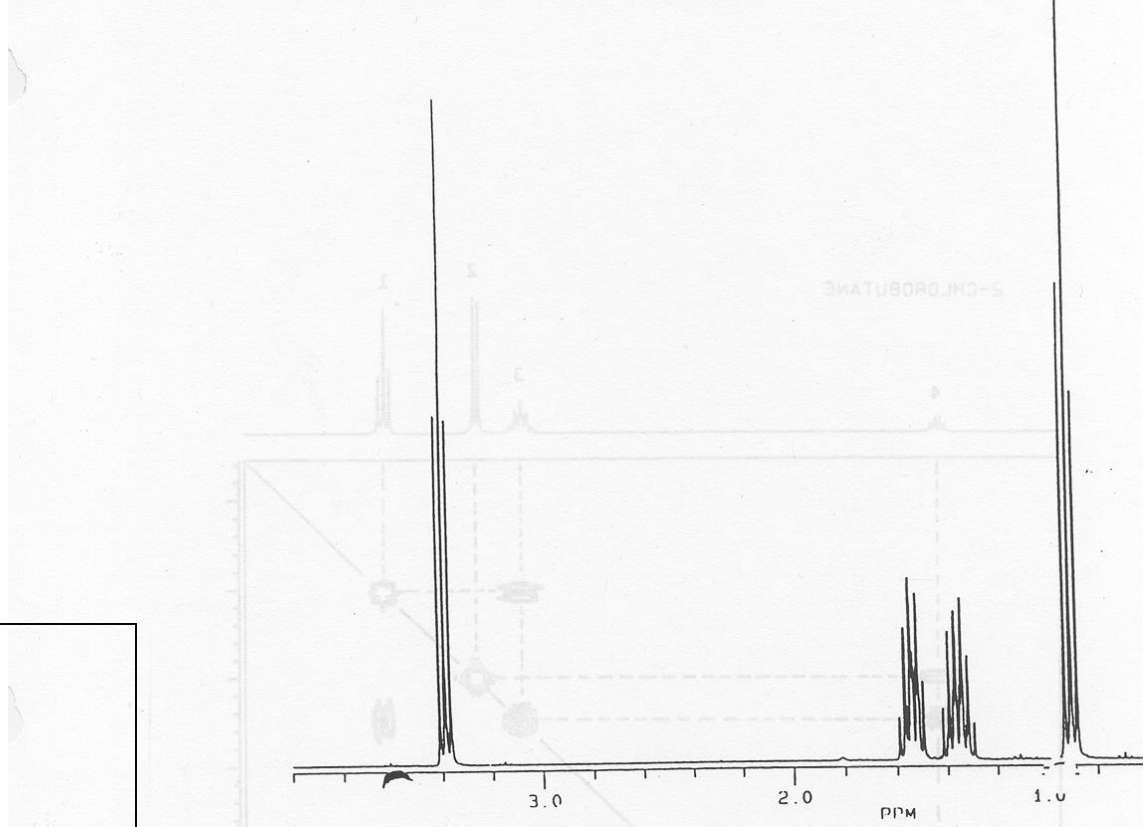
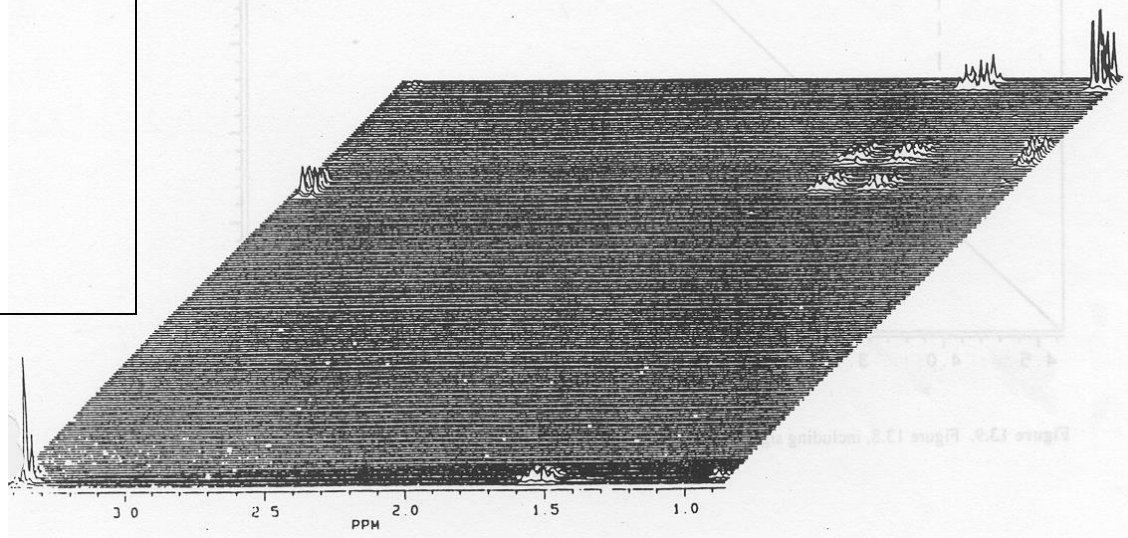
2D-NMR

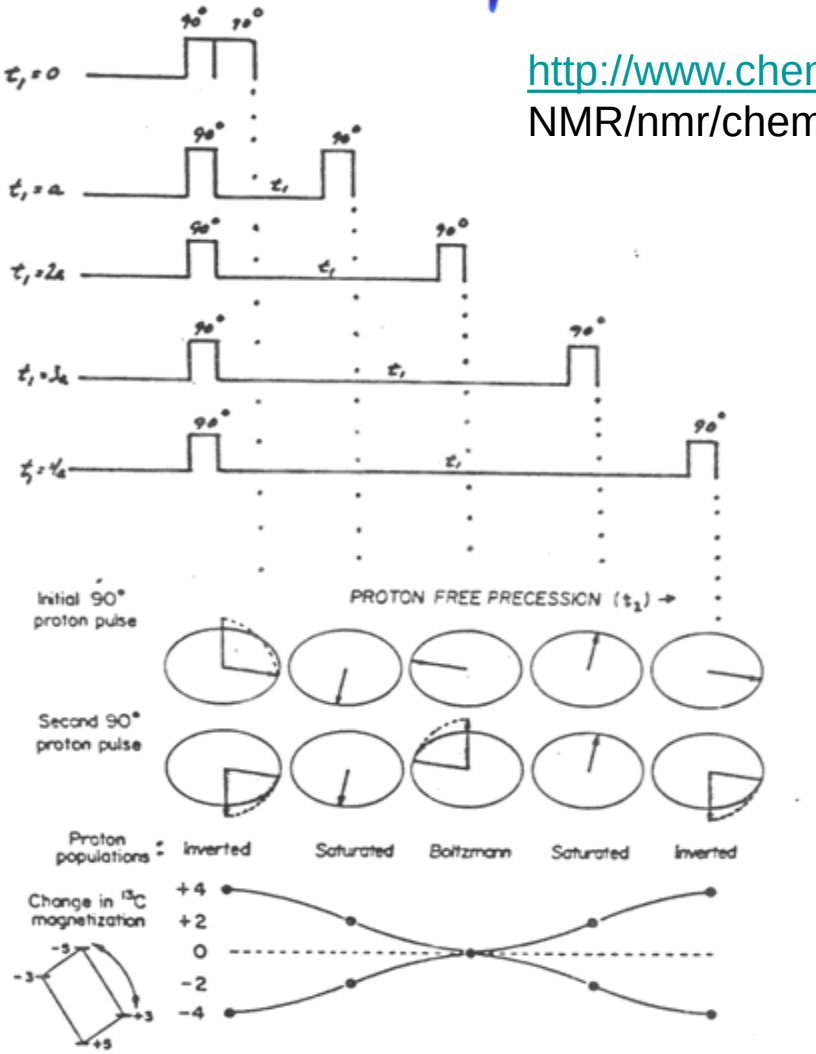
COSY, COrrellation SpectroscopY





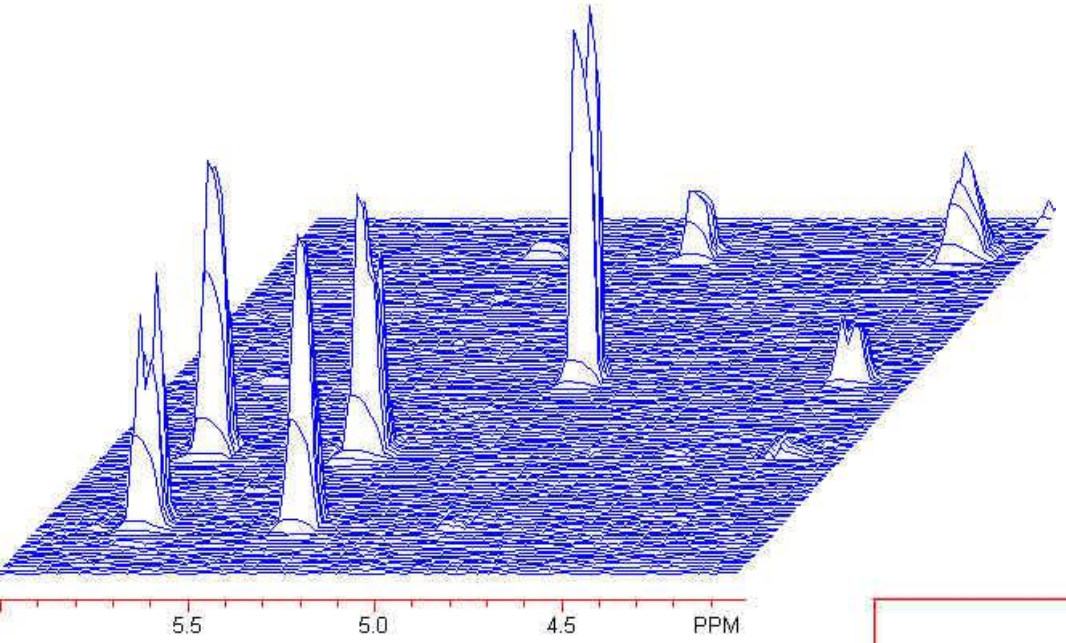
COSY : CORRELATED SPECTROSCOPY

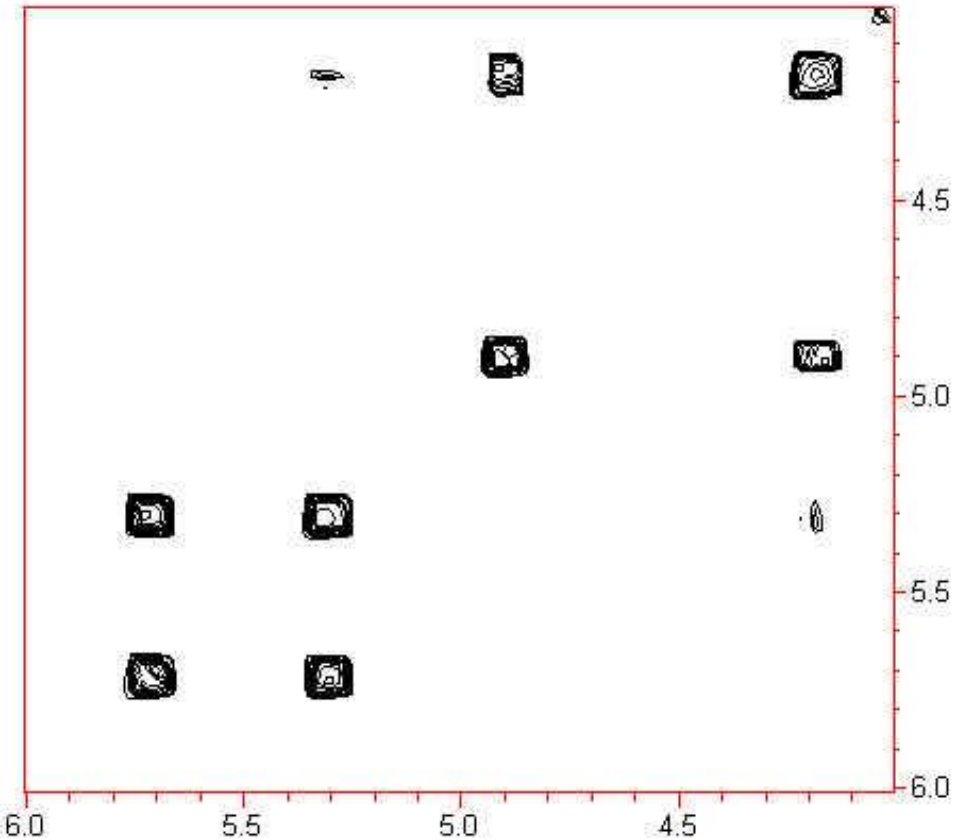
http://www.chem.queensu.ca/FACILITIES/NMR/nmr/chem806/Web/homo2_files/frame.htm



Magnetization transfer from protons to carbon-13 explained in terms of spin state populations. Free precession of the proton magnetizations during the t_1 period leaves the proton vectors in various possible positions in the XY plane, so that the second proton 90° pulse rotates the Y components of these magnetizations into the Z direction. The range of possible orientations in the XY plane at time t_1 leads to proton spin state populations that may be inverted, saturated, or at Boltzmann equilibrium. This results in changes to the population differences across carbon-13 transitions, modulating the longitudinal magnetization associated with these transitions as a function of t_1. This modulation may be mapped out as a function of t_1 by applying a 90° carbon pulse and measuring the resultant signal, "reading" the information coded into the t_1 dependence of the carbon magnetization.

COSY, COrrellation SpectroscopY

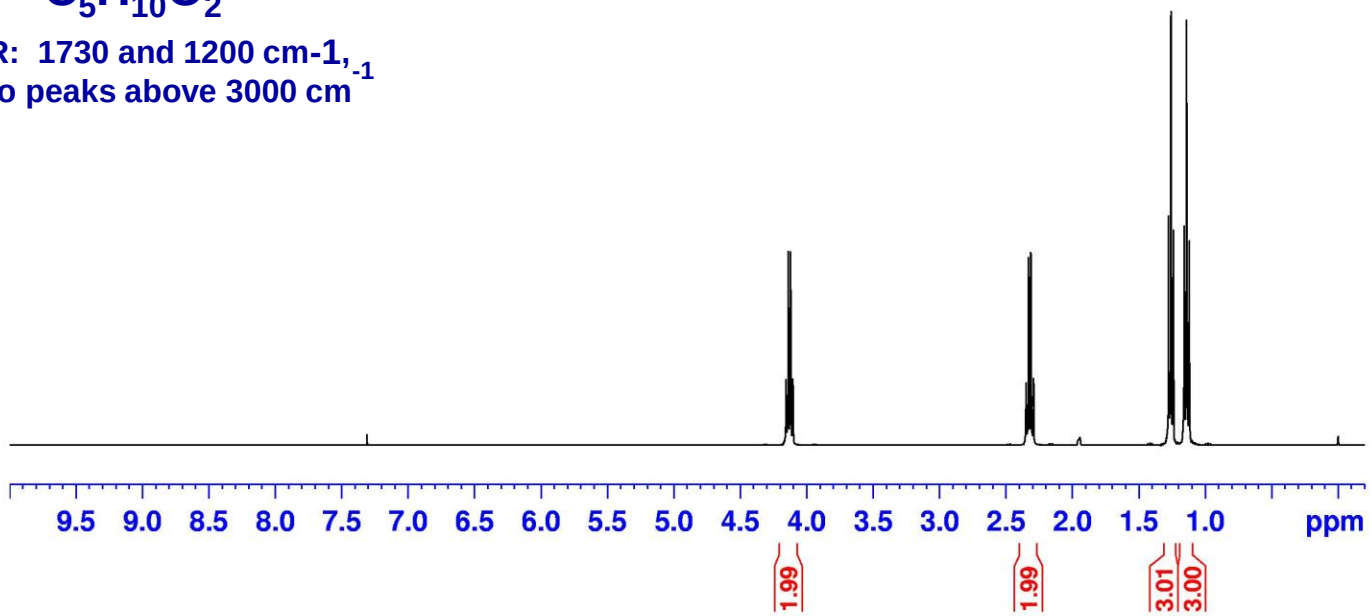




2D-NMR: COSY

$C_5H_{10}O_2$

IR: 1730 and 1200 cm-1, no peaks above 3000 cm^{-1}




```
Current Data Parameters
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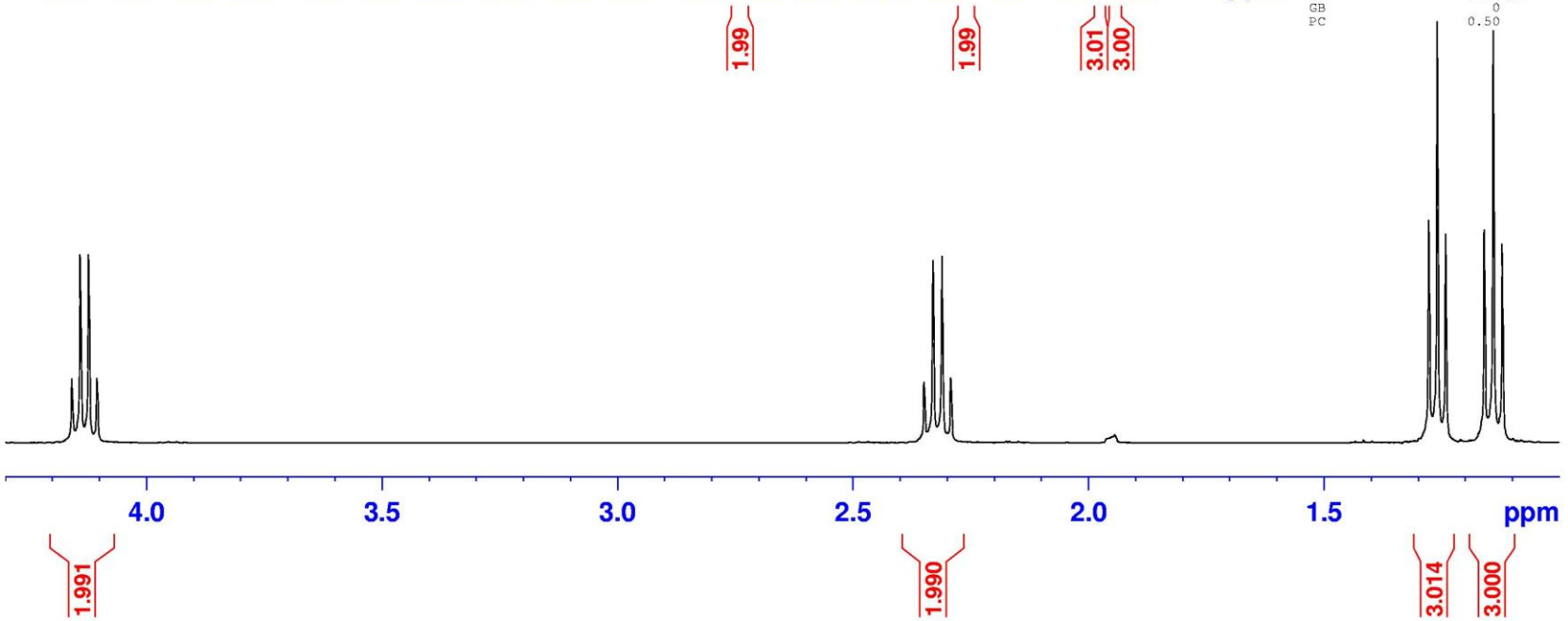
EXPNO                      1
PROCNO                     1

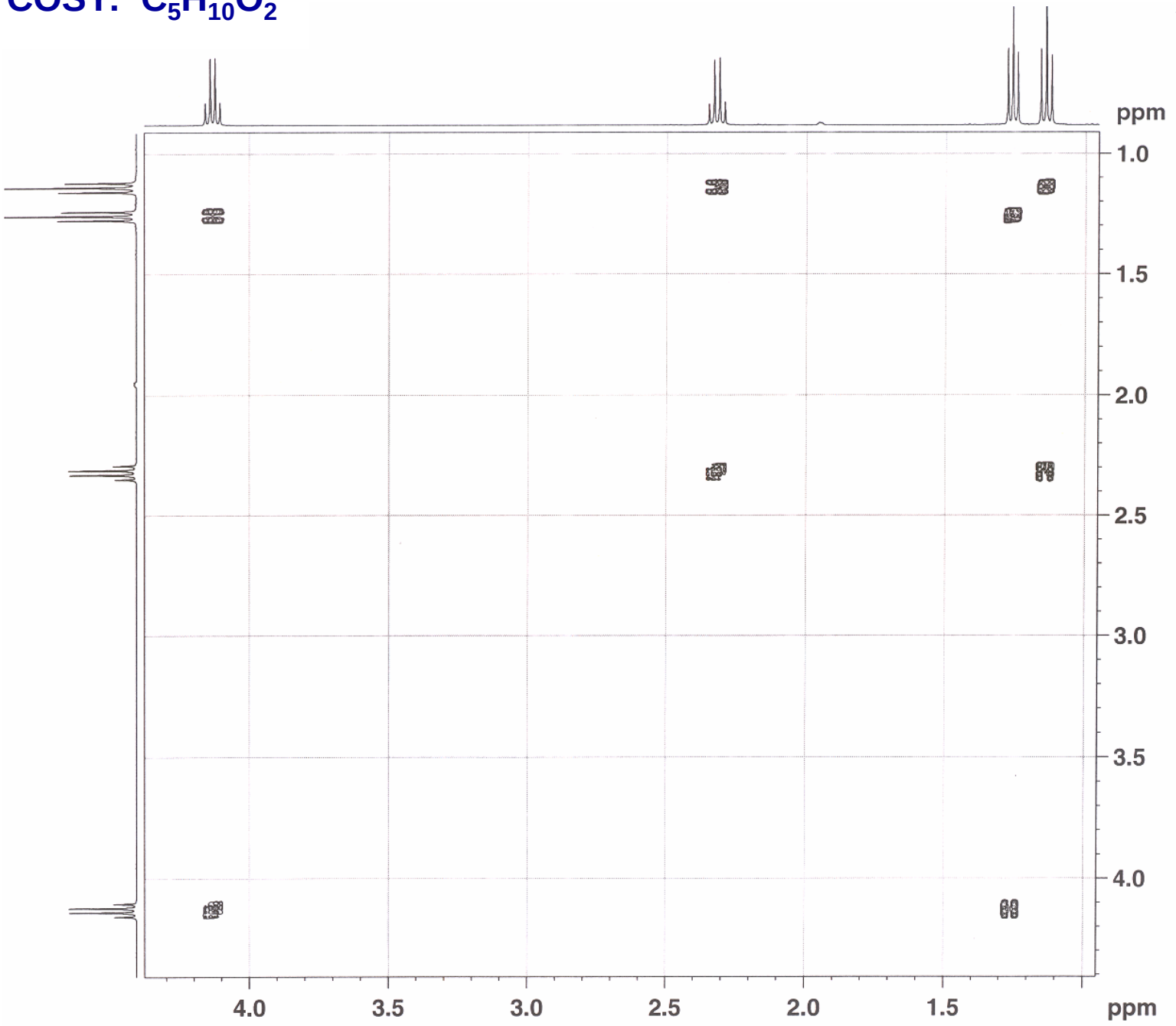
F2 - Acquisition Parameters
Date_              20070615
Time                  12.03
INSTRUM               spect
PROBHD    5 mm Multinucl
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               5208.333 Hz
FIDRES            0.079473 Hz
AQ                6.2915058 sec
RG                     35.9
DW                96.000 usec
DE                 6.00 usec
TE                 690.6 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                  7.50 usec
PL1                 -6.00 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                        32768
SF              400.1299890 MHz
WDW                       EM
SSB                        0
LB                  0.10 Hz
GB                         0
PC                  0.50
```



COSY: $C_5H_{10}O_2$

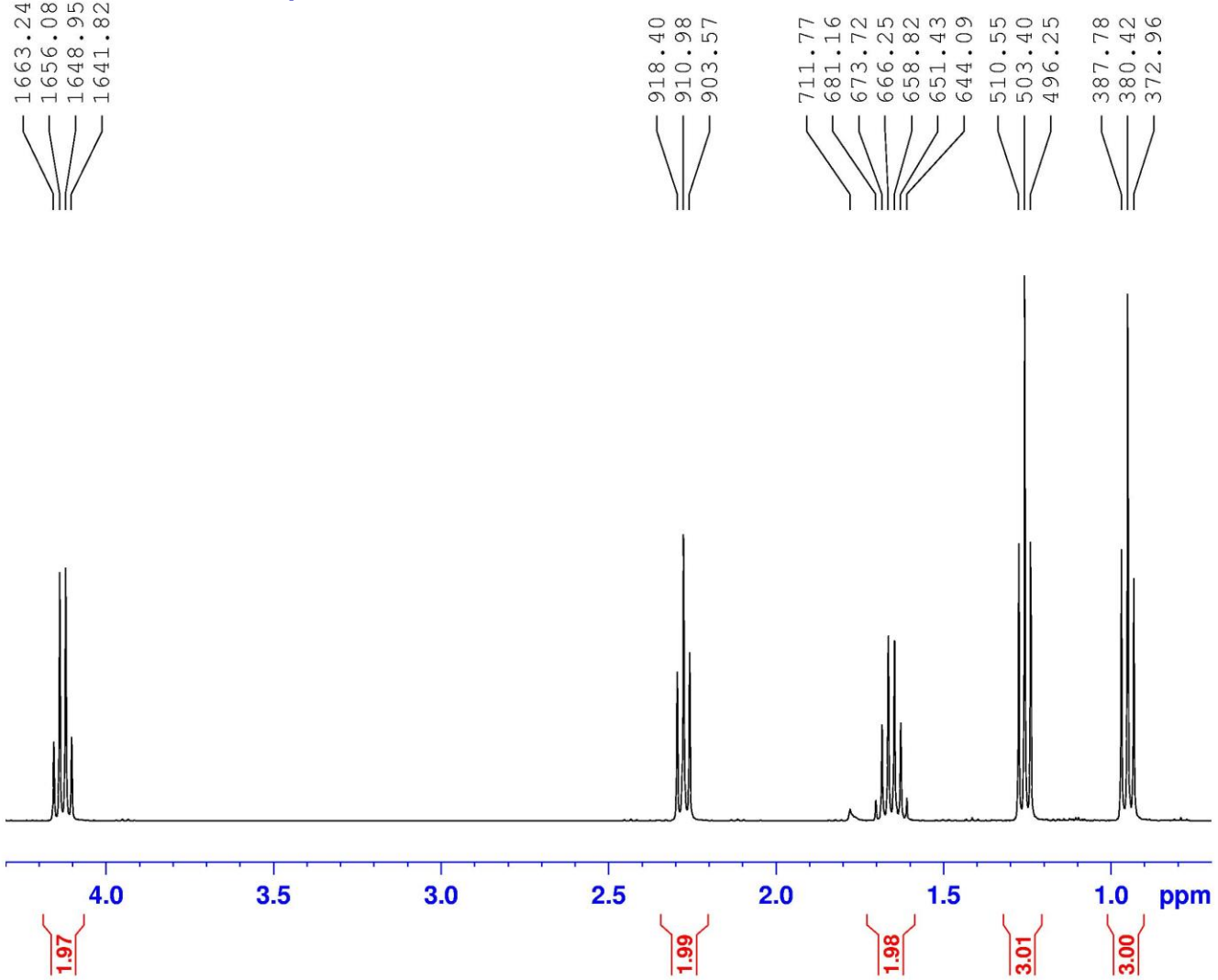


$C_6H_{12}O_2$

2D-NMR: COSY

C6H12O2

IR: 1730 and 1200 cm-1, $^{-1}$
no peaks above 3000 cm




```
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EXPNO                   1
PROCNO                  1

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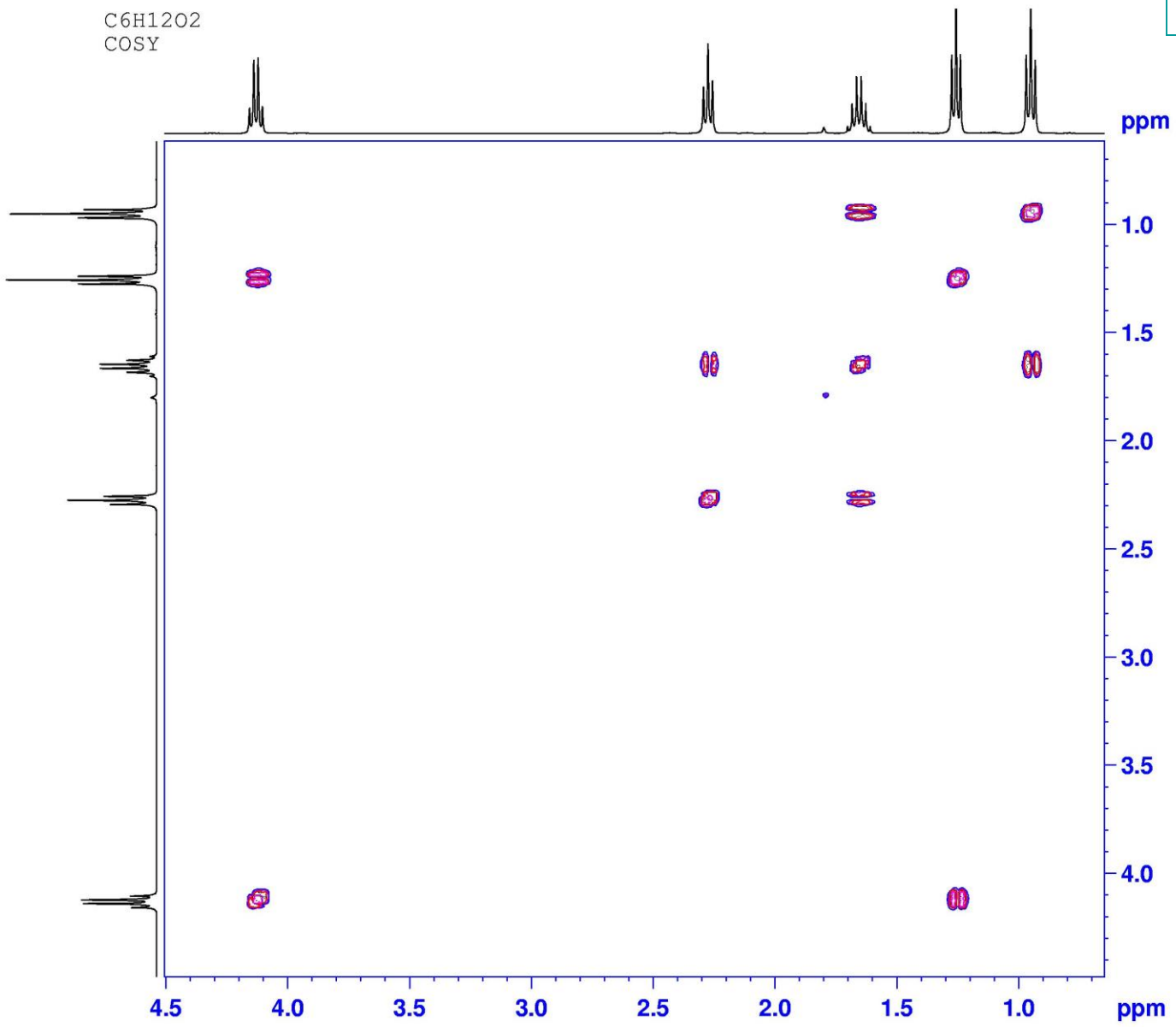
Time                13.16
INSTRUM             spect
PROBHD   5 mm Multinucl
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8250.825
FIDRES           0.125898
AQ               3.9715316
RG                     57
DW                 60.600
DE                   6.00
TE                  690.1
D1             1.00000000
TD0                     1

======== CHANNEL f1 ===
NUC1                   1H
P1                   7.50
PL1                 -6.00
SFO1          400.1320563

F2 - Processing paramet
SI                  32768
SF            400.1299982
WDW                    EM
SSB                     0
LB                   0.30
GB                      0
PC                   1.00
```

2D-NMR: COSY

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Current Data Parameters
NAME         512unknownJ
EXPNO                203
PROCNO                 1

F2 - Acquisition Parameters
Date_             20060226
Time                 13.20
INSTRUM              spect
PROBHD    5 mm TXI 13C Z
PULPROG          cosygpqf
TD                   2048
SOLVENT               DMSO
NS                       1
DS                       8
SWH              3623.188 Hz
FIDRES           1.769135 Hz
AQ               0.2826740 sec
RG                      64
DW                138.000 usec
DE                  6.00 usec
TE                 692.4 K
d0               0.00000300 sec
D1               1.48689198 sec
d13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00027600 sec

======== CHANNEL f1 ========
NUC1                    1H
P0                   9.00 usec
P1                   9.00 usec
PL1                 -2.00 dB
SFO1          400.1319991 MHz

====== GRADIENT CHANNEL =====
GPNAM1            SINE.100
GPNAM2            SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                10.00 %
GPZ2                10.00 %
P16               1000.00 usec

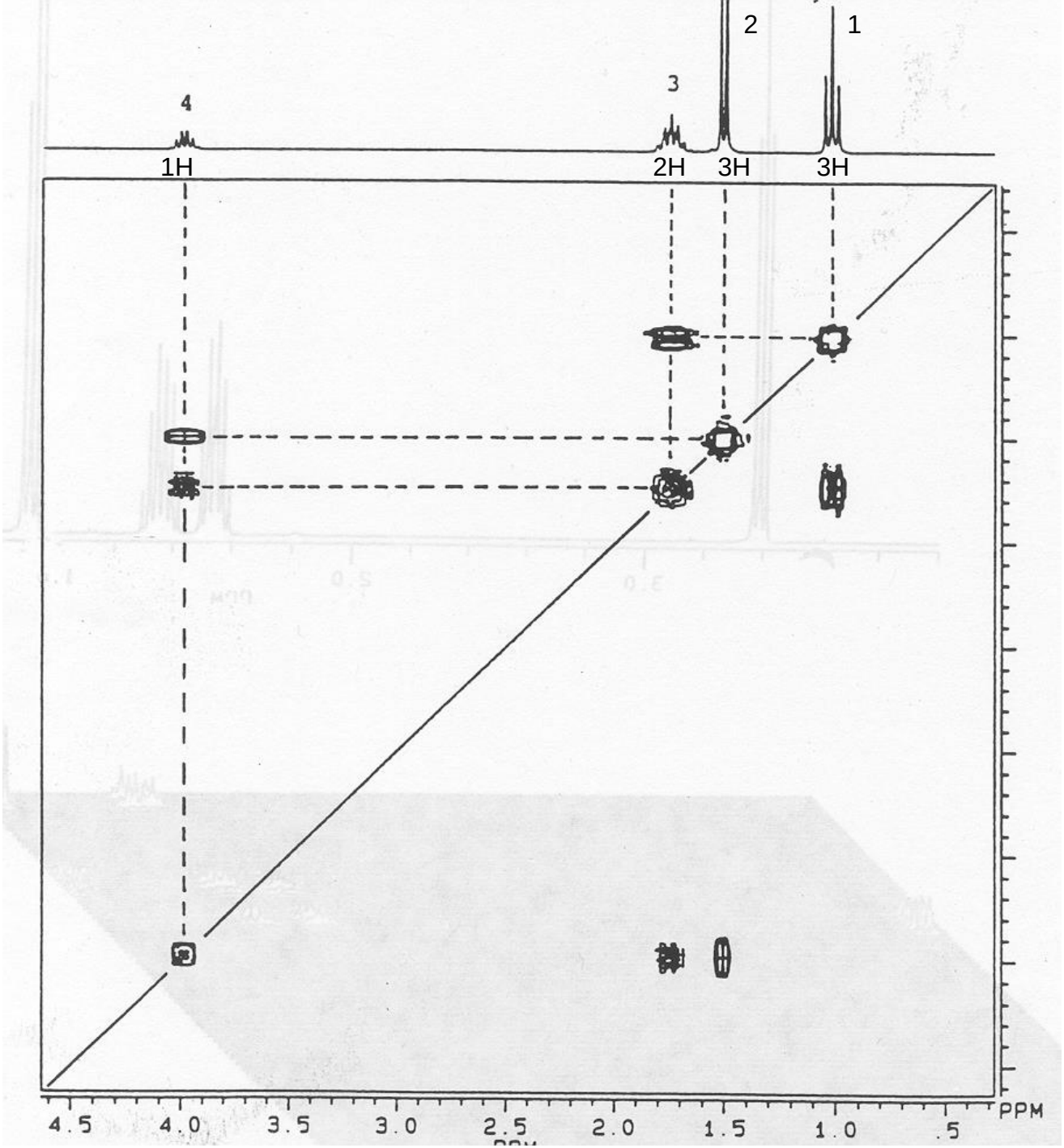
F1 - Acquisition parameters
ND0                      1
TD                     128
SFO1            400.132 MHz
FIDRES         28.306160 Hz
SW                 9.055 ppm
FnMODE                QF

F2 - Processing parameters
SI                    1024
SF            400.1300000 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00

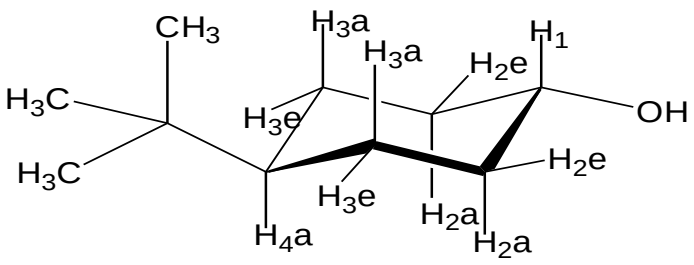
F1 - Processing parameters
SI                    1024
MC2                     QF
SF            400.1300000 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
```

2D-NMR: COSY

C_4H_9Cl



C10H18O

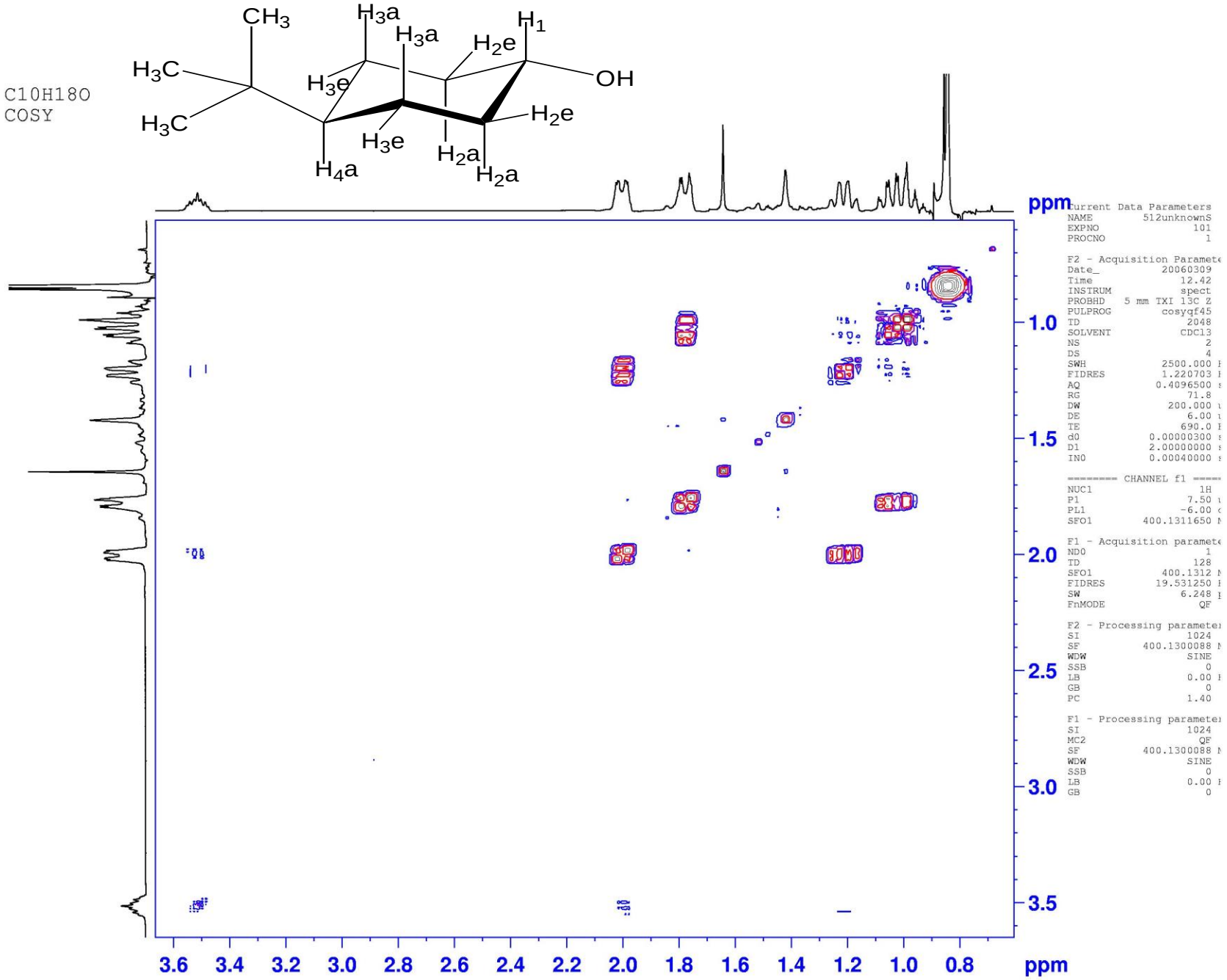



```
Current Data Parameters
NAME          512unknownS
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20060309
Time                12.30
INSTRUM             spect
PROBHD   5 mm TXI 13C Z
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8250.825 Hz
FIDRES           0.125898 Hz
AQ               3.9715316 sec
RG                   90.5
DW                 60.600 usec
DE                  6.00 usec
TE                 690.0 K
D1              1.00000000 sec
TD0                     1

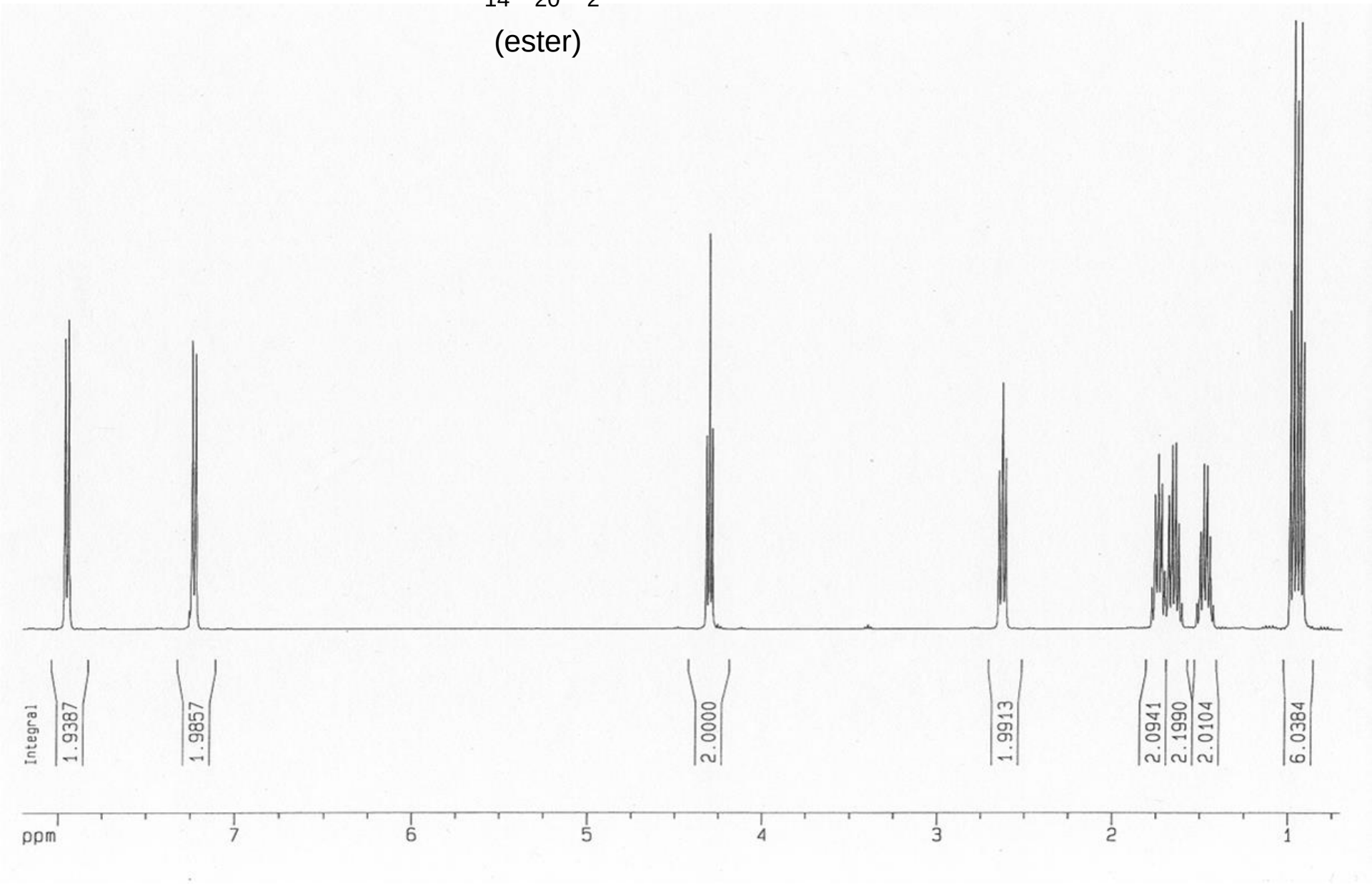
======== CHANNEL f1 ========
NUC1                   1H
P1                  7.50 usec
PL1                -6.00 dB
SFO1         400.1320563 MHz

F2 - Processing parameters
SI                  32768
SF           400.1300088 MHz
WDW                    EM
SSB                     0
LB                   0.20 Hz
GB                      0
PC                   1.00
```

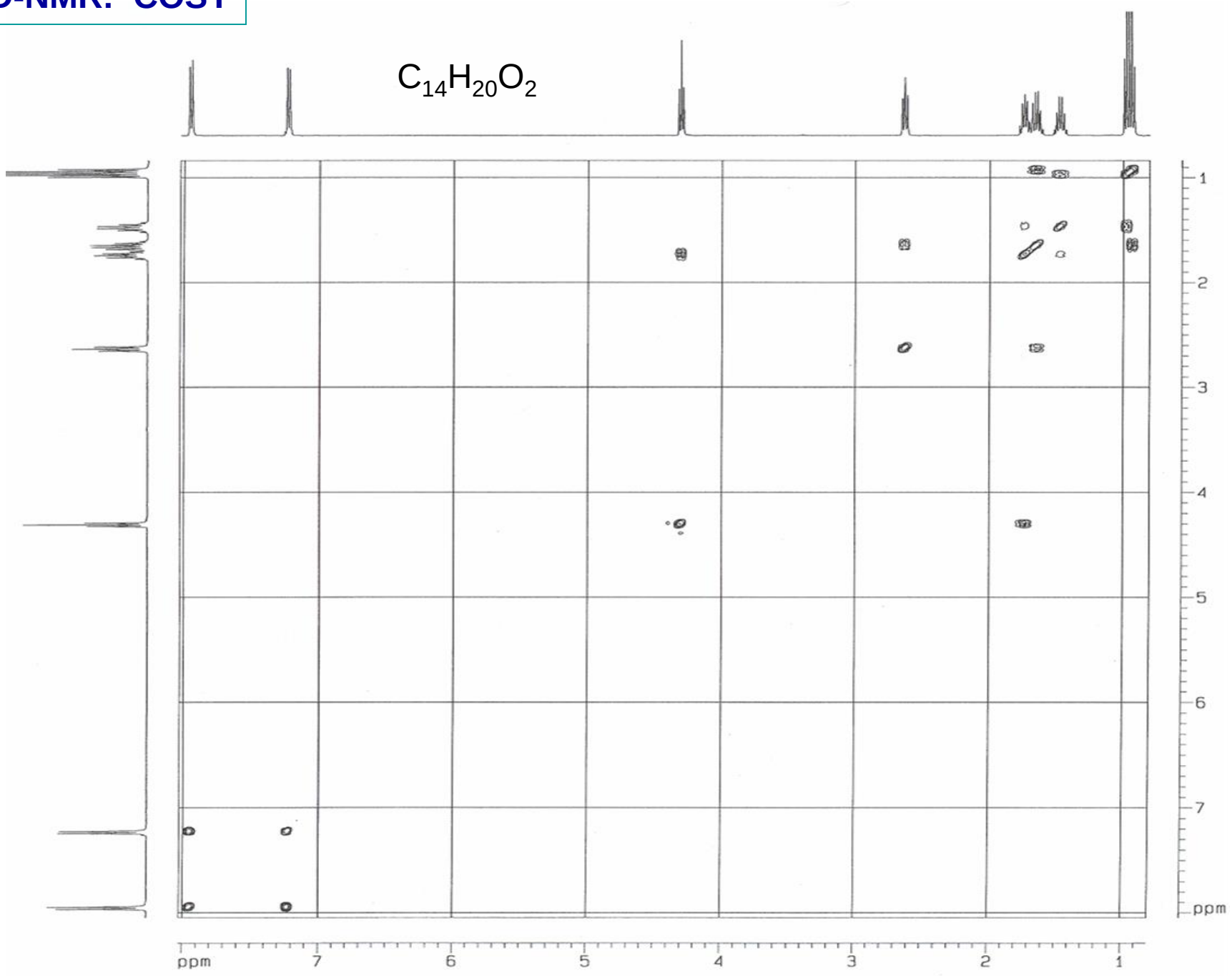

C10H18O
COSY
CH3
H3C
H3C
H3a
H3a
H3e
H3e
H4a
H2a
H2a
H2e
H2e
H1
OH
ppm
1.0
1.5
2.0
2.5
3.0
3.5
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
ppm
Current Data Parameters
NAME 512unknownS
EXPNO 101
PROCNO 1
F2 - Acquisition Paramete
Date_ 20060309
Time 12.42
INSTRUM spect
PROBHD 5 mm TXI 13C Z
PULPROG cosyqf45
TD 2048
SOLVENT CDCl3
NS 2
DS 4
SWH 2500.000
FIDRES 1.220703
AQ 0.4096500
RG 71.8
DW 200.000
DE 6.00
TE 690.0
d0 0.00000300
D1 2.00000000
IN0 0.00040000
CHANNEL f1
NUC1 1H
P1 7.50
PL1 -6.00
SFO1 400.1311650
F1 - Acquisition paramete
ND0 1
TD 128
SFO1 400.1312
FIDRES 19.531250
SW 6.248
FnMODE QF
F2 - Processing parameter
SI 1024
SF 400.1300088
WDW SINE
SSB 0
LB 0.00
GB 0
PC 1.40
F1 - Processing parameter
SI 1024
MC2 QF
SF 400.1300088
WDW SINE
SSB 0
LB 0.00
GB 0

$C_{14}H_{20}O_2$

(ester)

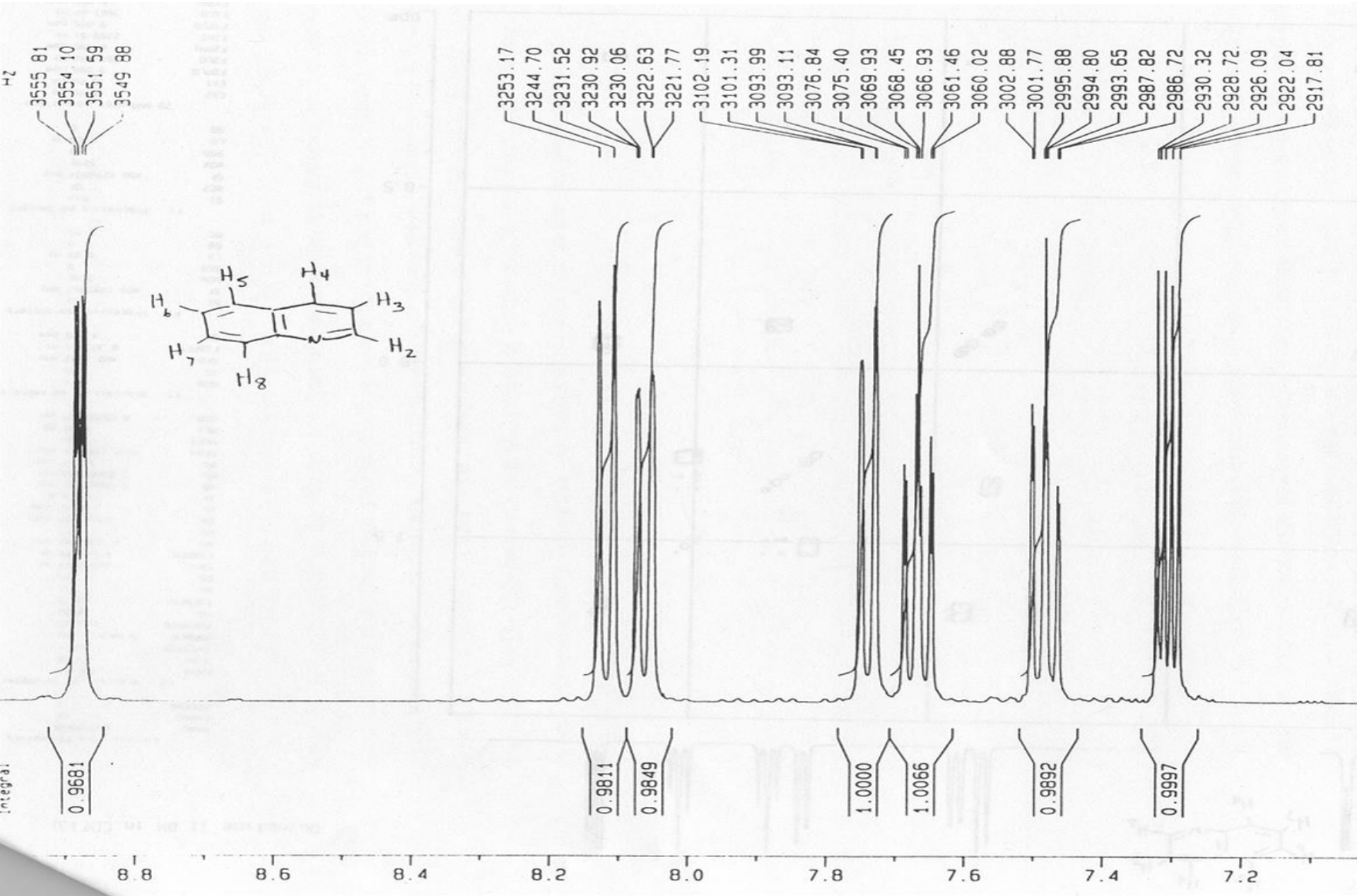


2D-NMR: COSY

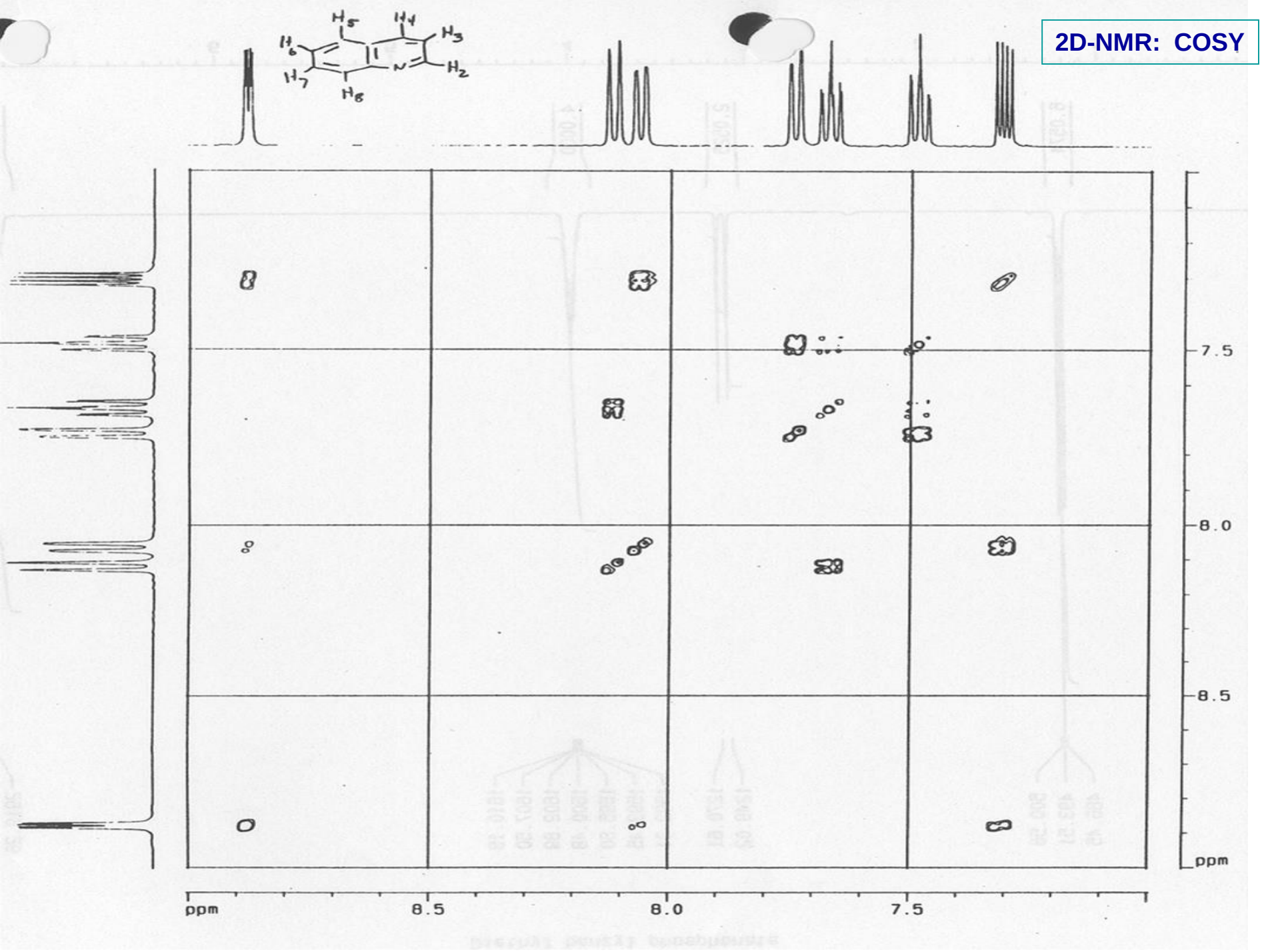


2D-NMR: COSY

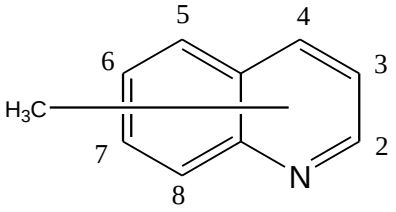
Given the COSY on the next page, assign all protons and calculate coupling constants, J_{23}, J_{24} and J_{34}? (Because of the heterocyclic ring, H-2 has the highest chemical shift and the *ortho* coupling constant $J_{2\text{-}3}$ ~ 4Hz, significantly smaller than a normal *ortho* coupling constant.



2D-NMR: COSY

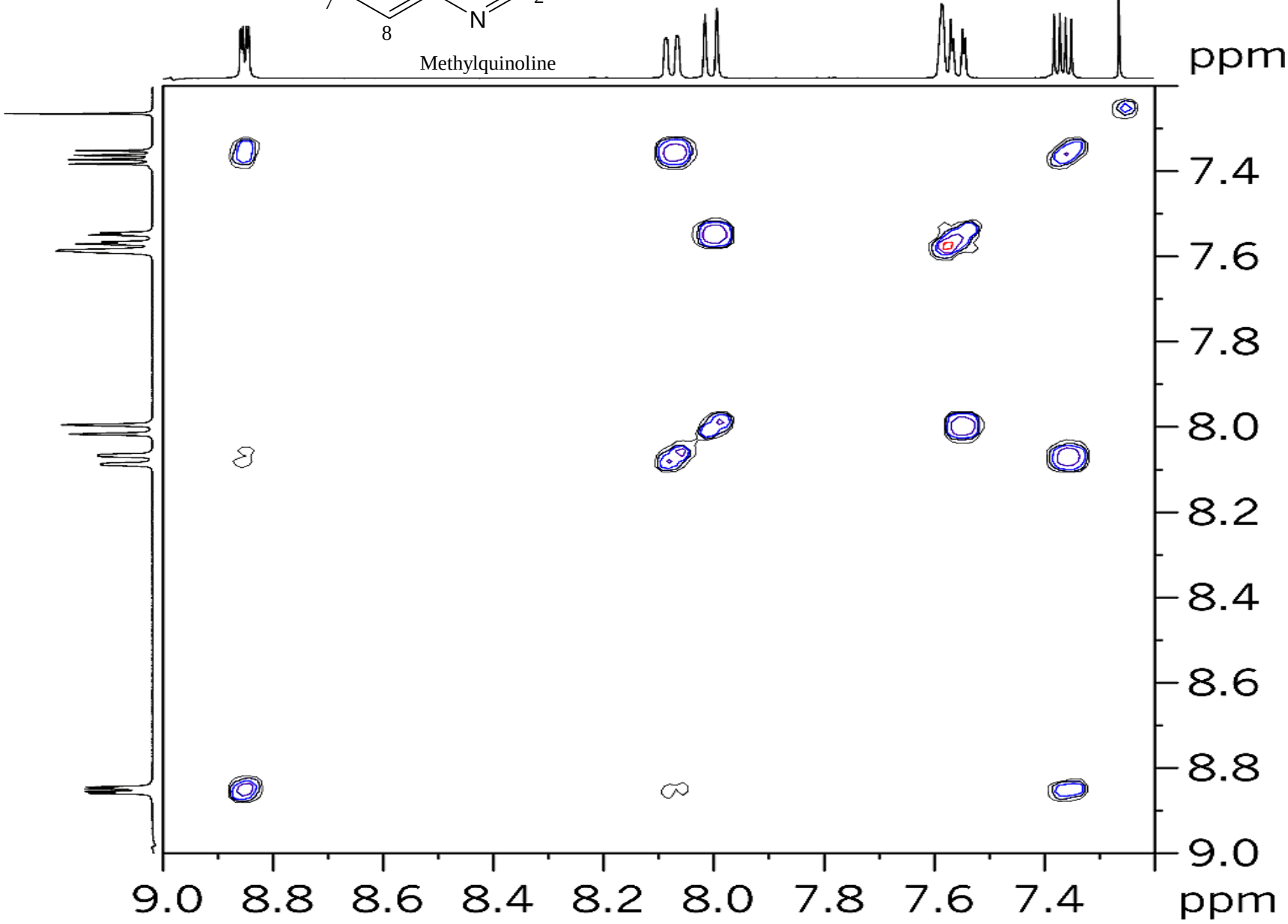


2D-NMR: COSY



Methylquinoline

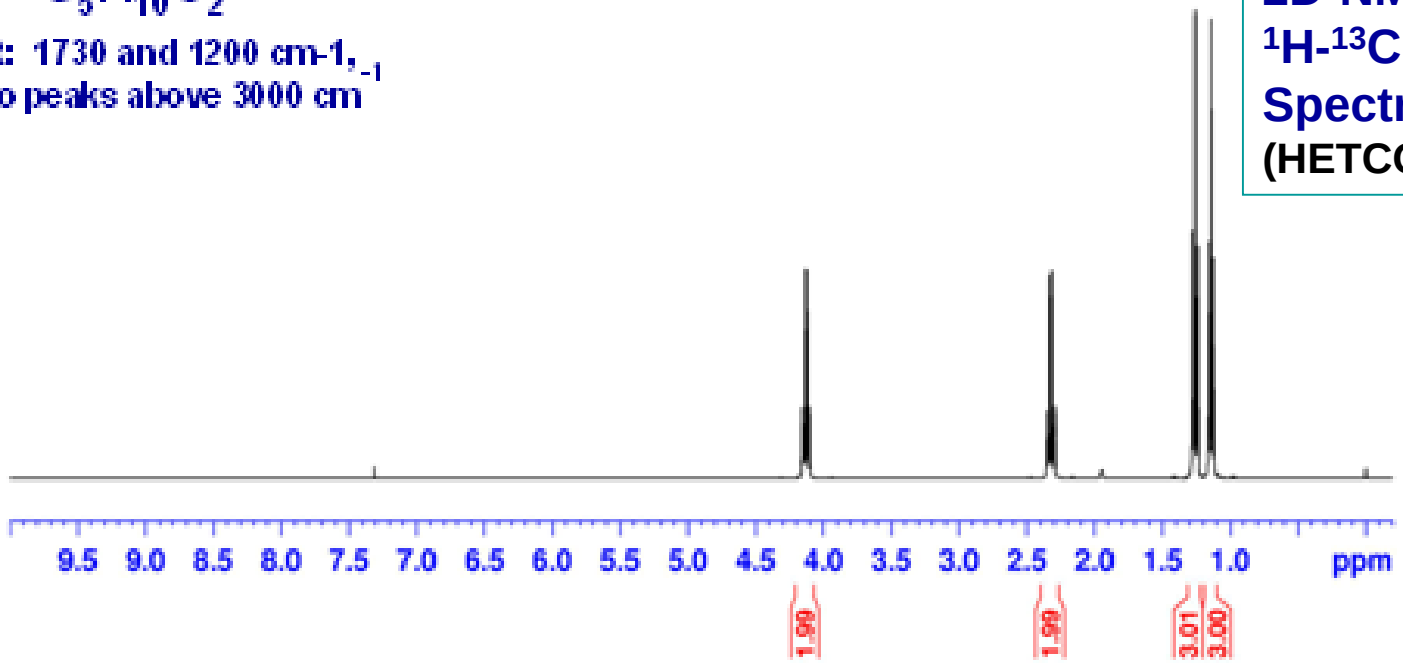
Problem - Identify where the methyl is located on the quinoline Ring and assign all protons. Show correlation lines on the COSY spectrum to support your assignments.

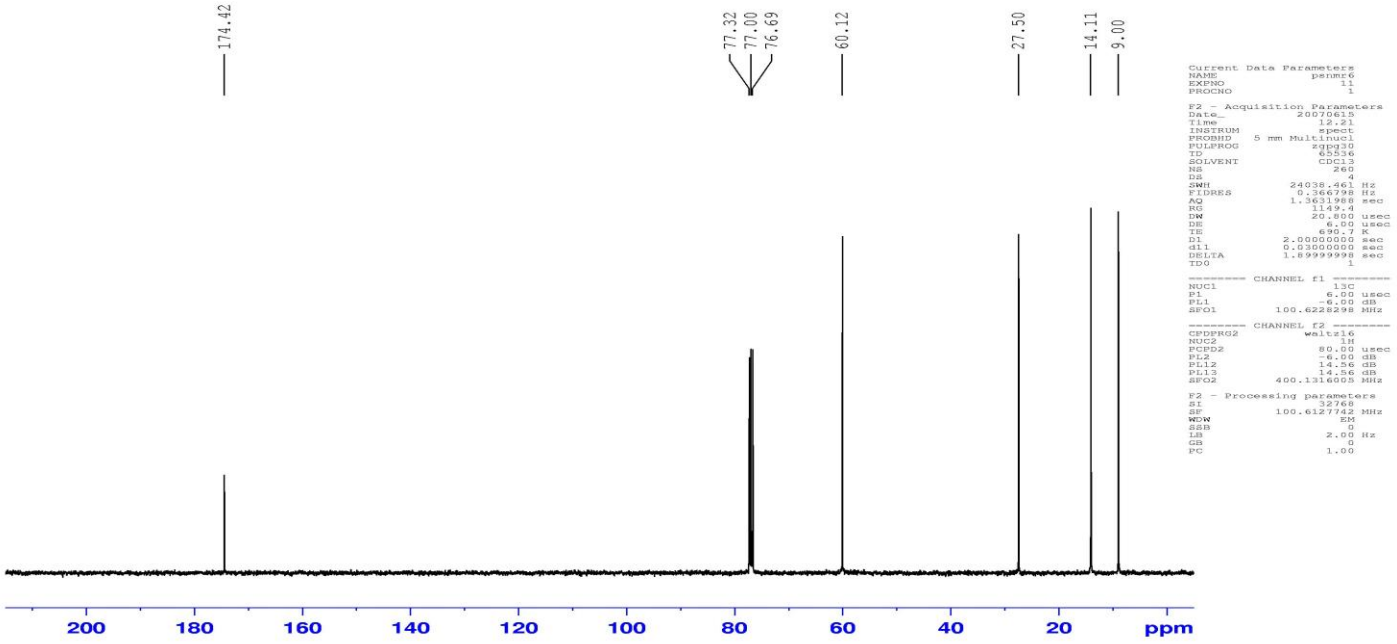


$C_5H_{10}O_2$

IR: 1730 and 1200 cm-1, no peaks above 3000 cm^{-1}

2D-NMR
^1H-^{13}C Correllation Spectroscopy
(HETCOR, HMQC, HSQC)






```
Current Data Parameters
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EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
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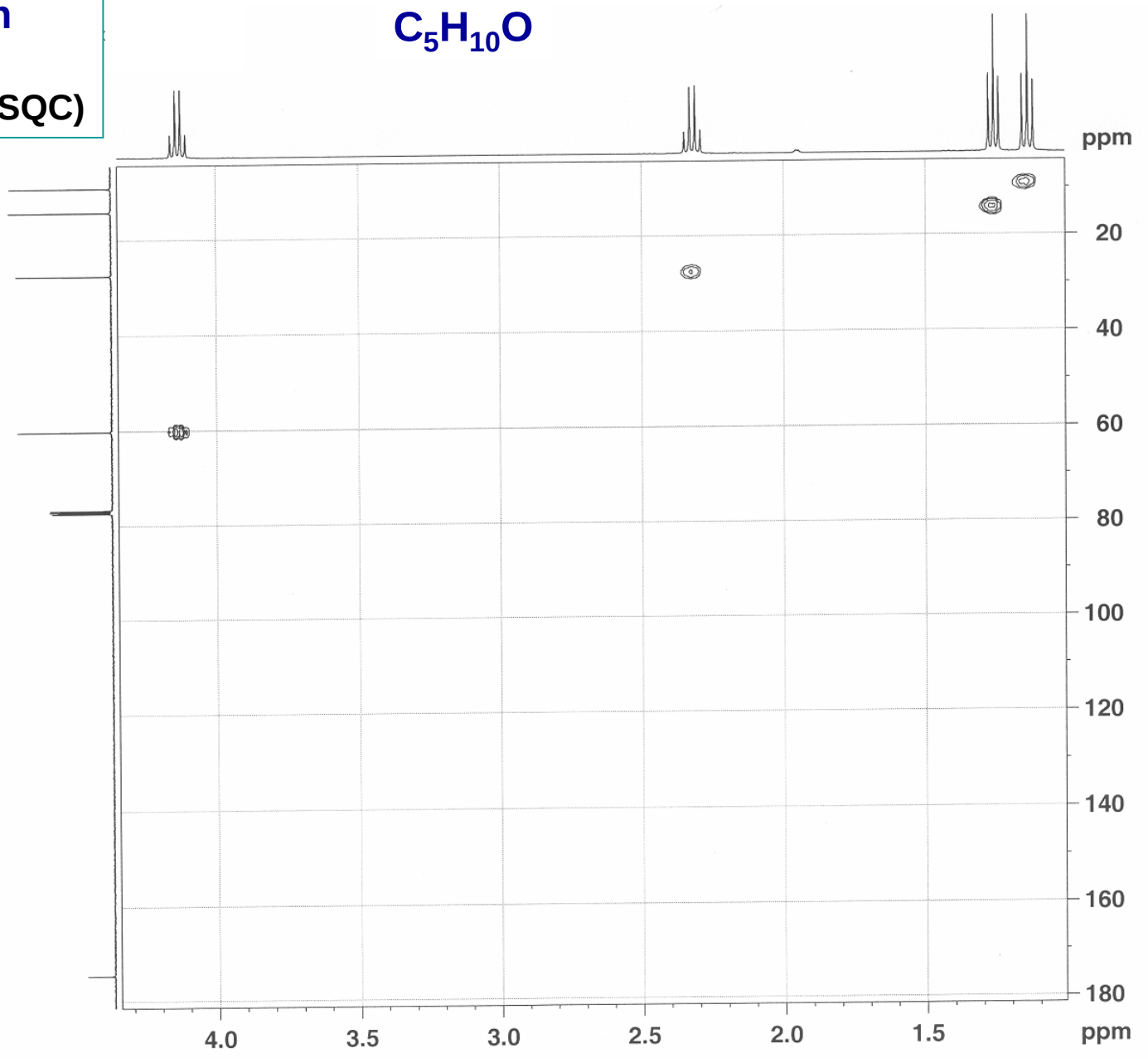
Time                  12:21
INSTRUM                spect
PROBHD   5 mm Multinucl
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     260
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                  1149.4
DW                 20.800 usec
DE                  6.00 usec
TE                 296.7 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                        1

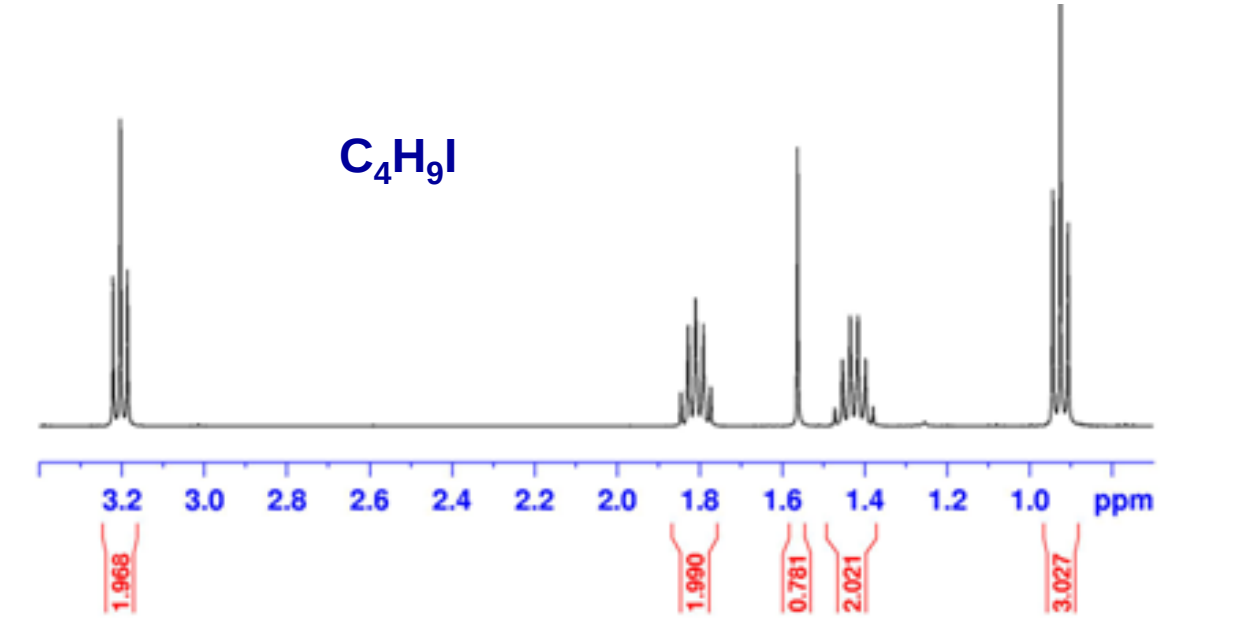
======== CHANNEL f1 ========
NUC1                     13C
P1                  6.00 usec
PL1                 -6.00 dB
SFO1          100.6228298 MHz

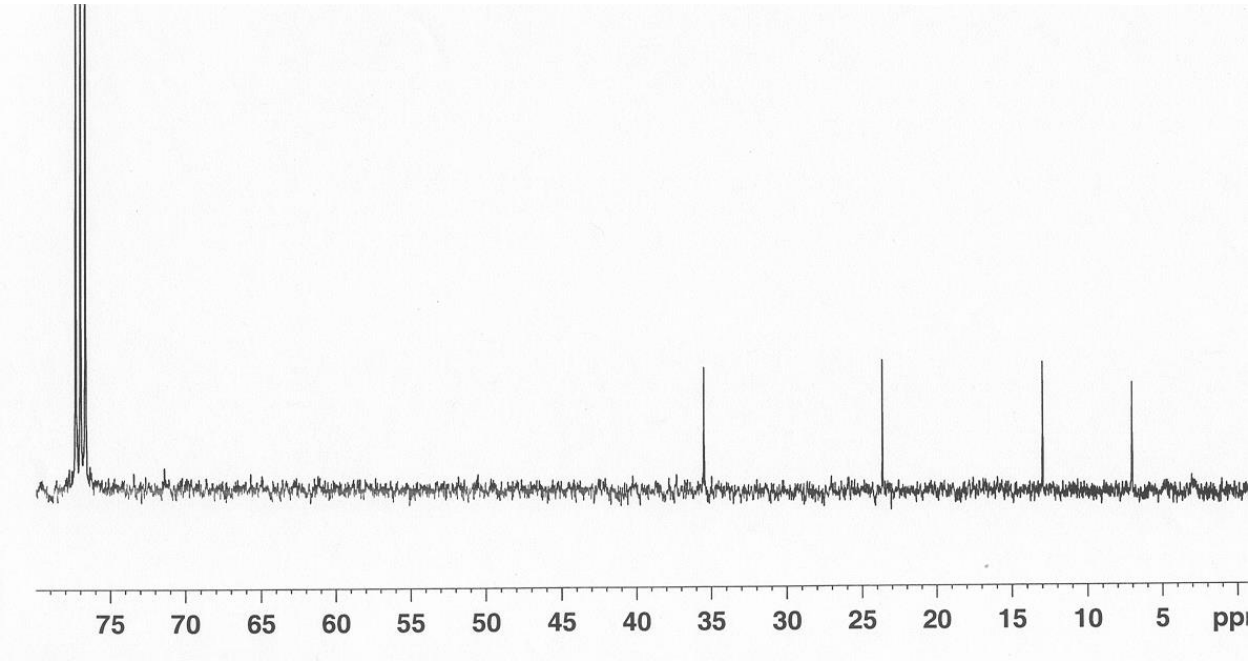
======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2               80.00 usec
PL2                 -6.00 dB
PL12                14.56 dB
PL13                14.56 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF            100.6127742 MHz
WDW                         EM
SSB                          0
LB                    2.00 Hz
GB                           0
PC                    1.00
```

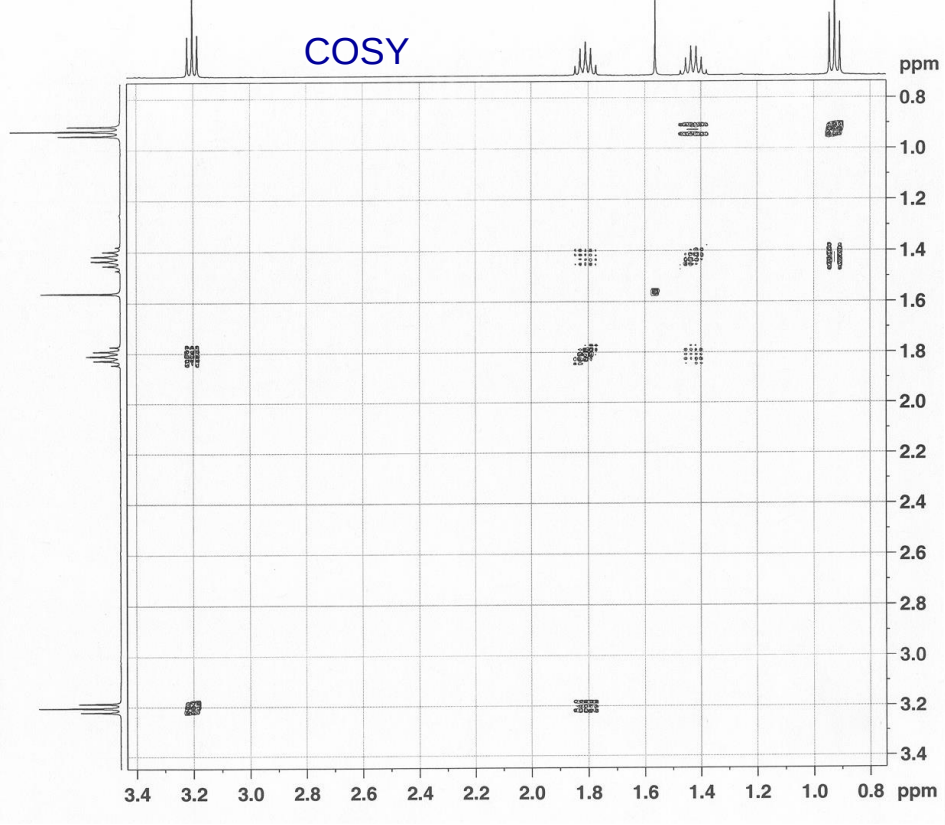
2D-NMR
^{1}H-^{13}C Correllation Spectroscopy
(HETCOR, HMQC, HSQC)




C_4H_9I
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
ppm
1.968
1.990
0.781
2.021
3.027

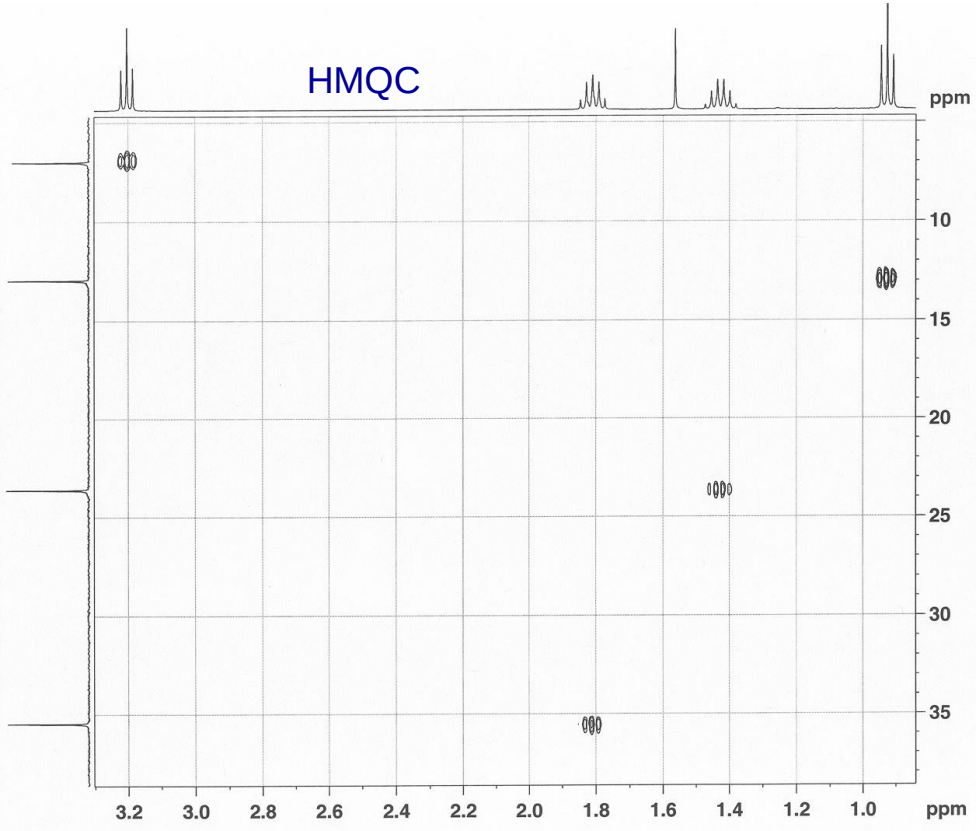

75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
ppi

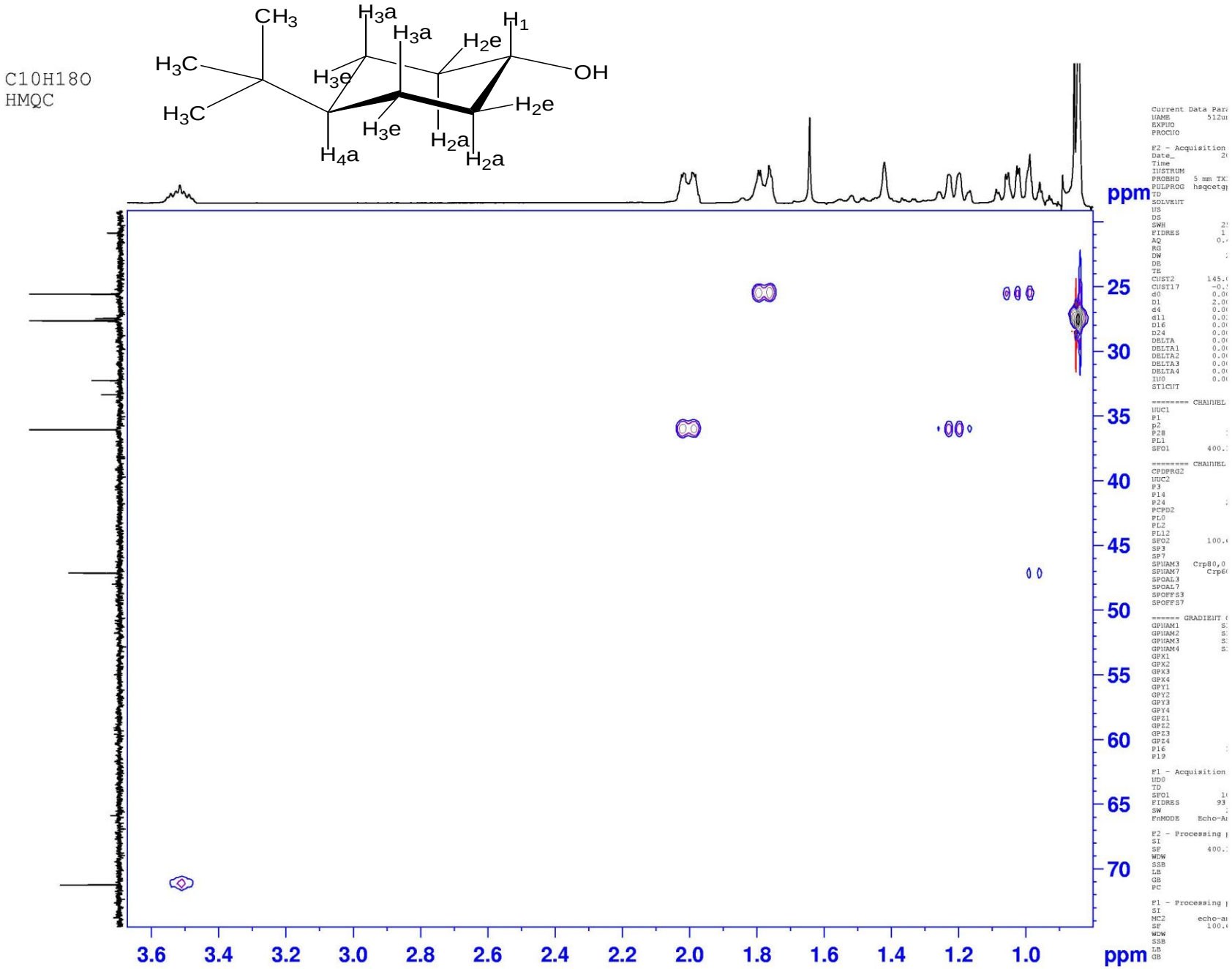
COSY



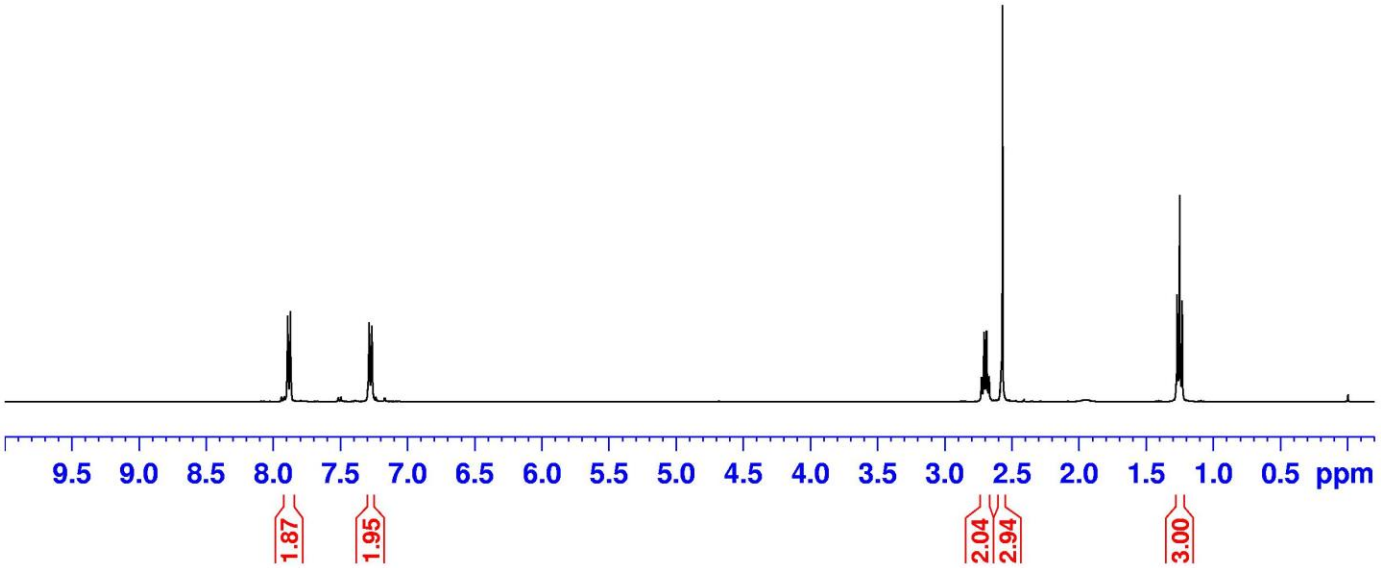
C_4H_9I

HMQC




C10H18O
HMQC
CH3
H3C
H3C
H3a
H3a
H3e
H3e
H4a
H2e
H1
OH
H2e
H2a
H2a
ppm
25
30
35
40
45
50
55
60
65
70
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
ppm

Unknown: $C_{10}H_{12}O$

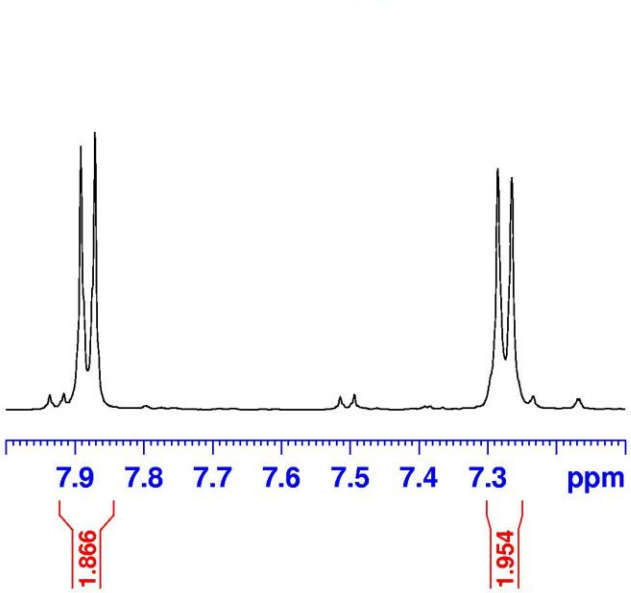


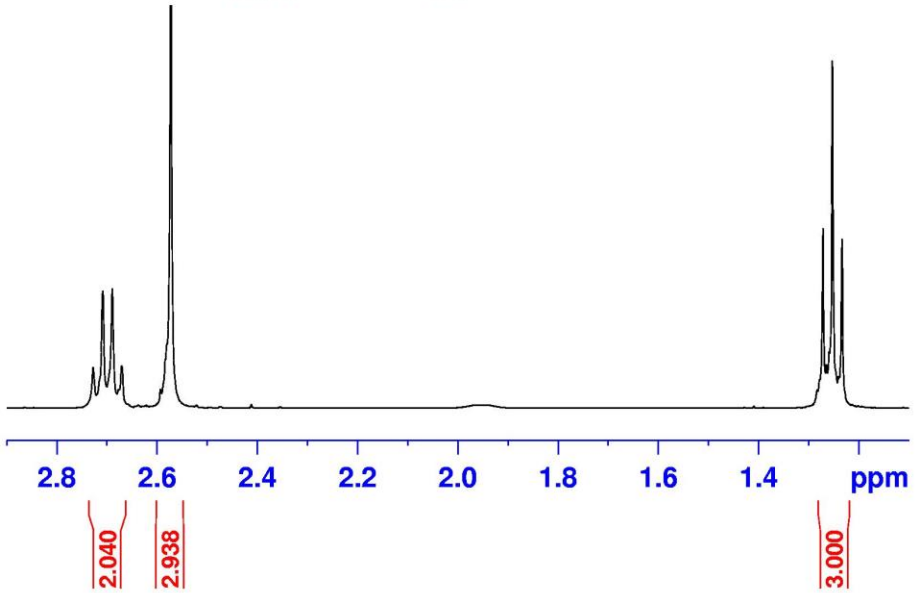

```
Current Data Parameters
NAME                  psnmr20
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20070618
Time                  17.32
INSTRUM               spect
PROBHD     5 mm Multinucl
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               5208.333 Hz
FIDRES           0.079473 Hz
AQ               6.2915058 sec
RG                      57
DW                 96.000 usec
DE                  6.00 usec
TE                  691.8 K
D1              1.00000000 sec
TD0                      1

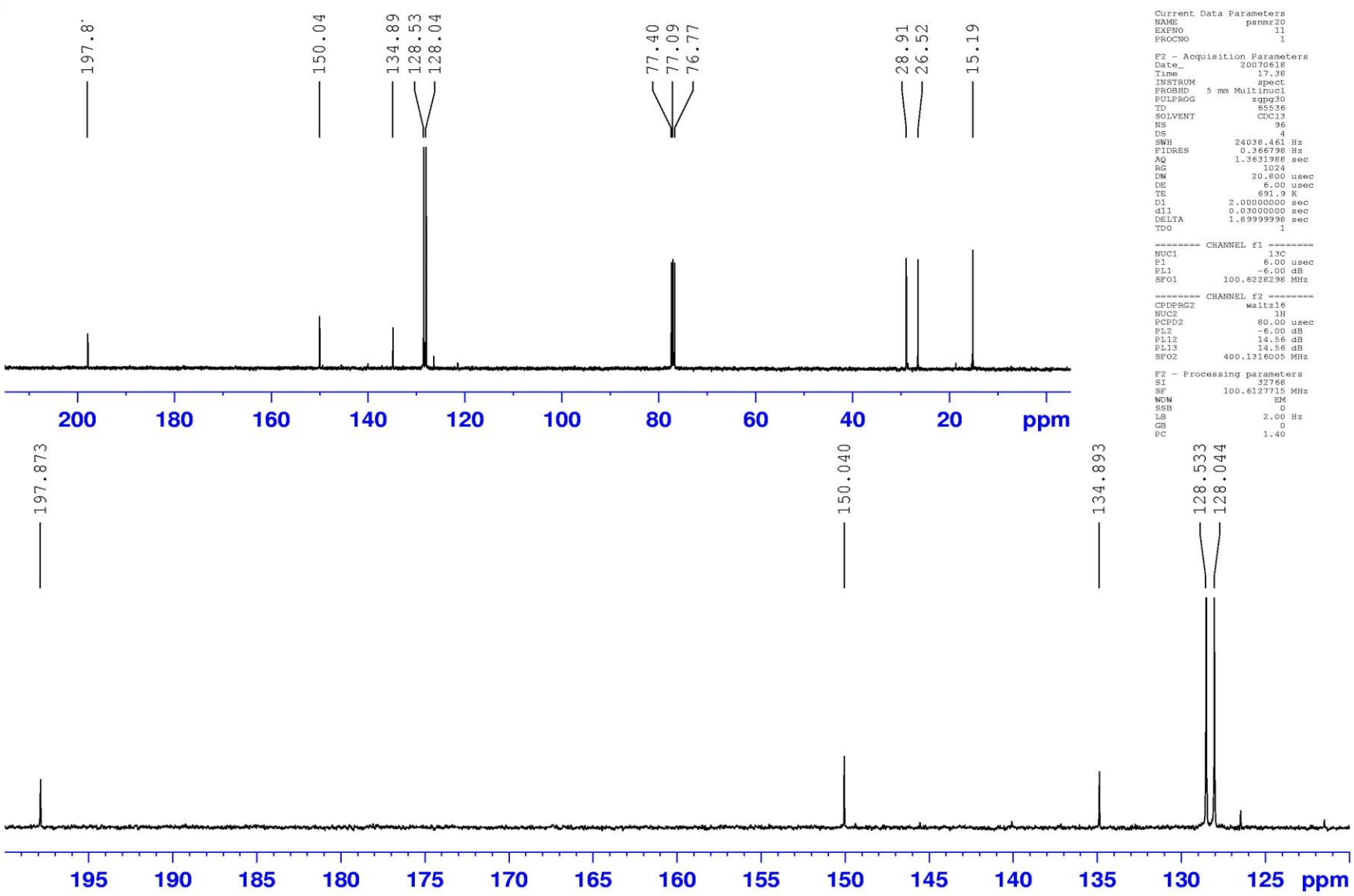
======== CHANNEL f1 ========
NUC1                    1H
P1                   7.50 usec
PL1                 -6.00 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                   32768
SF            400.1300066 MHz
WDW                     EM
SSB                      0
LB                    0.70 Hz
GB                       0
PC                    0.50
```





Unknown: $C_{10}H_{12}O$




```
Current Data Parameters
NAME                  psnmr20
EXPNO                      11
PROCNO                      1

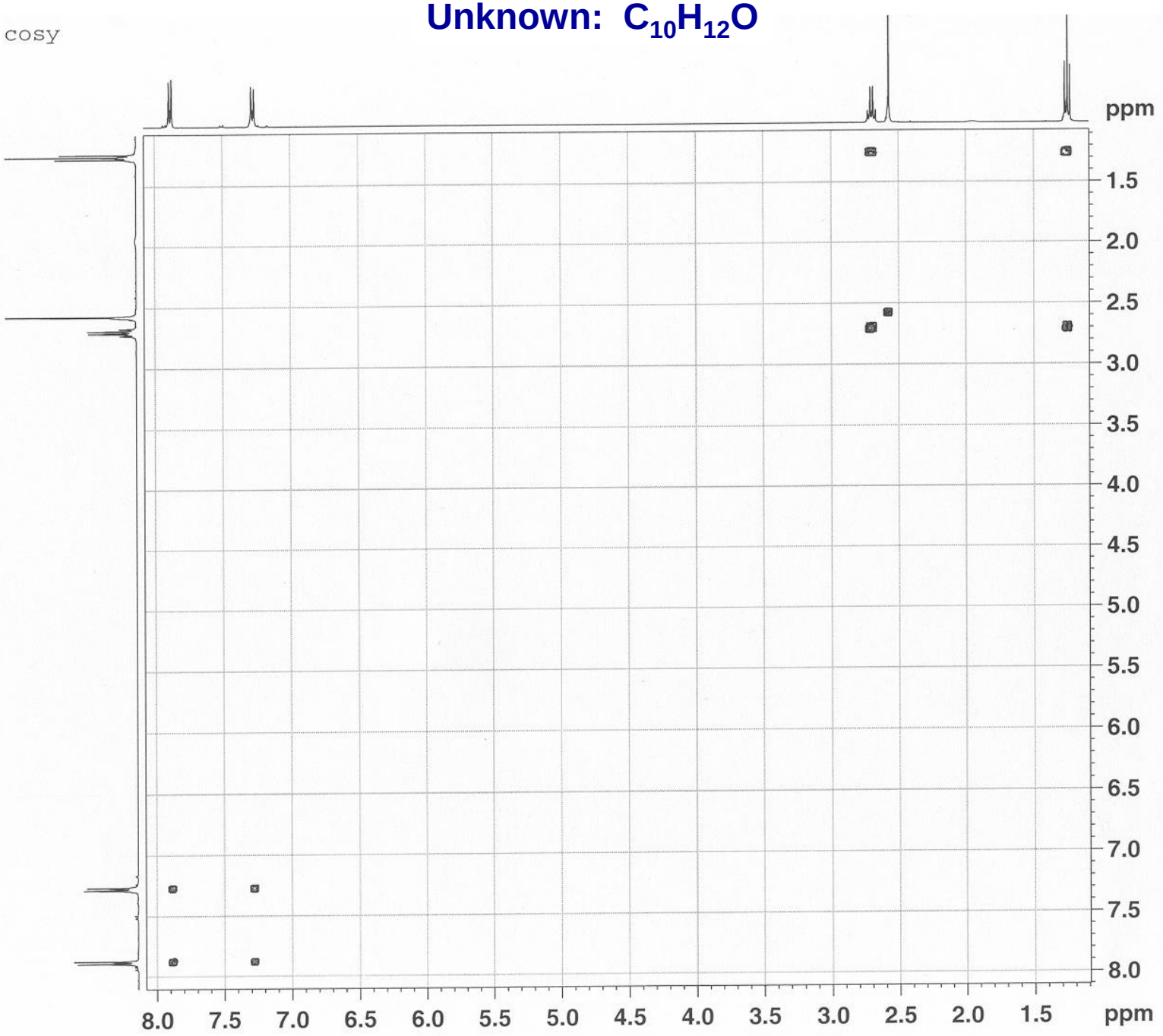
F2 - Acquisition Parameters
Date_               20070618
Time                   17.38
INSTRUM                spect
PROBHD     5 mm Multinucl
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        96
DS                         4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      1024
DW                   20.800 usec
DE                    6.00 usec
TE                   691.9 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                    6.00 usec
PL1                  -6.00 dB
SFO1            100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                  -6.00 dB
PL12                 14.56 dB
PL13                 14.56 dB
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF              100.6127715 MHz
WDW                         EM
SSB                          0
LB                    2.00 Hz
GB                           0
PC                        1.40
```

Unknown: $C_{10}H_{12}O$



Unknown: $C_{10}H_{12}O$