

Supporting Information (SI-2) for

Both D- and L-glucose polyphosphates mimic D-myo-inositol 1,4,5-trisphosphate: new synthetic agonists and partial agonists at the Ins(1,4,5)P₃ receptor

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[†]Drug Discovery & Medicinal Chemistry, Department of Pharmacology, University of Oxford, Mansfield Road, OX1 3QT, United Kingdom

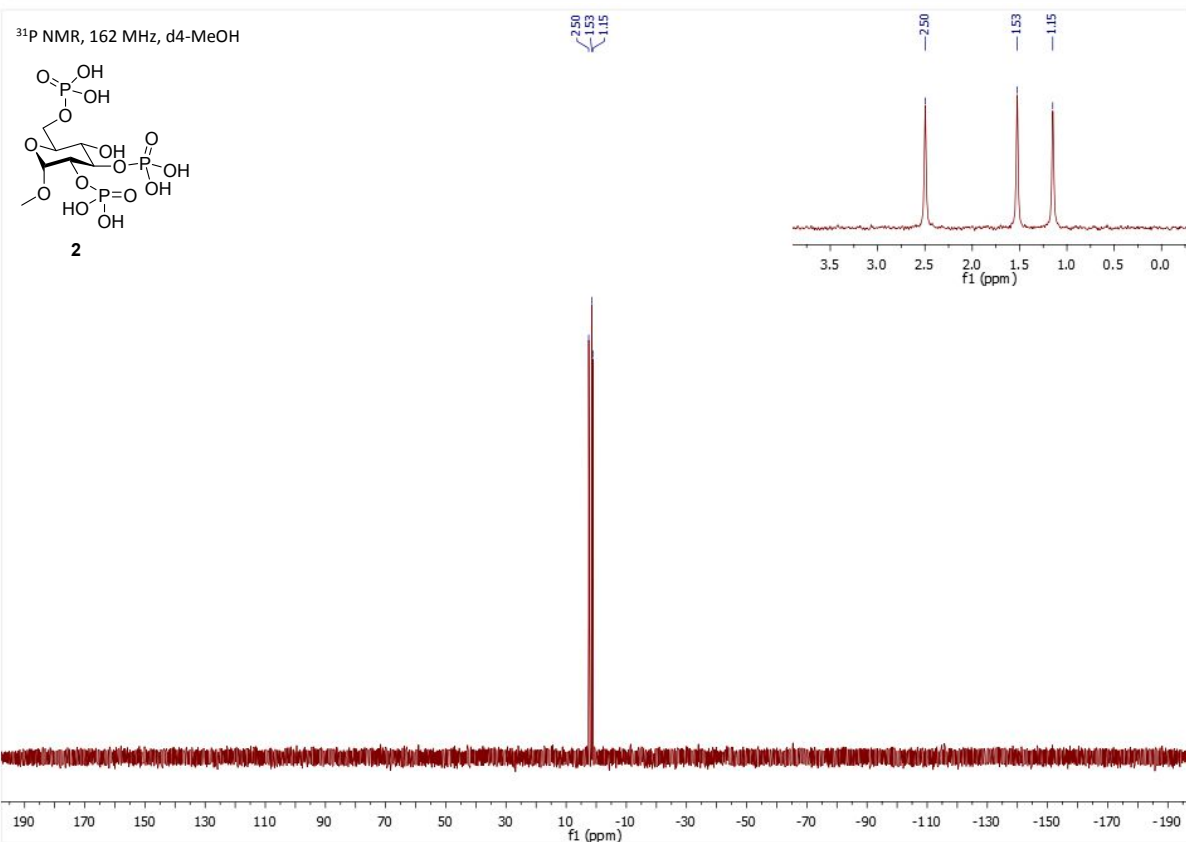
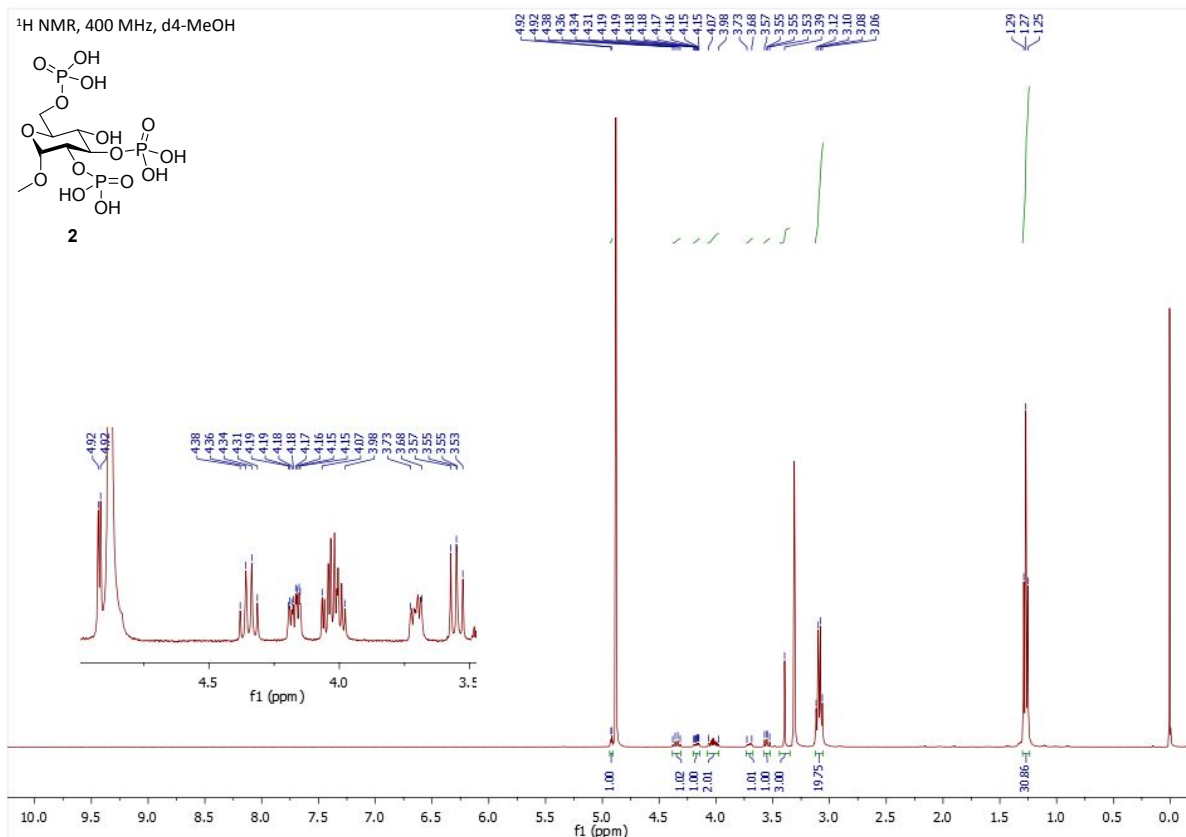
[‡]Department of Pharmacology, Tennis Court Road, University of Cambridge, CB2 1PD, United Kingdom

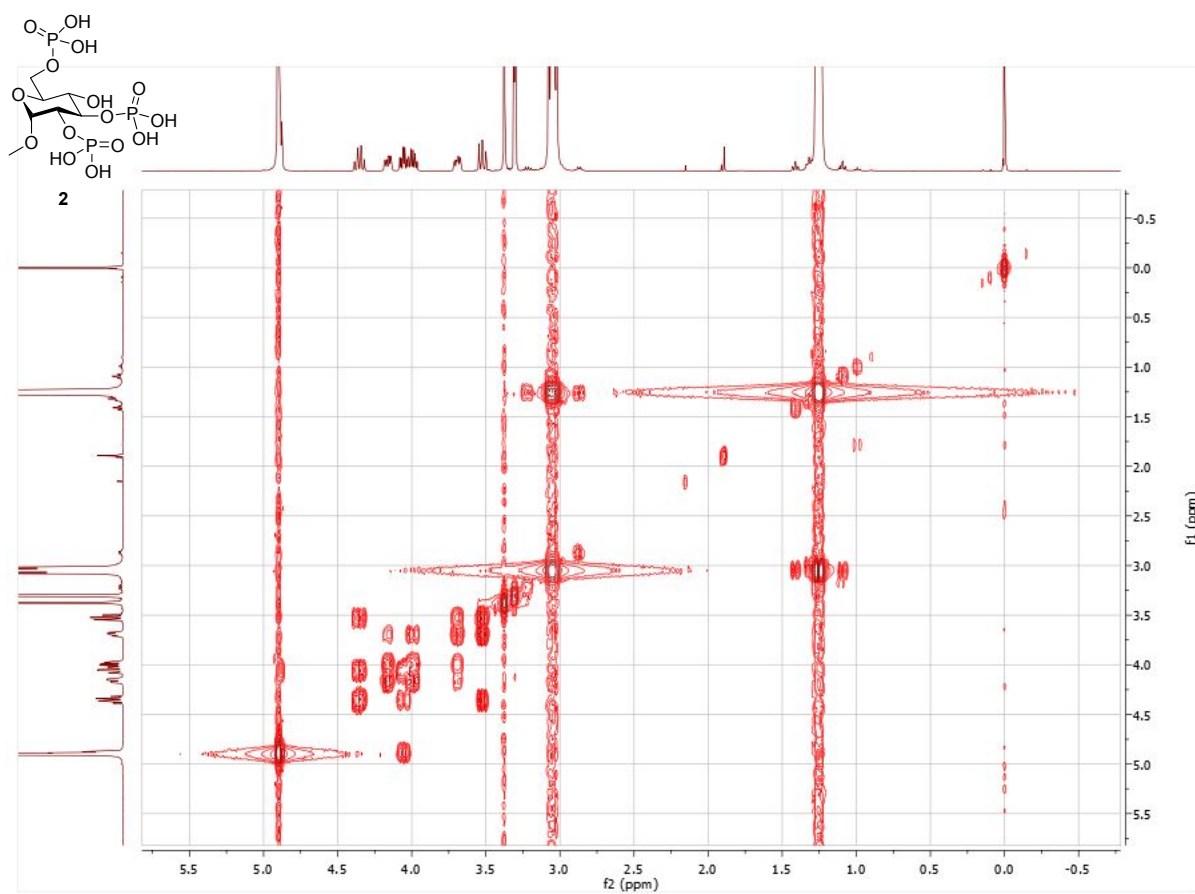
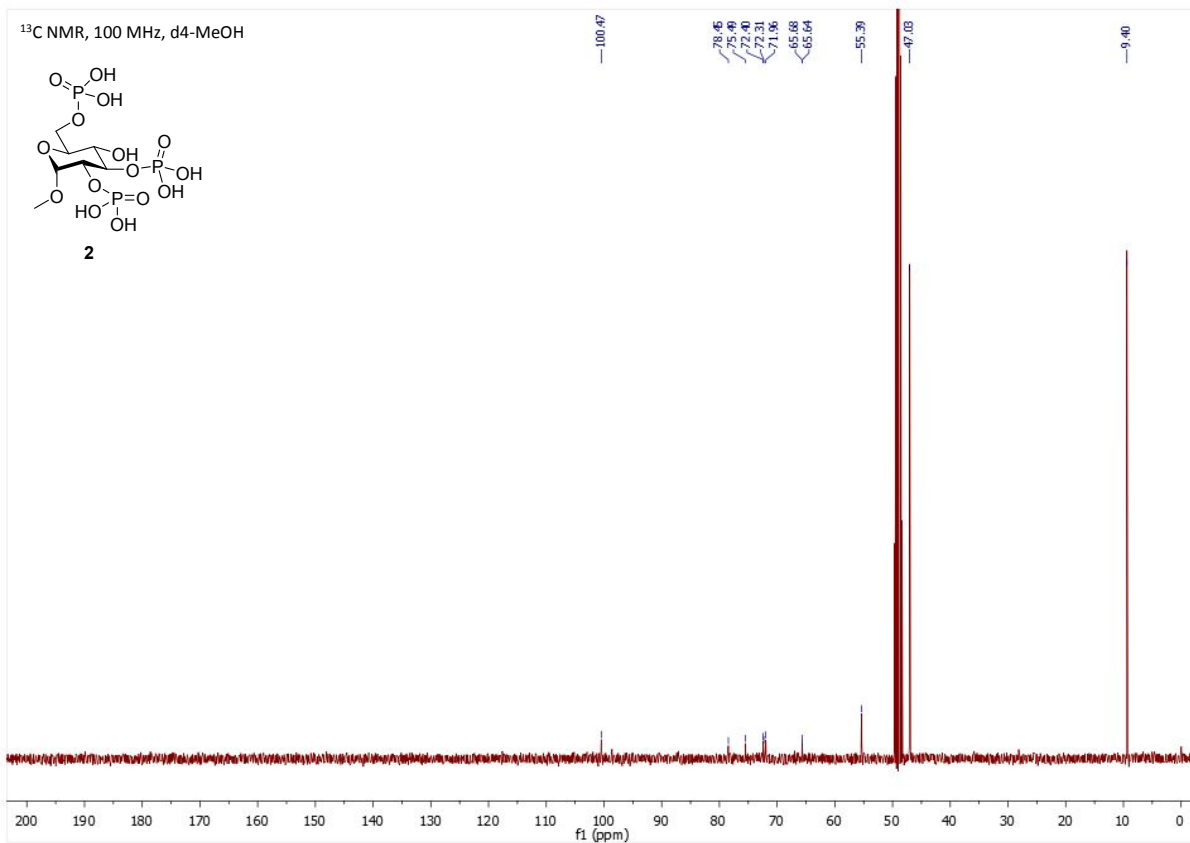
[§]School of Biological Sciences, University of East Anglia, Norwich Research Park, Norwich NR4 7TJ, United Kingdom

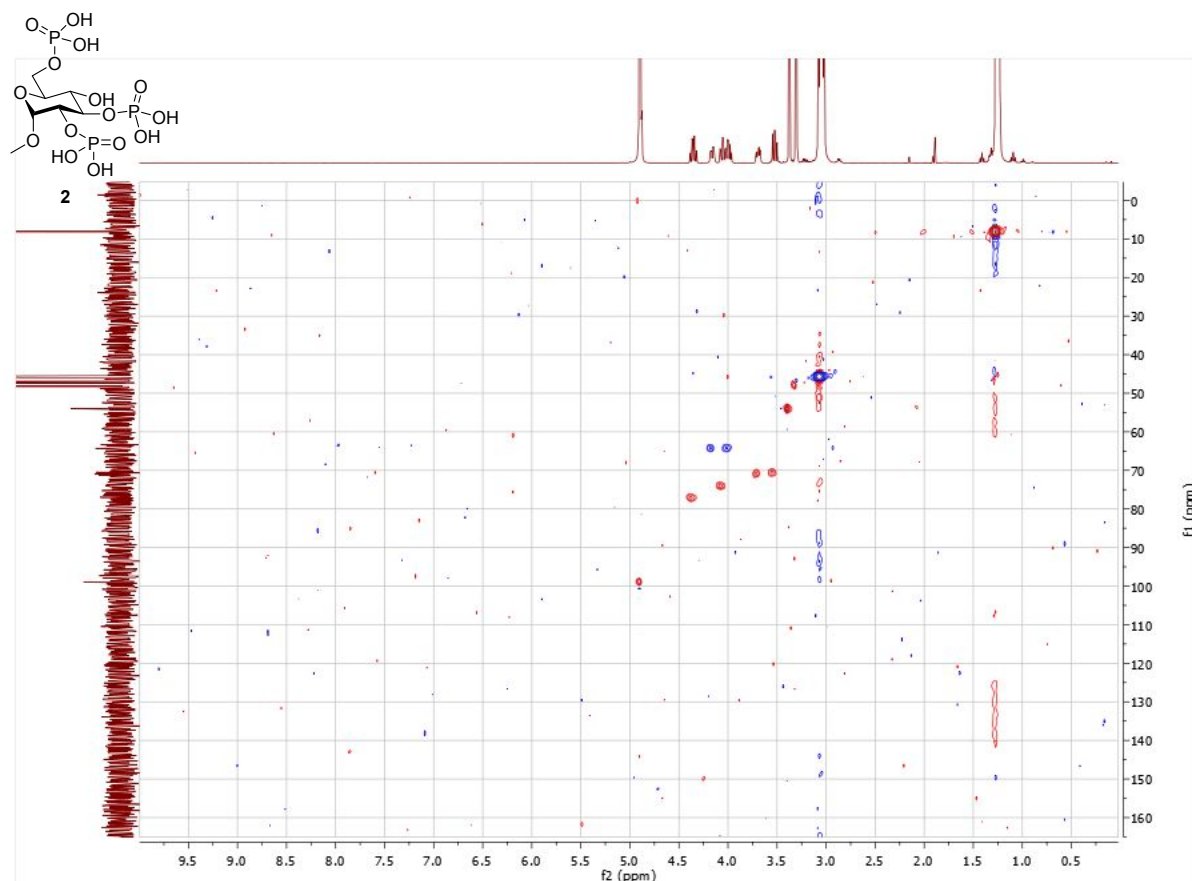
INDEX

1	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 2	S2-S4
2	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 3	S4-S6
3	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 4	S7-S9
4	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 5	S9-S11
5	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 6	S12-S14
6	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 7	S14-S16
7	¹ H NMR, ¹³ C NMR of 8	S17
8	¹ H NMR, ¹³ C NMR of 9	S18
9	¹ H NMR, ¹³ C NMR of 10	S19
10	¹ H NMR, ¹³ C NMR, ³¹ P NMR of 11	S20-S21
11	¹ H NMR, ¹³ C NMR, COSY, HSQC of 12	S21-S23
12	¹ H NMR, ¹³ C NMR, COSY, HSQC of 13	S23-S25
13	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 14	S25-27
14	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 17	S28-S30
15	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 18	S30-S32
16	¹ H NMR, ¹³ C NMR, COSY, HSQC of 21	S33-S34
17	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 22	S35-S37
18	¹ H NMR, ¹³ C NMR, COSY, HSQC of 23	S37-S39
19	¹ H NMR, ¹³ C NMR, COSY, HSQC of 24	S39-S41
20	¹ H NMR, ¹³ C NMR, ³¹ P NMR, COSY, HSQC of 25	S41-S43

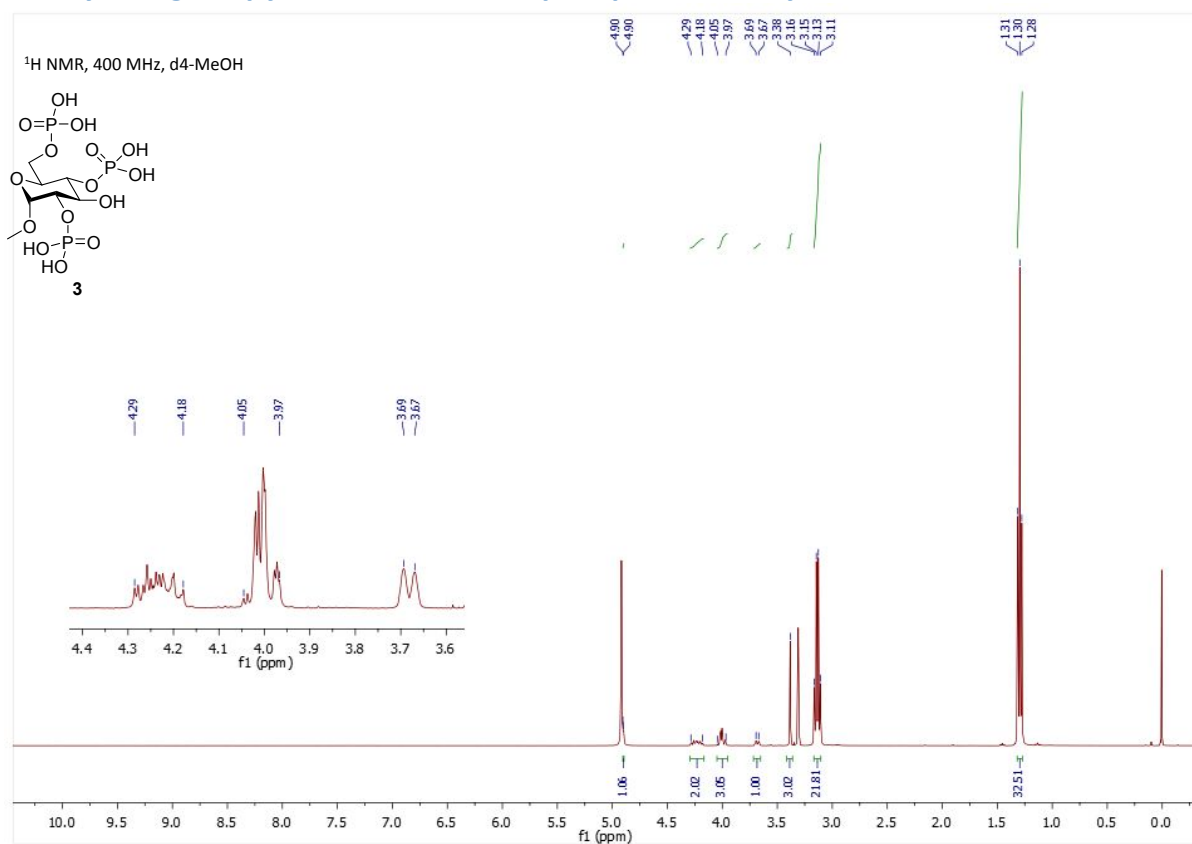
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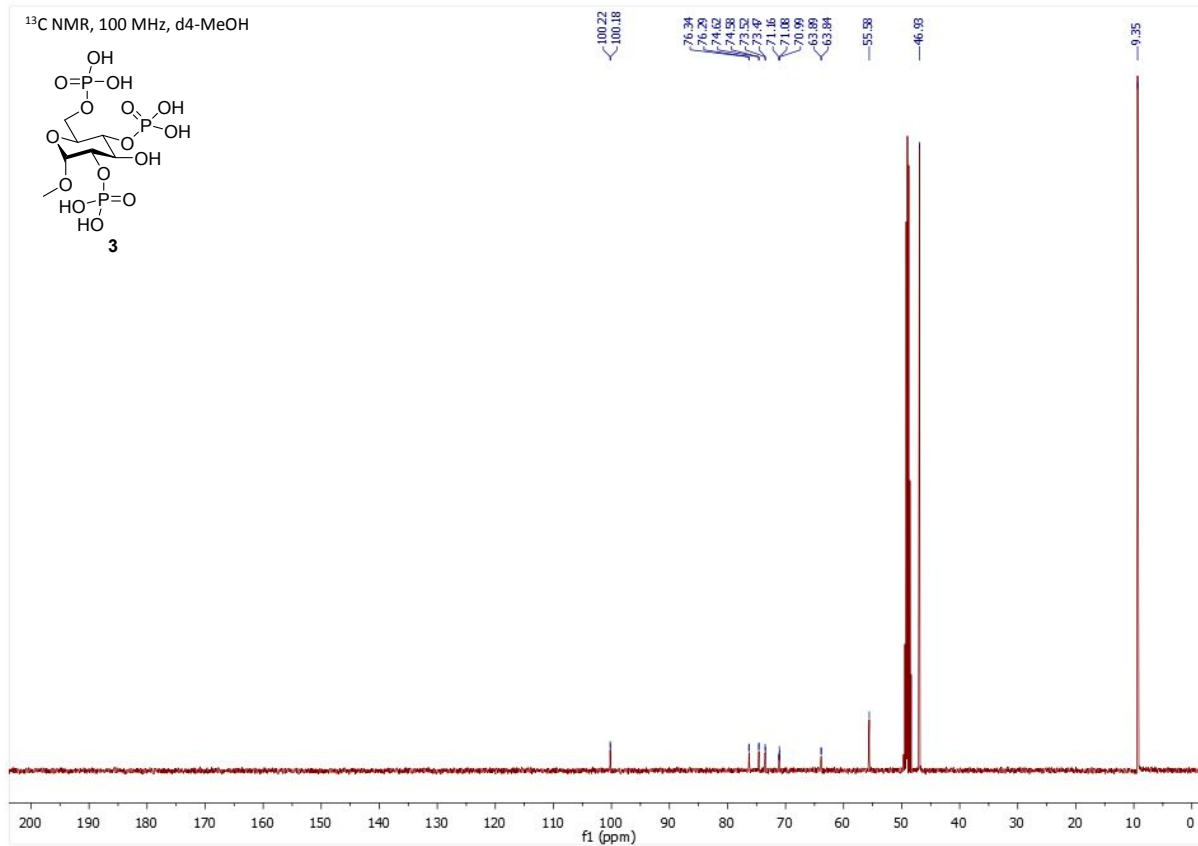
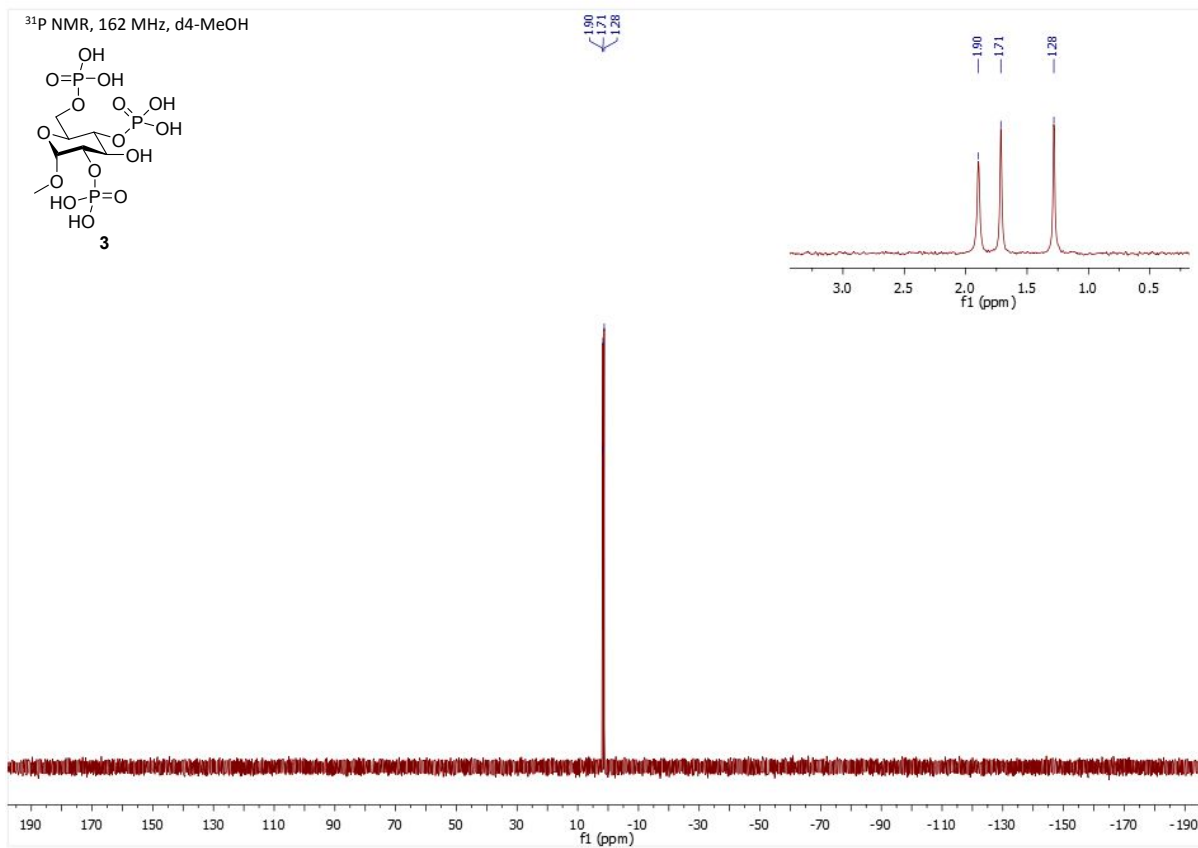


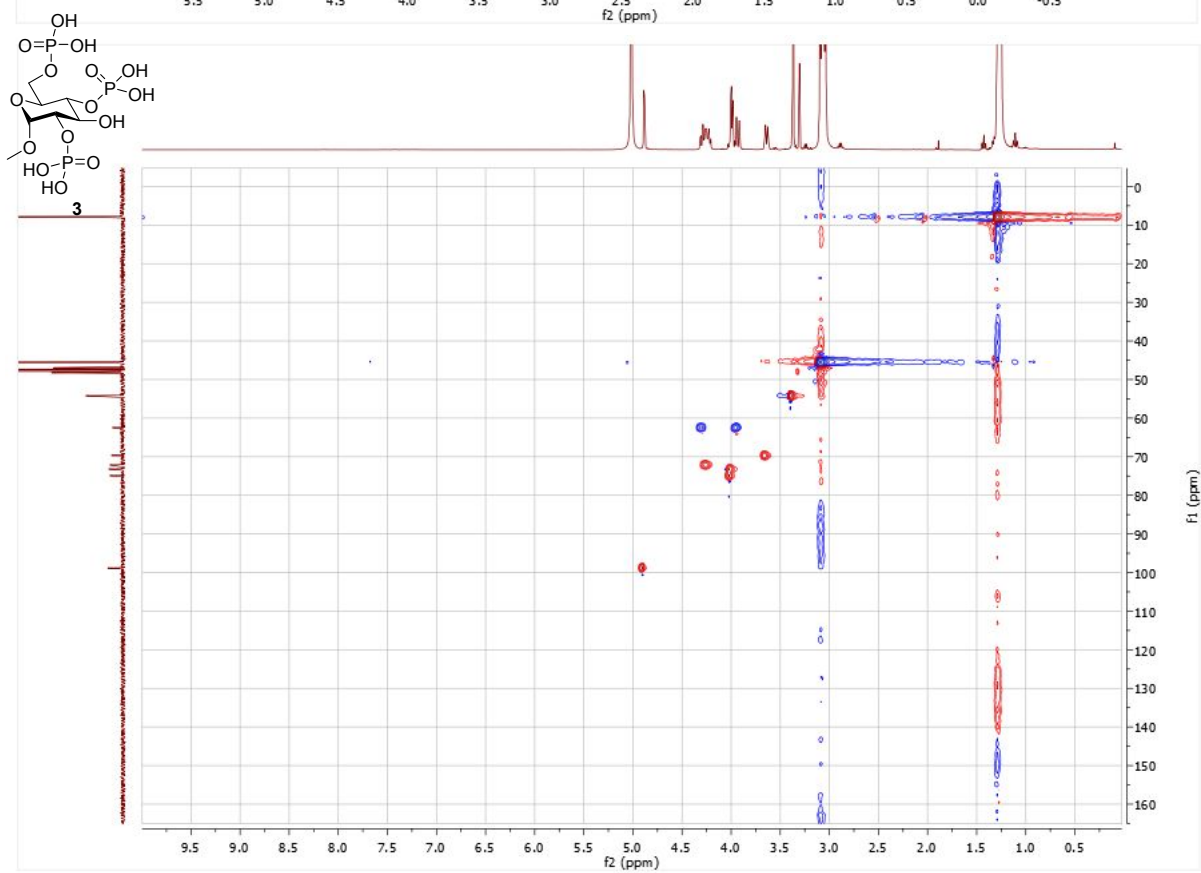
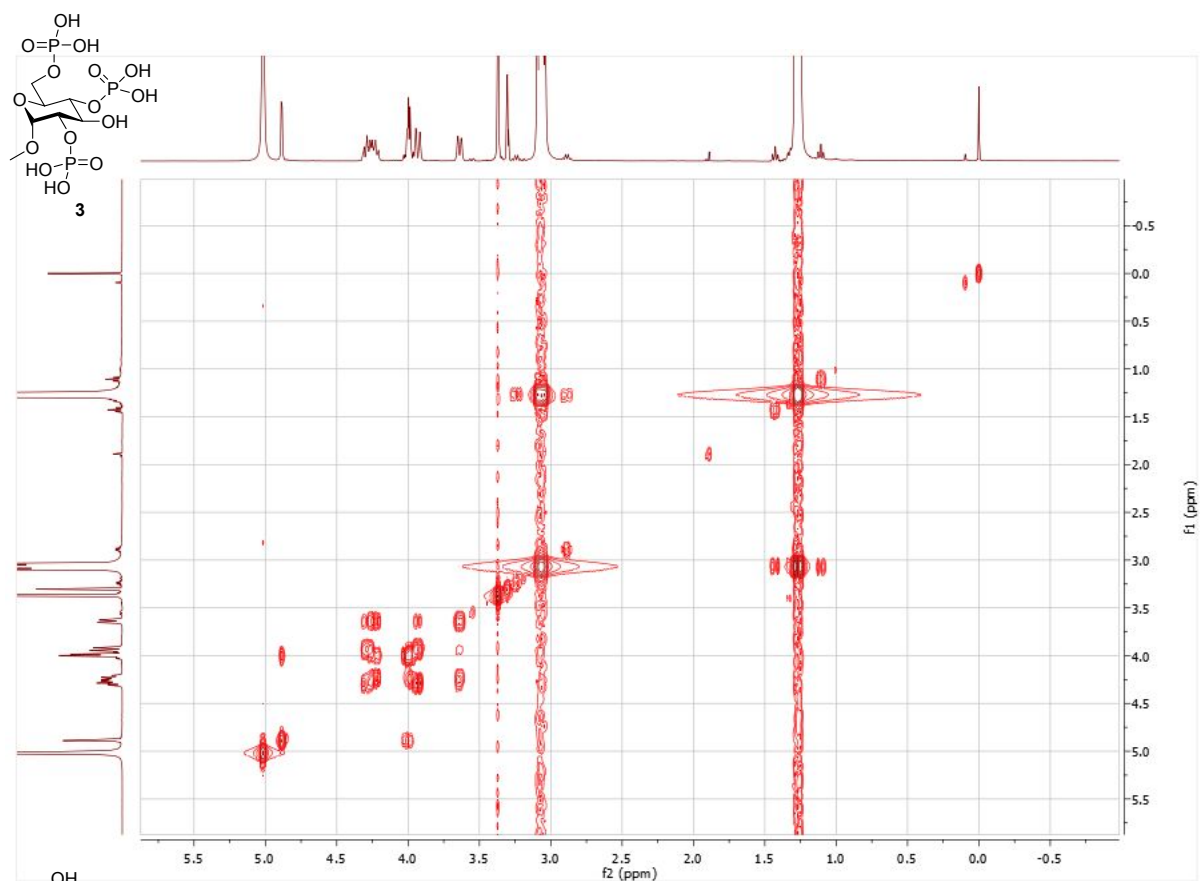


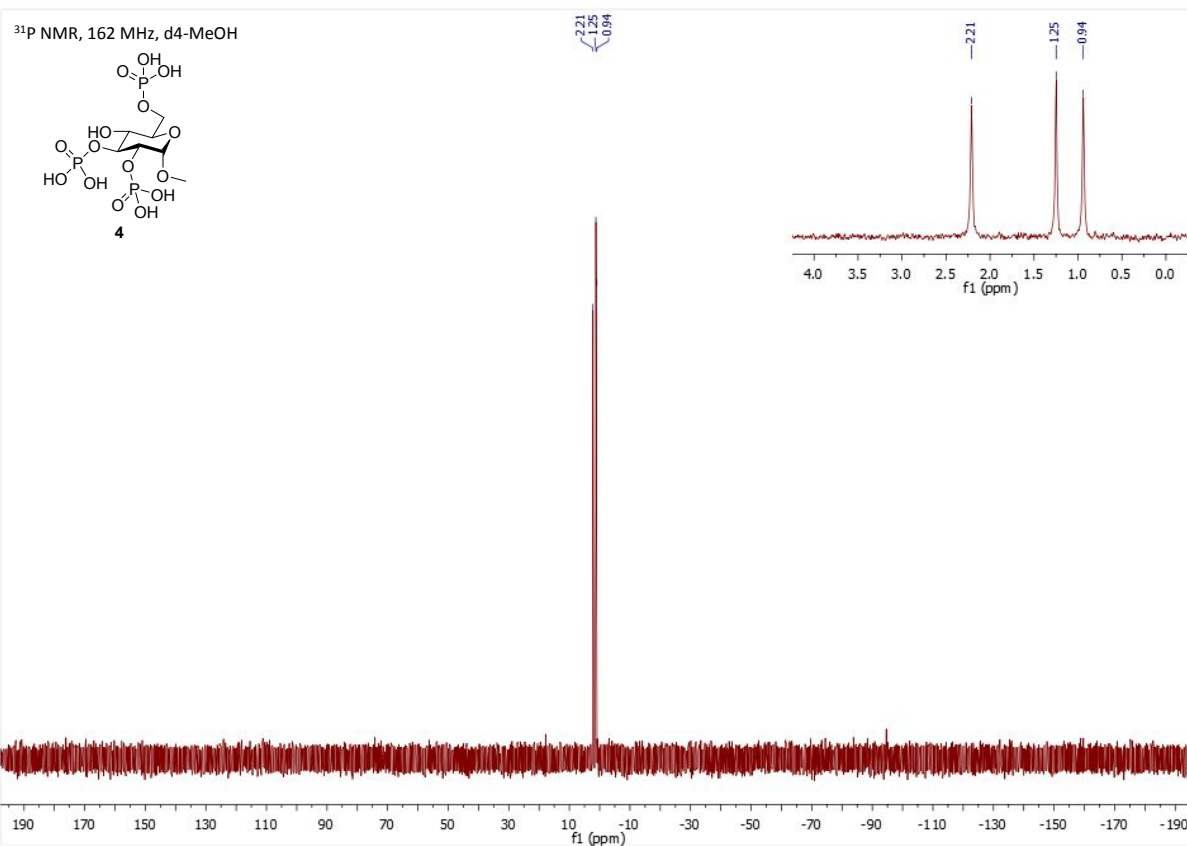
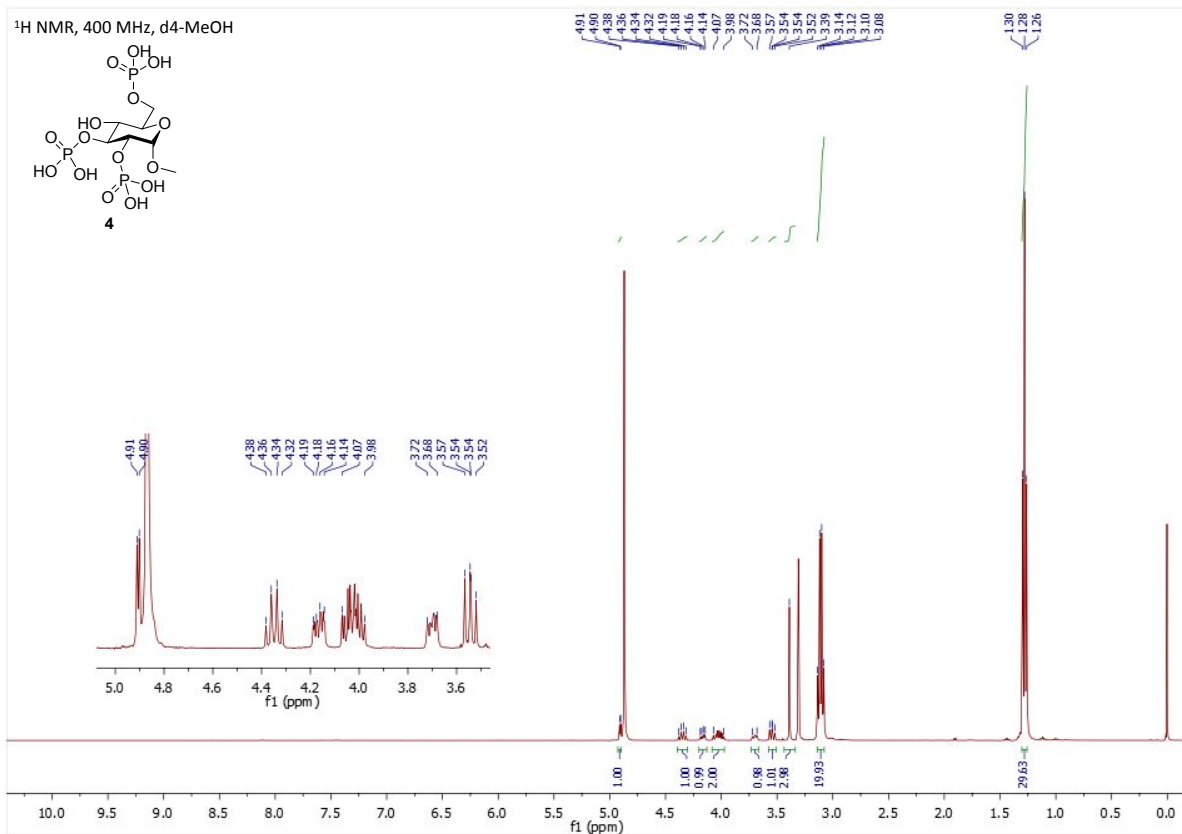


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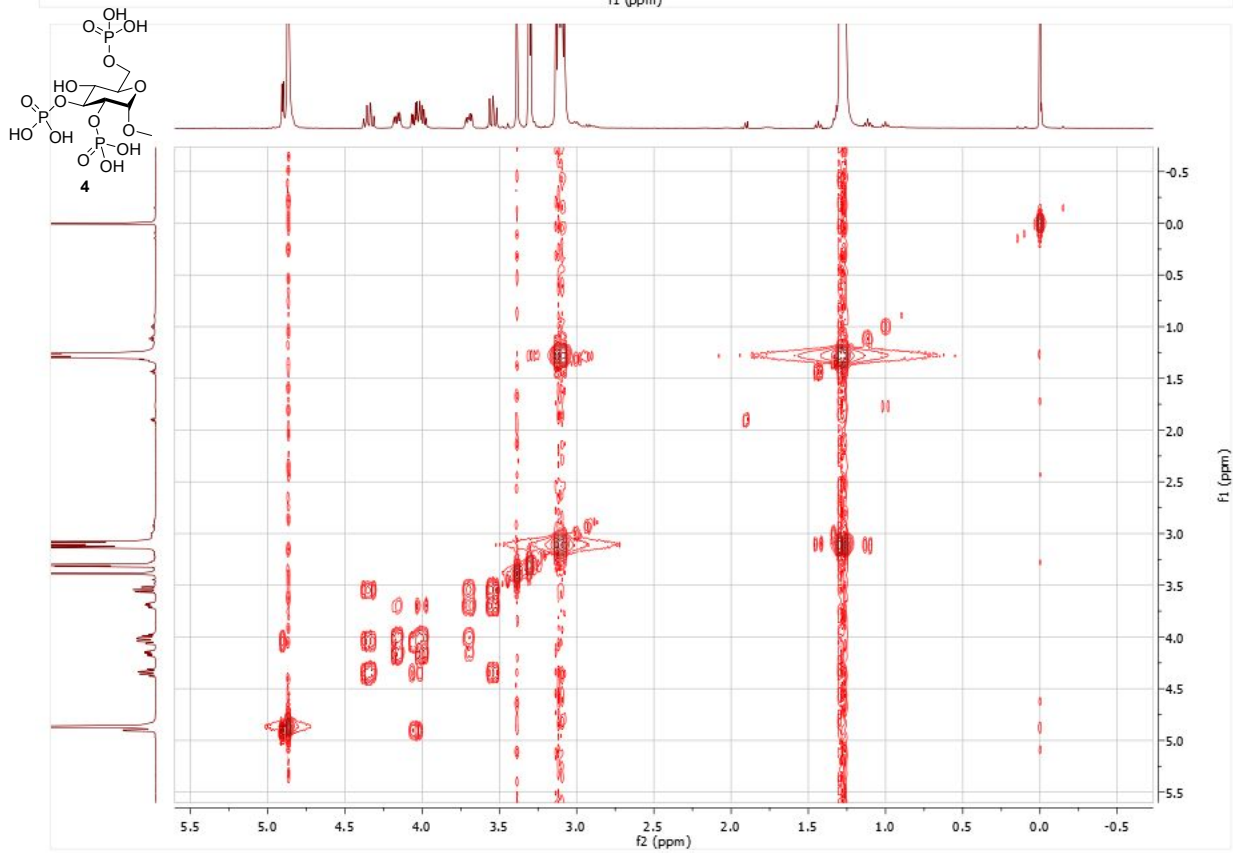
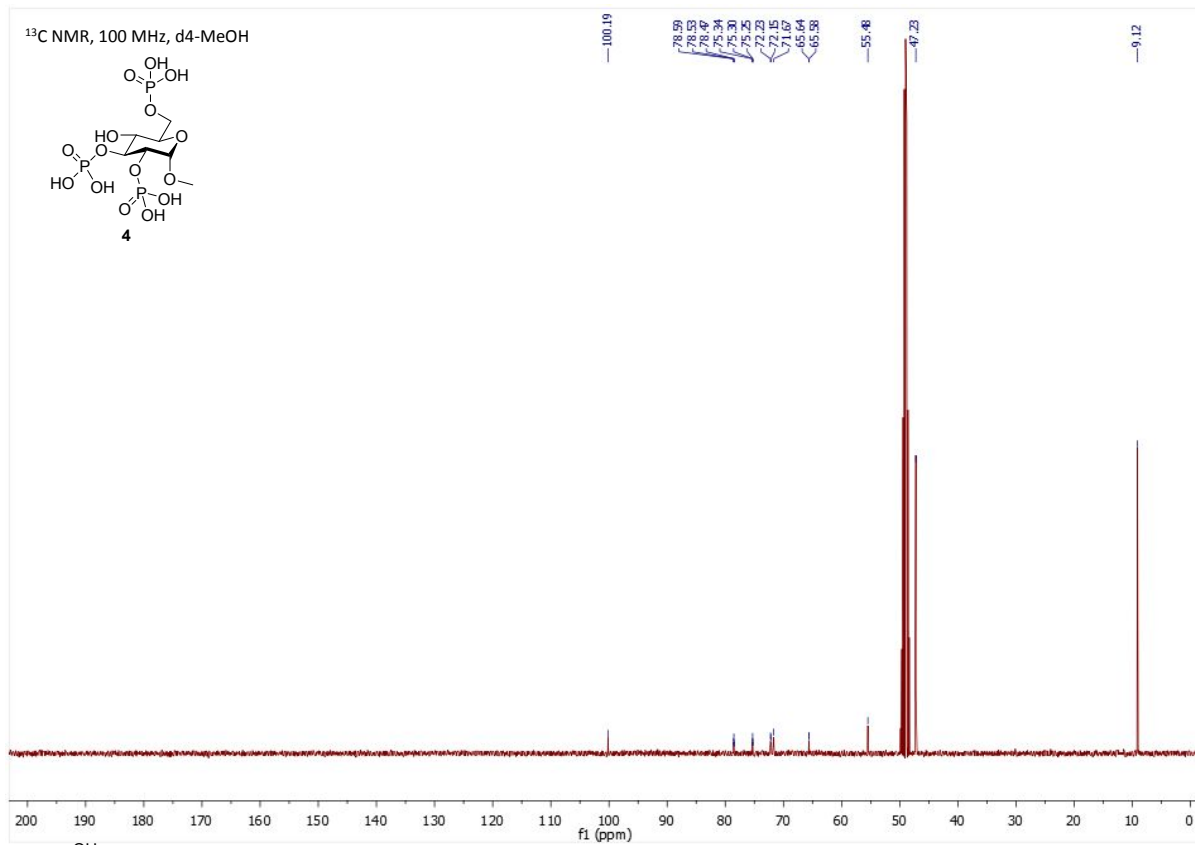
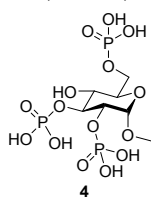


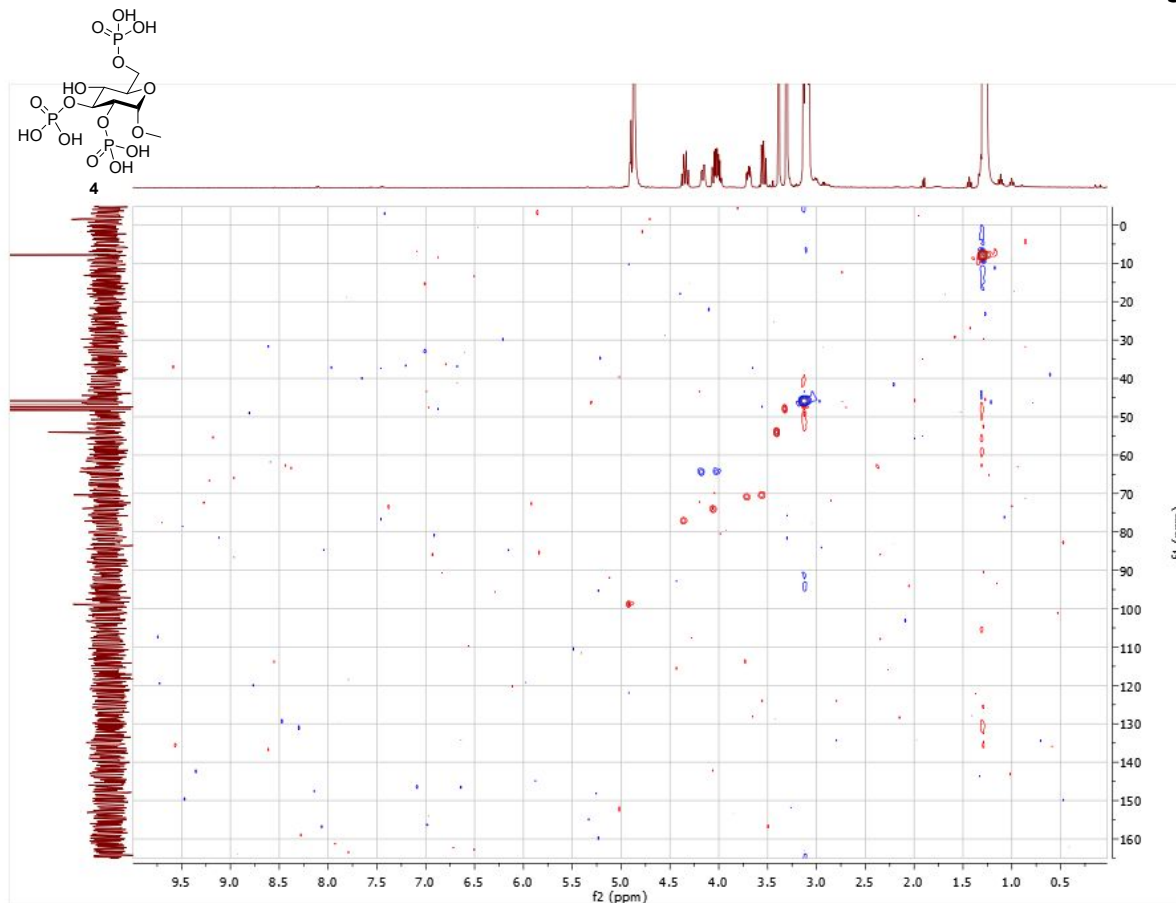




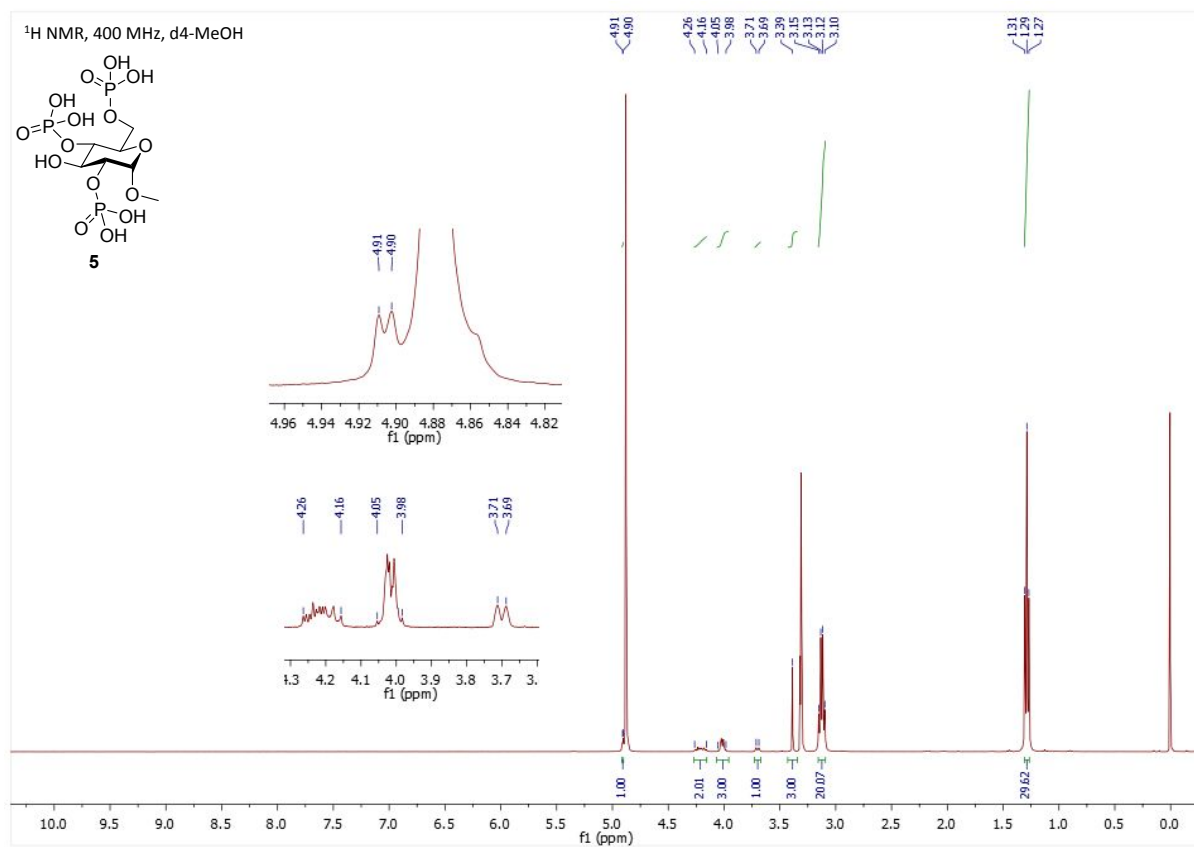
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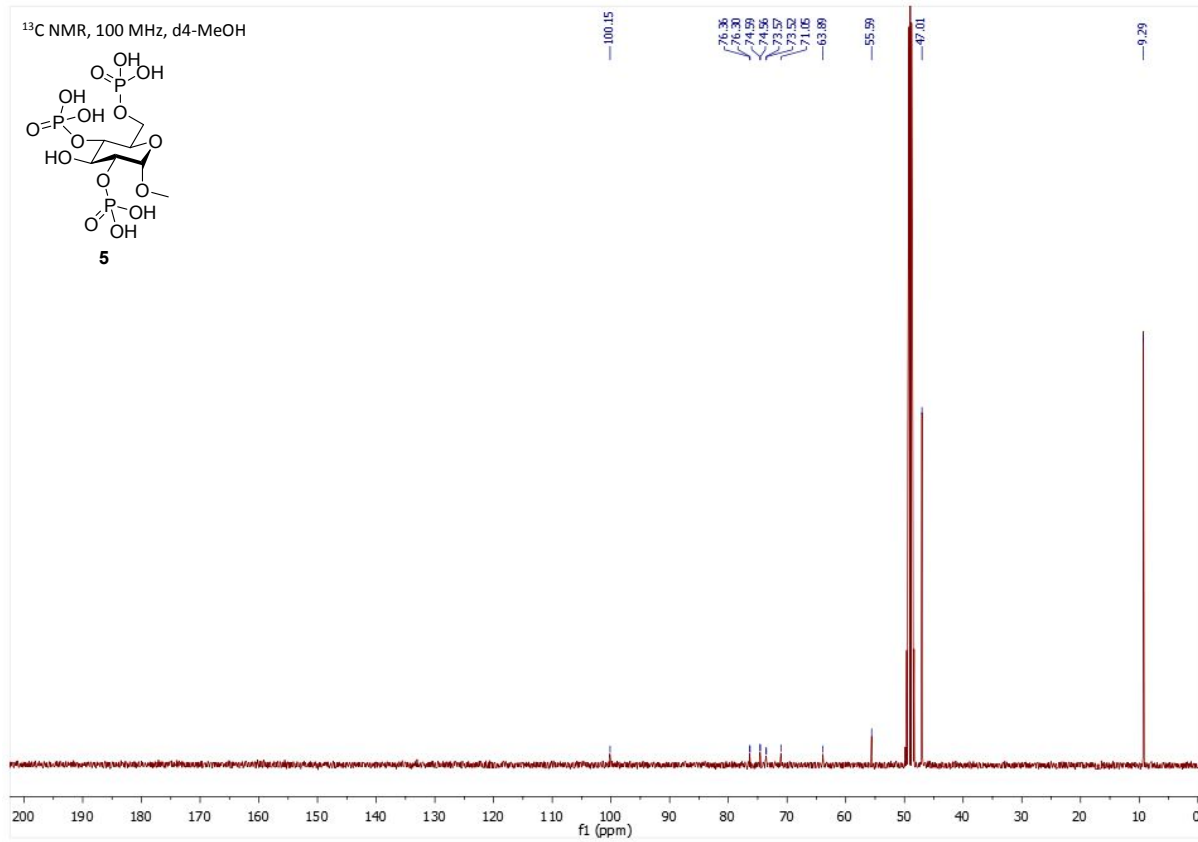
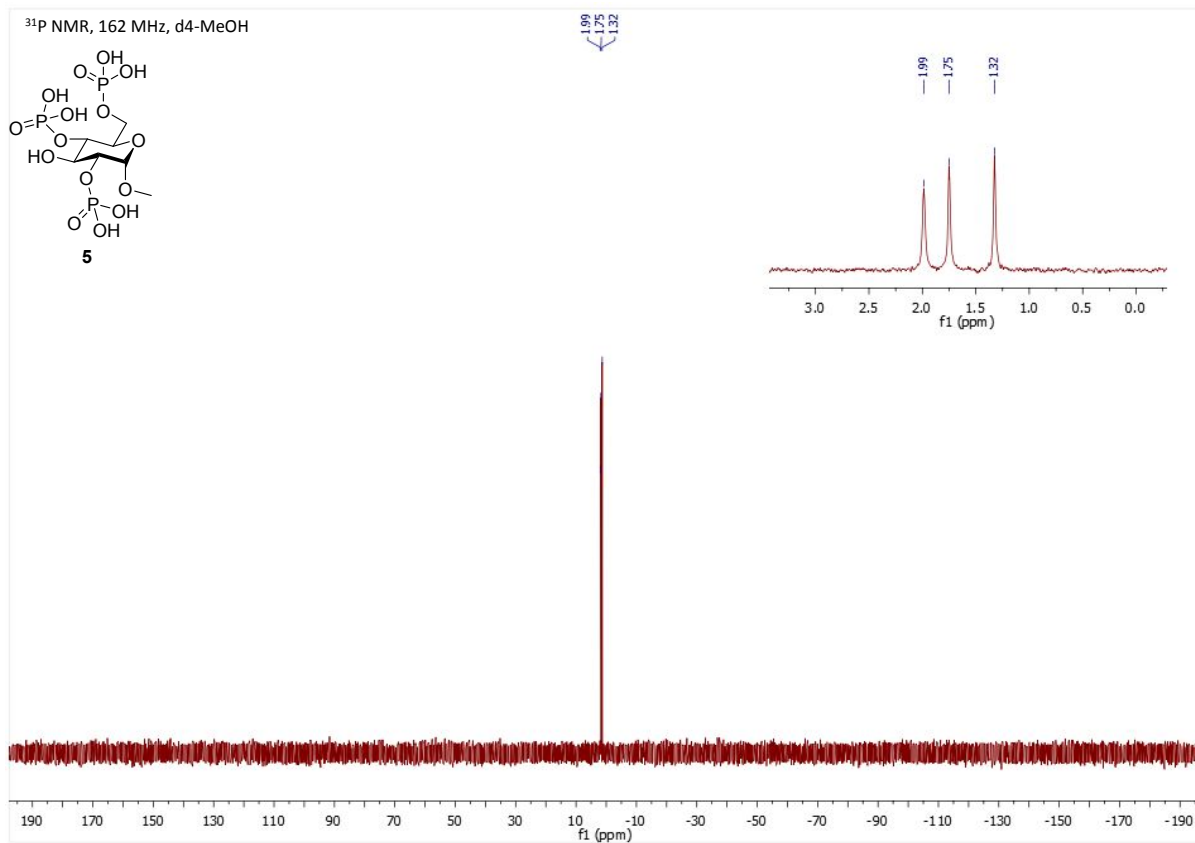
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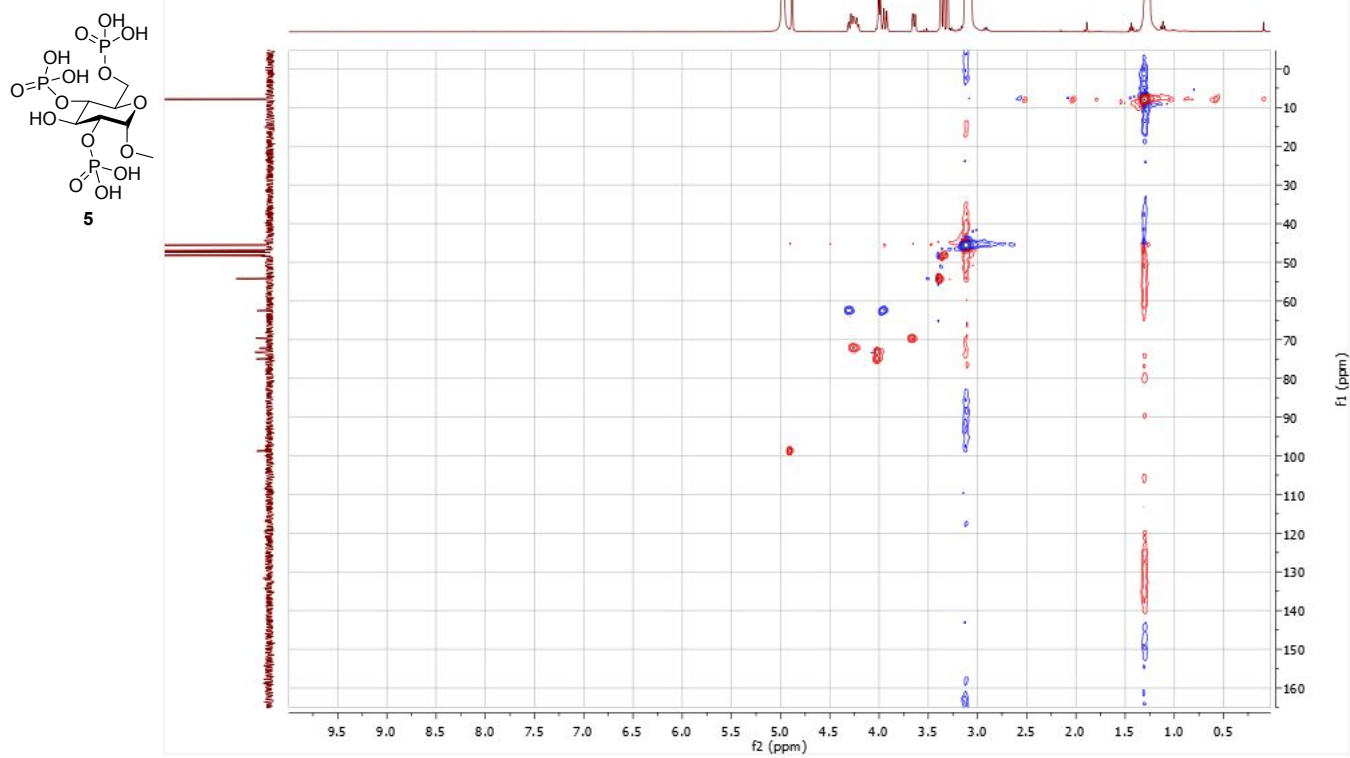
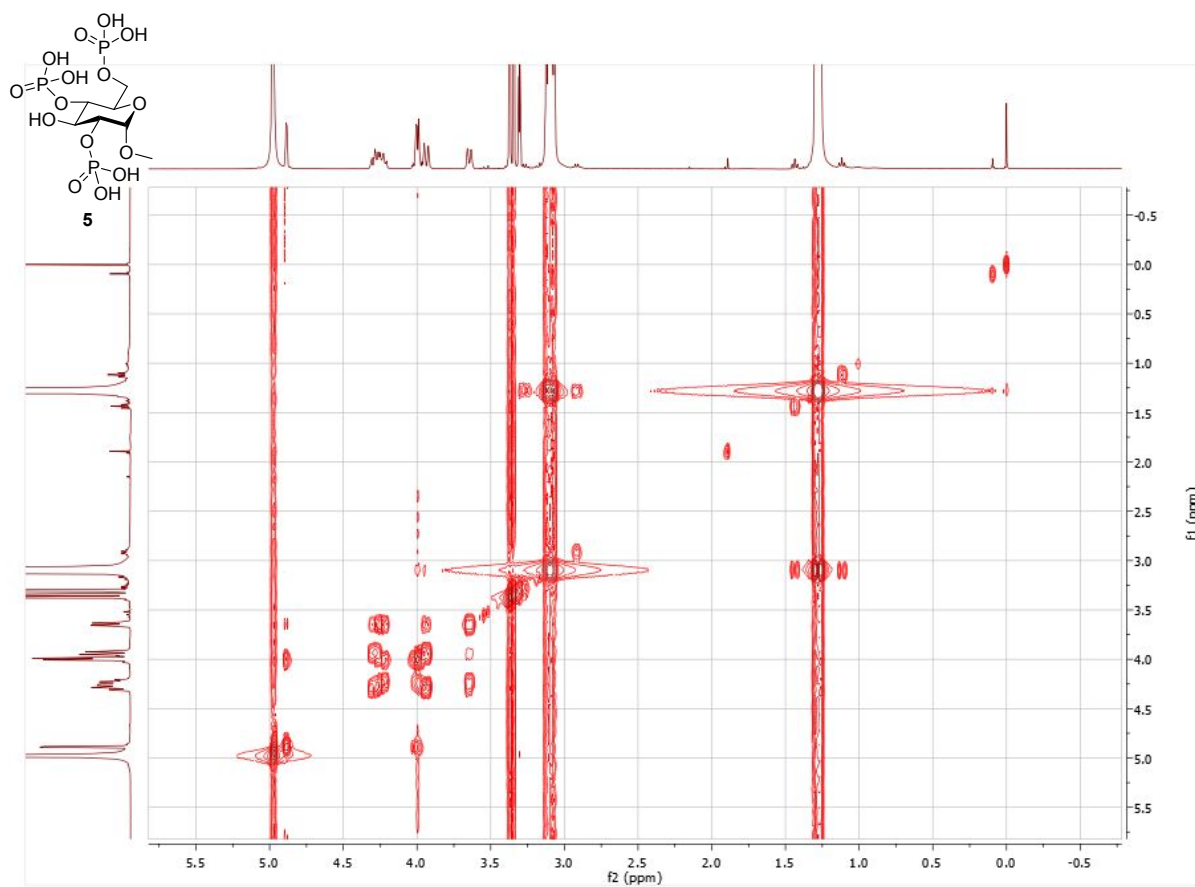


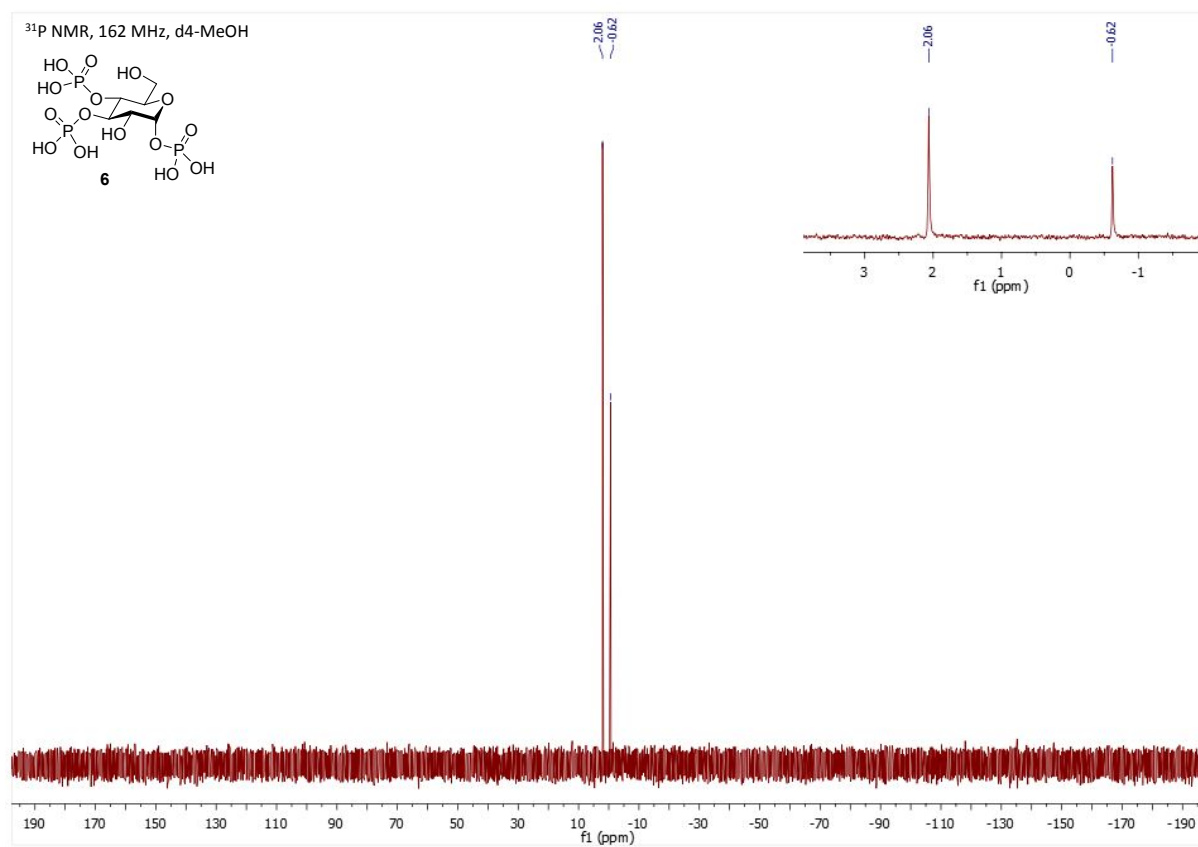
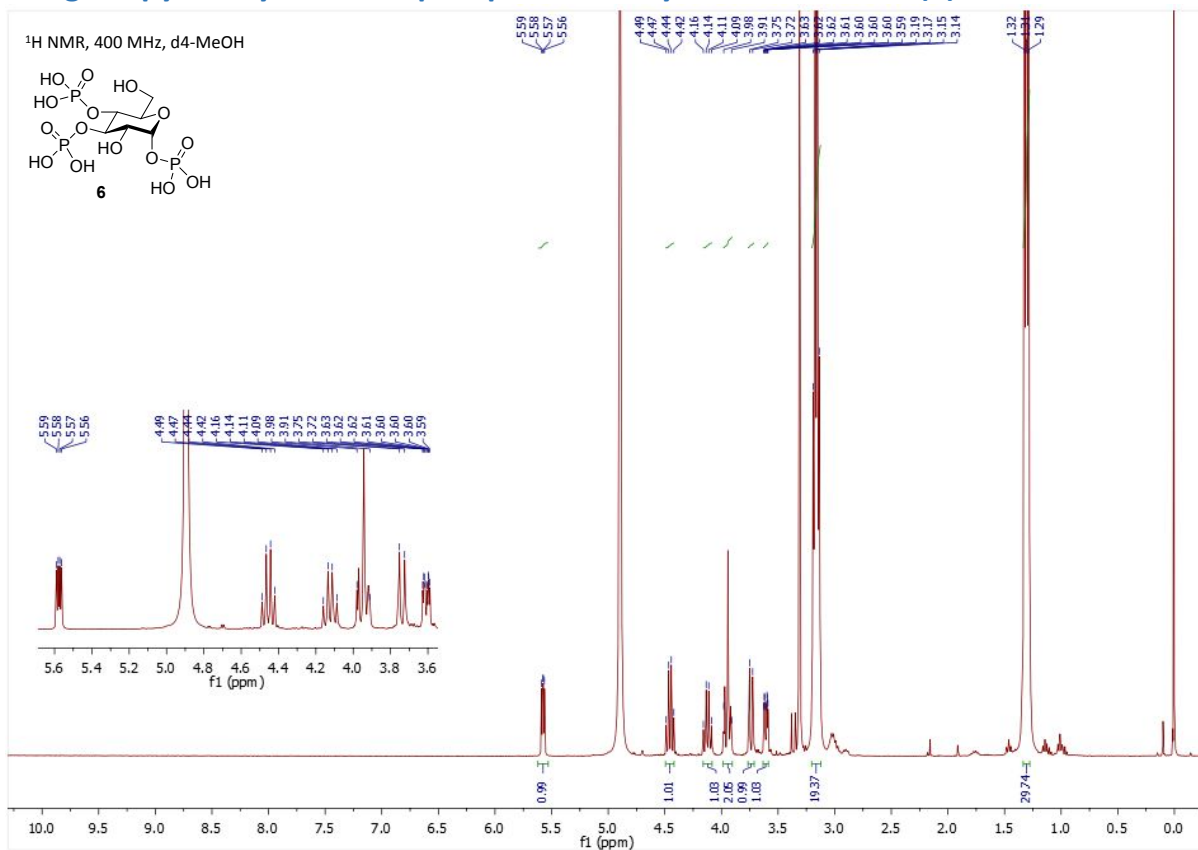


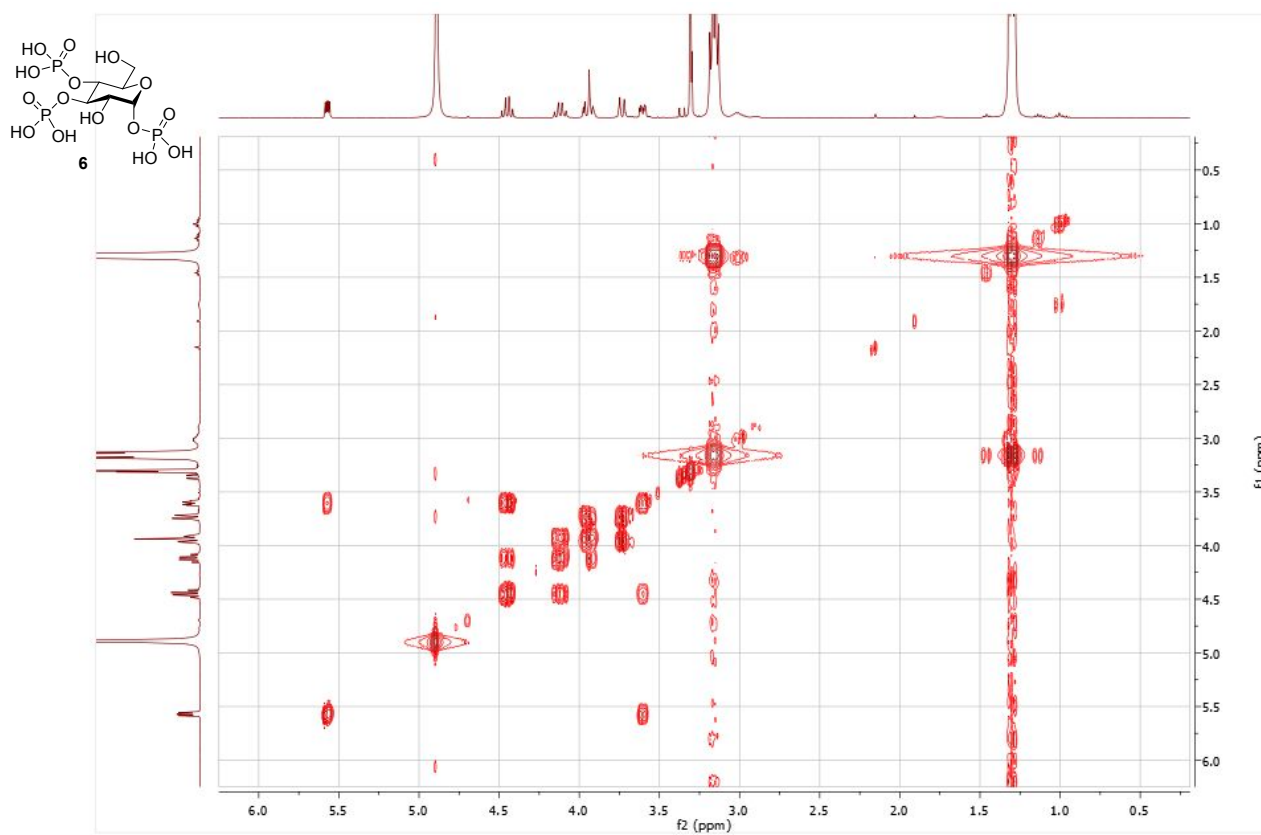
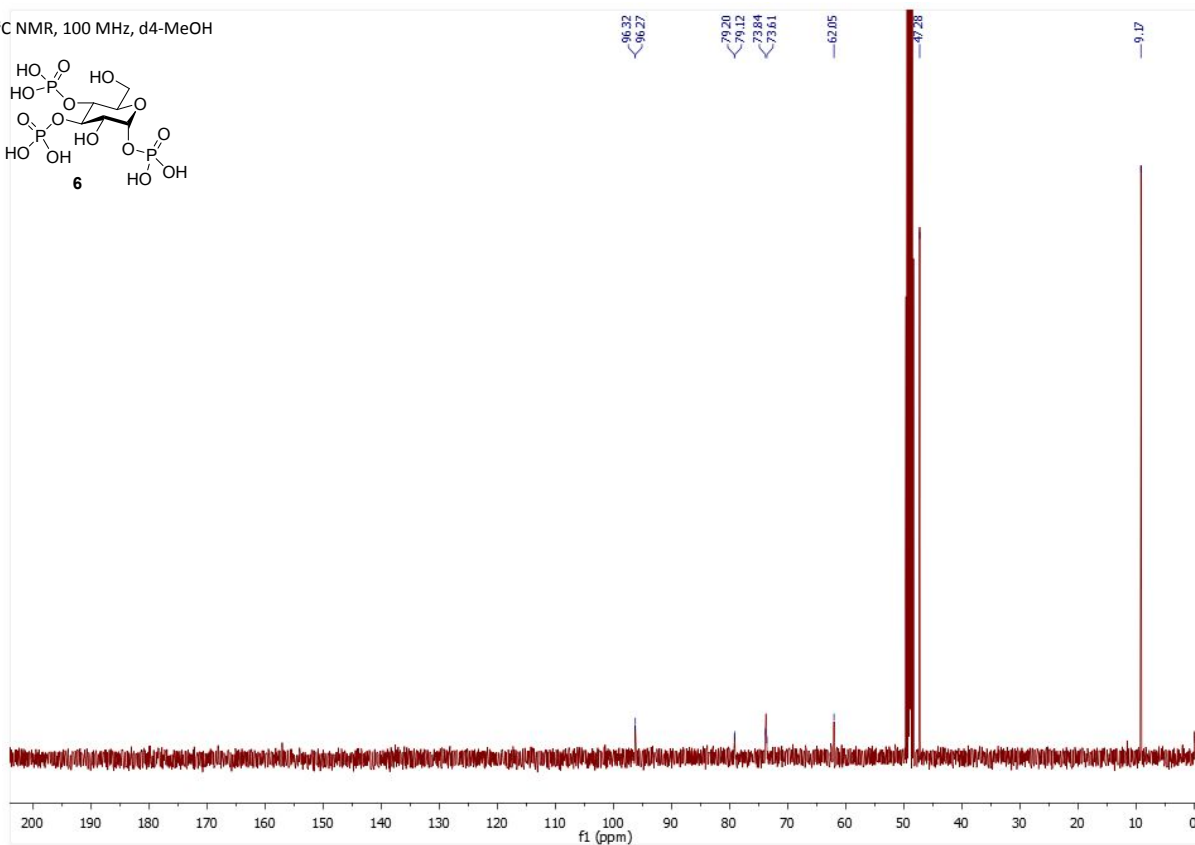
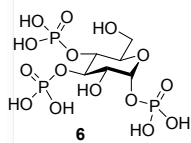
Methyl α -D-glucopyranoside 2,4,6-trisphosphate triethylammonium salt (**5**)

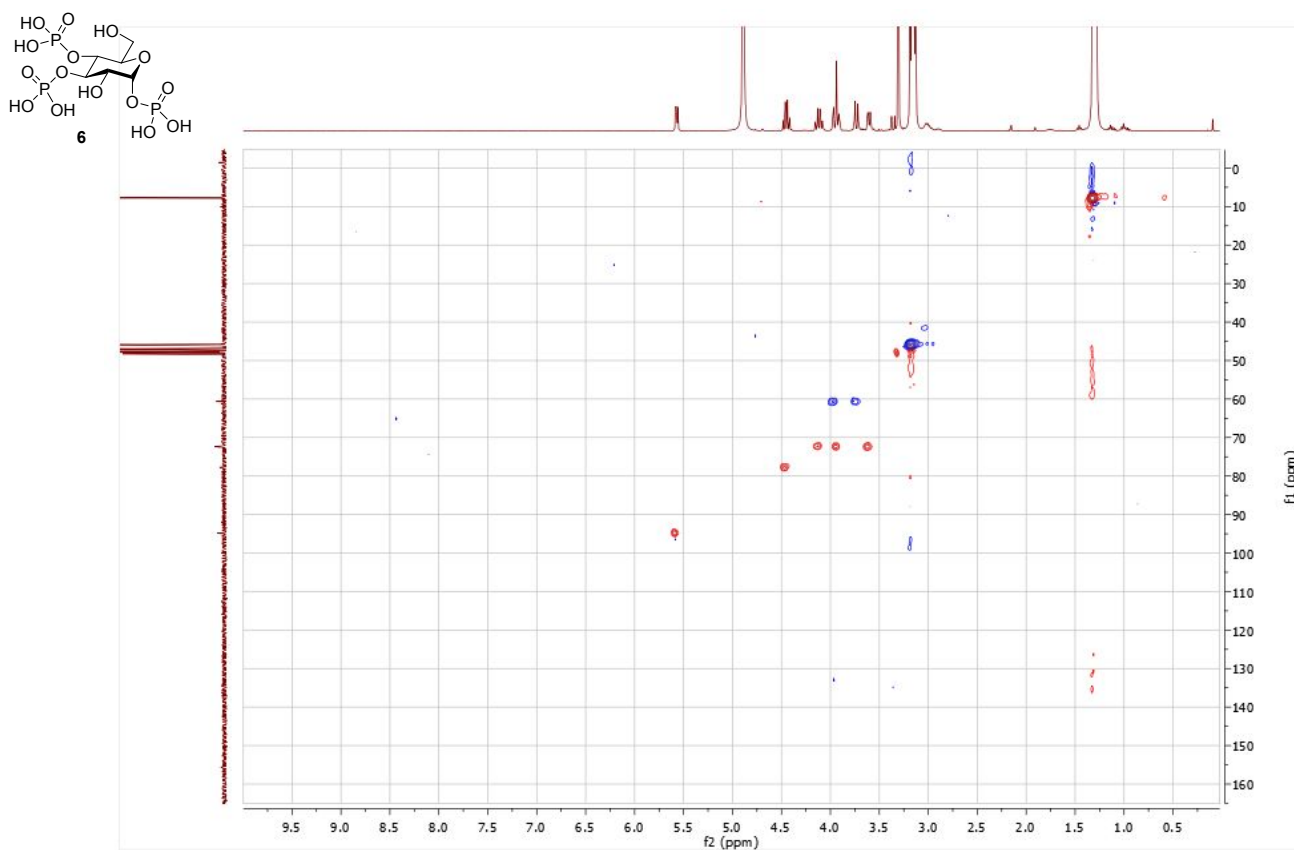




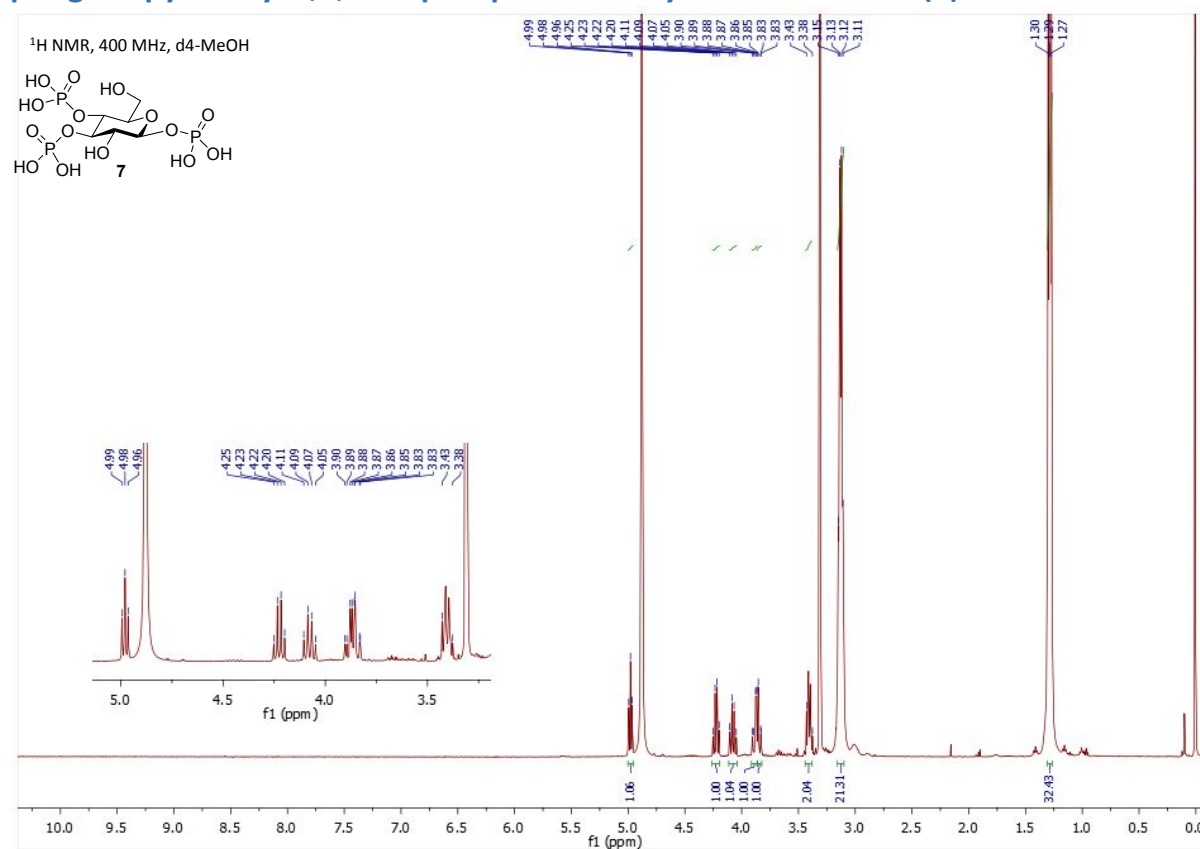


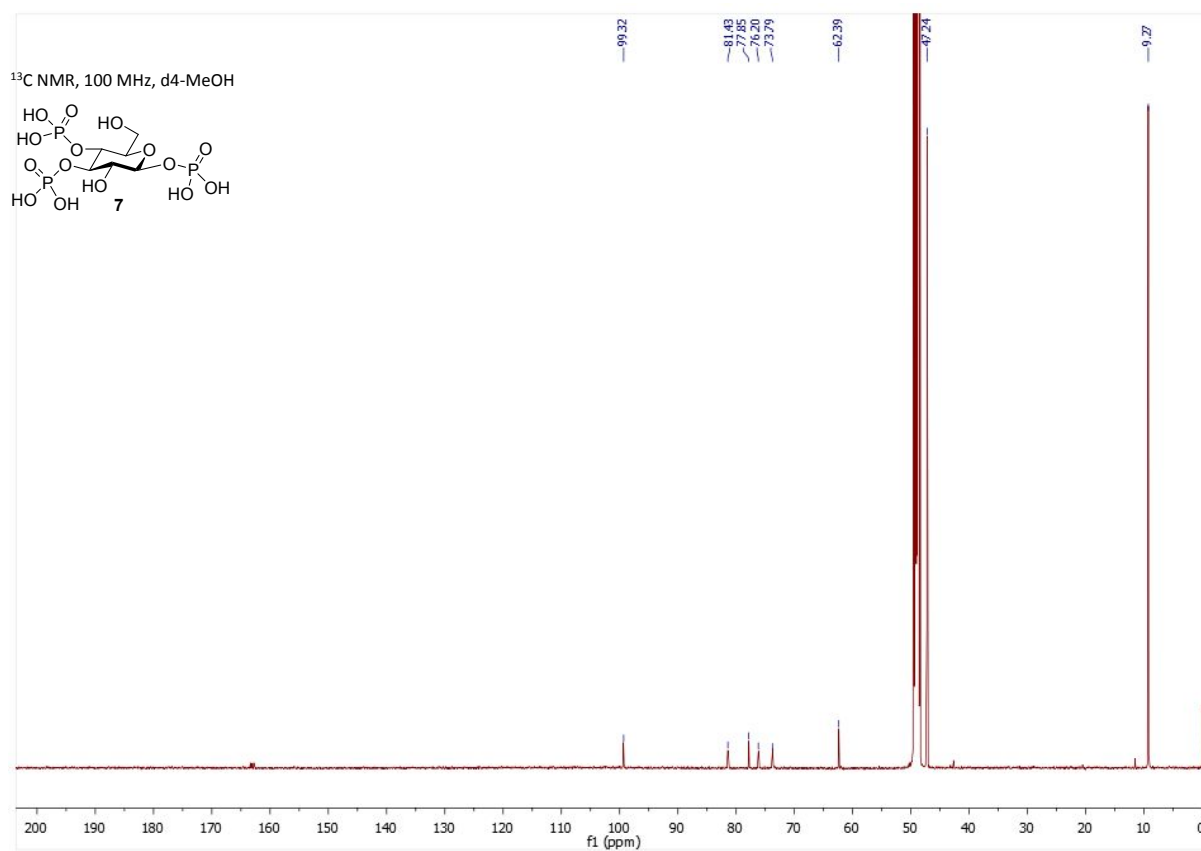
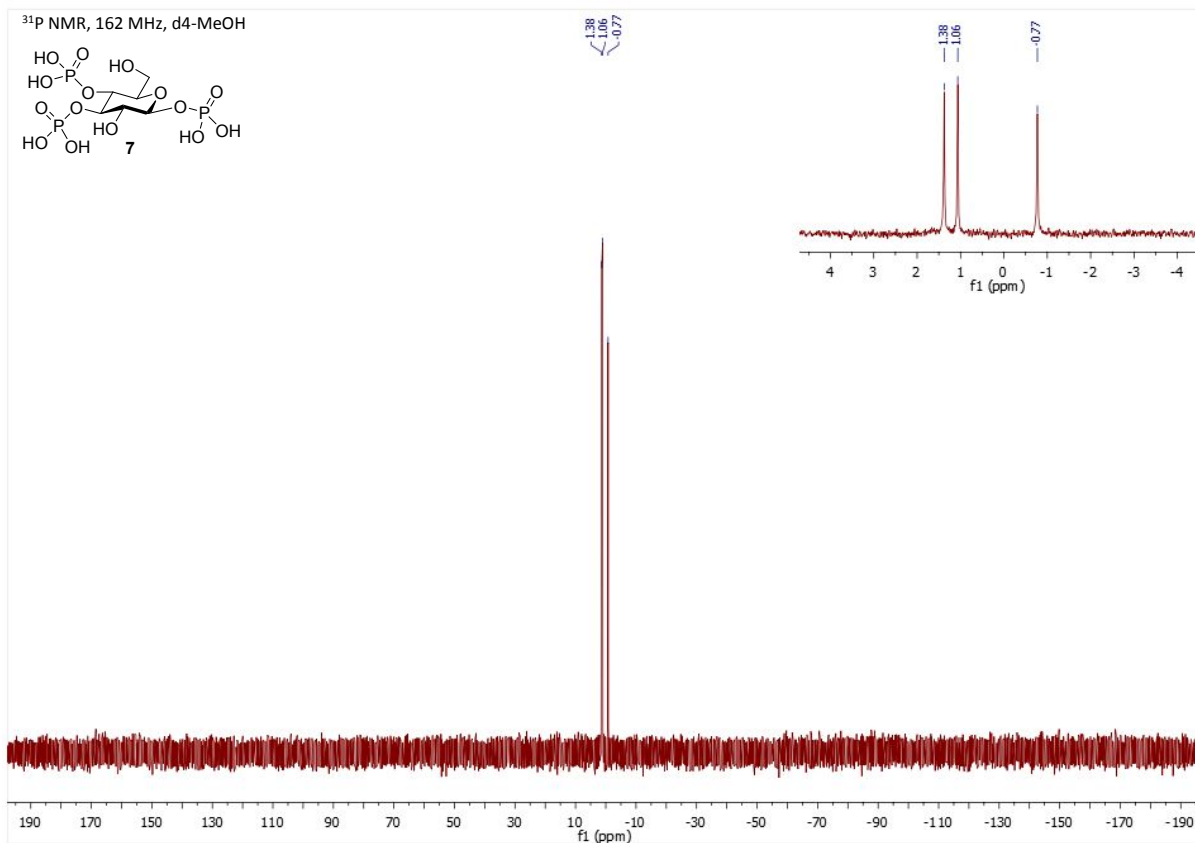
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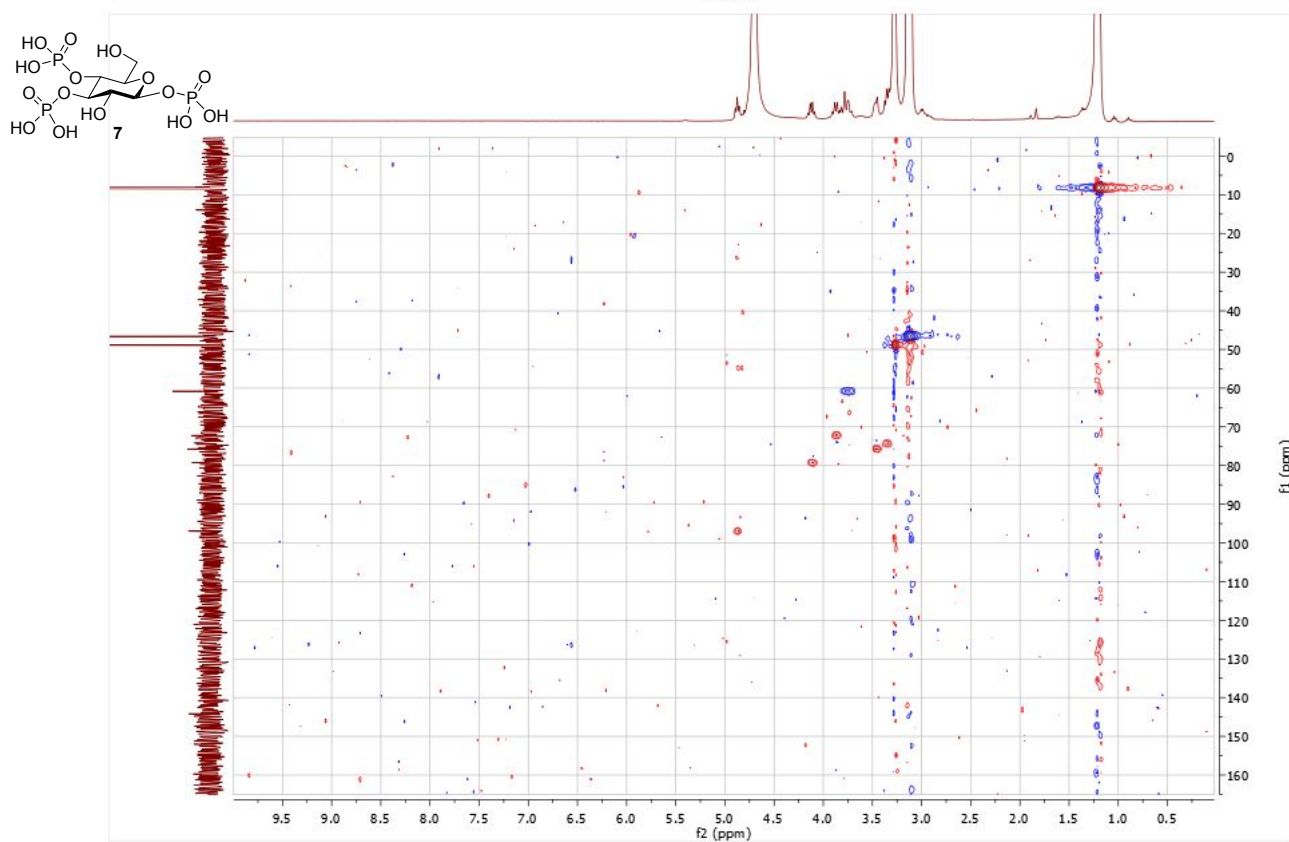
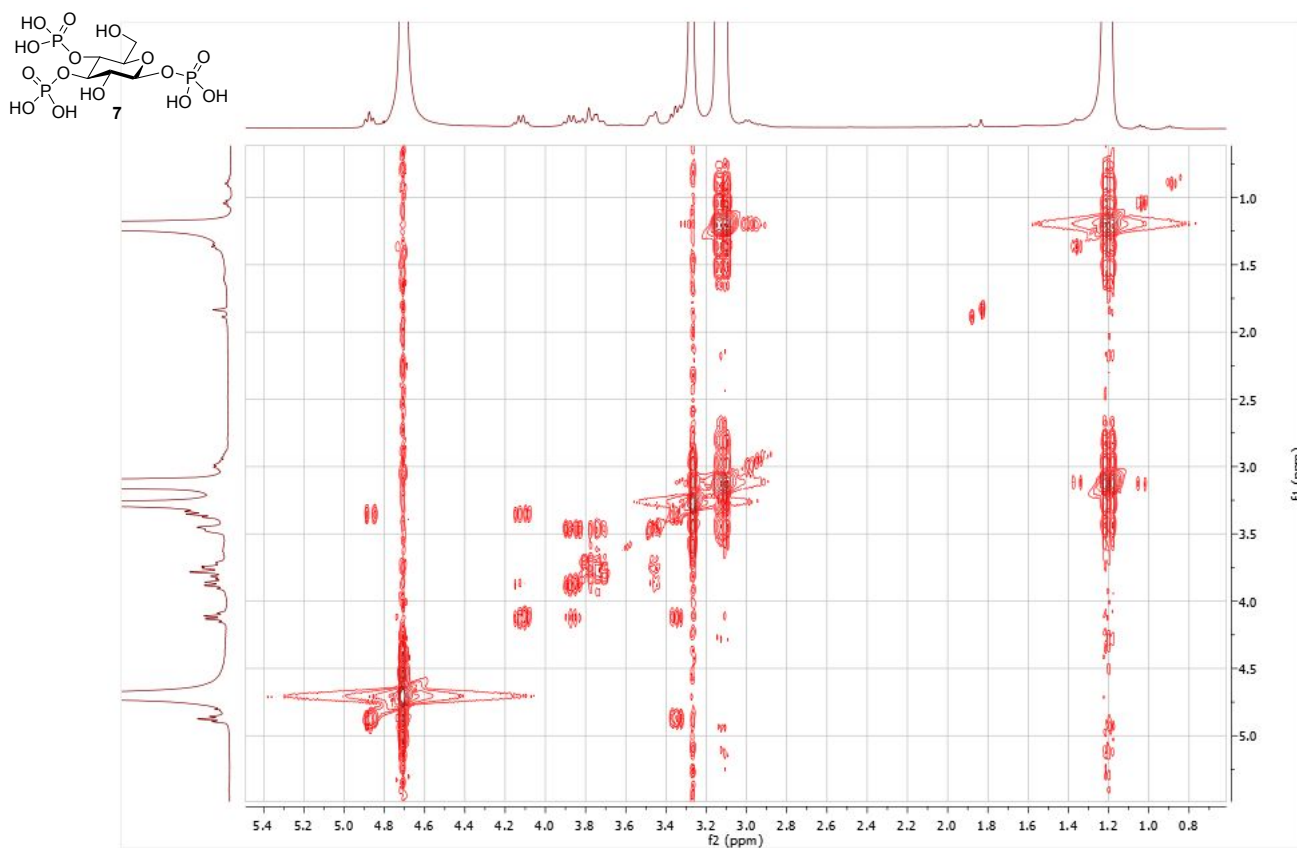
¹³C NMR, 100 MHz, d4-MeOH

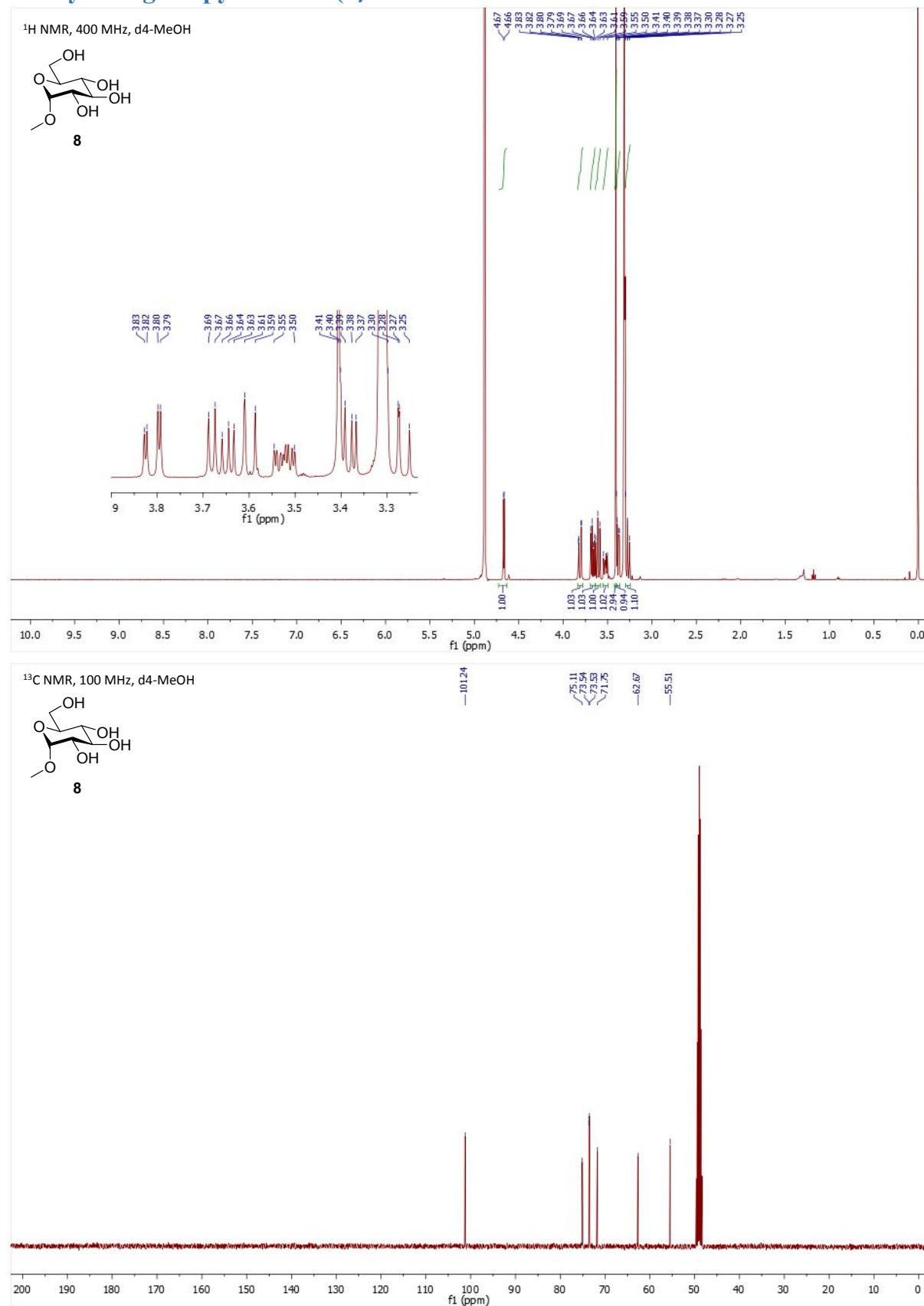


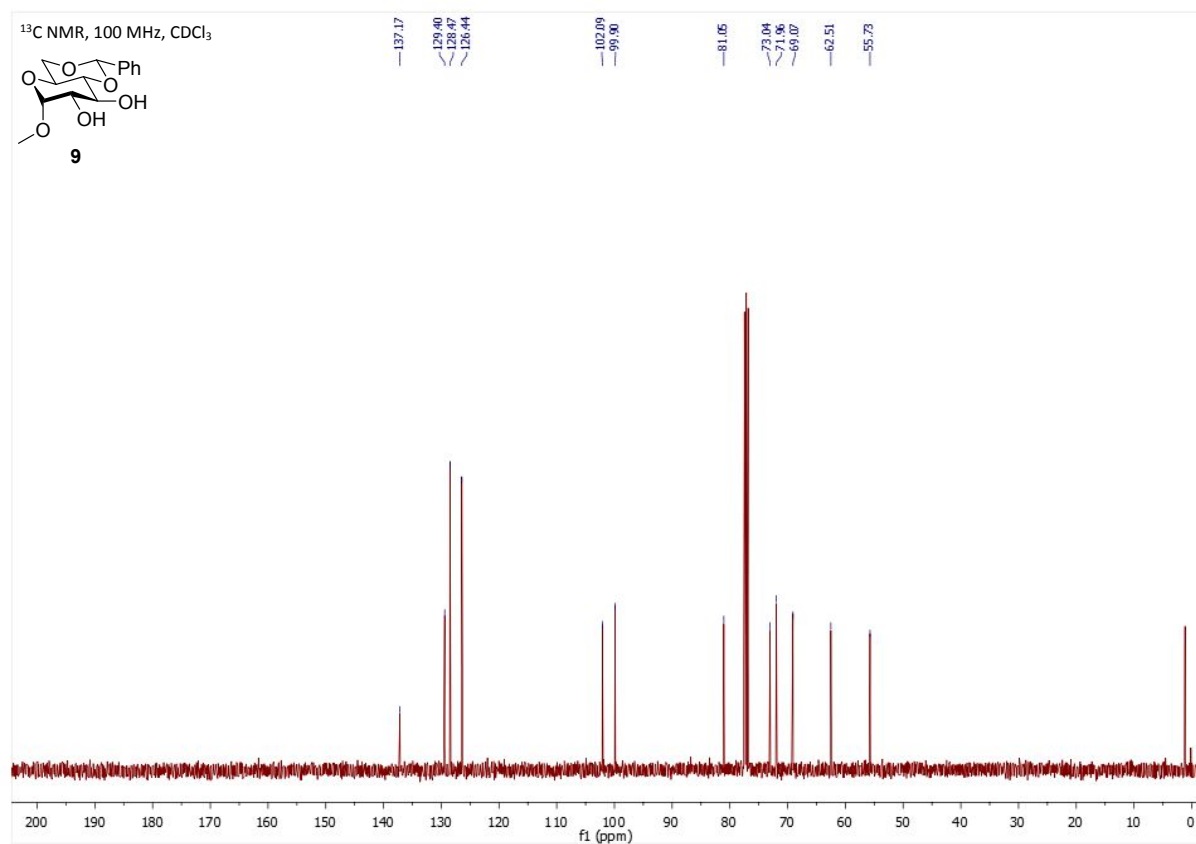
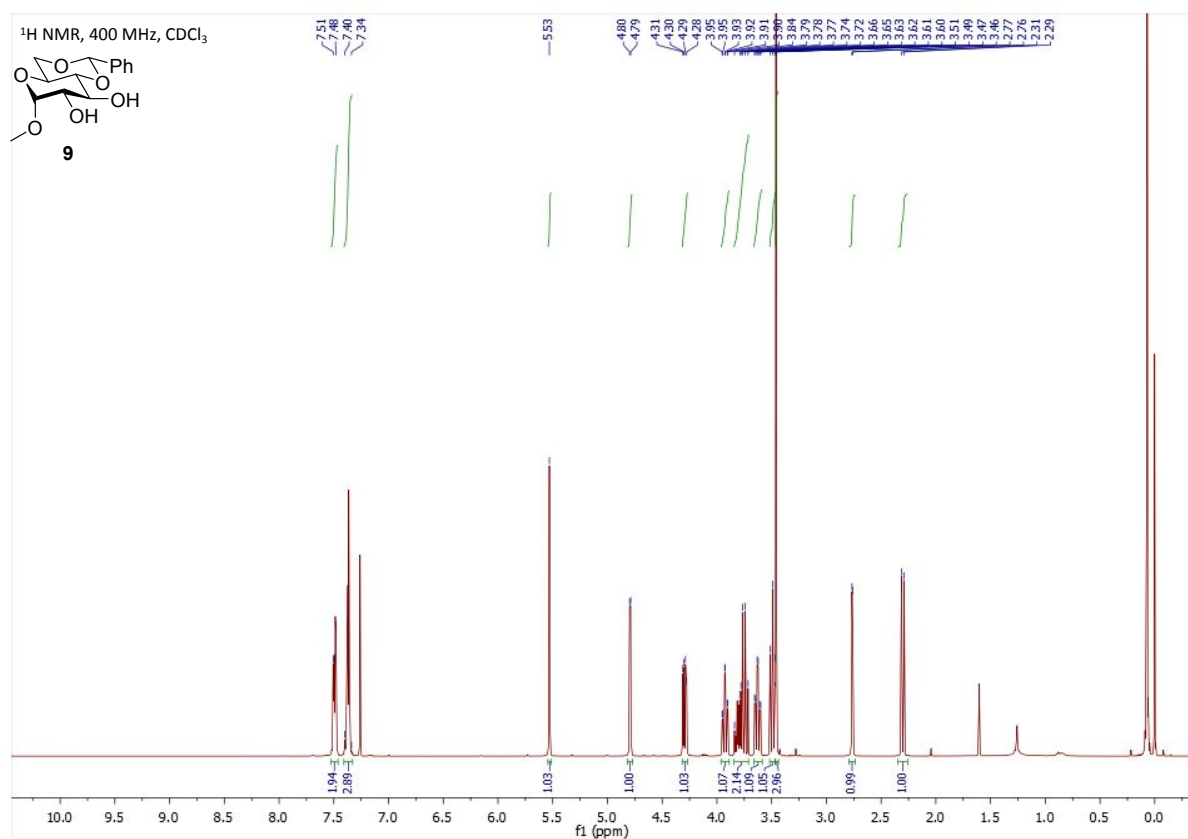
β -D-glucopyranosyl 1,3,4-trisphosphate triethylammonium salt (7)

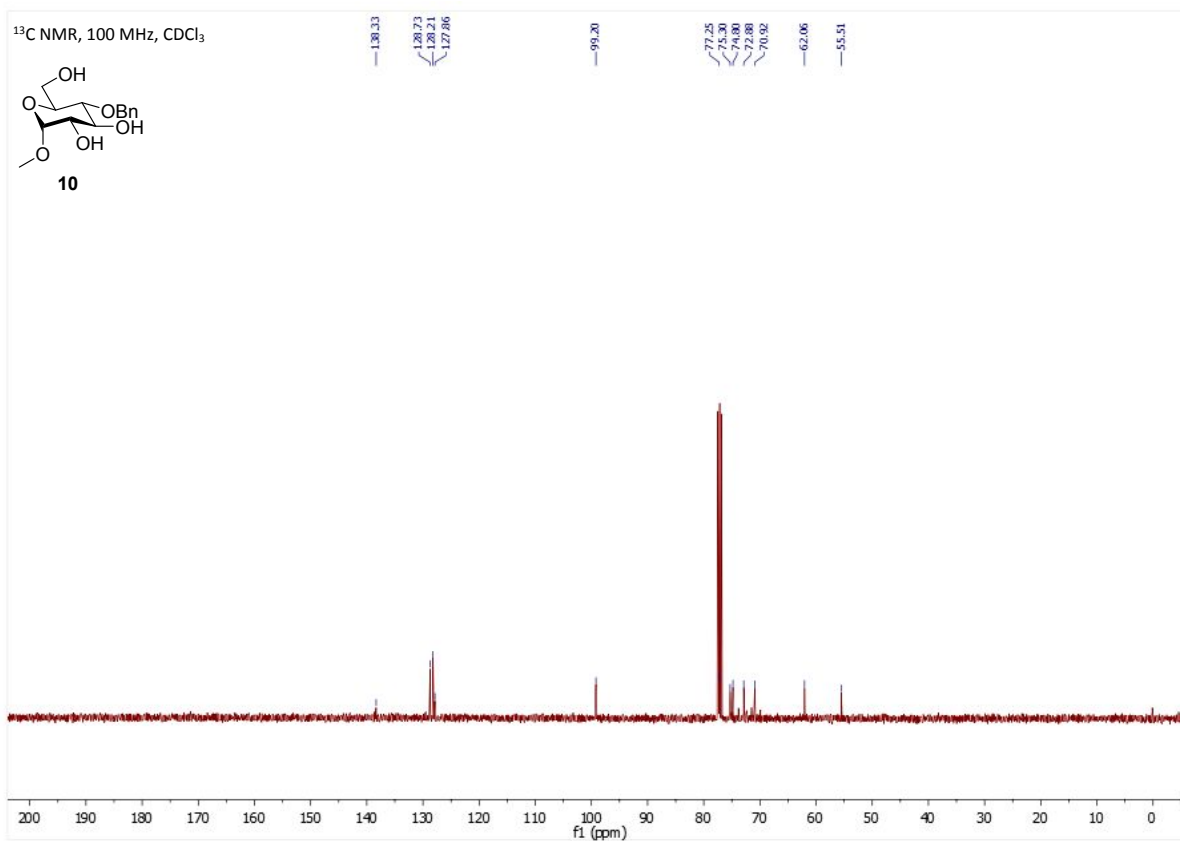
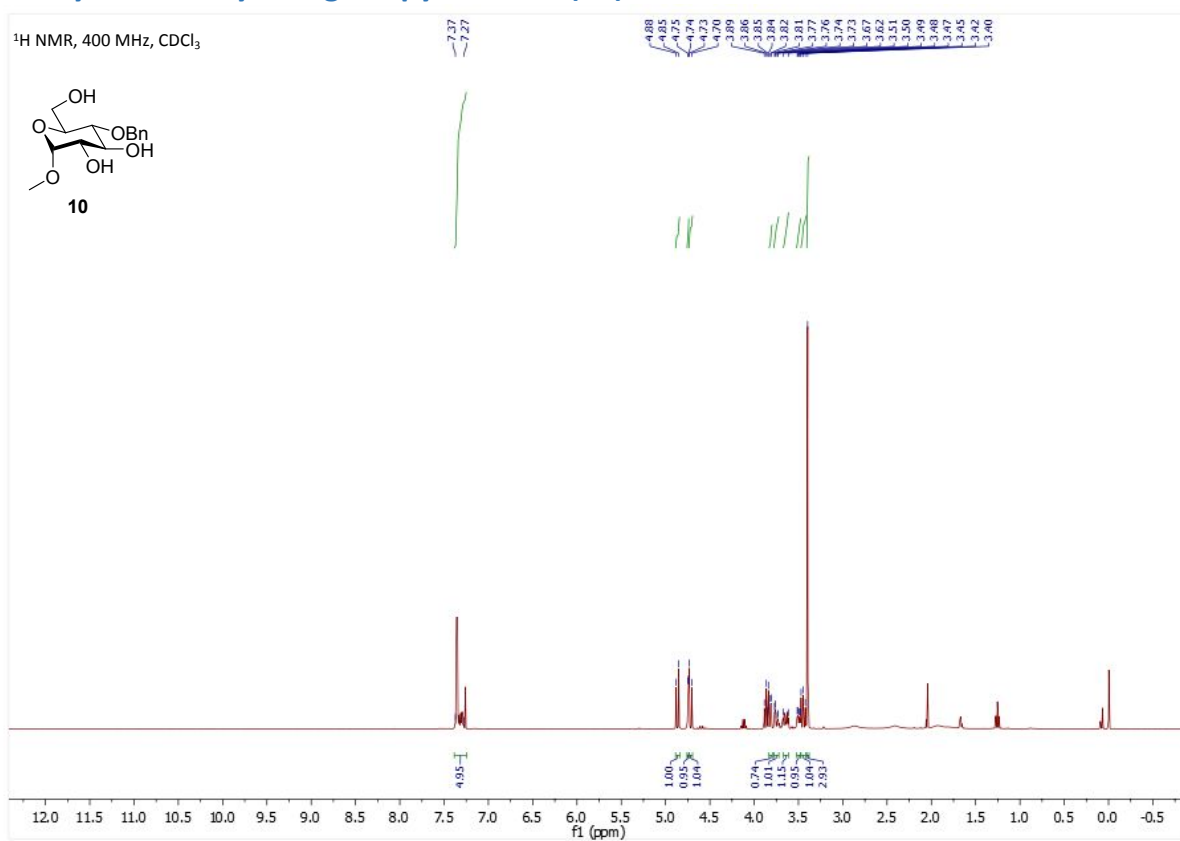


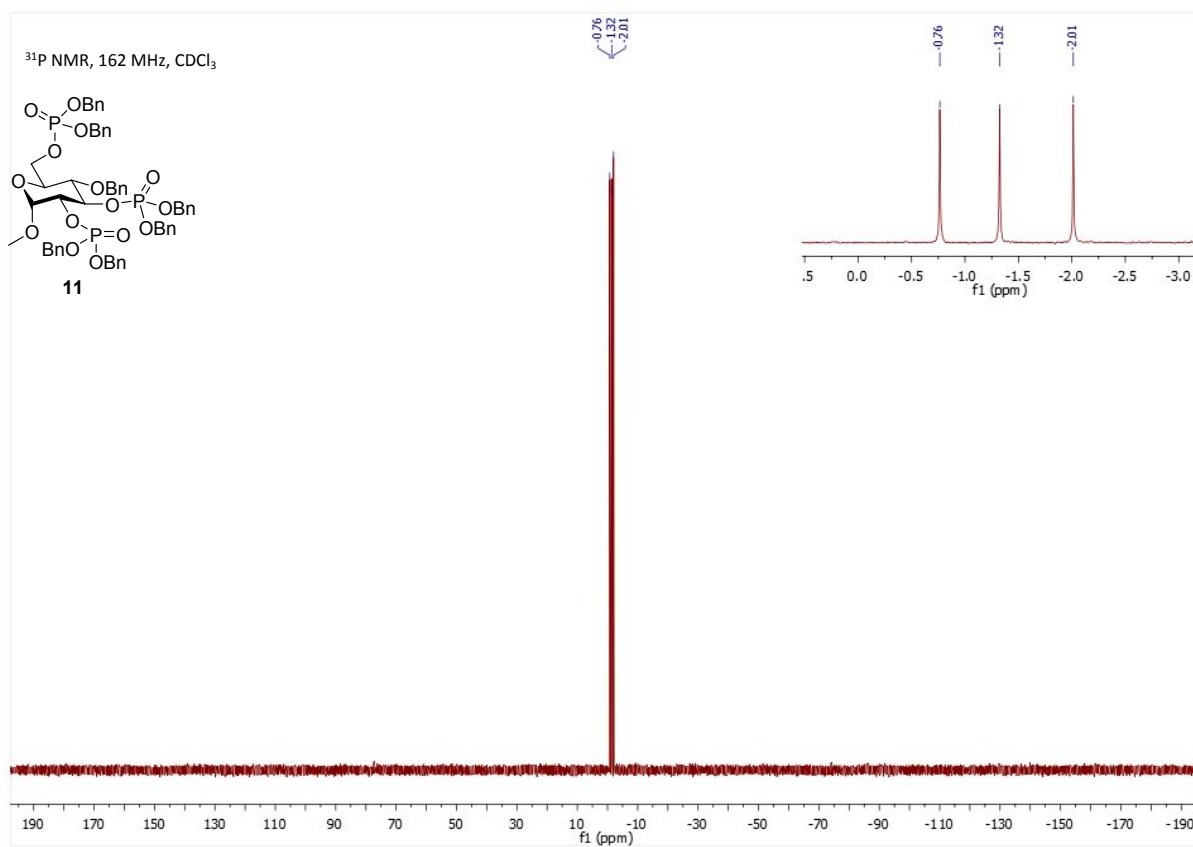
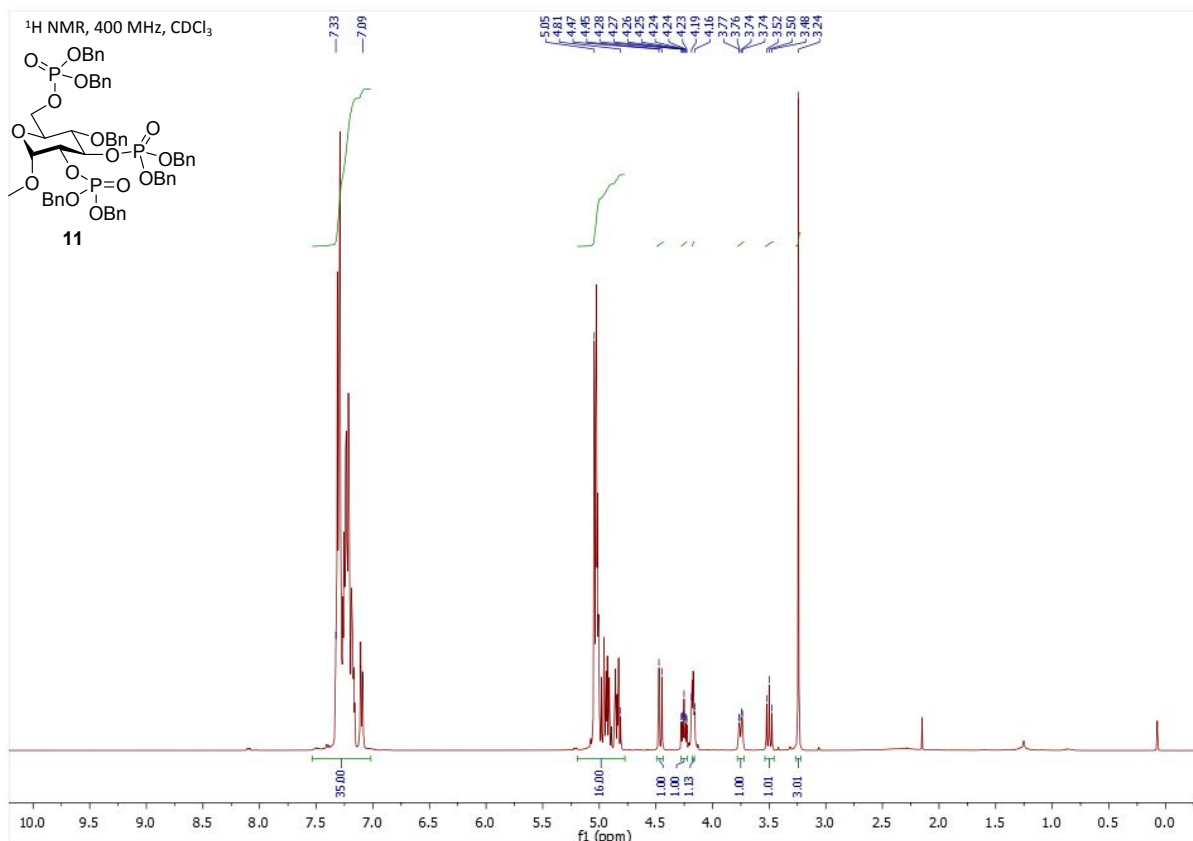


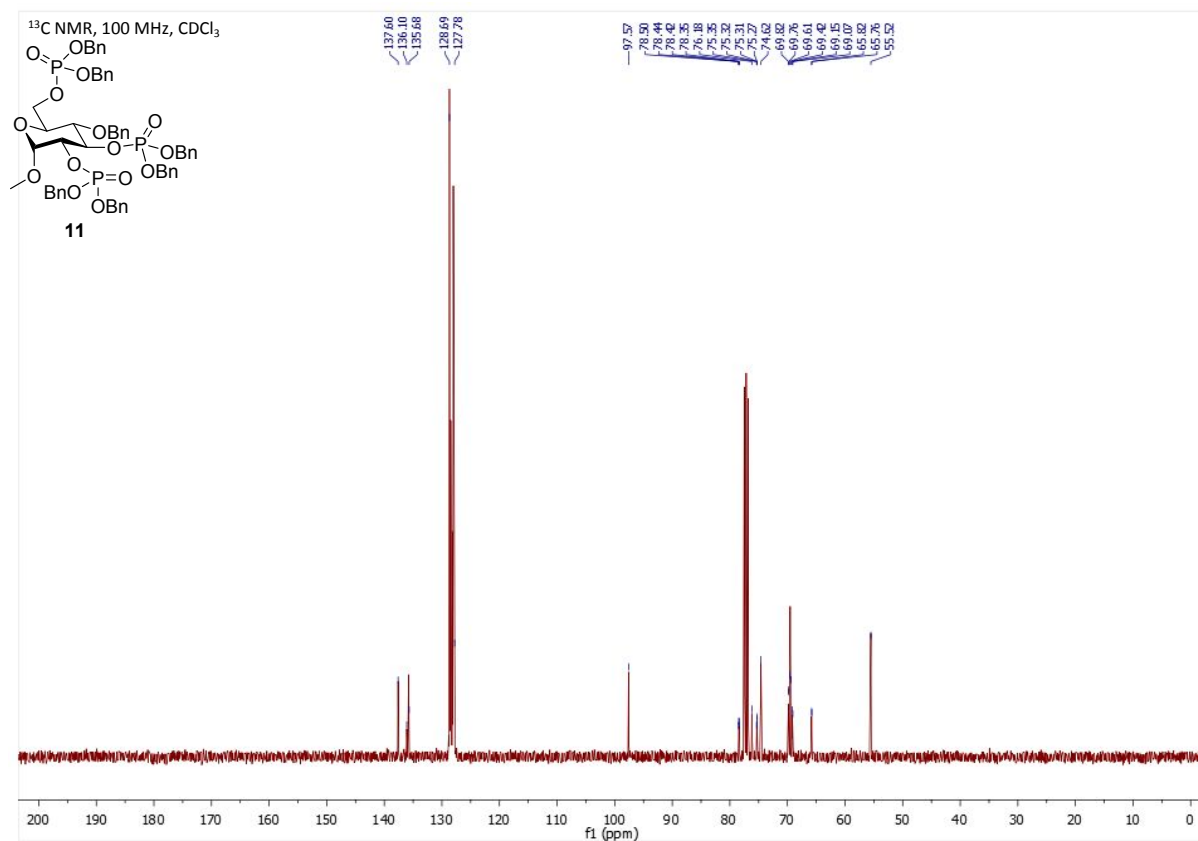


Methyl α -L-glucopyranoside (8)

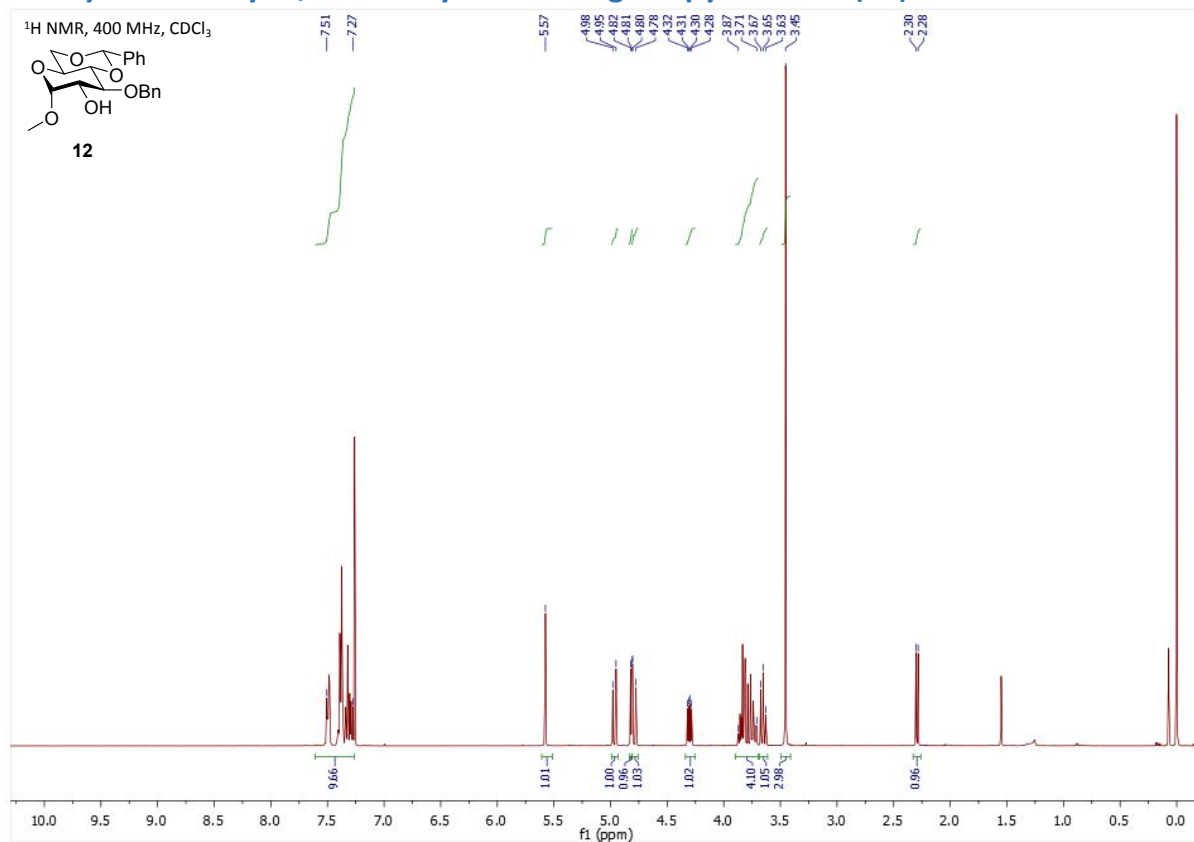
Methyl 4,6-O-benzylidene- α -L-glucopyranoside (**9**)

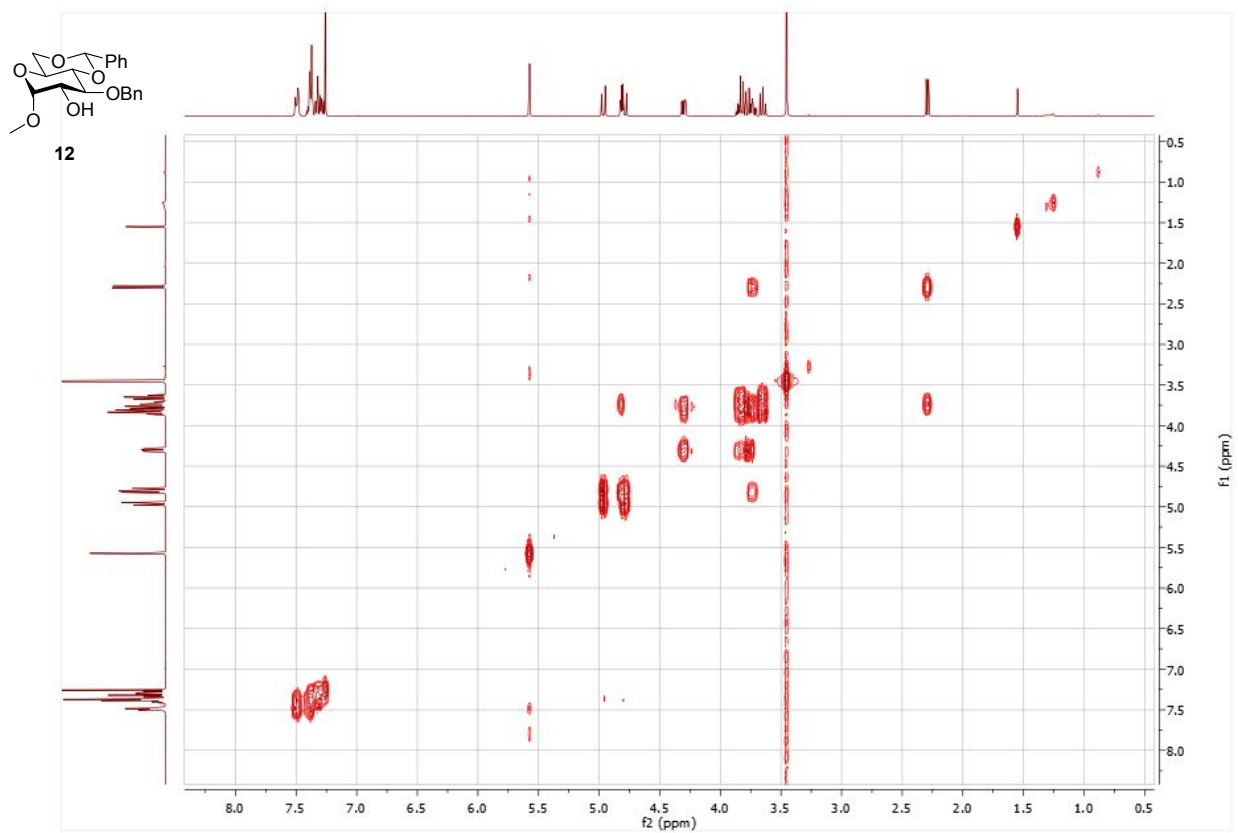
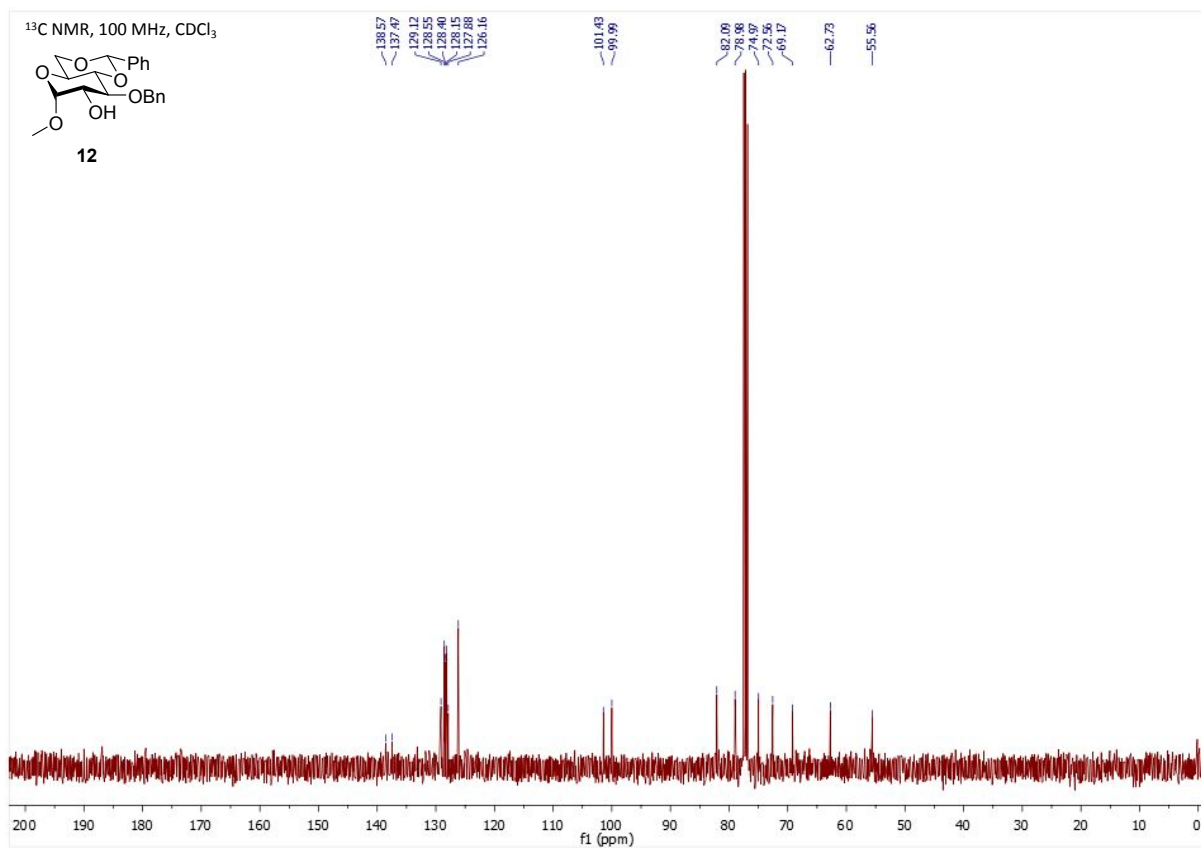
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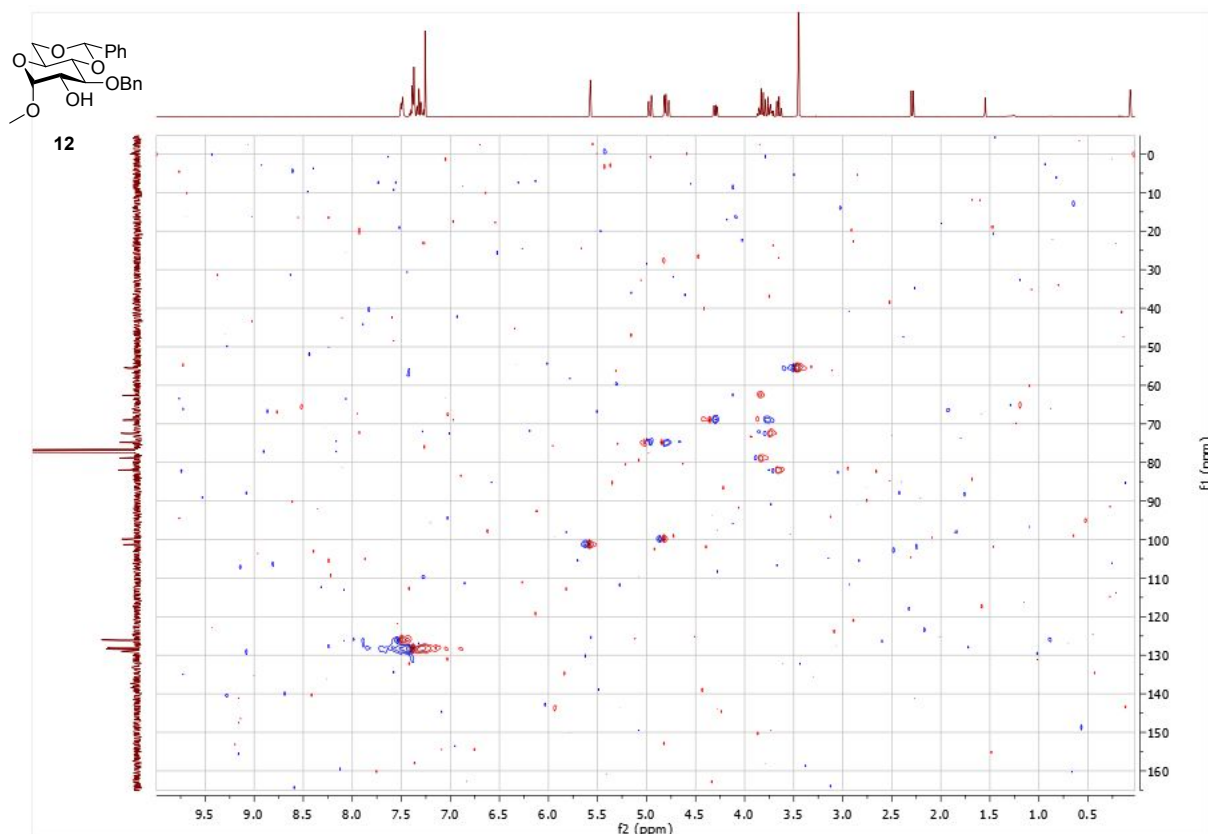
Methyl 4-O-benzyl- α -L-glucopyranoside 2,3,6-tris(dibenzyl phosphate) (**11**)



Methyl 3-O-benzyl-4,6-O-benzylidene- α -L-glucopyranoside (**12**)

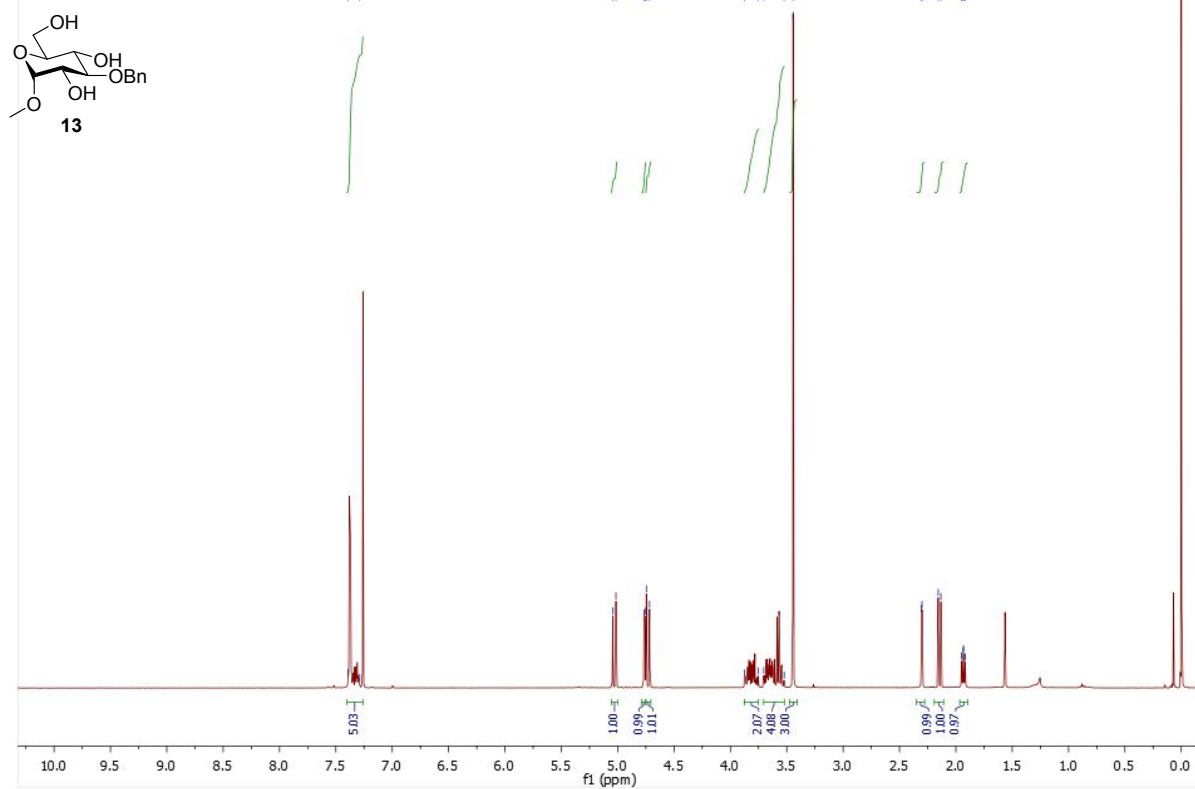


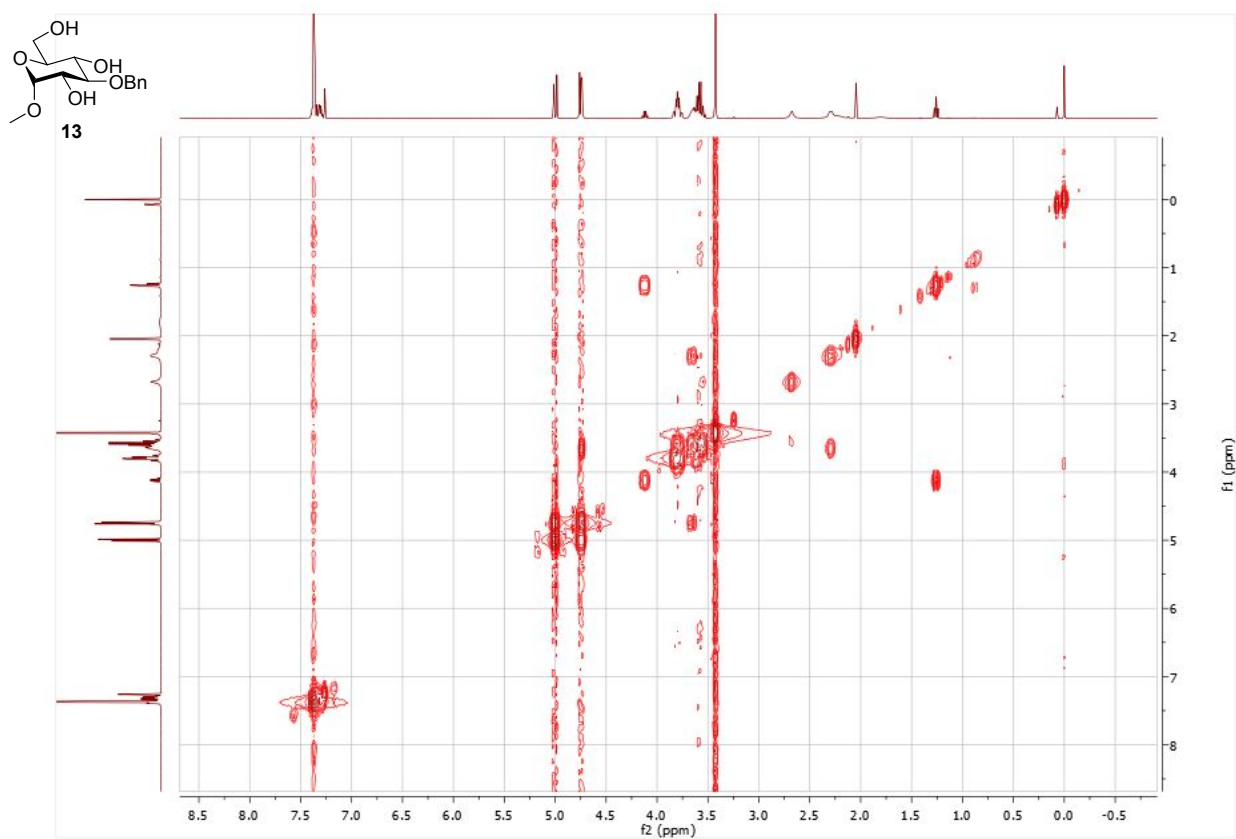
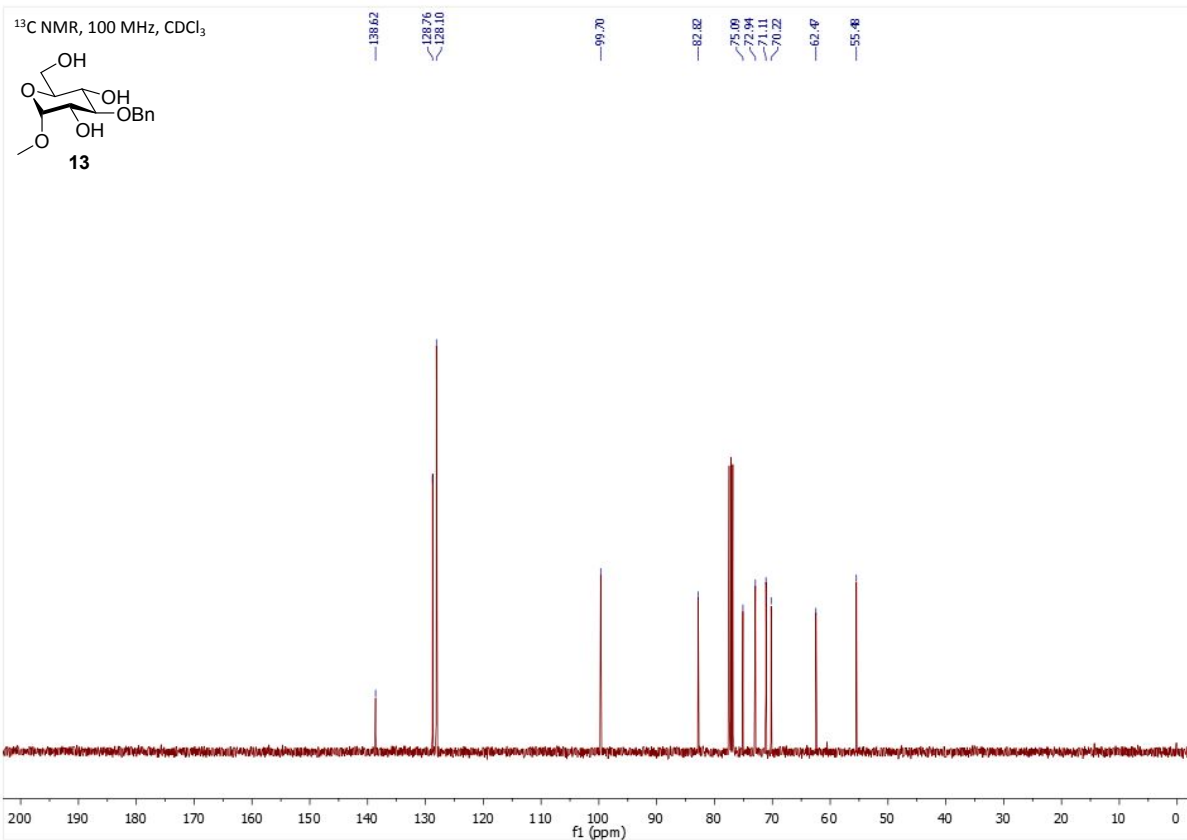


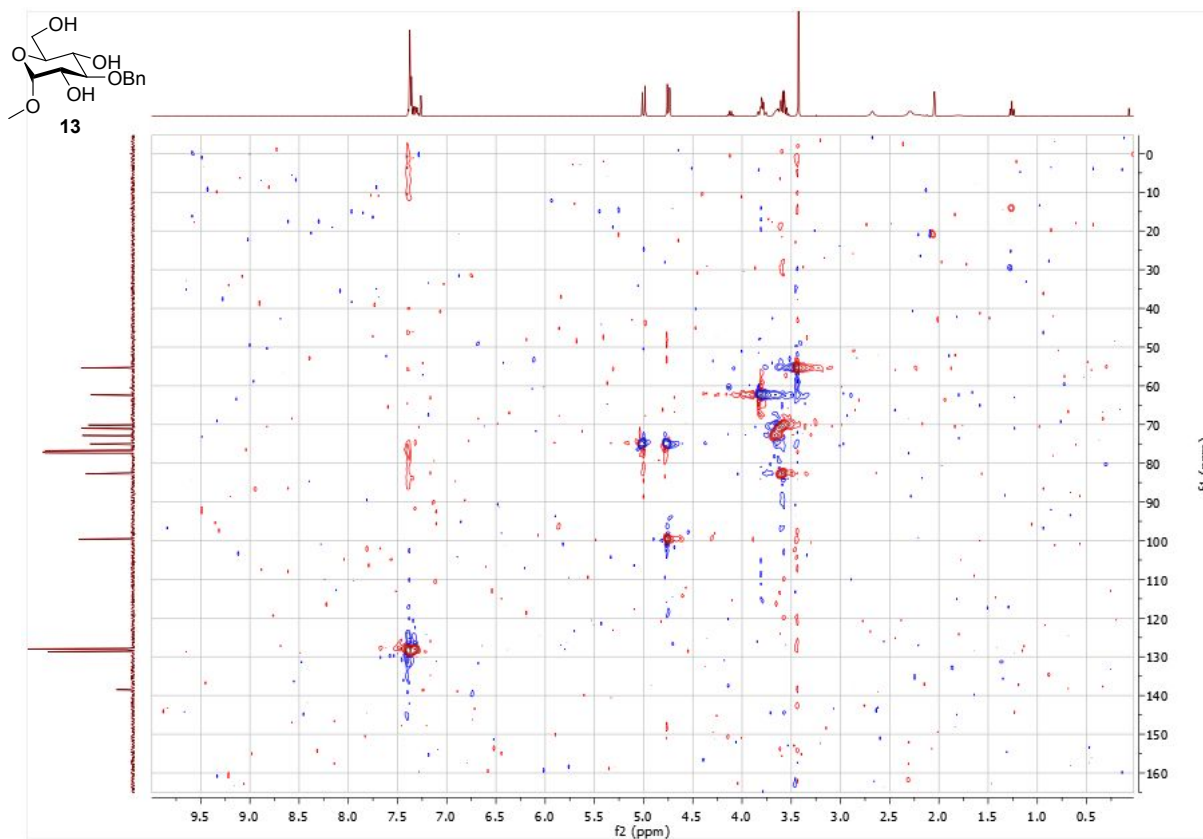


Methyl 3-O-benzyl- α -L-glucopyranoside (**13**)

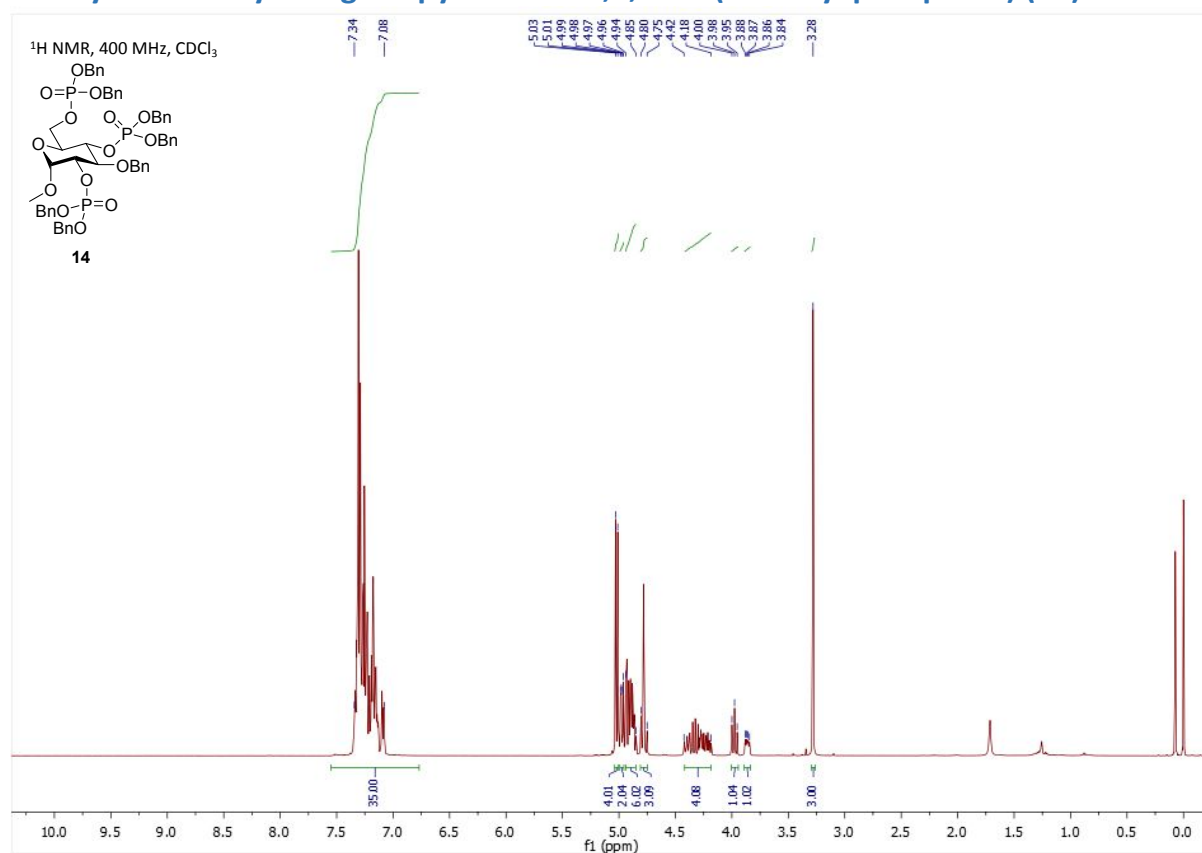
^1H NMR, 400 MHz, CDCl_3

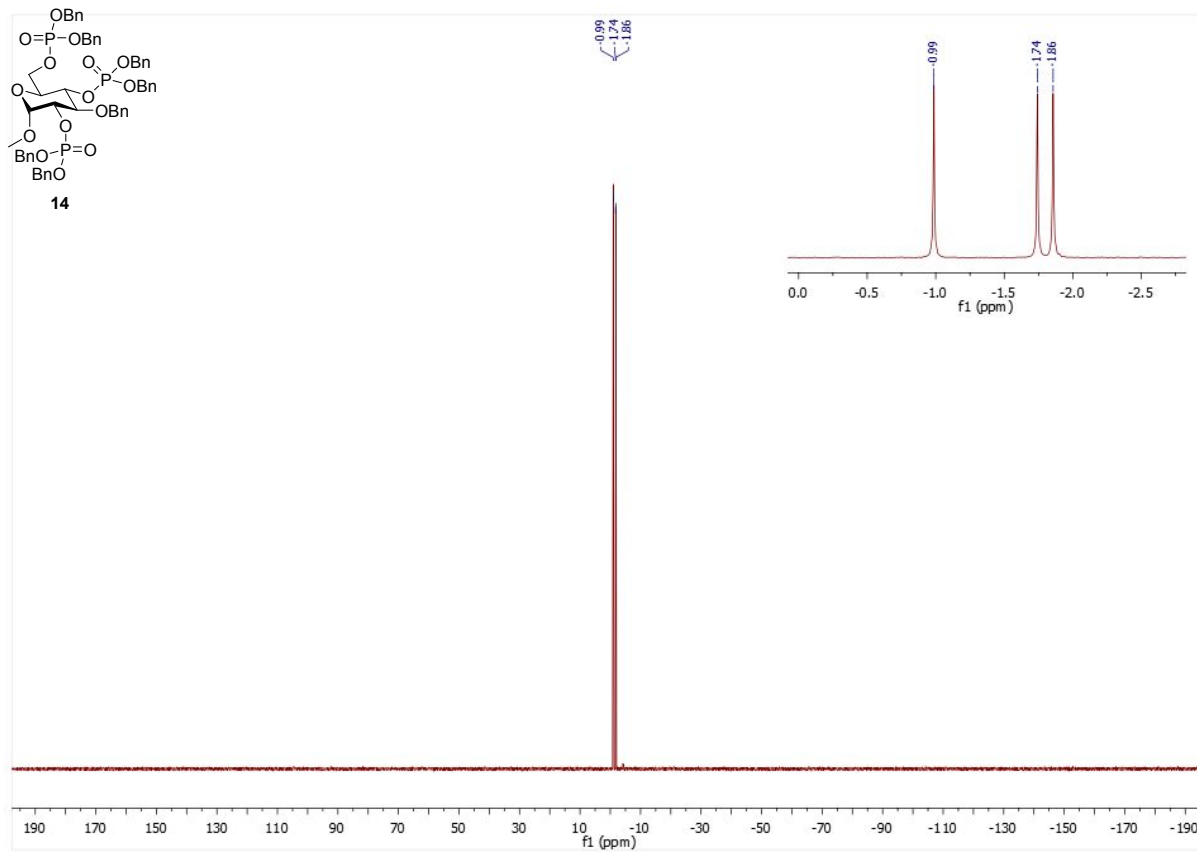
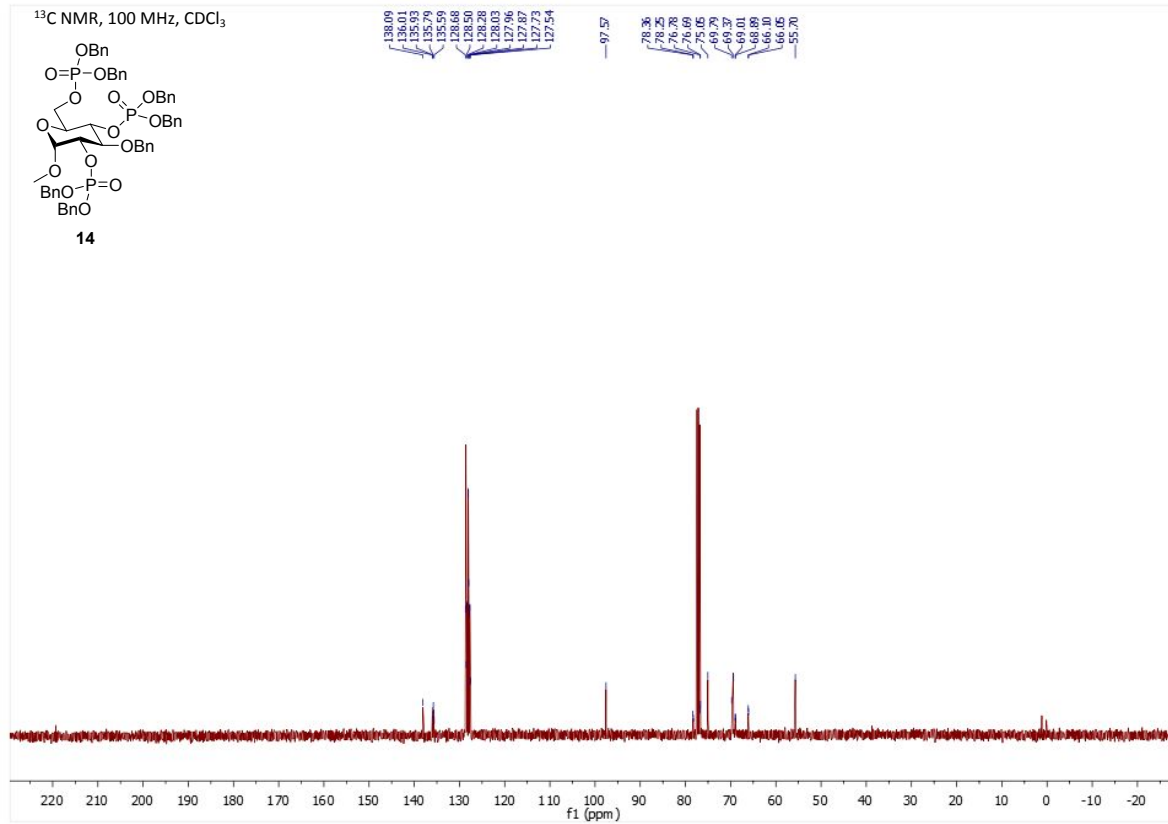


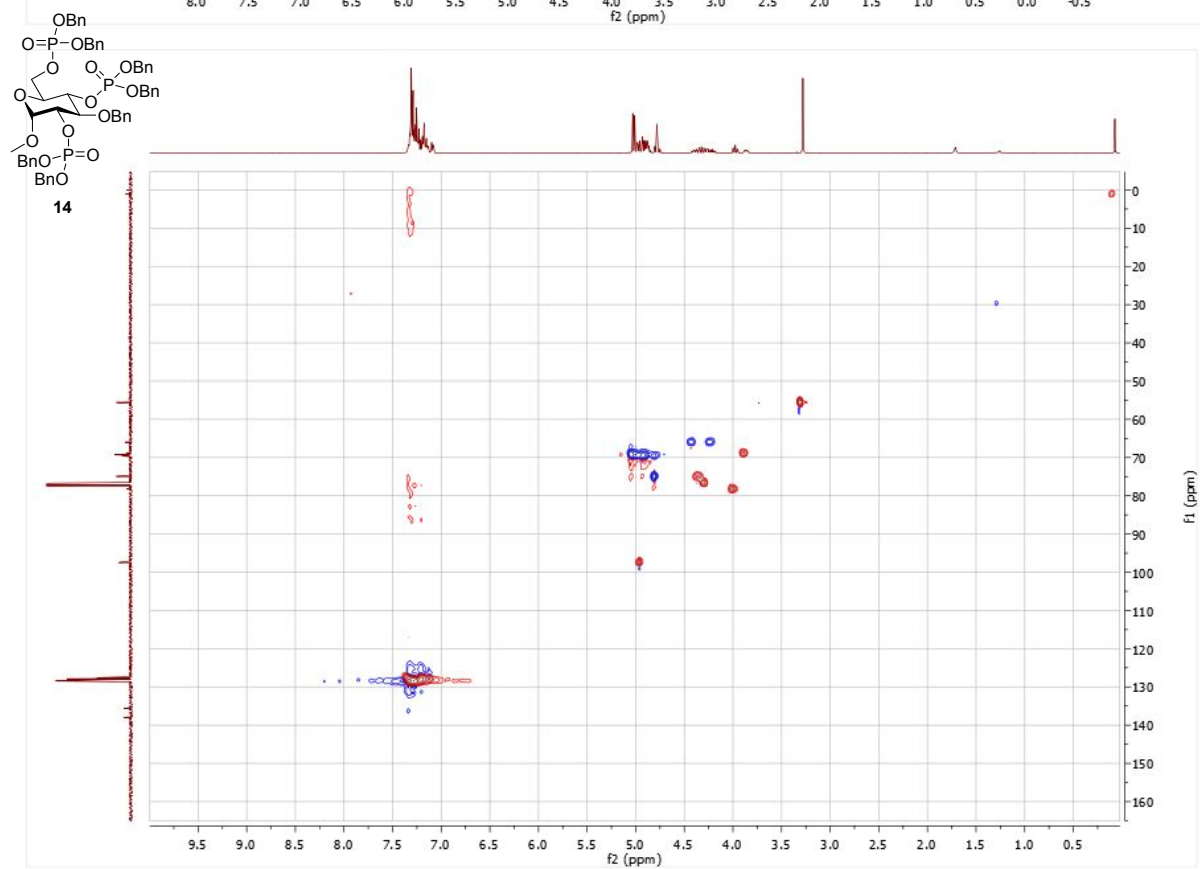
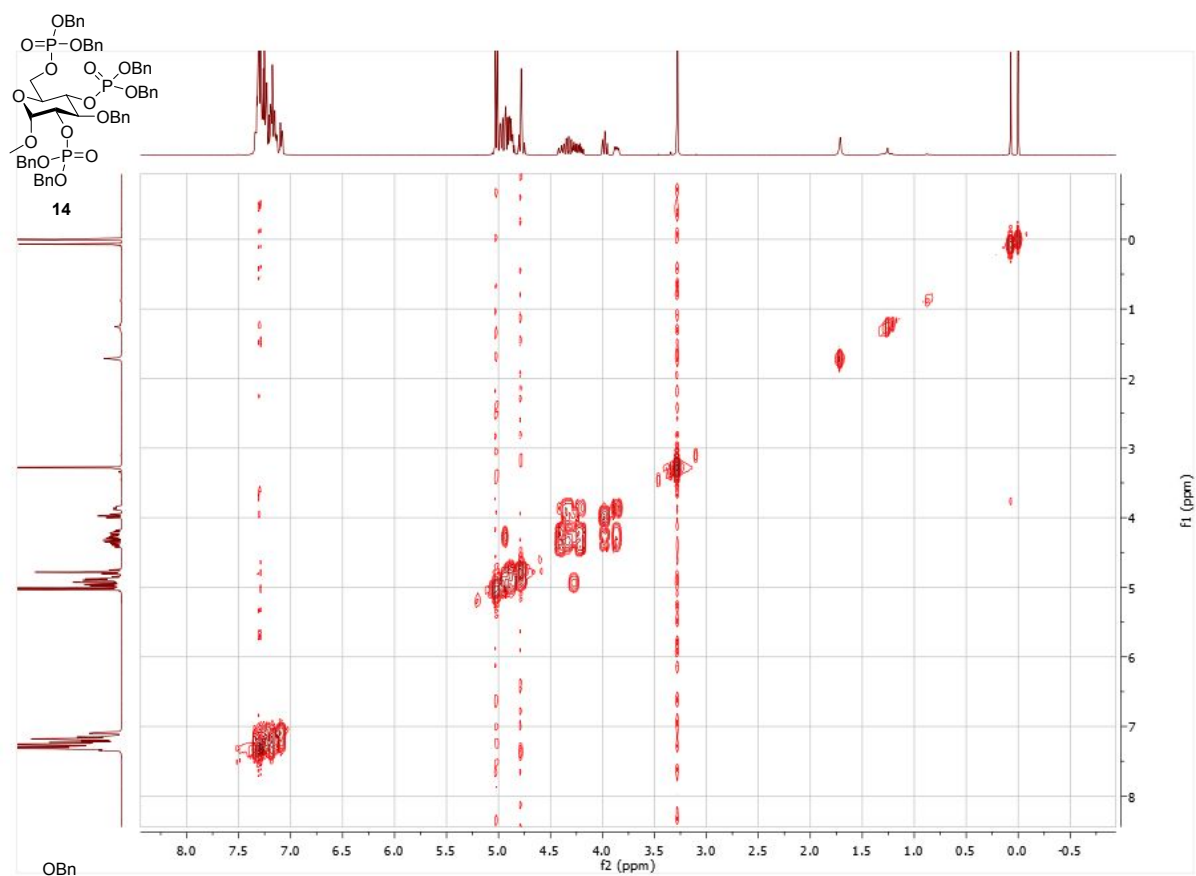


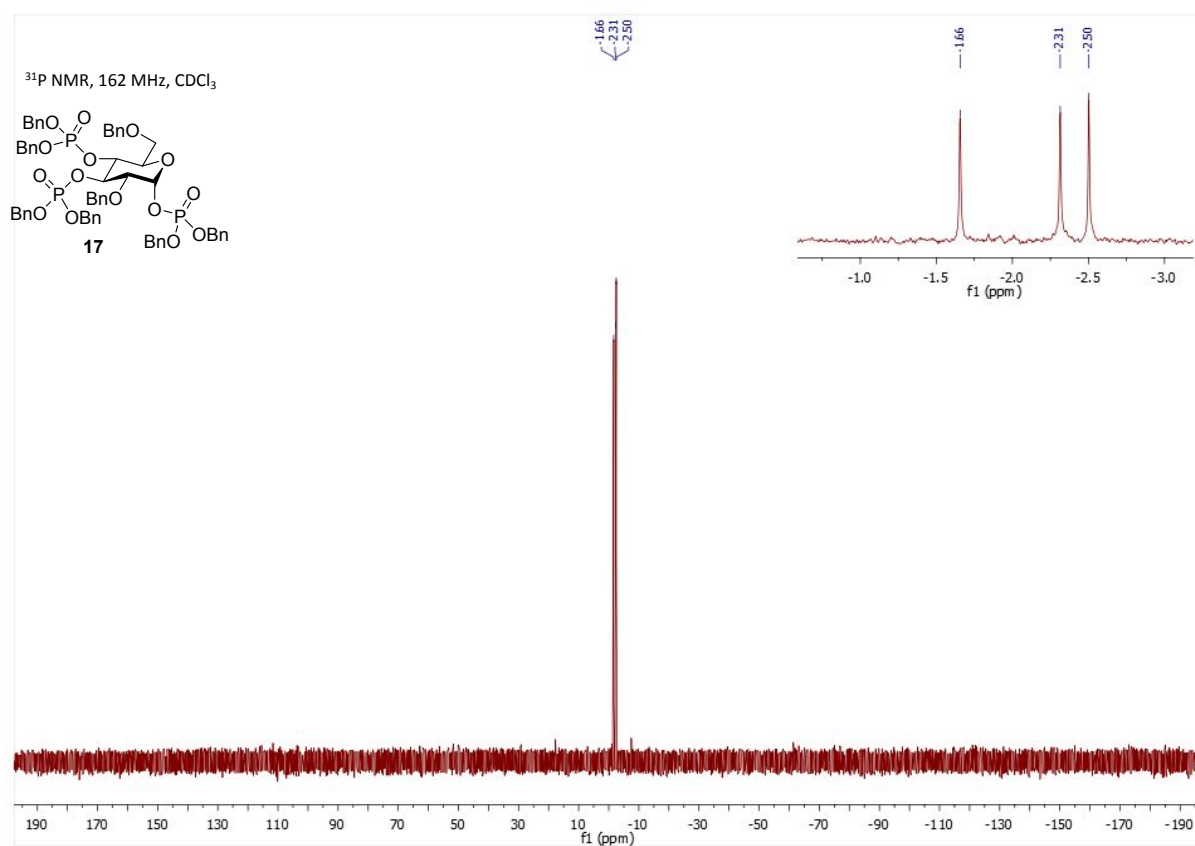
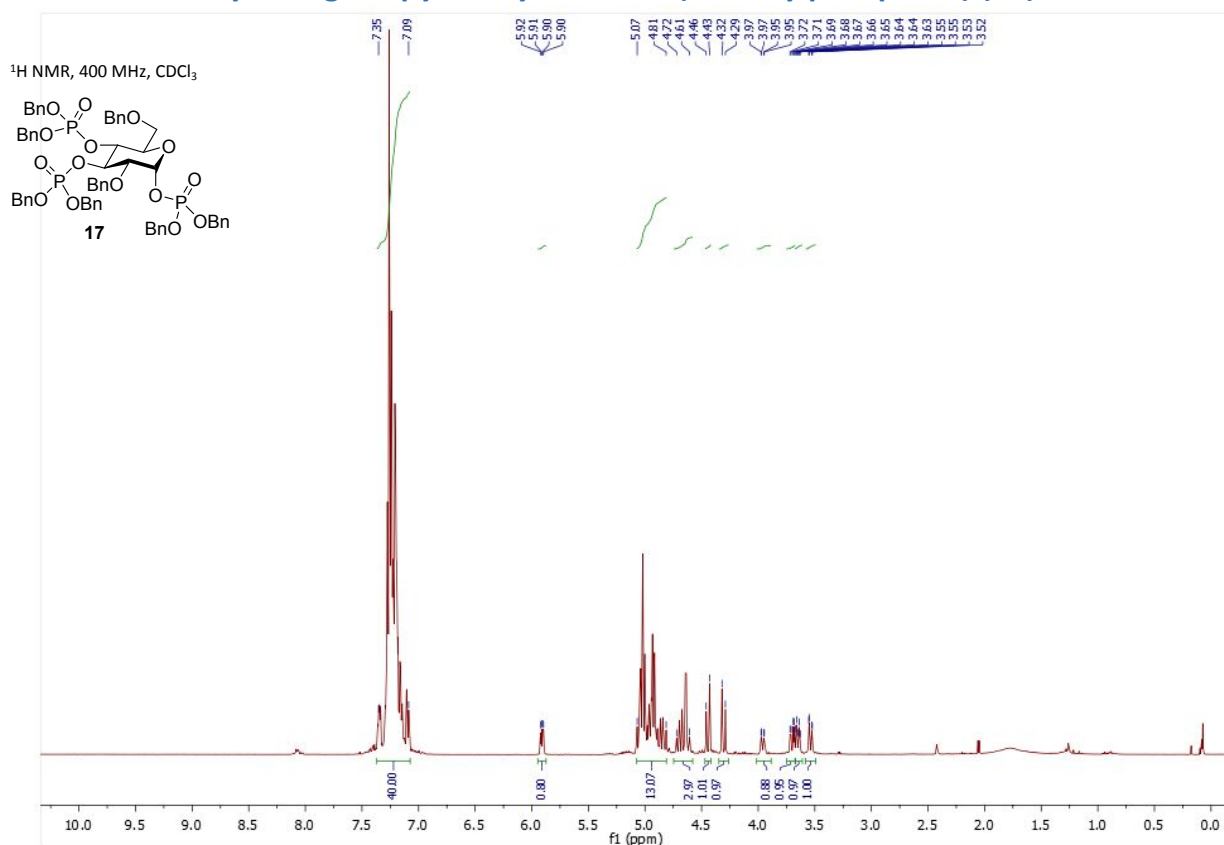


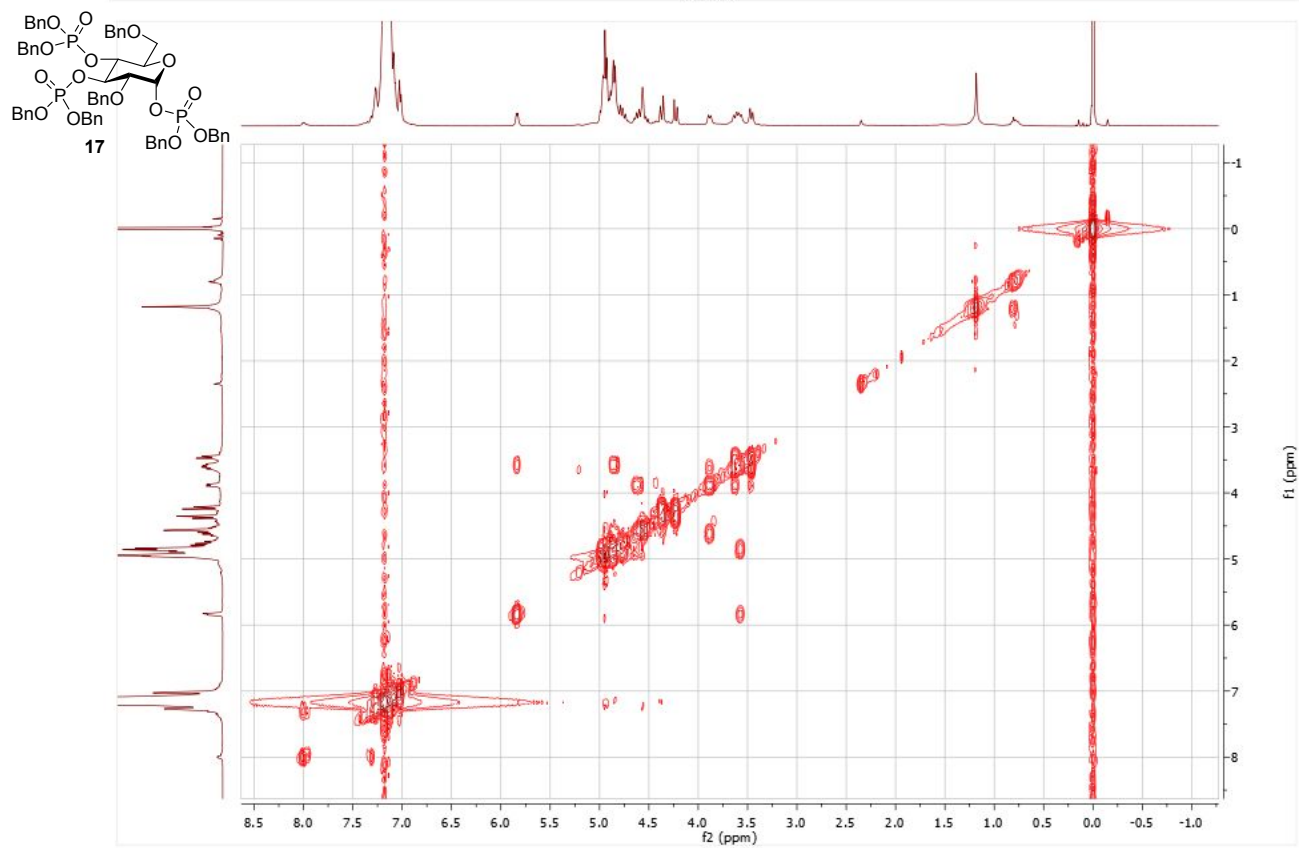
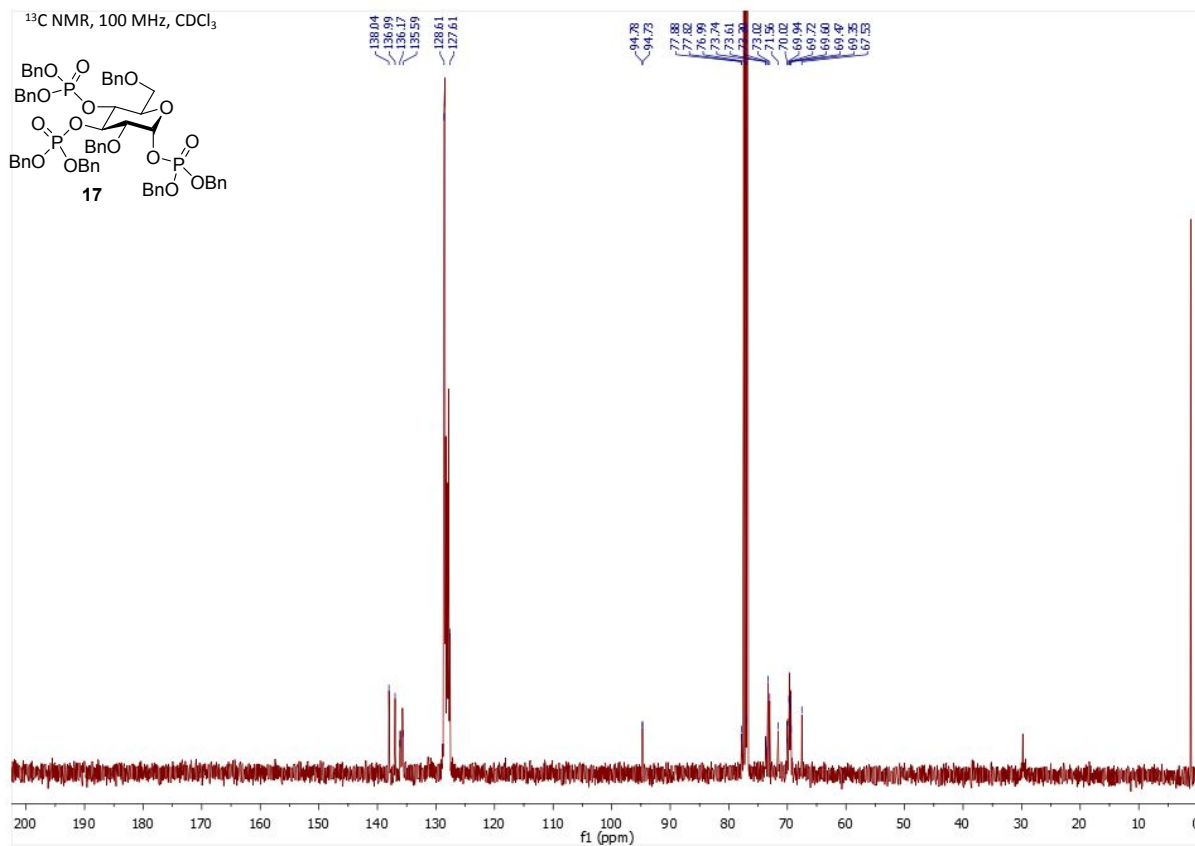
Methyl 3-O-benzyl- α -L-glucopyranoside 2,4,6-tris(dibenzyl phosphate) (**14**)

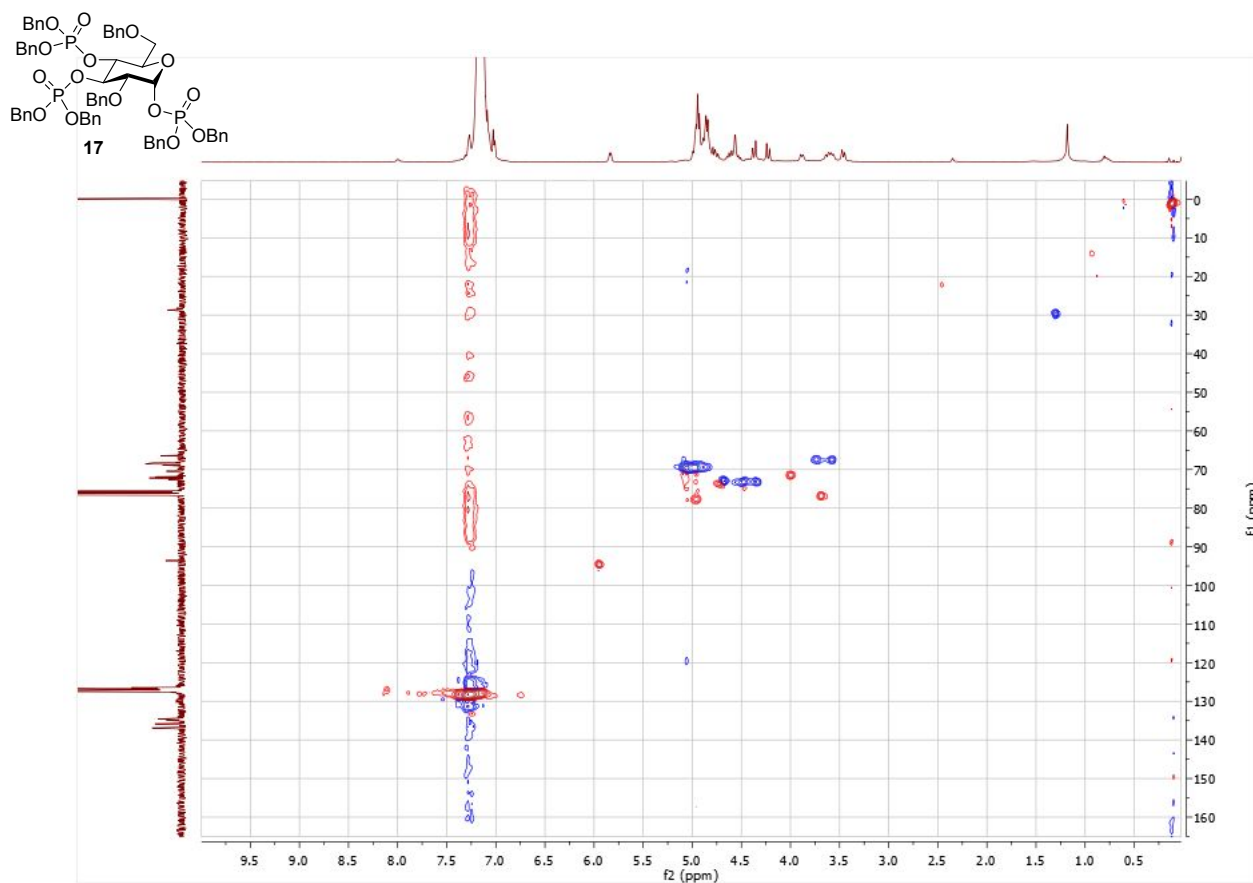


^{31}P NMR, 162 MHz, CDCl_3  ^{13}C NMR, 100 MHz, CDCl_3 

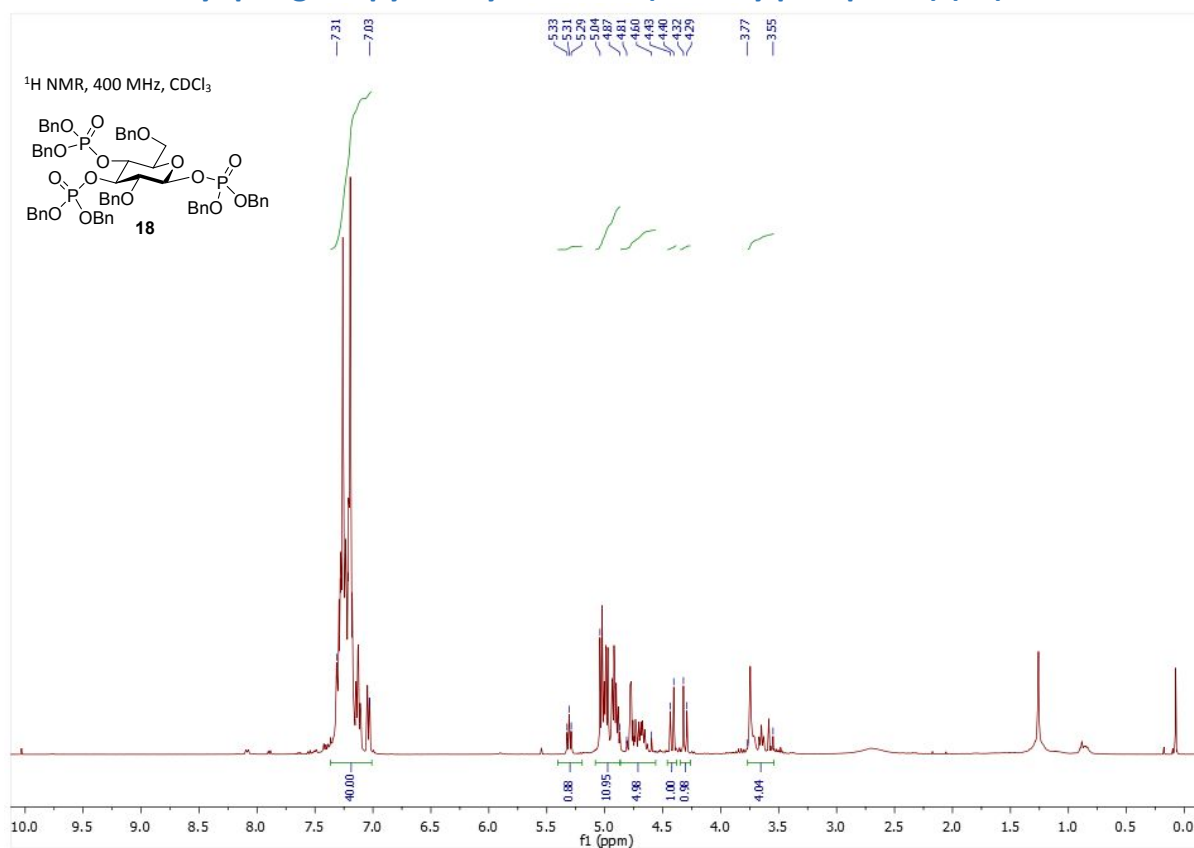


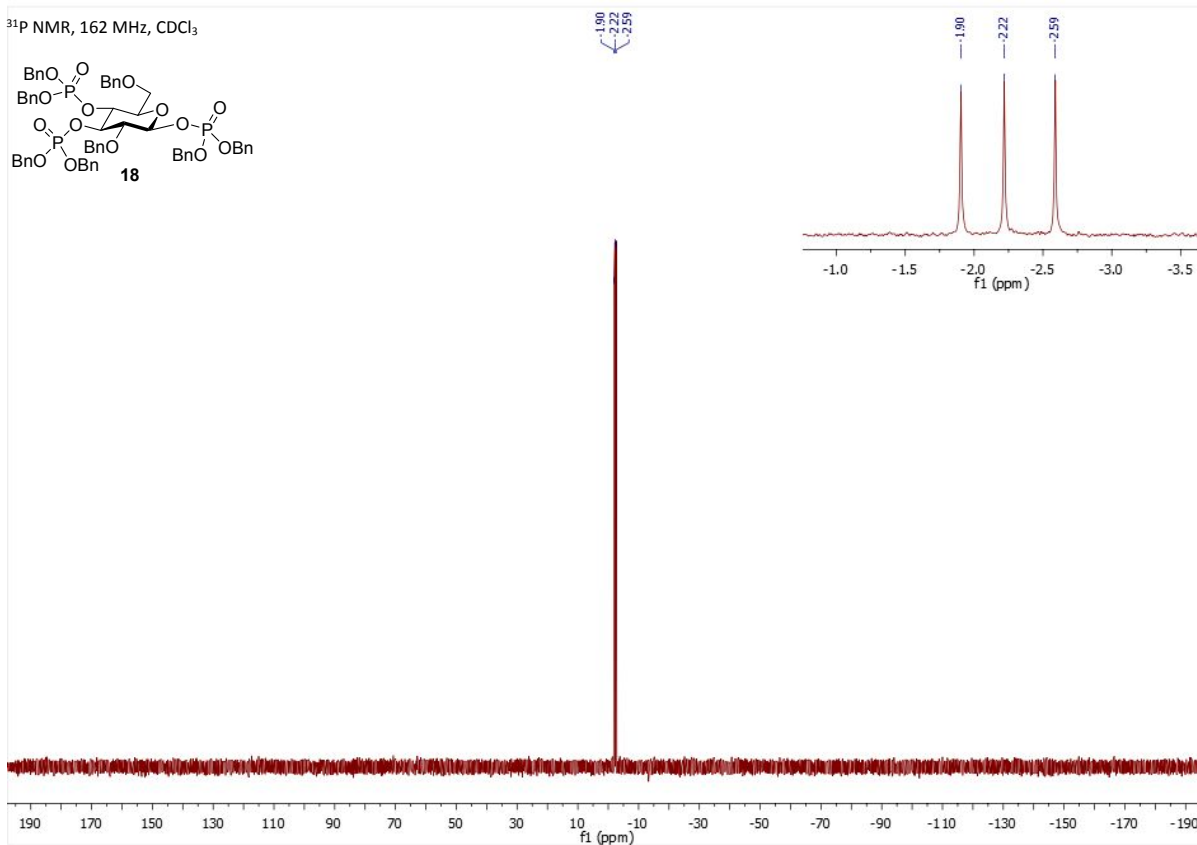
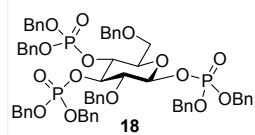
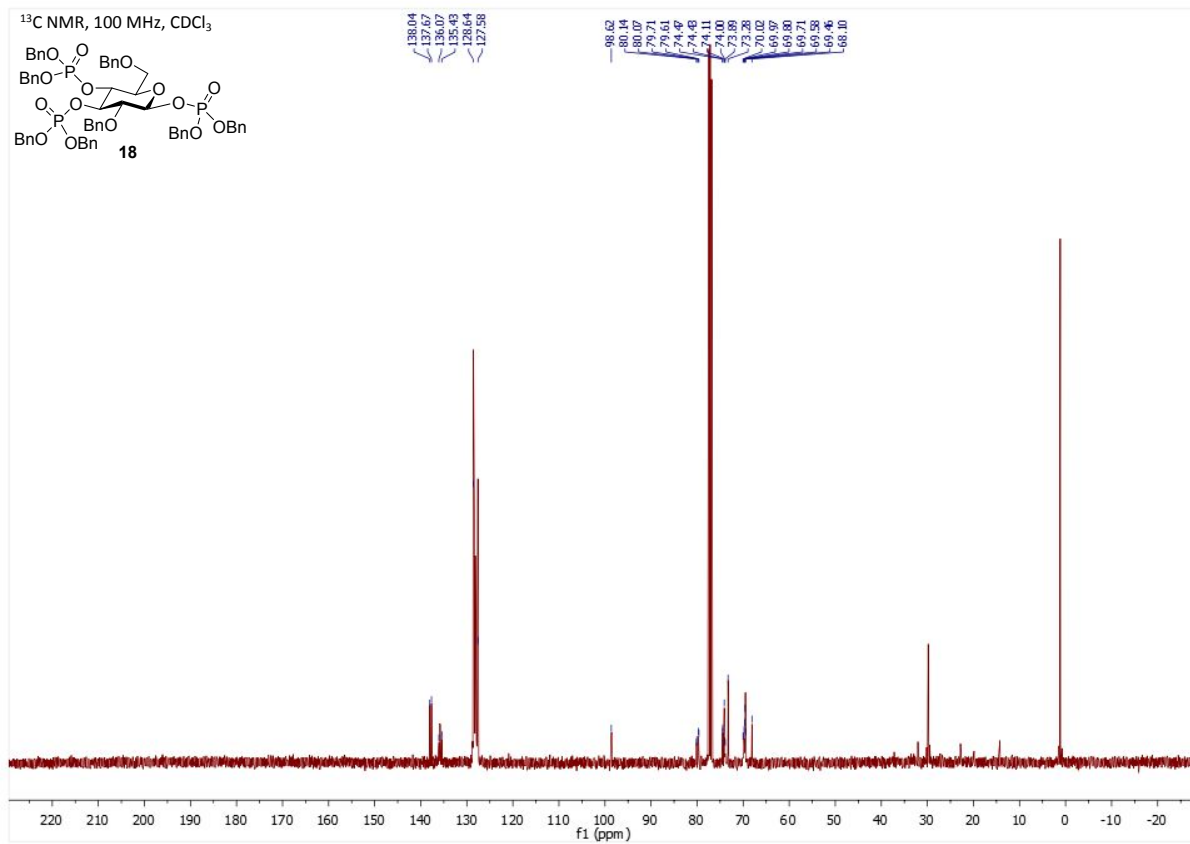
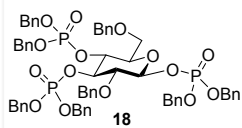
2,6-di-O-benzyl- α -D-glucopyranosyl 1,3,4-tris(dibenzylphosphate) (17)

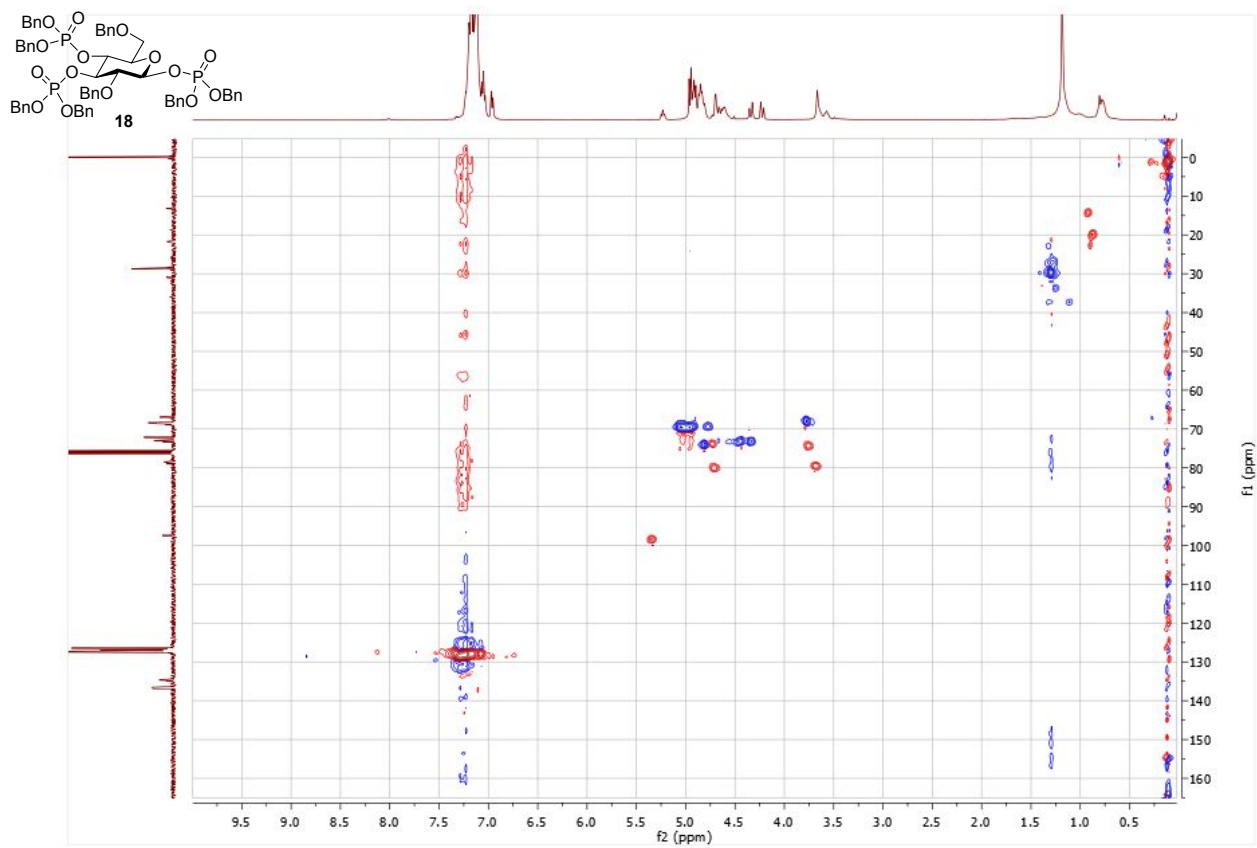
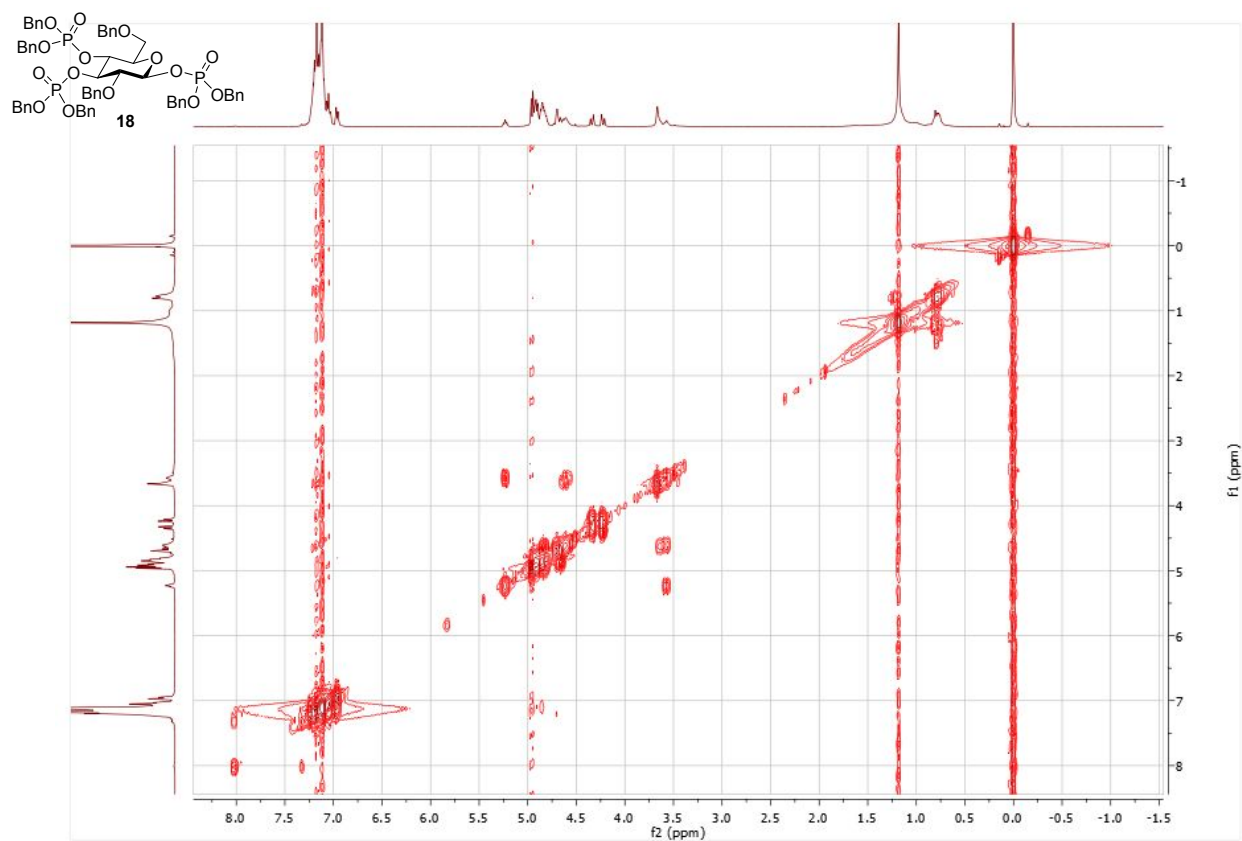


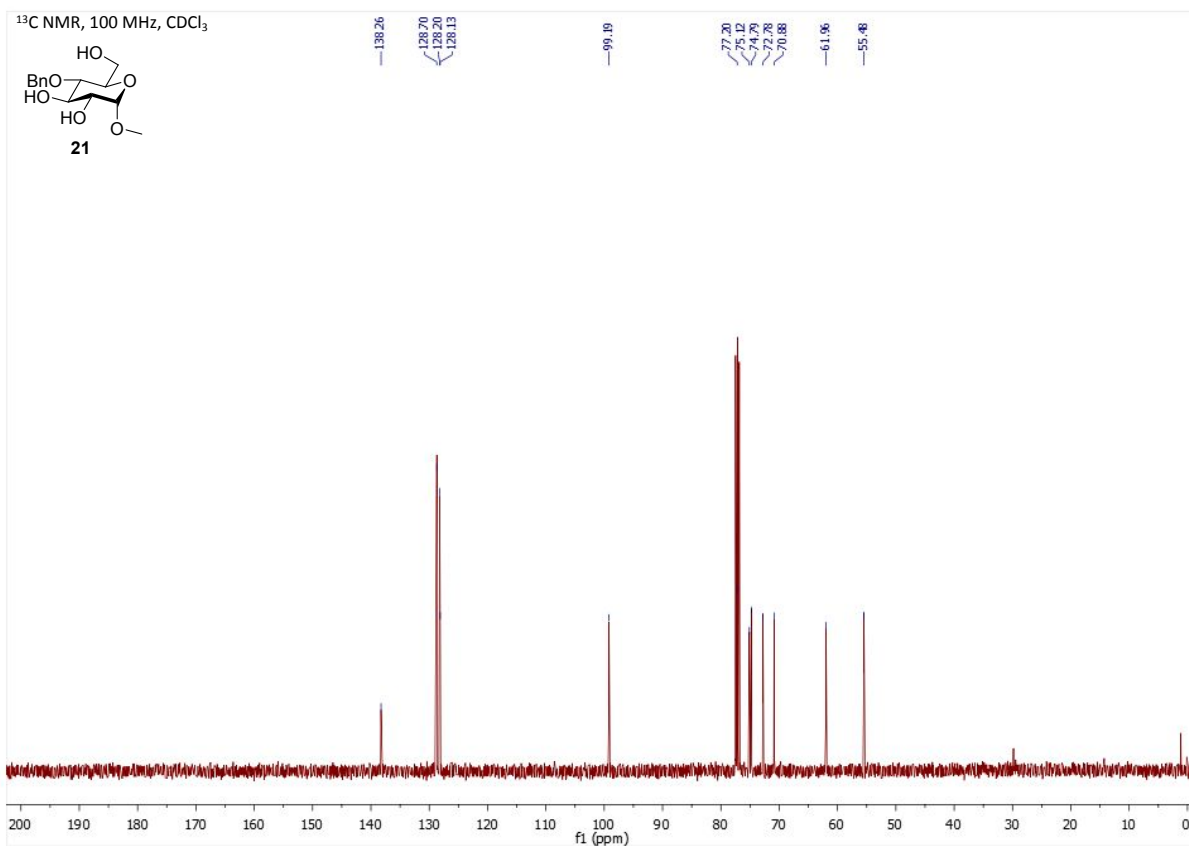
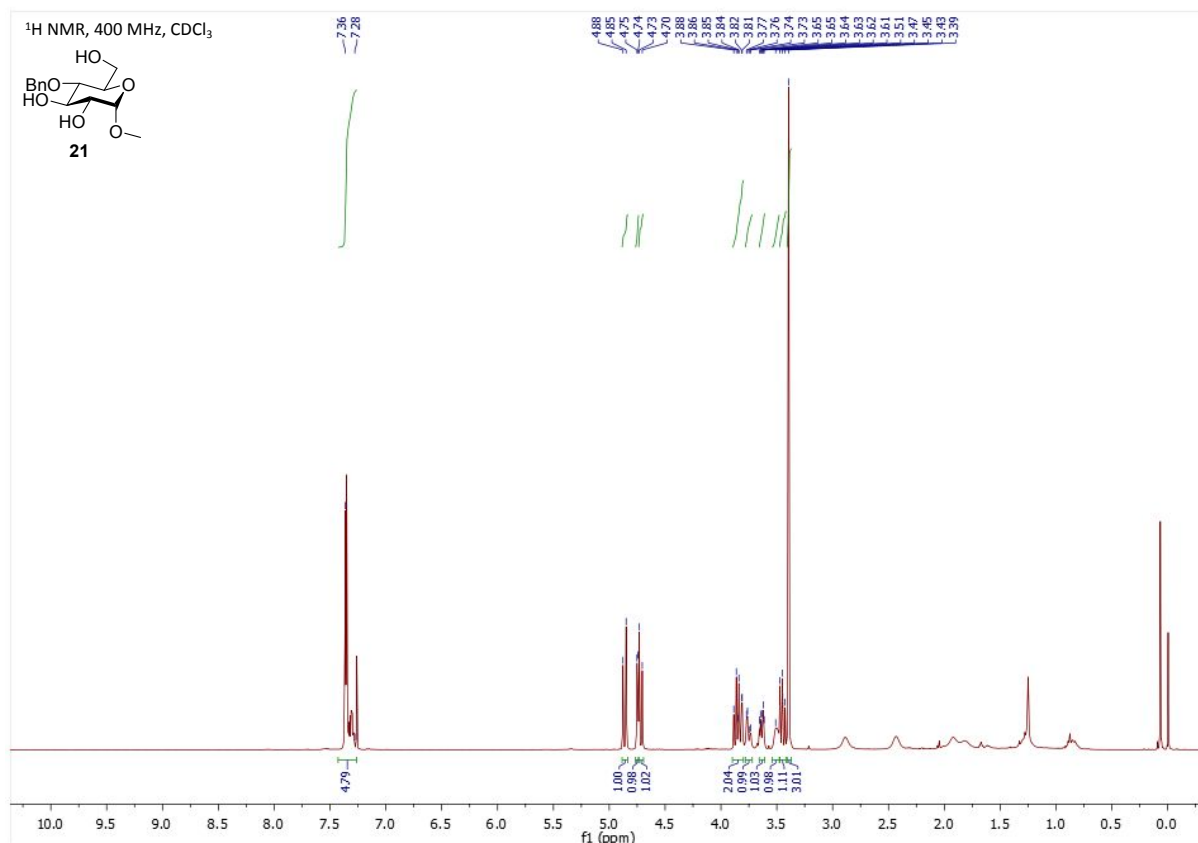


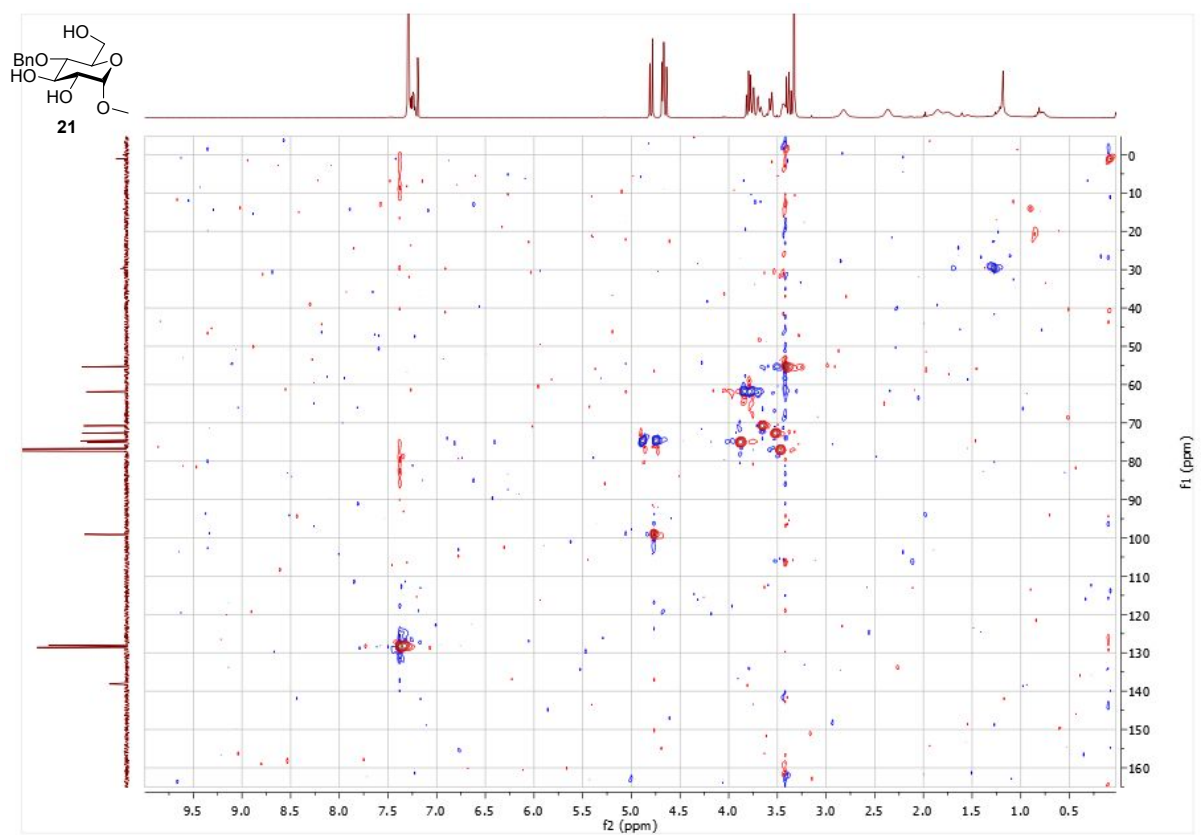
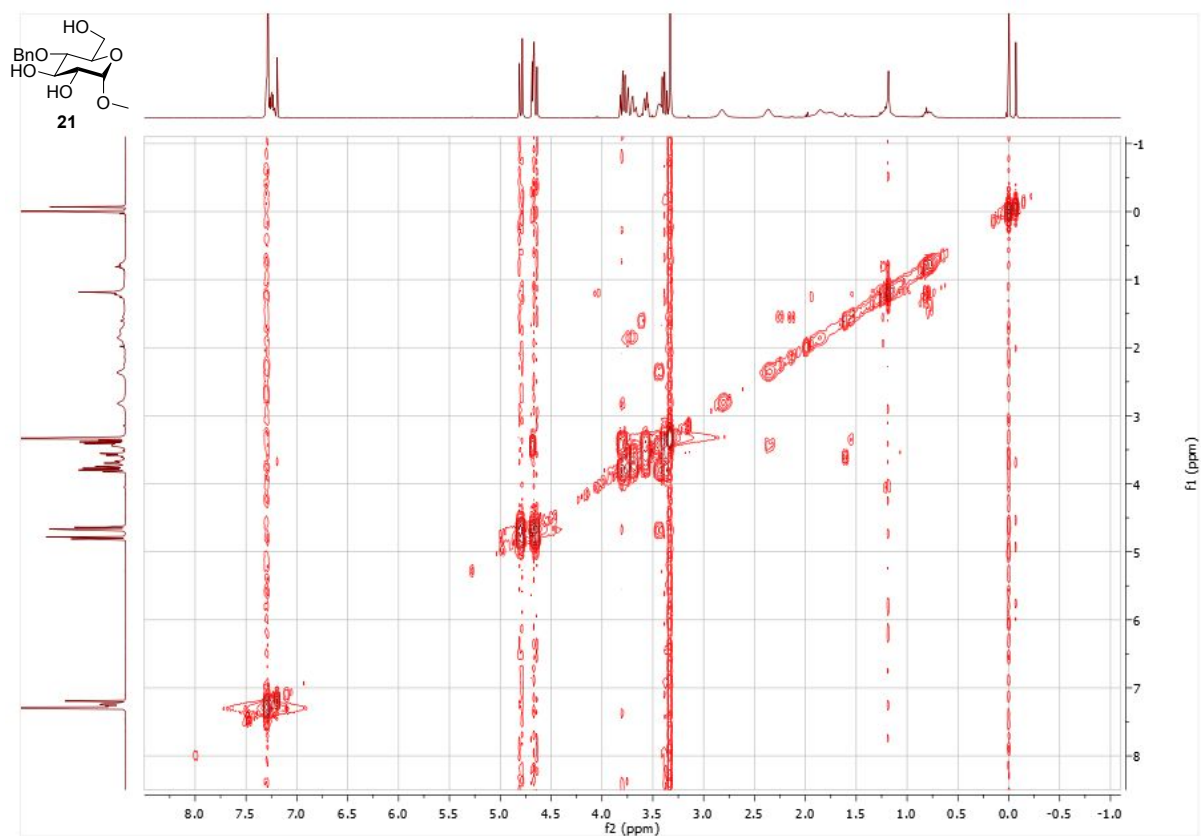
2,6-di-O-benzyl- β -D-glucopyranosyl 1,3,4-tris(dibenzylphosphate) (18)

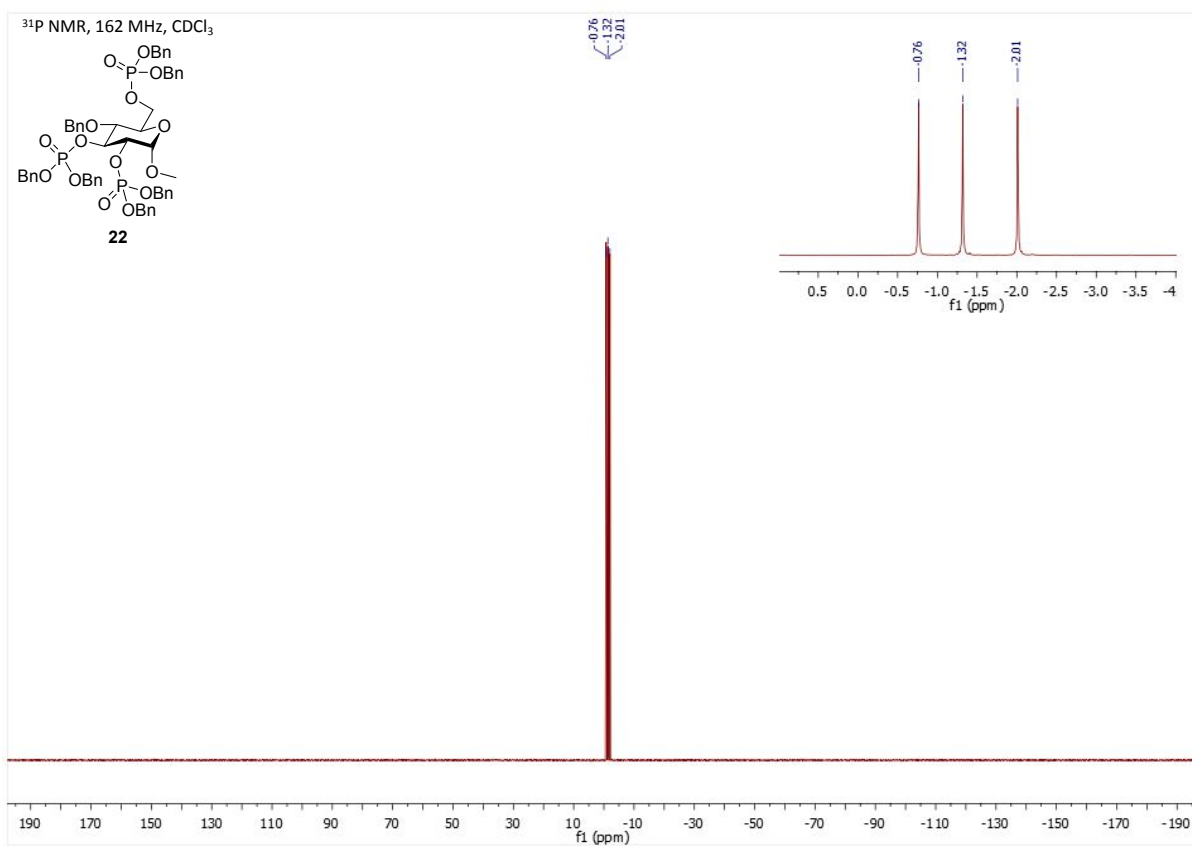
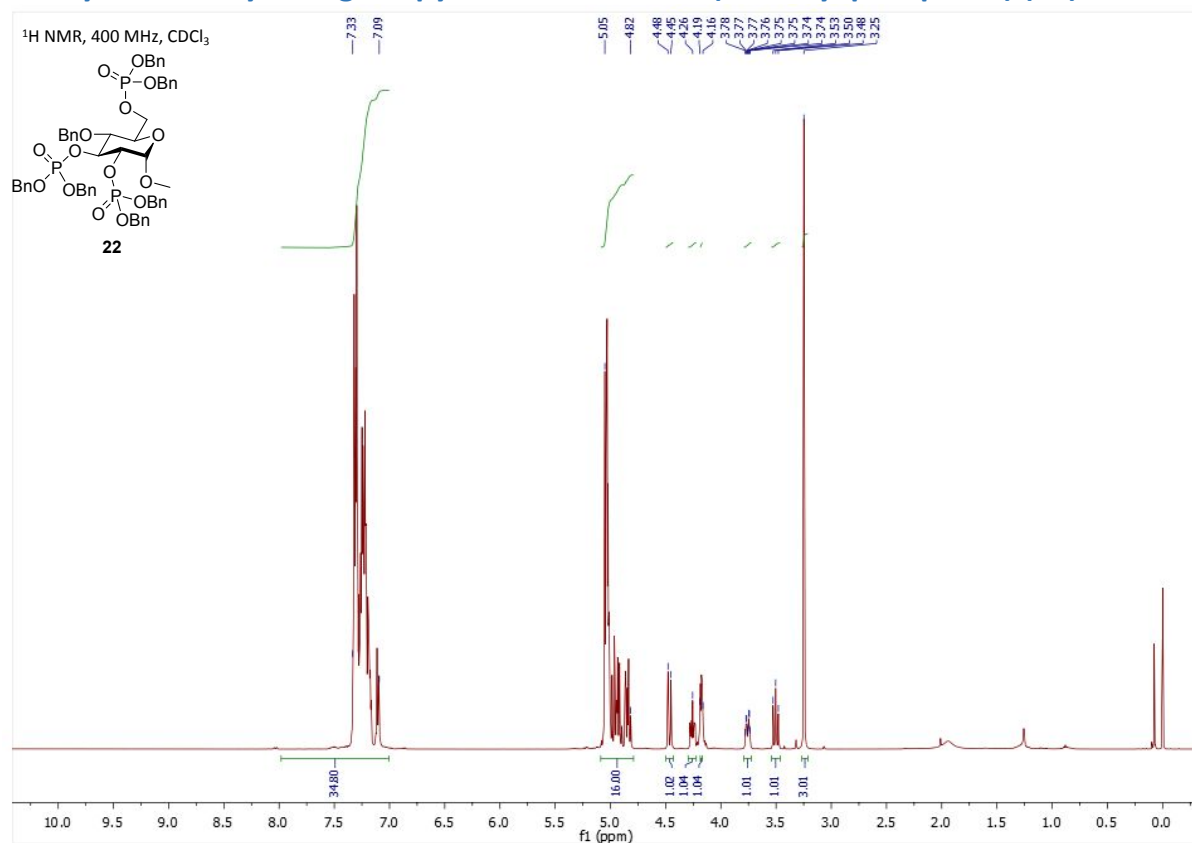


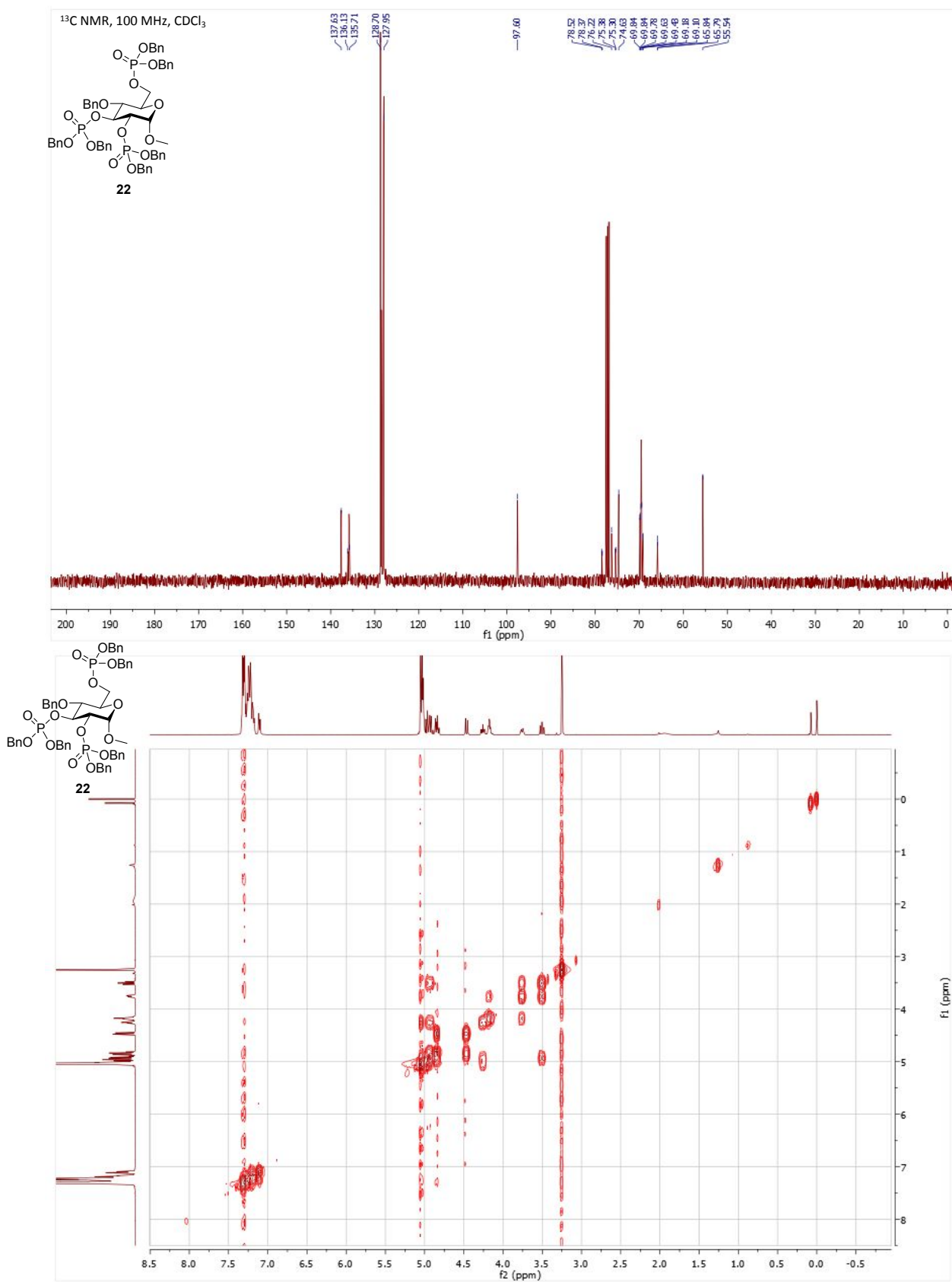
³¹P NMR, 162 MHz, CDCl₃¹³C NMR, 100 MHz, CDCl₃

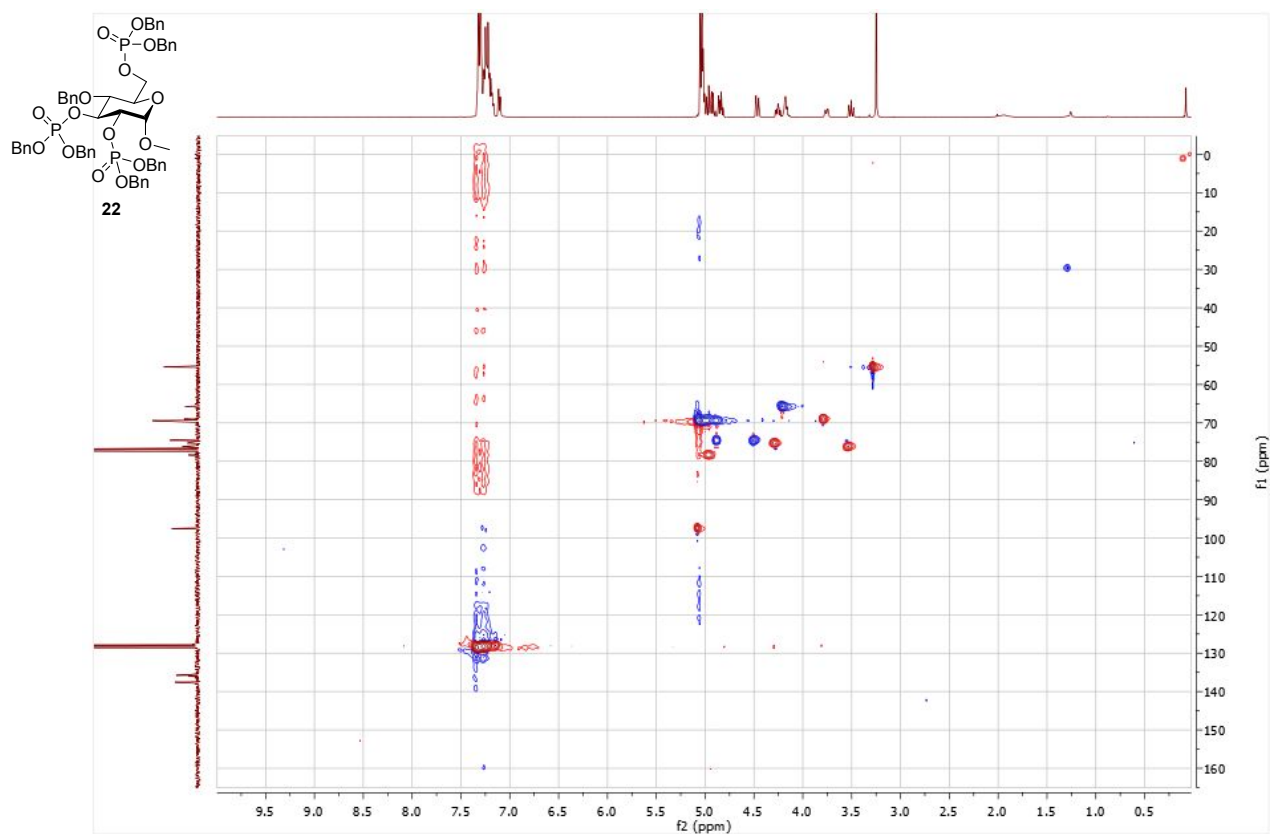


Methyl 4-O-benzyl- α -D-glucopyranoside (21)

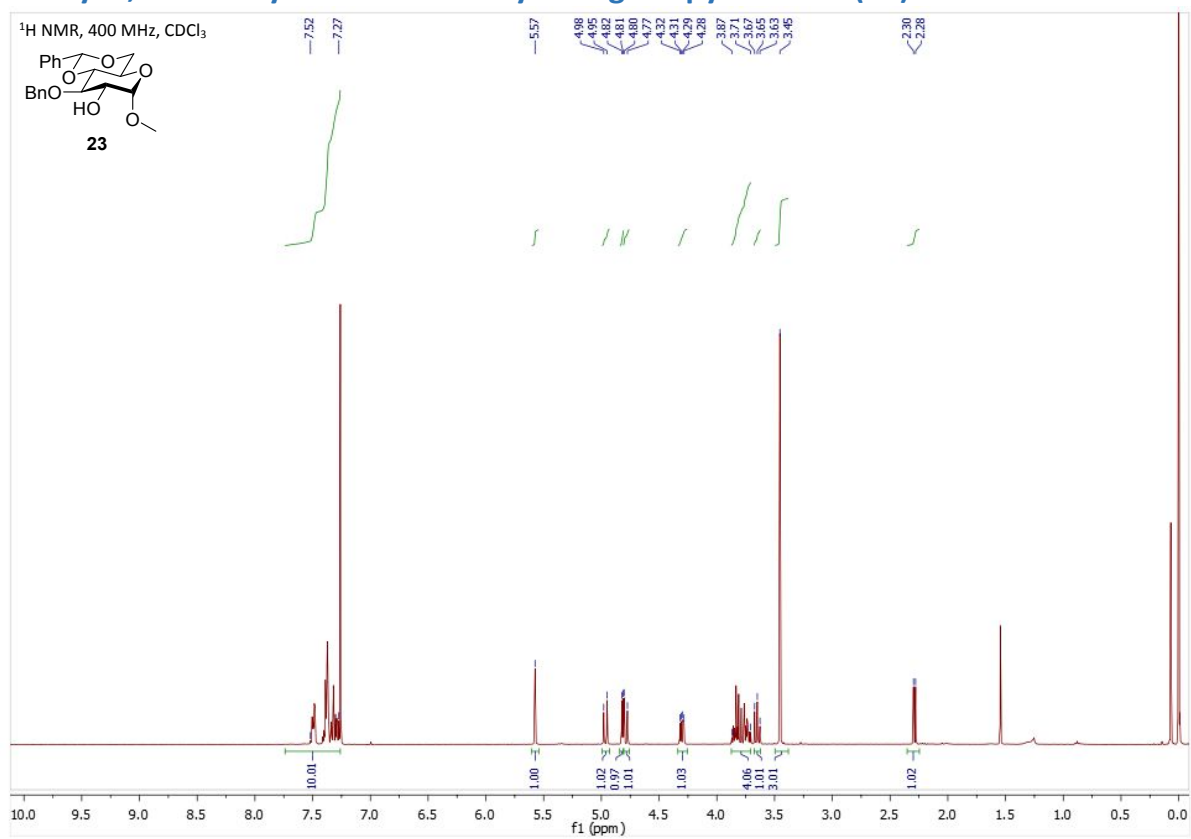


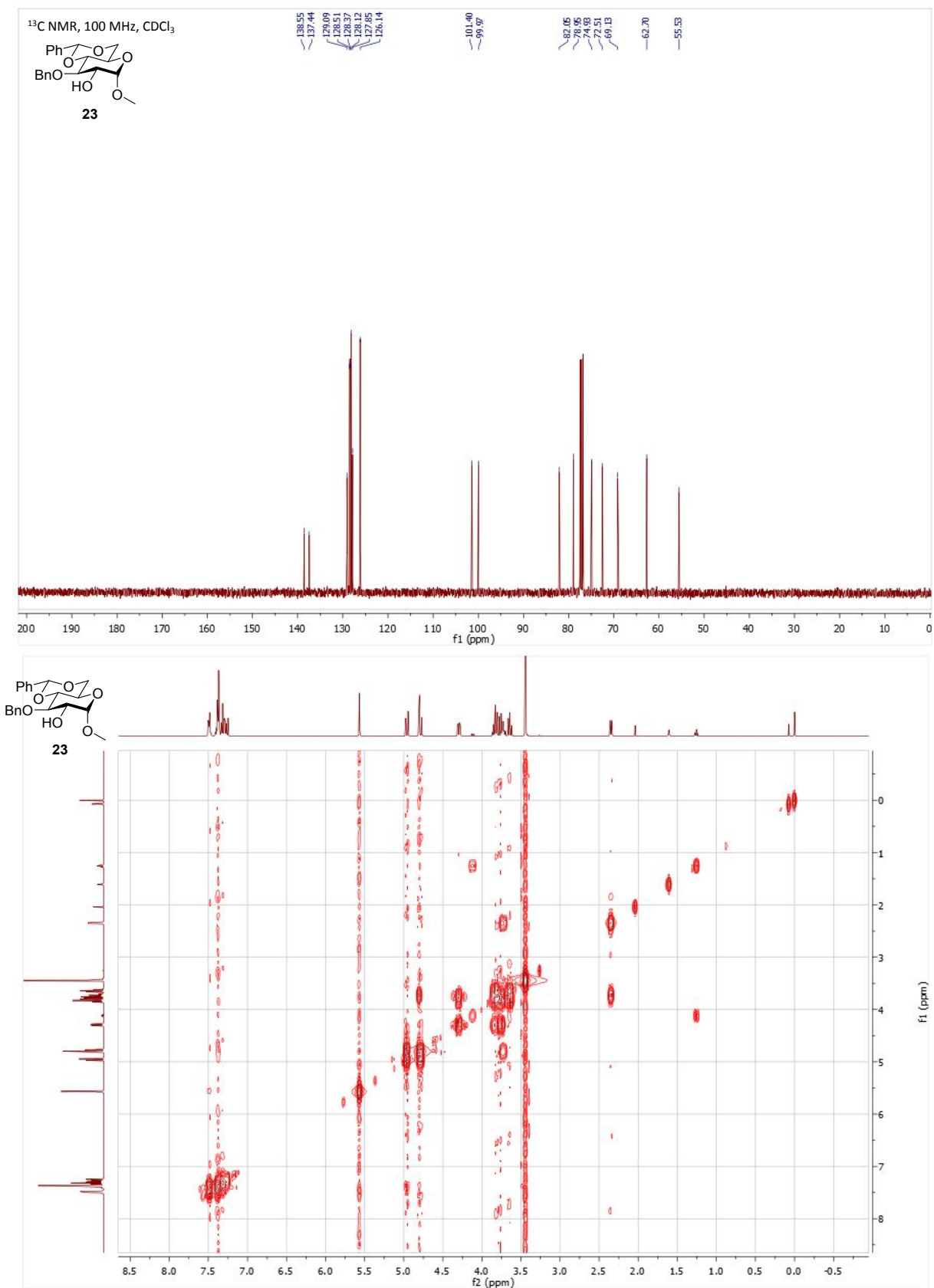
Methyl 4-O-benzyl- α -D-glucopyranoside 2,3,6-tris(dibenzyl phosphate) (22)

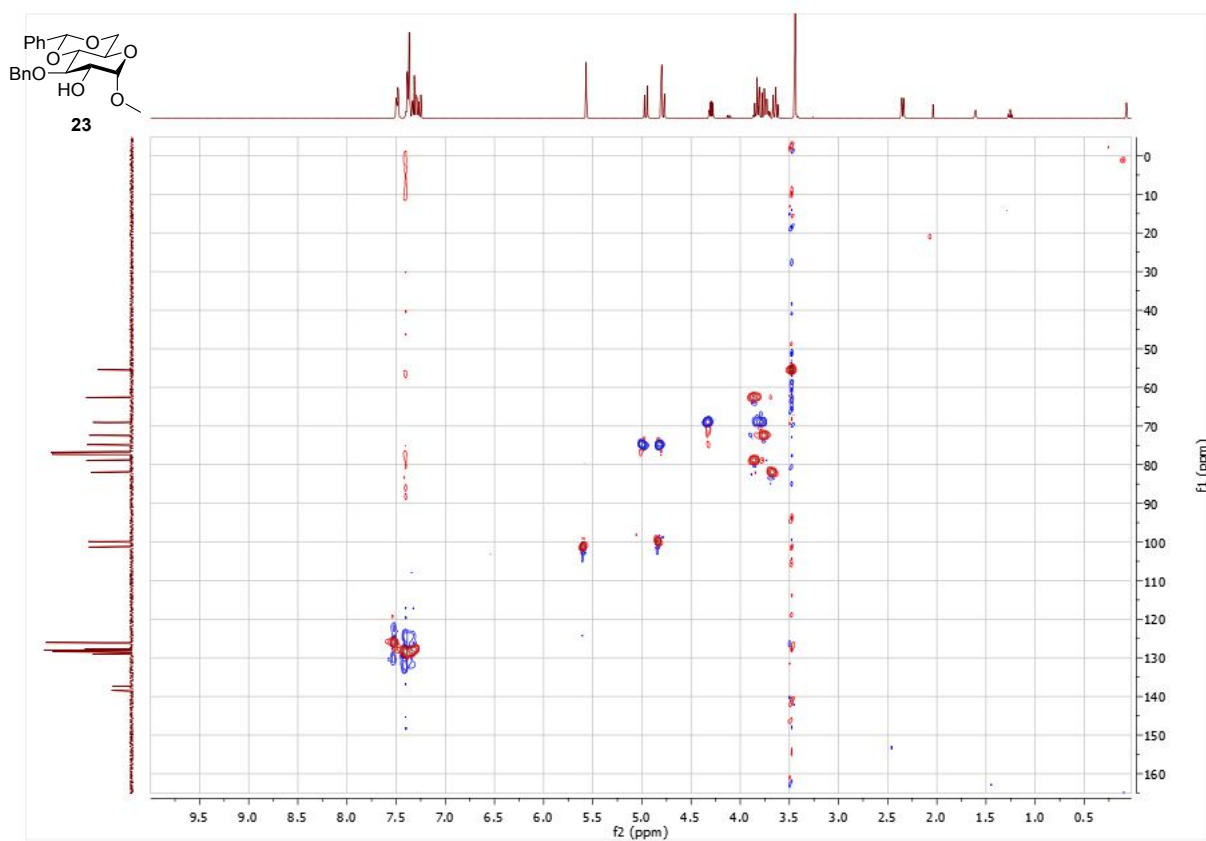




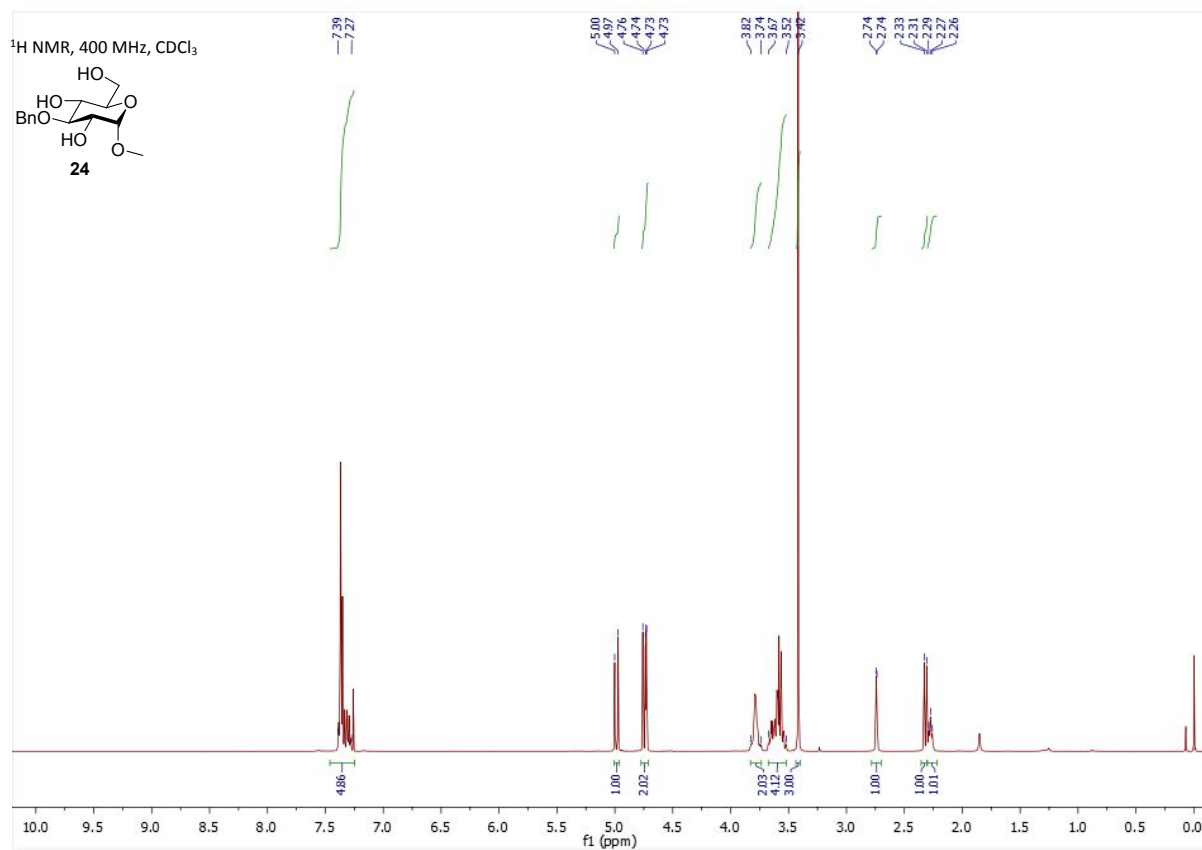
Methyl 4,6-O-benzylidene-3-O-benzyl- α -D-glucopyranoside (**23**)

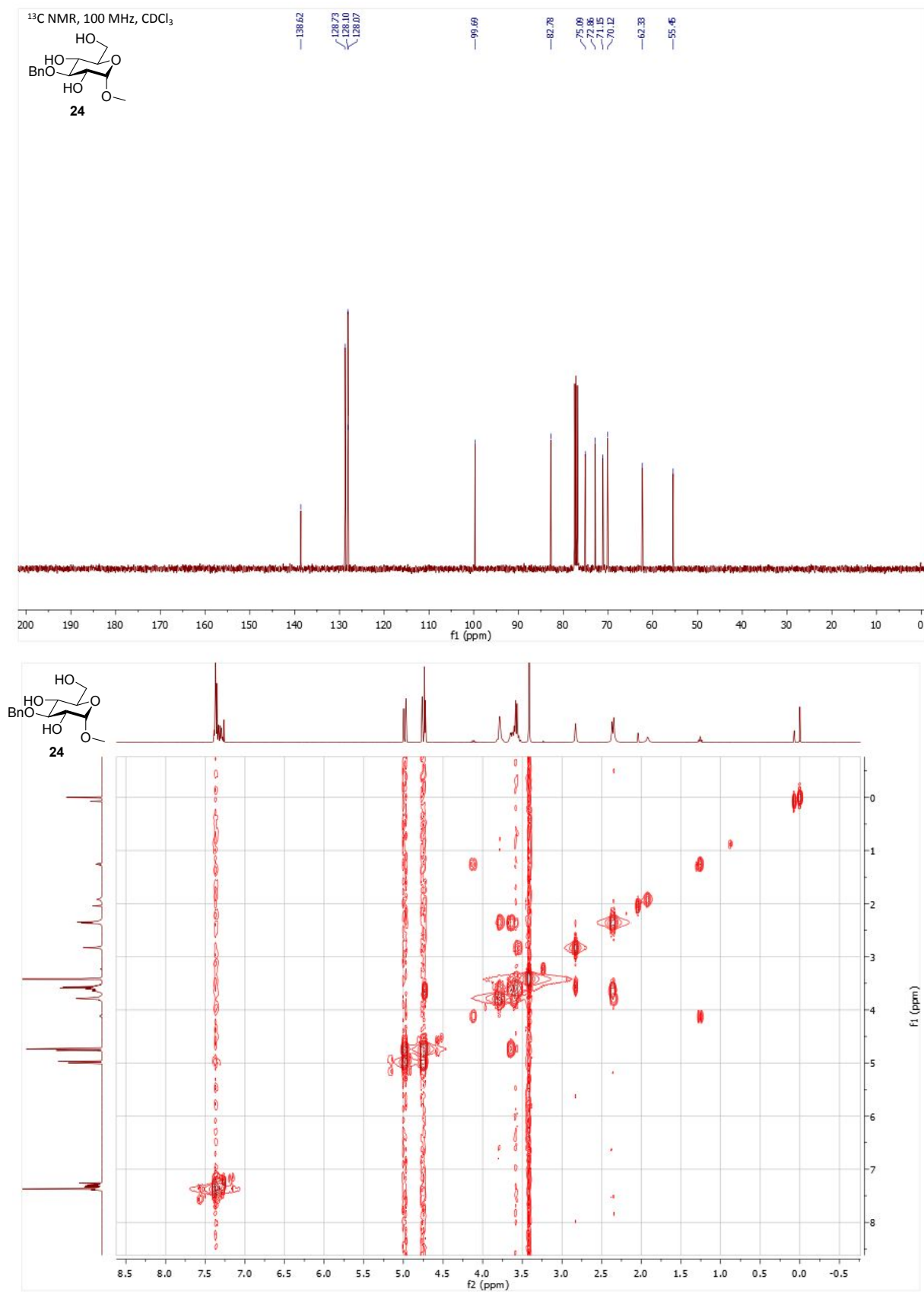


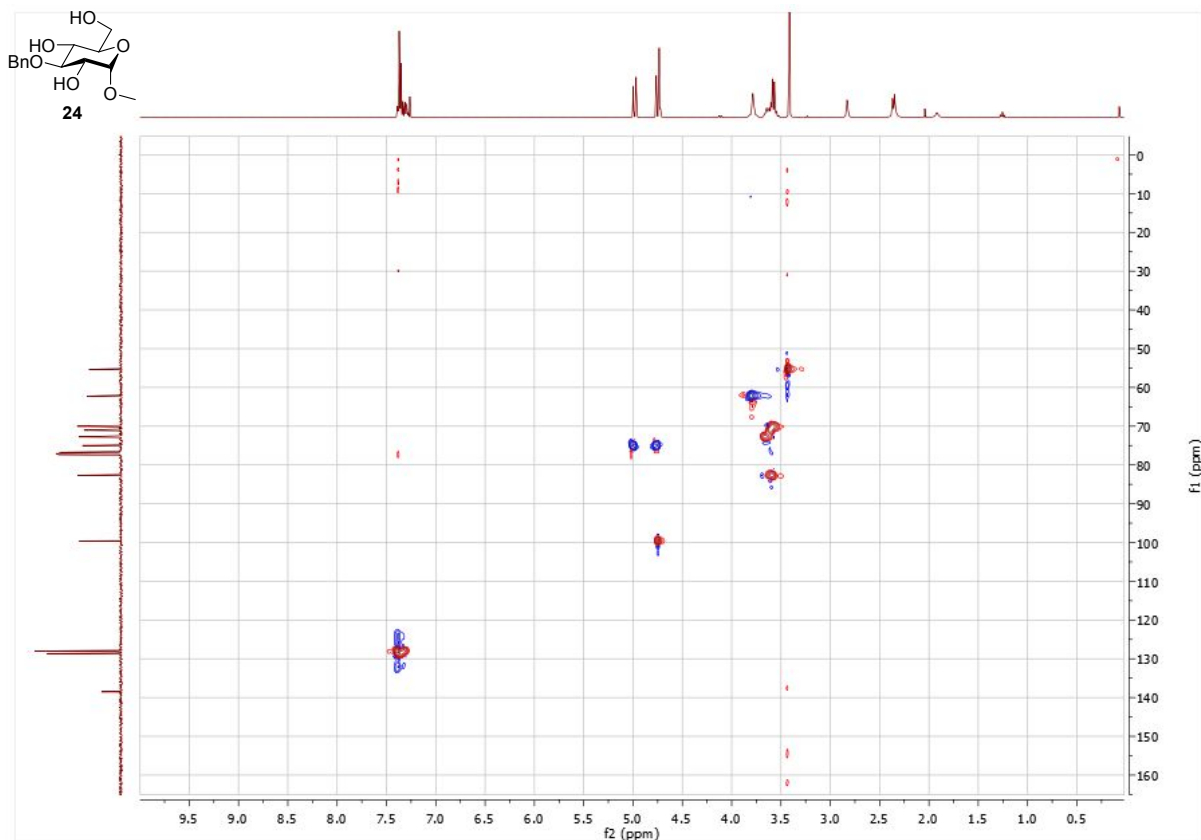




Methyl 3-*O*-benzyl- α -D-glucopyranoside (**24**)







Methyl 3-O-benzyl- α -D-glucopyranoside 2,4,6-tris(dibenzyl phosphate) (**25**)

