Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting information for

Introduction of *C*-alkyl branches to L-iminosugars changes their active site binding orientation

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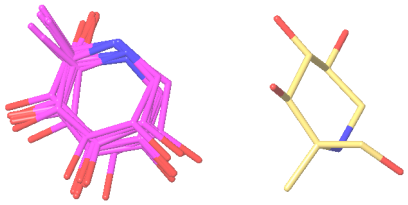
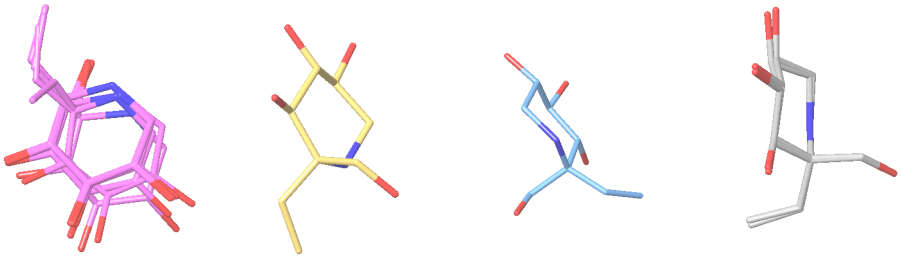
Figure S1 docking score top 10 poses generated by the docking analyses.

5-*C*-Methyl-L-*ido*-DNJ



5-*C*-Ethyl-L-*ido*-DNJ



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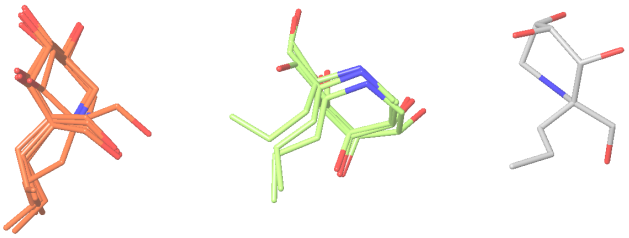

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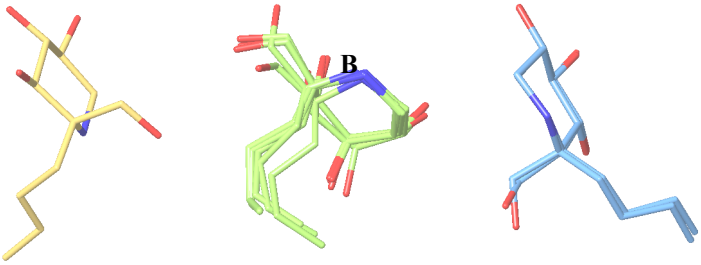

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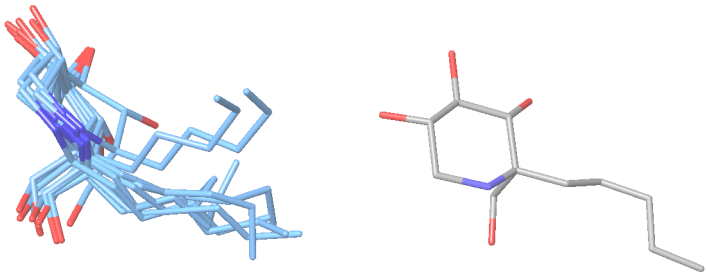


5-*C*-Hexyl-L-*ido*-DNJ

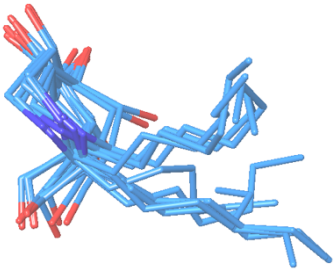
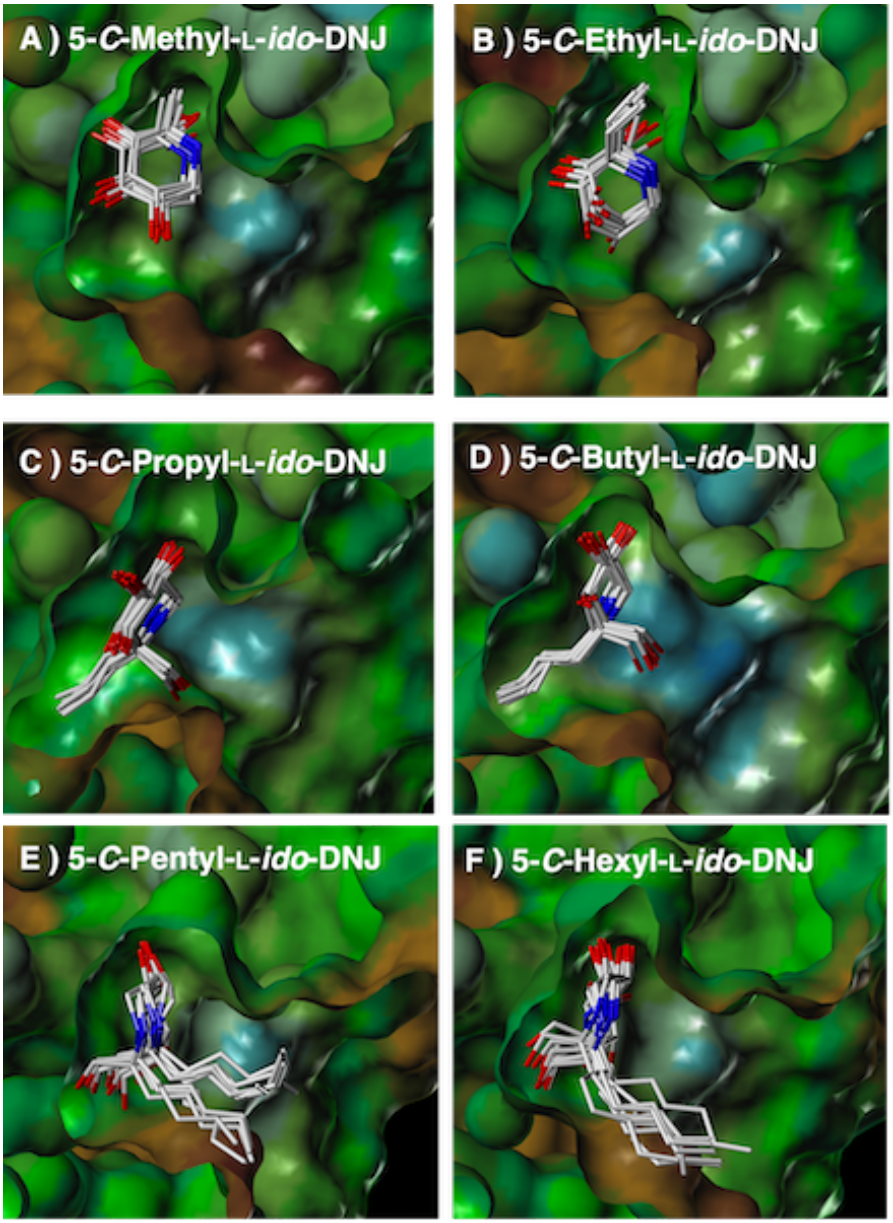


Figure S2 The binding poses of 5-*C*-alkyl-L-ido-DNJs extracted from the MD trajectory.

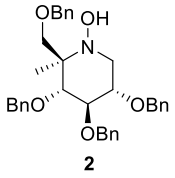


The molecular surfaces of GAA are rendered by lipophilic potential.

The 10 binding poses sampled from the MD trajectory are shown.

Compound 2

768a



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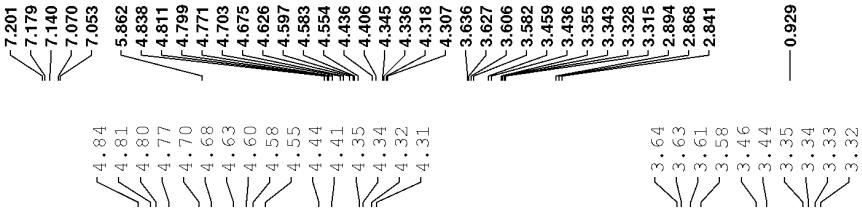

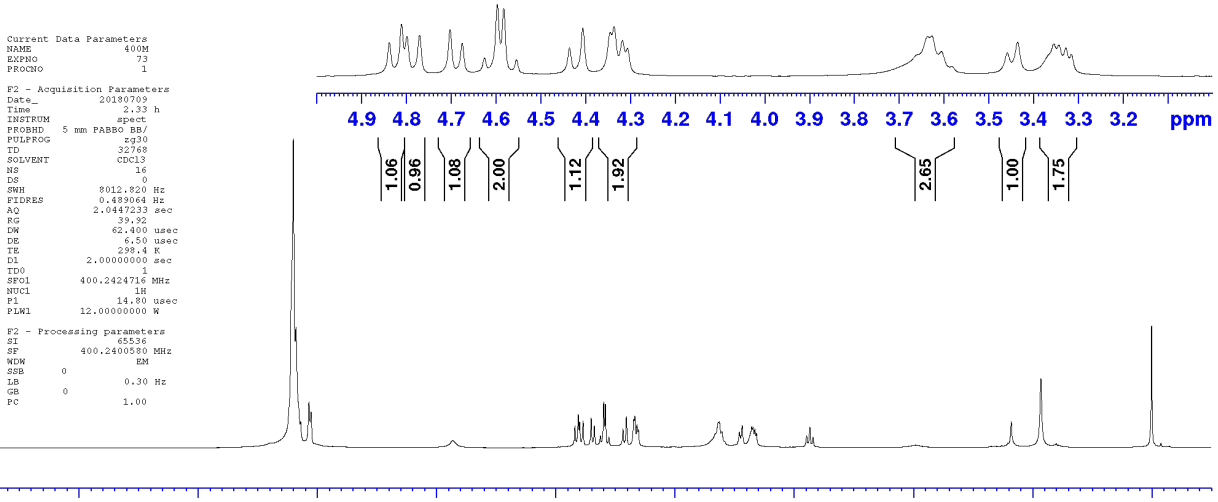

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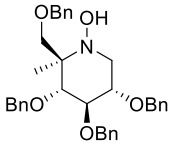

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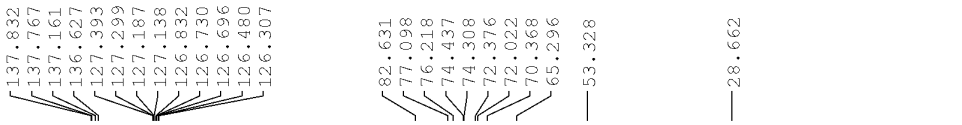
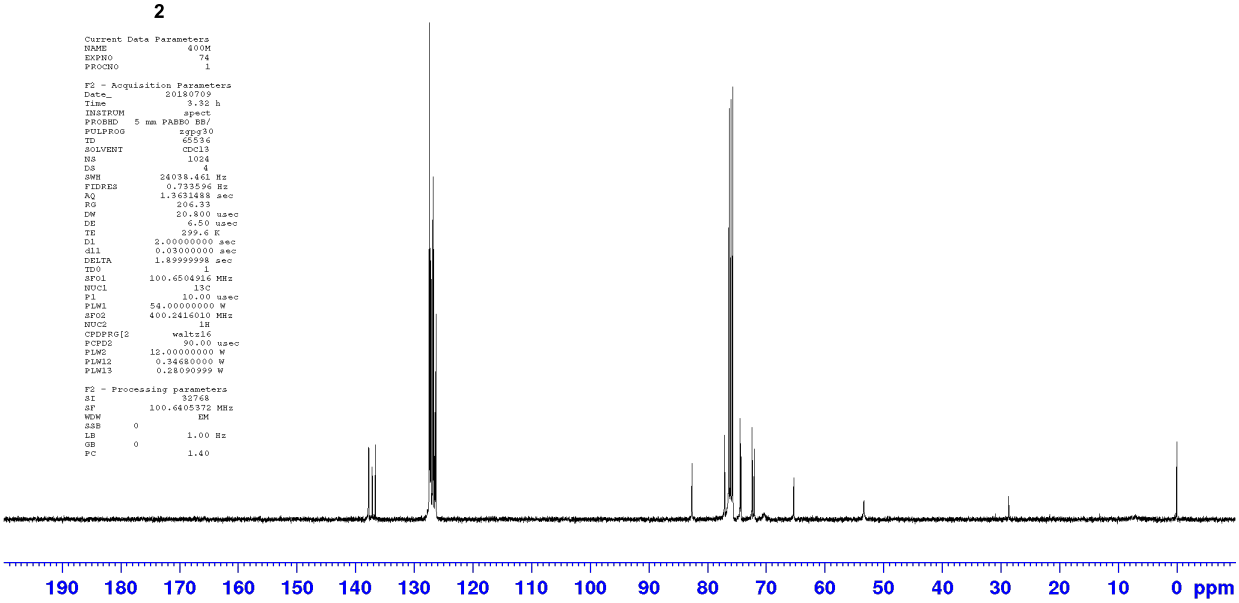
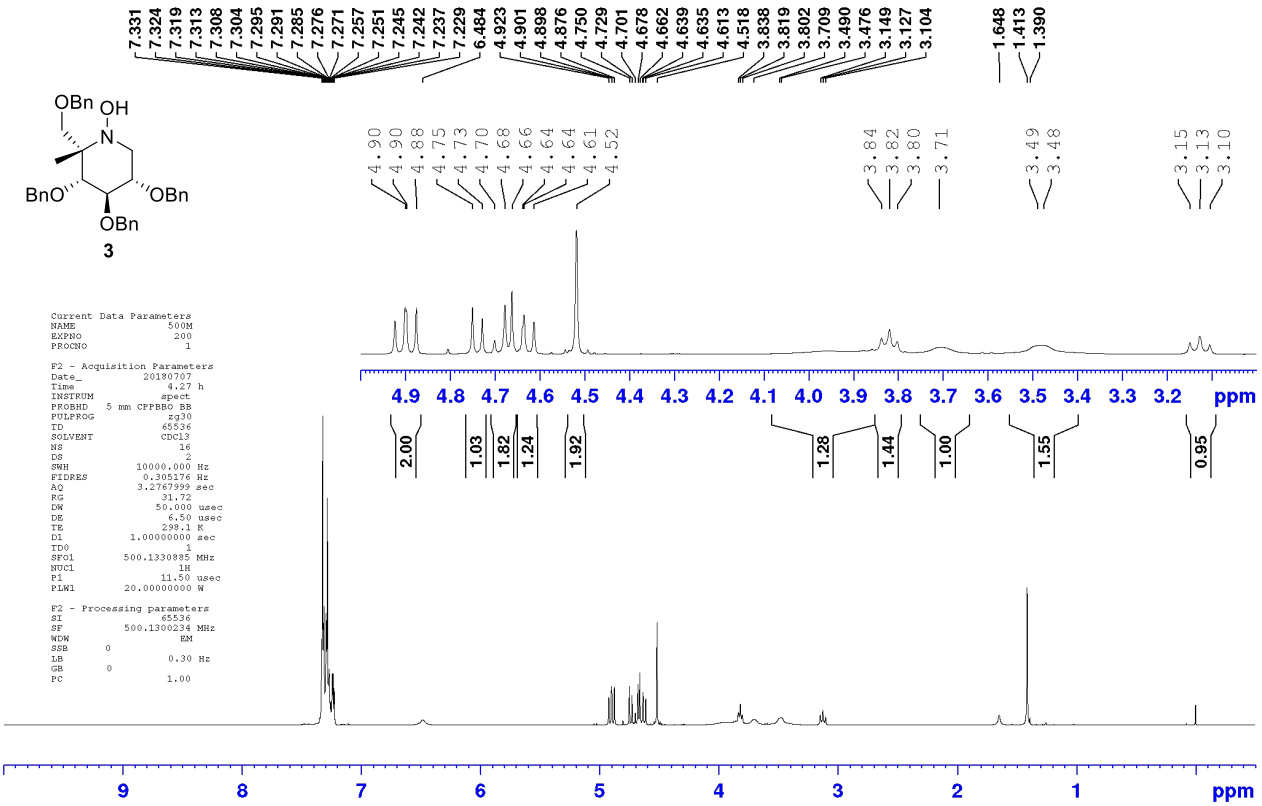




Compound 3

768b



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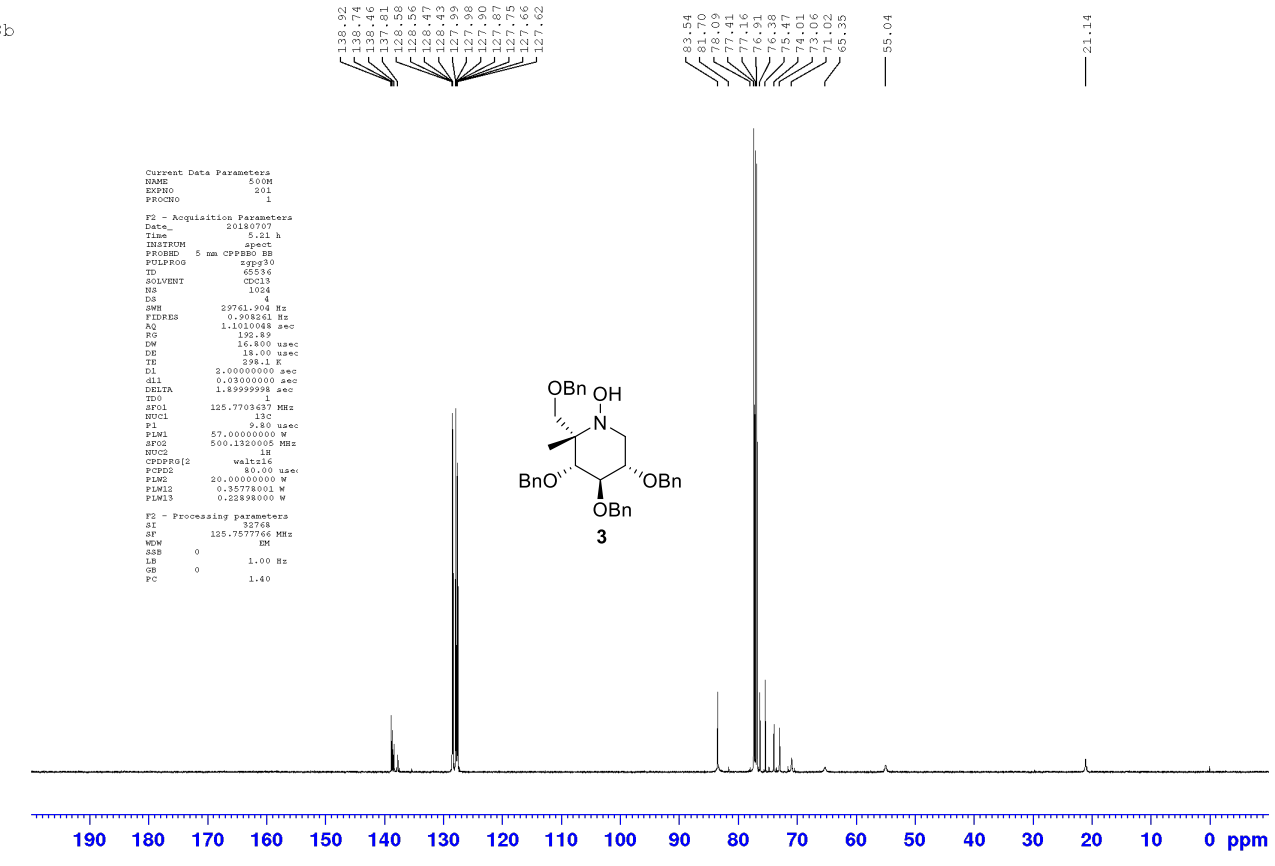
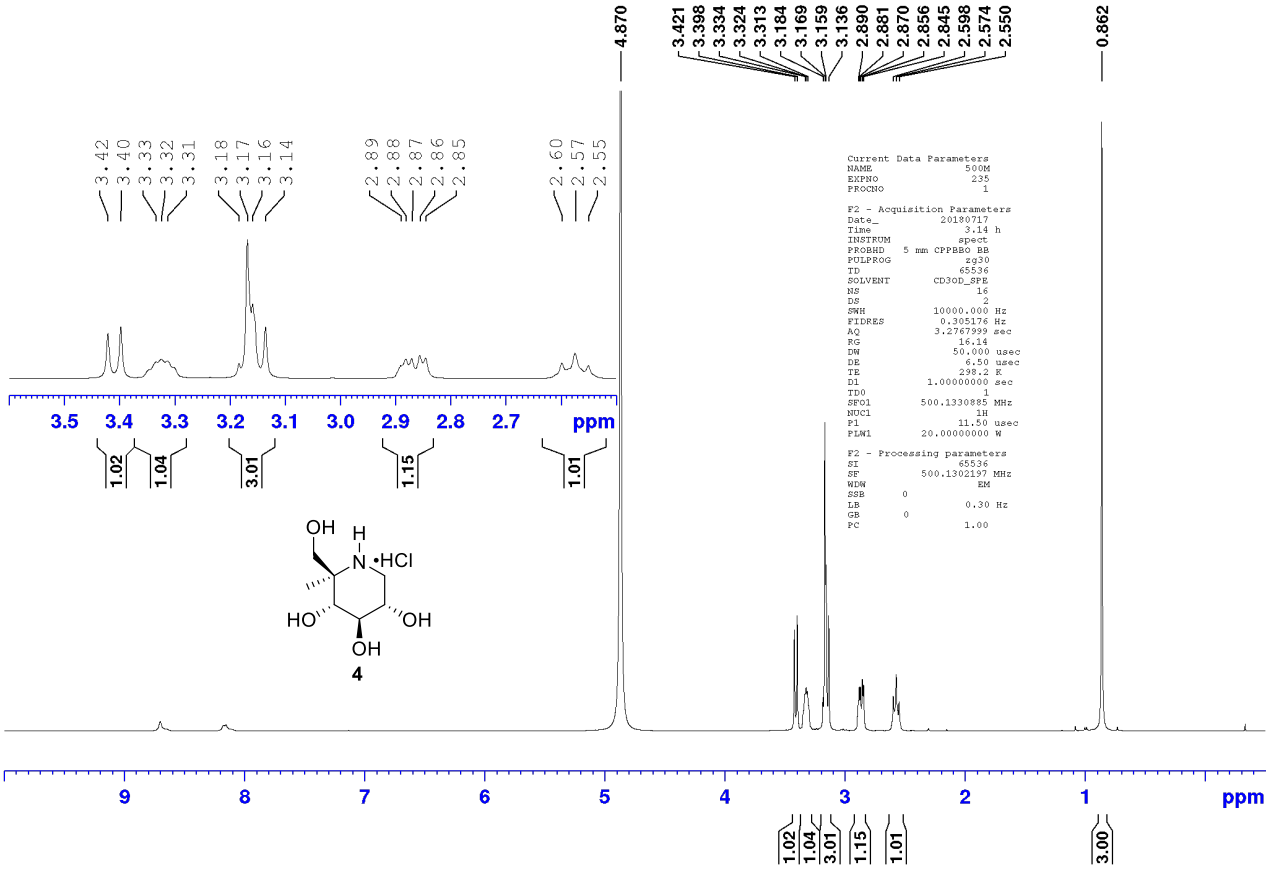


Compound 4

778



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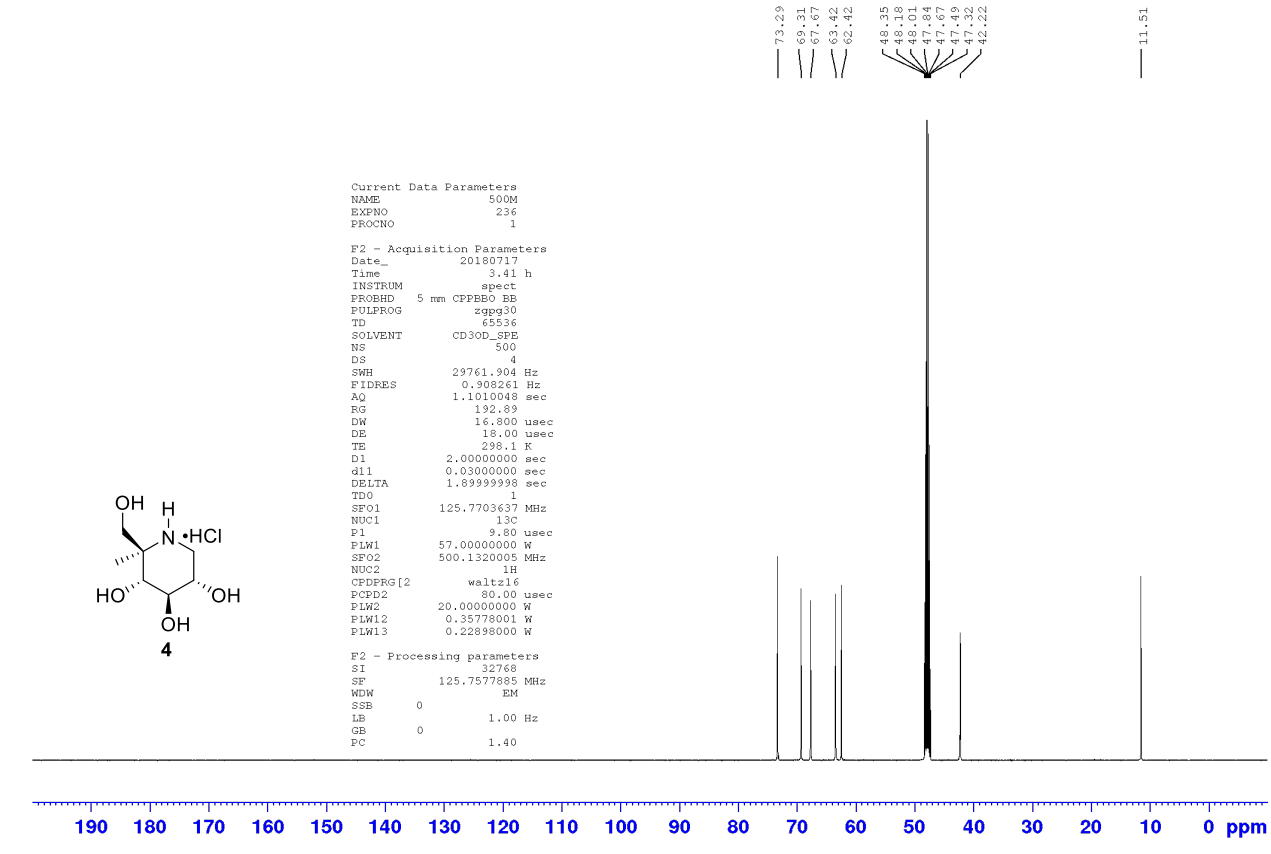

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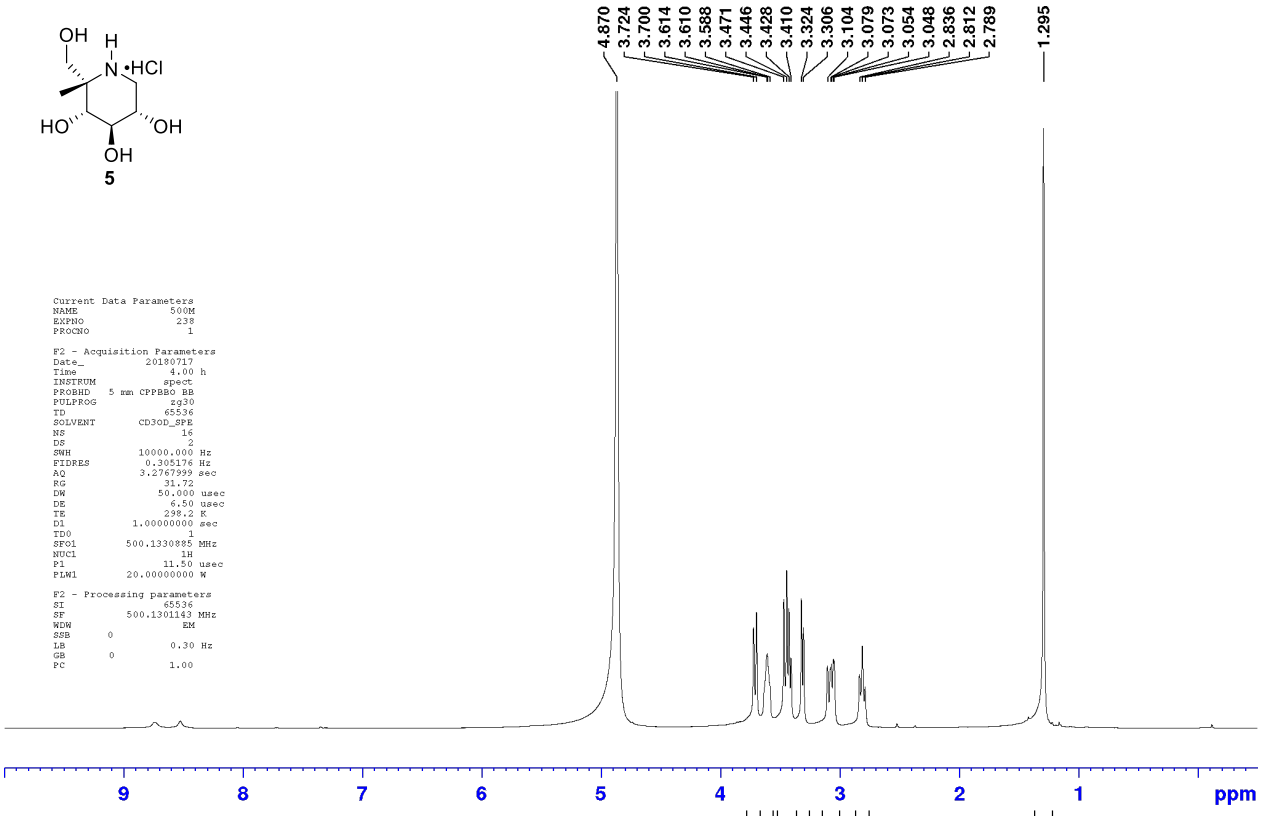

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