

Supporting Information

Gram scale production of 1-azido- β -D-glucose via enzyme catalysis for the synthesis of 1,2,3-triazole-glucosides

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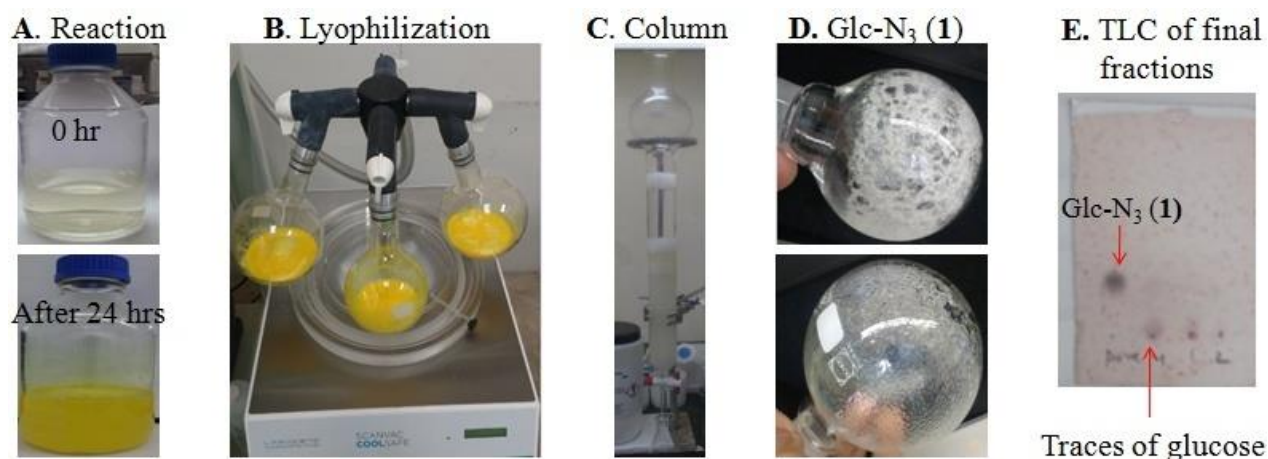


Figure S1. Reaction and first purification. (A). Transglucosylation reaction from 0 hr to 24 hrs, (B) H₂O drying by lyophilization, (C) Silica gel column purification, (D) Glc-N₃ **1** [Impure (top), 800 mg pure (bottom)], (E) TLC profile of final fractions from silica gel column.

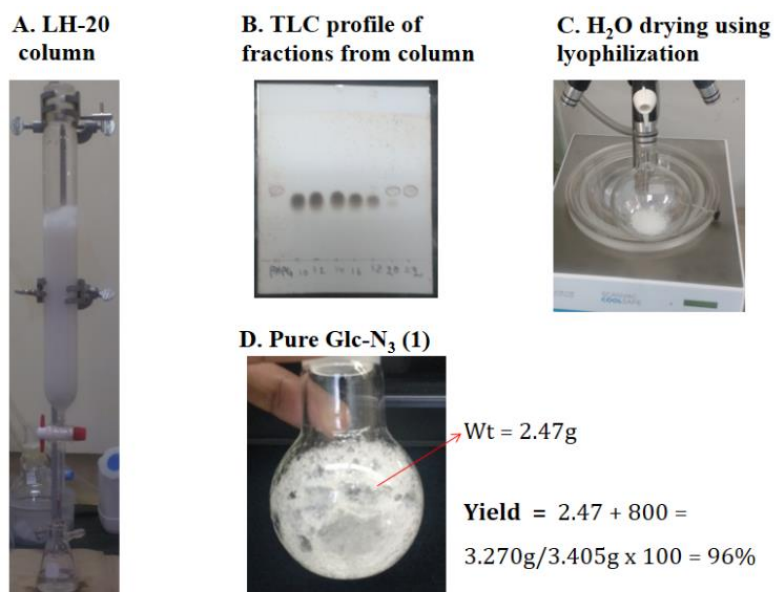
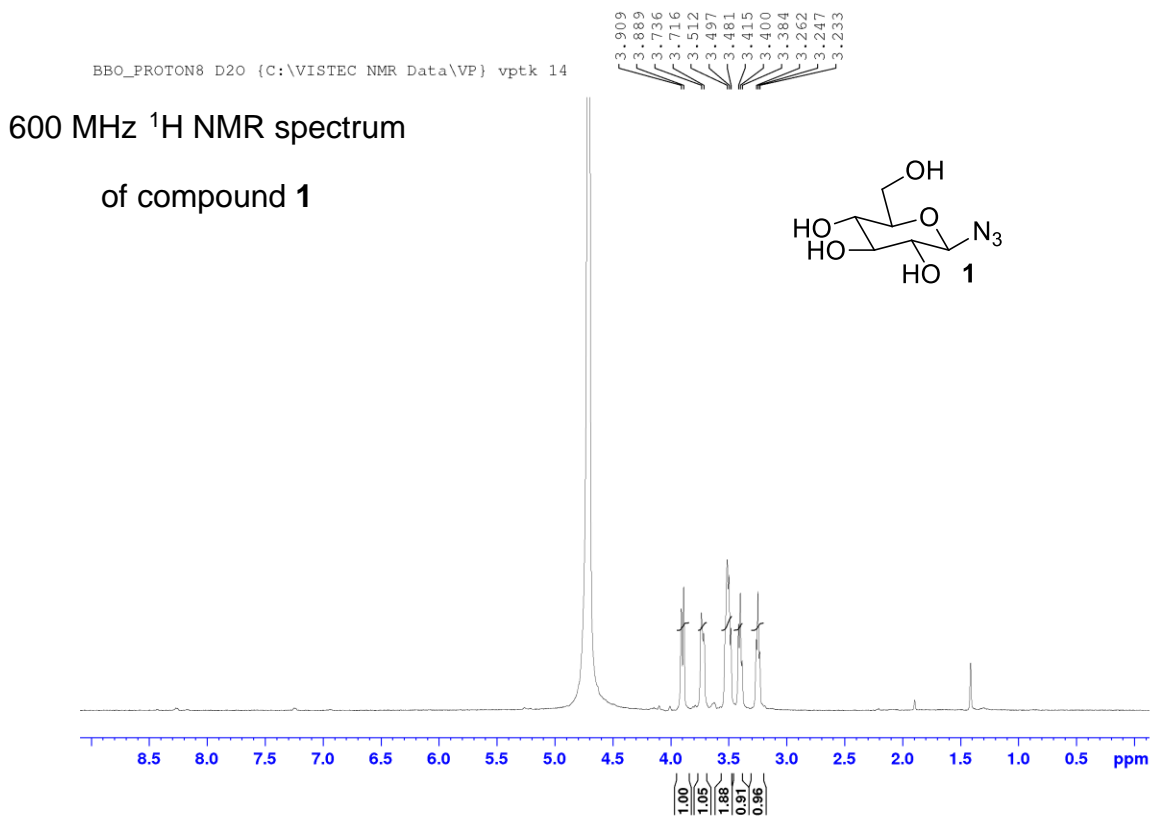


Figure S2. Second purification. (A). Sephadex LH-20 column (B) TLC profile of fractions from column (C) H₂O drying using lyophilization (D) Pure 1-azido- β -D-glucose (**1**).



400 MHz ¹H NMR spectra of compound **1**

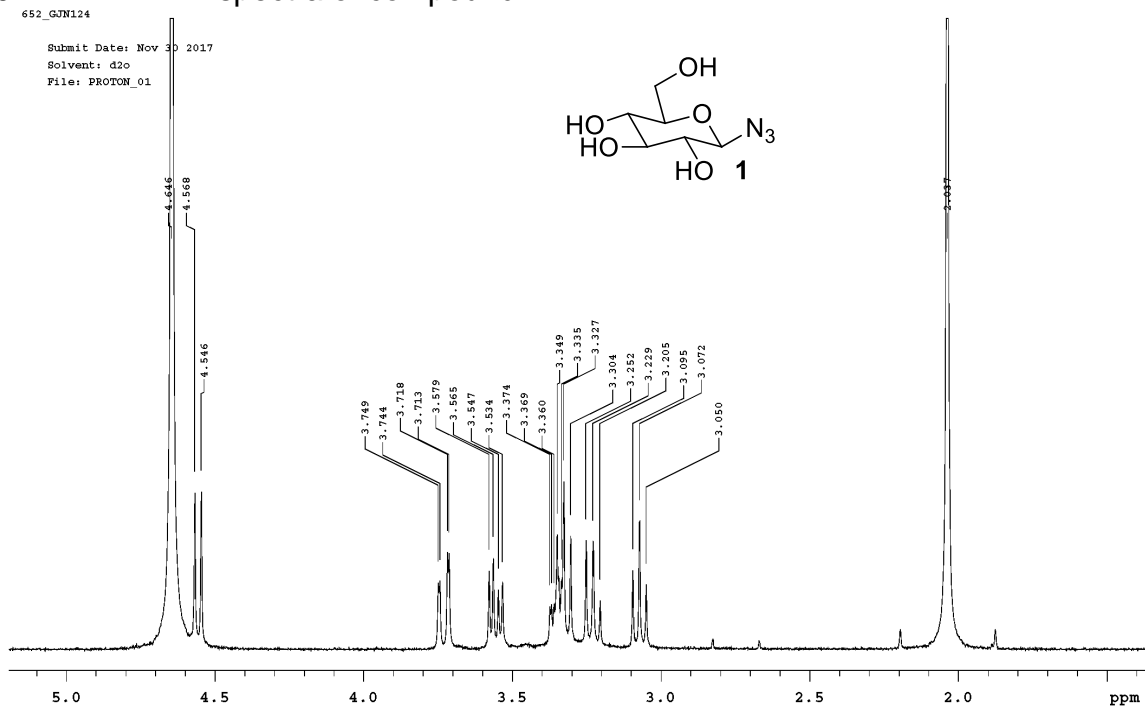


Figure S3. ¹H NMR Spectra of compound **1** at 600 and 400 MHz

BBO_C13CPD256 D2O {C:\VISTEC NMR Data\VP} vptk 14

90.14
77.94
75.79
72.88
69.23
60.60

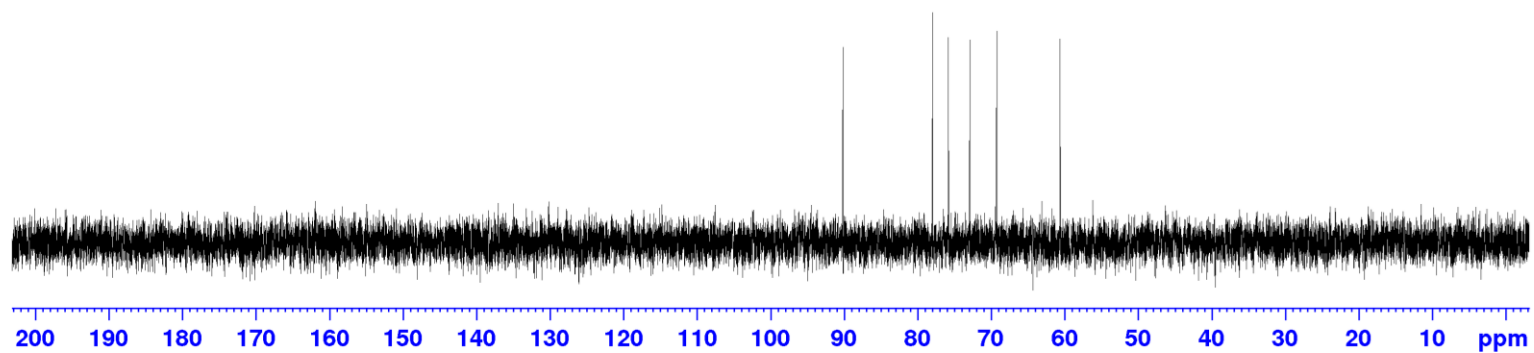
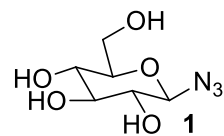
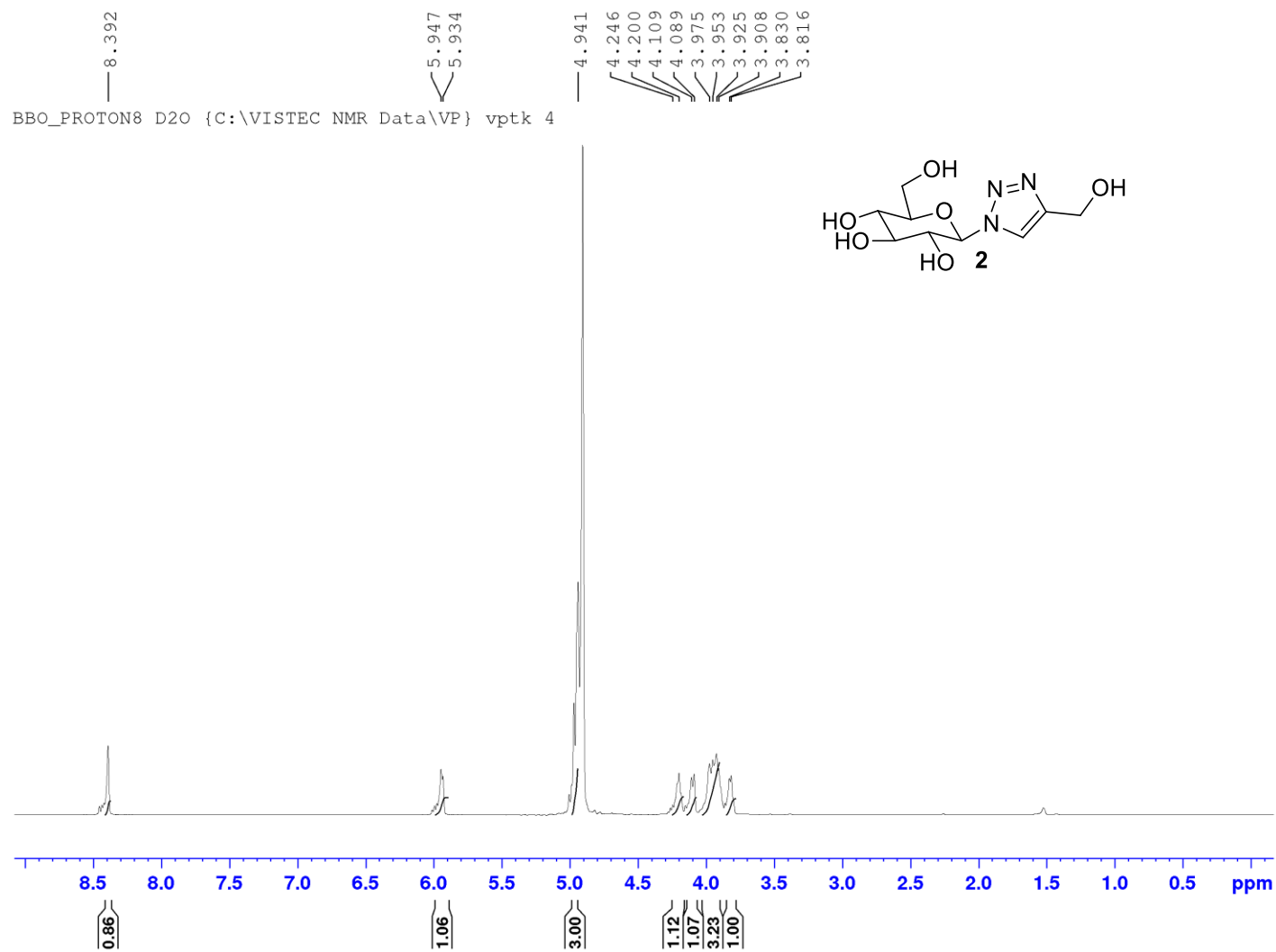


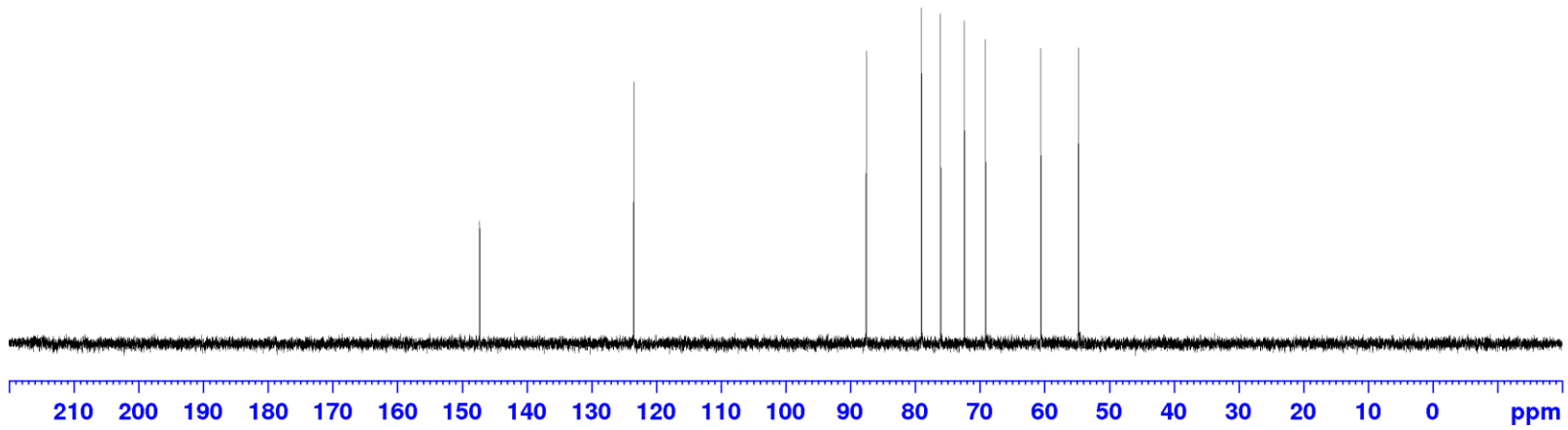
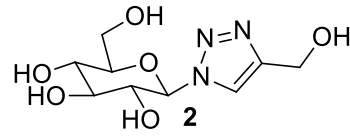
Figure S4. ^{13}C NMR Spectrum of Compound **1**.

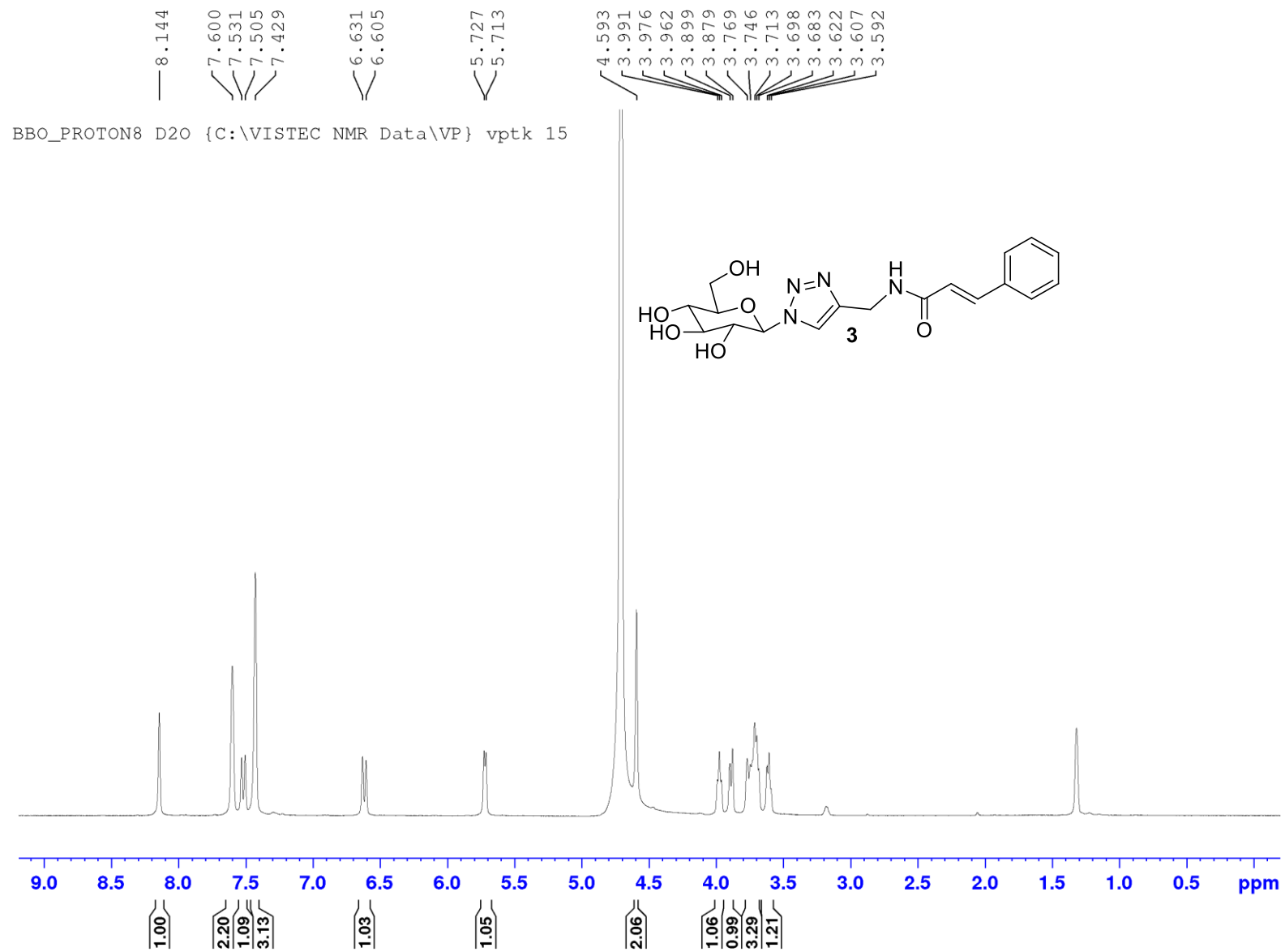
Figure S5 ^1H and ^{13}C NMR Spectra of Compounds **2-16**.



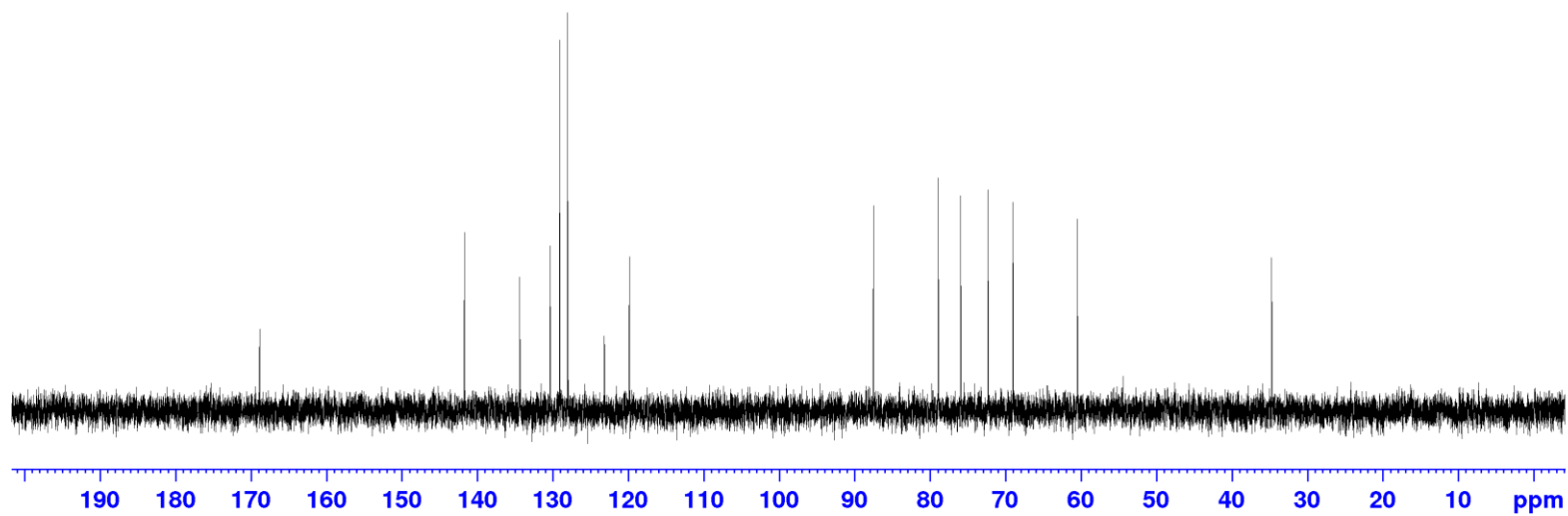
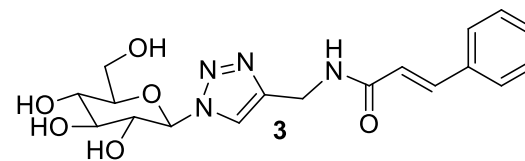
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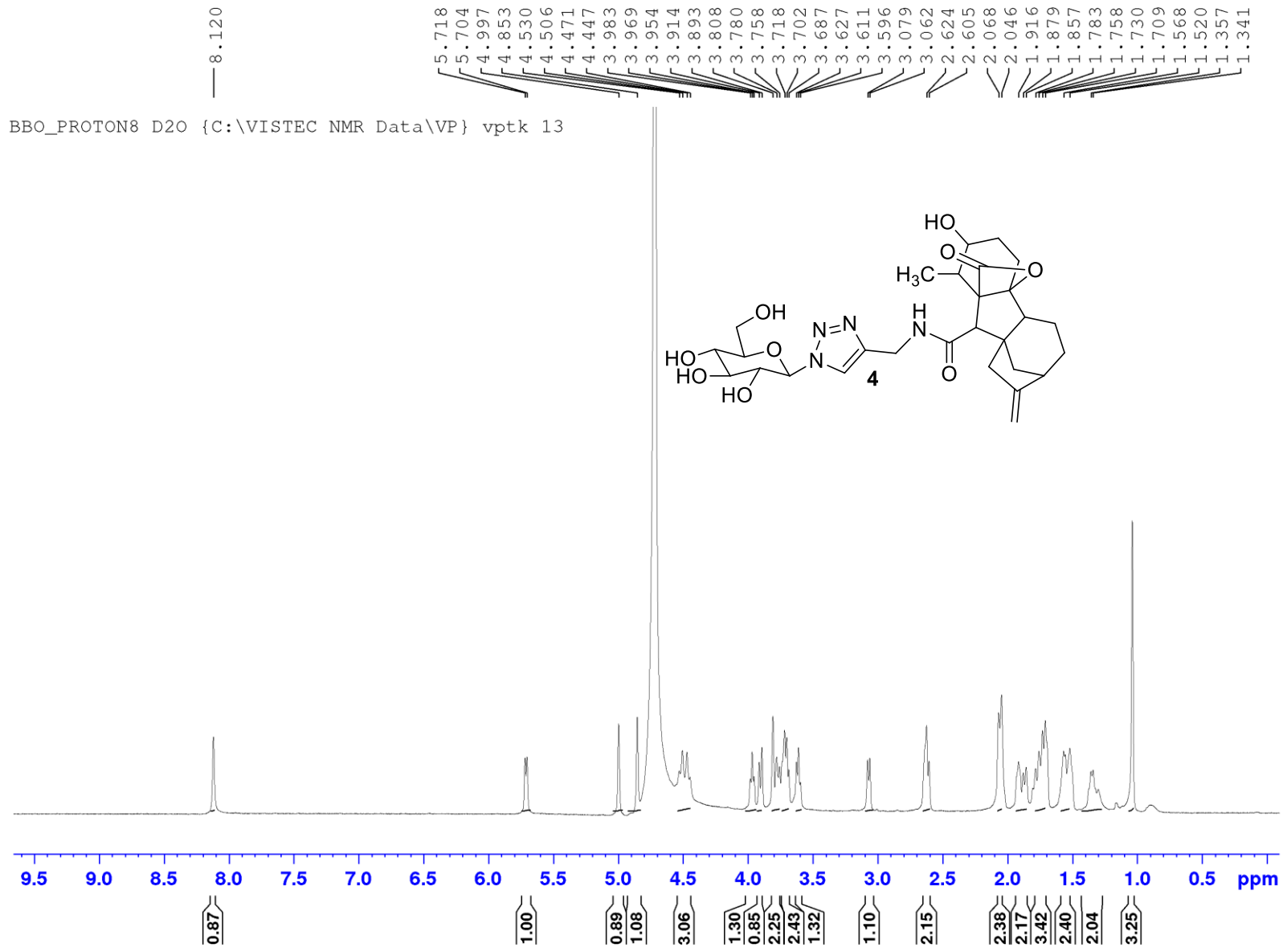
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123.43
87.51
78.98
76.03
72.35
69.08
60.53
54.71



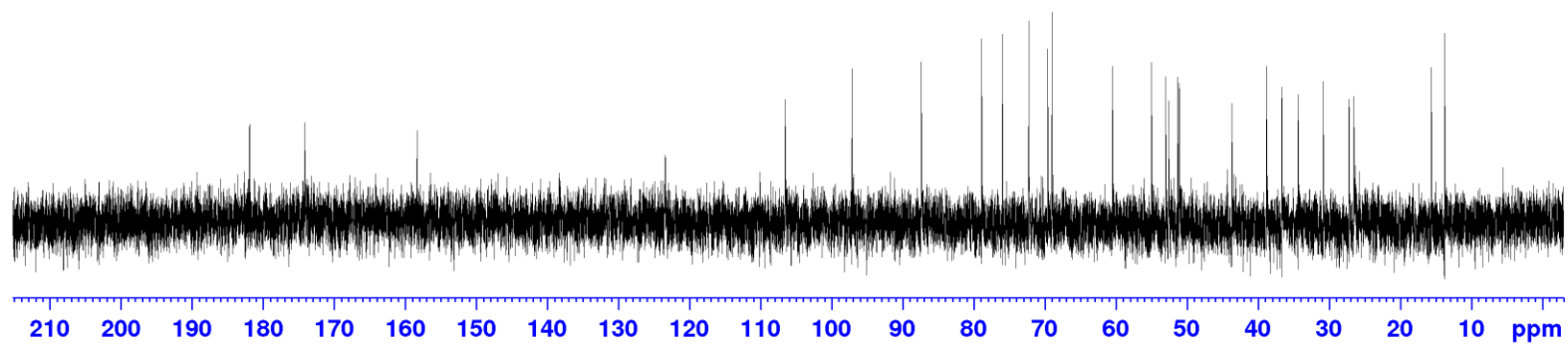
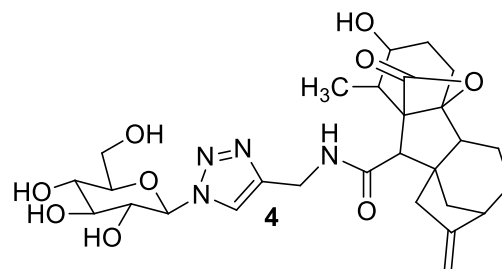


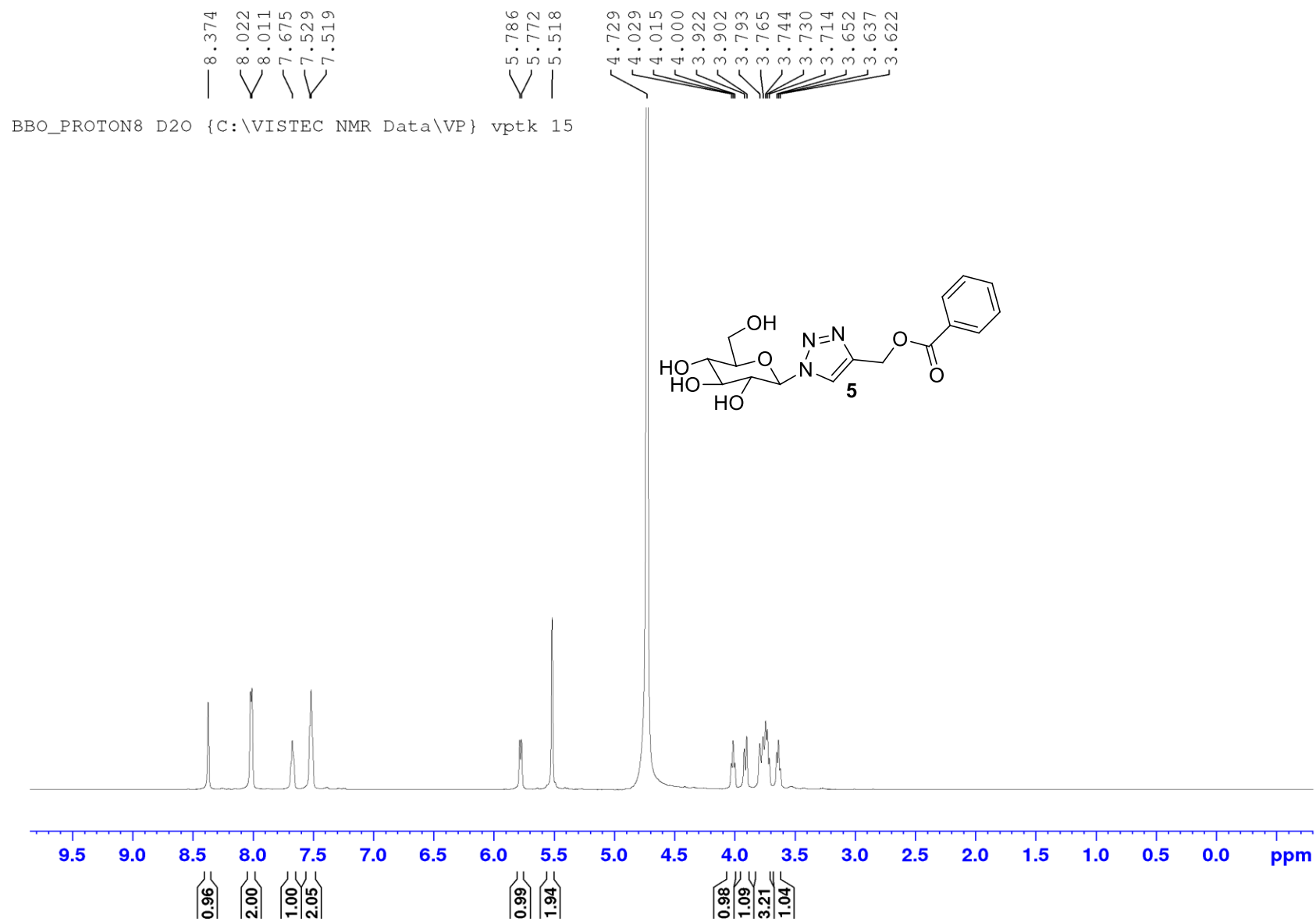
BBO_C13CPD256 D2O {C:\VISTEC NMR Data\VP} vptk 3





BBO_C13CPD256 D2O {C:\VISTEC NMR Data\VP} vptk 1





BBO_C13CPD256 D2O {C:\VISTEC NMR Data\VP} vptk 15

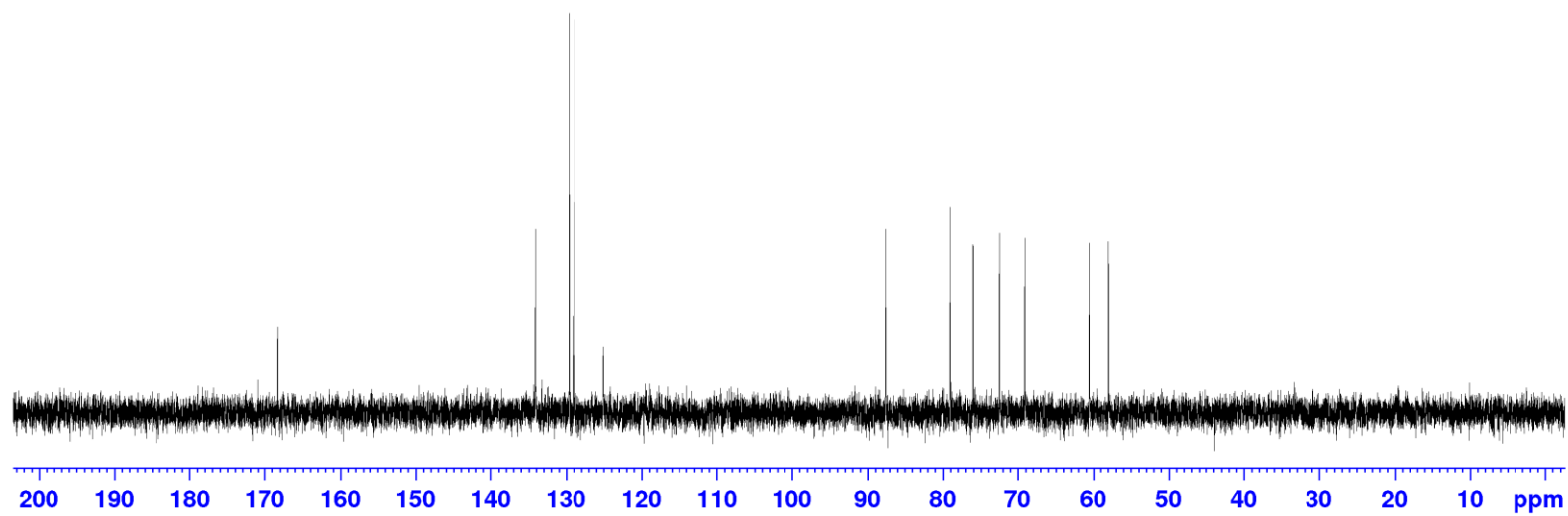
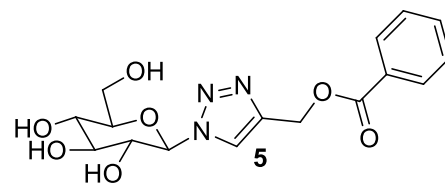
168.28

134.06
129.59
129.06
128.82
125.04

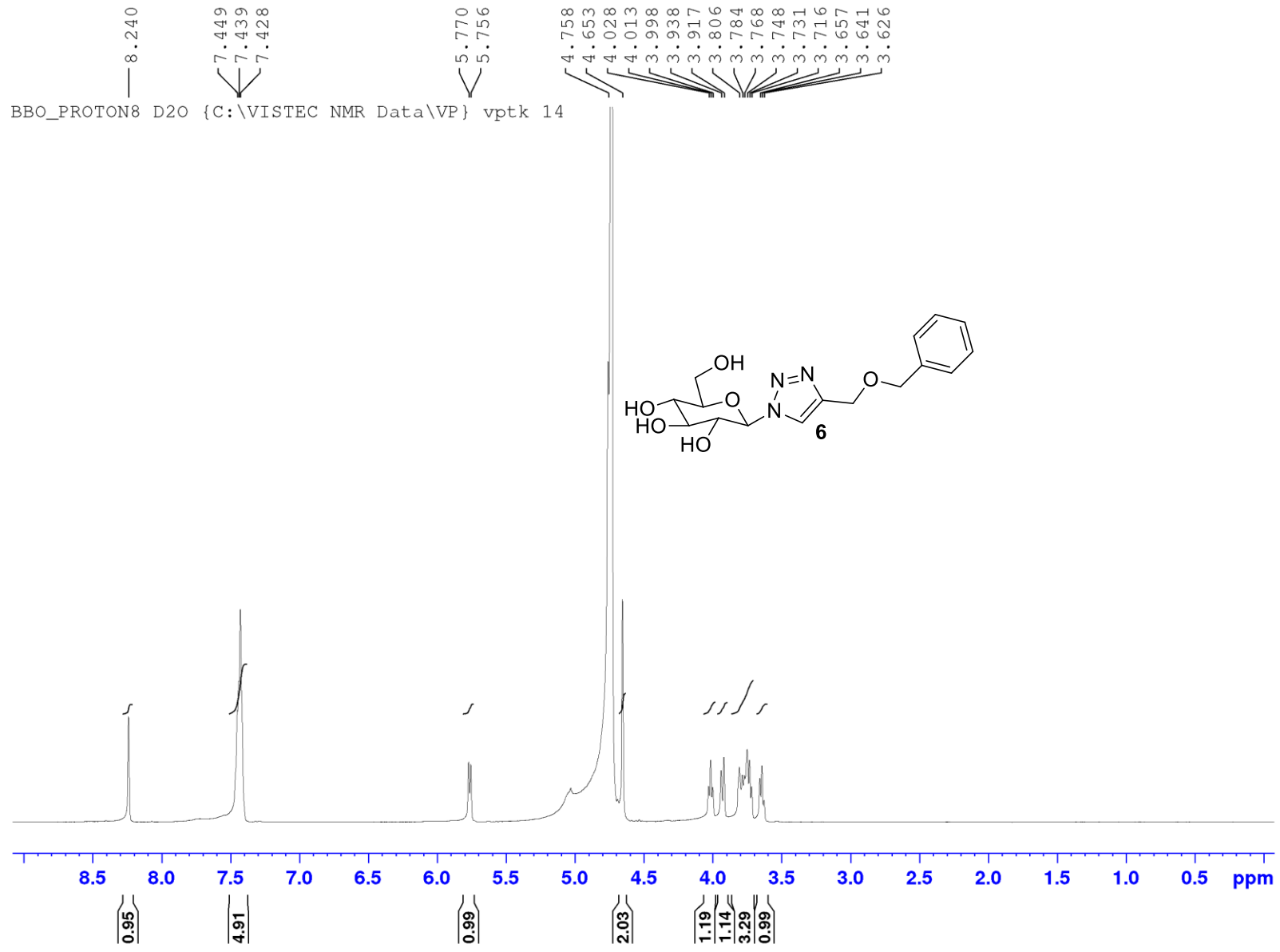
87.61

78.98
75.99
72.38
69.04

60.51
57.91

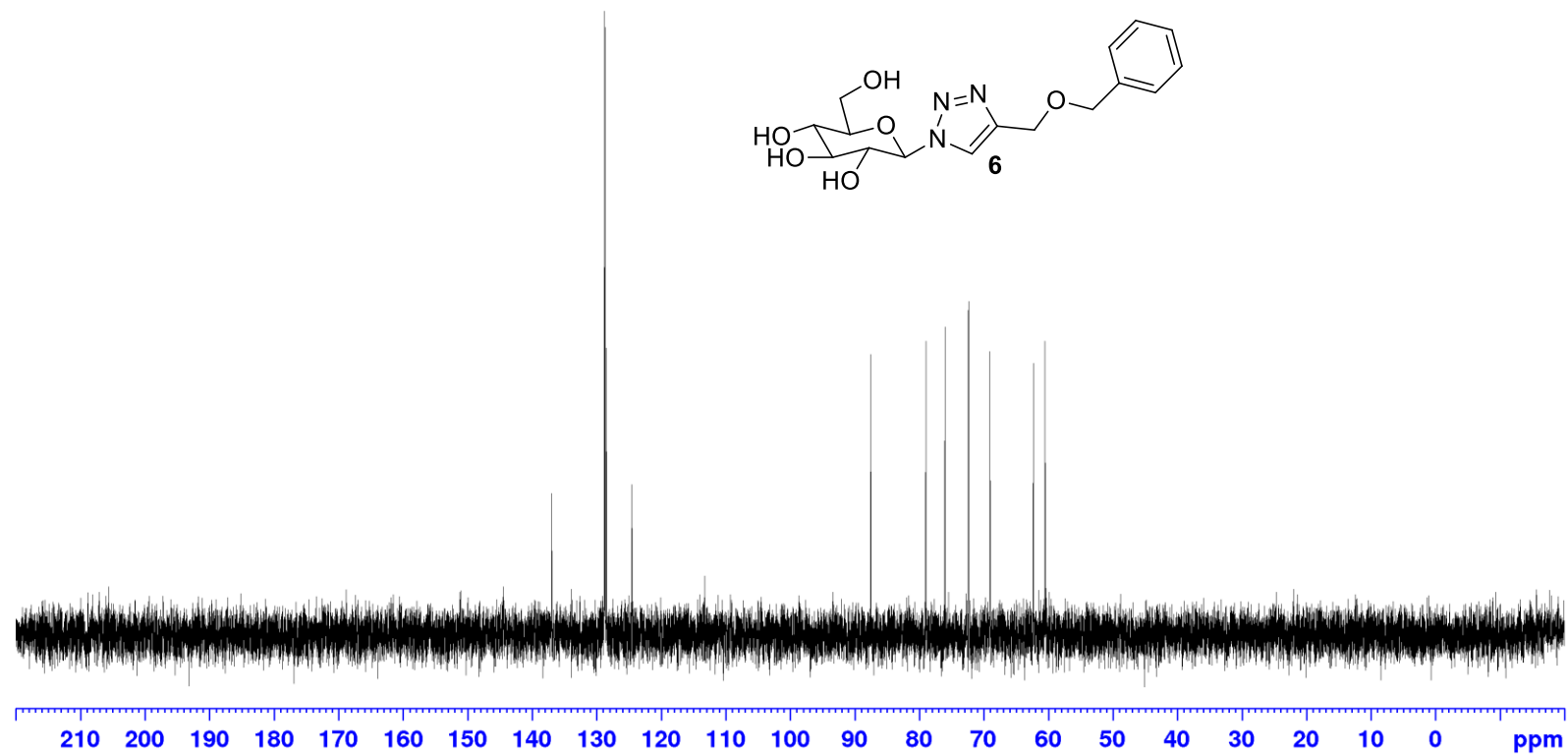


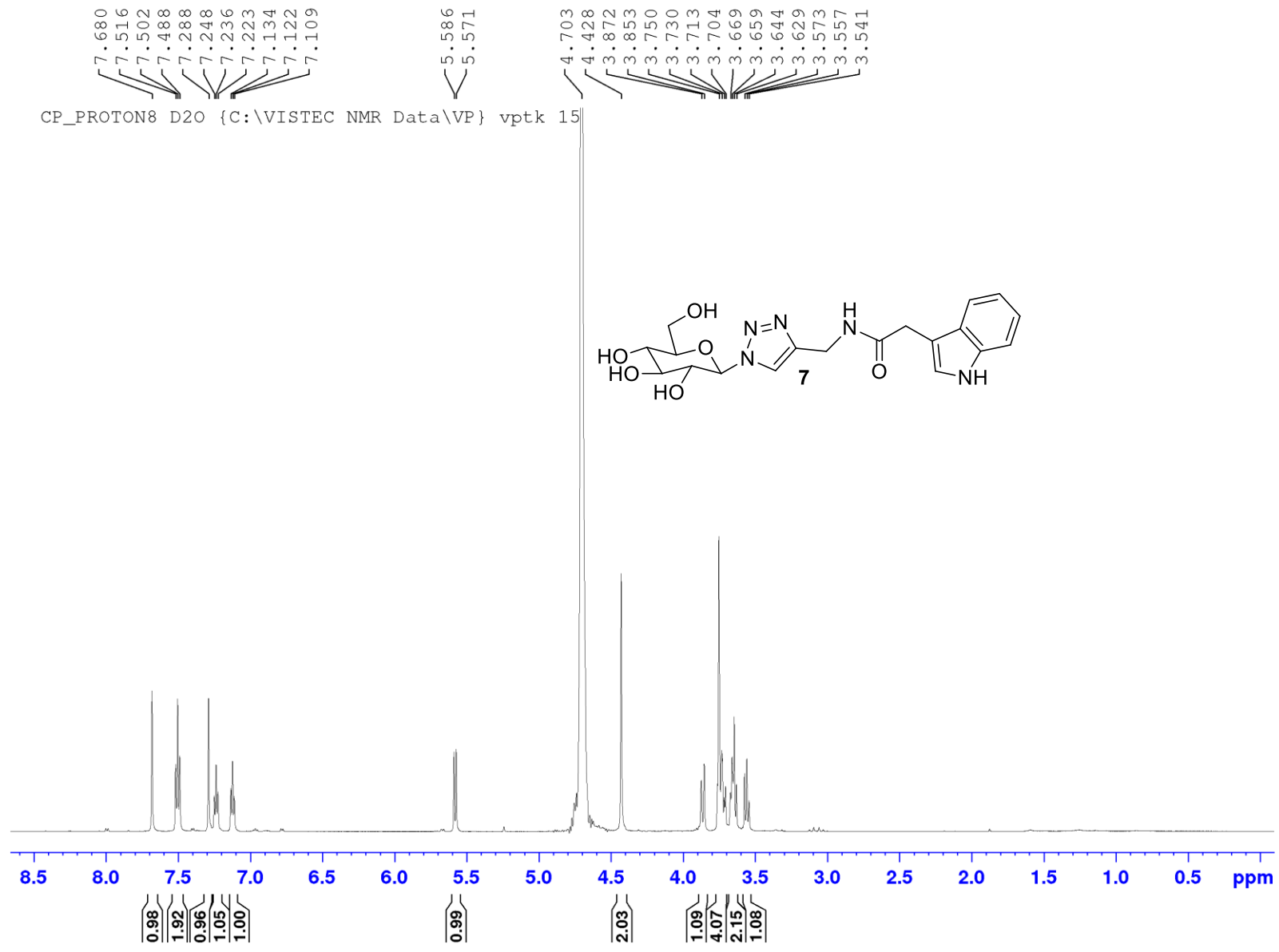
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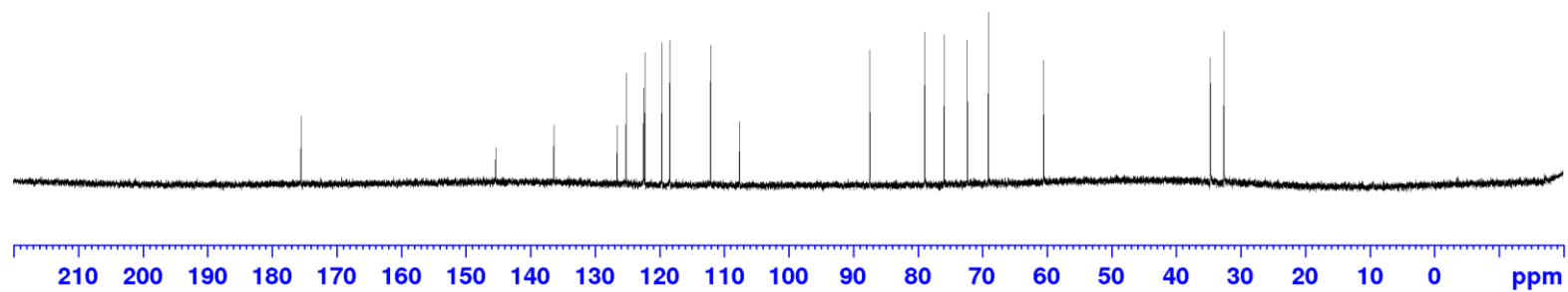
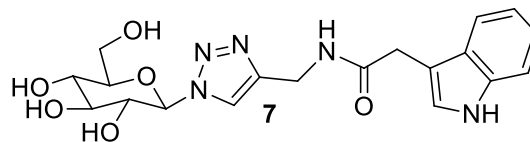
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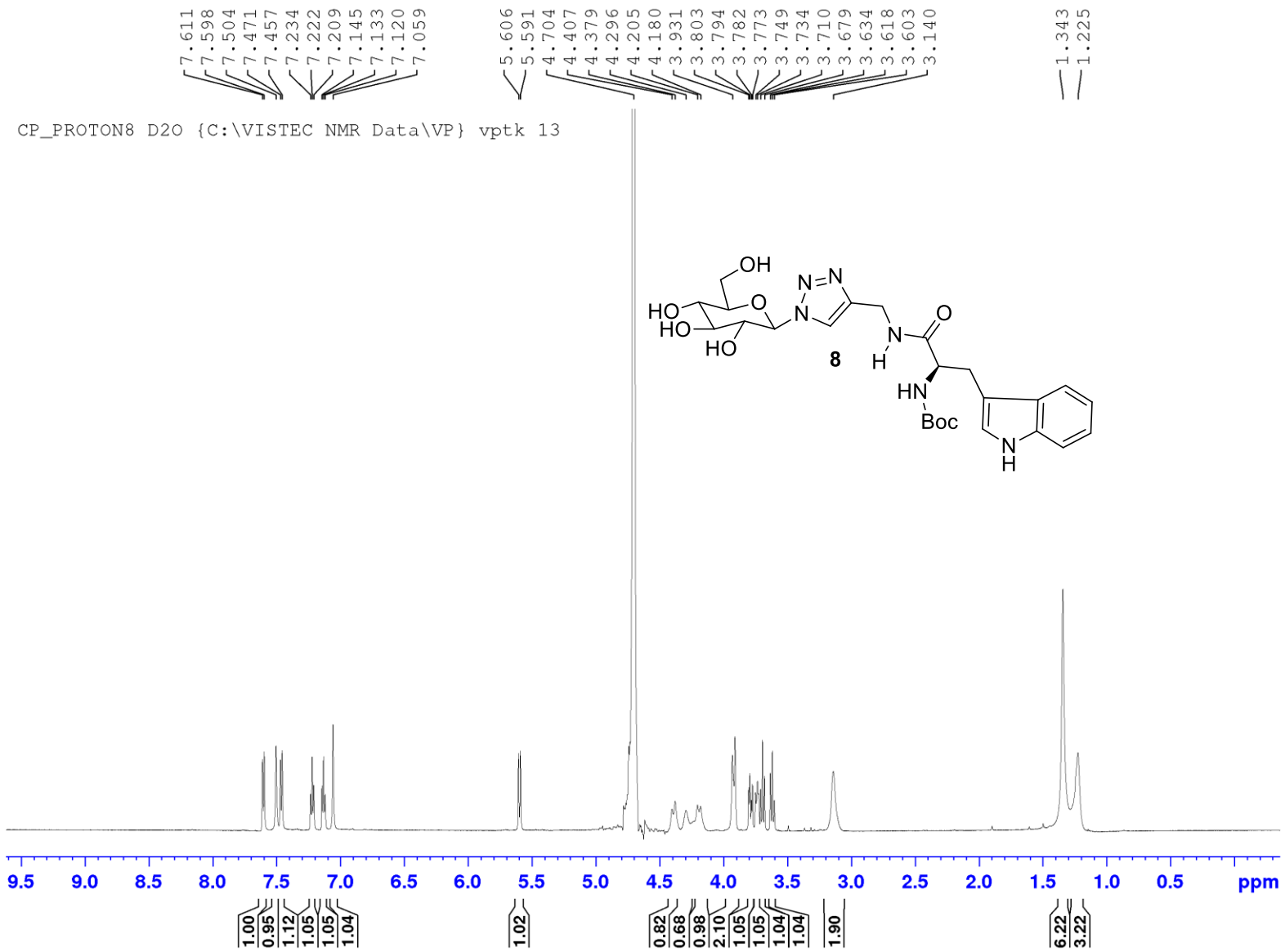
136.97
128.82
128.70
128.50
124.54
87.49
78.94
75.99
72.37
72.31
69.02
62.27
60.49

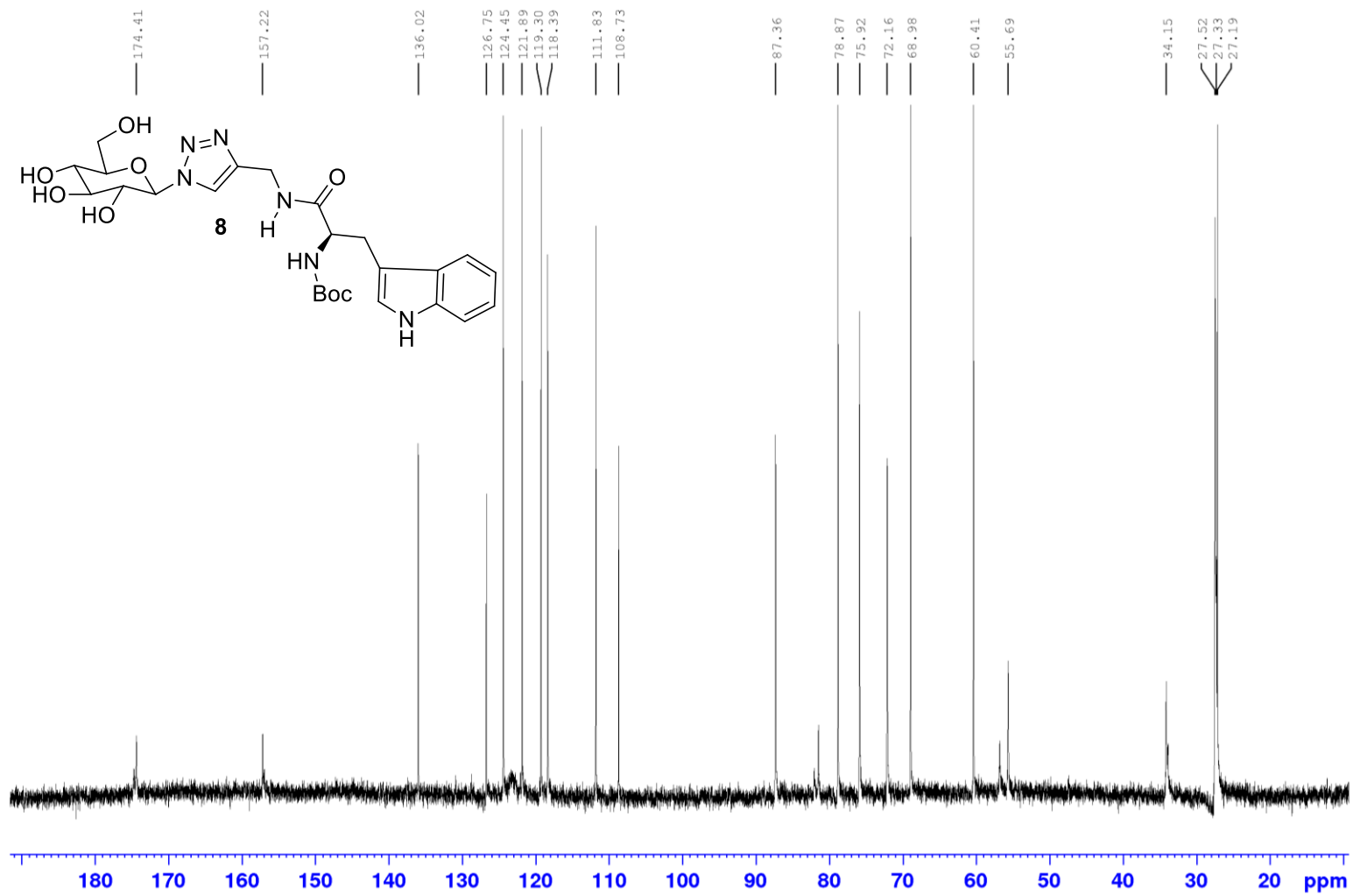


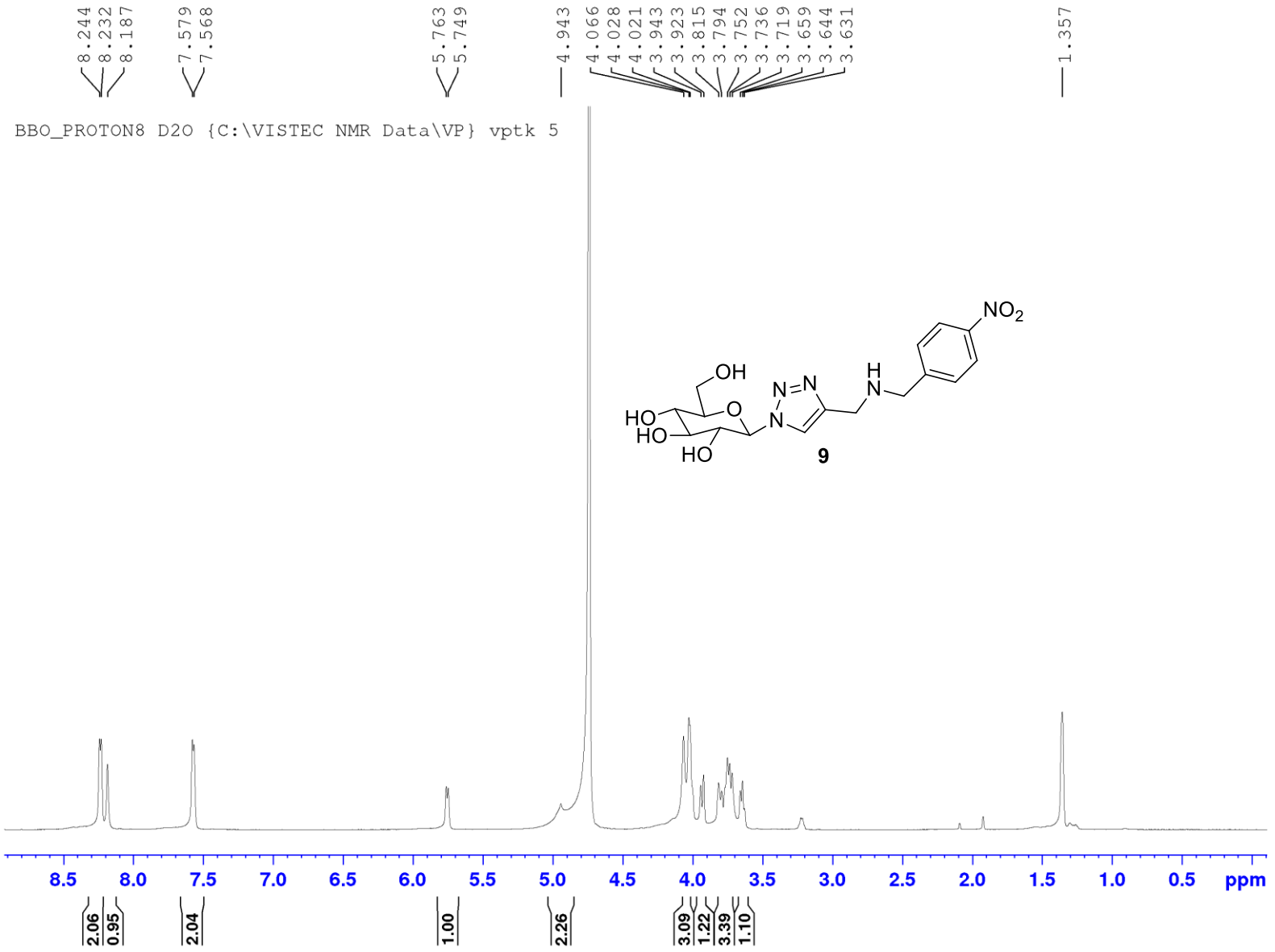


CP_C13CPD32_DE12 D2O {C:\VISTEC NMR Data\VP} vptk 6

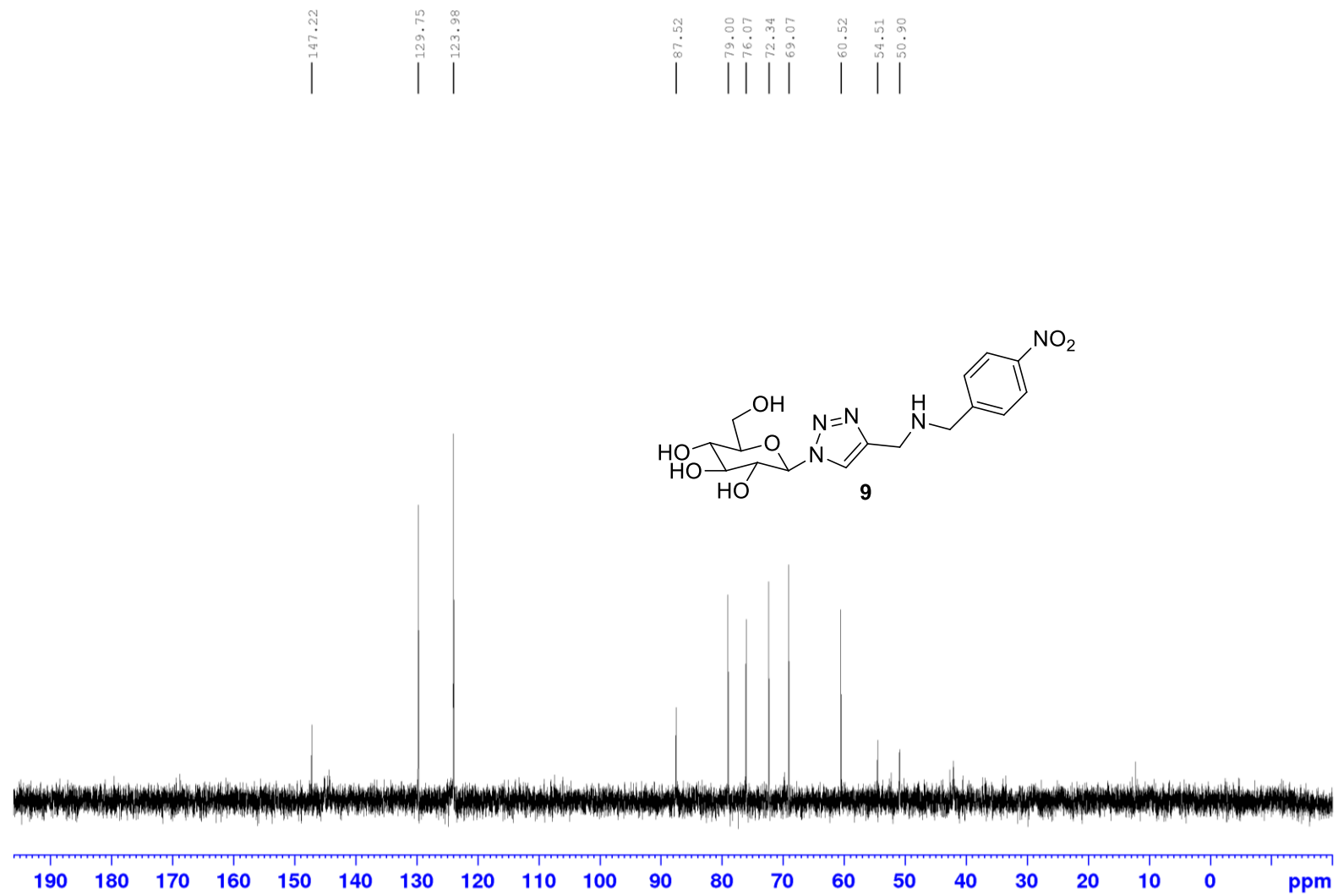


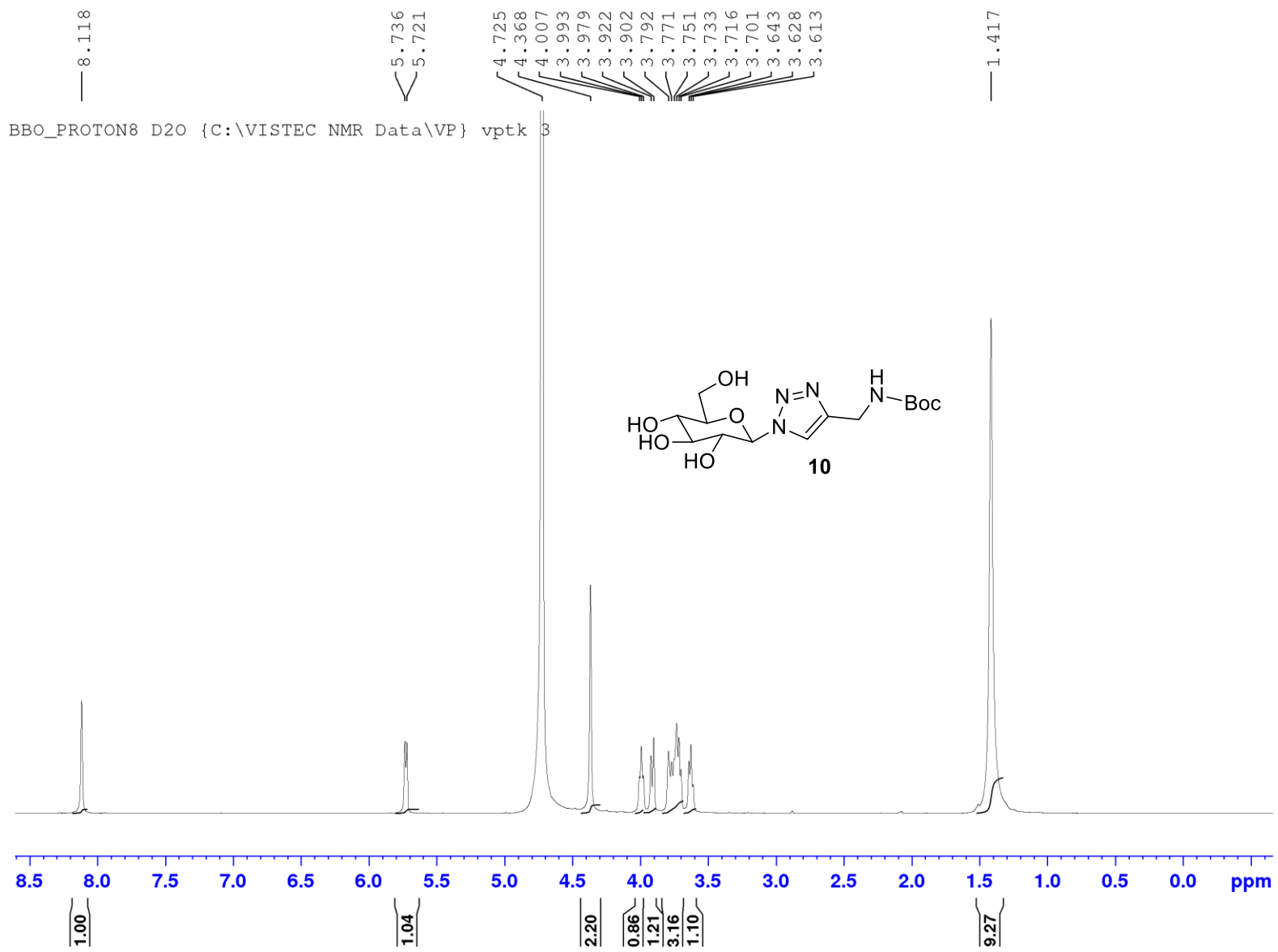




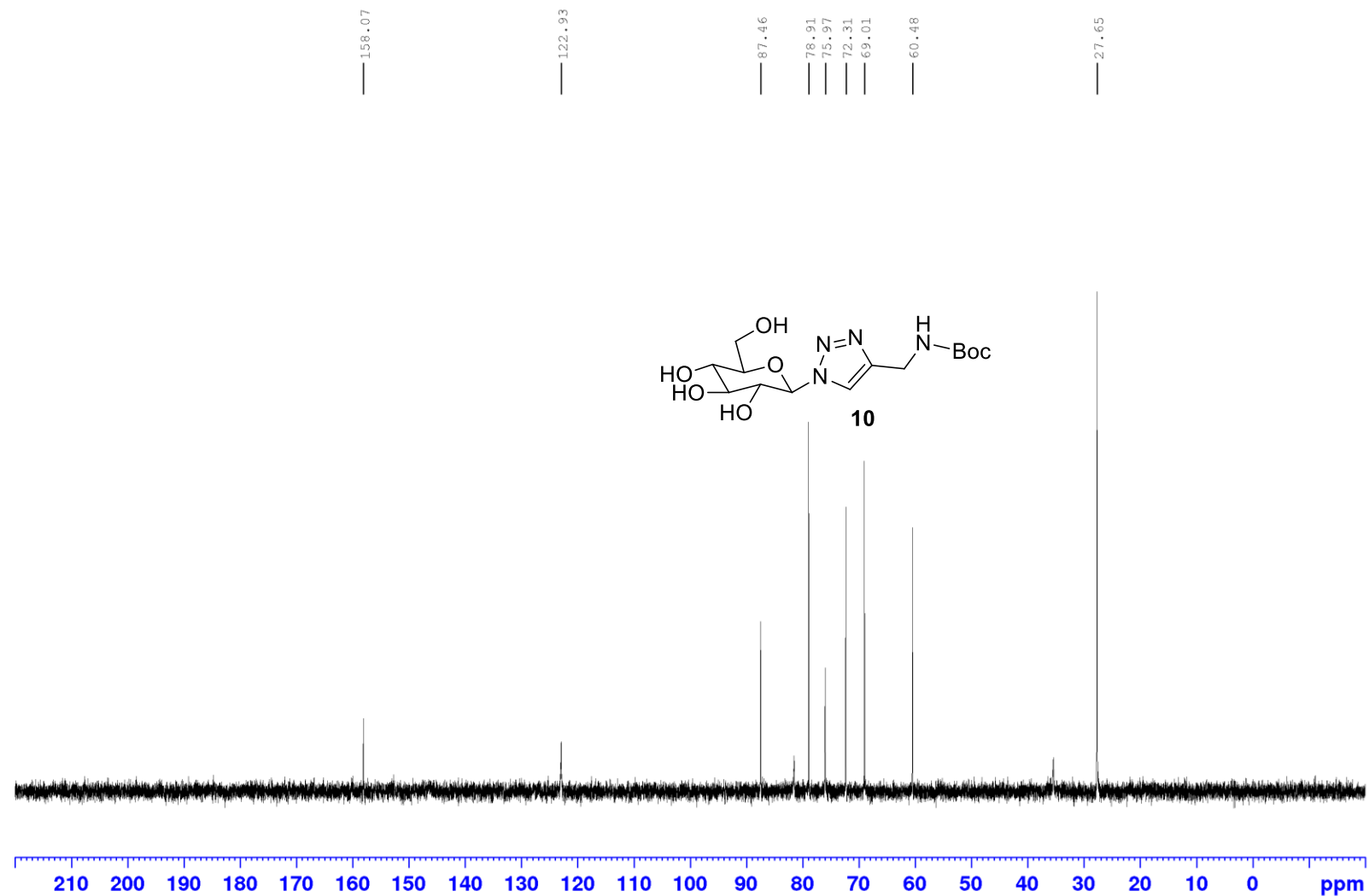


BBO_C13CPD256 D2O {C:\VISTEC NMR Data\VP} vptk 5

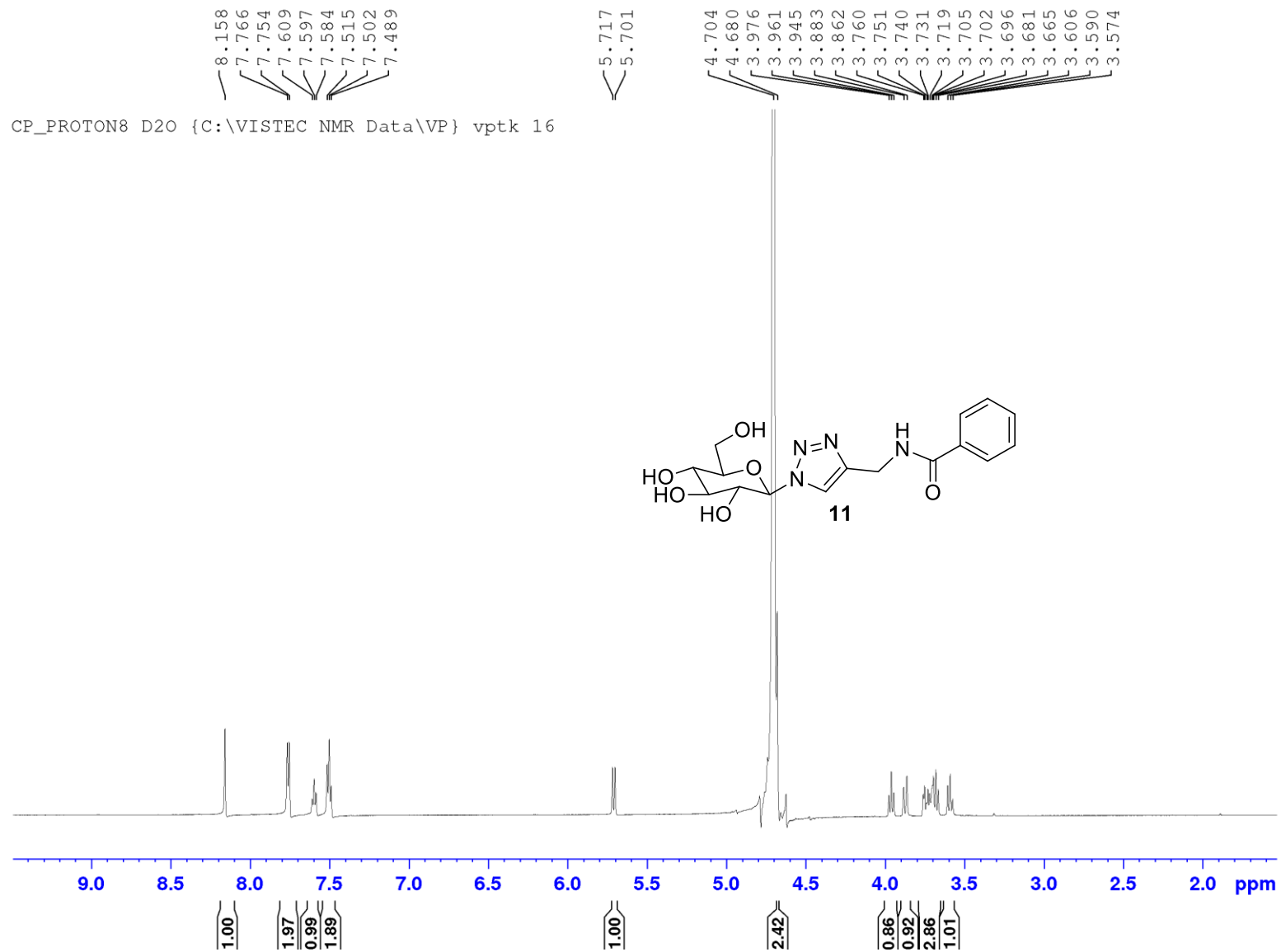




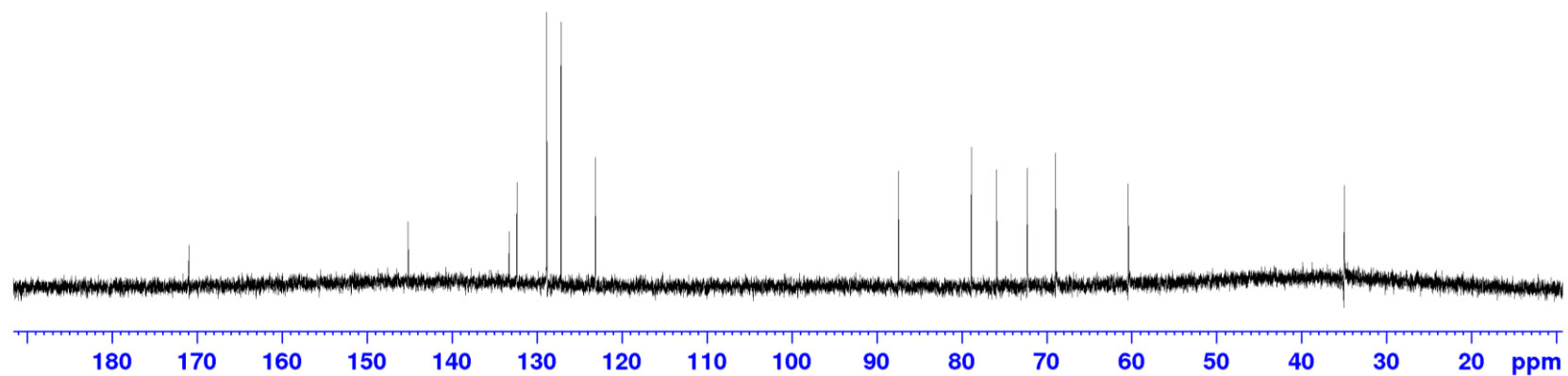
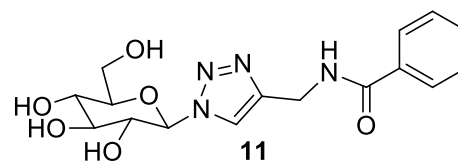
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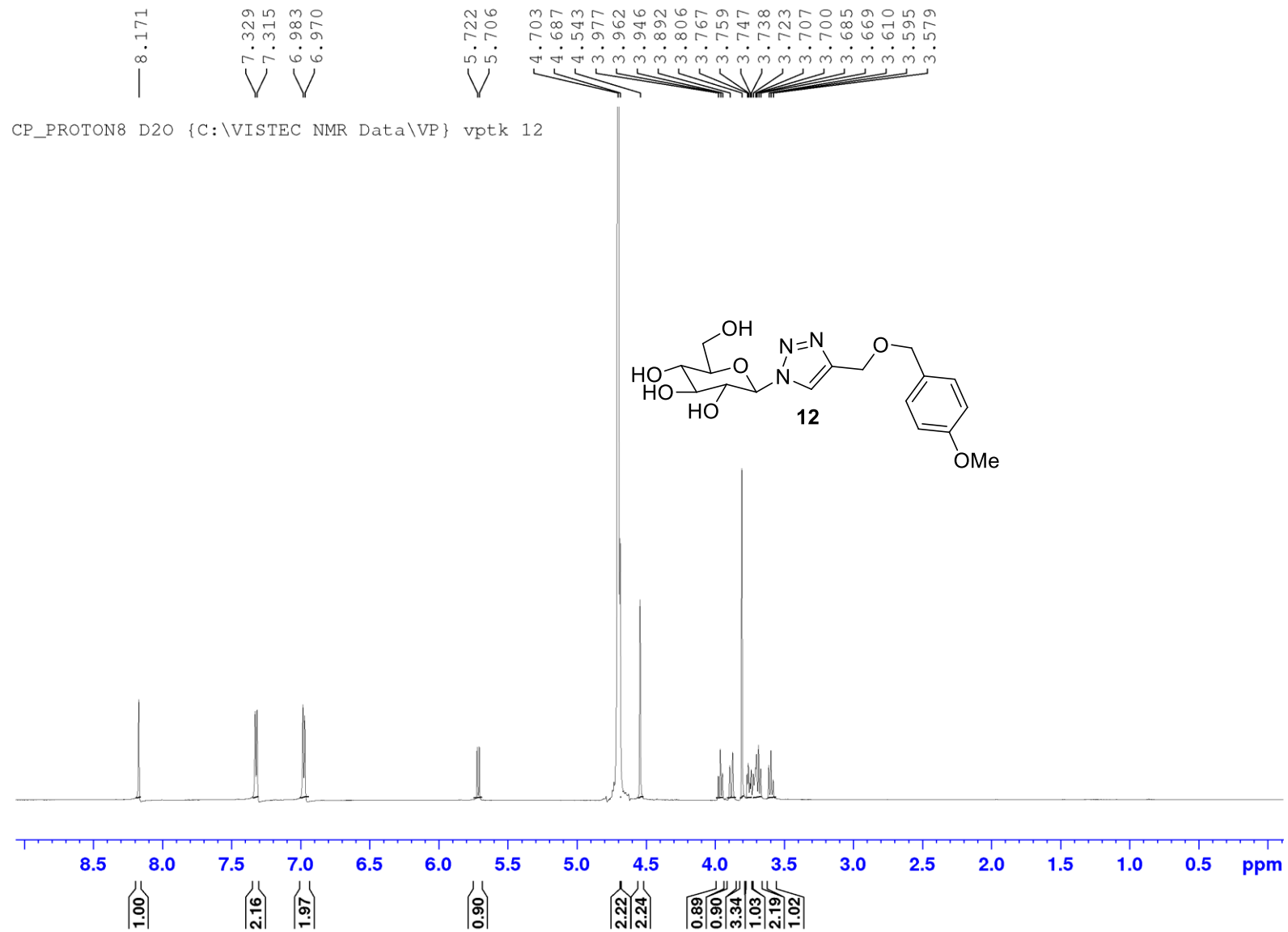


CP_PROTON8 D2O {C:\VISTEC NMR Data\VP} vptk 16

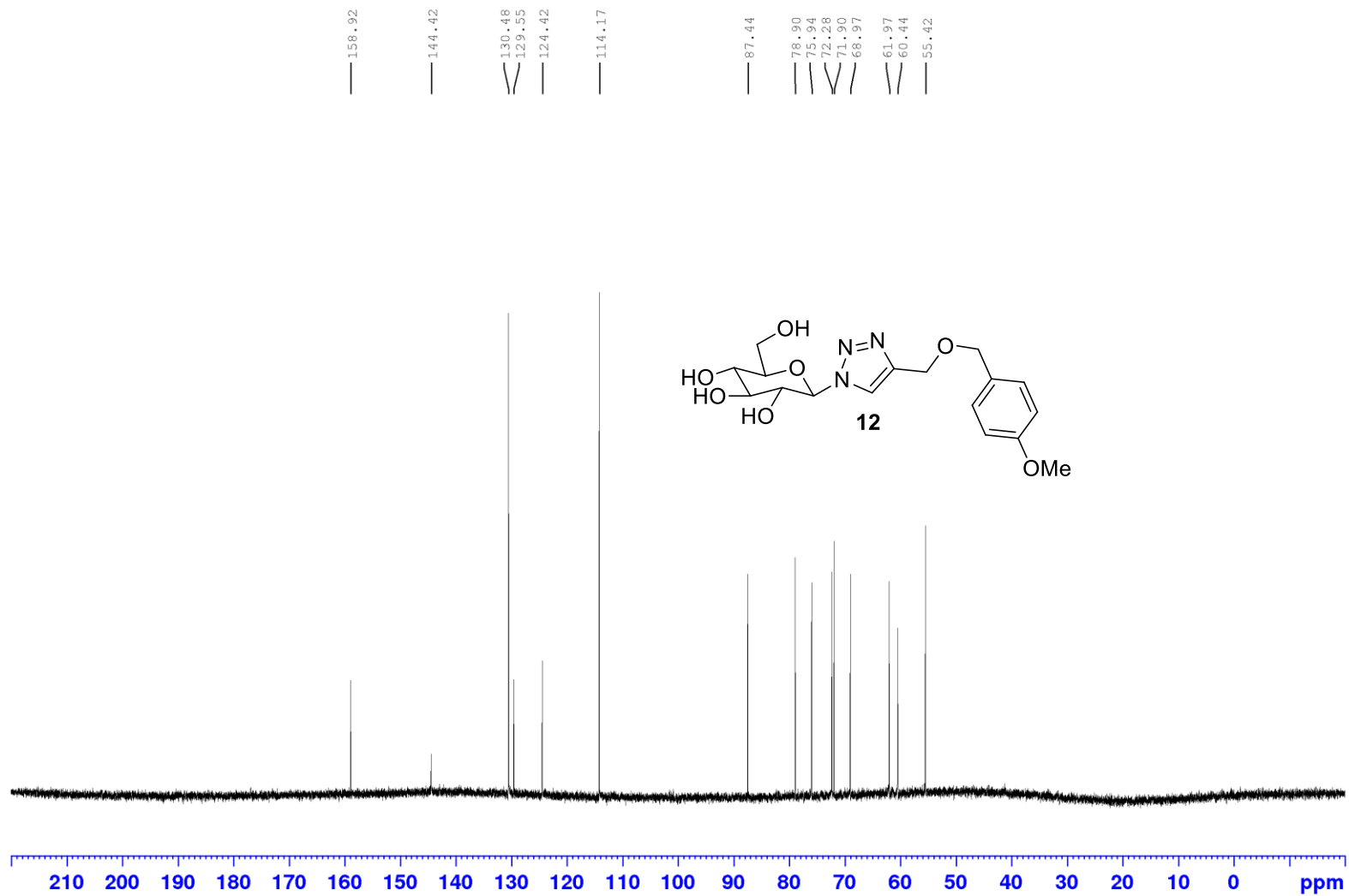


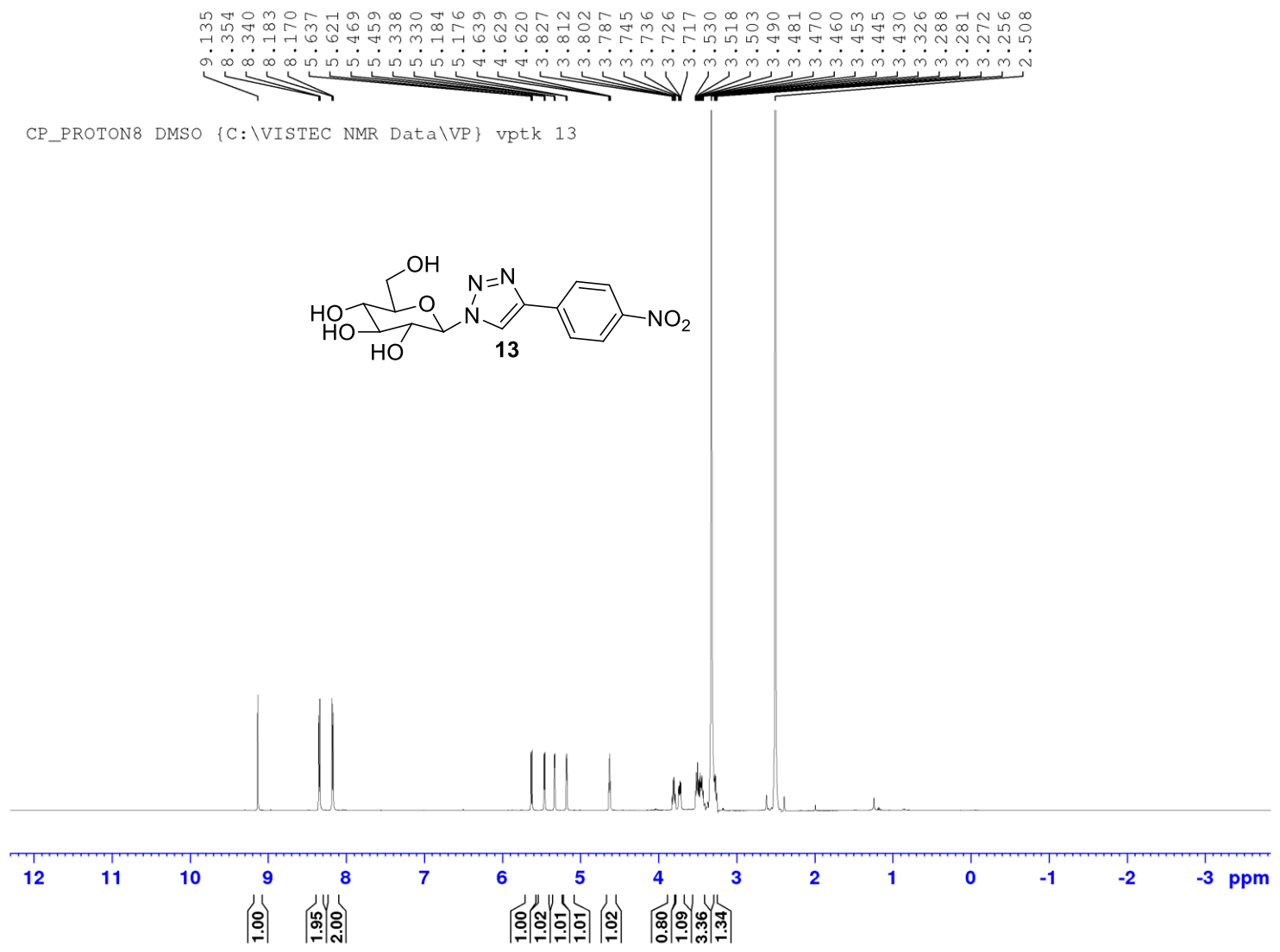
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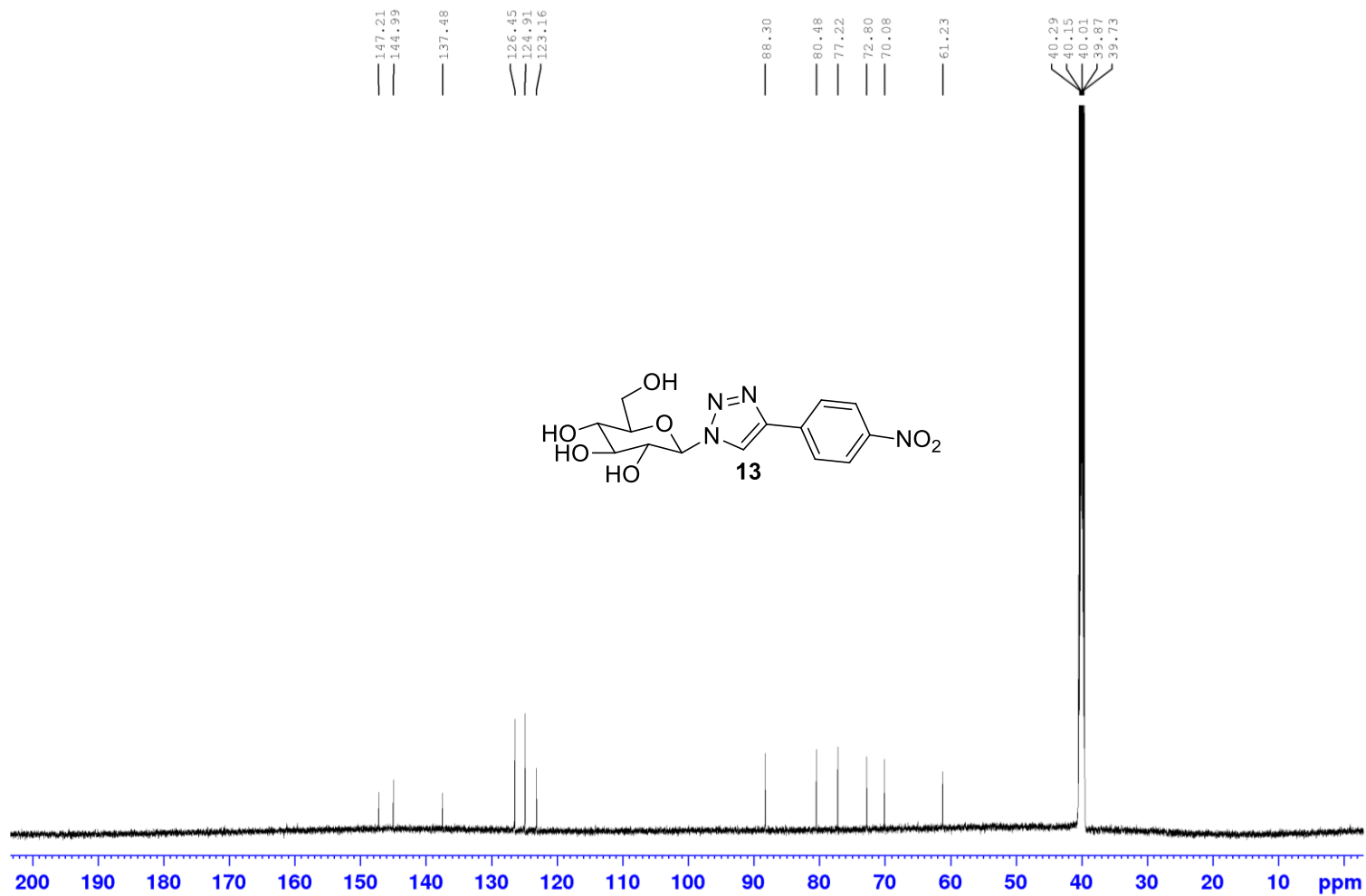


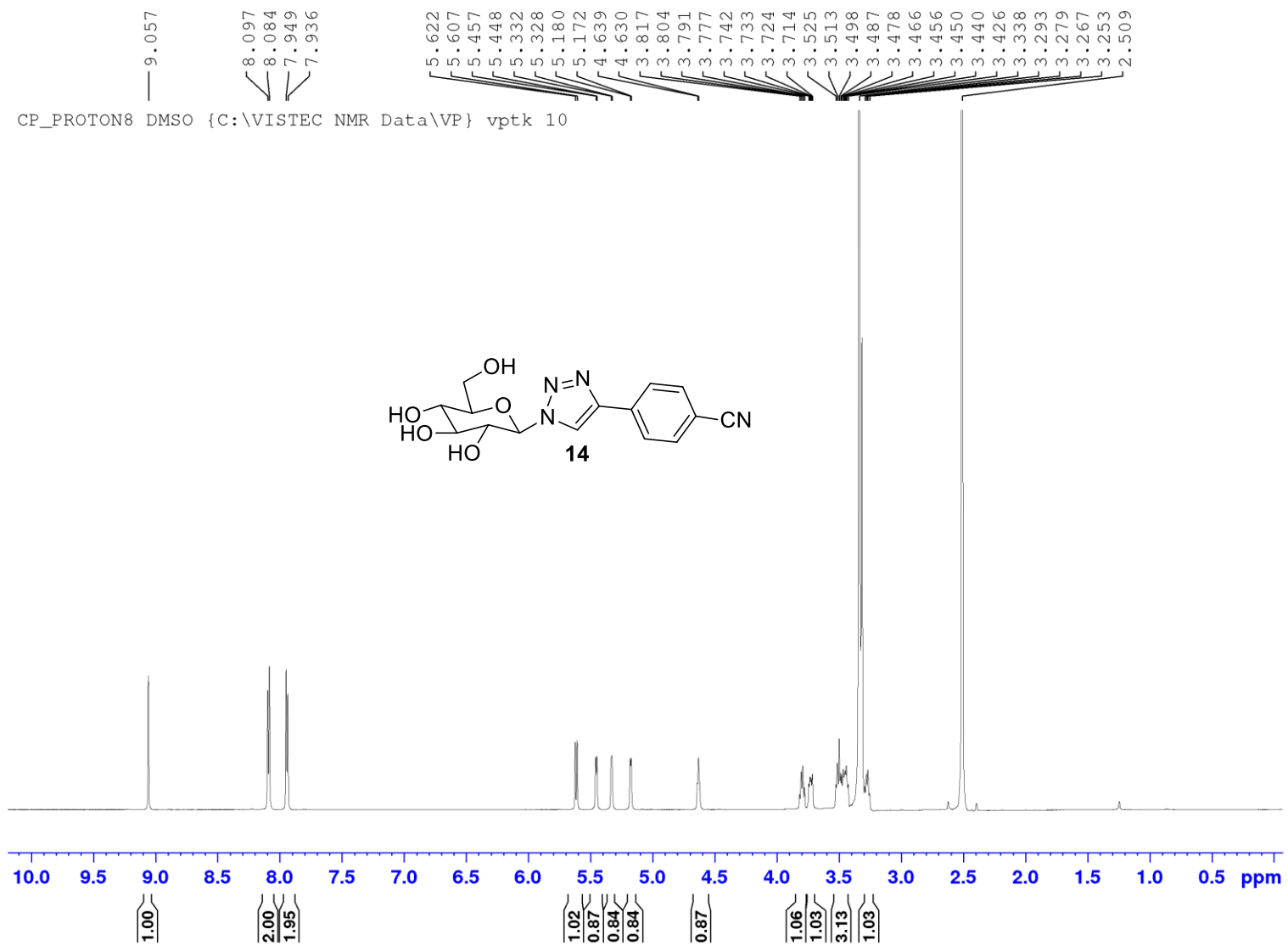
CP_C13CPD32_DE12 D2O {C:\VISTEC NMR Data\VP} vptk 9



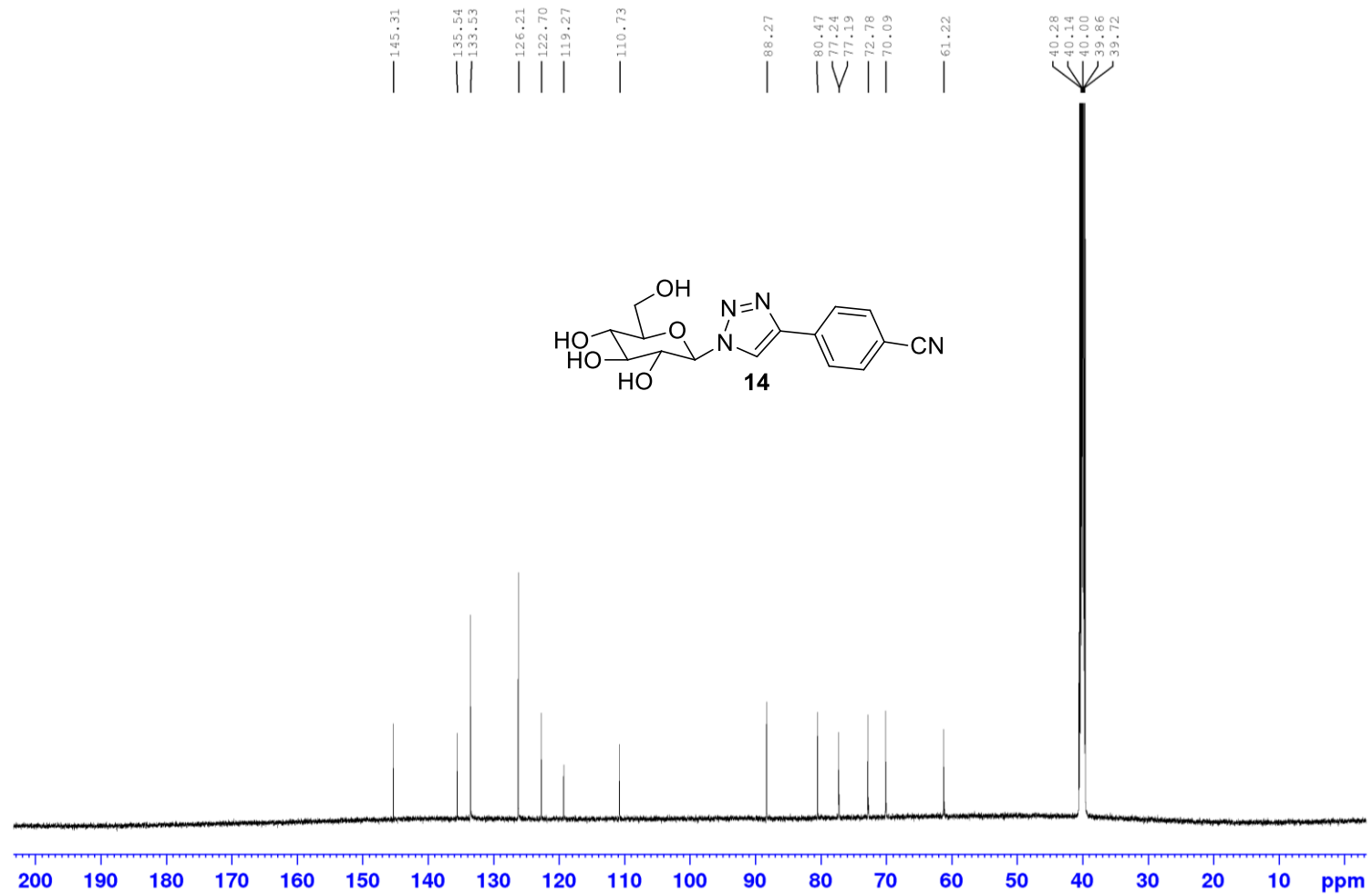


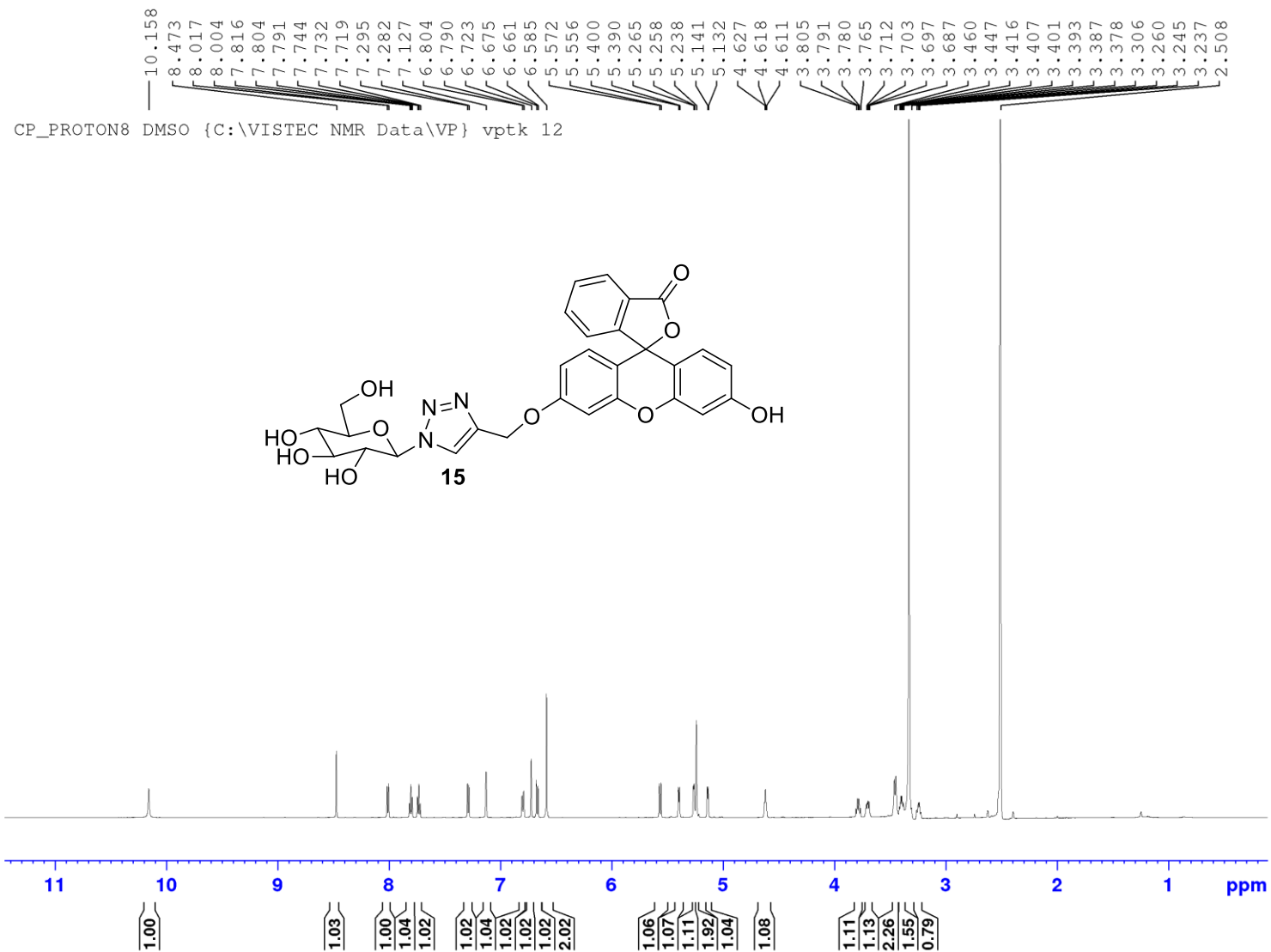
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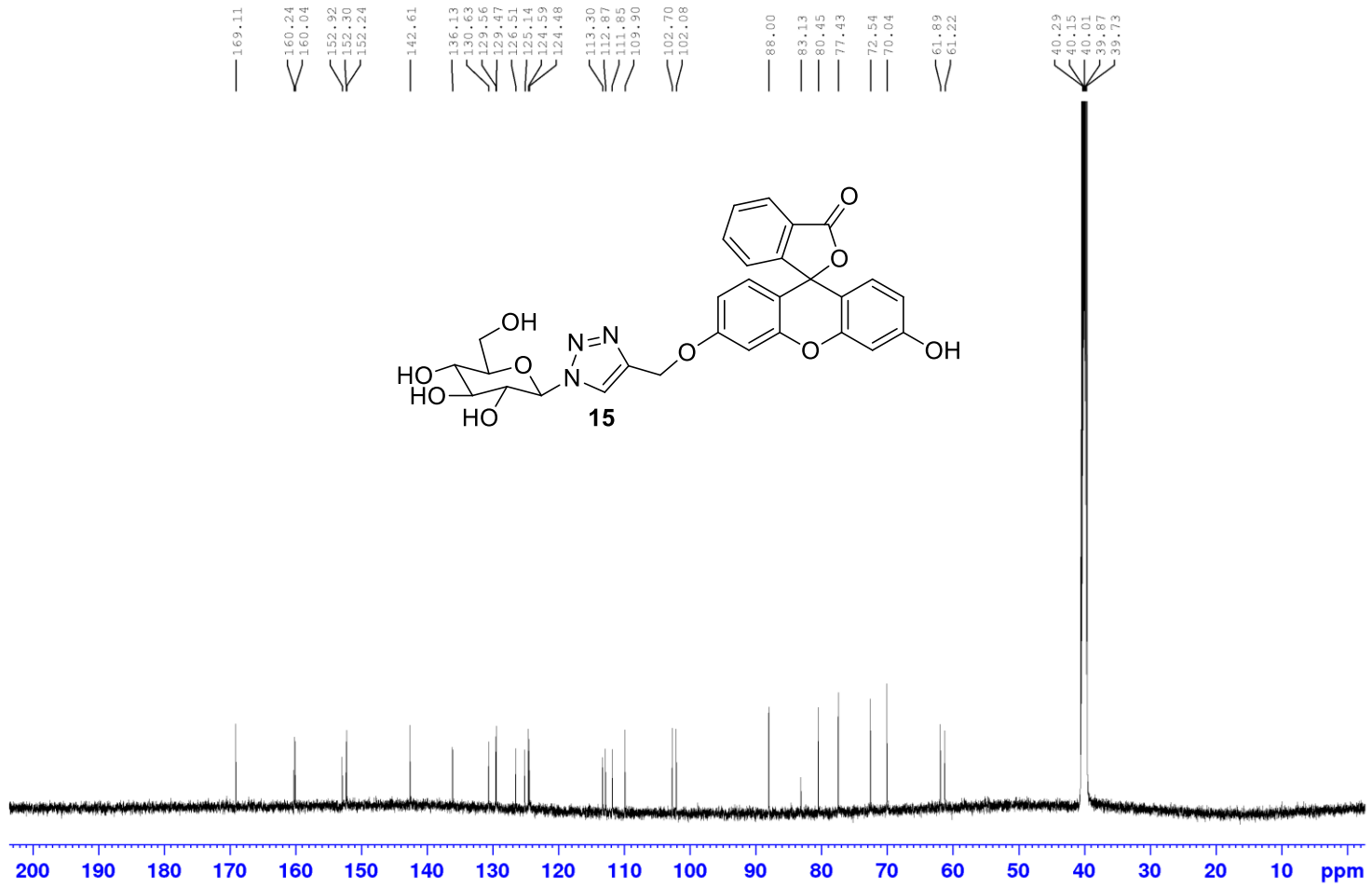


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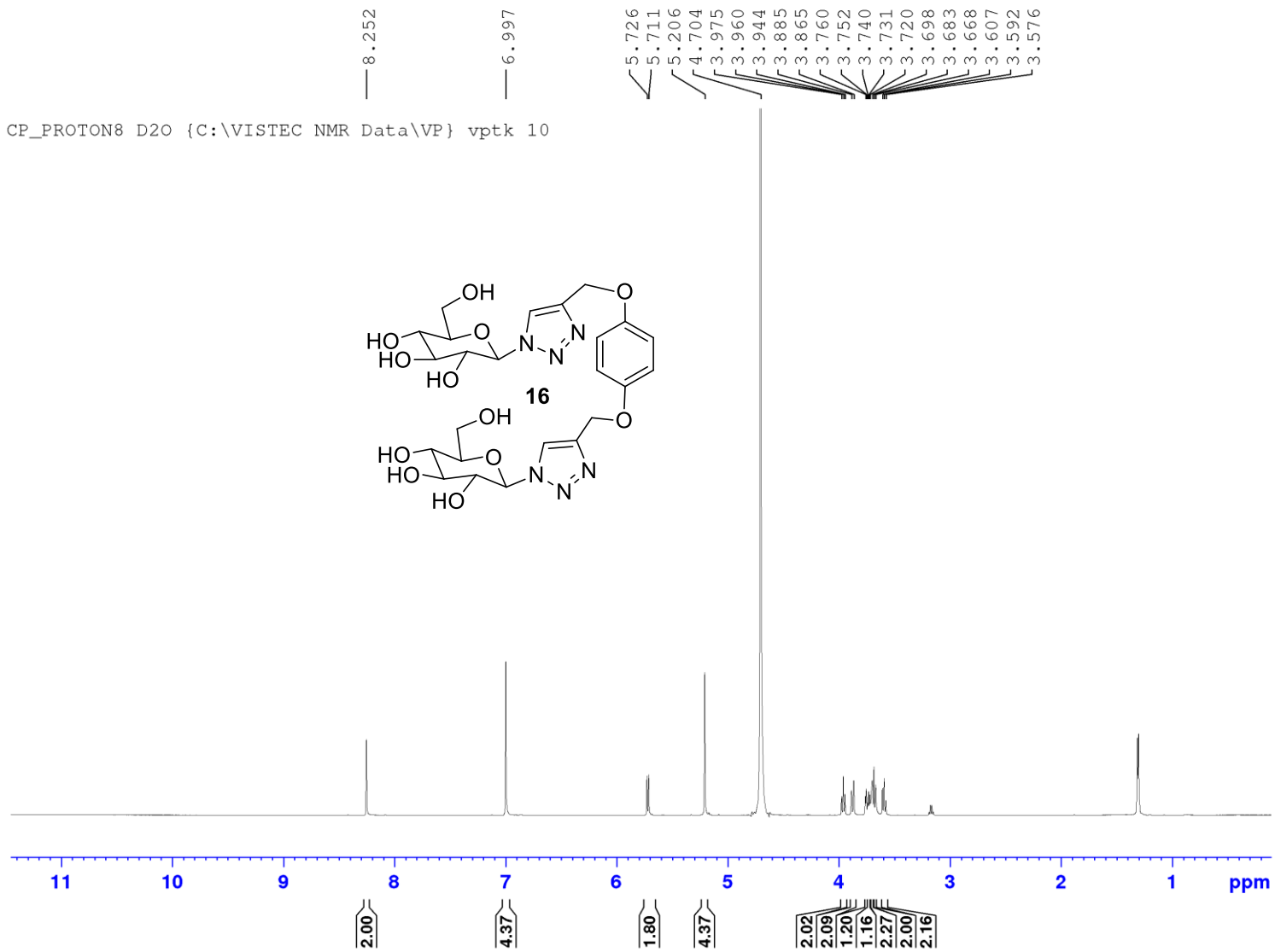




CP_C13CPD32_DE12 DMSO {C:\VISTEC NMR Data\VP} vptk 3

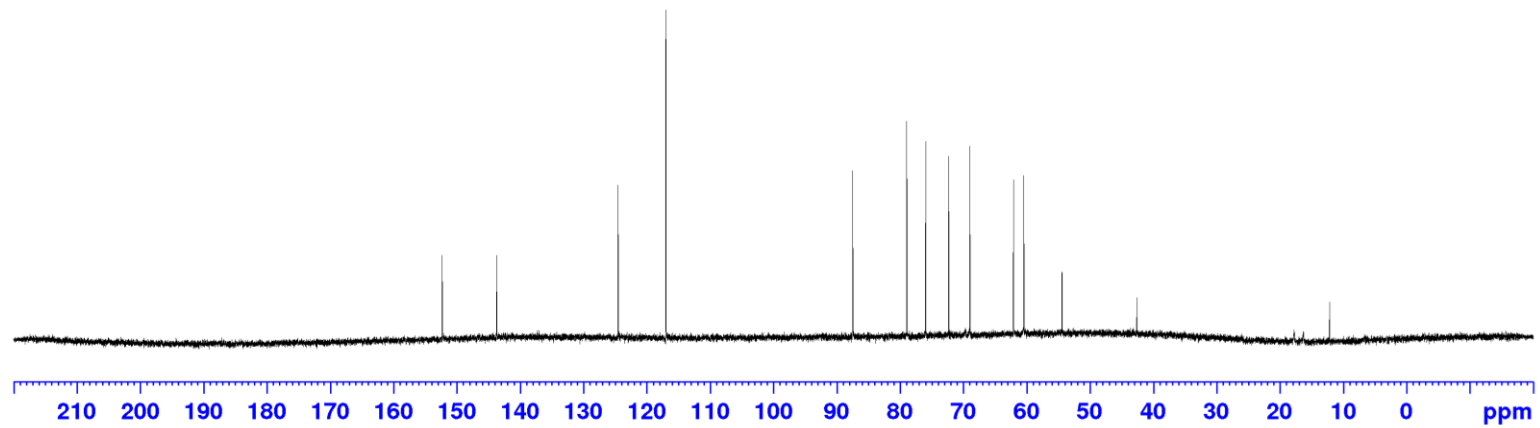
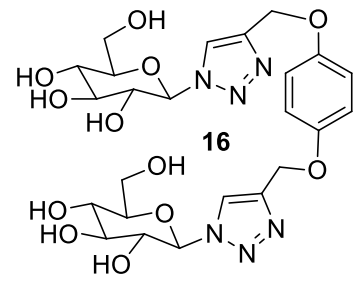


CP_PROTON8 D2O {C:\VISTEC NMR Data\VP} vptk 10



CP_C13CPD32_DE12 D2O {C:\VISTEC NMR Data\VP} vptk 2

152.31
143.72
124.52
116.98
87.48
78.91
75.93
72.29
68.97
62.06
60.43
54.40
42.57



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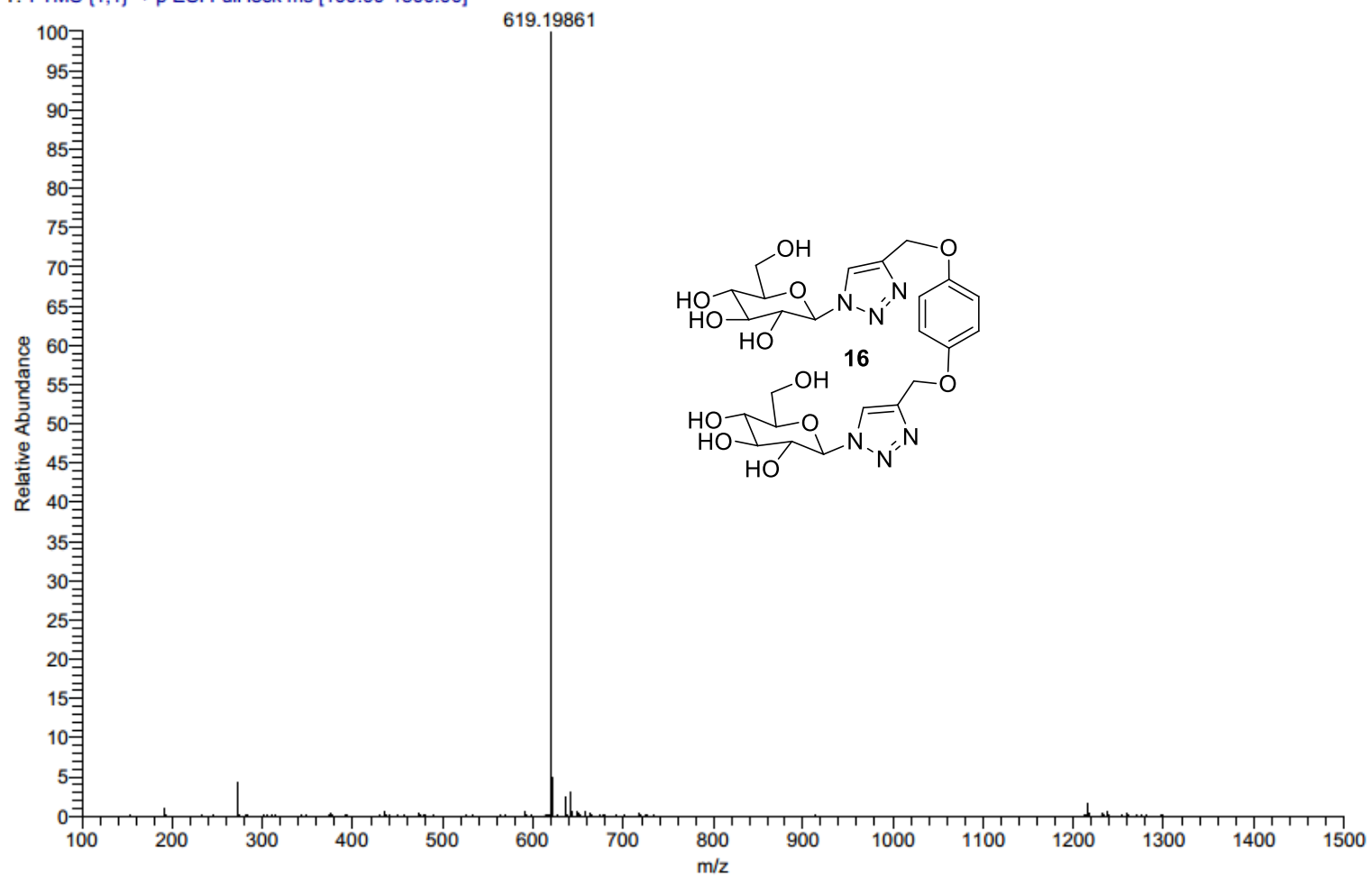


Figure S6. HR-ESI-MS Spectrum of Compound 16