

## **Total synthesis of 7-*des*-O-pivaloyl-7-O-benzylbryostatin 10**

Simon Hardy, Anthony P. Green, Alan T. L. Lee and Eric J. Thomas

### **Supplementary data**

Copies of  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra.



Current Data Parameters  
NAME 2007-08-01-ejt-20  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070802

Time 8.46

INSTRUM spect

PROBHD 5 mm TXI 1H/D-

PULPROG zg30b

TD 65536

SOLVENT CDCl3

NS 16

DS 0

SWH 10330.578 Hz

FIDRES 0.157632 Hz

AQ 3.171923 sec

RG 90.5

DW 48.400 usec

DE 13.76 usec

TE 300.0 K

DI 1.00000000 sec

TD0 1

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

NUC1 1H

P1 7.80 usec

PL1 3.25 dB

SFO1 500.1330885 MHz

F2 - Processing parameters

SI 32768

SF 500.1300444 MHz

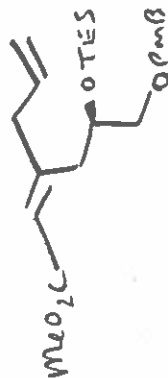
WDW EM

SSB 0

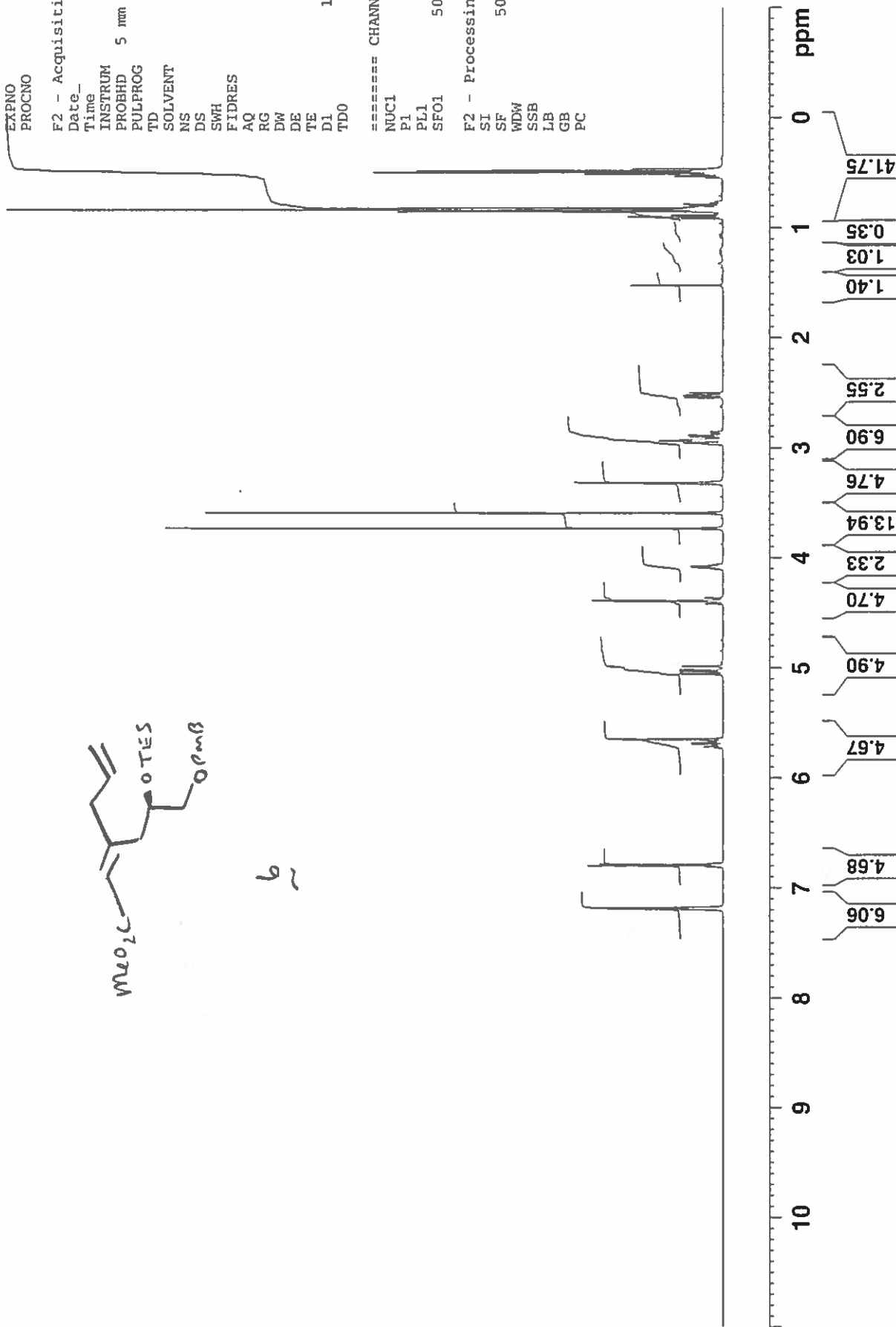
LB 0.30 Hz

GB 0

PC 1.00

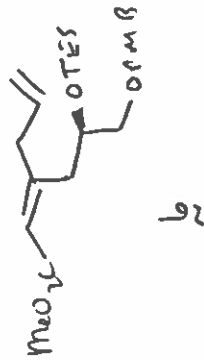
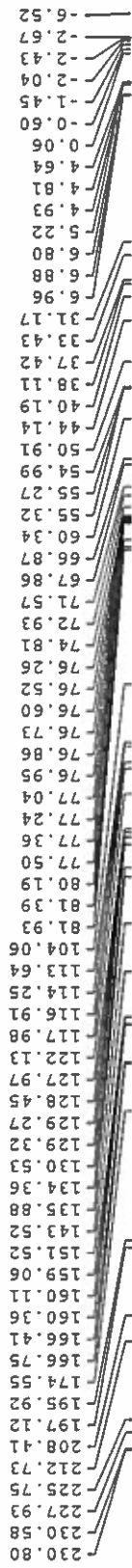


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atlites

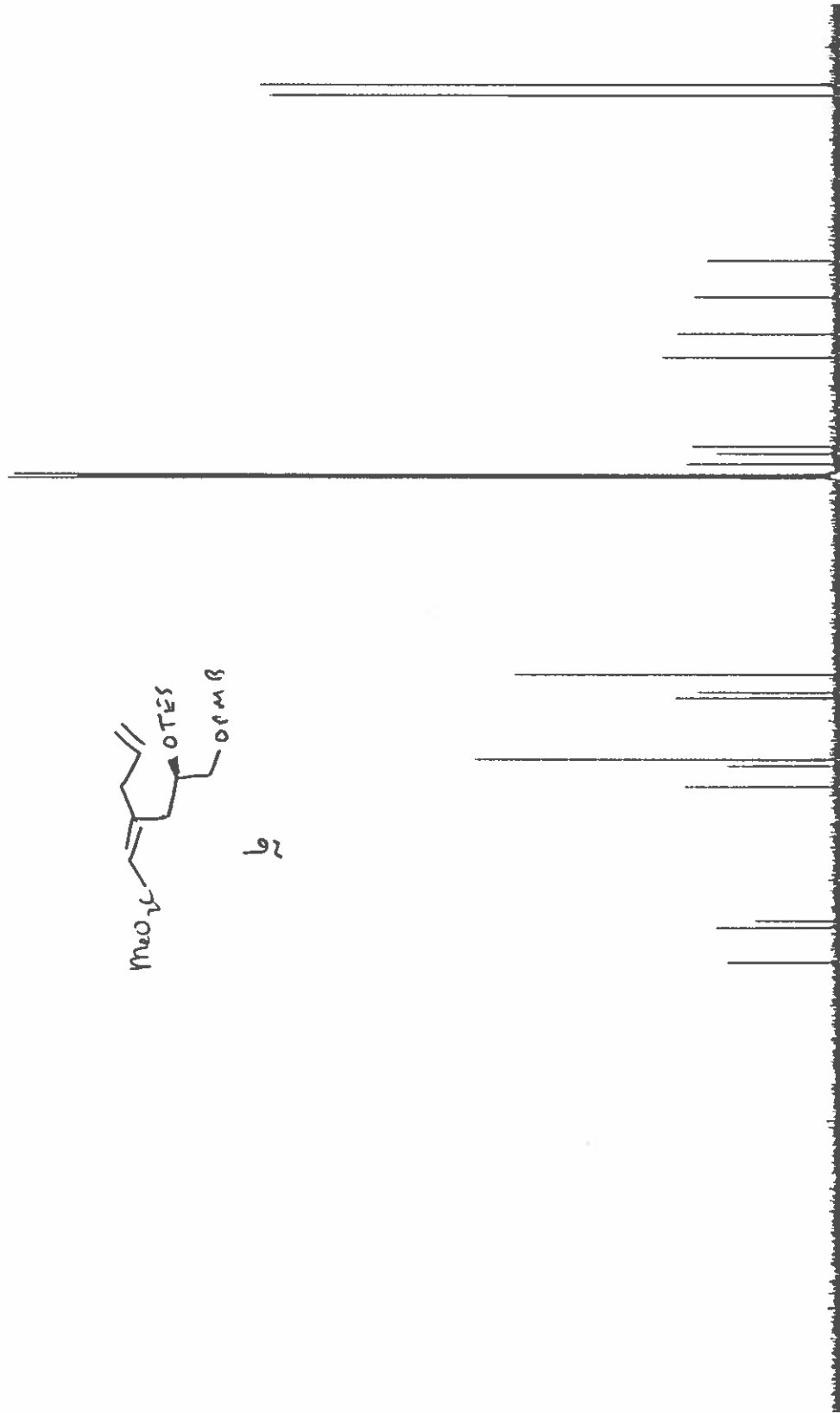
mCARBON CDCl3 {e:\bruk400data\2009\Feb} ejt 14



2009-02-13-ejt-14  
10  
NAME EXPNO  
PROCNO 1  
Date 20090213  
Time 16.41  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 256  
DS 2  
SWH 30241.936 Hz  
FIDRES 0.461455 Hz  
AQ 1.0835786 sec  
RG 512  
DW 16.533 usec  
DE 7.83 usec  
TE 293.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 34.91522217 W  
SFO1 100.6241042 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.60 dB  
PL12 15.31 dB  
PL13 18.00 dB  
PL2W 17.83863831 W  
PL12W 0.22927761 W  
PL13W 0.12341322 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 0.20



240 220 200 180 160 140 120 100 80 60 40 20 ppm

atlftips

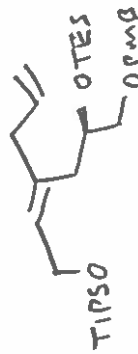
mPROTON CDCl3 {e:\bruk400data\2009\Feb} ejt 23



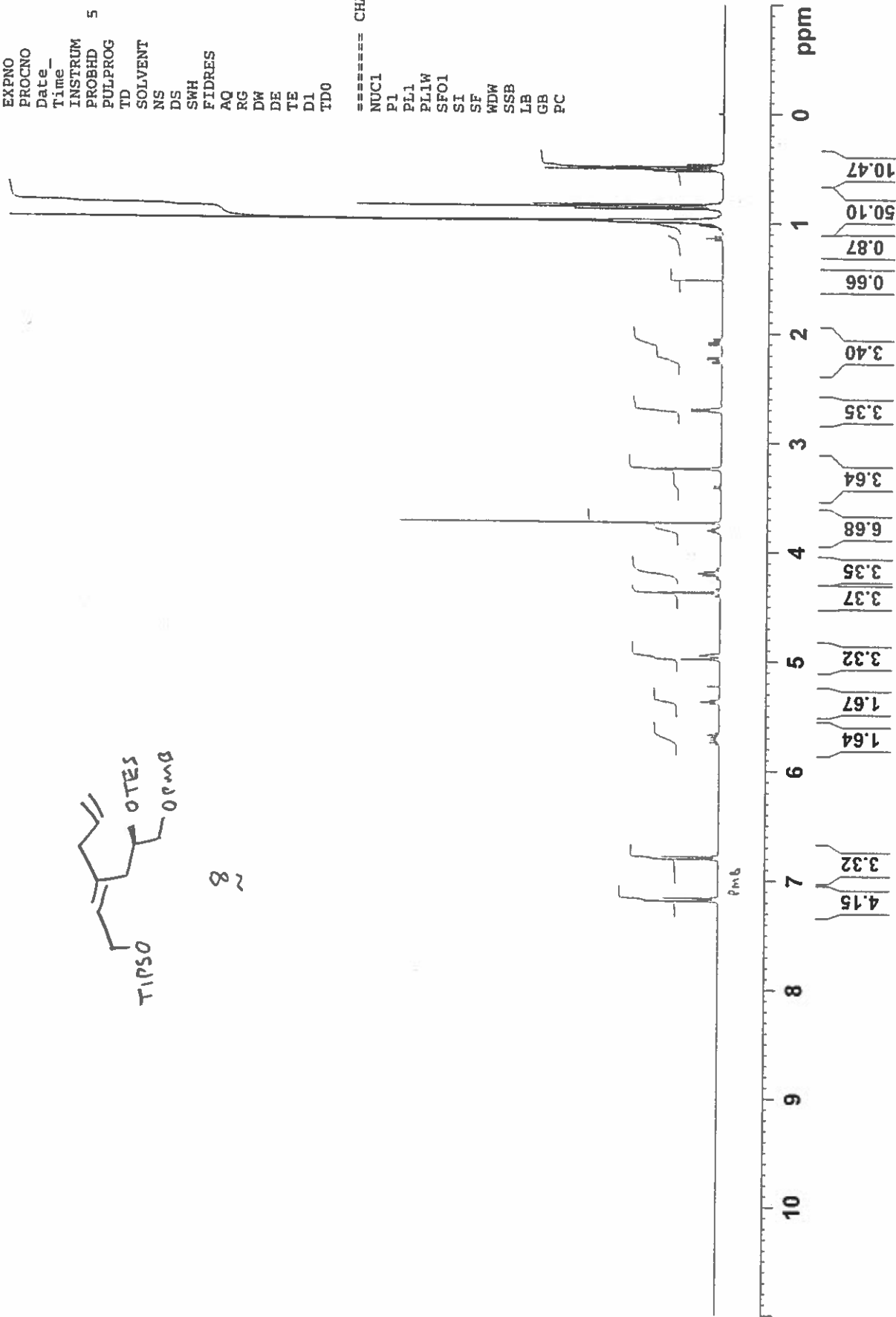
NAME 2009-02-18-ejt-23

EXPNO 10  
PROCNO 1  
Date\_ 20090218  
Time 14.01  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 114  
DW 60.500 usec  
DE 9.40 usec  
TE 293.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300384 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



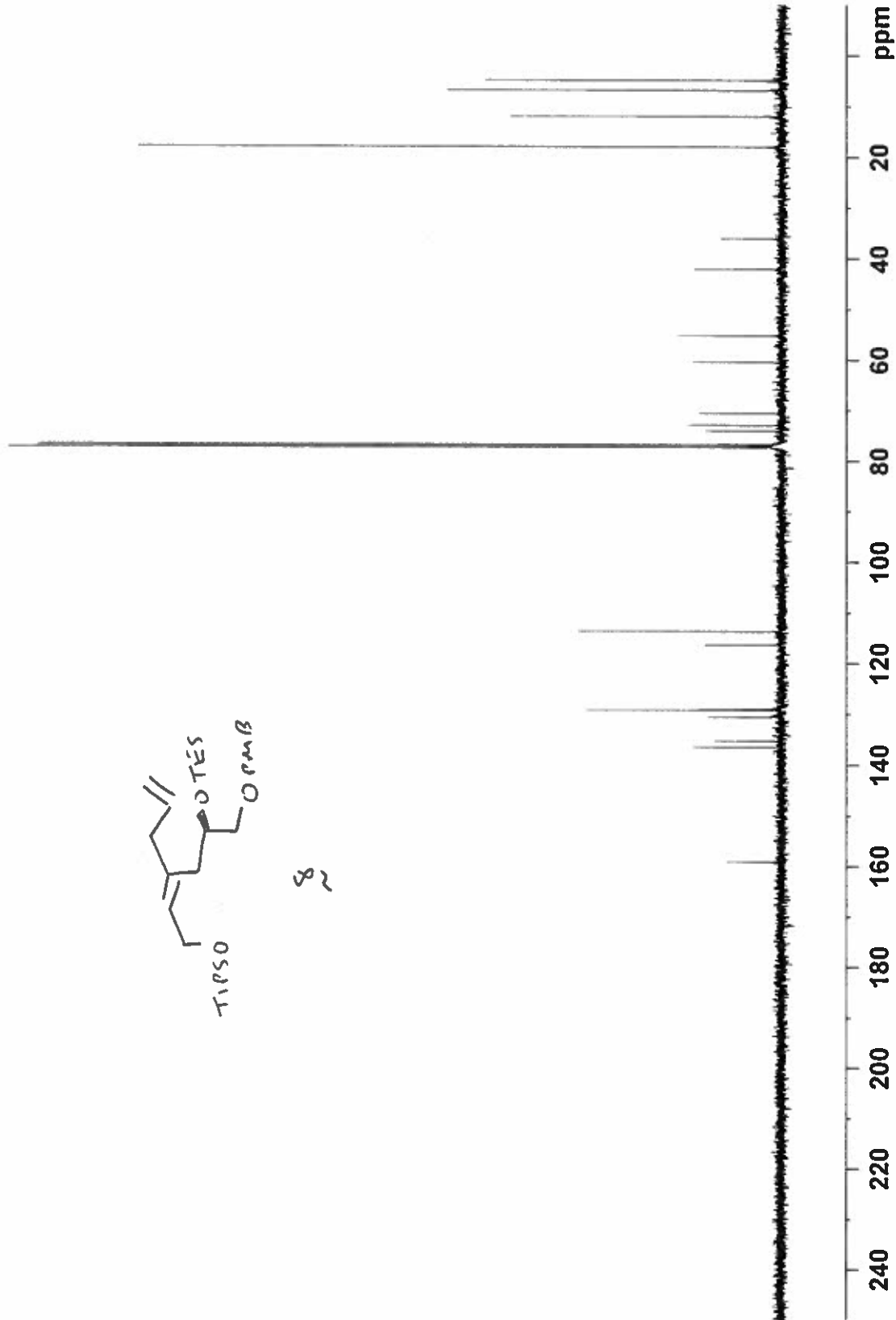
8





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NAME	EXPNO	PROCNO	Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FIDRES	AQ	RQ	DW	DE	TE	D1	D11	TD0
2003-02-18-ejt-46	10	1	20030218	17.28	AV400	5 mm PABBO BB-	ZDQ930	65536	CDC13	256	2	30241.936 Hz	0.461455 Hz	1.0835786 sec	512	16.533 usec	7.83 usec	293.7 K	2.00000000 sec	0.03000000 sec	1
===== CHANNEL f1 =====																					
NUC1	P1	8.00 usec																			
PL1	0.00 dB																				
PL1W	34.91523217 W																				
SF01	100.6241042 MHz																				
===== CHANNEL f2 =====																					
CPDPRG2	waitz16																				
NUC2	1H																				
PCPD2	90.00 usec																				
PL2	-3.60 dB																				
PL12	15.31 dB																				
PL13	18.00 dB																				
PL2W	17.83863831 W																				
PL12W	0.22927761 W																				
PL13W	0.12341332 W																				
SF02	400.1316005 MHz																				
SI	32768																				
SF1	100.6127690 MHz																				
WDW	EM																				
SSB	0																				
LB	1.00 Hz																				
GB	0																				
PC	0.20																				



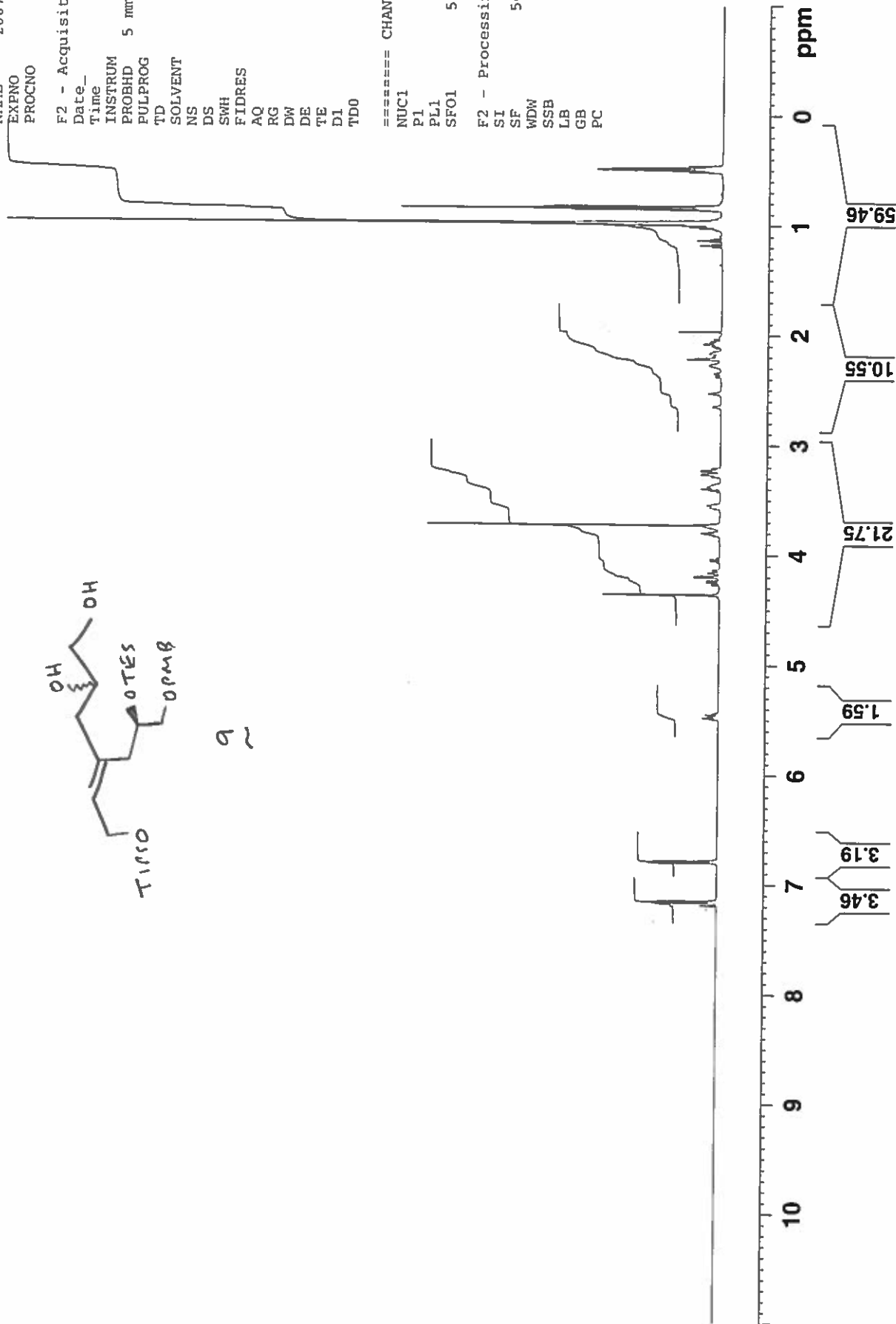
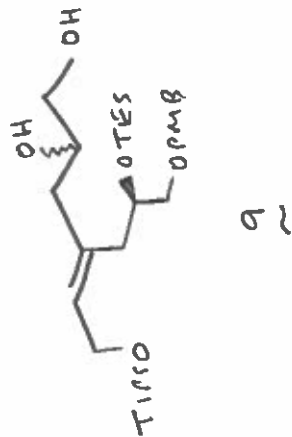


Current Data Parameters  
NAME 2007-08-16-ejt-1  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070816  
Time 15.37  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 22.6  
DW 48.400 usec  
DE 13.76 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 7.80 usec  
PL1 3.25 dB  
SFO1 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300433 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



atl1152

mCARBONnight CDCI3 /opt/topspin jpc 30



77.31  
77.06  
76.81  
73.97  
73.83  
73.00  
71.15  
70.65  
69.76  
66.54  
66.50  
65.86  
60.42  
60.18  
60.16  
55.25  
55.24  
41.93  
41.40  
36.08  
35.81  
21.04  
18.00  
17.42  
15.26  
14.19  
12.22  
11.99  
11.75  
11.47  
6.83  
5.10  
4.86  
4.63

159.16  
133.95  
133.39  
131.63  
131.09  
130.23  
129.24  
113.70

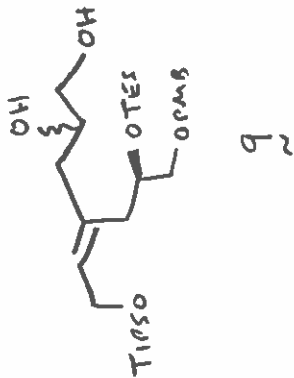
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NAME 2007-08-16-jpc-30  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070819  
Time 17.06  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCI3  
NS 256  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 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 11.50 usec  
PL1 -4.20 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL12 20.00 dB  
PL13 23.00 dB  
PL2 3.25 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7577890 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



200 180 160 140 120 100 80 60 40 20 0 ppm

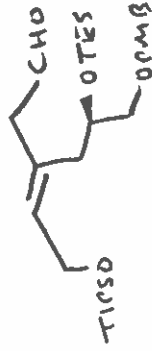


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NAME 2007-08-17-ejt-25  
EXPNO 10  
PROCNO 1

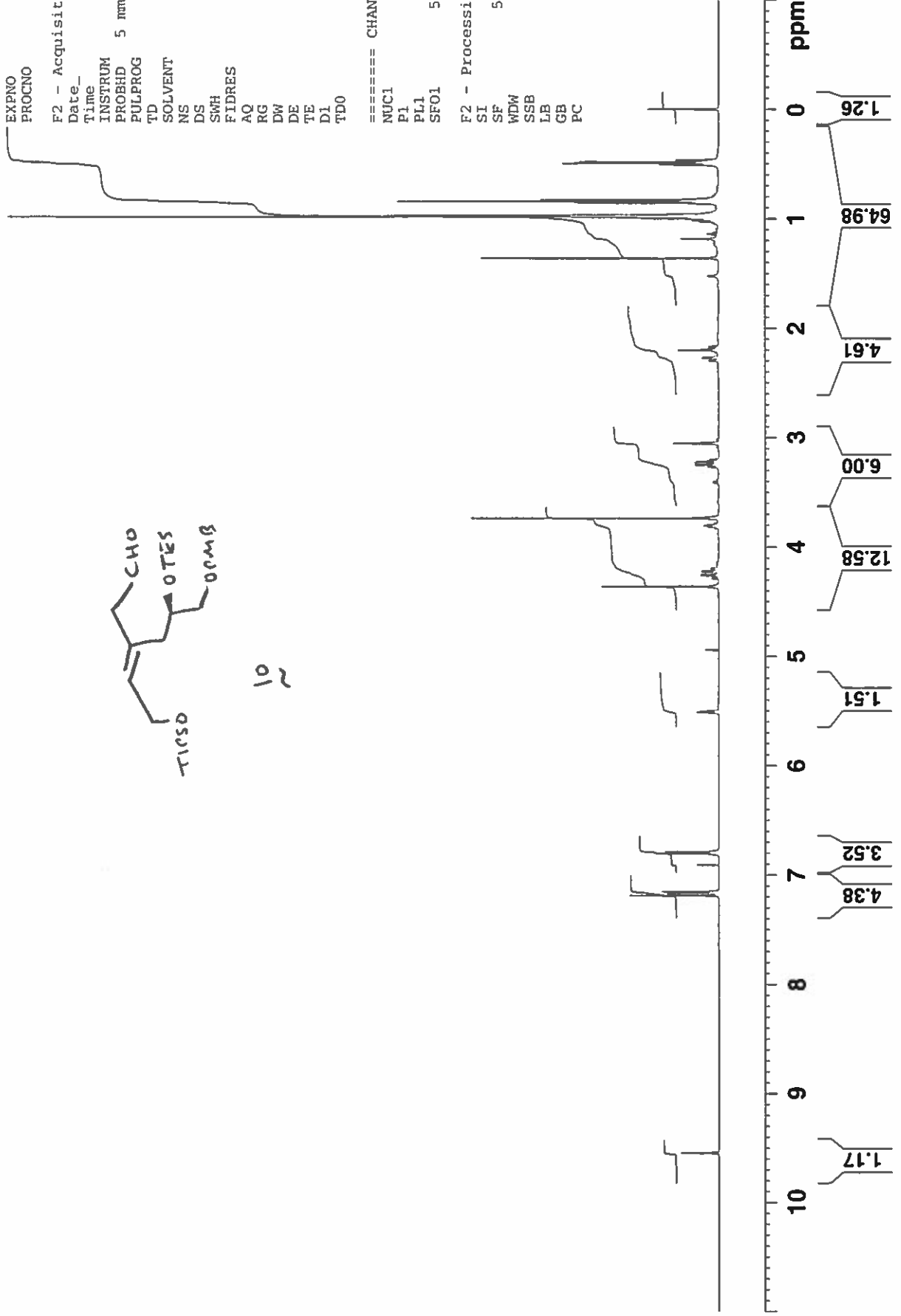
F2 - Acquisition Parameters  
Date\_ 20070817  
Time 13.40  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 144  
DW 48.400 usec  
DE 13.76 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 7.80 usec  
PL1 3.25 dB  
SFO1 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300442 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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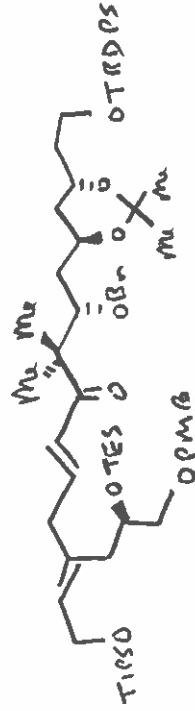


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EXPNO 10  
PROCNO 1

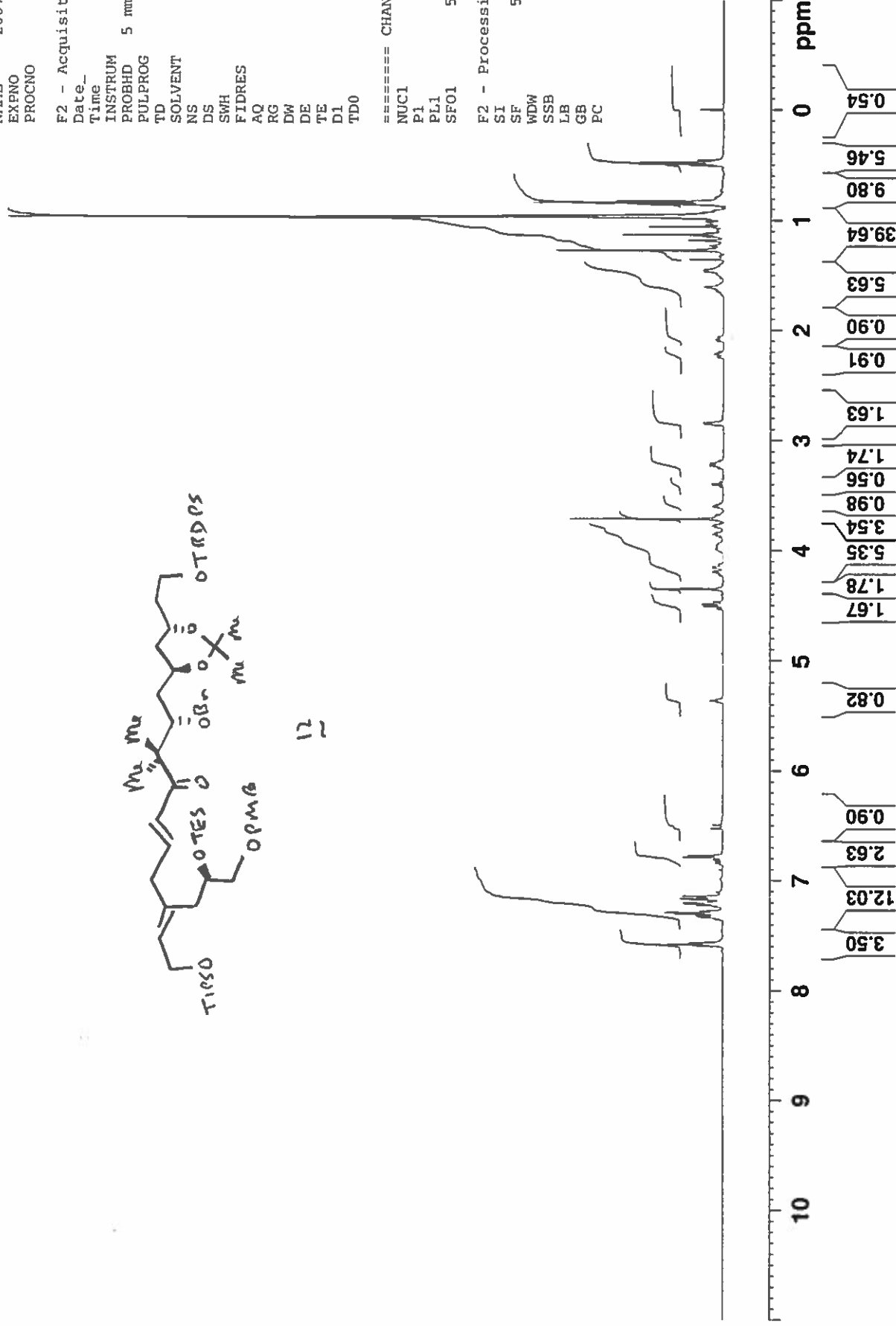
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Date\_ 20070925  
Time 3.06  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 20.2  
DW 48.400 usec  
DE 13.76 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 7.80 usec  
PL1 3.25 dB  
SF01 500.1330885 MHz

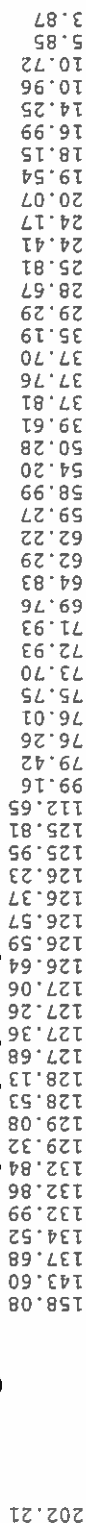
F2 - Processing parameters  
SI 32768  
SF 500.1300541 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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atll phosphate coupling  
mCARBONnight CDC13 /opt/topspin ejt 6



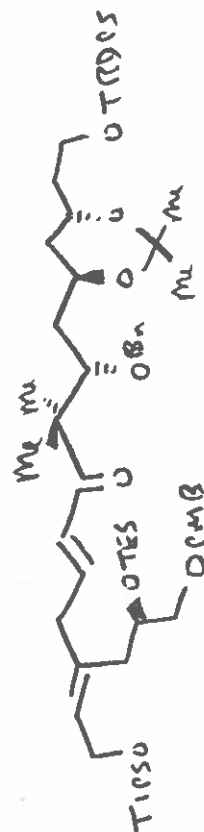
Current Data Parameters  
NAME 2007-09-24-ejt-6  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070925  
Time 3.20  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 256  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 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 11.50 usec  
PL1 -4.20 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL12 20.00 dB  
PL13 23.00 dB  
PL2 3.25 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7579214 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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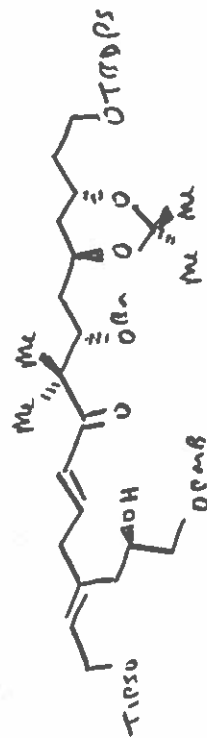


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EXPNO 10  
PROCNO 1

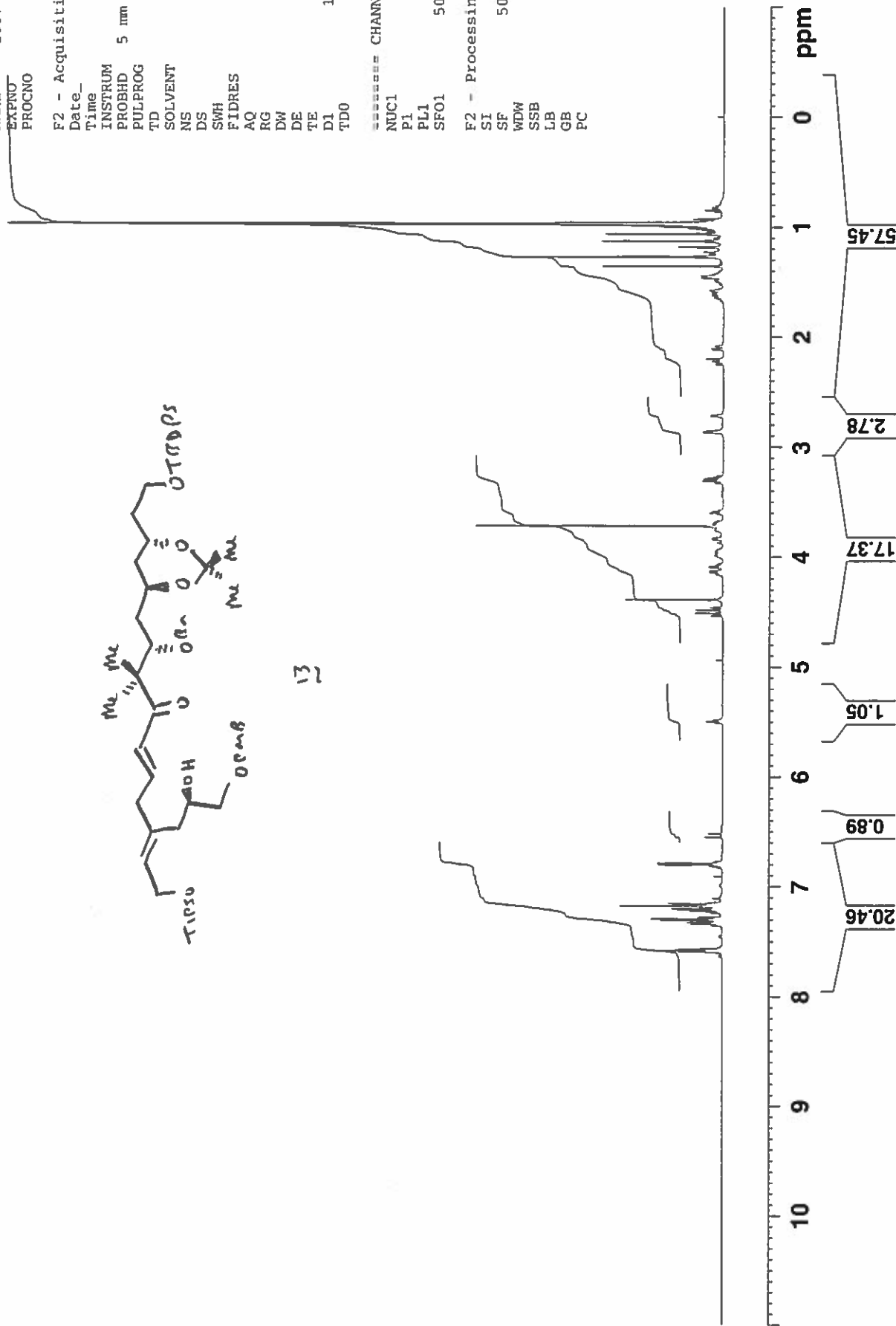
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Date\_ 20070831  
Time 14.31  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 57  
DW 48.400 usec  
DE 13.76 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 7.80 usec  
PL1 3.25 dB  
SFO1 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300501 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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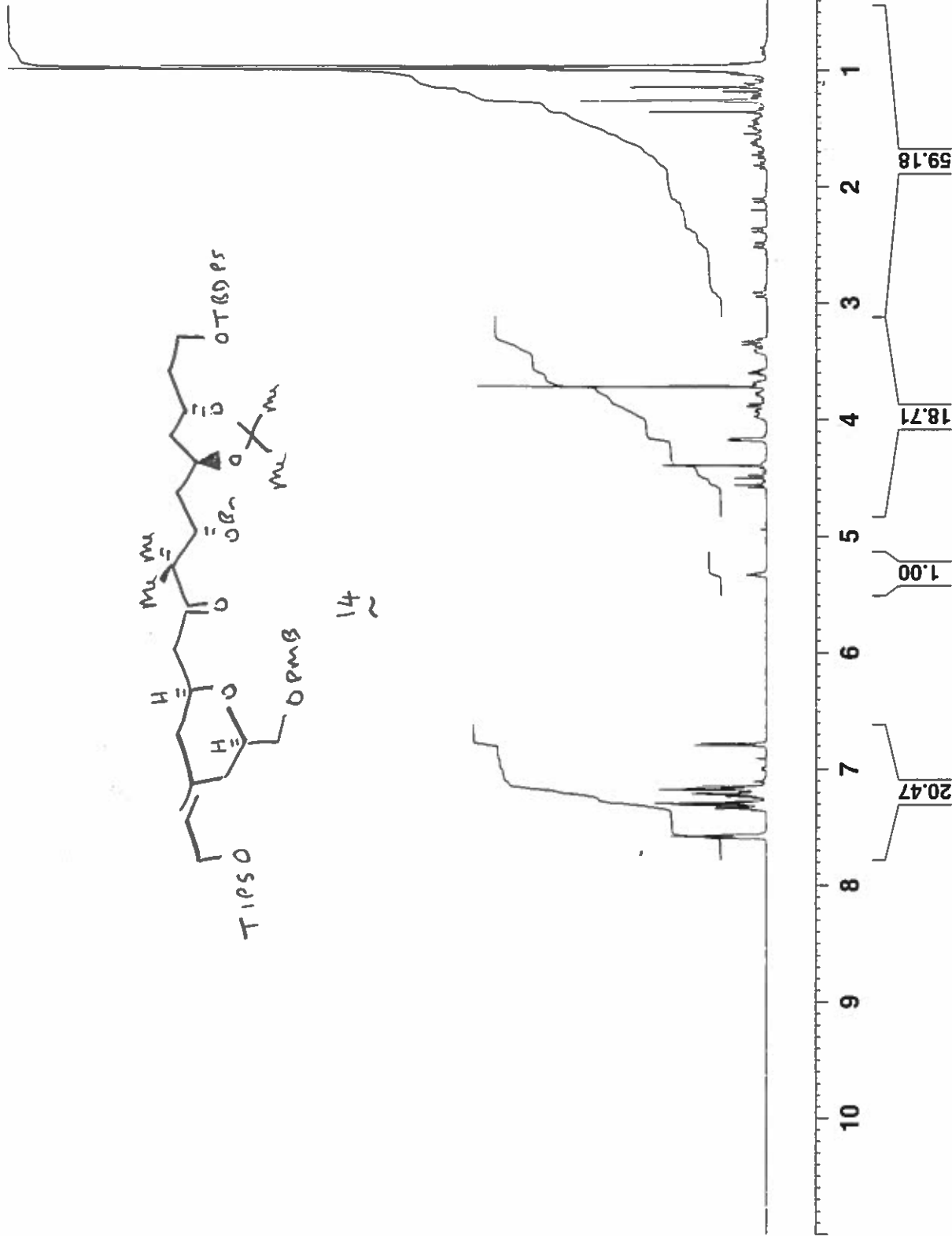


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NAME 2007-09-03-ejt-10  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070903  
Time 14.58  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 57  
DE 48.400 usec  
TE 13.76 usec  
TD0 1  
D1 300.0 K  
D0 1.0000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 7.80 usec  
PL1 3.25 dB  
SFO1 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300501 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



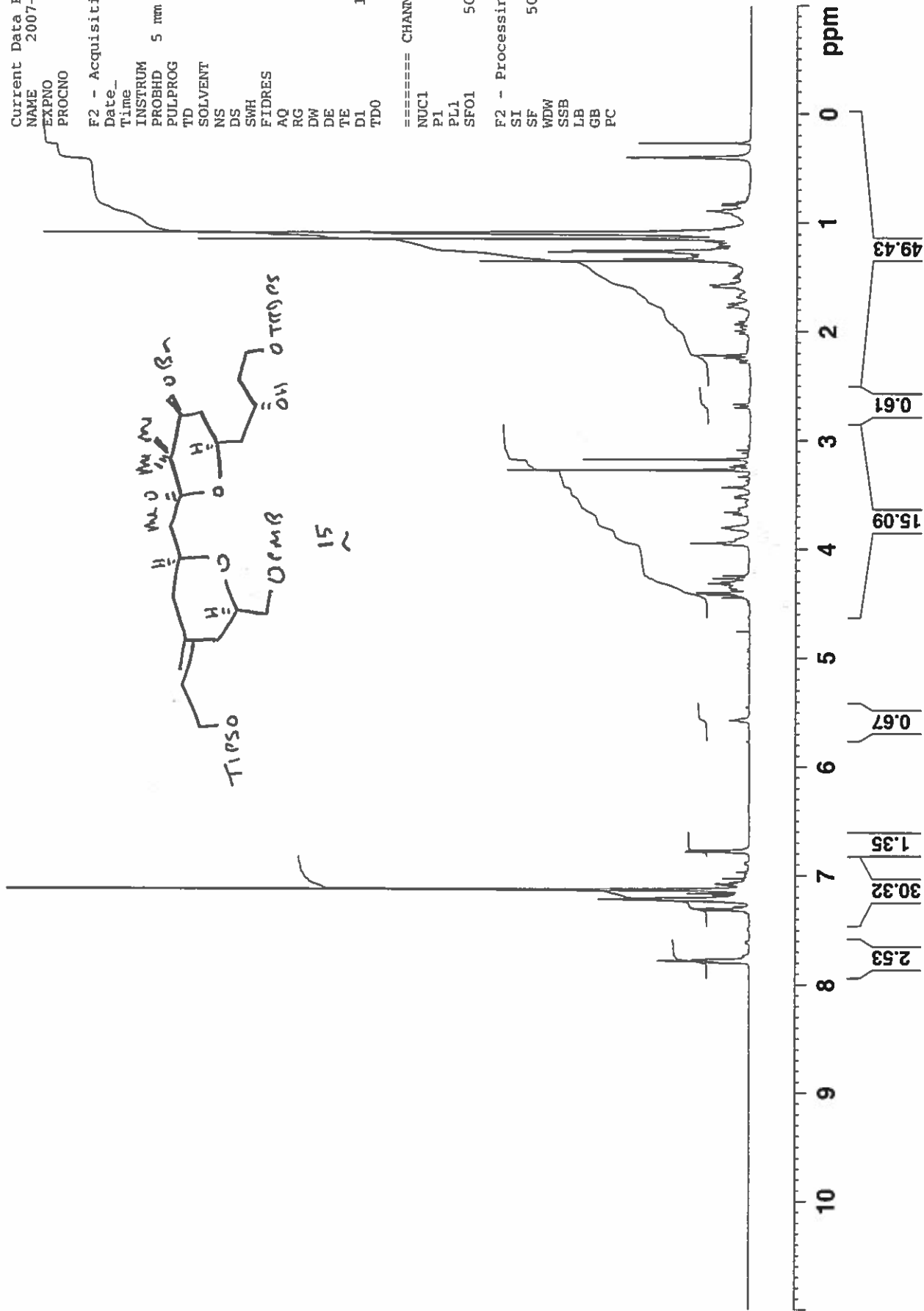


Current Data Parameters  
NAME 2007-09-07-ejt-30  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070907  
Time 16.27  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 161  
DW 48.400 usec  
DE 10.97 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

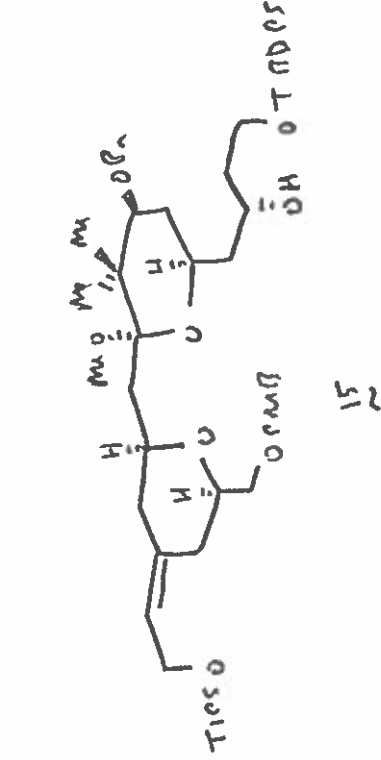
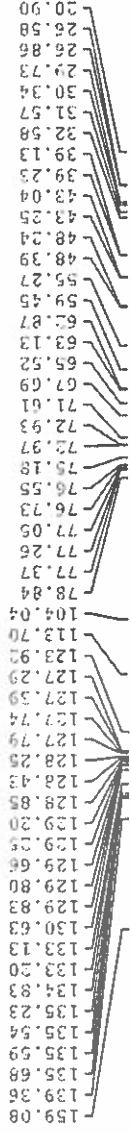
===== CHANNEL f1 =====  
NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
SFO1 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300695 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



atl1abC3OHC1OTBDPS  
mCARBONnight CDCI3

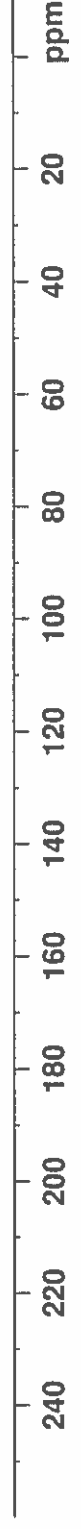
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NAME 2011-08-20-ejt-10  
EXPNO 14  
PROCNO 1  
Date\_ 20110820  
Time\_ 23.43  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCI3  
NS 3072  
DS 2  
SWH 30241.936 Hz  
FIDRES 0.461455 Hz  
AQ 1.0835786 sec  
RG 512  
DE 16.533 usec  
TE 293.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D10 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 34.91522217 W  
SFO1 100.6241042 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.60 dB  
PL12 15.31 dB  
PL13 18.00 dB  
PL2W 17.83863831 W  
PL12W 0.22927761 W  
PL13W 0.12341322 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

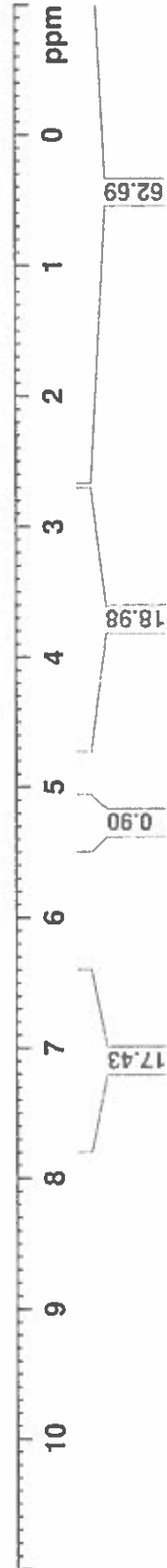
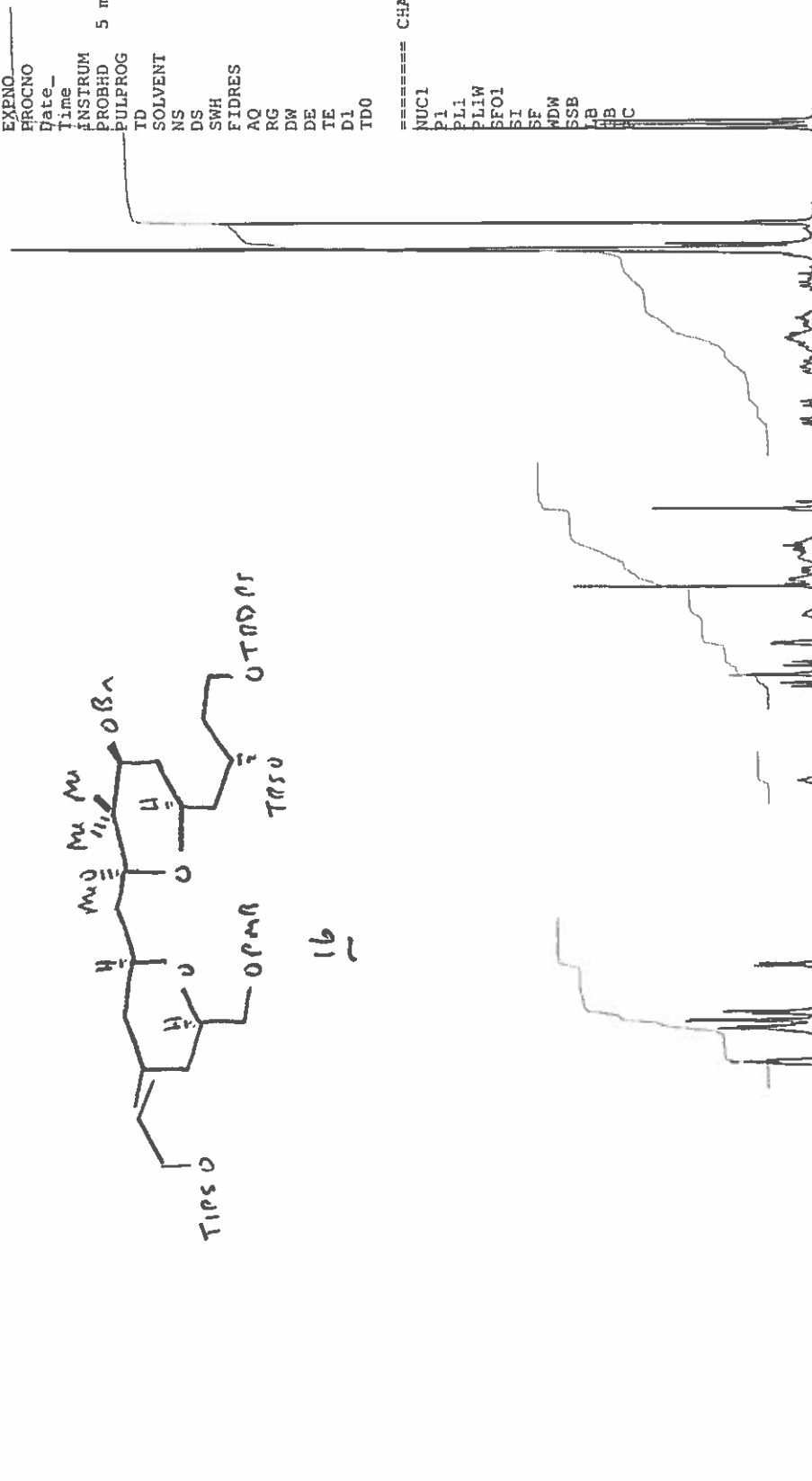
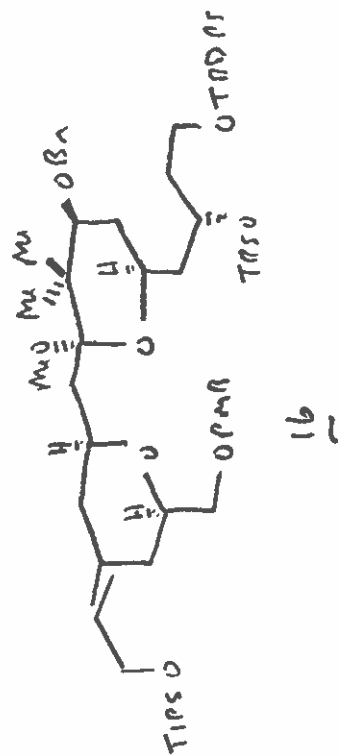


c1otbdps  
mPROTONnight CDCI3 {e:\bruk400data\2011\Aug} PB 34

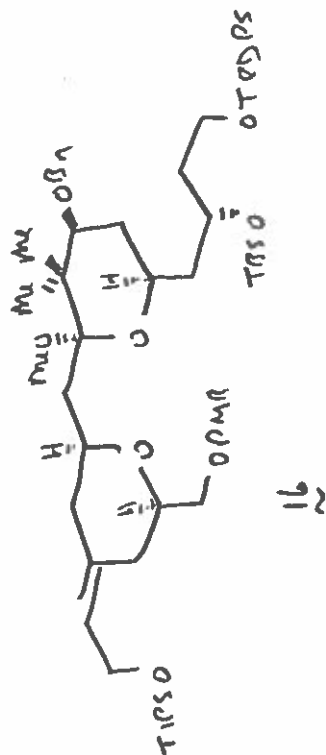
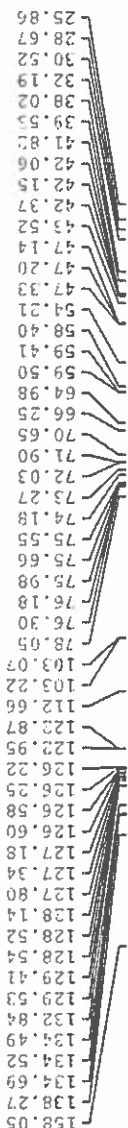


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EXPNO 10  
PROCNO 1  
Date\_ 20110828  
Time 20.15  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCI3  
NS 32  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 90.5  
DM 60.500 usec  
DE 9.40 usec  
TE 292.4 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300446 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



c1otbdps  
mCARBONnight CDCI3 {e:\bruk400data\2011\Aug} PB 34



NAME 2011-08-28-PB-34  
EXPNO 11  
PROCNO 1  
Date\_ 20110828  
Time\_ 22.56  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCI3  
NS 3072  
DS 2  
SWH 30241.936 Hz  
FIDRES 0.461455 Hz  
AQ 1.0835786 sec  
RG 512  
DW 16.533 usec  
DE 7.83 usec  
TE 293.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 34.9152217 W  
SFO1 100.6241042 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.60 dB  
PL12 15.31 dB  
PL13 18.00 dB  
PL2W 17.83863831 W  
PL12W 0.22927761 W  
PL13W 0.12341322 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6128759 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

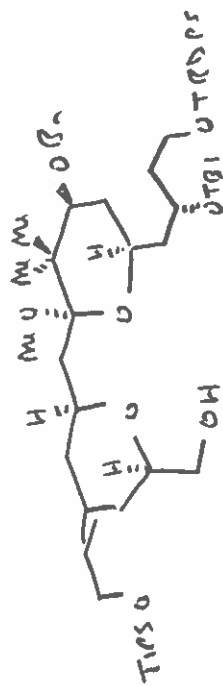
240 220 200 180 160 140 120 100 80 60 40 20 ppm



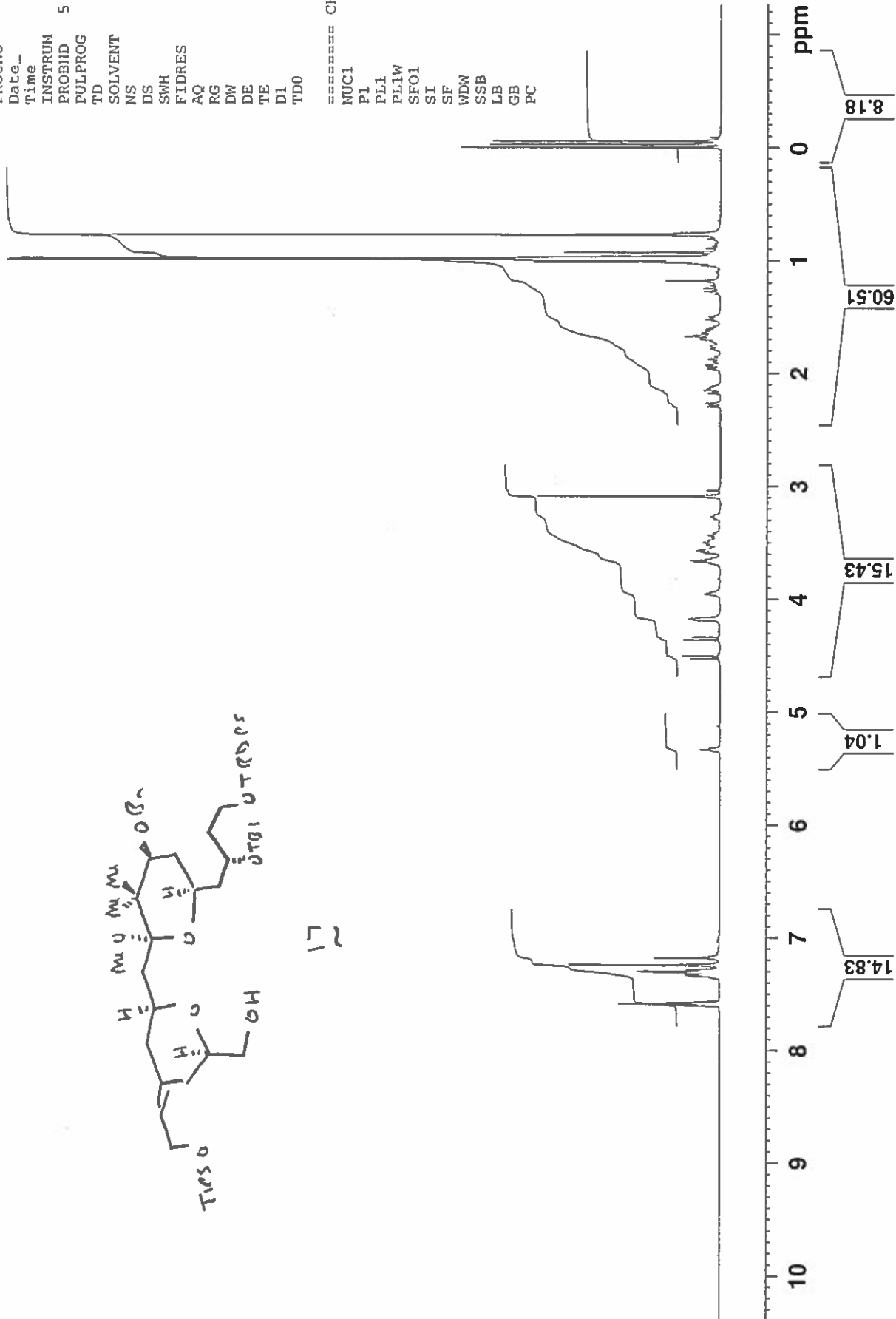


NAME 2011-08-30-ejt-3  
EXPNO 20  
PROCNO 1  
Date\_ 20110830  
Time 21.03  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCI3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 90.5  
DW 48.400 usec  
DE 13.38 usec  
TE 295.1 K  
D1 1.00000000 sec  
D1 1  
TD0 1

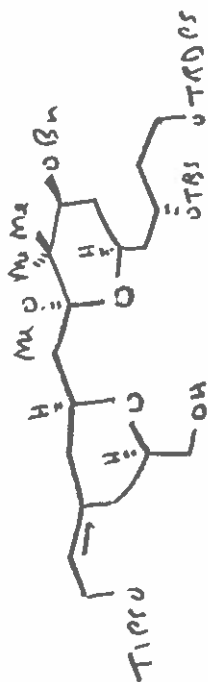
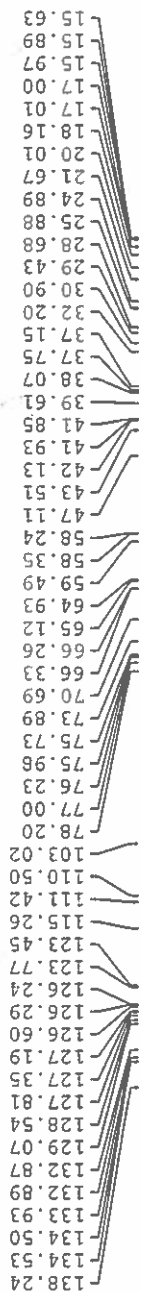
===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300521 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



17



atl1c1otbdpsc16oh  
mCARBONnight CDCl3 /opt/bruk500data/2011/Aug ejt 3

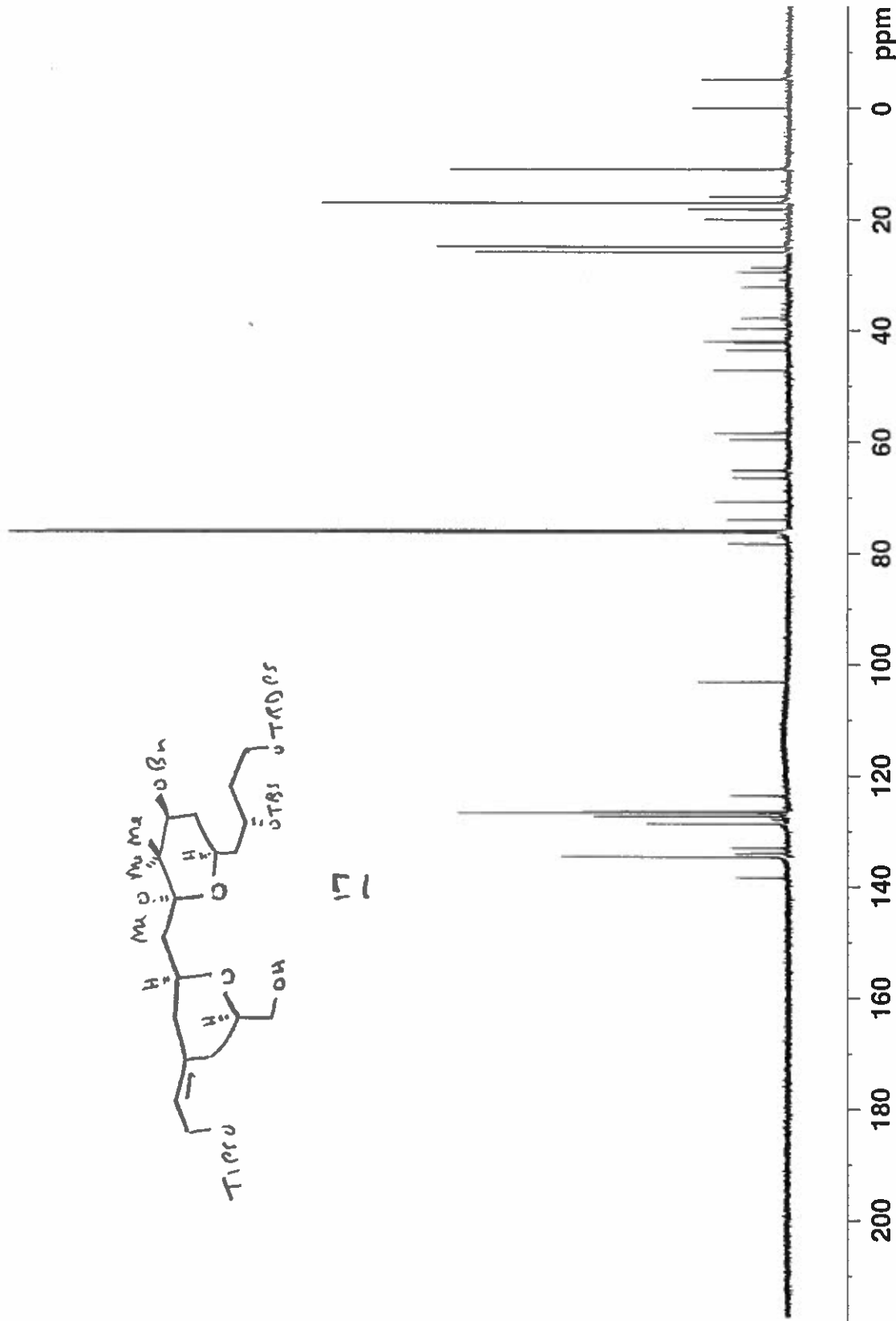


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2011-08-30-ejt-3  
NAME  
EXPNO 22  
PROCNO 1  
Date\_ 20110830  
Time 23:55  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 3072  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 usec  
DE 32.21 usec  
TE 295.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 11.50 usec  
PL1 -4.20 dB  
PL1W 218.02882385 W  
SFO1 125.7703643 MHz

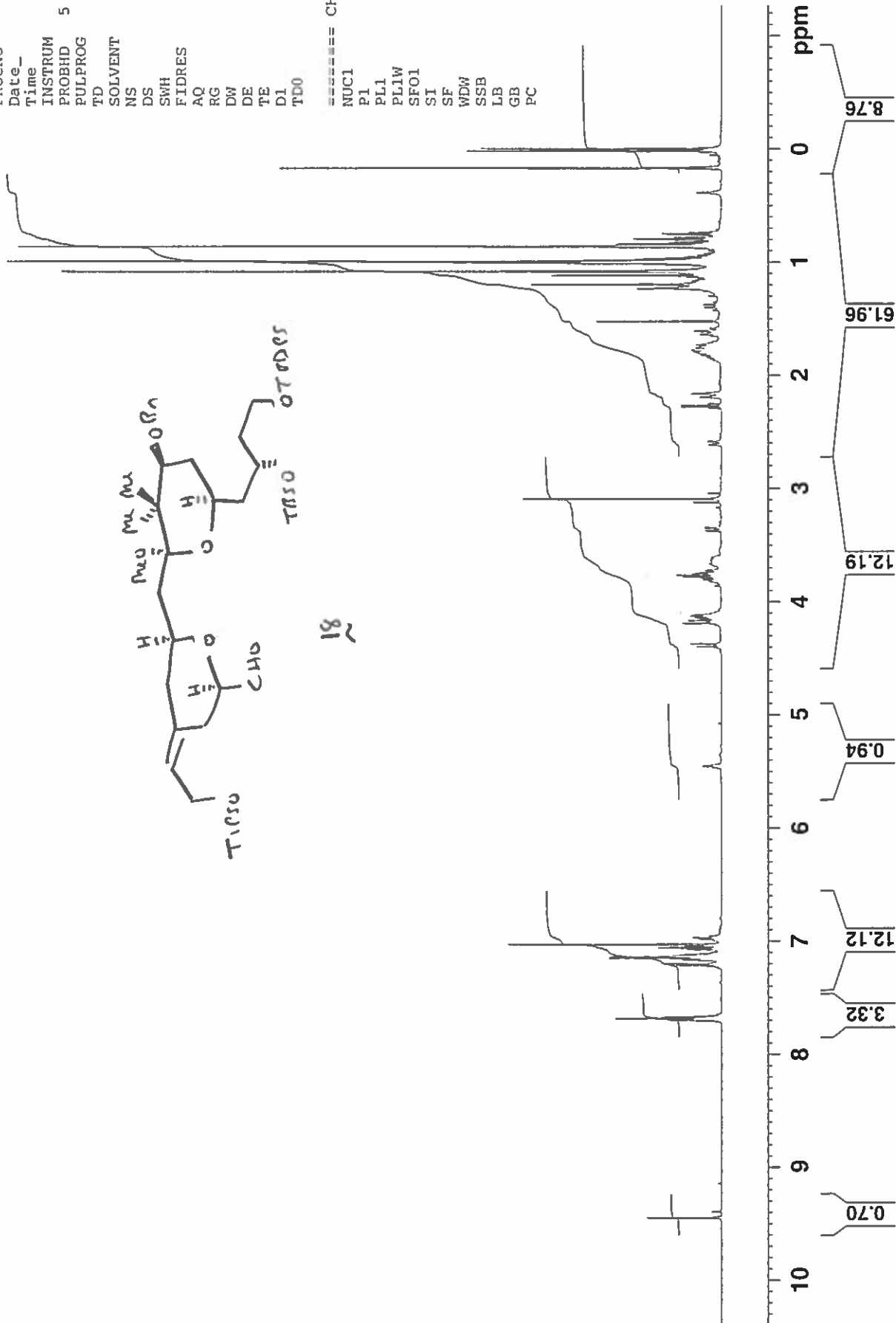
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 4.20 dB  
PL12 23.99 dB  
PL13 23.00 dB  
PL2W 9.74092484 W  
PL12W 0.10223514 W  
PL13W 0.12841040 W  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7579202 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

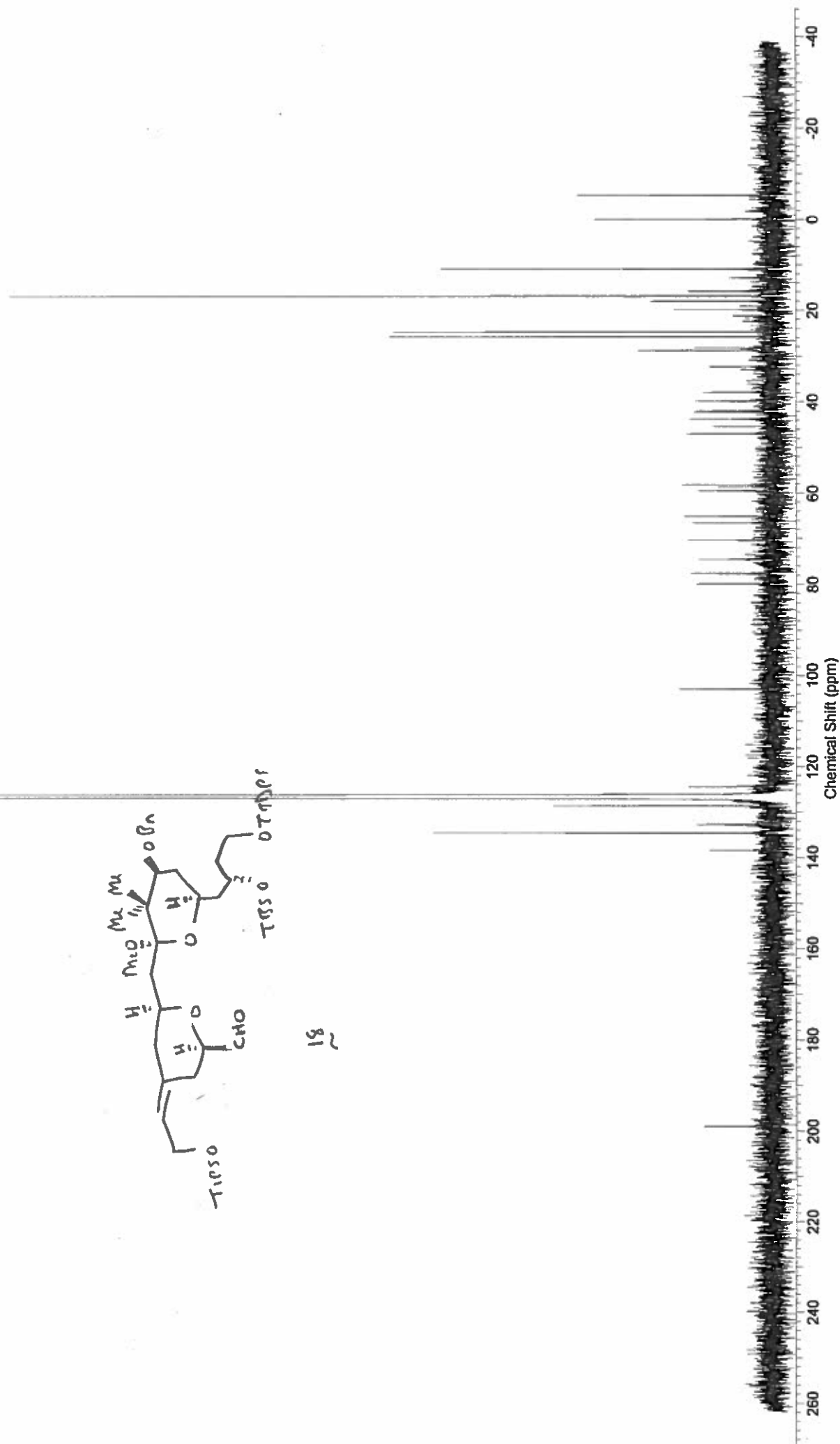
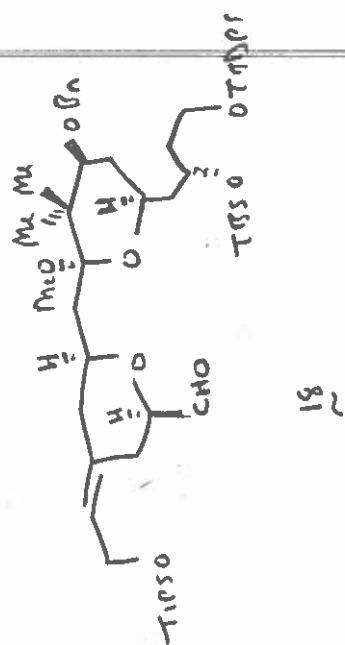




NAME 2011-09-06-ejt-31  
EXPNO 10  
PROCNO 1  
Date\_ 20110906  
Time 16.40  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 64  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 90.5  
DW 48.400 usec  
DE 10.67 usec  
TE 294.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SF01 500.1330885 MHz  
SI 32768  
SF 500.1301190 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

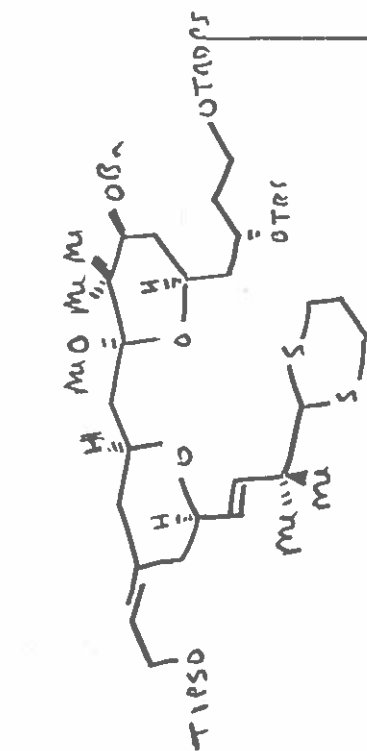




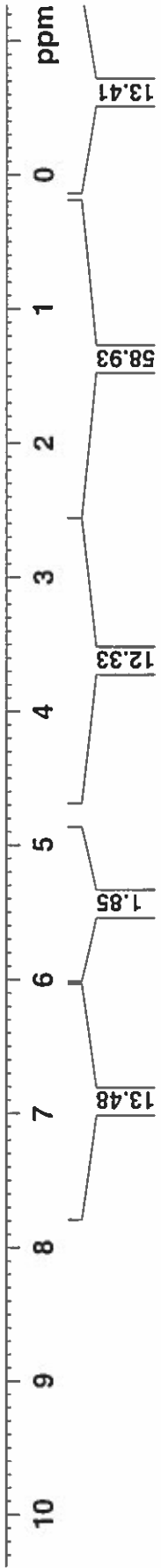
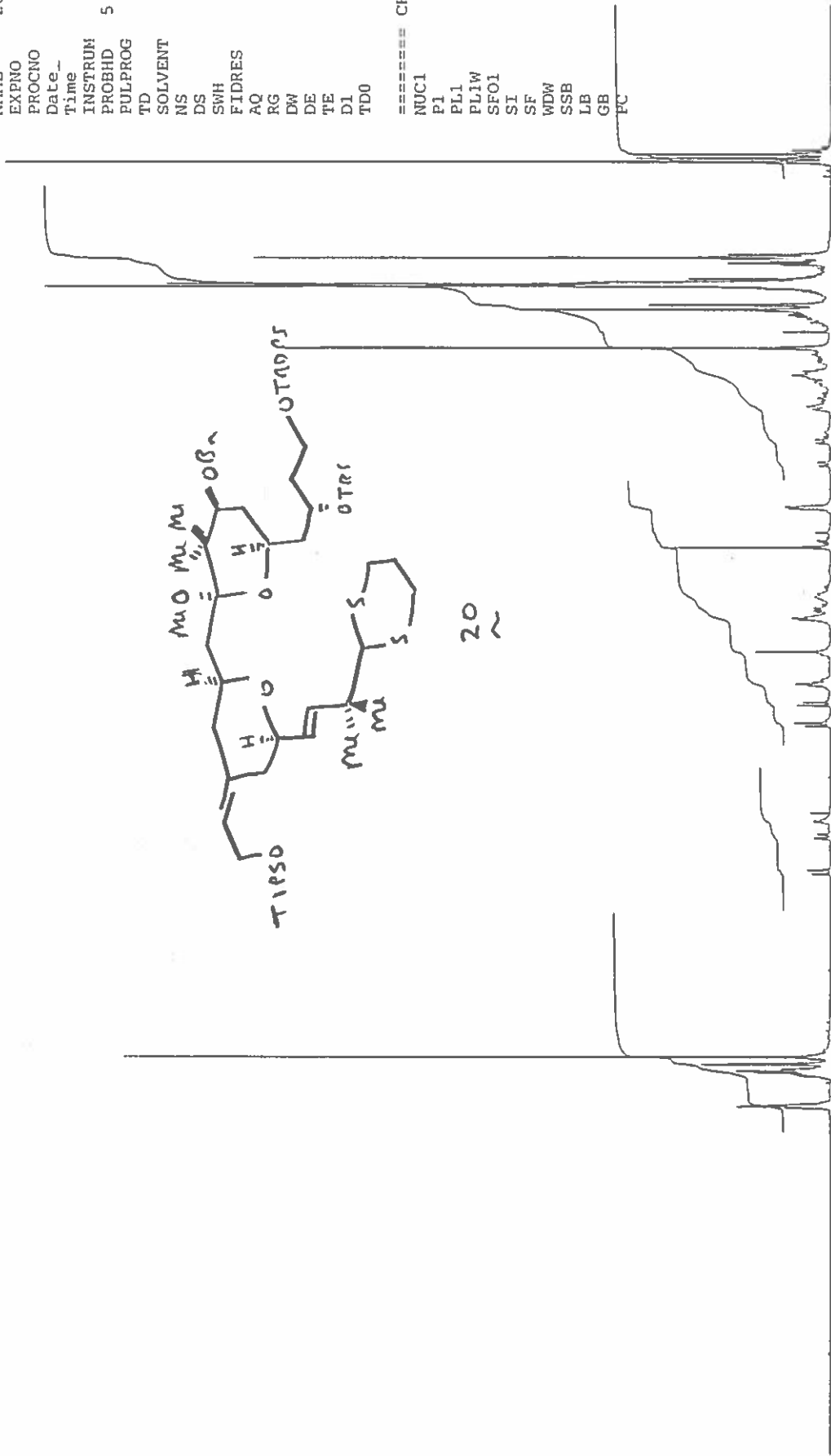


NAME 2011-08-30-ejt-4  
EXPNO 10  
PROCNO 1  
Date\_ 20110831  
Time 5.32  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 512  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 256  
DW 48.400 usec  
DE 13.38 usec  
TE 295.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300482 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



20 ~



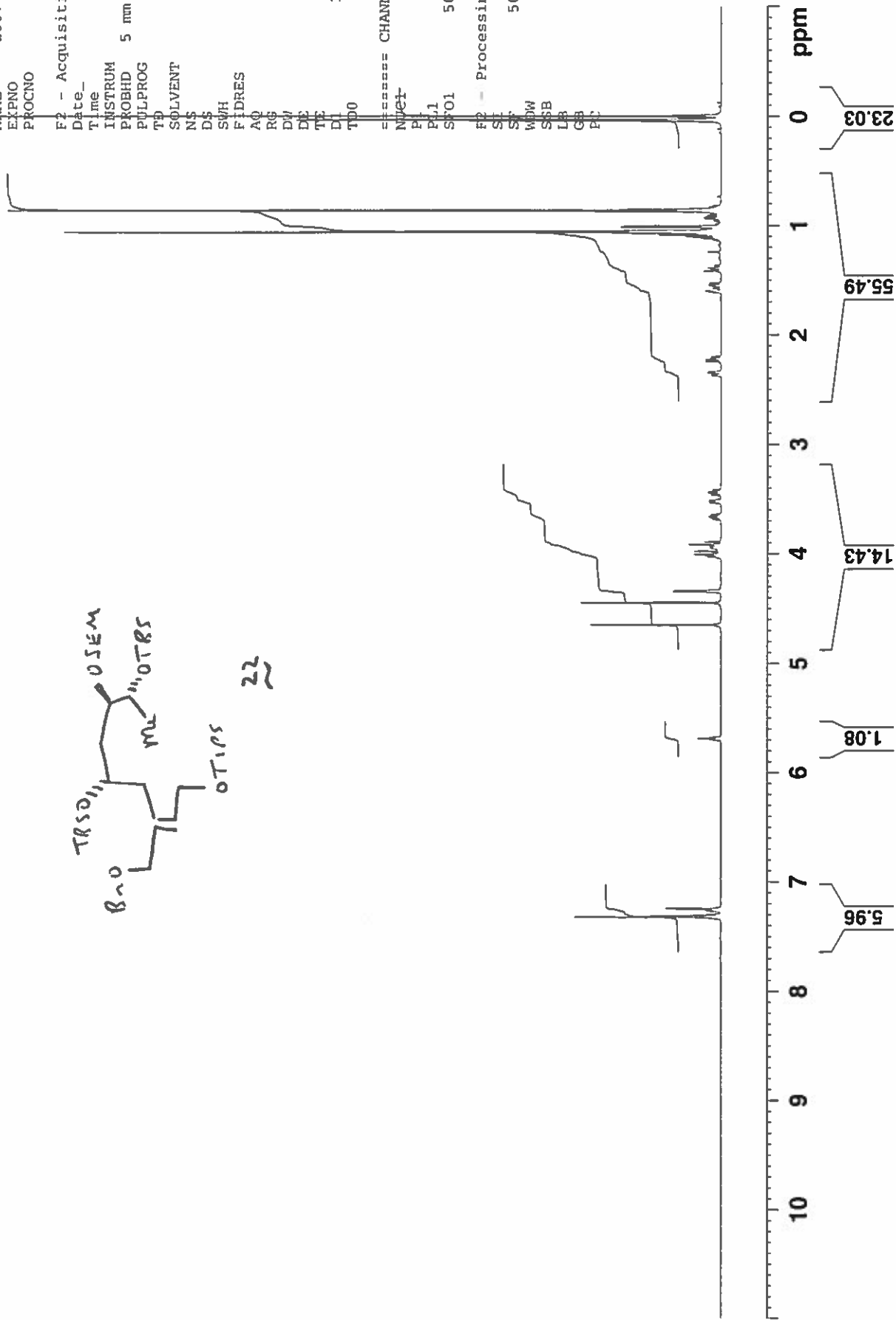


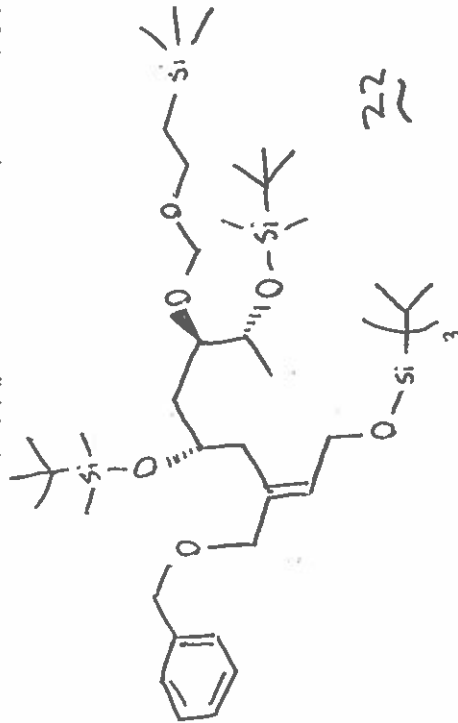
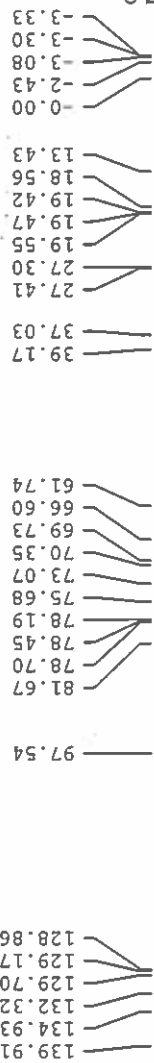
Current Data Parameters  
 NAME 2007-08-24-ejt-9  
 EXPNO 14  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20070828  
 Time 2.32  
 INSTRUM spect  
 PROBHD 5 mm TXI 1H/D-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1719923 sec  
 RG 32  
 DQ 48.400 usec  
 DE 13.76 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.80 usec  
 PL1 3.25 dB  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300163 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





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Current Data Parameters  
NAME 2007-08-24-ejt-9  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070828  
Time 2.30  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCI3  
NS 256  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 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 11.50 usec  
PL1 -4.20 dB  
SFO1 125.7703643 MHz

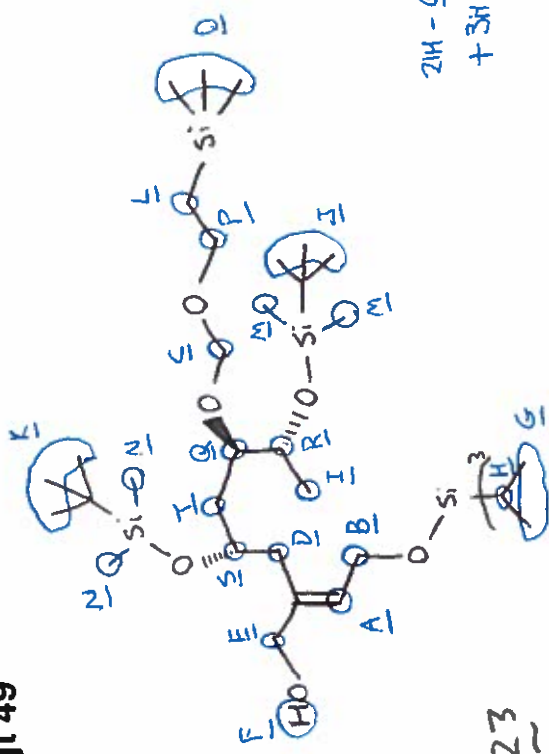
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL12 20.00 dB  
PL13 23.00 dB  
PL2 3.25 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7576096 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm



20H-3, K, L



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Current Data Parameters  
NAME 2007-08-30-ejt-49  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070830  
Time 14.37  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCI3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 25.4  
DW 48.400 usec  
DE 13.76 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 7.80 usec  
PL1 3.25 dB  
SFO1 500.1330885 MHz

FP - Processing parameters  
SI 32768  
SF 500.1300176 MHz  
WDW EM  
SSB 0  
LB 0  
GB 0  
PC 1.00

6H, 6H-M, N

9H-O

2H-G+H  
+ 3H-I

4H-E, S, R  
1H-P

1H, 1H-J  
1H-I

1H-F  
1H, 1H-D, D

2H-C

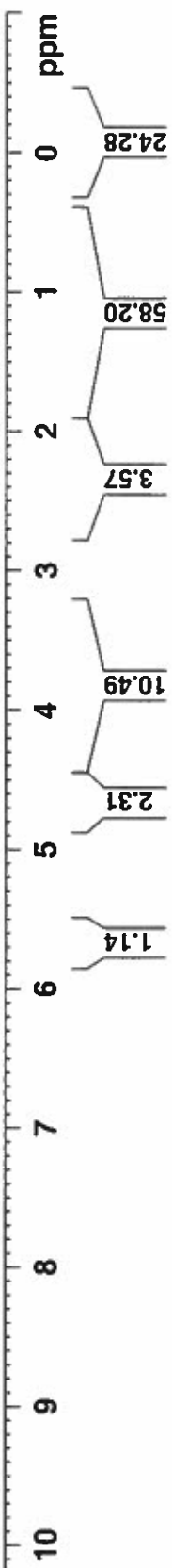
1H-A

2H-B

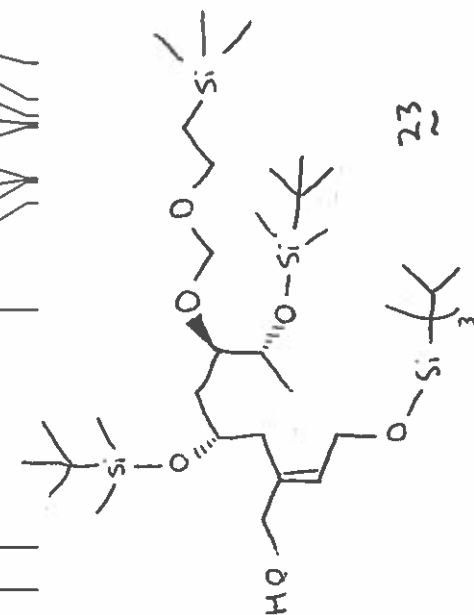
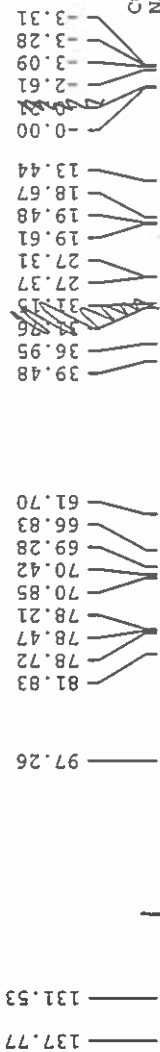
1H-P

2H-P, Q

1H, 1H-J







Current Data Parameters  
NAME 2007-08-30-ejt-49  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070831  
Time 1.32  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DE 16.800 usec  
TE 6.00 usec  
300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

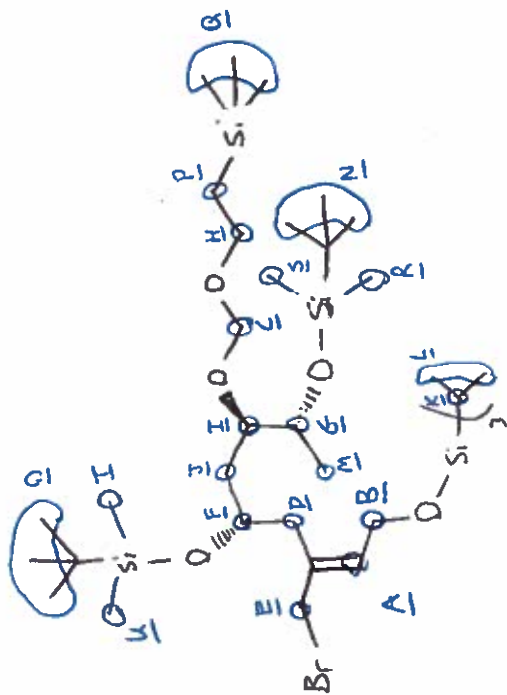
===== CHANNEL f1 =====  
NUC1 13C  
P1 11.50 usec  
PL1 -4.20 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL12 20.00 dB  
PL13 23.00 dB  
PL2 3.25 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7576067 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

SH337\_A  
mPROTONight CDCl3 /opt/topspin ejt 16



Current Data Parameters  
NAME 2007-08-31-ejt-16  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070902  
Time 10.38  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 64  
DW 48.400 usec  
DE 13.76 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 7.80 usec  
PL1 3.25 dB  
SFO1 500.1330885 MHz  
F2 - Processing parameters  
SF 32768  
SFO 500.1300195 MHz  
EM 0  
GB 0.30 Hz  
PC 0  
PR 1.00

24H-  
K, L, M

20H-  
N, O, P

1H, 1H  
-D, D'

3H  
-E, E'

1H-E  
1H-H  
2H-H+I

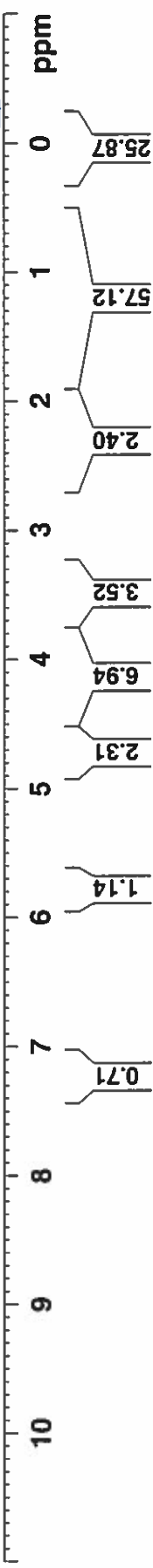
2H-B  
2H-C

1H-A  
2H-C

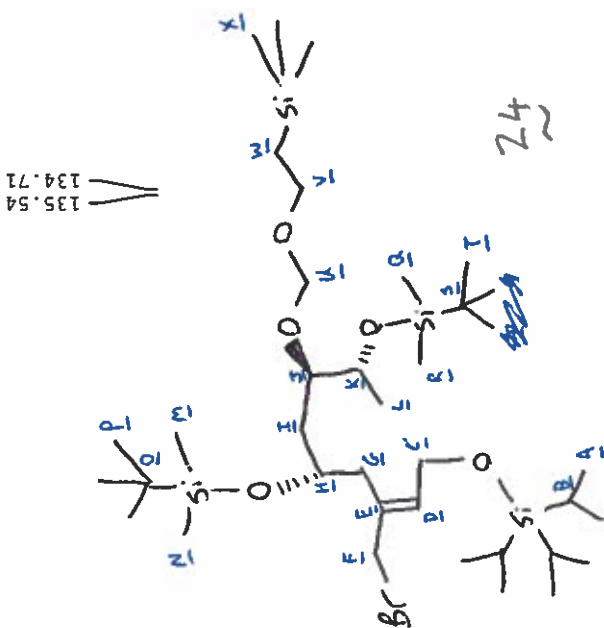
CHCl3

9H-Q

12H total,  
R, S, T, U,  
-1, -2, -3, -4



# SH337\_A mCARBONnight CDCl3 /opt/topspin ejt 16



Current Data Parameters  
NAME 2007-08-31-ejt-16  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070902  
Time 11.22  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 512  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 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 11.50 usec  
PL1 -4.20 dB  
SFO1 125.7703643 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL12 20.00 dB  
PL13 23.00 dB  
PL2 3.25 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7576096 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

M, N, O, R

200 180 160 140 120 100 80 60 40 20 0 ppm

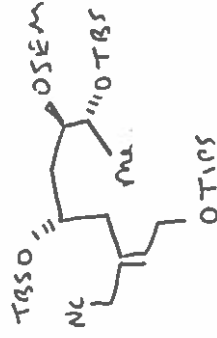


Current Data Parameters  
NAME 2007-09-21-ejt-15  
EXPNO 11  
PROCNO 1

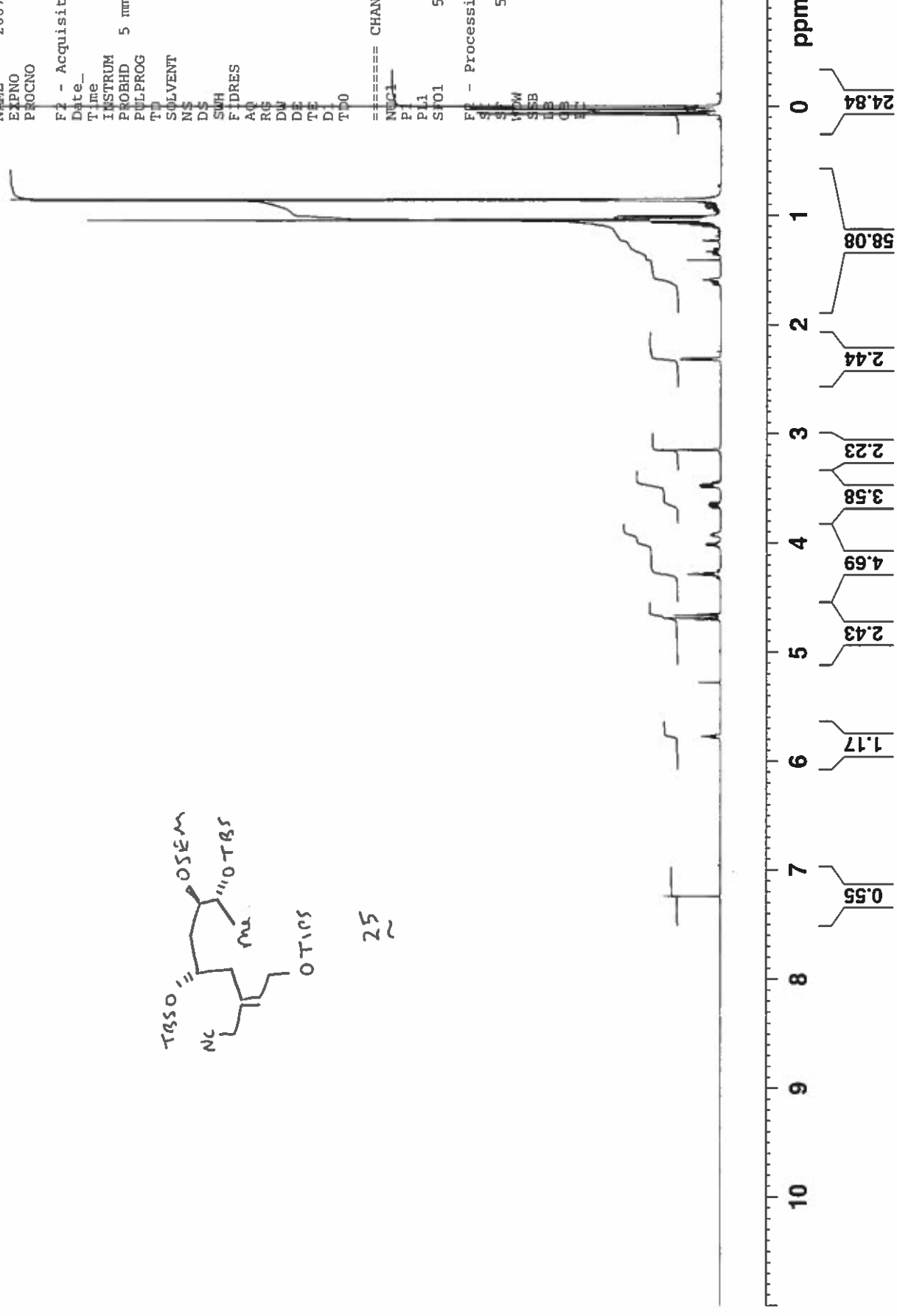
F2 - Acquisition Parameters  
Date\_ 20070923  
Time 0.26  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 28.5  
DW 48.400 usec  
DE 13.76 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 7.80 usec  
PL1 3.25 dB  
SFO1 500.1330885 MHz

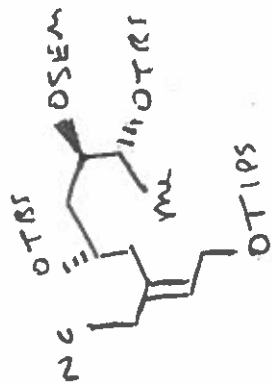
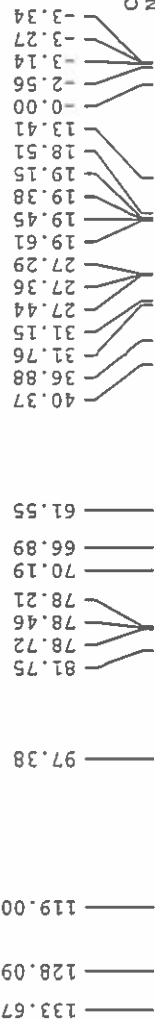
F2 - Processing parameters  
SI 32768  
SF 500.1300180 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
CB 1.00



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SH350\_A  
mCARBONnight CDCl3 /opt/topspin ejt 15



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Current Data Parameters  
NAME 2007-09-21-ejt-15  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070923  
Time 0.48  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 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 11.50 usec  
PL1 -4.20 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL12 20.00 dB  
PL13 23.00 dB  
PL2 3.25 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7576070 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

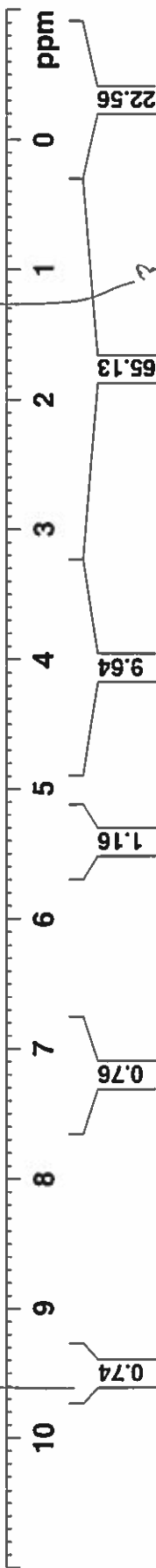
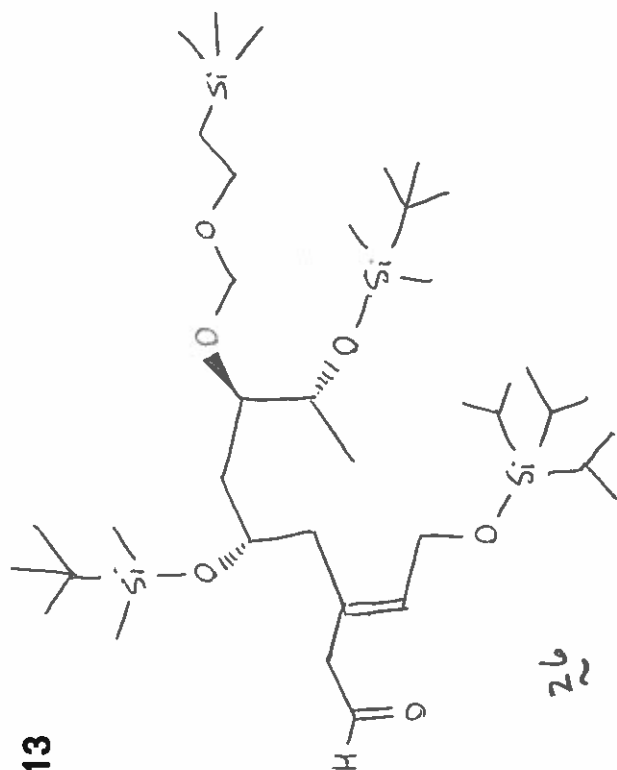
F2 - Acquisition Parameters	
Date_	Time_
20070914	11.00
INSTRUM	spect
PROBHD	5 mm TXI 1H/D-
PULPROG	zg30b
TD	65536
SOLVENT	CDCl3
NS	32
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	45.2
DN	48.400 usec
DE	13.76 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1

```

===== CHANNEL f1 =====
1H
7.80 usec
3.25 dB
500.1330885 MHz
SFO1

F7 - Processing parameters
SI 32768
SF 500.1300167 MHz
WDW EM
SSB 0
LFB 0
CB 0
PC 1.00

```





Current Data Parameters  
NAME 2007-09-27-ejt-50  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070928  
Time 1.53

INSTRUM spect  
PROBHD 5 mm TXI 1H/D-

PULPROG zg30b  
TD 65536

SOLVENT CDCl3  
NS 16

DS 0  
SWH 10330.578 Hz

FIDRES 0.157632 Hz  
AQ 3.171923 sec

RG 22.6  
DW 48.400 usec

DE 13.76 usec  
TE 300.0 K

D1 1.00000000 sec  
TD0 1

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

PC 7.80 usec  
PL 3.25 dB

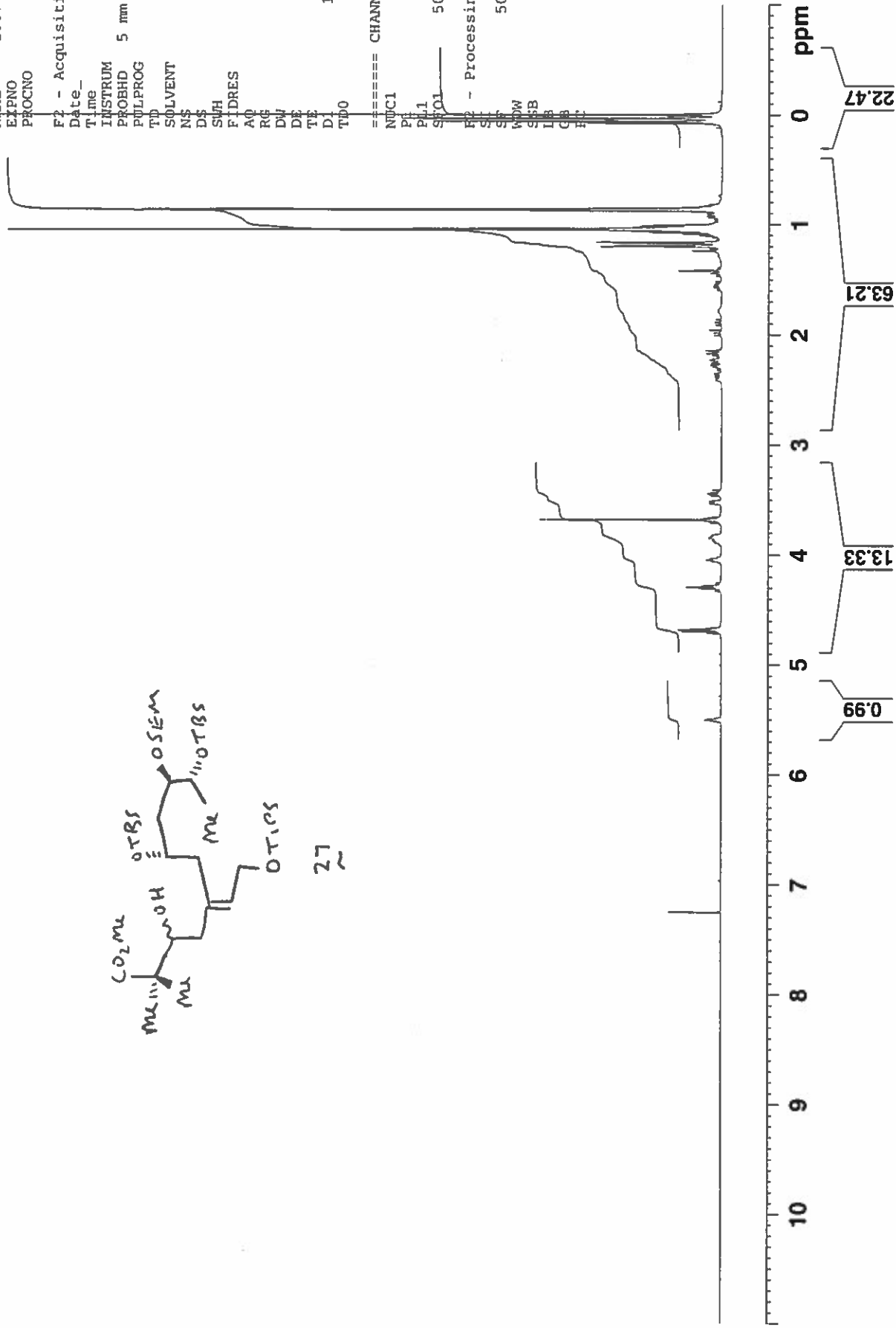
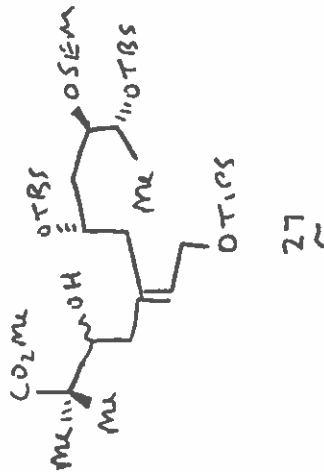
SR01 500.1330885 MHz

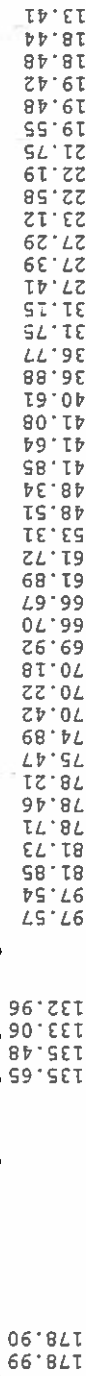
F2 - Processing parameters  
SI 32768

ST 500.1300121 MHz  
WDW EM

SSB 0  
LB 0.30 Hz

GB 0  
PC 1.00





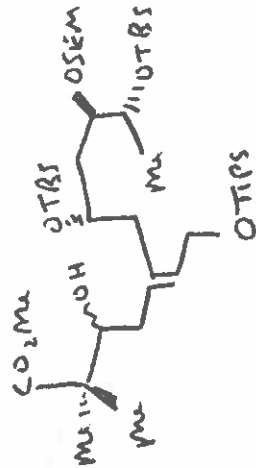
Current Data Parameters  
NAME 2007-09-27-ejt-50  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070928  
Time 1.52  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 11.50 usec  
PL1 -4.20 dB  
SFO1 125.7703643 MHz

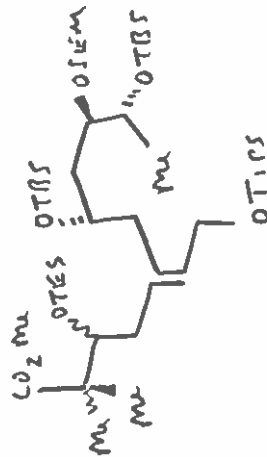
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL12 20.00 dB  
PL13 23.00 dB  
PL2 3.25 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7576076 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



200 180 160 140 120 100 80 60 40 20 0 ppm



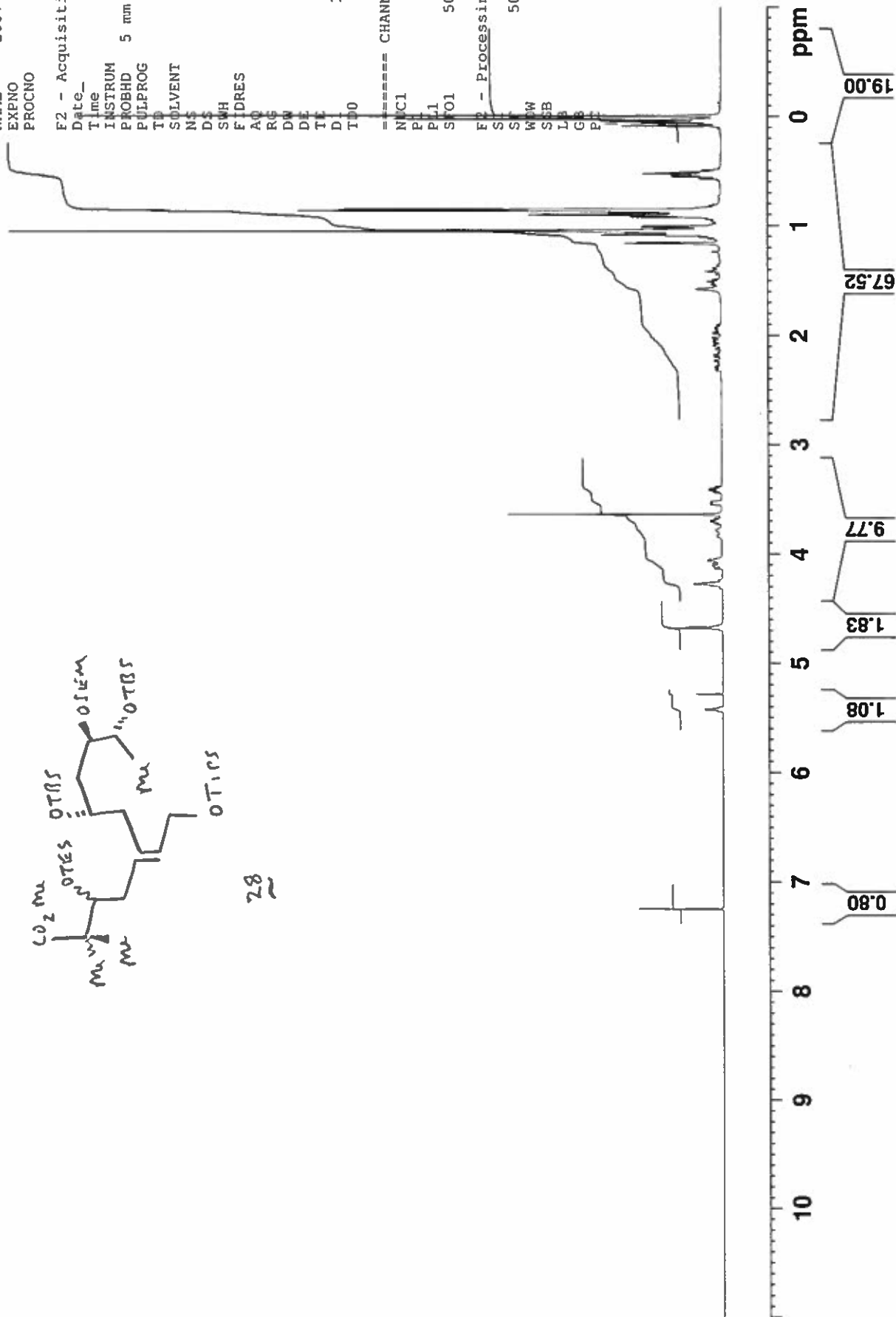


Current Data Parameters  
NAME 2007-11-20-ejt-6  
EXPNO 10  
PROCNO 1

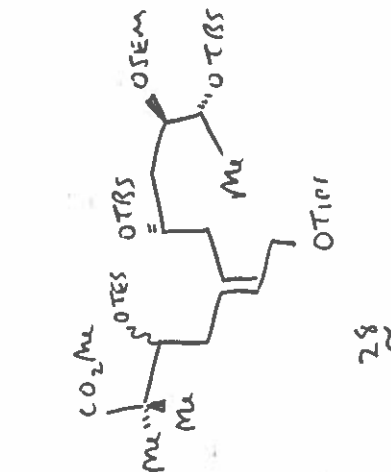
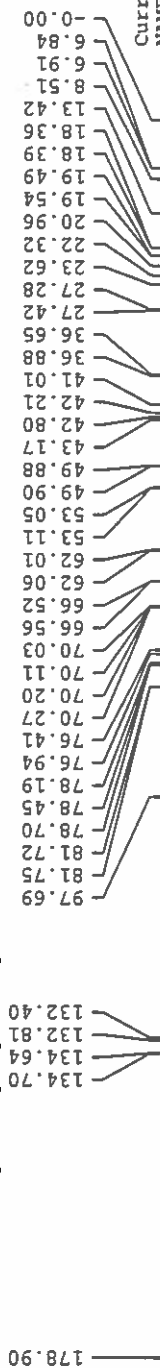
F2 - Acquisition Parameters  
Date\_ 20071121  
Time 6.09  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 48  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 90.5  
DW 48.400 usec  
DE 13.76 usec  
TE 300.0 K  
D1 1.00000000 sec  
T1 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 7.80 usec  
PL1 3.25 dB  
SFO1 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300142 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



SH383\_A  
mCARBONnight CDCI3 /opt/topspin ejt 37



Current Data Parameters  
NAME 2007-11-21-ejt-37  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20071122  
Time 4.30  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCI3  
NS 1024  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 11.50 usec  
PL1 -4.20 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL12 20.00 dB  
PL13 23.00 dB  
PL2 3.25 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7576078 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

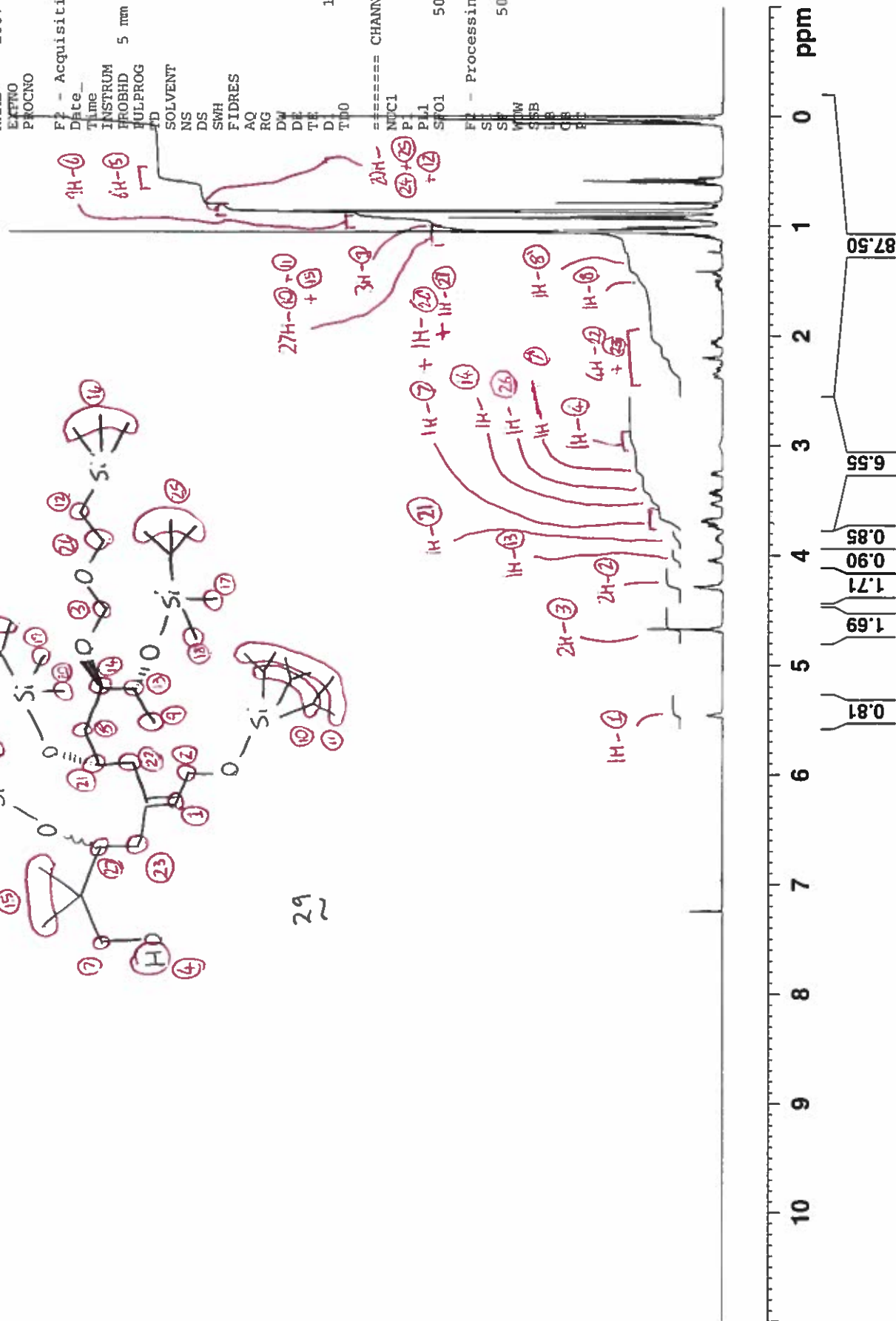
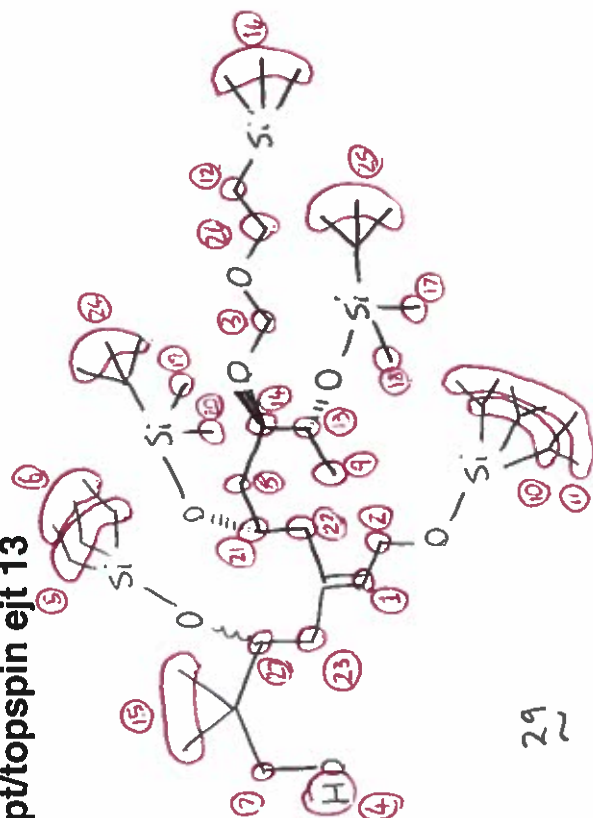
BRUKER

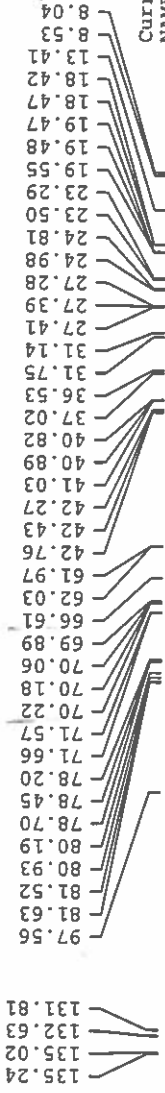
```

FF2 - Acquisition Parameters
Date_      20071123
Time       6.54
INSTRUM    spect
PROBHD     5 mm TXI 1H/D-
PULPROG    zg30b
TD         65536
SOLVENT    CDCl3
NS         32
DS         0
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1719923 sec
RG         22.6
DW         48.400 usec
DE         13.76 usec
TE         300.0 K
D1         1.00000000 sec
T100      1

```

FT	Processing parameters
SI	32768
SR	500.1300146 MHz
SWH	EM
SSB	0
GB	0.30 Hz
CR	0
PR	1.00





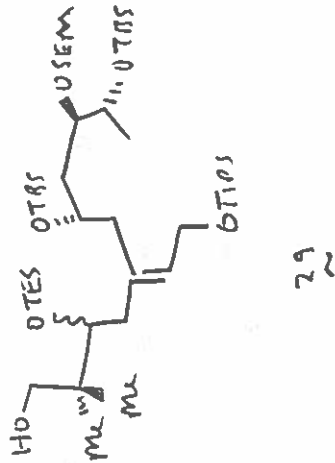
Current Data Parameters  
NAME 2007-11-22-ejt-13  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20071123  
Time 7.21  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 512  
DS 2  
SMH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

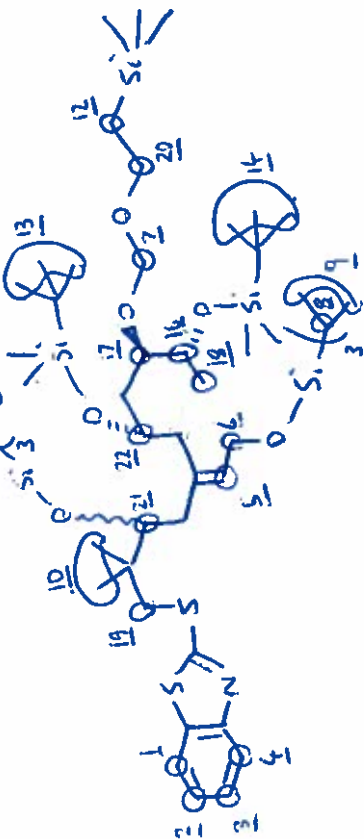
===== CHANNEL f1 =====  
NUC1 13C  
P1 11.50 usec  
PL1 -4.20 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL12 20.00 dB  
PL13 23.00 dB  
PL2 3.25 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7576081 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



SH390\_A  
mPROTONnight CDCl3 /opt/topspin ejt 17



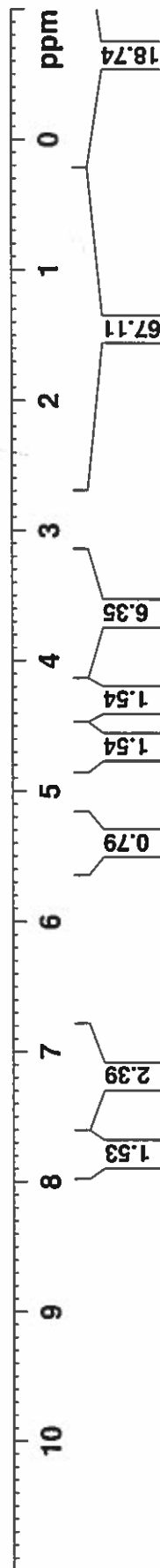
Current Data Parameters  
NAME 2007-11-27-ejt-17  
EXPNO 10  
PROCNO 1

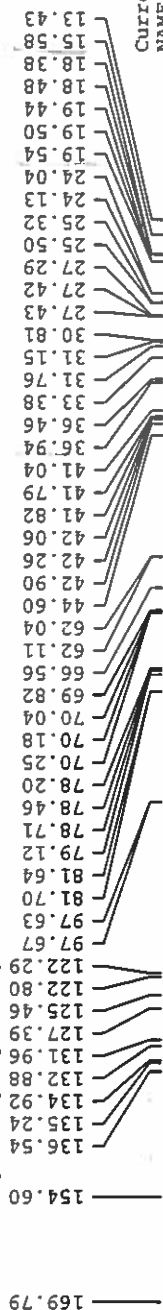
F2 - Acquisition Parameters  
Date\_ 20071127  
Time 21.44  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 90.5  
DW 48.400 usec  
DE 13.76 usec  
TE 300.0 K  
D 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P 7.80 usec  
PL1 3.25 dB  
SFO1 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300108 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
CB 1.00

For better 'H,  
See Bruker 300  
Dec 4, 2007,  
File 1202.





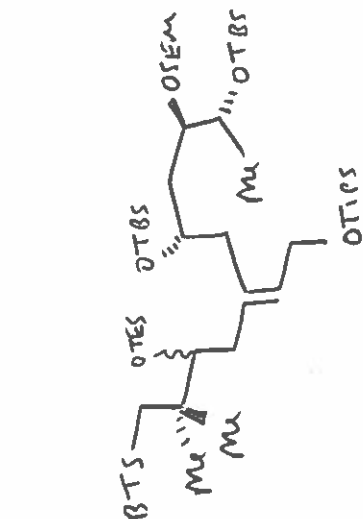
Current Data Parameters  
NAME 2007-11-27-ejt-17  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20071127  
Time 22.38  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DE 16.800 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 11.50 usec  
PL1 -4.20 dB  
SFO1 125.7703643 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL12 22.50 dB  
PL13 23.00 dB  
PL2 2.50 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7576079 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



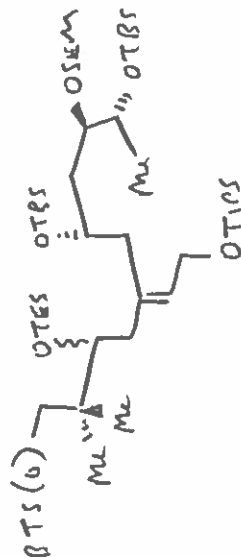
30

200 180 160 140 120 100 80 60 40 20 0 ppm

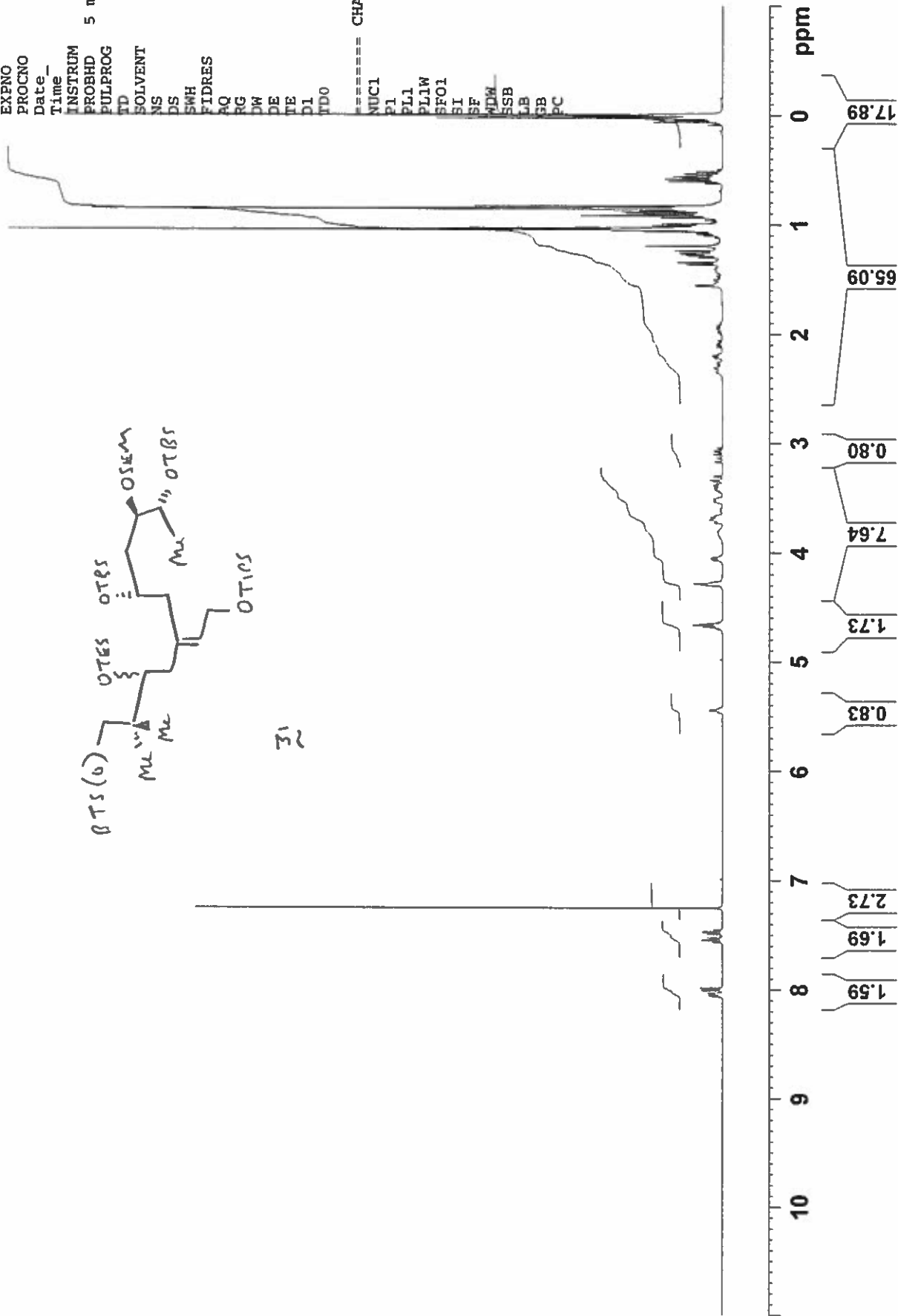
SH sulfoxide  
mPROTONnight CDC13 {C:\bruk400data\2008\Oct} ejt 8



NAME 2008-10-31-ejt-8  
 EXPNO 20  
 PROCNO 1  
 Date\_ 20081031  
 Time\_ 14.20  
 INSTRUM AV400  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDCl3  
 NS 64  
 DS 0  
 SWH 8264.463 Hz  
 FIDRES 0.126106 Hz  
 AQ 3.9649780 sec  
 RG 322  
 DW 60.500 usec  
 DE 9.40 usec  
 TE 292.8 K  
 D1 1.00000000 sec  
 TDO 1  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 -3.60 dB  
 PL1W 17.83863831 W  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300129 MHz  
 NDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



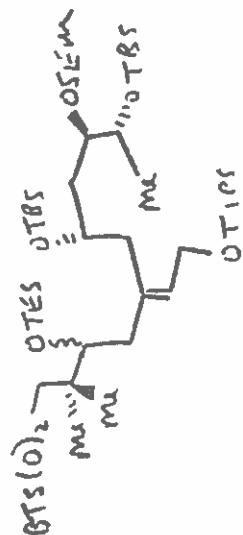
31



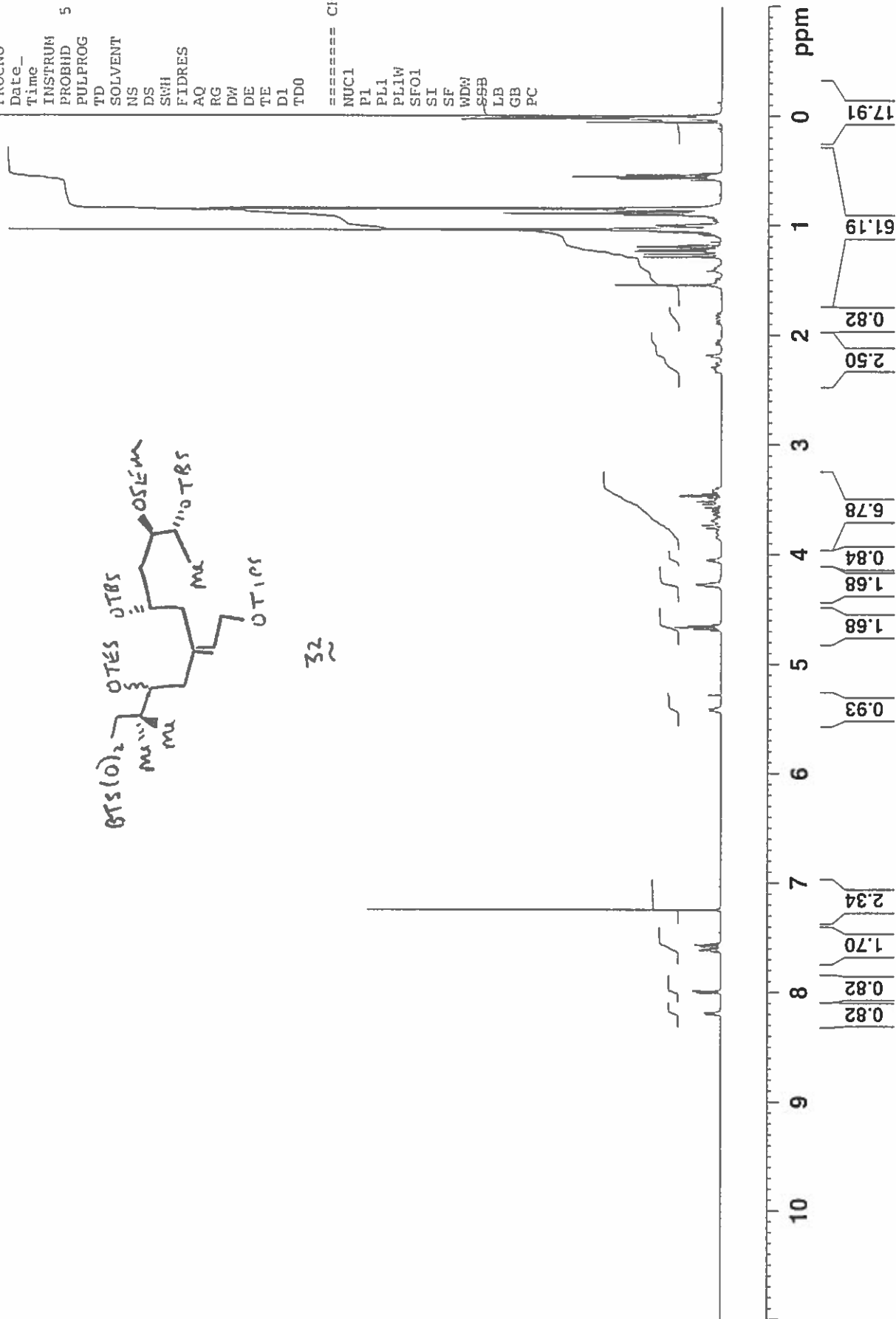


NAME 2009-04-08-ejt-43  
EXPNO 10  
PROCNO 1  
Date\_ 20090408  
Time 10.32  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SCH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 161  
DW 48.400 usec  
DE 13.38 usec  
TE 295.9 K  
D1 1.0000000 sec  
TD0 1

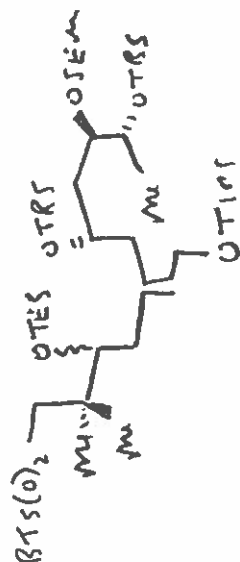
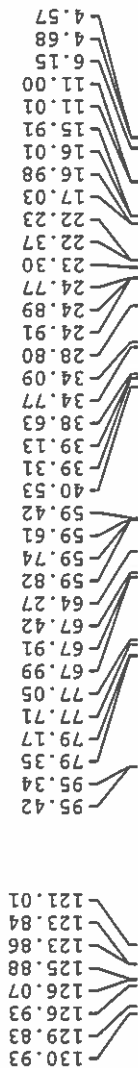
===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300192 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



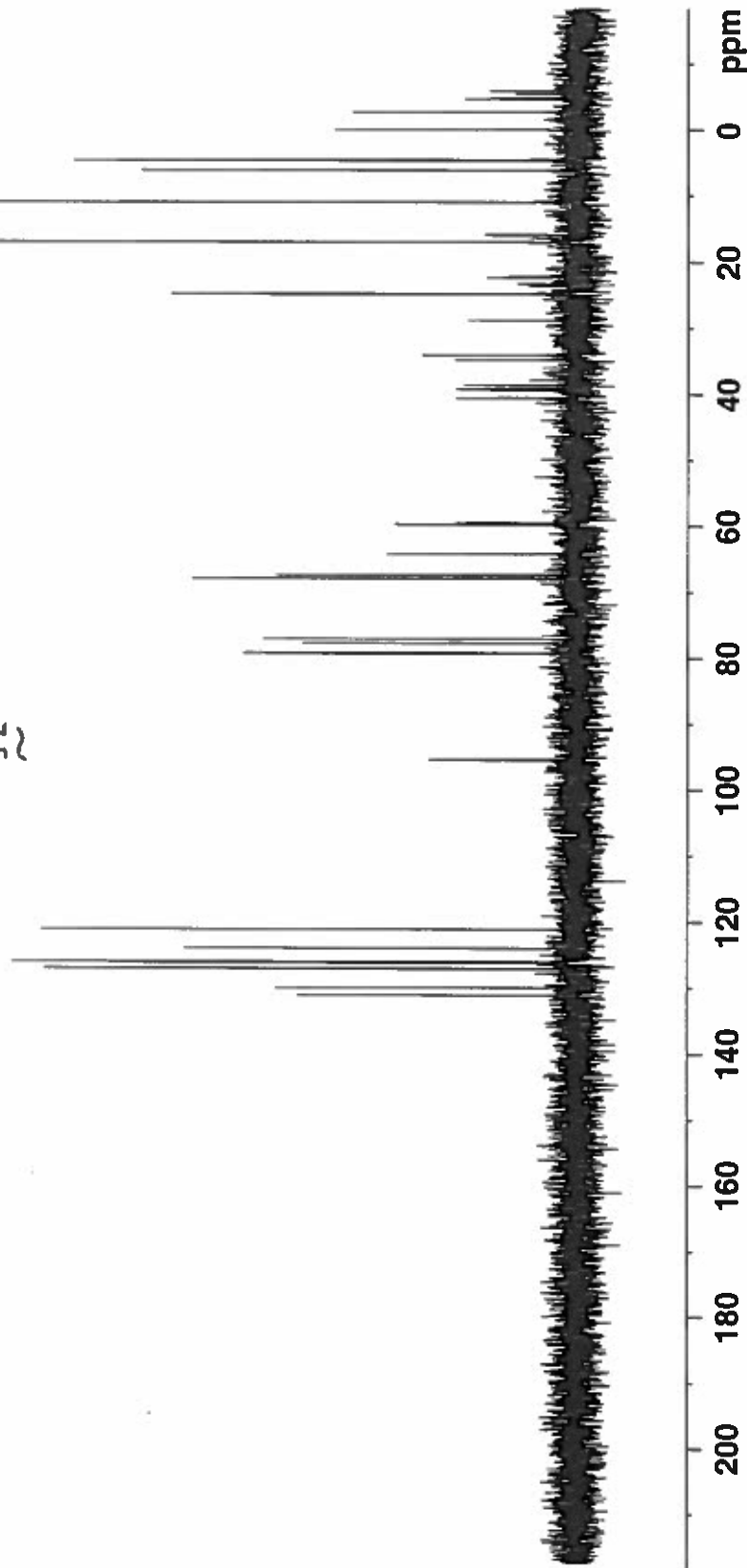
32







322



NAME	EXPNO	PROCNO	Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DE	DM	TE	CNST2	D1	D2	D12	TD0
2008-01-31-jct-34	14	1	20080131	12.51	spec	5 mm TXI 1H/D-	dept90.m	55536	C6D6	256	4	29761.904 Hz	0.454131 Hz	1.1010548 sec	512	16.800 usec	6.00 usec	300.0 K	145.0000000	2.000000000 sec	0.00344828 sec	0.000020000 sec	1

```
===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
P2        19.00 usec
PL1       -4.20 dB
PL1W      218.03882385 W
SF01      125.7703643 MHz
```

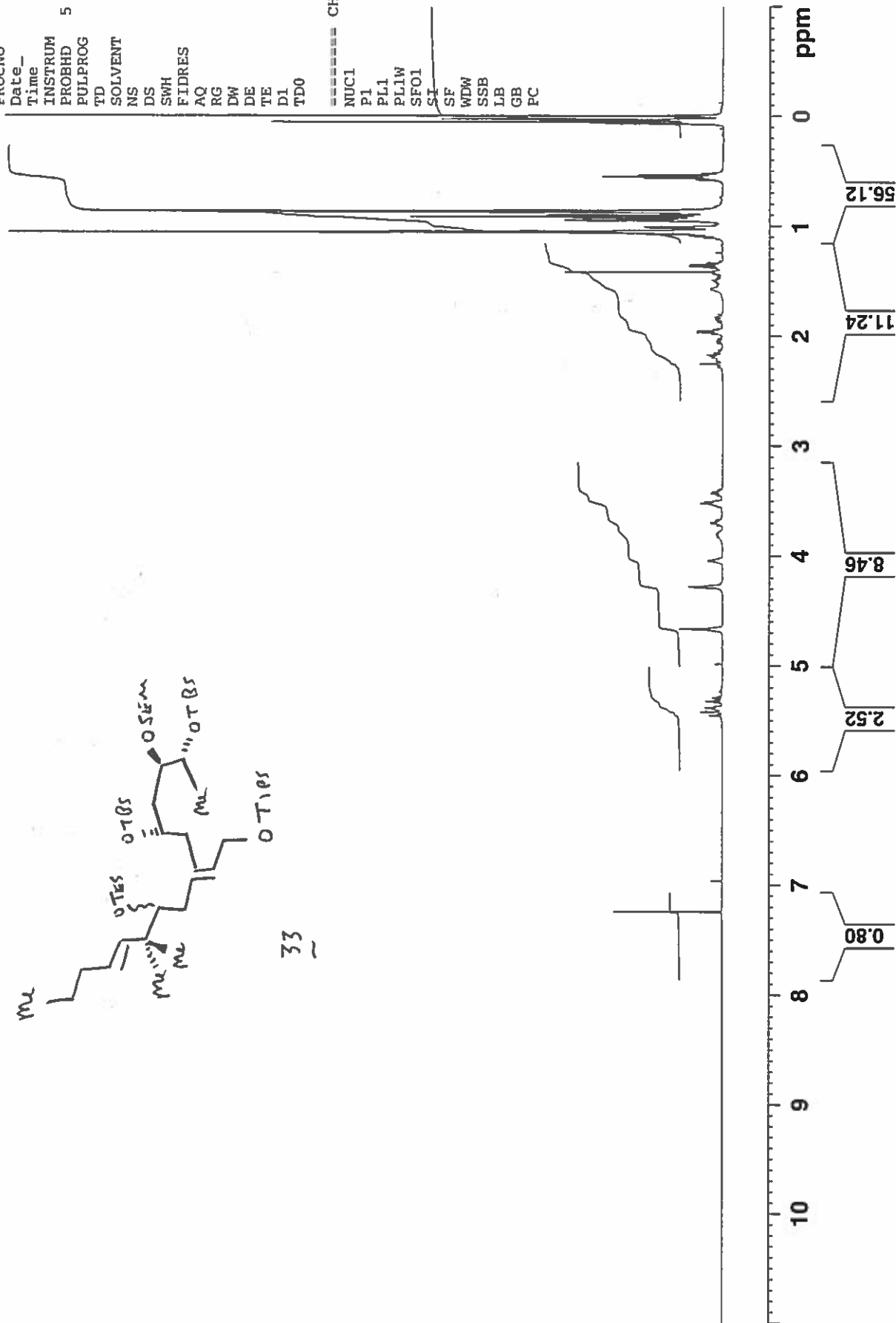
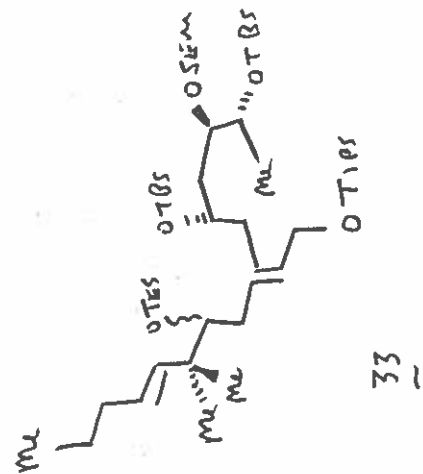
```
===== CHANNEL f2 =====
CPDPRG2      waitz16      IH
NUC02
P3           21.07 usec
P4           42.14 usec
PCPD2       80.00 usec
PL2         4.20 dB
PL12        15.79 dB
          9.74092484 W
PL2W        0.67546082 W
PL12W       500.1320005 MHz
SFO2        32768
SI          125.7579321 MHz
SF          EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
```

SH397

mPROTONnight CDCl<sub>3</sub> /opt/bruk500data/2008/Jan ejt 6

2008-01-31-ejt-6  
 NAME EXPNO 11  
 PROCNO 1  
 Date\_ 20080201  
 Time 5.20  
 INSTRUM spect  
 PROBHD 5 mm TXI 1H/D-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 96  
 DS 0  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.1719923 sec  
 RG 64  
 DW 48.400 usec  
 DE 13.46 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.80 usec  
 PL1 3.25 dB  
 PL1W 12.12272263 W  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1300154 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





NAME 2008-01-16-ejt-52

EXPNO 10

PROCNO 1

Date\_ 20080116

Time 17.04

INSTRUM spect

PROBHD 5 mm TXI 1H/D-

PULPROG zg30b

TD 65536

SOLVENT C6D6

NS 64

DS 0

SWH 10330.578 Hz

FIDRES 0.157632 Hz

AQ 3.1719923 sec

RG 90.5

DW 48.400 usec

DE 10.67 usec

TE 300.0 K

D1 3.0000000 sec

TD0 1

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

NUC1 1H

P1 21.07 usec

PL1 3.25 dB

PL1W 12.12272263 W

SFO1 500.1330885 MHz

SI 32768

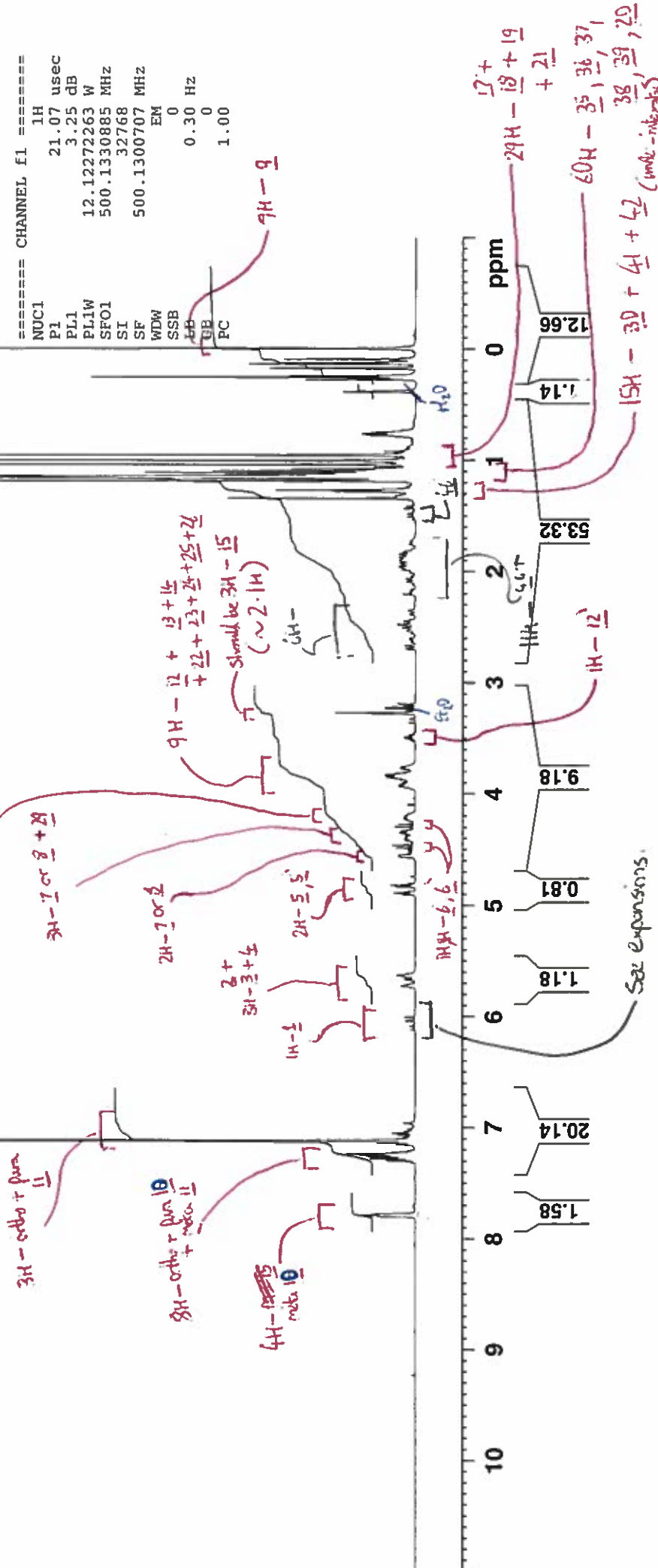
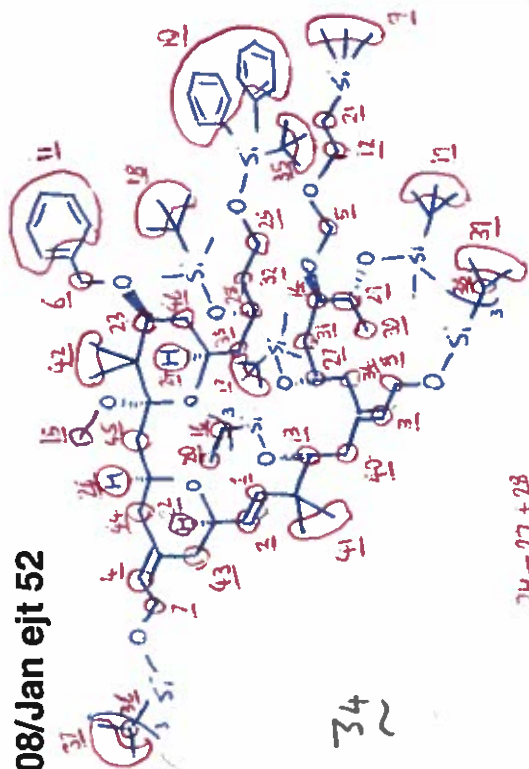
SF 500.1300707 MHz

WDW EM

SSB 0

GB 0.30 Hz

PC 1.00



Si411

mPROTON C6D6 /opt/bruk500data/2008/Feb ejt 17

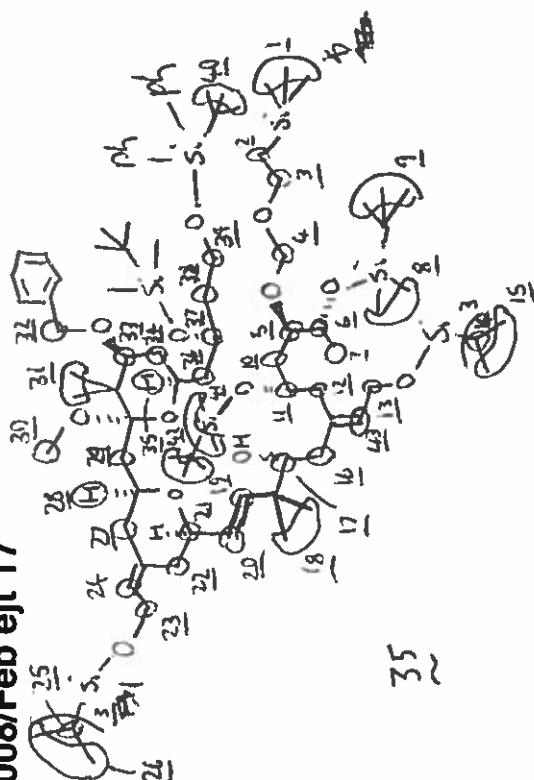


2008-02-26-ejt-17

NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20080226  
Time 11.22  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 64  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 90.5  
DW 48.400 usec  
DE 10.67 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

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

NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300688 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



41-32+13+23

+6+37

+11

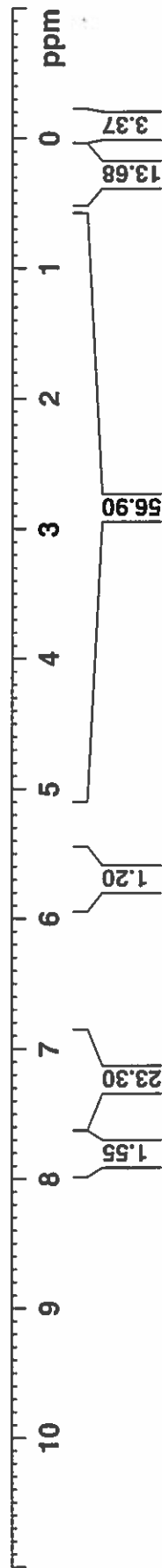
41-

24-4

41-43+20

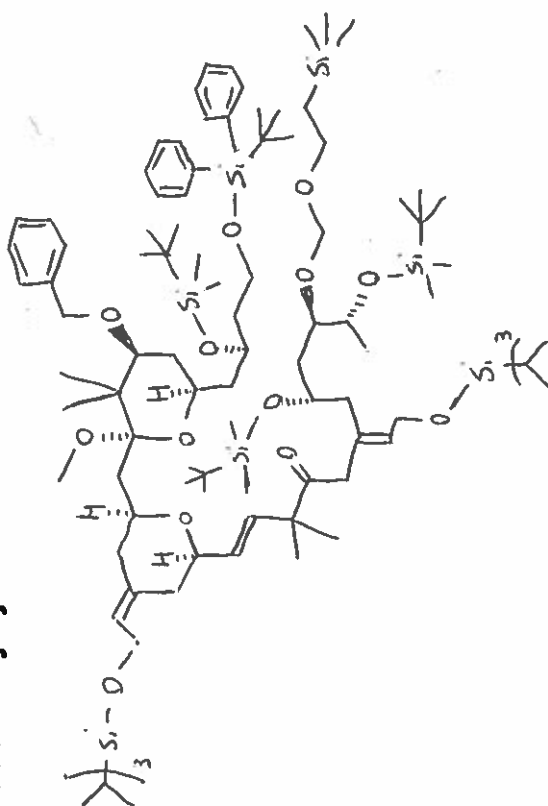
+24

14-19

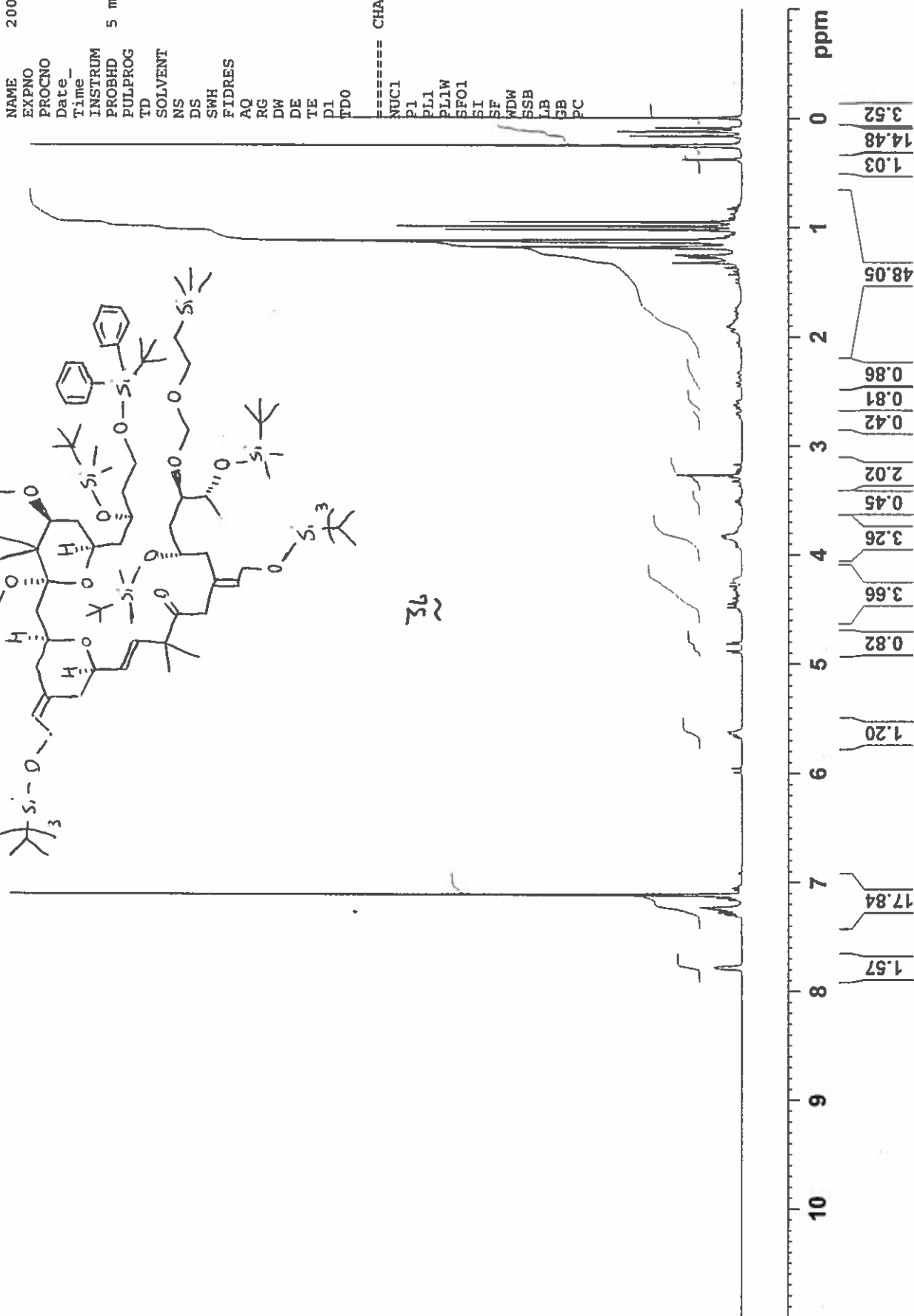


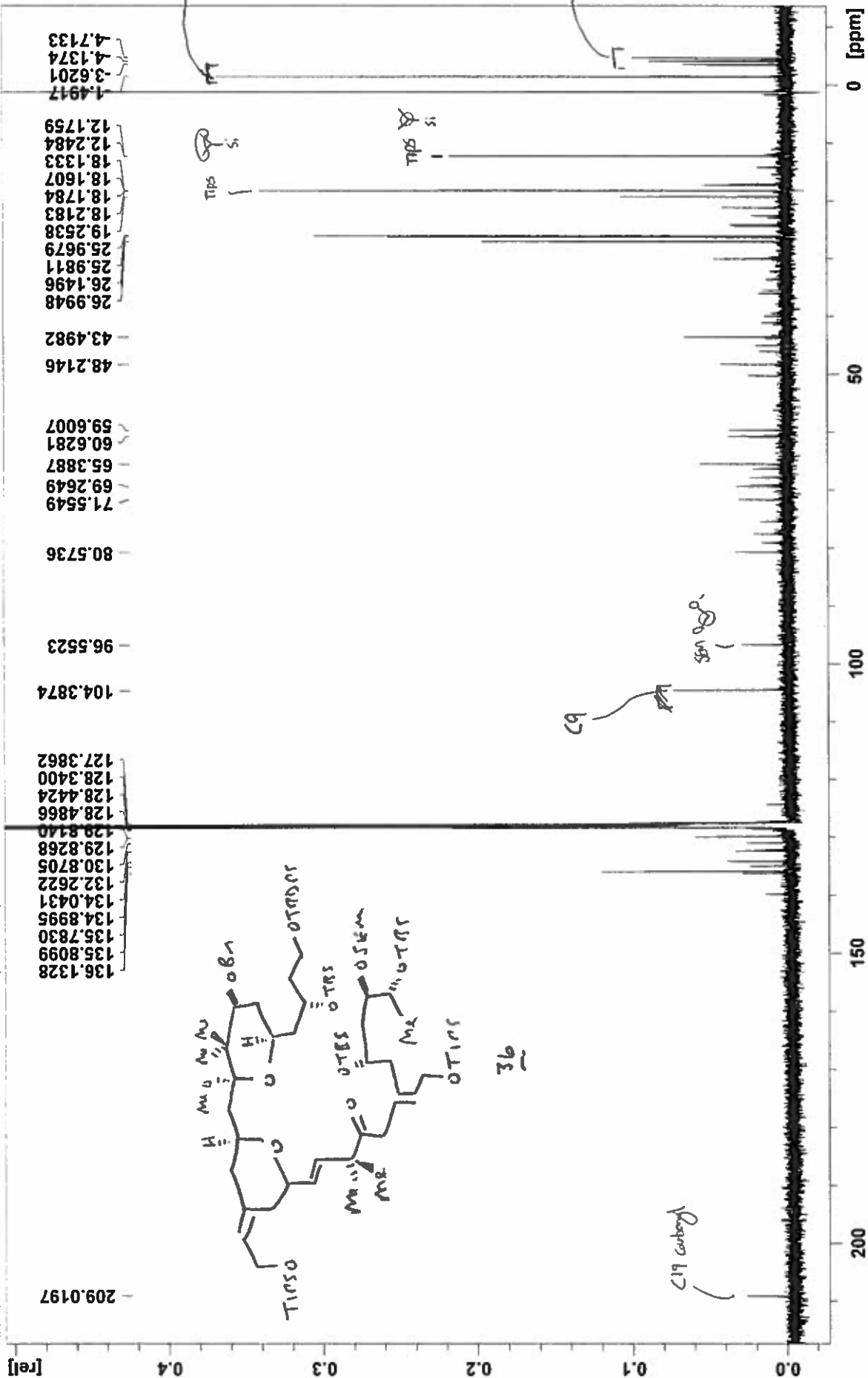
SH412

mPROTON C6D6 {C:\bruk400data\2008\Feb} ejt 58



NAME 2008-02-29-ejt-58  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20080229  
 Time\_ 10.36  
 INSTRUM AV400  
 PROBD 5 mm PABBO BB-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT C6D6  
 NS 64  
 DS 0  
 SWH 8264.463 Hz  
 FIDRES 0.126106 Hz  
 AQ 3.9649780 sec  
 RG 181  
 DW 60.500 usec  
 DE 9.40 usec  
 TE 293.6 K  
 D1 1.00000000 sec  
 TDO 1  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 -3.60 dB  
 PL1W 17.83863831 W  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300615 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00







2010-02-09-ejt-7

NAME

EXPNO

PROCNO

Date\_

Time

INSTRUM

PROBHD

PULPROG

TD

SOLVENT

NS

DS

SWH

FIDRES

AQ

RG

DW

DE

TE

D1

TD0

20100209  
18.17  
spect  
5 mm TXI 1H/D-  
zg30b  
65536  
C6D6  
64  
0

10330.578 Hz

0.157632 Hz

3.1719923 sec

28.5

48.400 usec

10.67 usec

294.8 K

1.00000000 sec

1

=====

CHANNEL f1

=====

NUC1

1H

P1

21.07 usec

PL1

3.25 dB

PL1W

12.12272263 W

SFO1

500.1330885 MHz

SI

32768

SF

500.1300000 MHz

WDW

EM

SSB

0

LB

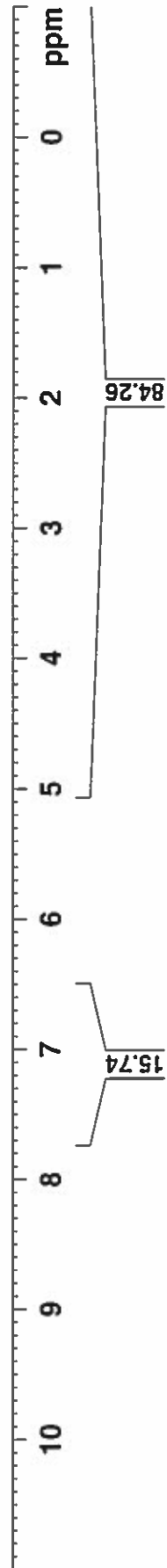
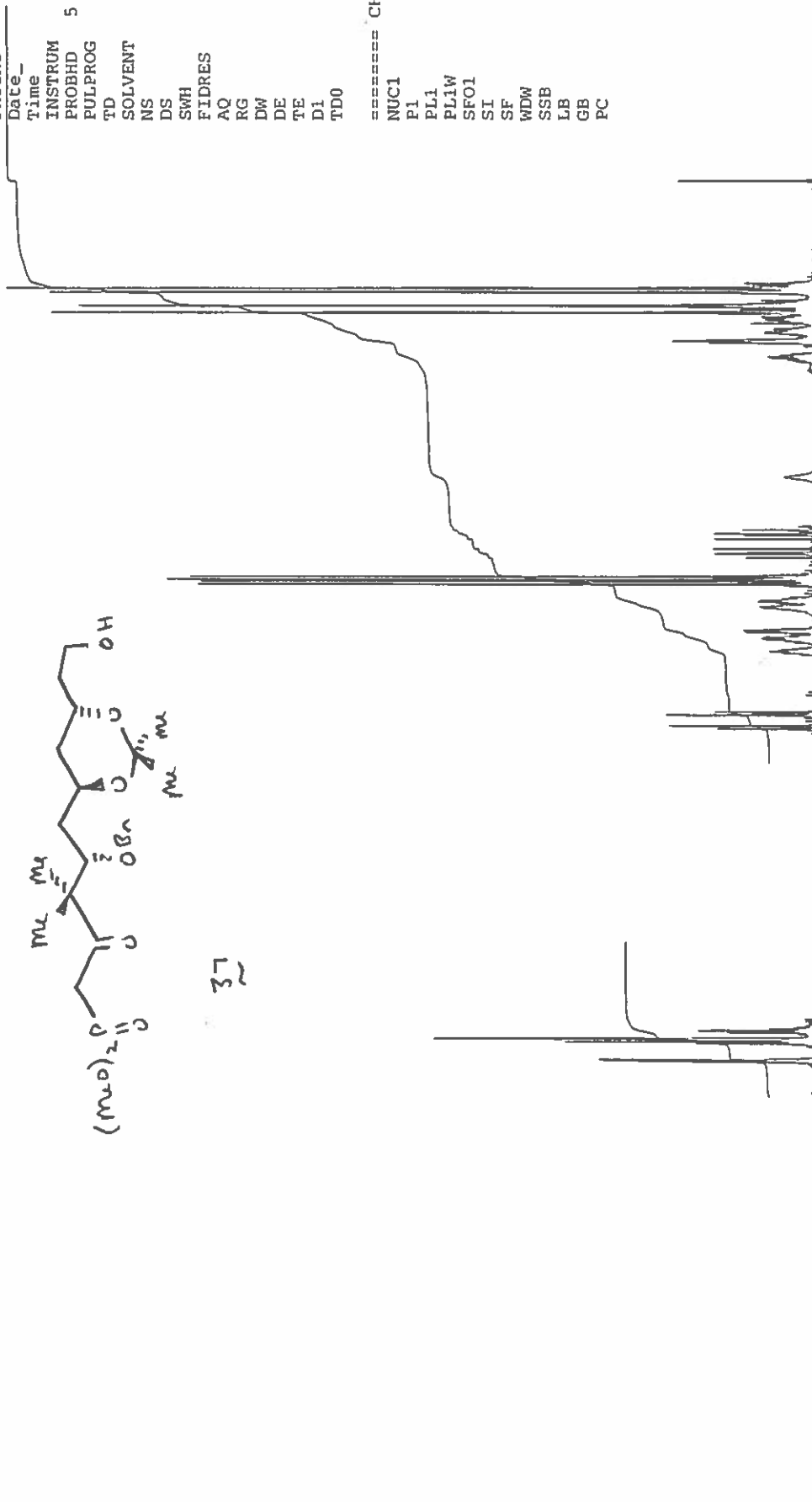
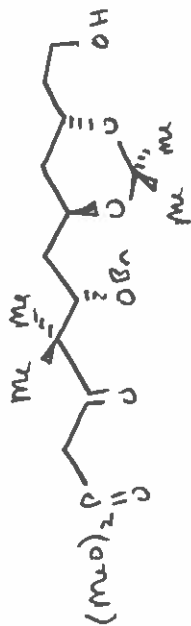
0.30 Hz

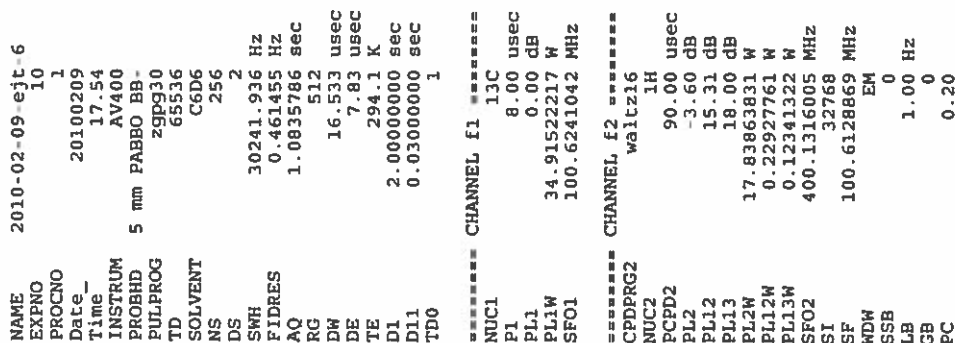
GB

0

PC

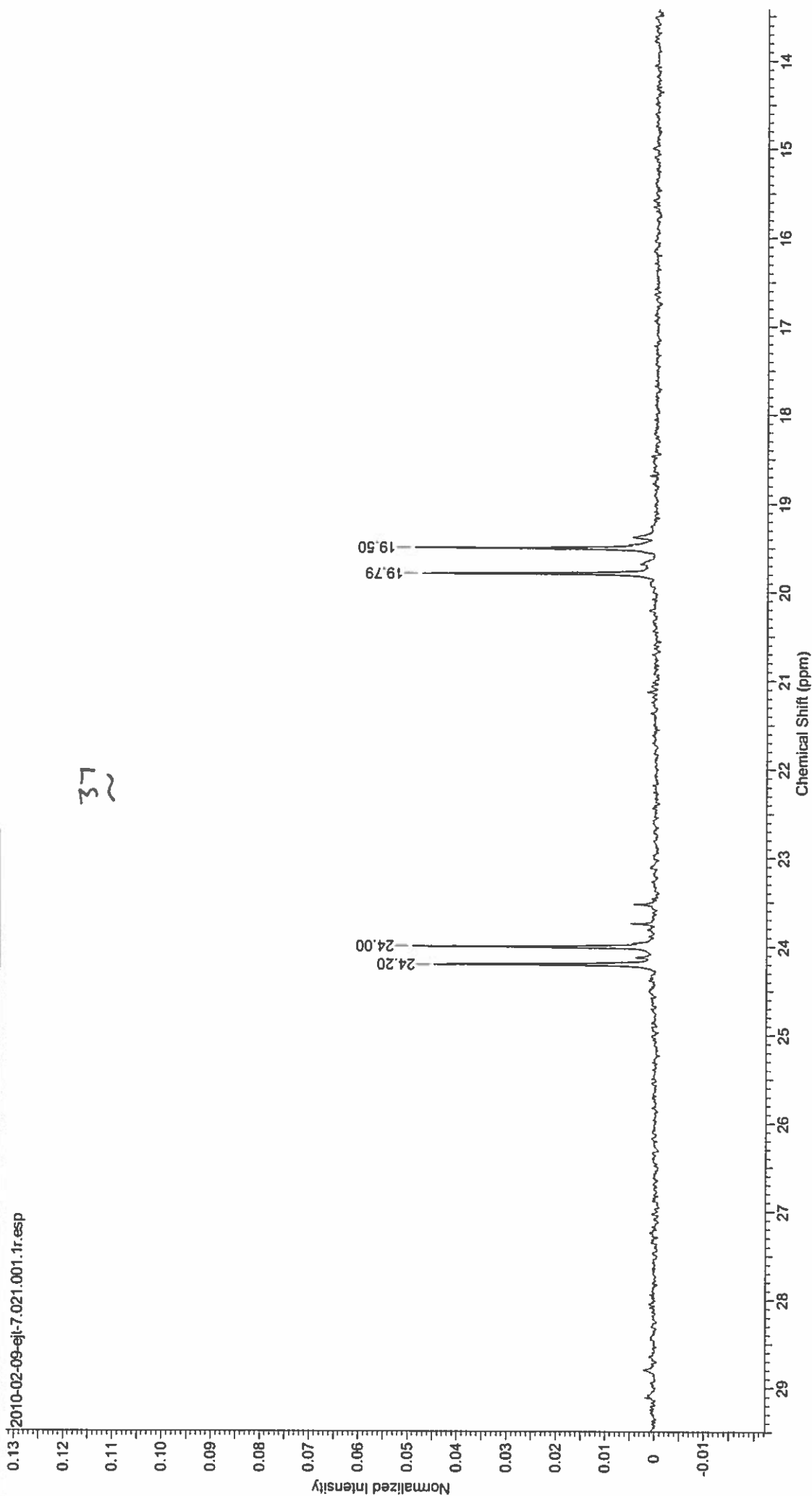
1.00



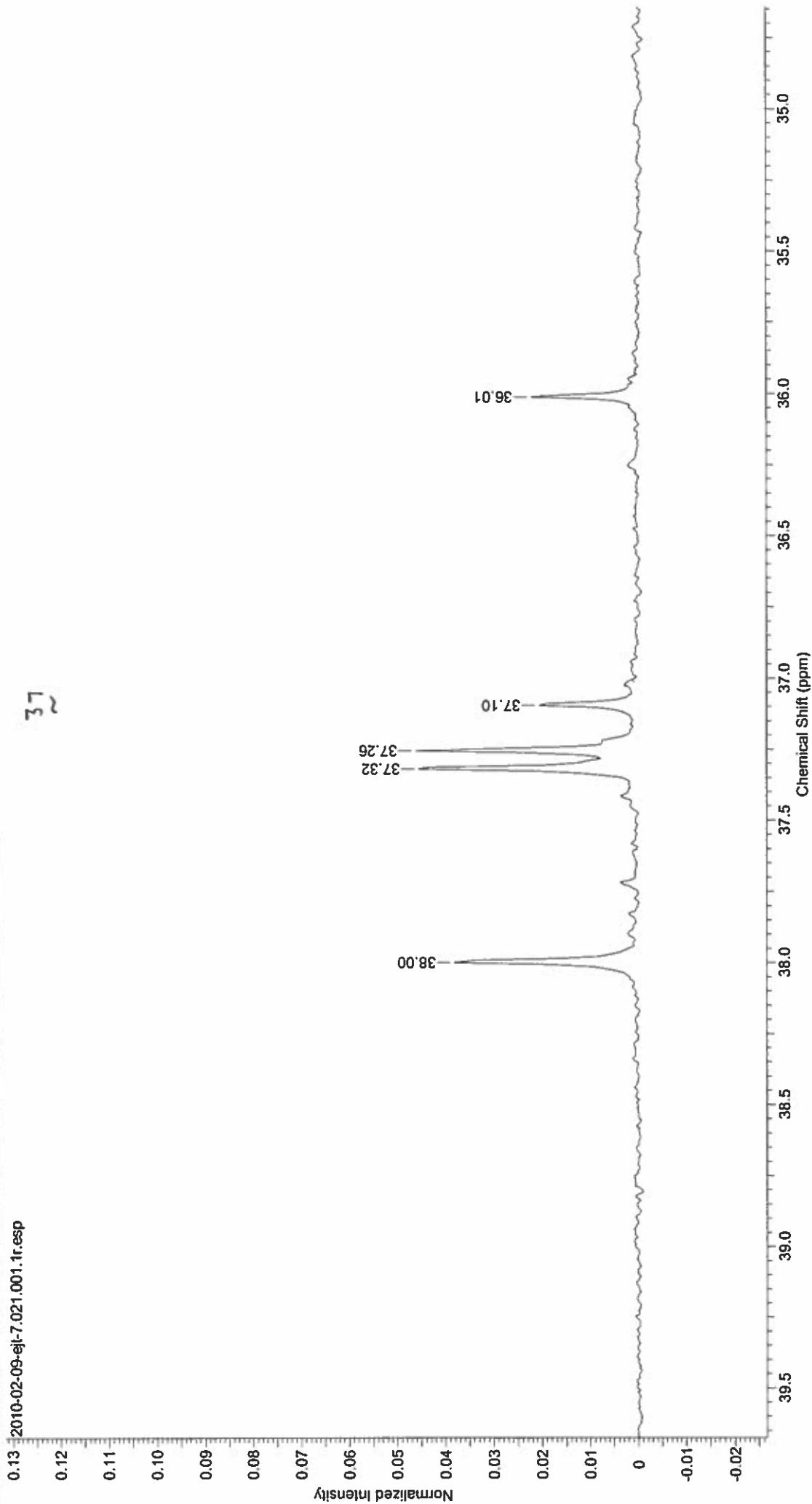




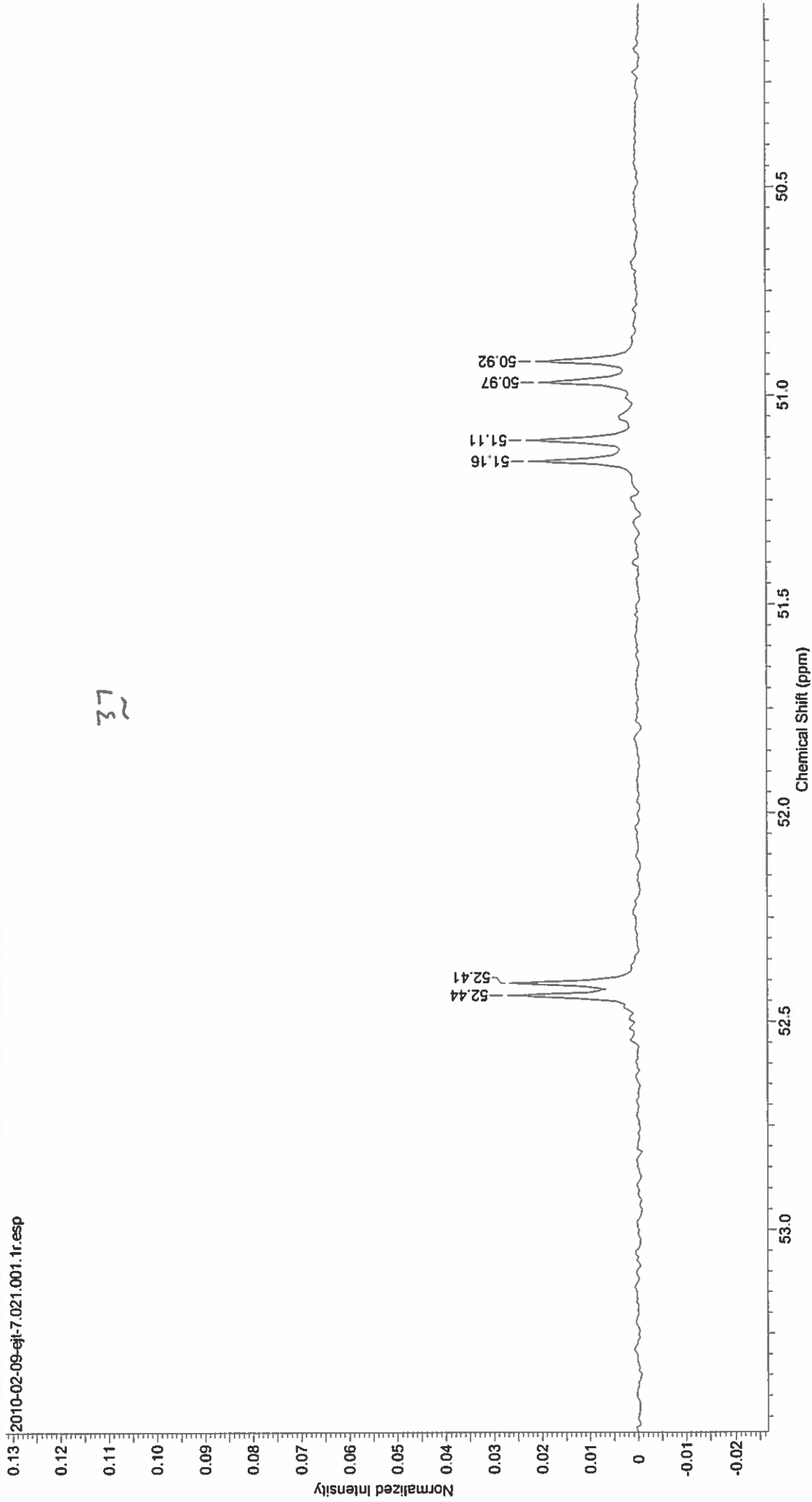
Acquisition Time (sec)	1.1010	Comment	allphosch mCARBONnight C6D6 /op/bruk500data/2010/Feb ejl 7	Date	09 Feb 2010 19:12:00
Date Stamp	09 Feb 2010 19:12:00				
File Name	C:\Documents and Settings\ejl\My Documents\Alan\Chem Communi\Phosphonate\2010-02-09-ejl-7\21\pdata\1\1r				
Nucleus	13C	Number of Transients	1024	Origin	spect
Owner	vmr1	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	29761.90	Solvent	BENZENE-d6	Spectrum Offset (Hz)	12428.5029
Sweep Width (Hz)	29761.00	Temperature (degree C)	22.268	Spectrum Type	STANDARD



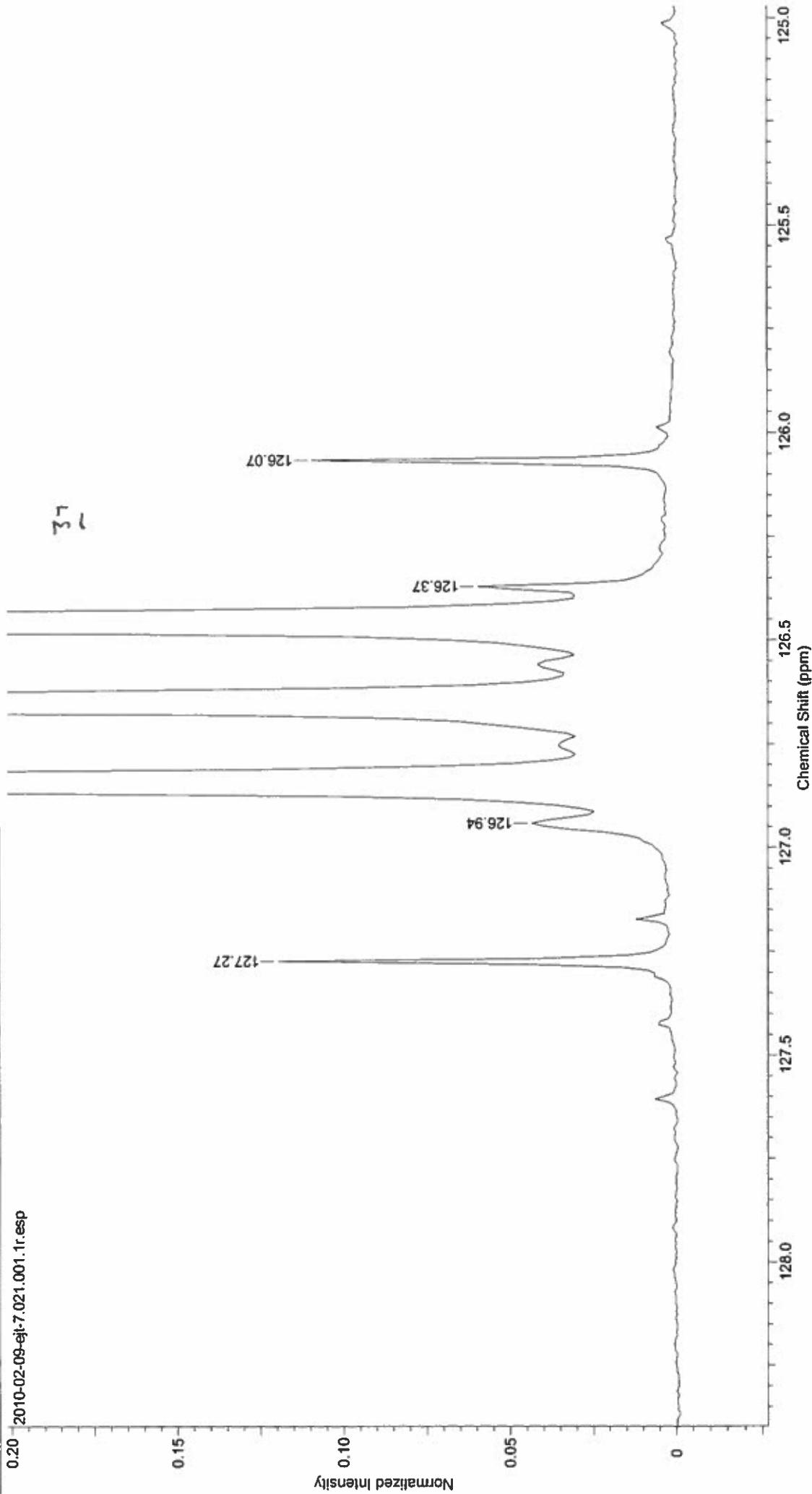
Acquisition Time (sec)	1.1010	Comment	allphosch mCARBONnight C6D6 /opt/bruk500data/2010/Feb ejl 7	Date	09 Feb 2010 19:12:00
Date Stamp	09 Feb 2010 19:12:00				
File Name	C:\Documents and Settings\Alan\Chem Communi\Phosphonate\2010-02-09-ejl-7\21\pdata\1\1r				
Nucleus	<sup>13</sup> C	Number of Transients	1024	Origin	spect
Owner	vnmr1	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	29761.90	Solvent	BENZENE-d6	Spectrum Offset (Hz)	12428.5029
Sweep Width (Hz)	29761.00	Temperature (degree C)	22.268	Receiver Gain	512.00
				Spectrum Type	STANDARD



Acquisition Time (sec)	1.1010	Comment	allphosch mCARBONnight C6D6 /opt/bruk500data/2010/Feb ejt 7	Date	09 Feb 2010 19:12:00
Date Stamp	09 Feb 2010 19:12:00				
File Name	C:\Documents and Settings\ejt\My Documents\Alan\Chem Communi\Phosphonate\2010-02-09-ejt-7\21\pdata\111r				
Nucleus	13C	Number of Transients	1024	Origin	spect
Owner	vmr1	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	29761.90	Solvent	BENZENE-d6	Spectrum Offset (Hz)	12428.5029
Sweep Width (Hz)	29761.00	Temperature (degree C)	22.268	Receiver Gain	512.00
				Spectrum Type	STANDARD
				Frequency (MHz)	125.76
				Original Points Count	32768
	</				

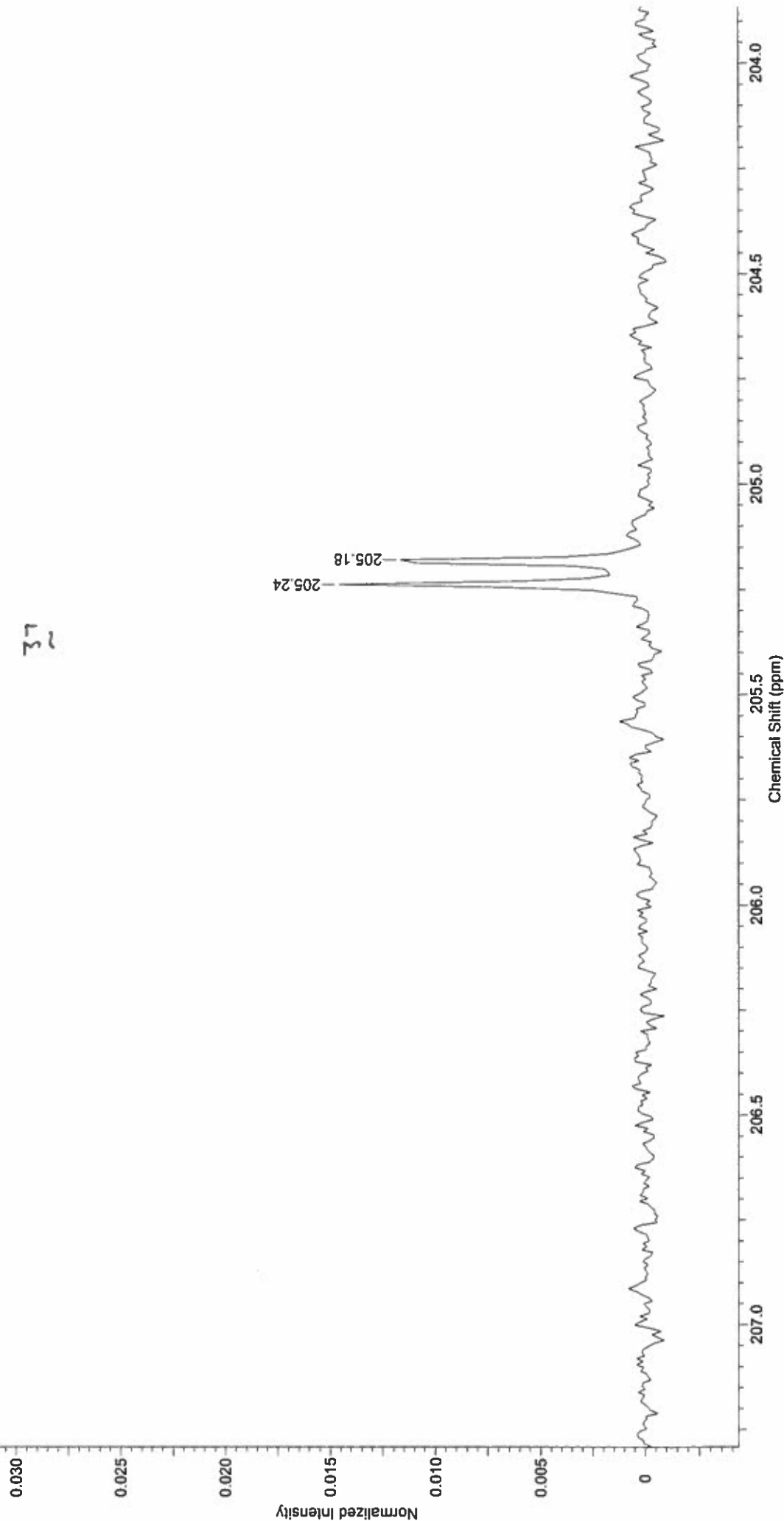


Acquisition Time (sec)	1.1010	Comment	allphosoh mCARBONnight C6D6 /opt/bruk500data/2010/Feb ejl 7	Date	09 Feb 2010 19:12:00
Date Stamp	09 Feb 2010 19:12:00				
File Name	C:\Documents and Settings\Alan\Chem Communi\Phosphonate\2010-02-09-ejl-7\21\pdata\1\1r				
Nucleus	13C	Number of Transients	1024	Origin	spect
Owner	vmr1	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	29761.90	Solvent	BENZENE-d6	Spectrum Offset (Hz)	12428.5029
Sweep Width (Hz)	29761.00	Temperature (degree C)	22.268	Spectrum Type	STANDARD



Acquisition Time (sec)	1.1010	Comment	allphosch mCARBONNIGHT C6D6 /op/bruk500data/2010/Feb ejt 7	Date	09 Feb 2010 19:12:00
Date Stamp	09 Feb 2010 19:12:00				
File Name	C:\Documents and Settings\ejt\My Documents\Alan\Chem Communi\Phosphonate\2010-02-09-ejt-7\21\pdata\111r				
Nucleus	13C	Number of Transients	1024	Origin	spect
Owner	vmr1	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	29761.90	Solvent	BENZENE-d6	Spectrum Offset (Hz)	12428.5029
Sweep Width (Hz)	29761.00	Temperature (degree C)	22.268	Receiver Gain	512.00
				Spectrum Type	STANDARD

2010-02-09-ejt-7.021.001.1r.esp



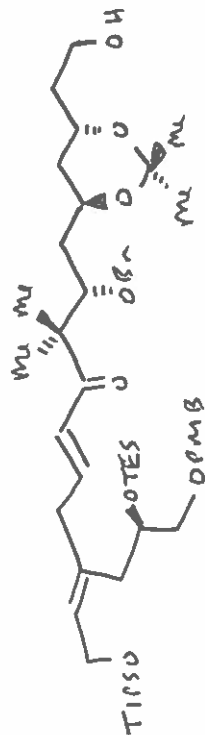
atlhwe-oh  
mPROTON CDCl3 {e:\bruk400data\2008\Nov} ejt 52



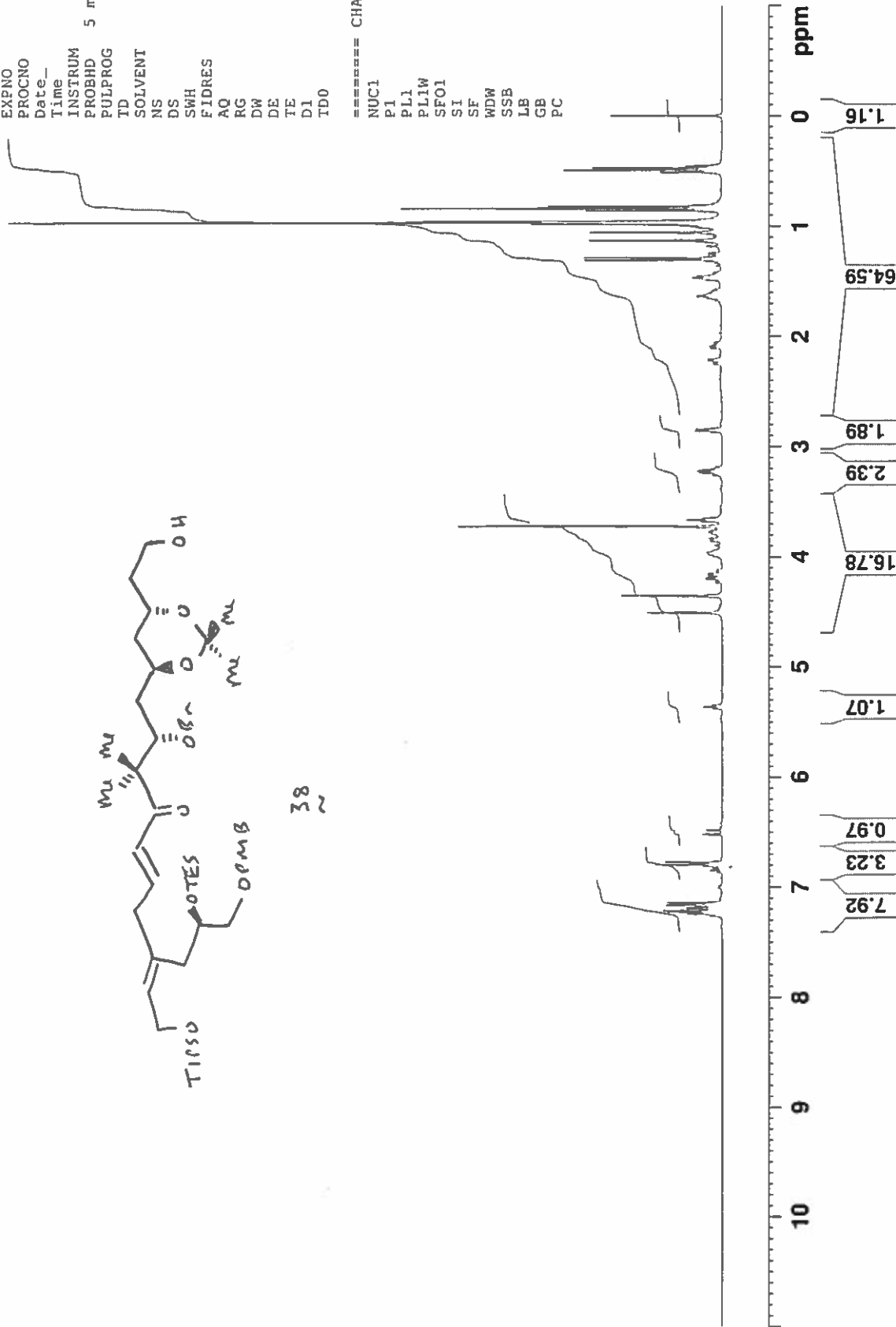
2008-11-12-ejt-52

NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20081112  
Time 12.08  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 57  
DW 60.500 usec  
DE 9.40 usec  
TE 293.7 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300380 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



38

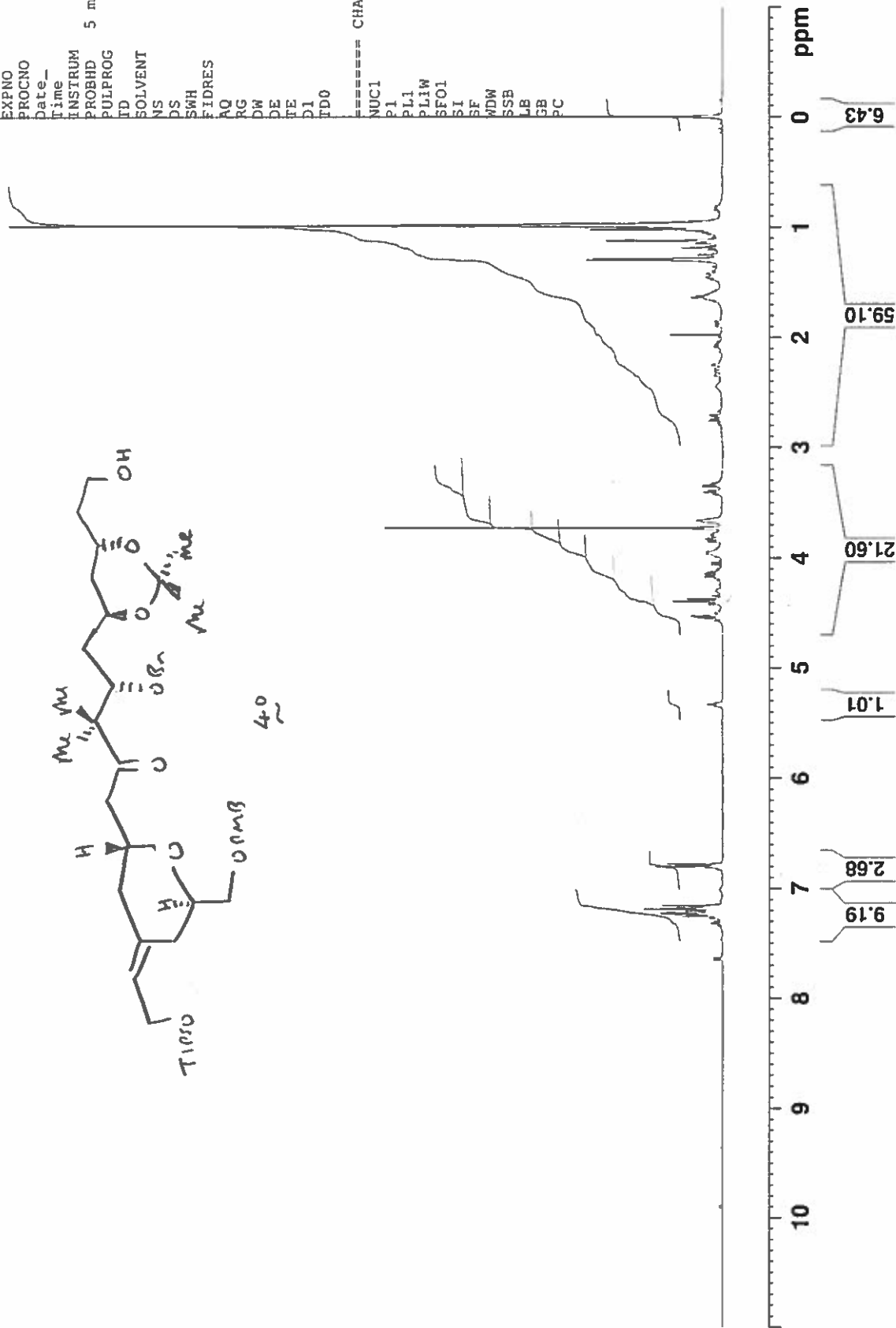




atlhfpv  
mPROTON CDCl3 {C:\bruk400data\2008\Oct} ejt 59



NAME 2008-10-30-ejt-59  
EXPNO 10  
PROCNO 1  
Date\_ 20081030  
Time 15.39  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 90.5  
DW 60.500 usec  
DE 9.40 usec  
TE 292.6 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300374 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





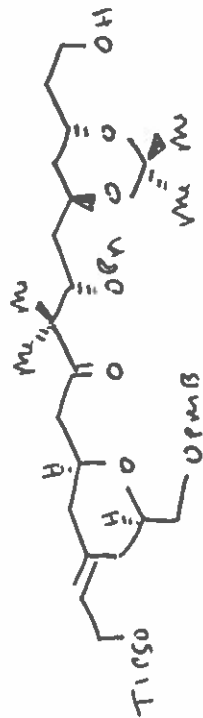
atllkotbu

mPROTONnight CDCI3 {e:\bruk400data\2008\Nov} ejt 2

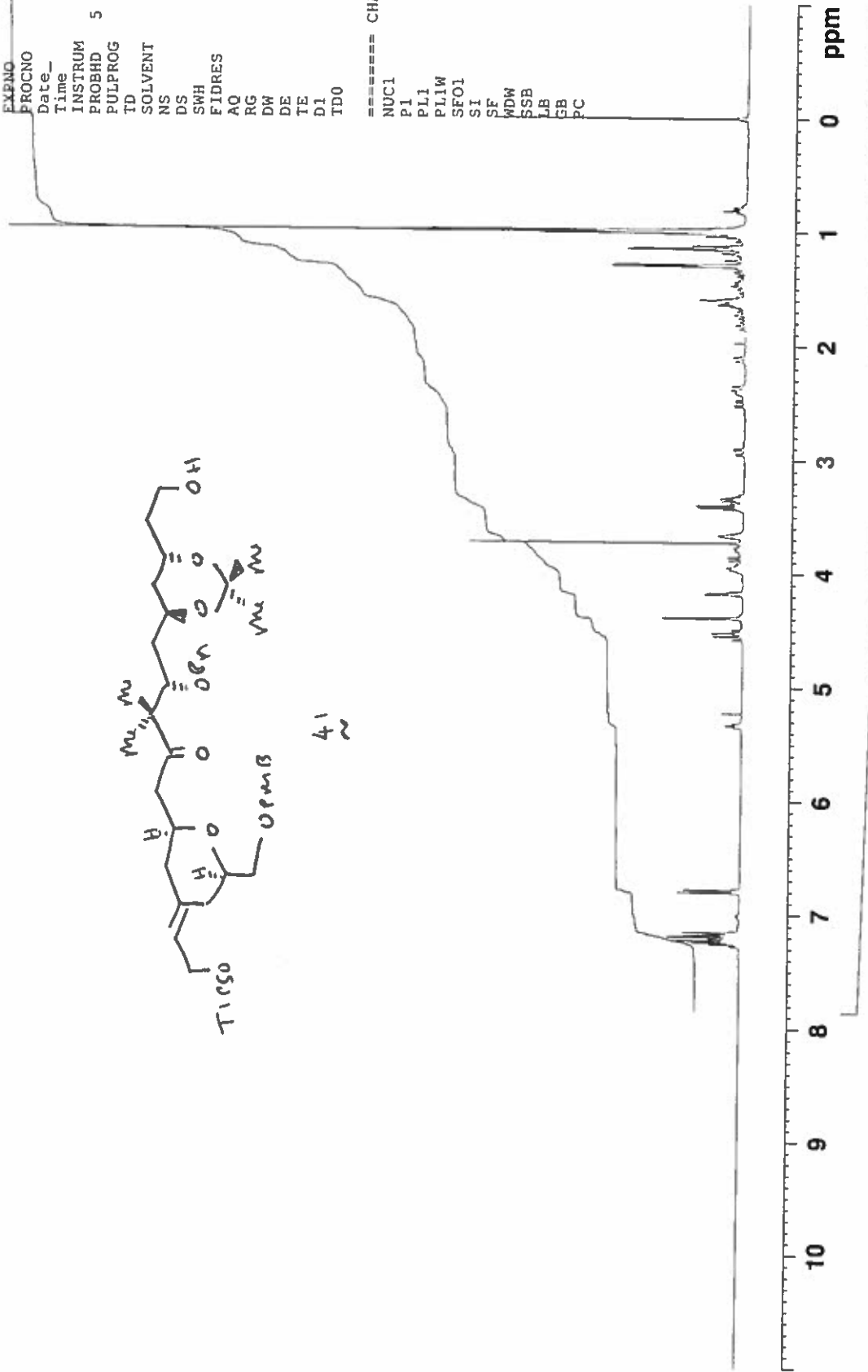


NAME 2008-11-13-ejt-2  
EXPNO 10  
PROCNO 1  
Date\_ 20081114  
Time 0.24  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCI3  
NS 128  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 144  
DW 60.500 usec  
DE 9.40 usec  
TE 293.5 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300369 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

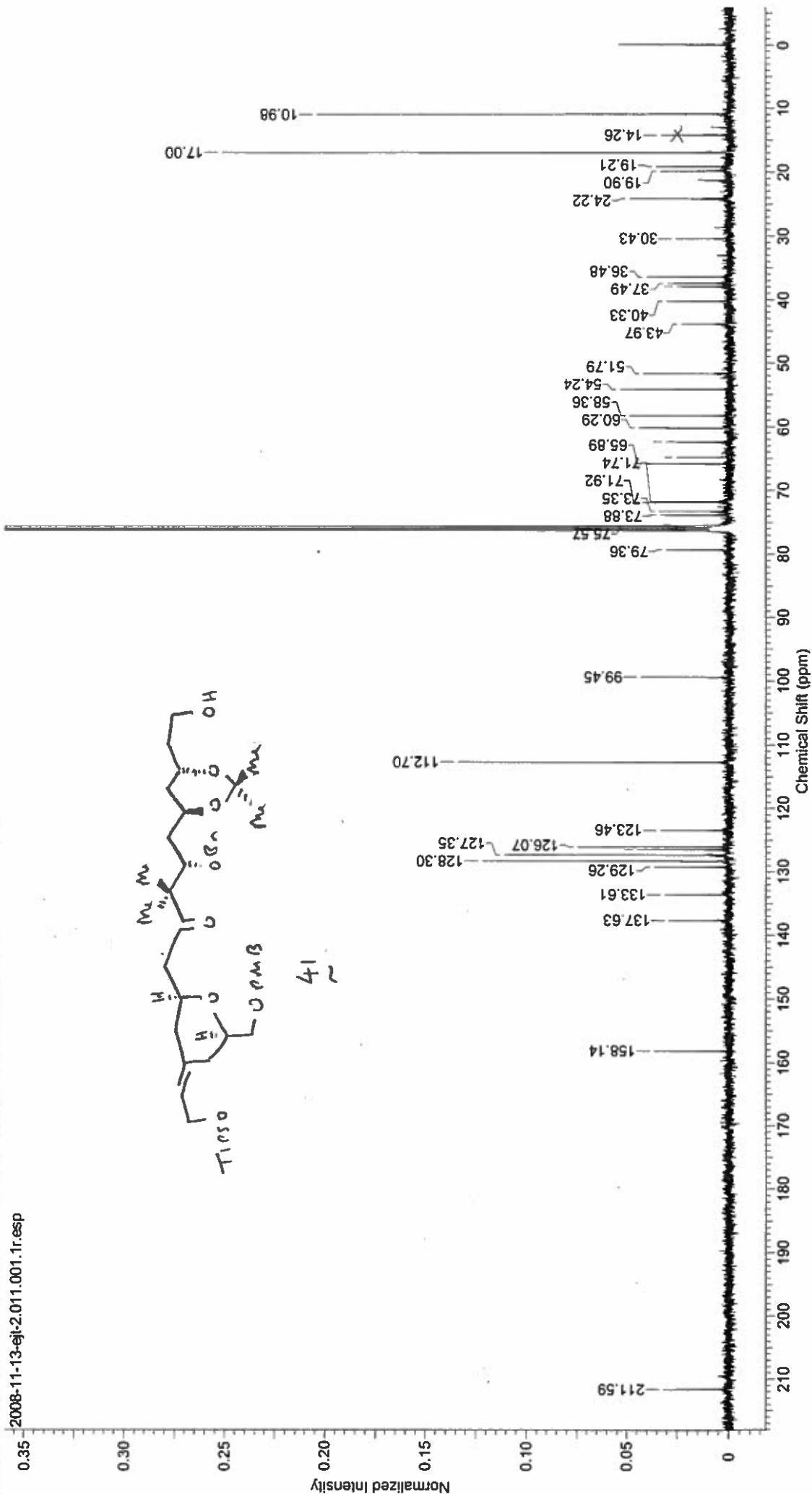


41



100.00

Acquisition Time (sec)	1.0835	Comment	allkolbu mCARBONight CDCl3 (e:\bruk400data\2008\Nov)\ejl 2	Date	14 Nov 2008 02:12:16
Date Stamp	14 Nov 2008 02:12:16				
File Name	C:\Documents and Settings\lej\My Documents\Alani\Chem Commun\B C1OH\2008-11-13-ejl-2\11\pdata\111r				
Nucleus	13C	Number of Transients	2048	Origin	AV400
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	11230.8027
Sweep Width (Hz)	30241.01	Temperature (degree C)	21.200	Spectrum Type	STANDARD





2008-11-05-ejt-22

NAME

EXPNO

PROCNO

Date\_

Time\_

INSTRUM

PROBHD

PULPROG

TD

SOLVENT

NS

DS

SWH

FIDRES

AQ

RG

DW

DE

TE

D1

TD0

=====

CHANNEL f1

=====

NUC1

P1

PL1

PL1W

SF01

SI

SF

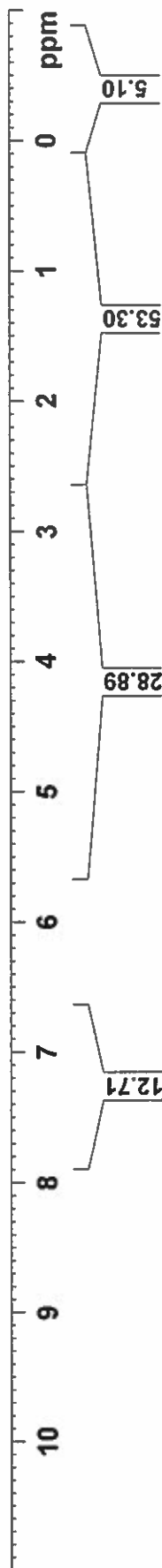
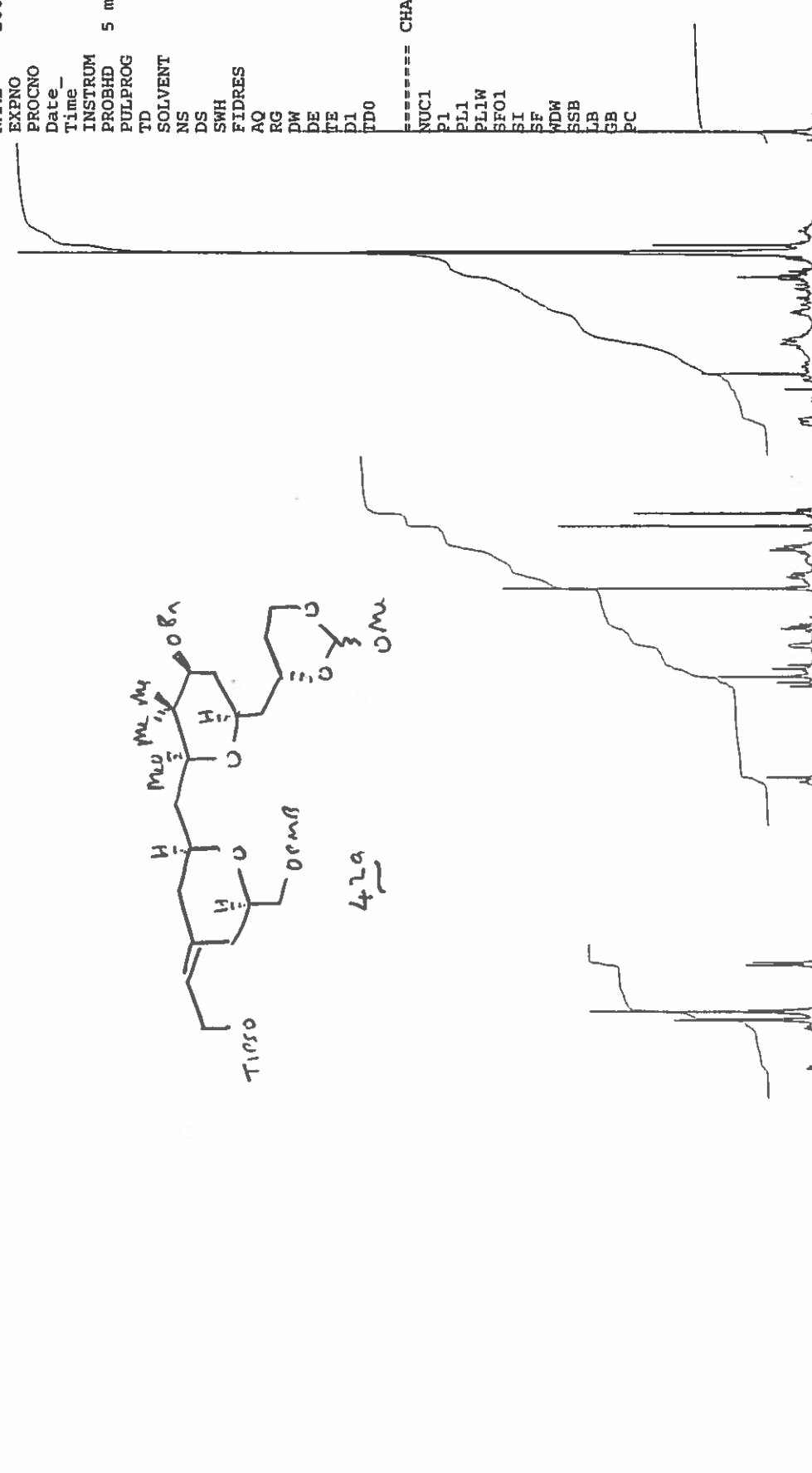
WDW

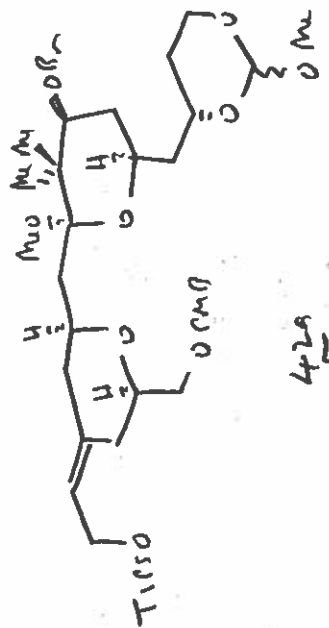
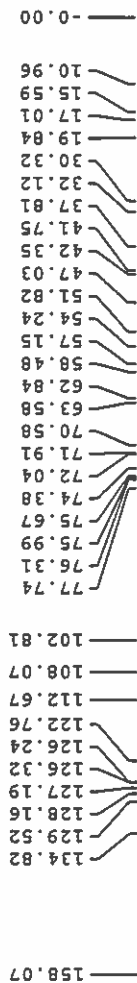
SSB

LB

GB

PC





```

NAME      2008-11-06-ejt-16
EXPNO     11
PROCNO    1
Date_      20081107
Time       4:57
INSTRUM    AV400
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         1024
DS         2
SWH         30241.936 Hz
FIDRES     0.461455 Hz
AQ         1.0835786 sec
RG         512
DW         16.533 usec
DE         7.83 usec
TE         294.5 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         8.00 usec
PL1        0.00 dB
PL1W       34.9152217 W
SFO1       100.6241042 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2      90.00 usec
PL2        -3.60 dB
PL12       15.31 dB
PL13       18.00 dB
PL2W       17.83863831 W
PL12W      0.22927761 W
PL13W      0.12341322 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6128735 MHz
WDW         EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40

```

240 220 200 180 160 140 120 100 80 60 40 20 ppm



2008-11-05-ejt-23

NAME  
EXPNO 10  
PROCNO 1

Date\_ 20081105

Time\_ 14.32

INSTRUM AV400

PROBHD 5 mm PABBO BB-

PULPROG zg30b

TD 65536

SOLVENT CDCl3

NS 16

DS 0

SWH 8264.463 Hz

FIDRES 0.126106 Hz

AQ 3.9649780 sec

RG 322

DW 60.500 usec

DE 9.40 usec

TE 293.7 K

D1 1.0000000 sec

TD0 1

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

NUC1 1H

P1 10.00 usec

PL1 -3.60 dB

PL1W 17.83863031 W

SFO1 400.1324710 MHz

SI 32768

SF 400.1300369 MHz

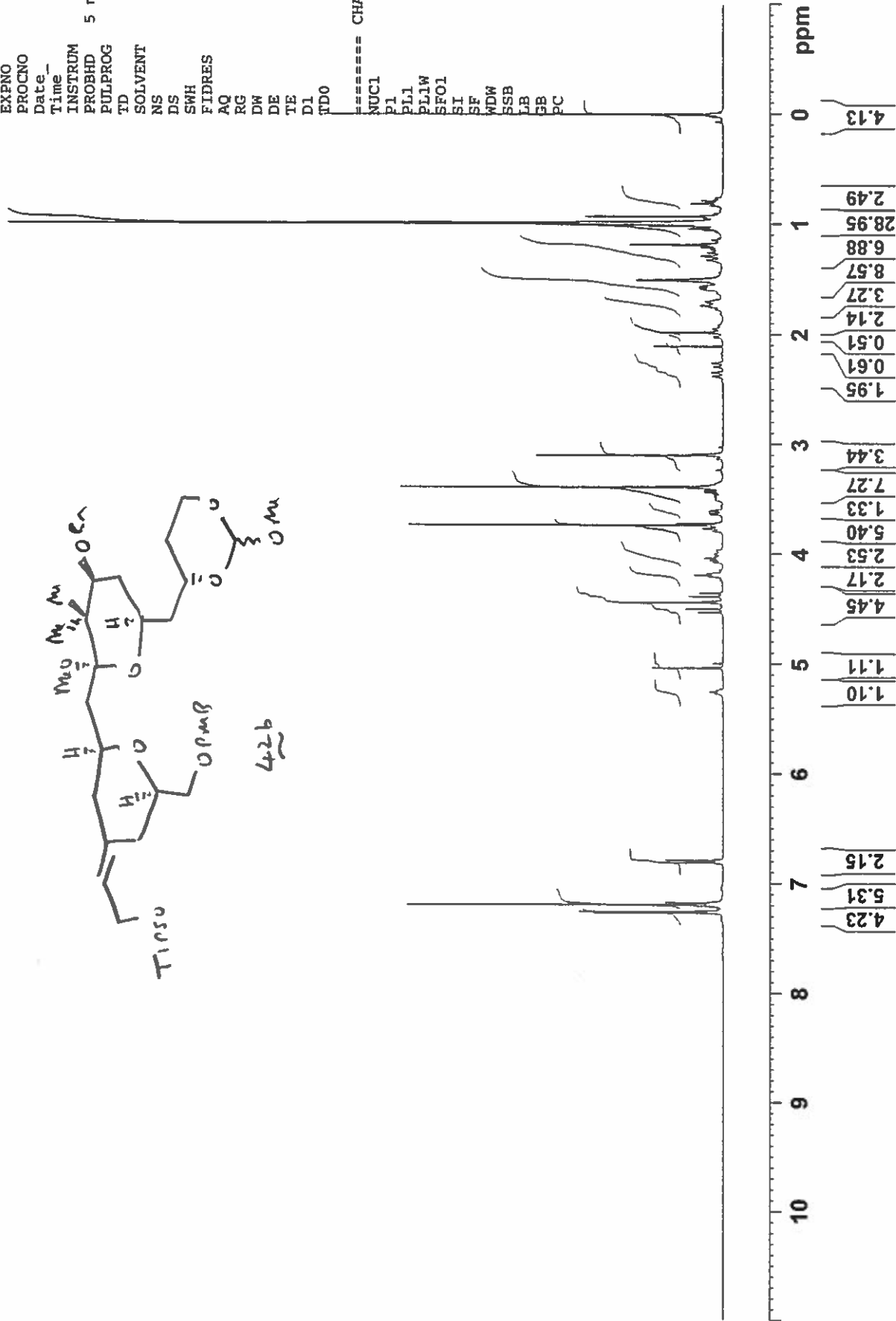
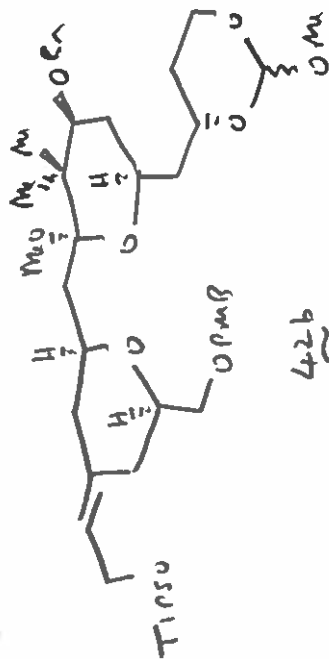
WDW EM

SSB 0

LB 0.30 Hz

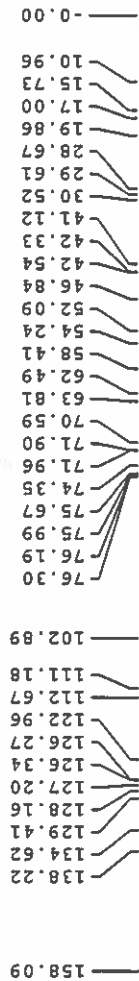
GB 0

PC 1.00



atl1ppts/2

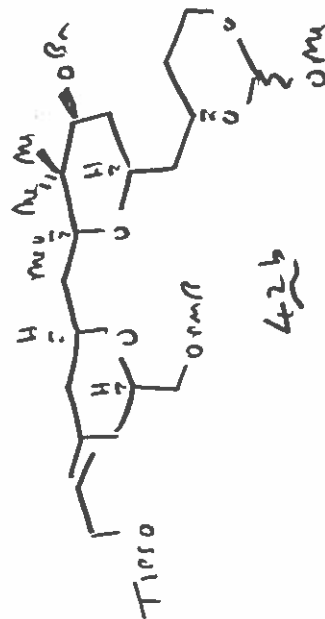
mCARBONnight CDCI3 {e:\bruk400data\2008\Nov} ejt 13



2008-11-16-ejt-13  
 EXPNO 21  
 PROCNO 1  
 Date\_ 20081117  
 Time\_ 2.21  
 INSTRUM AV400  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCI3  
 NS 3072  
 DS 2  
 SWH 30241.936 Hz  
 FIDRES 0.461455 Hz  
 AQ 1.0835786 sec  
 RG 512  
 DW 16.533 usec  
 DE 7.83 usec  
 TE 293.6 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.00 usec  
 PL1 0.00 dB  
 PL1W 34.91522217 W  
 SFO1 100.6241042 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -3.60 dB  
 PL12 15.31 dB  
 PL13 18.00 dB  
 PL2W 17.83863831 W  
 PL12W 0.22927761 W  
 PL13W 0.12341322 W  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6128742 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



240 220 200 180 160 140 120 100 80 60 40 20 ppm



2008-12-18-ejt-45

NAME  
EXPNO  
PROCNO

10  
1  
20081218

Date  
Time

22.51

INSTRUM

AV400

PROBHD

5 mm PABBO BB-

PULPROG

zg30b

TD

65536

SOLVENT

CDCl<sub>3</sub>

128

DS

0

8264.463 Hz

0.126106 Hz

3.9649780 sec

456

60.500 usec

9.40 usec

293.1 K

1.00000000 sec

1

ITD0

1

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

NUC1

1H

PL1

10.00 usec

-3.60 dB

PL1W

17.83863831 W

SFO1

400.1324710 MHz

SI

32768

SF

400.1300363 MHz

EM

0

SSB

0.30 Hz

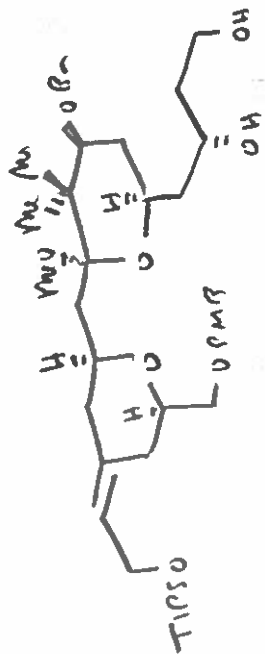
LB

0

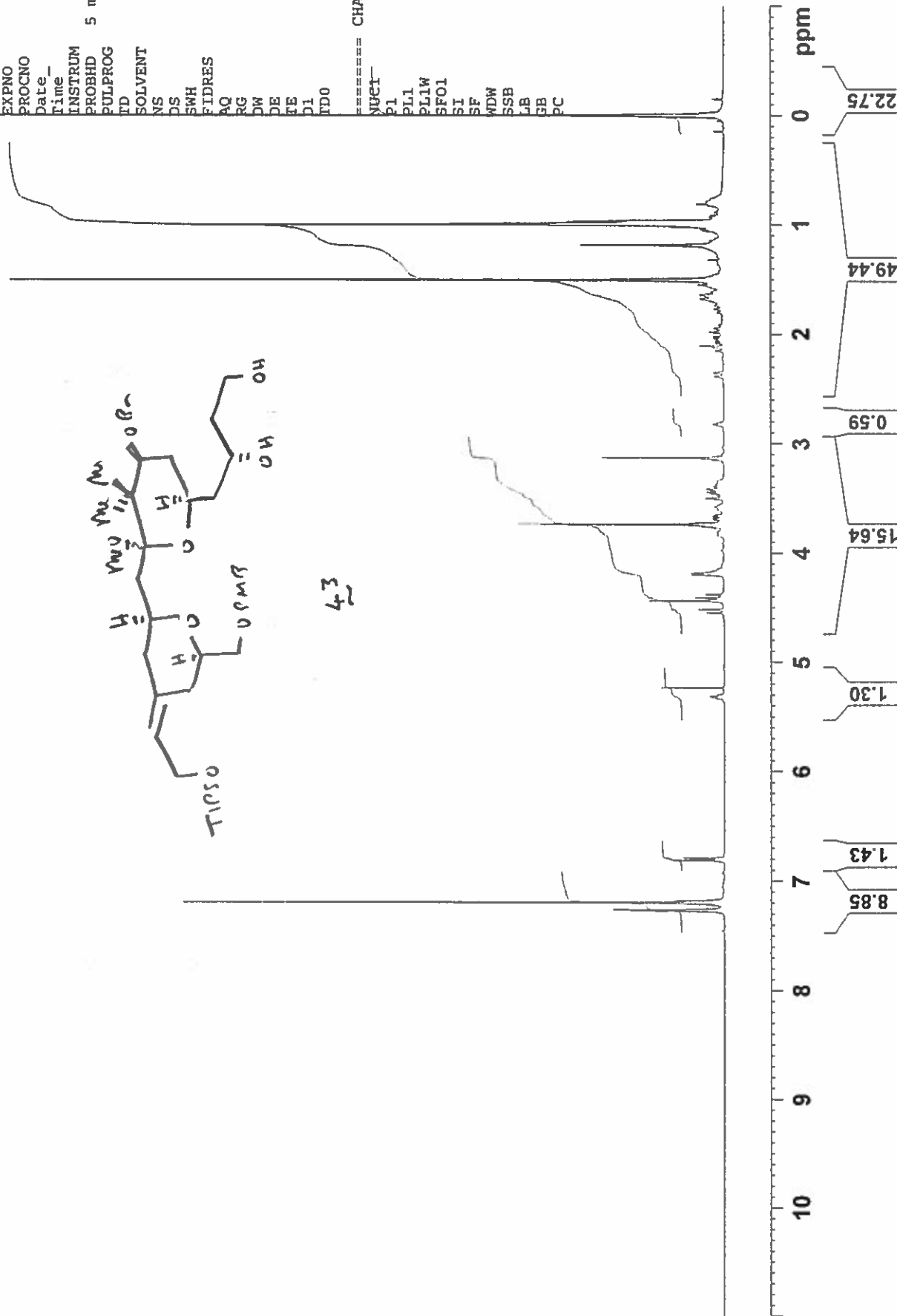
GB

1.00

PC

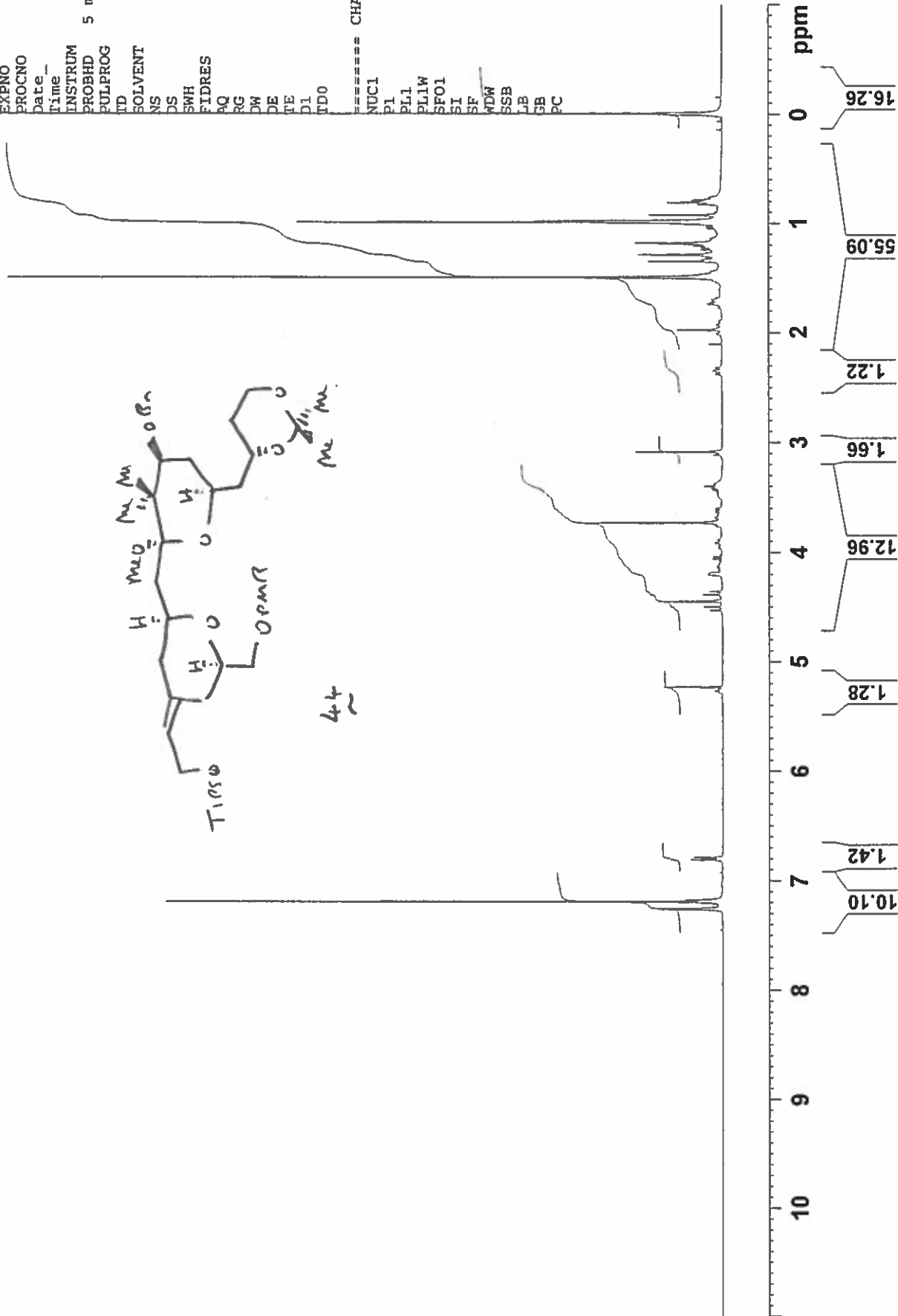


4.3





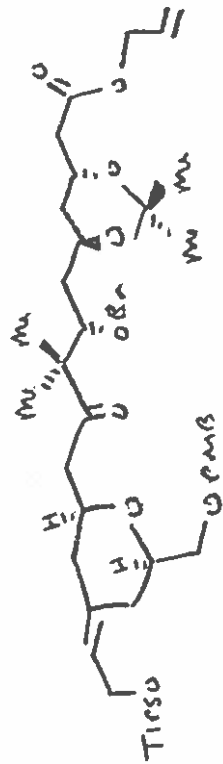
2008-12-18-ejt-44  
NAME  
EXPNO 20  
PROCNO 1  
Date\_ 20081218  
Time\_ 21.32  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 128  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 512  
DW 60.500 usec  
DE 9.40 usec  
TE 293.3 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SF01 400.1324710 MHz  
SI 32768  
SF 400.1300368 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





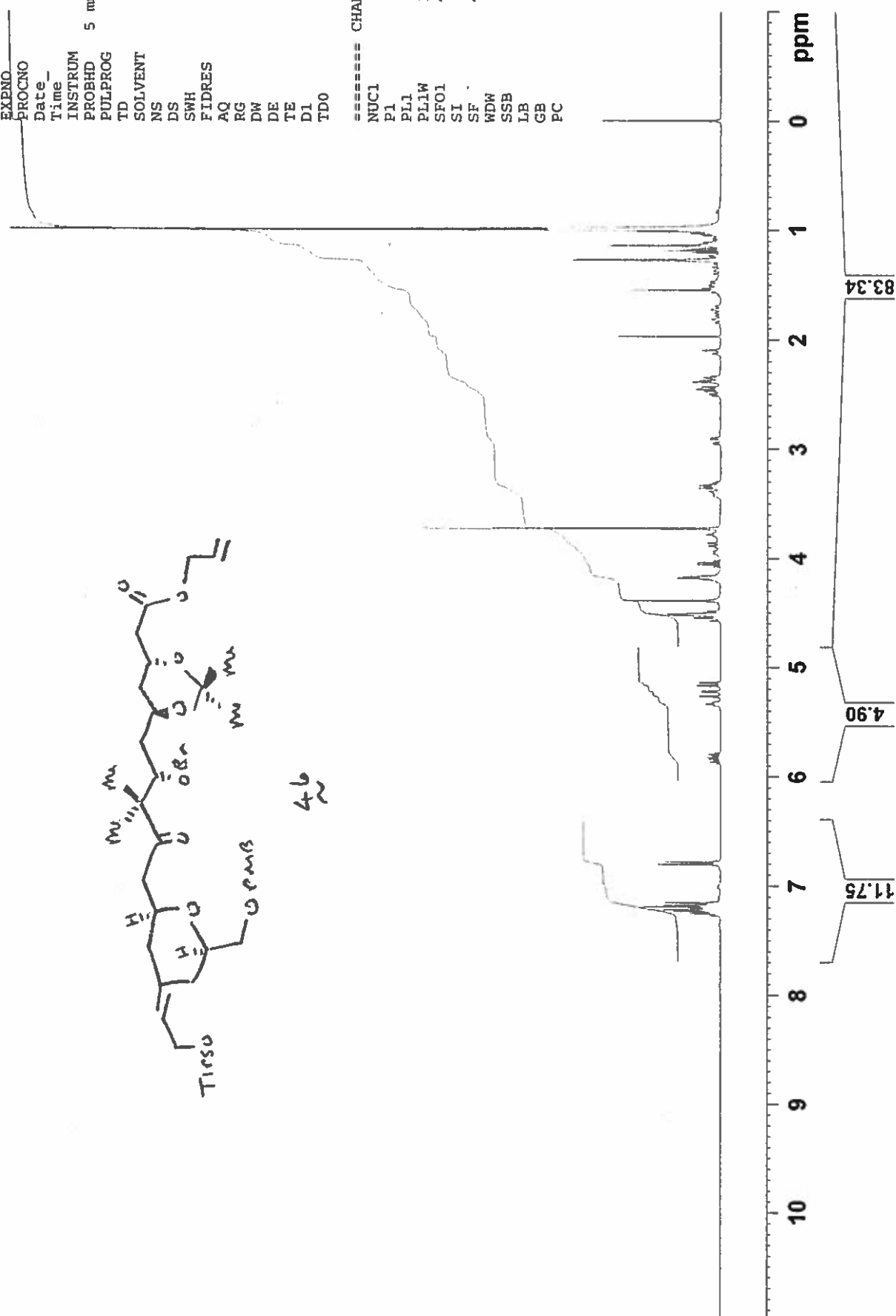
atlester

mPROTONnight CDCl3 {e:\bruk400data\2009\Apr} ejt 11

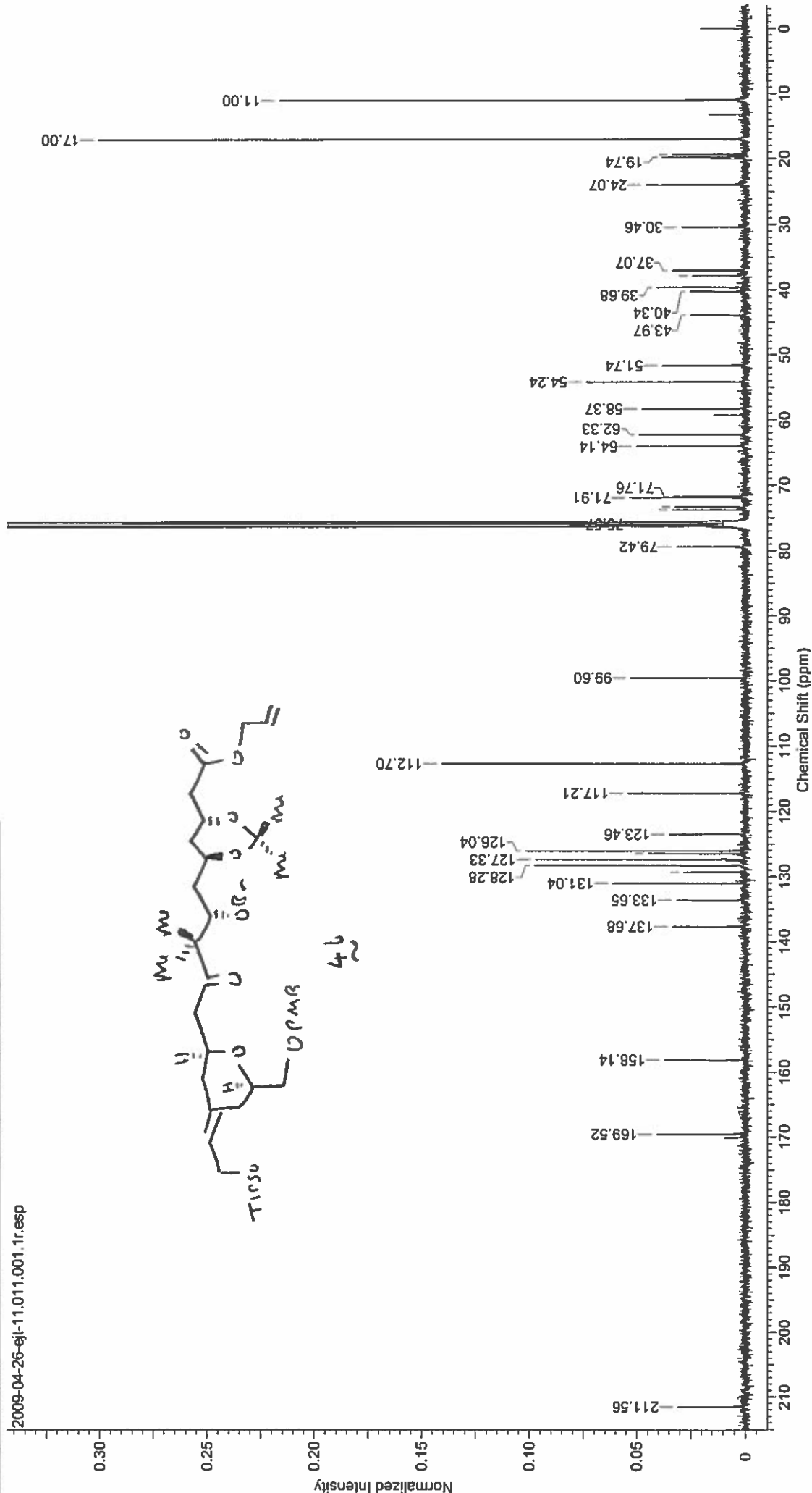


NAME 2009-04-26-ejt-11  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20090426  
 Time 21.02  
 INSTRUM AV400  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDCl3  
 NS 128  
 DS 0  
 SWH 8264.463 Hz  
 FIDRES 0.126106 Hz  
 AQ 3.9649780 sec  
 RG 144  
 DW 60.500 usec  
 DE 9.40 usec  
 TE 295.3 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 -3.60 dB  
 PL1W 17.83863831 W  
 SF01 400.1324710 MHz  
 SI 32768  
 SF 400.1300376 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Acquisition Time (sec)	1.0835	Comment	allister mCARBONnight CDC13 (e:\bruk400data\2009\Apr) ejt 11	Date	26 Apr 2009 23:43:12
Date Stamp	26 Apr 2009 23:43:12				
File Name	C:\Documents and Settings\ejt\My Documents\Alan\Chem Comm\unIB C1\test\2009-04-26-ejt-11\111\pdata\111r				
Nucleus	13C	Number of Transients	3072	Origin	AV400
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	11231.0420
Sweep Width (Hz)	30241.01	Temperature (degree C)	22.900	Spectrum Type	STANDARD

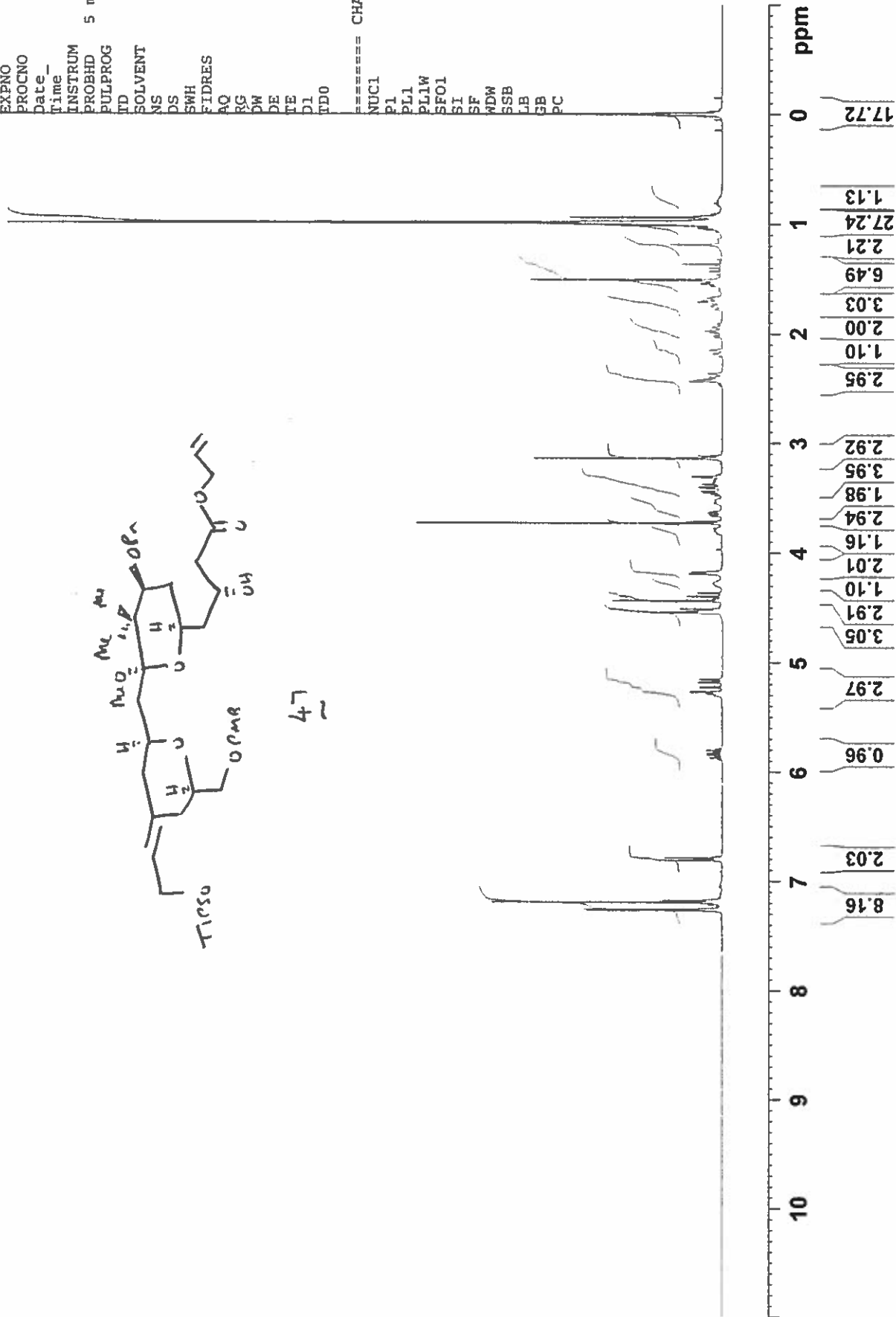
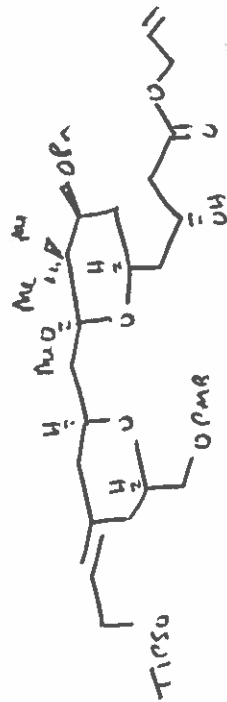


atllabester

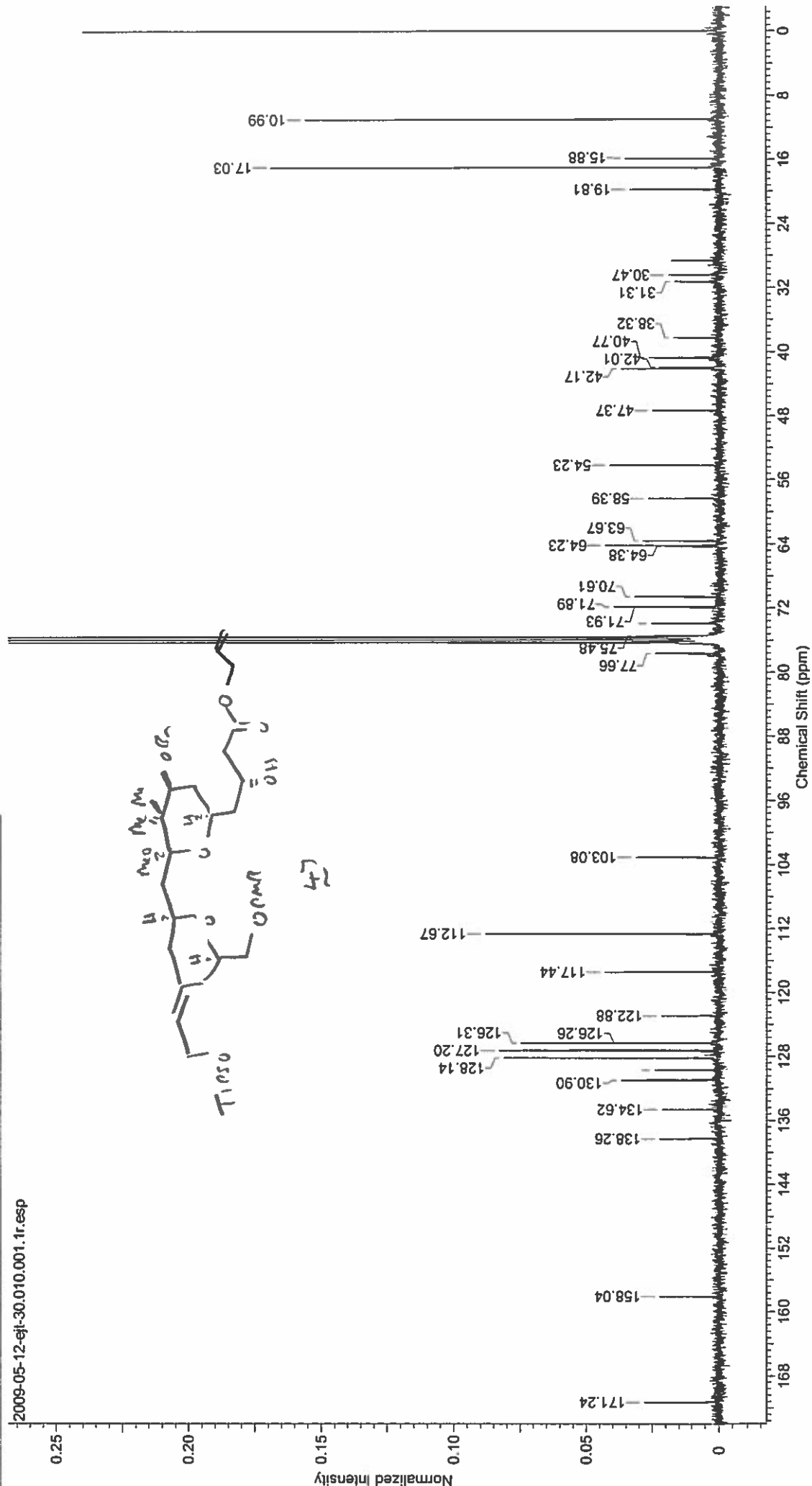
mPROTON CDCI3 {e:\bruk400data\2009\May} ejt 8



2009-05-11-ejt-8  
 NAME  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20090511  
 Time 9.57  
 INSTRUM AV400  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8264.463 Hz  
 FIDRES 0.126106 Hz  
 AQ 3.9649780 sec  
 RG 228  
 DW 60.500 usec  
 DE 9.40 usec  
 TE 293.9 K  
 D1 1.00000000 sec  
 TD0 1  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 -3.60 dB  
 PL1W 17.83863831 W  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300374 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



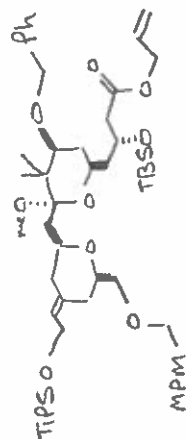
Acquisition Time (sec)	1.0835	Comment	allabester mCARBONnight CDCI3 (e:\bruk400data\2009May) ejt 30	Date	13 May 2009 04:56:48
Date Stamp	13 May 2009 04:56:48				
File Name	C:\Documents and Settings\ejt\My Documents\Alani\Chem Commun\AB C3OH\2009-05-12-ejt-30\10\pdata\111r				
Nucleus	13C	Number of Transients	3072	Origin	AV400
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	11230.8525
Sweep Width (Hz)	30241.01	Temperature (degree C)	21.900	Spectrum Type	STANDARD



```

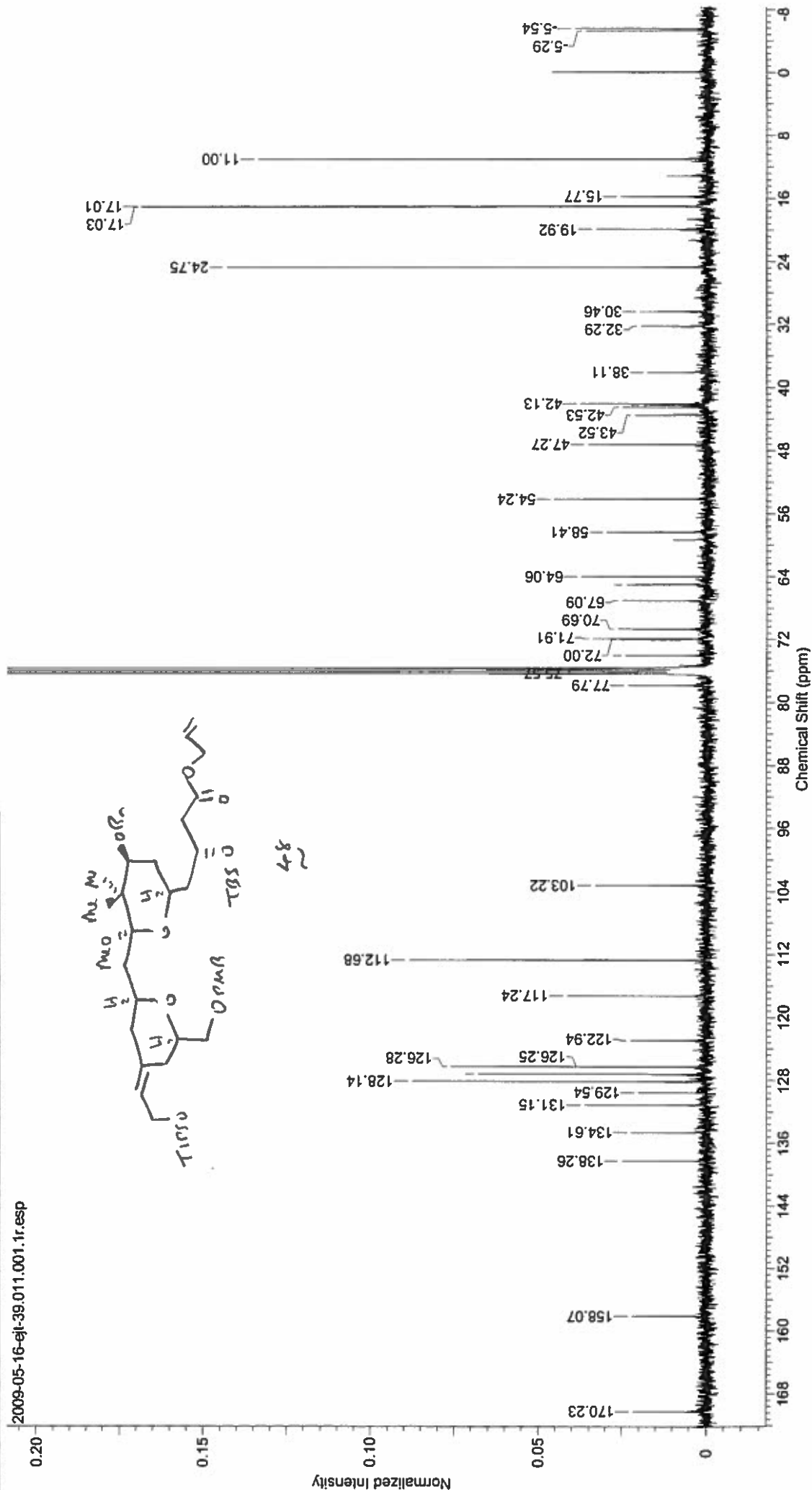
===== CHANNEL f1 =====
NUC1      1H
P1         8.20 usec
PL1        3.25 dB
PL1W       12.12272363 W
SF01       500.1330885 MHz
SI         32768
SF         500.1300490 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```



48

<b>Acquisition Time (sec)</b>	1.0835	<b>Comment</b>	allIABOTBS mCARBONnight CDCI3 (e:\bruk400data\2009\May)\ejl_39	<b>Date</b>	16 May 2009 22:58:24
<b>Date Stamp</b>	16 May 2009 22:58:24				
<b>File Name</b>	C:\Documents and Settings\ejl\My Documents\Alan\Chem Commun\IAB C3OTBS\2009-05-16-ejl-39\11\pdata\11\1r				
<b>Nucleus</b>	13C	<b>Number of Transients</b>	3072	<b>Origin</b>	AV400
<b>Owner</b>	Administrator	<b>Points Count</b>	32768	<b>Pulse Sequence</b>	zgpg30
<b>SW(cyclical) (Hz)</b>	30241.94	<b>Solvent</b>	CHLOROFORM-d	<b>Spectrum Offset (Hz)</b>	11230.9316
<b>Sweep Width (Hz)</b>	30241.01	<b>Temperature (degree C)</b>	22.400	<b>Spectrum Type</b>	STANDARD



abesterc16oh

mPROTONnight C6D6 {e:\bruk400data\2010\Mar} ejt 3



NAME 2010-03-18-ejt-3

EXPNO 10

PROCNO 1

Date\_ 20100319

Time 3.07

INSTRUM AV400

PROBHD 5 mm PABBO BB-

PULPROG zg30b

TD 65536

SOLVENT C6D6

NS 16

DS 0

SWH 8264.463 Hz

FIDRES 0.126106 Hz

AQ 3.9649780 sec

RG 90.5

DW 60.500 usec

DE 9.40 usec

TE 295.4 K

D1 1.00000000 sec

TD0 1

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

NUC1 1H

P1 10.00 usec

PL1 -3.60 dB

PL1W 17.83863831 W

SFO1 400.1324710 MHz

SI 32768

SF 400.1300981 MHz

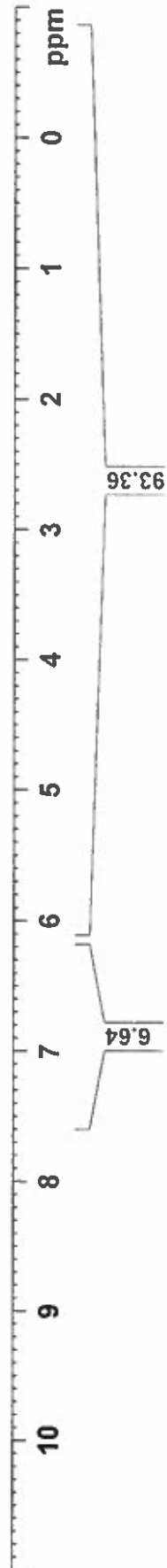
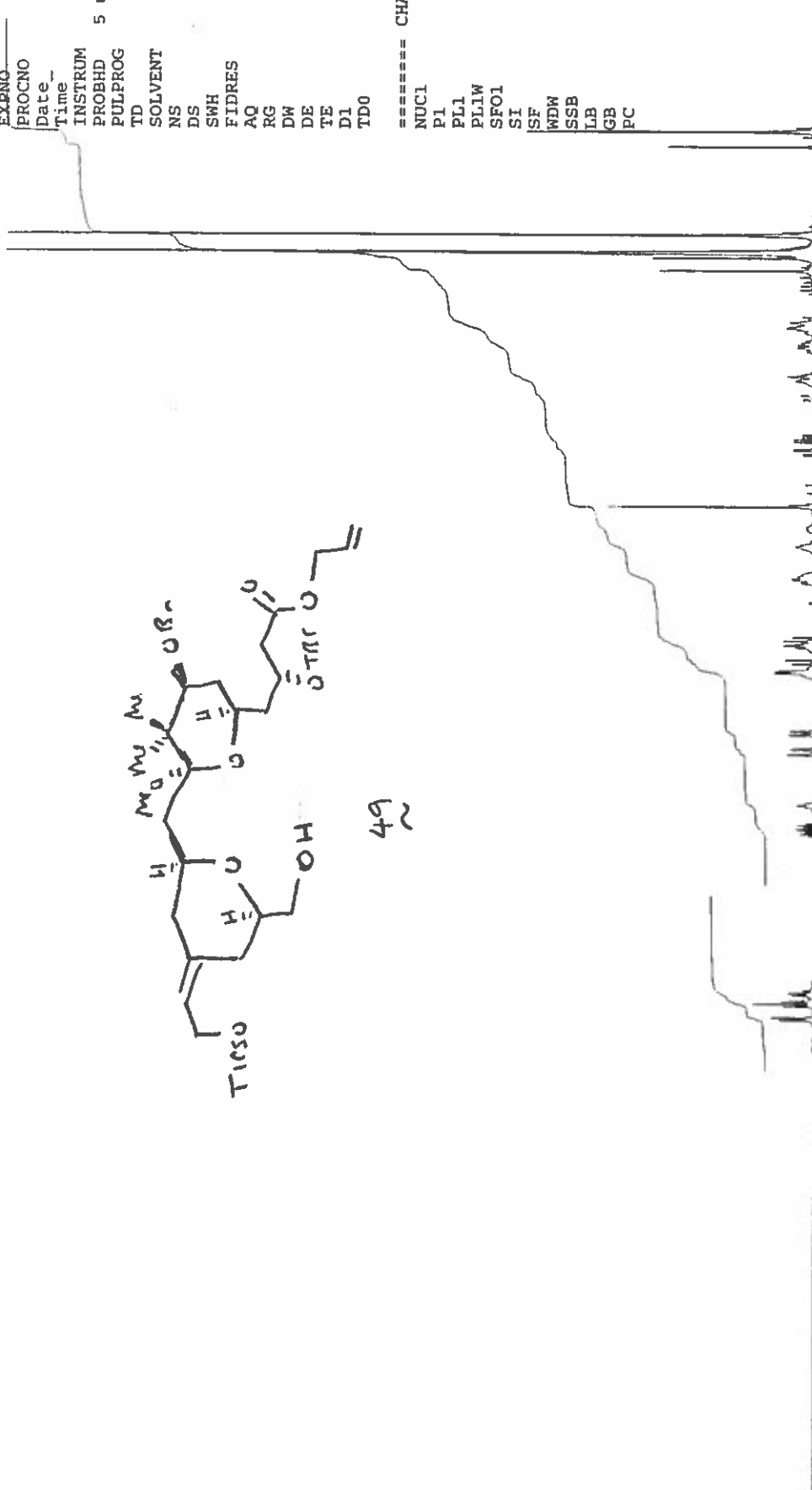
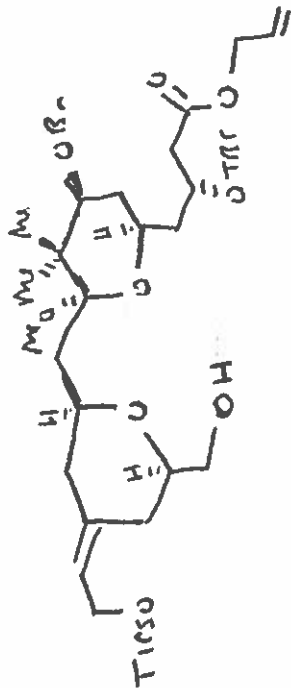
WDW EM

SSB 0

LB 0.30 Hz

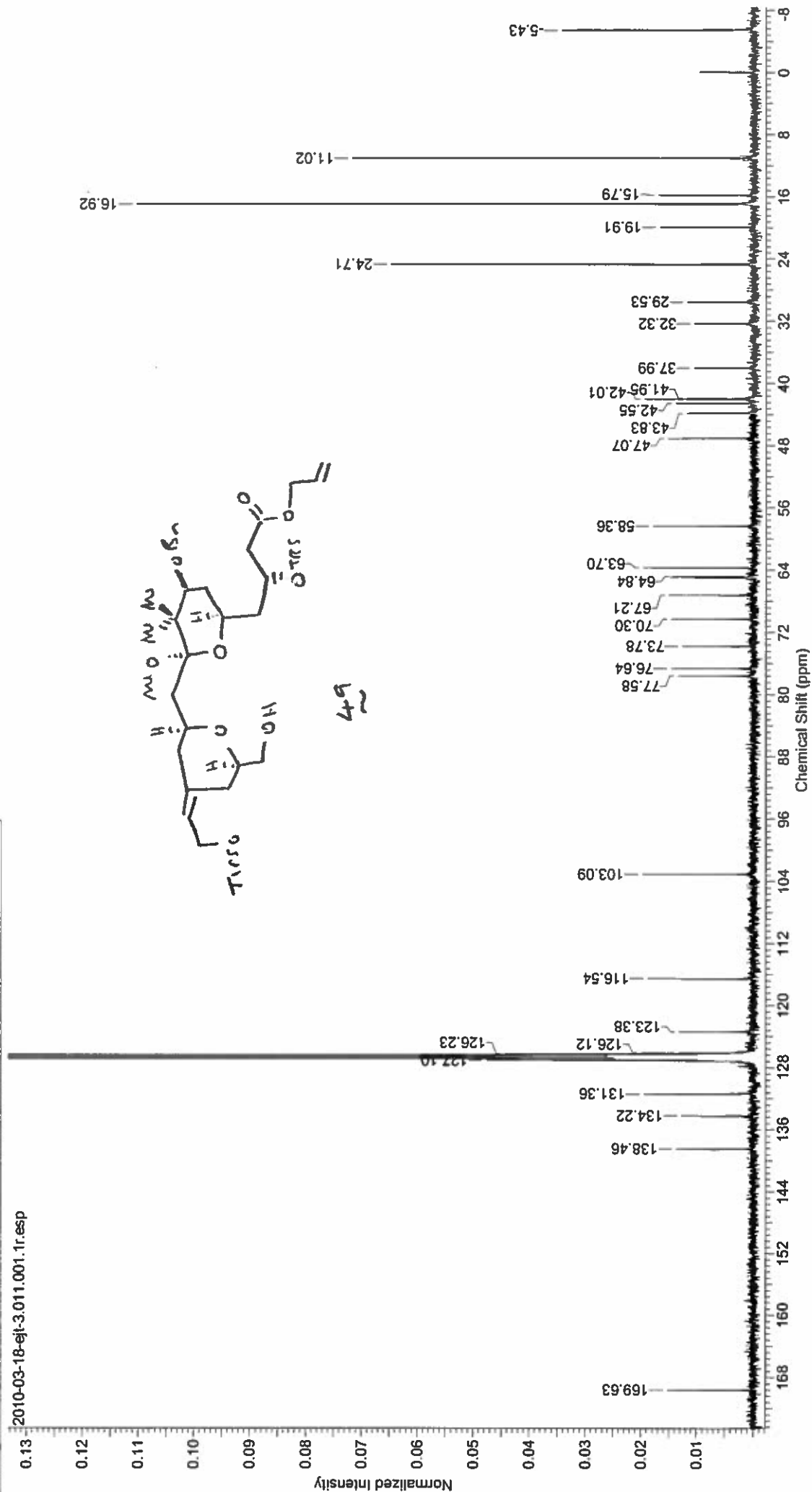
GB 0

PC 1.00

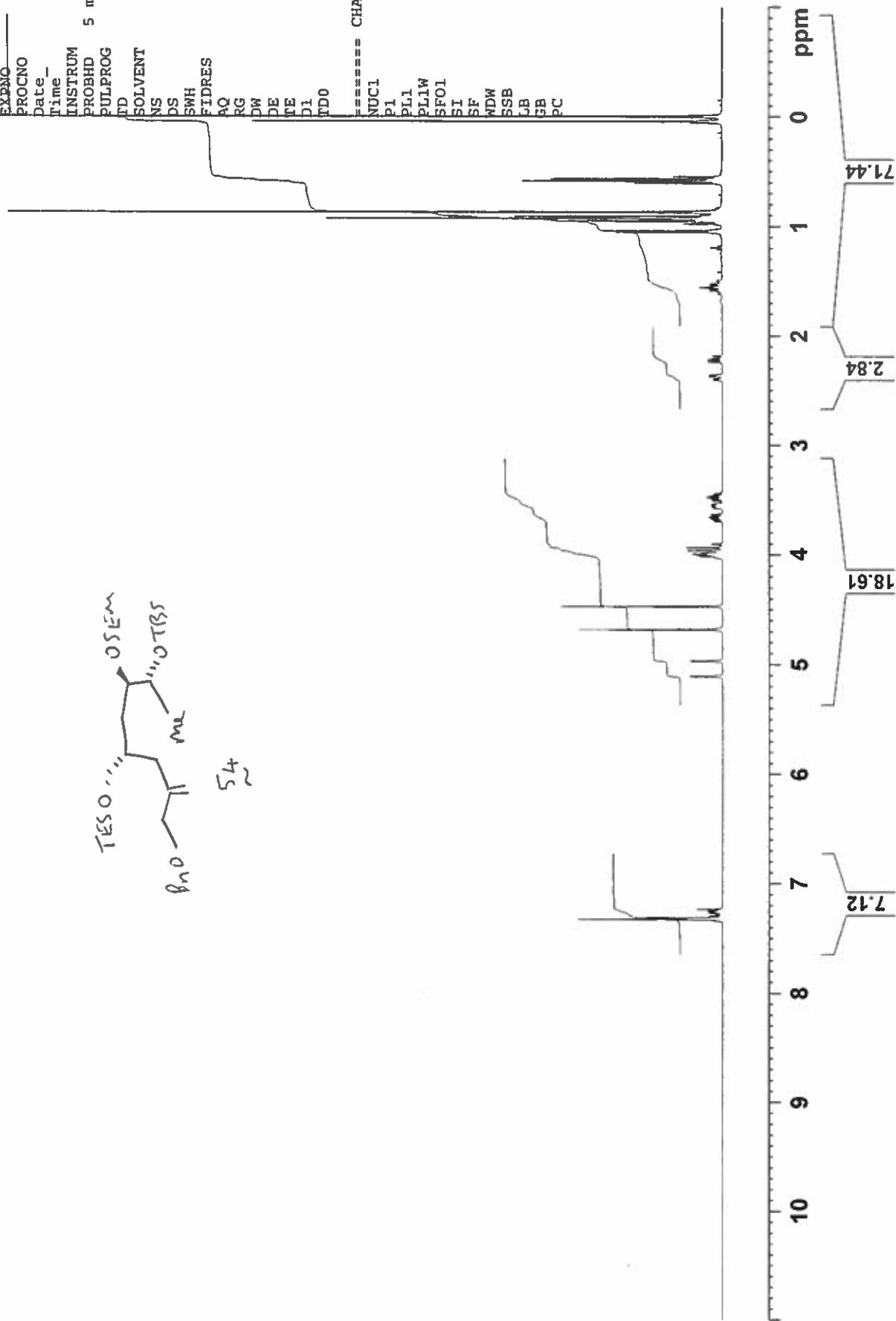
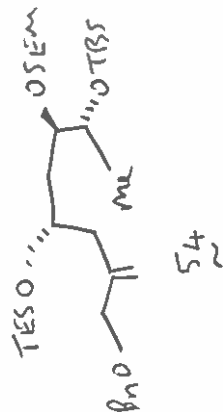


11/08/2010 18:37:56

Acquisition Time (sec)	1.0835	Comment	abesterc:16dh mCARBONnight C6D6 (e:\bruk400data\2010\Mar) ejt 3	Date	19 Mar 2010 04:01:04
Date Stamp	19 Mar 2010 04:01:04				
File Name	C:\Documents and Settings\ejt\My Documents\Alan\Chem Commun\AB C16OH\2010-03-18-ejt-3\11\data\111r				
Nucleus	13C	Number of Transients	1024	Origin	AV400
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	BENZENE-d6	Spectrum Offset (Hz)	11218.3389
Sweep Width (Hz)	30241.01	Temperature (degree C)	22.900	Spectrum Type	STANDARD

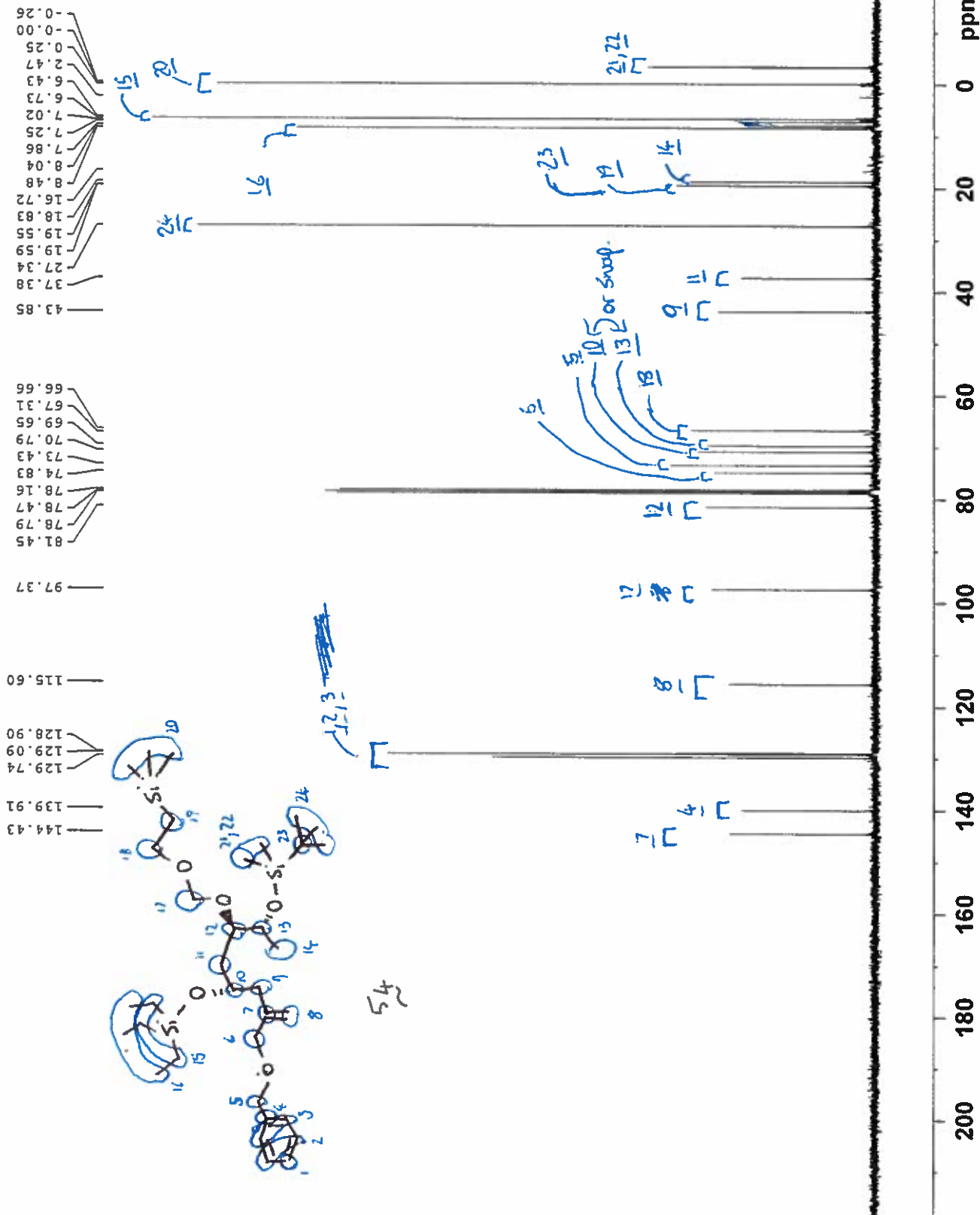




SH467  
mPROTONnight CDCI3 {C:\bruk400data\2008\Jul} ejt 33[illegible]

SH467

mCARBONnight CDCI3 {C:\bruk400data\2008\Jul} ejt 33



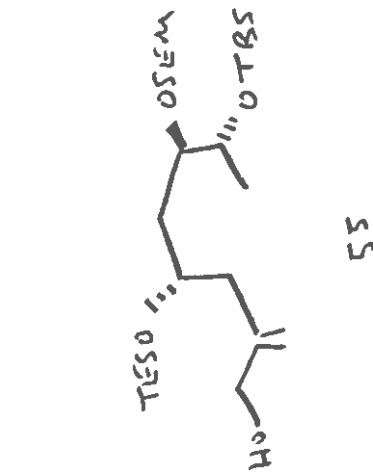
NAME 2008-07-23-ejt-33  
EXPNO 23  
PROCNO 1  
Date 20080724  
Time 4.13  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCI3  
NS 256  
DS 2  
SWH 23809.523 Hz  
FIDRES 0.363304 Hz  
AQ 1.3763061 sec  
RG 512  
DW 21.000 usec  
DE 7.66 usec  
TE 296.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 34.91522217 W  
SF01 100.6228294 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.60 dB  
PL12 13.80 dB  
PL13 14.00 dB  
PL1W 17.83863831 W  
PL12W 0.32460985 W  
PL13W 0.31000000 W  
SF02 400.1316005 MHz  
SI 32768  
SF 100.6126234 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

SH468

mPROTON CDCl3 {C:\bruk400data\2008\Jul} ejt 57

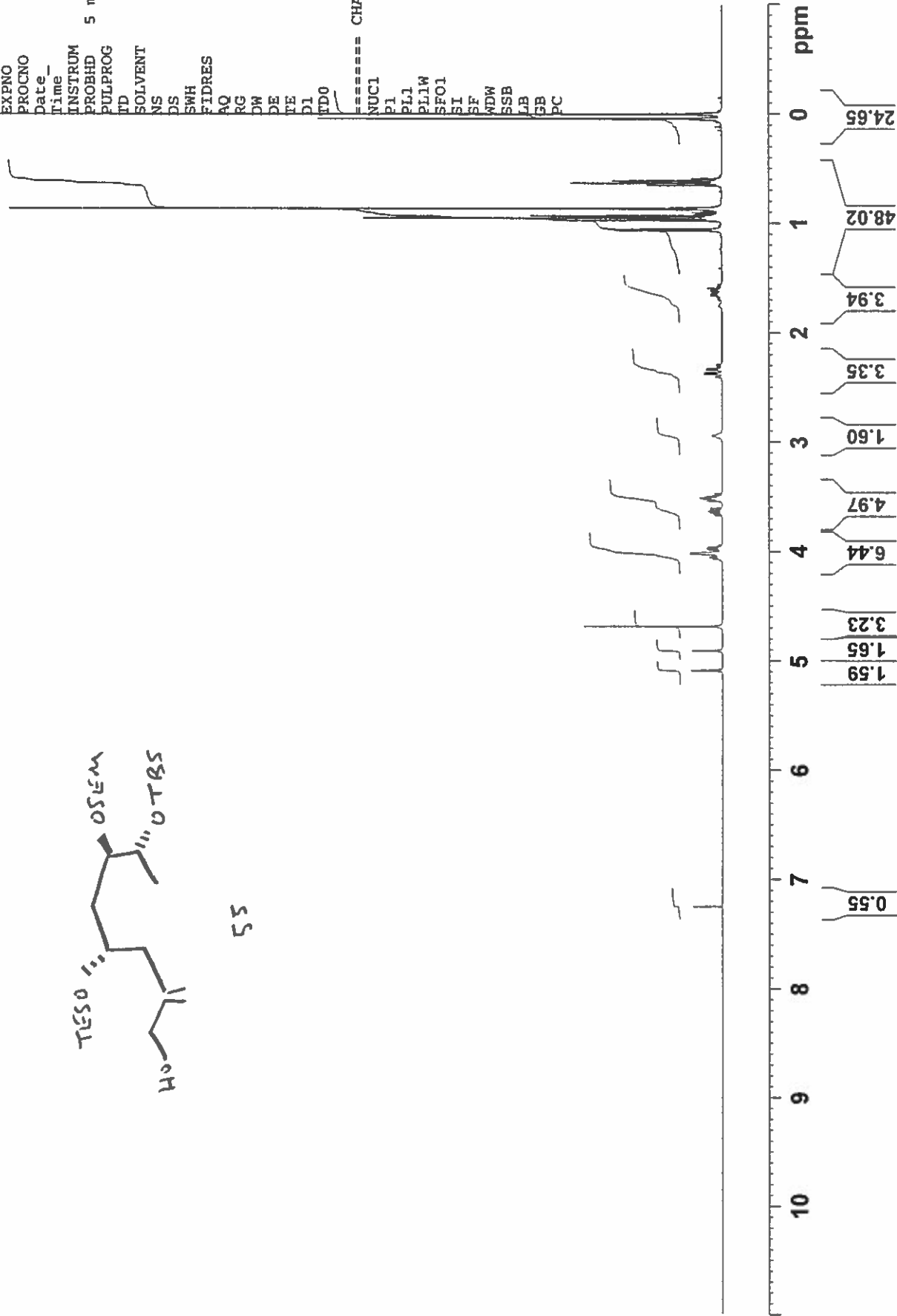


2008-07-24-ejt-57

NAME	EXPNO	PROCNO	Date_	Time
	10	1	20080724	17.56
INSTRUM	PROBHD	AV400		
	5 mm PABBO BB-			
PULPROG	zg30b			
TD	65536			
SOLVENT	CDCl3			
NS	16			
DS	0			
SWH	8264.463 Hz			
FIDRES	0.126106 Hz			
AQ	3.9649780 sec			
RG	36			
DW	60.500 usec			
DE	9.40 usec			
TE	295.2 K			
D1	1.00000000 sec			
TD0	1			

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

NUC1	1H
P1	10.00 usec
PL1	-3.60 dB
PL1W	17.83863831 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300097 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

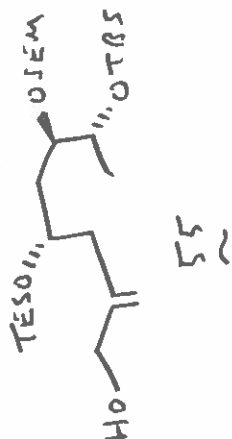
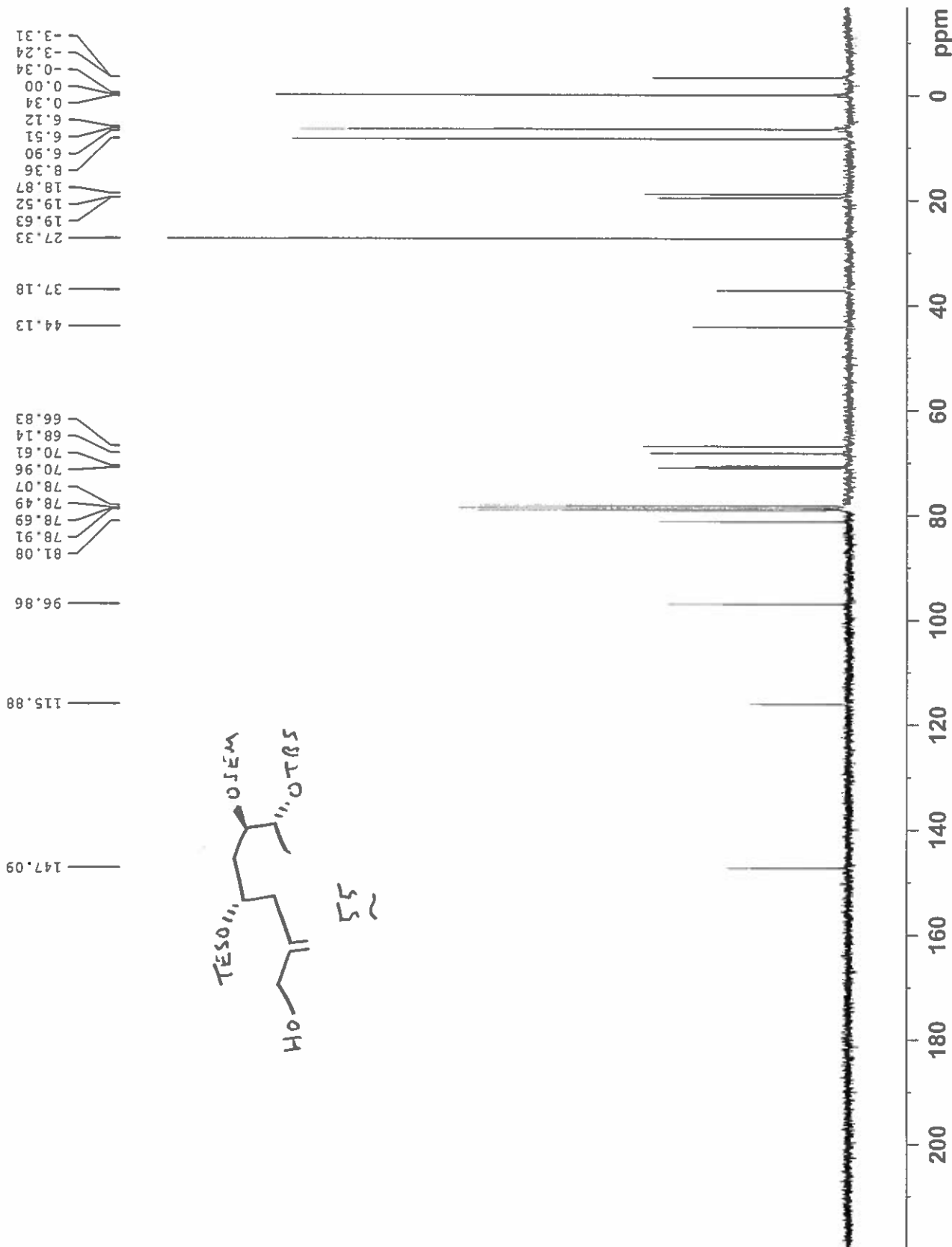




F2 - Acquisition Parameters	
Date_	20090128
Time_	12.23
INSTRUM	DPX300
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	2
SWH	17857.143 Hz
FIDRES	0.272478 Hz
AQ	1.8350580 sec
RG	16384
WDW	28.000 usec
DE	6.00 usec
TE	300.0 K
DD1	2.00000000 sec
dd1	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

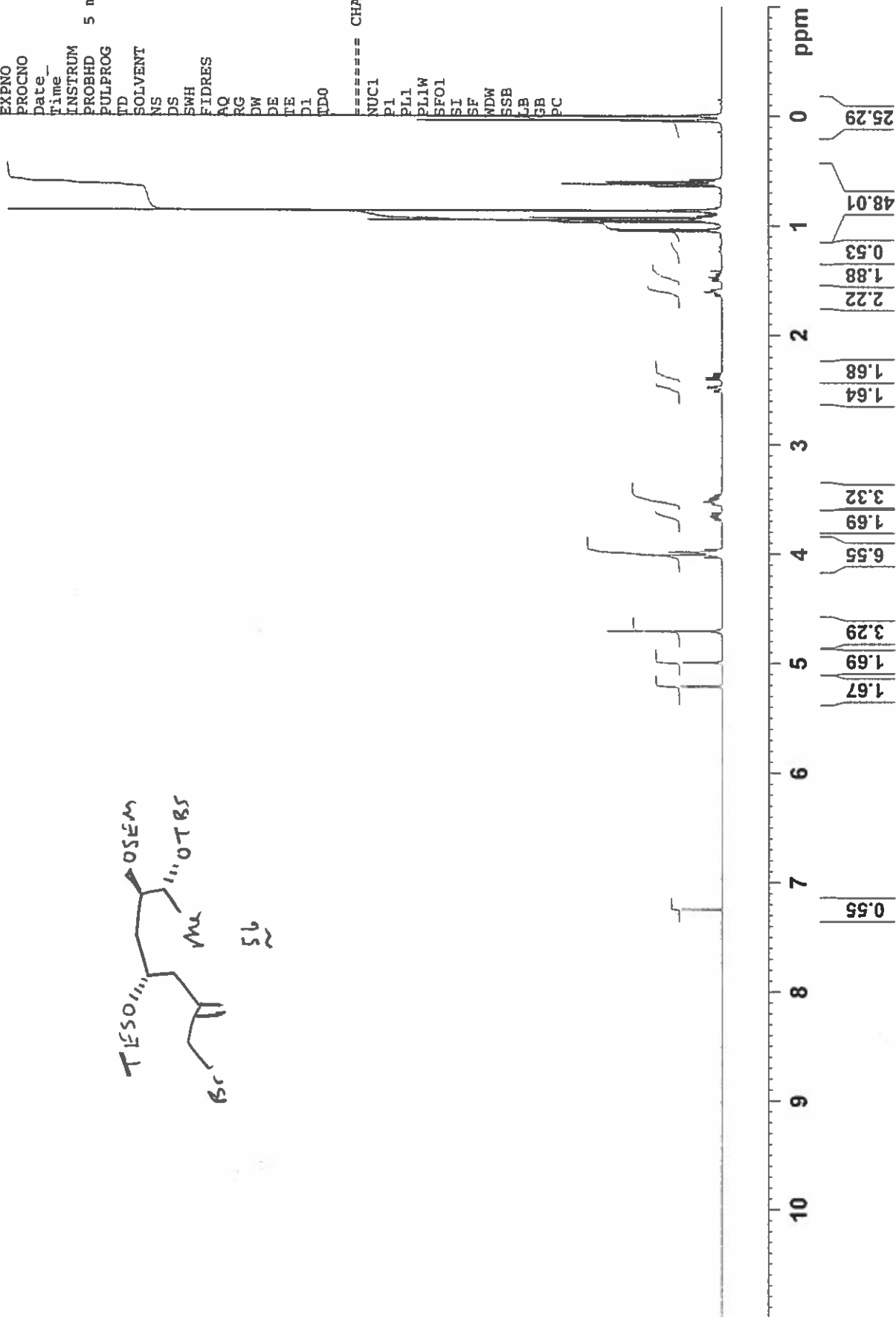
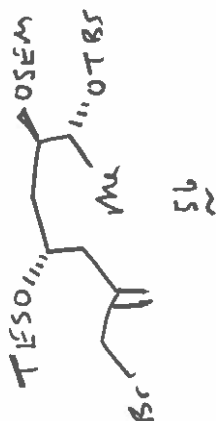
```
===== CHANNEL f2 =====
CPDPRG2      waitz16
UCP2         ih
NVC2         80.00 usec
PL12         -2.60 dB
PL11         14.50 dB
PL13         15.00 dB
SF02         299.9512000 MHz
```

F2 - Processing parameters	
SI	32768
SF	75.4223766 MHz
NDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

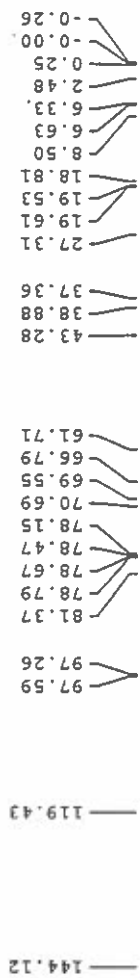




2009-02-01-ejt-10  
NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20090201  
Time 13.12  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 71.8  
DW 60.500 usec  
DE 9.40 usec  
TE 290.0 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300158 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



apgbromination  
mCARBON CDC13 {e:\bruk400data\2009\Jan} ejt 10

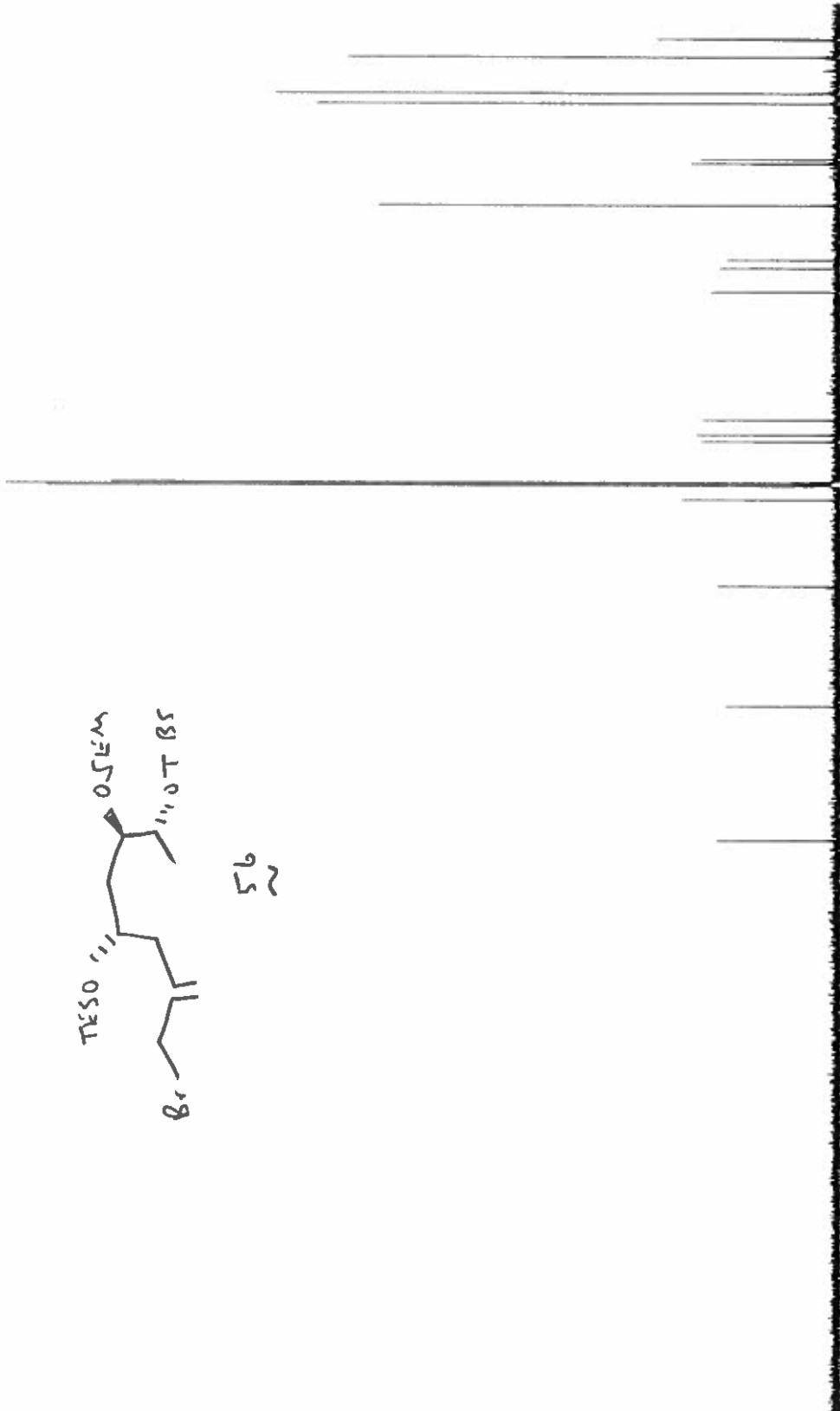


56

NAME 2009-02-01-ejt-10  
EXPNO 12  
PROCNO 1  
Date\_ 20090201  
Time\_ 13.34  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 2  
SWH 30241.936 Hz  
FIDRES 0.461455 Hz  
AQ 1.0835786 sec  
RG 512  
DW 16.533 usec  
DE 7.83 usec  
TE 290.7 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 34.91522217 W  
SFO1 100.6241042 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.60 dB  
PL12 15.31 dB  
PL13 18.00 dB  
PL2W 17.83863831 W  
PL12W 0.22927761 W  
PL13W 0.12341322 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6126251 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 0.20

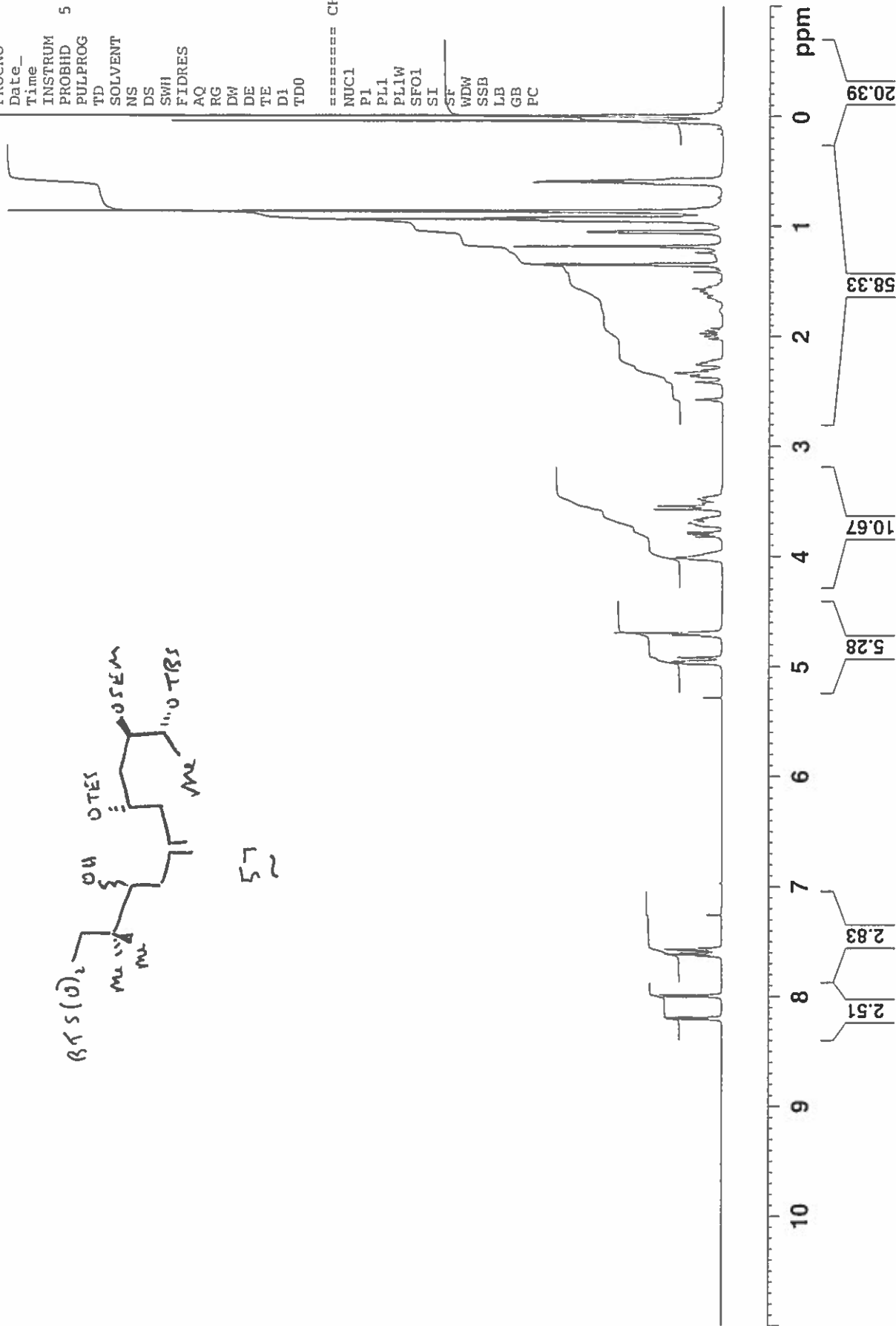
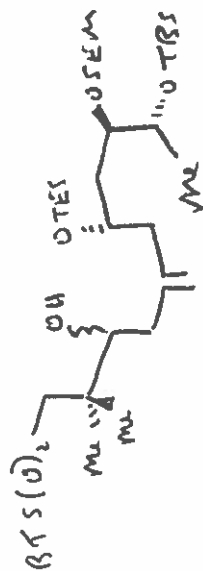


240 220 200 180 160 140 120 100 80 60 40 20 ppm



NAME 2009-06-02-ejt-48  
EXPNO 10  
PROCNO 1  
Date\_ 20090602  
Time 15.42  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 18  
DE 48.400 usec  
TE 13.38 usec  
TD0 1  
D1 290.6 K  
D0 1.00000000 sec

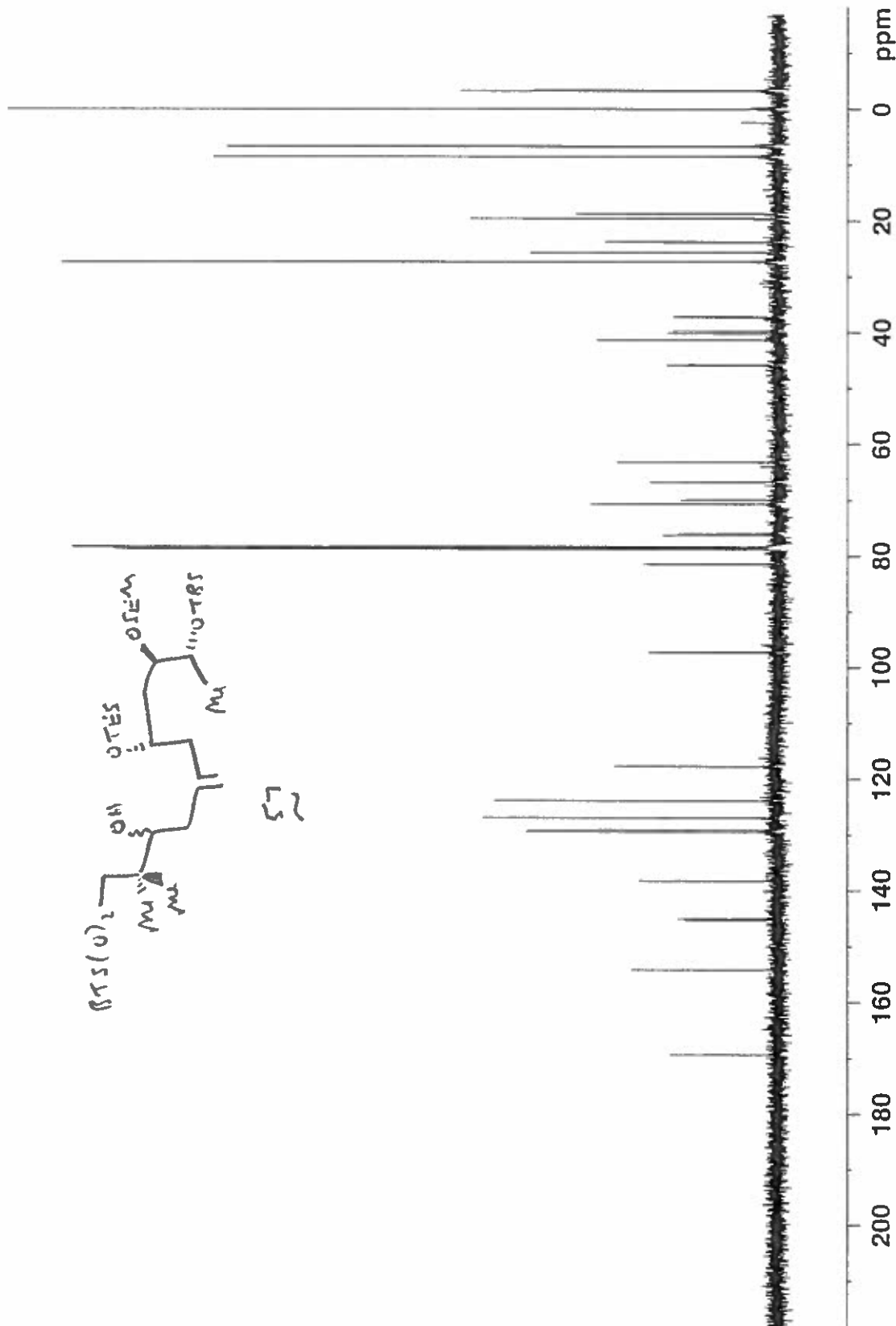
===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300138 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



NAME		2009-06-02-ejt-48
EXPNO	PROCNO	11
Date_	Date_	20090602
Time		15:55
INSTRUM	spect	
PROBHD	5 mm TXI 1H/D-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDC13	
N5	N5	256
DS	DS	2
SWH	29761.904 Hz	
FIDRES	0.454131 Hz	
AQ	1.1010548 sec	
RQ	512	
DW	16.800 usec	
DE	32.21 usec	
TE	291.4 K	
D1	2.00000000 sec	
d11	0.03000000 sec	
TD0		1

```
===== CHANNEL f1 =====
NUC1      13C
P1        11.50 usec
PL1       -4.20 dB
PL1W      218.0282385 W
SF01      125.7703643 MHz
```

```
===== CHANNEL f2 =====
CPDRPG2          waitz16
NUC2             1H
PCPD2            80.00 usec
PLP12            4.20 dB
PL12             23.99 dB
PL13             23.00 dB
PL12W            9.74092484 W
PL12W            0.10223514 W
PL13W            0.12841040 W
SF02             500.1320005 MHz
SI               32768
SF               125.7576101 MHz
WDW              EM
SDB              0
LB              1.00 Hz
GB              0
PC              1.40
```





SH502

mPROTONnight CDCl3 {C:\bruk400data\2008\Sep} ejt 56



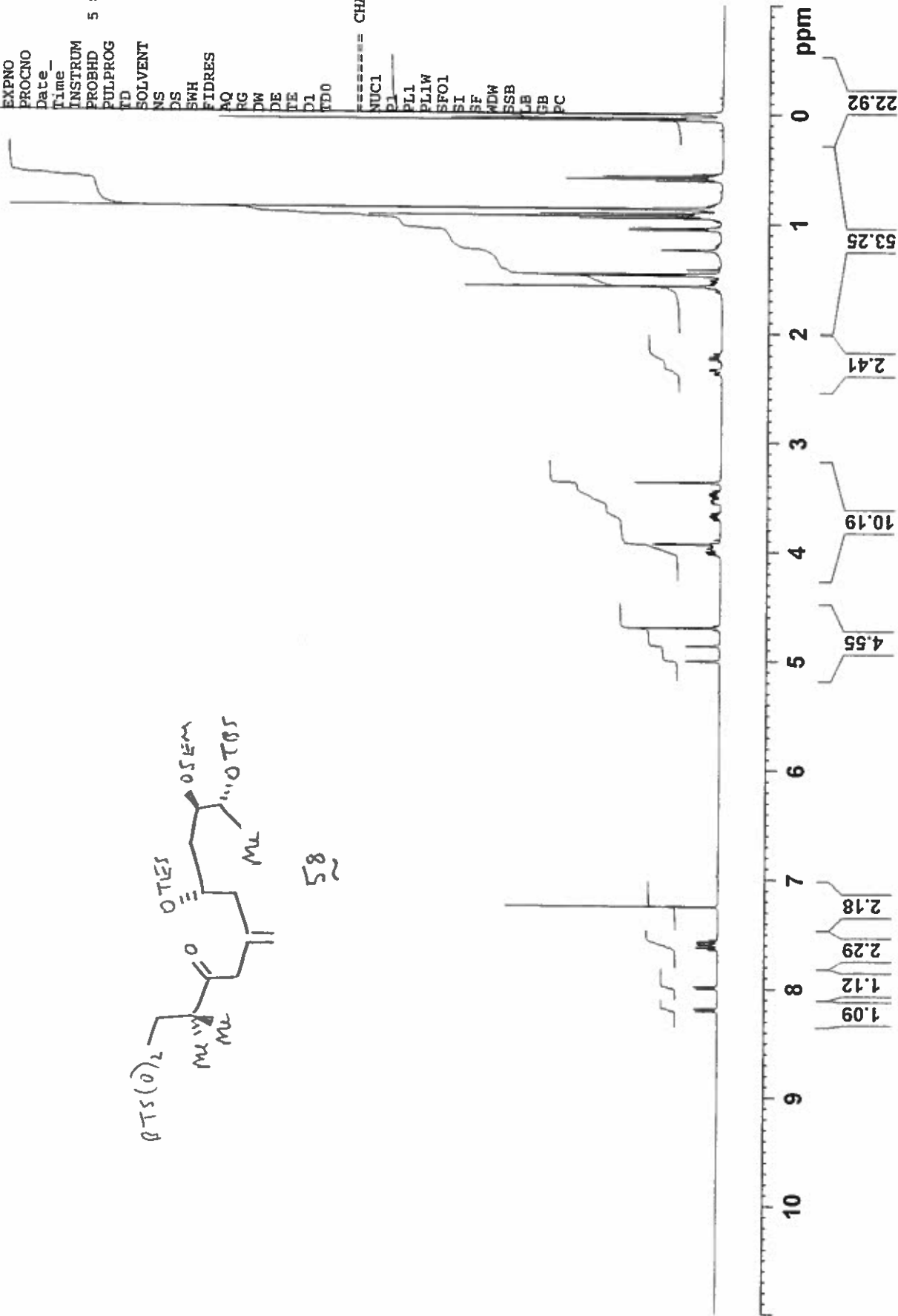
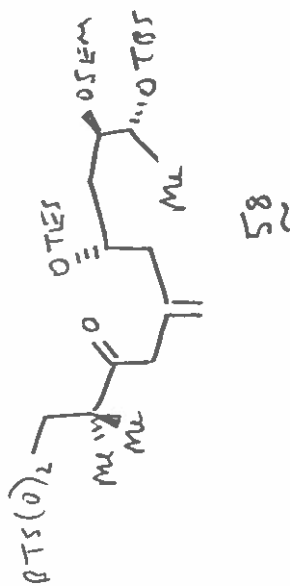
2008-09-18-ejt-56

NAME EXPNO PROCNO Date\_ Time INSTRUM PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG DW DE TE D1 TD0

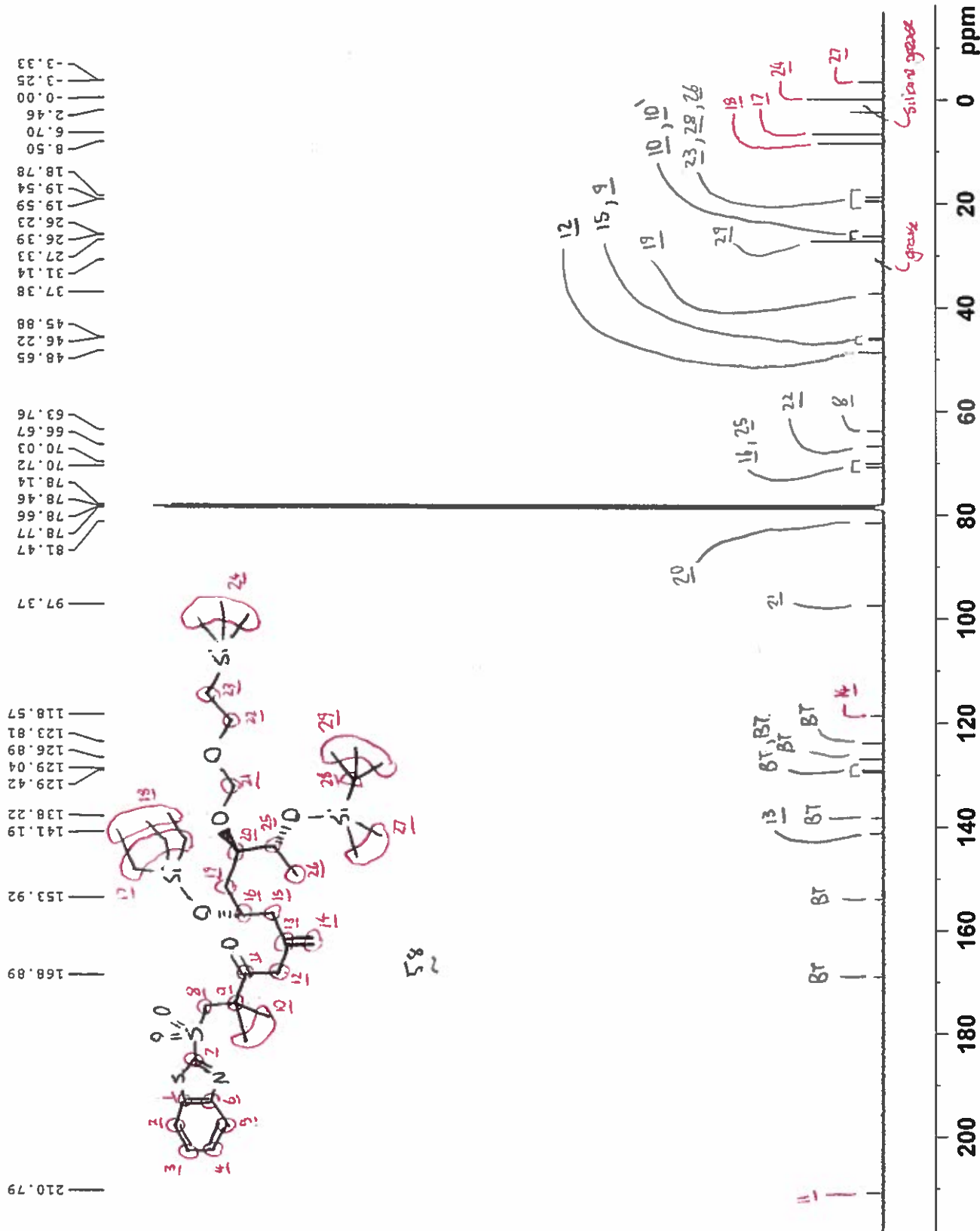
11 1 20080919 2.17 AV400 5 mm PABBO BB- 2930b 65536 CDCl3 64 0 8264.463 Hz 0.126106 Hz 3.9649780 sec 287 60.500 usec 9.40 usec 294.8 K 1.00000000 sec 1

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

NUC1 1H PL1 10.00 usec -3.60 dB PL1W 17.83863831 W SFO1 400.1324710 MHz SI 32768 SF 400.1300139 MHz MDW EM 0 SSB 0 LB 0 GB 0 PC 1.00



SH502

mCARBONnight CDCl<sub>3</sub> {C:\bruk400data\2008\Sep} ejt 56

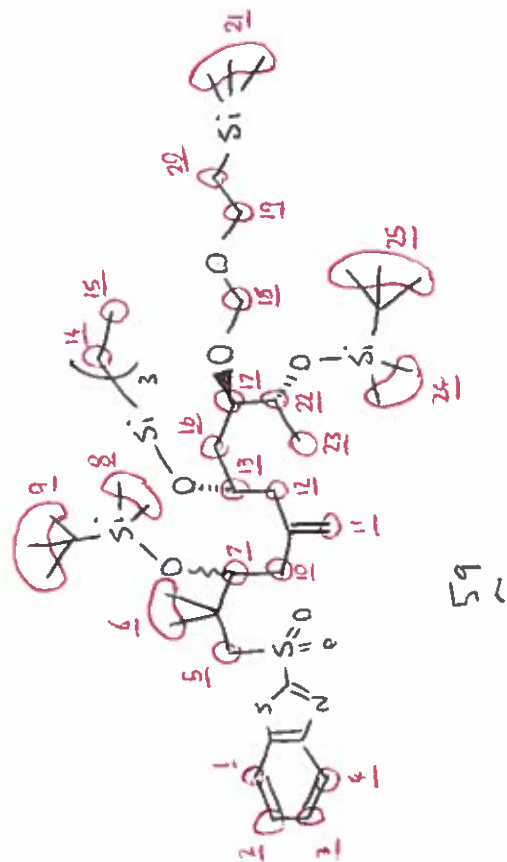
```

NAME      2008-09-18-ejt-56
EXPNO     10
PROCNO     1
Date_      20080919
Time       2.11
INSTRUM    AV400
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         2560
DS         2
SWH         23809.523 Hz
FIDRES     0.363304 Hz
AQ         1.3763061 sec
RG         512
DE         21.000 usec
TE         7.66 usec
D1         295.4 K
D11        2.0000000 sec
TD0        0.0300000 sec
===== CHANNEL f1 =====
NUC1       13C
P1         8.00 usec
PL1        0.00 dB
PL1W       34.91522217 W
SFO1       100.6228294 MHz
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -3.60 dB
PL12       15.31 dB
PL13       18.00 dB
PL2W       17.83863831 W
PL12W      0.22927761 W
PL13W      0.12341322 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6126249 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

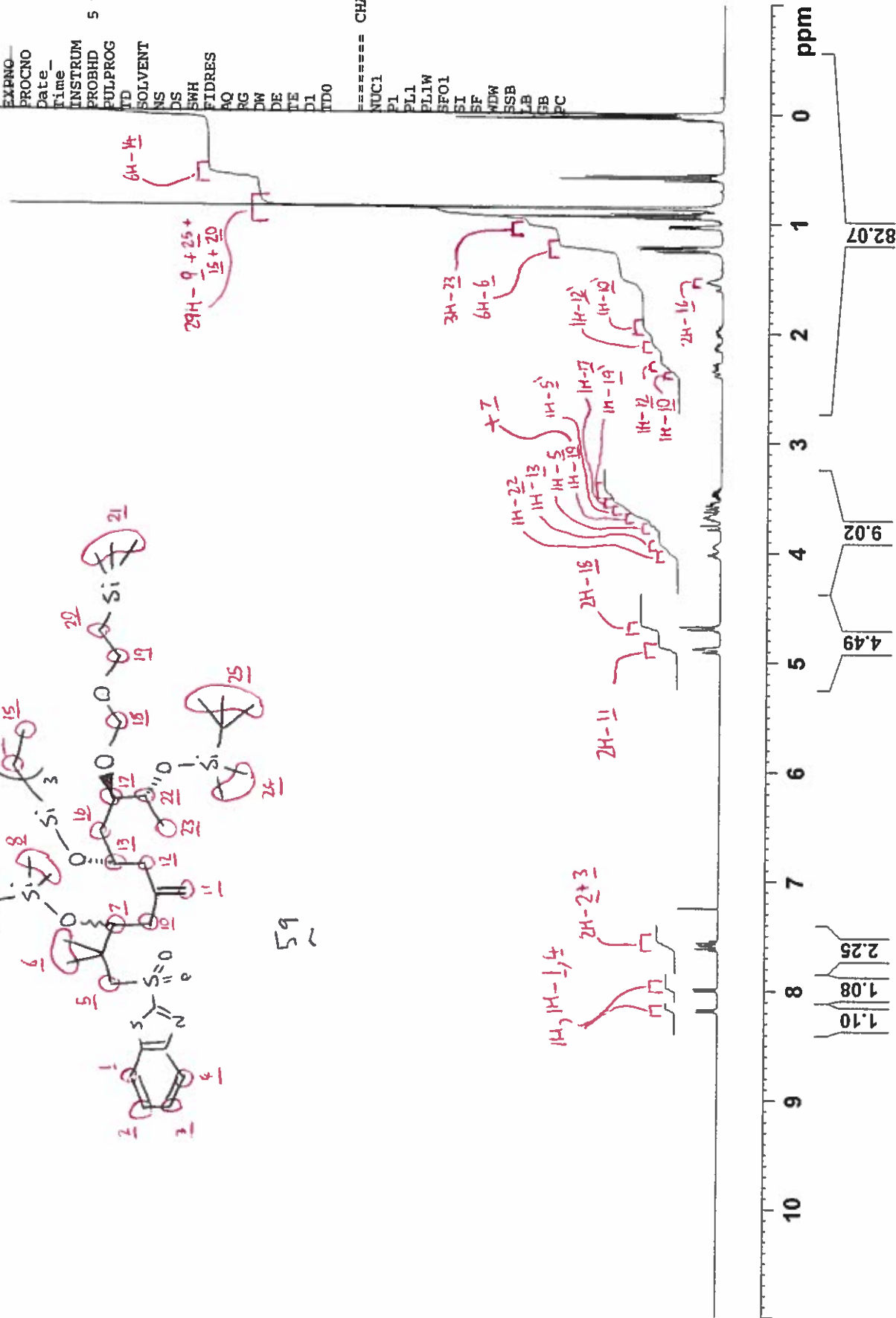
SH512

mPROTONight CDC13 {C:\bruk400data\2008\Oct} ejt 23



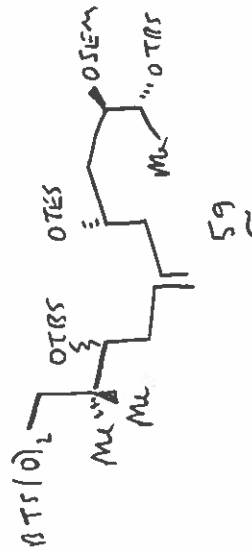
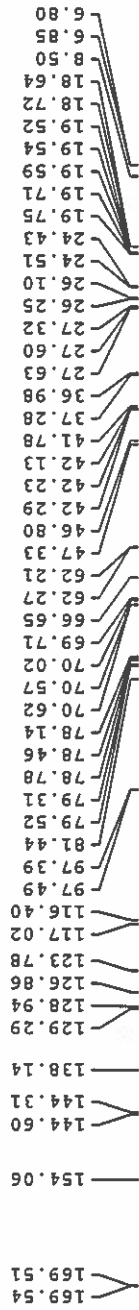
NAME 2008-10-01-ejt-23  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20081002  
 Time 3.27  
 INSTRUM AV400  
 PROBD 5 mm PABBO BB-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 0  
 SWH 8264.463 Hz  
 FIDRES 0.126106 Hz  
 AQ 3.9649780 sec  
 RG 90.5  
 DW 60.500 usec  
 DE 9.40 usec  
 TE 294.2 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 -3.60 dB  
 PL1W 17.83863831 W  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300137 MHz  
 NDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



SH512

mCARBONnight CDC13 {C:\bruk400data\2008\Oct} ejt 23



NAME 2008-10-01-ejt-23  
 EXPNO 12  
 PROCNO 1  
 Date 20081002  
 Time 4.05  
 INSTRUM AV400  
 PROBD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 512  
 DS 2  
 SWH 23809.523 Hz  
 FIDRES 0.363304 Hz  
 AQ 1.3763061 sec  
 RG 512  
 DW 21.000 usec  
 DE 7.66 usec  
 TE 294.8 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.00 usec  
 PL1 0.00 dB  
 PL1W 34.91522217 W  
 SFO1 100.628294 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -3.60 dB  
 PL12 15.31 dB  
 PL13 18.00 dB  
 PL2W 17.83863831 W  
 PL12W 0.22927761 W  
 PL13W 0.12341322 W  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6126250 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

SH513

mPROTON CDC13 {C:\bruk400data\2008\Oct} ejt 29

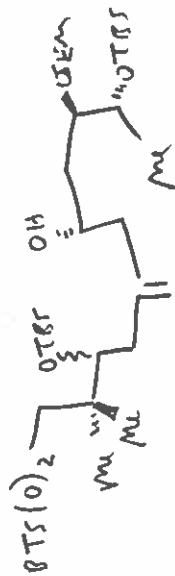


2008-10-03-ejt-29

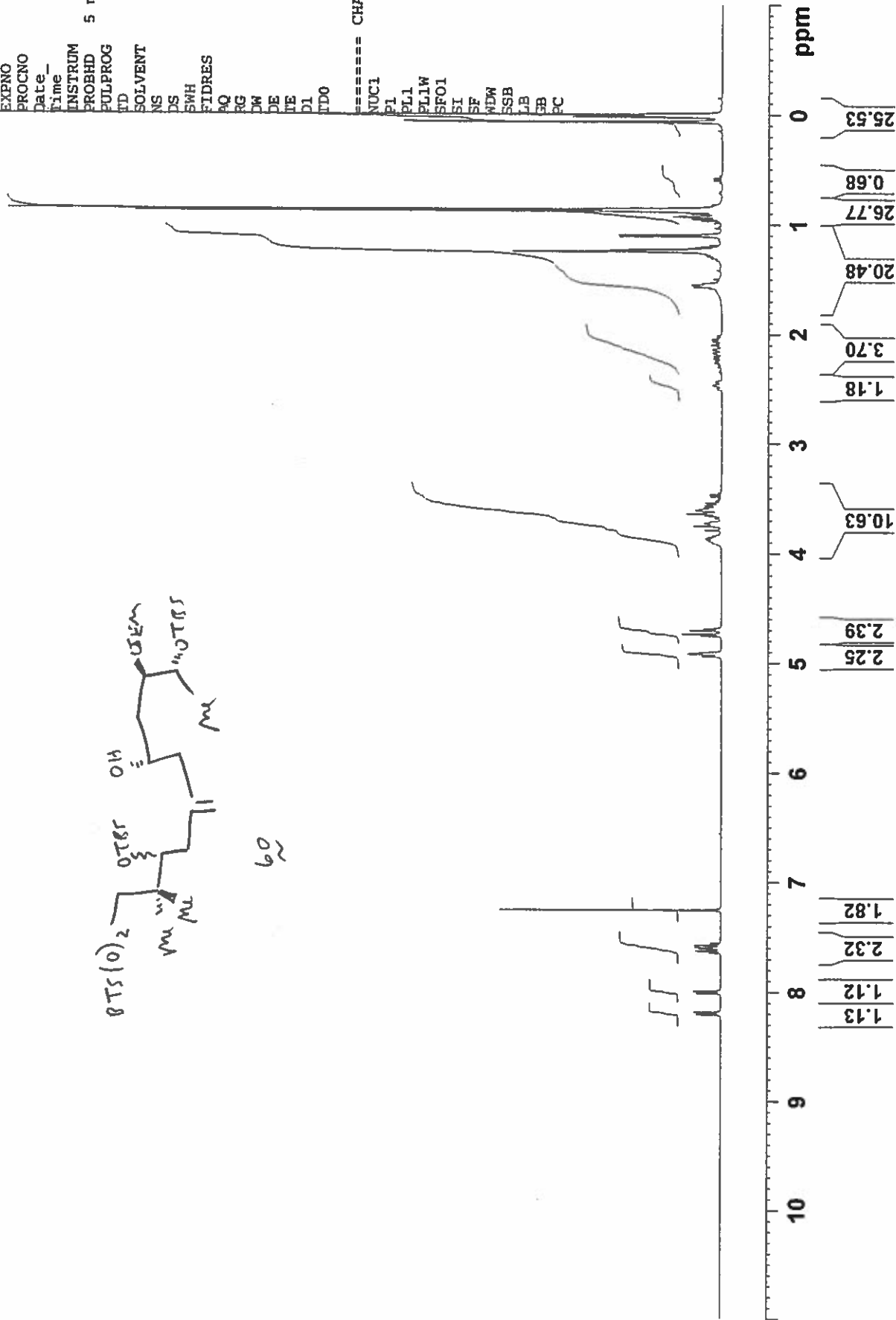
NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20081003  
Time 11:52  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDC13  
NS 64  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 287  
DW 60.500 usec  
DE 9.40 usec  
TE 293.9 K  
D1 1.00000000 sec  
TDO 1

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

NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300115 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

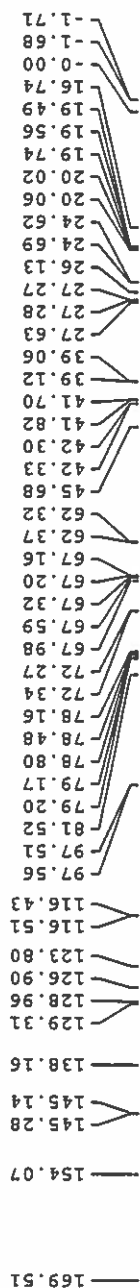


60



SH515

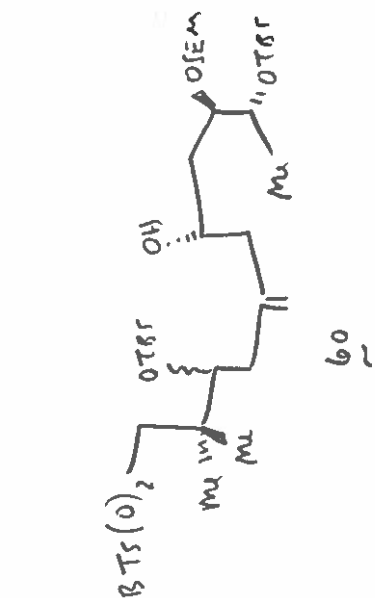
mCARBONnight CDCI3 {C:\bruk400data\2008\Oct} ejt 16



2008-10-05-ejt-16  
 NAME EXPNO 12  
 PROCNO 1  
 Date\_ 20081006  
 Time\_ 7.33  
 INSTRUM AV400  
 PROBD 5 mm PABBO BE-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCI3  
 NS 512  
 DS 2  
 SWH 23809.523 Hz  
 FIDRES 0.363304 Hz  
 AQ 1.3763061 sec  
 RG 512  
 DW 21.000 usec  
 DE 7.66 usec  
 TE 294.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.00 usec  
 PL1 0.00 dB  
 PL1W 34.9152217 W  
 SFO1 100.6228294 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -3.60 dB  
 PL12 15.31 dB  
 PL13 18.00 dB  
 PL2W 17.83863831 W  
 PL12W 0.22927761 W  
 PL13W 0.12341322 W  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6126233 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



200 180 160 140 120 100 80 60 40 20 0 ppm

SH516

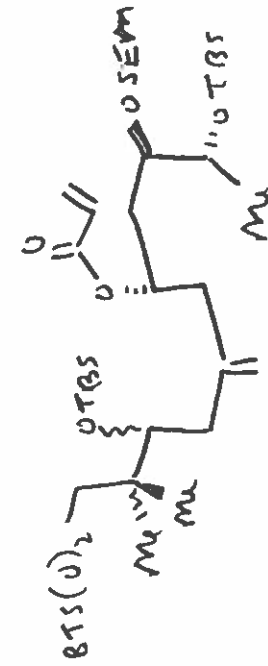
mPROTON CDCl<sub>3</sub> {C:\bruk400data\2008\Oct} ejt 15

2008-10-09-ejt-15

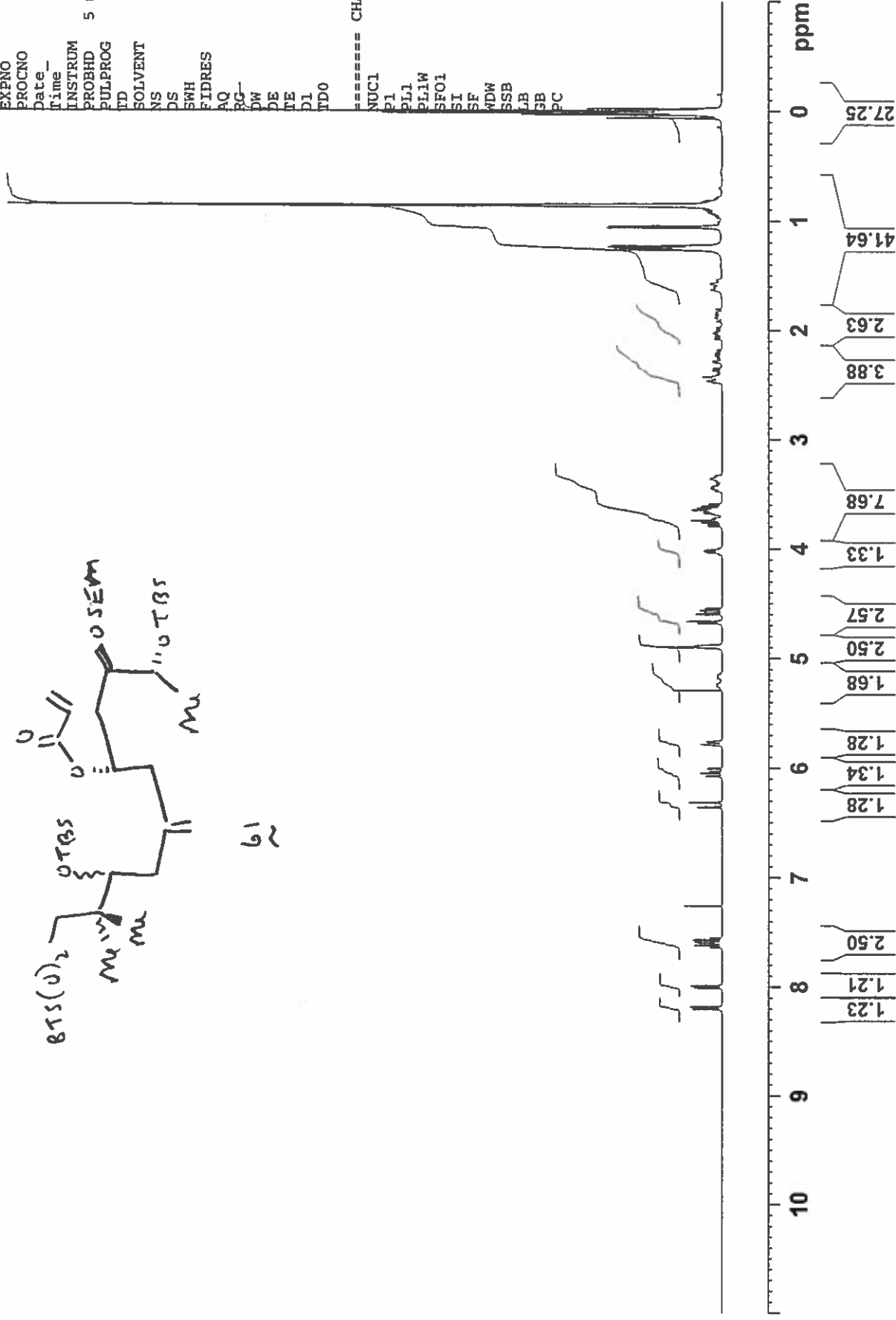
NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20081009  
Time\_ 8.51  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 32  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 80.6  
DW 60.500 usec  
DE 9.40 usec  
TE 294.0 K  
D1 1.00000000 sec  
TD0 1

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

NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300106 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

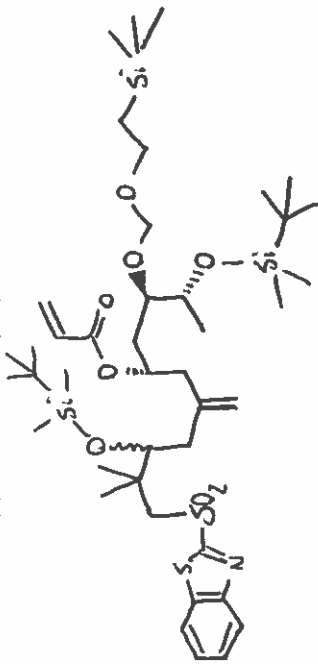
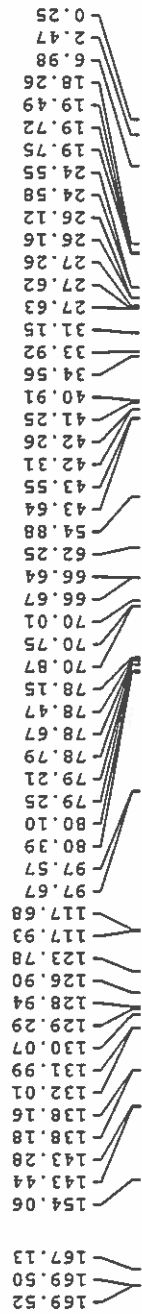


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SH516\_C

mCARBONnight CDC13 {C:\bruk400data\2008\Oct} ejt 15



NAME 2008-10-08-ejt-15  
 EXPNO 11  
 PROCNO 1  
 Date\_ 20081009  
 Time\_ 7.42  
 INSTRUM AV400  
 PROBD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 1024  
 DS 2  
 SWH 23809.523 Hz  
 FIDRES 0.363304 Hz  
 AQ 1.3763061 sec  
 RG 512  
 DW 21.000 usec  
 DE 7.66 usec  
 TE 294.8 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.00 usec  
 PL1 0.00 dB  
 PL1W 34.91522217 W  
 SFO1 100.6228294 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -3.60 dB  
 PL12 15.31 dB  
 PL13 18.00 dB  
 PL2W 17.83863831 W  
 PL12W 0.22927761 W  
 PL13W 0.12341322 W  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6126240 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

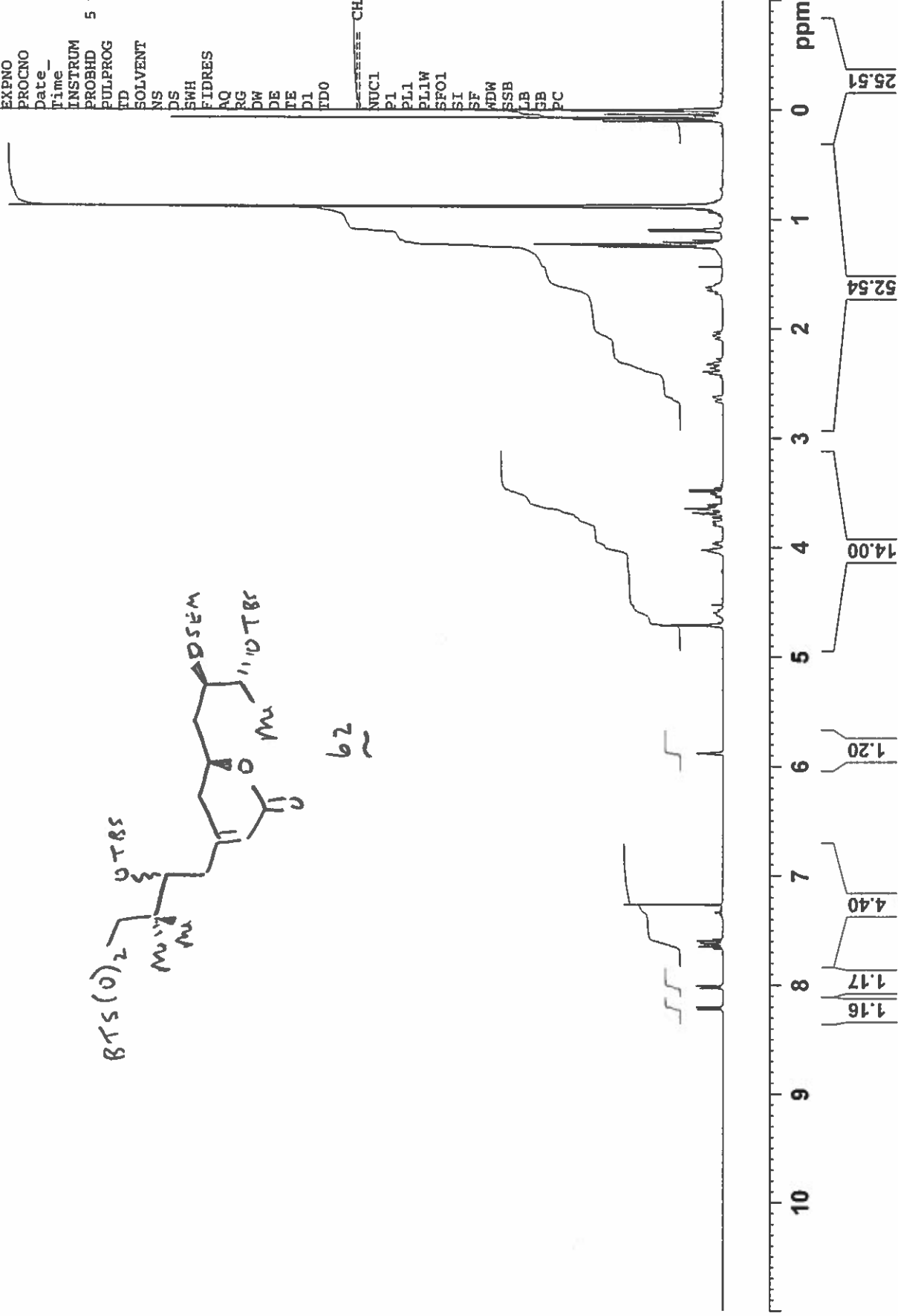
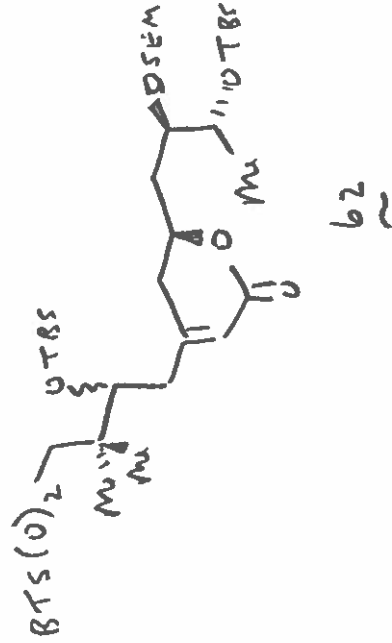


SH520

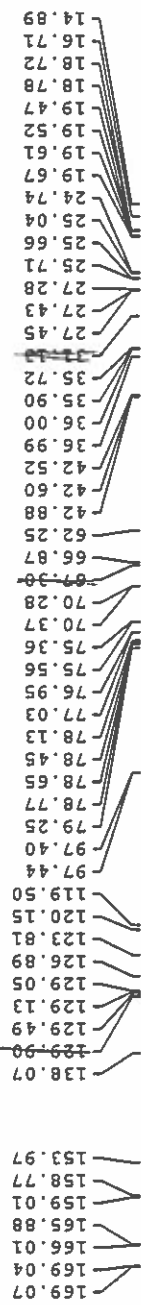
mPROTONnight CDCl3 {C:\bruk400data\2008\Oct} ejt 55



2008-10-17-ejt-55  
 NAME EXPNO 13  
 PROCNO 1  
 Date\_ 20081017  
 Time 21.12  
 INSTRUM AV400  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDCl3  
 NS 64  
 DS 0  
 SWH 8264.463 Hz  
 FIDRES 0.126106 Hz  
 AQ 3.9649780 sec  
 RG 203  
 DW 60.500 usec  
 DE 9.40 usec  
 TE 294.5 K  
 D1 1.00000000 sec  
 TDO 1  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 -3.60 dB  
 PL1W 17.83863831 W  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300073 MHz  
 ADW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



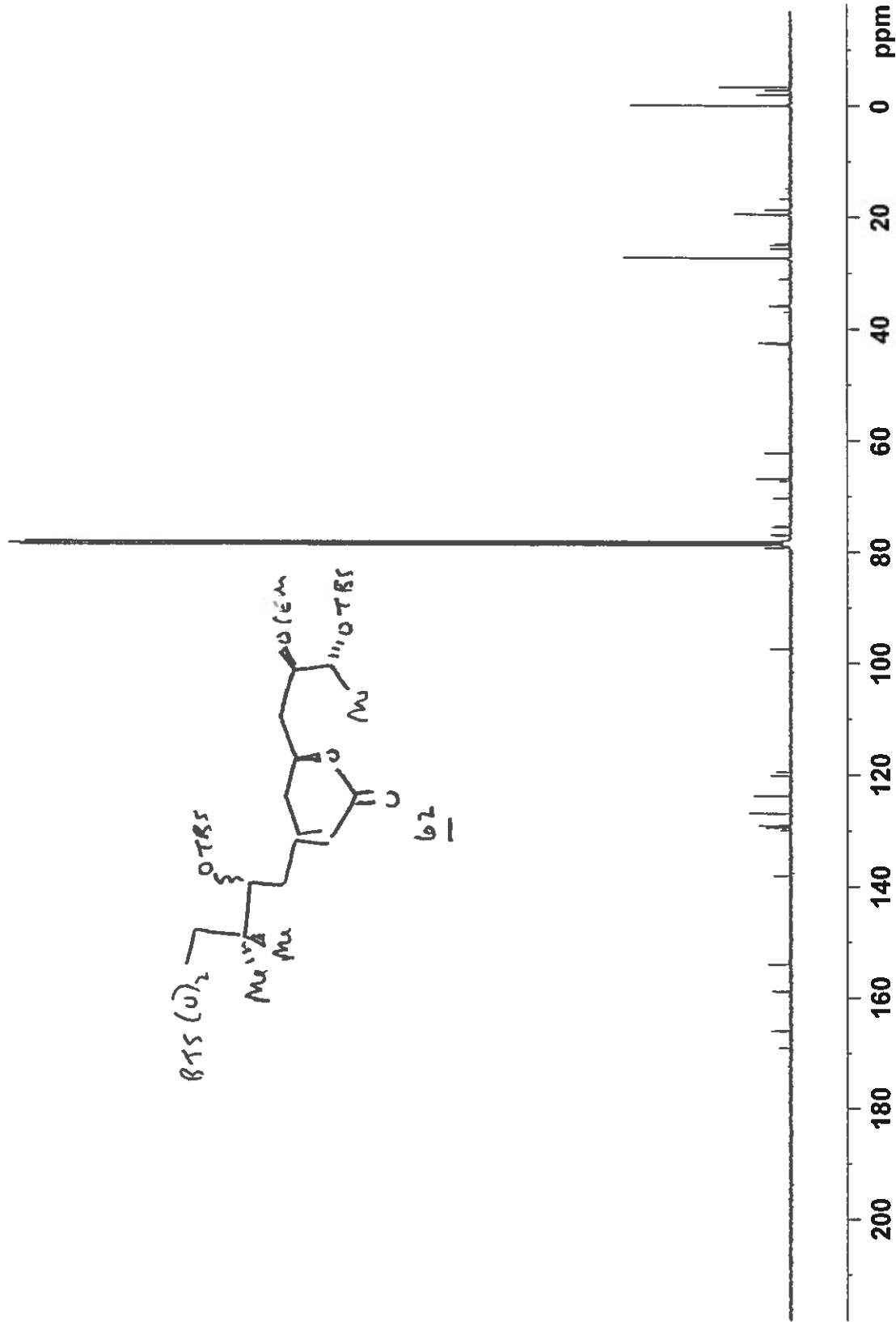
SH520

mCARBONnight CDCl<sub>3</sub> {C:\bruk400data\2008\Oct} ejt 55

2008-10-17-ejt-55  
 EXPNO 12  
 PROCNO 1  
 Date 20081017  
 Time 21.07  
 INSTRUM AV400  
 PROBD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 3072  
 DS 2  
 SMH 23809.523 Hz  
 FIDRES 0.363304 Hz  
 AQ 1.3763061 sec  
 RG 512  
 DW 21.000 usec  
 DE 7.66 usec  
 TE 295.1 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 8.00 usec  
 PL1 0.00 dB  
 PL1W 34.9152217 W  
 SFO1 100.6228294 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 90.00 usec  
 PL2 -3.60 dB  
 PL12 15.31 dB  
 PL13 18.00 dB  
 PL2W 17.83863831 W  
 PL12W 0.22927761 W  
 PL13W 0.12341322 W  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6126256 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



SH521

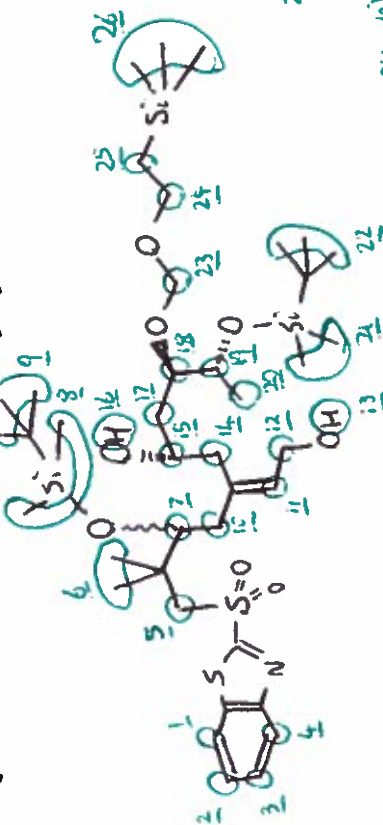
mPROTONight CDCl<sub>3</sub> {C:\bruk400data\2008\Oct} ejt 7

2008-10-19-ejt-7

NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20081019  
Time\_ 15.54  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 64  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 203  
DW 60.500 usec  
DE 9.40 usec  
TE 294.1 K  
D1 1.00000000 sec  
TD0 1

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

NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300078 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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2H-1 + 22  
+ 256H-6  
3H-20

2H-10 + 14

2H-10  
+ 14

2H-13 + 16

2H-17

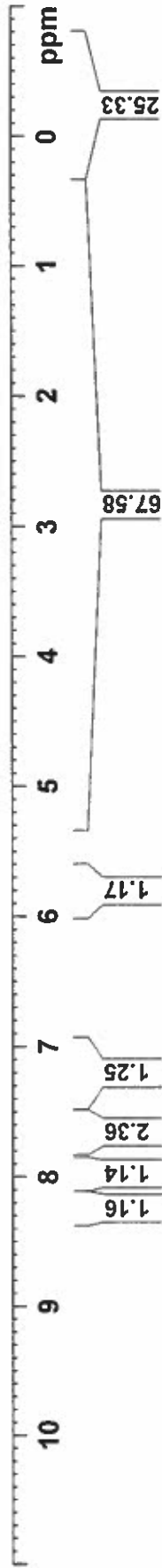
10H-12 + 24  
+ 24 + 2 + 15  
+ 18 + 10  
+ 5 + 5

2H-2 + 3

1H, 1H-1, 4

1H-12

2H-23

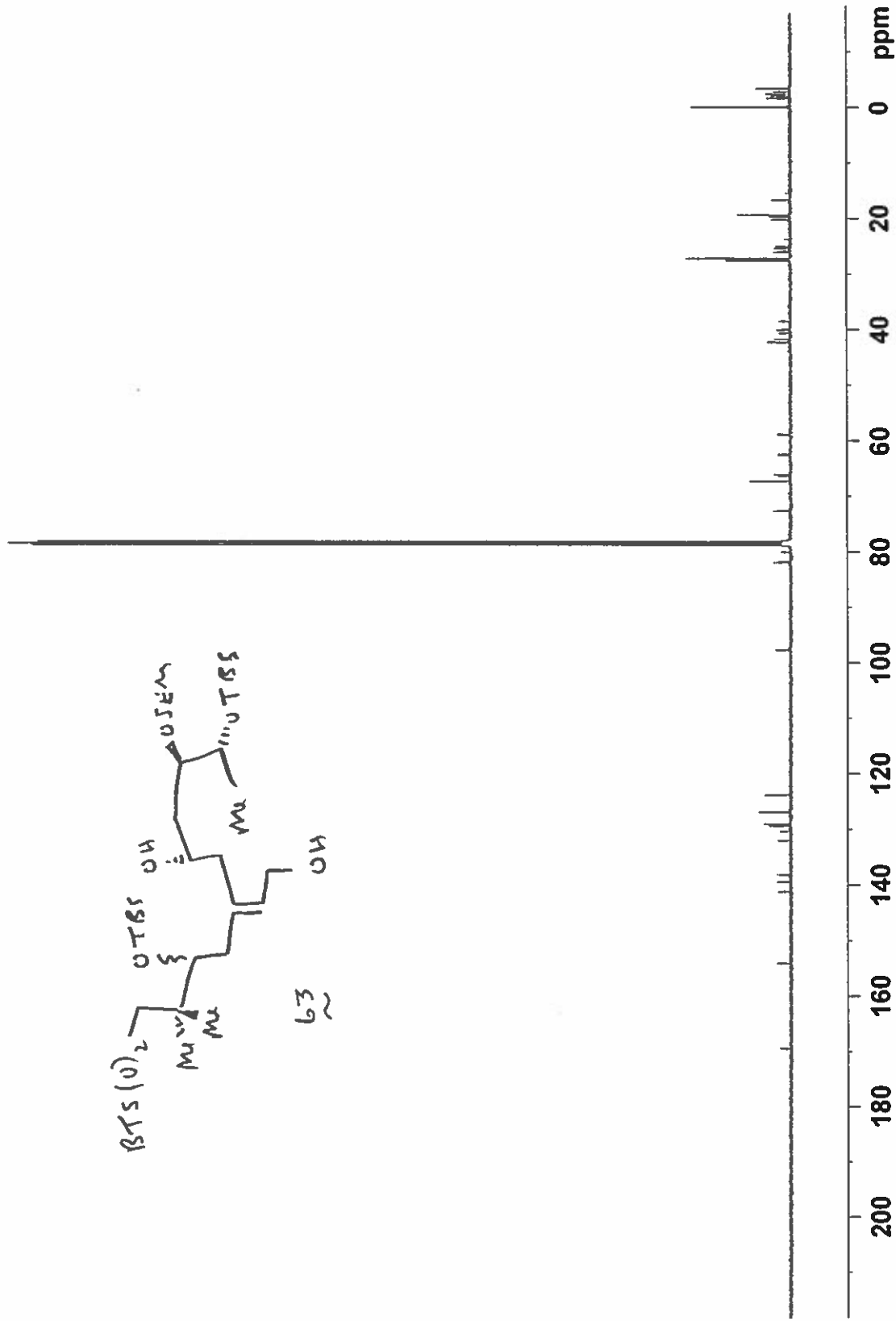
2H-8 + 21  
+ 26



NAME		2008-10-19-ejt-7
EXPNO	1	11
PROCNO	1	
Date_	20081019	
Time	18.51	
INSTRUM	AV400	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDC13	
NS	3072	
DS	2	
SWH	23809.523 Hz	
FIDRES	0.363304	
AQ	1.3763061 sec	
RQ	512	
DW	21.000 us	
DE	7.66 us	
TE	295.0 K	
D1	2.00000000 sec	
D11	0.03000000 sec	
TD0	1	

```
===== CHANNEL f1 =====
NUC1      13C
P1         8.00 usec
PL1        0.00 dB
PL1W       34.91522217 W
SF01      100.6228294 MHz
```

```
===== CHANNEL f2 =====
CPDRG2      waltz16      1H
NUC2
PCPD2        90.00 usec
PL12         -3.60 dB
PL22         15.31 dB
PL12         18.00 dB
PL2W         17.83863831 W
PL12W        0.22927761 W
PL13W        0.12341322 W
SP02         400.1316005 MHz
SI            32768
SF            100.6126238 MHz
WDW           EM
SSB            0
LB            1.00 Hz
PC            1.40
```

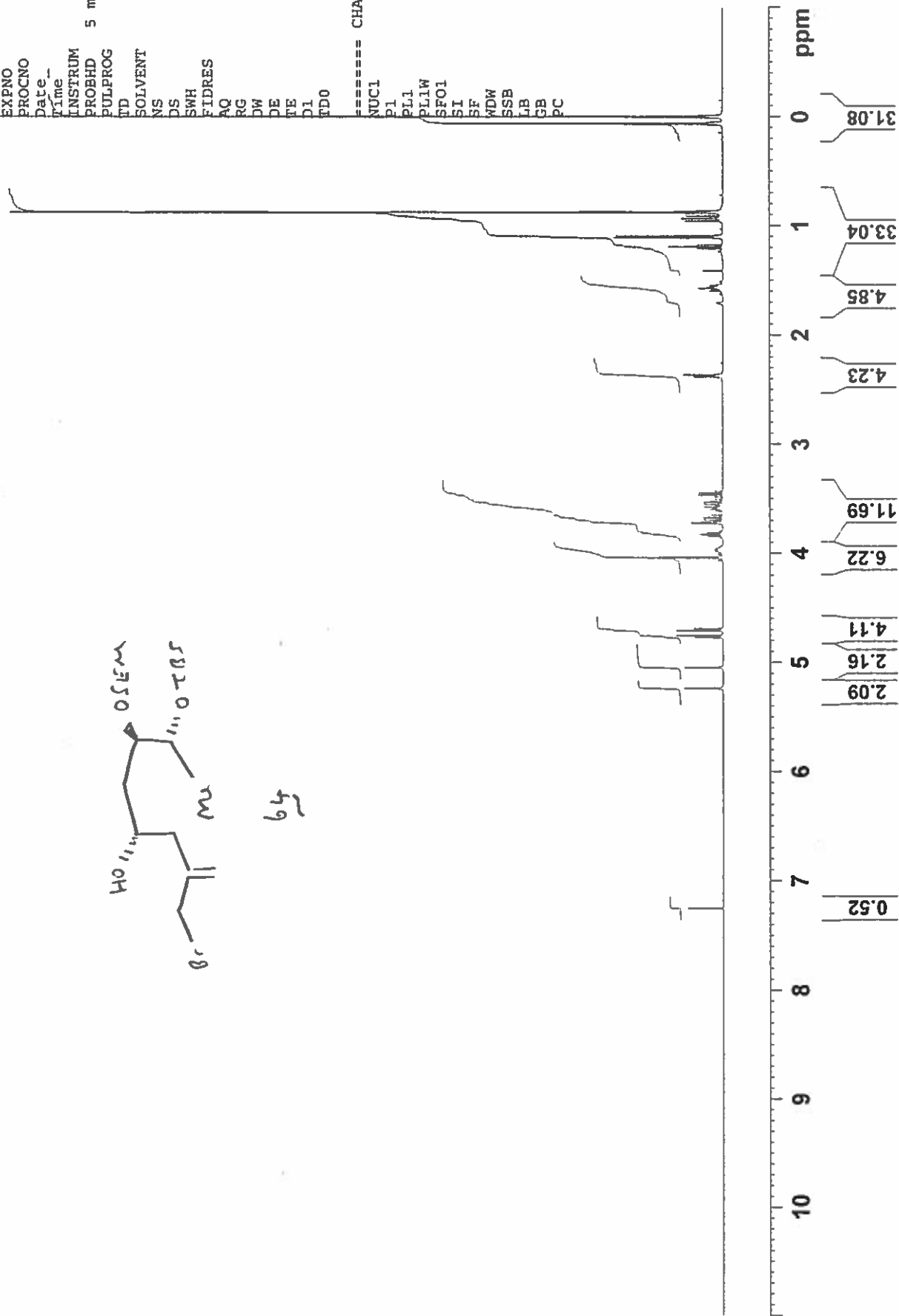


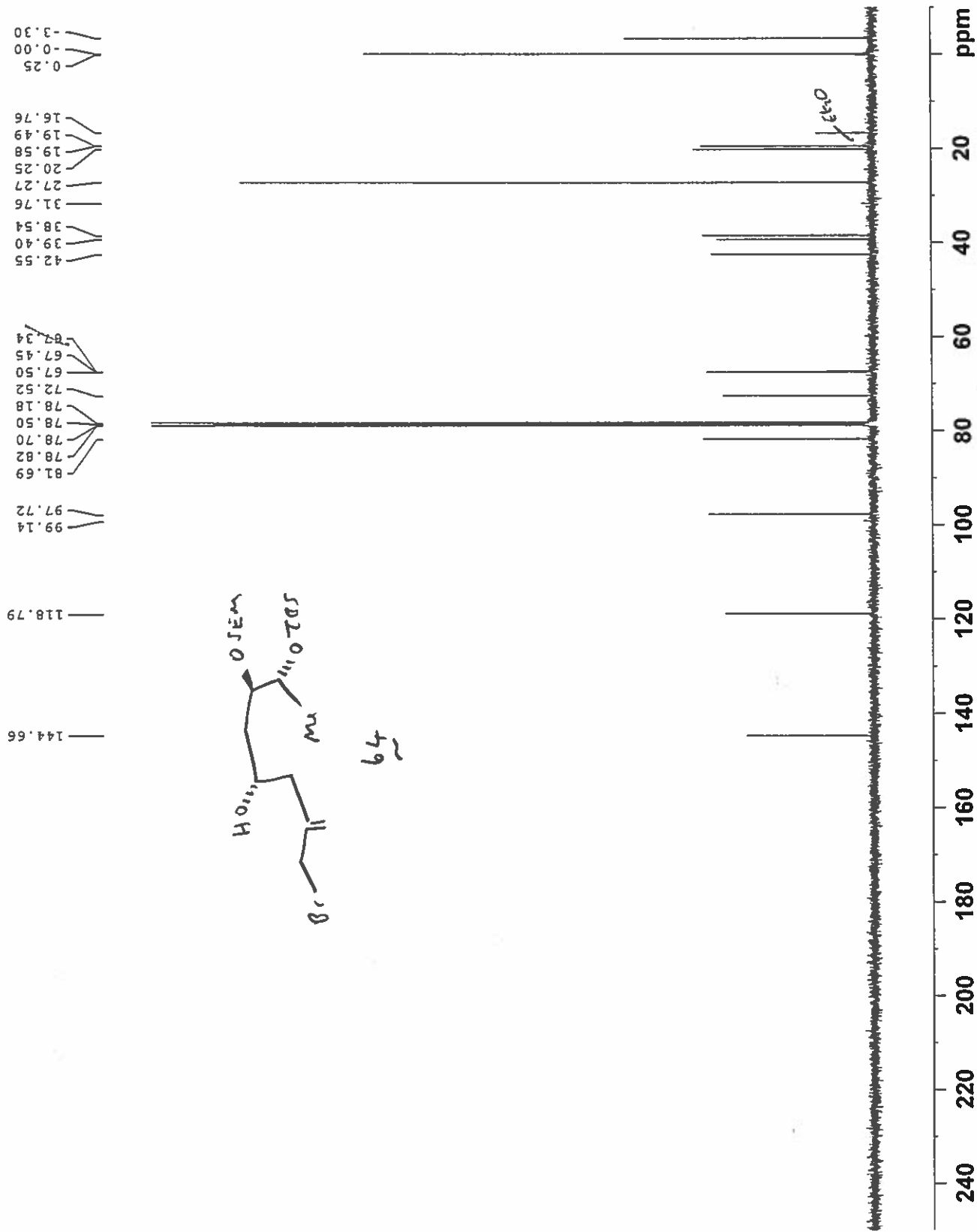


2009-02-02-ejt-49  
NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20090202  
Time\_ 17.23  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 64  
DW 60.500 usec  
DE 9.40 usec  
TE 289.9 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PLW 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300127 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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NAME 2009-02-02-ejt-49  
 EXPNO 12  
 PROCNO 1  
 Date\_ 20090202  
 Time\_ 17.46  
 INSTRUM AV400  
 PROBD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 DS 2  
 SWH 30241.936 Hz  
 FIDRES 0.461455 Hz  
 AQ 1.0835786 sec  
 RG 512  
 DW 16.533 usec  
 DE 7.83 usec  
 TE 290.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 8.00 usec  
 PL1 0.00 dB  
 PL1W 34.91522217 W  
 SFO1 100.6241042 MHz

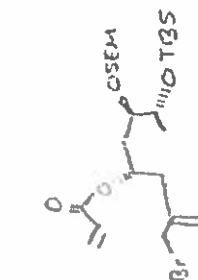
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -3.60 dB  
 PL12 15.31 dB  
 PL13 18.00 dB  
 PL2W 17.83863831 W  
 PL12W 0.2292761 W  
 PL13W 0.12341322 W  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6126234 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 0.20



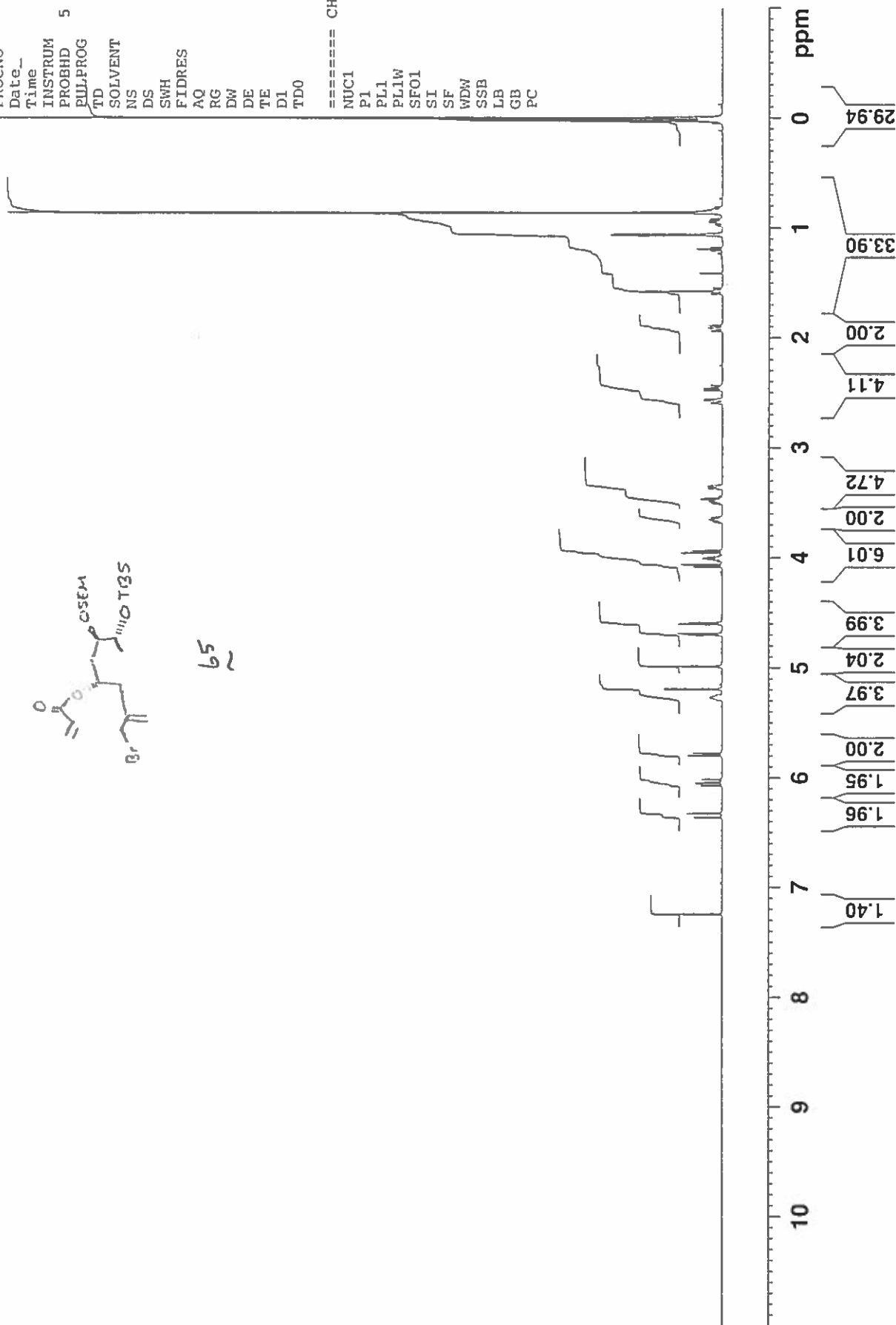
NAME 2009-02-03-ejt-12

EXPNO 10  
PROCNO 1  
Date\_ 20090203  
Time 16.50  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 90.5  
DW 48.400 usec  
DE 13.38 usec  
TE 292.4 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300199 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

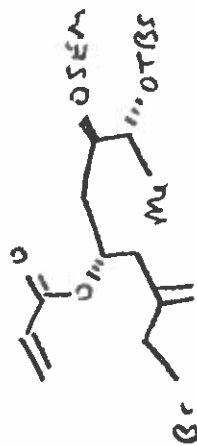
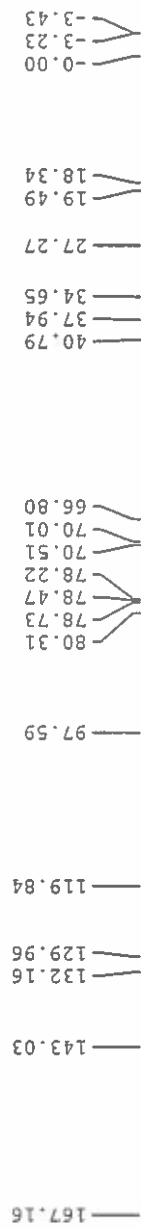


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apgacrylate

mCARBONnight CDCl3 /opt/bruk500data/2009/Feb ejt 14



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NAME 2009-02-03-ejt-14  
EXPNO 10  
PROCNO 1  
Date\_ 20090203  
Time 17.45  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 512  
DW 16.800 usec  
DE 32.21 usec  
TE 293.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 11.50 usec  
PL1 -4.20 dB  
PL1W 218.02882385 W  
SFO1 125.7703643 MHz

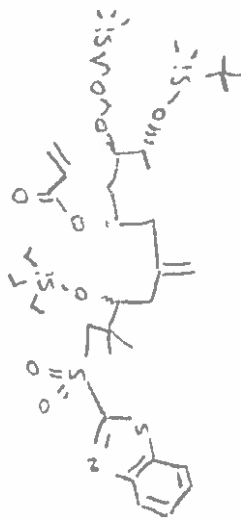
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 4.20 dB  
PL12 23.99 dB  
PL13 23.00 dB  
PL12W 9.74092484 W  
PL12W 0.10223514 W  
PL13W 0.12841040 W  
SFO2 500.1320005 MHz  
SI 32768  
SF 125.7576077 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

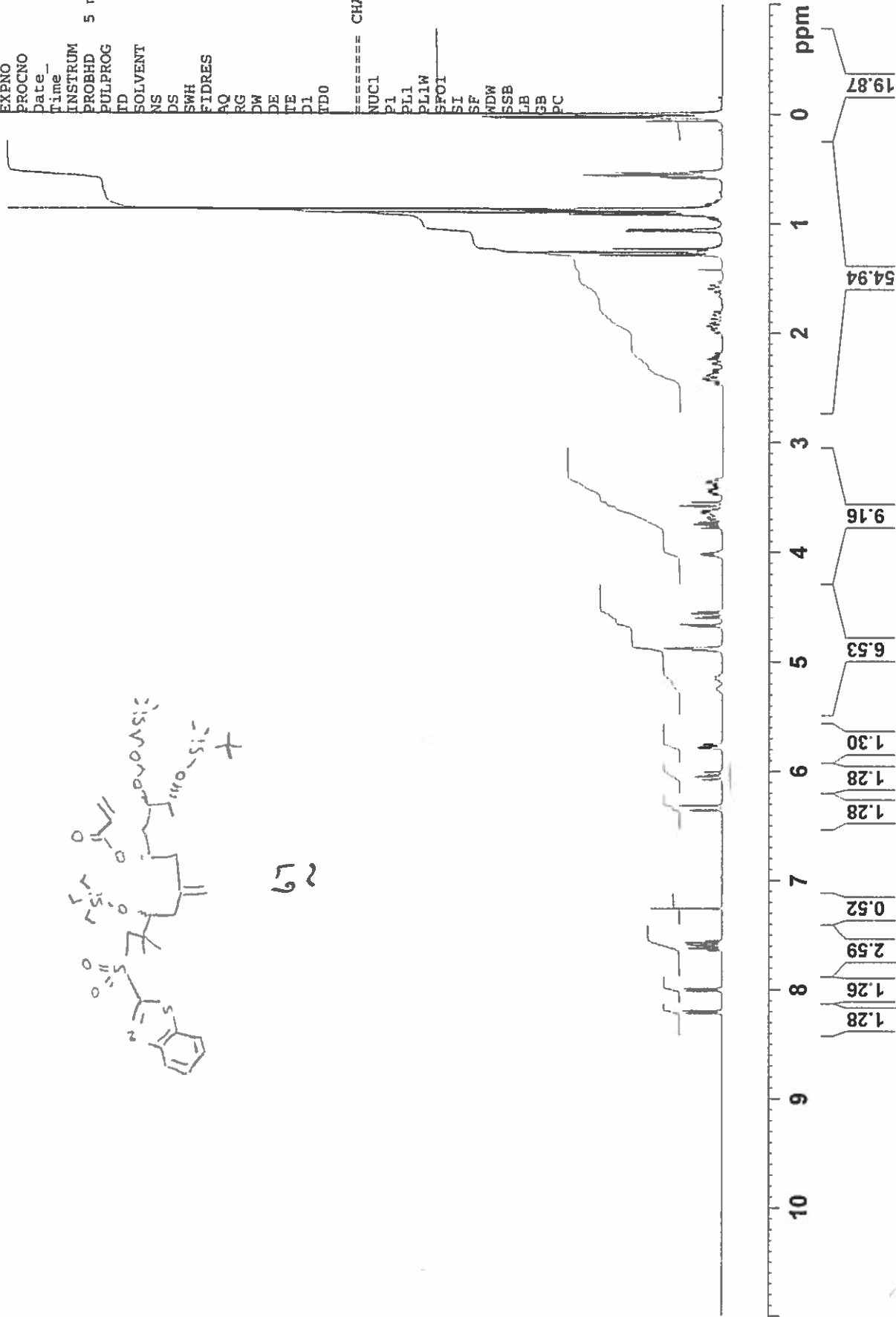




2009-02-18-ejt-1  
NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20090219  
Time 1.10  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 64  
DW 60.500 usec  
DE 9.40 usec  
TE 292.7 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300093 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

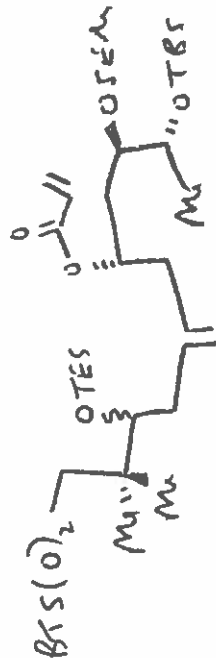


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169.51  
169.46  
167.10  
154.10  
143.30  
143.02  
138.20  
131.99  
130.09  
130.07  
129.30  
128.96  
128.95  
126.89  
123.79  
118.01  
117.72  
97.68  
97.56  
80.41  
80.16  
80.06  
80.00  
78.80  
78.69  
78.49  
78.17  
70.93  
70.73  
70.02  
69.99  
66.67  
66.64  
62.14  
43.35  
43.27  
42.14  
42.11  
40.99  
40.65  
34.67  
33.84  
31.76  
31.15  
27.26  
26.12  
24.74  
24.66  
19.47  
18.28

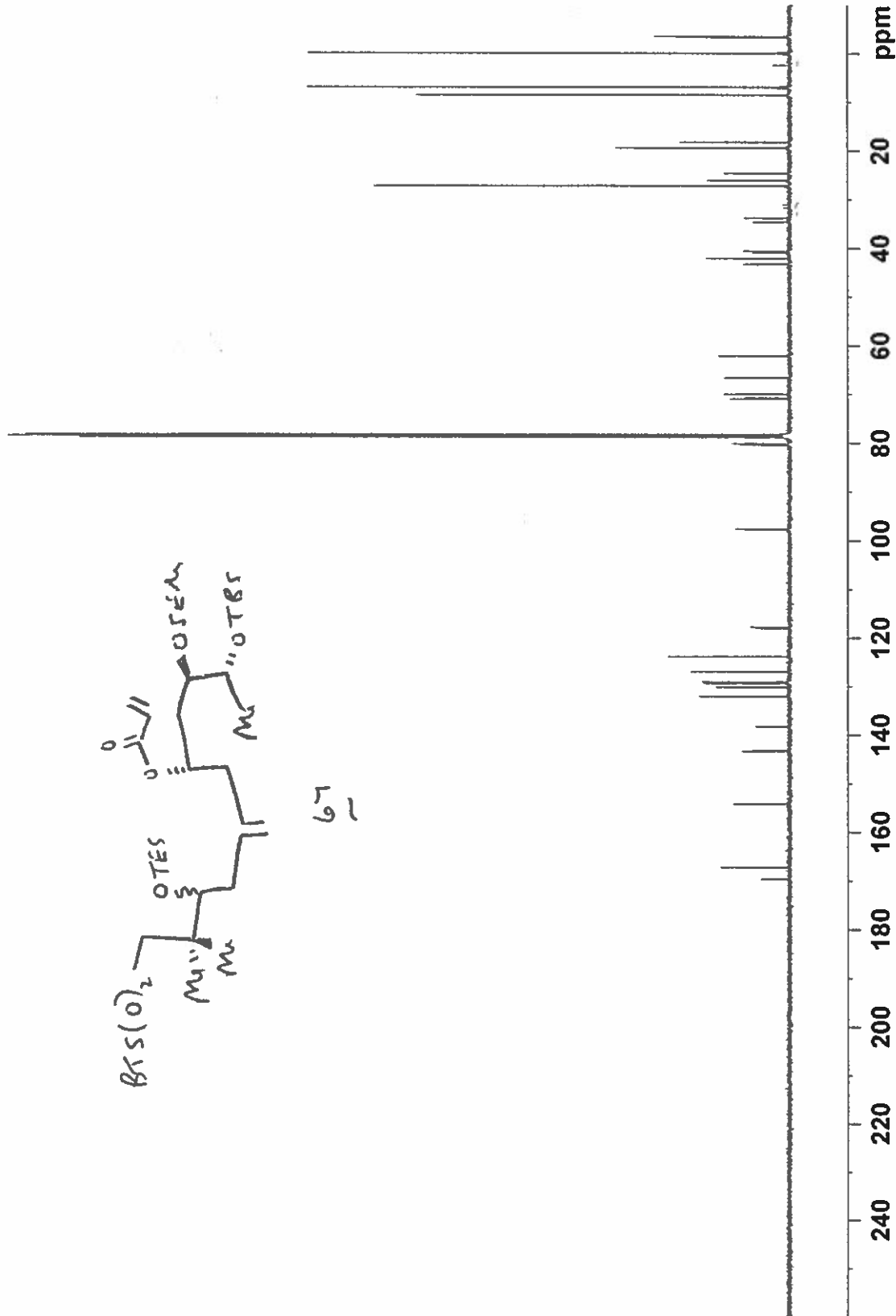


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NAME 2009-02-18-ejt-1  
EXPNO 12  
PROCNO 1  
Date\_ 20090219  
Time\_ 2.22  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1200  
DS 2  
SWH 30241.936 Hz  
FIDRES 0.461455 Hz  
AQ 1.0835786 sec  
RG 512  
DW 16.533 usec  
DE 7.83 usec  
TE 293.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

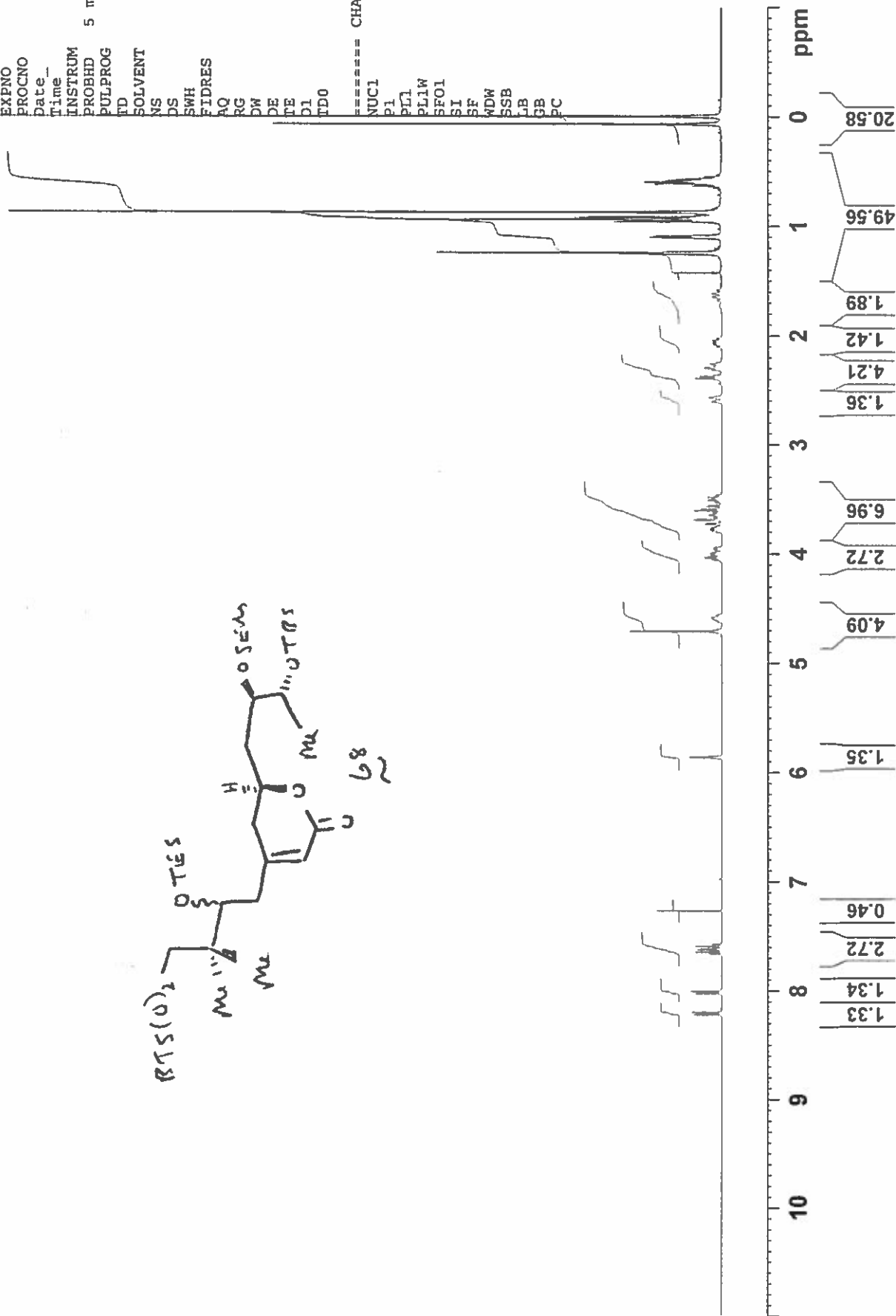
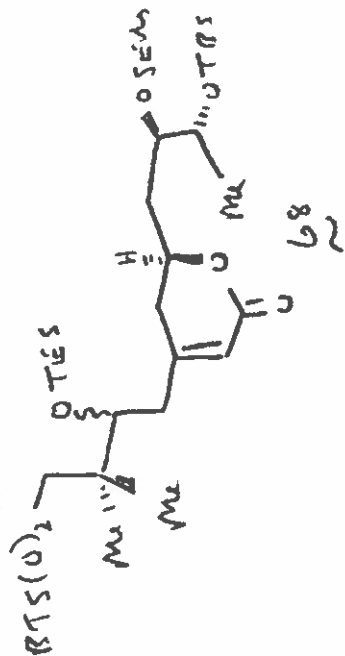
===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 34.91522217 W  
SFO1 100.6241042 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.60 dB  
PL12 15.31 dB  
PL13 18.00 dB  
PL2W 17.83863831 W  
PL12W 0.22927761 W  
PL13W 0.12341322 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6126241 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



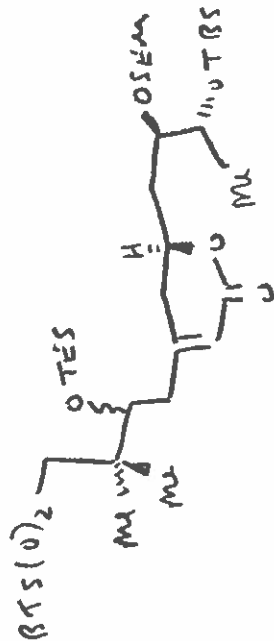
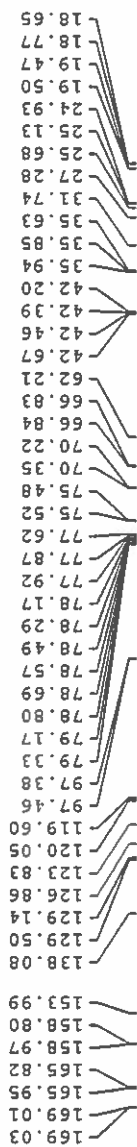


2009-02-20-ejt-13  
NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20090220  
Time 10.50  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 64  
DW 60.500 usec  
DE 9.40 usec  
TE 292.5 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
BF01 400.1324710 MHz  
SI 32768  
SF 400.1300066 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



apgmetathesis

mCARBON CDCl3 {e:\bruk400data\2009\Feb} ejt 5



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```

NAME      2009-02-20-ejt-5
EXPNO     11
PROCNO     1
Date_      20090220
Time_      10.09
INSTRUM    AV400
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD          65536
SOLVENT     CDCl3
NS          256
DS          2
SMH         30241.936 Hz
FIDRES     0.461455 Hz
AQ          1.0835786 sec
RG          512
DW          16.533 usec
DE          7.83 usec
TE          293.0 K
D1          2.0000000 sec
D11         0.0300000 sec
TD0         1

===== CHANNEL f1 =====
NUC1       13C
P1          8.00 usec
PL1         0.00 dB
PL1W        34.91522217 W
SFO1        100.6241042 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       90.00 usec
PL2         -3.60 dB
PL12        15.31 dB
PL13        18.00 dB
PL2W        17.83863831 W
PL12W       0.22927761 W
PL13W       0.12341322 W
SFO2        400.1316005 MHz
SI          32768
SF          100.6126258 MHz
WDW         EM
SSB          0
LB          1.00 Hz
GB          0
PC          0.20
  
```

240 220 200 180 160 140 120 100 80 60 40 20 ppm



2009-02-26-ejt-22\_01000007

VerticalScaleFactor = 1

0.025

0.020

0.015

0.010

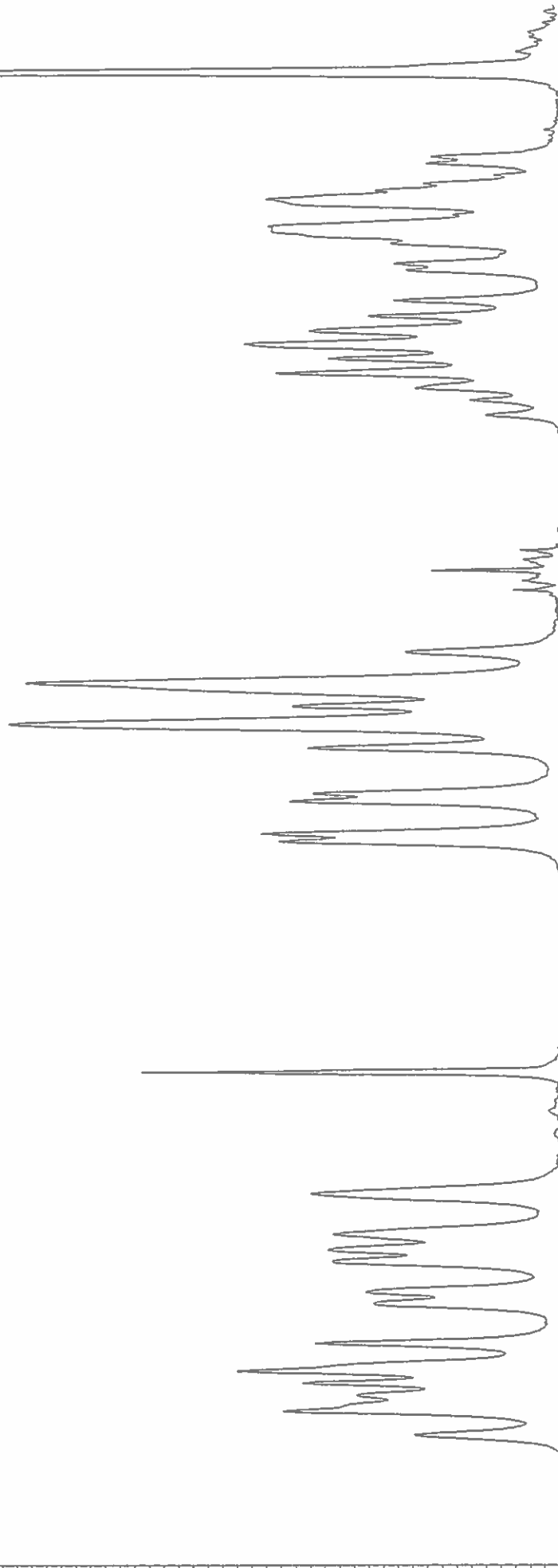
0.005

0

-0.005

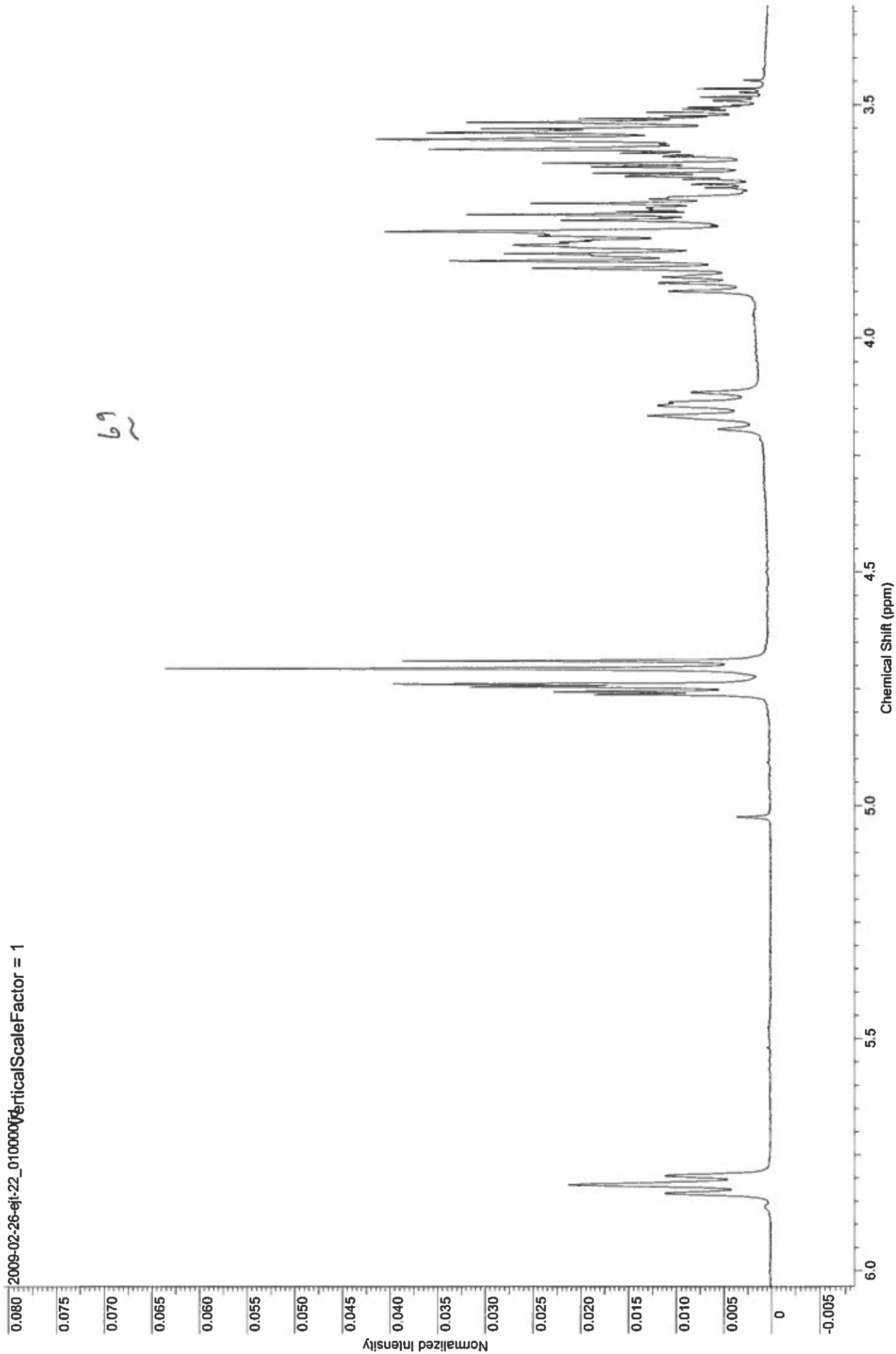
Normalized Intensity

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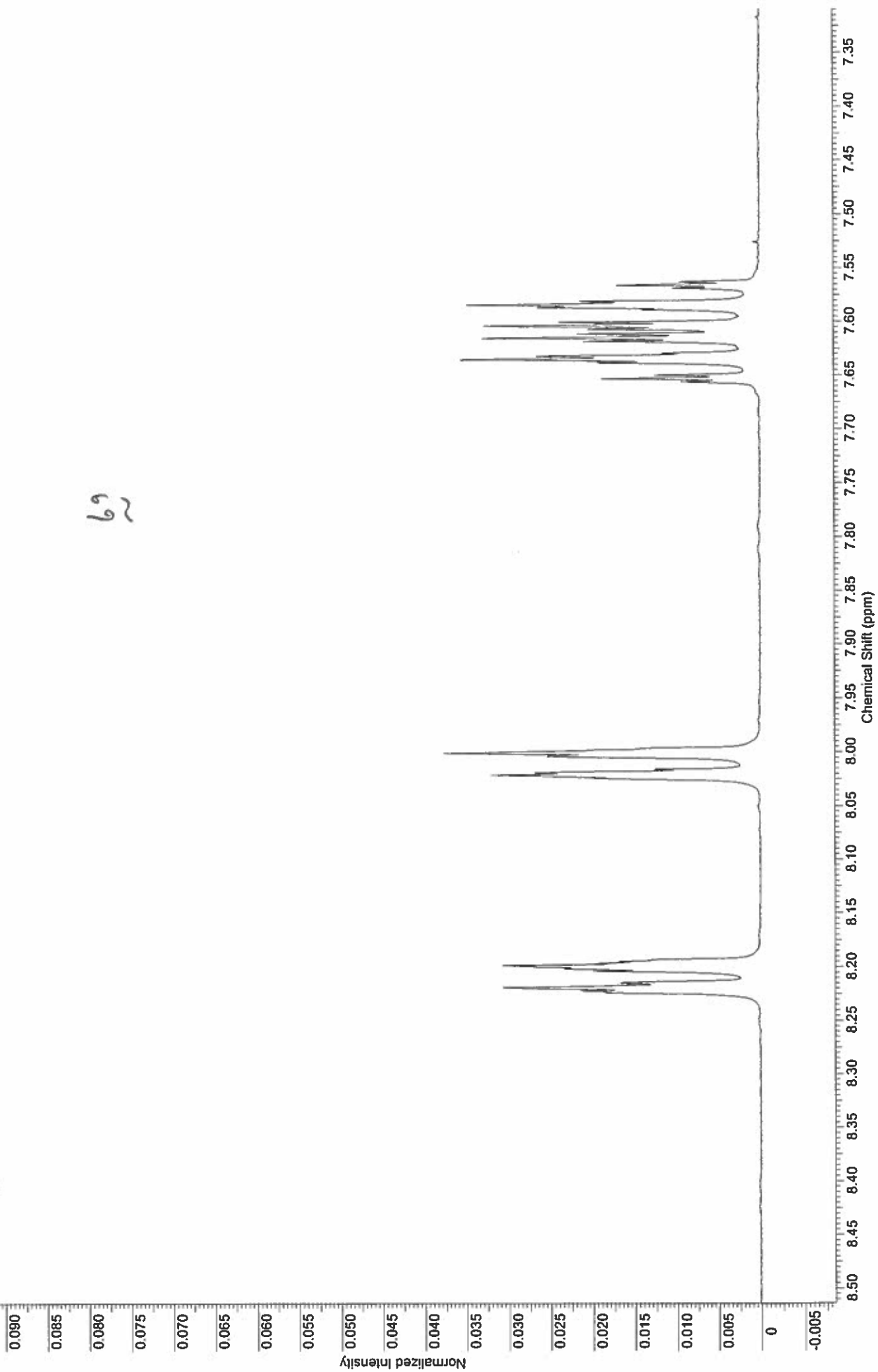


Chemical Shift (ppm)

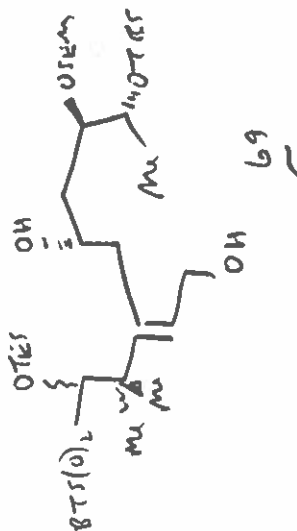
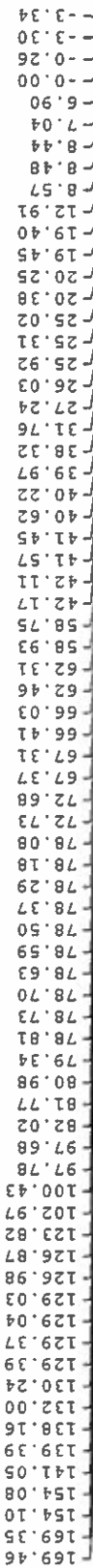
2009-02-26-ej-22\_010000VerticalScaleFactor = 1



2009-02-26-el-22\_0100000f VerticalScaleFactor = 1







```

NAME      2009-02-26-ejt-22
EXPNO     12
PROCNO     1
Date_      20090226
Time       9.06
INSTRUM    AV400
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT     CDCl3
NS         256
DS         2
SWH        30241.936 Hz
FIDRES     0.461455 Hz
AQ         1.0835786 sec
RG         512
DW         16.533 usec
DE         7.83 usec
TE         293.3 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         8.00 usec
PL1        0.00 dB
PL1W       34.91522217 W
SFO1       100.6241042 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -3.60 dB
PL12       15.31 dB
PL13       18.00 dB
PL2W       17.83863831 W
PL12W      0.22927761 W
PL13W      0.12341322 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6126235 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         0.20
    
```

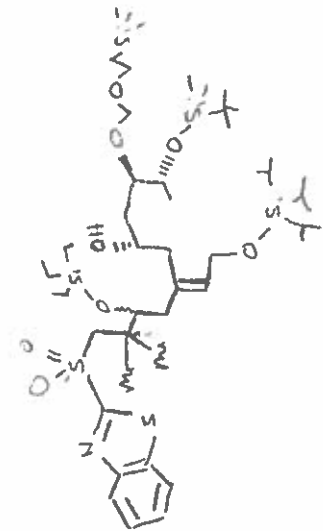
240 220 200 180 160 140 120 100 80 60 40 20 ppm



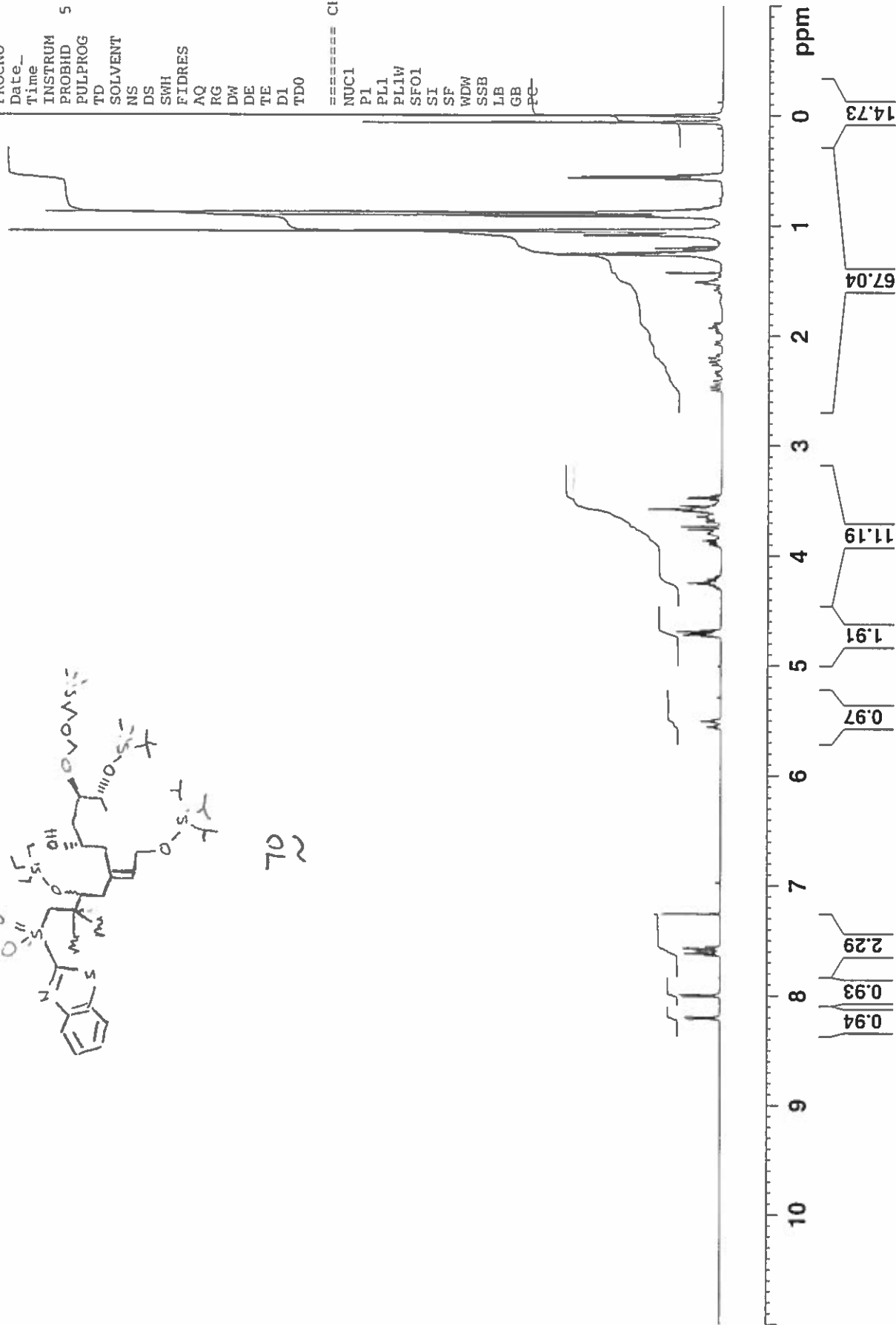
NAME 2009-02-27-ejt-11

EXPNO 10  
PROCNO 1  
Date\_ 20090227  
Time 18.43  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCI3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 40.3  
DW 48.400 usec  
DE 13.38 usec  
TE 295.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300125 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

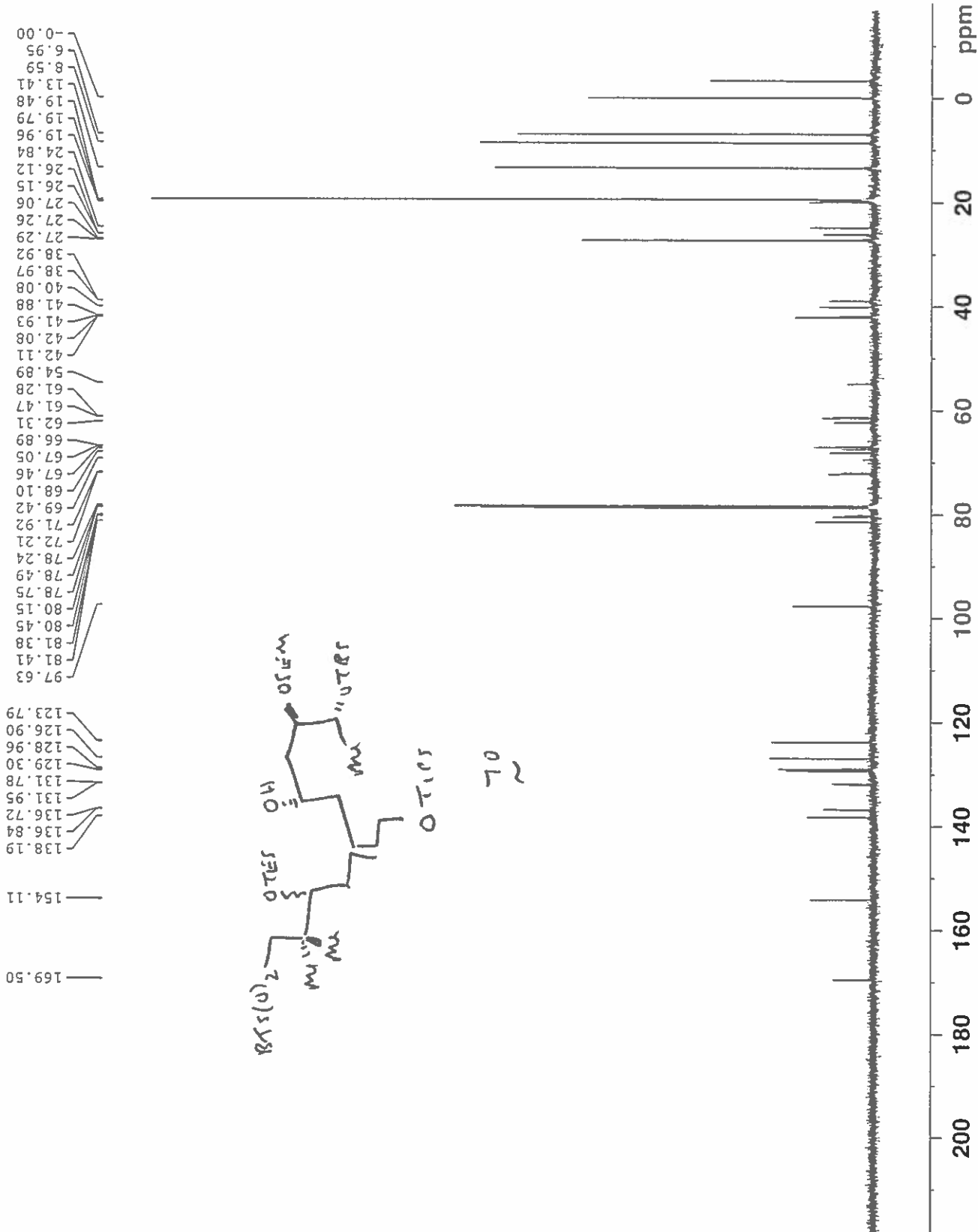


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apgtipsprot

mCARBON CDC13 /opt/bruk500data/2009/Feb ejt 17



```

NAME      2009-03-02-ejt-17
EXPNO     11
PROCNO    1
Date_     20090302
Time      8.07
INSTRUM   spect
PROBHD    5 mm TXI 1H/D-
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         256
DS         2
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010548 sec
RG         512
DW         16.800 usec
DE         32.21 usec
TE         294.1 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         11.50 usec
PL1        -4.20 dB
PL1W       218.02882385 W
SFO1       125.7703643 MHz

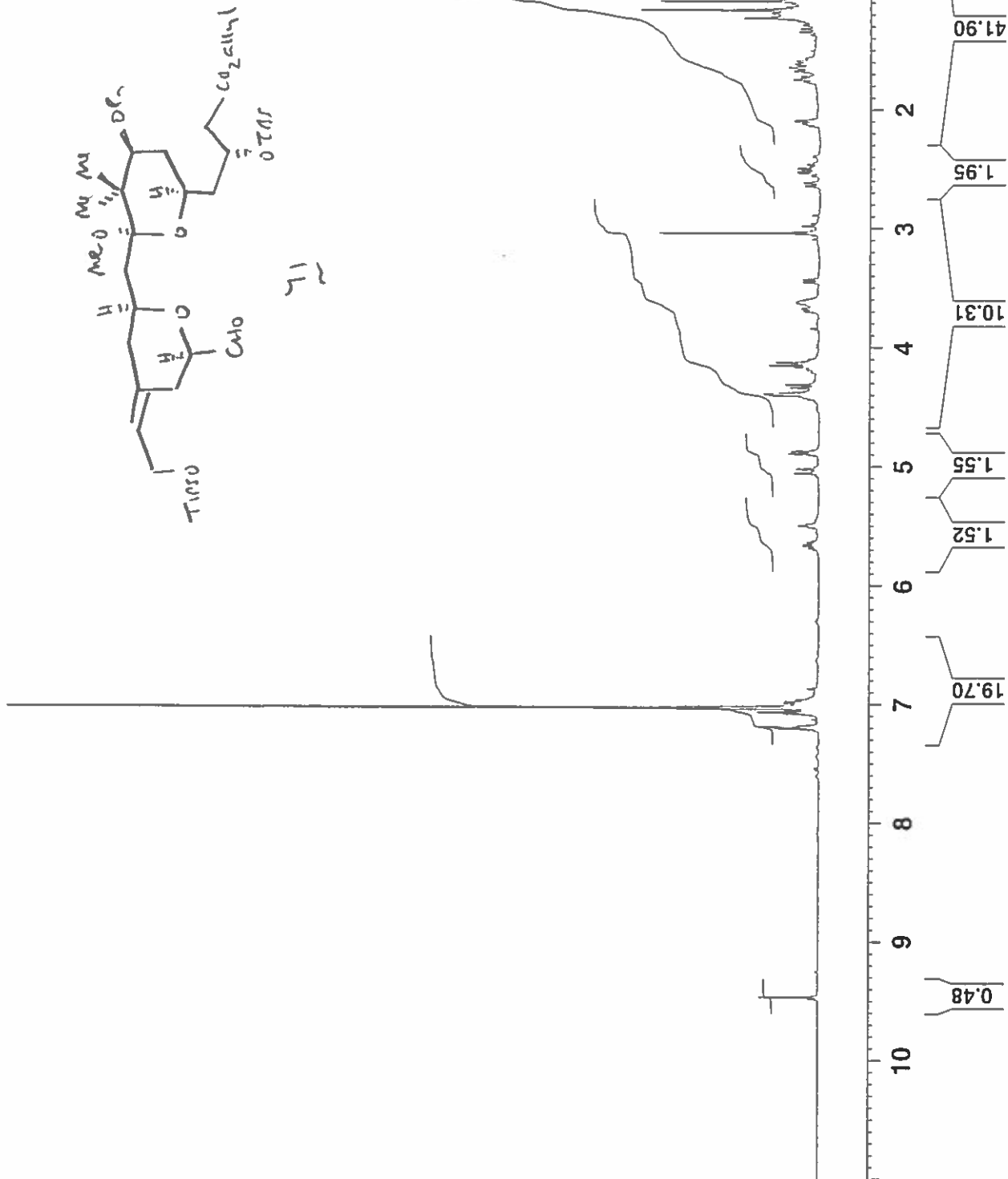
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        4.20 dB
PL12       23.99 dB
PL13       23.00 dB
PL12W      9.74092484 W
PL12W      0.10223514 W
PL13W      0.12841040 W
SFO2       500.1320005 MHz
SI         32768
SF         125.7576075 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

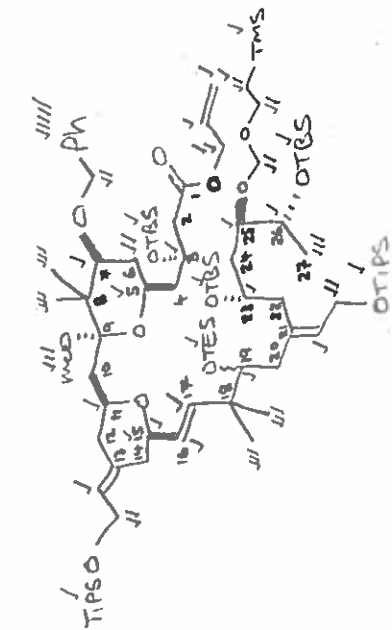
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NAME 2009-06-01-ejt-44  
EXPNO 10  
PROCNO 1  
Date\_ 20090601  
Time 14.49  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 144  
DW 48.400 usec  
DE 10.67 usec  
TE 291.5 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1301211 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

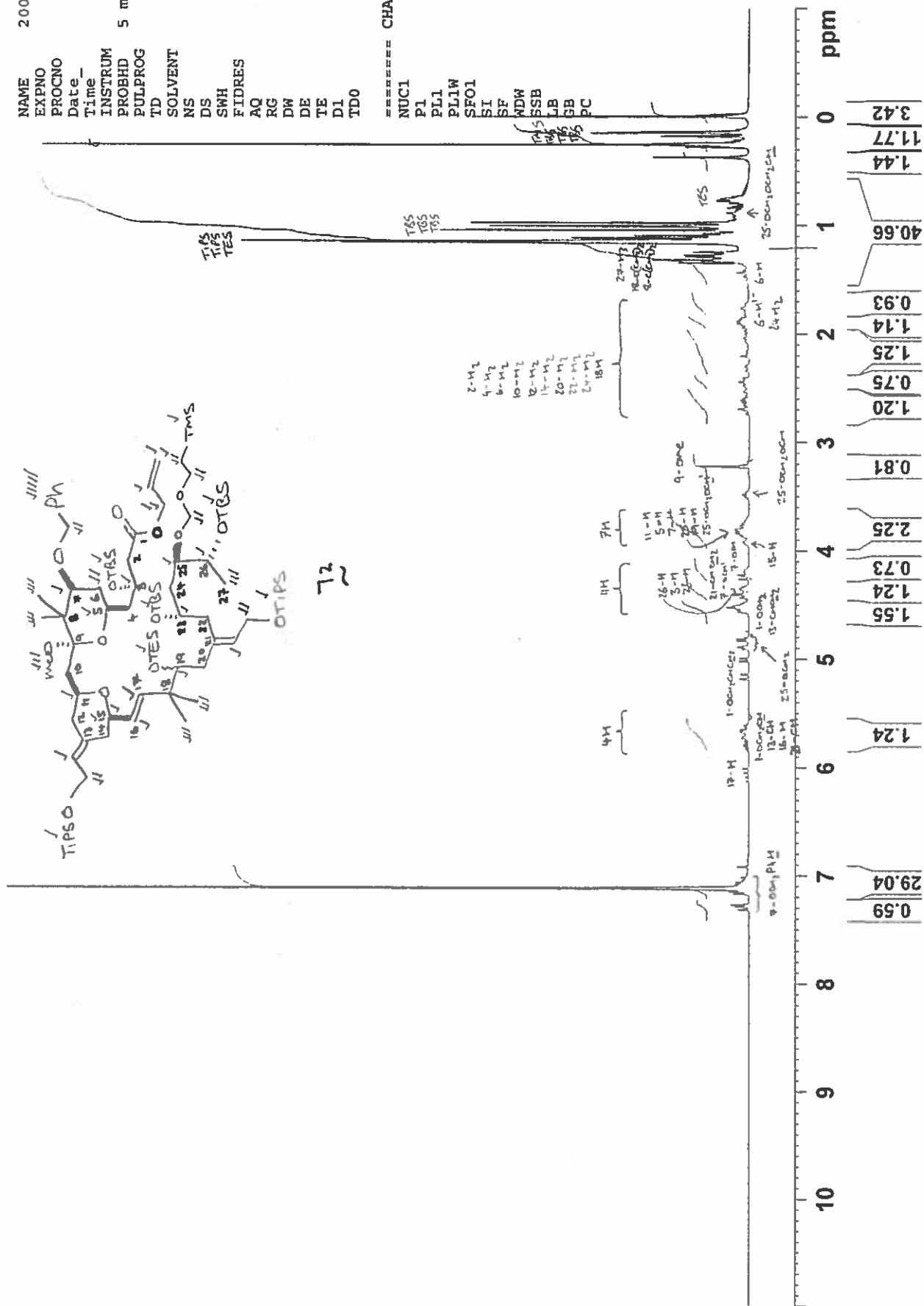




2009-06-11-ejt-8  
NAME  
EXPNO 10  
PROCNO 1  
Date 20090611  
Time 10.36  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 64  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 256  
DW 60.500 usec  
DE 9.40 usec  
TE 295.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300604 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

21  
11  
9  
9  
6  
9  
17  
6





NAME 2009-06-15-ejt-55  
EXPNO 10  
PROCNO 1

Date\_ 20090615  
Time 12.50

INSTRUM spect

PROBHD 5 mm TXI 1H/D-

PULPROG zg30b

TD 65536

SOLVENT C6D6

NS 64

DS 0

SWH 10330.578 Hz

FIDRES 0.157632 Hz

AQ 3.171923 sec

RG 161

DW 48.400 usec

DE 10.67 usec

TE 294.2 K

D1 1.00000000 sec

TD0 1

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

NUC1 1H

PL1 21.07 usec

PL1 3.25 dB

PL1W 12.12272263 W

SFO1 500.1330885 MHz

SI 32768

SF 500.1300802 MHz

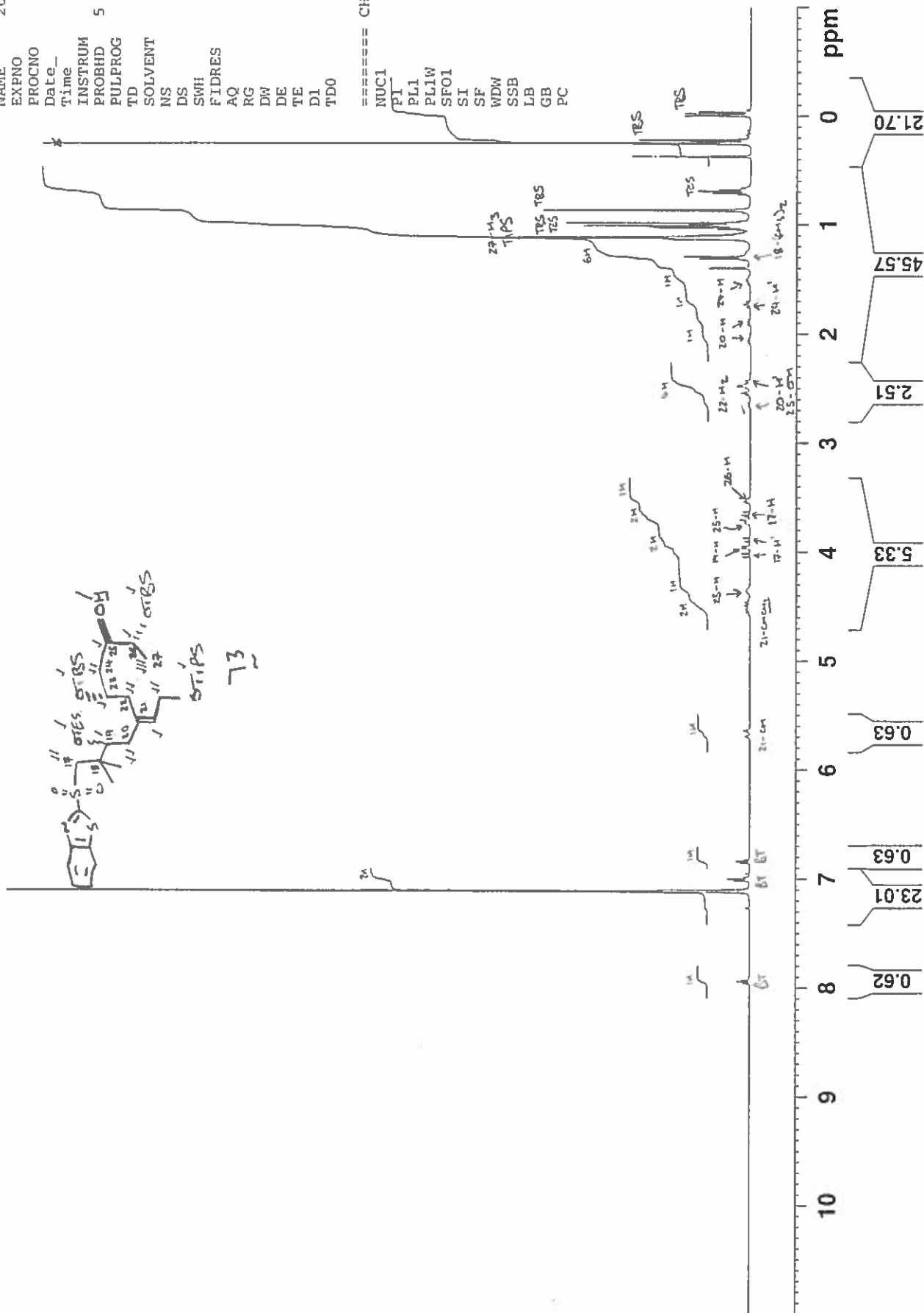
WDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.00



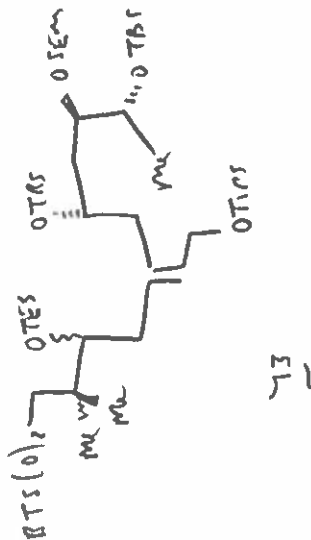
atilisulfone  
mCARBONnight

CDCl<sub>3</sub> {e:\bruk400data\2010\Mar} ejt 47



170.11  
167.04  
167.02  
151.63  
135.72  
132.44  
132.34  
130.39  
129.98  
126.82  
126.48  
124.41  
121.31

78.30  
77.98  
76.31  
75.99  
75.68  
71.05  
70.90  
67.83  
67.70  
59.83  
59.75  
59.44  
59.35  
39.62  
39.55  
39.44  
39.38  
39.32  
39.04  
38.11  
24.88  
24.80  
23.77  
23.63  
22.30  
22.26  
20.02  
18.86  
17.00  
16.65



NAME 2010-03-10-ejt-47  
EXPNO 11  
PROCNO 1  
Date 20100311  
Time 20.37  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 1024  
DS 2  
SWH 30241.936 Hz  
FIDRES 0.461455 Hz  
AQ 1.0835786 sec  
RG 512  
DW 16.533 usec  
DE 7.83 usec  
TE 296.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

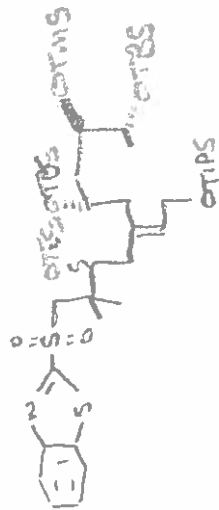
===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 34.91522217 W  
SFO1 100.6241042 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.60 dB  
PL12 15.31 dB  
PL13 18.00 dB  
PL2W 17.83863831 W  
PL12W 0.22927761 W  
PL13W 0.12341322 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6128724 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

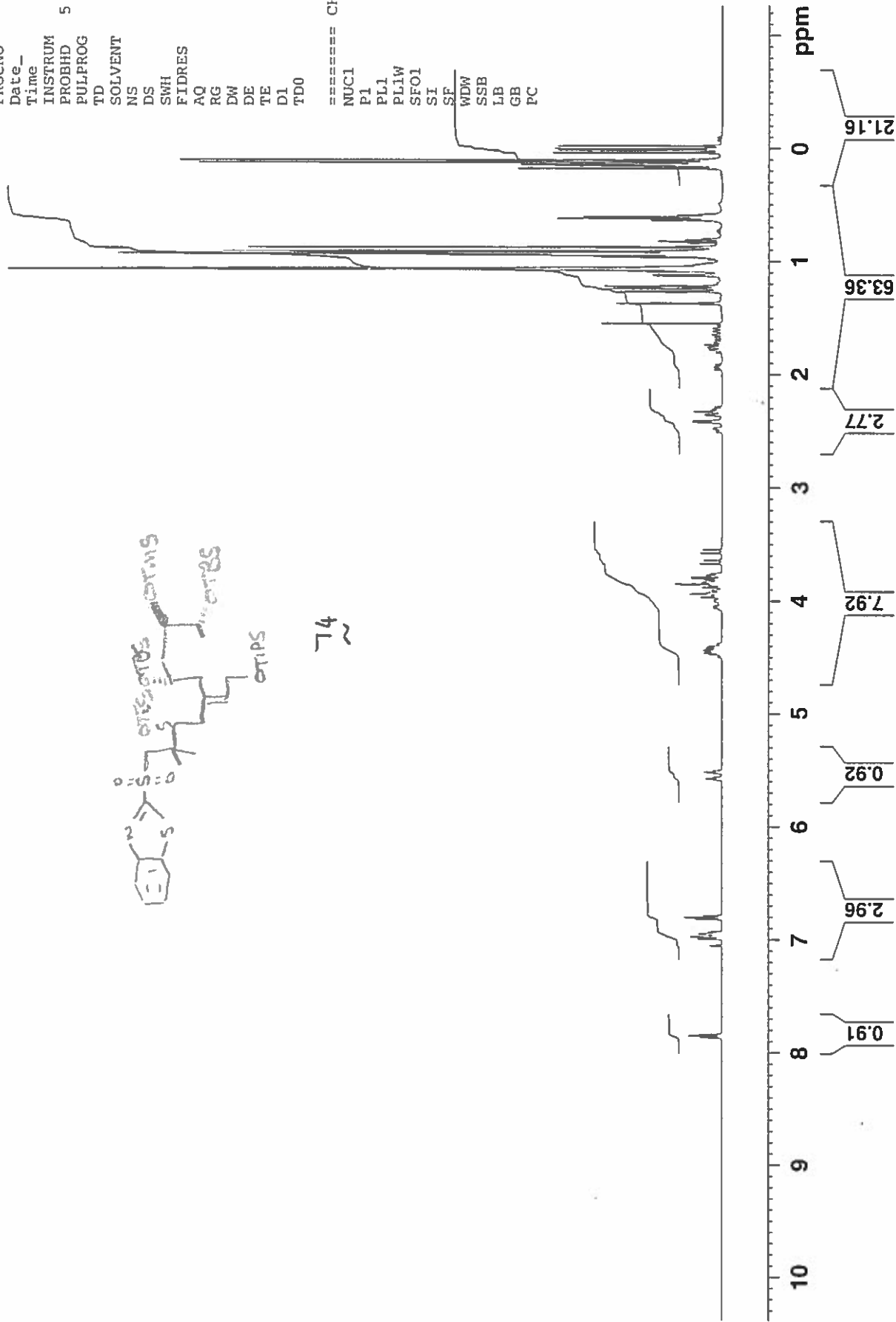
240 220 200 180 160 140 120 100 80 60 40 20 ppm



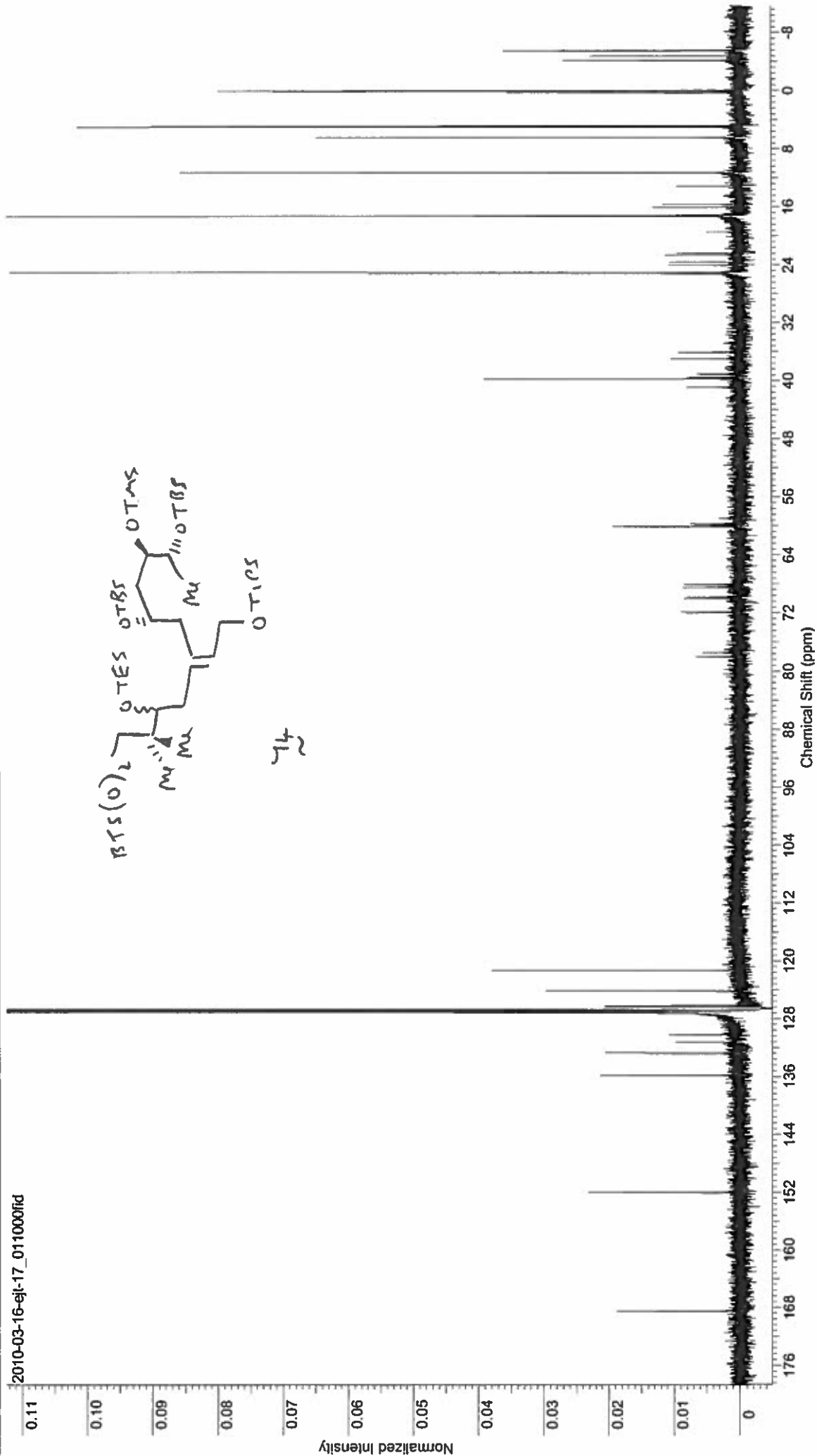
NAME 2010-03-16-ejt-17  
EXPNO 14  
PROCNO 1  
Date\_ 20100317  
Time 2.40  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 32  
DW 48.400 usec  
DE 10.67 usec  
TE 296.6 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1301092 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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2009-07-23-ejt-36

NAME  
EXPNO 10  
PROCNO 1

Date\_ 20090723  
Time 9.32

INSTRUM AV400

PROBHD 5 mm PABBO BB-

PULPROG zg30b

TD 65536

SOLVENT C6D6

NS 64

DS 0

SWH 8264.463 Hz

FIDRES 0.126106 Hz

AQ 3.9649780 sec

RG 256

DW 60.500 usec

DE 9.40 usec

TE 293.3 K

D1 1.0000000 sec

TD0 1

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

NUC1 1H

P1 10.00 usec

PL1 -3.60 dB

PL1W 17.83863831 W

SFO1 400.1324710 MHz

SI 32768

SF 400.1300903 MHz

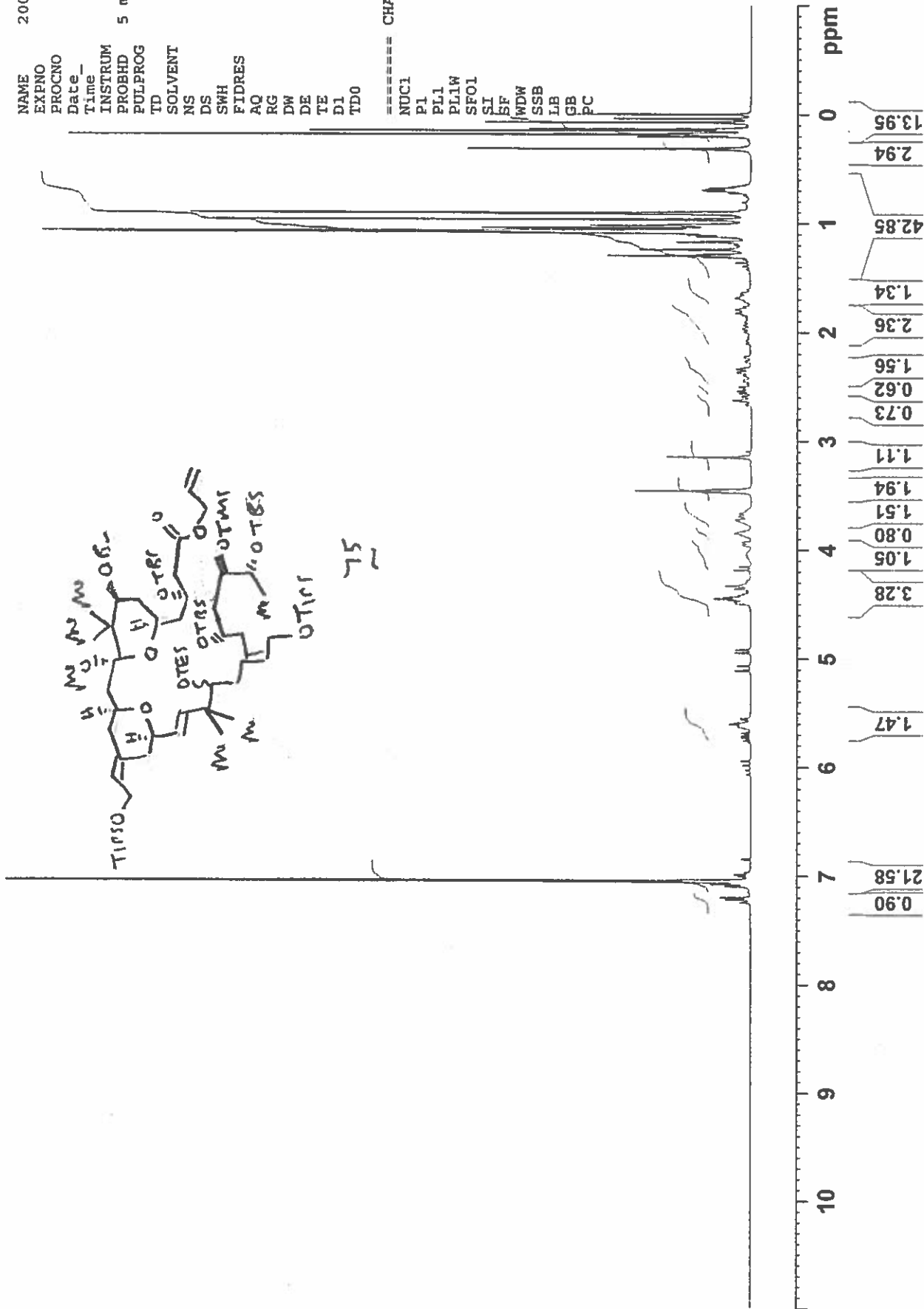
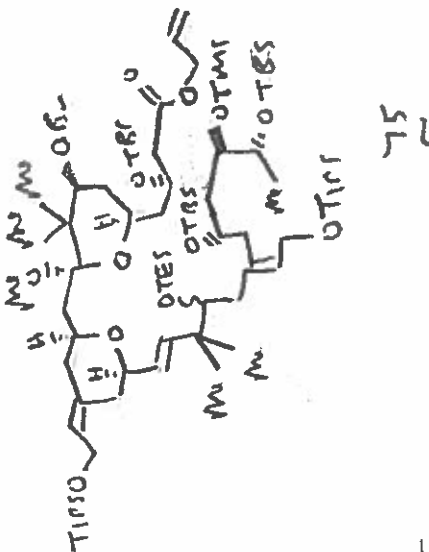
WDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.00

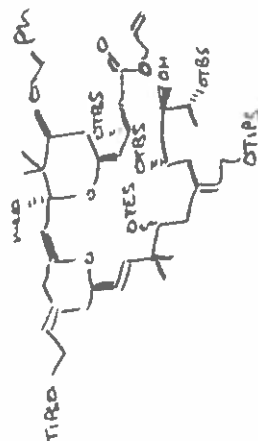




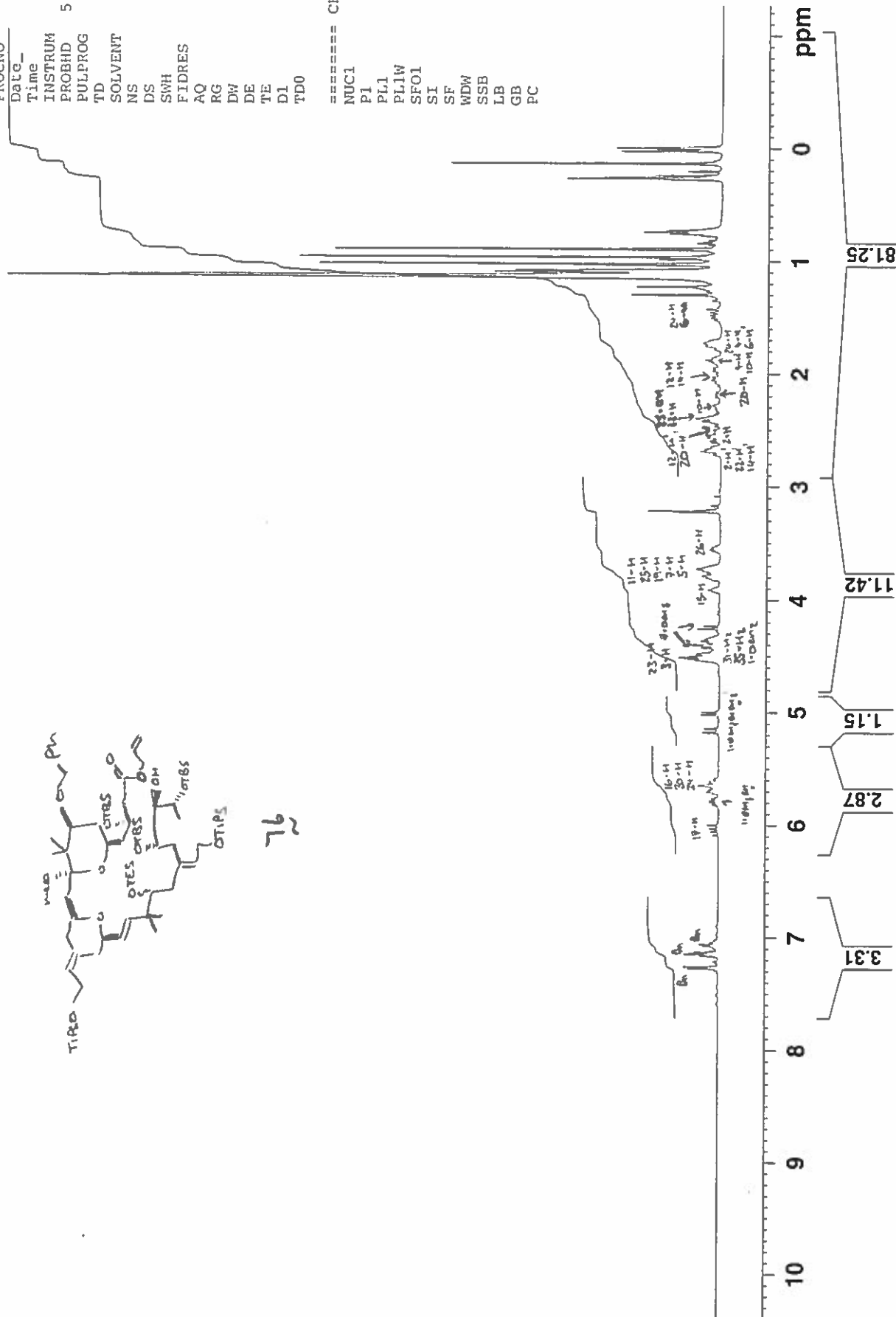
NAME 2010-04-11-ejt-5  
EXPNO 10  
PROCNO 1

Date\_ 20100411  
Time 15.30  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 16  
DW 48.400 usec  
DE 10.67 usec  
TE 297.3 K  
D1 1.00000000 sec  
TD0 1

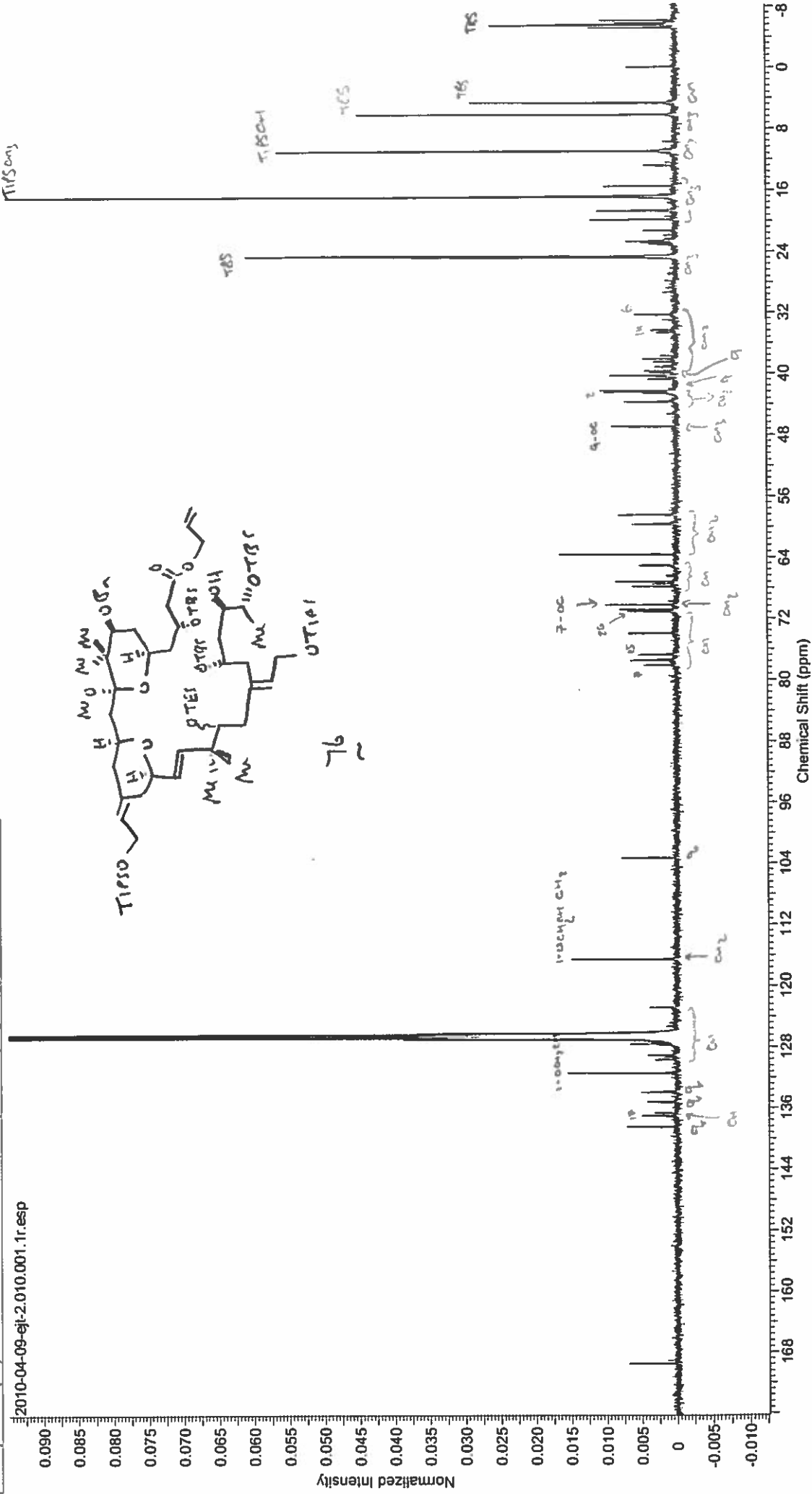
===== CHANNEL f1 =====  
NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300715 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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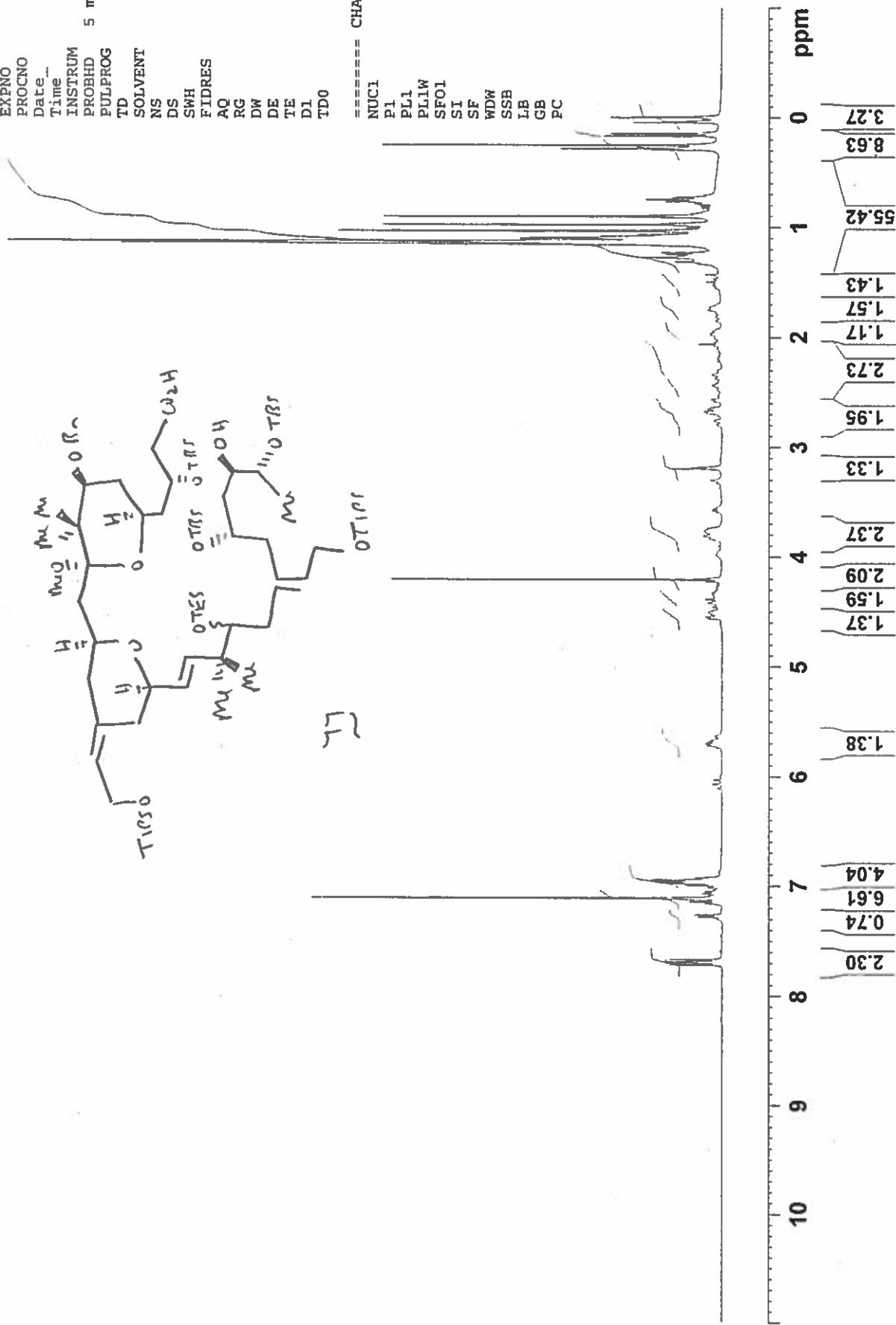
Acquisition Time (sec)	1.0835	Comment	alljuliac25ch mCARBONnight C6D6 (e:\bruk400data\2010\Apr) ejt 2	Date	10 Apr 2010 06:49:52
Date Stamp	10 Apr 2010 06:49:52				
File Name	C:\Documents and Settings\j\My Documents\Alan\Chem Comm\Julia C25OH\2010-04-09-ejt-2\110\pdata\111r				
Nucleus	13C	Number of Transients	3072	Origin	AV400
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	BENZENE-d6	Spectrum Offset (Hz)	11219.2842
Sweep Width (Hz)	30241.01	Temperature (degree C)	22.800	Spectrum Type	STANDARD





NAME 2009-08-27-ejt-47  
EXPNO 10  
PROCNO 1  
Date\_ 20090827  
Time 13.53  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 64  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 322  
DW 60.500 usec  
DE 9.40 usec  
TE 293.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300640 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

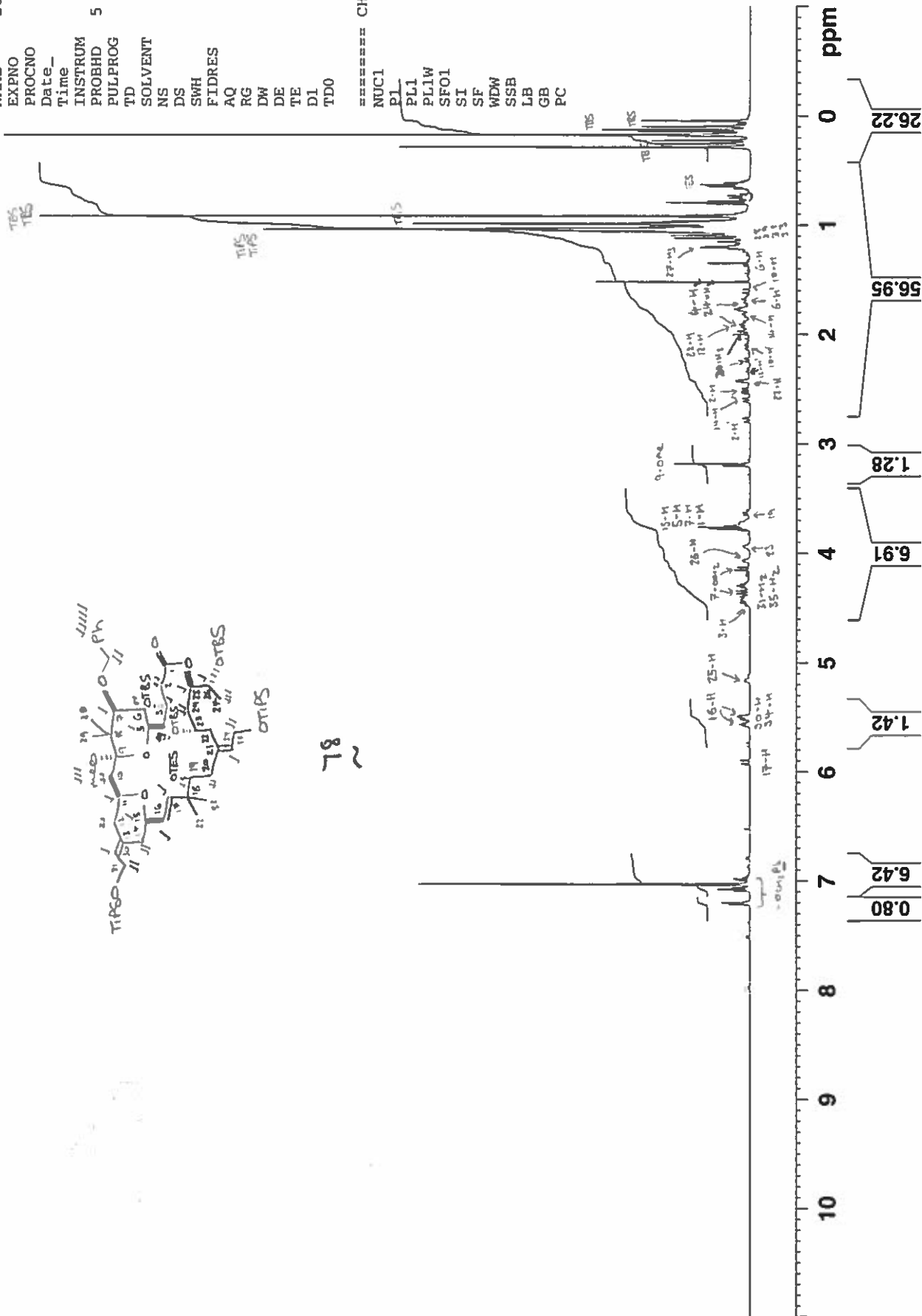




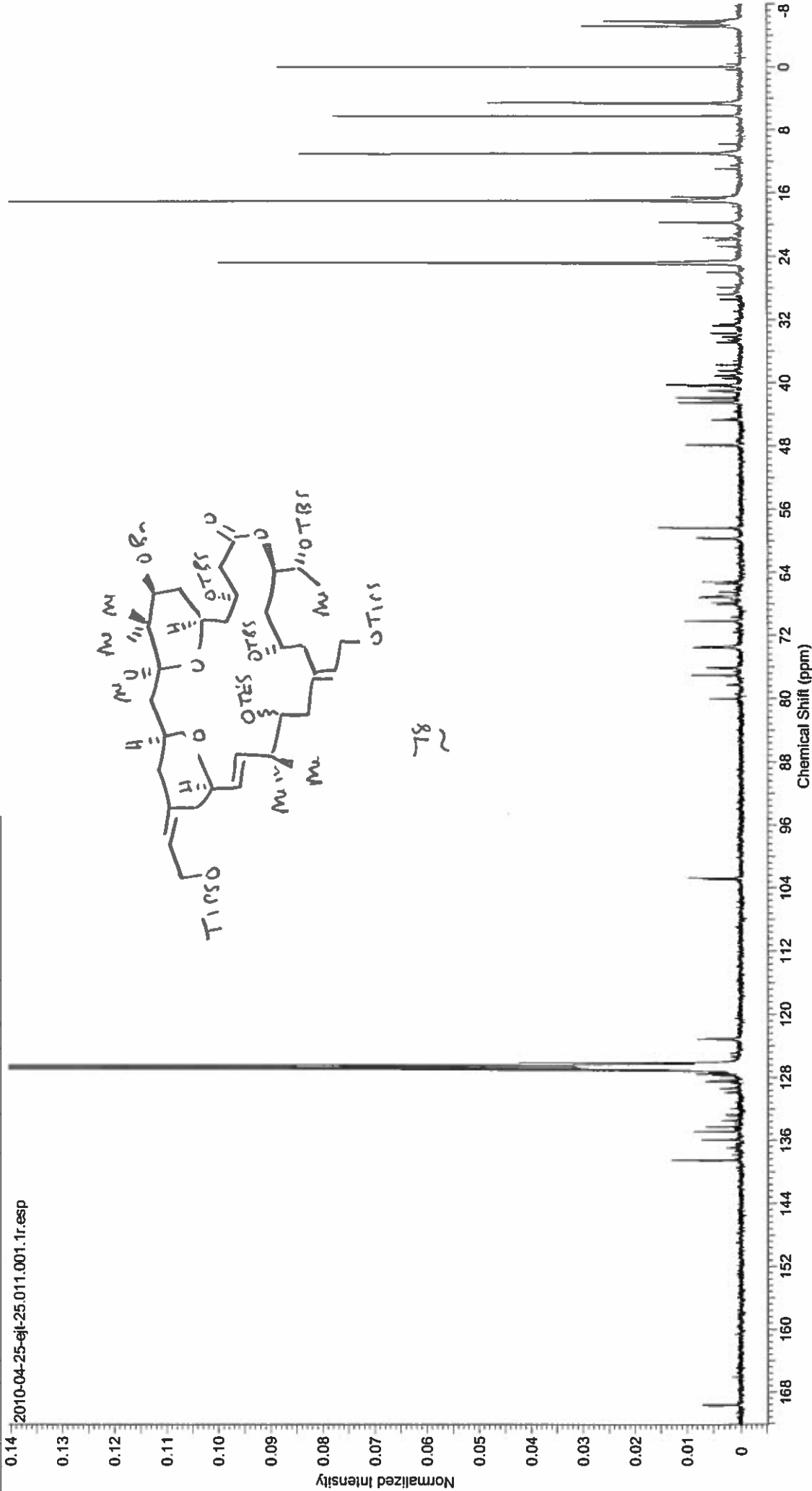
NAME 2009-08-07-ejt-11

EXPNO 10  
PROCNO 1  
Date\_ 20090807  
Time 10.47  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 64  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 322  
DW 48.400 usec  
DE 10.67 usec  
TE 293.3 K  
D1 1.00000000 sec  
TD0 1

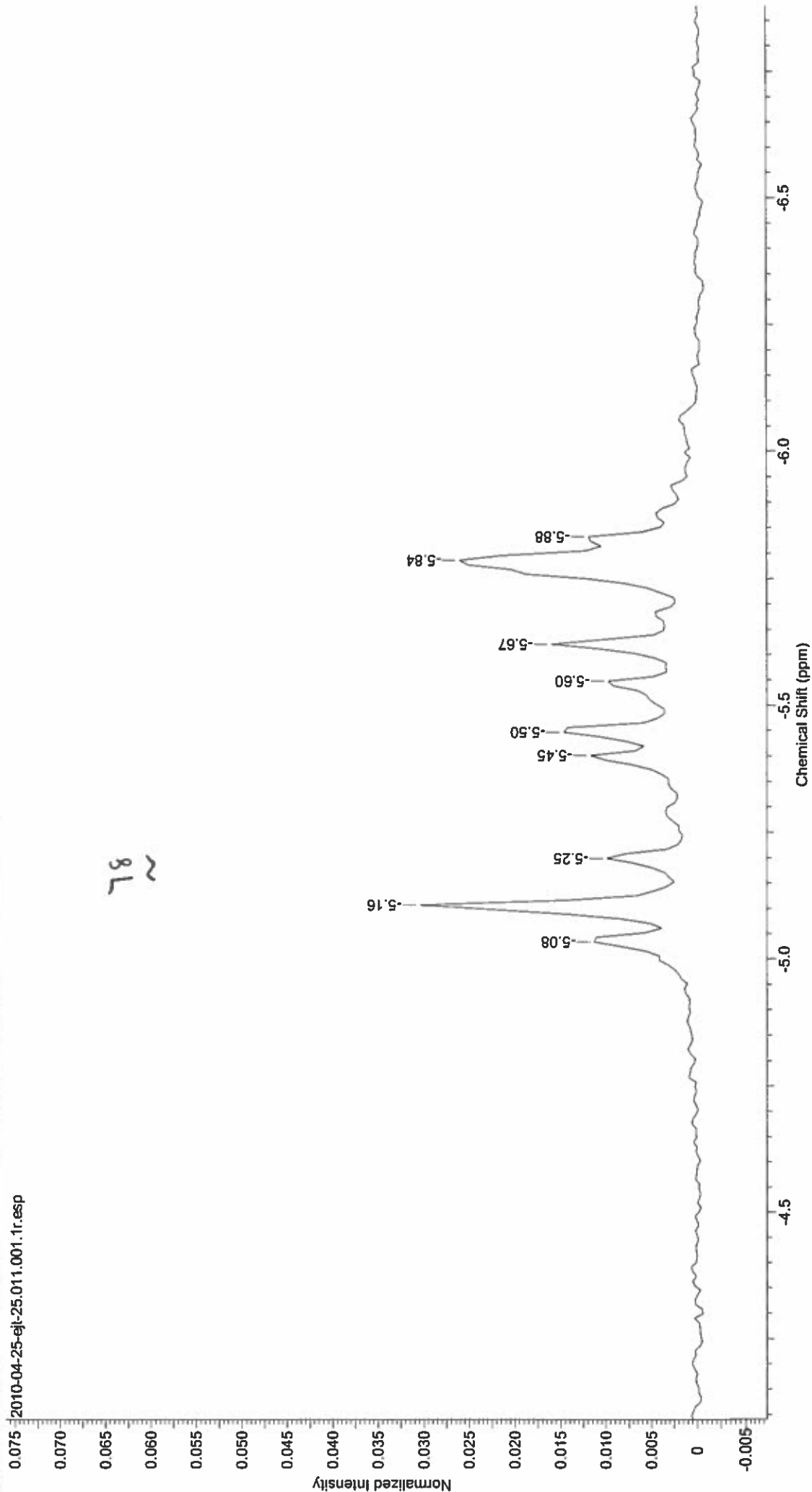
===== CHANNEL f1 =====  
NUC1 1H  
PL 21.07 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1301196 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Acquisition Time (sec)	1.0835	Comment	allyyamaguchi mCARBONnight C6D6 (e:\bruk400data\2010\Apr) ejt 25	Date	25 Apr 2010 18:59:28
Date Stamp	25 Apr 2010 18:59:28				
File Name	C:\Documents and Settings\ejt\My Documents\Alan\Chem Comm\Yamaguchi\2010-04-25-ejt-25\11\pdata\111r				
Nucleus	13C	Number of Transients	3072	Origin	AV400
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	BENZENE-d6	Spectrum Offset (Hz)	11221.0137
Sweep Width (Hz)	30241.01	Temperature (degree C)	22.100	Spectrum Type	STANDARD

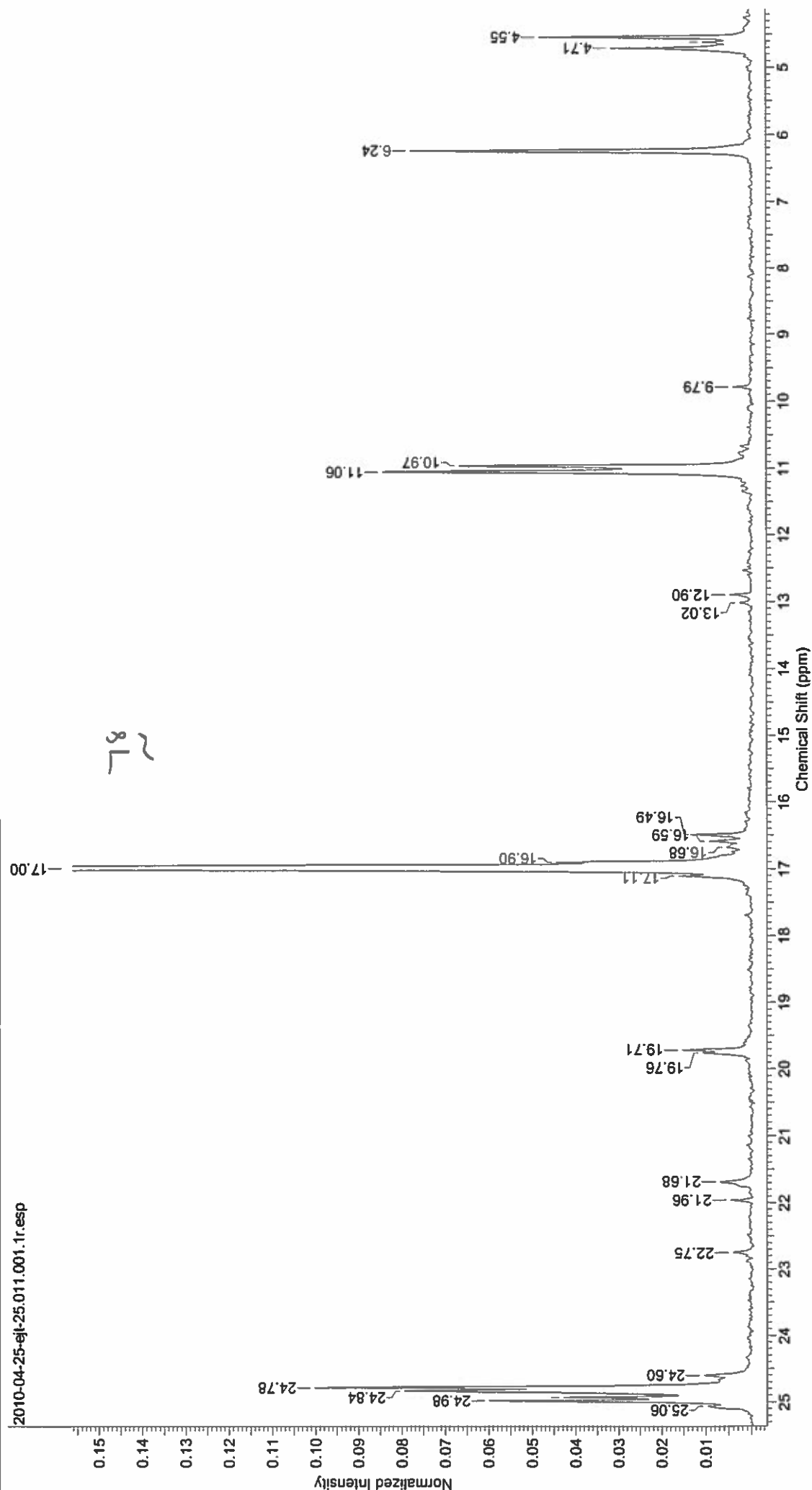


Acquisition Time (sec)	1.0835	Comment	allyyamaguchi mCARBONnight C6D6 (e:\bruk400data\2010\Apr) ejt 25	Date	25 Apr 2010 18:59:28
Date Stamp	25 Apr 2010 18:59:28				
File Name	C:\Documents and Settings\My Documents\Alan\Chem Comm\Yamaguchi\2010-04-25-ejt-25\11\data\11r				
Nucleus	13C	Number of Transients	3072	Origin	AV400
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	BENZENE-d6	Spectrum Offset (Hz)	11221.0137
Sweep Width (Hz)	30241.01	Temperature (degree C)	22.100	Spectrum Type	STANDARD





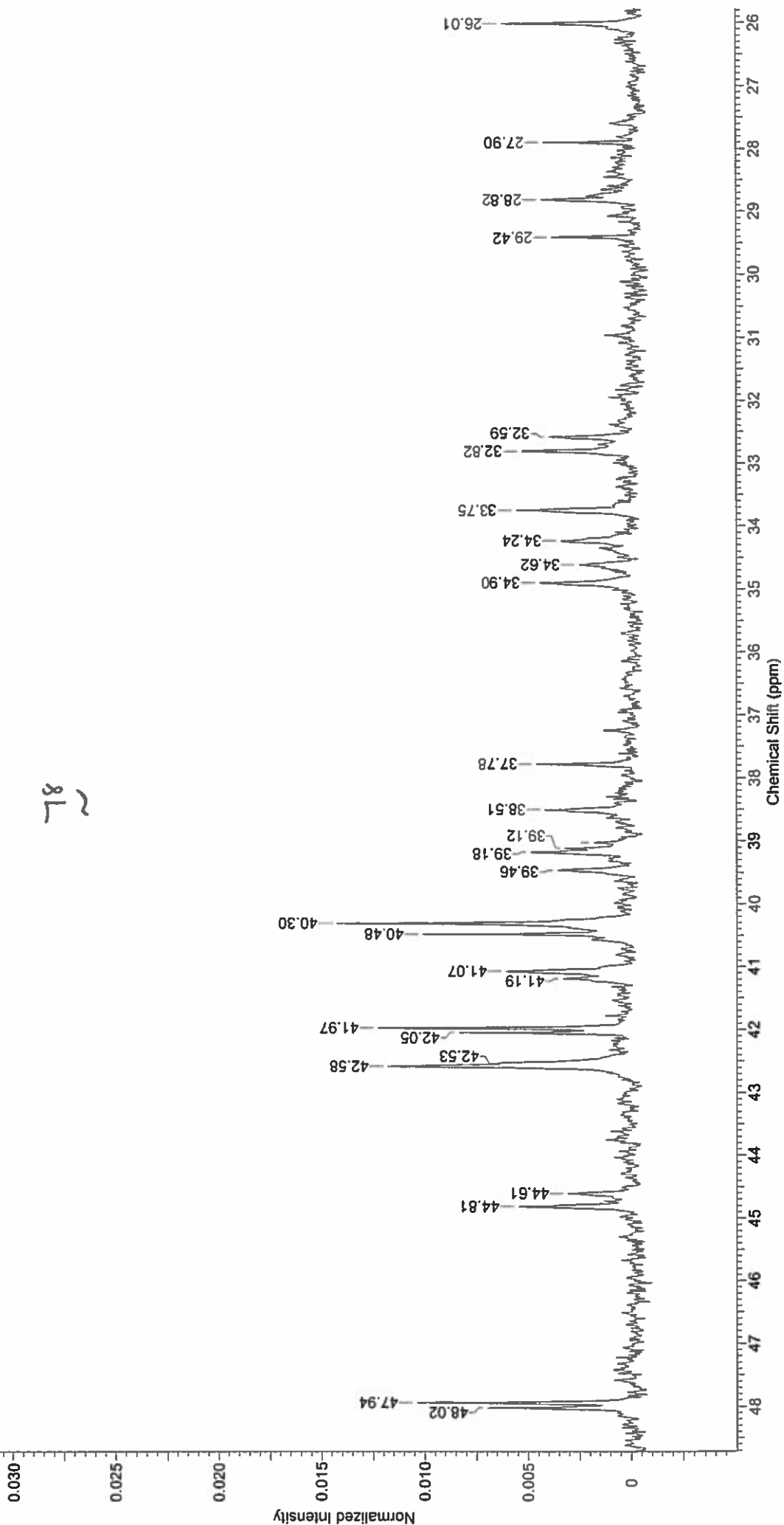
<b>Acquisition Time (sec)</b>	1.0835	<b>Comment</b>	allyyamaguchi mCARBONnight C6D6 (e:\bruk400data\2010\Apr) ejt 25	<b>Date</b>	25 Apr 2010 18:59:28
<b>Date Stamp</b>	25 Apr 2010 18:59:28				
<b>File Name</b>	C:\Documents and Settings\ejt\My Documents\Alan\Chem Communi\Yamaguchi\2010-04-25-ejt-25\11\data\11r				
<b>Nucleus</b>	13C	<b>Number of Transients</b>	3072	<b>Origin</b>	AV400
<b>Owner</b>	Administrator	<b>Points Count</b>	32768	<b>Pulse Sequence</b>	zgpg30
<b>SW(cyclical) (Hz)</b>	30241.94	<b>Solvent</b>	BENZENE-d6	<b>Spectrum Offset (Hz)</b>	11221.0137
<b>Sweep Width (Hz)</b>	30241.01	<b>Temperature (degree C)</b>	22.100	<b>Spectrum Type</b>	STANDARD



12/08/2010 14:13:01

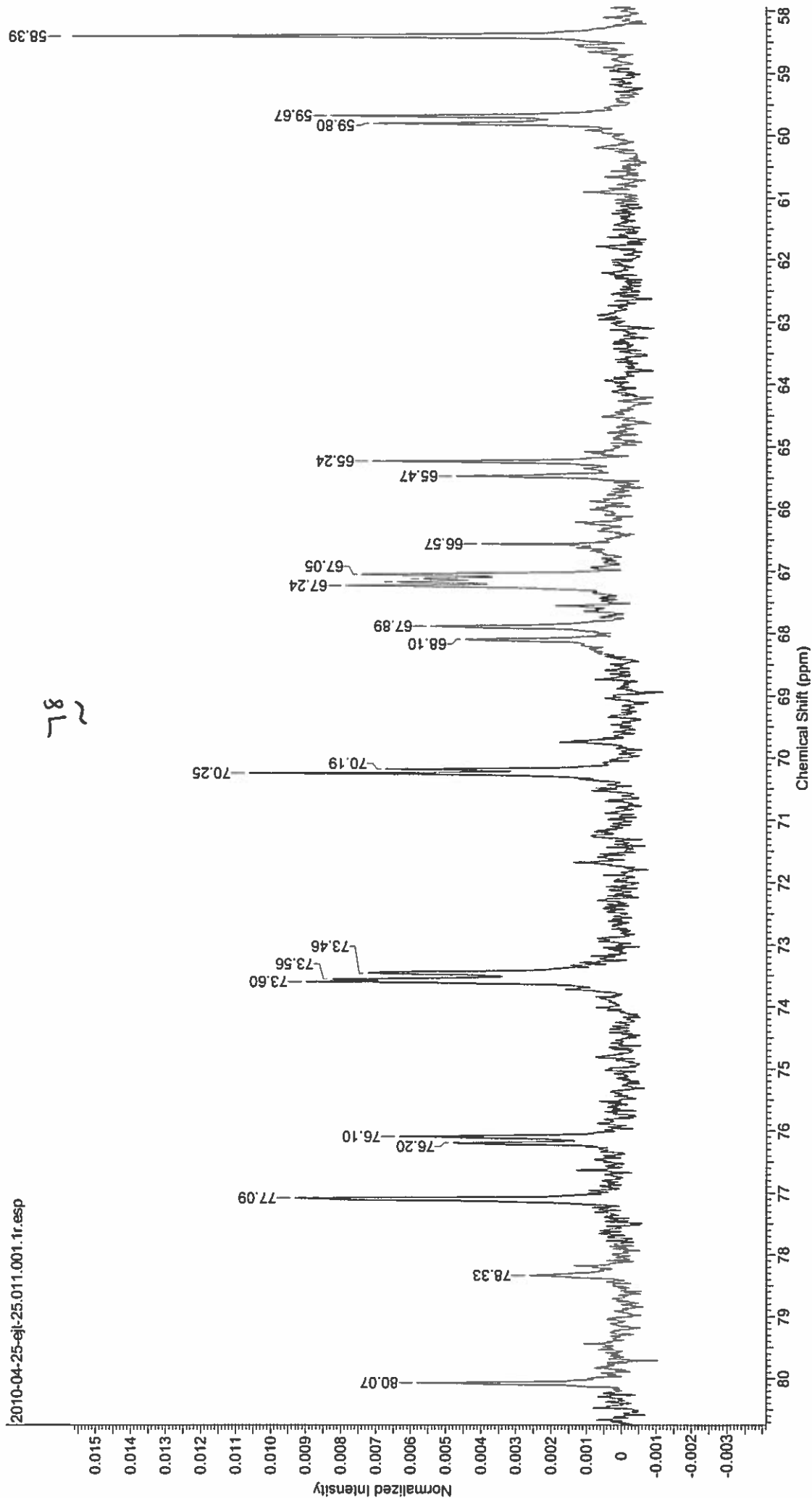
Acquisition Time (sec)	1.0835	Comment	atl-yamaguchi mCARBONnight C6D6 (e:\bruk400data\2010\Apr) ejl 25	Date	25 Apr 2010 18:59:28
Date Stamp	25 Apr 2010 18:59:28				
File Name	C:\Documents and Settings\lej\My Documents\Alan\Chem Comm\unYamaguchi\2010-04-25-ejl-25111\data\111r				
Nucleus	13C	Number of Transients	3072	Origin	AV400
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	BENZENE-d6	Spectrum Offset (Hz)	11221.0137
Sweep Width (Hz)	30241.01	Temperature (degree C)	22.100	Spectrum Type	STANDARD

2010-04-25-ejl-25.011.001.1r.esp



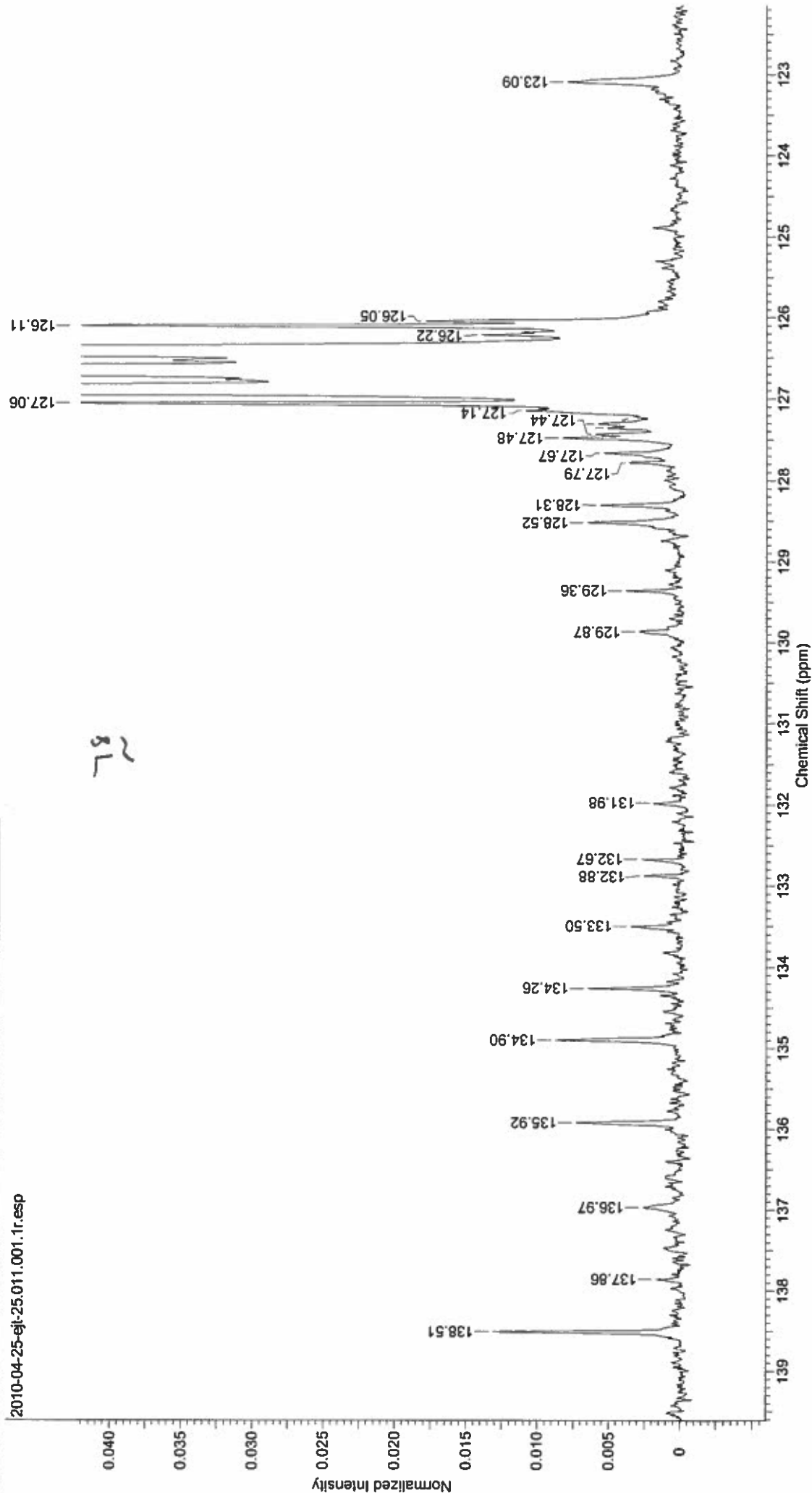
12/08/2010 14:15:32

Acquisition Time (sec)	1.0835	Comment	allyyamaguchi mCARBONight C6D6 (e:\bruk400data\2010\Apr) ejl 25	Date	25 Apr 2010 18:59:28
Date Stamp	25 Apr 2010 18:59:28				
File Name	C:\Documents and Settings\lej\My Documents\Alan\Chem Commun\Yamaguchi\2010-04-25-ejl-25111\data\11r				
Nucleus	13C	Number of Transients	3072	Origin	AV400
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	BENZENE-d6	Spectrum Offset (Hz)	11221.0137
Sweep Width (Hz)	30241.01	Temperature (degree C)	22.100	Spectrum Type	STANDARD

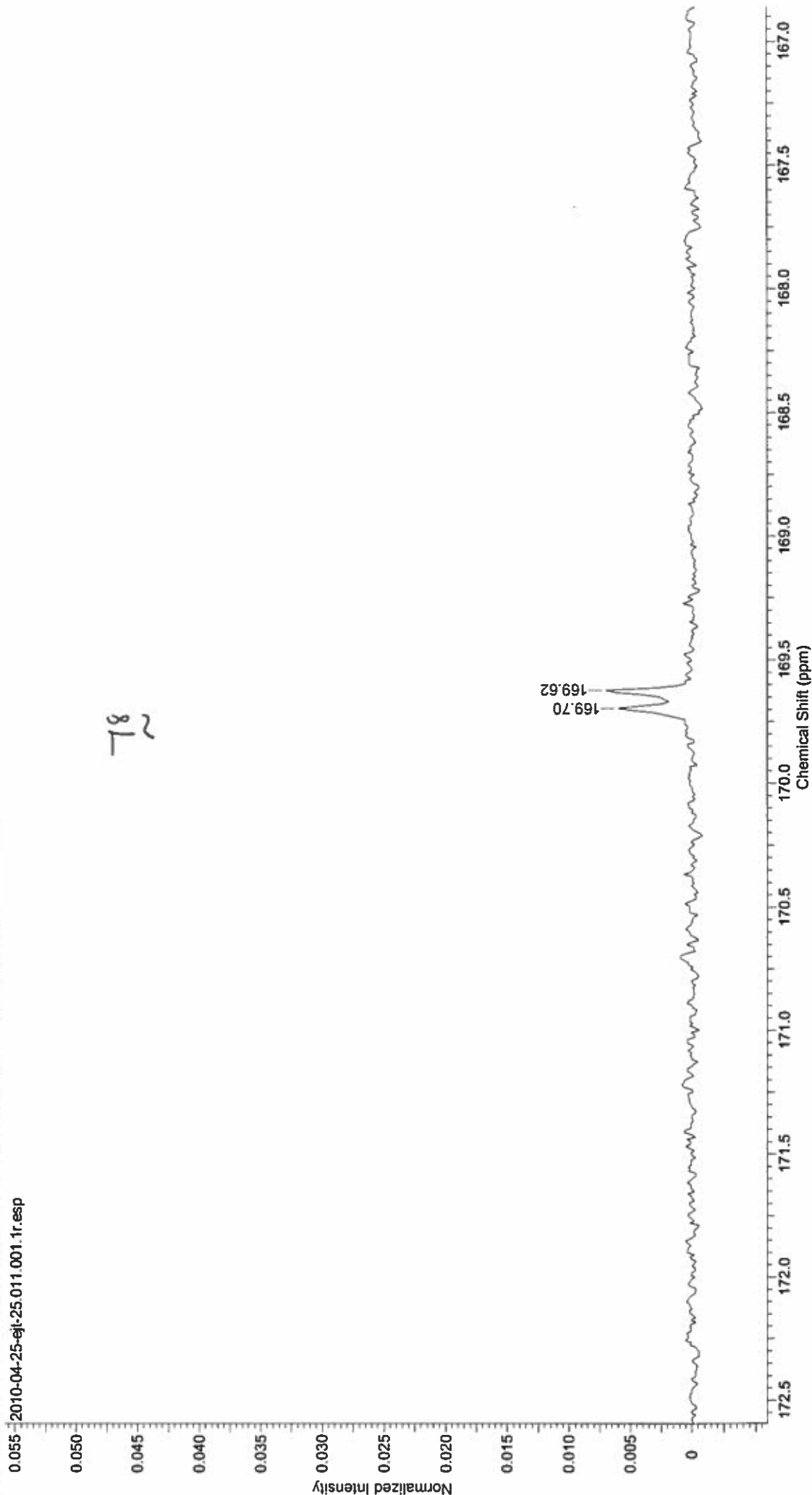


Acquisition Time (sec)	1.0835	Comment	allylamaguchi mCARBONnight C6D6 (e:\bruk400data\2010\Apr) ejt 25	Date	25 Apr 2010 18:59:28
Date Stamp	25 Apr 2010 18:59:28				
File Name	C:\Documents and Settings\ejt\My Documents\Alan\Chem Commum\Yamaguchi\2010-04-25-ejt-25\11\data\111r				
Nucleus	13C	Number of Transients	3072	Origin	AV400
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	BENZENE-d6	Spectrum Offset (Hz)	11221.0137
Sweep Width (Hz)	30241.01	Temperature (degree C)	22.100	Spectrum Type	STANDARD

2010-04-25-ejt-25.011.001.1r.esp



Acquisition Time (sec)	1.0835	Comment	allylamaguchi mCARBONnight C6D6 (e:\bruk400data\2010\Apr) ejt 25	Date	25 Apr 2010 18:59:28
Date Stamp	25 Apr 2010 18:59:28				
File Name	C:\Documents and Settings\ejt\My Documents\Alan\Chem Commu\Yamaguchi\2010-04-25-ejt-25\11\data\11.r	Frequency (MHz)	100.61		
Nucleus	13C	Number of Transients	3072	Original Points Count	32768
Owner	Administrator	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	30241.94	Solvent	BENZENE-d6	Receiver Gain	512.00
Sweep Width (Hz)	30241.01	Temperature (degree C)	22.100	Spectrum Type	STANDARD
2010-04-25-ejt-25.011.001.1r.esp					

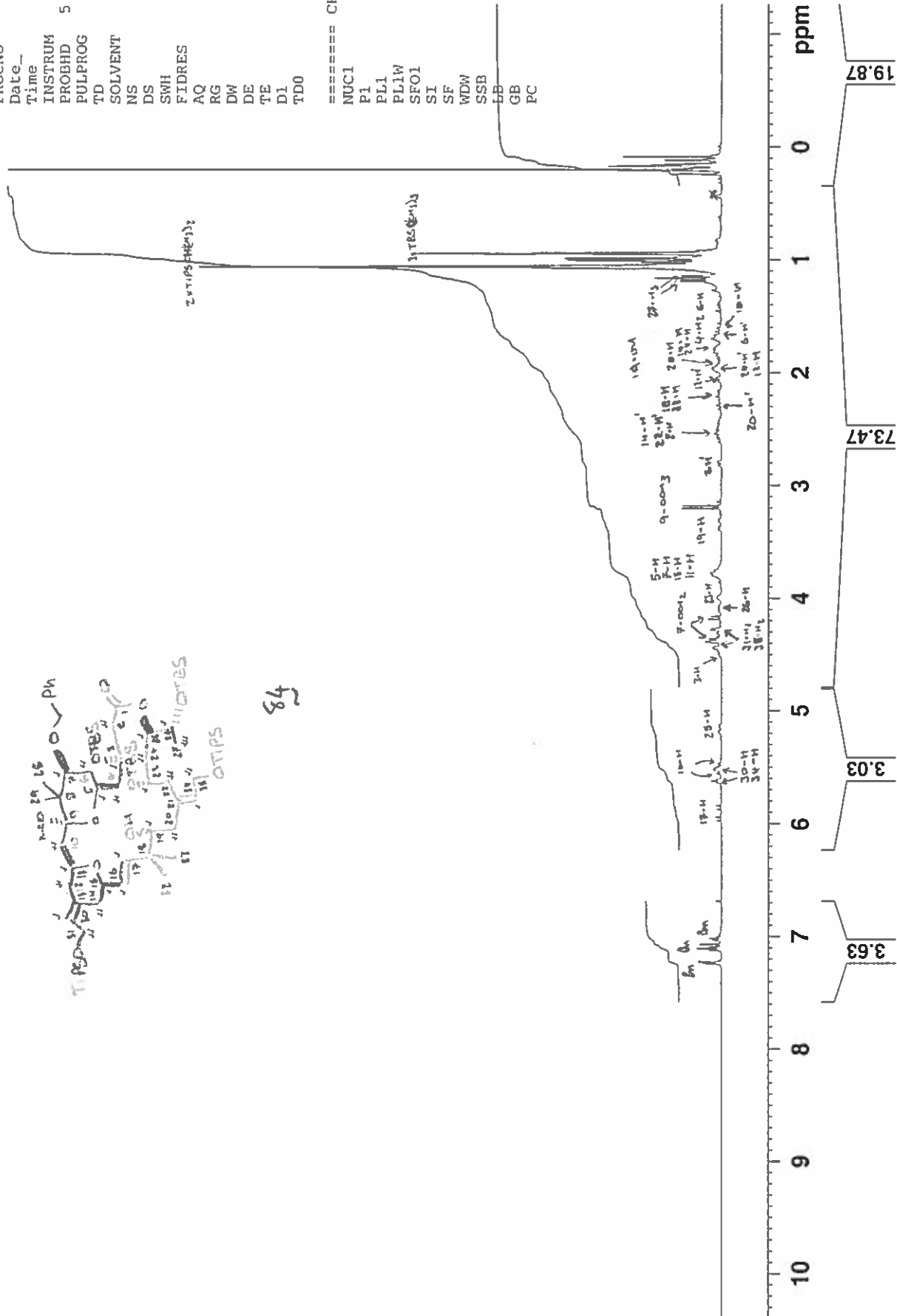




NAME 2010-05-17-ejt-22

EXPNO 10  
PROCNO 1  
Date\_ 20100517  
Time 15.19  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 64  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 64  
DW 48.400 usec  
DE 10.67 usec  
TE 298.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300999 MHz  
WDW EM  
SSB 0  
BB 0.30 Hz  
GB 0  
PC 1.00



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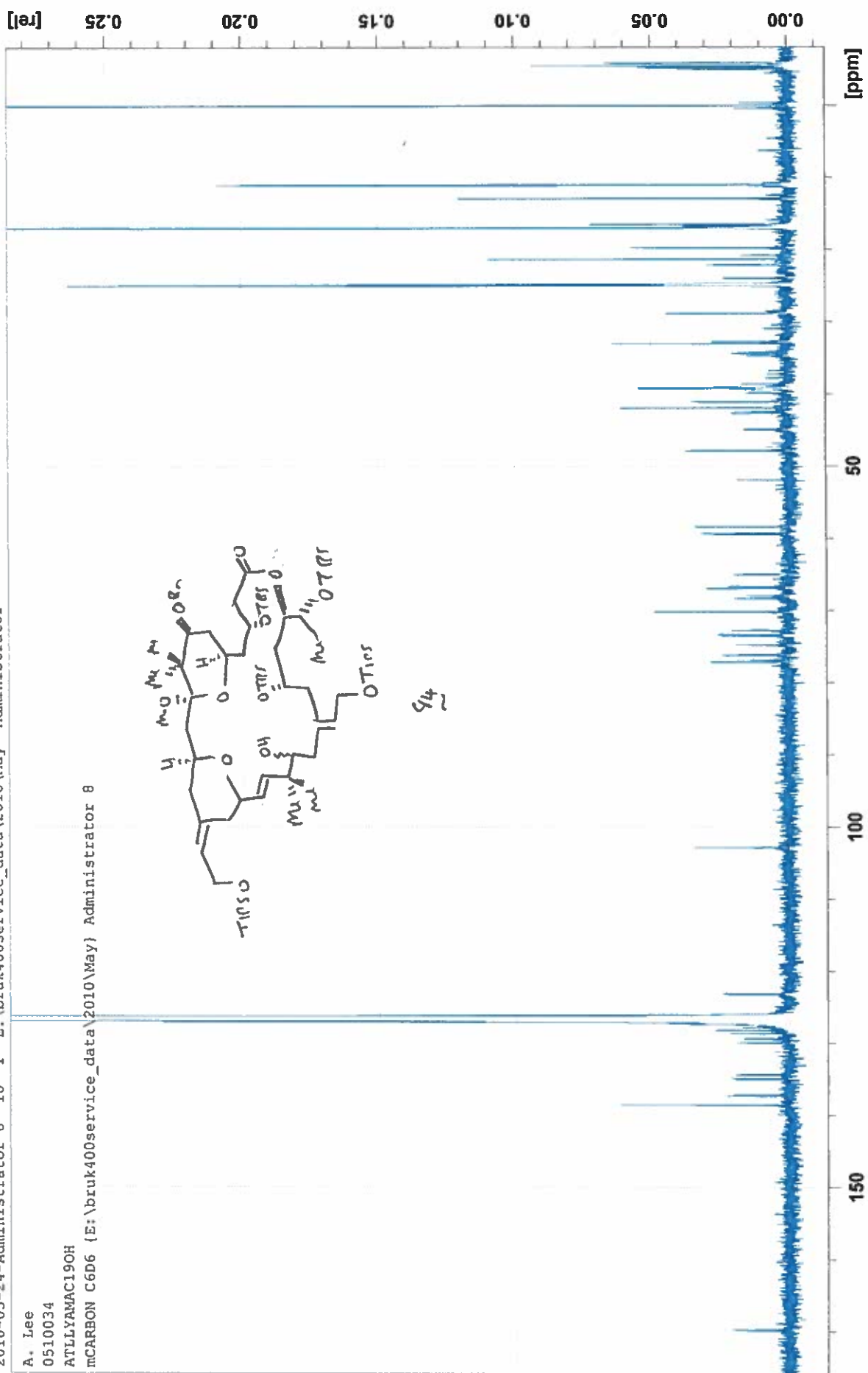
2010-05-24-Administrator-8 10 1 E:\bruk400service\_data\2010\May Administrator

A. Lee

0510034

ATLLYAMAC19OH

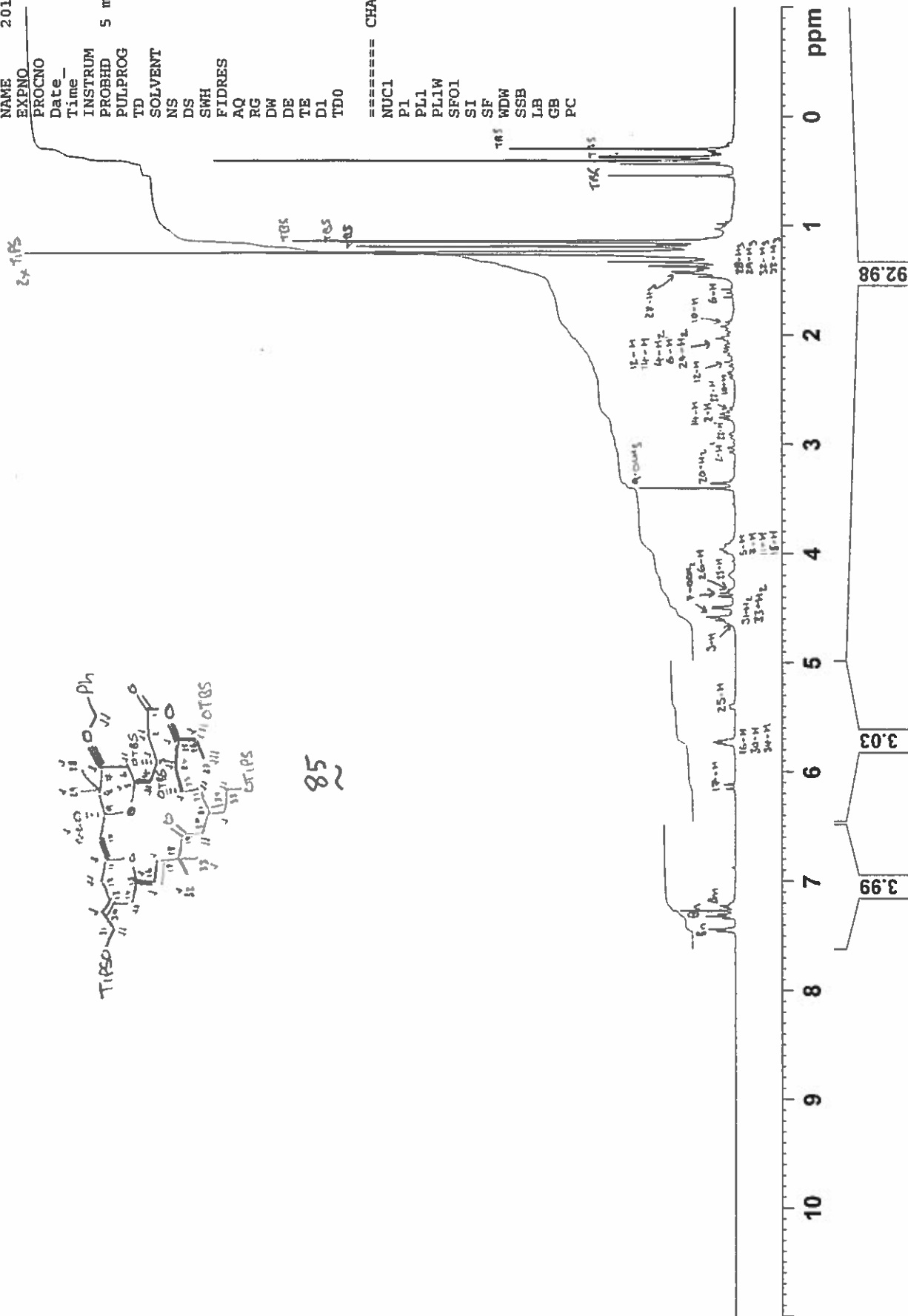
mCARBON C6D6 (E:\bruk400service\_data\2010\May) Administrator 8





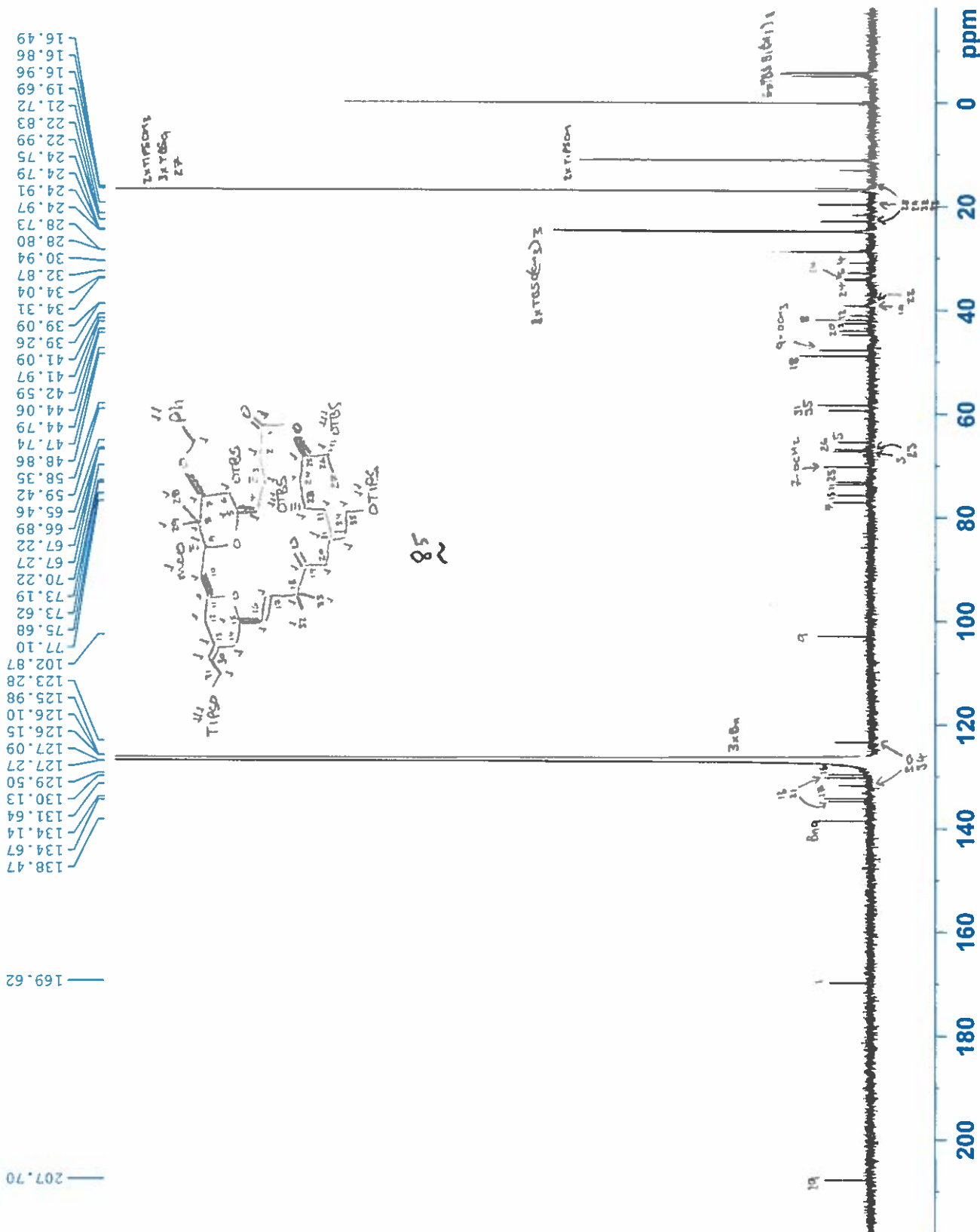
NAME 2010-05-30-ejt-9  
EXPNO 11  
PROCNO 1  
Date\_ 20100530  
Time\_ 18.01  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 128  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 228  
DW 60.500 usec  
DE 9.40 usec  
TE 293.8 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





# A Lee 0510-041 atll c19 ketone mCARBON C6D6 {E:\bruk400service\_data\2010\Jun} Administrator 37



```

NAME      2010-06-02-Administrator-37
EXPNO     11
PROCNO    1
Date_     20100602
Time      14.02
INSTRUM   AV400 5
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         36000
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631888 sec
RG         2050
DM         20.800 usec
DE         6.50 usec
TE         296.6 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         8.00 usec
PL1        0.00 dB
PL1W       33.91046524 W
SFO1       100.6479773 MHz

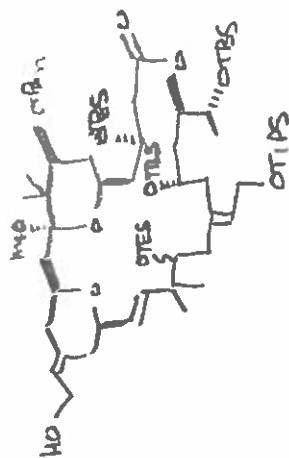
===== CHANNEL f2 =====
CPDPRG2    waitz16
NUC2        1H
PCPD2       90.00 usec
P2         -3.60 dB
PL2        15.31 dB
PL12       18.00 dB
PL13       18.9851721 W
PL12W      0.24406971 W
PL13W      0.13137537 W
SFO2       400.2316009 MHz
SI         32768
SF         100.6380921 MHz
RG         0
MEAS       1.00 Hz
LB         0
GB         1.40
PC
  
```



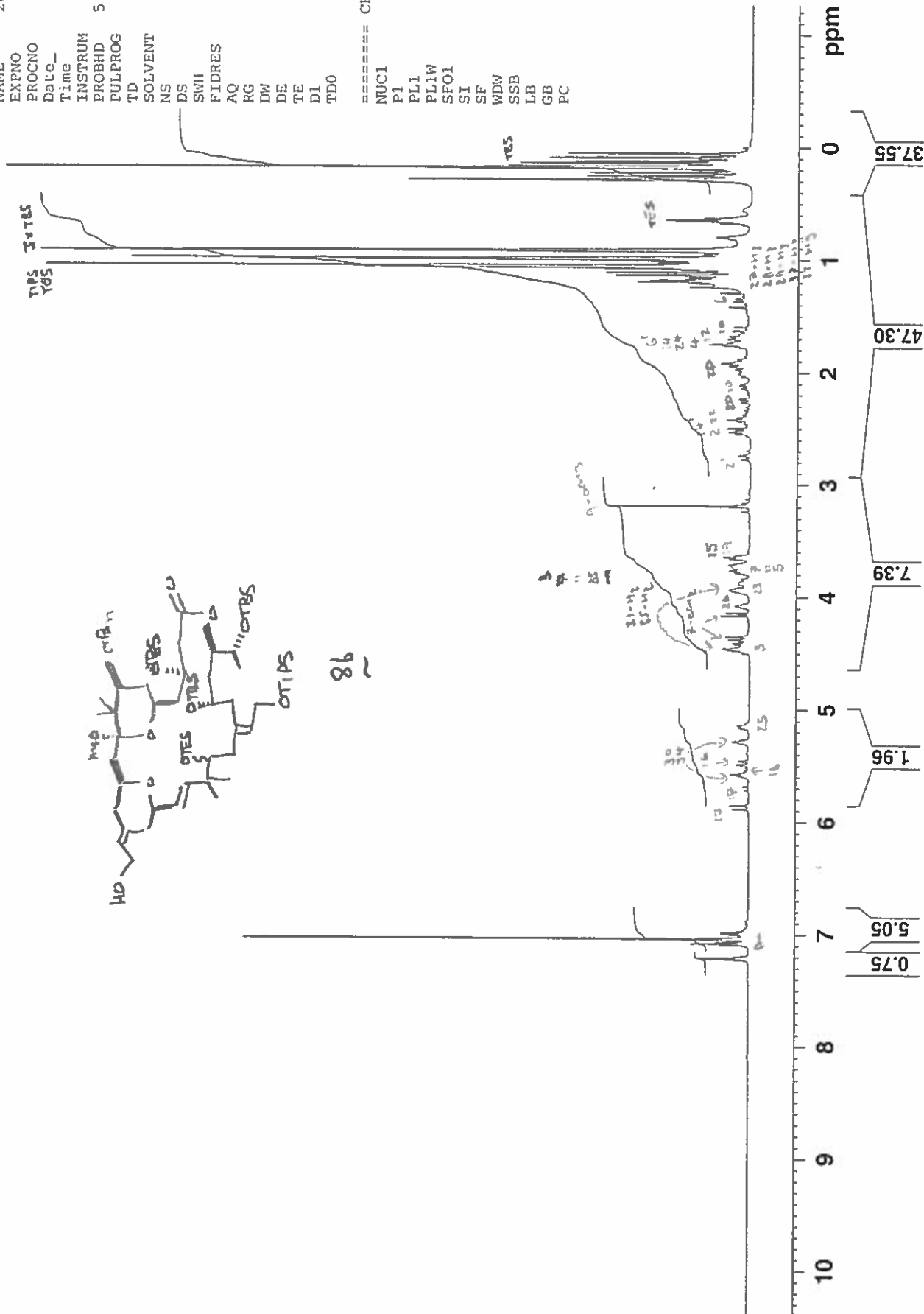
2010-05-17-ejt-15

NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20100517  
Time 12.43  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 64  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 287  
DW 48.400 usec  
DE 10.67 usec  
TE 298.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1301171 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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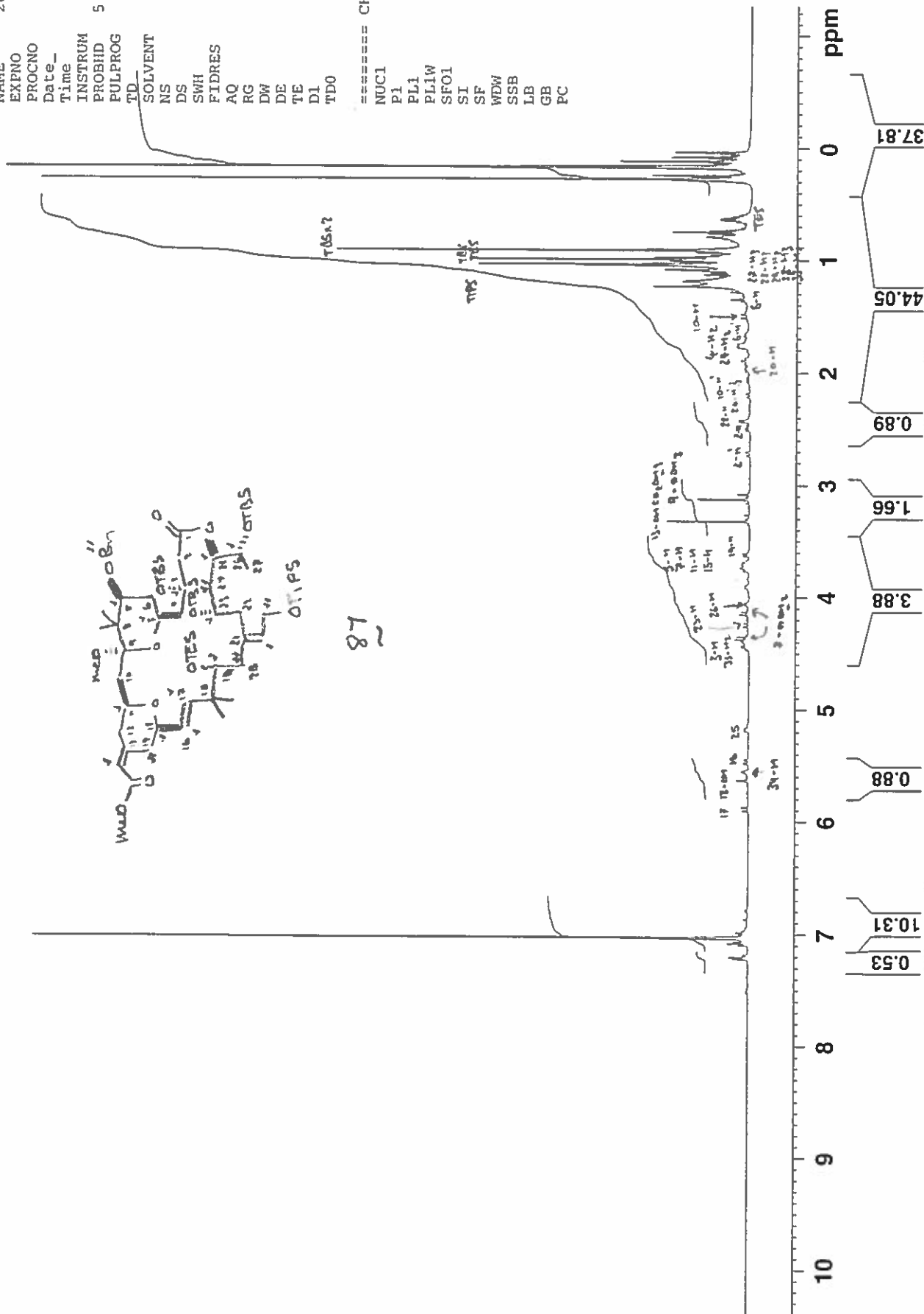
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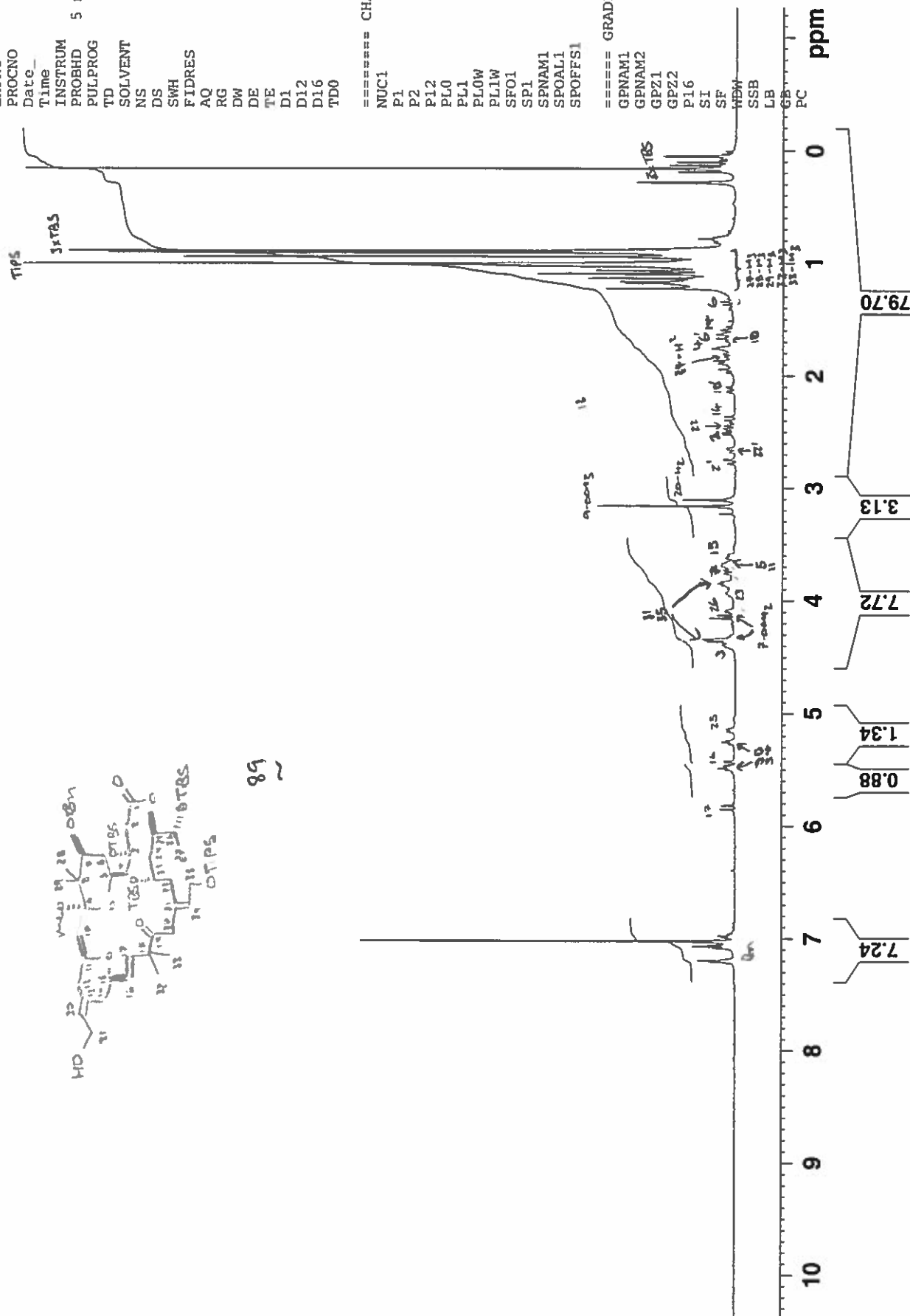
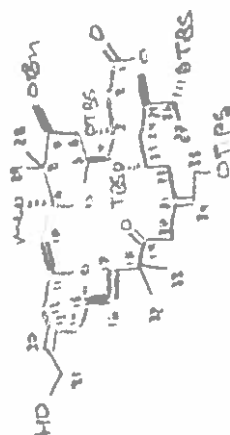
mPROTONight C6D6 /opt/bruk500data/2010/Jun ejt 4



2010-06-14-ejt-4  
 NAME EXPNO 10  
 PROCNO 1  
 Date\_ 20100614  
 Time 15.02  
 INSTRUM spect  
 PROBHD 5 mm TXI 1H/D-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT C6D6  
 NS 128  
 DS 0  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.171923 sec  
 RG 406  
 DW 48.400 usec  
 DE 10.67 usec  
 TE 294.3 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 21.07 usec  
 PL1 3.25 dB  
 PL1W 12.12272263 W  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1301213 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





2010-07-13-mib-31					
NAME	EXPNO	PROCNO	Date_	Time	
	10	1	20100713	10.03	
INSTRUM			Spect		
FIDRES	5 mm TXI 1H/D-				
PULPROG	zgpgsp				
TD	65536				
SOLVENT	C6D6				
DS	16				
NS	2				
SWH	10330.578 Hz				
FIDRES	0.157632 Hz				
AQ	3.1719923 sec				
RG	322				
DW	48.400 usec				
DE	9.05 usec				
TE	298.2 K				
DD1	2.40000010 sec				
DD12	0.00002000 sec				
DD16	0.00010000 sec				
TD0	1				
===== CHANNEL f1 =====					
NUC1	1H				
P1	21.07 usec				
P2	42.14 usec				
P12	2400.00 usec				
PL0	120.00 dB				
PL1	3.25 dB				
PFL0	0.00000000 W				
PFL1	12.12372263 W				
SFO1	500.1302054 MHz				
SP1	42.39 dB				
SPNAM1	Sinc1.1000				
SPOAL1	0.500				
SPOFFS1	0.00 Hz				

```

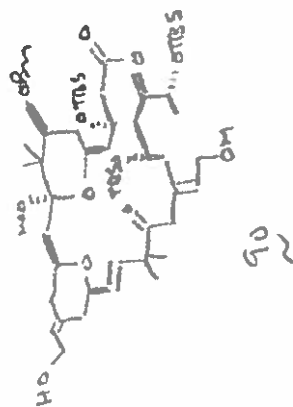
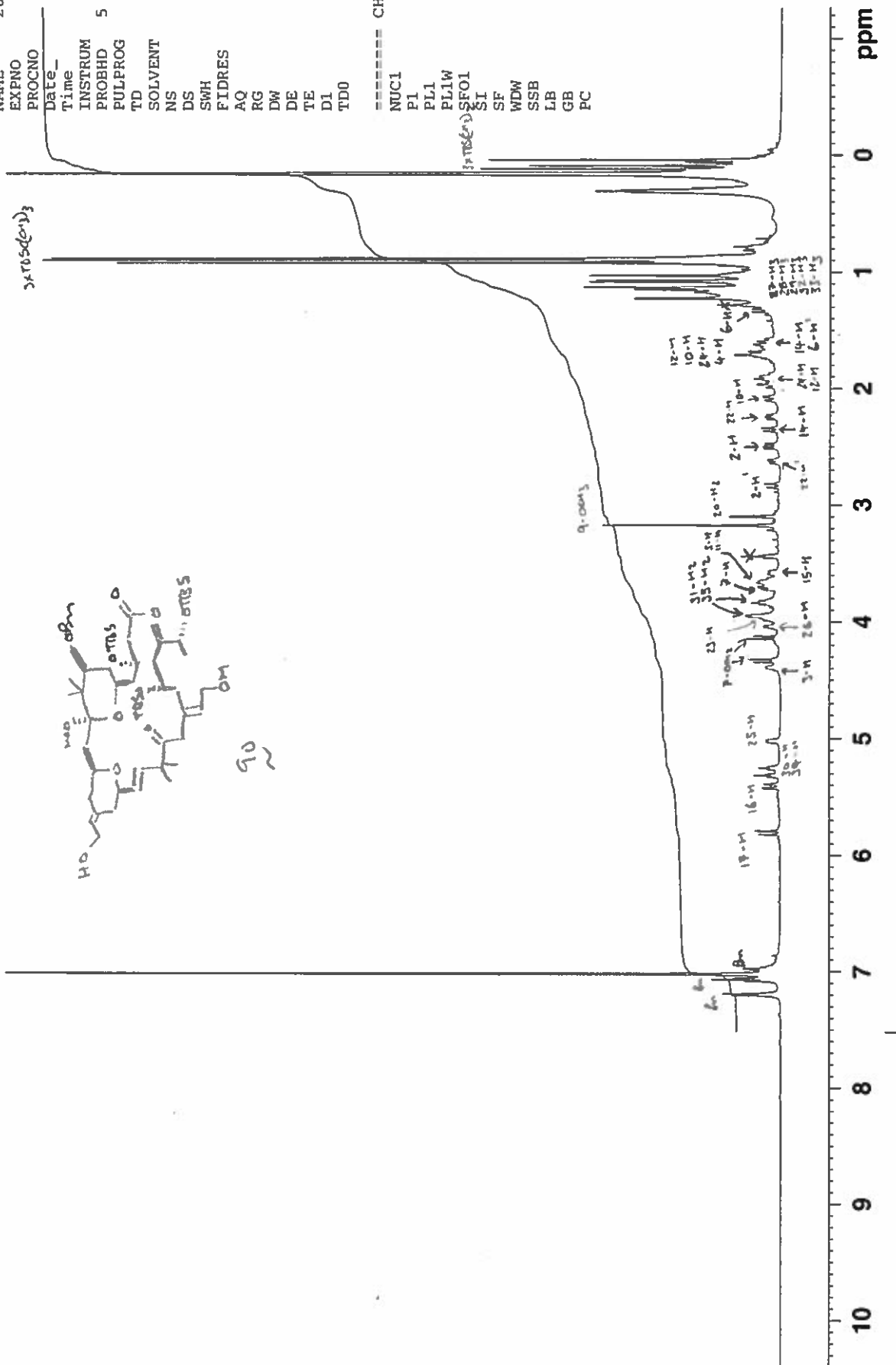
===== GRADIENT CHANNEL =====
GPNAM1      SINE.100
GPNAM2      SINE.100
GPZ1        31.00 %
GP22        11.00 %
P16         1000.00 usec
SI          32768
SF          500.1301243 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

```



NAME 2010-07-12-ejt-29  
EXPNO 10  
PROCNO 1  
Date\_ 20100713  
Time 1.07  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 512  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 362  
DW 48.400 usec  
DE 10.67 usec  
TE 298.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
PL1W 12.1272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1301242 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



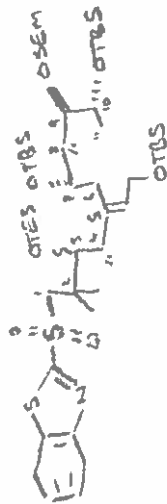
100.00



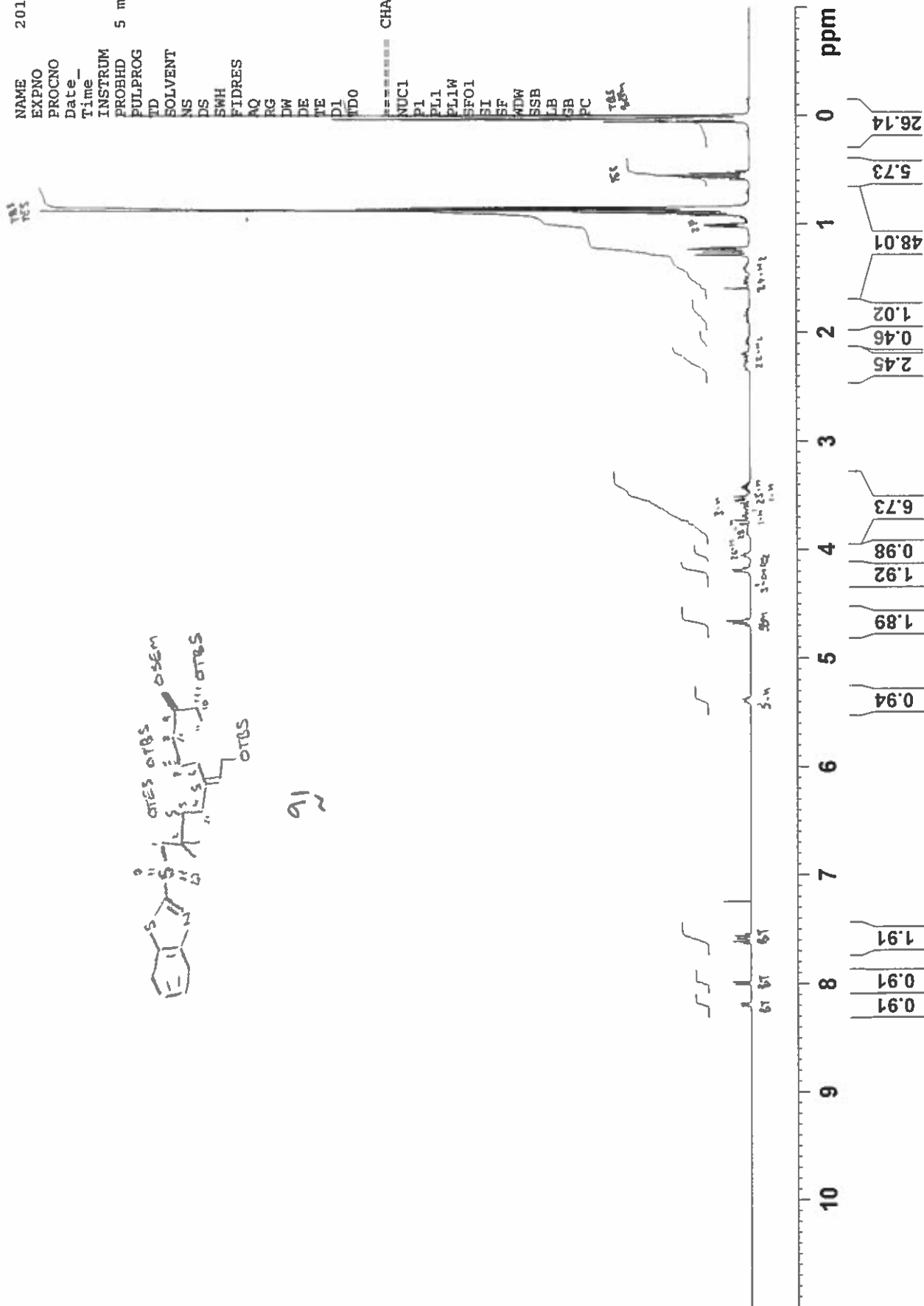
2011-06-12-ejt-24

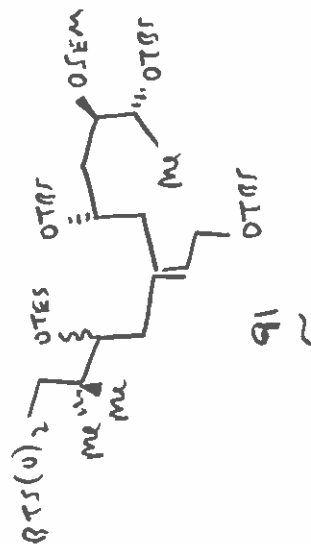
NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20110612  
Time 16.00  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 80.6  
DW 60.500 usec  
DE 9.40 usec  
TE 295.2 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PL1W 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300133 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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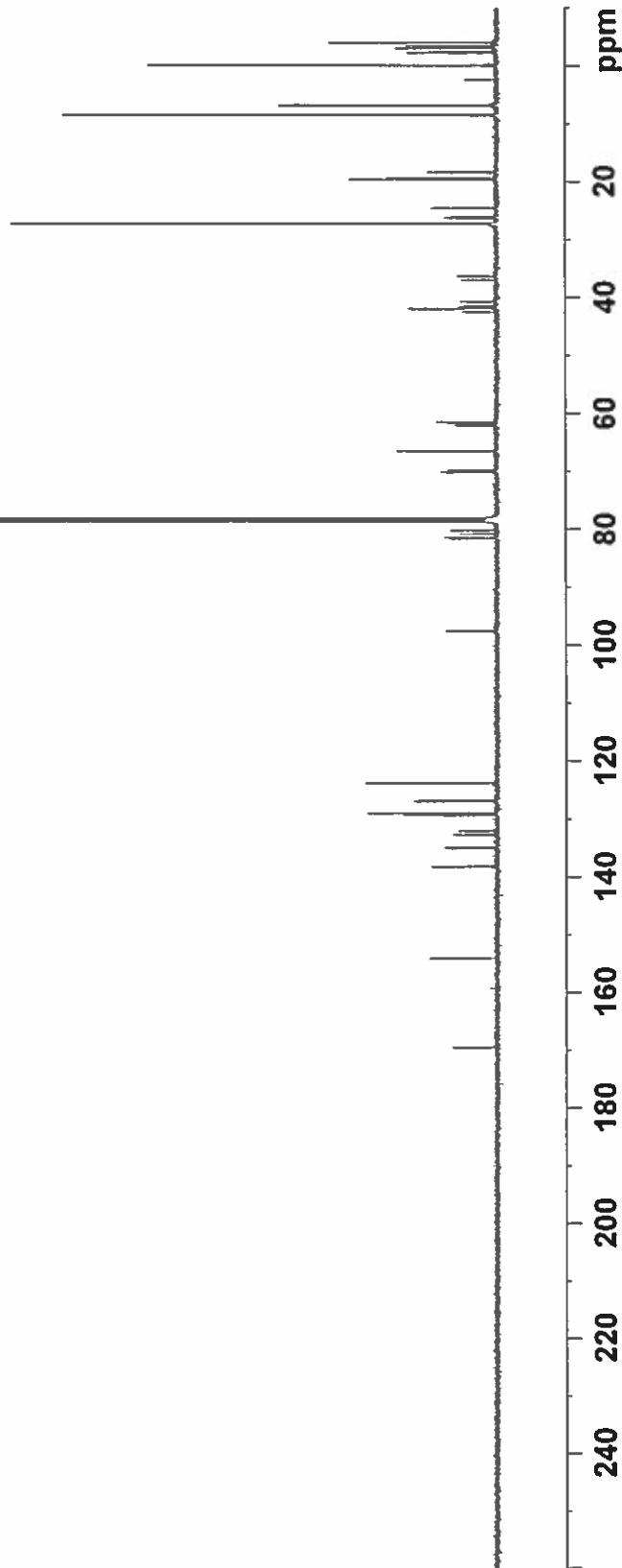




NAME 2011-06-12-ejt-24  
EXPNO 21  
PROCNO 1  
Date\_ 20110612  
Time\_ 19.08  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 3072  
DS 2  
SWH 30241.936 Hz  
FIDRES 0.461455 Hz  
AQ 1.0835786 sec  
RG 512  
DW 16.533 usec  
DE 7.83 usec  
TE 296.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 34.91522217 W  
SFO1 100.6241042 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.60 dB  
PL12 15.31 dB  
PL13 18.00 dB  
PL2W 17.83863831 W  
PL12W 0.22927761 W  
PL13W 0.12341322 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6126266 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

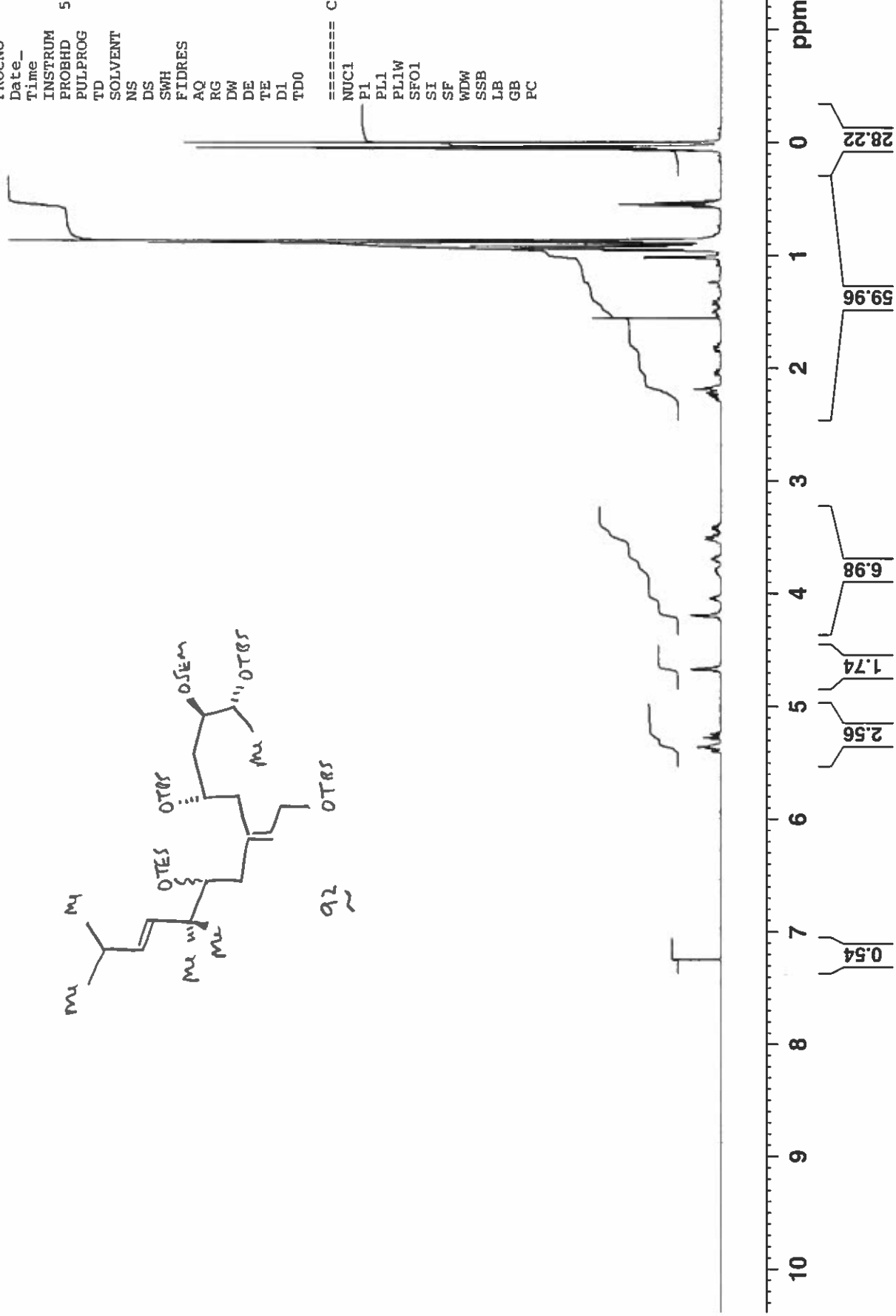
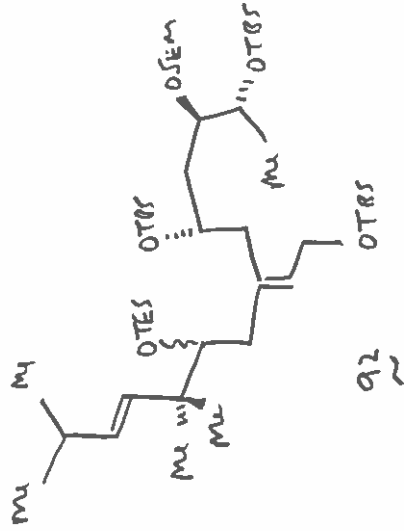


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mPROTON CDC13 /opt/bruk500data/2010/Sep ejt 17



NAME 2010-09-20-ejt-17  
 EXPNO 10  
 PROCNO 1  
 Date\_ 20100920  
 Time 14.02  
 INSTRUM spect  
 PROBHD 5 mm TXI 1H/D-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 0  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.171923 sec  
 RG 90.5  
 DW 48.400 usec  
 DE 13.38 usec  
 TE 294.5 K  
 D1 1.00000000 sec  
 TD0 1  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.20 usec  
 PL1 3.25 dB  
 PL1W 12.12272263 W  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1300197 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





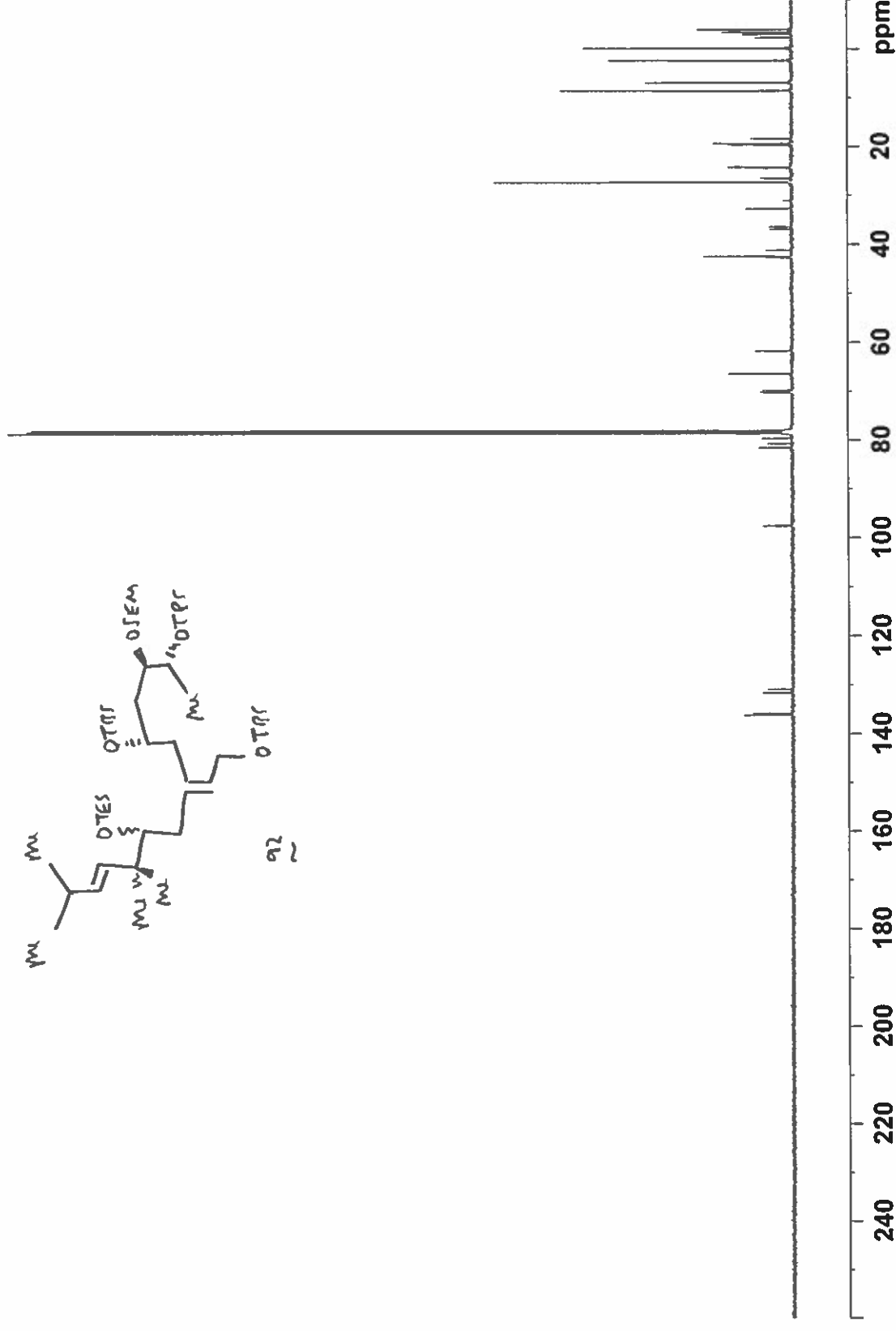
atlItristbsjulia  
mCARBONnight CDCI3 {e:\bruk400data\2011\Jun} ejt 7



NAME	EXPNO	PROCNO	Date_	Time_	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DW	DE	TE	D1	D11	TD0
2011-06-14-ejt-7	13	1	20110615	2.19	AV400	5 mm PABBO BB-	zgpg30	6536	CDC13	3072	2	30241.936 Hz	0.461455 Hz	1.0835786 sec	512	16.533 usec	7.83 usec	295.9 K	2.00000000 sec	0.03000000 sec	1

```
===== CHANNEL f1 =====
NUC1      13C      8.00 usec
P1         0.00 dB
PL1
PL1W      34.9152217 W
SF01     100.6241042 MHz
```

CHANNEL f2	
CDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL1	-3.60 dB
PL12	15.31 dB
PL13	18.00 dB
PL1W	17.83683831 W
PL12W	0.22927761 W
PL13W	0.12341322 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6126253 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



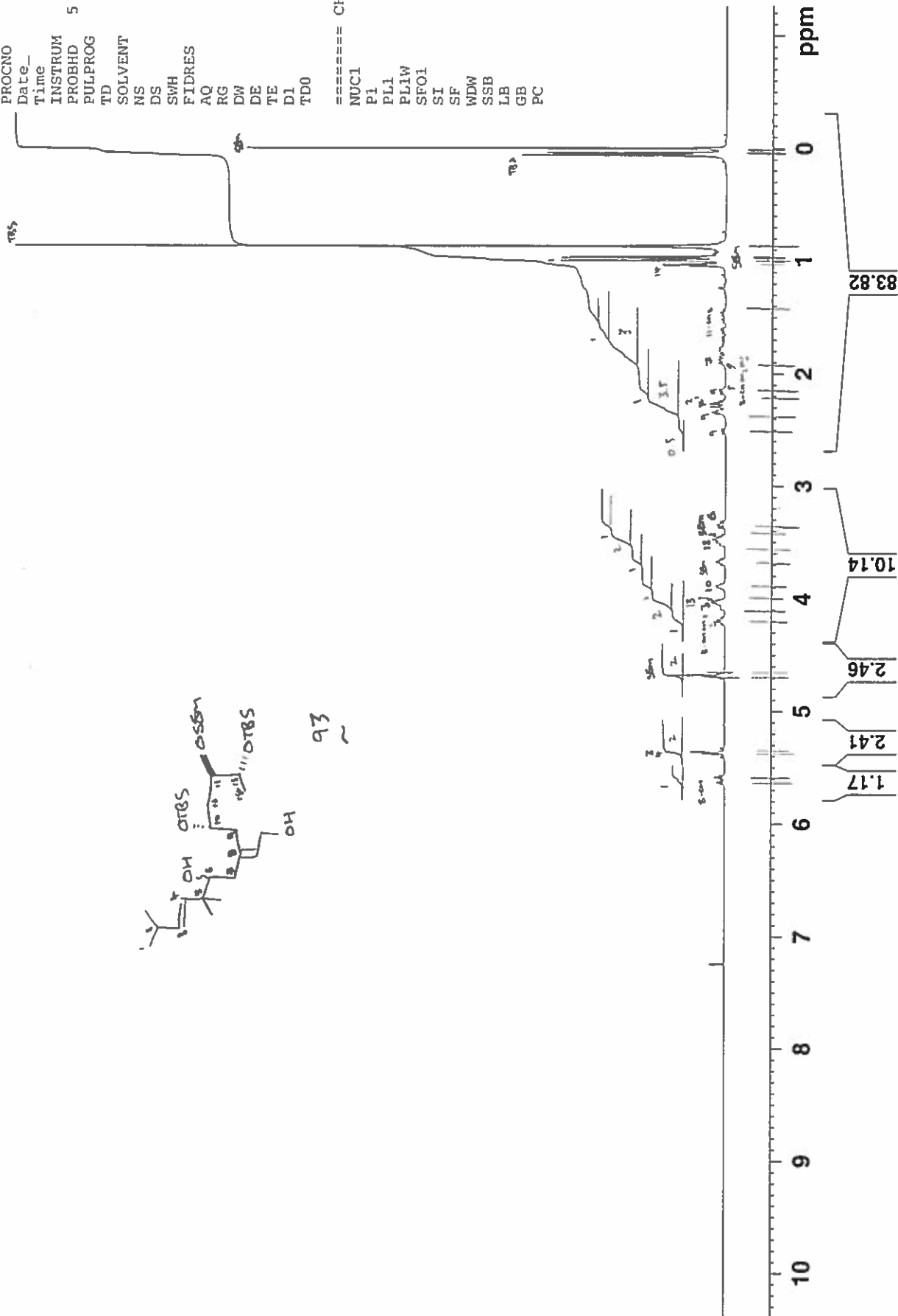
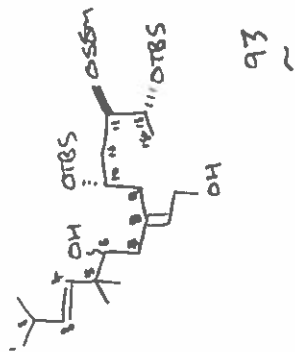


2011-06-20-ejt-5

NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20110620  
Time 11.49  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 45.2  
DW 48.400 usec  
DE 13.38 usec  
TE 298.2 K  
D1 1.00000000 sec  
TD0 1

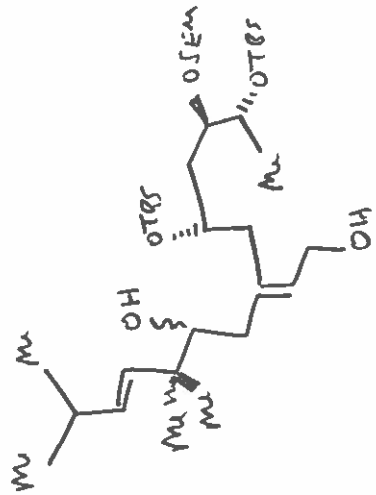
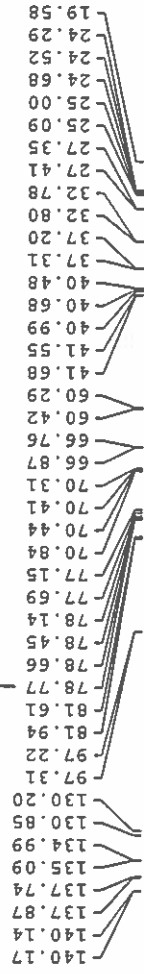
===== CHANNEL f1 =====

NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300191 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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mCARBONight CDC13 {e:\bruk400data\2011\Jun} ejt 1



```

NAME      2011-06-19-ejt-1
EXPNO     13
PROCNO    1
Date_     20110619
Time      22.21
INSTRUM   AV400
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         3072
DS         2
SWH        30241.936 Hz
FIDRES     0.461455 Hz
AQ         1.0835786 sec
RG         512
DE         16.533 usec
TE         296.9 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         8.00 usec
PL1        0.00 dB
PL1W       34.91522217 W
SFO1       100.6241042 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2      90.00 usec
PL2        -3.60 dB
PL12       15.31 dB
PL13       18.00 dB
PL2W       17.83863831 W
PL12W      0.22927761 W
PL13W      0.12341322 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6126230 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

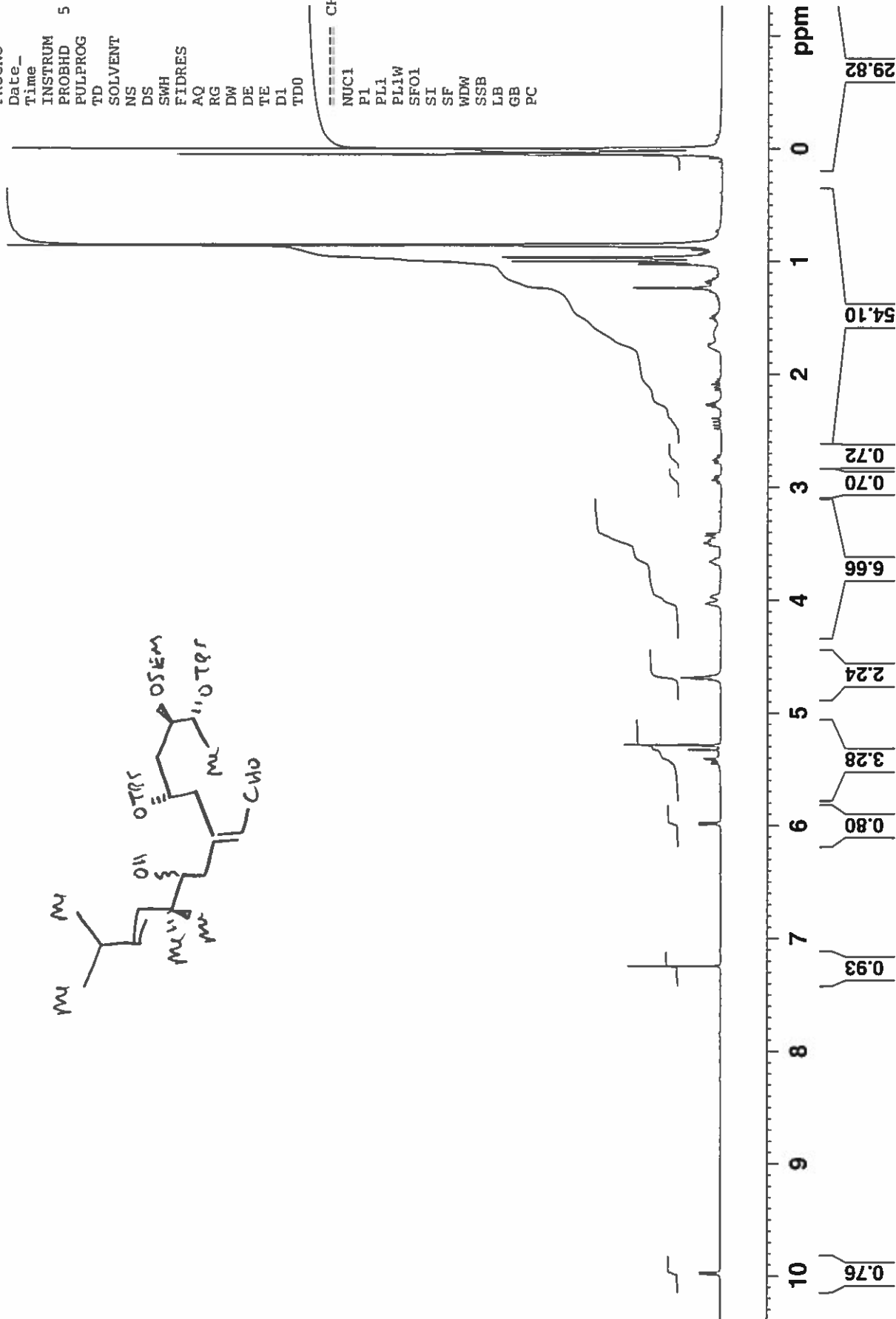
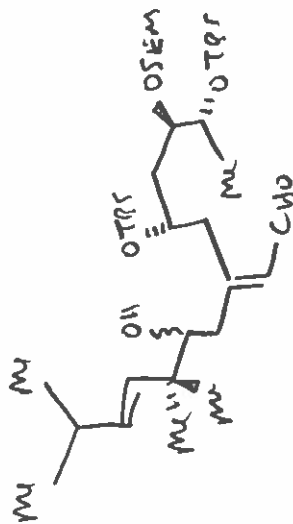
```

240 220 200 180 160 140 120 100 80 60 40 20 ppm



NAME 2010-11-08-ejt-17  
EXPNO 10  
PROCNO 1  
Date\_ 20101108  
Time 16.39  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 90.5  
DW 48.400 usec  
DE 13.38 usec  
TE 294.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300199 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





2011-06-25-ejt-56

NAME  
EXPNO 13  
PROCNO 1

Date\_ 20110625  
Time\_ 18.10

INSTRUM AV400

PROBHD 5 mm PABBO BB-

PULPROG zg30b

TD 65536

SOLVENT CDCl3

NS 128

DS 0

SWH 8264.463 Hz

FIDRES 0.126106 Hz

AQ 3.9649780 sec

RG 90.5

DW 60.500 usec

DE 9.40 usec

TE 293.7 K

D1 1.00000000 sec

TD0 1

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

NUC1 1H

P1 10.00 usec

PL1 -3.60 dB

PL1W 17.83863831 W

SFO1 400.1324710 MHz

SI 32768

SF 400.1300115 MHz

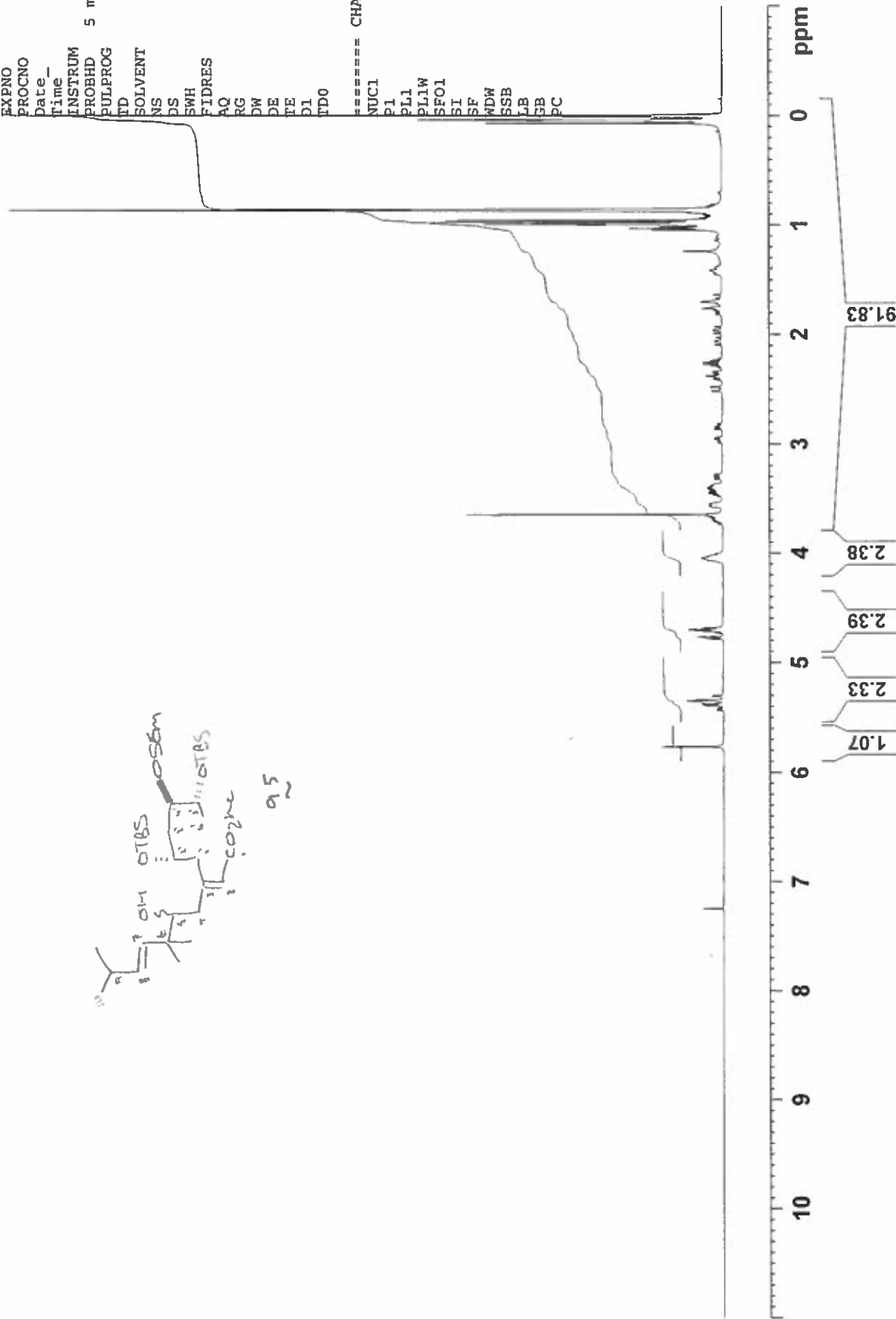
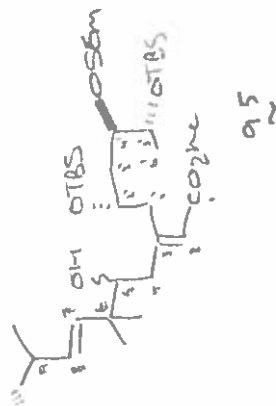
WDW EM

SSB 0

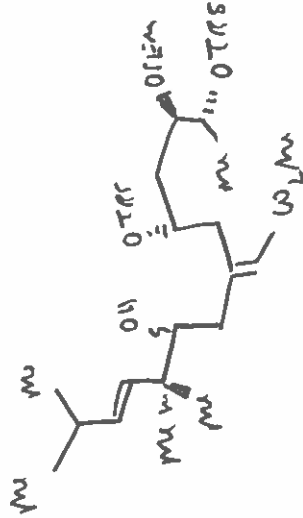
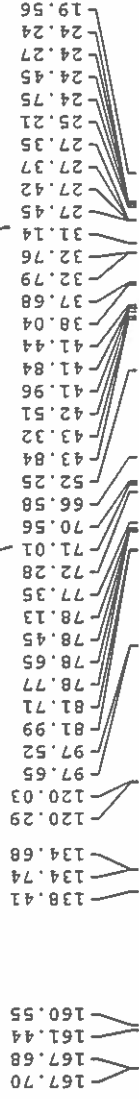
LB 0.30 Hz

GB 0

PC 1.00



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mCARBONight CDCl3 {e:\bruk400data\2011\Jun} ejt 56



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```

NAME      2011-06-25-ejt-56
EXPNO     14
PROCNO    1
Date_     20110625
Time      20.52
INSTRUM   AV400
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         3072
DS         2
SWH        30241.936 Hz
FIDRES     0.461455 Hz
AQ         1.0835786 sec
RG         512
DW         16.533 usec
DE         7.83 usec
TE         294.5 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         8.00 usec
PL1        0.00 dB
PL1W       34.91522217 W
SFO1       100.6241042 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -3.60 dB
PL12       15.31 dB
PL13       18.00 dB
PL2W       17.83863831 W
PL12W      0.22927761 W
PL13W      0.12341322 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6126241 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

240 220 200 180 160 140 120 100 80 60 40 20 ppm

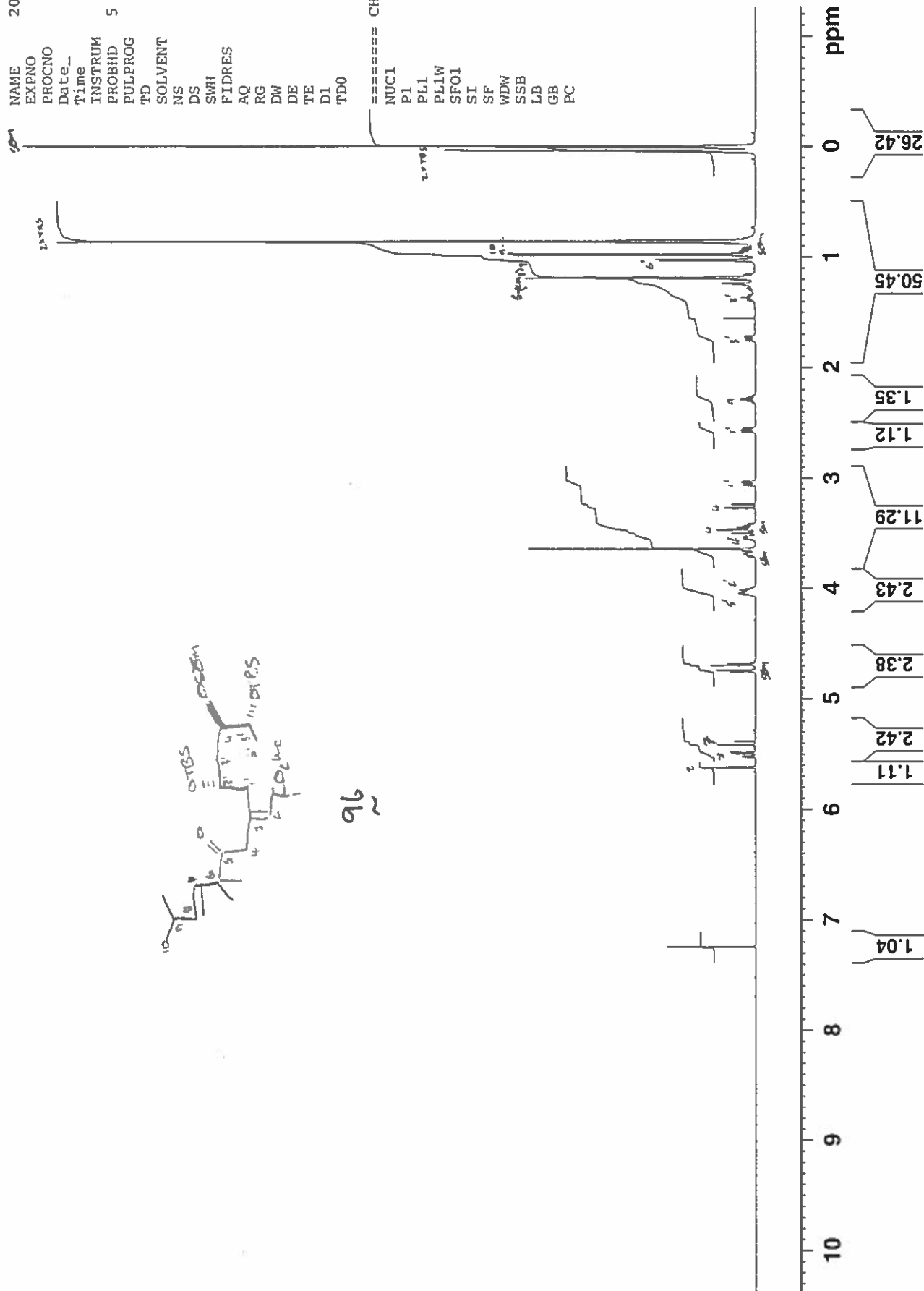


NAME 2011-07-05-ejt-18  
EXPNO 12  
PROCNO 1  
Date\_ 20110705  
Time 22.53  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 144  
DW 48.400 usec  
DE 13.38 usec  
TE 298.2 K  
D1 1.0000000 sec  
D1 1  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 8.20 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SF01 500.1330885 MHz  
SI 32768  
SF 500.1300198 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

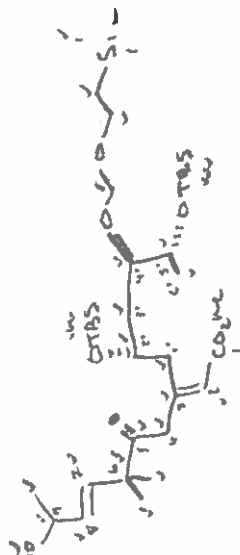
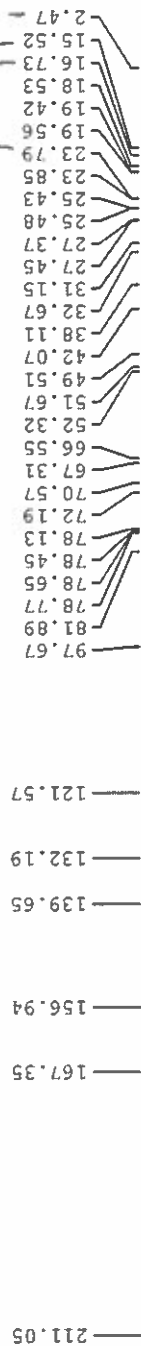


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mCARBONight CDCI3 {e:\bruk400data\2011\Jul} ejt 37



96  
2



240 220 200 180 160 140 120 100 80 60 40 20 ppm

NAME 2011-07-05-ejt-37  
EXPNO 11  
PROCNO 1  
Date\_ 20110706  
Time 1.58  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCI3  
NS 3072  
DS 2  
SWH 30241.936 Hz  
FIDRES 0.461455 Hz  
AQ 1.0835786 sec  
RG 512  
DW 16.533 usec  
DE 7.83 usec  
TE 295.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 34.91522217 W  
SFO1 100.6241042 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.60 dB  
PL12 15.31 dB  
PL13 18.00 dB  
PL2W 17.83863831 W  
PL12W 0.22927761 W  
PL13W 0.12341322 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6126242 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





2011-09-17-ejt-41

NAME  
EXPNO 12  
PROCNO 1

Date 20110917  
Time 19.51

INSTRUM AV400

PROBHD 5 mm PABBO BB-

PULPROG zg30b

TD 65536

SOLVENT CDCl3

NS 128

DS 0

SWH 8264.463 Hz

FIDRES 0.126106 Hz

AQ 3.9649780 sec

RG 362

DW 60.500 usec

DE 9.40 usec

TE 292.1 K

D1 1.00000000 sec

TD0 1

CHANNEL f1 =====

NUC1 1H

P1 10.00 usec

PL1 -3.60 dB

PL1W 17.83863831 W

SFO1 400.1324710 MHz

SI 32768

SF 400.1300124 MHz

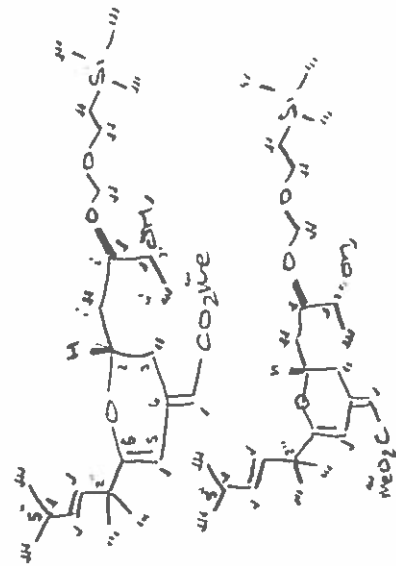
WDW EM

SSB 0

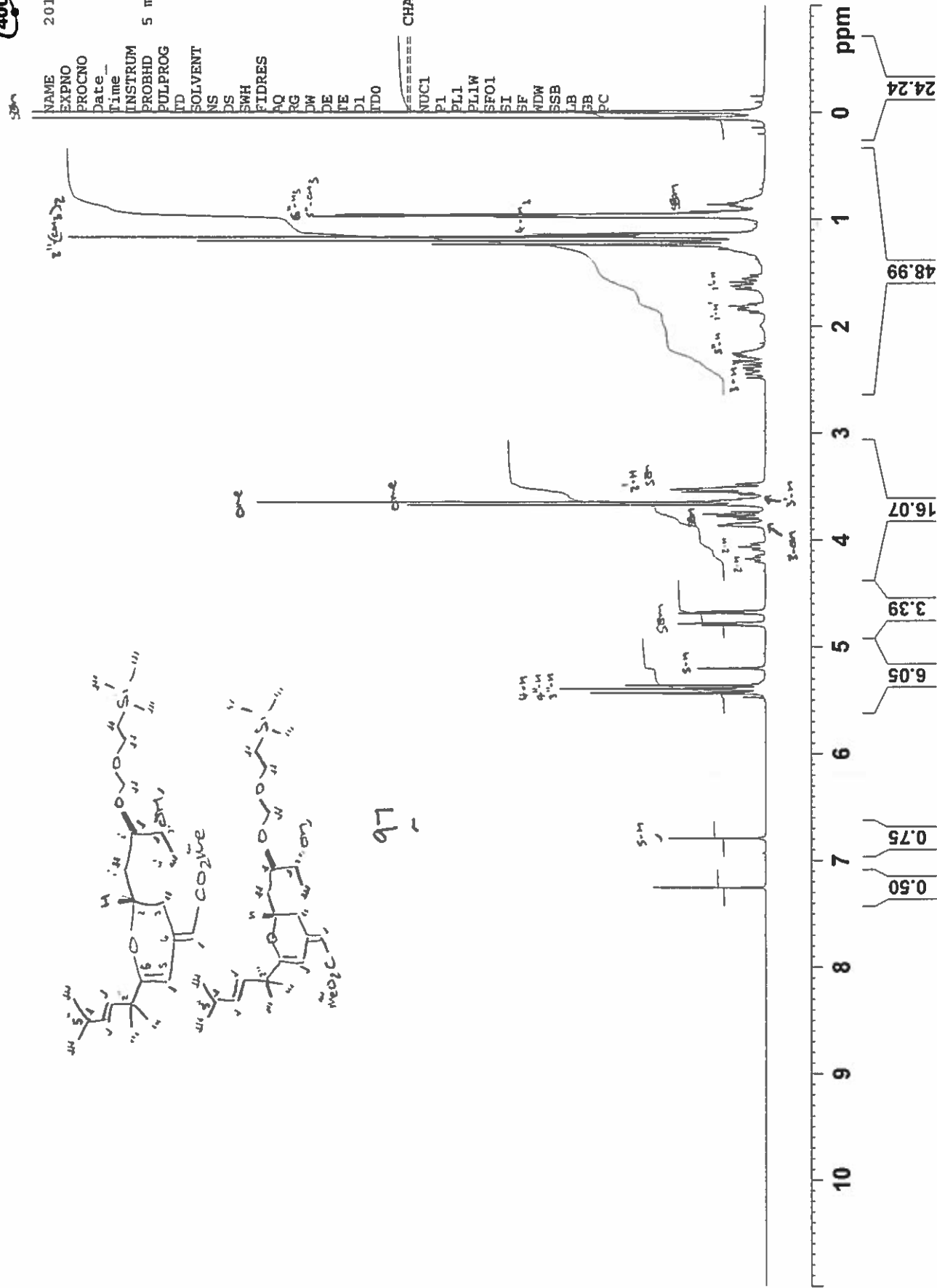
LB 0.30 Hz

GB 0

PC 1.00



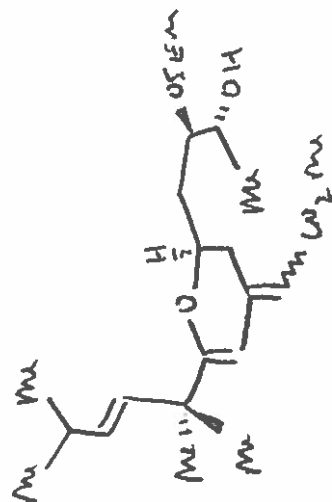
97



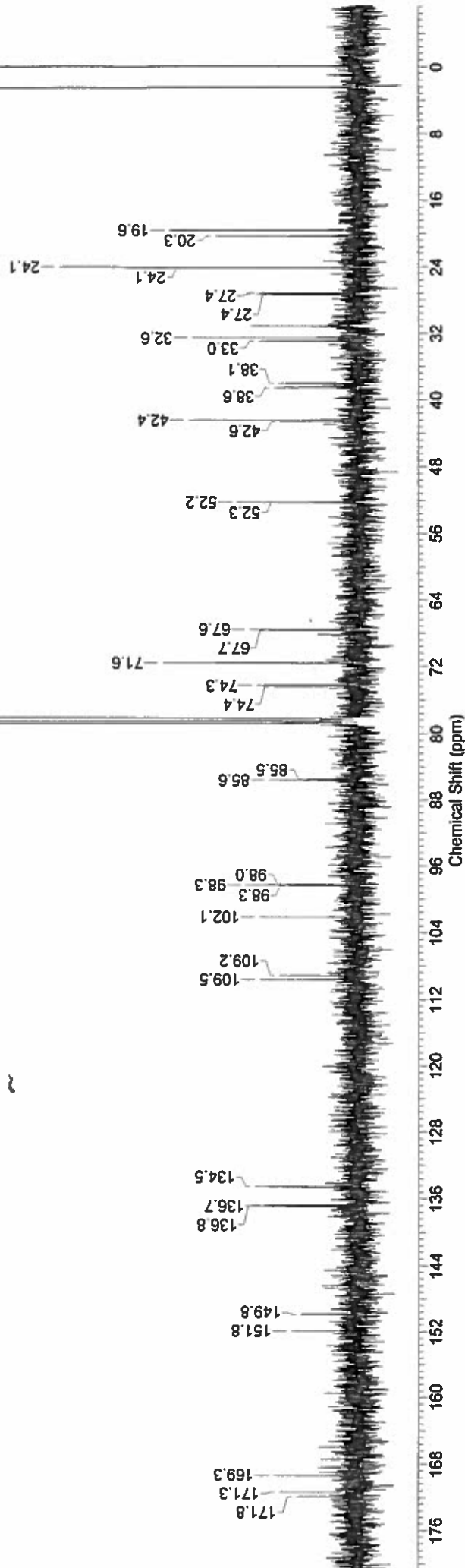
Acquisition Time (sec)	1.0835	Comment	allendelthemodel mCARBONnight CDC13 (e:\bruk400data\2011\1Sep) ejt 41
Date	17 Sep 2011 22:34:56	Date Stamp	17 Sep 2011 22:34:56
File Name	\\ss7a.ds.man.ac.uk\vd5\vd3\users\snmrdata\bruk400data\2011\1Sep\data\11r	Origin	AV400
Nucleus	13C	Number of Transients	3072
Owner	Administrator	Points Count	32768
SW(cyclical) (Hz)	30241.94	Solvent	CHLOROFORM-d
Sweep Width (Hz)	30241.01	Temperature (degree C)	20.100
		Pulse Sequence	zgpg30
		Spectrum Offset (Hz)	11484.7109
		Spectrum Type	STANDARD
		Frequency (MHz)	100.61
		Original Points Count	32768
		Receiver Gain	512.00

2011-09-17-ejt-41.013.001.1r.esp

TMS



17

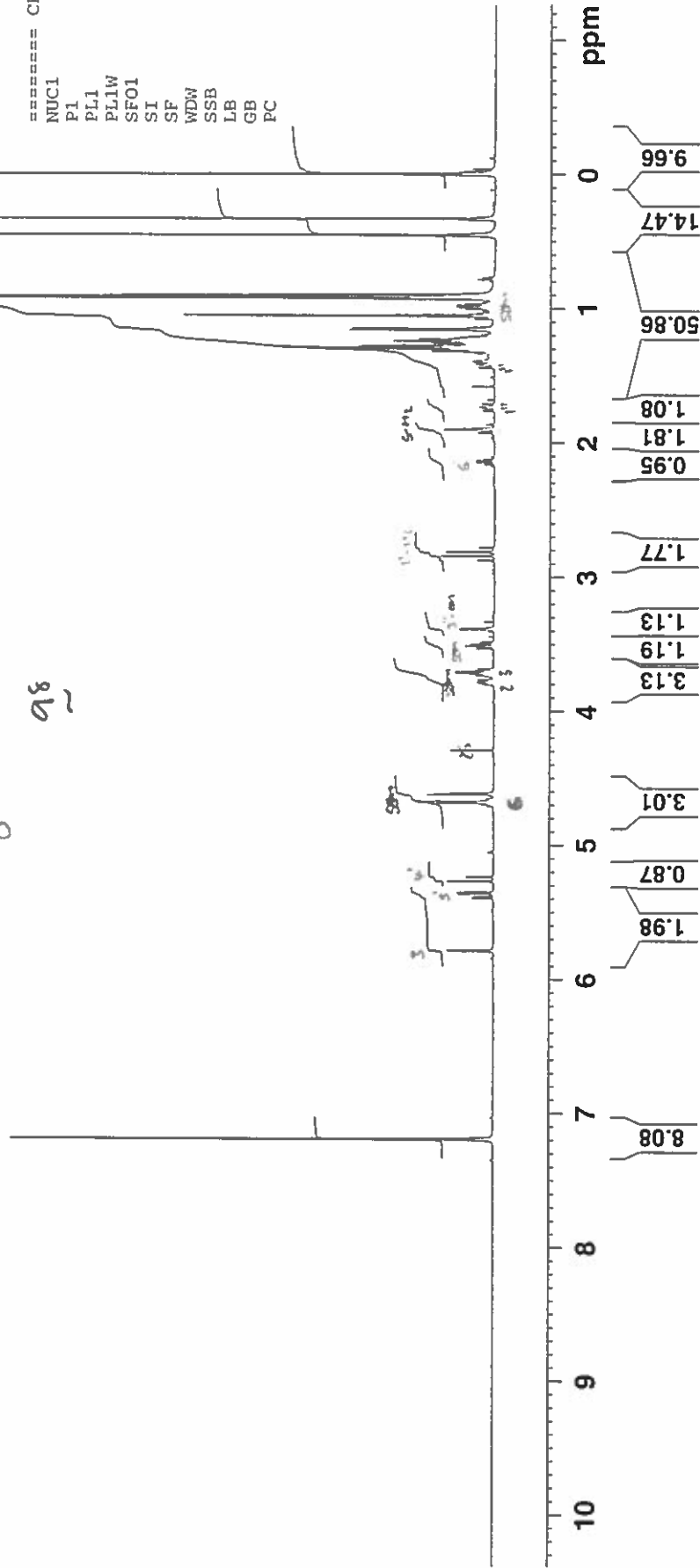
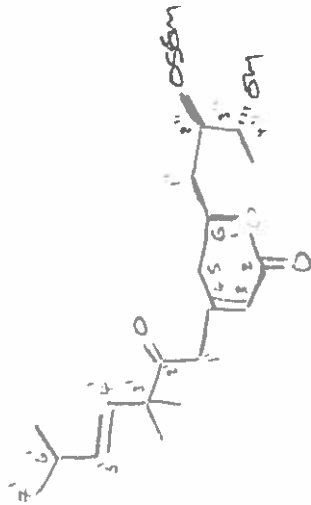




2011-09-06-ejt-30

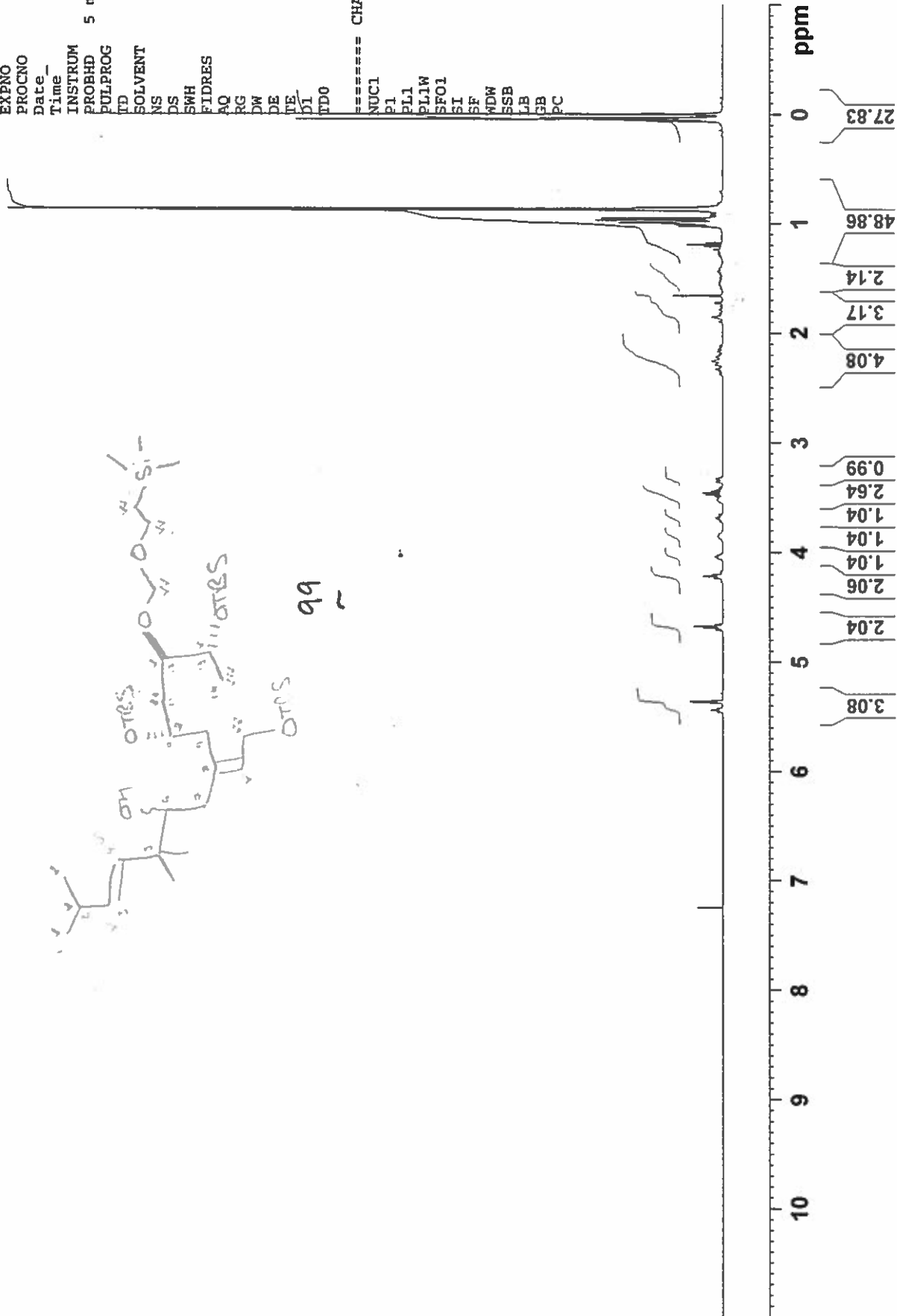
NAME  
EXPNO 12  
PROCNO 1  
Date\_ 20110906  
Time 16.20  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT CDC13  
NS 64  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 512  
DW 48.400 usec  
DE 10.67 usec  
TE 294.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1300201 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





NAME 2010-10-29-ejt-7  
 EXNO 10  
 PROCNO 1  
 Date\_ 20101029  
 Time\_ 15.26  
 INSTRUM AV400  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8264.463 Hz  
 FIDRES 0.126106 Hz  
 AQ 3.9649780 sec  
 RG 101  
 DW 60.500 usec  
 DE 9.40 usec  
 TE 293.4 K  
 D1 1.00000000 sec  
 TD0 1  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 -3.60 dB  
 PL1W 17.83863831 W  
 SFO1 400.1324710 MHz  
 SI 32768  
 SF 400.1300144 MHz  
 NDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

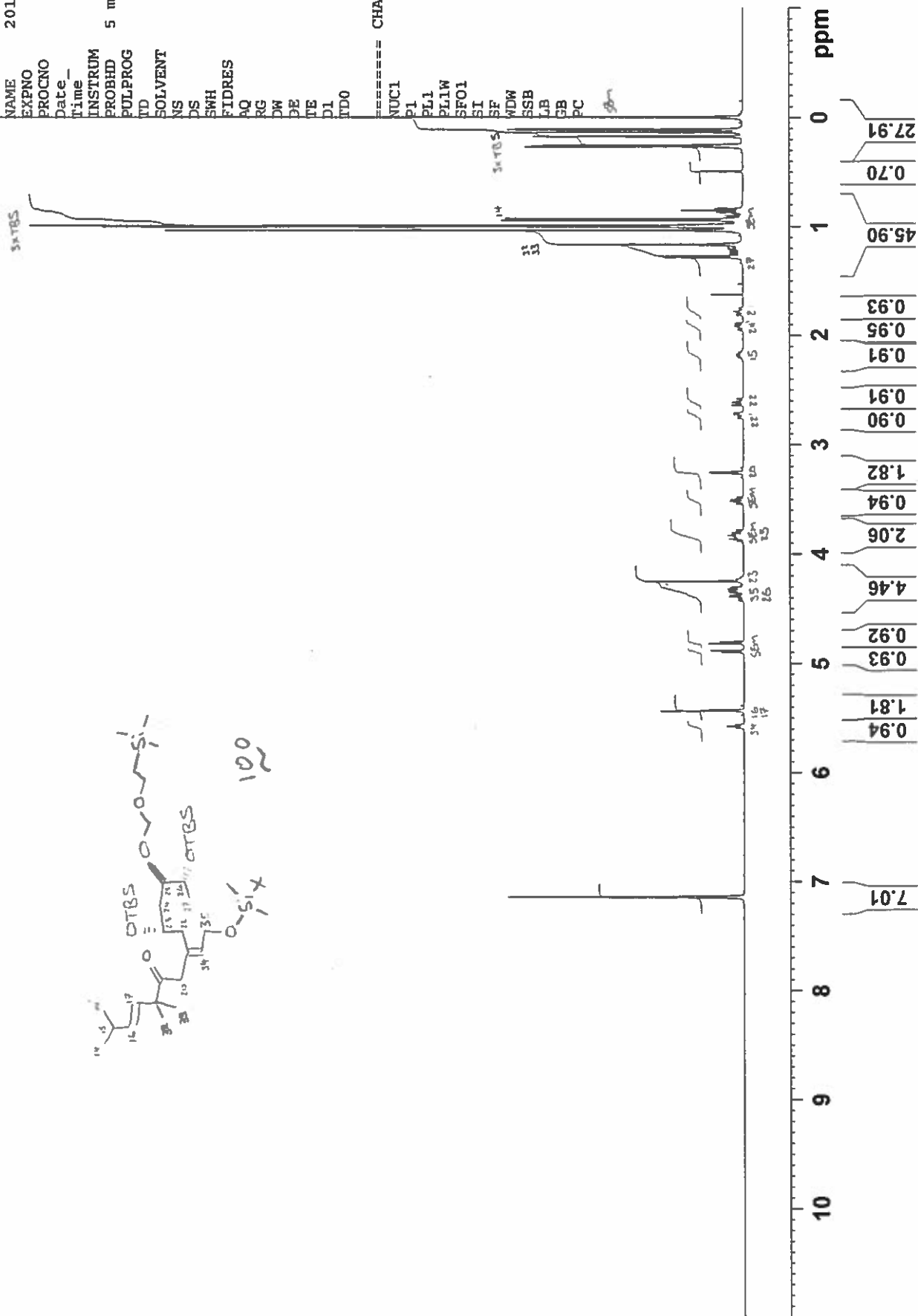
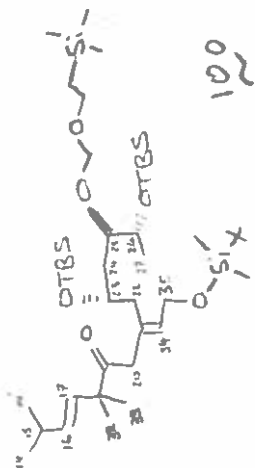


atlltristbsketone  
mPROTON C6D6 {e:\bruk400data\2010\Oct} ejt 32



2010-10-31-ejt-32  
NAME  
EXNO 10  
PROCNO 1  
Date 20101031  
Time 23.28  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 101  
DW 60.500 usec  
DE 9.40 usec  
TE 293.1 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
PLW 17.83863831 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300529 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

3xTBS

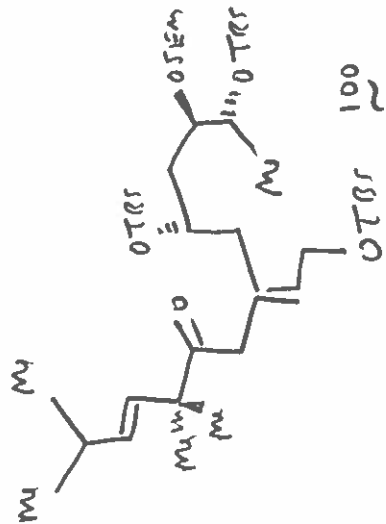


atltristbketone  
mCARBON C6D6 {e:\bruk400data\2010\Oct} ejt 32



138.71  
133.35  
133.35  
129.59  
129.47  
129.35  
129.23  
129.11

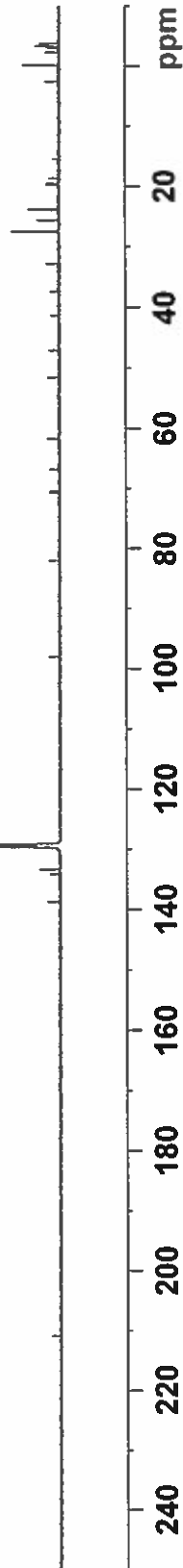
32.89  
27.65  
27.52  
27.50  
25.70  
23.93  
19.83  
19.72  
19.67  
19.65  
2.71  
-0.00  
-2.16  
-2.87



NAME 2010-11-01-ejt-32  
EXPNO 20  
PROCNO 1  
Date 20101101  
Time 8.31  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT C6D6  
NS 256  
DS 2  
SWH 30241.936 Hz  
FIDRES 0.461455 Hz  
AQ 1.0835786 sec  
RG 512  
DW 16.533 usec  
DE 7.83 usec  
TE 293.8 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

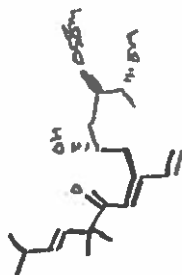
===== CHANNEL f1 =====  
NUC1 13C  
P1 8.00 usec  
PL1 0.00 dB  
PL1W 34.91522217 W  
SFO1 100.6241042 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.60 dB  
PL12 15.31 dB  
PL13 18.00 dB  
PL2W 17.83863831 W  
PL12W 0.22927761 W  
PL13W 0.12341322 W  
SFO2 400.1316005 MHz  
SI 32768  
SF 100.6126143 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 0.20

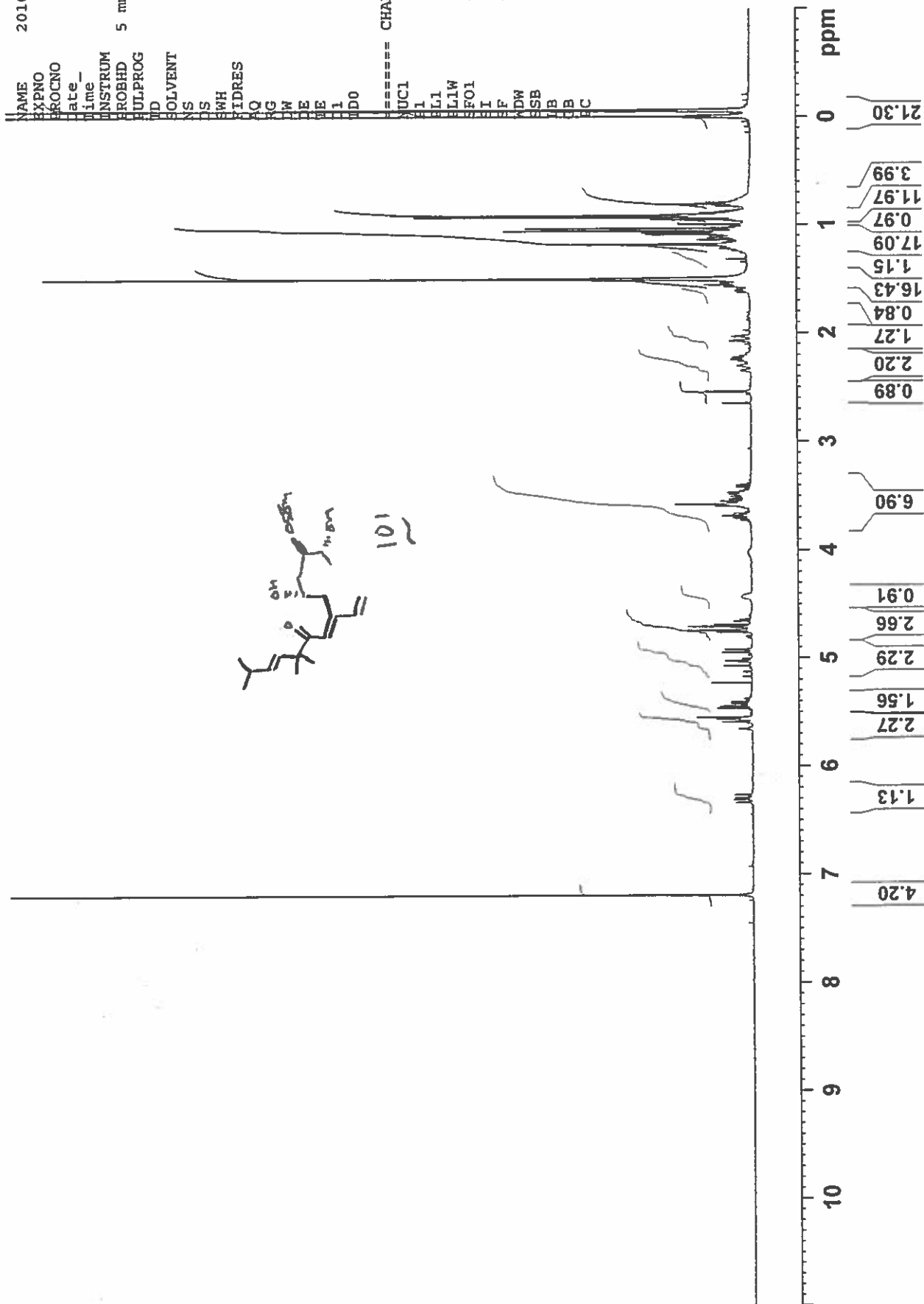




NAME 2010-11-05-ejt-11  
EXPNO 10  
PROCNO 1  
Date\_ 20101105  
Time\_ 11.45  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 406  
LW 60.500 usec  
DE 9.40 usec  
WE 293.1 K  
F1 1.00000000 sec  
F2 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
LLW 17.83863831 W  
SFO1 400.1324710 MHz  
FI 32768  
SF 400.1300364 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



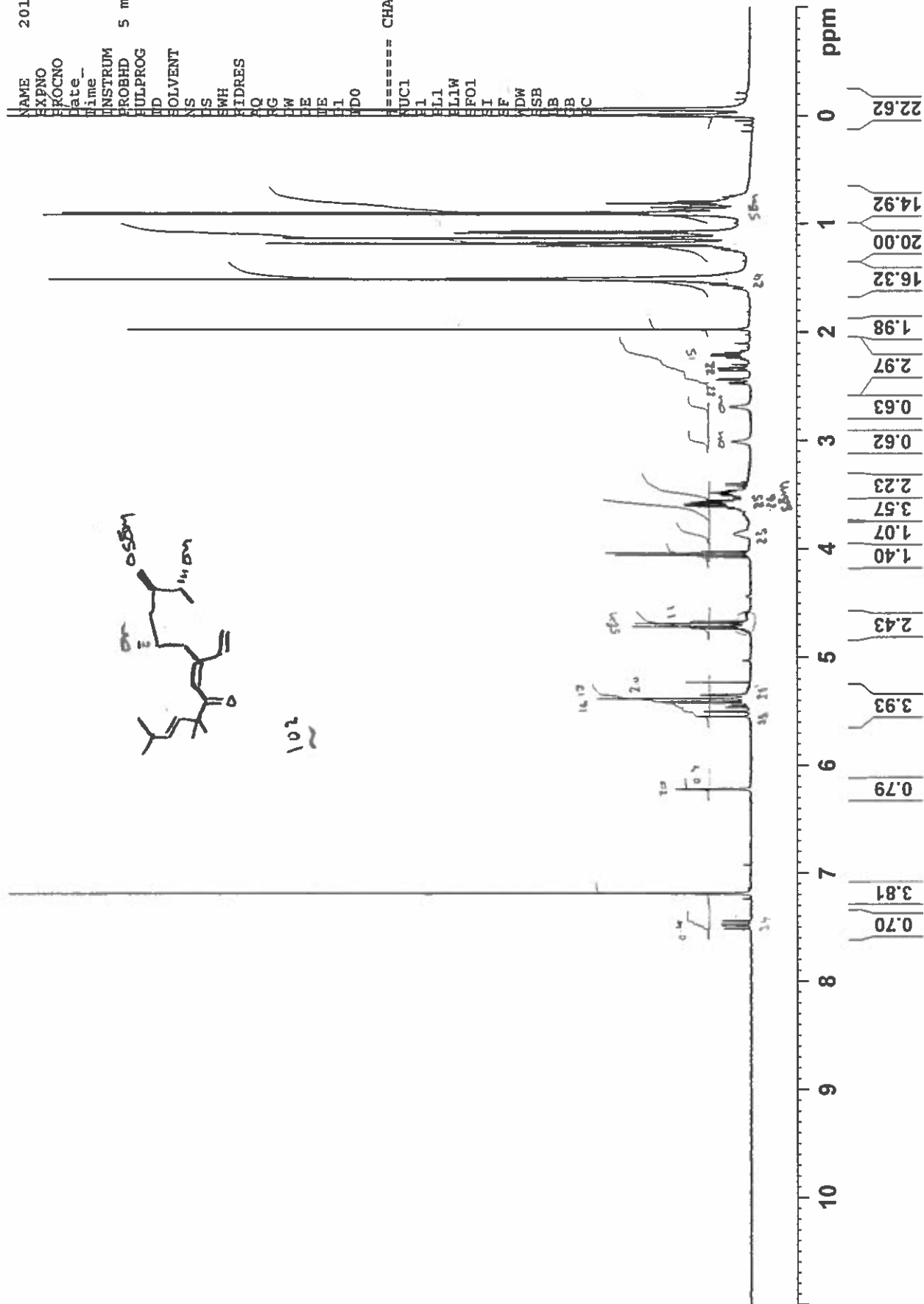
(101)



atl1tristbketonetbaf2  
mPROTON CDC13 {e:\bruk400data\2010\Nov} ejt 12



NAME 2010-11-05-ejt-12  
EXPNO 10  
PROCNO 1  
Date\_ 20101105  
Time 11.59  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zg30b  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 0  
SWH 8264.463 Hz  
FIDRES 0.126106 Hz  
AQ 3.9649780 sec  
RG 406  
LW 60.500 usec  
DE 9.40 usec  
TE 293.1 K  
F1 1.00000000 sec  
FID0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -3.60 dB  
FLW 17.83863831 W  
FOL 400.1324710 MHz  
FI 32768  
SF 400.1300362 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





NAME \_\_\_\_\_

EXPNO

10  
20  
30  
40  
50  
60

**NUC1**

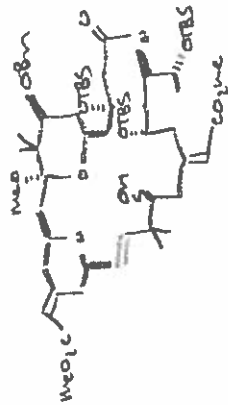




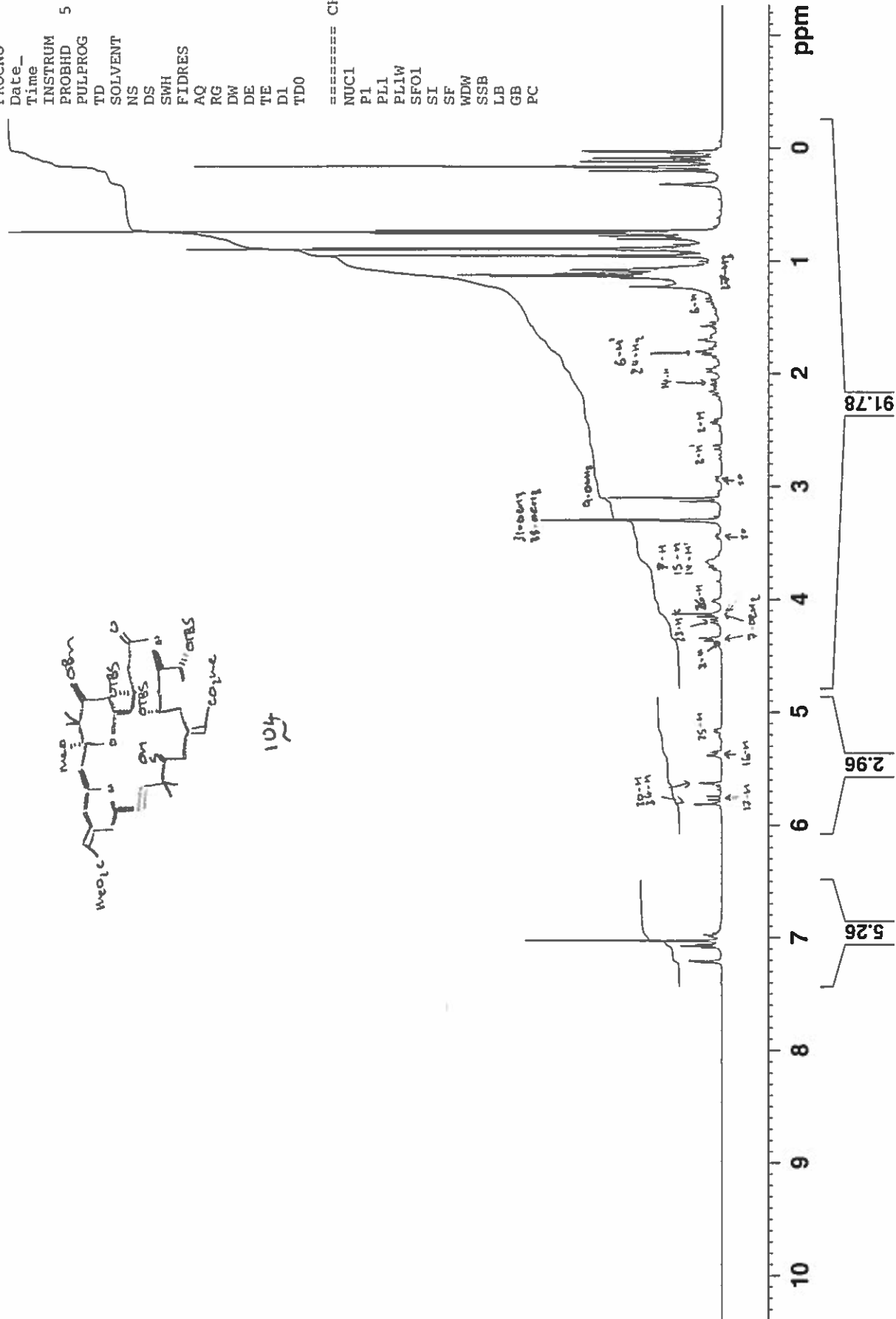
2011-02-22-ejt-14

NAME  
EXPNO 10  
PROCNO 1  
Date\_ 20110223  
Time 7.56  
INSTRUM spect  
PROBHD 5 mm TXI 1H/D-  
PULPROG zg30b  
TD 65536  
SOLVENT C6D6  
NS 64  
DS 0  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 228  
DW 48.400 usec  
DE 10.67 usec  
TE 294.7 K  
D1 1.00000000 sec  
TD0 1

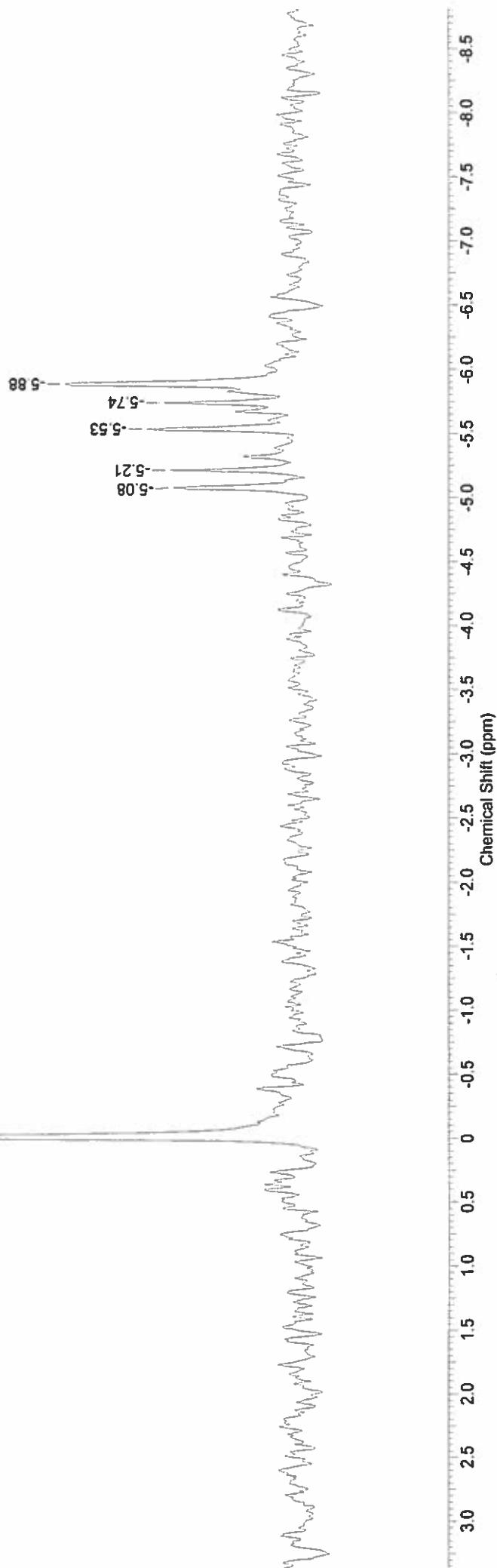
===== CHANNEL f1 =====  
NUC1 1H  
P1 21.07 usec  
PL1 3.25 dB  
PL1W 12.12272263 W  
SFO1 500.1330885 MHz  
SI 32768  
SF 500.1301224 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

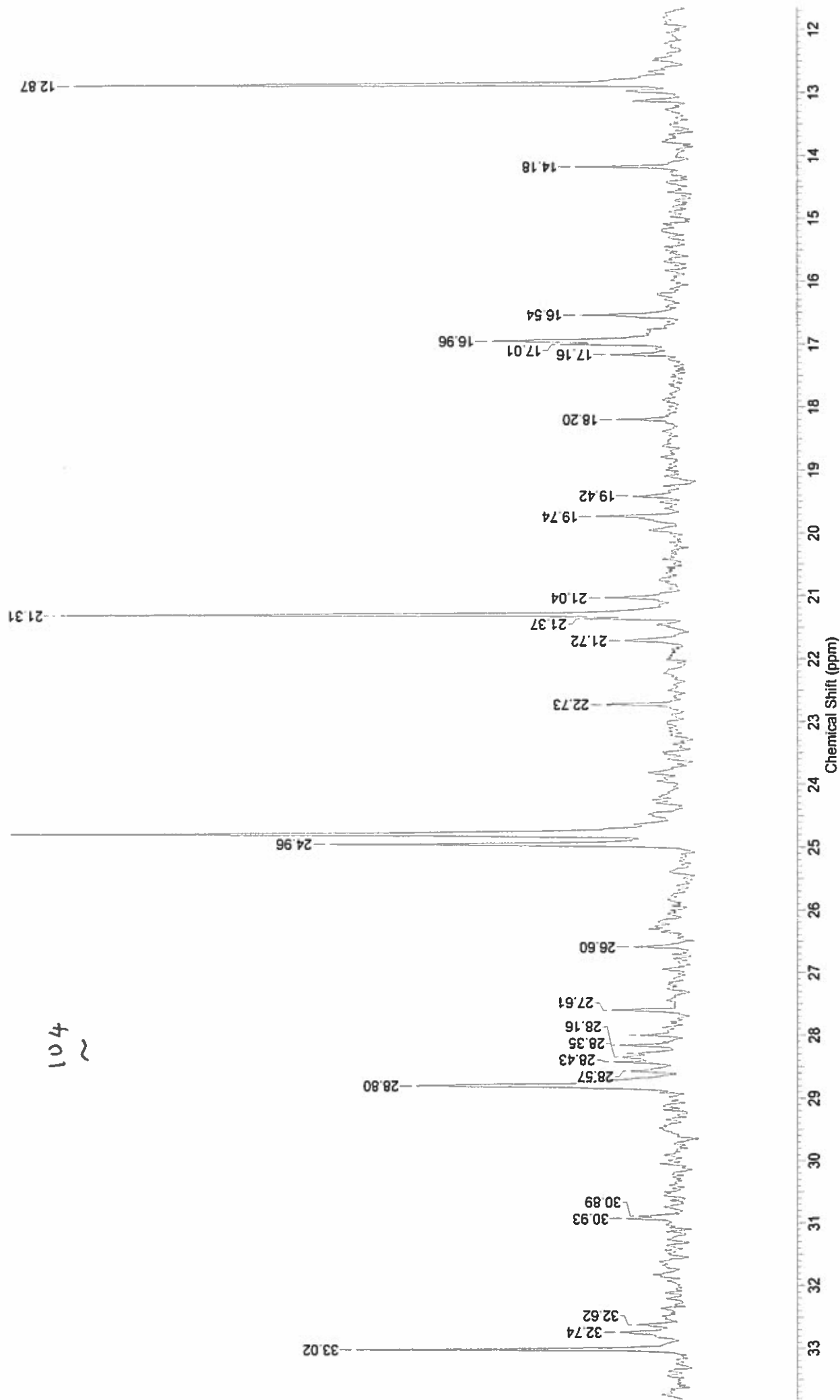


104

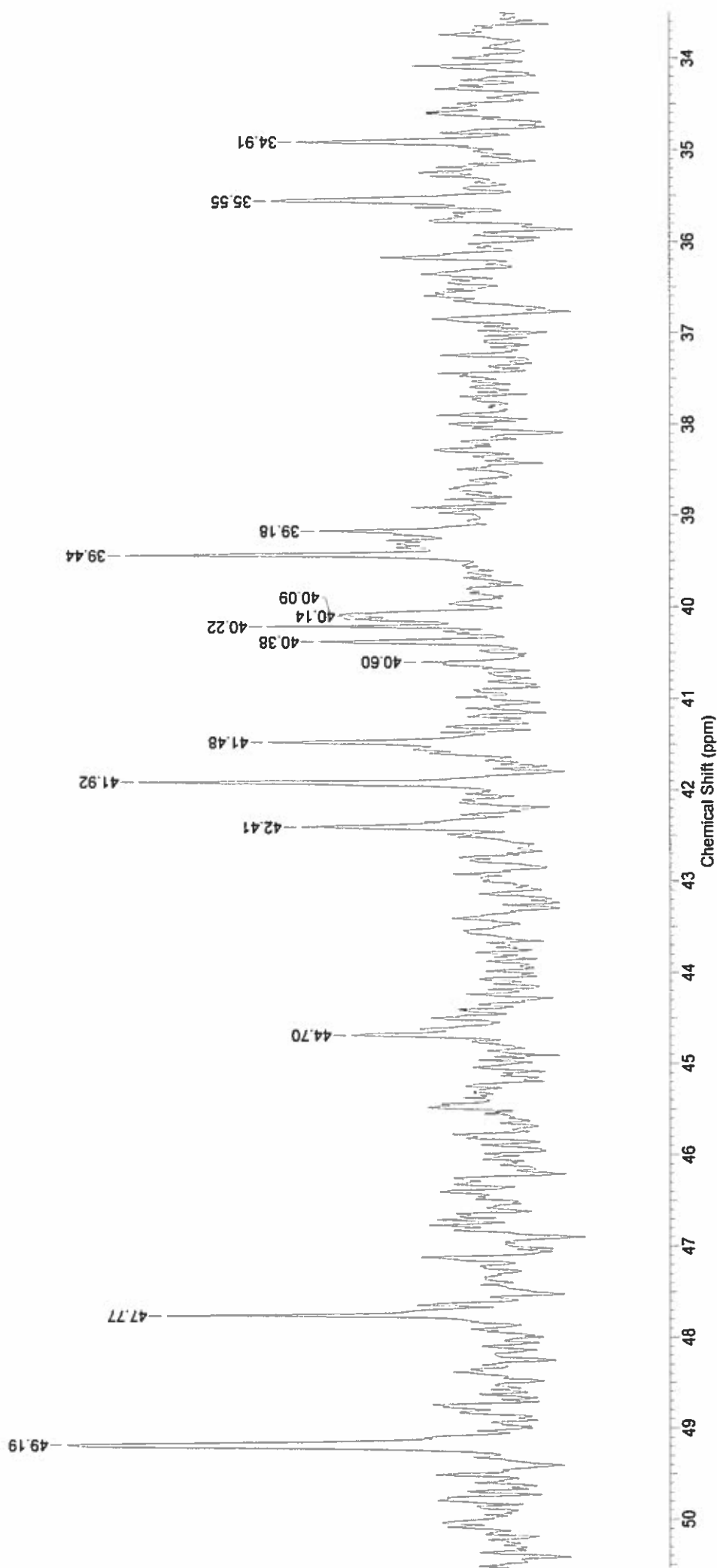


104  
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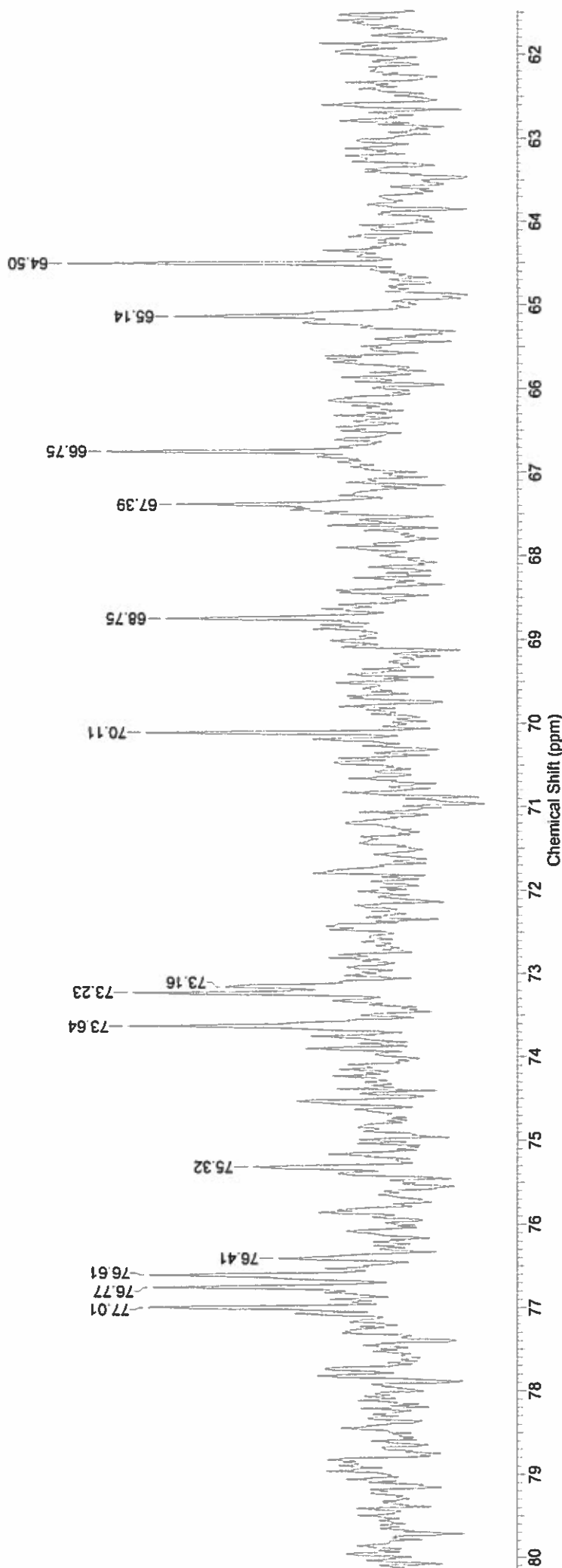




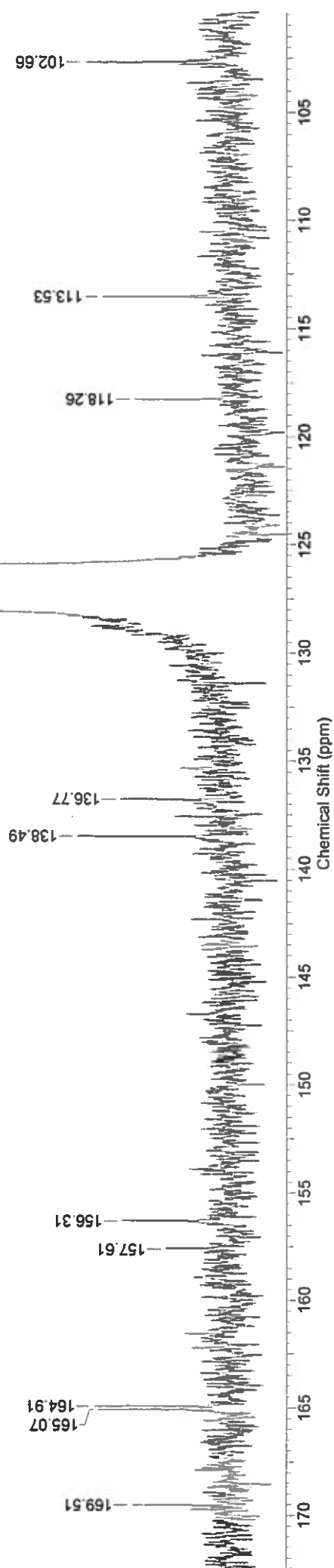
201

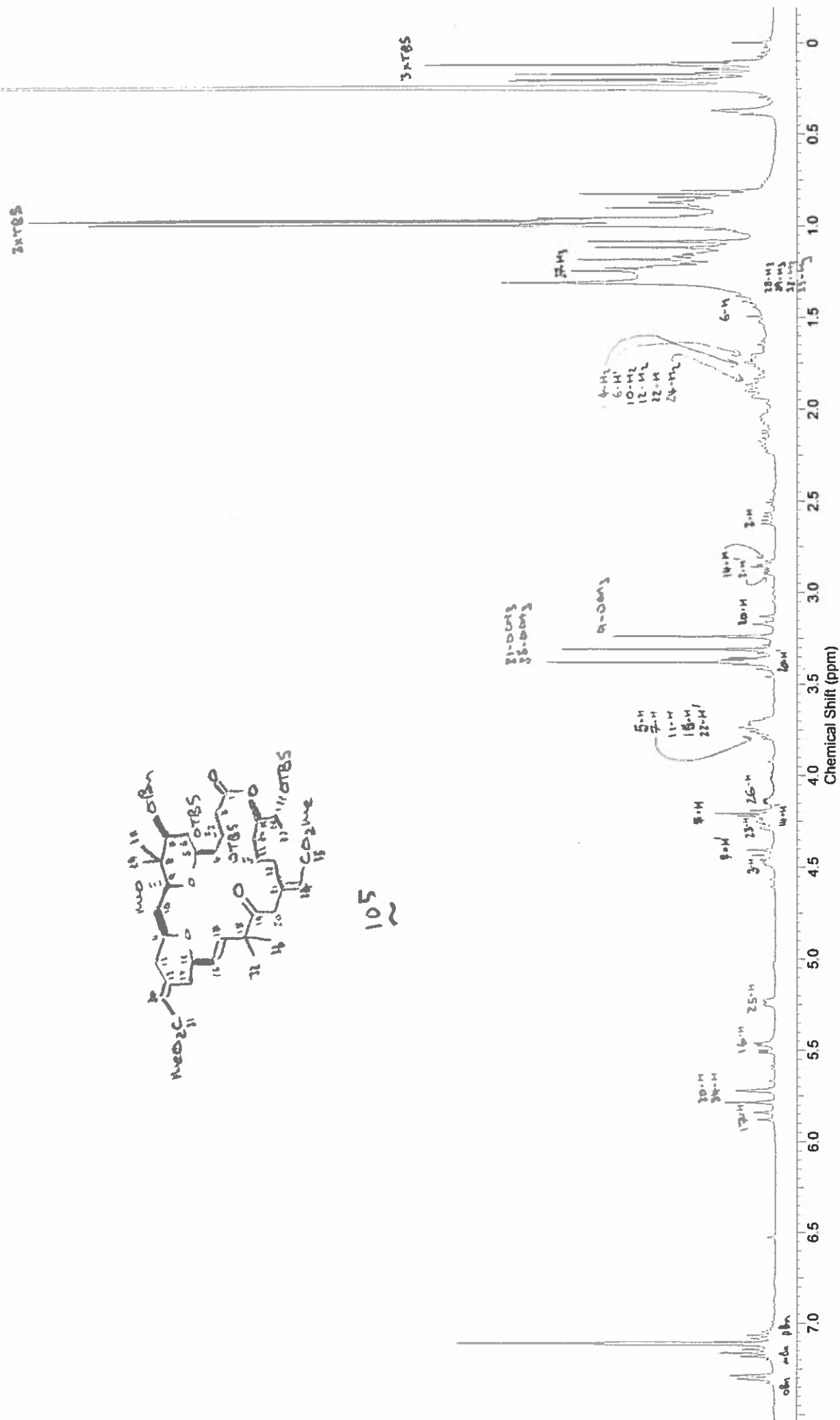


104



104



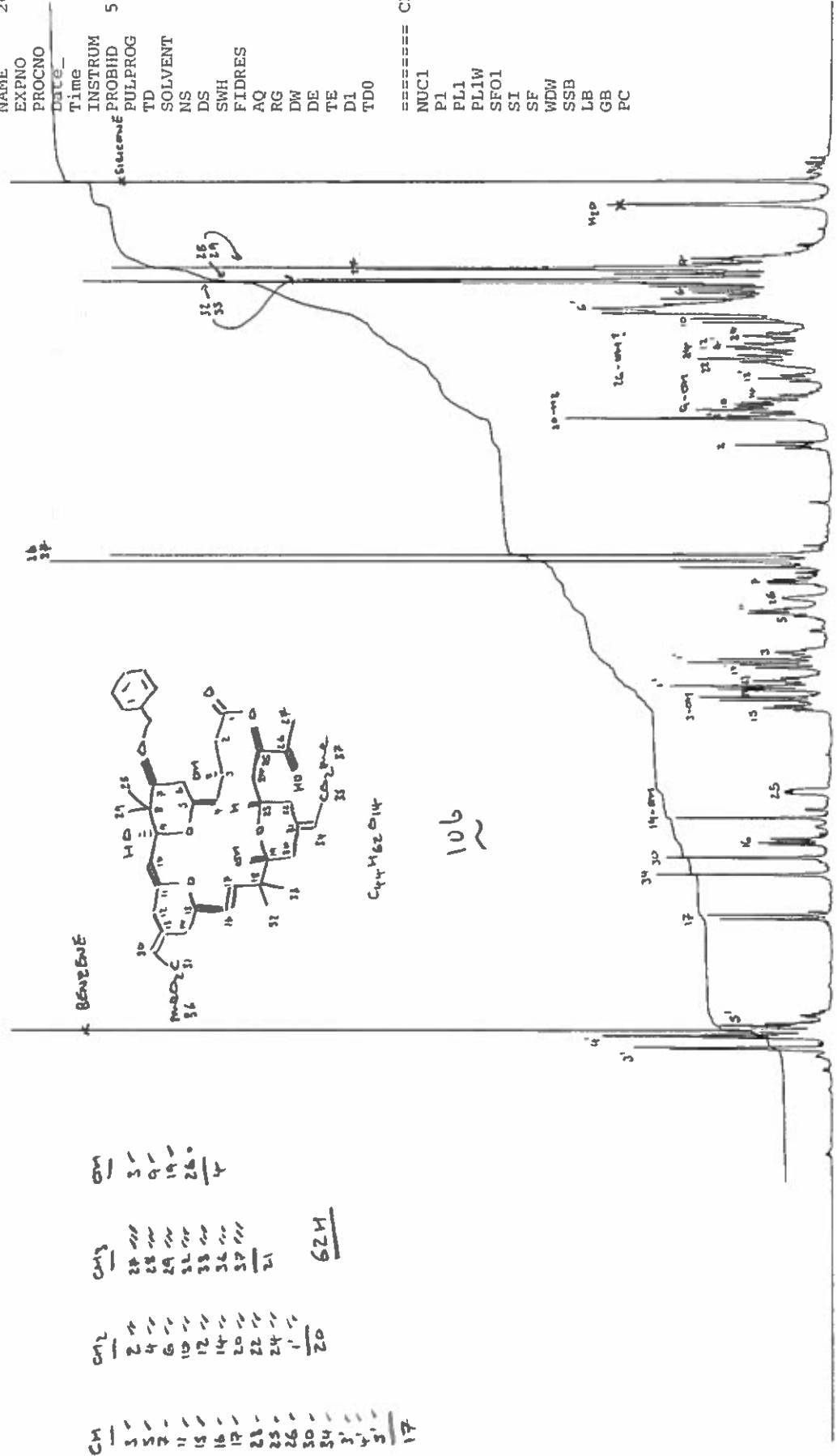






NAME 2011-04-12-ejt-54  
 EXPNO 20  
 PROCNO 1  
 Date\_ 20110413  
 Time 0.19  
 INSTRUM spect  
 PROBHD 5 mm TXI 1H/D-  
 PULPROG zg30b  
 TD 65536  
 SOLVENT C6D6  
 NS 2048  
 DS 0  
 SWH 10330.578 Hz  
 FIDRES 0.157632 Hz  
 AQ 3.171923 sec  
 RG 406  
 DW 48.400 usec  
 DE 10.67 usec  
 TE 296.4 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 21.07 usec  
 PL1 3.25 dB  
 PL1W 12.12272263 W  
 SFO1 500.1330885 MHz  
 SI 32768  
 SF 500.1301088 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



mCARBON c6d6{E:\bruk400service\_data\2011\Mar} Administrator 23  
 Alan Lee 0311-039  
 ATLL 7 O-Bn-Bryostatins16



2011-03-29-Administrator-61

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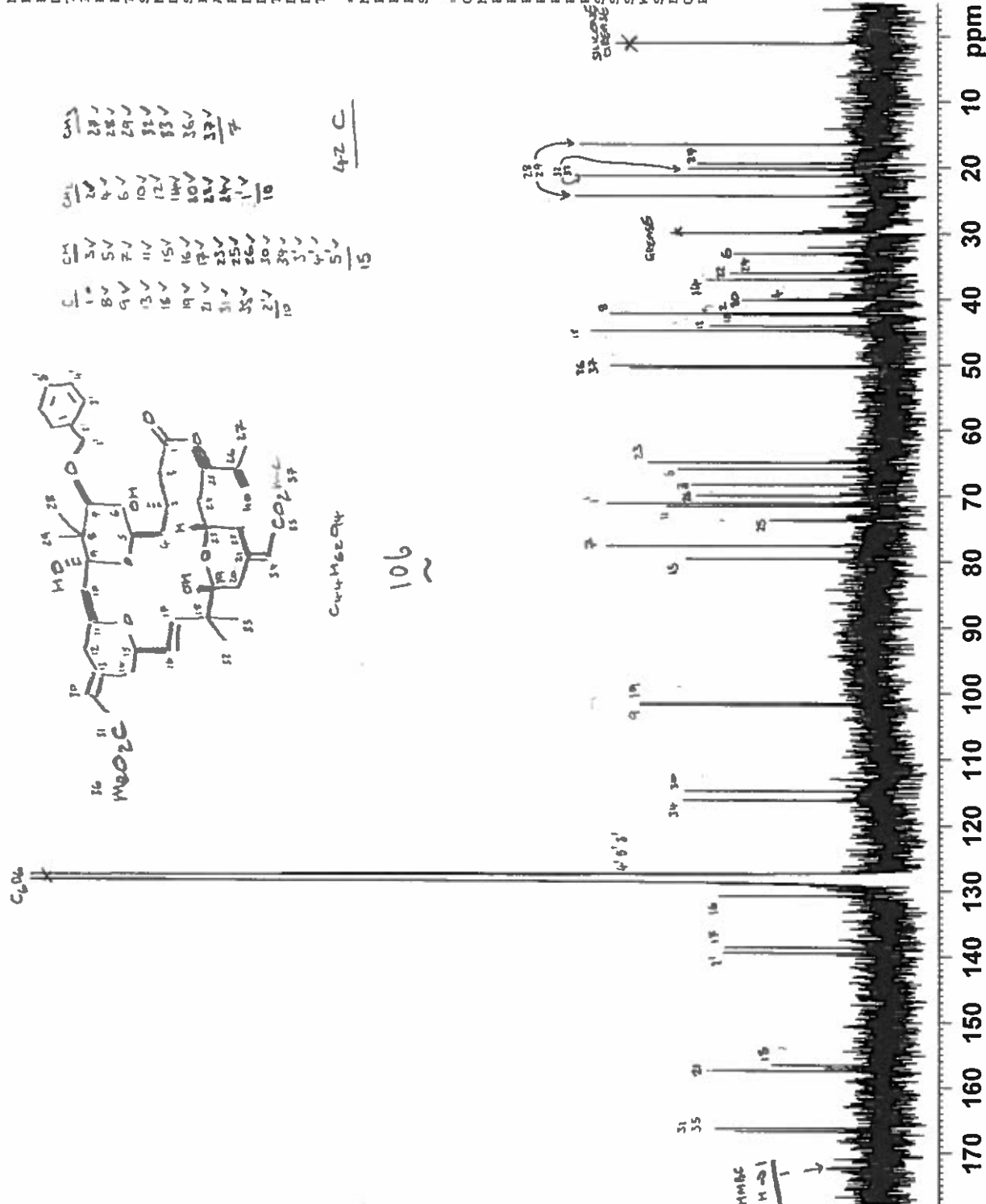
NAME EXPNO 11
PROCNO 1
Date_ 20110329
Time_ 12.56
INSTRUM AV400 S
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 98150
SOLVENT C6D6
NS 112634
DS 4
SWH 24038.461 Hz
FIDRES 0.250010 Hz
AQ 1.9999700 sec
RG 2050
DM 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1
  
```

```

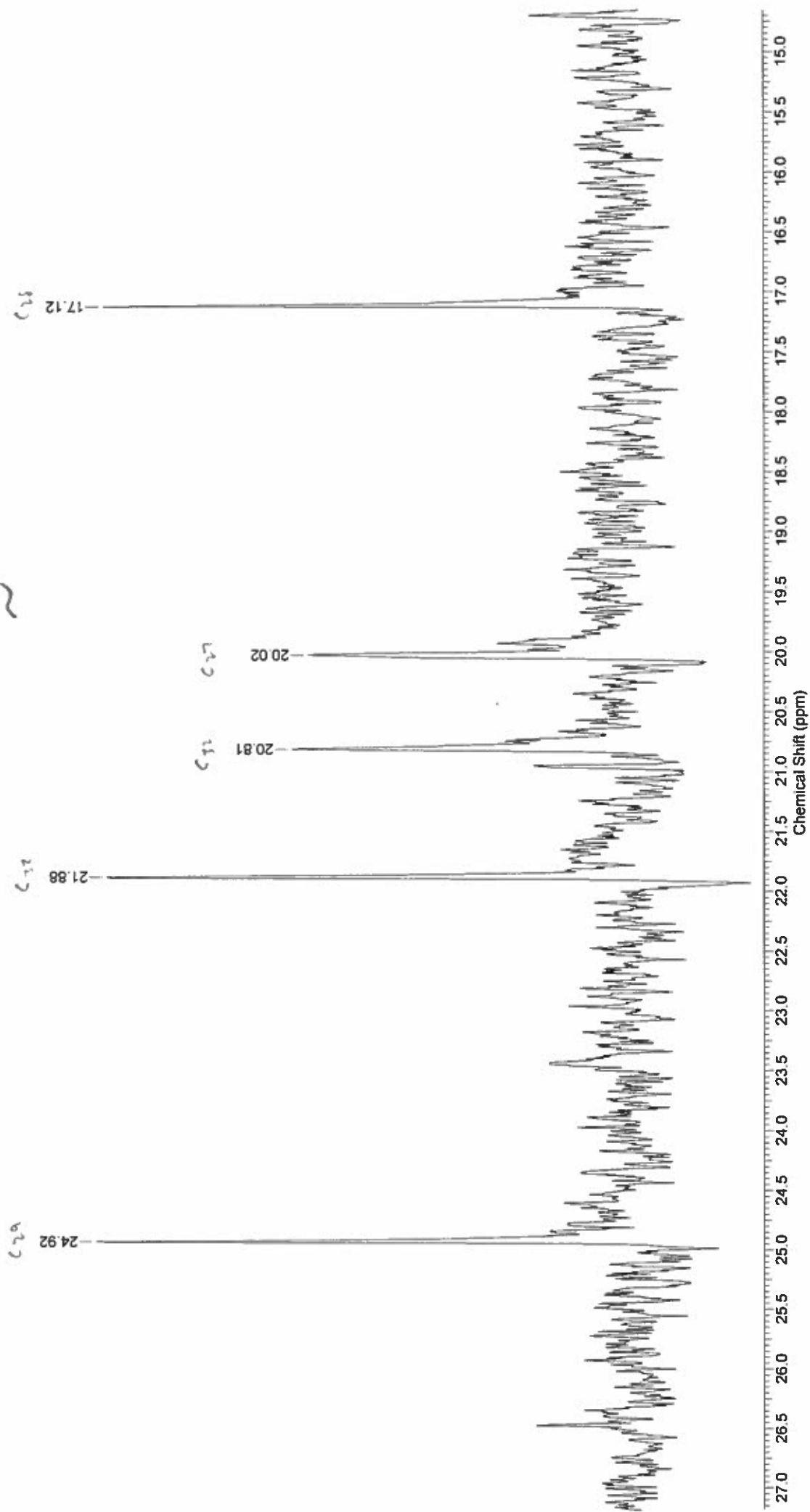
===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 33.91046524 W
SFO1 100.6479773 MHz
  
```

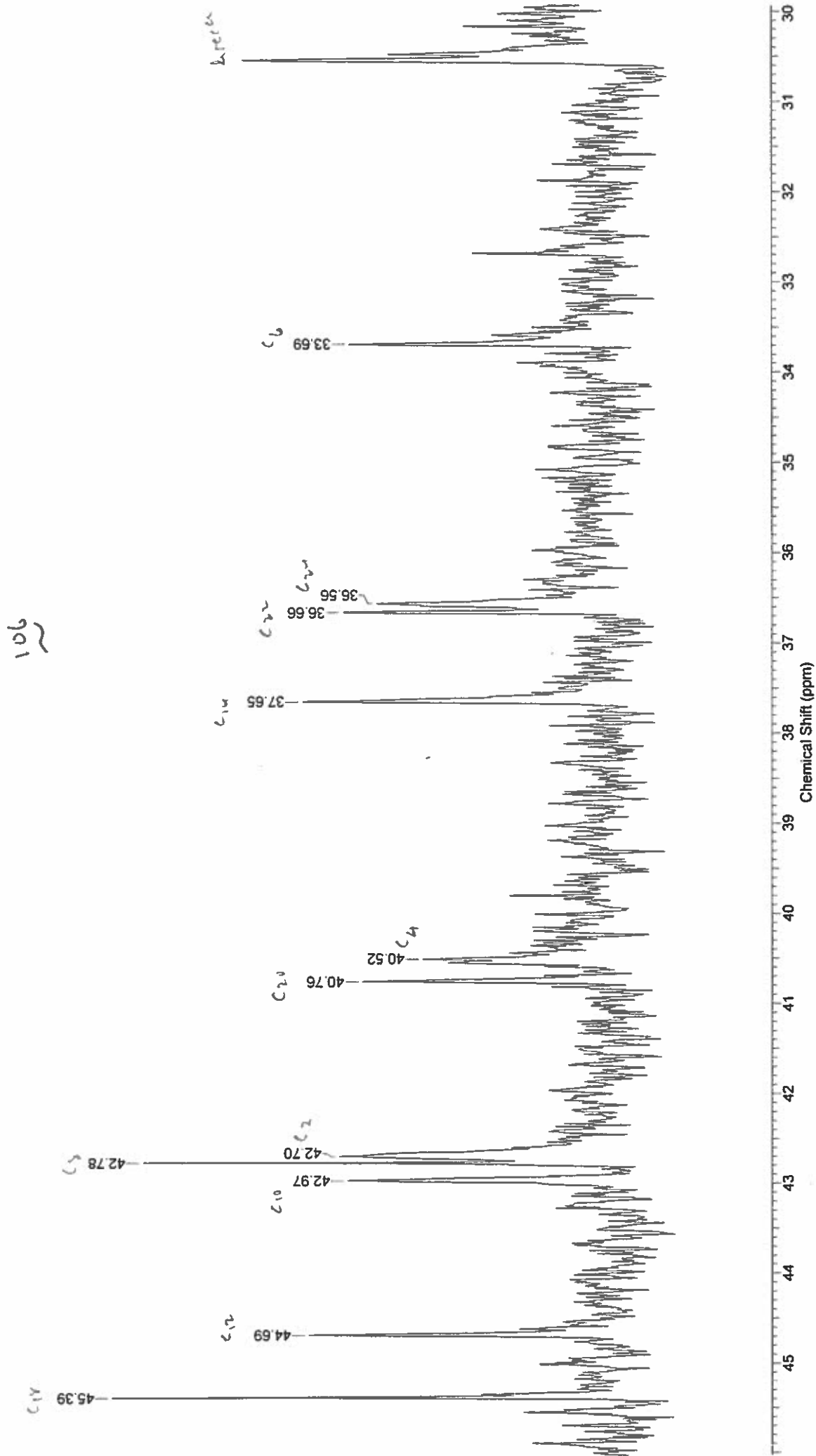
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===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.60 dB
PL12 15.31 dB
PL13 18.00 dB
PL12W 18.98951721 W
PL12W 0.24406971 W
PL13W 0.13137537 W
SFO2 400.2316009 MHz
SI 32768
SF 100.6379140 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```



106





106

C77

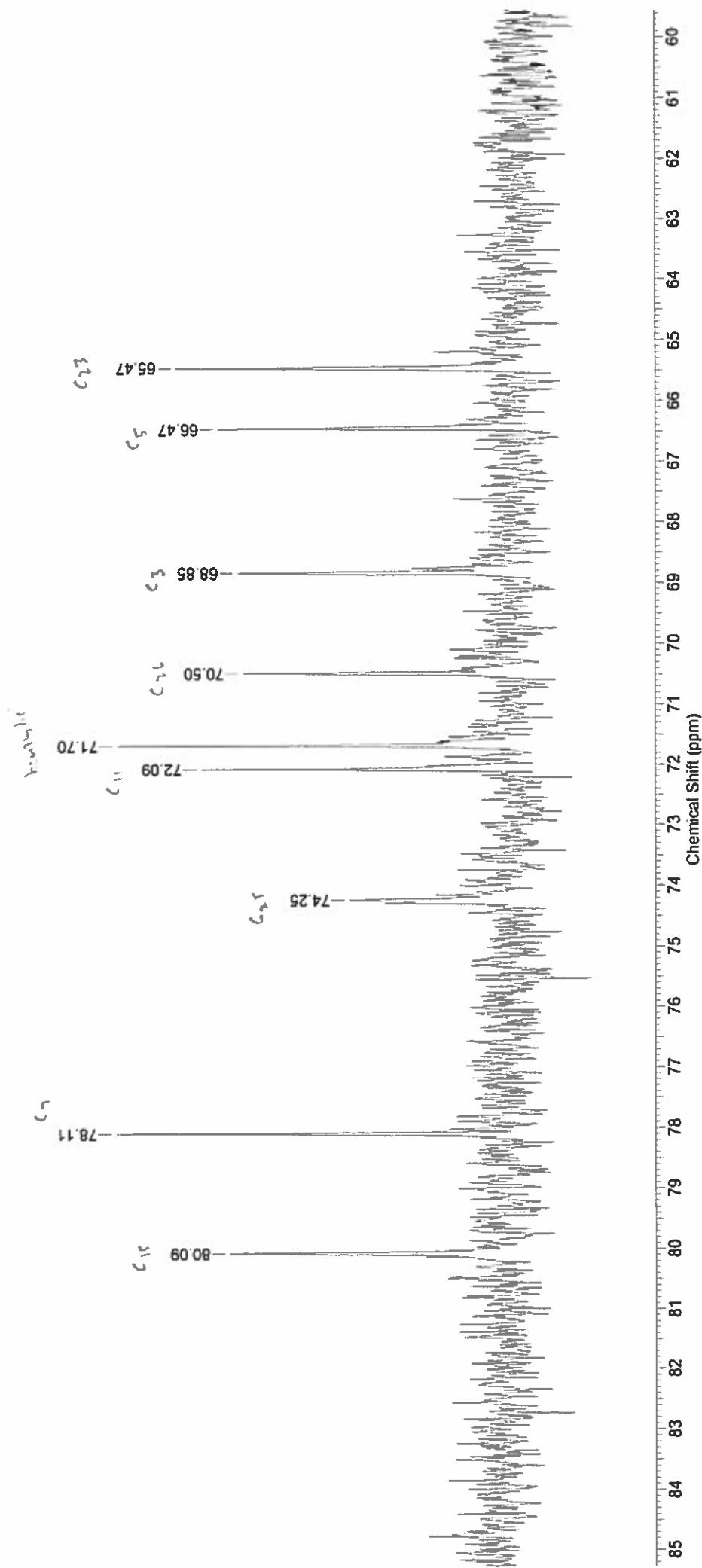
50.76

C36

51.05

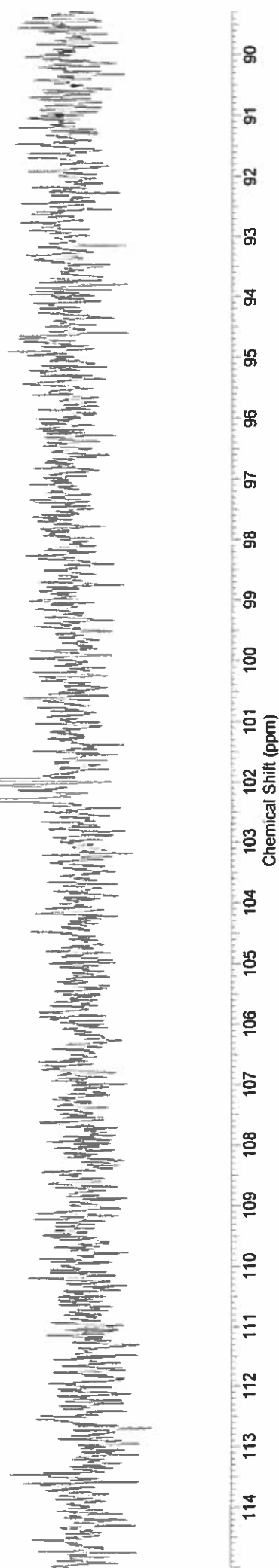


106  
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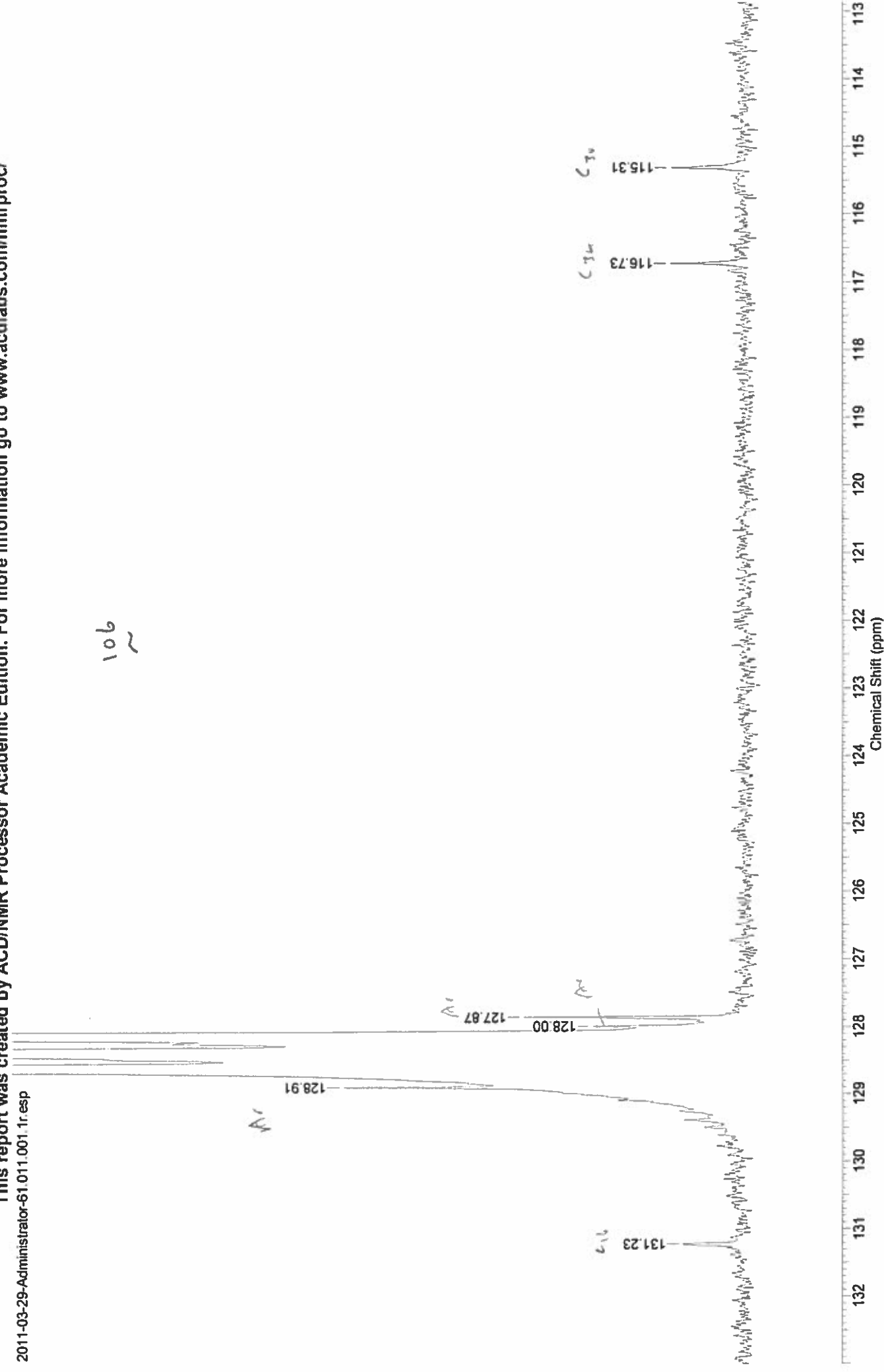
106

102.30  
101.97



2011-03-29-Administrator-61.011.001.1r.esp

106  
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106

