Microbial Biotransformation of the Sesquiterpene Carotol: Generation of Hydroxylated Metabolites with Potential Cytotoxic and Target-Specific Binding Activities

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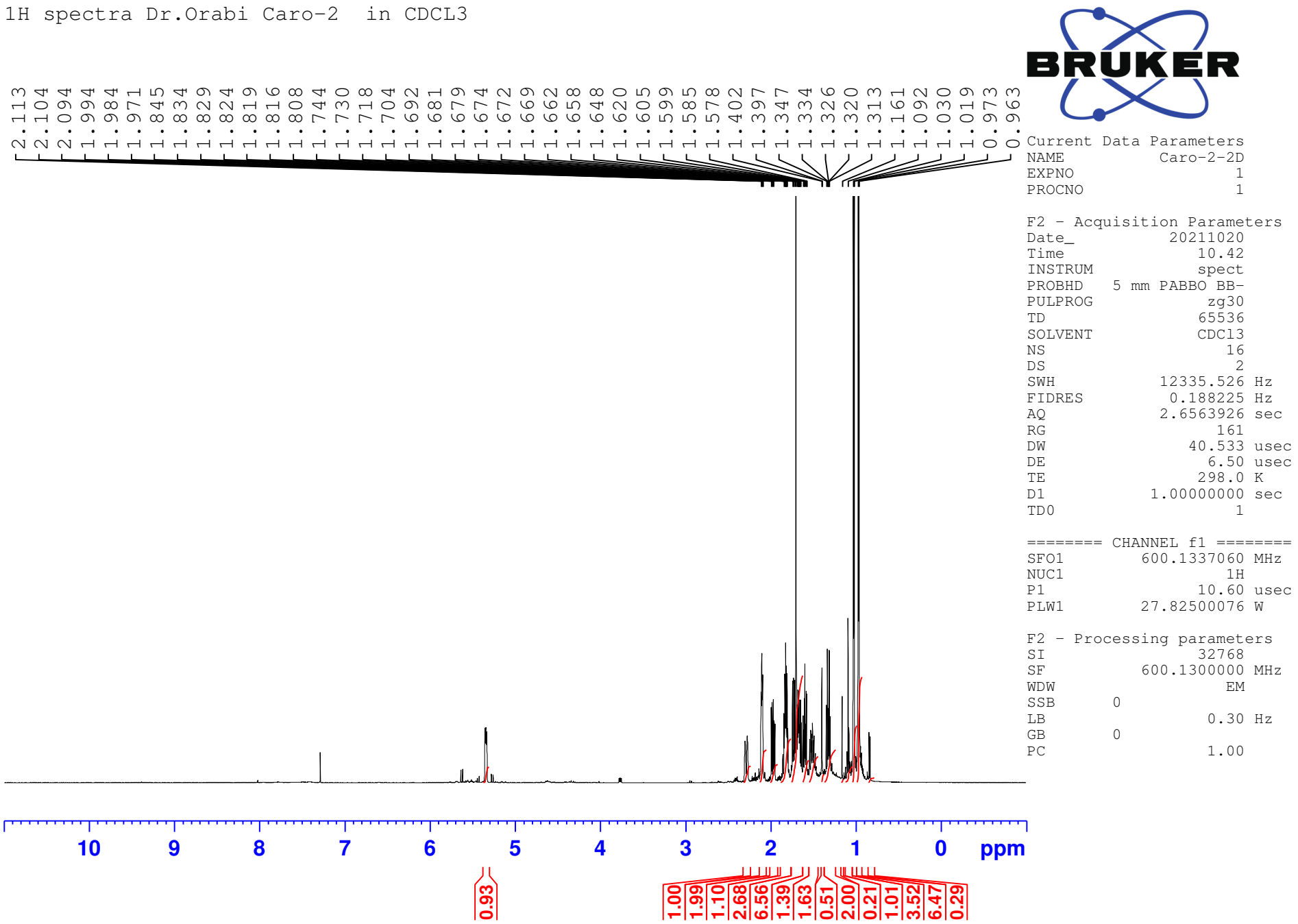
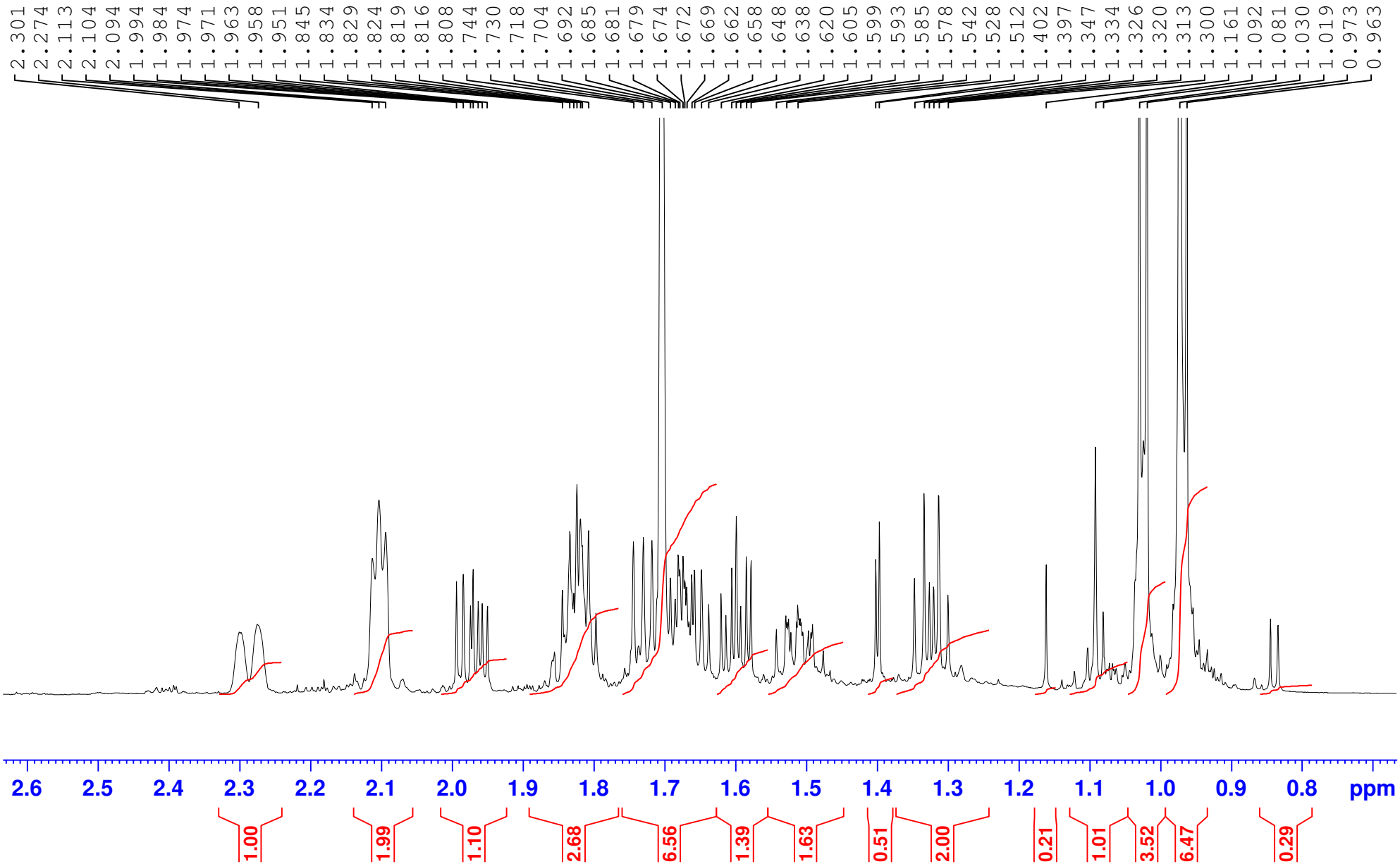
CONTENTS

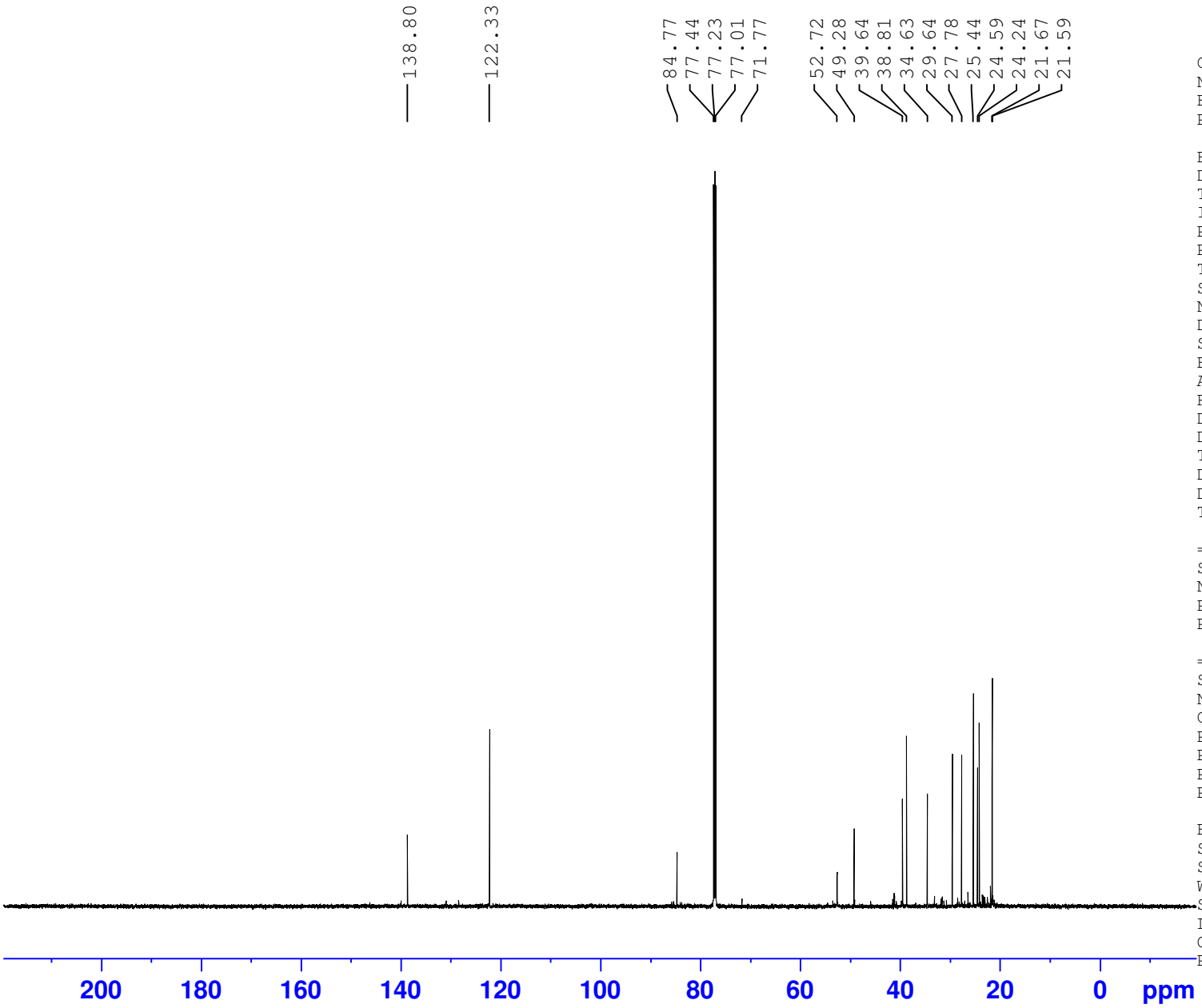
S1: ^{1}H, ^{13}C, DEPT-135, HSQC, HMBC and COSY spectra of carotol (**1**)



1H spectra Dr.Orabi Caro-2 in CDCL3



13C decoupled spectra Dr.Orabi Caro-2 in CDCL3



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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
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FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 150.9178979 MHz
NUC1 13C
P1 8.80 usec
PLW1 78.13500214 W

======== CHANNEL f2 ========
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W
PLW13 0.32093000 W

F2 - Processing parameters
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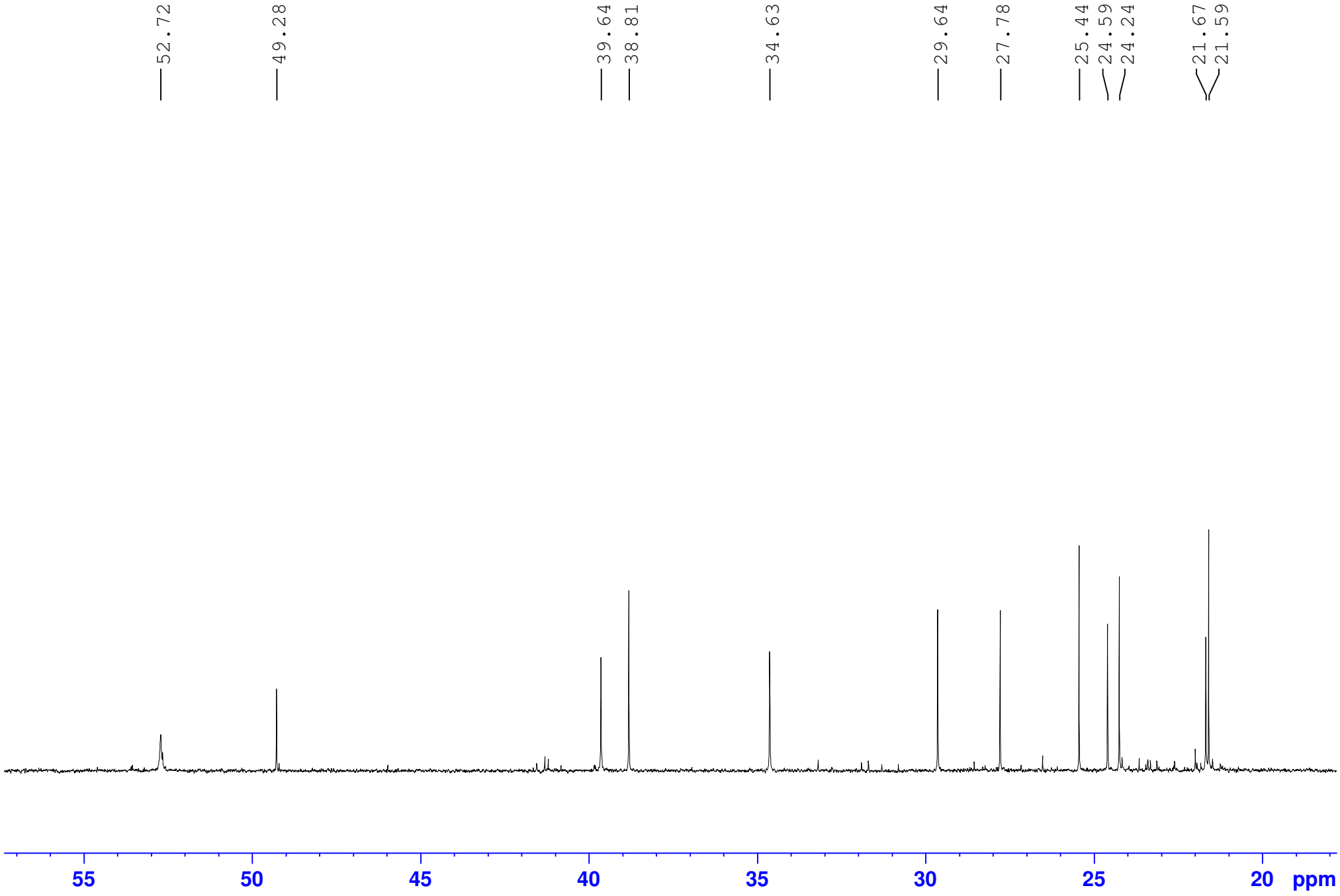
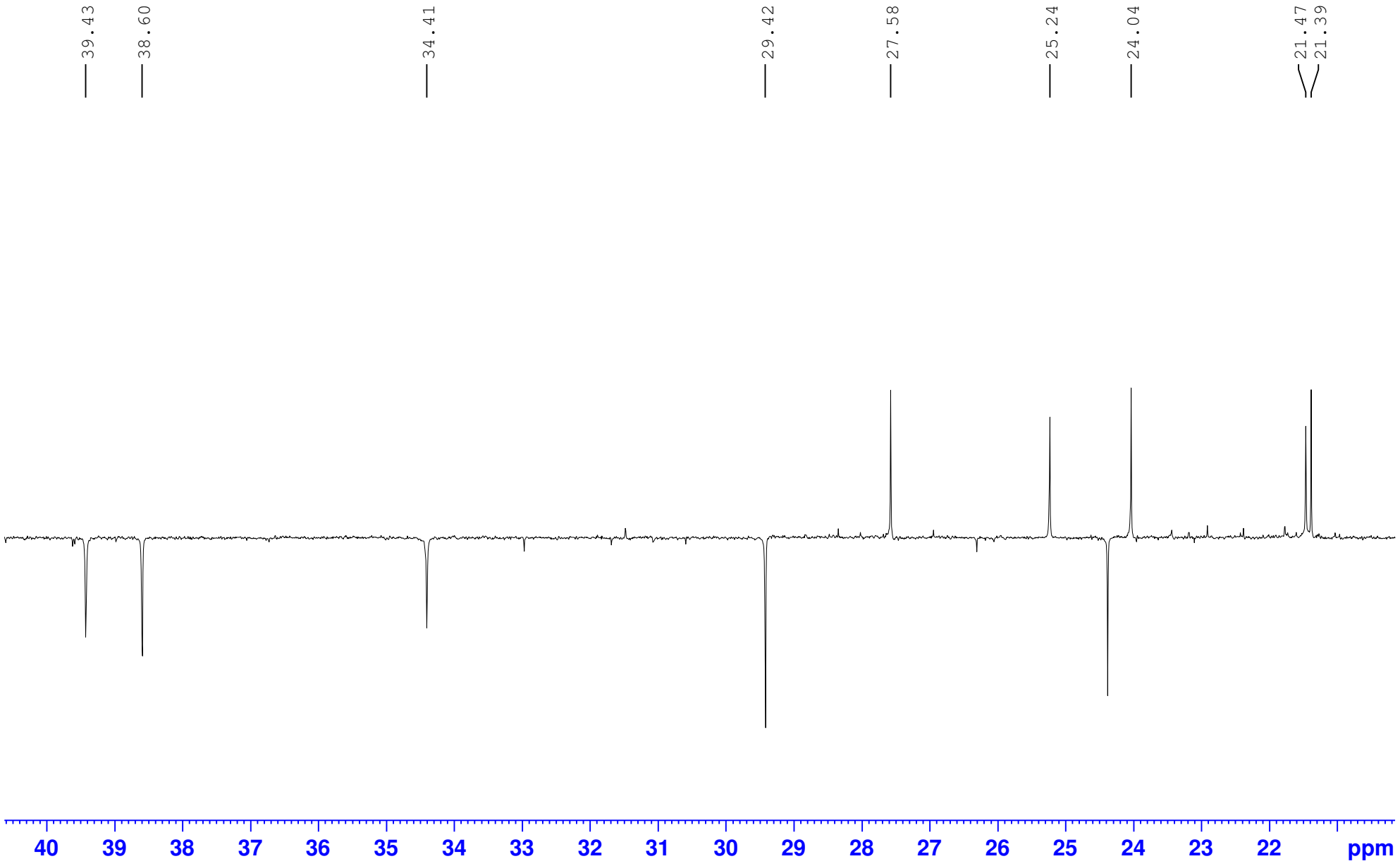
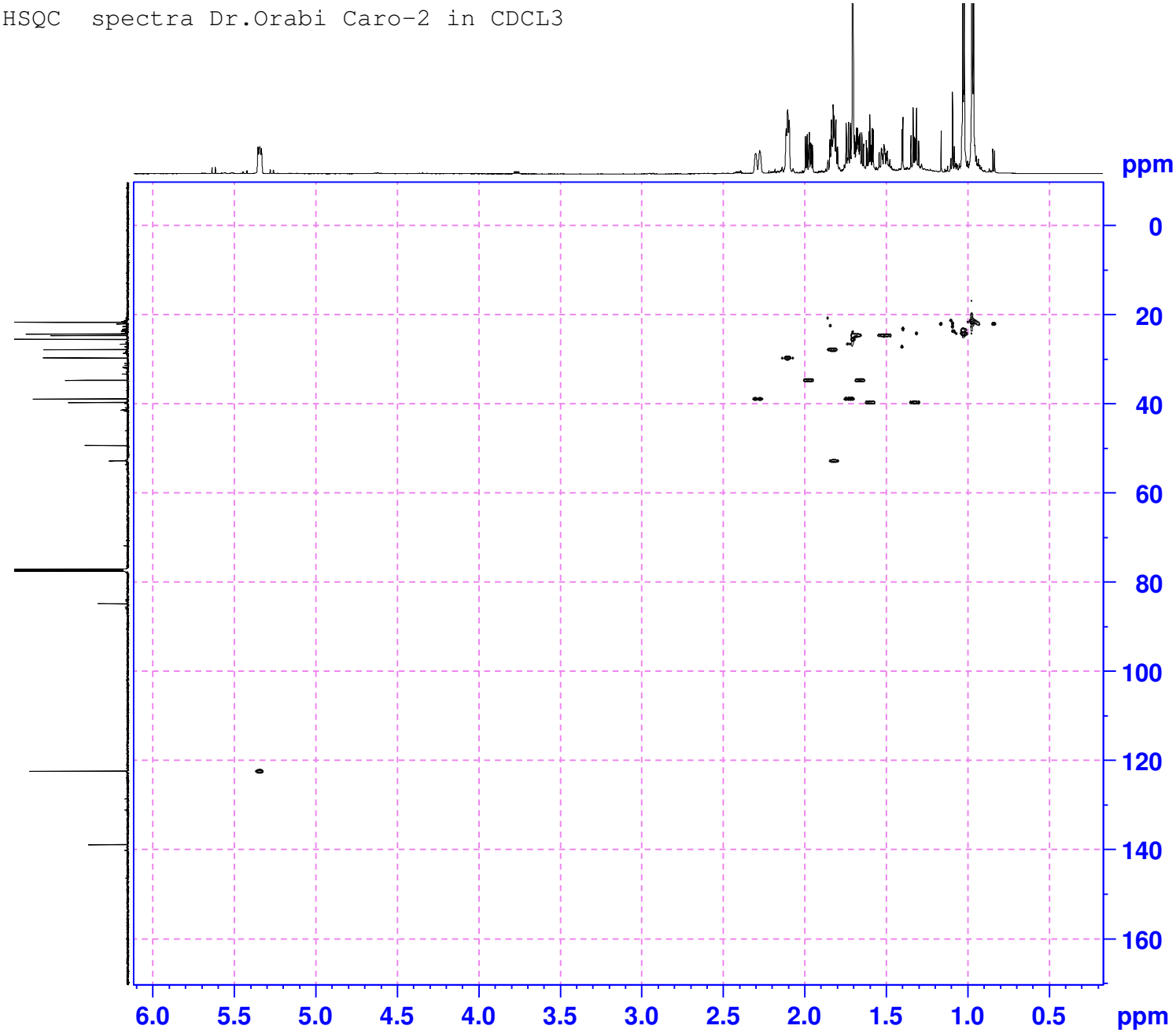
13C decoupled spectra Dr.Orabi Caro-2 in CDCL3



DEPT 135 spectra Dr.Orabi Caro-1 in CDCL3



13C HSQC spectra Dr.Orabi Caro-2 in CDCL3



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EXPNO                   4
PROCNO                  1

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Time               5.26
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG   hsqcetgpsp.2
TD                 2048
SOLVENT            CDCl3
NS                    8
DS                   16
SWH             3571.428 Hz
FIDRES          1.743862 Hz
AQ              0.2867200 sec
RG                  203
DW               140.000 usec
DE                6.50 usec
TE                298.5 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.81977606 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
IN0           0.00001840 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1         600.1318862 MHz
NUC1                1H
P1                10.60 usec
P2                21.20 usec
P28             1000.00 usec
PLW1         27.82500076 W

======== CHANNEL f2 ========
SFO2         150.9148803 MHz
NUC2                13C
CPDPRG[2            garp4
P3                 8.80 usec
P14              500.00 usec
P24             2000.00 usec
PCPD2             60.00 usec
PLW0      0 W
PLW2         78.13500214 W
PLW12         1.68079996 W
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SPW3          9.24489975 W
SPNAM[7]     Crp60comp.4
SPOAL7             0.500
SPOFFS7   0 Hz
SPW7          9.24489975 W

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GPNAM[2]         SINE.100
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GPZ2                20.10 %
P16               1000.00 usec

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SW               180.061 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  2048
SF            600.1300000 MHz
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SSB                     2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
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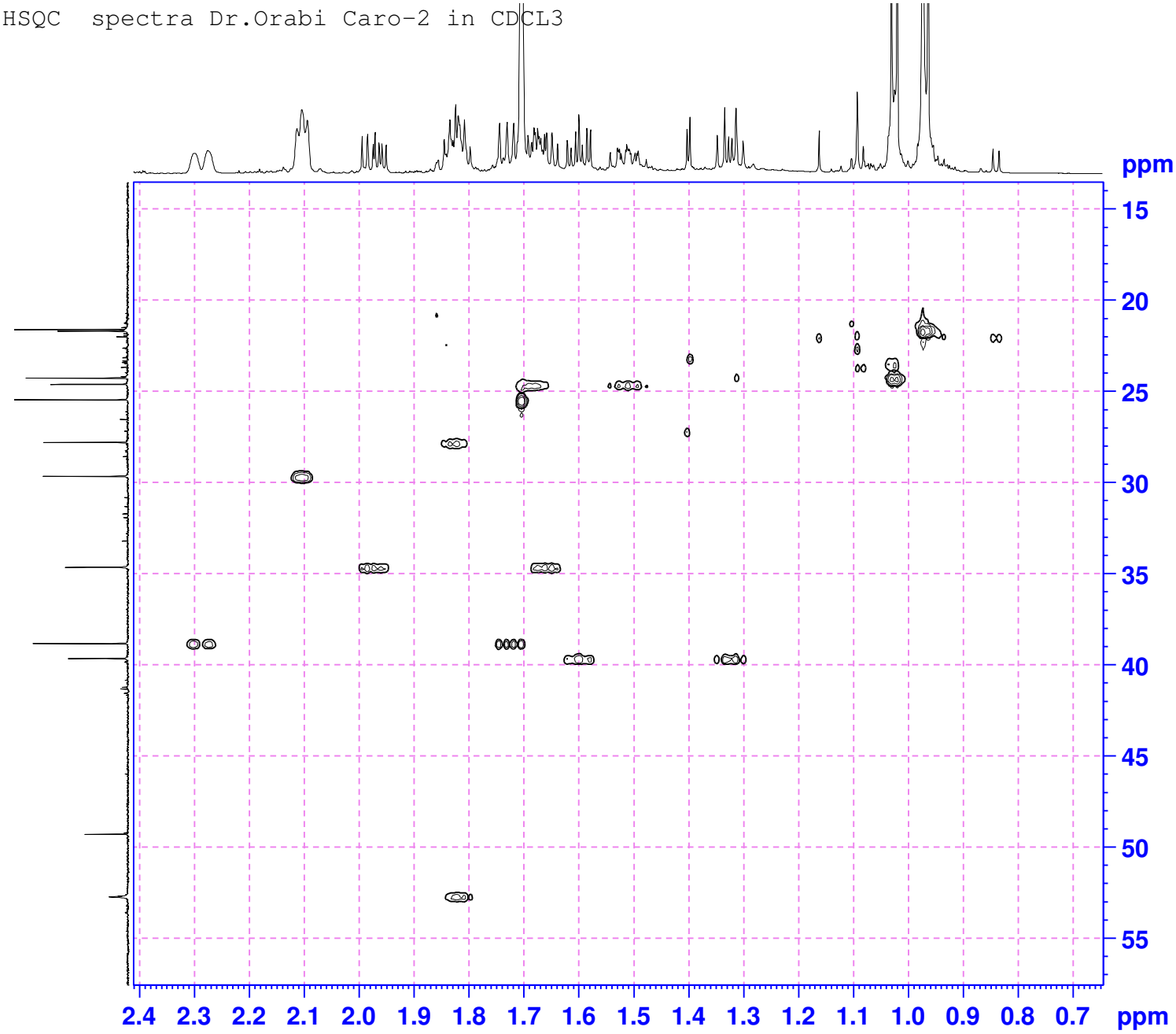

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Current Data Parameters
NAME            Caro-2-2D
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20211021
Time                5.26
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG    hsqcetgpsp.2
TD                  2048
SOLVENT            CDCl3
NS                     8
DS                    16
SWH             3571.428 Hz
FIDRES          1.743862 Hz
AQ              0.2867200 sec
RG                   203
DW               140.000 usec
DE                 6.50 usec
TE                298.5 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.81977606 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
IN0           0.00001840 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1         600.1318862 MHz
NUC1                1H
P1                10.60 usec
P2                21.20 usec
P28             1000.00 usec
PLW1         27.82500076 W

======== CHANNEL f2 ========
SFO2         150.9148803 MHz
NUC2                13C
CPDPRG[2           garp4
P3                 8.80 usec
P14              500.00 usec
P24             2000.00 usec
PCPD2             60.00 usec
PLW0      0 W
PLW2         78.13500214 W
PLW12         1.68079996 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3             0.500
SPOFFS3   0 Hz
SPW3          9.24489975 W
SPNAM[7]     Crp60comp.4
SPOAL7             0.500
SPOFFS7   0 Hz
SPW7          9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]         SINE.100
GPNAM[2]         SINE.100
GPZ1               80.00 %
GPZ2               20.10 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   512
SFO1            150.9149 MHz
FIDRES         53.074047 Hz
SW              180.061 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  2048
SF           600.1300000 MHz
WDW                QSINE
SSB                    2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           150.9027685 MHz
WDW                QSINE
SSB                    2
LB        0 Hz
GB        0
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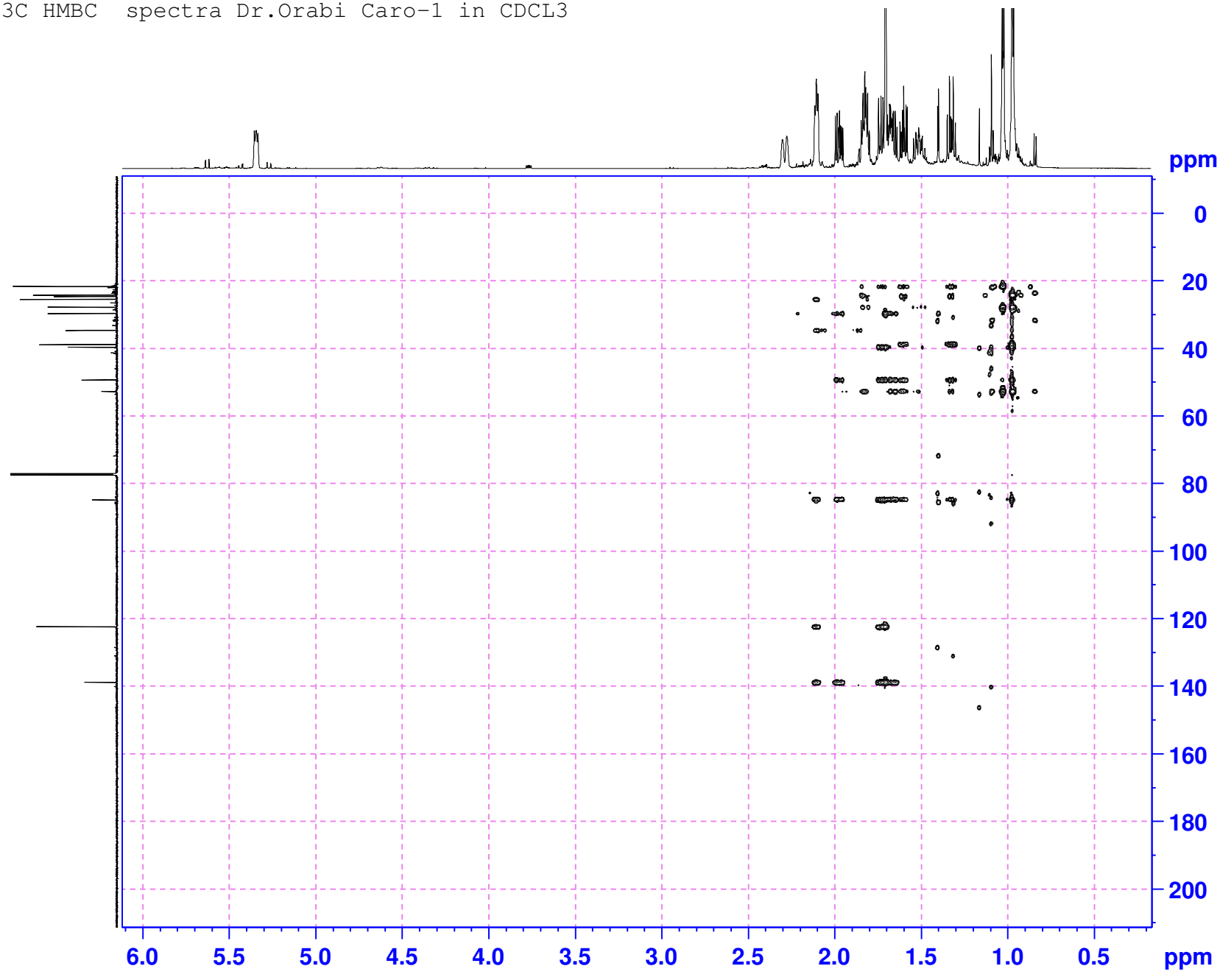
13C HMBC spectra Dr.Orabi Caro-1 in CDCL3

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Current Data Parameters
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PROCNO                        1

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Date_                  20211021
Time                       7.55
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG     hmbcetgp12nd
TD                         2048
SOLVENT                   CDCl3
NS                           32
DS                           16
SWH                  3571.428 Hz
FIDRES               1.743862 Hz
AQ                   0.2867200 sec
RG                         203
DW                   140.000 usec
DE                     6.50 usec
TE                     297.9 K
CNST6               125.0000000
CNST7               165.0000000
CNST13               10.0000000
CNST30                0.5981148
D0                   0.00000300 sec
D1                   1.34435201 sec
D6                   0.05000000 sec
D16                  0.00020000 sec
IN0                  0.00001490 sec

======== CHANNEL f1 ========
SFO1                600.1318862 MHz
NUC1                        1H
P1                       10.60 usec
P2                       21.20 usec
PLW1                27.82500076 W

======== CHANNEL f2 ========
SFO2                150.9178738 MHz
NUC2                        13C
P3                        8.80 usec
P24                    2000.00 usec
PLW2                78.13500214 W
SPNAM[7]            Crp60comp.4
SPOAL7                    0.500
SPOFFS7   0 Hz
SPW7                 9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]              SINE.100
GPNAM[3]              SINE.100
GPNAM[4]              SINE.100
GPNAM[5]              SINE.100
GPZ1                     80.00 %
GPZ3                     15.00 %
GPZ4                    -10.00 %
GPZ5                     -5.00 %
P16                    1000.00 usec

F1 - Acquisition parameters
TD                         256
SFO1                150.9179 MHz
FIDRES              131.082214 Hz
SW                    222.353 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                         2048
SF                  600.1300000 MHz
WDW                        SINE
SSB       0
LB        0 Hz
GB        0
PC                        1.40

F1 - Processing parameters
SI                          512
MC2          echo-antiecho
SF                  150.9027541 MHz
WDW                        SINE
SSB                           2
LB        0 Hz
GB        0
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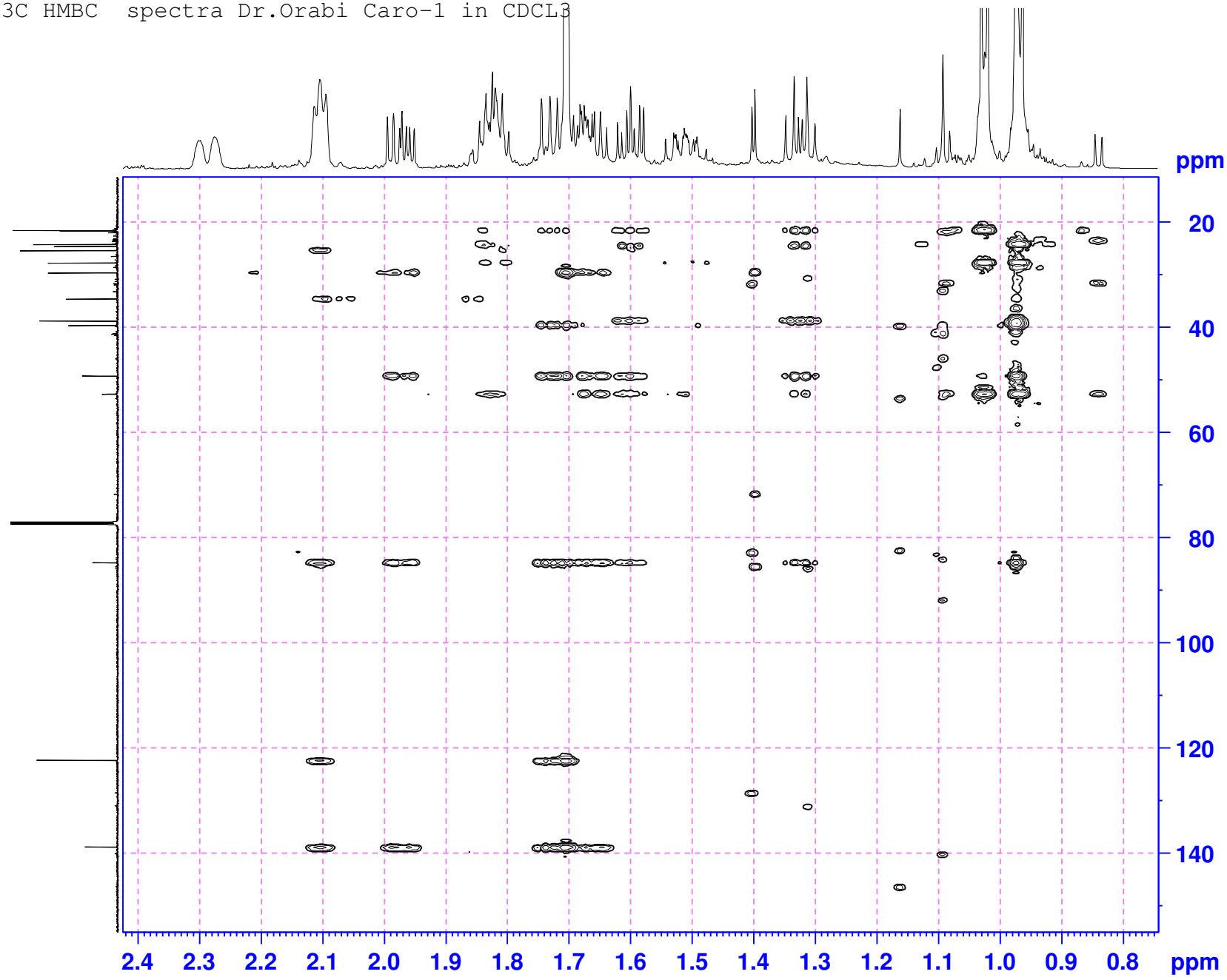
13C HMBC spectra Dr.Orabi Caro-1 in CDCL3



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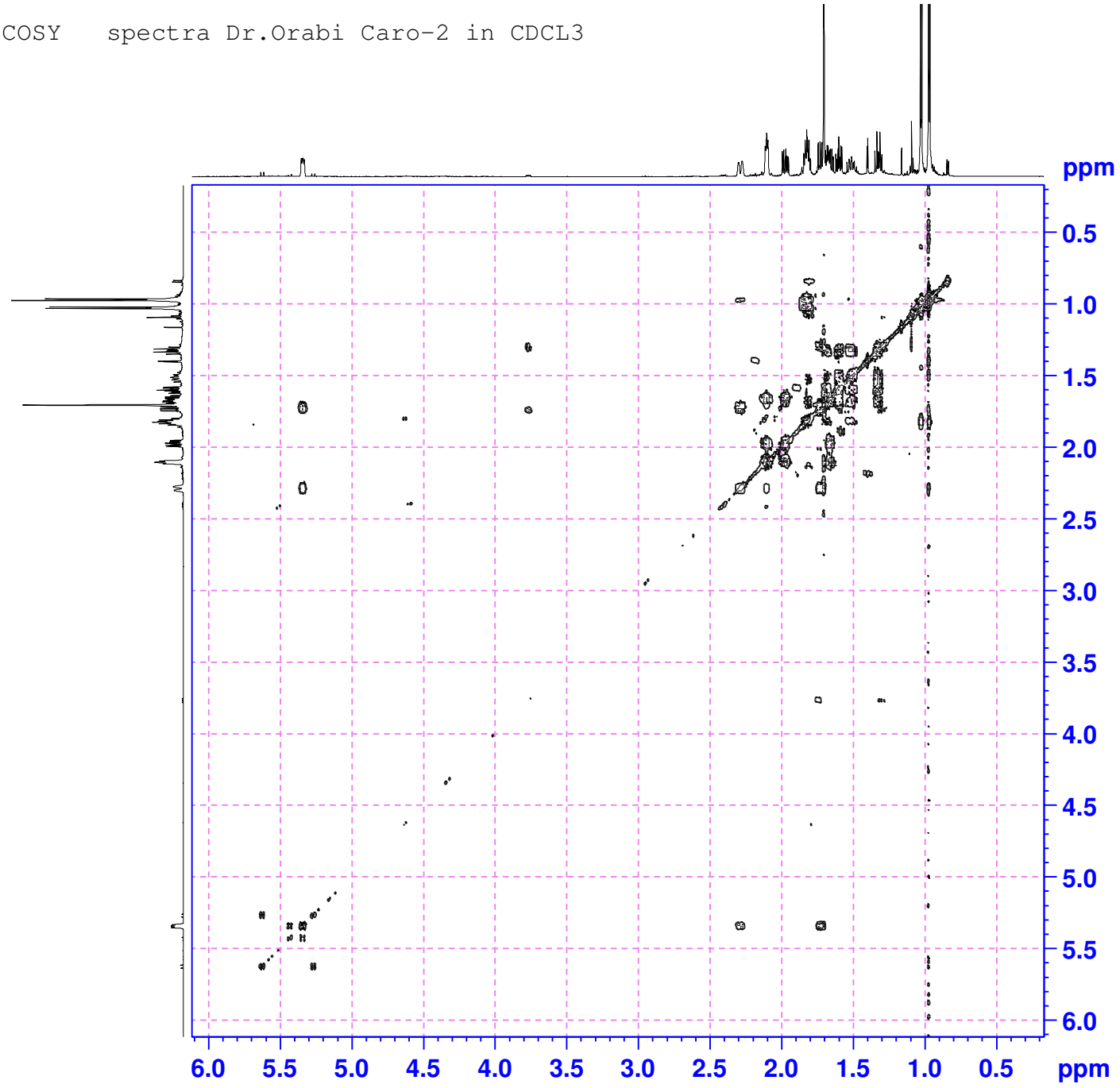
```
Current Data Parameters
NAME                  Caro-2-2D
EXPNO                         5
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20211021
Time                       7.55
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG     hmbcetgp12nd
TD                         2048
SOLVENT                   CDCl3
NS                           32
DS                           16
SWH                  3571.428 Hz
FIDRES               1.743862 Hz
AQ                   0.2867200 sec
RG                         203
DW                   140.000 usec
DE                     6.50 usec
TE                     297.9 K
CNST6               125.0000000
CNST7               165.0000000
CNST13               10.0000000
CNST30                0.5981148
D0                   0.00000300 sec
D1                   1.34435201 sec
D6                   0.05000000 sec
D16                  0.00020000 sec
IN0                  0.00001490 sec

======== CHANNEL f1 ========
SFO1                600.1318862 MHz
NUC1                        1H
P1                       10.60 usec
P2                       21.20 usec
PLW1                27.82500076 W

======== CHANNEL f2 ========
SFO2                150.9178738 MHz
NUC2                        13C
P3                        8.80 usec
P24                    2000.00 usec
PLW2                78.13500214 W
SPNAM[7]            Crp60comp.4
SPOAL7                    0.500
SPOFFS7   0 Hz
SPW7                 9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]               SINE.100
GPNAM[3]               SINE.100
GPNAM[4]               SINE.100
GPNAM[5]               SINE.100
GPZ1                      80.00 %
GPZ3                      15.00 %
GPZ4                     -10.00 %
GPZ5                      -5.00 %
P16                    1000.00 usec

F1 - Acquisition parameters
TD                           256
SFO1                150.9179 MHz
FIDRES               131.082214 Hz
SW                     222.353 ppm
FnMODE          Echo-Antiecho

F2 - Processing parameters
SI                         2048
SF                  600.1300000 MHz
WDW                        SINE
SSB          0
LB           0 Hz
GB           0
PC                         1.40

F1 - Processing parameters
SI                          512
MC2              echo-antiecho
SF                  150.9027541 MHz
WDW                        SINE
SSB                           2
LB           0 Hz
GB           0
```

COSY spectra Dr.Orabi Caro-2 in CDCL3



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Current Data Parameters
NAME            Caro-2-2D
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20211021
Time                5.01
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                      4
DS                      8
SWH              3571.428 Hz
FIDRES           1.743862 Hz
AQ               0.2867200 sec
RG                   90.5
DW                140.000 usec
DE                  6.50 usec
TE                 298.0 K
D0               0.00000300 sec
D1               0.59107488 sec
D11              0.03000000 sec
D12              0.00002000 sec
D13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00028000 sec

======== CHANNEL f1 ========
SFO1          600.1318862 MHz
NUC1                  1H
P0                 10.60 usec
P1                 10.60 usec
P17              2500.00 usec
PLW1          27.82500076 W
PLW10          5.00229979 W

====== GRADIENT CHANNEL =====
GPNAM[1]         SINE.100
GPZ1                20.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    320
SFO1             600.1319 MHz
FIDRES          11.160714 Hz
SW                  5.951 ppm
FnMODE                QF

F2 - Processing parameters
SI                   2048
SF            600.1300000 MHz
WDW                  SINE
SSB       0
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                   2048
MC2                    QF
SF            600.1300000 MHz
WDW                  SINE
SSB       0
LB        0 Hz
GB        0
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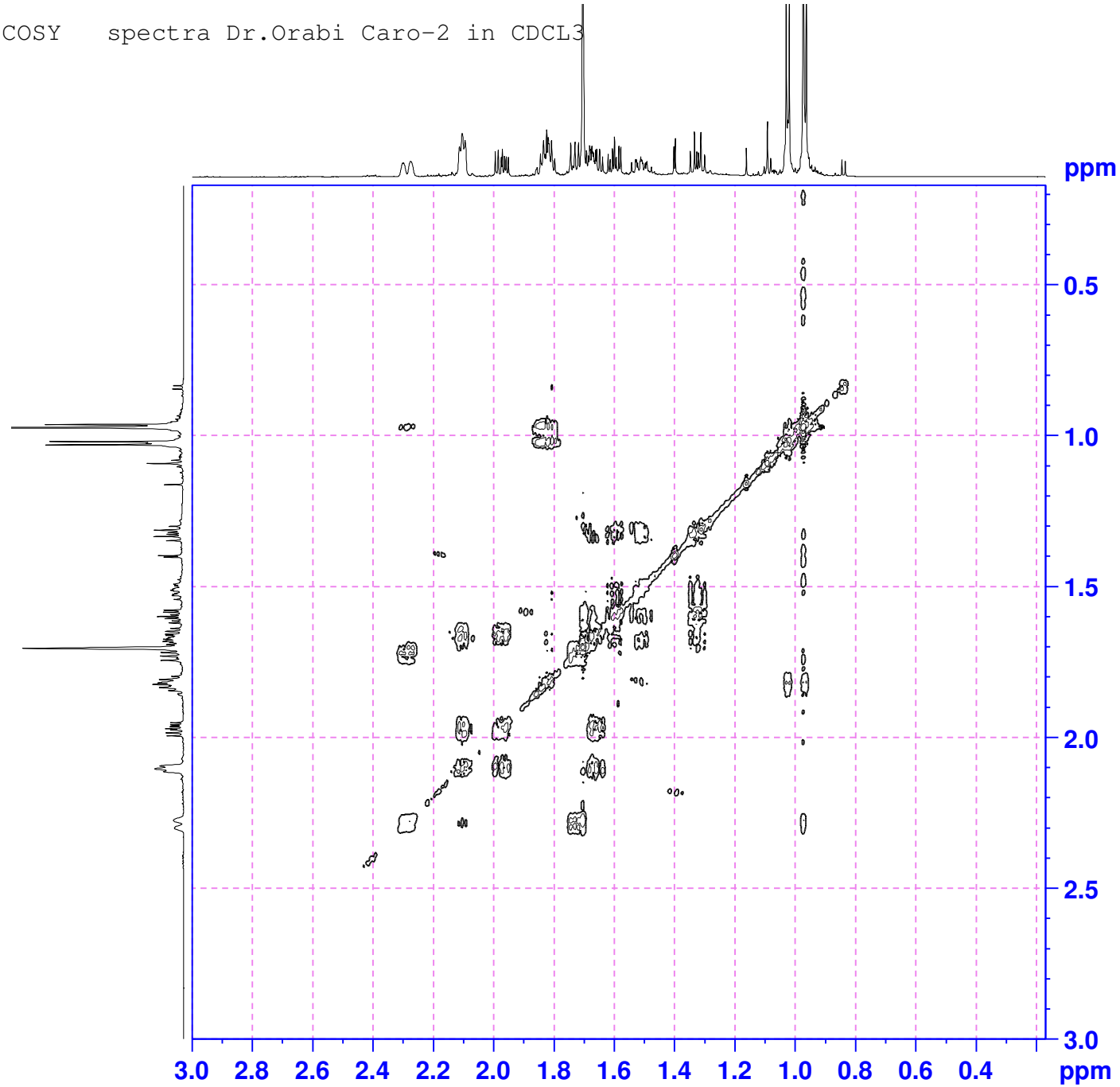
COSY spectra Dr.Orabi Caro-2 in CDCL3



Current Data Parameters
NAME Caro-2-2D
EXPNO 3
PROCNO 1

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INSTRUM spect
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PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 3571.428 Hz
FIDRES 1.743862 Hz
AQ 0.2867200 sec
RG 90.5
DW 140.000 usec
DE 6.50 usec
TE 298.0 K
D0 0.00000300 sec
D1 0.59107488 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00028000 sec

======== CHANNEL f1 ========
SFO1 600.1318862 MHz
NUC1 1H
P0 10.60 usec
P1 10.60 usec
P17 2500.00 usec
PLW1 27.82500076 W
PLW10 5.00229979 W

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPZ1 20.00 %
P16 1000.00 usec

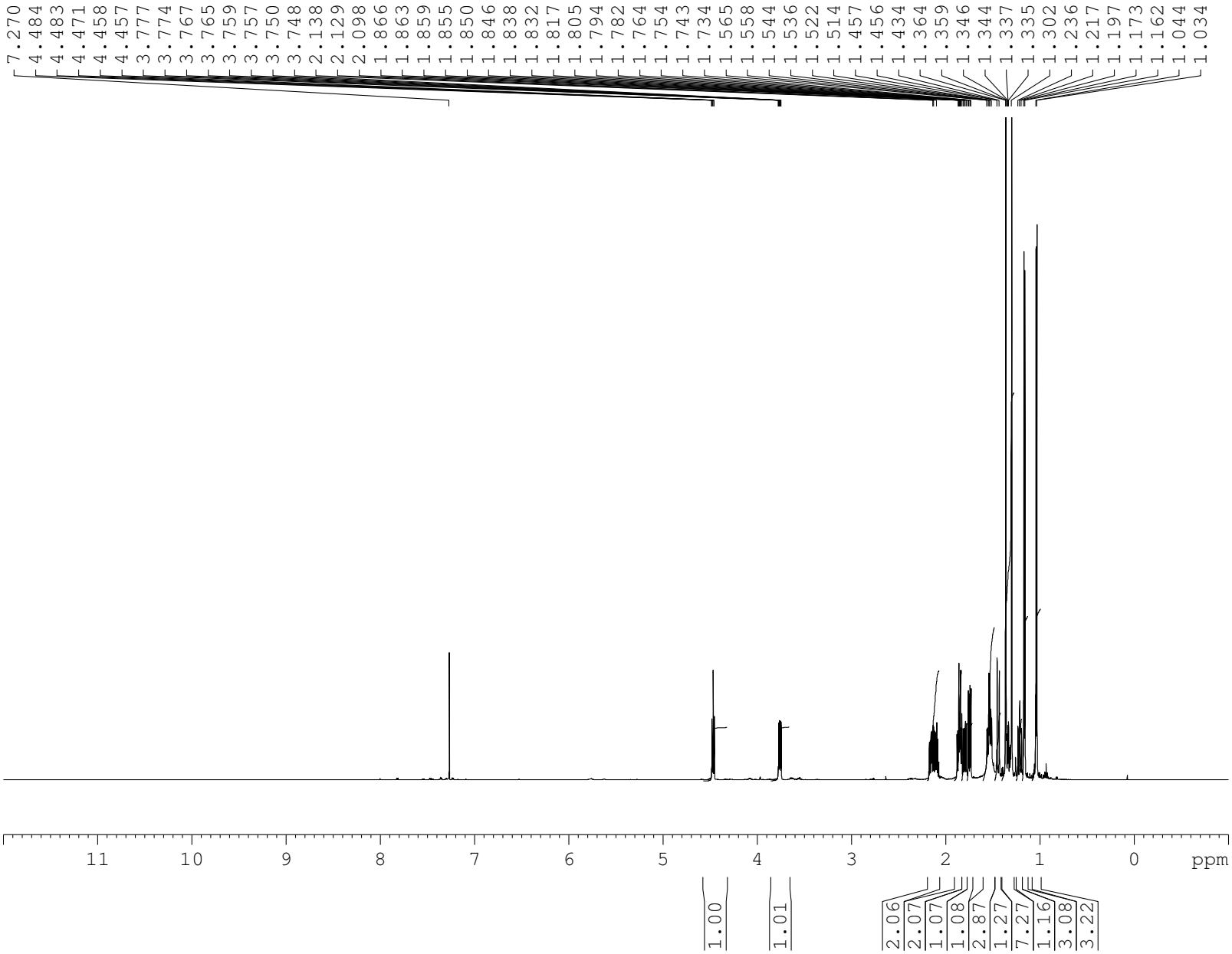
F1 - Acquisition parameters
TD 320
SFO1 600.1319 MHz
FIDRES 11.160714 Hz
SW 5.951 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 2048
MC2 QF
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

S2: 1H, 13C, DEPT-135, HSQC, HMBC and COSY spectra of CM1 (**2**)

1H spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



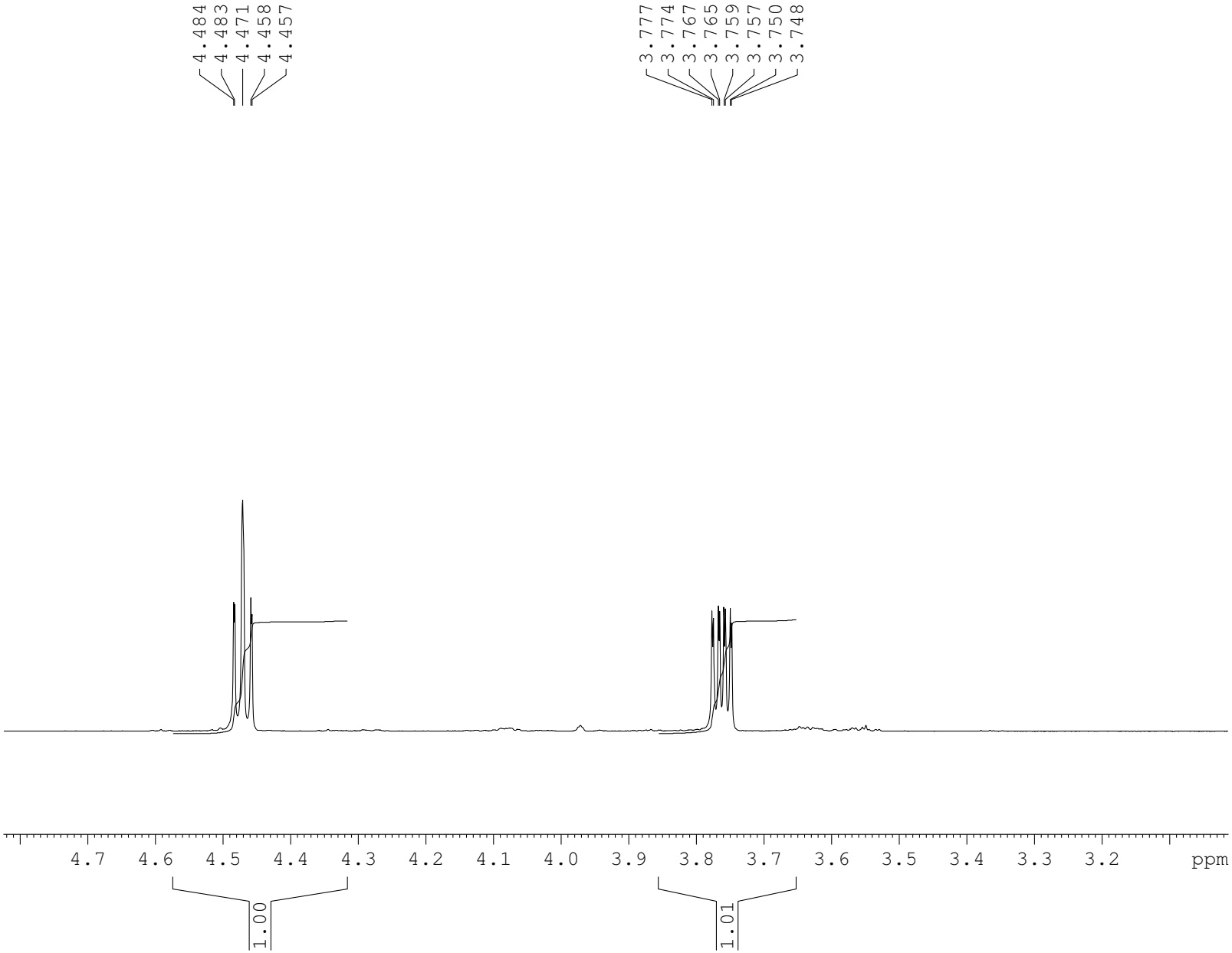
Current
NAME HGS-V-Caro85A-2D
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220524
Time 11.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 181
DW 40.533 usec
DE 20.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 600.1337060 MHz
NUC1 1H
P1 10.60 usec
PLW1 27.82500076 W

F2 - Processing parameters
SI 32768
SF 600.1300115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1H spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



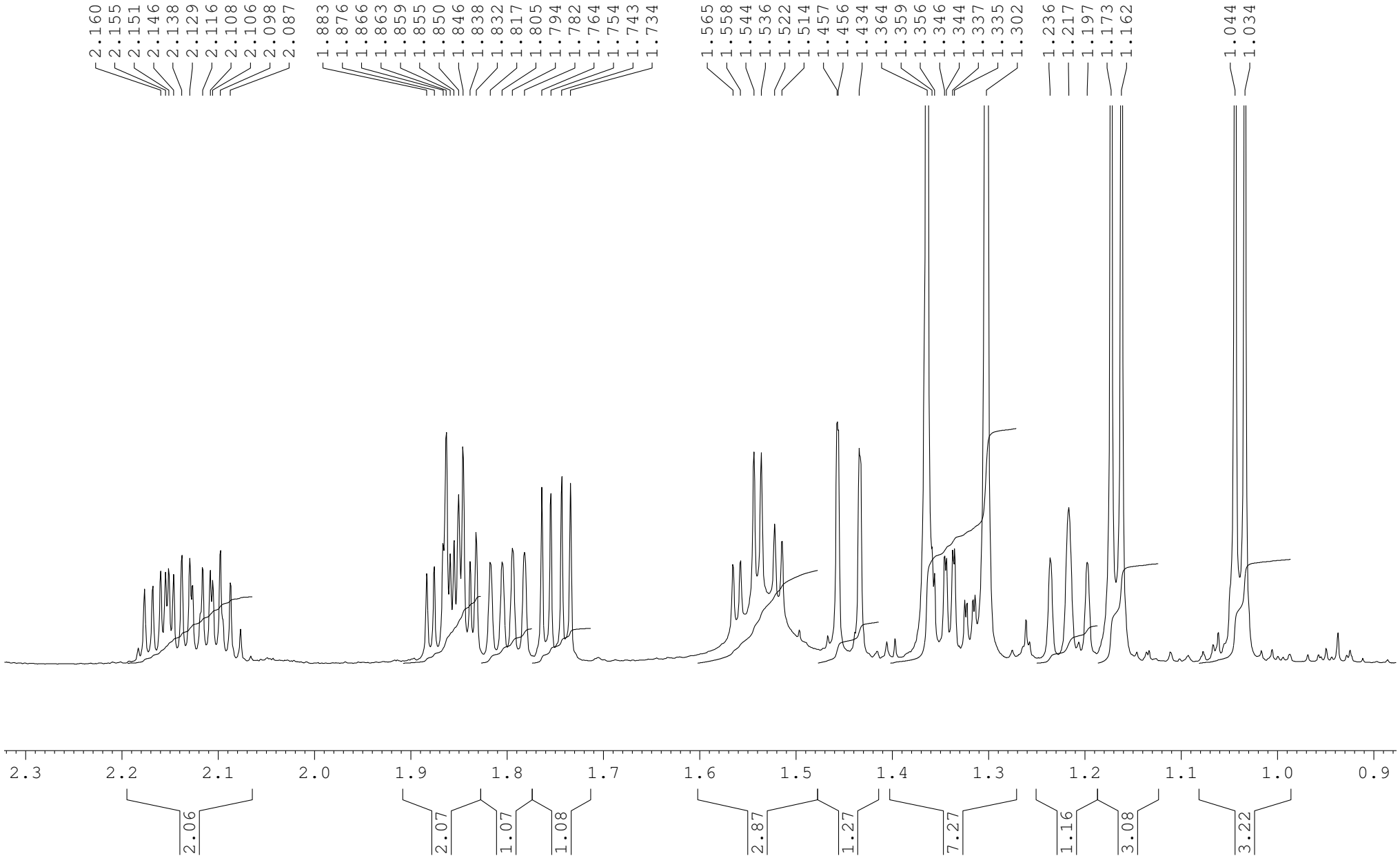
Current
NAME HGS-V-Caro85A-2D
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220524
Time 11.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 181
DW 40.533 usec
DE 20.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

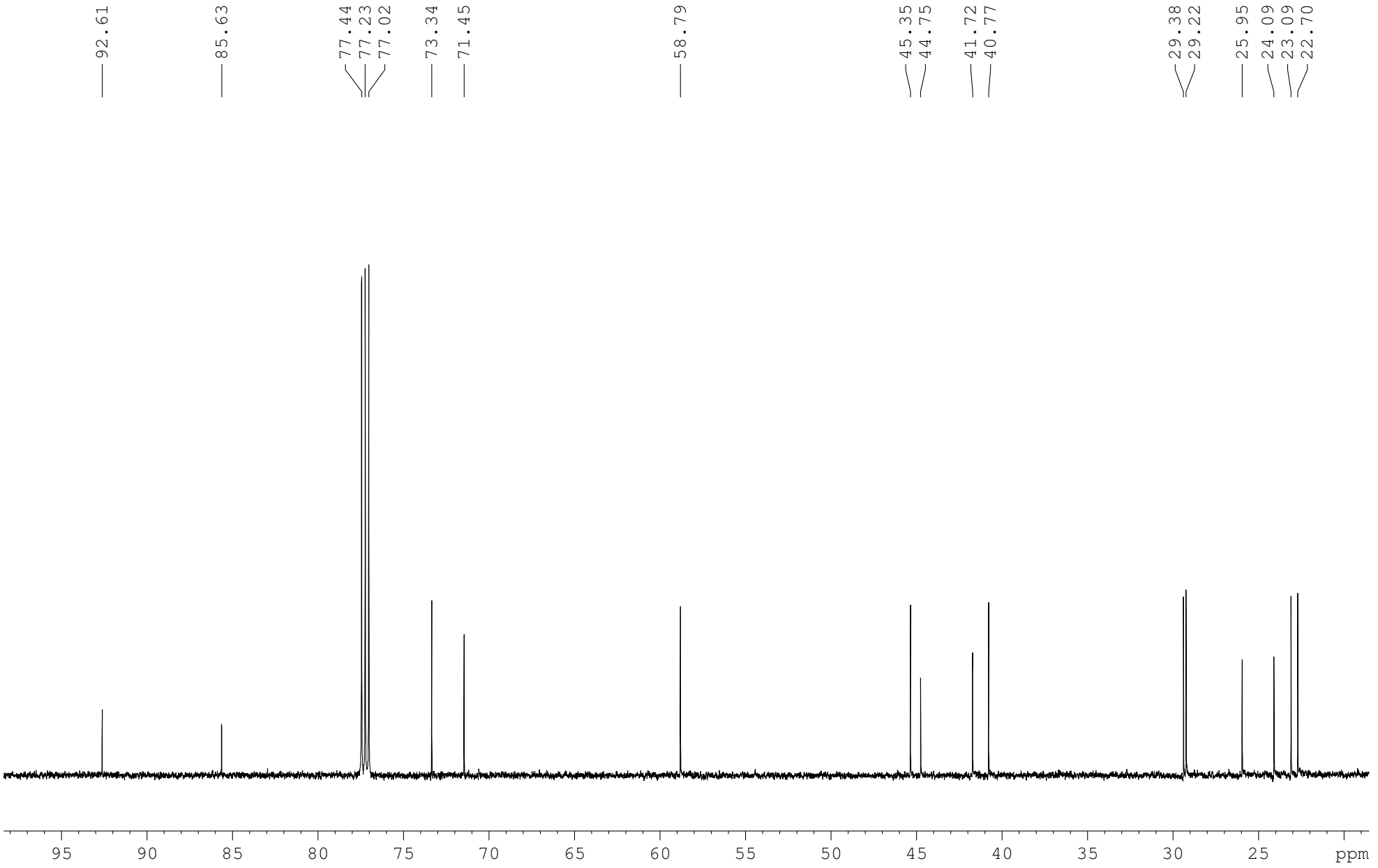
======== CHANNEL f1 ========
SFO1 600.1337060 MHz
NUC1 1H
P1 10.60 usec
PLW1 27.82500076 W

F2 - Processing parameters
SI 32768
SF 600.1300115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

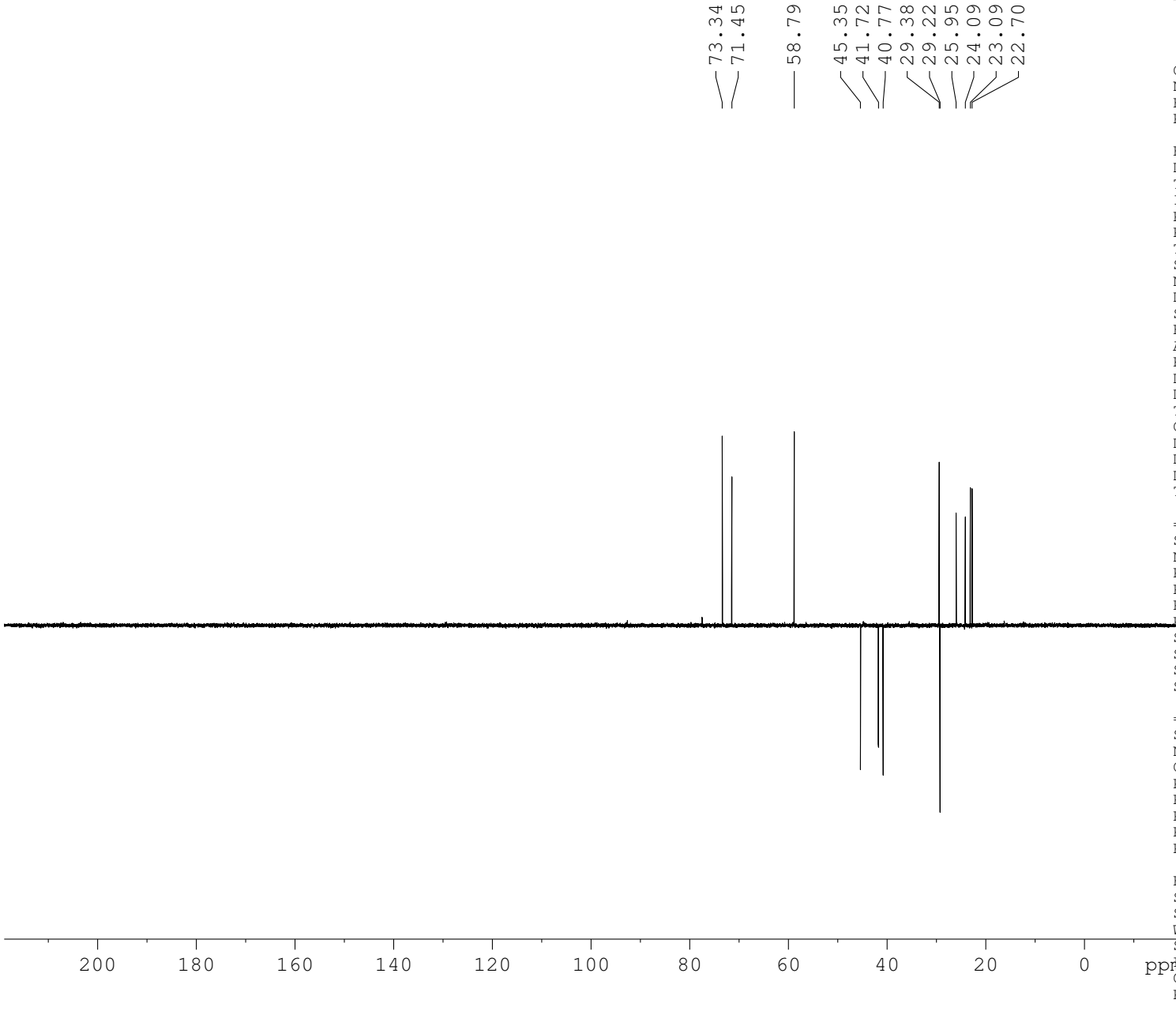
1H spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



13C decoupled spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



13C DEPT 135 spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



Current Data Parameters
NAME HGS-V-Caro85A-2D
EXPNO 5
PROCNO 1

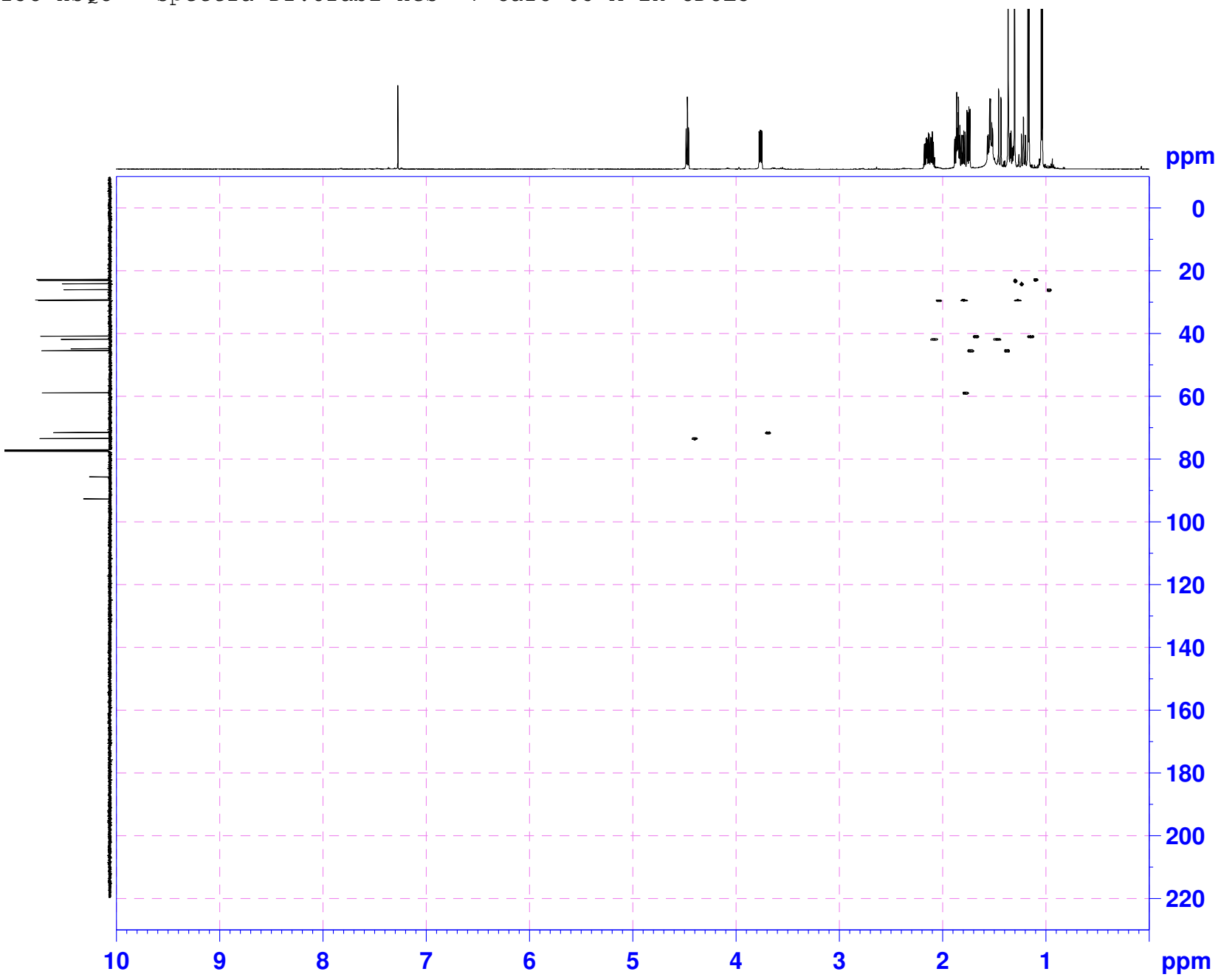
F2 - Acquisition Parameters
Date_ 20220524
Time 23.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 298.0 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 150.9178979 MHz
NUC1 13C
P1 8.80 usec
P13 2000.00 usec
PLW0 0 W
PLW1 78.13500214 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 9.24489975 W

======== CHANNEL f2 ========
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz65
P3 10.60 usec
P4 21.20 usec
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W

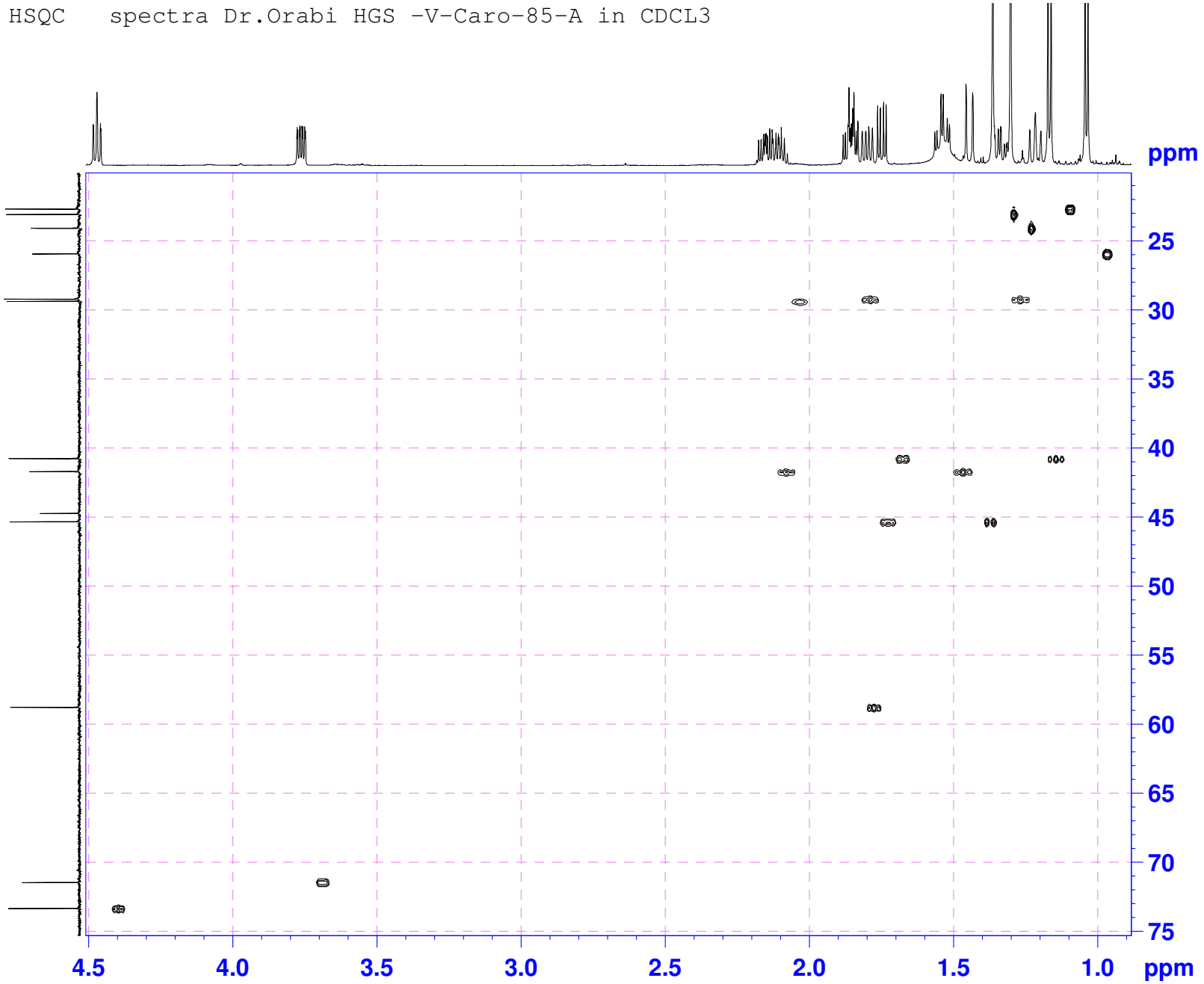
F2 - Processing parameters
SI 32768
SF 150.9027781 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13C HSQC spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



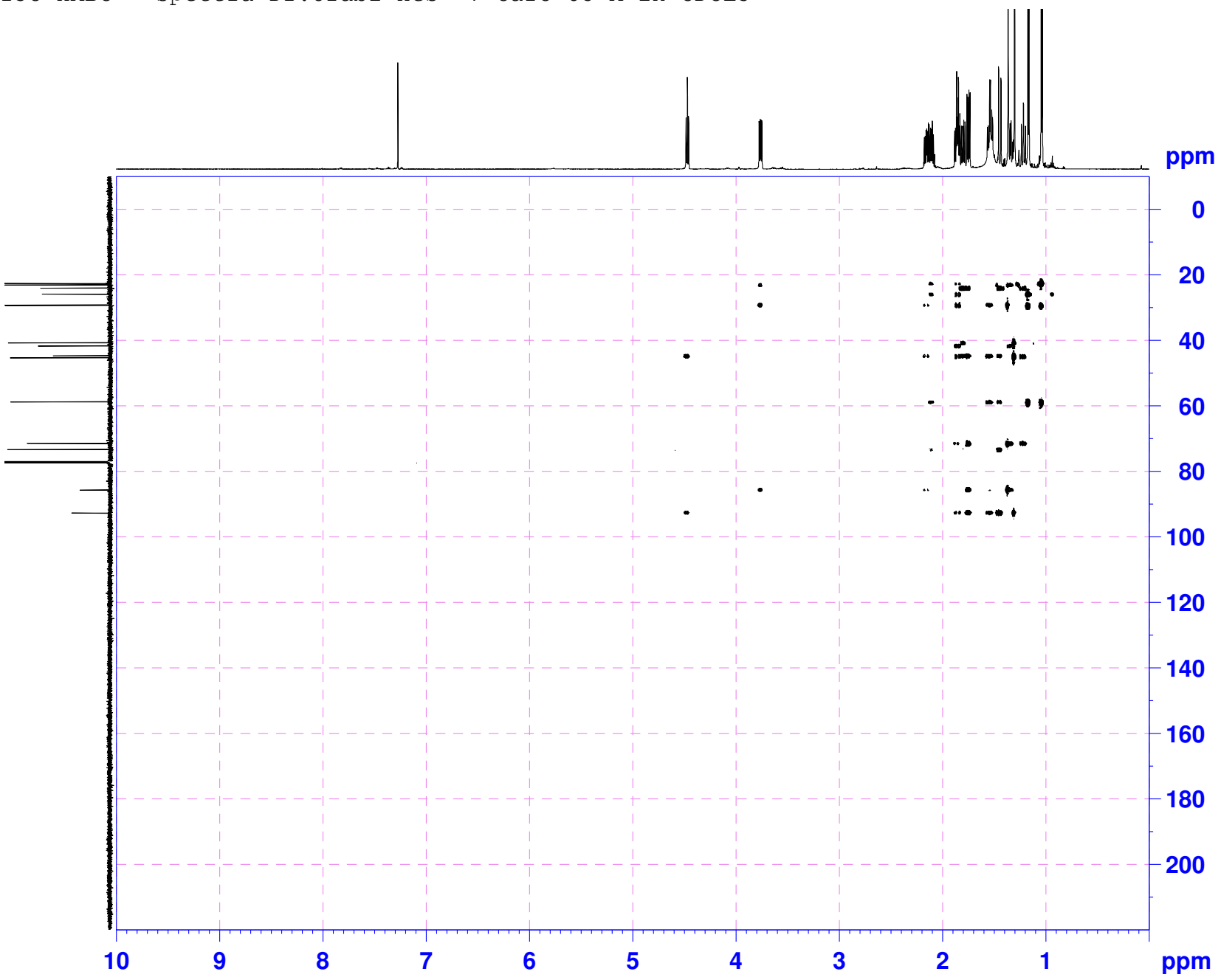

```
Current Data Parameters
NAME      HGS-V-Caro85A-2D
EXPNO                    7
PROCNO                   1

F2 - Acquisition Parameters
Date_             20220525
Time                  0.12
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG    hsqcetgpsp.2
TD                    2048
SOLVENT             CDCl3
NS                       4
DS                      16
SWH              4672.897 Hz
FIDRES           2.281688 Hz
AQ               0.2191360 sec
RG                     203
DW                107.000 usec
DE                 20.00 usec
TE                 298.1 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.88735998 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
IN0            0.00001840 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1          600.1324588 MHz
NUC1                    1H
P1                  10.60 usec
P2                  21.20 usec
P28               1000.00 usec
PLW1          27.82500076 W

======== CHANNEL f2 ========
SFO2          150.9148803 MHz
NUC2                   13C
CPDPRG[2             garp4
P3                   8.80 usec
P14                500.00 usec
P24               2000.00 usec
PCPD2               60.00 usec
PLW0       0 W
PLW2          78.13500214 W
PLW12          1.68079996 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3               0.500
SPOFFS3  0 Hz
SPW3           9.24489975 W
SPNAM[7]    Crp60comp.4
SPOAL7               0.500
SPOFFS7  0 Hz
SPW7           9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]         SINE.100
GPNAM[2]         SINE.100
GPZ1                80.00 %
GPZ2                20.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     512
SFO1            150.9149 MHz
FIDRES          53.074047 Hz
SW                180.061 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    2048
SF            600.1300553 MHz
WDW                 QSINE
SSB                     2
LB         0 Hz
GB         0
PC                   1.40

F1 - Processing parameters
SI                    1024
MC2         echo-antiecho
SF              150.9027623 MHz
WDW                 QSINE
SSB                     2
LB         0 Hz
```

13C HSQC spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



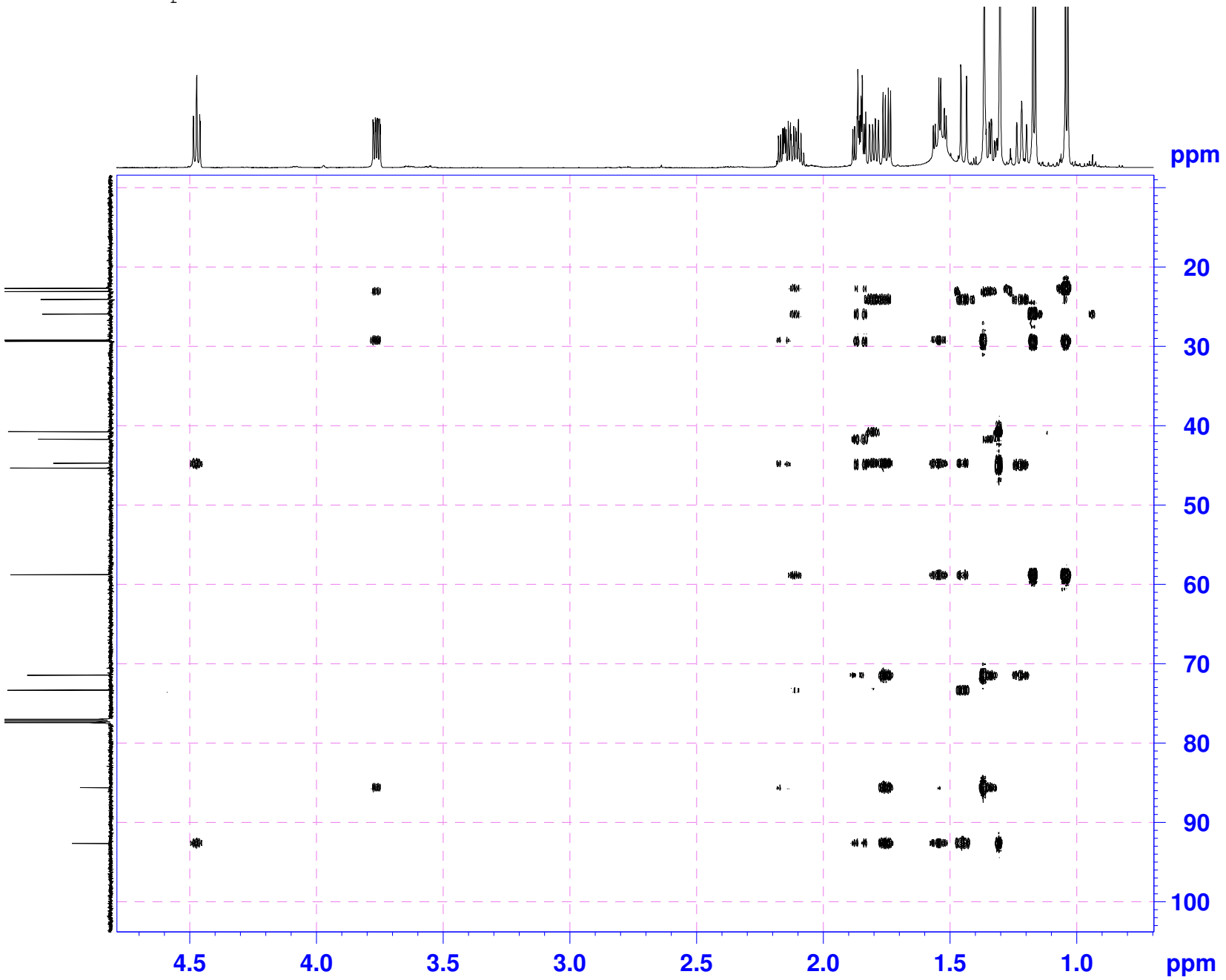

```
Current Data Parameters
NAME      HGS-V-Caro85A-2D
EXPNO                    7
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220525
Time                0.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG    hsqcetgpsp.2
TD                  2048
SOLVENT            CDCl3
NS                     4
DS                    16
SWH             4672.897 Hz
FIDRES          2.281688 Hz
AQ              0.2191360 sec
RG                   203
DW                107.000 usec
DE                 20.00 usec
TE                 298.1 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.88735998 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
IN0            0.00001840 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1         600.1324588 MHz
NUC1                   1H
P1                  10.60 usec
P2                  21.20 usec
P28               1000.00 usec
PLW1         27.82500076 W

======== CHANNEL f2 ========
SFO2         150.9148803 MHz
NUC2                  13C
CPDPRG[2            garp4
P3                   8.80 usec
P14                500.00 usec
P24               2000.00 usec
PCPD2               60.00 usec
PLW0       0 W
PLW2          78.13500214 W
PLW12          1.68079996 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3               0.500
SPOFFS3  0 Hz
SPW3           9.24489975 W
SPNAM[7]    Crp60comp.4
SPOAL7               0.500
SPOFFS7  0 Hz
SPW7           9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]        SINE.100
GPNAM[2]        SINE.100
GPZ1                80.00 %
GPZ2                20.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                   512
SFO1            150.9149 MHz
FIDRES          53.074047 Hz
SW                180.061 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  2048
SF           600.1300553 MHz
WDW                 QSINE
SSB                     2
LB         0 Hz
GB         0
PC                   1.40

F1 - Processing parameters
SI                  1024
MC2         echo-antiecho
SF            150.9027623 MHz
WDW                 QSINE
SSB                     2
LB         0 Hz
```

13C HMBC spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



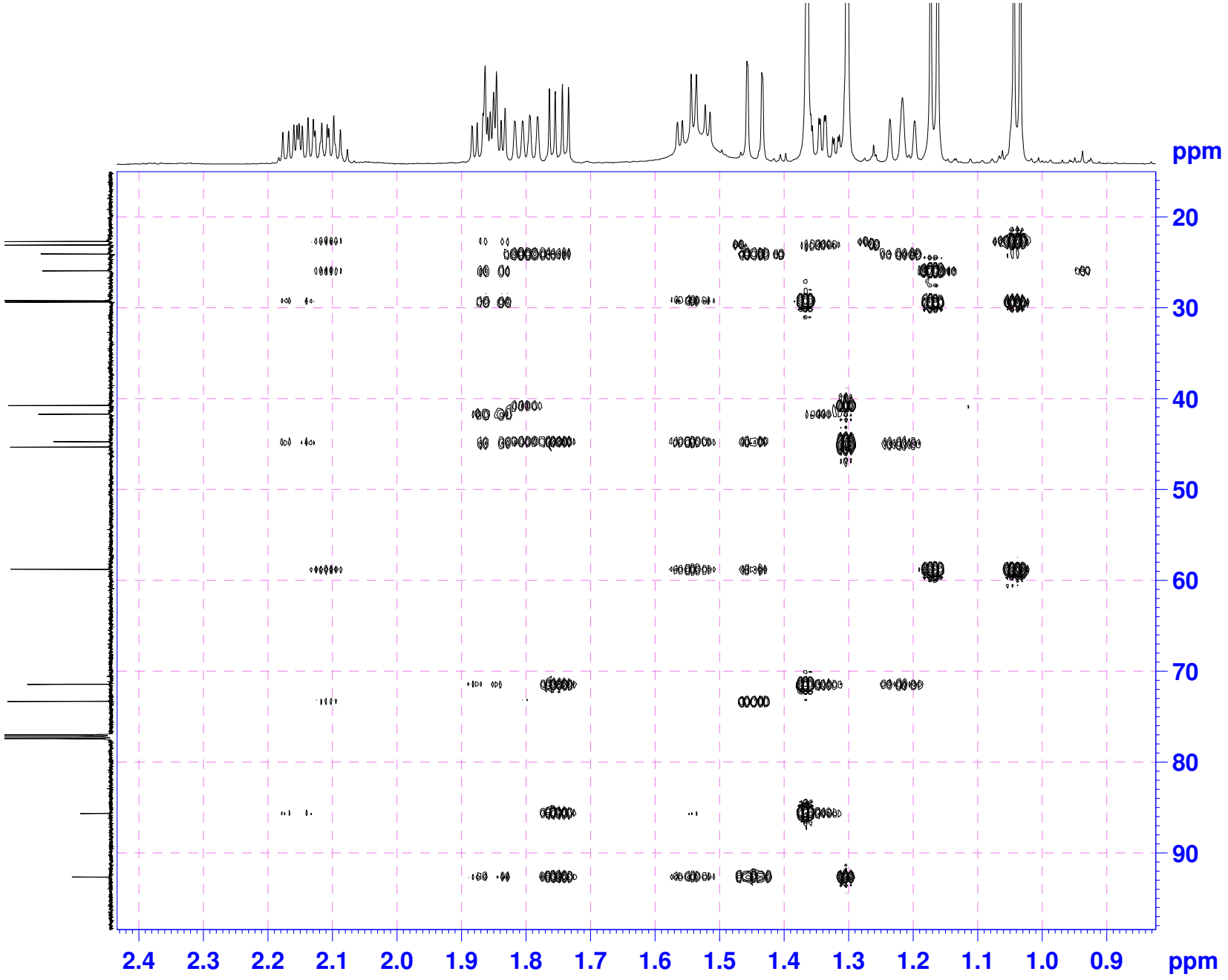

```
Current Data Parameters
NAME      HGS-V-Caro85A-2D
EXPNO                    8
PROCNO                   1

F2 - Acquisition Parameters
Date_             20220525
Time                 1.28
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG     hmbcetgpl2nd
TD                   2048
SOLVENT              CDCl3
NS                     16
DS                     16
SWH              4672.897 Hz
FIDRES           2.281688 Hz
AQ               0.2191360 sec
RG                   203
DW                107.000 usec
DE                 20.00 usec
TE                 297.9 K
CNST6         125.0000000
CNST7         165.0000000
CNST13         10.0000000
CNST30          0.5981151
D0            0.00000300 sec
D1            1.41193604 sec
D6            0.05000000 sec
D16           0.00020000 sec
IN0           0.00001490 sec

======== CHANNEL f1 ========
SFO1         600.1324588 MHz
NUC1                   1H
P1                 10.60 usec
P2                 21.20 usec
PLW1         27.82500076 W

======== CHANNEL f2 ========
SFO2         150.9178738 MHz
NUC2                  13C
P3                  8.80 usec
P24              2000.00 usec
PLW2         78.13500214 W
SPNAM[7]     Crp60comp.4
SPOAL7             0.500
SPOFFS7   0 Hz
SPW7          9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]         SINE.100
GPNAM[3]         SINE.100
GPNAM[4]         SINE.100
GPNAM[5]         SINE.100
GPZ1                80.00 %
GPZ3                15.00 %
GPZ4               -10.00 %
GPZ5                -5.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            150.9179 MHz
FIDRES        131.082214 Hz
SW              222.353 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                   2048
SF           600.1300104 MHz
WDW                  SINE
SSB       0
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                    512
MC2        echo-antiecho
SF            150.9027493 MHz
WDW                  SINE
SSB                     2
LB        0 Hz
```

13C HMBC spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



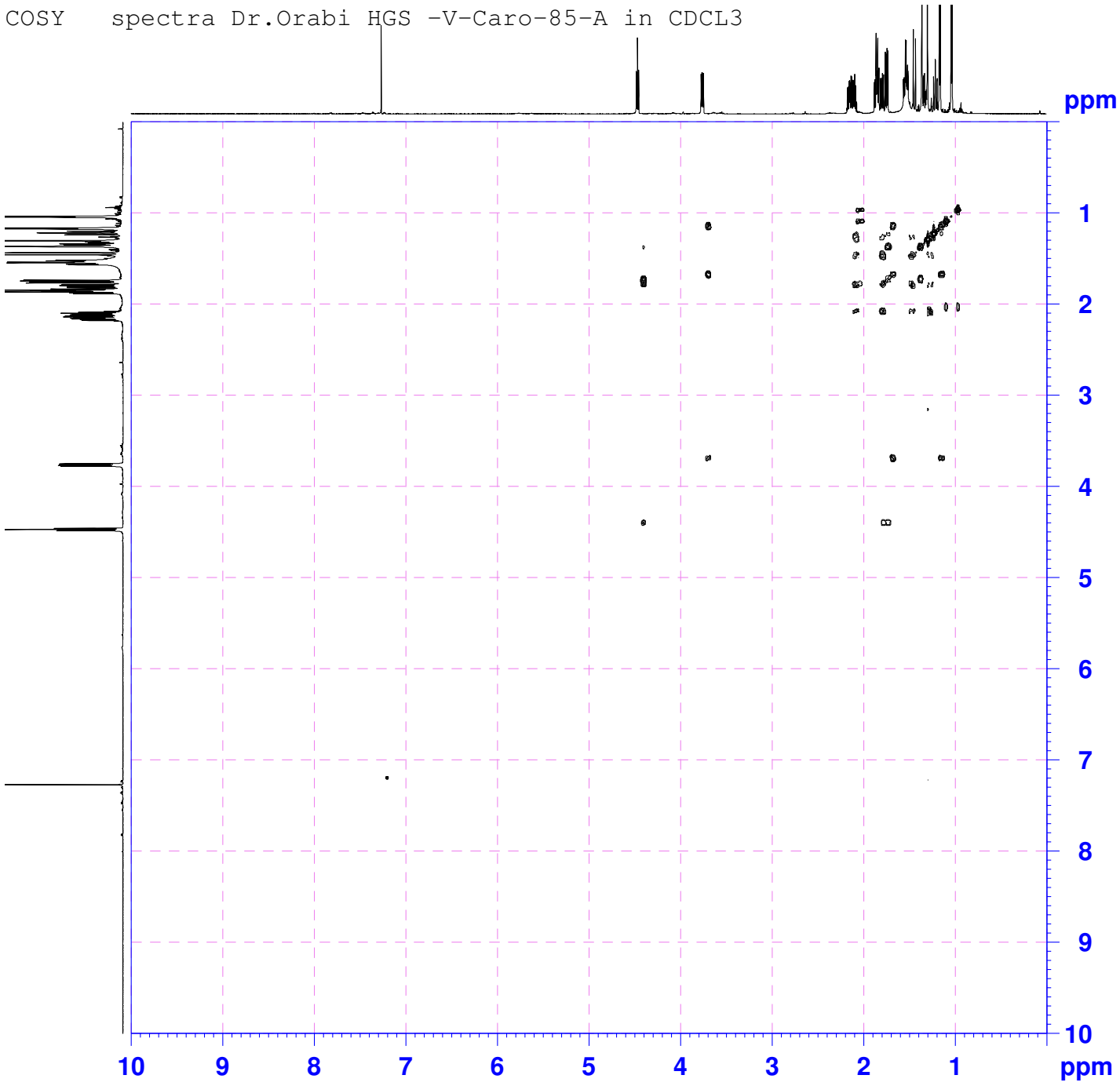

```
Current Data Parameters
NAME      HGS-V-Caro85A-2D
EXPNO                    8
PROCNO                   1

F2 - Acquisition Parameters
Date_             20220525
Time                 1.28
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG     hmbcetgpl2nd
TD                   2048
SOLVENT              CDCl3
NS                     16
DS                     16
SWH               4672.897 Hz
FIDRES            2.281688 Hz
AQ                0.2191360 sec
RG                     203
DW                107.000 usec
DE                 20.00 usec
TE                 297.9 K
CNST6         125.0000000
CNST7         165.0000000
CNST13         10.0000000
CNST30          0.5981151
D0             0.00000300 sec
D1             1.41193604 sec
D6             0.05000000 sec
D16            0.00020000 sec
IN0            0.00001490 sec

======== CHANNEL f1 ========
SFO1          600.1324588 MHz
NUC1                    1H
P1                  10.60 usec
P2                  21.20 usec
PLW1          27.82500076 W

======== CHANNEL f2 ========
SFO2          150.9178738 MHz
NUC2                   13C
P3                   8.80 usec
P24               2000.00 usec
PLW2          78.13500214 W
SPNAM[7]     Crp60comp.4
SPOAL7             0.500
SPOFFS7   0 Hz
SPW7           9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]         SINE.100
GPNAM[3]         SINE.100
GPNAM[4]         SINE.100
GPNAM[5]         SINE.100
GPZ1                80.00 %
GPZ3                15.00 %
GPZ4               -10.00 %
GPZ5                -5.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     256
SFO1            150.9179 MHz
FIDRES         131.082214 Hz
SW               222.353 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    2048
SF           600.1300104 MHz
WDW                   SINE
SSB        0
LB         0 Hz
GB         0
PC                    1.40

F1 - Processing parameters
SI                     512
MC2         echo-antiecho
SF            150.9027493 MHz
WDW                   SINE
SSB                      2
LB         0 Hz
```

13C HMBC spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3




```
Current Data Parameters
NAME      HGS-V-Caro85A-2D
EXPNO                    8
PROCNO                   1

F2 - Acquisition Parameters
Date_             20220525
Time                 1.28
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG     hmbcetgpl2nd
TD                   2048
SOLVENT              CDCl3
NS                     16
DS                     16
SWH               4672.897 Hz
FIDRES            2.281688 Hz
AQ                0.2191360 sec
RG                     203
DW                107.000 usec
DE                 20.00 usec
TE                 297.9 K
CNST6          125.0000000
CNST7          165.0000000
CNST13          10.0000000
CNST30           0.5981151
D0               0.00000300 sec
D1               1.41193604 sec
D6               0.05000000 sec
D16              0.00020000 sec
IN0              0.00001490 sec

======== CHANNEL f1 ========
SFO1          600.1324588 MHz
NUC1                    1H
P1                   10.60 usec
P2                   21.20 usec
PLW1          27.82500076 W

======== CHANNEL f2 ========
SFO2          150.9178738 MHz
NUC2                   13C
P3                    8.80 usec
P24                2000.00 usec
PLW2          78.13500214 W
SPNAM[7]     Crp60comp.4
SPOAL7               0.500
SPOFFS7   0 Hz
SPW7           9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]         SINE.100
GPNAM[3]         SINE.100
GPNAM[4]         SINE.100
GPNAM[5]         SINE.100
GPZ1                80.00 %
GPZ3                15.00 %
GPZ4               -10.00 %
GPZ5                -5.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    256
SFO1            150.9179 MHz
FIDRES        131.082214 Hz
SW              222.353 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                   2048
SF            600.1300104 MHz
WDW                  SINE
SSB       0
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                    512
MC2         echo-antiecho
SF            150.9027493 MHz
WDW                  SINE
SSB                     2
LB        0 Hz
```

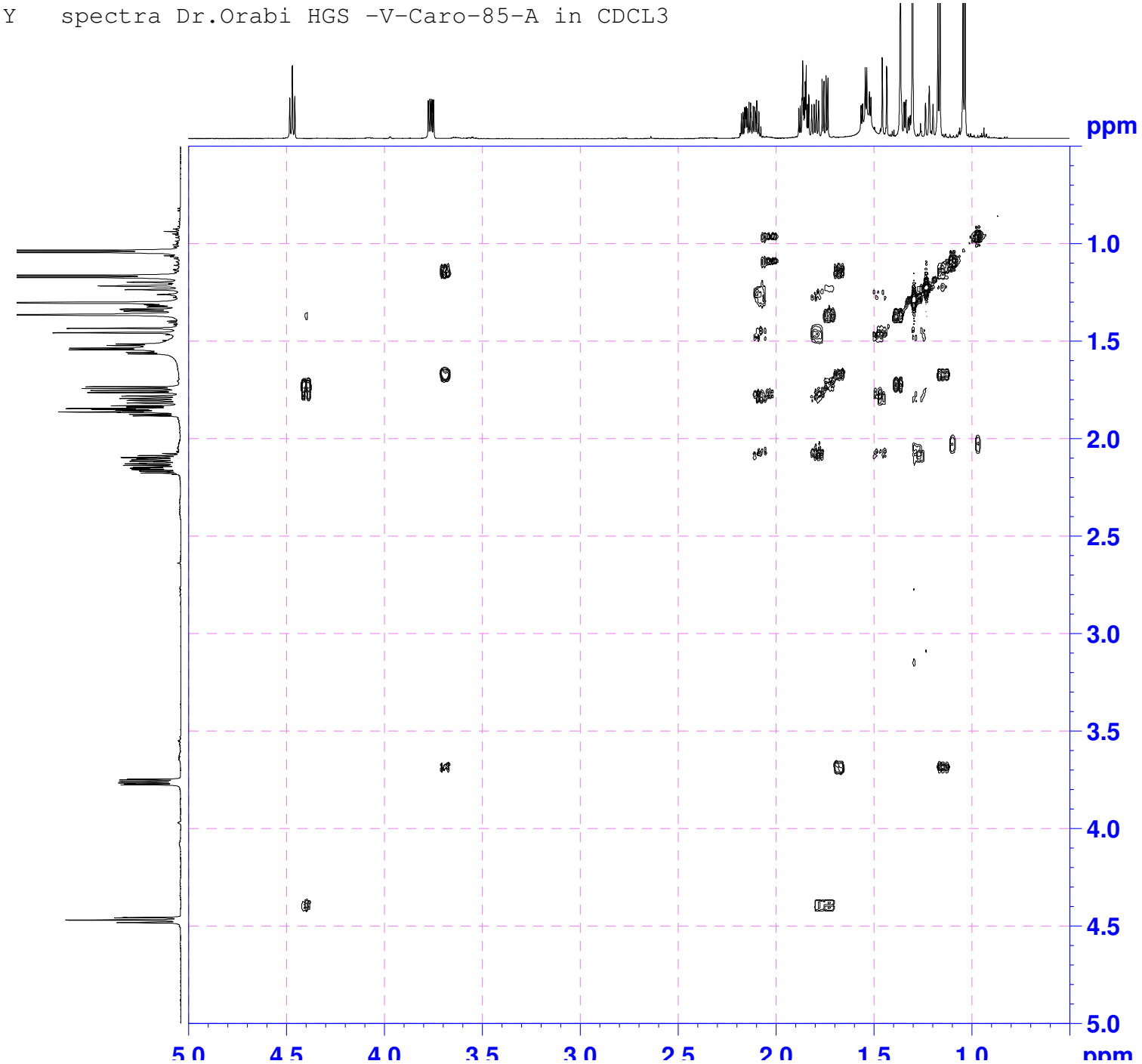
COSY spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



BRUKER

```
Current Data Parameters
NAME      HGS-V-Caro85A-2D
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220524
Time               23.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG      cosygpppqf
TD                 2048
SOLVENT            CDCl3
NS                    2
DS                    8
SWH             4672.897 Hz
FIDRES          2.281688 Hz
AQ              0.2191360 sec
RG                 90.5
DW               107.000 usec
DE                20.00 usec
TE                297.9 K
D0            0.00000300 sec
D1            0.65865898 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00021400 sec

======== CHANNEL f1 ========
SFO1         600.1323807 MHz
NUC1                1H
P0                10.60 usec
P1                10.60 usec
P17             2500.00 usec
PLW1         27.82500076 W
PLW10         4.62489986 W

====== GRADIENT CHANNEL =====
GPNAM[1]        SINE.100
GPZ1               20.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                  320
SFO1            600.1324 MHz
FIDRES         14.602804 Hz
SW                 7.786 ppm
FnMODE                QF

F2 - Processing parameters
SI                  2048
SF           600.1300549 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                  2048
MC2                   QF
SF           600.1300578 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
```

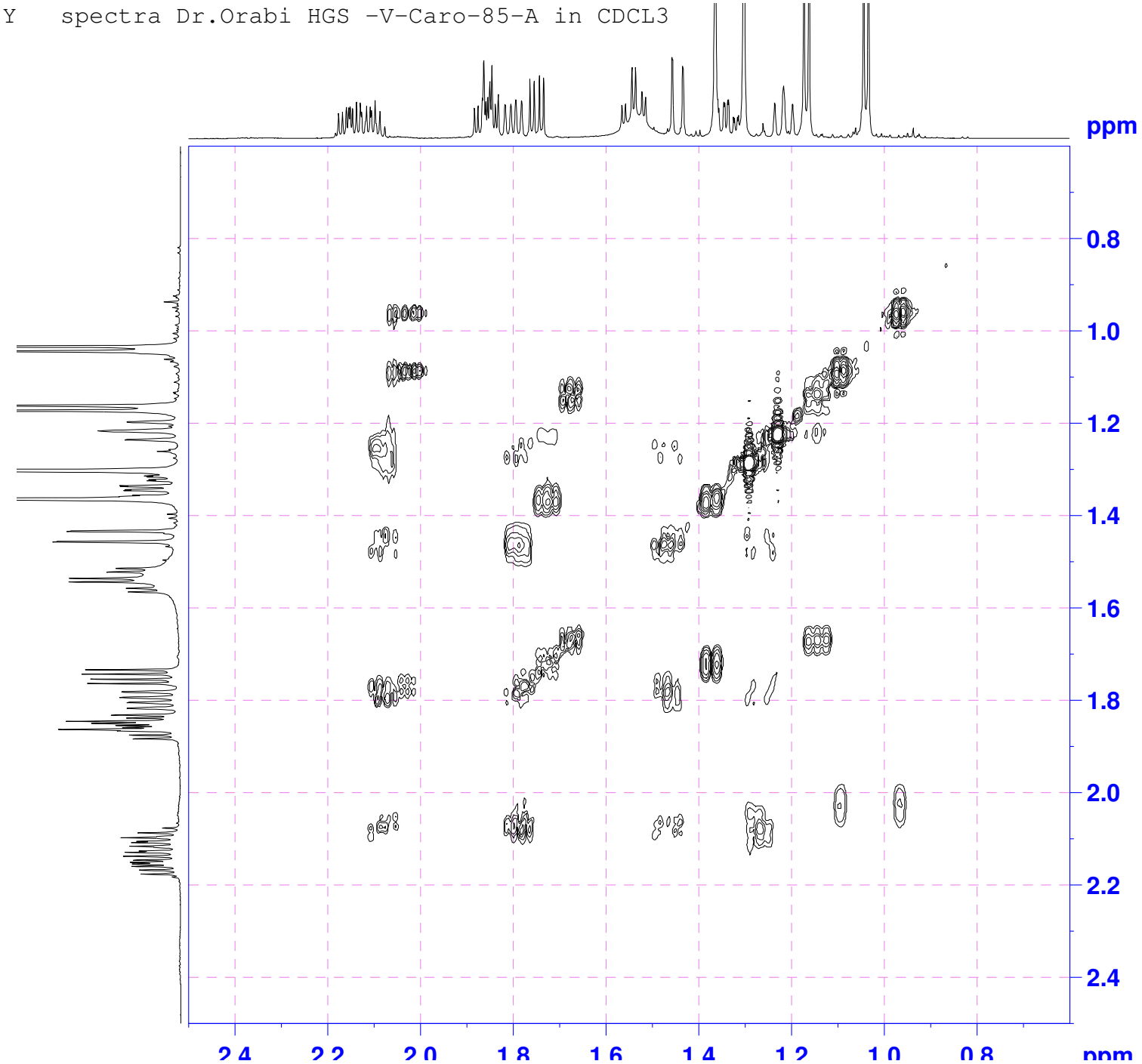
COSY spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3



BRUKER

```
Current Data Parameters
NAME      HGS-V-Caro85A-2D
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_             20220524
Time                 23.58
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG       cosygpppqf
TD                   2048
SOLVENT              CDCl3
NS                       2
DS                       8
SWH               4672.897 Hz
FIDRES            2.281688 Hz
AQ               0.2191360 sec
RG                    90.5
DW                 107.000 usec
DE                  20.00 usec
TE                  297.9 K
D0               0.00000300 sec
D1               0.65865898 sec
D11              0.03000000 sec
D12              0.00002000 sec
D13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00021400 sec

======== CHANNEL f1 ========
SFO1          600.1323807 MHz
NUC1                     1H
P0                  10.60 usec
P1                  10.60 usec
P17               2500.00 usec
PLW1          27.82500076 W
PLW10          4.62489986 W

====== GRADIENT CHANNEL =====
GPNAM[1]         SINE.100
GPZ1                20.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    320
SFO1             600.1324 MHz
FIDRES          14.602804 Hz
SW                  7.786 ppm
FnMODE                 QF

F2 - Processing parameters
SI                    2048
SF            600.1300549 MHz
WDW                   SINE
SSB          0
LB           0 Hz
GB           0
PC                    1.40

F1 - Processing parameters
SI                    2048
MC2                     QF
SF            600.1300578 MHz
WDW                   SINE
SSB          0
LB           0 Hz
GB           0
```

COSY spectra Dr.Orabi HGS -V-Caro-85-A in CDCL3

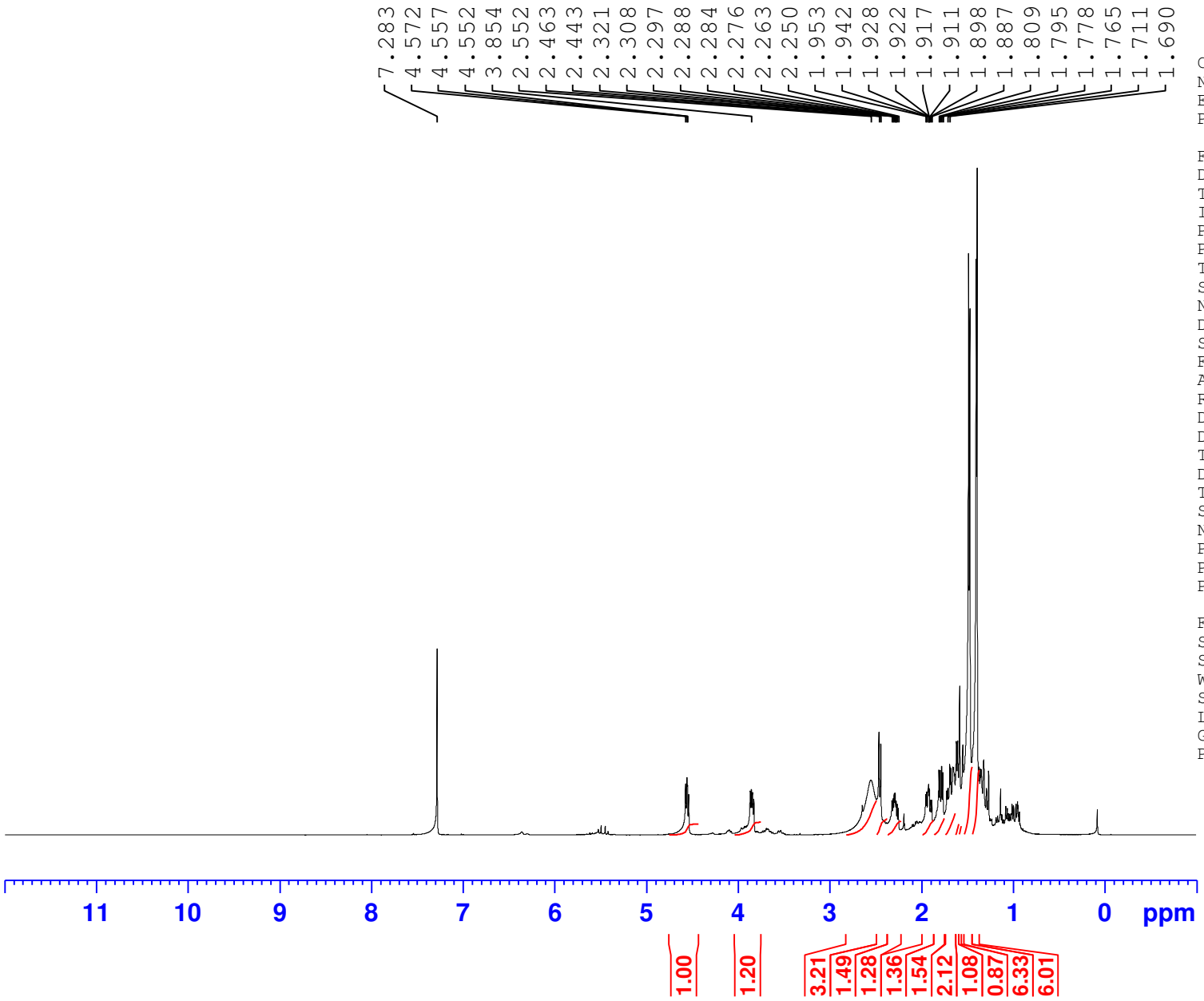


BRUKER

```
Current Data Parameters
NAME      HGS-V-Caro85A-2D
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220524
Time               23.58
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG       cosygpppqf
TD                 2048
SOLVENT            CDCl3
NS                    2
DS                    8
SWH             4672.897 Hz
FIDRES          2.281688 Hz
AQ             0.2191360 sec
RG                  90.5
DW               107.000 usec
DE                20.00 usec
TE                297.9 K
D0             0.00000300 sec
D1             0.65865898 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00021400 sec

======== CHANNEL f1 ========
SFO1         600.1323807 MHz
NUC1                 1H
P0                10.60 usec
P1                10.60 usec
P17             2500.00 usec
PLW1         27.82500076 W
PLW10         4.62489986 W

====== GRADIENT CHANNEL =====
GPNAM[1]        SINE.100
GPZ1               20.00 %
P16              1000.00 usec

F1 - Acquisition parameters
TD                  320
SFO1            600.1324 MHz
FIDRES         14.602804 Hz
SW                 7.786 ppm
FnMODE                QF

F2 - Processing parameters
SI                  2048
SF           600.1300549 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                  2048
MC2                   QF
SF           600.1300578 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
```

S3: 1H, 13C, DEPT-135, HSQC, HMBC and COSY spectra of CM2 (**3**)

1H SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3

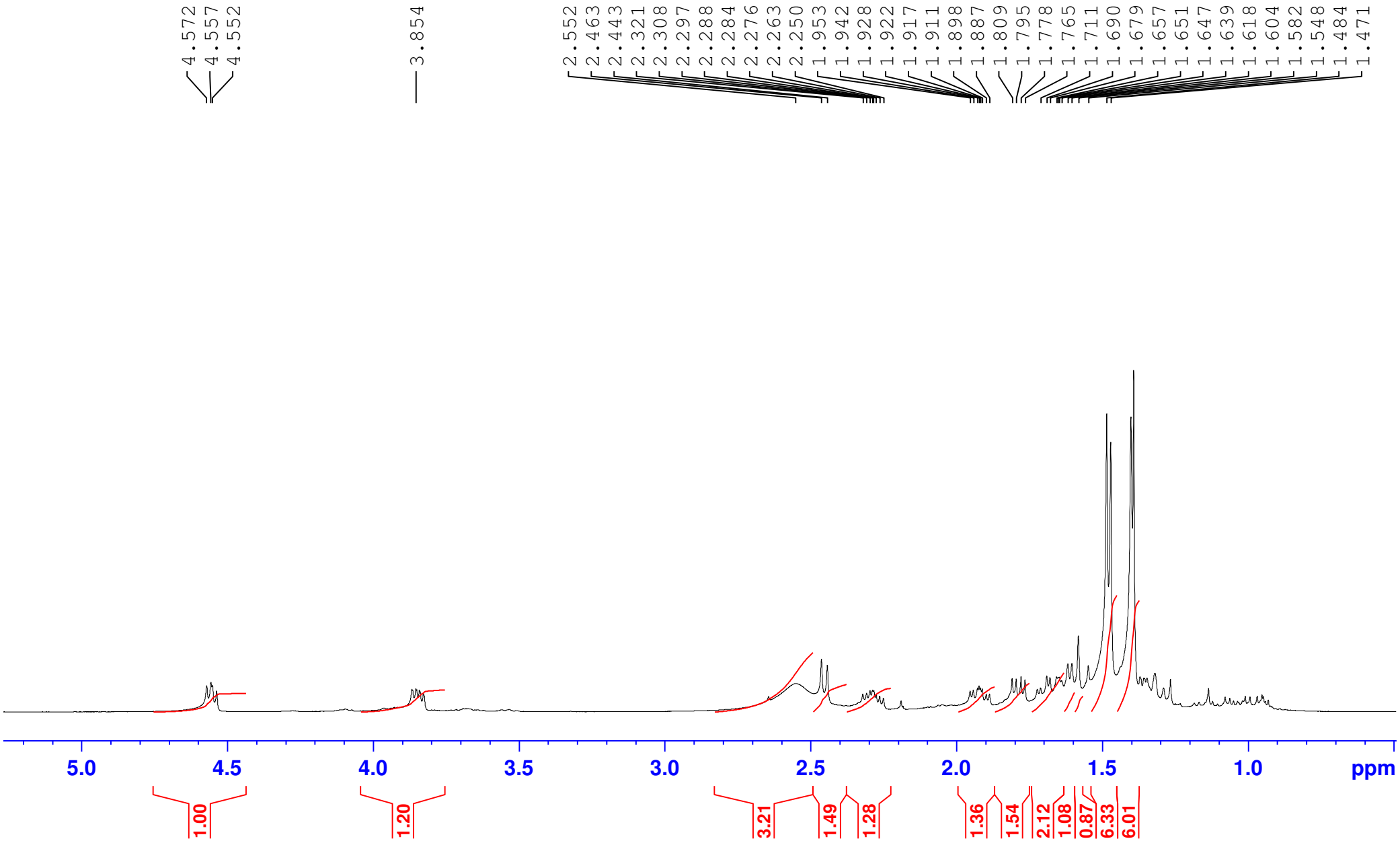


Current Data Parameters
NAME HGSVcaro86-2D
EXPNO 10
PROCNO 1

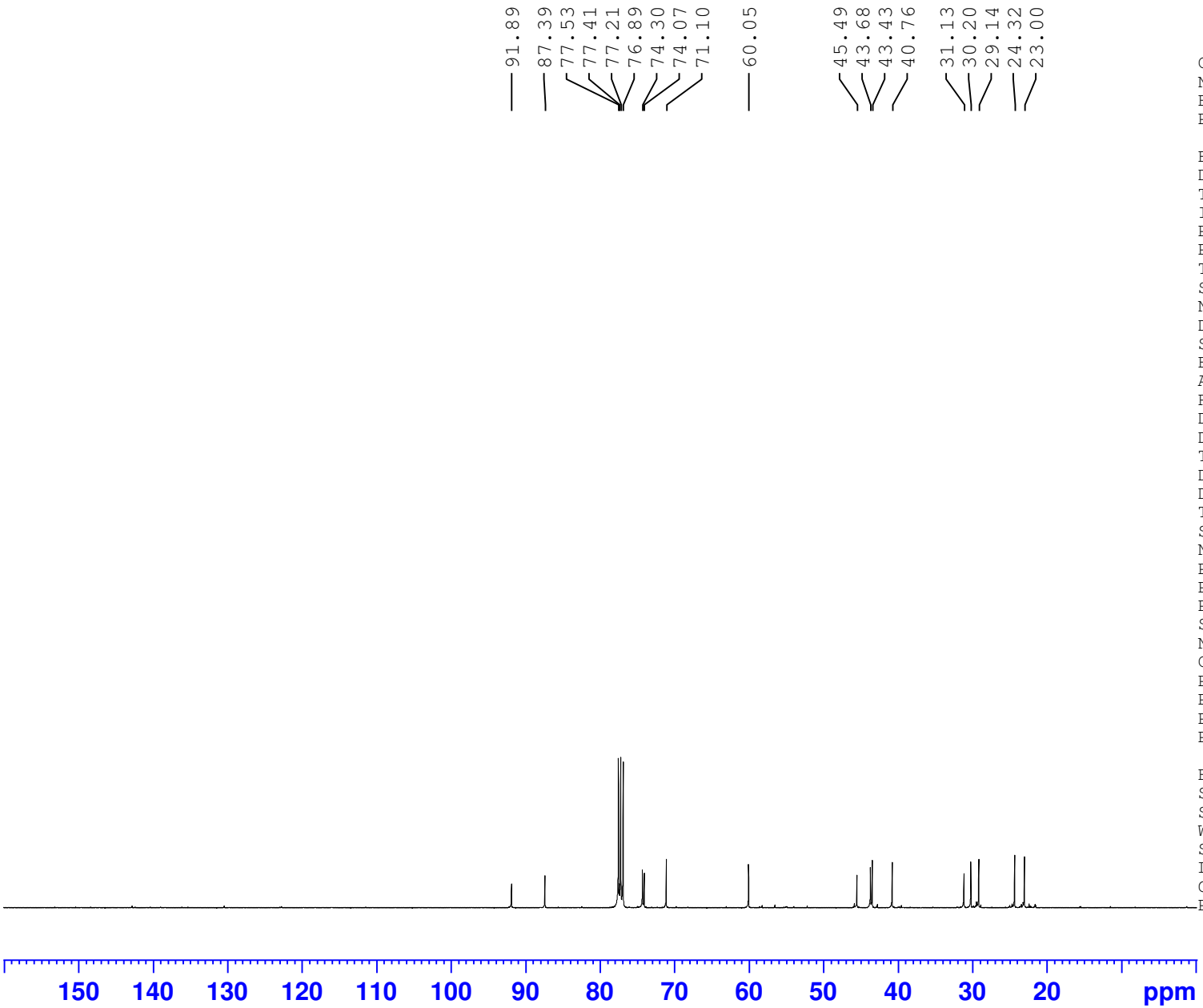
F2 - Acquisition Parameters
Date_ 20220522
Time 14.12 h
INSTRUM Avance AV Neo 400
PROBHD Z108618_0912 (
PULPROG zg30
TD 65536
SOLVENT CH3OH
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 13.01399994 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1H SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3



13C DECOUPLED SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3

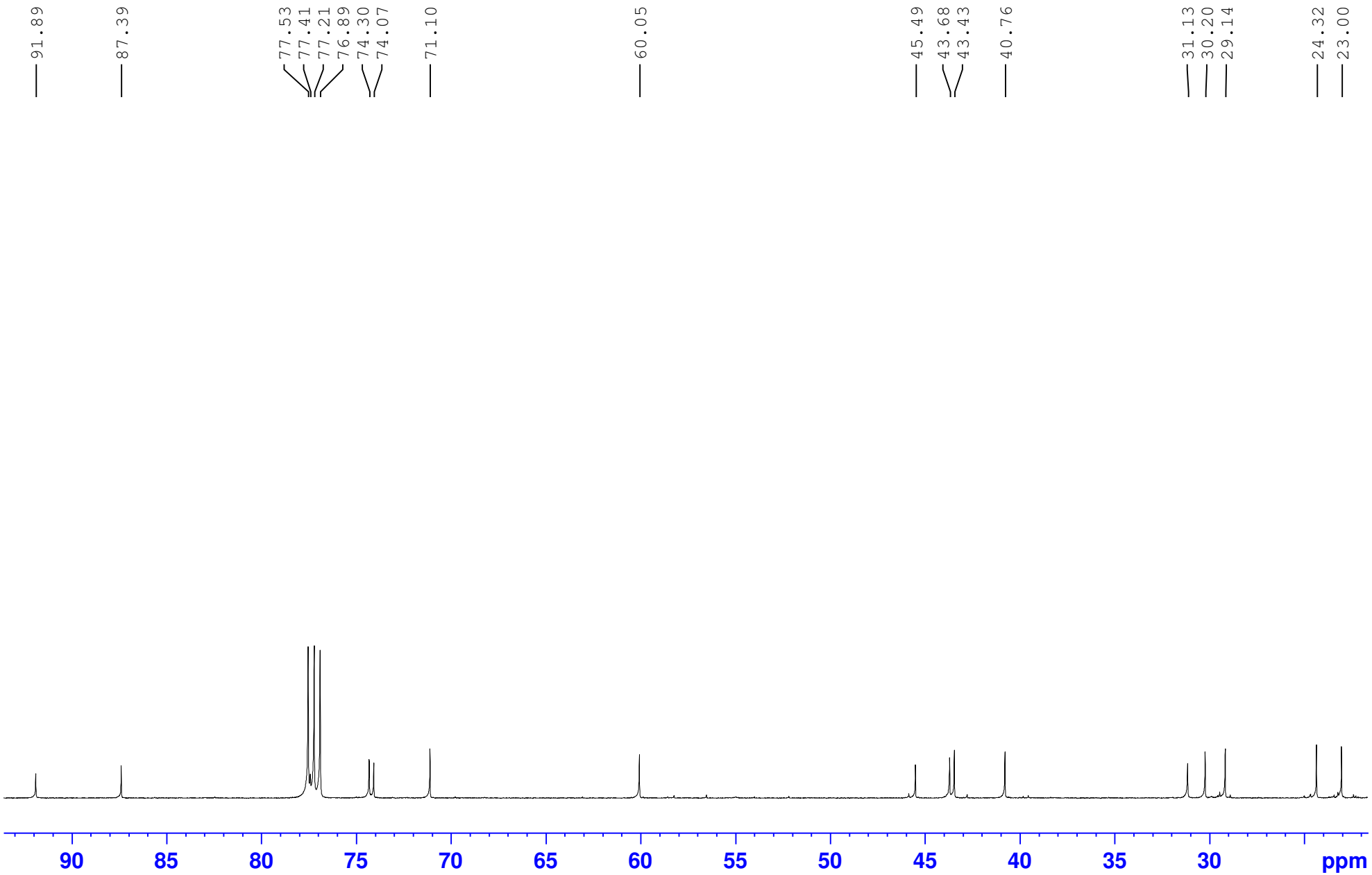


Current Data Parameters
NAME HGSVcaro86-2D
EXPNO 11
PROCNO 1

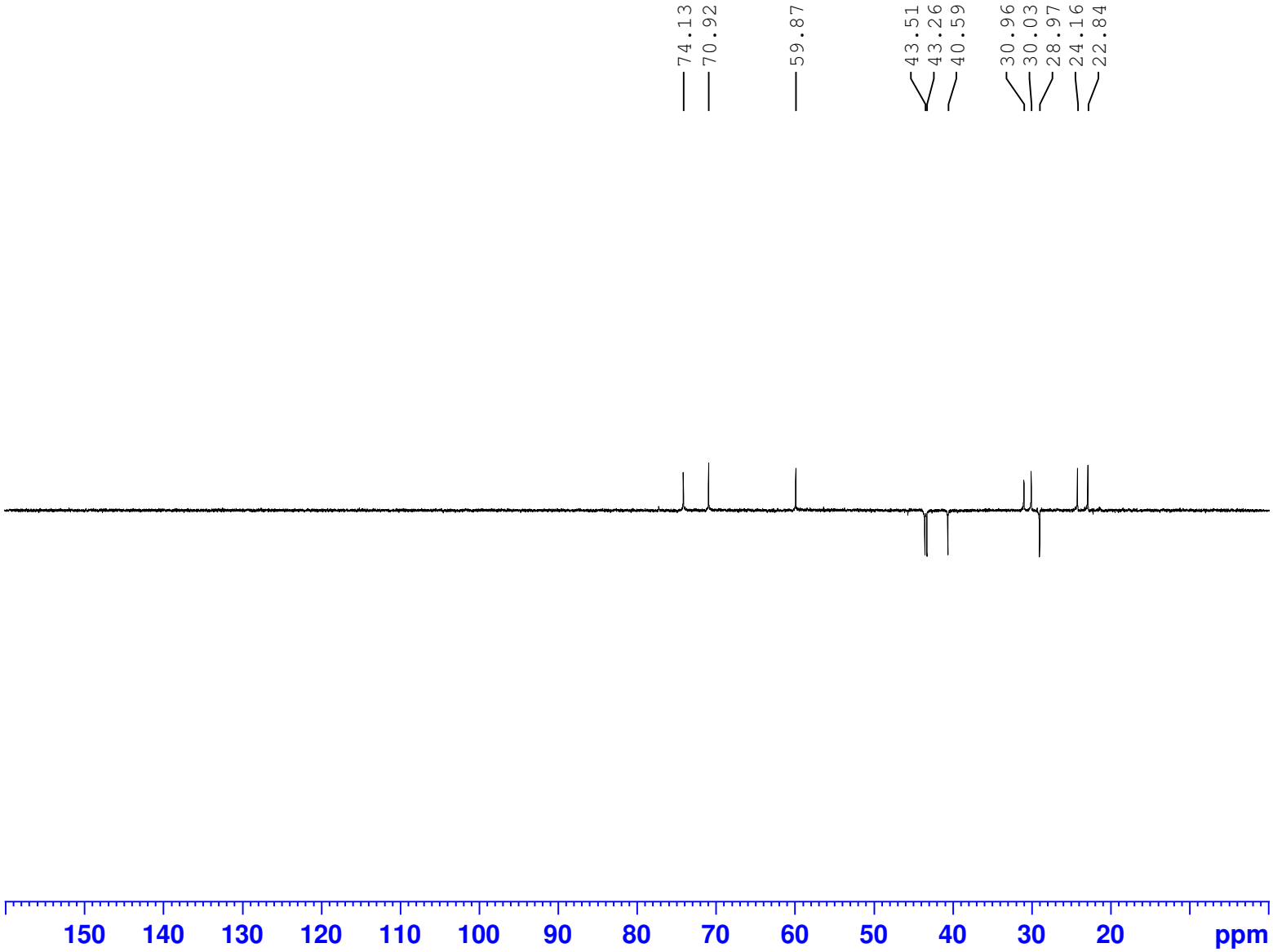
F2 - Acquisition Parameters
Date_ 20220523
Time 5.21 h
INSTRUM Avance AV Neo 400
PROBHD Z108618_0912 (
PULPROG zgpg30
TD 65536
SOLVENT CH3OH
NS 15360
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 29.8117
DW 21.000 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 53.78799820 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 13.01399994 W
PLW12 0.31492001 W
PLW13 0.15840000 W

F2 - Processing parameters
SI 32768
SF 100.6127514 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13C DECOUPLED SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3

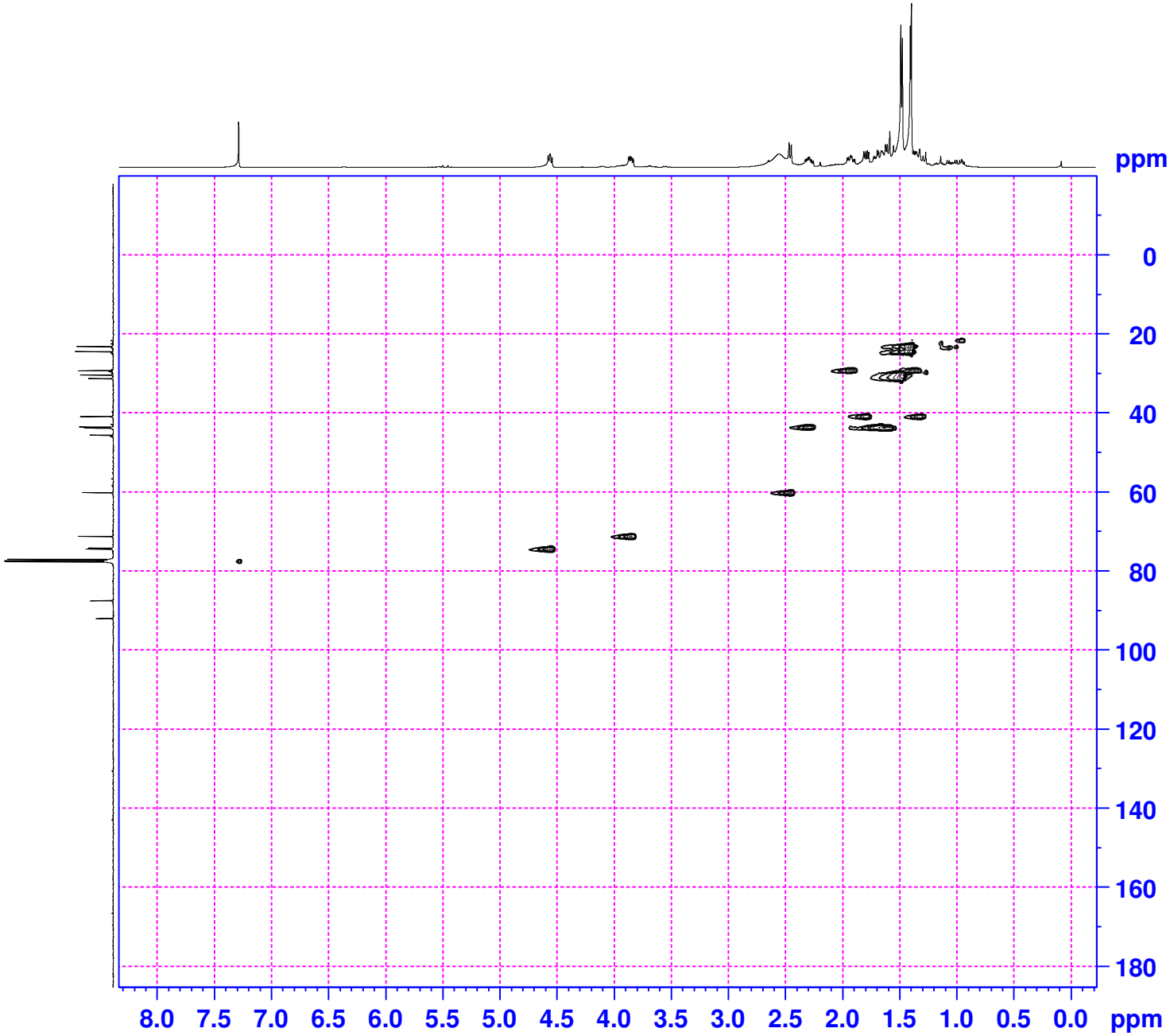


DEPT 135 SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3



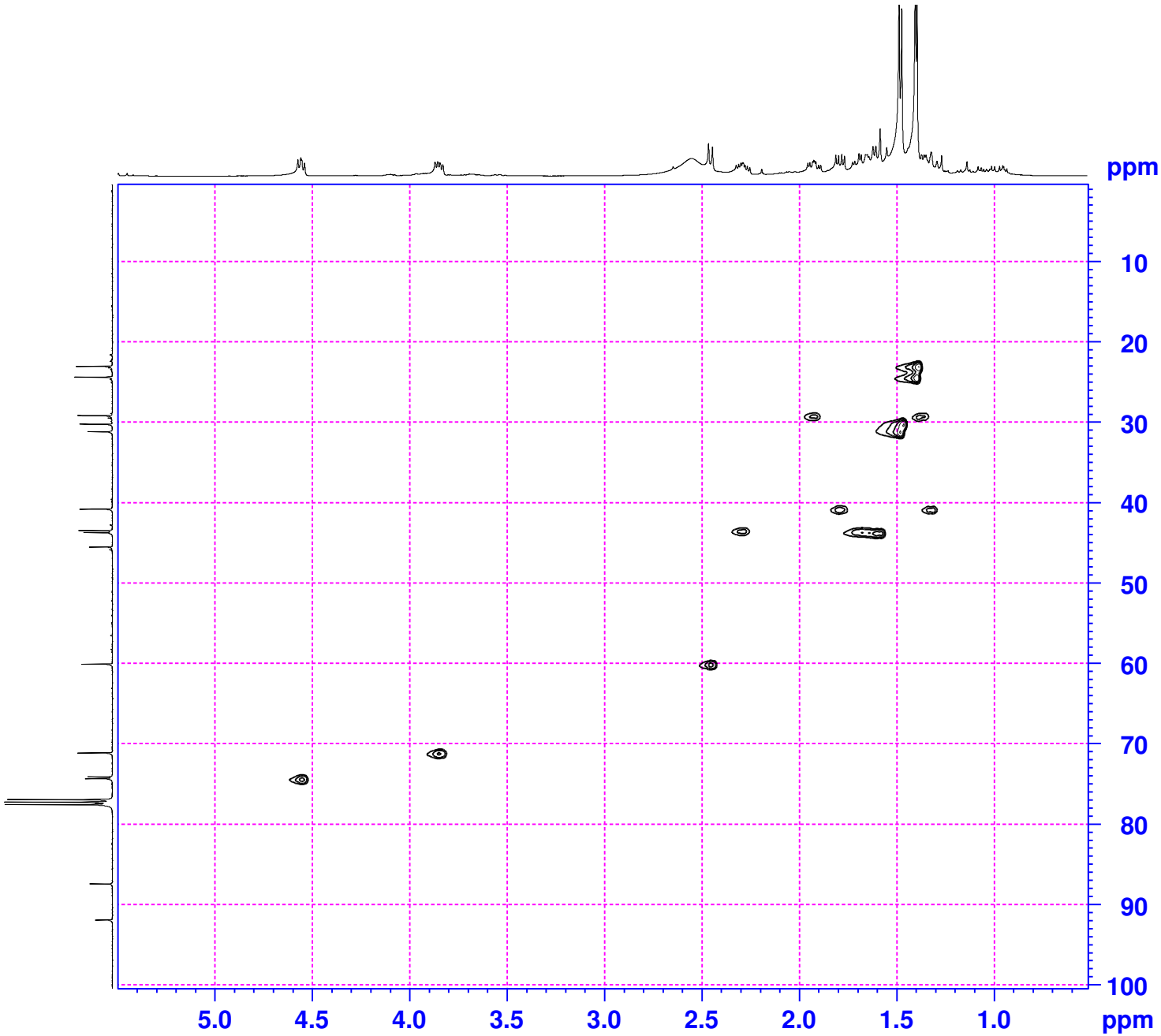

```
Current Data Parameters
NAME      HGSVcaro86-2D
EXPNO                16
PROCNO                1

F2 - Acquisition Parameters
Date_          20220523
Time               12.57 h
INSTRUM  Avance AV Neo 400
PROBHD   Z108618_0912 (
PULPROG       deptsp135
TD                65536
SOLVENT           CH3OH
NS                  256
DS                    8
SWH           16129.032 Hz
FIDRES         0.492219 Hz
AQ            2.0316160 sec
RG              46.3268
DW               31.000 usec
DE                6.50 usec
TE                298.5 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1
SFO1         100.6208175 MHz
NUC1                13C
P1                10.00 usec
P13             2000.00 usec
PLW0                  0 W
PLW1         53.78799820 W
SPNAM[5]     Crp60comp.4
SPOAL5            0.500
SPOFFS5               0 Hz
SPW5          8.21819973 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz65
P3                14.00 usec
P4                28.00 usec
PCPD2             90.00 usec
PLW2         13.01399994 W
PLW12         0.31492001 W

F2 - Processing parameters
SI                32768
SF           100.6127685 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

HSQC SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3



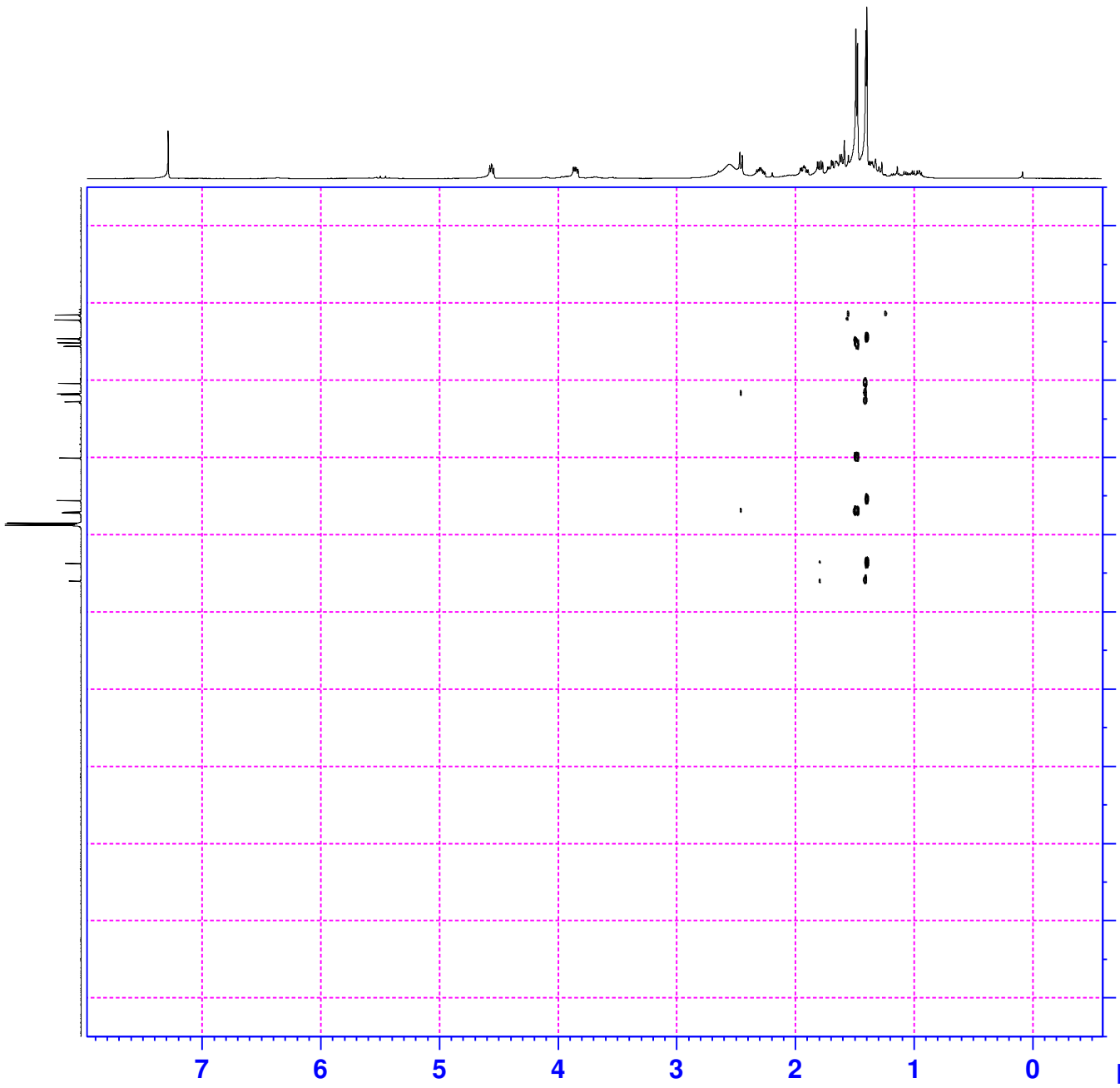

```
Current Data Parameters
NAME      HGSVcaro86-2D
EXPNO               15
PROCNO               1

F2 - Acquisition Parameters
Date_          20220523
Time              12.38 h
INSTRUM  Avance AV Neo 400
PROBHD   Z108618_0912 (
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT           CH3OH
NS                  32
DS                  16
SWH           3424.657 Hz
FIDRES        6.688784 Hz
AQ            0.1495040 sec
RG                 101
DW              146.000 usec
DE                6.50 usec
TE                298.1 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D16          0.00020000 sec
D24          0.00086207 sec
IN0          0.00002259 sec
TDav                 1
ZGOPTNS
SFO1        400.1316262 MHz
NUC1                1H
P1                14.00 usec
P2                28.00 usec
PLW1        13.01399994 W
SFO2        100.6203145 MHz
NUC2                13C
CPDPRG[2           garp
P3                10.00 usec
P4                20.00 usec
PCPD2             80.00 usec
PLW2        53.78799820 W
PLW12        0.84043998 W
GPNAM[1]     SMSQ10.100
GPZ1              80.00 %
GPNAM[2]     SMSQ10.100
GPZ2              20.10 %
GPNAM[3]     SMSQ10.100
GPZ3              11.00 %
GPNAM[4]     SMSQ10.100
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

======== F1 INDIRECT DIMENSION ========
td1      256
sw_F1    220.000000

F1 - Acquisition parameters
TD                 256
SFO1          100.6203 MHz
FIDRES       172.938568 Hz
SW             219.997 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                1024
SF          400.1300038 MHz
WDW               QSINE
SSB                  2
LB                   0 Hz
GB                   0
PC                1.40

F1 - Processing parameters
SI                1024
MC2       echo-antiecho
SF          100.6127390 MHz
WDW               QSINE
SSB                  2
LB                   0 Hz
GB                   0
```

HSQC SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3



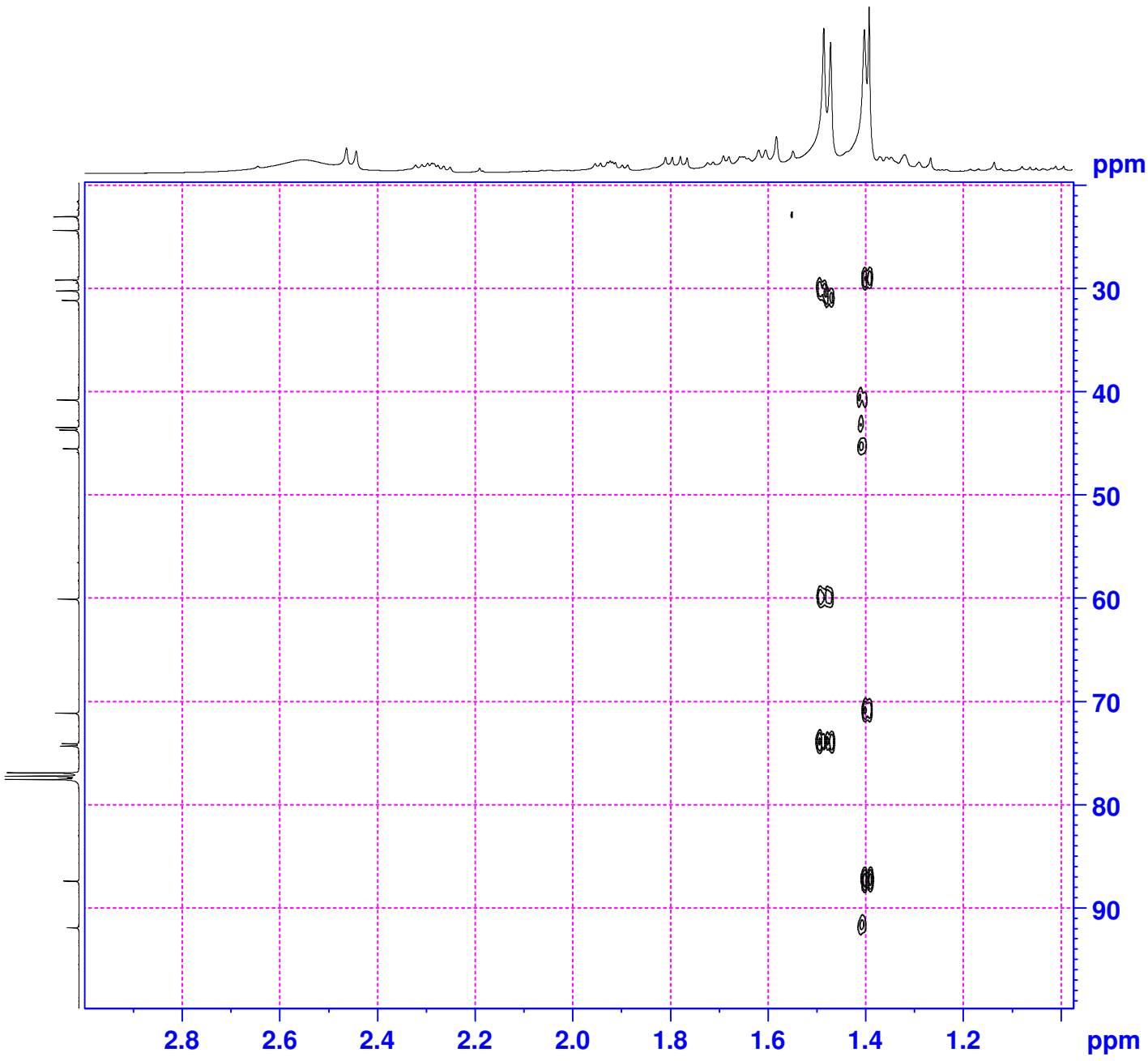

```
Current Data Parameters
NAME      HGSVcaro86-2D
EXPNO               15
PROCNO               1

F2 - Acquisition Parameters
Date_          20220523
Time              12.38 h
INSTRUM  Avance AV Neo 400
PROBHD   Z108618_0912 (
PULPROG     hsqcetgpsi2
TD              1024
SOLVENT          CH3OH
NS                 32
DS                 16
SWH          3424.657 Hz
FIDRES       6.688784 Hz
AQ           0.1495040 sec
RG                101
DW            146.000 usec
DE              6.50 usec
TE             298.1 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D16          0.00020000 sec
D24          0.00086207 sec
IN0          0.00002259 sec
TDav                1
ZGOPTNS
SFO1        400.1316262 MHz
NUC1               1H
P1               14.00 usec
P2               28.00 usec
PLW1        13.01399994 W
SFO2        100.6203145 MHz
NUC2               13C
CPDPRG[2          garp
P3               10.00 usec
P4               20.00 usec
PCPD2            80.00 usec
PLW2        53.78799820 W
PLW12        0.84043998 W
GPNAM[1]     SMSQ10.100
GPZ1             80.00 %
GPNAM[2]     SMSQ10.100
GPZ2             20.10 %
GPNAM[3]     SMSQ10.100
GPZ3             11.00 %
GPNAM[4]     SMSQ10.100
GPZ4             -5.00 %
P16            1000.00 usec
P19             600.00 usec

======== F1 INDIRECT DIMENSION ========
td1      256
sw_F1    220.000000

F1 - Acquisition parameters
TD               256
SFO1          100.6203 MHz
FIDRES       172.938568 Hz
SW             219.997 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI              1024
SF          400.1300038 MHz
WDW             QSINE
SSB                2
LB                 0 Hz
GB                 0
PC              1.40

F1 - Processing parameters
SI              1024
MC2       echo-antiecho
SF          100.6127390 MHz
WDW             QSINE
SSB                2
LB                 0 Hz
GB                 0
```

HMBC SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3



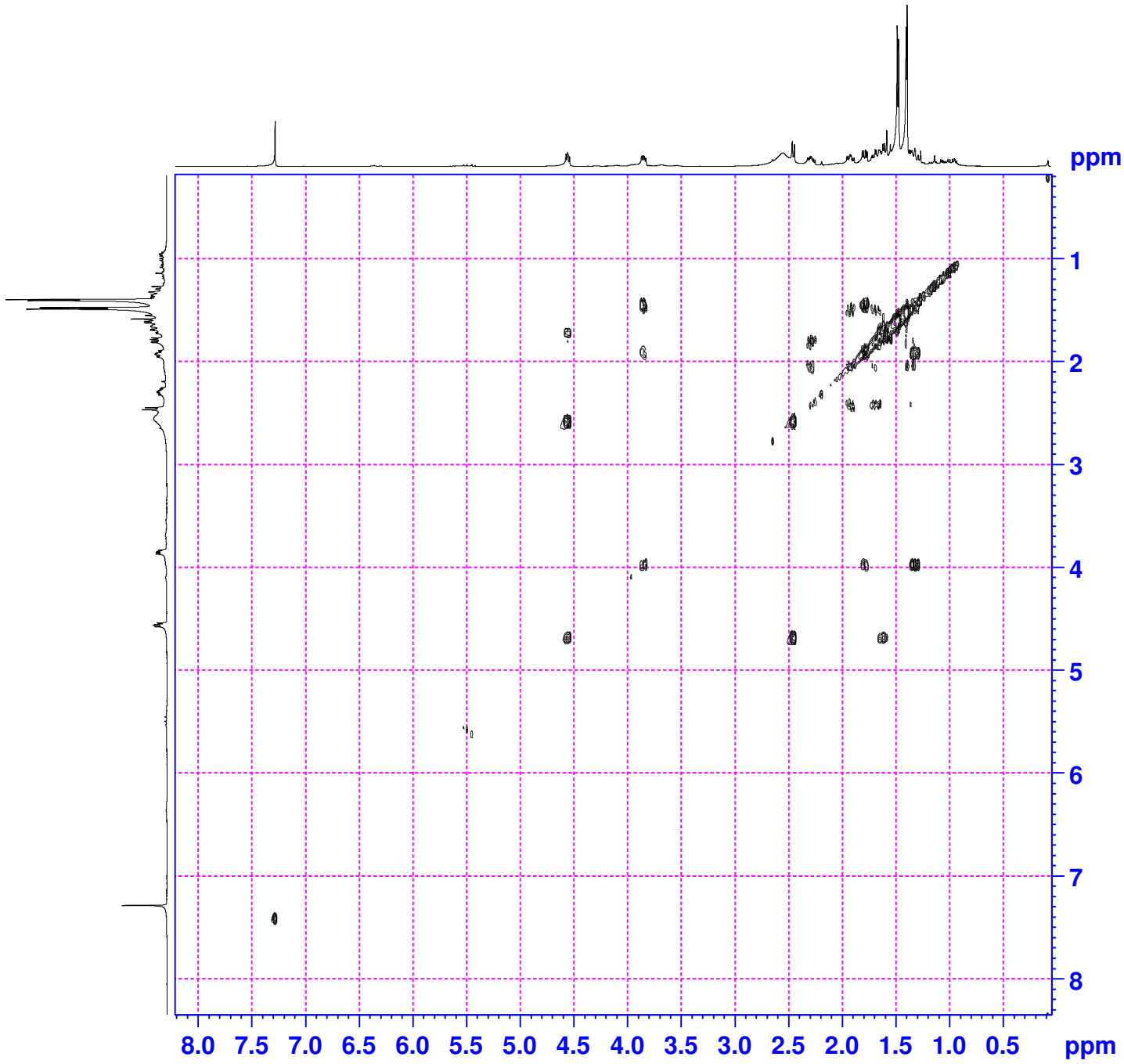

```
Current Data Parameters
NAME       HGSVcaro86-2D
EXPNO                14
PROCNO                1

F2 - Acquisition Parameters
Date_          20220523
Time               8.50 h
INSTRUM  Avance AV Neo 400
PROBHD   Z108618_0912 (
PULPROG    hmbcgplpndqf
TD                 4096
SOLVENT            CH3OH
NS                   32
DS                   16
SWH             3424.657 Hz
FIDRES          1.672196 Hz
AQ             0.5980160 sec
RG                  101
DW                146.000 usec
DE                  6.50 usec
TE                297.9 K
CNST2        145.0000000
CNST13        10.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D2             0.00344828 sec
D6             0.05000000 sec
D16            0.00020000 sec
IN0            0.00002259 sec
TDav                  1
SFO1         400.1314729 MHz
NUC1                 1H
P1                14.00 usec
P2                28.00 usec
PLW1         13.01399994 W
SFO2         100.6228298 MHz
NUC2                 13C
P3                10.00 usec
PLW2         53.78799820 W
GPNAM[1]      SMSQ10.100
GPZ1              50.00 %
GPNAM[2]      SMSQ10.100
GPZ2              30.00 %
GPNAM[3]      SMSQ10.100
GPZ3              40.10 %
P16             1000.00 usec

======== F1 INDIRECT DIMENSION ========
td1       128
sw_F1     220.000000

F1 - Acquisition parameters
TD                 128
SFO1            100.6228 MHz
FIDRES        345.877136 Hz
SW               219.991 ppm
FnMODE                QF

F2 - Processing parameters
SI                 4096
SF           400.1299966 MHz
WDW                QSINE
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.40

F1 - Processing parameters
SI                 1024
MC2                  QF
SF           100.6127685 MHz
WDW                QSINE
SSB                    0
LB                     0 Hz
GB                     0
```

HMBC SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3



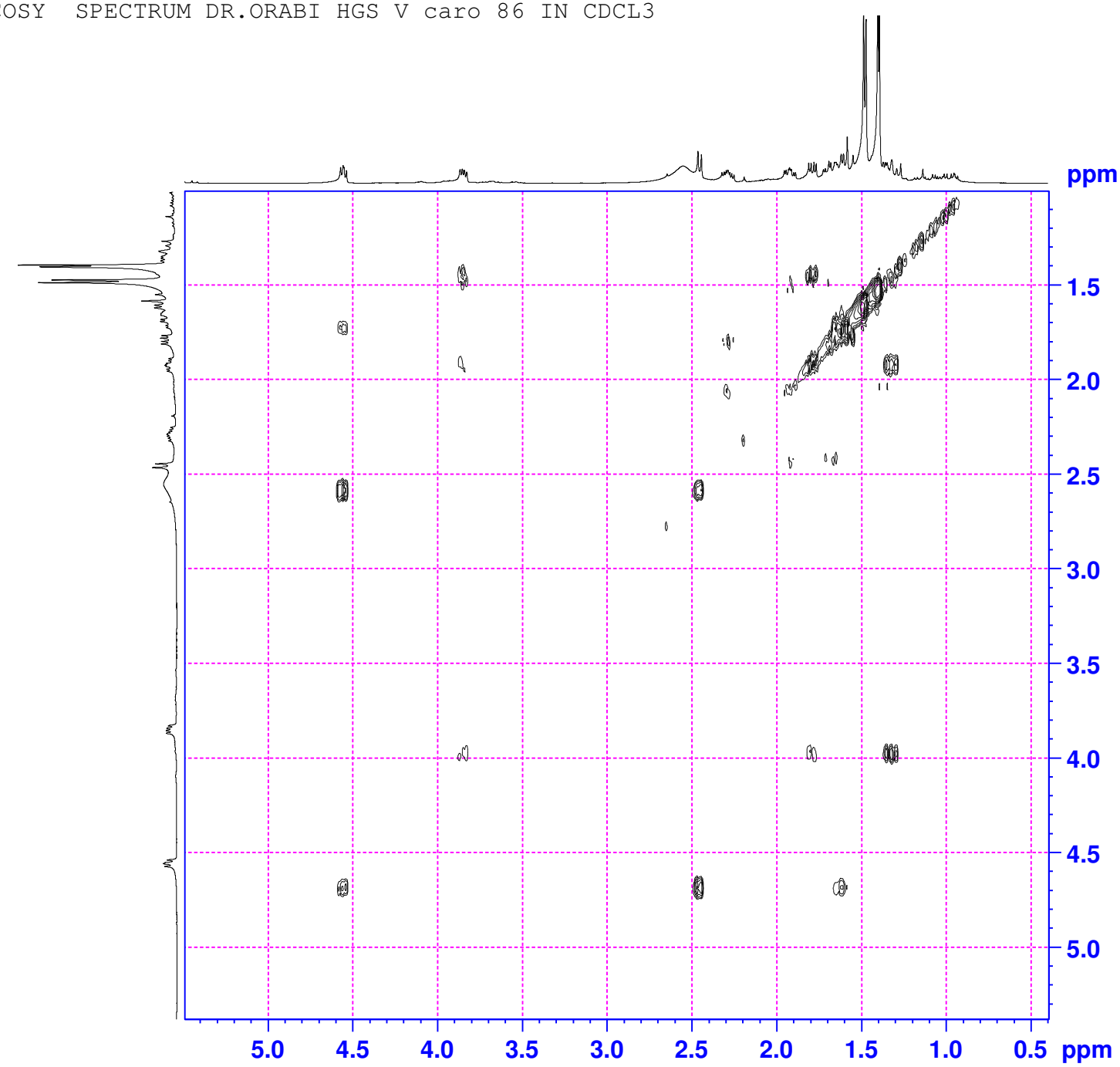

```
Current Data Parameters
NAME       HGSVcaro86-2D
EXPNO                14
PROCNO                1

F2 - Acquisition Parameters
Date_          20220523
Time               8.50 h
INSTRUM  Avance AV Neo 400
PROBHD   Z108618_0912 (
PULPROG    hmbcgplpndqf
TD                 4096
SOLVENT            CH3OH
NS                   32
DS                   16
SWH             3424.657 Hz
FIDRES          1.672196 Hz
AQ             0.5980160 sec
RG                  101
DW                146.000 usec
DE                  6.50 usec
TE                297.9 K
CNST2        145.0000000
CNST13        10.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D2             0.00344828 sec
D6             0.05000000 sec
D16            0.00020000 sec
IN0            0.00002259 sec
TDav                  1
SFO1         400.1314729 MHz
NUC1                  1H
P1                 14.00 usec
P2                 28.00 usec
PLW1         13.01399994 W
SFO2         100.6228298 MHz
NUC2                 13C
P3                 10.00 usec
PLW2         53.78799820 W
GPNAM[1]      SMSQ10.100
GPZ1               50.00 %
GPNAM[2]      SMSQ10.100
GPZ2               30.00 %
GPNAM[3]      SMSQ10.100
GPZ3               40.10 %
P16              1000.00 usec

======== F1 INDIRECT DIMENSION ========
td1       128
sw_F1     220.000000

F1 - Acquisition parameters
TD                   128
SFO1             100.6228 MHz
FIDRES        345.877136 Hz
SW               219.991 ppm
FnMODE                QF

F2 - Processing parameters
SI                  4096
SF            400.1299966 MHz
WDW                 QSINE
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF            100.6127685 MHz
WDW                 QSINE
SSB                     0
LB                      0 Hz
GB                      0
```

COSY SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3




```
Current Data Parameters
NAME       HGSVcaro86-2D
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220523
Time                6.00 h
INSTRUM  Avance AV Neo 400
PROBHD   Z108618_0912 (
PULPROG      cosygpppqf
TD                  2048
SOLVENT            CH3OH
NS                     8
DS                    16
SWH             3267.974 Hz
FIDRES             3.191381 Hz
AQ              0.3133440 sec
RG                   101
DW                153.000 usec
DE                  6.50 usec
TE                298.4 K
D0             0.00000300 sec
D1             1.88735998 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00030600 sec
TDav                   1
SFO1         400.1316515 MHz
NUC1                  1H
P0                 14.00 usec
P1                 14.00 usec
P17              2500.00 usec
PLW1         13.01399994 W
PLW10         2.83430004 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

======== F1 INDIRECT DIMENSION ========
td1       128
sw_F1     8.167247

F1 - Acquisition parameters
TD                   128
SFO1            400.1317 MHz
FIDRES          51.062092 Hz
SW                 8.167 ppm
FnMODE                QF

F2 - Processing parameters
SI                  1024
SF           400.1299976 MHz
WDW                 QSINE
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1299447 MHz
WDW                 QSINE
SSB                     0
LB                      0 Hz
GB                      0
```

COSY SPECTRUM DR.ORABI HGS V caro 86 IN CDCL3



Current Data Parameters
NAME HGSVcaro86-2D
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220523
Time 6.00 h
INSTRUM Avance AV Neo 400
PROBHD Z108618_0912 (
PULPROG cosygpppqf
TD 2048
SOLVENT CH3OH
NS 8
DS 16
SWH 3267.974 Hz
FIDRES 3.191381 Hz
AQ 0.3133440 sec
RG 101
DW 153.000 usec
DE 6.50 usec
TE 298.4 K
D0 0.00000300 sec
D1 1.88735998 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00030600 sec
TDav 1
SFO1 400.1316515 MHz
NUC1 1H
P0 14.00 usec
P1 14.00 usec
P17 2500.00 usec
PLW1 13.01399994 W
PLW10 2.83430004 W
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

======== F1 INDIRECT DIMENSION ========
td1 128
sw_F1 8.167247

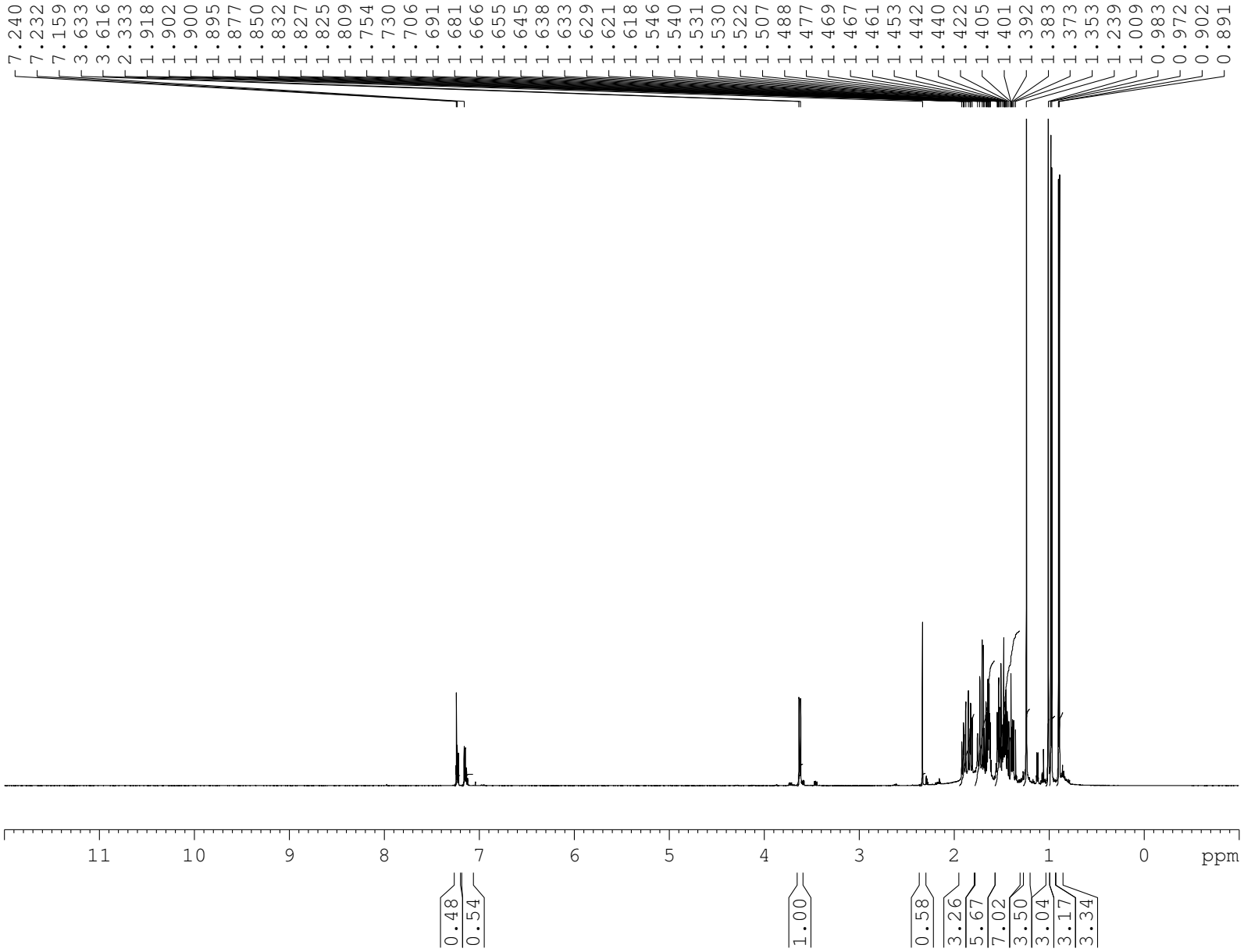
F1 - Acquisition parameters
TD 128
SFO1 400.1317 MHz
FIDRES 51.062092 Hz
SW 8.167 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1299976 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1299447 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

S4: 1H, 13C, DEPT-135, HSQC, HMBC and COSY spectra of CM3 (**4**)

1H spectra Dr.Orabi Caro M3 in CDCL3



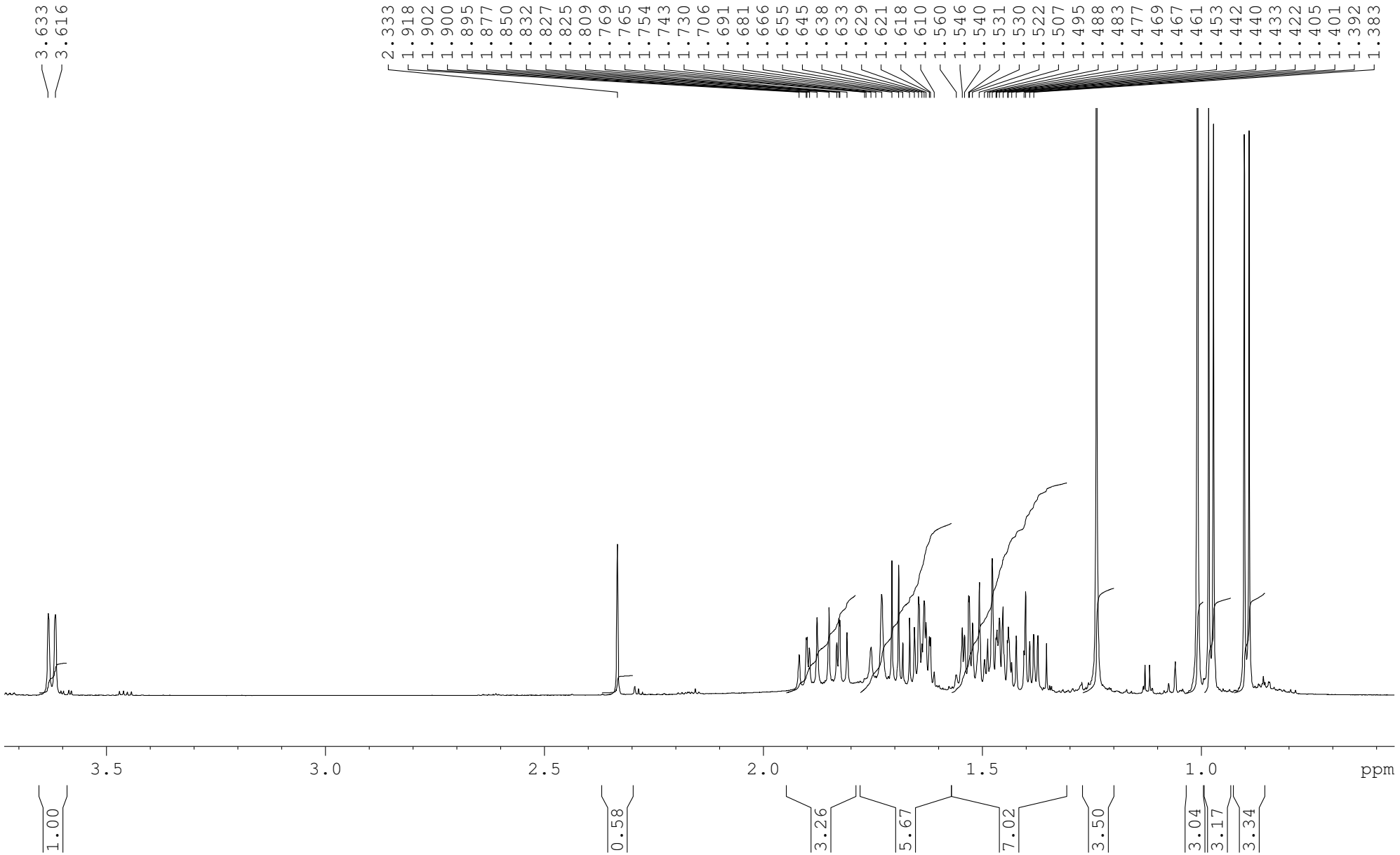
Current Data Parameters
NAME CaroM3-2D
EXPNO 2
PROCNO 1

F2 - Acquisition Parameter
Date_ 20220630
Time 14.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 se
RG 203
DW 40.533 us
DE 20.00 us
TE 298.0 K
D1 1.00000000 se
TD0 1

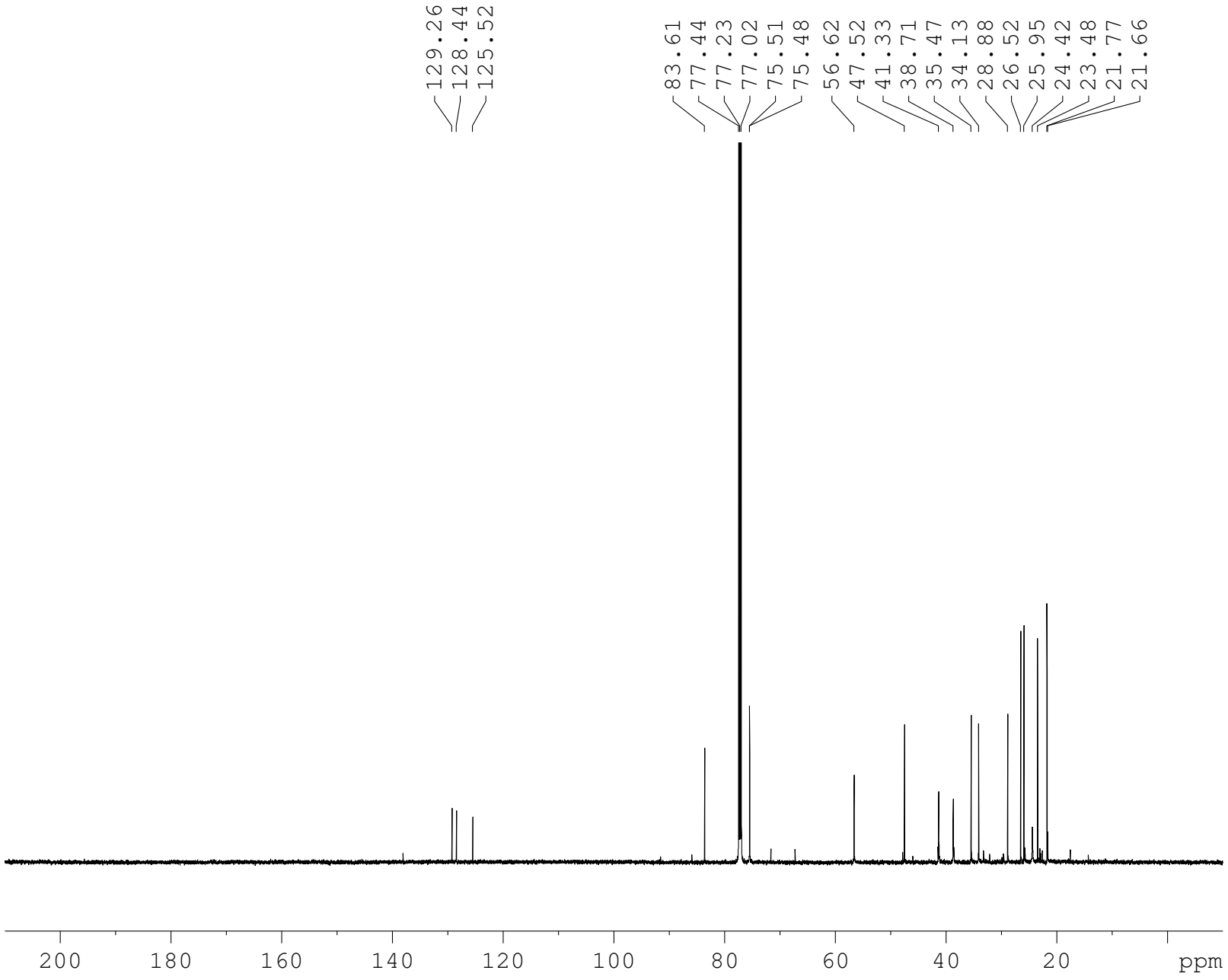
======== CHANNEL f1 ======
SFO1 600.1337060 MH
NUC1 1H
P1 10.60 us
PLW1 27.82500076 W

F2 - Processing parameters
SI 32768
SF 600.1300280 MH
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1H spectra Dr.Orabi Caro M3 in CDCL3



13C decoupled spectra Dr.Orabi Caro M3 in CDCL3



Current Data Parameters
NAME CaroM3-2D
EXPNO 3
PROCNO 1

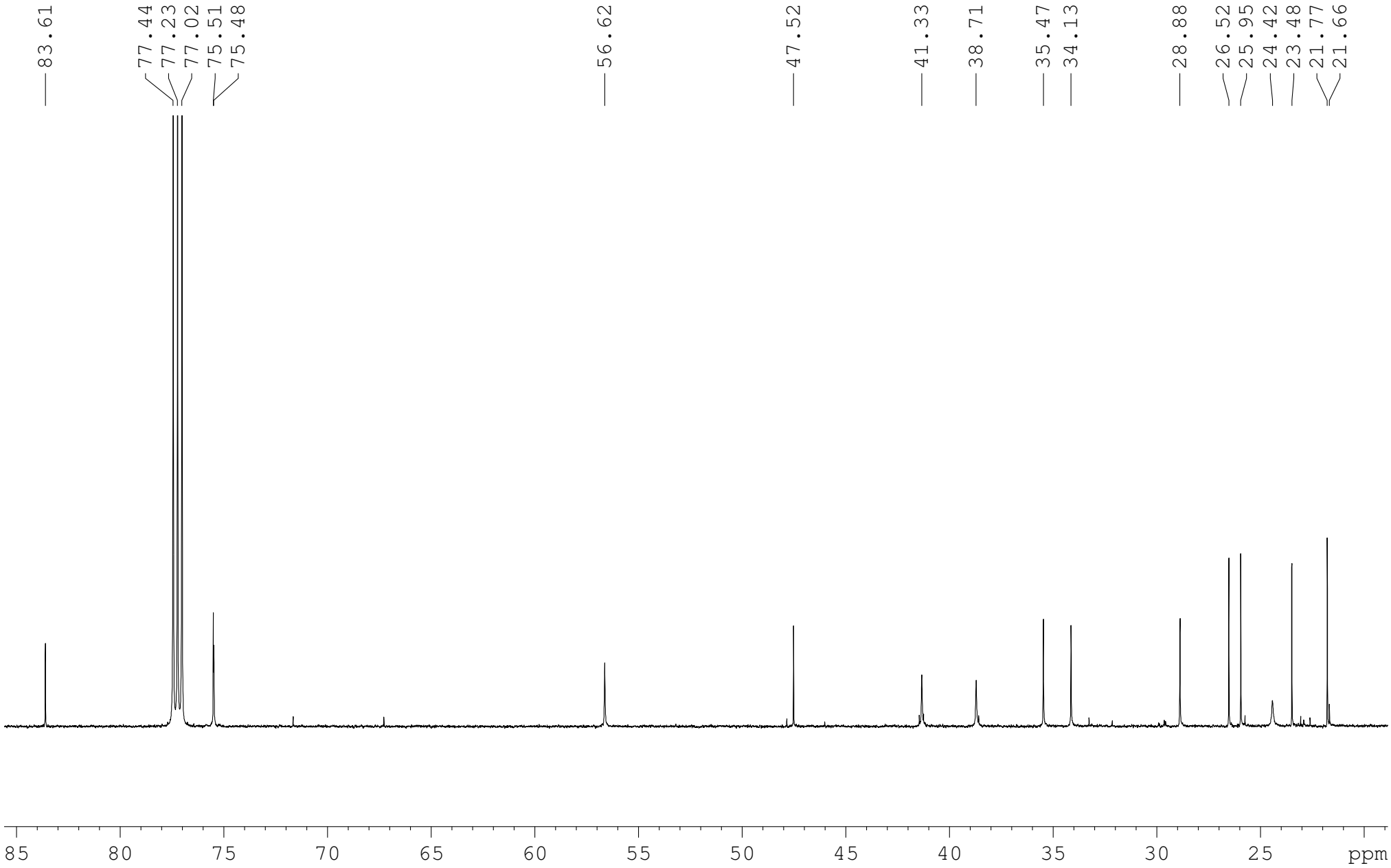
F2 - Acquisition Parameters
Date_ 20220630
Time 22.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10240
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 150.9178979 MHz
NUC1 13C
P1 8.80 usec
PLW1 78.13500214 W

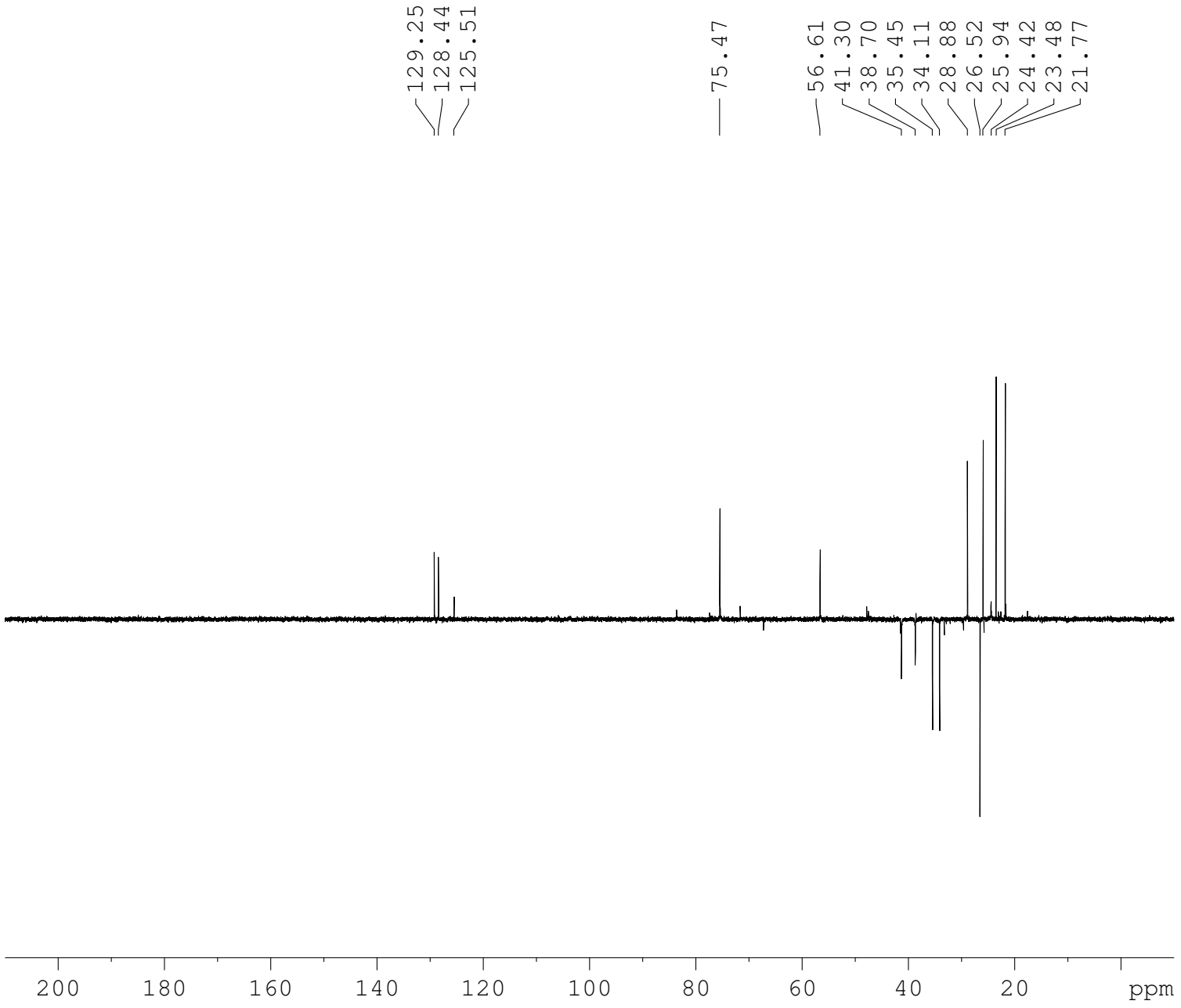
======== CHANNEL f2 ========
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W
PLW13 0.31264001 W

F2 - Processing parameters
SI 32768
SF 150.9027757 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13C decoupled spectra Dr.Orabi Caro M3 in CDCL3



DEPT 135 spectra Dr.Orabi Caro M3 in CDCL3



Current Data Parameters
NAME CaroM3-2D
EXPNO 6
PROCNO 1

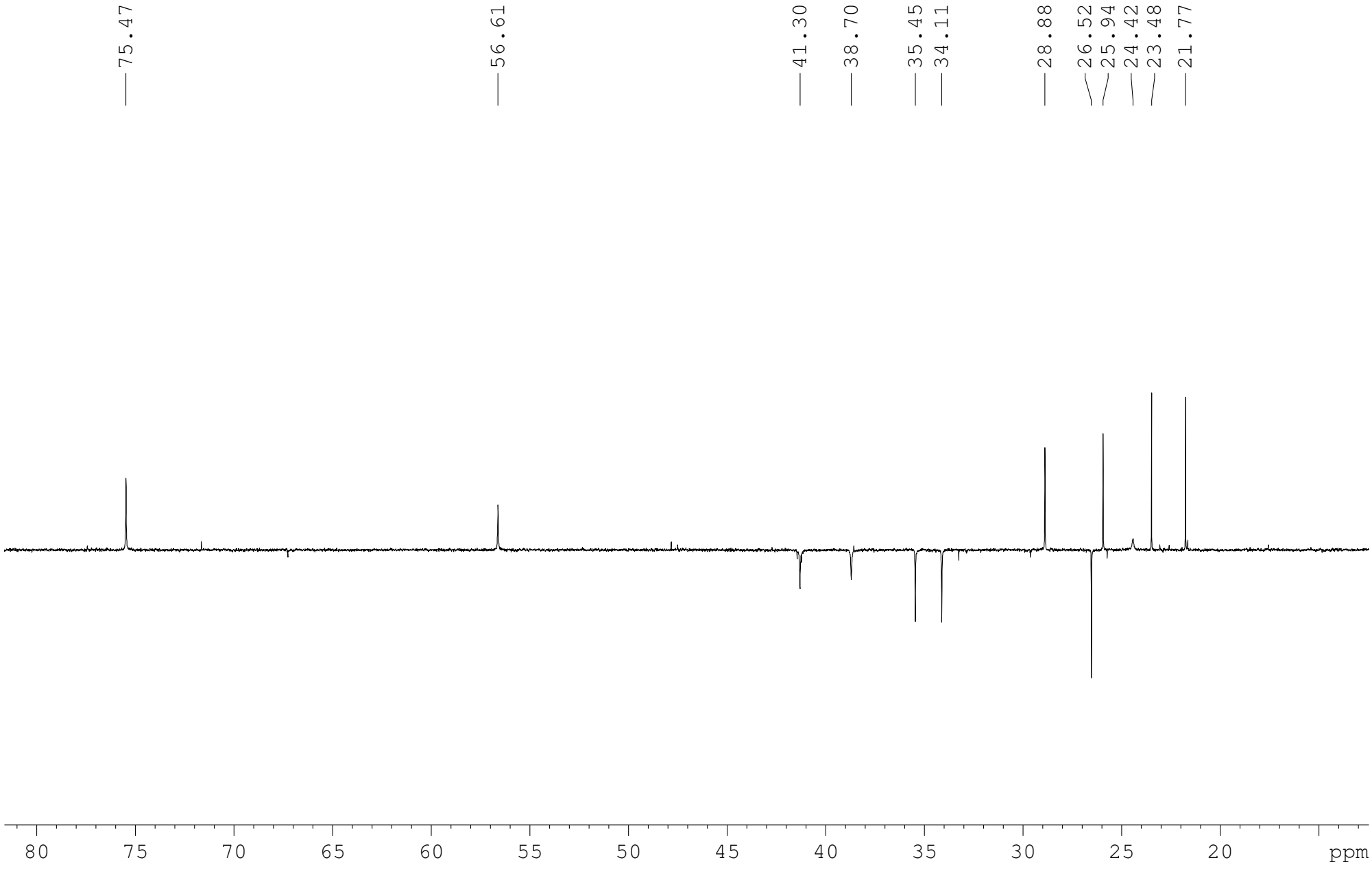
F2 - Acquisition Parameters
Date_ 20220701
Time 8.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 299.4 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 150.9178979 MHz
NUC1 13C
P1 8.80 usec
P13 2000.00 usec
PLW0 0 W
PLW1 78.13500214 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 9.24489975 W

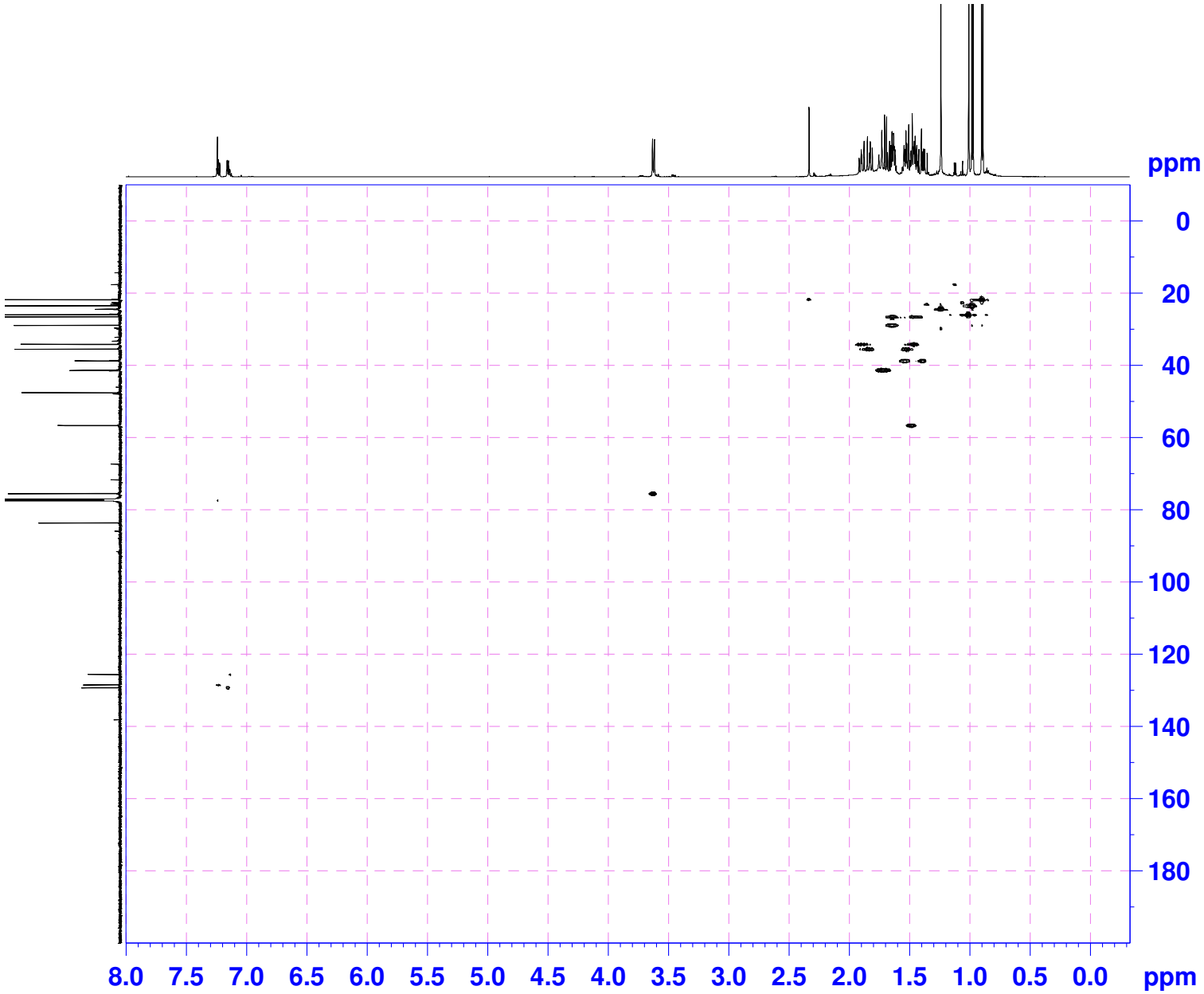
======== CHANNEL f2 ========
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz65
P3 10.60 usec
P4 21.20 usec
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W

F2 - Processing parameters
SI 32768
SF 150.9027774 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DEPT 135 spectra Dr.Orabi Caro M3 in CDCL3



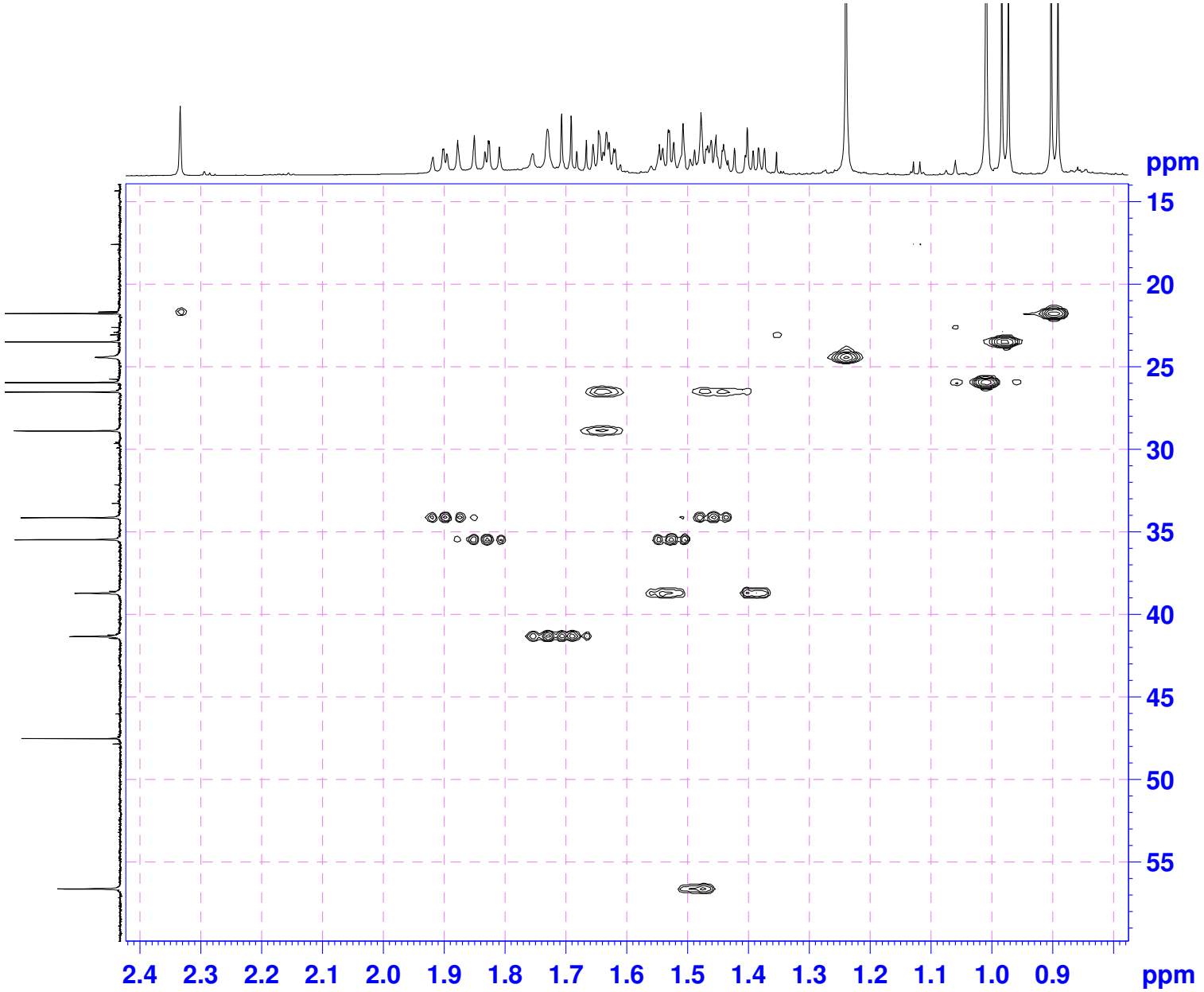
13C HSQC spectra Dr.Orabi Caro M3 in CDCL3



BRUKER

```
Current Data Parameters
NAME                  CaroM3-2D
EXPNO                         8
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20220701
Time                       9.35
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG     hsqcetgpsp.2
TD                         2048
SOLVENT                   CDC13
NS                           16
DS                           16
SWH                  5000.000 Hz
FIDRES               2.441406 Hz
AQ                   0.2048000 sec
RG                         203
DW                   100.000 usec
DE                    20.00 usec
TE                    299.1 K
CNST2               145.0000000
D0                   0.00000300 sec
D1                   1.90169597 sec
D4                   0.00172414 sec
D11                  0.03000000 sec
D16                  0.00020000 sec
IN0                  0.00001840 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1                600.1323288 MHz
NUC1                        1H
P1                    10.60 usec
P2                    21.20 usec
P28                 1000.00 usec
PLW1               27.82500076 W

======== CHANNEL f2 ========
SFO2                150.9178993 MHz
NUC2                        13C
CPDPRG[2                 garp4
P3                     8.80 usec
P14                  500.00 usec
P24                 2000.00 usec
PCPD2                 60.00 usec
PLW0          0 W
PLW2               78.13500214 W
PLW12               1.68079996 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                 0.500
SPOFFS3  0 Hz
SPW3                9.24489975 W
SPNAM[7]    Crp60comp.4
SPOAL7                 0.500
SPOFFS7  0 Hz
SPW7                9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]              SINE.100
GPNAM[2]              SINE.100
GPZ1                     80.00 %
GPZ2                     20.10 %
P16                   1000.00 usec

F1 - Acquisition parameters
TD                         512
SFO1                150.9179 MHz
FIDRES              53.074047 Hz
SW                   180.058 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                         2048
SF                  600.1300268 MHz
WDW                       QSINE
SSB                           2
LB                0 Hz
GB                0
PC                        1.40

F1 - Processing parameters
SI                         1024
MC2               echo-antiecho
SF                  150.9027635 MHz
WDW                       QSINE
SSB                           2
LB                0 Hz
GB                0
```

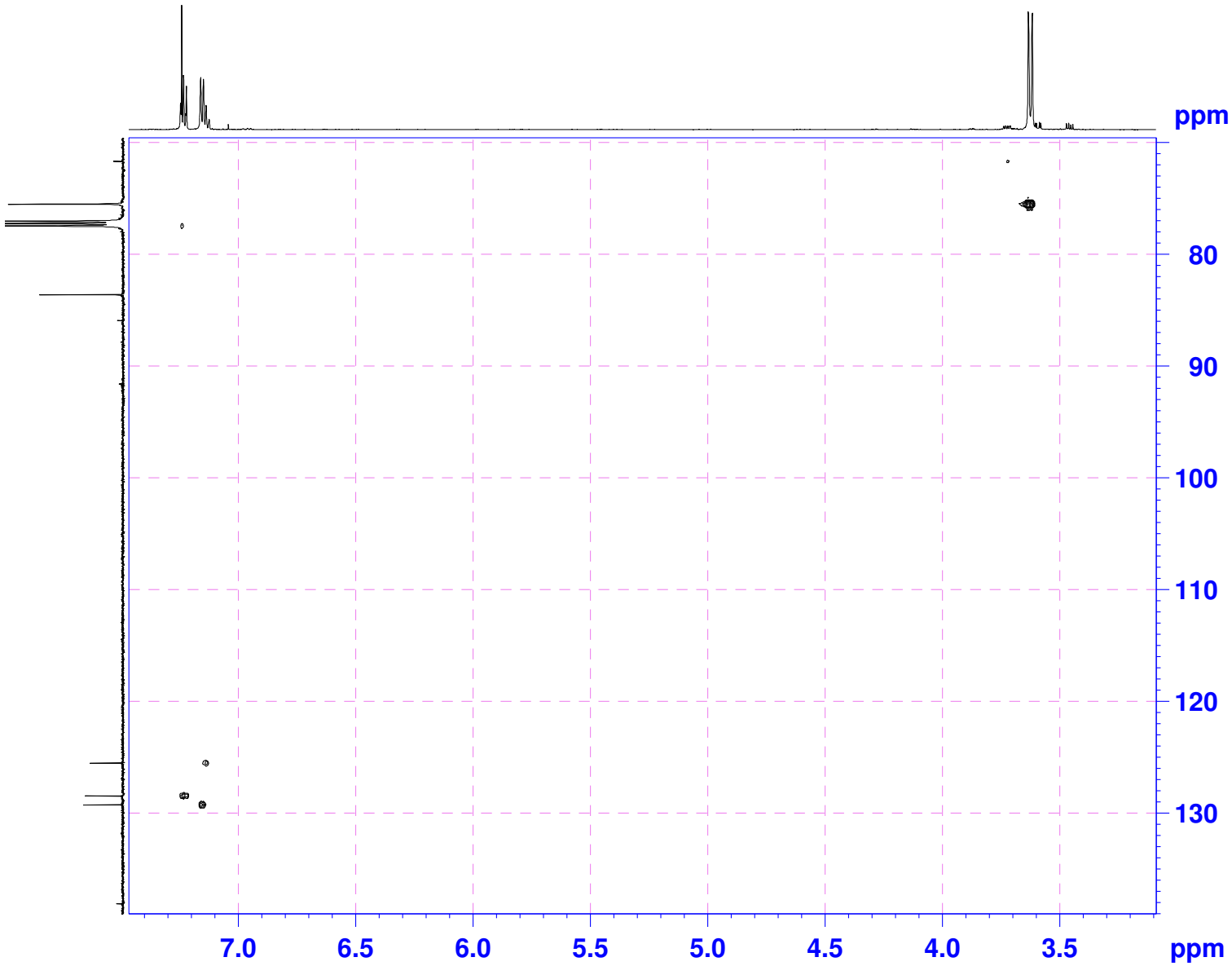
13C HSQC spectra Dr.Orabi Caro M3 in CDCL3



BRUKER

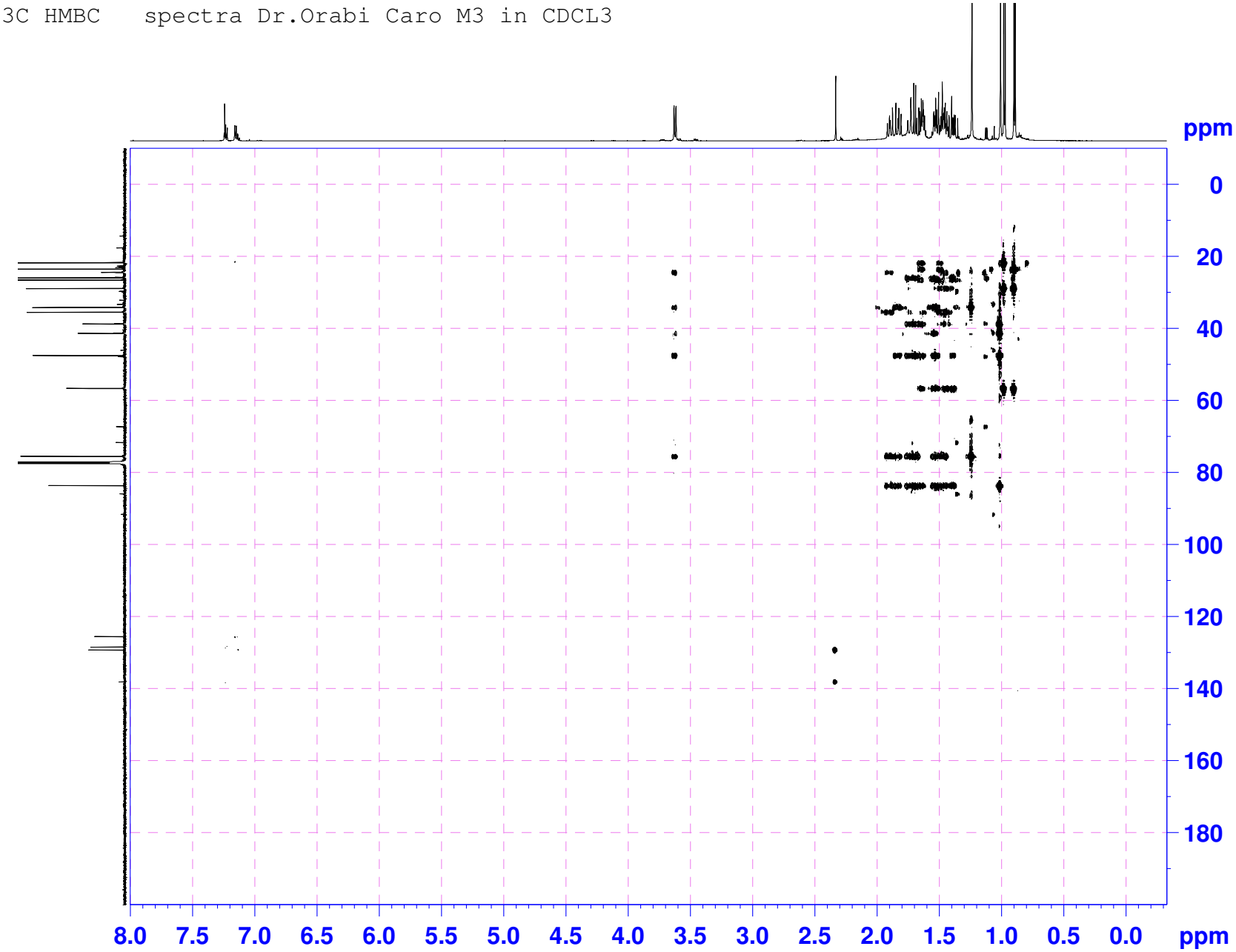
```
Current Data Parameters
NAME                  CaroM3-2D
EXPNO                         8
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20220701
Time                       9.35
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG     hsqcetgpsp.2
TD                         2048
SOLVENT                   CDCl3
NS                           16
DS                           16
SWH                5000.000 Hz
FIDRES                2.441406 Hz
AQ                 0.2048000 sec
RG                         203
DW                   100.000 usec
DE                    20.00 usec
TE                    299.1 K
CNST2              145.0000000
D0                 0.00000300 sec
D1                 1.90169597 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D16                0.00020000 sec
IN0                0.00001840 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1             600.1323288 MHz
NUC1                       1H
P1                    10.60 usec
P2                    21.20 usec
P28                 1000.00 usec
PLW1              27.82500076 W

======== CHANNEL f2 ========
SFO2             150.9178993 MHz
NUC2                      13C
CPDPRG[2                garp4
P3                     8.80 usec
P14                  500.00 usec
P24                 2000.00 usec
PCPD2                 60.00 usec
PLW0          0 W
PLW2             78.13500214 W
PLW12             1.68079996 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                 0.500
SPOFFS3  0 Hz
SPW3              9.24489975 W
SPNAM[7]     Crp60comp.4
SPOAL7                 0.500
SPOFFS7  0 Hz
SPW7              9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]            SINE.100
GPNAM[2]            SINE.100
GPZ1                  80.00 %
GPZ2                  20.10 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                         512
SFO1                150.9179 MHz
FIDRES             53.074047 Hz
SW                  180.058 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                         2048
SF                600.1300268 MHz
WDW                       QSINE
SSB                           2
LB             0 Hz
GB             0
PC                         1.40

F1 - Processing parameters
SI                         1024
MC2             echo-antiecho
SF                150.9027635 MHz
WDW                       QSINE
SSB                           2
LB             0 Hz
GB             0
```

13C HSQC spectra Dr.Orabi Caro M3 in CDCL3




```
Current Data Parameters
NAME                  CaroM3-2D
EXPNO                         8
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20220701
Time                       9.35
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG     hsqcetgpsp.2
TD                         2048
SOLVENT                   CDC13
NS                           16
DS                           16
SWH                5000.000 Hz
FIDRES              2.441406 Hz
AQ                 0.2048000 sec
RG                         203
DW                   100.000 usec
DE                    20.00 usec
TE                    299.1 K
CNST2             145.0000000
D0                 0.00000300 sec
D1                 1.90169597 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D16                0.00020000 sec
IN0                0.00001840 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1             600.1323288 MHz
NUC1                       1H
P1                    10.60 usec
P2                    21.20 usec
P28                 1000.00 usec
PLW1             27.82500076 W

======== CHANNEL f2 ========
SFO2             150.9178993 MHz
NUC2                      13C
CPDPRG[2                garp4
P3                     8.80 usec
P14                  500.00 usec
P24                 2000.00 usec
PCPD2                 60.00 usec
PLW0          0 W
PLW2            78.13500214 W
PLW12            1.68079996 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3                0.500
SPOFFS3  0 Hz
SPW3             9.24489975 W
SPNAM[7]     Crp60comp.4
SPOAL7                0.500
SPOFFS7  0 Hz
SPW7             9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]            SINE.100
GPNAM[2]            SINE.100
GPZ1                  80.00 %
GPZ2                  20.10 %
P16                 1000.00 usec

F1 - Acquisition parameters
TD                          512
SFO1                150.9179 MHz
FIDRES             53.074047 Hz
SW                   180.058 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                         2048
SF                600.1300268 MHz
WDW                       QSINE
SSB                           2
LB             0 Hz
GB             0
PC                         1.40

F1 - Processing parameters
SI                         1024
MC2               echo-antiecho
SF                150.9027635 MHz
WDW                       QSINE
SSB                           2
LB             0 Hz
GB             0
```

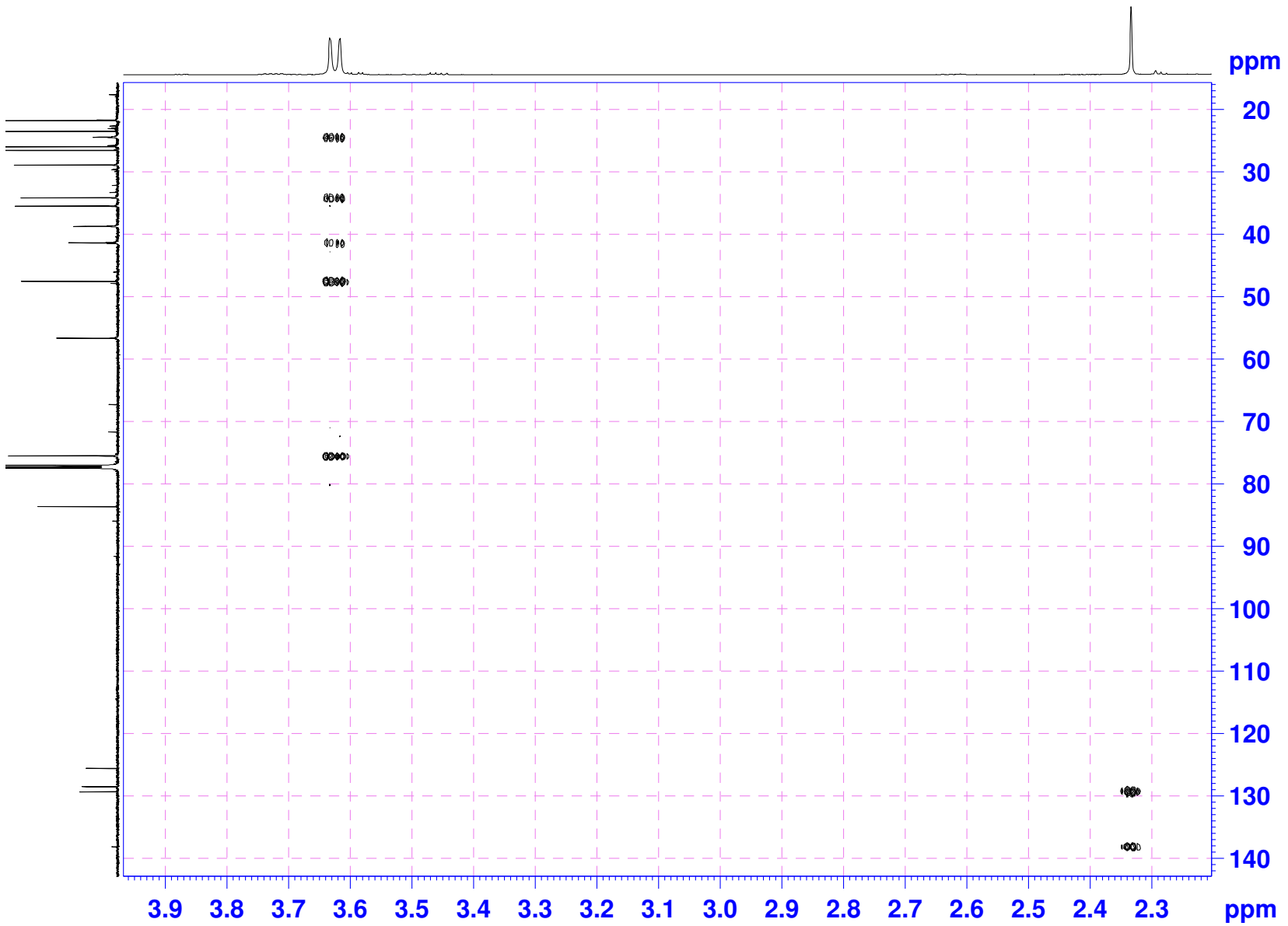
13C HMBC spectra Dr.Orabi Caro M3 in CDCL3



BRUKER

```
Current Data Parameters
NAME          CaroM3-2D
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Date_          20220701
Time              14.29
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG   hmbcetgpl2nd
TD                2048
SOLVENT           CDCl3
NS                  32
DS                  16
SWH         5000.000 Hz
FIDRES      2.441406 Hz
AQ          0.2048000 sec
RG                 203
DW           100.000 usec
DE            20.00 usec
TE            298.8 K
CNST6       125.0000000
CNST7       165.0000000
CNST13       10.0000000
CNST30        0.5981151
D0         0.00000300 sec
D1         1.42627203 sec
D6         0.05000000 sec
D16        0.00020000 sec
IN0        0.00001490 sec

======== CHANNEL f1 ========
SFO1        600.1323288 MHz
NUC1               1H
P1              10.60 usec
P2              21.20 usec
PLW1        27.82500076 W

======== CHANNEL f2 ========
SFO2        150.9178738 MHz
NUC2               13C
P3               8.80 usec
P24           2000.00 usec
PLW2        78.13500214 W
SPNAM[7]    Crp60comp.4
SPOAL7           0.500
SPOFFS7  0 Hz
SPW7         9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]       SINE.100
GPNAM[3]       SINE.100
GPNAM[4]       SINE.100
GPNAM[5]       SINE.100
GPZ1             80.00 %
GPZ3             15.00 %
GPZ4            -10.00 %
GPZ5             -5.00 %
P16           1000.00 usec

F1 - Acquisition parameters
TD                 256
SFO1          150.9179 MHz
FIDRES       131.082214 Hz
SW            222.353 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                2048
SF          600.1300257 MHz
WDW               SINE
SSB       0
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                 512
MC2        echo-antiecho
SF          150.9027314 MHz
WDW               SINE
SSB                  2
LB        0 Hz
GB        0
```

13C HMBC spectra Dr.Orabi Caro M3 in CDCL3



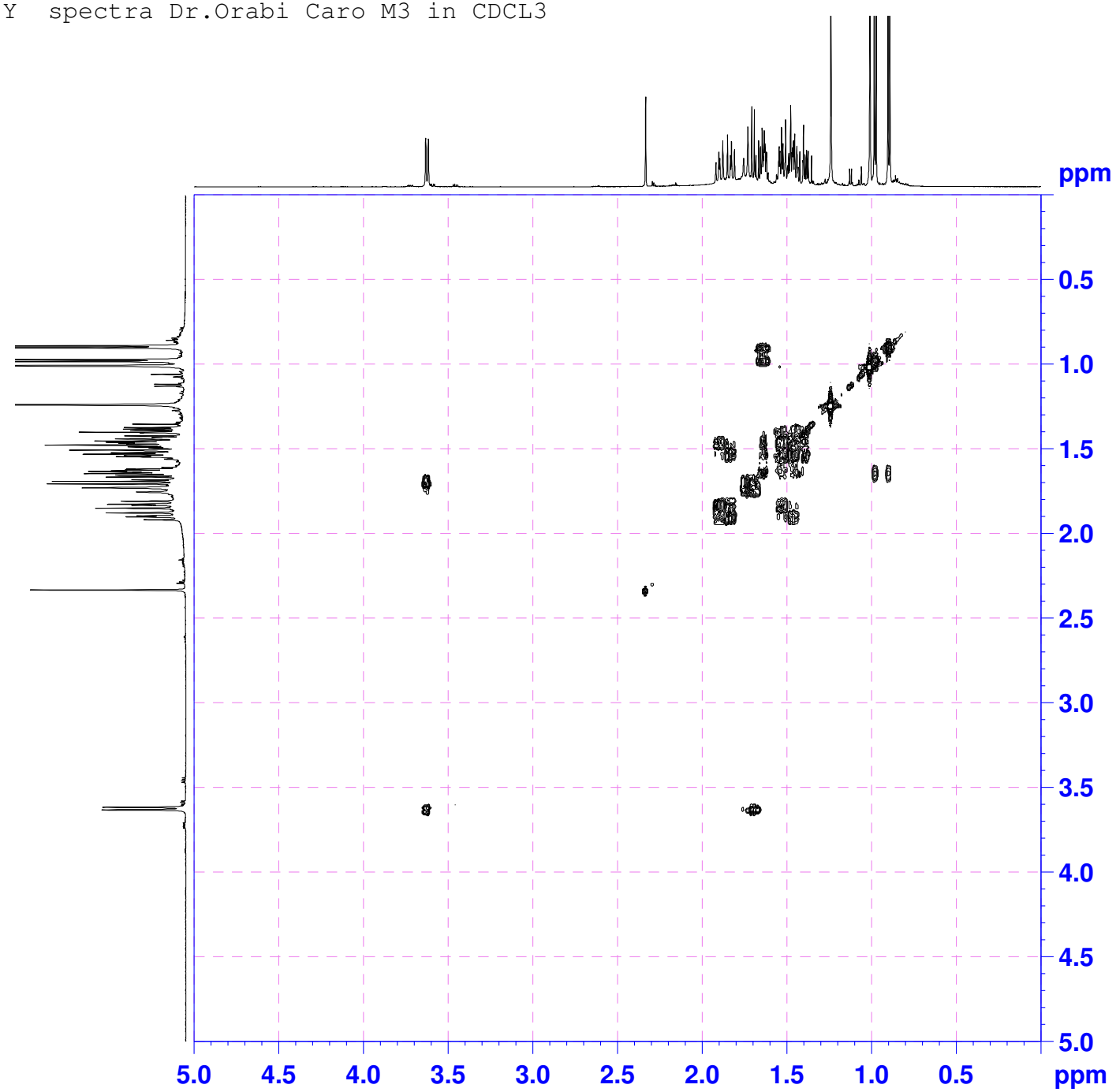

```
Current Data Parameters
NAME          CaroM3-2D
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Date_          20220701
Time              14.29
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG   hmbcetgpl2nd
TD                2048
SOLVENT           CDCl3
NS                  32
DS                  16
SWH           5000.000 Hz
FIDRES        2.441406 Hz
AQ            0.2048000 sec
RG                203
DW              100.000 usec
DE               20.00 usec
TE               298.8 K
CNST6       125.0000000
CNST7       165.0000000
CNST13       10.0000000
CNST30        0.5981151
D0          0.00000300 sec
D1          1.42627203 sec
D6          0.05000000 sec
D16         0.00020000 sec
IN0         0.00001490 sec

======== CHANNEL f1 ========
SFO1        600.1323288 MHz
NUC1                1H
P1                10.60 usec
P2                21.20 usec
PLW1        27.82500076 W

======== CHANNEL f2 ========
SFO2        150.9178738 MHz
NUC2                13C
P3                 8.80 usec
P24             2000.00 usec
PLW2        78.13500214 W
SPNAM[7]    Crp60comp.4
SPOAL7            0.500
SPOFFS7  0 Hz
SPW7         9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]       SINE.100
GPNAM[3]       SINE.100
GPNAM[4]       SINE.100
GPNAM[5]       SINE.100
GPZ1              80.00 %
GPZ3              15.00 %
GPZ4             -10.00 %
GPZ5              -5.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                 256
SFO1           150.9179 MHz
FIDRES        131.082214 Hz
SW             222.353 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                2048
SF          600.1300257 MHz
WDW               SINE
SSB       0
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                 512
MC2        echo-antiecho
SF          150.9027314 MHz
WDW               SINE
SSB                  2
LB        0 Hz
GB        0
```

13C HMBC spectra Dr.Orabi Caro M3 in CDCL3

BRUKER

```
Current Data Parameters
NAME          CaroM3-2D
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Date_          20220701
Time              14.29
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG   hmbcetgpl2nd
TD                2048
SOLVENT           CDCl3
NS                  32
DS                  16
SWH           5000.000 Hz
FIDRES        2.441406 Hz
AQ            0.2048000 sec
RG                203
DW             100.000 usec
DE              20.00 usec
TE              298.8 K
CNST6       125.0000000
CNST7       165.0000000
CNST13       10.0000000
CNST30        0.5981151
D0          0.00000300 sec
D1          1.42627203 sec
D6          0.05000000 sec
D16         0.00020000 sec
IN0         0.00001490 sec

======== CHANNEL f1 ========
SFO1        600.1323288 MHz
NUC1                1H
P1                10.60 usec
P2                21.20 usec
PLW1        27.82500076 W

======== CHANNEL f2 ========
SFO2        150.9178738 MHz
NUC2                13C
P3                 8.80 usec
P24             2000.00 usec
PLW2        78.13500214 W
SPNAM[7]    Crp60comp.4
SPOAL7            0.500
SPOFFS7  0 Hz
SPW7         9.24489975 W

====== GRADIENT CHANNEL =====
GPNAM[1]        SINE.100
GPNAM[3]        SINE.100
GPNAM[4]        SINE.100
GPNAM[5]        SINE.100
GPZ1              80.00 %
GPZ3              15.00 %
GPZ4             -10.00 %
GPZ5              -5.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                 256
SFO1           150.9179 MHz
FIDRES        131.082214 Hz
SW              222.353 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                2048
SF          600.1300257 MHz
WDW               SINE
SSB       0
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                 512
MC2        echo-antiecho
SF          150.9027314 MHz
WDW               SINE
SSB                  2
LB        0 Hz
GB        0
```

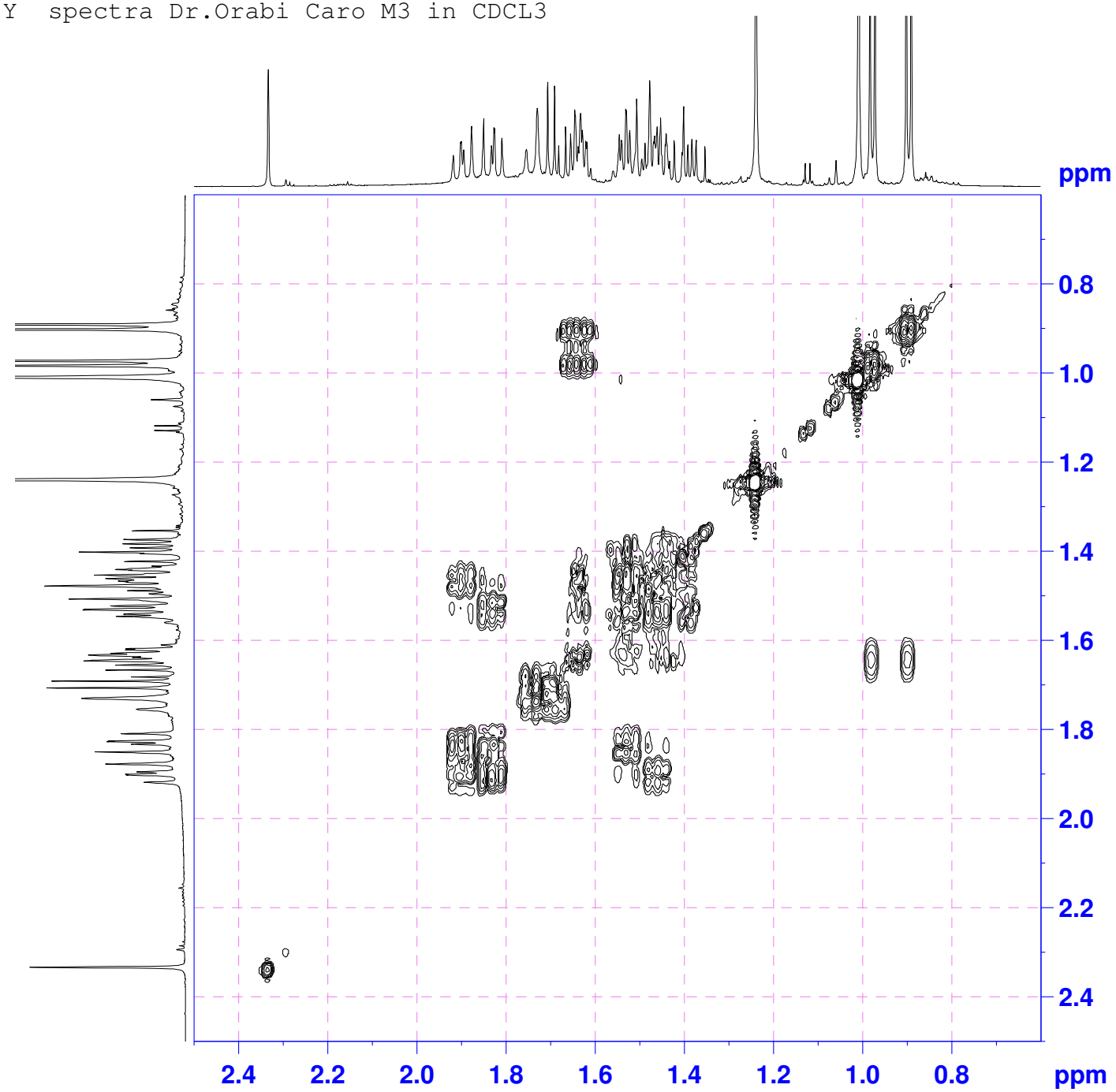
COSY spectra Dr.Orabi Caro M3 in CDCL3



BRUKER

```
Current Data Parameters
NAME            CaroM3-2D
EXPNO                   7
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220701
Time                8.50
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                      8
DS                      8
SWH              4854.369 Hz
FIDRES           2.370297 Hz
AQ               0.2109440 sec
RG                   90.5
DW                 103.000 usec
DE                  20.00 usec
TE                  298.8 K
D0               0.00000300 sec
D1               0.66685098 sec
D11              0.03000000 sec
D12              0.00002000 sec
D13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00020600 sec

======== CHANNEL f1 ========
SFO1          600.1322713 MHz
NUC1                  1H
P0                  10.60 usec
P1                  10.60 usec
P17               2500.00 usec
PLW1         27.82500076 W
PLW10         4.62489986 W

====== GRADIENT CHANNEL =====
GPNAM[1]         SINE.100
GPZ1                20.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    320
SFO1             600.1323 MHz
FIDRES          15.169903 Hz
SW                  8.089 ppm
FnMODE                QF

F2 - Processing parameters
SI                    2048
SF           600.1300250 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                    2048
MC2                   QF
SF           600.1300235 MHz
WDW                 SINE
SSB       0
LB        0 Hz
GB        0
```

COSY spectra Dr.Orabi Caro M3 in CDCL3



Current Data Parameters
NAME CaroM3-2D
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220701
Time 8.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 8
DS 8
SWH 4854.369 Hz
FIDRES 2.370297 Hz
AQ 0.2109440 sec
RG 90.5
DW 103.000 usec
DE 20.00 usec
TE 298.8 K
D0 0.00000300 sec
D1 0.66685098 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00020600 sec

======== CHANNEL f1 ========
SFO1 600.1322713 MHz
NUC1 1H
P0 10.60 usec
P1 10.60 usec
P17 2500.00 usec
PLW1 27.82500076 W
PLW10 4.62489986 W

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPZ1 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 320
SFO1 600.1323 MHz
FIDRES 15.169903 Hz
SW 8.089 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.1300250 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 2048
MC2 QF
SF 600.1300235 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0