

Tentamen "Structuuropheldering"

Docent: Prof.dr. J. Lugtenburg

23 december 2003, collegezaal 1
9.00 uur - 12.30 uur

In alle onderstaande vraagstukken wordt gevraagd van een onbekende verbinding de structuur te bepalen. Geef hierbij een zo volledig mogelijke motivering. Ken in de spectra zoveel mogelijk pieken toe, in MS spectra en in IR spectra in elk geval de meest relevante pieken.

LEES DE VRAAGSTUKKEN VOORAL GOED !

1. Het IR spectrum van een verbinding met molecuulgewicht 79
2. Van de verbinding $C_8H_8O_3$ zijn de volgende spectra gegeven:
 - 2a. 600 MHz 1H NMR spectrum. Het signaal bij 7.14 ppm is afkomstig van het oplosmiddel hexadeuterobenzeen
 - 2b. het gebied tussen 7.3 en 6.7 ppm
 - 2c. het COSY spectrum in dit gebied
 - 2d. het ^{13}C APT spectrum
 - 2e. het NOESY spectrum
3. Van de verbinding $C_9H_8O_4$ zijn de volgende spectra gegeven:
 - 3a. het 600 MHz 1H NMR spectrum
 - 3b. het spectrum tussen 7.6 en 6.00 ppm
 - 3c. de ppm waarden van de signalen in het 1H NMR spectrum
 - 3d. het COSY spectrum
 - 3e. het ^{13}C APT spectrum
 - 3f. het 1H ^{13}C gecorreleerde spectrum
4. Fig. 4a en 4b: een combinatie probleem
5. Figuur 5a en 5b: een combinatie probleem

Fig. 1

(d) A compound with a molecular weight of 79.

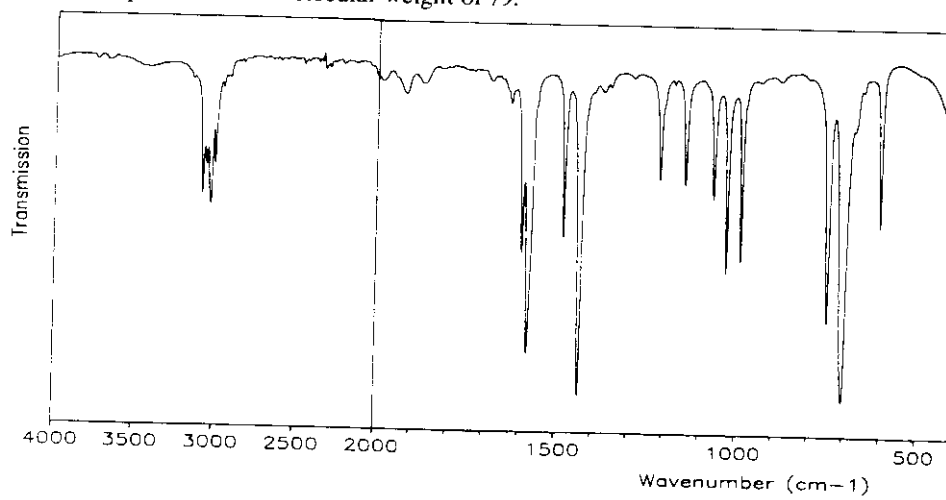


Fig. 2 A

1h NMR in C6D6 dmx-600

Current Data Parameters
 NAME vac
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20031217
 Time 3.48
 INSTRUM dmx600
 PROHD 5 mm TXI-2 ZB-
 PULPROG zg
 TD 65536
 SOLVENT Aceton
 NS 14
 DS 2
 SWH 7597.507 Hz
 FIDRES 0.114555 Hz
 AQ 4.3647475 sec
 RG 64
 DW 66.600 usec
 DE 4.50 usec
 TE 293.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUCL LH
 PL 4.00 usec
 PL1 3.00 dB
 SFO1 600.1332442 MHz

F2 - Processing parameters
 SI 32768
 SF 600.1299976 MHz
 WDW mc
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 24.00 cm
 CY 15.00 cm
 FLP 10.000 deg
 F1 6001.50 Hz
 F2P 0.000 ppr
 F2 0.00 Hz
 PPMCM 0.41667 PPM/
 RZCM 250.05417 Hz/er

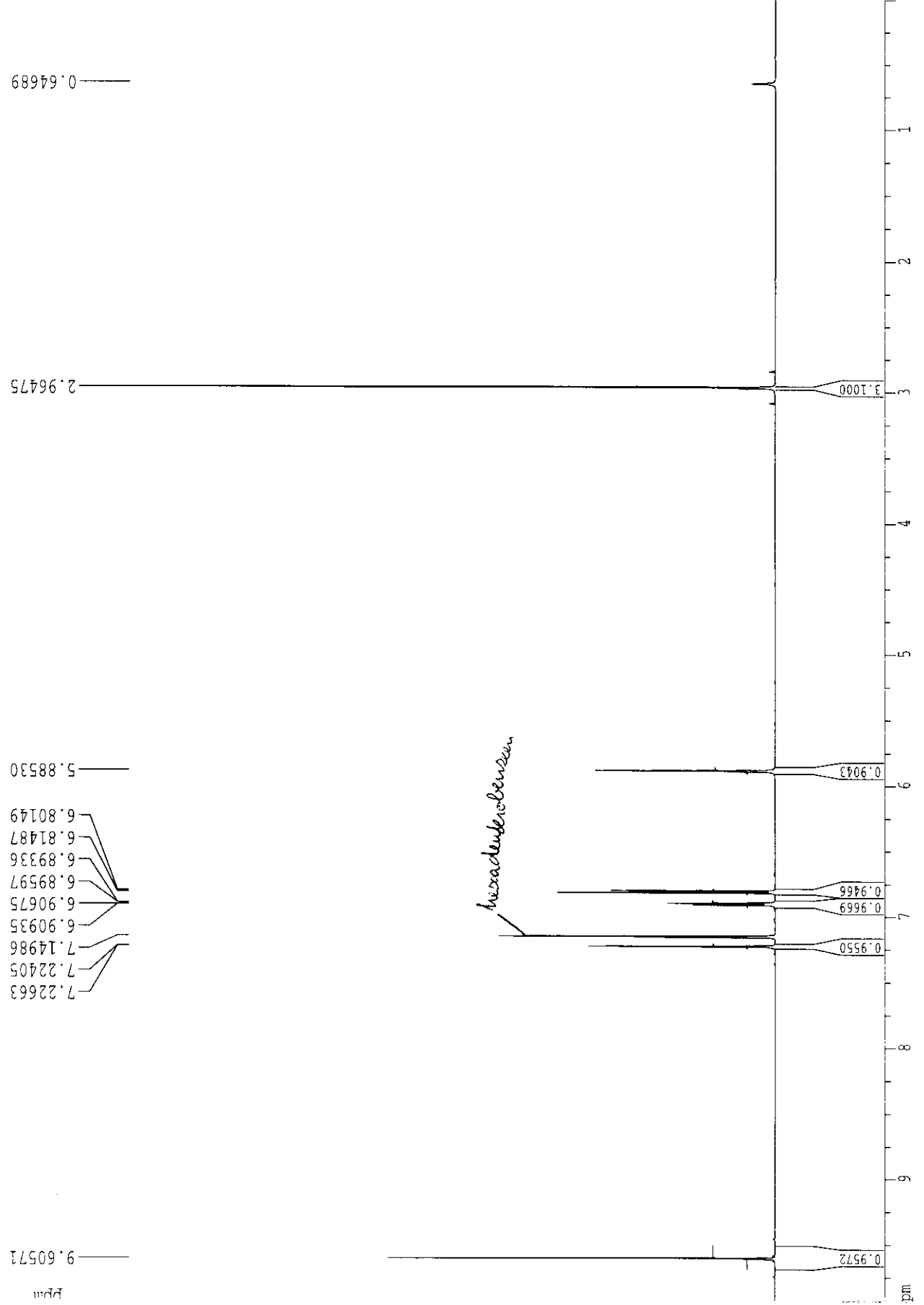


FIG. 2 B

1h NMR in C6D6 dmx-600

```

Current Data Parameters
NAME      van
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20031217
Time      8.48
INSTRUM   dmx600
PROBHD    5 mm TXI-2 ZG1
PULPROG   zg
TD         65536
SOLVENT   Aceton
NS         14
DS         2
SWH        7507.507 Hz
FIDRES     0.114555 Hz
AQ         4.3647475 sec
RG         64
DW         66.600 usec
DE         4.50 usec
TE         293.0 K
D1         2.00000000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         4.00 usec
PL1        3.00 dB
SFO1       600.1332442 MHz

F2 - Processing parameters
SI         32768
SF         600.1299976 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00

ID NMR plict parameters
CX         24.00 cm
CY         19.00 cm
FLP        7.270 ppm
F1         4162.79 Hz
F2         5.699 ppm
F3         4021.26 Hz
PPMCH      0.02175 ppm/1
HZCM       14.27195 Hz/ct
    
```

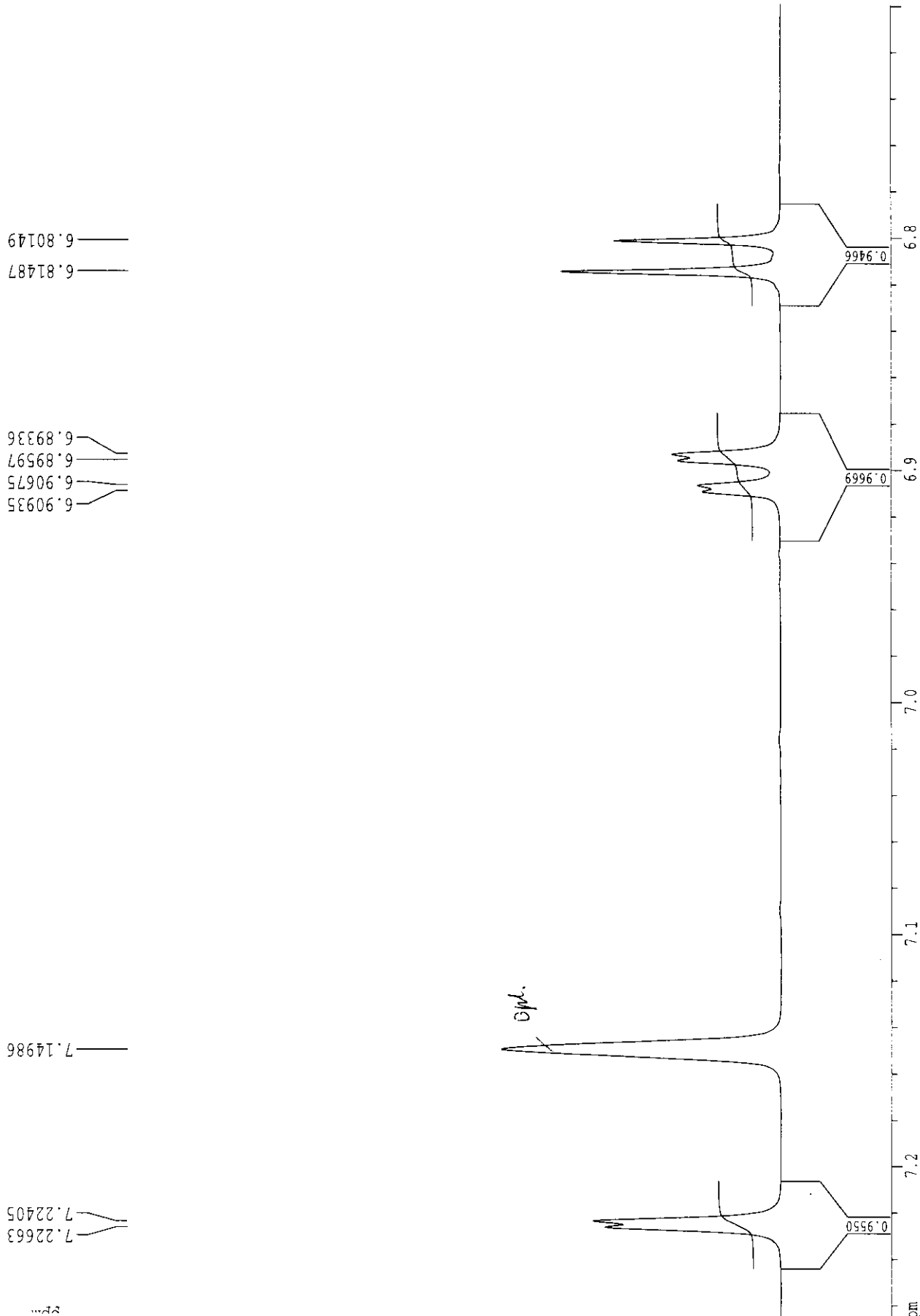
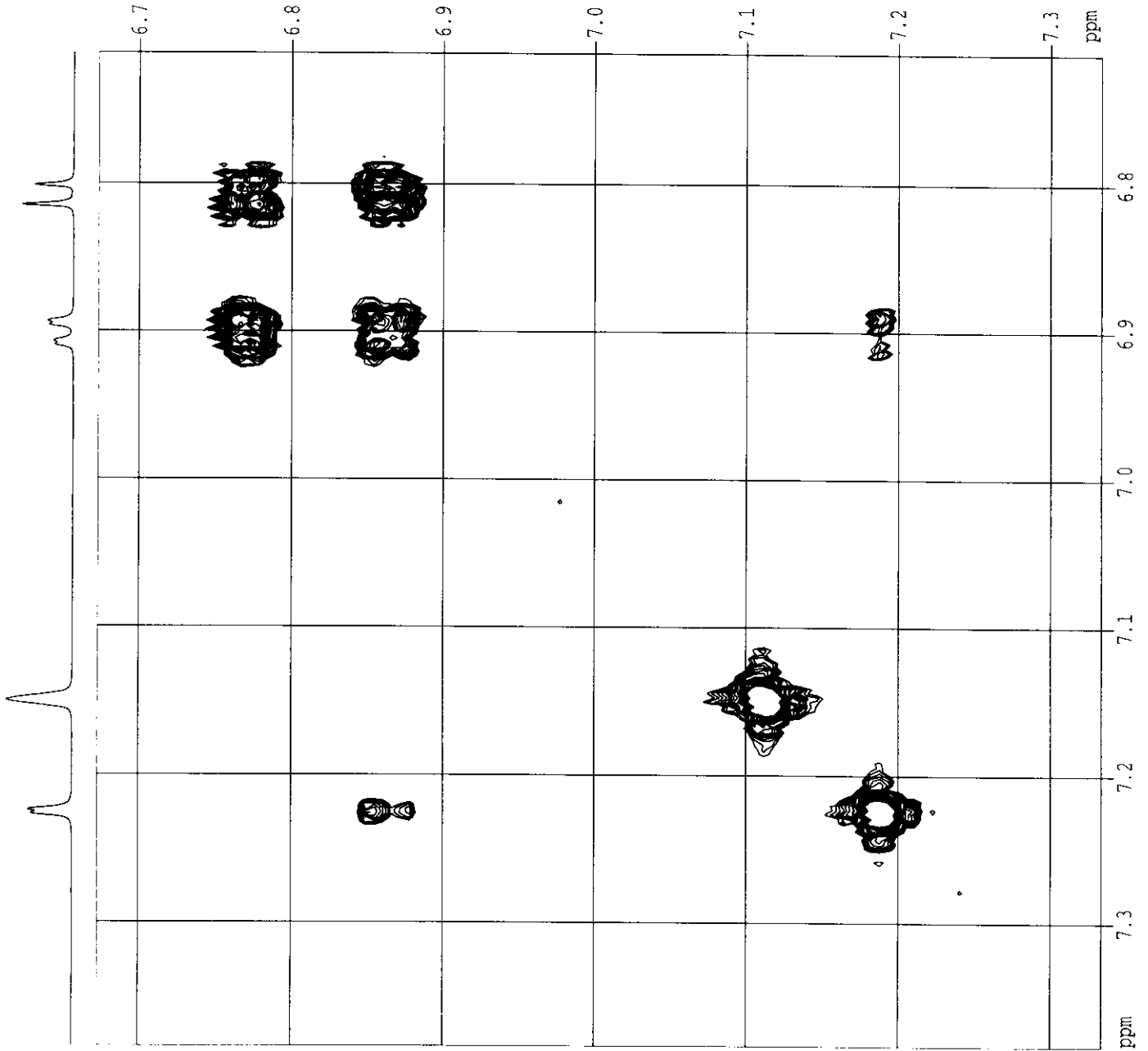


Fig. 2c

1h NMR 2D-COSYgp in C6D6 dmx600



```

=====
NAME                               1h NMR 2D-COSYgp in C6D6 dmx600
EXPNO                               1
PROCNO                               1
PR.CH                                1
=====
F2 - Acquisition Parameters
Date_                               20111113
Time                                  15:57
INSTRUM                               spect
PRORUN                               dmx600
F2 F0 FID                               600.1342 MHz
F2 F1 FID                               14.031071 Hz
PULPROG                               zgpg30
TD                                      1024
SOLVENT                               CDCl3
NS                                      1
DS                                      2
SWH                                      1795.977 Hz
FIDRES                                  1.751864 Hz
AQ                                       0.2851216 sec
RG                                       256
DE                                       278.460 usec
TE                                       300.2 K
D0                                       0.06500170 sec
d1                                       1.06500000 sec
d13                                      0.06000000 sec
d16                                      0.05000000 sec
TD0                                       0.06555897 sec
MKSYST                                  0.00000000 sec
MCREF                                  1.00000000 sec
===== CHANNEL f1 =====
NUC1                                   13
P1                                       12.00 usec
PL1                                       0.00 dB
PC1                                       1.00 dB
SFO1                                   600.1342619 MHz
===== CHANNEL CHANNEL =====
GRAB1                                  SINE 100
GRAB2                                  SINE 100
SFO2                                  0.00 MHz
SFO1                                  0.00 MHz
SFO2                                  0.00 MHz
SFO1                                  10.00 MHz
SFO2                                  10.00 MHz
P16                                    1.000.00 usec
=====
F1 - Acquisition Parameters
RG0                                    1
TD                                      128
SFO1                                   600.1342 MHz
FIDRES                                  14.031071 Hz
SFO2                                   2.951 ppm
PULPROG                               zgpg30
=====
F2 - Processing Parameters
SI                                       132
SF                                       600.1342619 MHz
WDW                                       SINE
SSB                                       0
LB                                       0.00 Hz
GB                                       0
PC                                       1.00
=====
F1 - Processing Parameters
SI                                       522
SF                                       600.1342619 MHz
WDW                                       SINE
SSB                                       0
LB                                       0.00 Hz
GB                                       0
PC                                       1.00
=====
2D NMR plot parameters
CX2                                     16.00 cm
CY1                                     16.00 cm
F2 F2                                     3.284 ppm
F2 F1                                     4831.35 Hz
F2 F0                                     4571.12 ppm
F1 F2                                     7.135 Hz
F1 F0                                     4401.28 ppm
F1 F1                                     6.453 Hz
F1 F0                                     4264.91 Hz
F2 F2 CM                                0.04203 ppm/cm
F2 F1 CM                                25.21209 Hz/cm
F1 F2 CM                                0.04128 ppm/cm
F1 F1 CM                                24.77362 Hz/cm

```

Fig. 20

13C APT in C6D6 dmx600

```

Current Data Parameters
NAME          Var.
EXPAC         5
PRGNO        11

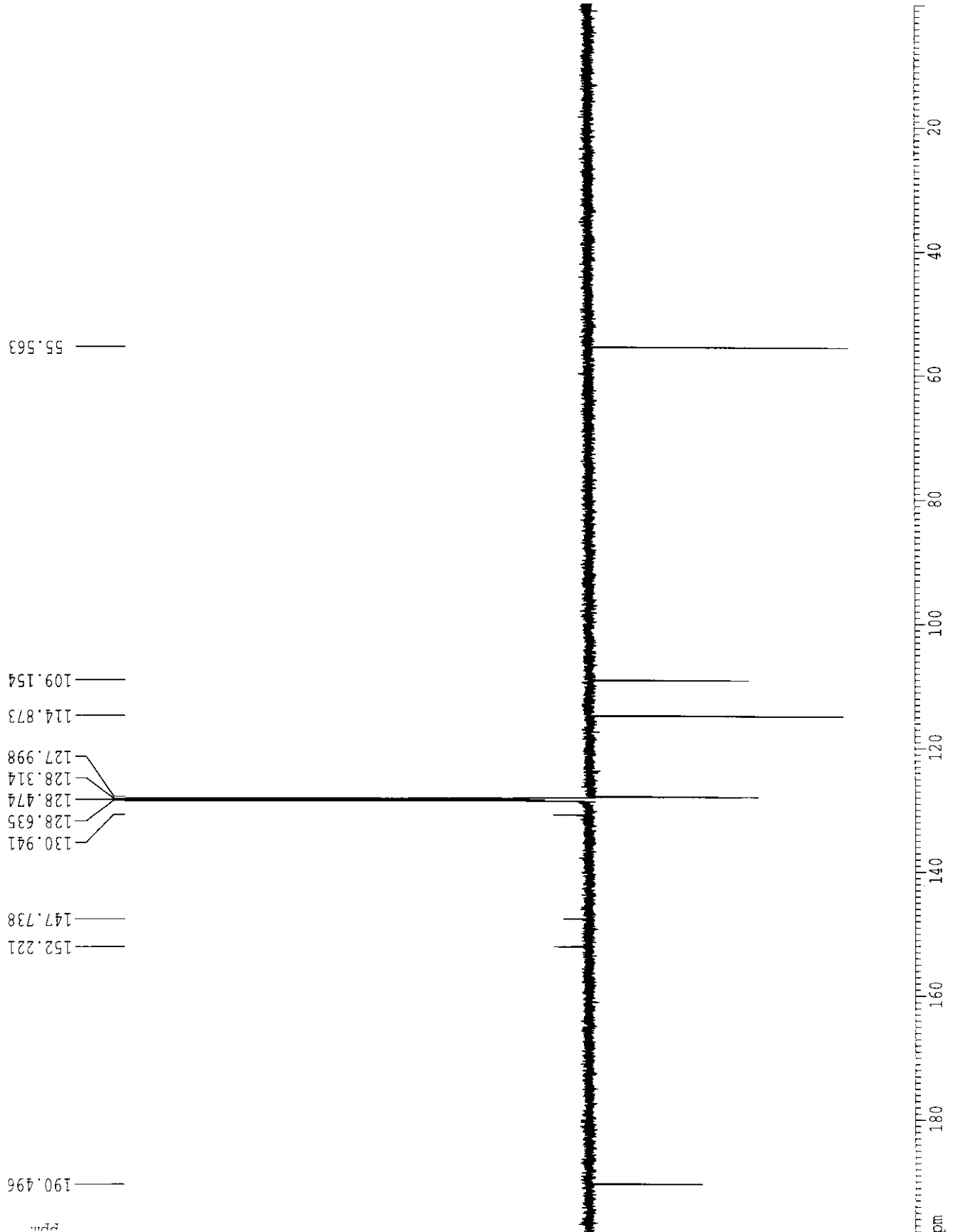
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INSTRUM      dmx600
PROBHD       5 mm TXI-2 Z81
PULPROG      jmod
TD           131072
SOLVENT      CDCl3
NS           519
DS           8
SWH          34722.223 Hz
FIDRES       0.264910 Hz
AQ           1.8874868 sec
RG           8192
DW           14.400 usec
DE           4.50 usec
TE           294.4 K
CNST2       155.0000000
CNST11      1.0000000
D1           1.00000000 sec
d13          0.00000300 sec
d2c         0.00645161 sec
DELTA       0.00001528 sec

===== CHANNEL f1 =====
NUC1         13C
P1           12.00 usec
P2           24.00 usec
PL1          3.00 dB
SFO1        150.9185938 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2         1H
PCPD2        90.00 usec
PL2          3.00 dB
PL12        25.69 dB
SFO2        600.1330606 MHz

F2 - Processing parameters
SI           65536
SF          150.9026925 MHz
RG          65536
SSB          0
LS          1.50 Hz
GB          0
PC          1.00

ID NMR plot parameters
CX          23.00 cm
CY          30.60 cm
F1P        200.000 ppm
F1         30180.54 Hz
F2P        0.000 ppm
F2         0.00 Hz
PPMCM      8.69565 ppm/cm
HZCM       1312.19739 Hz/cm
    
```



```

Current Data Parameters
NAME      van
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20031217
Time     9:00
INSTRUM  dmx600
PROBHD   5 mm TXI-2 Z41
PULPROG  noesymp1ph
TD       2688
SOLVENT  H2O:D2O
NS       4
DS       2
SFR      4807.692 Hz
FIDRES   2.347506 Hz
AQ       0.2130420 sec
RG       256
DW       104.000 usec
DE       4.50 usec
TE       298.0 K
d0       0.0000000 sec
d1       0.8000001 sec
d8       1.0000000 sec
d16      0.0005000 sec
d20      0.4885000 sec
IN0       0.0020000 sec
MCPROG   0.0000000 sec
MCWPRG   0.8000001 sec

===== CHANNEL f1 =====
NUC1      13C
P1        6.50 usec
P2        13.00 usec
PL1       3.00 dB
PL2       3.00 dB
SFO1      600.1336008 MHz

===== GRADIENT CHANNEL =====
GPMAX1    SINE 100
GPMAX2    SINE 100
GPA1      0.00 %
GPA2      0.00 %
GPA3      0.00 %
GPA4      0.00 %
GPA5      0.00 %
GPA6      0.00 %
GPA7      0.00 %
GPA8      0.00 %
GPA9      0.00 %
GPA10     0.00 %
GPA11     0.00 %
GPA12     0.00 %
GPA13     0.00 %
GPA14     0.00 %
GPA15     0.00 %
GPA16     0.00 %
GPA17     0.00 %
GPA18     0.00 %
GPA19     0.00 %
GPA20     0.00 %
GPA21     0.00 %
GPA22     0.00 %
GPA23     0.00 %
GPA24     0.00 %
GPA25     0.00 %
GPA26     0.00 %
GPA27     0.00 %
GPA28     0.00 %
GPA29     0.00 %
GPA30     0.00 %
GPA31     0.00 %
GPA32     0.00 %
GPA33     0.00 %
GPA34     0.00 %
GPA35     0.00 %
GPA36     0.00 %
GPA37     0.00 %
GPA38     0.00 %
GPA39     0.00 %
GPA40     0.00 %
GPA41     0.00 %
GPA42     0.00 %
GPA43     0.00 %
GPA44     0.00 %
GPA45     0.00 %
GPA46     0.00 %
GPA47     0.00 %
GPA48     0.00 %
GPA49     0.00 %
GPA50     0.00 %
GPA51     0.00 %
GPA52     0.00 %
GPA53     0.00 %
GPA54     0.00 %
GPA55     0.00 %
GPA56     0.00 %
GPA57     0.00 %
GPA58     0.00 %
GPA59     0.00 %
GPA60     0.00 %
GPA61     0.00 %
GPA62     0.00 %
GPA63     0.00 %
GPA64     0.00 %
GPA65     0.00 %
GPA66     0.00 %
GPA67     0.00 %
GPA68     0.00 %
GPA69     0.00 %
GPA70     0.00 %
GPA71     0.00 %
GPA72     0.00 %
GPA73     0.00 %
GPA74     0.00 %
GPA75     0.00 %
GPA76     0.00 %
GPA77     0.00 %
GPA78     0.00 %
GPA79     0.00 %
GPA80     0.00 %
GPA81     0.00 %
GPA82     0.00 %
GPA83     0.00 %
GPA84     0.00 %
GPA85     0.00 %
GPA86     0.00 %
GPA87     0.00 %
GPA88     0.00 %
GPA89     0.00 %
GPA90     0.00 %
GPA91     0.00 %
GPA92     0.00 %
GPA93     0.00 %
GPA94     0.00 %
GPA95     0.00 %
GPA96     0.00 %
GPA97     0.00 %
GPA98     0.00 %
GPA99     0.00 %
GPA100    0.00 %

F1 - Acquisition parameters
NUC0      13C
TD        227
SFO0      600.1337 MHz
FIDRES    21.178262 Hz
SFO1      600.1336008 MHz
SFO2      600.1336008 MHz
SFO3      600.1336008 MHz
SFO4      600.1336008 MHz
SFO5      600.1336008 MHz
SFO6      600.1336008 MHz
SFO7      600.1336008 MHz
SFO8      600.1336008 MHz
SFO9      600.1336008 MHz
SFO10     600.1336008 MHz
SFO11     600.1336008 MHz
SFO12     600.1336008 MHz
SFO13     600.1336008 MHz
SFO14     600.1336008 MHz
SFO15     600.1336008 MHz
SFO16     600.1336008 MHz
SFO17     600.1336008 MHz
SFO18     600.1336008 MHz
SFO19     600.1336008 MHz
SFO20     600.1336008 MHz
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SFO35     600.1336008 MHz
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SFO81     600.1336008 MHz
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SFO91     600.1336008 MHz
SFO92     600.1336008 MHz
SFO93     600.1336008 MHz
SFO94     600.1336008 MHz
SFO95     600.1336008 MHz
SFO96     600.1336008 MHz
SFO97     600.1336008 MHz
SFO98     600.1336008 MHz
SFO99     600.1336008 MHz
SFO100    600.1336008 MHz

F2 - Processing parameters
SI        2048
SF        600.1336976 MHz
WDW       COSYME
SSB       0
LB        0.00 Hz
GB        0
CB        0
PC        1.00

F1 - Processing parameters
SI        1024
SF        600.1336885 MHz
WDW       COSYME
SSB       0
LB        0.00 Hz
GB        0
CB        0
PC        1.00

2D NMR Plot parameters
CZ2       15.705 cm
CZ1       15.705 cm
F2F2G     5.754 ppm
F2F2C     5.853 ppm
F2F2H     2.717 ppm
F2F2I     1630.78 Hz
F2F2J     9.762 ppm
F2F2K     5858.48 Hz
F2F2L     2.745 ppm
F2F2M     1647.06 Hz
F2F2N     0.46914 ppm/cm
F2F2O     281.54425 Hz/cm
F2F2P     0.46783 ppm/cm
F2F2Q     280.76172 Hz/cm
    
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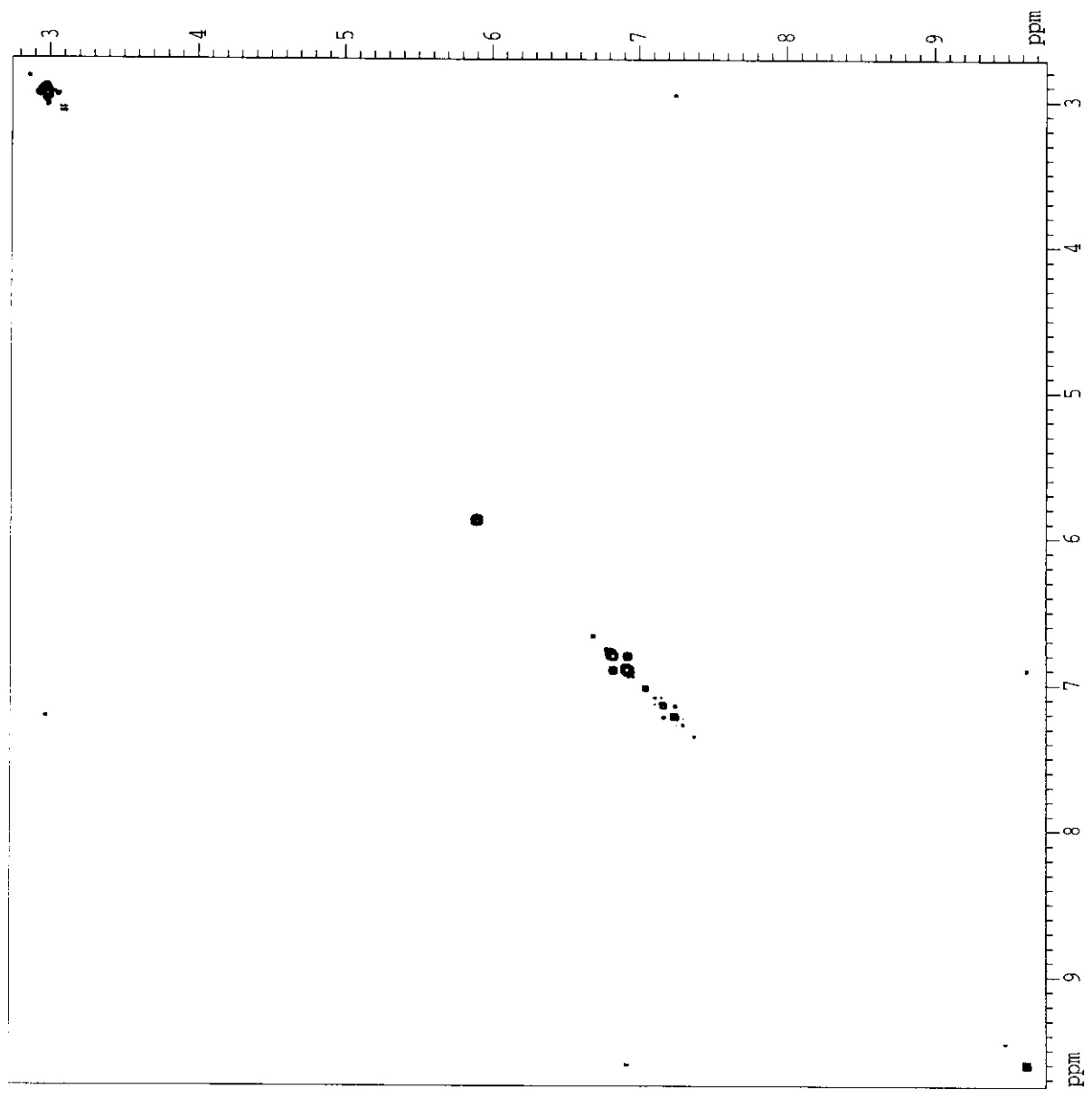


Fig. 3A

1h NMR dmx-600 solvent: CD3OD

```

Current Data Parameters
NAME          caf
EXPNO        3
PROCNO       1

F2 - Acquisition Parameters
Date_        20031215
Time         8.35
INSTRUM      dmx600
PROBHC       5 mm TXI-Z 261
PULPROG      zg
TD           65536
SOLVENT      MeOH
NS           10
DS           2
SWH          8992.896 Hz
FIDRES       0.137219 Hz
AQ           3.6438515 sec
RG           64
DW           55.600 usec
DE           4.50 usec
TE           293.0 K
D1           2.0000000 sec

===== CHANNEL f1 =====
NUC1         1H
P1           11.30 usec
PA1         3.00 dB
SFO1        600.1339008 MHz

F2 - Processing parameters
SI           32768
SF           600.1300199 MHz
WDW          EM
SSB          0
LB           0.15 Hz
GB           0
PC           1.00

1D NMR plot parameters
CX           24.00 cm
CY           10.00 cm
FIP          16.000 ppm
F1           6661.30 Hz
F2           0.000 ppm
PPMCM        0.00 Hz
HZCM         6.44667 ppm/c
            250.05417 Hz/c
    
```

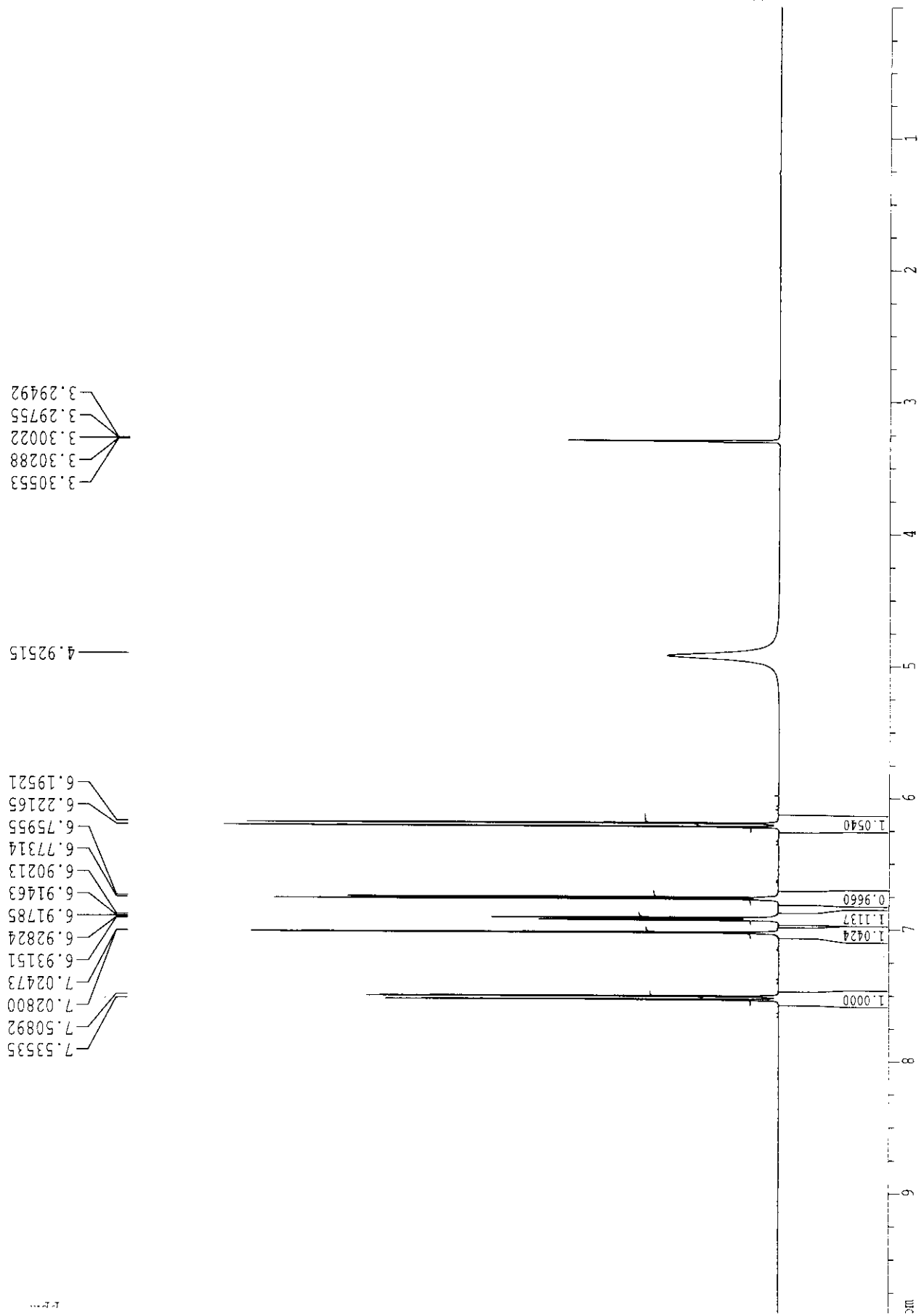


Fig. 3B

1h NMR dmx-600 solvent: CD3OD

```

Current Data Parameters
NAME          caf
EAPNC         3
PROCNO        1

F2 - Acquisition Parameters
Date_         20031215
Time_         8.35
INSTRUM       dmx600
PROBHD        5 mm TX-2 Z81
PULPROG       zg
TD             65536
SOLVENT        MeOH
NS             10
DS             2
SWH            8992.806 Hz
FIDRES         0.137219 Hz
AQ             3.6436515 sec
RG             64
DW             55.600 usec
DE             4.50 usec
TE             293.0 K
D1             2.00000000 sec

===== CHANNEL f1 =====
NUC1           1H
P1             11.30 usec
PL1            3.00 dB
SFO1           600.1339008 MHz

F2 - Processing parameters
SI             32768
SF            600.1300199 MHz
WDW            EM
SSB            0
LB             0.15 Hz
GB             0
PC             1.00

ID NMR Plot parameters
CX            24.00 cm
CY            16.00 cm
F1P           7.820 ppm
F1            4667.24 Hz
F2P           5.772 ppm
F2            3453.53 Hz
PPMCM         0.04496 ppm/Hz
HZCM          50.98762 Hz/cm
    
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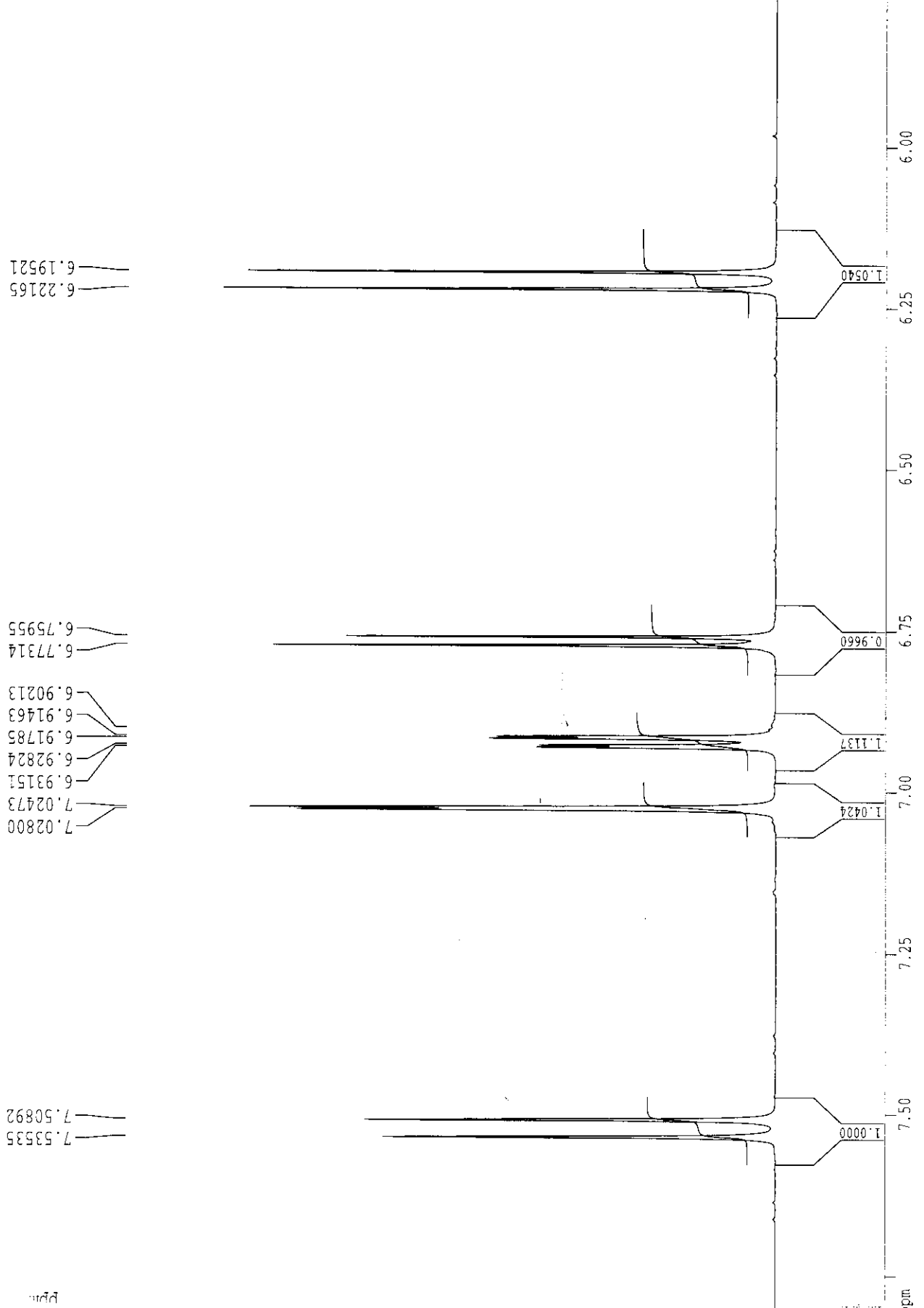


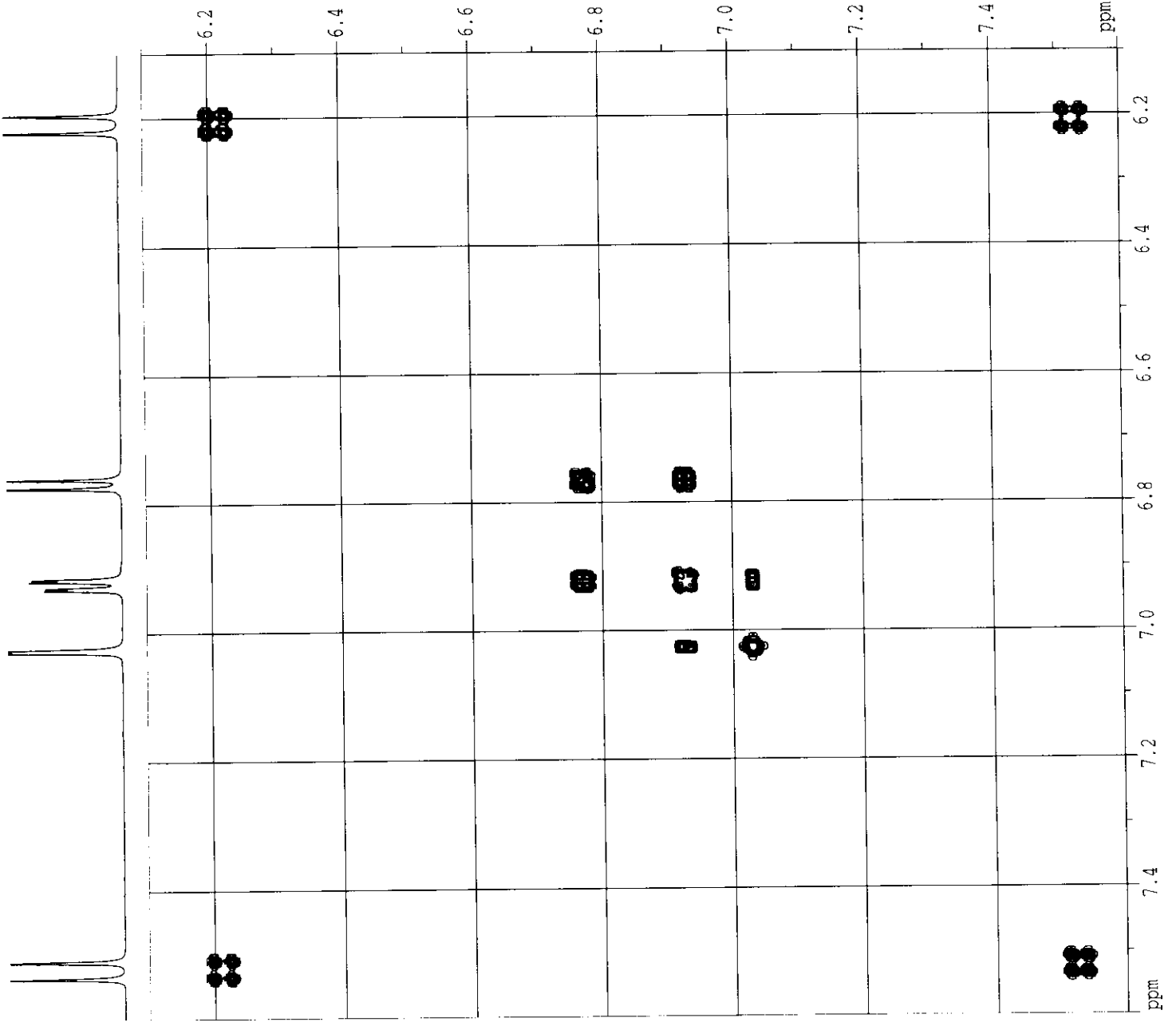
Fig. 3c

DU=/u, USER=nmrafd, NAME=caf, EXPNO=3, PROCNO=1
F1=7.810ppm, F2=5.771ppm, MI=0.12cm, MAXI=10000.00cm, PC=1.000

#	ADDRESS	FREQUENCY		INTENSITY
		[Hz]	[PPM]	
1	14047.3	4522.189	7.5353	7.13
2	14105.1	4506.326	7.5089	7.42
3	15156.8	4217.711	7.0280	8.65
4	15163.9	4215.751	7.0247	9.49
5	15367.8	4159.806	6.9315	4.31
6	15375.0	4157.842	6.9282	4.25
7	15397.7	4151.608	6.9178	5.19
8	15404.7	4149.674	6.9146	5.04
9	15432.0	4142.173	6.9021	0.12
10	15714.1	4064.767	6.7731	9.09
11	15743.8	4056.608	6.7595	7.78
12	16920.1	3733.797	6.2216	10.00
13	16977.9	3717.929	6.1952	9.57

Fig. 3d

1h NMR 2D-COSYgp dmx600



Cont'd. Para. Parameters
NAME: cas1
EXPNO: 4
PROCNO: 1

F1 - Processing Parameters
Date_ 20070218
Time 8:13
INSTRUM spect
PROBHD 5 mm TSI-CSI
PULPROG zgpg30
TD 65536
SFO F2
AQ 1.00
RG 320
DE 1592.434 Hz
PC 1.467191 Hz
DC 0.2498772 sec
AS 256
VA 332.857 usec
TE 300.0 K
DE 4.56 usec
SFO 600.1370189 MHz
AQ 1.0000000 sec
PC 1.0000000 sec
SFO 600.1370189 MHz
AQ 1.0000000 sec
PC 1.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 1.76 usec
PL 0.00 dB
PC 1.00 dB
SFO1 600.1370189 MHz

===== CHANNEL f2 =====
CPDPRG2 SINE_V06
OPWA2 100
GPR2 5.00 kHz
GR2 6.00 kHz
GR1 6.00 kHz
GR2 6.00 kHz
GR1 10.00 kHz
GR2 10.00 kHz
P15 1.000.00 usec

F1 - Acquisition Parameters
NUC 13C
TD 256
SFO1 600.1370189 MHz
SFO2 600.1370189 MHz
SF 600.1370189 MHz
PULPROG zgpg30

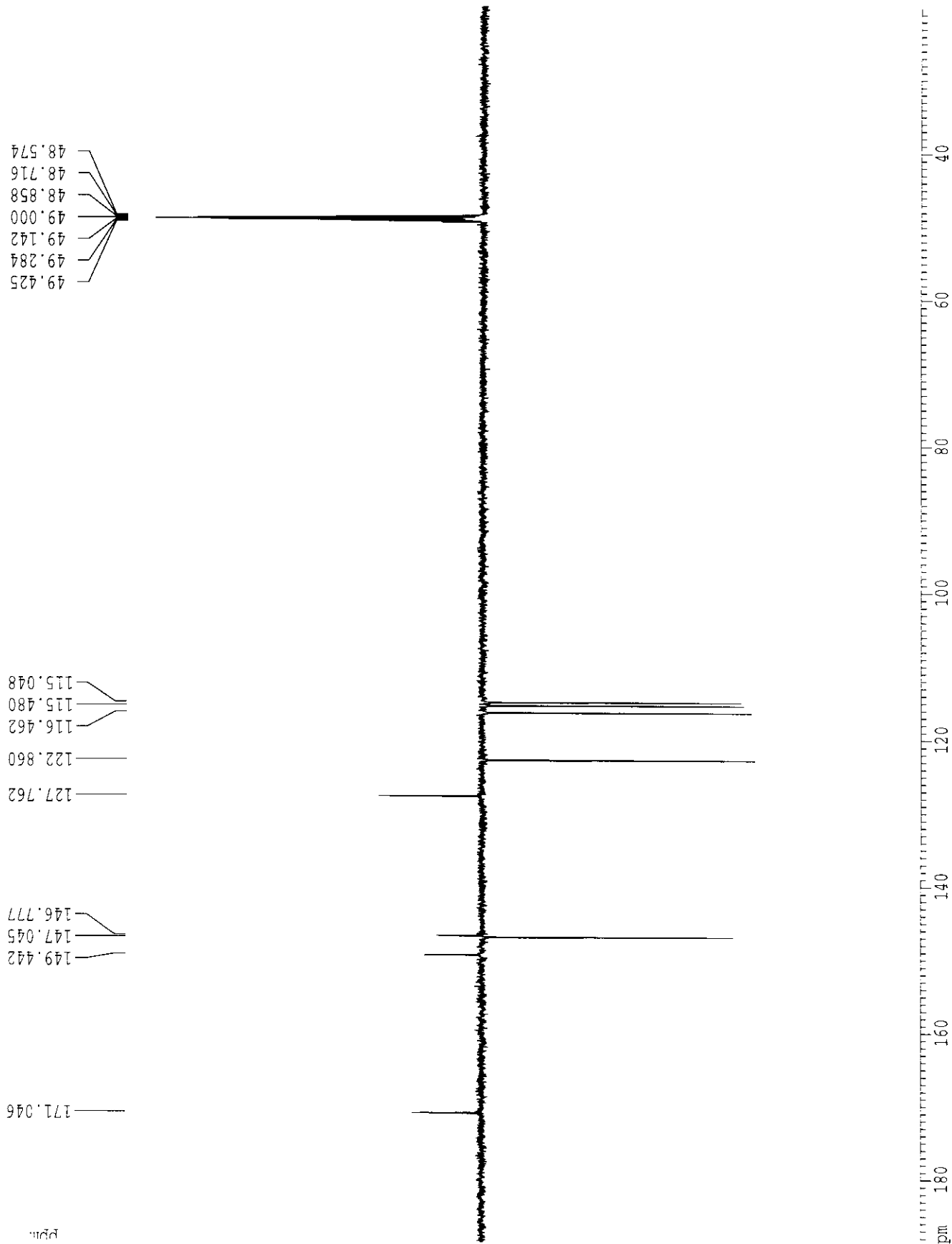
F2 - Processing Parameters
SI 2048
SF 600.1370189 MHz
SFO 600.1370189 MHz
SFB 9
LX 9
LB 9.60 Hz
GB 0
PC 1.00

F1 - Processing Parameters
SI 2048
SF 600.1370189 MHz
SFO 600.1370189 MHz
SFB 9
LX 9
LB 9.60 Hz
GB 0
PC 1.00

===== F2 P15 Parameters =====
CA 10.00 usec
SI 1000
PC 1.00 usec
SFO 600.1370189 MHz
SFB 9
LX 9
LB 9.60 usec
GB 0
PC 1.00 usec
SFO 600.1370189 MHz
SFB 9
LX 9
LB 9.60 usec
GB 0
PC 1.00 usec

Fig. 3e

¹³C APT dmx-600 in CD3OD



Current Data Parameters
 NAME caf
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20011212
 Time 14.03
 INSTRUM dmx600
 PROBHD 5 mm Multinuc
 PULPROG jmc3
 TD 131072
 SOLVENT CDCl3
 NS 76
 DS 2
 SWH 34722.223 Hz
 FIDRES 0.264910 Hz
 AQ 1.8874868 sec
 RG 6192
 BW 14.400 usec
 DE 4.50 usec
 TE 299.0 K
 CNST2 155.0000000
 CNST11 1.0000000
 S1 2.0000000 sec
 d13 0.0000300 sec
 d20 0.00645161 sec
 DELTA 0.0000789 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 6.20 usec
 P2 12.40 usec
 PL1 4.00 dB
 SF01 150.9165938 MHz

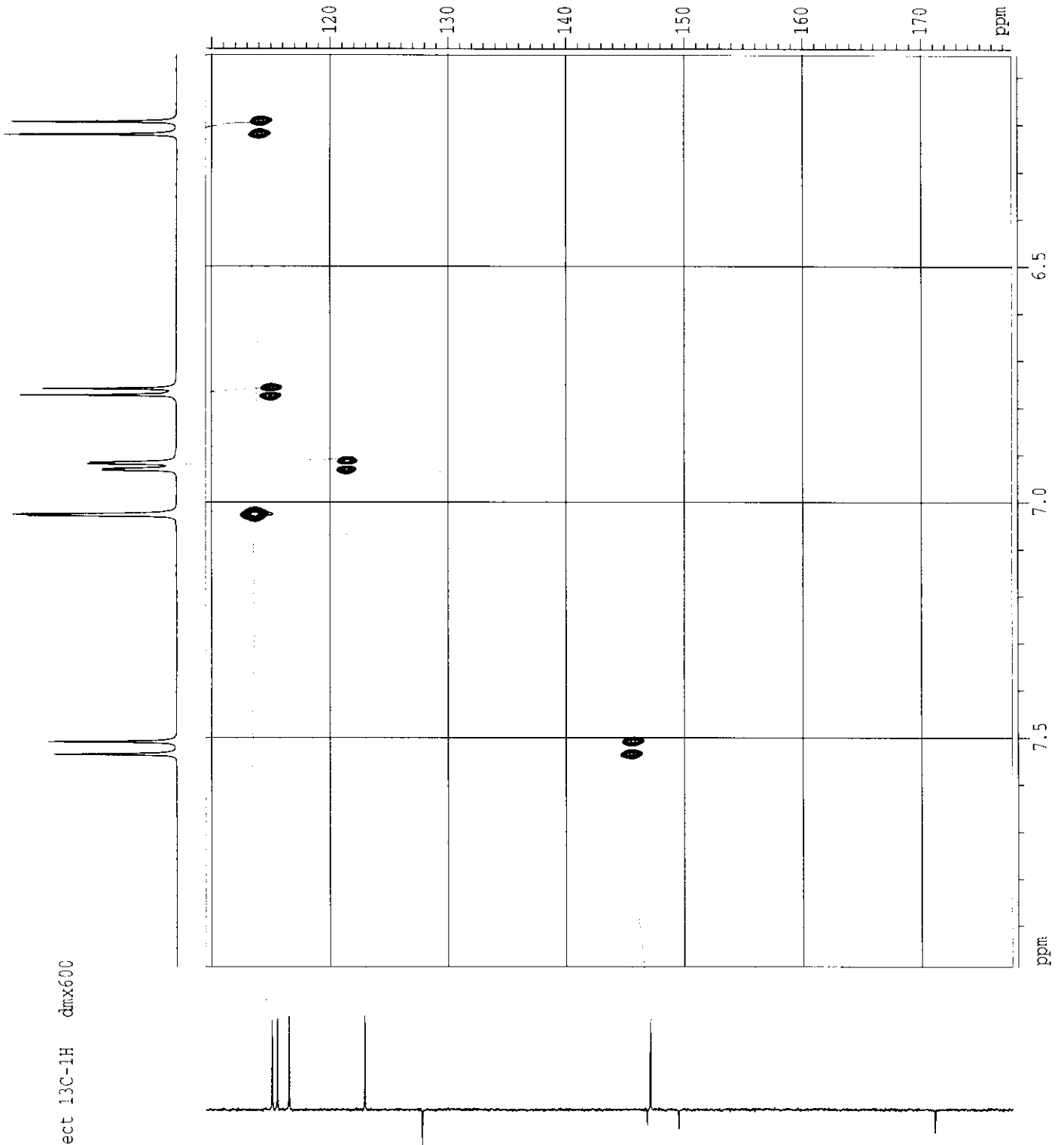
===== CHANNEL f2 =====
 CPDPR2 waltz16
 NUC2 ¹H
 PCPD2 95.00 usec
 PL2 3.00 dB
 PL12 21.02 dB
 SF02 600.1330066 MHz

F2 - Processing parameters
 SI 65536
 SF 150.9026017 MHz
 WDW EM
 SSB 0
 LB 3.50 Hz
 GB 0
 PC 1.00

1D NMR F2 parameters
 CX 23.00 cm
 CY 6.00 cm
 F1P 130.000 ppm
 F1 28671.49 Hz
 F2P 20.000 ppm
 F2 3018.05 Hz
 PPMCM 7.39130 ppm/cm
 HZCM 1115.36694 Hz/cm

Fig. 3 F

HMOCGS direct 13C-1H dmx600



----- Data Parameters

NAME: 13C-1H
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters

NAME: 13C-1H
Time: 3.47
INSTRUM: dmhsc
PROBHD: 5 mm QNP1H CP
PULPROG: zgpg30
SOLVENT: DMSO
NS: 1
DS: 1
SWH: 15904.24 Hz
FIDRES: 1.450194 Hz
AQ: 0.140331 sec
RG: 327.5
AQ2: 32.75 sec
TE: 300.2 K
TE2: 4.50 sec
SFO1: 125.761 MHz
SFO2: 150.916 MHz

----- CHANNEL f1 -----

NUC1: 13C
P1: 7.72 usec
PL1: 15.45 usec
PC1: 3.00 dB
SFO1: 125.761605 MHz

----- CHANNEL f2 -----

NUC2: 1H
P2: 4.50 usec
PL2: 65.00 usec
PC2: 3.00 dB
SFO2: 400.147 MHz

----- CHANNEL CHANNEL -----

ORIG1: SINE 100
ORIG2: SINE 100
ORIG3: SINE 100
SFO1: 500.136 MHz
SFO2: 500.136 MHz
SFO3: 500.136 MHz
SFO4: 500.136 MHz
SFO5: 500.136 MHz
SFO6: 500.136 MHz
SFO7: 500.136 MHz
SFO8: 500.136 MHz
SFO9: 500.136 MHz
SFO10: 500.136 MHz
SFO11: 500.136 MHz
SFO12: 500.136 MHz
SFO13: 500.136 MHz
SFO14: 500.136 MHz
SFO15: 500.136 MHz
SFO16: 500.136 MHz
SFO17: 500.136 MHz
SFO18: 500.136 MHz
SFO19: 500.136 MHz
SFO20: 500.136 MHz

----- Processing Parameters -----

SI: 327.5
SF: 600.136055 MHz
WDW: EM
SSB: 0
GB: 0
PC: 0.20 dB
SC: 3.00 Hz
SD: 0.30 Hz
FI: 0.30

F3 - Processing Parameters

SI: 327.5
SF: 600.136055 MHz
WDW: EM
SSB: 0
GB: 0
PC: 0.20 dB
SC: 3.00 Hz
SD: 0.30 Hz
FI: 0.30

F4 - Processing Parameters

SI: 327.5
SF: 600.136055 MHz
WDW: EM
SSB: 0
GB: 0
PC: 0.20 dB
SC: 3.00 Hz
SD: 0.30 Hz
FI: 0.30

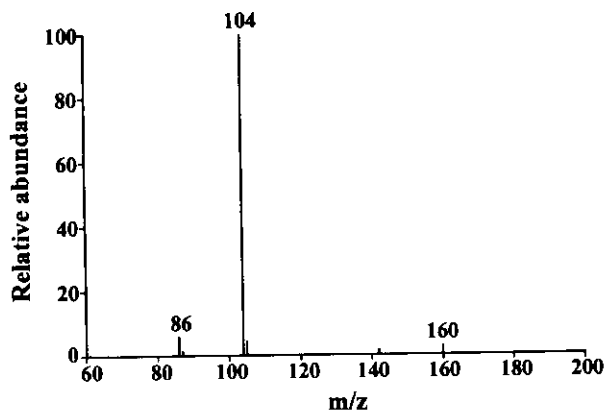
F5 - Processing Parameters

SI: 327.5
SF: 600.136055 MHz
WDW: EM
SSB: 0
GB: 0
PC: 0.20 dB
SC: 3.00 Hz
SD: 0.30 Hz
FI: 0.30

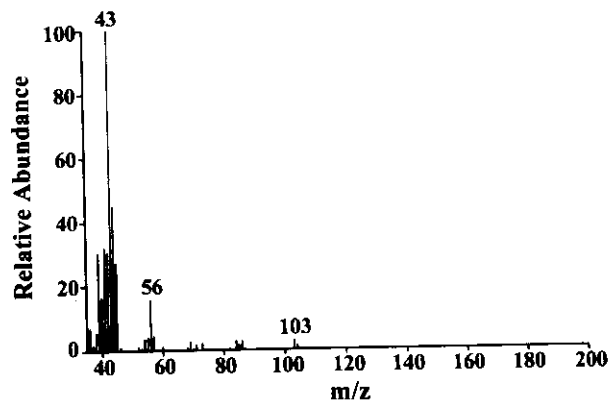
Fig. 4A

PROBLEM 16-15

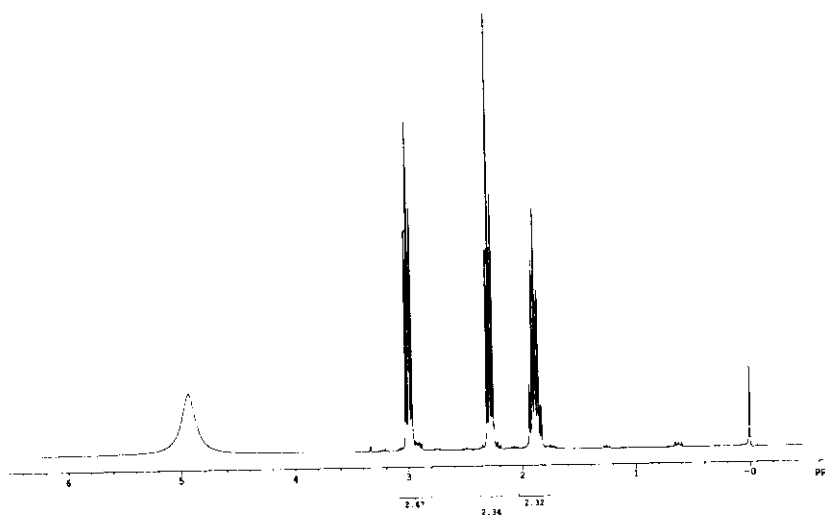
Mass spectrum (CI)



Mass spectrum (EI)



Proton NMR spectrum (D₂O)



Carbon-13 NMR spectrum

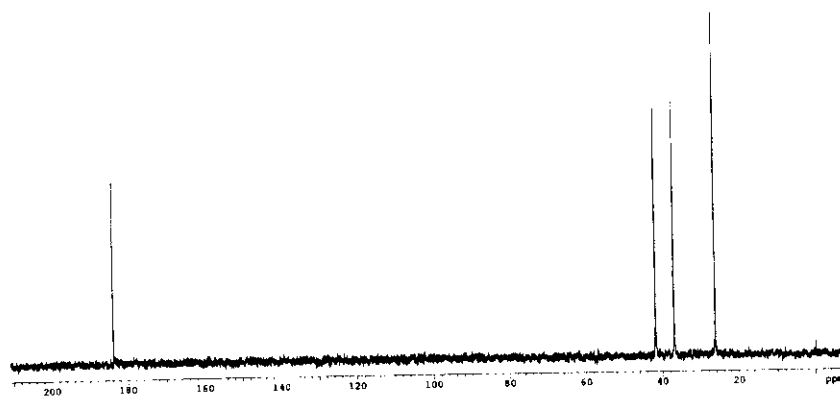
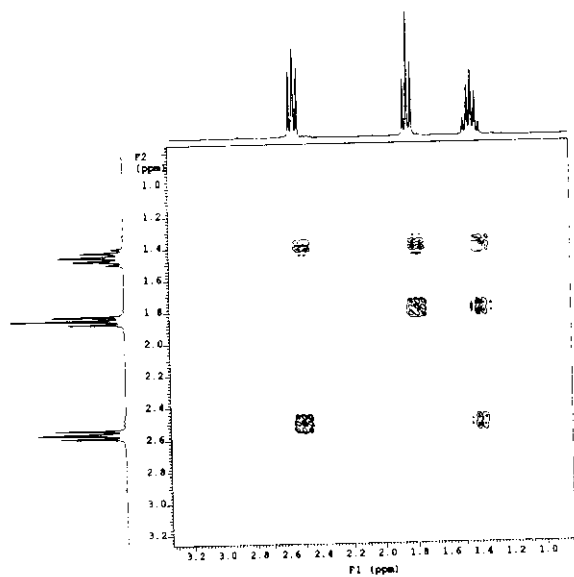
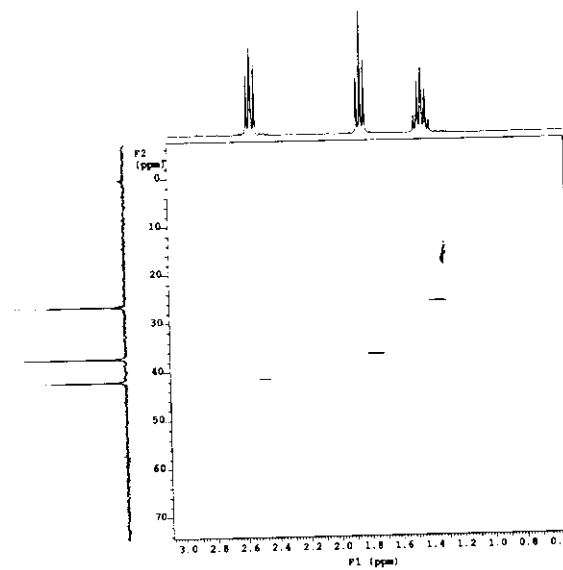


Fig. 4b

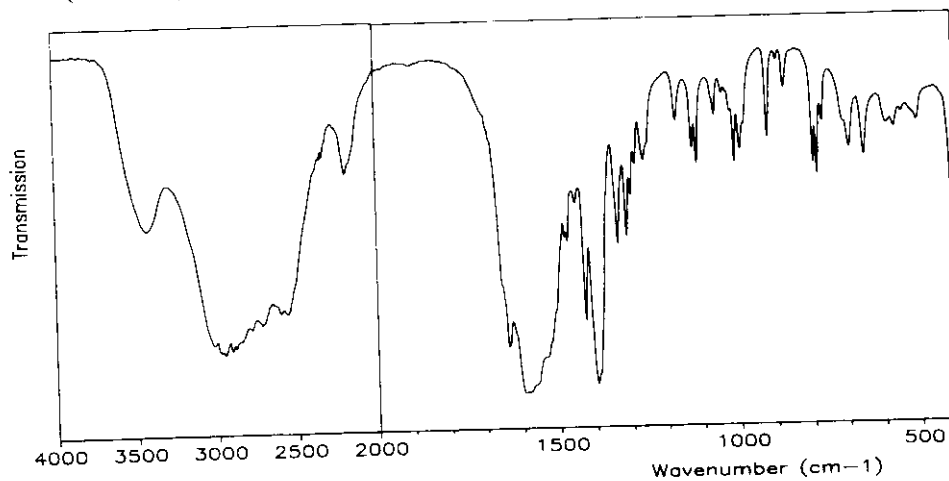
COSY spectrum



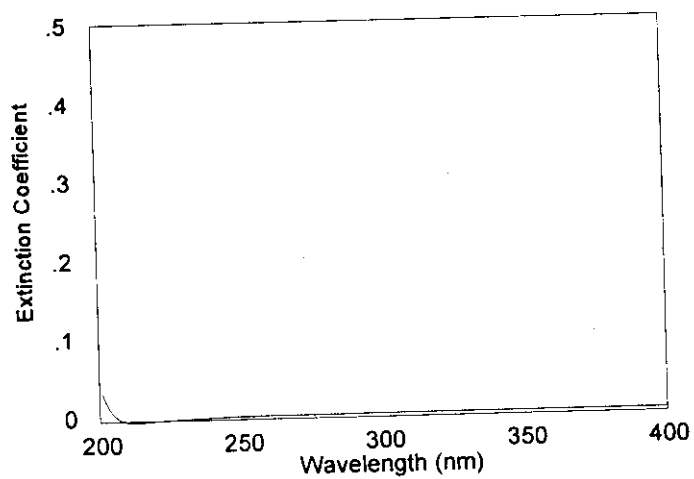
HETCOR spectrum



Infrared spectrum (KBr disc)

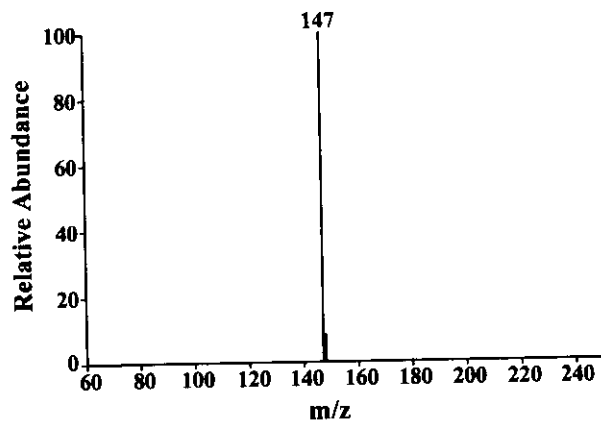


Ultraviolet-visible spectrum (EtOH)

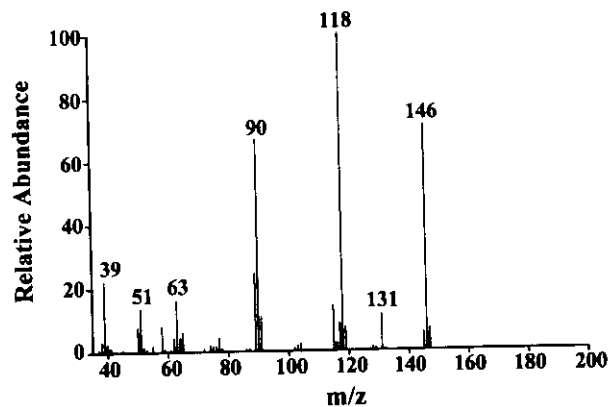


PROBLEM 16-28

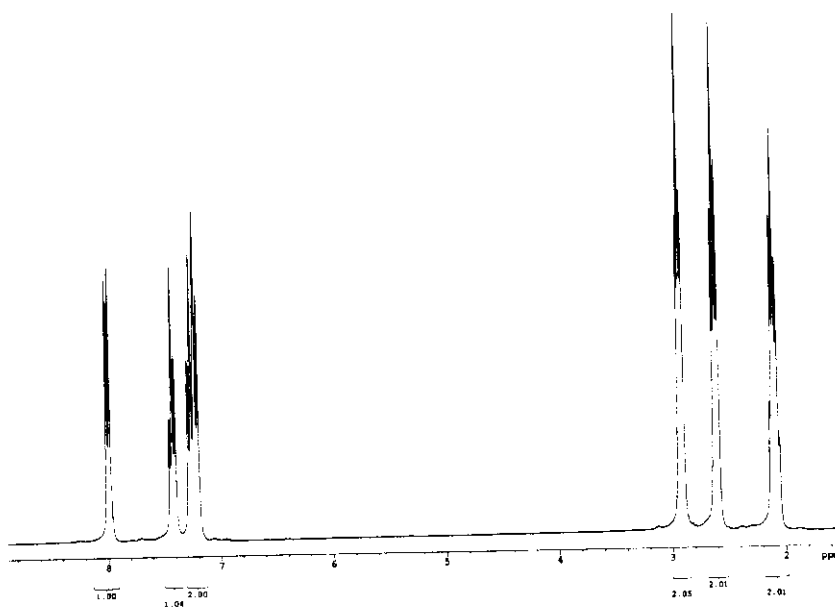
Mass spectrum (CI)



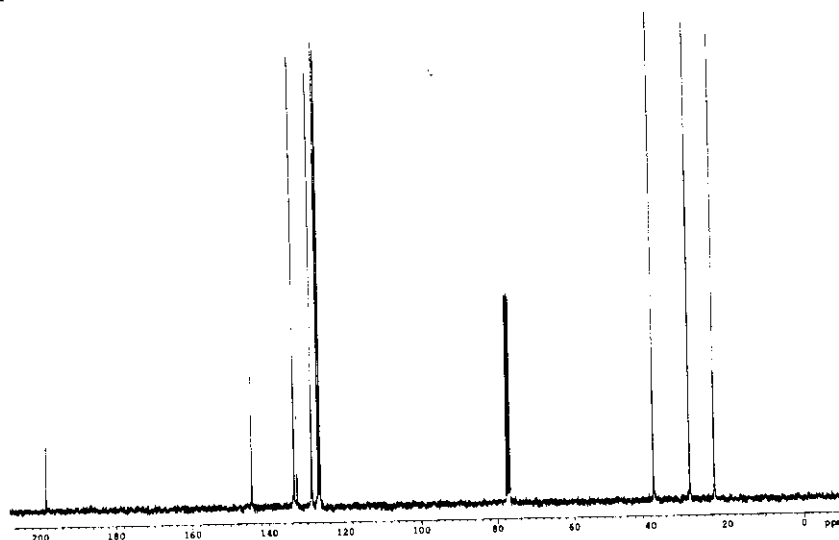
Mass spectrum (EI)



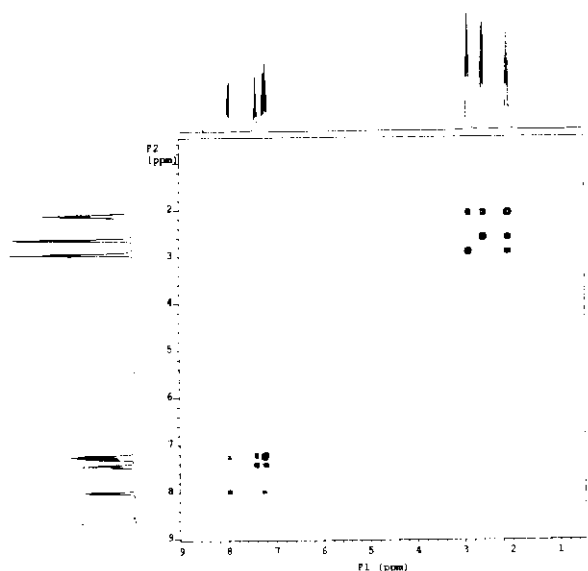
Proton NMR spectrum ($CDCl_3$)



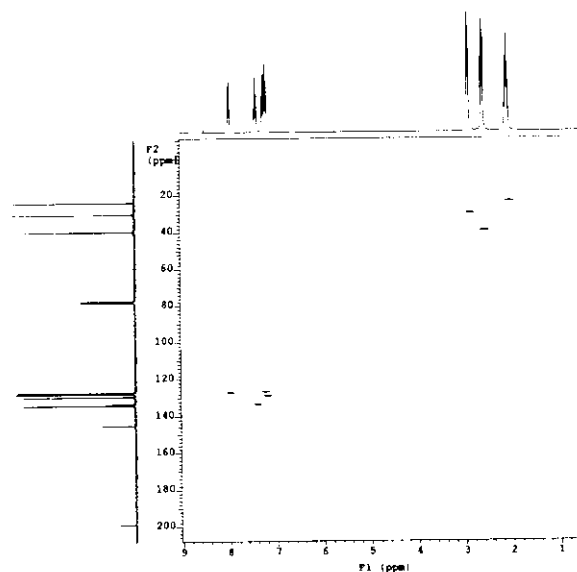
Carbon-13 NMR spectrum



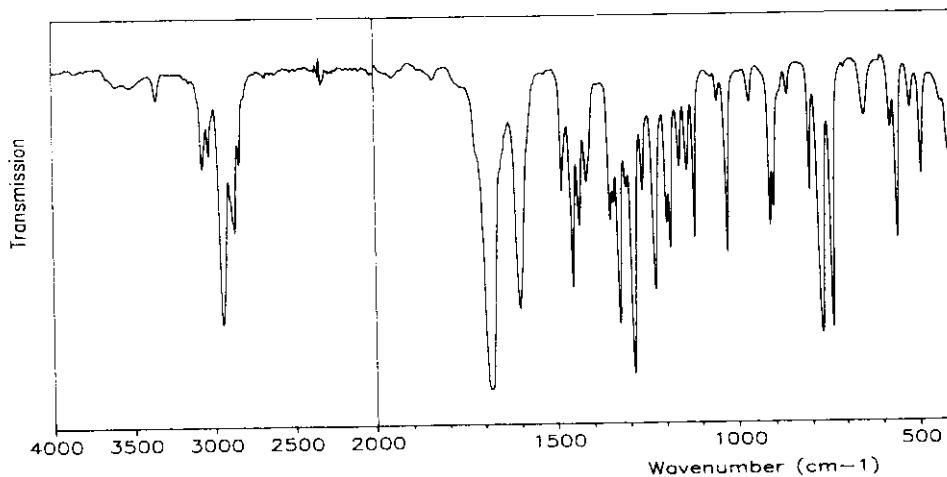
COSY spectrum



HETCOR spectrum



Infrared spectrum (neat)



Ultraviolet-visible spectrum (EtOH, ϵ [206] 24,500, ϵ [248] 12,200, ϵ [291] 2200)

