

Electronic Supporting Information

Synthesis and Biological Evaluation of Phosphatidylinositol Phosphate Affinity Probes

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^a Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK.

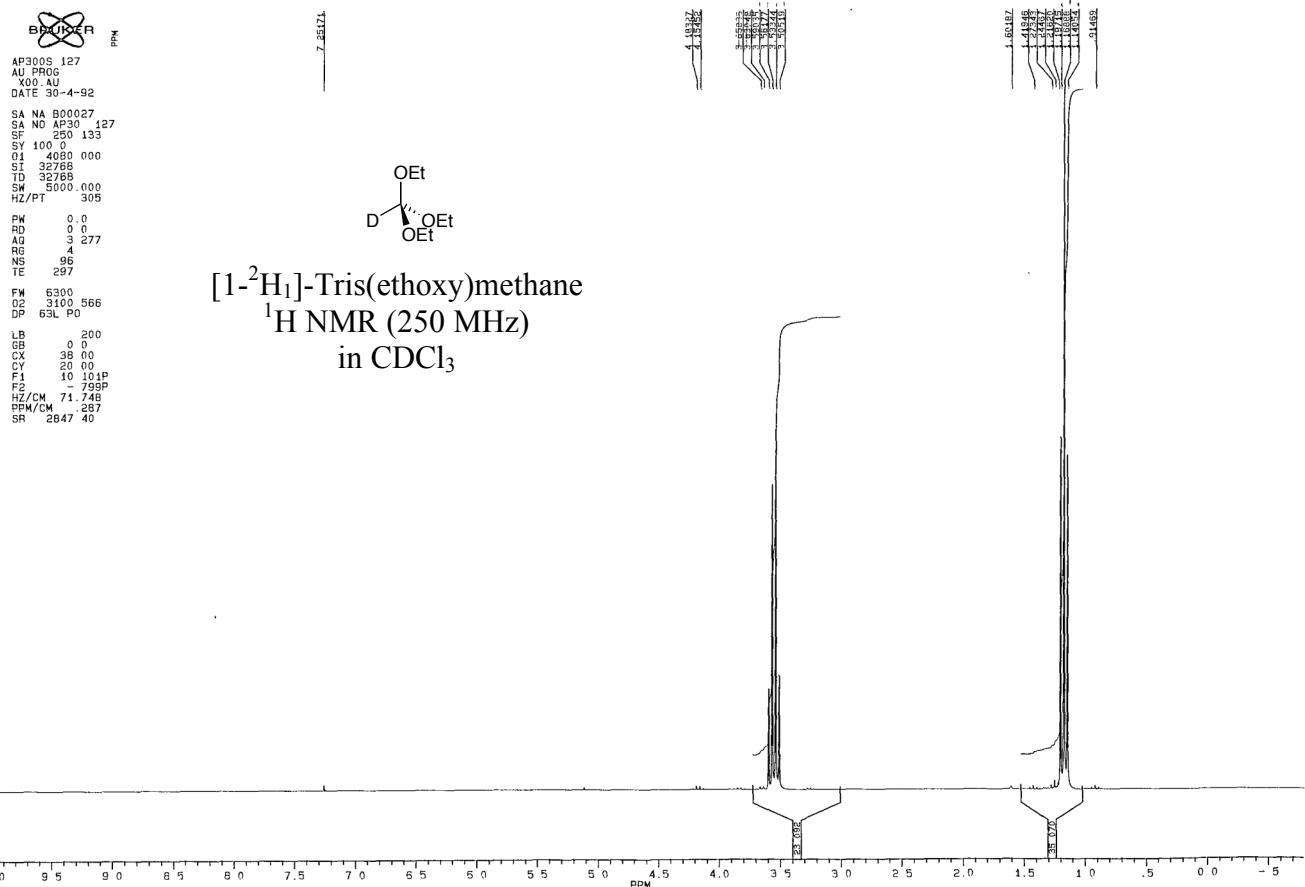
^b School of Chemistry, Bio21 Institute, University of Melbourne, Building 102, 30 Flemington Road, Parkville, Victoria 3010, Australia

^c Ludwig Institute for Cancer Research, Melbourne Tumour Biology Branch, Royal Melbourne Hospital, Parkville, Victoria, 3052, Australia

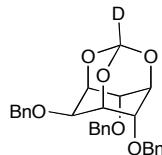
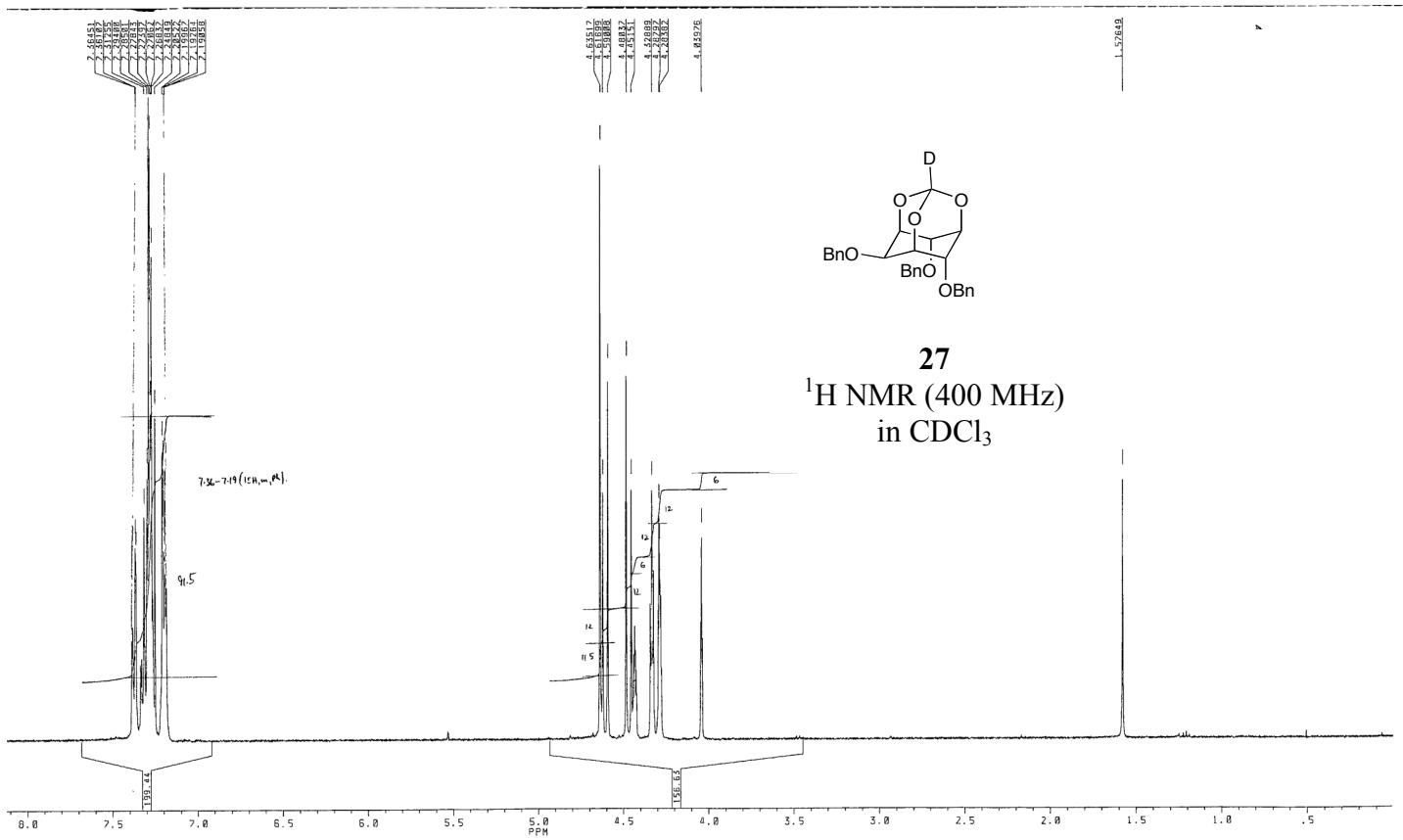
^d Babraham Institute, Department of Signalling, Inositide Laboratory, Cambridge, CB2 4AT, UK

NMR Spectra (¹H, ¹³C or ³¹P) for the following compounds:

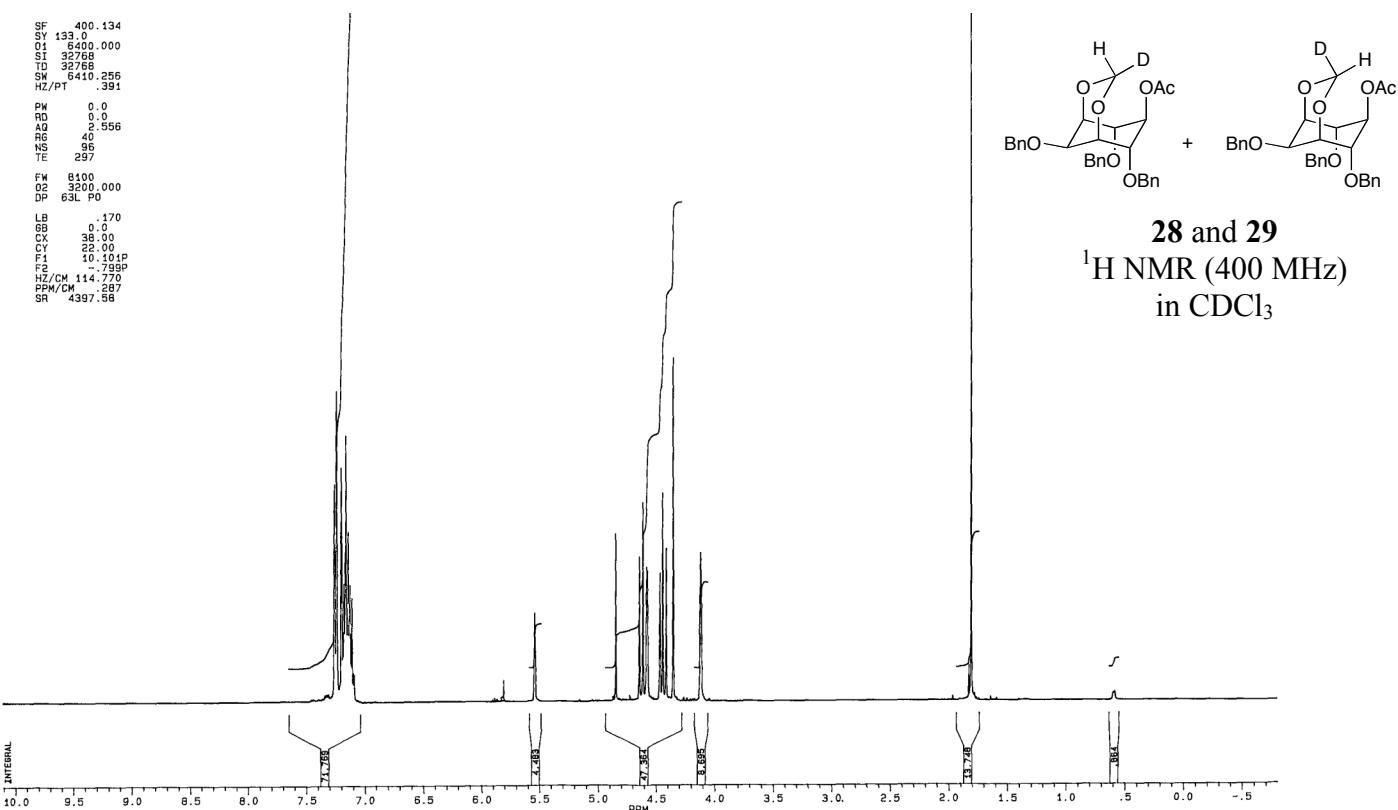
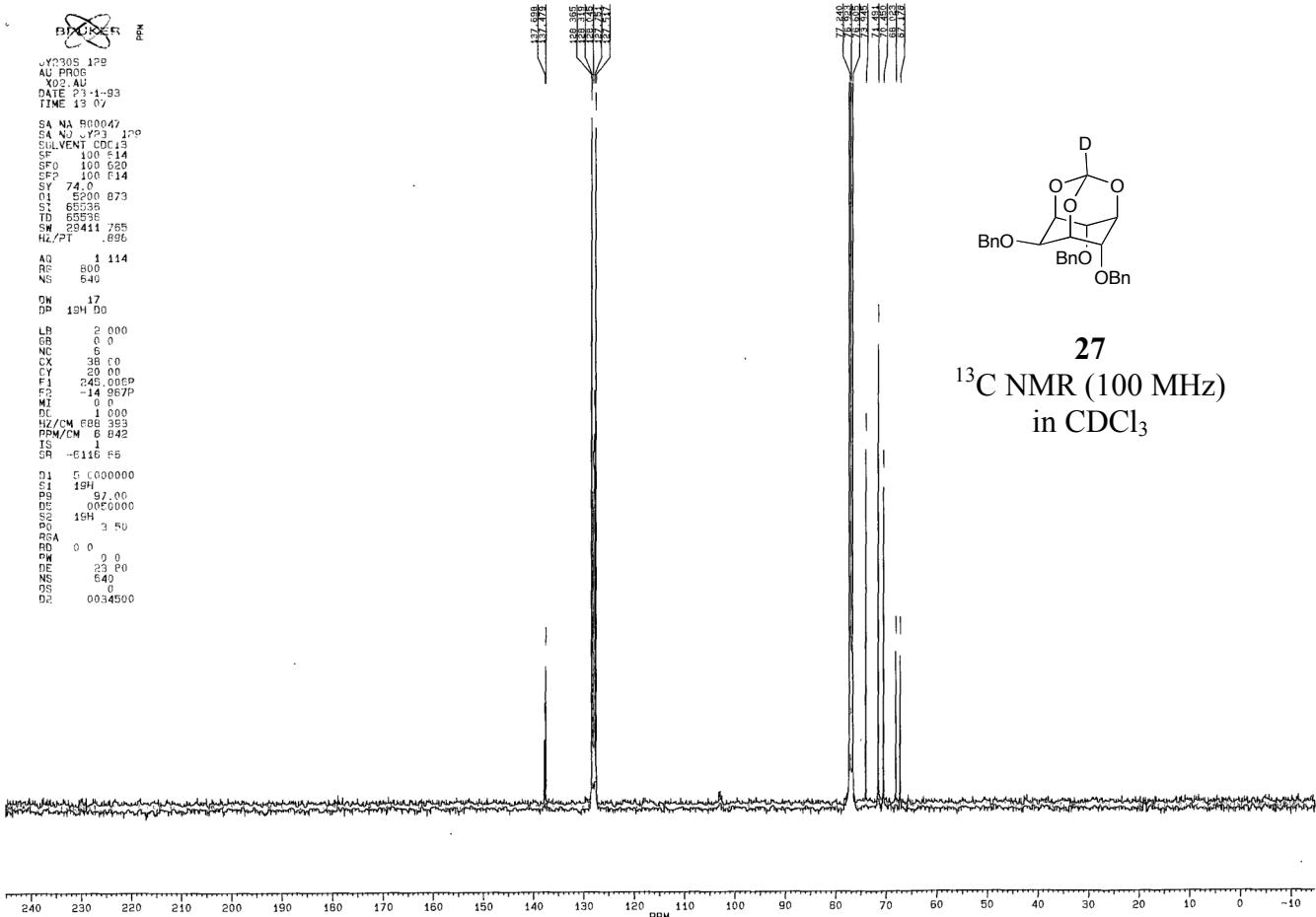
[1-²H]-Tris(ethoxy)methane, **27-29, S2, 39-42, S5, 44, 49, 51, 54-59, 61, 71, S6, 62-67, 75, 77, 81, 83, 90, 92, S8, S9, 102, 105, 108, 106, 109, S10, S11, 104, 107, 110.**



[1-²H₁]-Tris(ethoxy)methane
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in CDCl₃



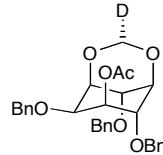
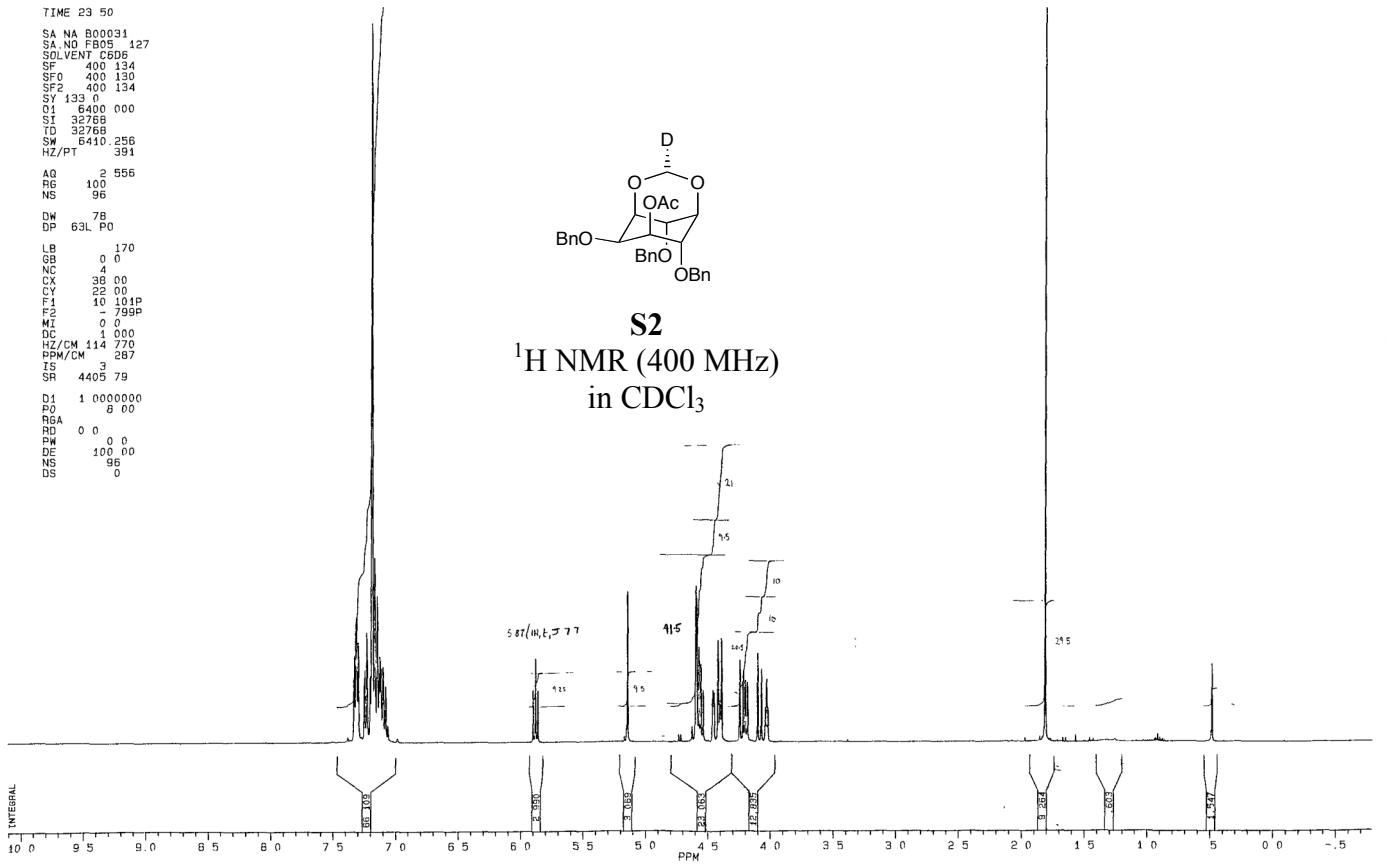
27
¹H NMR (400 MHz)
 in CDCl₃



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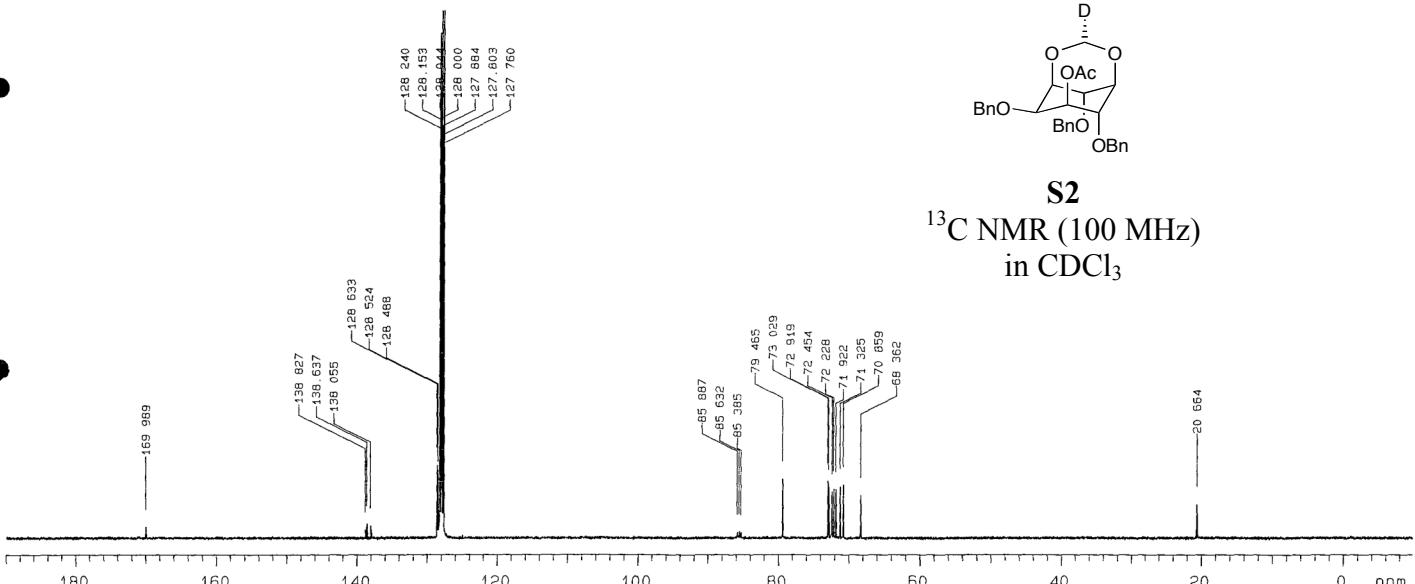
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S2

¹³C NMR (100 MHz)

in CDCl₃

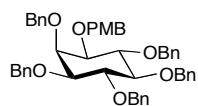


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 Date May 20 93
 Chemist Simon Grove
 Lab P5PR2

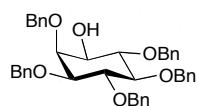
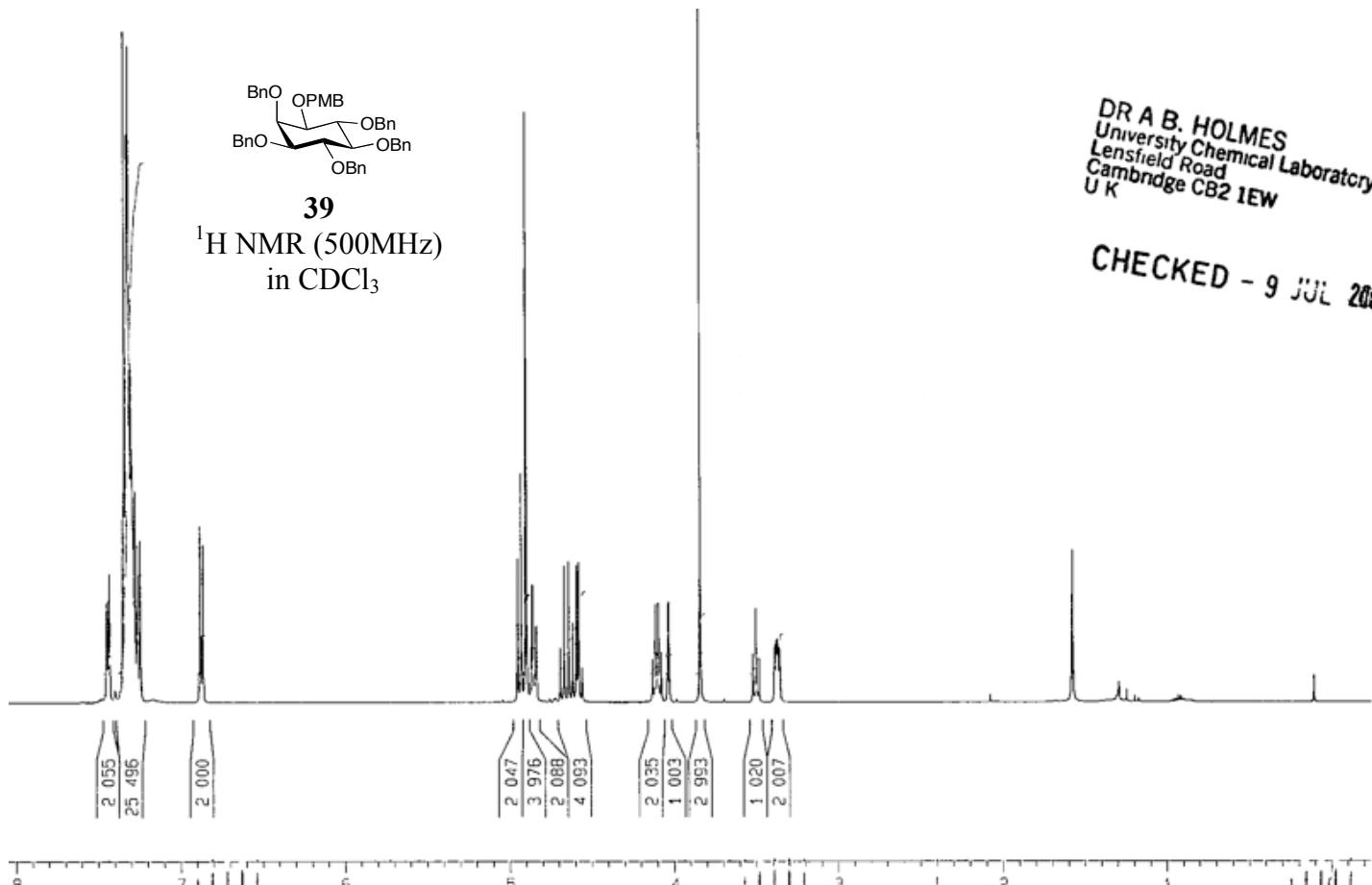


39

^1H NMR (500MHz)
in CDCl_3

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UK

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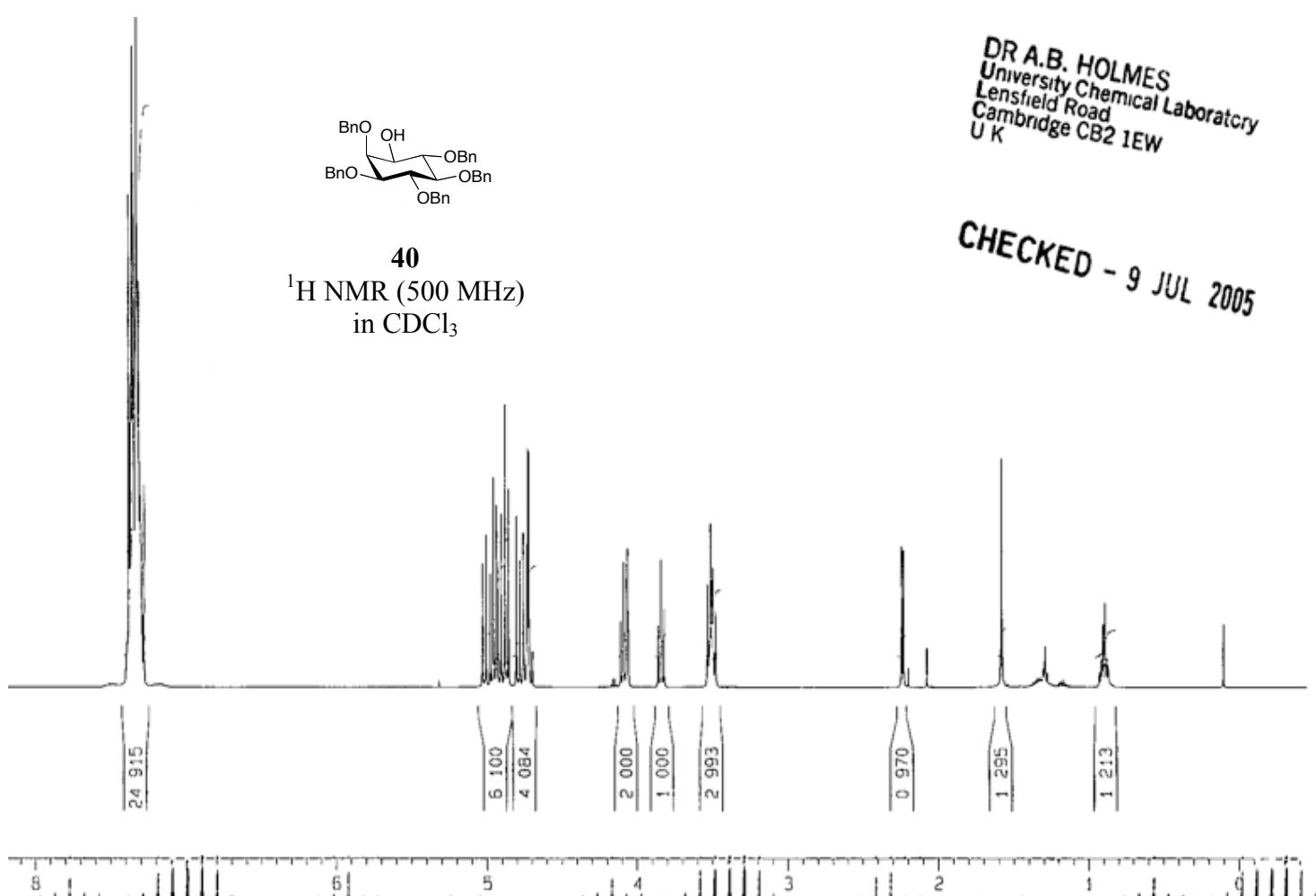


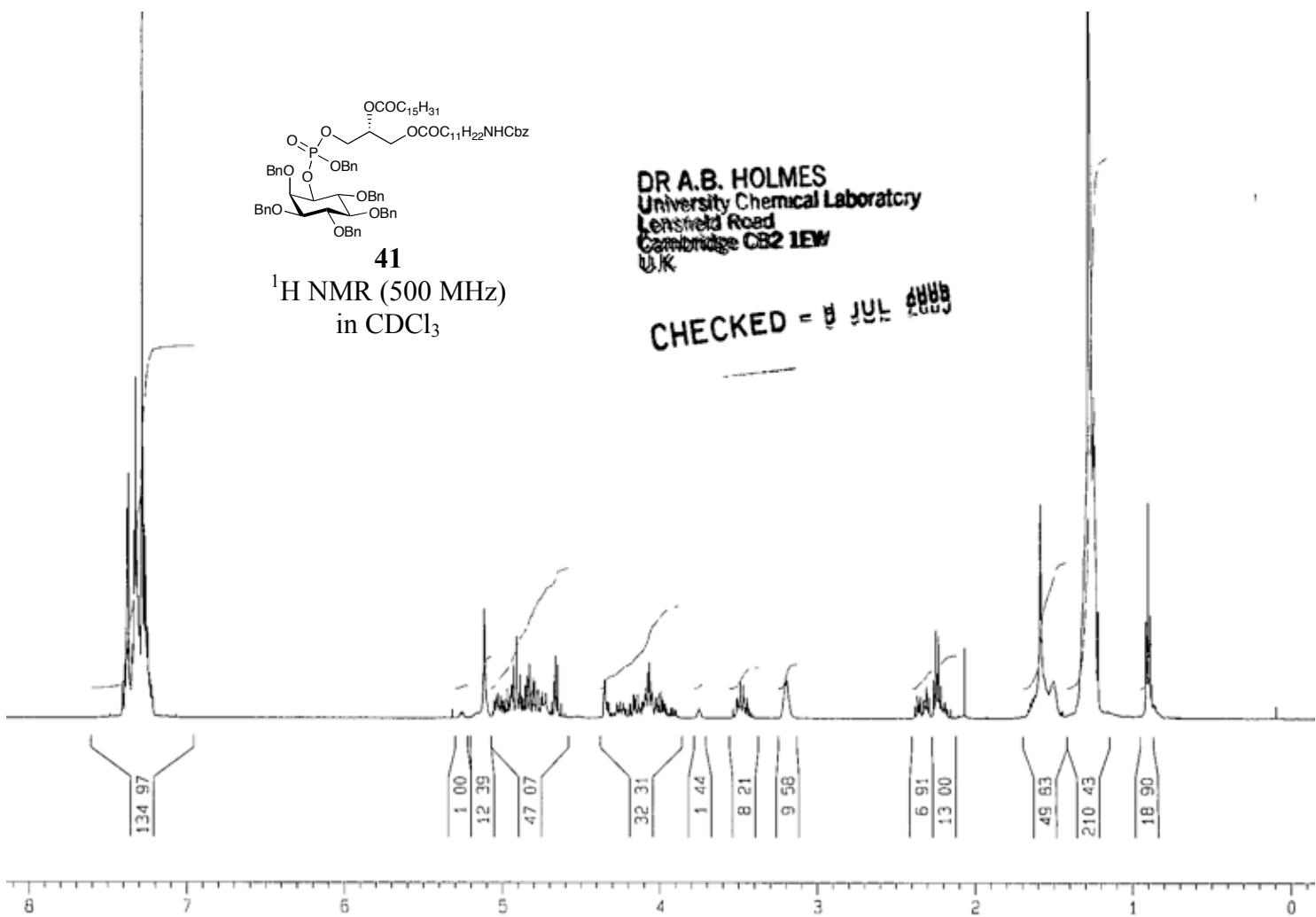
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^1H NMR (500 MHz)
in CDCl_3

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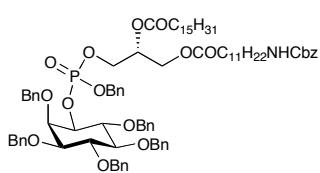
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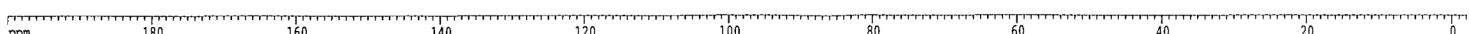


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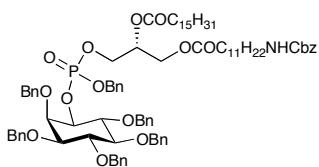


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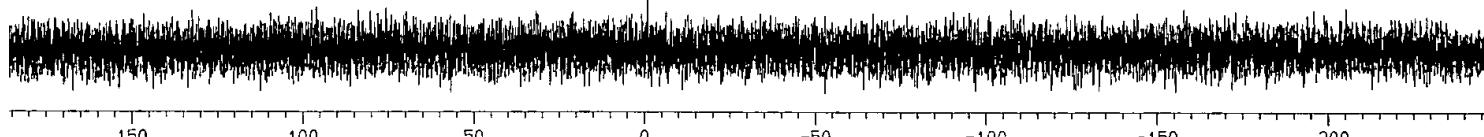


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U.K.

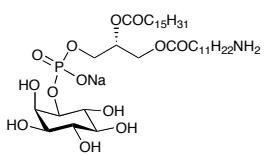
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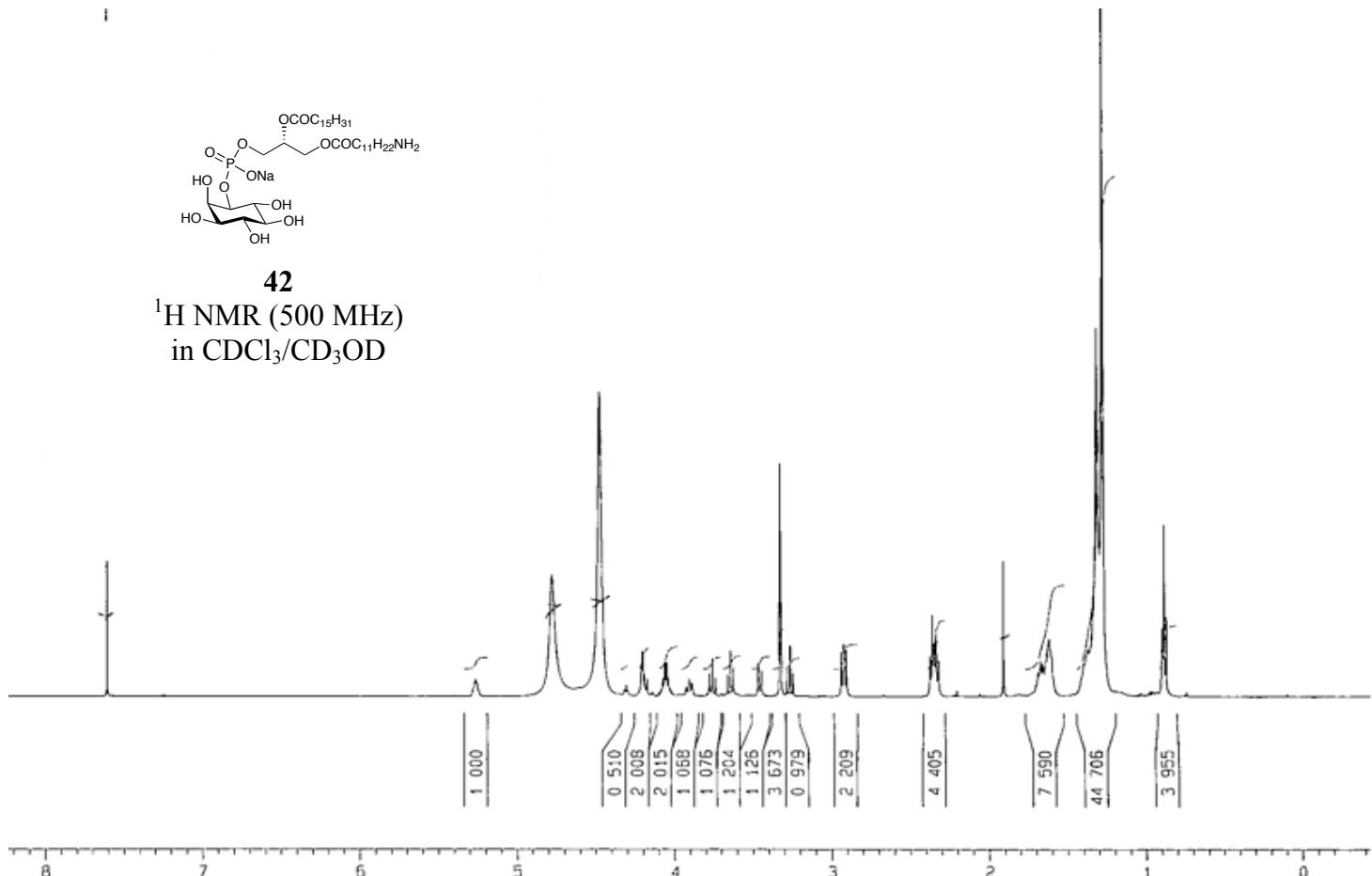
41
 ^{31}P NMR (202 MHz)
in CDCl_3



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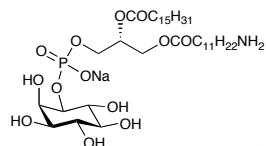


42
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in $\text{CDCl}_3/\text{CD}_3\text{OD}$



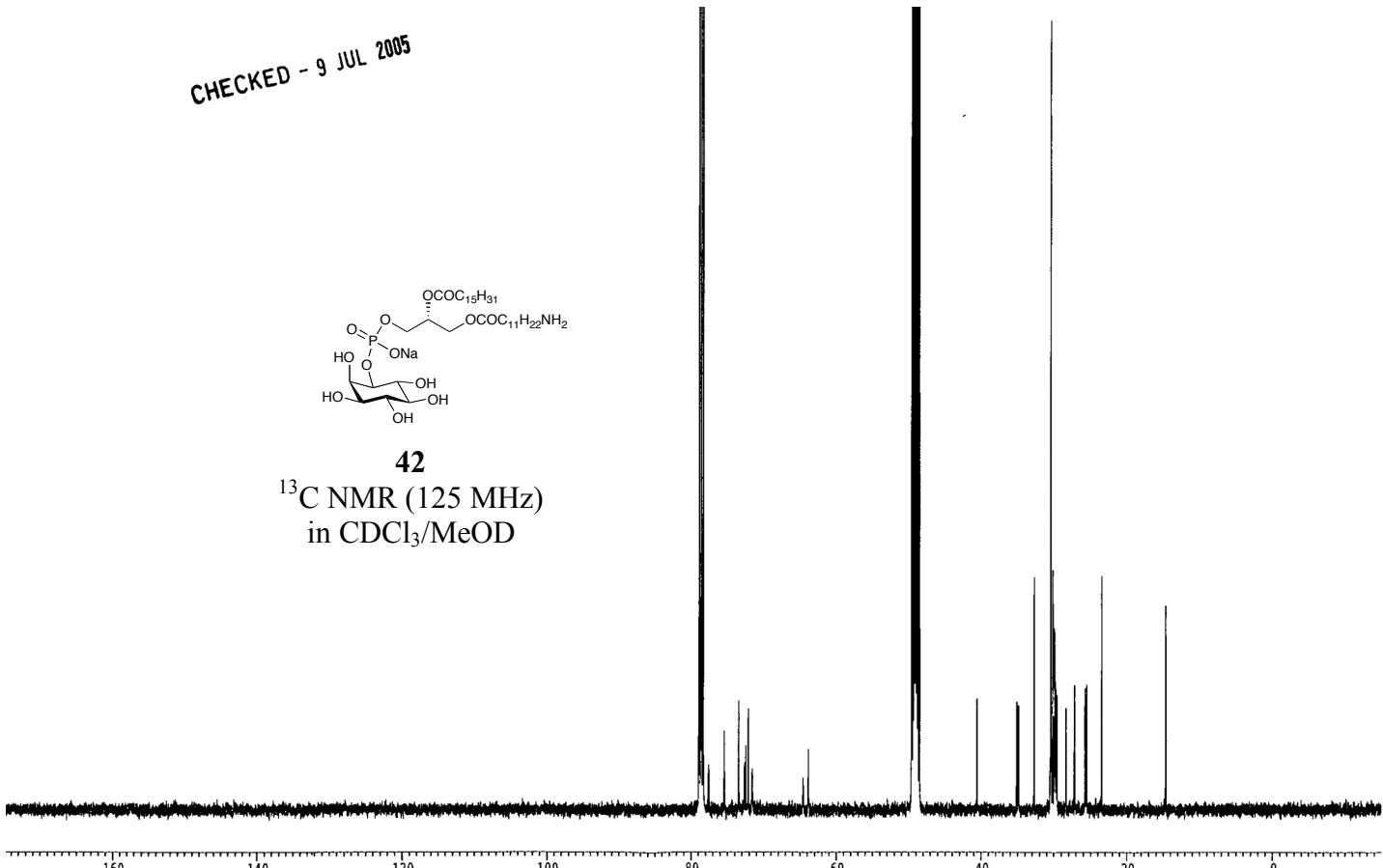
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42

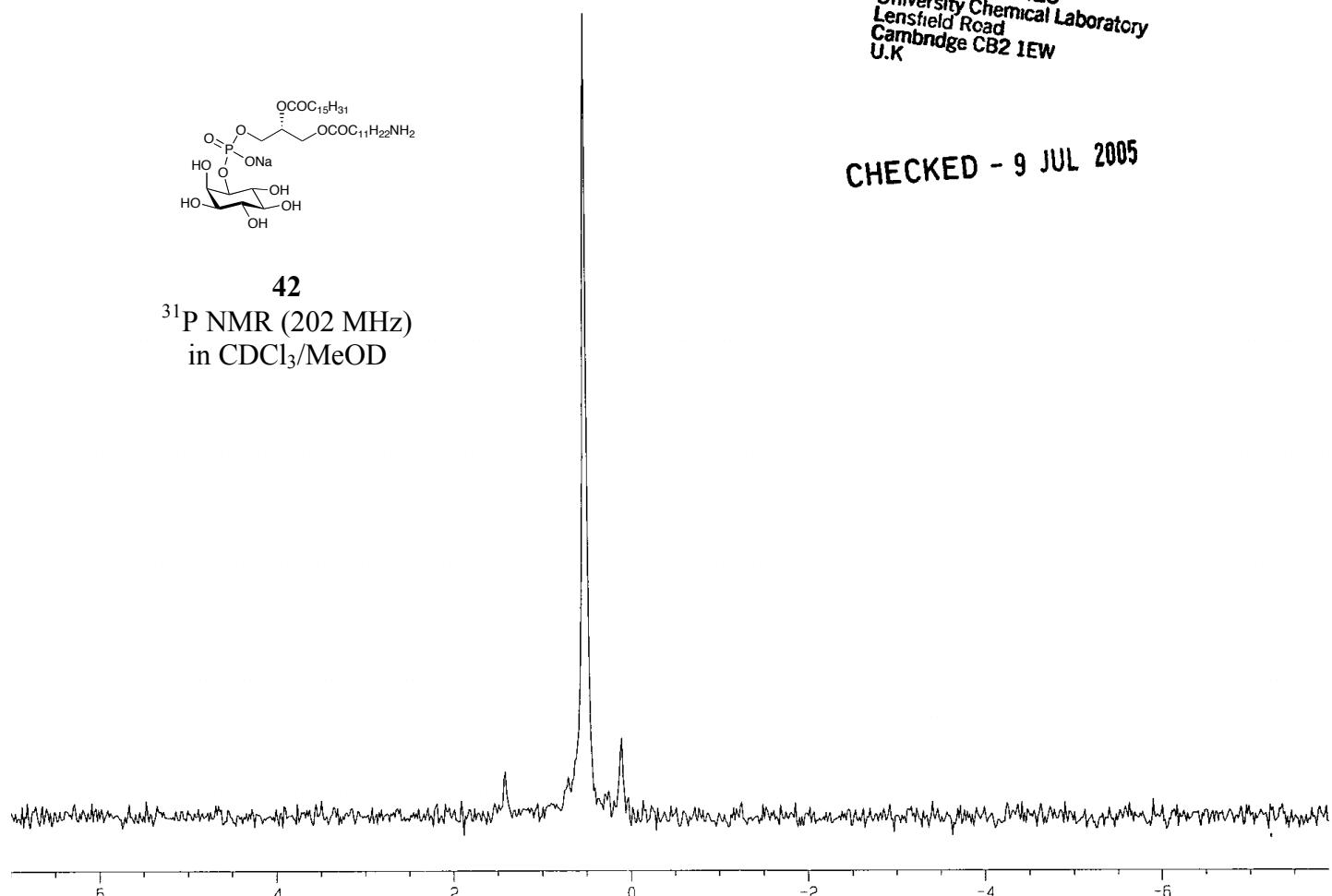
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in $\text{CDCl}_3/\text{MeOD}$

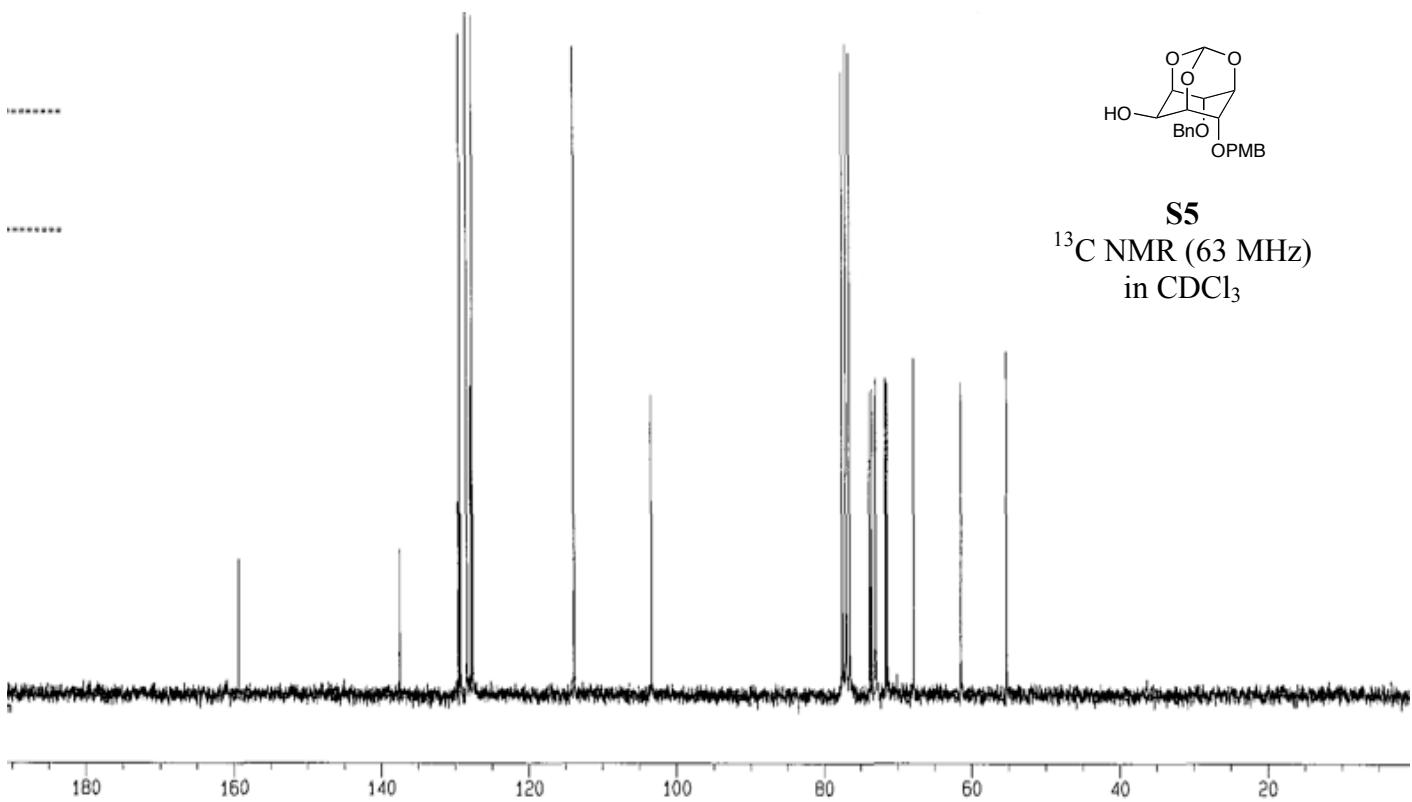
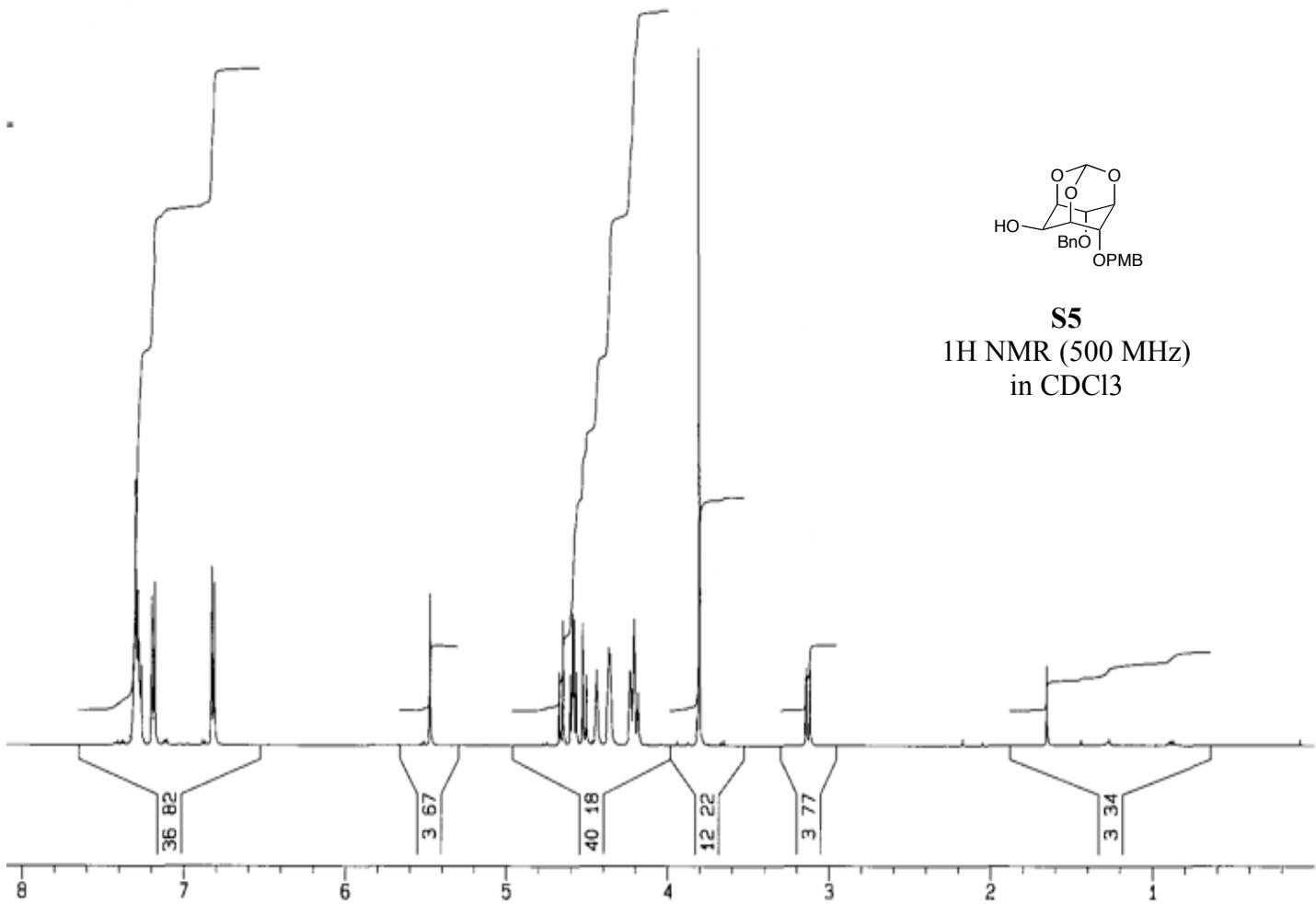


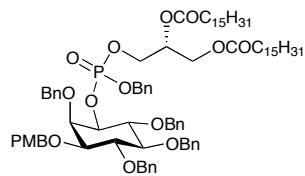
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42

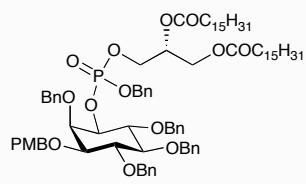
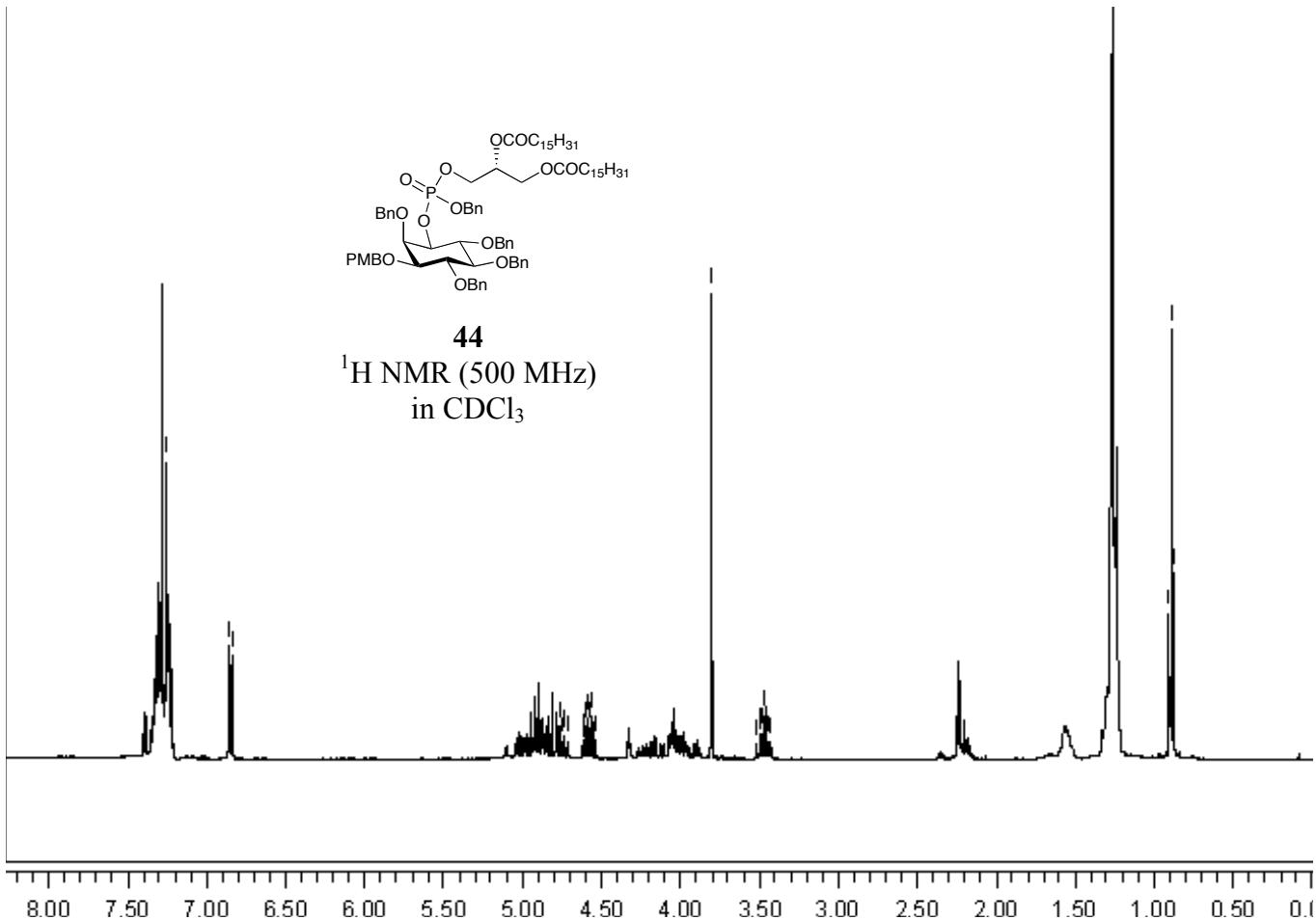
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in $\text{CDCl}_3/\text{MeOD}$



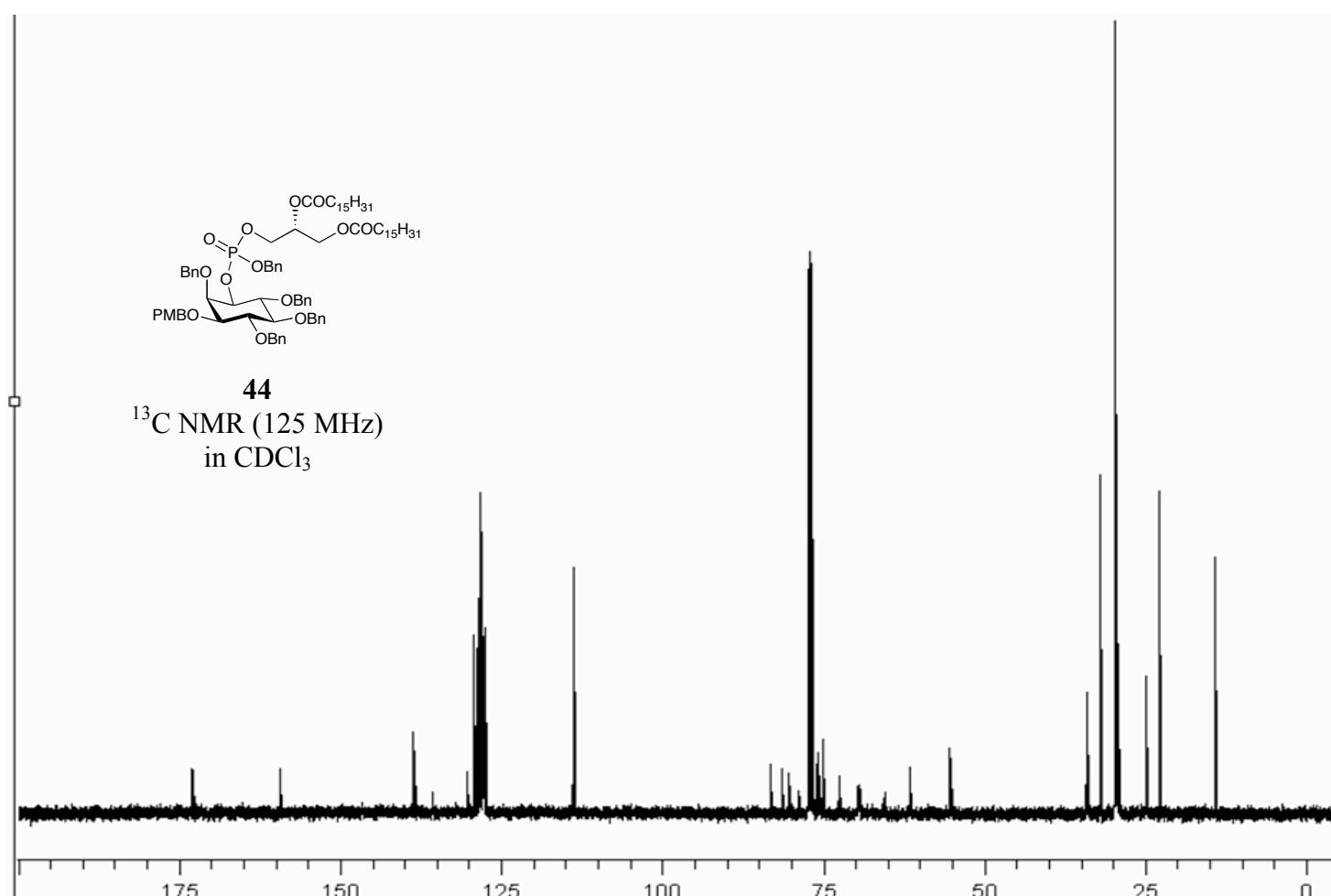


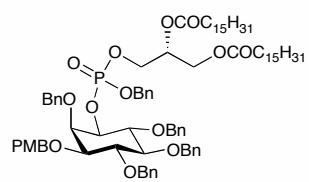


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in CDCl_3



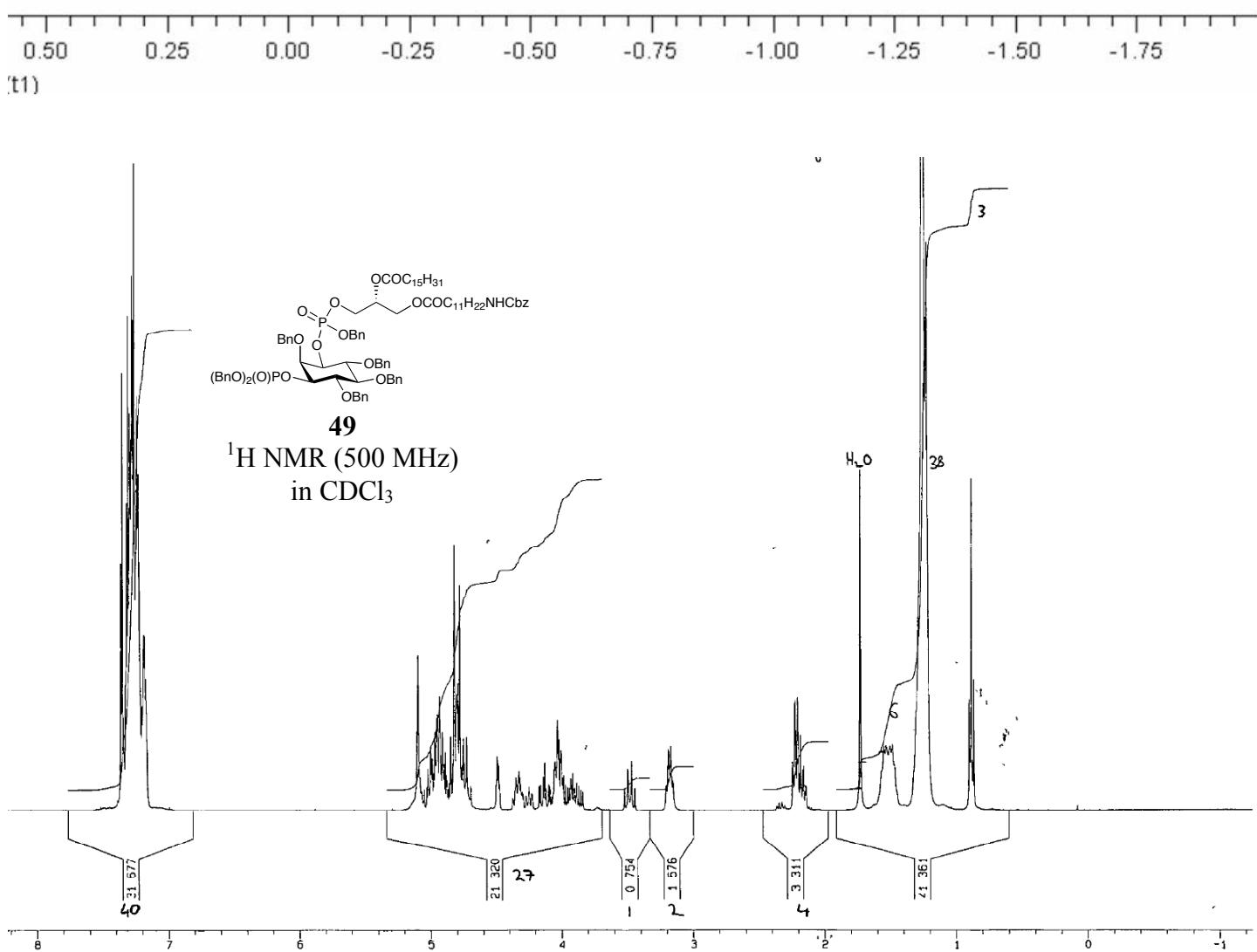
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in CDCl_3

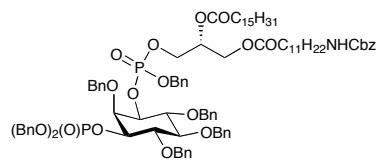




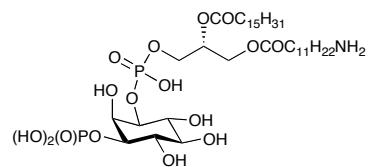
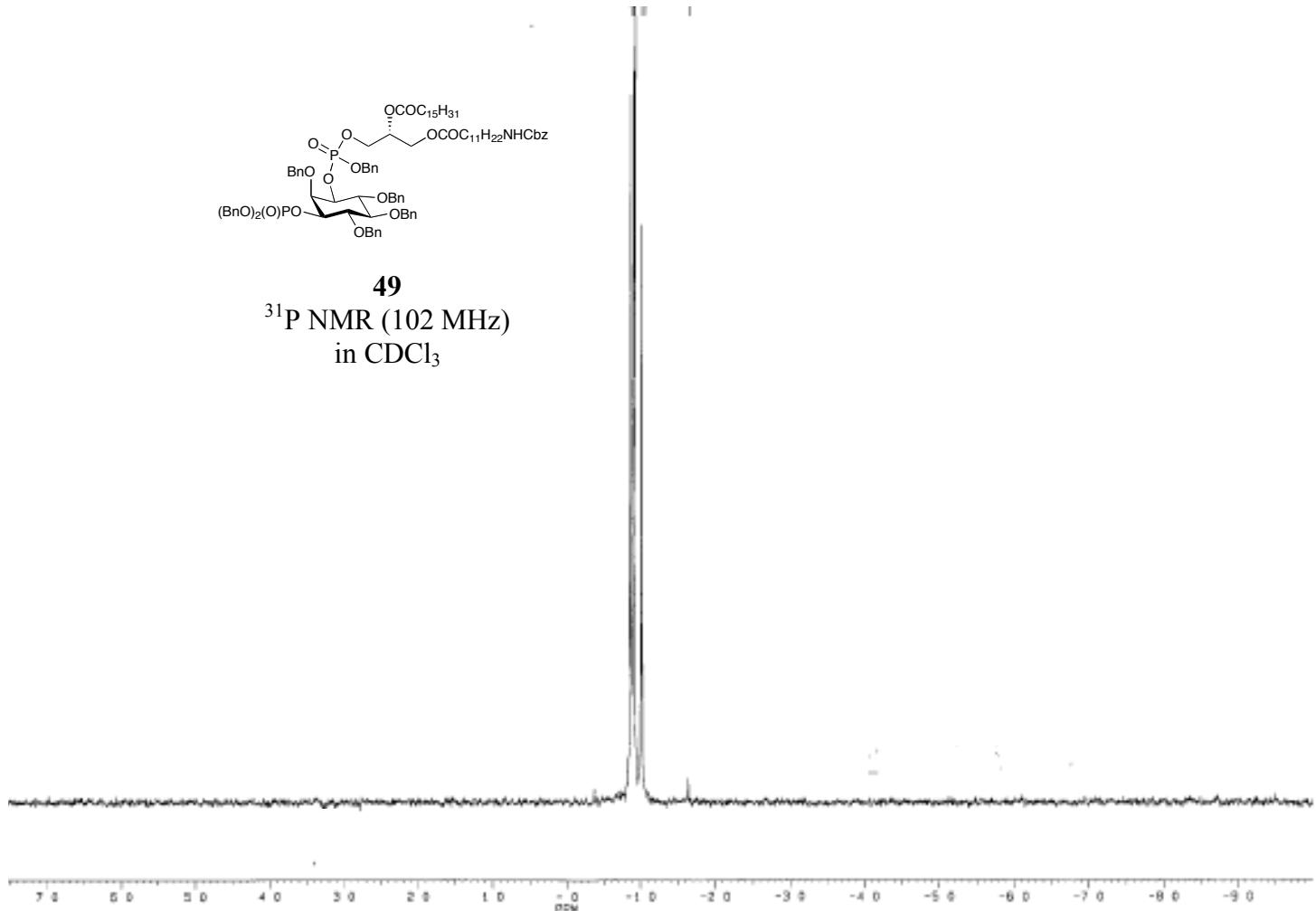
44

³¹P NMR (202 MHz)
in CDCl₃

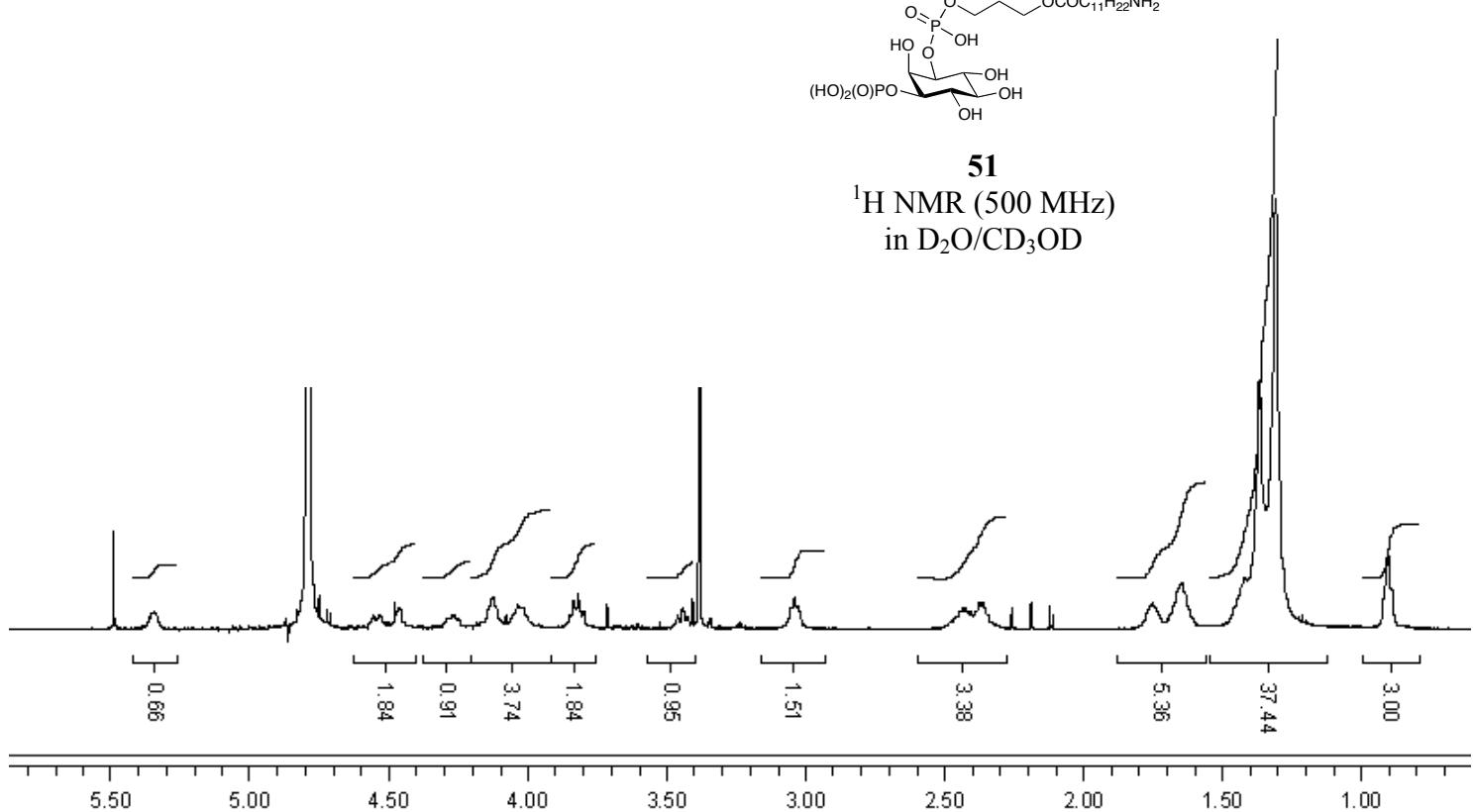


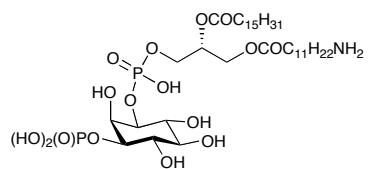


49
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in CDCl_3

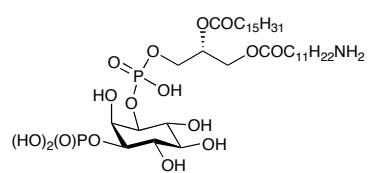
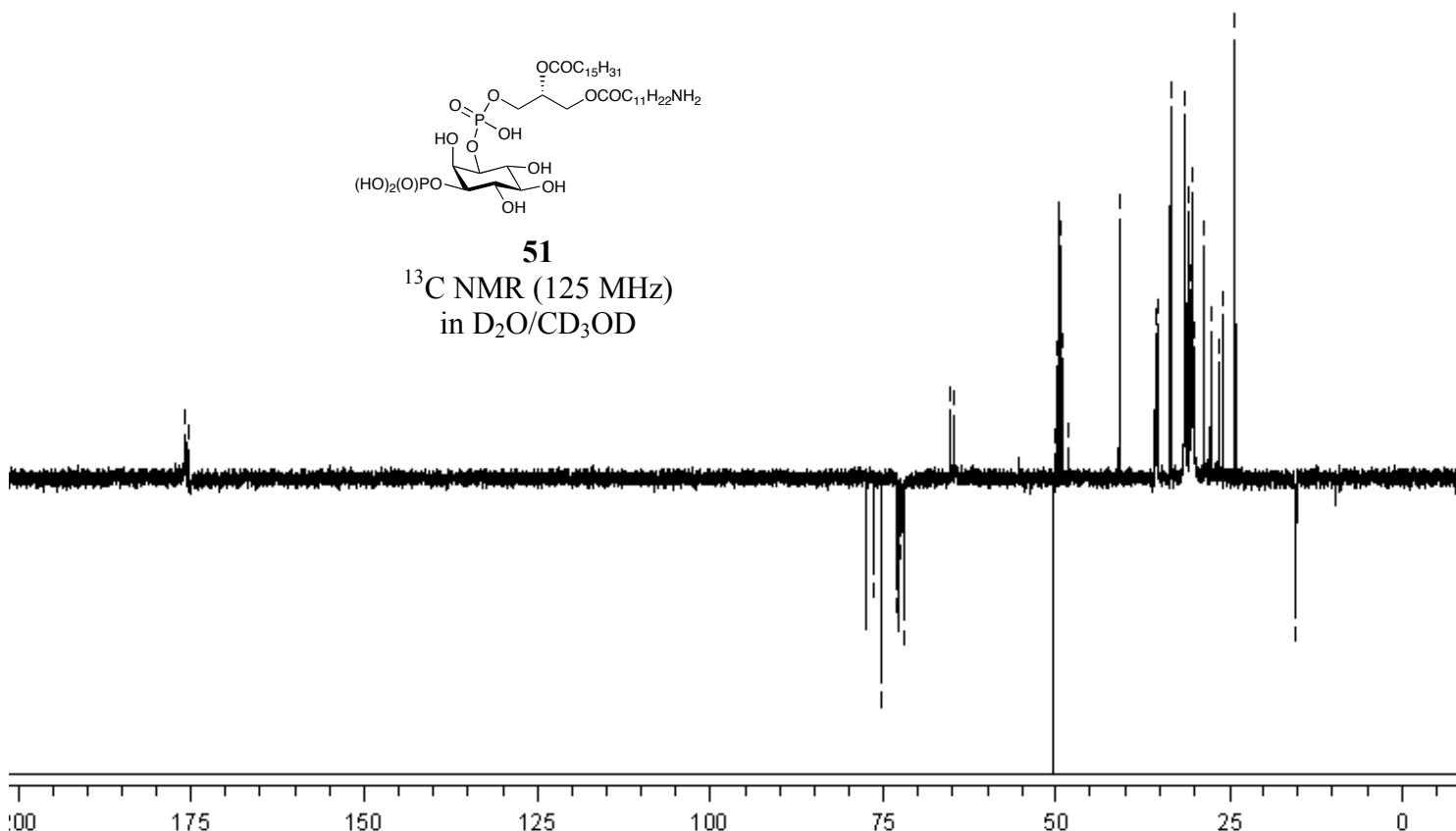


51
 ^1H NMR (500 MHz)
in $\text{D}_2\text{O}/\text{CD}_3\text{OD}$

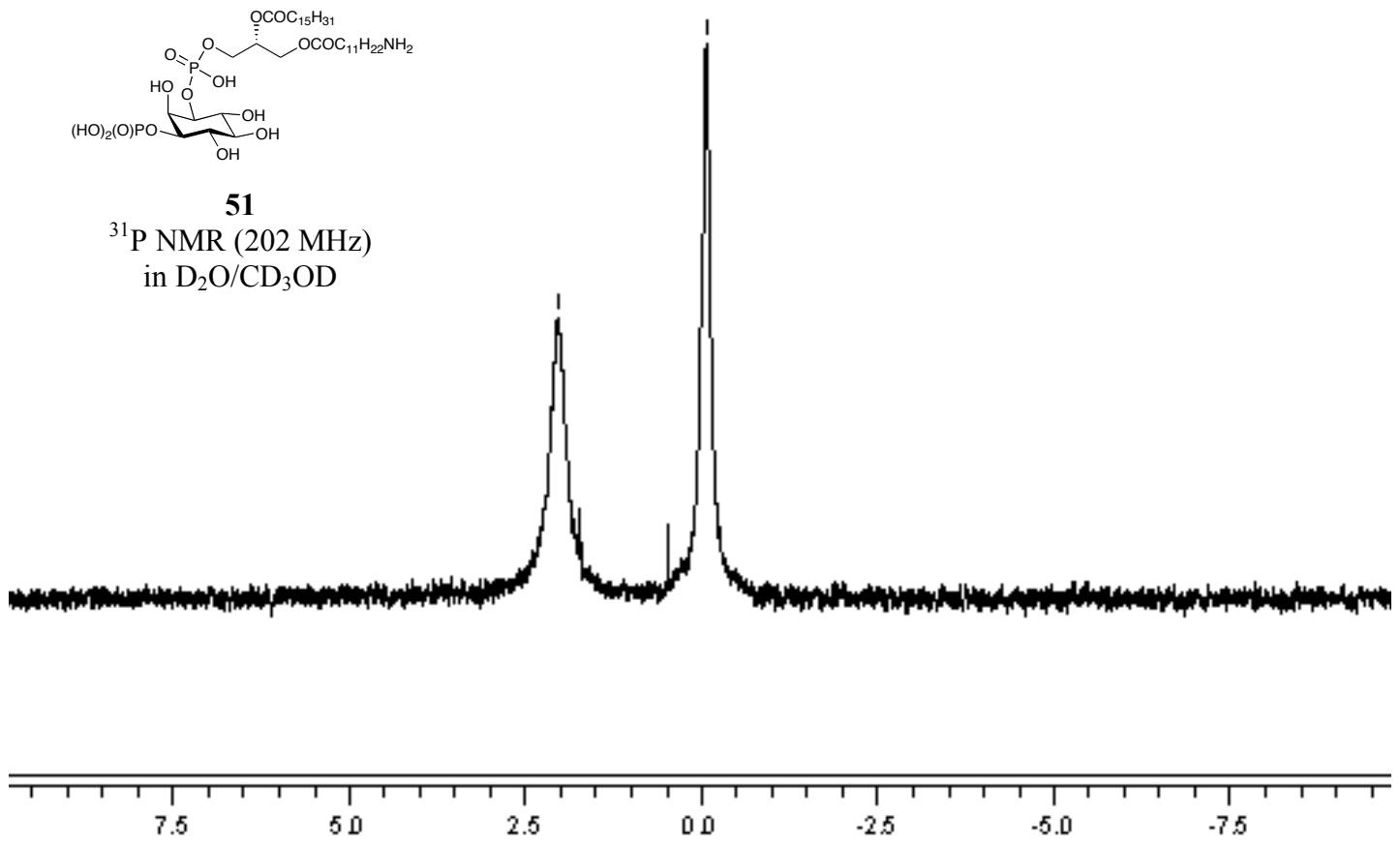


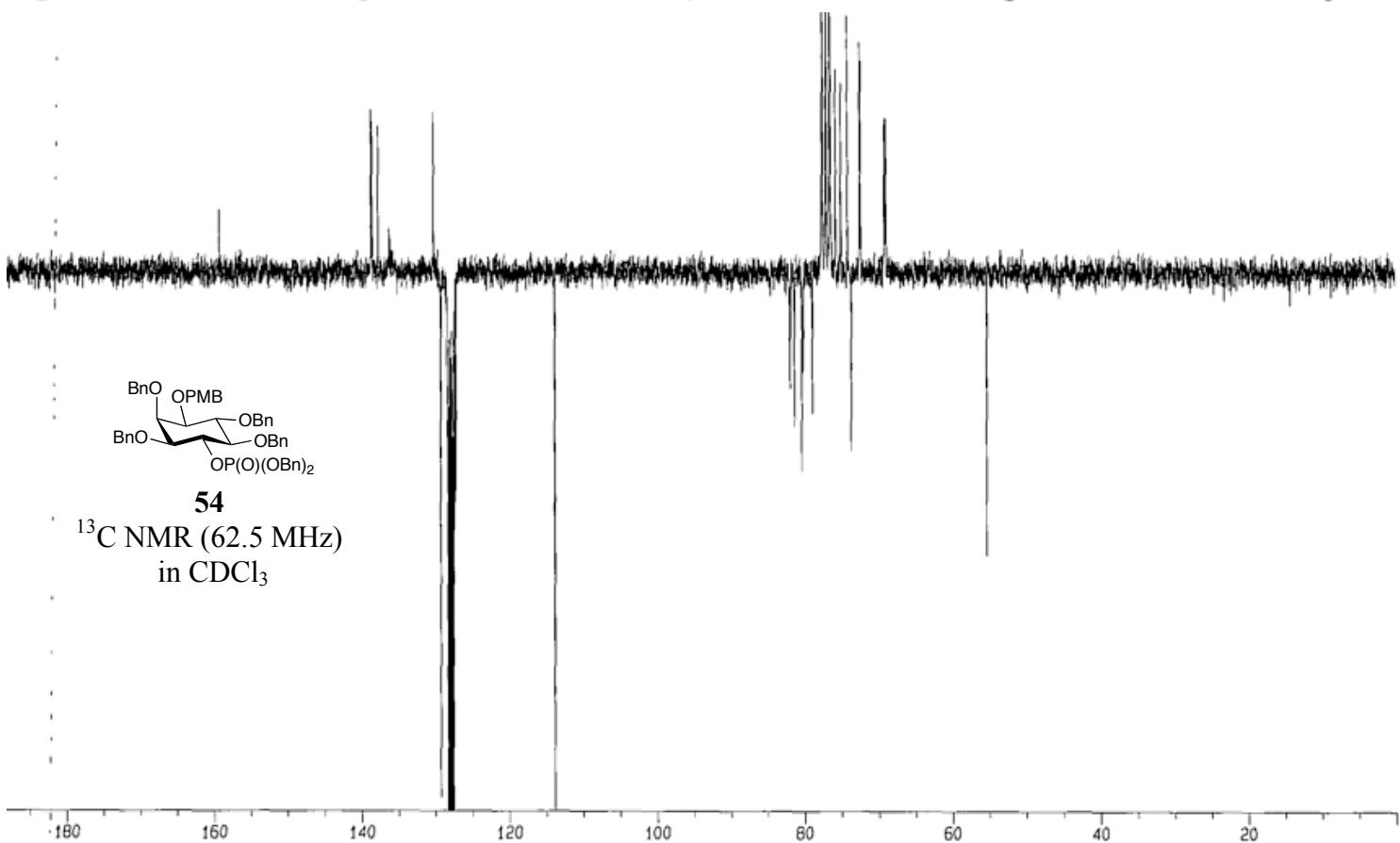
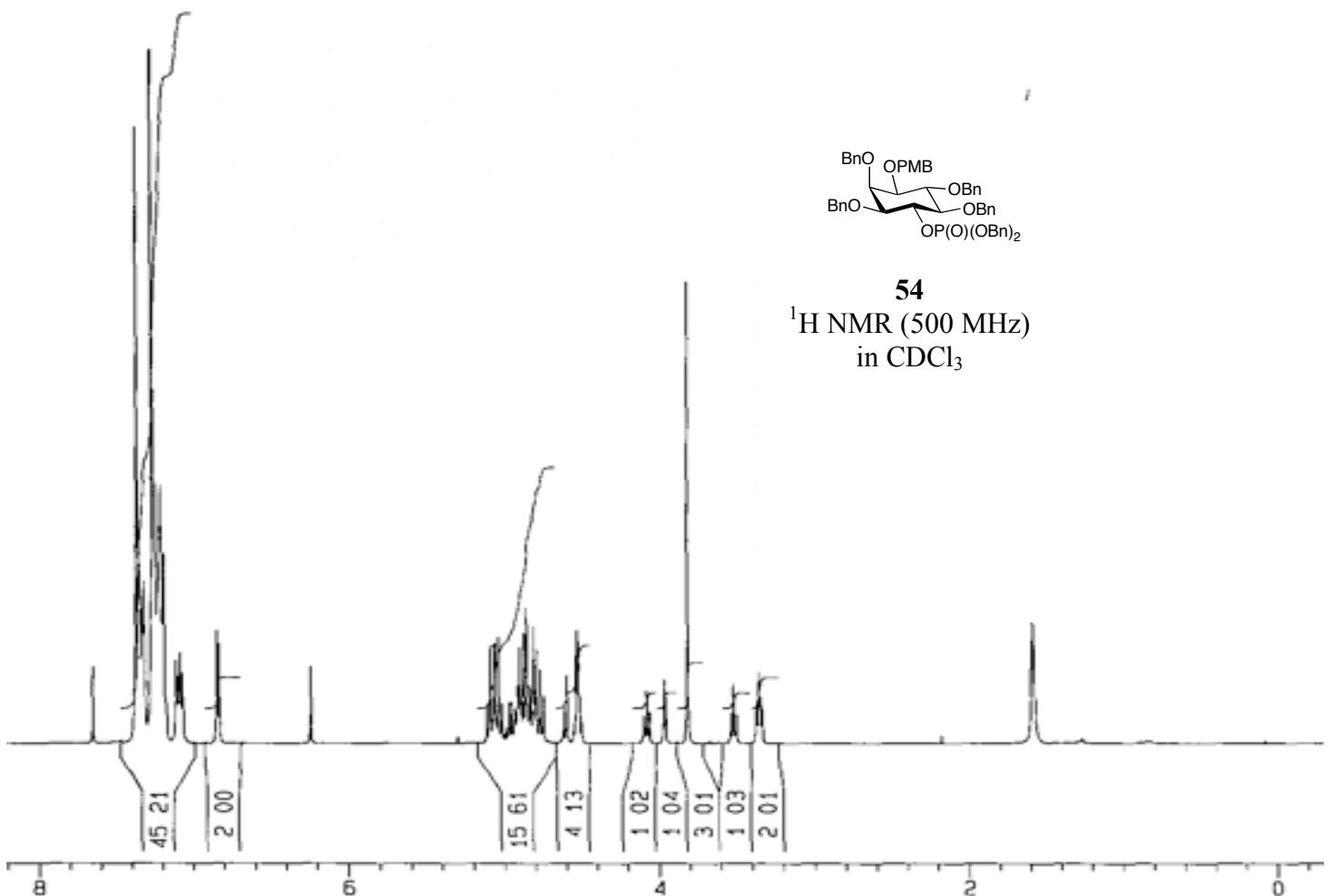


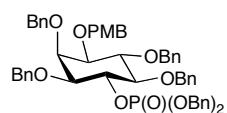
51
 ^{13}C NMR (125 MHz)
in $\text{D}_2\text{O}/\text{CD}_3\text{OD}$



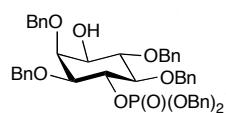
51
 ^{31}P NMR (202 MHz)
in $\text{D}_2\text{O}/\text{CD}_3\text{OD}$



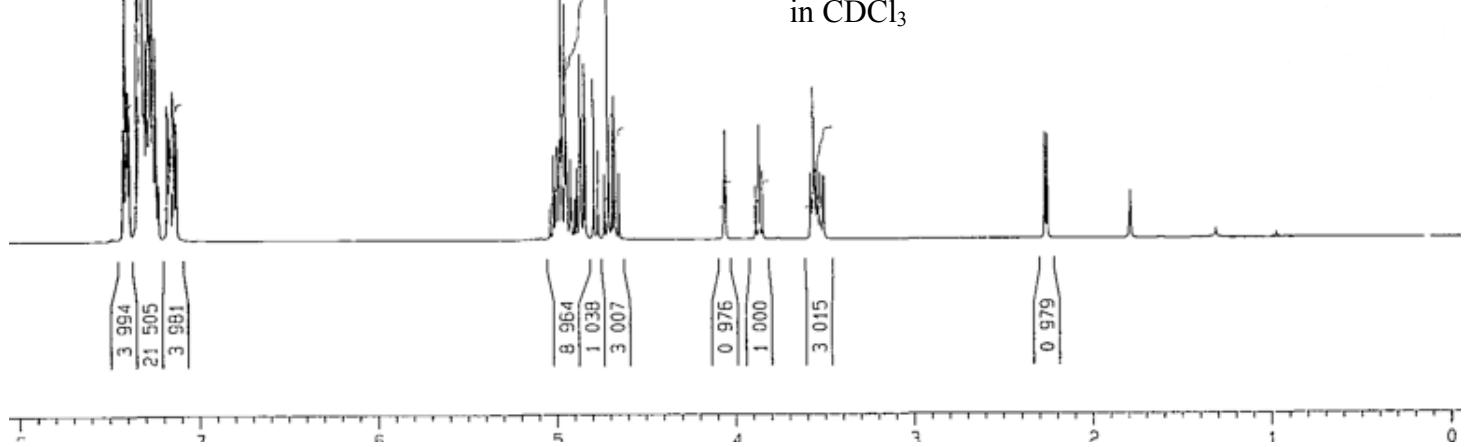




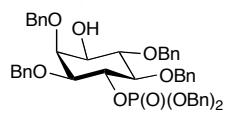
54
³¹P NMR (162 MHz)
in CDCl₃



55
¹H NMR (500 MHz)
in CDCl₃



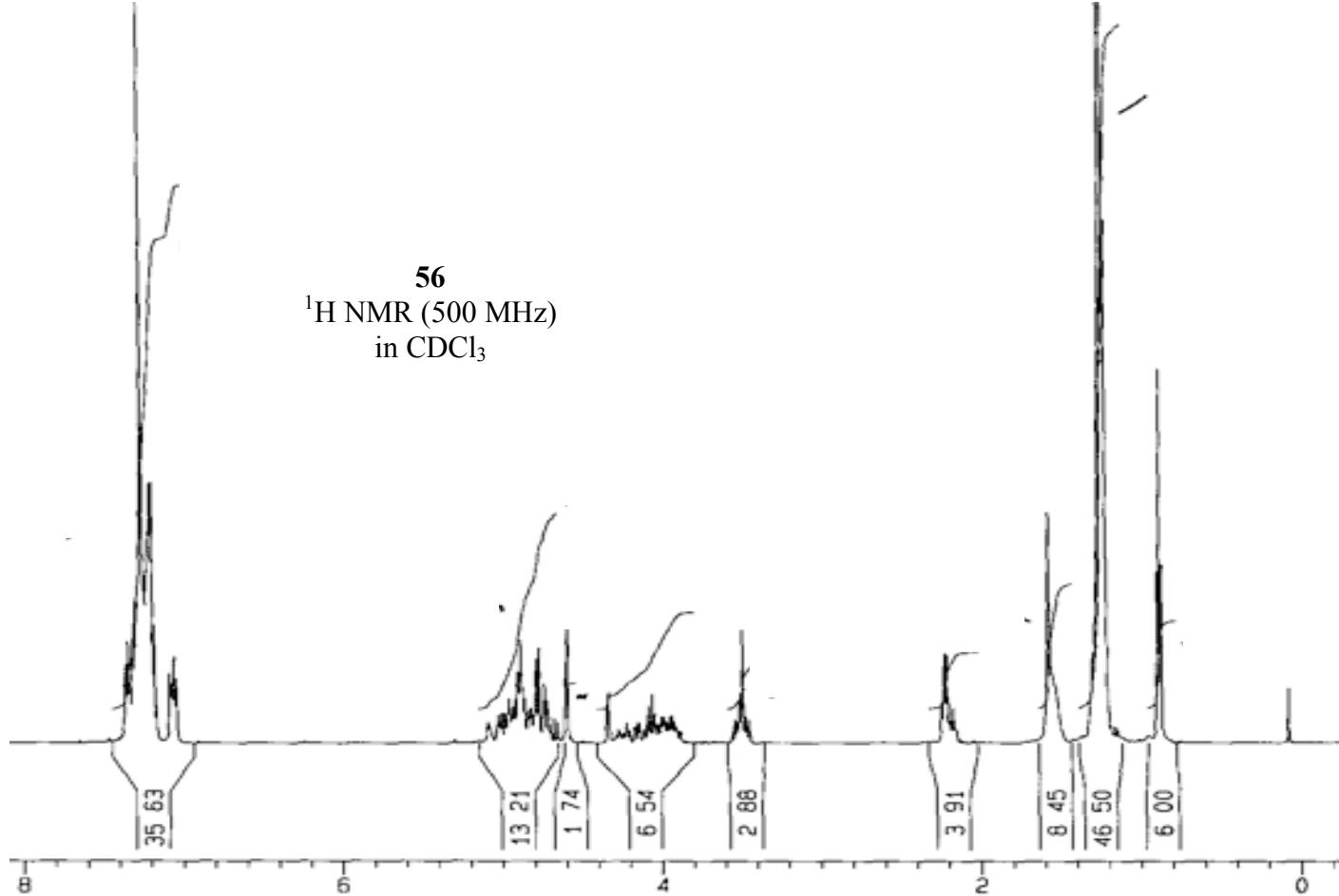
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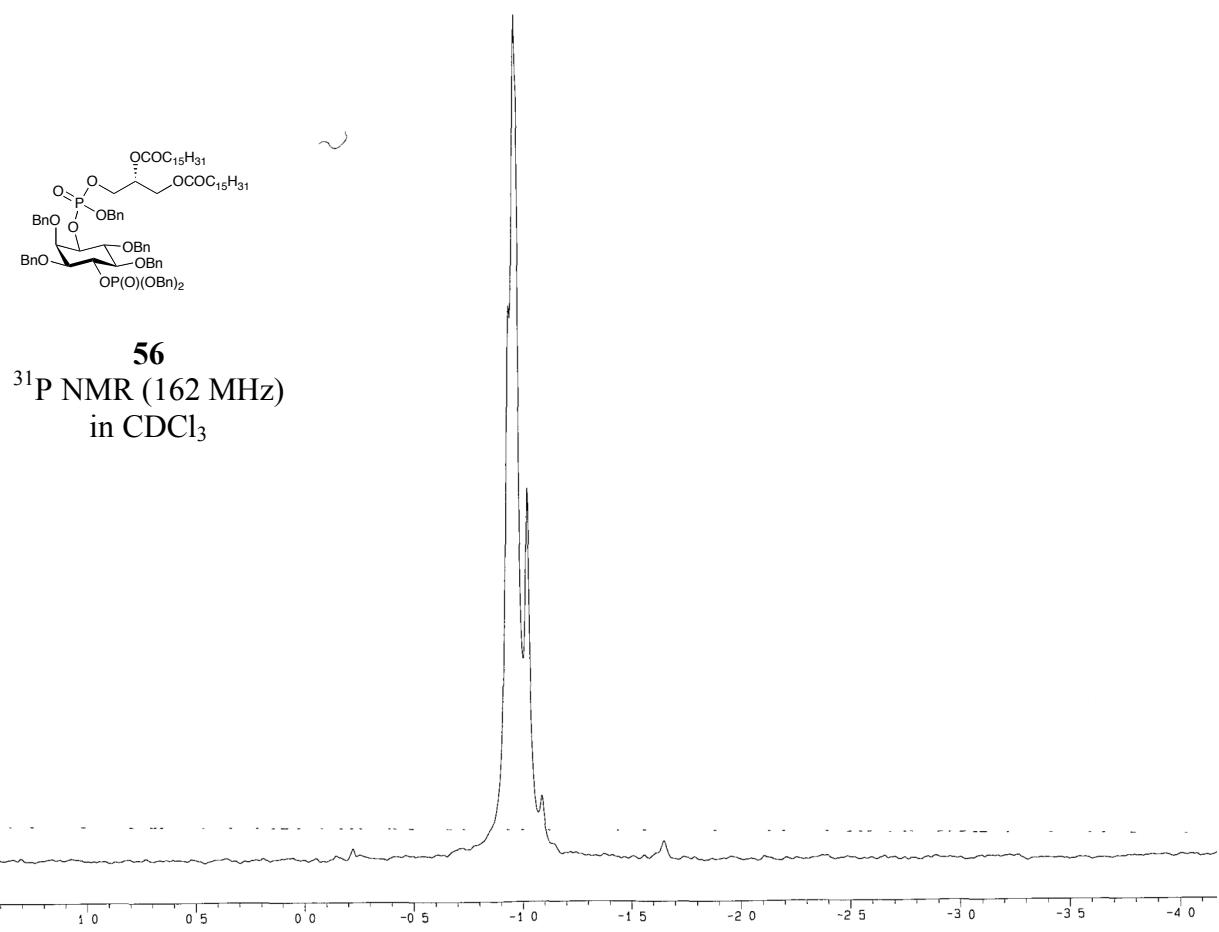
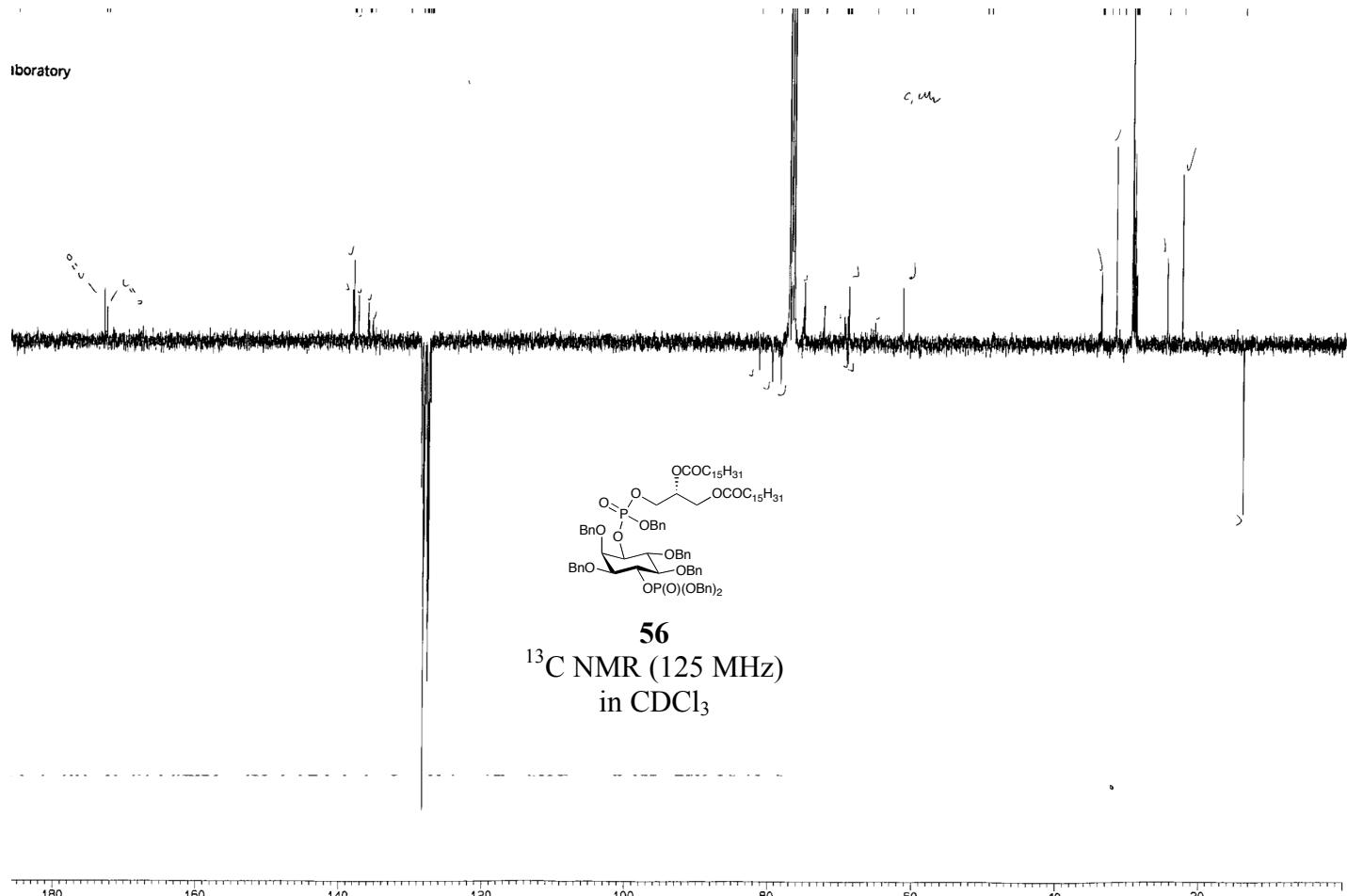


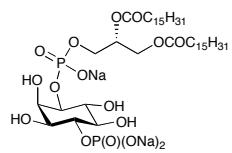
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 ^{31}P NMR (202 MHz)
in CDCl_3



56
 ^1H NMR (500 MHz)
in CDCl_3

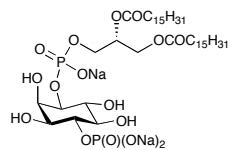
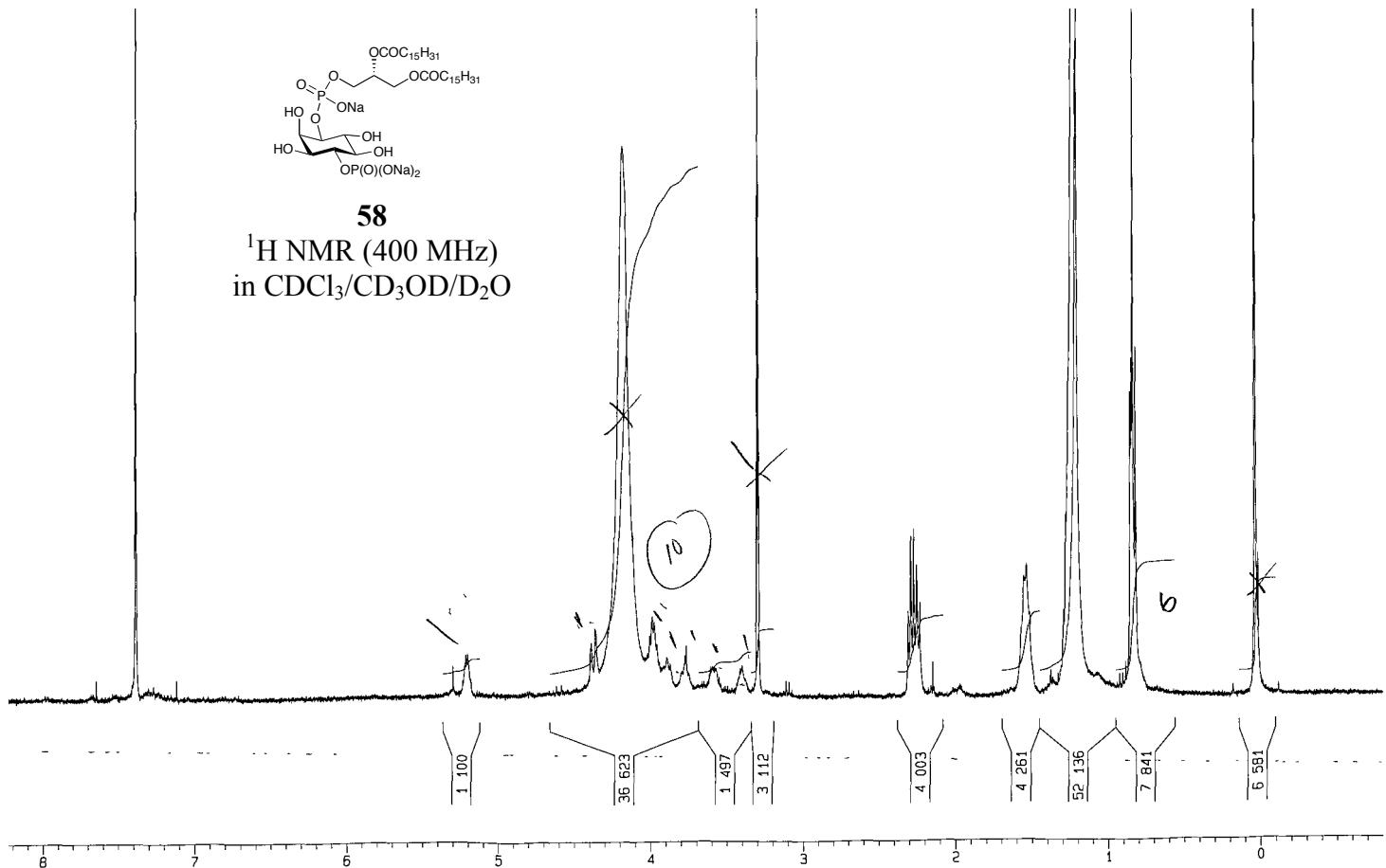






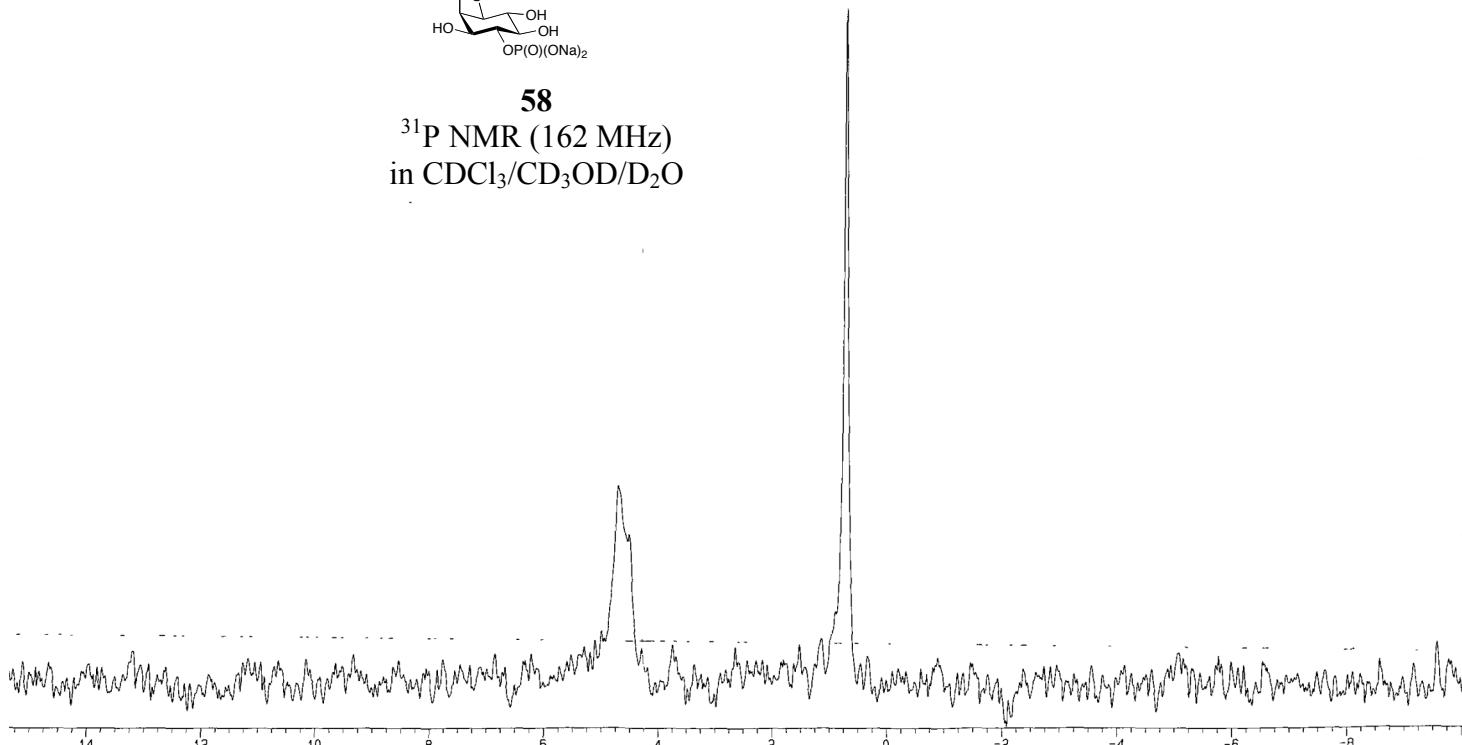
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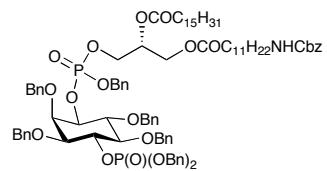
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in $\text{CDCl}_3/\text{CD}_3\text{OD}/\text{D}_2\text{O}$



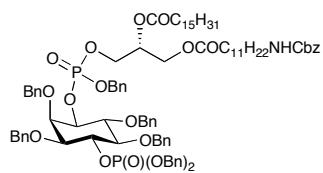
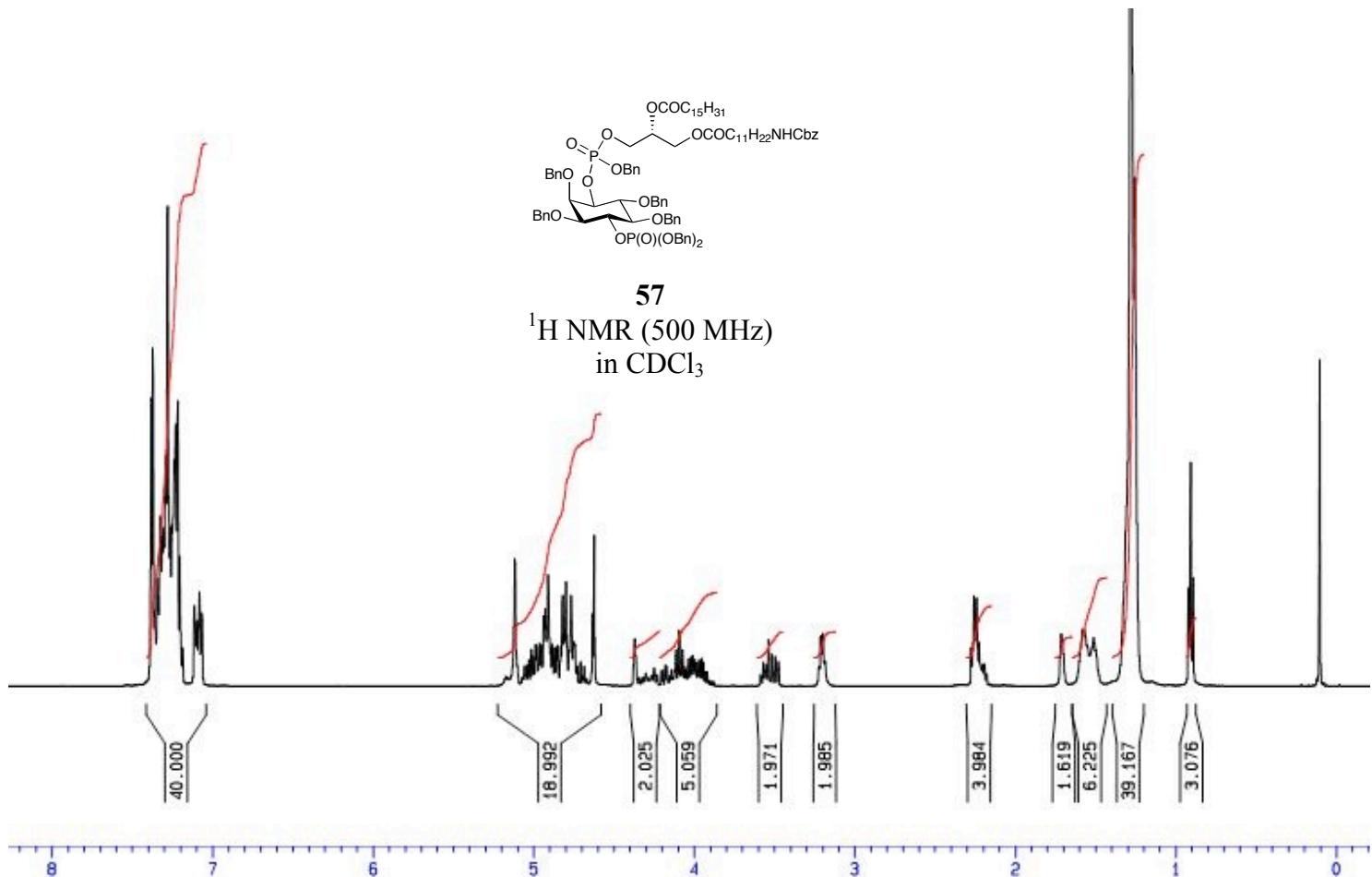
58

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in $\text{CDCl}_3/\text{CD}_3\text{OD}/\text{D}_2\text{O}$

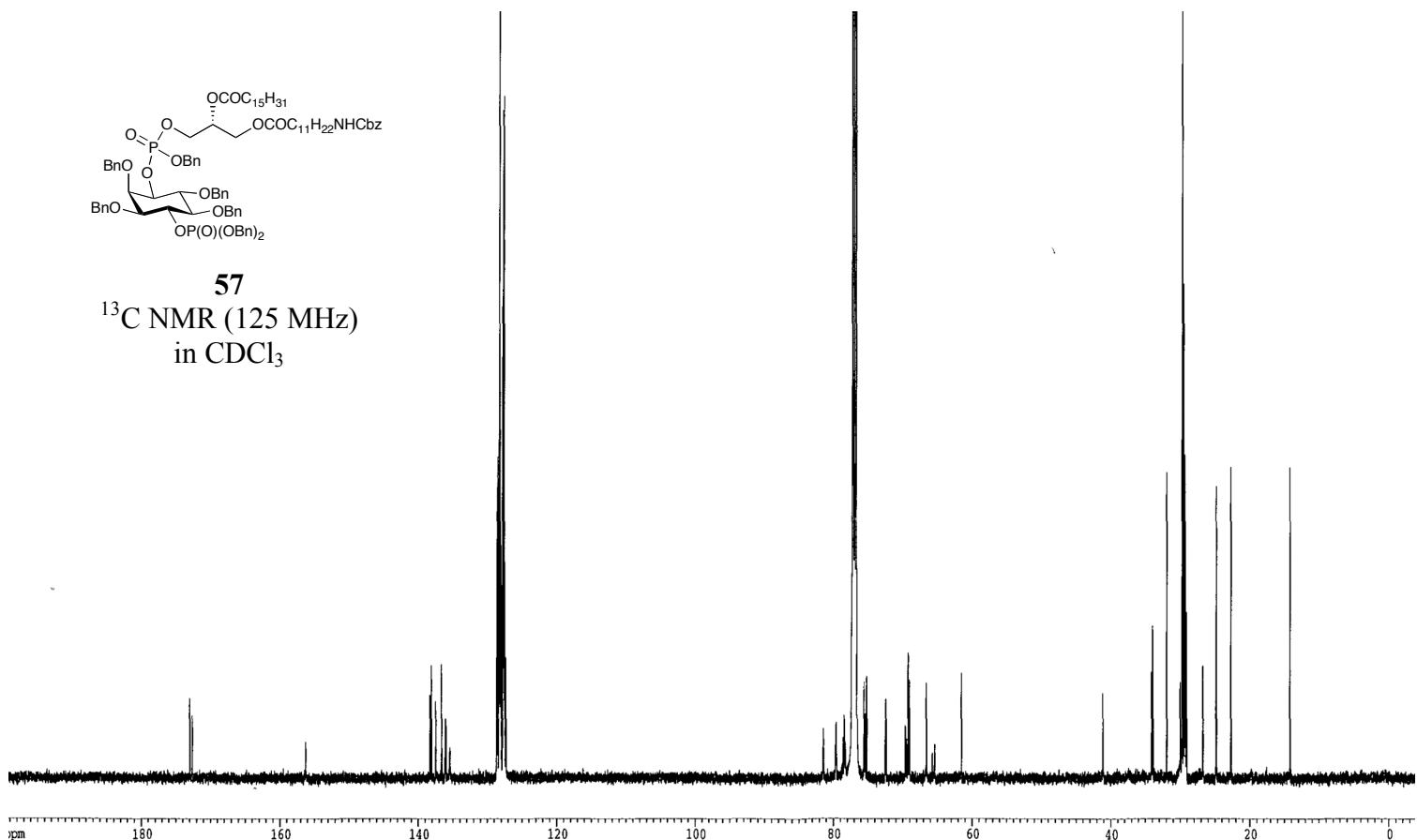


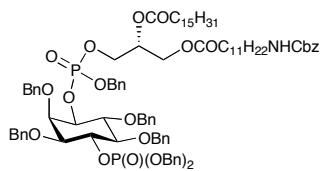


57
¹H NMR (500 MHz)
in CDCl₃



57
¹³C NMR (125 MHz)
in CDCl₃

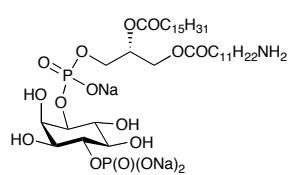




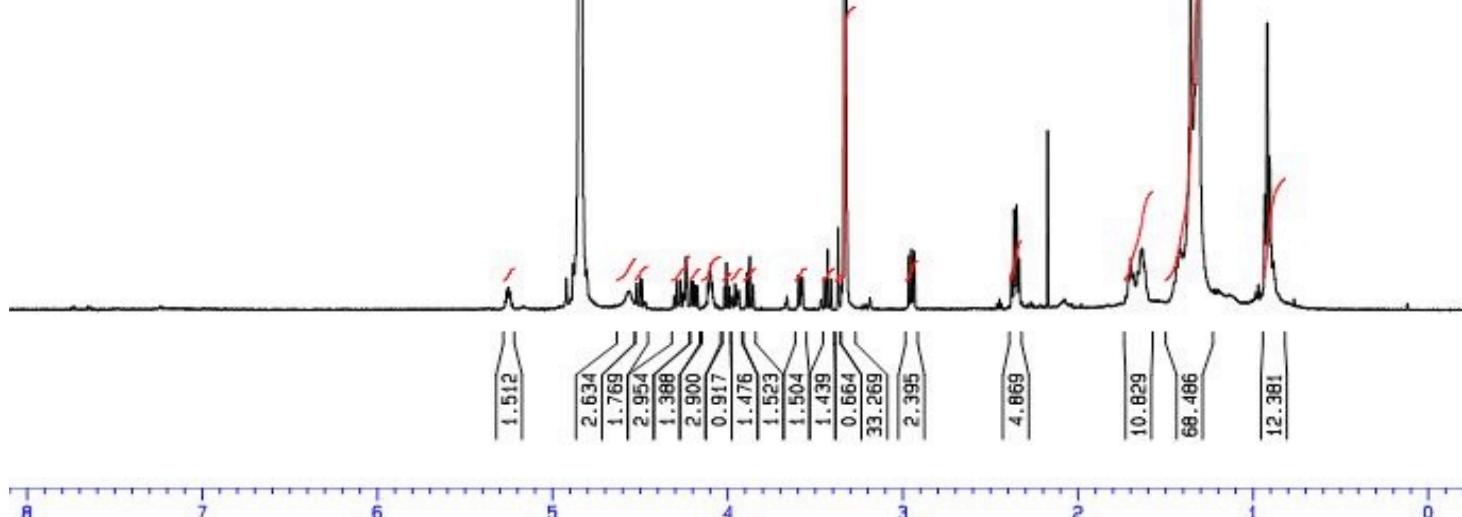
^{31}P NMR (162 MHz)
in CDCl_3



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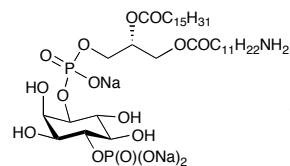


59
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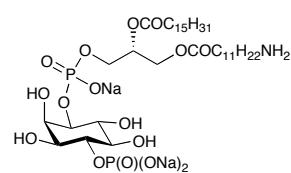
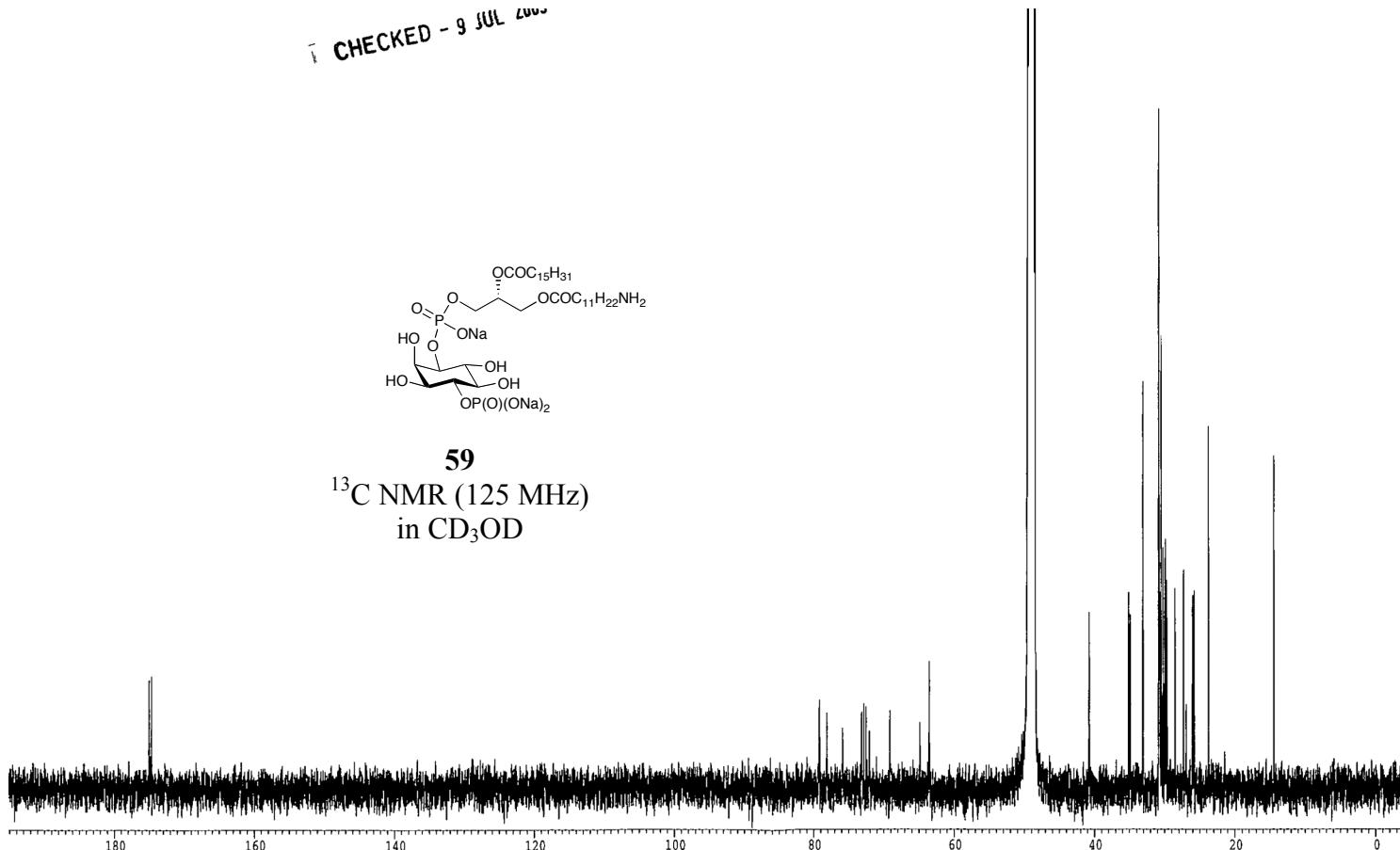


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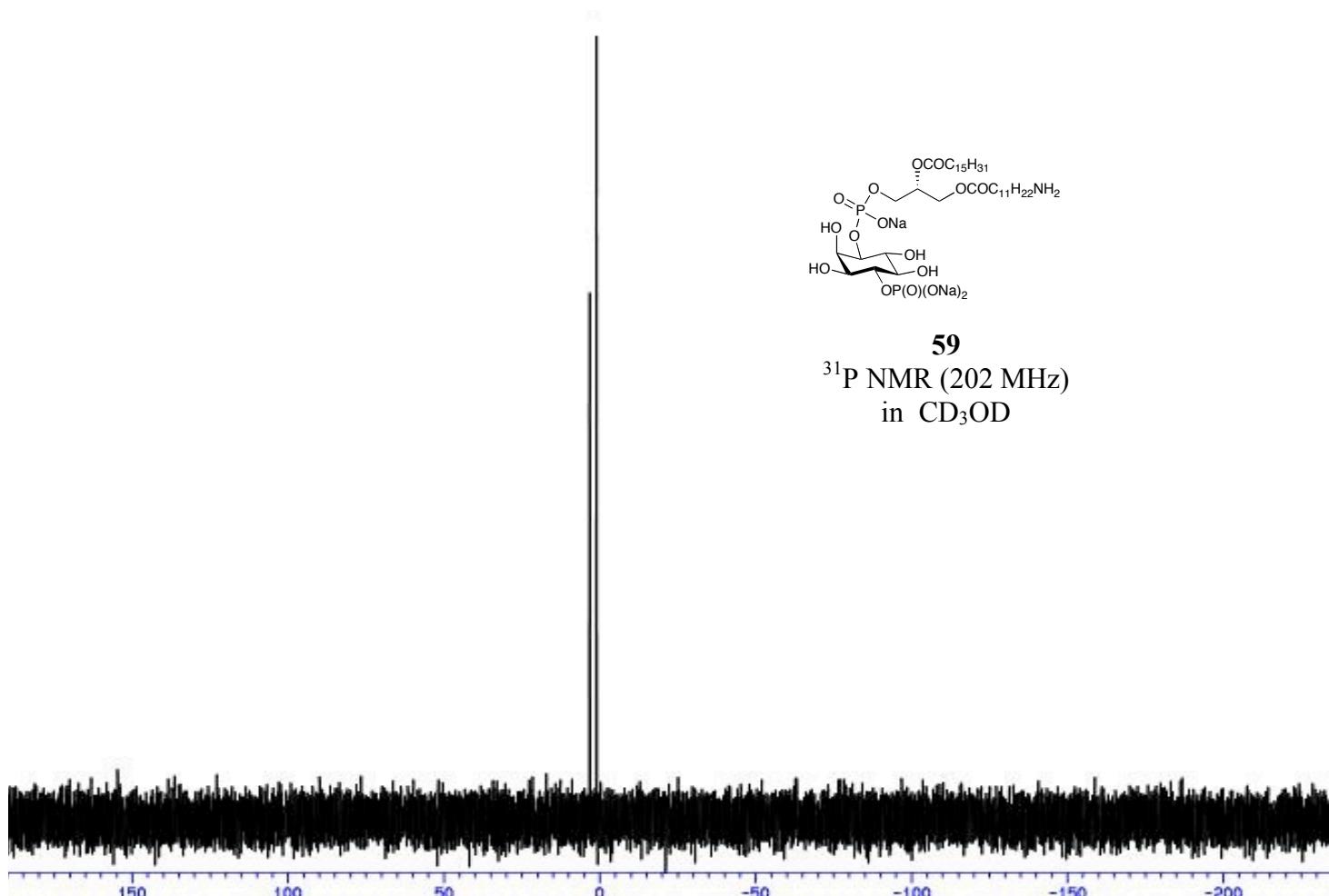
✓ CHECKED - 9 JUL 2000



59
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in CD_3OD

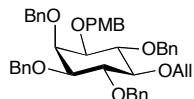


59
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in CD_3OD

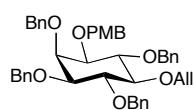
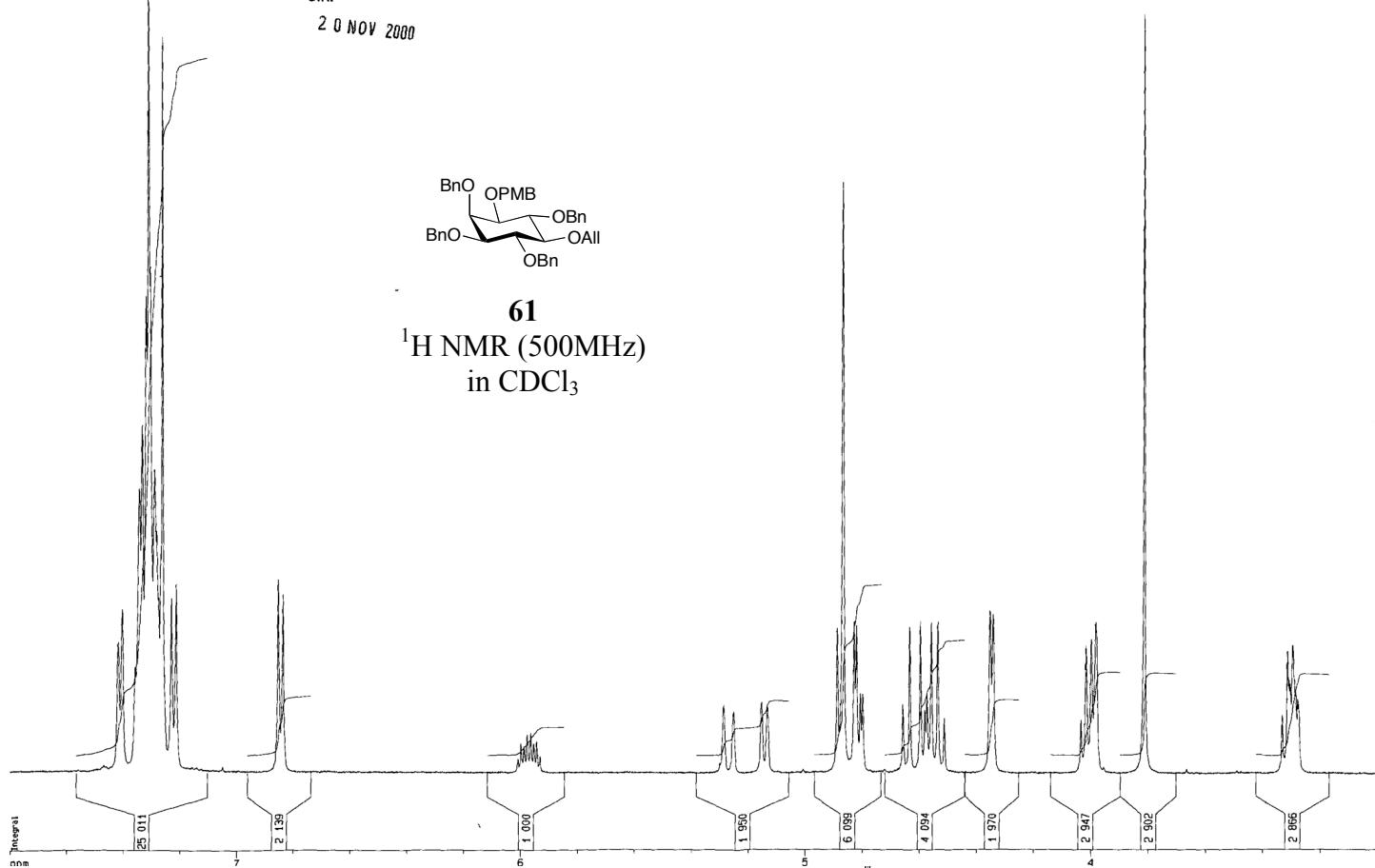


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U.K.

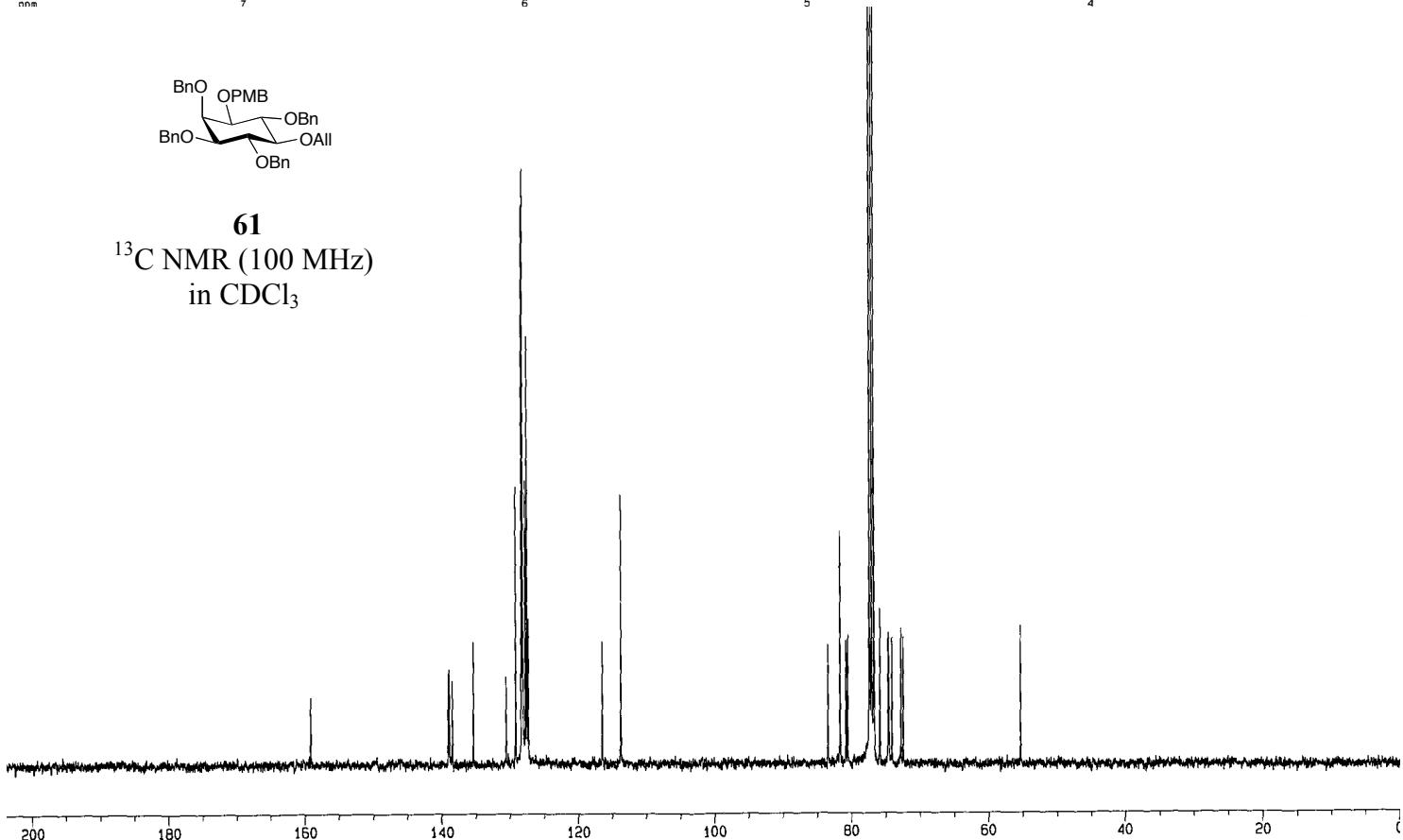
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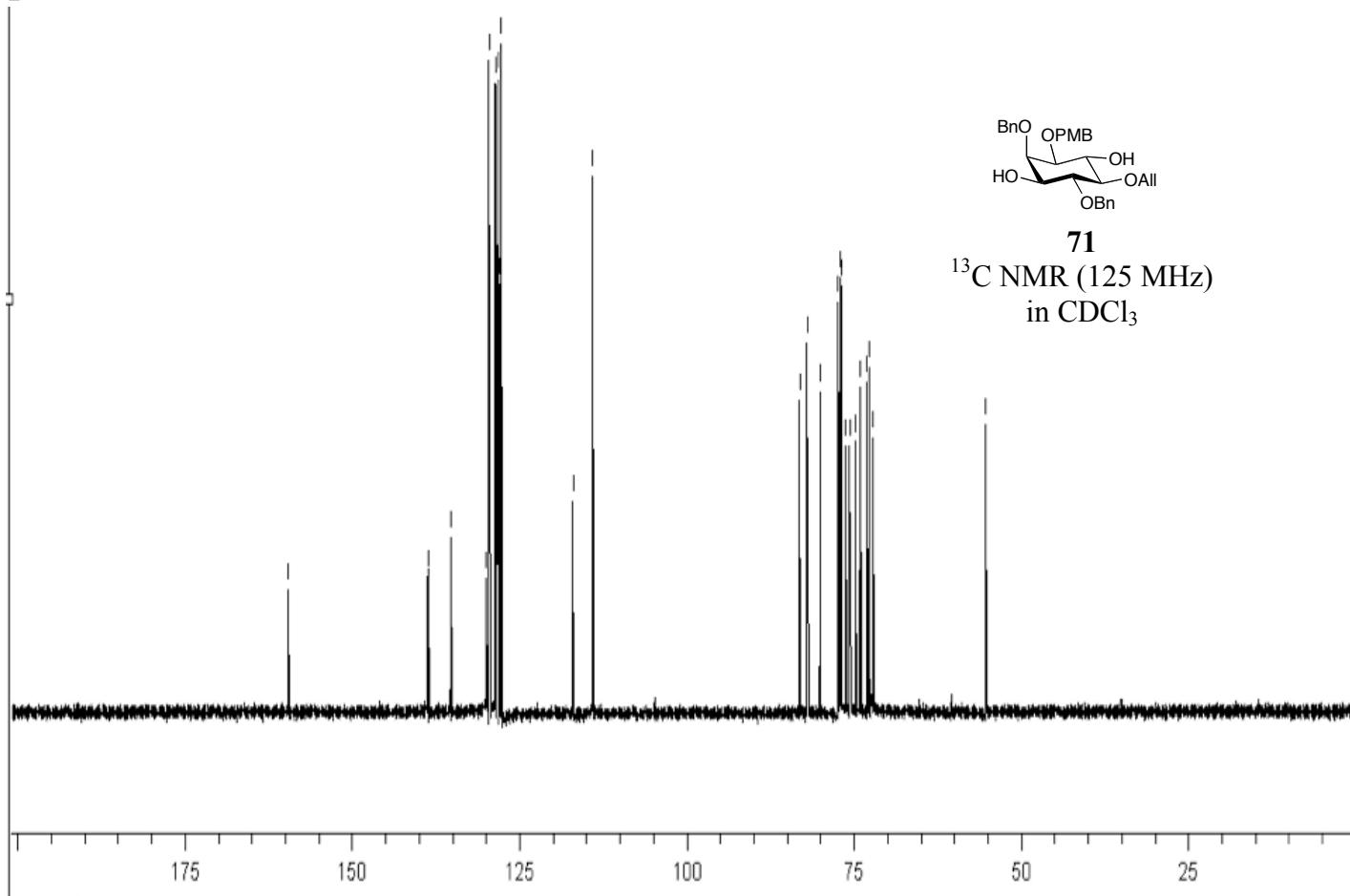
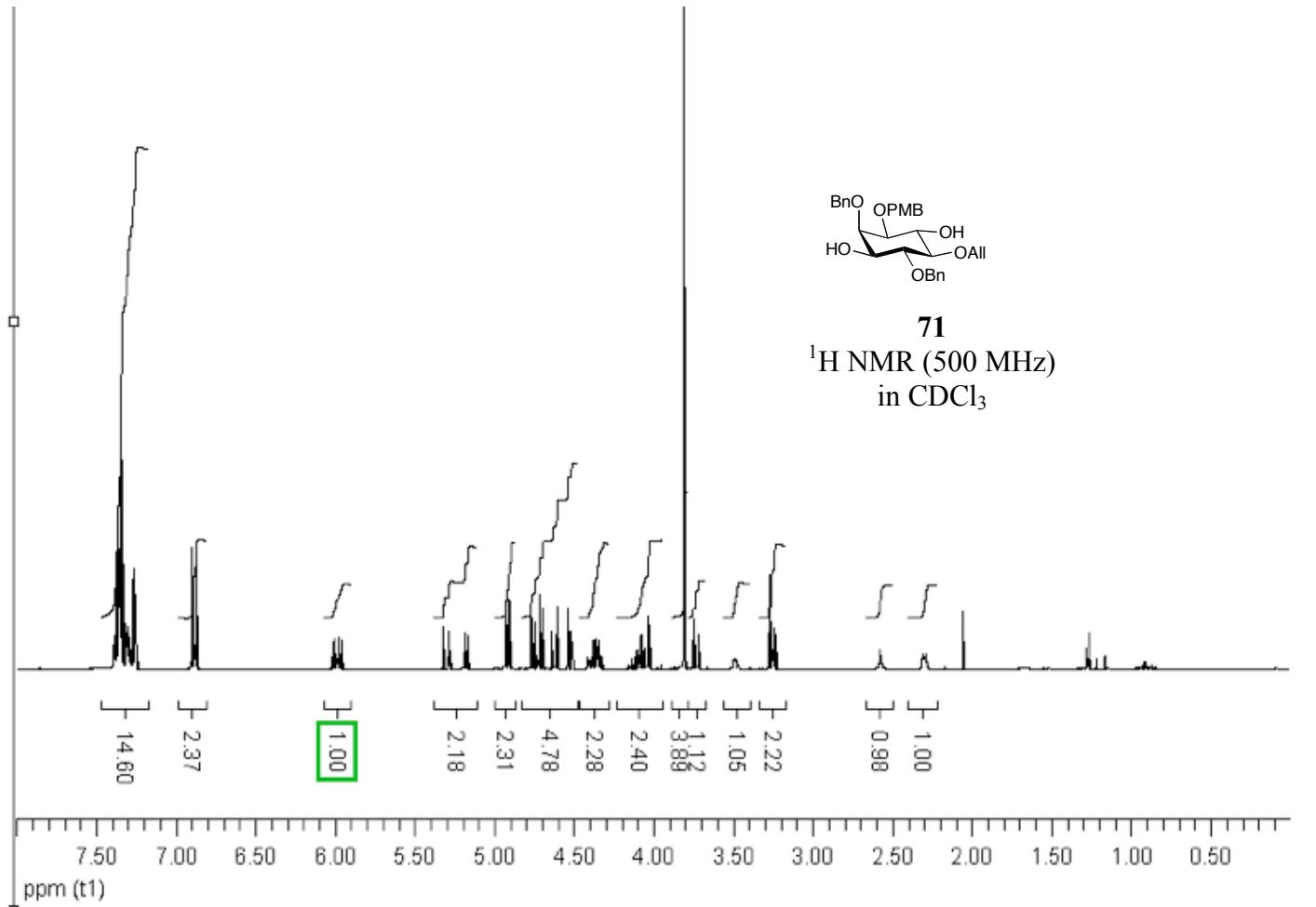


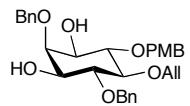
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in CDCl_3



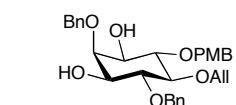
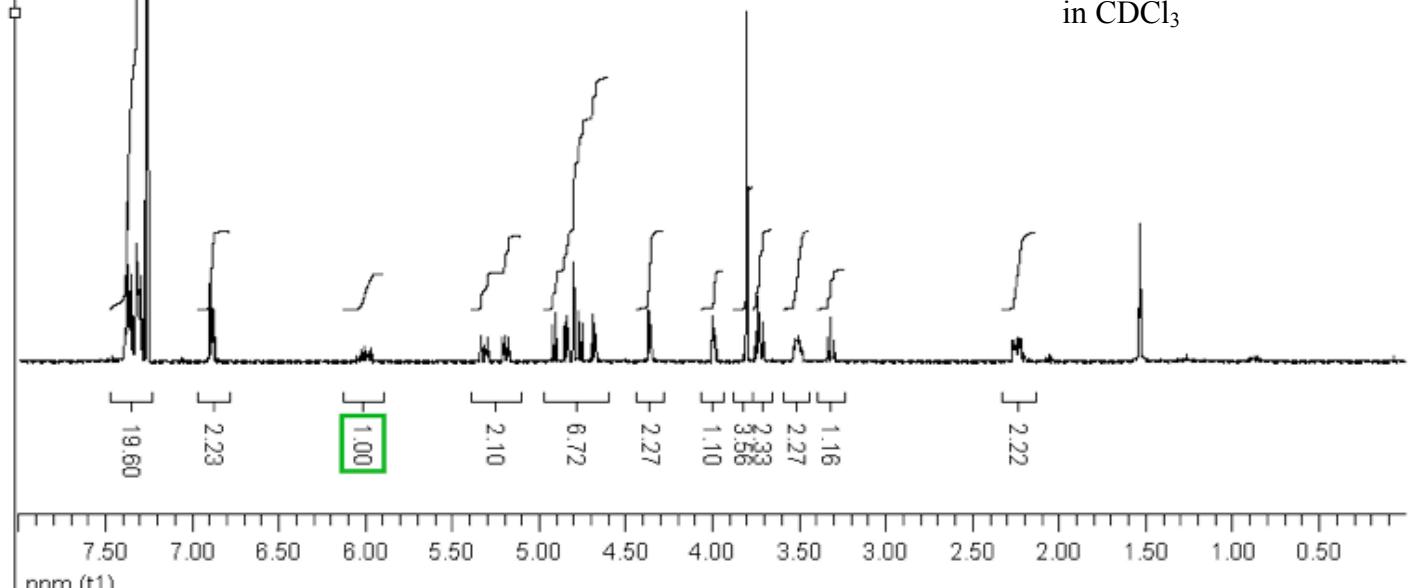
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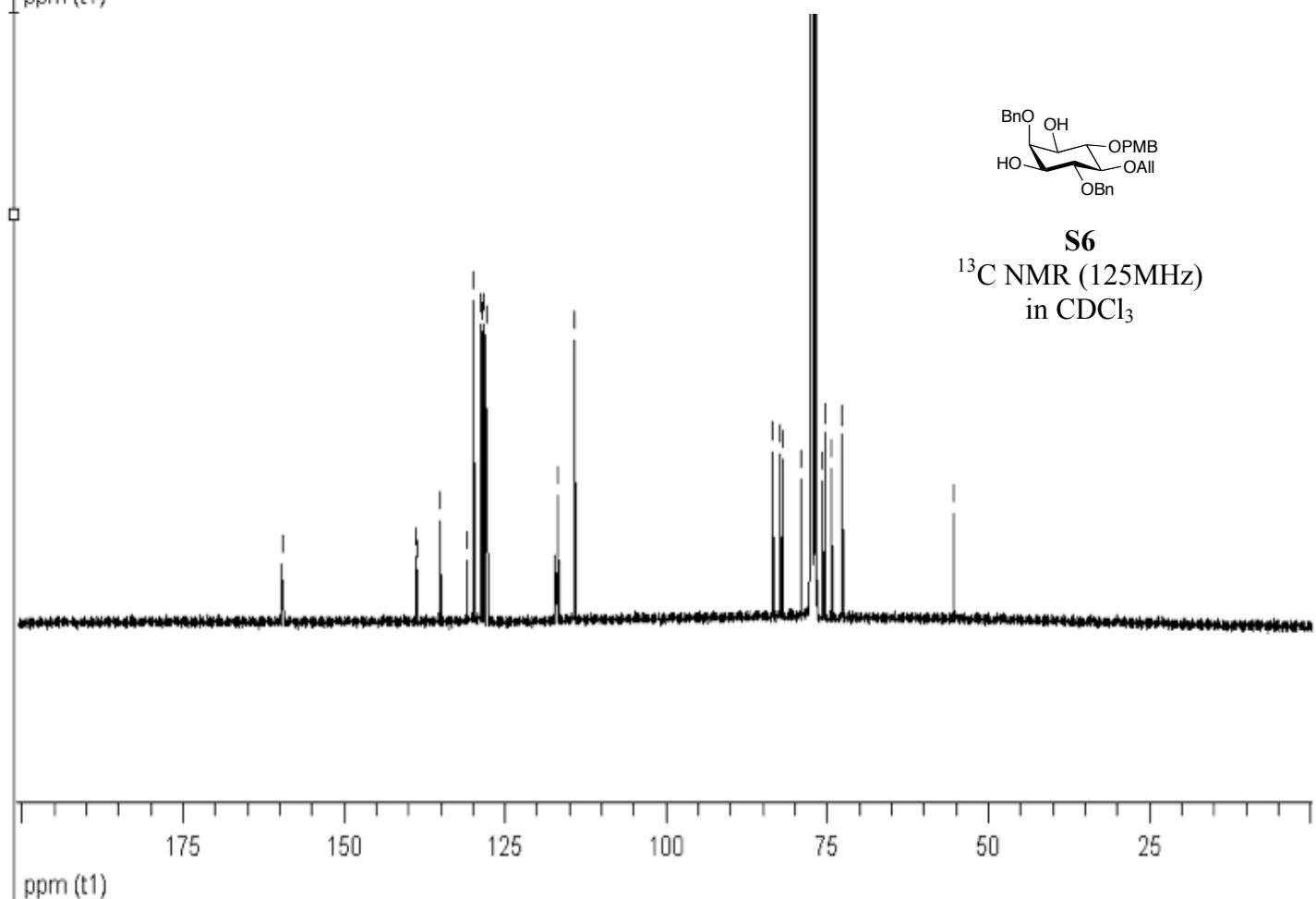


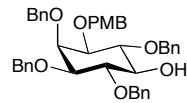


S6
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in CDCl_3

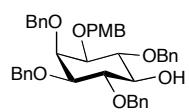
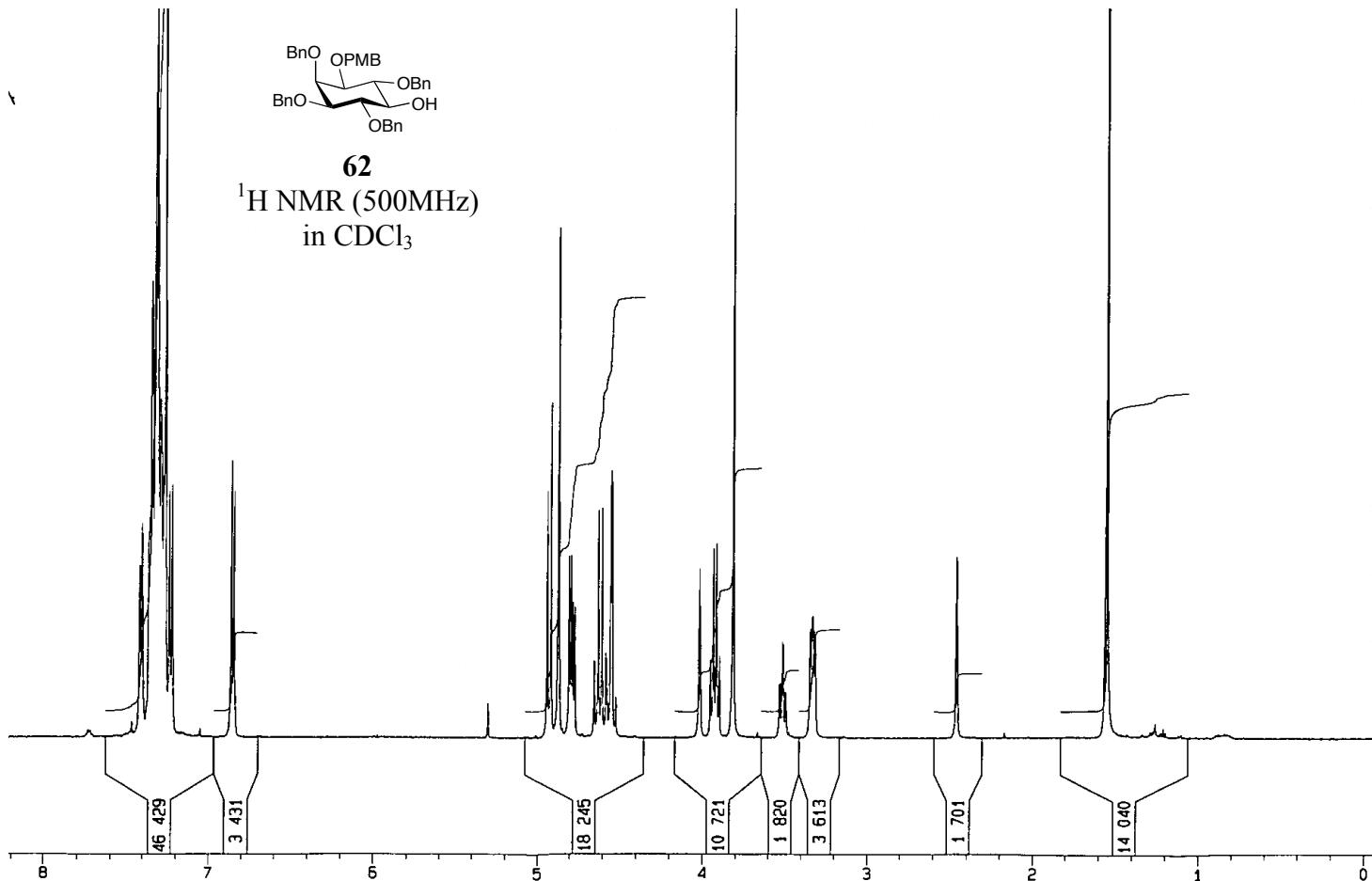


S6
 ^{13}C NMR (125MHz)
in CDCl_3

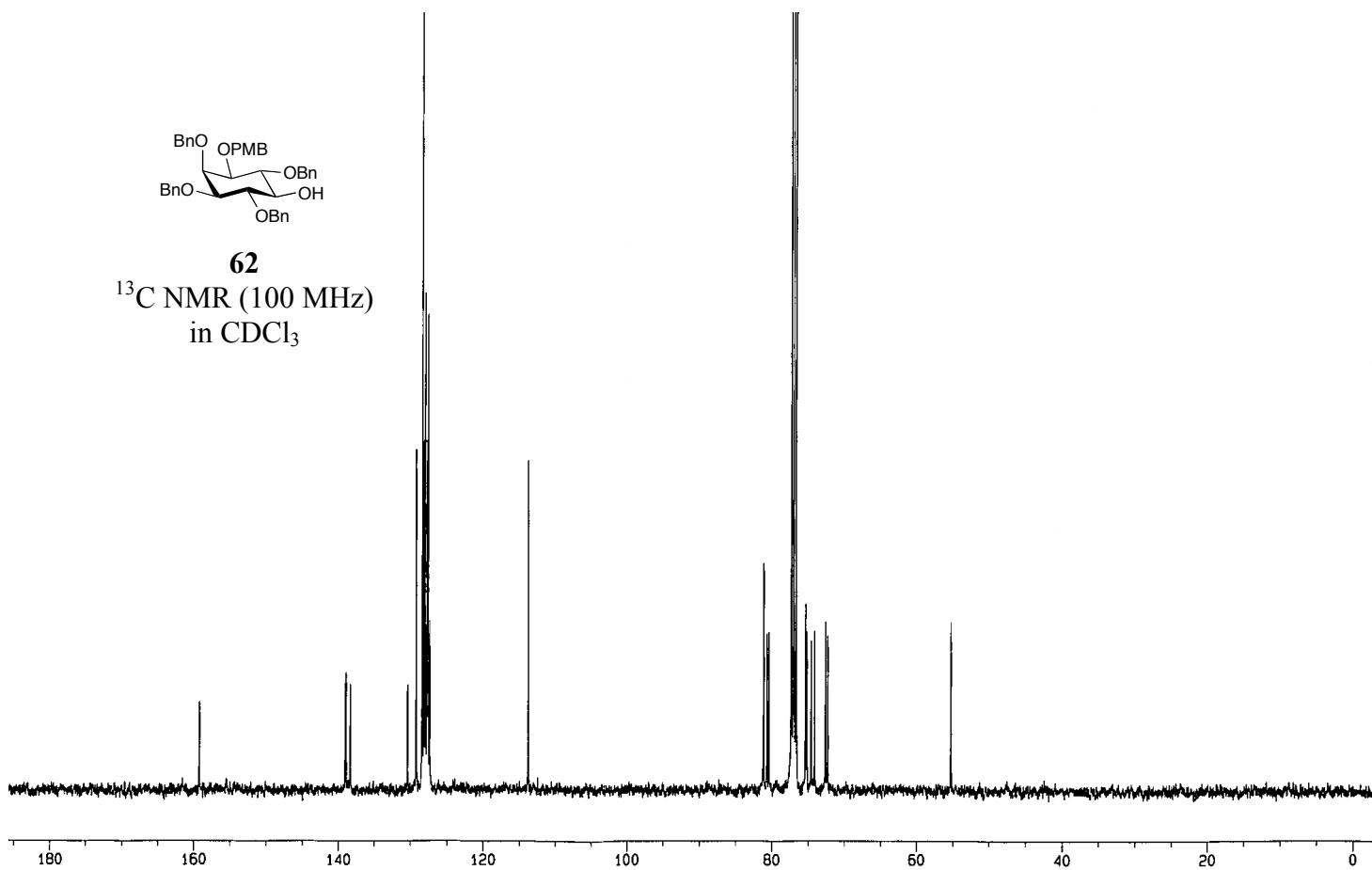


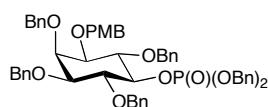


62
 ^1H NMR (500MHz)
in CDCl_3

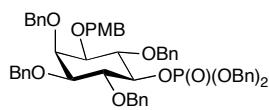
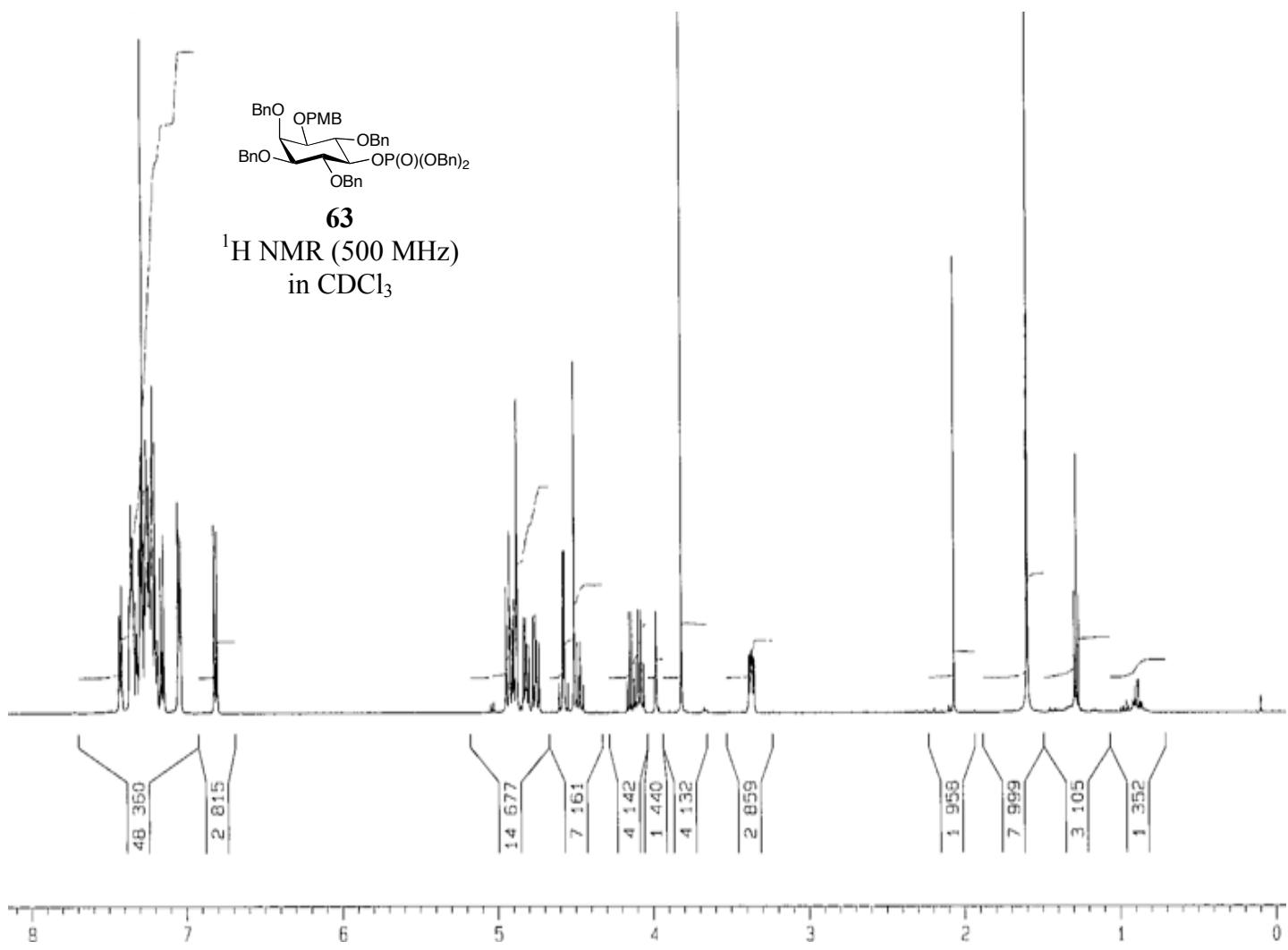


62
 ^{13}C NMR (100 MHz)
in CDCl_3

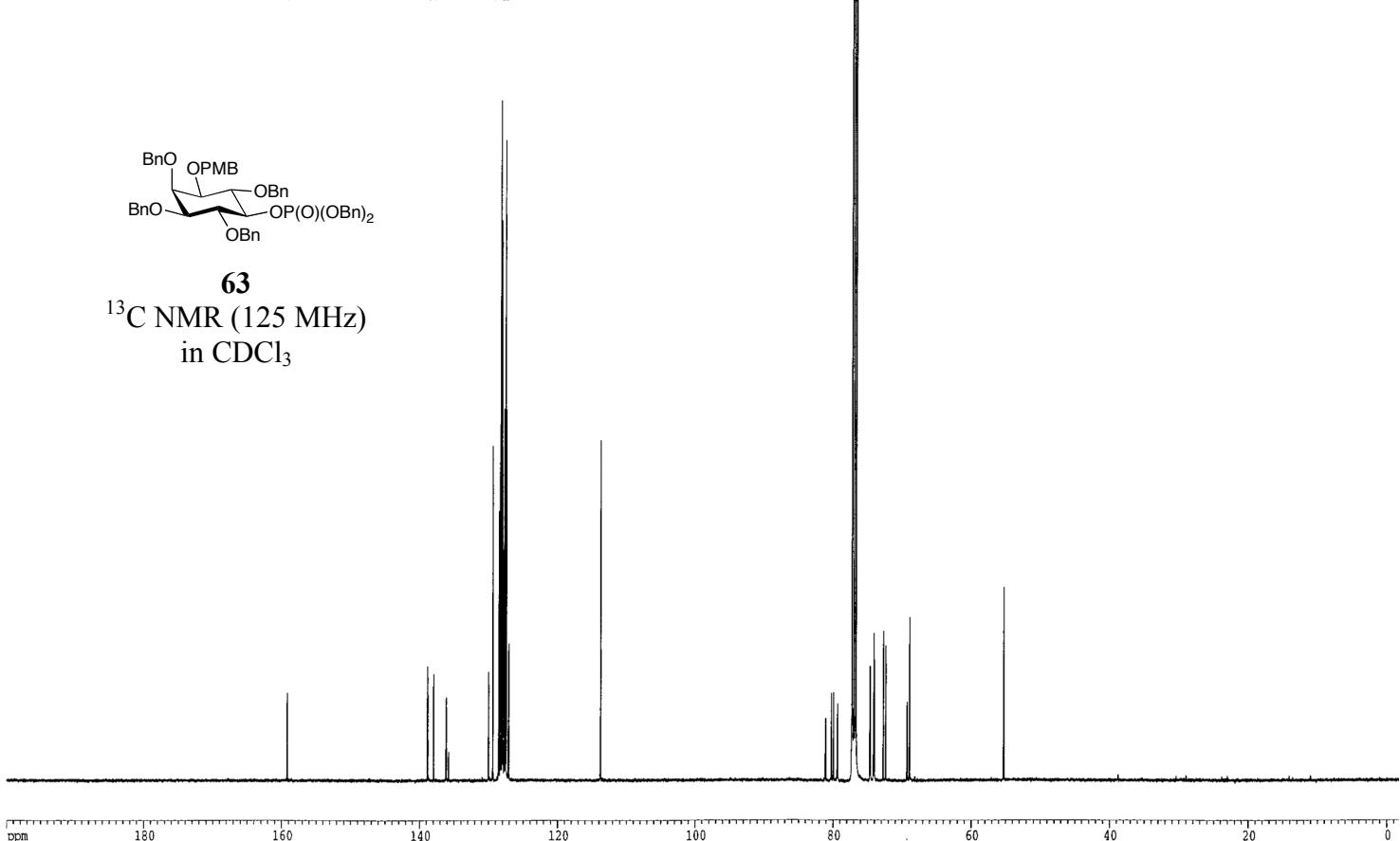


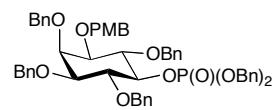


63
 ^1H NMR (500 MHz)
in CDCl_3

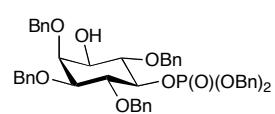
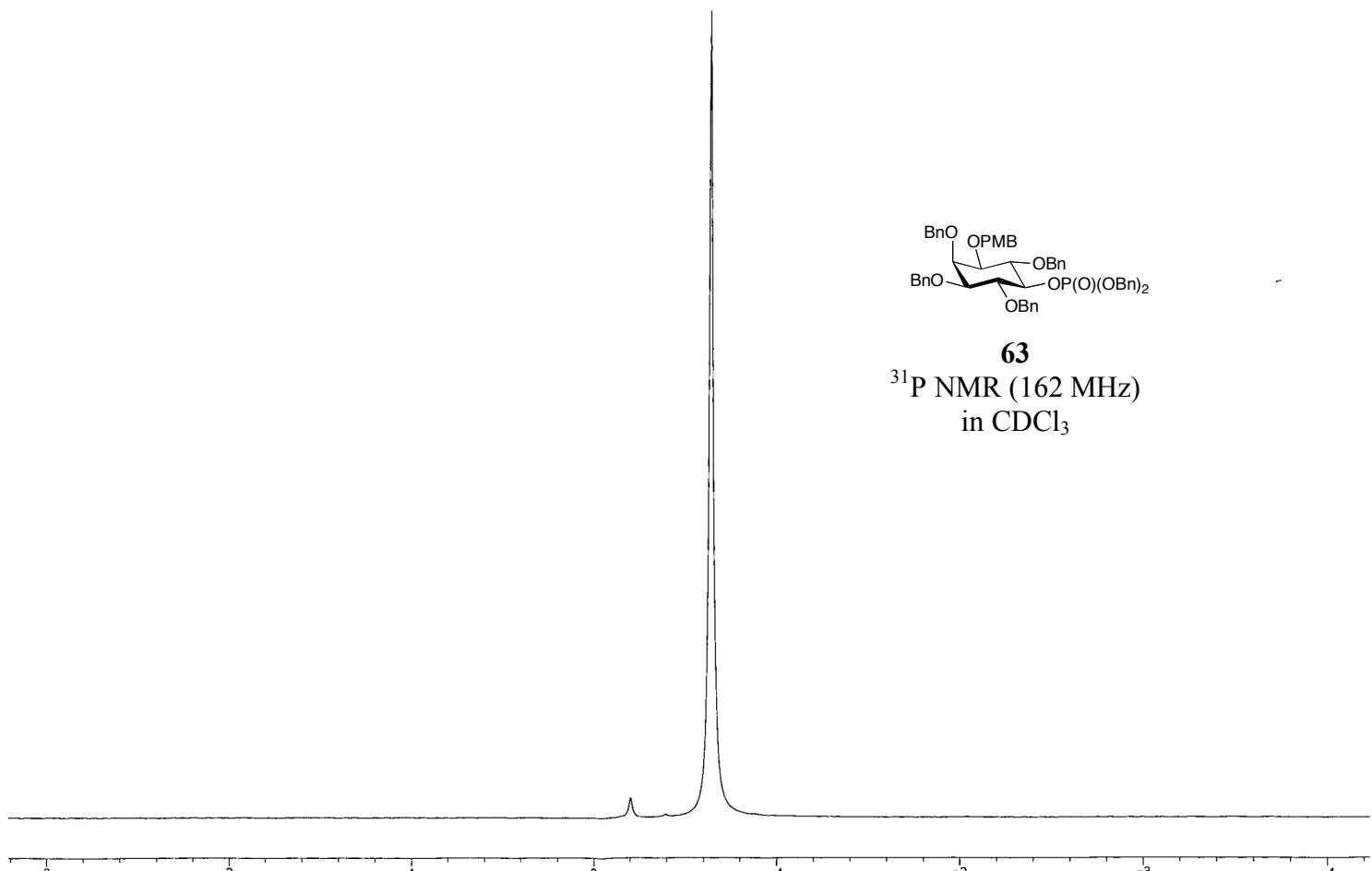


63
 ^{13}C NMR (125 MHz)
in CDCl_3

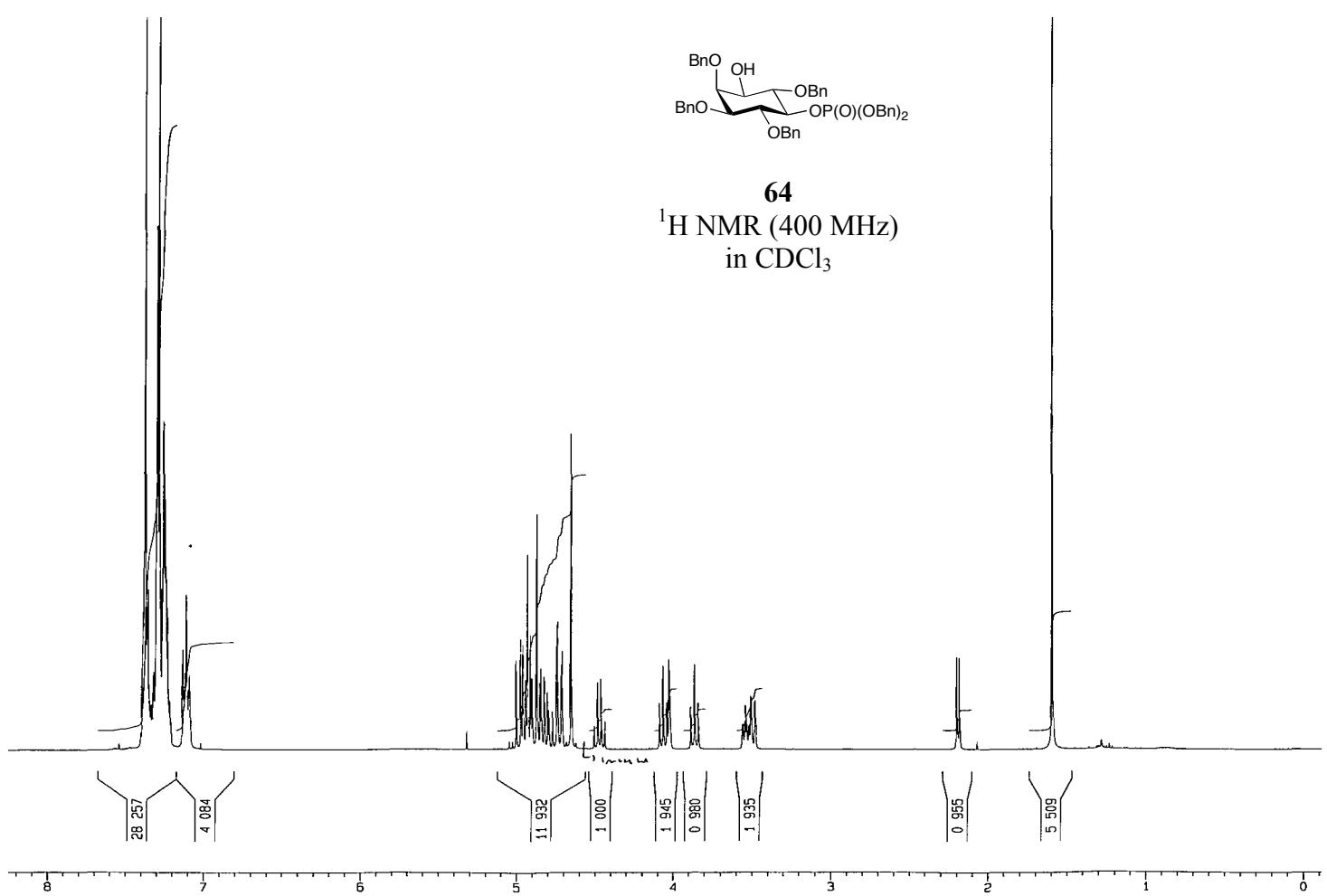


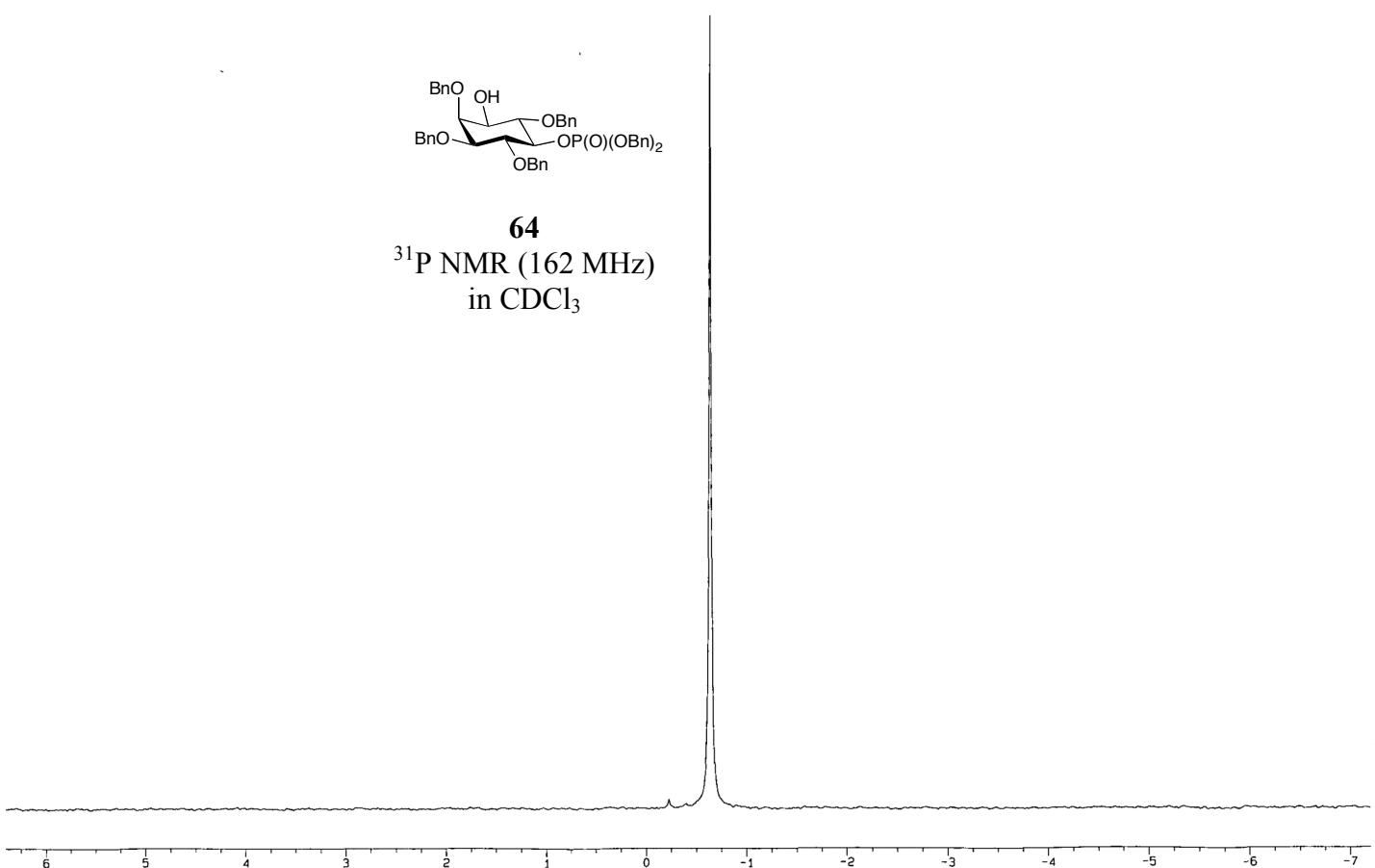
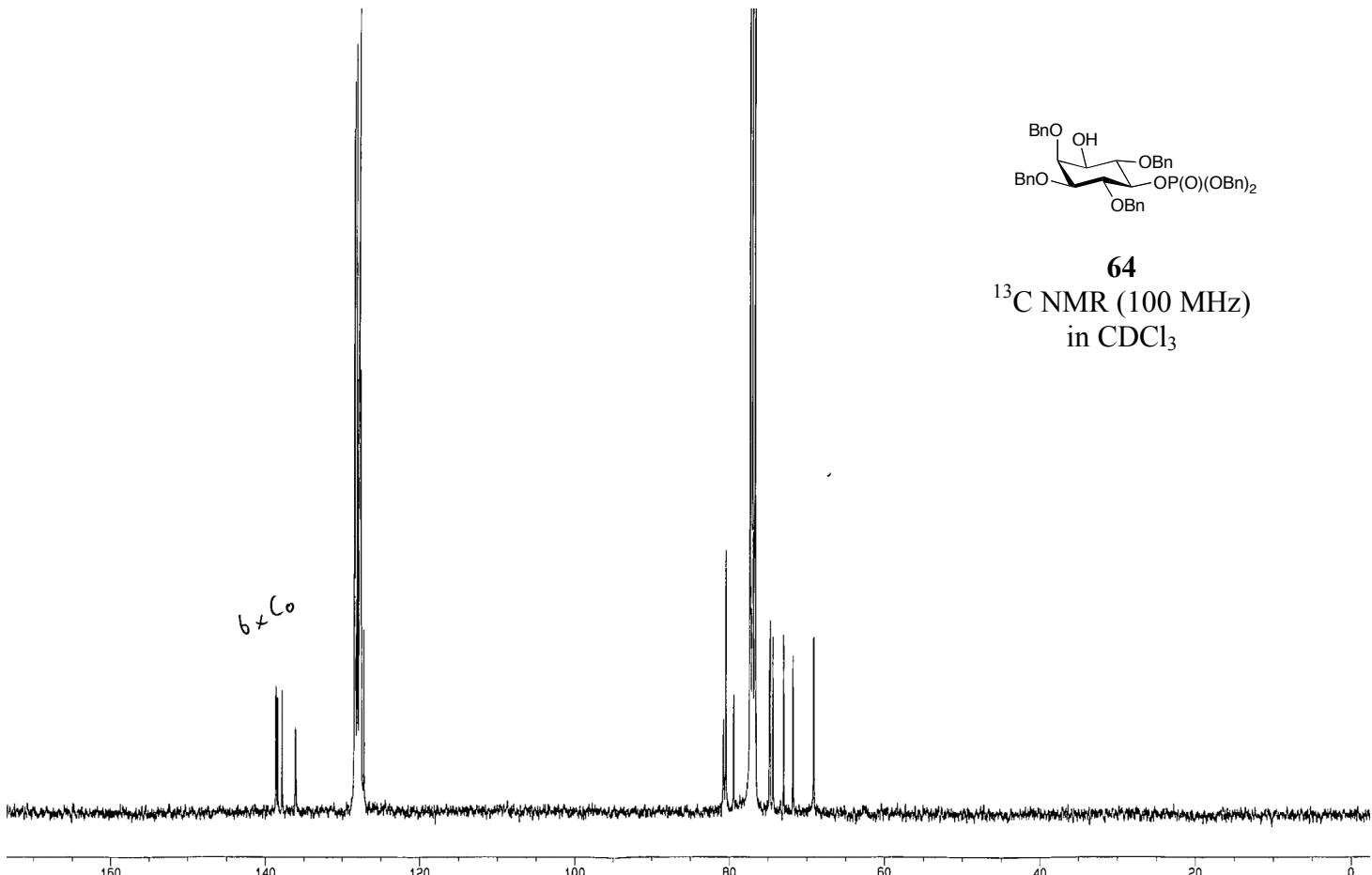


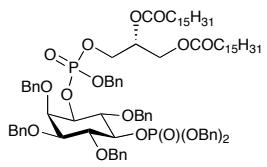
63
 ^{31}P NMR (162 MHz)
 in CDCl_3



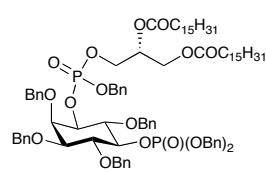
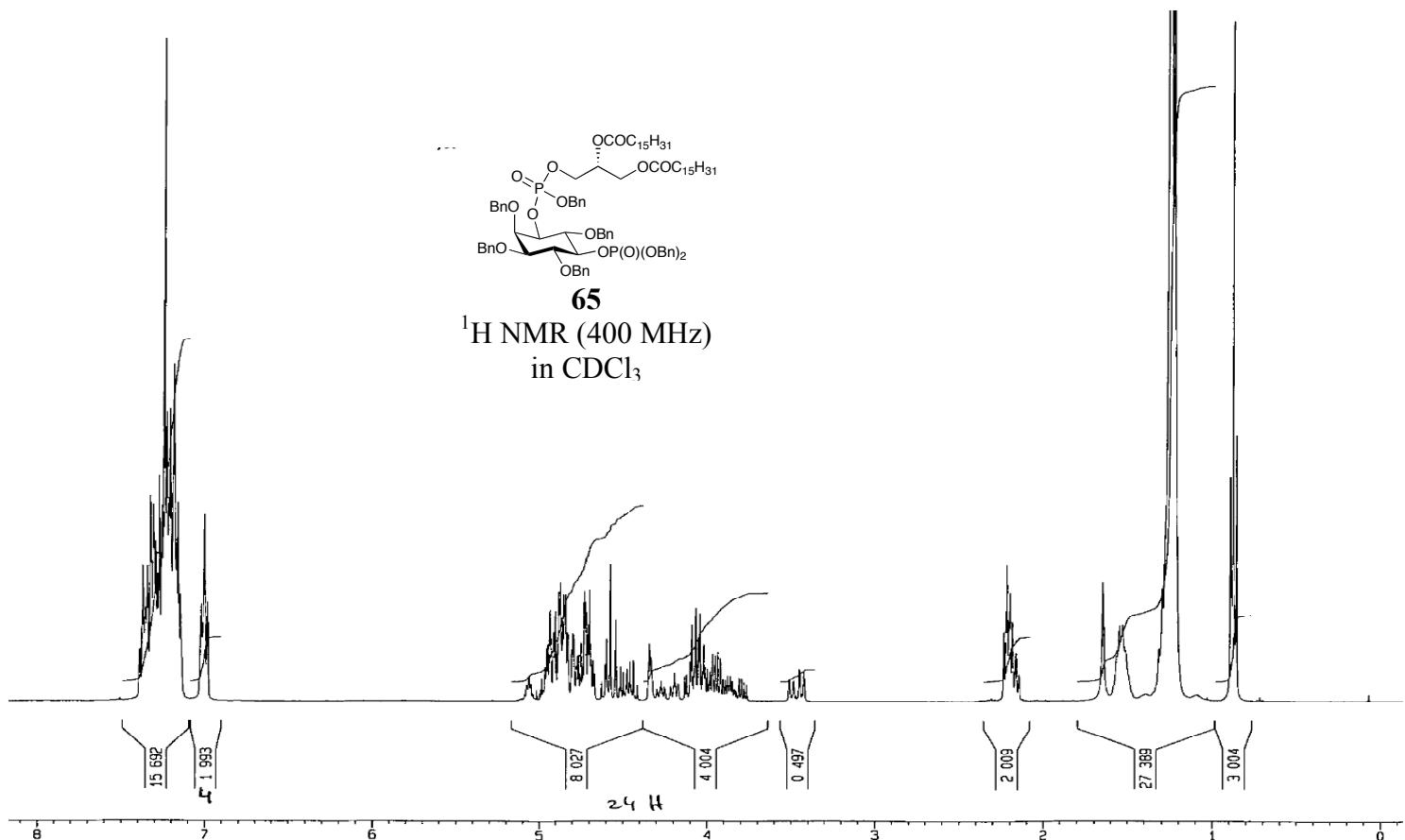
64
 ^1H NMR (400 MHz)
 in CDCl_3



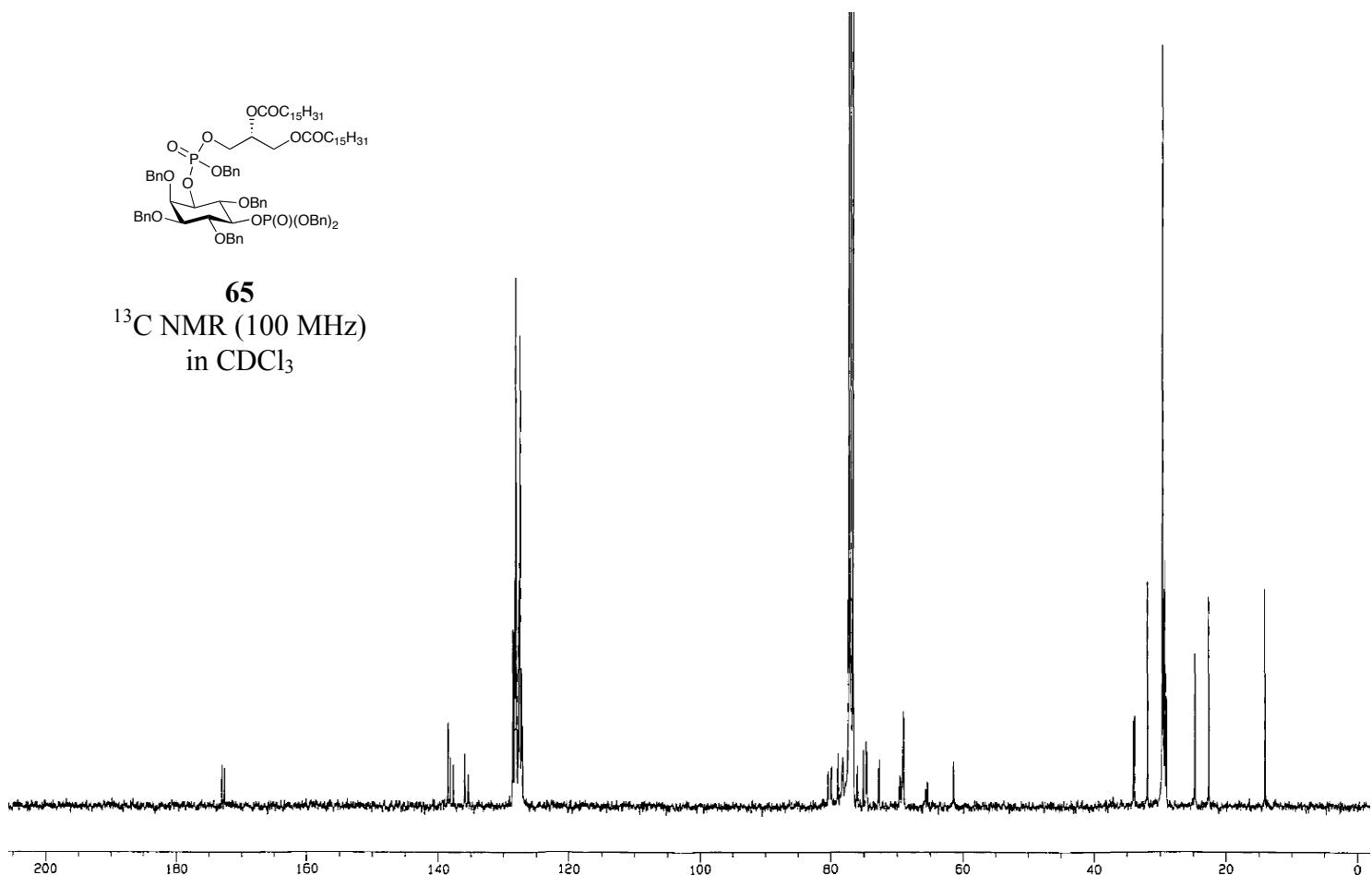


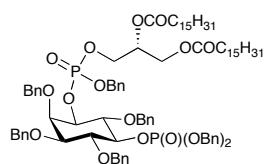


65
 ^1H NMR (400 MHz)
in CDCl_3

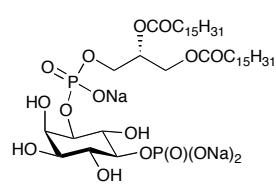
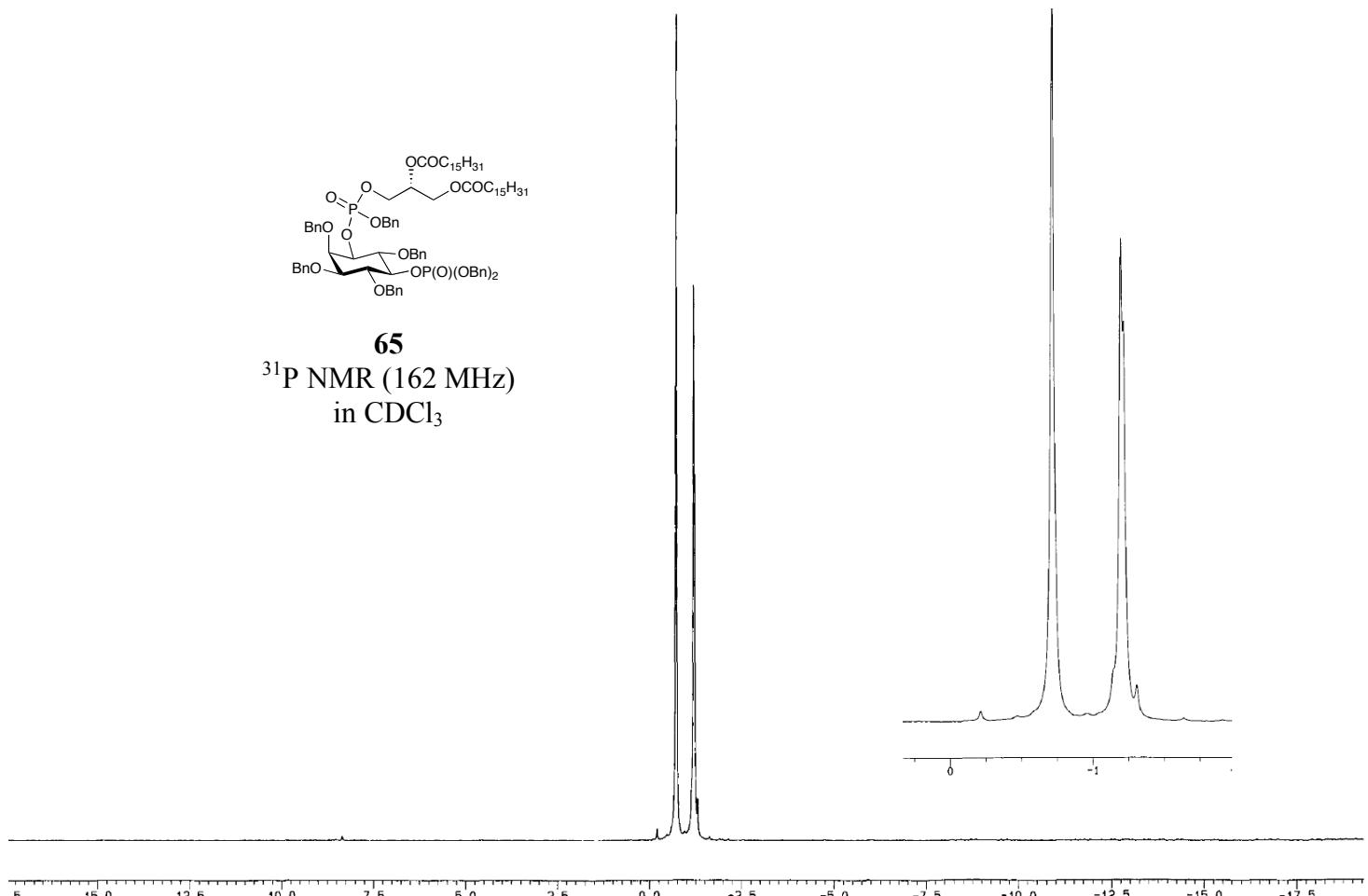


65
 ^{13}C NMR (100 MHz)
in CDCl_3

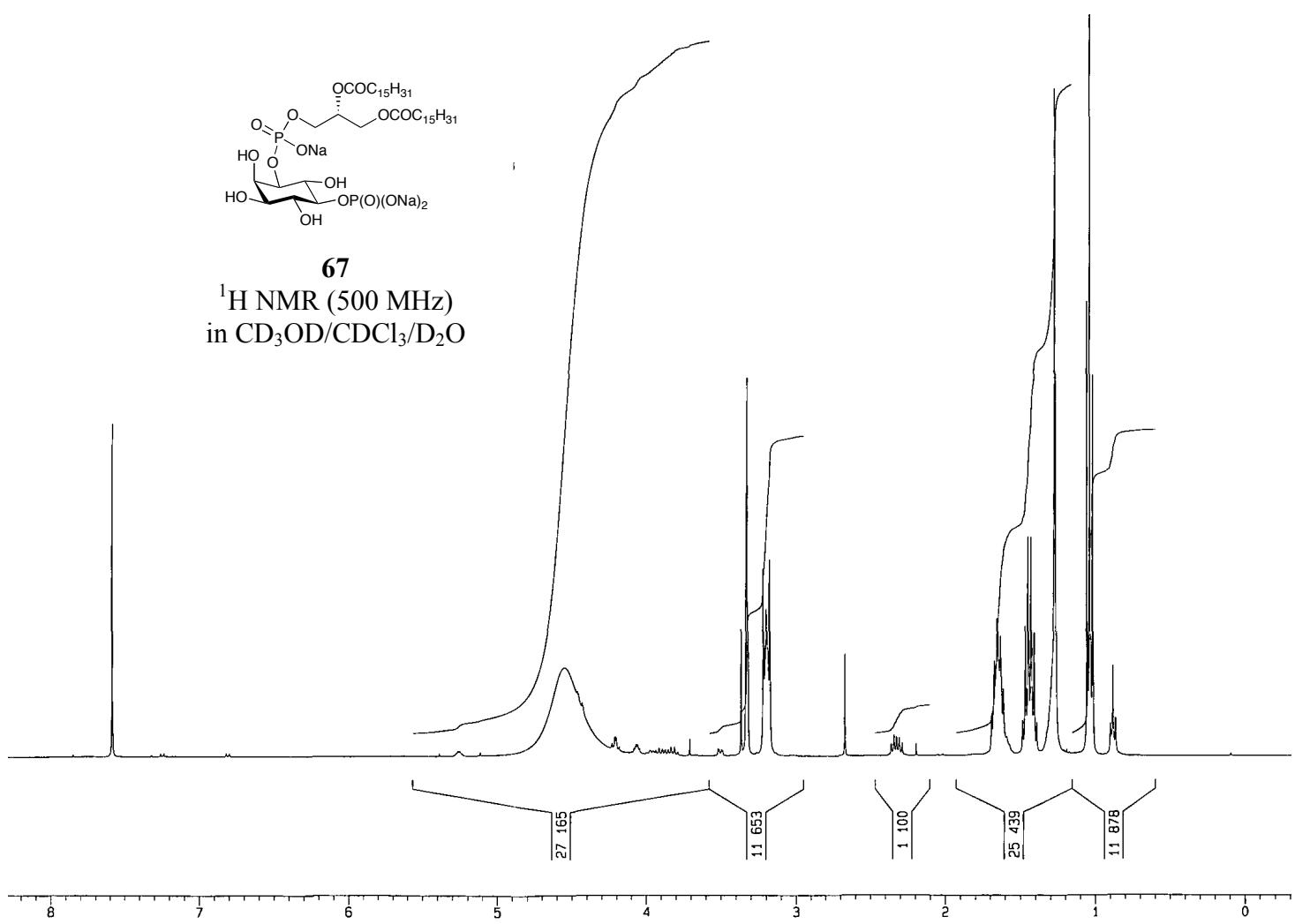


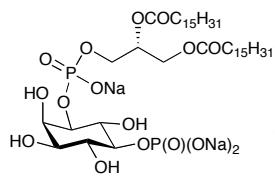


65
³¹P NMR (162 MHz)
in CDCl₃

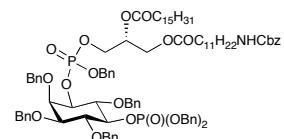
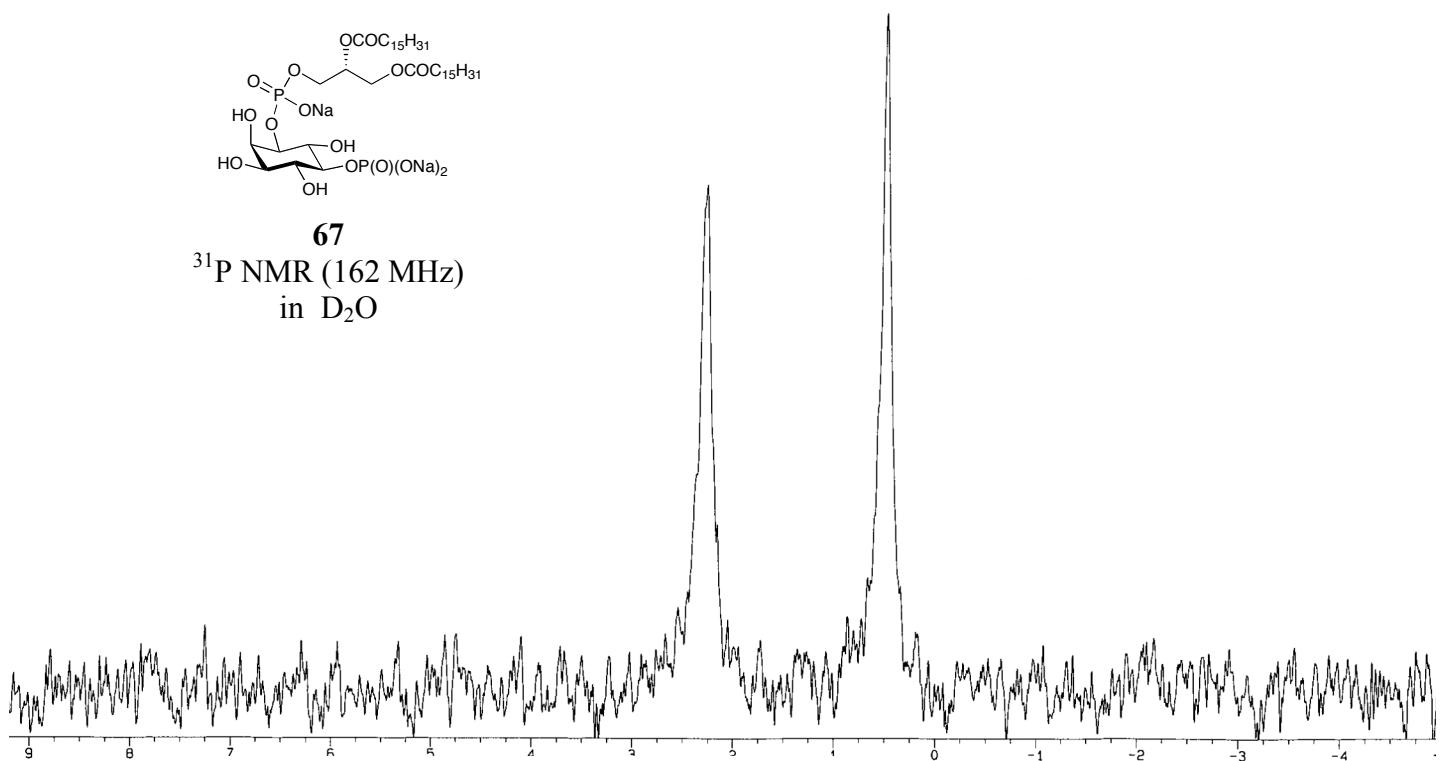


67
¹H NMR (500 MHz)
in CD₃OD/CDCl₃/D₂O

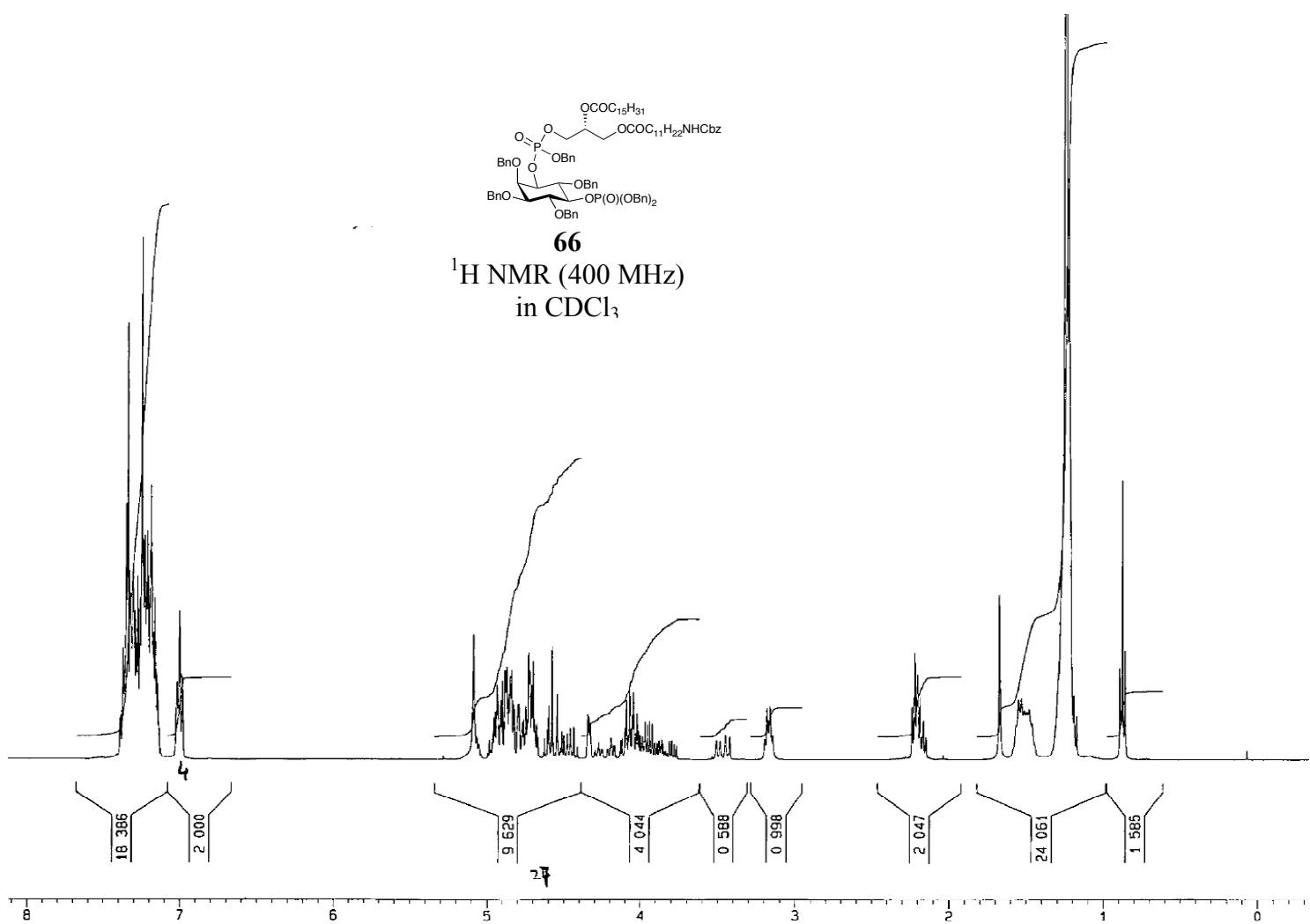


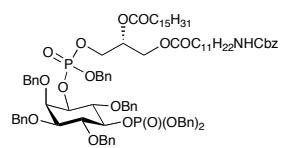


67
 ^{31}P NMR (162 MHz)
 in D_2O

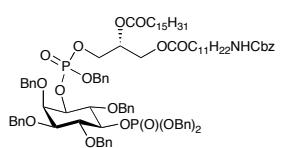
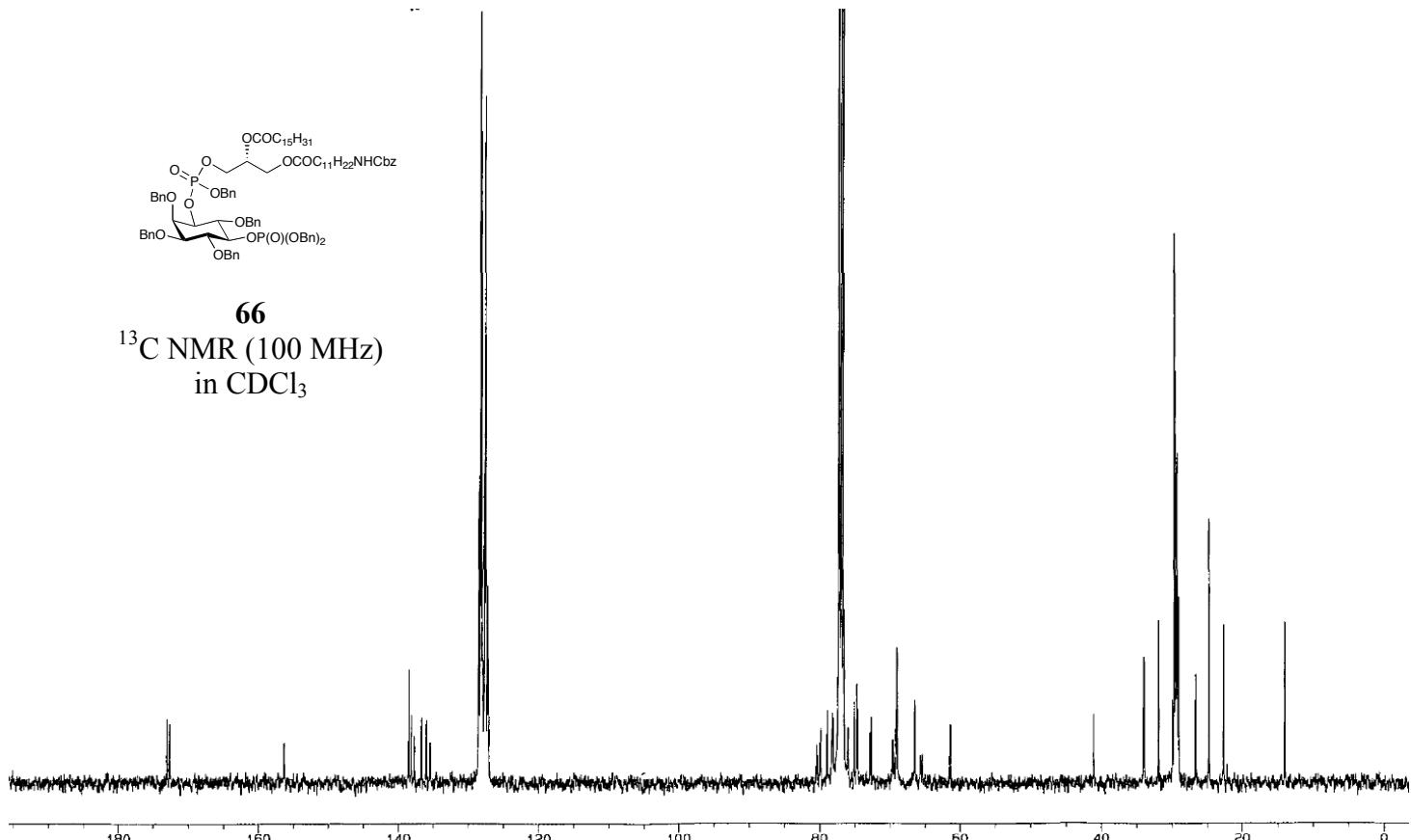


66
 ^1H NMR (400 MHz)
 in CDCl_3

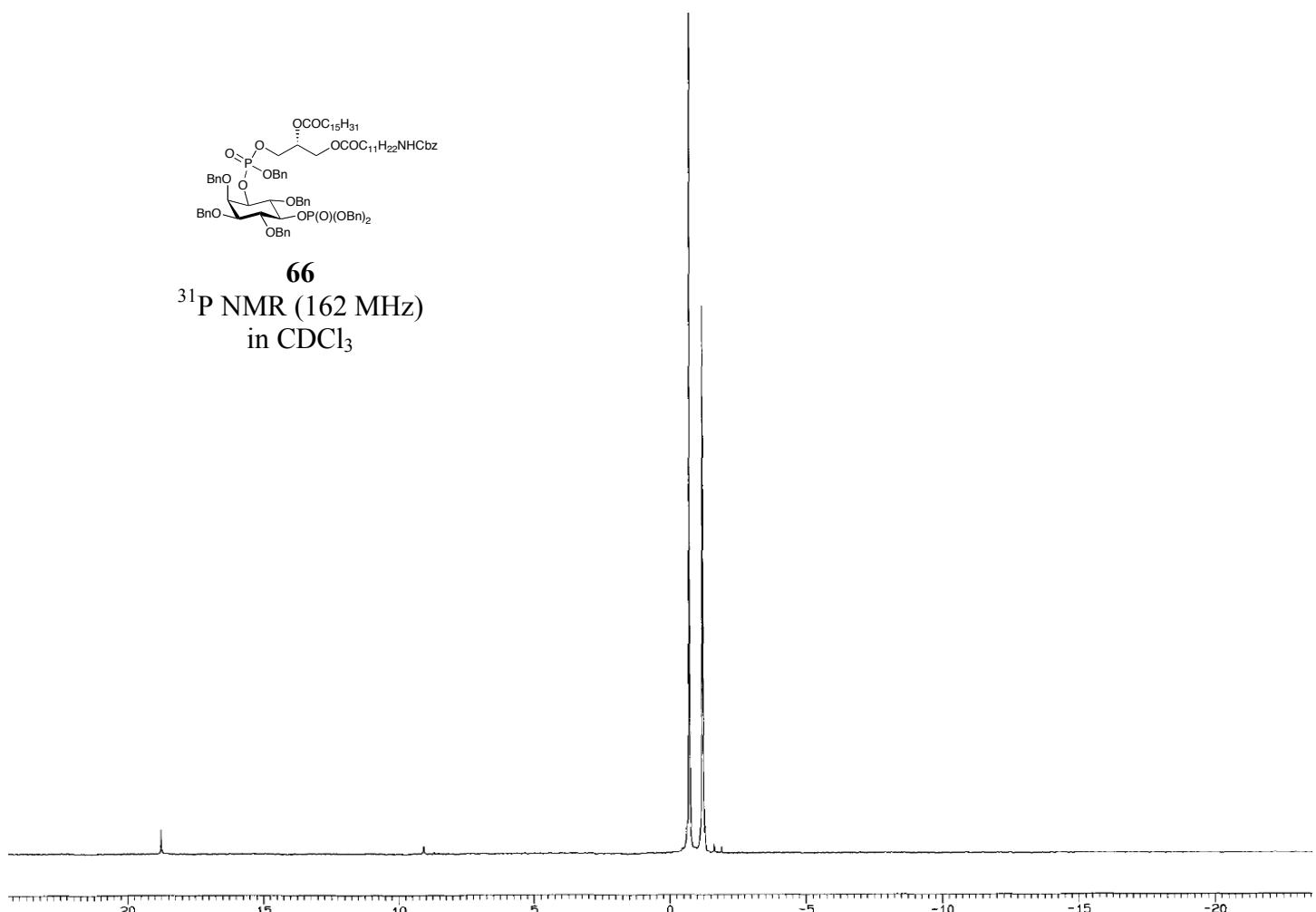




66
¹³C NMR (100 MHz)
in CDCl₃



66
³¹P NMR (162 MHz)
in CDCl₃



```

meters
22
38
It
4

30
34
13
21
4

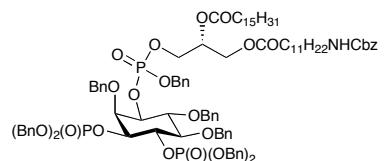
36 Hz
99 Hz
16 sec
55

00 usec
50 usec
0 K
00 sec
40 usec
08 MHz
1H
00 dB

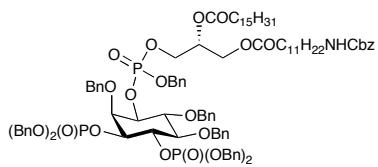
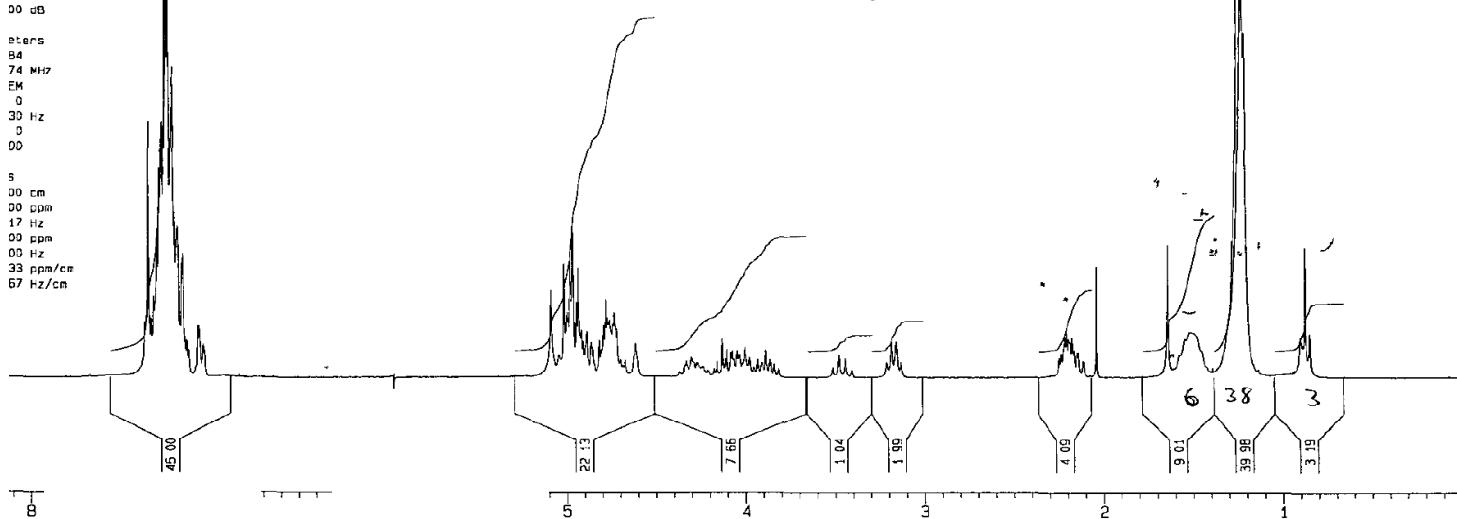
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eters
 B4
 74 MHz
 EM
 0
 30 Hz
 0
 00

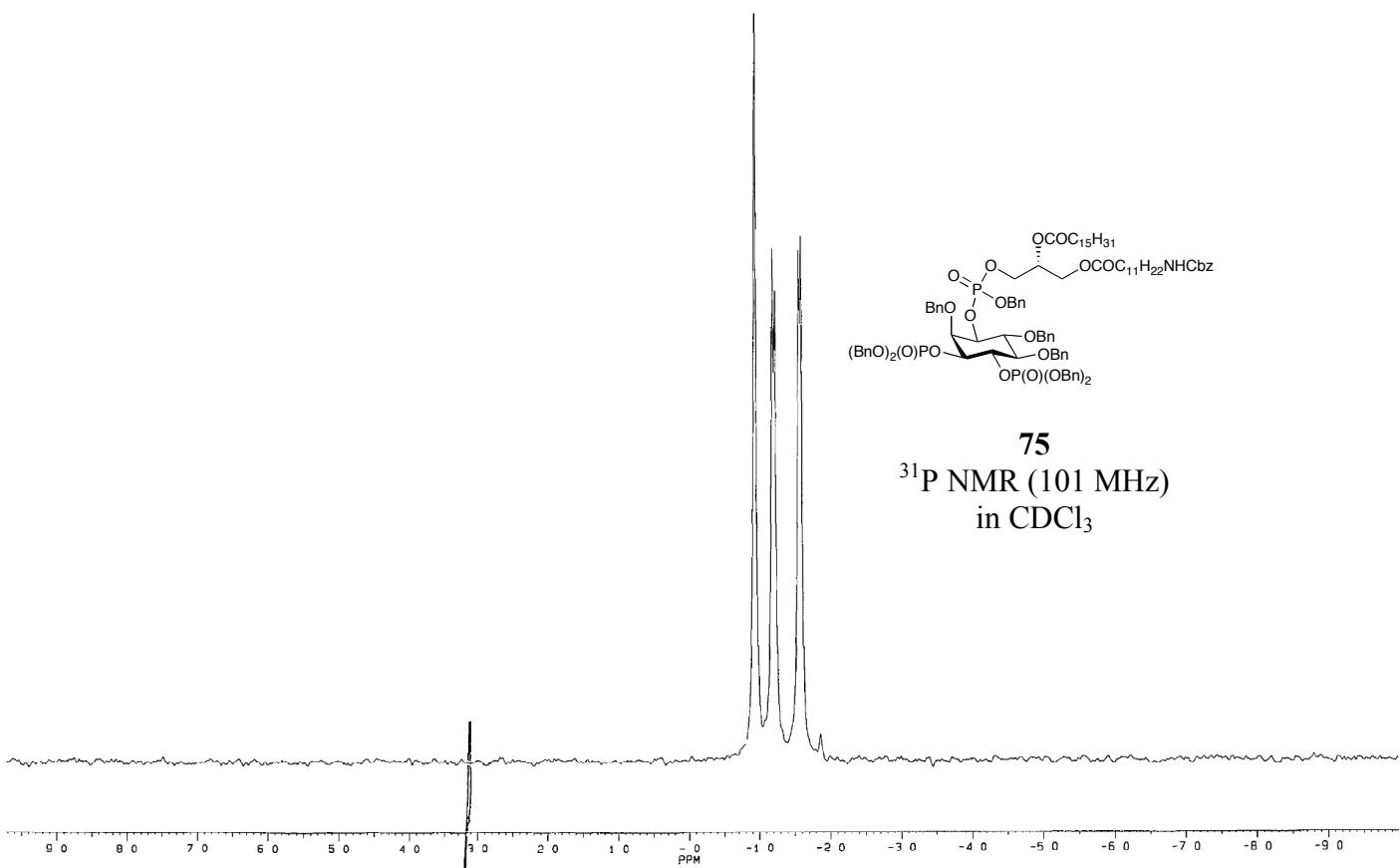
 5
 00 cm
 00 ppm
 17 Hz
 00 ppm
 00 Hz
 33 ppm/cm
 67 Hz/cm



75
¹H NMR (250 MHz)
 in CDCl₃

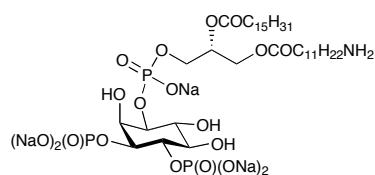


75
 ^{31}P NMR (101 MHz)
in CDCl_3

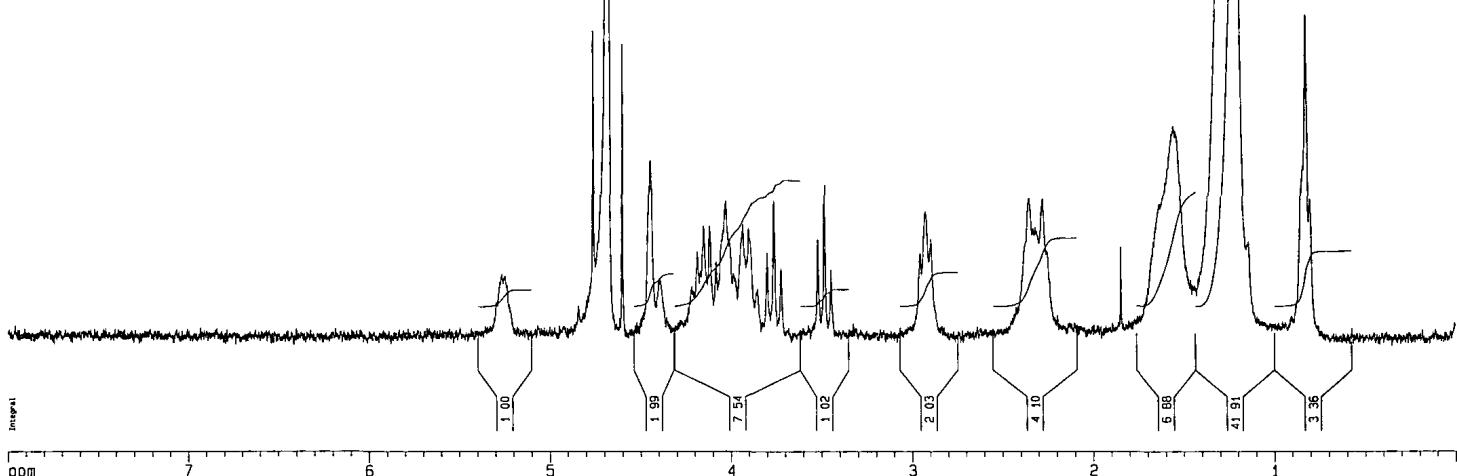


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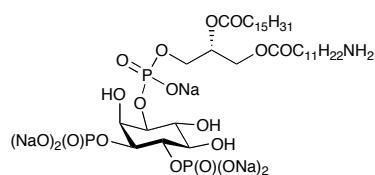


77
 ^1H NMR (250 MHz)
in D_2O

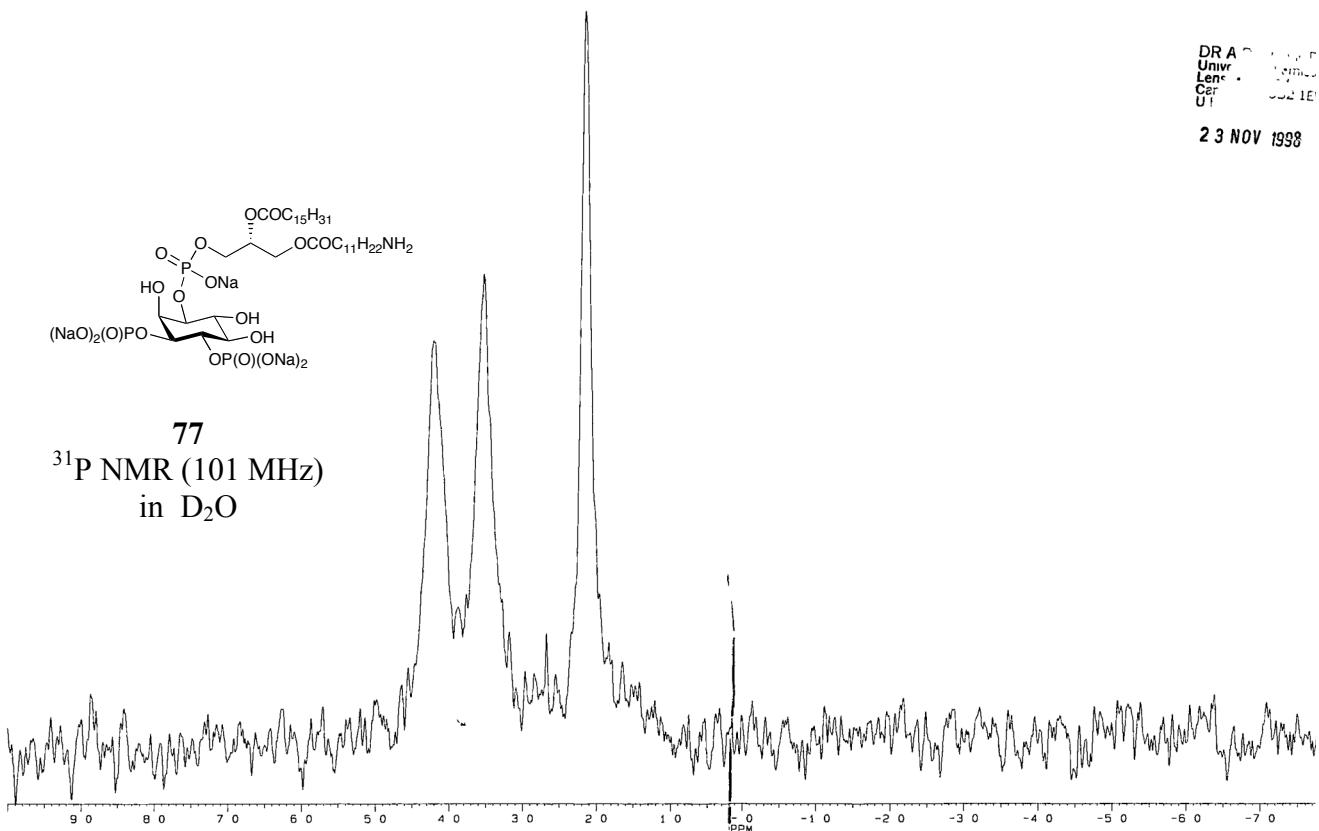


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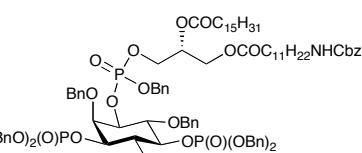
23 NOV 1998



77
 ^{31}P NMR (101 MHz)
in D_2O

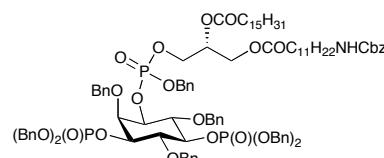
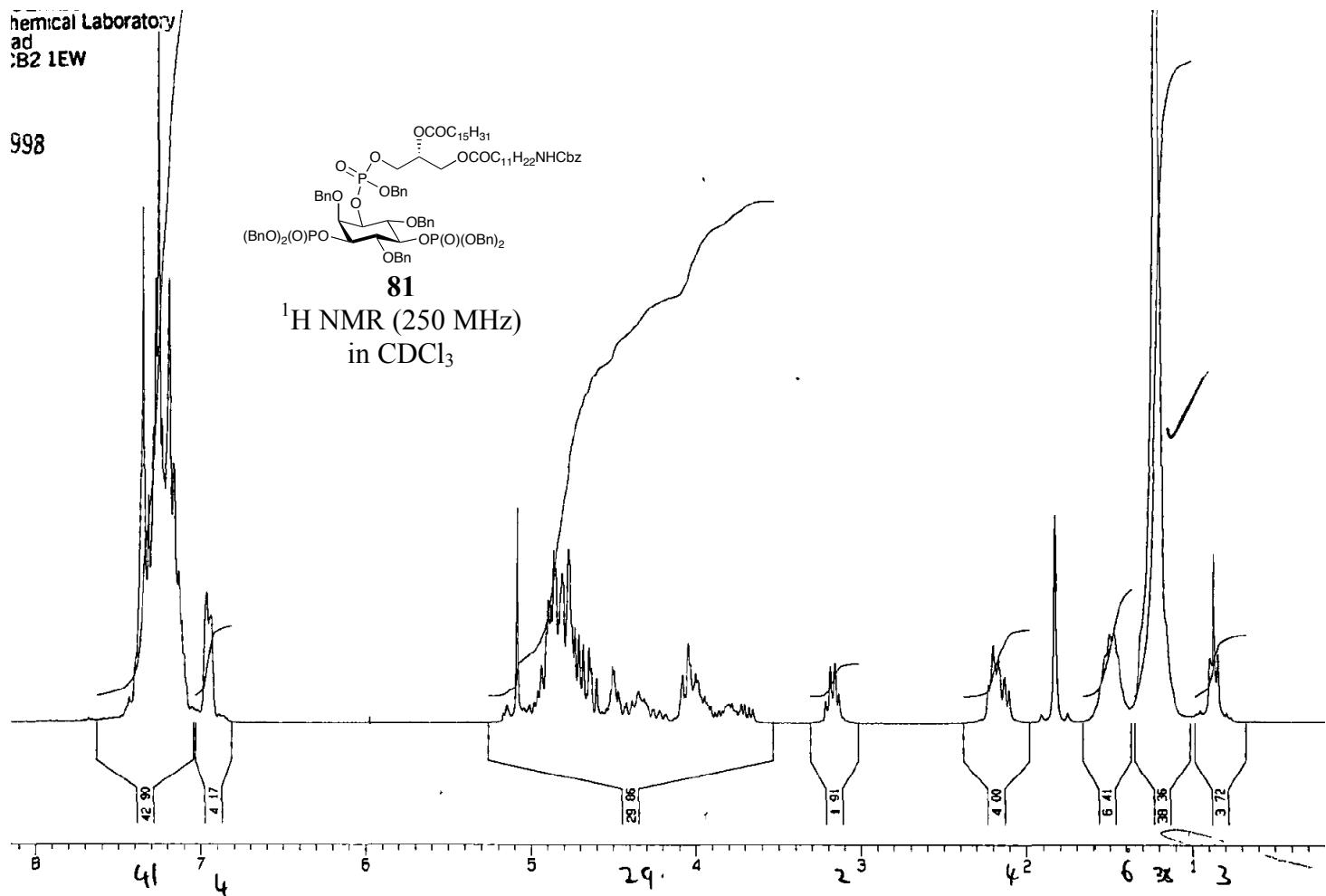


998



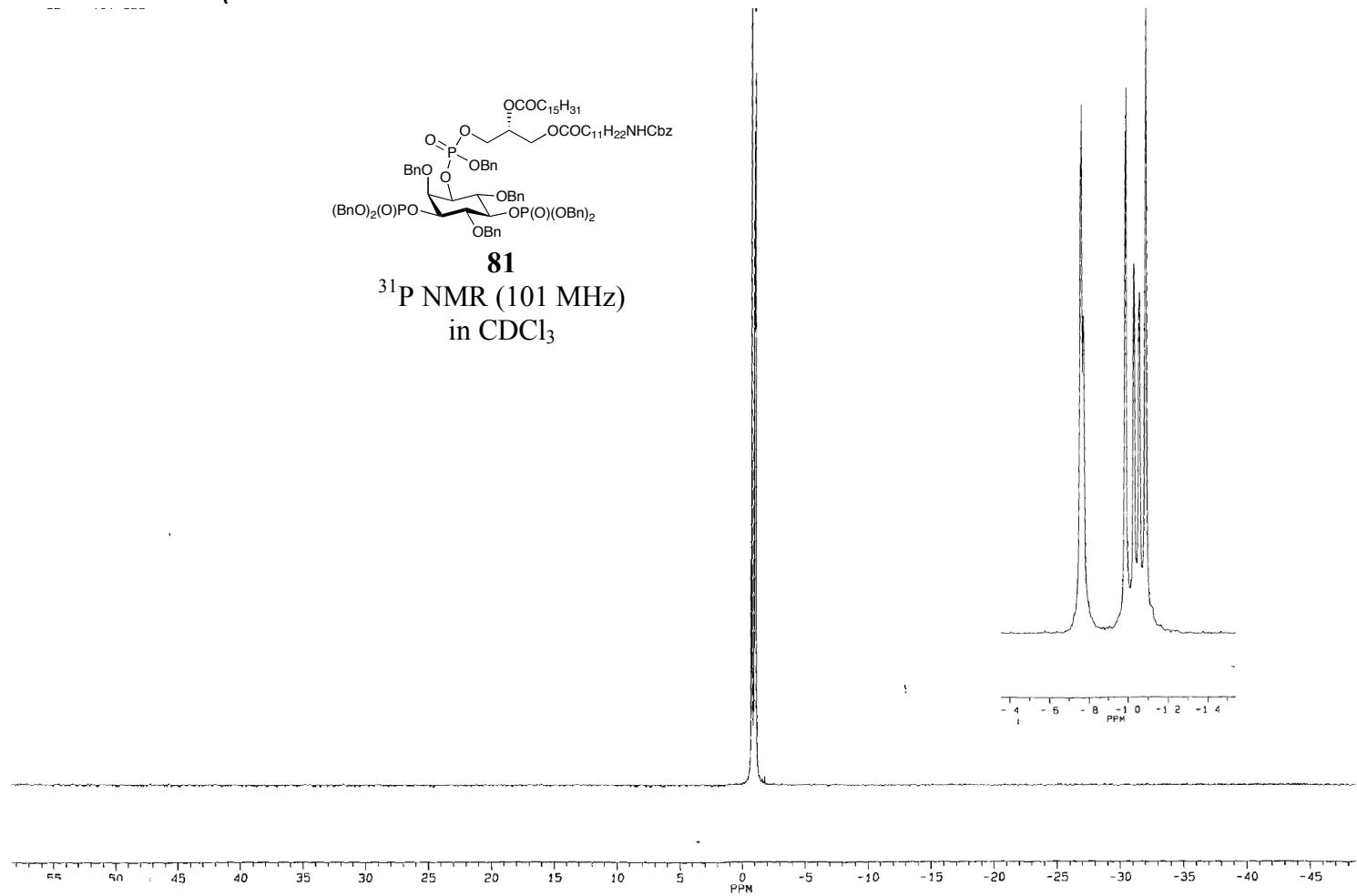
81

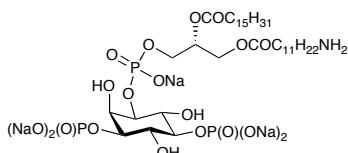
¹H NMR (250 MHz)
in CDCl₃



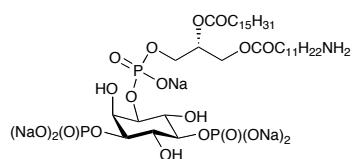
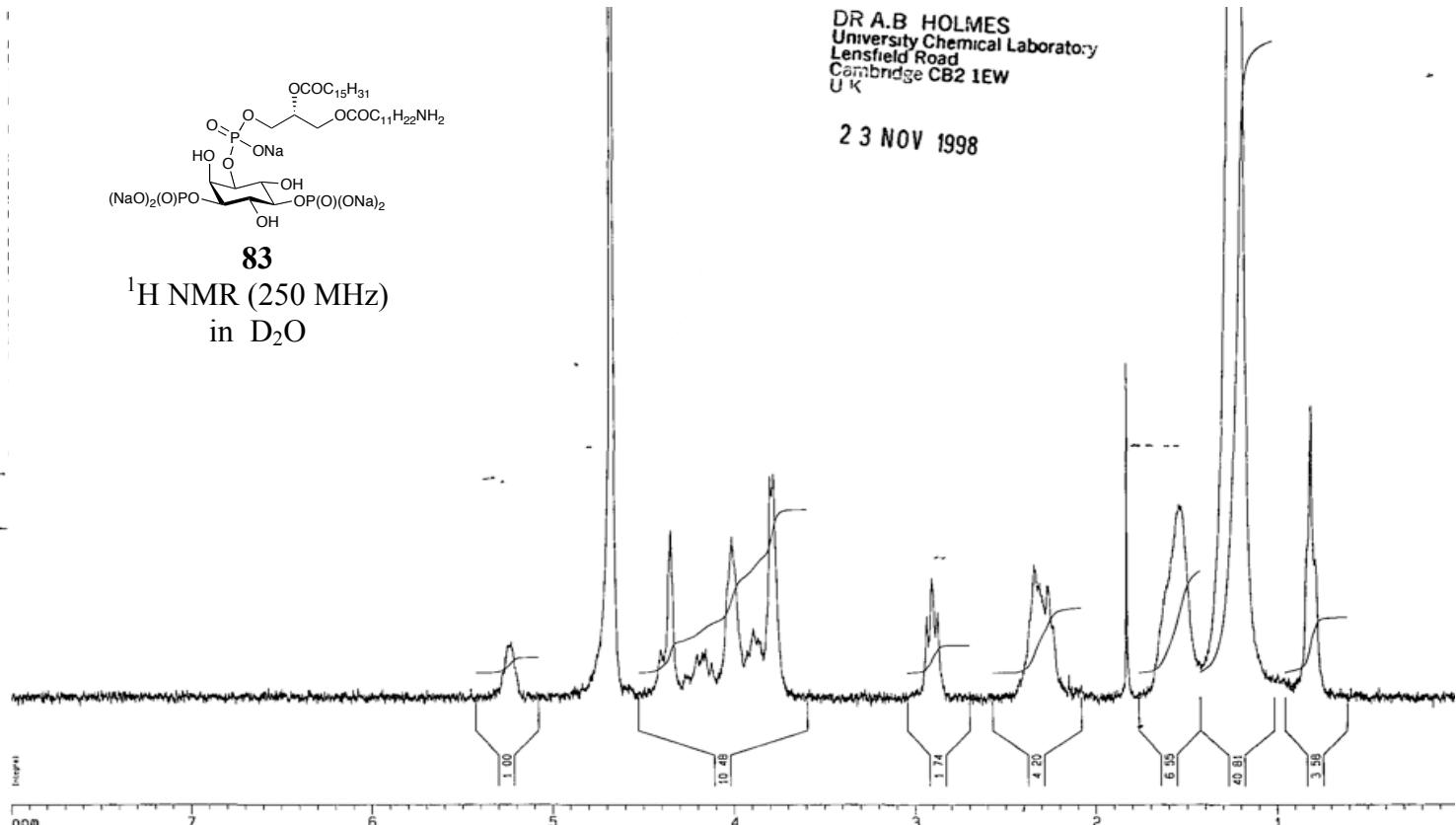
81

³¹P NMR (101 MHz)
in CDCl₃

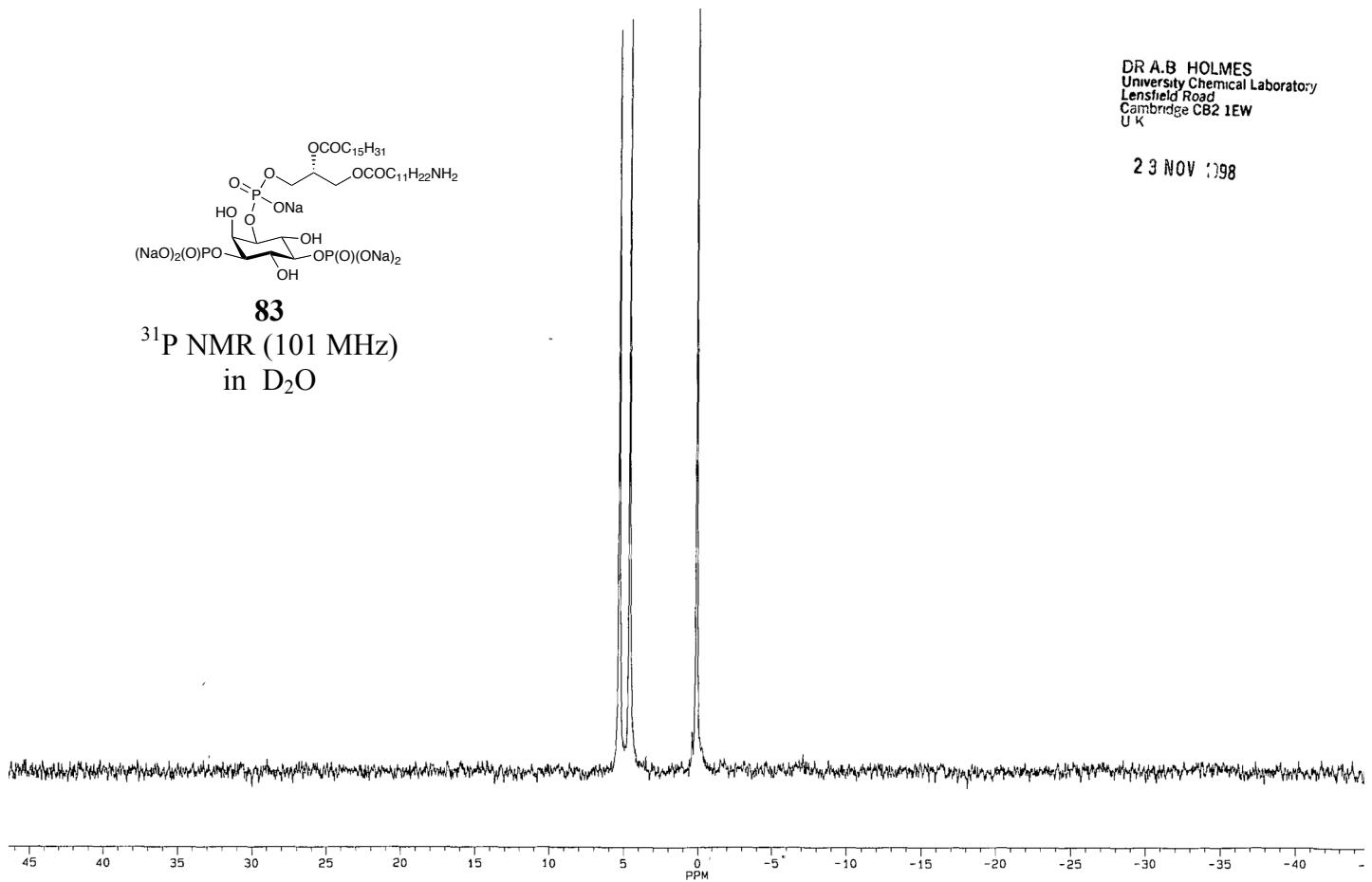




83
¹H NMR (250 MHz)
 in D₂O



83
³¹P NMR (101 MHz)
in D₂O

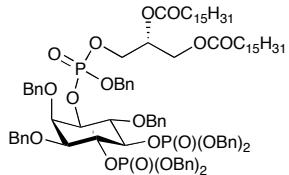


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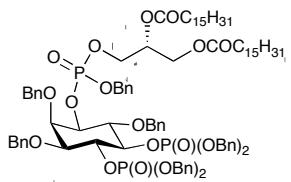
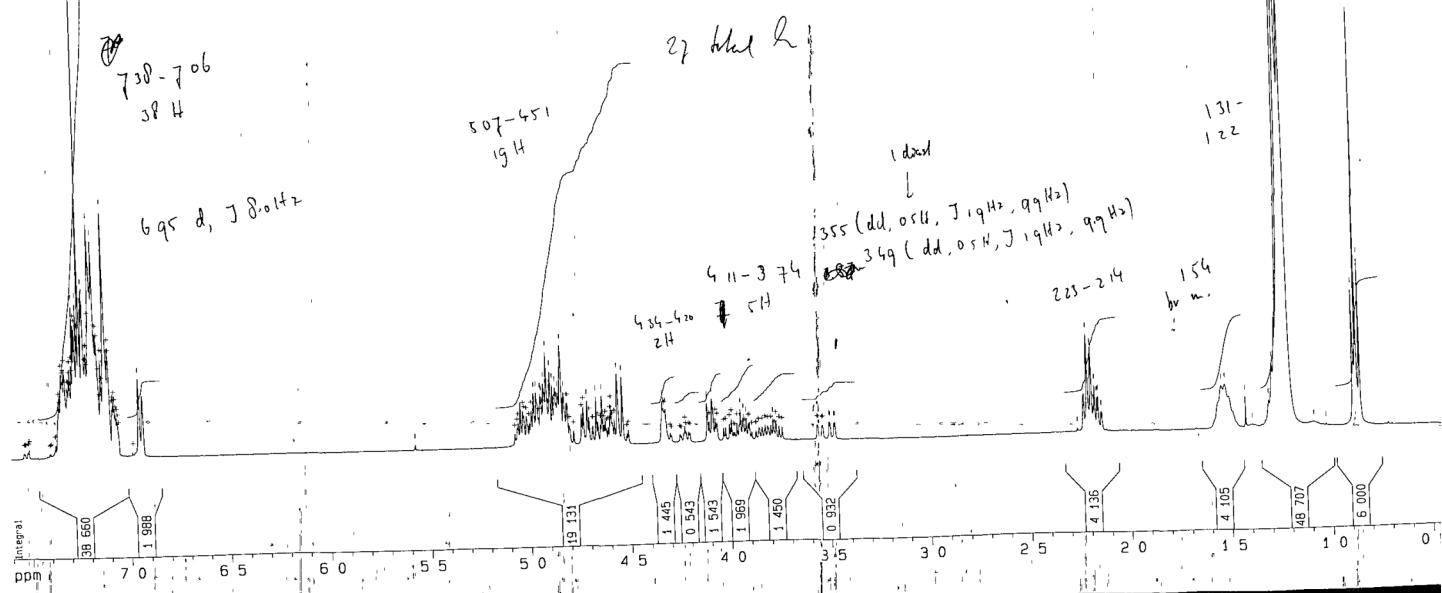
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U.K.

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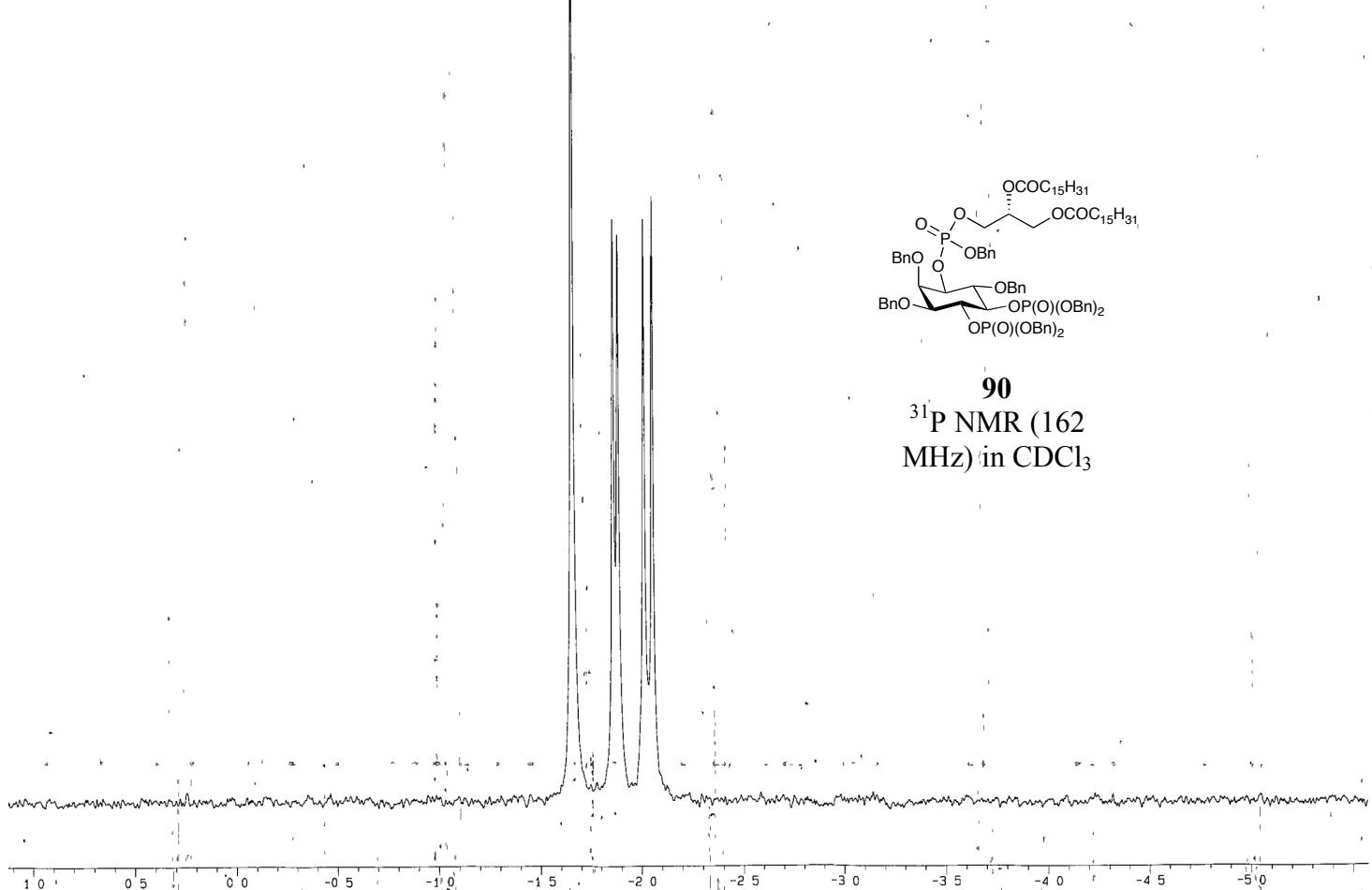
90

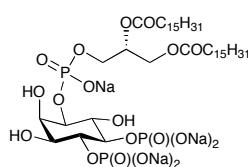
^1H NMR (400 MHz)
in CDCl_3



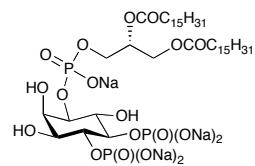
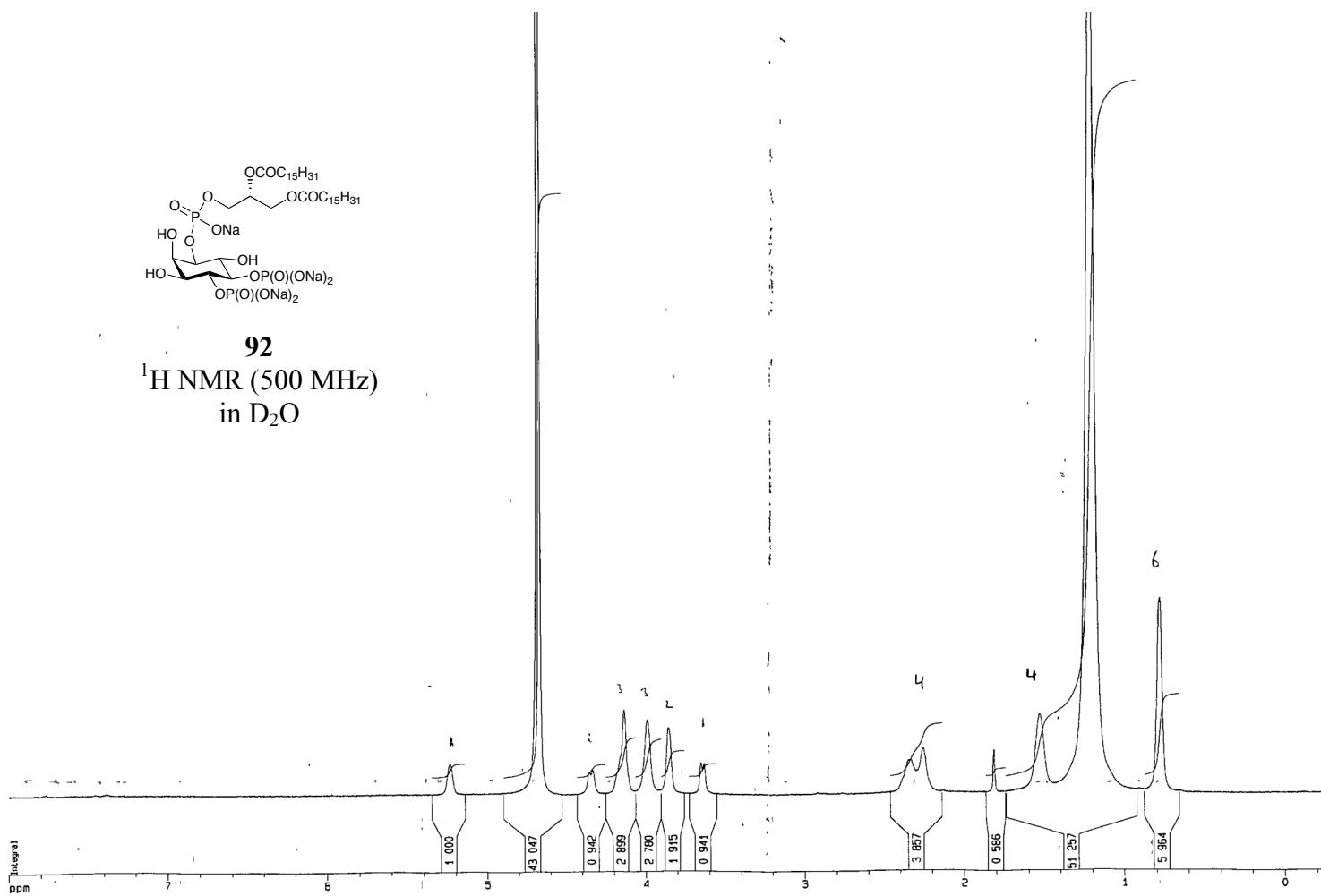
90

^{31}P NMR (162 MHz) in CDCl_3

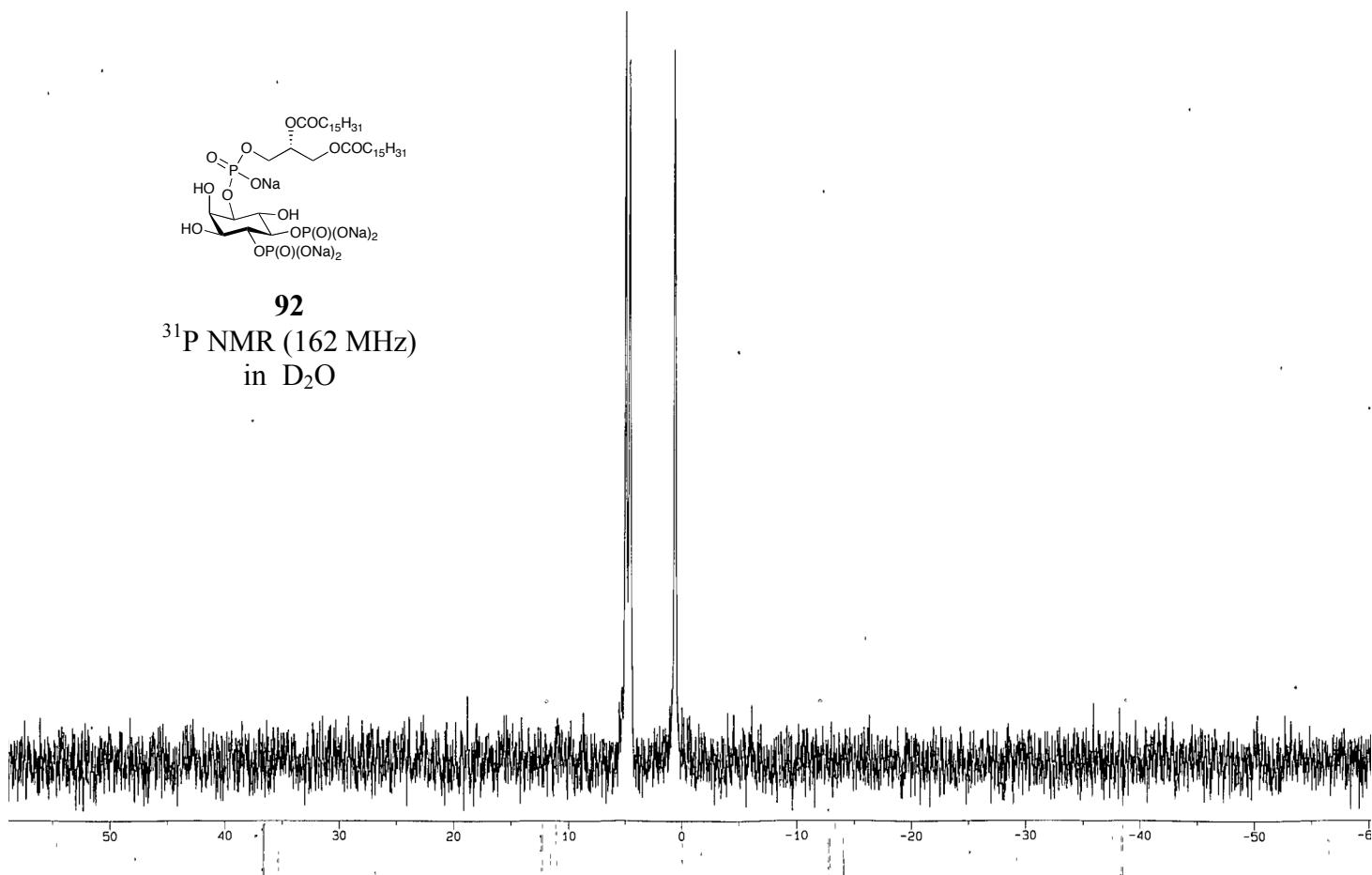




92
 ^1H NMR (500 MHz)
 in D_2O



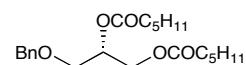
92
 ^{31}P NMR (162 MHz)
 in D_2O



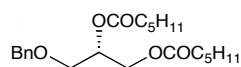
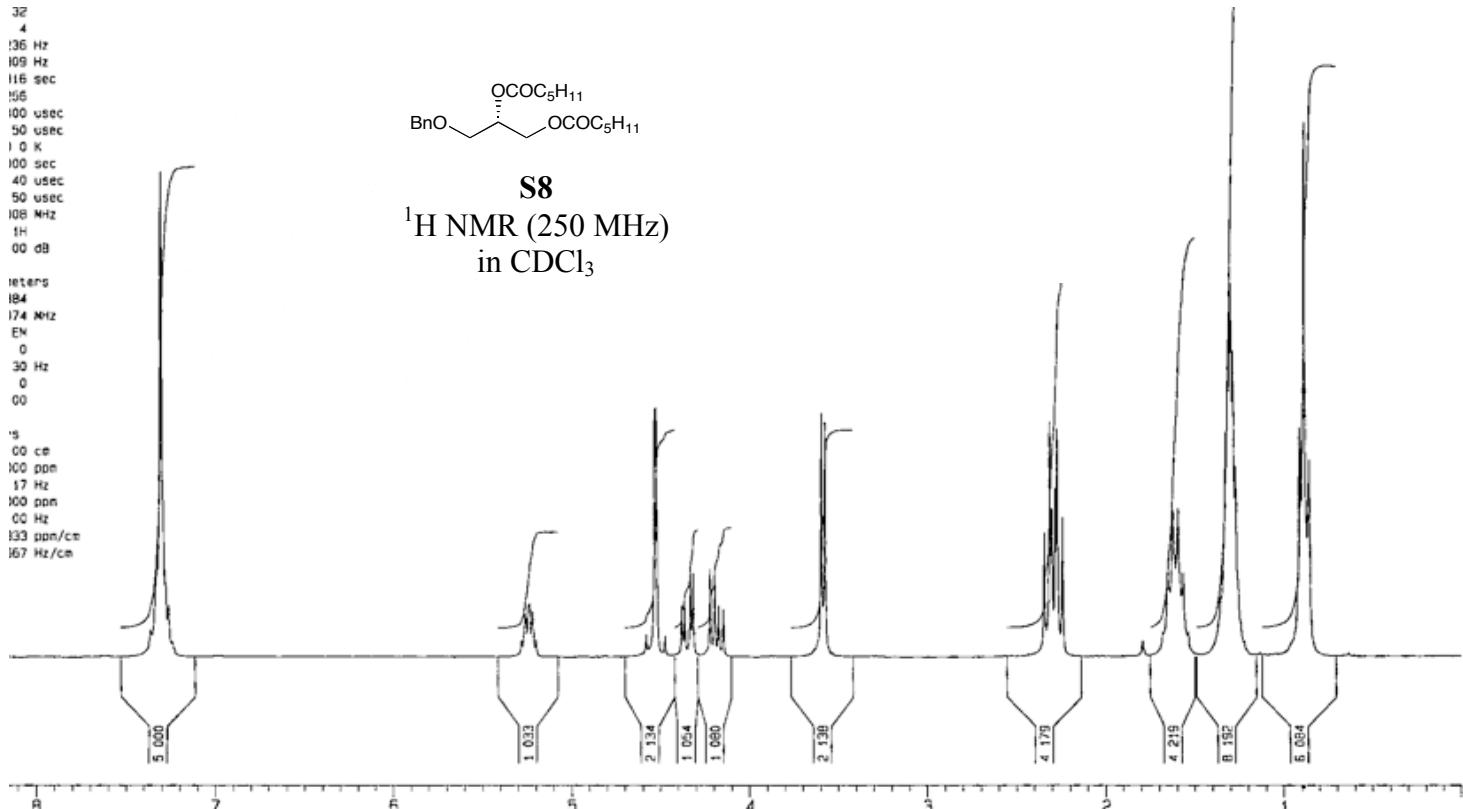
32
4
136 Hz
109 Hz
116 sec
156
100 usec
50 usec
1.0 K
100 sec
40 usec
50 usec
108 MHz
1H
00 dB

meters
184
174 MHz
EM
0
30 Hz
0
00

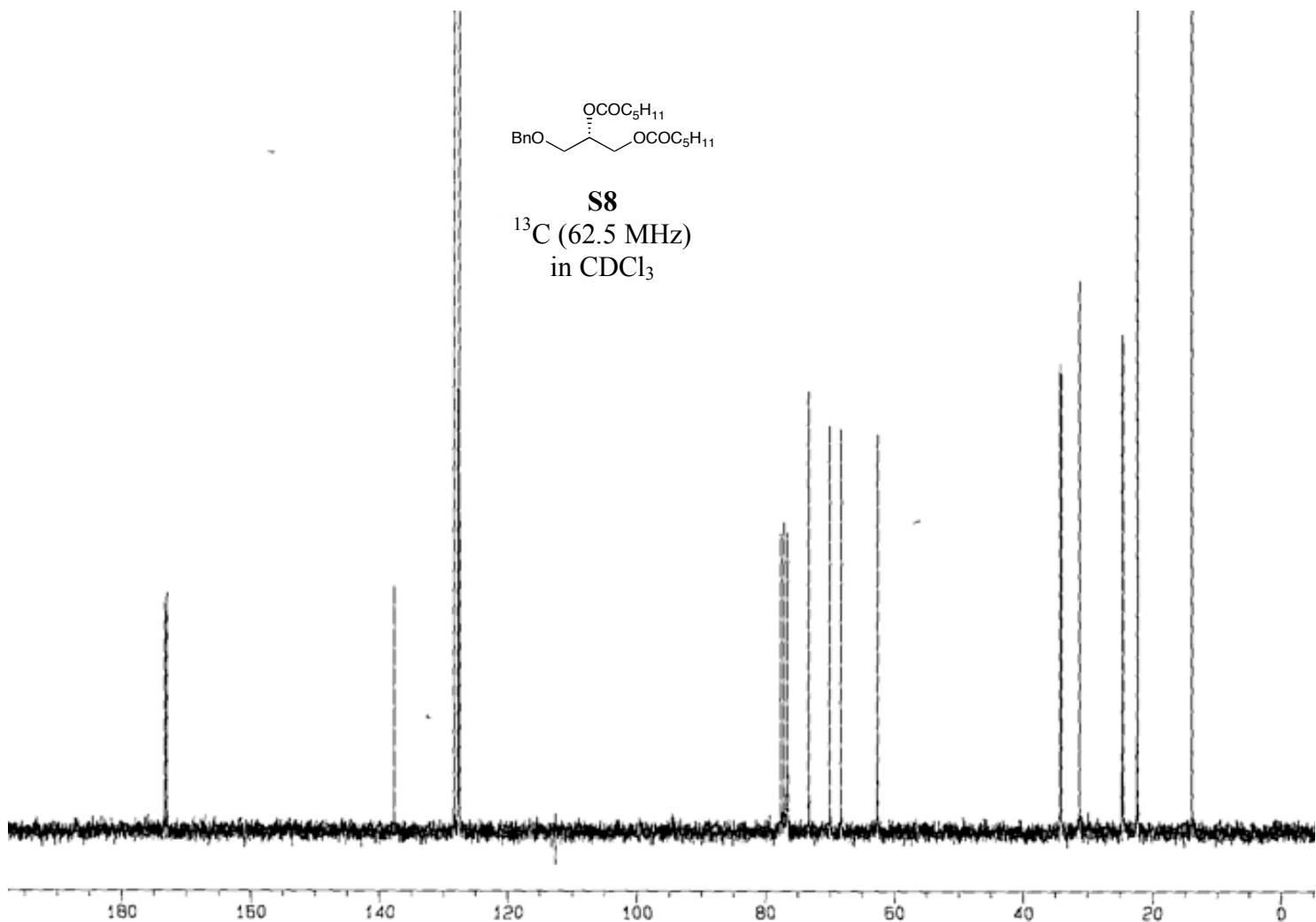
'S
00 cps
100 ppm
17 Hz
100 ppm
00 Hz
133 ppm/cps
167 Hz/cm



S8
 ^1H NMR (250 MHz)
in CDCl_3

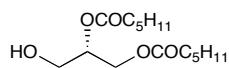


S8
 ^{13}C (62.5 MHz)
in CDCl_3



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2 2 Nov 1988



S9

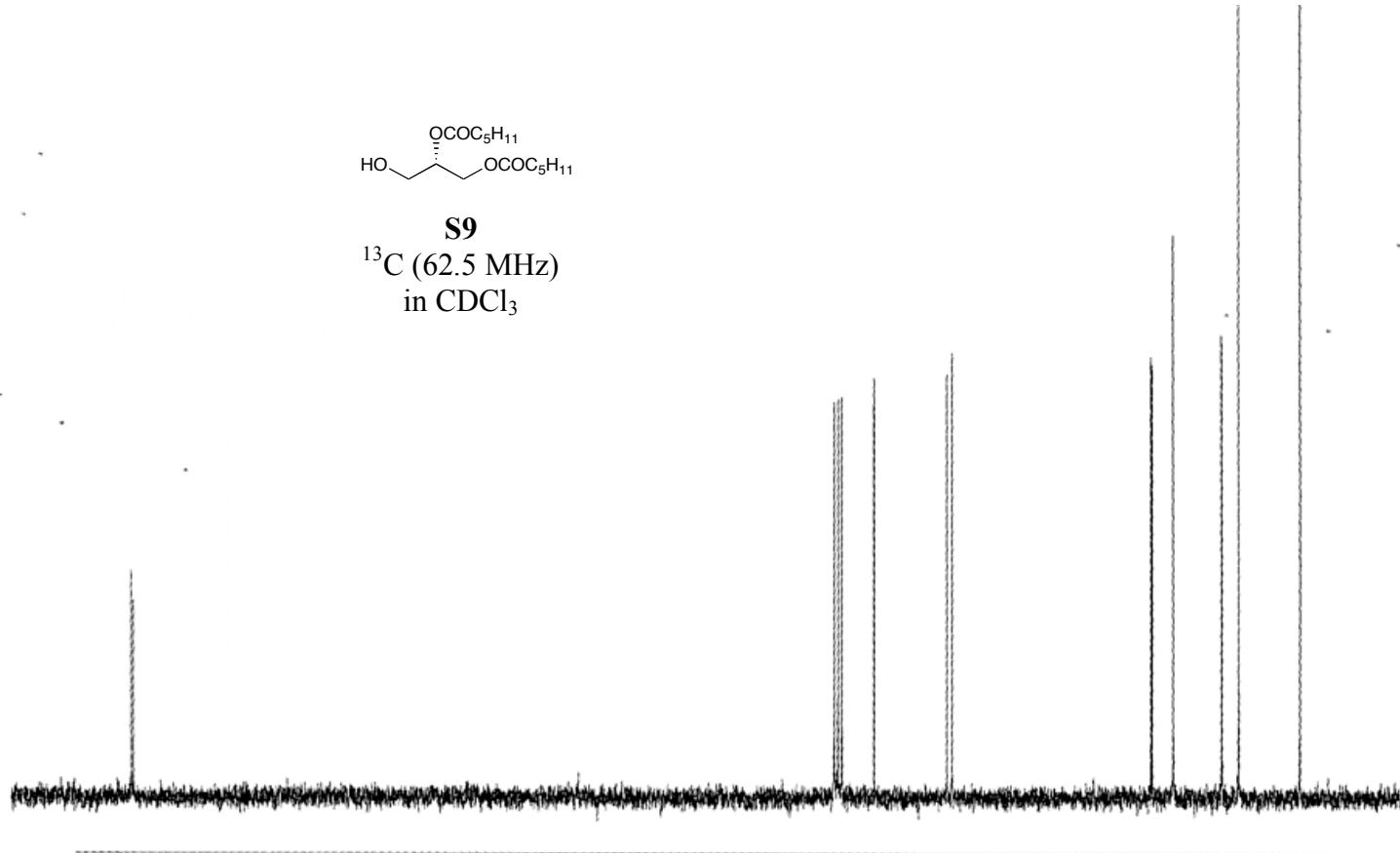
^1H NMR (250 MHz)
in CDCl_3

meters
04
06
ct
1H
30
84
13
32
4
35 Hz
09 Hz
16 sec
56
00 usec
50 usec
0 K
00 sec
40 usec
50 usec
08 MHz
1H
00 dB

eterns
B4
74 MHz
EM
0
30 Hz
0
40

5 cm
00 ppm
17 Hz
00 ppm
00 Hz
33 ppm/cm
57 Hz/cm

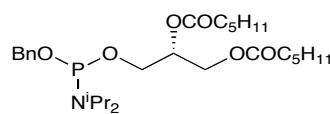
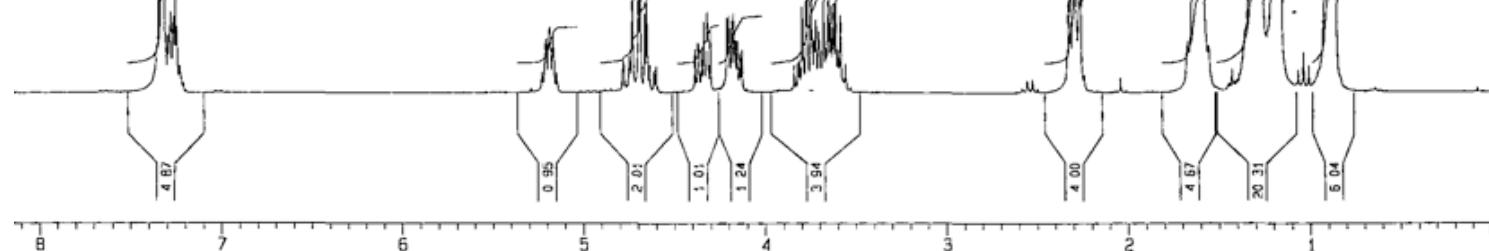
7 6 5 4 3 2 1



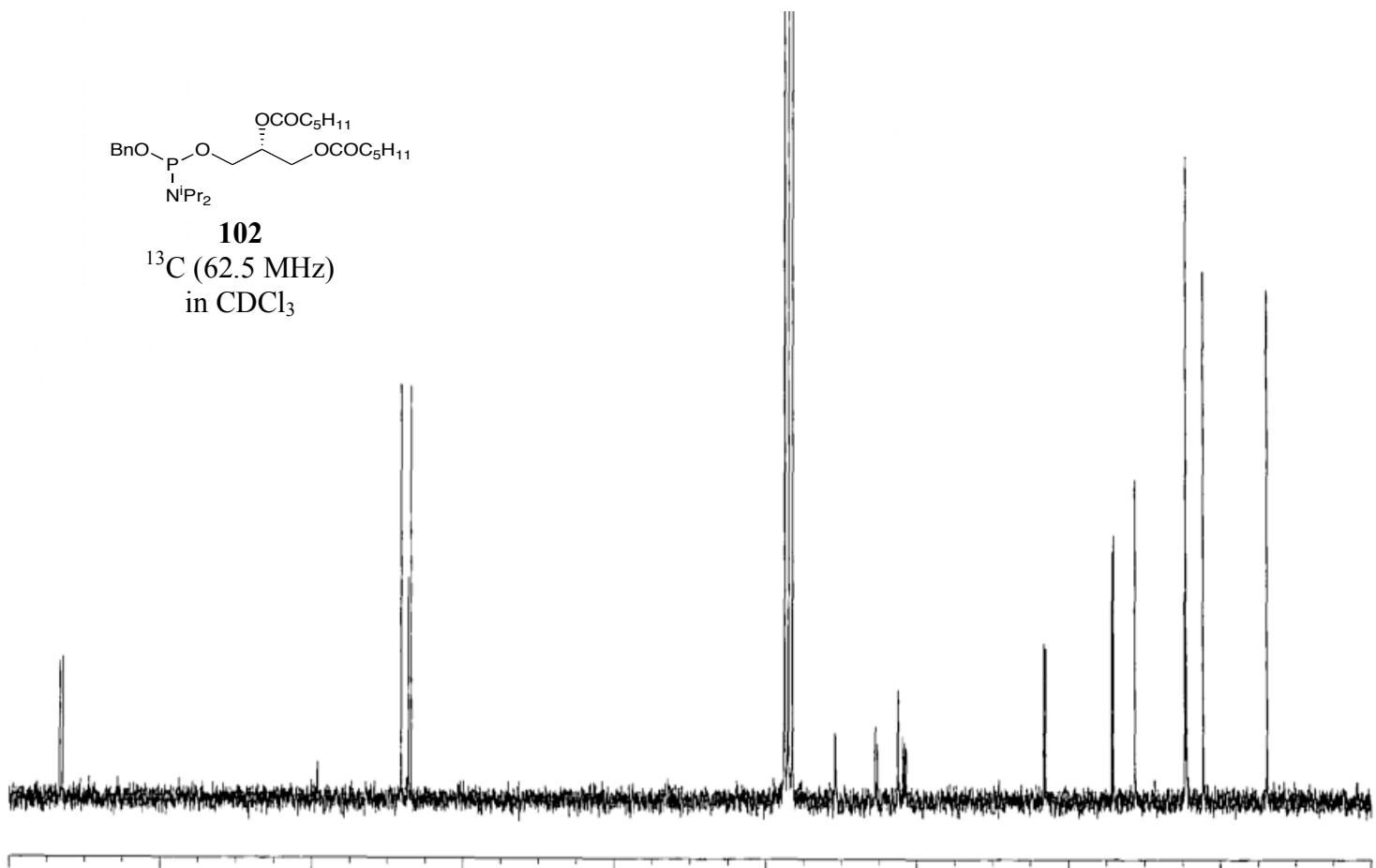
Meters
0.6
40
1ct
1H
13C
32
4
135 Hz
109 Hz
116 sec
156
100 usec
50 usec
1.0 K
100 sec
40 usec
50 usec
108 MHz
1H
00 dB

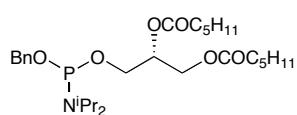
Meters
184
174 MHz
EM
0
30 Hz
0
00

's
00 cm
100 ppm
17 Hz
100 ppm
00 Hz
133 ppm/cm
167 Hz/cm

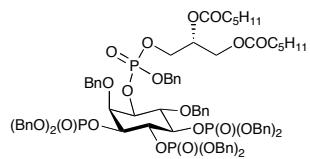
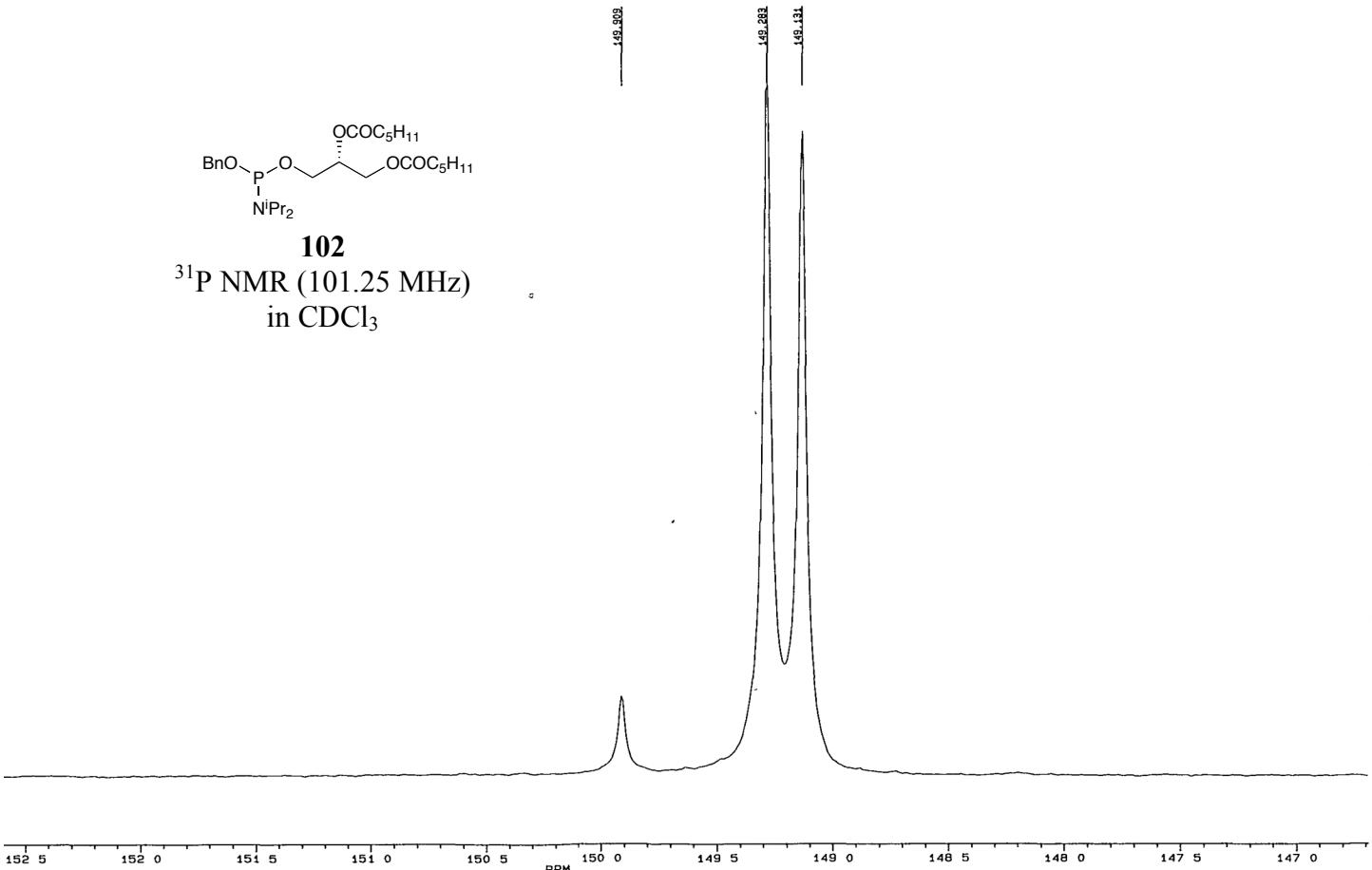


^{13}C (62.5 MHz)
in CDCl_3

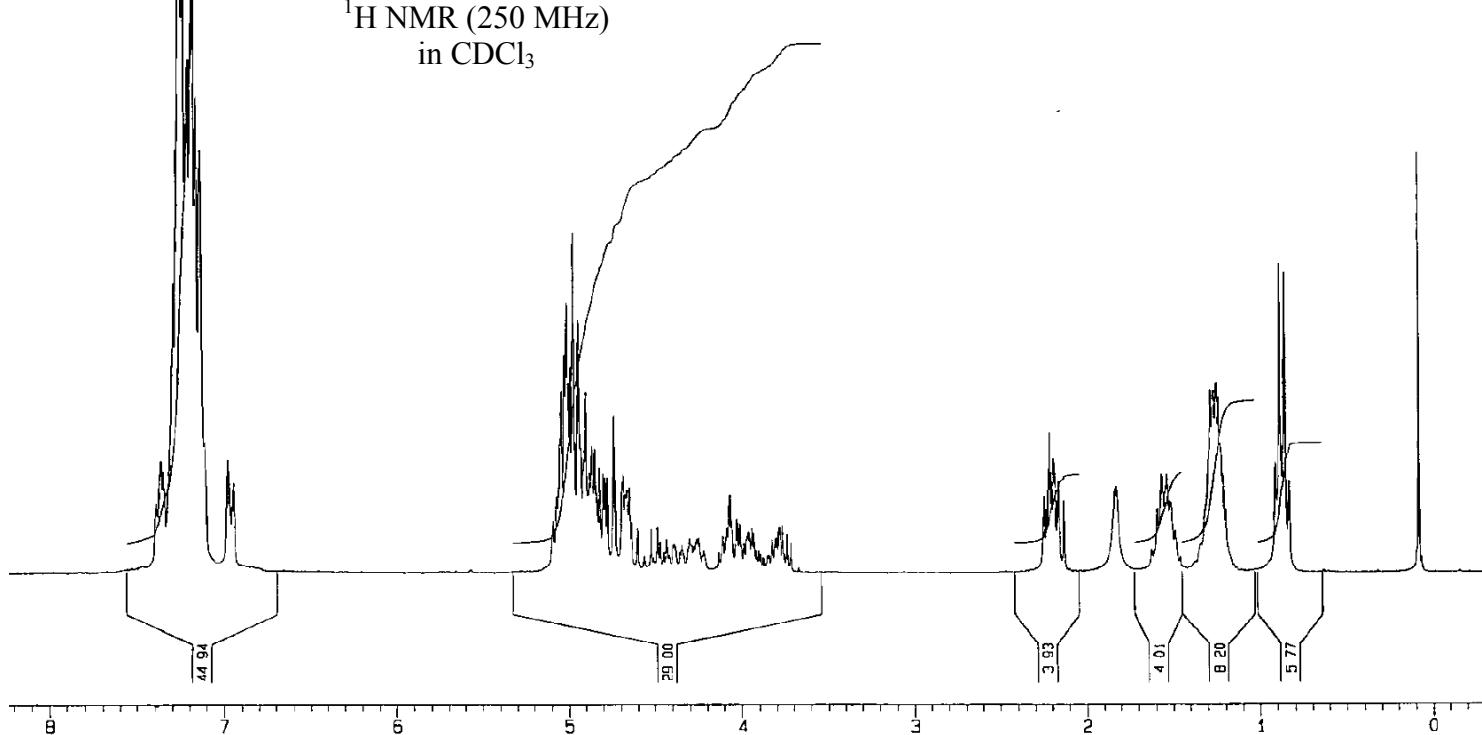


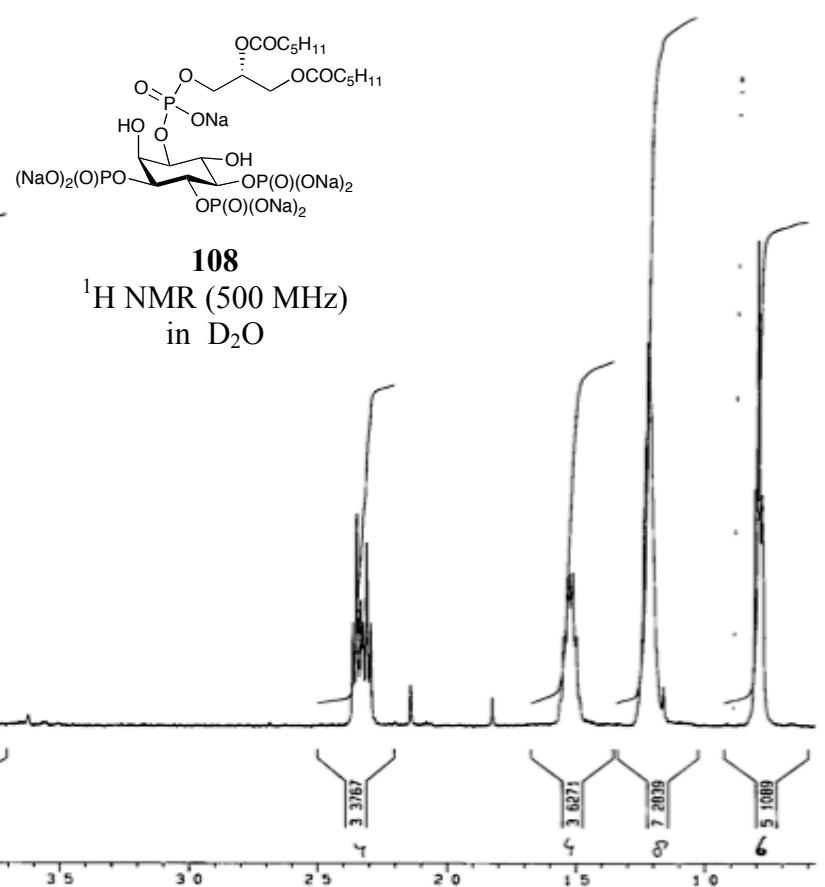
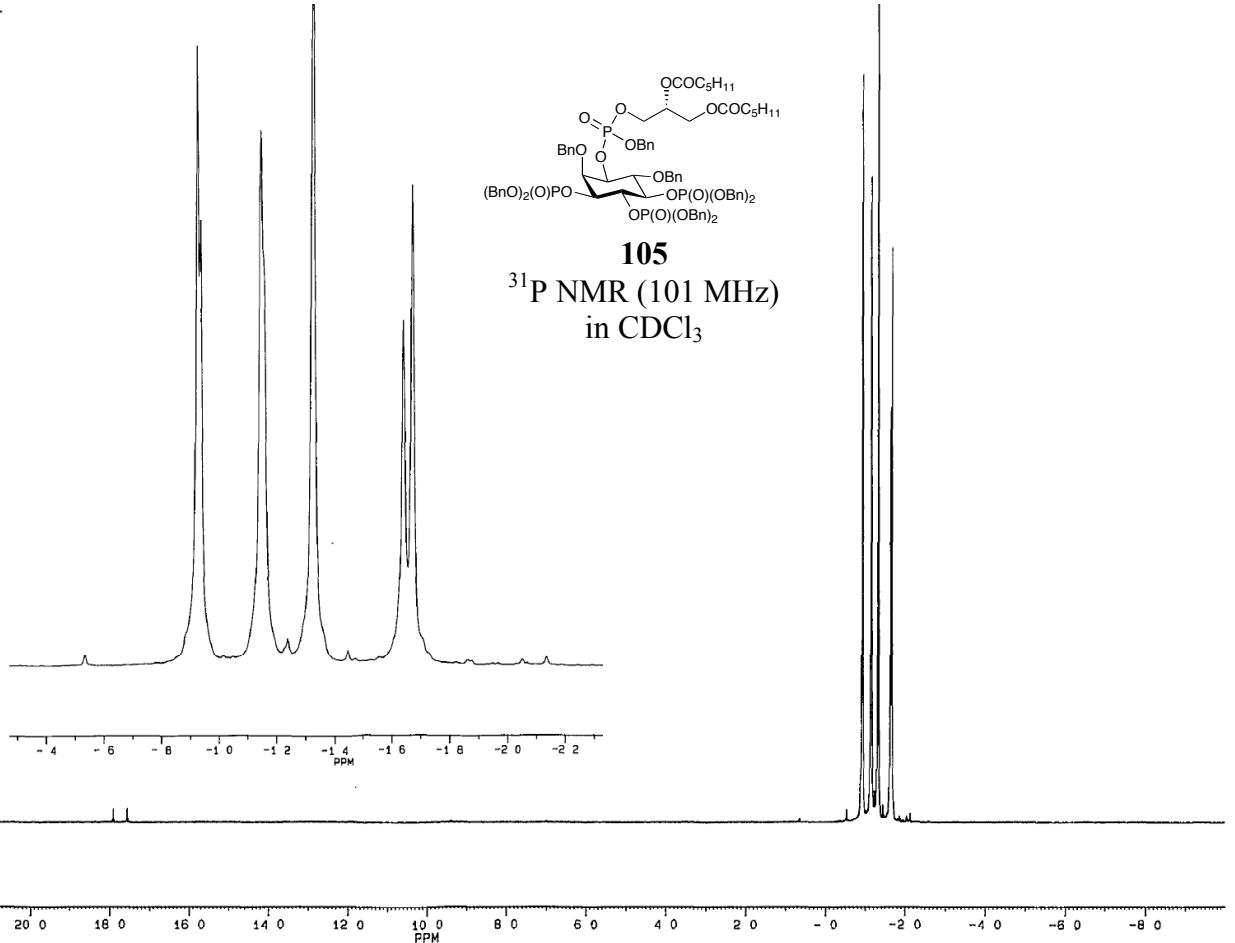


^{31}P NMR (101.25 MHz)
in CDCl_3

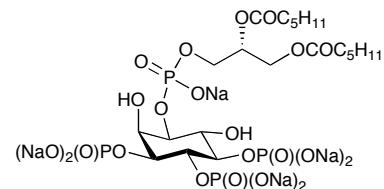


^1H NMR (250 MHz)
in CDCl_3

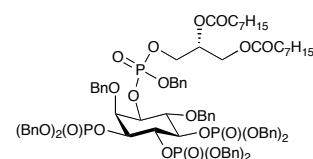
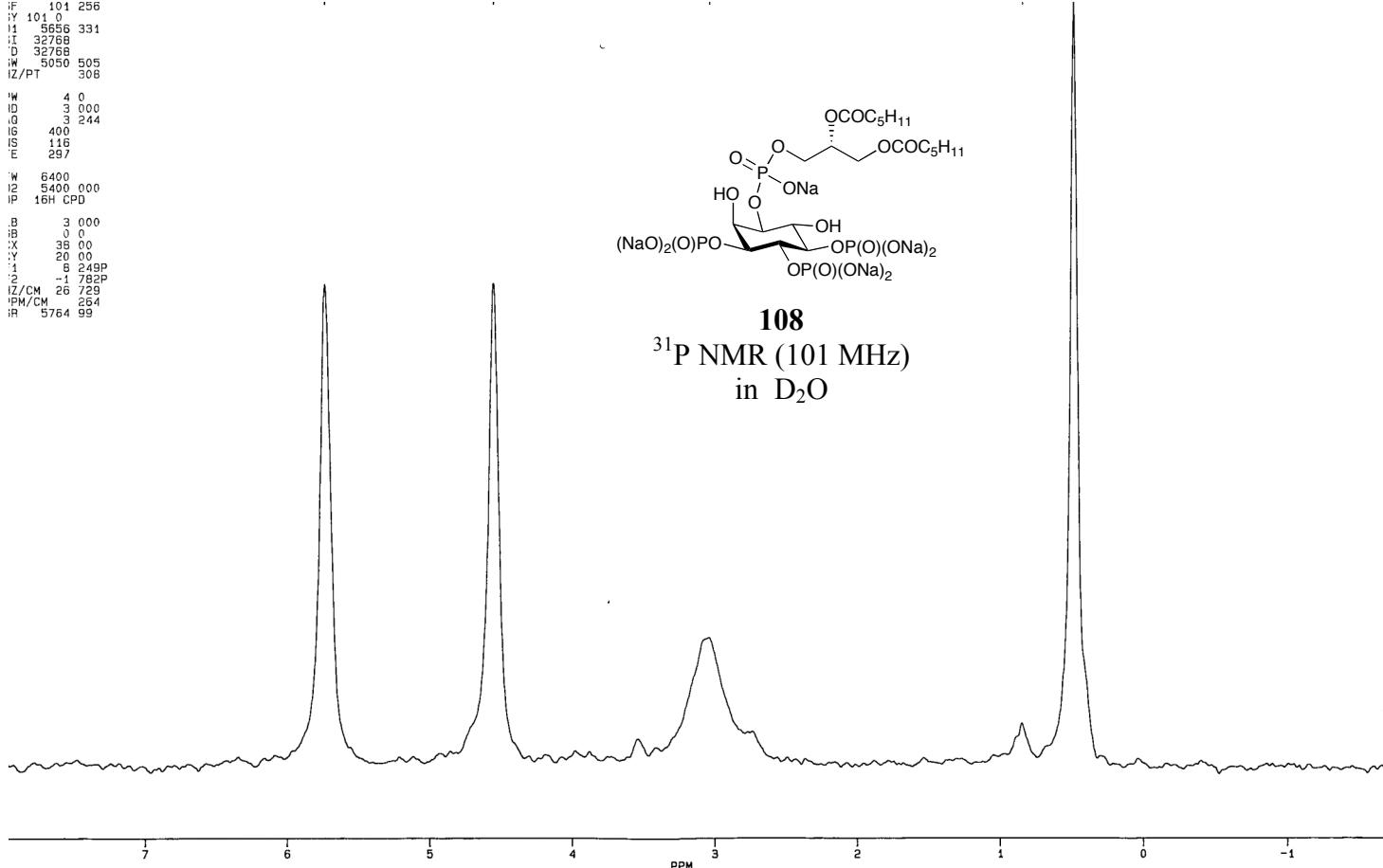




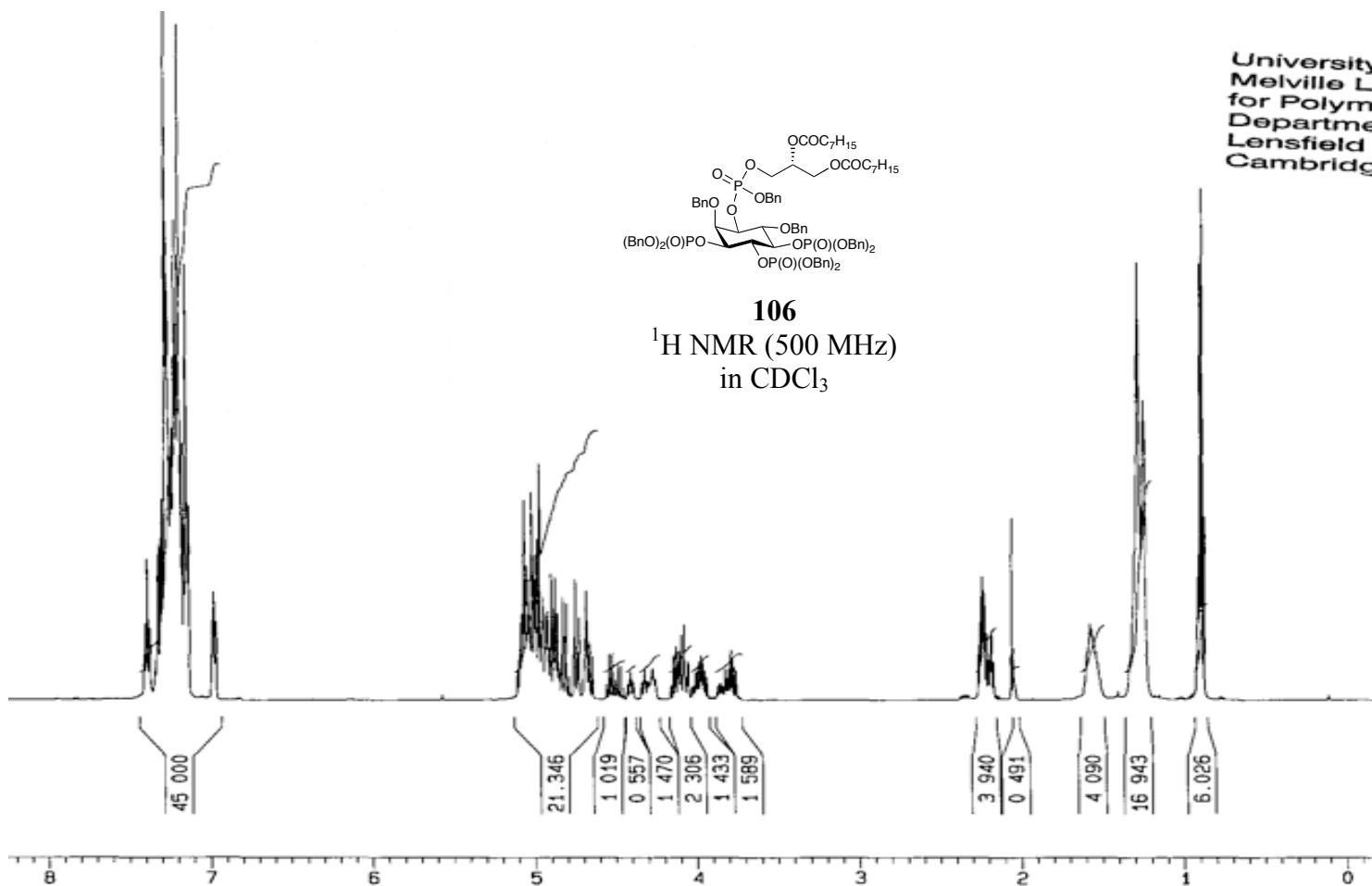
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 iY 104.0 5656 331
 iI 32768
 iD 32768
 iW 5050 505
 IZ/PT 308
 iW 4 0
 iD 3 000
 iG 3 244
 iE 400
 iL 116
 iS 297
 iW 6400
 iD 5400 000
 iCPD 16H CPD
 iB 3 000
 iC 3 000
 iX 35 00
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 iI 200 00
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 iW -1 782P
 iZ/CM 26 729
 iPM/CM 26 254
 iW 5764 99



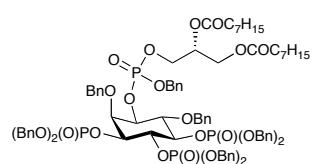
108
 ^{31}P NMR (101 MHz)
 in D_2O



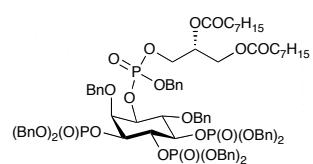
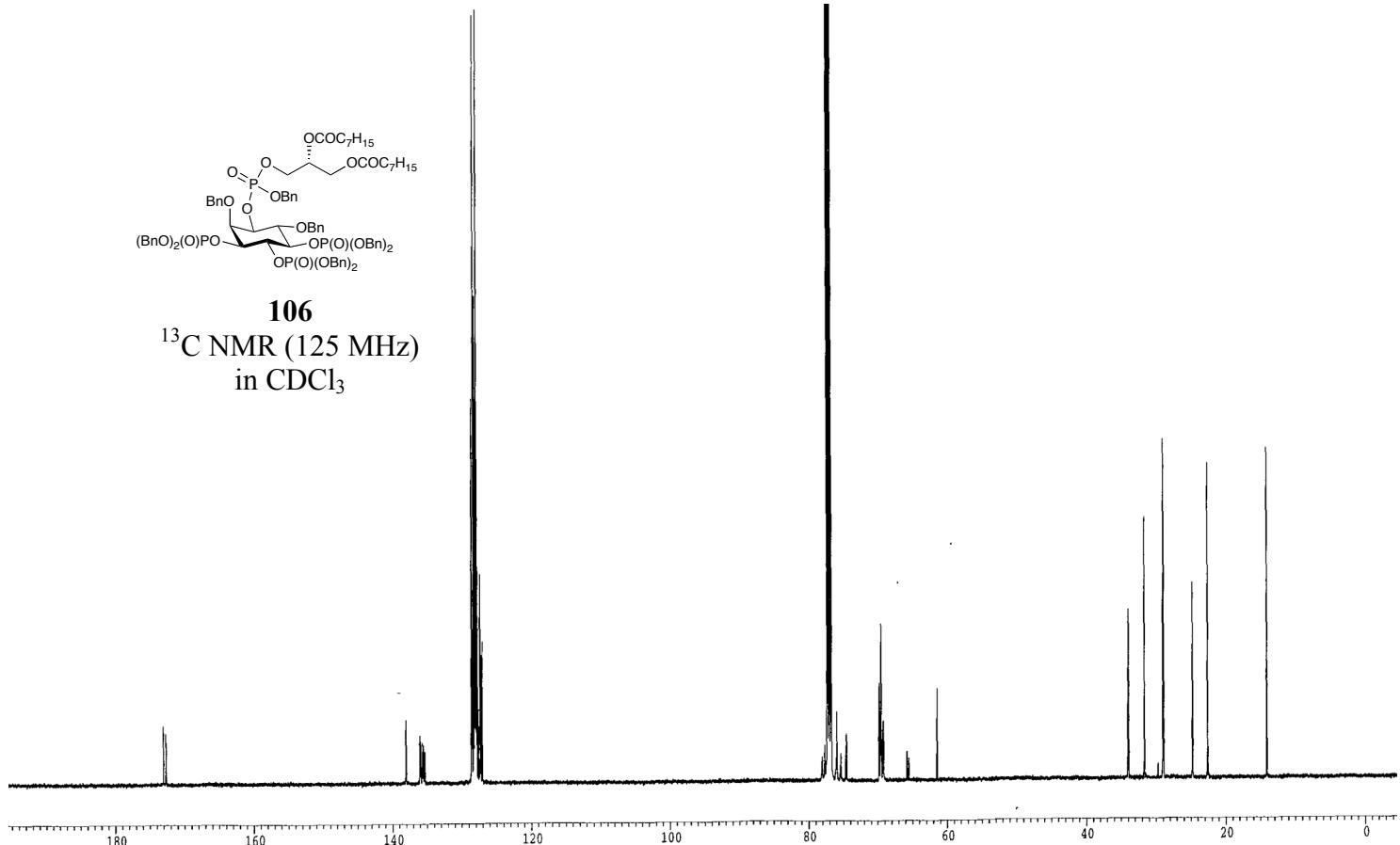
106
 ^1H NMR (500 MHz)
 in CDCl_3



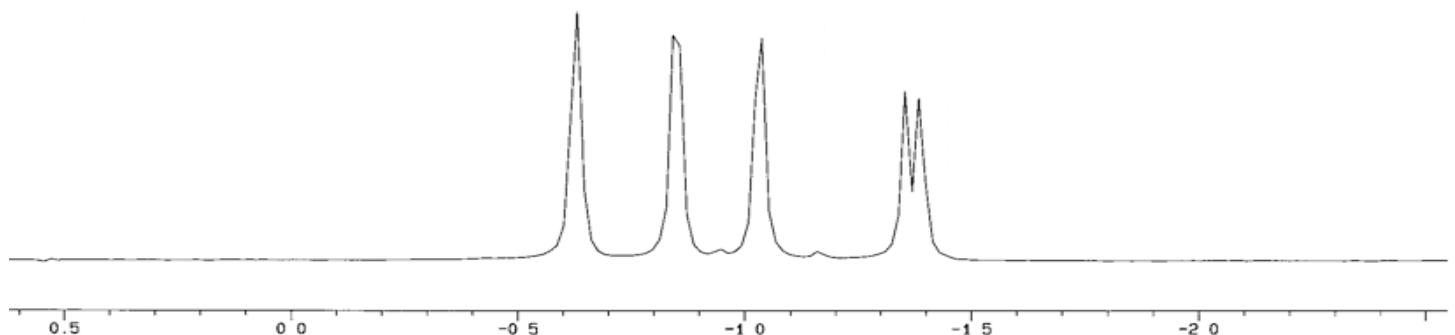
University
 Melville Li
 for Polym
 Departme
 Lensfield
 Cambridge

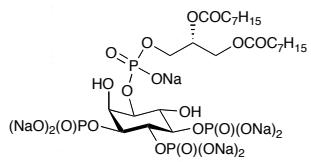


106
¹³C NMR (125 MHz)
in CDCl₃

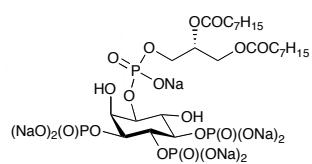
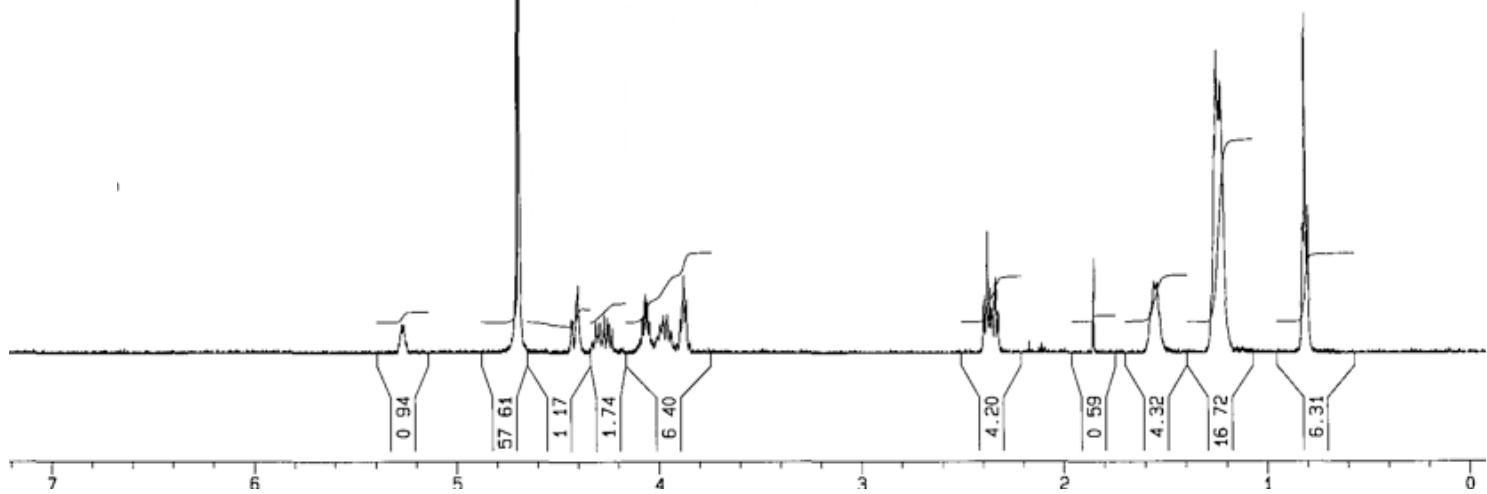


106
³¹P NMR (202 MHz)
in CDCl₃

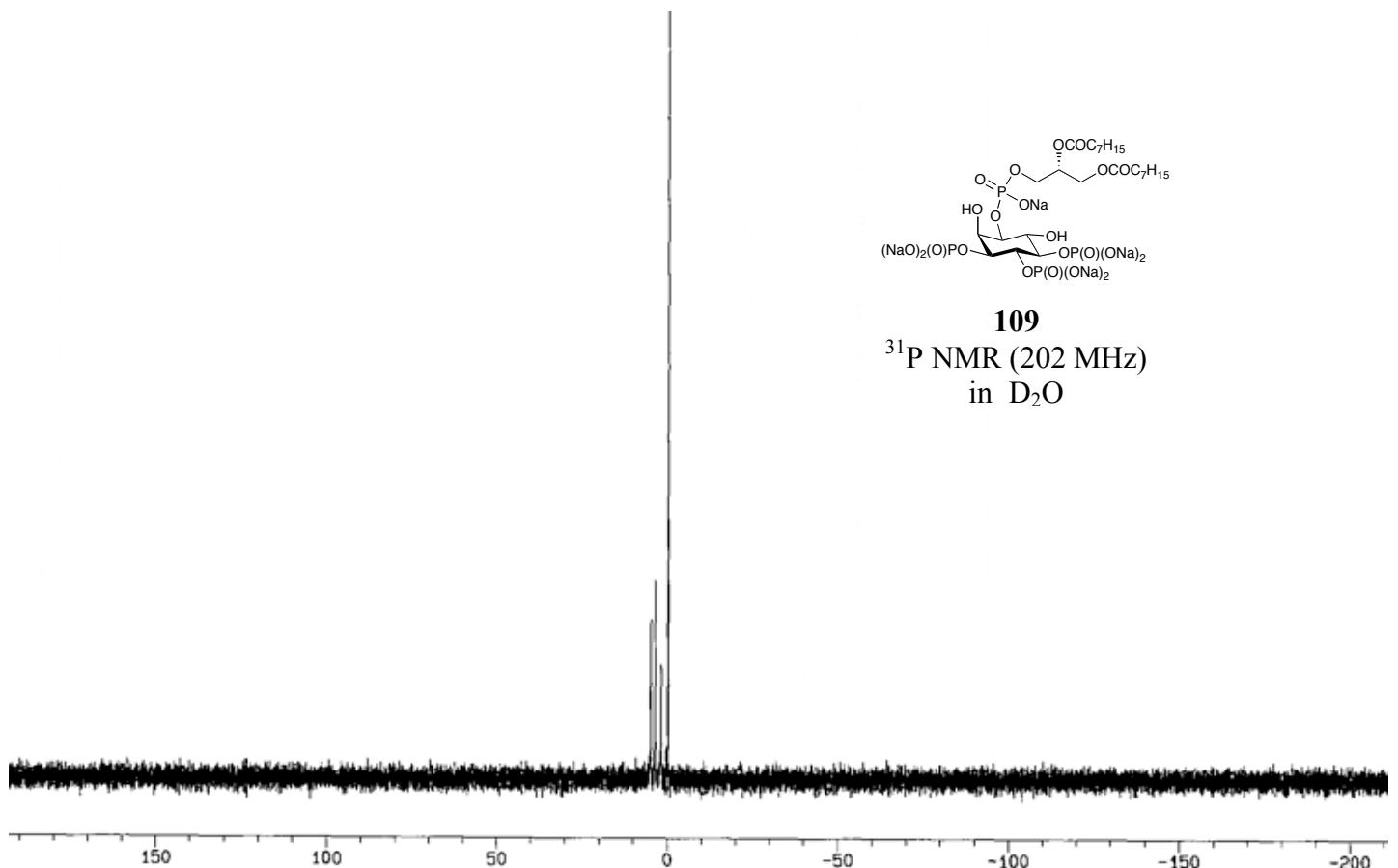


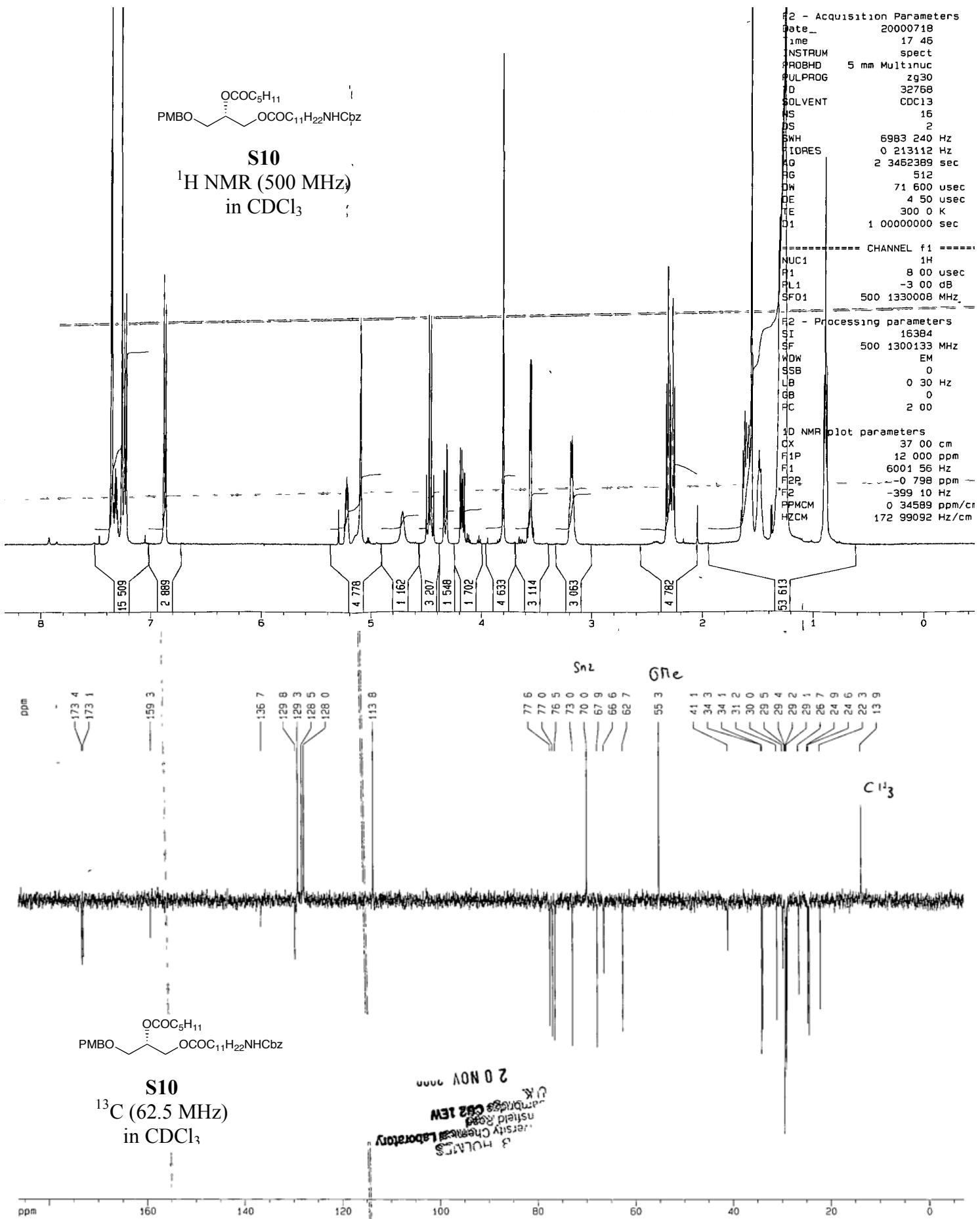


109
 ^1H NMR (500 MHz)
 in D_2O

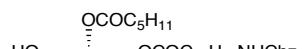


109
 ^{31}P NMR (202 MHz)
 in D_2O



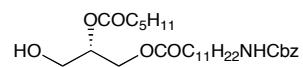
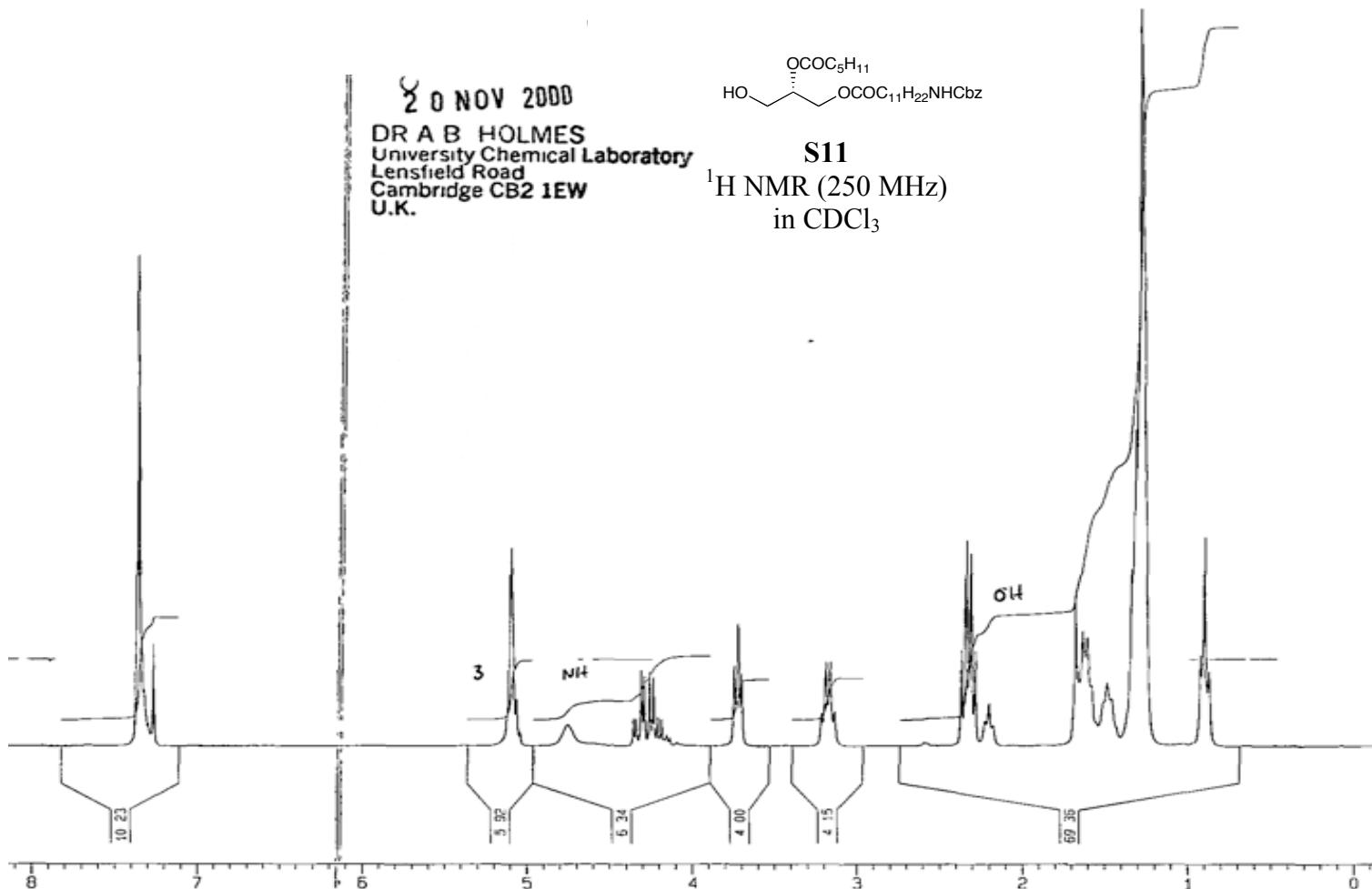


20 NOV 2000
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U.K.



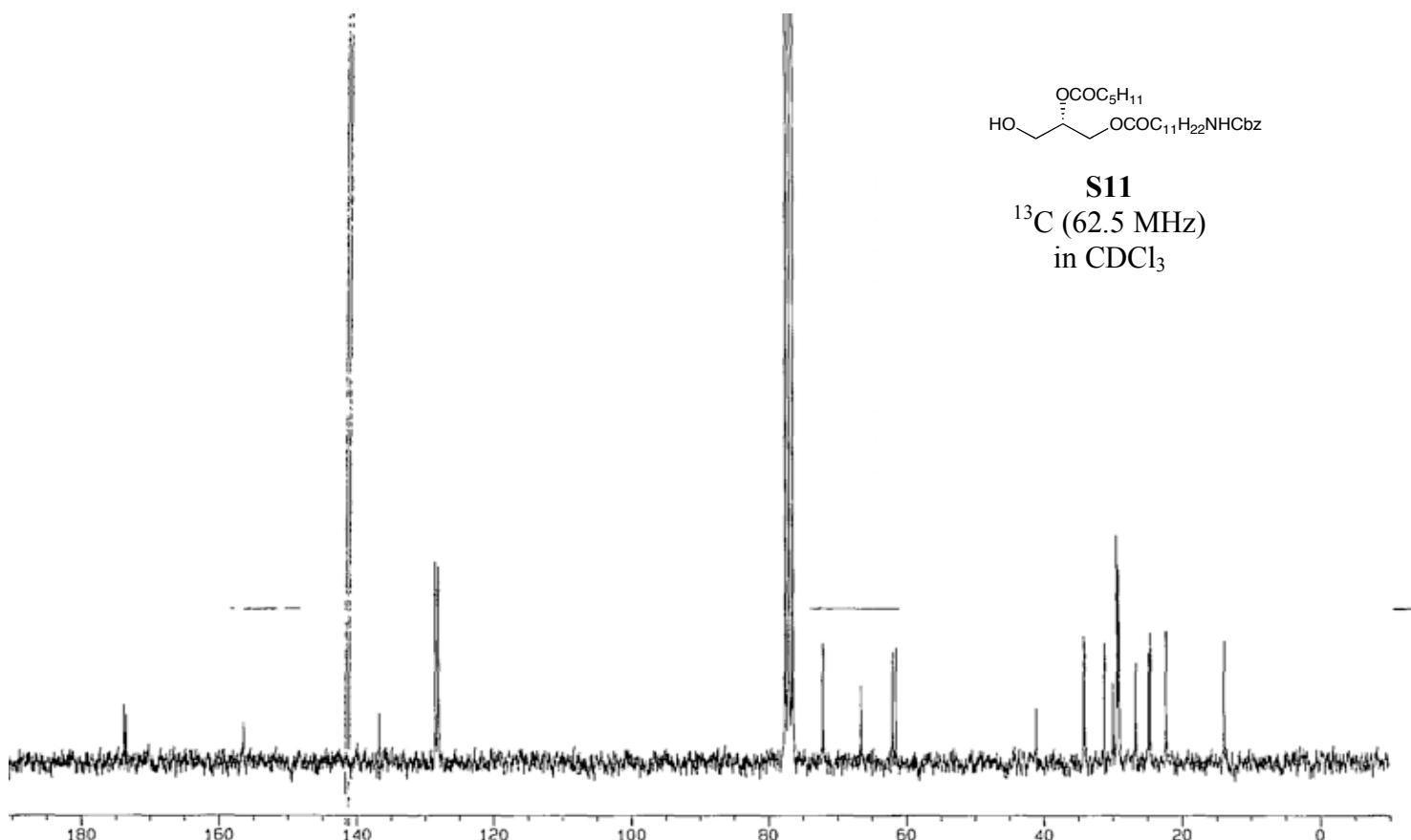
S11

^1H NMR (250 MHz)
in CDCl_3



S11

^{13}C (62.5 MHz)
in CDCl_3



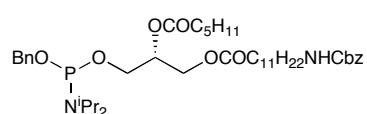
Current Data Parameters
 • NAME jta16960b
 • EXPNO 1
 • PROBNO 1

F2 - Acquisition Parameters
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 Time 14 56
 INSTRUM spect
 PROBHD 5 mm Multinuc
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWF 6983 240 Hz
 FIDRES 0 213112 Hz
 AQ 2 3462389 sec
 RG 362
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 DE 4 50 usec
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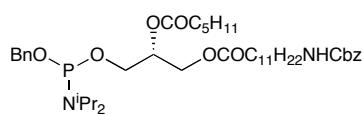
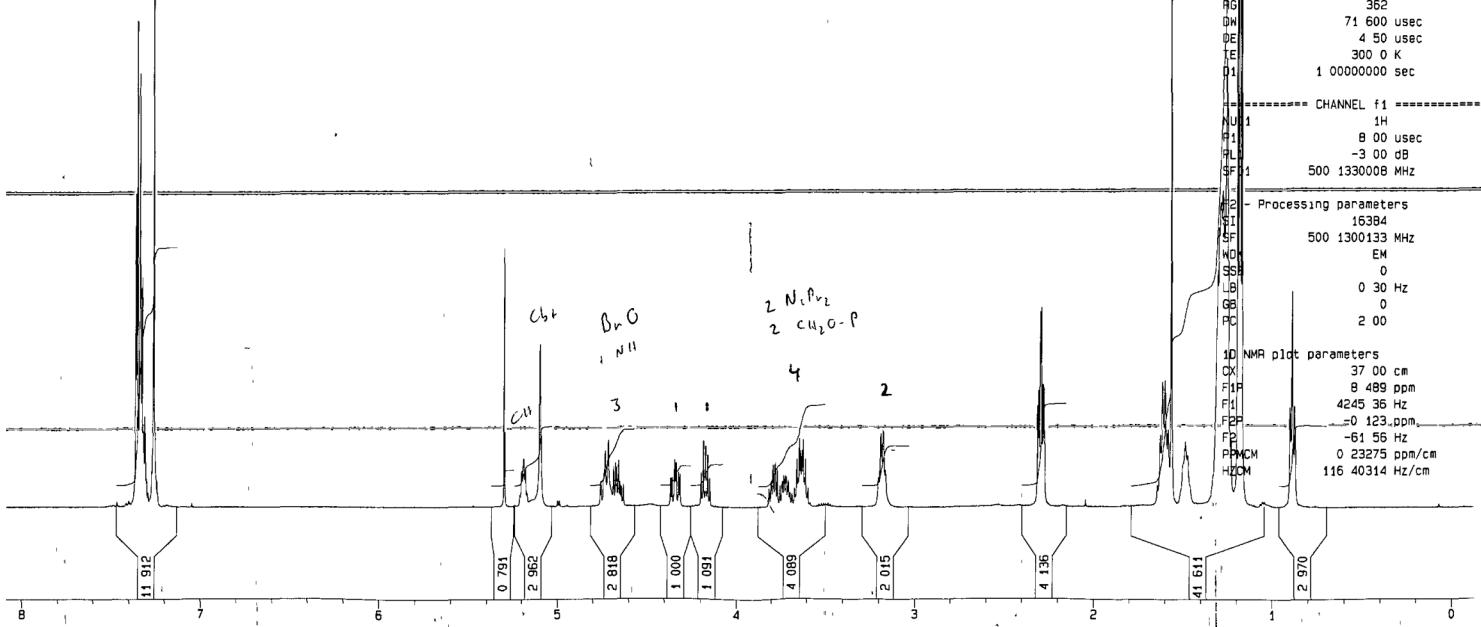
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 NU 1H
 F1 8 00 usec
 RL -3 00 dB
 SF 500 1330008 MHz

Processing parameters
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 500 1300133 MHz
 EM 0
 O 0 30 Hz
 LB 0
 OB 0
 PC 2 00

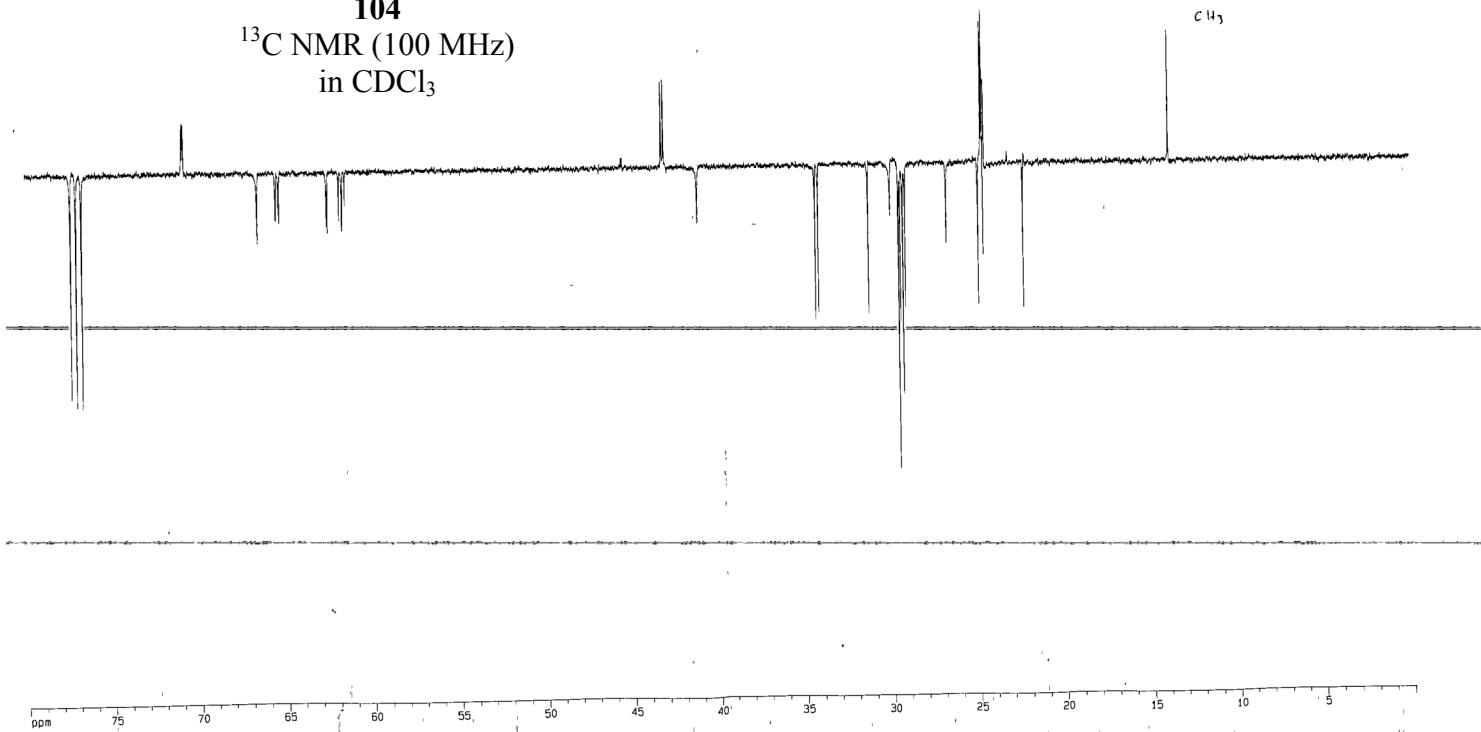
1D NMR plot parameters
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 F1 4245 36 Hz
 F2P -61 56 Hz
 F2 PPMCM 0 23275 ppm/cm
 HZCM 116 40314 Hz/cm

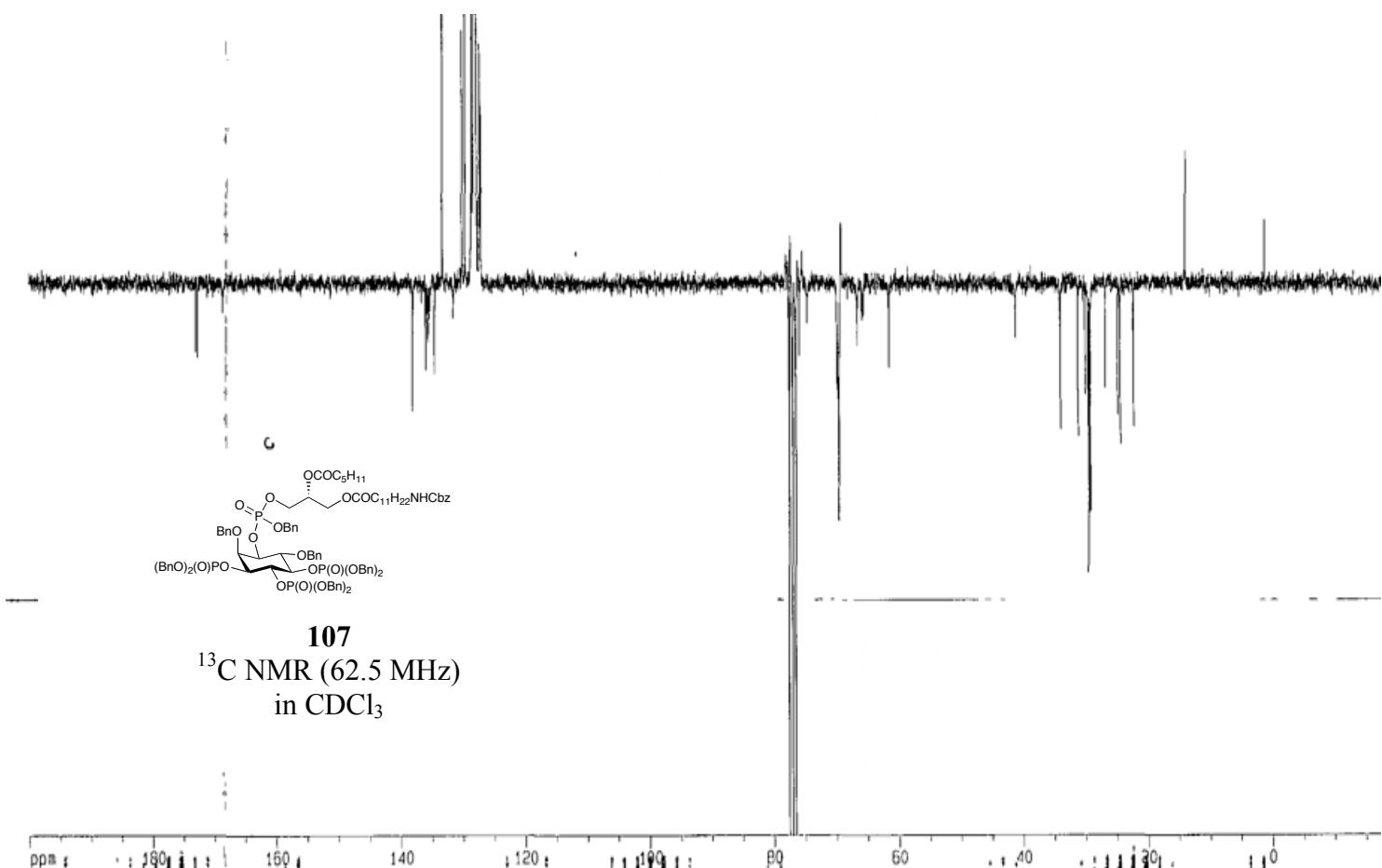
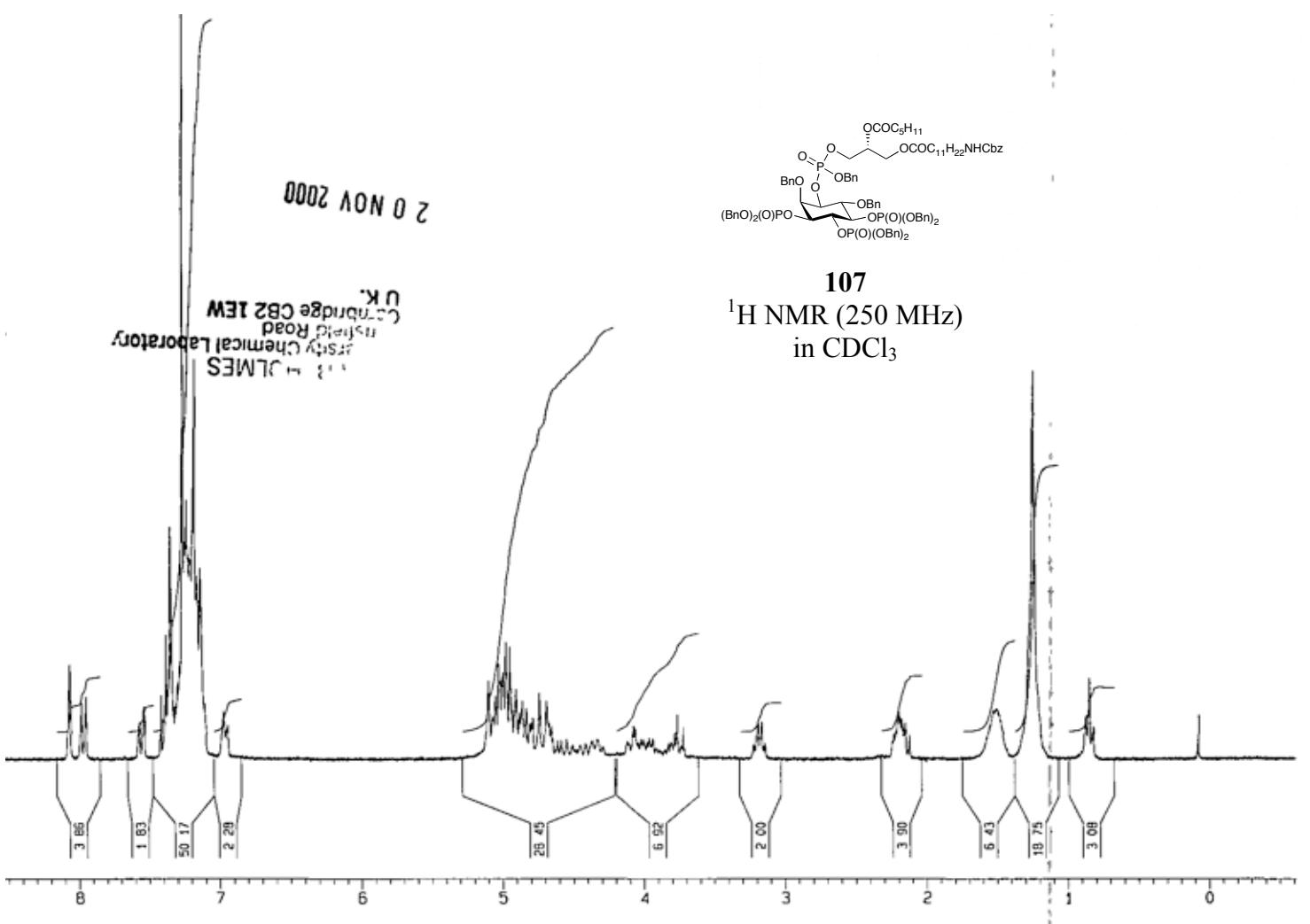


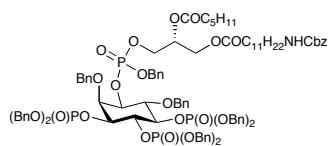
¹H NMR (500 MHz)
 in CDCl₃



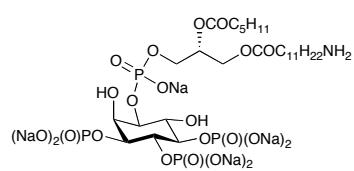
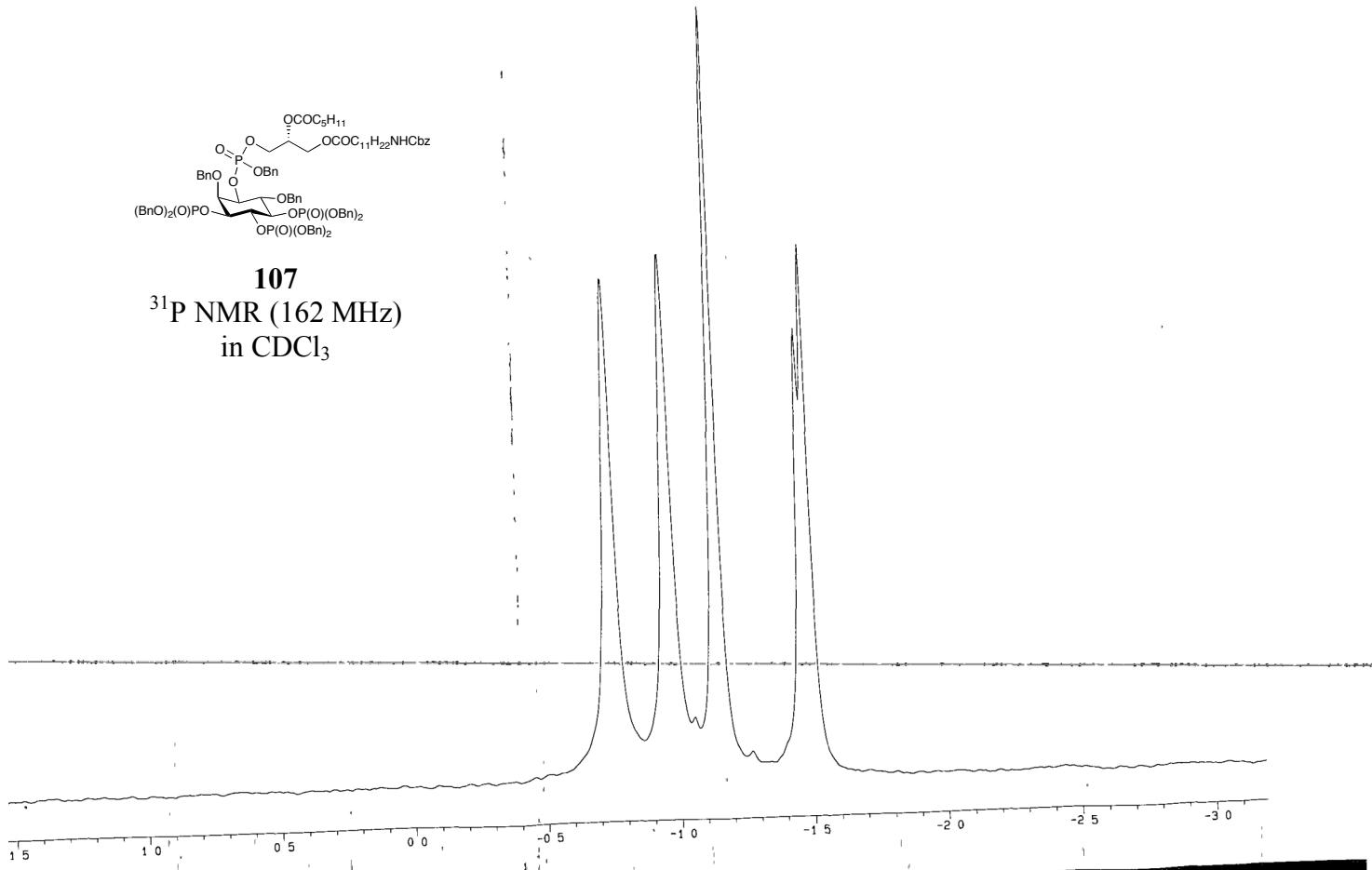
104
¹³C NMR (100 MHz)
 in CDCl₃



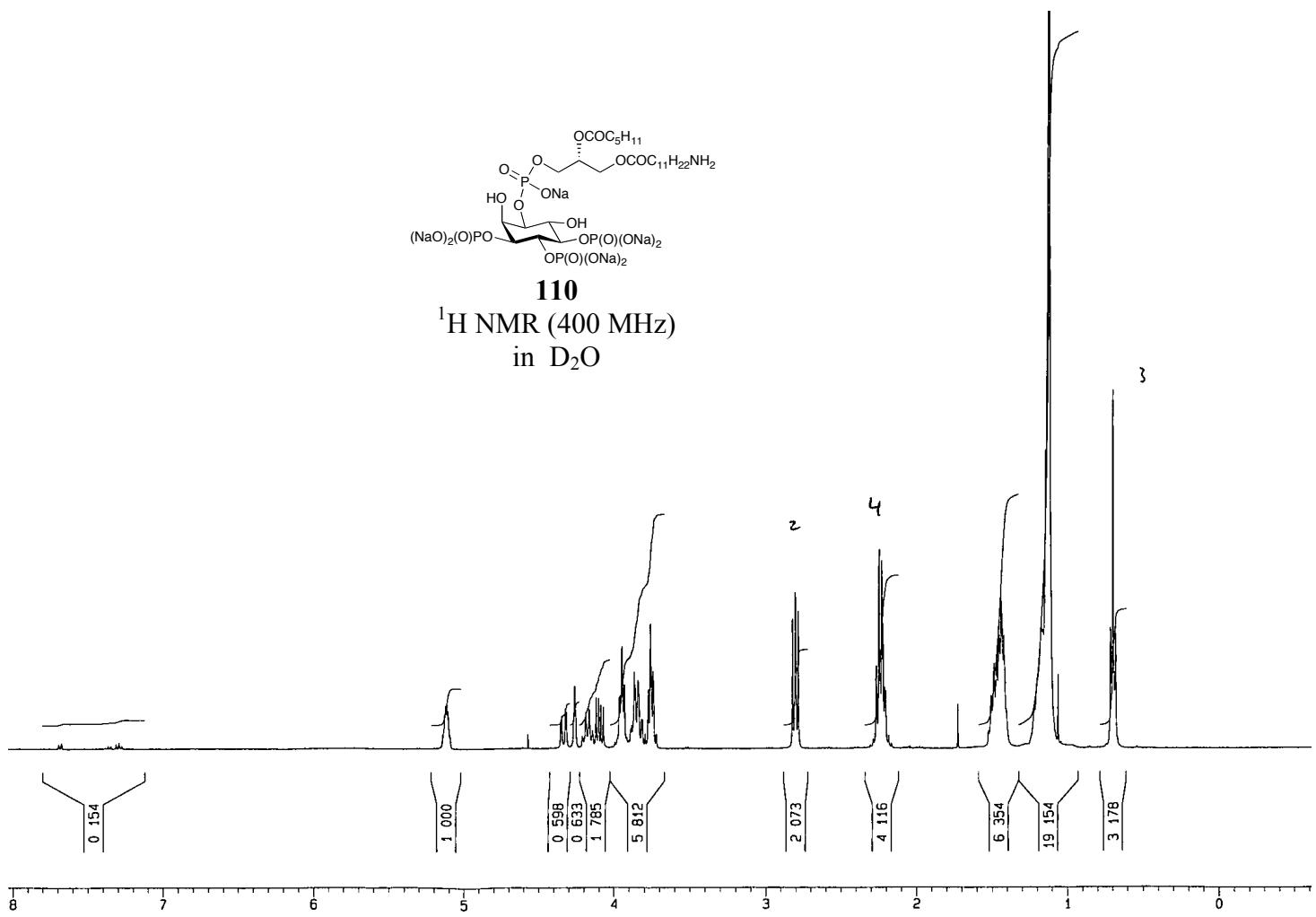


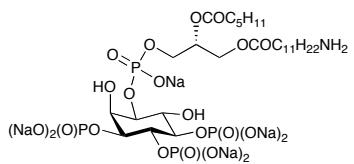


107
 ^{31}P NMR (162 MHz)
 in CDCl_3



110
 ^1H NMR (400 MHz)
 in D_2O





110

^{31}P NMR (162 MHz)
in D_2O

