

Supporting Information

for

An efficient synthesis of 1,6-anhydro-*N*-acetylmuramic acid from *N*-acetylglucosamine

Matthew B. Calvert^{1,2}, Christoph Mayer³, Alexander Titz^{1,2,4*}

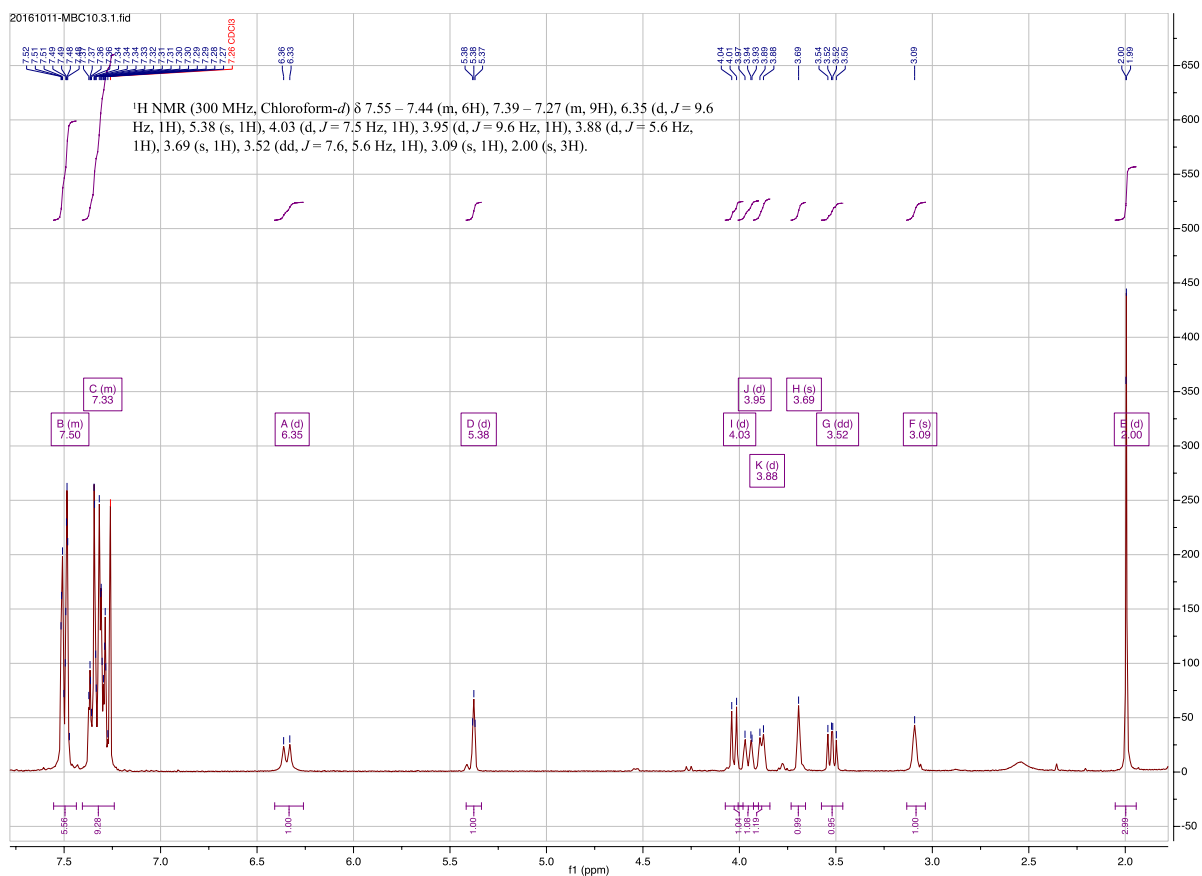
Address: ¹Chemical Biology of Carbohydrates, Helmholtz Institute for Pharmaceutical Research Saarland (HIPS), D-66123 Saarbrücken, Germany, ²Deutsches Zentrum für Infektionsforschung (DZIF), Standort Hannover-Braunschweig, Germany, ³Interfaculty Institute of Microbiology and Infection Medicine Tübingen (IMIT), Department of Microbiology and Biotechnology, University of Tübingen, Germany and ⁴Department of Pharmacy, Saarland University, Saarbrücken, Germany

Email: Alexander Titz - alexander.titz@helmholtz-hzi.de *Corresponding author

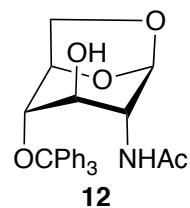
Contents

Table of Contents	S1
Confirming the reported structure of 12	S2
¹ H NMR data for 12 in CDCl ₃ , table of observed and reported proton shifts	S2
HMBC data for 12 (acetone- <i>d</i> ₆) with key correlations indicated	S3
NOESY data for 12 (acetone- <i>d</i> ₆) with key correlations indicated	S4
¹H and ¹³C NMR data	S5
¹ H NMR data for 12	S5
¹³ C NMR data for 12	S6
¹ H NMR data for 13	S7
¹³ C NMR data for 13	S8
¹ H NMR data for 1	S9
¹³ C NMR data for 1	S10
¹ H NMR data for 5	S11
¹³ C NMR data for 5	S12

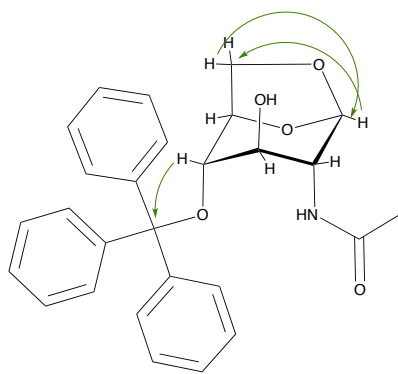
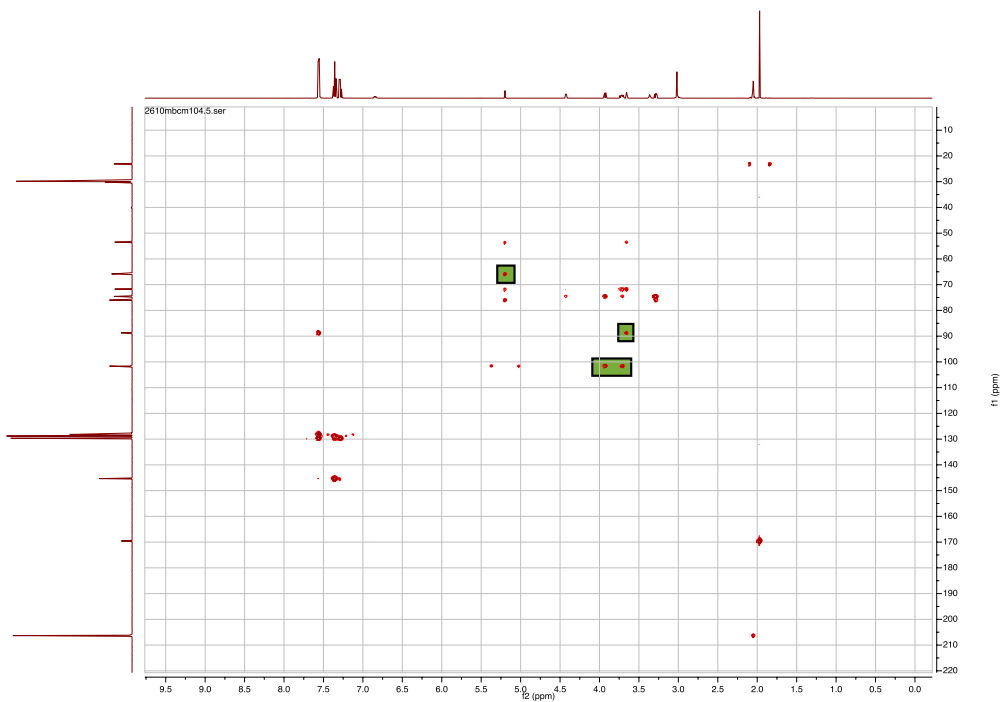
Confirming the reported structure of **12**



	Observed	Reported
H-1	5.38	5.40
H-2	3.95	3.973
H-3	3.09	3.080
H-4	3.69	3.705
H-5	3.88	3.910
H-6a	4.03	4.350
H-6b	3.52	3.538
NHAc	6.35	6.350
Ac	2.00	2.198
Ar	7.27-7.55	7.28-7.55

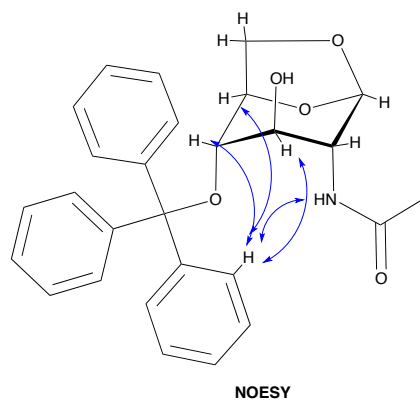
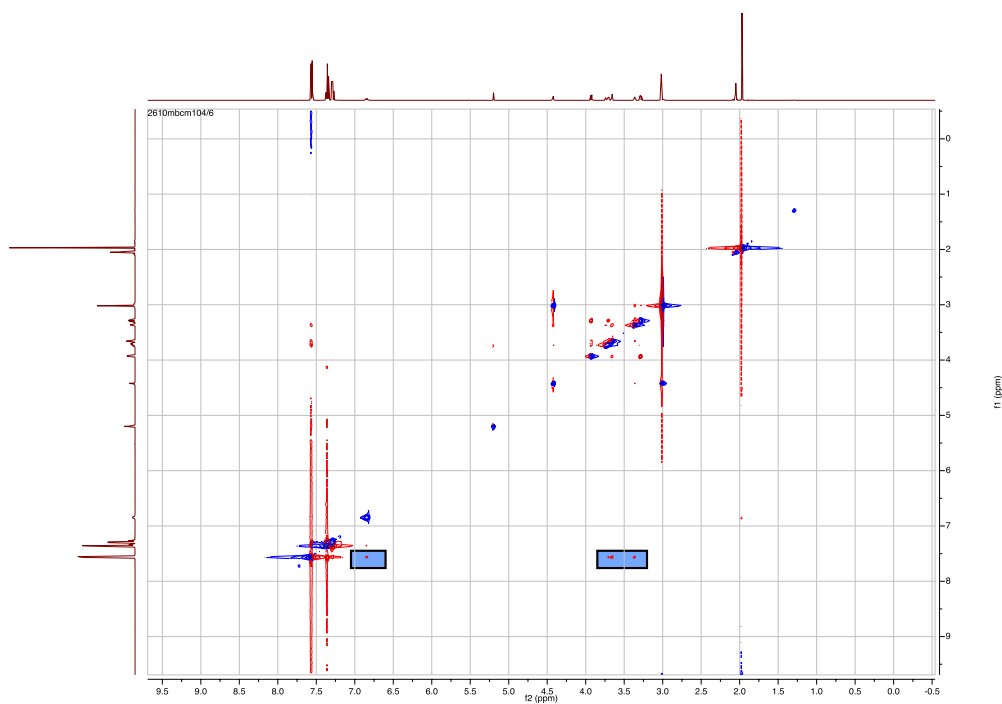


¹H NMR data for **12** (CDCl₃); Literature data from Tyrtys, T. V.; Byramova, N. E.; Bovin, N. V. *Russian Journal of Bioorganic Chemistry*, **2000**, 26, 414-418.

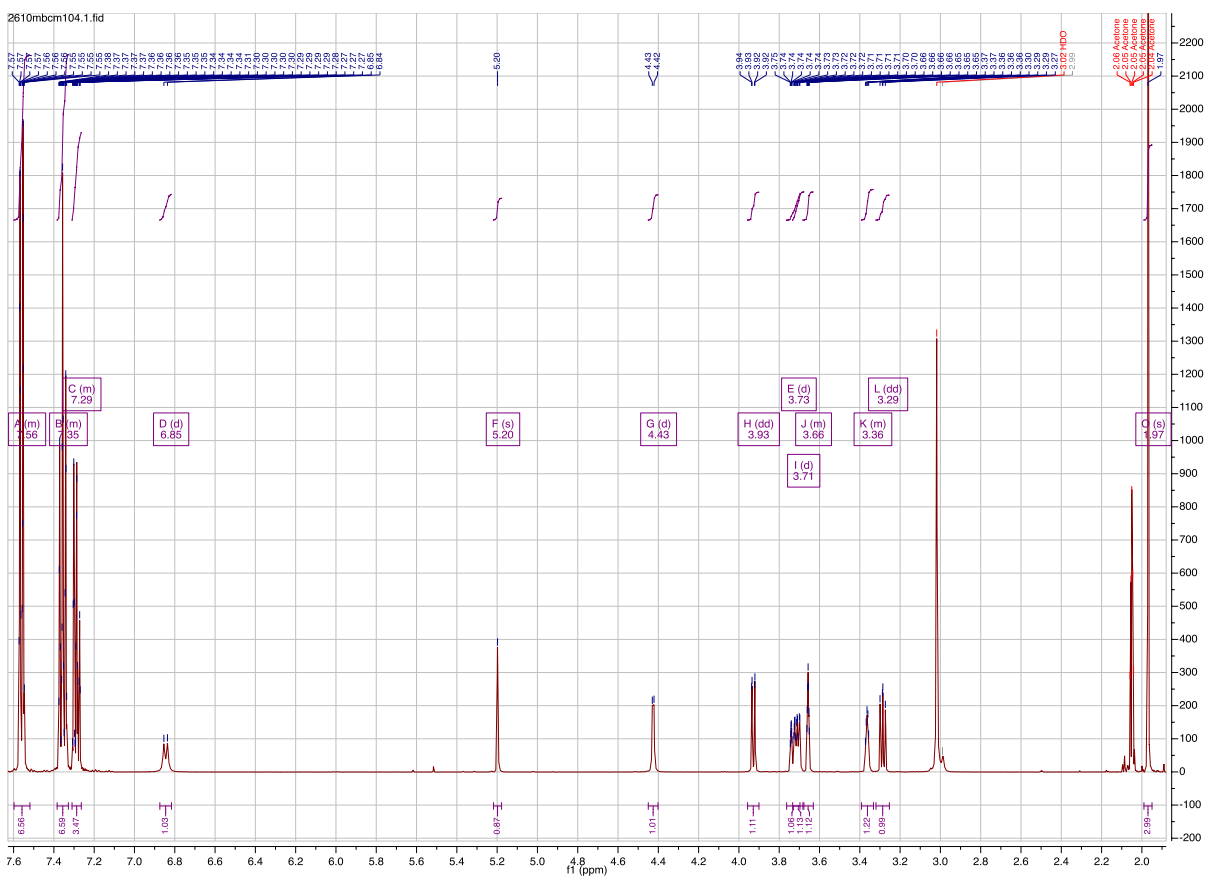
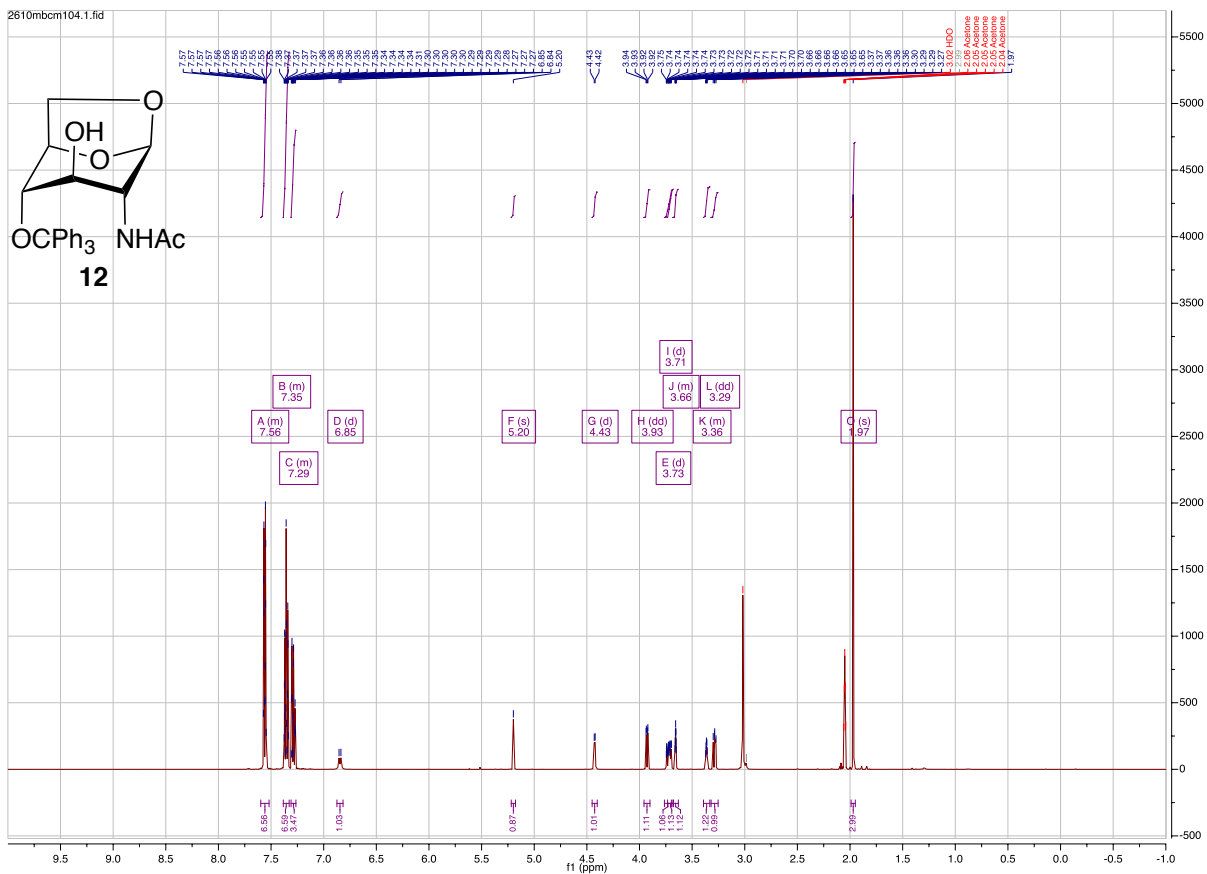


HMBC

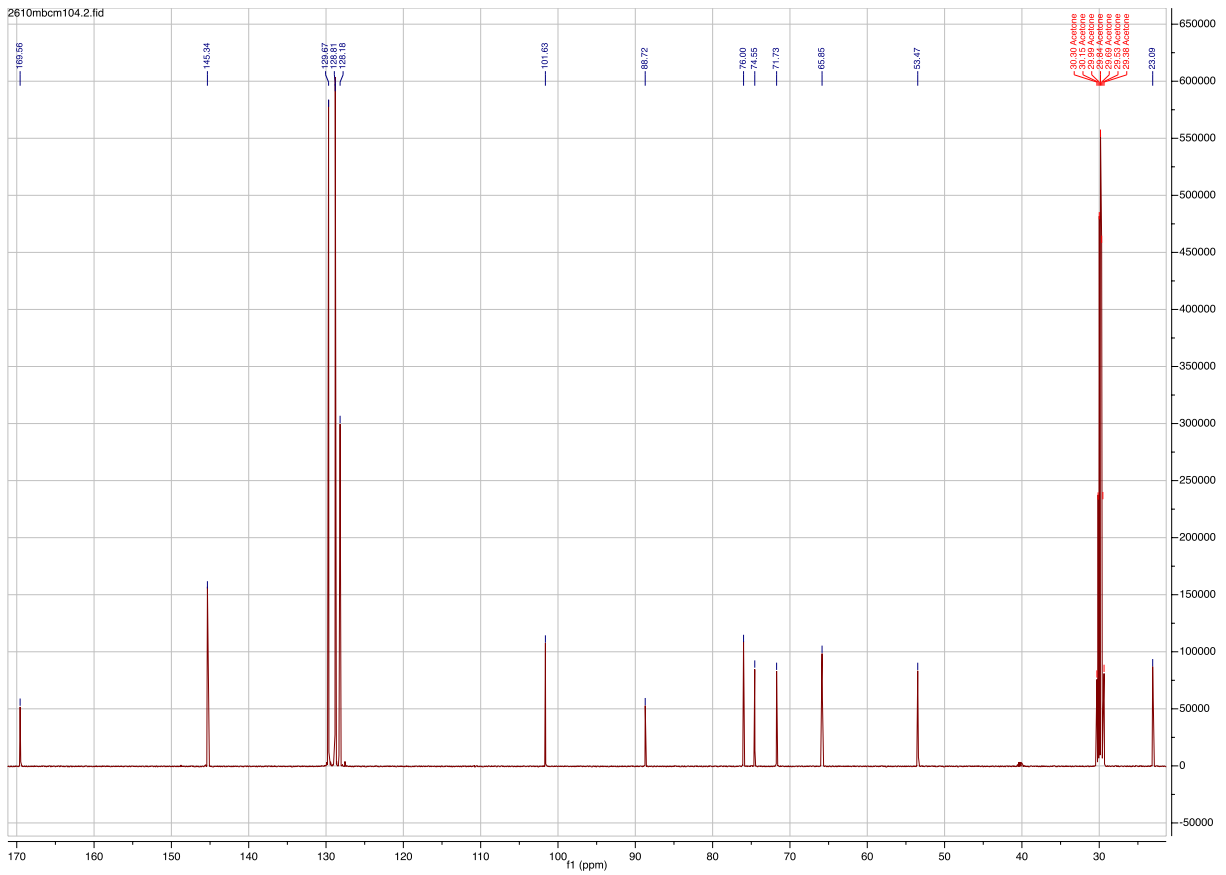
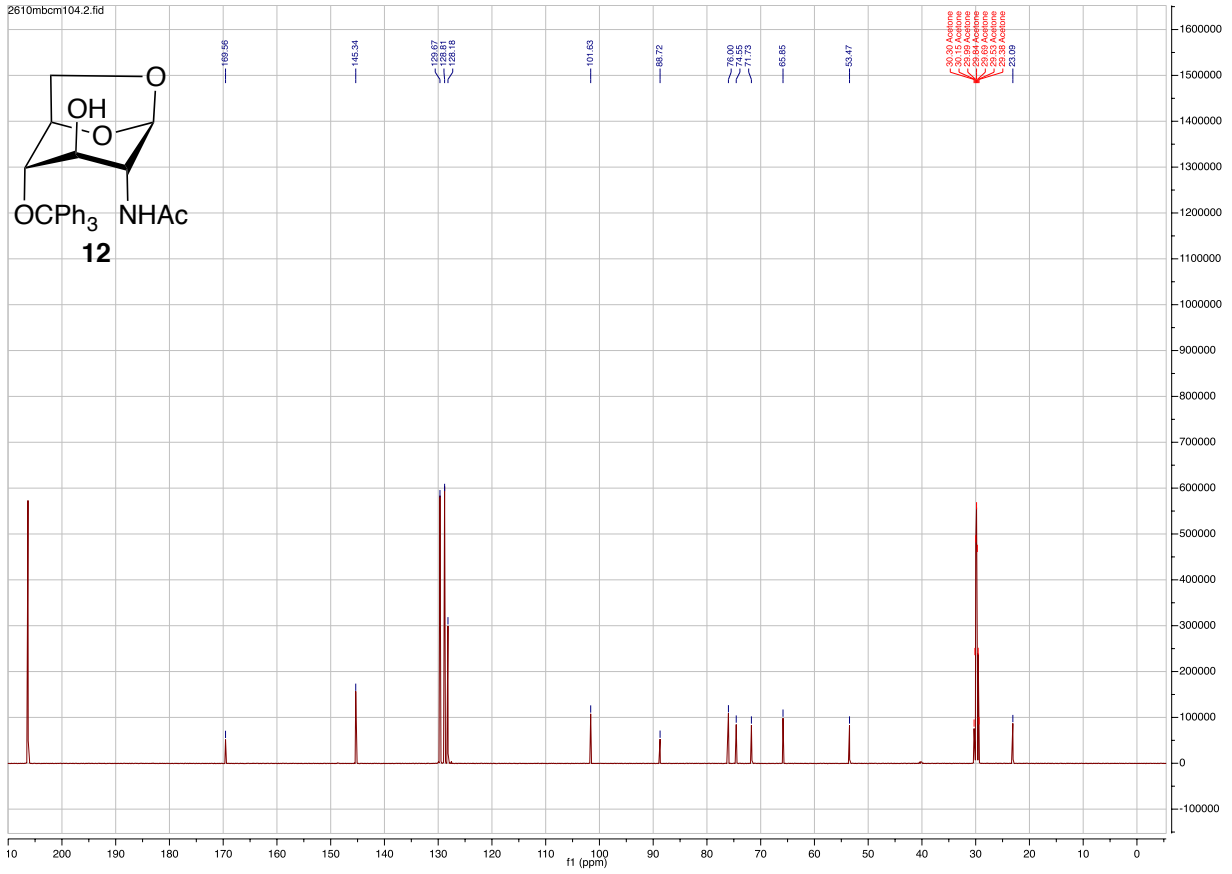
HMBC spectrum for **12** with key correlations indicated on spectrum and structure



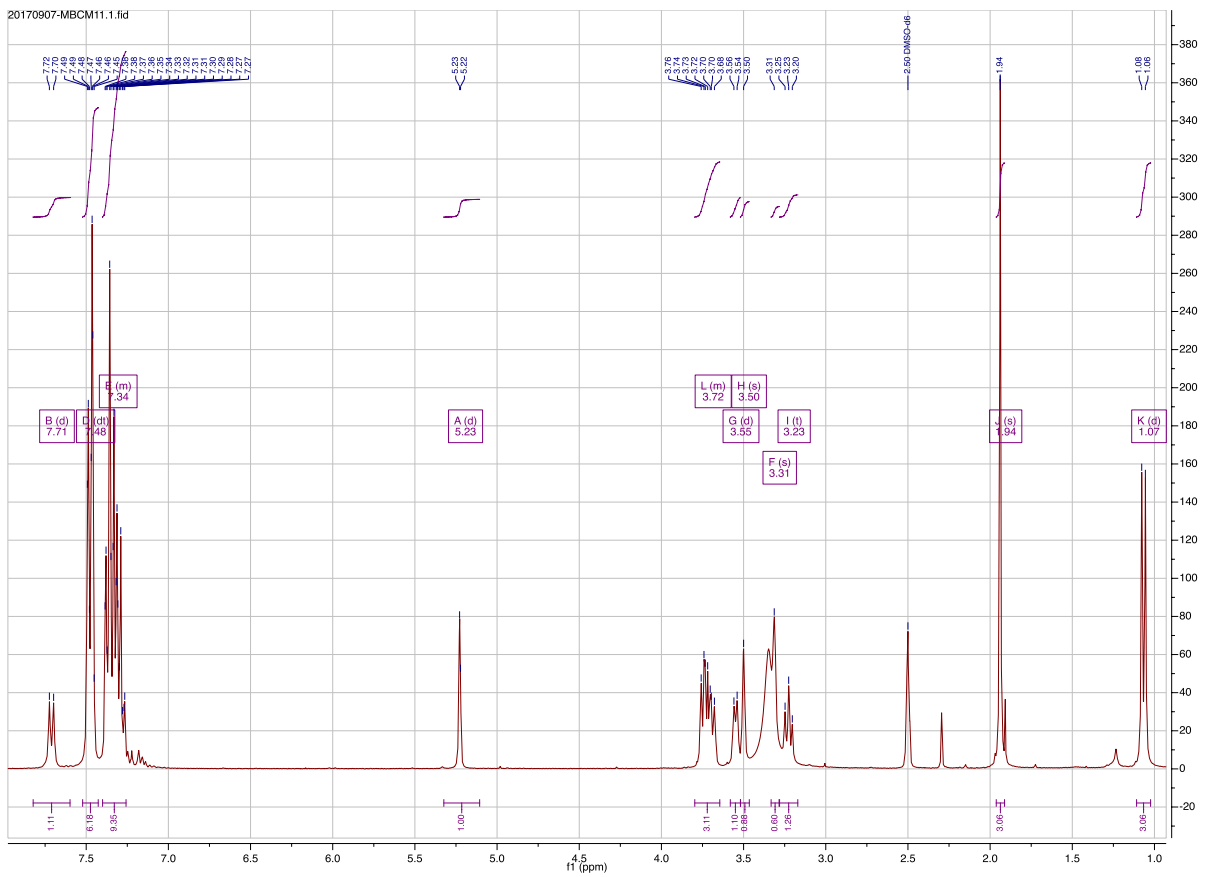
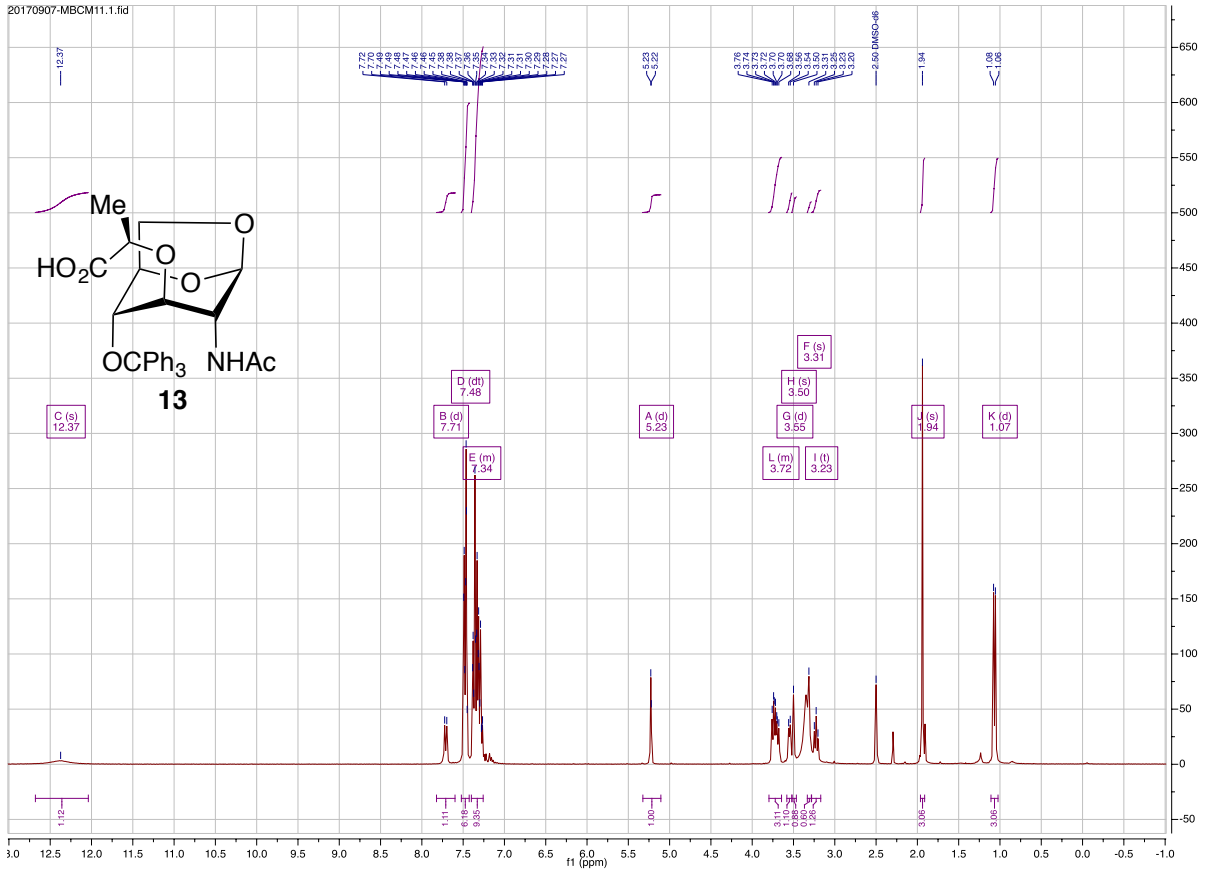
NOESY spectrum for **12** with key correlations indicated on spectrum and structure



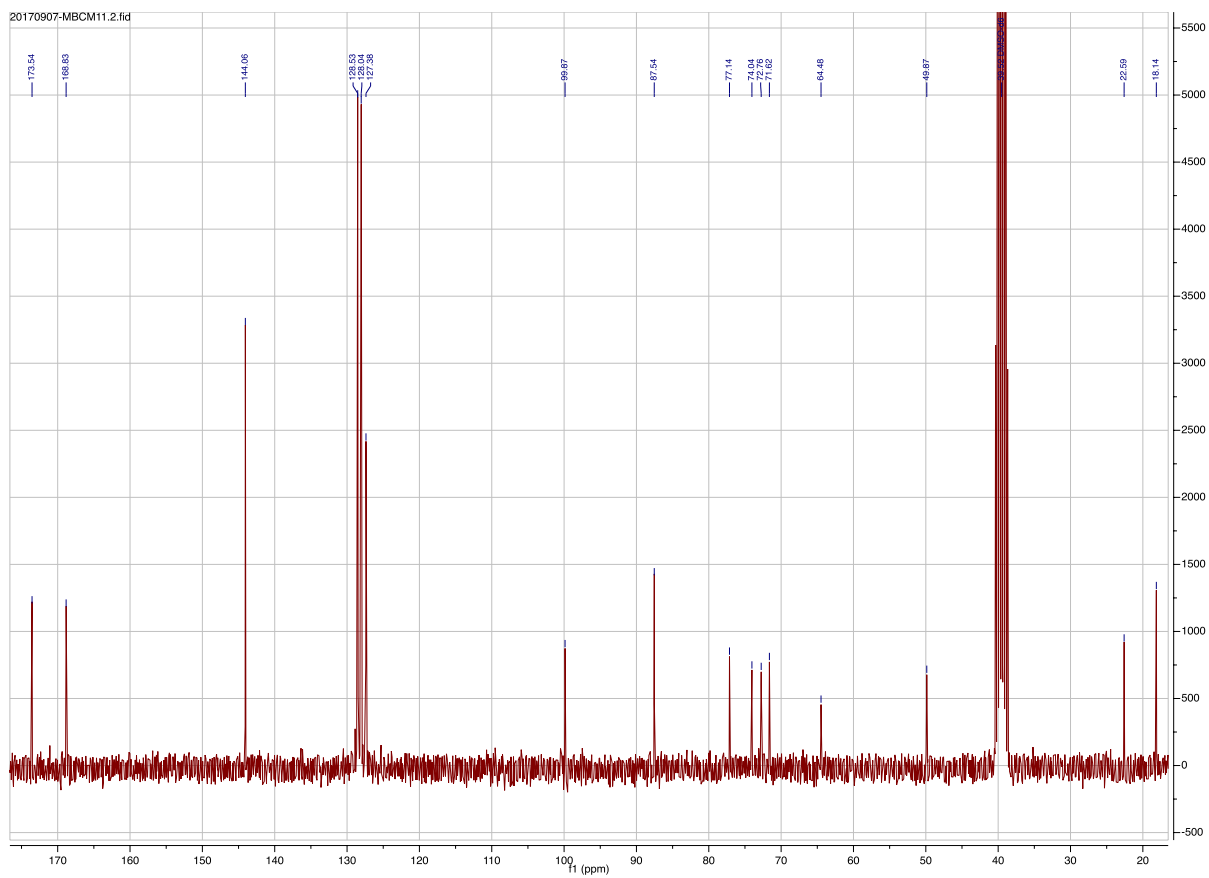
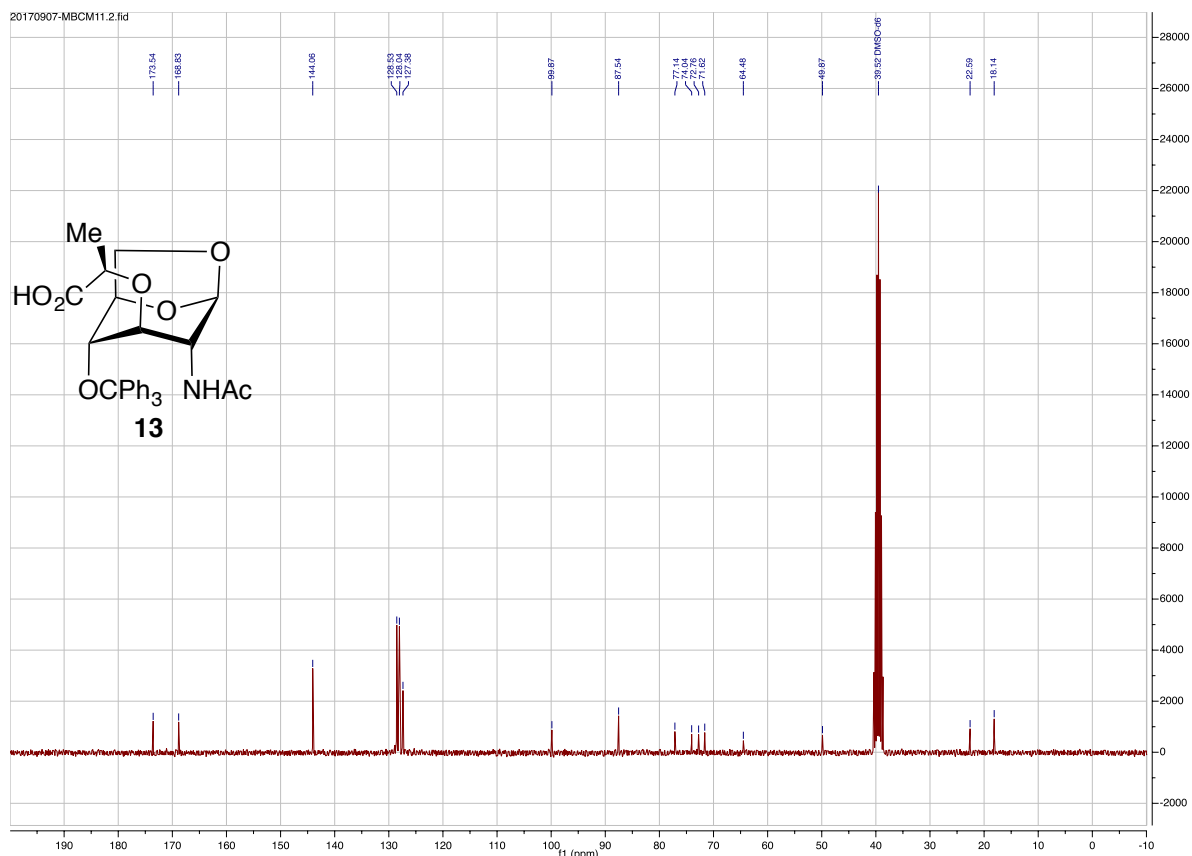
^1H NMR data for **12**



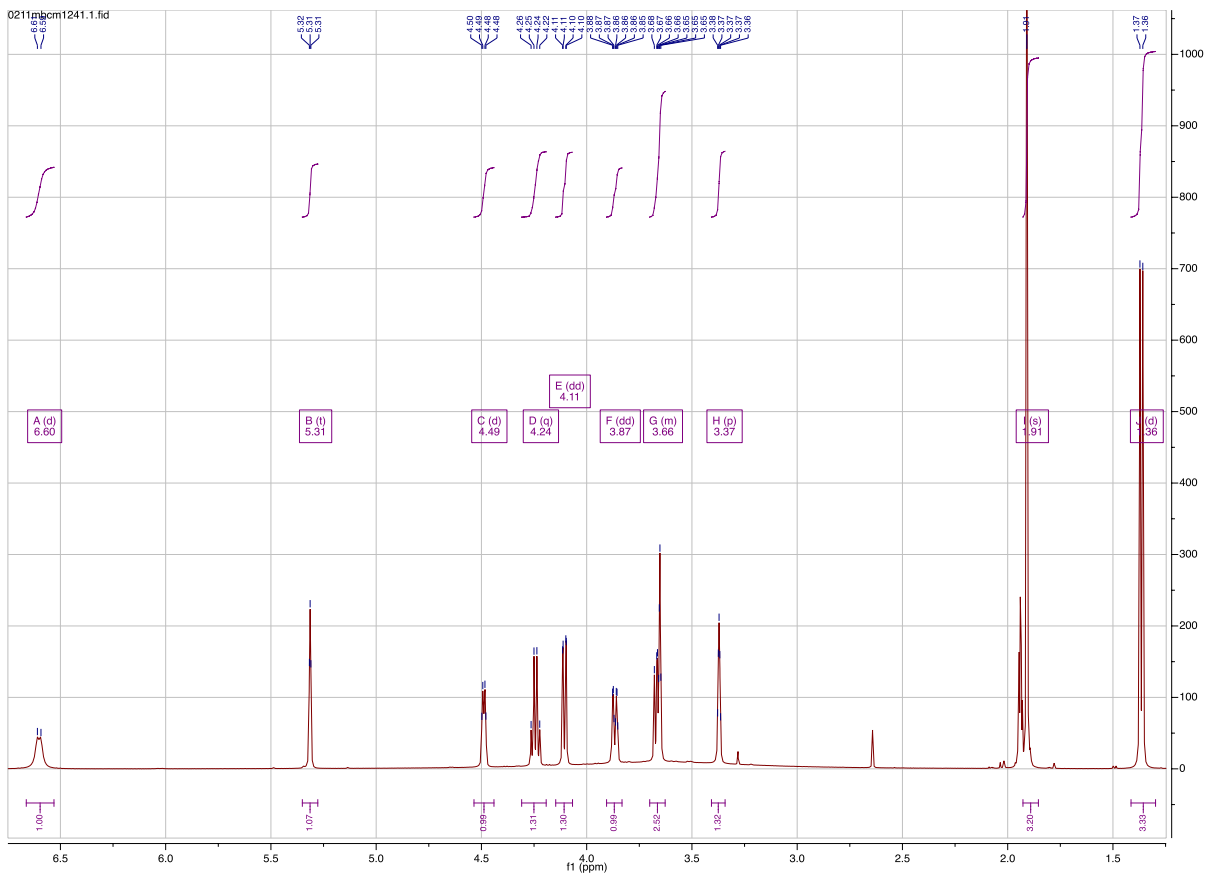
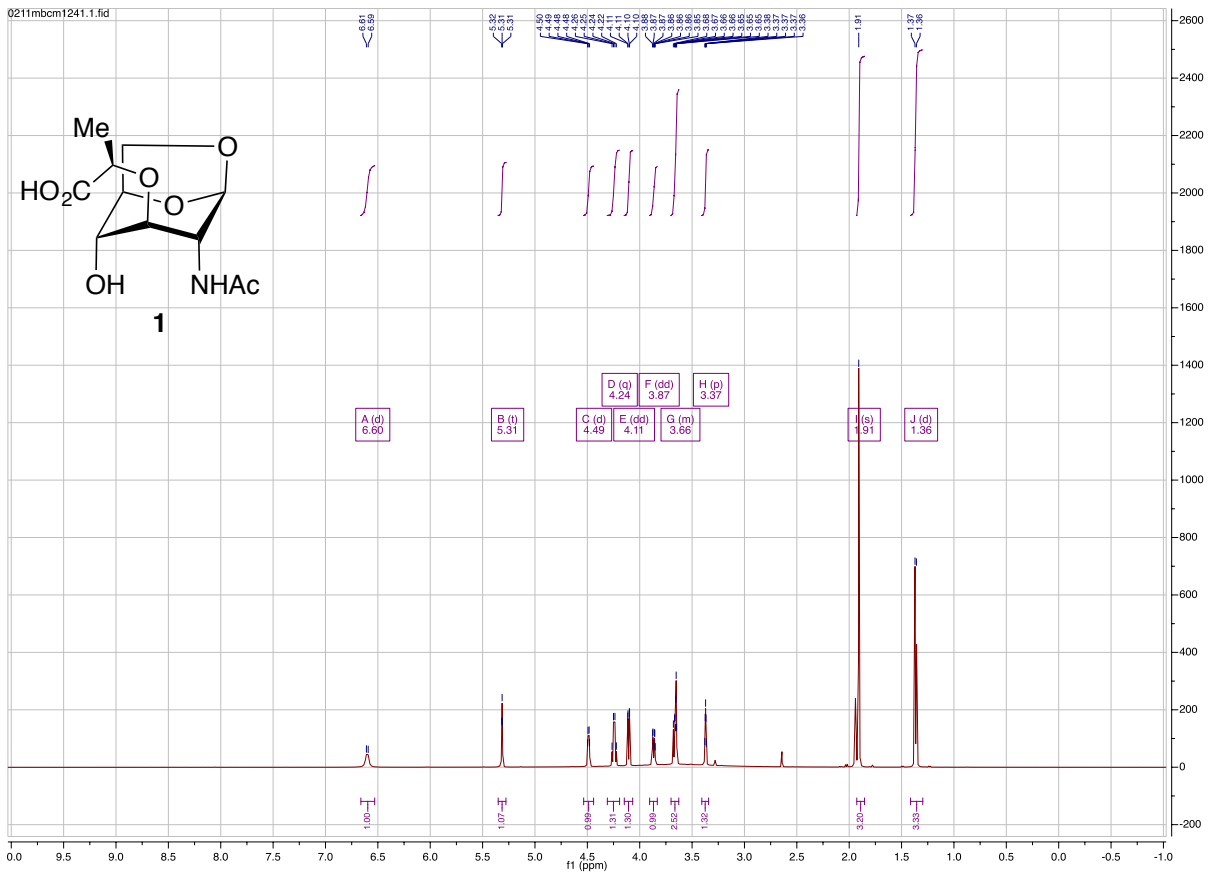
¹³C NMR data for **12**



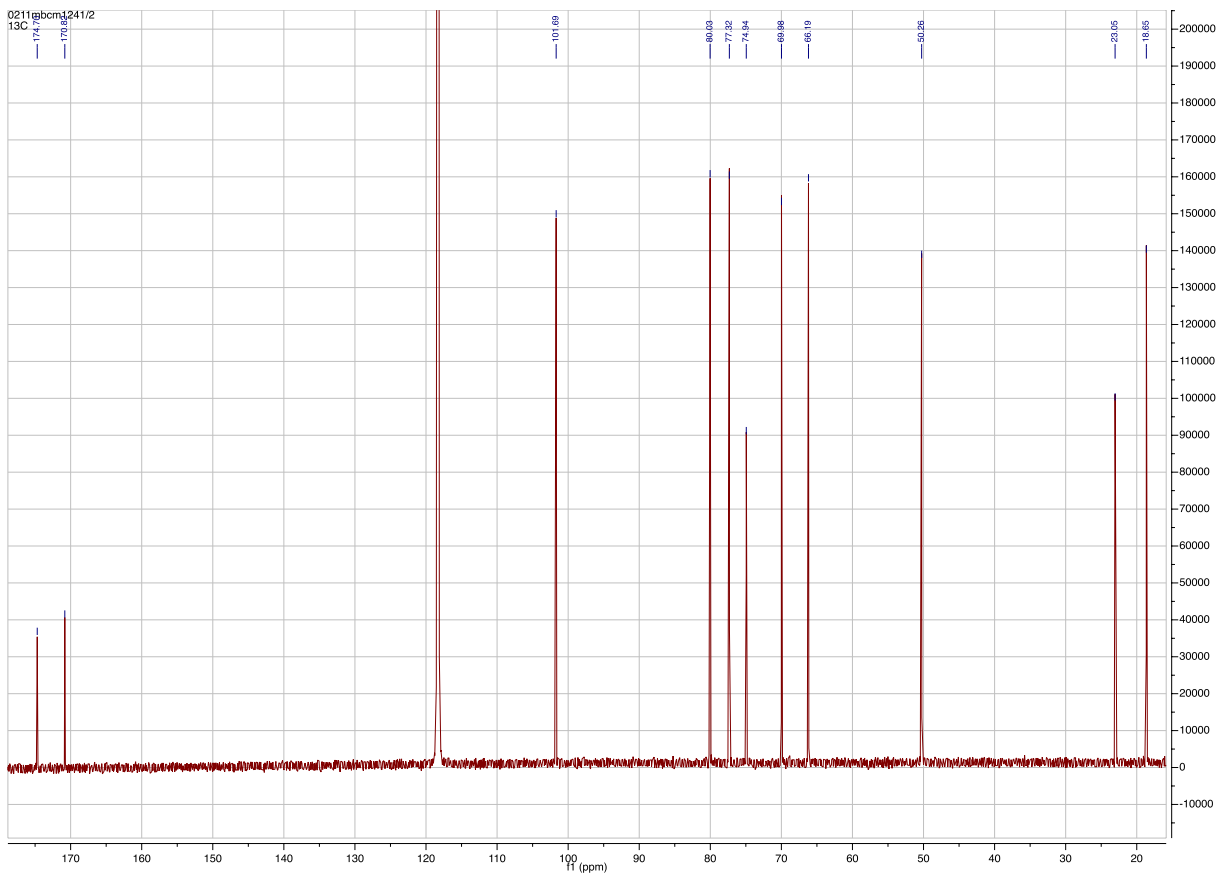
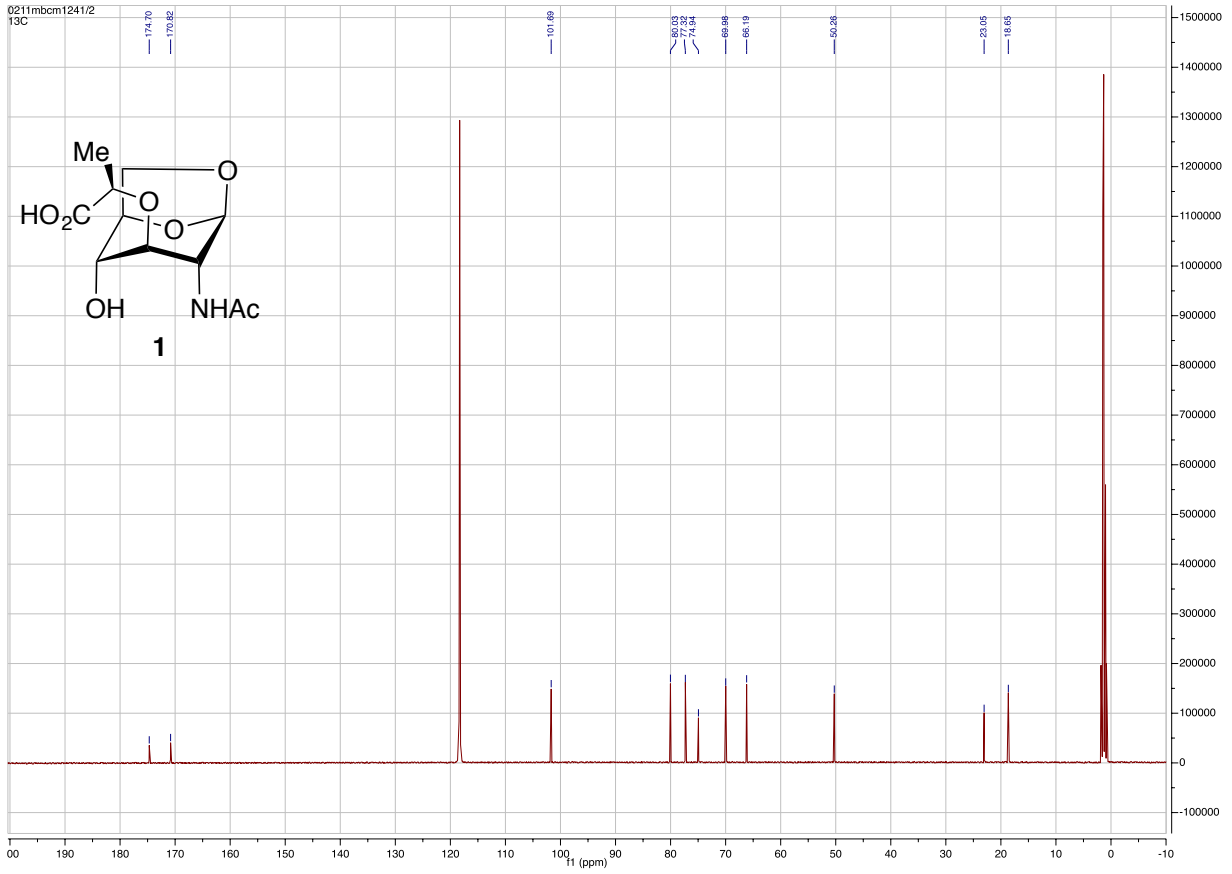
¹H NMR data for **13**



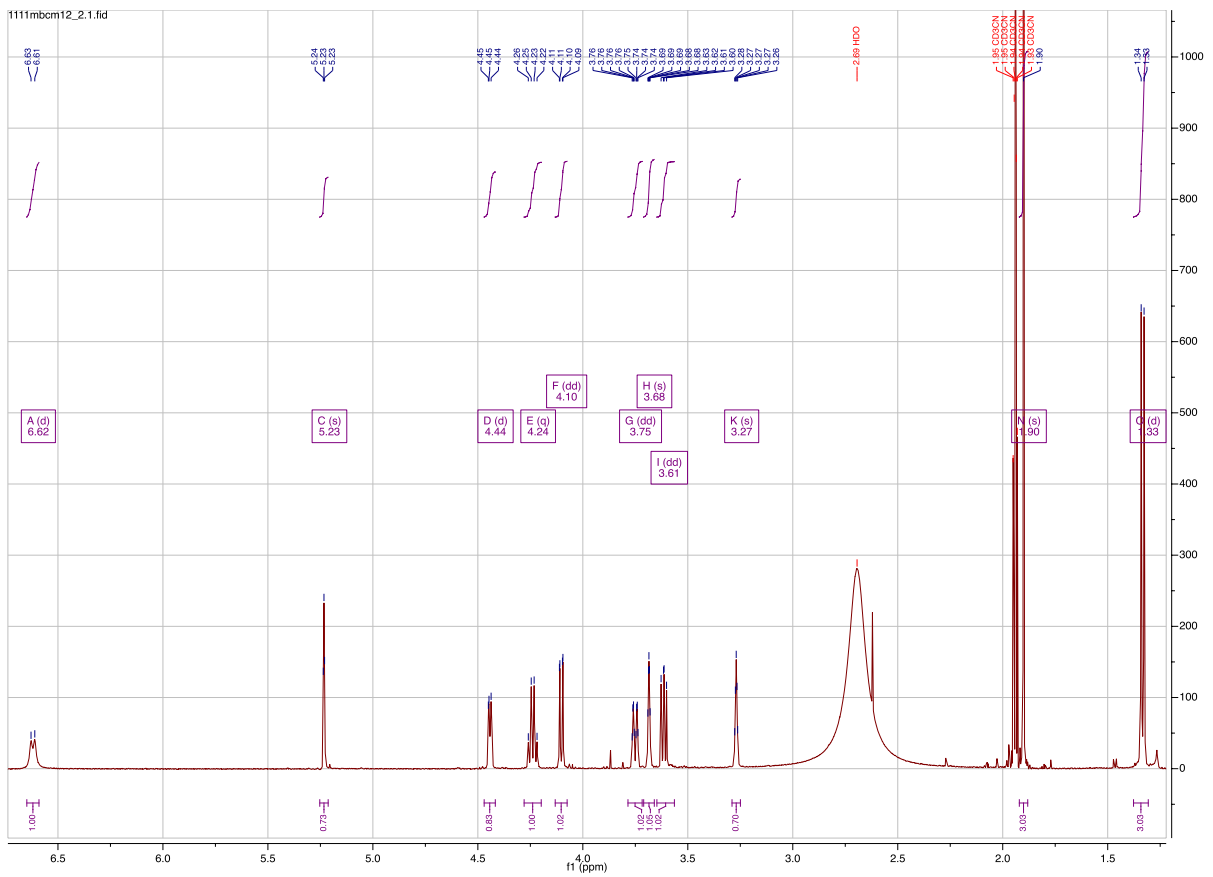
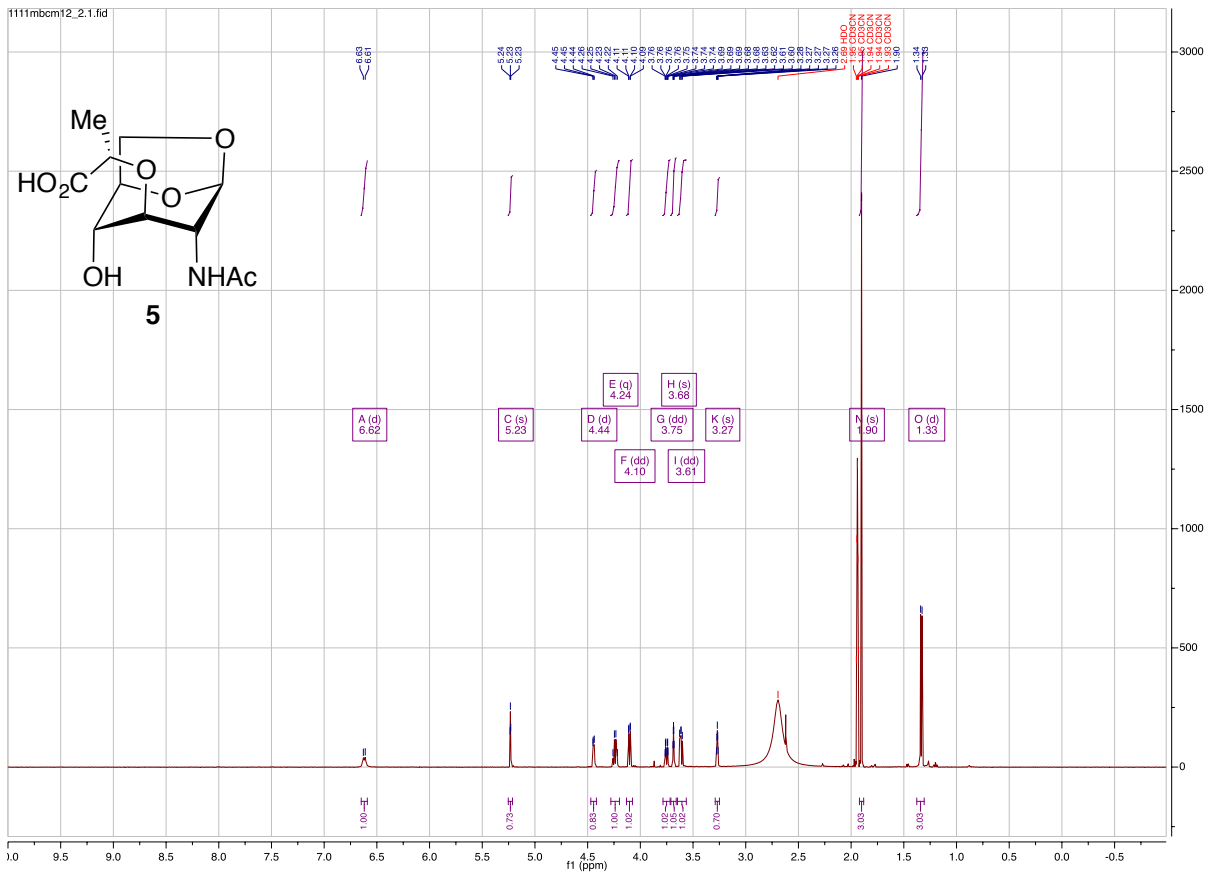
¹³C NMR data for **13**



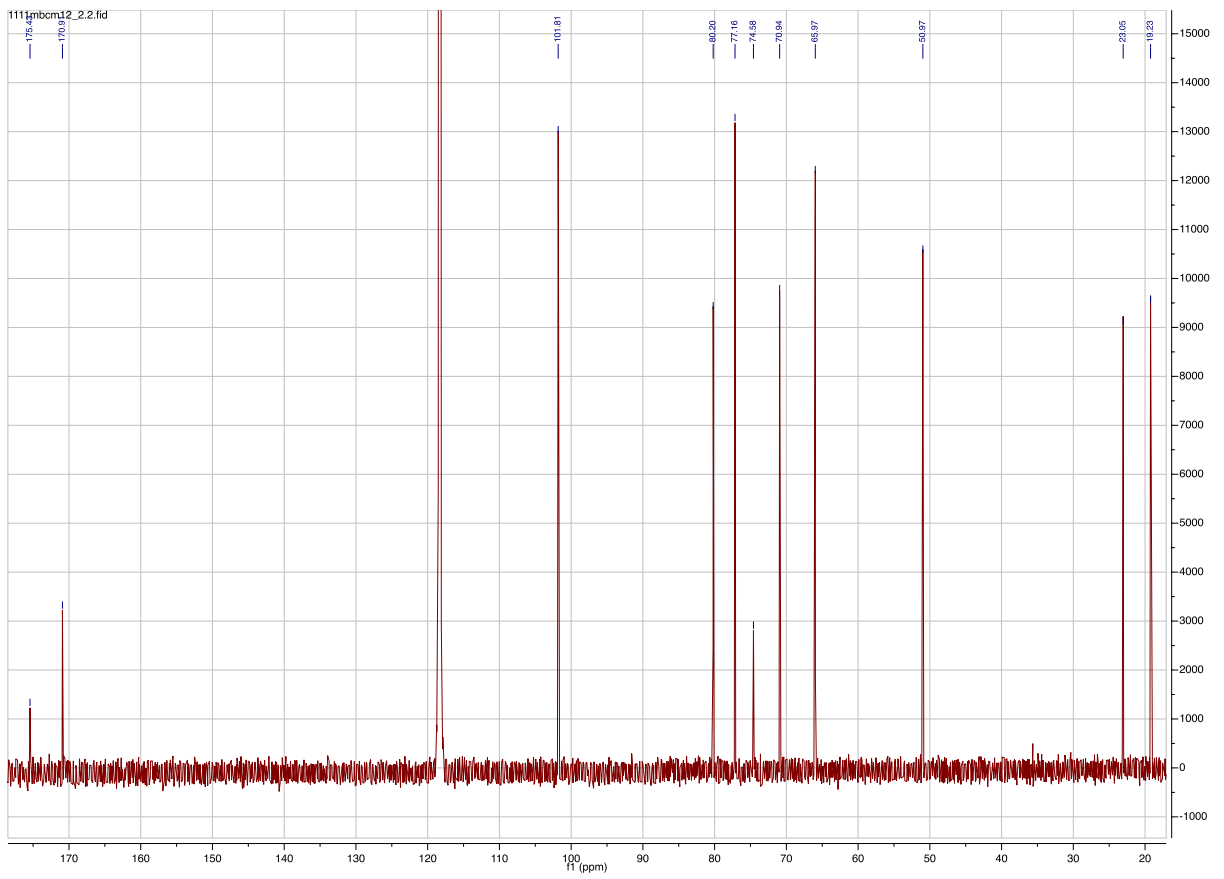
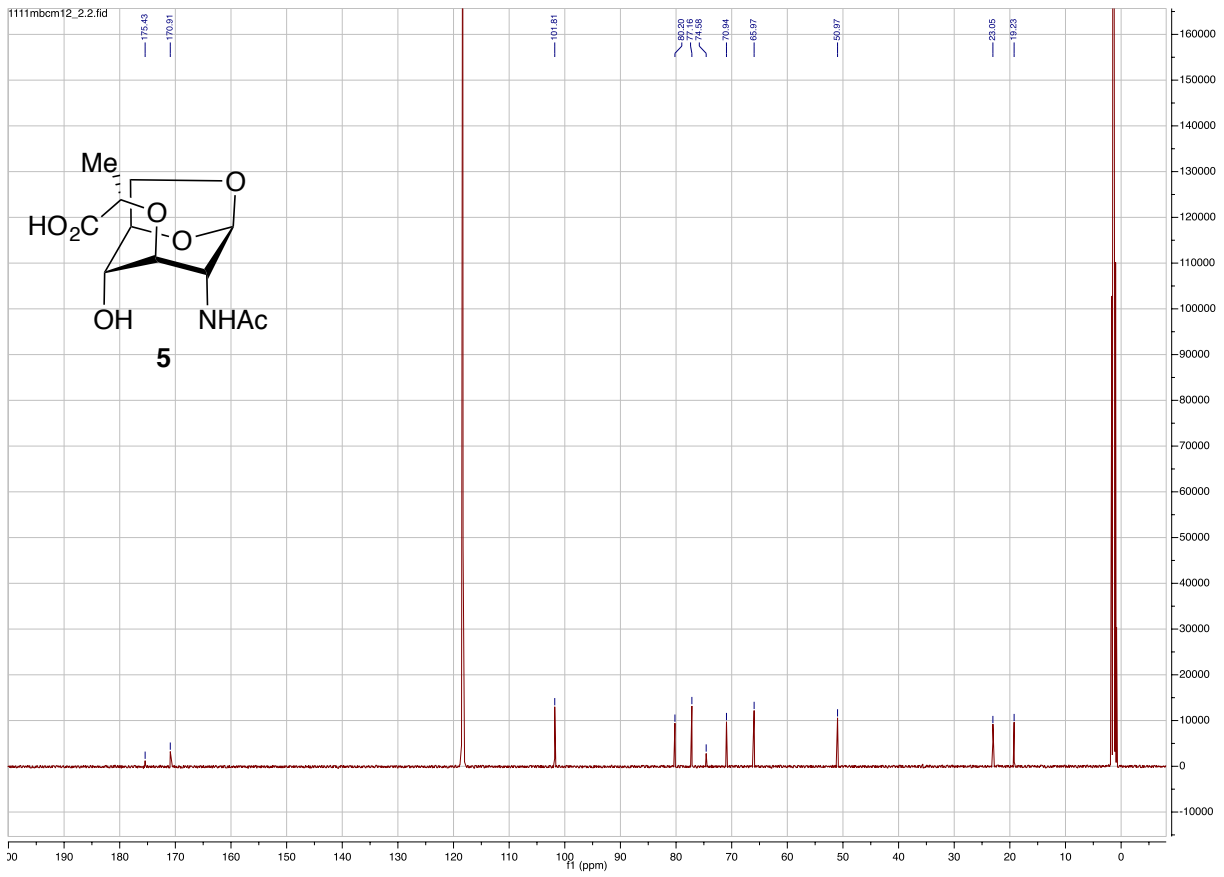
¹H NMR data for **1**



¹³C NMR data for **1**



¹H NMR data for **5**



^{13}C NMR data for **5**