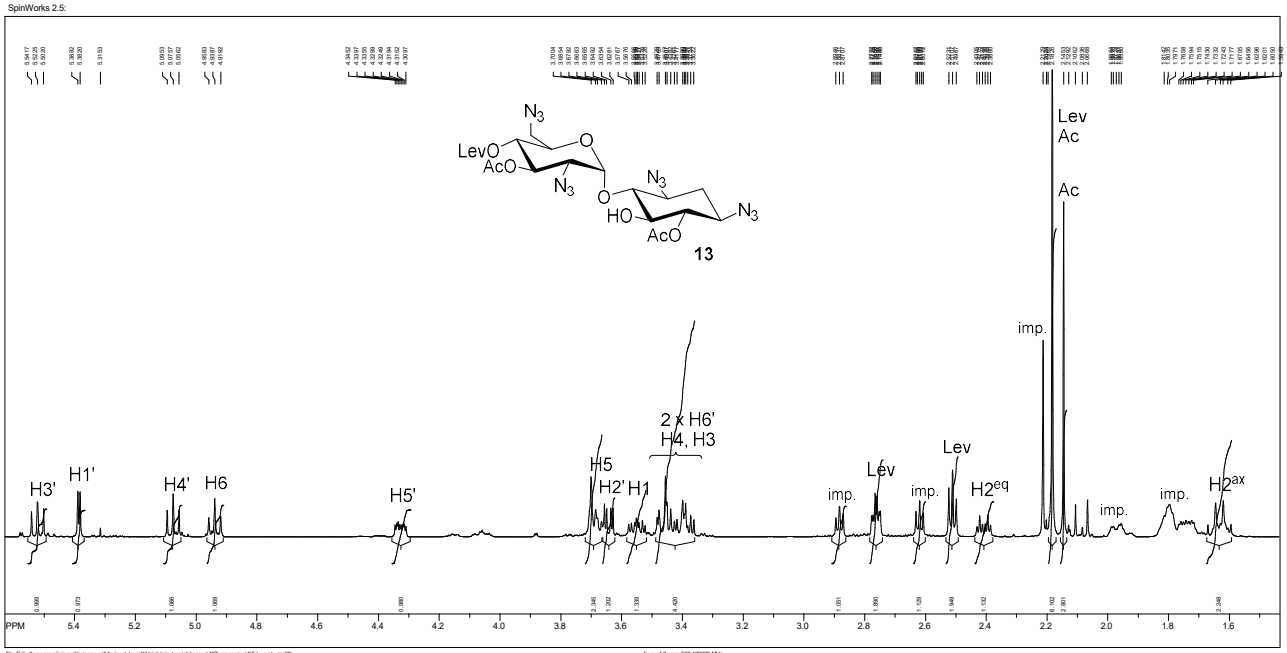


Figure S31. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **13**.

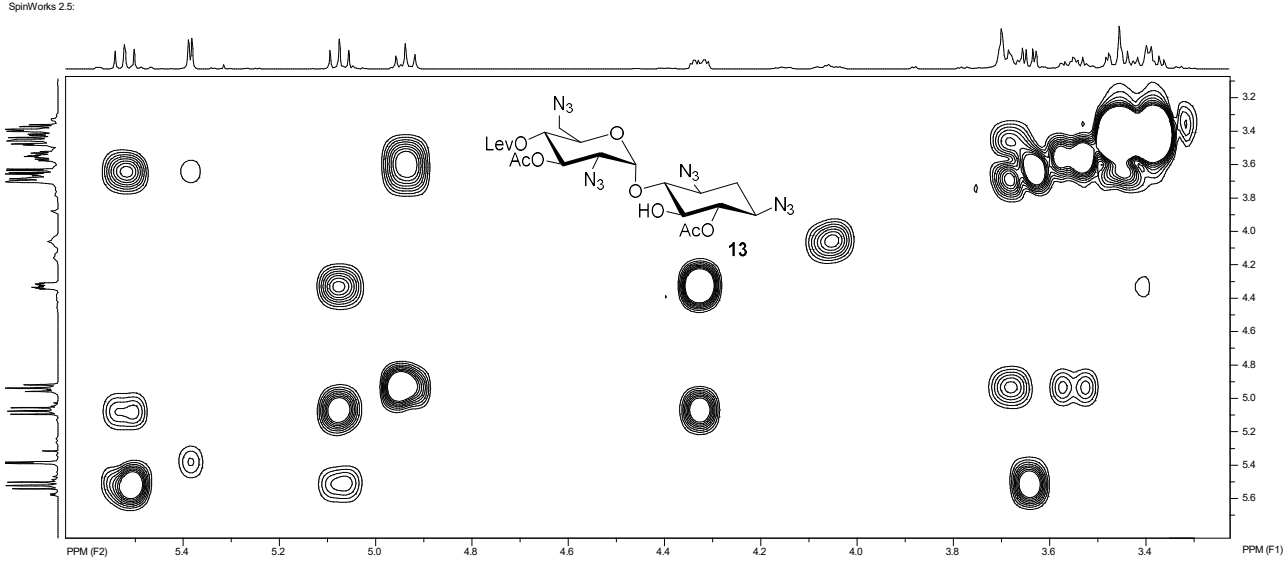


Figure S32. COSY spectrum of **13**.

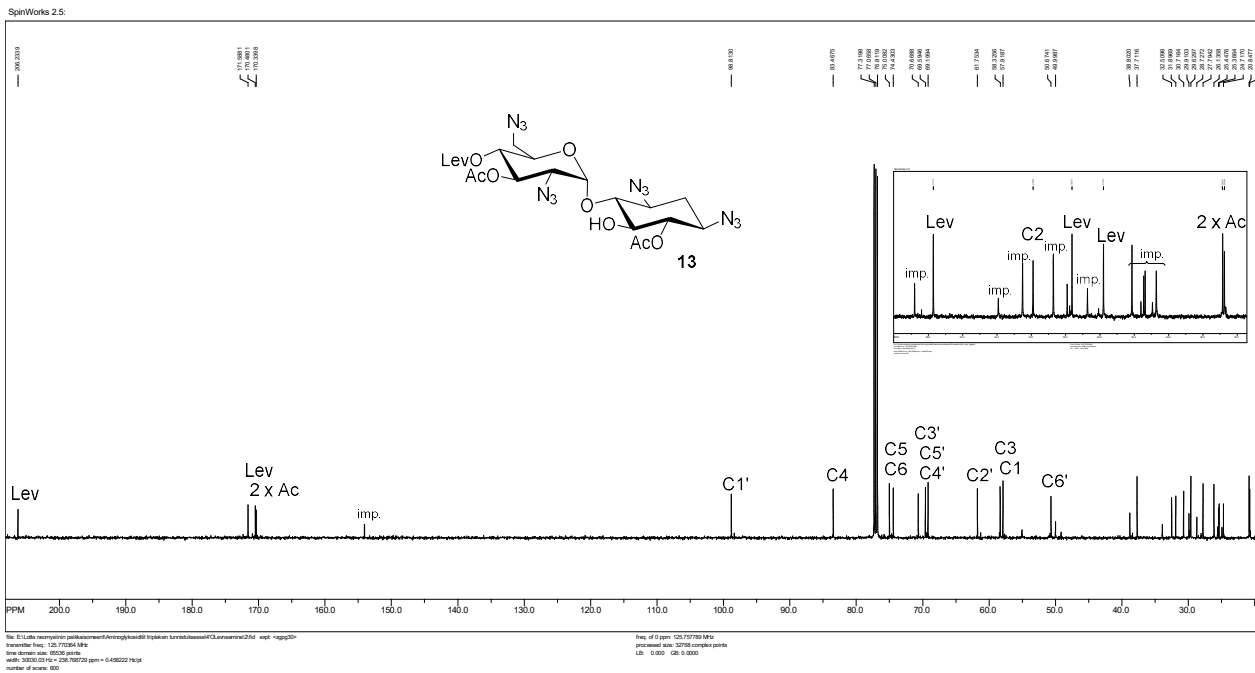


Figure S33.  $^{13}C$  NMR (125 MHz,  $CDCl_3$ ) spectrum of **13**.

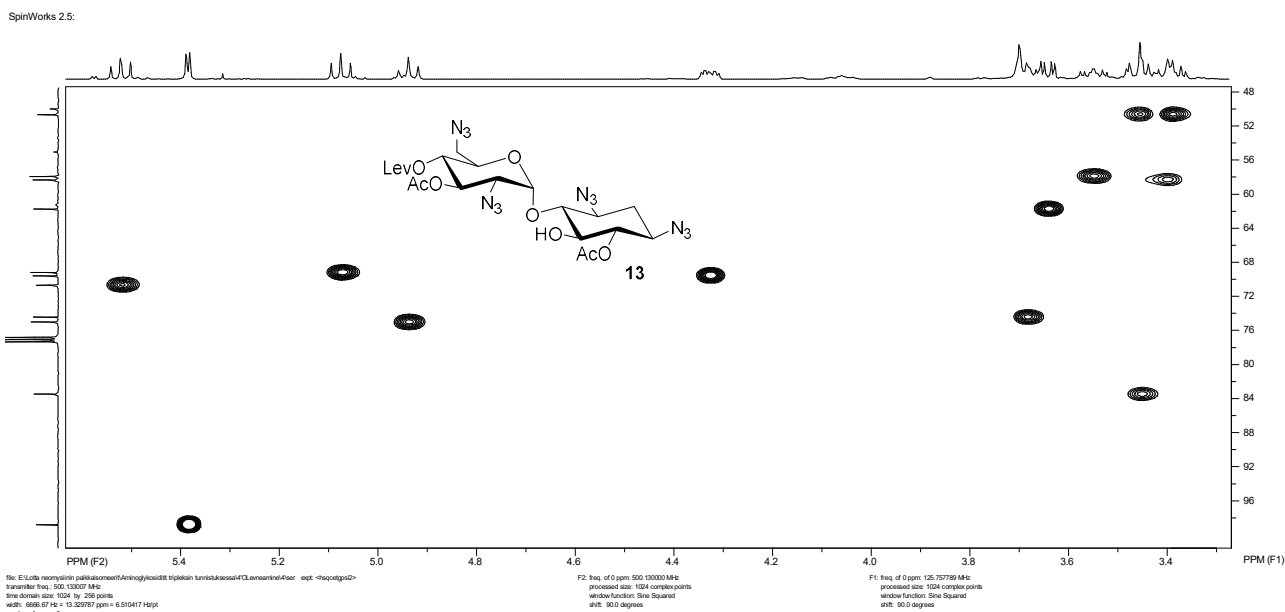
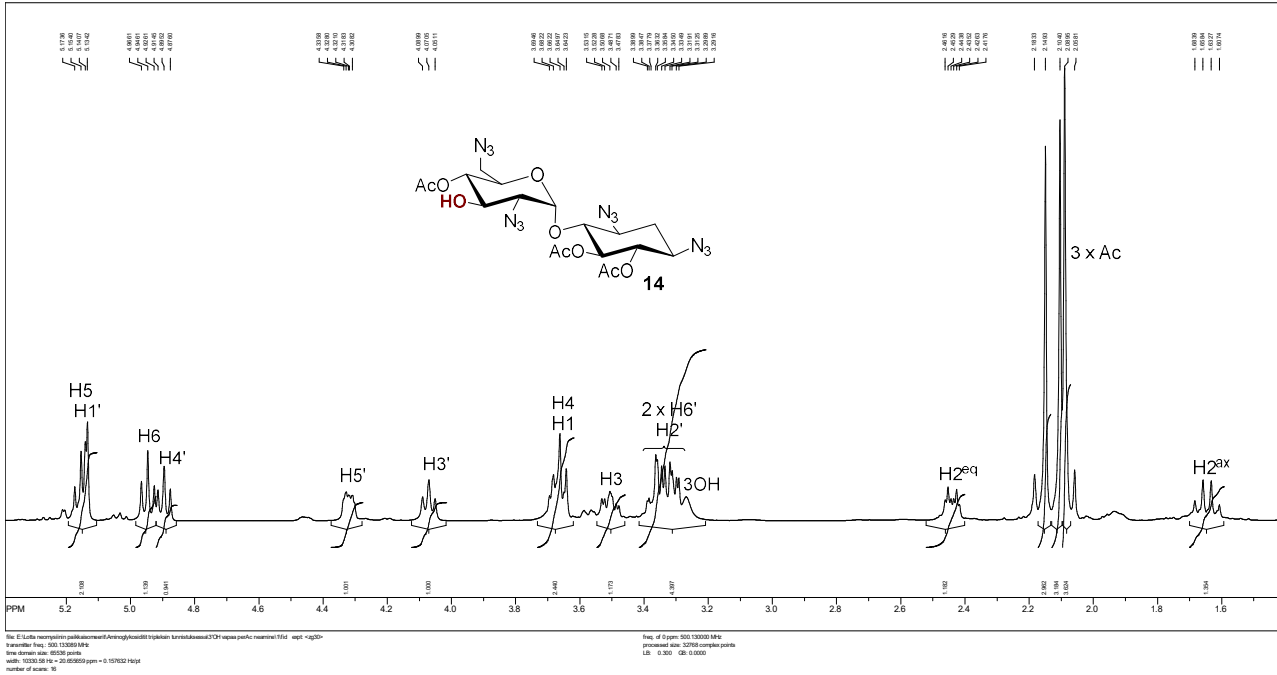


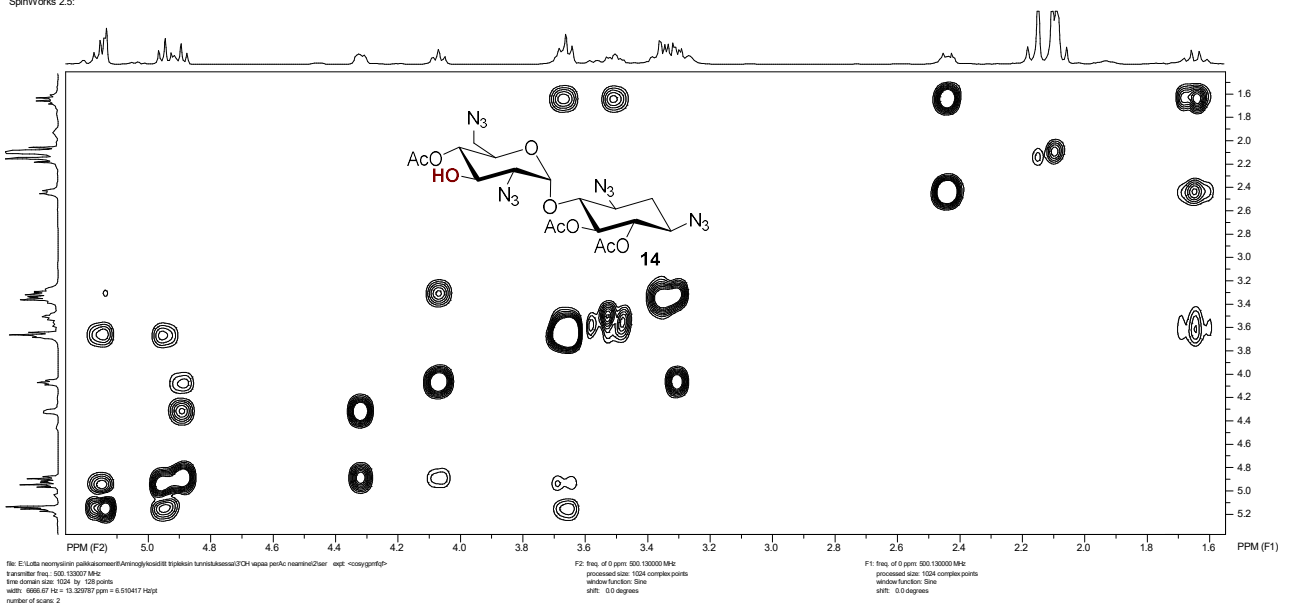
Figure S34. HSQC spectrum of **13**.

SpinWorks 2.5:

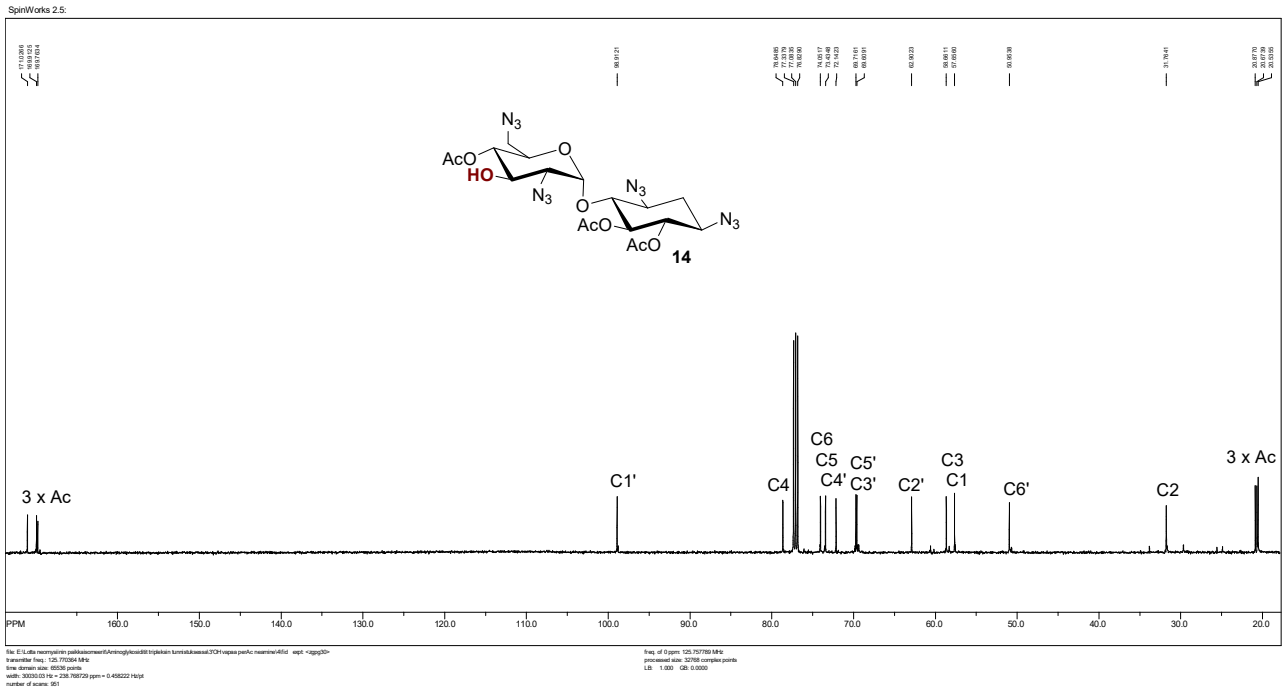


**Figure S35.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **14**.

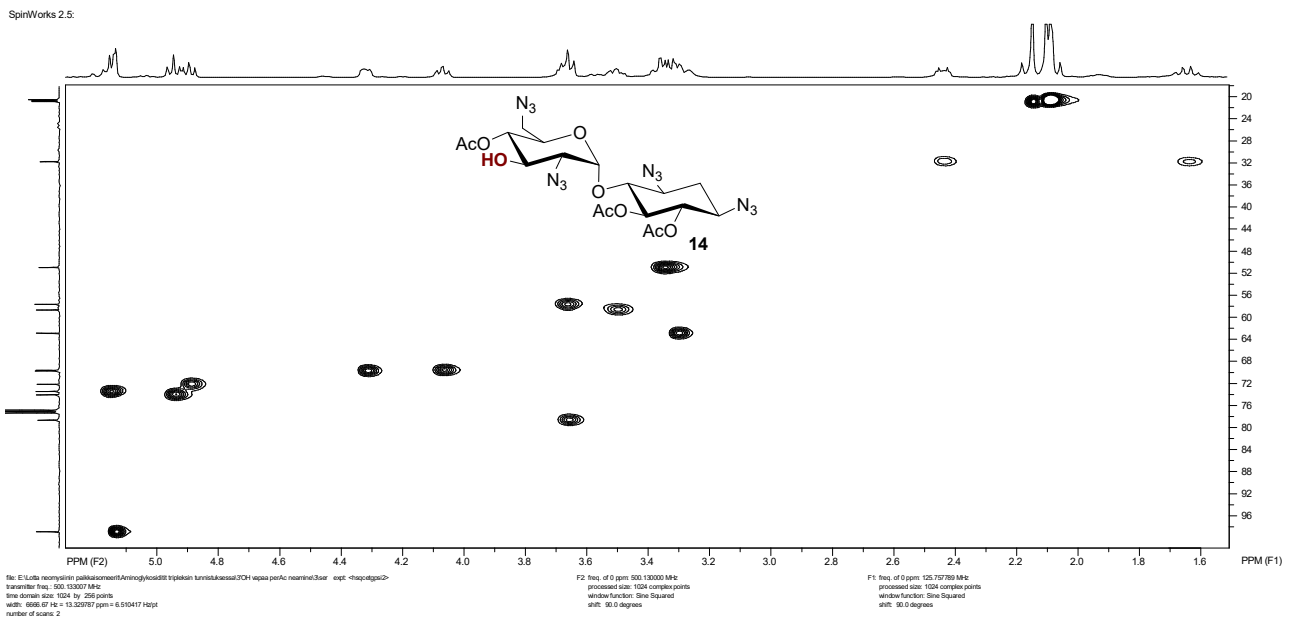
SpinWorks 2.5:



**Figure S36.** COSY spectrum of **14**.

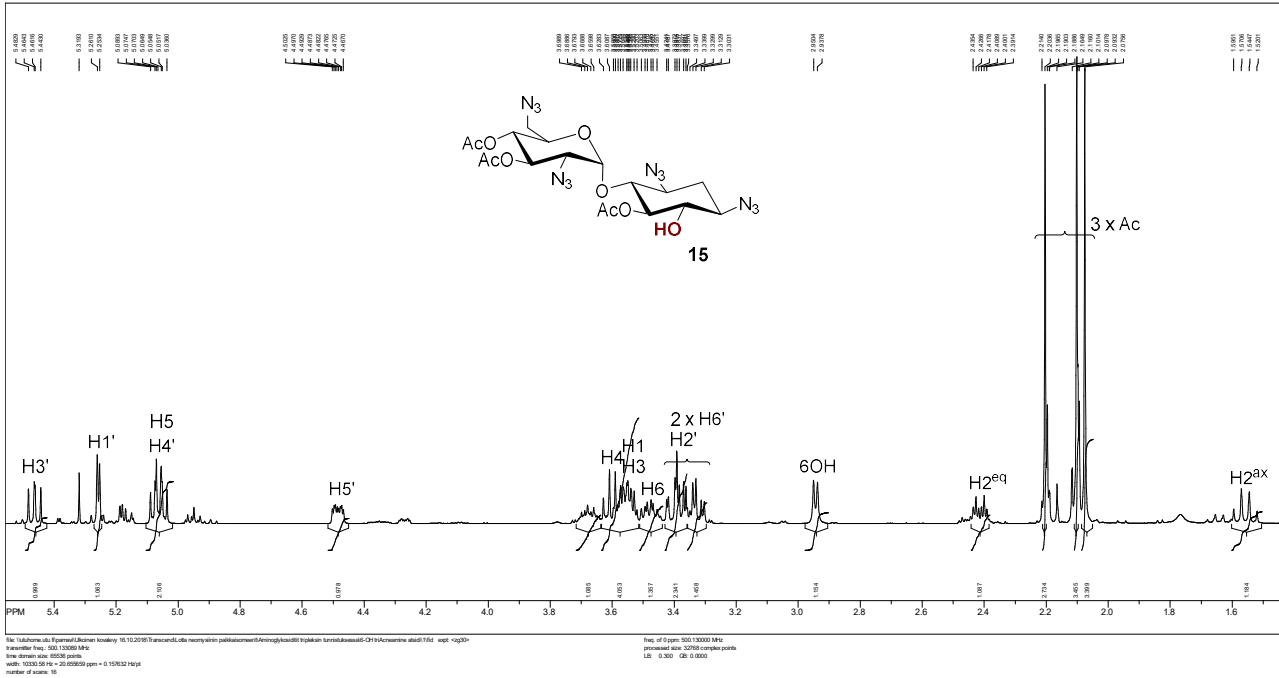


**Figure S37.** <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) spectrum of **14**.



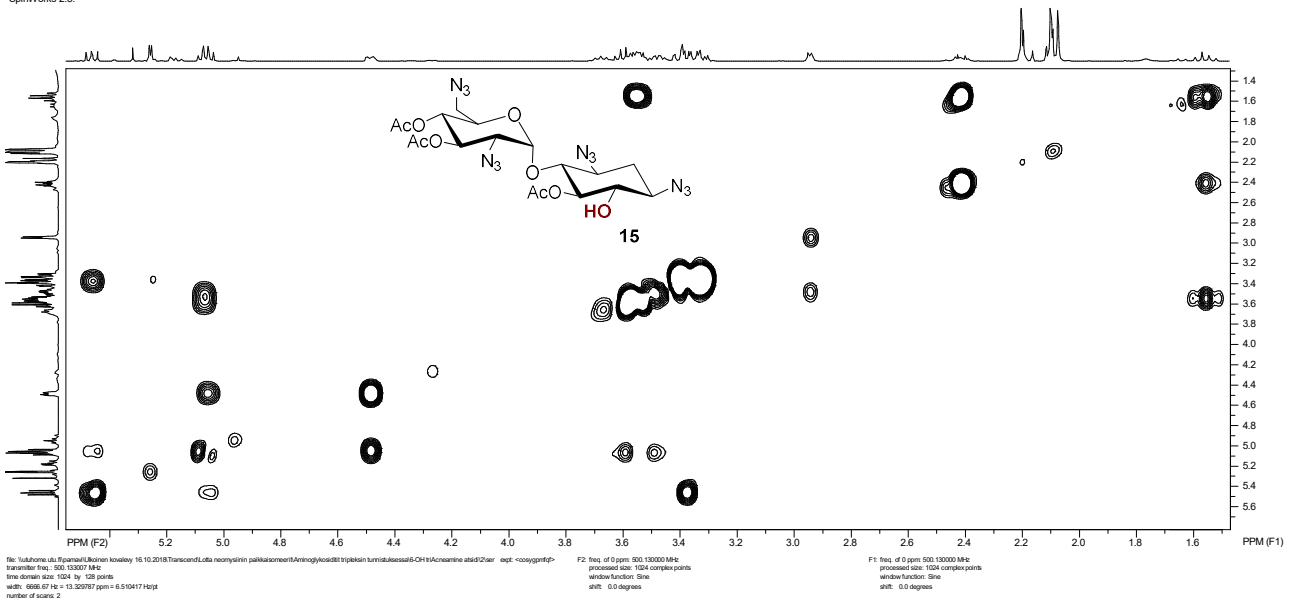
**Figure S38.** HSQC spectrum of **14**.

SpinWorks 2.5:

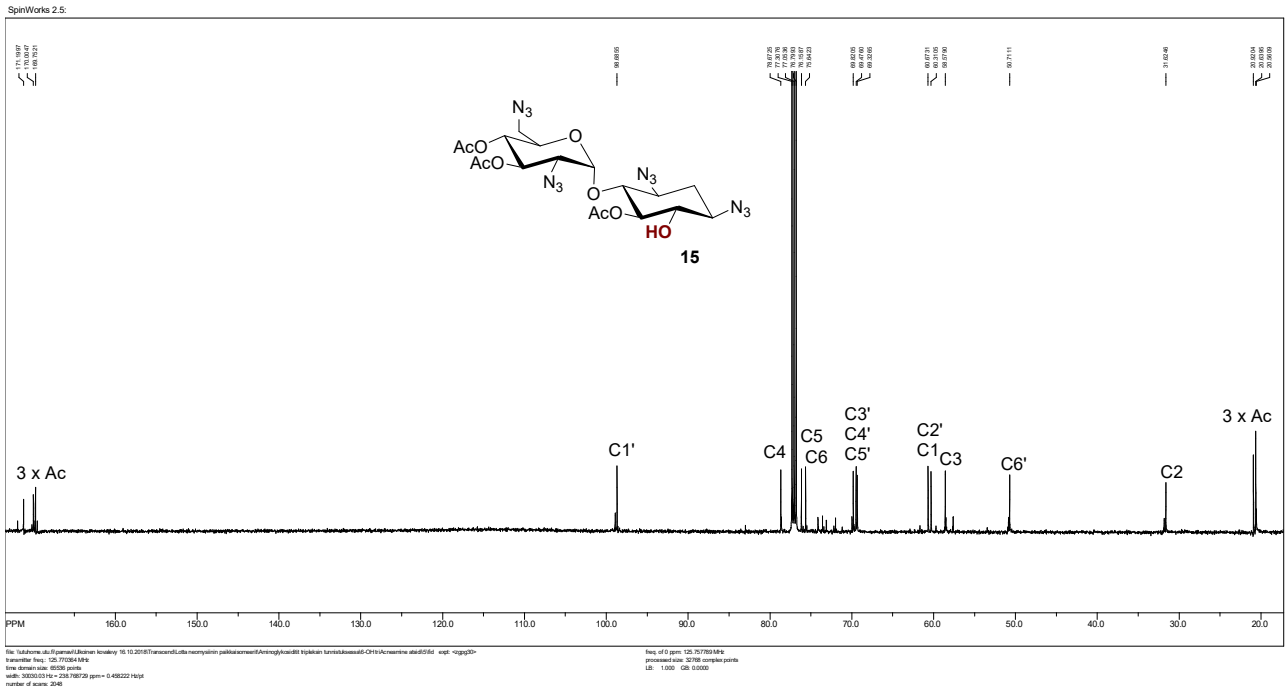


**Figure S39.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **15**.

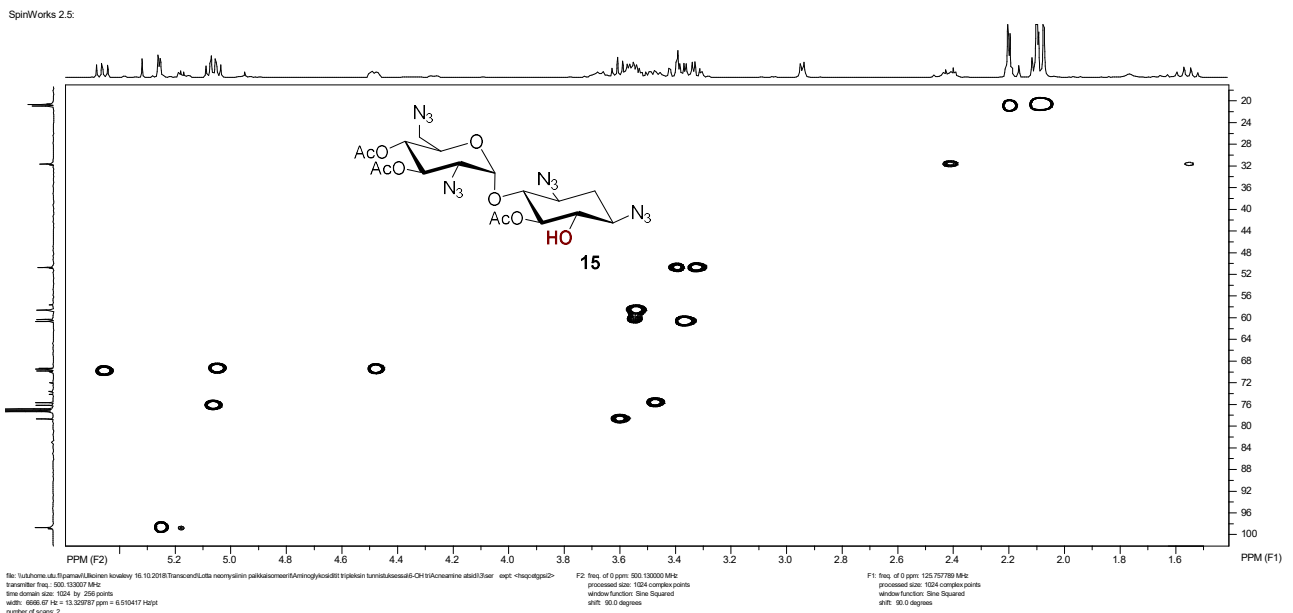
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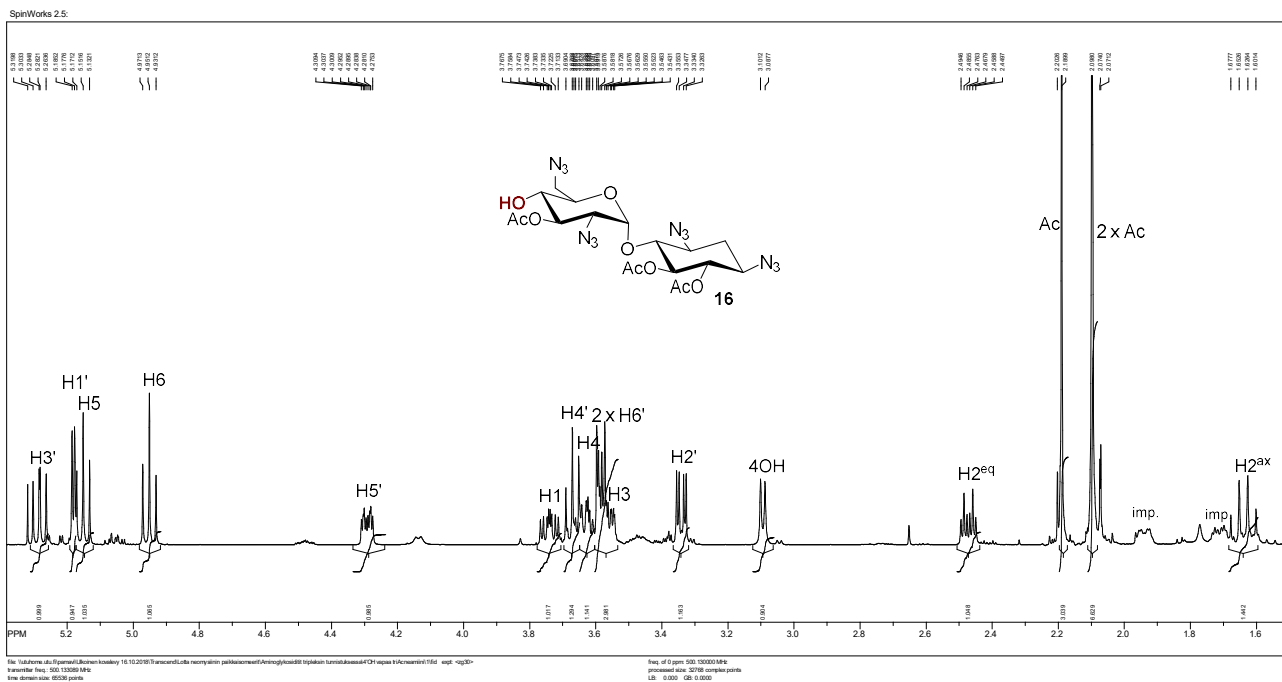
**Figure S40.** COSY spectrum of **15**.



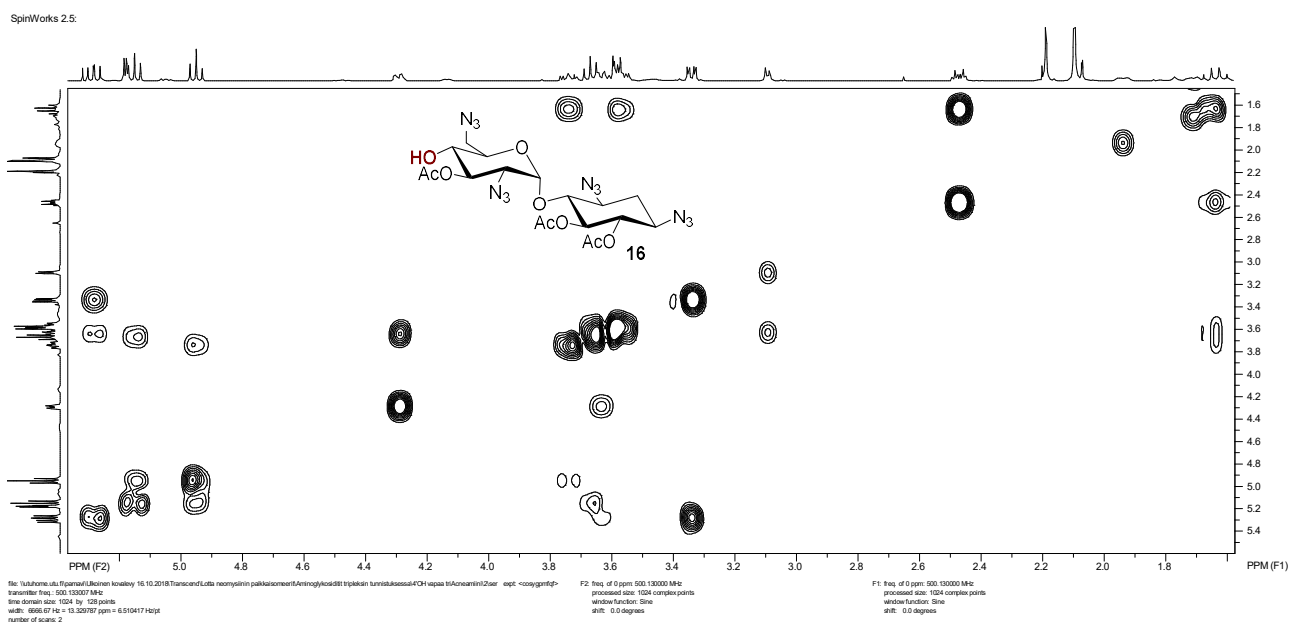
**Figure S41.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of **15**.



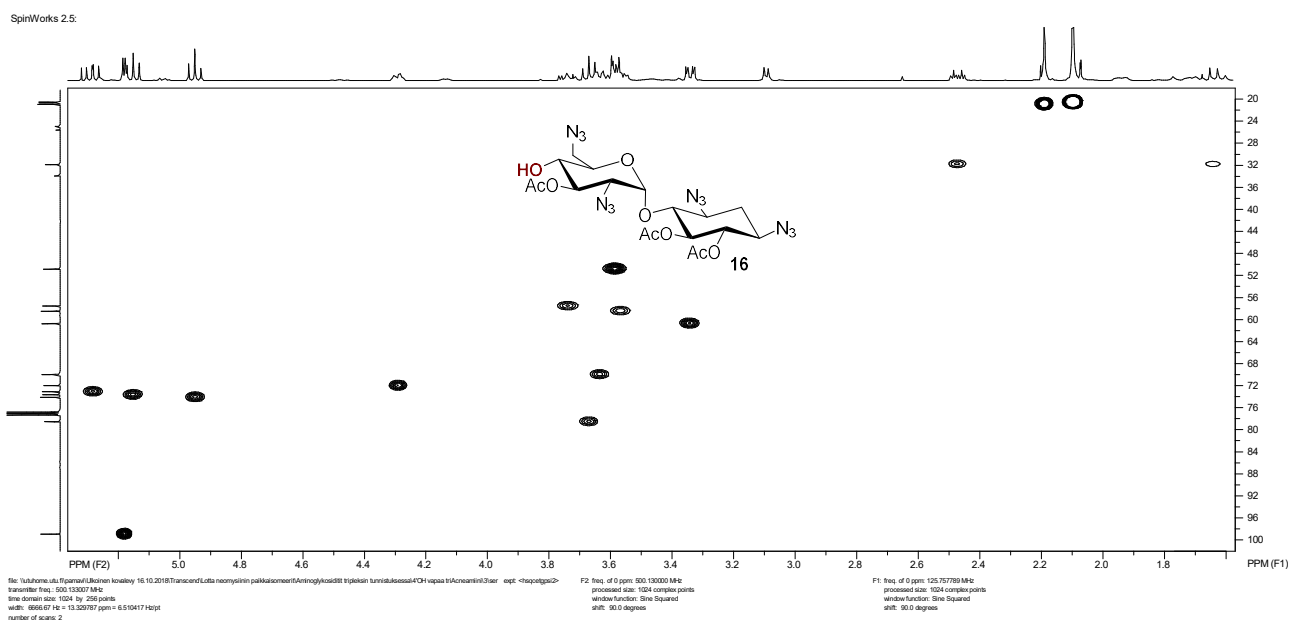
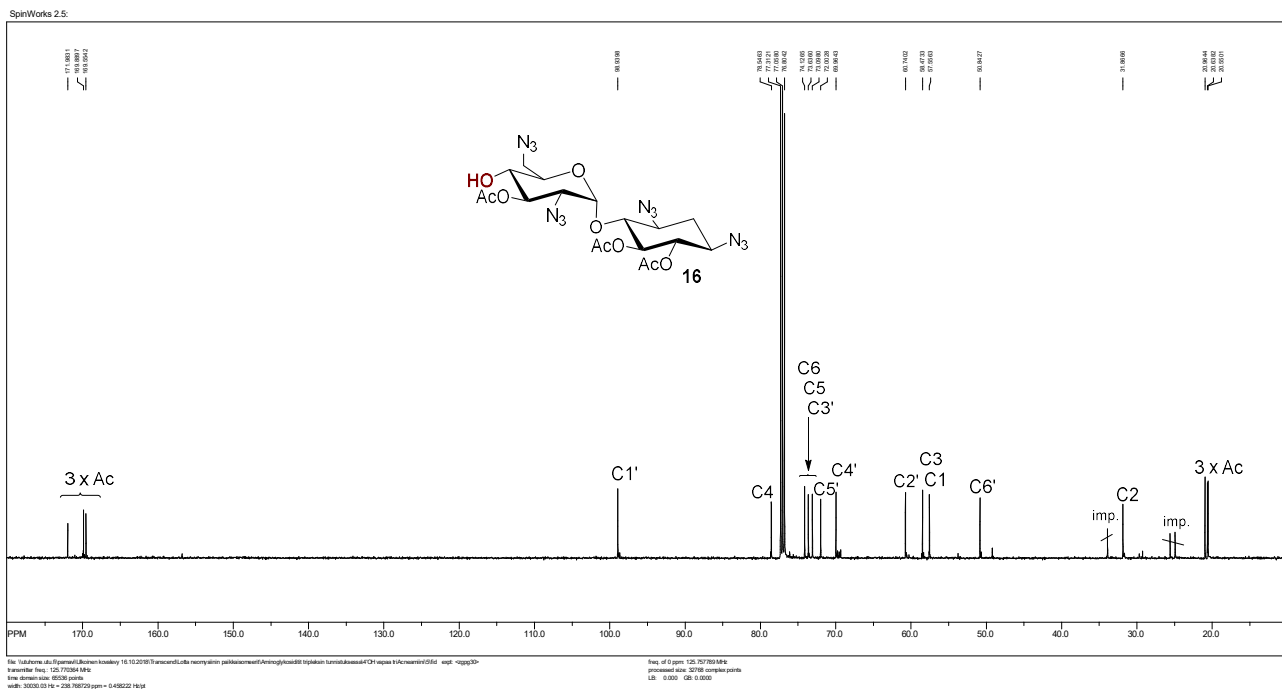
**Figure S42.** HSQC spectrum of **15**.



**Figure S43.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **16**.



**Figure S44.** COSY spectrum of **16**.





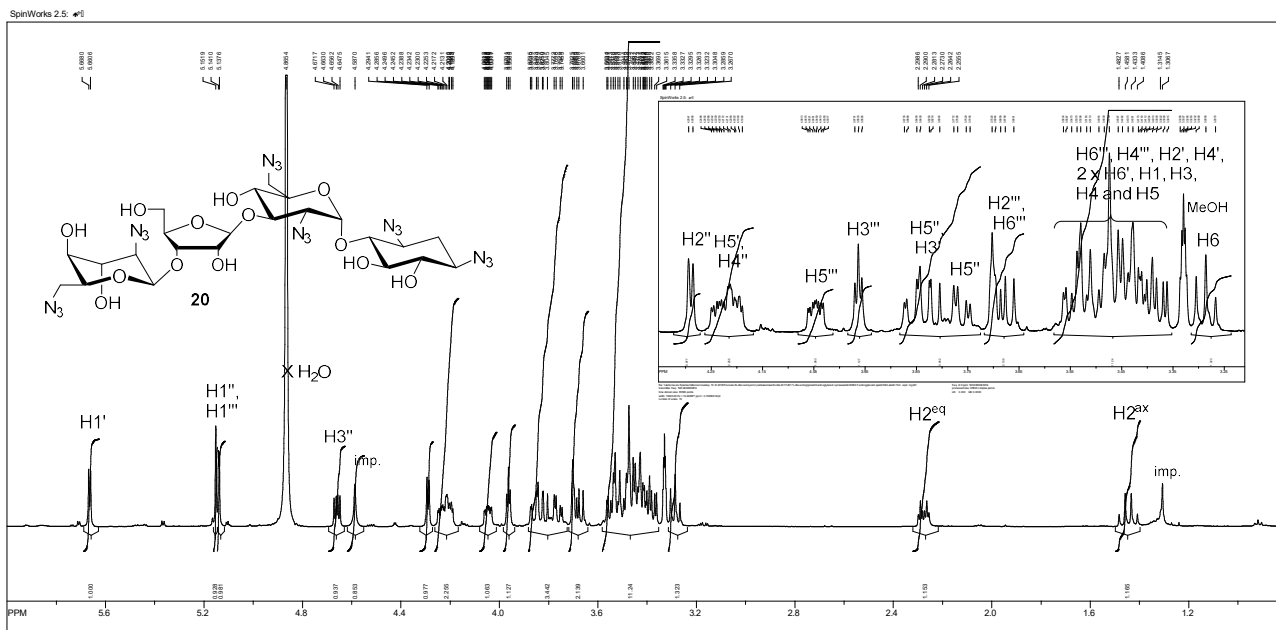


Figure S47.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **20**.

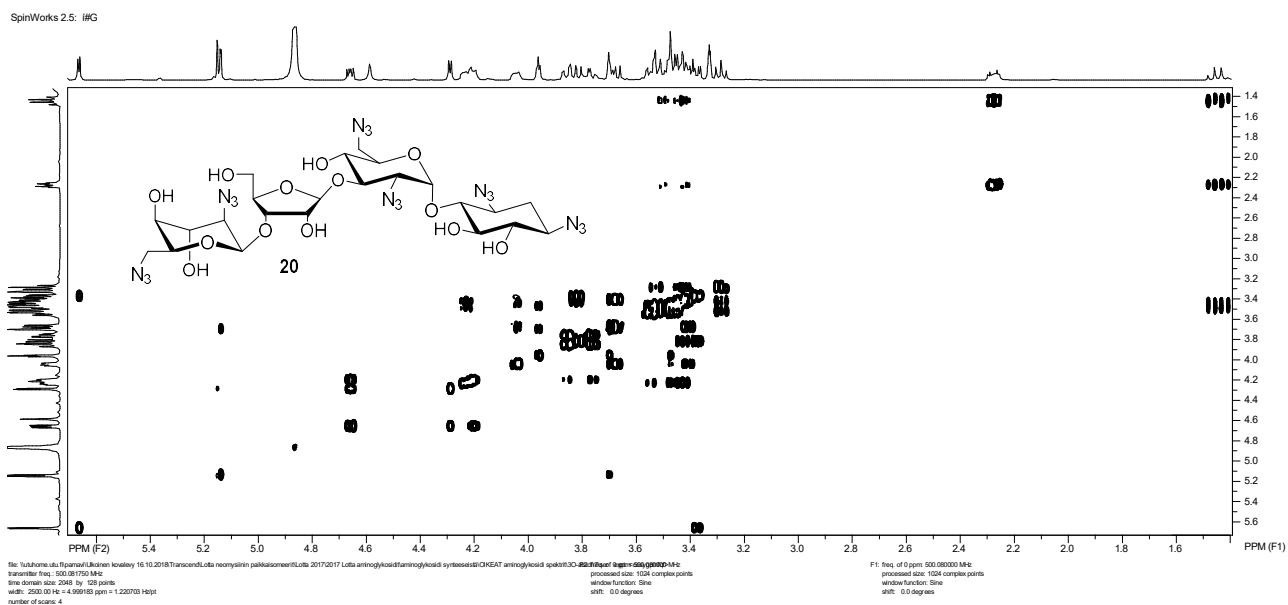


Figure S48. COSY spectrum of **20**.

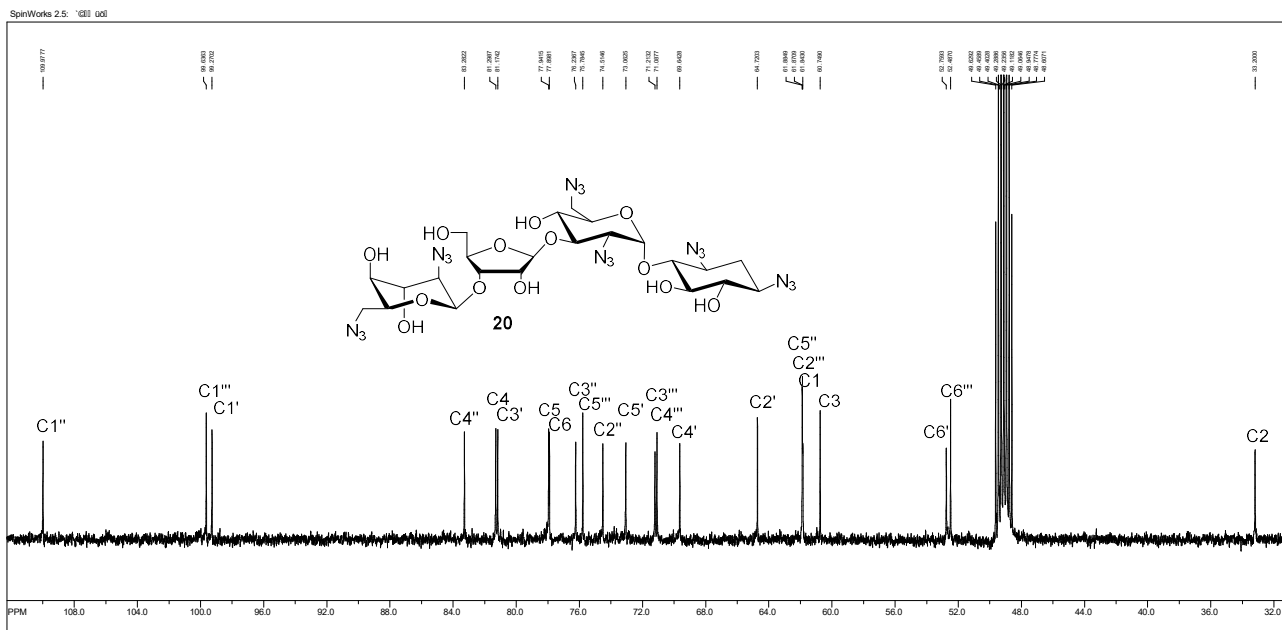


Figure S49.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of **20**.

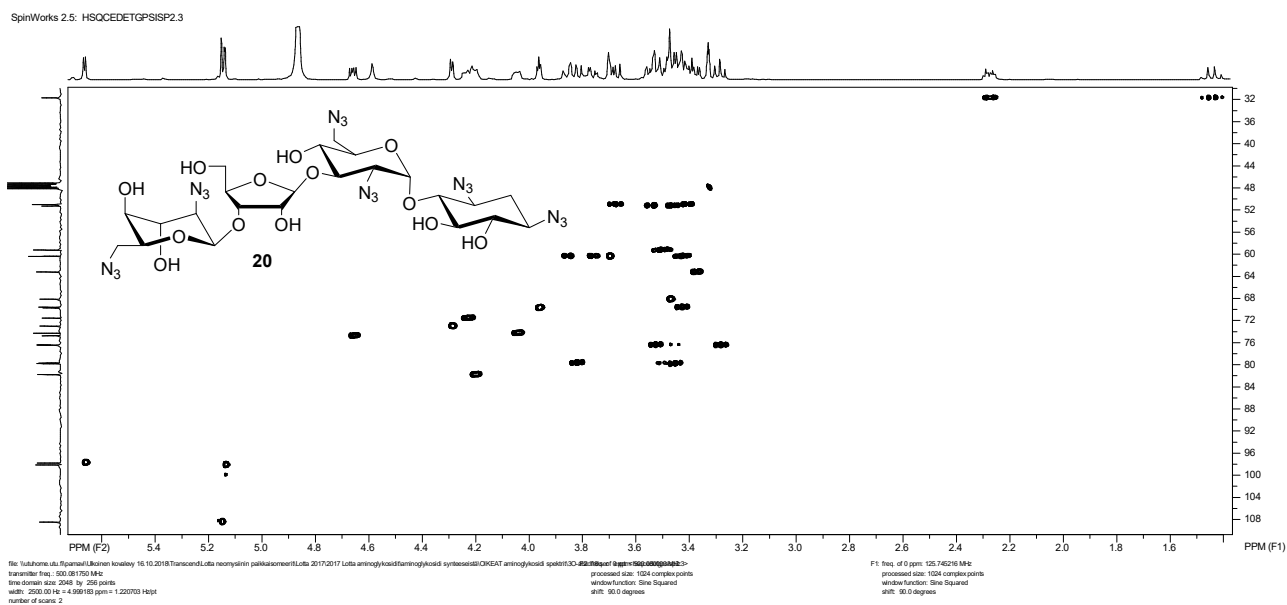


Figure S50. HSQC spectrum of **20**.





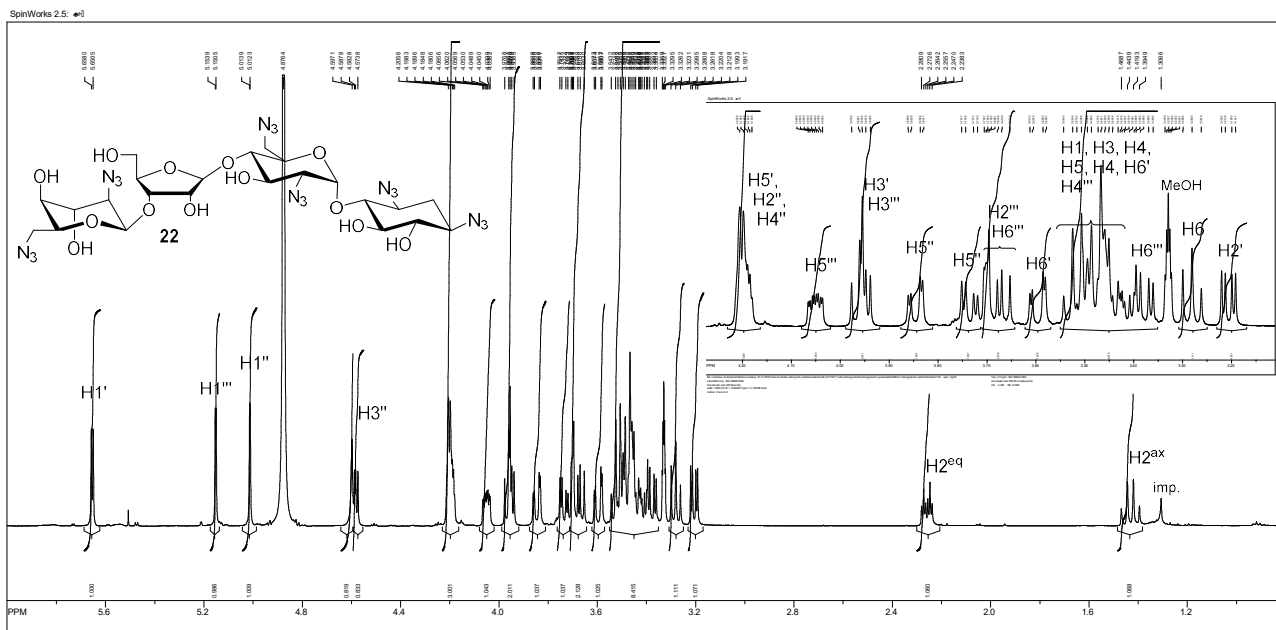


Figure S55.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **22**.

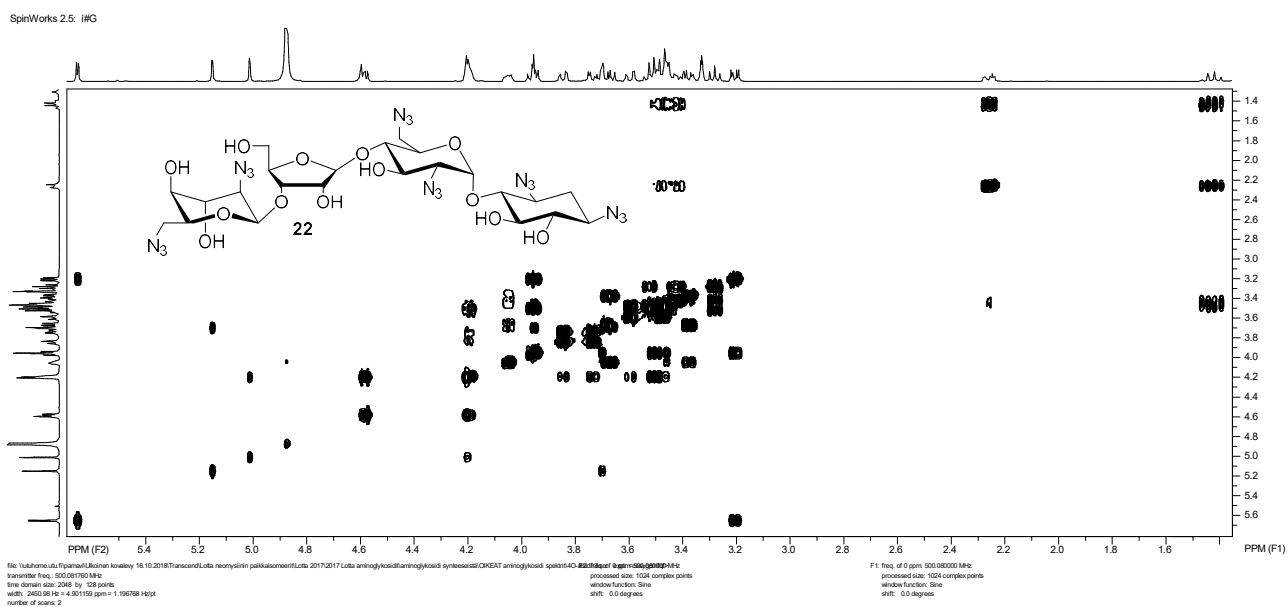


Figure S56. COSY spectrum of **22**.



SpinWorks 2.5:

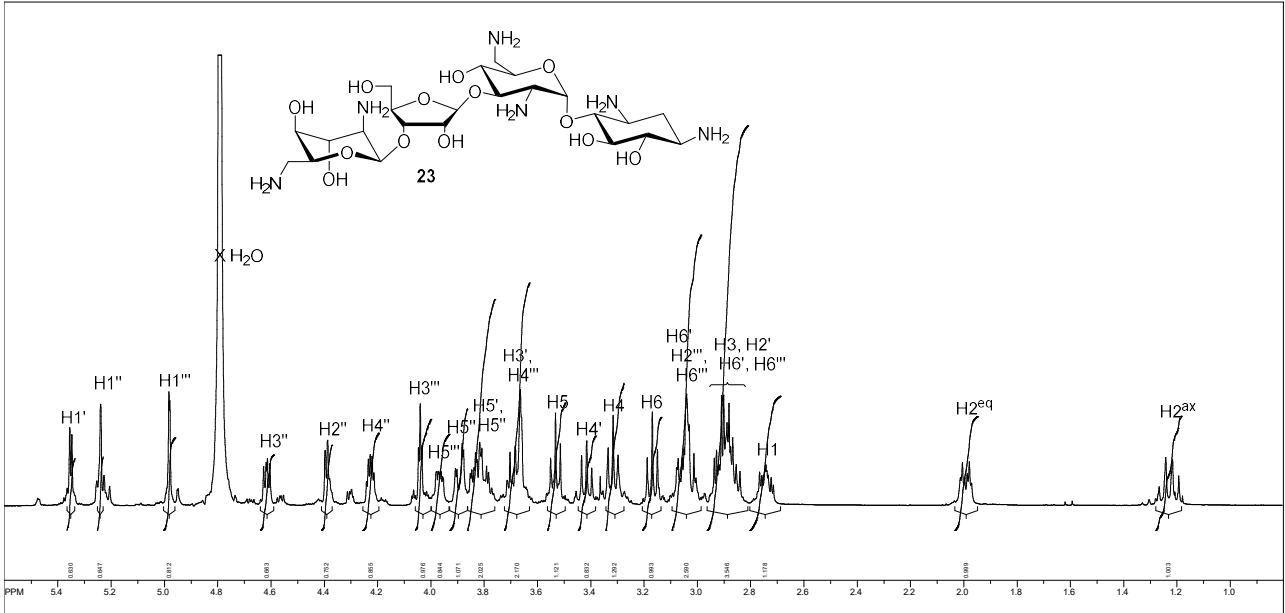


Figure S59.  $^1\text{H}$  NMR (500 MHz,  $\text{D}_2\text{O}$ ) spectrum of **23**.

SpinWorks 2.5:

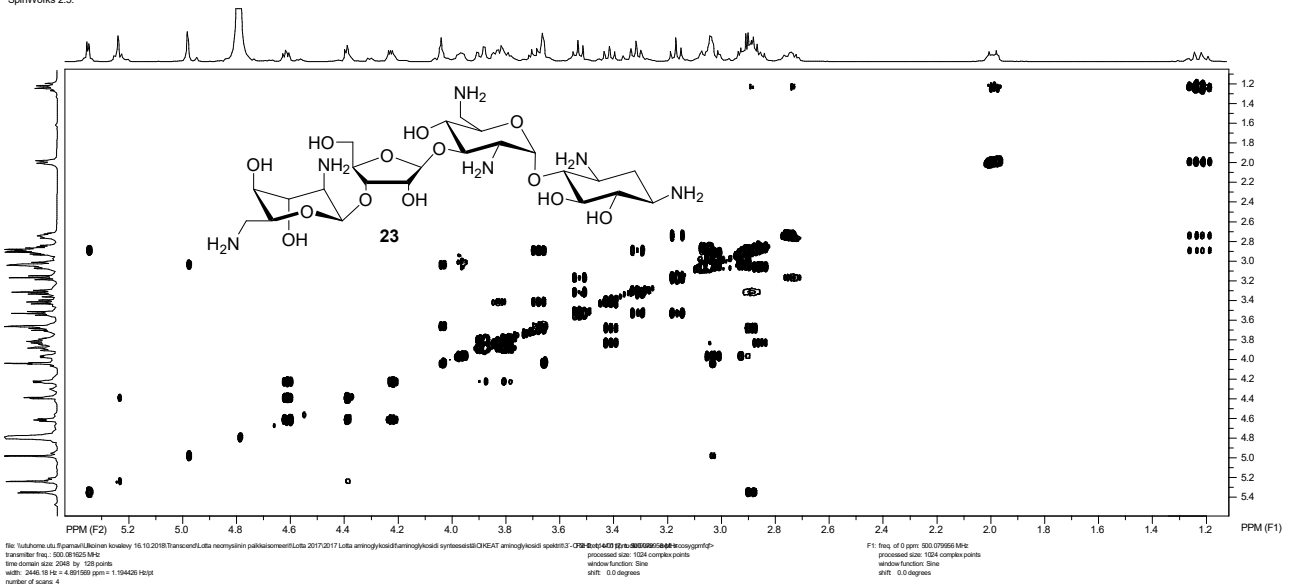


Figure S60. COSY spectrum of **23**.

SpinWorks 2.5:

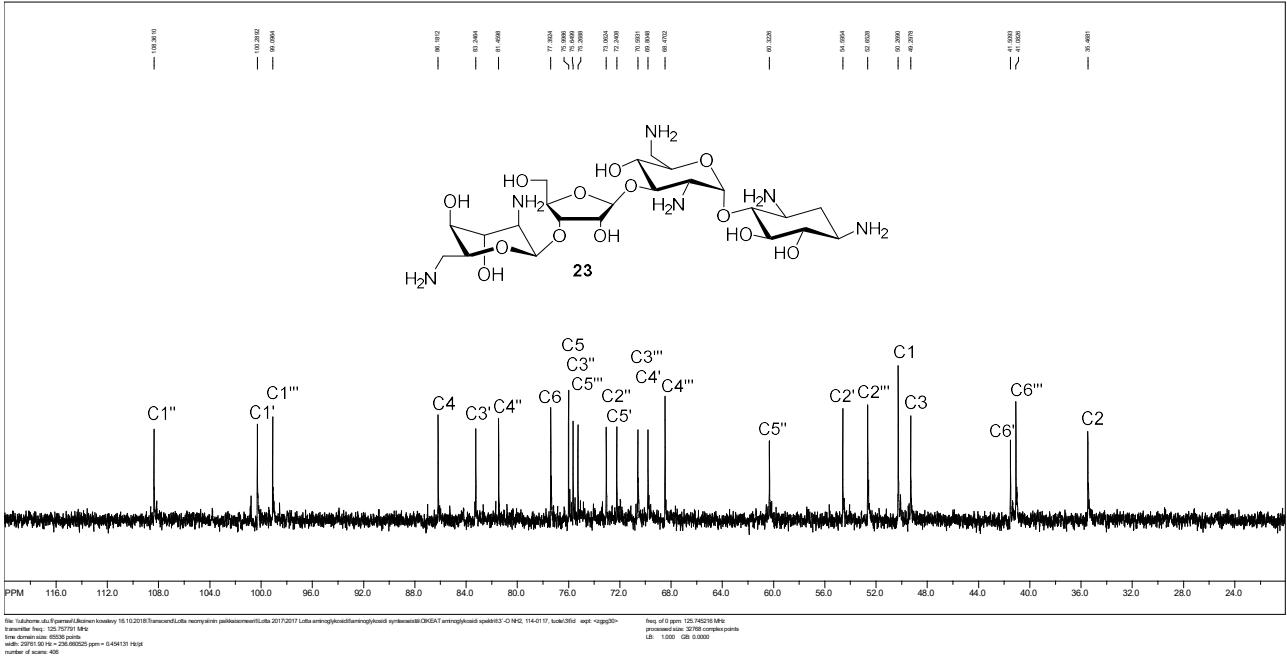


Figure S61. <sup>13</sup>C NMR (125 MHz, D<sub>2</sub>O) spectrum of **23**.

SpinWorks 2.5: HSOCEDETGPSISP2.3

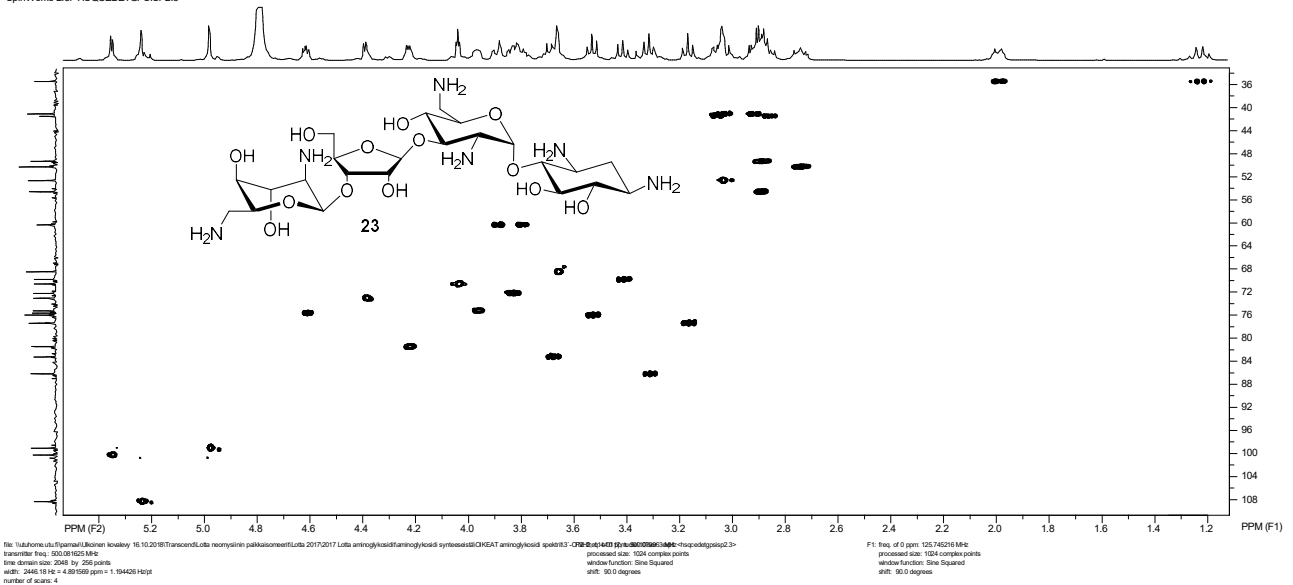


Figure S62. HSQC spectrum of **23**.



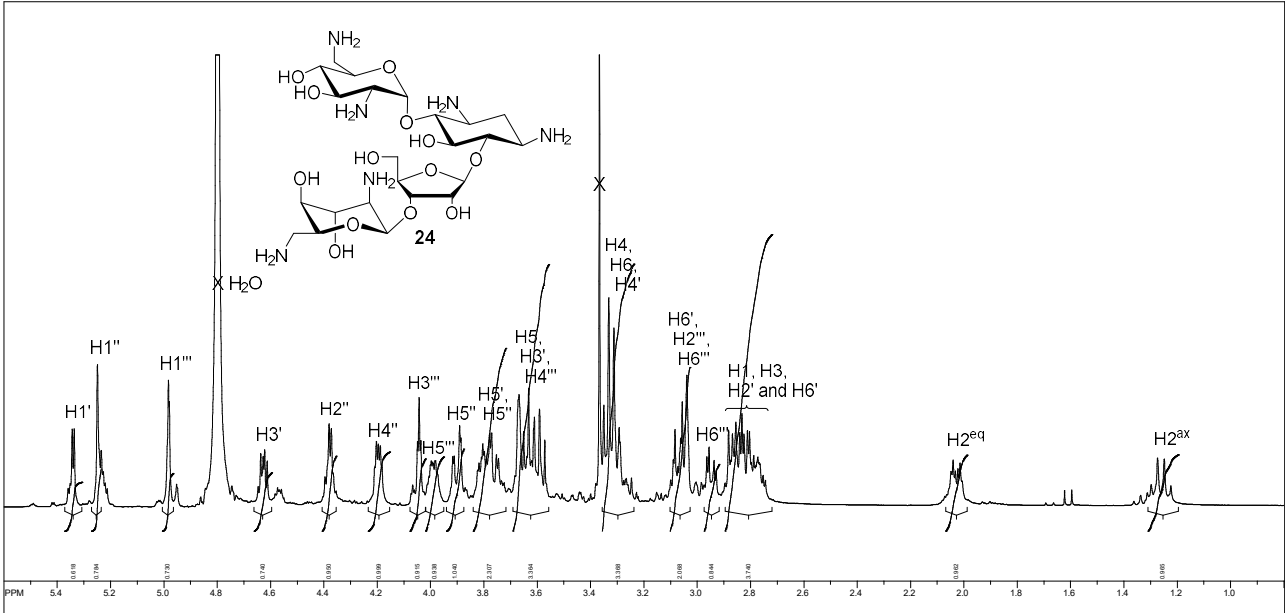


Figure S63.  $^1\text{H}$  NMR (500 MHz,  $\text{D}_2\text{O}$ ) spectrum of **24**.

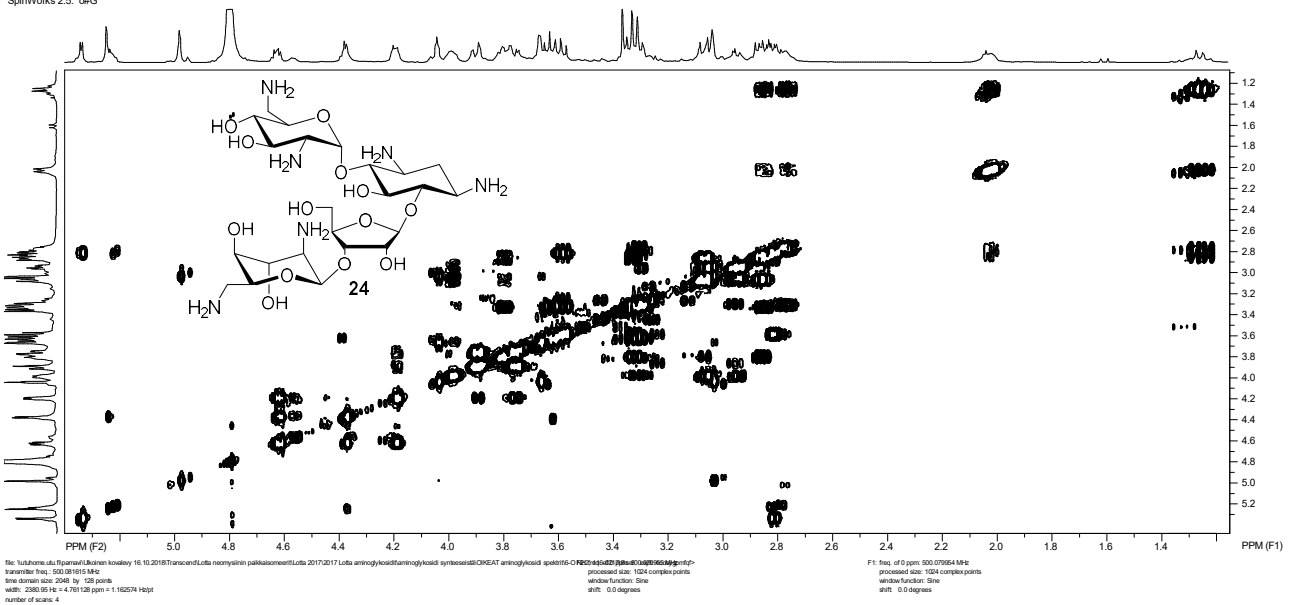


Figure S64. COSY spectrum of **24**.

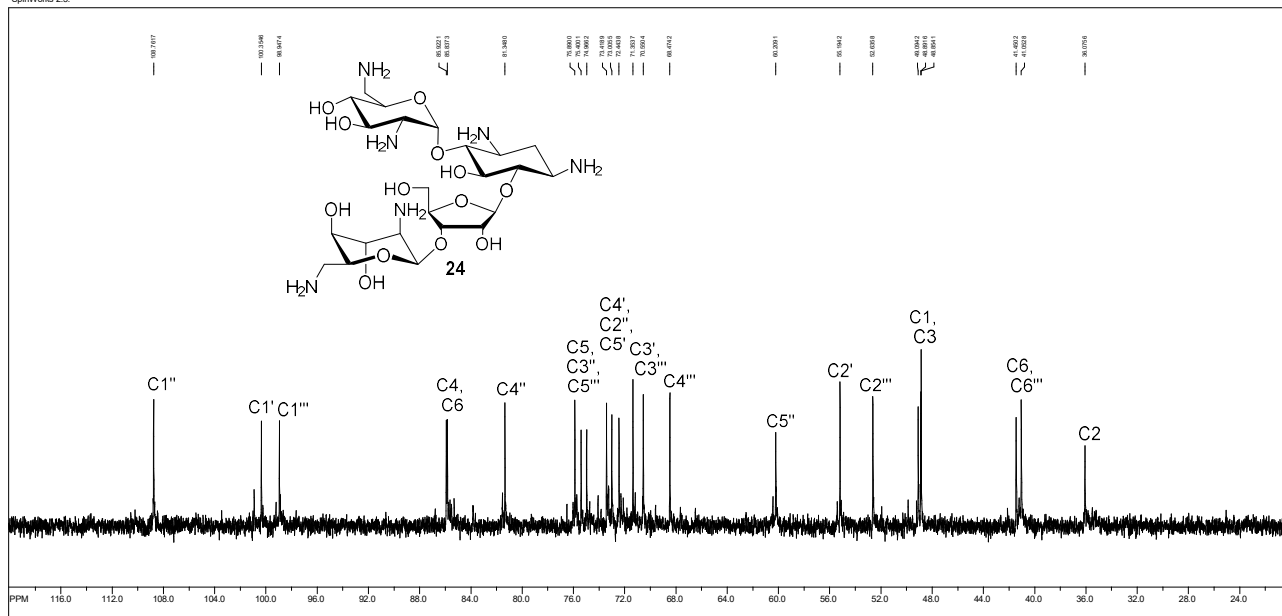


Figure S65. <sup>13</sup>C NMR (125 MHz, D<sub>2</sub>O) spectrum of 24.

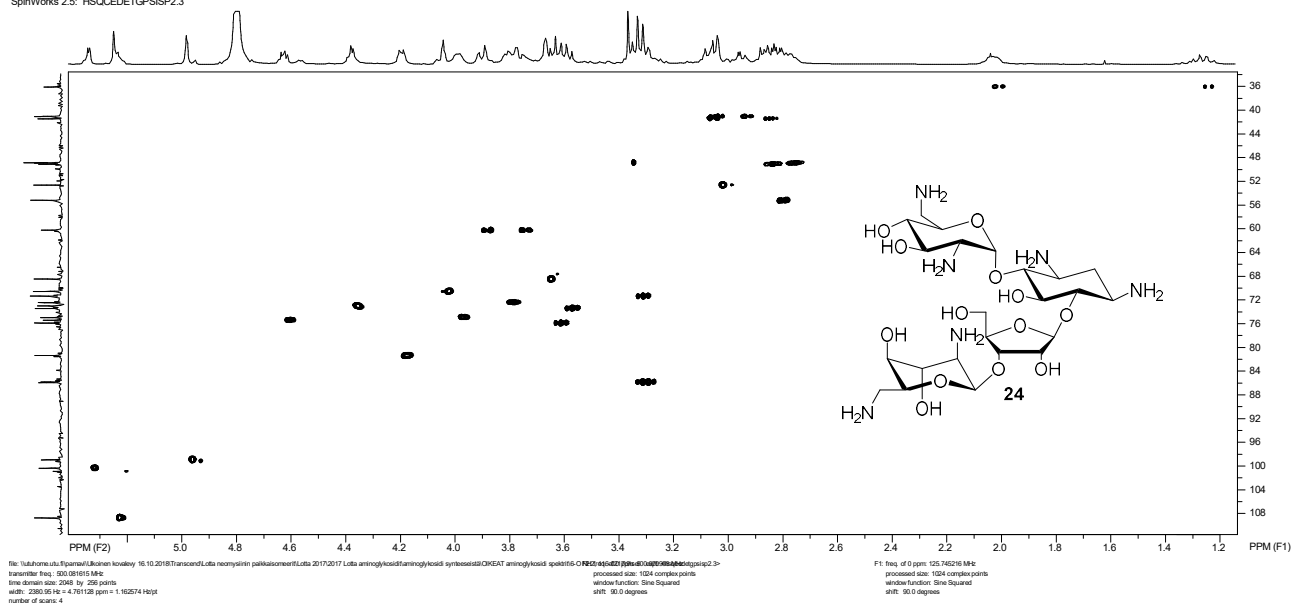


Figure S66. HSQC spectrum of 24.



