

Supporting Information to

**Synthesis of Mannoheptose Derivatives and their Evaluation as Inhibitors of the Lectin LecB
from the Opportunistic Pathogen *Pseudomonas aeruginosa***

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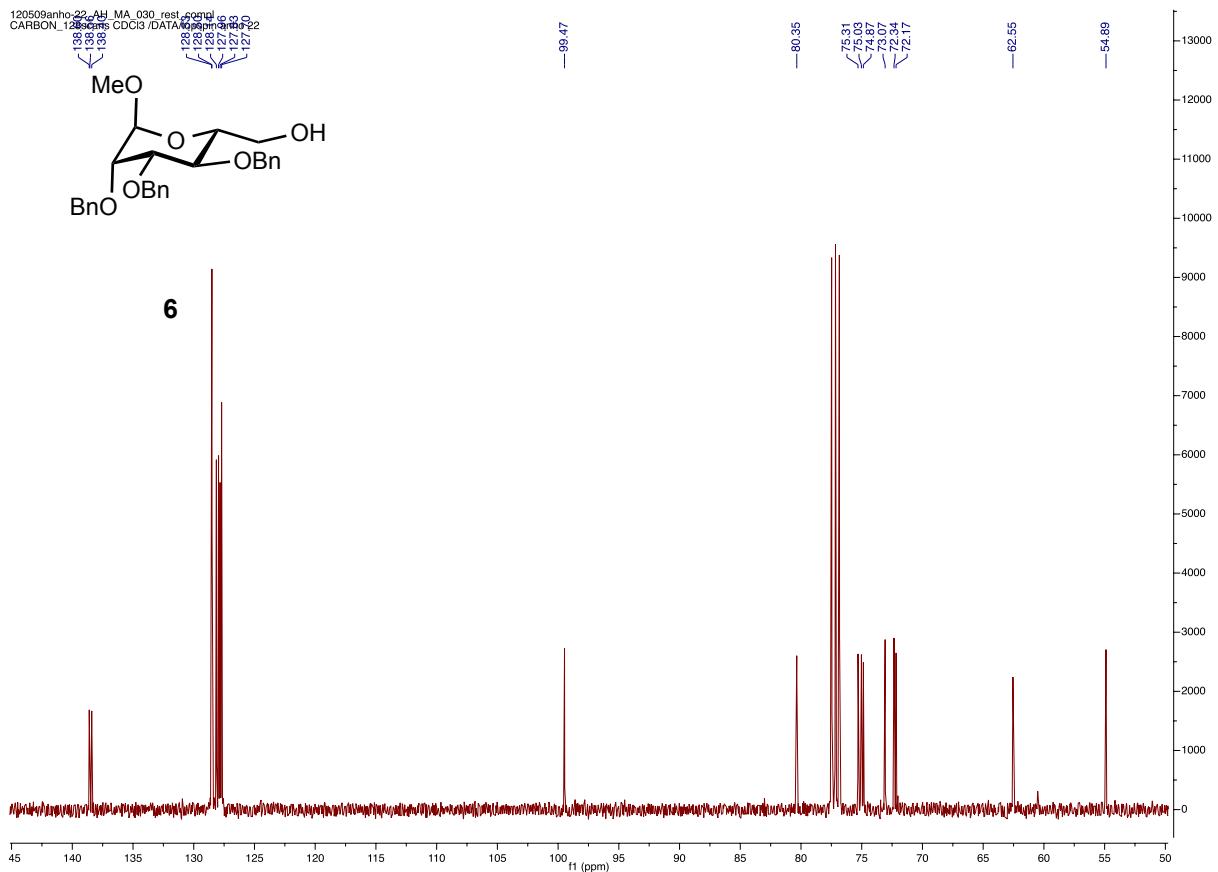
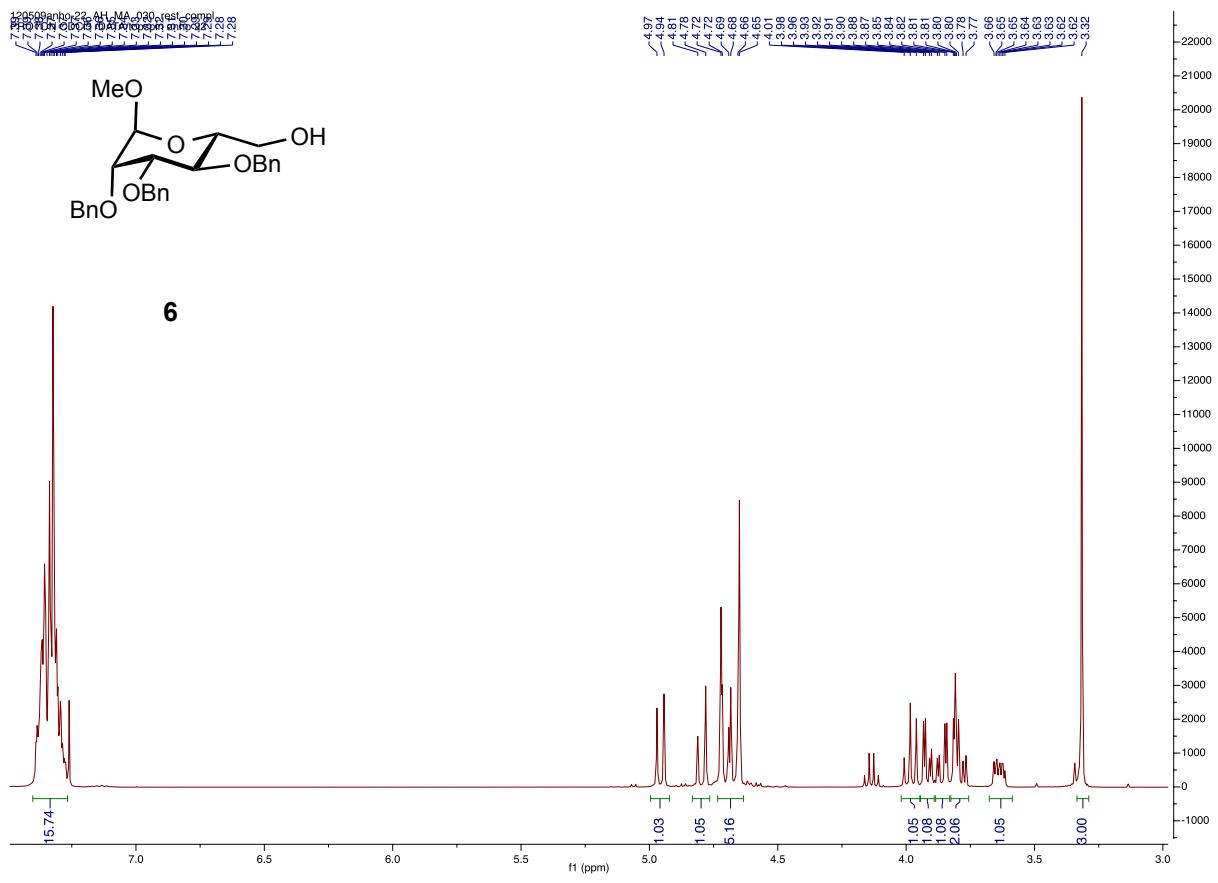
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Würzburg, Germany

#both authors contributed equally

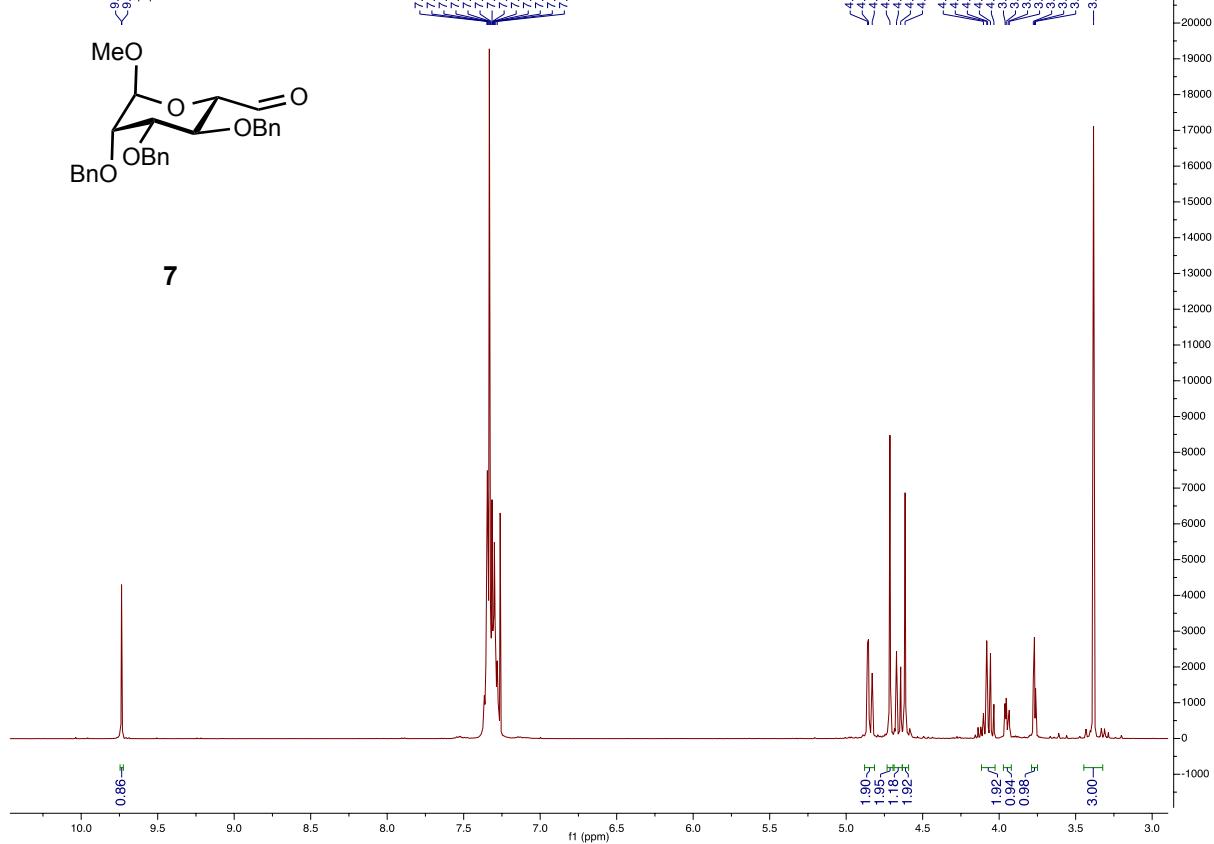
* corresponding author

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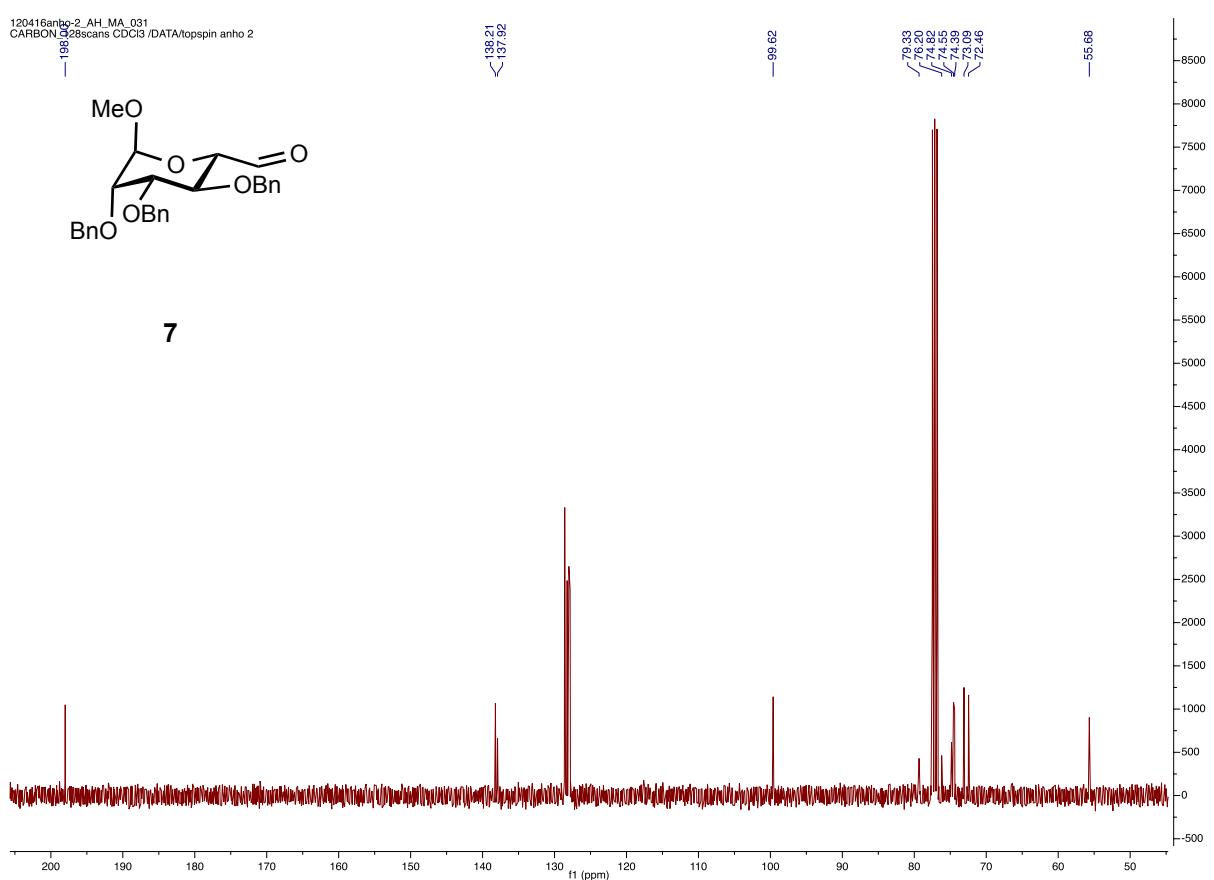
¹H-NMR and ¹³C-NMR traces of synthesized compounds

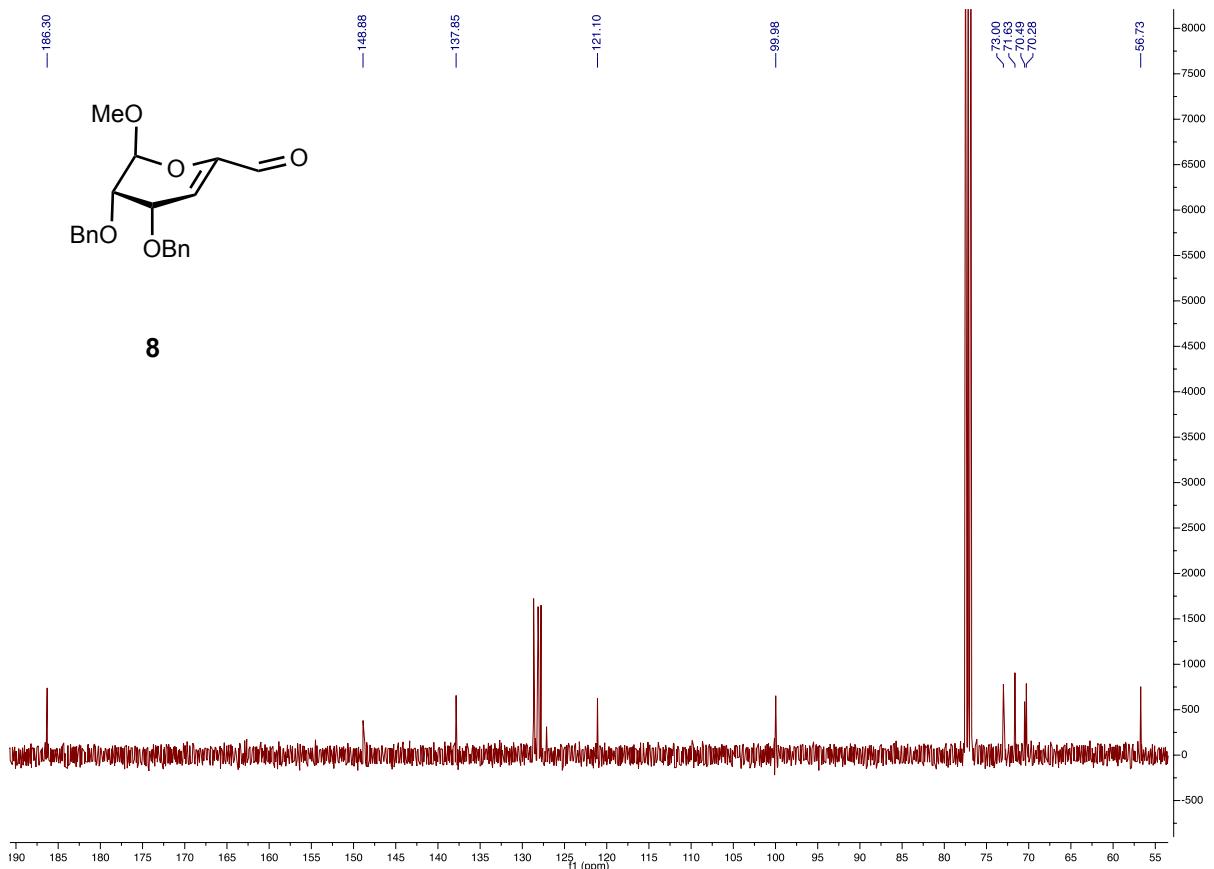
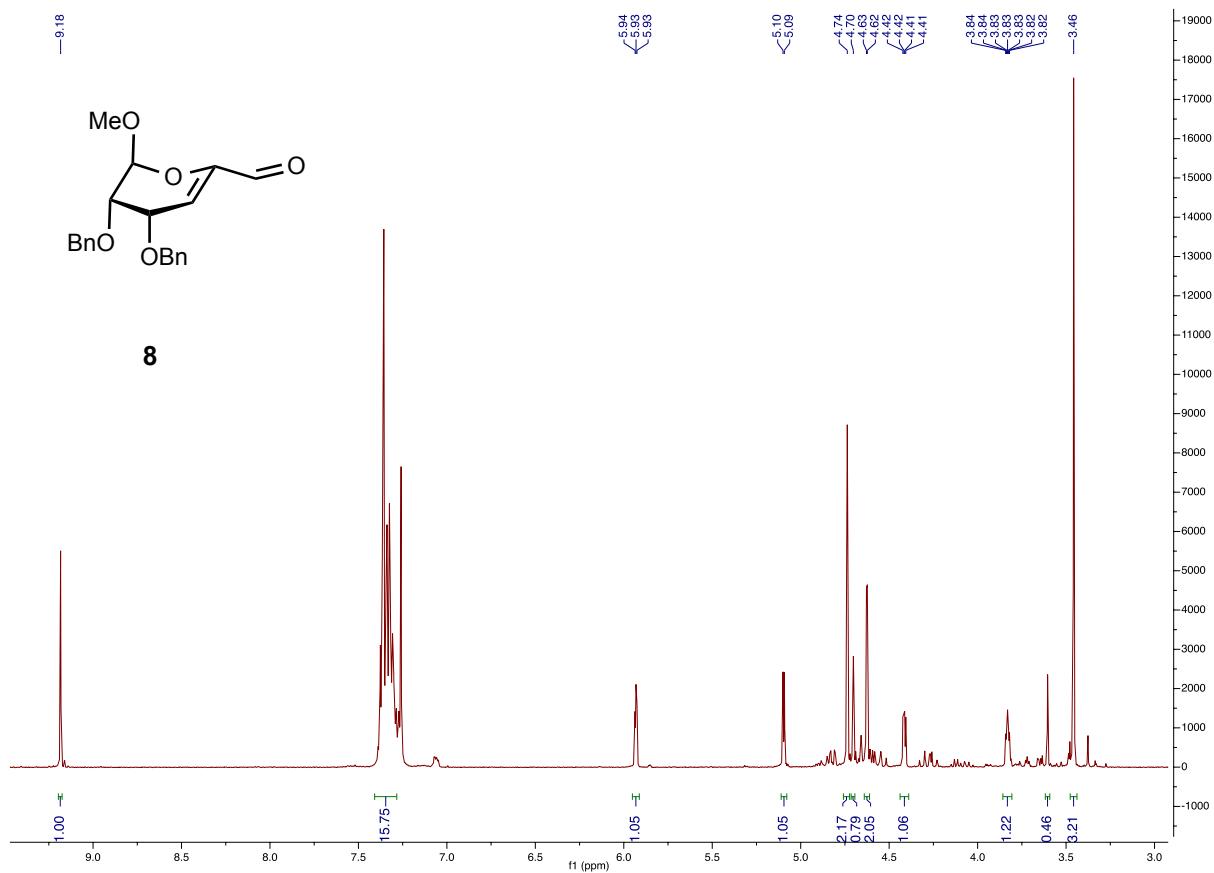


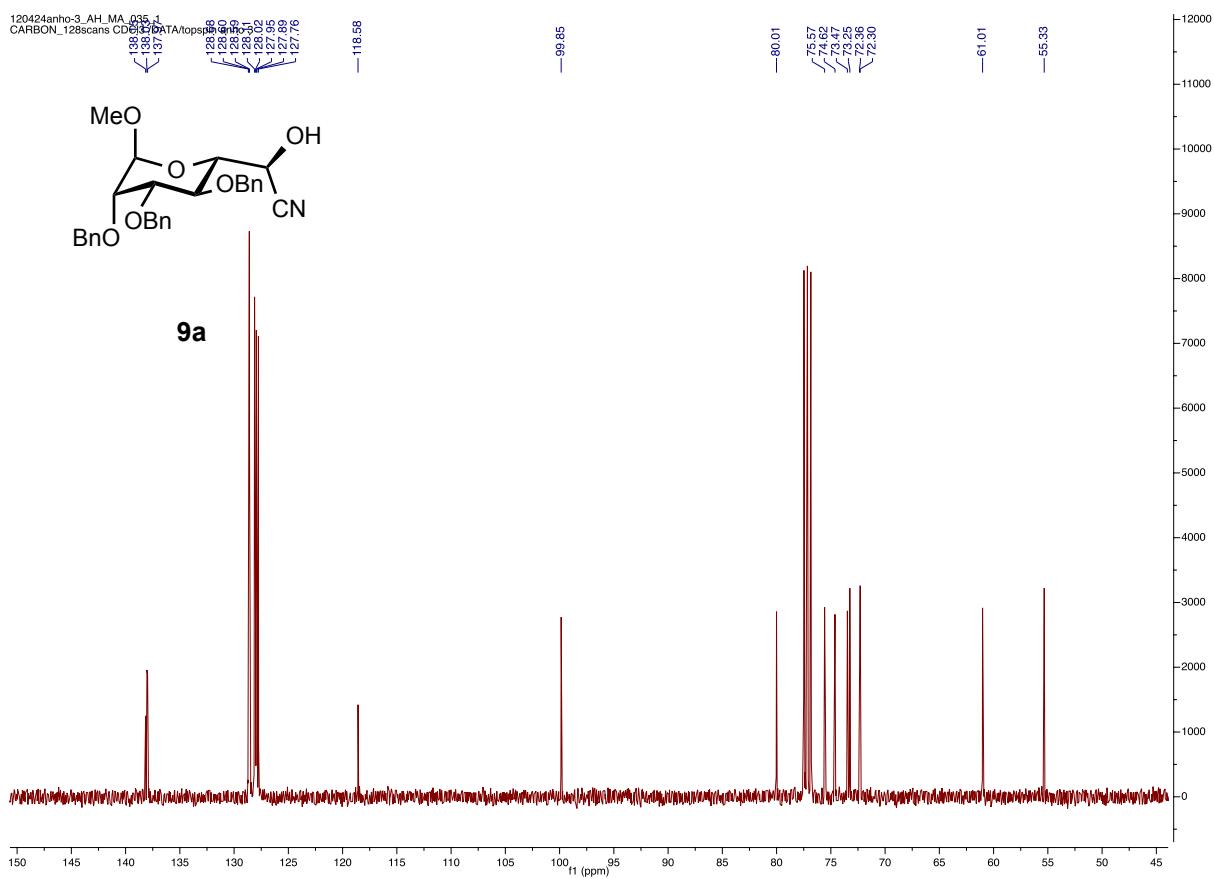
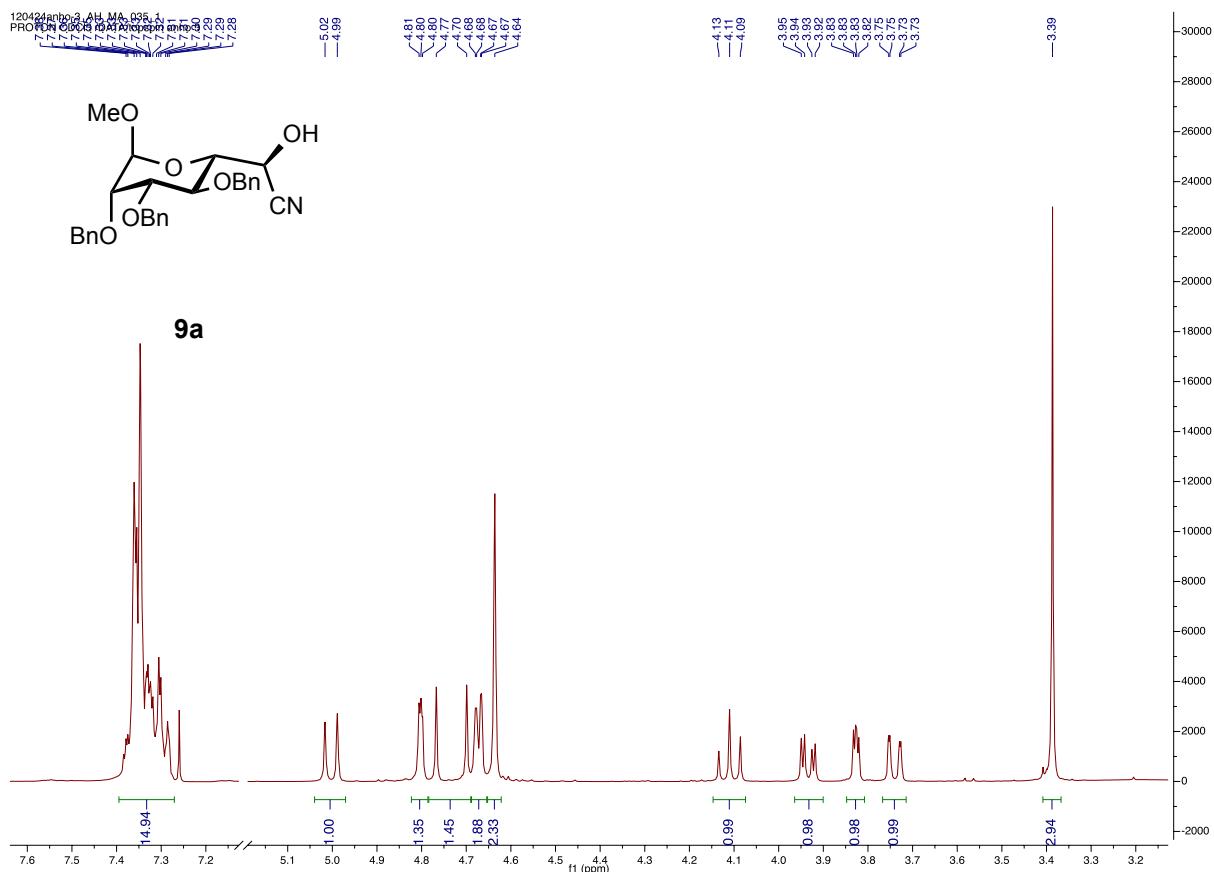
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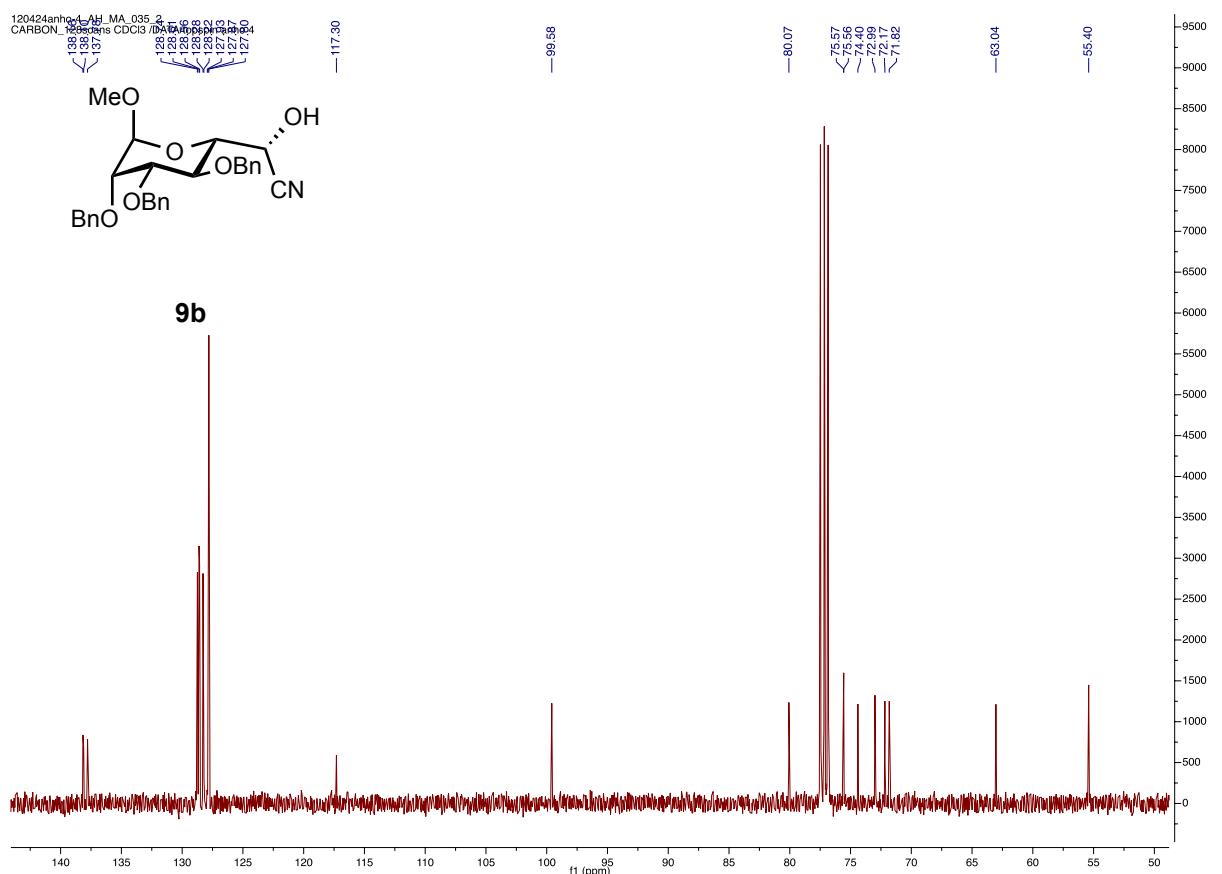
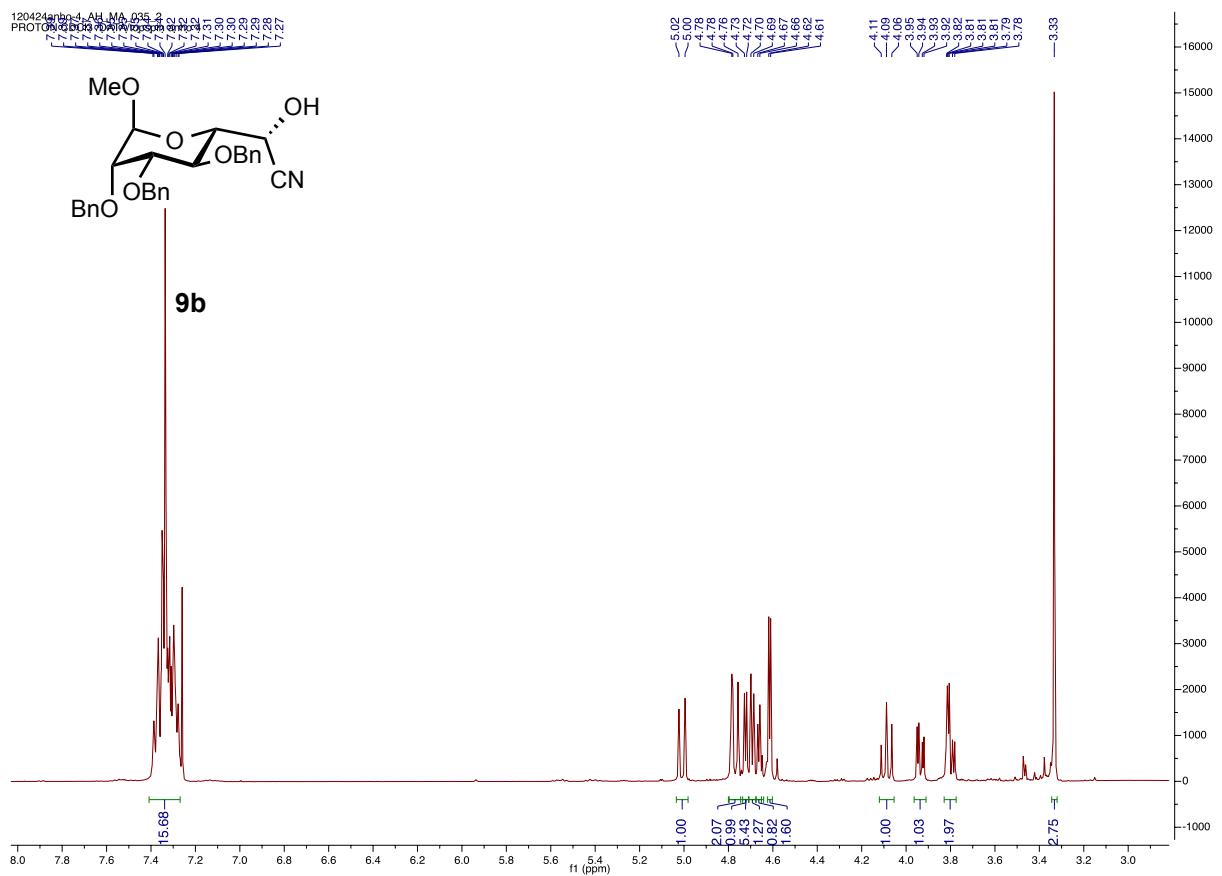


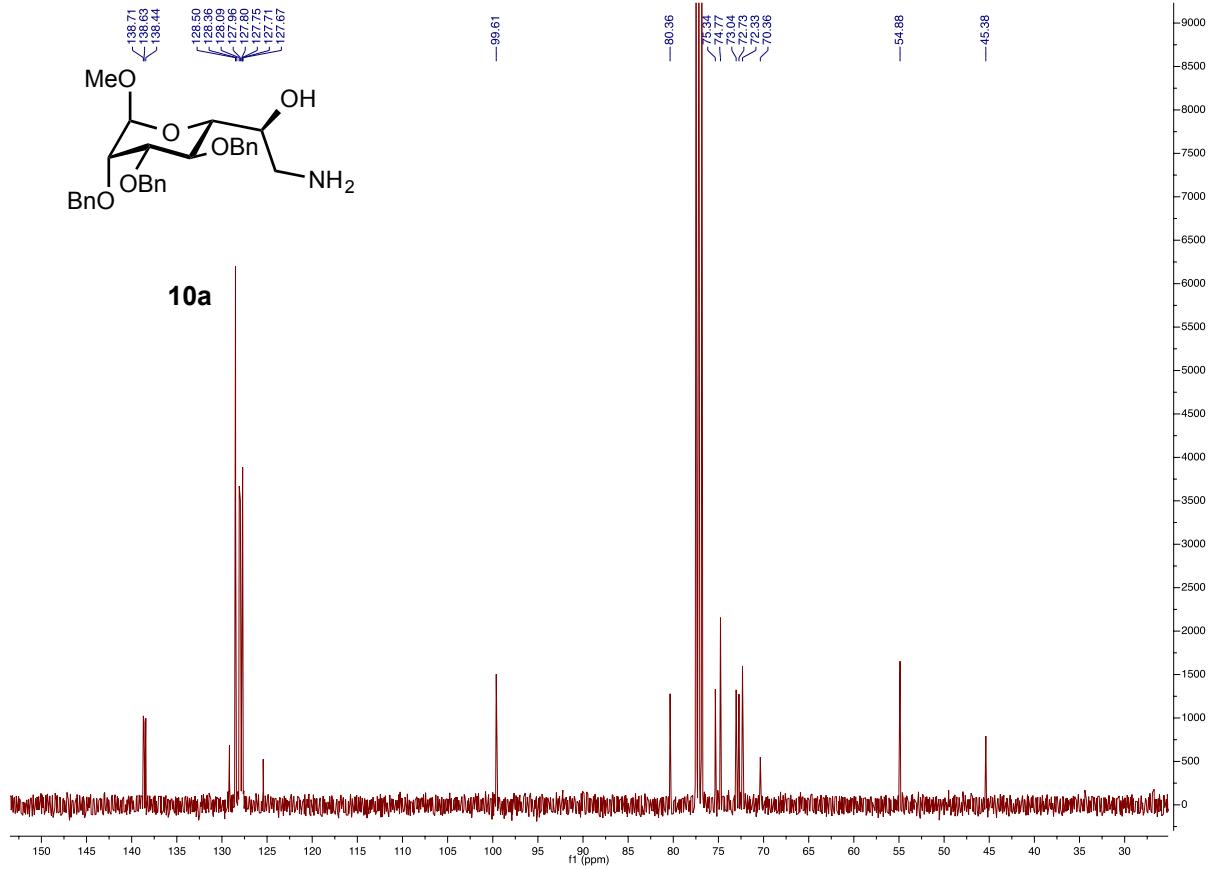
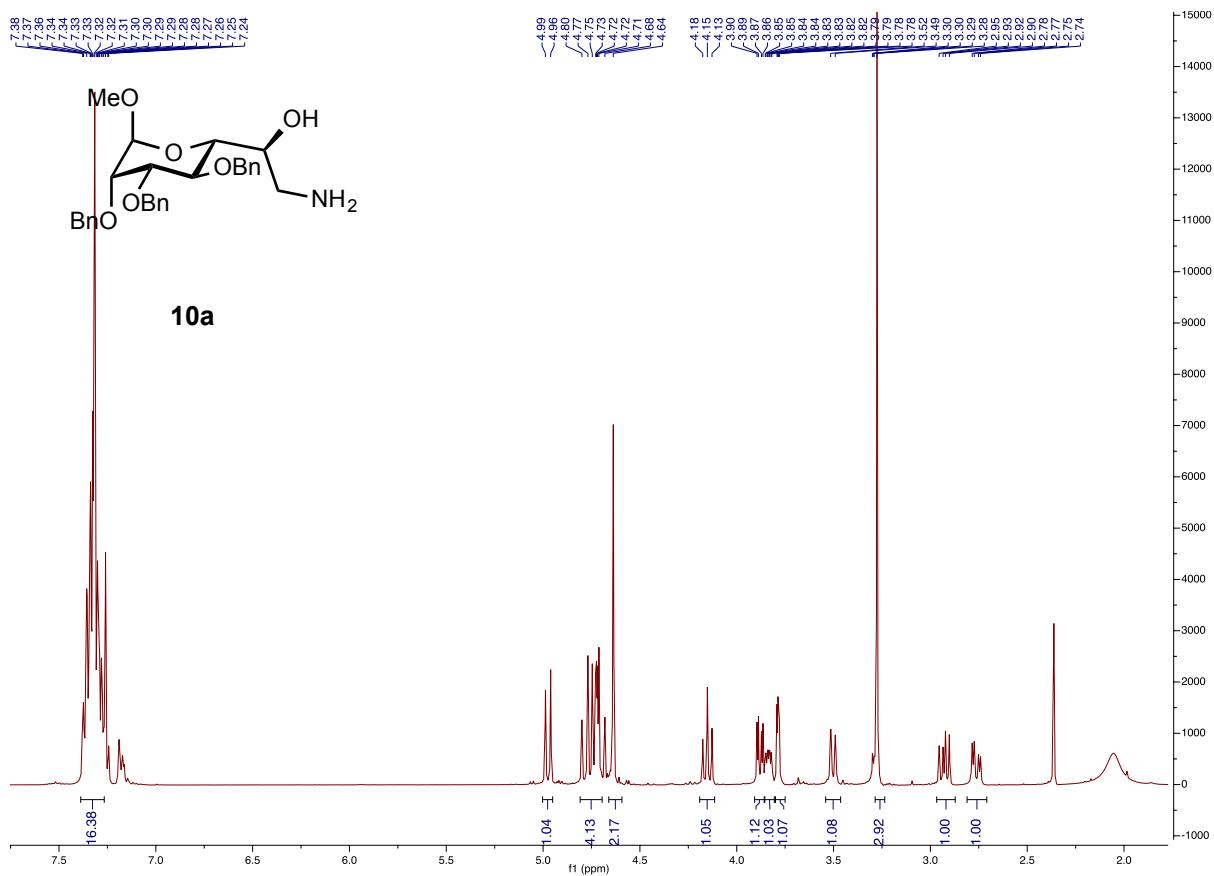
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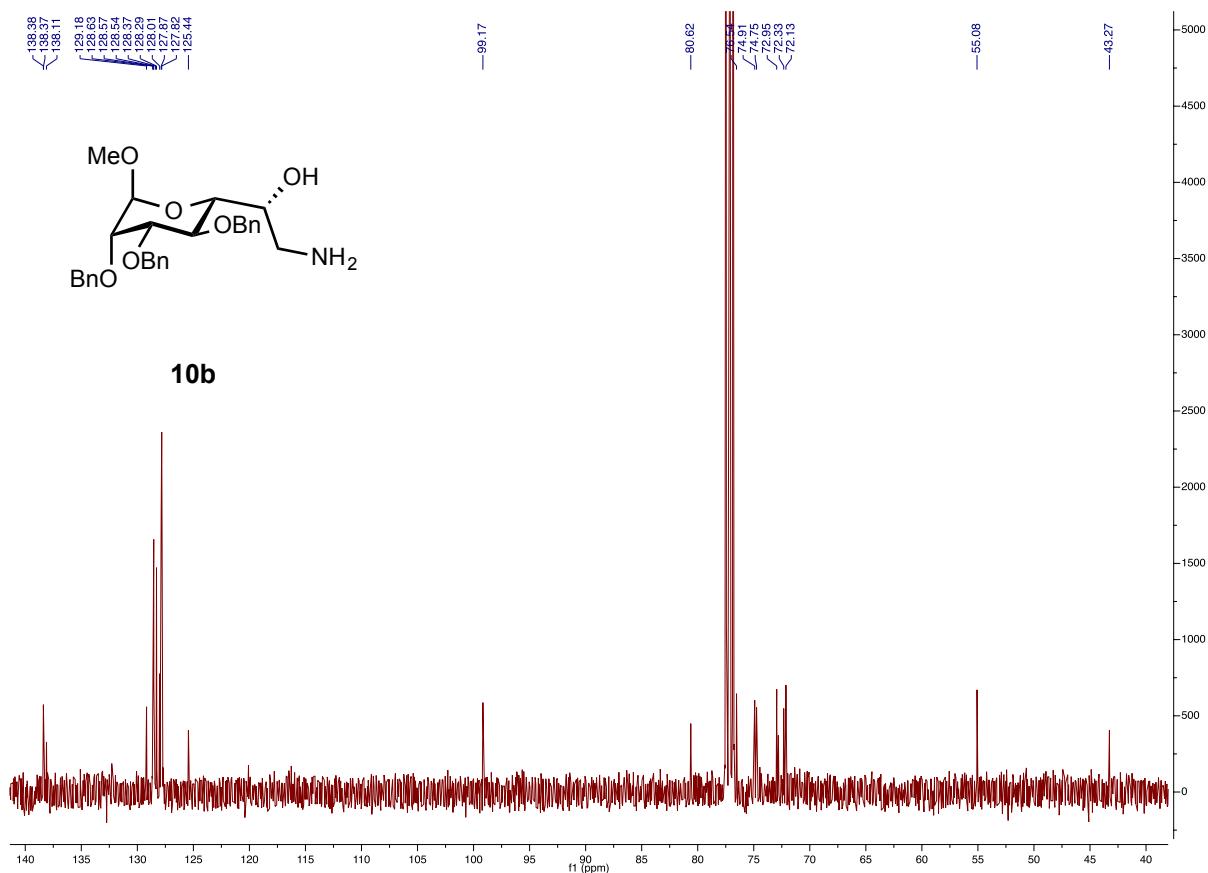
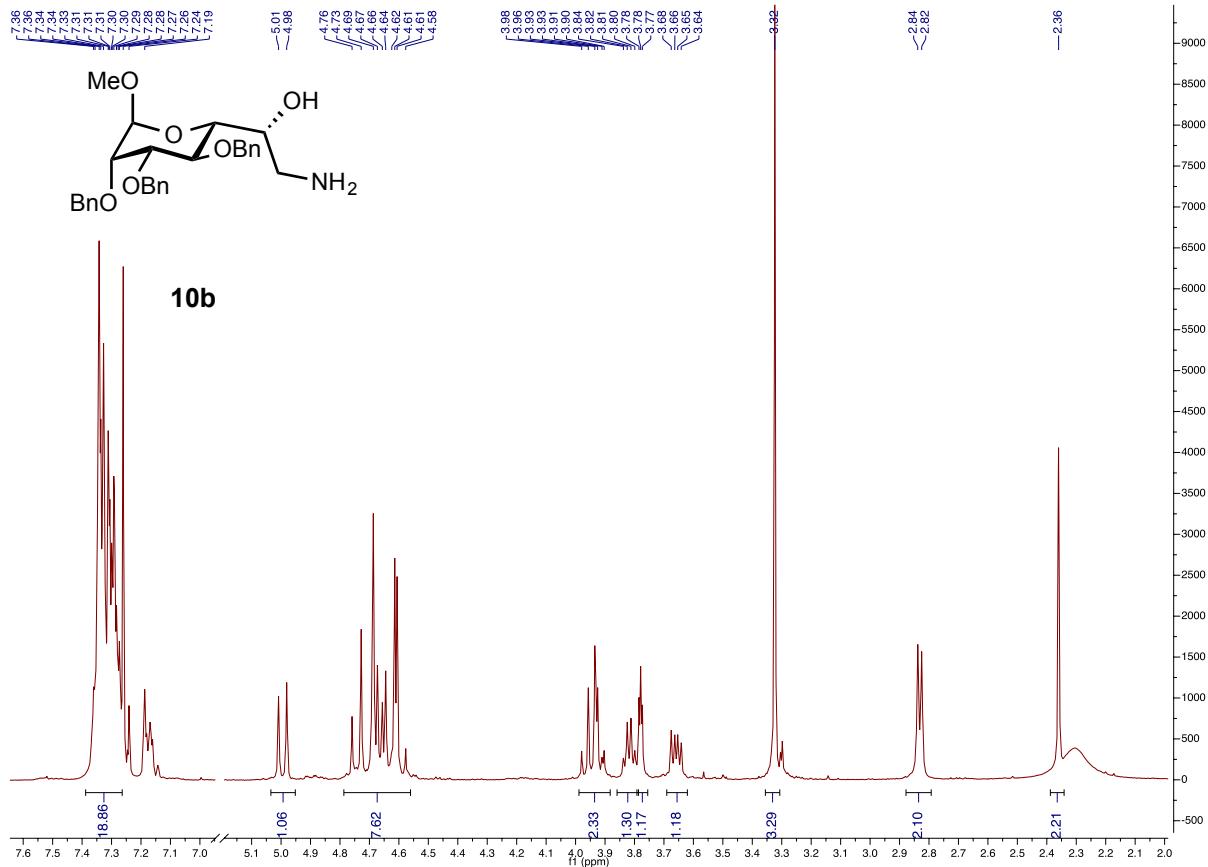


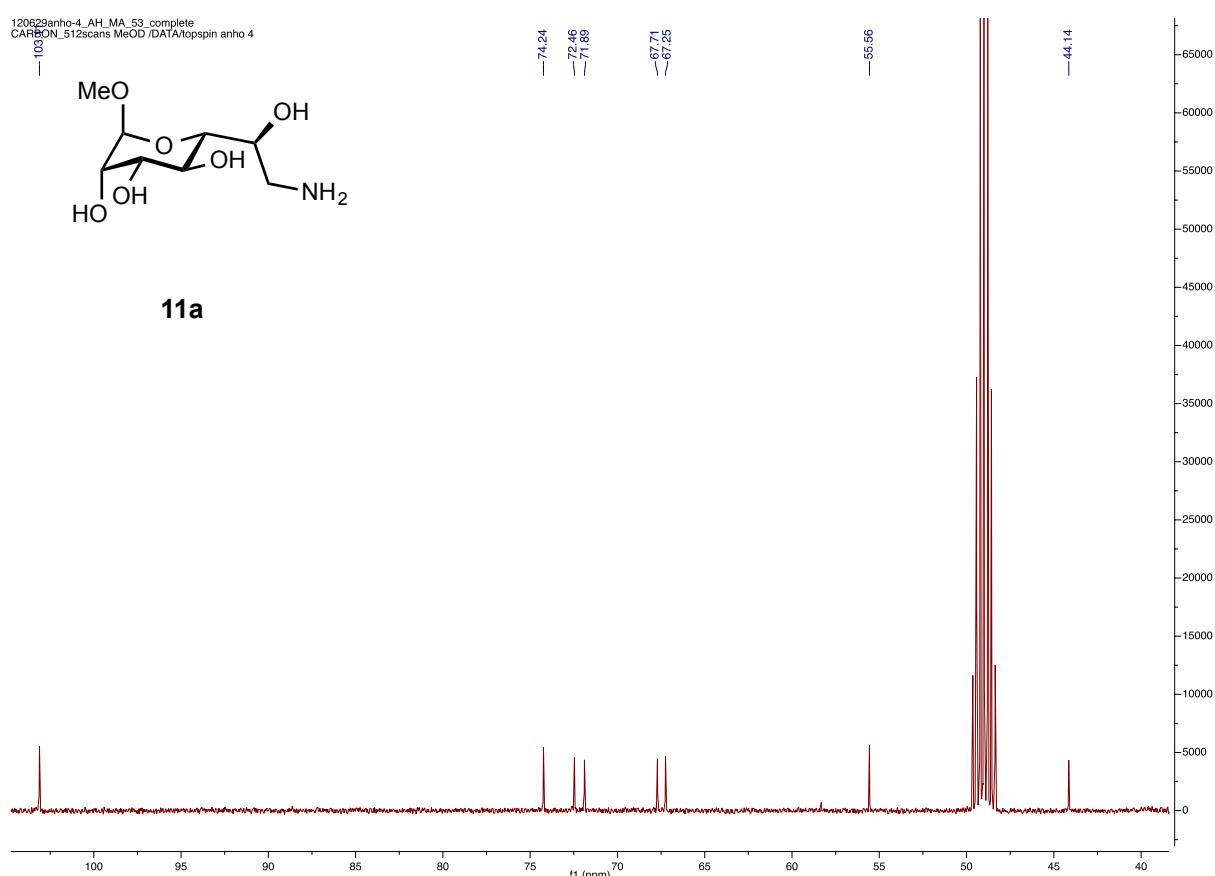
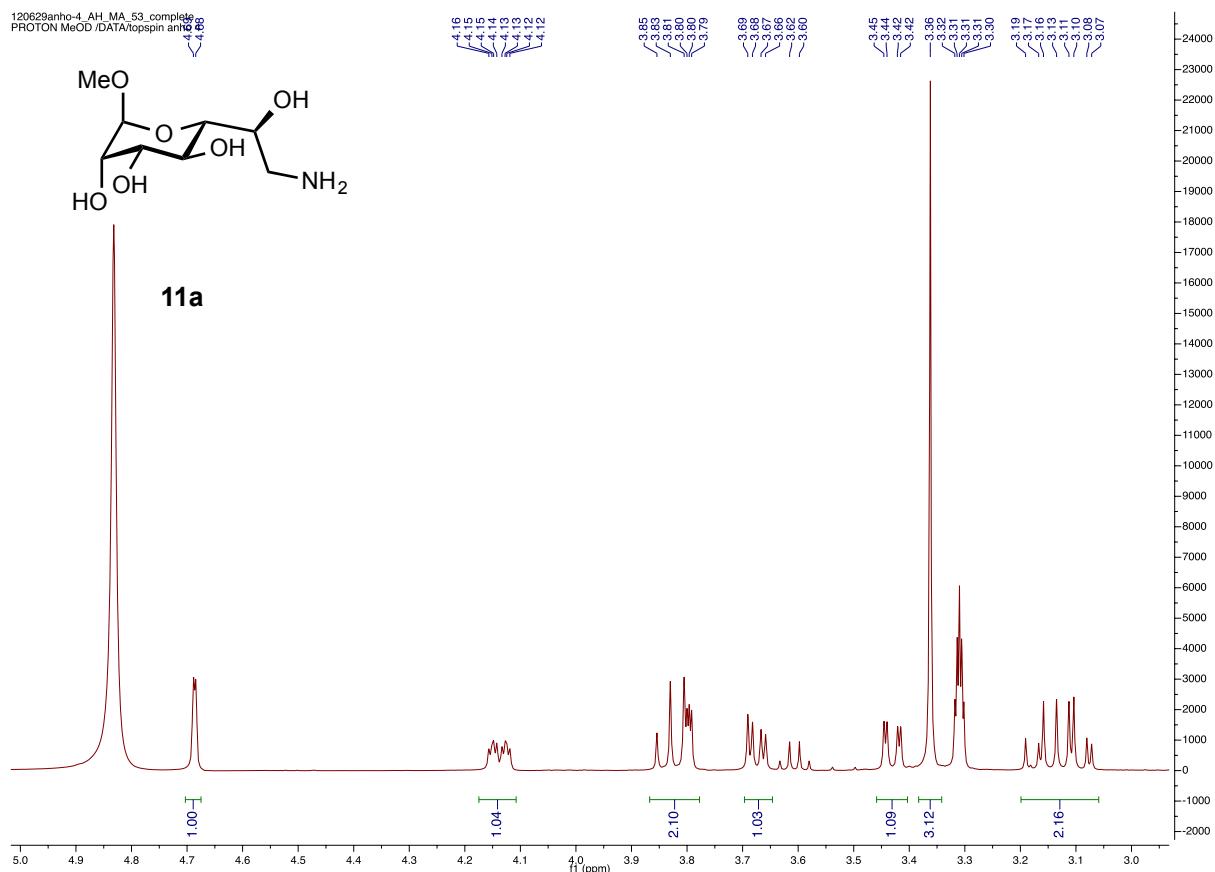


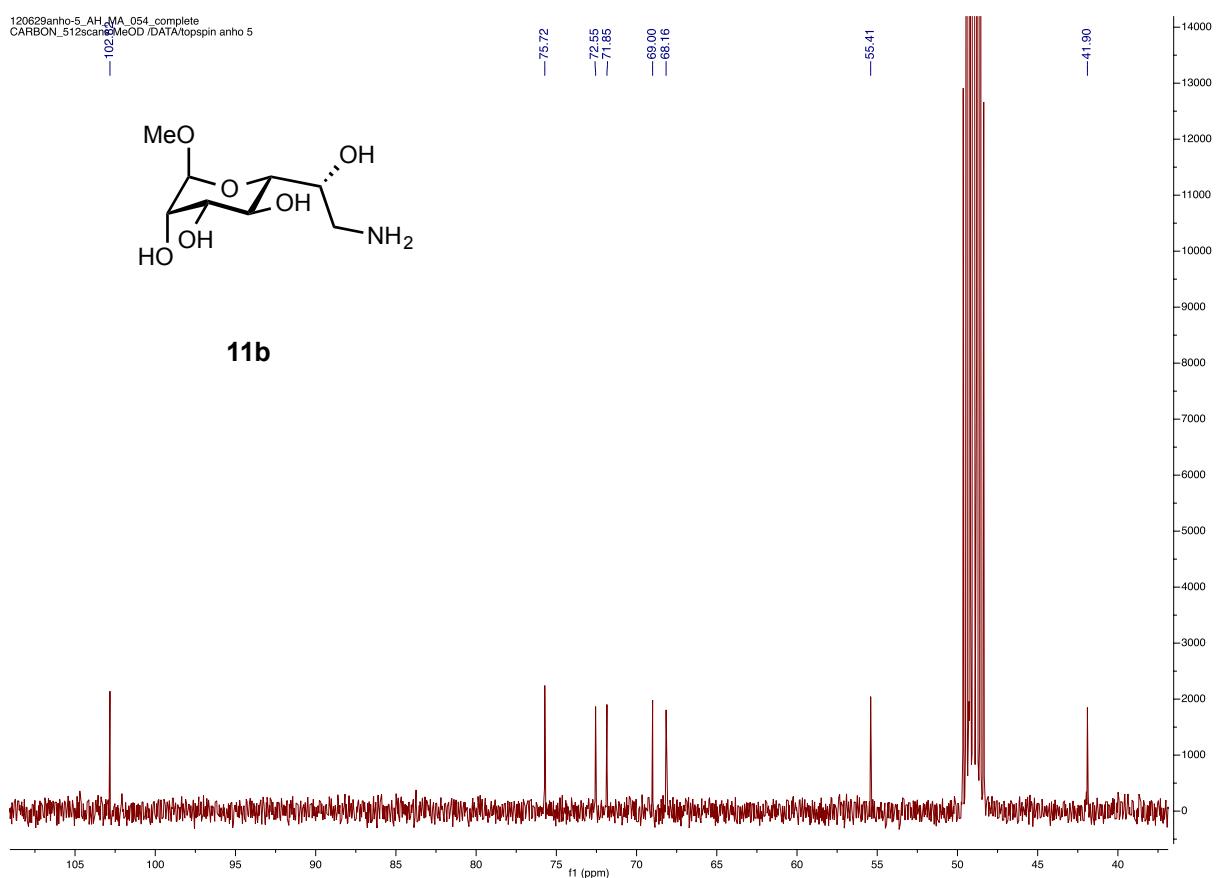
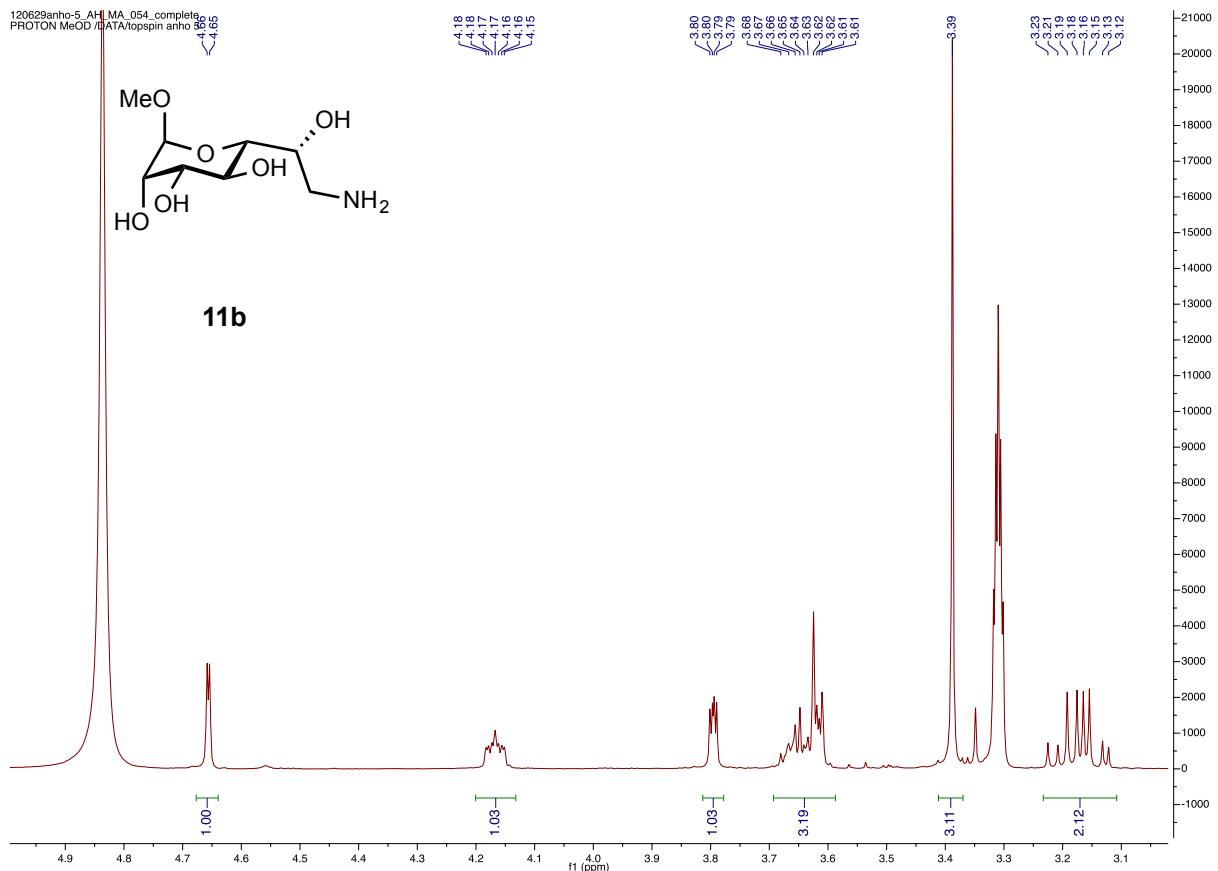


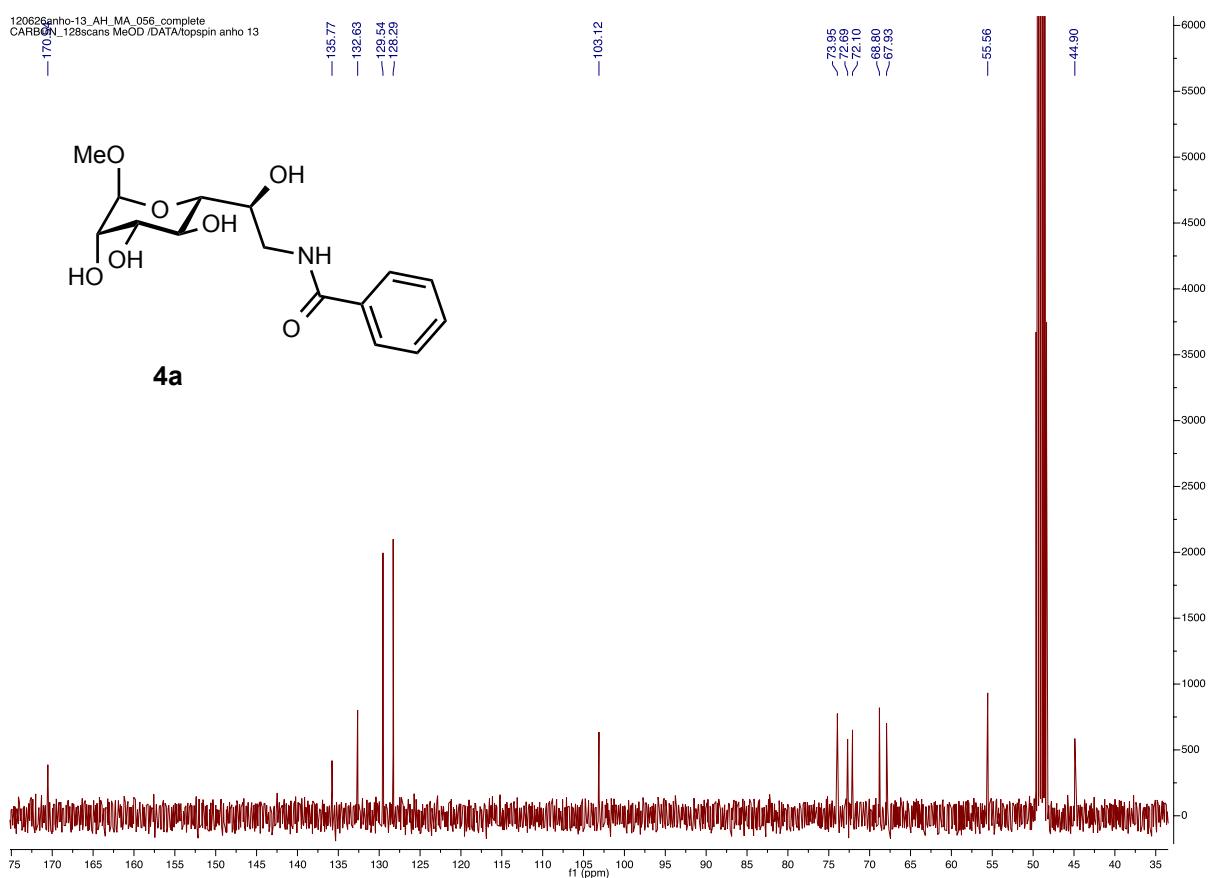
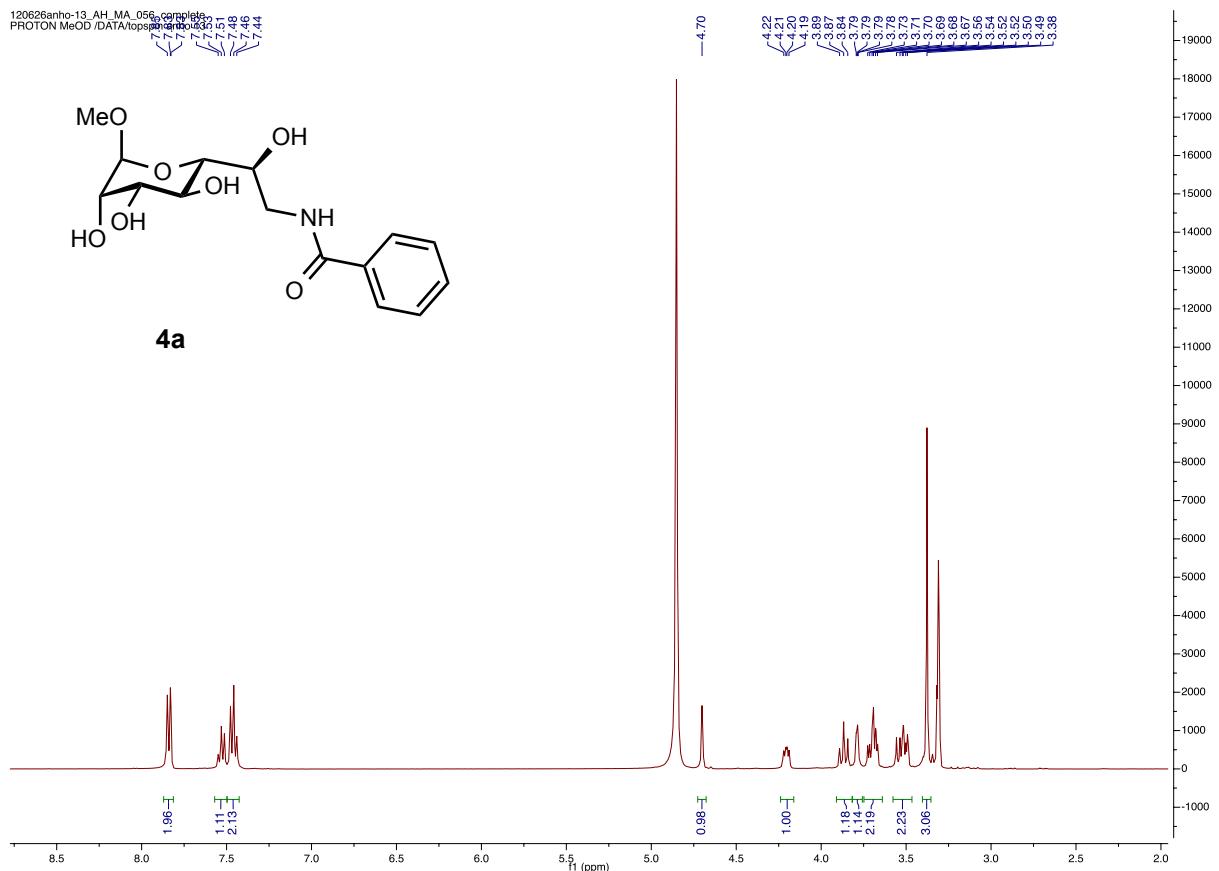


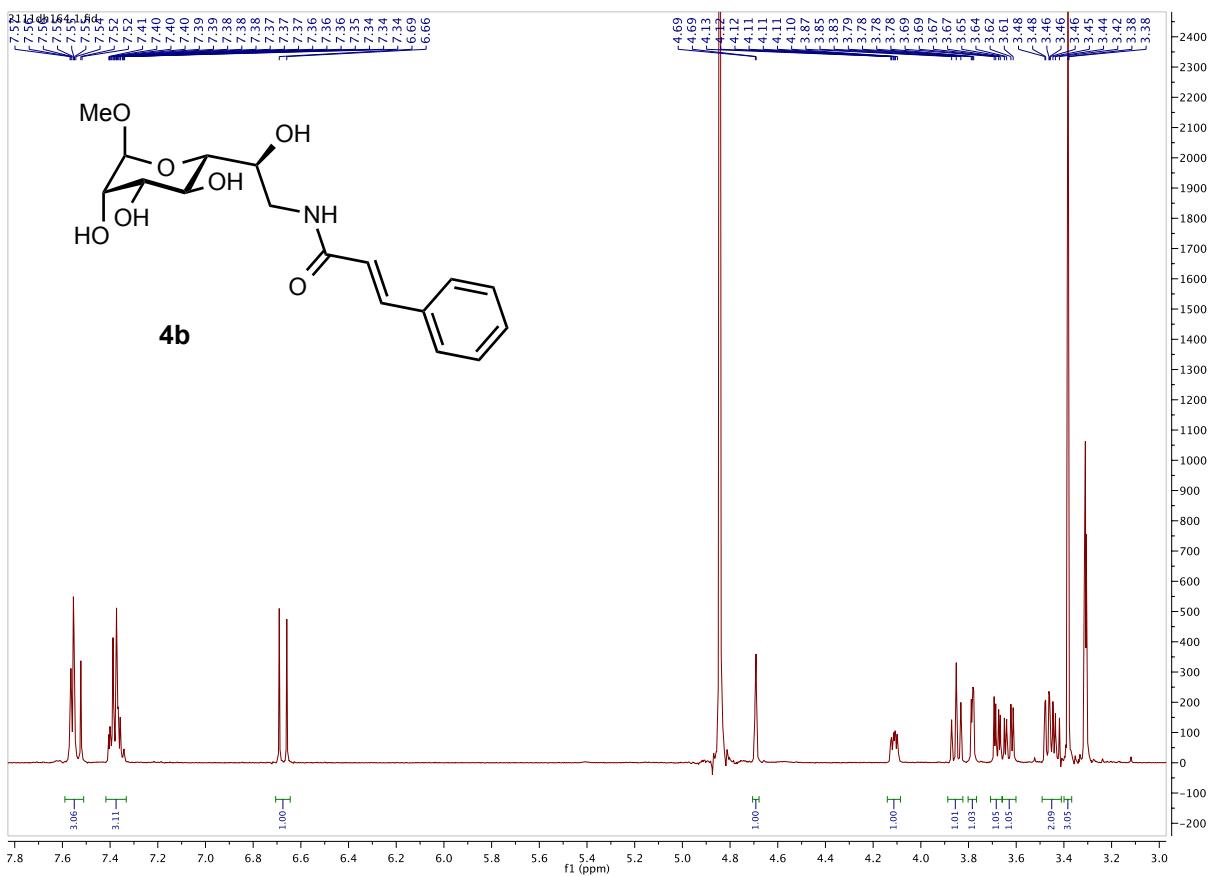


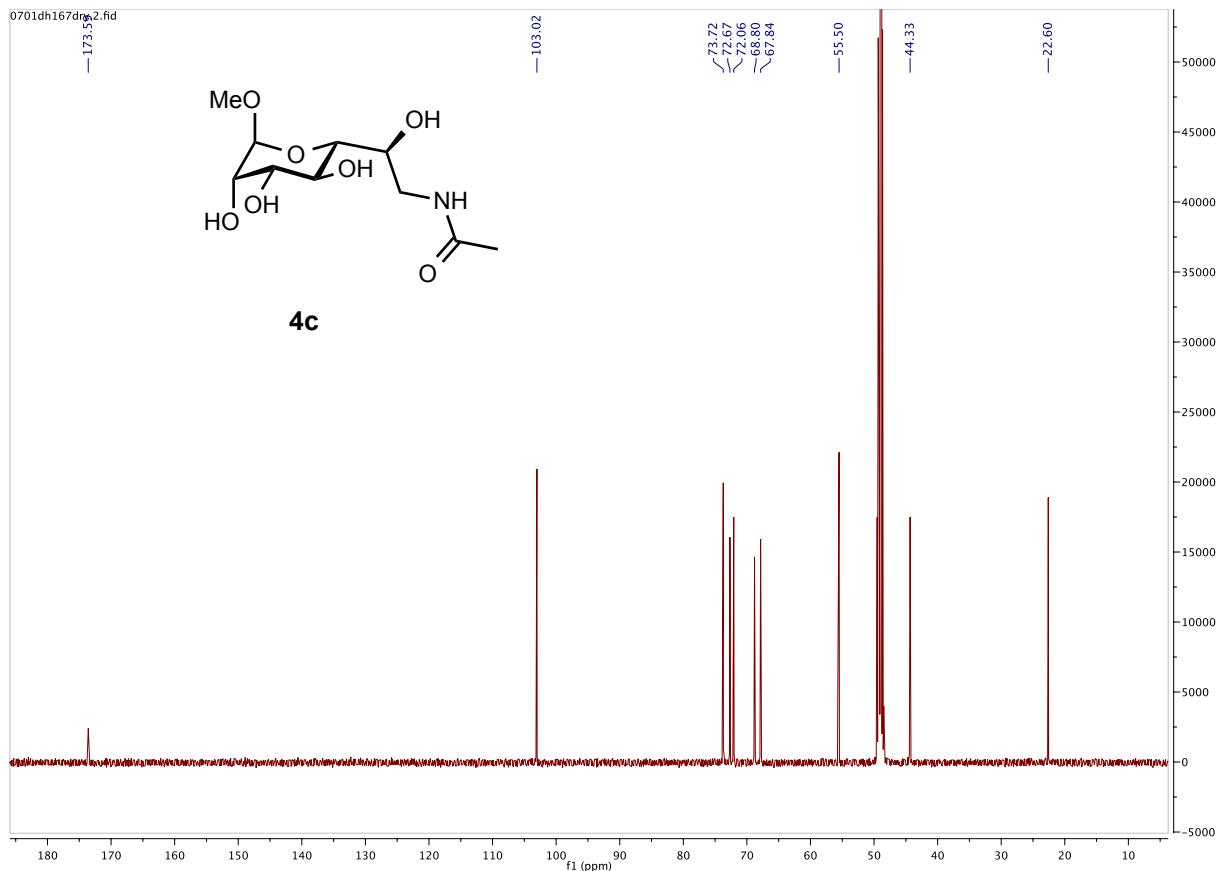
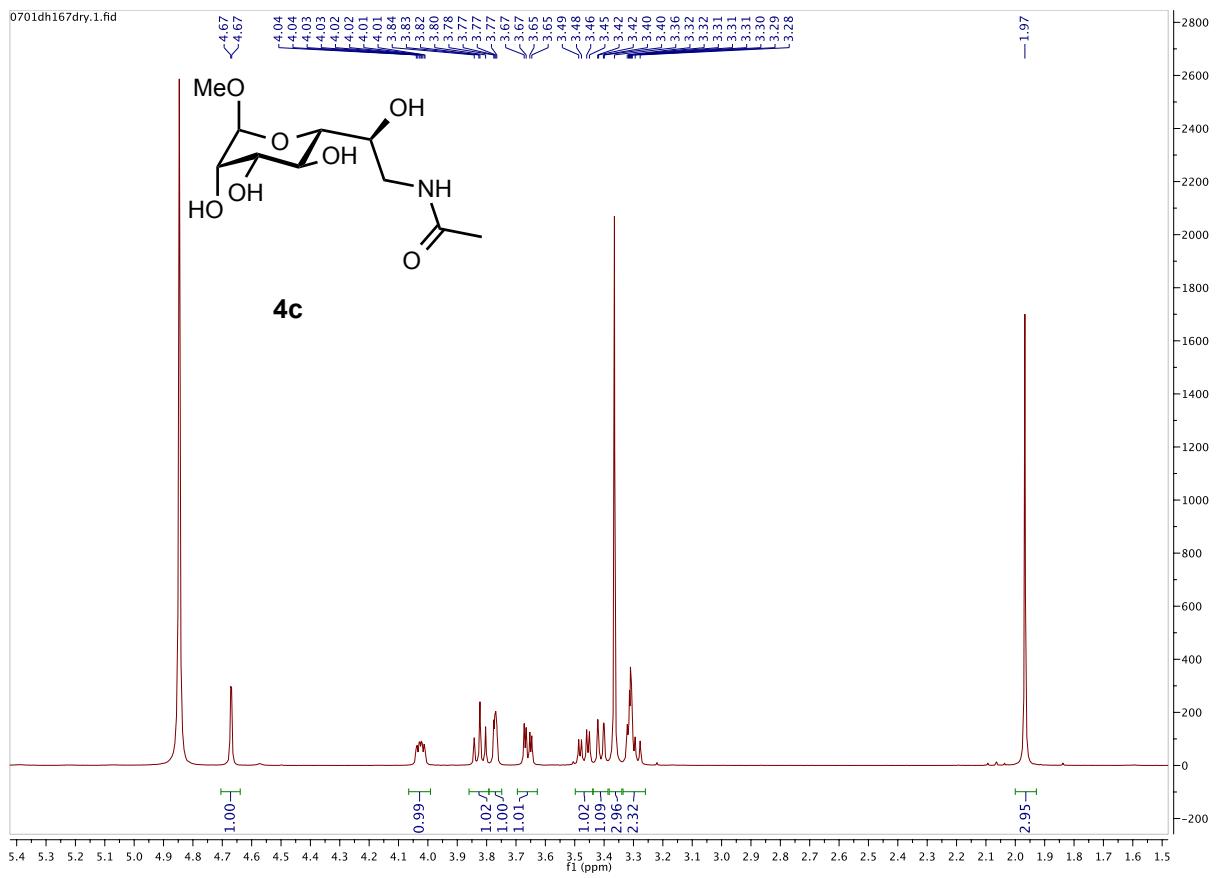


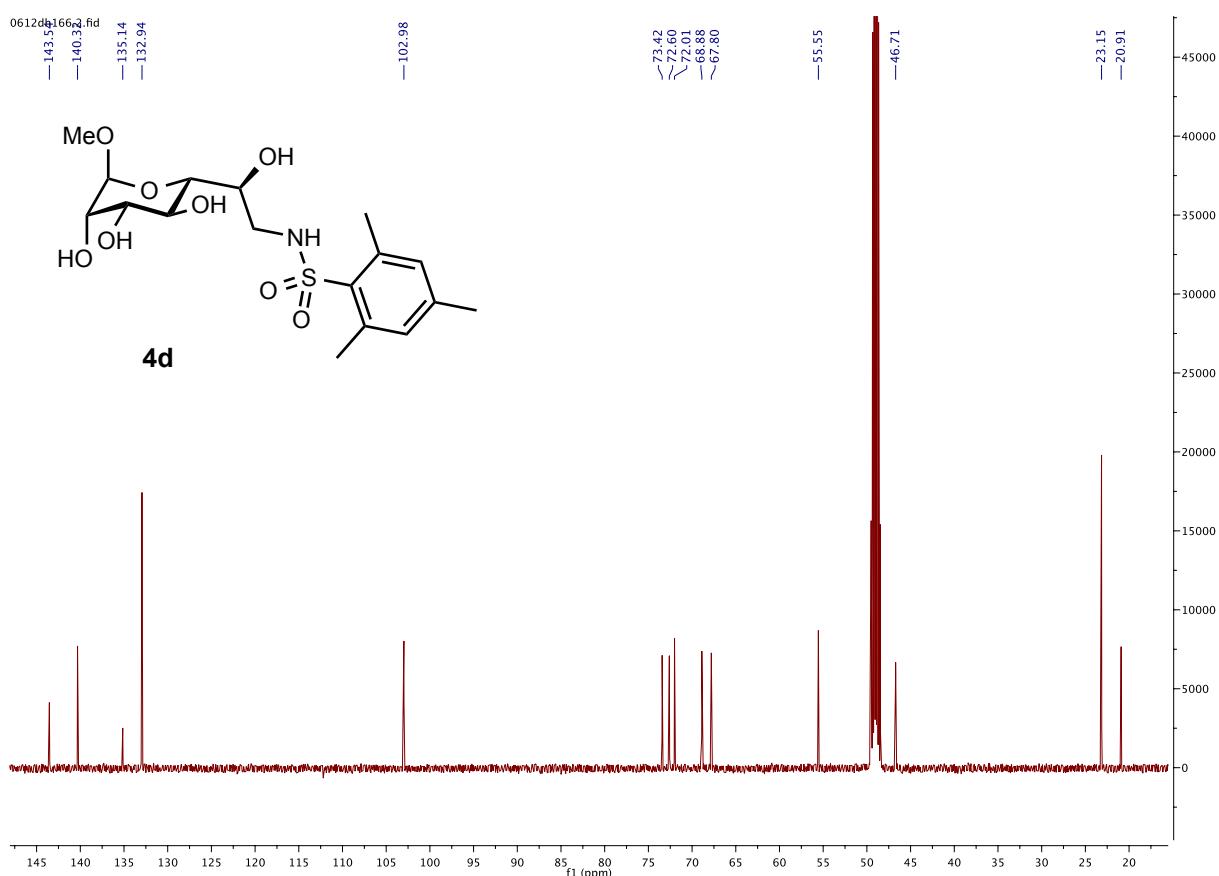
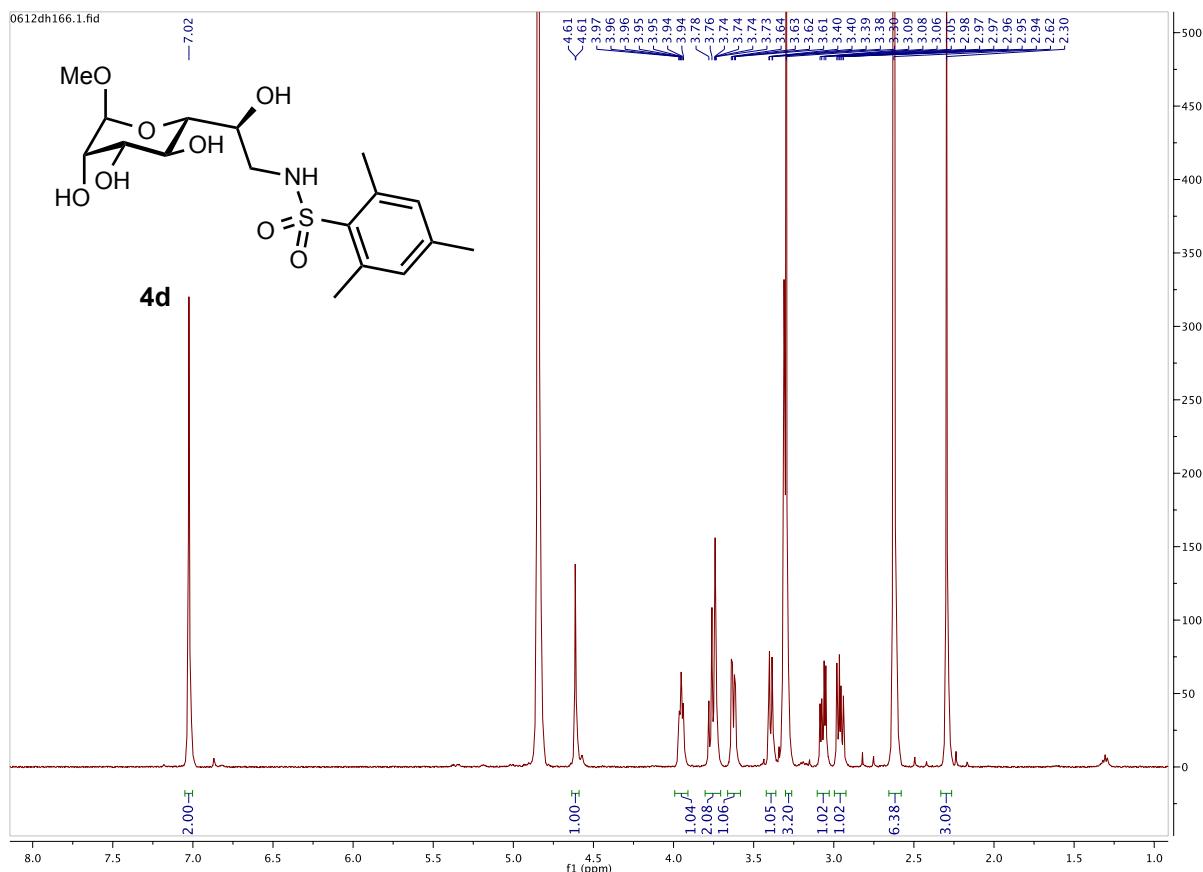


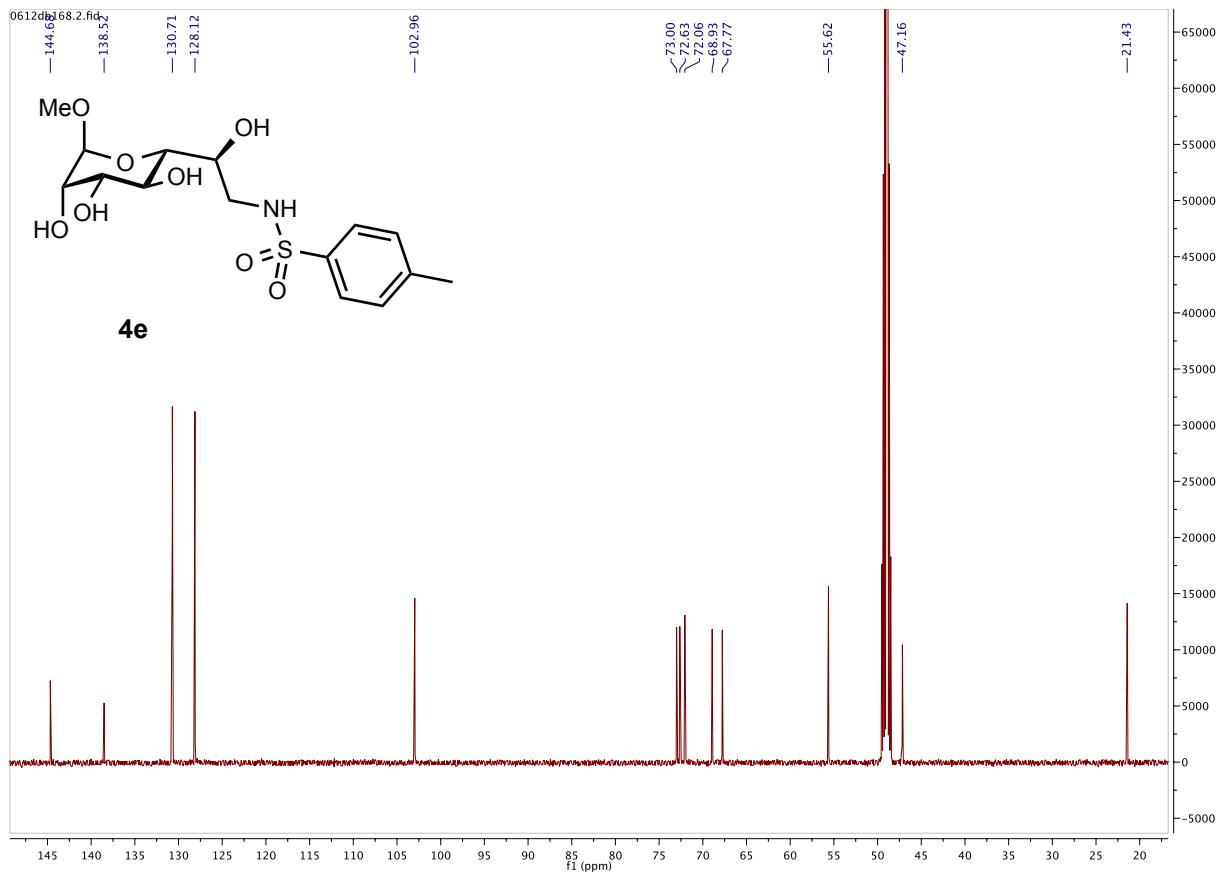
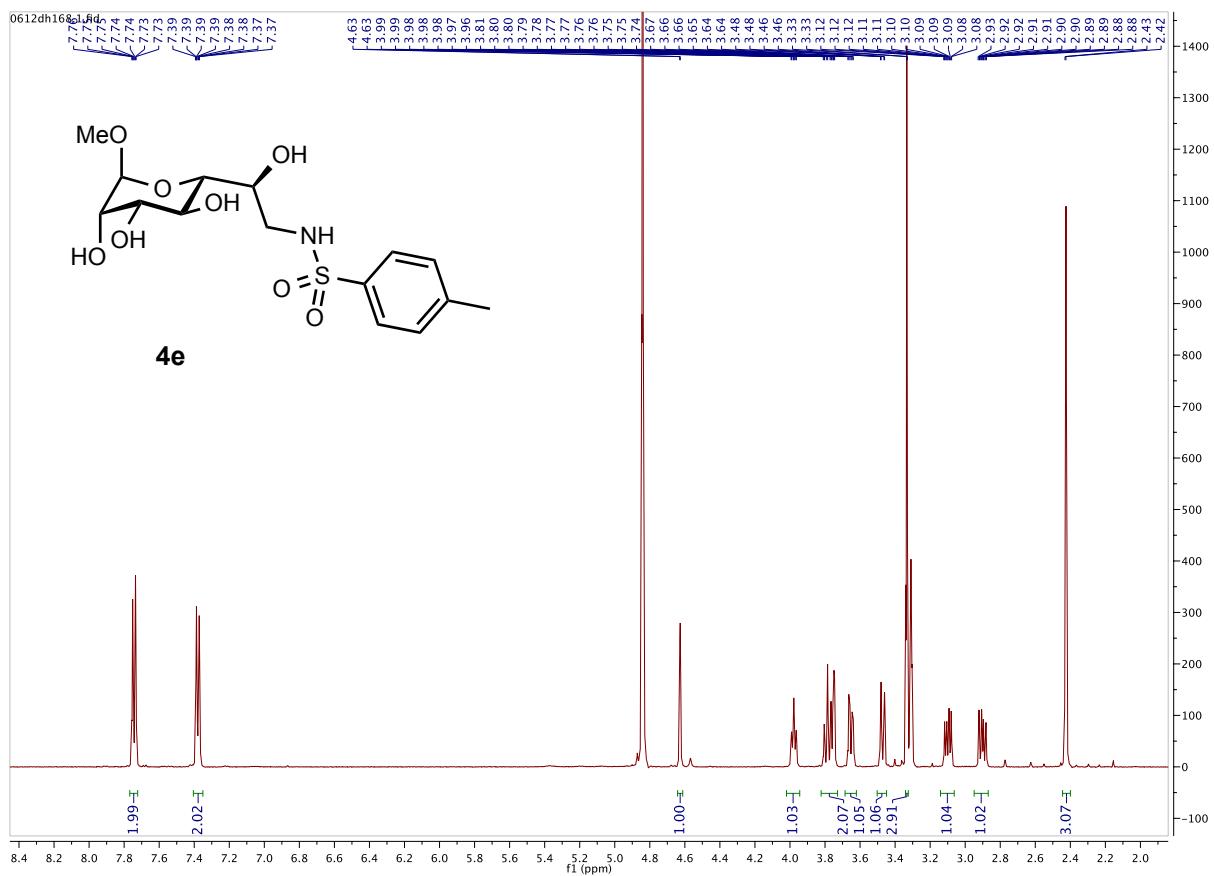




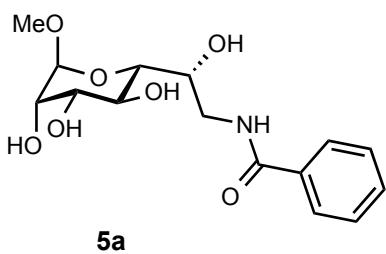




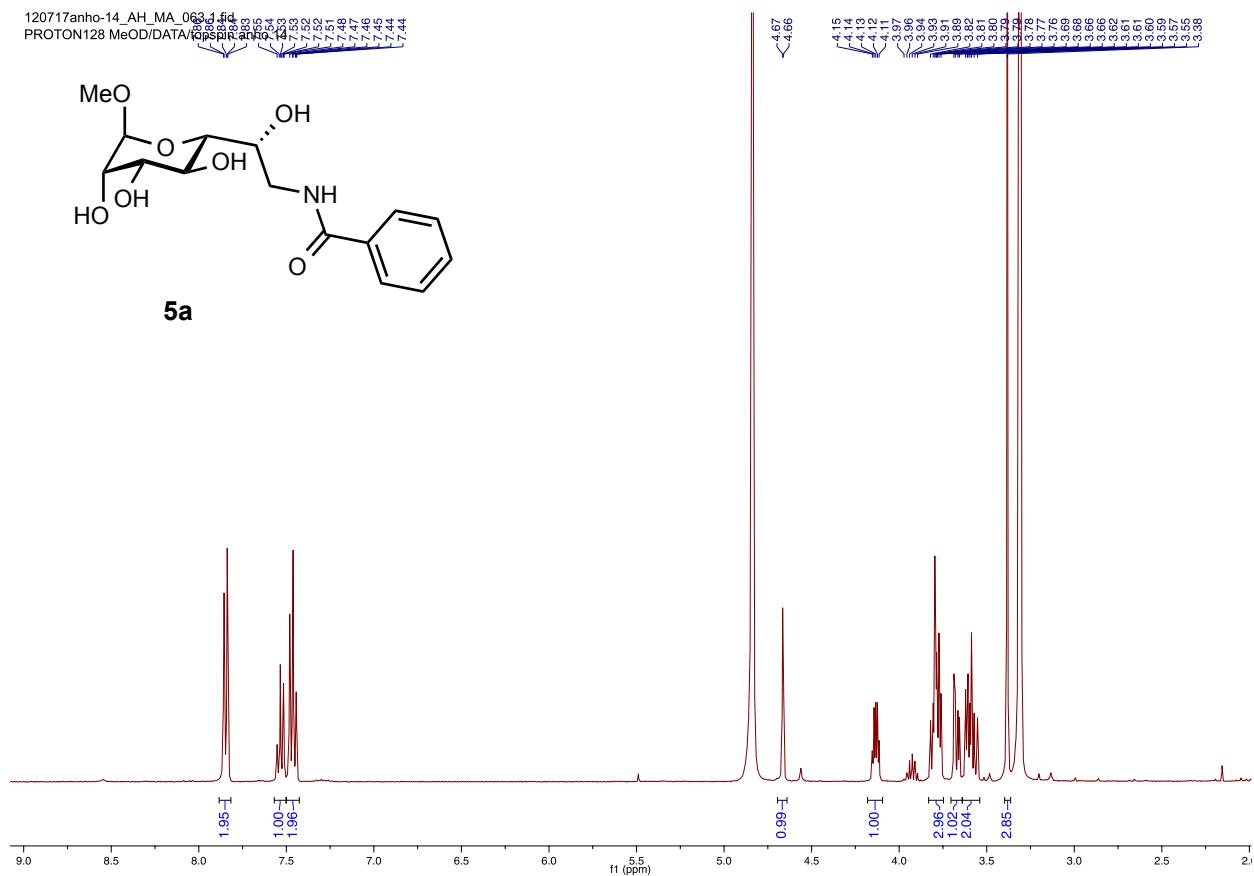




120717anho-14_AH_MA_063.6.fid
PROTON128 MeOD/DATA/topspin anho 14



5a



120717anho-14_AH_MA_063.6.fid
CARBON_1024scans MeOD/DATA/topspin anho 14

— 175.64
— 135.74
— 132.67
— 129.57
— 128.32

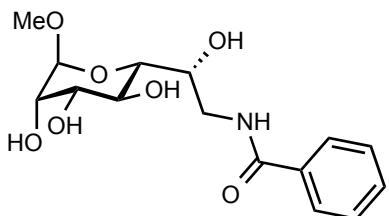
— 102.87

— 74.95
— 72.72
— 71.90
— 71.72
— 69.88

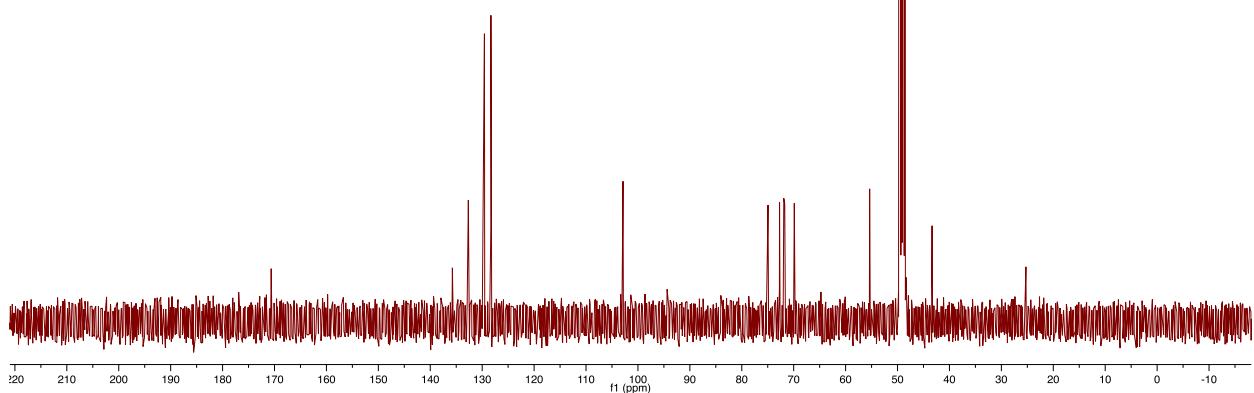
— 55.37

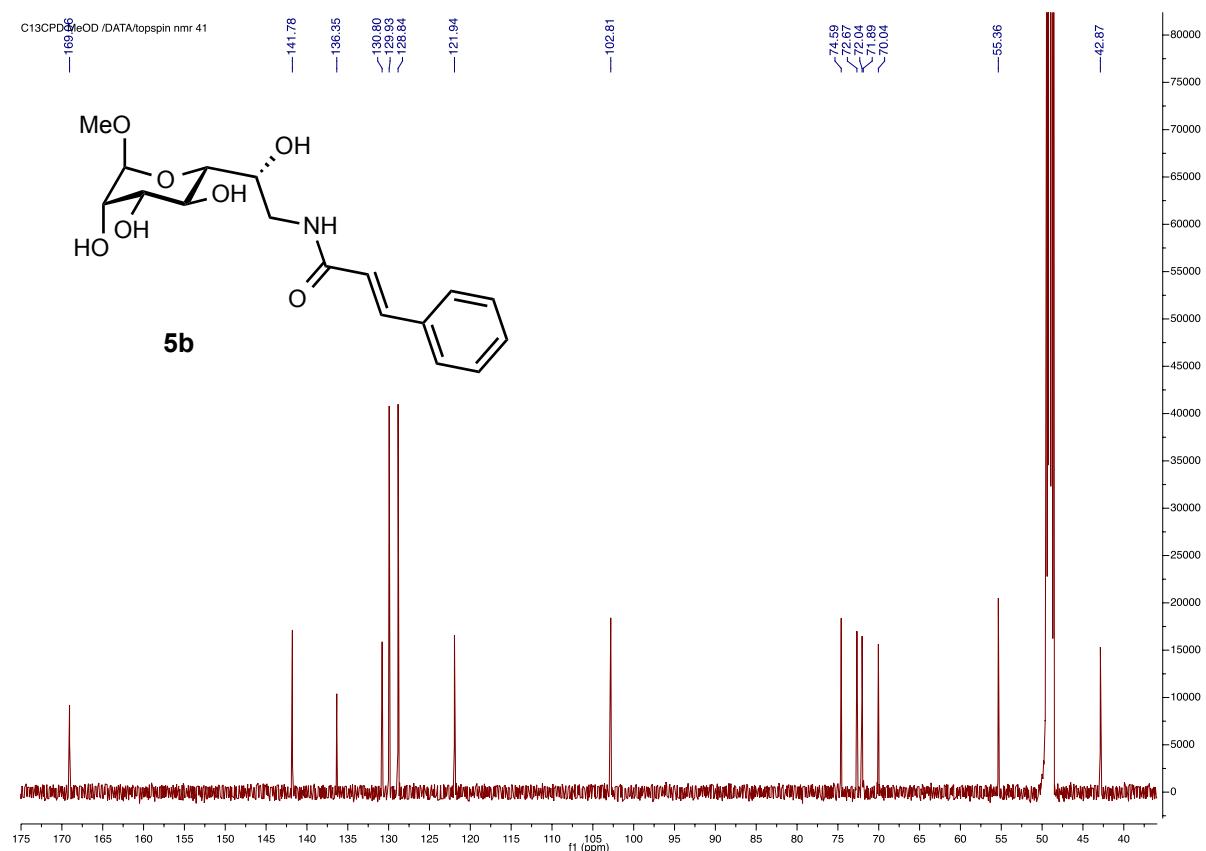
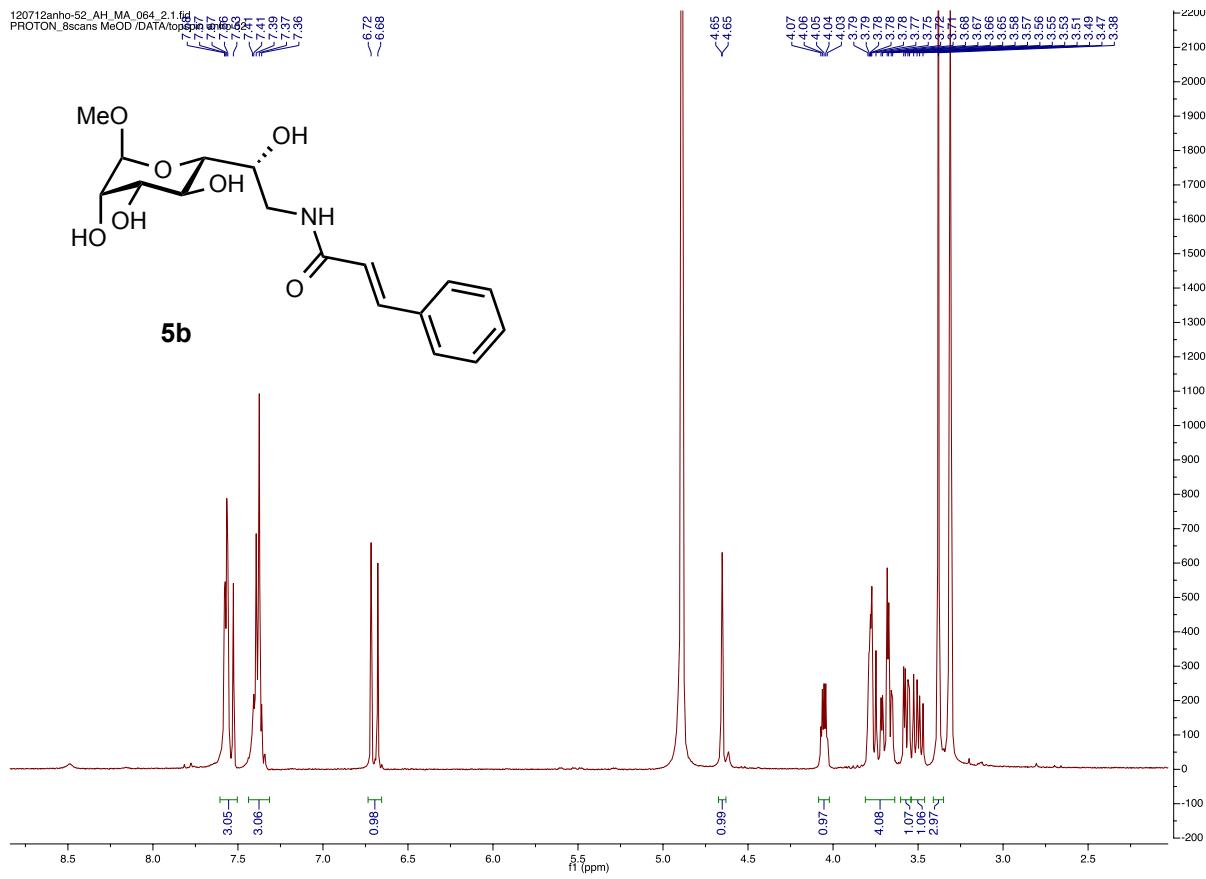
— 43.35

— 25.27



5a





Temperature-dependent ^1H -NMR for **9a** and **9b**

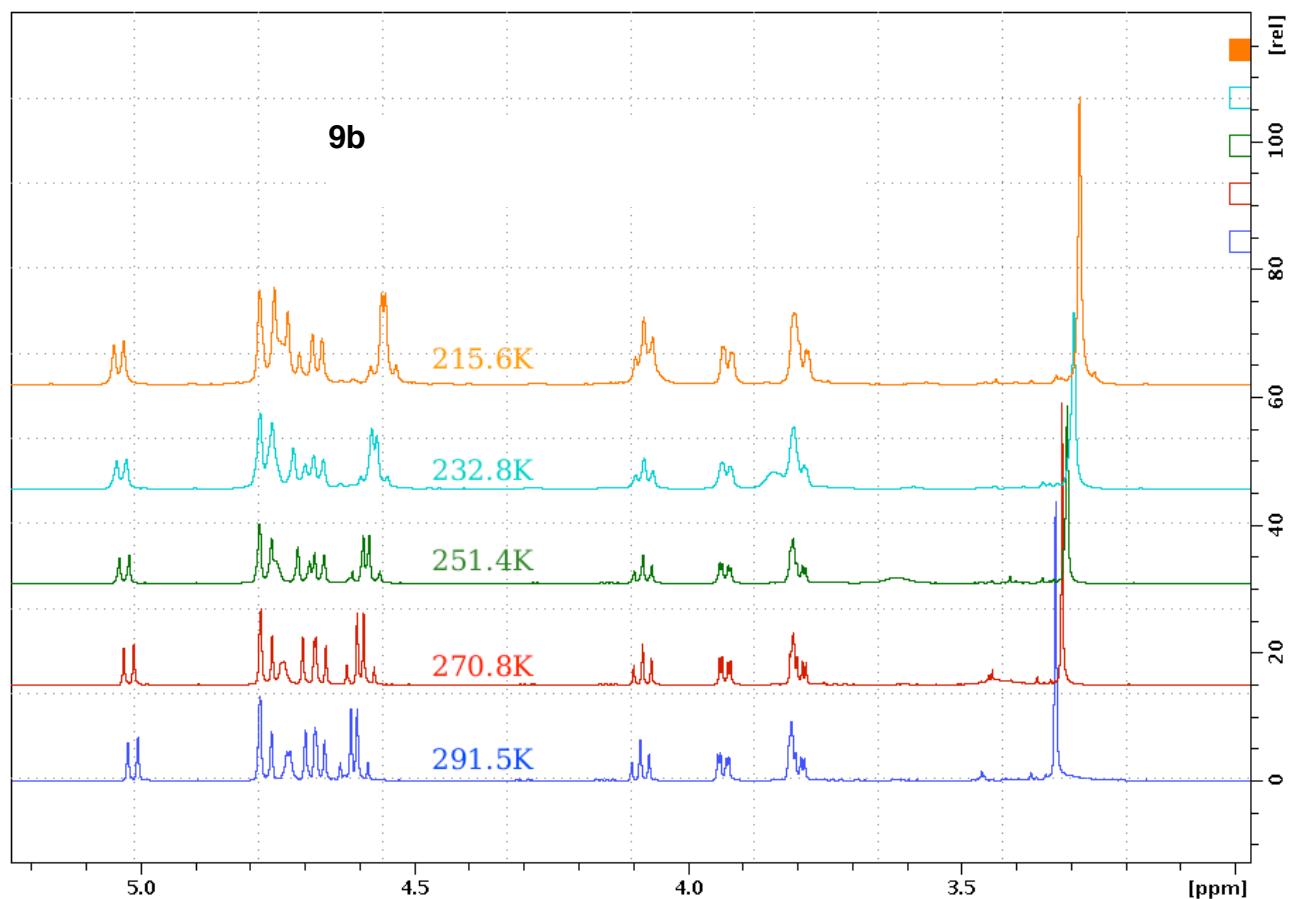
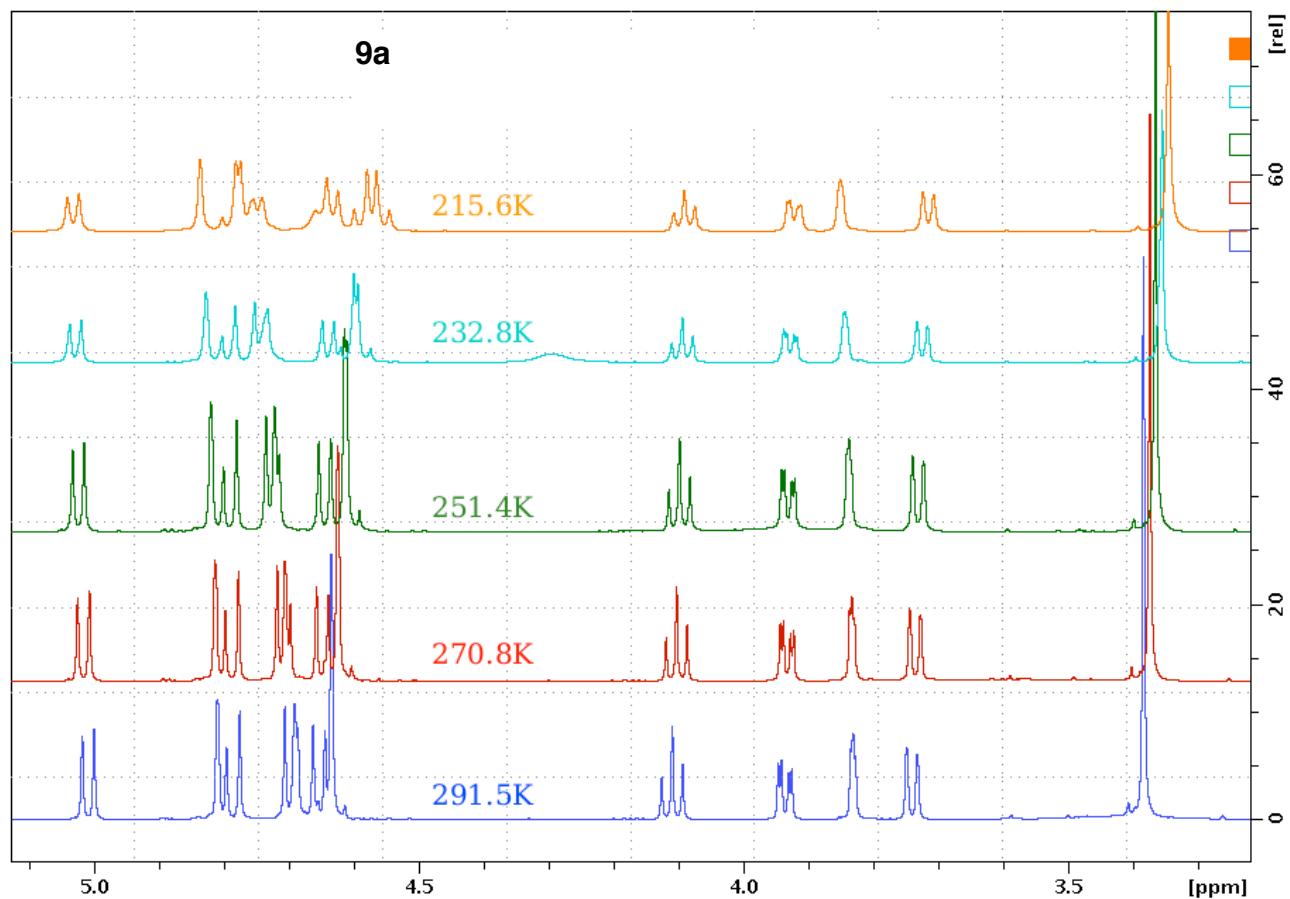


Table S1: Stereochemical analysis of **9a** and **9b** by NMR: $^3J_{CH}$ -HMBC coupling constants between H5 and CN group of the diastereomers **9a** and **9b** were recorded in the temperature range of 292 to 223 K.

T [K]	9a , $^3J_{CH}$ -HMBC [Hz]	9b , $^3J_{CH}$ -HMBC [Hz]
292	9.9 Hz	8.8 Hz
274	8.7 Hz	8.4 Hz
257	8.7 Hz	8.5 Hz
240	9.3 Hz	8.8 Hz
223	8.8 Hz	8.7 Hz

Table S2. Crystal data and structure refinement for cyanohydrin **9a**.

Identification code	z:012_011AH_Titz	
Empirical formula	C ₂₉ H ₃₁ N O ₆	
Formula weight	489.55	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 5.6943(3) Å	α= 90°.
	b = 10.5141(7) Å	β= 90°.
	c = 42.648(2) Å	γ = 90°.
Volume	2553.4(3) Å ³	
Z	4	
Density (calculated)	1.273 Mg/m ³	
Absorption coefficient	0.089 mm ⁻¹	
F(000)	1040	
Crystal size	0.450 x 0.250 x 0.150 mm ³	
Theta range for data collection	1.91 to 25.30°.	
Index ranges	-6<=h<=6, -12<=k<=12, -48<=l<=51	
Reflections collected	20891	
Independent reflections	4657 [R(int) = 0.0569]	
Completeness to theta = 25.30°	99.8 %	
Absorption correction	Integration	
Max. and min. transmission	0.9877 and 0.9665	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4657 / 0 / 331	
Goodness-of-fit on F ²	0.947	
Final R indices [I>2sigma(I)]	R1 = 0.0320, wR2 = 0.0690	
R indices (all data)	R1 = 0.0428, wR2 = 0.0723	
Extinction coefficient	0.0111(8)	
Largest diff. peak and hole	0.144 and -0.141 e.Å ⁻³	