

## **SUPPLEMENTARY DATA**

### **Chemo-Enzymatic Synthesis of C-9 Acetylated Sialosides**

Jana Rauvolfova, Andre Venot, Geert-Jan Boons\*

Complex Carbohydrate Research Center, University of Georgia, 315 Riverbend Road,  
Athens, Georgia 30602, USA.

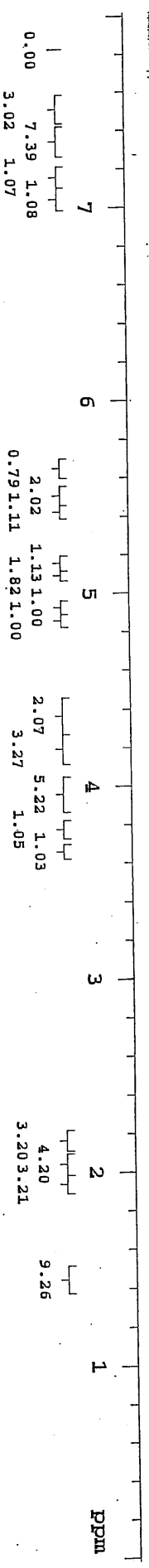
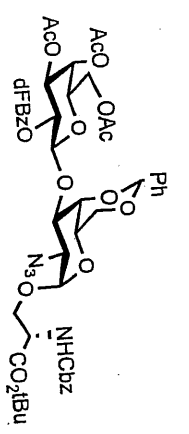
\*Corresponding author. Fax: (706)-542-4412; E-mail: [gjboons@ccrc.uga.edu](mailto:gjboons@ccrc.uga.edu).

Archive directory: /export/home/avenot/vmmr/sys/data  
 Sample directory: /export/home/avenot/vmmr/sys/data/avenot\_260an2005  
 File: PROTON

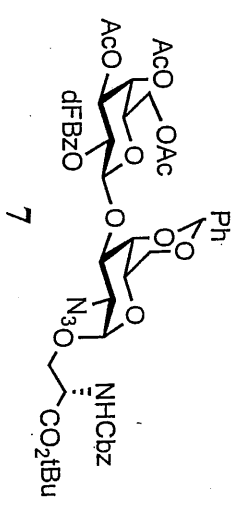
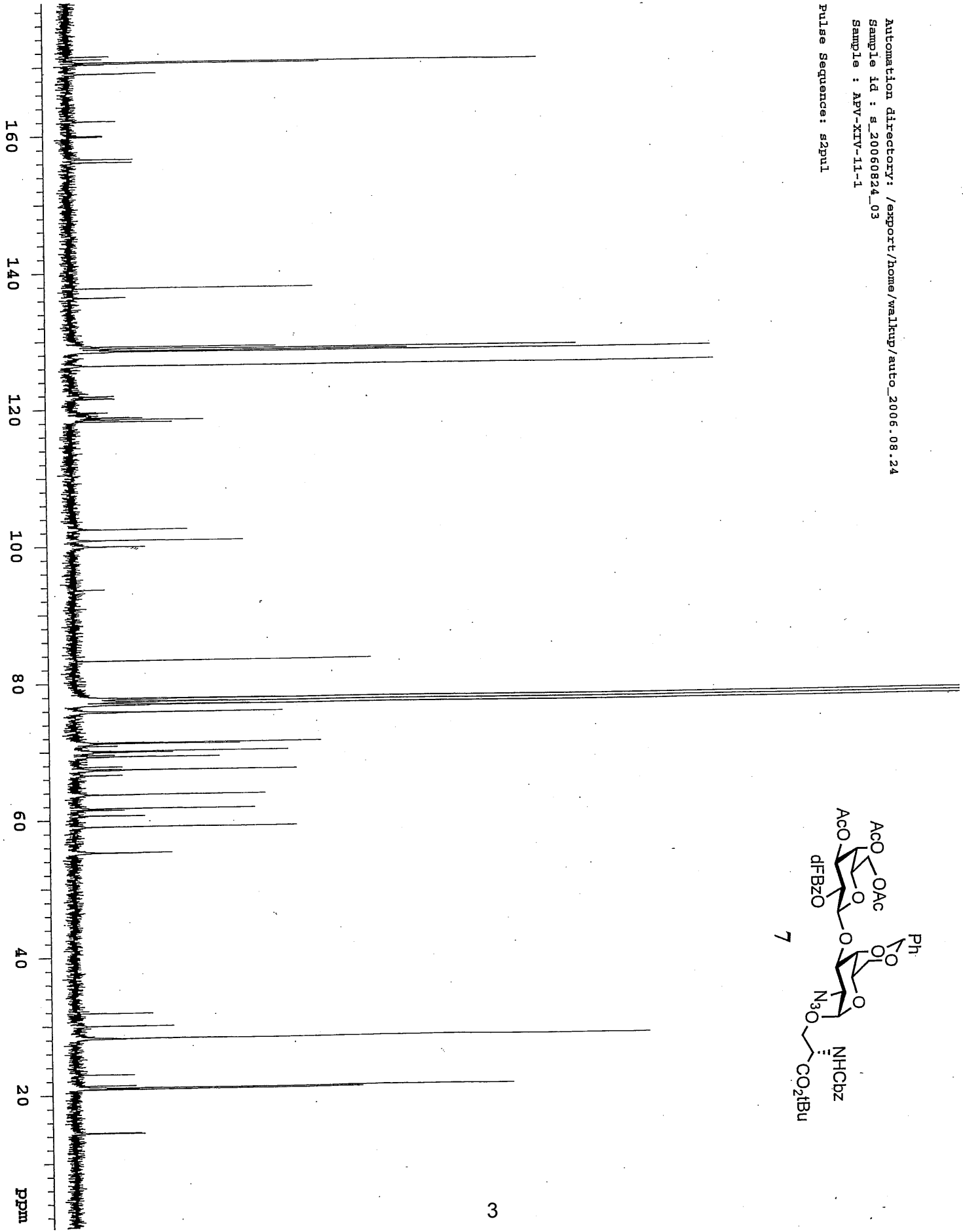
Pulse sequence: s2pul  
 Solvent: CHCl3  
 Temp: 25.0 C / 298.1 K  
 Operator: avenot  
 Mercury-300db "merc300"

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.998 sec  
 Width 5000.0 Hz

32 repetitions  
 OBSERVE H1, 300.0804015 MHz  
 DATA PROCESSING  
 Line broadening 0.3 Hz  
 F2 size 12768  
 Total time 1. min, 39 sec

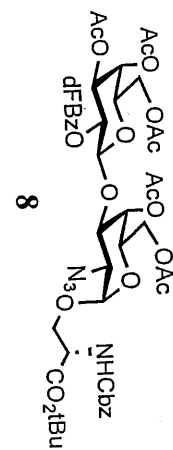
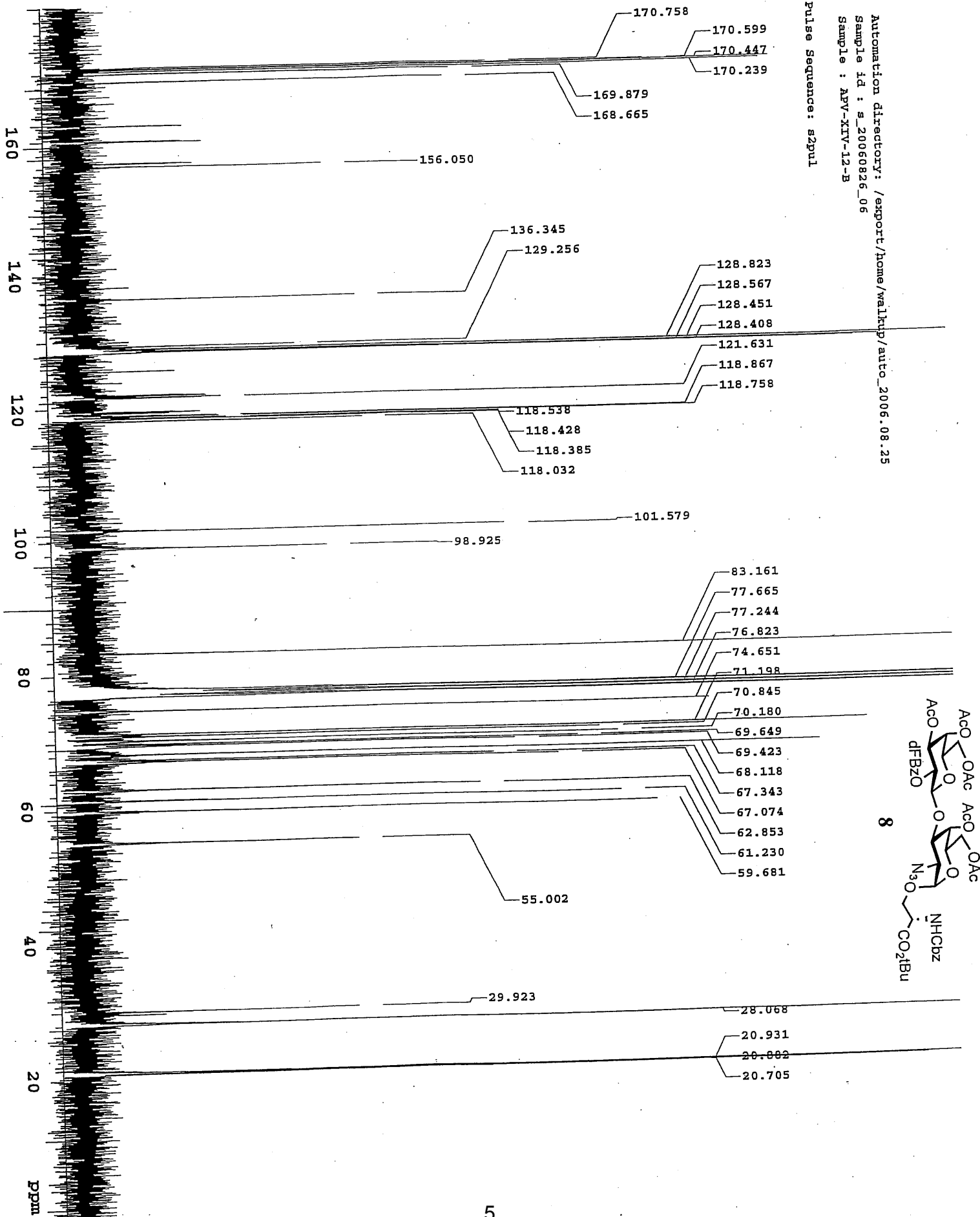


Automation directory: /export/home/walkup/autoc\_2006.08.24  
Sample id : s\_20060824\_03  
Sample : APV-XIV-11-1  
Pulse Sequence: s2pml





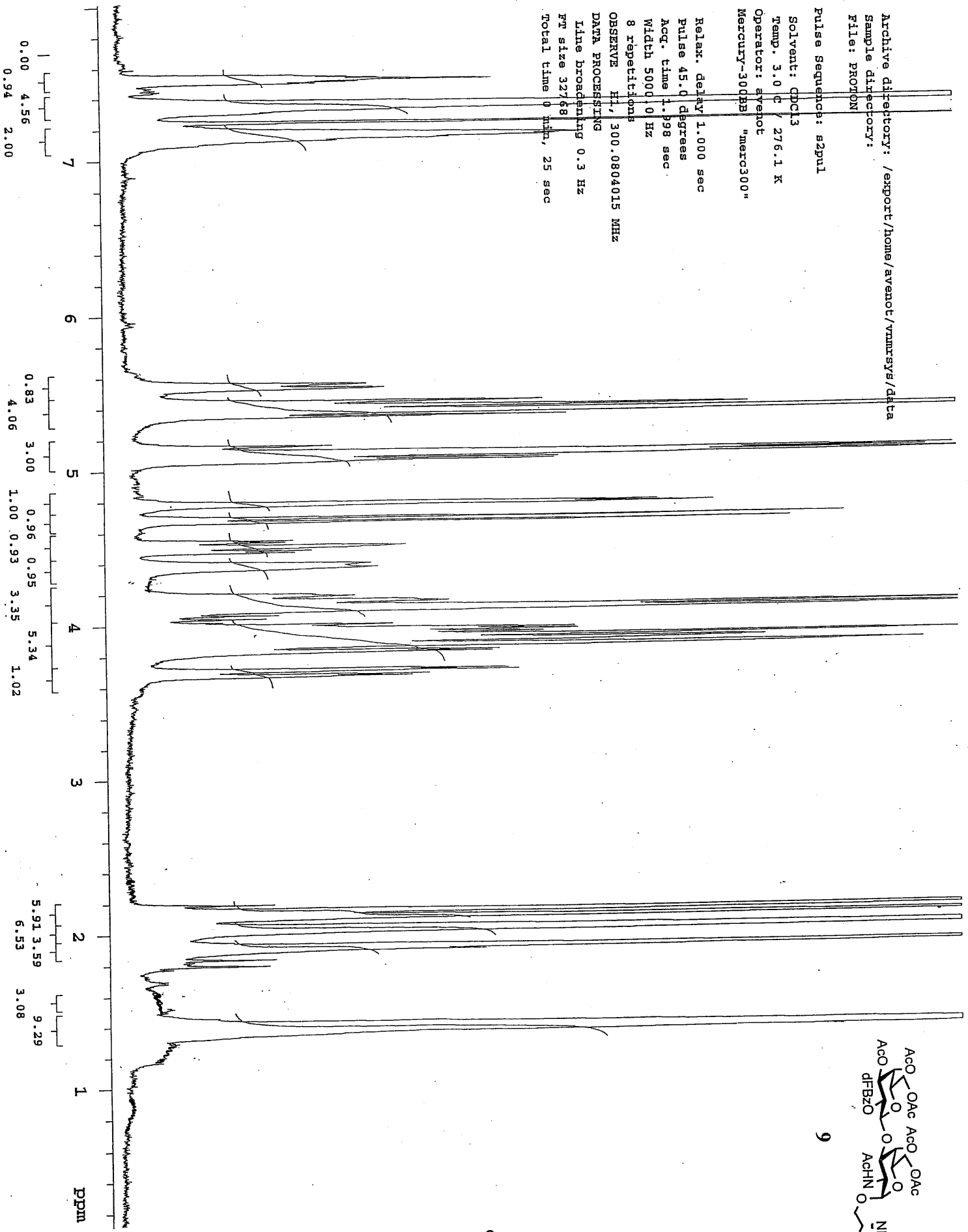
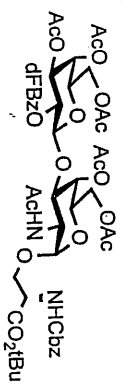
Automation directory: /export/home/waltrip/auto\_2006\_08.25  
 Sample id : s\_20060826\_06  
 Sample : APV-XIV-12-B  
 Pulse Sequence: s2pul



Archive directory: /export/home/avenot/vnmrSYS/d41ca  
 Sample directory:  
 File: PROTON

Pulse Sequence: s2pul  
 Solvent: CDCl3  
 Temp. 3.0 C / 276.1 K  
 Operator: avenot  
 Mercury-300MB "merc300"

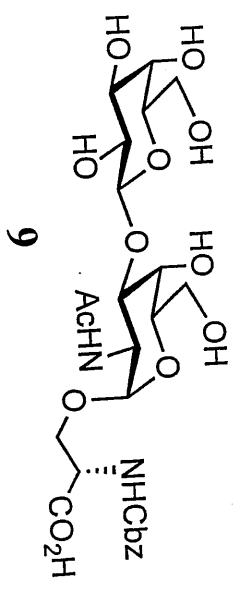
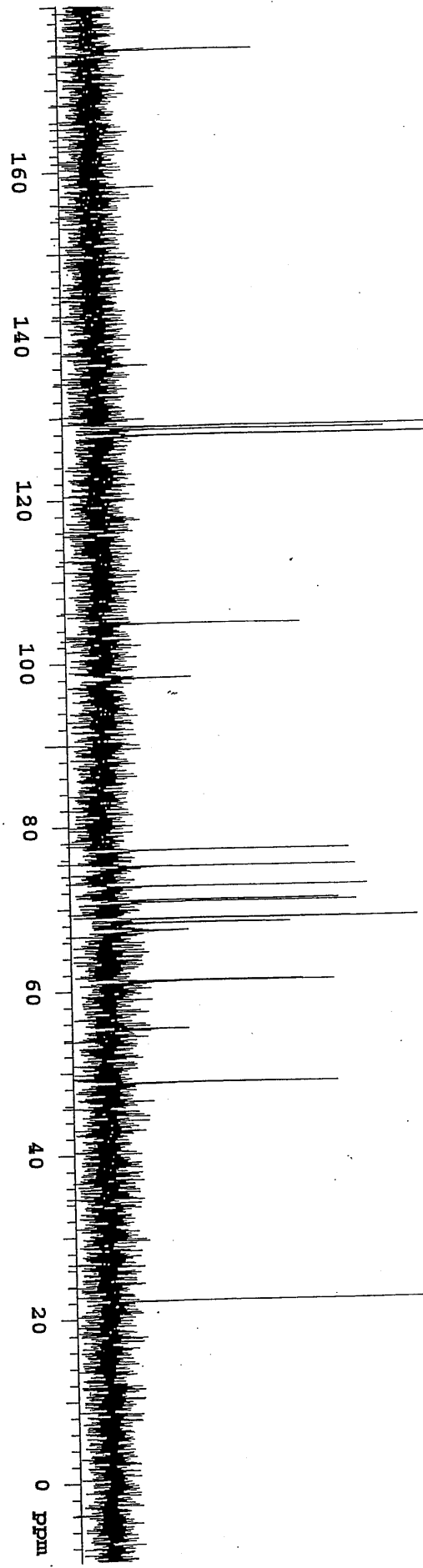
Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.898 sec  
 Width 5000.0 Hz  
 8 repetitions  
 OBSERVE H1, 300.0804015 MHz  
 DATA PROCESSING  
 Line broadening 0.3 Hz  
 FM size 32768  
 Total time 0 min, 25 sec



Automation directory: /export/home/walkrup/autoc\_2006.09.06  
 ep08\_01\_fid

Sample : APV-XIV-15-2-H  
 SPECTRAL  
 Reference: 2995ul temp 25.0  
 solvent d2o gain 20  
 file /export/home/- spin not used  
 walkrup/vmrsvs/dst-hst 0.008  
 a/avenoc/APV-XIV-1- pw90 6.500  
 5-2-H\_Carbon\_2006S- alfa 10.000

ep08\_01\_fid  
 ACQUISITION  
 sw 15083.0 in n  
 at 1.301 dp y  
 np 39232 hs m  
 fb 8400  
 bs 64 lb  
 dl 1.000 fn not used  
 nt 22000  
 ct 22000 sp DISPLAY -732.8  
 TRANSMITTER  
 tn C13 rfi 14324.0  
 sfid 75.460 rfp 750.7  
 lof -762.8 rp 142.6  
 tpwr 60 lp -132.6  
 pw 3.250 PLOT  
 DECOUPLER  
 dn wg 250  
 dn H1 sc 0  
 dof 0 vs 23295  
 dm YYY th 12  
 dmm w al cdc ph  
 dipwr 37  
 dmf 11000



Archive directory: /export/home/avenot/vnmrsvs/Data  
Sample directory: \_05Mar2005  
File: PROTON

Pulse Sequence: s2pul

Solvent: D3OD

Temp. 25.0 C / 298.1 K

Operator: avenot

INOVA-500 "Inova500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.890 sec

Width 5000.3 Hz

32 repetitions

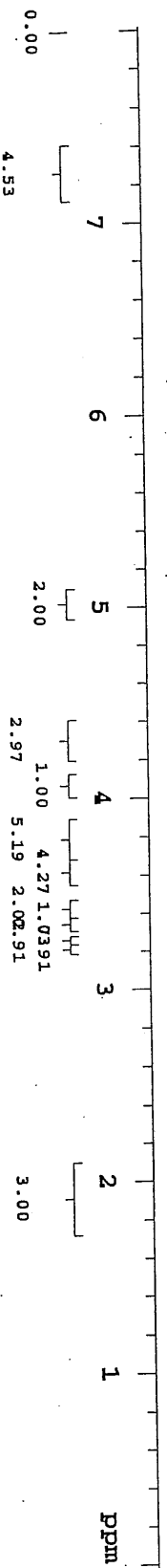
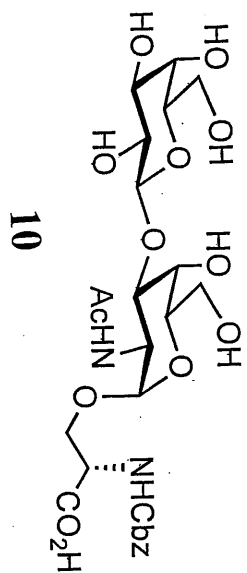
OBSERVE 1, 499.9531770 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 32768

Total time 1 min, 32 sec





13C OBSERVE

Archive directory: /export/home/avenot/vmrtye/data  
Sample directory:  
File: CARBON

Pulse Sequence: s3pul

Solvent: CDCl3  
Temp. 3.0 C / 276.1 K  
Operator: avenot  
Mercury-300BB "merc300"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

1440 repetitions

OBSERVE C13, 75.4552776 MHz

DECOUPLE H1, 300.0819042 MHz

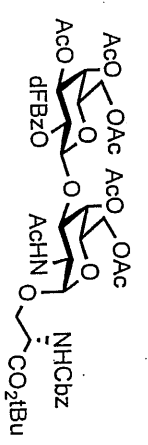
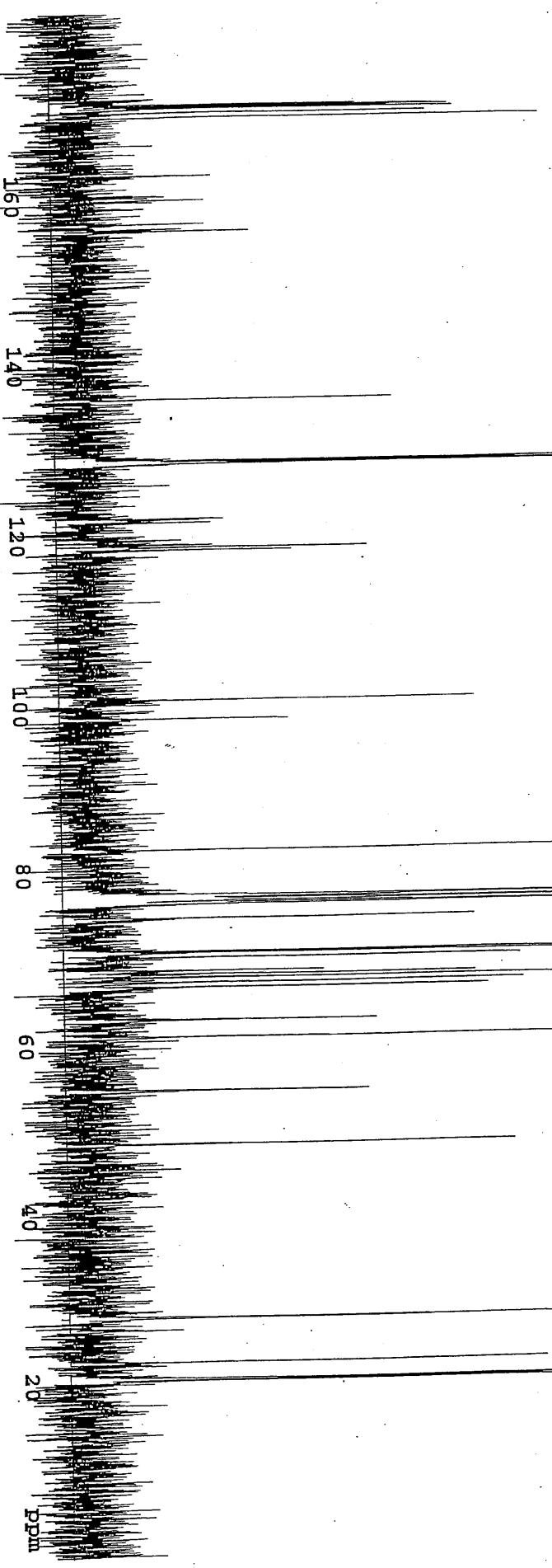
Power 37 db

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz  
FT size 131072  
Total time 2 hr, 36 min, 35 sec

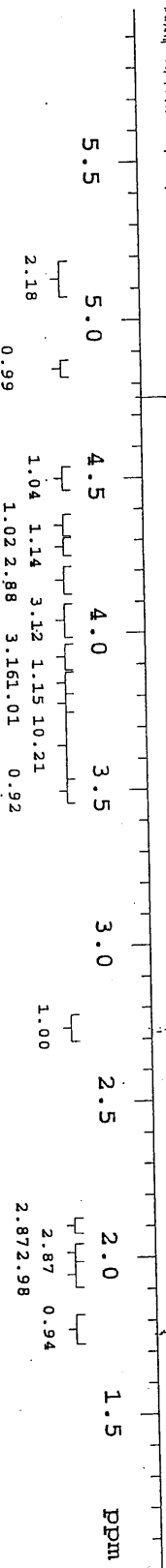


Sample directory: 20Apr2005\_20Apr2005  
File: PROTON

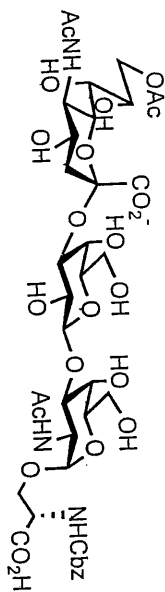
Pulse Sequence: PRESAT

Solvent: D2O  
Temp. 25.0 C / 298.1 K  
Operator: avenot  
INOVA-600 "Inova600"

Relax. delay 0.200 sec  
Pulse 45.0 degrees  
Acq. time 1.892 sec  
Width 5000.0 Hz  
64 repetitions  
OBSERVE H1, 599.7388725 MHz  
DATA PROCESSING  
Gauss apodization 0, 874 sec  
F2 size 32768  
Total time 3 min, 18 sec



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XII-125 900MHz

Pulse Sequence: s2pu1

Solvent: D2O

Temp. 25.0 C / 298.1 K

Operator: ftian

File: avenot\_xii\_125

Relax. delay 3.000 sec

Pulse 63.5 degrees

Acq. time 2.000 sec

Width 14524.3 Hz

32 repetitions

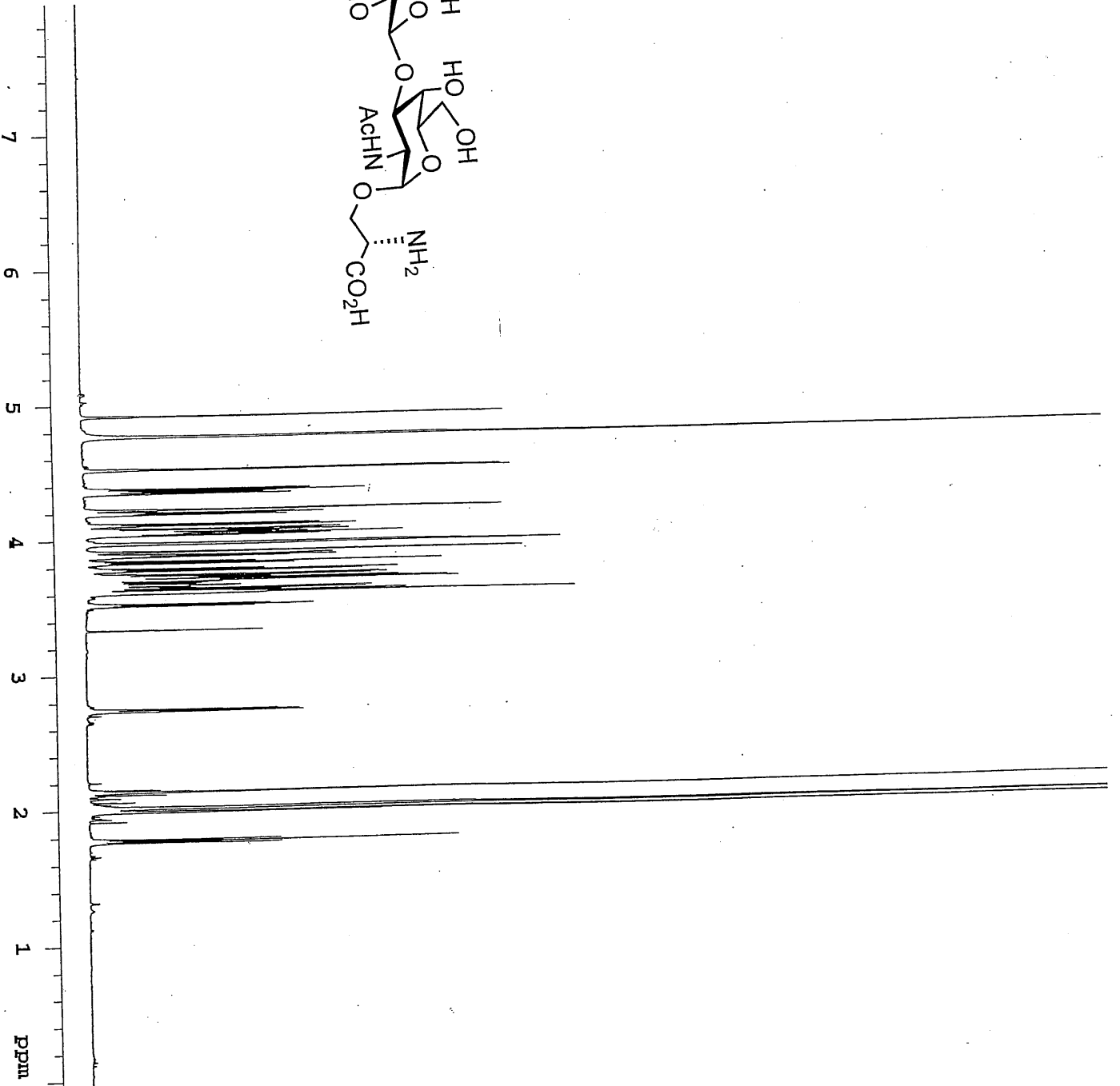
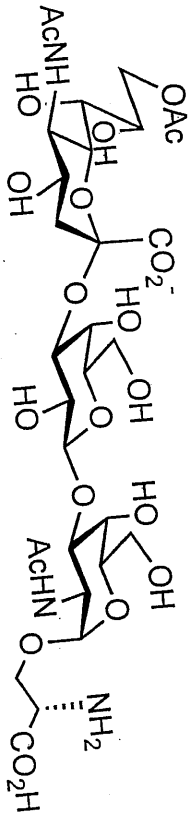
OBSERVE F1: 899.8162543 MHz

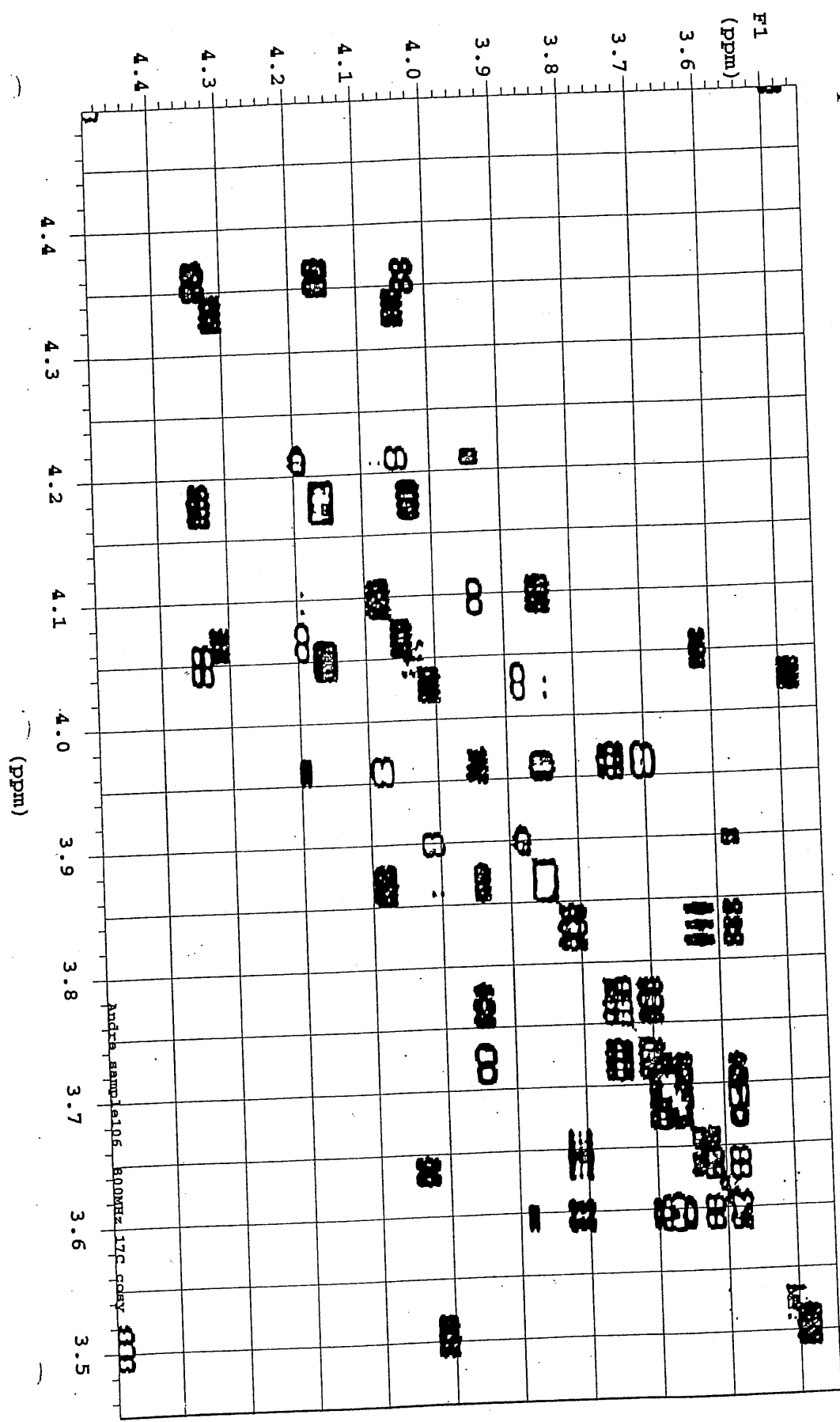
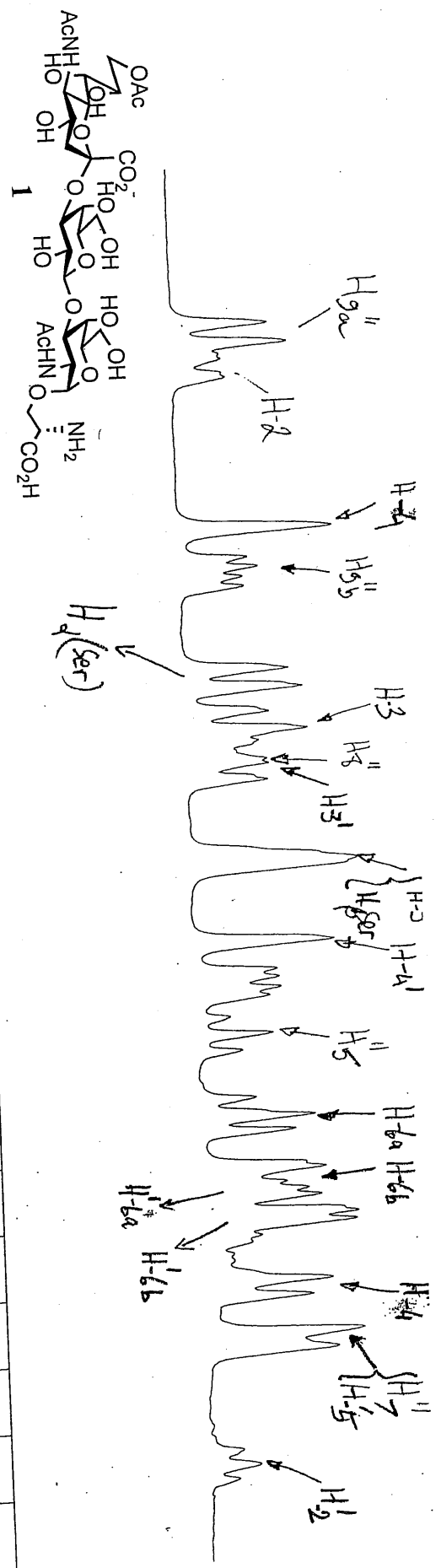
DATA PROCESSING

line broadening 0.3 Hz

FT size 65536

Total time 2 min, 40 sec





Andre sample106  
800MHz 17C hsqc

Pulse Sequence: ghsqc  
Solvent: D2O  
Temp. 17.0 C / 290.1 K  
file: andre\_s106\_hsqc

Relax. delay 1.000 sec  
Acq. time 0.146 sec  
Width 3508.8 Hz  
2D Width 17094.0 Hz  
8 repetitions  
2 x 128 increments  
OBSERVE H1, 799.7285583 MHz  
DECOUPLE C13, 201.1069847 MHz  
Power 44 dB  
on during acquisition  
off during delay  
W40\_HCN\_160 modulated  
DATA PROCESSING  
Gauss apodization 0.067 sec  
F1 DATA PROCESSING  
Gauss apodization 0.007 sec  
FT size 2048 x 512  
Total time 40 min, 56 sec

