

**Synthesis and in vitro characterization of trehalose-based inhibitors of
mycobacterial trehalose 6-phosphate phosphatases**

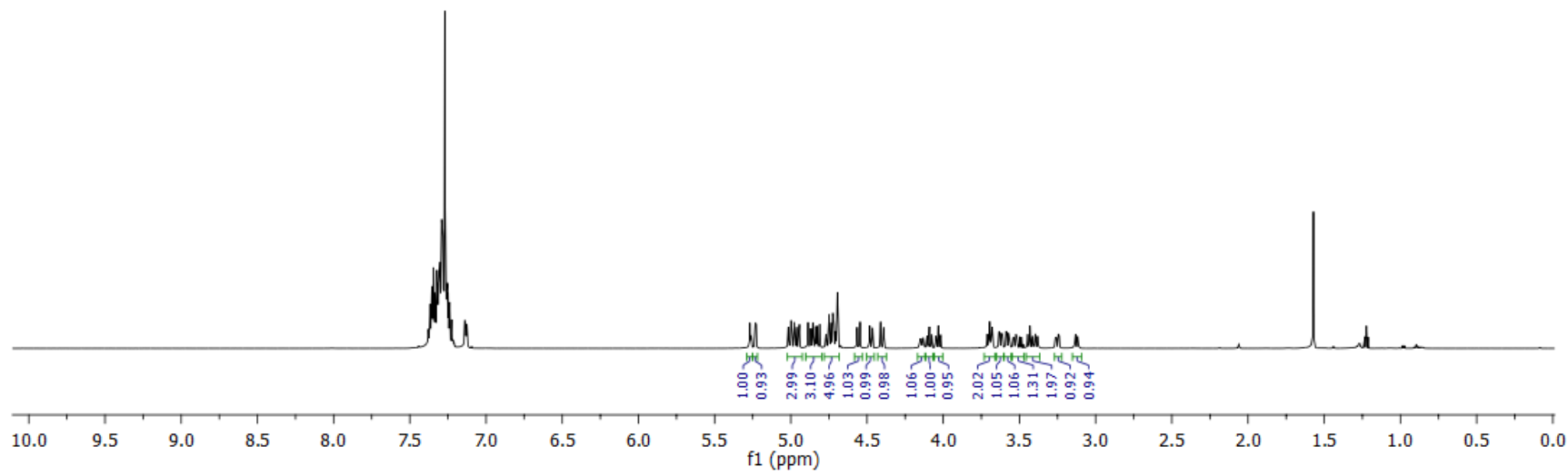
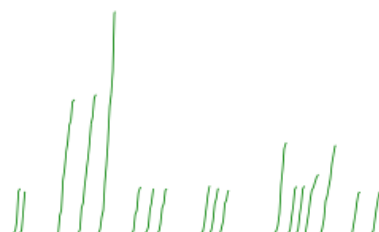
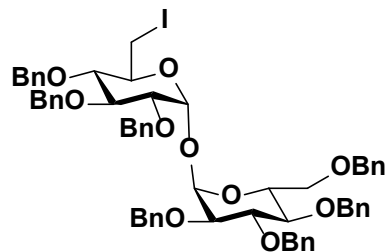
**Sunayana Kapil[‡], Cecile Petit[‡], Victoria N. Drago, Donald R. Ronning* and Steven
J. Sucheck*^[a]**

Contents:

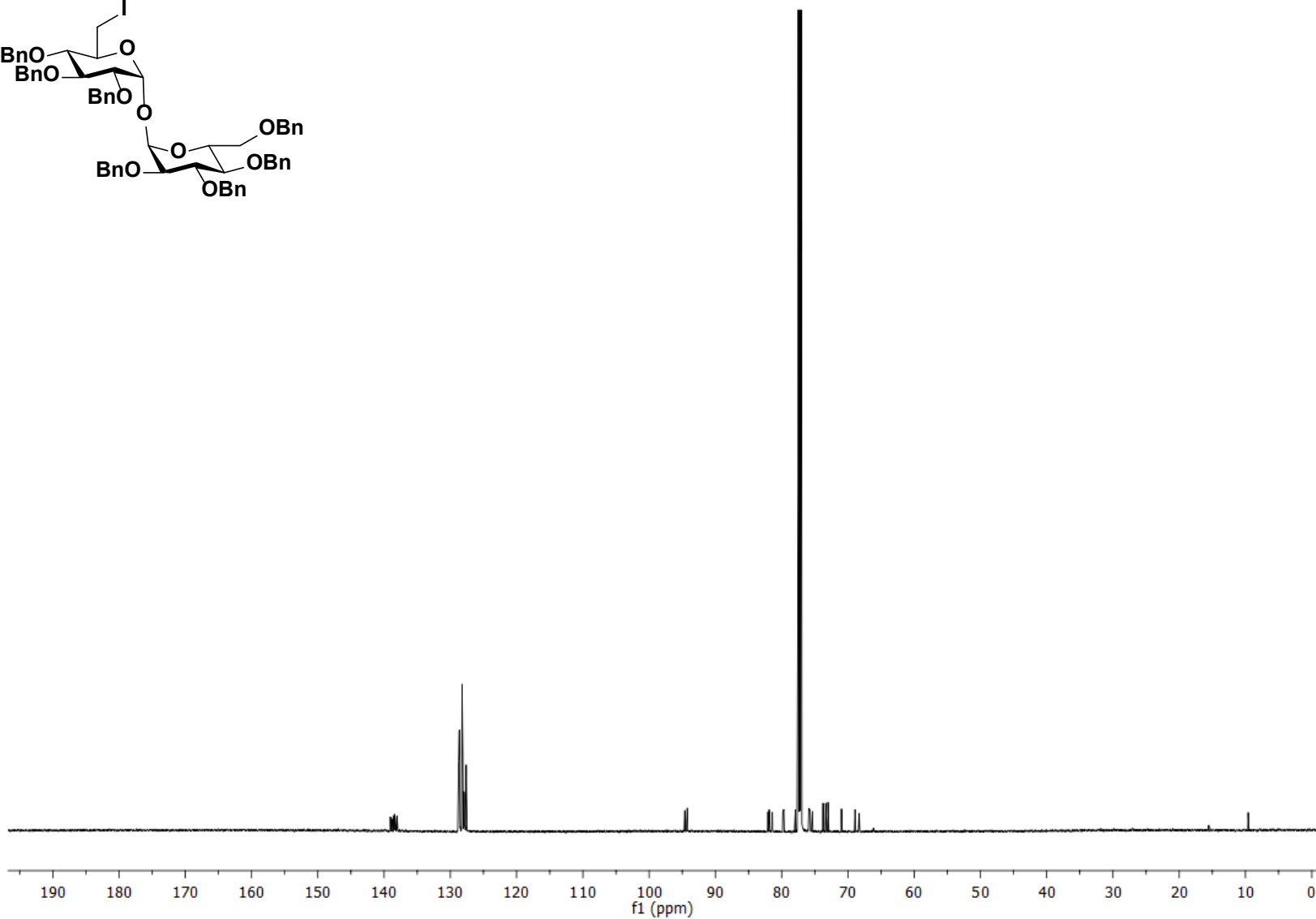
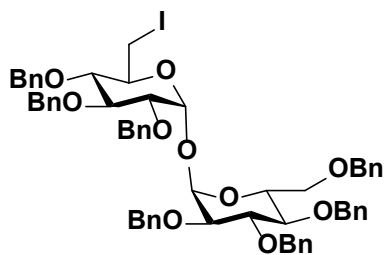
- S4 ¹H NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-iodo-6-deoxy- α -D-glucopyranosyl-(1 \rightarrow 1)- α -D-glucopyranoside (9)
- S5 ¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-iodo-6-deoxy- α -D-glucopyranosyl-(1 \rightarrow 1)- α -D-glucopyranoside (9)
- S6 ¹H NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-deoxy-6-phosphonate- α -D-glucopyranosyl-(1 \rightarrow 1)- α -D-glucopyranoside (10)
- S7 ¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-deoxy-6-phosphonate- α -D-glucopyranosyl-(1 \rightarrow 1)- α -D-glucopyranoside (10)
- S8 ³¹P NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-deoxy-6-phosphonate- α -D-glucopyranosyl-(1 \rightarrow 1)- α -D-glucopyranoside (10)
- S9 ¹H NMR 6-(phosphonic acid)-6-deoxy- α,α' -trehalose (4)
- S10 ¹³C NMR 6-(phosphonic acid)-6-deoxy- α,α' -trehalose (4)
- S11 ³¹P NMR 6-(phosphonic acid)-6-deoxy- α,α' -trehalose (4)
- S12 ¹H NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-carbaldehyde- α -D-glucopyranosyl-(1 \rightarrow 1)- α -D-glucopyranoside (12)
- S13 ¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-carbaldehyde- α -D-glucopyranosyl-(1 \rightarrow 1)- α -D-glucopyranoside (12)
- S14 ¹H NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-deoxy-6E-(dimethyl vinylphosphonate)- α,α' -trehalose (13)
- S15 ¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-deoxy-6E-(dimethyl vinylphosphonate)- α,α' -trehalose (13)
- S16 ³¹P NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-deoxy-6E-(dimethyl vinylphosphonate)- α,α' -trehalose (13)
- S17 ¹H NMR 6-(Methylenephosphonic acid)- α,α' -trehalose (5)
- S18 ¹³C NMR 6-(Methylenephosphonic acid)- α,α' -trehalose (5)
- S19 ³¹P NMR 6-(Methylenephosphonic acid)- α,α' -trehalose (5)
- S20 ¹H NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-Deoxy-6-azido- α,α' -trehalose (15)
- S21 ¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-Deoxy-6-azido- α,α' -trehalose (15)
- S22 ¹H NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-Deoxy-6-amino- α,α' -trehalose (16)
- S23 ¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-Deoxy-6-amino- α,α' -trehalose (16)
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- S26 ³¹P 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-Deoxy-6-dibenzylphosphoramidate)- α,α' -trehalose (17)
- S27 ¹H NMR 6-(phosphoramidic acid)- α,α' -trehalose (6)
- S28 ¹³C NMR 6-(phosphoramidic acid)- α,α' -trehalose (6)
- S29 ³¹P NMR 6-(phosphoramidic acid)- α,α' -trehalose (6)
- S30 ¹H NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-deoxy-6-ethynyl- α,α' -trehalose (18)

- S31 ¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-deoxy-6-ethynyl- α,α' -trehalose (18)
- S32 ¹H NMR 2,2',3,3',4,4',6'-Hepta-O-acetyl-6-Deoxy-6-vinyl- α,α' -trehalose (19)
- S33 ¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-acetyl-6-Deoxy-6-vinyl- α,α' -trehalose (19)
- S34 ¹H NMR 2,2',3,3',4,4',6'-Hepta-O-acetyl-6-Deoxy-6-oxiranyl- α,α' -trehalose (20)
- S35 ¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-acetyl-6-Deoxy-6-oxiranyl- α,α' -trehalose (20)
- S36 ¹H NMR 6-Deoxy-6-oxiranyl- α,α' -trehalose (7)
- S37 ¹³C NMR 6-Deoxy-6-oxiranyl- α,α' -trehalose (7)

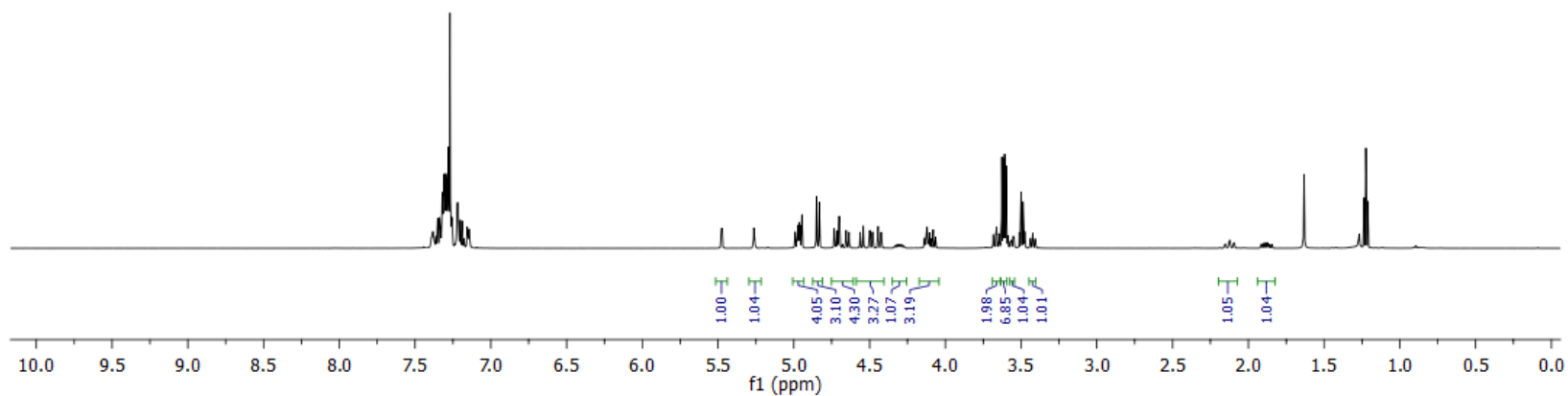
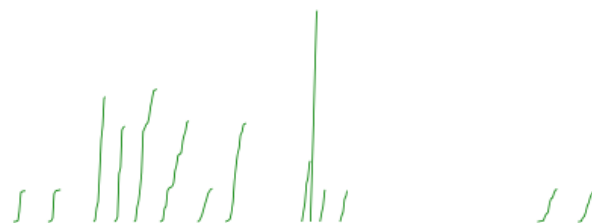
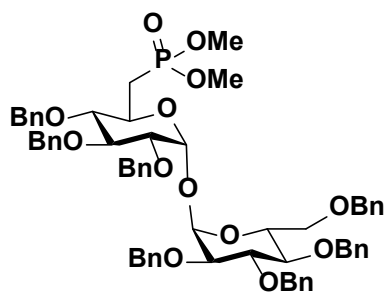
¹H NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-iodo-6-deoxy- α -D-glucopyranosyl-(1 \rightarrow 1)- α -D-glucopyranoside (9)



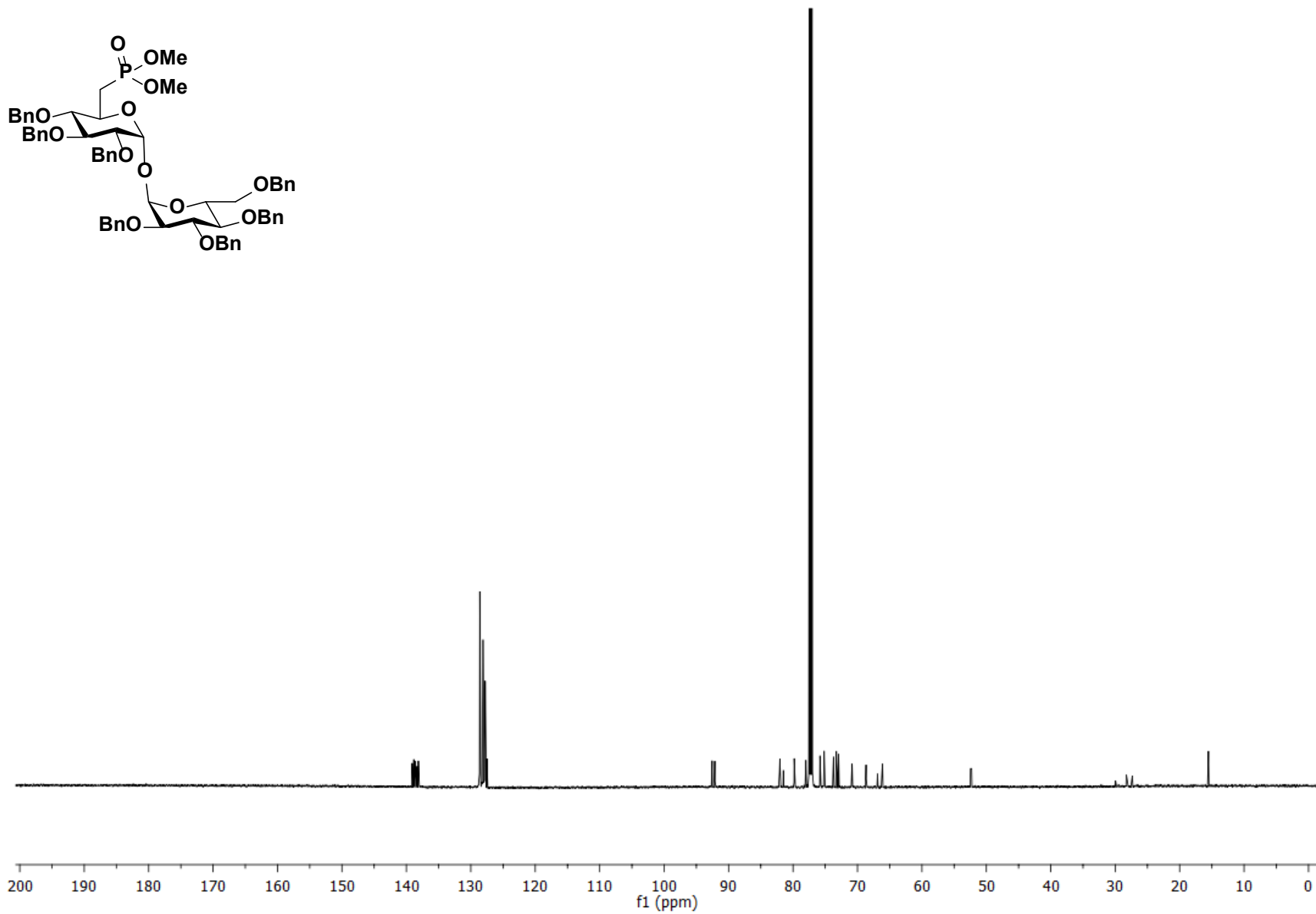
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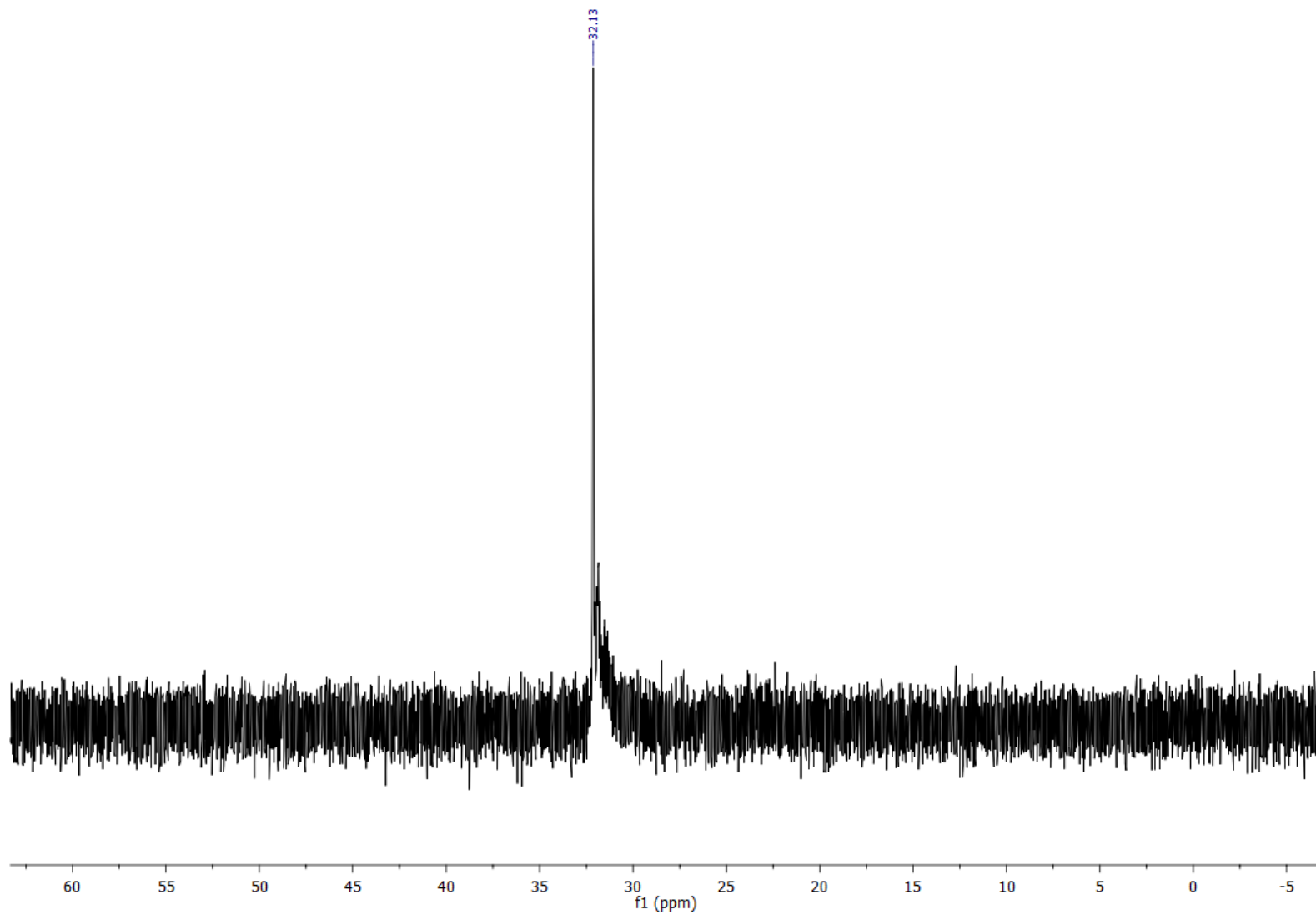
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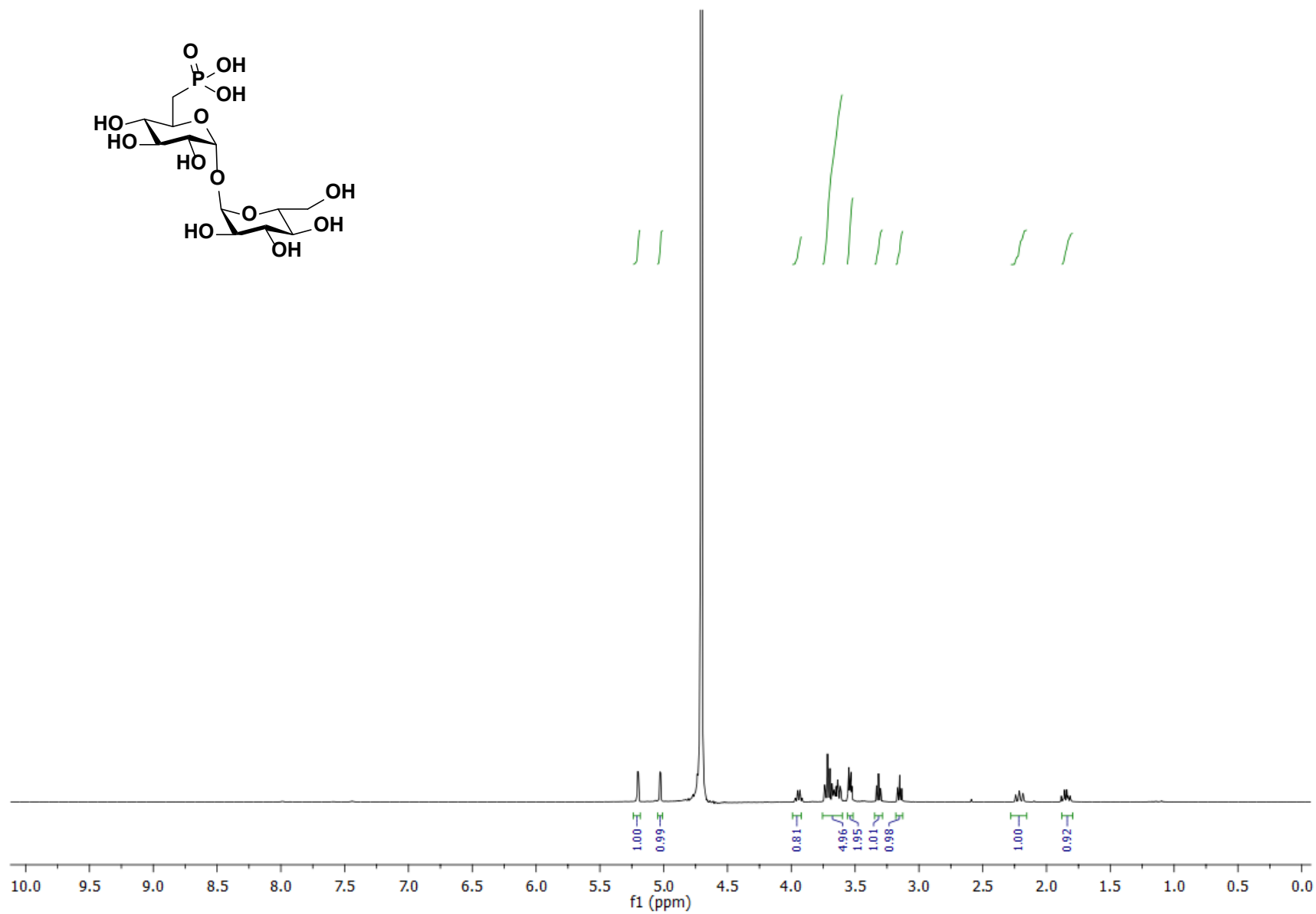
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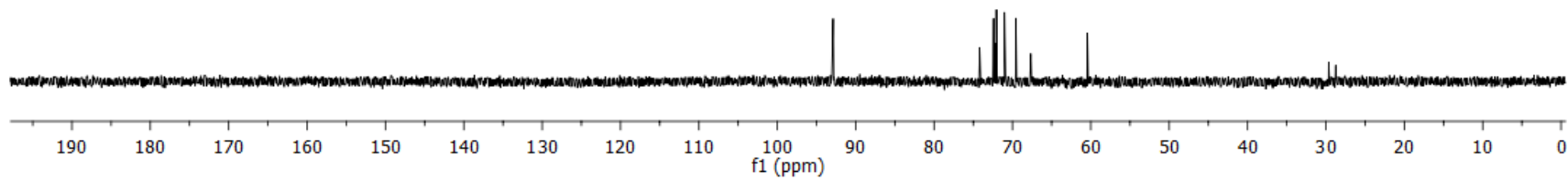
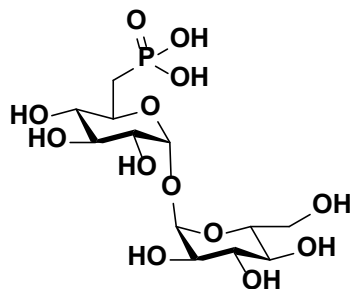
^{31}P NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-deoxy-6-phosphonate- α -D-glucopyranosyl-(1 \rightarrow 1)- α -D-glucopyranoside (10)



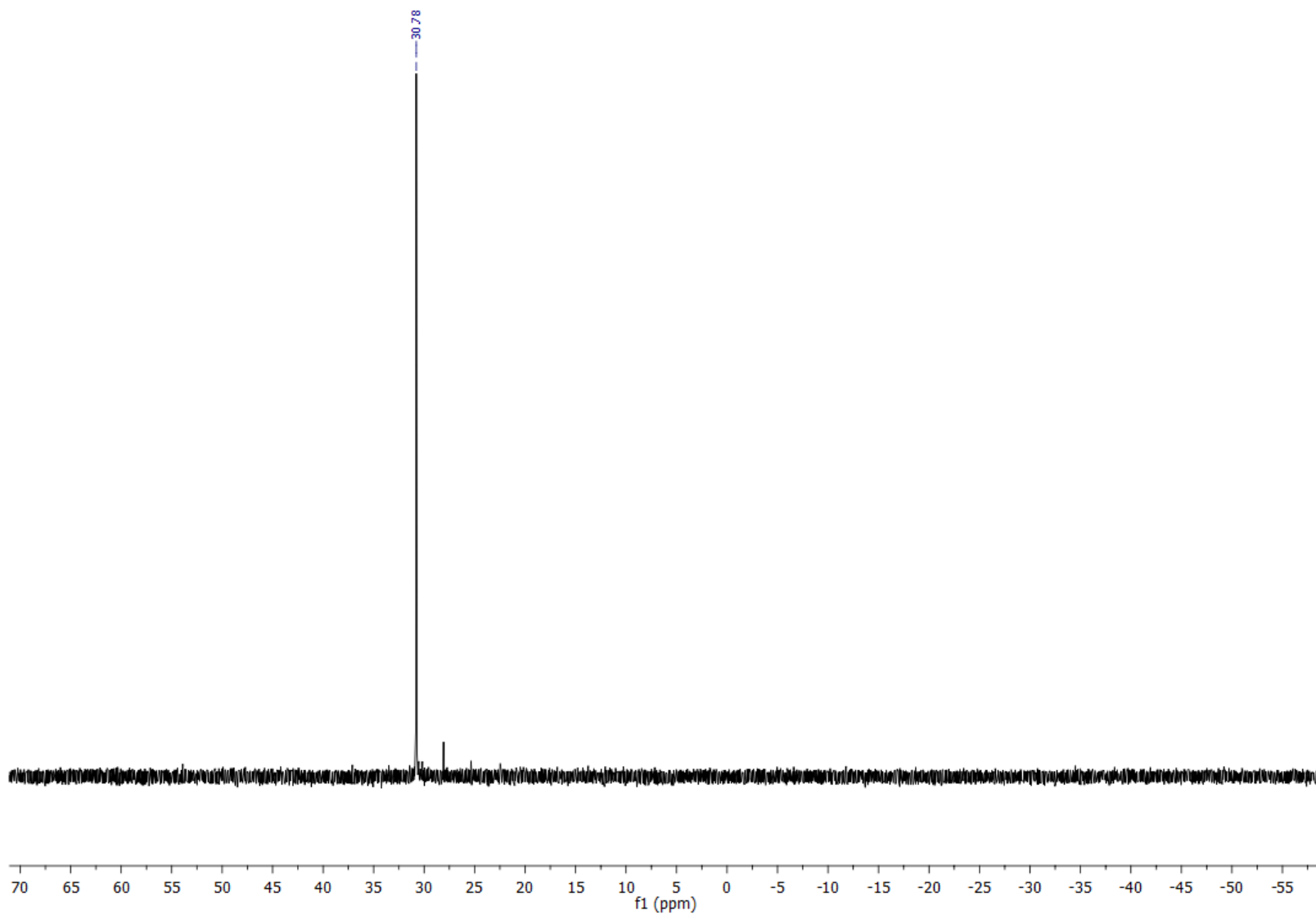
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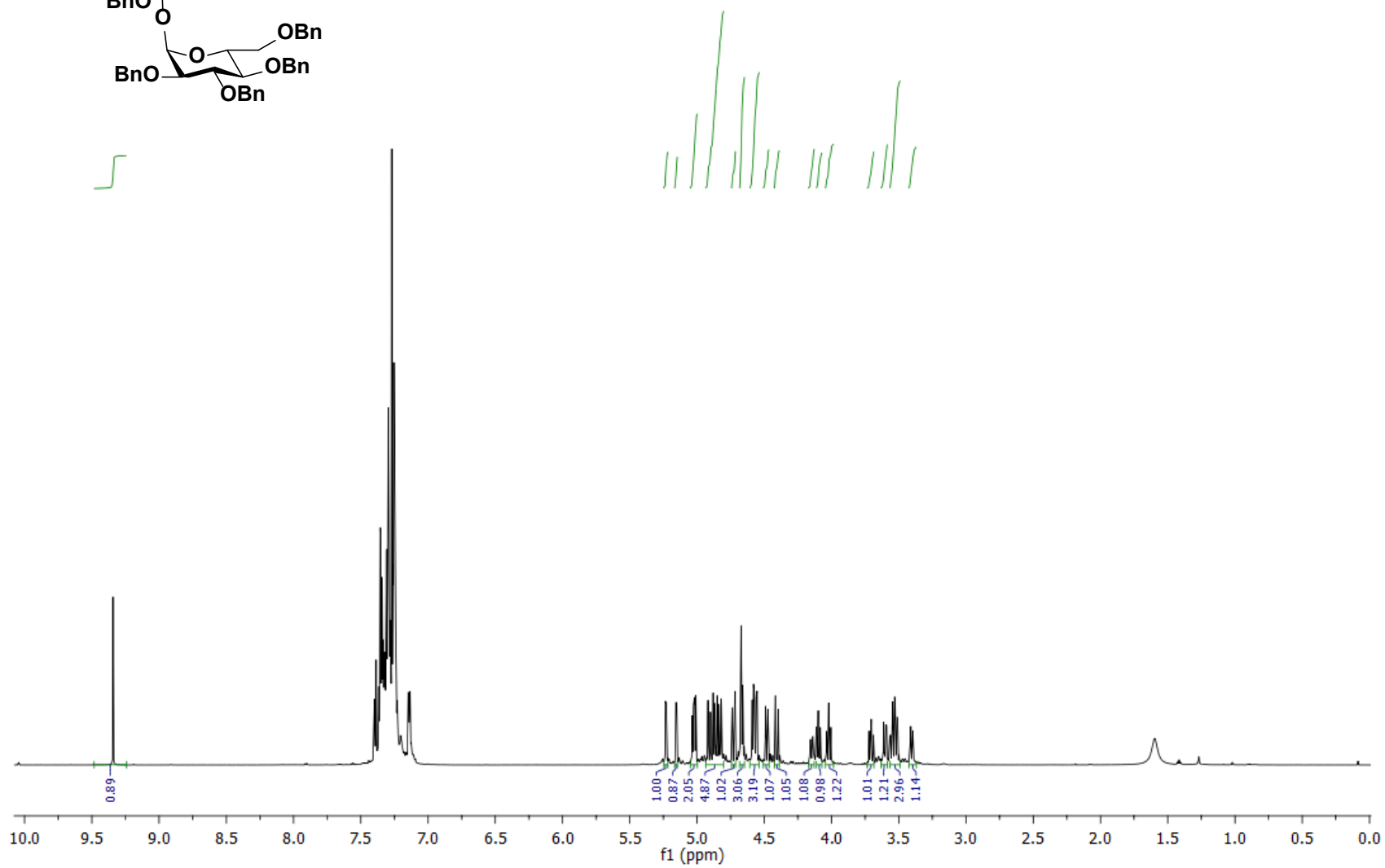
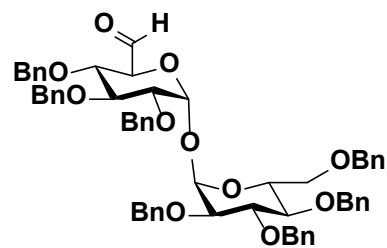
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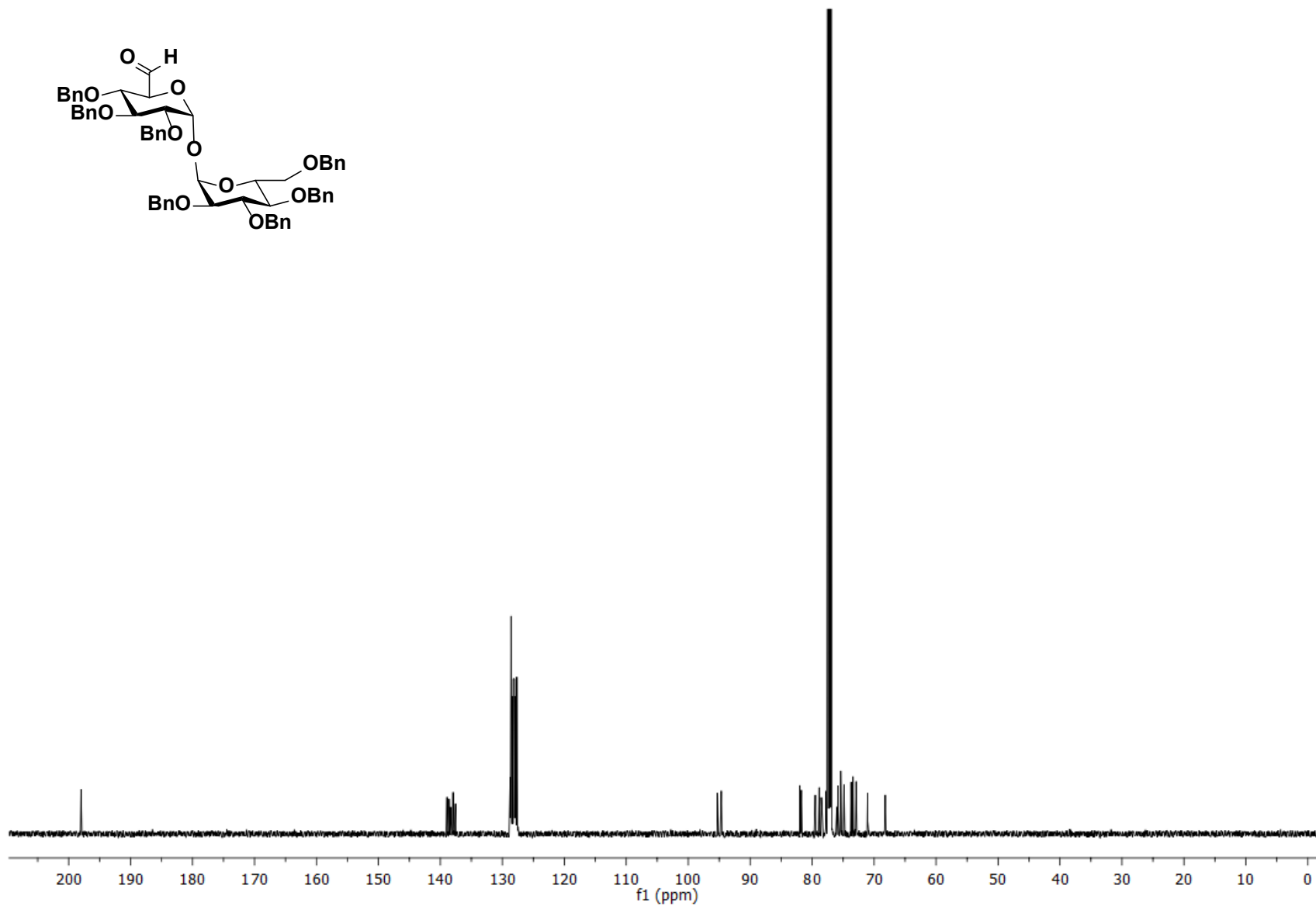
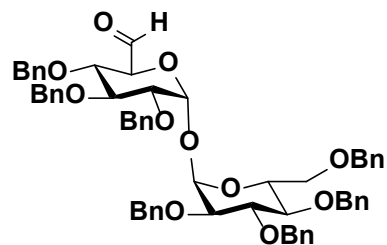
^{31}P NMR NMR 6-(phosphonic acid)-6-deoxy- α,α' -trehalose (4)



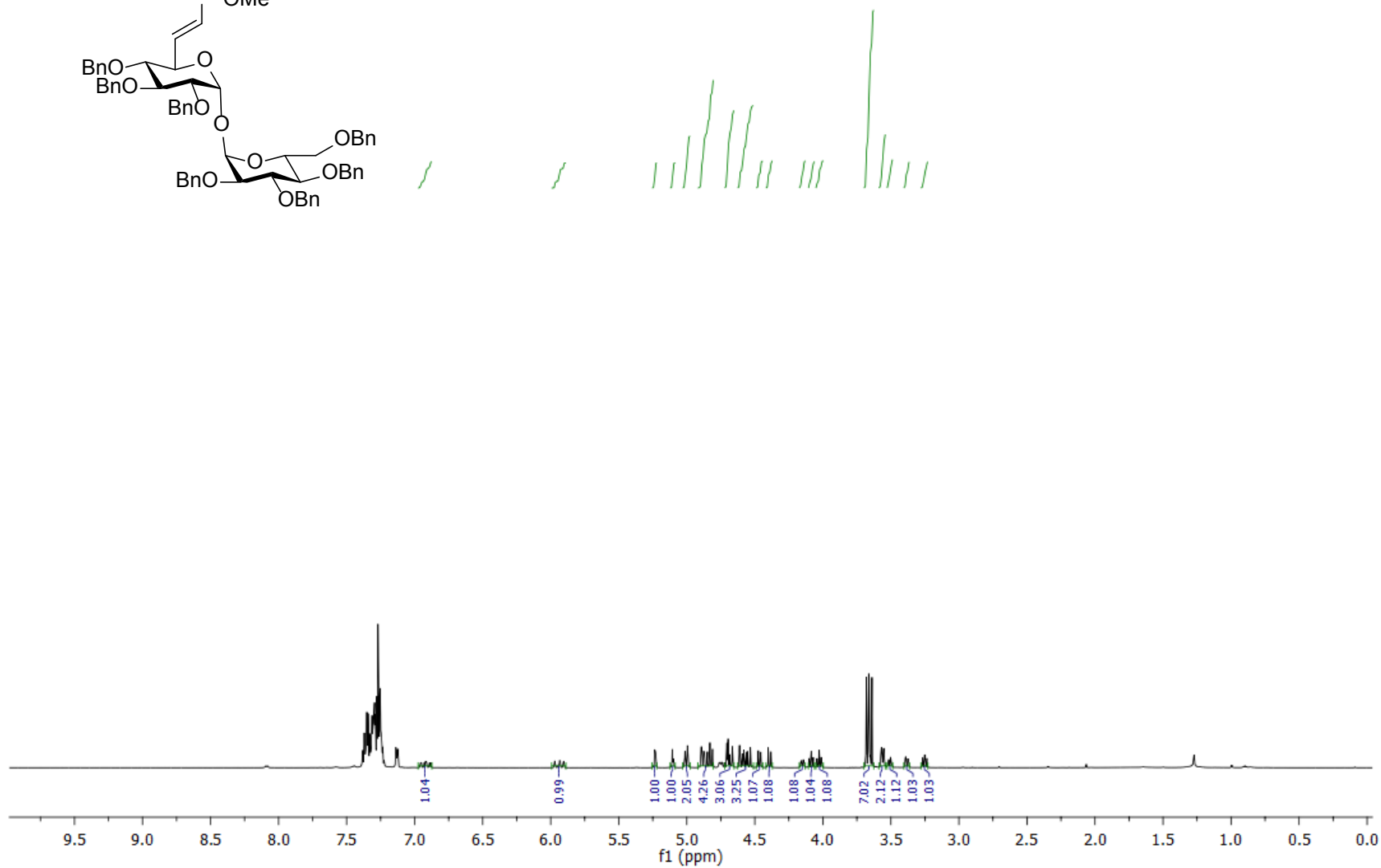
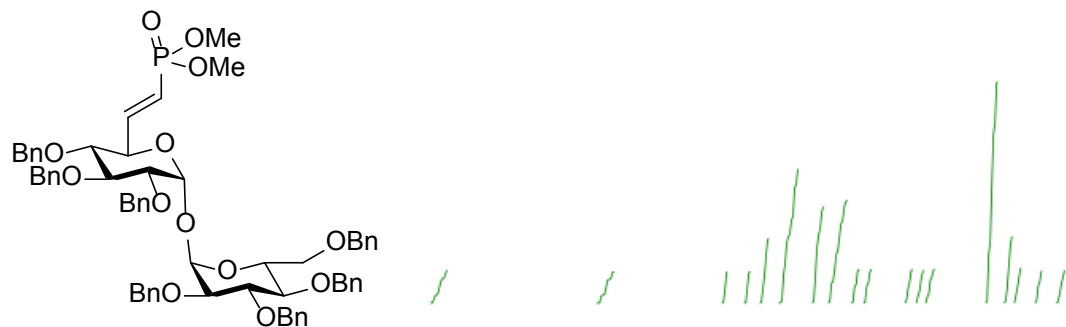
¹H NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-carbaldehyde- α -D-glucopyranosyl-(1 \rightarrow 1)- α -D-glucopyranoside (12)



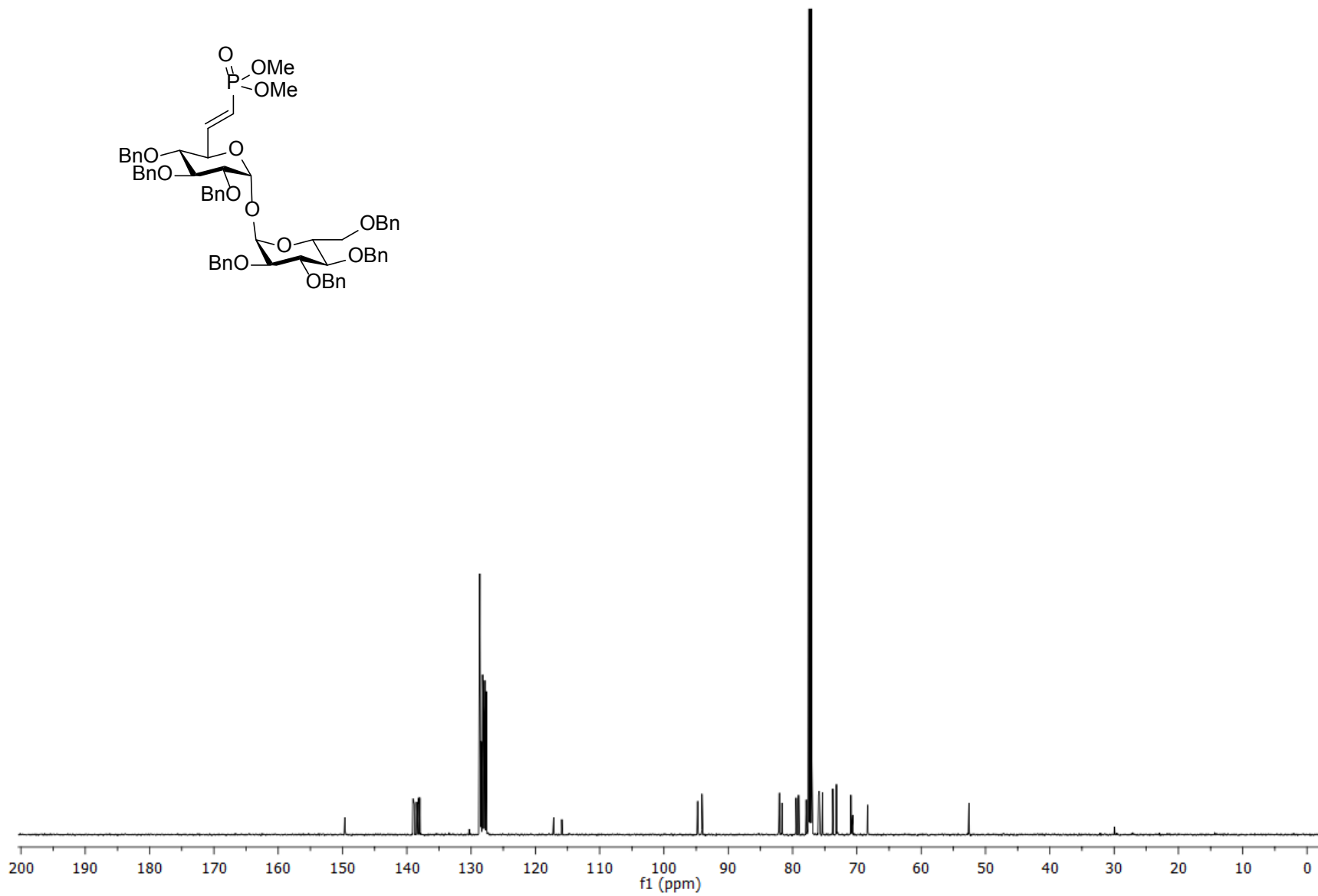
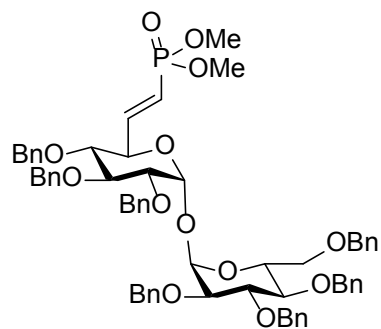
¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-carbaldehyde-α-D-glucopyranosyl-(1→1)-α-D-glucopyranoside (12)



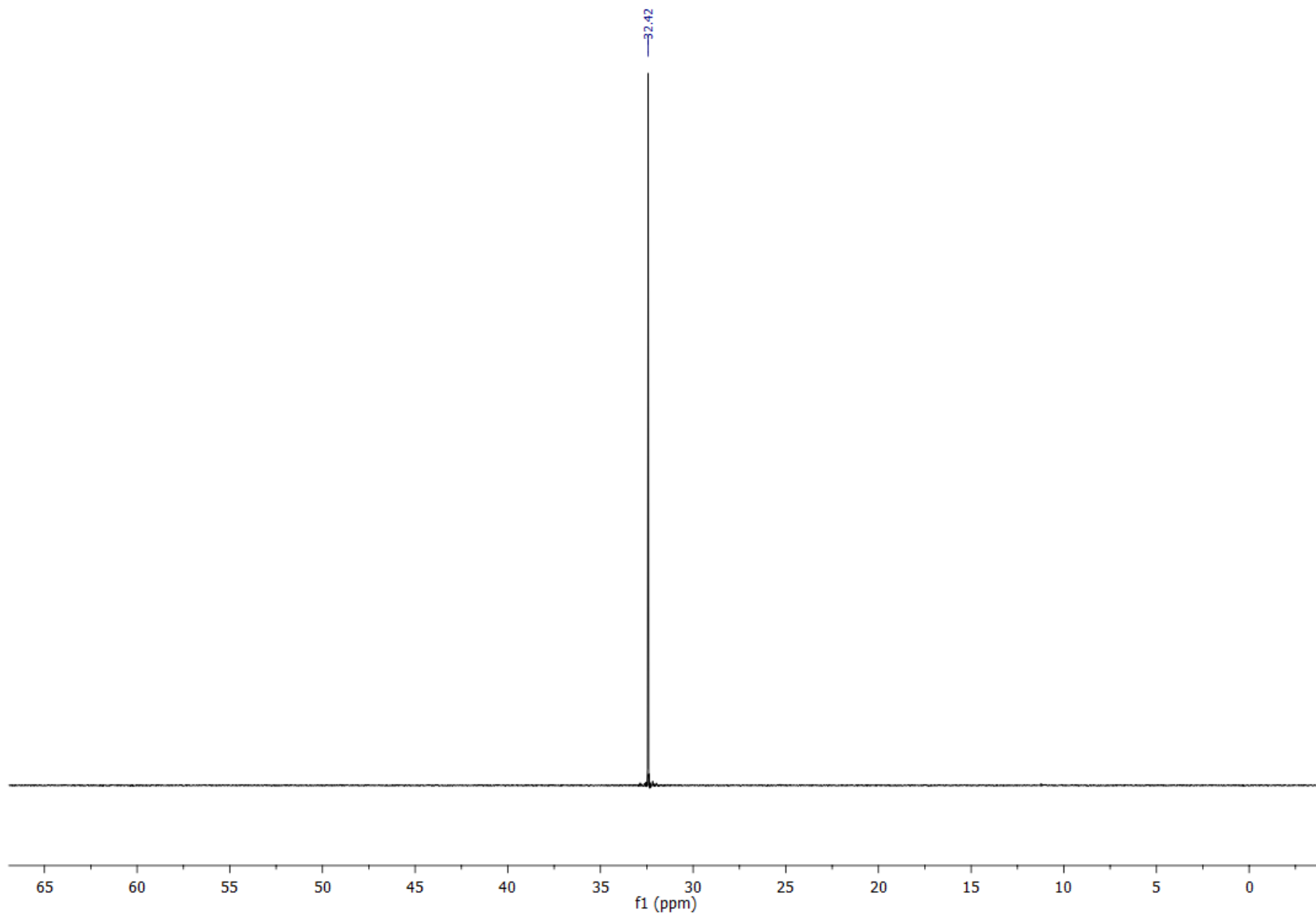
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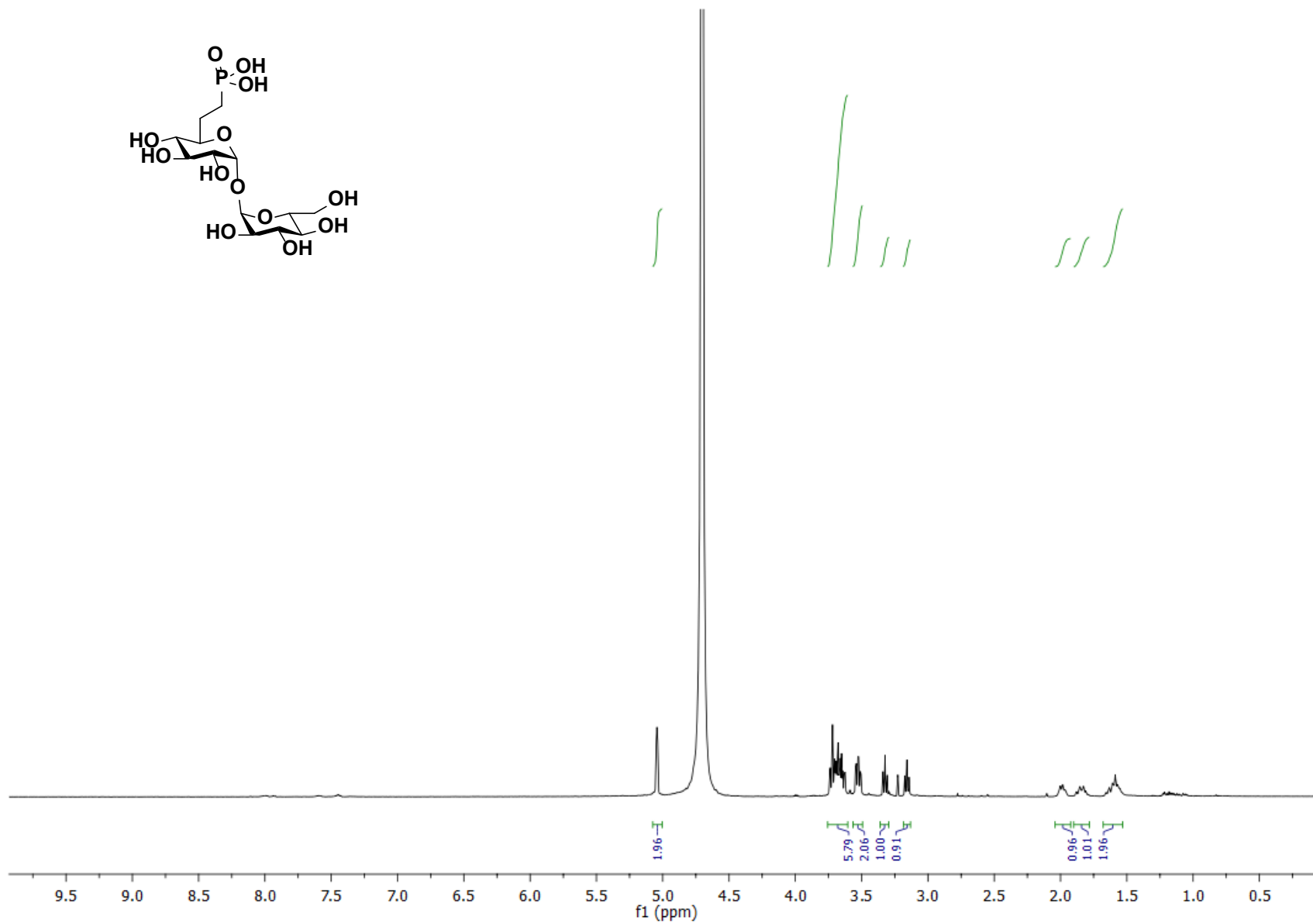
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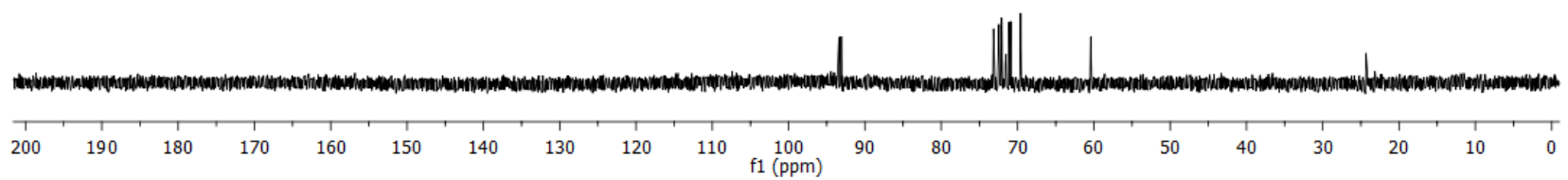
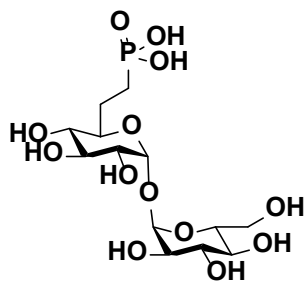
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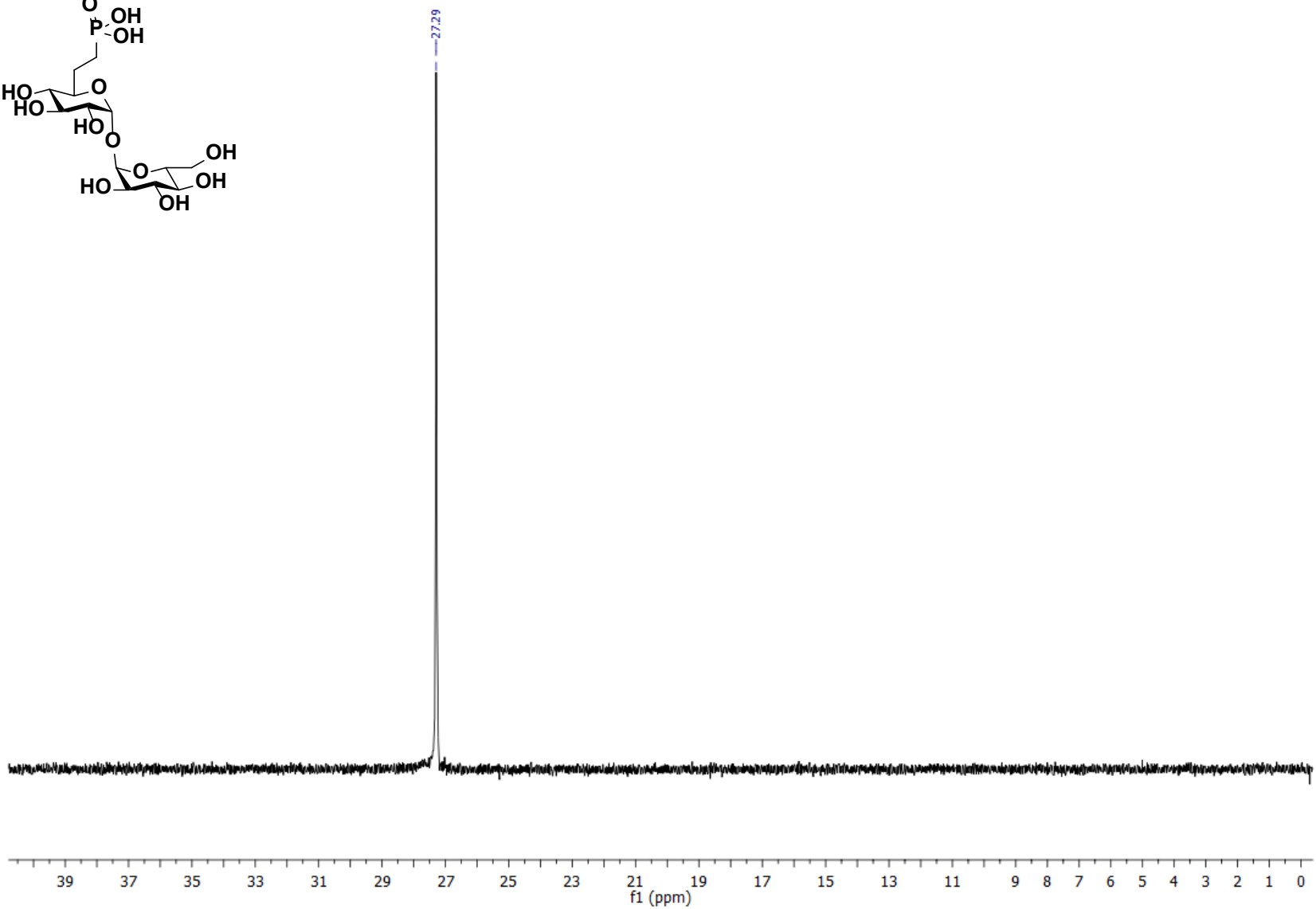
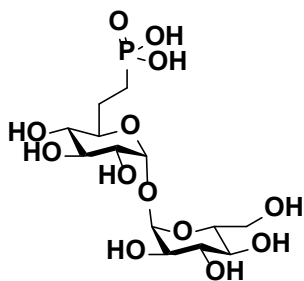
¹H NMR 6-(Methylenephosphonic acid)- α,α' -trehalose (5)



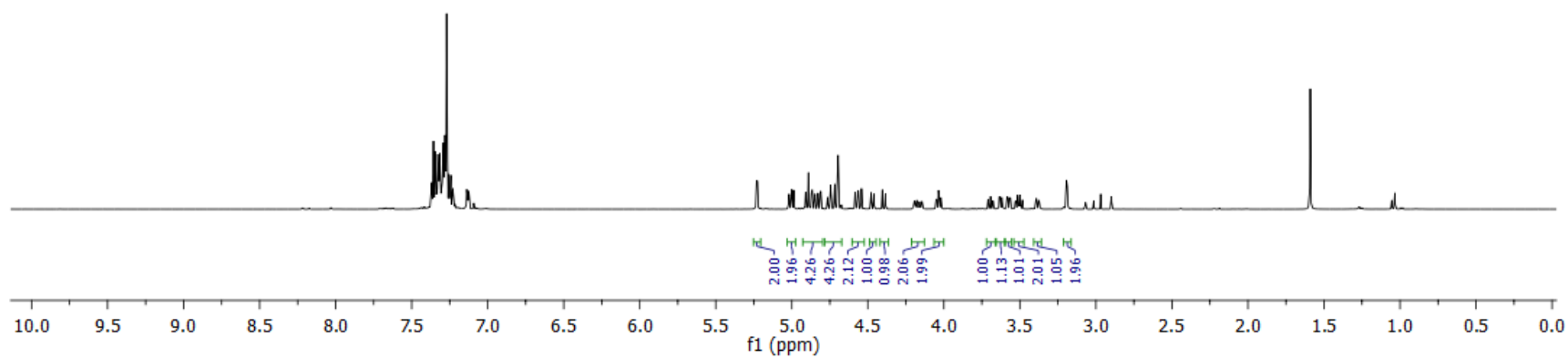
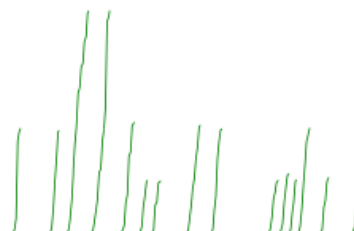
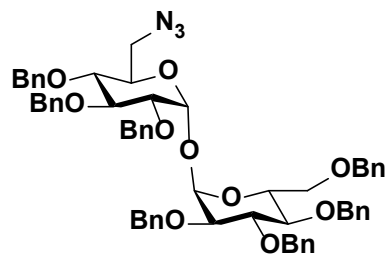
^{13}C NMR 6-(Methylenephosphonic acid)- α,α' -trehalose (5)



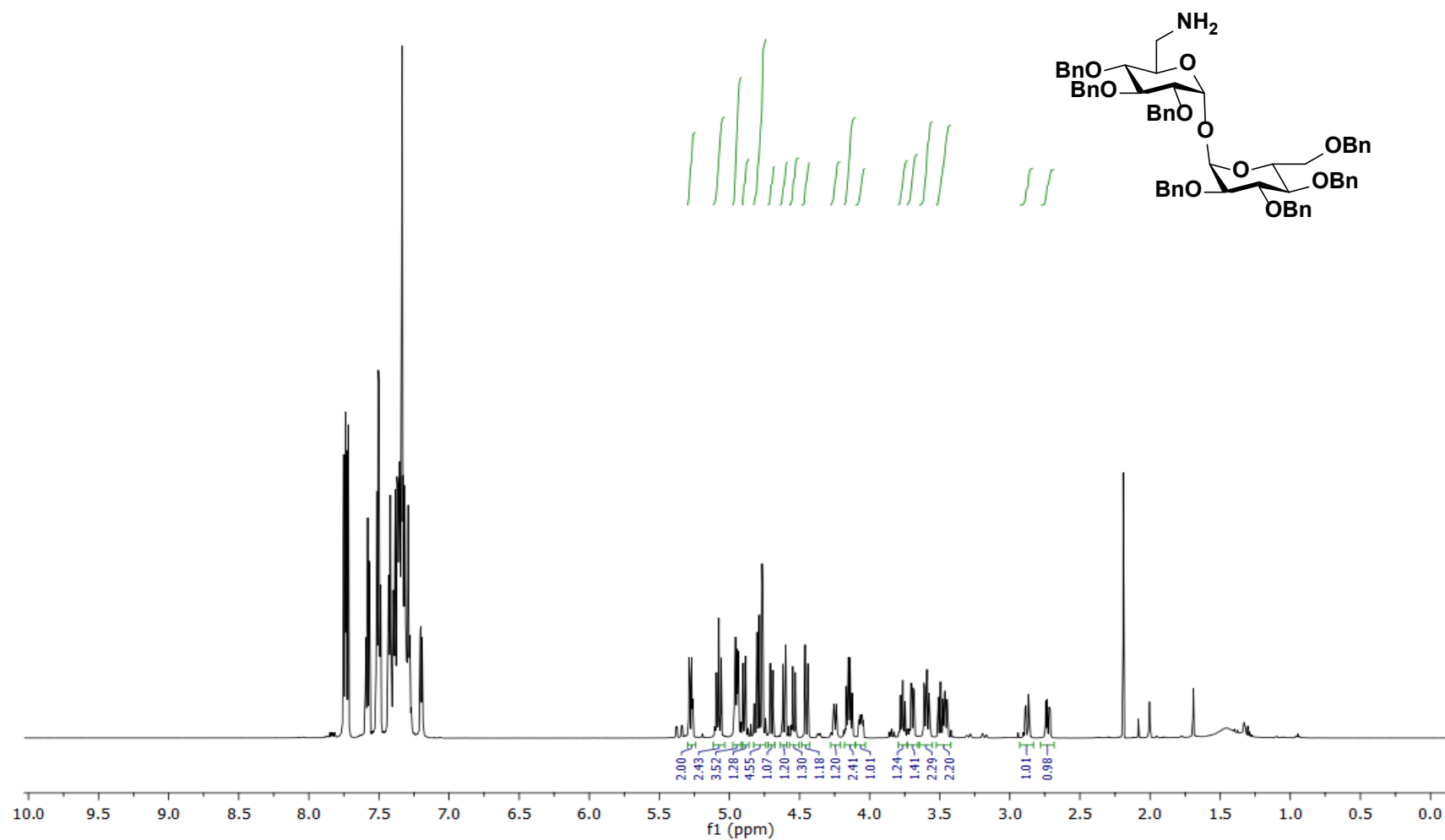
³¹P NMR 6-(Methylenephosphonic acid)- α,α' -trehalose (5)



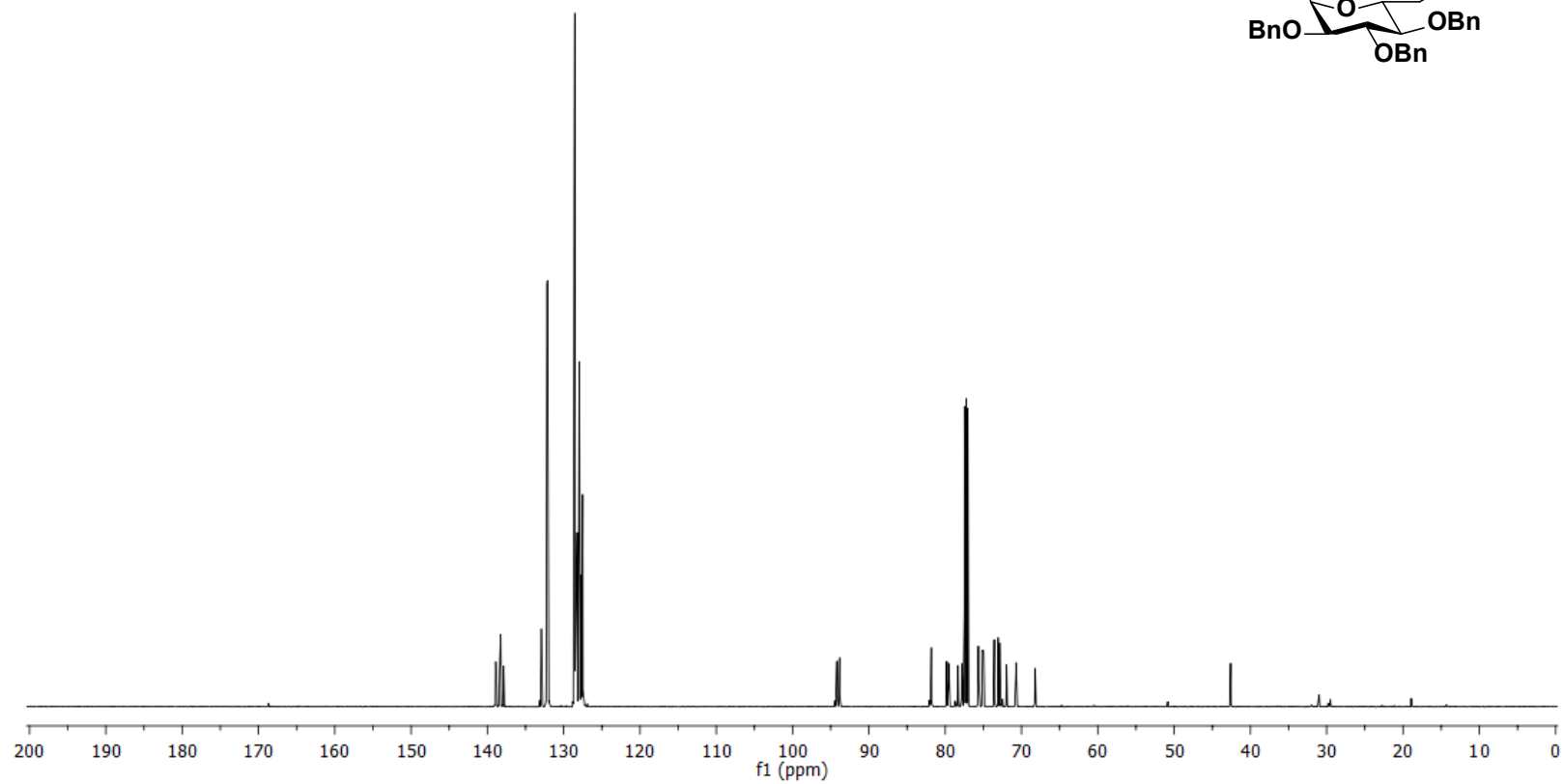
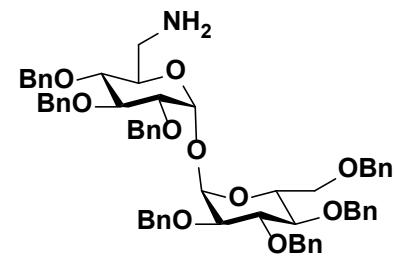
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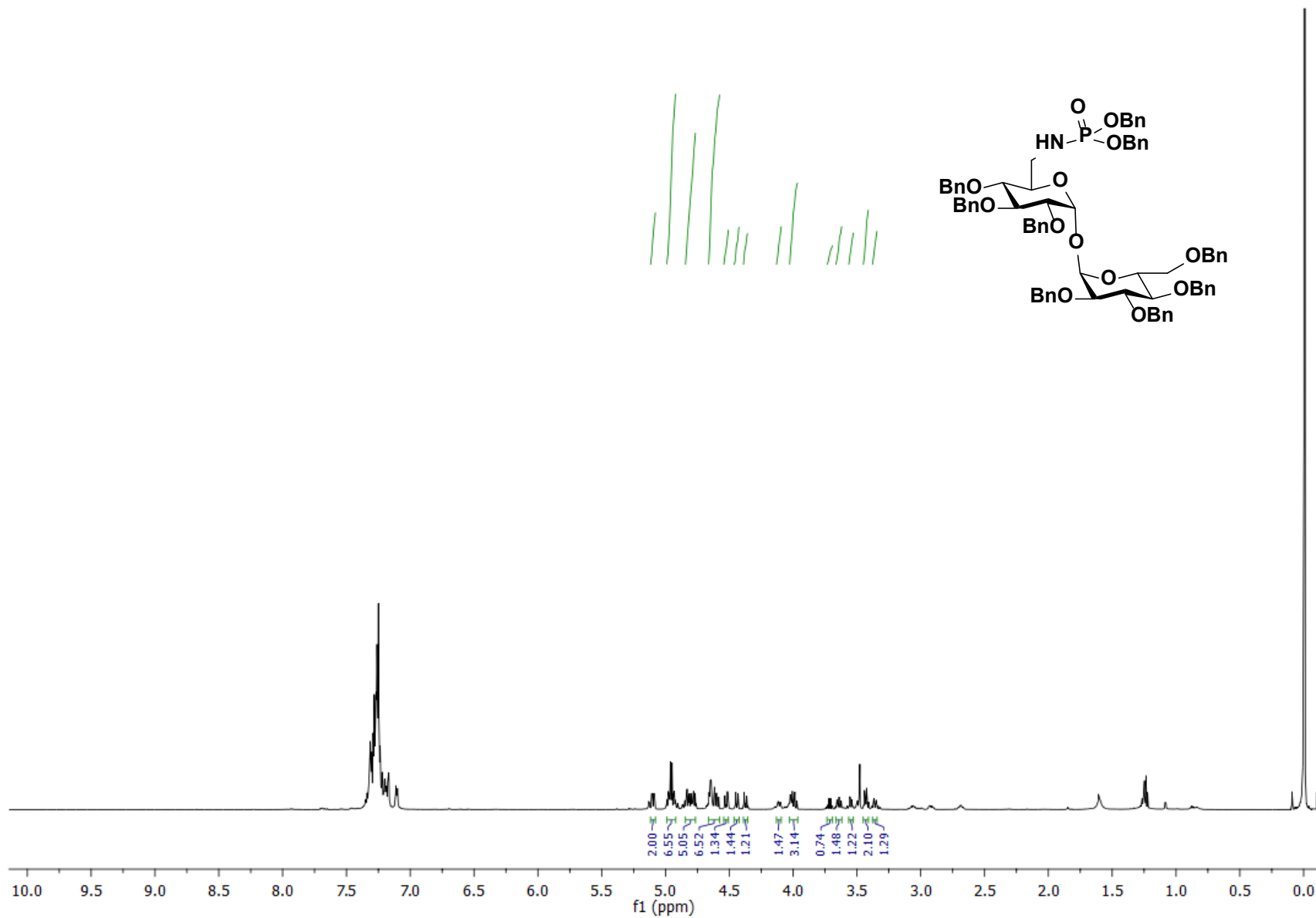
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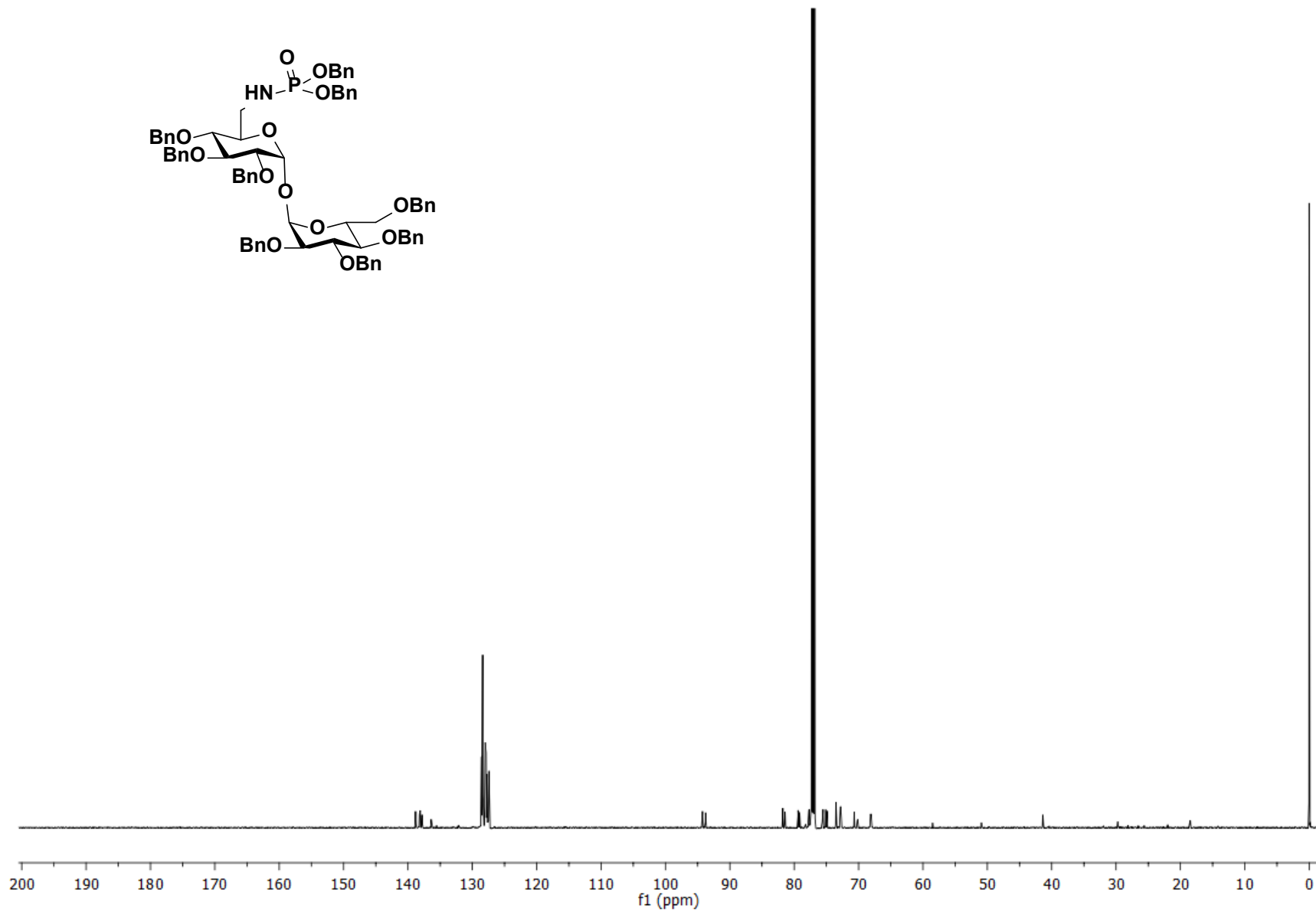
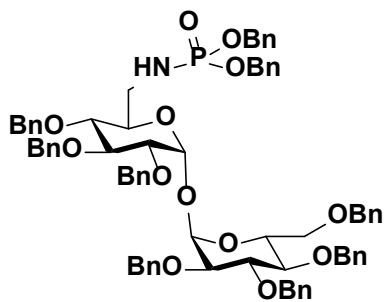
^{13}C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-Deoxy-6-amino- α,α' -trehalose (16)



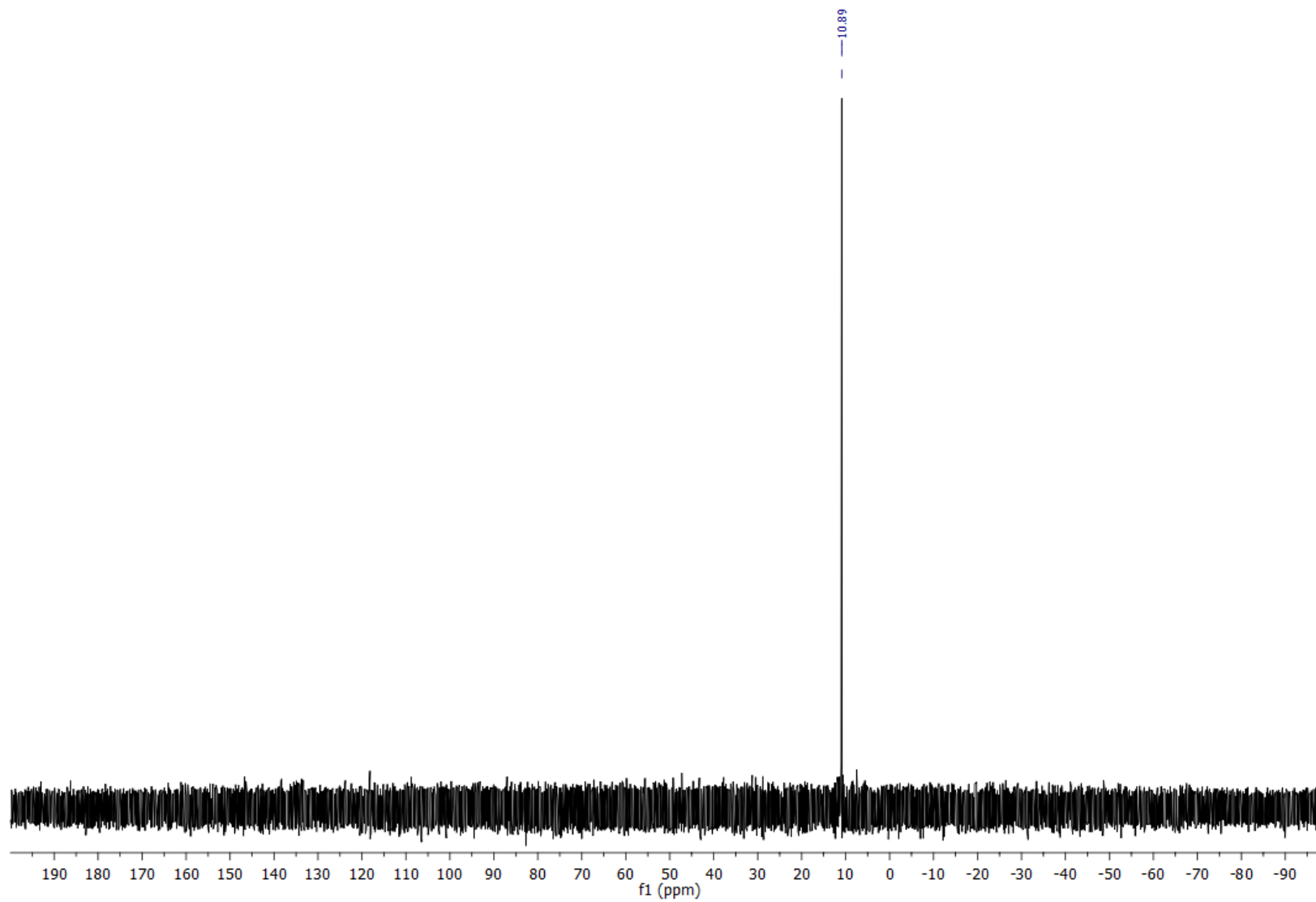
¹H NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-Deoxy-6-dibenzylphosphoramidate)-α,α'-trehalose (17)



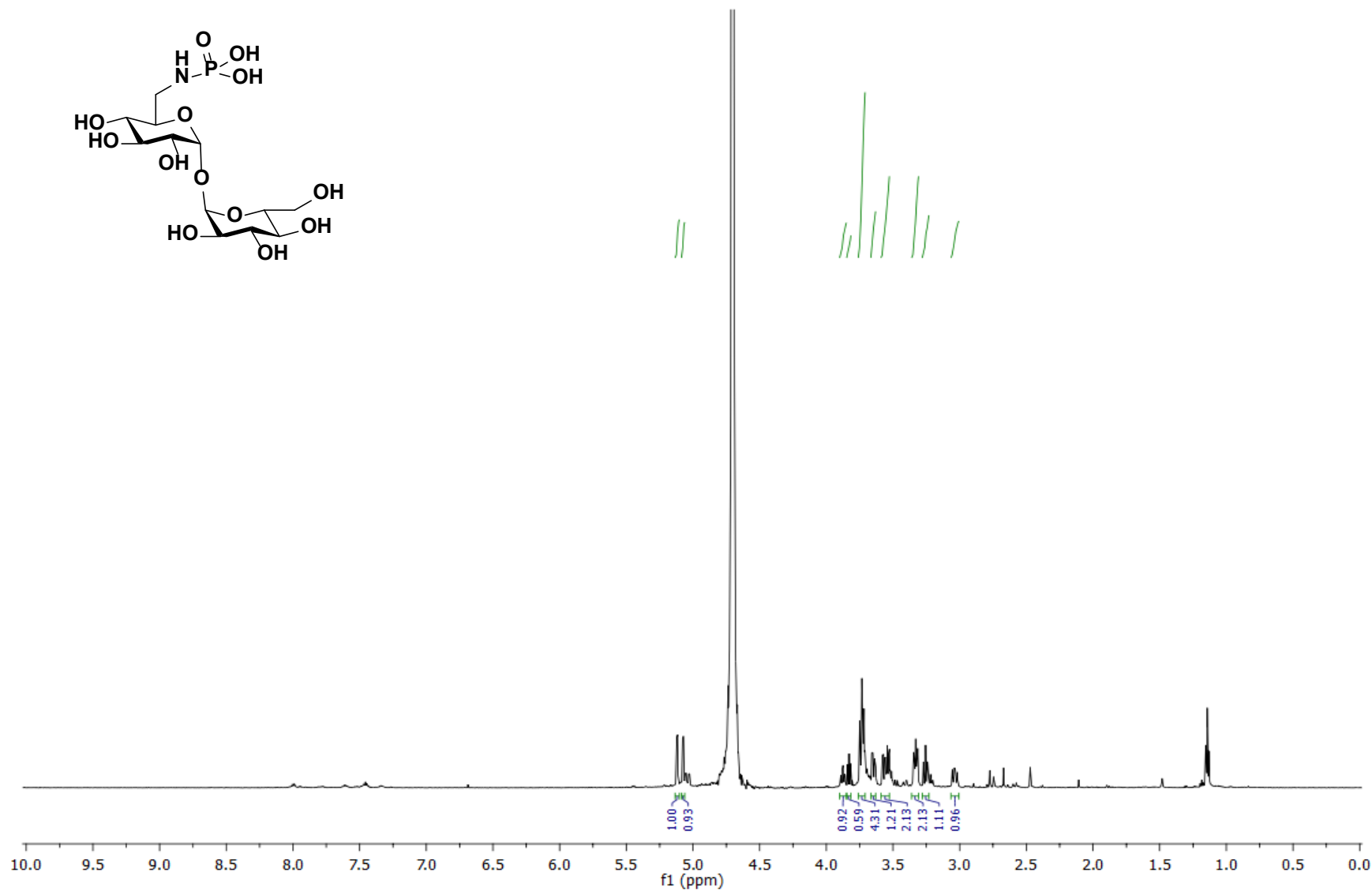
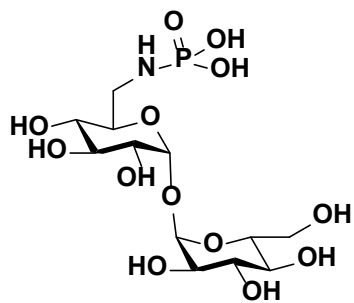
¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-Deoxy-6-dibenzylphosphoramidate)-α,α'-trehalose (17)



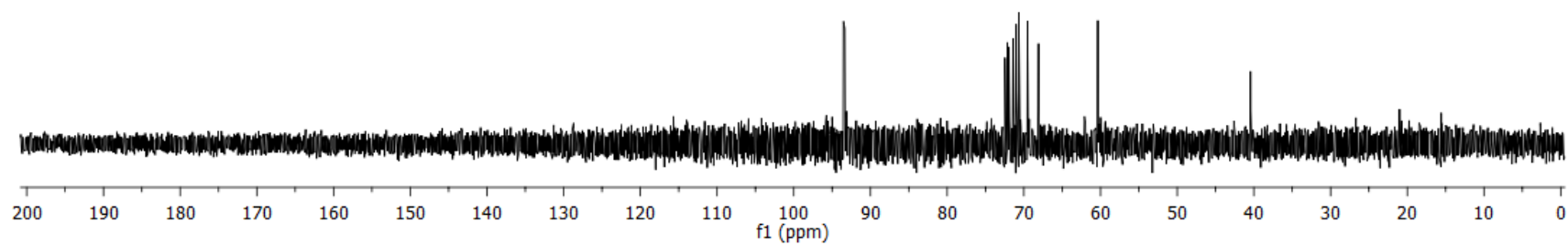
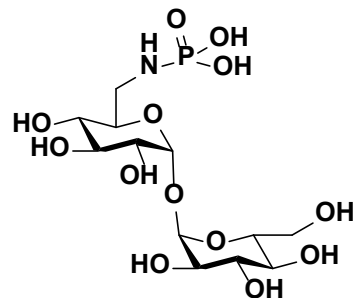
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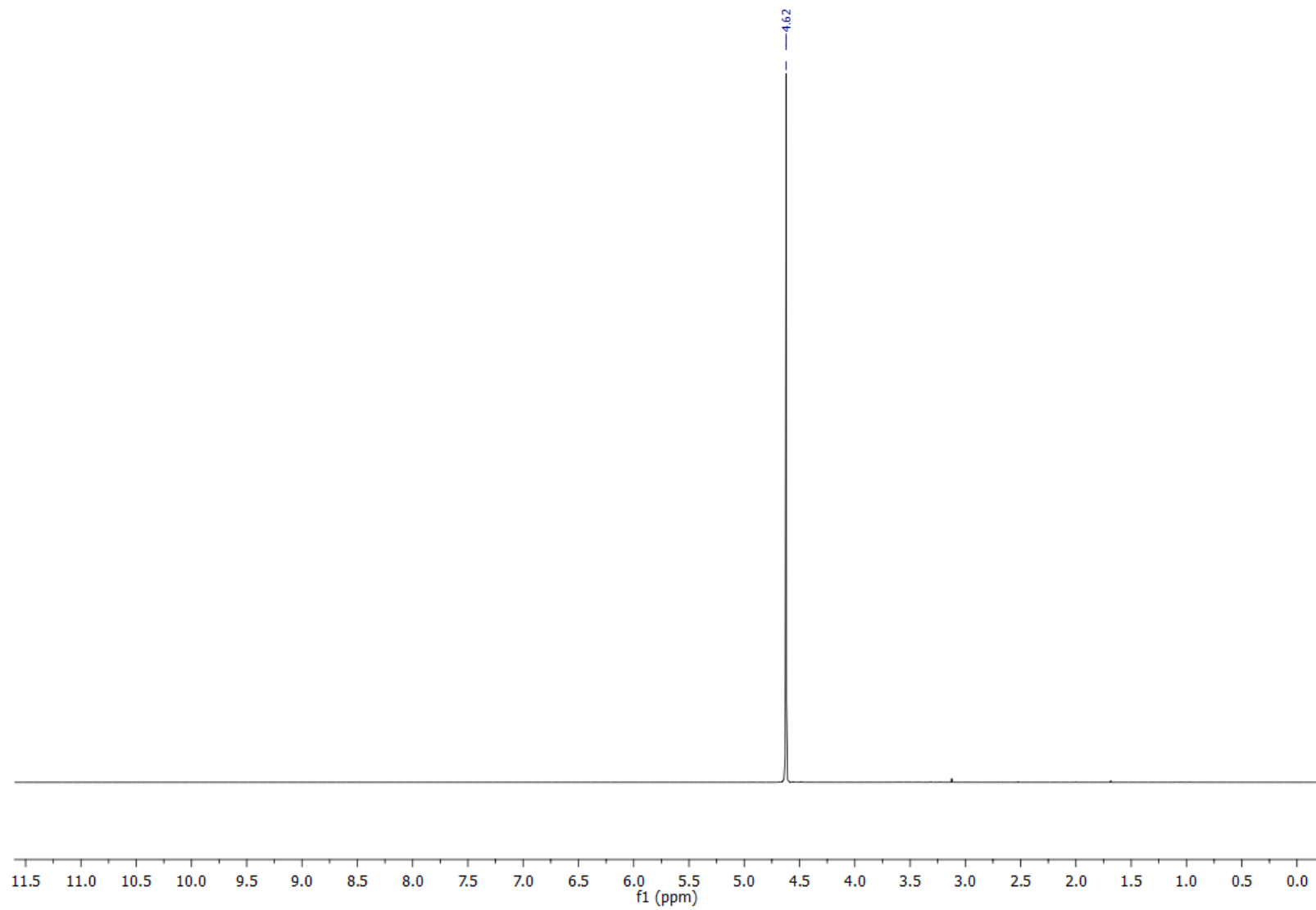
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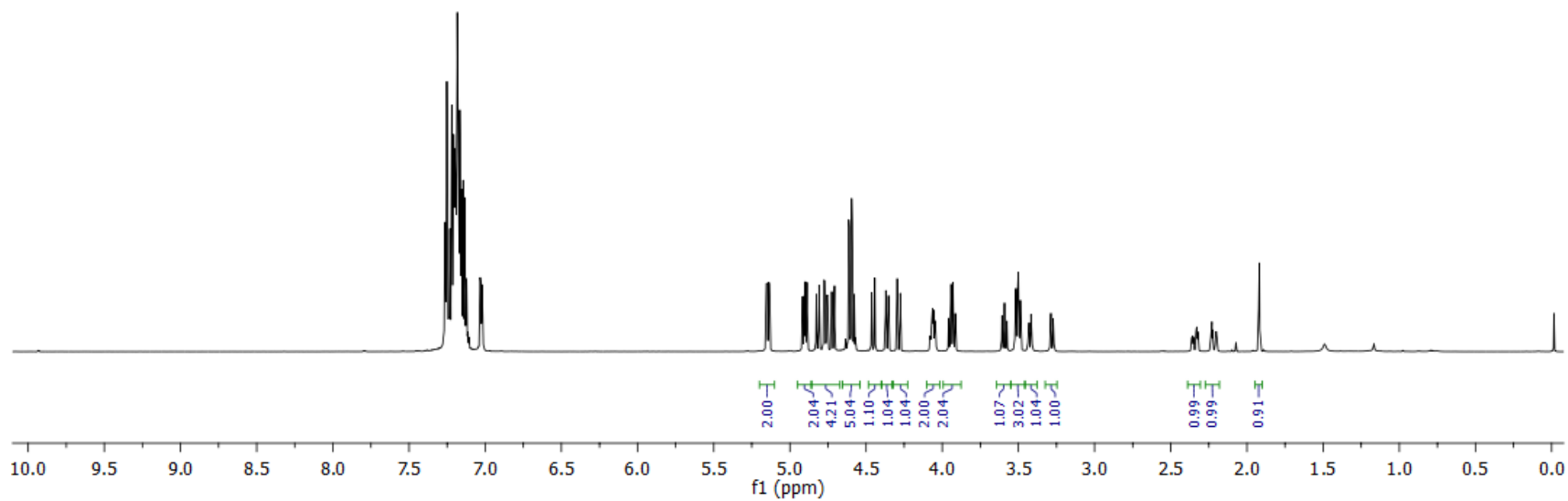
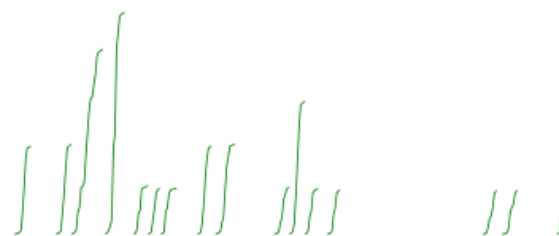
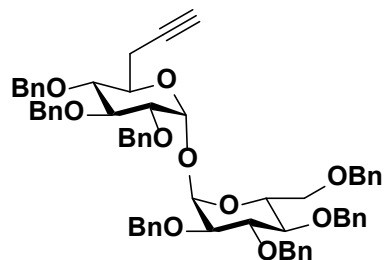
¹³C NMR 6-(phosphoramidic acid)- α,α' -trehalose (6)



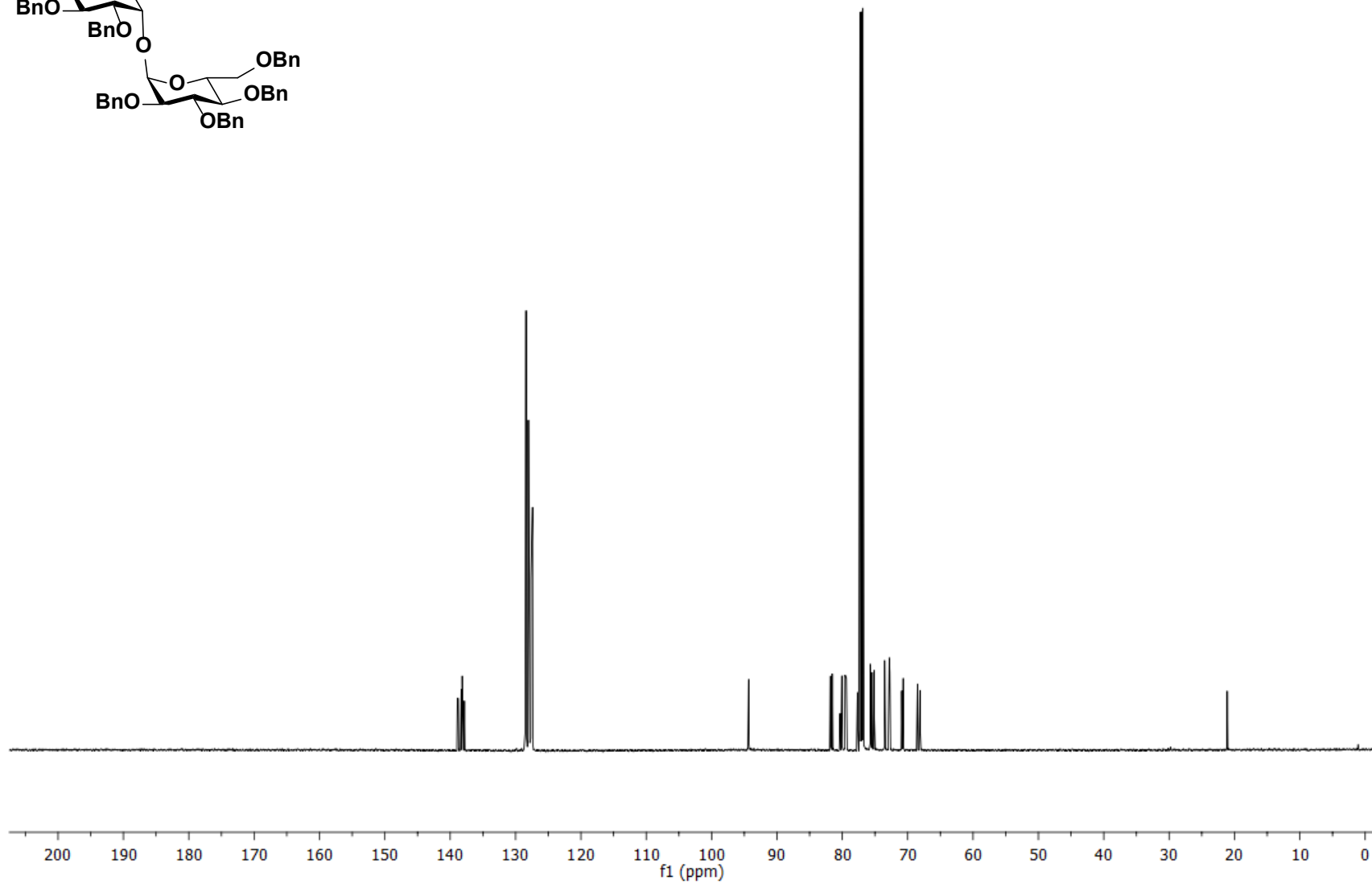
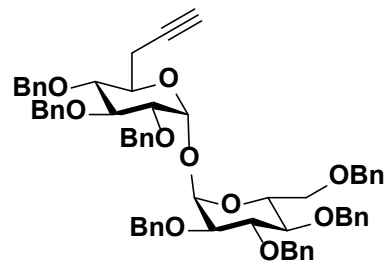
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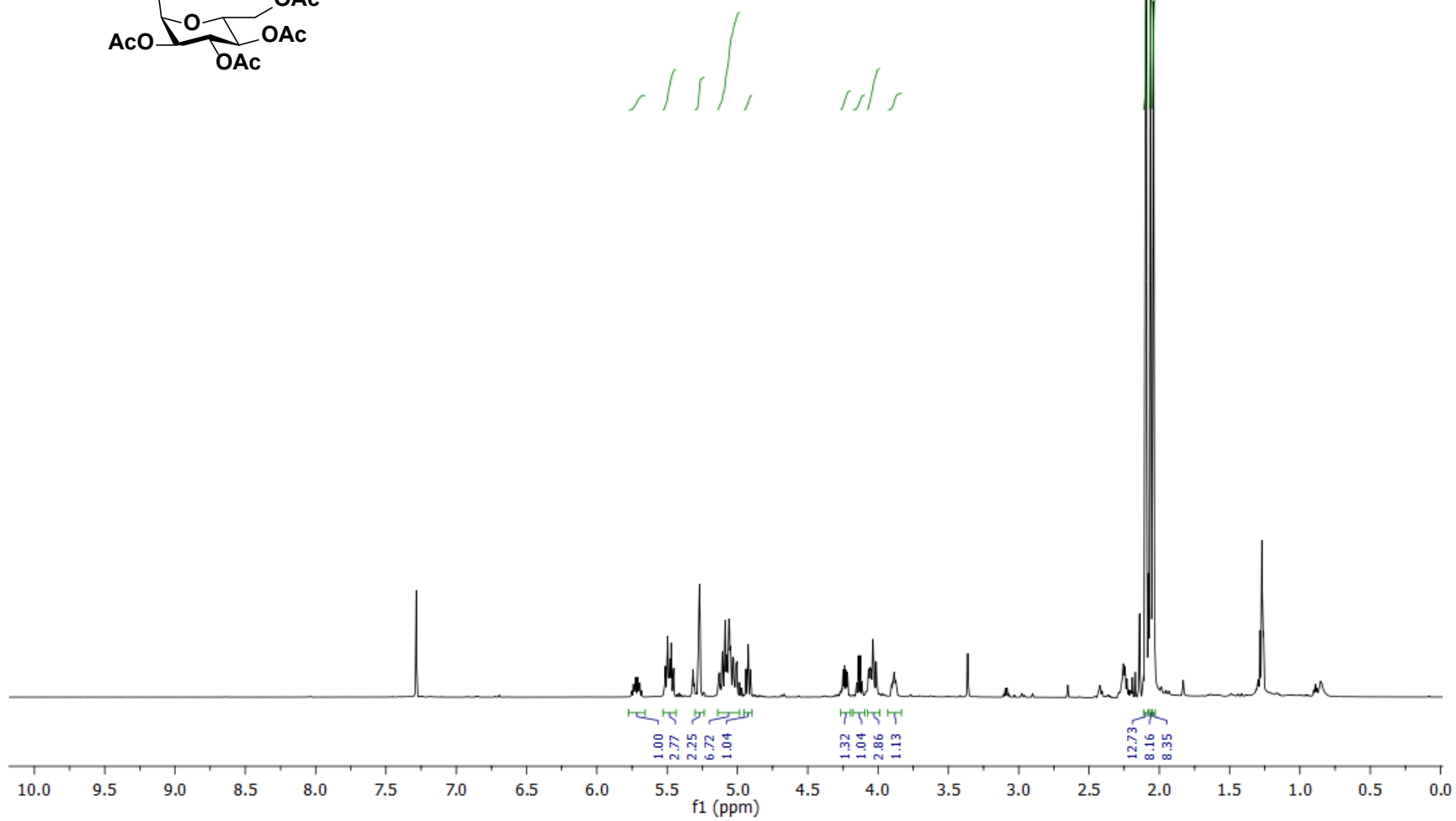
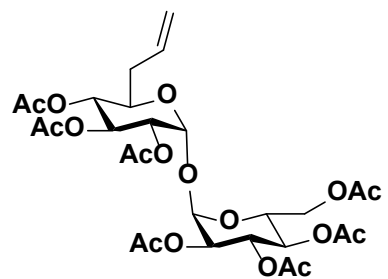
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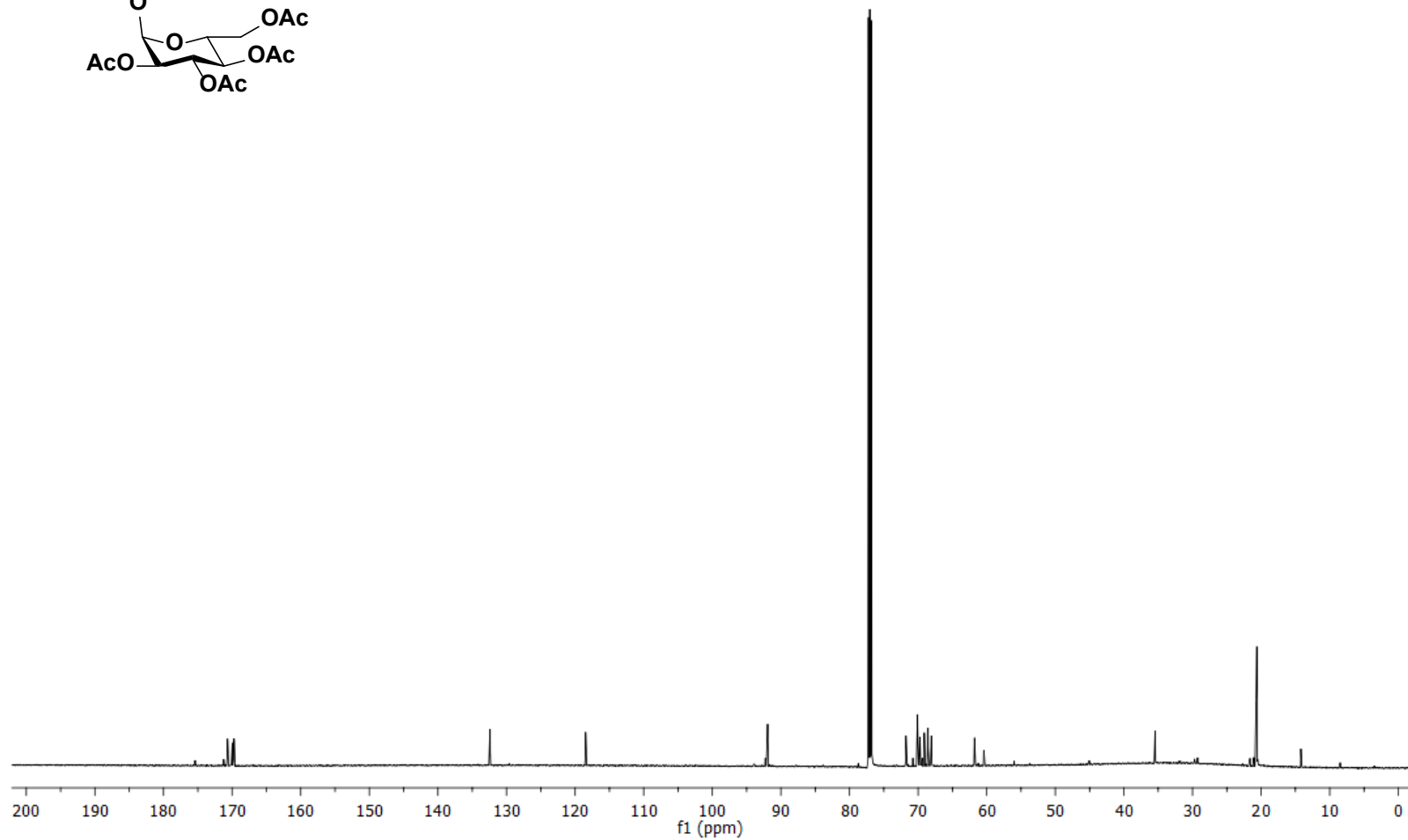
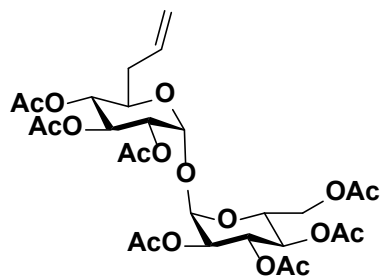
^{13}C NMR 2,2',3,3',4,4',6'-Hepta-O-benzyl-6-deoxy-6-ethynyl- α,α' -trehalose (18)



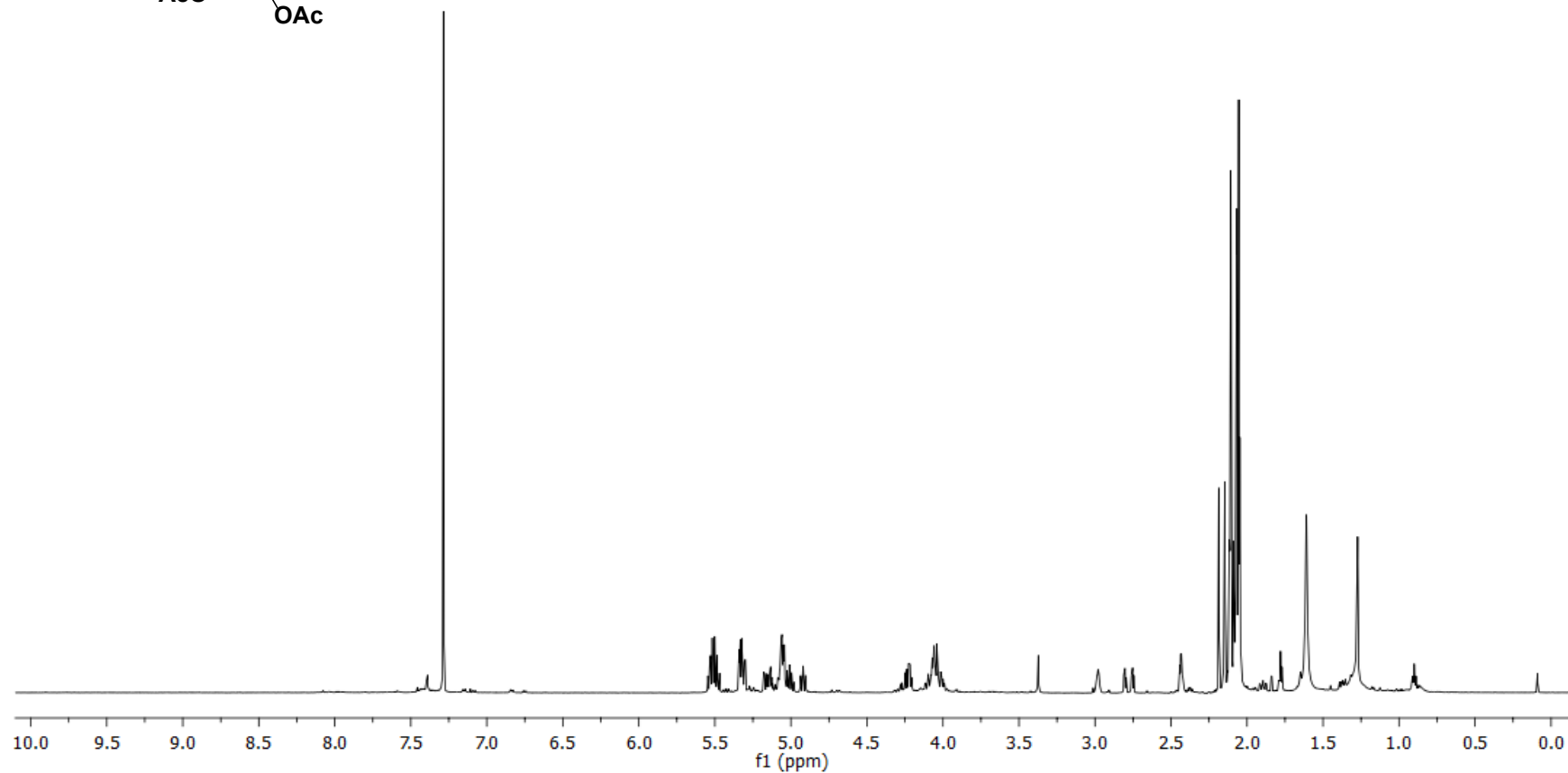
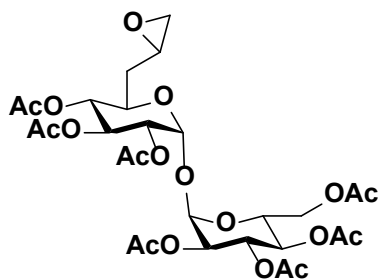
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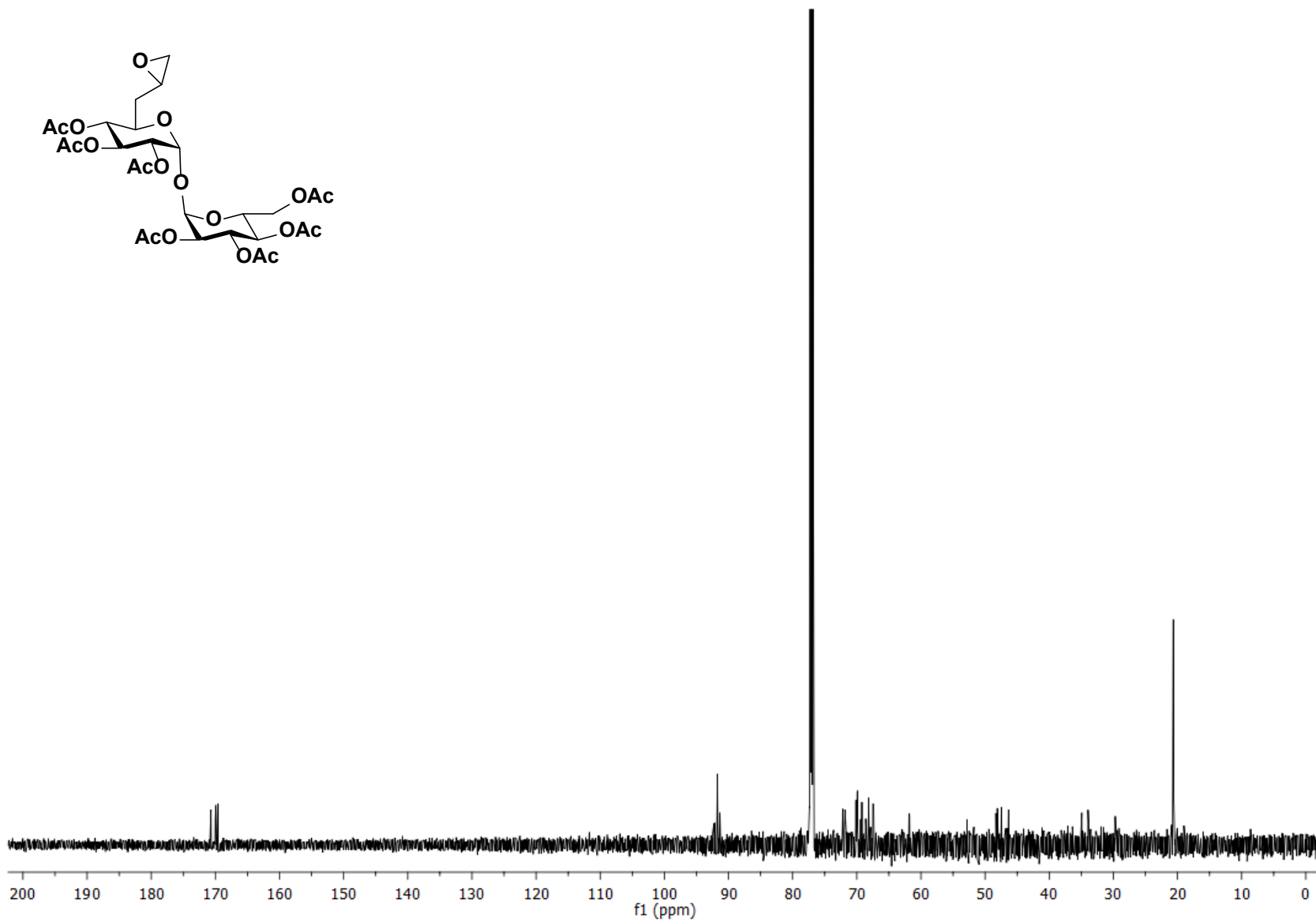
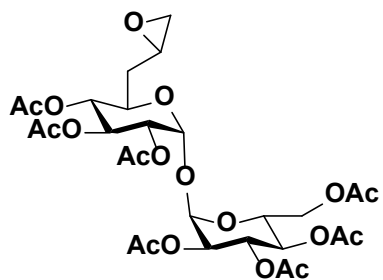
¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-acetyl-6-Deoxy-6-vinyl- α,α' -trehalose (19)



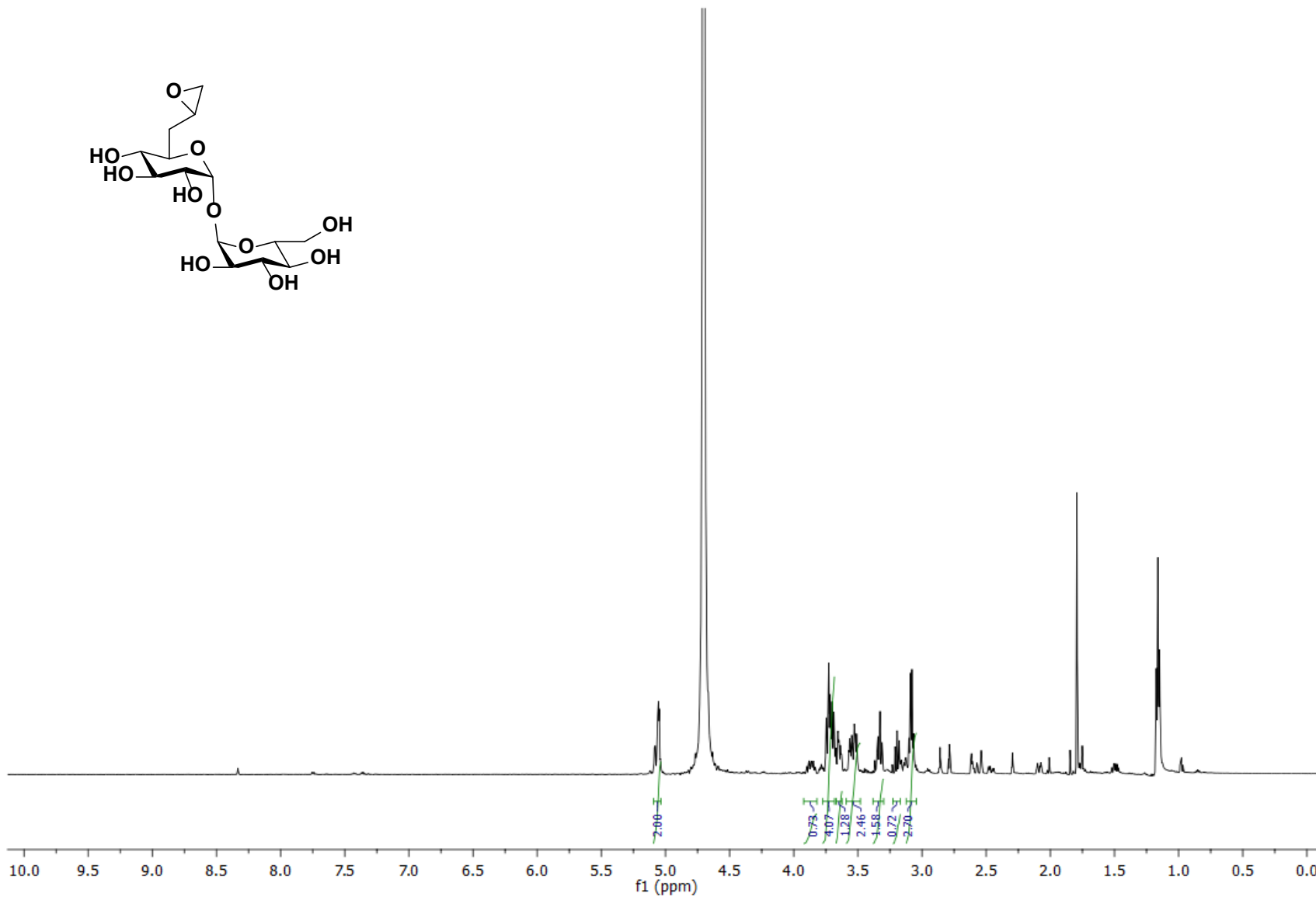
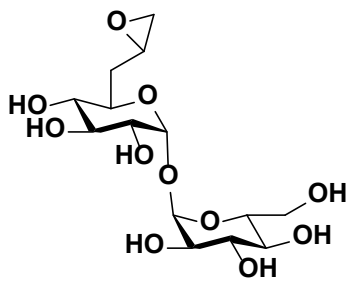
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¹³C NMR 2,2',3,3',4,4',6'-Hepta-O-acetyl-6-Deoxy-6-oxiranyl- α,α' -trehalose (20)



¹H NMR 6-Deoxy-6-oxiranyl- α,α' -trehalose (7)



¹³C NMR 6-Deoxy-6-oxiranyl- α,α' -trehalose (7)

