

Synthesis of QS21-based Immunoadjuvants

Pengfei Wang,^{*†} Qipu Dai,[†] Punith Thogaripally,[†] Ping Zhang,[‡] and Suzanne M. Michalek[§]

[†]Department of Chemistry, [‡]Department of Pediatric Dentistry, [§]Department of Microbiology, University of Alabama at Birmingham, 901 14th Street South, Birmingham, Alabama 35294, United States

Table of Content

	Page
Table of content	S1
Immunological data 2b	S2
¹ H NMR spectra of known compounds 5 and 6	S3-4
¹ H and ¹³ C NMR spectra of 7	S5-6
¹ H and ¹³ C NMR spectra of 9	S7-8
¹ H and ¹³ C NMR spectra of 10	S9-10
¹ H NMR spectrum of known compound 11	S11
¹ H and ¹³ C NMR spectra of 12	S12-13
¹ H and ¹³ C NMR spectra of 13a	S14-15
¹ H and ¹³ C NMR spectra of 13b	S16-17
¹ H and ¹³ C NMR spectra of 13c	S18-19
¹ H and ¹³ C NMR spectra of 4a	S20-21
¹ H and ¹³ C NMR spectra of 4b	S22-23
¹ H and ¹³ C NMR spectra of 4c	S24-25
¹ H and ¹³ C NMR spectra of 14a	S26-27
¹ H and ¹³ C NMR spectra of 14b	S28-29
¹ H and ¹³ C NMR spectra of 14c	S30-31
¹ H and ¹³ C NMR spectra of 15a	S32-33
¹ H and ¹³ C NMR spectra of 15b	S34-35
¹ H and ¹³ C NMR spectra of 15c	S36-37
¹ H and ¹³ C NMR spectra of 2a	S38-39
¹ H and ¹³ C NMR spectra of 2b	S40-41
¹ H and ¹³ C NMR spectra of 2c	S42-44
¹ H NMR spectrum of the intermediate S2	S45

Table S1. Weight monitoring of mice immunized by s.c. route with rHagB alone or with GPI-0100 or **2b** over time.^a

Group	mice	Weight (g)				
		Week 0	Week 2	Week 4	Week 6	Week 12
1 no adjuvant	A1	18.6	19.8	20.9	22.6	27.4
	A2	18.1	19.8	20.6	21.6	26.6
	A3	17.6	18.7	19.6	20.5	25.9
	A4	18.8	20.9	20.5	22.3	27.1
	A5	18.9	20.8	21.5	22.8	26.9
	A6	18.2	18.9	19.6	20.9	26.4
	mean	18.4	19.8	20.5	21.8	26.7
2 GPI-0100 ^b	B1	19.0	21.4	22.6	23.1	27.5
	B2	17.0	18.1	18.9	19.2	26.8
	B3	19.6	21.6	22.1	23.2	28.2
	B4	17.3	19.2	20.2	20.0	27.1
	B5	19.1	20.6	21.1	21.8	27.3
	B6	18.1	19.6	20.0	20.7	26.2
	mean	18.4	20.1	20.9	21.4	27.2
3 2b ^c	C1	16.8	18.6	19.4	20.4	26.7
	C2	16.0	16.9	18.3	18.5	25.8
	C3	18.8	20.5	21.6	23.0	27.9
	C4	17.9	19.3	21.0	21.8	26.2
	C5	17.5	18.7	21.4	22.6	26.3
	C6	16.7	17.6	19.0	19.8	25.3
	mean	17.3	18.6	20.2	21.1	26.4

^aFemale BALB/c mice (8-10 weeks of age); ^b100 µg of GPI-0100; ^c100 µg of **2b**.

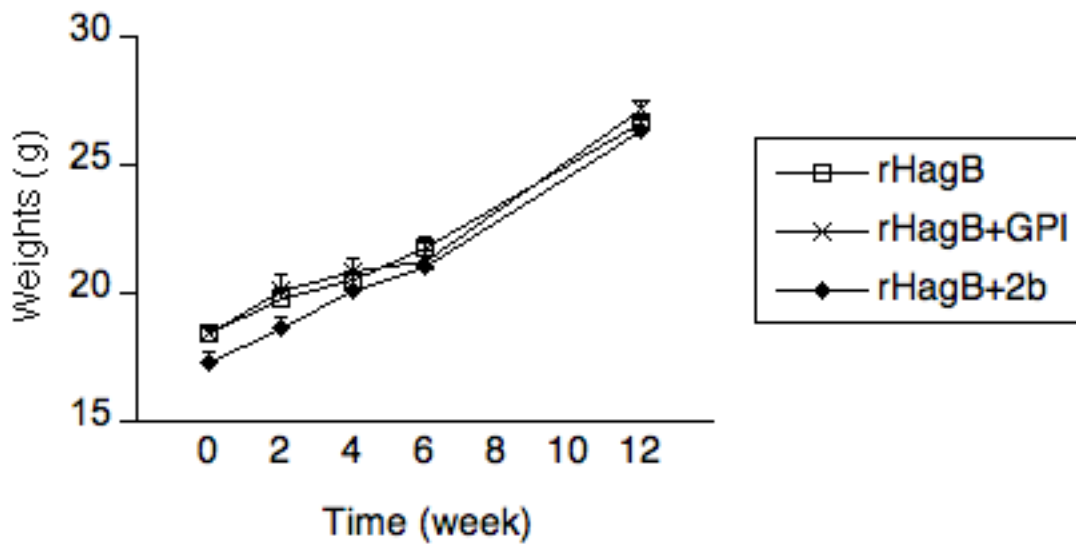
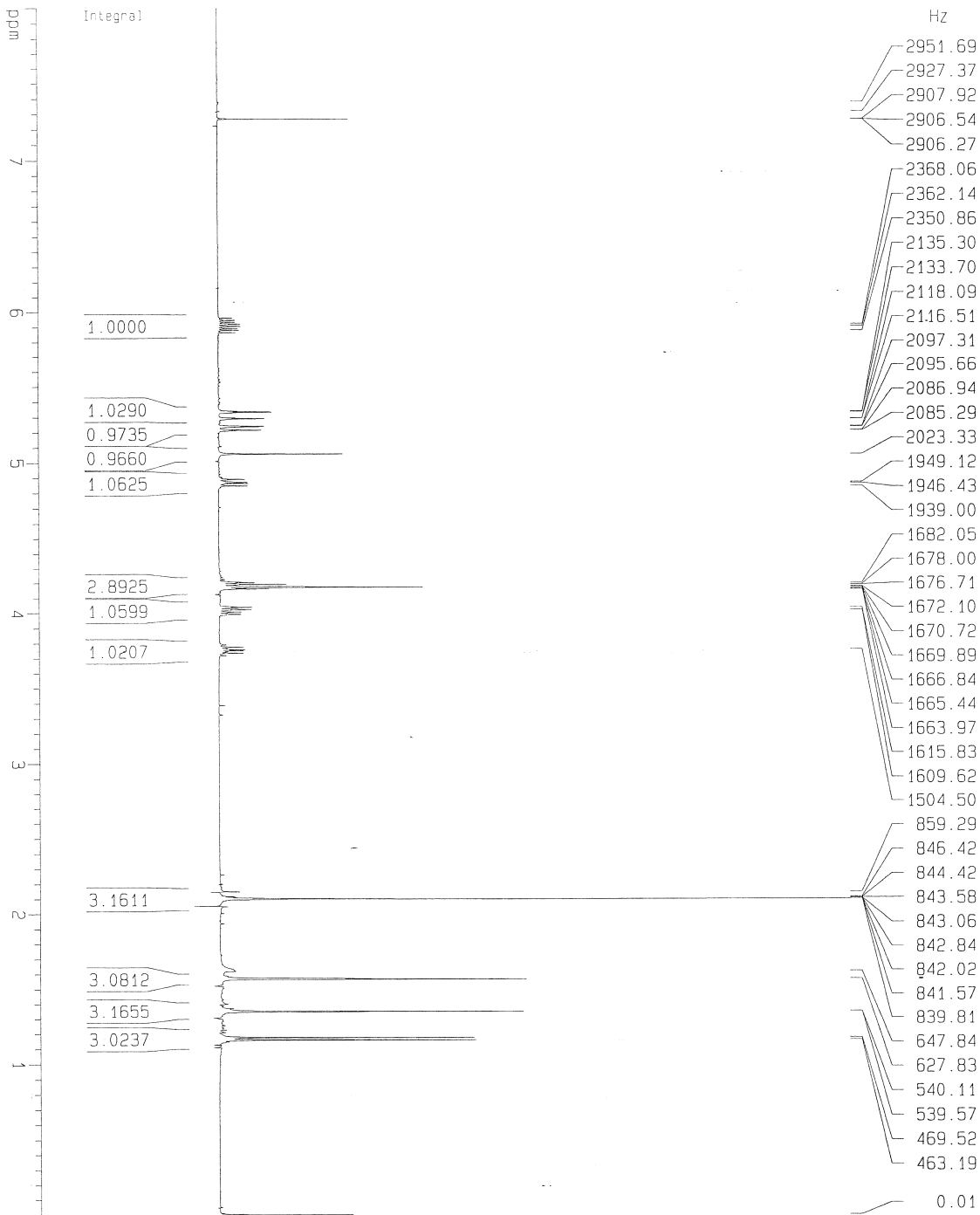
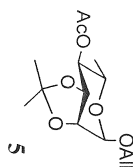


Figure S1. Weight of mice following s.c. immunized with rHagB alone or with GPI-0100 or **2b** over time. Mice were immunized on days 0, 14 and 28. Mice were weighed prior to each immunization and at 6 and 12 weeks following the initial immunization. Values are expressed as mean \pm SEM.



Current Data Parameters
 NAME PW-V-SM3-R2
 EXPNO 1
 PROCNO 1

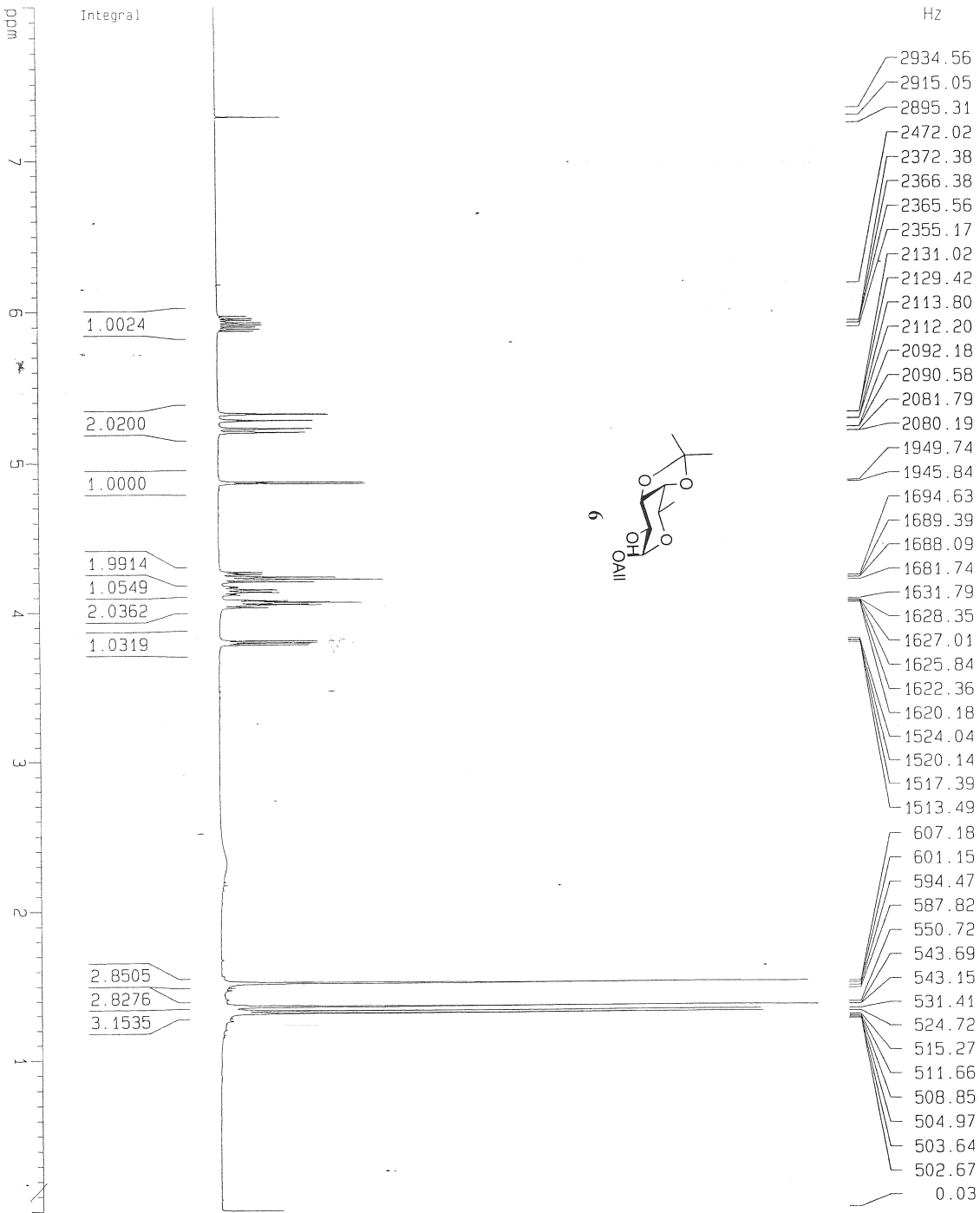
F2 - Acquisition Parameters
 Date_ 20110826
 Time 11.07
 INSTRUM drx400
 PROBDH 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 287.4
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 131072
 SF 400.1300662 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 3201.04 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPM1CM 0.40000 ppm/cm
 HZCM 160.05200 Hz/cm

PW-V-38-C1



Current Data Parameters
 NAME PW-V-38-C1
 EXPNO 1
 PROCNO 1

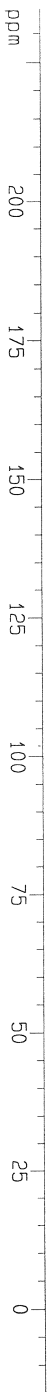
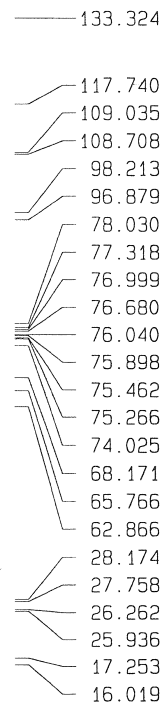
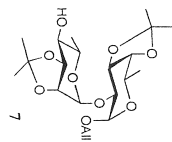
F2 - Acquisition Parameters
 Date_ 20110901
 Time 13.29
 INSTRUM dfrx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT COC13
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 71.8
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 131072
 SF 400.1299990 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 3201.04 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPKMCH 0.40000 ppm/cm
 HZCM 160.05200 Hz/cm

13C w/ 1H decoupling



Current Data Parameters
NAME PW-VI-34-C3C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120521
Time 9.48

INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 80
DS 4

SWH 25125.629 Hz
FIDRES 0.383367 Hz
AQ 1.3042164 sec

RG 32768
DM 19.900 usec
DE 6.00 usec
TE 300.0 K

D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

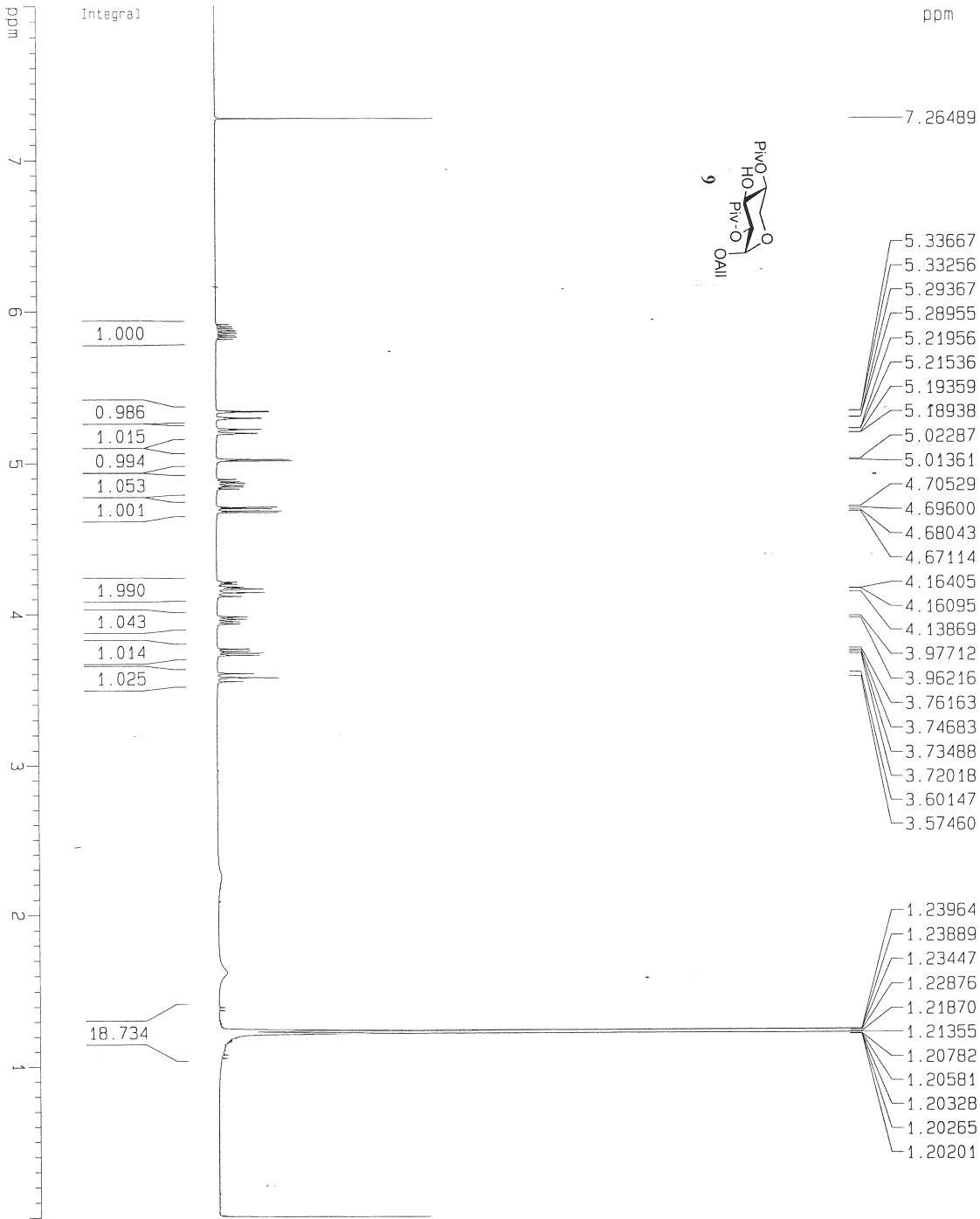
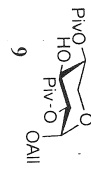
==== CHANNEL f1 =====
NUC1 13C
P1 16.00 usec
PL1 0.00 dB
SF01 100.6237959 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 102.00 usec
PL2 0.00 dB
PL12 23.00 dB
PL13 23.00 dB
SF02 400.1318005 MHz

F2 - Processing Parameters
SI 131072
SF 100.6127844 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 234.308 ppm
F1 23674.34 Hz
F2P -15.418 ppm
F2 -1951.29 Hz
PNUCM 12.48630 ppm/cm
HZCM 1256.28149 Hz/cm

PW-V-SM4-X2A
XYLOSE W/ 2 PIV



Current Data Parameters

NAME PW-V-SM4-X2A

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20110826

Time 11.13

INSTRUM drx400

PROBHD 5 mm Multinu

PULPROG zg30

TD 65536

SOLVENT CDCl3

NS 16

DS 2

SWH 8278.146 HZ

FIDRES 0.126314 HZ

AQ 3.9584243 sec

RG 256

DW 60.400 usec

DE 6.00 usec

TE 300.0 K

D1 1.00000000 sec

==== CHANNEL f1 =====

NUC1 1H

P1 6.50 usec

PL1 0.00 dB

SFO1 400.1324710 MHz

F2 - Processing parameters

SF 400.1300073 MHz

SI 131072

WDW no

SSB 0

LB 0.00 HZ

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

F1P 8.000 ppm

F1 3201.04 HZ

F2P 0.000 ppm

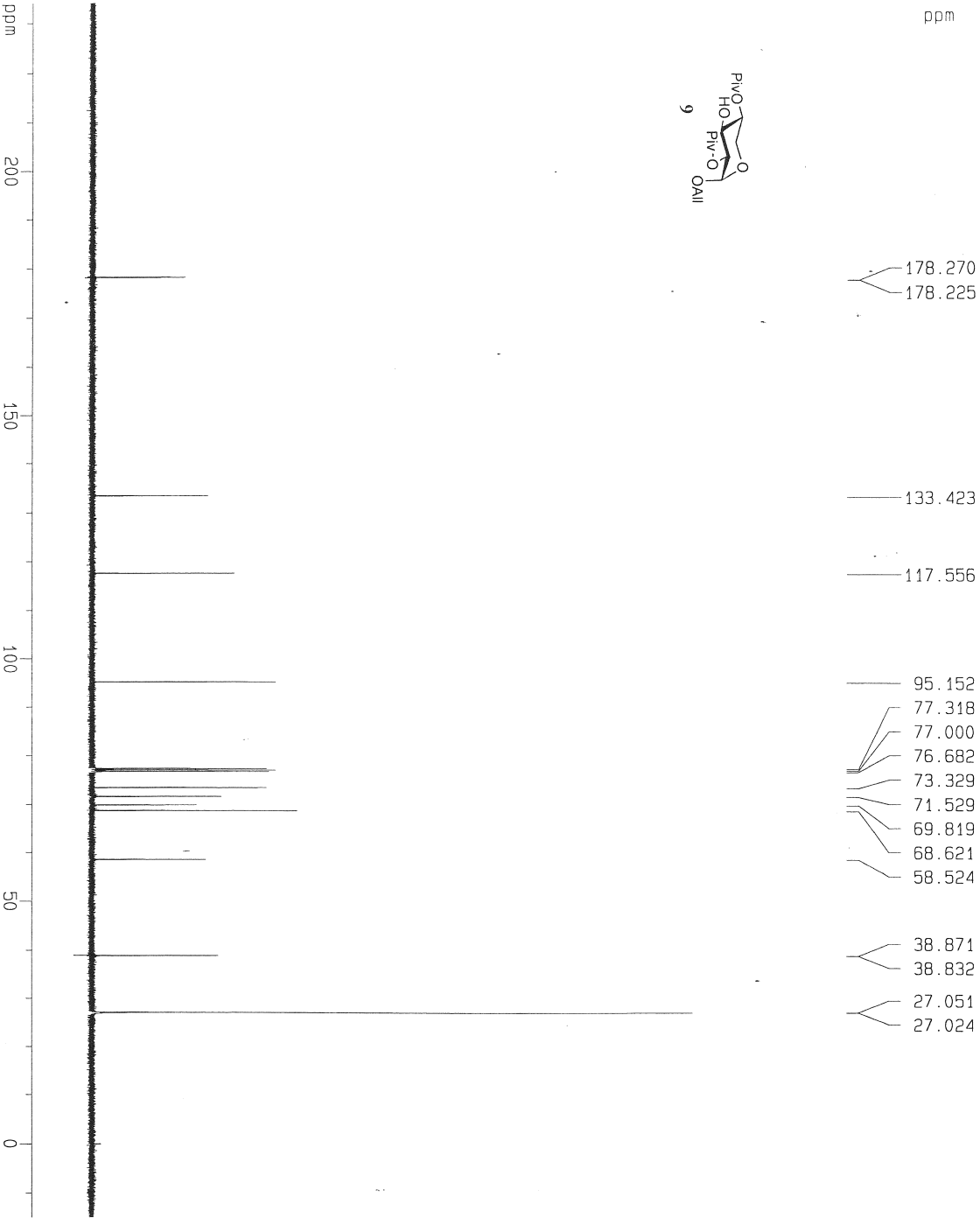
F2 0.00 HZ

PPMCM 0.40000 ppm/cm

HZCM 160.05200 HZ/cm



ppm



Current Data Parameters
 NAME Pw-VI-29-1-C3c
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20120309
 Time 13.15
 INSTRUM drx400
 PROBH0 5 mm Multinu
 PULPROG zgpg30
 TD 83536
 SOLVENT CDCl3
 NS 1244
 DS 4
 SMH 25125.629 Hz
 FIDRES 0.383387 Hz
 AQ 1.3042164 sec
 RG 32789
 DM 19.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

==== CHANNEL f1 =====

NUC1 13C
 P1 16.00 usec
 PL1 0.00 dB
 SF01 100.6237959 MHz

==== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 102.00 usec
 PL2 0.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SF02 400.1316005 MHz

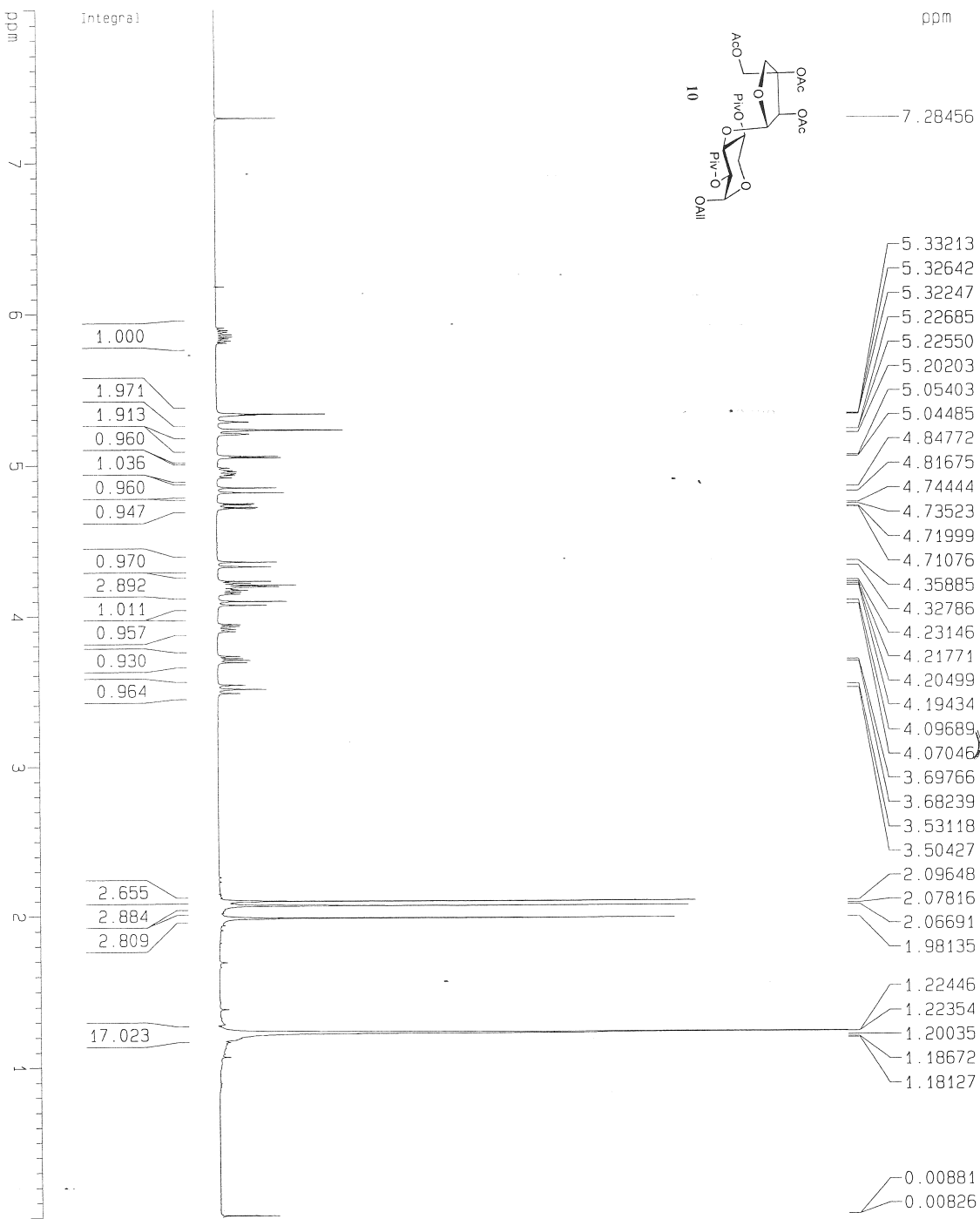
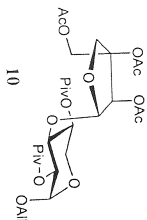
F2 - Processing parameters

SI 131072
 SF 100.6127733 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters

CX 20.00 cm
 F1P 234.000 ppm
 F1 23543.39 Hz
 F2P -15.000 ppm
 F2 -1509.19 Hz
 PPMCM 12 45000 ppm/cm
 HZCM 1252.62903 Hz/cm

PM-VI-APIXYL
 Check ap1-xy1-a11y1



Current Data Parameters
 NAME PM-VI-APIXYL
 EXPNO 1
 PROCNO 1

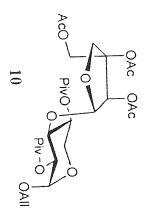
F2 - Acquisition Parameters
 Date_ 20130416
 Time 14.55
 INSTRUM drx400
 PROBD 5 mm WU11nu
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AG 3.9584243 sec
 RG 90.5
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 S1 131072
 SF 400.1299992 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 3201.04 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPKCM 0.40000 ppm/cm
 HZCM 160.05200 Hz/cm

177.14
177.00
176.04
168.29
168.48



133.06

117.55

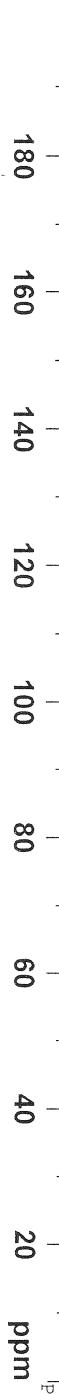
103.95

94.38

83.38
77.42
76.99
76.57
76.23
75.80
72.80
71.77
69.13
68.37
62.10
58.01

38.54
38.38

28.83
28.65
20.69
20.31
20.10



Current Data Parameters
NAME QD-I-138b-CC
EXPNO 1
PROCNO 1

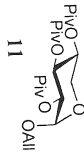
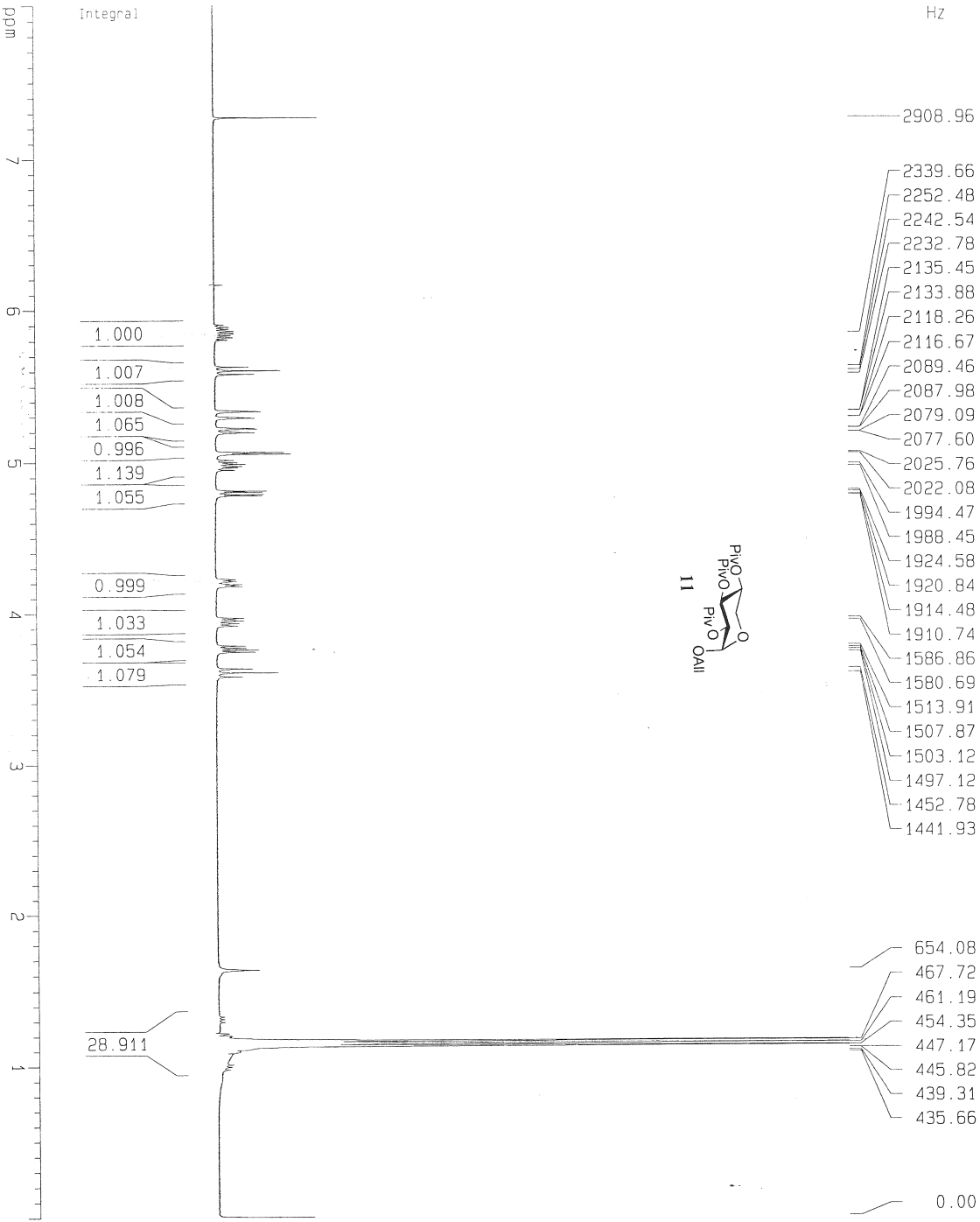
F2 - Acquisition Parameters
Date_ 20130223
Time 15.37
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 109
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DE 27.800 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 -1.80 dB
SFO1 75.4124265 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 -2.50 dB
PL12 11.48 dB
PL13 12.00 dB
SFO2 299.8811995 MHz

F2 - Processing parameters
SI 32768
SF 75.4049004 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PW-V-43-C1



```

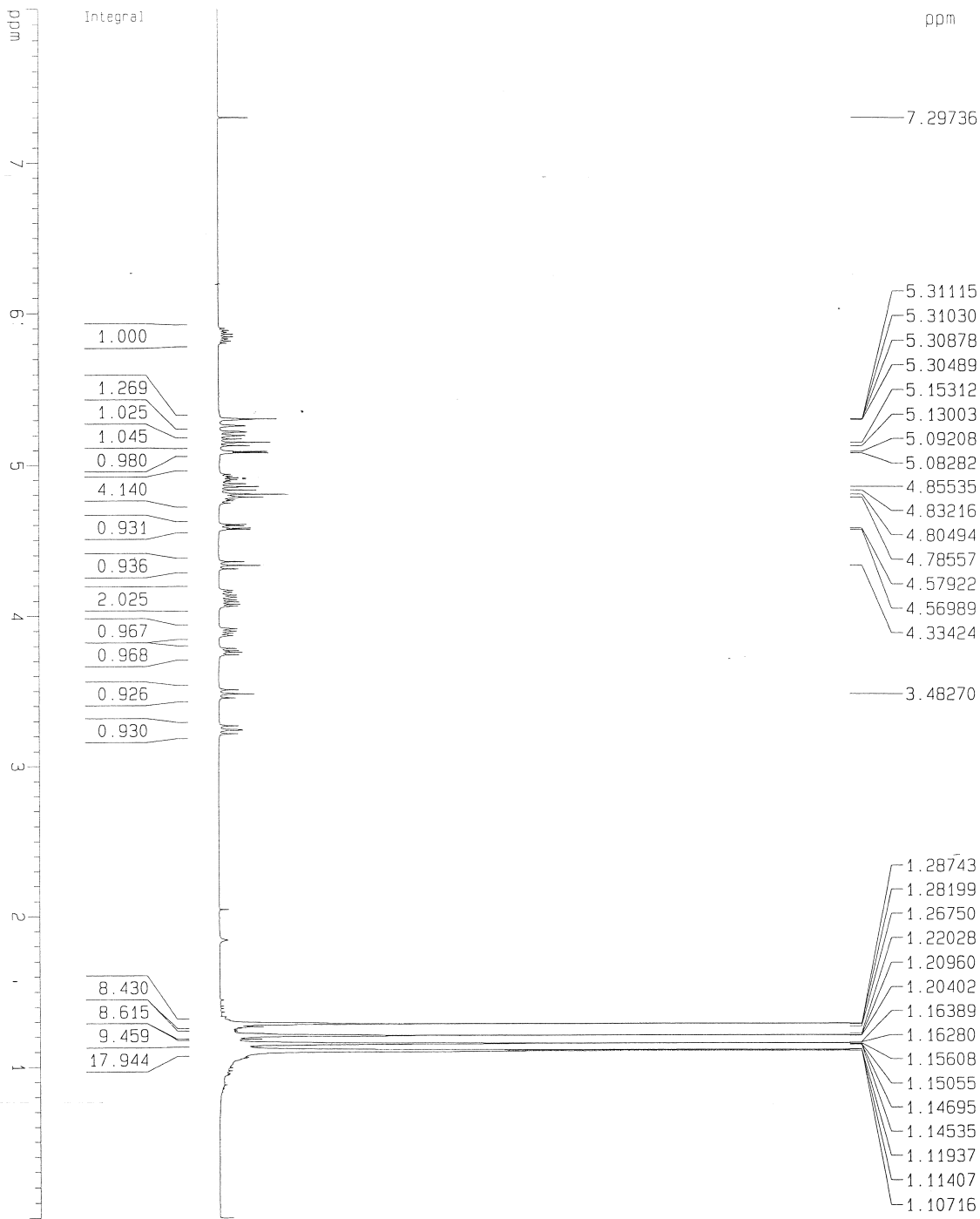
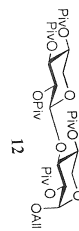
Current Data Parameters
NAME          PW-V-43-C1
EXPNO        1
PROCNO       1

F2 - Acquisition Parameters
Date_        20110919
Time         12.29
INSTRUM      drx400
PROBHD       5 mm Multinu
PULPROG      zg30
TD            65536
SOLVENT      CDCl3
NS            8
DS            2
SMH           8278.146 Hz
FIDRES       0.126314 Hz
AQ           3.9584243 sec
RG            512
DE            60.400 usec
TE            300.0 K
D1            1.00000000 sec

===== CHANNEL f1 =====
NUC1          1H
P1            6.50 usec
PL1           0.00 dB
SF01         400.1324710 MHz

F2 - Processing parameters
SI            131072
SF            400.130054 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.00

1D NMR plot parameters
CX            20.00 cm
F1P           8.000 ppm
F1            3201.04 Hz
F2P           0.000 ppm
F2            0.00 Hz
PPMCKM       0.40000 ppm/cm
HZCKM        160.05200 Hz/cm
  
```



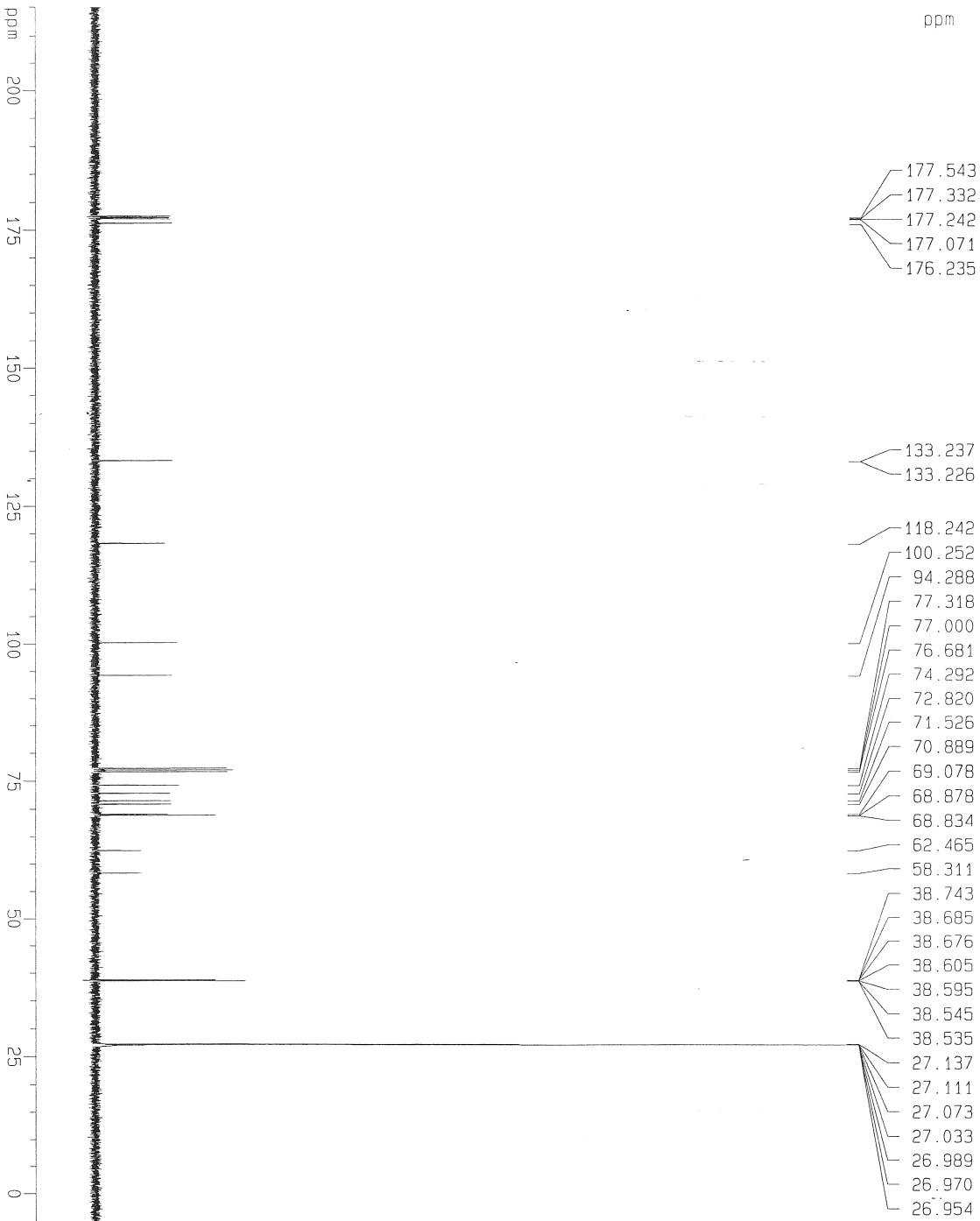
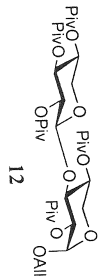
Current Data Parameters
 NAME Pw-V-49-C3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111017
 Time 12.58
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 40.3
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 S1 131072
 SF 400.1299941 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 3201.04 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PRXCM 0.40000 ppm/cm
 HZCM 160.05200 Hz/cm



Current Data Parameters
 NAME PM-V-49-C3C13
 EXPNO 1
 PROCNO 1

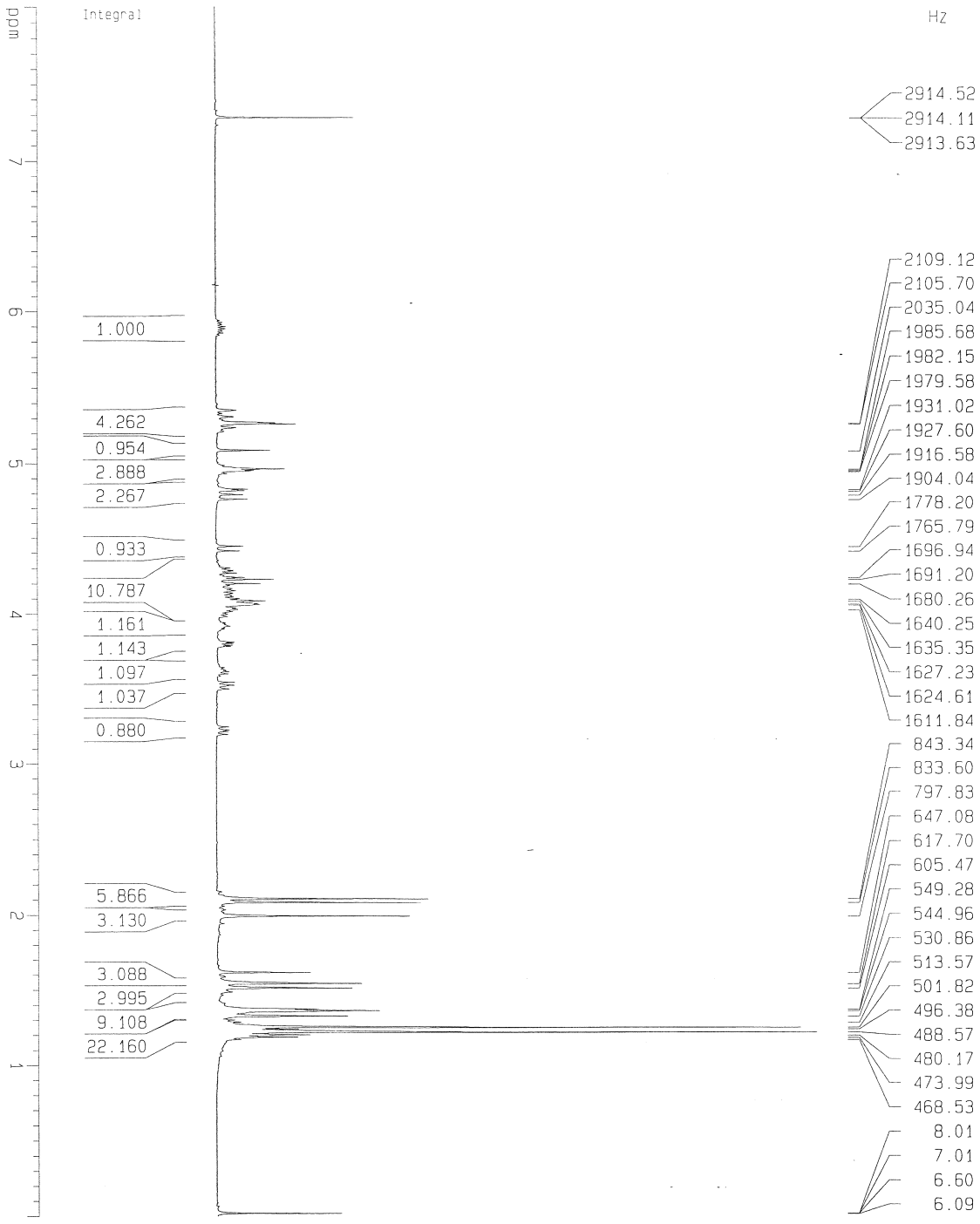
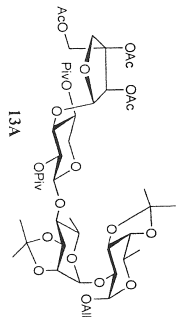
F2 - Acquisition Parameters
 Date_ 20111017
 Time 13.25
 INSTRUM drx400
 PROBRD 5 mm Multinu
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 359
 DS 4
 SWH 25125.629 Hz
 FIDRES 0.383387 Hz
 AQ 1.3042164 sec
 RG 32768
 DW 19.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 16.00 usec
 PL1 0.00 dB
 SF01 100.6237959 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 102.00 usec
 PL2 0.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 131072
 SF 100.6127744 MHz
 WDM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 215.000 ppm
 F1 21631.75 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.74060 Hz/cm



Current Data Parameters
 NAME PM-VI-51-SW2
 EXPNO 1
 PROCNO 1

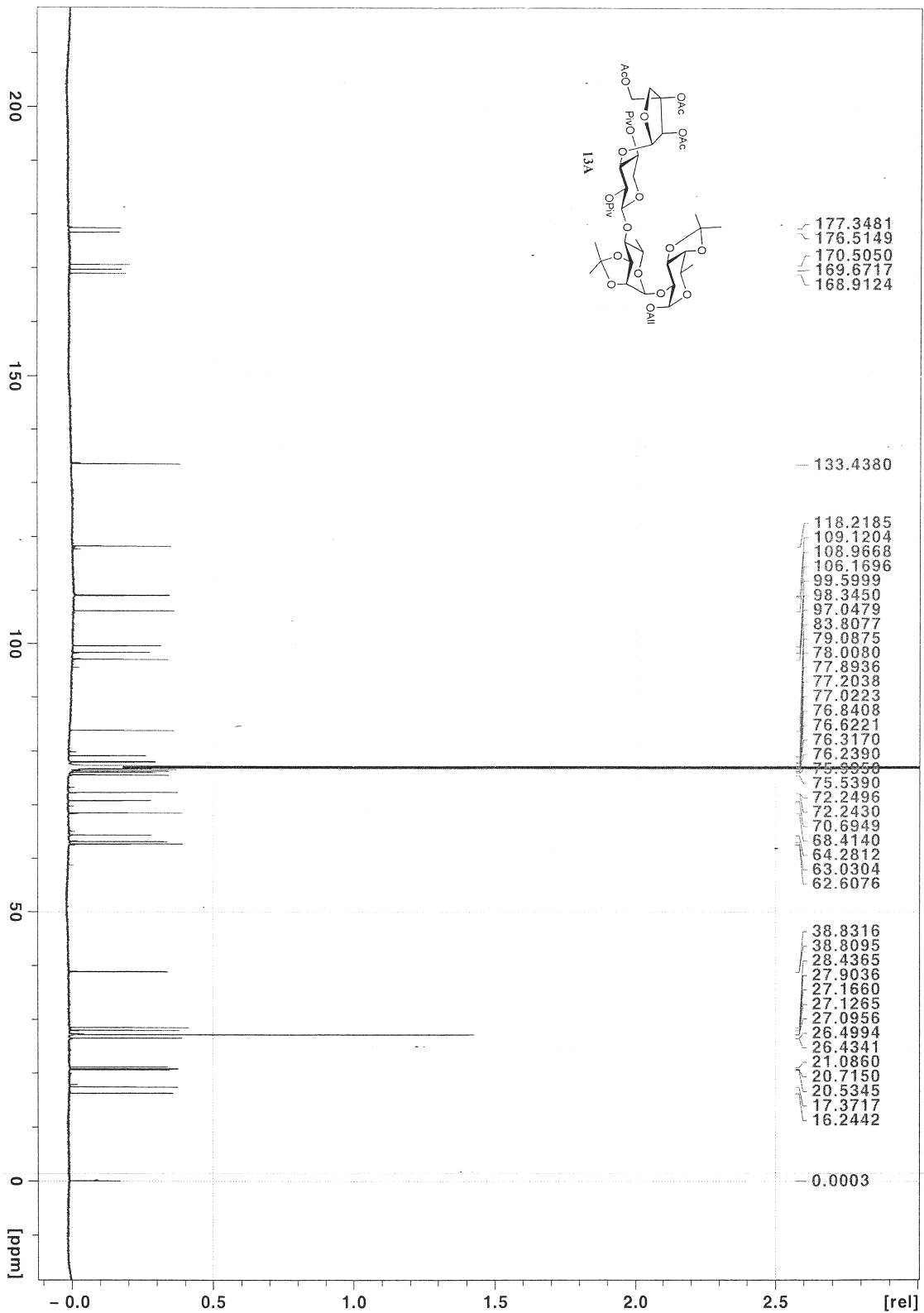
F2 - Acquisition Parameters
 Date_ 20130306
 Time 14.45
 INSTRUM drx400
 PROBD 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 287.4
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

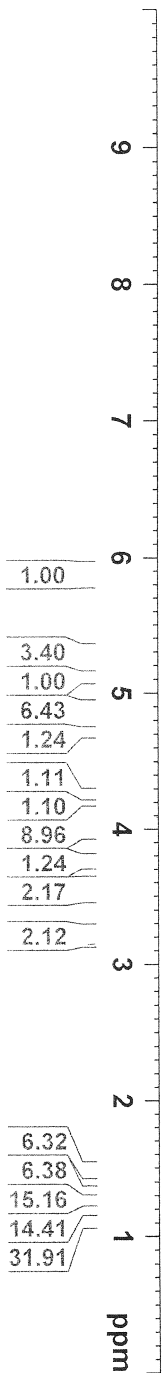
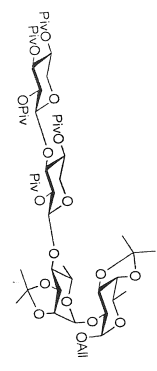
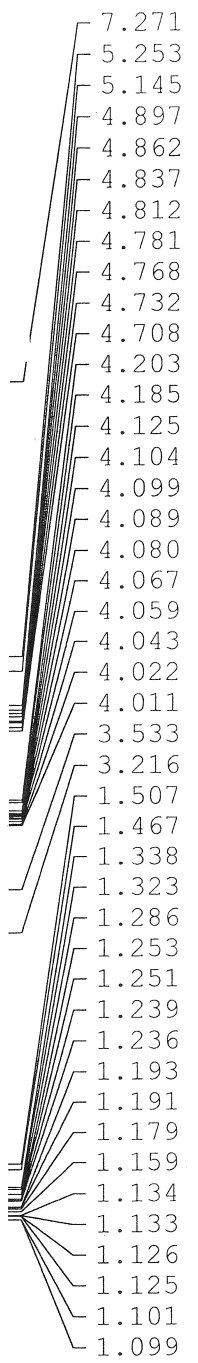
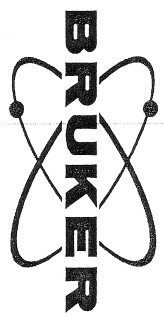
CHANNEL f1

NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 131072
 SF 400.1299995 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 3201.04 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPKCM 0.40000 ppm/cm
 HZCM 160.05200 Hz/cm





Current Data Parameters
 NAME QD-1-166-pure-11
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130419
 Time 8.46
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 57
 DW 80.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -2.50 dB
 SFO1 299.8818519 MHz

F2 - Processing parameters
 SI 32768
 SF 299.8800004 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME QD-I-166-pure-11C
 EXPNO 1
 PROCNO 1

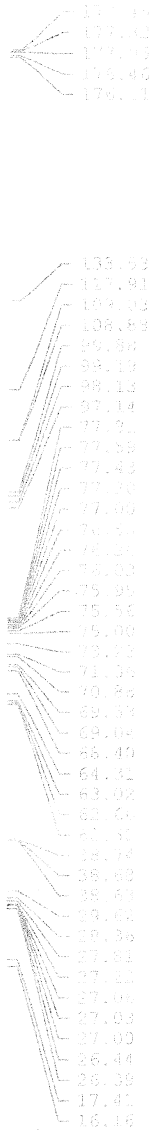
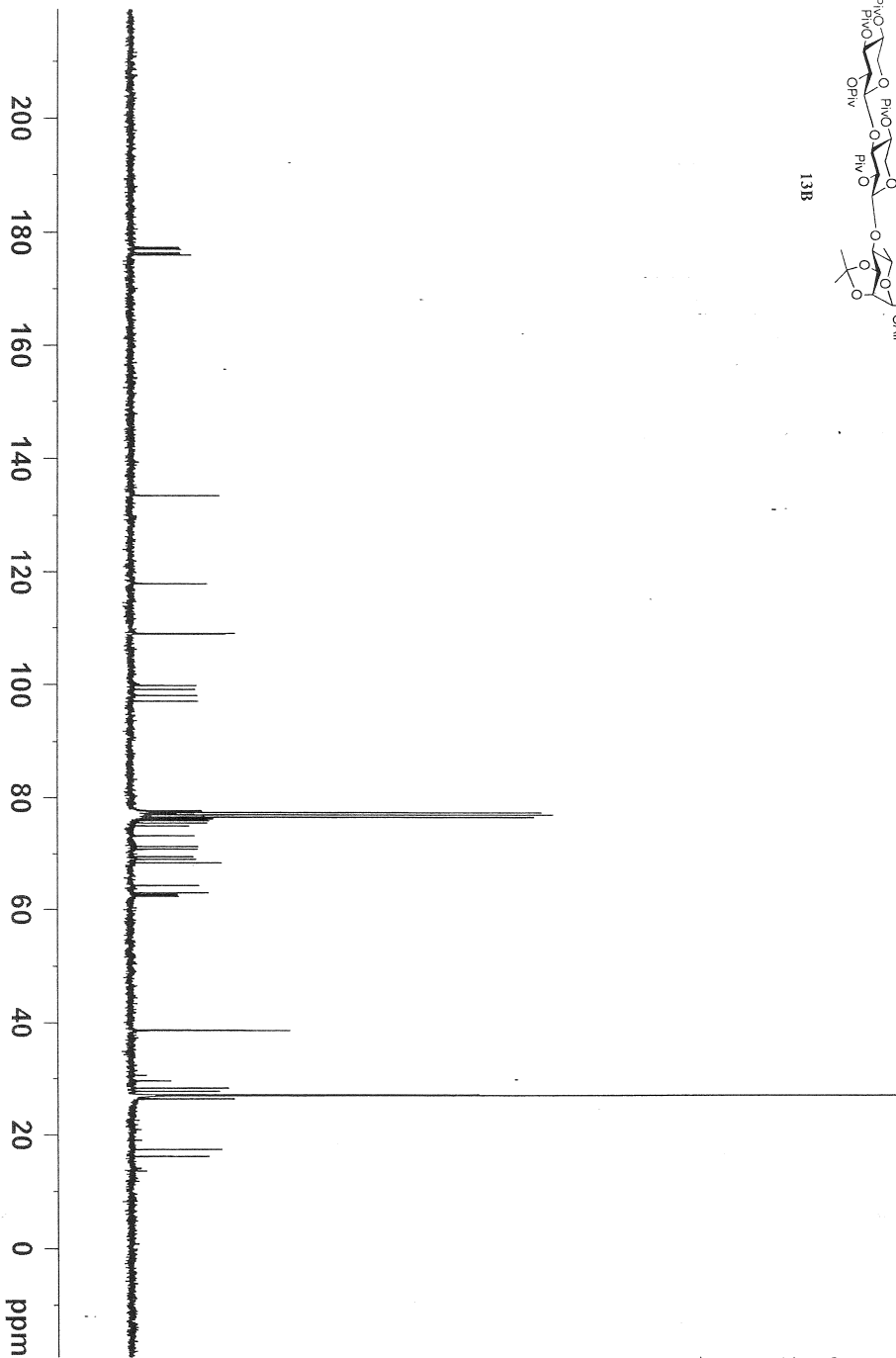
F2 - Acquisition Parameters

Date_ 20130419
 Time 8.50
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 448
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 32768
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -1.80 dB
 SFO1 75.4124265 MHz

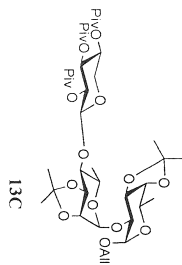
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 75.00 usec
 PL2 -2.50 dB
 PL12 11.48 dB
 PL13 12.00 dB
 SFO2 299.8811995 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4048878 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

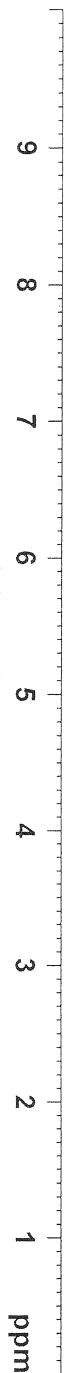




Current Data Parameters
 NAME QD-I-159-111
 EXPNO 1
 PROCNO 1



- 7.270
- 5.309
- 5.251
- 5.235
- 5.212
- 5.208
- 5.178
- 4.984
- 4.969
- 4.960
- 4.954
- 4.925
- 4.784
- 4.772
- 4.221
- 4.207
- 4.189
- 4.123
- 4.105
- 4.101
- 4.090
- 4.070
- 4.060
- 4.051
- 4.036
- 4.028
- 4.018
- 4.010
- 3.781
- 3.769
- 3.753
- 3.549
- 3.525
- 1.504
- 1.494
- 1.335
- 1.322
- 1.312
- 1.302
- 1.176
- 1.151
- 1.132
- 1.117
- 1.101

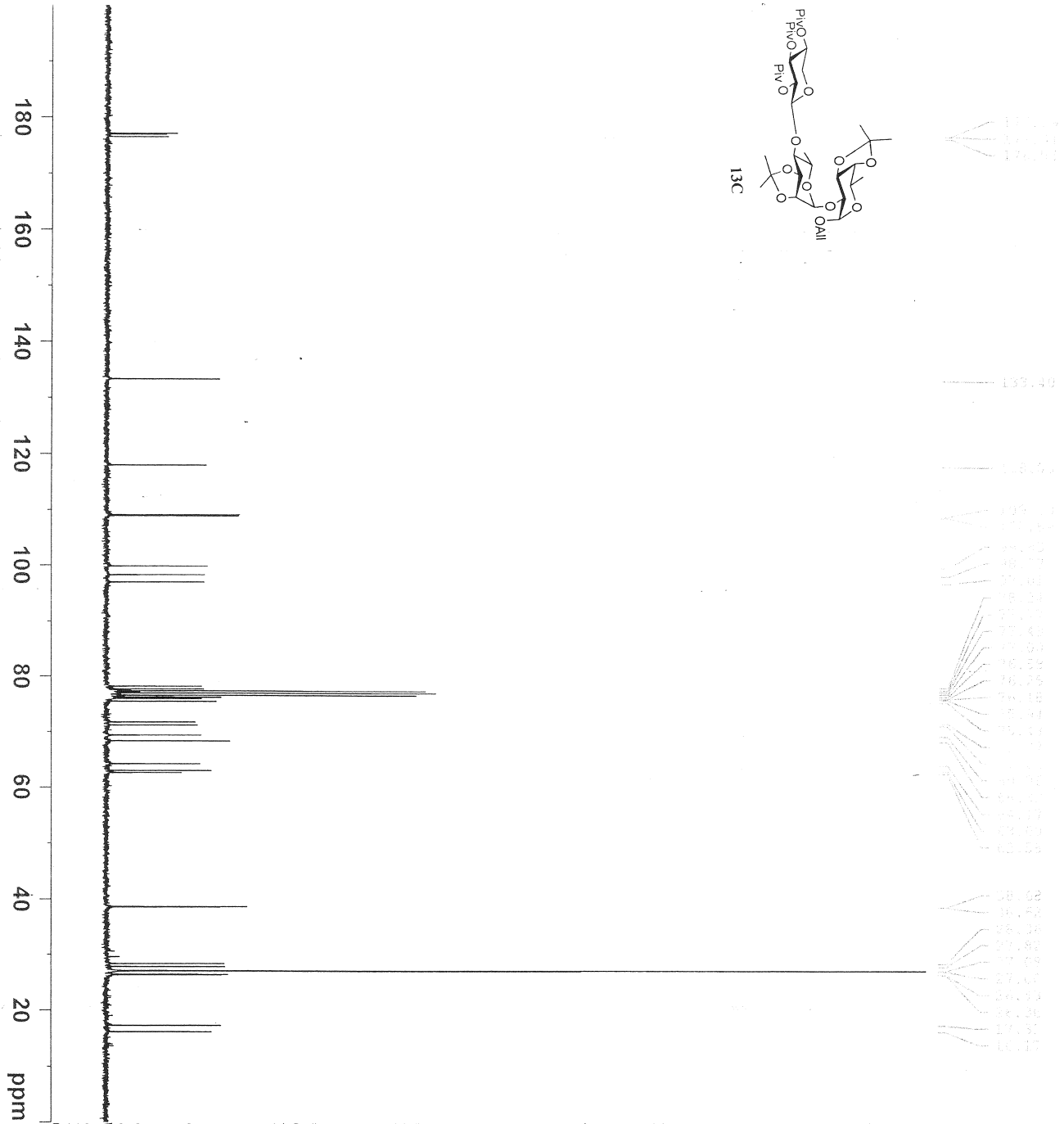
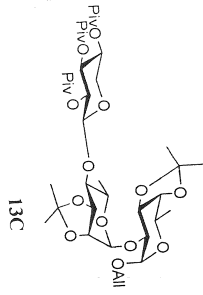


1.00
 2.99
 1.11
 3.03
 1.02
 2.02
 6.44
 1.10
 1.99
 1.00
 6.08
 9.24
 12.73
 18.33

F2 - Acquisition Parameters
 Date_ 20130420
 Time_ 11.12
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 71.8
 DW 80.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -2.50 dB
 SFO1 299.8818519 MHz

F2 - Processing parameters
 SI 32768
 SF 299.8800004 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME QD-I-159-111C
 EXPNO 1
 PROCNO 1

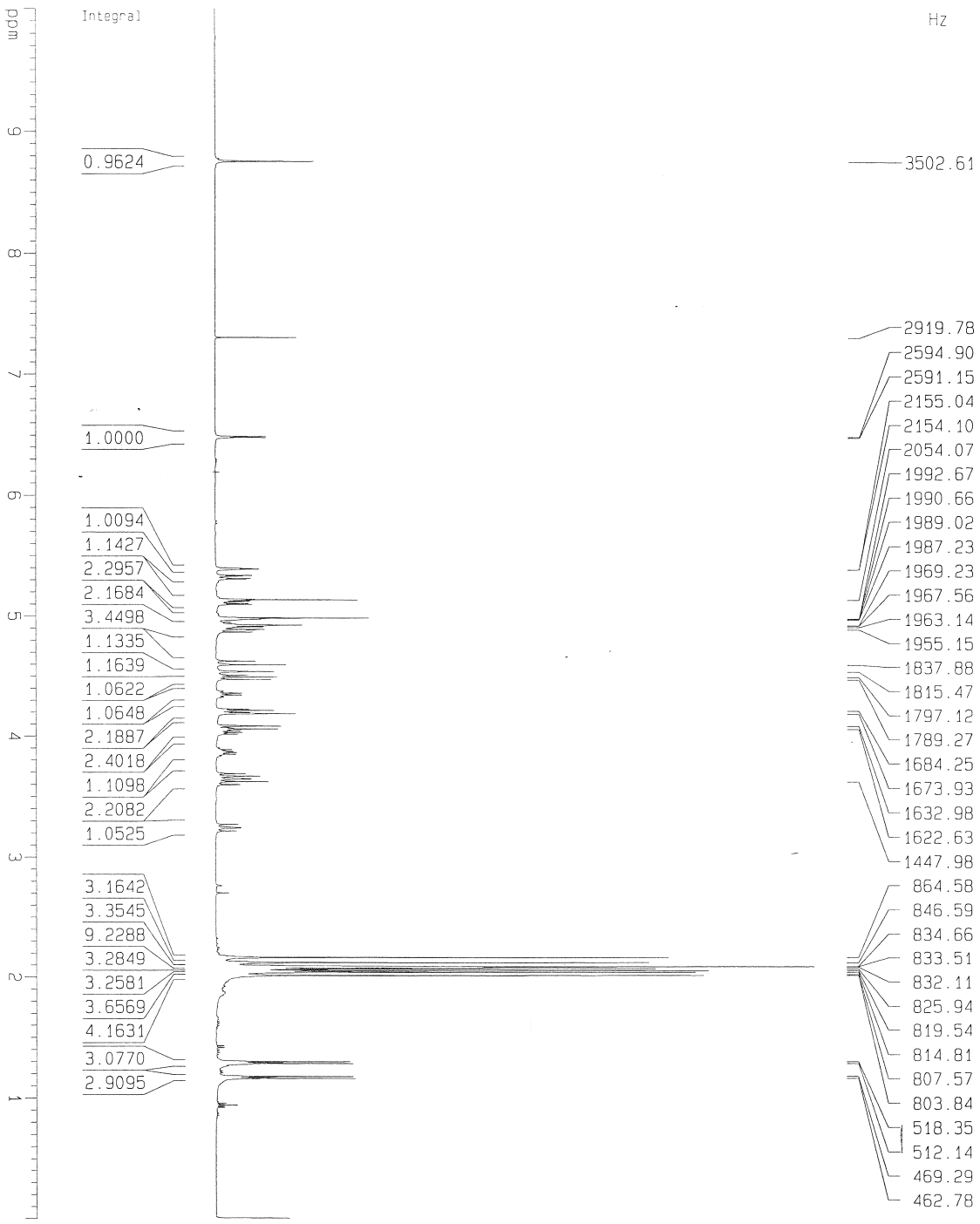
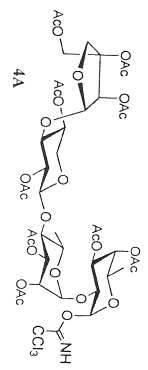
F2 - Acquisition Parameters

Date_ 20130420
 Time 11.27
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SMH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 32768
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL F1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -1.80 dB
 SFO1 75.4124265 MHz

==== CHANNEL F2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 75.00 usec
 PL2 -2.50 dB
 PL12 11.48 dB
 PL13 12.00 dB
 SFO2 299.8811995 MHz

F2 - Processing Parameters
 SI 32768
 SF 75.4048877 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



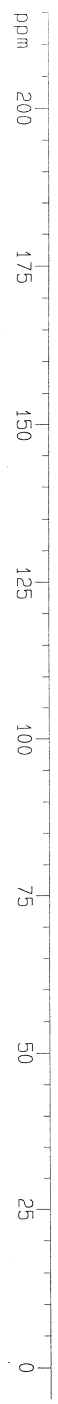
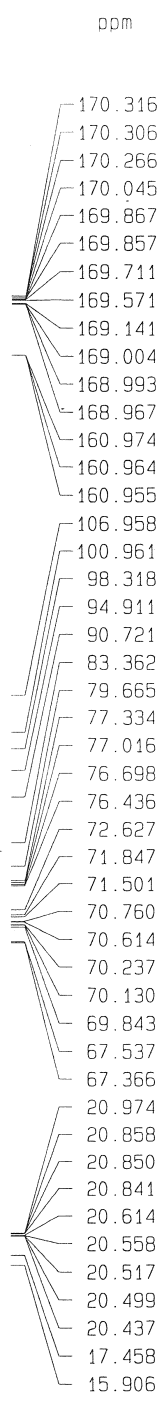
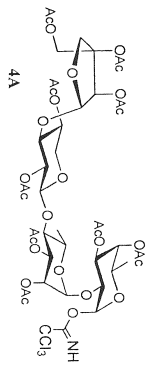
Current Data Parameters
 NAME PW-VI-55-3-BH
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130304
 Time 16.40
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 57
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 131072
 SF 400.1299339 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1p 10.000 ppm
 F1 4001.30 Hz
 F2p 0.000 ppm
 F2 0.00 Hz
 PPMCK 0.50000 ppm/cm
 HZCM 200.06500 Hz/cm



```

Current Data Parameters
NAME          PM-VI-55-38C
EXPNO         1
PROCNO        1

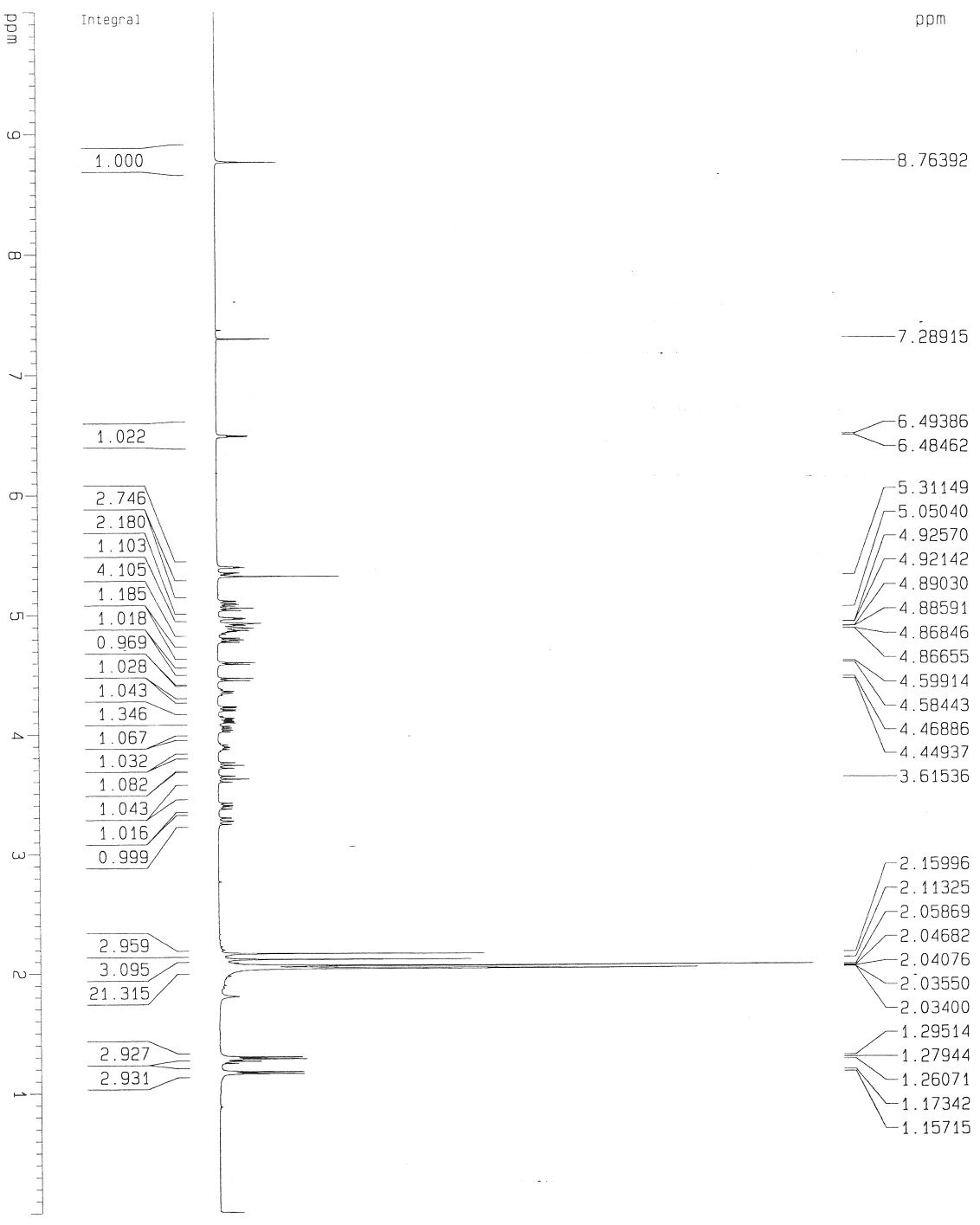
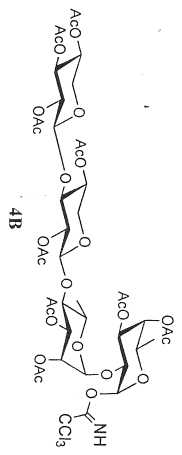
F2 - Acquisition Parameters
Date_         20130304
Time          16.53
INSTRUM      drx400
PROBHD       5 mm Multinu
PULPROG      zgpg30
TD            65536
SOLVENT      CDCl3
NS            16004
DS            4
SWH           25125.629 Hz
FIDRES        0.38387 Hz
AQ            1.3042164 sec
RG            32768
DM            19.900 usec
DE            6.00 usec
TE            300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

===== CHANNEL f1 =====
NUC1          13C
P1            16.00 usec
PL1           0.00 dB
SF01          100.6237959 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        102.00 usec
PL2           0.00 dB
PL12         23.00 dB
PL13         23.00 dB
SF02          400.1316005 MHz

F2 - Processing parameters
SI            131072
SF            100.6127754 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.40

1D NMR plot parameters
CX            20.00 cm
F1p           215.000 ppm
F1            21631.75 Hz
F2p           -5.000 ppm
F2            -503.06 Hz
PMCKM        11.00000 ppm/cm
HZCM         1106.74060 Hz/cm
  
```



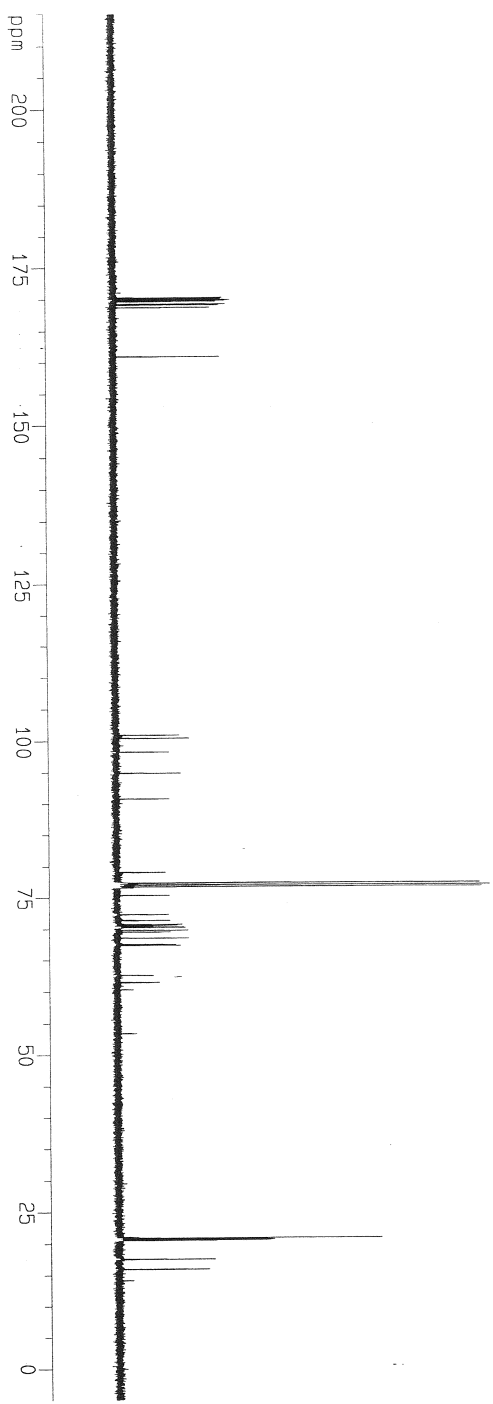
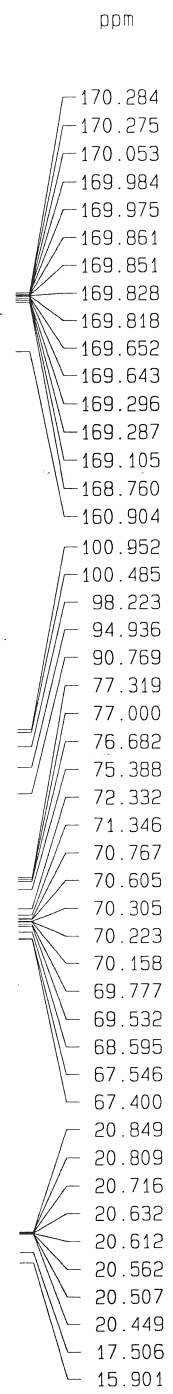
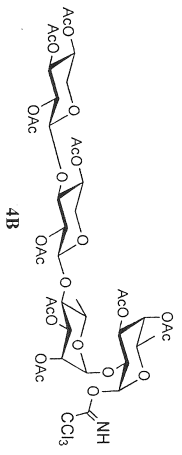
Current Data Parameters
 NAME PW-VI-25-C1B
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120206
 Time 13.04
 INSTRUM drx400
 PULPROG 5 mm Multinu
 PROBD 2g30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 114
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 131072
 SF 400.1299974 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 0.50000 ppm/cm
 HZCM 200.065500 Hz/cm



```

Current Data Parameters
NAME      PK-VI-25-C18-C
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20120206
Time     13.16
INSTRUM  drx400
PROBHD   5 mm Multinu
PULPROG  zgpg30
TD        65536
SOLVENT  DMS-D3
NS        3144
DS        4
SMH       25125.629 Hz
FIDRES    0.383987 Hz
AQ         1.3042164 sec
RG         32768
DM         19.900 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00020000 sec

===== CHANNEL f1 =====
NUC1      13C
P1        16.00 usec
PL1       0.00 dB
SF01      100.6237959 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     102.00 usec
PL2       0.00 dB
PL12      23.00 dB
PL13      23.00 dB
SF02      400.1316005 MHz

F2 - Processing parameters
SI         131072
SF         100.6127759 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         20.00 cm
F1P       215.000 ppm
F1        21631.75 Hz
F2P       -5.000 ppm
F2        -503.06 Hz
PPHMC     11.00000 ppm/cm
HZCW     1106.74050 Hz/cm
  
```

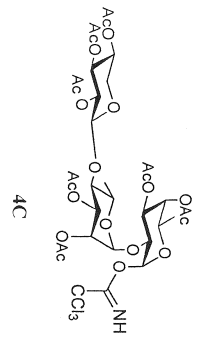


Current Data Parameters
 NAME QD-I-180-aH
 EXPNO 1
 PROCNO 1

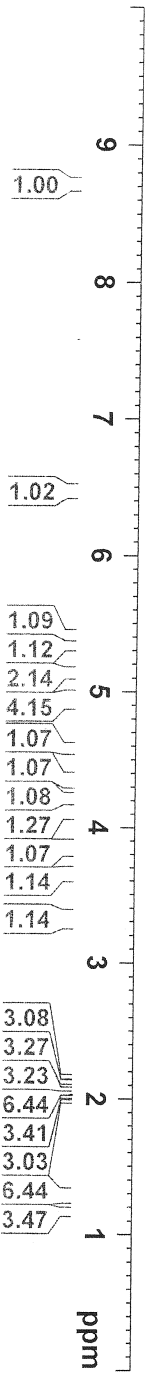
F2 - Acquisition Parameters
 Date_ 20130503
 Time_ 13.17
 INSTRUM spect
 PROBH1 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 322.5
 DW 80.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL F1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -2.50 dB
 SFO1 299.8818519 MHz

F2 - Processing parameters
 SI 32768
 SF 299.8800004 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



- 8.707
- 7.270
- 6.477
- 6.464
- 5.396
- 5.388
- 5.344
- 5.309
- 5.152
- 5.140
- 5.123
- 5.107
- 5.091
- 4.984
- 4.978
- 4.973
- 4.967
- 4.946
- 4.928
- 4.923
- 4.907
- 4.881
- 4.875
- 4.849
- 4.585
- 4.559
- 4.224
- 4.212
- 4.177
- 3.671
- 3.639
- 2.161
- 2.124
- 2.064
- 2.042
- 2.034
- 2.012
- 1.976
- 1.648
- 1.312
- 1.291
- 1.253
- 1.176
- 1.154





Current Data Parameters
 NAME QD-I-180-ac
 EXPNO 1
 PROCNO 1

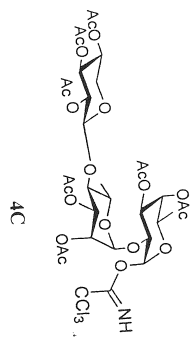
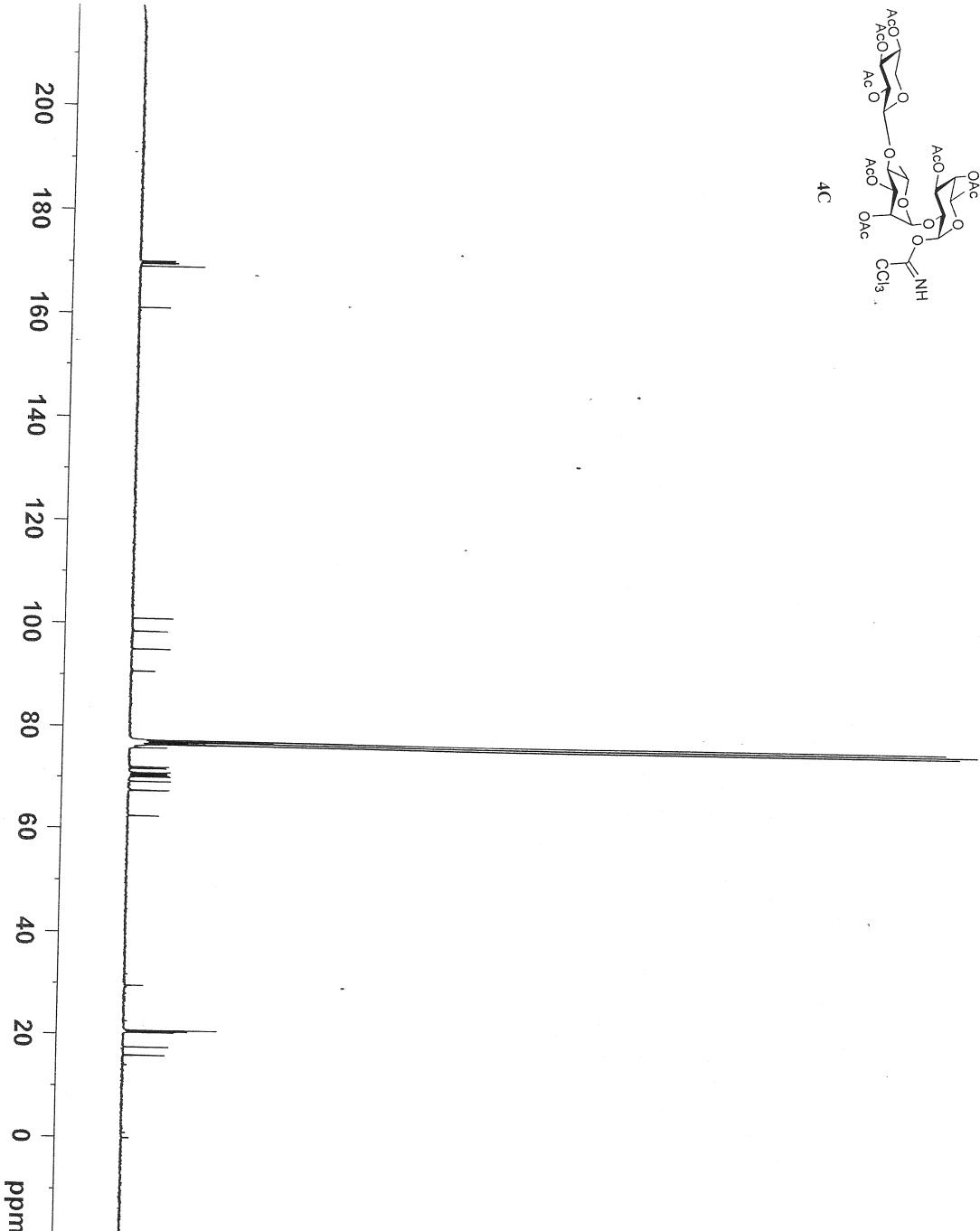
F2 - Acquisition Parameters

Date_ 20130503
 Time 17.35
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10240
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 32768
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUCL1 13C
 P1 8.00 usec
 PL1 -1.80 dB
 SFO1 75.4124265 MHz

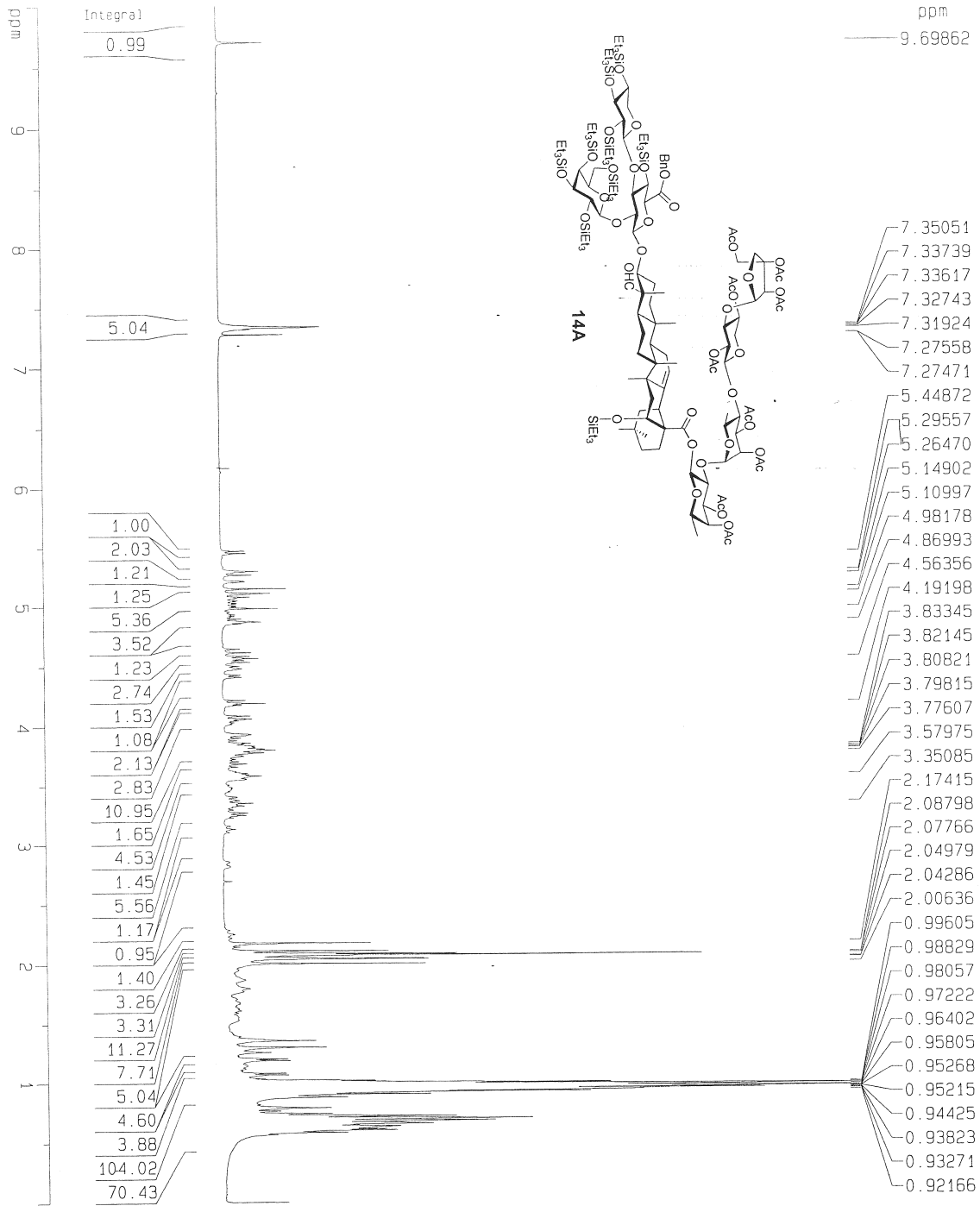
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUCC2 1H
 PCPD2 75.00 usec
 PL2 -2.50 dB
 PL12 11.48 dB
 PL13 12.00 dB
 SFO2 299.8811995 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4048867 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



- 170.29
- 170.17
- 170.09
- 169.90
- 169.78
- 169.29
- 161.14
- 100.96
- 98.47
- 95.06
- 90.82
- 77.43
- 77.31
- 77.00
- 76.59
- 75.89
- 72.11
- 71.79
- 71.02
- 70.84
- 70.58
- 70.32
- 70.12
- 69.27
- 67.56
- 67.47
- 62.53
- 29.78
- 29.68
- 29.67
- 29.63
- 29.60
- 29.54
- 29.36
- 17.53
- 15.96

PW-VI-59-2-C2A



Current Data Parameters

NAME PW-VI-59-2-C2A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20130308
 Time 9.08
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 57
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

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

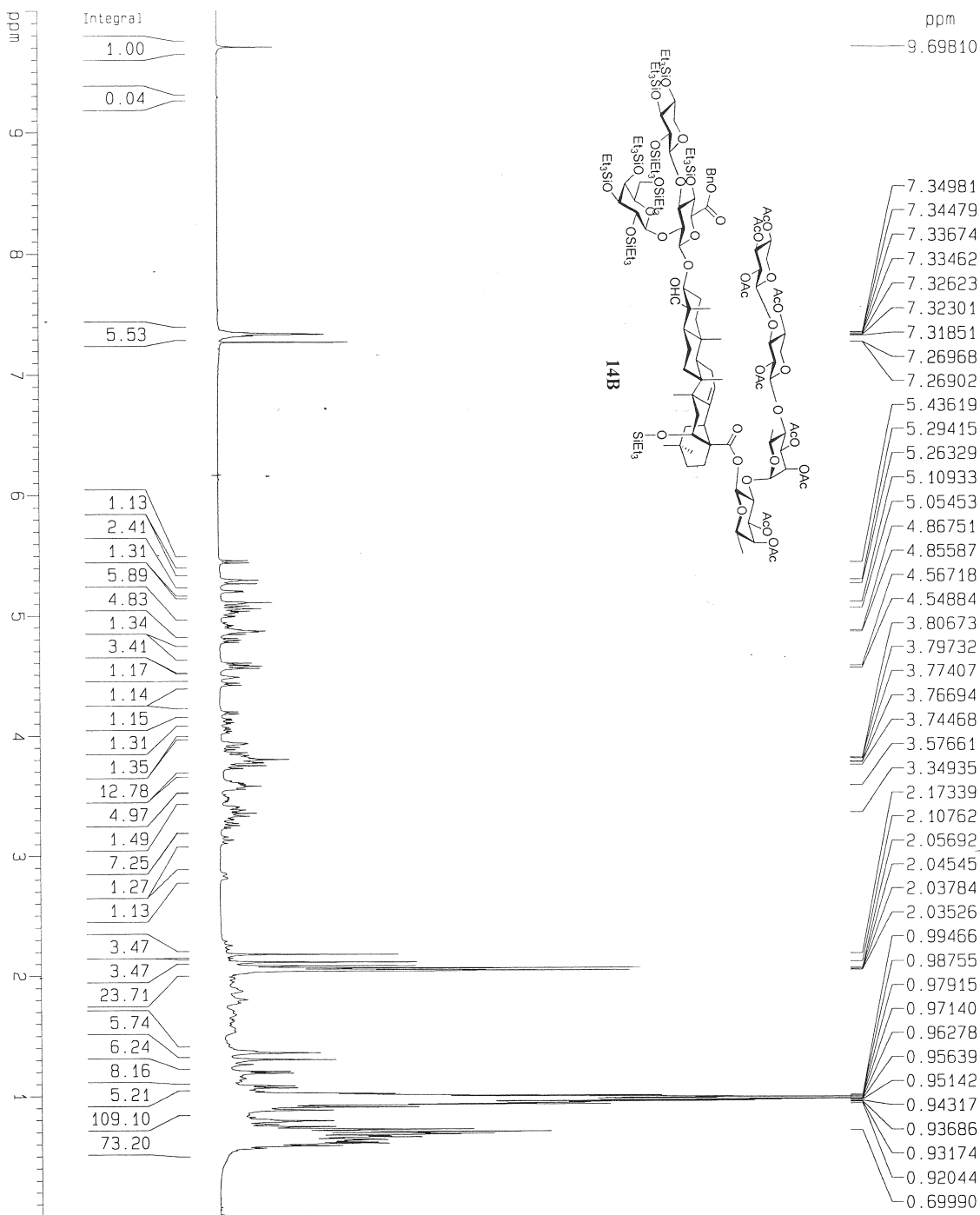
NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters

SF 400.130028 MHz
 SI 131072
 SF 400.130028 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

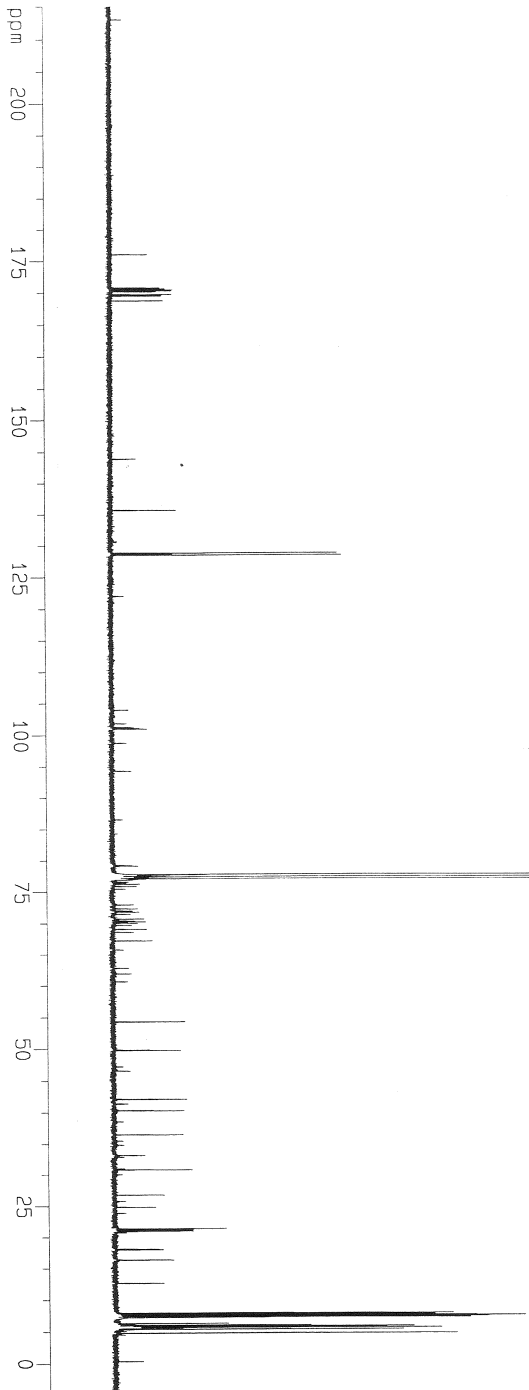
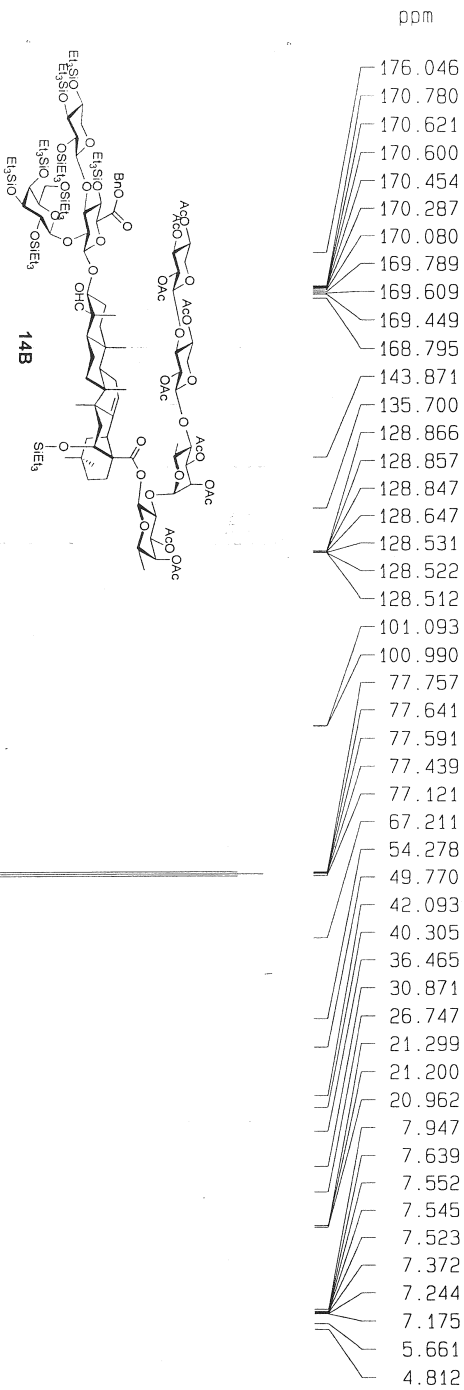
CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 0.50000 ppm/cm
 HZCM 200.06500 Hz/cm



Current Data Parameters
 NAME PM-VI-26-B-H
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20120211
 Time 12.34
 INSTRUM drx400
 PROBNR 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT CUC13
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 45.3
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 131072
 SF 400.1300054 MHz
 KW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPKCM 0.50000 ppm/cm
 HZCM 200.06500 Hz/cm

PW-VI-26-B-C13
 13C w/ 1H decoupling



```

Current Data Parameters
NAME      PW-VI-26-B-C13
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20120211
Time     12.43
INSTRUM  drx400
PROBHD   5 mm Multinu
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        26521
DS         4
SWH       25125.629 Hz
FIDRES    0.38387 Hz
AQ         1.3042164 sec
RG         32768
DE         19.900 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00002000 sec

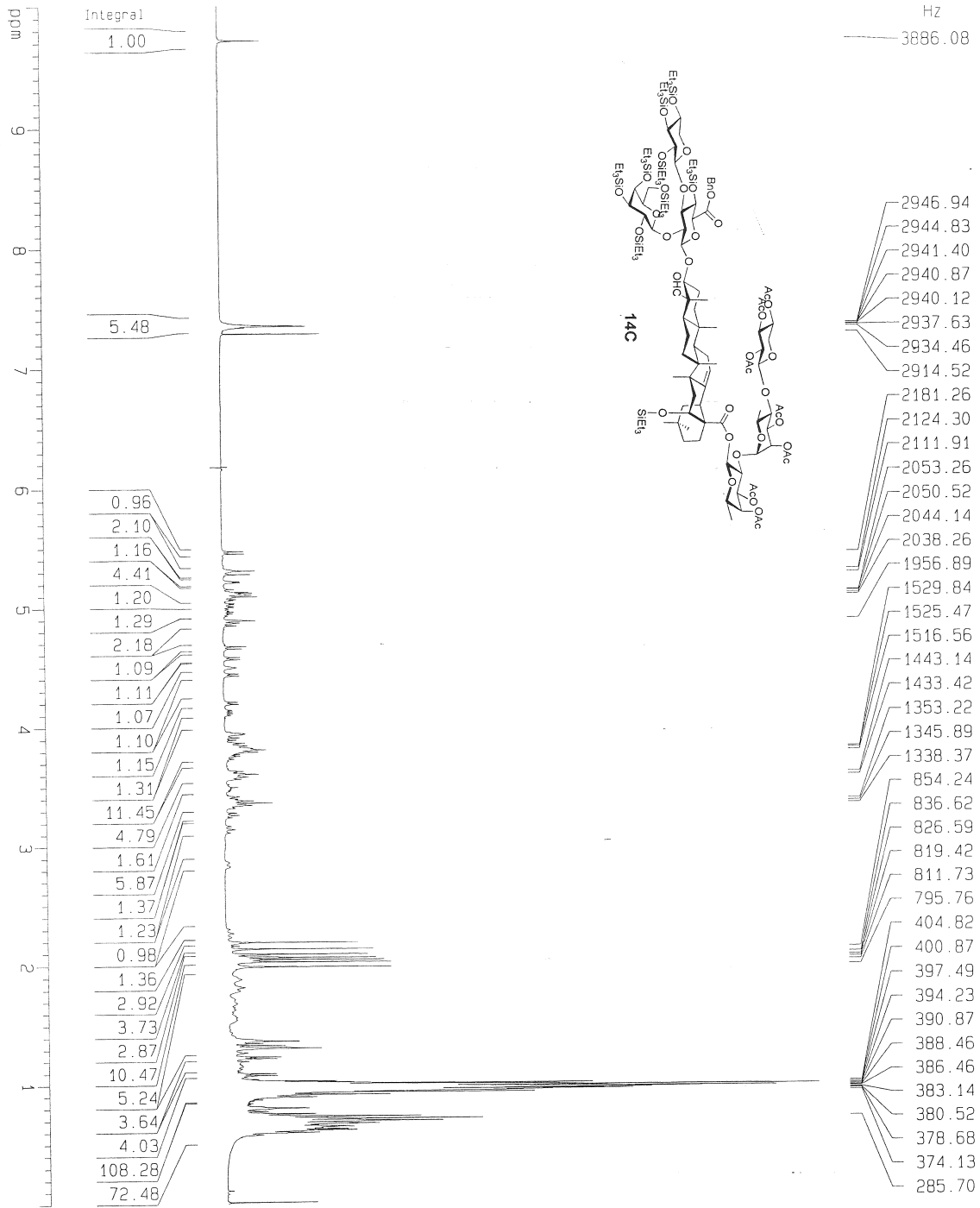
===== CHANNEL f1 =====
NUC1      13C
P1        16.00 usec
PL1       0.00 dB
SF01      100.6237959 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     102.00 usec
PL2       0.00 dB
PL12      23.00 dB
PL13      23.00 dB
SF02      400.1316005 MHz

F2 - Processing parameters
SI         131072
SF         100.6127290 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

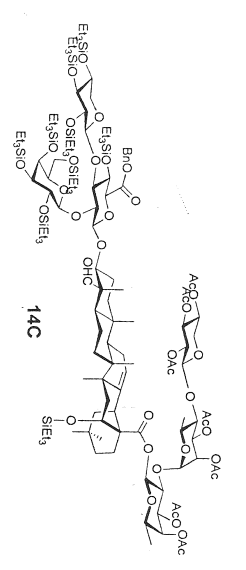
1D NMR plot parameters
CX         20.00 cm
F1P        215.000 ppm
F1         21631.74 Hz
F2P        -5.000 ppm
F2         -503.06 Hz
PPM/CW     11.00000 ppm/cm
HZ/CW     1106.73999 Hz/cm
  
```

PW-VI-57-C3A



Integral
1.00

Hz
3886.08



ppm
9
8
7
6
5
4
3
2
1

0.96
2.10
1.16
4.41
1.20
1.29
2.18
1.09
1.11
1.07
1.10
1.15
1.31
11.45
4.79
1.61
5.87
1.37
1.23
0.98
1.36
2.92
3.73
2.87
10.47
5.24
3.64
4.03
108.28
72.48

2946.94
2944.83
2941.40
2940.87
2940.12
2937.63
2934.46
2914.52
2181.26
2124.30
2111.91
2053.26
2050.52
2044.14
2038.26
1956.89
1529.84
1525.47
1516.56
1443.14
1433.42
1353.22
1345.89
1338.37
854.24
836.62
826.59
819.42
811.73
795.76
404.82
400.87
397.49
394.23
390.87
388.46
386.46
383.14
380.52
378.68
374.13
285.70

Current Data Parameters
NAME PW-VI-57-C3a
EXPNO 1
PROCNO 1

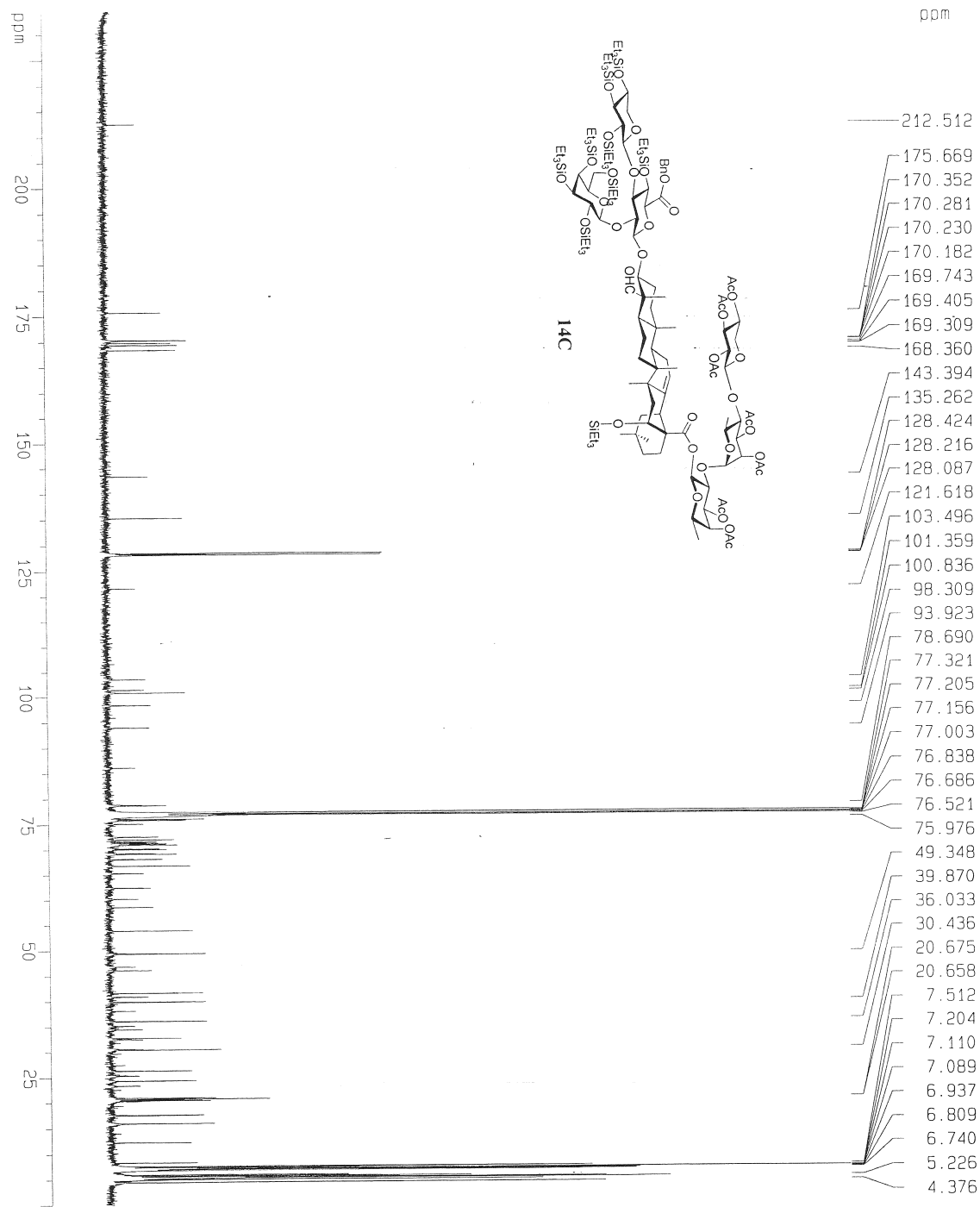
F2 - Acquisition Parameters
Date_ 20130306
Time 14.52
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 64
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.50 usec
PL1 0.00 dB
SF01 400.1324710 MHz

F2 - Processing Parameters
SI 131072
SF 400.1299995 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.50000 ppm/cm
HZCM 200.06500 Hz/cm

PW-VI-57-C3C13



```

Current Data Parameters
NAME      PW-VI-57-C3C13
EXPNO     1
PROCNO    1

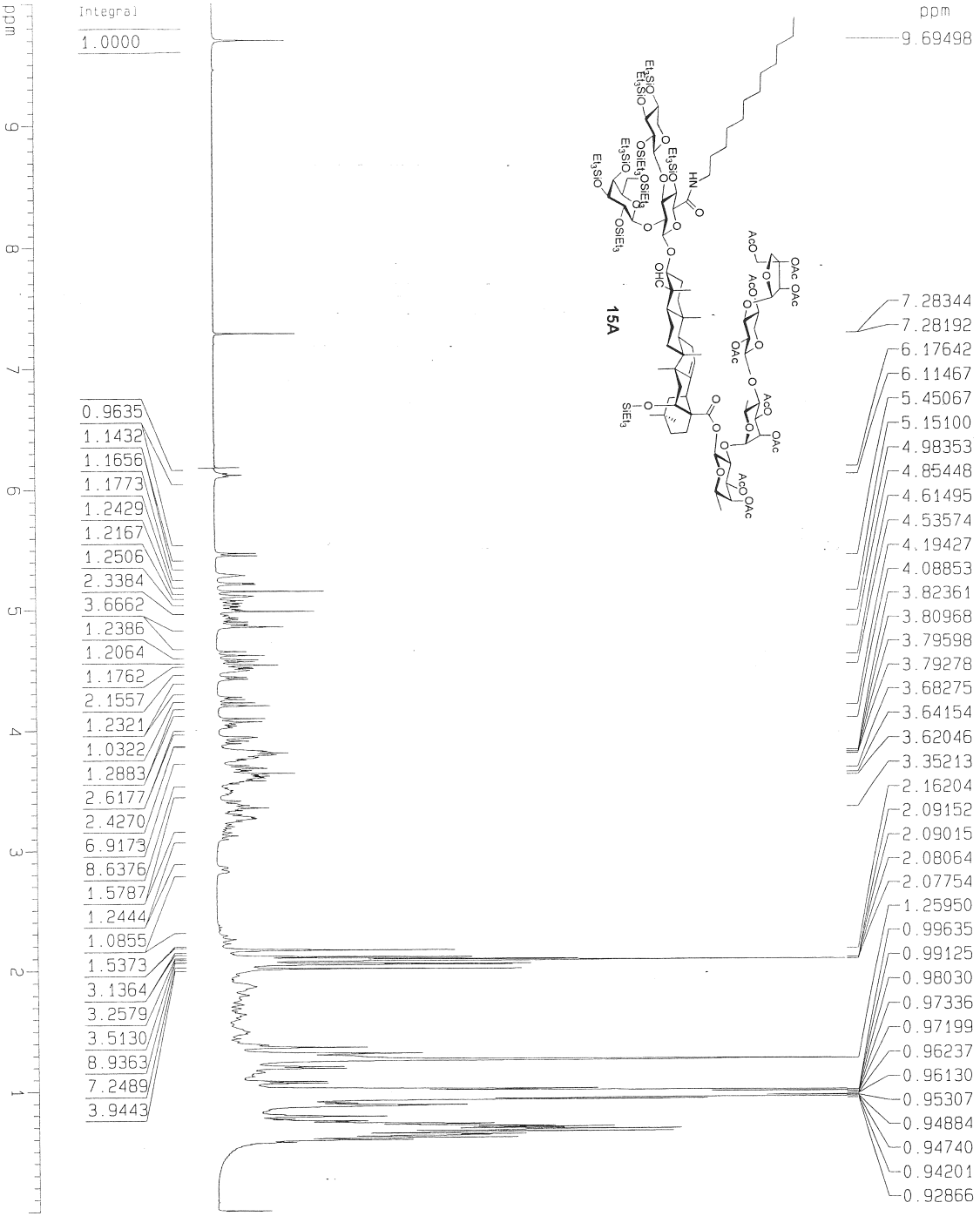
F2 - Acquisition Parameters
Date_     20130306
Time      15.52
INSTRUM   drx400
PROBHD    zgpg30
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16522
DS         4
SWH        25125.629 Hz
FIDRES     0.38387 Hz
AQ         1.3042184 sec
RG         32768
DE         19.500 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00020000 sec

===== CHANNEL f1 =====
NUC1      13C
P1         16.00 usec
PL1        0.00 dB
SF01      100.627959 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      102.00 usec
PL2         0.00 dB
PL12       23.00 dB
PL13       23.00 dB
SF02      400.1315005 MHz

F2 - Processing parameters
SI         131072
SF         100.6127727 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         20.00 cm
F1P        235.000 ppm
F1         236.4400 Hz
F2P        0.000 ppm
F2         0.00 Hz
PPMCK      11.75000 ppm/cm
HZCM       1.18220007 Hz/cm
  
```



Current Data Parameters
 NAME PW-VI-63-3-h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130320
 Time 15.36

INSTRUM drx400

PROBHD 5 mm Multinu

PULPROG zg30

TD 65536

SOLVENT CDCl3

NS 16

DS 2

SWH 8278.146 Hz

FTORES 0.126314 Hz

AQ 3.9584243 sec

RG 40.3

DW 60.400 usec

DE 5.00 usec

TE 300.0 K

D1 1.00000000 sec

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

NUC1 1H

P1 6.50 usec

PL1 0.00 dB

SFO1 400.1324710 MHz

F2 - Processing parameters

SI 131072

SF 400.1299997 MHz

WDW no

SSB 0

LB 0.00 Hz

GB 0

PC 1.00

1D NMR p1ot parameters

CX 20.00 cm

F1P 10.000 ppm

F1 4001.30 Hz

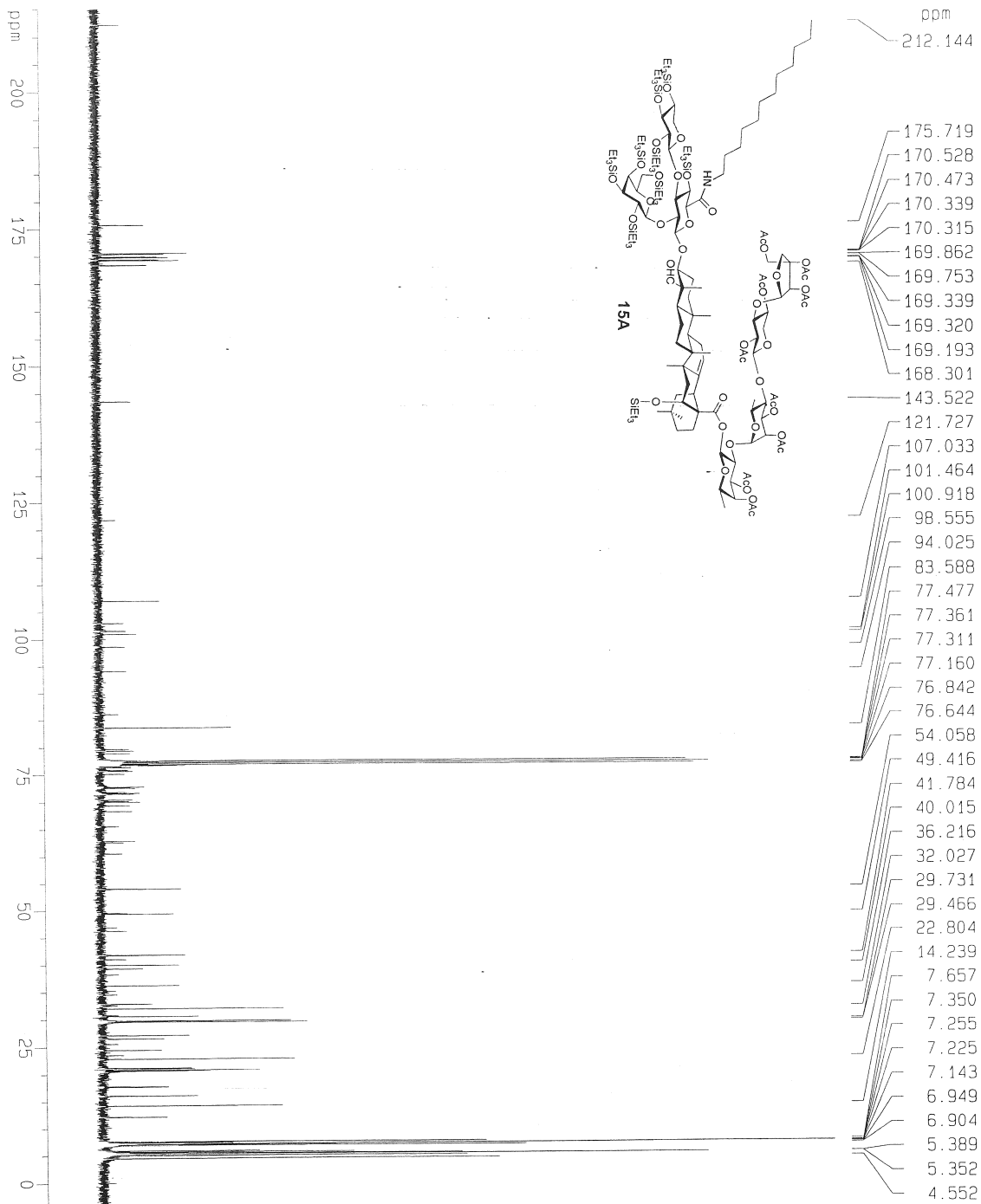
F2P 0.000 ppm

F2 0.00 Hz

PPMKCM 0.50000 pDm/cm

HZCM 200.06500 Hz/cm

PW-VI-63-3-C13



Current Data Parameters
 NAME PW-VI-63-3C13
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130320
 Time 15:57
 INSTRUM drx400
 PROBHD 5 mm MUltinu
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1782
 DS 4
 SMH 25125.629 Hz
 FIDRES 0.38387 Hz
 AQ 1.3042164 sec
 RG 32768
 DW 19.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 D12 0.0002000 sec

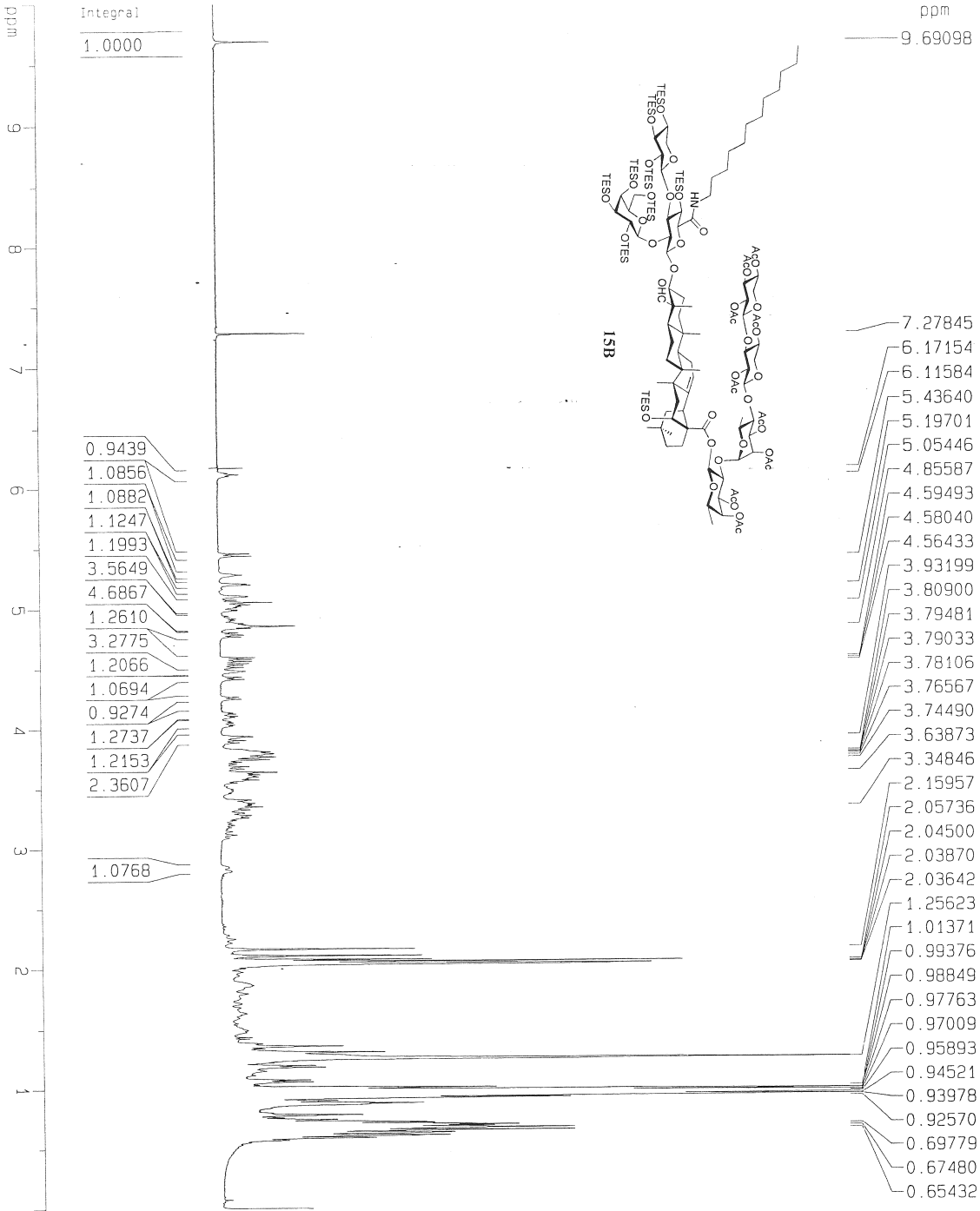
==== CHANNEL f1 =====
 NUC1 13C
 P1 16.00 usec
 PL1 0.00 dB
 SF01 100.6237959 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 102.00 usec
 PL2 0.00 dB
 PL12 23.00 dB
 PL13 23.00 dB
 SF02 400.1315005 MHz

F2 - Processing parameters
 SI 131072
 SF 100.6127564 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 215.000 dpm
 F1 21631.74 Hz
 F2P -5.000 dpm
 F2 -503.06 Hz
 PPMCM 11.00000 dpm/cm
 HZCM 1106.74036 Hz/cm

PW-VI-40-H



Integral
1.0000

- 0.9439
- 1.0856
- 1.0882
- 1.1247
- 1.1993
- 3.5649
- 4.6867
- 1.2610
- 3.2775
- 1.2066
- 1.0694
- 0.9274
- 1.2737
- 1.2153
- 2.3607

1.0768

ppm
9.69098

- 7.27845
- 6.17154
- 6.11584
- 5.43640
- 5.19701
- 5.05446
- 4.85587
- 4.59493
- 4.58040
- 4.56433
- 3.93199
- 3.80900
- 3.79481
- 3.79033
- 3.78106
- 3.76567
- 3.74490
- 3.63873
- 3.34846
- 2.15957
- 2.05736
- 2.04500
- 2.03870
- 2.03642
- 1.25623
- 1.01371
- 0.99376
- 0.98849
- 0.97763
- 0.97009
- 0.95893
- 0.94521
- 0.93978
- 0.92570
- 0.69779
- 0.67480
- 0.65432

```

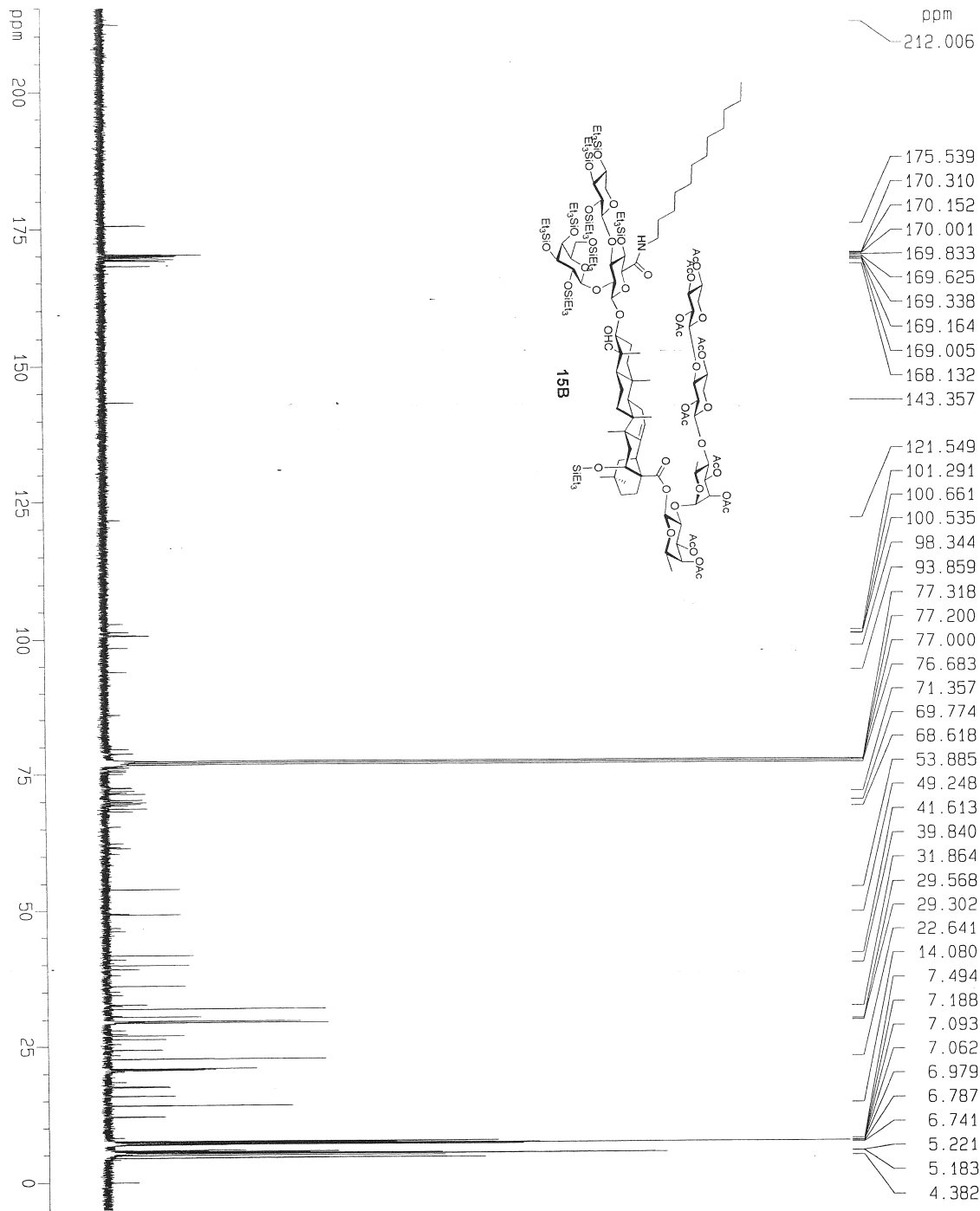
Current Data Parameters
NAME PW-VI-40-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121008
Time 16.28
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zg30
TD 65536
SOLVENT COC13
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 40.3
DE 60.400 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.50 usec
PL1 0.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 131072
SF 400.1300015 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.50000 ppm/cm
HZCM 200.06500 Hz/cm
  
```



13C w/ 1H decoupling

Current Data Parameters

NAME PW-VI-40-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20121008
Time 16.52
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zpg30
TO 65536
SOLVENT CDCl3
NS 16311
DS 4
SMH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 32768
DM 19.900 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

CHANNEL f1

NUC1 13C
P1 16.00 usec
PL1 0.00 dB
SF01 100.6237959 MHz

CHANNEL f2

CPDPRG2 waltz16
NUC2 1H
PCPD2 102.00 usec
PL2 0.00 dB
PL12 23.00 dB
PL13 23.00 dB
SF02 400.1316005 MHz

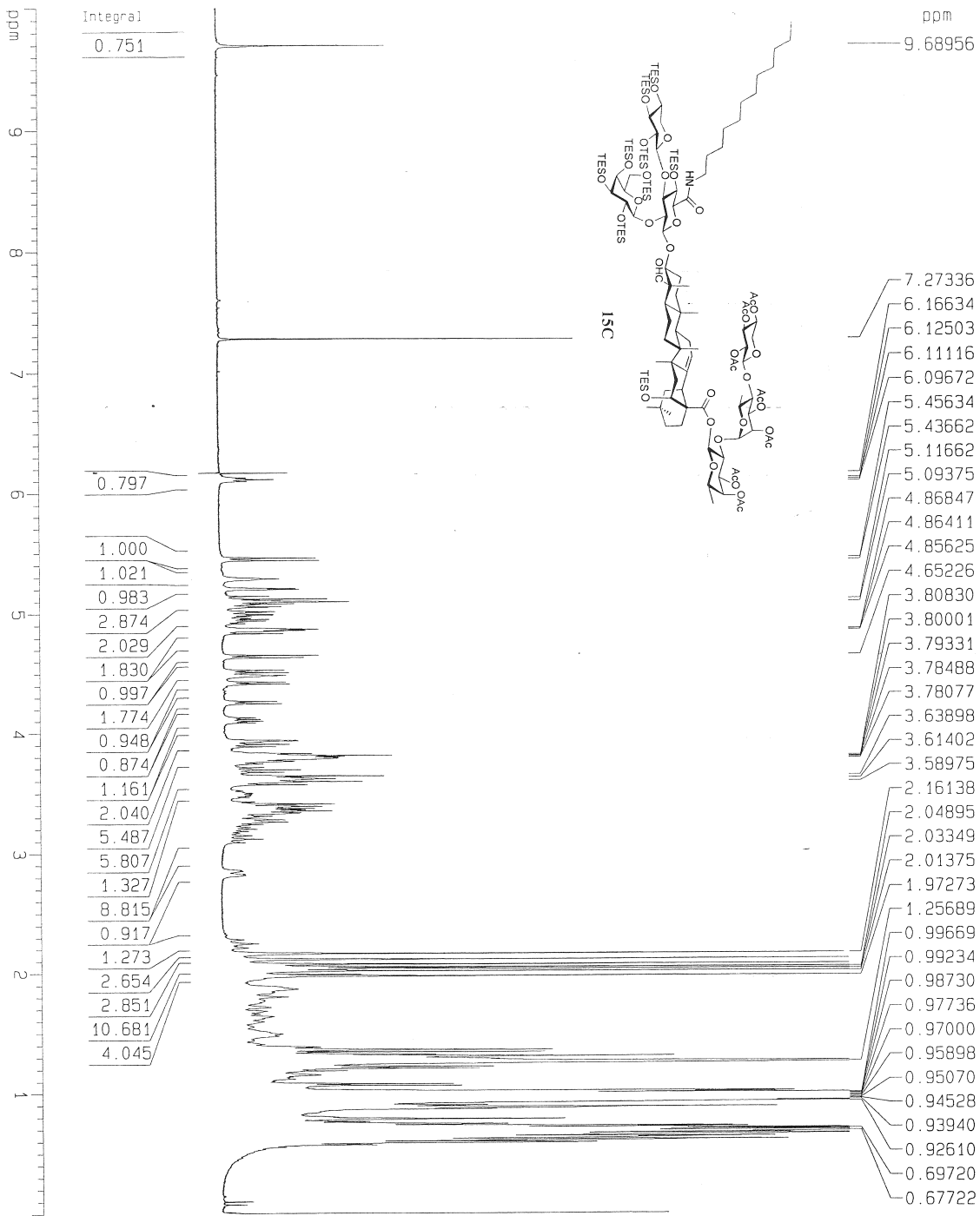
F2 - Processing parameters

SF 131072
SF 100.6127736 MHz
KIDK no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
F1P 215.000 ppm
F1 21631.75 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCK 11.00000 ppm/cm
HZCM 1106.74048 Hz/cm

PW-VI-62-C2-H



Current Data Parameters
 NAME PW-VI-62-C2-H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130315
 Time 15.57
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 50.8
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUCl1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

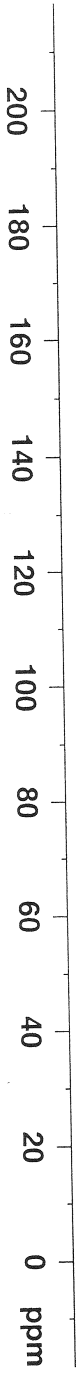
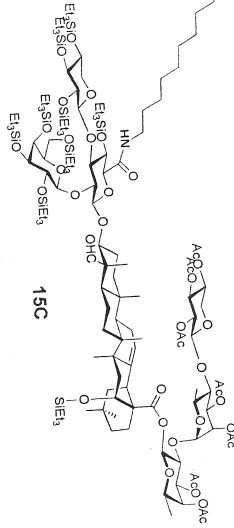
F2 - Processing parameters
 S1 131072
 SF 400.1300036 MHz
 WDM no
 SSB no
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCK 0.50000 ppm/cm
 HZCM 200.06500 Hz/cm

VI-62

700MHz

170.33
170.28
170.21
169.44
169.35
169.31
169.29
109.89
98.40
77.23
77.05
76.86
76.00
72.01
71.15
70.95
69.14
68.17
58.60
53.93
49.31
41.66
39.89
39.22
36.10
32.78
31.92
30.47
29.71
29.66
29.63
29.61
29.60
29.36
29.33
26.99
26.37
24.35
22.70
20.97
20.92
20.72
20.70
20.54
20.41
17.64
17.50
15.92
15.90
14.15
12.10
8.32
7.96
7.46
7.25
7.16
7.13
7.04
6.85
6.80
5.86
5.65
5.43
5.34
5.27
5.24
4.96
4.43



```

NAME PW-VI-62
EXPNO 702
PROCNO 1
Date_ 20130315
Time 9.02
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 3829
DS 4
SWH 41666.668 Hz
FIDRES 0.635783 Hz
AQ 0.7864820 sec
RG 64
DW 12.000 usec
DE 20.00 usec
TE 298.0 K
D1 3.20000005 sec
D11 0.03000000 sec
TD0 1

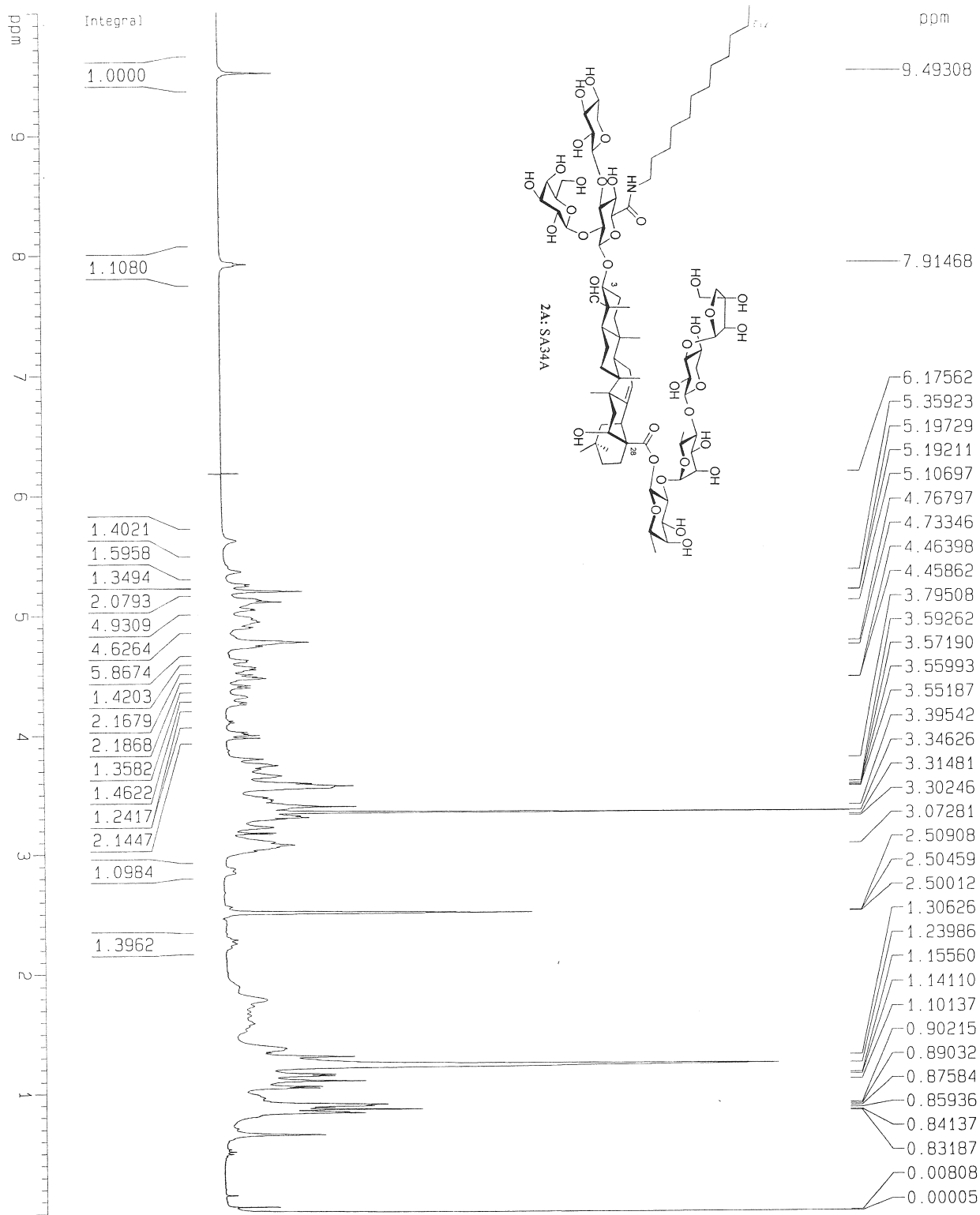
===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 -1.30 dB
PL1W 128.76077271 W
SFO1 176.0377710 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 65.00 usec
PL2 1.30 dB
PL12 19.50 dB
PL13 19.50 dB
PL2W 6.88972235 W
PL12W 0.10428017 W
PL13W 0.10428017 W
SFO2 700.0228001 MHz
SI 131072
SF 176.0201697 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```



PW-VI-65-4



Current Data Parameters
 NAME PW-VI-65-4
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20130416
 Time 9.01
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SMH 8278.146 HZ
 FIDRES 0.126314 HZ
 AQ 3.9584243 sec
 RG 90.5
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

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

NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

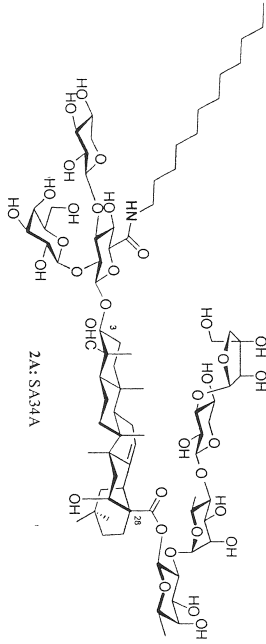
F2 - Processing parameters

SF 131072
 SF 400.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 HZ
 GB 0
 PC 1.00

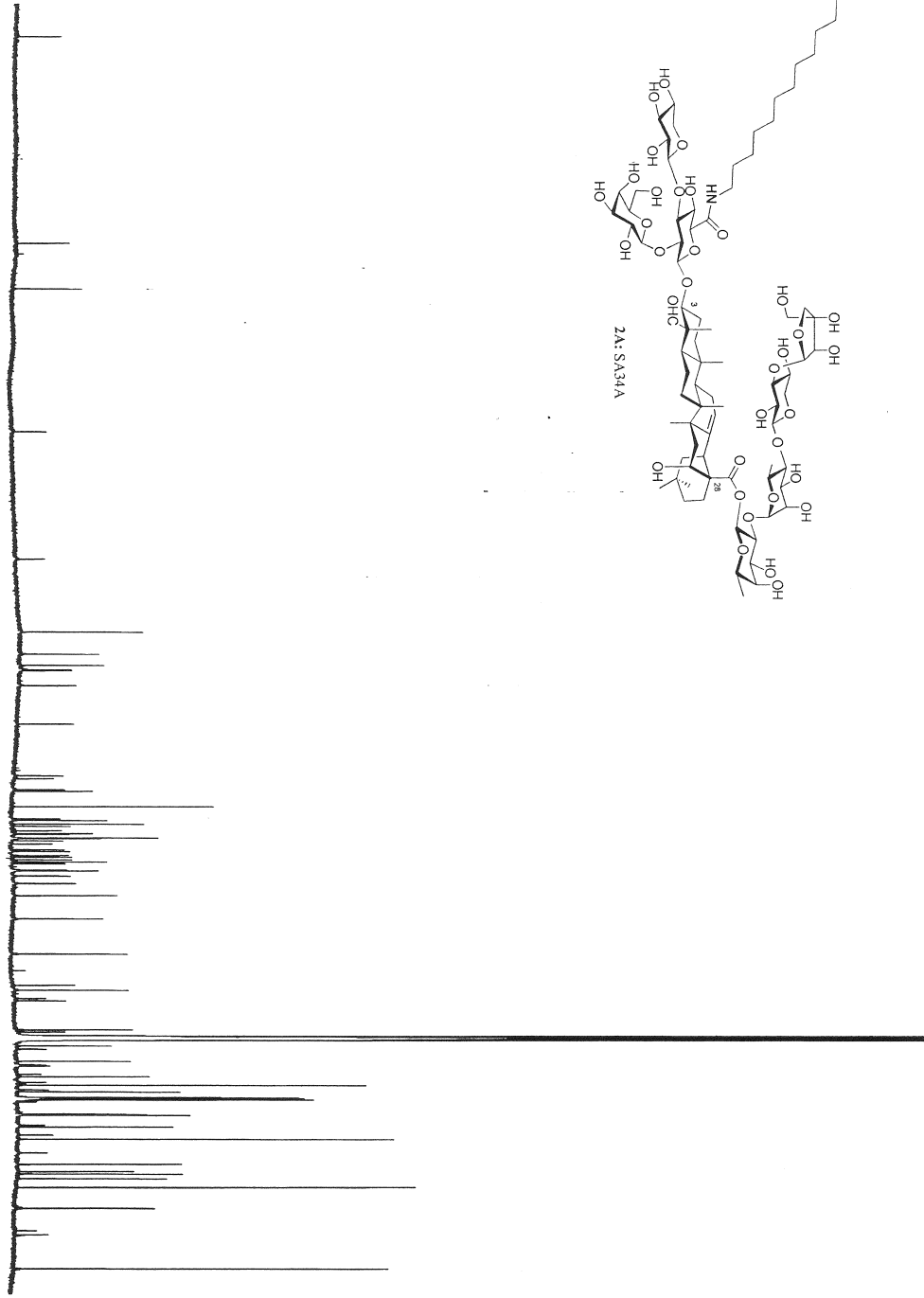
1D NMR plot parameters

CX 20.00 cm
 F4P 10.000 ppm
 F1 4001.30 HZ
 F2P 0.000 ppm
 F2 0.00 HZ
 PPMCM 0.50000 ppm/cm
 HZCM 200.06500 HZ/cm

VI-65-4
700MHz



200 180 160 140 120 100 80 60 40 20 ppm



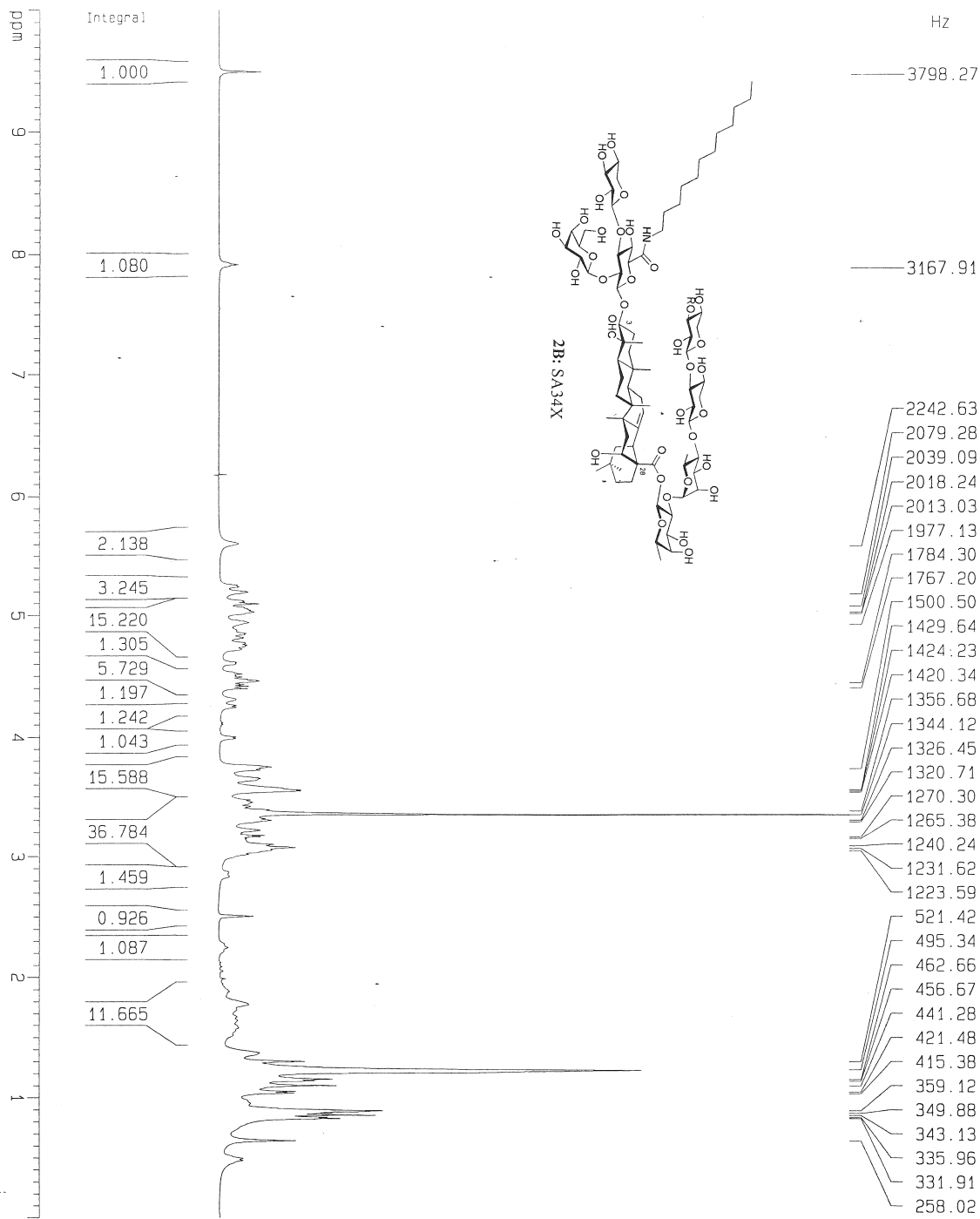
```

NAME VI-65-4a
EXPNO 702
PROCNO 1
Date_ 20130417
Time 16.39
INSTRUM spect
PROBHD 5 mm CPXI 1H-
PULPROG zgpg30
TD 65336
SOLVENT DMSO
NS 4096
DS 4
SWH 41666.668 Hz
FIDRES 0.635783 Hz
AQ 0.7864820 sec
RG 64
DW 12.000 usec
DE 20.00 usec
TE 306.4 K
D1 4.19999981 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL F1 =====
NUC1 13C
P1 11.00 usec
PL1 -1.30 dB
PL1W 128.76077271 W
SFO1 176.0395312 MHz

===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 65.00 usec
PL2 1.30 dB
PL12 19.50 dB
PL13 19.50 dB
PL2W 6.88972235 W
PL12W 0.10428017 W
PL13W 0.10428017 W
SFO2 700.0228001 MHz
SI 131072
SF 176.0202699 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```



Current Data Parameters
 NAME PW-VI-448
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121016
 Time 12.23
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 64
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 S1 131072
 SF 400.1300000 MHz
 KDW no
 SSB no
 LB 0.00 Hz
 GB 0
 PC 1.00

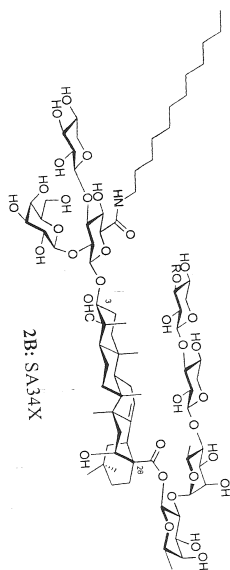
1D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPKCM 0.50000 ppm/cm
 HZCM 200.06500 Hz/cm

PW-VI-43B-DMSO

After H-D exchange to remove all OH's peaks.

Hz

3814.63



- 2296.05
- 2112.19
- 2105.04
- 2077.17
- 1820.64
- 1807.11
- 1793.51
- 1786.13
- 1529.02
- 1522.98
- 1508.02
- 1491.34
- 1453.94
- 1451.89
- 1448.03
- 1294.97
- 1035.45
- 1033.65
- 1031.84
- 837.47
- 835.00
- 832.54
- 830.07
- 827.60
- 544.01
- 518.46
- 511.73
- 492.56
- 486.78
- 464.91
- 381.12
- 366.45
- 359.18
- 356.43

Integral

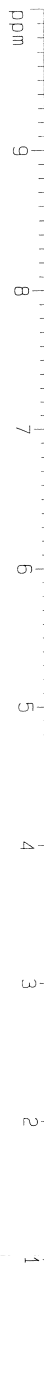
1.0000

2.2535
1.1517

1.1935
3.5192
2.5879

1.3126

1.3357



```

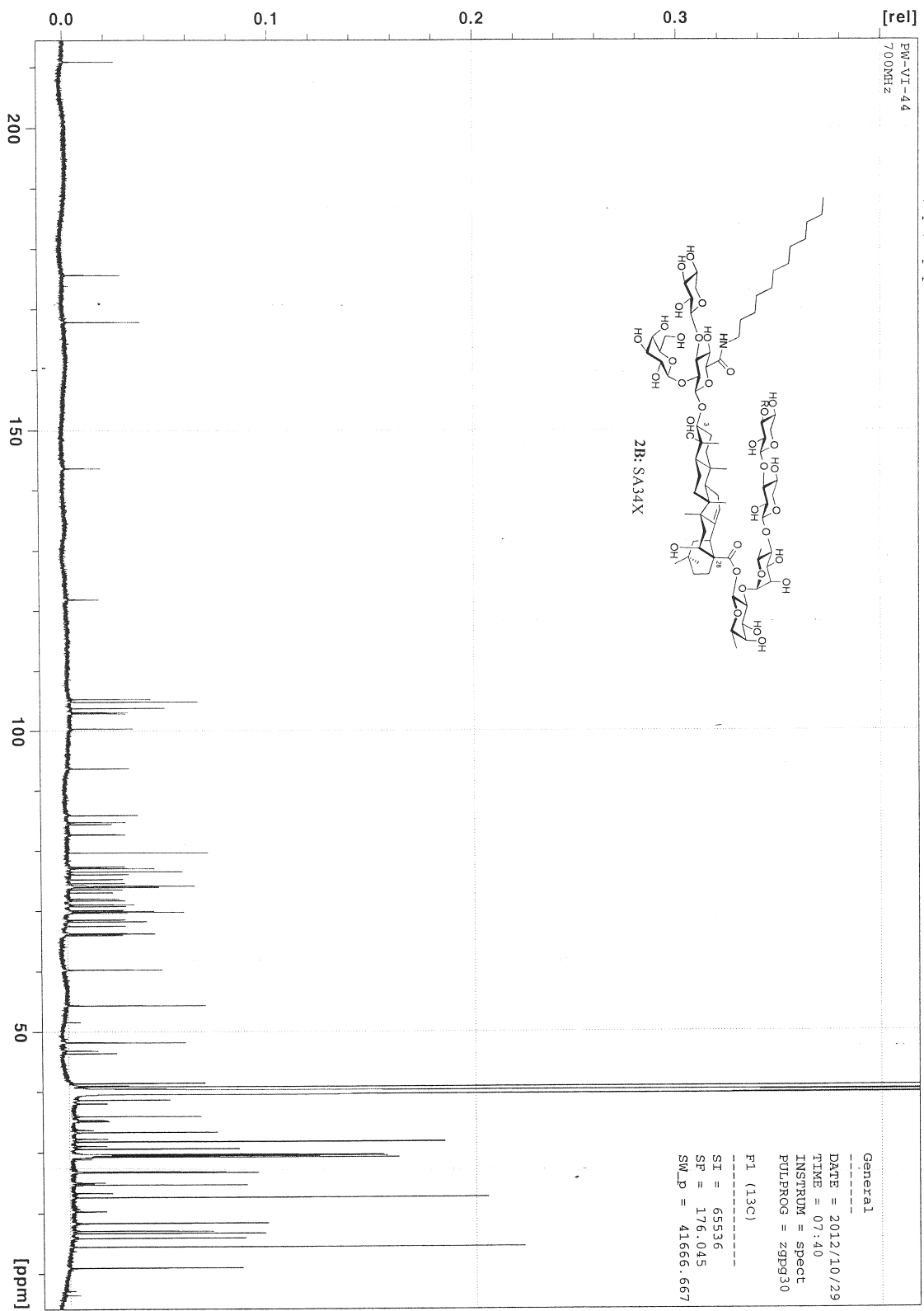
Current Data Parameters
NAME      PW-VI-43B-DMSO
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20121011
Time      8:54
INSTRUM   drx400
PROBHD    5 mm Multinu
PULPROG   zg30
TD         65536
SOLVENT   D2O
NS         64
DS         2
SWH        8278.146 Hz
FIDRES     0.126314 Hz
AQ         3.9584243 sec
RG         143.7
DE         60.400 usec
TE         300.0 K
D1         1.00000000 sec

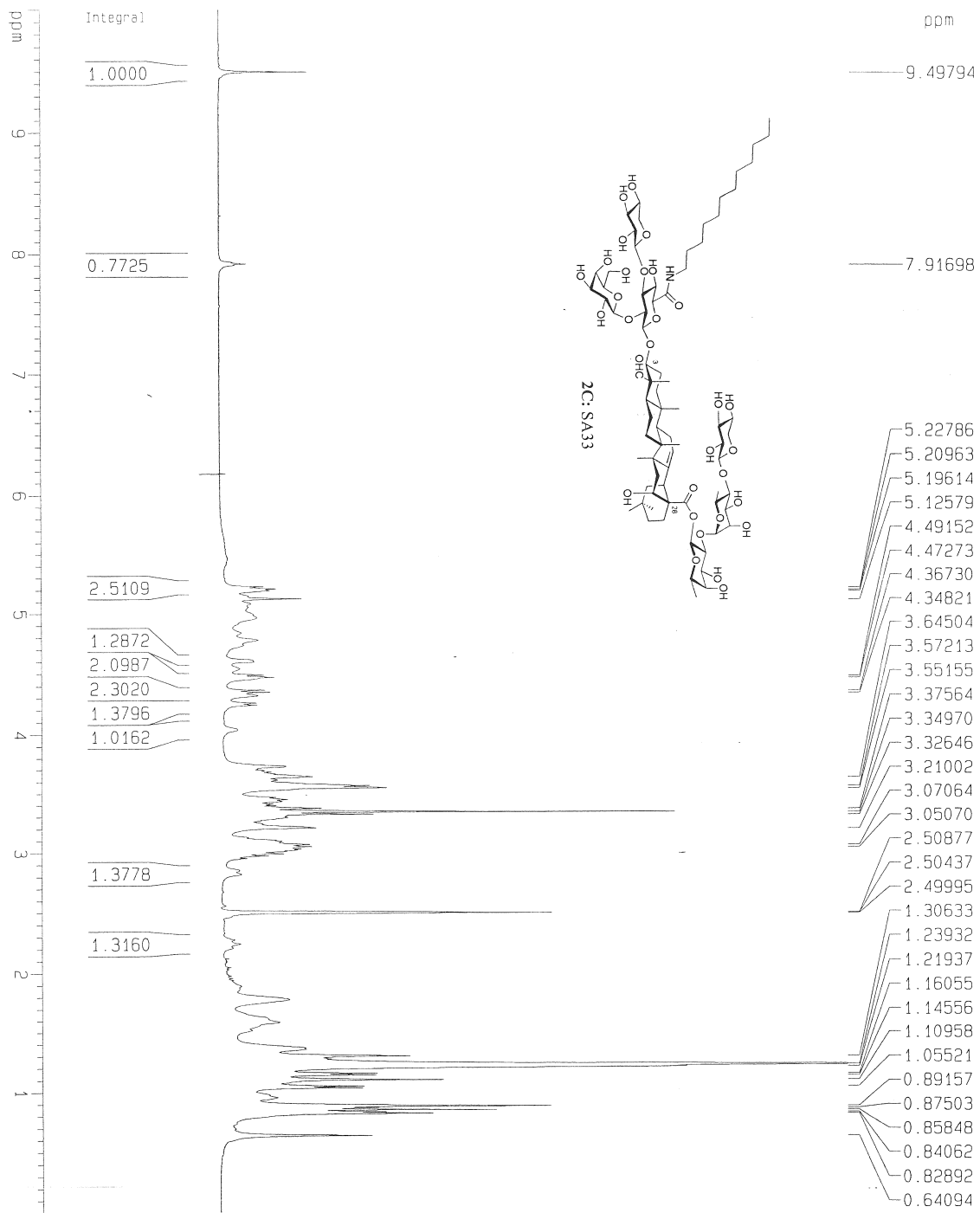
===== CHANNEL f1 =====
NUC1       1H
P1         6.50 usec
PL1        0.00 dB
SF01       400.1324710 MHz

F2 - Processing parameters
S1         131072
SF         400.1299693 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00

1D NMR plot parameters
CX         20.00 cm
F1P        10.000 ppm
F1         4001.30 Hz
F2P        0.000 ppm
F2         0.00 Hz
PPMCM      0.50000 ppm/cm
HZCM       200.06499 Hz/cm
  
```



PW-VI-64-2-H



Current Data Parameters
 NAME PW-VI-64-2-H
 EXPNO 1
 PROCNO 1

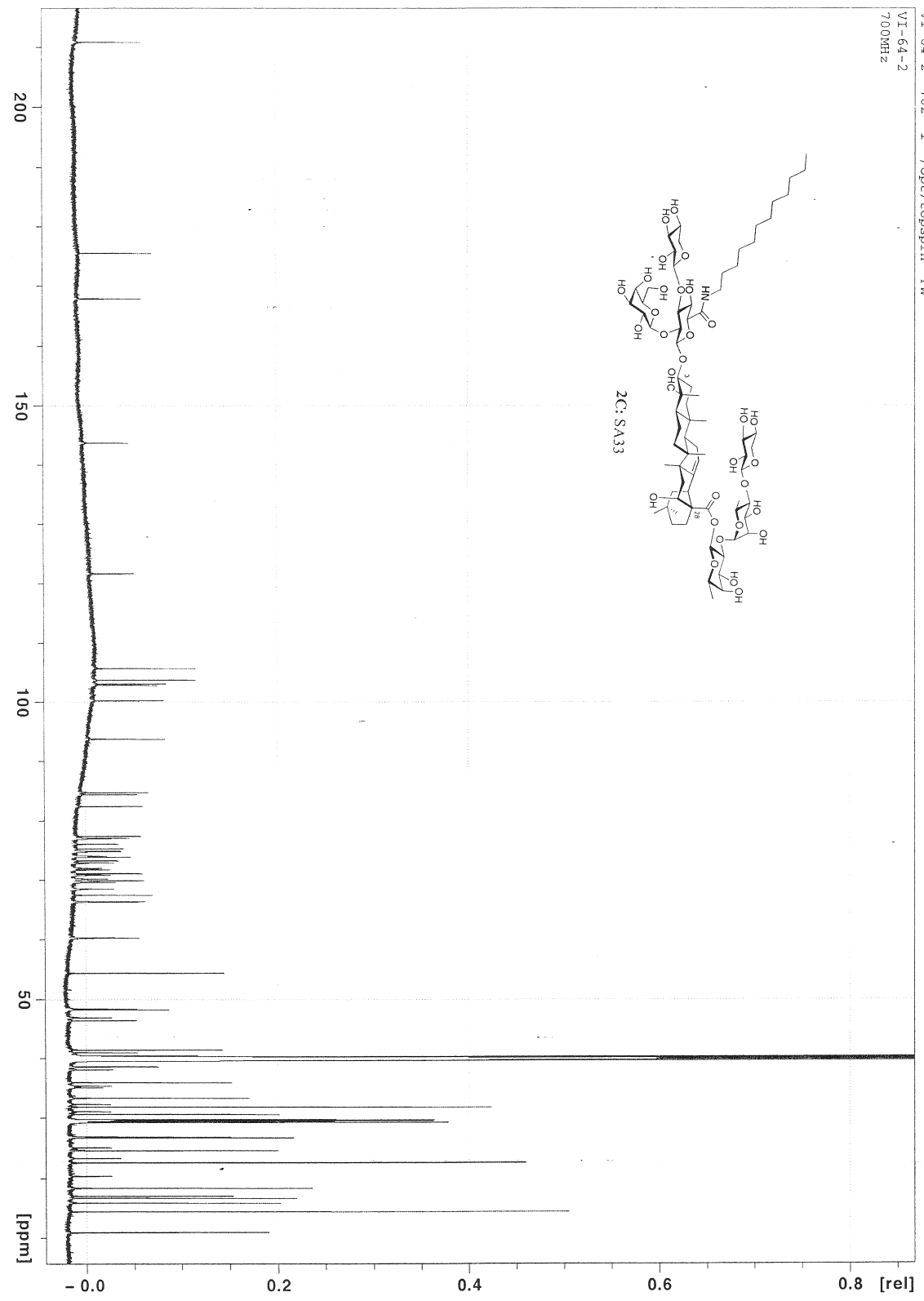
F2 - Acquisition Parameters
 Date_ 20130328
 Time 15.39
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 80.5
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

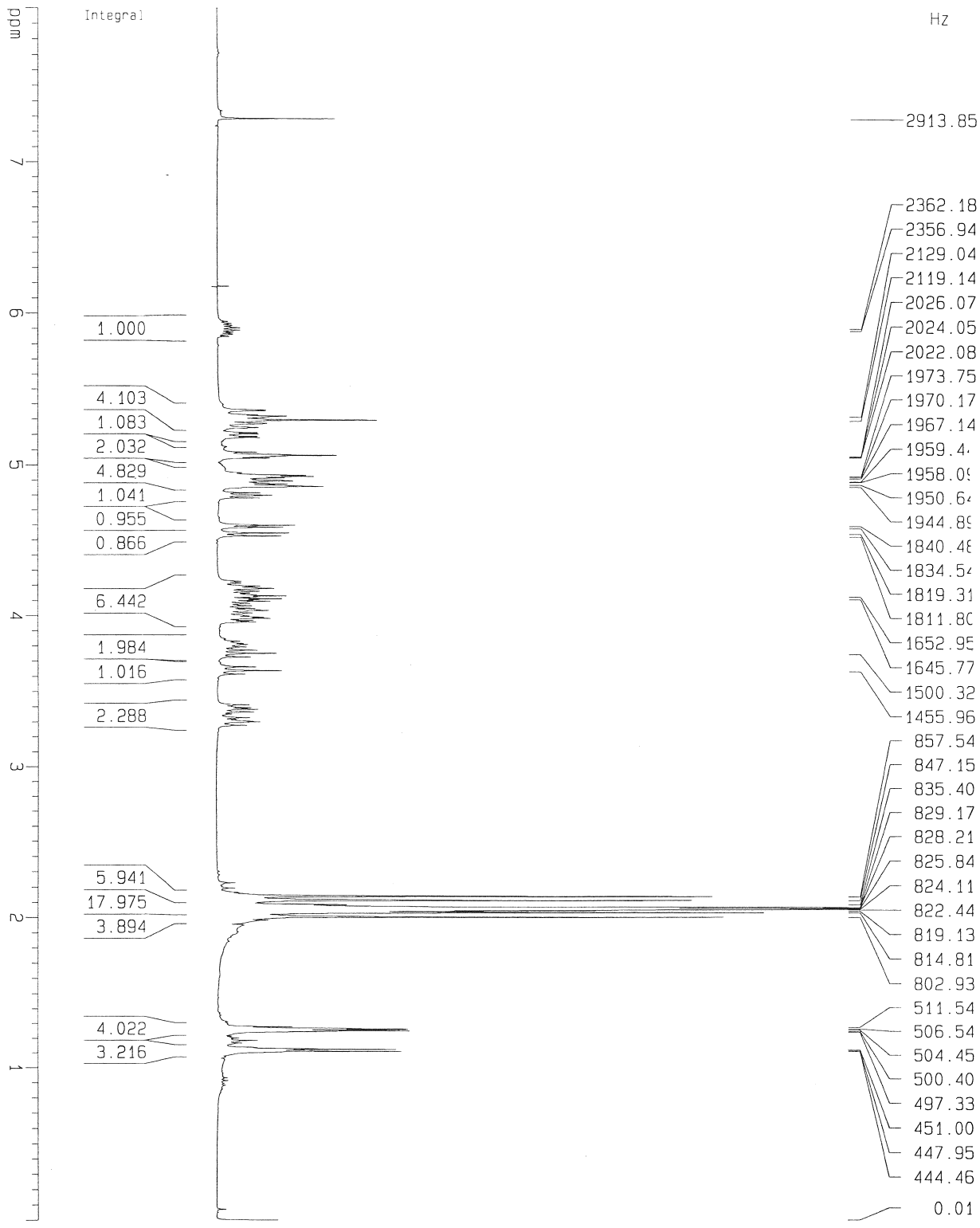
===== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 131072
 SF 400.1300000 MHz
 WDW no
 SSB no
 LB 0
 GB 0
 PC 1.00

1D NMR plot parameters
 CK 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPKCM 0.50000 ppm/cm
 HZCM 200.06500 Hz/cm

VI-64-2 702 1 /opt/lopssp1n PW
VI-64-2
700MHz





Current Data Parameters
 NAME PW-VI-5
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120105
 Time 13.52
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 101.6
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 S1 131072
 SF 400.1300002 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 3201.04 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCK 0.40000 ppm/cm
 HZCM 160.05200 Hz/cm