

Supporting Information
for
**De novo macrolide – glycolipid macrolactone hybrids:
Synthesis, structure and antibiotic activity of
carbohydrate-fused macrocycles**

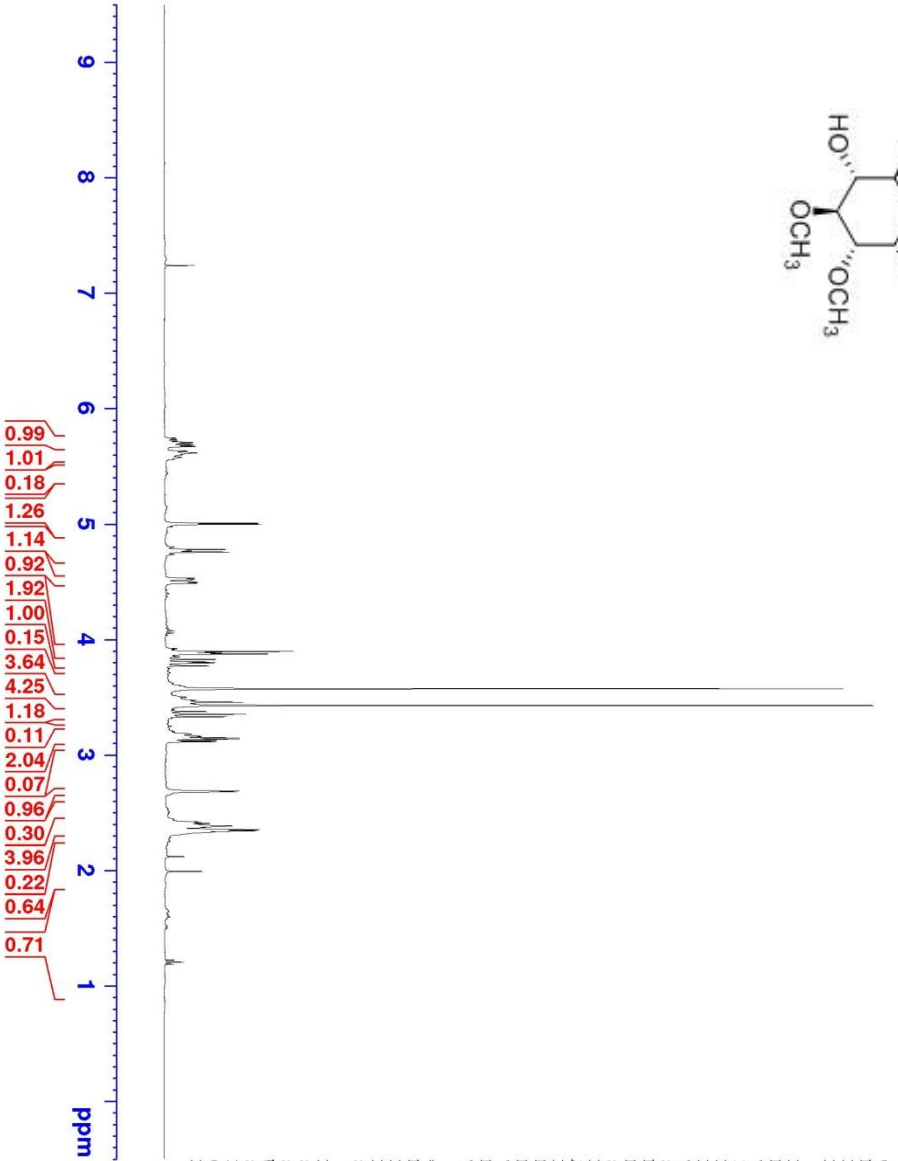
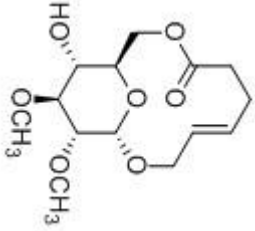
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Email: Mark W. Peczuh - mark.peczuh@uconn.edu

Characterization data including ¹H and ¹³C NMR spectra of all new compounds and ORTEP figures for **5** and **6**.

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Current Data Parameters
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 PROCNO 1

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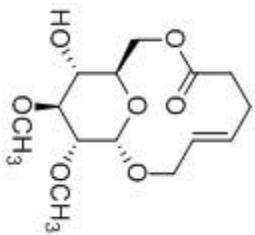
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 NS 32
 DS 2
 SMH 8012.820 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999423 sec
 RG 36
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

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 P1M1 12.00000000 W
 SFO1 400.1464009 MHz

F2 - Processing parameters

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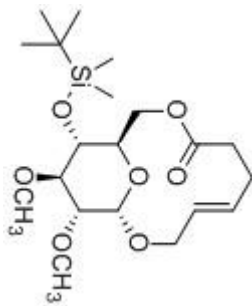
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 FIDRES 0.550104 Hz
 AQ 0.9089184 sec
 RG 203
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 TE 298.0 K
 D1 1.50000000 sec
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 SFO1 100.6263500 MHz

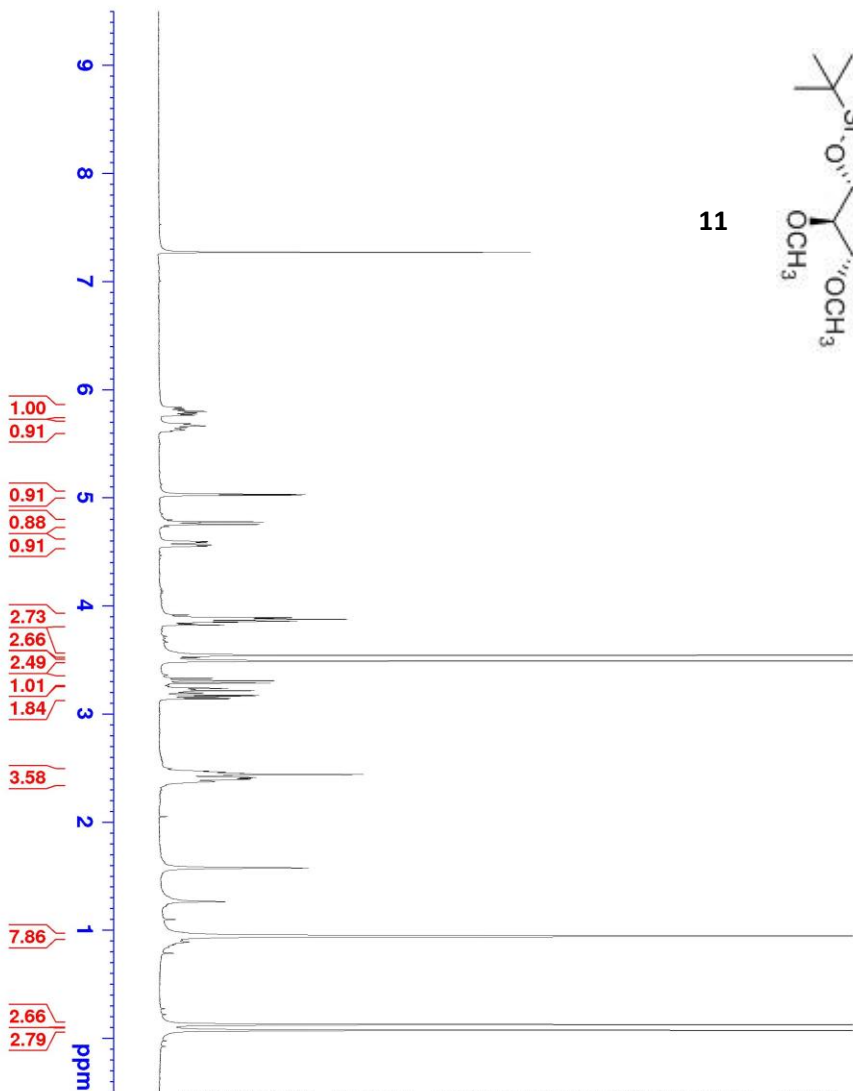
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 PLM13 0.27000001 W
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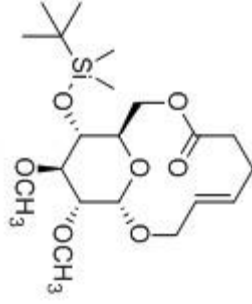
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 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

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 SFO1 400.1464009 MHz

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11



Current Data Parameters
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 PROCNO 1

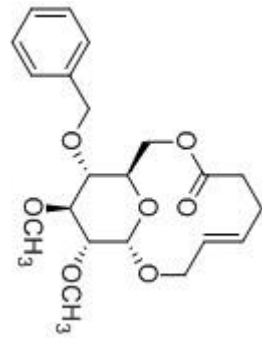
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 NS 444
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.550104 Hz
 AQ 0.9089184 sec
 RG 203
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 DE 6.50 usec
 TE 300.1 K
 D1 1.5000000 sec
 D11 0.0300000 sec
 TD0 1

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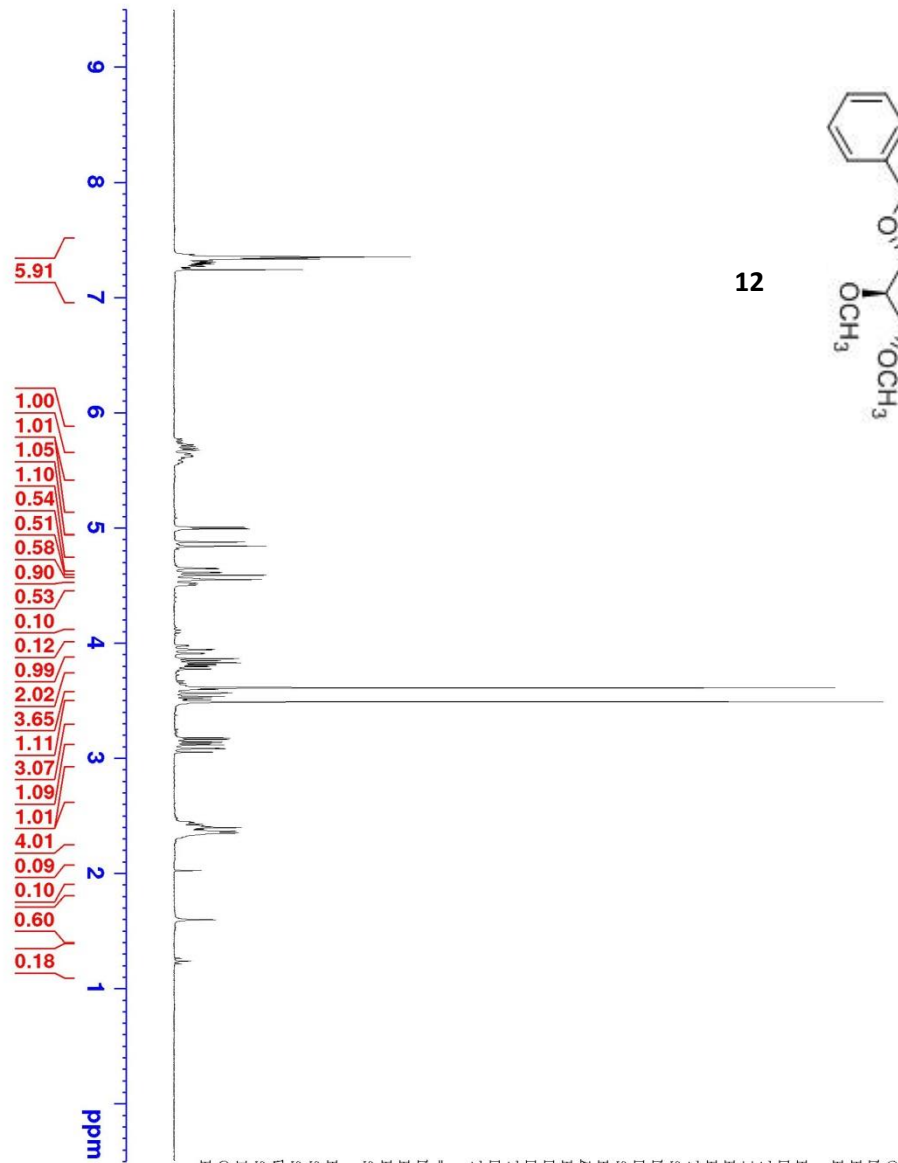
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 PLW12 0.33333001 W
 PLW13 0.27000001 W
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F2 - Processing parameters
 SI 131072
 SF 100.6162577 MHz
 WDW EM
 SSB 0
 GB 0
 PC 1.40





12



Current Data Parameters
NAME Ftd-111-19-p3
EXNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110811
Time_ 16.22

INSTRUM spect
PROBHD 5 mm Maltinact

PULPROG zg30
TD 32768

SOLVENT CDCl3
NS 16

DS 2
SMH 4789.272 Hz

FIDRES 0.146157 Hz
AQ 3.4209793 sec

RG 4
DW 104.400 usec

DE 6.50 usec
TE 271.8 K

D1 1.50000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H

P1 8.20 usec
PL1 0 dB

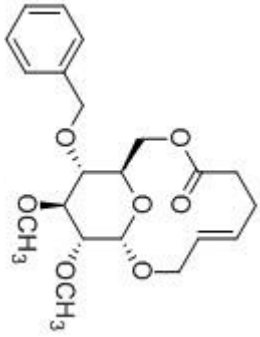
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F2 - Processing parameters
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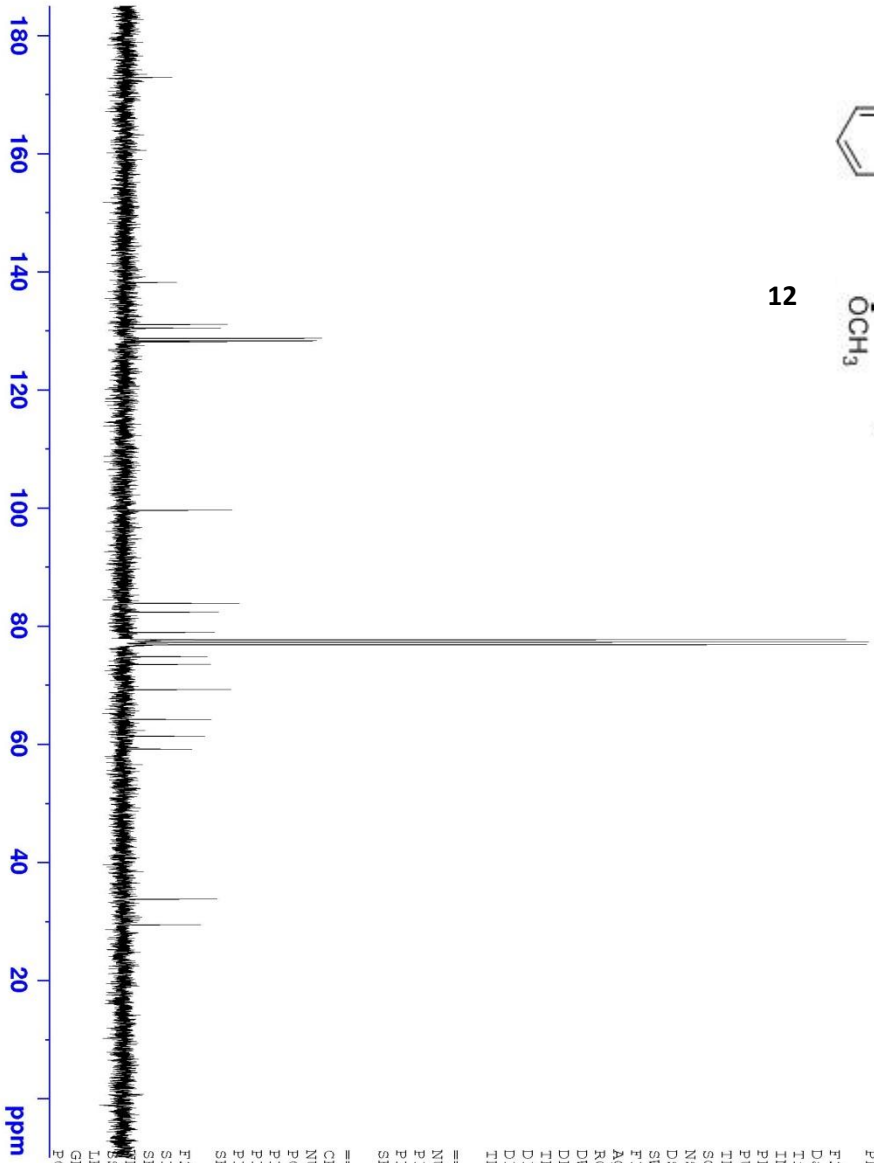
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IB 0.30 Hz

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12



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PROCNO 1

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Time_ 16.27

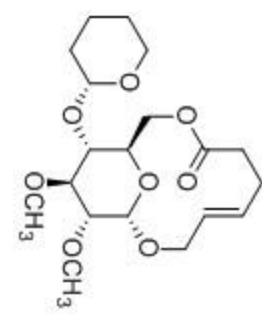
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PROBHD 5 mm Maltinact
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 191

DS 4
SMH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219008 sec
RG 32768
DW 27.800 usec
DE 6.50 usec
TE 274.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

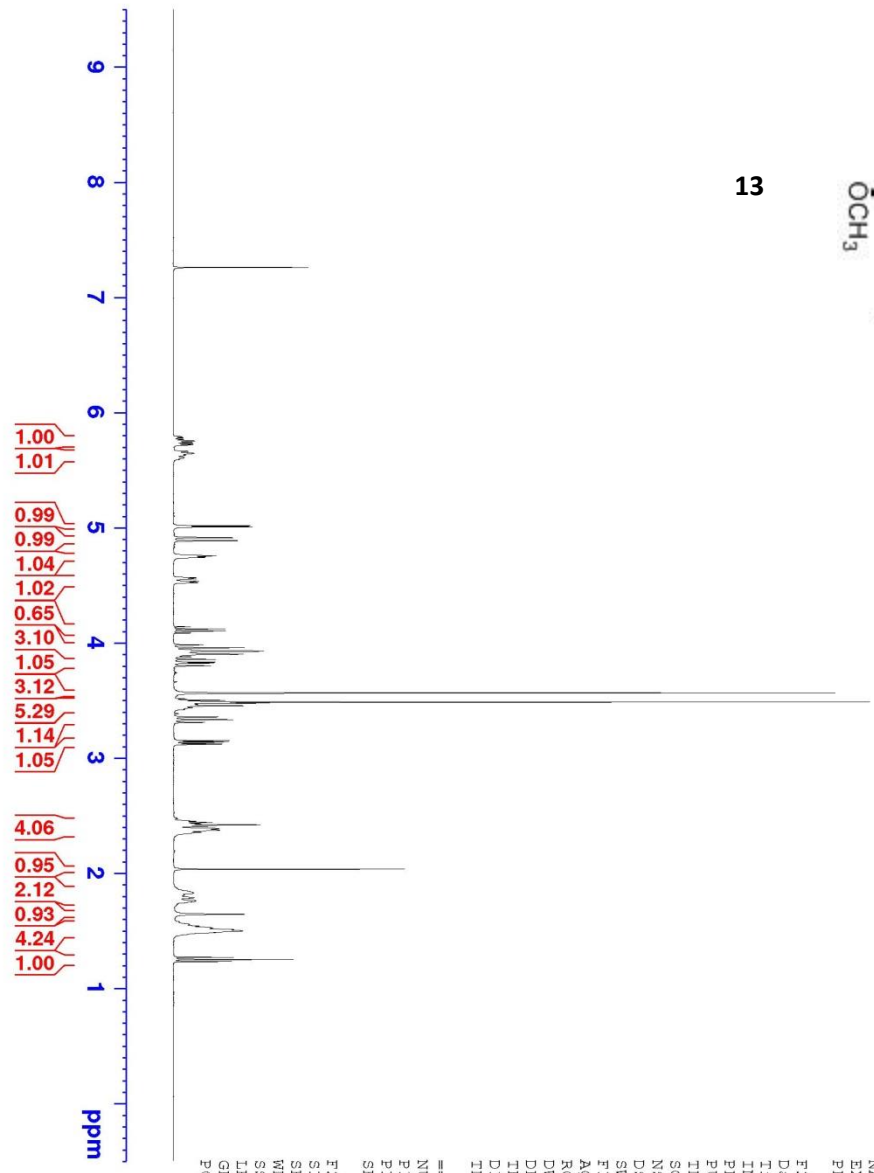
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NUC1 13C
P1 7.50 usec
PL1 0 dB
SFO1 75.4752953 MHz

==== CHANNEL f2 =====
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NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
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SF 75.4679856 MHz
WDW EM
SSB 0
GB 0
PC 1.40



13



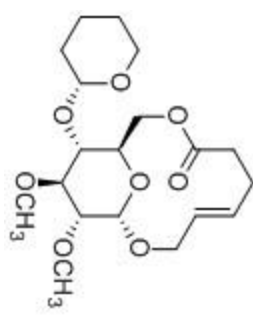
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 EXNO 1
 PROCNO 1

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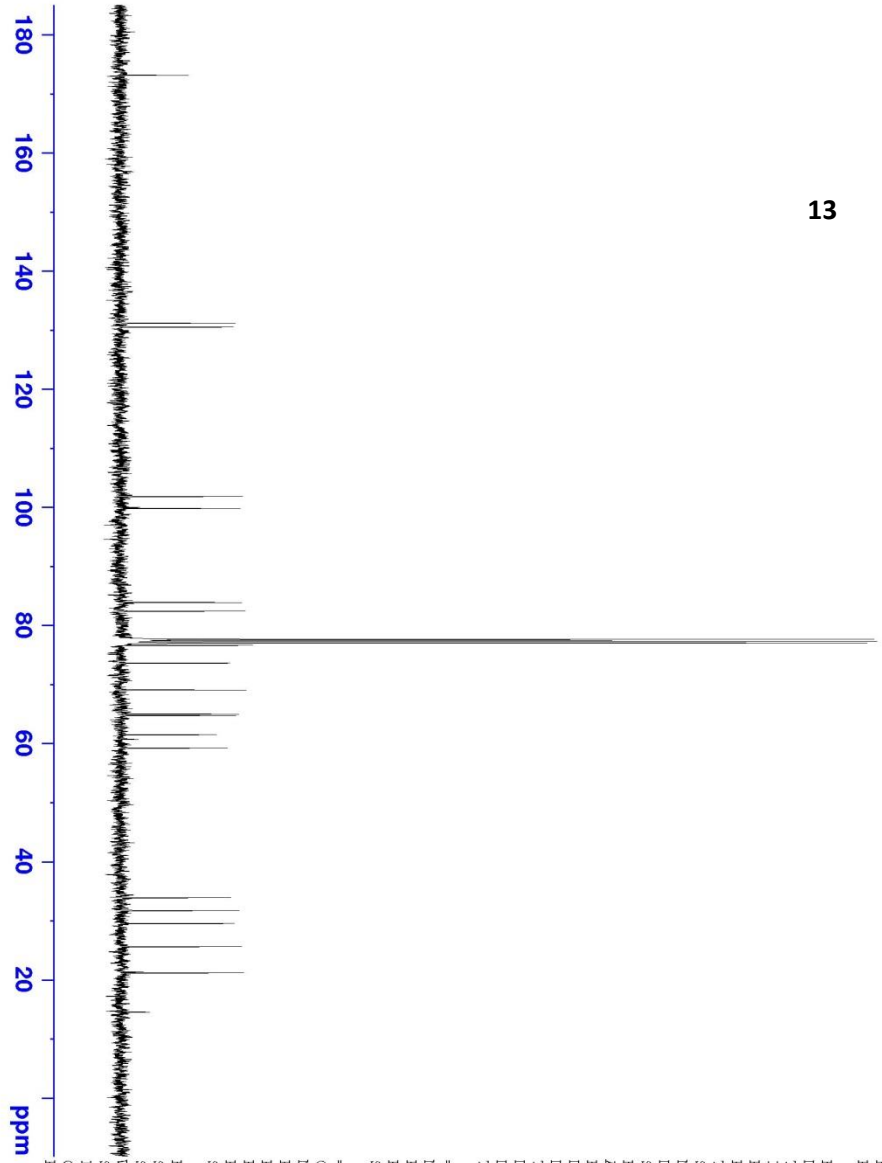
Date_ 20130917
 Time_ 15.12
 INSTRUM spect
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 PULPROG zg30
 TD 48076
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 8012.820 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999423 sec
 RG 80.6
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUCL 1H
 P1 15.20 usec
 PLW 12.00000000 W
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 321072
 SF 400.144094 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00



13



Current Data Parameters
NAME am-113-coll-178
EXNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130917
Time 15.15

INSTRUM spect
PROBHD 5 mm PABBO BBI/

PULPROG zgpg30
TD 43698

SOLVENT CDCl3
NS 157

DS 4
SMH 24038.461 Hz

FIDRES 0.550104 Hz
AQ 0.9089184 sec

RG 203
DW 20.800 usec

DE 6.50 usec
TE 300.1 K

D1 1.50000000 sec
D11 0.03000000 sec

TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec

PLM1 50.00299835 W
SFO1 100.6263500 MHz

===== CHANNEL f2 =====
CPDPRGf2 waltz16

NUC2 1H
PCPD2 90.00 usec

PLM2 12.00000000 W
PLM12 0.33333001 W

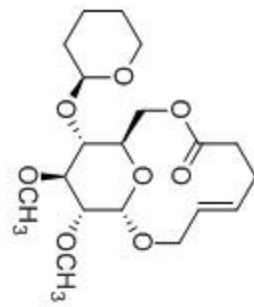
PLM13 0.27000001 W
SFO2 400.1456006 MHz

F2 - Processing parameters
SI 131072

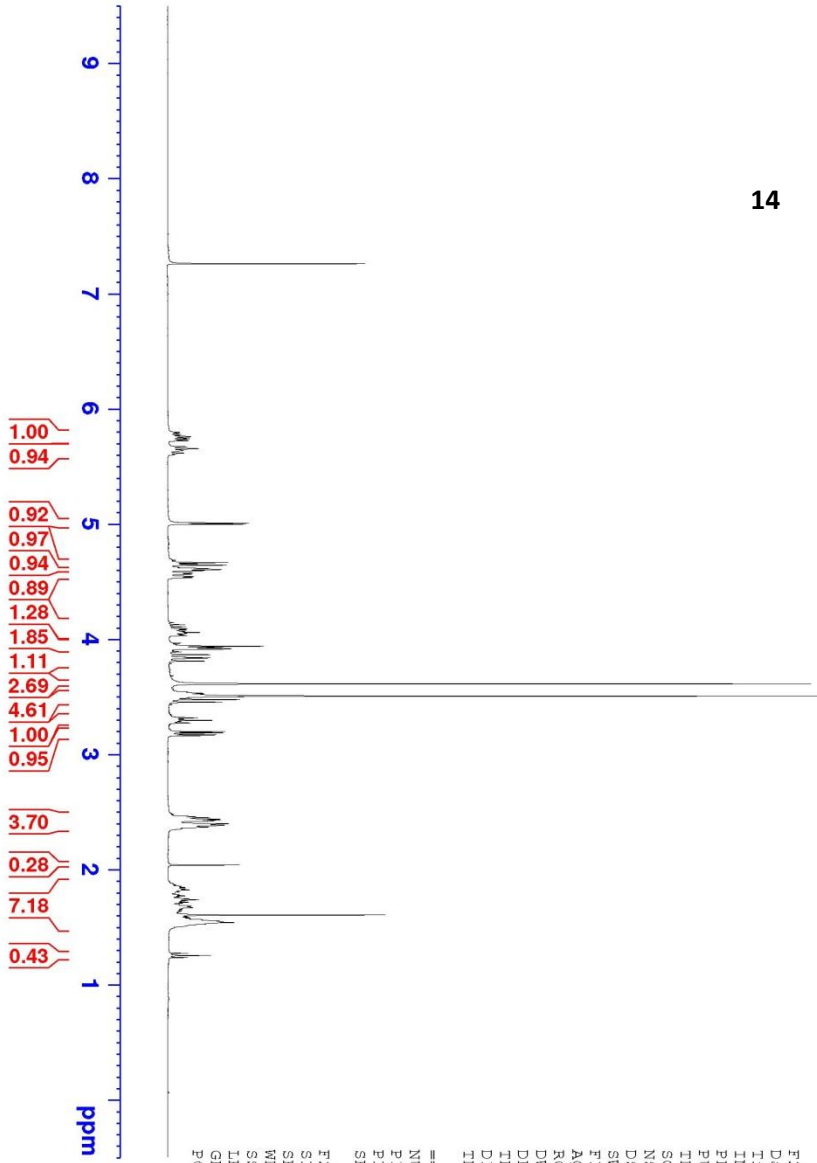
SF 100.6162656 MHz
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SSB 0
LB 2.50 Hz

GB 0
PC 1.40



14



Current Data Parameters
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 PROCNO 1

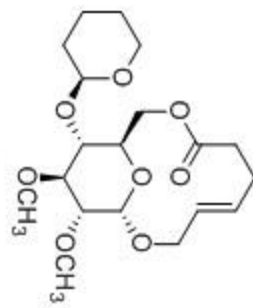
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 Time 15.29

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 PULPROG zg30
 TD 48076
 SOLVENT CDCl3
 NS 16
 DS 2

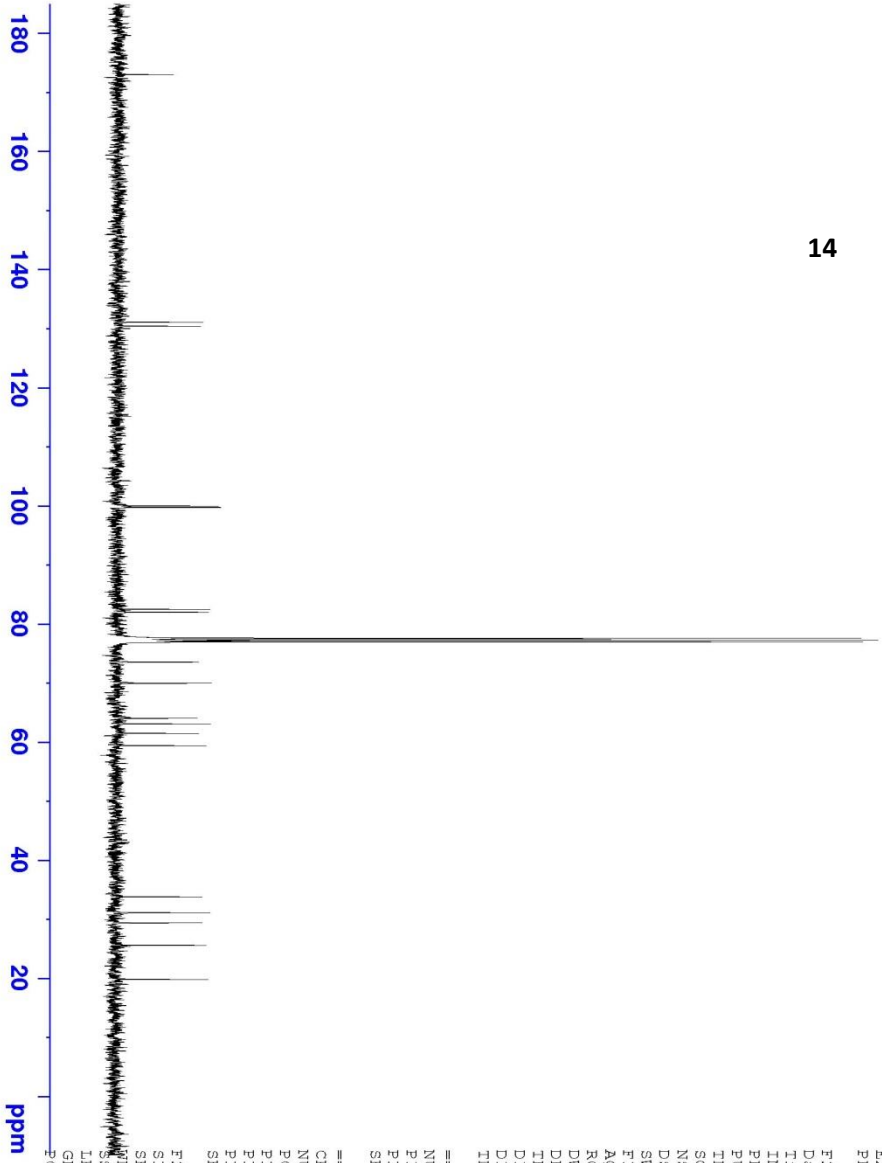
SMH 8012.820 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999423 sec
 RG 90.5
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUCL 1H
 P1 15.20 usec
 PLW1 12.00000000 W
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 321072
 SF 400.144095 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00



14



Current Data Parameters
 NAME am-113-coll-F16
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130917
 Time 15.35

INSTRUM spect
 PROBHD 5 mm PABBO BBI
 PULPROG zgpg30
 TD 43698
 SFO1 CDC13
 SOLVENT NS
 NS 235
 DS 4

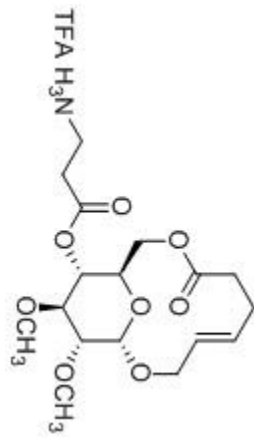
SMH 24038.461 Hz
 FIDRES 0.550104 Hz
 AQ 0.9089184 sec
 RG 203

DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

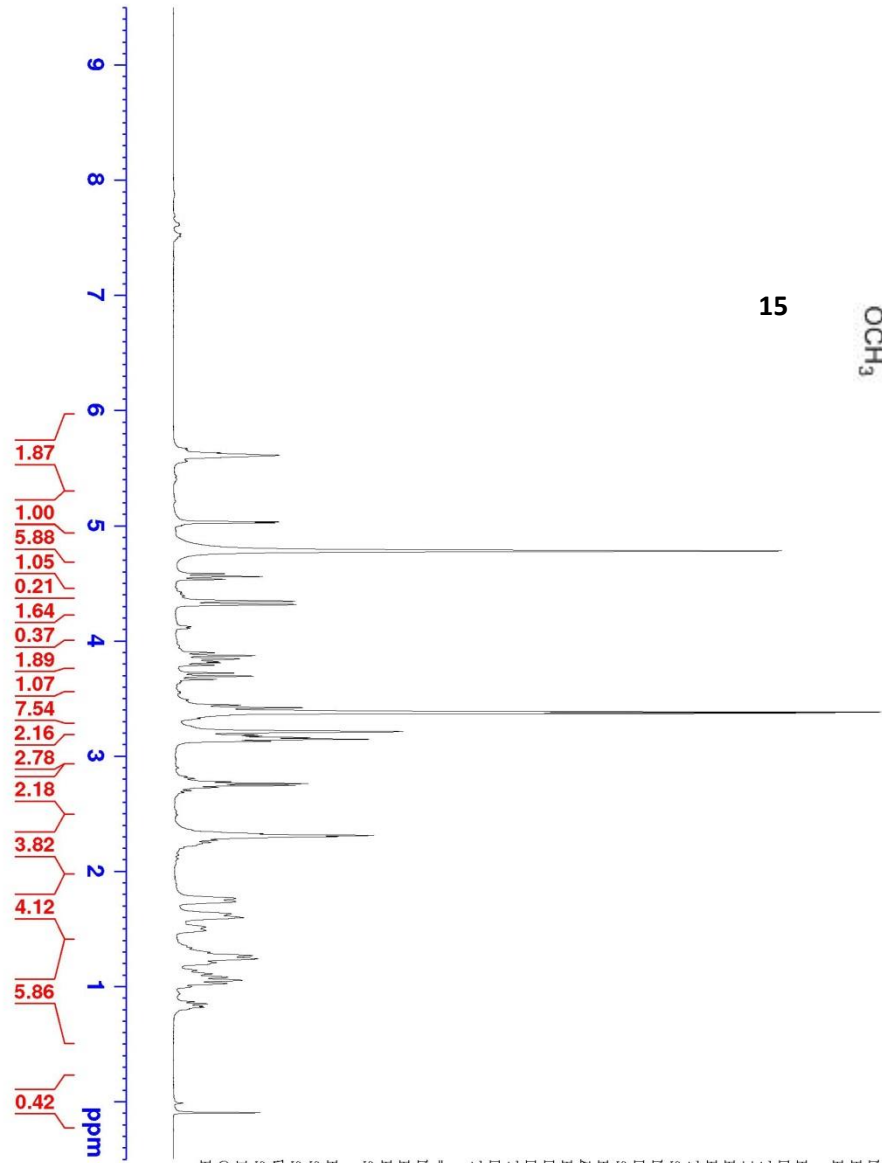
==== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PLW1 50.00299835 W
 SFO1 100.6263500 MHz

==== CHANNEL f2 =====
 CPDPRG12 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.33333001 W
 PLW13 0.27000001 W
 SFO2 400.1456006 MHz

F2 - Processing parameters
 SI 131072
 SF 100.6162656 MHz
 ADW EM
 SSB 0
 GB 0
 PC 1.40



15



Current Data Parameters
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 PROCNO 1

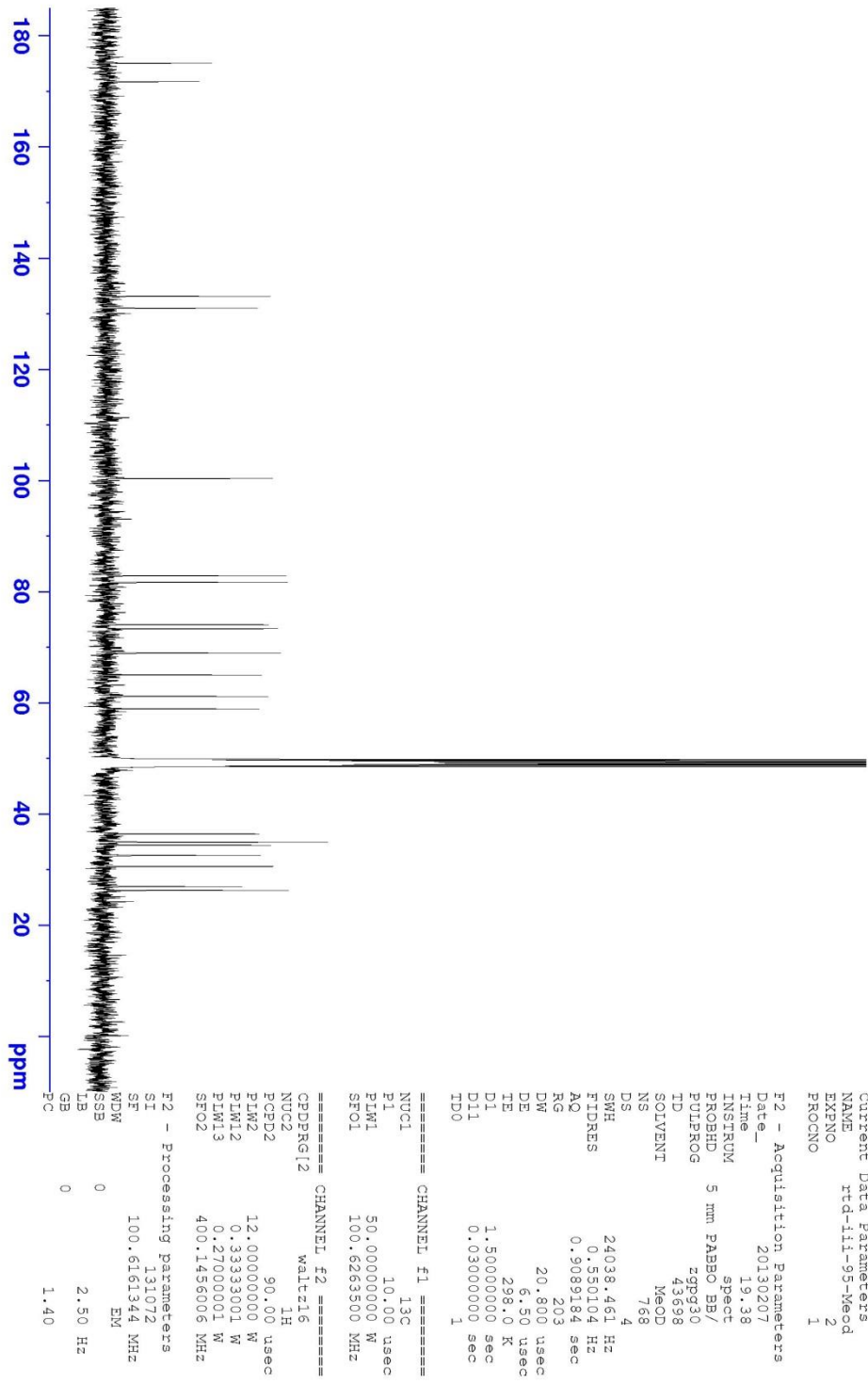
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 Time 19.30

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 PROBHD zg30
 PULPROG zgpg30
 TD 48076
 SOLVENT MeOD
 NS 32
 DS 2

SMH 8012.820 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999423 sec
 RG 80.6
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.22 usec
 PL1 12.00000000 W
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 321072
 SF 400.1464009 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00





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 PROCNO 1

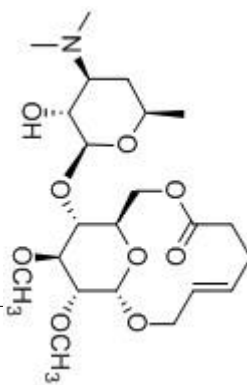
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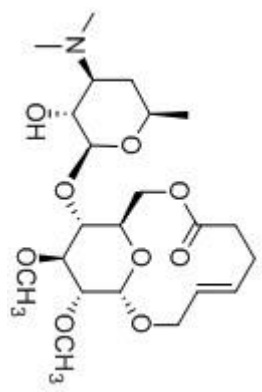
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 PULPROG zg30
 TD 48076
 SOLVENT CDCl3
 NS 16
 DS 2

SWH 8012.820 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999423 sec
 RG 203
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 DE 6.50 usec
 TE 300.0 K
 DI 2.00000000 sec
 TD0 1

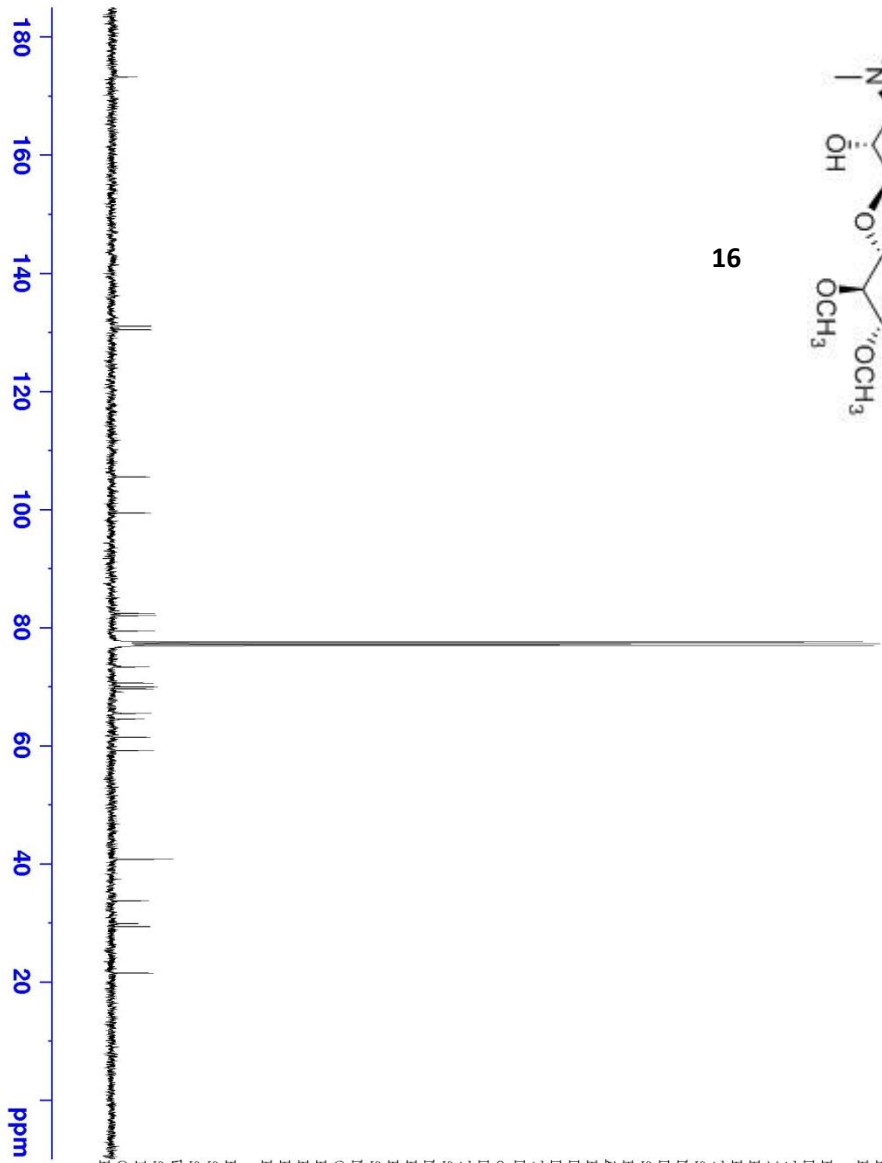
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 P1 15.20 usec
 P1M1 12.00000000 W
 SFO1 400.1464009 MHz

F2 - Processing parameters
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 SF 400.1440000 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00





16



Current Data Parameters
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 EXPRNO 2
 PROCNO 1

F2 - Acquisition Parameters
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 Time_ 15.48

INSTRUM spect
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 PULPROG zgpg30
 TD 43698
 SOLVENT CDCl3
 NS 253
 DS 4

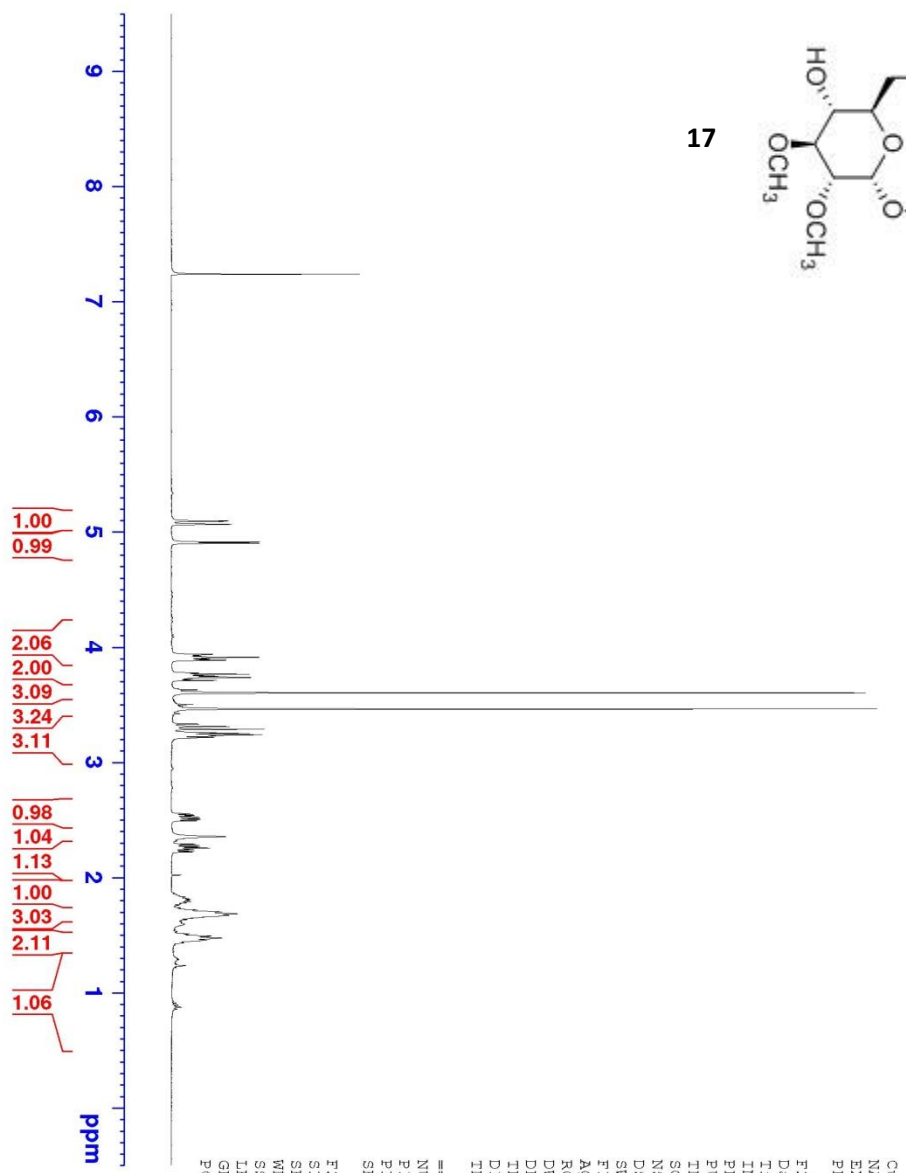
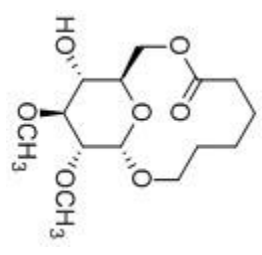
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 FIDRES 0.550104 Hz
 AQ 0.9089184 sec
 RG 114
 DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K

D1 1.50000000 sec
 d11 0.03000000 sec
 DELTA 1.39999998 sec
 ID0 1
 SFO1 100.6263500 MHz
 NUC1 13C

P1 10.00 usec
 PLW1 50.00299835 W
 SFO2 400.1456006 MHz
 NUC2 1H
 CPDPRG12 waltz16

PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLWI2 0.33333001 W
 PLWI3 0.270000001 W

F2 - Processing parameters
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 SF 100.6162684 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

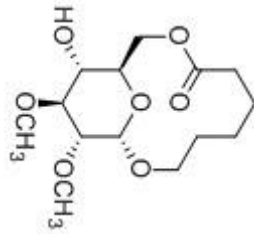


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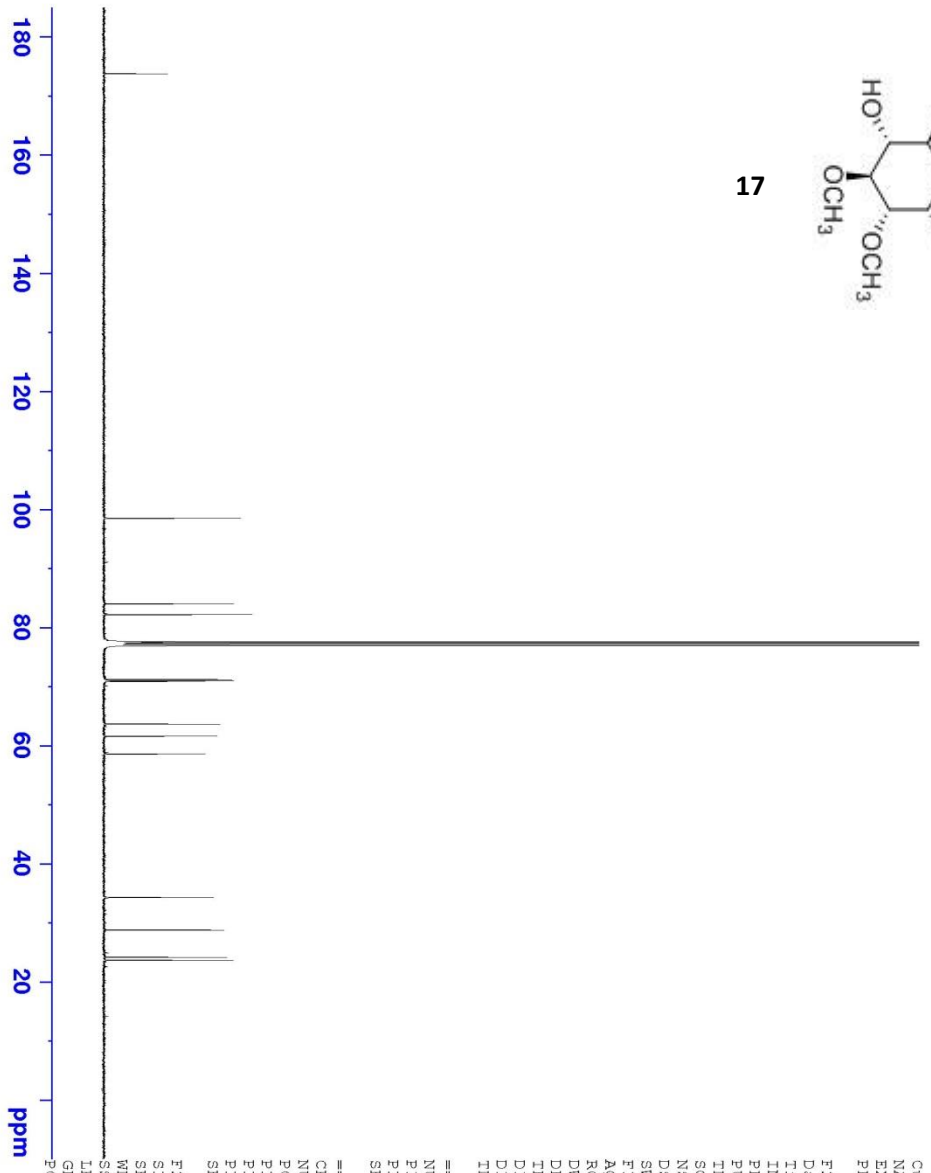
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 PROBHD 5 mm PABBO BBI
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 8012.820 Hz
 FIDRES 0.122256 Hz
 AQ 4.0894463 sec
 RG 181
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUCL1 1H
 P1 15.00 usec
 PLW1 12.00000000 W
 SFO1 400.1464711 MHz

F2 - Processing parameters
 SI 65536
 SE 400.1440175 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



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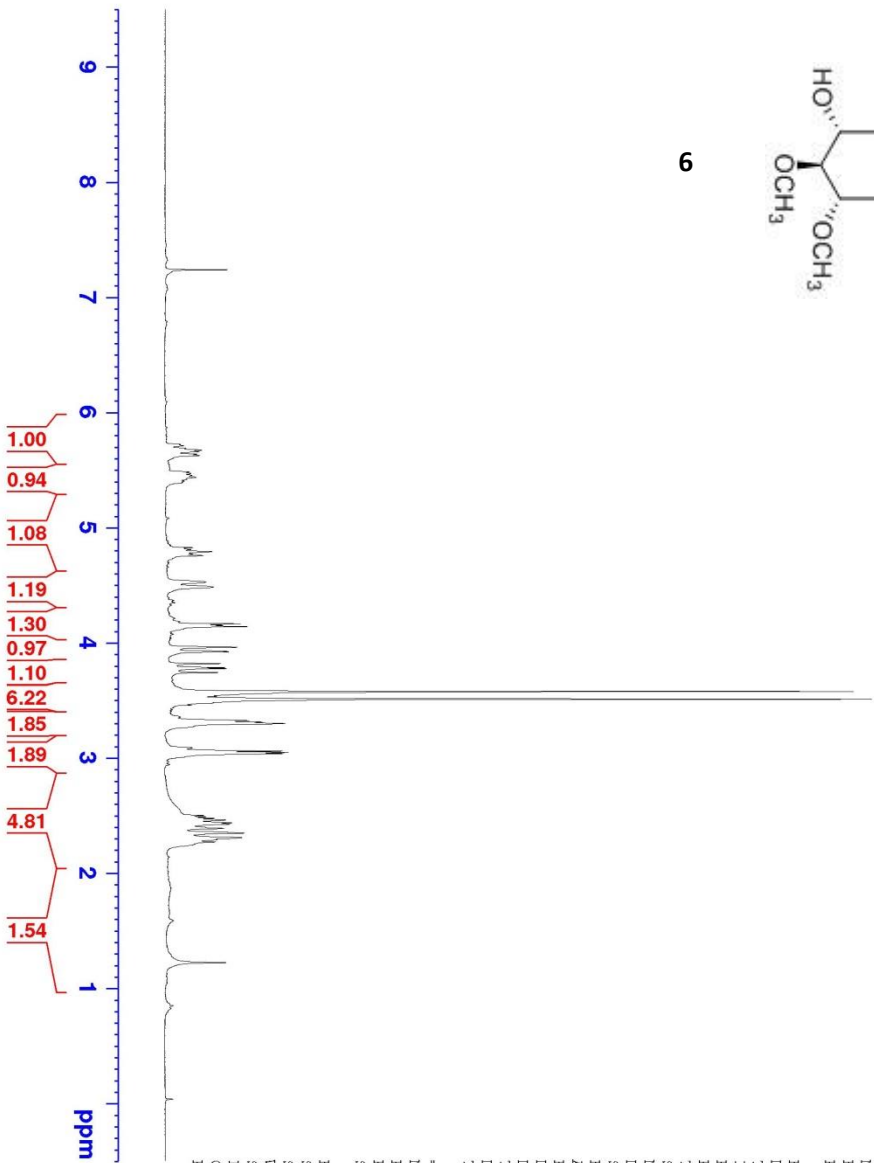
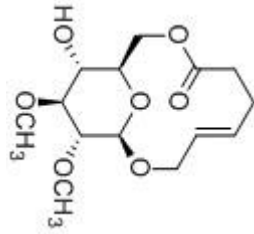
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 13673
 DS 4
 SMH 24038.461 Hz
 FIDRES 0.36798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUCl 13C
 P1 10.00 usec
 PLW1 50.00000000 W
 SFO1 100.6263500 MHz

==== CHANNEL f2 =====
 CPDPRGf2 waltz16
 NUCl 1H
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.33333001 W
 PLW13 0.27000001 W
 SFO2 400.1456006 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6162656 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
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 EXPRNO 1
 PROCNO 1

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 Time 21.10

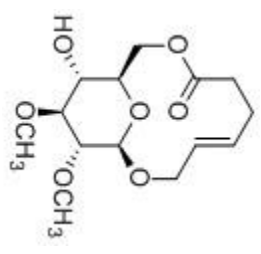
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 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 128

DS 2
 SMH 3906.250 Hz
 FIDRES 0.119209 Hz
 AQ 4.1949040 sec

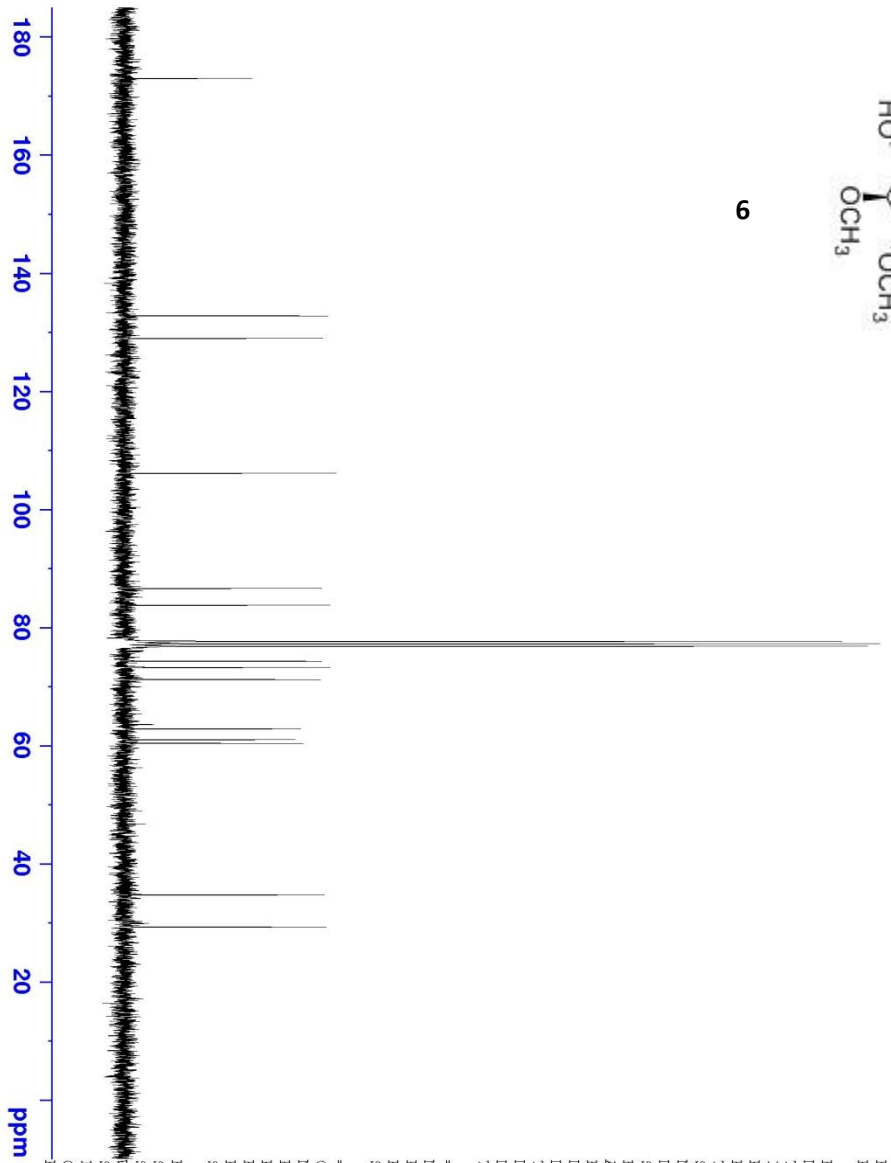
RG 256
 DW 128.000 usec
 DE 6.50 usec
 TE 300.2 K
 D1 1.50000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 8.20 usec
 PL1 0 dB
 SFO1 300.1326507 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1310160 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



9



Current Data Parameters
 NAME ftd-11-204-f2a
 EXFNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110602
 Time_ 2.53

INSTRUM spect
 PROBHD 5 mm Multinuc1
 PULPROG zgpg30
 TD 65536
 SFO1 302.0 K
 SOLVENT CDCl3
 NS 5120
 DS 4

SMH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219008 sec
 RG 32768
 DW 27.800 usec
 DE 6.50 usec
 TE 302.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 7.50 usec
 PL1 0 dB
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====
 CPDPRGf2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -2.00 dB
 PL12 15.00 dB
 PL13 15.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4679850 MHz
 HYDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



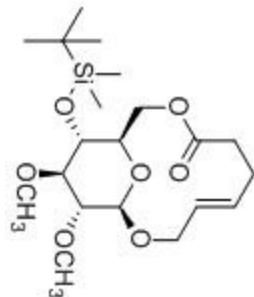
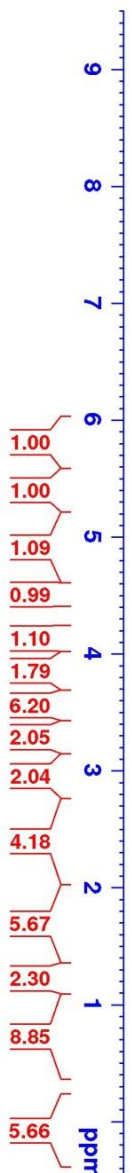
Current Data Parameters
NAME rtd-111-104-p2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130807
Time 12.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 48076
SOLVENT CDCl3
NS 32
DS 2

SWH 8012.820 Hz
FIDRES 0.166670 Hz
AQ 2.9999423 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.20 usec
PLM1 12.00000000 W
SFO1 400.1464009 MHz

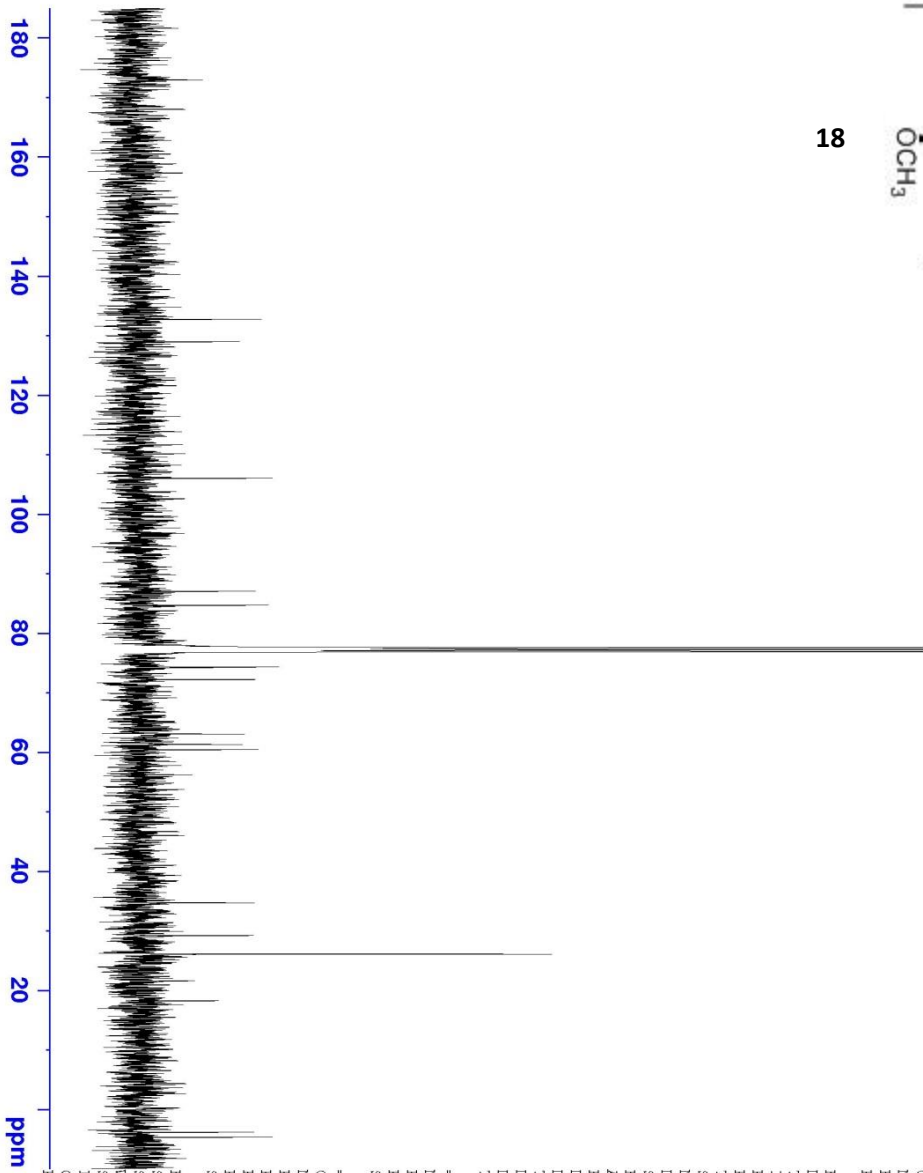
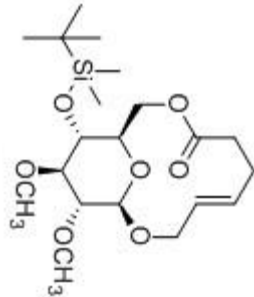
F2 - Processing parameters
SI 131072
SF 400.1440177 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00



18



18



Current Data Parameters
NAME rtd-111-104-p2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130807
Time 12.05

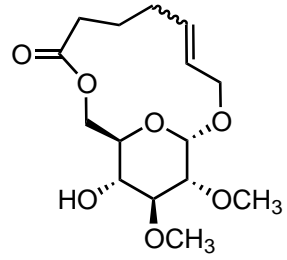
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 43698
SOLVENT CDCl3
NS 512
DS 4

SWH 24038.461 Hz
FIDRES 0.550104 Hz
AQ 0.9089184 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 300.2 K
D1 1.5000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PLW1 50.00229835 W
SFO1 100.6263500 MHz

===== CHANNEL f2 =====
CPDPRGf2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.33333001 W
PLW13 0.27000001 W
SFO2 400.1456006 MHz

F2 - Processing parameters
SI 131072
SF 100.6162693 MHz
WDW EM
SSB 0
LB 2.50 Hz
GB 0
PC 1.40



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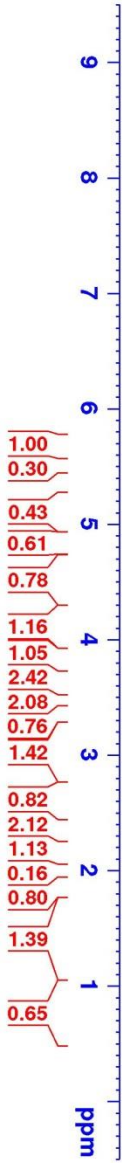
Current Data Parameters
 NAME rtd-111-1-p3 a
 EXPNO 1
 PROCNO 1

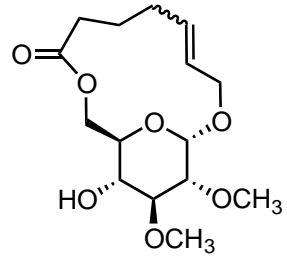
F2 - Acquisition Parameters

Date_ 20110610
 Time 14.07
 INSTRUM spect
 FROSHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 5592.841 Hz
 FIDRES 0.170689 Hz
 AQ 2.9294591 sec
 RG 181
 DW 89.400 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.50000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.20 usec
 P1L -2.00 dB
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1440169 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





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Current Data Parameters
 NAME red-f11-1-p3 a
 EXENO 2
 PROCNO 1

F2 - Acquisition Parameters

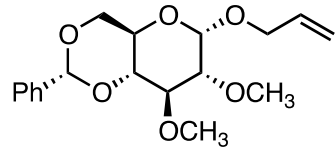
Date_ 20110610
 Time_ 14.44
 INSTRUM spect
 PROBDW 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 368
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.363218 Hz
 AQ 1.3684236 sec
 RG 32768
 DW 20.850 usec
 DE 6.00 usec
 TE 300.2 K
 D1 6.00000000 sec
 d11 0.03000000 sec
 DELTA 5.90000010 sec
 TD0 1

==== CHANNEL F1 =====
 NUCL1 13C
 P1 10.00 usec
 P11 0 dB
 SF01 100.6263500 MHz

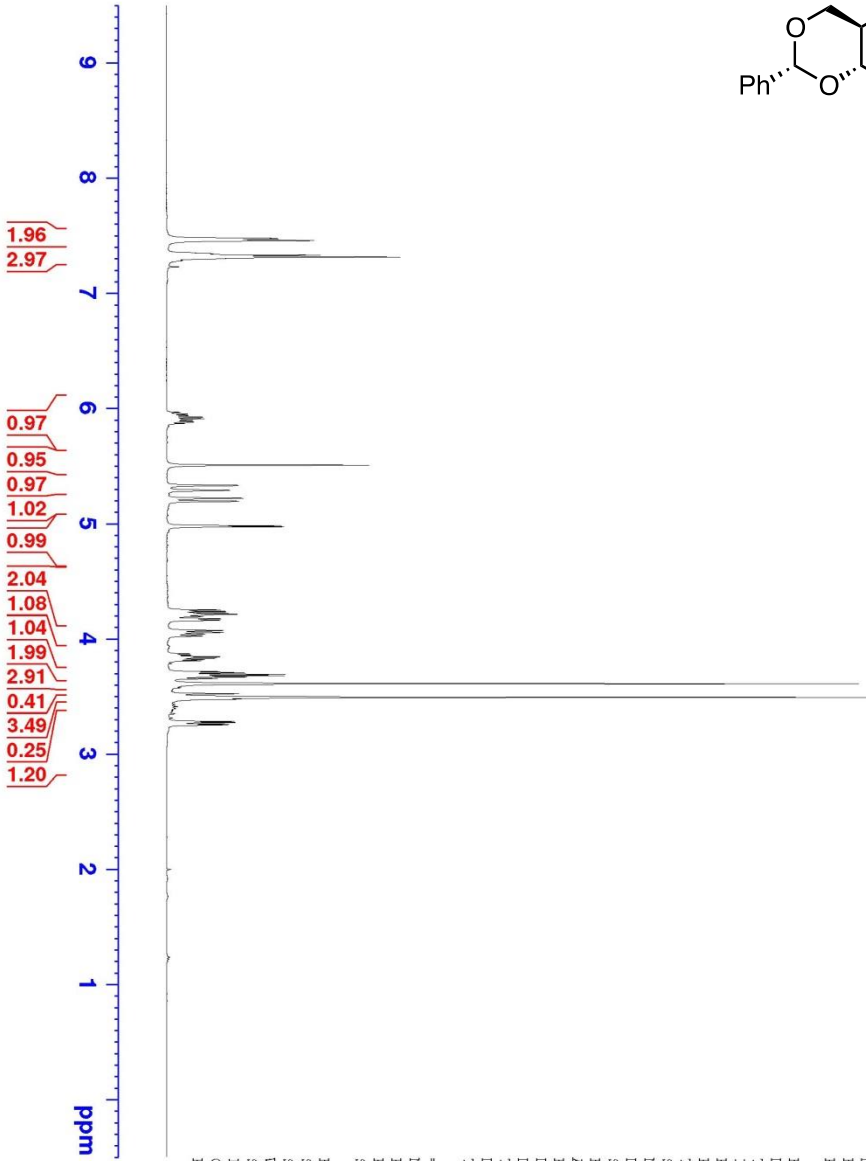
==== CHANNEL F2 =====
 CDPDRG12 waltz16
 NUCL2 1H
 PCPD2 110.00 usec
 P12 12.00 dB
 P112 13.00 dB
 P113 13.00 dB
 SF02 400.1496010 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6162685 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





8a



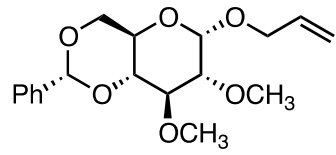
Current Data Parameters
 NAME Ftd-11-194-b2
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20110315
 Time_ 14.44
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9294591 sec
 RG 35.9
 DW 89.400 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.50000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.20 usec
 PL1 -2.00 dB
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1440204 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



8a



Current Data Parameters
 NAME Ftd-11-194-D2
 EXFNO 2
 PROCNO 1

F2 - Acquisition Parameters

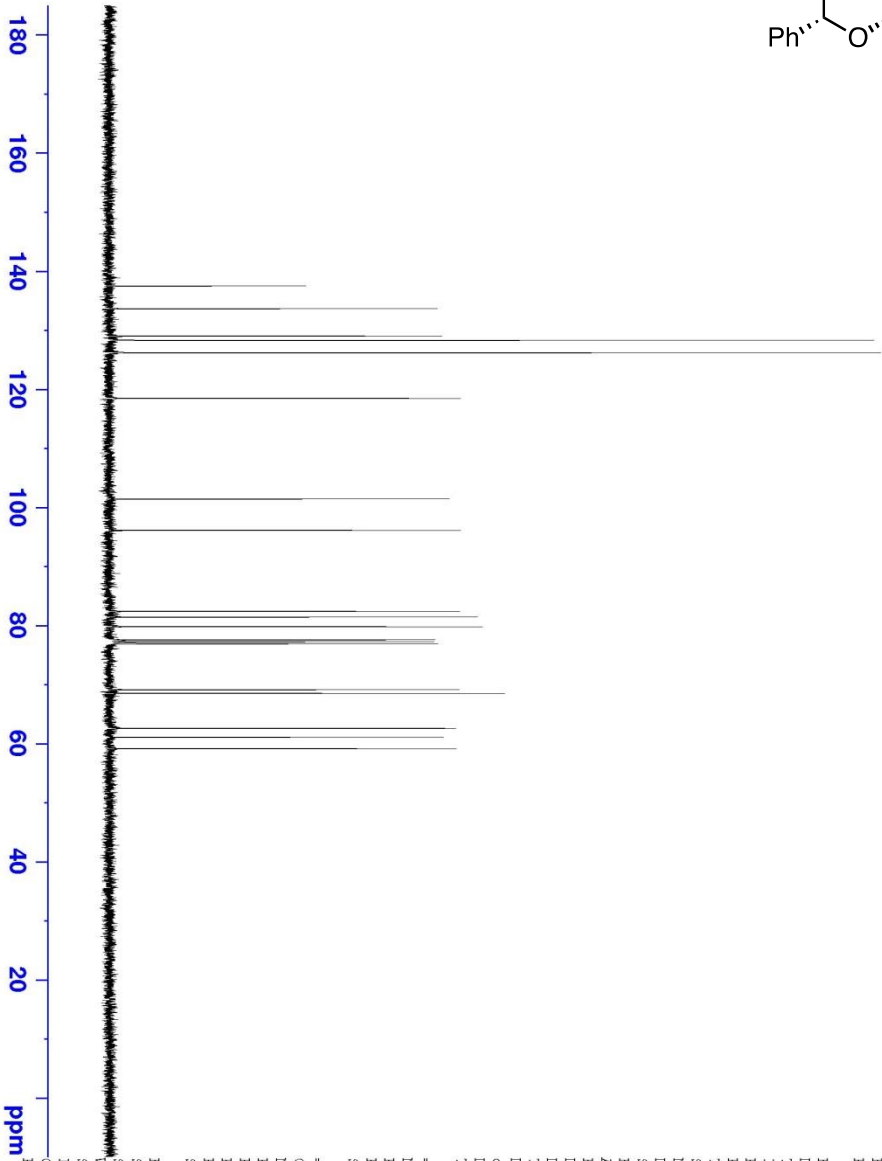
Date_ 20110315
 Time_ 14.49
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 77
 DS 4
 SMH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3684258 sec
 RG 32768
 DW 20.850 usec
 DE 6.00 usec
 TE 300.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 ID0 1

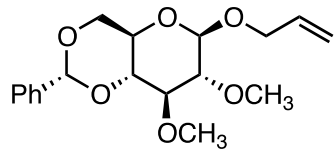
===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0 dB
 SFO1 100.6283500 MHz

===== CHANNEL f2 =====
 CPDPRG12 waltz16
 NUC2 1H
 PCPD2 110.00 usec
 PL2 -2.00 dB
 PL12 19.00 dB
 PL13 19.00 dB
 SFO2 400.1456010 MHz

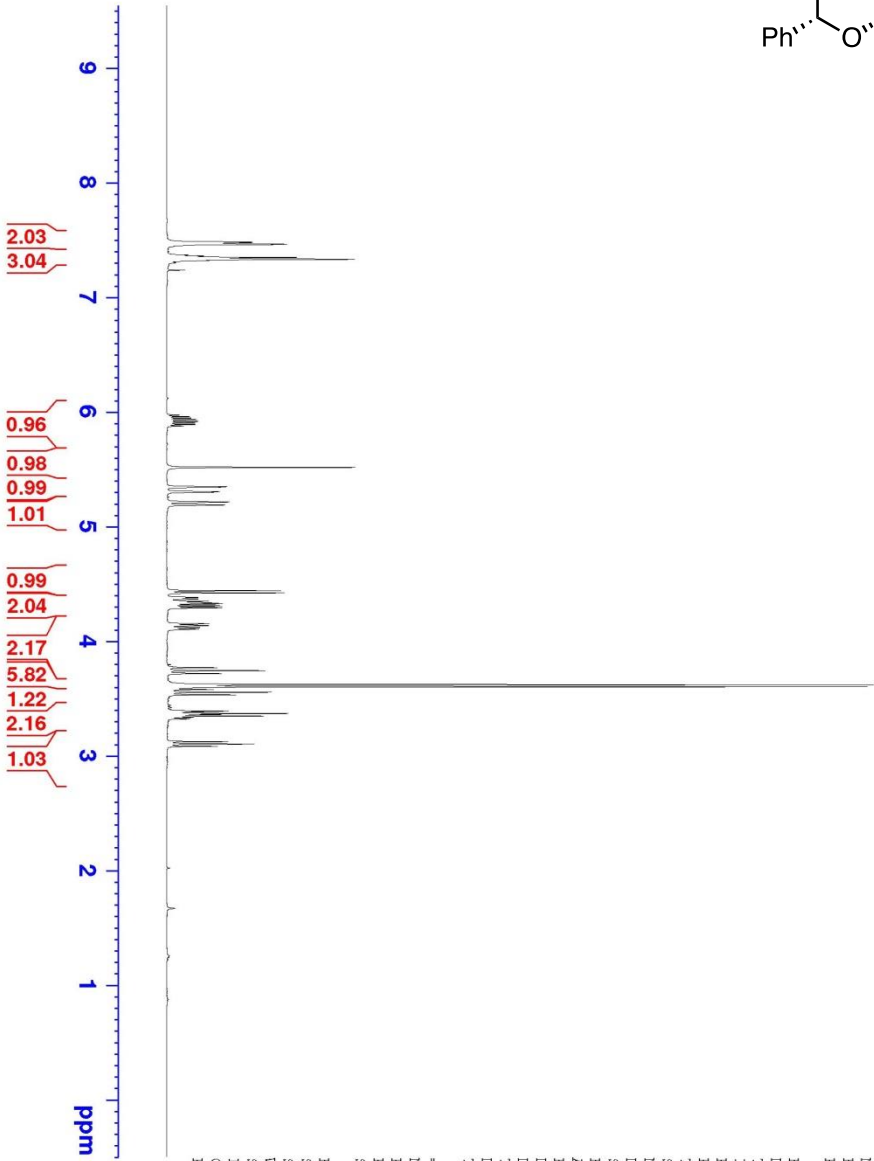
F2 - Processing parameters

SI 32768
 SF 100.6162806 MHz
 MDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





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Current Data Parameters
 NAME Ftd-11-195-P1
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110316
 Time_ 15.17

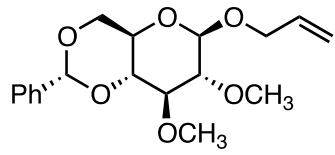
INSTRUM spect
 PROBHD 1H/1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2

SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9294591 sec
 RG 57

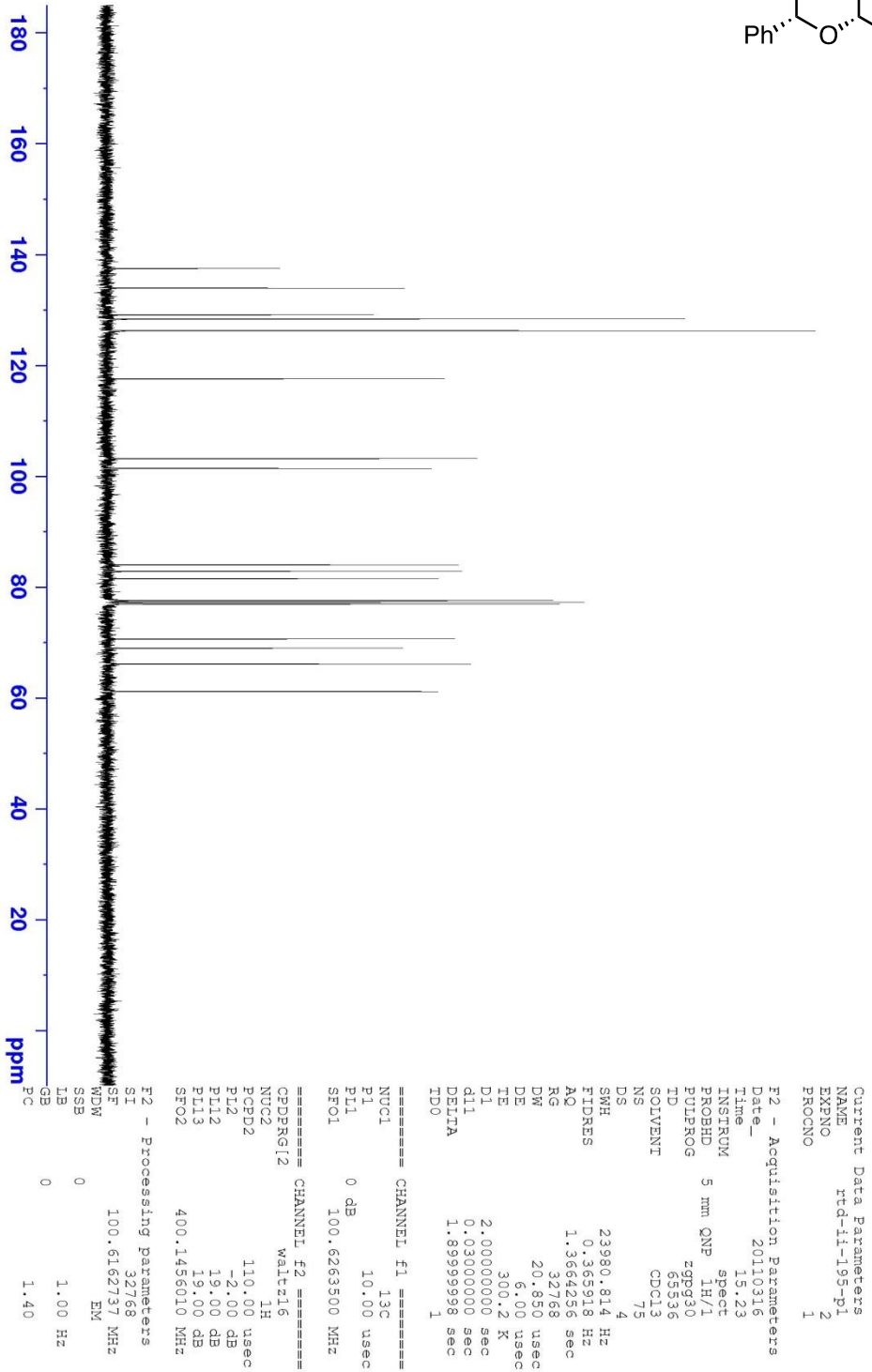
DW 89.400 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.50000000 sec
 TD0 1

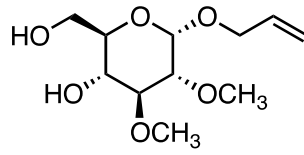
==== CHANNEL f1 =====
 NUC1 1H
 P1 9.20 usec
 PL1 -2.00 dB
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1440164 MHz
 WDW EM
 SSB 0
 IB 0.30 Hz
 GB 0
 PC 1.00

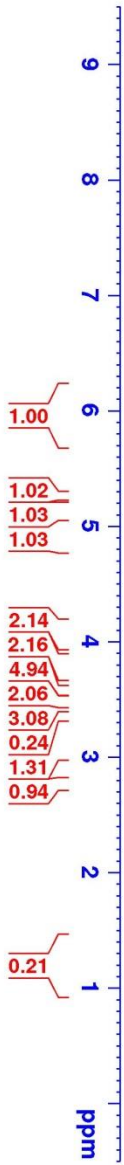


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9a



Current Data Parameters
 NAME Ftd-11-196-p1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110317
 Time 9.27
 INSTRUM spect
 PULPROG 5 mm QNP 1H/1
 F2 - Processing parameters
 SFO1 400.1464009 MHz
 SI 32768
 SF 400.1440172 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.20 usec
 P1L -2.00 dB
 SFO1 400.1464009 MHz

F2 - Acquisition Parameters
 Date_ 20110317
 Time 9.27
 INSTRUM spect
 PULPROG 5 mm QNP 1H/1
 F2 - Processing parameters
 SFO1 400.1464009 MHz
 SI 32768
 SF 400.1440172 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.20 usec
 P1L -2.00 dB
 SFO1 400.1464009 MHz

===== CHANNEL f2 =====
 NUC2 13C
 P2 12.00 usec
 P2L -2.00 dB
 SFO2 101.2519046 MHz

===== CHANNEL f3 =====
 NUC3 13C
 P3 12.00 usec
 P3L -2.00 dB
 SFO3 101.2519046 MHz

===== CHANNEL f4 =====
 NUC4 13C
 P4 12.00 usec
 P4L -2.00 dB
 SFO4 101.2519046 MHz

===== CHANNEL f5 =====
 NUC5 13C
 P5 12.00 usec
 P5L -2.00 dB
 SFO5 101.2519046 MHz

===== CHANNEL f6 =====
 NUC6 13C
 P6 12.00 usec
 P6L -2.00 dB
 SFO6 101.2519046 MHz

===== CHANNEL f7 =====
 NUC7 13C
 P7 12.00 usec
 P7L -2.00 dB
 SFO7 101.2519046 MHz

===== CHANNEL f8 =====
 NUC8 13C
 P8 12.00 usec
 P8L -2.00 dB
 SFO8 101.2519046 MHz

===== CHANNEL f9 =====
 NUC9 13C
 P9 12.00 usec
 P9L -2.00 dB
 SFO9 101.2519046 MHz

===== CHANNEL f10 =====
 NUC10 13C
 P10 12.00 usec
 P10L -2.00 dB
 SFO10 101.2519046 MHz

===== CHANNEL f11 =====
 NUC11 13C
 P11 12.00 usec
 P11L -2.00 dB
 SFO11 101.2519046 MHz

===== CHANNEL f12 =====
 NUC12 13C
 P12 12.00 usec
 P12L -2.00 dB
 SFO12 101.2519046 MHz

===== CHANNEL f13 =====
 NUC13 13C
 P13 12.00 usec
 P13L -2.00 dB
 SFO13 101.2519046 MHz

===== CHANNEL f14 =====
 NUC14 13C
 P14 12.00 usec
 P14L -2.00 dB
 SFO14 101.2519046 MHz

===== CHANNEL f15 =====
 NUC15 13C
 P15 12.00 usec
 P15L -2.00 dB
 SFO15 101.2519046 MHz

===== CHANNEL f16 =====
 NUC16 13C
 P16 12.00 usec
 P16L -2.00 dB
 SFO16 101.2519046 MHz

===== CHANNEL f17 =====
 NUC17 13C
 P17 12.00 usec
 P17L -2.00 dB
 SFO17 101.2519046 MHz

===== CHANNEL f18 =====
 NUC18 13C
 P18 12.00 usec
 P18L -2.00 dB
 SFO18 101.2519046 MHz

===== CHANNEL f19 =====
 NUC19 13C
 P19 12.00 usec
 P19L -2.00 dB
 SFO19 101.2519046 MHz

===== CHANNEL f20 =====
 NUC20 13C
 P20 12.00 usec
 P20L -2.00 dB
 SFO20 101.2519046 MHz

===== CHANNEL f21 =====
 NUC21 13C
 P21 12.00 usec
 P21L -2.00 dB
 SFO21 101.2519046 MHz

===== CHANNEL f22 =====
 NUC22 13C
 P22 12.00 usec
 P22L -2.00 dB
 SFO22 101.2519046 MHz

===== CHANNEL f23 =====
 NUC23 13C
 P23 12.00 usec
 P23L -2.00 dB
 SFO23 101.2519046 MHz

===== CHANNEL f24 =====
 NUC24 13C
 P24 12.00 usec
 P24L -2.00 dB
 SFO24 101.2519046 MHz

===== CHANNEL f25 =====
 NUC25 13C
 P25 12.00 usec
 P25L -2.00 dB
 SFO25 101.2519046 MHz

===== CHANNEL f26 =====
 NUC26 13C
 P26 12.00 usec
 P26L -2.00 dB
 SFO26 101.2519046 MHz

===== CHANNEL f27 =====
 NUC27 13C
 P27 12.00 usec
 P27L -2.00 dB
 SFO27 101.2519046 MHz

===== CHANNEL f28 =====
 NUC28 13C
 P28 12.00 usec
 P28L -2.00 dB
 SFO28 101.2519046 MHz

===== CHANNEL f29 =====
 NUC29 13C
 P29 12.00 usec
 P29L -2.00 dB
 SFO29 101.2519046 MHz

===== CHANNEL f30 =====
 NUC30 13C
 P30 12.00 usec
 P30L -2.00 dB
 SFO30 101.2519046 MHz

===== CHANNEL f31 =====
 NUC31 13C
 P31 12.00 usec
 P31L -2.00 dB
 SFO31 101.2519046 MHz

===== CHANNEL f32 =====
 NUC32 13C
 P32 12.00 usec
 P32L -2.00 dB
 SFO32 101.2519046 MHz

===== CHANNEL f33 =====
 NUC33 13C
 P33 12.00 usec
 P33L -2.00 dB
 SFO33 101.2519046 MHz

===== CHANNEL f34 =====
 NUC34 13C
 P34 12.00 usec
 P34L -2.00 dB
 SFO34 101.2519046 MHz

===== CHANNEL f35 =====
 NUC35 13C
 P35 12.00 usec
 P35L -2.00 dB
 SFO35 101.2519046 MHz

===== CHANNEL f36 =====
 NUC36 13C
 P36 12.00 usec
 P36L -2.00 dB
 SFO36 101.2519046 MHz

===== CHANNEL f37 =====
 NUC37 13C
 P37 12.00 usec
 P37L -2.00 dB
 SFO37 101.2519046 MHz

===== CHANNEL f38 =====
 NUC38 13C
 P38 12.00 usec
 P38L -2.00 dB
 SFO38 101.2519046 MHz

===== CHANNEL f39 =====
 NUC39 13C
 P39 12.00 usec
 P39L -2.00 dB
 SFO39 101.2519046 MHz

===== CHANNEL f40 =====
 NUC40 13C
 P40 12.00 usec
 P40L -2.00 dB
 SFO40 101.2519046 MHz

===== CHANNEL f41 =====
 NUC41 13C
 P41 12.00 usec
 P41L -2.00 dB
 SFO41 101.2519046 MHz

===== CHANNEL f42 =====
 NUC42 13C
 P42 12.00 usec
 P42L -2.00 dB
 SFO42 101.2519046 MHz

===== CHANNEL f43 =====
 NUC43 13C
 P43 12.00 usec
 P43L -2.00 dB
 SFO43 101.2519046 MHz

===== CHANNEL f44 =====
 NUC44 13C
 P44 12.00 usec
 P44L -2.00 dB
 SFO44 101.2519046 MHz

===== CHANNEL f45 =====
 NUC45 13C
 P45 12.00 usec
 P45L -2.00 dB
 SFO45 101.2519046 MHz

===== CHANNEL f46 =====
 NUC46 13C
 P46 12.00 usec
 P46L -2.00 dB
 SFO46 101.2519046 MHz

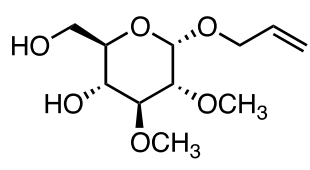
===== CHANNEL f47 =====
 NUC47 13C
 P47 12.00 usec
 P47L -2.00 dB
 SFO47 101.2519046 MHz

===== CHANNEL f48 =====
 NUC48 13C
 P48 12.00 usec
 P48L -2.00 dB
 SFO48 101.2519046 MHz

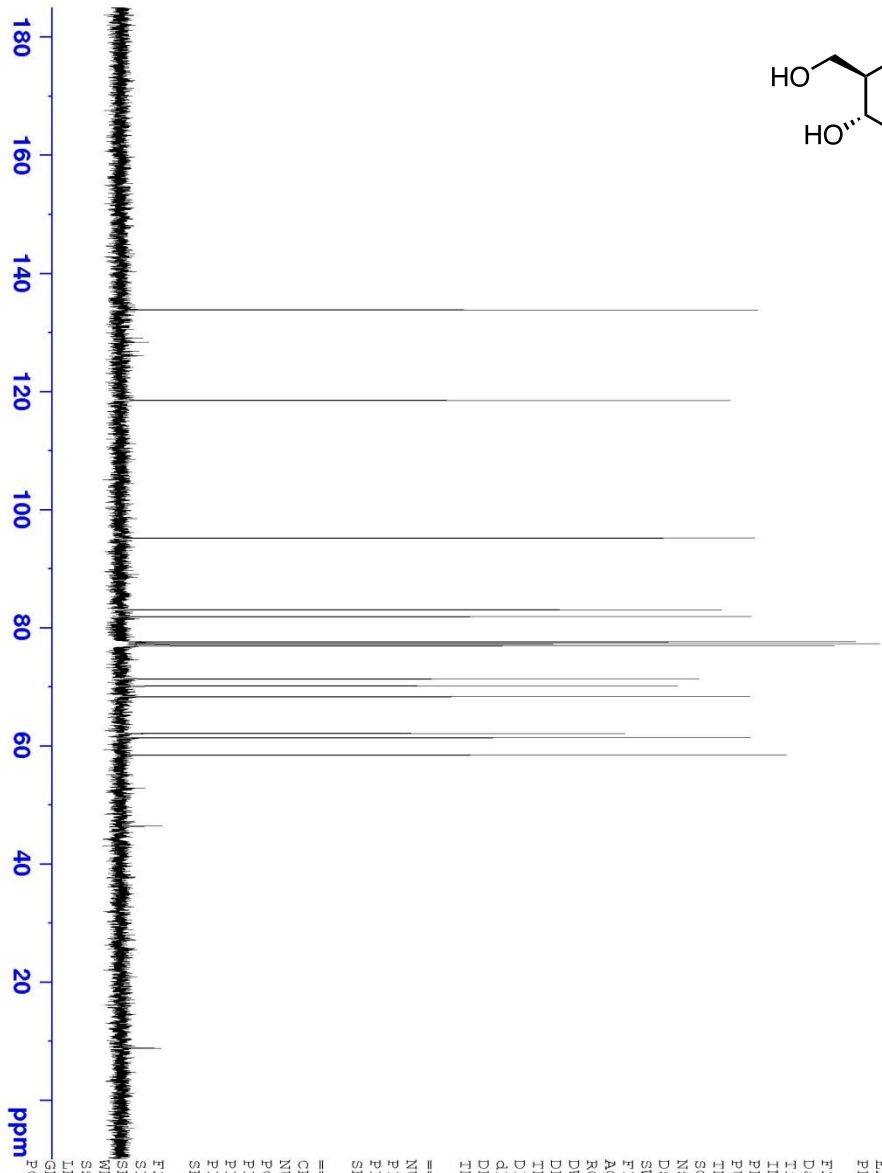
===== CHANNEL f49 =====
 NUC49 13C
 P49 12.00 usec
 P49L -2.00 dB
 SFO49 101.2519046 MHz

===== CHANNEL f50 =====
 NUC50 13C
 P50 12.00 usec
 P50L -2.00 dB
 SFO50 101.2519046 MHz





9a



Current Data Parameters
 NAME Ftd-11-196-P1
 EXNO 2
 PROCNO 1

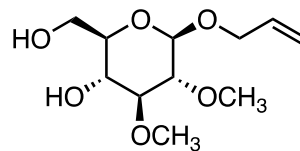
F2 - Acquisition Parameters
 Date_ 20110317
 Time_ 9.34

INSTRUM spect
 PROBHD 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 118
 DS 4
 SMH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3684258 sec
 RG 32768
 DW 20.850 usec
 DE 6.00 usec
 TE 300.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 ID0 1

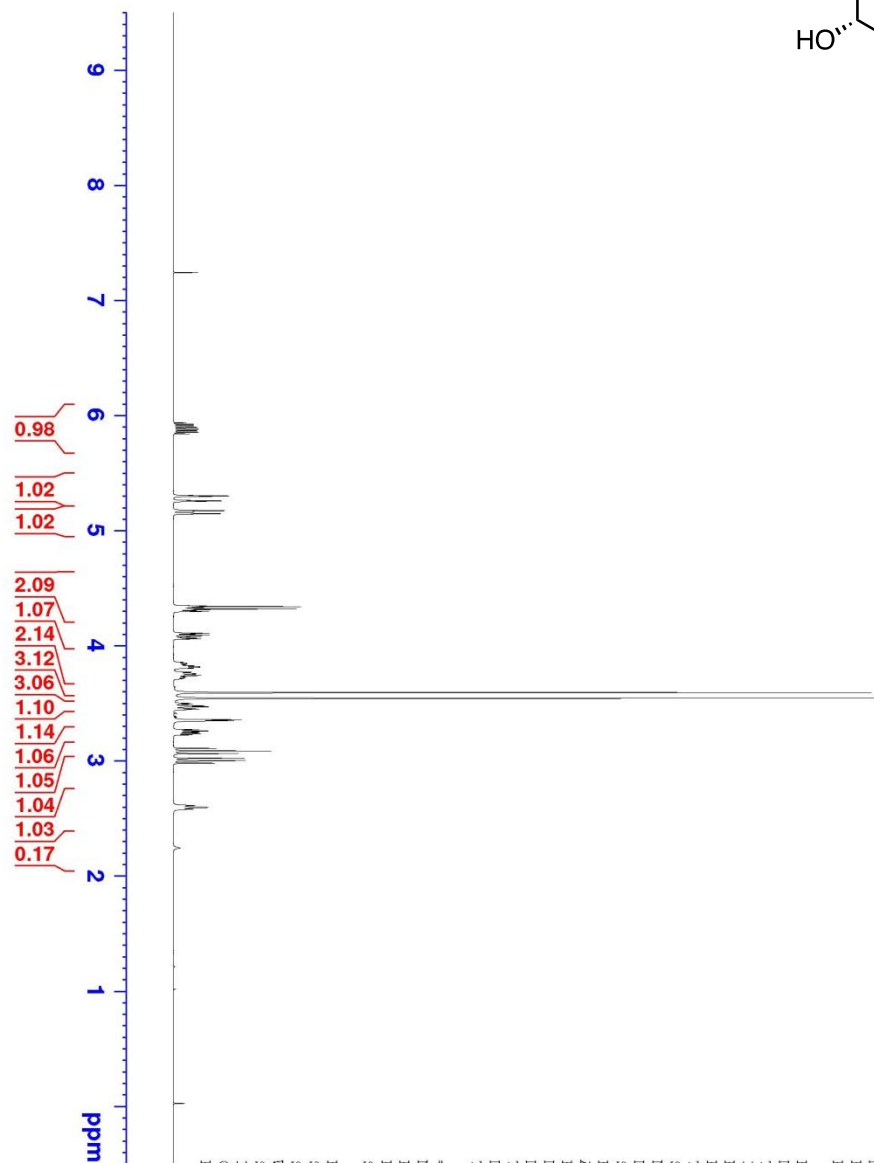
===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0 dB
 SFO1 100.6283500 MHz

===== CHANNEL f2 =====
 CPDPRG12 waltz16
 NUC2 1H
 PCPD2 110.00 usec
 PL2 -2.00 dB
 PL12 19.00 dB
 PL13 19.00 dB
 SFO2 400.1456010 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6162746 MHz
 MDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



9b



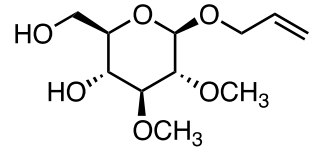
Current Data Parameters
 NAME Ftd-11-202-p2
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110516
 Time 12.05
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 ID 32768
 SOLVENT CDCl3
 NS 16
 DS 2

SMH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9294921 sec
 RG 57
 DE 89.400 usec
 TE 300.2 K
 D1 1.50000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUCL 1H
 P1 9.20 usec
 PL1 -2.00 dB
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1440167 MHz
 WDW EM
 SSB 0
 IB 0.30 Hz
 GB 0
 PC 1.00



9b



Current Data Parameters
 NAME rtd-11-203-p2-400
 EXPRNO 2
 PROCNO 1

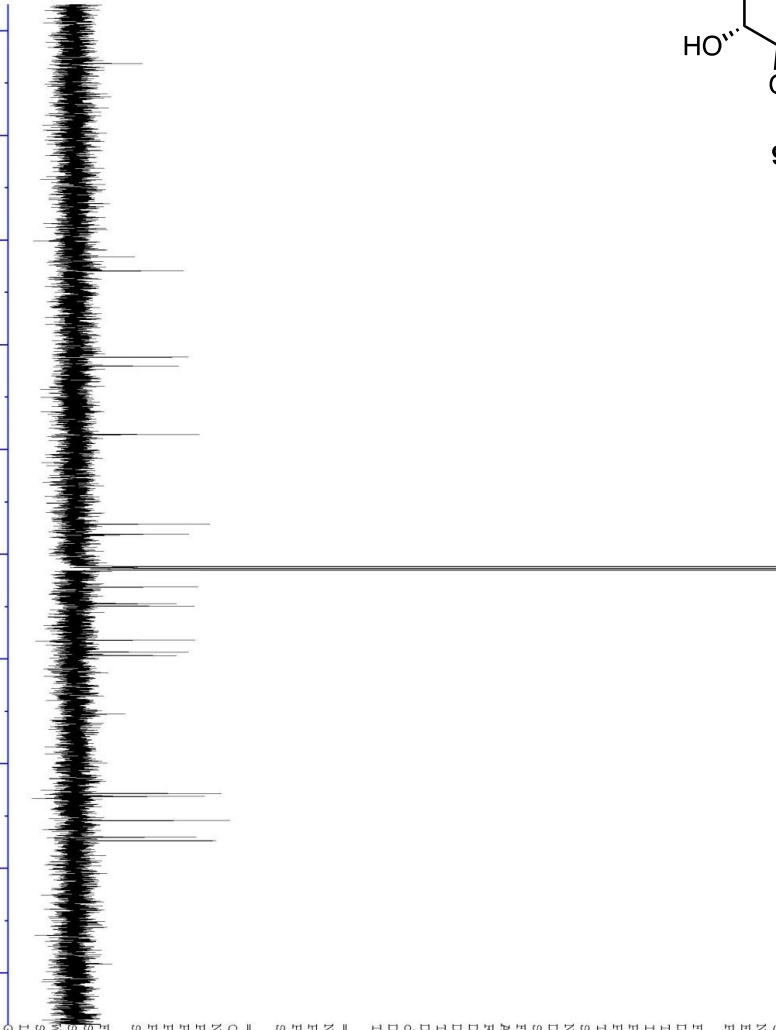
F2 - Acquisition Parameters
 Date_ 20110517
 Time 15.22
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 137
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664256 sec
 RG 32768
 DW 20.850 usec
 DE 6.00 usec
 TE 300.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

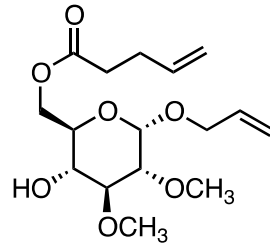
===== CHANNEL F1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0 dB
 SFO1 100.6263500 MHz

===== CHANNEL F2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 110.00 usec
 PL2 -2.00 dB
 PL12 19.00 dB
 PL13 19.00 dB
 SFO2 400.1456010 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6162876 MHz
 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

180 160 140 120 100 80 60 40 20 ppm





10a



Current Data Parameters
 NAME rtd-111-90-p2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130125
 Time 10.45

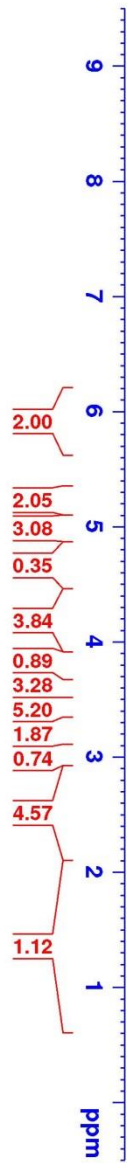
INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 48076
 SOLVENT CDCl₃
 NS 32
 DS 2

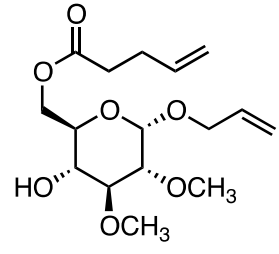
SWH 8012.820 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999423 sec
 RG 22.6

DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 DI 2.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 15.22 usec
 P1M1 12.00000000 W
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 131072
 SF 400.1440177 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00





10a

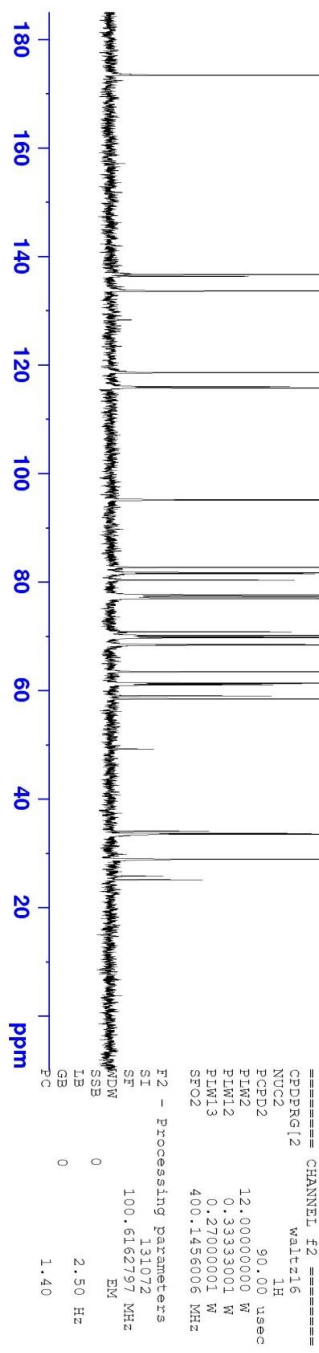


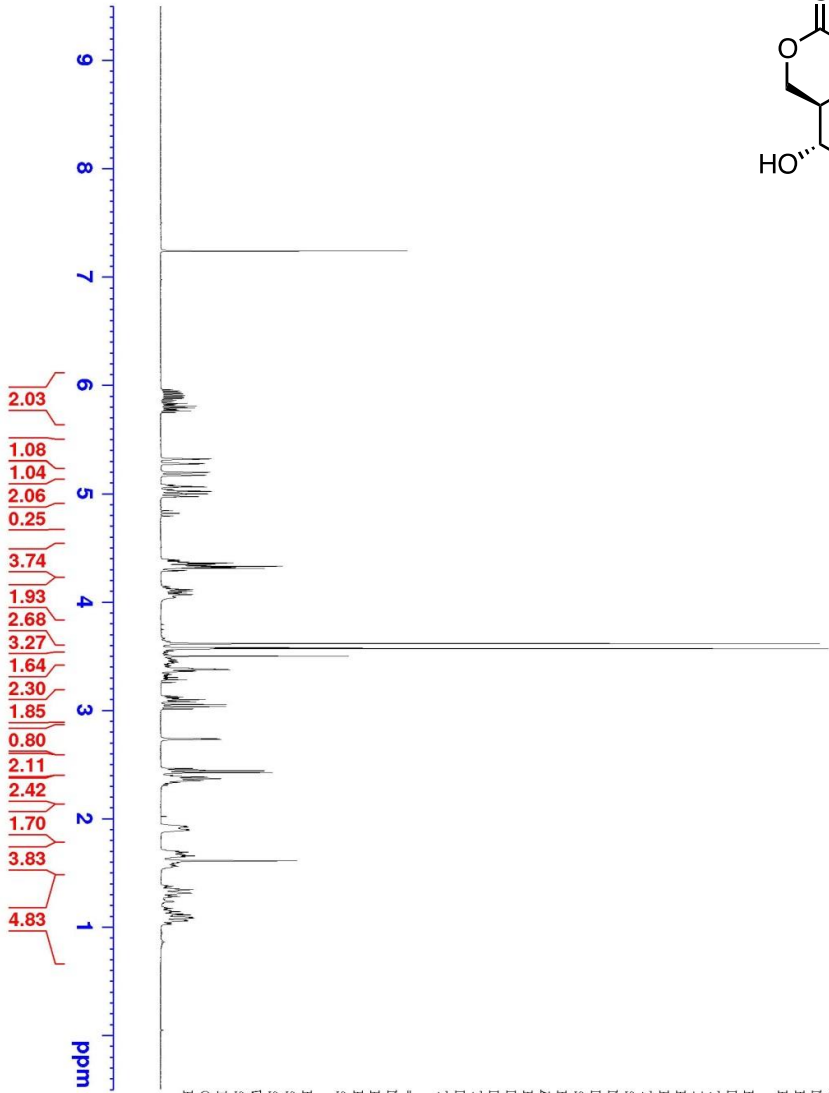
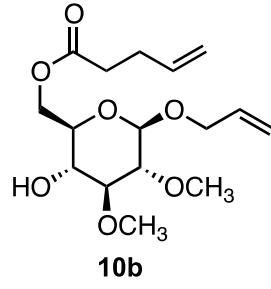
Current Data Parameters
 NAME rtd-111-90-p2
 EXNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130125
 Time_ 10.50
 INSTRUM spect
 PROBD 5 mm BBO-5B/1
 PULPROG zgpg30
 ID zgpg30
 SOLVENT CDCl₃
 NS 238
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.550104 Hz
 AQ 0.9089184 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PLW1 50.00000000 W
 SFO1 100.6263500 MHz

===== CHANNEL f2 =====
 CPDPRG12 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PFM2 12.00000000 W
 FMI2 33333001 W
 FMI3 27000001 W
 SFO2 400.1436006 MHz





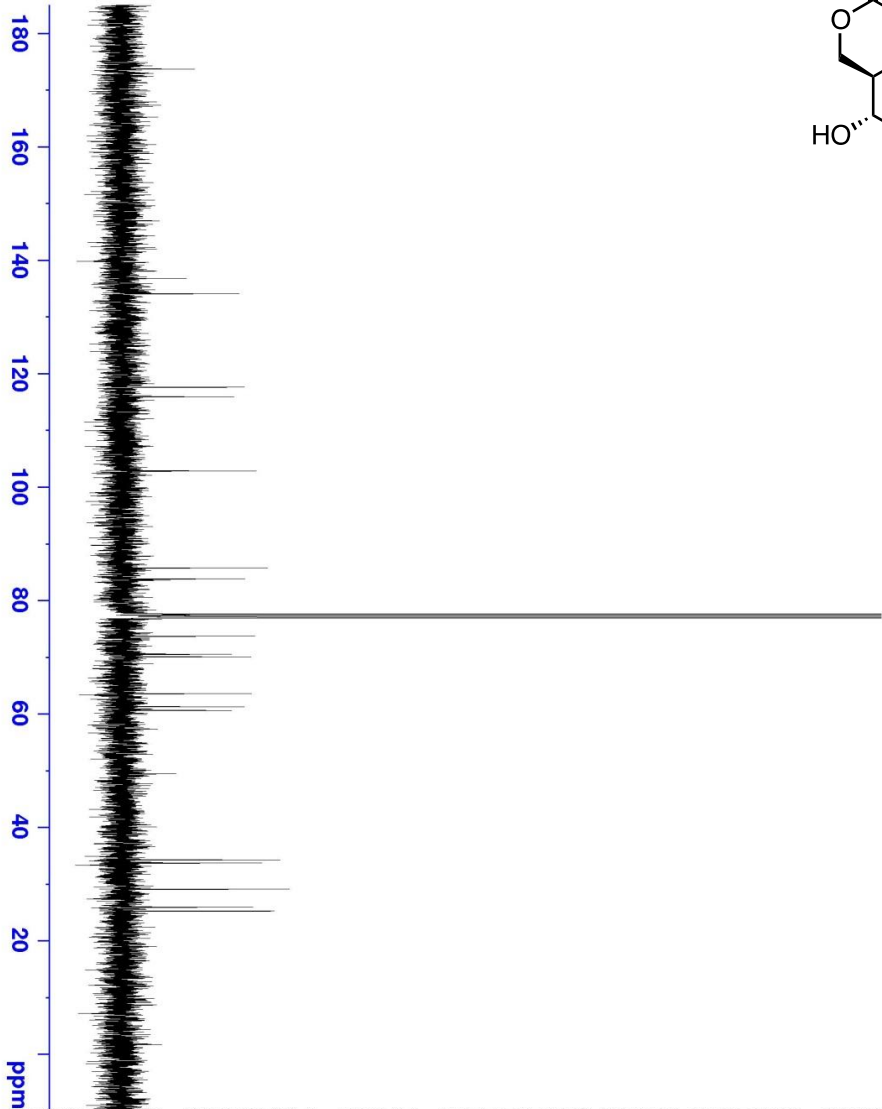
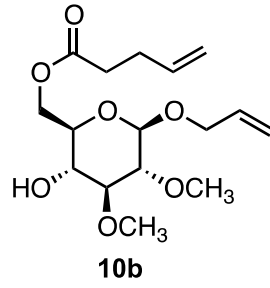
Current Data Parameters
 NAME rtd-11-203-p2-400
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110517
 Time 15.17
 INSTRUM spect
 PROBD 5 mm QNP
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2

SWH 5392.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9294591 sec
 RG 322.5
 DW 89.400 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.50000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.20 usec
 PL1 -2.00 dB
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1440168 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME rtd-11-203-p2-400
 EXPNO 2
 PROCNO 1

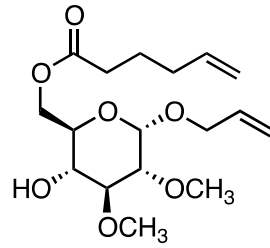
F2 - Acquisition Parameters
 Date_ 20110517
 Time 15:22
 INSTRUM spect
 PROBD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 ID CDD13
 SOLVENT CDCl3
 NS 137
 DS 4

SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3864256 sec
 RG 32768
 DM 20.850 usec
 DE 6.00 usec
 TE 300.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 ID0 1

===== CHANNEL f1 =====
 NUCL 13C
 P1 10.00 usec
 PL1 0 dB
 SFO1 100.6263500 MHz

===== CHANNEL f2 =====
 CPDPRG12 waltz16
 NUCL2 1H
 PULPROG2 110.00 usec
 PL2 -2.00 dB
 PL12 19.00 dB
 PL13 19.00 dB
 SFO2 400.1456010 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6162676 MHz
 MDW EM
 SSB 0
 GB 0
 PC 1.40



10c



Current Data Parameters
 NAME rtd-11-207-p2
 EXPNO 1
 PROCNO 1

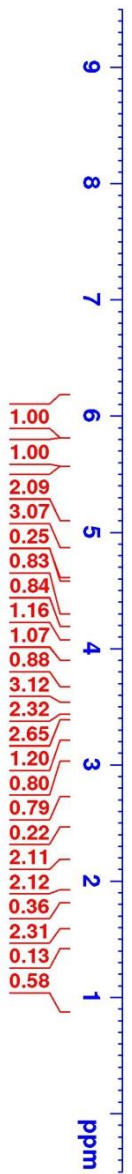
F2 - Acquisition Parameters
 Date_ 20110603
 Time 16.04

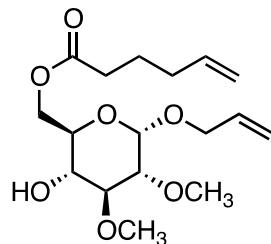
INSIRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9294591 sec

RG 57
 DW 89.400 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.50000000 sec
 ID0 1

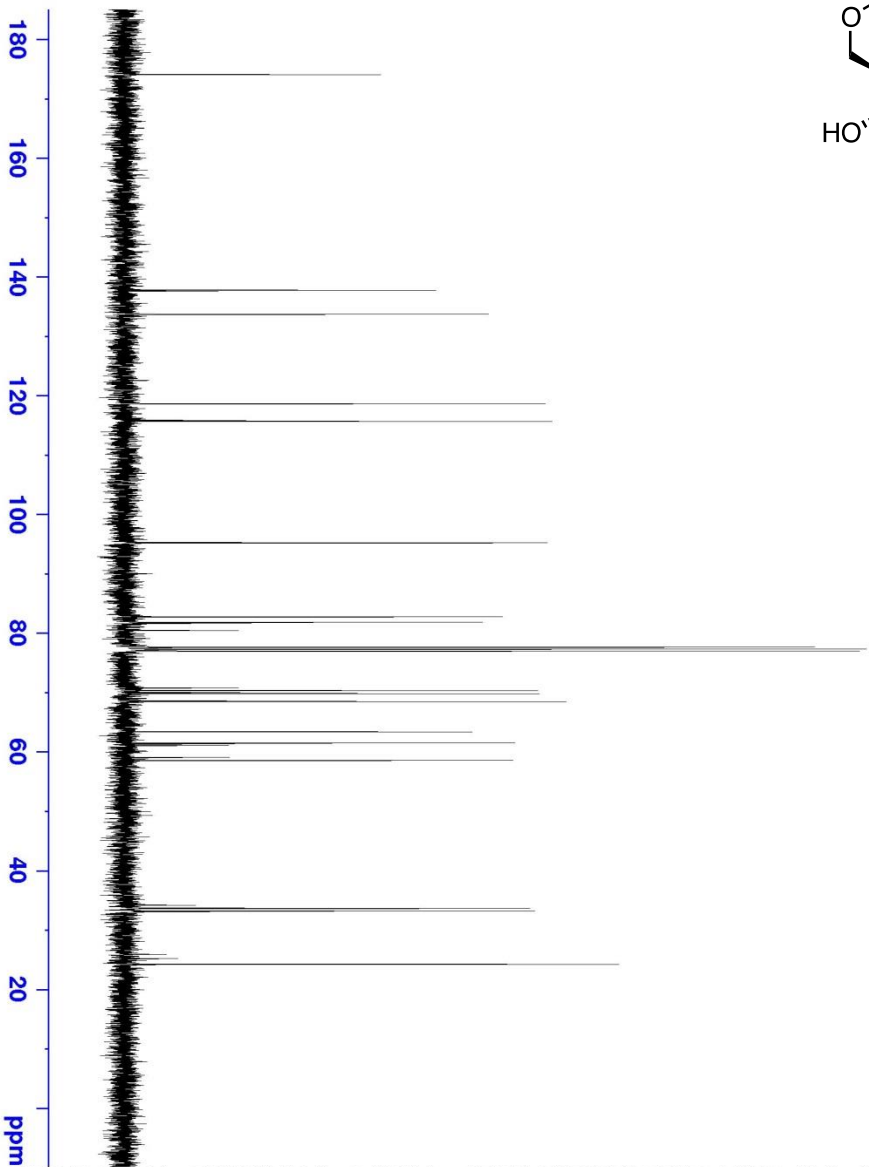
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.20 usec
 PL1 -2.00 dB
 SFO1 400.1464009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1440169 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





10c



Current Data Parameters
 NAME rtd-f1-207-p2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20110603
 Time 16:09
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3864256 sec
 RG 32768
 DW 20.850 usec
 DE 6.00 usec
 IE 300.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0 dB
 SFO1 100.6263500 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P1 110.00 usec
 PCPD2 110.00 usec
 PL2 -2.00 dB
 PL12 19.00 dB
 PL13 19.00 dB
 SFO2 400.1456010 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6162730 MHz
 WDW EM
 SSB 0
 GB 0

PC 1.40



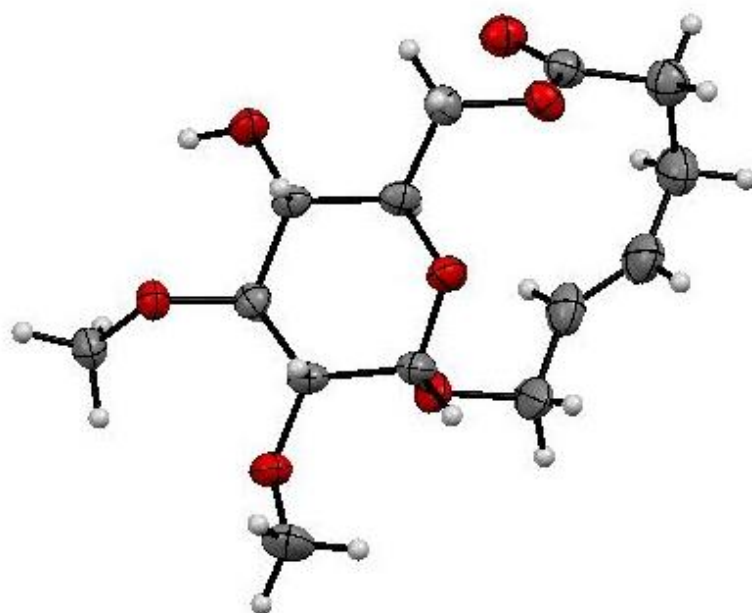


Figure S1. ORTEP of compound 5.

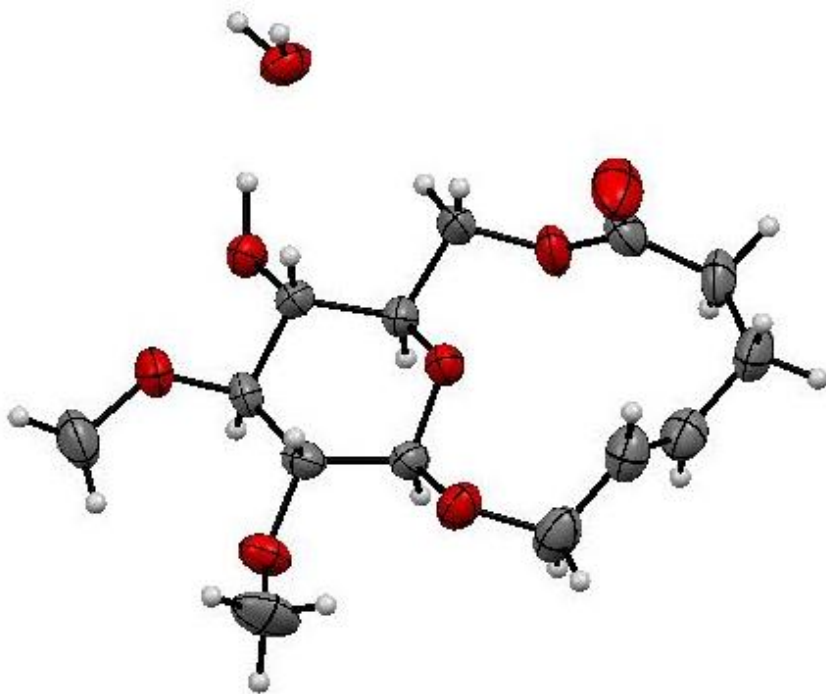


Figure S2. ORTEP of compound **6**.