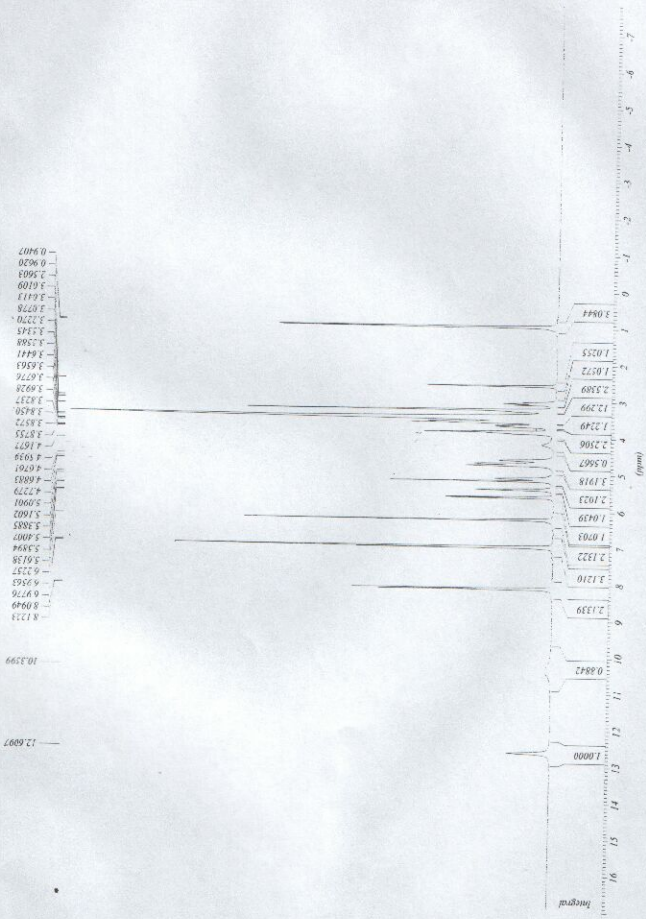


DM12-4



Current Data Parameters  
 NAME DWB-4  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

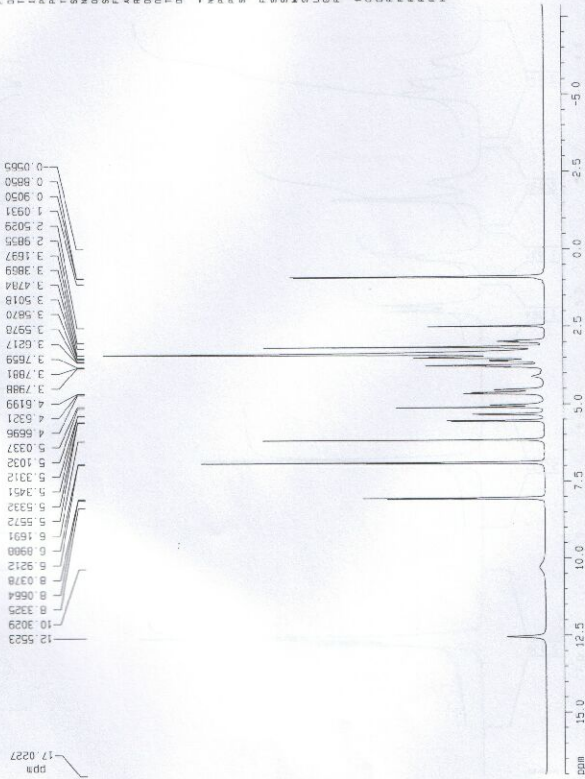
Date\_ 20050622  
 Time 17:39  
 INSTRUM spect  
 PULPROG 5 mm BBP BH-1H  
 TO 10.30  
 SOLVENT 16384  
 NS 16  
 DS 0  
 SWH 7465.030 Hz  
 FWHZ 0.450000 Hz  
 AQUE 1.0945013 sec  
 RG 181  
 DM 66.800 uPFC  
 SF 6.00 uPFC  
 TE 300.0 K  
 D1 2.0000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*

MU1 0p  
 P1 11.75 uPFC  
 PL 1  
 LOFF 3.00 dB  
 FREQ 300.1313730 MHz

F2 - Processing Parameters

SF 300.1313730 MHz  
 WDW EM  
 SSB 0  
 GB 0  
 PC 1.00  
 10 MHz PLOT PARAMETERS  
 PL 0.00 cm  
 SL 12.00 cm  
 F1/P 17.040 ppm  
 F1 5114.22 Hz  
 F2/P -7.859 ppm  
 F2 -2370.81 Hz  
 PPHON 1.10159 ppm/cm  
 HCON 356.02559 Hz/cm



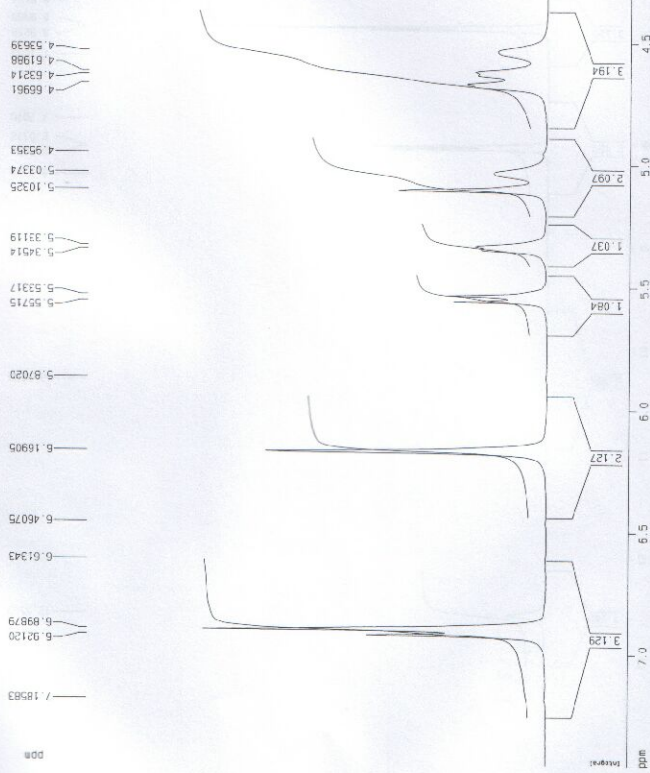
17.0227  
 ppm

Current Data Parameters  
 Name: DMF-4  
 ExpNO: 1  
 PROCNO: 1

F2 - Acquisition Parameters  
 Date\_: 20050622  
 Time: 7.59  
 HostNO: 1  
 PROCNO: 1  
 F2: 300.1300013 MHz  
 TO: 0.30 Hz  
 SOLVENT: DMSO  
 NS: 16  
 DS: 0  
 SWH: 7495.030 Hz  
 FIDRES: 6.408566 Hz  
 AQ: 1.0945013 SEC  
 RG: 327.5  
 DM: 65.800 uSAC  
 DE: 5.00 uSAC  
 TE: 300.0 K  
 D1: 2.00000000 SEC

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUCL1: 13  
 P1: 11.35 uSAC  
 PL1: 3.00 dB  
 SF01: 300.1313730 MHz  
 F2 - Processing parameters  
 S1: 8152  
 SF: 300.1300013 MHz  
 SWH: 0  
 SFO: 0  
 LE: 0.30 Hz  
 GB: 0  
 PC: 1.00

1D NMR plot parameters  
 CX: 21.00 cm  
 CY: 7.00 cm  
 FID: 1.00  
 F1: 2039.37 Hz  
 F2: 4.310 009  
 FWHM: 1.990 50 Hz  
 PPMXN: 0.15007 ppm/cm  
 HZCN: 45.04160 Hz/cm



Current Data Parameters  
 NAME DMF-d  
 DATE 1  
 300200

6.6134  
 6.8988  
 6.9212  
 7.1858  
 7.7970  
 8.0378  
 8.0564  
 8.3325

10.3029

12.5523

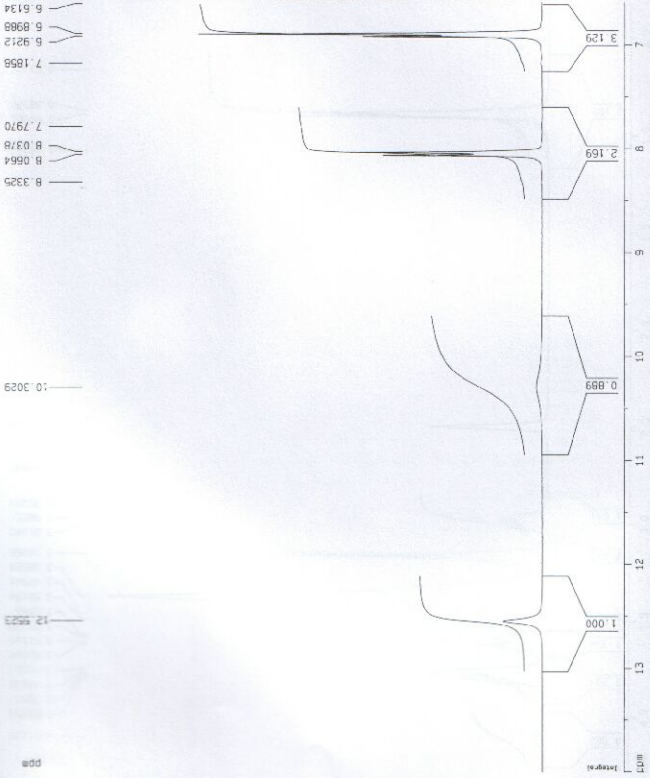
ppm

F2 - Acquisition Parameters  
 Date\_ 20050522  
 Time 7.59  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 0  
 SWH 7485.020 Hz  
 FIDRES 0.456850 Hz  
 AQ 1.356013 sec  
 RG 327.5  
 DW 800.000 nsec  
 DE 6.000 nsec  
 TE 300.0 K  
 SE 1  
 SI 1  
 2.03000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUCL1 1H  
 P1 11.20 nsec  
 PL1 1.00 dB  
 SFO1 300.1311330 MHz

F2 - Processing parameters  
 SI 8192  
 SF 300.1300013 MHz  
 SDM SM  
 SFO2 300.1300013 MHz  
 LB 6.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 21.00 cm  
 CY 12.00 cm  
 FIP 4300.000 Hz  
 F2D 6.593 Hz  
 F2 1978.70 Hz  
 PRINOM 3.3532 deg/cx  
 HZDM 105.04236 Hz/cm



Current Data Parameters  
 NAME DMT-4  
 EPOCH 1  
 PUNCH 1

F2 - Acquisition Parameters  
 DATE 20050622  
 TIME 7.55

INSTRAN spect  
 PULPROG 5 ms BBO BB-14  
 TO 79.36  
 10 108.24  
 16 108.24

SOLVENT DMF0  
 DS 0  
 SS 0

SMH 7485.030 Hz  
 FIDRES 0.466550 Hz  
 AQ 1.0945013 sec

RG 81  
 GB 64  
 GC 6.00 usec  
 GZ 300.0 K  
 D1 2.00000000 sec

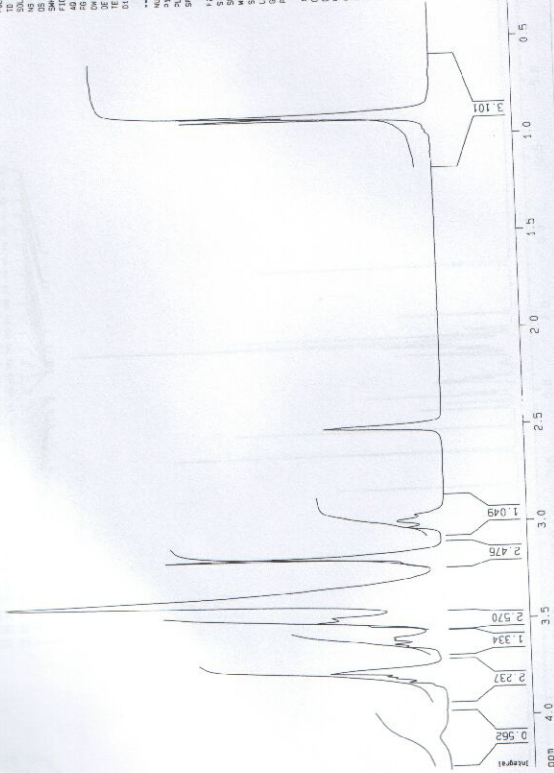
\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 11.75 usec  
 PL 1.4  
 PR 300.1313700 MHz  
 SFO1 570.1

F2 - Processing parameters  
 SI 8192  
 SF 300.1300013 MHz  
 WDW EM  
 SS 0  
 LB 0.3 Hz  
 GB 0  
 PC 1.00

10 NMR plot parameters  
 CX 21.00 cm  
 CY 17.00 cm  
 CZ 4.285 000  
 IZ 1285.05 000  
 IY 0.11 000  
 IZ 54.40 000  
 FWHM 3.88007 000/cm  
 HZSM 56.74507 MHz/cm

0.67407  
 0.88500  
 0.90501  
 1.09312

2.50286  
 2.72940  
 2.95422  
 2.98258  
 3.01590  
 3.03965  
 3.26089  
 3.47947  
 3.50394  
 3.52637  
 3.59779  
 3.62166  
 3.63600  
 3.75909  
 3.78808  
 3.79877  
 3.81956  
 4.11120



Current Data Parameters  
 NAME Dns-4  
 EPOCH 1  
 PRODIG 1

#2 - Acquisition Parameters

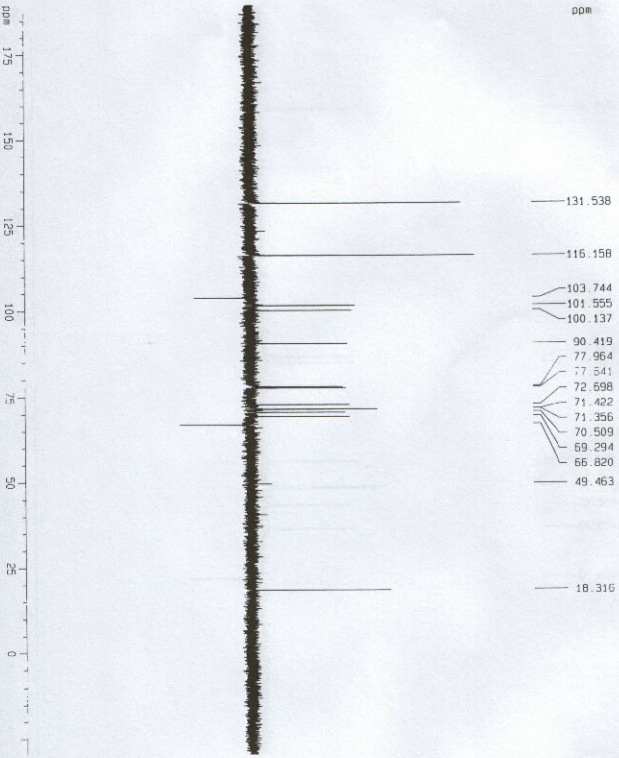
DATE 20050622  
 TIME 8.38  
 INSTRUM SECT1  
 PRODIG 5 m BRU BR1  
 P1/PROD 06/11/25  
 T0 06/23/05  
 SC VENT HIGH  
 NS 259  
 OS 1  
 SMH 16556.291 Hz  
 F1/DRES 0.2456629 Hz  
 AQ 1 97923172 SMC  
 NO 183950 #  
 SW 30.200 uS/C  
 SC 8.00 uS/C  
 ZE 32000 K  
 CRSTR 145.0000000  
 T 0.00000001 sec  
 R2 0.00000000 sec  
 R12 0.00002000 sec  
 DELTA 0.00001000 sec

\*\*\*\*\* CHANNEL 11 \*\*\*\*\*  
 WACT 13C  
 P1 8.50 uS/C  
 S2 17.00 uS/C  
 S1 1.00 sec  
 S/T0 75.4173264 sec

\*\*\*\*\* CHANNEL 12 \*\*\*\*\*  
 CHOPRG w12r16  
 WACT 1H  
 P1 11.75 uS/C  
 S2 23.50 uS/C  
 S1 100.00 uS/C  
 P12 3.20 sec  
 P12 22.00 sec  
 S/T0 300.1155007 sec

#2 - Processing Parameters  
 F1 32768  
 S1 75.4637150 sec  
 MON FM  
 SSB 0  
 LB 0.50 Hz  
 GB 0  
 PC 1.40

10 NMR D1/D2 Parameters  
 CA 29.00 cm  
 CR 1.00 cm  
 F1P 189.801 sec  
 S1 1.6415 56 Hz  
 F2P -29.681 sec  
 F2 -22.46 73 Hz  
 PPHCM 10.95912 sec/cm  
 HZCM R27 81.464 Hz/cm



Current Data Parameters  
Date: 20050822  
Time: 8:38  
INSTRUM: 5 ma 880 MR-14  
PROCNO: 3661135  
COLPRNO: 05236  
TO: VENT  
NS: VENT  
VS: VENT  
05: 195  
06: 1  
07: 1  
08: 1  
09: 1  
10: 1  
11: 1  
12: 1  
13: 1  
14: 1  
15: 1  
16: 1  
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18: 1  
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96: 1  
97: 1  
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99: 1  
100: 1

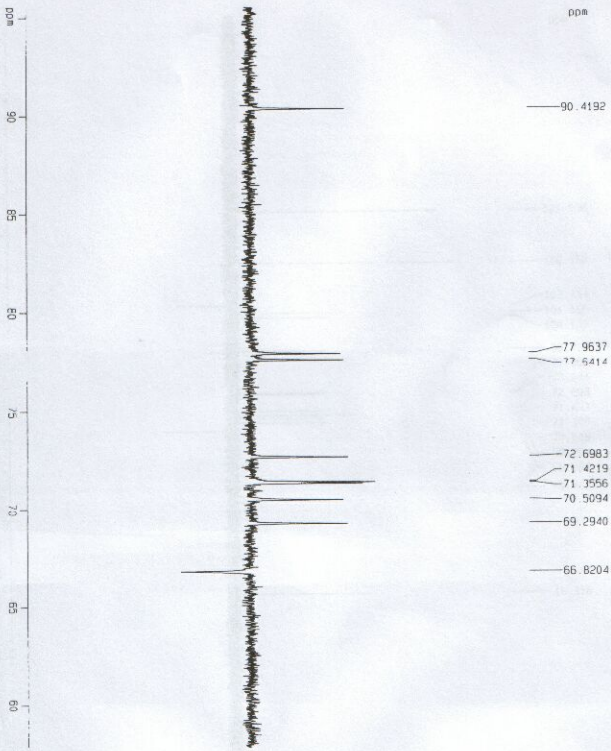
F2 - Acquisition Parameters  
Date: 20050822  
Time: 8:38  
INSTRUM: 5 ma 880 MR-14  
PROCNO: 3661135  
COLPRNO: 05236  
TO: VENT  
NS: VENT  
VS: VENT  
05: 195  
06: 1  
07: 1  
08: 1  
09: 1  
10: 1  
11: 1  
12: 1  
13: 1  
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96: 1  
97: 1  
98: 1  
99: 1  
100: 1

F2 - Processing Parameters  
SI: 32768  
SF: 75.4627180 MHz  
MOM: EM  
SSB: 0  
LB: 0.50 Hz  
GB: 0  
PC: 1.40

10 MAG D101 Parameters  
CX: 20.00 CM  
CY: 6.00 CM  
FIP: 95.408 DPM  
F1: 7215.30 Hz  
F2p: 57.643 DPM  
F2: 4365.31 Hz  
PRMCM: 1.68025 DPM/CM  
HZCM: 1.424584 Hz/1cm

\*\*\*\*\* CHANNEL 11 \*\*\*\*\*  
NUC1: 13C  
NUC2: 13C  
E1: 8.50 uSRT  
E2: 17.00 uSRT  
SFO1: 75.4737554 MHz  
DELTA: 0.000103925 SEC

\*\*\*\*\* CHANNEL 12 \*\*\*\*\*  
PROB02: wj1115  
IH: 1H  
NUC1: 11H  
NUC2: 11H  
E1: 11.75 uSRT  
E2: 23.50 uSRT  
ROCC2: 100.00 uSRT  
R12: 1.00 DB  
FL12: 22.00 DB  
SFO2: 200.1315007 MHz



ppm

ppm  
200  
175  
150  
125  
100  
75  
50  
25  
0

178.507	-	177.680
161.083	-	160.256
157.316	-	156.489
154.806	-	153.979
152.489	-	151.668
141.252	-	140.425
133.576	-	132.749
131.532	-	130.705
130.226	-	129.399
121.360	-	120.533
116.151	-	108.304
107.743	-	106.976
103.737	-	102.910
101.550	-	100.129
100.129	-	99.308
90.413	-	89.588
77.958	-	77.191
77.639	-	76.812
72.697	-	71.87
71.350	-	70.508
70.508	-	69.296
69.296	-	68.469
66.810	-	65.983
49.467	-	
41.156	-	
40.880	-	
40.604	-	
40.327	-	
40.047	-	
39.765	-	
39.486	-	
18.312	-	17.48

```

Current Data Parameters
NAME: 1
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_ 20050622
Time 8:17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SFO 500.136
GAMMA 160.00
SOLVENT
NS 1024
DS 2
SWH 18832.793 Hz
FIDRES 1.149438 Hz
AQ 0.4782452 sec
RG 8192
AQ 0.4782452 sec
DE 26.950 uS/cK
TE 300.0 K
1.50000000 Hz
0.03000000 Hz
0.00000000 Hz
0.00000000 Hz

***** CHANNEL f1 *****
NUC1 13C
P1 8.00 uS/cK
PL1 0.25 dB
SFO1 75.480204 MHz

***** CHANNEL f2 *****
DEPHAS2
NUC2 13C
P2 100.00 uS/cK
PL2 0.00 dB
SFO2 150.000000 MHz
SFO2 300.1312055 MHz

F2 - Processing Parameters
SI 8192
SF 75.4827190 MHz
AQ 1.00 uS
GB 0
DC 1.40

10 MHz B101 Parameters
CX 20.00 cm
CY 25.00 cm
F1P 238.731 GHz
F1 1231.65 MHz
F2P 14.731 GHz
F2 1231.65 MHz
SFO 123.4713 MHz
SFO2 300.1312055 MHz
AQ 0.4782452 sec
  
```



13C (zgpg30)

ppm

ppm 82 80 78 76 74 72 70 68 66 64

77.9579  
77.6386

72.6972

71.3503

70.523

70.5076

69.2960

66.8104



Current Data Parameters  
NAME 1  
EXPNO 5  
PROCNO 1  
PROCIN 1

F2 - Acquisition Parameters  
Date\_ 20050622

Time 6.17  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1024  
DS 2  
SWH 18832.393 Hz  
FIDRES 1.149458 Hz  
AQ 0.4385452 sec  
RG 655  
GZ 0.032  
SFO 500.136 MHz  
CZ 5.00 usec  
TE 300.2 K  
D1 1.50000000 sec  
d11 0.02000000 sec  
d12 0.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 13C  
P1 8.00 usec  
PL1 0.25 dB  
SFO1 75.4763004 MHz

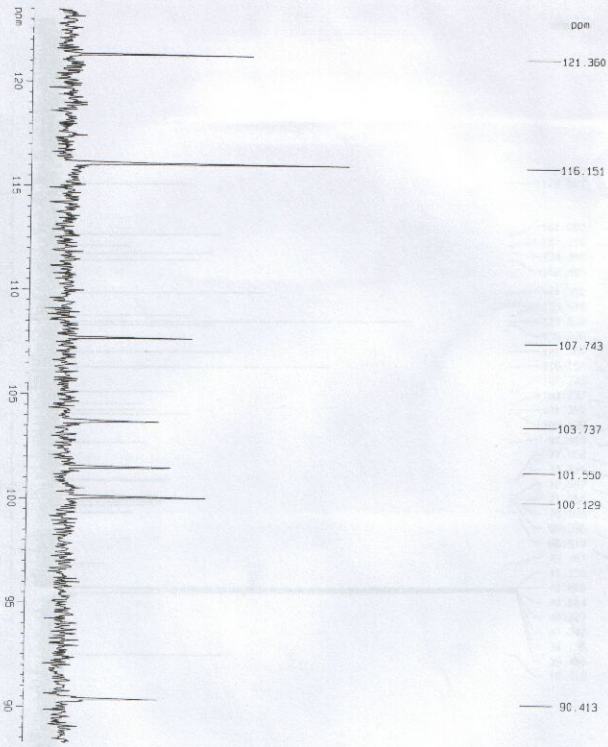
\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
COPROG2 waltz16  
NUC2 13C  
P2 8.00 usec  
PL2 0.00 dB  
PL12 18.00 dB  
PL13 40.00 dB  
SFO2 300.1310005 MHz

F2 - Processing Parameters  
SI 8192  
SF 75.467150 MHz  
WDW EM  
SS 18  
LB 1.00 Hz  
GB 0  
PC 1.40

ID NAME D131 PARAMETERS  
C3 28.00 usec  
C4 0.00 usec  
C5 0.00 usec  
C6 5.28.04 usec  
C7 63.444 usec  
C8 4.81.95 usec  
C9 0.99320 usec  
PC 74.99484 Hz

42CM

13C 1:299330



Current Data Parameters  
 NAME  
 EXPTNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 DATE\_ 20050622  
 TIME 8:17

INSTRUM spect  
 PROBHD 5 mm BBO spect  
 PULPROG zgpg30  
 TO 16384  
 SOLVENT DMSO  
 NS 1524  
 DS 2

SI 188012.393 Hz  
 FIDRES 1.164428 Hz  
 AQ 0.430025 sec  
 RG 327.5  
 DM 36.580 dB  
 DE 6.00 dB  
 TE 300.0 K  
 O1 1.50000000 38C  
 D11 0.03000000 sec  
 R12 0.03002000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 8.30 dB  
 PL1 0.25 dB  
 SFO1 75.4752014 MHz

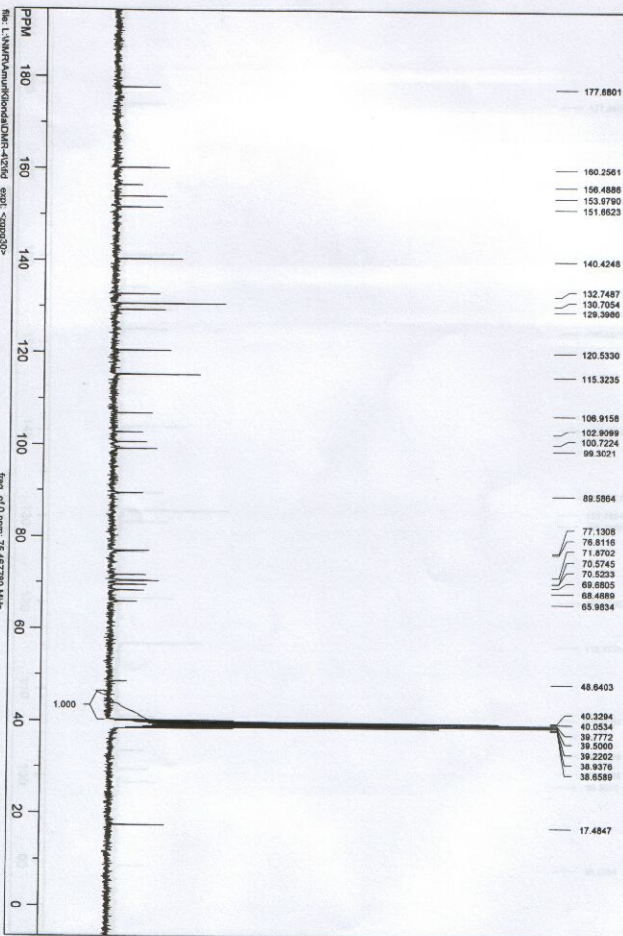
\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG23 waltz16  
 NUC2 13C  
 P2 100.00 dB  
 PL2 0.00 dB  
 PL3 18.00 dB  
 PL4 40.00 dB  
 SFO2 300.1312025 MHz

F2 - Processing Parameters  
 SI 188012.393 Hz  
 SF 75.4657120 MHz  
 WDM 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

3D NMR Data Parameters  
 CX 15.00 cm  
 F1P 123.333 GHz  
 F1 9322.71 MHz  
 F2P 66.724 GHz  
 F2 6661.81 MHz  
 PCHN 1.76794 DM/CM

131 CASY 02/20M

## SpinWorks 2.4: 13C (zqpg30)



file: L:\MTR\Run\kilonca\DMR-4216d exp1 <zqpg30>  
 transmitter freq.: 75.476020 MHz  
 time domain size: 16384 points  
 width: 18632.36 Hz = 249.514900 ppm = 1.149438 Hz/pt  
 number of scans: 1024

freq. of 0 ppm: 75.467780 MHz  
 processed size: 8192 complex points  
 LB: 1.000 GB: 0.0000  
 Hd/cm: 606.772 ppm/cm: 8.03927

<sup>13</sup>C (zgpg30)

77.1308  
78.8116

71.8702

70.5745  
70.5233

68.8905

66.4689

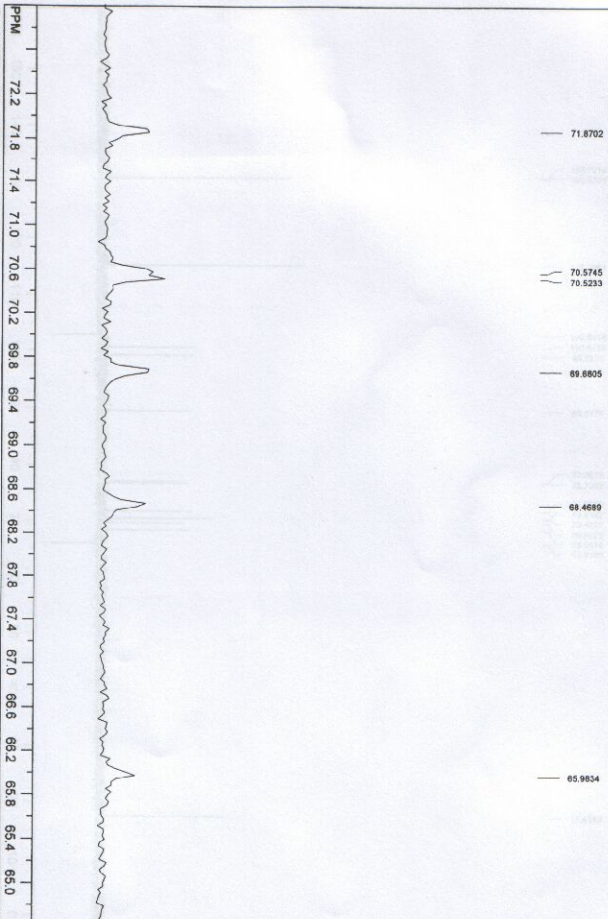
65.9634



data:DMR-4121fid exp1: <zgpg30>  
9020 MHz  
4 points  
49.514900 ppm = 1.149438 Hz/pt

freq. of 0 ppm: 75.467780 MHz  
processed size: 8192 complex points  
LB: 1.000 GB: 0.0000  
Hz/cm: 98.076 ppm/cm: 1.29943

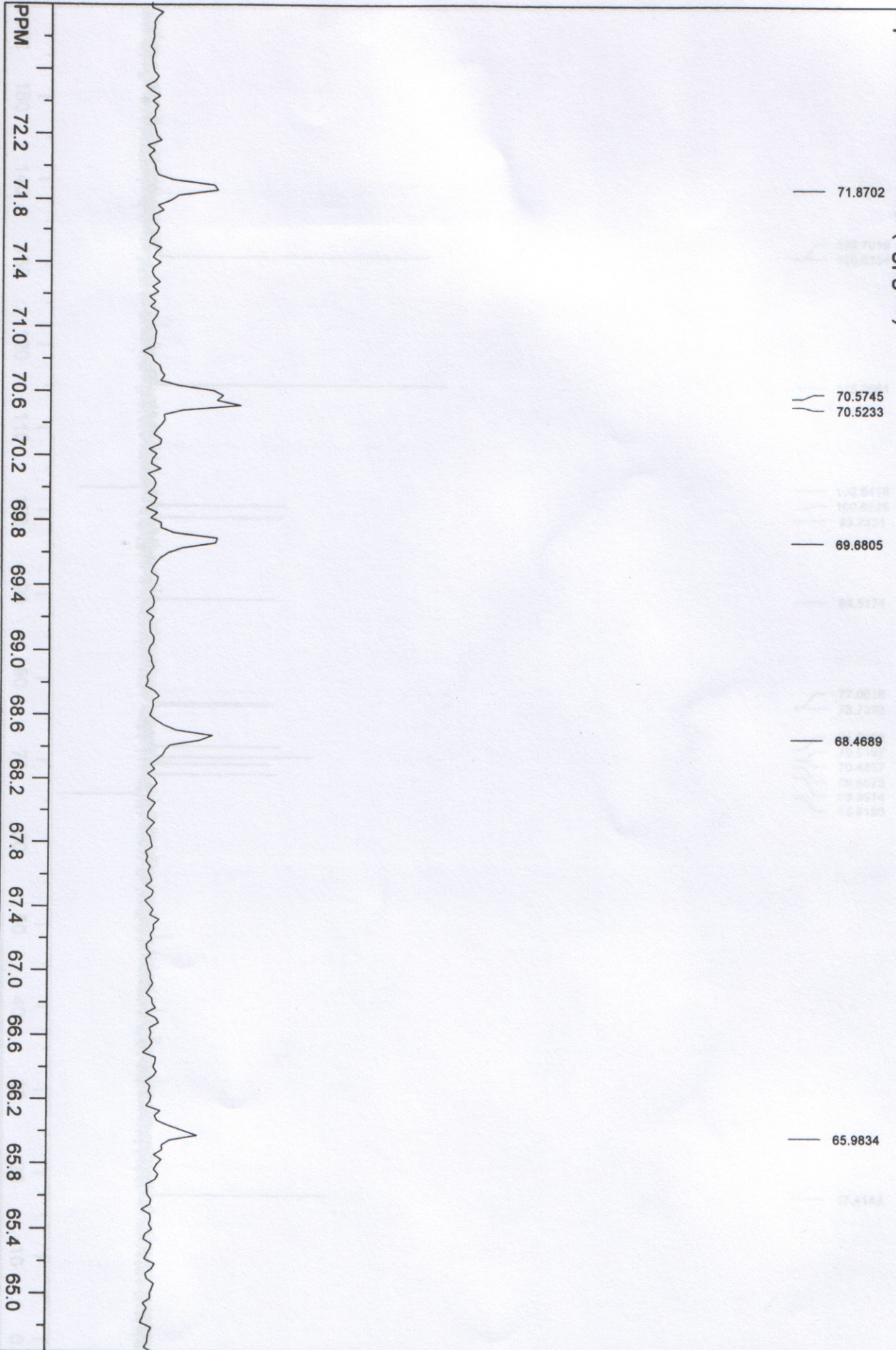
SpinWorks 2.4: 13C (zgpg30)



file: L:\NMR\Amurk\donald\DMR-42\fid exp1: <zgpg30>  
transmitter freq.: 75.479020 MHz  
line domain size: 16384 points  
width: 18832.39 Hz = 249.514900 ppm = 1.149438 Hz/pt  
number of scans: 1024

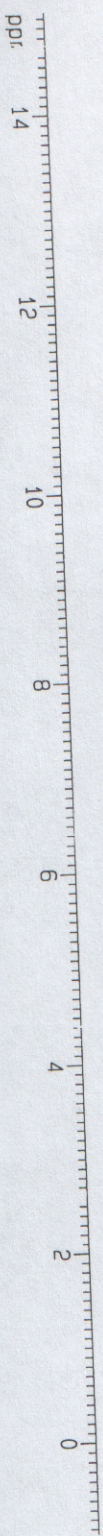
freq. of 0 ppm: 75.467780 MHz  
processed size: 8192 complex points  
LB: 1.0000 GIG: 0.0000  
Hz/cm: 25.251 ppm/cm: 0.33456

SpinWorks 2.4: 13C (zgpg30)



file: L:\NMR\Amunkilondal\DMR-4\2\fid exp: <zgpg30>  
transmitter freq.: 75.476020 MHz  
time domain size: 16384 points  
width: 18832.39 Hz = 249.514900 ppm = 1.149438 Hz/pt  
number of scans: 1024

freq. of 0 ppm: 75.467780 MHz  
processed size: 8192 complex points  
LB: 1.000 GB: 0.0000  
Hz/cm: 25.251 ppm/cm: 0.33456



Integral

1.0000

0.8565

2.0992

3.0696

2.1153

2.1371

2.0533

1.2091

7.6370

1.1409

8.10339  
8.08171

6.96579  
6.94225

6.21847  
5.42689

5.40975  
5.36891

5.07591  
4.97307

3.71428  
3.70226

3.68585  
3.67371

3.34951  
3.29152

3.27106  
3.25111

3.06848  
3.04319

3.01688  
2.55184

He

Current Data Parameters  
NAME DMR-1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20050627  
Time 13.00  
INSTRUM spect  
PROBHD 5 mm Multinu  
PULPROG zg30  
TD 32768  
SOLVENT COC13  
NS 16  
DS 2  
SWH 6250.000 HZ  
FIDRES 0.190735 HZ  
AQ 2.6214900 sec  
RG 256  
DK 80.000 usec  
DE 100.00 usec  
TE 298.0 K  
HL1 3 dB  
D1 2.51999998 sec  
P1 7.50 usec  
SF01 400.1390253 MHz  
NUCLEUS 1H

F2 - Processing parameters

SI 32768  
SF 400.1362675 MHz  
WDW EM  
SSB 0  
LB 0.20 HZ  
GB 0  
PC 1.00

10 NMR plot parameters

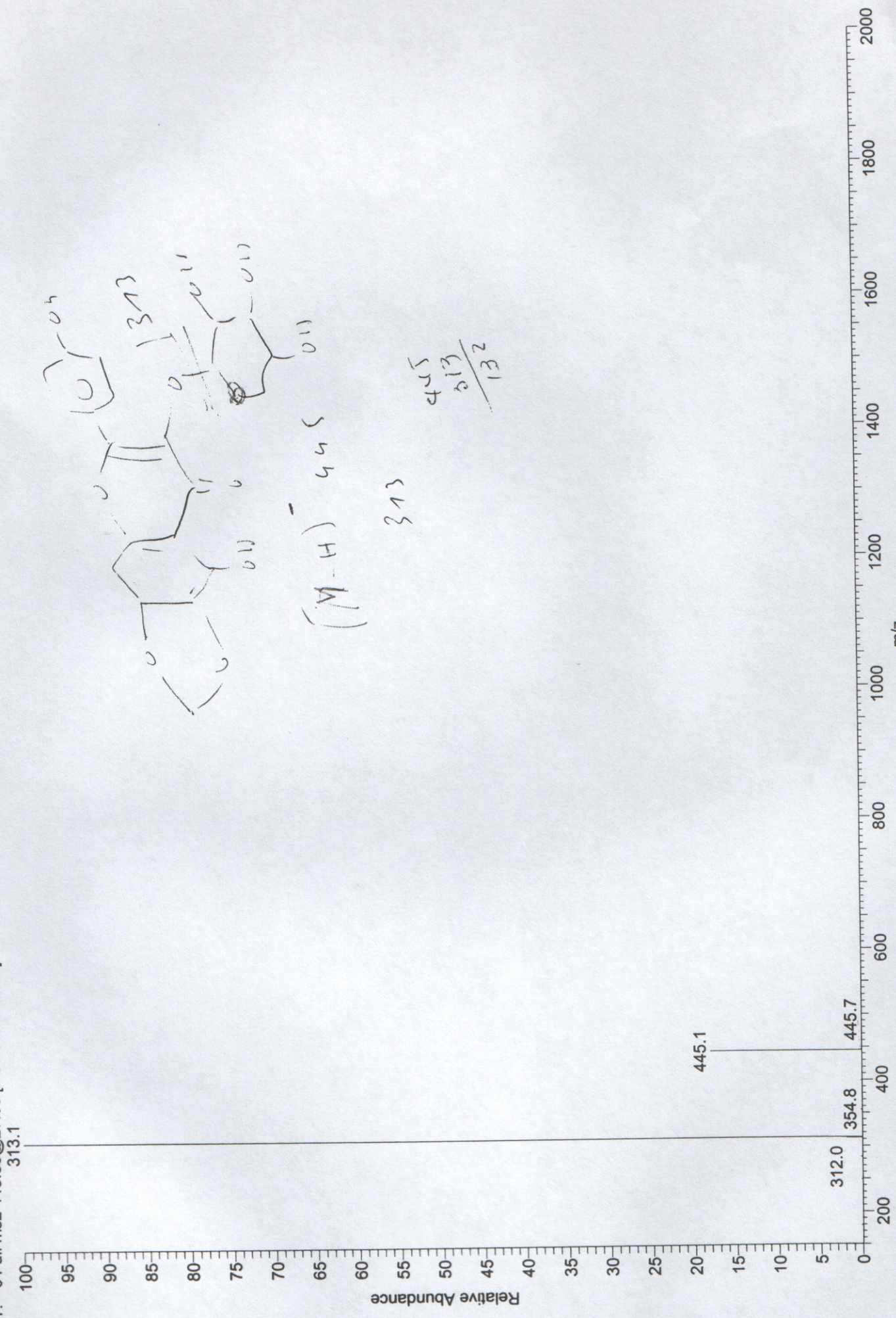
CX 20.00 cm  
F1P 15.062 ppm  
F1 6027.02 Hz  
F2P -0.956 ppm  
F2 -363.23 Hz  
PPMCM 0.80101 ppm/cm  
HZCM 320.51282 Hz/cm

File Name F:\Data\2005\losh\101SPN0810

MeOH

101SPN0810 #136-145 RT: 4.78-5.10 AV: 10 NL: 8.74E4

T: - c Full ms2 445.00@27.00 [ 150.00-2000.00]





HMOyc H-C

+ Wasser

across 186728 dmsd

Current Data Parameters  
 NAME EXPNO PROCNO  
 DMS-1 4 1

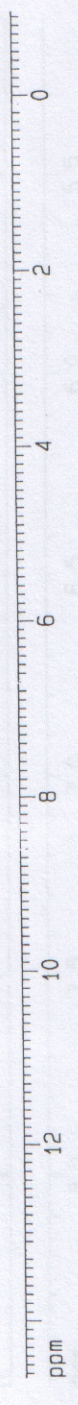
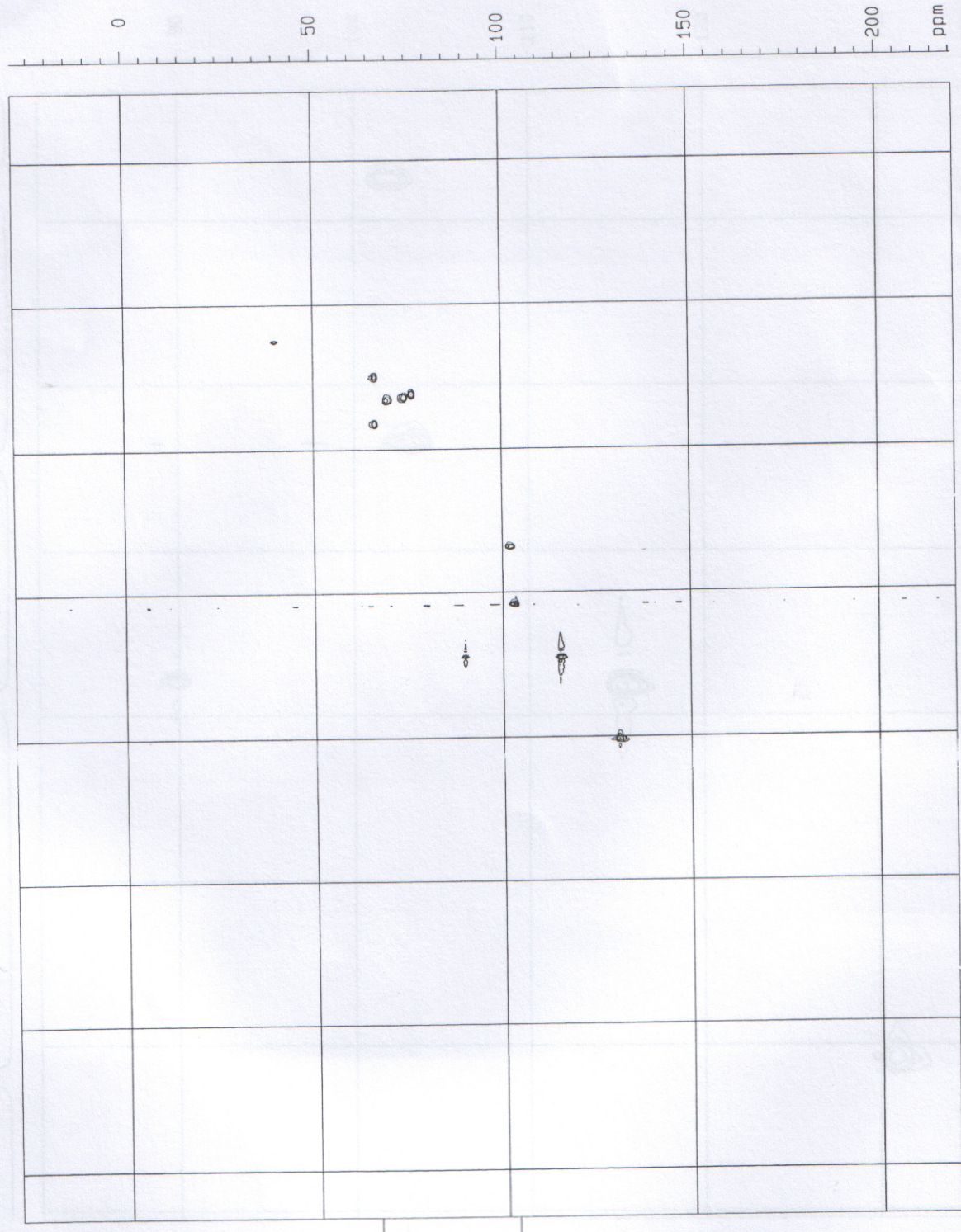
F2 - Acquisition Parameters  
 Date\_ 20050627  
 Time 13.22  
 INSTRUM Spect  
 PROBHD 5 mm Multinu  
 PULPROG zgpg30  
 TD 65536  
 SFO1 400.146301  
 ACQFSZ 4  
 NS 2  
 DS 8  
 SMH 6250.000 Hz  
 FIDRES 3.051798 Hz  
 AQ 0.1638900 sec  
 RG 16384  
 DM 80.000 usec  
 DE 114.28 usec  
 TE 290.0 K  
 P16 1000.00 usec  
 L21 100  
 D2 0.00345000 sec  
 D16 0.00010000 sec  
 RL1 0  
 RL2 0  
 RL3 0.03000000 sec  
 D17 18.00 dB  
 D18 18.00 dB  
 D19 1.25000000 sec  
 P1 7.31 usec  
 D4 0.0017250 sec  
 P2 14.62 usec  
 P4 19.50 usec  
 SFO2 100.624000 MHz  
 DECNLC 13C  
 P3 9.75 usec  
 D0 0.00000300 sec  
 D13 0.00000300 sec  
 D19 0.000000 sec  
 D27 0.000000 sec  
 D28 0.000000 sec  
 D29 0.0033400 sec  
 SF01 400.1360252 MHz  
 NUCLEUS 1H  
 CHPRG 80PD  
 P31 100.00 usec  
 INO 0.00000584 sec

F1 - Acquisition Parameters  
 NDD 4  
 TD 256  
 SFO1 100.624 MHz  
 FIDRES 98.26663 Hz  
 SW 250.000 ppm

F2 Processing parameters  
 SI 1024  
 ST 400.1362851 MHz  
 MDM 2  
 OSINE 0.00 Hz  
 LB 0  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 256  
 MCF 1191  
 SF 100.6143000 MHz  
 MDM 2  
 OSINE 0.00 Hz  
 LB 0  
 GB 0

20 NMR plot parameters  
 CX2 18.00 cm  
 CX1 15.00 cm  
 F2PLO 14.655 ppm  
 F2LO 5864.13 Hz  
 F2PHI -0.964 ppm  
 F2K1 -385.87 Hz  
 F1PLO 250.750 ppm  
 F1LO 250.750 ppm  
 F1K1 -2945.41 Hz  
 F2PCKM 0.66776 ppm/cm  
 F1PCKM 347.22223 Hz/cm  
 F1HZCM 15.66826 ppm/cm  
 F1HZCM 1677.06653 Hz/cm



acros 186728 dms0

Current Data Parameters  
 NAME DMR-1  
 EXPNO 4  
 PROCNO 1

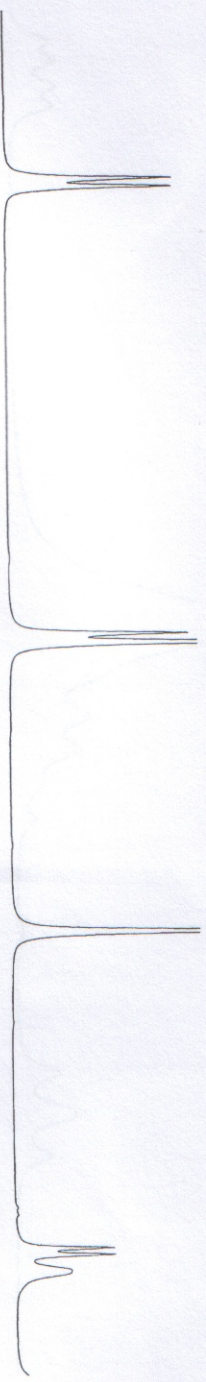
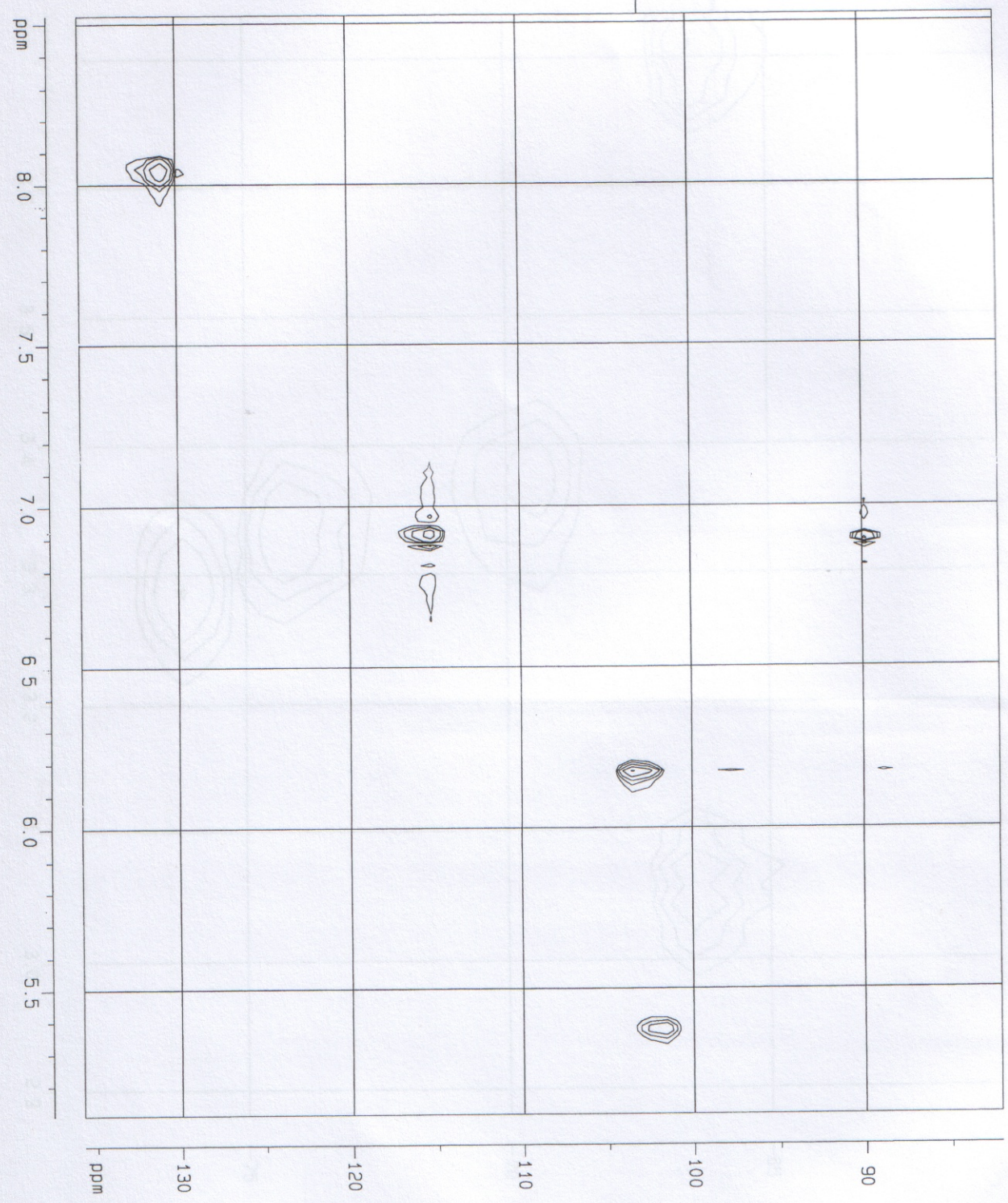
F2 - Acquisition Parameters  
 Date\_ 2003.12.22  
 Time\_ 13.22  
 INSTRUM spect  
 PROBRW 5 mm Multinu  
 PULPROG zgpg30  
 SFO 200.6  
 VFO 200.6  
 NS 4  
 DS 4  
 SMH 6250.000 Hz  
 FIDRES 3.051758 Hz  
 AQ 0.163900 sec  
 RG 15384  
 DM 60.000 USEC  
 DE 1.4  
 TE 290.0 K  
 PC 1000.00 usec  
 L2 100  
 D2 0.0034000 sec  
 D16 0.00010000 sec  
 H4 1 3.49  
 O1 1 0.03000000 sec  
 O0 18.00 dB  
 P1 1 25000000 sec  
 P1 7.31 usec  
 P2 0.0017250 sec  
 P3 1.4 62 usec  
 P4 1.4 62 usec  
 SFO2 100.624000 MHz  
 DECPHASE 13C

F1 - Acquisition Parameters  
 NO 256  
 SFO1 100.624 MHz  
 FIDRES 98.265629 Hz  
 SW 250.000 ppm  
 NUCLEUS 1H  
 CPDPRG 98PP  
 P31 100.00 usec  
 INO 0.0000354 sec

F2 - Processing Parameters  
 S1 1024  
 SM 400.1362861 MHz  
 SFO 531.15  
 SSF 0.00 Hz  
 LB 0  
 GB 0  
 PC 1.00

F1 - Processing Parameters  
 S1 256  
 NC2 100.6143574 MHz  
 SF 531.15  
 WDM 0.00 Hz  
 SSB 2  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

20 NMR Data Parameters  
 CX2 19.00 cm  
 CX1 15.00 cm  
 F2PULP 8.523 ppm  
 F2LLO 3410.52 Hz  
 F2MH1 5.107 ppm  
 F2H1 2043.33 Hz  
 F1PULP 135.781 ppm  
 F1LLO 13861.48 Hz  
 F1MH1 522.053 ppm  
 F1H1 0.18883 ppm/c  
 F2PULPC 75.95465 Hz/c  
 F1PULPC 3.58107 ppm/c  
 F1HZCM 360.30726 Hz/c



across 186728 dms0

Current Data Parameters  
 NAME DMR-1  
 FAPNO 4  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20050727  
 TIME 17:32  
 INSTRUM spect  
 PROBRG 5 mm Multinu  
 PULPROG inv45SD  
 TD 2048  
 SOLVENT dmsd5  
 NS 4  
 DS B  
 QS 6250.000 Hz  
 SNR 3.05798 Hz  
 AQ 0.1639500 sec  
 RG 16384  
 DM 0.000000 sec  
 DE 114.20 usec  
 TE 290.0 K  
 TC 1000.00 usec  
 L21 100  
 L22 100

D2 0.00345000 sec  
 D3 0.00010000 sec  
 HL1 3 dB  
 HL2 3 dB  
 D11 0.03000000 sec  
 D12 18.00 dB  
 D13 1.25000000 sec  
 P1 7.31 usec  
 P2 0.0017250 sec  
 P3 19.50 usec  
 P4 19.50 usec  
 F2 100.6240000 MHz  
 BECNUC 13C

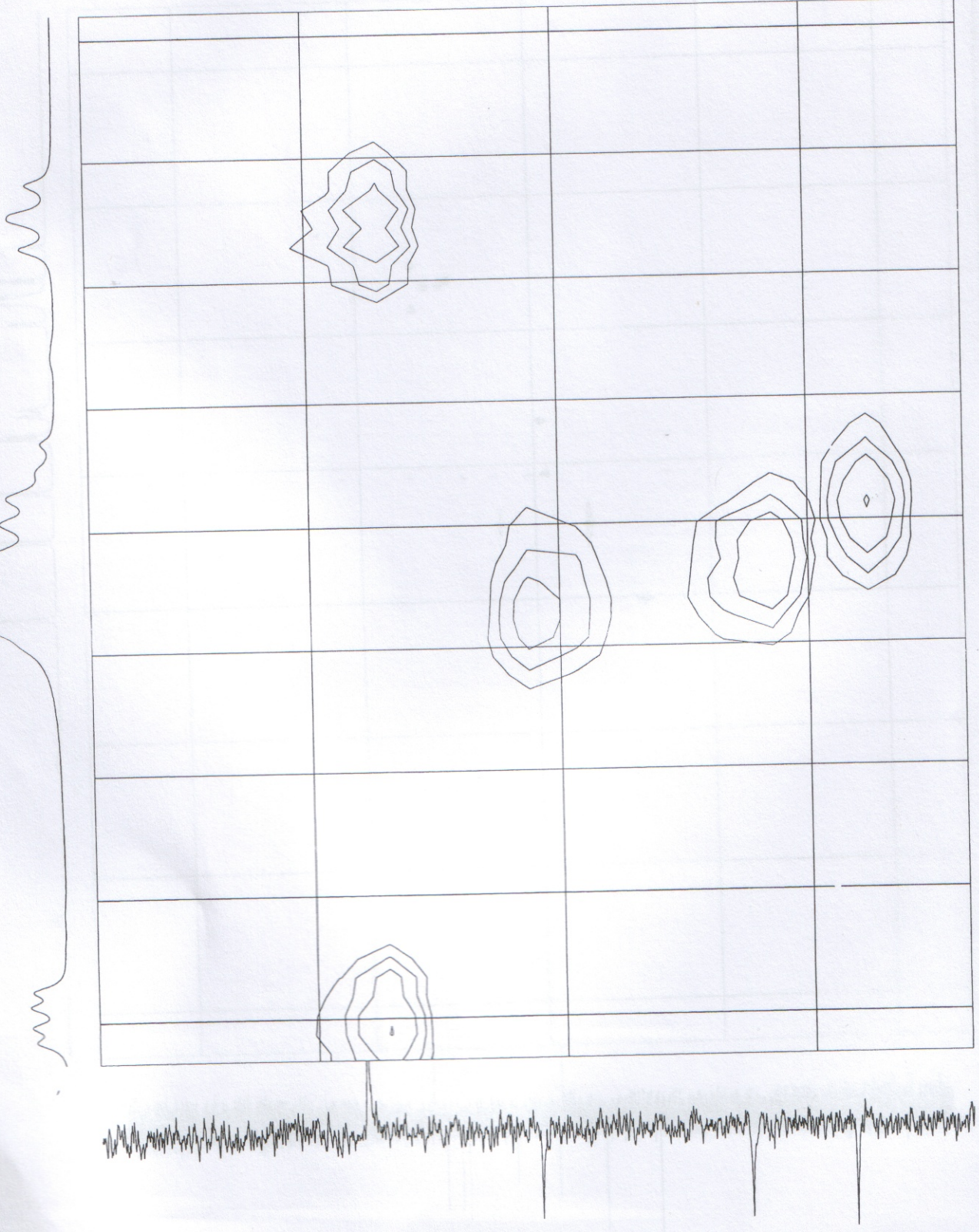
P3 9.75 usec  
 D0 0.00000300 sec  
 D13 0.00000300 sec  
 D27 0.00000800 sec  
 D20 0.00062500 sec  
 D21 0.0023460 sec  
 SF01 400.1390232 MHz  
 NUC1EUS 1H  
 CPDPRG 3P  
 P31 100.00 usec  
 INO 0.0000994 sec

F1 - Acquisition Parameters  
 NDO 4  
 TD 256  
 SF01 100.624 MHz  
 FIDRES 88.26565 Hz  
 SN 250.000 ppm

F2 Processing Parameters  
 SI 400.1390232 MHz  
 SF 400.1390232 MHz  
 SCA 0.00 Hz  
 LB 2  
 GB 0  
 PC 1.00

F1 - Processing Parameters  
 SI 100.624 MHz  
 MC2 100.6143674 MHz  
 SF 100.6143674 MHz  
 WDW USINE  
 SSB 0.00 Hz  
 LB 0  
 GB 0

20 NMR plot parameters  
 CX2 18.00 cm  
 CX1 15.00 cm  
 F2PLO 3.734 ppm  
 F2LO 1494.02 Hz  
 F2PHI 2.880 ppm  
 F2H1 135.25 Hz  
 F1PLO 78.110 ppm  
 F1LO 785.578 ppm  
 F1PH1 6095.03 Hz  
 F2PROM 0.04746 ppm/cm  
 F2MCM 18.98874 Hz/cm  
 F1PROM 1.17199 ppm/cm  
 F1MCM 117.91874 Hz/cm



ppm 2.9 3.0 3.1 3.2 3.3 3.4 3.5 3.6 ppm

Current Data Parameters  
 NAME DMR 1  
 EXPNO 3  
 PROCNO 4

F2 - Acquisition Parameters

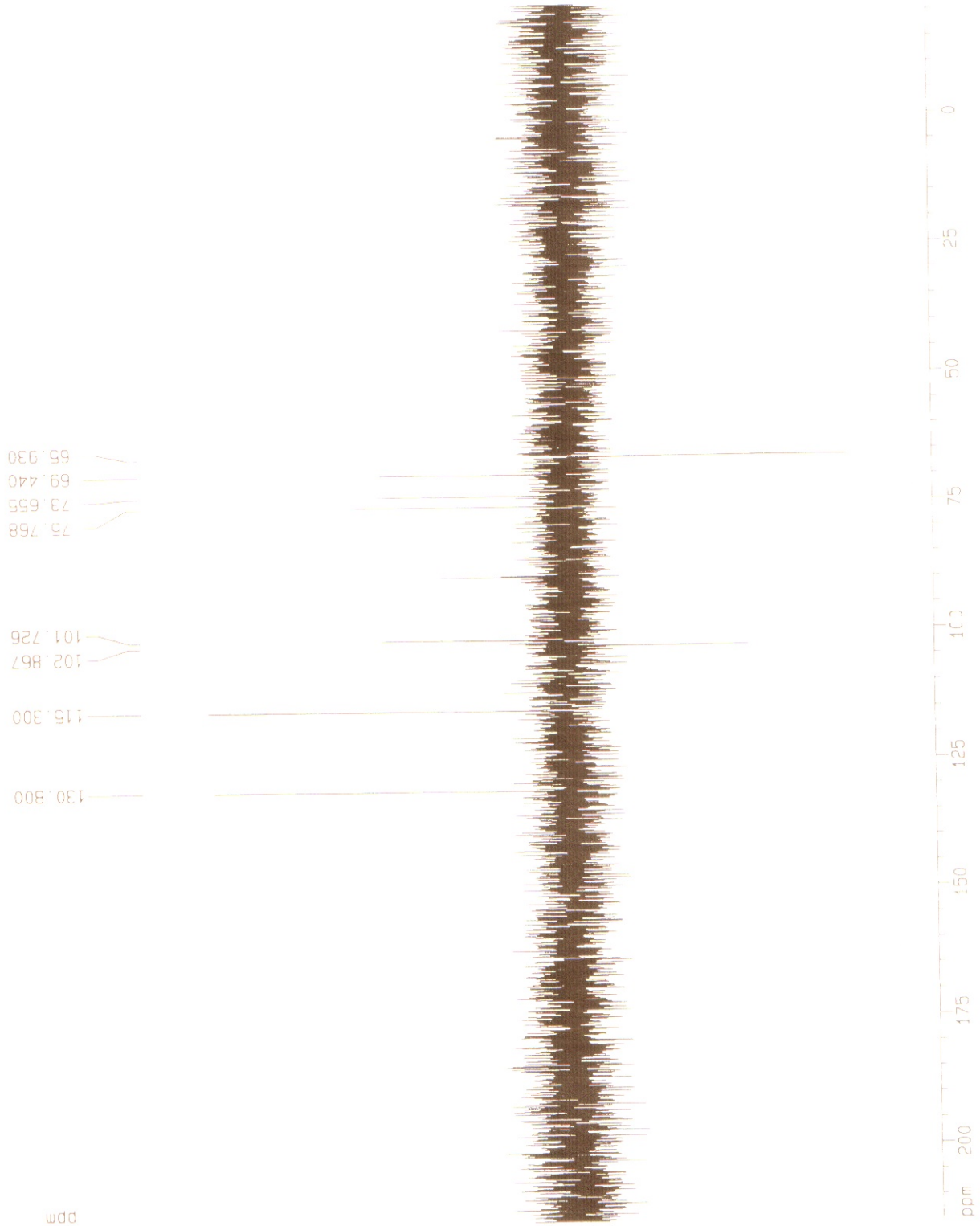
Date\_ 20050627  
 Time 13 22  
 INSTRUM spect  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT dmsc  
 NS 256  
 DS 4  
 SWH 23809.521 Hz  
 FIDRES 0.126509 Hz  
 AQ 0.6881780 sec  
 RG 32768  
 DW 21.000 usec  
 DE 26.274 usec  
 TE 300.2 K  
 HLT 1.05  
 D1 0.80000000 sec  
 S1 1.00  
 P3 7.41 usec  
 SF02 400.1467000 MHz  
 DECNJC \*\*\*  
 D2 0.00340000 sec  
 P4 14.87 usec  
 P1 10.50 usec  
 P2 21.00 usec  
 D13 0.00000400 sec  
 S2 28.00  
 SF01 100.6241000 MHz  
 NUCLEUS 13C  
 CPDPRG waltz16  
 P31 100.00 usec

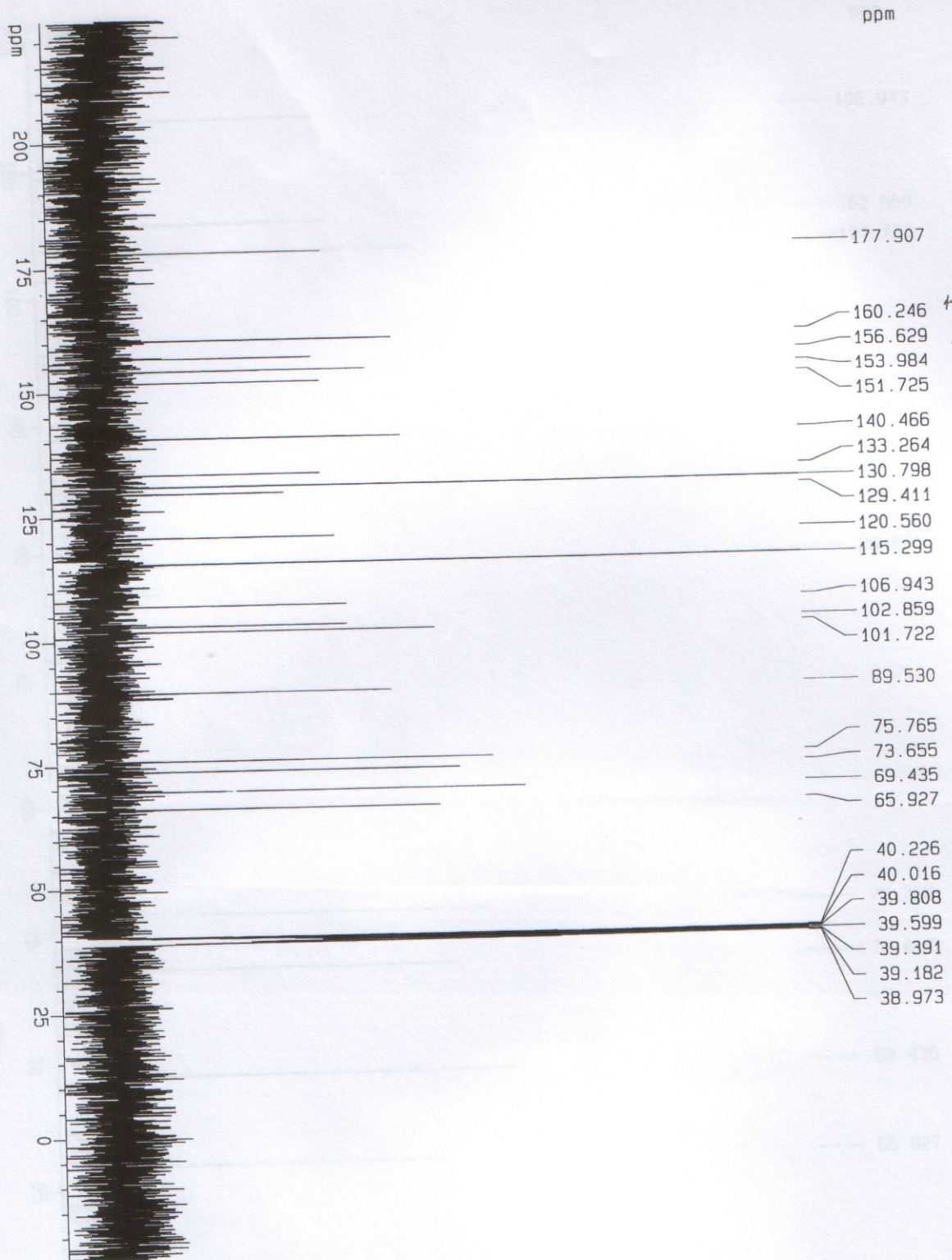
F3 - Processing Parameters

SI 32768  
 SF 100.6183560 MHz  
 WDA EM  
 SSB 0  
 LB 1.50 Hz  
 GB 0  
 PC 2.00

1D NMR 0101 parameters

DS 20.00 cm  
 F1P 214.872 ppm  
 F1 24519.24 Hz  
 F2P -21.769 ppm  
 F2 -2190.28 Hz  
 PRGCM 1: 83207 ppm/cm  
 HZCM 1190.47620 Hz/cm





Current Data Parameters  
 NAME DMR-1  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050627  
 Time 13.04

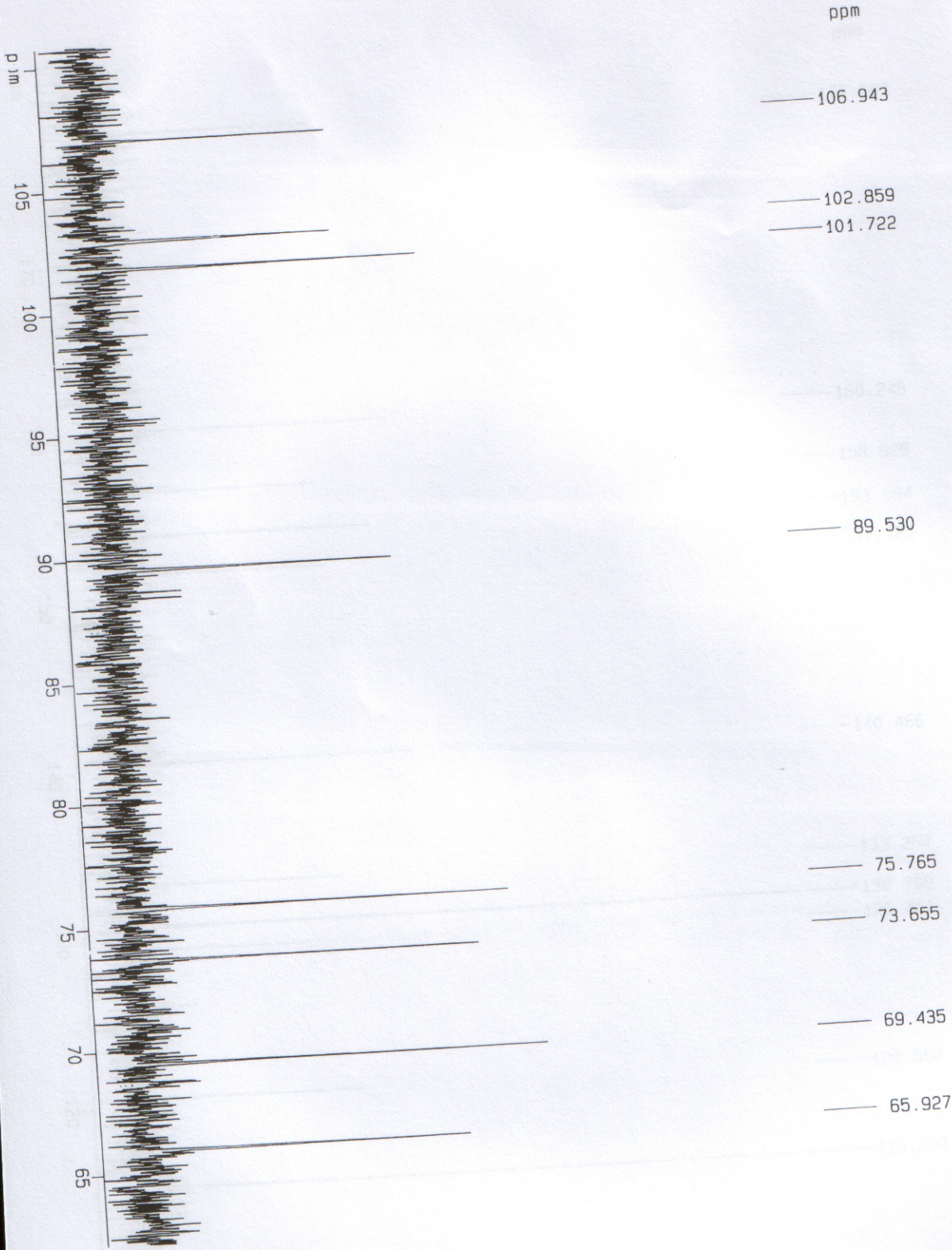
INSTRUM spect  
 PROBHID 5 mm Multinu  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT dmsod6  
 NS 512  
 DS 2  
 SMH 25000.000 Hz  
 FIDRES 0.762939 Hz  
 AQ 0.6554100 sec  
 RG 16384

DW 20.000 usec  
 DE 25.00 usec  
 TE 298.0 K  
 HL1 1 dB  
 D1 1.00000000 sec  
 CPDPRG waltz16

P31 100.00 usec  
 S4 35 dB  
 D11 0.03000000 sec  
 S2 32 dB  
 P1 12.00 usec  
 SF01 100.6244403 MHz  
 NUCLEUS 13C

F2 - Processing parameters  
 SI 32768  
 SF 100.6143960 MHz  
 KDW EM  
 SSB 0  
 LB 1.50 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 224.066 ppm  
 F1 22544.21 Hz  
 F2P -24.408 ppm  
 F2 -2455.78 Hz  
 PPKCM 12.42367 ppm/cm  
 HZCM 1249.99986 Hz/cm



Current Data Parameters  
 NAME DKR-1  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050627  
 Time 13.04

INSTRUM spect  
 PROBHD 5 mm Multinu  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT dmsod6  
 NS 512  
 DS 2

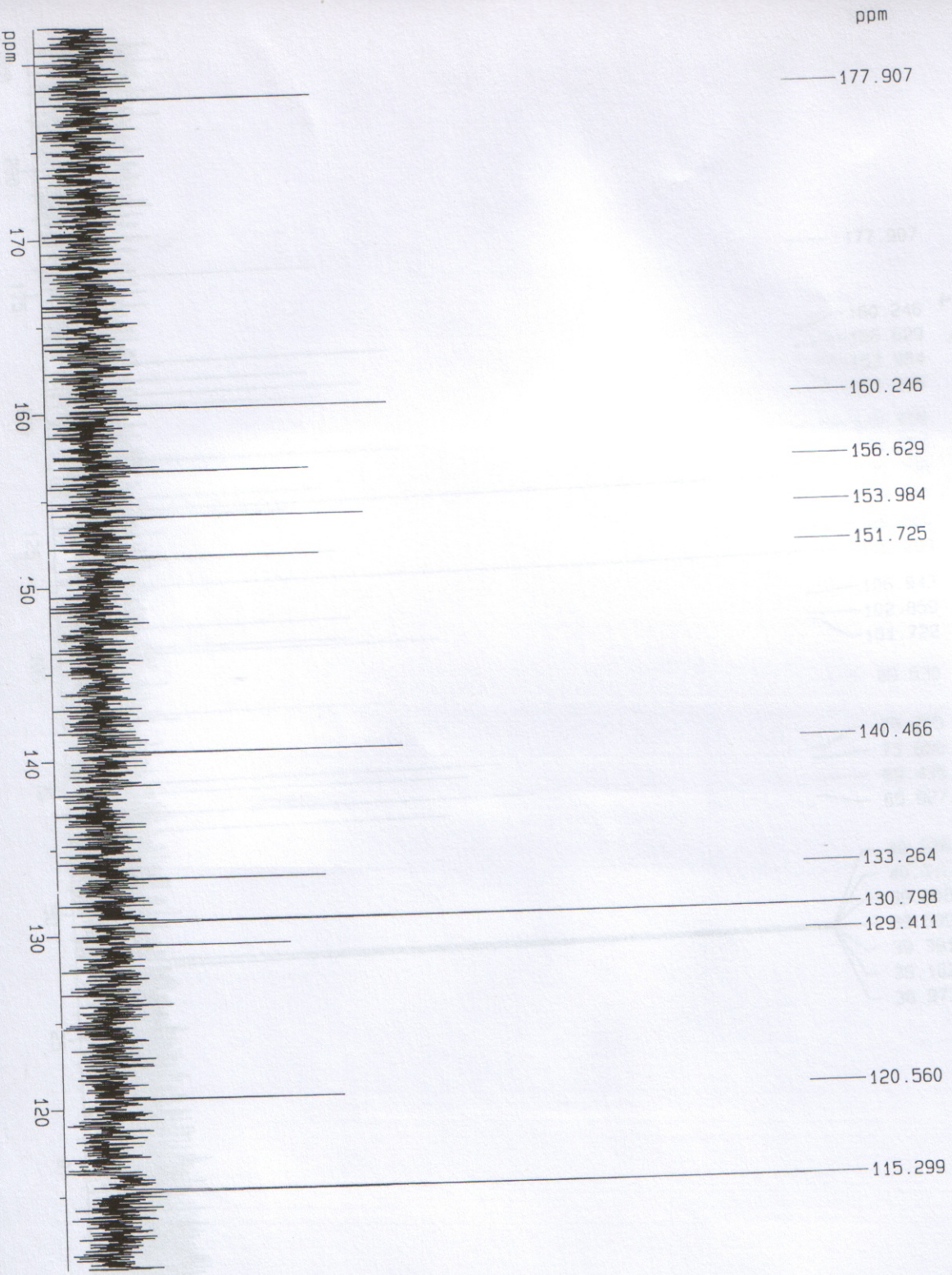
SWH 25000.000 Hz  
 FIDRES 0.762939 Hz  
 AQ 0.6554100 sec  
 RG 16384  
 DM 20.000 usec  
 DE 25.00 usec  
 TE 298.0 K  
 HL 1  
 D1 1.00000000 sec

waitz16  
 CPDPRG 100.00 usec  
 P31 35 dB  
 S4 0.03000000 sec  
 D11 32 dB  
 S2 12.00 usec  
 P1 100.6244403 MHz  
 SF01 13C

NUCLEUS 13C

F2 - Processing parameters  
 SI 32768  
 SF 100.6143960 MHz  
 SF EM  
 MDM 0  
 SSB 1.50 Hz  
 LB 0  
 GB 1.40  
 PC

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 110.746 ppm  
 F1 11142.66 Hz  
 F2P 62.102 ppm  
 F2 6248.33 Hz  
 PPMCM 2.43222 ppm/cm  
 HZCM 244.71634 Hz/cm



Current Data Parameters  
 NAME DMH-1  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20050627  
 Time 13.04  
 INSTRUM spect  
 PROBHD 5 mm Multinu  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT dmsod6  
 NS 512  
 DS 2  
 SMH 25000.000 Hz  
 FIDRES 0.762939 Hz  
 AQ 0.6554100 sec  
 RG 16384  
 DW 20.000 usec  
 DE 25.00 usec  
 TE 298.0 K  
 HL1 1 dB  
 D1 1.00000000 sec  
 CPDPRG waltz16  
 P31 100.00 usec  
 S4 35 dB  
 D11 0.03000000 sec  
 S2 32 dB  
 P1 12.00 usec  
 SF01 100.6244403 MHz  
 NUCLEUS 13C

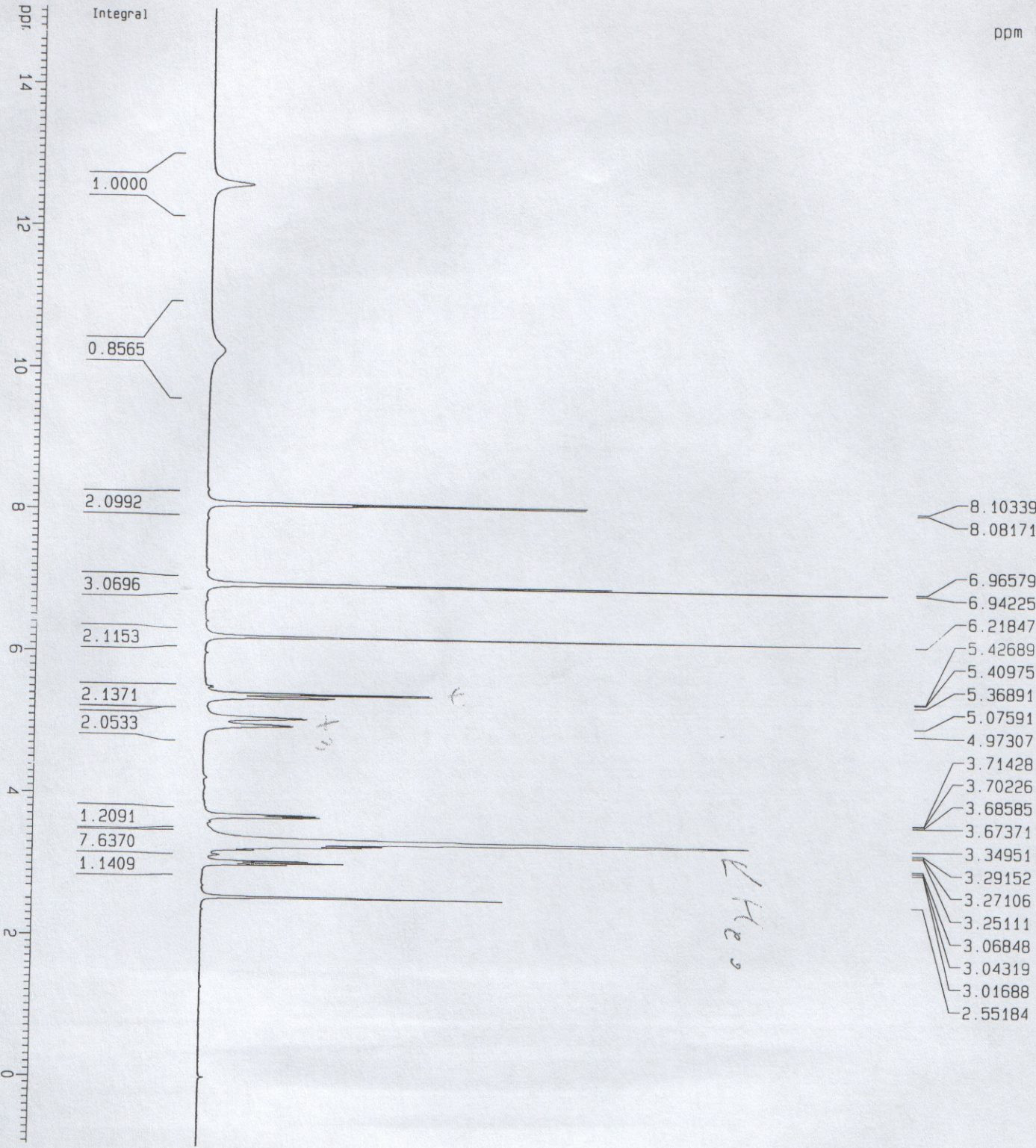
F2 - Processing parameters

SI 32768  
 SF 100.6143960 MHz  
 MDW EM  
 SSB 0  
 LB 1.50 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters

CX 20.00 cm  
 F1P 182.054 ppm  
 F1 18317.30 Hz  
 F2P 110.746 ppm  
 F2 11142.66 Hz  
 PPMCM 3.56541 ppm/cm  
 HZCM 358.73193 Hz/cm

ppm



Current Data Parameters  
 NAME DMR-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050627  
 Time 13.00

INSTRUM spect  
 PROBD 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2

SMH 6250.000 HZ  
 FIDRES 0.190735 HZ  
 AQ 2.6214900 sec  
 RG 256  
 DM 80.000 usec  
 DE 100.00 usec  
 TE 298.0 K  
 HL1 3 dB  
 D1 2.51999998 sec  
 P1 7.50 usec  
 SF01 400.1390253 MHZ  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 32768  
 SF 400.1362675 MHZ  
 MDM EM  
 SSB 0  
 LB 0.20 HZ  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 15.062 ppm  
 F1 6027.02 Hz  
 F2P -0.958 ppm  
 F2 -383.23 Hz  
 PPMCK 0.80101 ppm/cm  
 HZCM 320.51282 Hz/cm

303 K DMR-1



3637K

Current Data Parameters  
 NAME DMR-1.363  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050627  
 Time 15.21

INSTNUM 5 mm Multinu  
 PROBHD spect  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2

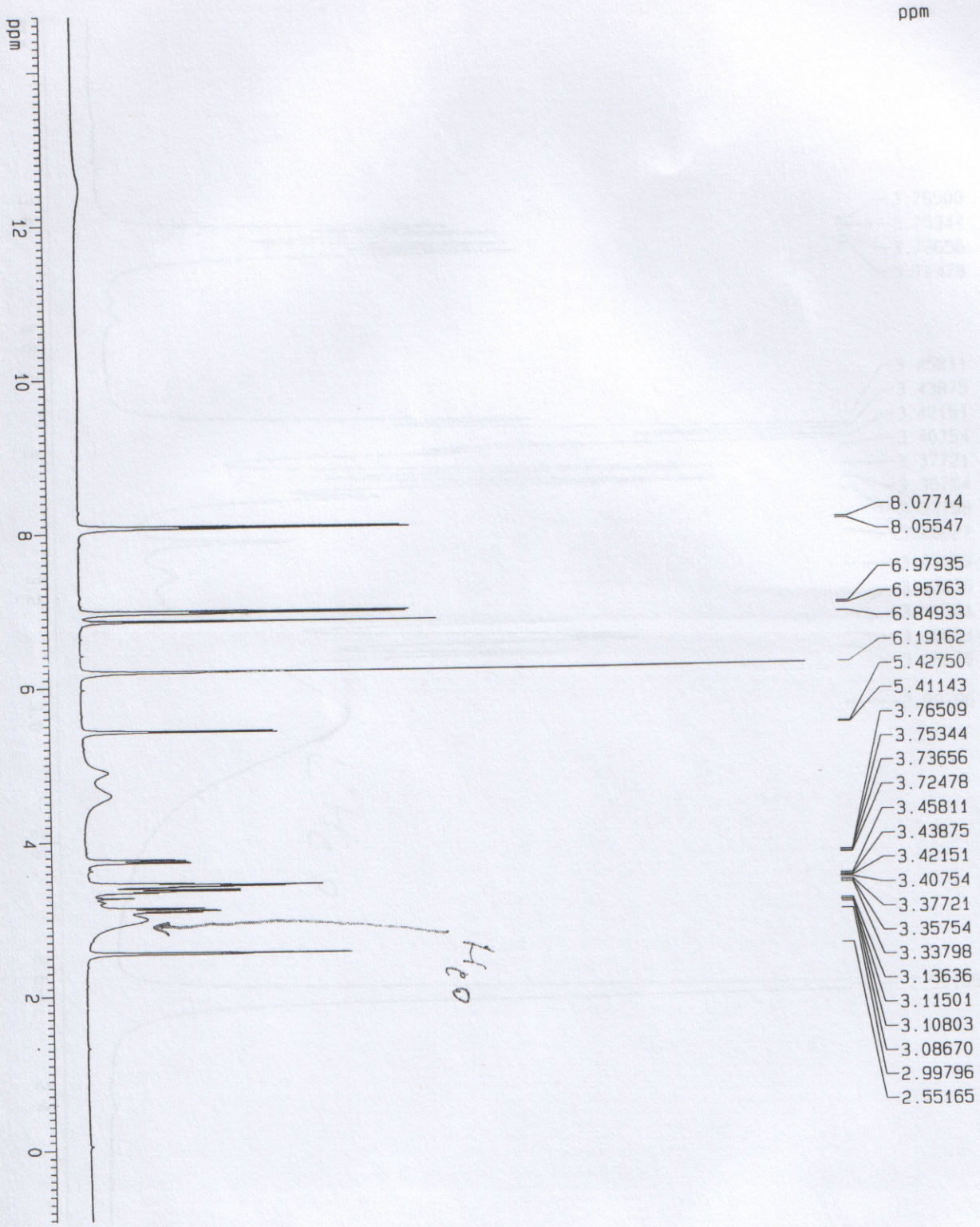
SMH 6250.000 Hz  
 FIDRES 0.190735 Hz  
 AQ 2.6214900 sec  
 RG 256

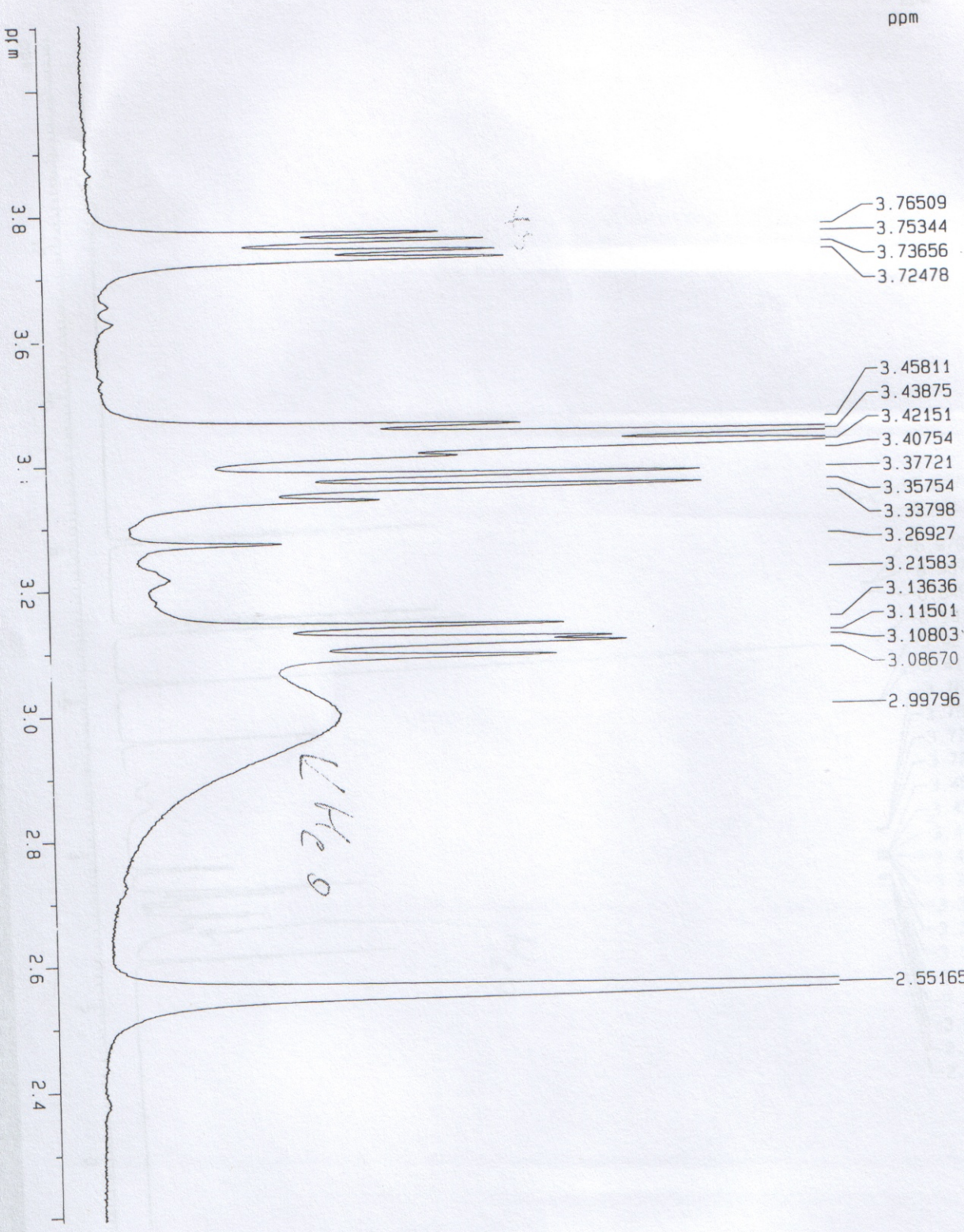
DW 80.000 usec  
 DE 100.00 usec  
 TE 298.0 K

HL1 3 dB  
 D1 2.51999998 sec  
 P1 7.50 usec  
 SF01 400.1390253 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 32768  
 SF 400.1362675 MHz  
 WDW EM  
 SSB 0  
 LB 0.20 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 14.702 ppm  
 F1 5882.73 Hz  
 F2P -367.27 Hz  
 F2 0.78098 ppm/cm  
 PPKCM 312.50000 Hz/cm  
 HZCM





ppm

W  
H<sub>2</sub>O

4.5

H<sub>2</sub>O

365 R

DMR-1

Current Data Parameters  
 NAME DMR-1.363  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050627  
 Time 15.21  
 INSTRUM spect  
 PROBHD 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SMH 6250.000 Hz  
 FIDRES 0.190735 Hz  
 AQ 2.6214900 sec  
 RG 256  
 DW 80.000 usec  
 DE 100.00 usec  
 TE 298.0 K  
 HL1 3 dB  
 D1 2.5199998 sec  
 P1 7.50 usec  
 SF01 400.1390253 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 32768  
 SF 400.1362675 MHz  
 MDW EM  
 SSB 0  
 LB 0.20 Hz  
 GB 0  
 PC 1.00

10 NMR plot parameters  
 CX 20.00 cm  
 F1p 4.103 ppm  
 F1 1641.90 Hz  
 F2p 2.192 ppm  
 F2 877.17 Hz  
 PPMCM 0.09556 ppm/cm  
 HZCM 38.23693 Hz/cm

acros 179179 dms0

Current Data Parameters

NAME DM1-1  
 EXPNO 6  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20050627  
 Time 14.13  
 INSTRUM spect  
 PROBD 5 mm Multinu  
 PULPROG zgpg30  
 TD 1024  
 SOLVENT dmsd06  
 NS 2  
 DS 8  
 SFO 6250.000 MHz  
 FIDRES 6.103316 Hz  
 AQ 0.0819700 sec  
 RG 128  
 DM 80.000 usec  
 DE 114.29 usec  
 TE 303.0 K  
 P16 1000.00 usec  
 L21 100  
 hL1 3 GB  
 O1 1.25000000 sec  
 P1 7.31 usec  
 D0 0.00000300 sec  
 D27 0.00000600 sec  
 D16 0.00050000 sec  
 P0 7.31 usec  
 D13 0.00000300 sec  
 SFO1 400.1390252 MHz  
 NUC1US 1H  
 INO 0.00016010 sec

F1 - Acquisition Parameters

ND0 256  
 TD 1  
 SFO1 400.139 MHz  
 FIDRES 24.395092 Hz  
 SN 13.610 ppm

F2 - Processing Parameters

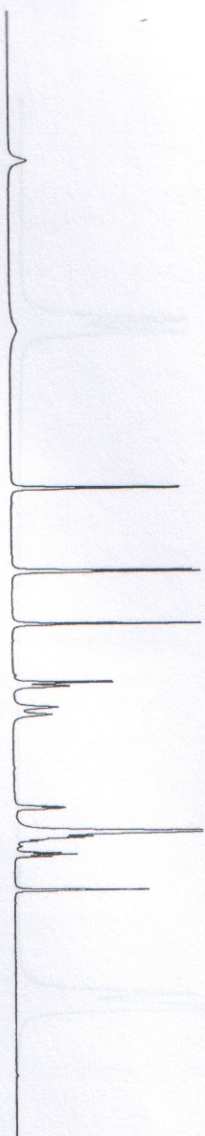
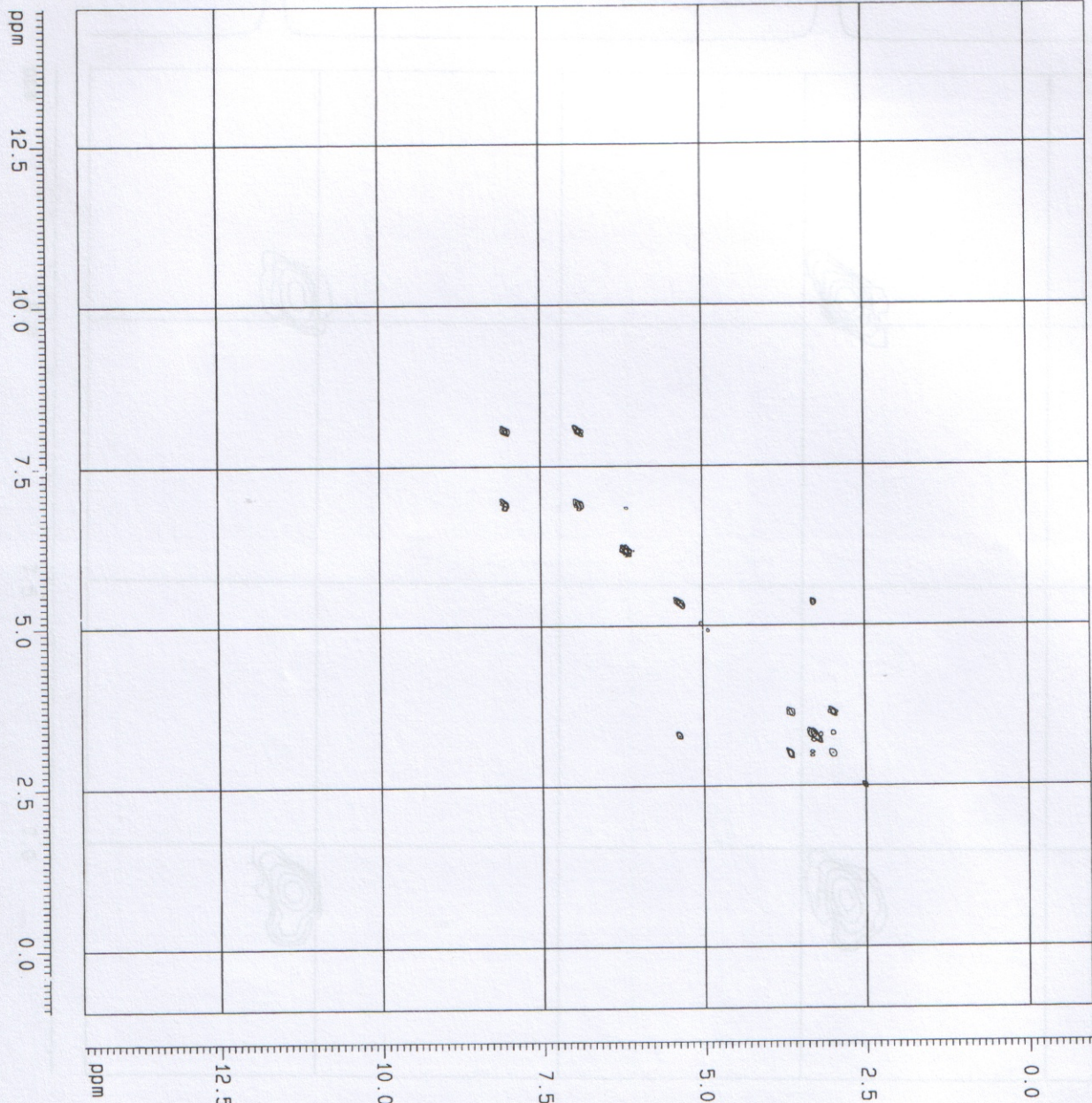
SF 1024  
 SF 400.1362864 MHz  
 MCM SINE  
 SSB 0.5  
 LB 0.00 Hz  
 GB 0  
 PC 1.40

F1 - Processing Parameters

SF 1024  
 OF  
 MCF 400.1362864 MHz  
 SINE  
 SSB 0.5  
 LB 0.00 Hz  
 GB 0

20 NMR plot parameters

CX2 15.00 cm  
 CK1 15.00 cm  
 F2PH0 14.656 ppm  
 F2L0 5864.44 Hz  
 F2PH1 -0.964 ppm  
 F2L1 -385.36 Hz  
 F1PH0 14.650 ppm  
 F1L0 5861.32 Hz  
 F1PH1 -0.960 ppm  
 F1L1 -384.25 Hz  
 F2PPOCK 1.04131 ppm/cm  
 F2RZCK 416.56569 Hz/cm  
 F1PPOCK 1.04067 ppm/cm  
 F1RZCK 416.41101 Hz/cm



ACROS 179179 DMSO

Current Data Parameters

NAME DMP-1  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20050627  
Time 14.13  
INSTRUM spect  
PROBHD 5 mm MLI1nu  
PULPROG cosyg8  
TD 1024  
SOLVENT dmsod6  
NS 2  
DS 8  
SH 6250.000 Hz  
FIDRES 6.102916 Hz  
AQ 0.0819700 sec  
RG 128  
DM 80.000 usec  
DE 114.29 usec  
TE 303.0 K  
P16 1000.00 usec  
L21 100  
H1 3 dB  
D1 1.25000000 sec  
P1 7.31 usec  
D2 0.00000300 sec  
D27 0.00000800 sec  
D16 0.00050000 sec  
P0 7.31 usec  
D13 0.00000300 sec  
SF01 400.1390252 MHz  
NUCLEUS 1H  
IN0 0.00016010 sec

F1 - Acquisition Parameters

NO0 1  
TD 256  
SF01 400.139 MHz  
FIDRES 24.399082 Hz  
SFORES 15.610 ppm  
SK

F2 - Processing Parameters

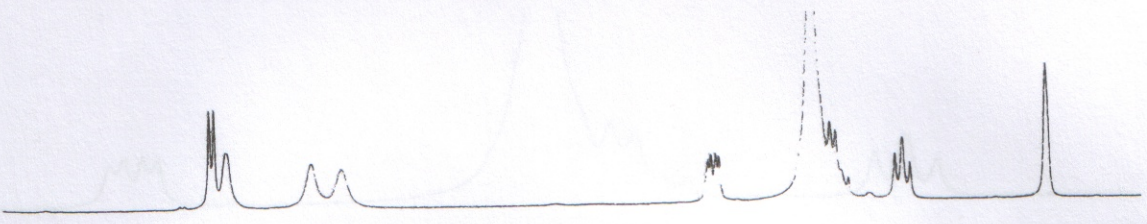
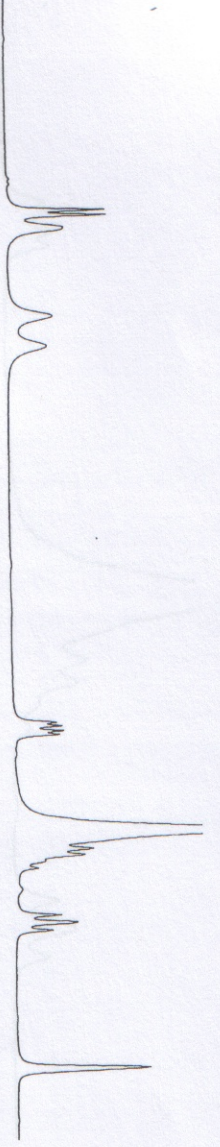
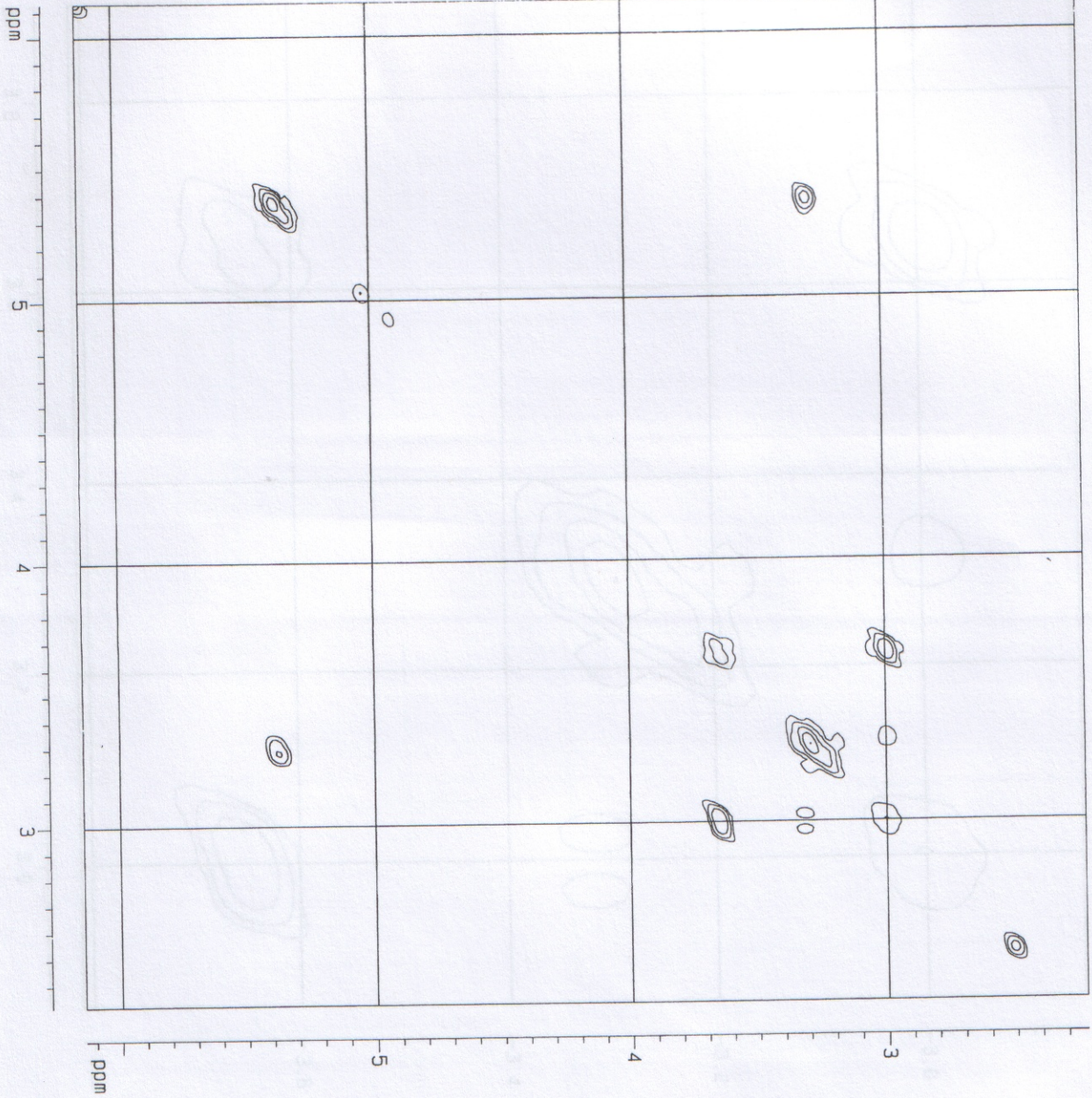
SI 1024  
SF 400.1362988 MHz  
WDW SINE  
SSB 0.5  
LB 0.00 Hz  
GB 0  
PC 1.40

F1 - Processing Parameters

SI 1024  
SF 400.1362984 MHz  
WDW SINE  
SSB 0.5  
LB 0.00 Hz  
GB 0

2D NMR Plot Parameters

CX2 15.00 cm  
CX1 15.00 cm  
F2DLO 6.129 ppm  
F2LO 2482.57 Hz  
F2PHI 2.316 ppm  
F2HI 926.69 Hz  
F1PLO 6.144 ppm  
F1LO 2459.24 Hz  
F1PHI 2.226 ppm  
F1HI 690.60 Hz  
FAPPNCK 0.25423 ppm/cm  
FAHZCK 101.72226 Hz/cm  
FJPNCK 0.26118 ppm/cm  
FAHZCK 104.50941 Hz/cm



acros 179179 dms0

Current Data Parameters

NAME DMH-1  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20050627  
Time 14.13  
INSTRUM spect  
PROBHD 5 mm Multinu  
PULPROG cosyg5  
TD 1024  
SOLVENT dms0d6  
NS 2  
DS 6  
SWH 6230.000 Hz  
FIDRES 6.103516 Hz  
AQ 0.0815700 sec  
RG 128  
RW 80.000 usec  
DM 114.29 usec  
DE 303.0 K  
TE 1000.00 usec  
P16 100  
L21 3 dB  
HL1 1.25000000 sec  
D1 7.31 usec  
P1 0.00000300 sec  
D0 0.00000800 sec  
D27 0.00050000 sec  
P0 7.31 usec  
P013 0.00000300 sec  
SF01 400.1390252 MHz  
NUC1EUS 1H  
IN0 0.00016010 sec

F1 - Acquisition parameters

MD0 1  
TD 256  
SF01 400.139 MHz  
FIDRES 24.395082 Hz  
SM 15.610 ppm  
SI 1024  
SF 400.1362858 MHz  
KQW SINE  
SSB 0.5  
LB 0.00 Hz  
GB 0  
PC 1.40

F1 - Processing parameters

SI 1024  
MC2 GF  
SF 400.1362858 MHz  
KQW SINE  
SSB 0.5  
LB 0.00 Hz  
GB 0

2D NMR plot parameters

CX2 15.00 cm  
CX1 15.00 cm  
F2PUL0 31.902 ppm  
F2L0 1561.46 Hz  
F2PH1 2.850 ppm  
F2H1 1140.32 Hz  
F1PUL0 3.811 ppm  
F1L0 1524.98 Hz  
F1PH1 2.851 ppm  
F1H1 1140.59 Hz  
F2PQCN 0.07017 ppm/cm  
F2HZCN 28.07617 Hz/cm  
F1PQCN 0.06403 ppm/cm  
F1HZCN 25.61904 Hz/cm





acros 186728 DMSO

Current Data Parameters  
 NAME DMS-1  
 EXPRNO 5  
 PROCNO 1

F2 - Acquisition Parameters

DATE\_ 20060627  
 TIME 13 47  
 INSTNM spect  
 PRBBDW 5 mm WALTDM  
 PULPROG invgqsig11m  
 TD 2048  
 SCLVENT dmsd0e  
 NS 16  
 DS 16  
 SH 650.000 Hz  
 FIDRES 3.051758 Hz  
 AQ 0.1628500 sec  
 RG 16384  
 DM 80.000 USEC  
 DE 114.25 USEC  
 TE 303.0 K  
 P16 1000.00 USEC  
 L21 100  
 H.L1 3.08  
 D1 1.25000000 sec  
 P1 / 31 usec  
 D2 0.00345000 sec  
 P3 9.75 usec  
 SF02 100.6244000 MHz  
 DECNLC 13C  
 D6 0.05000000 sec  
 D0 0.00000300 sec  
 D27 0.00000800 sec  
 D16 0.00010000 sec  
 P2 14.62 usec  
 D13 0.00000300 sec  
 SF01 400.1380252 MHz  
 NUCLEUS 1H  
 INO 0.00002559 sec

F1 - Acquisition Parameters

NOO 2  
 TD 256  
 SF01 100.6244 MHz  
 FIDRES 66.474129 Hz  
 SM 220.000 DPM

F2 - Processing Parameters

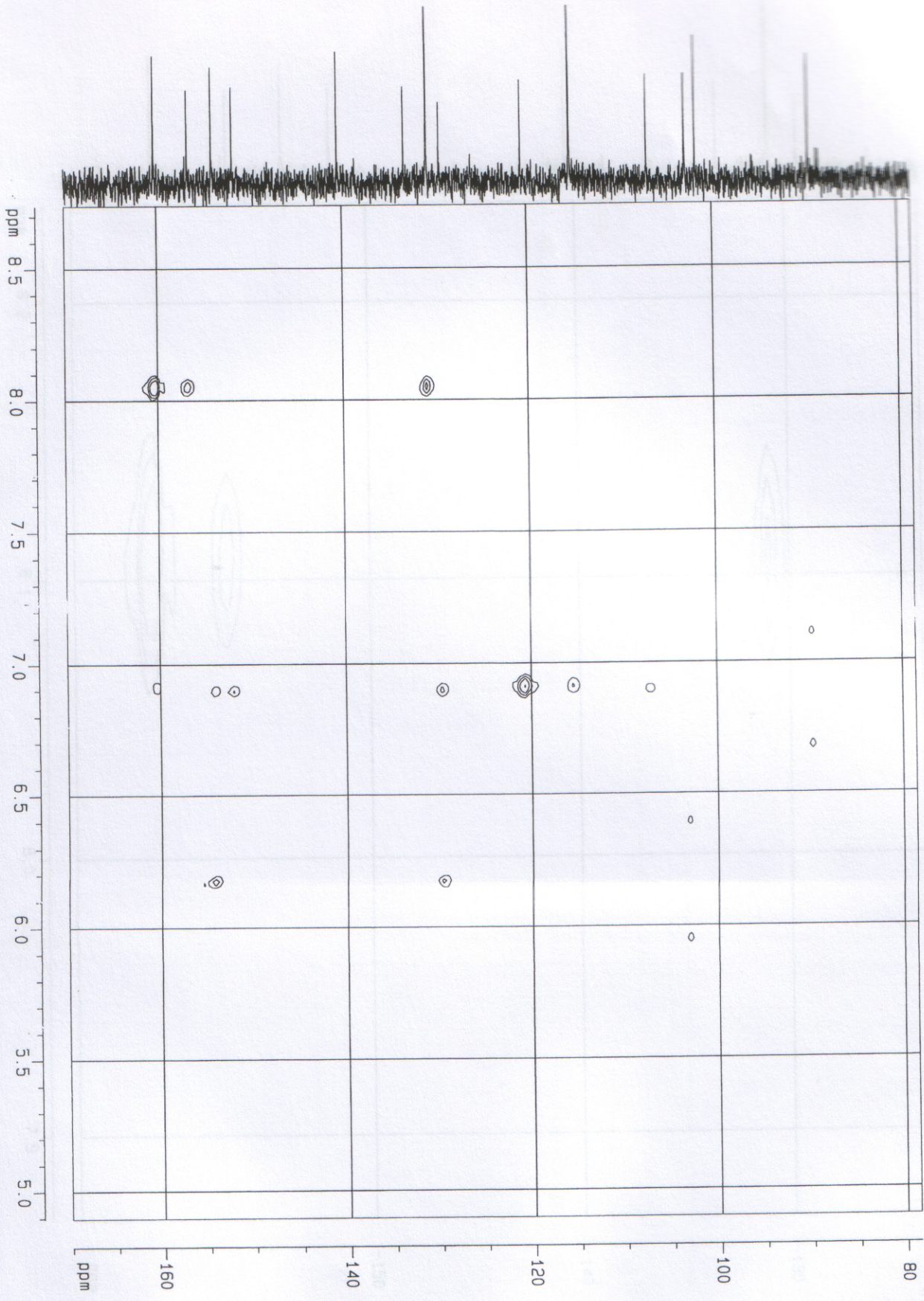
SI 1024  
 SF 400.1382853 MHz  
 MDM 051MC  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40

F1 - Processing Parameters

SI 512  
 SF 100.6143774 MHz  
 MDM SINE  
 SSB 2  
 LB 0.00 Hz  
 GB 0

2D NMR plot parameters

CX2 18.00 cm  
 CK1 15.00 cm  
 F2PUL0 8.739 DPM  
 FALO 3496.81 Hz  
 F2PH1 4.895 DPM  
 F2M1 1.968 72 Hz  
 F1PUL0 1.170 090 DPM  
 F1LO 1711.46 Hz  
 F1PH1 78.557 DPM  
 F1M1 7903.56 Hz  
 F2P2CM 0.21355 JPM/cm  
 F2HZCM 85.44823 Hz/m  
 F1P2CM 6.10217 JPM/cm  
 F1HZCM 613.96531 Hz/cm



Current Data Parameters  
 NAME: DM1  
 EXPRNO: 5  
 PROCNO: 1

F2 - Acquisition Parameters

Date\_: 20050527  
 Time: 13.47  
 INSTRUM: spect  
 PROBHD: 5 mm WALTRO  
 PULPROG: zgpg30  
 TD: 2048  
 SOLVENT: dmso-d  
 NS: 16  
 DS: 16  
 SH: 6250.000 Hz  
 FIDRES: 3.021125 Hz  
 AQ: 0.163800 sec  
 RG: 16384  
 DM: 80.000 USEC  
 DE: 114.75 USEC  
 TE: 303.0 K  
 P16: 1000.00 USEC  
 L21: 100  
 H1: 3.08  
 D1: 1.2500000 sec  
 P1: 7.31 USEC  
 P2: 0.0734500 sec  
 P3: 9.75 USEC  
 SF02: 100.6244000 MHz  
 DECNLC: 13C  
 D6: 0.0500000 sec  
 D0: 0.0000000 sec  
 D27: 0.0000060 sec  
 D16: 0.0001000 sec  
 P2: 14.62 USEC  
 D13: 0.0000000 sec  
 SF01: 400.1398252 MHz  
 NUCLEUS: 1H  
 INO: 0.00002259 sec

F1 - Acquisition Parameters

NDO: 2  
 TD: 256  
 SF01: 100.6244 MHz  
 FIDRES: 86.474129 Hz  
 SM: 720.000 DPM

F2 - Processing Parameters

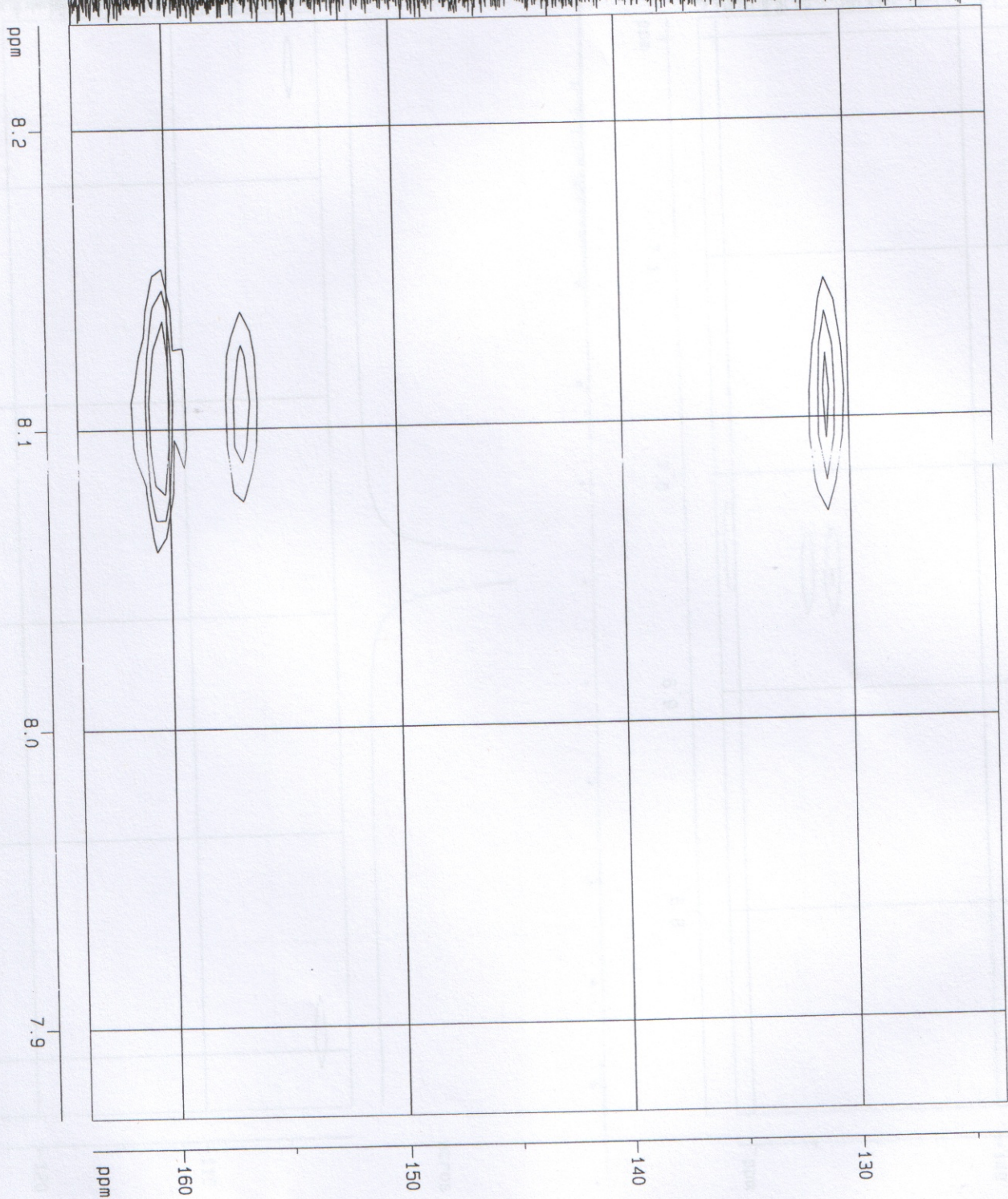
SF: 1024  
 SF: 400.1398252 MHz  
 MDM: 0.0516  
 SSB: 0  
 LB: 0.00 Hz  
 GB: 0  
 PC: 1.40

F1 - Processing Parameters

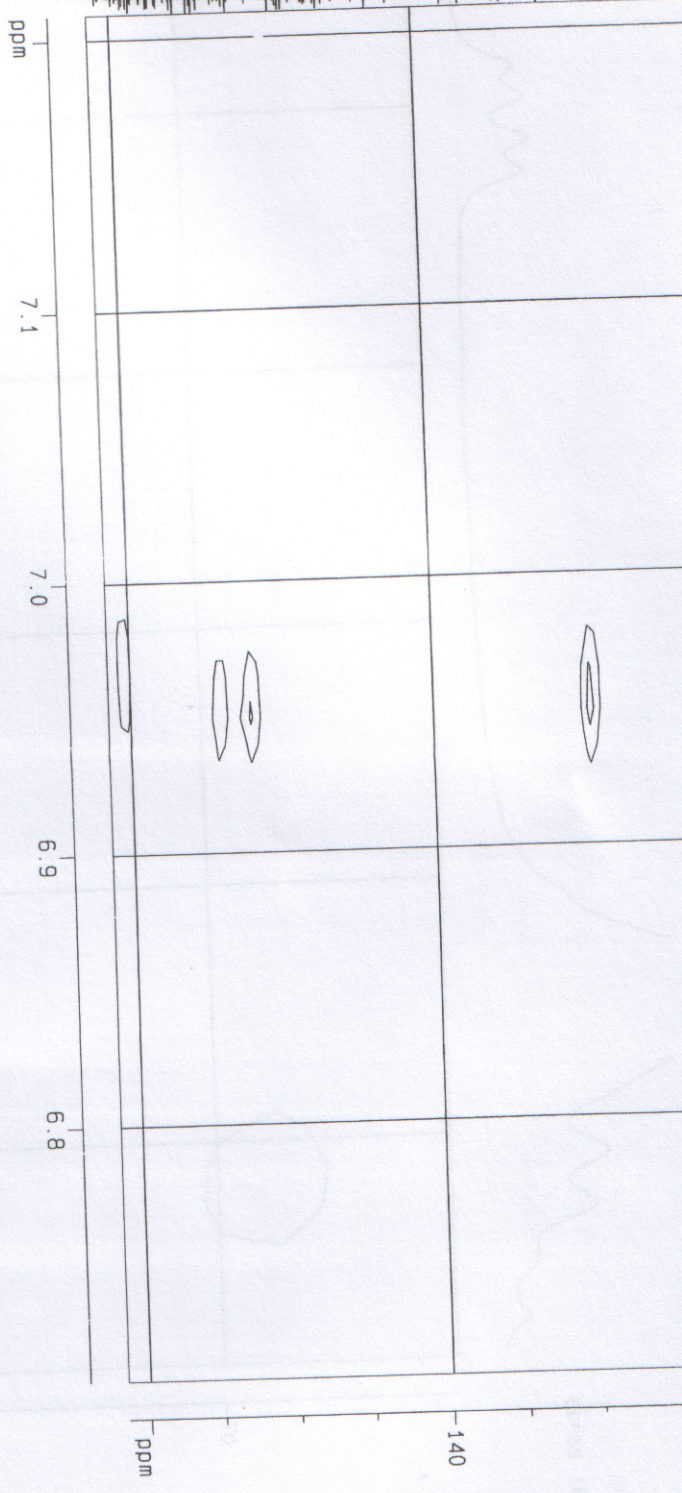
SF: 512  
 SF: 100.6143774 MHz  
 MDM: 0.0516  
 SSB: 2  
 LB: 0.00 Hz  
 GB: 0

20 NMR D101 parameters

CX2: 18.00 cm  
 CX1: 15.00 cm  
 F2P1.0: 8.236 DPM  
 F2L0: 3295.39 Hz  
 F2P11: 7.870 DPM  
 F2P11: 3148.90 Hz  
 F1P1.0: 164.073 DPM  
 F1L0: 16508.14 Hz  
 F1P11: 123.679 DPM  
 F1P11: 12443.86 Hz  
 F2P111C4: 0.020134 DPM/cm  
 F2H2C4: 8.13802 Hz/cm  
 F1P111C4: 2.69298 DPM/cm  
 F1H2C4: 270.95520 Hz/cm







20 NMR plot parameters

CK2	18.00 cm
CK1	18.00 cm
F2PL0	7.208 ppm
F2L0	288.82 Hz
F2PH1	706 ppm
F2H1	2883.20 Hz
F1PL0	1.06 ppm
F1L0	15246.12 Hz
F1PH1	662.29 ppm
F1H1	8662.23 Hz
F2PRCKM	0.002366 ppm/cm
F2PRCK	11.16977 Hz/cm
F1PRCKM	3.01359 ppm/cm
F1PRCK	504.43623 Hz/cm

f1 Processing Parameters

S1	312
MCF	100
SF	100.614374 MHz
WDR	512
SSB	0.00 Hz
LB	0
GB	0

f2 Processing Parameters

S1	1024
SF	400.1362673 MHz
WDR	0.00 Hz
SSB	0
LB	0
GB	0
PC	1.40

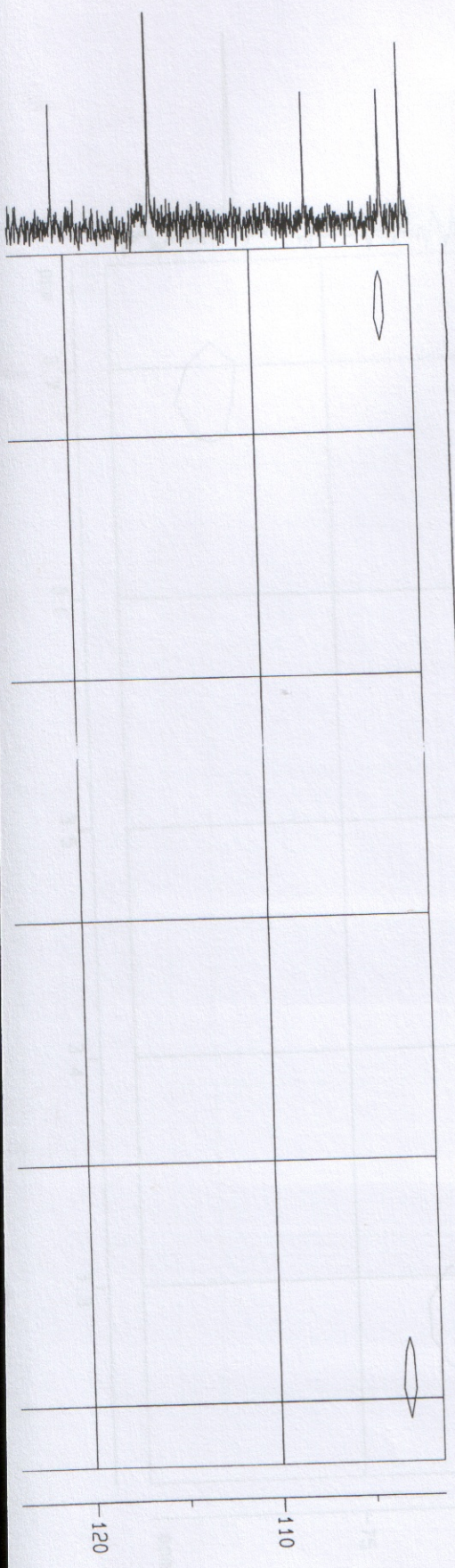
acros 186728 dms0

Current Data Parameters

NAME DMS-1  
 EXPNO 5  
 PROCNO 1

f2 Acquisition Parameters

Date\_ 20050627  
 Time 13.47  
 INSTRUM spect  
 PROBHD 5 mm WJ11nu  
 PULPROG zgpg30  
 TD 2048  
 SOLVENT dmsd06  
 NS 4  
 DS 16  
 SM 6250.000 Hz  
 FIDRES 3.051758 Hz  
 AQ 0.1638900 sec  
 RG 16384  
 DM 80.000 usec  
 DE 114.29 usec  
 TE 303.0 K  
 P16 1000.00 usec  
 L21 100  
 H1 3.00  
 D1 1.25000000 sec  
 P1 1.31 usec  
 D2 0.00345000 sec  
 P3 9.75 usec  
 SF02 100.6144000 MHz  
 DECNLC 13C  
 DB 0.05000000 sec  
 DD 0.00000300 sec



across 186728 dms0



Current Data Parameters  
 NAME DMS-1  
 EXPNO 5  
 PROCNO 1

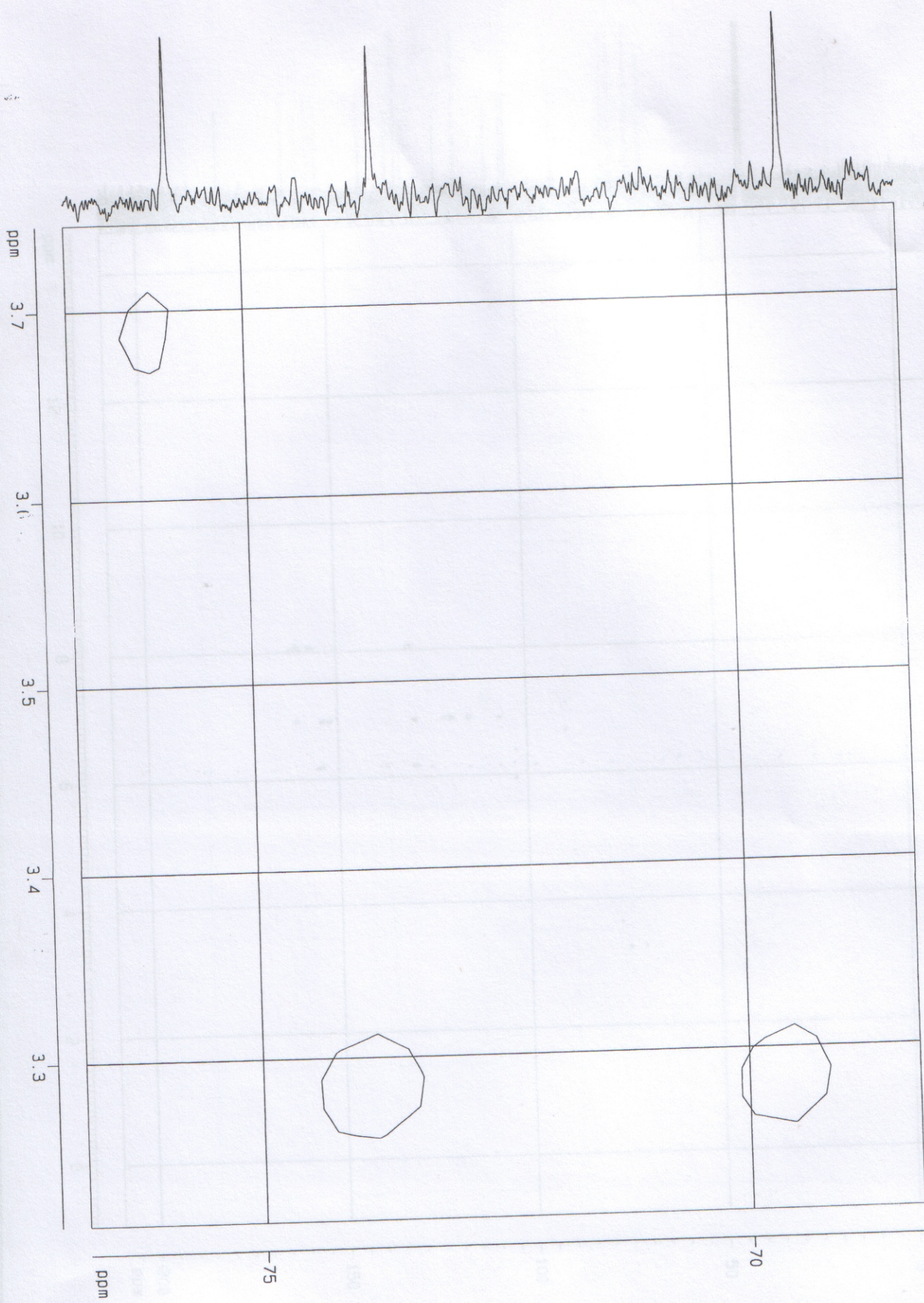
F2 - Acquisition Parameters  
 Date\_ 20050527  
 Time 13.47  
 INSTRUM spect  
 PROBRD 5 mm WJ11nu  
 PULPROG inv4gs1d1prnd  
 TD 2048  
 SOLVENT dmsd06  
 NS 4  
 DS 16  
 SFO 6250.000 Hz  
 SHH 3.051758 Hz  
 FIDRES 0.163990 sec  
 AQ 1.6384  
 RG 80.000 usec  
 DW 114.29 usec  
 DE 303.0 K  
 TE 303.0 K  
 YF 1000.00 usec  
 PL16 100  
 L21 3 dB  
 LC1 1  
 D1 1.25000000 sec  
 P1 7.31 usec  
 O1 0.00345000 sec  
 O2 9.75 usec  
 P2 100.6244000 MHz  
 SFO2 13C  
 DECNLC 0.05000000 sec  
 O3 0.00003000 sec  
 O27 0.00000080 sec  
 O16 0.00010000 sec  
 P2 14.62 usec  
 P2 0.00000300 sec  
 SFO1 400.1390252 MHz  
 NUCLEUS 1H  
 INO 0.00002529 sec

F1 - Acquisition Parameters  
 NDD 256  
 TD 100  
 SFO1 100.6244 MHz  
 FIDRES 86.474129 Hz  
 SM 220.000 ppm

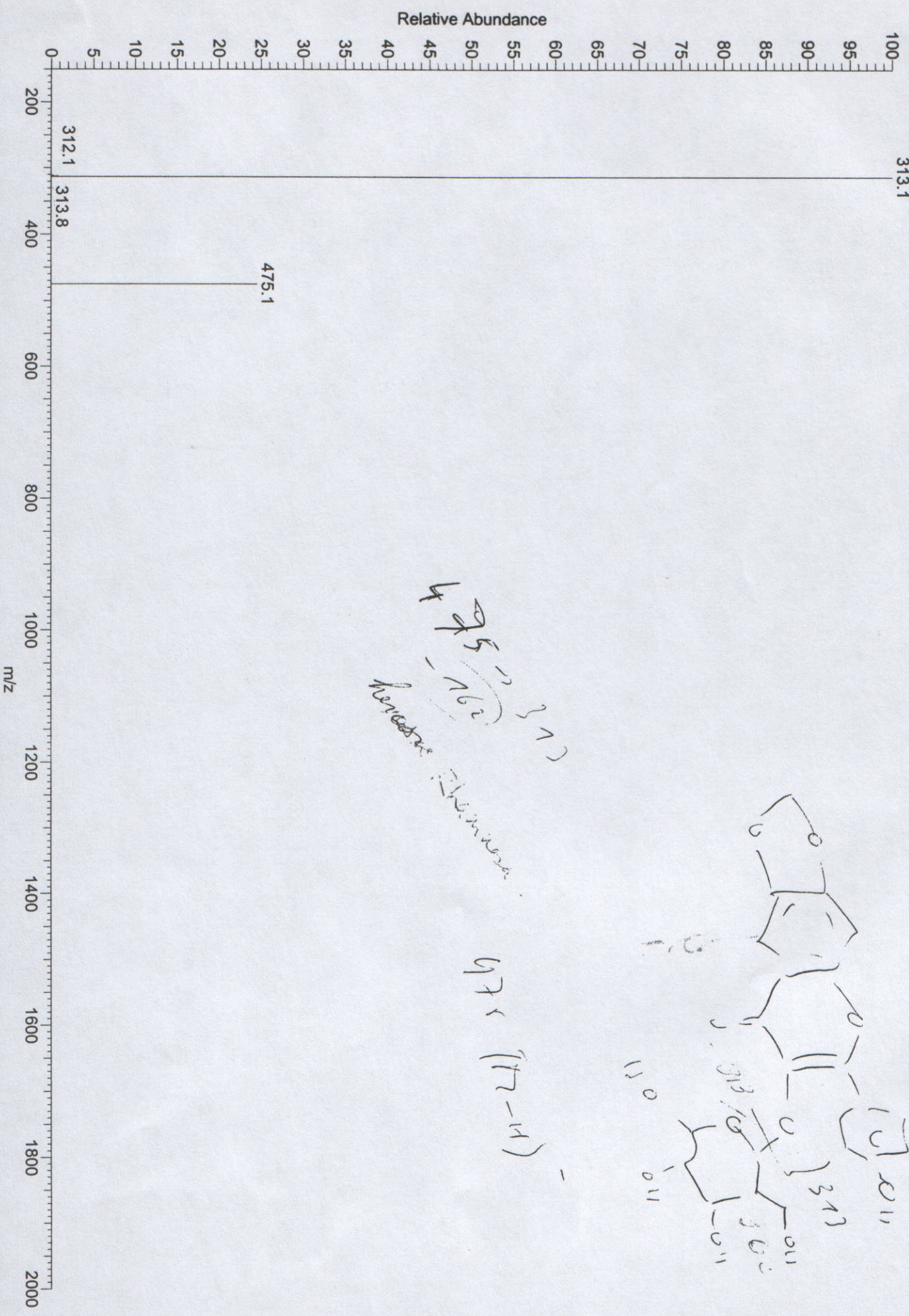
F2 - Processing Parameters  
 SI 1024  
 SF 400.1390252 MHz  
 DSINE 0  
 MDM 0  
 SSB 0.00 Hz  
 LB 0  
 GB 1.40  
 PC

F1 - Processing Parameters  
 SI 512  
 MC2 100.614377 MHz  
 SF 512  
 MDM 512  
 SSB 0.00 Hz  
 LB 0  
 GB 0

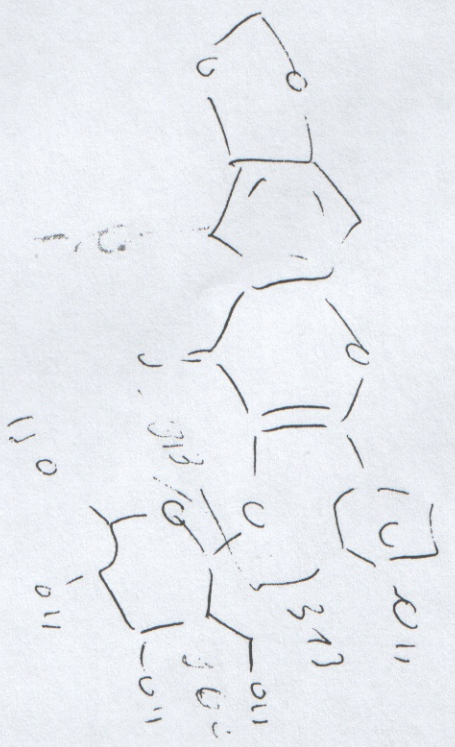
2D NMR Plot Parameters  
 CK2 18.00 cm  
 CK1 18.00 cm  
 F2PUL 3.747 DDM  
 F2LO 1499.12 Hz  
 F2PH1 3.413 DDM  
 F2PH2 1289.30 Hz  
 F1PUL 76.856 DDM  
 F1LO 7731.02 Hz  
 F1PH1 66.453 DDM  
 F1PH2 66.453 DDM  
 F2 PPM/cm 0.02986 DDM/cm  
 F2 ZC 11.86795 Hz/cm  
 F1 PPM/cm 0.57257 DDM/cm  
 F1 ZC 57.84944 Hz/cm



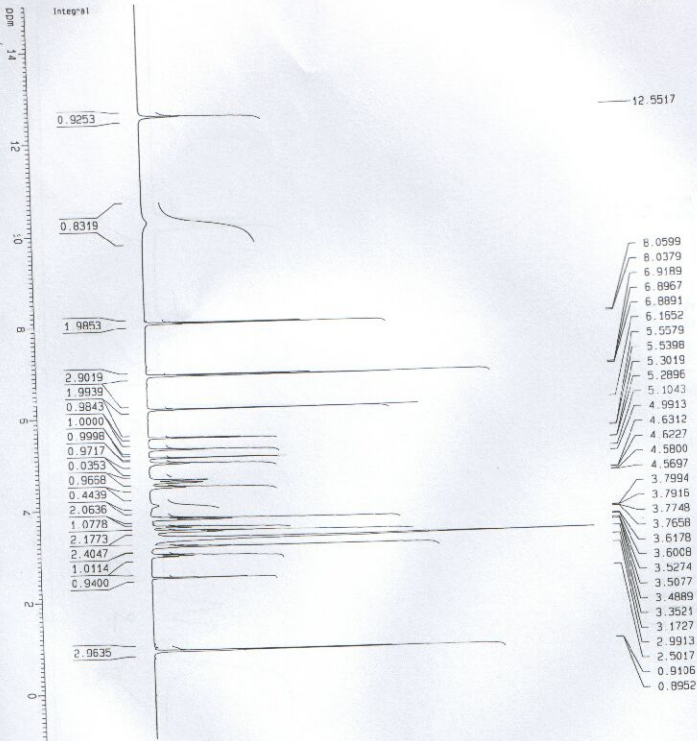
101SPN0812 #103-112 RT: 3.63-3.95 AV: 10 NL: 7.22E4  
T: - c Full ms2 475.00@27.00 [150.00-2000.00]



*Handwritten notes:*  
475 (172)  
Molecular weight  
475 (17-14)



12.5517



Current Data Parameters  
 NAME CSMS-4\_25  
 EXPNO 1  
 PROCNO 1

## F2 - Acquisition Parameters

Date\_ 20050624  
 Time 8:19  
 INSTRUM spect  
 PQCARD 5 mri Multiv  
 PU\_PROG 2930  
 TO SOLVENT 32768  
 CDC13  
 NS 8  
 DS 2  
 SMH 6410.256 Hz  
 FREQES 0.195625 MHz  
 AQ 2.5559540 sec  
 RG 64  
 DW 78.000 usec  
 DE 97.50 usec  
 TE 298.0 K  
 K1 3.08  
 D1 1.00000000 sec  
 P1 7.50 usec  
 SF01 400.1390934 MHz  
 NUC1EUS 1H

## F2 - Processing parameters

SF 327.68  
 SF 400.1390934 MHz  
 MCH EM  
 SSB 0  
 LB 0.20 Hz  
 DB 0  
 PC 1.00

## 10 NMR Plot Parameters

CK 20.00 cm  
 F1P 13.01C ppm  
 F1 6008.01 Hz  
 F2P -14.58 Hz  
 F2 0.80101 ppm/cm  
 HZCM 380.51289 Hz/cm



Current Data Parameters  
NAME DBM-4 20  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

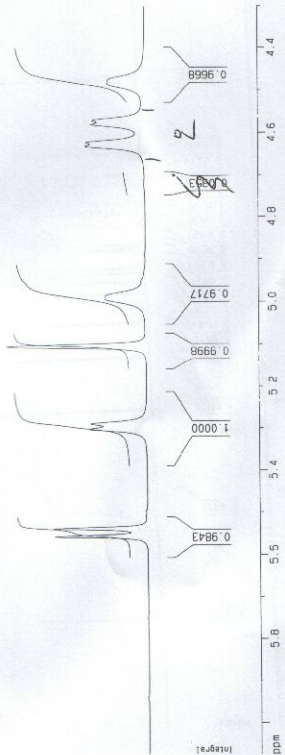
Date\_ 20050821  
Time 8 19  
INSTRUM spect  
PROBHD 5 mm Multino  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 2  
DS 2  
SWH 6410.255 Hz  
FIDRES 0.135673 Hz  
AQ 2.3555570 SEC  
RG 64  
AQ 79.000 USEC  
SFO1 400.136288 MHz  
NUC1 13C  
NUC2 1H

F2 - Processing parameters

SI 32768  
SF 400.136288 MHz  
WDW EM  
SSB 0  
GB 0.20 Hz  
PC 1.00

1D NMR plot parameters

CA 20.00 cm  
CX 5.074 ppm  
F1P 2430.46 Hz  
F2 175.97 ppm  
Z 2  
SFO1 0.08873 ppm/cm  
SFO2 38.36462 Hz/cm

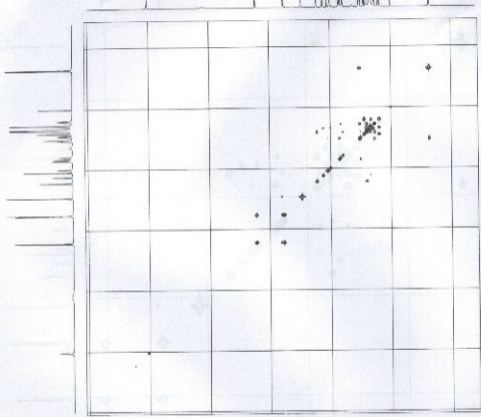


COSY

H-H

2 Keisler

acros 179179 dms



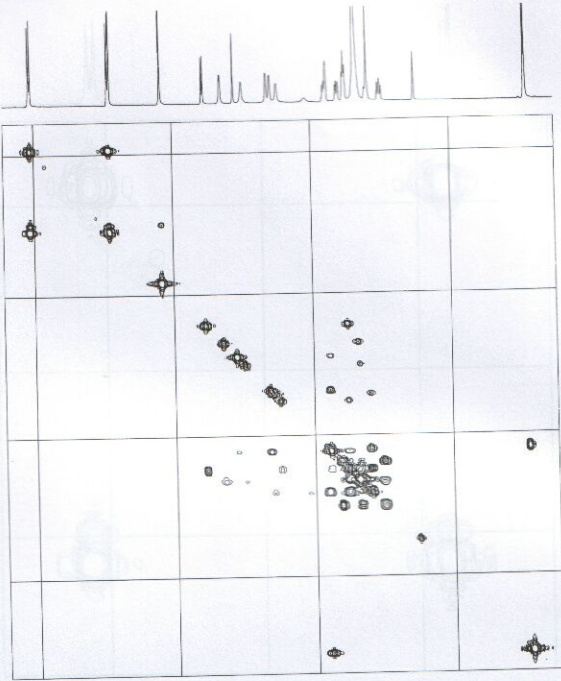
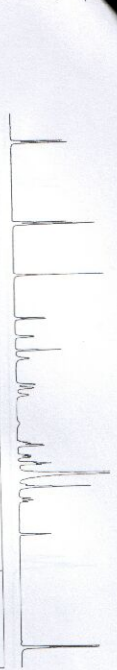
Vertical axis label: ppm

Horizontal axis label: ppm

General Data Parameters	
NAME	0841-4 20
EXPNO	4
F2PROC	1
F1 - Acquisition Parameters	
Date_	08/08/00
Time	8 11
INSTRUM	jeol
PROBHD	5 mm H-13C
PULPROG	zgpg30
TD	1310
SOFTW	jeol
SI	2
SS	8
DSM	6481 664 12
FIDRES	0.34708 Hz
AQ	0.020000 sec
RG	32
SD	17 000 4000
WDW	EM
SSB	0
LB	300.0 Hz
GB	0
PC	1000 00 0000
RG1	320
RG2	1 0000000 000
RG3	2 000 0000
RG4	0 000000 000
RG5	0 000000 000
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RG371	0 000000 000

across 179179 dmsu

Current Data Parameters  
 Date: 11/11/81  
 Time: 11:11  
 Name: 179179



12 - RESULTS OF PARAMETERS

DATA: 179179

NAME: 179179

INSTR: spect

PROBHD: 5 mm Maltinn

KA1 P105: C131194

SO1:V1:1

SO2:V1:1

NS: 8

DS: 2

PR1: 179179

PR2: 179179

PR3: 179179

PR4: 179179

PR5: 179179

PR6: 179179

PR7: 179179

PR8: 179179

PR9: 179179

PR10: 179179

PR11: 179179

PR12: 179179

PR13: 179179

PR14: 179179

PR15: 179179

PR16: 179179

PR17: 179179

PR18: 179179

PR19: 179179

PR20: 179179

PR21: 179179

PR22: 179179

PR23: 179179

PR24: 179179

PR25: 179179

PR26: 179179

PR27: 179179

PR28: 179179

PR29: 179179

PR30: 179179

PR31: 179179

F1 - Processing parameters

SI: 1600

DF: 1000

SR: 400 (MAGNA-400)

NUC1: 13C

PC: 0.000000

PR1: 179179

PR2: 179179

PR3: 179179

PR4: 179179

PR5: 179179

PR6: 179179

PR7: 179179

PR8: 179179

PR9: 179179

PR10: 179179

PR11: 179179

PR12: 179179

PR13: 179179

PR14: 179179

PR15: 179179

PR16: 179179

PR17: 179179

PR18: 179179

PR19: 179179

PR20: 179179

PR21: 179179

PR22: 179179

PR23: 179179

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PR25: 179179

PR26: 179179

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PR102: 179179

PR103: 179179

PR104: 179179

PR105: 179179

PR106: 179179

PR107: 179179

PR108: 179179

PR109: 179179

PR110: 179179

PR111: 179179

PR112: 179179

PR113: 179179

PR114: 179179

PR115: 179179

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PR160: 179179

PR161: 179179

PR162: 179179

PR163: 179179

PR164: 179179

PR165: 179179

PR166: 179179

PR167: 179179

PR168: 179179

PR169: 179179

PR170: 179179

PR171: 179179

PR172: 179179

PR173: 179179

PR174: 179179

PR175: 179179

PR176: 179179

PR177: 179179

PR178: 179179

PR179: 179179

PR180: 179179

PR181: 179179

PR182: 179179

PR183: 179179

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PR189: 179179

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PR191: 179179

PR192: 179179

PR193: 179179

PR194: 179179

PR195: 179179

PR196: 179179

PR197: 179179

PR198: 179179

PR199: 179179

PR200: 179179

PR201: 179179

PR202: 179179

PR203: 179179

PR204: 179179

PR205: 179179

PR206: 179179

PR207: 179179

PR208: 179179

PR209: 179179

PR210: 179179

PR211: 179179

PR212: 179179

PR213: 179179

8CROS 179179 0890

System Data Parameters  
 Name: 8CROS 179  
 PROGID: 1

F2 - Acquisition Parameters

Date\_: 20020921  
 Time: 8:17  
 Date\_: 09/21/02  
 PROGID: 5 48 PULL179  
 PULLPROG: CRYST  
 PULLTIME: 100  
 SOLVENT: 2  
 NS: 2  
 DS: 4  
 SWH: 6400.000 MHz  
 FIDRES: 0.361325 Hz  
 AC: 0.0389900 sec  
 DE: 17.000 MHz  
 FE: 115.00 MHz  
 FI18: 1500.000 MHz  
 L41: 100.000  
 L42: 100.000  
 L43: 1.0000000 sec  
 S1: 7.38 MHz  
 S2: 0.0000000 sec  
 S3: 0.0000000 sec  
 D1: 0.0000000 sec  
 D18: 0.0000000 sec  
 PG: 0.0000000 sec  
 S7: 0.0000000 sec  
 S7G: 400.1302004 MHz  
 NUC16U5: 0.0000000 sec  
 INC: 0.0000000 sec

F1 - Acquisition Parameters

NUC: 13C  
 PULPROG: zgpg30  
 PCPD: 400.1301 MHz  
 FIDRES: 25.0000000 MHz  
 SFO: 400.1301 MHz

F2 - Processing Parameters

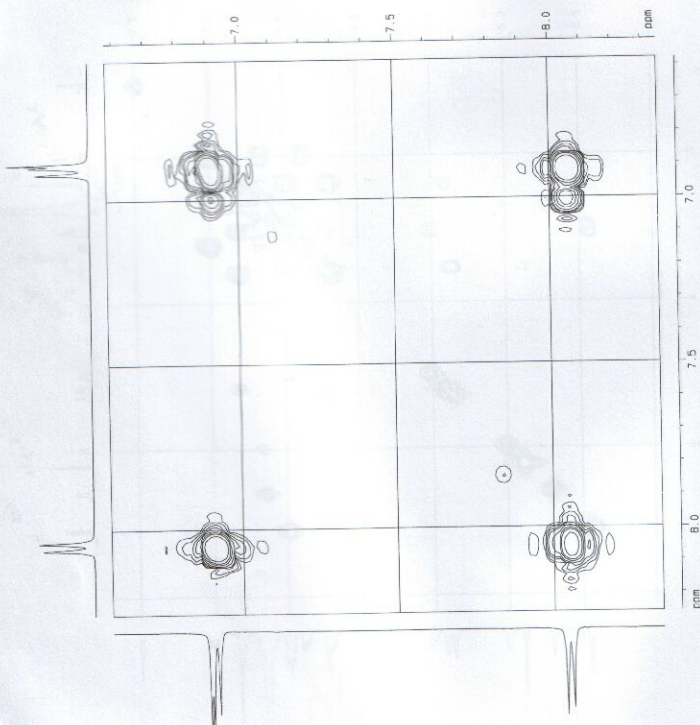
SI: 1  
 SF: 400.1302004 MHz  
 WHW: 5140  
 LB: 0.00 Hz  
 GB: 0  
 PC: 1.00

F1 - Processing Parameters

SI: 1  
 SF: 100.6261500 MHz  
 WHW: 400.1302004 MHz  
 LB: 0.00 Hz  
 GB: 0

25 - MR 13C1 Parameters

CH1: 13C  
 CH2: 13C  
 F2: 0  
 F2C: 200.415171 MHz  
 F2C2: 0.0000000 MHz  
 F4: 0  
 F4C: 334.915171 MHz  
 F4C2: 0.0000000 MHz  
 F1: 100.6261500 MHz  
 F1C2: 0.0000000 MHz  
 F1C3: 0.0000000 MHz  
 F1C4: 0.0000000 MHz  
 F1C5: 0.0000000 MHz  
 F1C6: 0.0000000 MHz  
 F1C7: 0.0000000 MHz  
 F1C8: 0.0000000 MHz  
 F1C9: 0.0000000 MHz  
 F1C10: 0.0000000 MHz  
 F1C11: 0.0000000 MHz  
 F1C12: 0.0000000 MHz  
 F1C13: 0.0000000 MHz  
 F1C14: 0.0000000 MHz  
 F1C15: 0.0000000 MHz  
 F1C16: 0.0000000 MHz  
 F1C17: 0.0000000 MHz  
 F1C18: 0.0000000 MHz  
 F1C19: 0.0000000 MHz  
 F1C20: 0.0000000 MHz













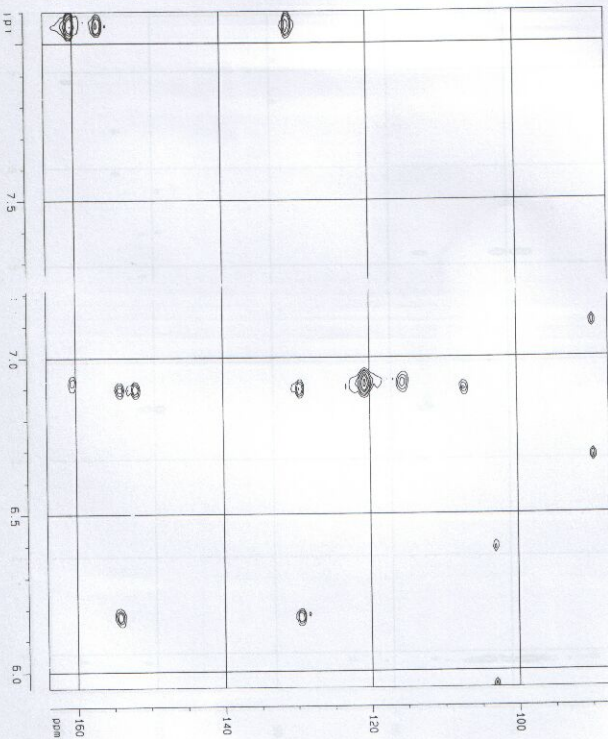




Chemical Shift Reference  
 Name: DMF-d7  
 Value: 29.29  
 Name: DMF-d7  
 Value: 29.29

13 C NMR (101 MHz, DMSO-d6)

Chemical Shift (ppm)	Assignment
160.0	C=O
155.0	C-O
150.0	C-O
145.0	C-O
140.0	C-O
135.0	C-O
130.0	C-O
125.0	C-O
120.0	C-O
115.0	C-O
110.0	C-O
105.0	C-O
100.0	C-O
95.0	C-O
90.0	C-O
85.0	C-O
80.0	C-O
75.0	C-O
70.0	C-O
65.0	C-O
60.0	C-O
55.0	C-O
50.0	C-O
45.0	C-O
40.0	C-O
35.0	C-O
30.0	C-O
25.0	C-O
20.0	C-O
15.0	C-O
10.0	C-O
5.0	C-O



Format: Data Output  
 Date: 11/11/83  
 Time: 11:30  
 Name: 186728.dms0



1. Acquisition Parameters  
 Date: 20080804  
 Time: 11:30  
 Name: 186728.dms0  
 Operator: [unreadable]  
 Instrument: spect  
 P1: 1.00  
 P2: 0.00  
 F1: 500.136  
 F2: 500.136  
 SFO: 500.136  
 AQ: 1.00  
 SI: 32768  
 SF: 500.136  
 AS: 32768  
 DS: 4  
 SS: 16  
 IS: 16  
 OS: 16  
 PS: 16  
 PC: 16  
 PD: 16  
 PE: 16  
 PF: 16  
 PG: 16  
 PH: 16  
 PI: 16  
 PJ: 16  
 PK: 16  
 PL: 16  
 PM: 16  
 PN: 16  
 PO: 16  
 PP: 16  
 PQ: 16  
 PR: 16  
 PS: 16  
 PT: 16  
 PU: 16  
 PV: 16  
 PW: 16  
 PX: 16  
 PY: 16  
 PZ: 16  
 Q1: 16  
 Q2: 16  
 Q3: 16  
 Q4: 16  
 Q5: 16  
 Q6: 16  
 Q7: 16  
 Q8: 16  
 Q9: 16  
 Q0: 16  
 R1: 16  
 R2: 16  
 R3: 16  
 R4: 16  
 R5: 16  
 R6: 16  
 R7: 16  
 R8: 16  
 R9: 16  
 R0: 16  
 S1: 16  
 S2: 16  
 S3: 16  
 S4: 16  
 S5: 16  
 S6: 16  
 S7: 16  
 S8: 16  
 S9: 16  
 S0: 16  
 T1: 16  
 T2: 16  
 T3: 16  
 T4: 16  
 T5: 16  
 T6: 16  
 T7: 16  
 T8: 16  
 T9: 16  
 T0: 16  
 U1: 16  
 U2: 16  
 U3: 16  
 U4: 16  
 U5: 16  
 U6: 16  
 U7: 16  
 U8: 16  
 U9: 16  
 U0: 16  
 V1: 16  
 V2: 16  
 V3: 16  
 V4: 16  
 V5: 16  
 V6: 16  
 V7: 16  
 V8: 16  
 V9: 16  
 V0: 16  
 W1: 16  
 W2: 16  
 W3: 16  
 W4: 16  
 W5: 16  
 W6: 16  
 W7: 16  
 W8: 16  
 W9: 16  
 W0: 16  
 X1: 16  
 X2: 16  
 X3: 16  
 X4: 16  
 X5: 16  
 X6: 16  
 X7: 16  
 X8: 16  
 X9: 16  
 X0: 16  
 Y1: 16  
 Y2: 16  
 Y3: 16  
 Y4: 16  
 Y5: 16  
 Y6: 16  
 Y7: 16  
 Y8: 16  
 Y9: 16  
 Y0: 16  
 Z1: 16  
 Z2: 16  
 Z3: 16  
 Z4: 16  
 Z5: 16  
 Z6: 16  
 Z7: 16  
 Z8: 16  
 Z9: 16  
 Z0: 16











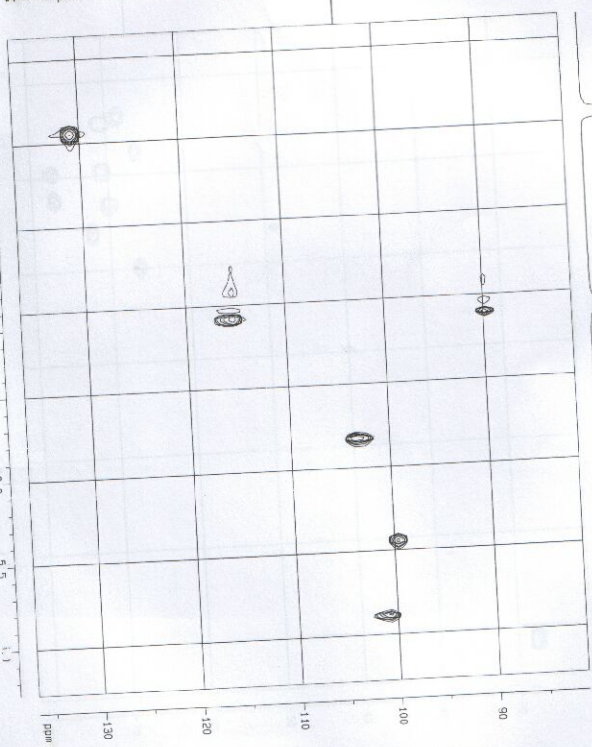
across 186/228 dmso

Current Data Parameters

NAME: 186/228  
 DATE: 08/18/77  
 RECD: 1

27 186/228 DMF/DMSO

FILE: 186/228  
 INSTR: 100 MHz  
 PULPROG: zgpg30  
 TD: 65536  
 SFO: 100.626130  
 AQ: 1.00000000  
 RG: 0.50000000  
 DELTA: 0.00000000  
 DE: 0.00000000  
 EC: 0.00000000  
 ZF2: 0.00000000  
 ZF1: 0.00000000  
 ZC: 0.00000000  
 ZB: 0.00000000  
 ZY: 0.00000000  
 ZX: 0.00000000  
 ZW: 0.00000000  
 ZV: 0.00000000  
 ZU: 0.00000000  
 ZT: 0.00000000  
 ZS: 0.00000000  
 ZR: 0.00000000  
 ZQ: 0.00000000  
 ZP: 0.00000000  
 ZO: 0.00000000  
 ZN: 0.00000000  
 ZM: 0.00000000  
 ZL: 0.00000000  
 ZK: 0.00000000  
 ZJ: 0.00000000  
 ZI: 0.00000000  
 ZH: 0.00000000  
 ZG: 0.00000000  
 ZF: 0.00000000  
 ZE: 0.00000000  
 ZD: 0.00000000  
 ZC: 0.00000000  
 ZB: 0.00000000  
 ZA: 0.00000000  
 Z9: 0.00000000  
 Z8: 0.00000000  
 Z7: 0.00000000  
 Z6: 0.00000000  
 Z5: 0.00000000  
 Z4: 0.00000000  
 Z3: 0.00000000  
 Z2: 0.00000000  
 Z1: 0.00000000



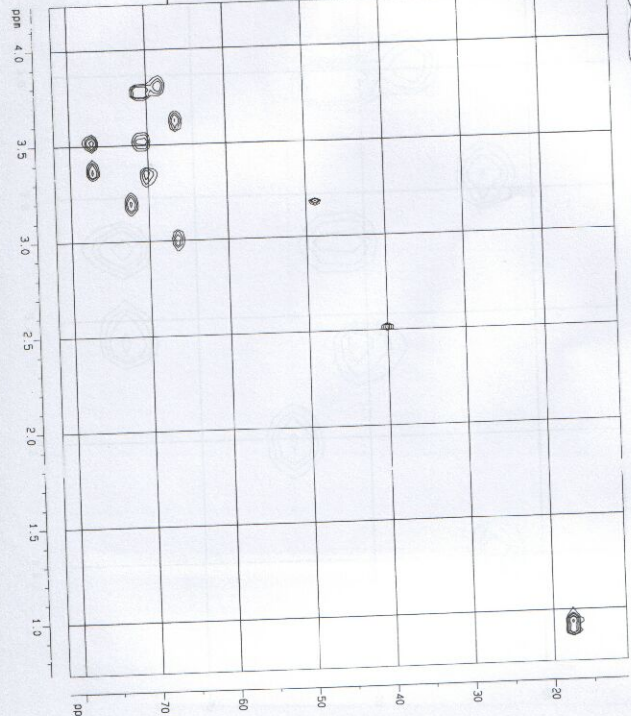
27 186/228 DMF/DMSO

FILE: 186/228  
 INSTR: 100 MHz  
 PULPROG: zgpg30  
 TD: 65536  
 SFO: 100.626130  
 AQ: 1.00000000  
 RG: 0.50000000  
 DELTA: 0.00000000  
 DE: 0.00000000  
 EC: 0.00000000  
 ZF2: 0.00000000  
 ZF1: 0.00000000  
 ZC: 0.00000000  
 ZB: 0.00000000  
 ZY: 0.00000000  
 ZX: 0.00000000  
 ZW: 0.00000000  
 ZV: 0.00000000  
 ZU: 0.00000000  
 ZT: 0.00000000  
 ZS: 0.00000000  
 ZR: 0.00000000  
 ZQ: 0.00000000  
 ZP: 0.00000000  
 ZO: 0.00000000  
 ZN: 0.00000000  
 ZM: 0.00000000  
 ZL: 0.00000000  
 ZK: 0.00000000  
 ZJ: 0.00000000  
 ZI: 0.00000000  
 ZH: 0.00000000  
 ZG: 0.00000000  
 ZF: 0.00000000  
 ZE: 0.00000000  
 ZD: 0.00000000  
 ZC: 0.00000000  
 ZB: 0.00000000  
 ZA: 0.00000000  
 Z9: 0.00000000  
 Z8: 0.00000000  
 Z7: 0.00000000  
 Z6: 0.00000000  
 Z5: 0.00000000  
 Z4: 0.00000000  
 Z3: 0.00000000  
 Z2: 0.00000000  
 Z1: 0.00000000

NAME: SC705 186728.DMSO  
 EXPNO: 2  
 PROCNO: 2  
 F2 - Acquisition Parameters

DATE\_: 20080827  
 TIME: 11.00  
 INSTRUM: spect  
 CHANNEL: zgpg30  
 PULPROG: zgpg30  
 PROCPRG: zgpg30  
 F2 - Processing parameters

SI - Processing parameters  
 SI 1: 400.146000 MHz  
 SI 2: 51.813000 MHz  
 SI 3: 51.813000 MHz  
 SI 4: 0.000000 MHz  
 SI 5: 0.000000 MHz  
 SI 6: 0.000000 MHz  
 SI 7: 0.000000 MHz  
 SI 8: 0.000000 MHz  
 SI 9: 0.000000 MHz  
 SI 10: 0.000000 MHz  
 SI 11: 0.000000 MHz  
 SI 12: 0.000000 MHz  
 SI 13: 0.000000 MHz  
 SI 14: 0.000000 MHz  
 SI 15: 0.000000 MHz  
 SI 16: 0.000000 MHz  
 SI 17: 0.000000 MHz  
 SI 18: 0.000000 MHz  
 SI 19: 0.000000 MHz  
 SI 20: 0.000000 MHz  
 SI 21: 0.000000 MHz  
 SI 22: 0.000000 MHz  
 SI 23: 0.000000 MHz  
 SI 24: 0.000000 MHz  
 SI 25: 0.000000 MHz  
 SI 26: 0.000000 MHz  
 SI 27: 0.000000 MHz  
 SI 28: 0.000000 MHz  
 SI 29: 0.000000 MHz  
 SI 30: 0.000000 MHz  
 SI 31: 0.000000 MHz  
 SI 32: 0.000000 MHz  
 SI 33: 0.000000 MHz  
 SI 34: 0.000000 MHz  
 SI 35: 0.000000 MHz  
 SI 36: 0.000000 MHz  
 SI 37: 0.000000 MHz  
 SI 38: 0.000000 MHz  
 SI 39: 0.000000 MHz  
 SI 40: 0.000000 MHz  
 SI 41: 0.000000 MHz  
 SI 42: 0.000000 MHz  
 SI 43: 0.000000 MHz  
 SI 44: 0.000000 MHz  
 SI 45: 0.000000 MHz  
 SI 46: 0.000000 MHz  
 SI 47: 0.000000 MHz  
 SI 48: 0.000000 MHz  
 SI 49: 0.000000 MHz  
 SI 50: 0.000000 MHz  
 SI 51: 0.000000 MHz  
 SI 52: 0.000000 MHz  
 SI 53: 0.000000 MHz  
 SI 54: 0.000000 MHz  
 SI 55: 0.000000 MHz  
 SI 56: 0.000000 MHz  
 SI 57: 0.000000 MHz  
 SI 58: 0.000000 MHz  
 SI 59: 0.000000 MHz  
 SI 60: 0.000000 MHz  
 SI 61: 0.000000 MHz  
 SI 62: 0.000000 MHz  
 SI 63: 0.000000 MHz  
 SI 64: 0.000000 MHz  
 SI 65: 0.000000 MHz  
 SI 66: 0.000000 MHz  
 SI 67: 0.000000 MHz  
 SI 68: 0.000000 MHz  
 SI 69: 0.000000 MHz  
 SI 70: 0.000000 MHz  
 SI 71: 0.000000 MHz  
 SI 72: 0.000000 MHz  
 SI 73: 0.000000 MHz  
 SI 74: 0.000000 MHz  
 SI 75: 0.000000 MHz  
 SI 76: 0.000000 MHz  
 SI 77: 0.000000 MHz  
 SI 78: 0.000000 MHz  
 SI 79: 0.000000 MHz  
 SI 80: 0.000000 MHz  
 SI 81: 0.000000 MHz  
 SI 82: 0.000000 MHz  
 SI 83: 0.000000 MHz  
 SI 84: 0.000000 MHz  
 SI 85: 0.000000 MHz  
 SI 86: 0.000000 MHz  
 SI 87: 0.000000 MHz  
 SI 88: 0.000000 MHz  
 SI 89: 0.000000 MHz  
 SI 90: 0.000000 MHz  
 SI 91: 0.000000 MHz  
 SI 92: 0.000000 MHz  
 SI 93: 0.000000 MHz  
 SI 94: 0.000000 MHz  
 SI 95: 0.000000 MHz  
 SI 96: 0.000000 MHz  
 SI 97: 0.000000 MHz  
 SI 98: 0.000000 MHz  
 SI 99: 0.000000 MHz  
 SI 100: 0.000000 MHz















hmbc\_106\_cdc13

Current Data Acquisition

NAME: hmbc\_106\_cdc13  
 EXPNO: 5  
 PROCNO: 1

PROBHD: zgpg30

PULPROG: zgpg30

PCPDPRG2: zgpg30

PCPDPRG1: zgpg30

PCPDPRG0: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

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PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

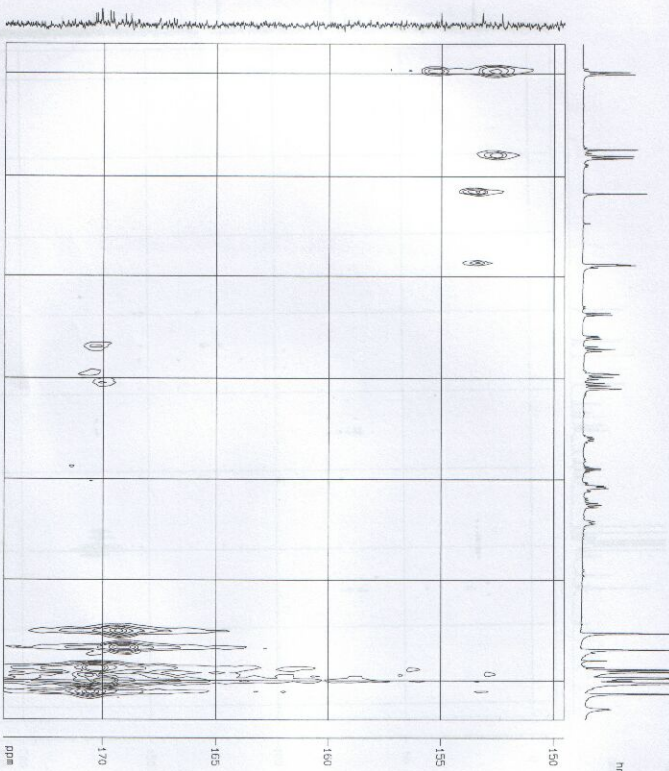
PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30

PCPDPRG: zgpg30



F1 - Acetone-d6, 120 MHz

F2 - Acetone-d6, 120 MHz

F3 - Acetone-d6, 120 MHz

F4 - Acetone-d6, 120 MHz

F5 - Acetone-d6, 120 MHz

F6 - Acetone-d6, 120 MHz

F7 - Acetone-d6, 120 MHz

F8 - Acetone-d6, 120 MHz

F9 - Acetone-d6, 120 MHz

F10 - Acetone-d6, 120 MHz

F11 - Acetone-d6, 120 MHz

F12 - Acetone-d6, 120 MHz

F13 - Acetone-d6, 120 MHz

F14 - Acetone-d6, 120 MHz

F15 - Acetone-d6, 120 MHz

LABOR H-1 NMR E-3 Lincom

INSTR: 105 CDC13

DATE: 10/10/77

NAME: H-1 NMR

EXPNO: 1

PROCNO: 1

PROG: 1

INSTR: 1

PROBHD: 5 mm NMR

PULPROG: zgpg30

TD: 32768

DELTA: 0.000000

DE: 0.000000

TE: 300.2 K

F2: 500.136 MHz

F1: 500.136 MHz

NUC1: 13C

NUC2: 1H

WALTZ16: 0.000000

WALTZ17: 0.000000

WALTZ18: 0.000000

WALTZ19: 0.000000

WALTZ20: 0.000000

WALTZ21: 0.000000

WALTZ22: 0.000000

WALTZ23: 0.000000

WALTZ24: 0.000000

WALTZ25: 0.000000

WALTZ26: 0.000000

WALTZ27: 0.000000

WALTZ28: 0.000000

WALTZ29: 0.000000

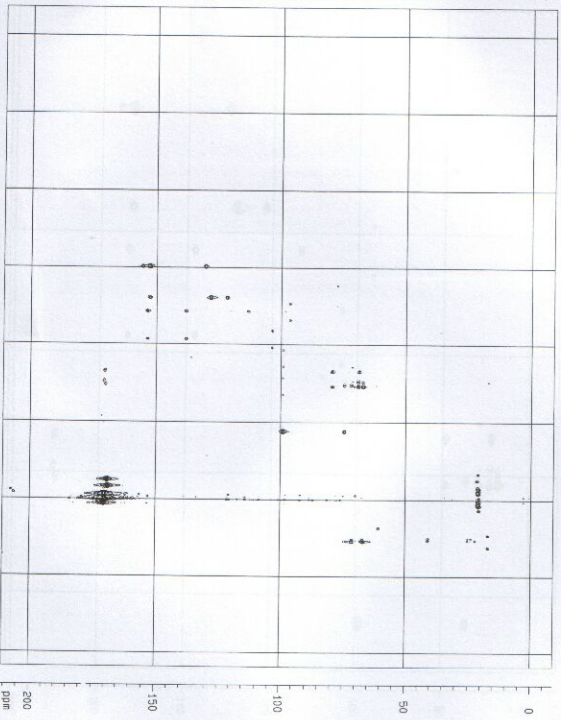
WALTZ30: 0.000000

WALTZ31: 0.000000

WALTZ32: 0.000000

WALTZ33: 0.000000

WALTZ34: 0.000000



F1: Processing parameters

SI: 32768

SD: 1

WDW: EM

SSB: 0

LB: 0.000000

GB: 0.000000

PC: 1.000000

CC: 0.000000

CD: 0.000000

CF: 0.000000

CH: 0.000000

CM: 0.000000

CO: 0.000000

CP: 0.000000

CQ: 0.000000

CR: 0.000000

CS: 0.000000

CT: 0.000000

CU: 0.000000

CV: 0.000000

CW: 0.000000

CX: 0.000000

CY: 0.000000

CZ: 0.000000

CA: 0.000000

CB: 0.000000

CC: 0.000000

CD: 0.000000

CE: 0.000000

CF: 0.000000

CG: 0.000000

CH: 0.000000

CI: 0.000000

CJ: 0.000000

CK: 0.000000

CL: 0.000000

CM: 0.000000

CN: 0.000000

CO: 0.000000

CP: 0.000000

CQ: 0.000000

CR: 0.000000

CS: 0.000000

CT: 0.000000

CU: 0.000000

CV: 0.000000

CW: 0.000000

CX: 0.000000

CY: 0.000000

CZ: 0.000000

CA: 0.000000

CB: 0.000000

CC: 0.000000

CD: 0.000000

CE: 0.000000

CF: 0.000000

CG: 0.000000

CH: 0.000000

CI: 0.000000

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CS: 0.000000

CT: 0.000000

CU: 0.000000

CV: 0.000000

CW: 0.000000

CX: 0.000000

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CV: 0.000000

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CX: 0.000000

CY: 0.000000

CZ: 0.000000

CA: 0.000000

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CE: 0.000000

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CO: 0.000000

CP: 0.000000

CQ: 0.000000

CR: 0.000000

CS: 0.000000

CT: 0.000000

CU: 0.000000

CV: 0.000000

CW: 0.000000

CX: 0.000000

CY: 0.000000

CZ: 0.000000

CA: 0.000000

CB: 0.000000

CC: 0.000000

CD: 0.000000

CE: 0.000000

CF: 0.000000

CG: 0.000000

CH: 0.000000

CI: 0.000000

CJ: 0.000000

CK: 0.000000

CL: 0.000000

CM: 0.000000

CN: 0.000000

CO: 0.000000

CP: 0.000000

CQ: 0.000000

CR: 0.000000

CS: 0.000000

CT: 0.000000

CU: 0.000000

CV: 0.000000

CW: 0.000000

CX: 0.000000

CY: 0.000000

CZ: 0.000000

CA: 0.000000

CB: 0.000000

CC: 0.000000

CD: 0.000000

CE: 0.000000

CF: 0.000000

CG: 0.000000

CH: 0.000000

CI: 0.000000

CJ: 0.000000

CK: 0.000000

CL: 0.000000

CM: 0.000000

CN: 0.000000

CO: 0.000000

CP: 0.000000

CQ: 0.000000

CR: 0.000000

CS: 0.000000

CT: 0.000000

CU: 0.000000

CV: 0.000000

CW: 0.000000

CX: 0.000000

CY: 0.000000

CZ: 0.000000

CA: 0.000000

CB: 0.000000

CC: 0.000000

CD: 0.000000

CE: 0.000000

CF: 0.000000

CG: 0.000000

CH: 0.000000

CI: 0.000000

CJ: 0.000000

CK: 0.000000

CL: 0.000000

CM: 0.000000

CN: 0.000000

CO: 0.000000

CP: 0.000000

CQ: 0.000000

CR: 0.000000

CS: 0.000000

CT: 0.000000

CU: 0.000000

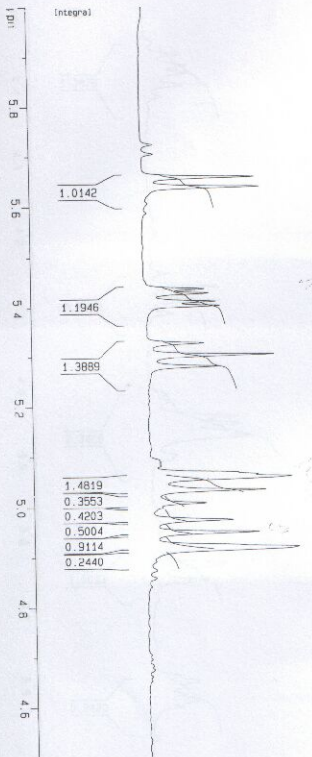
CV: 0.000000

CW: 0.00





- 5.65687
- 5.63769
- 5.43590
- 5.42734
- 5.41074
- 5.40216
- 5.32652
- 5.30296
- 5.27936
- 5.06291
- 5.05799
- 5.03228
- 5.00714
- 4.97244
- 4.94799
- 4.91765



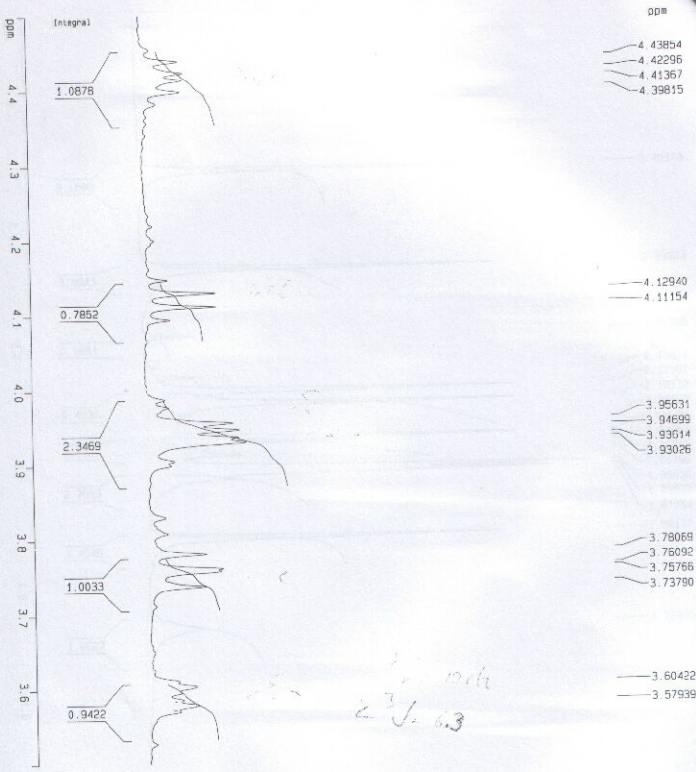
Current Data Parameters  
 NAME DMC-5a  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050808  
 Time 10.34  
 INSTRUM spect  
 PROCNO 5  
 PULPROG zgpg  
 TD 32768  
 SFO 300.13  
 ACQ 16  
 DS 2  
 SWH 6544.315 Hz  
 FIDRES 0.200028 Hz  
 AQ 2.989128 sec  
 RG 64  
 DM 73.000 USEC  
 DE 91.25 usec  
 TE 299.0 K  
 H1 3 dB  
 D1 2.00000000 sec  
 R1 7.50 usec  
 SFO1 400.1360532 MHz  
 NUC1 1H

F2 Processing parameters  
 SI 32768  
 SF 400.1343898 MHz  
 MD EN  
 SEB 0  
 LB 0.10 Hz  
 GB 0  
 PC 1.00

10 MHz pilot parameters  
 CV 20.00 CEM  
 F1P 5.000 CEM  
 F1 2400.91 Hz  
 F2 4.500 CEM  
 F2 1800.90 Hz  
 PPMOFC 0.07500 ppm/cm  
 MZCM 38.01000 Hz/cm



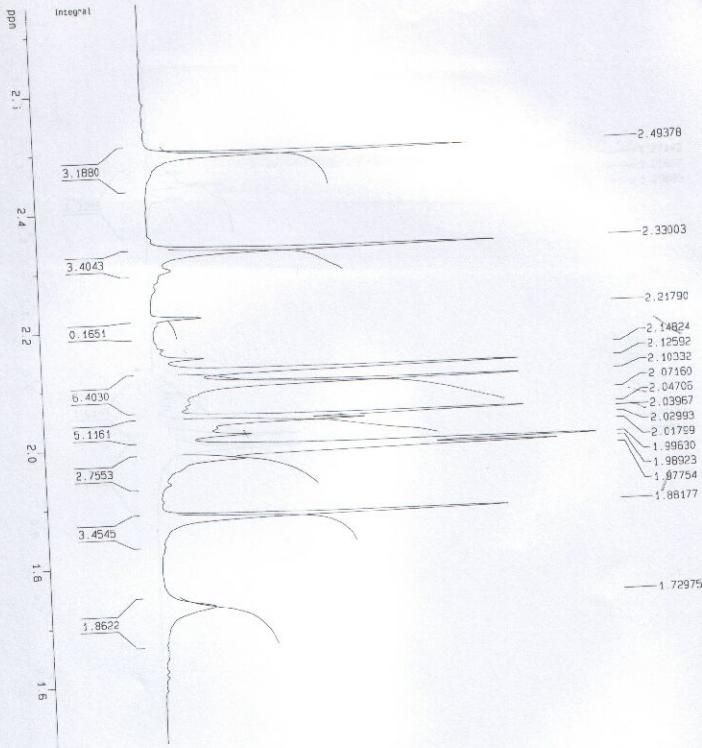


Current Data Parameters  
 NAME DM-5g  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050603  
 Time 10 34  
 INSTRUM spect  
 PROBRD 5 mm NUTYNU  
 PULPROG zg30  
 TD 32768  
 TO 22788  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6846.315 Hz  
 FIDRES 0.259075 Hz  
 AQ 2.3921139 sec  
 RG 64  
 RW 73.050 usec  
 DE 91.25 usec  
 TE 298.0 K  
 H4.1 3.08  
 D1 2.00000000 sec  
 D1.1 7.50 usec  
 SF01 400.1588032 Mhz  
 NUCLEN1 1H

F2 - Processing parameters  
 SI 32768  
 SF 400.1588039 Mhz  
 MM EM  
 SSB 0  
 LB 0.10 Hz  
 GB 0  
 PC 1.00

1D NMR plot characters  
 CX 20.00 cm  
 FV 4.500 um  
 F1 1800.60 Hz  
 F2 3.500 ppm  
 F3 1400.47 Hz  
 PPGM 0.00000 cm/cm  
 HZCM 20.00378 Hz/cm



Current Data Parameters  
 Name: DMS-5a  
 EXPNO: 1  
 PROCNO: 1

## F2 - Acquisition Parameters

Date\_: 200606  
 Time: 10.34  
 INSTRUM: spect  
 PROBNM: 5 ml MULLTPO  
 PULPROG: zgpg30  
 TD: 4930  
 SO: vent  
 CQ: 13  
 NS: 4  
 DS: 2

SB: 6646.315 Hz  
 FIDRES: 0.209525 Hz  
 AQ: 2.392138 sec

RG: 64  
 UM: 73.000 usec  
 DE: 51.25 usec  
 TE: 298.0 K

HL: 3.03  
 D1: 2.0000000 sec  
 P1: 7.50 usec

SC: 400.1368532 MHz  
 NUC1: 1H

## F2 - Processing parameters

SI: 32768  
 SF: 400.1368532 MHz  
 SM: EM  
 MM: 0  
 SSB: 0  
 LB: 0.10 Hz  
 GB: 0  
 PC: 1.00

## 1D NMR plot parameters

CK: 20.00 cm  
 F1: 2.750 dm  
 F1: 1100.37 Hz  
 F2: 1.500 dm  
 F2: 600.20 Hz  
 SFO: 400.1368532 MHz  
 H2O: 0.050 dm  
 CHCl3: 29.050 dm

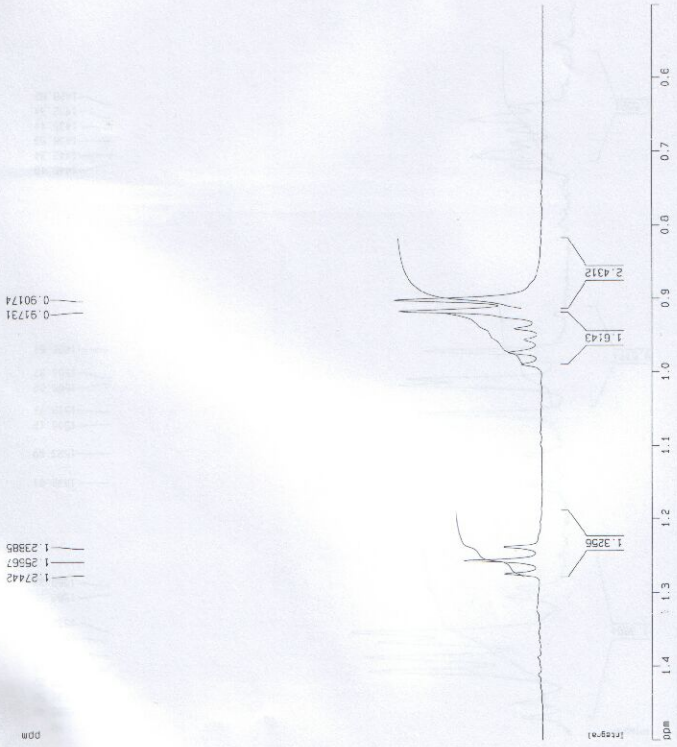
1.27442  
 1.25667  
 1.23985  
 0.91731  
 0.90174

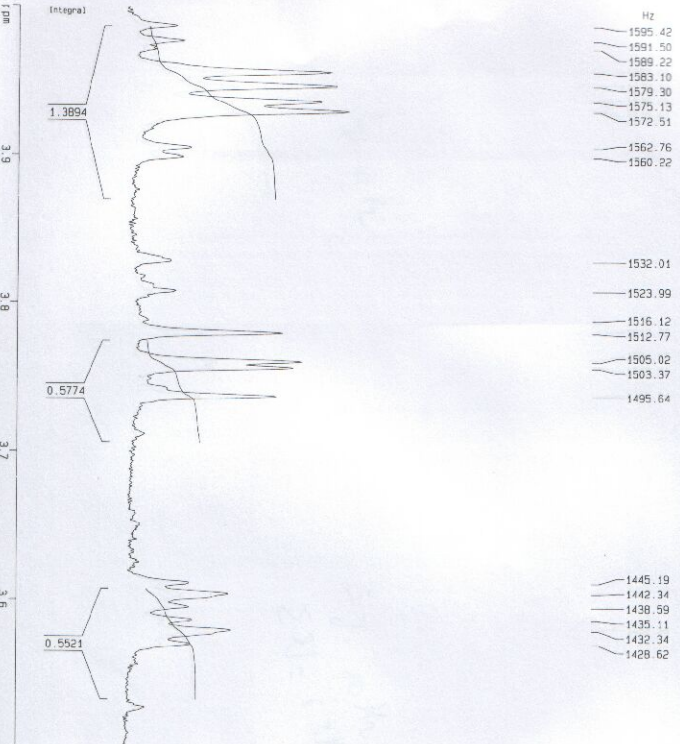
Current Data Parameters  
 NAME DMF-S  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050808  
 Time 10.34  
 INSTRUM spect  
 PROBO 5 mm MulticJ  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMS  
 NS 16  
 DS 2  
 SWH 6649.315 Hz  
 FIDRES 0.200025 Hz  
 AQ 2.3821139 sec  
 RG 64  
 CW 73.000 USEC  
 DE 91.25 USEC  
 TE 298.0 K  
 HL 3.60  
 D1 2.20000000 sec  
 P1 7.50 USEC  
 SF01 400.1368032 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 S1 32758  
 SF 400.1343888 MHz  
 MW CM  
 SSB 0  
 LB 0.10 Hz  
 GB 0  
 PC 1.00

10 NMR plot parameters  
 CX 20.00 cm  
 F1P 1.500 ppm  
 F1 650.30 Hz  
 F2 3.530 ppm  
 F2 200.37 Hz  
 PRGM  
 HZCM 20.00672 Hz/cm





- Hz
- 1595.42
- 1591.50
- 1589.22
- 1583.10
- 1579.30
- 1575.13
- 1572.51
- 1562.76
- 1560.22
- 1532.01
- 1523.99
- 1516.12
- 1512.77
- 1505.02
- 1503.37
- 1495.64
- 1445.19
- 1442.34
- 1438.59
- 1435.11
- 1432.34
- 1428.62

Current Data Parameters  
 NAME DMW-58  
 EXPNO 1  
 PROCNO 1

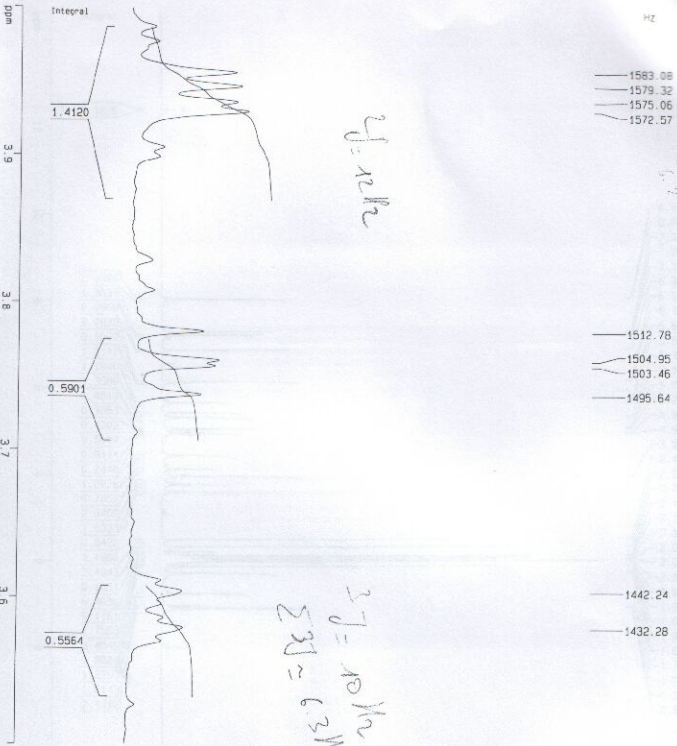
F2 - Acquisition Parameters

Date 20050605  
 Time 10:34  
 INSTRUM spect  
 PROBRG 8 mm MUX17V  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMS-D  
 NS 16  
 DS 2  
 SWH 6640.319 Hz  
 FIDRES 0.205529 Hz  
 AQ 2.1392129 sec  
 RG 64  
 WS 73.000 usec  
 CH 51.620 usec  
 TE 299.2 K  
 T1 3.03  
 T1 2.0000000 sec  
 T1 2.50 usec  
 SFO 400.1360625 MHz  
 NUCLEUS <sup>1</sup>H

F2 - Processing parameters

SF 400.1360625 MHz  
 NUC 1H  
 SSB 0  
 GB 0  
 PC 1.10  
 -1.00 Hz  
 0.5  
 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1-P 4.000 ppm  
 F1 1600.54 Hz  
 F2P 3.500 ppm  
 F2 1400.47 Hz  
 PPOUCH 0.02500 GHz/cm  
 HZCM (10) 00336 Hz/cm



Current Data Parameters  
 NAME: DMF-56  
 EXPNO: 1  
 PROCNO: 1

F2 - Acquisition Parameters

Date\_: 20050529  
 Time: 10:54  
 INSTRUM: spect  
 PROBRD: 5 mm Mx139v  
 PULPROG: zg30  
 PG2: 2c7f60  
 SOLVENT: DMS-D3  
 NS: 16  
 DS: 2  
 SWH: 6040.315 Hz  
 FIDRES: 0.205029 Hz  
 AQ: 2.3921139 sec  
 RG: 64  
 DM: 73.000 uSFC  
 DE: 91.25 uSFC  
 TE: 298.0 K  
 KL1: 3.05  
 F1: 2.00000000 sec  
 F2: 7.50 uSFC  
 SFO: 400.146082 MHz  
 NUCLEI: 1H

F2 - Processing parameters

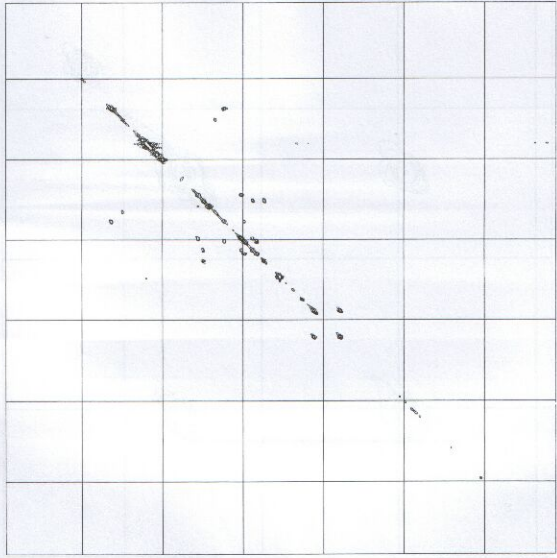
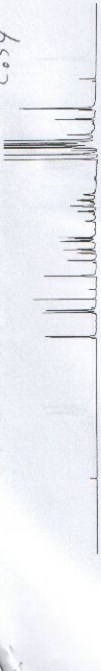
SI: 32768  
 SF: 400.146082 MHz  
 KW: 1342569.3  
 SSB: 0  
 LB: -0.52 Hz  
 GB: 0.23  
 PC: 1.00

1D NMR file parameters

OR: 1  
 CX: 1  
 F1P: 4.000 GHz  
 F1: 1650.54 MHz  
 F2P: 3.500 GHz  
 F2: 1400.47 MHz  
 PGMNAM: DQ32500 psm/cr  
 MZCM: 10.00336 Hz/Hz

0001001.D

COSY H-H 1 bin



Current Data Parameters  
 NAME 0001001.D  
 PDETC 1  
 1

F1 - Acquisition Parameters

Date\_ 11.30  
 Time 16:33  
 Name 0001001.D  
 PDETC 1  
 PAIRING COSY2D  
 Q 1  
 Q2 1  
 NS 2  
 DS 8  
 SWH 3.000 MHz  
 F1FREQ 6.0000000 MHz  
 A3 6.0745000 MHz  
 P3 75.000 MHz  
 P2 134.29 MHz  
 Q2 100.000 MHz  
 Q1 100.000 MHz  
 F1 1.0000000 Hz  
 F2 7.31 MHz  
 F3 0.0000000 Hz  
 F4 0.0000000 Hz  
 F5 0.0000000 Hz  
 F6 7.31 MHz  
 F7 0.0000000 Hz  
 F8 0.0000000 Hz  
 F9 7.31 MHz  
 F10 0.0000000 Hz  
 NUC1 1H  
 NUC2 1H  
 NUC3 1H  
 NUC4 1H  
 NUC5 1H  
 NUC6 1H  
 NUC7 1H  
 NUC8 1H  
 NUC9 1H  
 NUC10 1H  
 NUC11 1H  
 NUC12 1H  
 NUC13 1H  
 NUC14 1H  
 NUC15 1H  
 NUC16 1H  
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 NUC40 1H  
 NUC41 1H  
 NUC42 1H  
 NUC43 1H  
 NUC44 1H  
 NUC45 1H  
 NUC46 1H  
 NUC47 1H  
 NUC48 1H  
 NUC49 1H  
 NUC50 1H

F2 - Acquisition Parameters

Date\_ 11.30  
 Time 16:33  
 Name 0001001.D  
 PDETC 1  
 1

F3 - Processing Parameters

SI 32768  
 SF 400.13080 MHz  
 F2 FREQ 7.31 MHz  
 SI 131088  
 SF 400.13080 MHz  
 SFO 5196  
 SF 8.0 MHz  
 SFC 1.0 MHz  
 SFG 1.40 MHz

F4 - Processing Parameters

SI 131088  
 SF 400.13080 MHz  
 SFO 5196  
 SF 8.0 MHz  
 SFC 1.0 MHz  
 SFG 1.40 MHz

F5 - Processing Parameters

SI 131088  
 SF 400.13080 MHz  
 SFO 5196  
 SF 8.0 MHz  
 SFC 1.0 MHz  
 SFG 1.40 MHz

F6 - Processing Parameters

SI 131088  
 SF 400.13080 MHz  
 SFO 5196  
 SF 8.0 MHz  
 SFC 1.0 MHz  
 SFG 1.40 MHz

F7 - Processing Parameters

SI 131088  
 SF 400.13080 MHz  
 SFO 5196  
 SF 8.0 MHz  
 SFC 1.0 MHz  
 SFG 1.40 MHz

ppm 12.5 10.0 7.5 5.0 2.5 0.0

ppm 12.5 10.0 7.5 5.0 2.5 0.0

COZY ccc13

Current Data Acquisition

NAME: ccc13  
 EXPNO: 2  
 PROCNO: 1

F2 - Acquisition Parameters

INSTR: spect  
 DATE\_1: 11.30  
 TIME: 11.30  
 PULPROG: zgpg30  
 SOLVENT: POLY(ETHYLENE TEREPHTHALATE)  
 SOLVENT: POLY(ETHYLENE TEREPHTHALATE)  
 NS: 2  
 DS: 2  
 SWH: 6000.000 Hz  
 FWHM: 11.70 Hz  
 AQ: 0.00000000 sec  
 RG: 2048  
 ACQ: 23.400 sec  
 DE: 104.50 usec  
 TEM: 300.2 K  
 FIDRES: 0.00000000 Hz  
 AQRES: 0.00000000 Hz  
 SFO: 500.136363 MHz  
 NUC1: 13C  
 NUC2: 1H

F1 - Acquisition Parameters

INSTR: spect  
 DATE\_1: 11.30  
 TIME: 11.30  
 PULPROG: zgpg30  
 SOLVENT: POLY(ETHYLENE TEREPHTHALATE)  
 SOLVENT: POLY(ETHYLENE TEREPHTHALATE)  
 NS: 2  
 DS: 2  
 SWH: 6000.000 Hz  
 FWHM: 11.70 Hz  
 AQ: 0.00000000 sec  
 RG: 2048  
 ACQ: 23.400 sec  
 DE: 104.50 usec  
 TEM: 300.2 K  
 FIDRES: 0.00000000 Hz  
 AQRES: 0.00000000 Hz  
 SFO: 500.136363 MHz  
 NUC1: 13C  
 NUC2: 1H

F2 - Processing parameters

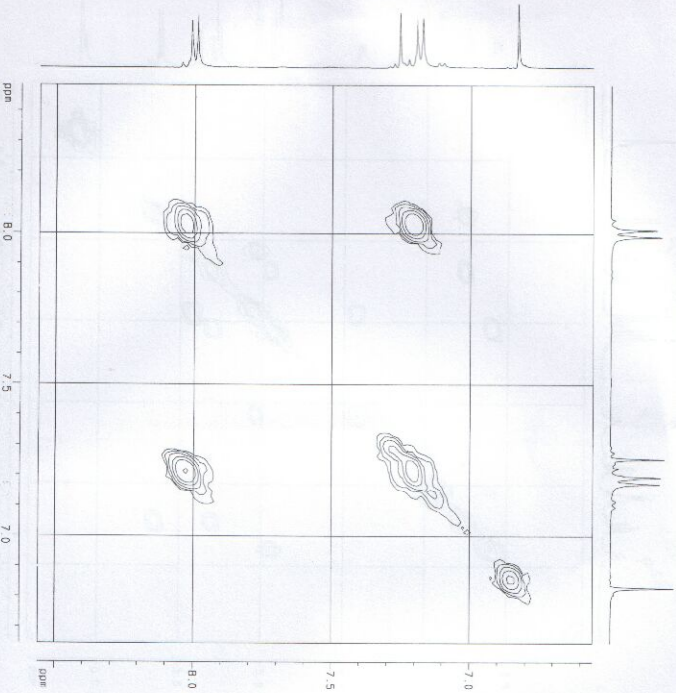
SI: 32768  
 SF: 500.136363 MHz  
 DS: 4  
 SWH: 6000.000000 MHz  
 FWHM: 11.700000 Hz  
 AQ: 0.00000000 sec  
 RG: 2048  
 DQ: 32768  
 SFO: 500.136363 MHz  
 NUC1: 13C  
 NUC2: 1H

F1 - Processing parameters

SI: 32768  
 SF: 500.136363 MHz  
 DS: 4  
 SWH: 6000.000000 MHz  
 FWHM: 11.700000 Hz  
 AQ: 0.00000000 sec  
 RG: 2048  
 DQ: 32768  
 SFO: 500.136363 MHz  
 NUC1: 13C  
 NUC2: 1H

2D NMR Data Acquisition

EXPNO: 2  
 F2PROC: 2  
 F1PROC: 1  
 SUBST: POLY(ETHYLENE TEREPHTHALATE)  
 SOLVENT: POLY(ETHYLENE TEREPHTHALATE)  
 NS: 2  
 DS: 2  
 SWH: 6000.000000 MHz  
 FWHM: 11.700000 Hz  
 AQ: 0.00000000 sec  
 RG: 2048  
 DQ: 32768  
 SFO: 500.136363 MHz  
 NUC1: 13C  
 NUC2: 1H







COSY cd13

NAME: CD13  
 EXPNO: 3  
 PROCNO: 1

Current Data Parameters

F2 - 13C NMR Shifts (ppm)

DATE\_ 20050711  
 TIME 11:36  
 INSTRUM spect  
 PULPROG zgpg30  
 AROBJ 3 W P-1313W  
 RNUC1 13C  
 TD 65536  
 F2 102.4  
 SFO 125.761  
 AQ 0.0113  
 LG 8  
 GB 0  
 SFR 320 Hz  
 BMRB 320 Hz  
 A1 1313W  
 AS 0.048500 sec  
 RG 32  
 HY 28  
 EX 100 Hz  
 DR 320 MHz  
 DE 353.3 K  
 FIDRES 0.000000 Hz  
 AQ 0.000000 sec  
 SFO 125.761  
 F2 102.4  
 C13 0.000000 sec  
 F22 0.000000 sec  
 C13 0.000000 sec  
 F22 0.000000 sec  
 SFO 125.761  
 F2 102.4

F1 - 13C NMR Shifts (ppm)

NAME: CD13  
 EXPNO: 3  
 PROCNO: 1  
 F1FRES 17.118 0.04

F2 - Processing parameters

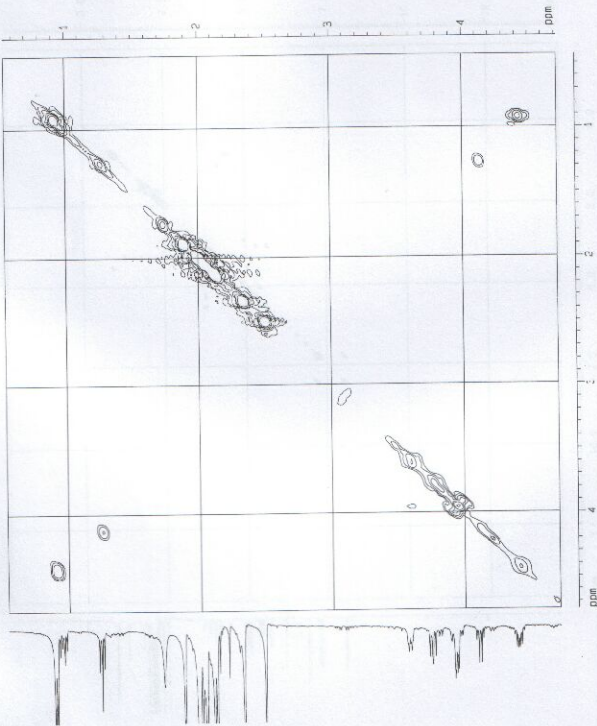
SI 0  
 SF 600.136261 MHz  
 SFO 125.761  
 AS 0.048500 sec  
 HY 28  
 EX 100

F1 - Processing parameters

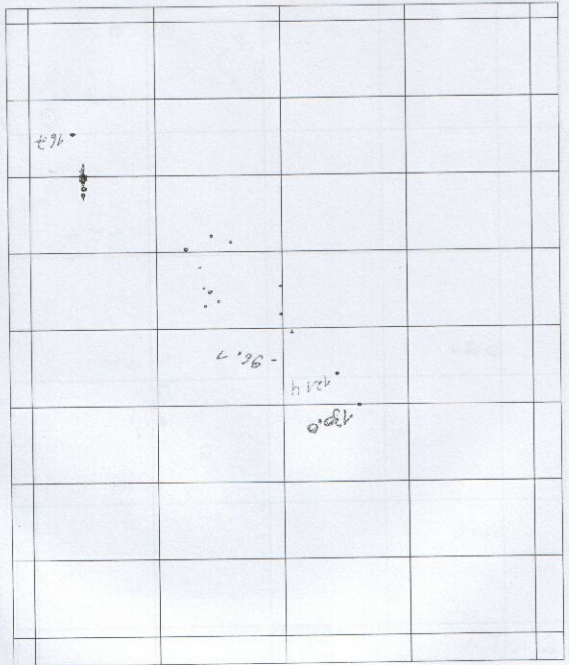
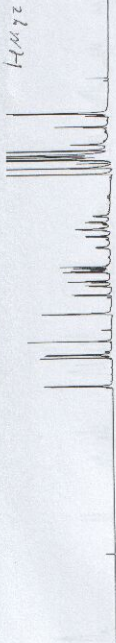
NAME: CD13  
 EXPNO: 3  
 PROCNO: 1  
 F1FRES 17.118 0.04

F2 - 13C NMR Shifts (ppm)

DATE\_ 20050711  
 TIME 11:36  
 INSTRUM spect  
 PULPROG zgpg30  
 AROBJ 3 W P-1313W  
 RNUC1 13C  
 TD 65536  
 F2 102.4  
 SFO 125.761  
 AQ 0.0113  
 LG 8  
 GB 0  
 SFR 320 Hz  
 BMRB 320 Hz  
 A1 1313W  
 AS 0.048500 sec  
 RG 32  
 HY 28  
 EX 100 Hz  
 DR 320 MHz  
 DE 353.3 K  
 FIDRES 0.000000 Hz  
 AQ 0.000000 sec  
 SFO 125.761  
 F2 102.4  
 C13 0.000000 sec  
 F22 0.000000 sec  
 C13 0.000000 sec  
 F22 0.000000 sec  
 SFO 125.761  
 F2 102.4



H<sub>2</sub>C I C<sub>13</sub> 10



BV-6598-C10-HMOC

NAME	FORMULA	EXP	ACQUISITION PARAMETERS
01	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
02	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
03	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
04	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
05	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
06	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
07	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
08	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
09	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
10	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
11	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
12	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
13	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
14	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
15	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
16	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
17	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
18	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
19	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
20	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
21	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
22	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
23	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
24	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
25	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
26	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
27	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
28	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
29	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
30	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
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35	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
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40	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
41	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
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44	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
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46	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
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64	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
65	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
66	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
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68	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
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70	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
71	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
72	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
73	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
74	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
75	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
76	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
77	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
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79	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
80	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
81	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
82	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
83	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
84	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
85	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
86	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
87	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
88	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
89	CH <sub>2</sub> CL <sub>2</sub>	1	100.624 MHz
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Current Data Parameters  
 NAME DMR-56  
 EXPNO 2  
 PROCNO 1

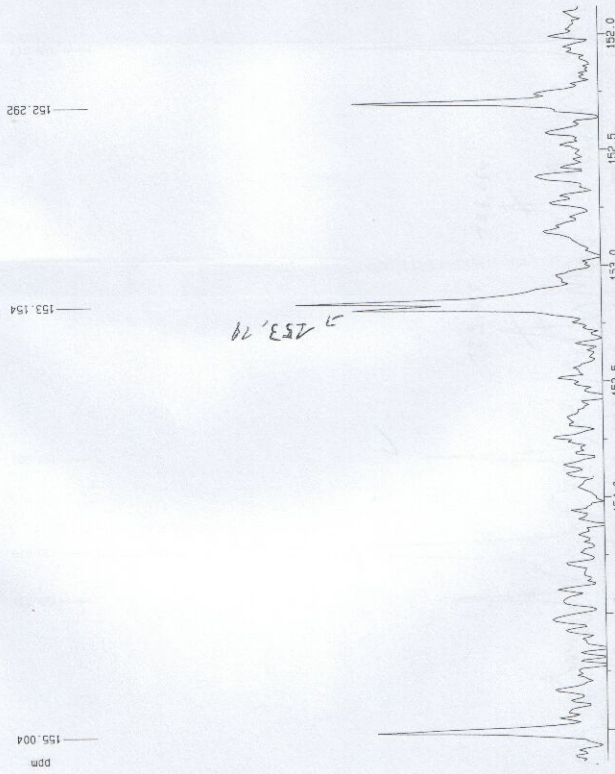
F2 - Acquisition Parameters  
 Date\_ 20030808  
 Time 13.00  
 INSTRUM spect  
 PROBNM 5 mm Multinu  
 PULPROG zgpg30  
 TO 32768  
 SOLVENT DMS-D  
 NS 1792  
 DS 2

SWH 25000.000 Hz  
 FIDRES 0.762538 Hz  
 AQ 0.655400 sec  
 RG 16384  
 DW 20.000 usec  
 DE 25.00 usec  
 TE 298.0 K  
 HL 1.00  
 H-1 1.00

D1 1.0000000 sec  
 CPDPRG waltz16  
 P31 100.00 usec  
 S4 35 dB  
 D11 0.0300000 sec  
 S2 32 dB  
 P1 11.00 usec  
 F1 100.6244403 MHz

NUCLEUS 13C  
 F2 - Processing parameters  
 SI 32768  
 SF 100.6130724 MHz  
 KW EM  
 SSB 0  
 LB 1.50 Hz  
 GB 0  
 PC 1.40

10 NMR plot parameters  
 CX 20.00 cm  
 F1P 135.135 ppm  
 F1 15608.76 Hz  
 F2P 151.878 ppm  
 F2 15281.06 Hz  
 PPM0 0.16285 ppm/cm  
 HZCM 16.39545 Hz/cm

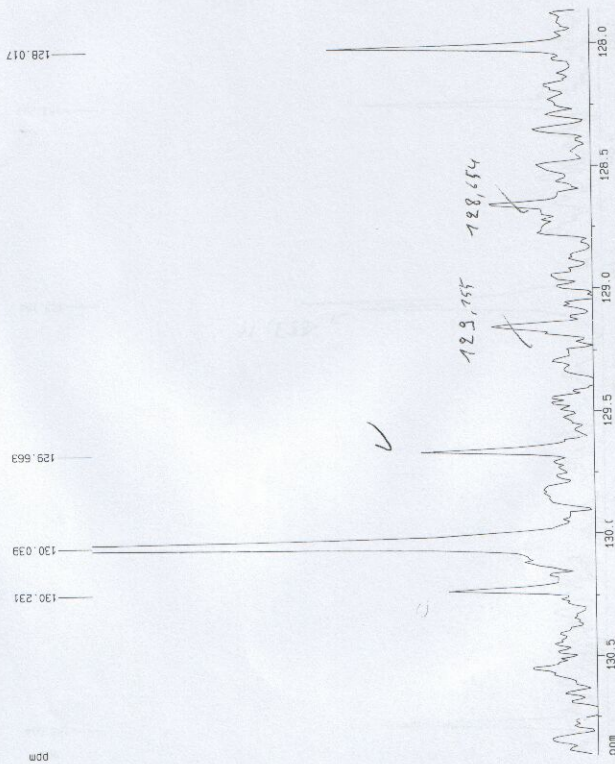


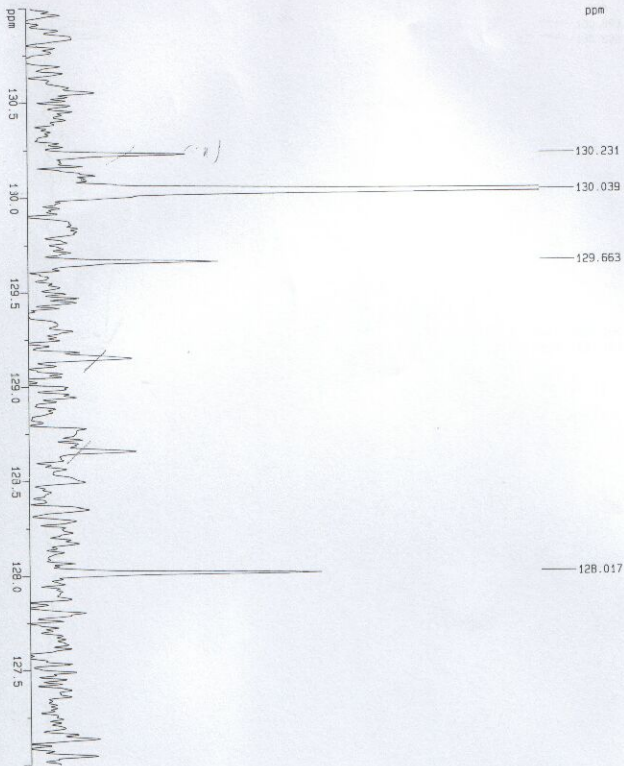
Current Date Parameters  
 NAME DMF-D5  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050808  
 TIME 13:00  
 INSTRUM spect  
 PROBHD 5 mm MULTIFU  
 PULPROG zgpg30  
 TO 32788  
 SOLVENT DMS-D6  
 NS 1792  
 US 2  
 SWH 25000.000 Hz  
 FIDRES 0.762359 Hz  
 AQ 0.6554100 sec  
 RG 16384  
 DW 20.000 USEC  
 DE 25.00 USEC  
 TE 293.0 K  
 HL1 1 CB  
 D1 1.00000000 sec  
 waitz16  
 P31 100.00 usec  
 S4 35 CB  
 D11 0.03000000 sec  
 S2 32 CB  
 P1 11.00 USEC  
 SFO1 100.6244403 MHz  
 NUCLEUS 13C

F2 - Processing parameters  
 S1 32768  
 SF 100.6138724 MHz  
 EQ  
 NQM  
 SSB  
 LB 1.50 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 FIP 130.953 ppm  
 F1 1377.865 Hz  
 F2 12562.56 Hz  
 PUNCH 15.210 ppm/cm  
 HZOM 15.31108 Hz/cm





Current Data Parameters  
 NAME DMF-5a  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20050808  
 Time 13.00  
 INSTRUM spect  
 PULPROG 5 mm Multis  
 PCPRG00 4puls2  
 TD 65536  
 SFO 299.62  
 SOLVENT DMSO  
 NS 1752  
 DS 2  
 SM 25000.000 Hz  
 FIDRES 0.182839 Hz  
 AQ 0.0354180 sec  
 RG 6584  
 DW 20.000 usec  
 DE 23.00 usec  
 TE 298.0 K  
 NL 1  
 NU 1.00

01 : 0.0000000 sec  
 DPGPRG wait1716  
 F31 100.00 usec  
 S4 50.00  
 S4 50.00  
 D11 0.0300000 sec  
 S2 32.00  
 P1 11.00 usec  
 SFO1 100.6244003 MHz  
 NUC1EUS 13C

F2 - Processing parameters

SI 60536  
 SF 100.619724 MHz  
 KW 64  
 SFS 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters

CK 20.00 cm  
 F1P 131.000 ppm  
 F1 13180.42 Hz  
 F2P 127.000 ppm  
 F2 12777.96 Hz  
 PRCKM 0.20000 ppm/cm  
 HZCM 20.12277 Hz/cm

Current Data Parameters  
 NAME: DMK 04  
 EX-NO: 7  
 SICOND: 1

F2 - Acquisition Parameters  
 Date: 20/05/2000  
 Time: 13:59

INSTRUM: SMC  
 ACQUIS: 5 MHz MULTIF  
 PULPROG: zgpg30  
 TD: 32768  
 SFO: 500.13  
 AQ: 0.72  
 DS: 5

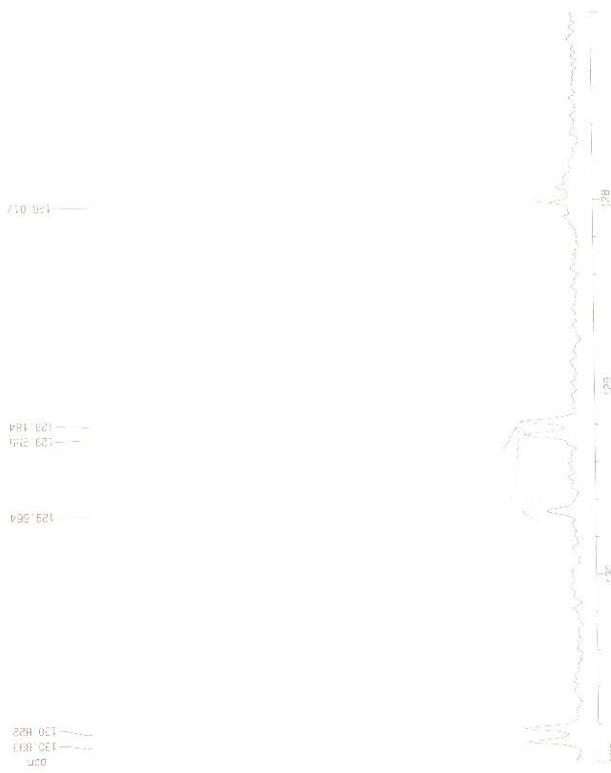
Q1: 25000.000 Hz  
 FIDRES: 0.356525 Hz  
 A1: 0.153420 SEC  
 T0: 10.000  
 INJ: 0.000 SEC  
 DE: 25.00 uL/SEC  
 T1: 200.0 X

C1: 0.2000000 SEC  
 SFO: 30.00  
 A1: 0.153420 SEC  
 T0: 10.000  
 INJ: 0.000 SEC  
 DE: 25.00 uL/SEC  
 T1: 200.0 X

C1: 0.2000000 SEC  
 SFO: 30.00 uL/SEC  
 T1: 200.0 X  
 SFO: 300.2246400 MHz  
 NUC1: 13C

F2 - Acquisition Parameters  
 SFO: 25.000 MHz  
 SFO: 100.6187524 MHz  
 INJ: 0.000 SEC  
 DE: 25.00 uL/SEC  
 T1: 200.0 X

1D MMR Plot Parameters  
 EX: 20.00.00  
 F1P: 171.200.000  
 F1: 13.80.40.00  
 F2: 127.000.000  
 F2: 12.777.68.00  
 H1-NUC: 13C  
 H2-NUC: 13C



Current Data Parameters  
 NAME DMR-5a  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

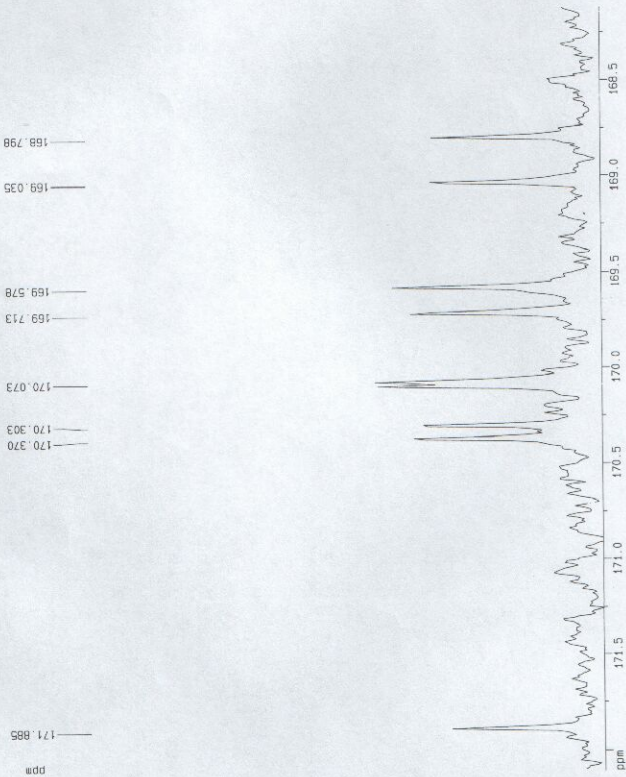
Date\_ 20050808  
 Time\_ 13.00  
 INSTRM spect  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CCl3  
 NS 1792  
 DS 2  
 SWH 28000.000 Hz  
 FIDRES 0.162538 Hz  
 AQ 0.6954100 sec  
 RG 16384  
 DM 20.000 usec  
 DE 25.00 usec  
 TE 298.0 K  
 HL 1.00  
 D1 1.00000000 sec  
 waitzr6  
 CPDPRG 100.00 usec  
 P31 35.68  
 S4 32.00 usec  
 D11 0.03000000 sec  
 S2 32.00 usec  
 P1 11.00 usec  
 SFO1 100.6244003 MHz  
 NUCLEUS 13C

F2 - Processing parameters

SI 32768  
 SF 100.6138724 MHz  
 WDW EM  
 SSB 0  
 LB 1.50 Hz  
 GB 0  
 PC 1.40

10 NMR plot parameters

CX 20.00 cm  
 FIP 172.164 ppm  
 F1 17316.04 Hz  
 F2P 168.118 ppm  
 F2 16915.13 Hz  
 PPMON 0.19923 ppm/cm  
 HZON 20.44524 Hz/cm





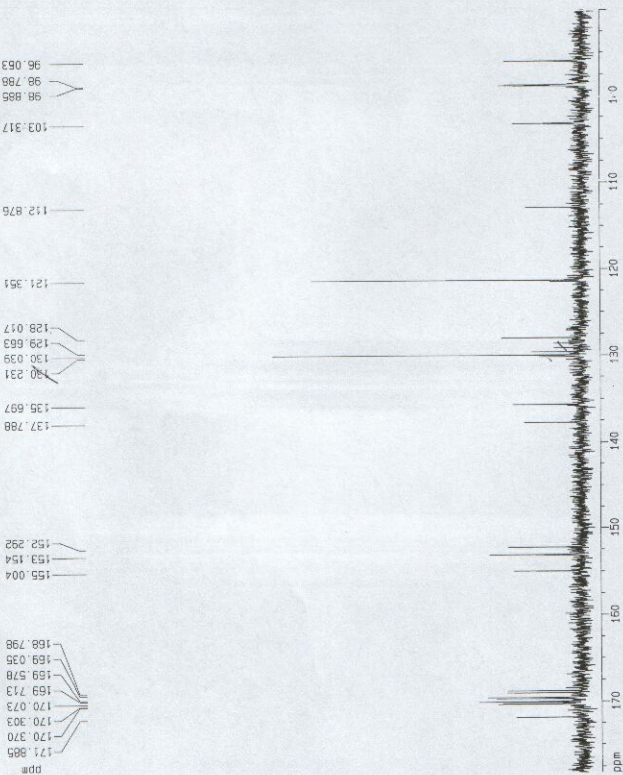
Current Data Parameters  
 NAME DMF-S9  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050808  
 TIME 13.00  
 INSTRUM spect  
 PROBHD 5 mm MUX110U  
 PULPROG zgpg30  
 TO 32768  
 SOLVENT CDCl3  
 NS 1792  
 DS 2

SWH 25000.000 Hz  
 FIDRES 0.789588 Hz  
 AQ 0.0594100 sec  
 RG 16384  
 DM 20.000 usec  
 DE 25.00 usec  
 TE 298.0 K  
 HL 1.28  
 D1 1.0000000 sec  
 waltz16  
 P31 100.00 usec  
 S4 35.85  
 O11 0.0300000 sec  
 S2 32.69  
 P1 11.00 usec  
 SFO1 100.6244403 MHz  
 NUC1EUS 13C

F2 - Processing parameters  
 SI 32768  
 SF 100.6138724 MHz  
 NQW EM  
 EN 0  
 SSB 0  
 LB 1.50 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 178.219 ppm  
 F1 17931.27 Hz  
 F2P 89.984 ppm  
 F2 9053.60 Hz  
 PPMCK 4.41175 ppm/cm  
 HZCM 443.88358 Hz/cm



Current Data Parameters

NAME DMF-5a  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20050808  
 Time 13.00  
 INSTRUM spect  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1752  
 DS 2

1D NMR plot parameters

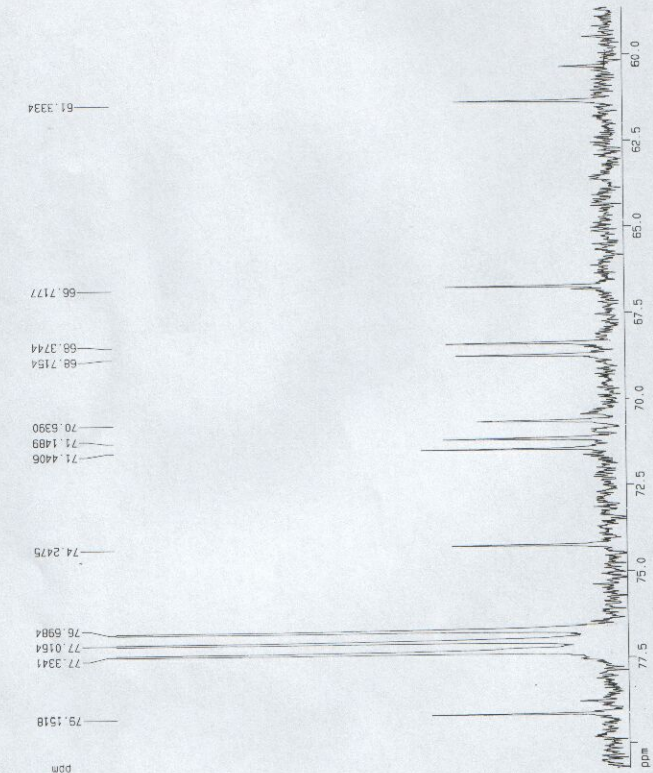
CX 20.00 cm  
 F1P 80.723 ppm  
 F1 8182.48 Hz  
 F2P 50.632 ppm  
 F2 9889.16 Hz  
 PPGNCH 1.10468 ppm/cm  
 HZCN 111.16857 Hz/cm

F2 - Processing parameters

SF 32768  
 SF 100.6138724 MHz  
 EQ  
 SSB 0  
 LB 1.50 Hz  
 GB 0  
 PC 1.40

F2 - Processing parameters

SI 32768  
 SF 100.6138724 MHz  
 EQ  
 SSB 0  
 LB 1.50 Hz  
 GB 0  
 PC 1.40



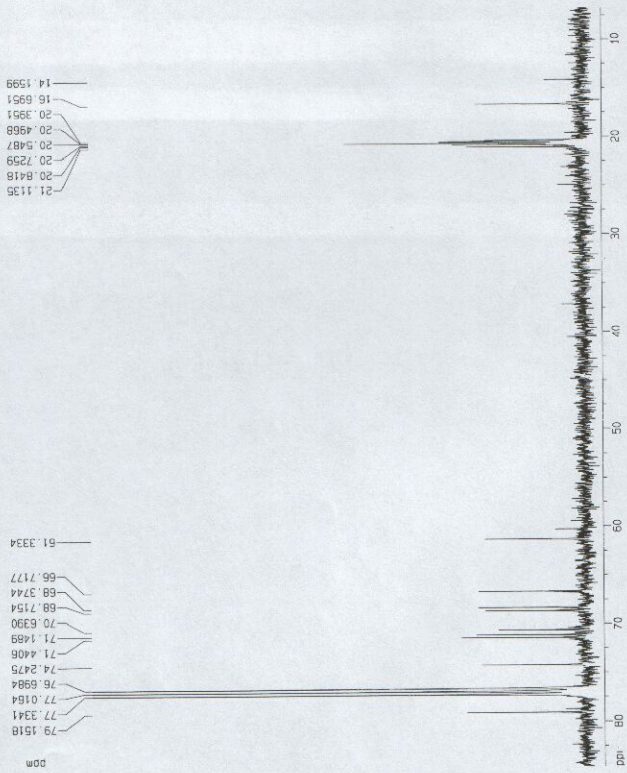
Current Data Parameters  
 NAME DWA-5a  
 EXPNO 2  
 PROCNO 1

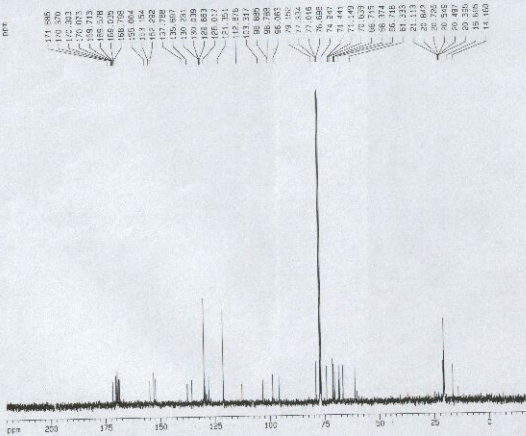
F2 - Acquisition Parameters  
 Date\_ 20050908  
 Time 13.00  
 INSTRUM spect  
 PROBRD 5 mm MUltiRU  
 PULPROG zgpg30  
 TO 32768  
 SOLVENT CDCl3  
 NS 1792  
 DS 2

SWH 20000.000 Hz  
 FIDRES 0.752028 Hz  
 AQ 0.6554100 sec  
 RG 1.63584  
 DM 20.000 usec  
 DE 23.00 usec  
 TE 298.0 K  
 H1 1  
 D1 1.00000000 sec  
 CPDPRG waltz16  
 P31 100.00 usec  
 S4 35 dB  
 O11 0.03000000 sec  
 S2 32 dB  
 P1 11.00 usec  
 SF01 100.6244403 MHz  
 NUC1EUS 13C

F2 - Processing parameters  
 S1 32768  
 SF 100.6138724 MHz  
 WDW EM  
 SSB 0  
 LB 1.50 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 84.613 ppm  
 F1 8513.20 Hz  
 F2P 6.702 ppm  
 F2 680.37 Hz  
 PRNCH 3.86256 ppm/ct  
 HZCM 391.64120 Hz/cm





Current Data Parameters  
NAME 2NF-58  
EXPNO 2  
PROCNO 1

## F2 - Acquisition Parameters

Date\_ 20090105  
Time 15:50  
INSTRUM spect  
PROBHD 5 mm HLTBHU  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 2  
DS 2  
SWH 25000.000 Hz  
FIDRES 0.162879 Hz  
AQ 0.6264100 sec  
RG 6254  
DA 20.000 sec  
DE 25.00 usec  
TE 296.2 K  
NUC1 13C  
D1 1.00000000 sec  
DEPRG waltz16  
PUL 100.00 usec  
SA 25.00  
D11 0.00000000 sec  
SFO 50.00 MHz  
PC 11.00 usec  
SFO1 100.6264100 MHz  
NUCLEUS 13C

## F2 - Processing parameters

SI 32768  
SF 100.6264100 MHz  
WDW EM  
SSB 0  
LB 1.50 Hz  
GB 0  
FC 1.40

## F2 NMR list parameters

CF 20.00 usec  
F1P 220.075 MHz  
F1 201.40 MHz  
F2P -10.300 MHz  
F2 -1500.00 MHz  
WINDM 11.05163 positions  
GCP 1190.47601 MHz/Hz

ppm  
 137.796  
 135.695  
 130.731  
 130.039  
 129.653  
 128.017  
 124.251

103.677

103.315

95.894  
 95.709

95.054



Current Data Parameters  
 NAME: DM4 5h  
 EXPNO: 2  
 PROCNU: 1

F2 - Acquisition Parameters

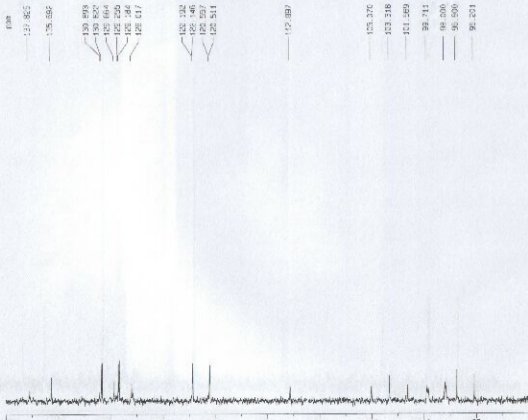
Date: 09/08/05  
 Time: 15.00  
 CHANNEL: spect  
 PULPROG: zgpg30  
 F2.FH1U: 200MHz  
 TC: 320K  
 SOLVENT: CDCl3  
 NS: 1700  
 DS: 2  
 SWH: 25000.000 Hz  
 FIDRES: 0.162500 Hz  
 AQ: 0.658400 sec  
 RG: 1024  
 IN: 20.000 MHz  
 DE: 35.000 dB  
 TL: 299.0 K  
 H1: 1.00  
 Dc: 1.0000000 MHz  
 DPREP0: waltz16  
 FSI: 100.00 MHz  
 S4: 35.00  
 S11: 0.0300000 sec  
 S2: 30.00  
 F1: 11.00 MHz  
 SFO1: 100.6264603 MHz  
 NUC1: 13C

F2 - Processing parameters

SI: 32768  
 SF: 100.6264603 MHz  
 WHW: 7M  
 SSF: 3  
 LG: 1.40 Hz  
 SR: 0  
 PC: 1.40

13C NMR plot parameters

CH: 20.00 Hz  
 F1: 140.000 MHz  
 F2: 140.000 MHz  
 F3: 30.000 MHz  
 F4: 0.000 MHz  
 SFO1: 250.000 MHz  
 SFO2: 0.000 MHz



Current Data Parameters

NAME DM-55  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20080808  
 Time 13:38  
 INSTRUM spect  
 PROBHD 5 mm P111nu  
 PULPROG zgpg30  
 F2 307.58  
 SFO 500.13  
 AS 3073  
 CS 2  
 SWH 9500.000 Hz  
 FIDRES 0.762535 Hz  
 AQ 0.0554100 sec  
 RG 15364  
 SW 26.000 usec  
 TE 25.00 usec  
 TC 299.0 K  
 DS 0.0300000 sec  
 SS 28.00  
 NL1 1.00  
 DS 2.0000000 sec  
 CHPROG waltz16  
 PS1 100.00 usec  
 P1 11.00 usec  
 SFO1 100.6244403 MHz  
 NUC1 F19  
 N2 F19

F2 - Processing parameters

SF 307.58  
 SF 100.6244403 MHz  
 HN 4  
 RB 0  
 LB 1.50 Hz  
 GB 0  
 PC 1.40

1D NMR processing parameters

OR 30.00 dB  
 F1 140.000 dB  
 F2 140.000 dB  
 F3 50.000 dB  
 F4 50.000 dB  
 F5 50.000 dB  
 F6 50.000 dB  
 F7 50.000 dB  
 F8 50.000 dB  
 F9 50.000 dB  
 F10 50.000 dB

Current Data Parameters  
 NAME DMF-D<sub>6</sub>  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050503  
 Time 13 30  
 INSTRUM spect  
 PULPROG zgpg30  
 5 mm MULTIPRO  
 dec:135

TO 30768  
 SOLVENT DMF-D<sub>6</sub>  
 NS 1152  
 DS 4  
 SWH 23805.523 Hz  
 FIDRES 0.725609 Hz  
 AQ 0.6881780 sec  
 RG 30768  
 DM 21.000 usec  
 DE 25.25 usec  
 TE 298.0 K  
 D1 1.00  
 D11 1.00  
 D12 1.00  
 D13 1.00

NUCLEUS 13C  
 CPDPRG2 waltz16  
 P31 100.00 usec  
 P32 100.00 usec  
 P33 100.00 usec  
 SF02 400.1367100 MHz  
 P3 7.31 usec  
 P31 3.00  
 P32 3.00  
 P33 3.00  
 DDCPRG mzgpg  
 C 0.00345000  
 S 14.52 usec  
 S2 10.50 usec  
 S3 21.00 usec  
 S4 21.00 usec  
 S5 21.00 usec  
 S6 21.00 usec  
 S7 21.00 usec  
 S8 21.00 usec  
 S9 21.00 usec  
 S10 21.00 usec  
 S11 21.00 usec  
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 S63 21.00 usec  
 S64 21.00 usec  
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 S67 21.00 usec  
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 S95 21.00 usec  
 S96 21.00 usec  
 S97 21.00 usec  
 S98 21.00 usec  
 S99 21.00 usec  
 S100 21.00 usec

F2 - Processing parameters  
 SI 30768  
 SF 100.6136724 MHz  
 EM EM  
 0  
 LB 1.50 Hz  
 GB 0  
 CB 0  
 PC 2.00

1D NMR plot parameters  
 CA 100.00 cm  
 CB 100.00 cm  
 CC 100.00 cm  
 CD 100.00 cm  
 CE 100.00 cm  
 CF 100.00 cm  
 CG 100.00 cm  
 CH 100.00 cm  
 CI 100.00 cm  
 CJ 100.00 cm  
 CK 100.00 cm  
 CL 100.00 cm  
 CM 100.00 cm  
 CN 100.00 cm  
 CO 100.00 cm  
 CP 100.00 cm  
 CQ 100.00 cm  
 CR 100.00 cm  
 CS 100.00 cm  
 CT 100.00 cm  
 CU 100.00 cm  
 CV 100.00 cm  
 CW 100.00 cm  
 CX 100.00 cm  
 CY 100.00 cm  
 CZ 100.00 cm  
 CA 100.00 cm  
 CB 100.00 cm  
 CC 100.00 cm  
 CD 100.00 cm  
 CE 100.00 cm  
 CF 100.00 cm  
 CG 100.00 cm  
 CH 100.00 cm  
 CI 100.00 cm  
 CJ 100.00 cm  
 CK 100.00 cm  
 CL 100.00 cm  
 CM 100.00 cm  
 CN 100.00 cm  
 CO 100.00 cm  
 CP 100.00 cm  
 CQ 100.00 cm  
 CR 100.00 cm  
 CS 100.00 cm  
 CT 100.00 cm  
 CU 100.00 cm  
 CV 100.00 cm  
 CW 100.00 cm  
 CX 100.00 cm  
 CY 100.00 cm  
 CZ 100.00 cm

