SUPPORTING INFORMATION

PART 2

Synthesis of a Versatile Building Block for the Preparation of 6-*N*-Derivatized α-Galactosyl Ceramides: Rapid Access to Biologically Active Glycolipids

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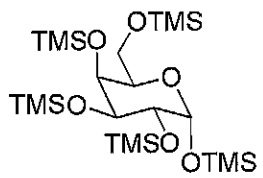
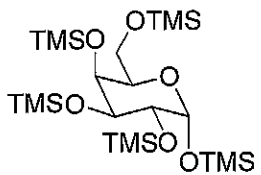
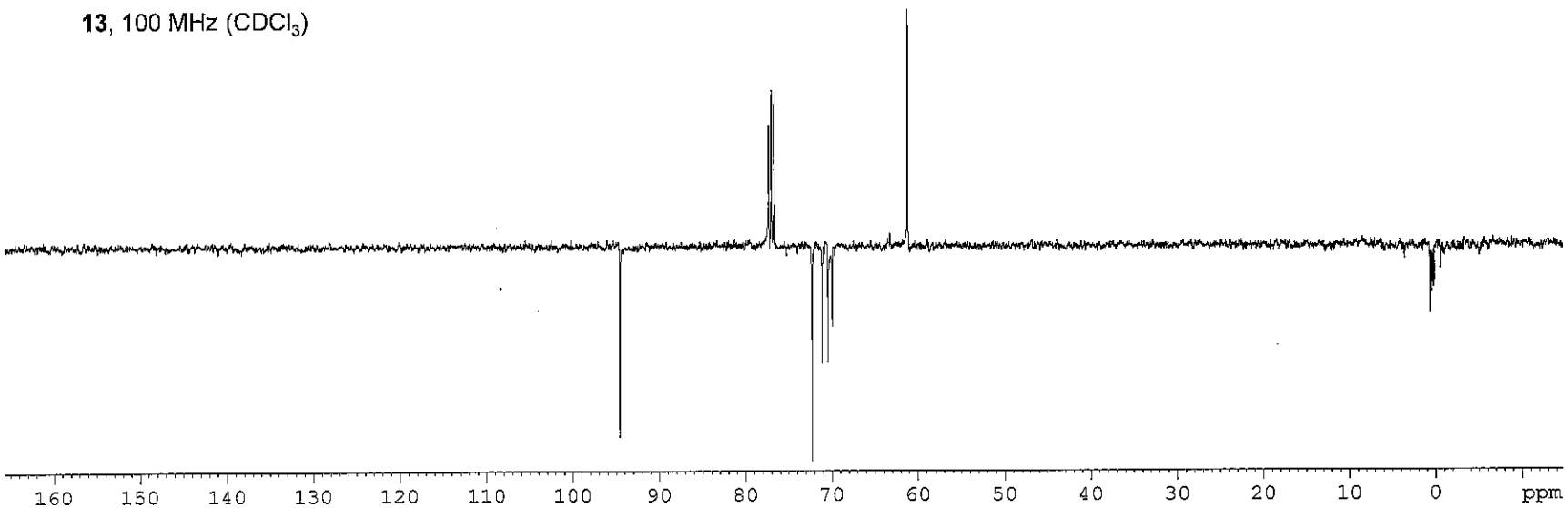
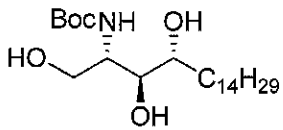


13, 300 MHz ($CDCl_3$)

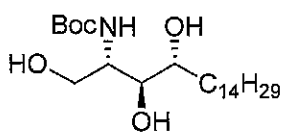


13, 100 MHz ($CDCl_3$)

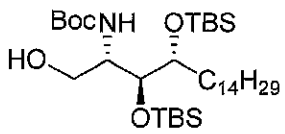




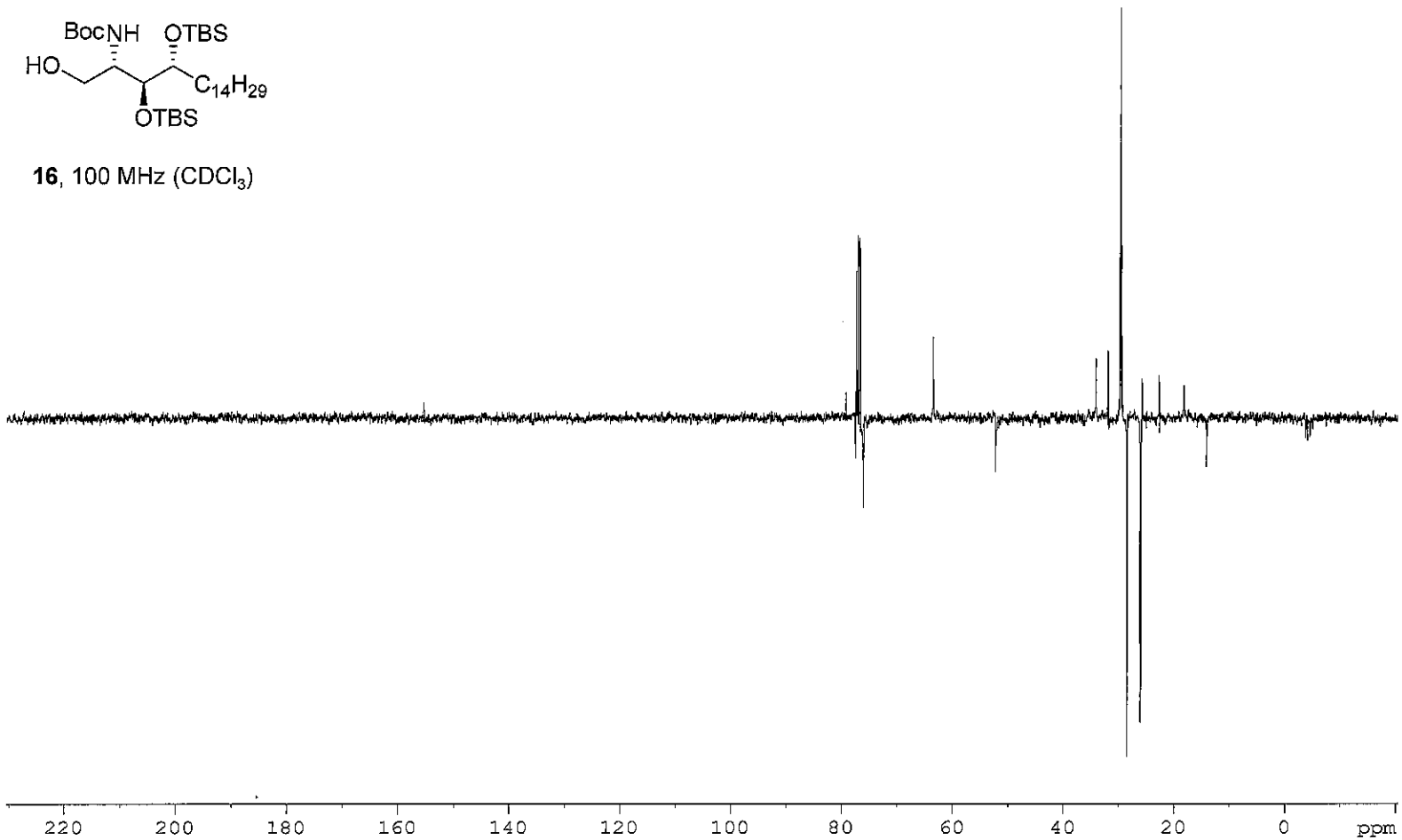
18, 300 MHz ($CDCl_3$)



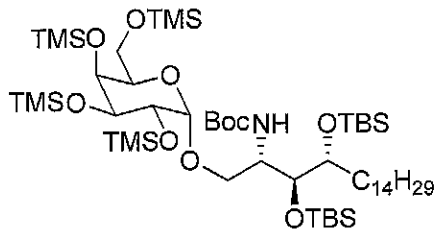
18, 100 MHz ($CDCl_3$)



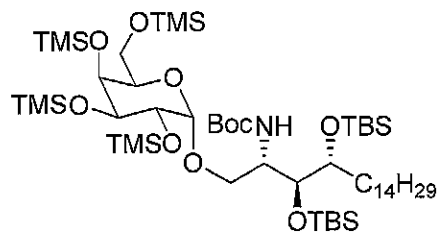
16, 300 MHz ($CDCl_3$)



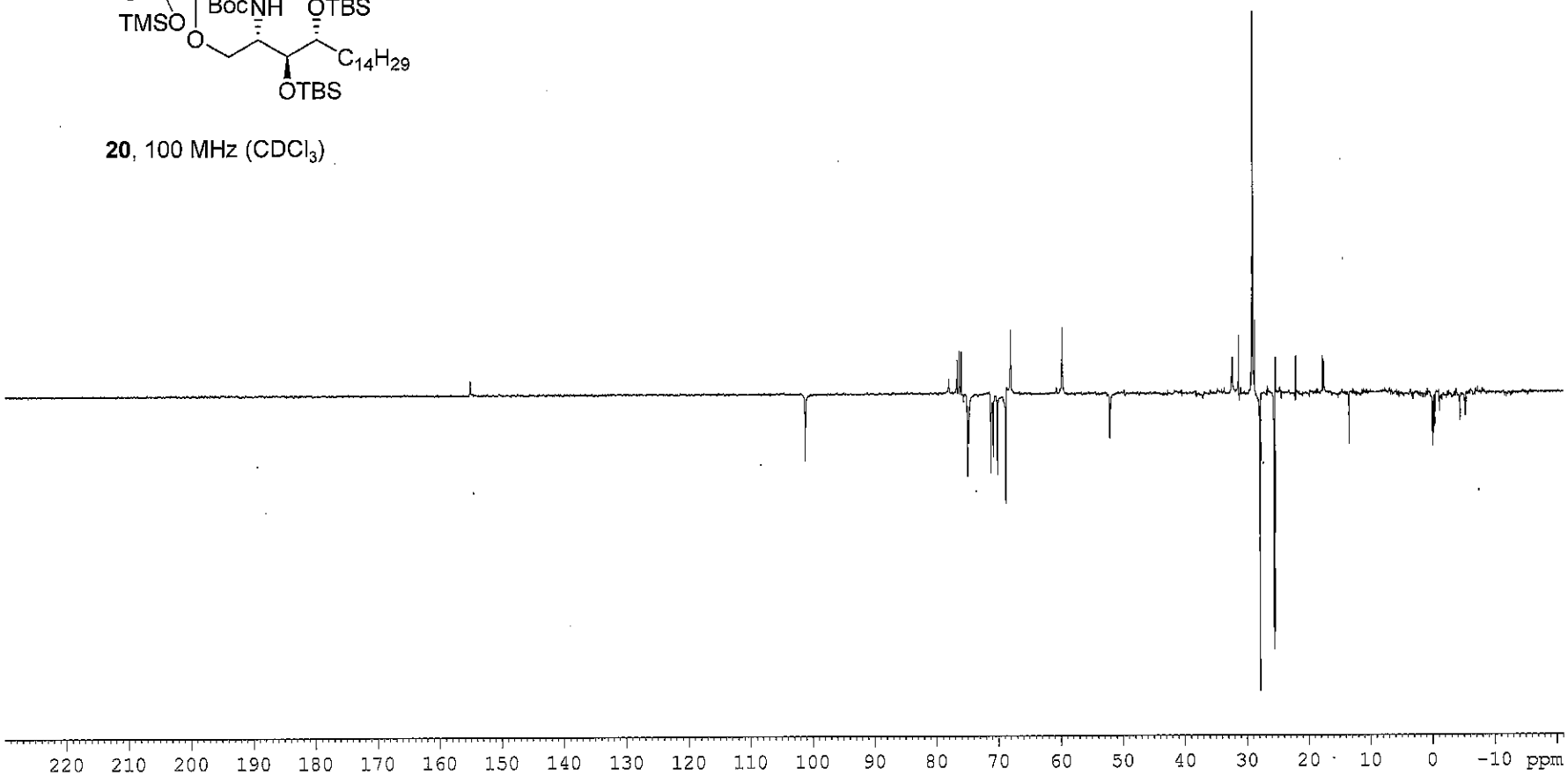
16, 100 MHz ($CDCl_3$)

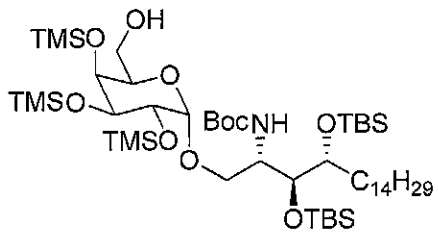


20, 300 MHz ($CDCl_3$)

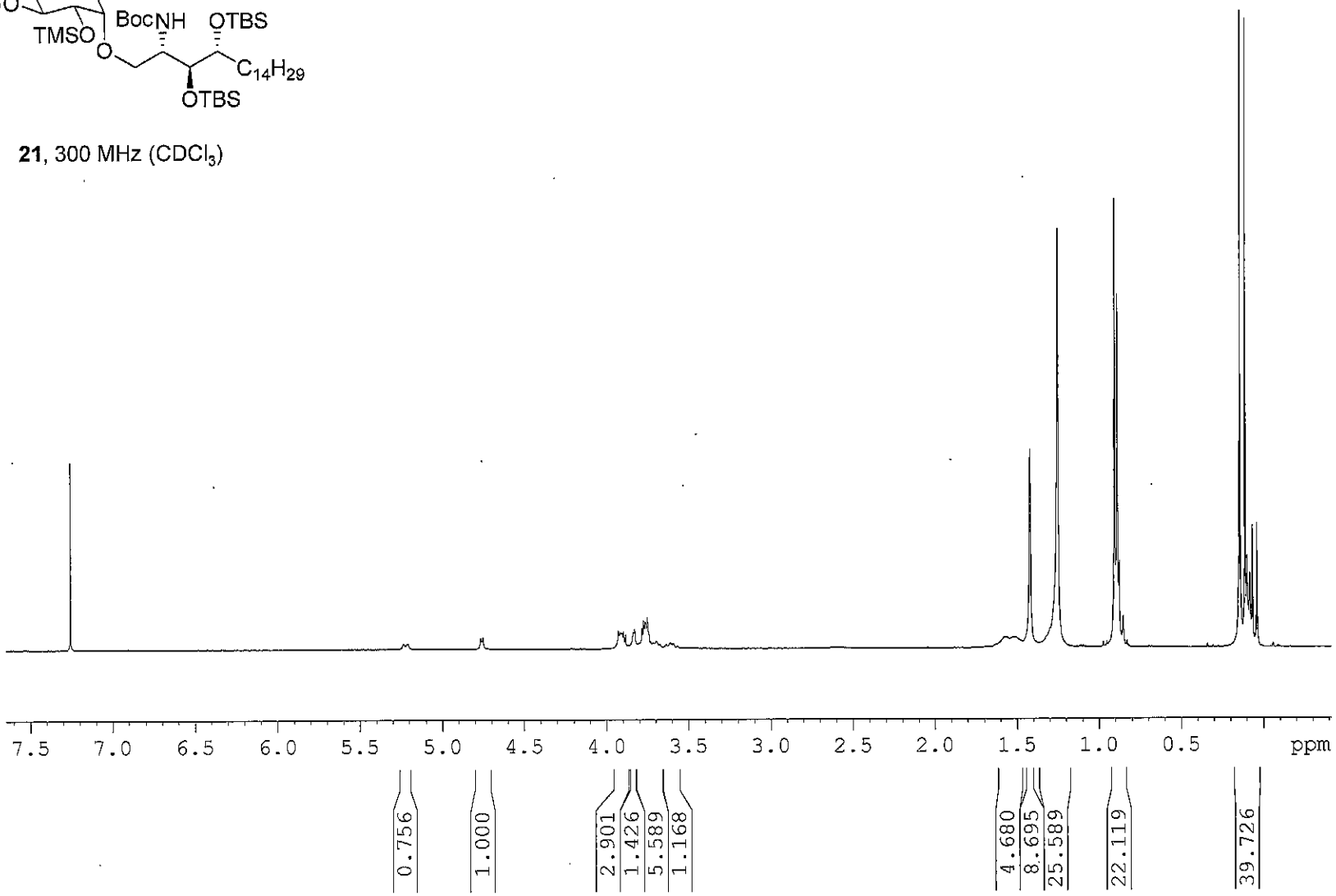


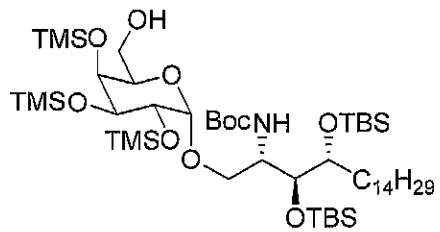
20, 100 MHz ($CDCl_3$)



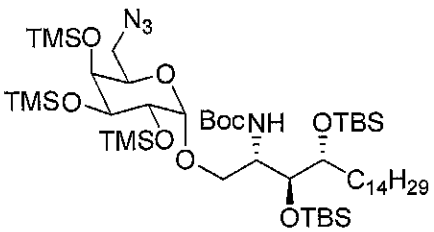


21, 300 MHz ($CDCl_3$)

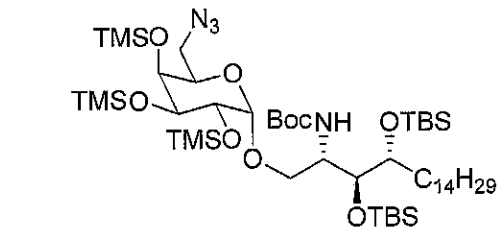




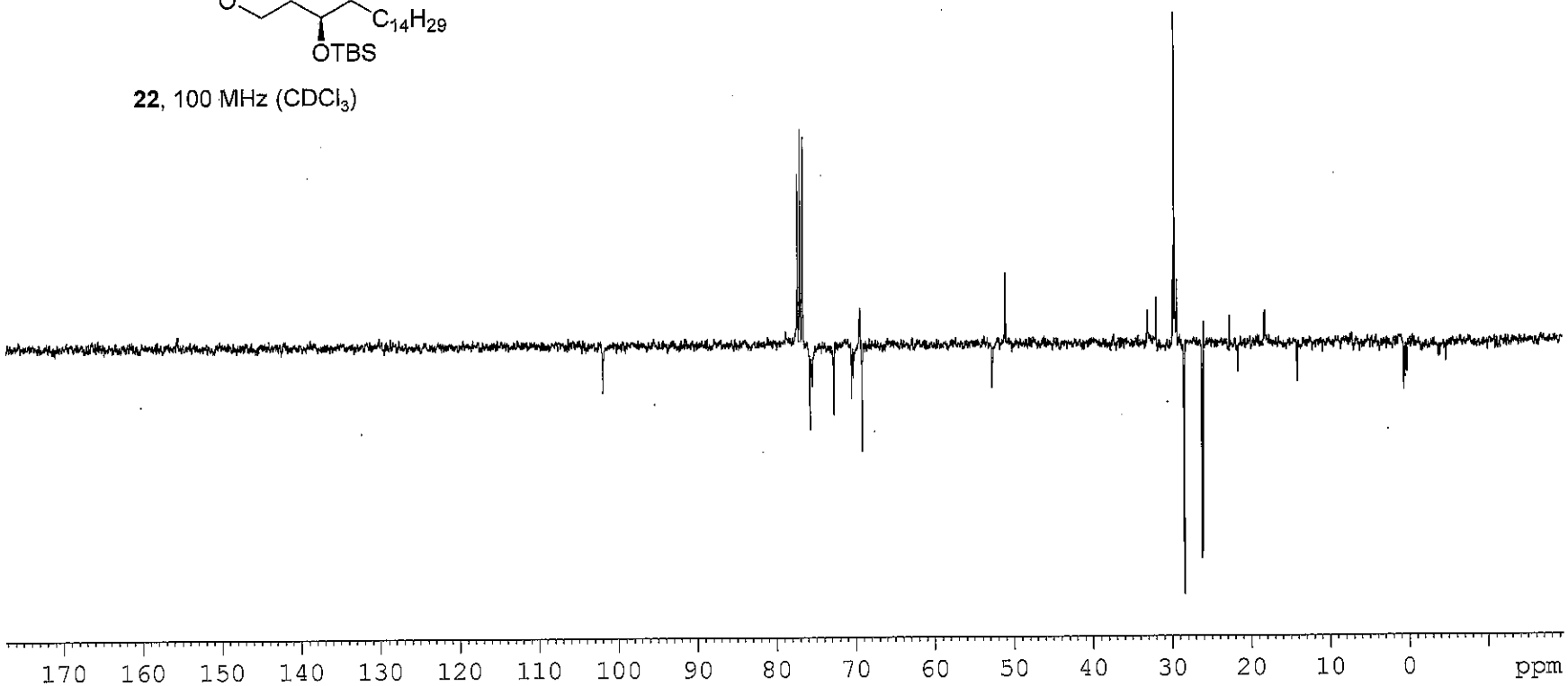
21, 100 MHz ($CDCl_3$)

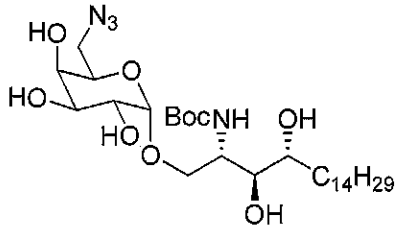


22, 300 MHz ($CDCl_3$)

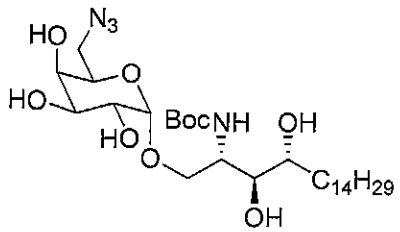


22, 100 MHz ($CDCl_3$)

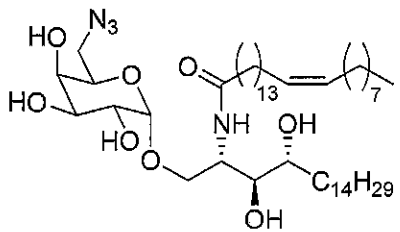




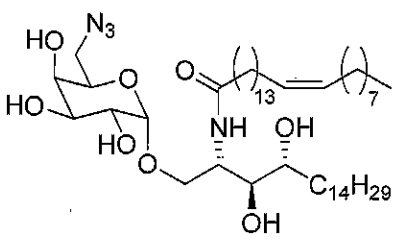
9, 300 MHz (2:1 $CDCl_3$:CD_3OD)



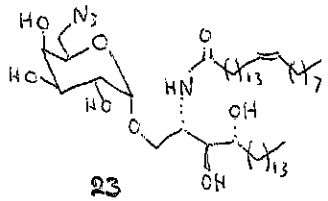
9, 100 MHz (2:1 $CDCl_3$:CD_3OD)



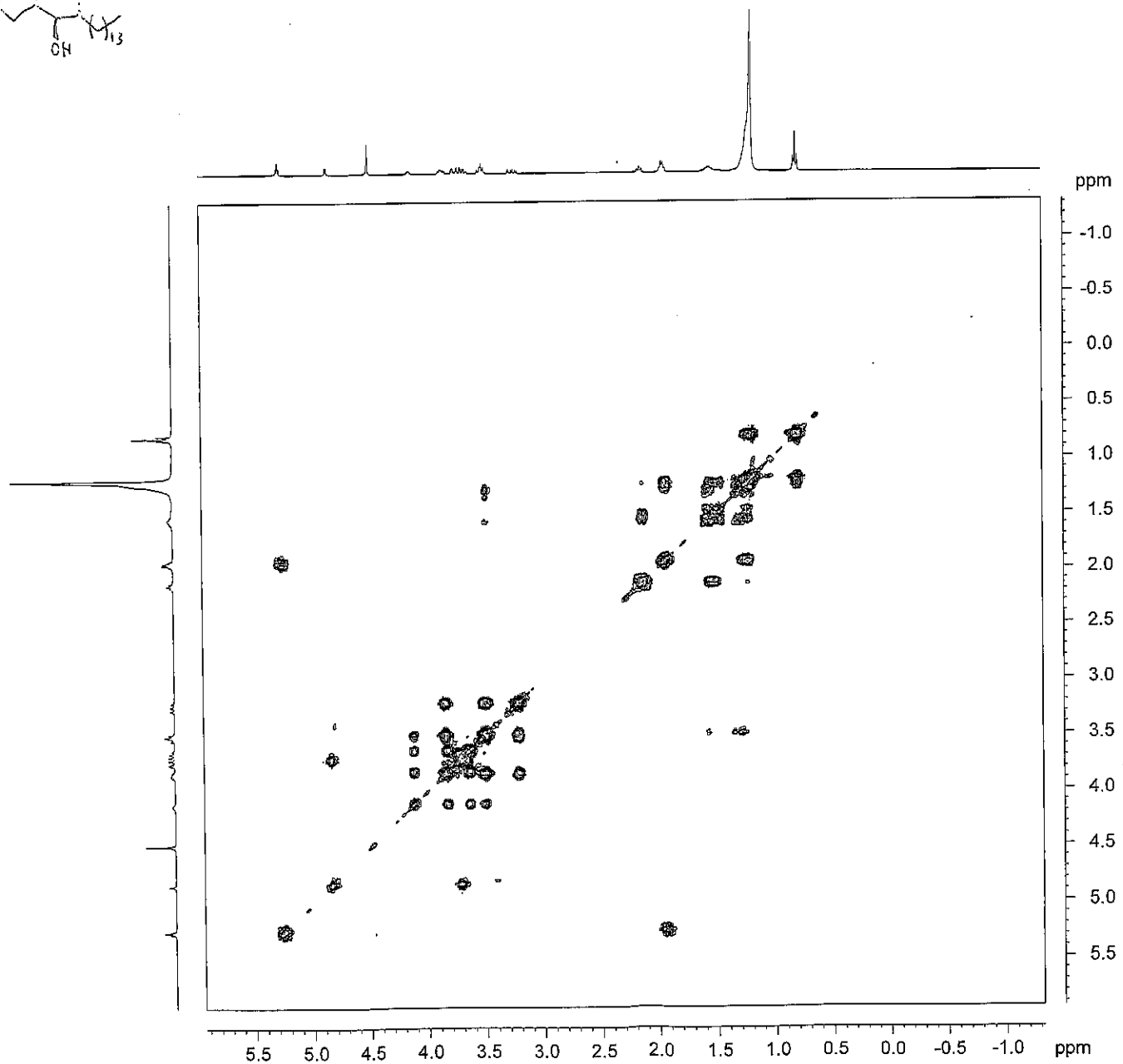
23, 400 MHz (2:1 $CDCl_3$:CD_3OD)



23, 100 MHz (2:1 $CDCl_3$:CD_3OD)



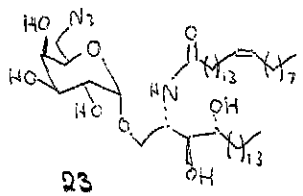
23



NAME 03-16-Besra-1
EXPNO 11
PROCNO 1
Date_ 20100316
Time 9.40
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG cosygpmfqf
TD 1024
SOLVENT MeOD
NS 4
DS 16
SWH 2906.977 Hz
FIDRES 2.838845 Hz
AQ 0.1761780 sec
RG 2050
DW 172.000 usec
DE 6.50 usec
TE 296.4 K
D0 0.00000300 sec
D1 1.40661001 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00034400 sec

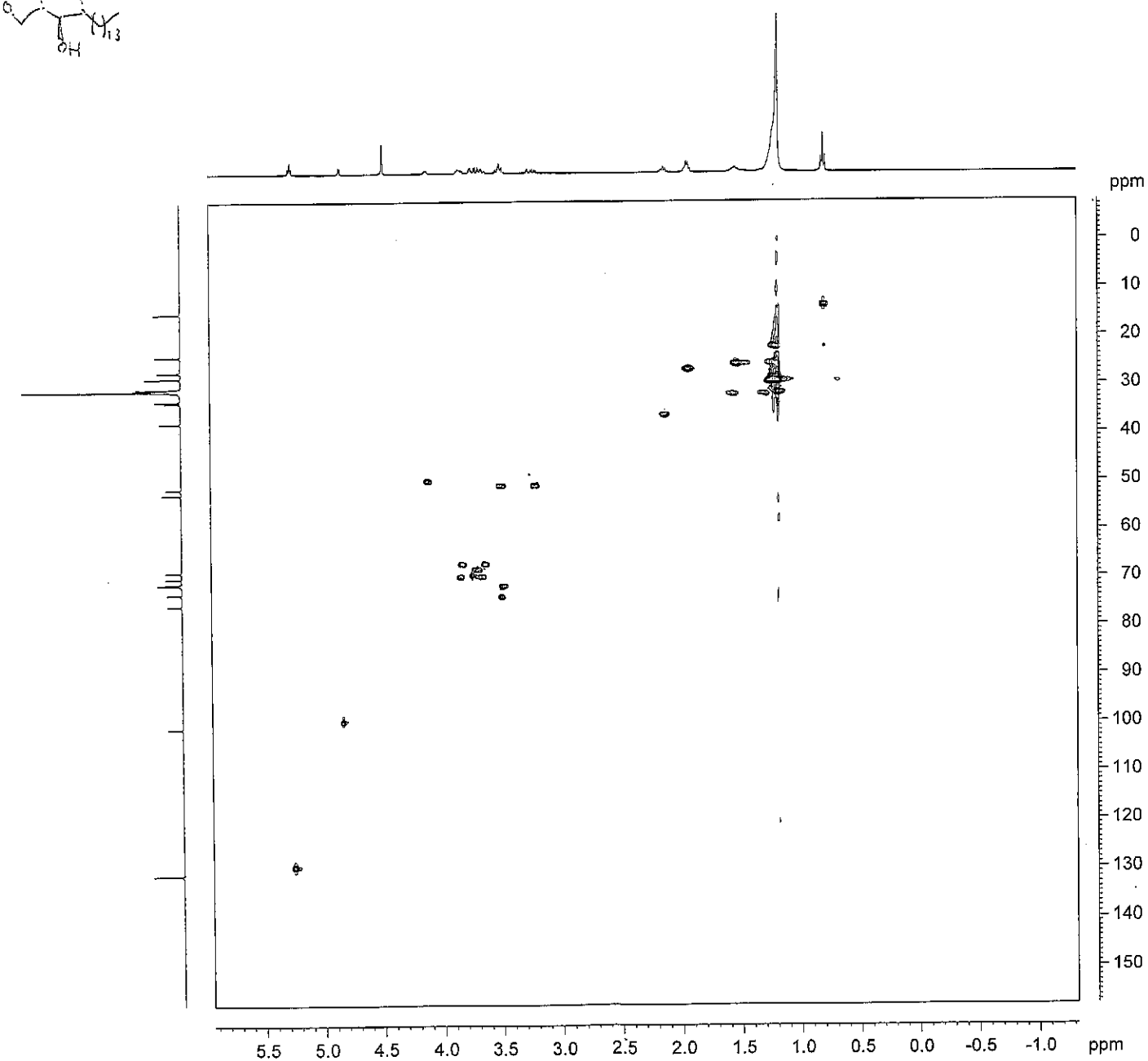
======== CHANNEL f1 ========
NUC1 1H
P1 9.50 usec
PL1 -4.00 dB
PL1W 24.29185867 W
SFO1 400.1309503 MHz

====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 400.131 MHz
FIDRES 11.355378 Hz
SW 7.265 ppm
FnMODE QF
SI 1024
SF 400.1300269 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 QF
SF 400.1300269 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

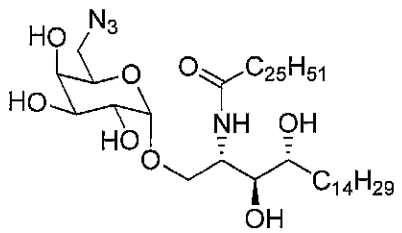


23

S43

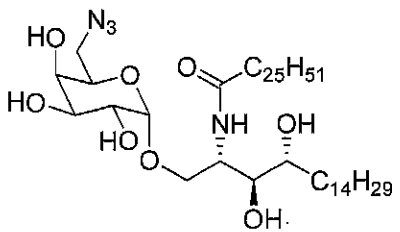



```
NAME      03-16-Besra-1
EXPNO             13
PROCNO             1
Date_       20100316
Time            10.35
INSTRUM          spect
PROBHD   5 mm PADUL 13C
PULPROG       hsqcetgp
TD                1024
SOLVENT           MeOD
NS                   4
DS                  16
SWH         2906.977 Hz
FIDRES      2.838845 Hz
AQ          0.1761780 sec
RG                2050
DW             172.000 usec
DE               6.50 usec
TE              297.1 K
CNST2       145.0000000
D0          0.00000300 sec
D1          1.41982295 sec
D4          0.00172414 sec
D11         0.03000000 sec
D13         0.00000400 sec
D16         0.00020000 sec
IN0         0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1               1H
P1               9.50 usec
P2              19.00 usec
P28              0.00 usec
PL1             -4.00 dB
PL1W        24.29185867 W
SFO1        400.1309503 MHz

======== CHANNEL f2 ========
CPDPRG2          garp
NUC2               13C
P3               8.90 usec
P4              17.80 usec
PCPD2           78.00 usec
PL2             -3.00 dB
PL12            16.00 dB
PL2W        58.63880457 W
PL12W        0.73822010 W
SFO2        100.6203124 MHz

====== GRADIENT CHANNEL =====
GPNAM1         SINE.100
GPNAM2         SINE.100
GPZ1             80.00 %
GPZ2             20.10 %
P16            1000.00 usec
ND0                  2
TD                 256
SFO1        100.6203 MHz
FIDRES      65.108421 Hz
SW          165.650 ppm
FnMODE     Echo-Antiecho
SI                1024
SF          400.1300259 MHz
WDW               QSINE
SSB                  2
LB              0.00 Hz
GB                   0
PC                1.40
SI                 512
MC2        echo-antiecho
SF          100.6127690 MHz
WDW               QSINE
SSB                  2
LB              0.00 Hz
GB                   0
```



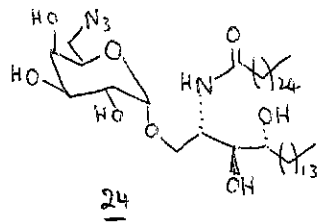
24, 400 MHz (2:1 $CDCl_3$:CD_3OD)

S44



24, 400 MHz (2:1 $CDCl_3$:CD_3OD)

P Jervis, 6-Azide C26



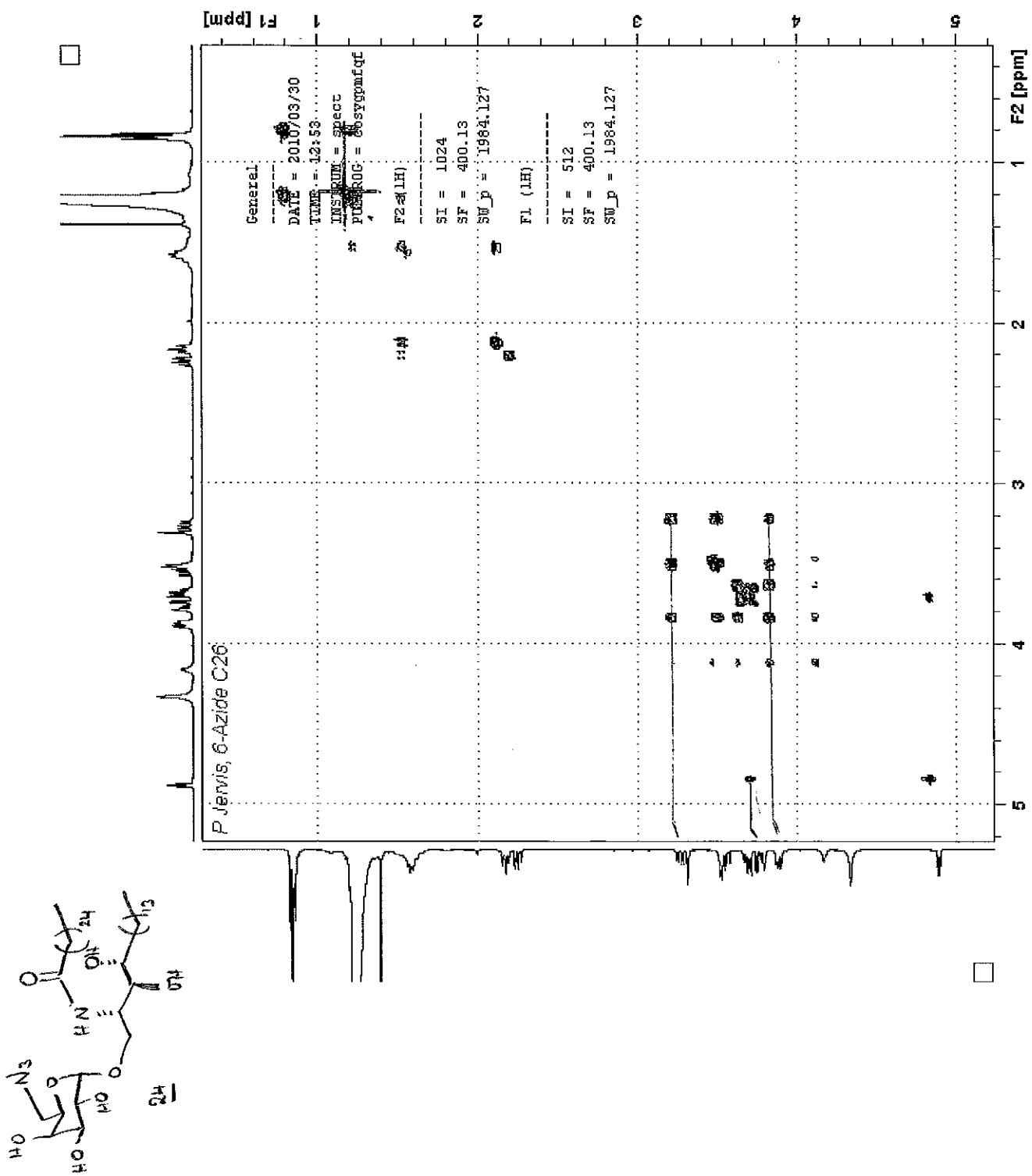
24

SH6

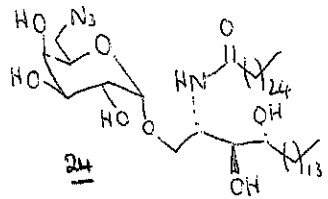
NAME 03-30-Besra-4
EXPNO 11
PROCNO 1
Date_ 20100330
Time 12.53
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG cosygpmfqf
TD 1024
SOLVENT MeOD
NS 4
DS 16
SWH 1984.127 Hz
FIDRES 1.937624 Hz
AQ 0.2580980 sec
RG 2050
DW 252.000 usec
DE 6.50 usec
TE 296.3 K
D0 0.00000300 sec
D1 1.32468998 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00050400 sec

======== CHANNEL f1 ========
NUC1 1H
P1 9.50 usec
PL1 -4.00 dB
PL1W 24.29185867 W
SFO1 400.1311256 MHz

====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 400.1311 MHz
FIDRES 7.750496 Hz
SW 4.959 ppm
FnMODE QF
SI 1024
SF 400.1300248 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 QF
SF 400.1300248 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0


F1 [ppm]
F2 [ppm]
P Jarvis, 6-Azide C26
General
DATE = 2010/03/30
TIME = 12:53
F2 (1H)
SI = 1024
SF = 400.13
SW_p = 1984.127
F1 (1H)
SI = 512
SF = 400.13
SW_p = 1984.127

P Jervis, 6-Azide C26



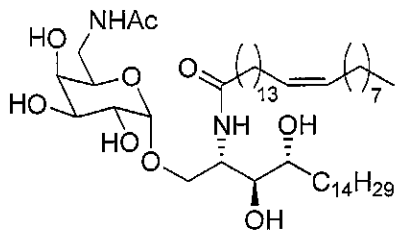
24

NAME 03-30-Besra-4
EXPNO 13
PROCNO 1
Date_ 20100330
Time 13.49
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG hsqcetgp
TD 1024
SOLVENT MeOD
NS 4
DS 16
SWH 1984.127 Hz
FIDRES 1.937624 Hz
AQ 0.2580980 sec
RG 2050
DW 252.000 usec
DE 6.50 usec
TE 297.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.33800304 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00003000 sec
ZGOPTNS

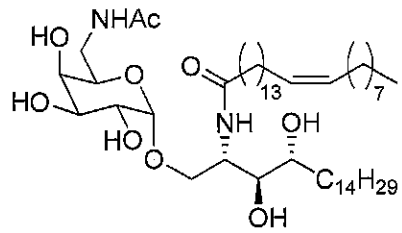
======== CHANNEL f1 ========
NUC1 1H
P1 9.50 usec
P2 19.00 usec
P28 0.00 usec
PL1 -4.00 dB
PL1W 24.29185867 W
SFO1 400.1311256 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 8.90 usec
P4 17.80 usec
PCPD2 78.00 usec
PL2 -3.00 dB
PL12 16.00 dB
PL2W 58.63890457 W
PL12W 0.73822010 W
SFO2 100.6203124 MHz

====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 100.6203 MHz
FIDRES 65.108421 Hz
SW 165.650 ppm
FnMODE Echo-Antiecho
SI 1024
SF 400.1300248 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 echo-antiecho
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

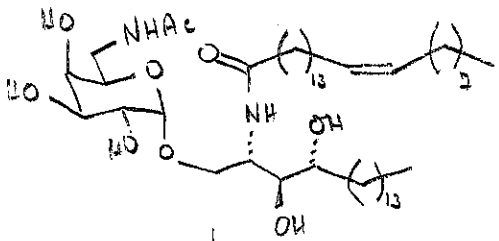


6, 400 MHz (2:1 $CDCl_3$:CD_3OD)



6, 100 MHz (2:1 $CDCl_3$:CD_3OD)

P Jervis, PBS-57 (6)

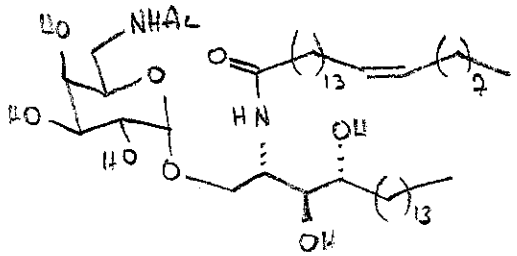


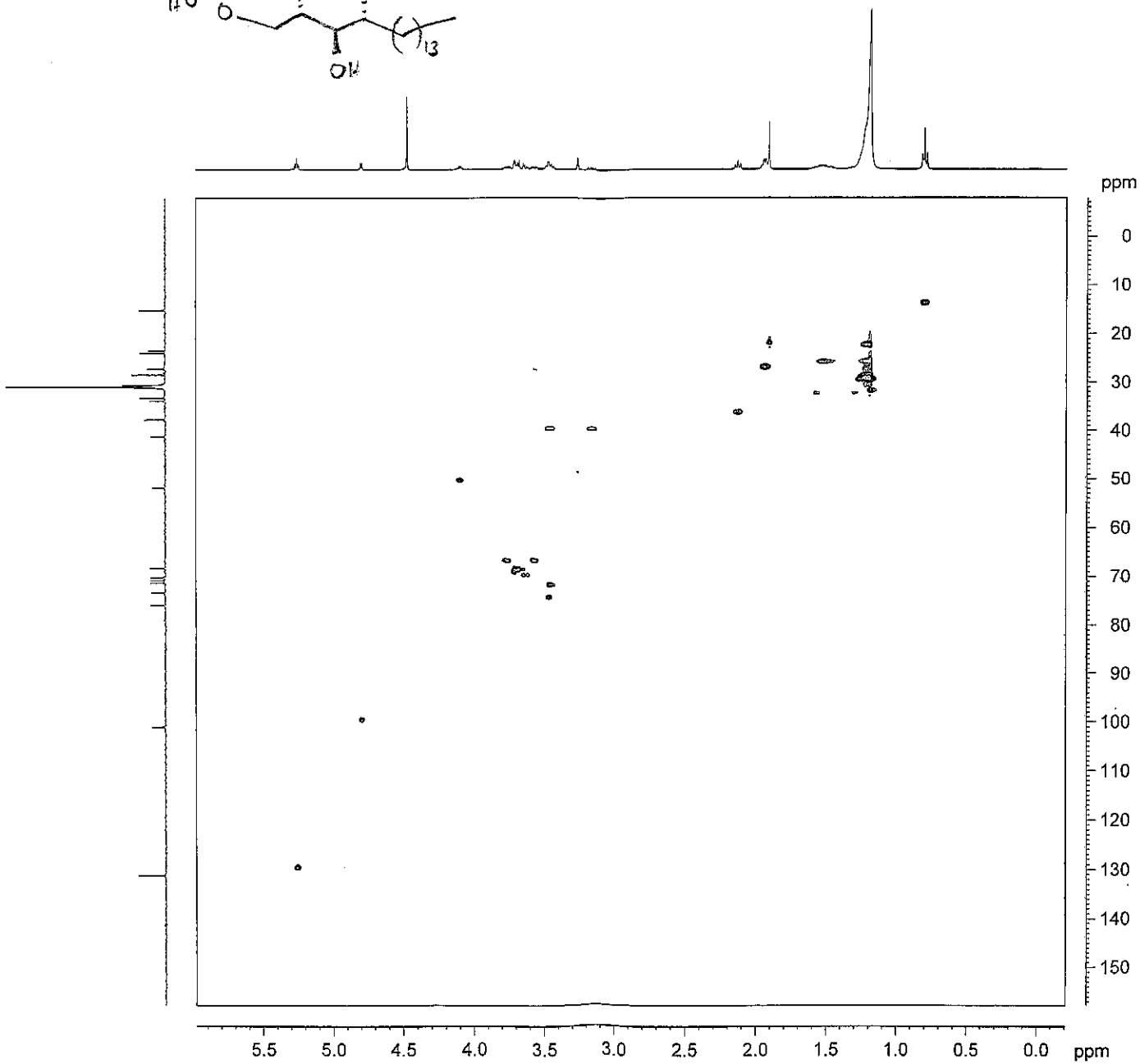
NAME 03-18-Besra-1
EXPNO 11
PROCNO 1
Date_ 20100318
Time 9.16
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG cosygpmfqf
TD 1024
SOLVENT MeOD
NS 4
DS 16
SWH 2475.248 Hz
FIDRES 2.417234 Hz
AQ 0.2068980 sec
RG 2050
DW 202.000 usec
DE 6.50 usec
TE 296.4 K
D0 0.00000300 sec
D1 1.37589002 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00040400 sec

======== CHANNEL f1 ========
NUC1 1H
P1 9.50 usec
PL1 -4.00 dB
PL1W 24.29185867 W
SFO1 400.1311815 MHz

====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 400.1312 MHz
FIDRES 9.668936 Hz
SW 6.186 ppm
FnMODE QF
SI 1024
SF 400.1300267 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 QF
SF 400.1300267 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

Jervis, PBS-57 (6)



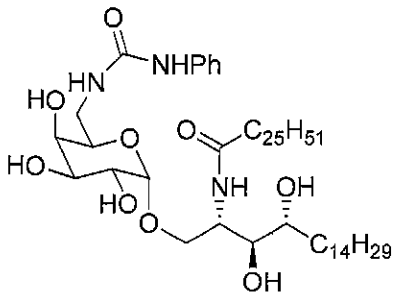


NAME 03-18-Besra-1
EXPNO 13
PROCNO 1
Date_ 20100318
Time 10.11
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG hsqcetgp
TD 1024
SOLVENT MeOD
NS 4
DS 16
SWH 2475.248 Hz
FIDRES 2.417234 Hz
AQ 0.2068980 sec
RG 2050
DW 202.000 usec
DE 6.50 usec
TE 297.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.38920295 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00003000 sec
ZGOPTNS

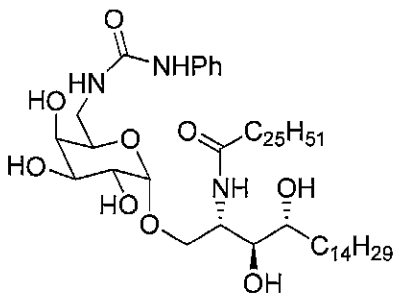
======== CHANNEL f1 ========
NUC1 1H
P1 9.50 usec
P2 19.00 usec
P28 0.00 usec
PL1 -4.00 dB
PL1W 24.29185867 W
SFO1 400.1311815 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 8.90 usec
P4 17.80 usec
PCPD2 78.00 usec
PL2 -3.00 dB
PL12 16.00 dB
PL2W 58.63890457 W
PL12W 0.73822010 W
SFO2 100.6203124 MHz

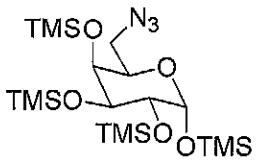
====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 100.6203 MHz
FIDRES 65.108421 Hz
SW 165.650 ppm
FnMODE Echo-Antiecho
SI 1024
SF 400.1300267 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 echo-antiecho
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0



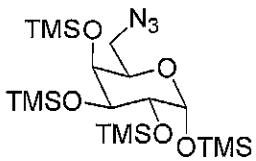
8, 300 MHz (2:1 $CDCl_3$:CD_3OD)



8, 100 MHz (2:1 $CDCl_3$:CD_3OD)



25, 300 MHz ($CDCl_3$)



25, 100 MHz ($CDCl_3$)