

SUPPLEMENTARY MATERIAL

Synthesis of Highly Water Soluble Adamantyl Phosphoinositide Derivatives

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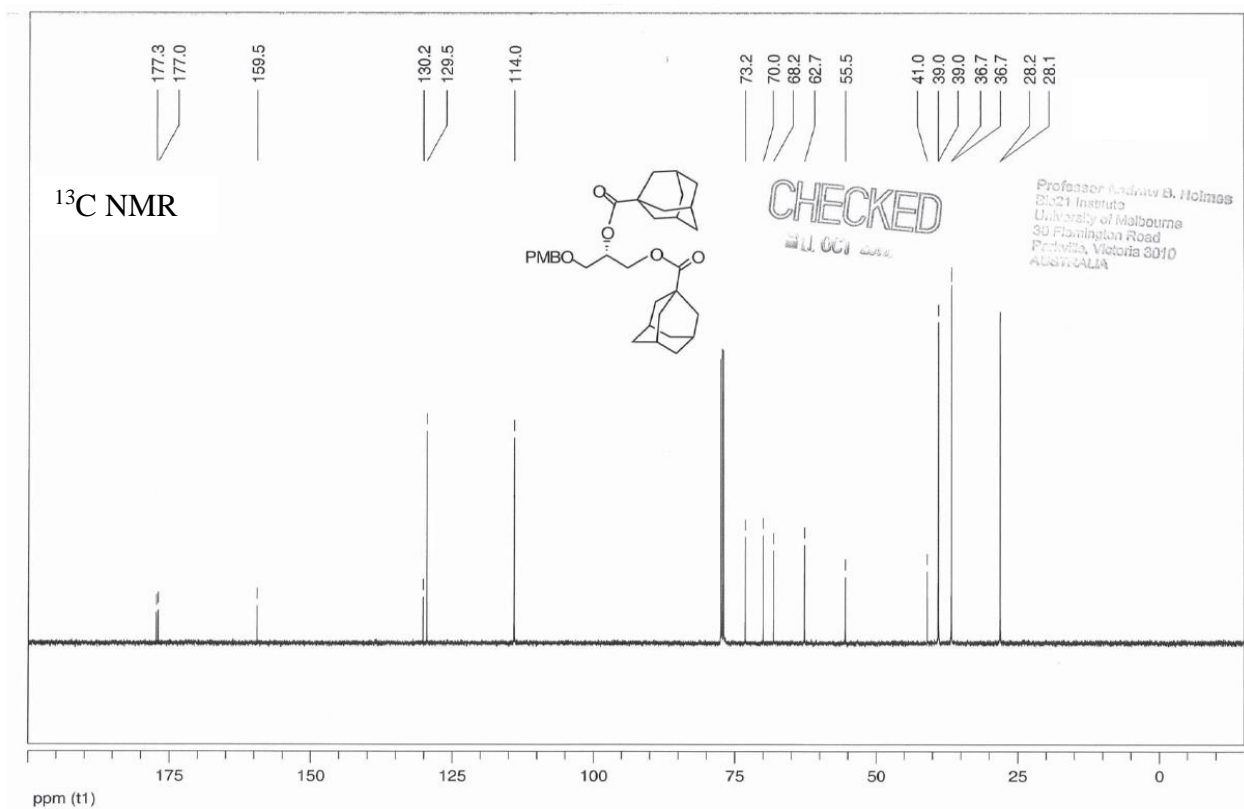
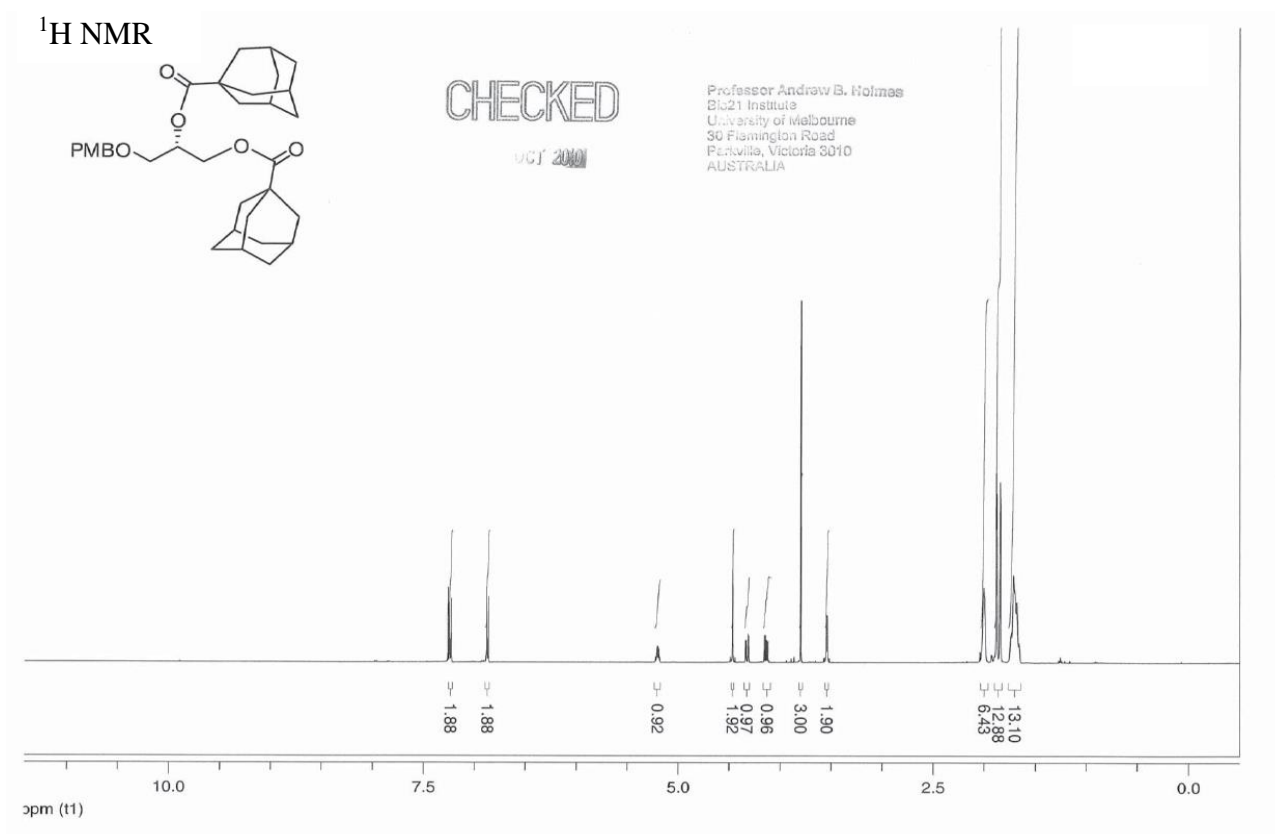
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NMR (¹H, ¹³C and ³¹P) and HRMS spectra for the following compounds: **3**, **4**, **5**, **8**, **9**, **10** and **11**.

3-O-Methoxybenzyl -1,2-di-O-adamantanecarbonyl-sn-glycerol (3)



HRMS

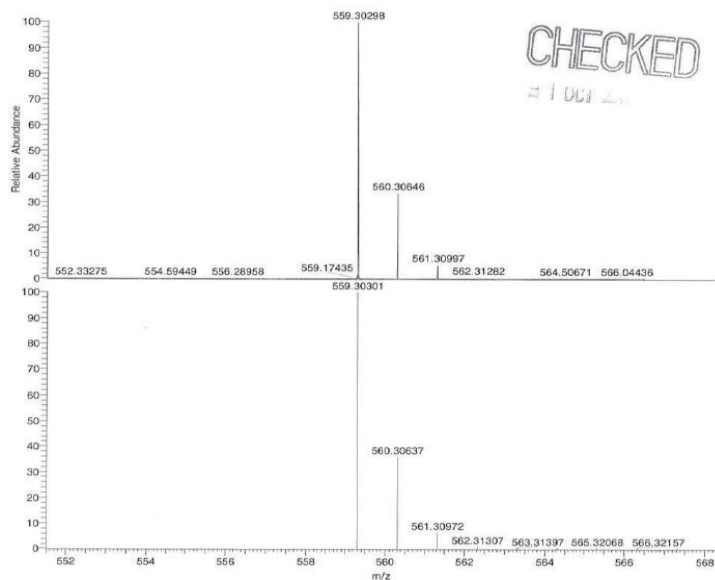
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Parkville, Victoria 3010
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SIMS

C:\calibur\...MSS-05-05-09_13SIM

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Vivian Yin VY-B-1

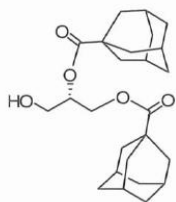


Experimental peaks

Simulated peaks

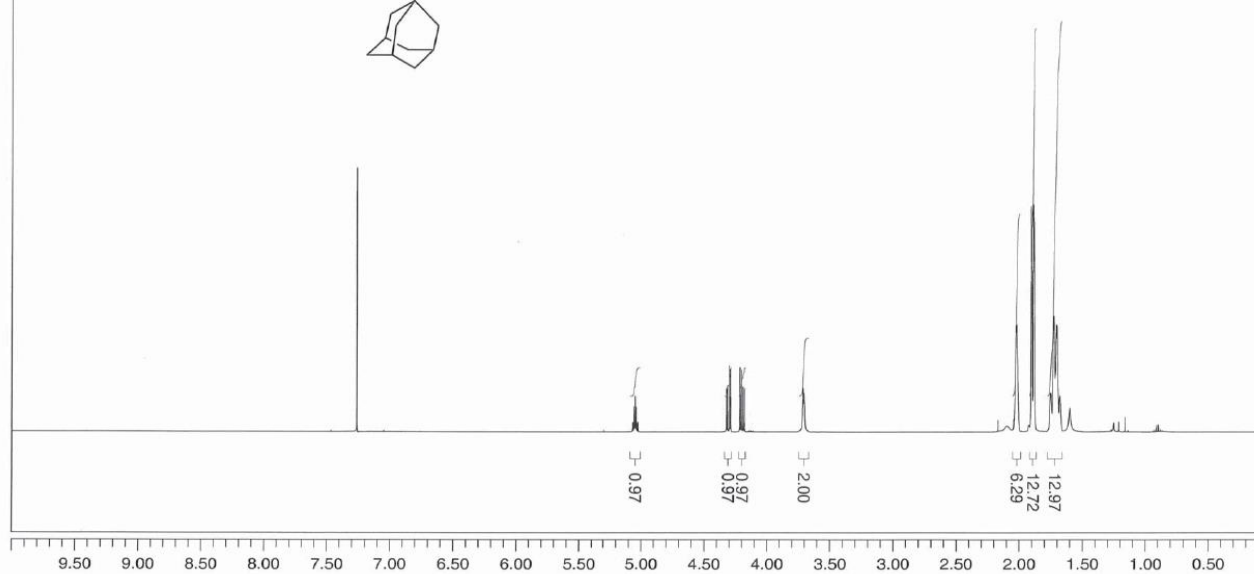
1,2-di-O-adamantanecarbonyl-sn-glycerol (4)

¹H NMR

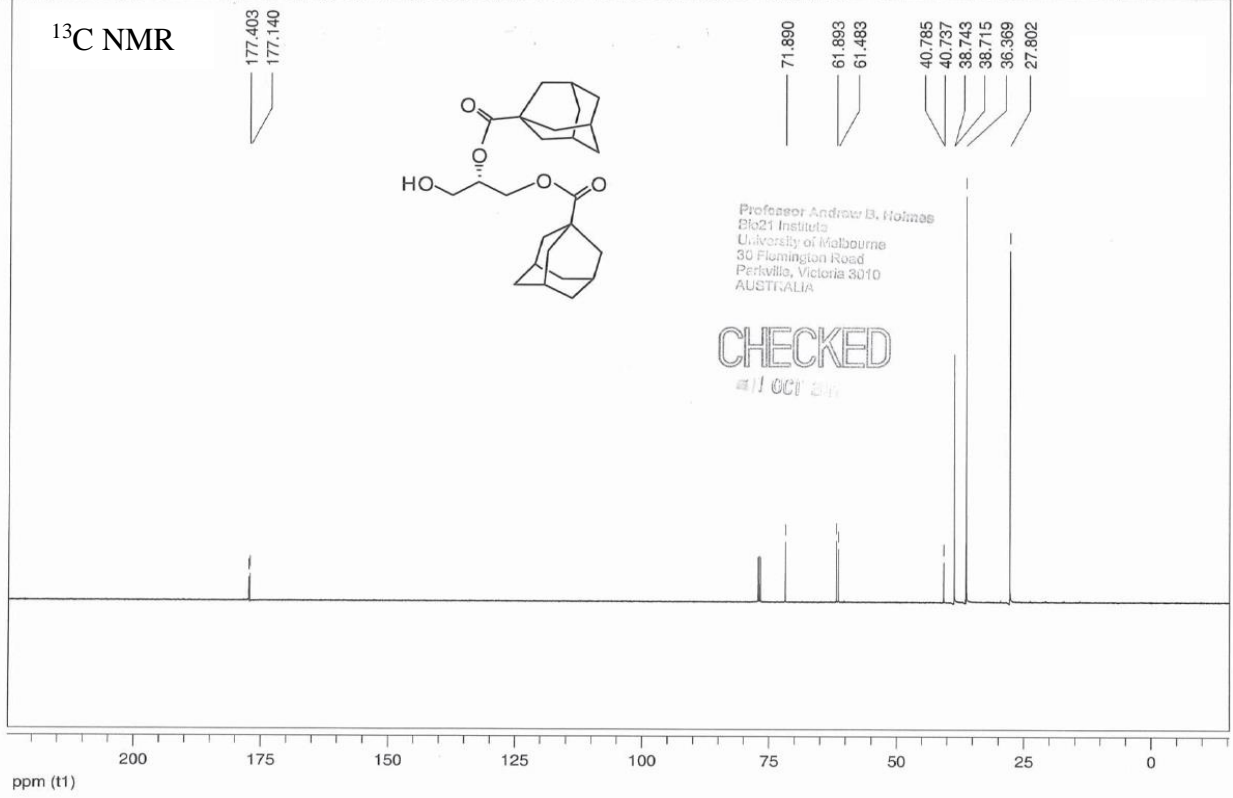


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OCT 2009

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¹³C NMR



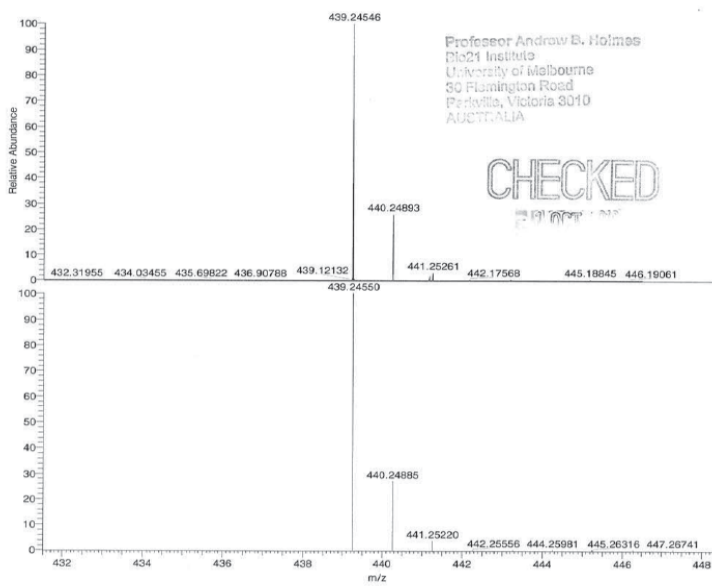
HRMS

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Vivien Yin VY-B-17

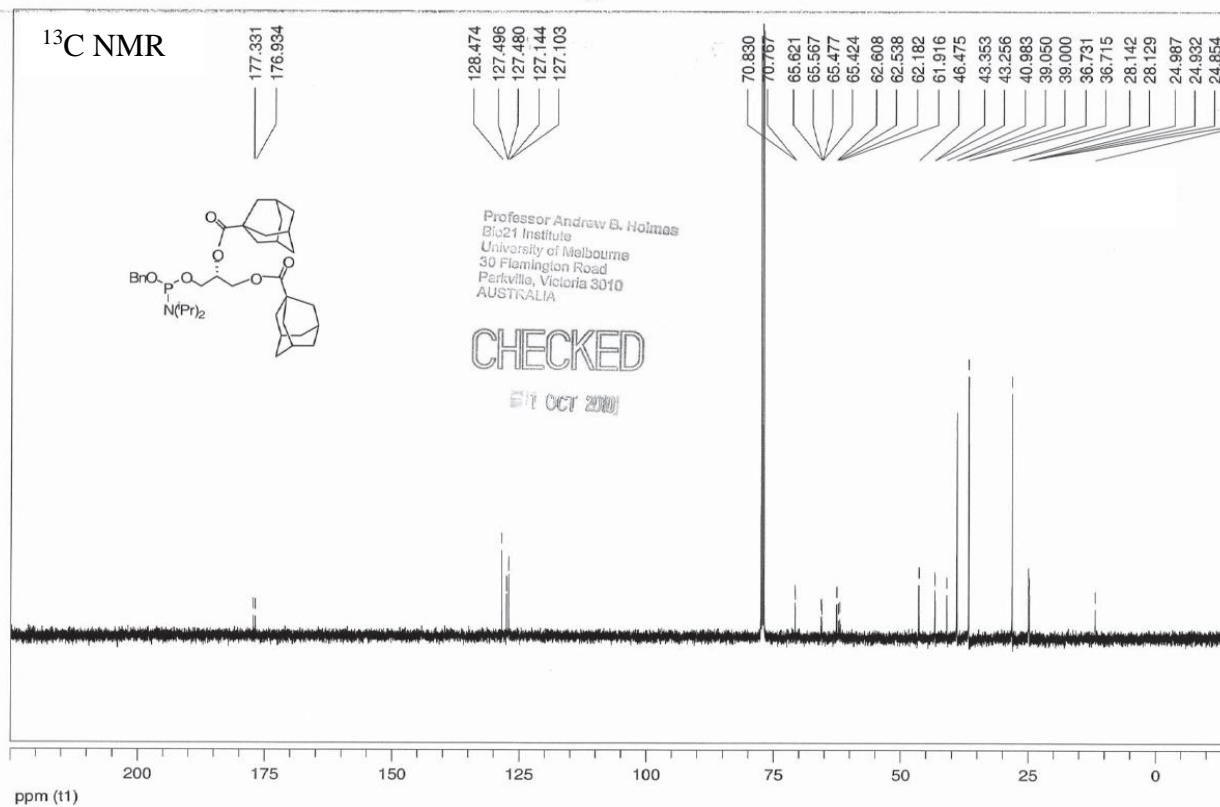
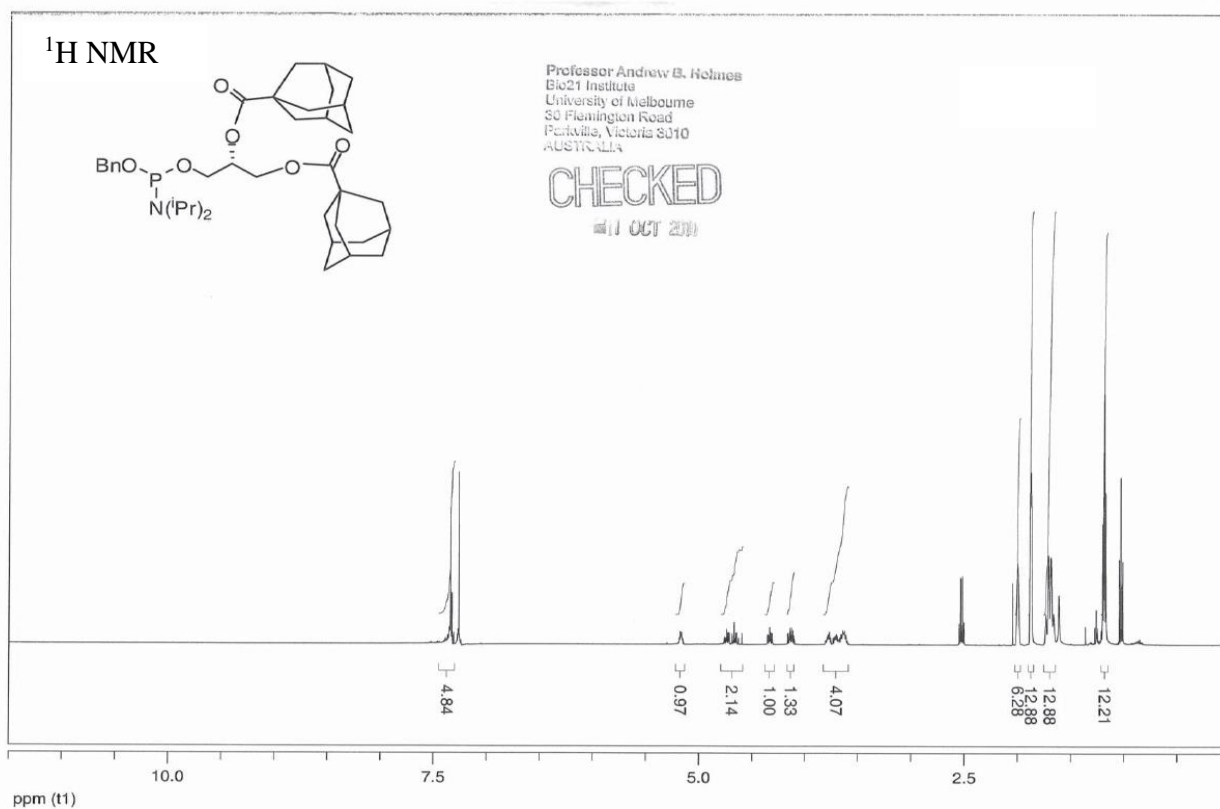
SIMS



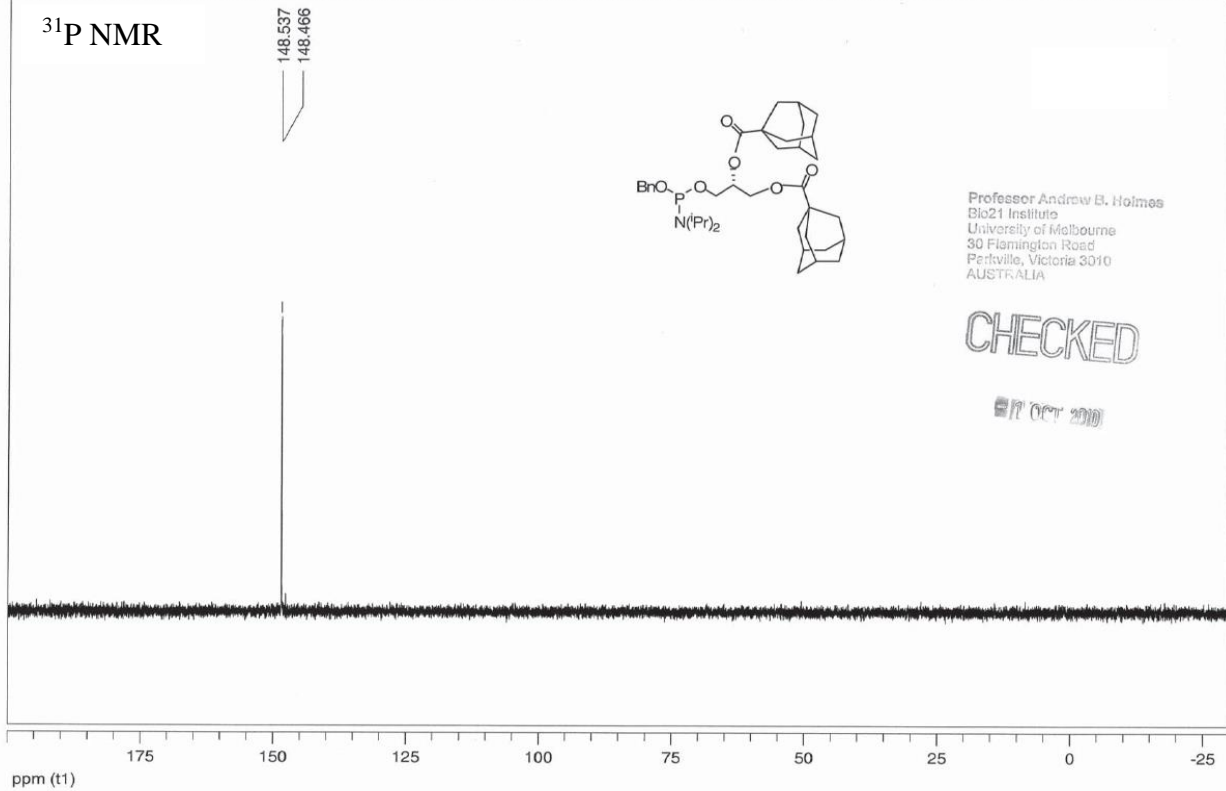
Experimental peaks

Simulated peaks

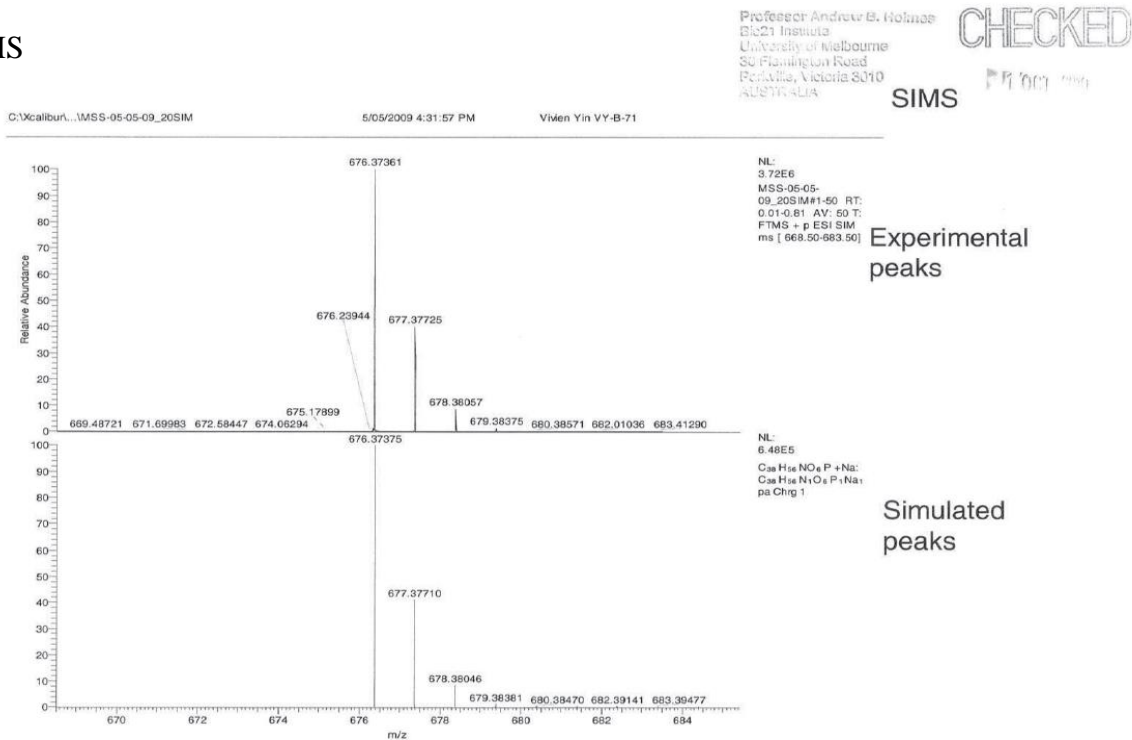
(+)-Benzoyloxy(*N,N*-diisopropylamino)(1,2-di-*O*-adamantanecarbonyl-*sn*-glycer-3-yl)phosphine (**5**)



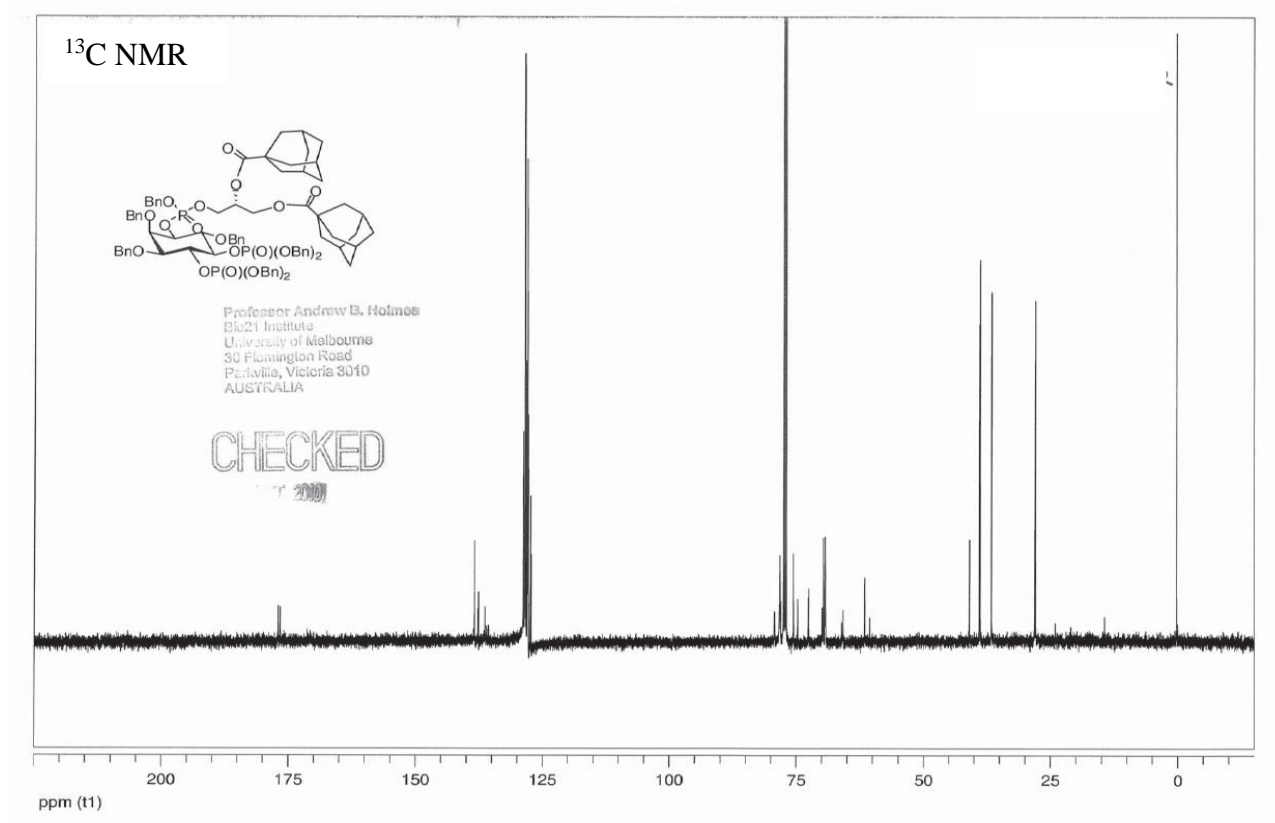
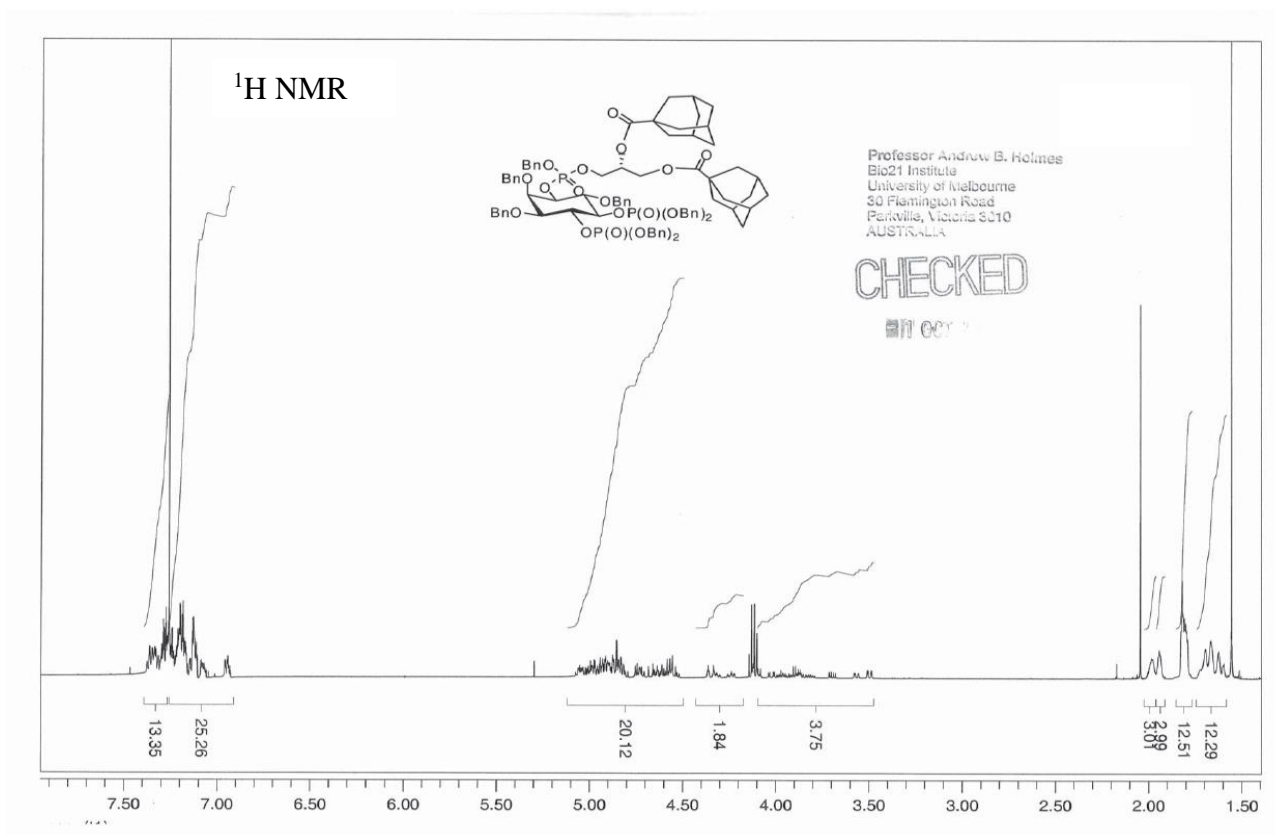
³¹P NMR

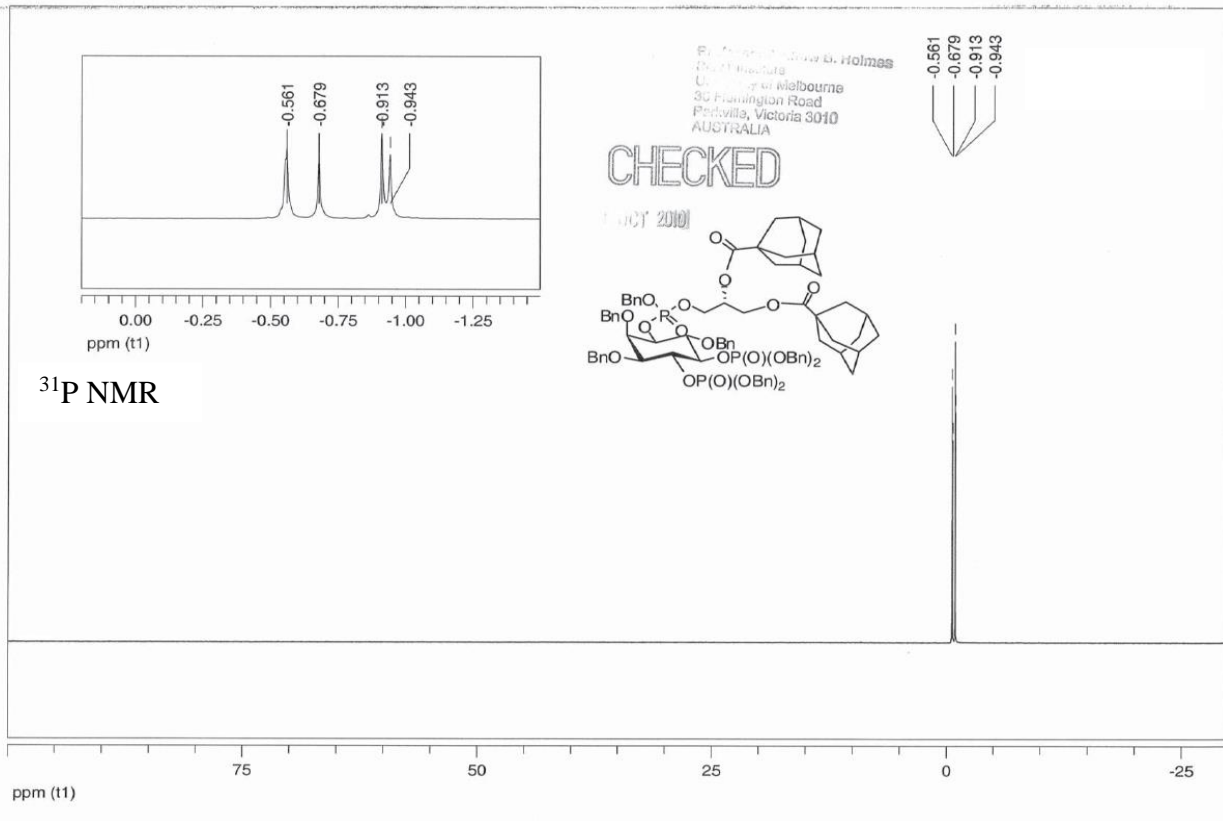


HRMS



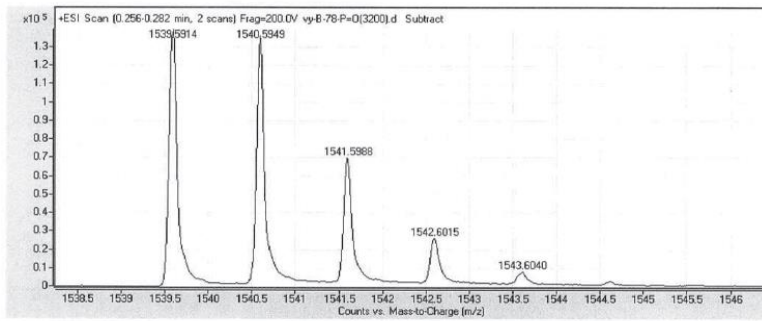
1D-2,3,6-Tri-O-benzyl-myo-inositol-[1',2'-di-O-adamantanecarbonyl-glycer-3'-yl benzyl phosphate] 4,5-bis(dibenzyl)phosphate (8)





HRMS

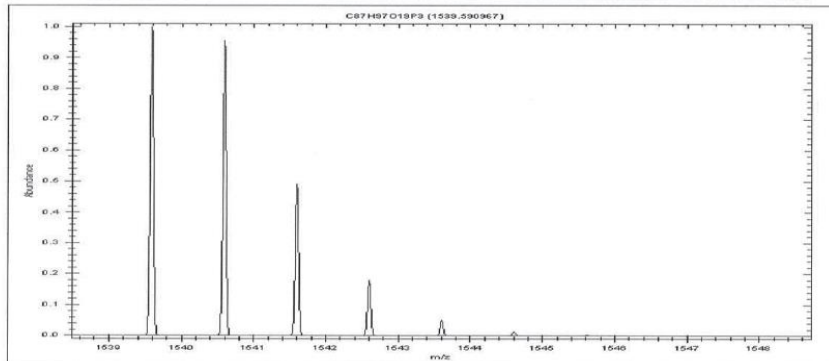
M+H



Experimental peaks

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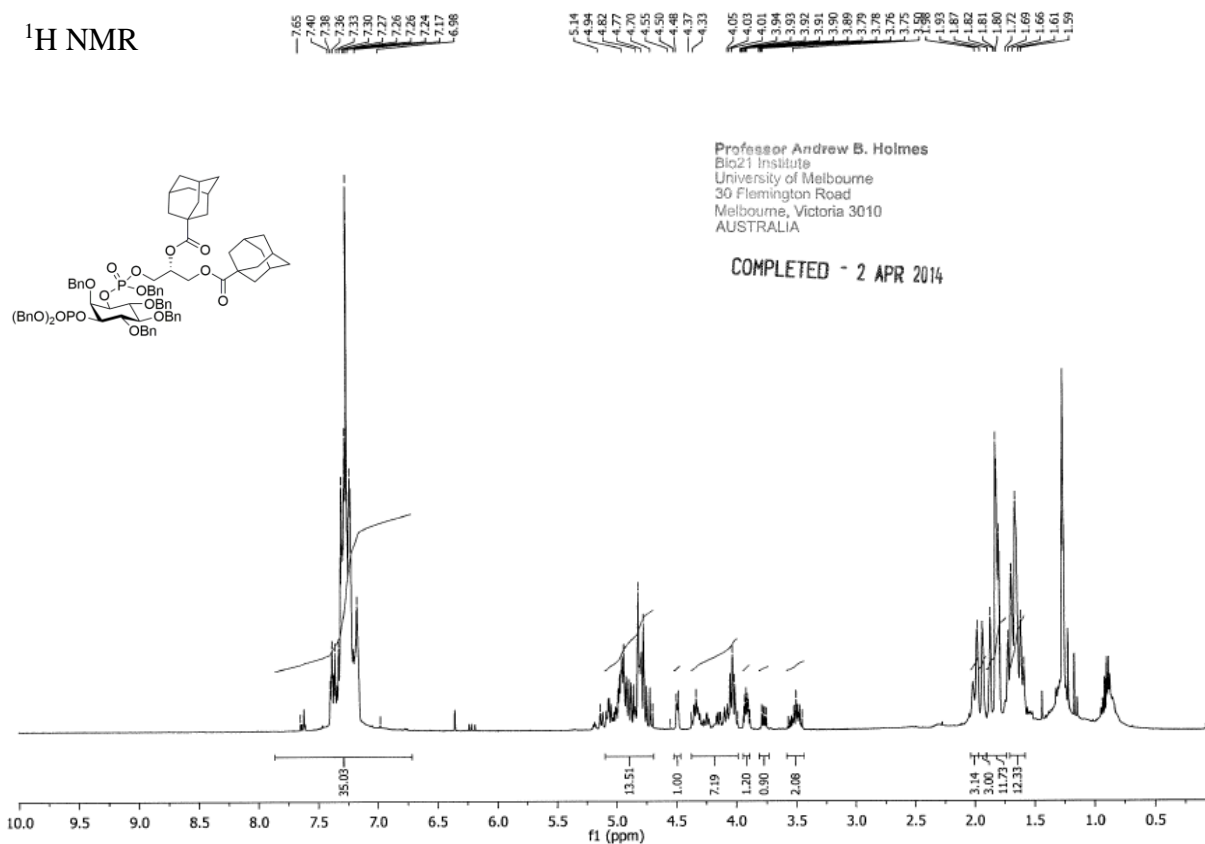
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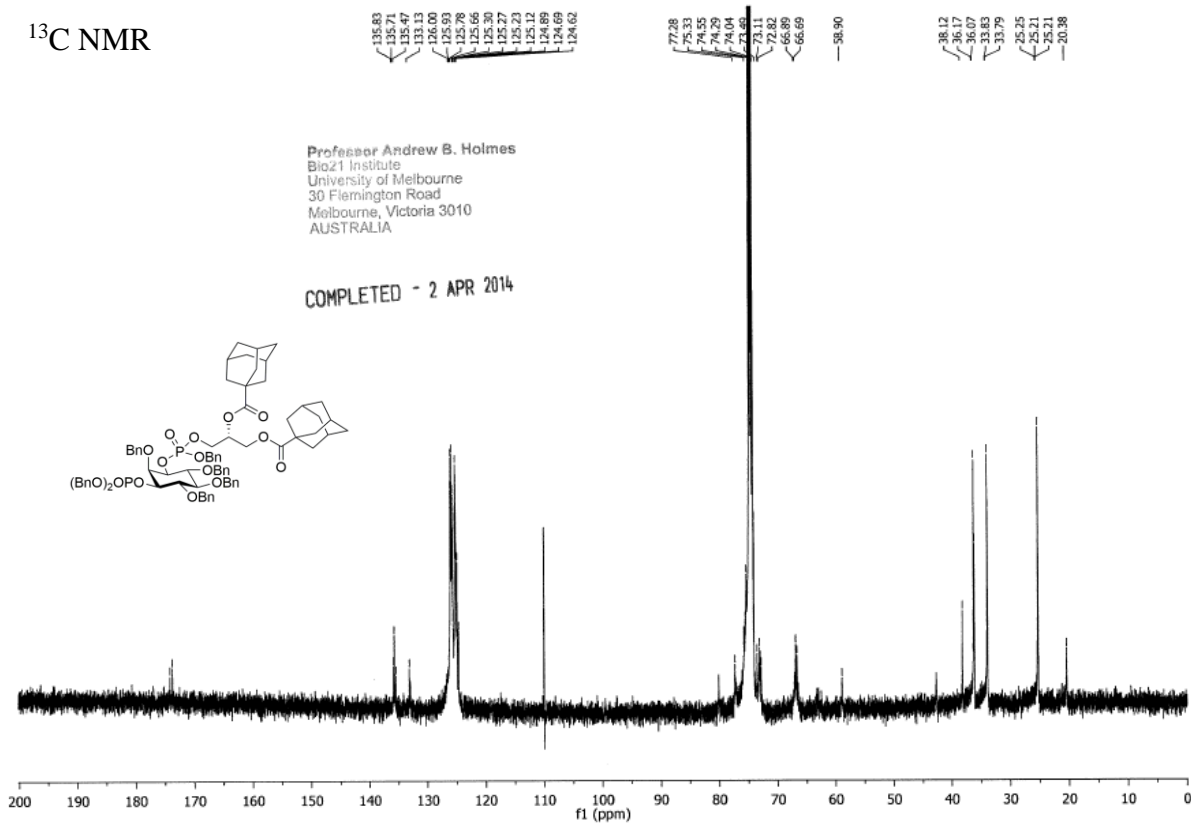
Simulated peaks

1D-2,4,5,6-Tetra-O-benzyl-myo-inositol-[1',2'-di-O-adamantanecarbonyl-glycer-3'-yl benzyl phosphate] 3(dibenzyl)phosphate (9)

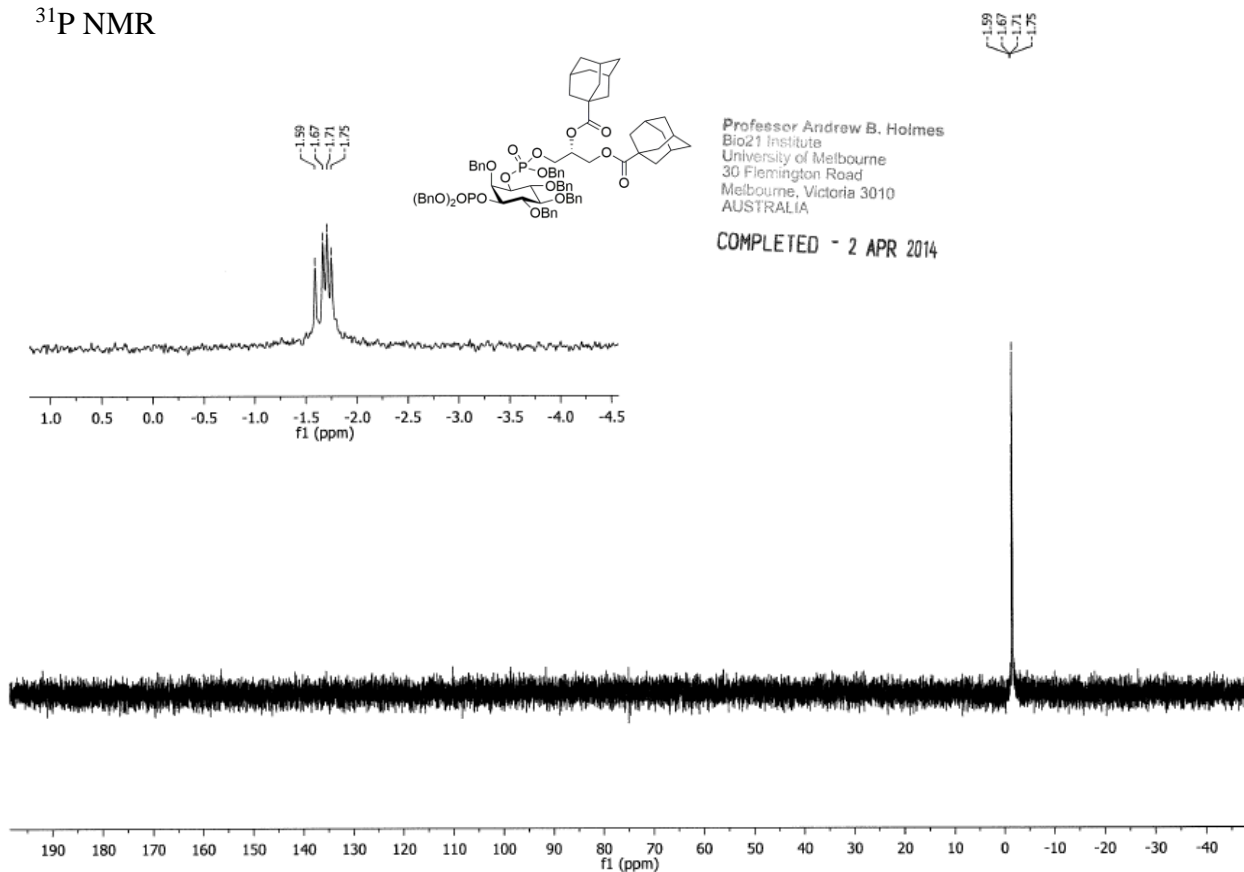
¹H NMR



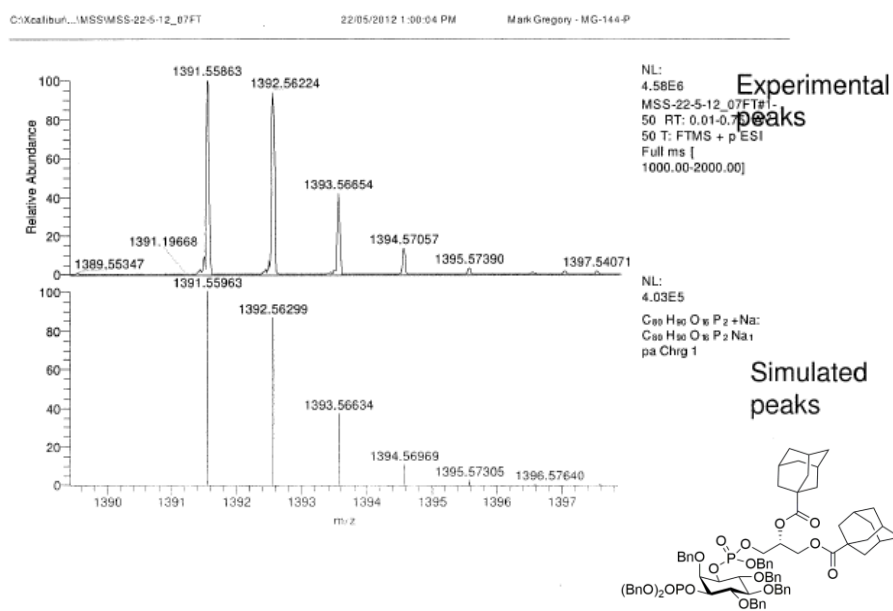
¹³C NMR



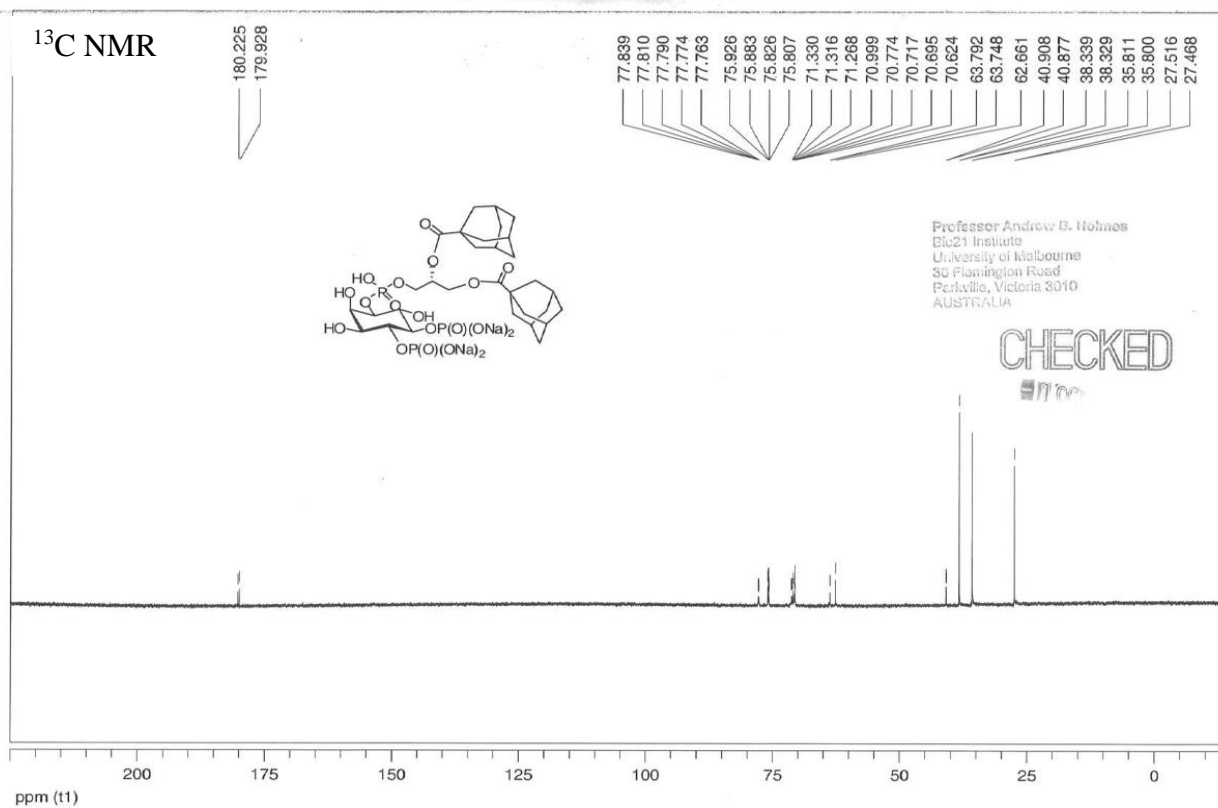
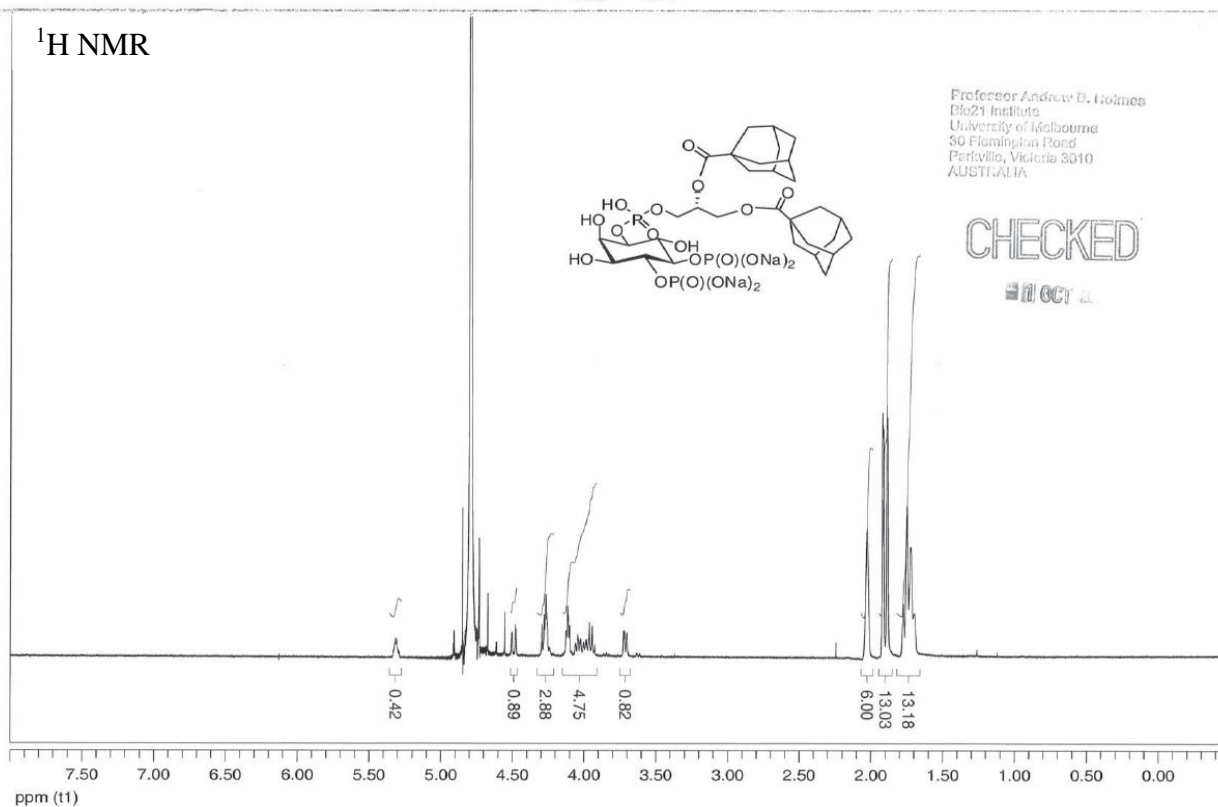
³¹P NMR



HRMS



1D-2,3,6-Tri-hydroxy-myo-inositol-[1',2'-di-O-adamantanecarbonyl-glycer-3'-yl phosphate] 4,5-bisphosphate (10)

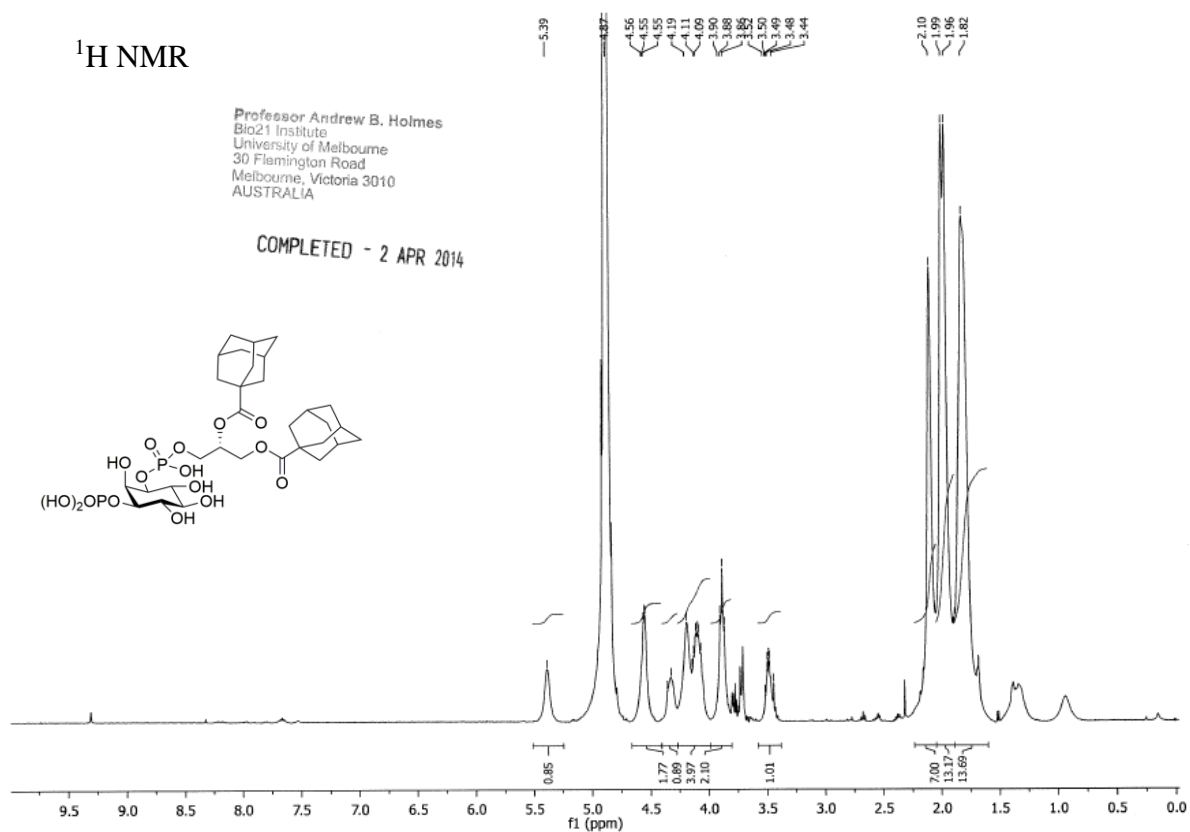


1D-2,4,5,6-Tetra-hydroxy-myo-inositol-[1',2'-di-O-adamantanecarbonyl-glycer-3'-yl phosphate] 3-phosphate (II)

¹H NMR

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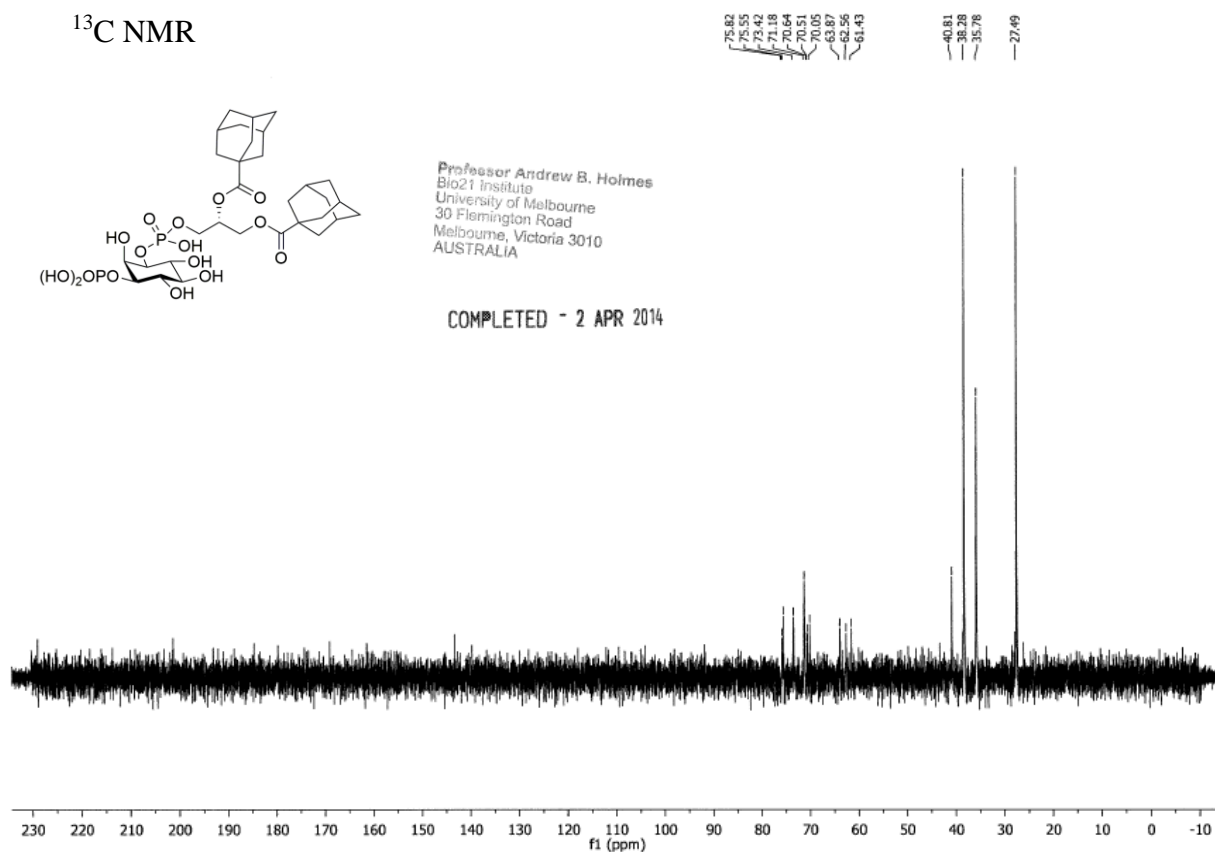
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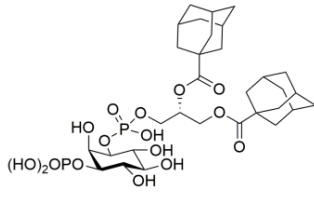
¹³C NMR

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COMPLETED - 2 APR 2014



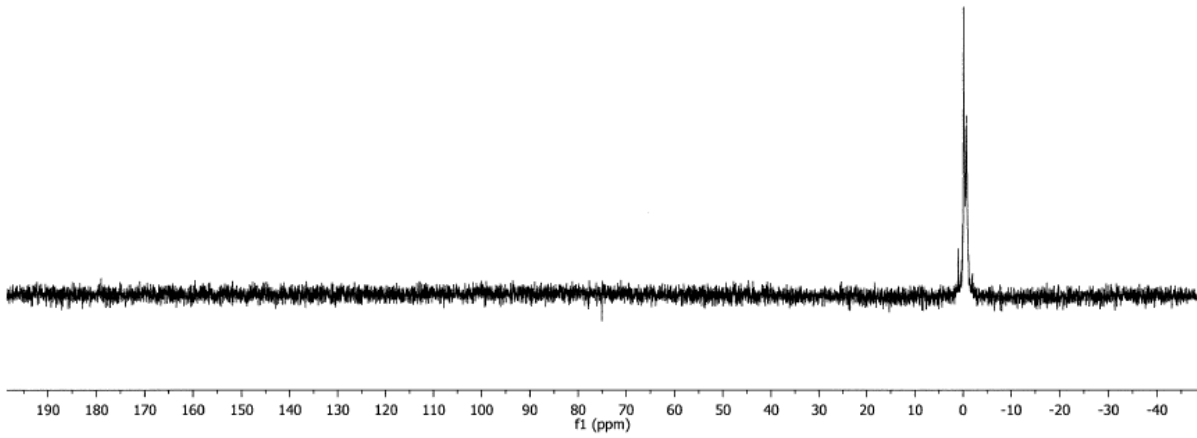
³¹P NMR



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0.35
 0.90



HRMS

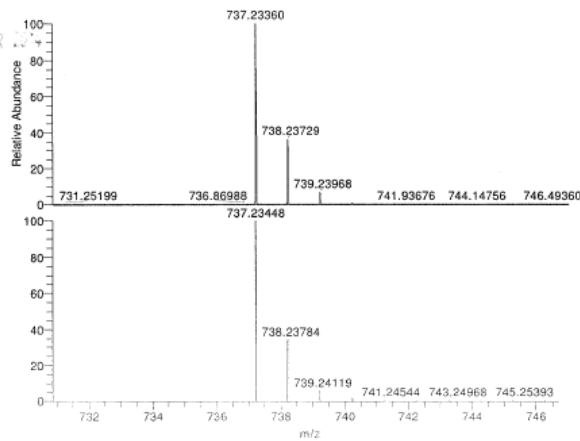
COMPLETED - 2 APR 2014

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Mark Gregory - MG-146-P

COMPLETED - 2 APR 2014



Experimental peaks

NL:
 3.83E5
 MSS-29-5-12_08FT#1-
 41 RT: 0.01-0.08
 41 T: FTMS - p ESI
 Full ms [
 500.00-1000.00]

Simulated peaks

NL:
 6.85E5
 C₃₁H₄₈O₈P₂+H:
 C₃₁H₄₇O₈P₂
 pa Chrg -1

