

Supporting Information

Synthesis and enzymatic evaluation of ketose phosphonates: the interplay between mutarotation, monofluorination and acidity

Stephanie M. Forget,^{§†} Debabrata Bhattasali,^{##‡} V. Catherine Hart,[#] T. Stanley Cameron,[§] Ray T. Syvitski[§] and David L. Jakeman^{#,§*}

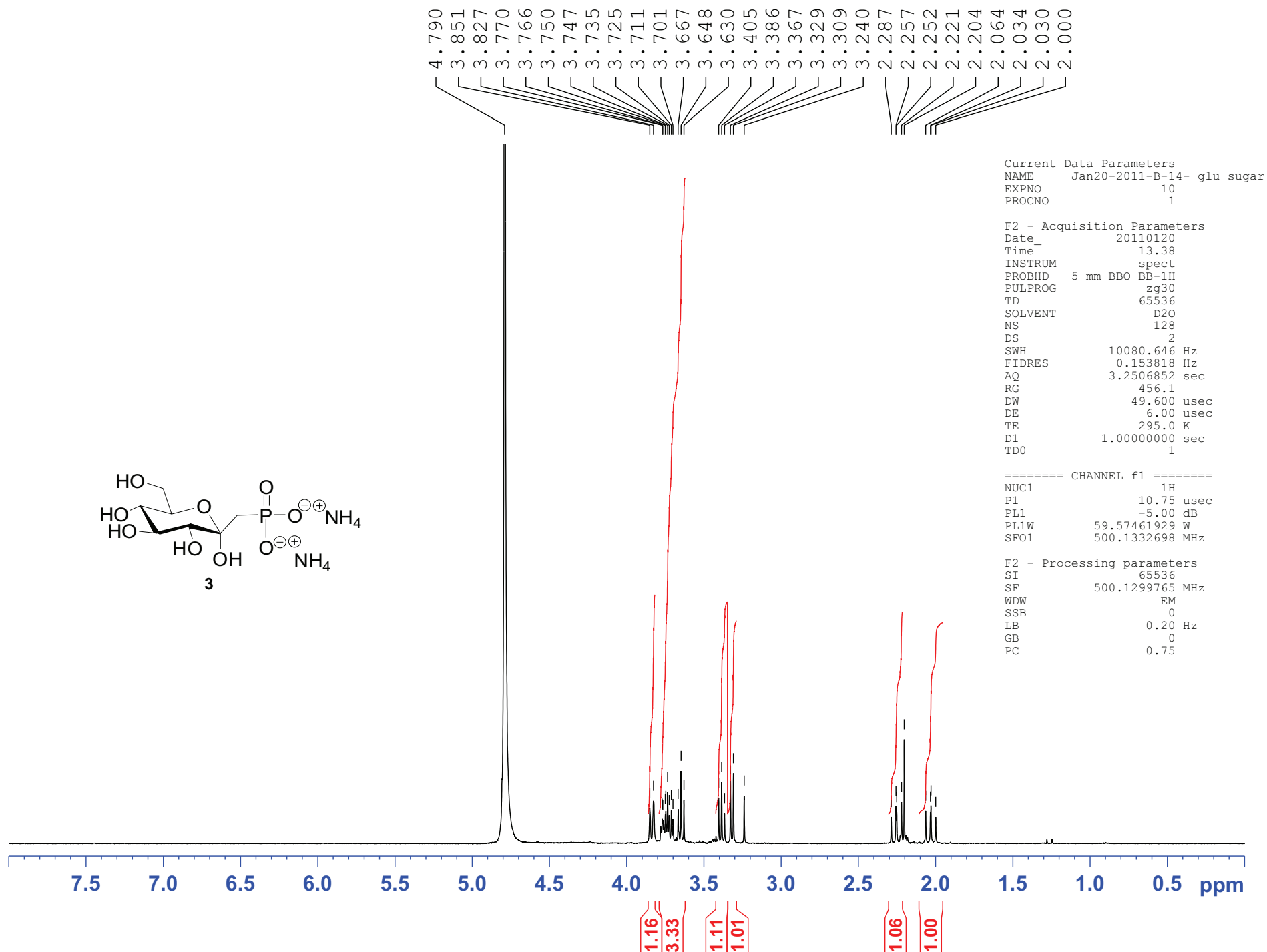
[#]College of Pharmacy, Dalhousie University, 5968 College St., PO Box 15,000, Halifax, Nova Scotia, B3H 4R2, Canada.

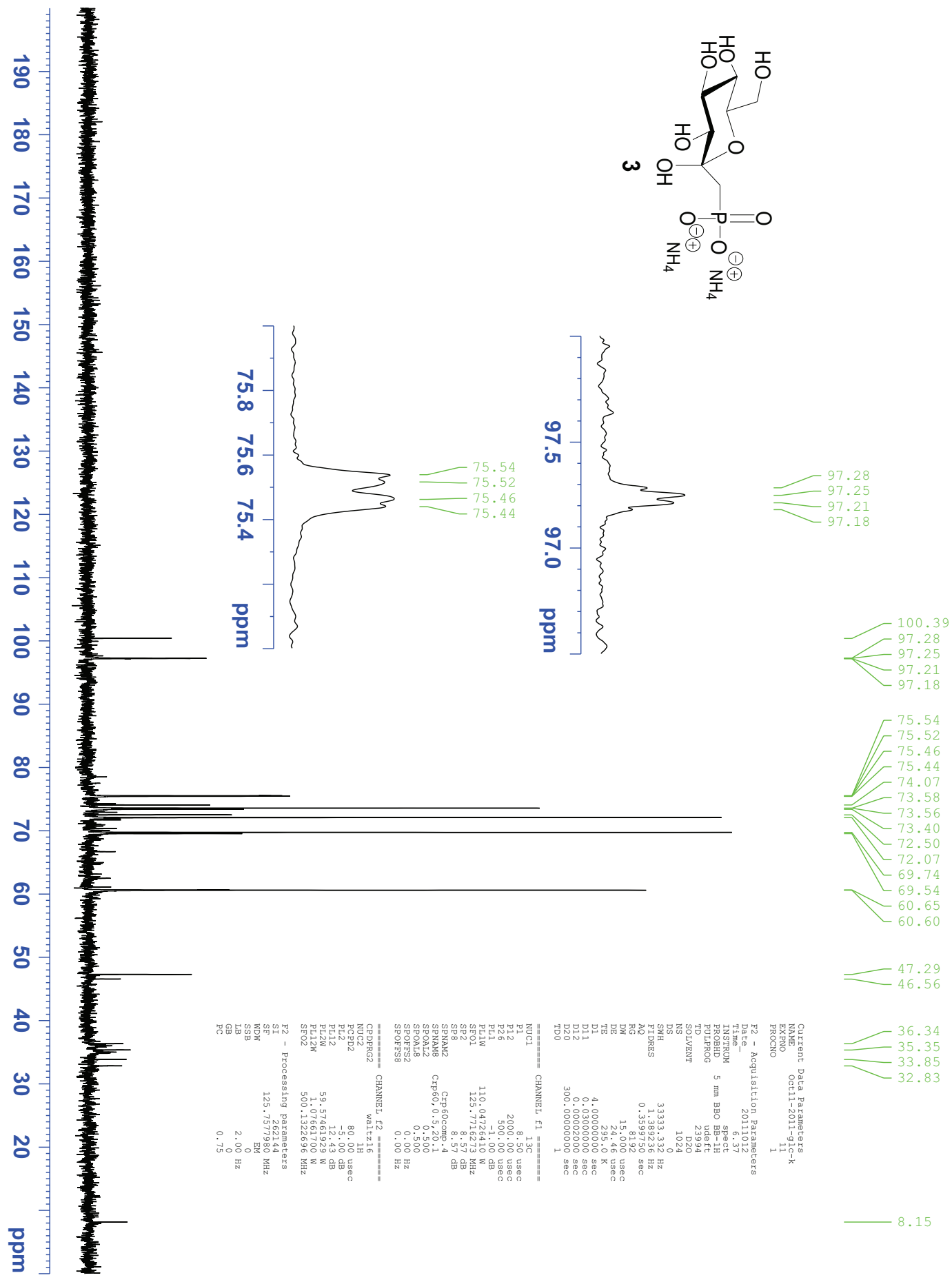
[§]Department of Chemistry, Dalhousie University, 6274 Coberg Rd., PO Box 15,000, Halifax, Nova Scotia, B3H 4R2, Canada.

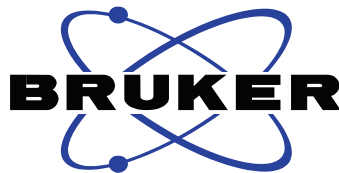
Supporting Information- Table of contents

¹ H, ¹³ C, ³¹ P{ ¹ H} and HSQC NMR spectra of compound 3	S3-S7
¹ H, ¹³ C, ³¹ P{ ¹ H}, ¹⁹ F{ ¹ H} and ¹⁹ F NMR spectra of compound 4	S8-S12
¹ H, ¹³ C, ³¹ P{ ¹ H}, ¹⁹ F{ ¹ H} and ¹⁹ F NMR spectra of compound 5	S13-S17
¹ H, ¹³ C, ³¹ P{ ¹ H}, and ¹⁹ F{ ¹ H} NMR spectra of compound 6	S18-S21
¹⁹ F{ ¹ H} NMR spectrum of compound 6 (free acid)	S22
¹ H, ¹³ C, and ³¹ P{ ¹ H} NMR spectra of compound 7	S23-S25
¹ H, ¹³ C, and ³¹ P{ ¹ H} NMR spectra of compound 8	S26-S28
¹ H, ¹³ C, and ³¹ P{ ¹ H} NMR spectra of compound 9	S29-S31
¹ H, ¹³ C, and ³¹ P{ ¹ H} NMR spectra of compound 12	S32-S34
¹ H, ¹³ C, and ³¹ P{ ¹ H} NMR spectra of compound 13	S35-S37
¹ H, ¹³ C, ³¹ P{ ¹ H}, ¹⁹ F{ ¹ H} and ¹⁹ F NMR spectra of compound 14	S38-S42
¹ H, ¹³ C, ³¹ P{ ¹ H}, ¹⁹ F{ ¹ H} and ¹⁹ F NMR spectra of compound 15	S43-S47
¹ H, ¹³ C, ³¹ P{ ¹ H}, ¹⁹ F{ ¹ H} and ¹⁹ F NMR spectra of compound 16	S48-S52
¹ H, ¹³ C, and ³¹ P{ ¹ H} NMR spectra of compound 17	S53-S55
¹ H, ¹³ C, ³¹ P{ ¹ H}, ¹⁹ F{ ¹ H} and ¹⁹ F NMR spectra of compound 18	S56-S60
¹ H, ¹³ C, and ³¹ P{ ¹ H} NMR spectra of compound 21	S61-S63

¹ H, and ³¹ P{ ¹ H} NMR spectra of compound 26	S64-S65
¹ H, and ³¹ P{ ¹ H} NMR spectra of compound 27	S66-S67
¹ H, ³¹ P{ ¹ H}, and ¹⁹ F{ ¹ H} NMR spectra of compound 28	S68-S70
Water LOGSY NMR spectrum of compound 1	S71
Water LOGSY NMR spectrum of compound 2	S72
Water LOGSY NMR spectrum of compound 3	S73
Water LOGSY NMR spectrum of compound 4	S74
Water LOGSY NMR spectrum of compound 5	S75
Water LOGSY NMR spectrum of compound 8	S76
Water LOGSY NMR spectrum of compound 9	S77
Water LOGSY NMR spectrum of compound 25	S78
Water LOGSY NMR spectrum of compound 26	S79
Water LOGSY NMR spectrum of compound 34	S80
Water LOGSY NMR spectrum of compound 6	S81
Table of HPLC retention times for Cps2L catalyzed reactions.....	S82







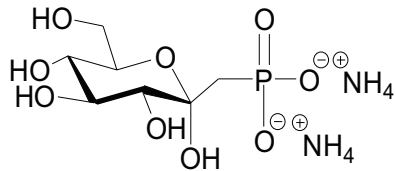
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PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 256
DS 4
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

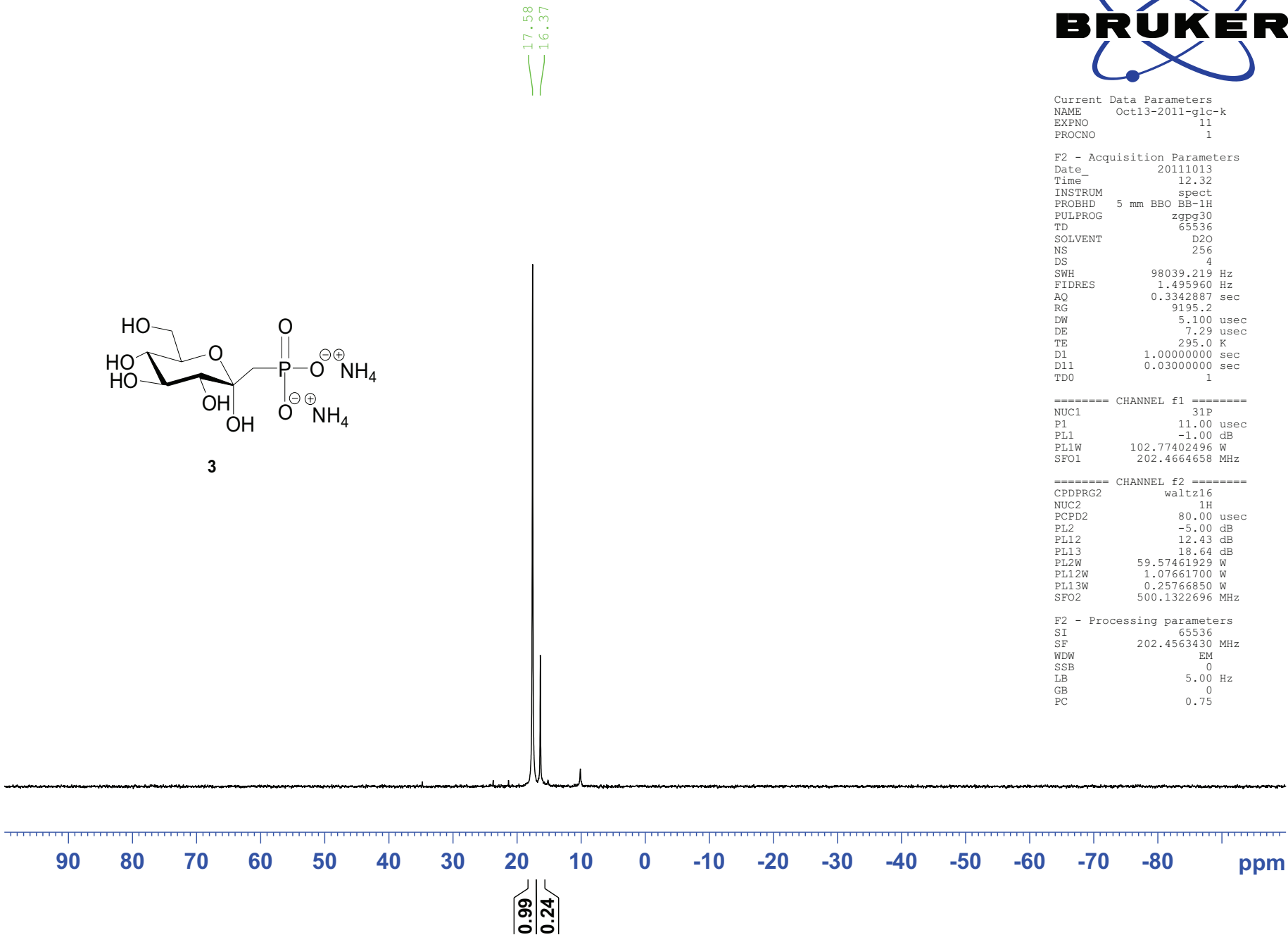
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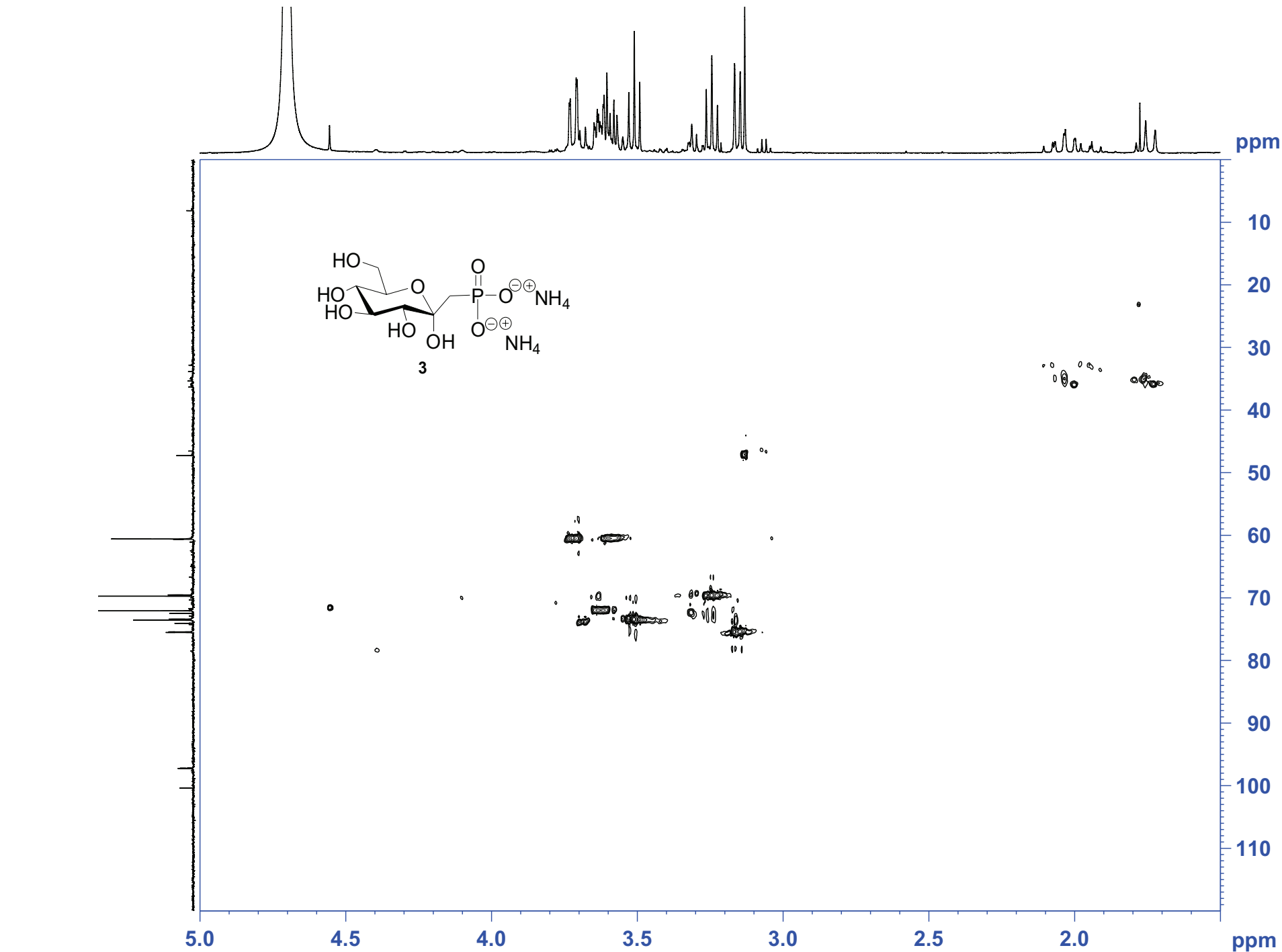
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PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
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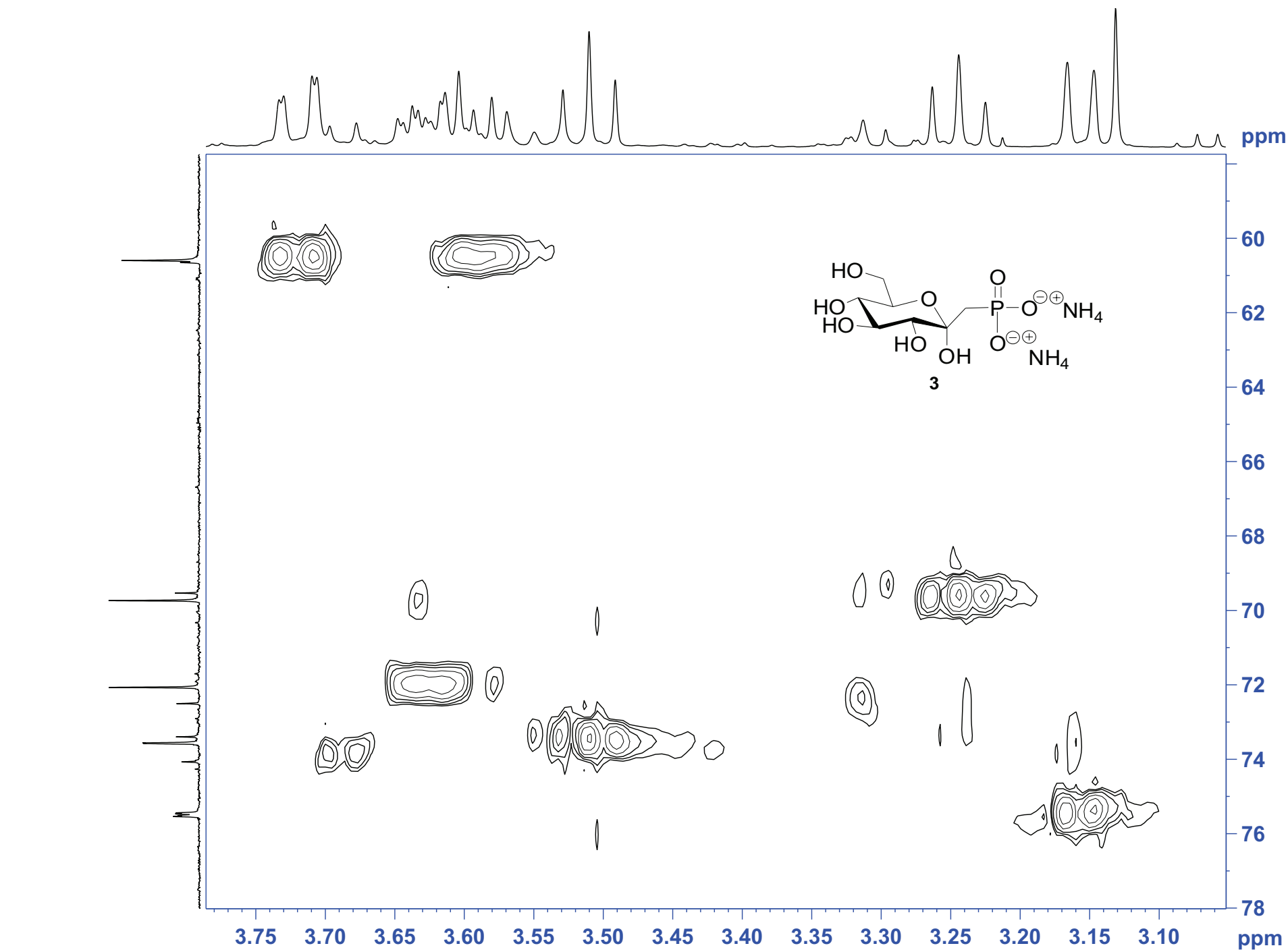
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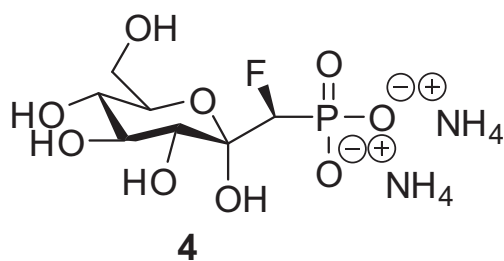


3









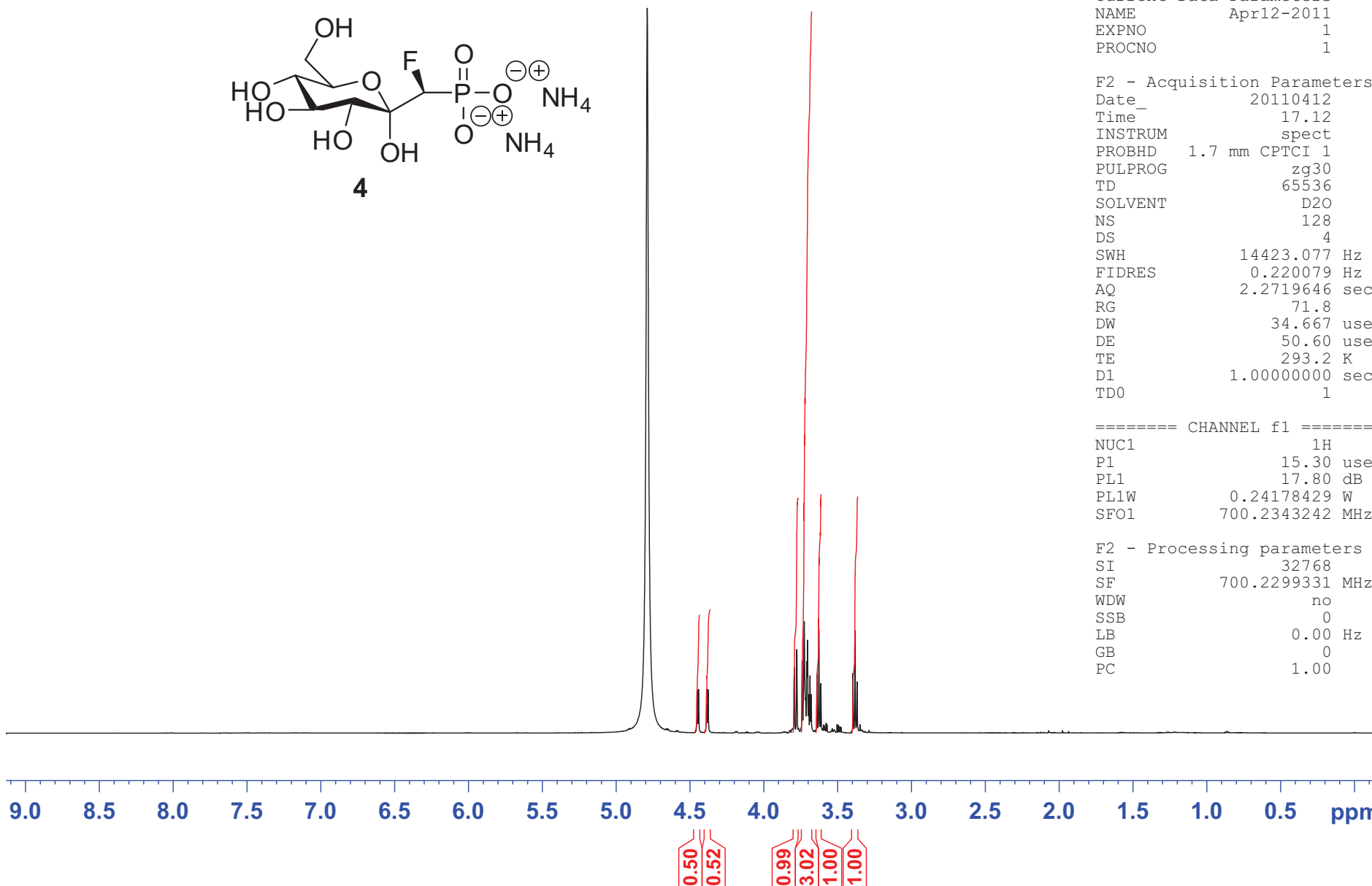
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3.72
3.70
3.68
3.63
3.38

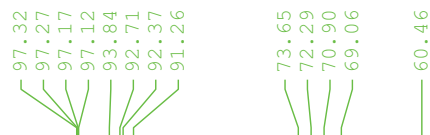
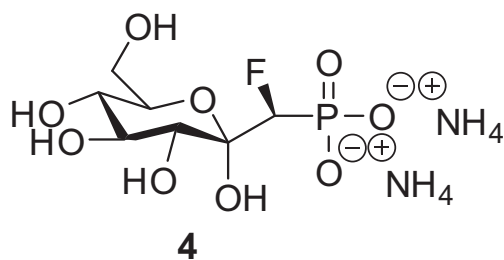
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PULPROG zg30
TD 65536
SOLVENT D2O
NS 128
DS 4
SWH 14423.077 Hz
FIDRES 0.220079 Hz
AQ 2.2719646 sec
RG 71.8
DW 34.667 usec
DE 50.60 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.30 usec
PL1 17.80 dB
PL1W 0.24178429 W
SFO1 700.2343242 MHz

F2 - Processing parameters
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PC 1.00





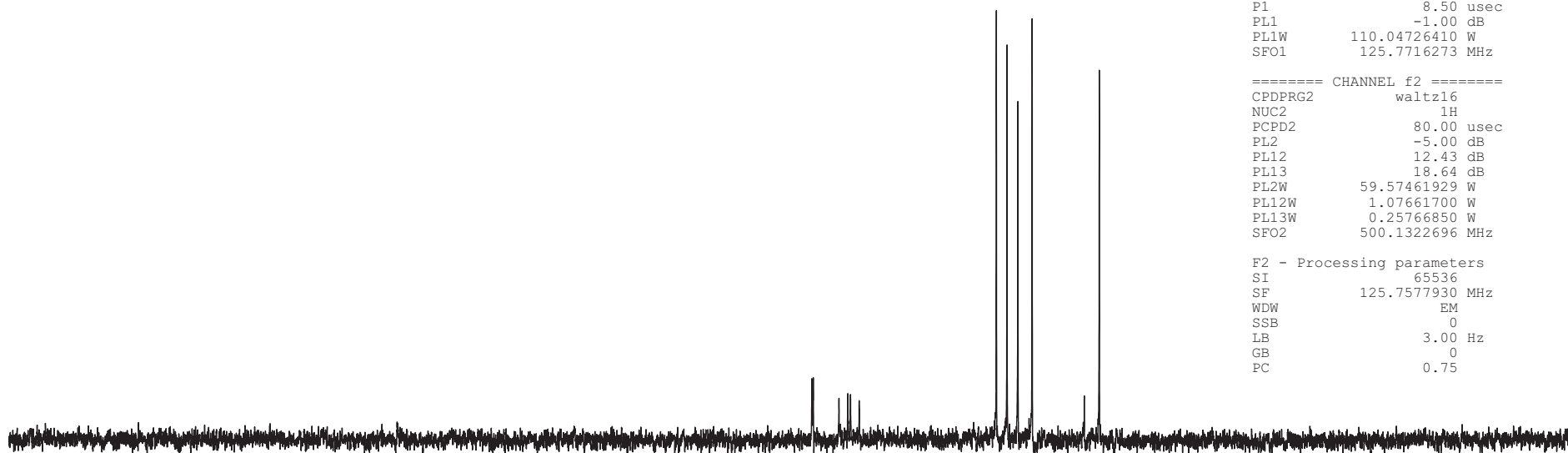
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 PULPROG zgpg30
 TD 54048
 SOLVENT D2O
 NS 2048
 DS 4
 SWH 33333.332 Hz
 FIDRES 0.616736 Hz
 AQ 0.8107850 sec
 RG 9195.2
 DW 15.000 usec
 DE 21.14 usec
 TE 295.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -1.00 dB
 PL1W 110.04726410 W
 SFO1 125.7716273 MHz

===== CHANNEL f2 =====
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 NUC2 1H
 PCPD2 80.00 usec
 PL2 -5.00 dB
 PL12 12.43 dB
 PL13 18.64 dB
 PL2W 59.57461929 W
 PL12W 1.07661700 W
 PL13W 0.25766850 W
 SFO2 500.1322696 MHz

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 GB 0
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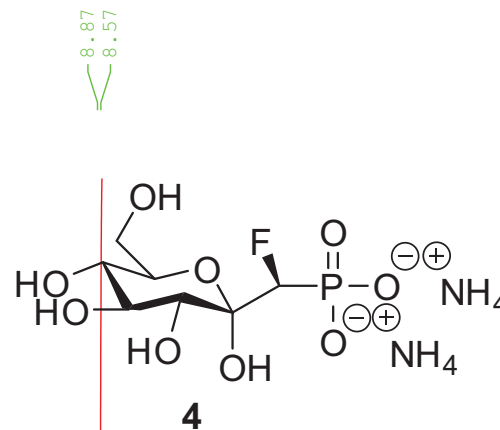
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PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 512
DS 4
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 2

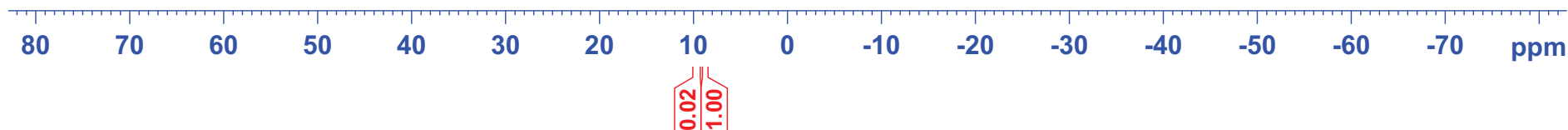
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PL1 -1.00 dB
PL1W 102.77402496 W
SFO1 202.4664658 MHz

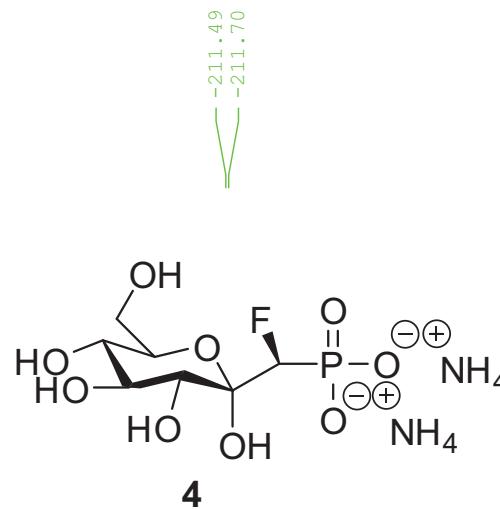
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NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
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GB 0
PC 0.75



8.87
8.57





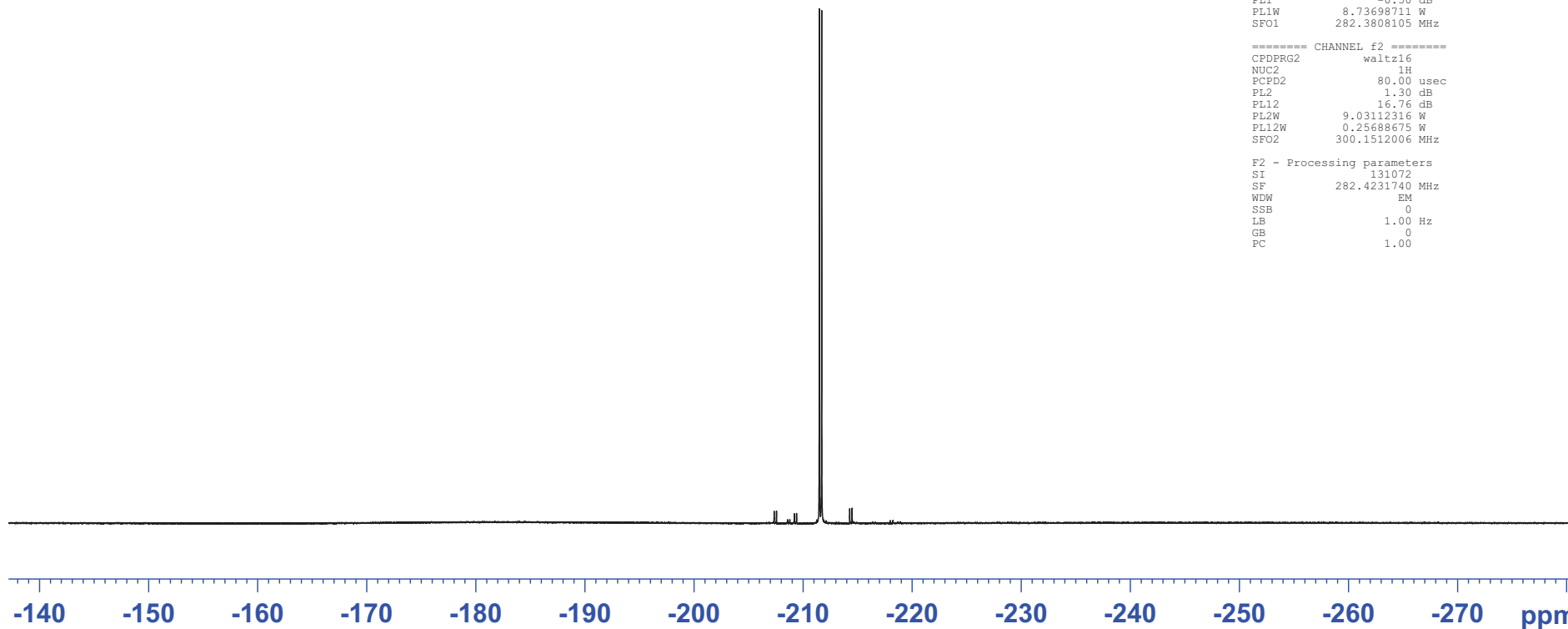
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EXPNO 3
PROCNO 1

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PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT D2O
NS 32
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716788 sec
RG 4100
DW 6.650 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.00 usec
PL1 -0.50 dB
PL1W 8.73698711 W
SFO1 282.3808105 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.76 dB
PL2W 9.03112316 W
PL12W 0.25688675 W
SFO2 300.1512006 MHz

F2 - Processing parameters
SI 131072
SF 282.4231740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



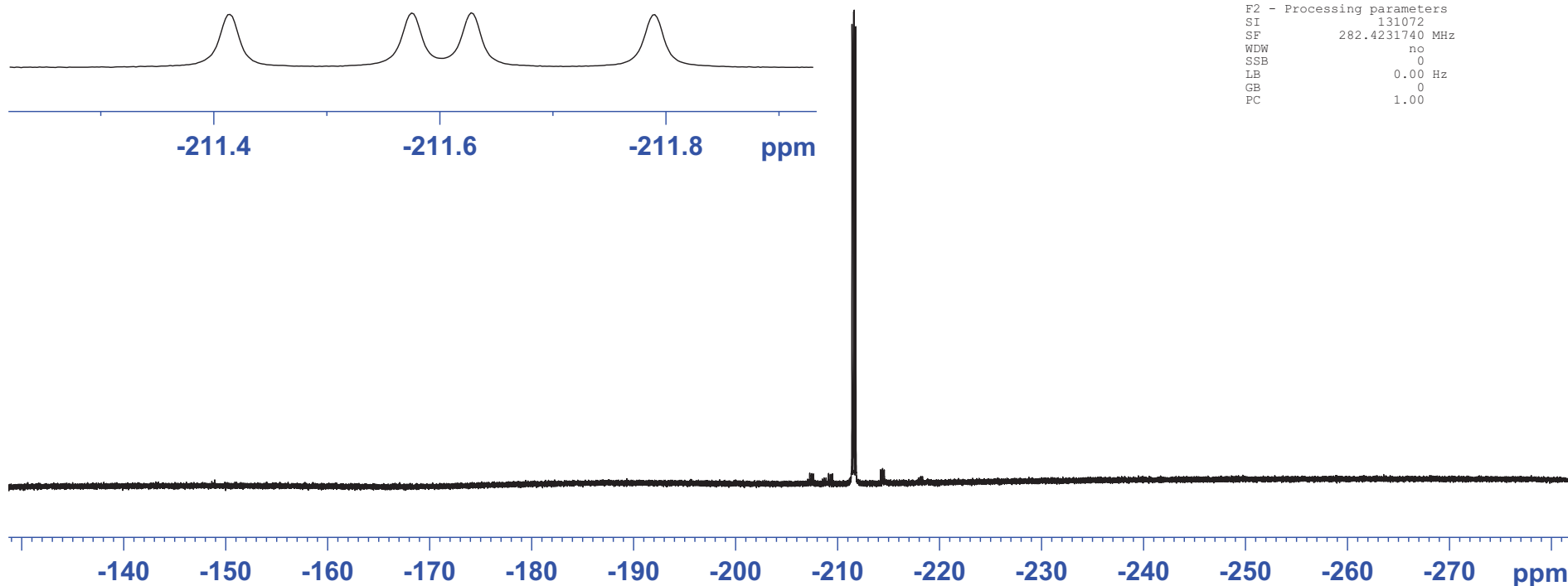
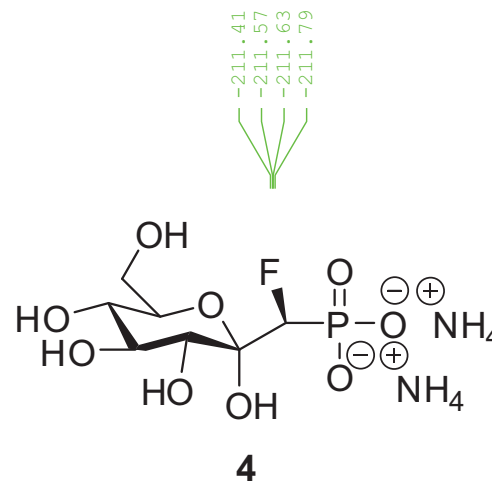


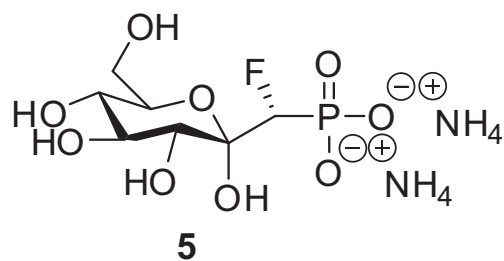
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 EXPNO 4
 PROCNO 1

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 PULPROG zgpg30
 TD 131072
 SOLVENT D2O
 NS 32
 DS 4
 SWH 75187.969 Hz
 FIDRES 0.573639 Hz
 AQ 0.8716788 sec
 RG 1440
 DW 6.650 usec
 DE 6.50 usec
 TE 297.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 14.00 usec
 PL1 -0.50 dB
 PL1W 8.73698711 W
 SFO1 282.3808105 MHz

F2 - Processing parameters
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 SF 282.4231740 MHz
 WDW no
 SSB 0
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 GB 0
 PC 1.00





Chemical shift values (ppm) for the peaks in the spectrum:

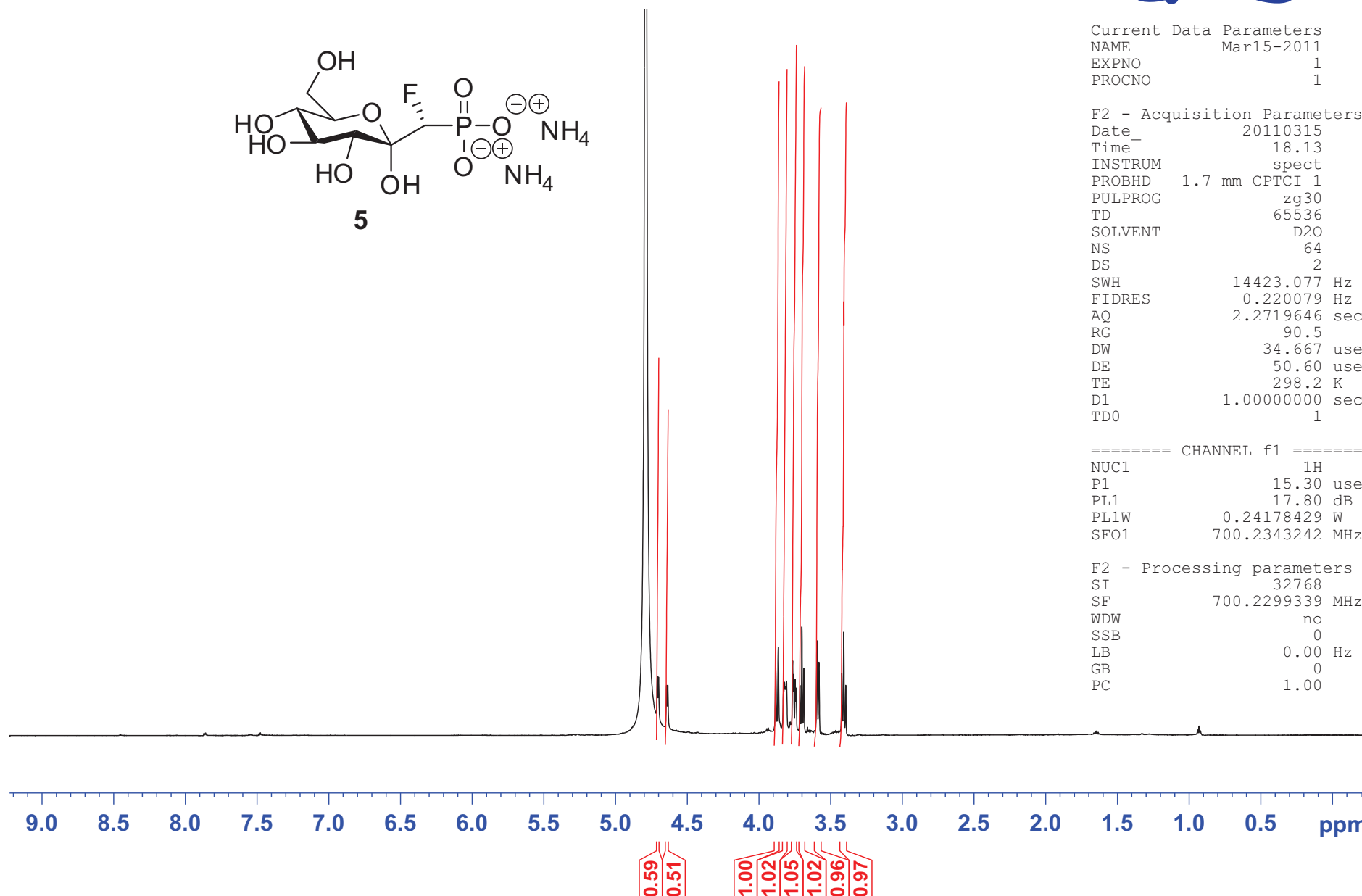
- 4.79, 4.71, 4.70, 4.64, 4.64, 3.88, 3.87, 3.83, 3.81, 3.77, 3.76, 3.75, 3.74, 3.70, 3.60, 3.58, 3.41

Current Data Parameters
 NAME Mar15-2011
 EXPNO 1
 PROCNO 1

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 Date_ 20110315
 Time_ 18.13
 INSTRUM spect
 PROBHD 1.7 mm CPTCI 1
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 64
 DS 2
 SWH 14423.077 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719646 sec
 RG 90.5
 DW 34.667 usec
 DE 50.60 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.30 usec
 PL1 17.80 dB
 PL1W 0.24178429 W
 SFO1 700.2343242 MHz

F2 - Processing parameters
 SI 32768
 SF 700.229339 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00





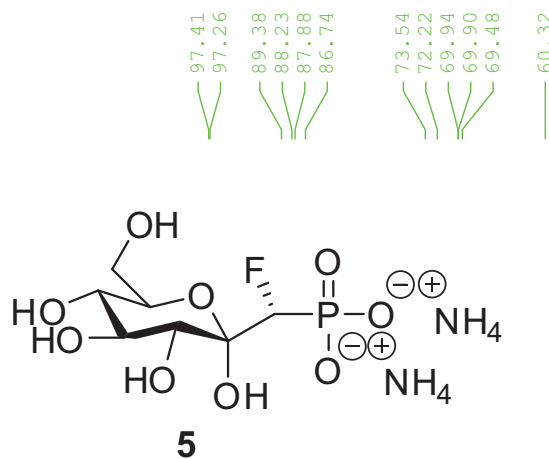
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NAME Feb28-2011-bhattasali
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zgpg30
TD 54048
SOLVENT D2O
NS 1024
DS 4
SWH 33333.332 Hz
FIDRES 0.616736 Hz
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RG 9195.2
DW 15.000 usec
DE 21.14 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

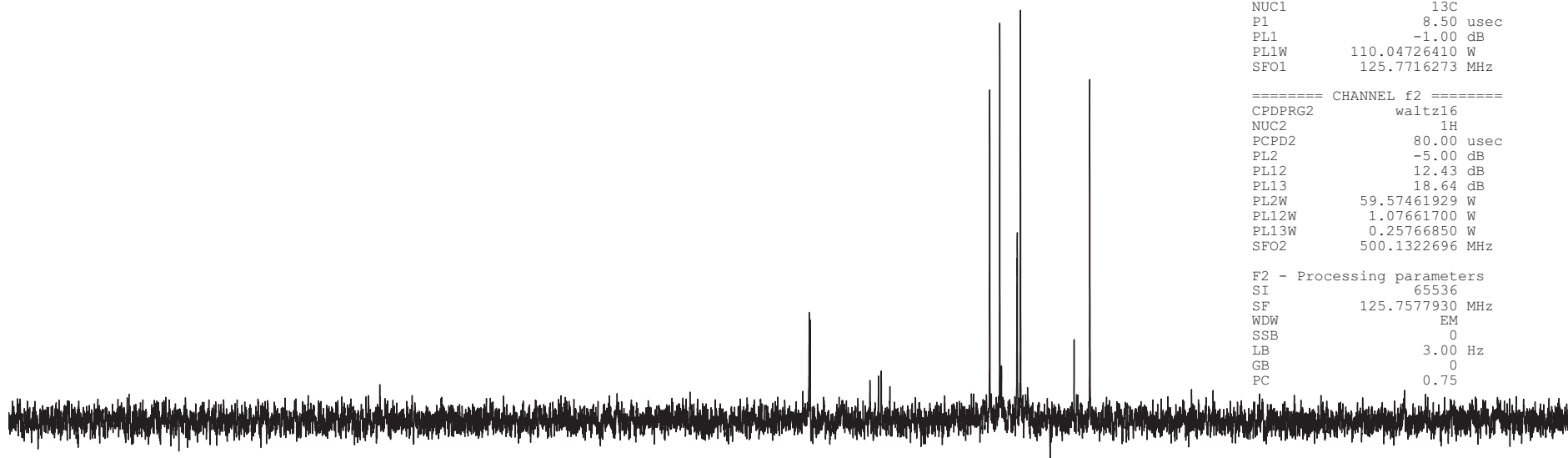
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NUC1 13C
P1 8.50 usec
PL1 -1.00 dB
PL1W 110.04726410 W
SFO1 125.7716273 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 125.7577930 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.75



97.41
97.26
89.38
88.23
87.88
86.74
73.54
72.22
69.94
69.90
69.48
60.32



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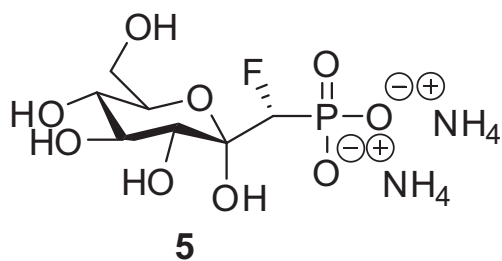
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 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 128
 DS 4
 SWH 98039.219 Hz
 FIDRES 1.495960 Hz
 AQ 0.3342887 sec
 RG 9195.2
 DW 5.100 usec
 DE 7.29 usec
 TE 295.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 31P
 P1 11.00 usec
 PL1 -1.00 dB
 PL1W 102.77402496 W
 SFO1 202.4664658 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -5.00 dB
 PL12 12.43 dB
 PL13 18.64 dB
 PL2W 59.57461929 W
 PL12W 1.07661700 W
 PL13W 0.25766850 W
 SFO2 500.1322696 MHz

F2 - Processing parameters
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 WDW no
 SSB 0
 LB 0.00 Hz
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 PC 0.75



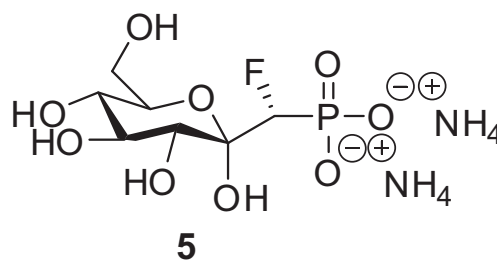
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8.96

0.04
1.00



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-213.03
 -213.27
 -214.27
 -214.48



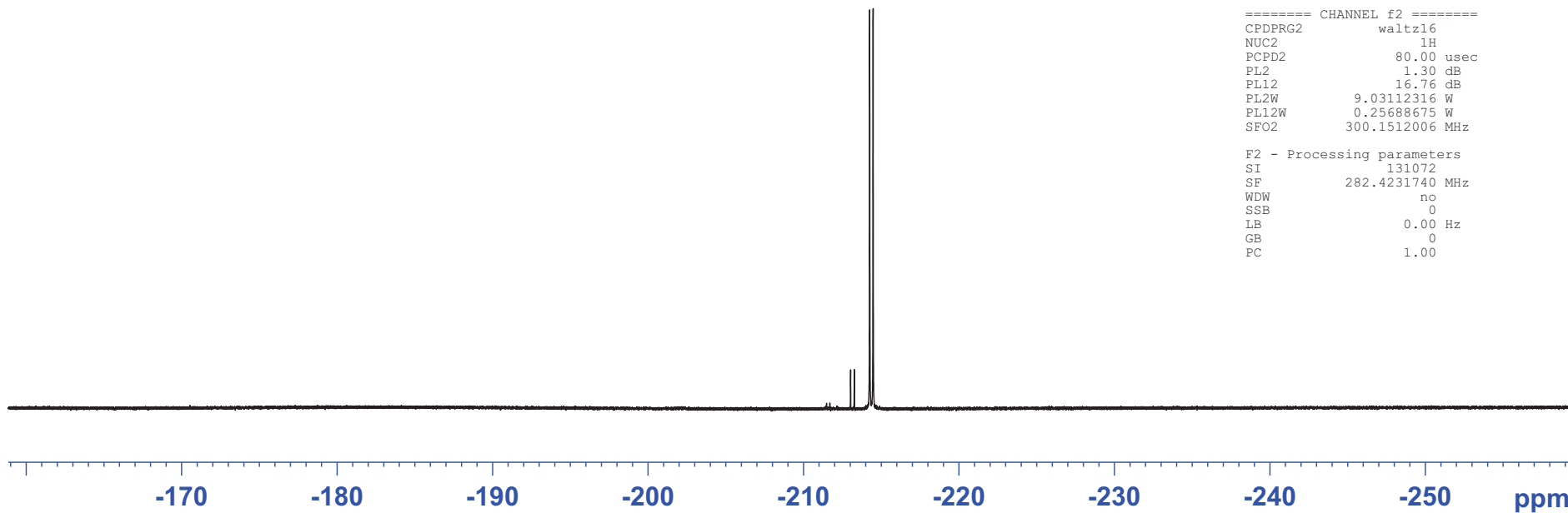
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F2 - Acquisition Parameters
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 PULPROG zgfhigqn
 TD 131072
 SOLVENT D2O
 NS 32
 DS 4
 SWH 75187.969 Hz
 FIDRES 0.573639 Hz
 AQ 0.8716788 sec
 RG 4100
 DW 6.650 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 14.00 usec
 PL1 -0.50 dB
 PL1W 8.73698711 W
 SFO1 282.3808105 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.30 dB
 PL12 16.76 dB
 PL2W 9.03112316 W
 PL12W 0.25688675 W
 SFO2 300.1512006 MHz

F2 - Processing parameters
 SI 131072
 SF 282.4231740 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



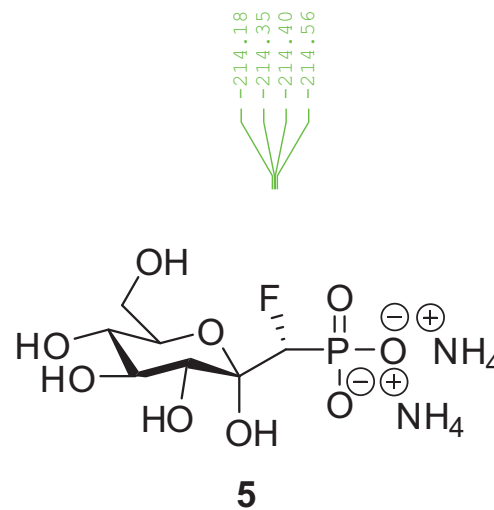


Current Data Parameters
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EXPNO 4
PROCNO 1

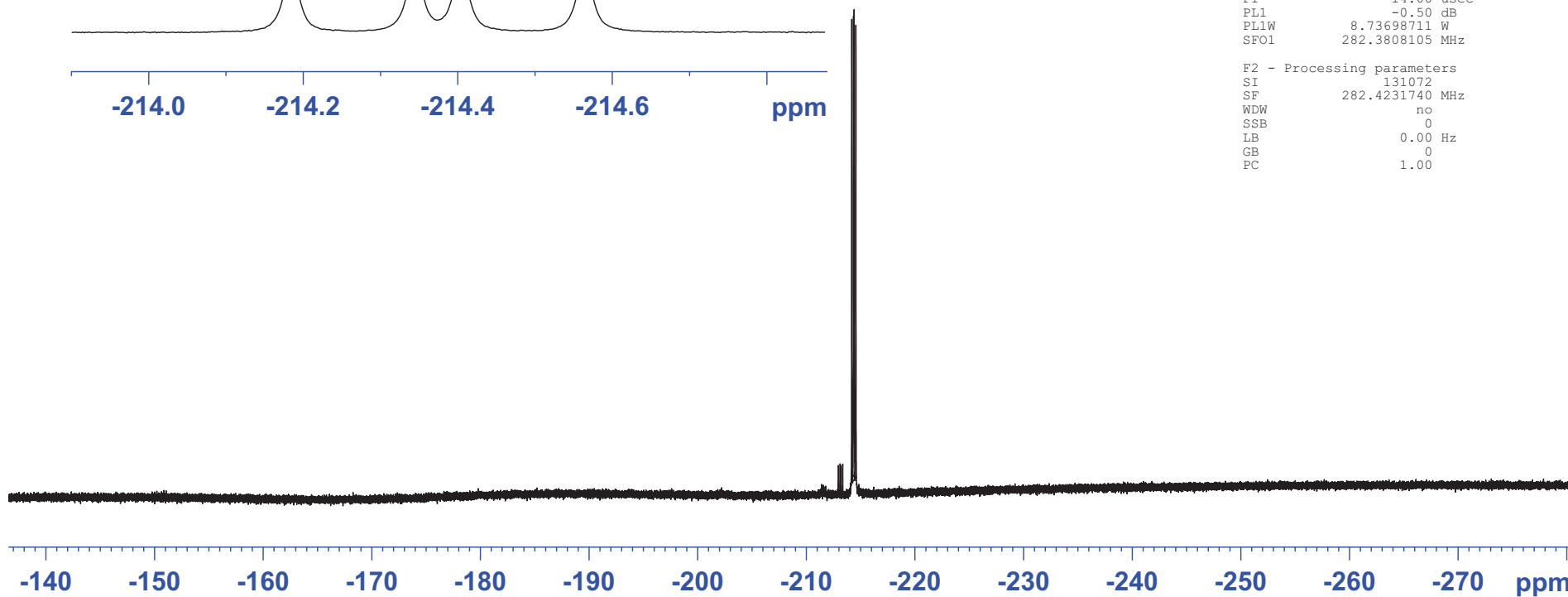
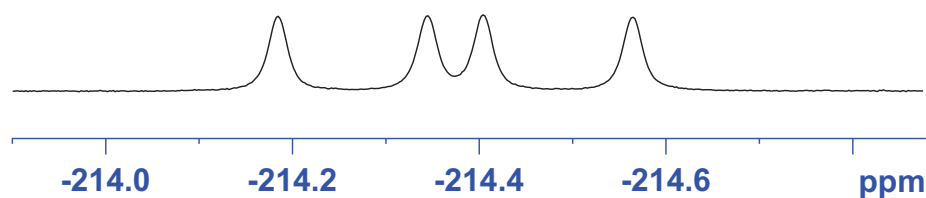
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PULPROG zgflgn
TD 131072
SOLVENT D2O
NS 32
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716788 sec
RG 1440
DW 6.650 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

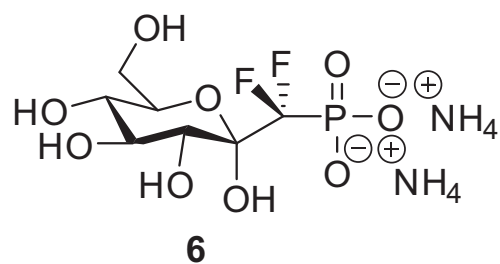
===== CHANNEL f1 =====
NUC1 19F
P1 14.00 usec
PL1 -0.50 dB
PL1W 8.73698711 W
SFO1 282.3808105 MHz

F2 - Processing parameters
SI 131072
SF 282.4231740 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



-214.18
-214.35
-214.40
-214.56





3.84
3.82
3.80
3.78
3.75
3.73
3.64
3.45

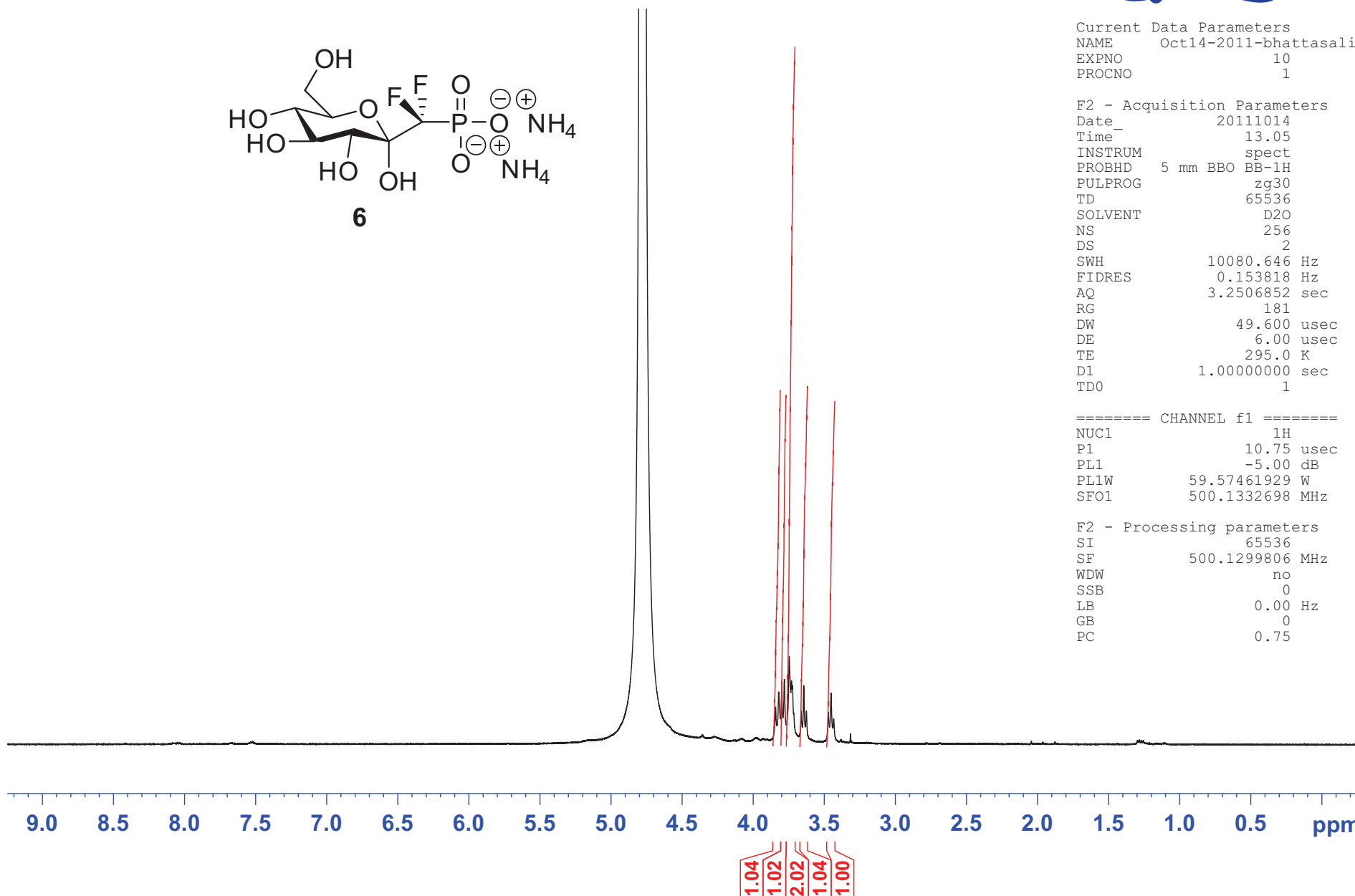


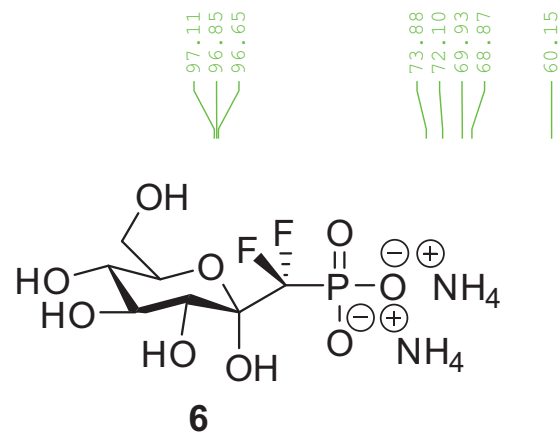
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 EXPNO 10
 PROCNO 1

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 Time 13.05
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 PULPROG zg30
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 SOLVENT D2O
 NS 256
 DS 2
 SWH 10080.646 Hz
 FIDRES 0.153818 Hz
 AQ 3.2506852 sec
 RG 181
 DW 49.600 usec
 DE 6.00 usec
 TE 295.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
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 P1 10.75 usec
 PL1 -5.00 dB
 PL1W 59.57461929 W
 SFO1 500.1332698 MHz

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 SI 65536
 SF 500.1299806 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 0.75





97.11
96.85
96.65
73.88
72.10
69.93
68.87
60.15



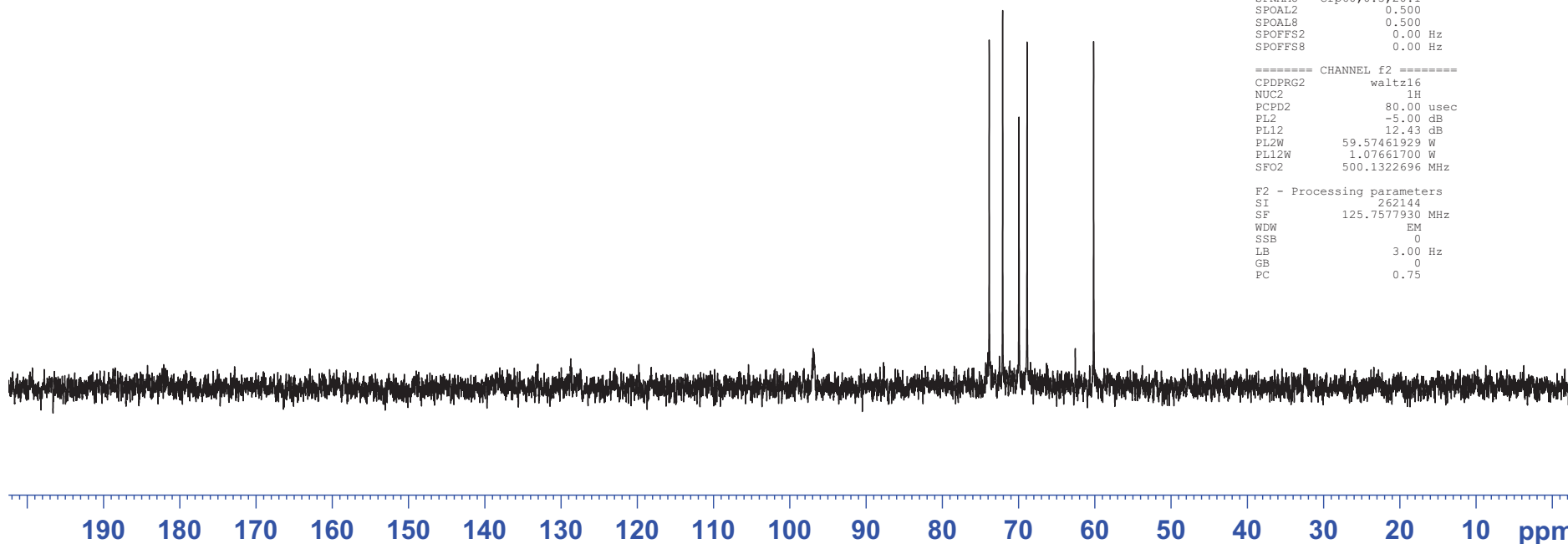
Current Data Parameters
 NAME Sep29-bhattachali
 EXPNO 12
 PROCNO 1

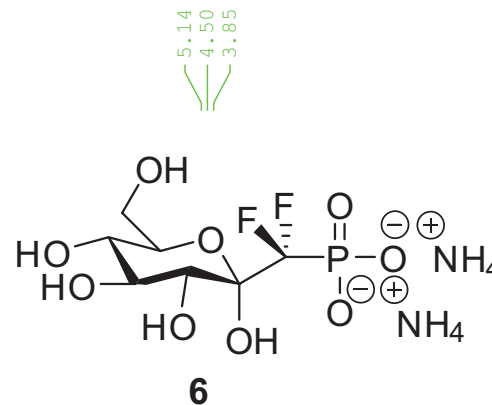
F2 - Acquisition Parameters
 Date_ 20110930
 Time 6.09
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG udeflt
 TD 23994
 SOLVENT D2O
 NS 1000
 DS 0
 SWH 33333.332 Hz
 FIDRES 1.389236 Hz
 AQ 0.3599750 sec
 RG 9195.2
 DW 15.000 usec
 DE 24.46 usec
 TE 295.5 K
 D1 4.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 D20 300.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P12 2000.00 usec
 P26 500.00 usec
 PL1 -1.00 dB
 PL1W 110.04726410 W
 SFO1 125.7716273 MHz
 SP2 8.57 dB
 SP8 8.57 dB
 SPNAM2 Crp60comp.4
 SPNAM8 Crp60,0.5,20.1
 SPOAL2 0.500
 SPOAL8 0.500
 SPOFFS2 0.00 Hz
 SPOFFS8 0.00 Hz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -5.00 dB
 PL12 12.43 dB
 PL2W 59.57461929 W
 PL12W 1.07661700 W
 SFO2 500.1322696 MHz

F2 - Processing parameters
 SI 262144
 SF 125.7577930 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.75





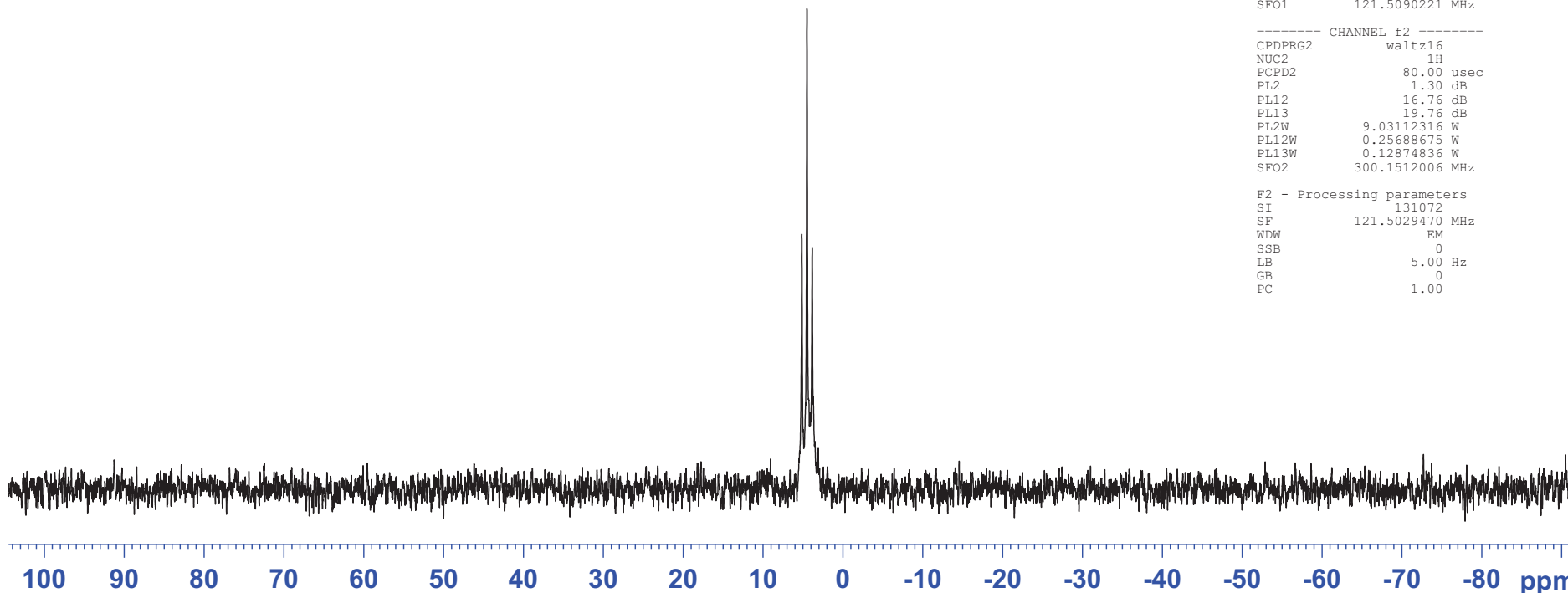
Current Data Parameters
 NAME deb_difluoroOH amine salt
 EXPNO 1
 PROCNO 1

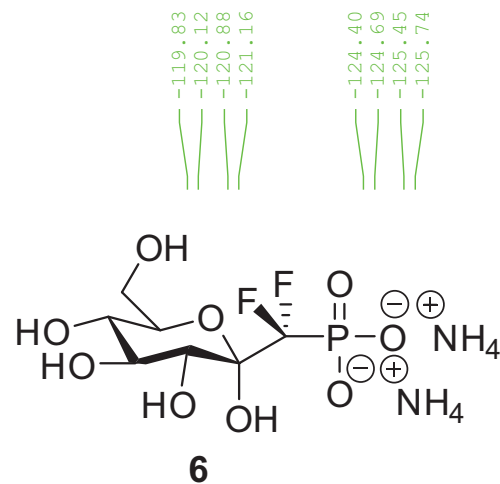
F2 - Acquisition Parameters
 Date_ 20110929
 Time_ 10.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 109284
 SOLVENT D2O
 NS 32
 DS 4
 SWH 54644.809 Hz
 FIDRES 0.500026 Hz
 AQ 0.9999986 sec
 RG 36800
 DW 9.150 usec
 DE 6.50 usec
 TE 301.3 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 31P
 P1 11.00 usec
 PL1 3.10 dB
 PL1W 12.91782284 W
 SFO1 121.5090221 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.30 dB
 PL12 16.76 dB
 PL13 19.76 dB
 PL2W 9.03112316 W
 PL12W 0.25688675 W
 PL13W 0.12874836 W
 SFO2 300.1512006 MHz

F2 - Processing parameters
 SI 131072
 SF 121.5029470 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.00





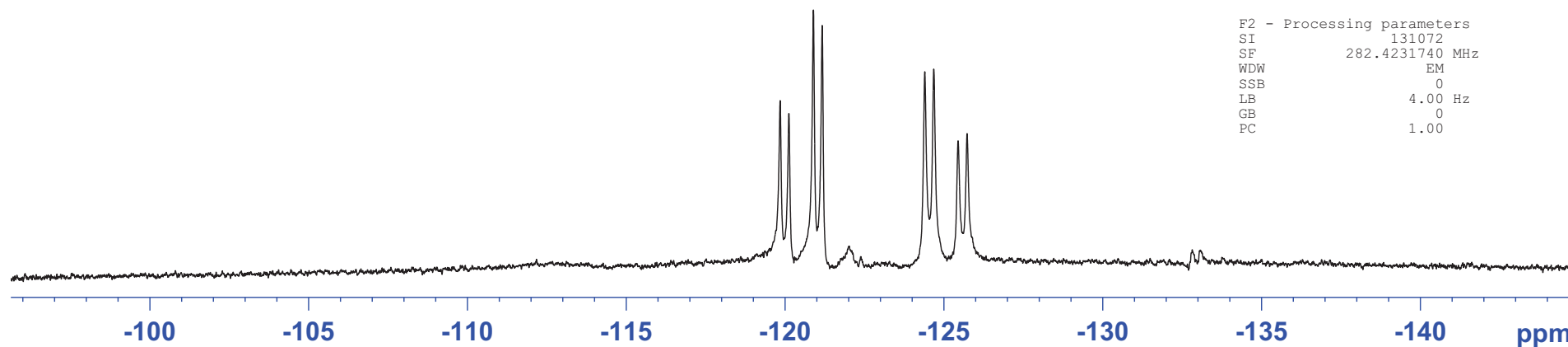
Current Data Parameters
NAME deb_TMSI_amine salt
EXPNO 1
PROCNO 1

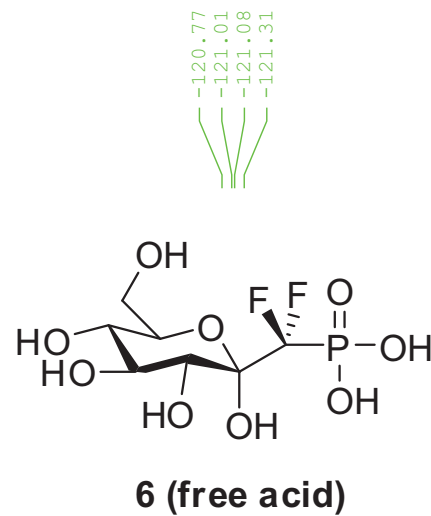
F2 - Acquisition Parameters
Date_ 20111014
Time_ 11.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT D2O
NS 512
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716788 sec
RG 4100
DW 6.650 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.00 usec
PL1 -0.50 dB
PL1W 8.73698711 W
SFO1 282.3808105 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.76 dB
PL2W 9.03112316 W
PL12W 0.25688675 W
SFO2 300.1512006 MHz

F2 - Processing parameters
SI 131072
SF 282.4231740 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 1.00





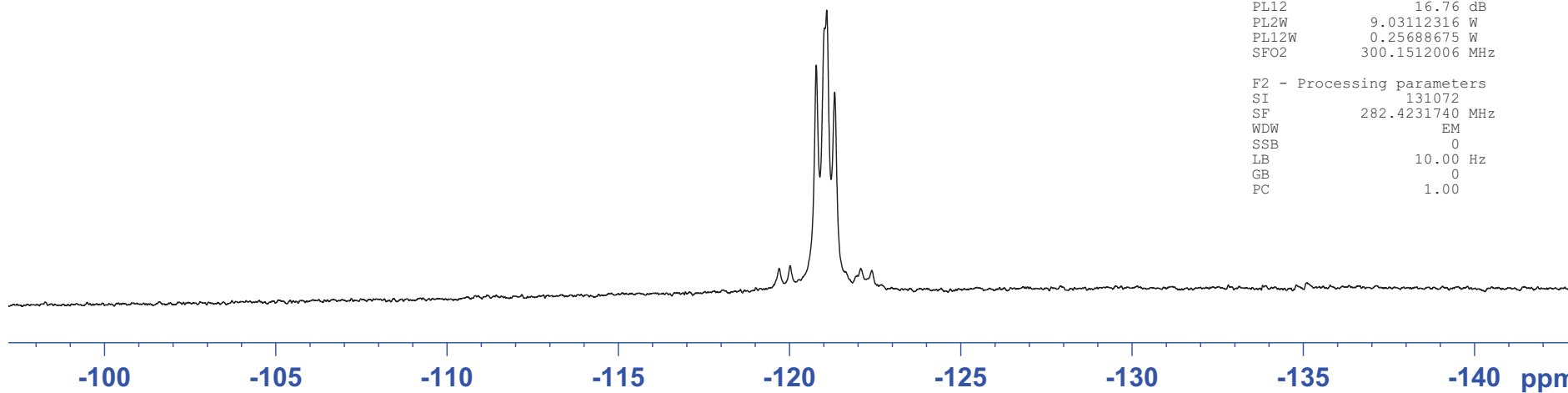
Current Data Parameters
NAME deb_TMSI_2ND BATCH_FREE ACID
EXPNO 2
PROCNO 1

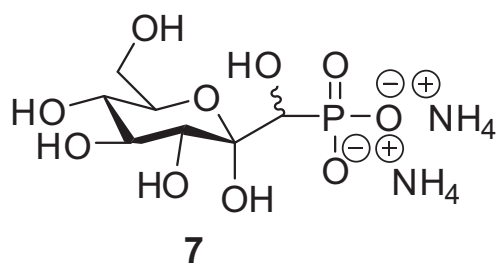
F2 - Acquisition Parameters
Date_ 20111013
Time_ 10.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhiggn
TD 131072
SOLVENT D2O
NS 256
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716788 sec
RG 4100
DW 6.650 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.00 usec
PL1 -0.50 dB
PL1W 8.73698711 W
SFO1 282.3808105 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.76 dB
PL2W 9.03112316 W
PL12W 0.25688675 W
SFO2 300.1512006 MHz

F2 - Processing parameters
SI 131072
SF 282.4231740 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.00





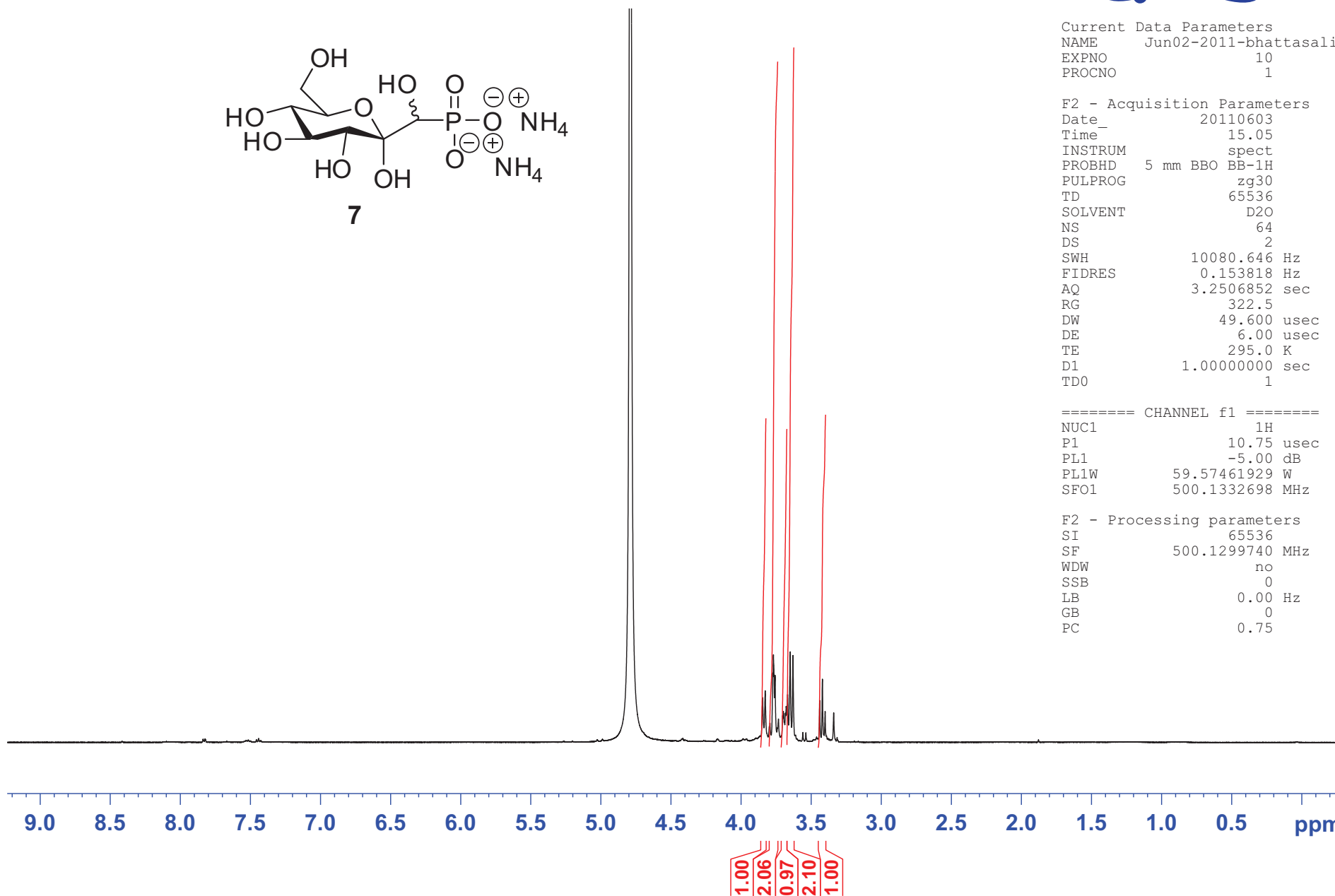
3.85
3.83
3.79
3.74
3.70
3.67
3.63
3.42

Current Data Parameters
 NAME Jun02-2011-bhattasali
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110603
 Time_ 15.05
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 64
 DS 2
 SWH 10080.646 Hz
 FIDRES 0.153818 Hz
 AQ 3.2506852 sec
 RG 322.5
 DW 49.600 usec
 DE 6.00 usec
 TE 295.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.75 usec
 PL1 -5.00 dB
 PL1W 59.57461929 W
 SFO1 500.1332698 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1299740 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 0.75





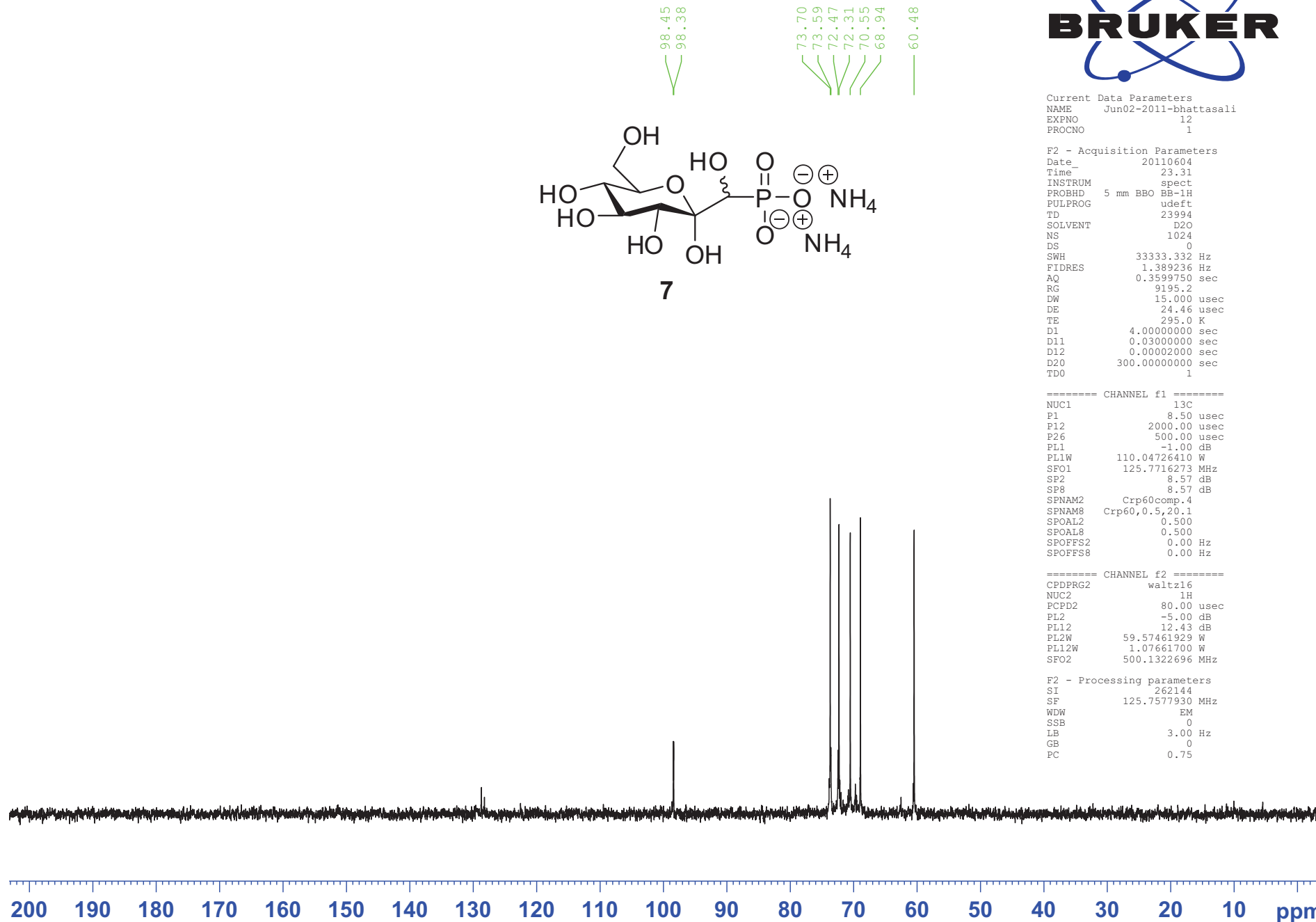
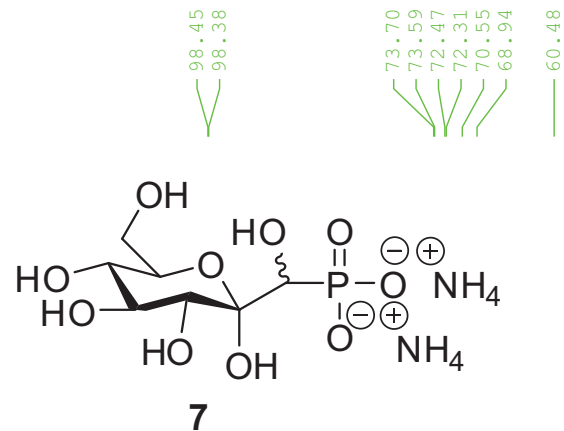
Current Data Parameters
NAME Jun02-2011-bhattasali
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110604
Time 23.31
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG udeflt
TD 23994
SOLVENT D2O
NS 1024
DS 0
SWH 33333.332 Hz
FIDRES 1.389236 Hz
AQ 0.3599750 sec
RG 9195.2
DW 15.000 usec
DE 24.46 usec
TE 295.0 K
D1 4.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D20 300.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
P12 2000.00 usec
P26 500.00 usec
PL1 -1.00 dB
PL1W 110.04726410 W
SFO1 125.7716273 MHz
SP2 8.57 dB
SP8 8.57 dB
SPNAM2 Crp60comp.4
SPNAM8 Crp60,0.5,20.1
SPOAL2 0.500
SPOAL8 0.500
SPOFFS2 0.00 Hz
SPOFFS8 0.00 Hz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 262144
SF 125.7577930 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.75





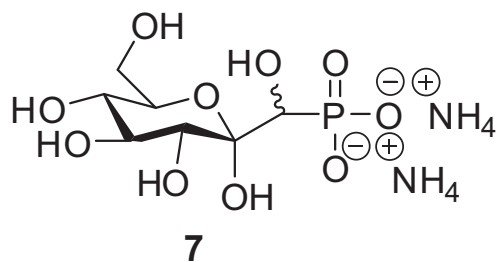
Current Data Parameters
 NAME Jun02-2011-bhattasali
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110605
 Time_ 2.11
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 256
 DS 4
 SWH 98039.219 Hz
 FIDRES 1.495960 Hz
 AQ 0.3342887 sec
 RG 9195.2
 DW 5.100 usec
 DE 7.29 usec
 TE 295.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

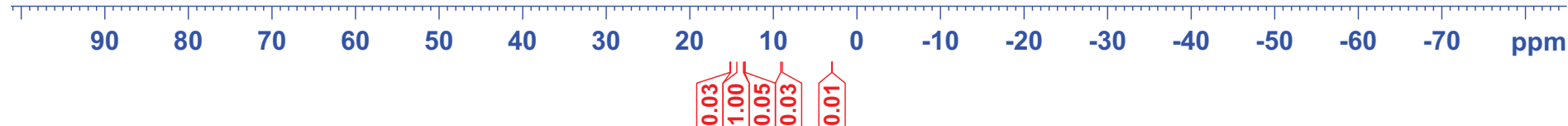
===== CHANNEL f1 =====
 NUC1 31P
 P1 11.00 usec
 PL1 -1.00 dB
 PL1W 102.77402496 W
 SFO1 202.4664658 MHz

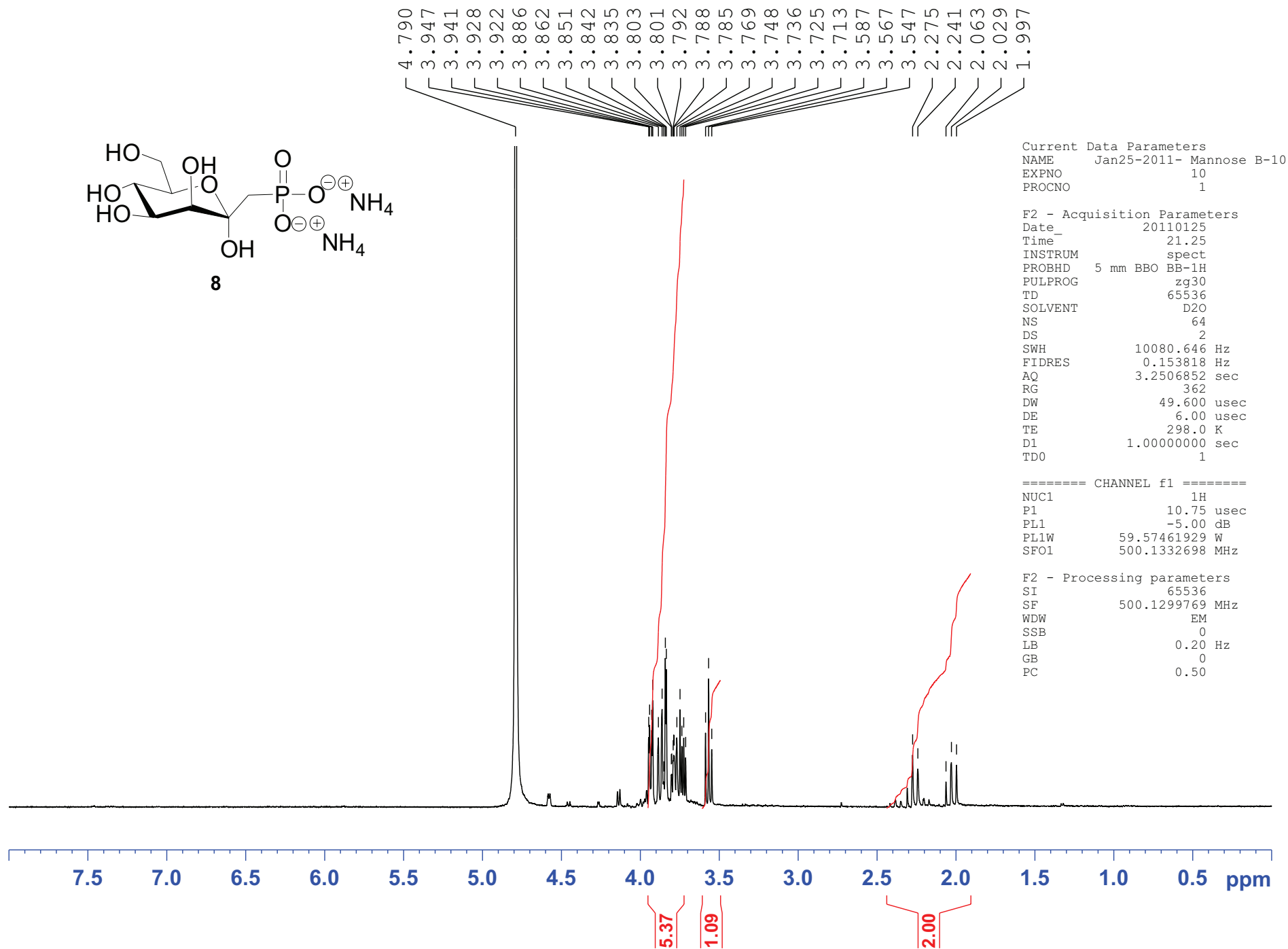
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -5.00 dB
 PL12 12.43 dB
 PL13 18.64 dB
 PL2W 59.57461929 W
 PL12W 1.07661700 W
 PL13W 0.25766850 W
 SFO2 500.1322696 MHz

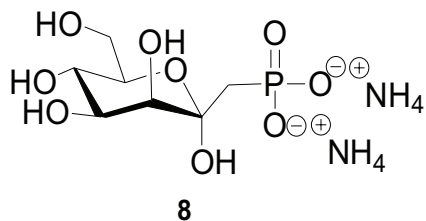
F2 - Processing parameters
 SI 65536
 SF 202.4563430 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 0.75



13.87







97.66

73.32

72.92

70.71

66.67

61.05

35.29
34.40

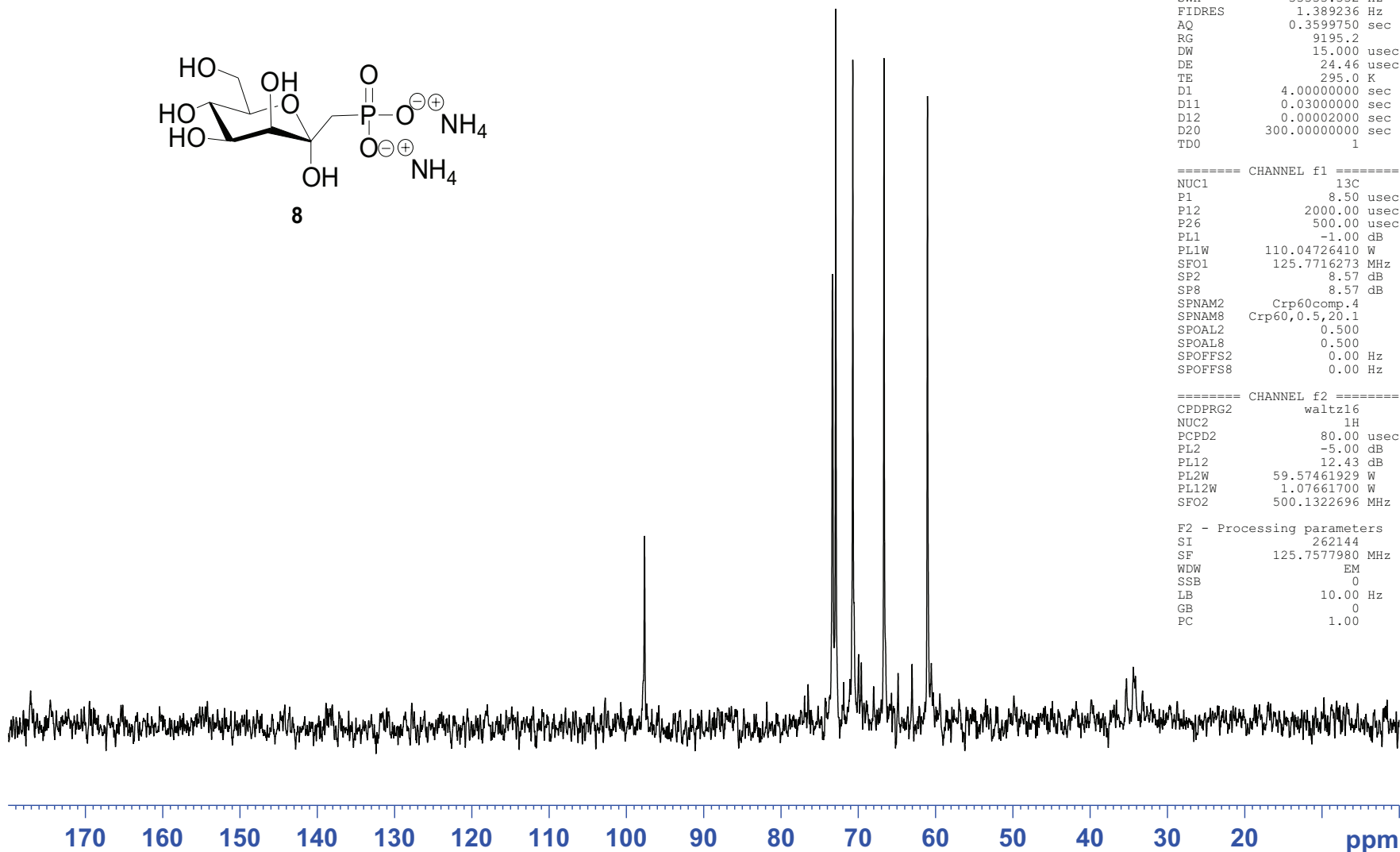
Current Data Parameters
NAME Oct11-2011-man-k
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111012
Time 17.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG udeflt
TD 23994
SOLVENT D2O
NS 1024
DS 0
SWH 33333.332 Hz
FIDRES 1.389236 Hz
AQ 0.3599750 sec
RG 9195.2
DW 15.000 usec
DE 24.46 usec
TE 295.0 K
D1 4.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D20 300.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
P12 2000.00 usec
P26 500.00 usec
PL1 -1.00 dB
PL1W 110.04726410 W
SFO1 125.7716273 MHz
SP2 8.57 dB
SP8 8.57 dB
SPNAM2 Crp60comp.4
SPNAM8 Crp60,0.5,20.1
SPOAL2 0.500
SPOAL8 0.500
SPOFFS2 0.00 Hz
SPOFFS8 0.00 Hz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 262144
SF 125.7577980 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.00



18.69
16.56



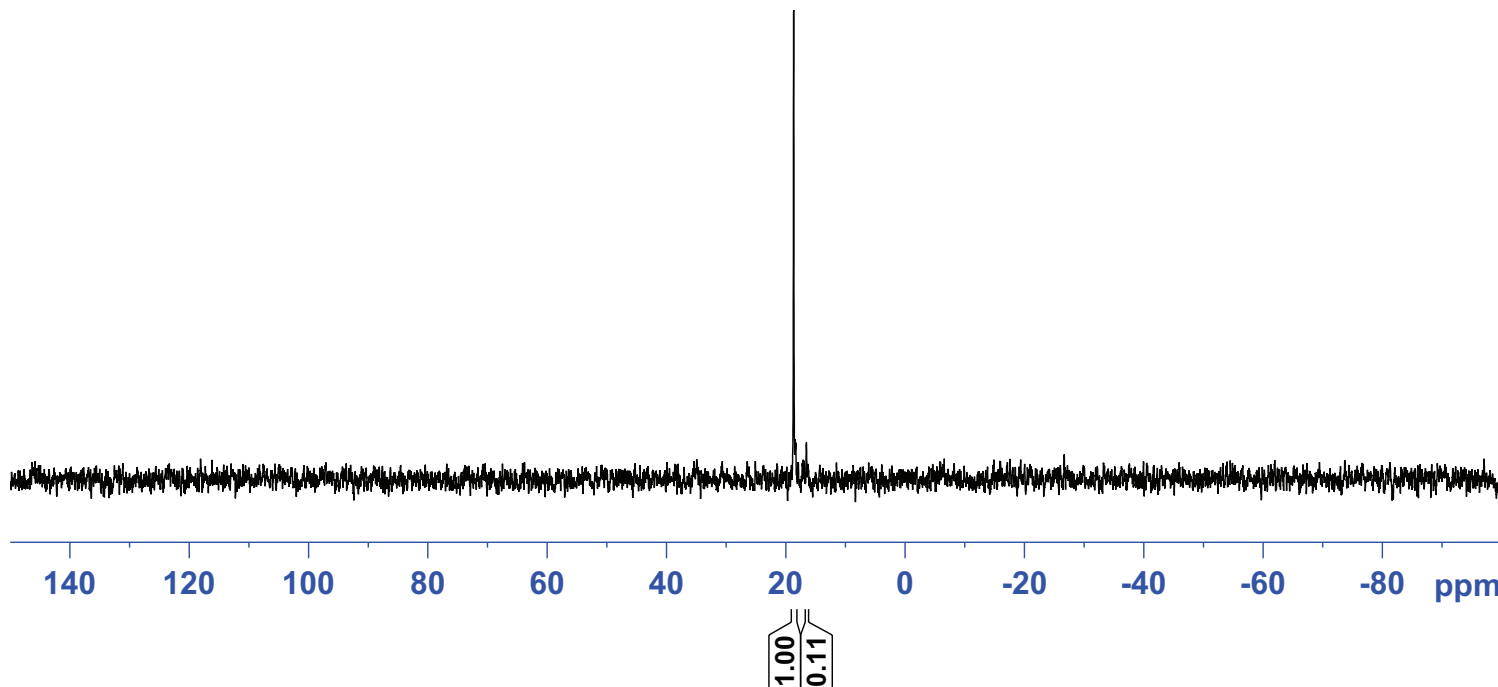
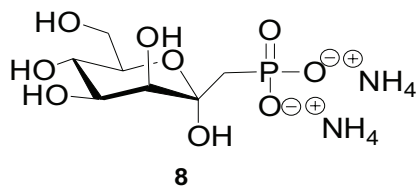
Current Data Parameters
NAME Jan24-2011-Mandprtd-B7
EXPNO 11
PROCNO 1

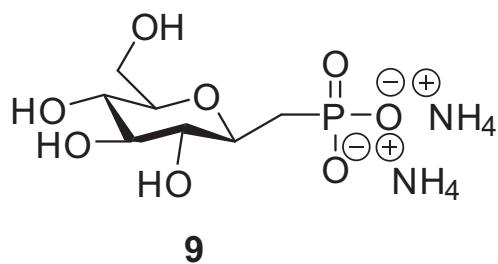
F2 - Acquisition Parameters
Date_ 20110124
Time_ 12.28
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 128
DS 4
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 -1.00 dB
PL1W 102.77402496 W
SFO1 202.4664658 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 202.4563430 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 0.75





3.85
3.83
3.61
3.60
3.59
3.58
3.55
3.54
3.53
3.52
3.51
3.42
3.38
3.35
3.27
3.21

1.91
1.90
1.88
1.87
1.86
1.85
1.82
1.81
1.80
1.79
1.78

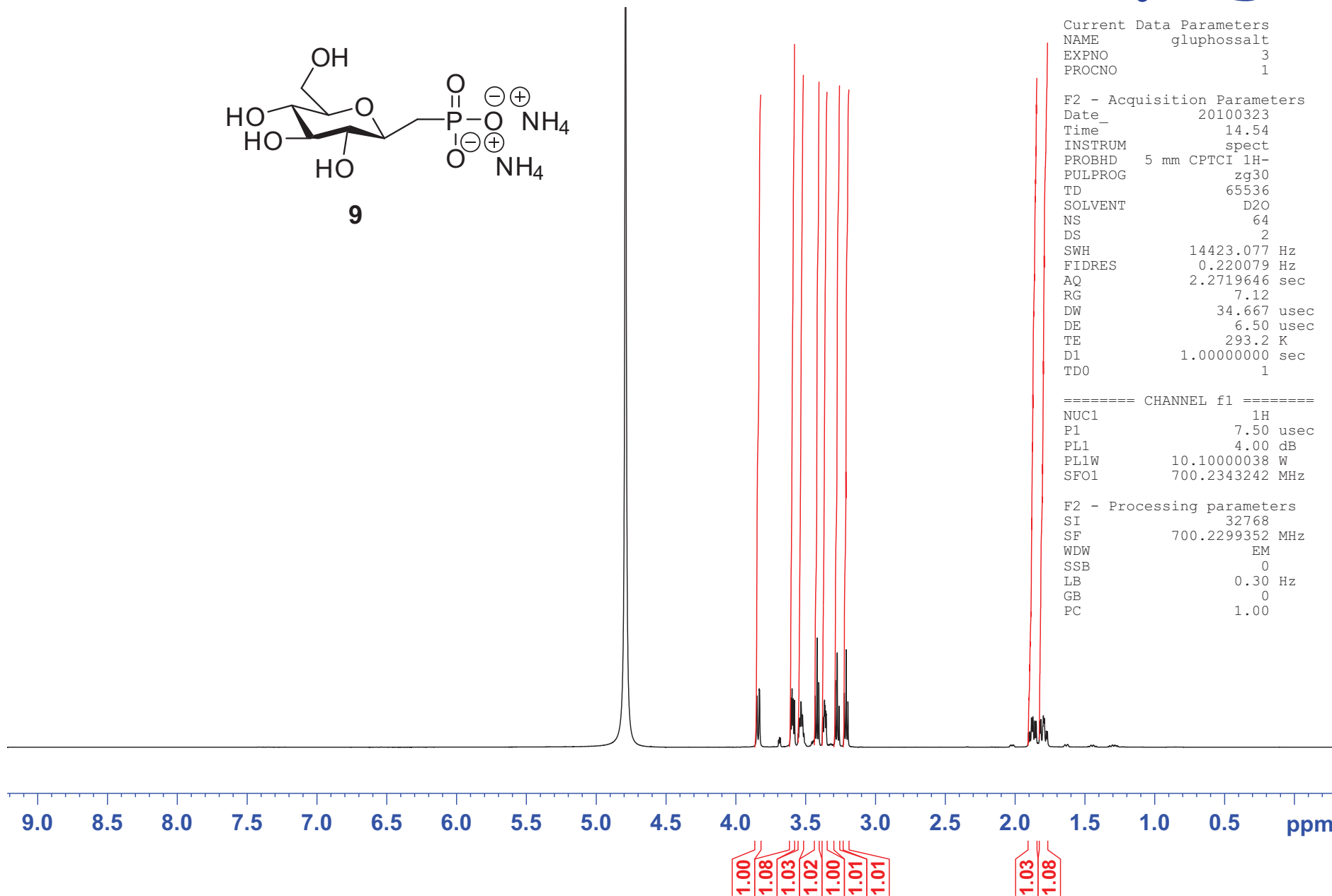


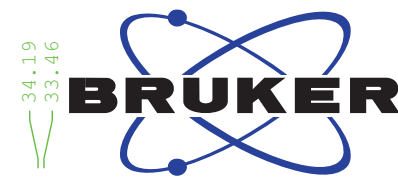
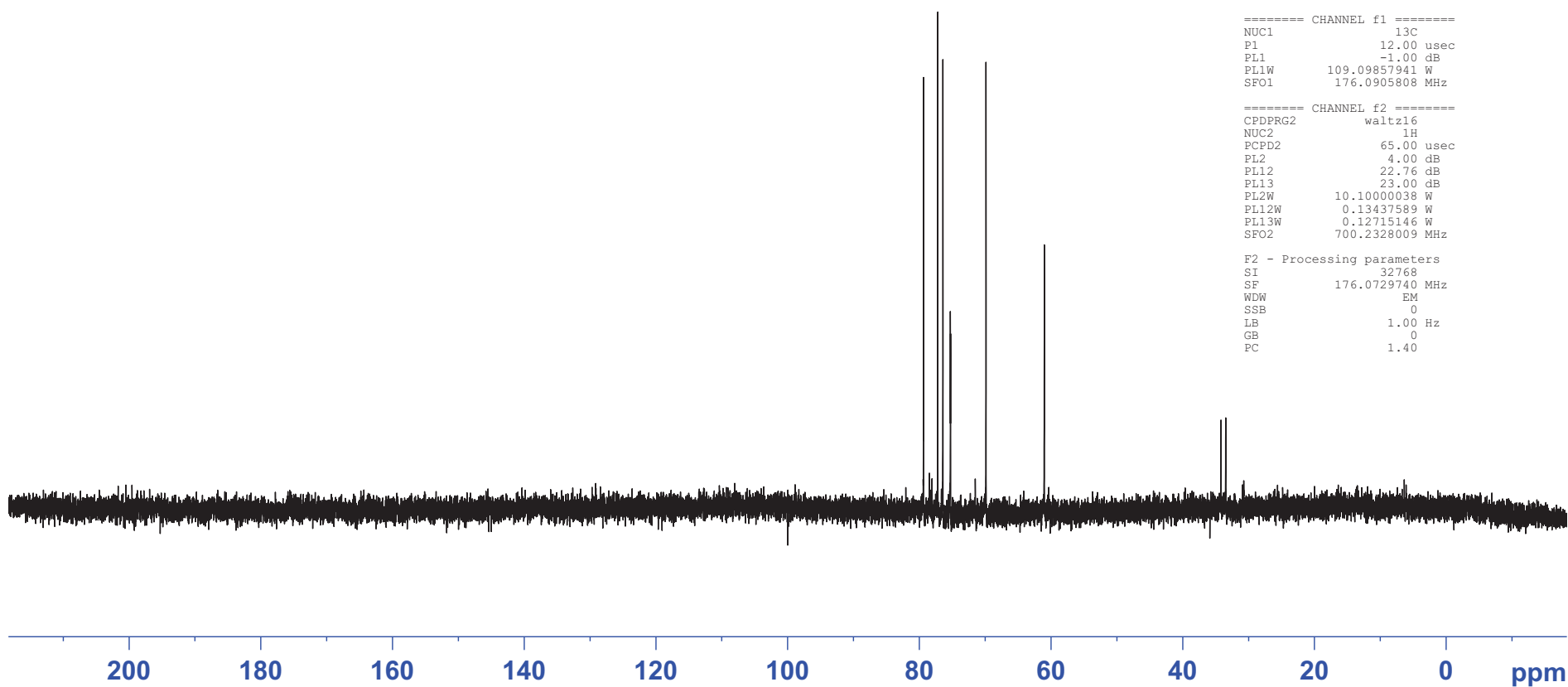
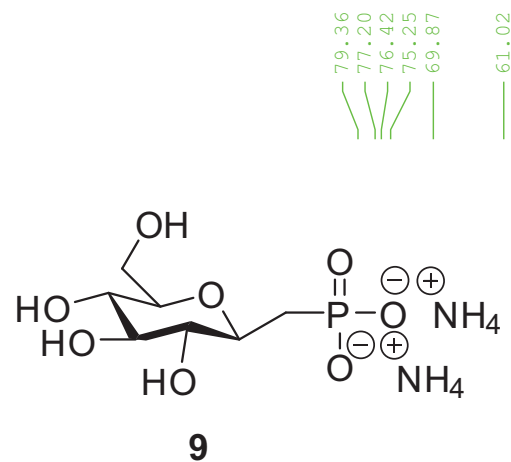
Current Data Parameters
 NAME gluphossalt
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100323
 Time 14.54
 INSTRUM spect
 PROBHD 5 mm CPTCI 1H-
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 64
 DS 2
 SWH 14423.077 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719646 sec
 RG 7.12
 DW 34.667 usec
 DE 6.50 usec
 TE 293.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 4.00 dB
 PL1W 10.10000038 W
 SFO1 700.2343242 MHz

F2 - Processing parameters
 SI 32768
 SF 700.2299352 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





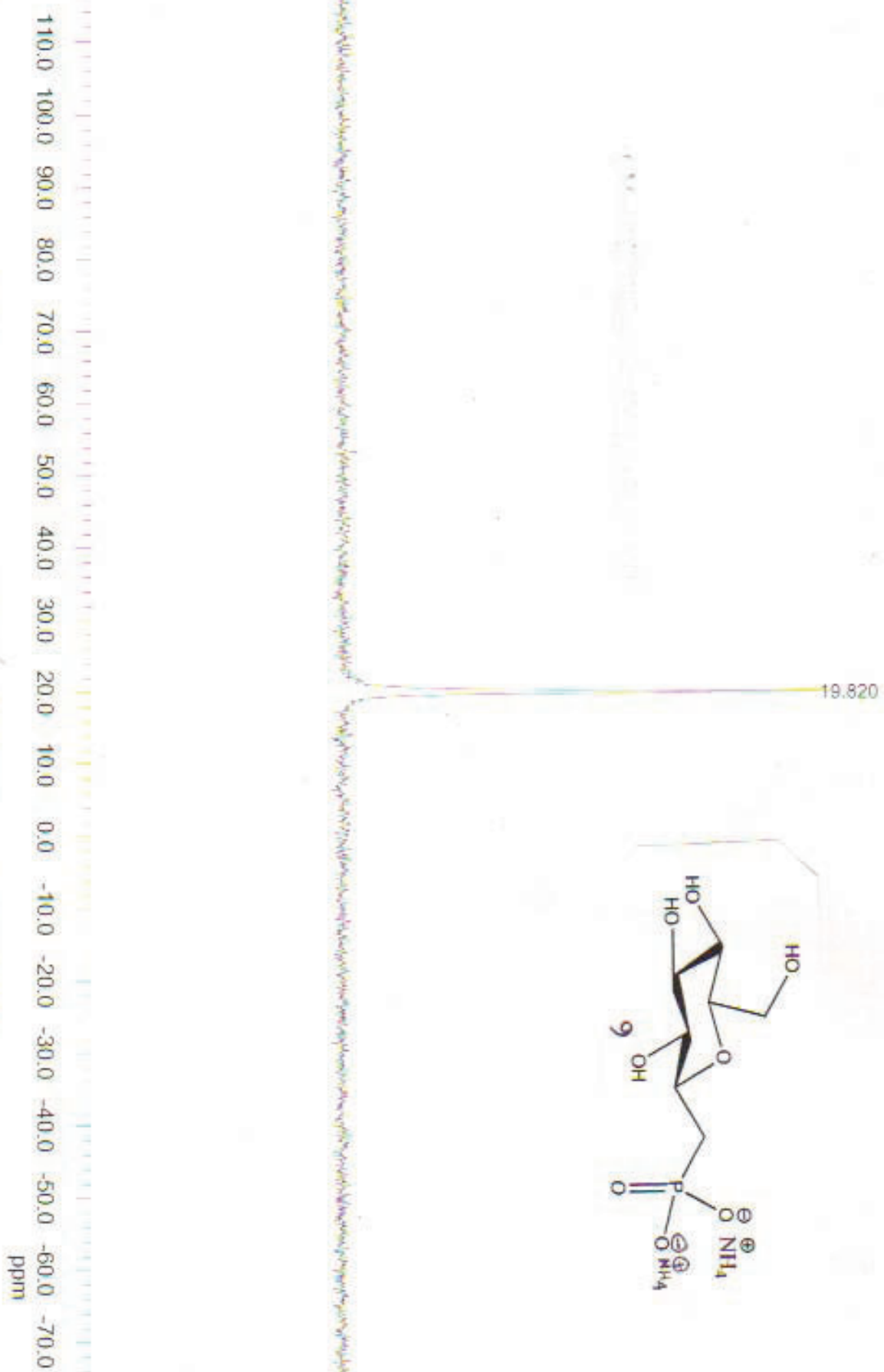
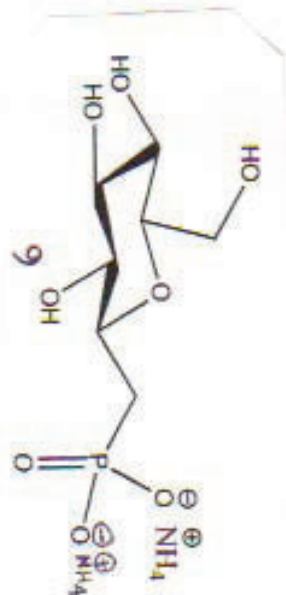
Current Data Parameters
NAME gluphossalt
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100323
Time 15.44
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 1024
DS 4
SWH 41666.668 Hz
FIDRES 0.635783 Hz
AQ 0.7864820 sec
RG 2.56
DW 12.000 usec
DE 6.50 usec
TE 293.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -1.00 dB
PL1W 109.09857941 W
SFO1 176.0905808 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 65.00 usec
PL2 4.00 dB
PL12 22.76 dB
PL13 23.00 dB
PL2W 10.10000038 W
PL12W 0.13437589 W
PL13W 0.12715146 W
SFO2 700.2328009 MHz

F2 - Processing parameters
SI 32768
SF 176.0729740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Acquisition
Date = 2010/02/25 13:24:34
Name = sample_001_1.f2
Start time = Wednesday, March 17, 2010 10:07:26
End time = Wednesday, March 17, 2010 10:10:26
Scan Rate = 100.625 MHz
Sweep = 32768
Pulse = zgpg30
Relax Time = 0.000000

Acquisition
Name = sample_001_1.f2
Date = 2010/02/25 13:24:34
Start time = Wednesday, March 17, 2010 10:07:26
End time = Wednesday, March 17, 2010 10:10:26
Scan Rate = 100.625 MHz
Sweep = 32768
Pulse = zgpg30
Relax Time = 0.000000

Sequence
Name = sample_001_1.f2
Date = 2010/02/25 13:24:34
Start time = Wednesday, March 17, 2010 10:07:26
End time = Wednesday, March 17, 2010 10:10:26
Scan Rate = 100.625 MHz
Sweep = 32768
Pulse = zgpg30
Relax Time = 0.000000

Frequency
Name = sample_001_1.f2
Date = 2010/02/25 13:24:34
Start time = Wednesday, March 17, 2010 10:07:26
End time = Wednesday, March 17, 2010 10:10:26
Scan Rate = 100.625 MHz
Sweep = 32768
Pulse = zgpg30
Relax Time = 0.000000

Frequency
Name = sample_001_1.f2
Date = 2010/02/25 13:24:34
Start time = Wednesday, March 17, 2010 10:07:26
End time = Wednesday, March 17, 2010 10:10:26
Scan Rate = 100.625 MHz
Sweep = 32768
Pulse = zgpg30
Relax Time = 0.000000



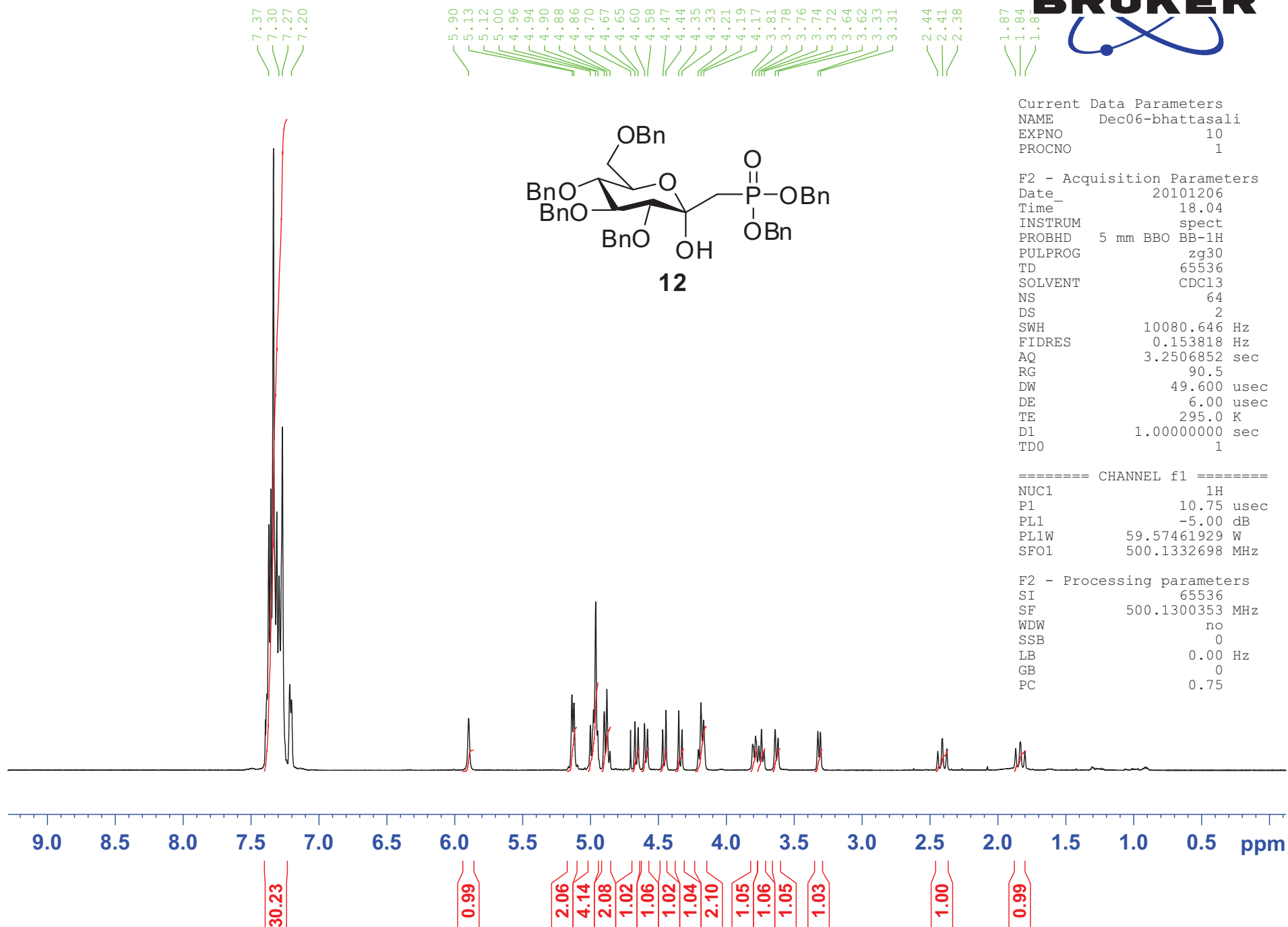
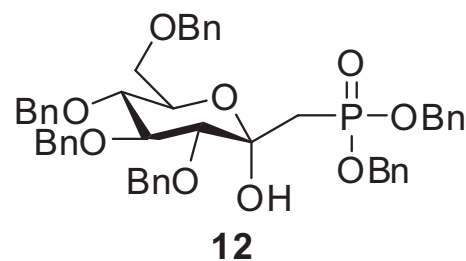
```

F2 - Acquisition Parameters
Date_                20101206
Time                 18.04
INSTRUM              spect
PROBHD      5 mm BBO BB-1H
PULPROG              zg30
TD                   65536
SOLVENT              CDCl3
NS                     64
DS                      2
SWH             10080.646 Hz
FIDRES           0.153818 Hz
AQ             3.2506852 sec
RG                90.5
DW              49.600 usec
DE              6.00 usec
TE              295.0 K
D1              1.00000000 sec
TD0              1

```

```
===== CHANNEL f1 =====
NUC1                      1H
P1                        10.75 usec
PL1                       -5.00 dB
PL1W                      59.57461929 W
SFO1                     500.1332698 MHz
```

```
F2 - Processing parameters
SI                      65536
SF                      500.1300353 MHz
WDW                      no
SSB                      0
LB                      0.00 Hz
GB                      0
PC                      0.75
```





```
Current Data Parameters
NAME      Dec06-bhattasali
EXPNO      11
PROCNO     1
```

```

F2 - Acquisition Parameters
Date_      20101206
Time       18.10
INSTRUM    spect
PROBHD     5 mm BBO BB-1H
PULPROG    zgpgp30
TD          54048
SOLVENT    CDC13
NS          512
DS          4
SWH         33333.332 Hz
FIDRES     0.616736 Hz
AQ          0.8107850 sec
RG          3649.1
DW          15.000 usec
DE          21.14 usec
TE          295.0 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0         1

```

```
===== CHANNEL f1 =====
NUC1          13C
P1             8.50 usec
PL1           -1.00 dB
PL1W          110.04726410 W
SFO1          125.7716273 MHz
```

```

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2         1H
PCPD2        80.00 usec
PL2          -5.00 dB
PL12         12.43 dB
PL13         18.64 dB
PL2W         59.57461929 W
PL12W        1.07661700 W
PL13W        0.25766850 W
SF02         500.1322696 MHz

```

F2 - Processing parameters	
SI	65536
SF	125.7578128 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	0.75



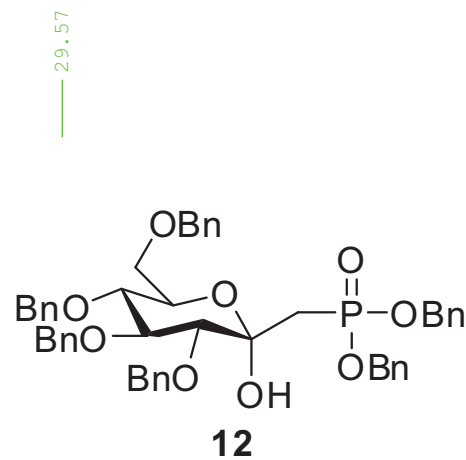
Current Data Parameters
NAME Dec06-bhattachali
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101206
Time 18.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 -1.00 dB
PL1W 102.77402496 W
SFO1 202.4664658 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 202.4563430 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.75



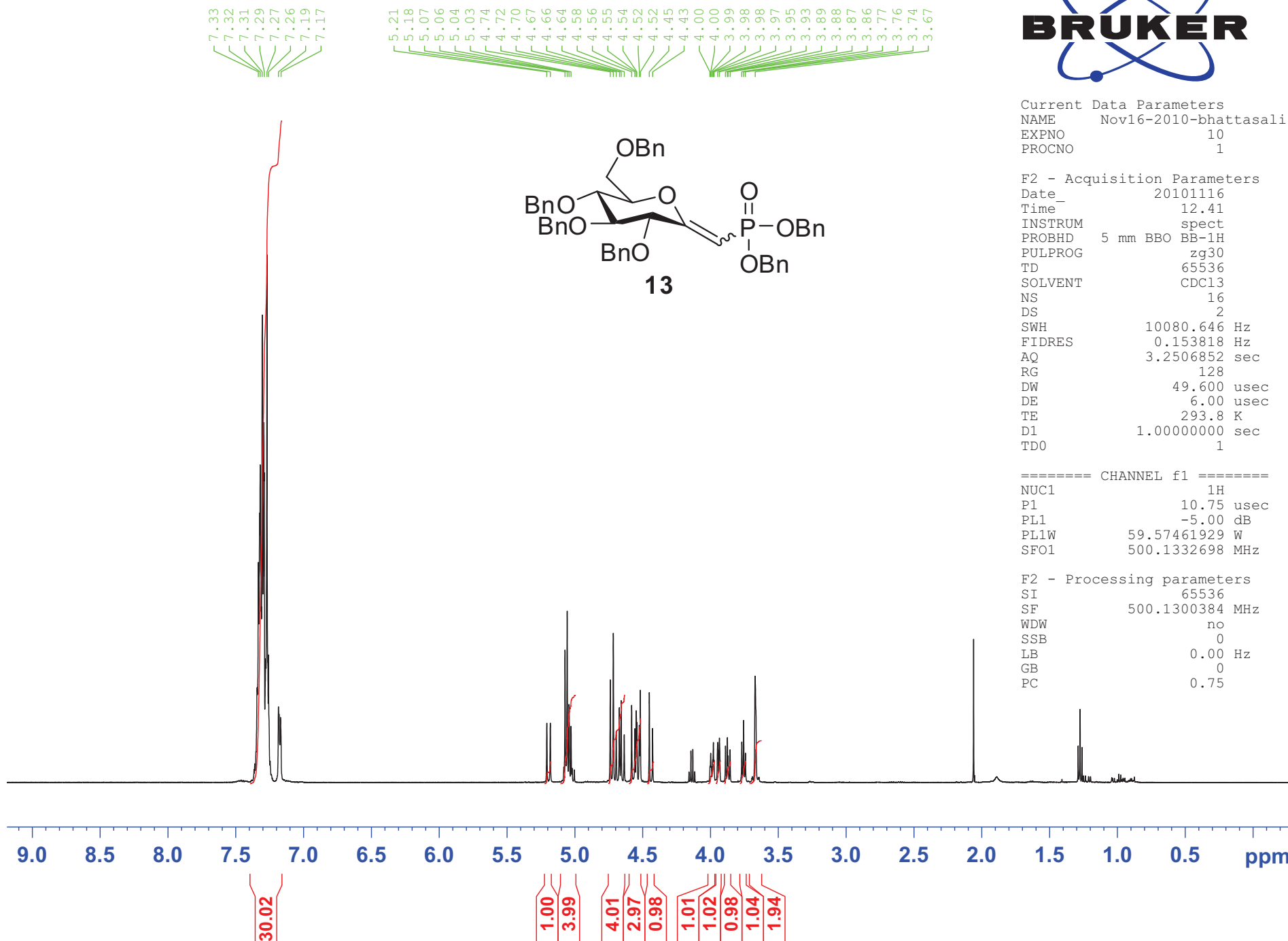
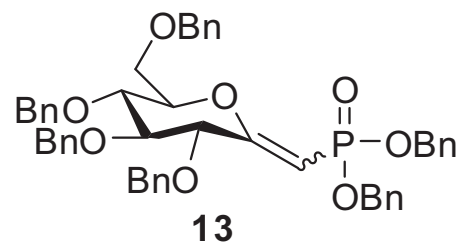


Current Data Parameters
 NAME Nov16-2010-bhattasali
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101116
 Time_ 12.41
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10080.646 Hz
 FIDRES 0.153818 Hz
 AQ 3.2506852 sec
 RG 128
 DW 49.600 usec
 DE 6.00 usec
 TE 293.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.75 usec
 PL1 -5.00 dB
 PL1W 59.57461929 W
 SFO1 500.1332698 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300384 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 0.75





```
Current Data Parameters
NAME      Nov16-2010-bhattasali
EXPNO      11
PROCNO     1
```

```

F2 - Acquisition Parameters
Date_                20101116
Time_                12.47
INSTRUM              spect
PROBHD               5 mm BBO BB-1H
PULPROG              zgpg30
TD                   54048
SOLVENT              CDCl3
NS                   600
DS                   4
SWH                  33333.332 Hz
FIDRES               0.616736 Hz
AQ                   0.8107850 sec
RG                   9195.2
DE                   15.000 usec
DW                   21.14 usec
TE                   294.2 K
D1                   1.00000000 sec
D11                  0.030000000 sec
TD0                  1

```

```
===== CHANNEL f1 =====
NUC1                13C
P1                  8.50 usec
PL1                 -1.00 dB
PL1W                110.04726410 W
SFO1                125.7716273 MHz
```

```

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2          -5.00 dB
PL12         12.43 dB
PL13         18.64 dB
PL2W         59.57461929 W
PL12W        1.07661700 W
PL13W        0.25766850 W
SFO2         500.1322696 MHz

```

```
F2 - Processing parameters
SI                      65536
SF                      125.7578074 MHz
WDW                      EM
SSB                      0
LB                      3.00 Hz
GB                      0
PC                      0.75
```



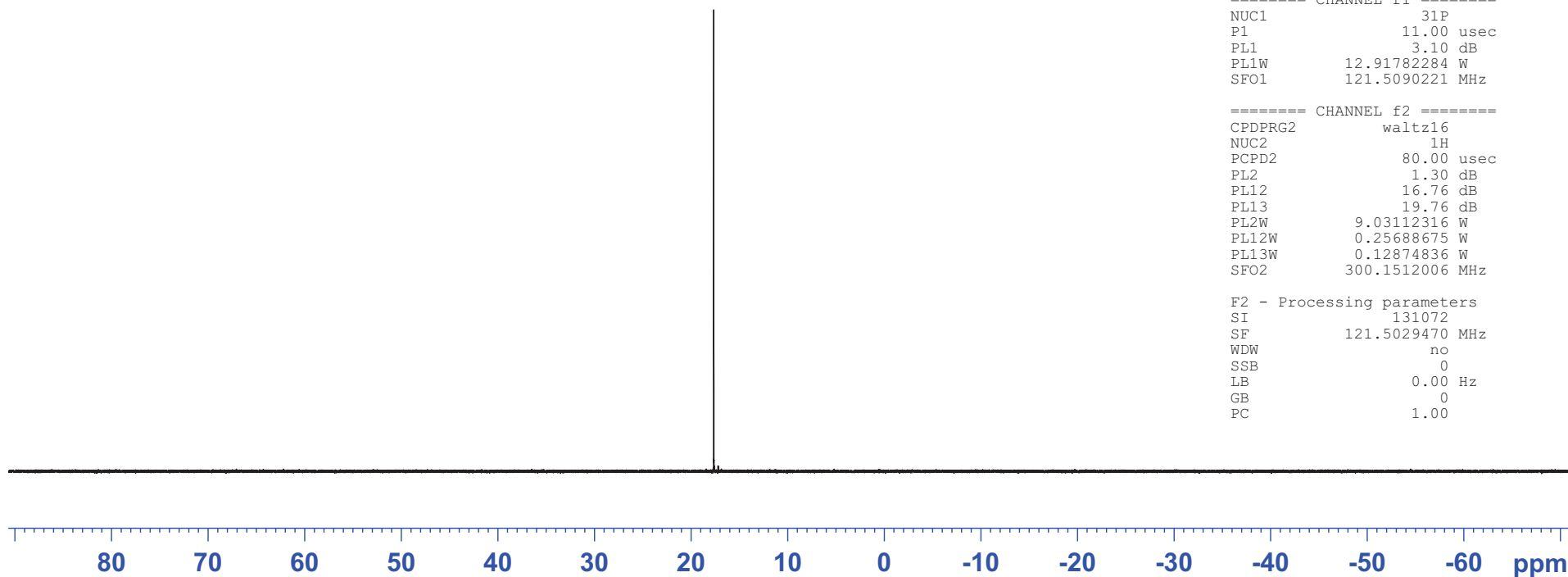
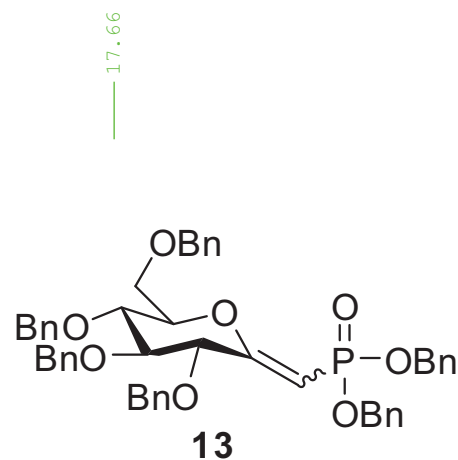
Current Data Parameters
NAME deb_benzyl_exoglycal
EXPNO 2
PROCNO 1

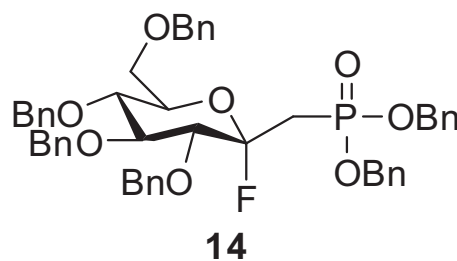
F2 - Acquisition Parameters
Date_ 20101116
Time 11.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 109284
SOLVENT CDCl3
NS 16
DS 4
SWH 54644.809 Hz
FIDRES 0.500026 Hz
AQ 0.9999986 sec
RG 23100
DW 9.150 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 3.10 dB
PL1W 12.91782284 W
SFO1 121.5090221 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.76 dB
PL13 19.76 dB
PL2W 9.03112316 W
PL12W 0.25688675 W
PL13W 0.12874836 W
SFO2 300.1512006 MHz

F2 - Processing parameters
SI 131072
SF 121.5029470 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



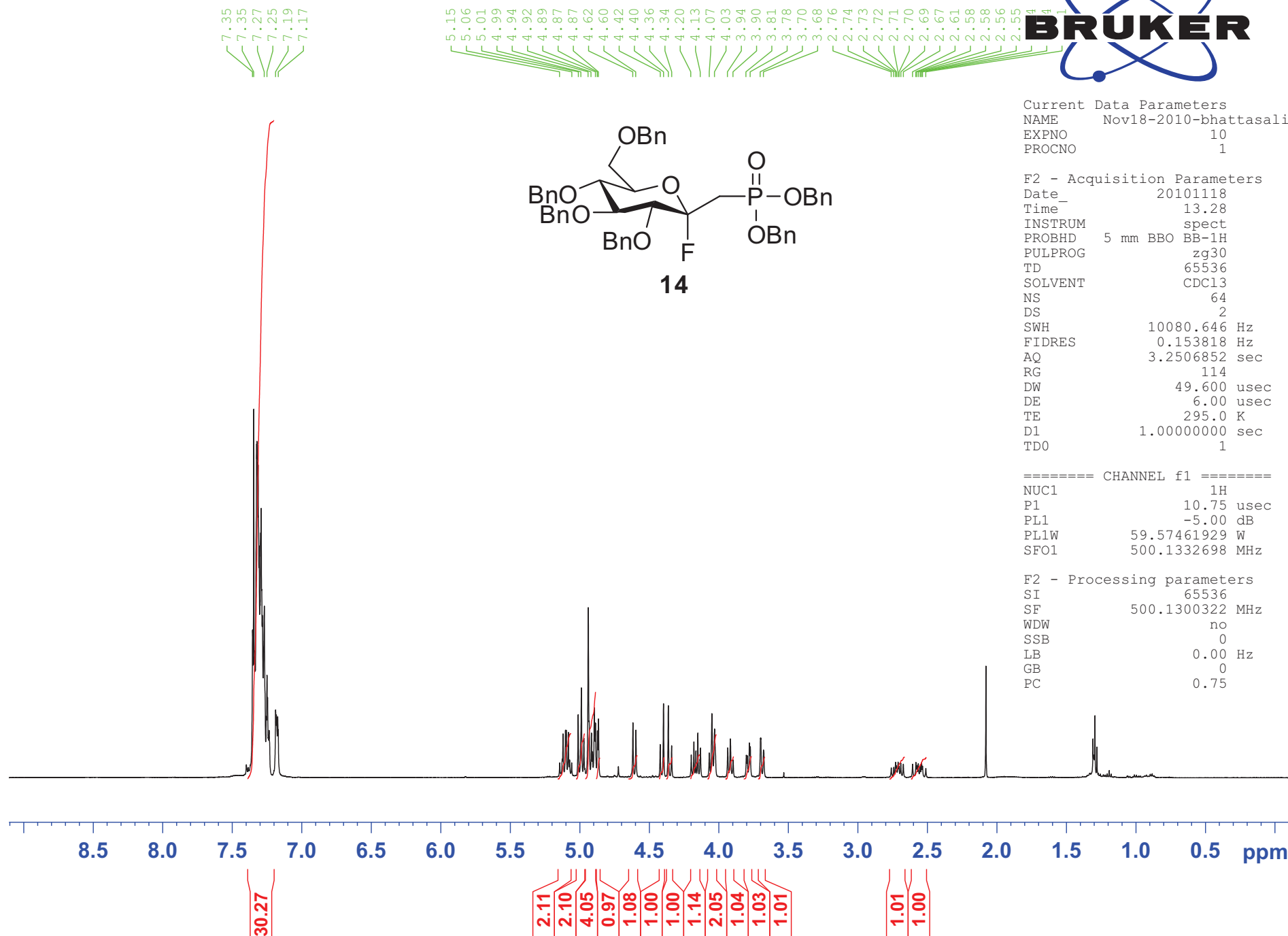


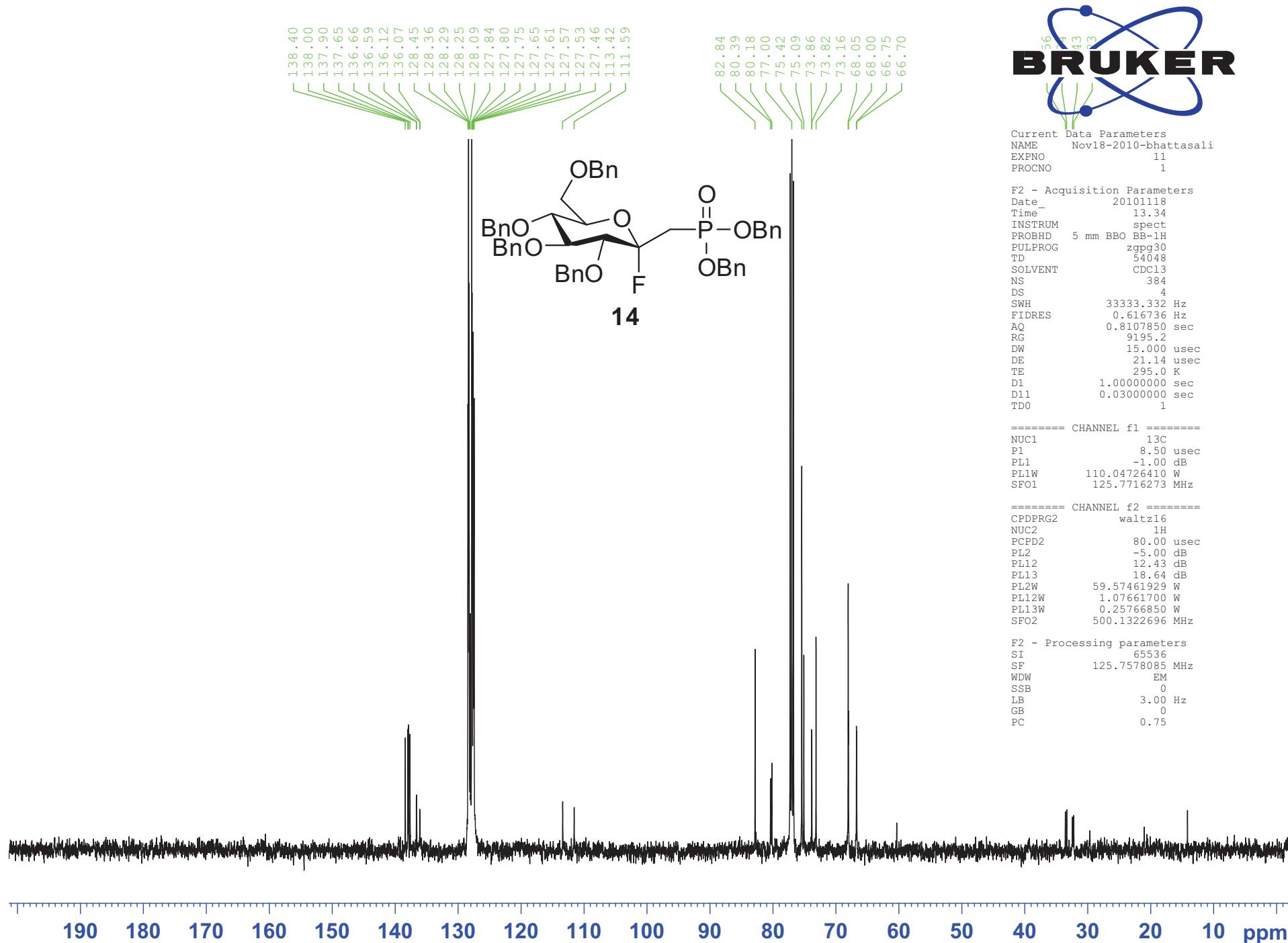
Current Data Parameters
 NAME Nov18-2010-bhattasali
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101118
 Time 13.28
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 10080.646 Hz
 FIDRES 0.153818 Hz
 AQ 3.2506852 sec
 RG 114
 DW 49.600 usec
 DE 6.00 usec
 TE 295.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.75 usec
 PL1 -5.00 dB
 PL1W 59.57461929 W
 SFO1 500.1332698 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300322 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 0.75





Current Data Parameters
 NAME Nov18-2010-bhattachali
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101118
 Time_ 13.34
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 54048
 SOLVENT CDCl3
 NS 384
 DS 4
 SWH 33333.332 Hz
 FIDRES 0.616736 Hz
 AQ 0.8107850 sec
 RG 9195.2
 DW 15.000 usec
 DE 21.14 usec
 TE 295.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -1.00 dB
 PL1W 110.04726410 W
 SFO1 125.7716273 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -5.00 dB
 PL12 12.43 dB
 PL13 18.64 dB
 PL2W 59.57461929 W
 PL12W 1.07661700 W
 PL13W 0.25766850 W
 SFO2 500.1322696 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578085 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 0.75



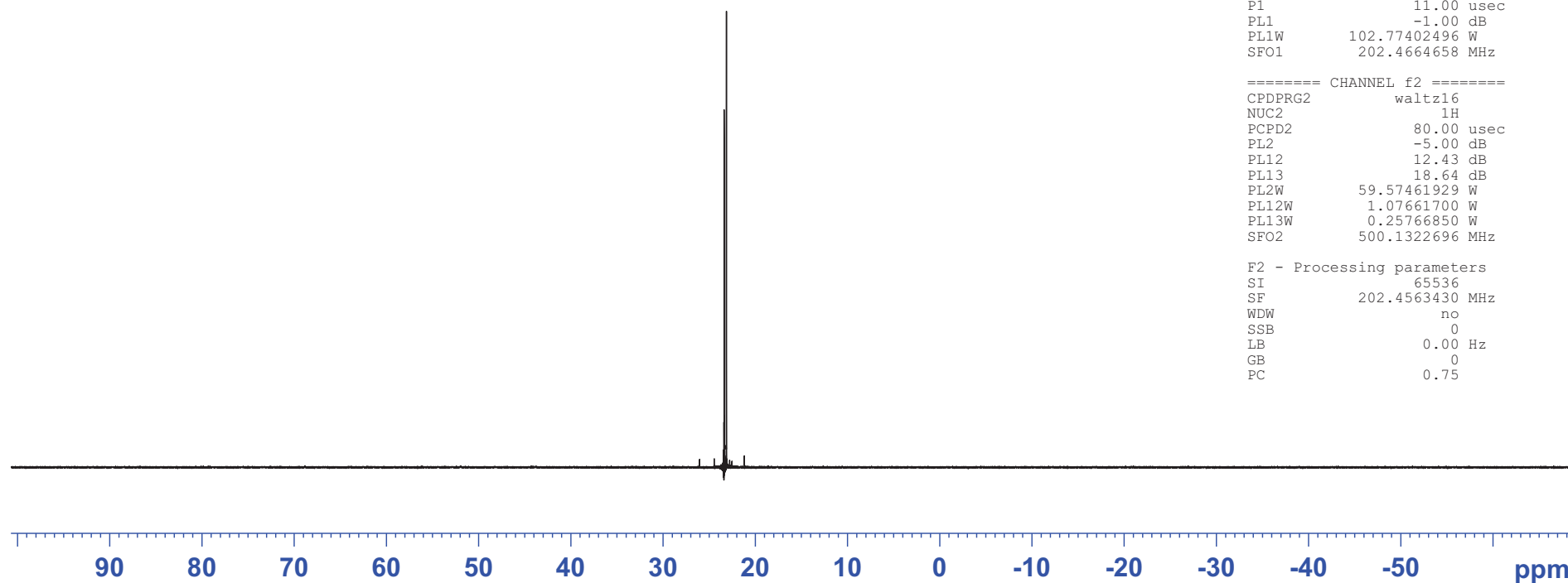
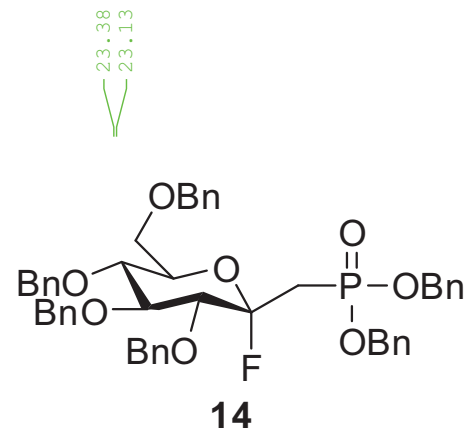
Current Data Parameters
NAME Nov18-2010-bhattasali
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101118
Time 13.54
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 4
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 -1.00 dB
PL1W 102.77402496 W
SFO1 202.4664658 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 202.4563430 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.75





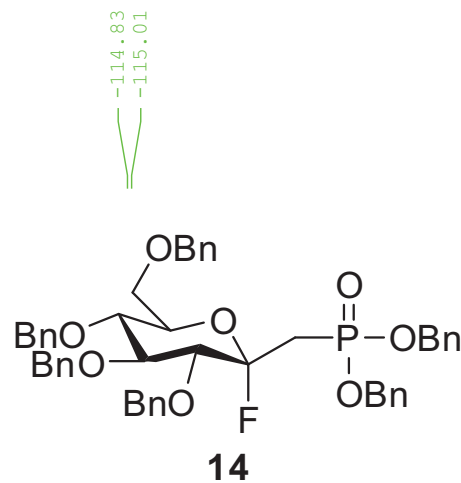
Current Data Parameters
NAME deb_benzyl_phos_anomeric_fluoride
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101118
Time 12.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716788 sec
RG 4100
DW 6.650 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

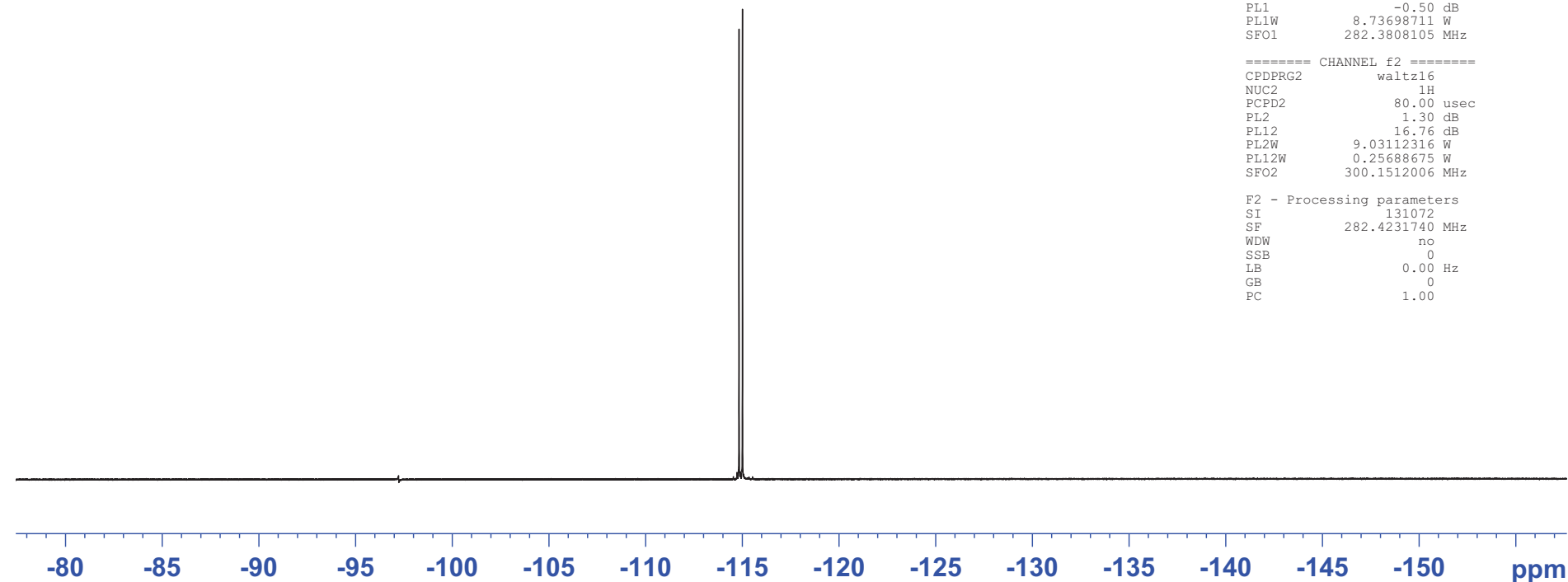
===== CHANNEL f1 =====
NUC1 19F
P1 14.00 usec
PL1 -0.50 dB
PL1W 8.73698711 W
SFO1 282.3808105 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.76 dB
PL2W 9.03112316 W
PL12W 0.25688675 W
SFO2 300.1512006 MHz

F2 - Processing parameters
SI 131072
SF 282.4231740 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



-114.83
-115.01



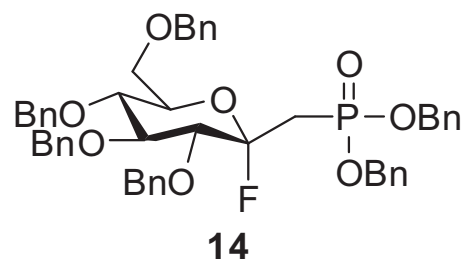


Current Data Parameters
 NAME deb_benzyl_phos_anomeric_fluoride
 EXPNO 3
 PROCNO 1

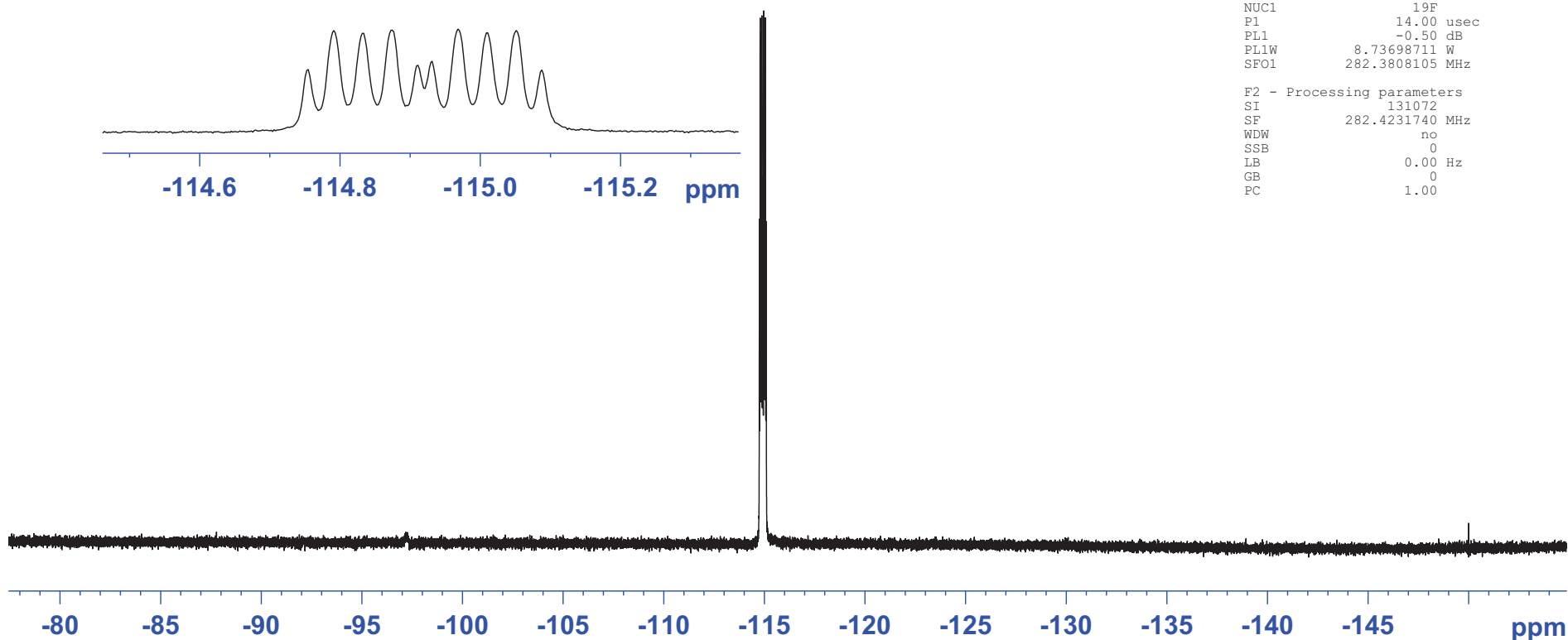
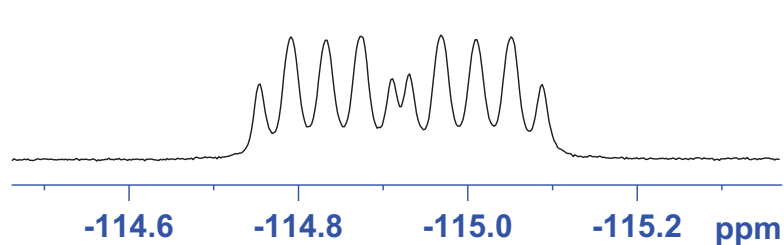
F2 - Acquisition Parameters
 Date_ 20101118
 Time_ 12.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 131072
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 75187.969 Hz
 FIDRES 0.573639 Hz
 AQ 0.8716788 sec
 RG 1440
 DW 6.650 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 14.00 usec
 PL1 -0.50 dB
 PL1W 8.73698711 W
 SFO1 282.3808105 MHz

F2 - Processing parameters
 SI 131072
 SF 282.4231740 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



-114.92



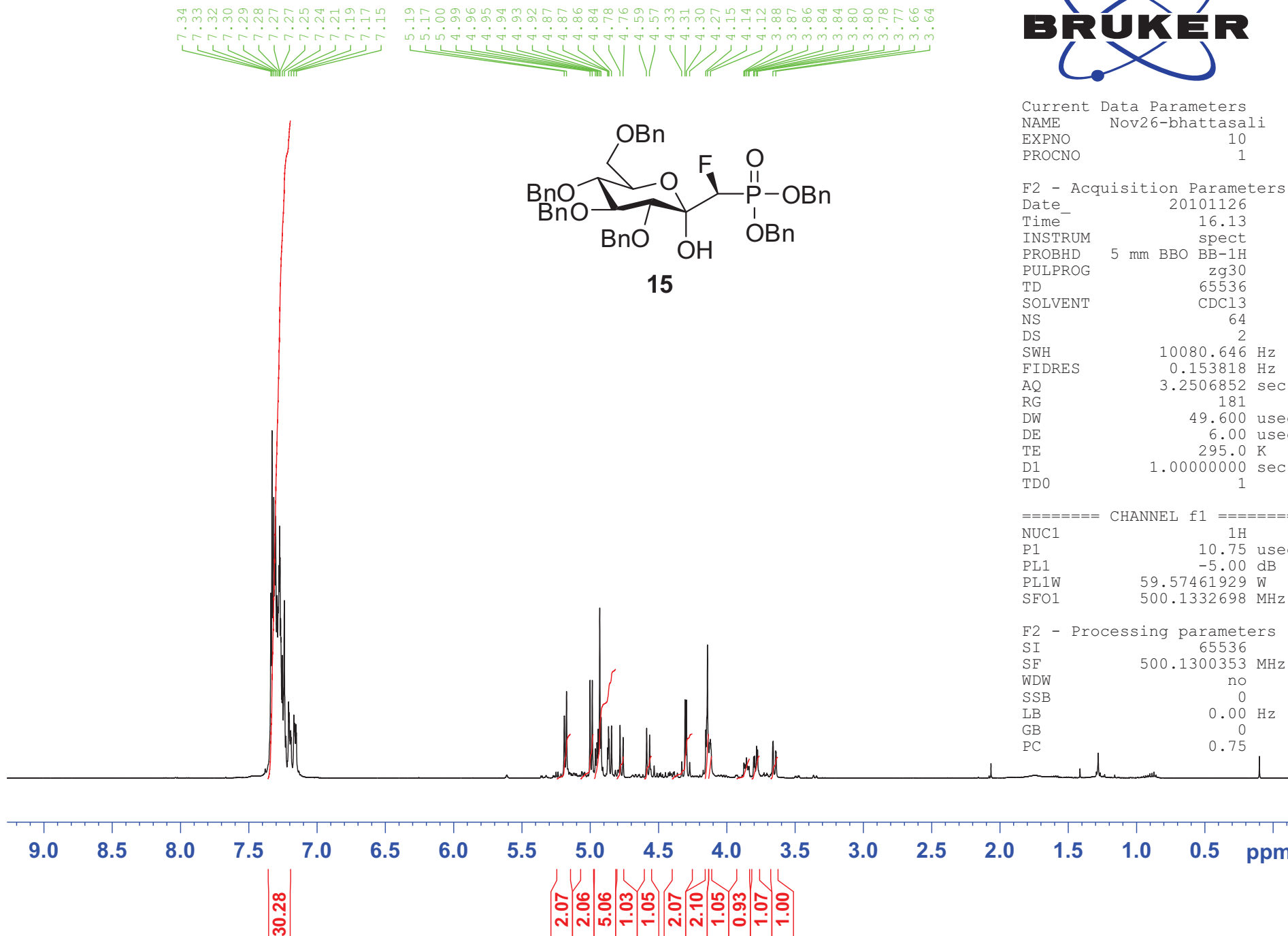
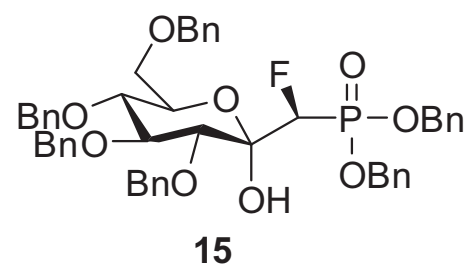


Current Data Parameters
NAME Nov26-bhattasali
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101126
Time_ 16.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 10080.646 Hz
FIDRES 0.153818 Hz
AQ 3.2506852 sec
RG 181
DW 49.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.75 usec
PL1 -5.00 dB
PL1W 59.57461929 W
SFO1 500.1332698 MHz

F2 - Processing parameters
SI 65536
SF 500.1300353 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.75





```
Current Data Parameters
NAME      Nov26-bhattachali
EXPNO      11
PROCNO     1
```

```

F2 - Acquisition Parameters
Date_                20101126
Time                 16.18
INSTRUM              spect
PROBHD               5 mm BBO BB-1H
PULPROG              zgpg30
TD                   54048
SOLVENT              CDC13
NS                   1664
DS                    4
SWH                  33333.332 Hz
FIDRES               0.616736 Hz
AQ                   0.8107850 sec
RG                   9195.2
DW                   15.000 usec
DE                   21.14 usec
TE                   295.0 K
D1                   1.00000000 sec
D11                  0.03000000 sec
TD0                  1

```

```
===== CHANNEL f1 =====
NUC1                13C
P1                   8.50 usec
PL1                  -1.00 dB
PL1W                110.04726410 W
SFO1                125.7716273 MHz
```

```

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2         1H
PCPD2        80.00 usec
PL2          -5.00 dB
PL12         12.43 dB
PL13         18.64 dB
PL2W         59.57461929 W
PL12W        1.07661700 W
PL13W        0.25766850 W
SF02         500.1322696 MHz

```

F2 - Processing parameters	
SI	65536
SF	125.7578043 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	0.75



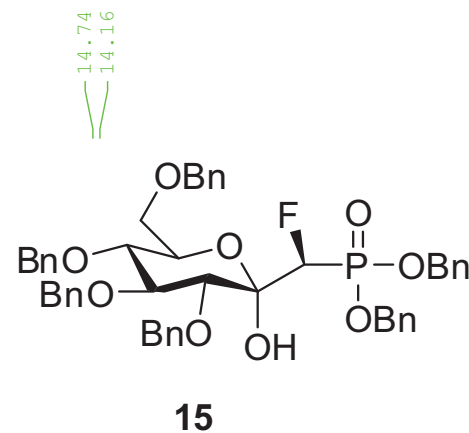
Current Data Parameters
NAME deb_SEL(B)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111012
Time 11.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 109284
SOLVENT CDC13
NS 128
DS 4
SWH 54644.809 Hz
FIDRES 0.500026 Hz
AQ 0.9999986 sec
RG 41200
DW 9.150 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 3.10 dB
PL1W 12.91782284 W
SFO1 121.5090221 MHz

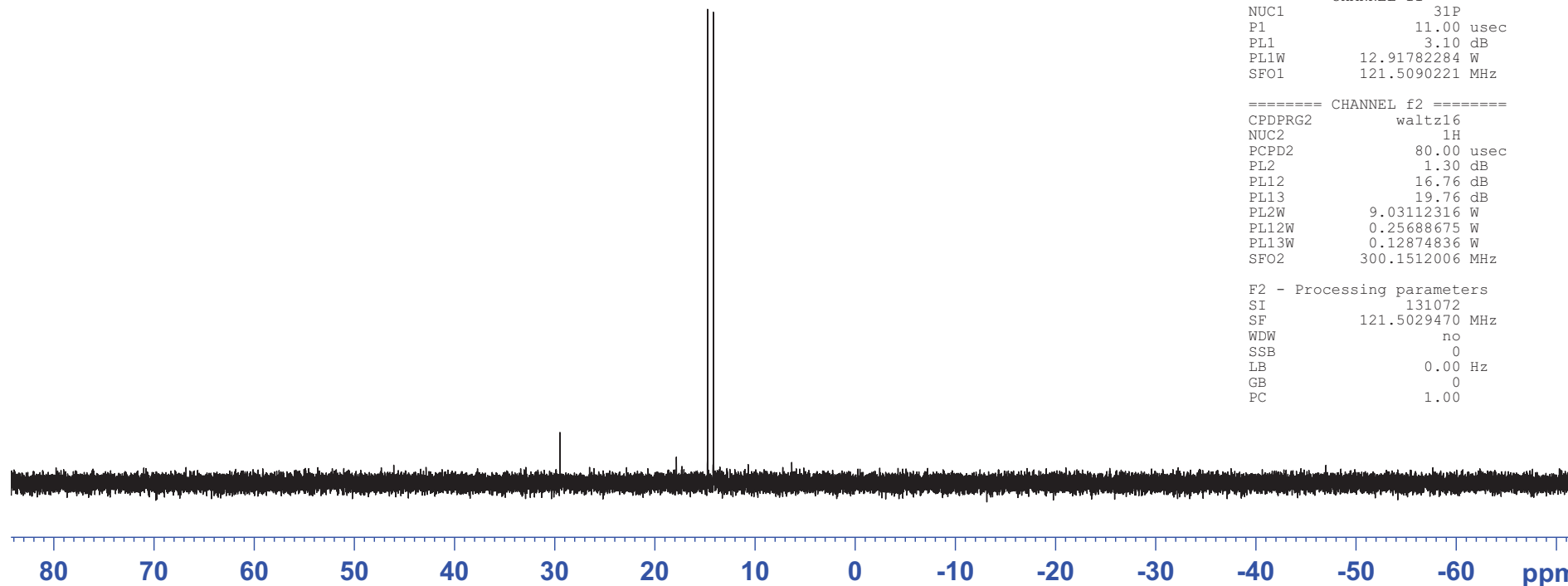
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.76 dB
PL13 19.76 dB
PL2W 9.03112316 W
PL12W 0.25688675 W
PL13W 0.12874836 W
SFO2 300.1512006 MHz

F2 - Processing parameters
SI 131072
SF 121.5029470 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



14.74
14.16

15





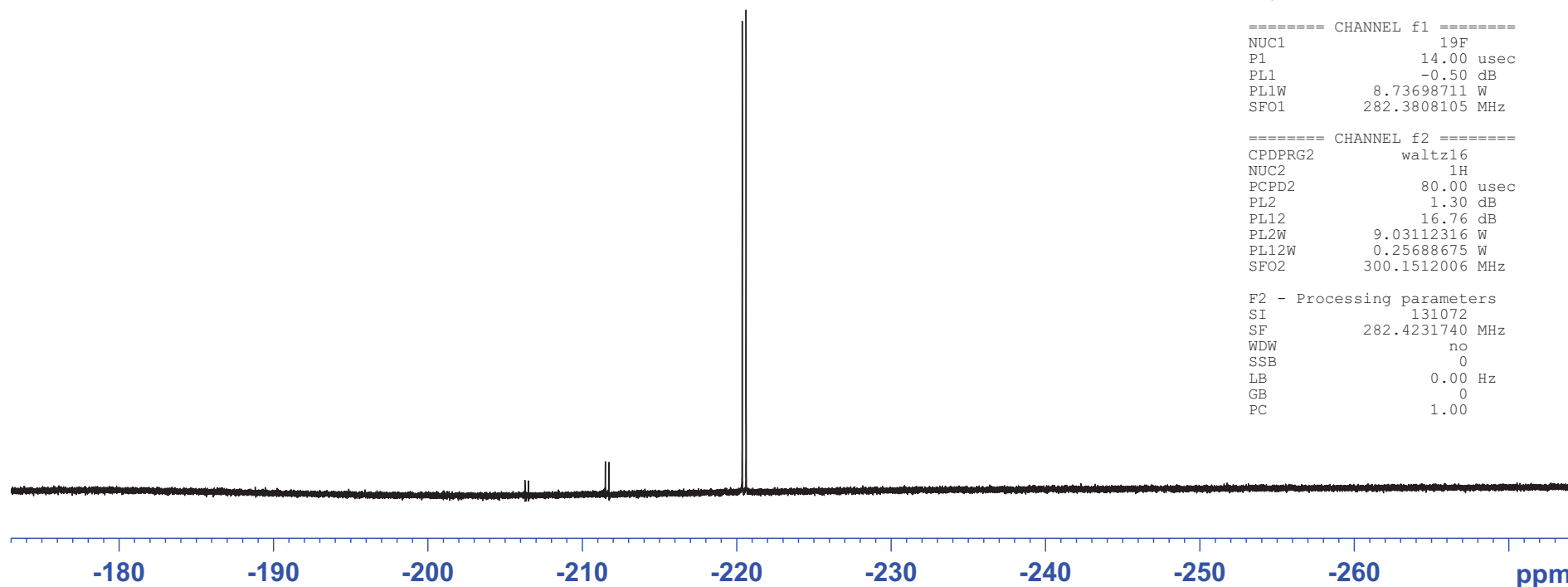
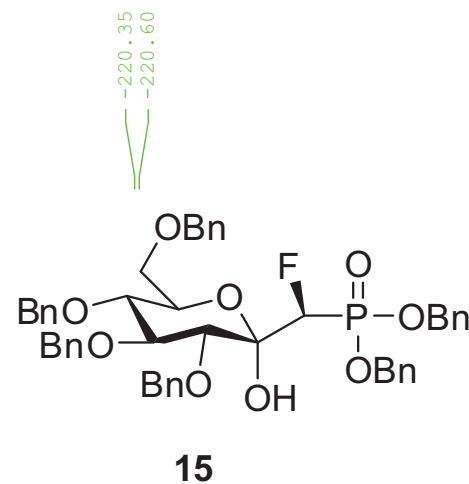
Current Data Parameters
 NAME deb_SEL(B)
 EXPNO 2
 PROCNO 1

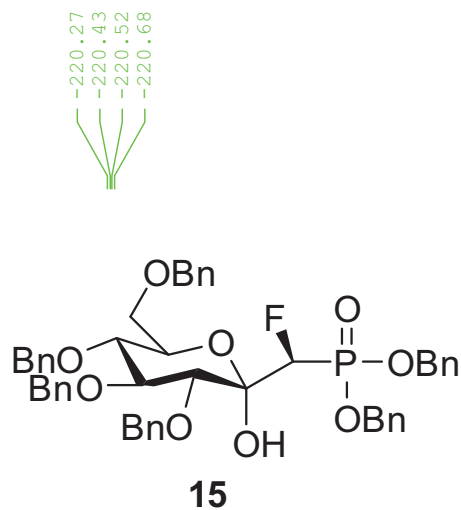
F2 - Acquisition Parameters
 Date_ 20111012
 Time 12.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 131072
 SOLVENT CDCl3
 NS 64
 DS 4
 SWH 75187.969 Hz
 FIDRES 0.573639 Hz
 AQ 0.8716788 sec
 RG 4100
 DW 6.650 usec
 DE 6.50 usec
 TE 298.8 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 14.00 usec
 PL1 -0.50 dB
 PL1W 8.73698711 W
 SFO1 282.3808105 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.30 dB
 PL12 16.76 dB
 PL2W 9.03112316 W
 PL12W 0.25688675 W
 SFO2 300.1512006 MHz

F2 - Processing parameters
 SI 131072
 SF 282.4231740 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



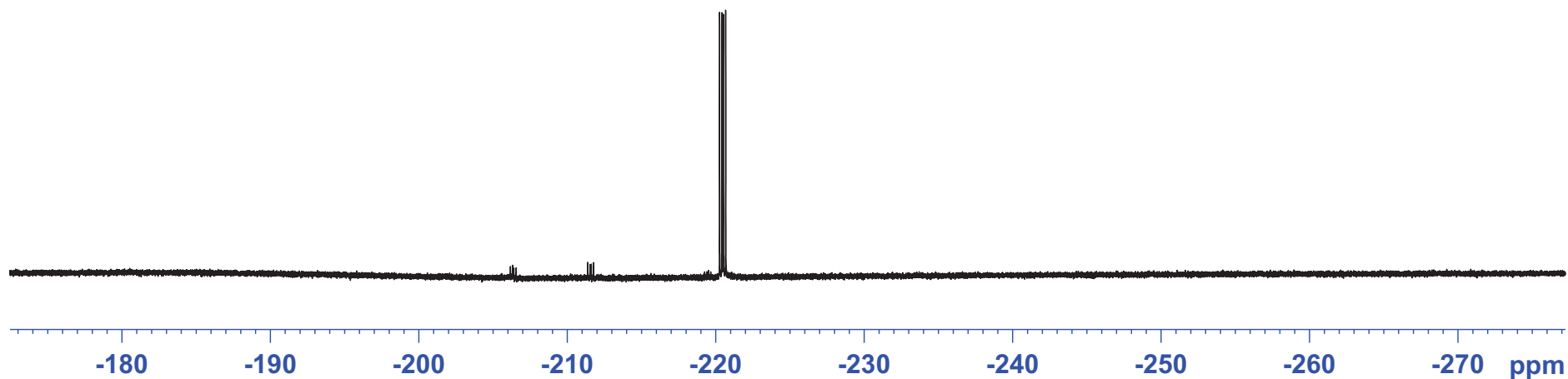
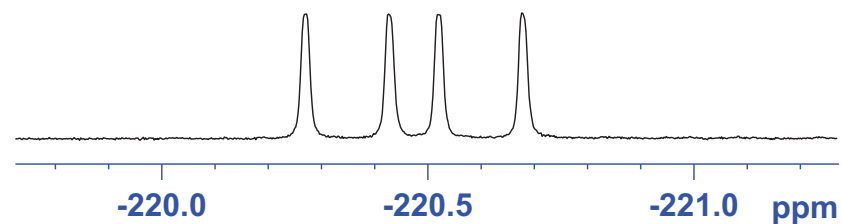


Current Data Parameters
NAME deb_selectfluor_BENZYL DERIVATIVE (BOTTOM SPOT)
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101124
Time 11.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716788 sec
RG 1440
DW 6.650 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.00 usec
PL1 -0.50 dB
PL1W 8.73698711 W
SFO1 282.3808105 MHz

F2 - Processing parameters
SI 131072
SF 282.4231740 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



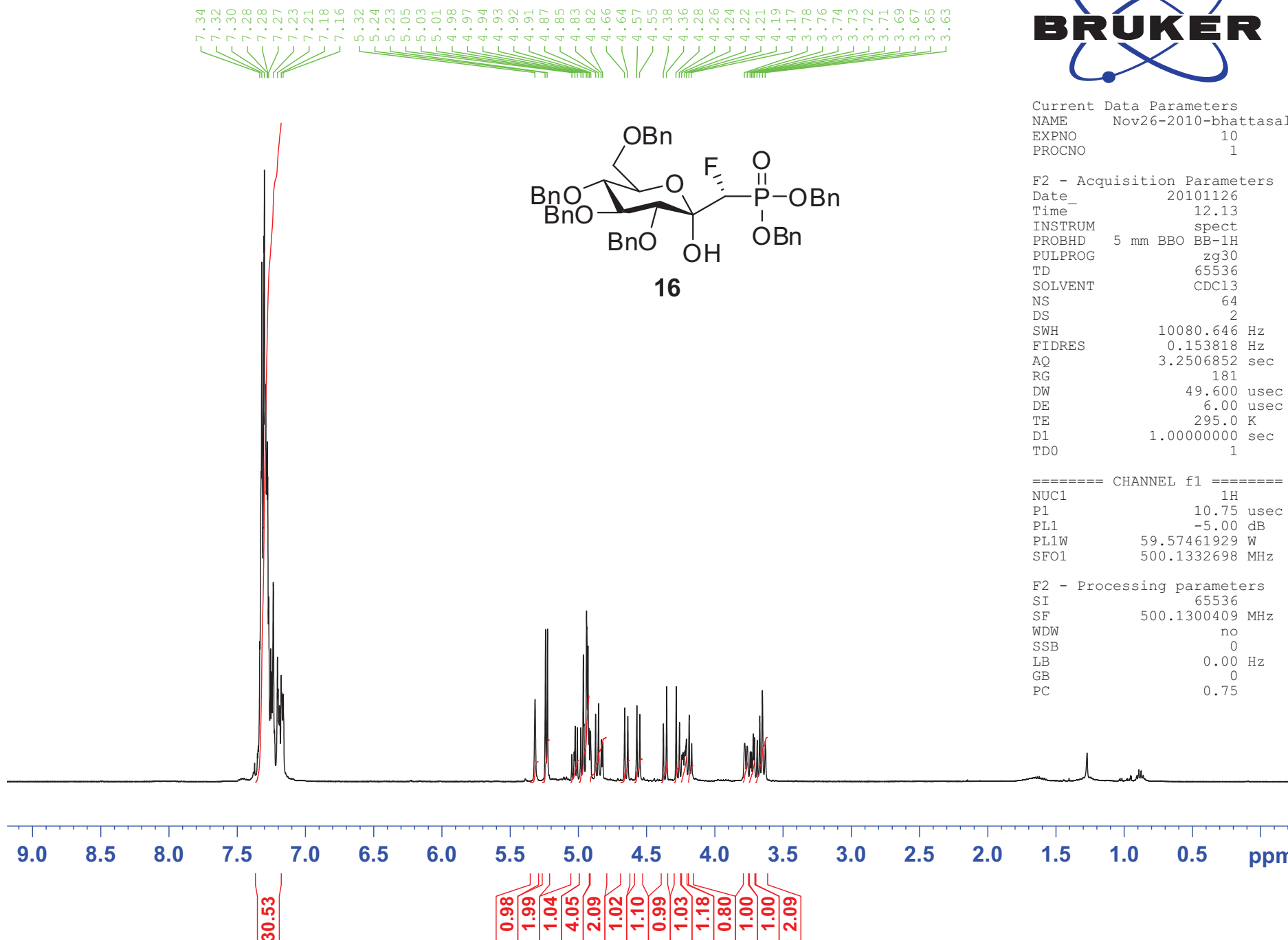
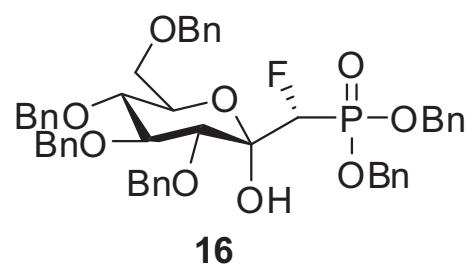


Current Data Parameters
 NAME Nov26-2010-bhattasali
 EXPNO 10
 PROCNO 1

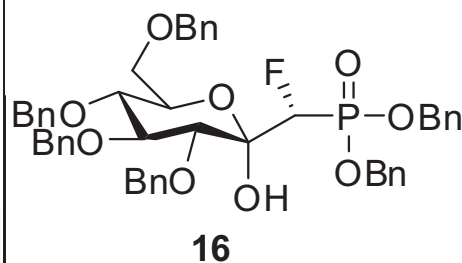
F2 - Acquisition Parameters
 Date_ 20101126
 Time_ 12.13
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 10080.646 Hz
 FIDRES 0.153818 Hz
 AQ 3.2506852 sec
 RG 181
 DW 49.600 usec
 DE 6.00 usec
 TE 295.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.75 usec
 PL1 -5.00 dB
 PL1W 59.57461929 W
 SFO1 500.1332698 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300409 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 0.75



138.44
137.99
137.76
135.99
135.93
135.18
135.13
128.64
128.58
128.50
128.40
128.34
128.26
128.19
128.06
127.85
127.74
127.66
127.60
127.55
97.58
97.38
87.16
85.92
85.56
84.32
82.78
78.15
77.70
77.64
76.99
75.65
75.44
75.01
73.08
71.77
69.80
69.77
68.75
68.12
68.08



Current Data Parameters
NAME Nov26-2010-bhattasali
EXPNO 11
PROCNO 1

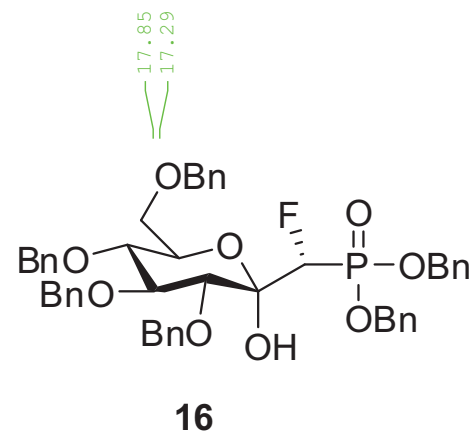
F2 - Acquisition Parameters
Date_ 20101126
Time_ 12.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 54048
SOLVENT CDCl3
NS 2048
DS 4
SWH 33333.332 Hz
FIDRES 0.616736 Hz
AQ 0.8107850 sec
RG 11585.2
DW 15.000 usec
DE 21.14 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -1.00 dB
PL1W 110.04726410 W
SFO1 125.7716273 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 125.7578053 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.75





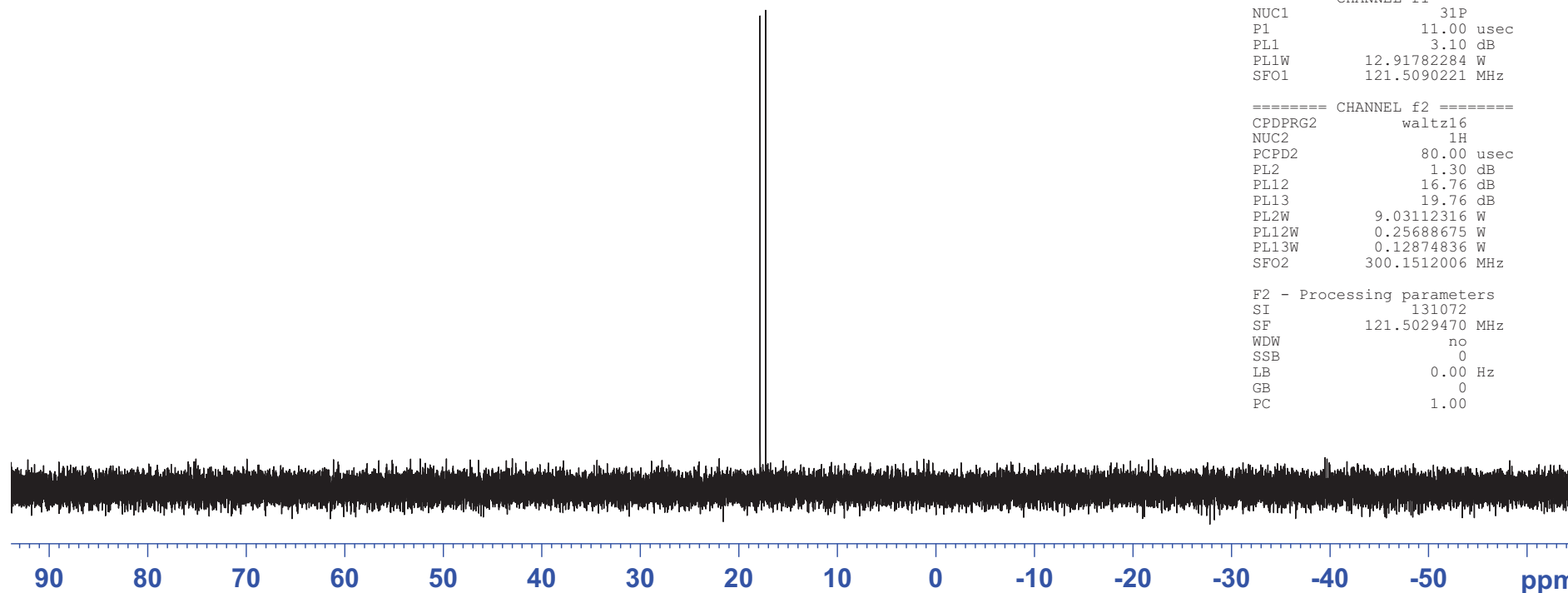
Current Data Parameters
NAME deb_SEL(T)
EXPNO 1
PROCNO 1

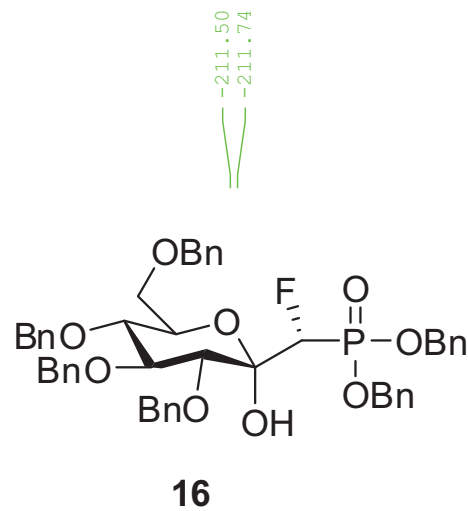
F2 - Acquisition Parameters
Date_ 20111012
Time 11.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 109284
SOLVENT CDCl3
NS 128
DS 4
SWH 54644.809 Hz
FIDRES 0.500026 Hz
AQ 0.9999986 sec
RG 23100
DW 9.150 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 3.10 dB
PL1W 12.91782284 W
SFO1 121.5090221 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.76 dB
PL13 19.76 dB
PL2W 9.03112316 W
PL12W 0.25688675 W
PL13W 0.12874836 W
SFO2 300.1512006 MHz

F2 - Processing parameters
SI 131072
SF 121.5029470 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00





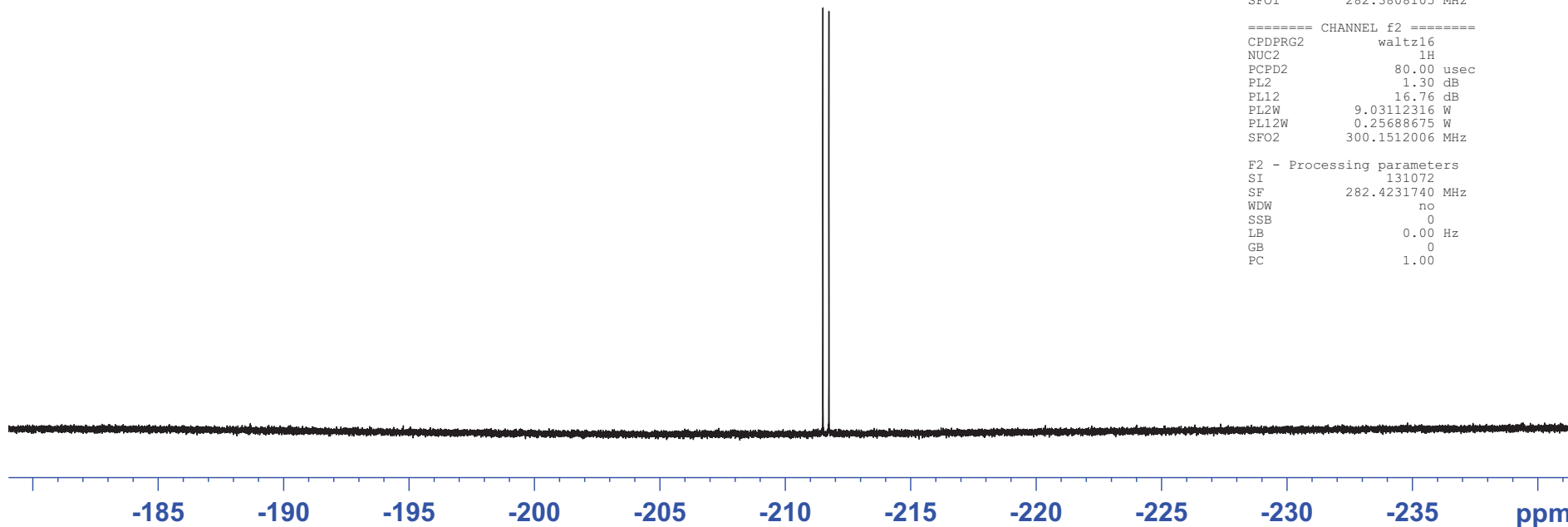
Current Data Parameters
 NAME deb_SEL(T)
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111012
 Time 11.30
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 131072
 SOLVENT CDCl3
 NS 64
 DS 4
 SWH 75187.969 Hz
 FIDRES 0.573639 Hz
 AQ 0.8716788 sec
 RG 4100
 DW 6.650 usec
 DE 6.50 usec
 TE 297.4 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

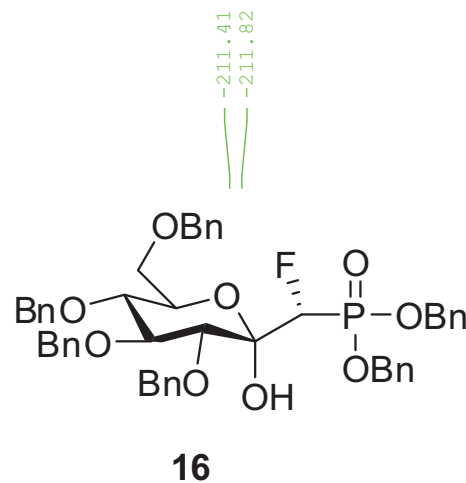
===== CHANNEL f1 =====
 NUC1 19F
 P1 14.00 usec
 PL1 -0.50 dB
 PL1W 8.73698711 W
 SFO1 282.3808105 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.30 dB
 PL12 16.76 dB
 PL2W 9.03112316 W
 PL12W 0.25688675 W
 SFO2 300.1512006 MHz

F2 - Processing parameters
 SI 131072
 SF 282.4231740 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



¹⁹F NMR

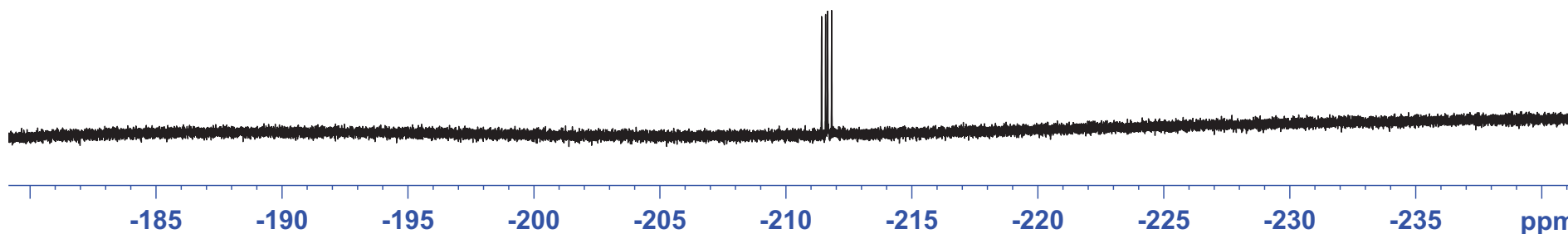
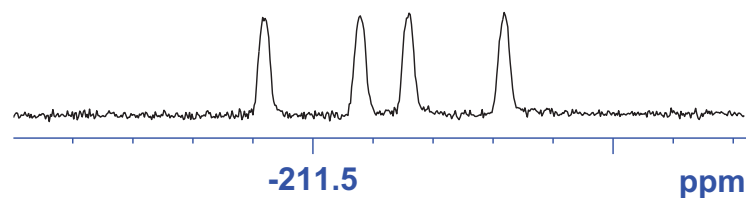


Current Data Parameters
NAME deb_SEL(T)
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111012
Time_ 11.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgflqn
TD 131072
SOLVENT CDC13
NS 64
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716788 sec
RG 1440
DW 6.650 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.00 usec
PL1 -0.50 dB
PL1W 8.73698711 W
SFO1 282.3808105 MHz

F2 - Processing parameters
SI 131072
SF 282.4231740 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



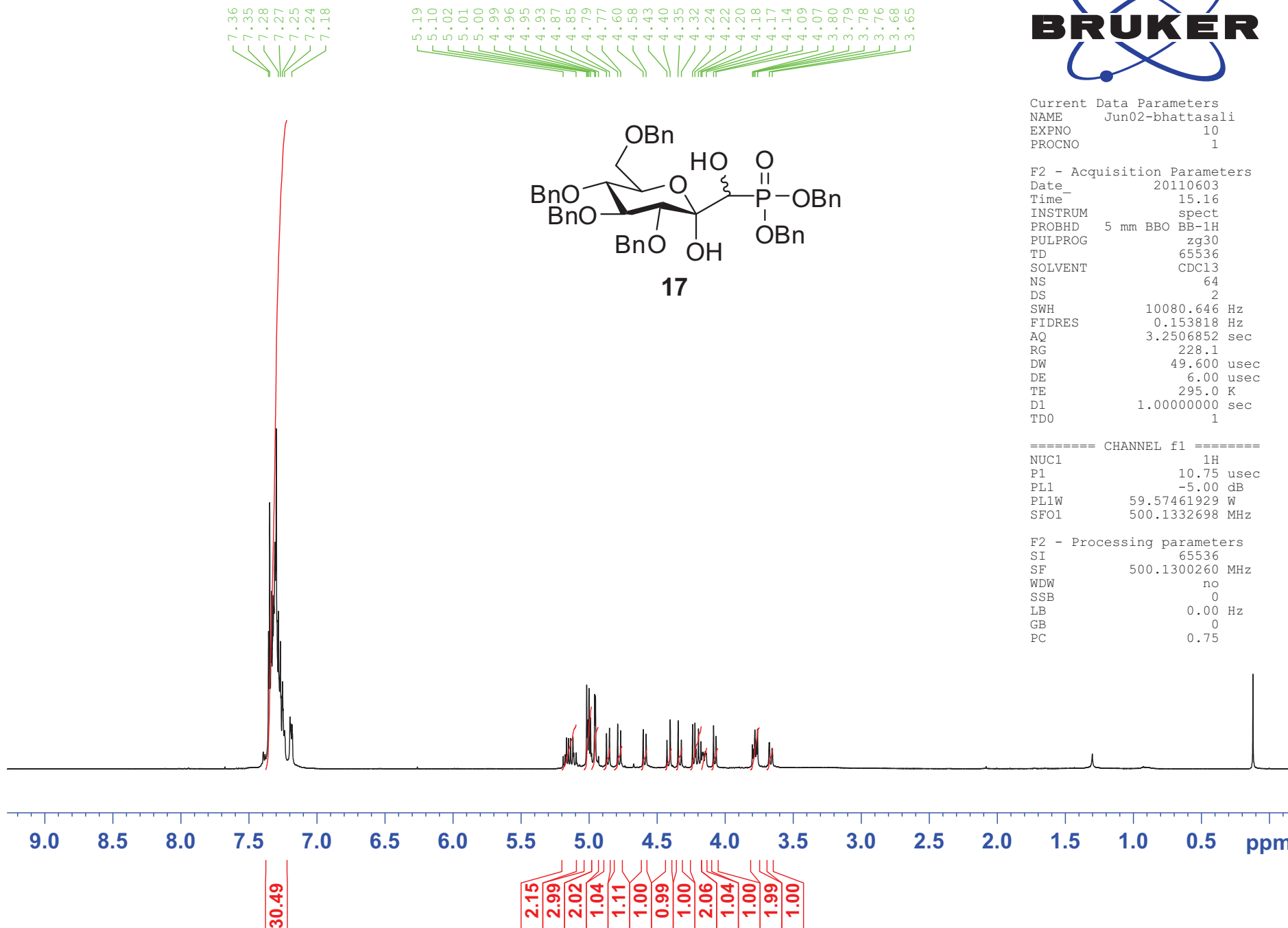
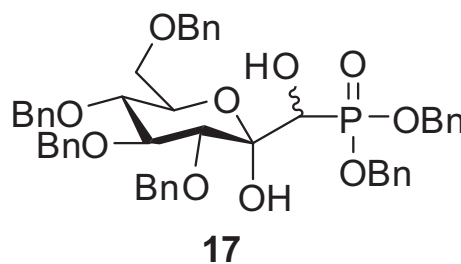


Current Data Parameters
NAME Jun02-bhattasali
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110603
Time_ 15.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 64
DS 2
SWH 10080.646 Hz
FIDRES 0.153818 Hz
AQ 3.2506852 sec
RG 228.1
DW 49.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.75 usec
PL1 -5.00 dB
PL1W 59.57461929 W
SFO1 500.1332698 MHz

F2 - Processing parameters
SI 65536
SF 500.1300260 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.75





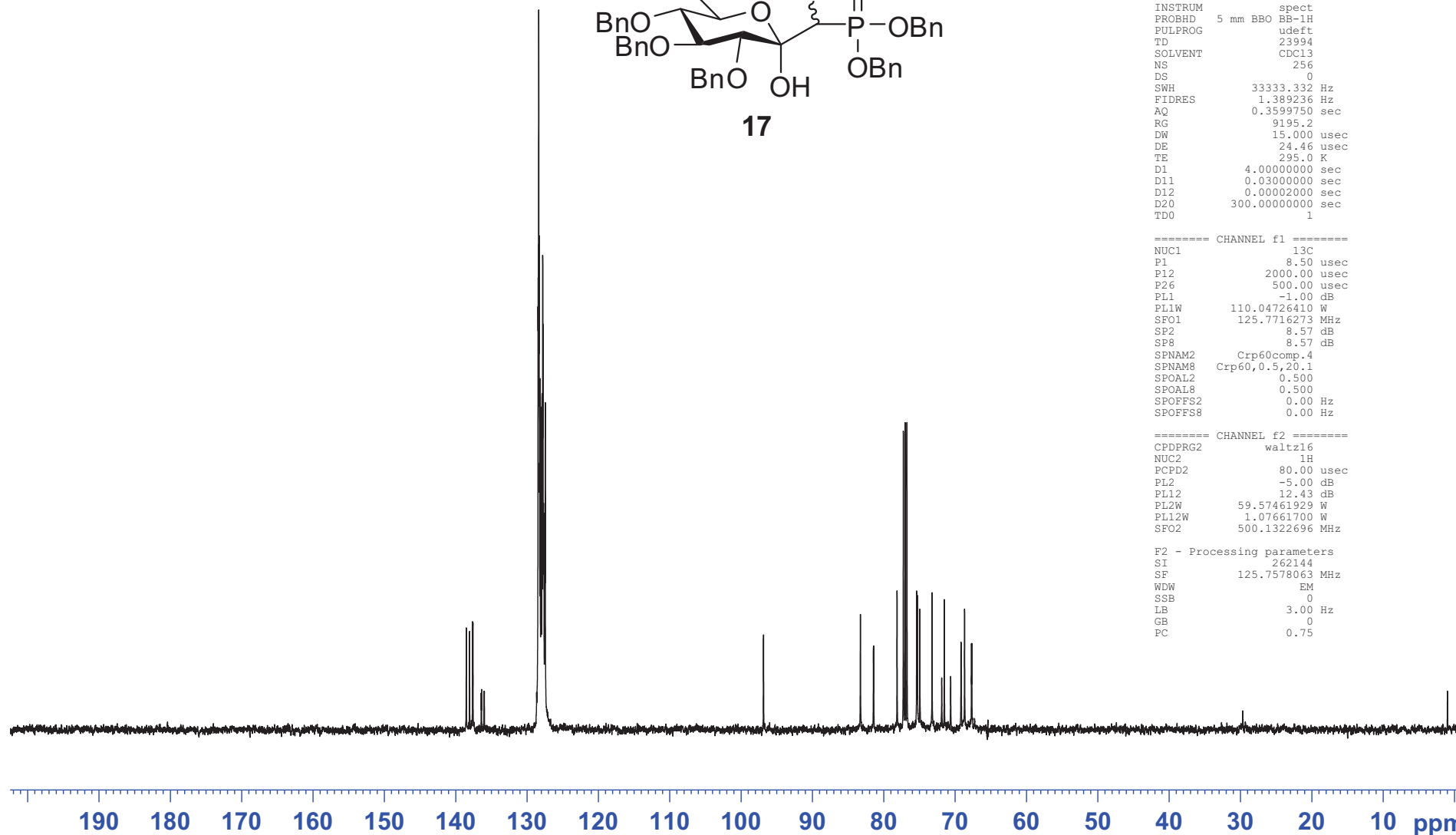
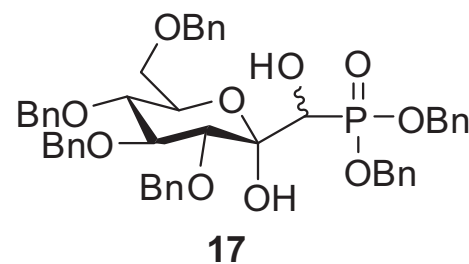
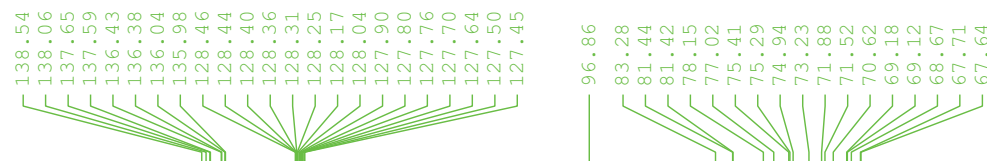
Current Data Parameters
NAME Jun02-bhattasali
EXPNO 12
PROCNO 1

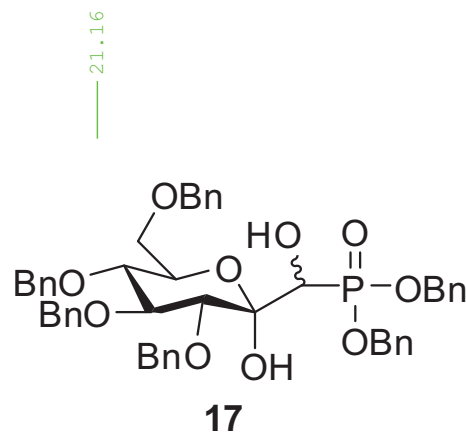
F2 - Acquisition Parameters
Date_ 20110605
Time 5.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG udeft
TD 23994
SOLVENT CDCl3
NS 256
DS 0
SWH 33333.332 Hz
FIDRES 1.389236 Hz
AQ 0.3599750 sec
RG 9195.2
DW 15.000 usec
DE 24.46 usec
TE 295.0 K
D1 4.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D20 300.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
P12 2000.00 usec
P26 500.00 usec
PL1 -1.00 dB
PL1W 110.04726410 W
SFO1 125.7716273 MHz
SP2 8.57 dB
SP8 8.57 dB
SPNAM2 Crp60comp.4
SPNAM8 Crp60,0.5,20.1
SPOAL2 0.500
SPOAL8 0.500
SPOFFS2 0.00 Hz
SPOFFS8 0.00 Hz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 262144
SF 125.7578063 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.75





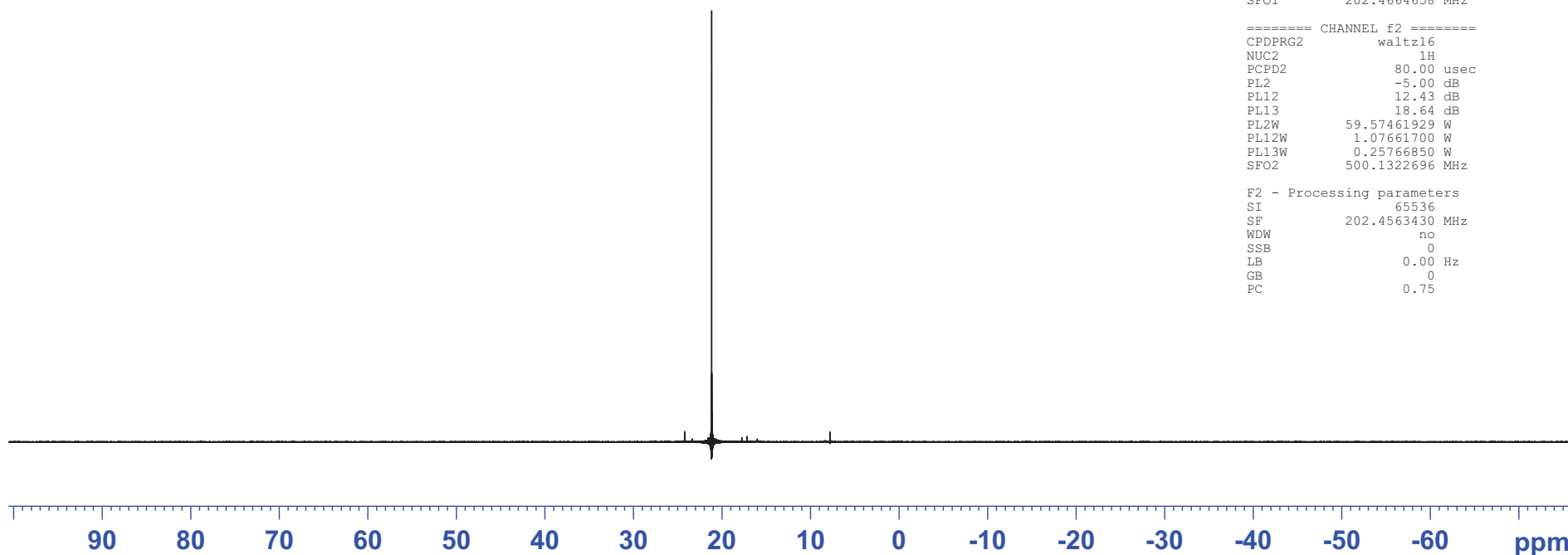
Current Data Parameters
NAME Jun02-bhattachali
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110603
Time 15.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 -1.00 dB
PL1W 102.77402496 W
SFO1 202.4664658 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 202.4563430 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.75



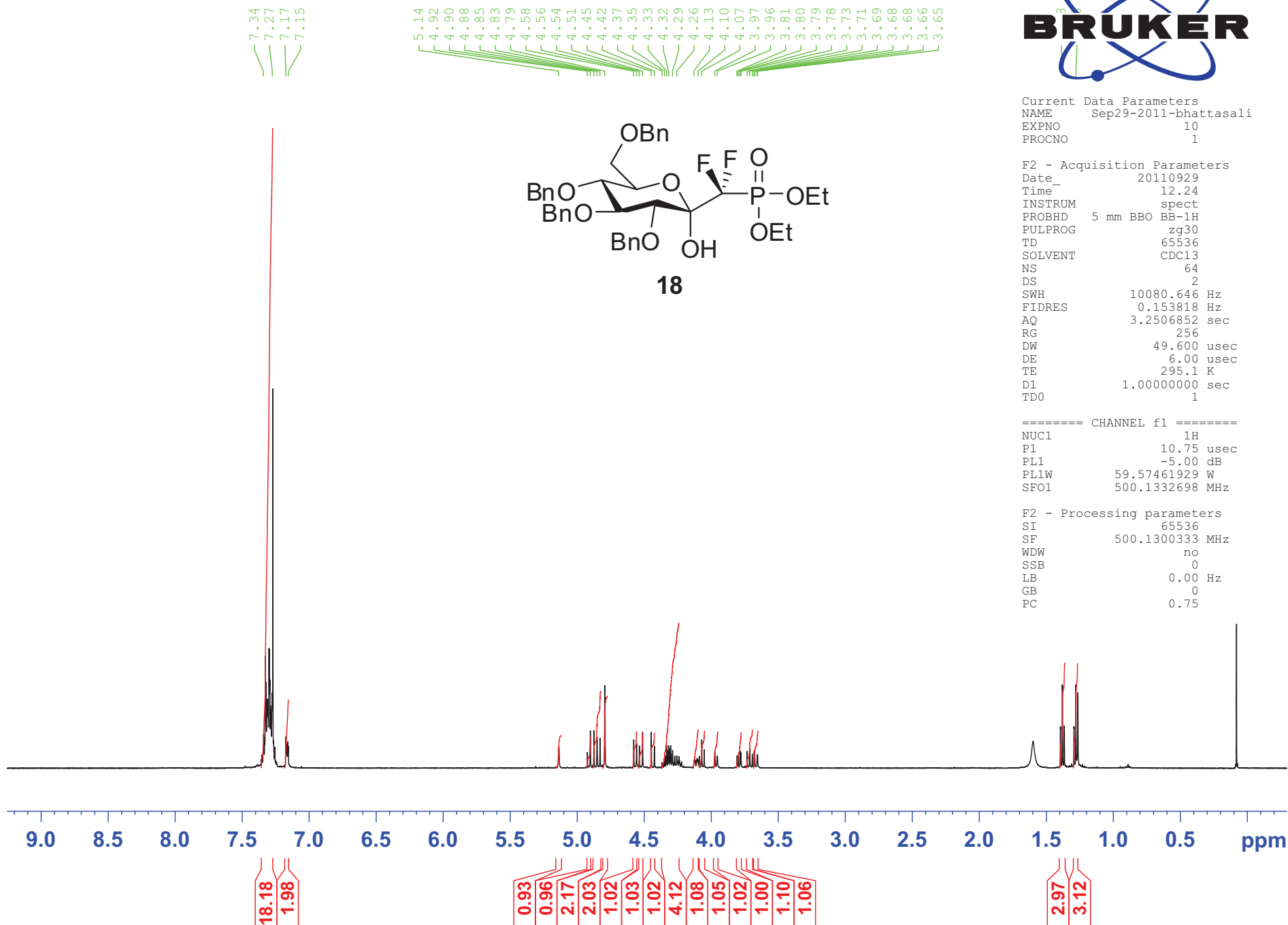
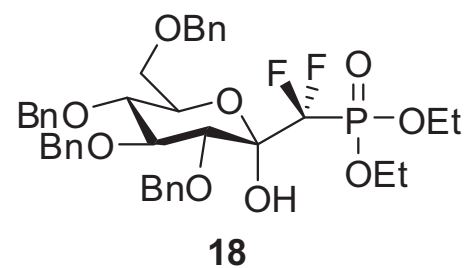


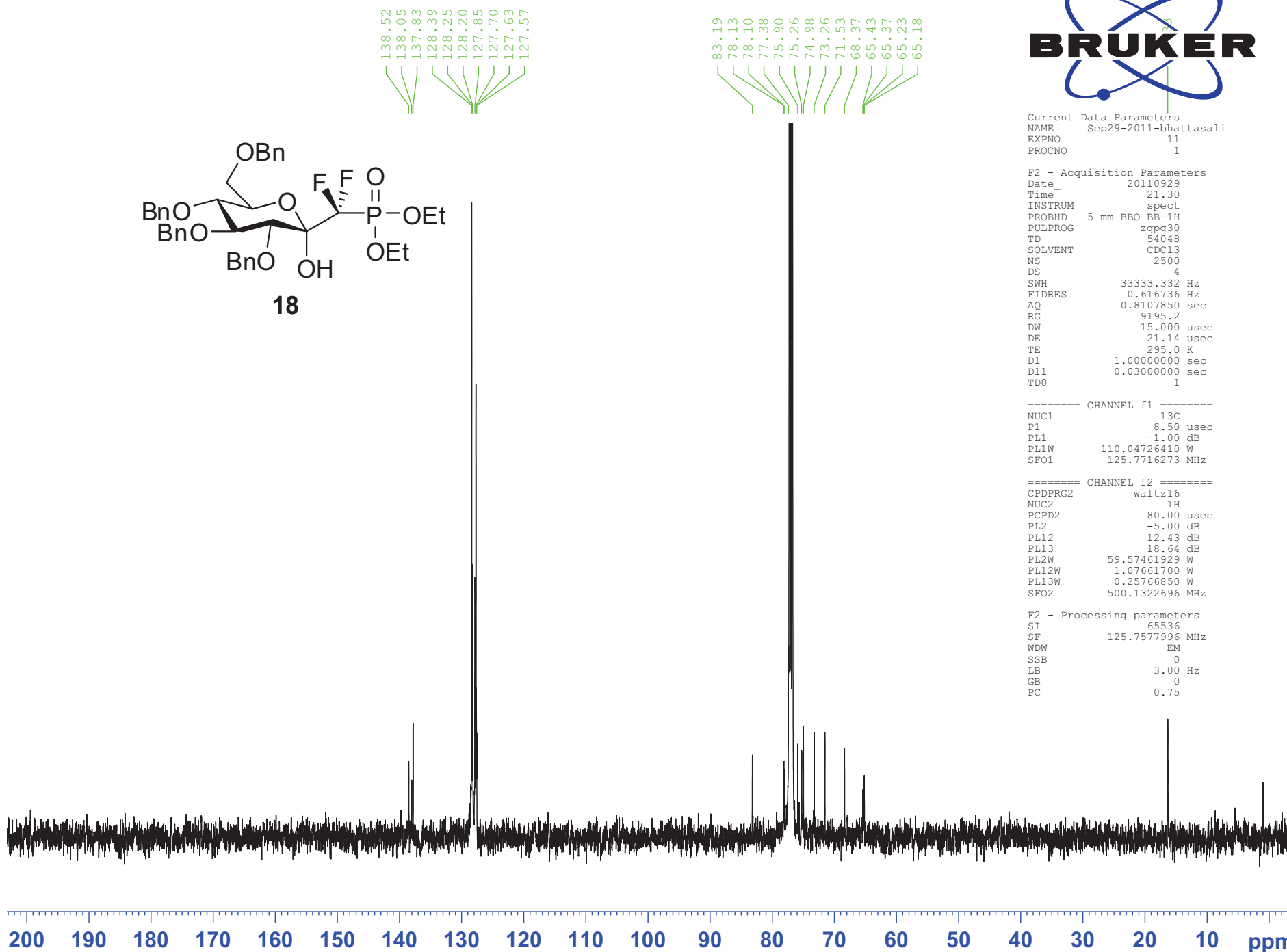
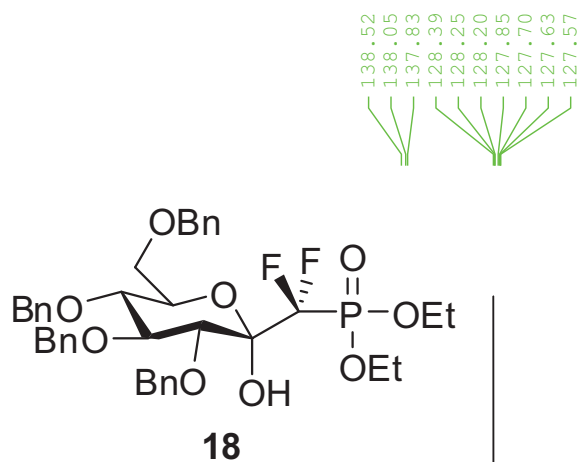
Current Data Parameters
NAME Sep29-2011-bhattasali
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110929
Time 12.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 10080.646 Hz
FIDRES 0.153818 Hz
AQ 3.2506852 sec
RG 256
DW 49.600 usec
DE 6.00 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.75 usec
PL1 -5.00 dB
PL1W 59.57461929 W
SFO1 500.1332698 MHz

F2 - Processing parameters
SI 65536
SF 500.1300333 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.75





Current Data Parameters
NAME Sep29-2011-bhattachali
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110929
Time_ 21.30
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 54048
SOLVENT CDCl3
NS 2500
DS 4
SWH 33333.332 Hz
FIDRES 0.616736 Hz
AQ 0.8107850 sec
RG 9195.2
DW 15.000 usec
DE 21.14 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -1.00 dB
PL1W 110.04726410 W
SFO1 125.7716273 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 125.7577996 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.75



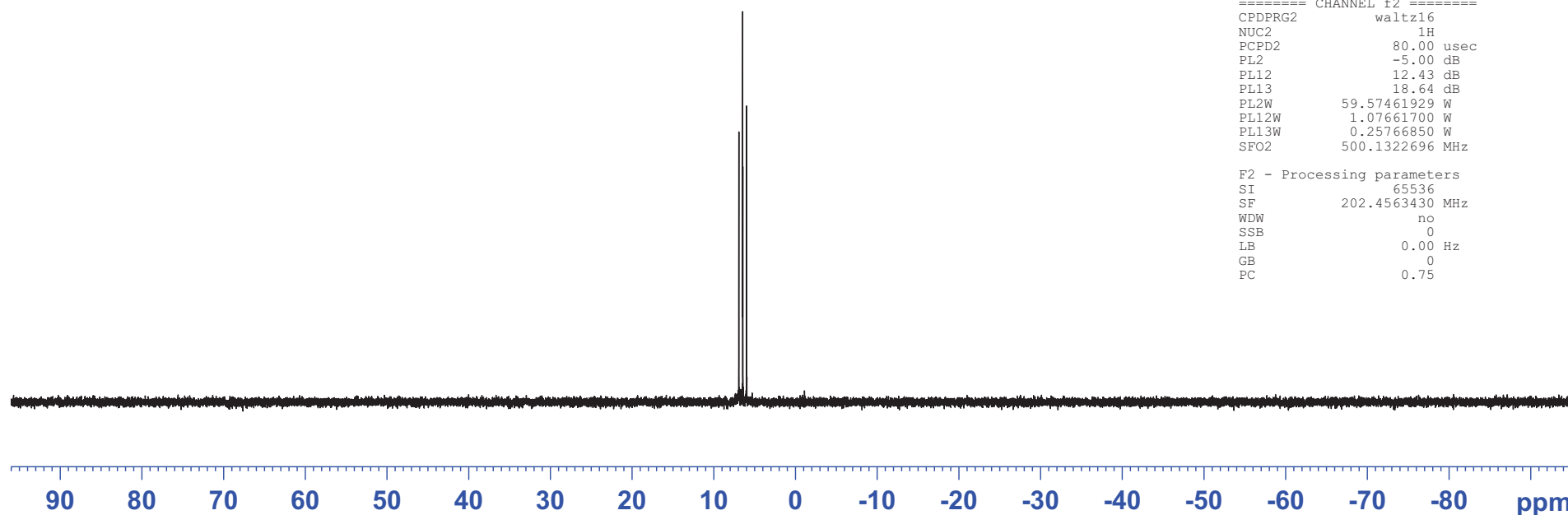
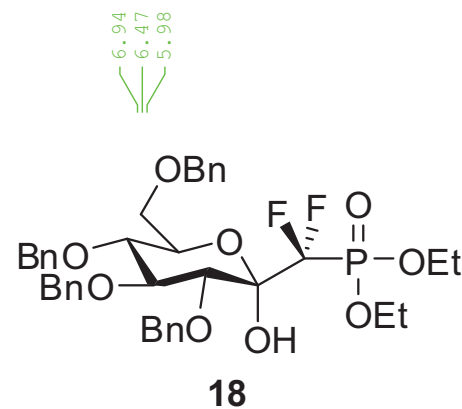
Current Data Parameters
NAME Sep29-2011-bhattasali
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110930
Time_ 1.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 295.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 2

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 -1.00 dB
PL1W 102.77402496 W
SFO1 202.4664658 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 202.4563430 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.75



-119.65
-119.73
-119.99
-120.08



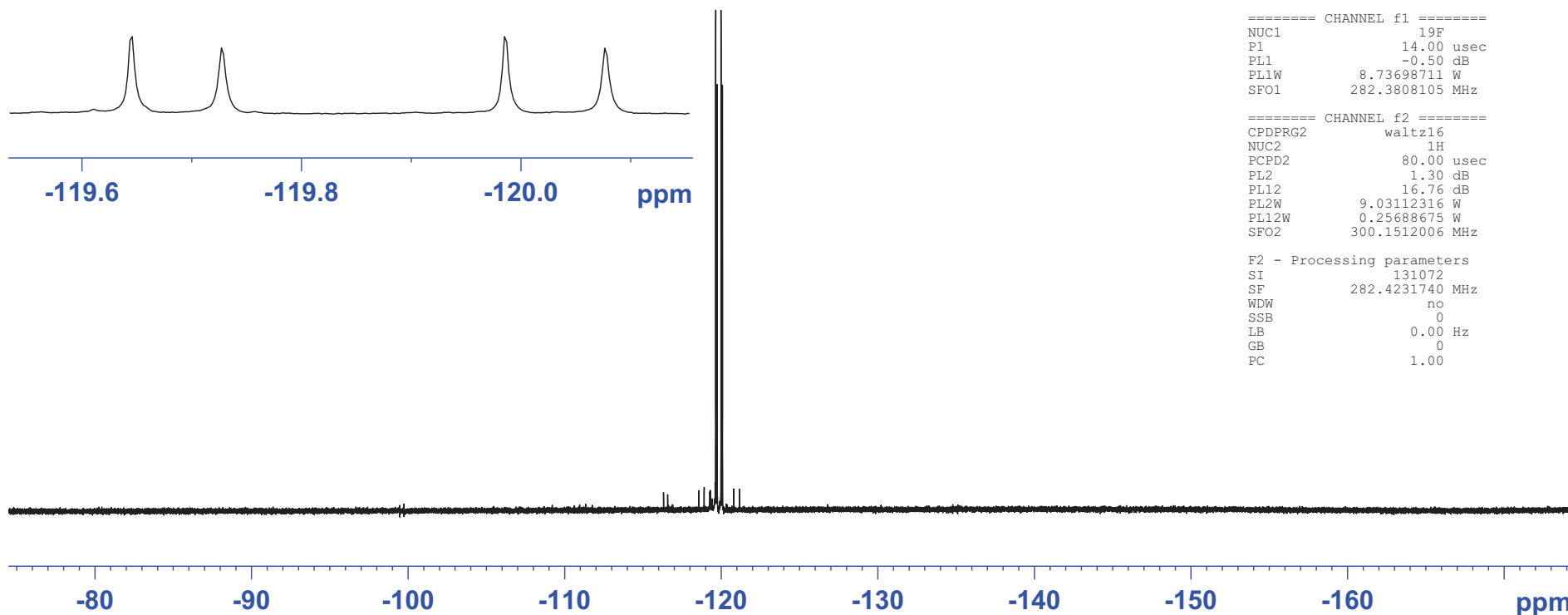
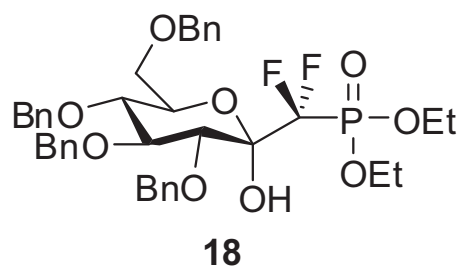
Current Data Parameters
NAME debdifluoro_column 2
EXPNO 1
PROCNO 1

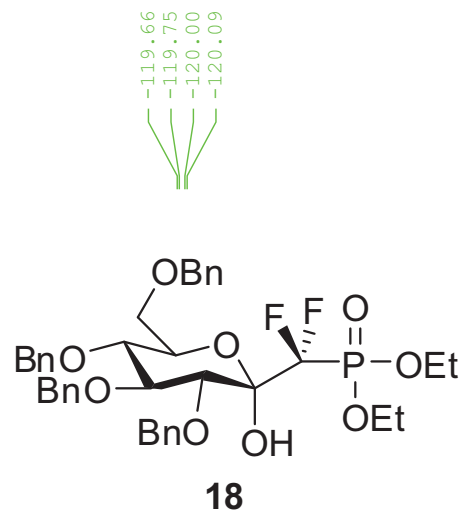
F2 - Acquisition Parameters
Date_ 20110914
Time_ 15.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhiggn
TD 131072
SOLVENT CDCl3
NS 32
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716788 sec
RG 4100
DW 6.650 usec
DE 6.50 usec
TE 305.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.00 usec
PL1 -0.50 dB
PL1W 8.73698711 W
SFO1 282.3808105 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.76 dB
PL2W 9.03112316 W
PL12W 0.25688675 W
SFO2 300.1512006 MHz

F2 - Processing parameters
SI 131072
SF 282.4231740 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



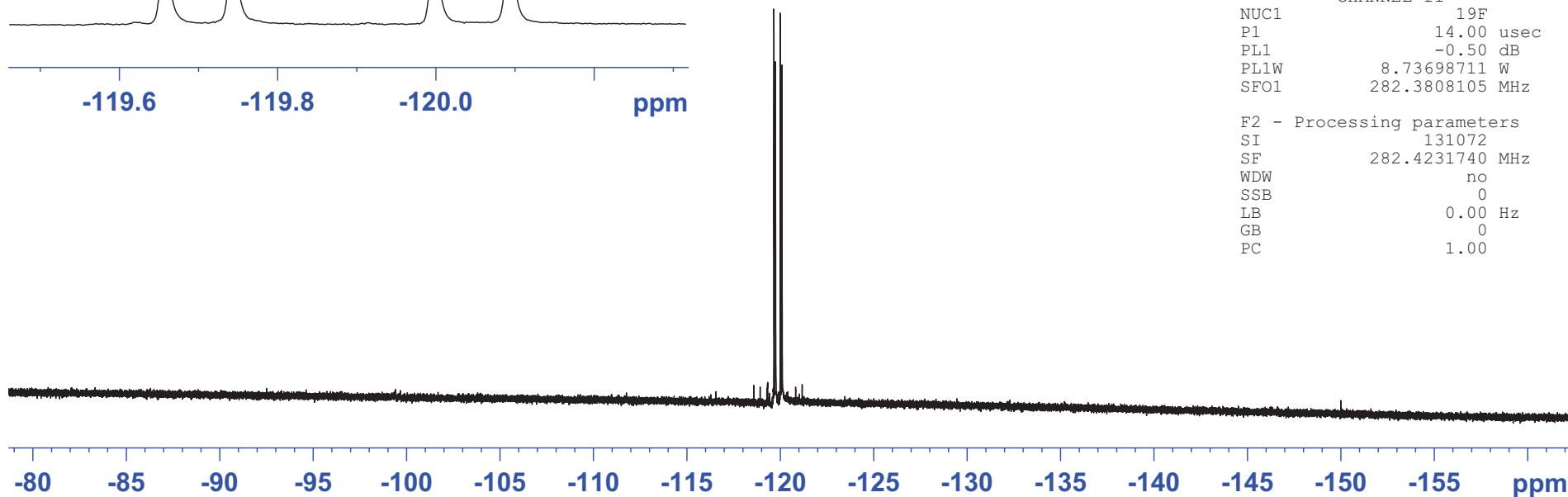
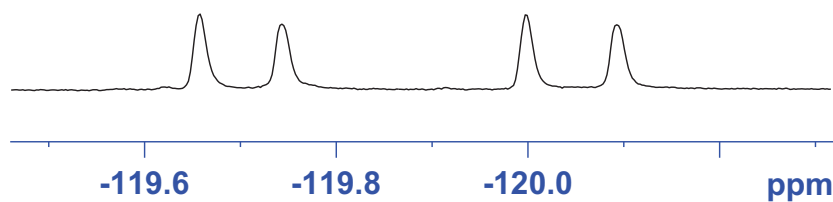


Current Data Parameters
NAME deb_difluoro_column 2
EXPNO 2
PROCNO 1

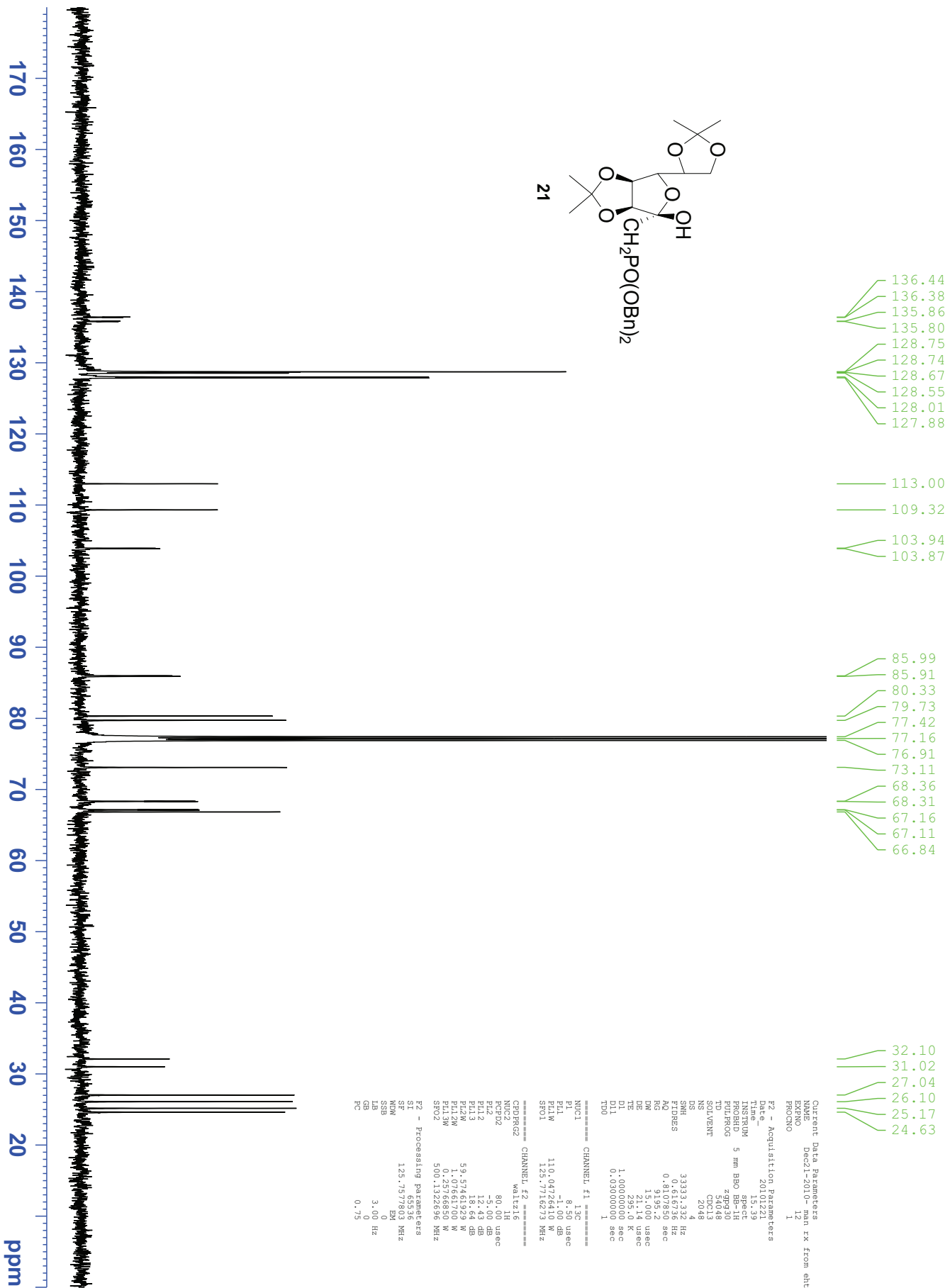
F2 - Acquisition Parameters
Date_ 20110914
Time_ 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 32
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716788 sec
RG 1440
DW 6.650 usec
DE 6.50 usec
TE 302.8 K
D1 1.00000000 sec
TD0 1

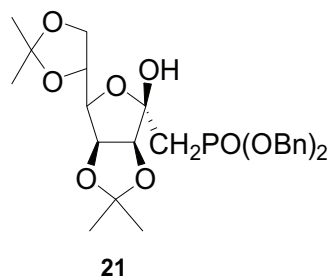
===== CHANNEL f1 =====
NUC1 19F
P1 14.00 usec
PL1 -0.50 dB
PL1W 8.73698711 W
SFO1 282.3808105 MHz

F2 - Processing parameters
SI 131072
SF 282.4231740 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00









29.67



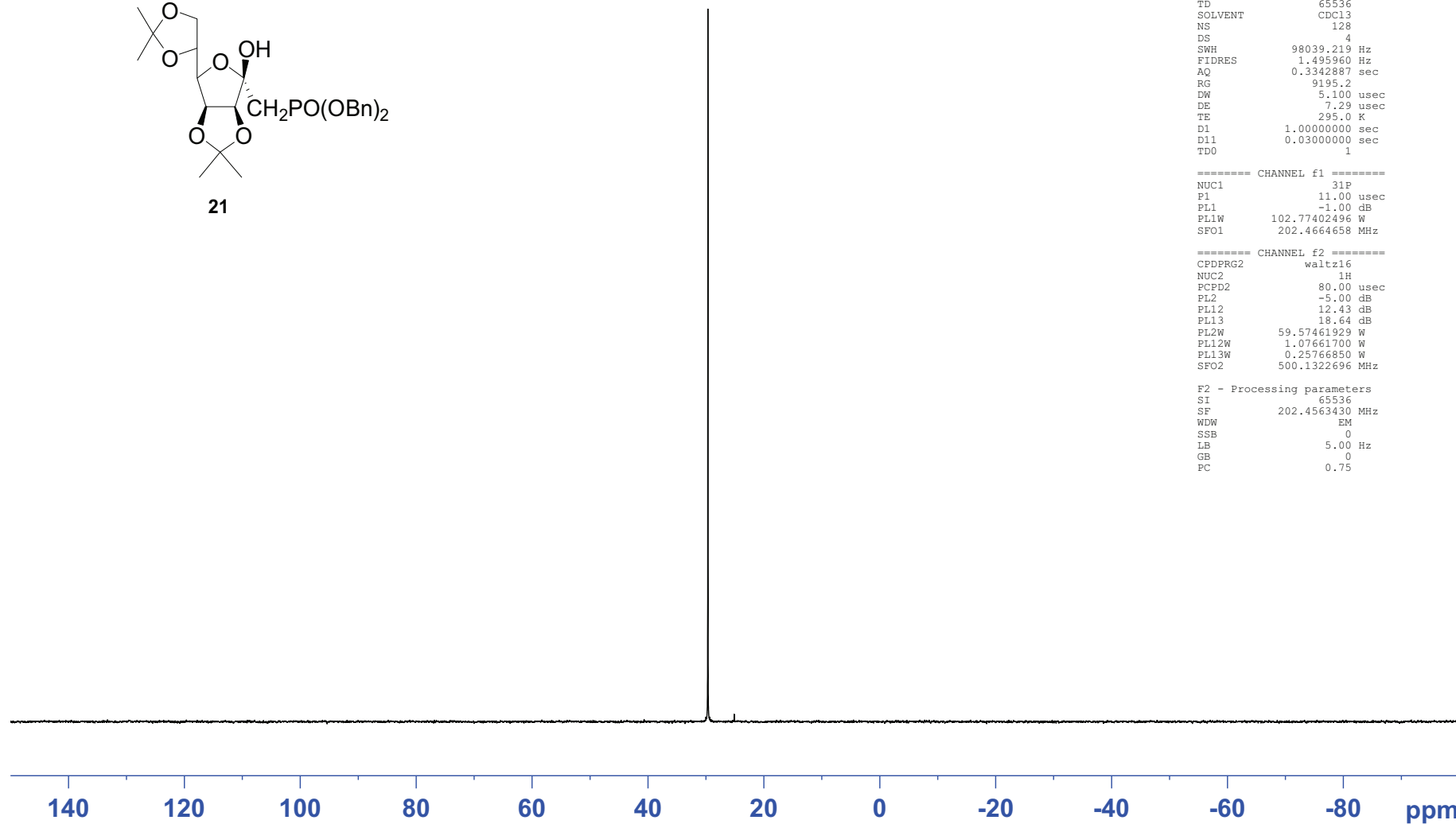
Current Data Parameters
NAME Dec21-2010- man rx from ehter hexanes
EXPNO 13
PROCNO 1

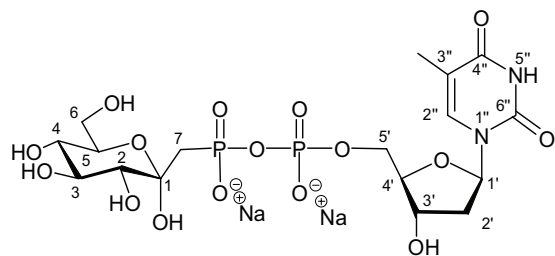
F2 - Acquisition Parameters
Date_ 20101221
Time 16.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 -1.00 dB
PL1W 102.77402496 W
SFO1 202.4664658 MHz

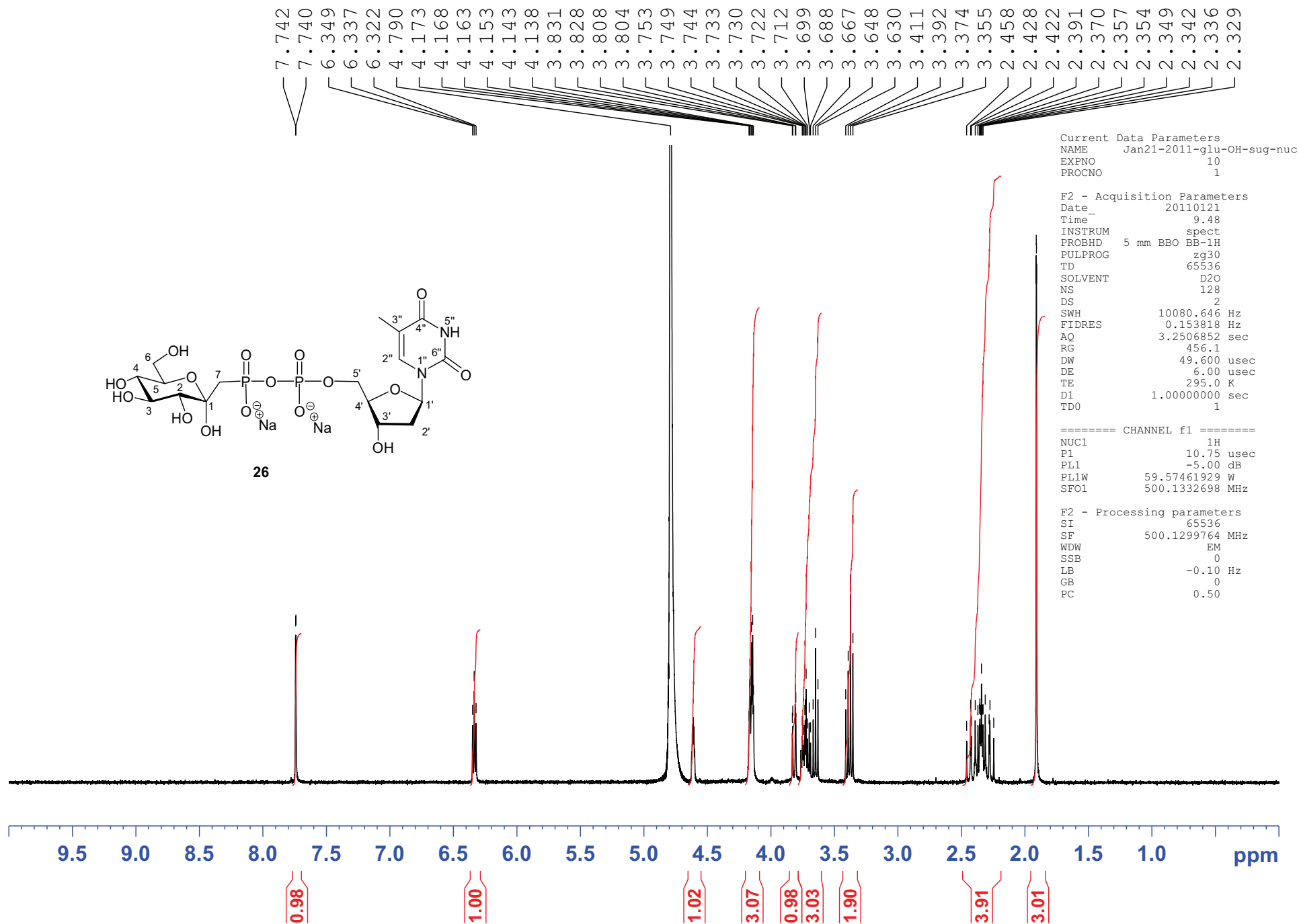
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 202.4563430 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 0.75





26





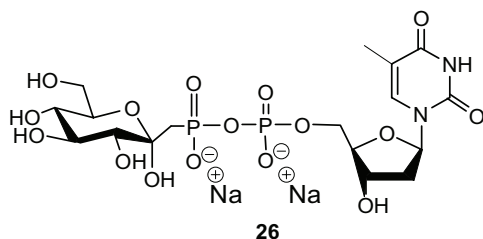
Current Data Parameters
NAME Jan21-2011-glu-OH-sug-nuc
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110121
Time 9.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 410
DS 4
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 -1.00 dB
PL1W 102.77402496 W
SFO1 202.4664658 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL13 18.64 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
PL13W 0.25766850 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 202.4563430 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 0.75

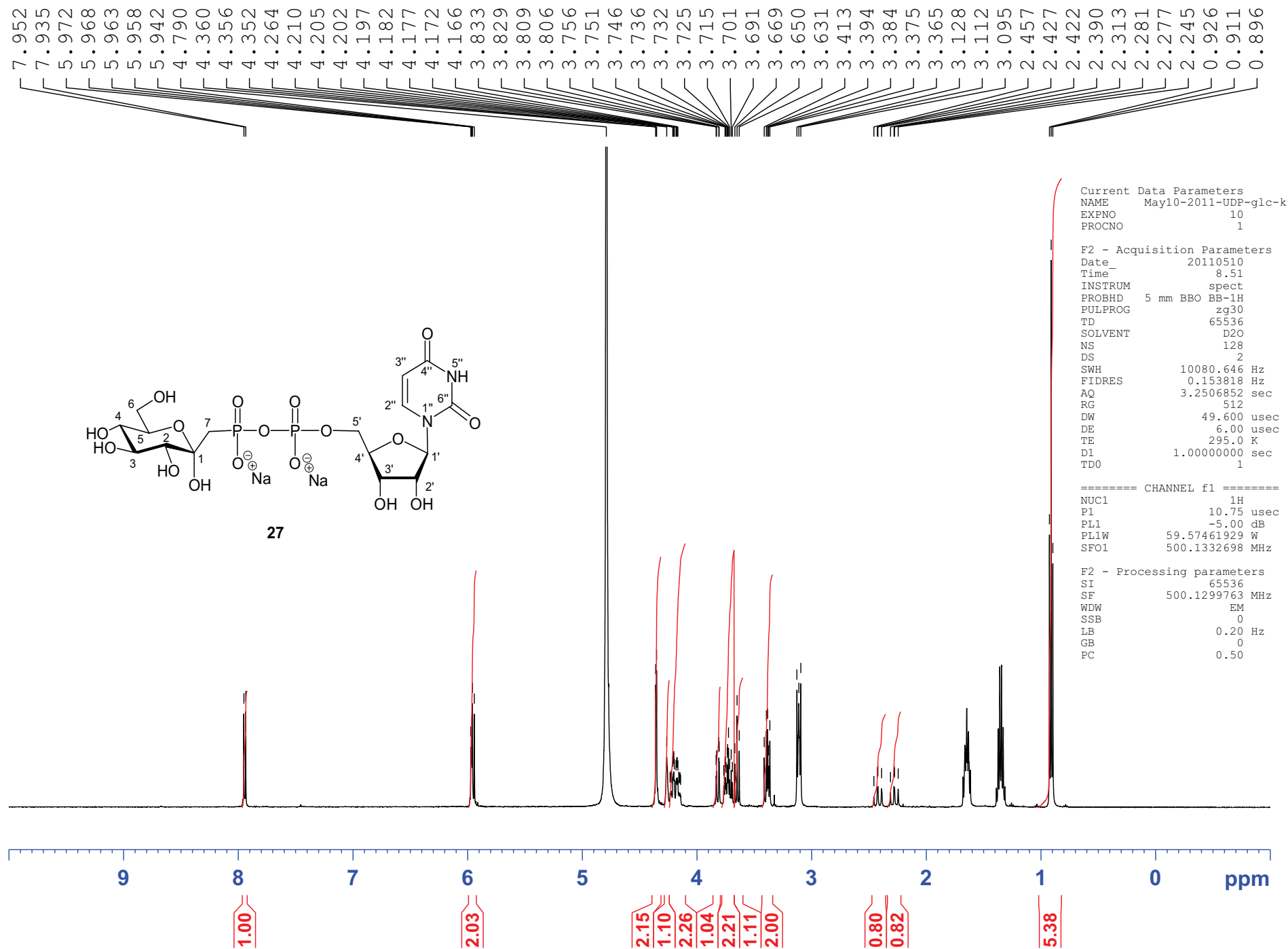


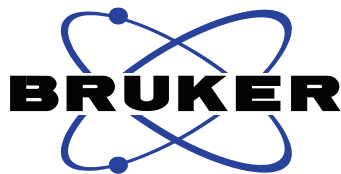
26

11.52
11.40
-11.77
-11.89



90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 ppm





Current Data Parameters
NAME May10-2011-UDP-glc-k
EXPNO 11
PROCNO 1

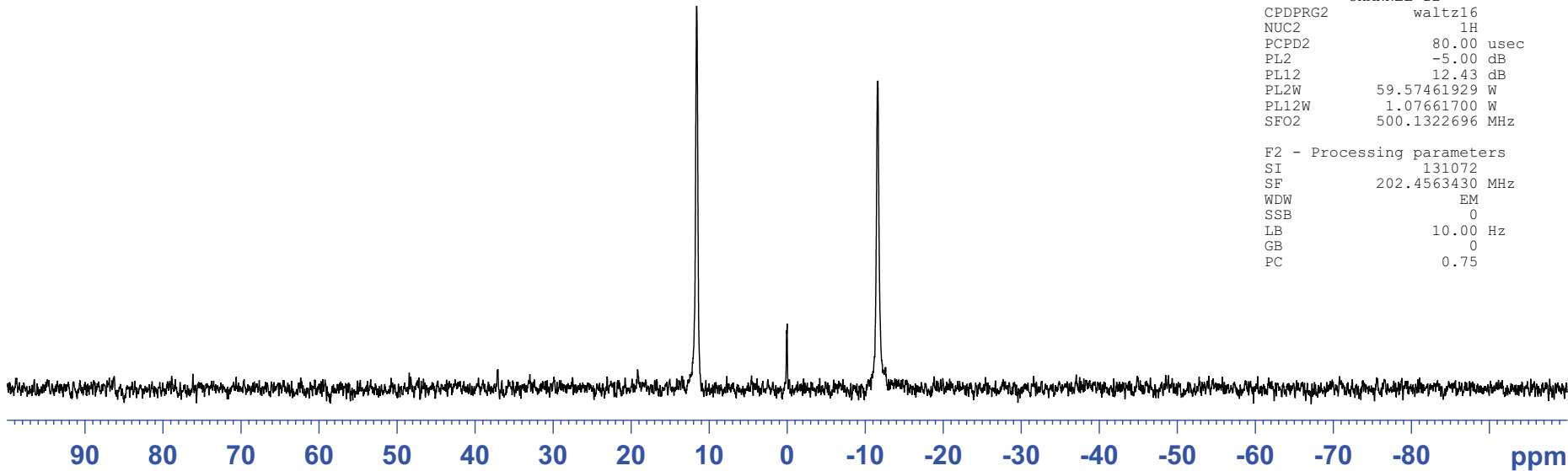
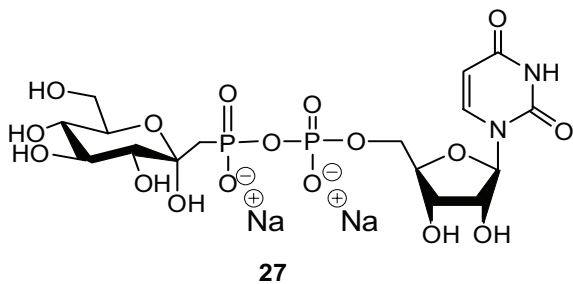
F2 - Acquisition Parameters
Date_ 20110510
Time 8.58
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 614
DS 2
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 2

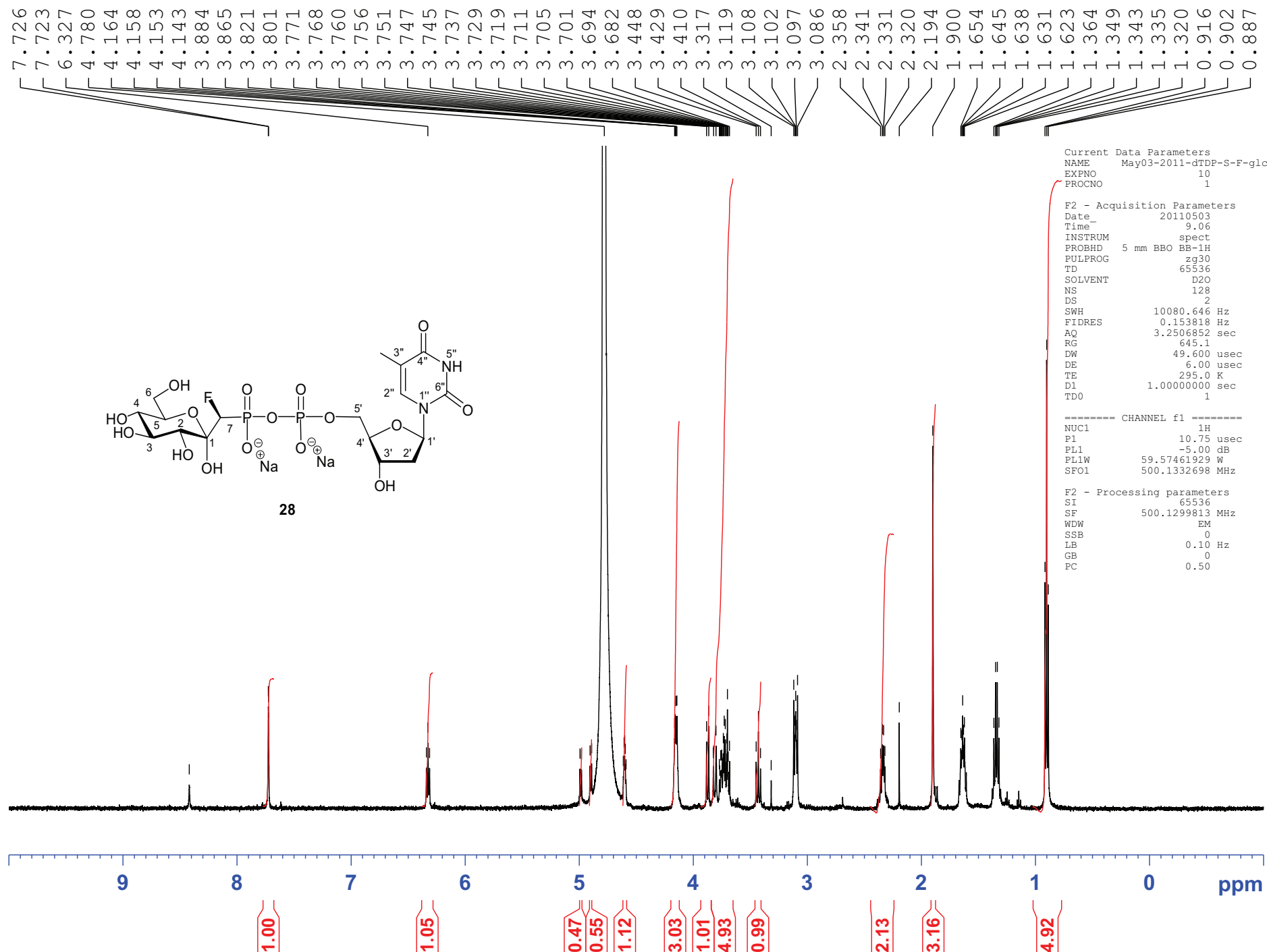
===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 -1.00 dB
PL1W 102.77402496 W
SFO1 202.4664652 MHz

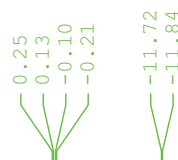
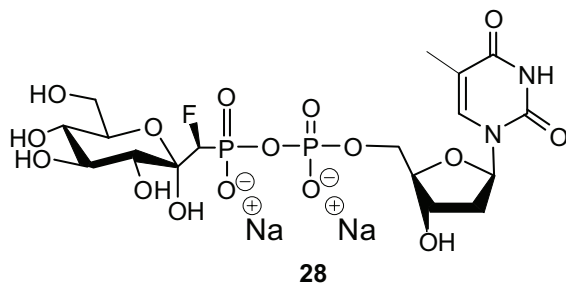
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 131072
SF 202.4563430 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 0.75

11.68
11.62
0.08
0.01
-11.58
-11.62







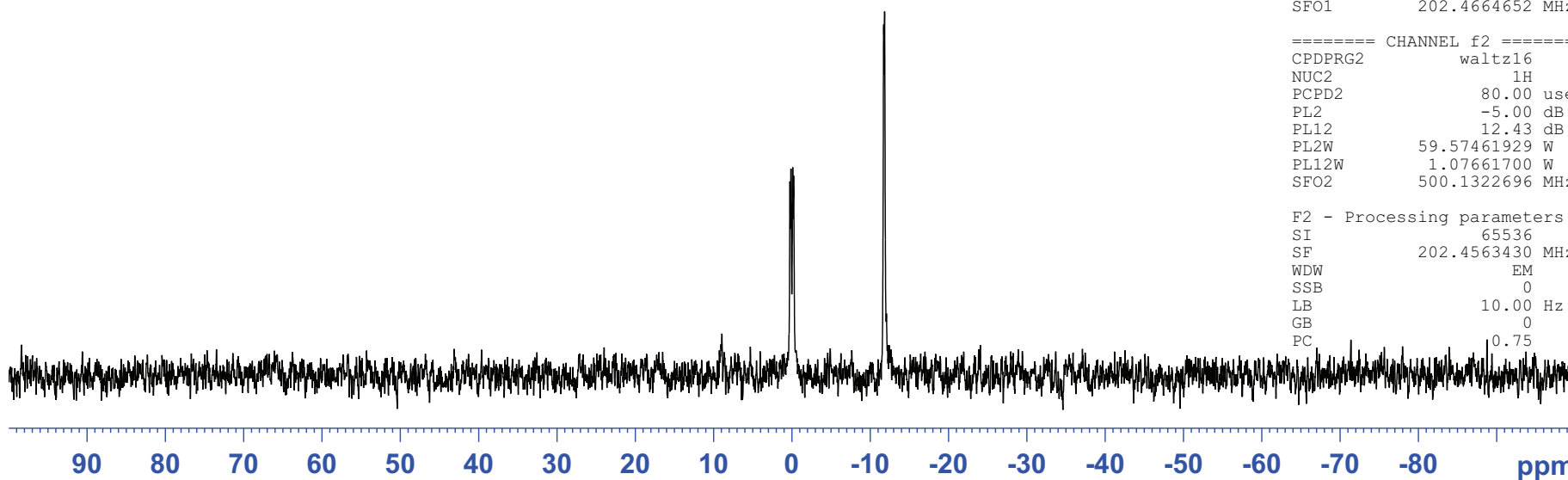
Current Data Parameters
NAME May03-2011-dTDP-S-F-glc
EXPNO 11
PROCNO 1

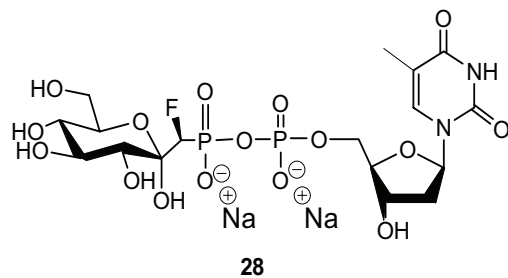
F2 - Acquisition Parameters
Date_ 20110503
Time_ 9.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 819
DS 2
SWH 98039.219 Hz
FIDRES 1.495960 Hz
AQ 0.3342887 sec
RG 9195.2
DW 5.100 usec
DE 7.29 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 3

===== CHANNEL f1 =====
NUC1 31P
P1 11.00 usec
PL1 -1.00 dB
PL1W 102.77402496 W
SFO1 202.4664652 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 12.43 dB
PL2W 59.57461929 W
PL12W 1.07661700 W
SFO2 500.1322696 MHz

F2 - Processing parameters
SI 65536
SF 202.4563430 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 0.75





-217.22
-217.48

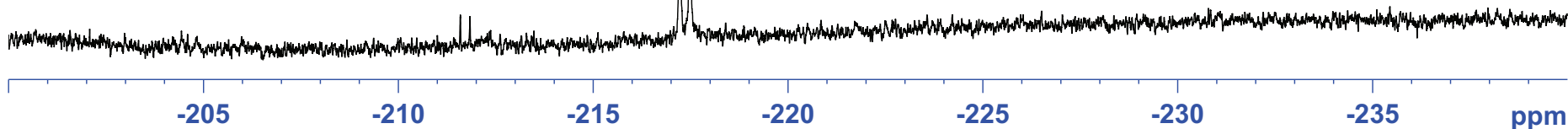
Current Data Parameters
 NAME dTDP-S-F-glc-19F
 EXPNO 1
 PROCNO 1

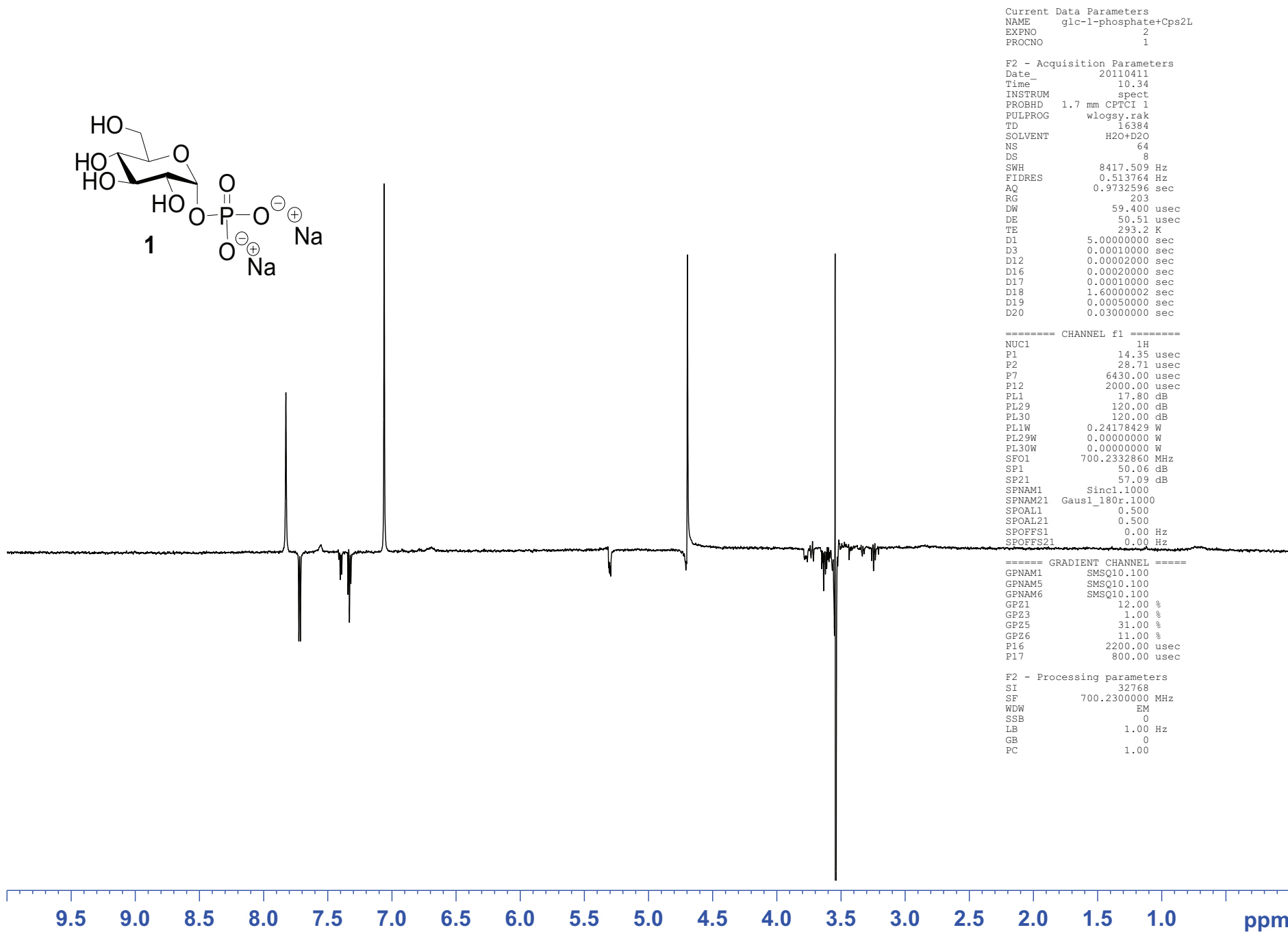
F2 - Acquisition Parameters
 Date_ 20110503
 Time_ 12.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgfhigqn
 TD 131072
 SOLVENT D2O
 NS 64
 DS 4
 SWH 70422.539 Hz
 FIDRES 0.537281 Hz
 AQ 0.9306612 sec
 RG 4100
 DW 7.100 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

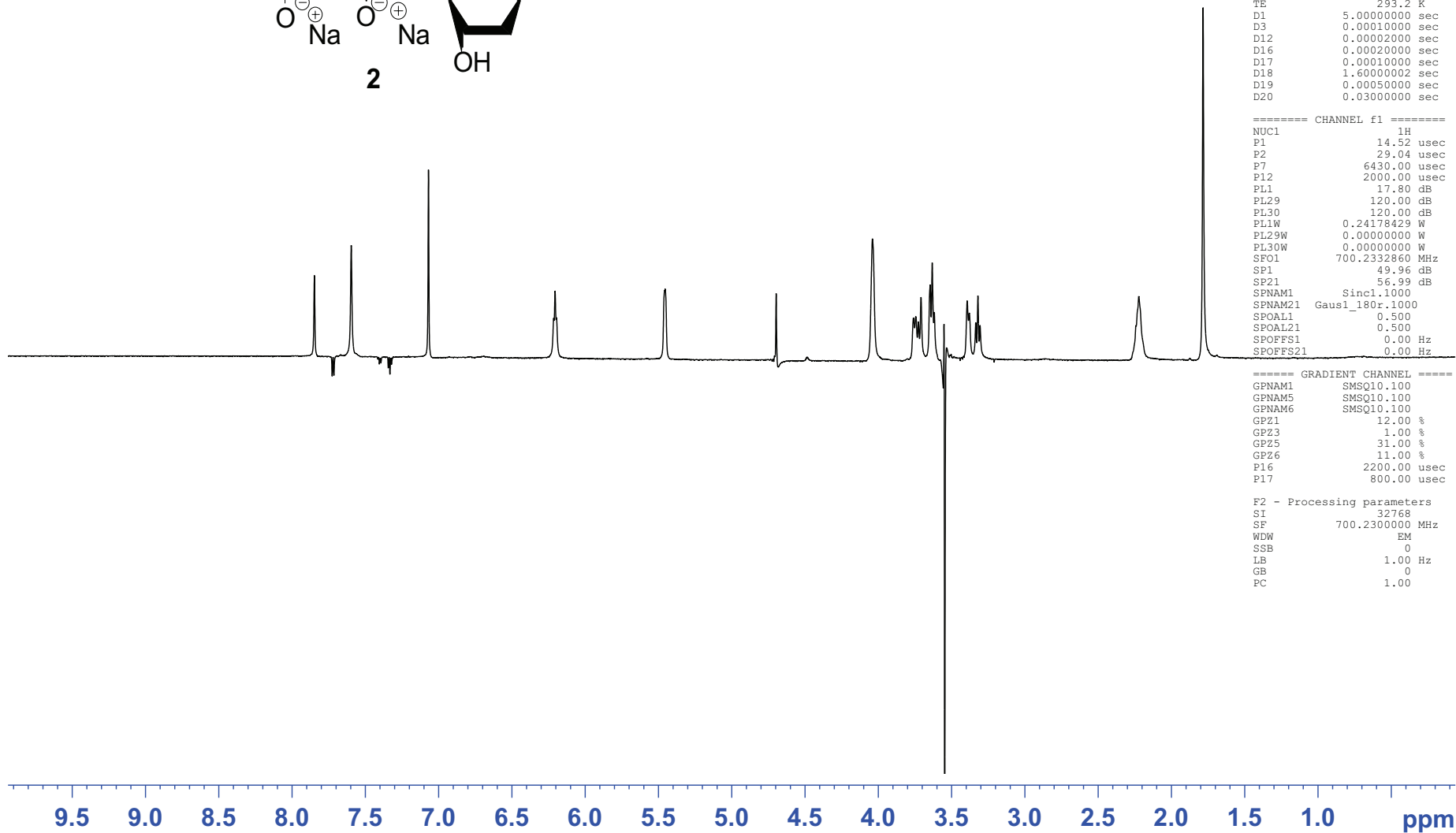
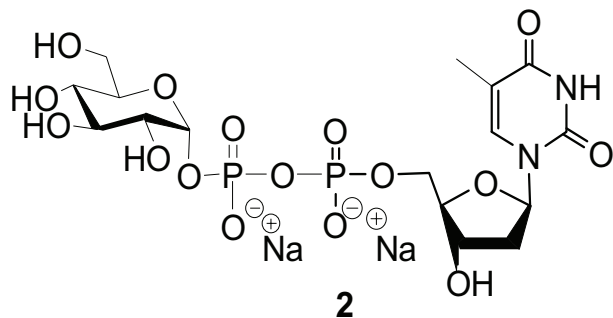
===== CHANNEL f1 =====
 NUC1 19F
 P1 14.00 usec
 PL1 -0.50 dB
 PL1W 8.73698711 W
 SFO1 282.3666894 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.30 dB
 PL12 16.76 dB
 PL2W 9.03112316 W
 PL12W 0.25688675 W
 SFO2 300.1512006 MHz

F2 - Processing parameters
 SI 131072
 SF 282.4231740 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00







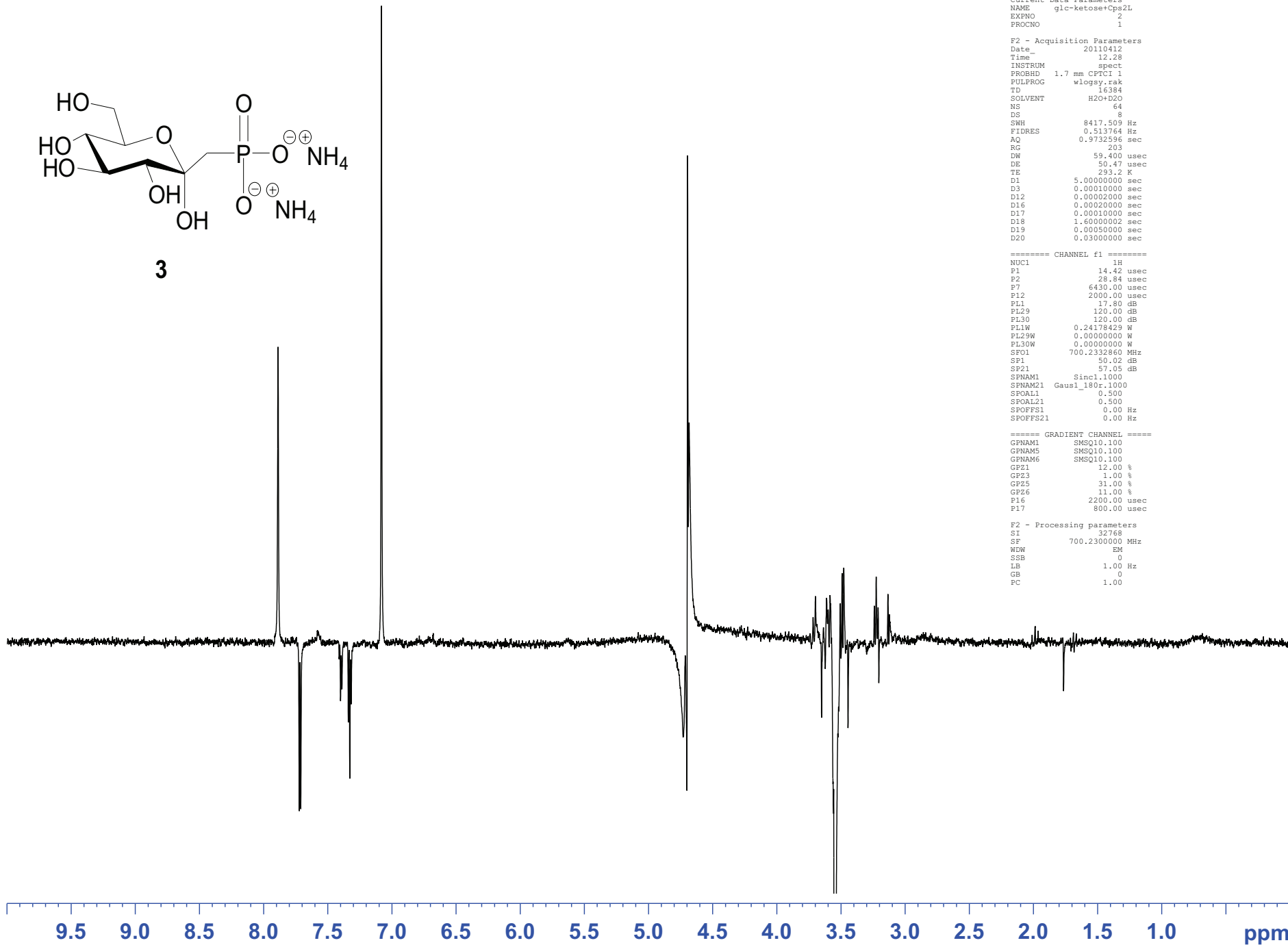
Current Data Parameters
NAME 2011_Apr12_dTDP-Glc_Cps2L
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110412
Time 14.37
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG wlogsy.rak
TD 16384
SOLVENT H2O+D2O
NS 64
DS 8
SWH 8417.509 Hz
FIDRES 0.513764 Hz
AQ 0.9732596 sec
RG 203
DW 59.400 usec
DE 50.40 usec
TE 293.2 K
D1 5.00000000 sec
D3 0.00010000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D17 0.00010000 sec
D18 1.60000002 sec
D19 0.00050000 sec
D20 0.03000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 14.52 usec
P2 29.04 usec
P7 6430.00 usec
P12 2000.00 usec
PL1 17.80 dB
PL29 120.00 dB
PL30 120.00 dB
PL1W 0.24178429 W
PL29W 0.00000000 W
PL30W 0.00000000 W
SFO1 700.2332860 MHz
SP1 49.96 dB
SP21 56.99 dB
SPNAM1 Sinc1.1000
SPNAM21 Gauss1.180r.1000
SPOAL1 0.500
SPOAL21 0.500
SPOFFS1 0.00 Hz
SPOFFS21 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM5 SMSQ10.100
GPNAM6 SMSQ10.100
GPZ1 12.00 %
GPZ3 1.00 %
GPZ5 31.00 %
GPZ6 11.00 %
P16 2200.00 usec
P17 800.00 usec

F2 - Processing parameters
SI 32768
SF 700.2300000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



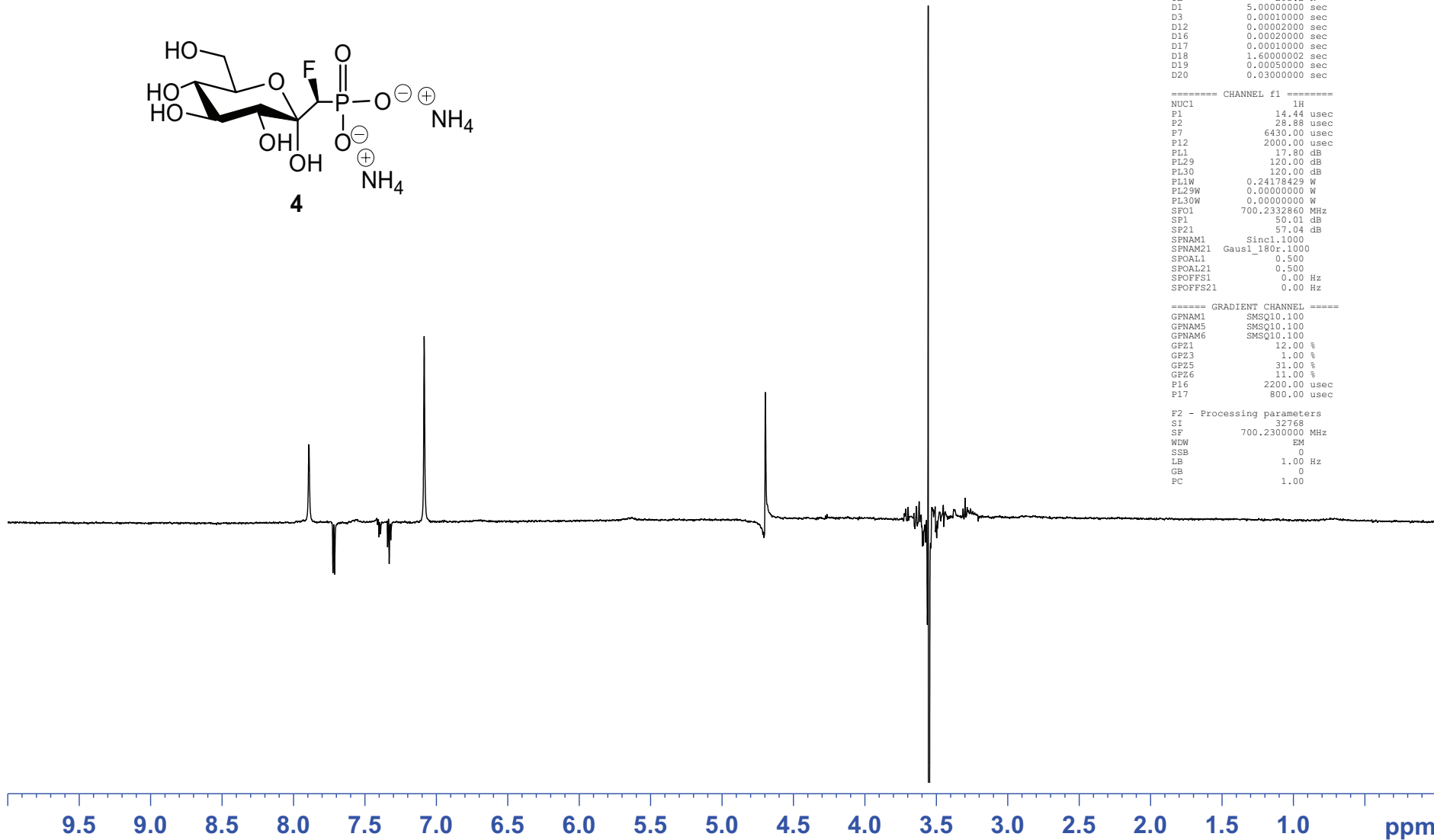
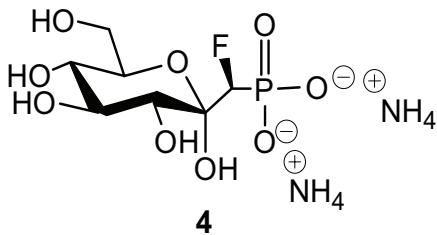
Current Data Parameters
NAME glc-ketose+Cps2L
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110412
Time 12.28
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG wlogsy.tak
TD 16384
SOLVENT H2O+D2O
NS 64
DS 8
SWH 8417.509 Hz
FIDRES 0.513764 Hz
AQ 0.9732596 sec
RG 203
DW 59.400 usec
DE 50.47 usec
TE 293.2 K
D1 5.00000000 sec
D3 0.00010000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D17 0.00010000 sec
D18 1.60000002 sec
D19 0.00050000 sec
D20 0.03000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 14.42 usec
P2 28.84 usec
P7 6430.00 usec
P12 2000.00 usec
PL1 17.80 dB
PL29 120.00 dB
PL30 120.00 dB
PL1W 0.24178429 W
PL29W 0.00000000 W
PL30W 0.00000000 W
SFO1 700.2332860 MHz
SP1 50.02 dB
SP21 57.05 dB
SPNAM1 Sinc1.1000
SPNAM21 Gaus1_180r.1000
SPOAL1 0.500
SPOAL21 0.500
SPOFFS1 0.00 Hz
SPOFFS21 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM5 SMSQ10.100
GPNAM6 SMSQ10.100
GP21 12.00 %
GP23 1.00 %
GP25 31.00 %
GP26 11.00 %
P16 2200.00 usec
P17 800.00 usec

F2 - Processing parameters
SI 32768
SF 700.2300000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



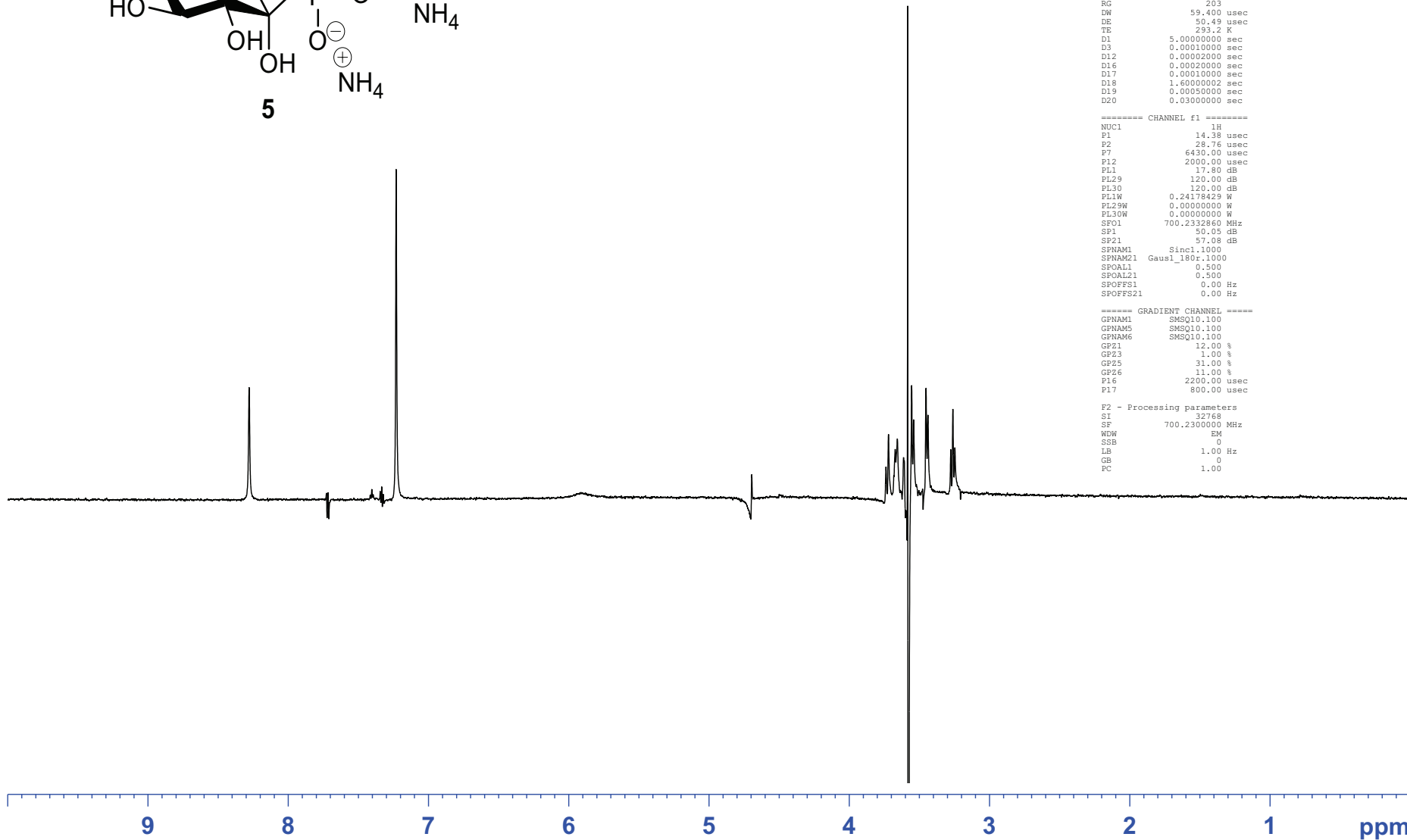
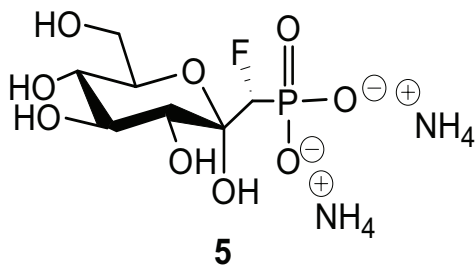
Current Data Parameters
NAME 5-F-glc-ketose-phosphonate+Cps2L
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110411
Time 11.00
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
FULPROG wlogsy.rak
TD 16384
SOLVENT H2O+D2O
NS 64
DS 8
SWH 8417.509 Hz
FIDRES 0.513764 Hz
AQ 0.9732596 sec
RG 203
DW 59.400 usec
DE 50.45 usec
TE 293.2 K
D1 5.00000000 sec
D3 0.00010000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D17 0.00010000 sec
D18 1.60000002 sec
D19 0.00050000 sec
D20 0.03000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 14.44 usec
P2 28.88 usec
P7 6430.00 usec
P12 2000.00 usec
PL1 17.80 dB
PL29 120.00 dB
PL30 120.00 dB
PL1W 0.24178429 W
PL29W 0.00000000 W
PL30W 0.00000000 W
SFO1 700.2332860 MHz
SF1 50.01 dB
SP21 57.04 dB
SPNAM1 Sinc1.1000
SPNAM21 Gaus1_180r.1000
SFOAL1 0.500
SFOAL21 0.500
SPOFFS1 0.00 Hz
SPOFFS21 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM5 SMSQ10.100
GPNAM6 SMSQ10.100
GPZ1 12.00 %
GPZ3 1.00 %
GPZ5 31.00 %
GPZ6 11.00 %
P16 2200.00 usec
P17 800.00 usec

F2 - Processing parameters
SI 32768
SF 700.2300000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



Current Data Parameters
NAME R-F-glc-ketose-phosphonate+Cps2L
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20110411
Time_ 11.20
INSTRUM spect
PROBHD 1.7 mm CPTC1
PULPROG wlogsy.rak
TD 16384
SOLVENT H2O+D2O
NS 64
DS 8
SWH 8417.509 Hz
FIDRES 0.513764 Hz
AQ 0.9732596 sec
RG 203
DW 59.400 usec
DE 50.49 usec
TE 293.2 K
D1 5.00000000 sec
D3 0.00010000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D17 0.00010000 sec
D18 1.60000002 sec
D19 0.00050000 sec
D20 0.03000000 sec

===== CHANNEL f1 =====

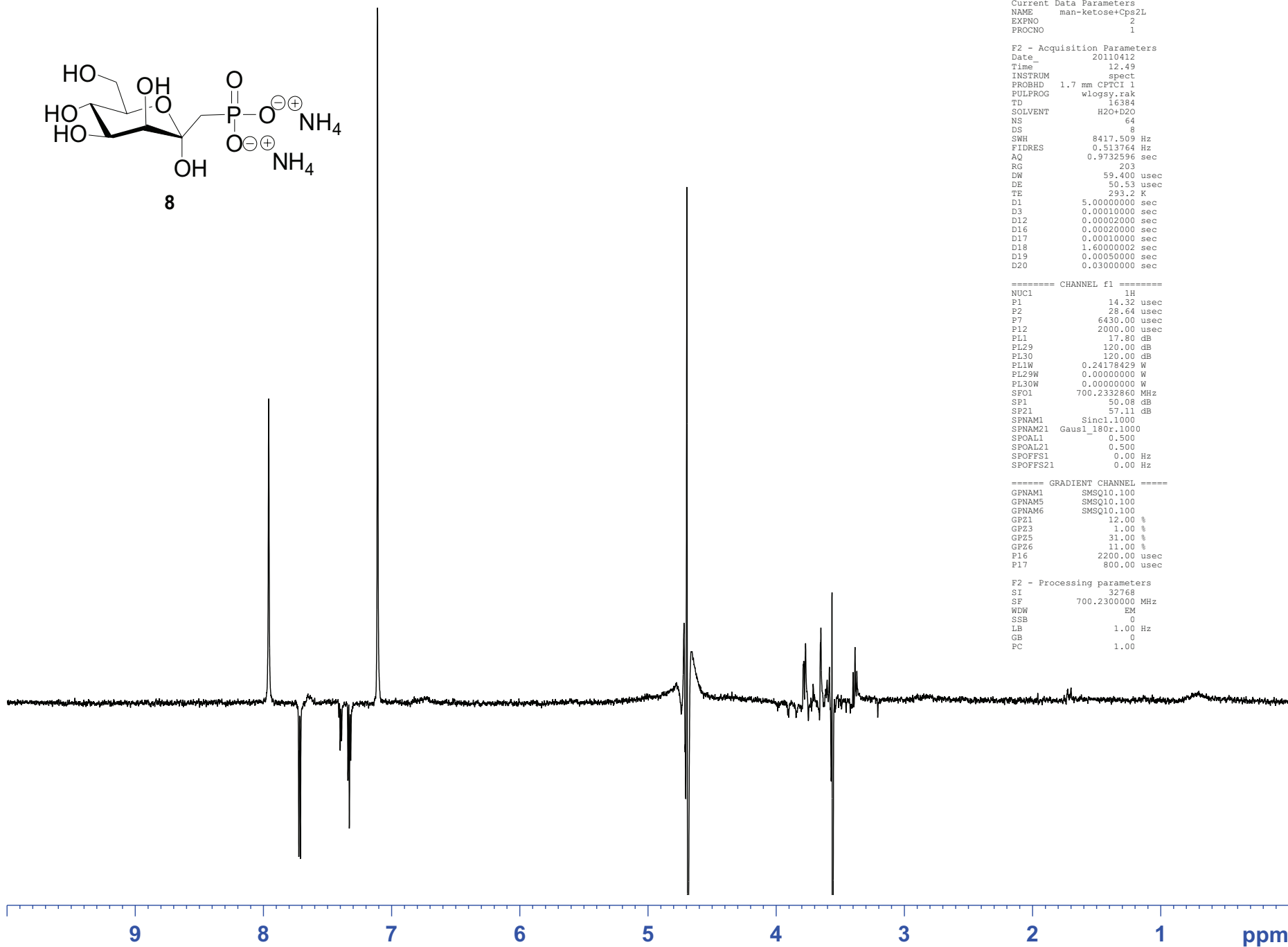
NUC1 1H
P1 14.38 usec
P2 28.76 usec
P7 6430.00 usec
P12 2000.00 usec
PL1 17.80 dB
PL29 120.00 dB
PL30 120.00 dB
PL1W 0.24178429 W
PL29W 0.00000000 W
PL30W 0.00000000 W
SFO1 700.2332860 MHz
SF1 50.05 dB
SF21 57.08 dB
SPNAM1 Sincl.1000
SPNAM21 Gaus1_180r.1000
SFOAL1 0.500
SFOAL21 0.500
SPOFFS1 0.00 Hz
SPOFFS21 0.00 Hz

===== GRADIENT CHANNEL =====

GPNAM1 SMSQ10.100
GPNAM5 SMSQ10.100
GPNAM6 SMSQ10.100
GP21 12.00 %
GP23 1.00 %
GP25 31.00 %
GP26 11.00 %
P16 2200.00 usec
P17 800.00 usec

F2 - Processing parameters

SI 32768
SF 700.2300000 MHz
WDW EW
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



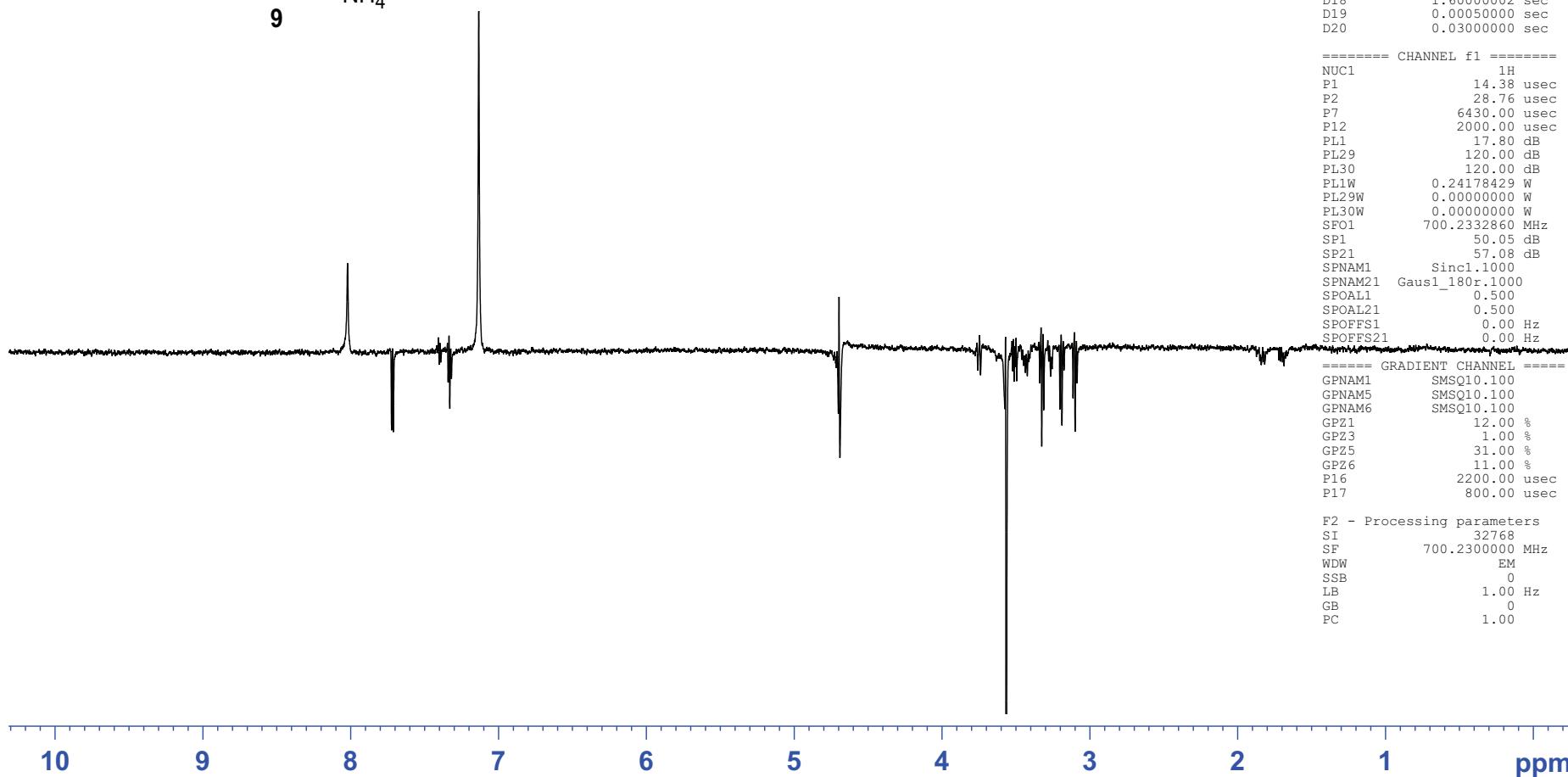
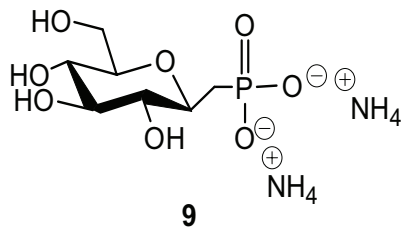
Current Data Parameters
NAME man-ketose+Cps2L
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110412
Time 12.49
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG wlogsy.rak
TD 16384
SOLVENT H2O+D2O
NS 64
DS 8
SWH 8417.509 Hz
FIDRES 0.513764 Hz
AQ 0.9732596 sec
RG 203
DW 59.400 usec
DE 50.53 usec
TE 293.2 K
D1 5.00000000 sec
D3 0.00010000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D17 0.00010000 sec
D18 1.60000002 sec
D19 0.00050000 sec
D20 0.03000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 14.32 usec
P2 28.64 usec
P7 6430.00 usec
P12 2000.00 usec
PL1 17.80 dB
PL29 120.00 dB
PL30 120.00 dB
PL1W 0.24178429 W
PL29W 0.00000000 W
PL30W 0.00000000 W
SF01 700.2332860 MHz
SP1 50.08 dB
SP21 57.11 dB
SPNAM1 Sinc1.1000
SPNAM21 Gaus1_180r.1000
SPOAL1 0.500
SPOAL21 0.500
SPOFFS1 0.00 Hz
SPOFFS21 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM5 SMSQ10.100
GPNAM6 SMSQ10.100
GPZ1 12.00 %
GPZ3 1.00 %
GPZ5 31.00 %
GPZ6 11.00 %
P16 2200.00 usec
P17 800.00 usec

F2 - Processing parameters
SI 32768
SF 700.2300000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



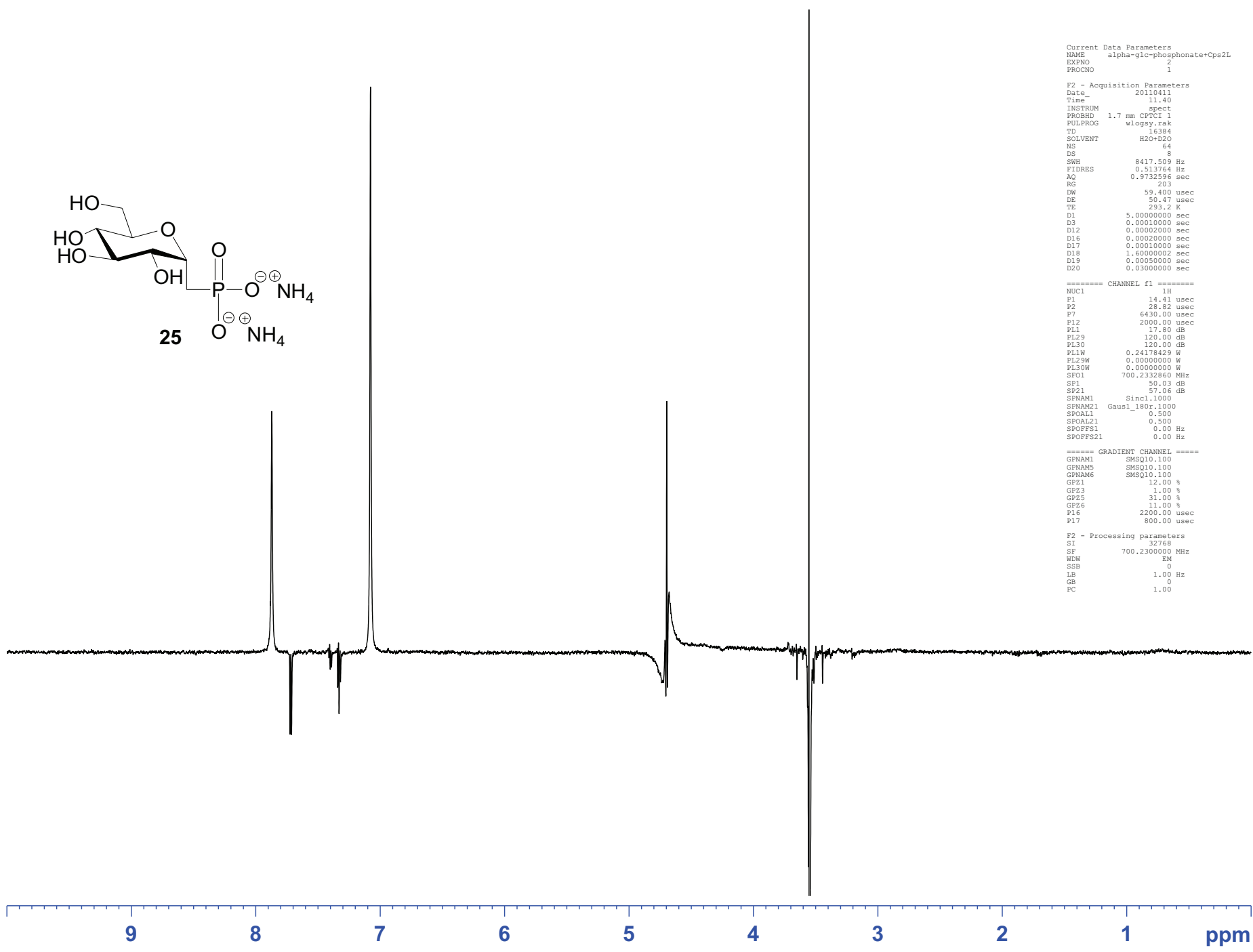
Current Data Parameters
NAME beta-glc-phosphonate+Cps2L
EXPNO 2
PROCNO 1

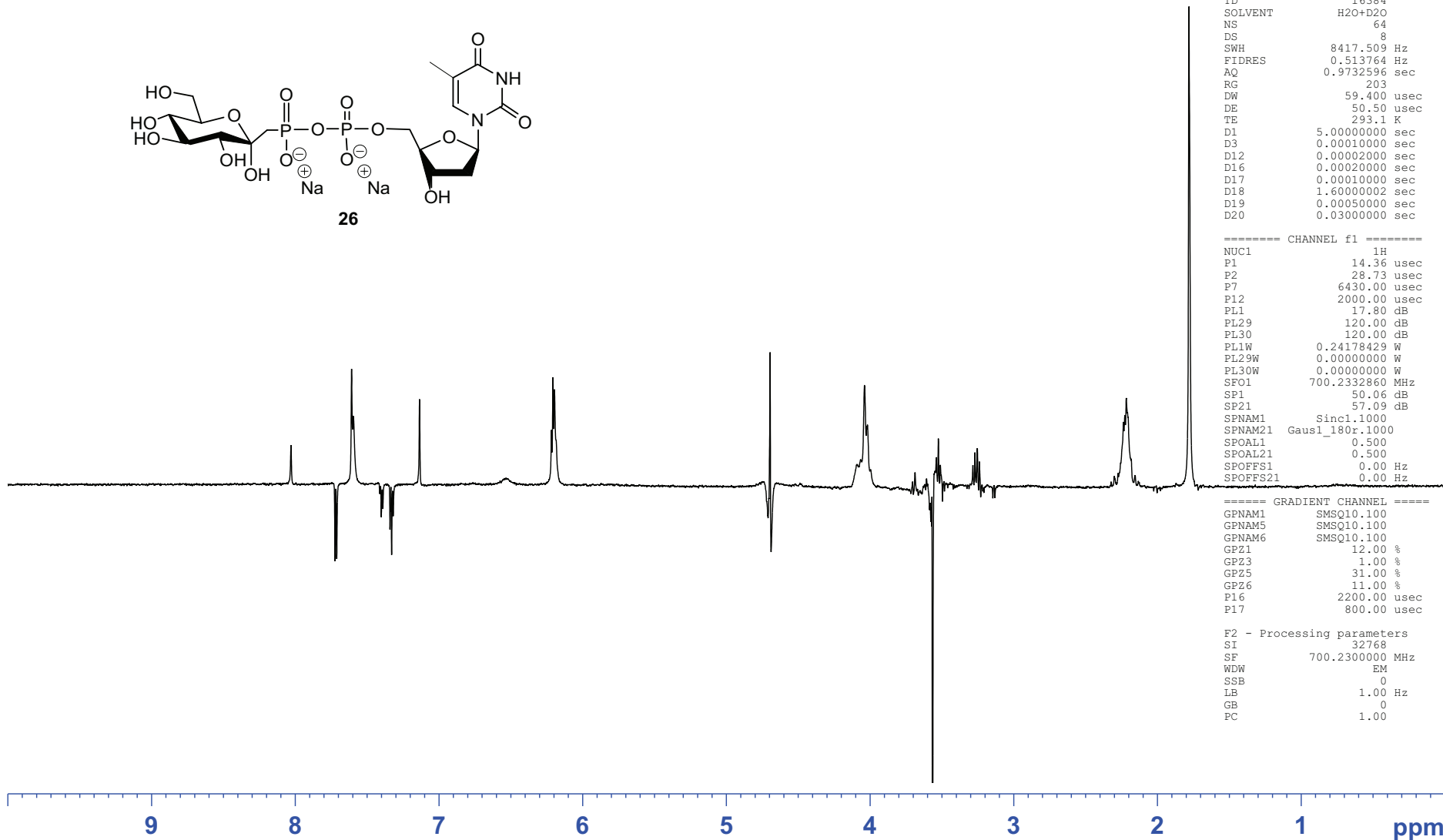
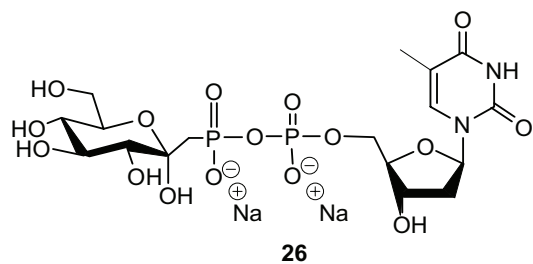
F2 - Acquisition Parameters
Date_ 20110411
Time_ 12.00
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG wlogsy.rak
TD 16384
SOLVENT H2O+D2O
NS 64
DS 8
SWH 8417.509 Hz
FIDRES 0.513764 Hz
AQ 0.9732596 sec
RG 203
DW 59.400 usec
DE 50.49 usec
TE 293.2 K
D1 5.0000000 sec
D3 0.0001000 sec
D12 0.0000200 sec
D16 0.0002000 sec
D17 0.0001000 sec
D18 1.6000000 sec
D19 0.0005000 sec
D20 0.0300000 sec

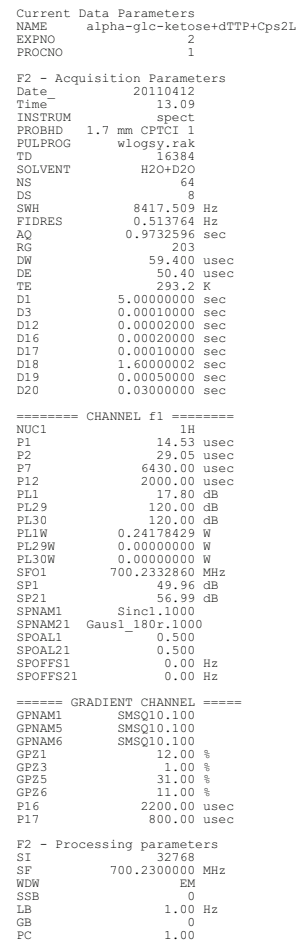
===== CHANNEL f1 =====
NUC1 1H
P1 14.38 usec
P2 28.76 usec
P7 6430.00 usec
P12 2000.00 usec
PL1 17.80 dB
PL29 120.00 dB
PL30 120.00 dB
PL1W 0.24178429 W
PL29W 0.00000000 W
PL30W 0.00000000 W
SF01 700.2332860 MHz
SP1 50.05 dB
SP21 57.08 dB
SPNAM1 Sinc1.1000
SPNAM21 Gaus1_180r.1000
SPOAL1 0.500
SPOAL21 0.500
SPOFFS1 0.00 Hz
SPOFFS21 0.00 Hz

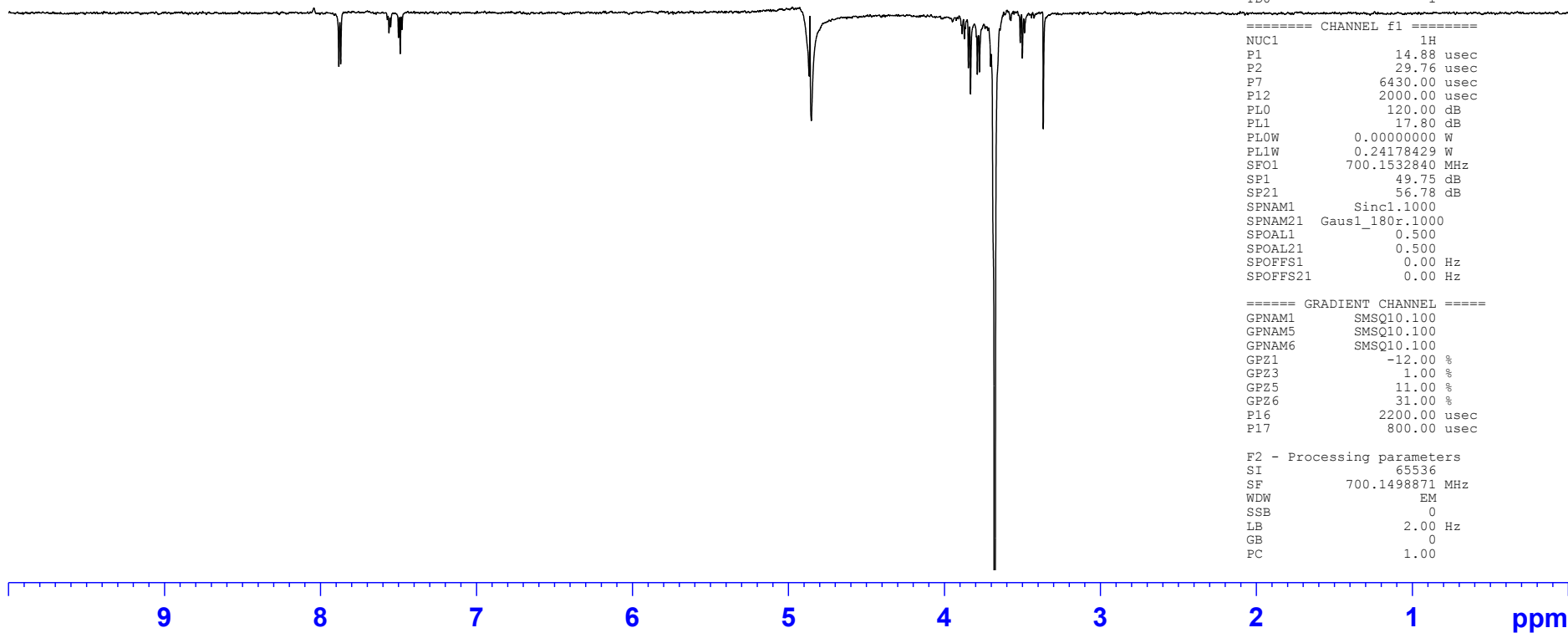
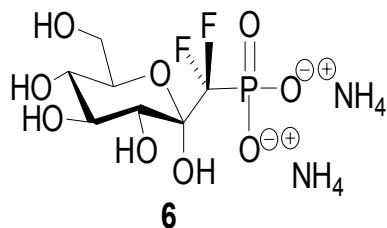
===== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM5 SMSQ10.100
GPNAM6 SMSQ10.100
GPZ1 12.00 %
GPZ3 1.00 %
GPZ5 31.00 %
GPZ6 11.00 %
P16 2200.00 usec
P17 800.00 usec

F2 - Processing parameters
SI 32768
SF 700.2300000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00









Current Data Parameters
NAME Feb14-2012-DiFglcketo-re
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120214
Time 19.10
INSTRUM spect
PROBHD 1.7 mm CPTCI 1
PULPROG imb_wlogsy
TD 32768
SOLVENT H2O+D2O
NS 64
DS 8
SWH 8417.509 Hz
FIDRES 0.256882 Hz
AQ 1.9464692 sec
RG 203
DW 59.400 usec
DE 27.90 usec
TE 293.2 K
D1 5.00000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
D18 1.20000005 sec
D19 0.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^1H
P1 14.88 usec
P2 29.76 usec
P7 6430.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 17.80 dB
PL0W 0.00000000 W
PL1W 0.24178429 W
SFO1 700.1532840 MHz
SP1 49.75 dB
SP21 56.78 dB
SPNAM1 Sinc1.1000
SPNAM21 Gaus1_180r.1000
SPOAL1 0.500
SPOAL21 0.500
SPOFFS1 0.00 Hz
SPOFFS21 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM5 SMSQ10.100
GPNAM6 SMSQ10.100
GPZ1 -12.00 %
GPZ3 1.00 %
GPZ5 11.00 %
GPZ6 31.00 %
P16 2200.00 usec
P17 800.00 usec

F2 - Processing parameters
SI 65536
SF 700.1498871 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

Table 1. Assay data including HPLC retention times for Cps2L-catalyzed reaction of sugar nucleotide phosphonate and keto-phosphonate analogues to NDP-sugars.

Substrate	NTP	Enzyme units	time (hours)	%conversion	Product	MS/MS (m/z)	NDP-sugar retention time (min)	NTP retention time (min)
3	dTTP	2	0.1	100	26	577, 321, 255	5.82	7.78
3	UTP	10	2.5	100	27	579,323, 255	5.36	7.60
3	GTP	10	1	0	-	-	-	8.04
3	CTP	10	1.5	0	-	-	-	8.21
3	ATP	2	1	0	-	-	-	8.67
4	dTTP	2	0.5	100	28	595, 321, 273	5.71	7.80
4	UTP	10	1	17	29	597,323,273	5.83	8.06
5	dTTP	10	1	18	30	595, 321, 273	6.02	8.33
5	UTP	10	6	3	-	-	5.69	8.37
6	dTTP	10	24	<1	-	-	5.59	7.46
7	dTTP	10	1	30*	*	-	5.67	7.68
8	dTTP	10	1	21	31	577, 321, 255	5.81	8.04
8	UTP	10	6	<1%	-	-	5.79	8.43
8	GTP	10	0	0	-	-	-	8.62
9	dTTP	10	42	100	32	561, 321	5.69	7.89