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Supporting Information

for

Zwitterionic pyrrolidine-phosphonates: Inhibitors of the glycoside hydrolase-like phosphorylase *Streptomyces coelicolor* GlgEI-V279S

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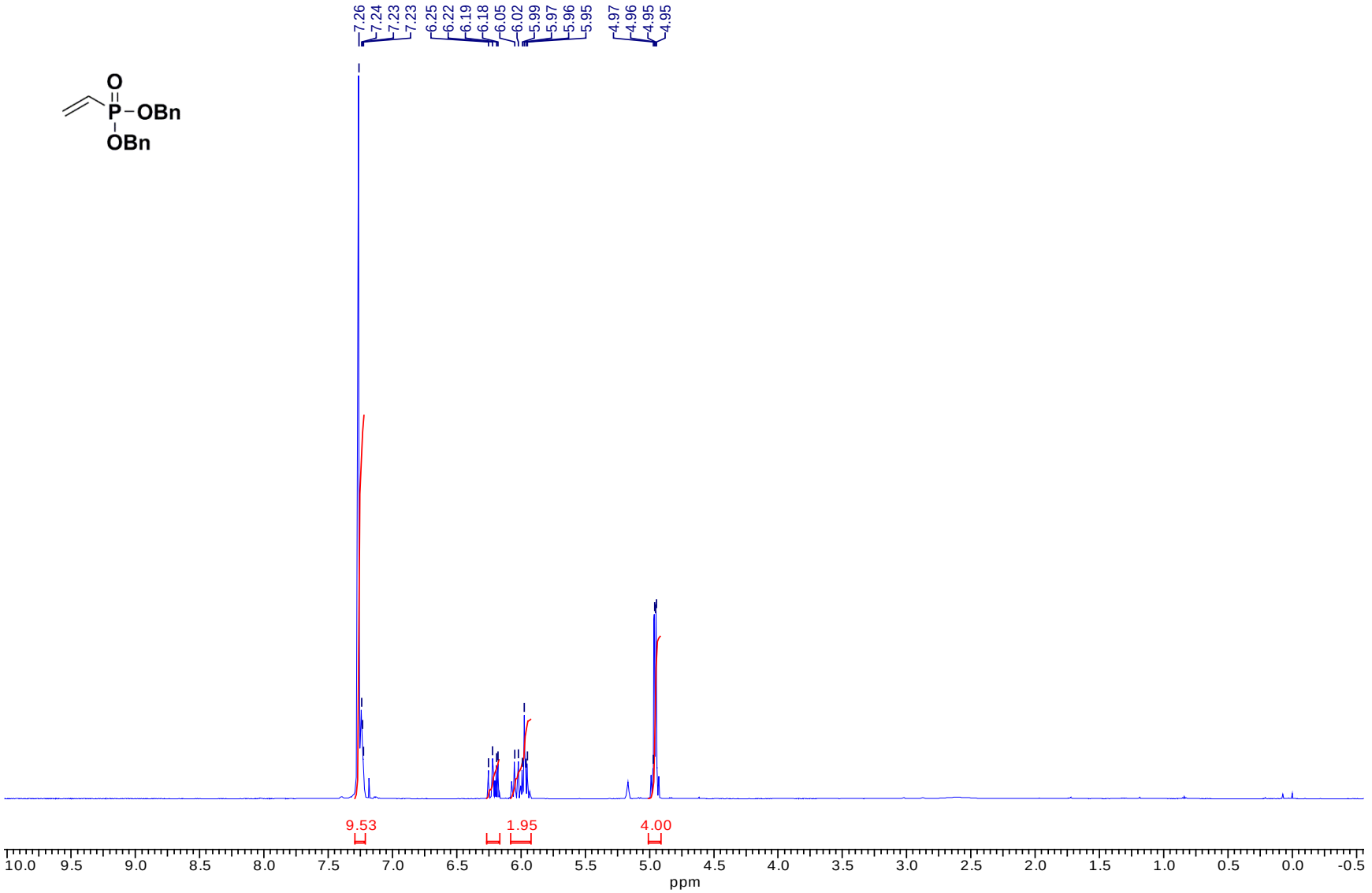
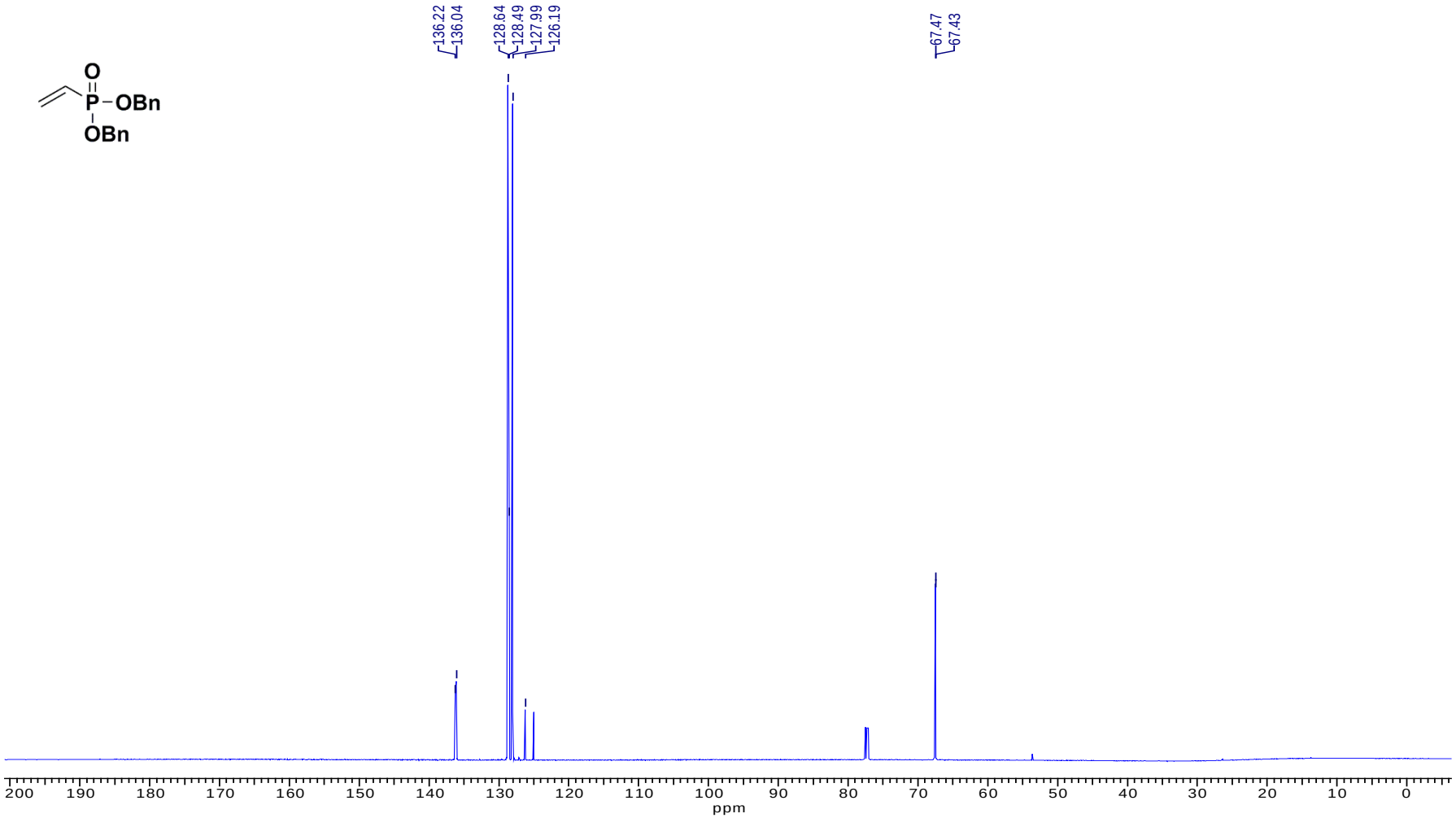
Table S1. Data collection and refinement statistics. The necessary data were obtained from one crystal. Values in parentheses are for the highest shells.

	Sco GlgEI-V279S-**5** complex	*Sco* GlgEI-V279S-**6** complex
Data collection		
Wavelength (Å)		
Space group	P 4_1	P 4_12_12
Cell dimensions		
a, b, c (Å)	113.3, 113.3 314.3	113.9, 113.9, 317.3
α, β, γ	90 °, 90 °, 90 °	90 °, 90 °, 90 °
Resolution (Å)	50.0 – 3.20	50.0 – 2.45
R_{merge}	12.4 (61.7)	17.2 (33.0)
$I/\sigma I$	11.5 (2.4)	14.8 (2.8)
Completeness (%)	99.6 (99.8)	99.1 (95.1)
Redundancy	4.3 (4.3)	12.7 (13.3
Refinement		
Resolution (Å)	39.06 – 3.21	45.88 – 2.45
No. unique reflections	64,431	76,413 (7,224)
R_{work}/R_{free} (%)	20.8/24.0	19.2/23.7
No. atoms		
Protein	20,461	10,724
Ligand/ion	108	64
Water	57	359
B-factors (Å^2)		
Protein	68.0	52.6
Ligand/ion	70.5	66.0
Water	50.8	47.1
R.m.s deviations		
Bond lengths (Å)	0.005	0.008
Bond angles (°)	1.047	1.18
Ramachandran		
Favored (%)	97.98	97.38
Outliers (%)	0.12	0.00

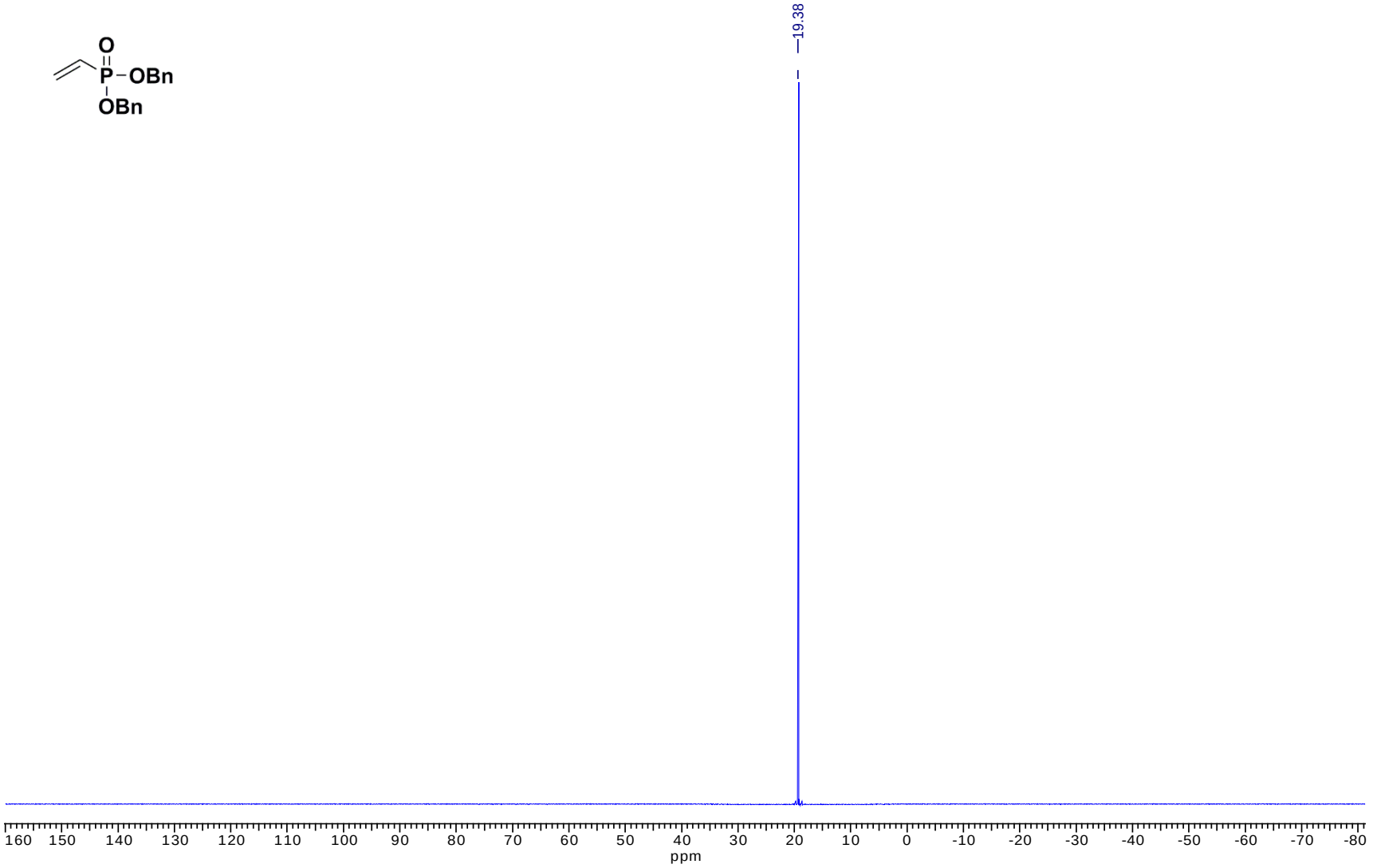
^{1}H NMR of Dibenzyl vinylphosphonate (10)



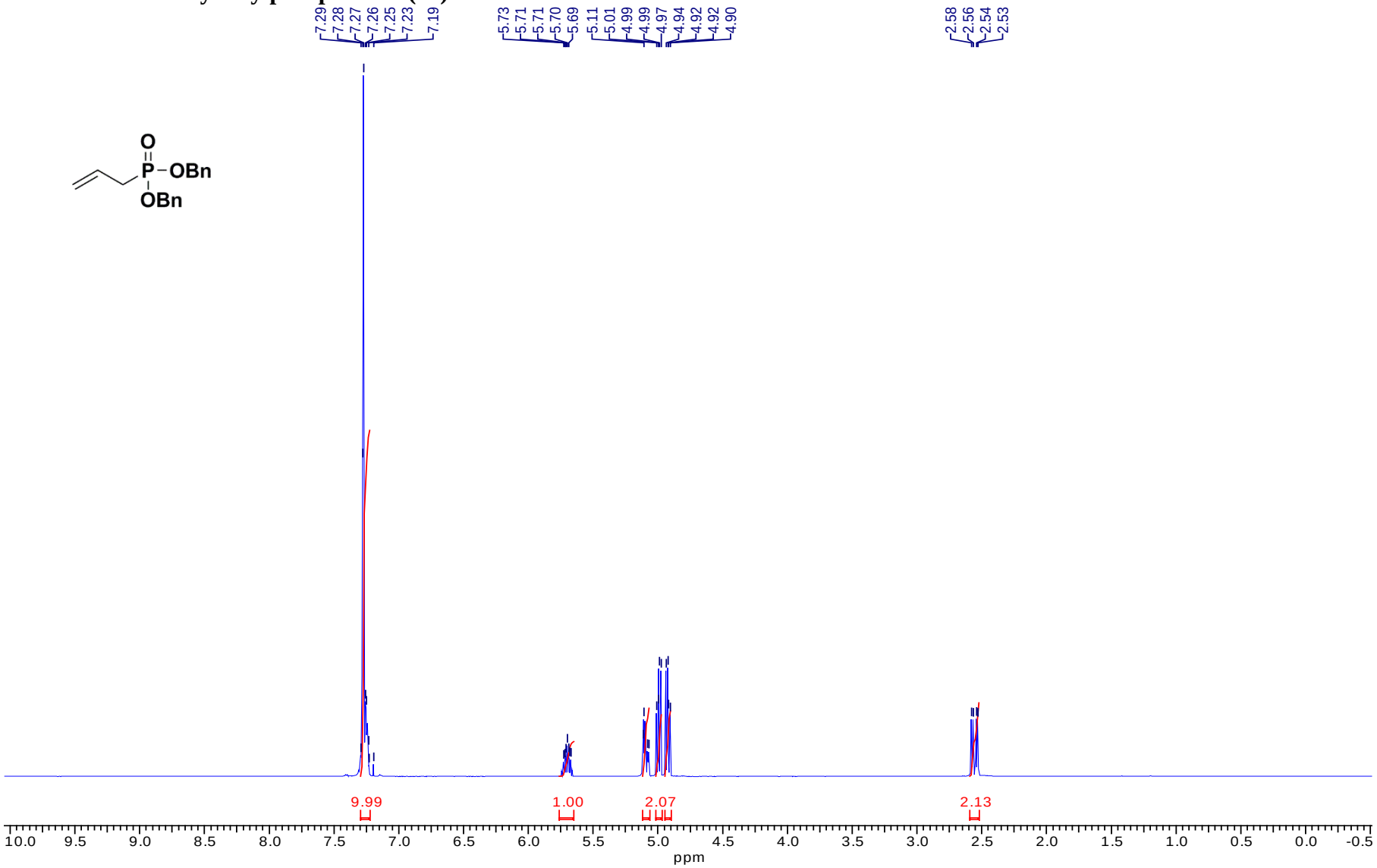
^{13}C NMR of Dibenzyl vinylphosphonate (10)



^{31}P NMR of Dibenzyl vinylphosphonate (10)



^{1}H NMR of Dibenzyl allylphosphonate (14)



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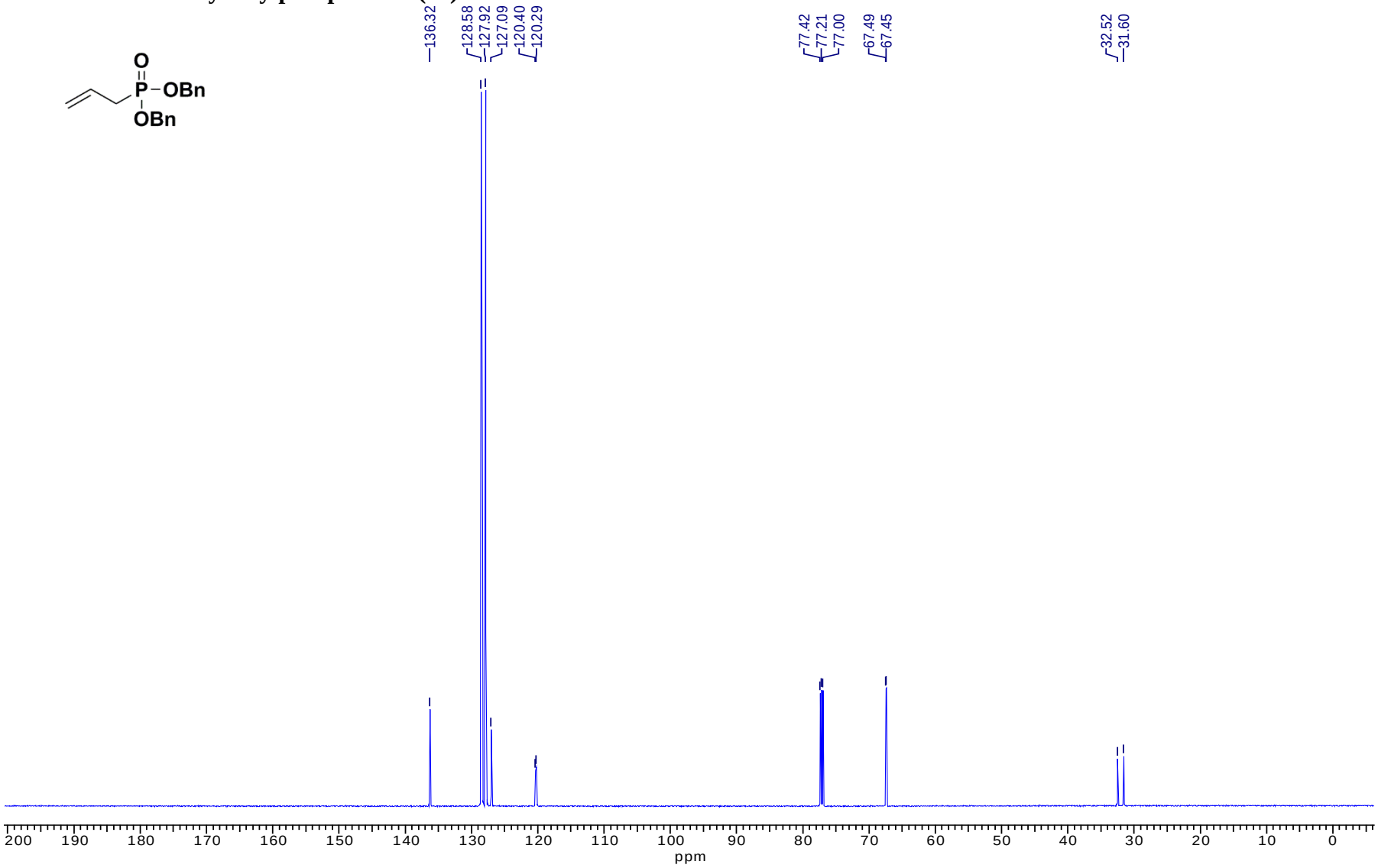
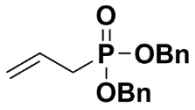
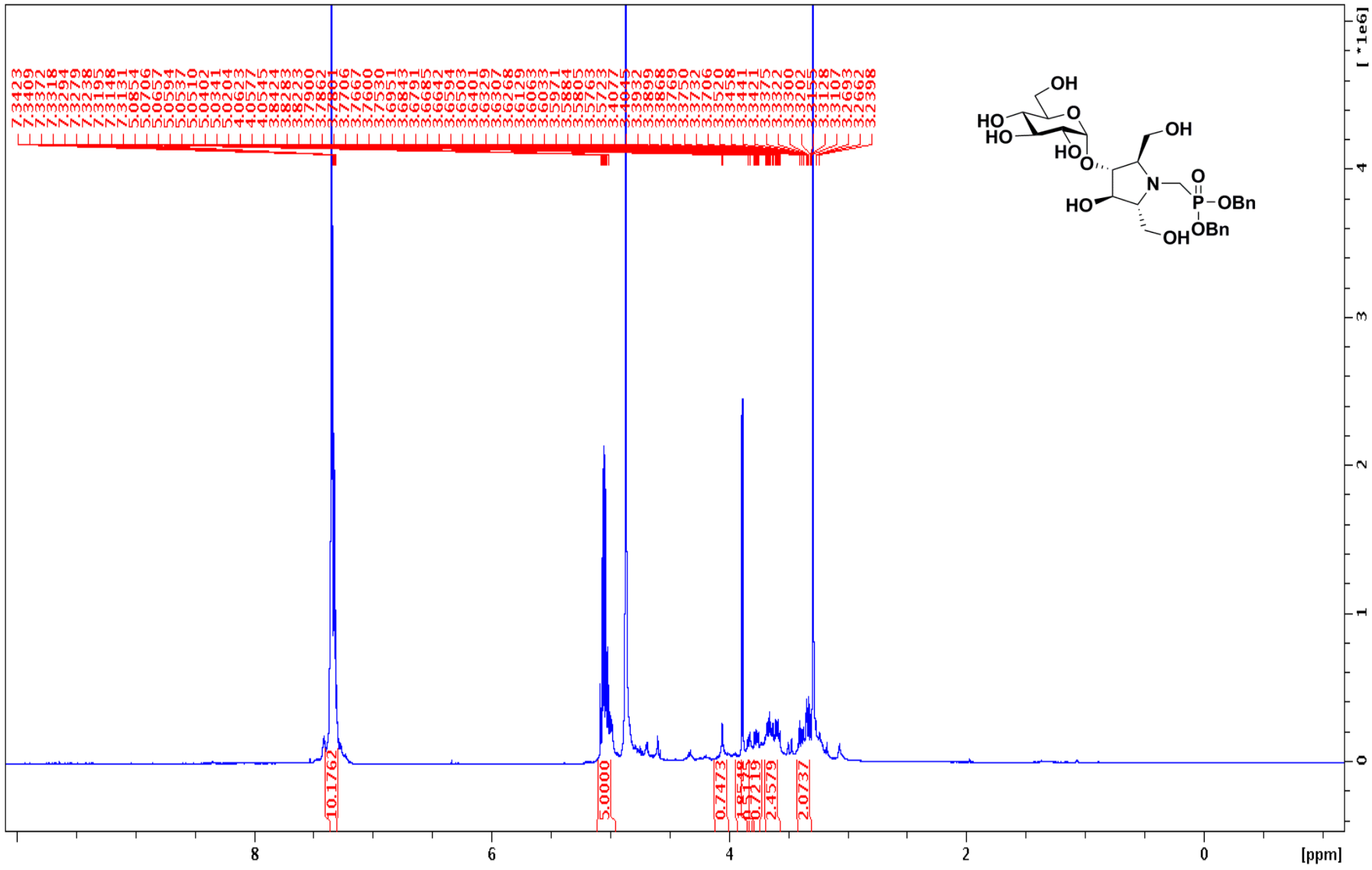


^{31}P NMR of Dibenzyl allylphosphonate (14)



^{1}H NMR of dibenzyl ((3-hydroxy-2,5-bis(hydroxymethyl)-(3-*O*-α-D-glucopyranosyl)pyrrolidin-1-yl)methyl)phosphonate (16):



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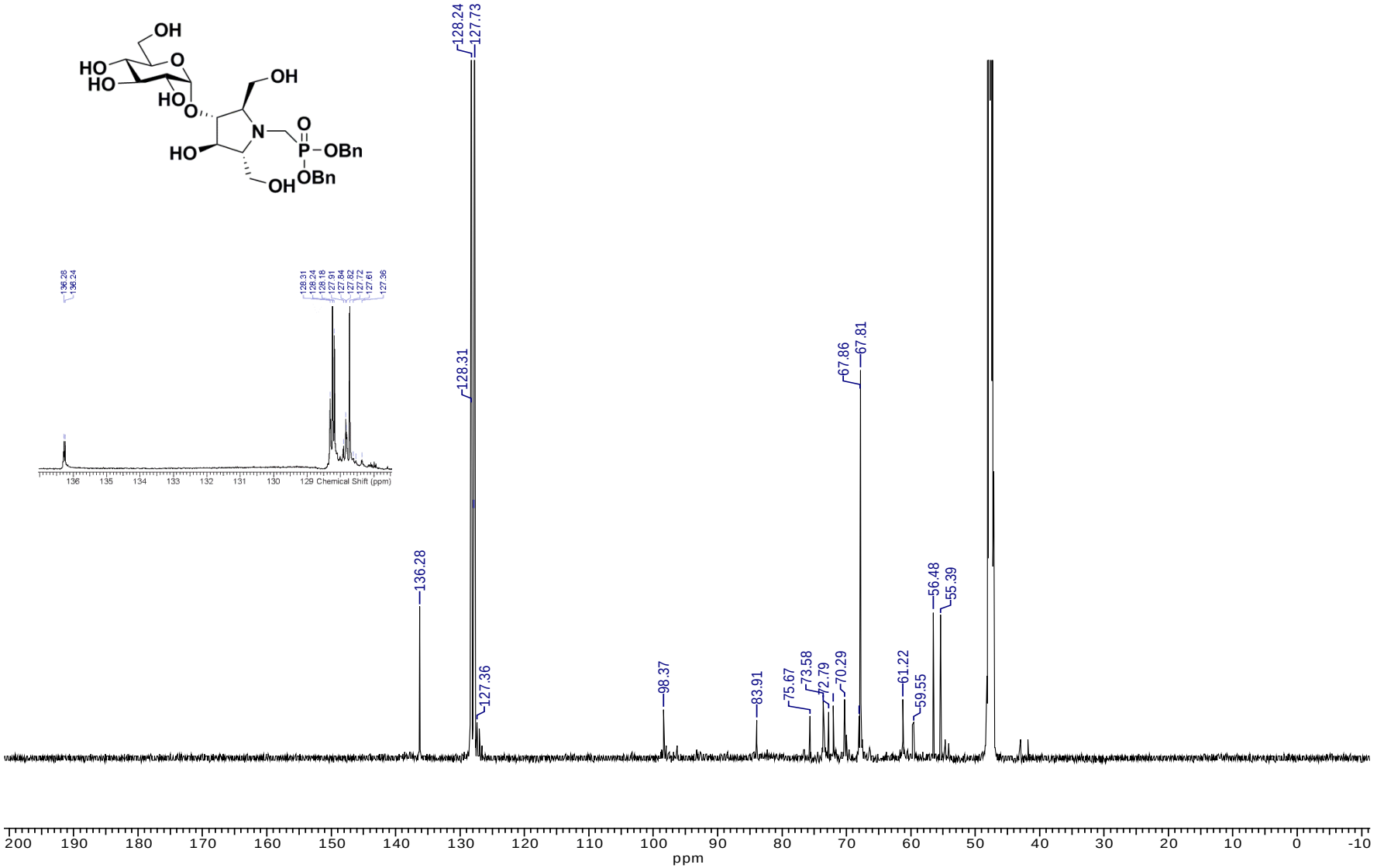

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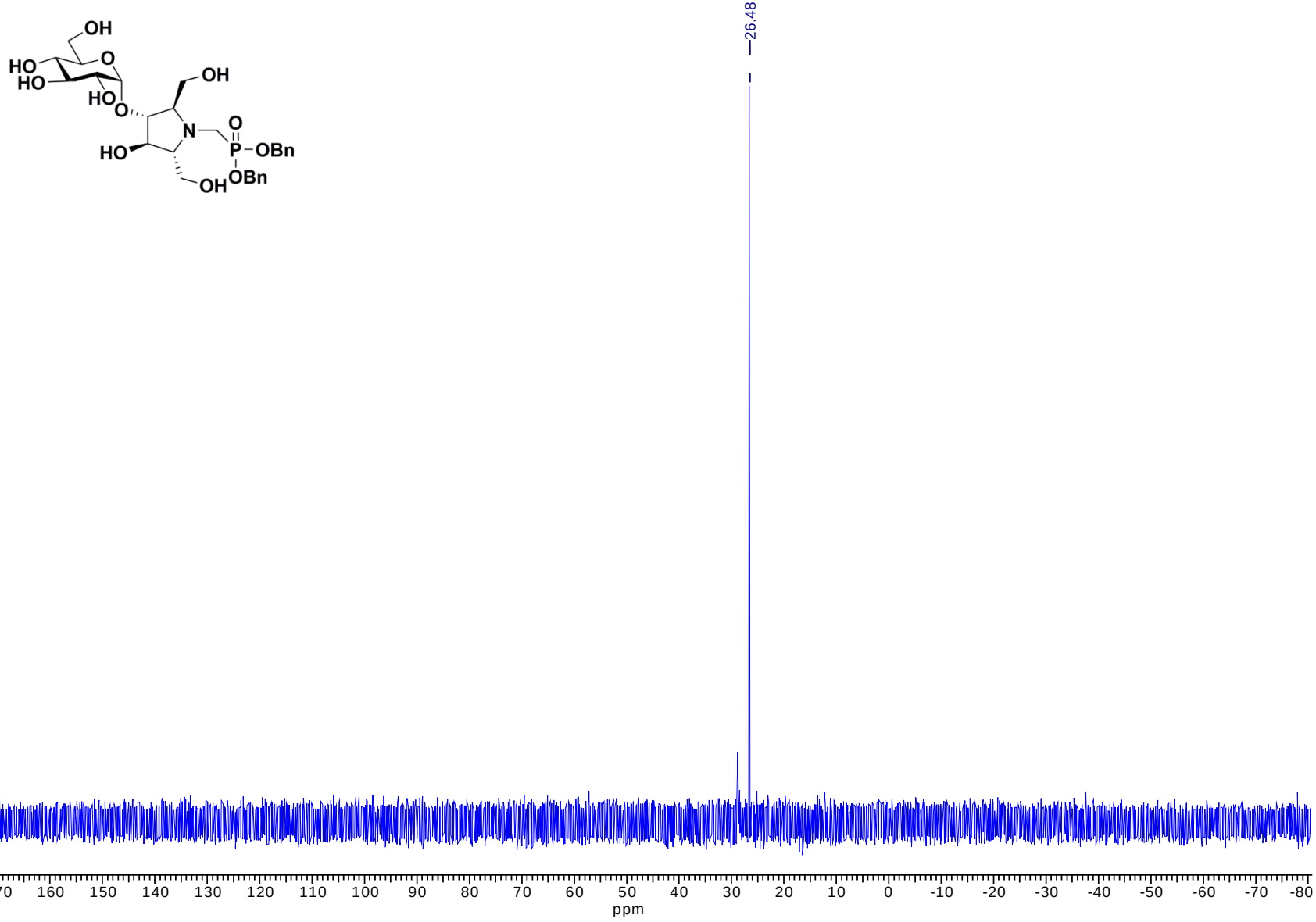
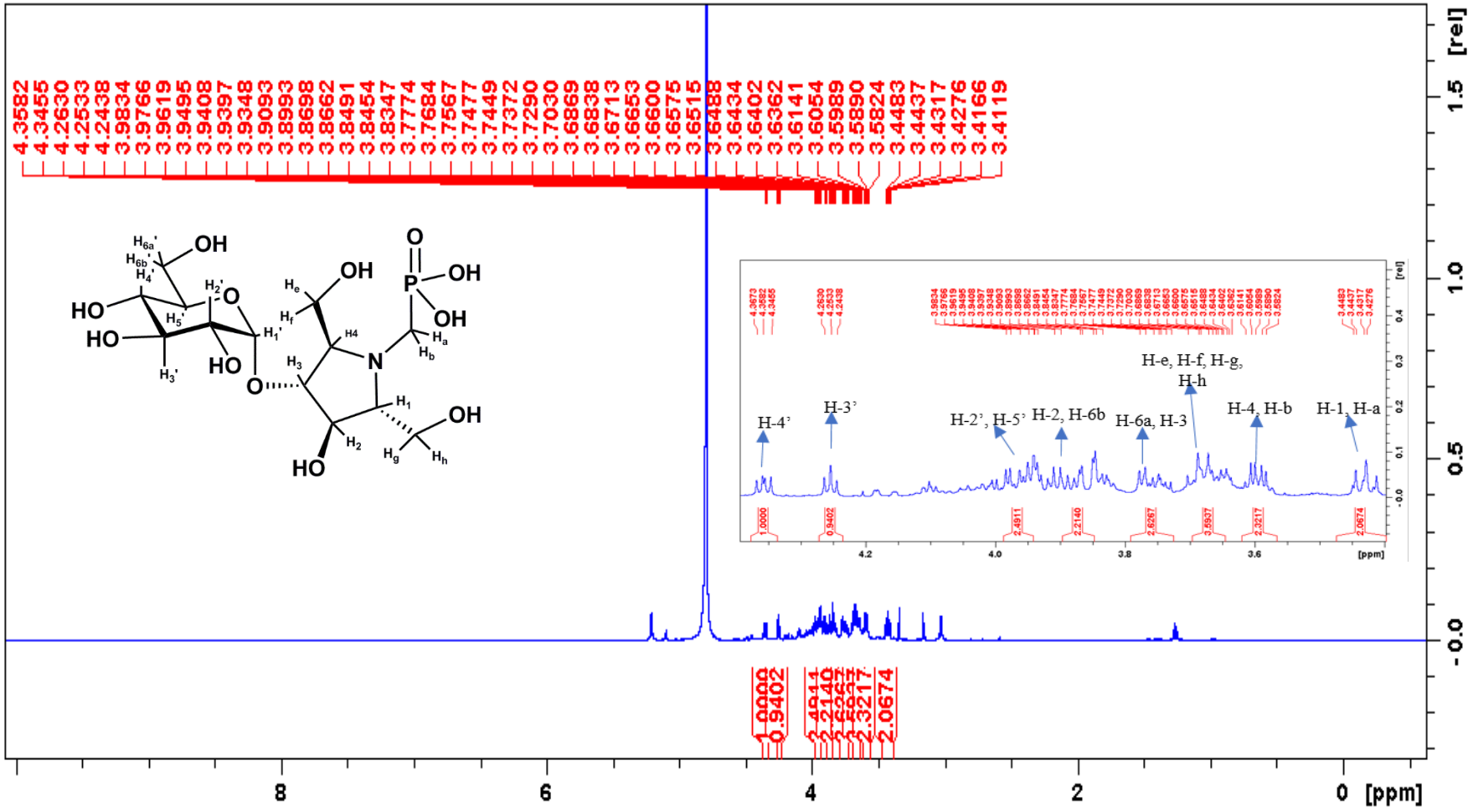


^{1}H NMR of ((3-hydroxy-2,5-bis(hydroxymethyl)-(3-*O*-α-D-glucopyranosyl)pyrrolidin-1-yl)methyl)phosphonic acid (5)



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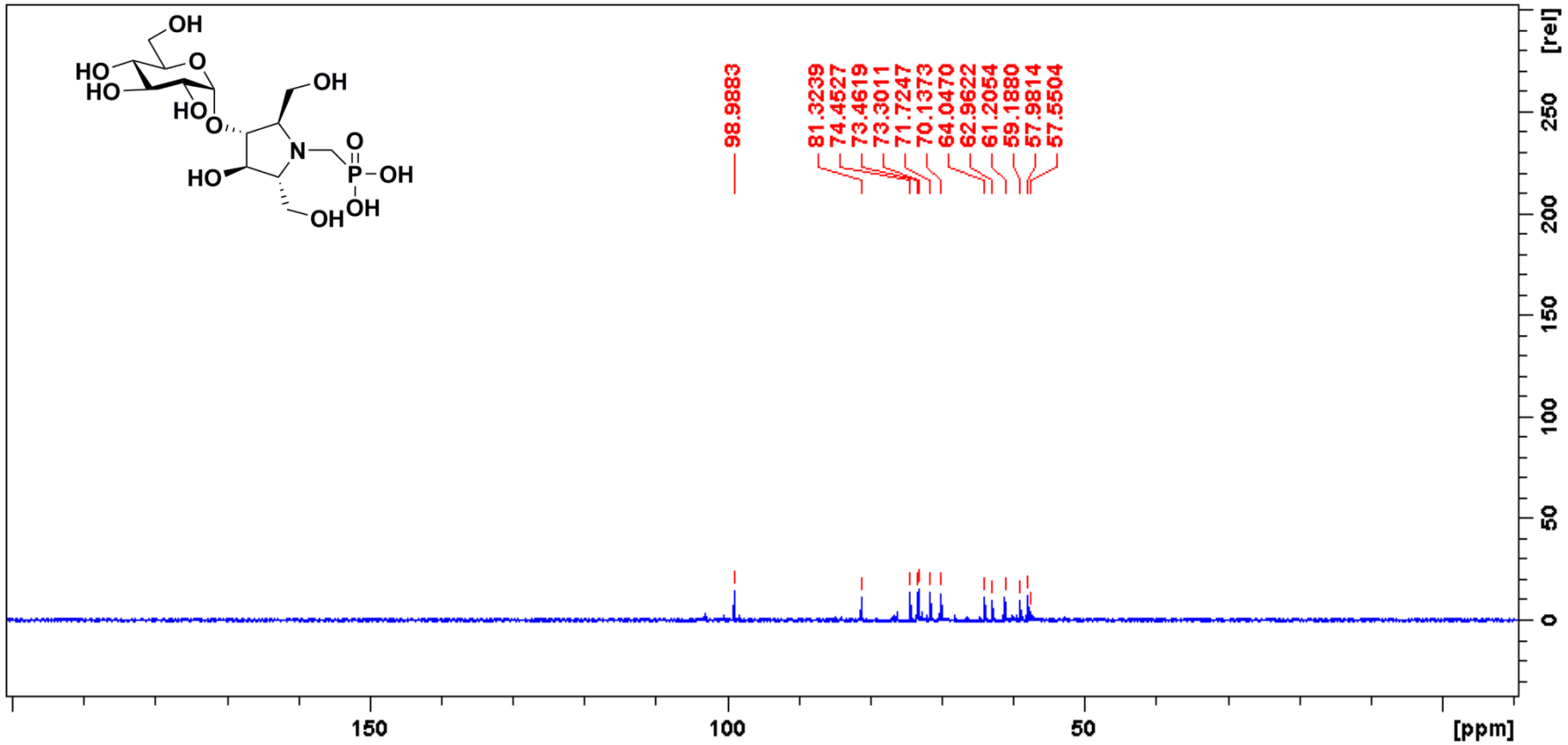
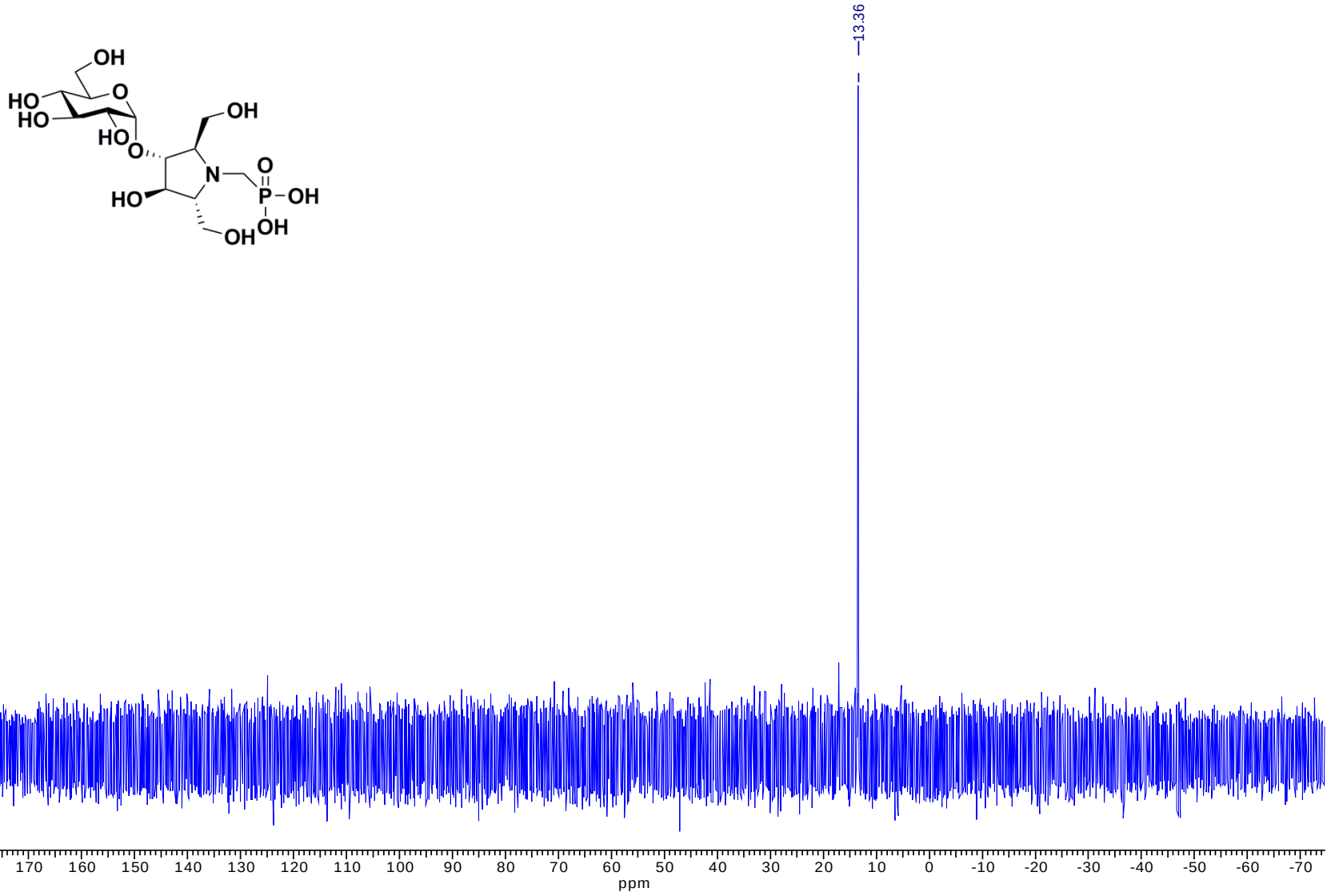
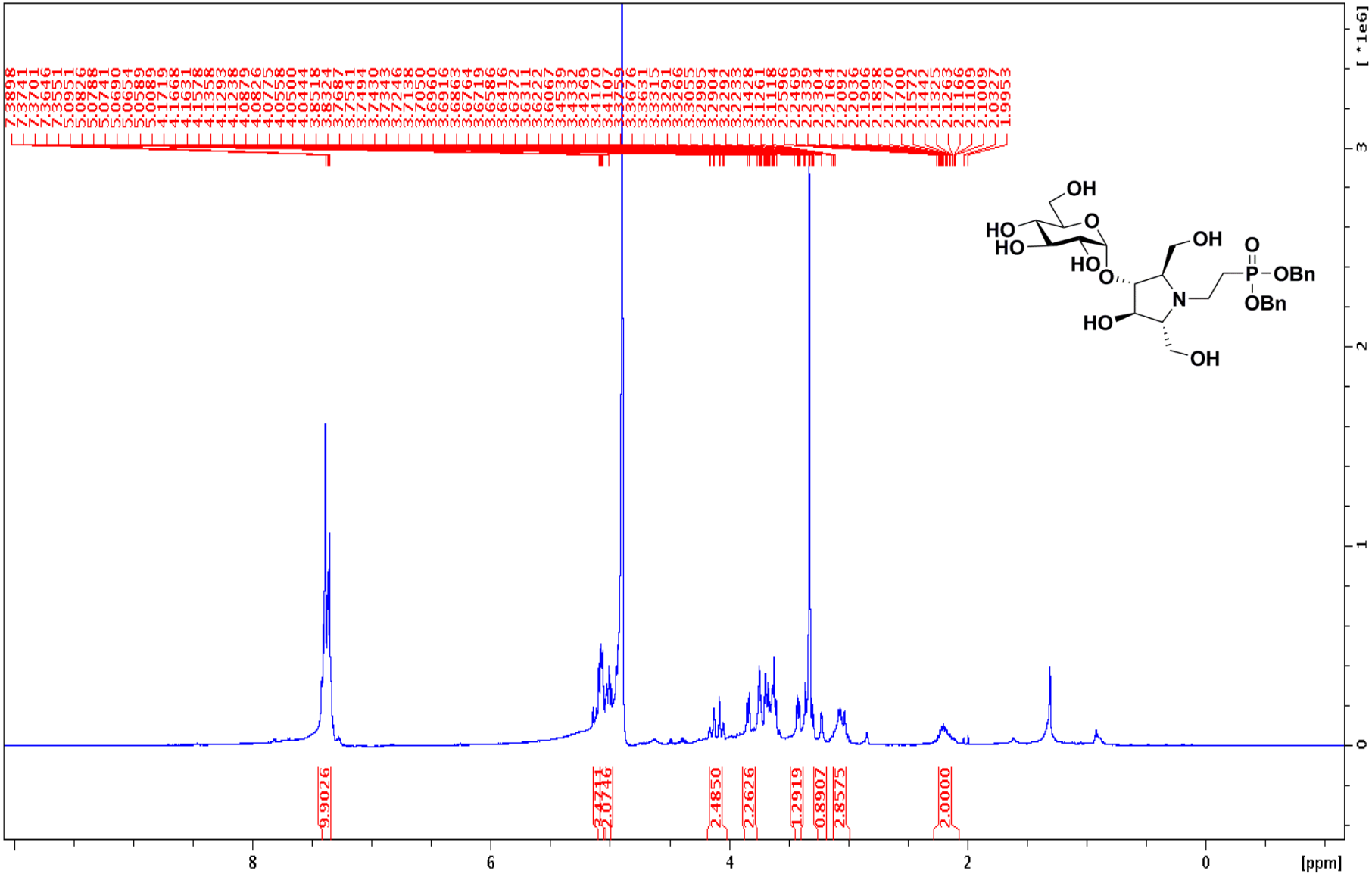


^{31}P NMR of ((3-hydroxy-2,5-bis(hydroxymethyl)-(3-*O*-α-D-glucopyranosyl)pyrrolidin-1-yl)methyl)phosphonic acid (5)



^{1}H NMR of dibenzyl ((3-hydroxy-2,5-bis(hydroxymethyl)-(3-*O*-α-D-glucopyranosyl)pyrrolidin-1-yl)ethyl)phosphonate (17)



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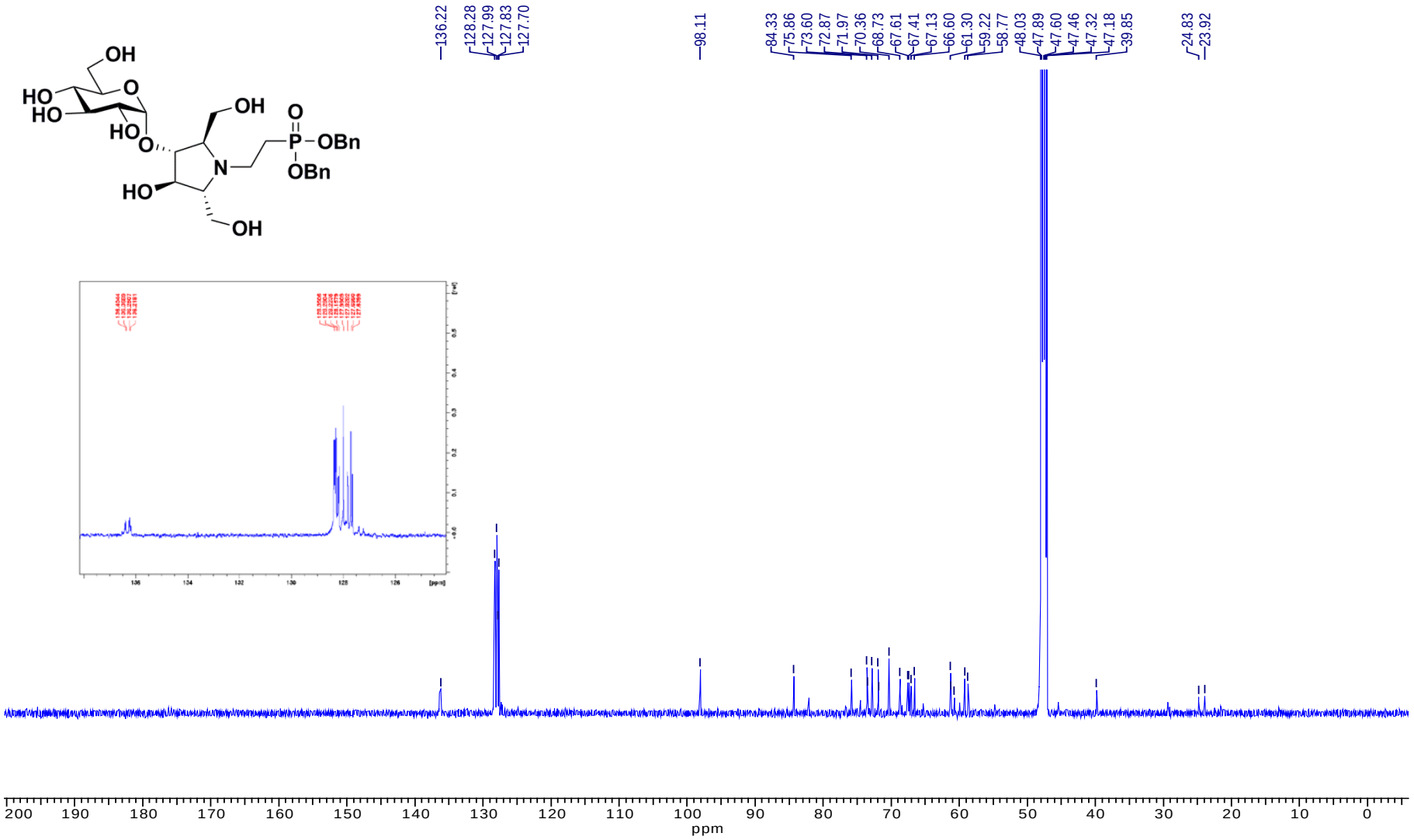

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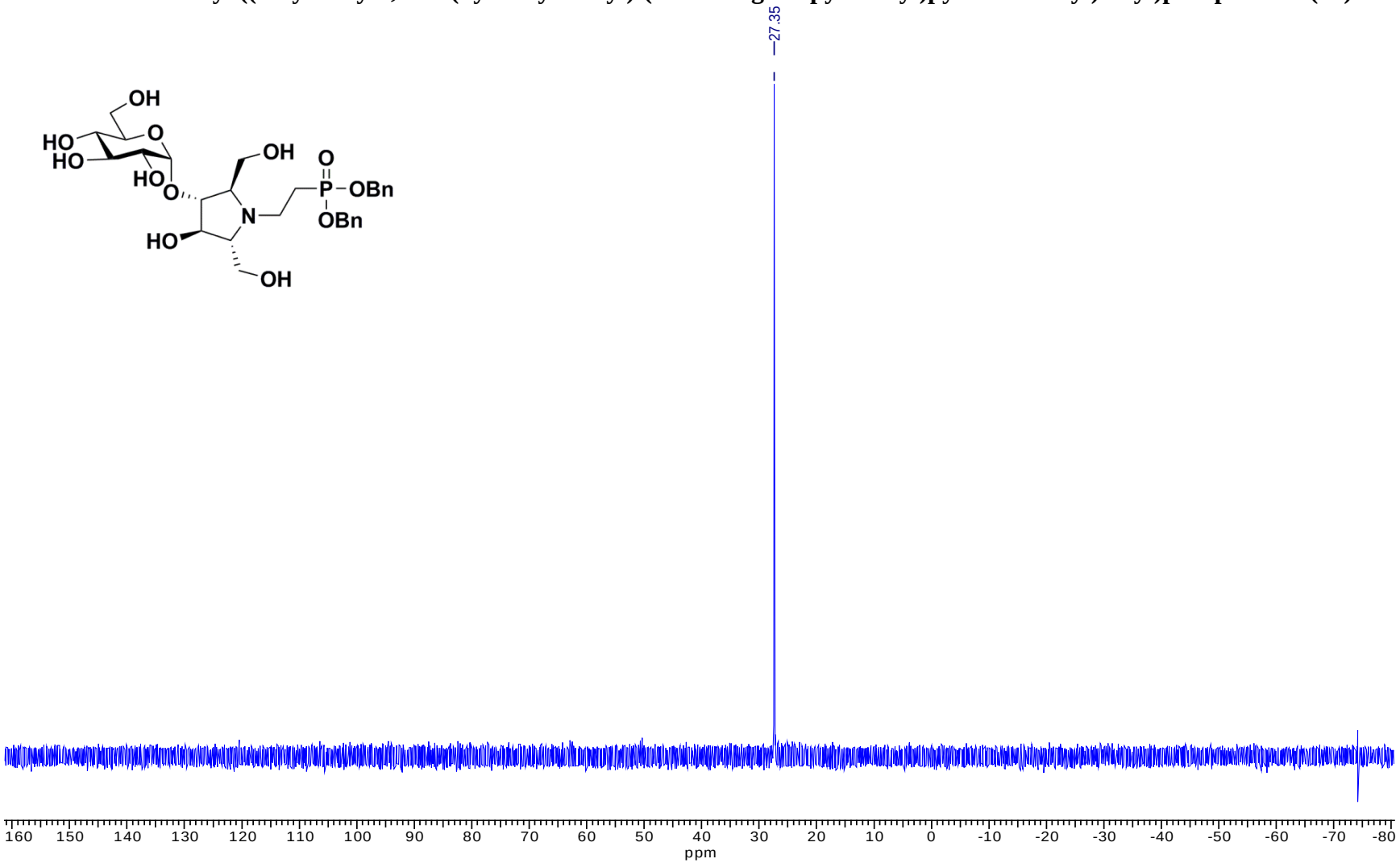
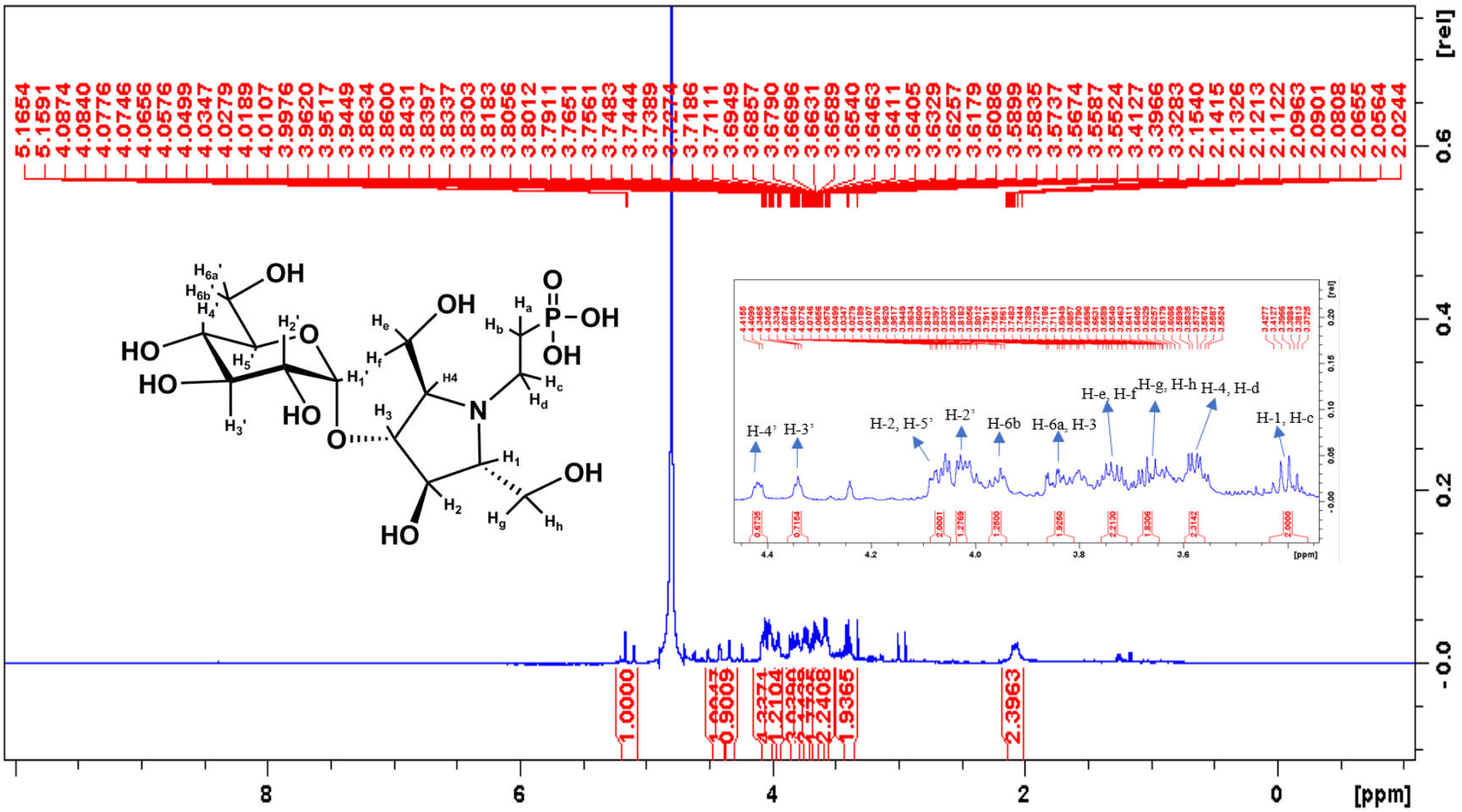


^{1}H NMR of ((3-hydroxy-2,5-bis(hydroxymethyl)-(3-*O*-α-D-glucopyranosyl)pyrrolidin-1-yl)ethyl)phosphonic acid (6)



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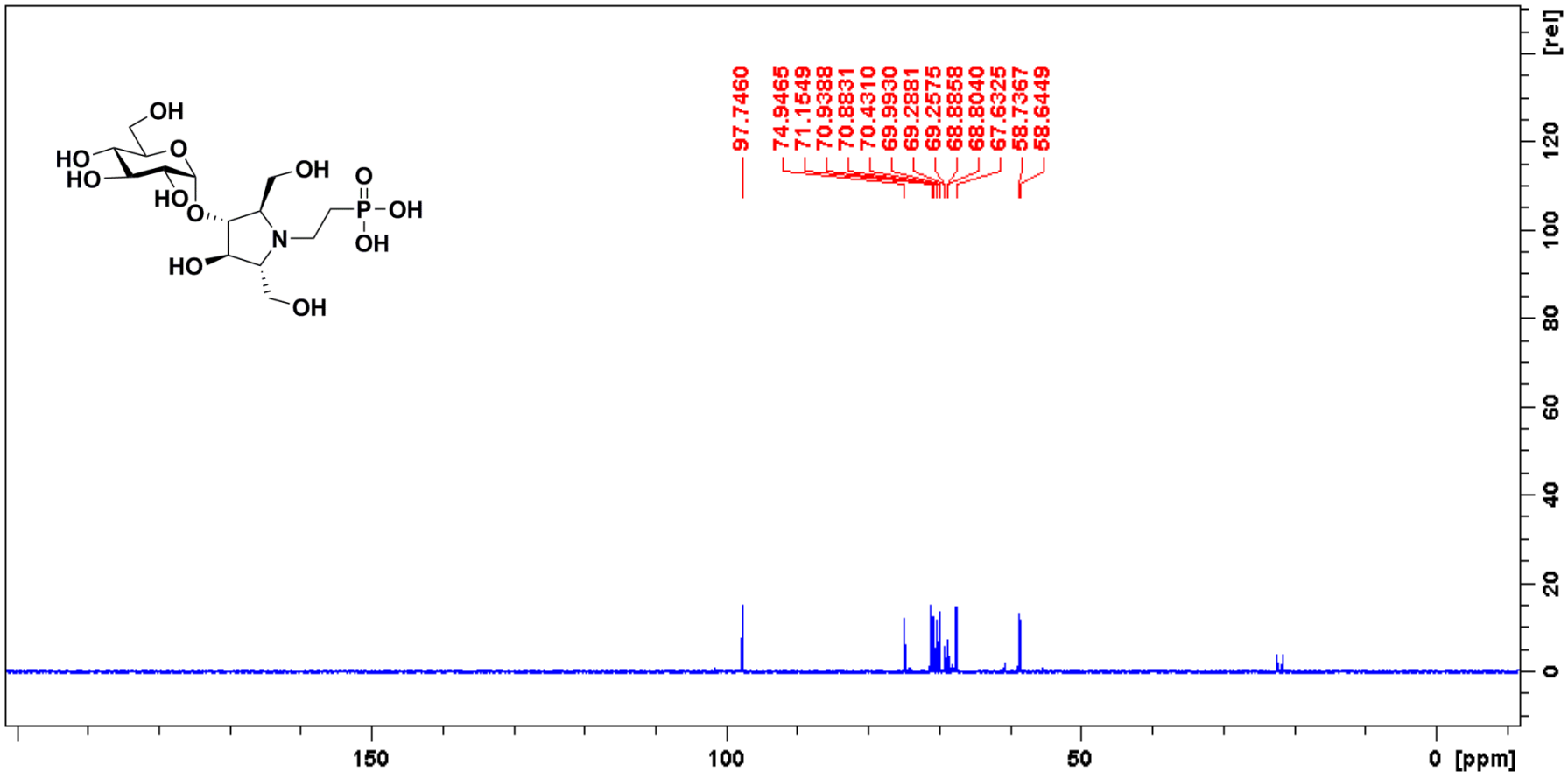

^{31}P NMR of ((3-hydroxy-2,5-bis(hydroxymethyl)-(3-*O*-α-D-glucopyranosyl)pyrrolidin-1-yl)ethyl)phosphonic acid (6)