

# Chemistry–A European Journal

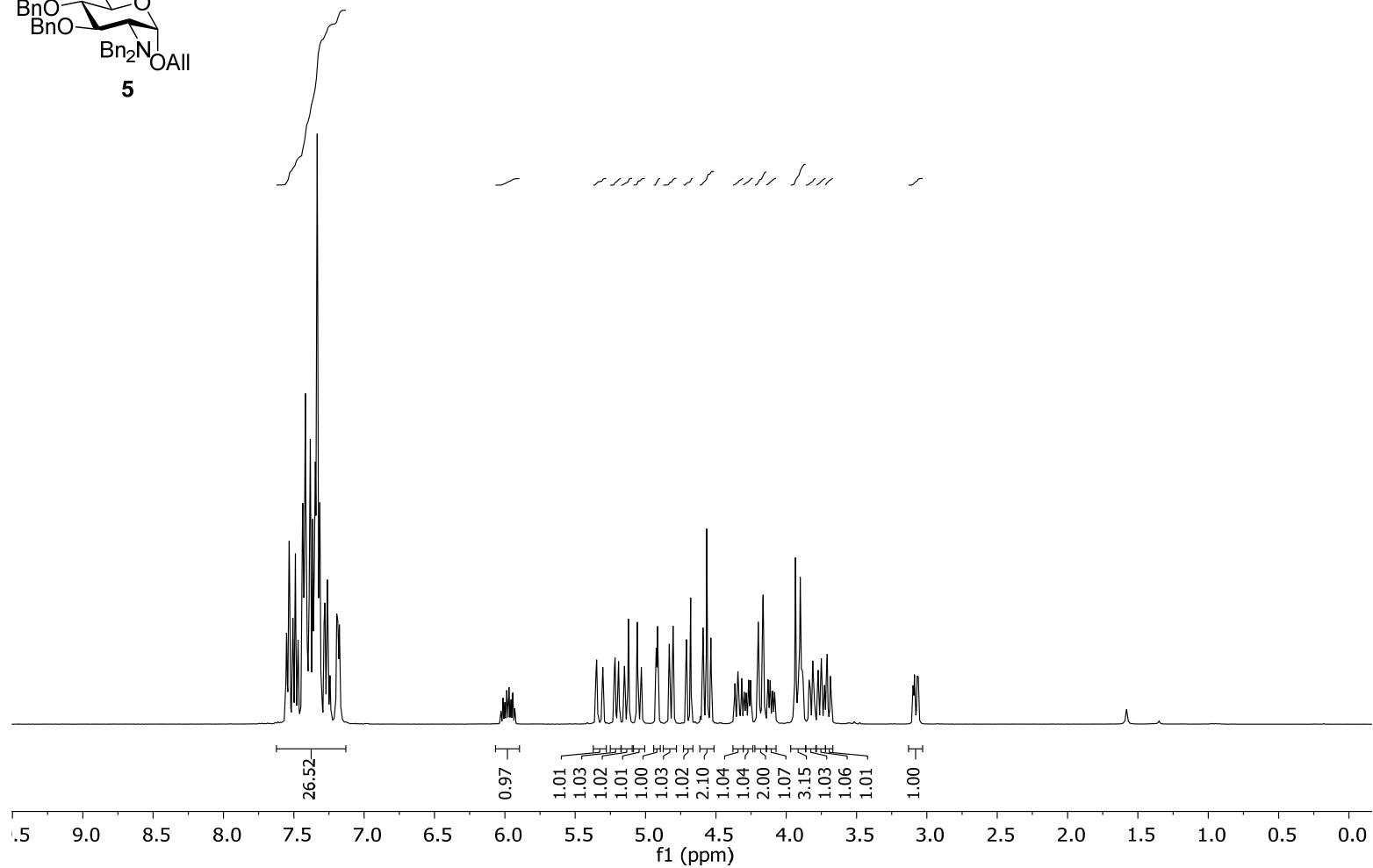
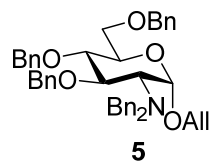
Supporting Information

## **Carba-Sugar Analogs of Glucosamine-6-Phosphate: New Activators for the *glmS* Riboswitch**

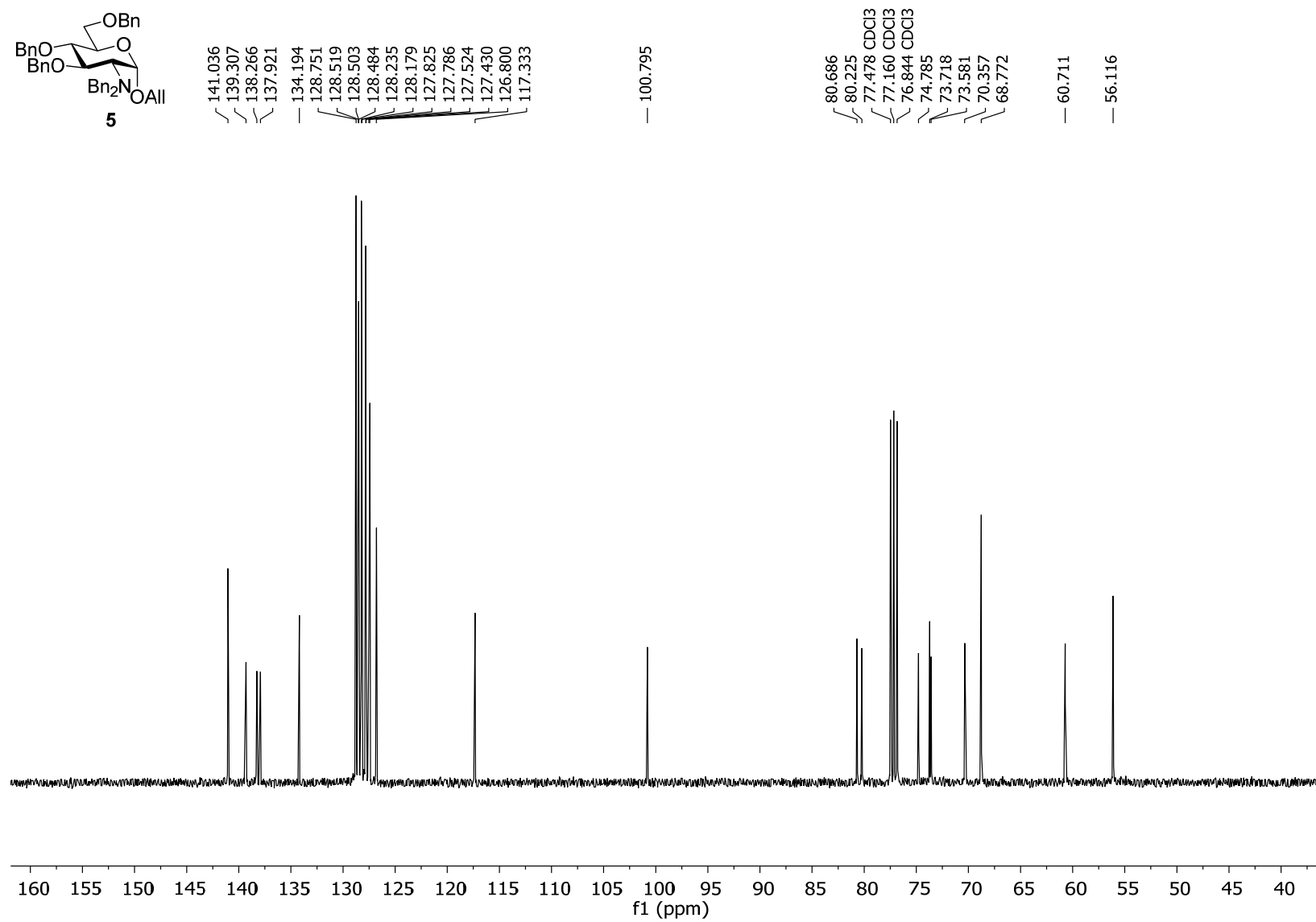
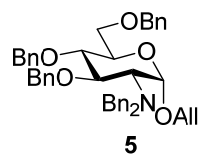
David Stängle, Bjarne Silkenath, Paul Gehle, Anna Esser, Günter Mayer,\* and  
Valentin Wittmann\*

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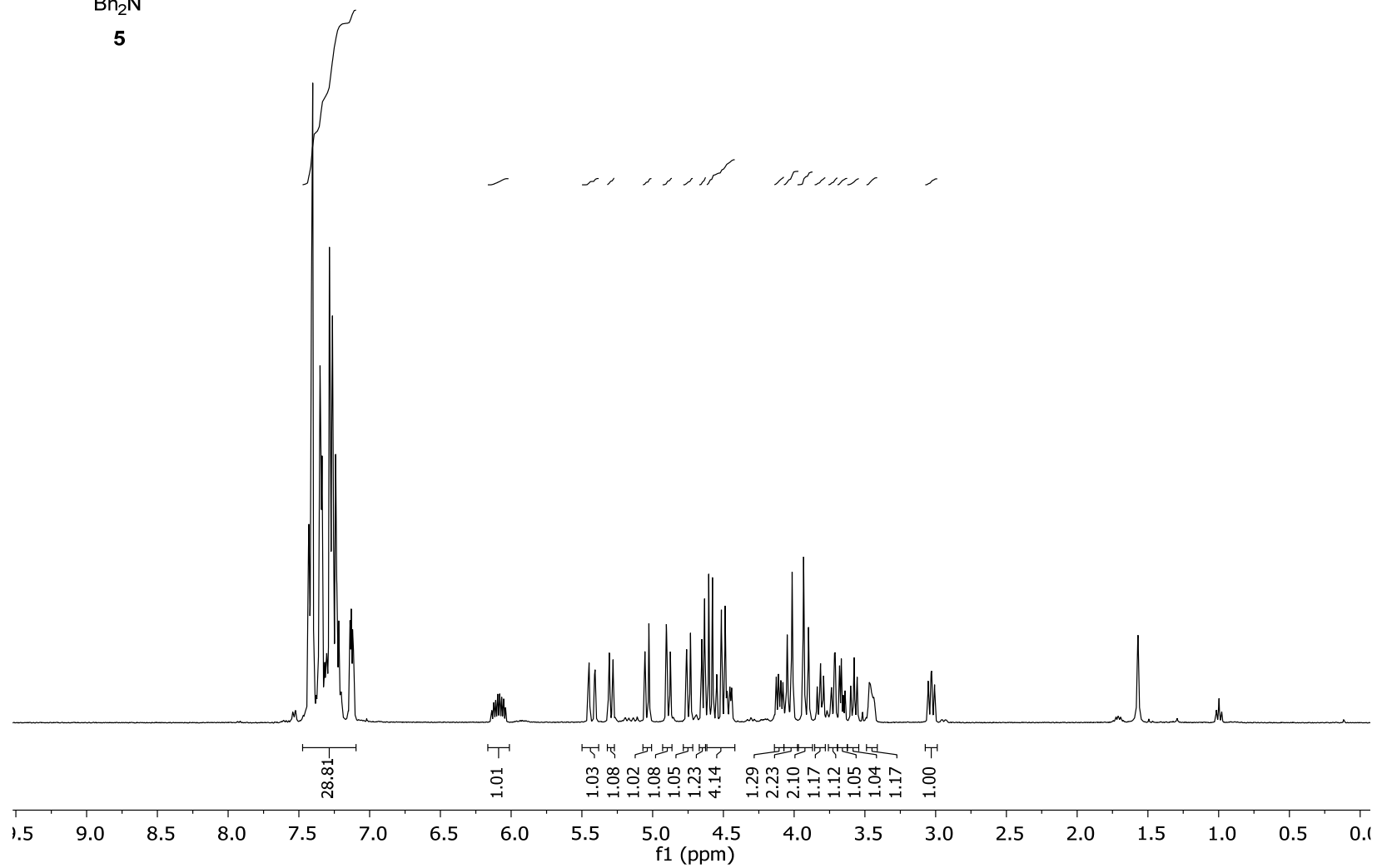
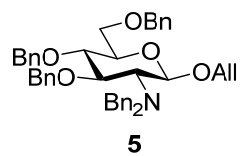
NMR spectra of synthesized compounds



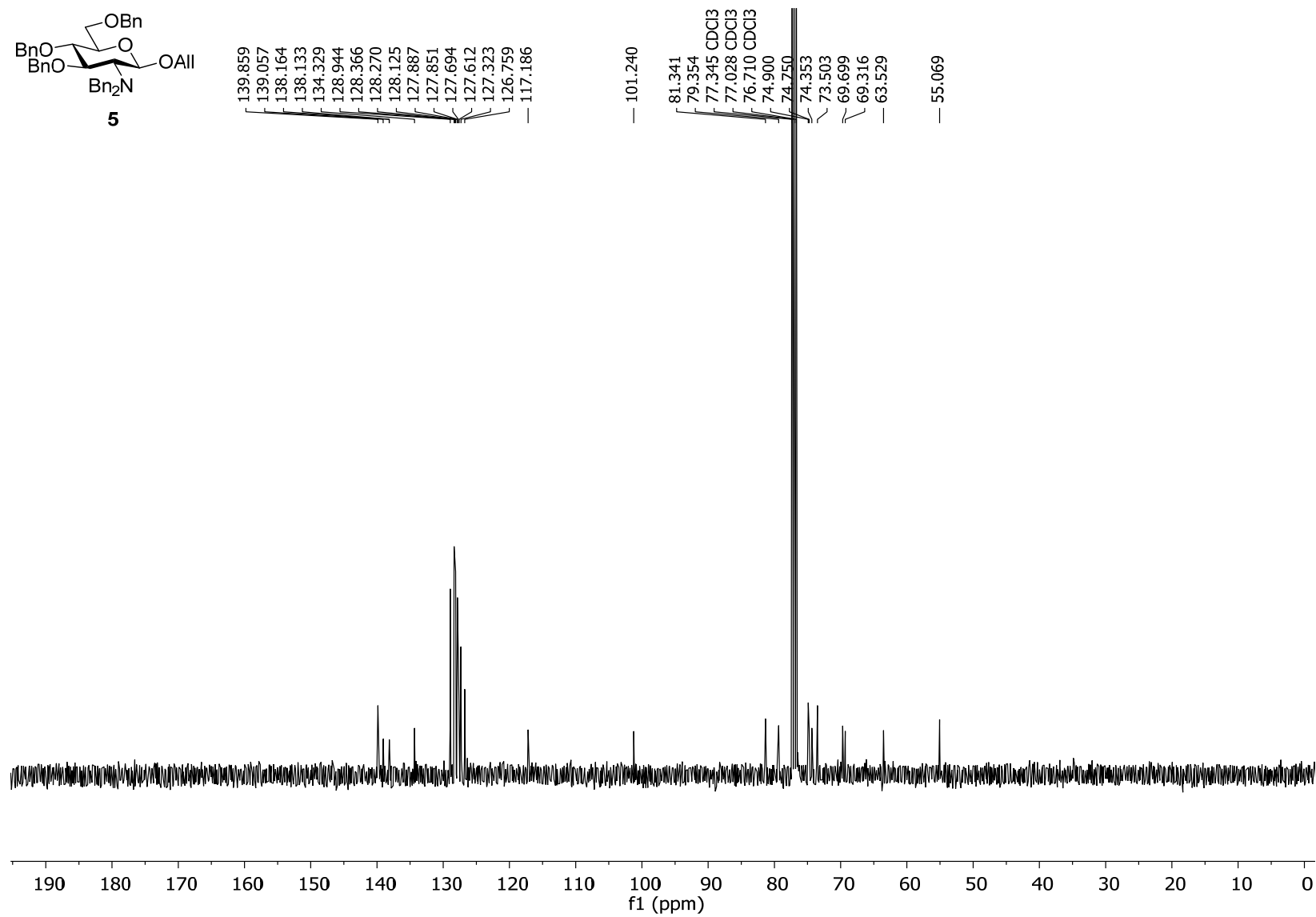
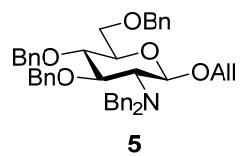
<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of **5a**



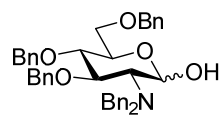
<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of **5a**



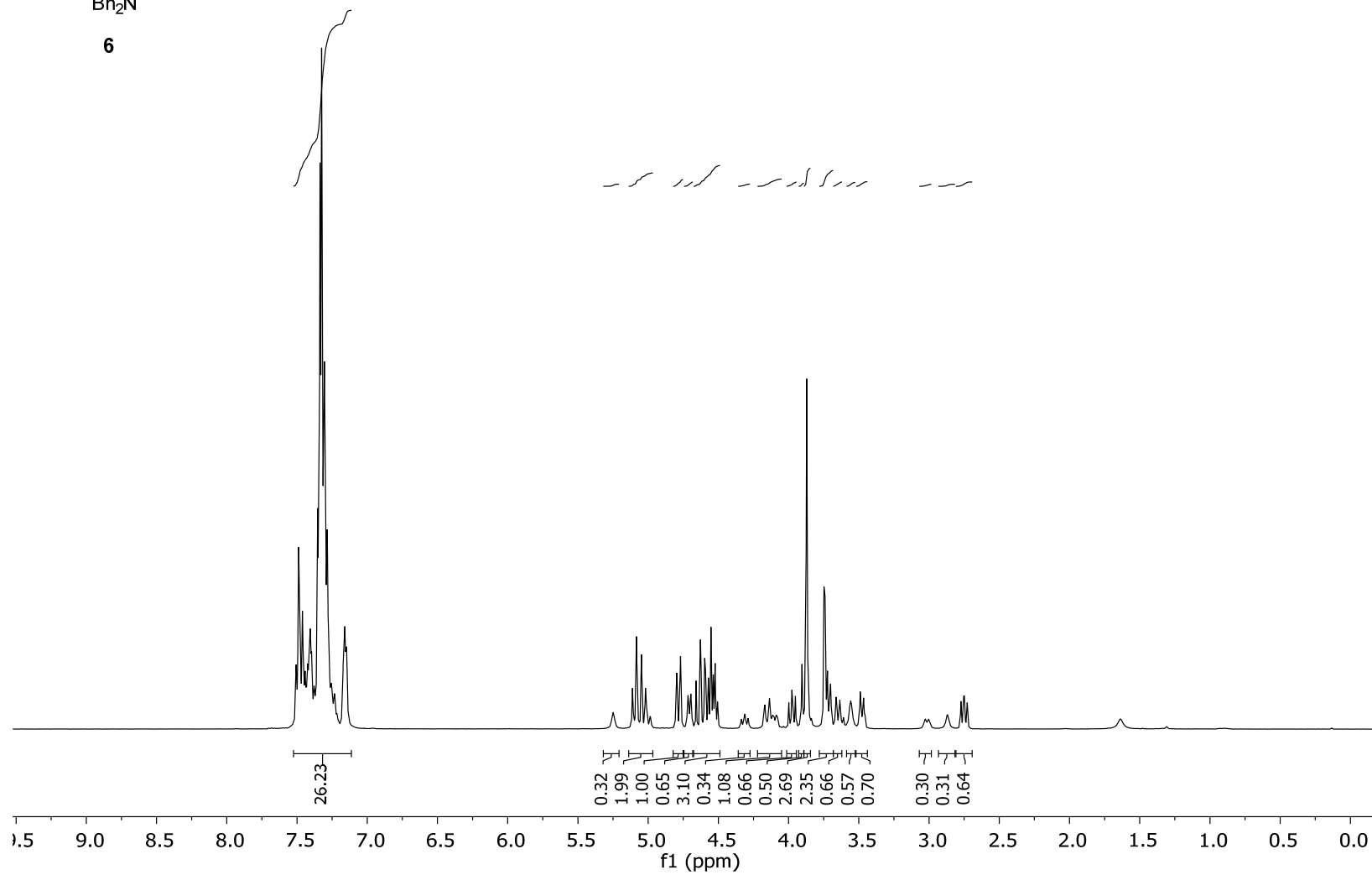
$^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of **5 $\beta$**



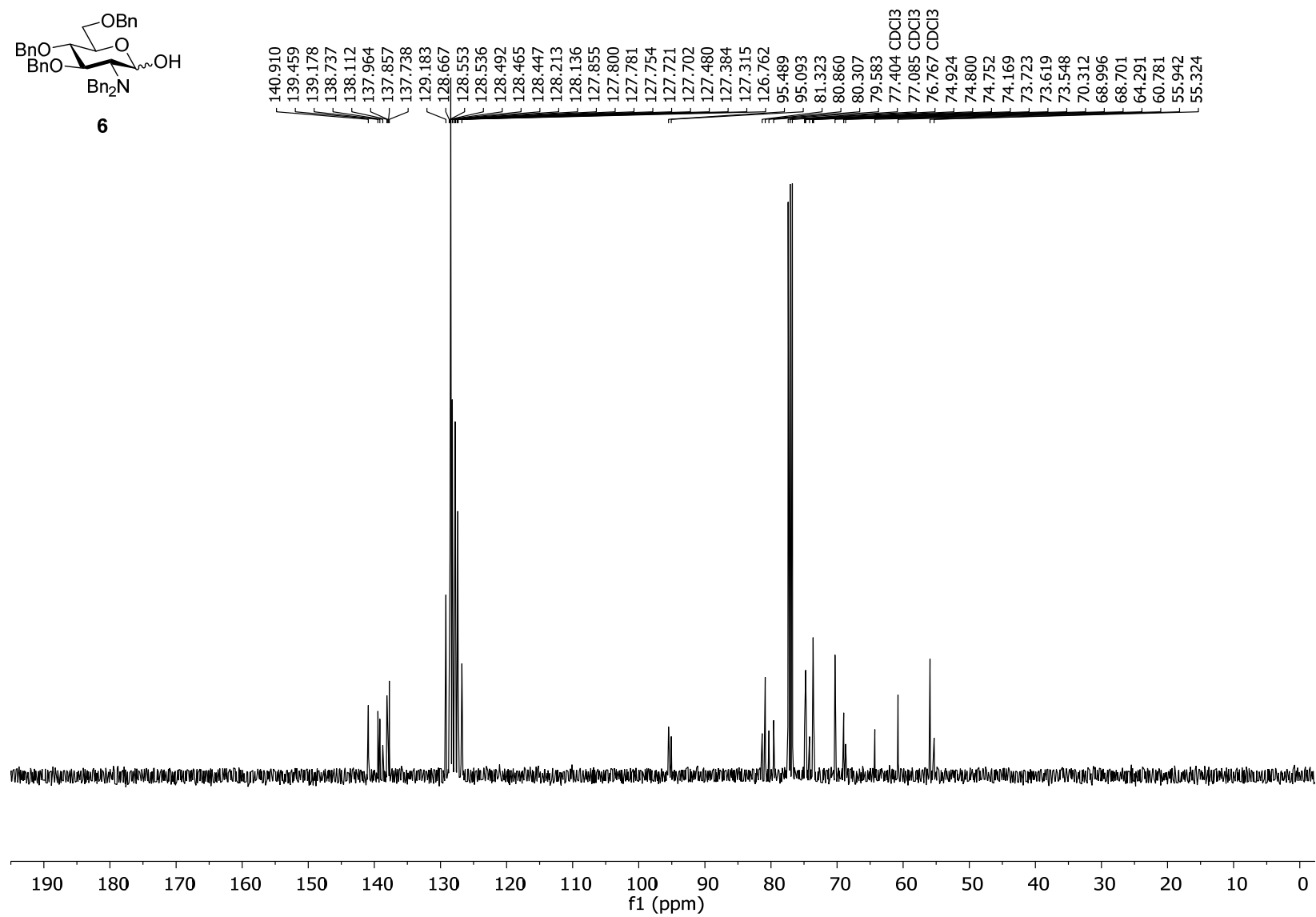
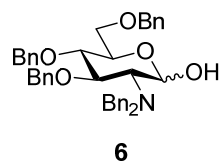
$^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of **5 $\beta$**



**6**

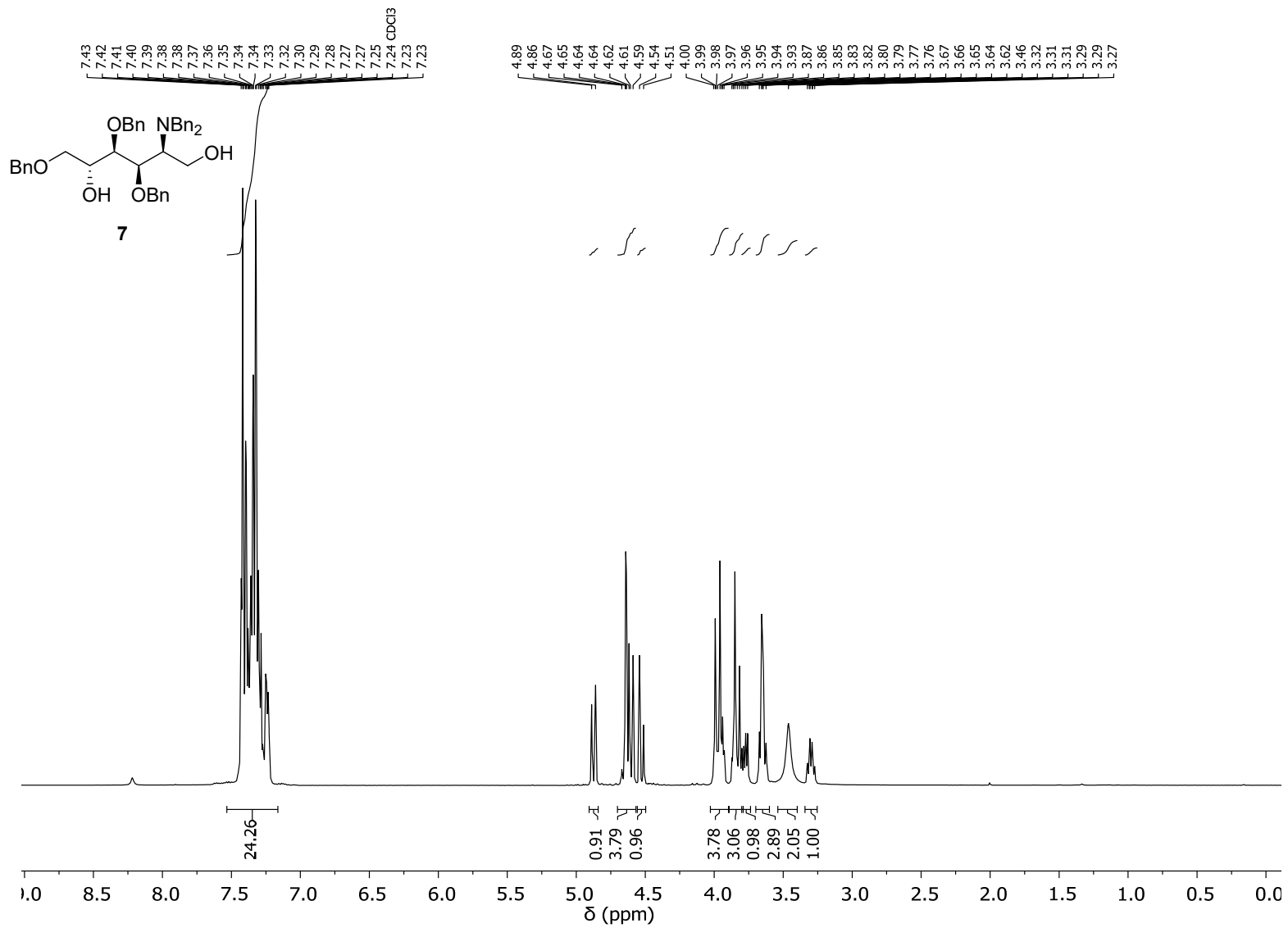


<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of **6**

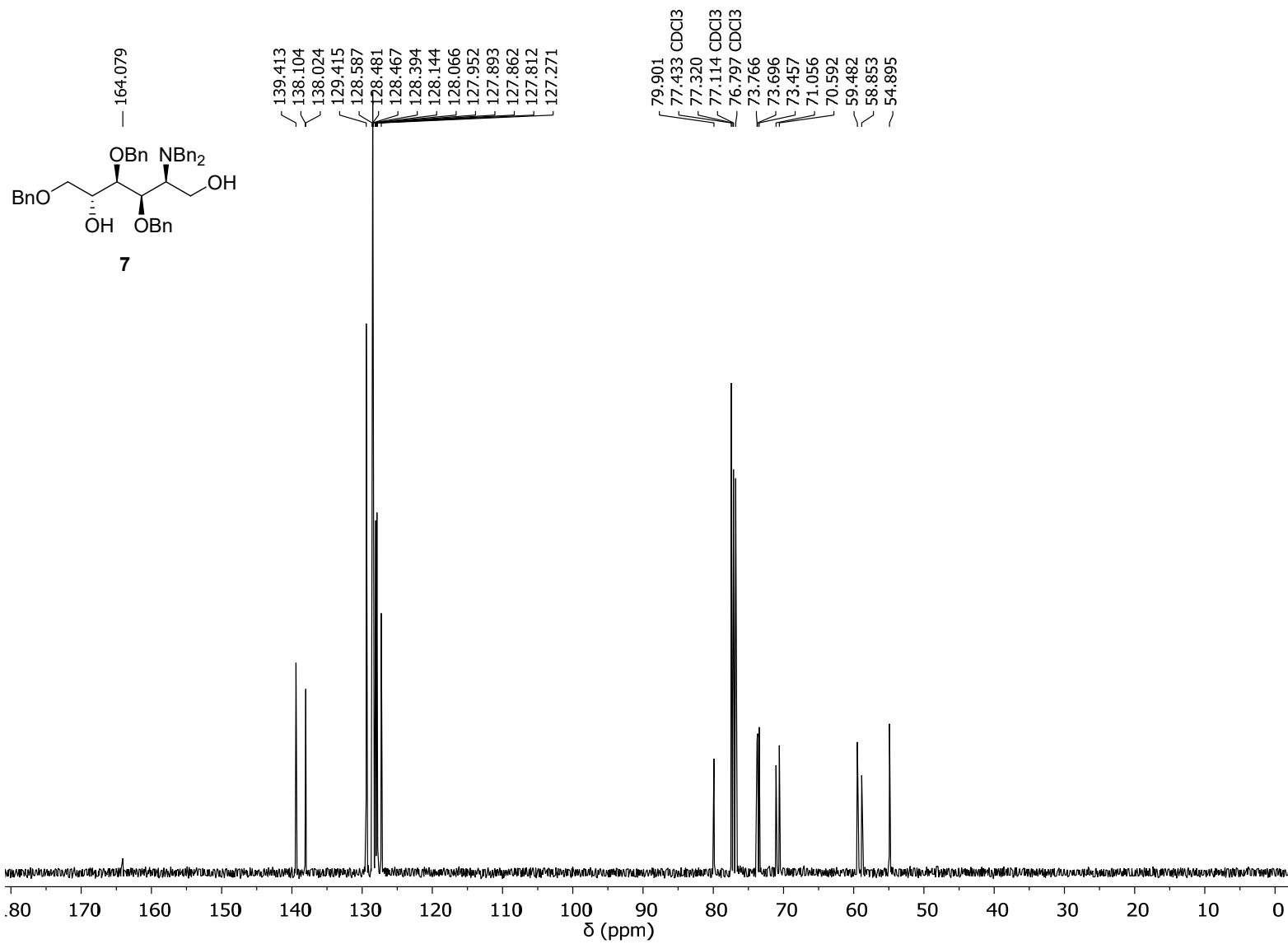


$^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of **6**

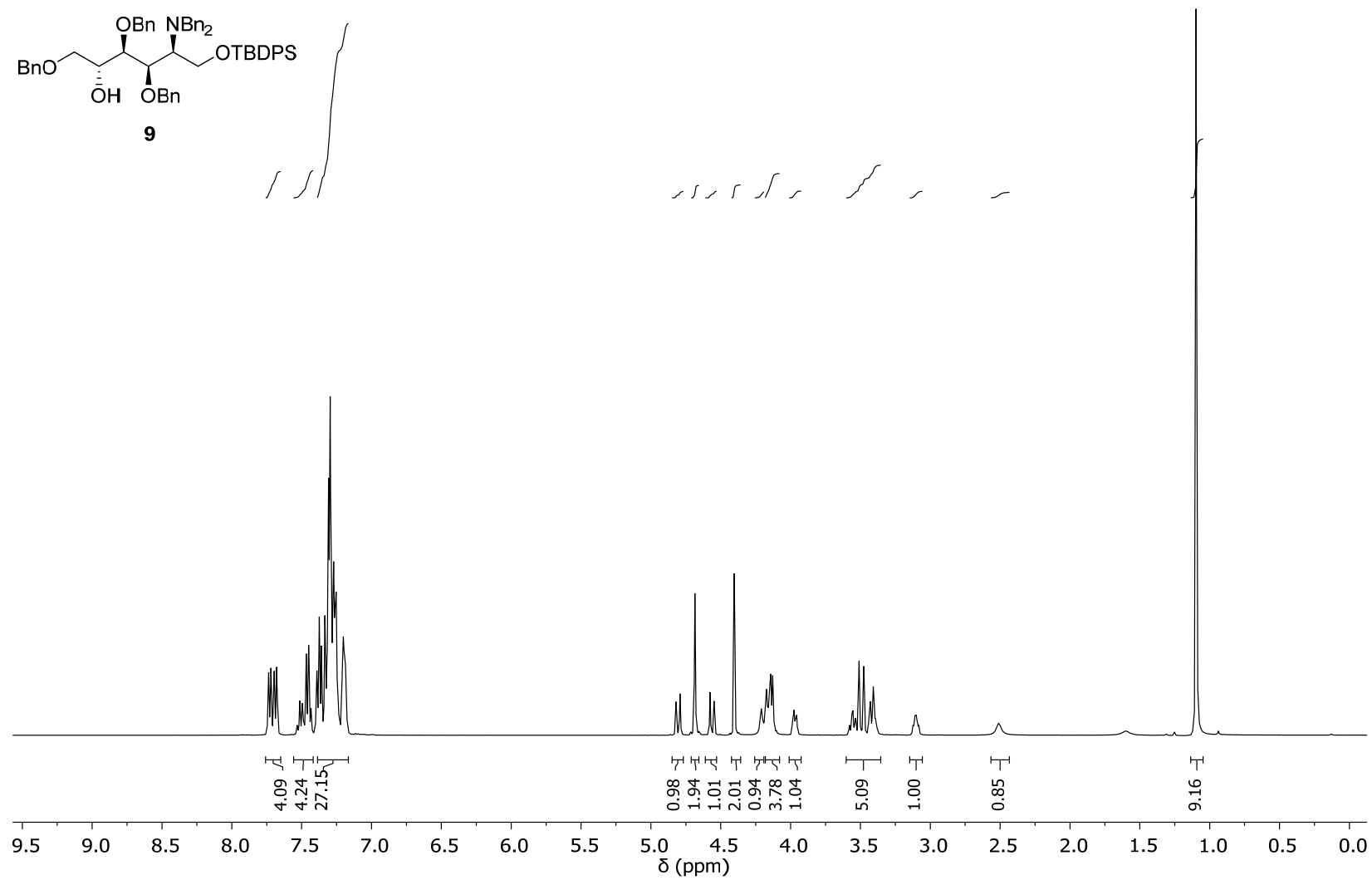
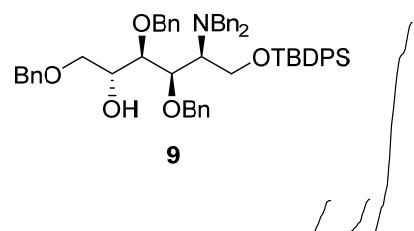




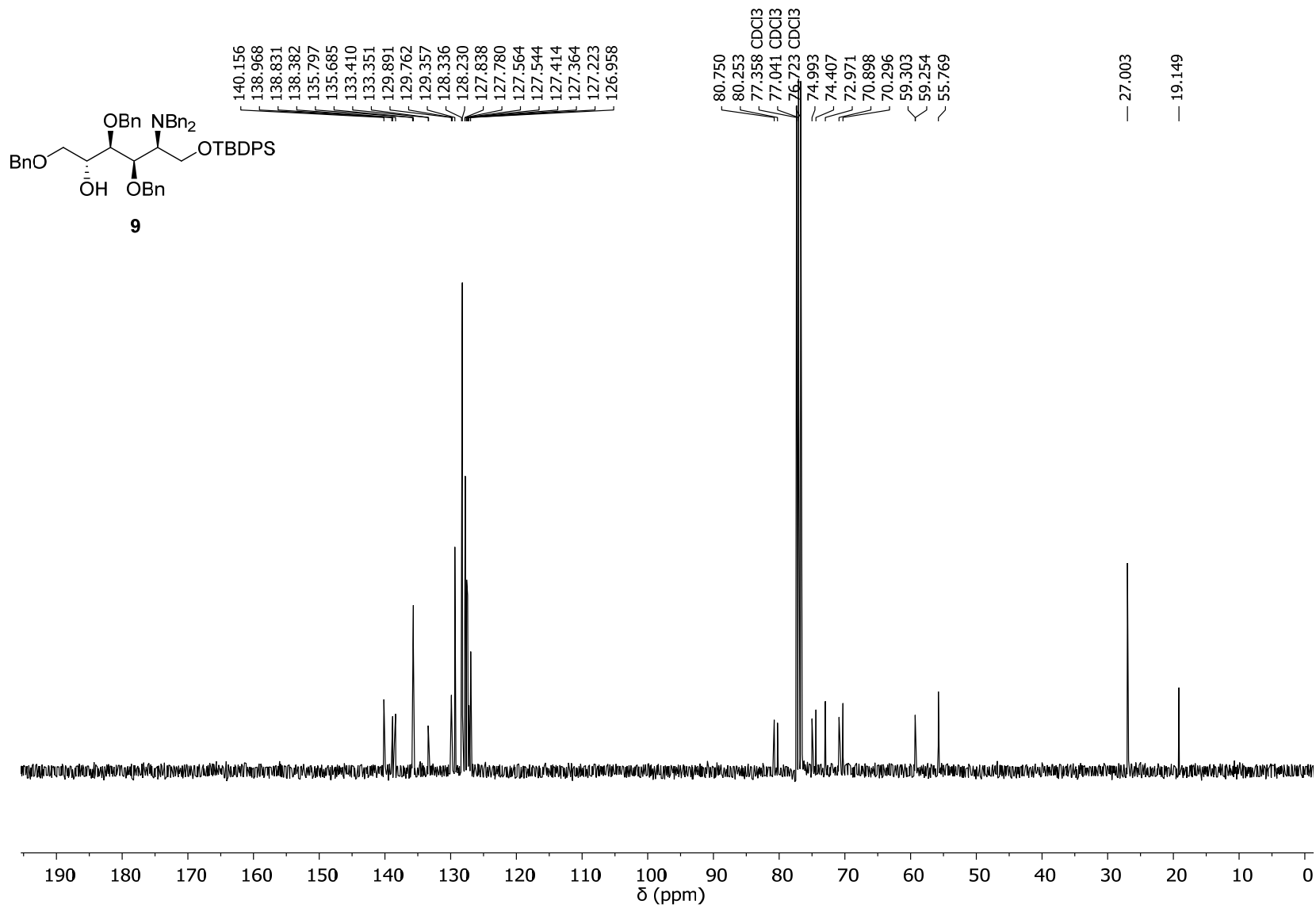
<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of **7**



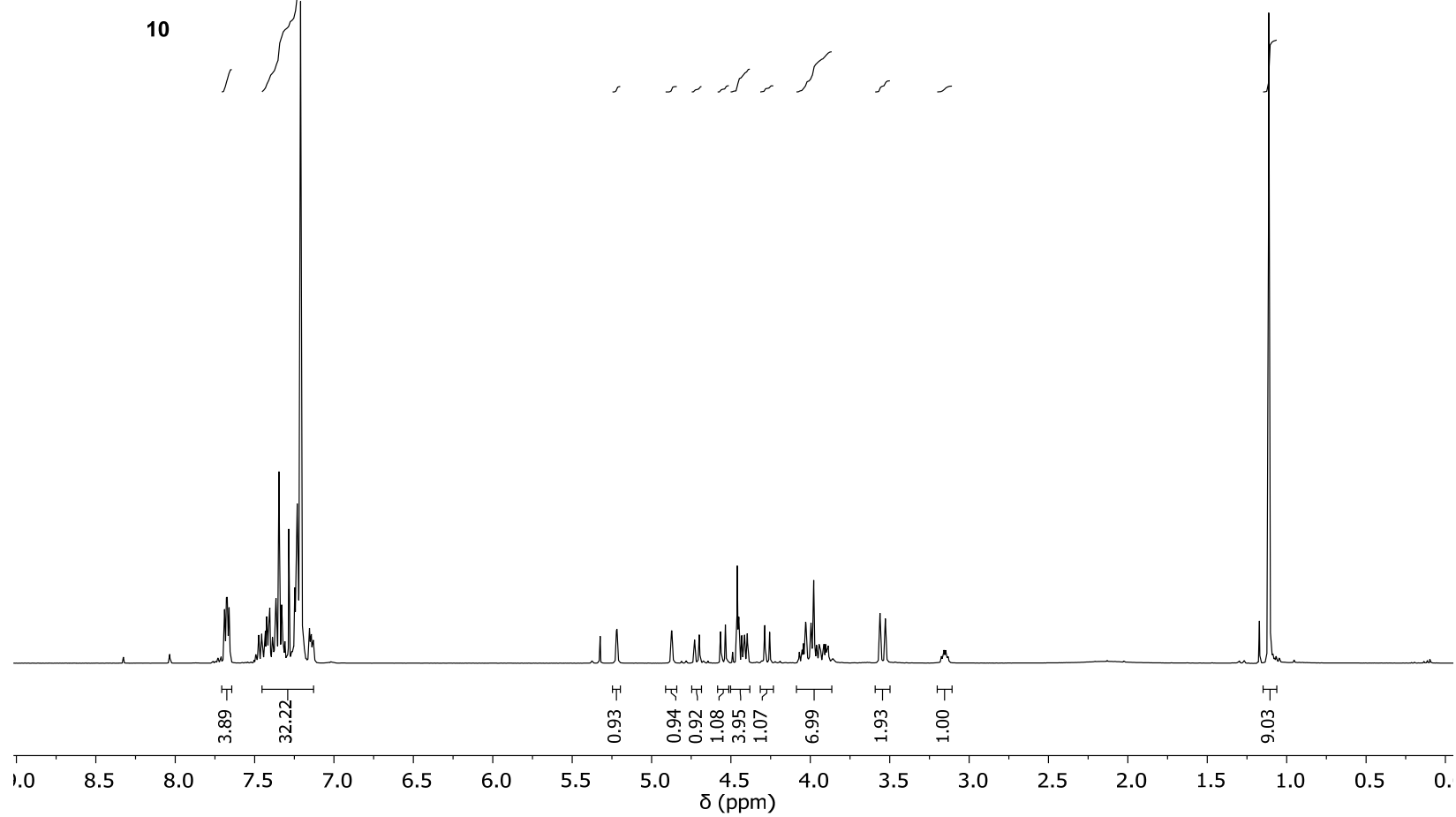
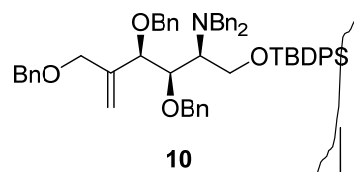
$^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of **7**



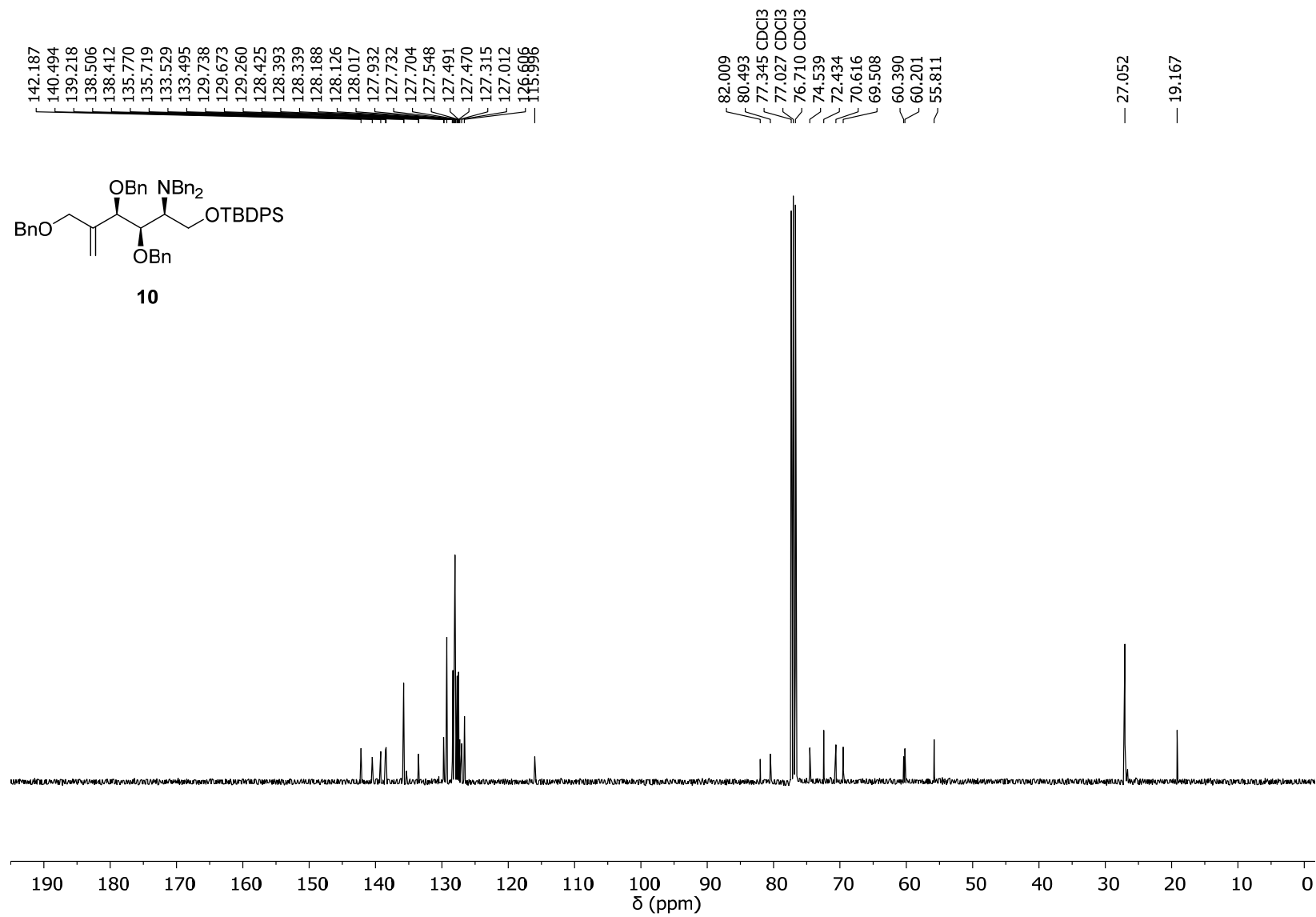
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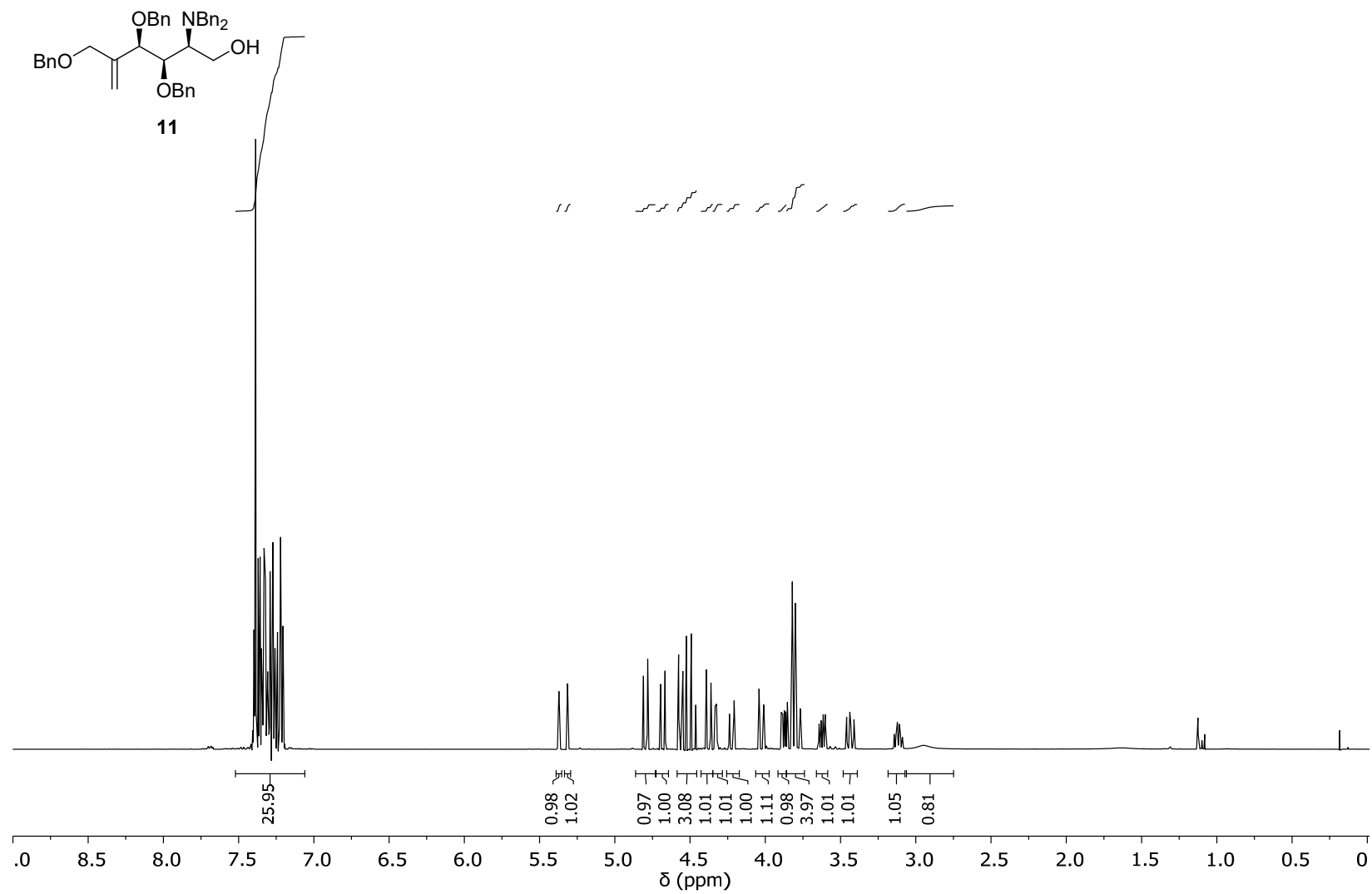
<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of **9**



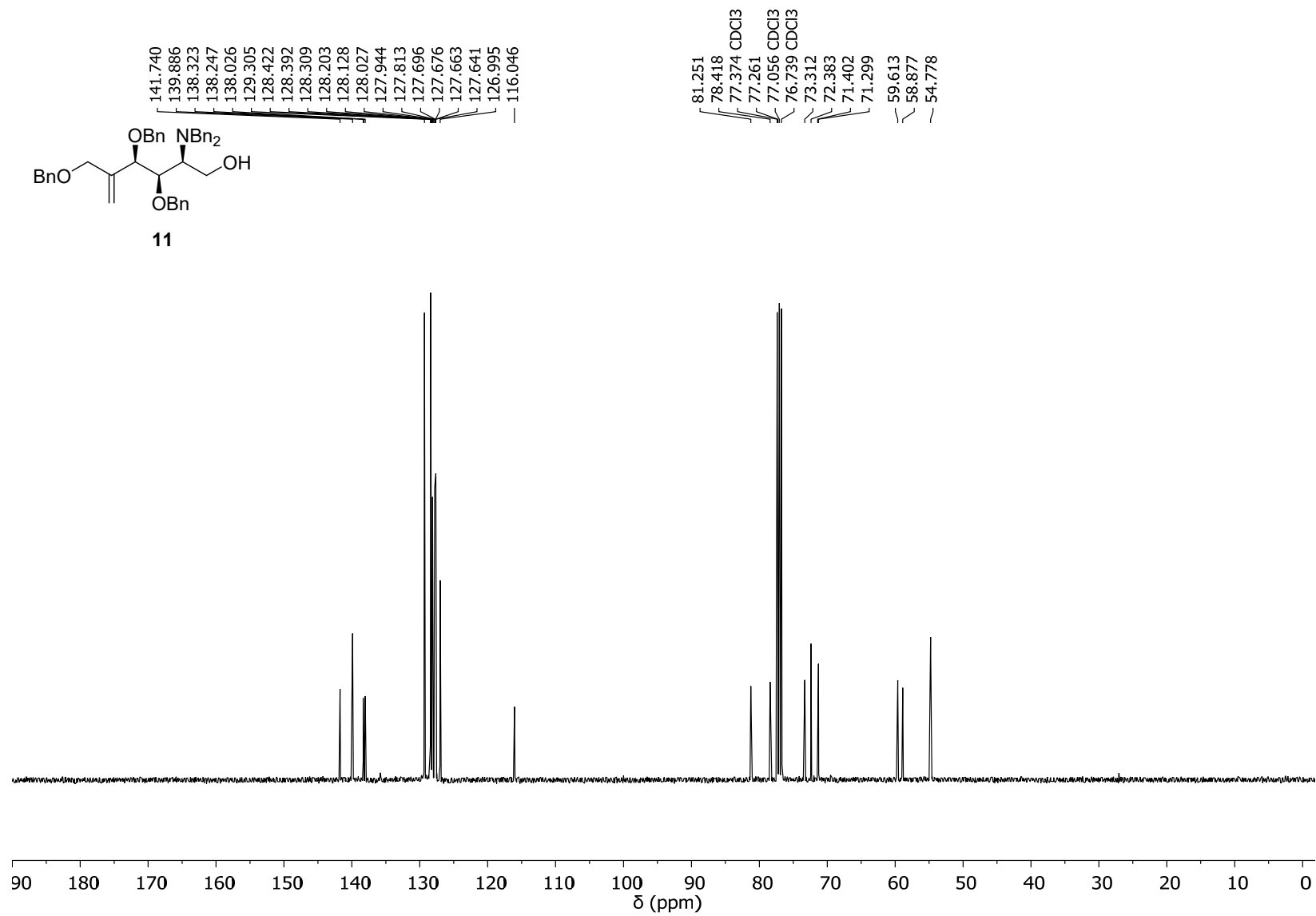
$^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of **10**



$^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of **10**

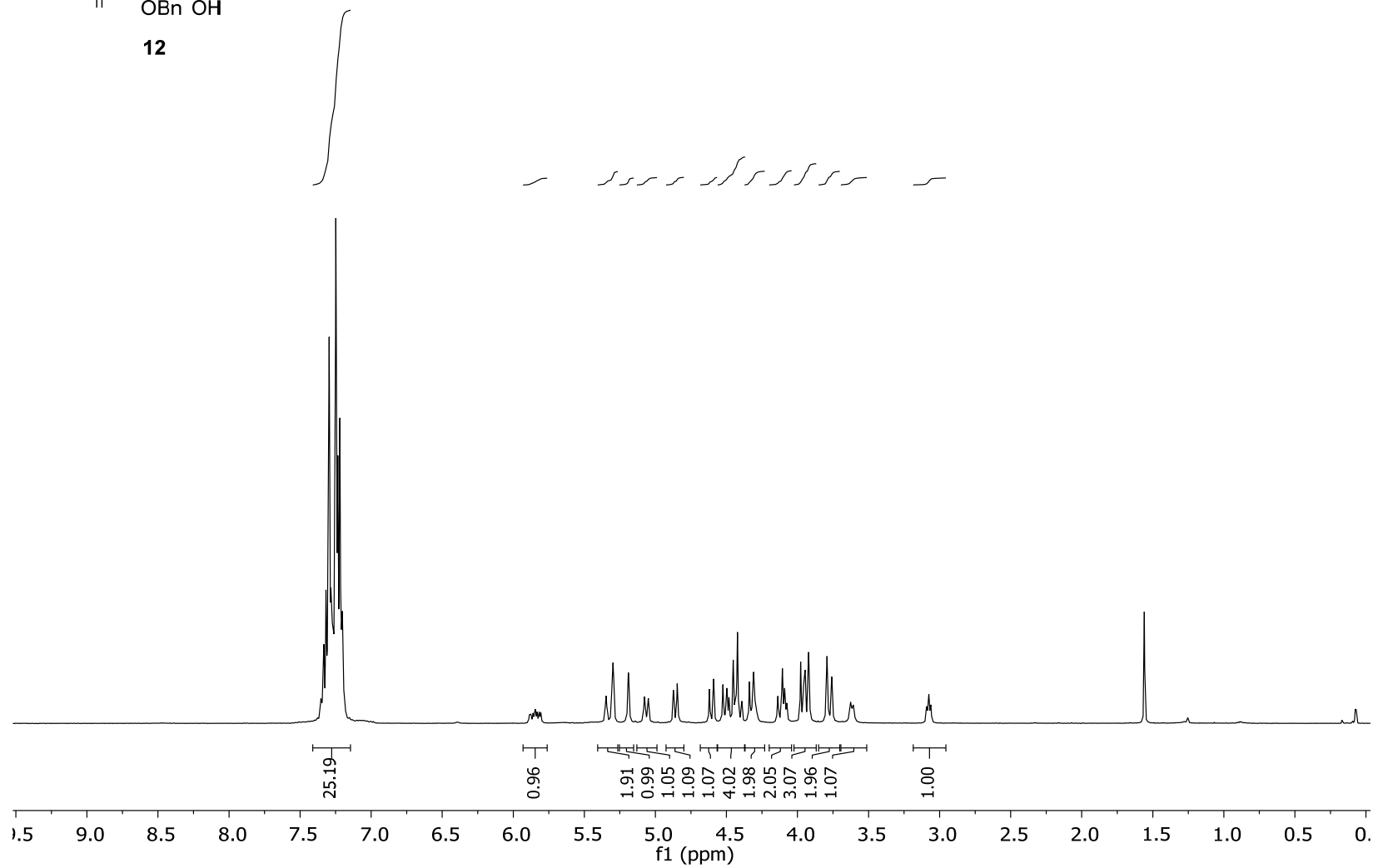
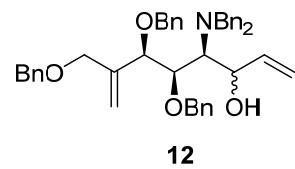


$^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of **11**

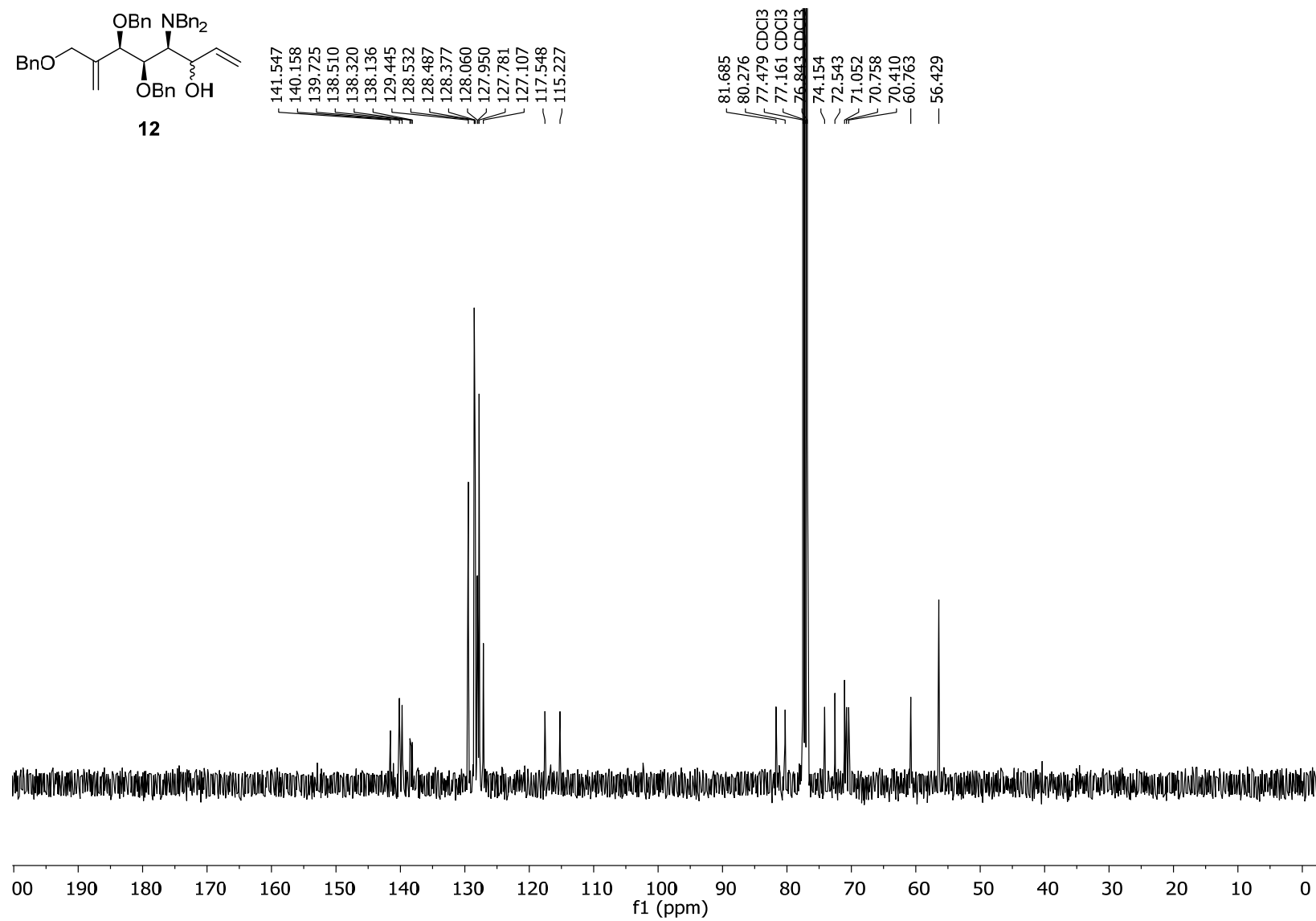
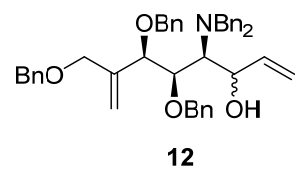


<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of **11**

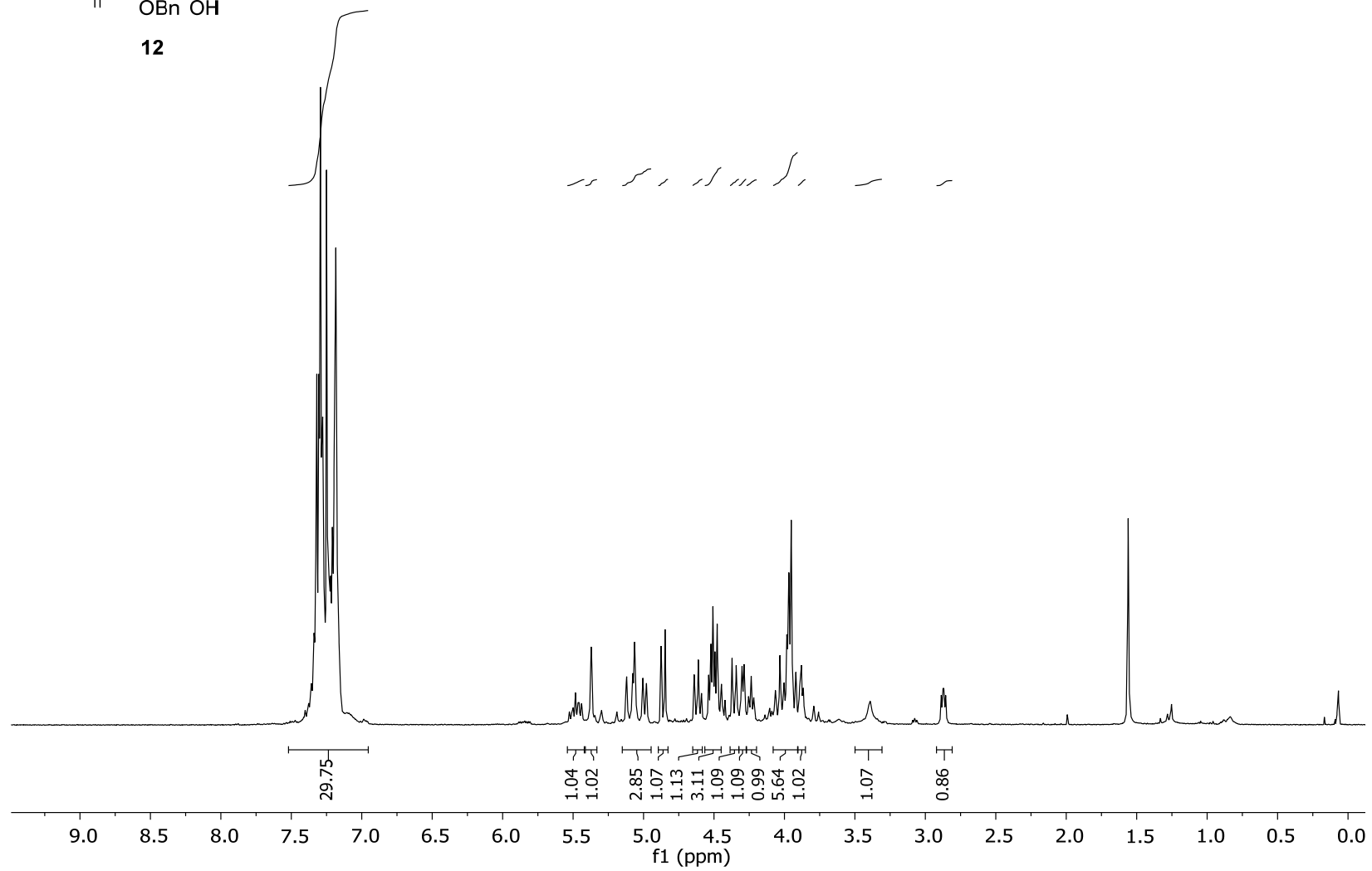
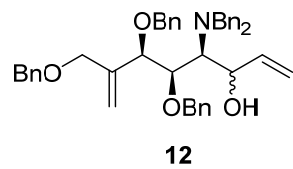




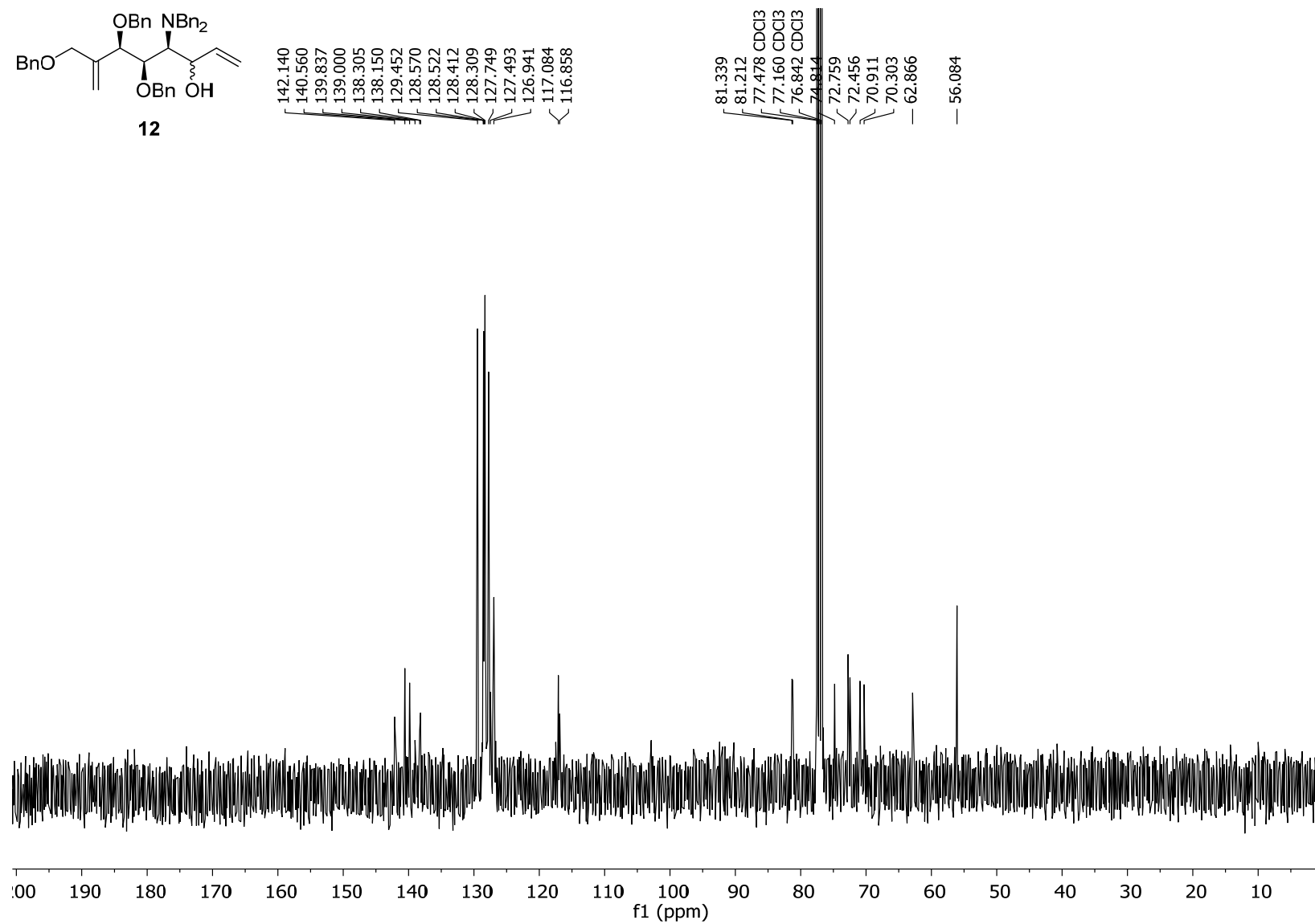
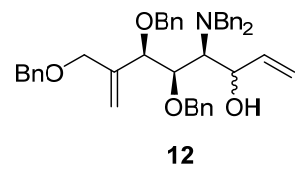
$^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of **12** (isomer 1)



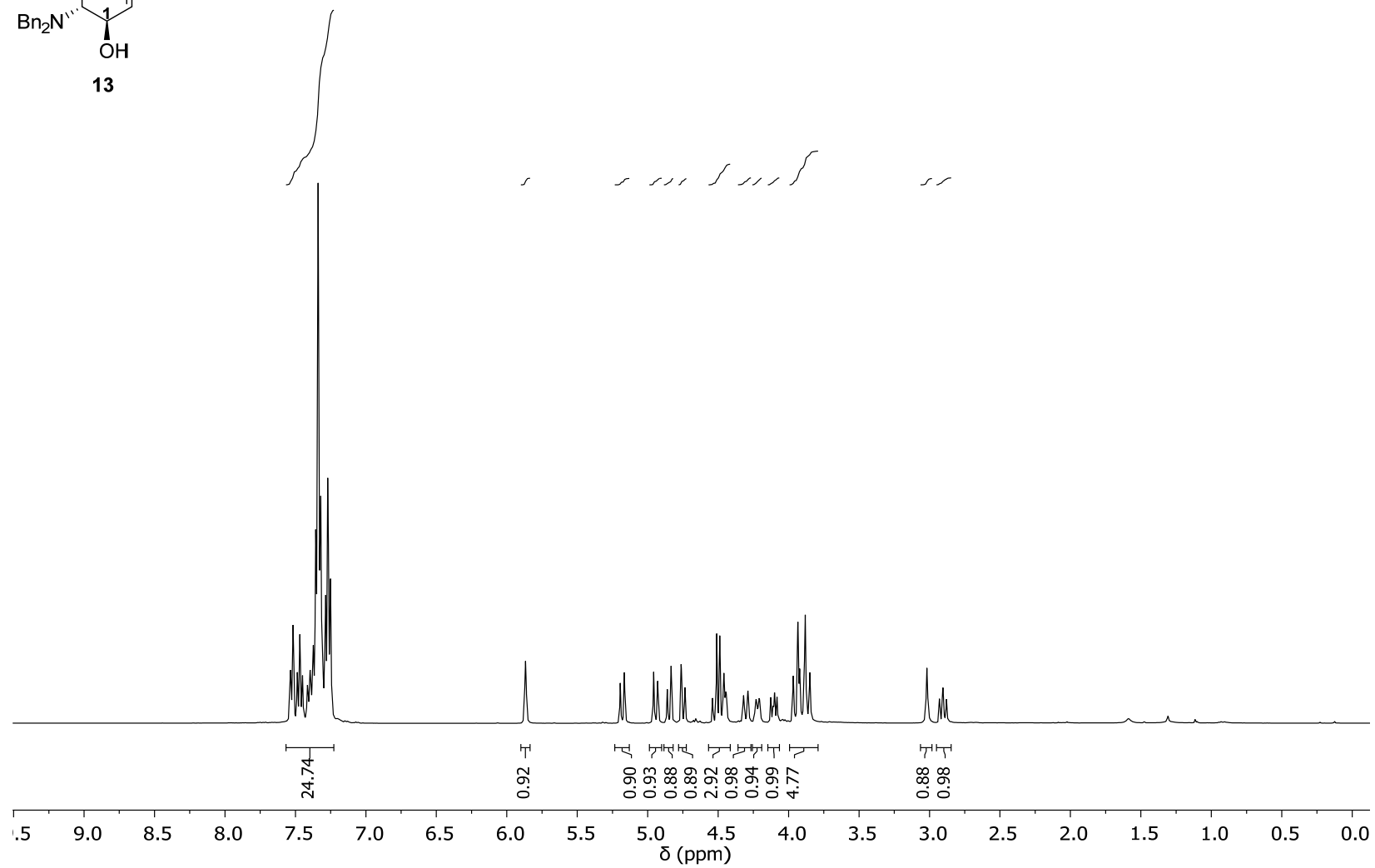
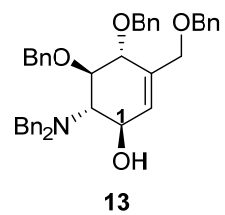
$^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of **12** (isomer 1)



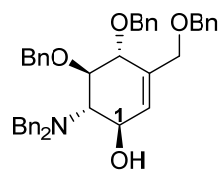
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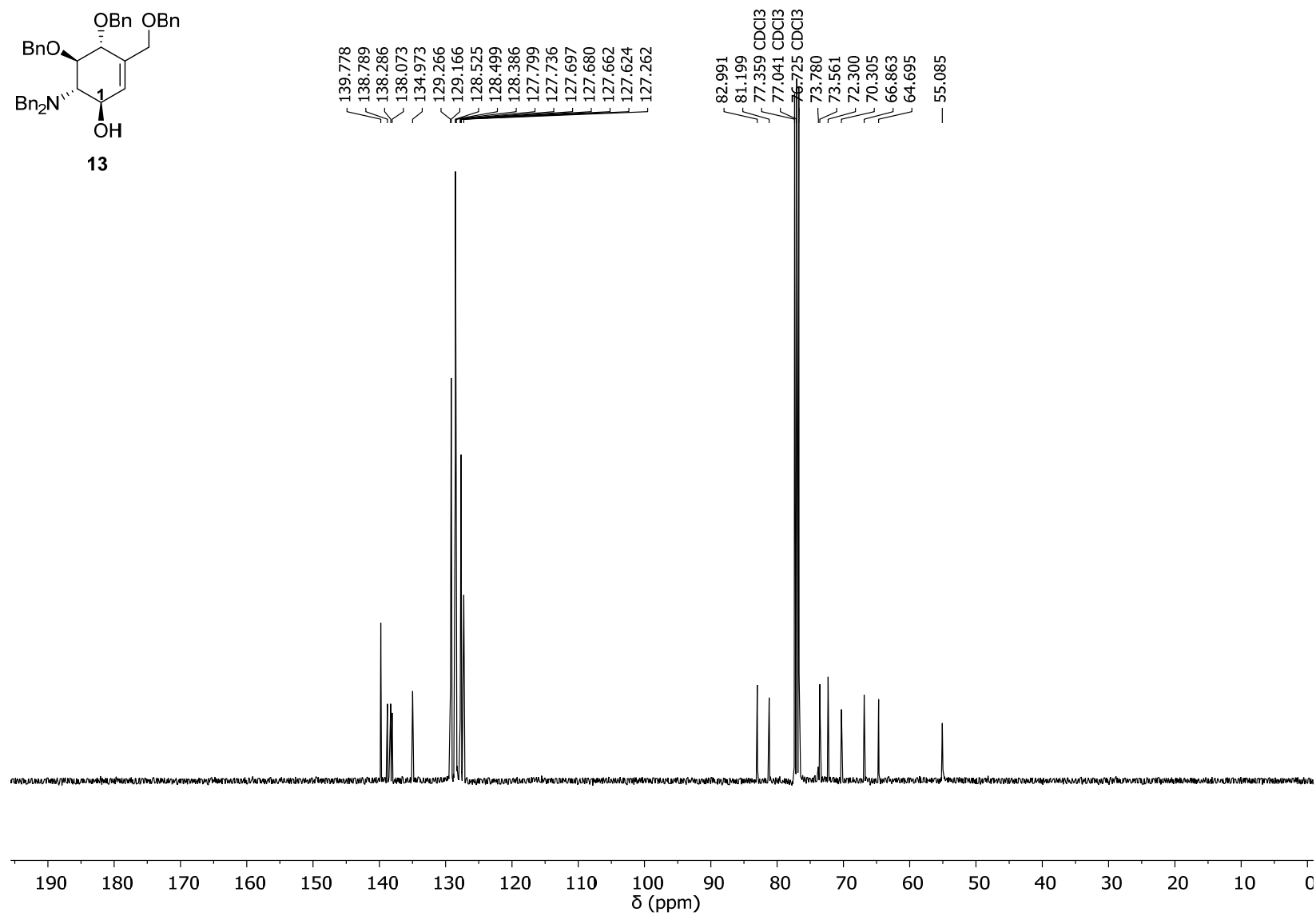
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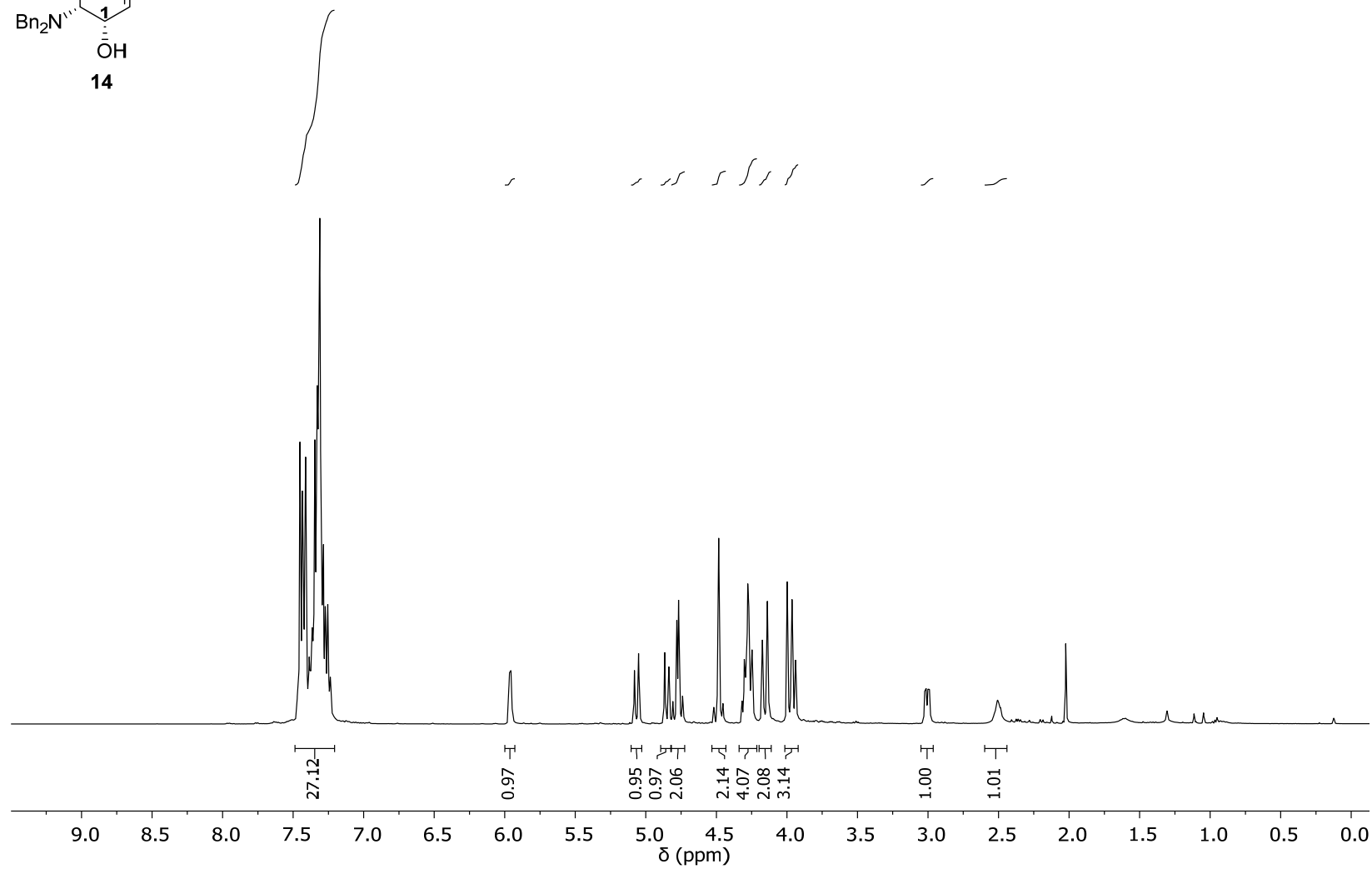
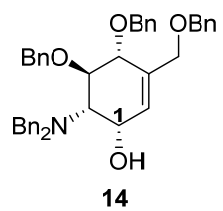
$^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of **13**



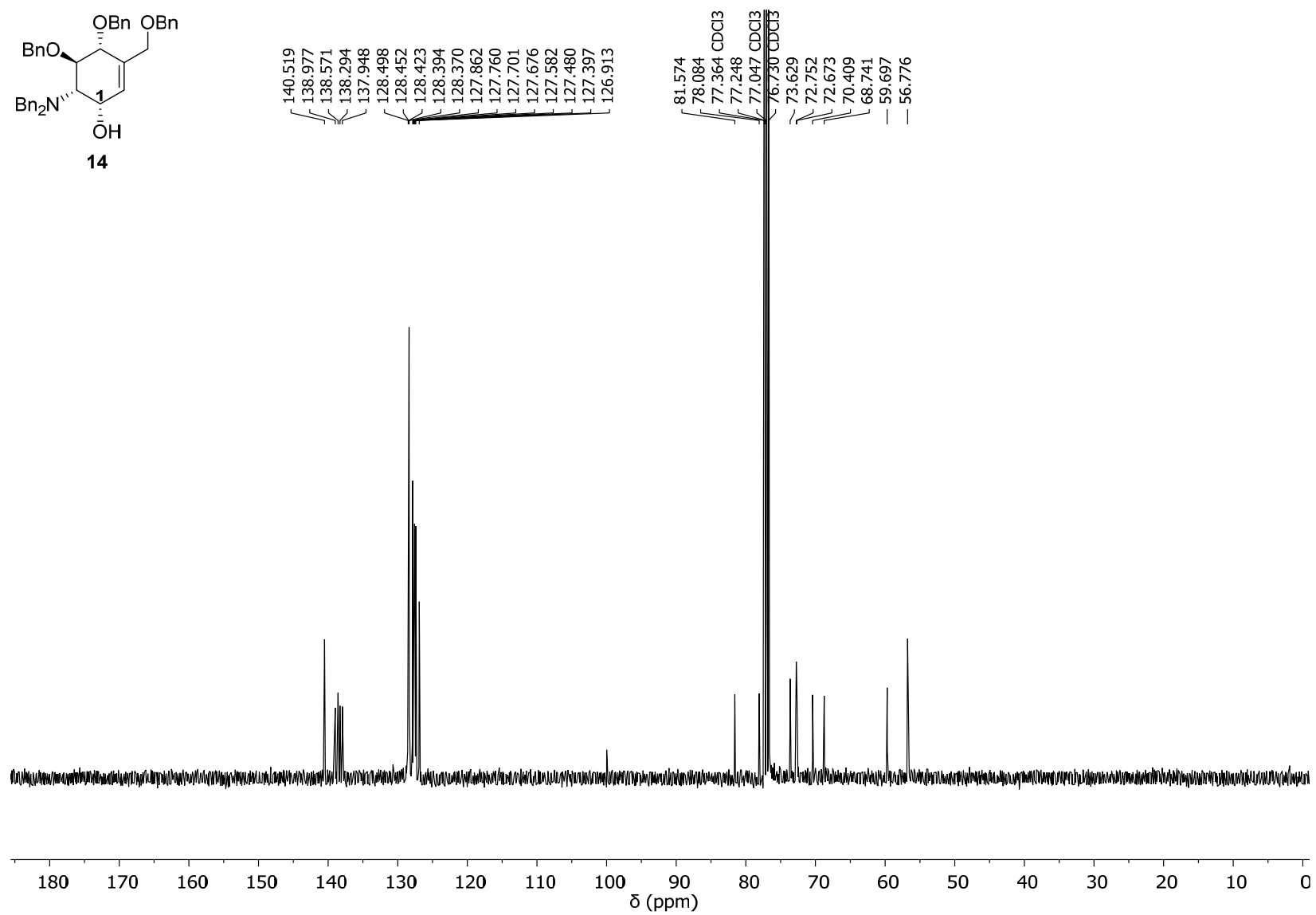
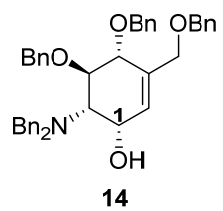
**13**



<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of **13**

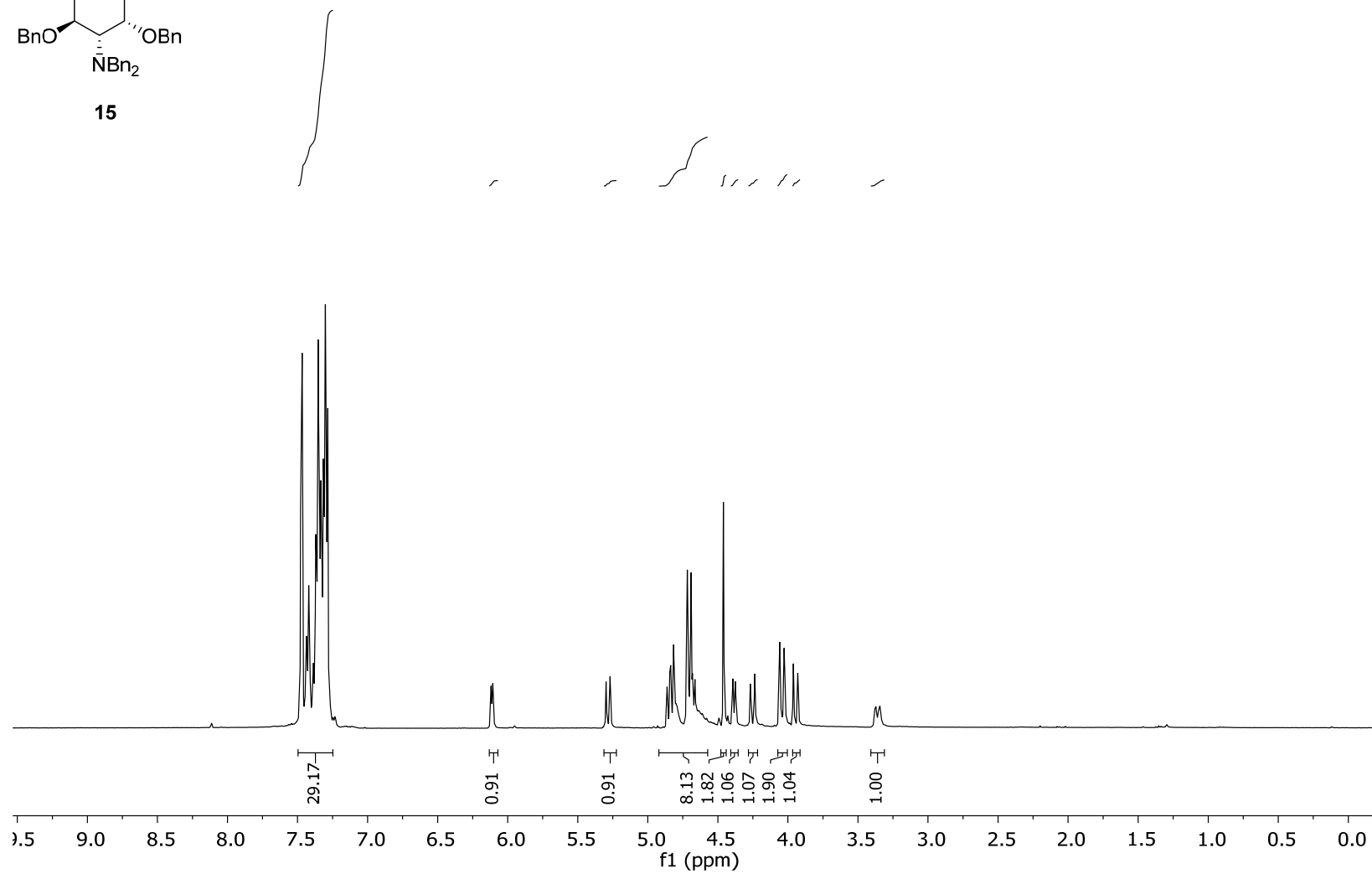
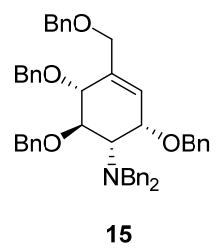


$^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of **14**

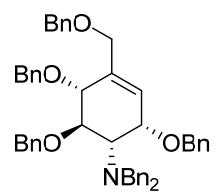


$^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of **14**

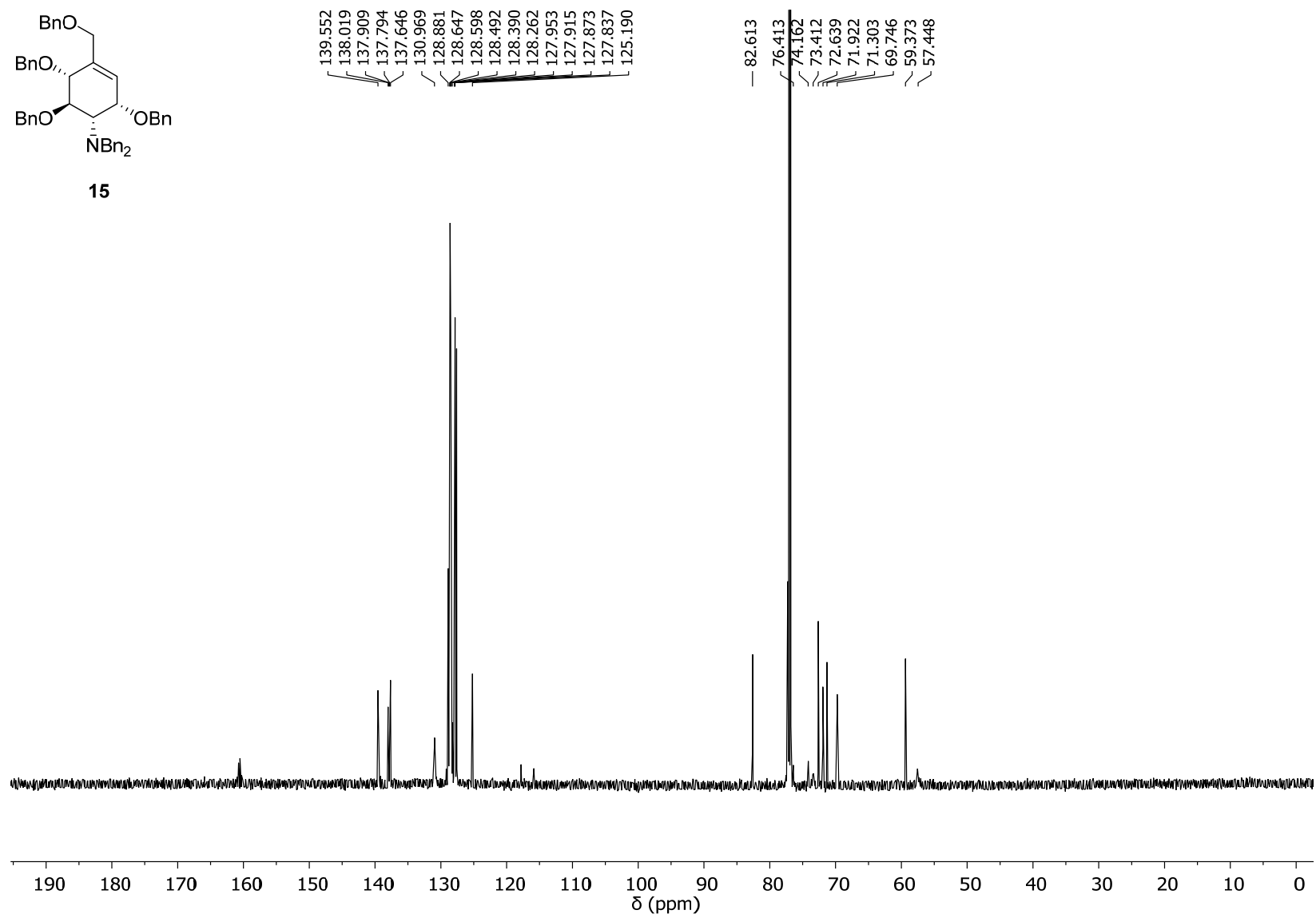




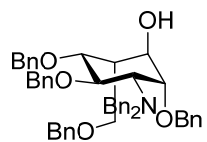
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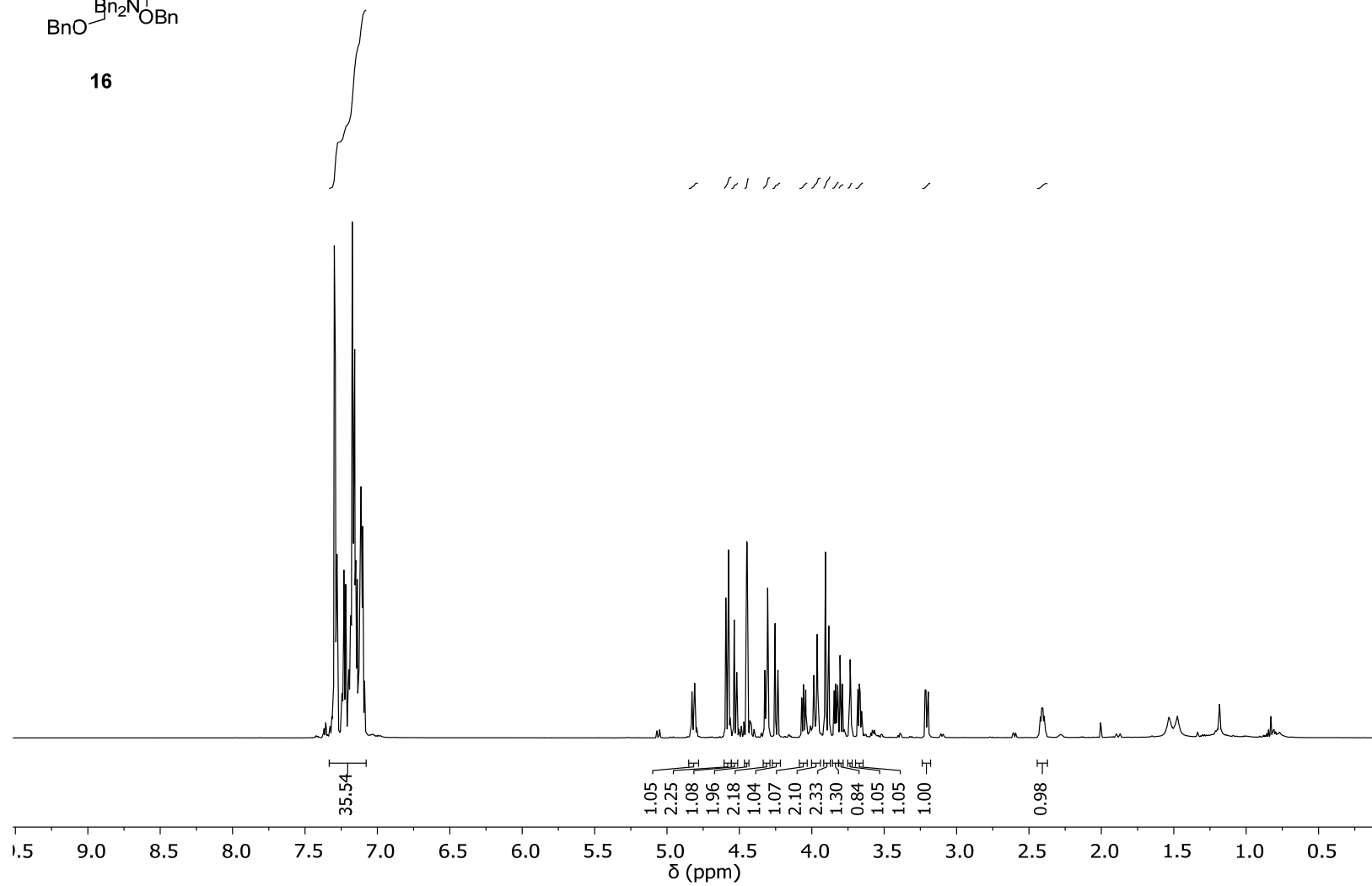
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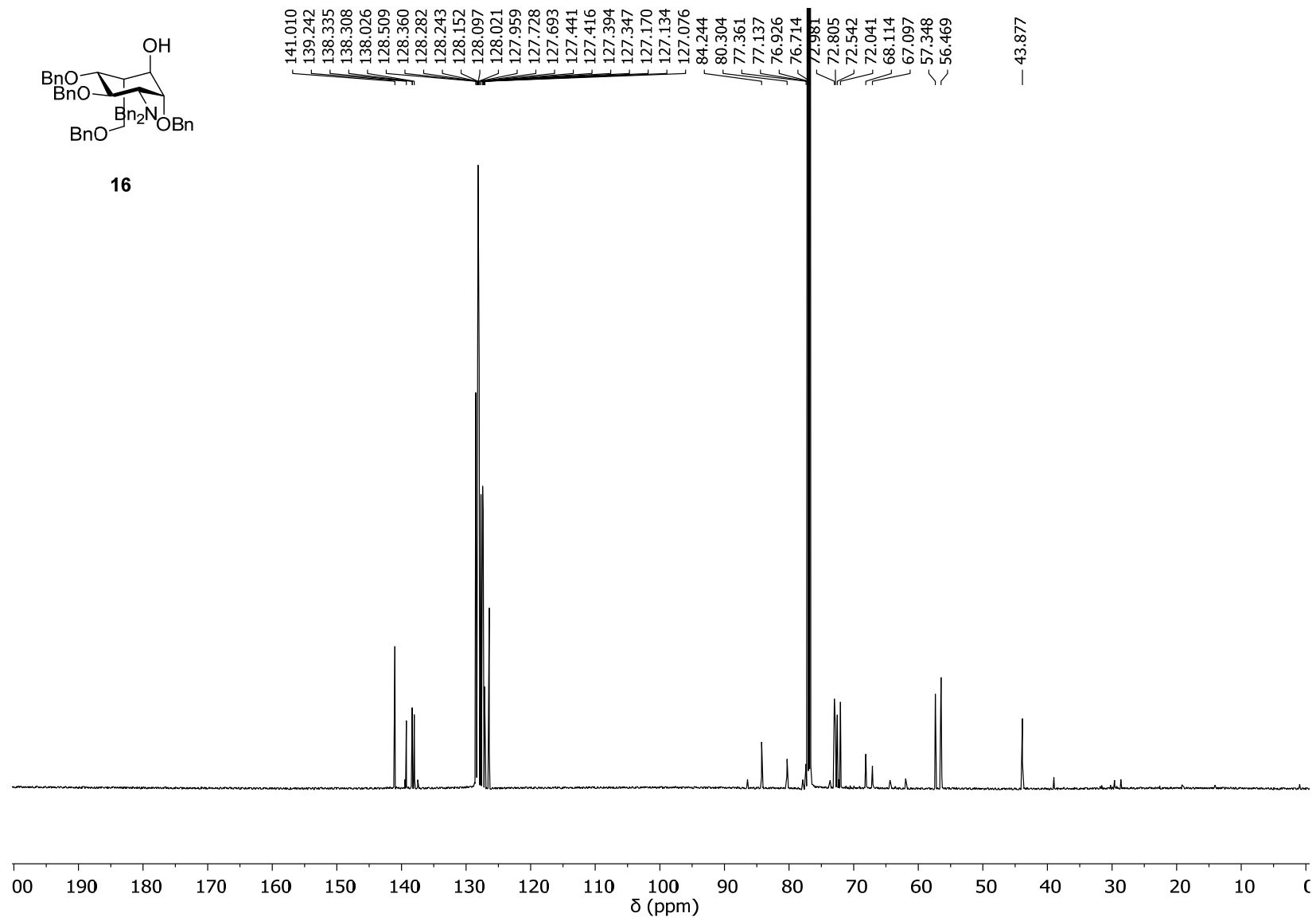
<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of **15**



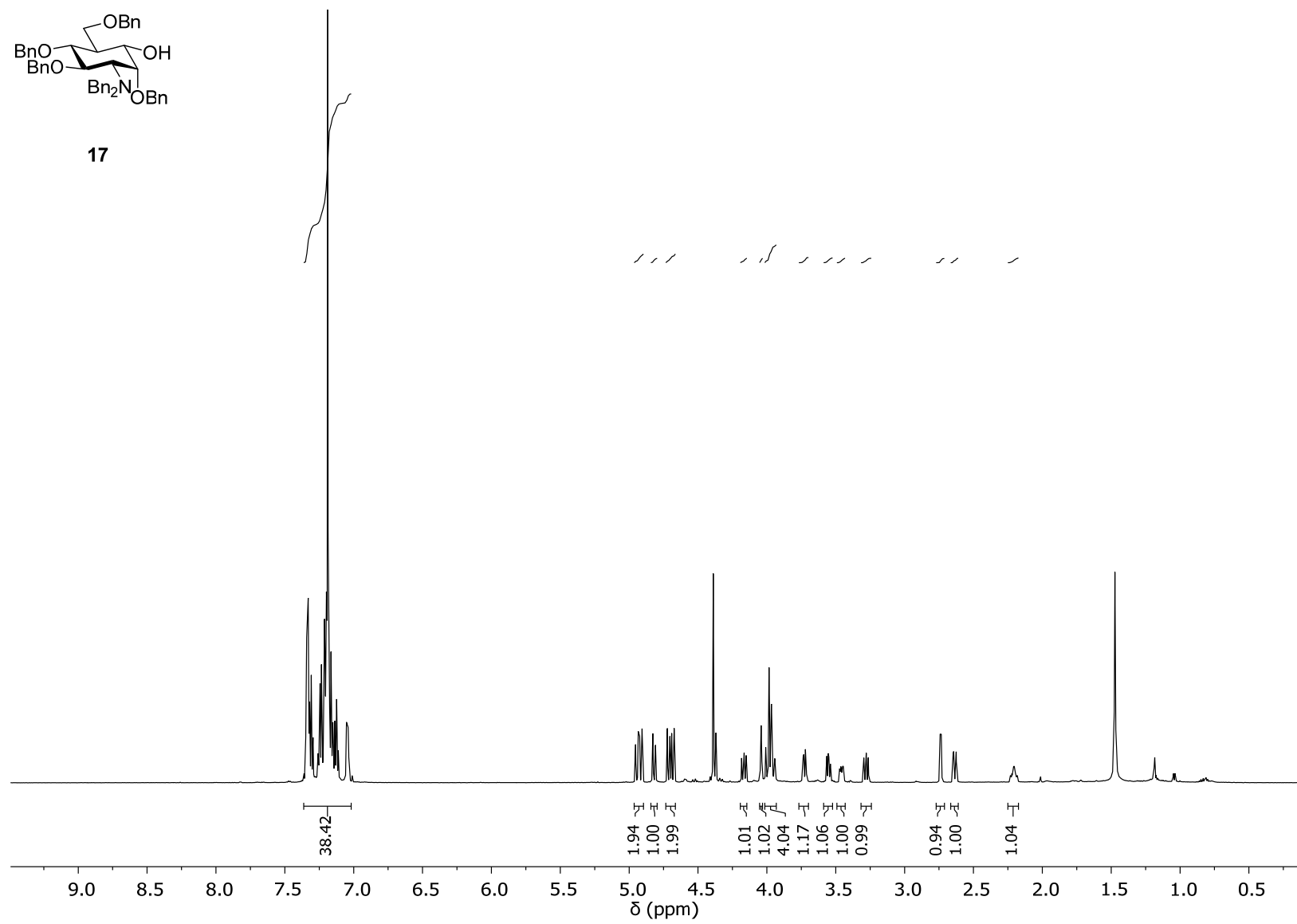
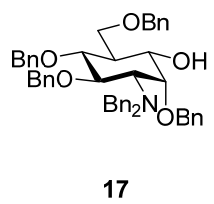
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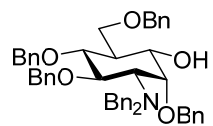
$^1\text{H}$  NMR spectrum (600 MHz,  $\text{CDCl}_3$ ) of **16**



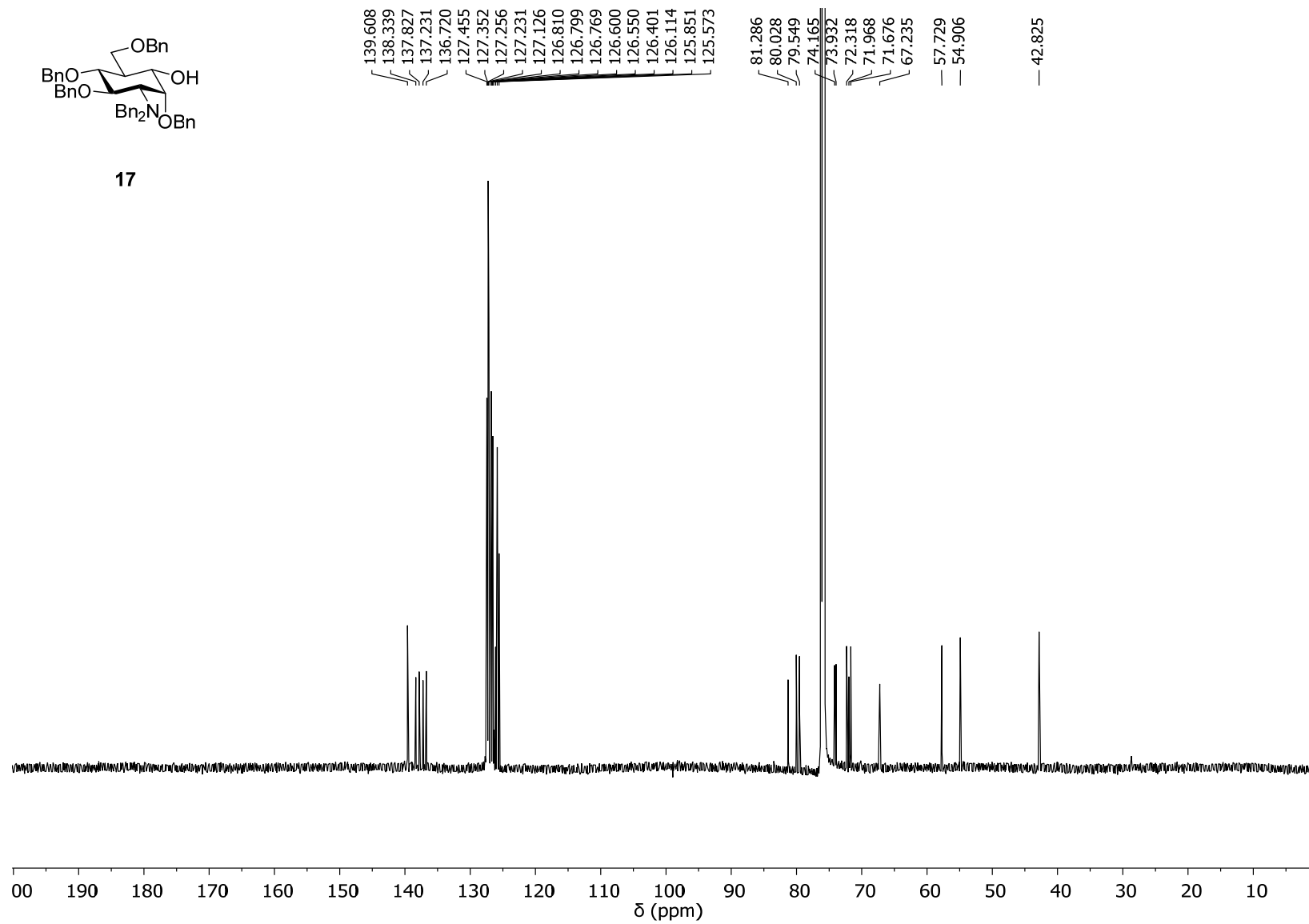
<sup>13</sup>C NMR spectrum (151 MHz, CDCl<sub>3</sub>) of **16**



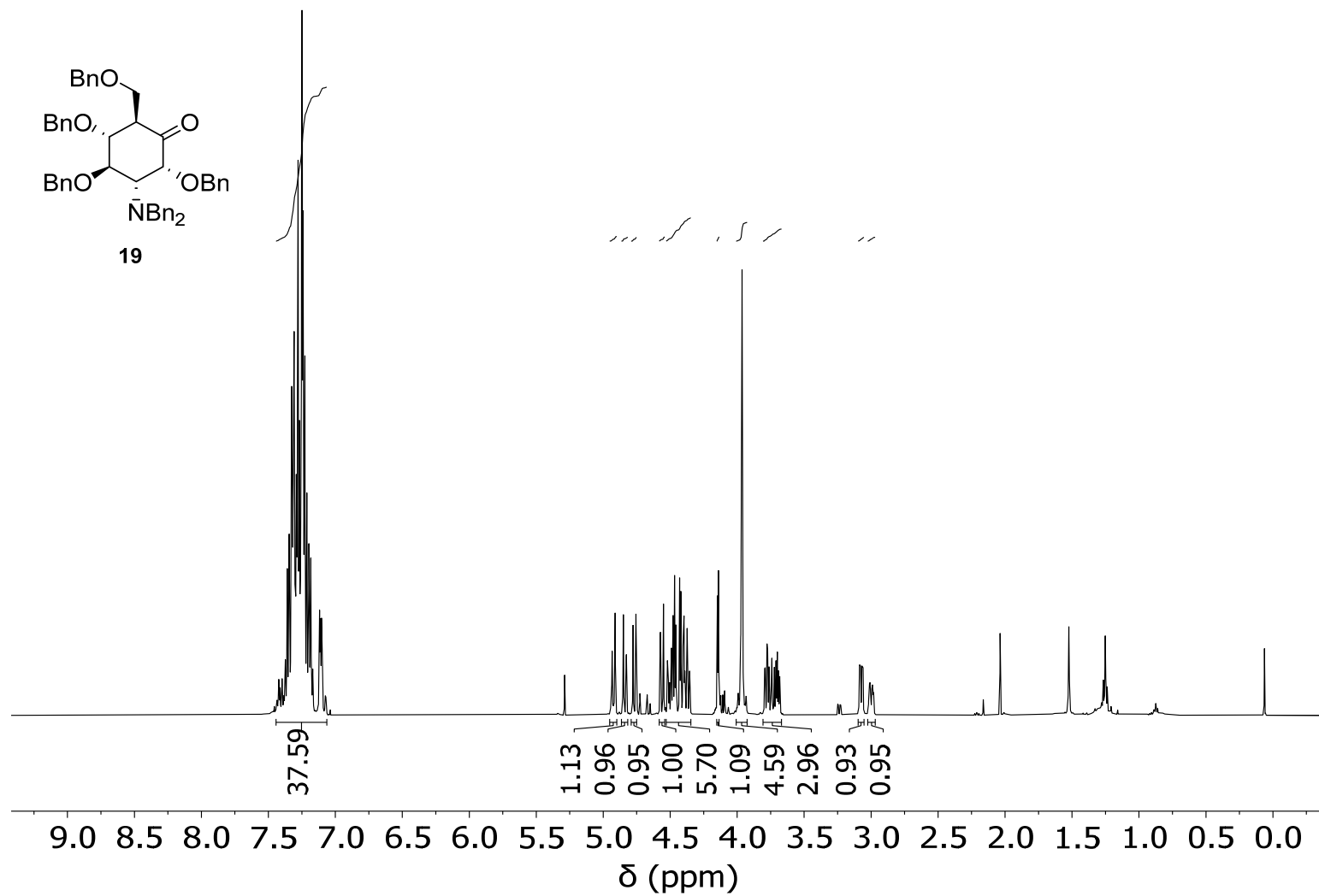
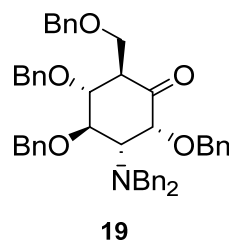
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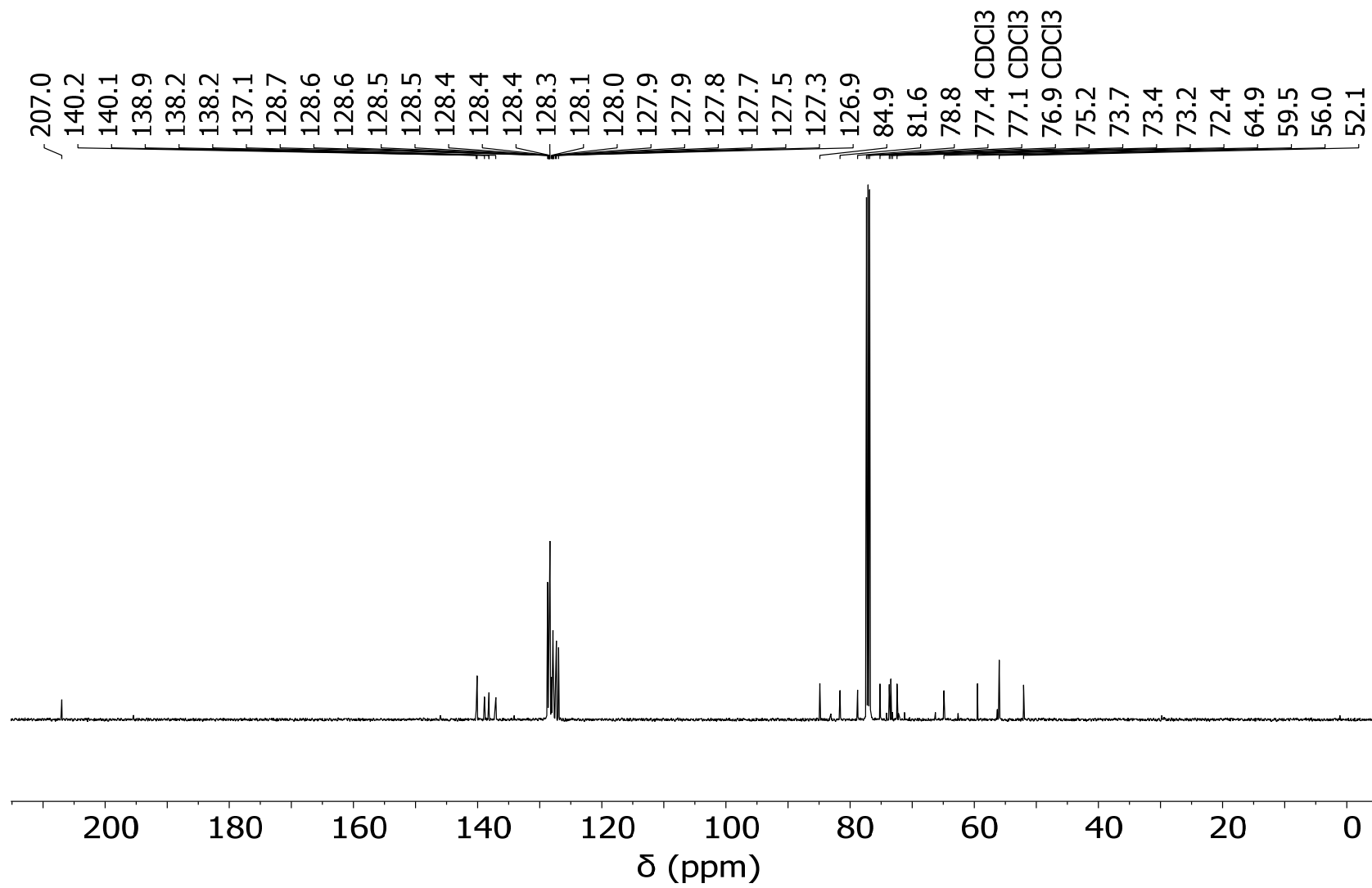
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$^{13}\text{C}$  NMR spectrum (151 MHz,  $\text{CDCl}_3$ ) of **17**

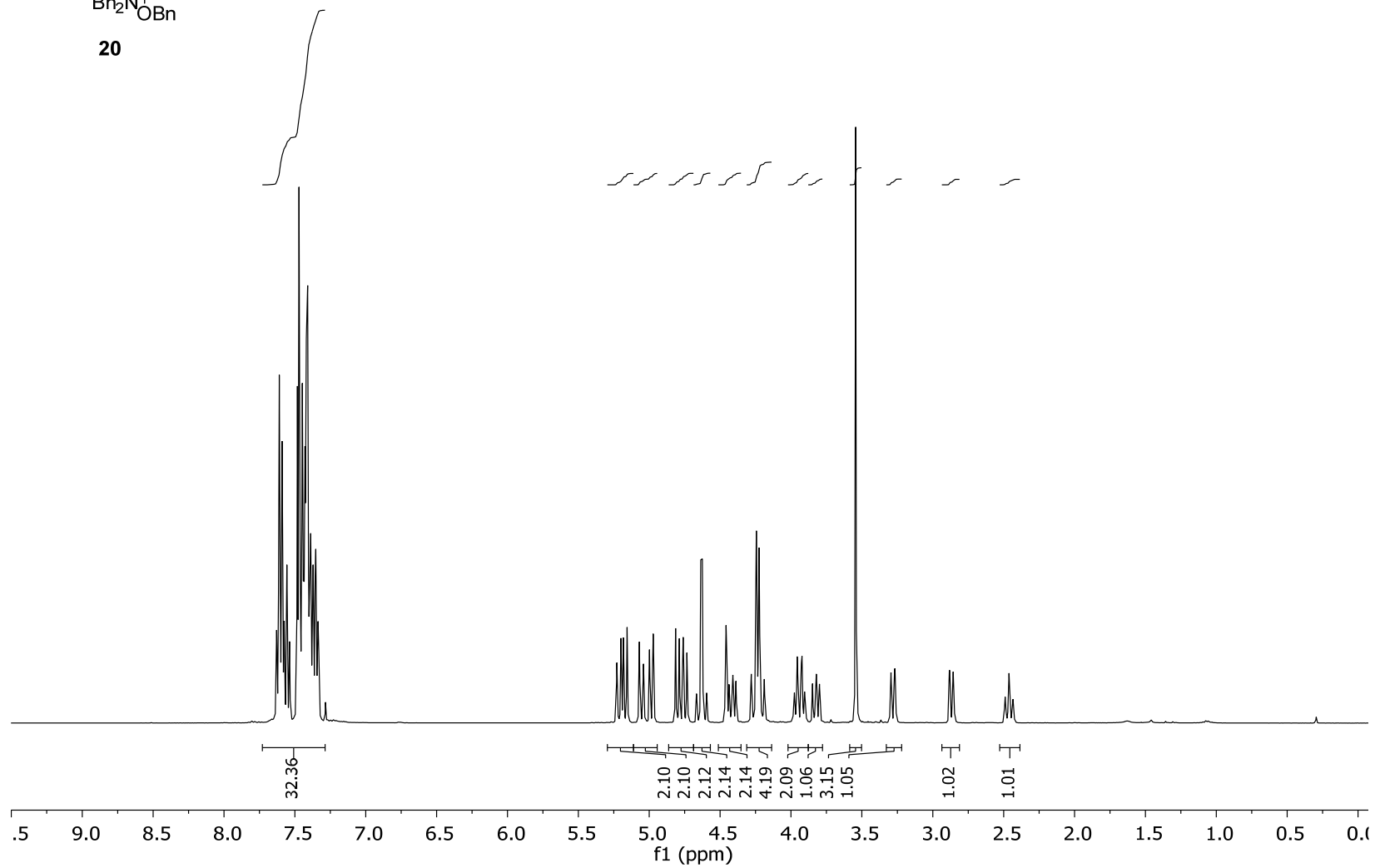
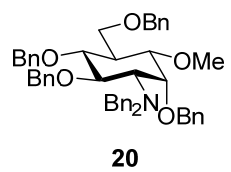


$^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of **19**

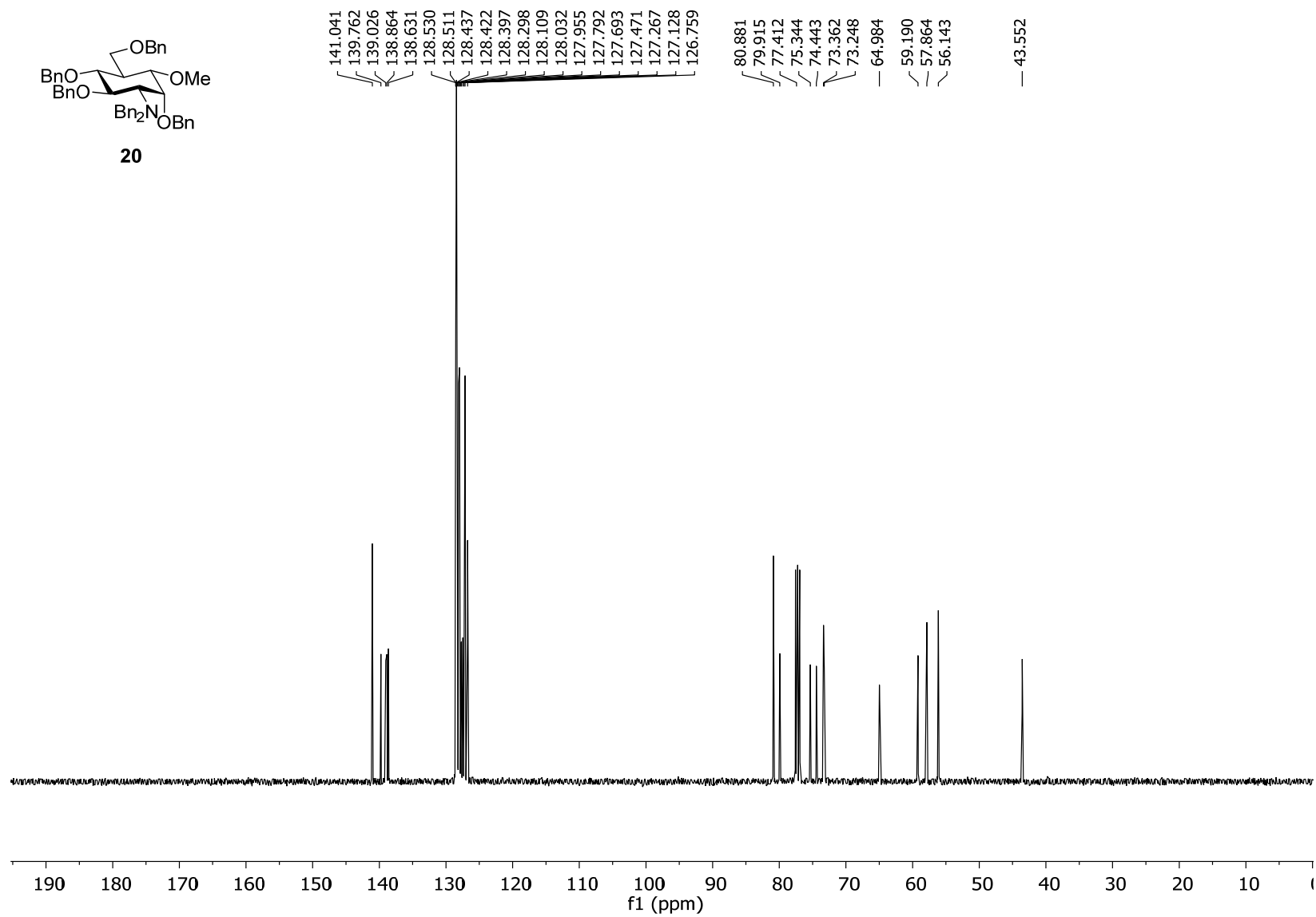


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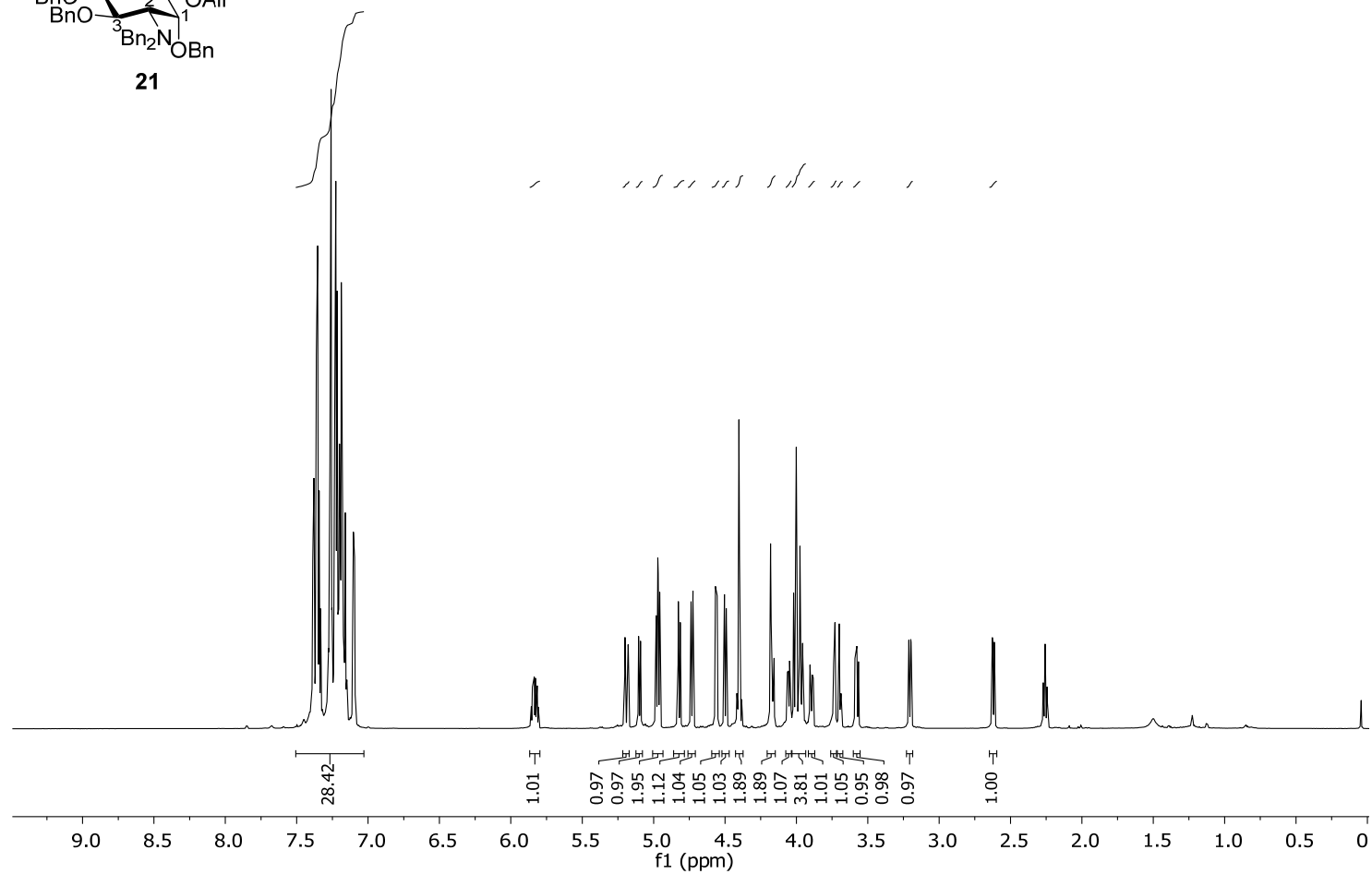
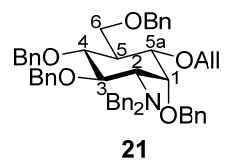




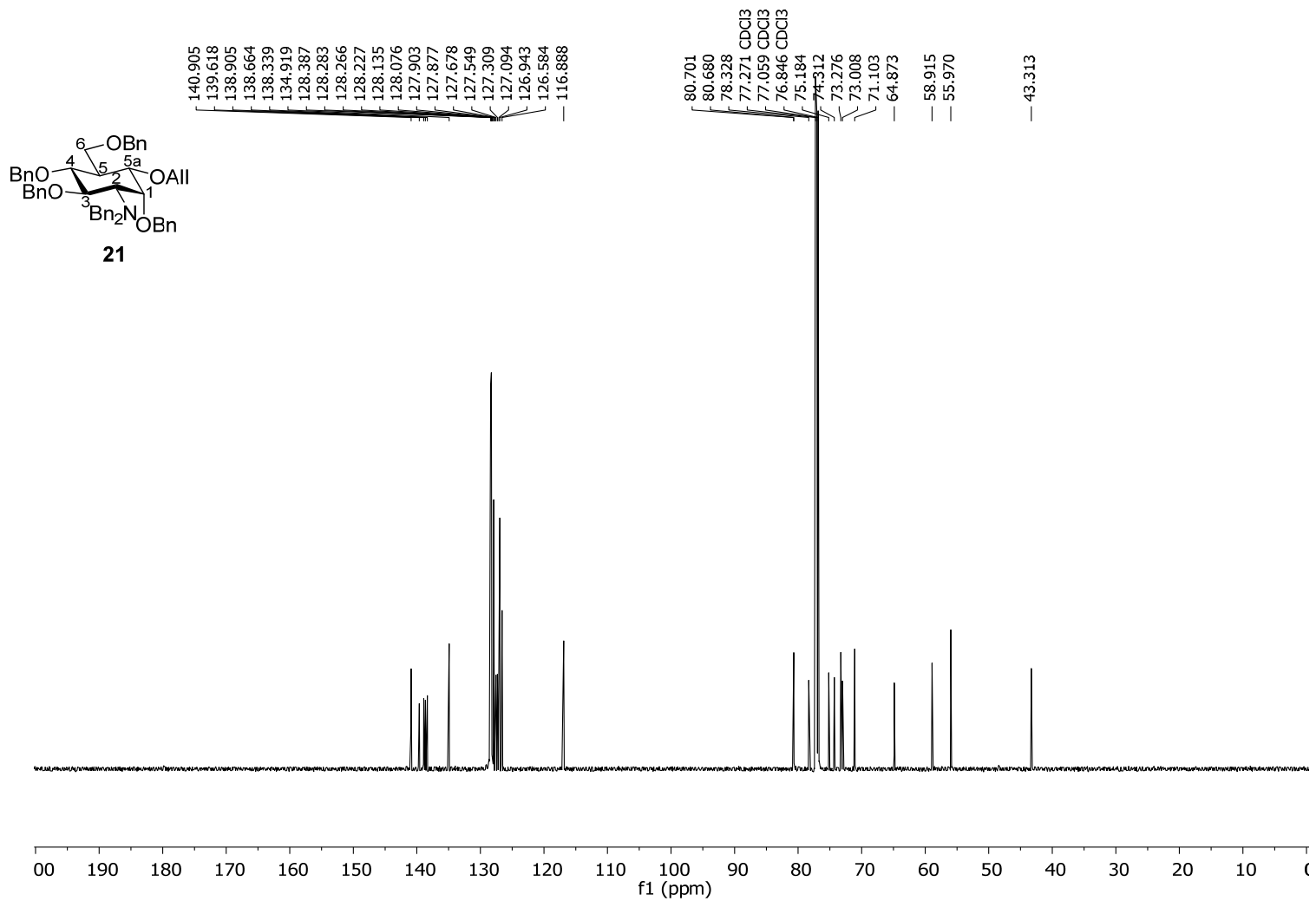
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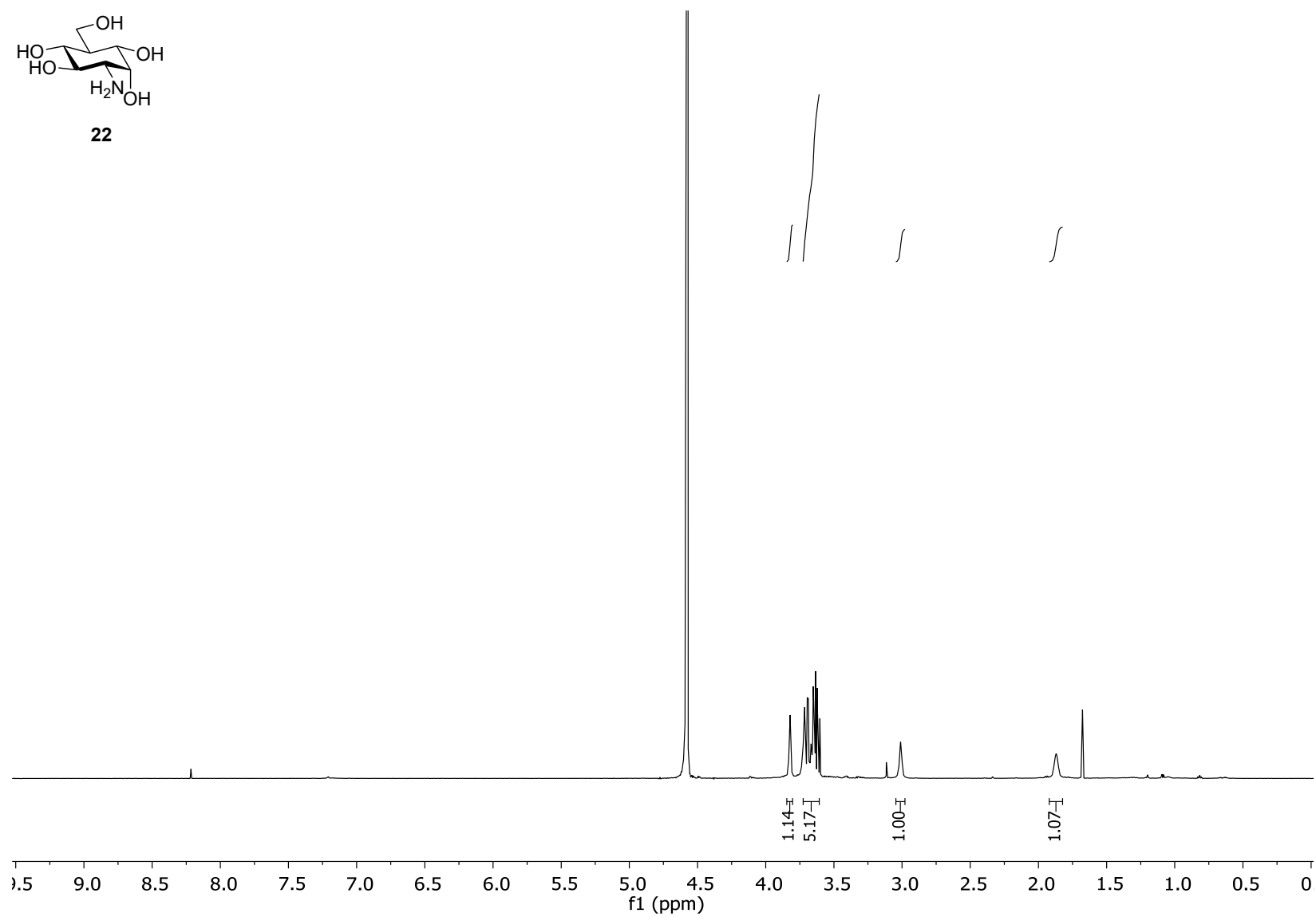
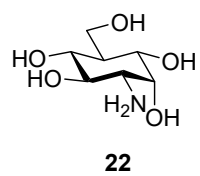


**<sup>13</sup>C NMR spectrum (101 MHz, CDCl<sub>3</sub>) of 20**

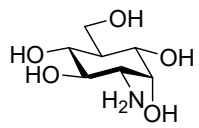


<sup>1</sup>H NMR spectrum (800 MHz, CDCl<sub>3</sub>) of **21**



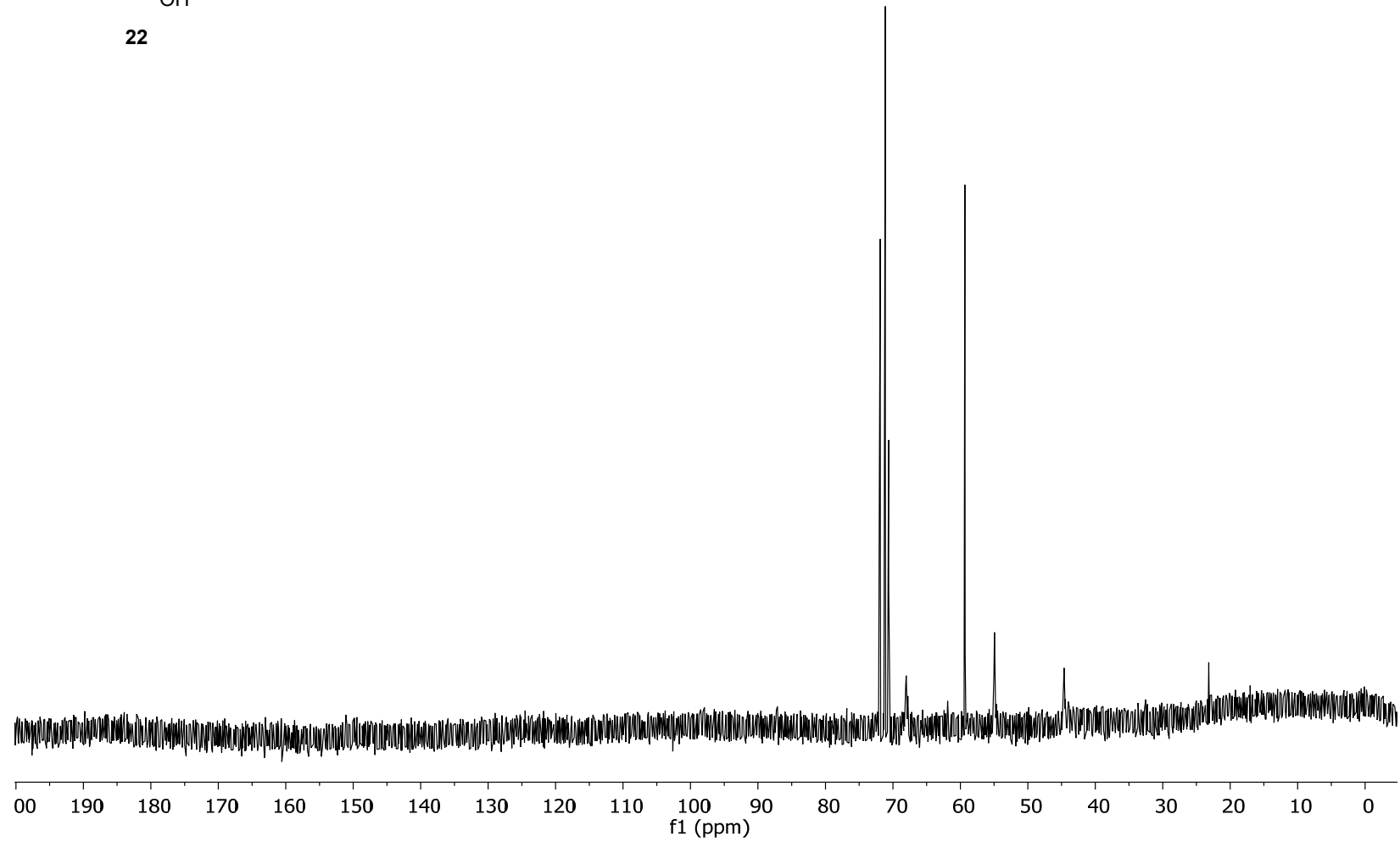


$^1\text{H}$  NMR spectrum (600 MHz,  $\text{D}_2\text{O}$ ) of **22**

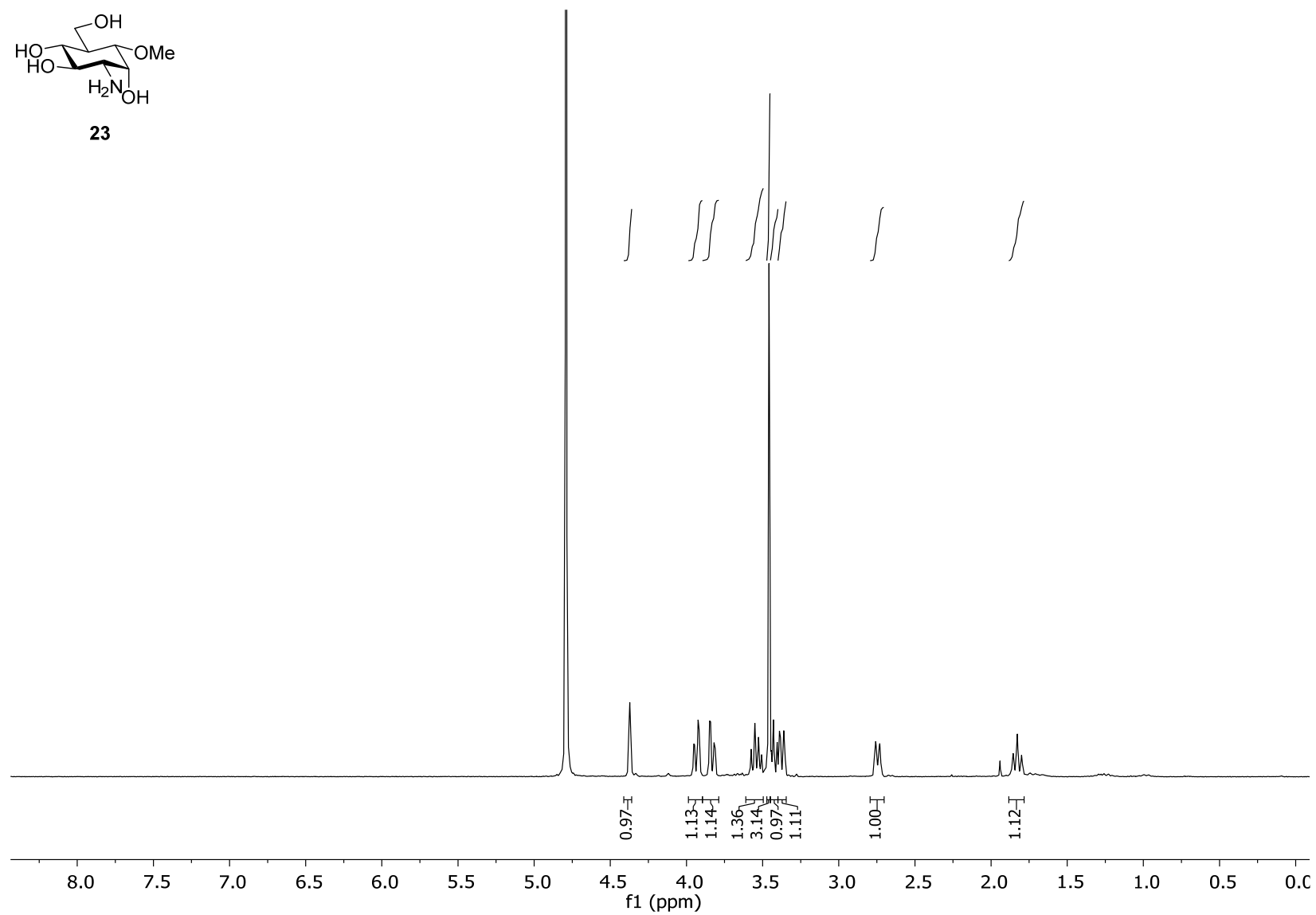
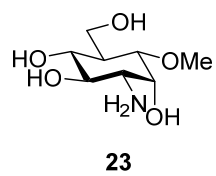


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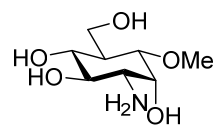
71.877  
71.121  
70.629  
68.018  
— 59.323  
— 54.942  
— 44.561



<sup>13</sup>C NMR spectrum (151 MHz, D<sub>2</sub>O) of 22

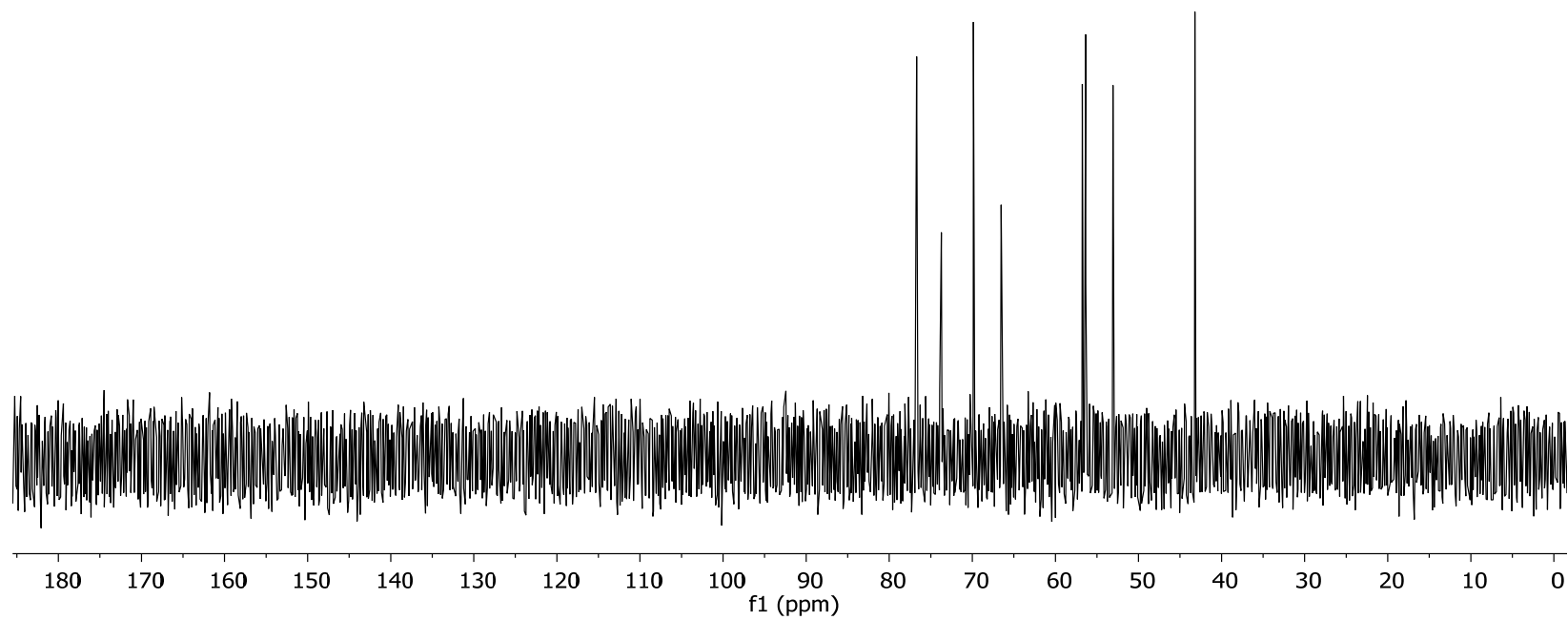


$^1\text{H}$  NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ ) of **23**



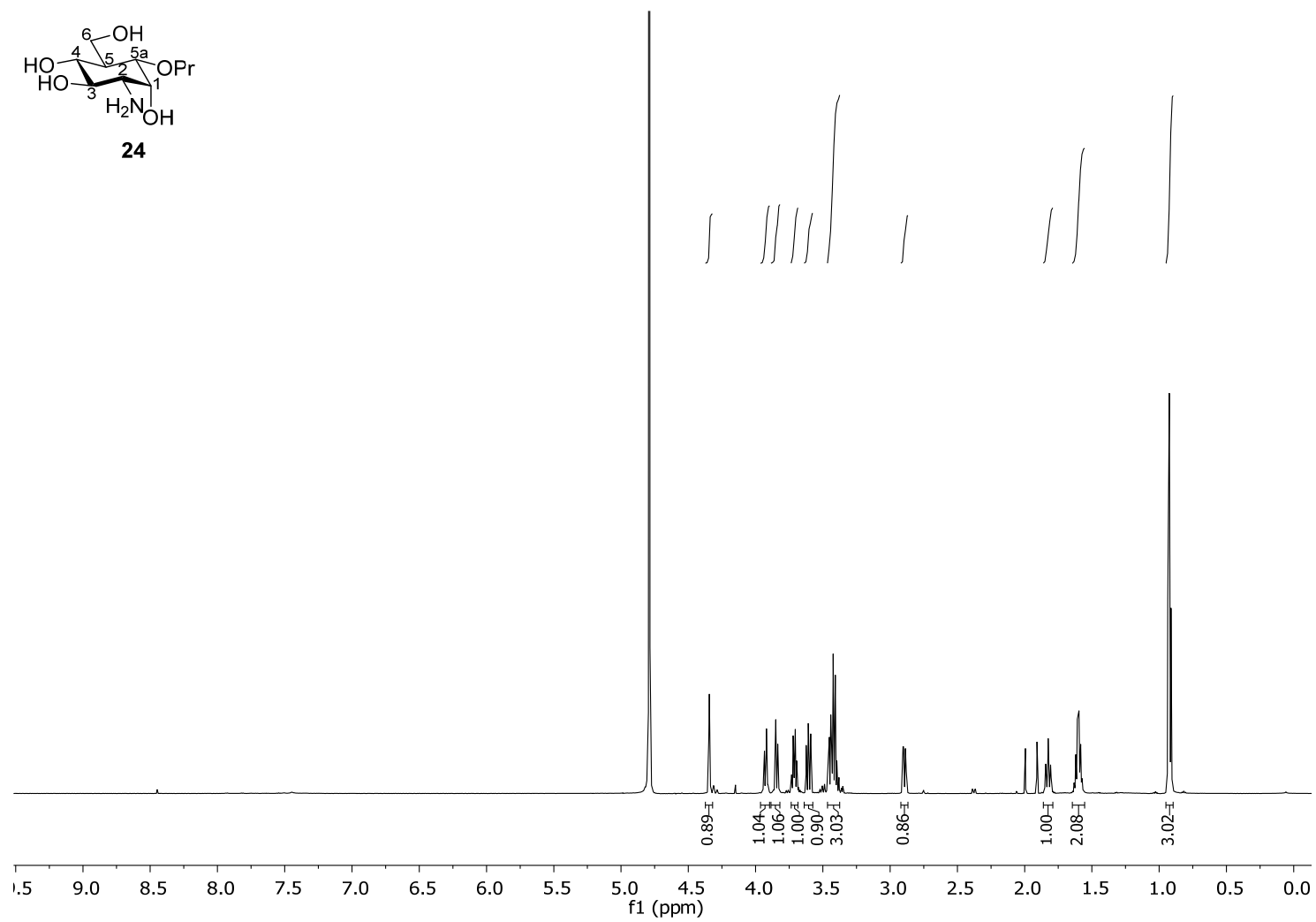
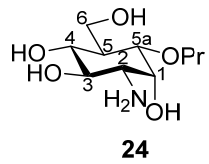
23

76.694  
73.721  
69.867  
66.520  
56.762  
56.351  
53.078  
43.200

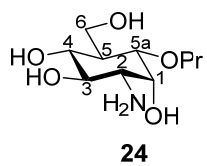


<sup>13</sup>C NMR spectrum (101 MHz, D<sub>2</sub>O) of 23

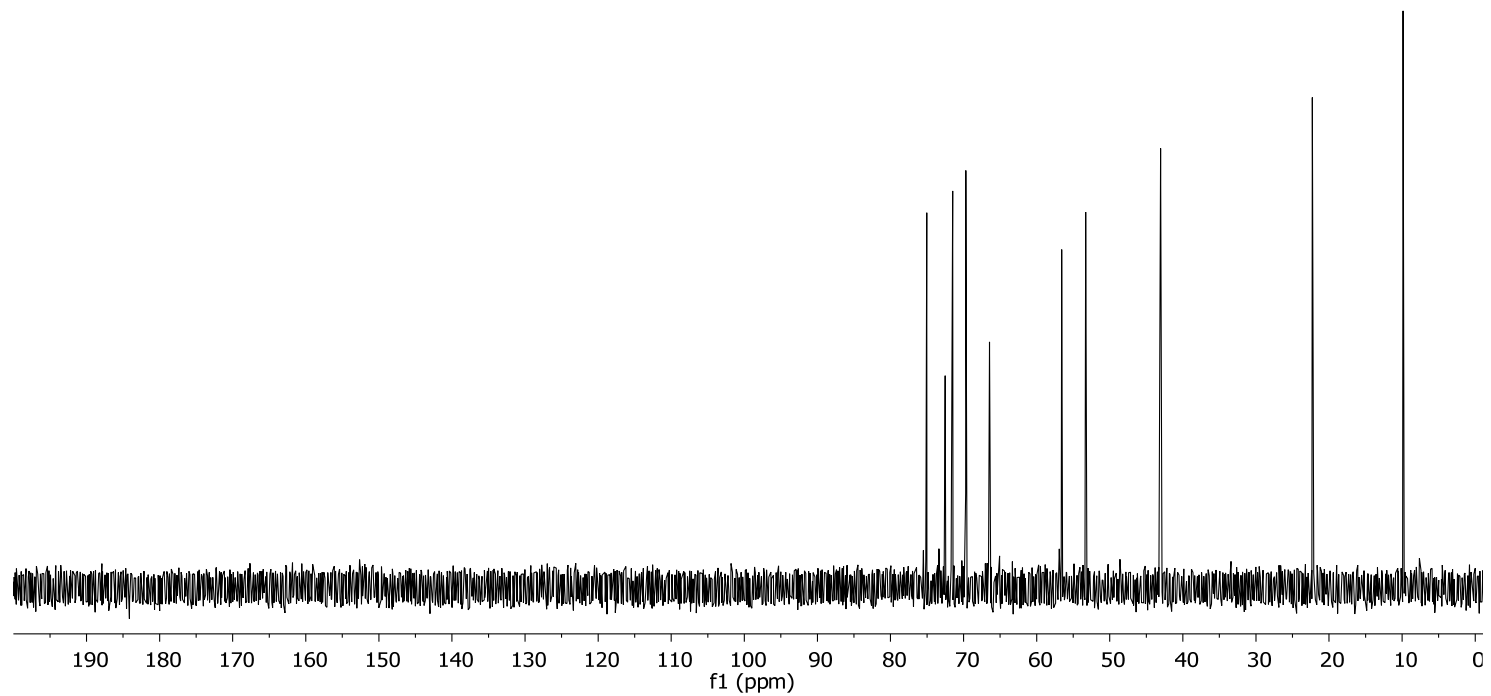




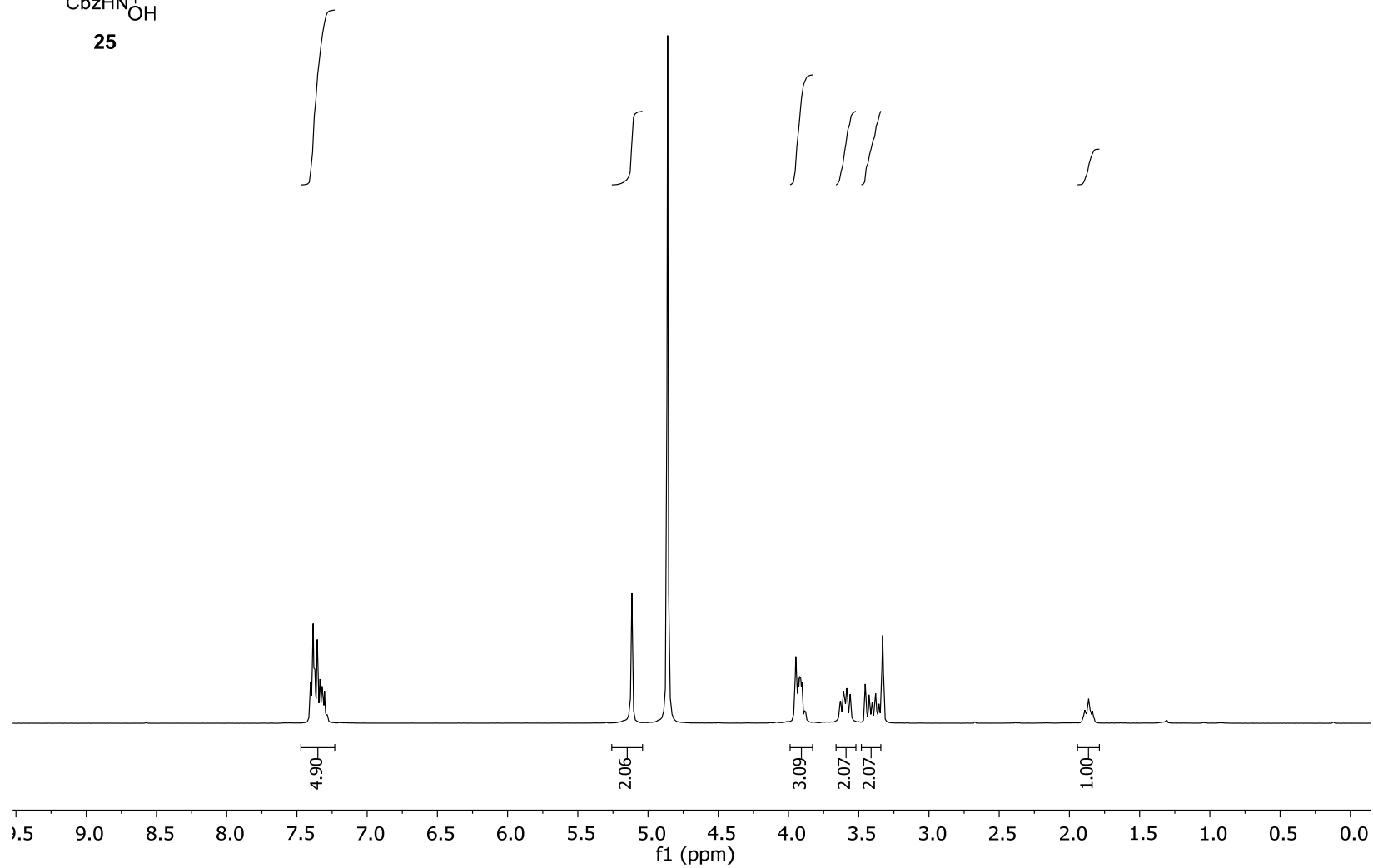
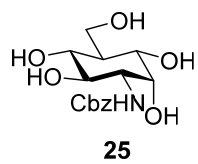
$^1\text{H}$  NMR spectrum (600 MHz,  $\text{D}_2\text{O}$ ) of **24**



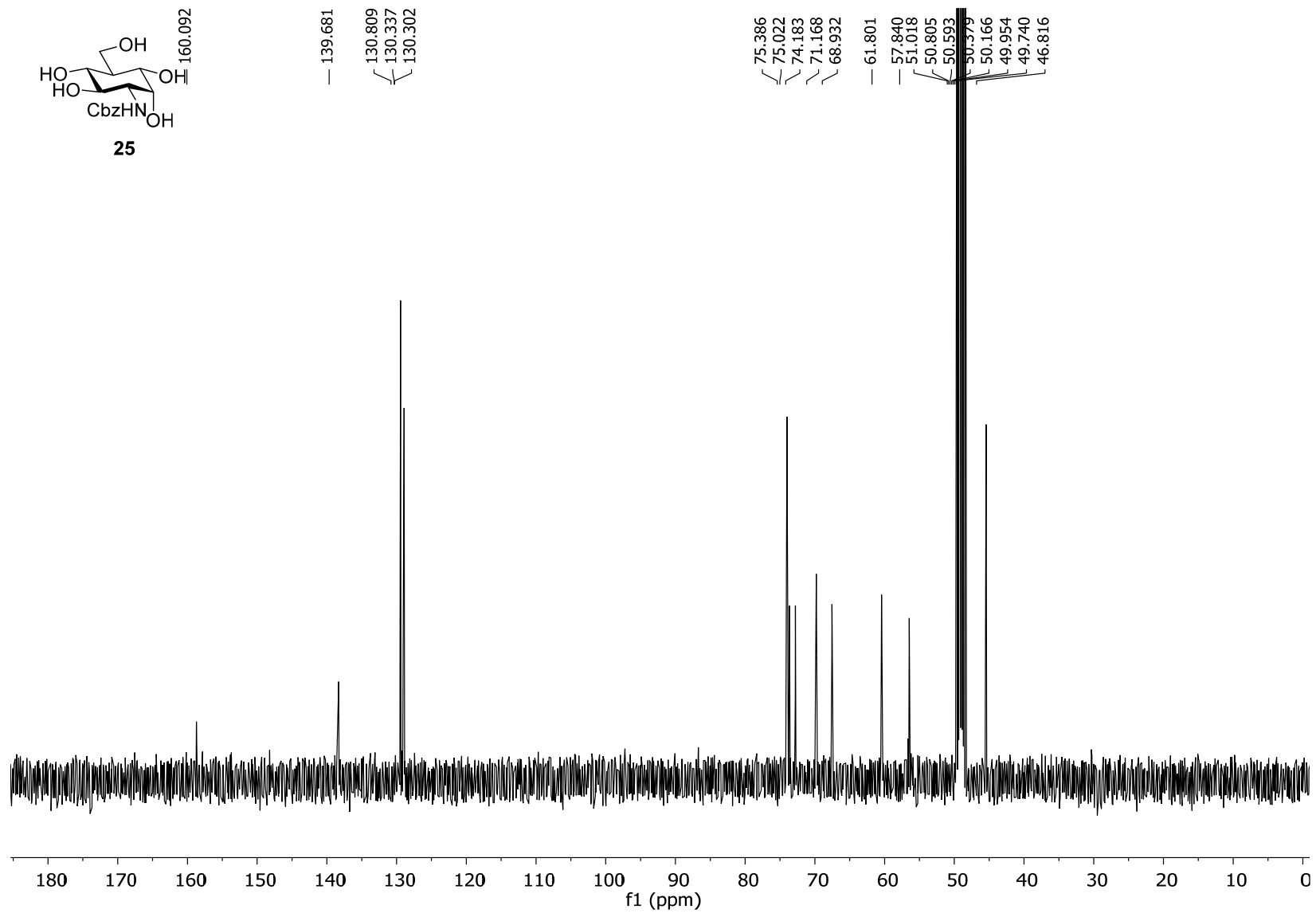
75.043  
72.526  
71.480  
69.694  
66.458  
56.581  
53.296  
43.048  
22.282  
9.855



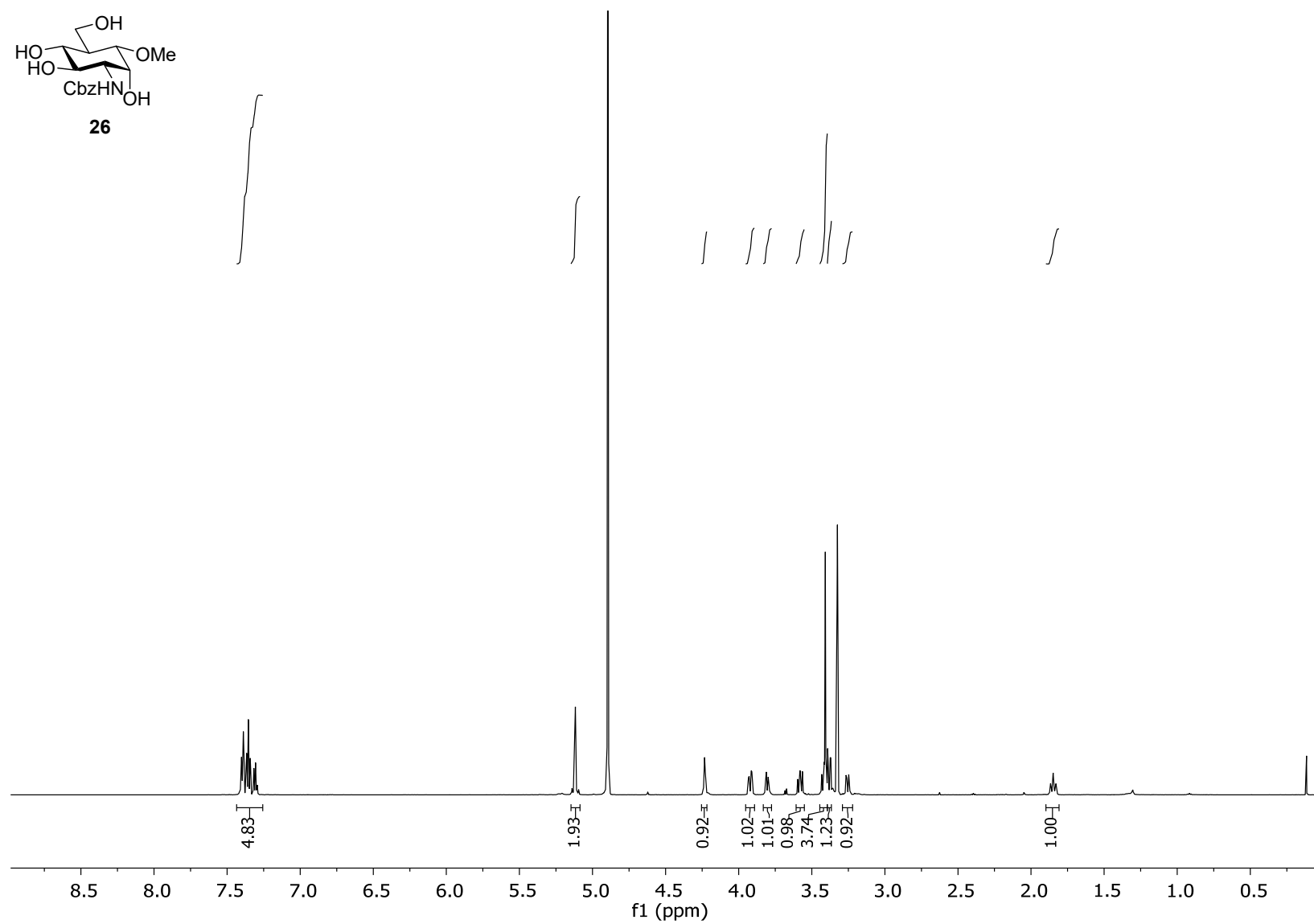
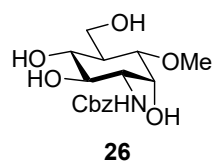
<sup>13</sup>C NMR spectrum (151 MHz, D<sub>2</sub>O) of **24**



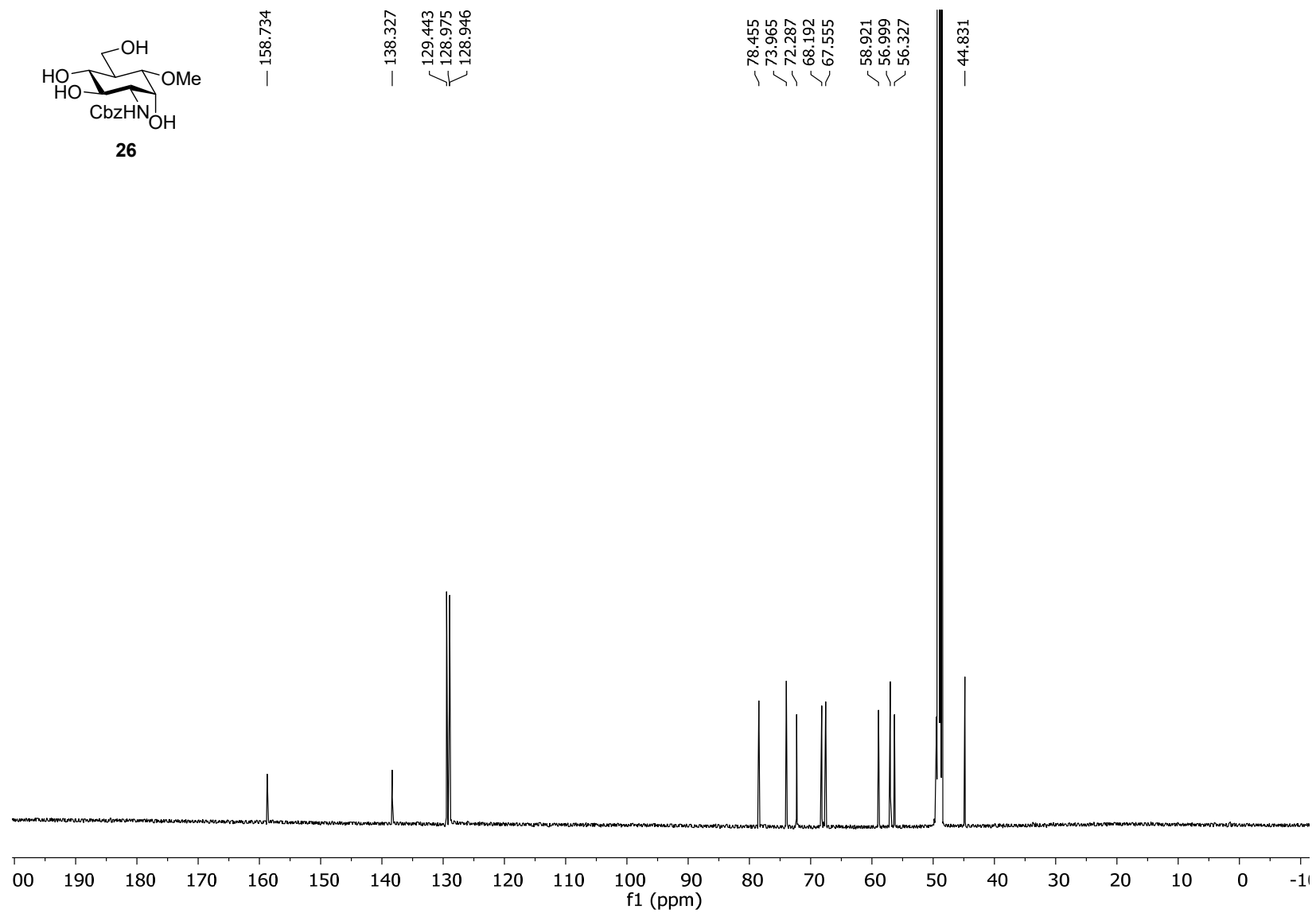
$^1\text{H}$  NMR spectrum (400 MHz,  $\text{CD}_3\text{OD}$ ) of **25**



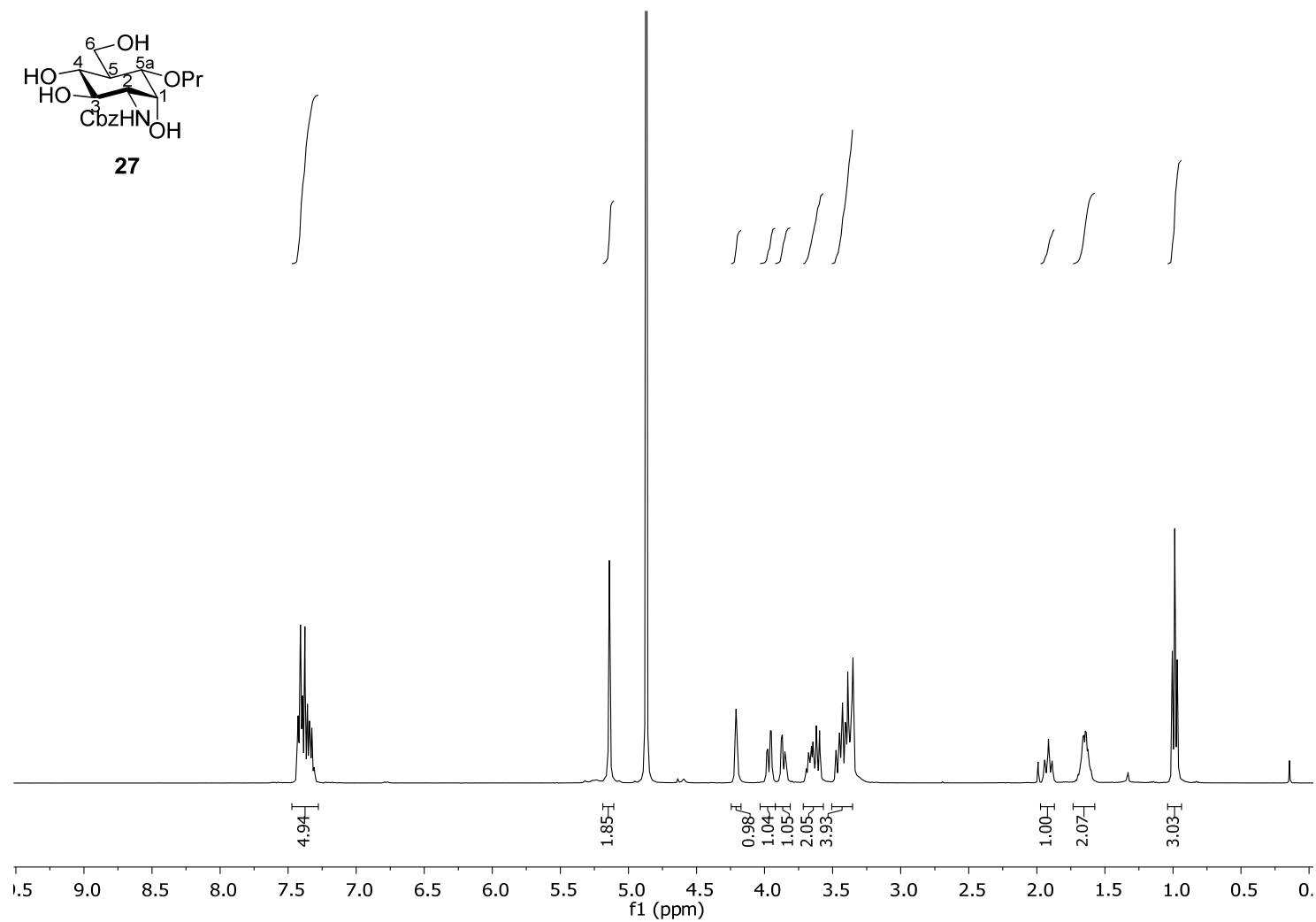
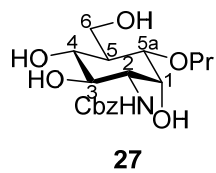
$^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CD}_3\text{OD}$ ) of **25**



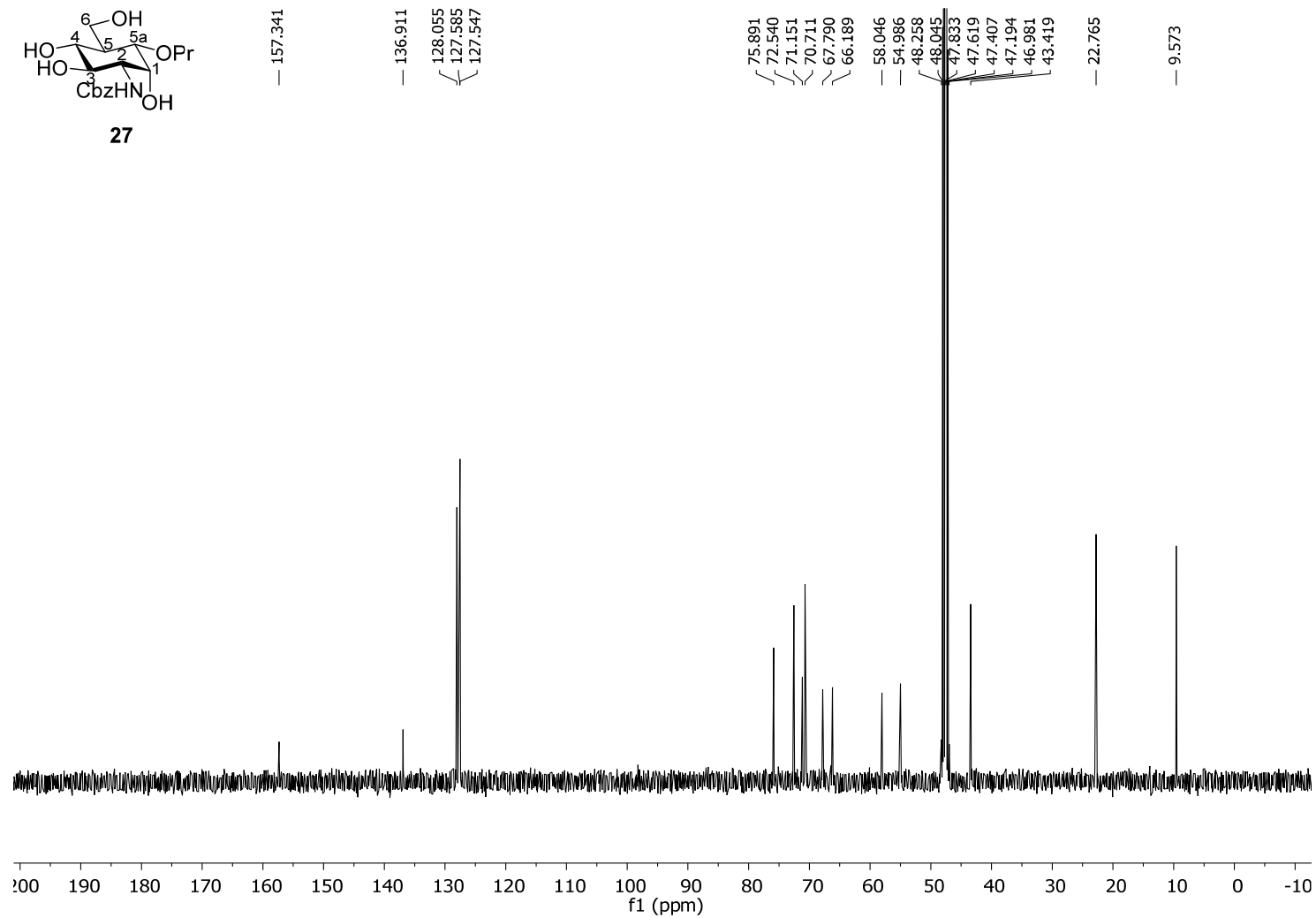
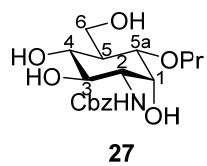
<sup>1</sup>H NMR spectrum (400 MHz, CD<sub>3</sub>OD) of **26**



<sup>13</sup>C NMR spectrum (101 MHz, CD<sub>3</sub>OD) of **26**

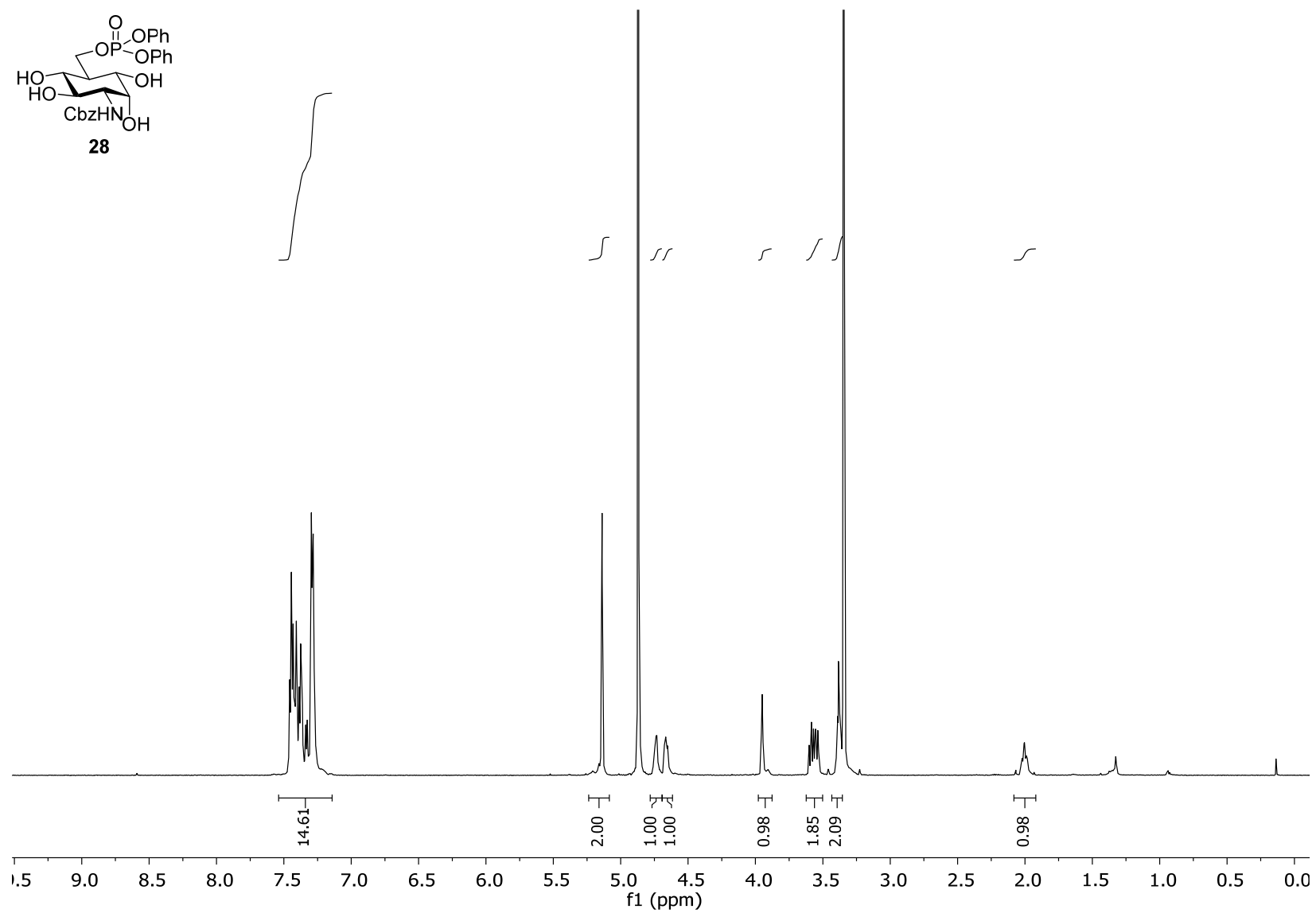
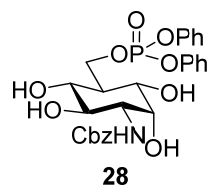


<sup>1</sup>H NMR spectrum (400 MHz, CD<sub>3</sub>OD) of **27**

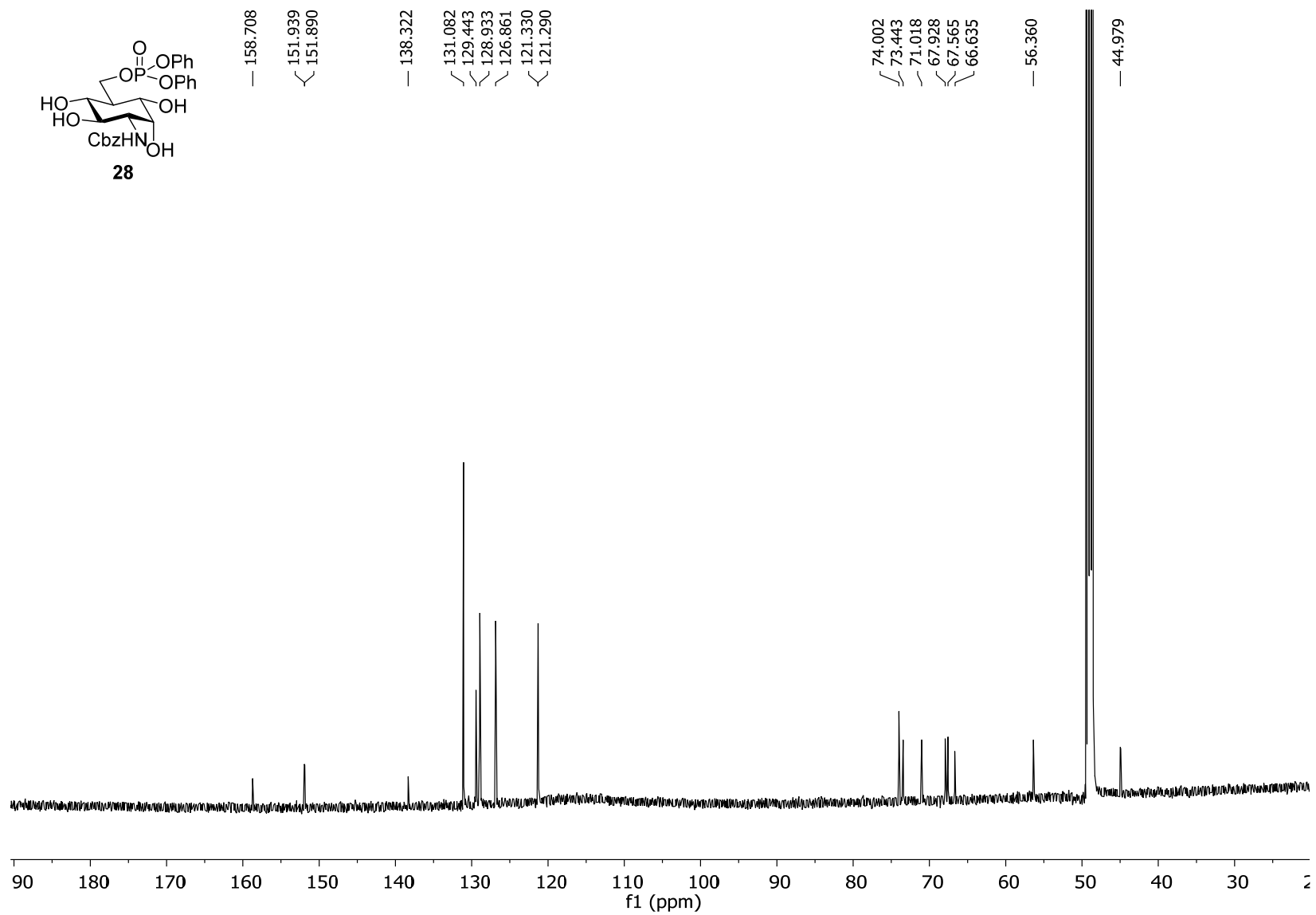


<sup>13</sup>C NMR spectrum (101 MHz, CD<sub>3</sub>OD) of **27**

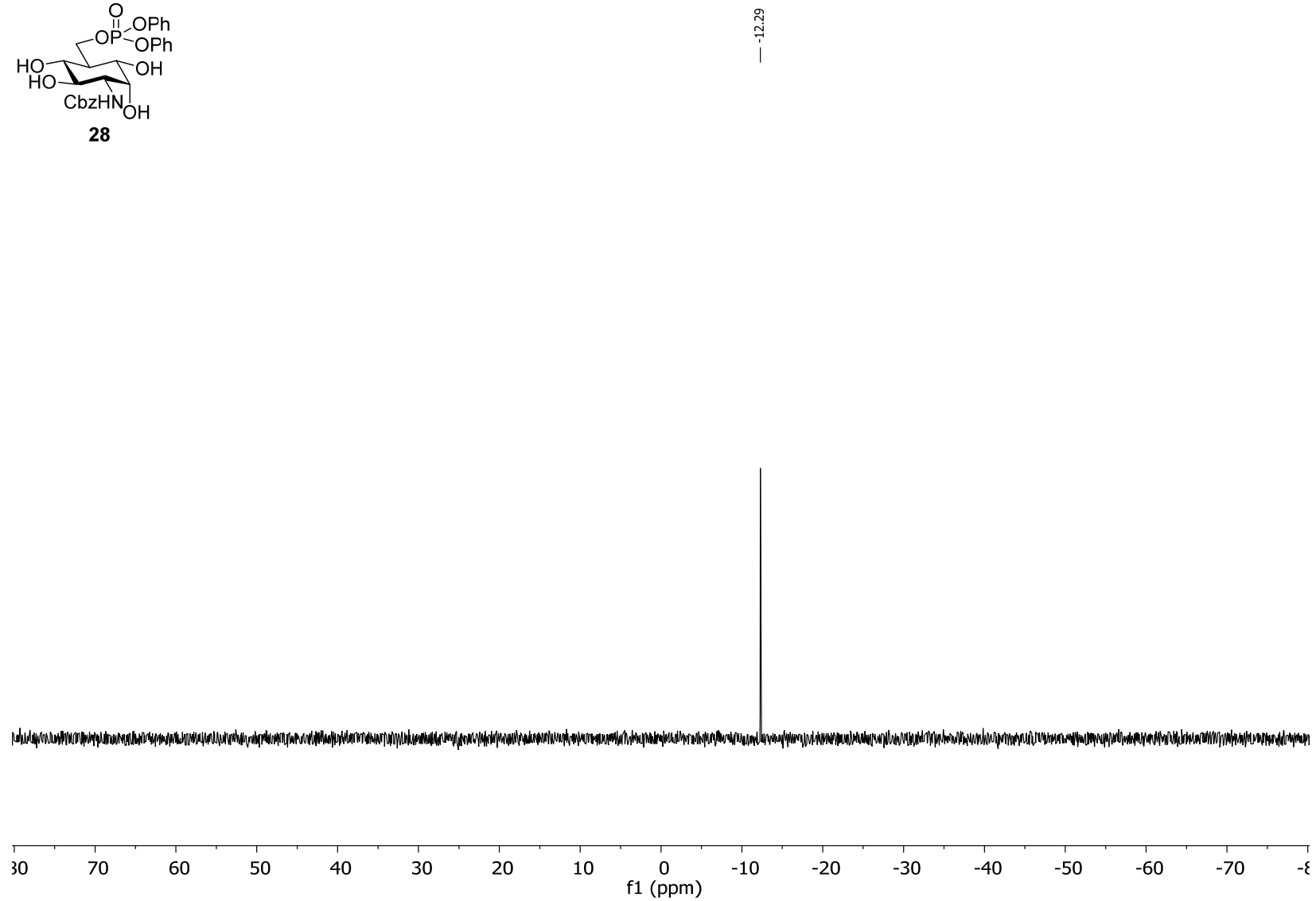
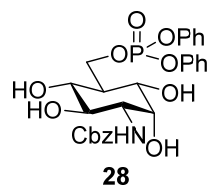




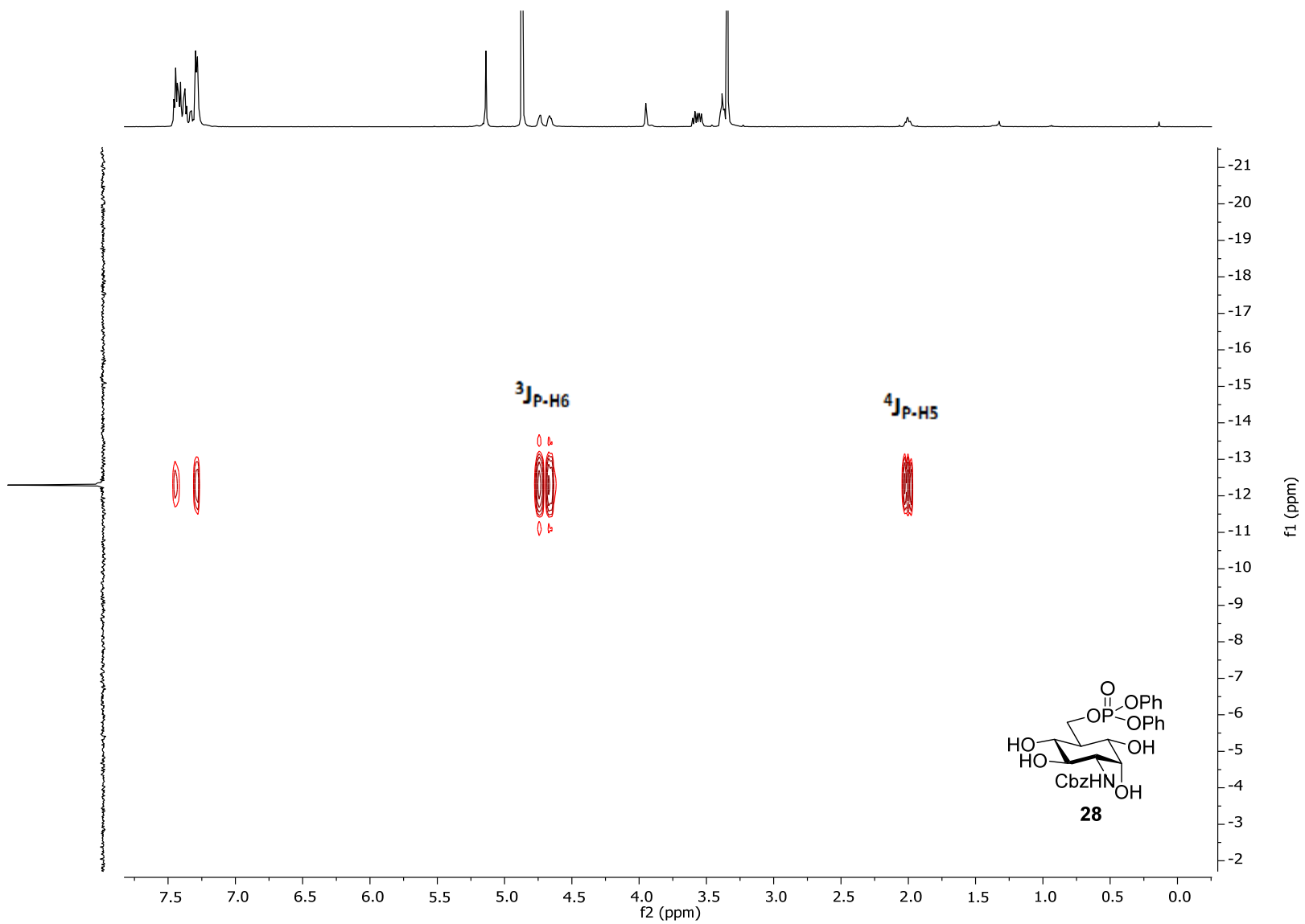
$^1\text{H}$  NMR spectrum (600 MHz,  $\text{CD}_3\text{OD}$ ) of **28**



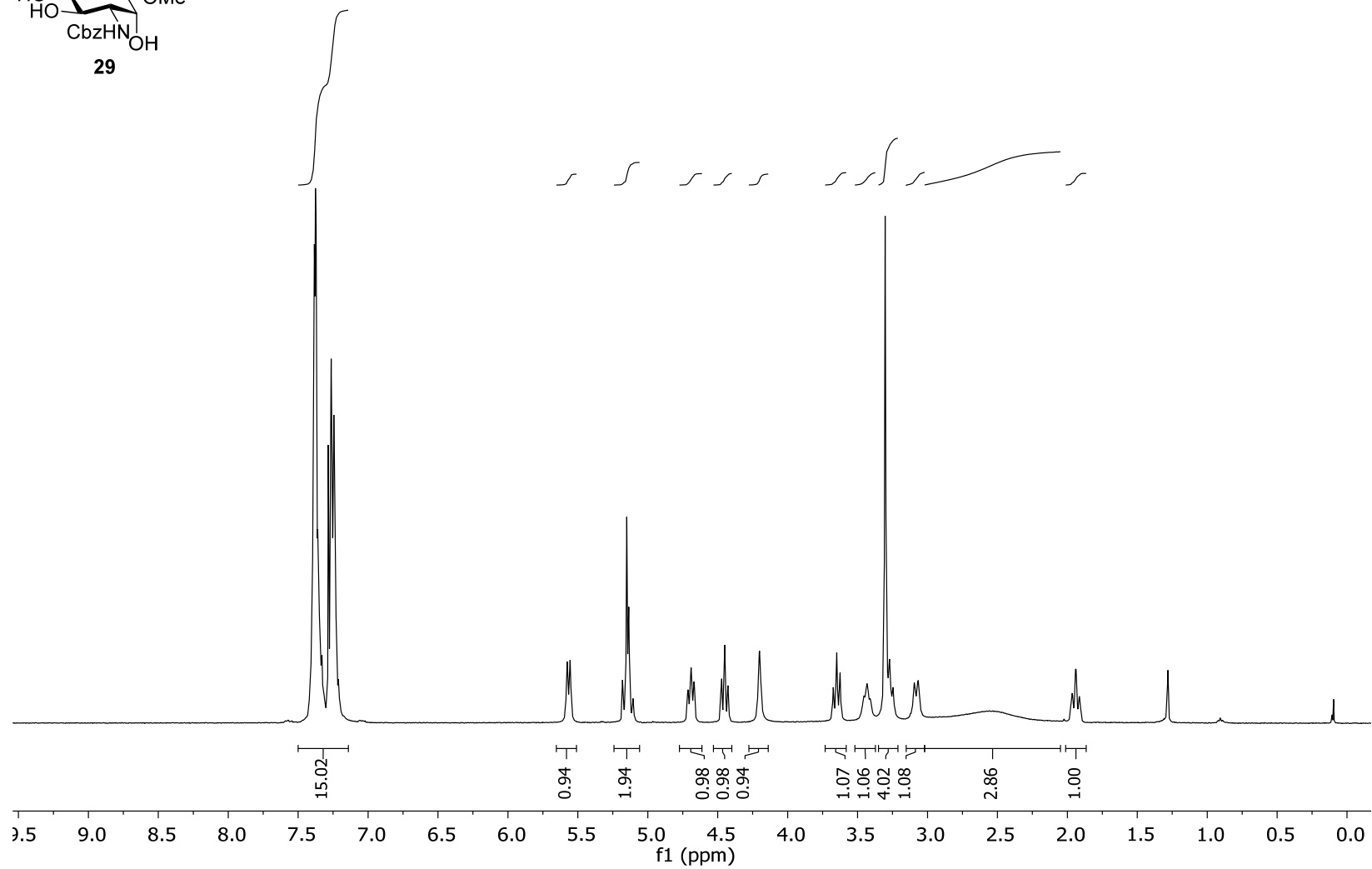
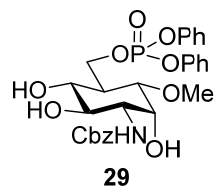
<sup>13</sup>C NMR spectrum (151 MHz, CD<sub>3</sub>OD) of **28**



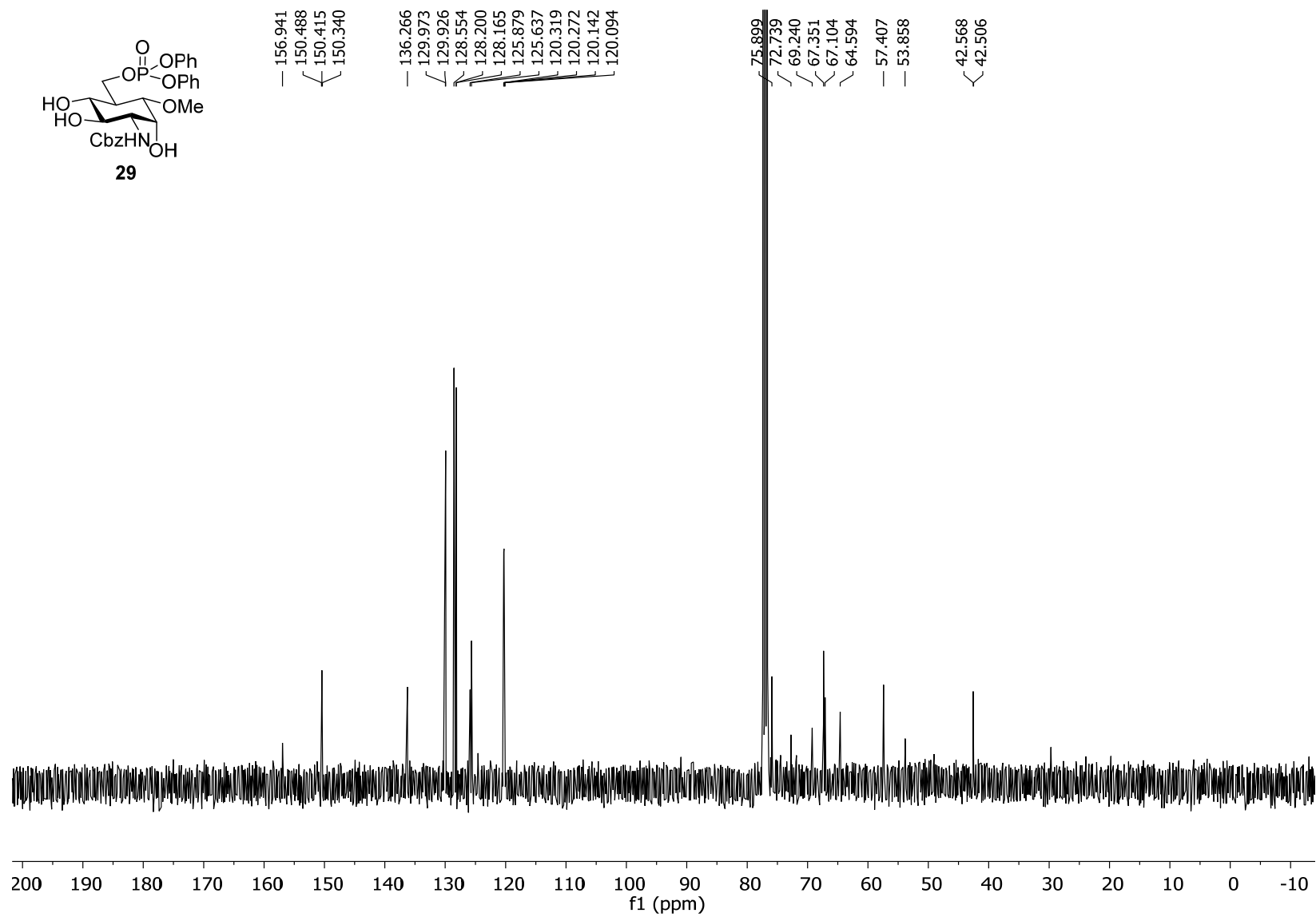
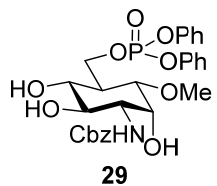
$^{31}\text{P}$  NMR spectrum (162 MHz,  $\text{CD}_3\text{OD}$ ) of **28**



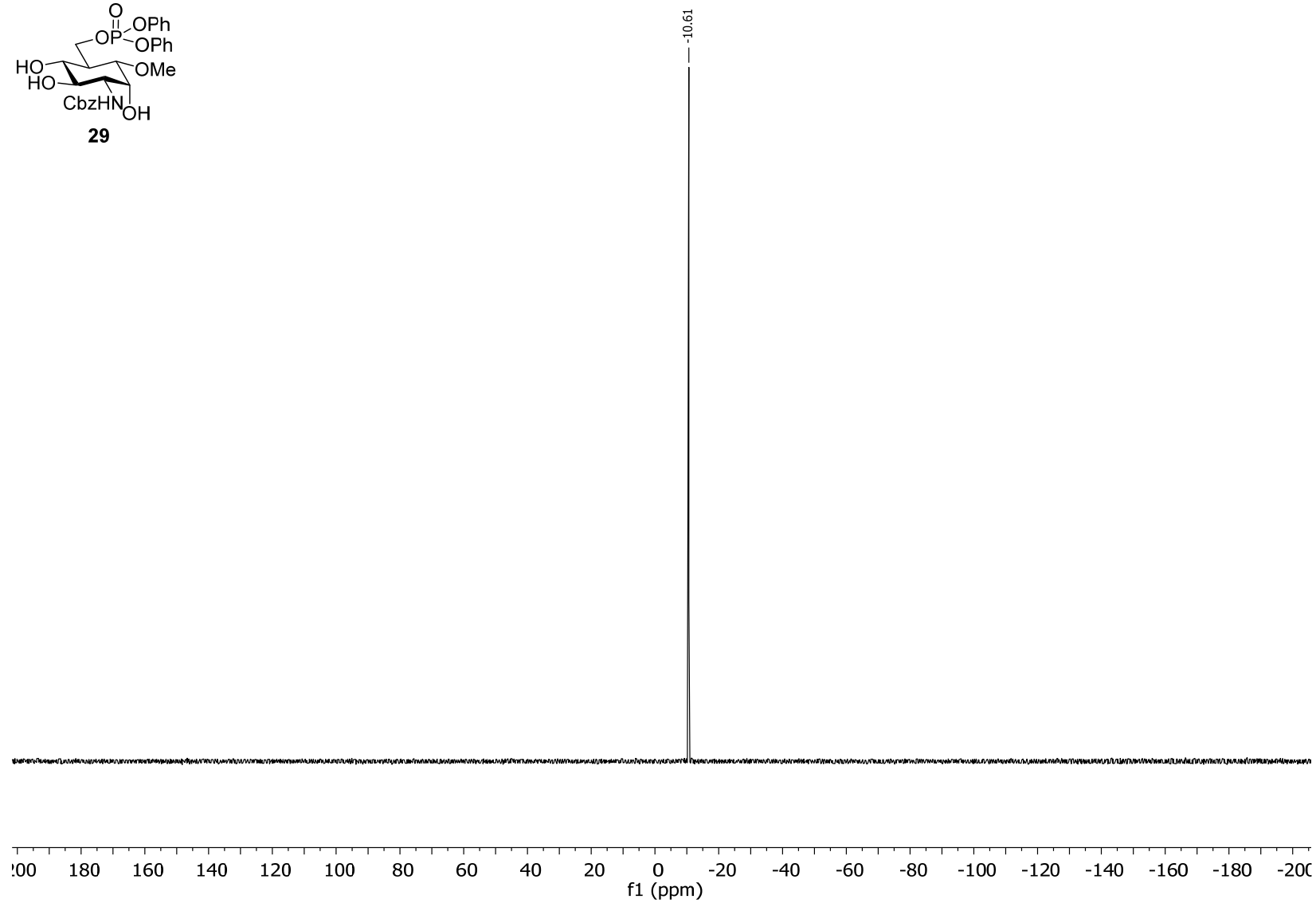
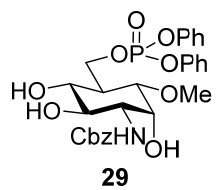
$^{31}\text{P}$ - $^1\text{H}$  HMBC NMR spectrum ( $\text{CD}_3\text{OD}$ ) of **28**



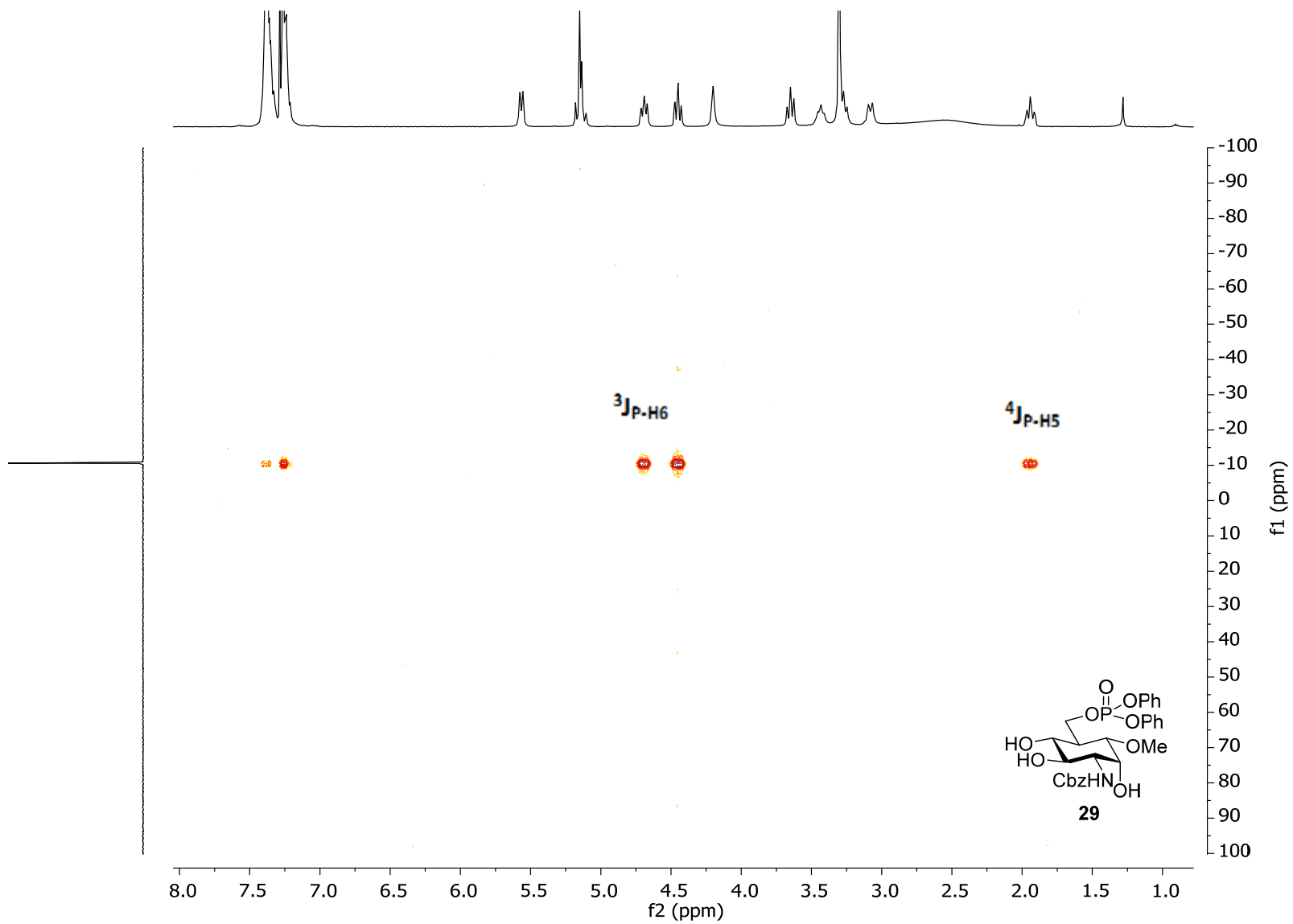
<sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of **29**



$^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of **29**

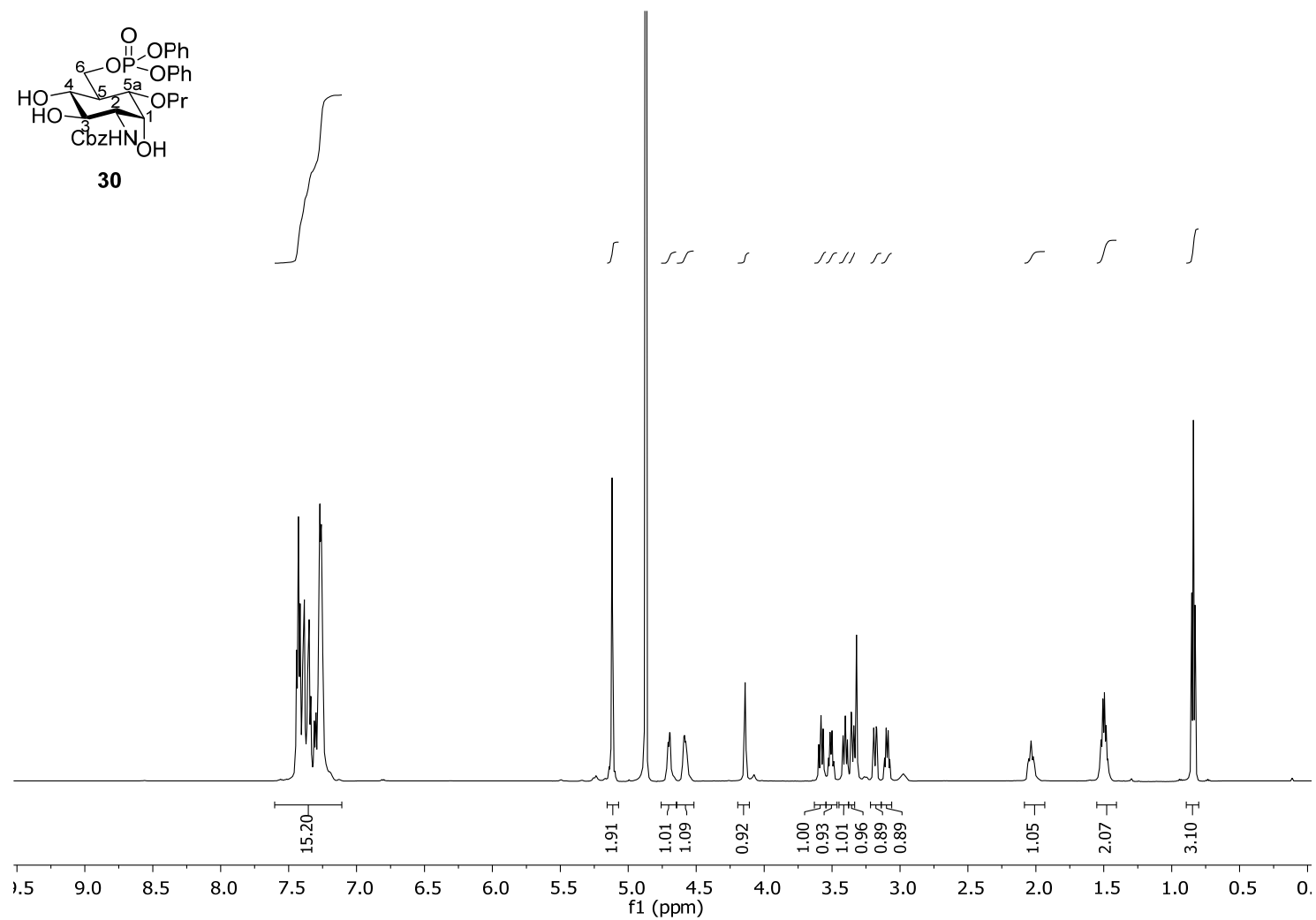
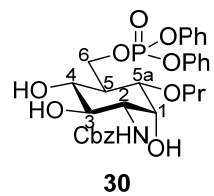


$^{31}\text{P}$  NMR spectrum (162 MHz,  $\text{CDCl}_3$ ) of **29**

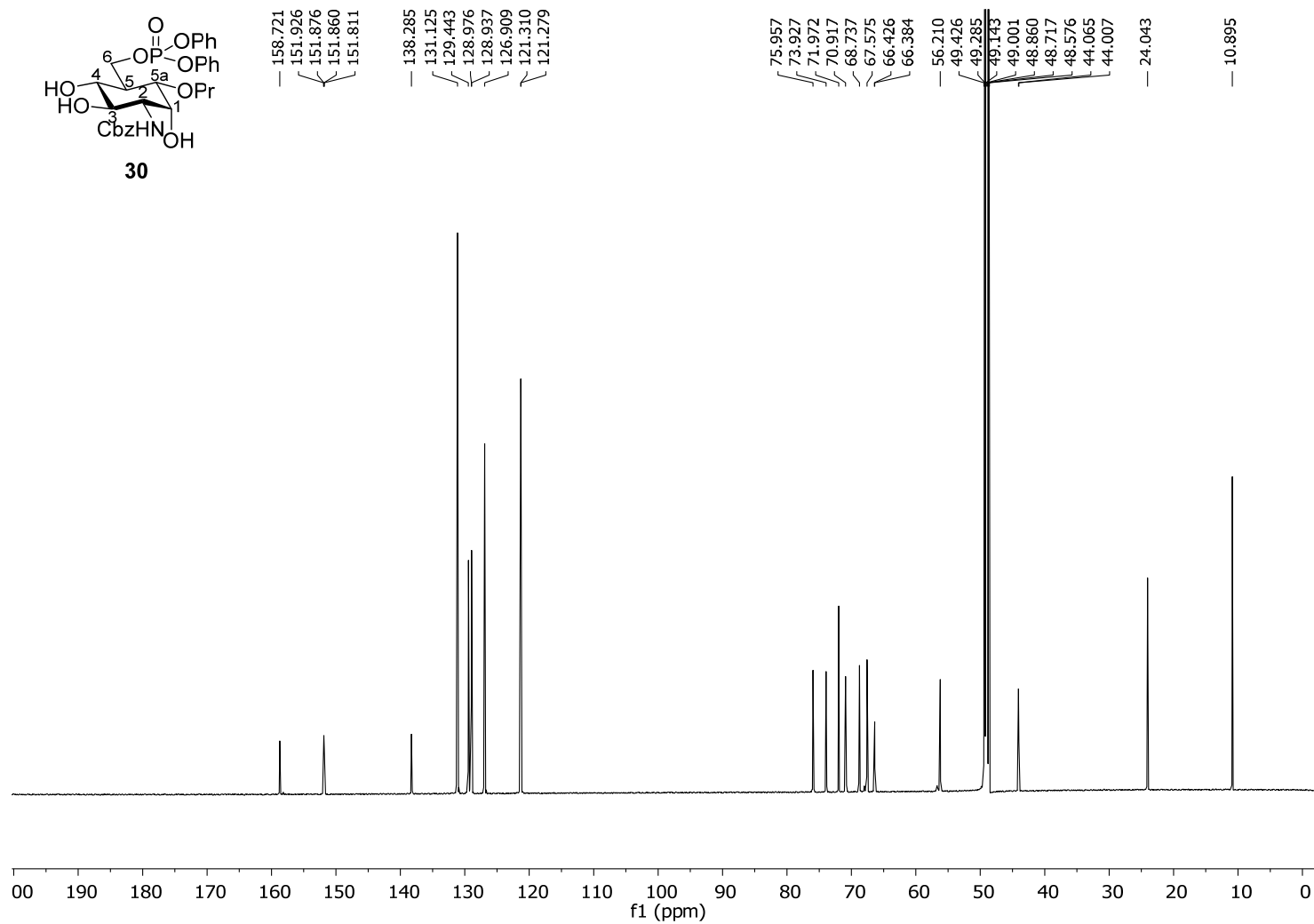


$^{31}\text{P}$ - $^1\text{H}$  HMBC NMR spectrum ( $\text{CDCl}_3$ ) of **29**

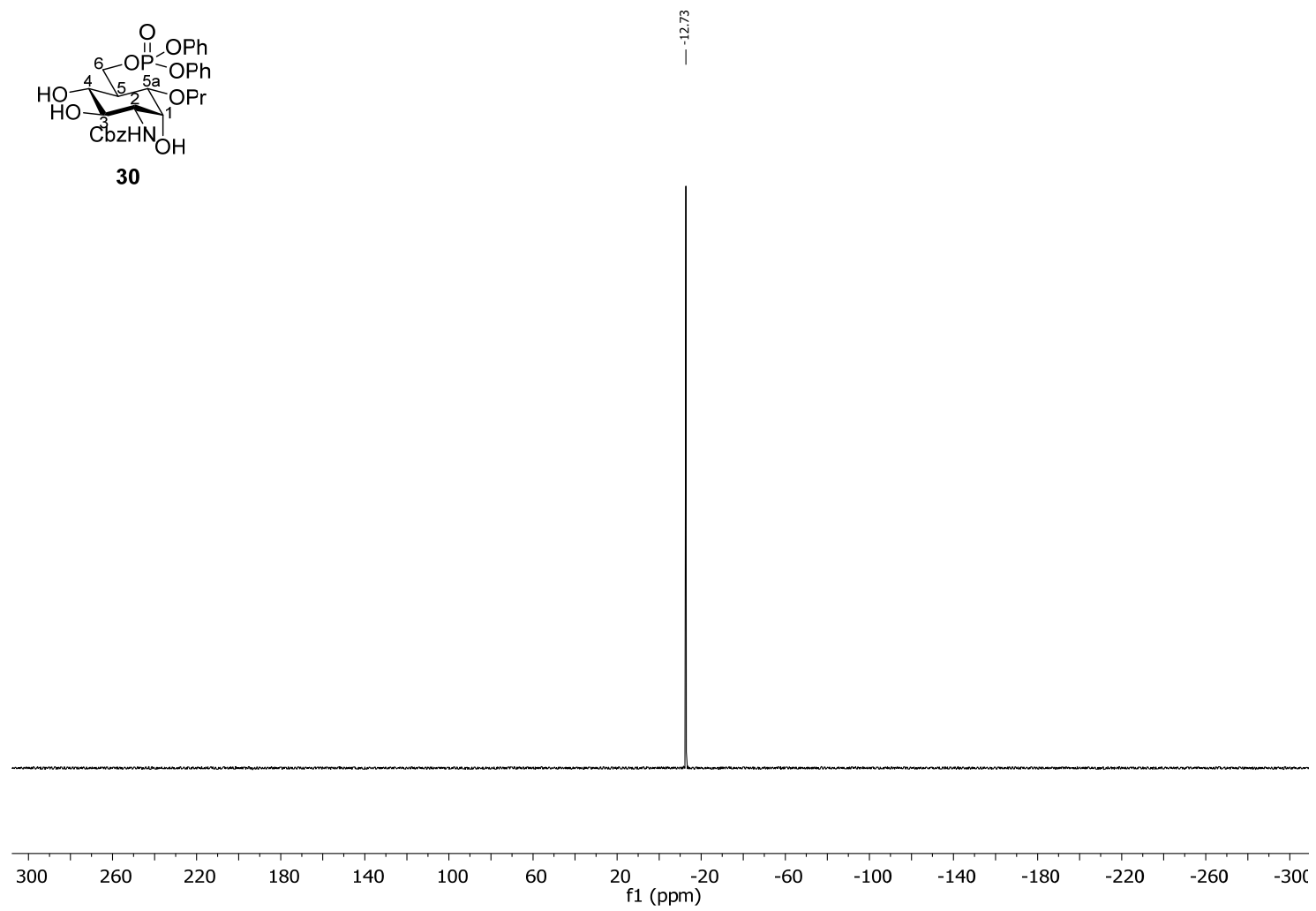
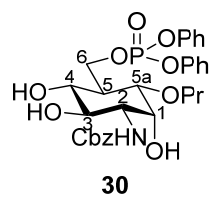




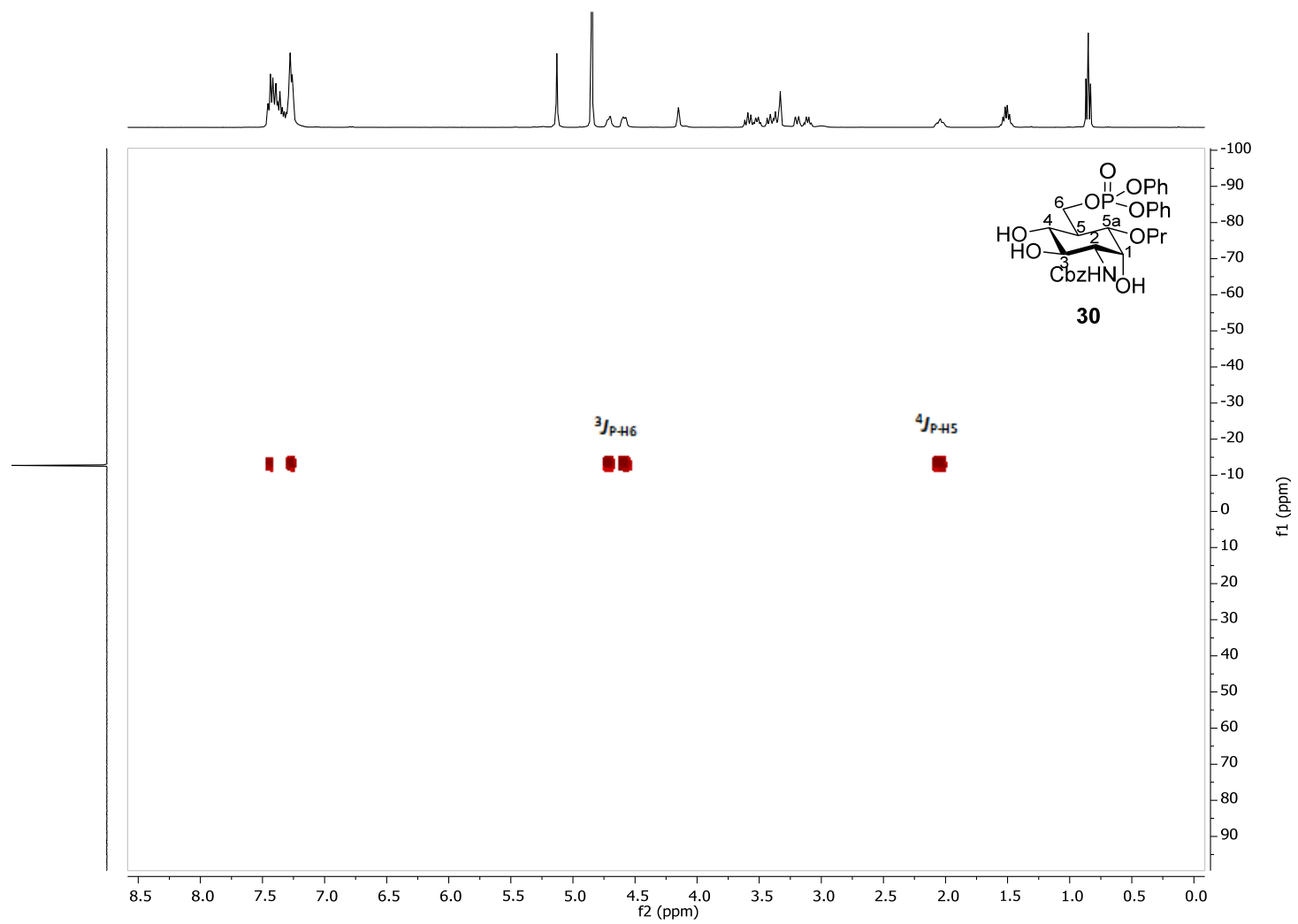
$^1\text{H}$  NMR spectrum (400 MHz,  $\text{CD}_3\text{OD}$ ) of **30**



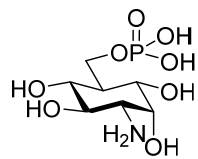
<sup>13</sup>C NMR spectrum (101 MHz, CD<sub>3</sub>OD) of **30**



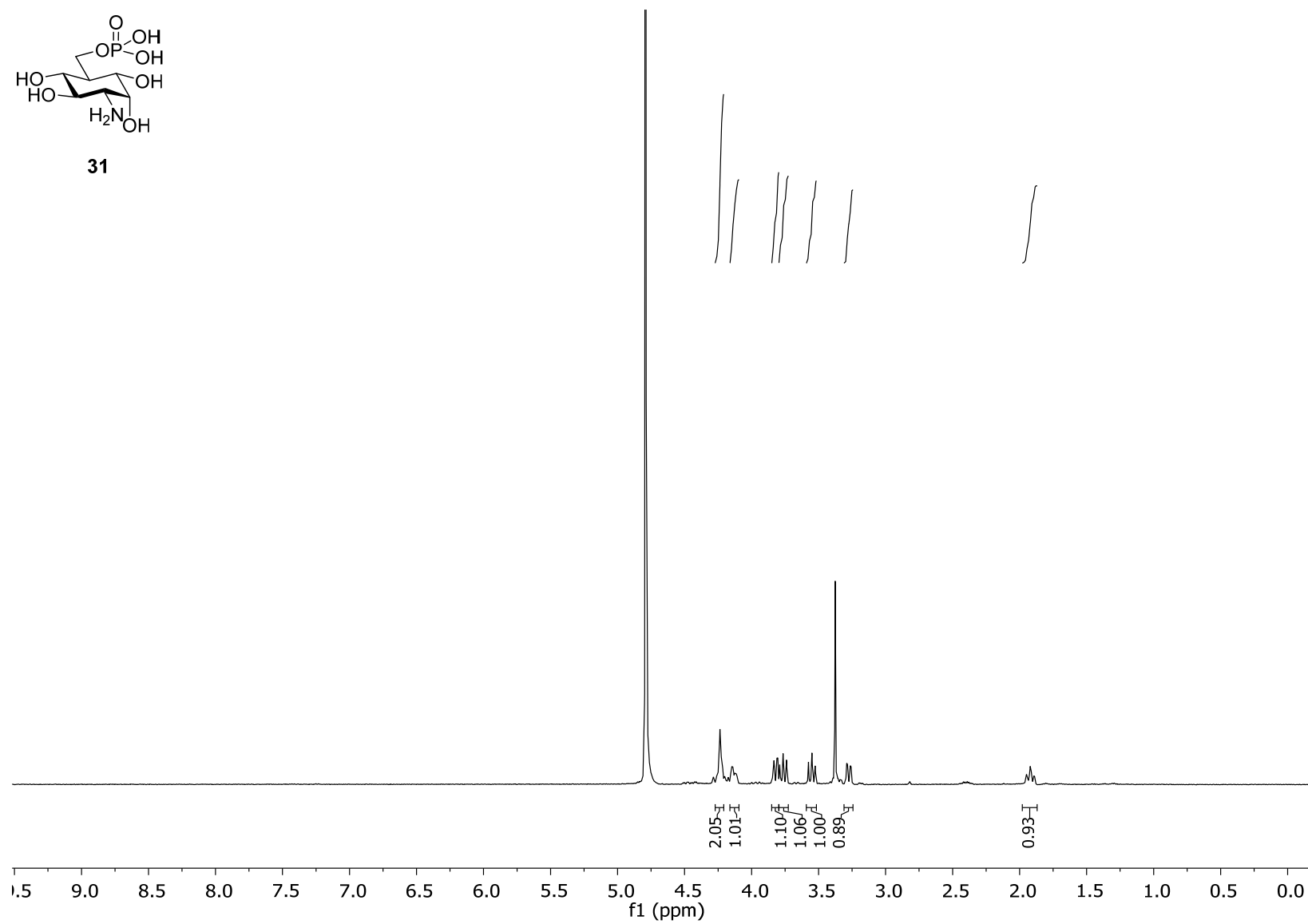
<sup>31</sup>P NMR spectrum (162 MHz, CD<sub>3</sub>OD) of **30**



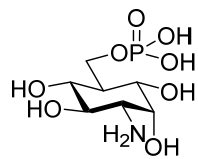
$^{31}\text{P}$ - $^1\text{H}$  HMBC NMR spectrum ( $\text{CD}_3\text{OD}$ ) of **30**



**31**

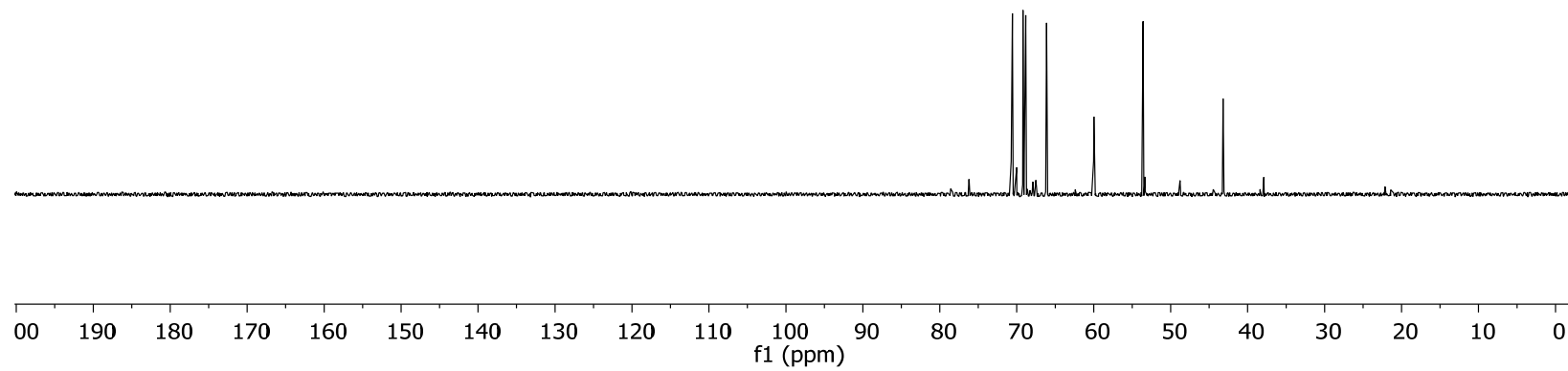


<sup>1</sup>H NMR spectrum (400 MHz, D<sub>2</sub>O) of **31**

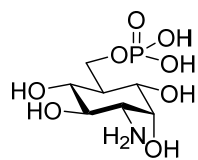


**31**

70.574  
69.200  
68.838  
66.127  
60.012  
59.979  
— 53.590  
43.190  
43.136

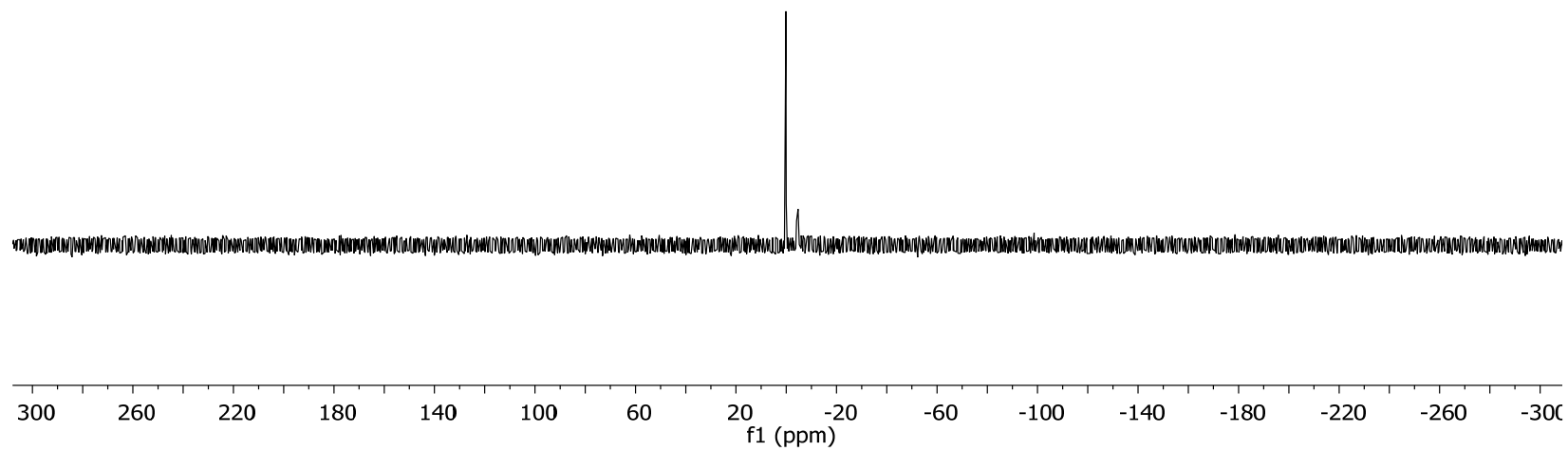


$^{13}\text{C}$  NMR spectrum (151 MHz,  $\text{D}_2\text{O}$ ) of **31**

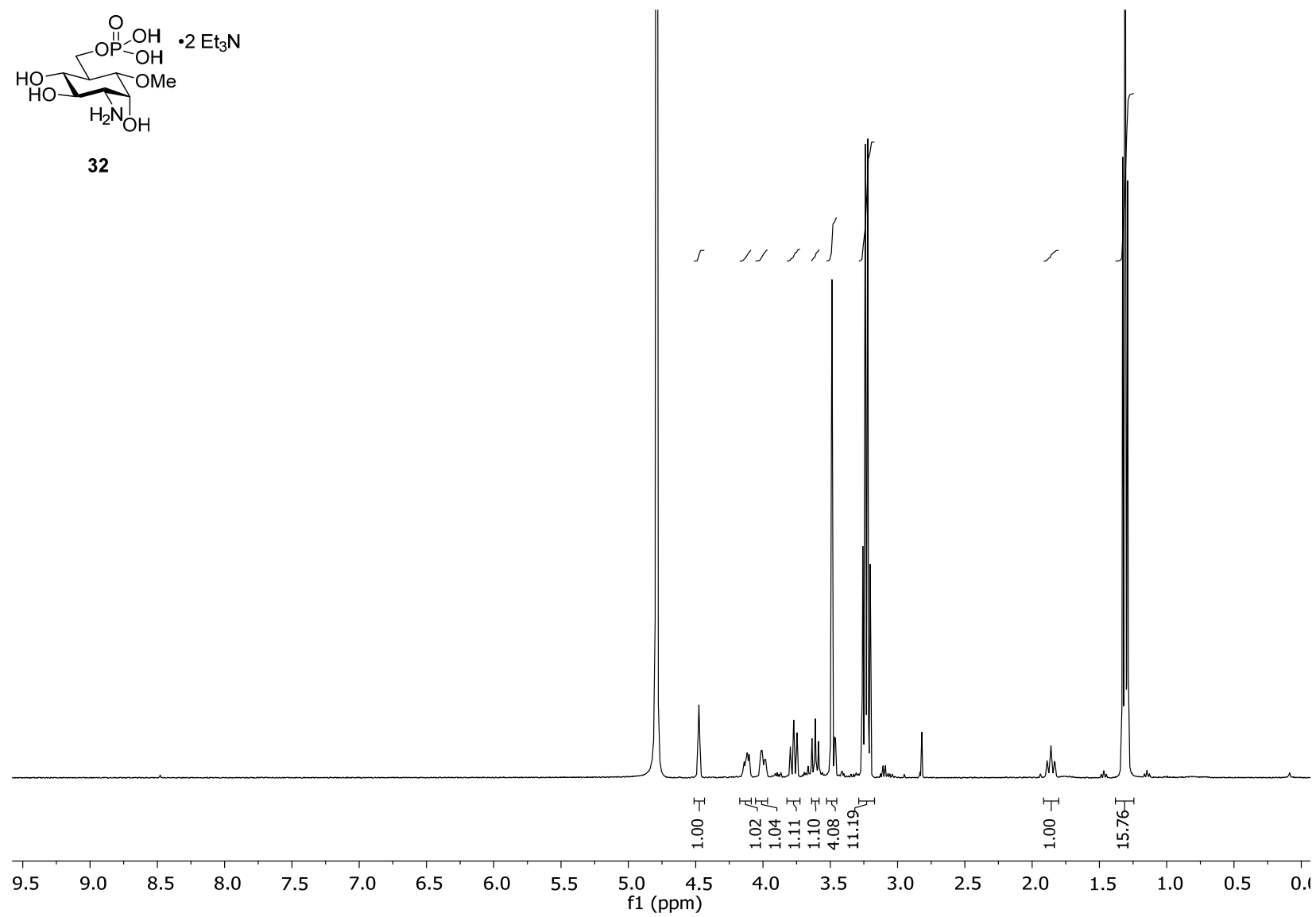
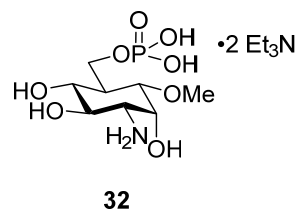


**31**

— 0.12

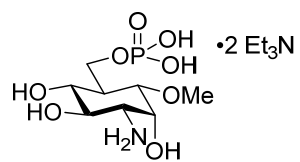


$^{31}\text{P}$  NMR spectrum (CDCl<sub>3</sub>) of **31**

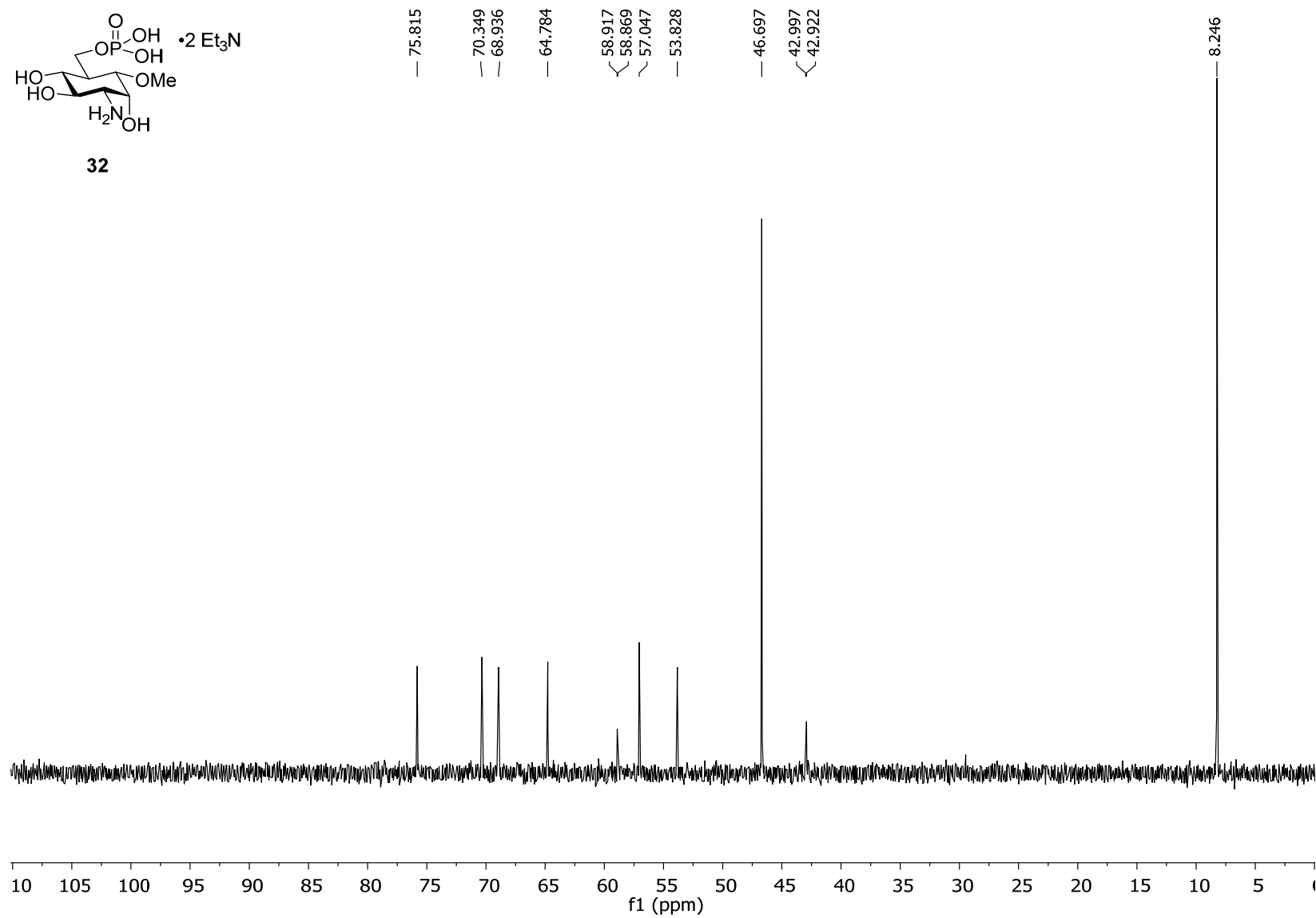


$^1\text{H}$  NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ ) of **32**

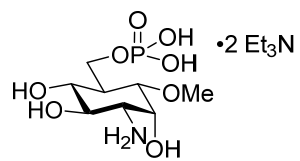




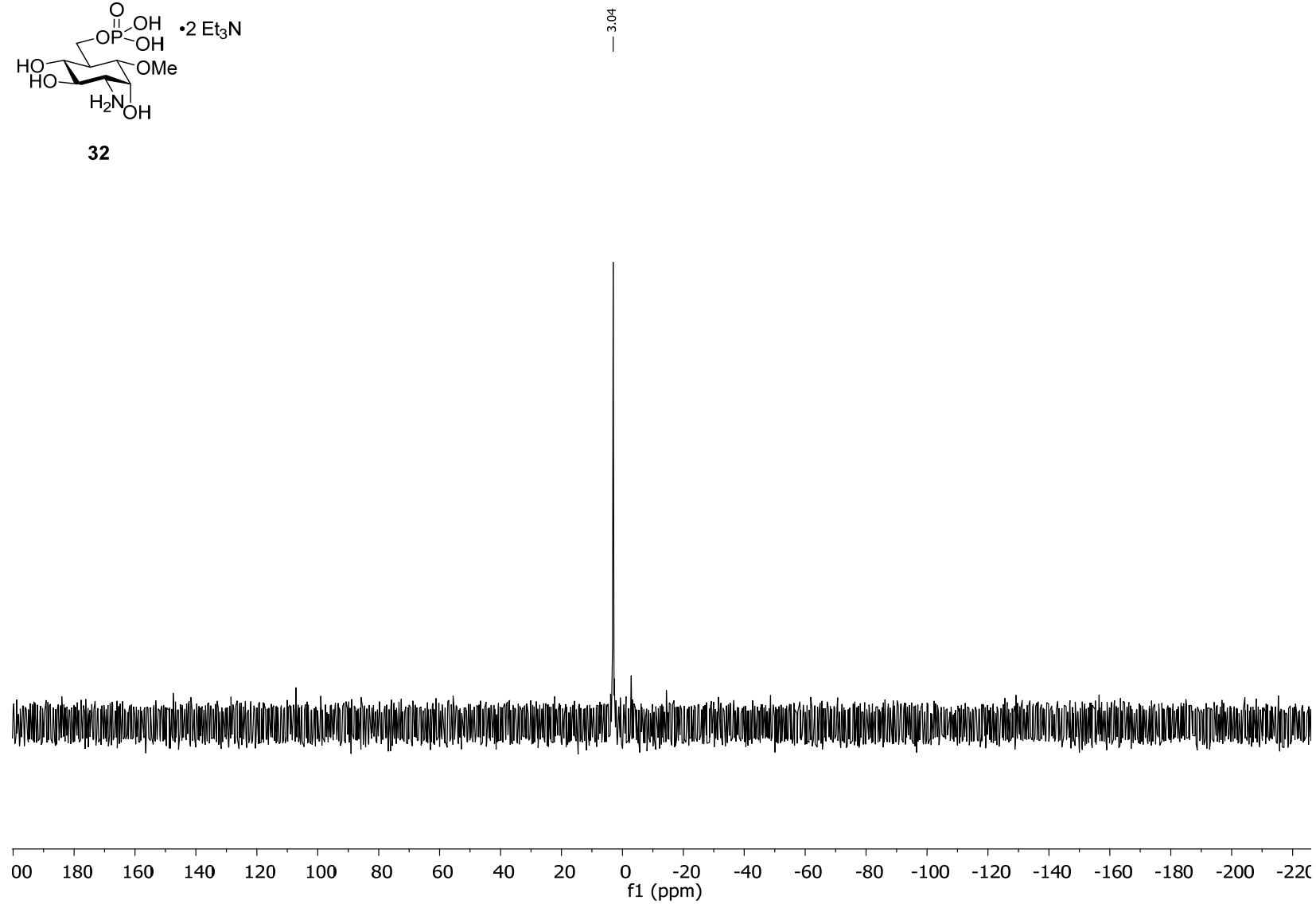
**32**



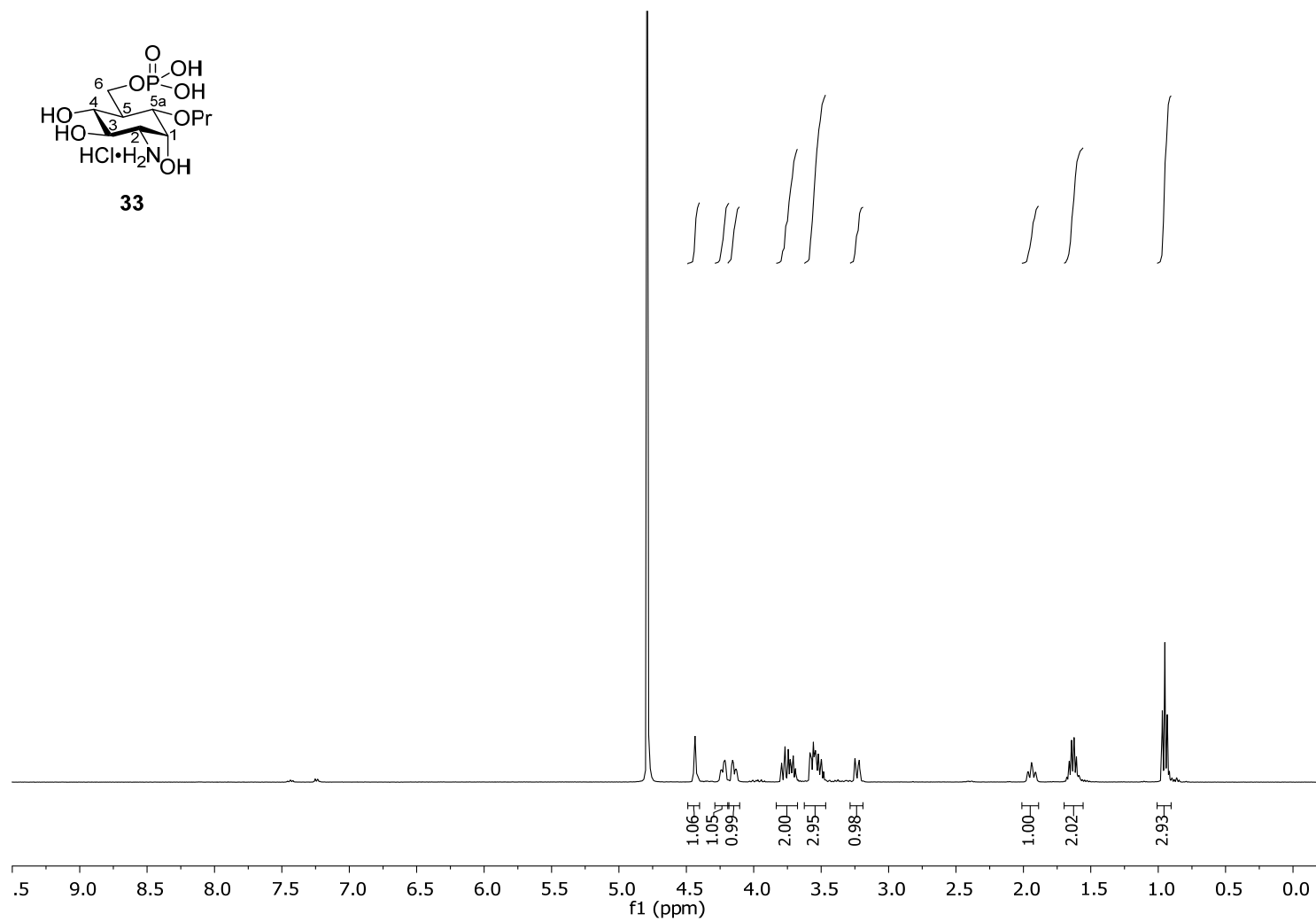
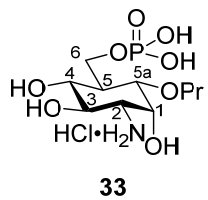
$^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{D}_2\text{O}$ ) of **32**



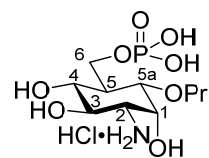
**32**



<sup>31</sup>P NMR spectrum (162 MHz, D<sub>2</sub>O) of **32**

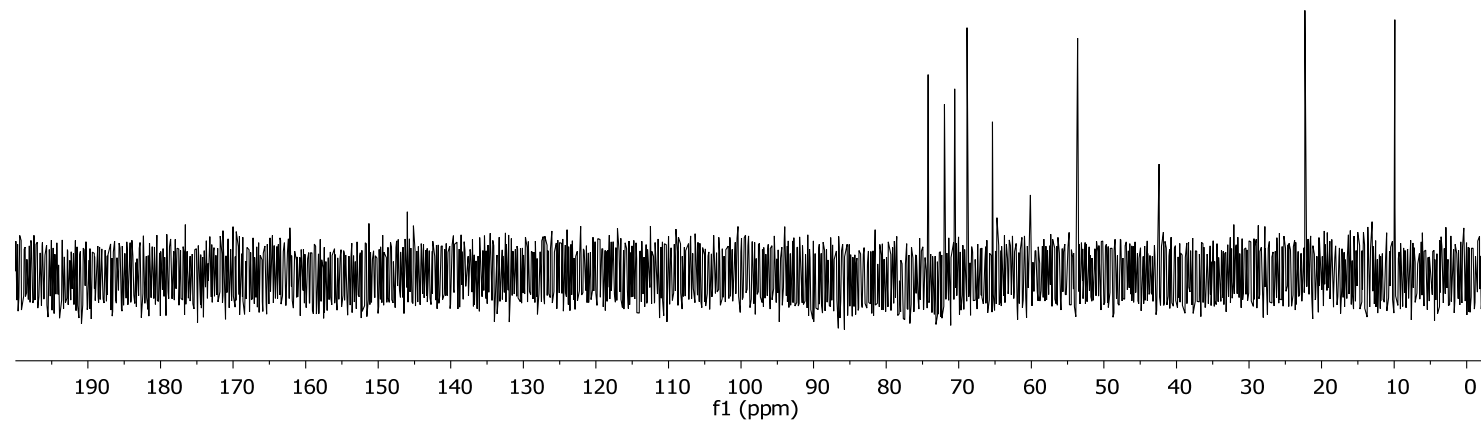


<sup>1</sup>H NMR spectrum (400 MHz, D<sub>2</sub>O) of **33**

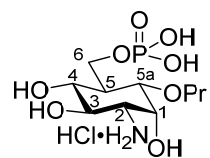


**33**

74.230  
71.959  
70.566  
68.853  
65.351  
60.161  
60.115  
53.610  
42.486  
42.393  
22.297  
9.904

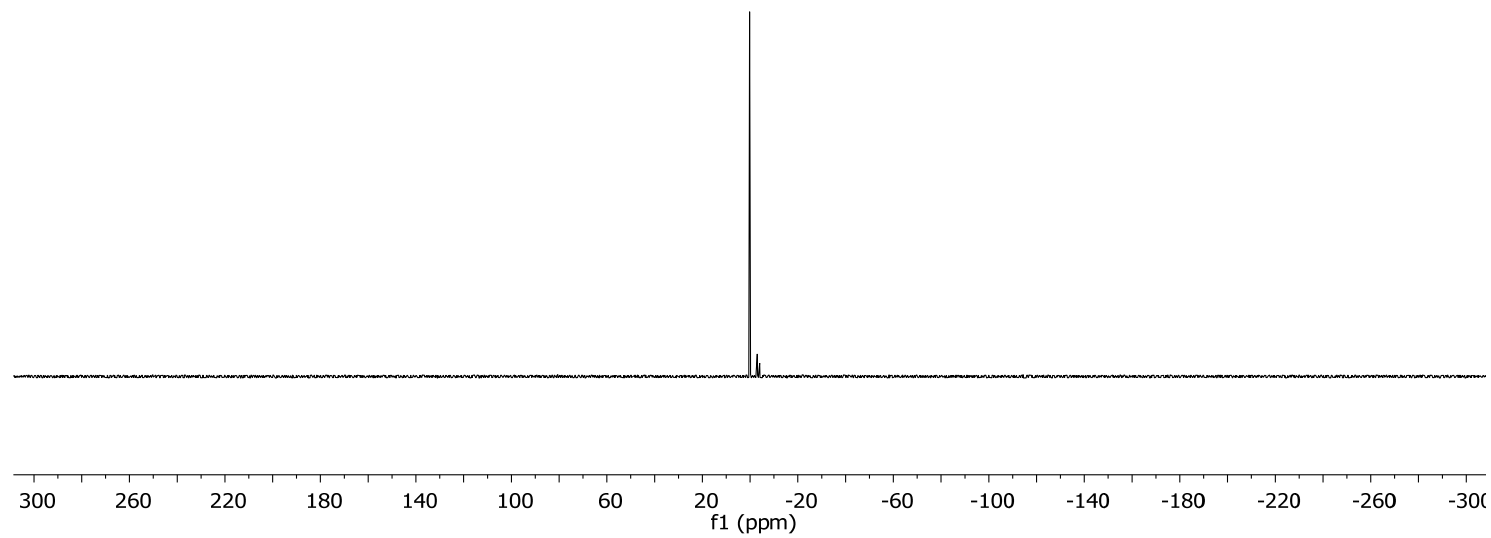


$^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{D}_2\text{O}$ ) of **33**



**33**

— 0.20



$^{31}\text{P}$  NMR spectrum (162 MHz,  $\text{D}_2\text{O}$ ) of **33**