

Supplementary Information

Terretonin, ophiobolin, and drimane terpenes with absolute configurations from an algicolous *Aspergillus ustus*

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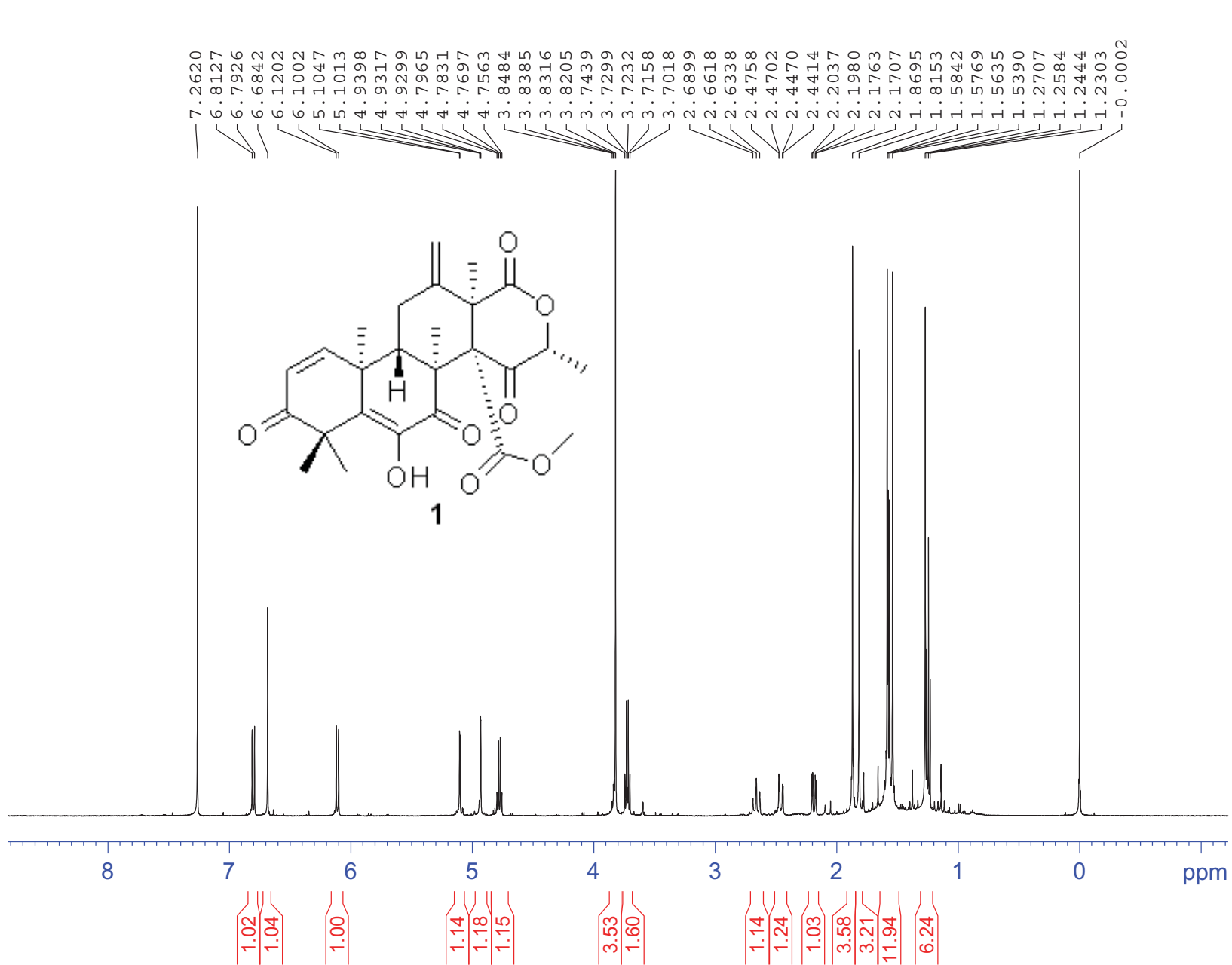
^b*University of Oklahoma, Norman, Oklahoma 73019, United States*

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- S4, ¹³C NMR and DEPT spectra of compound **1**;
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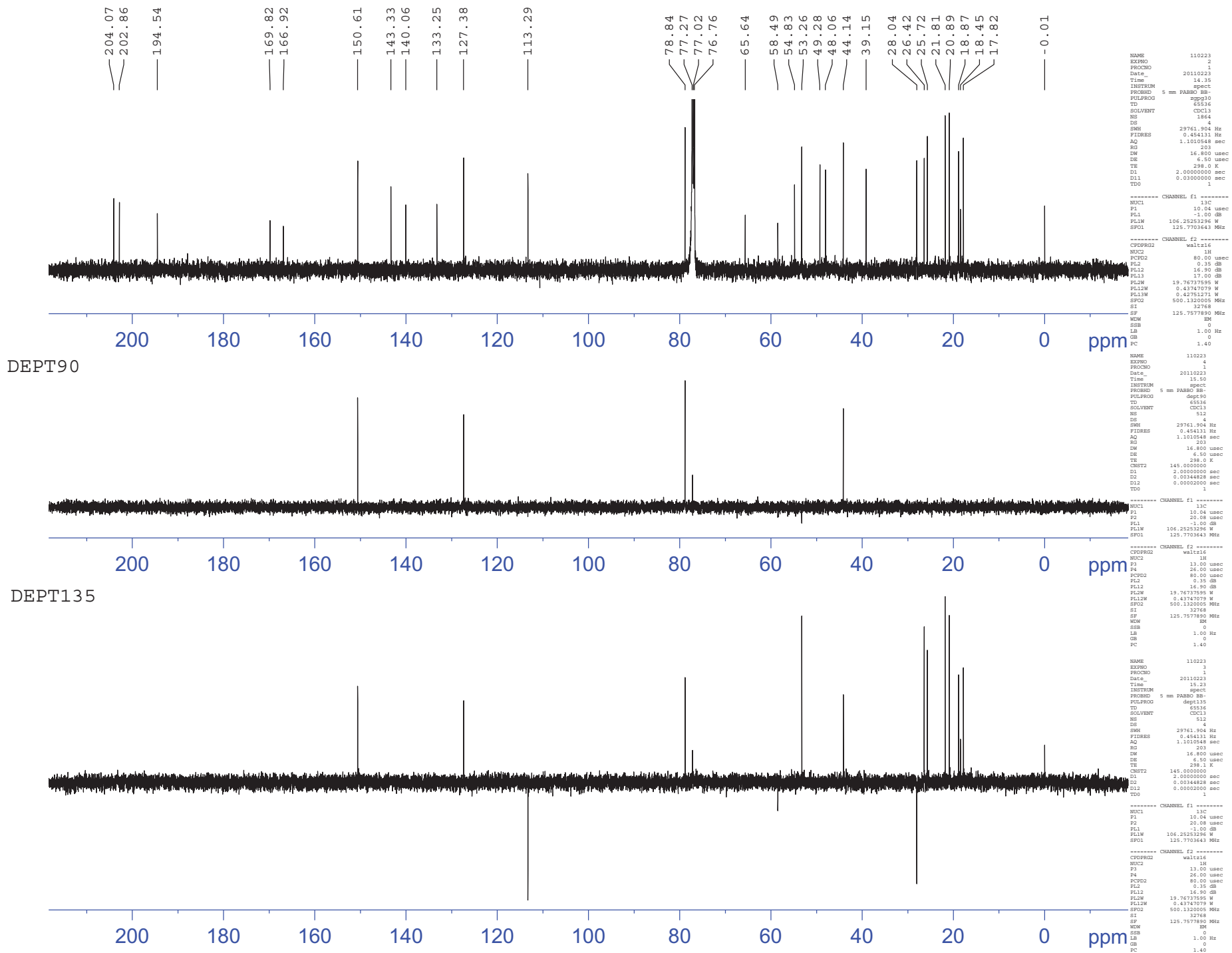
- S28, ^1H - ^1H COSY spectrum of compound **4**;
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- S59, Cartesian coordinates for energy-minimized conformer of **2** optimized at the B3LYP/6-31G(d) level in methanol;
- S60, Cartesian coordinates for energy-minimized conformer of **3** optimized at the B3LYP/6-31G(d) level in methanol;
- S61, Cartesian coordinates for energy-minimized conformer of **12** optimized at the B3LYP/6-31G(d) level in methanol.

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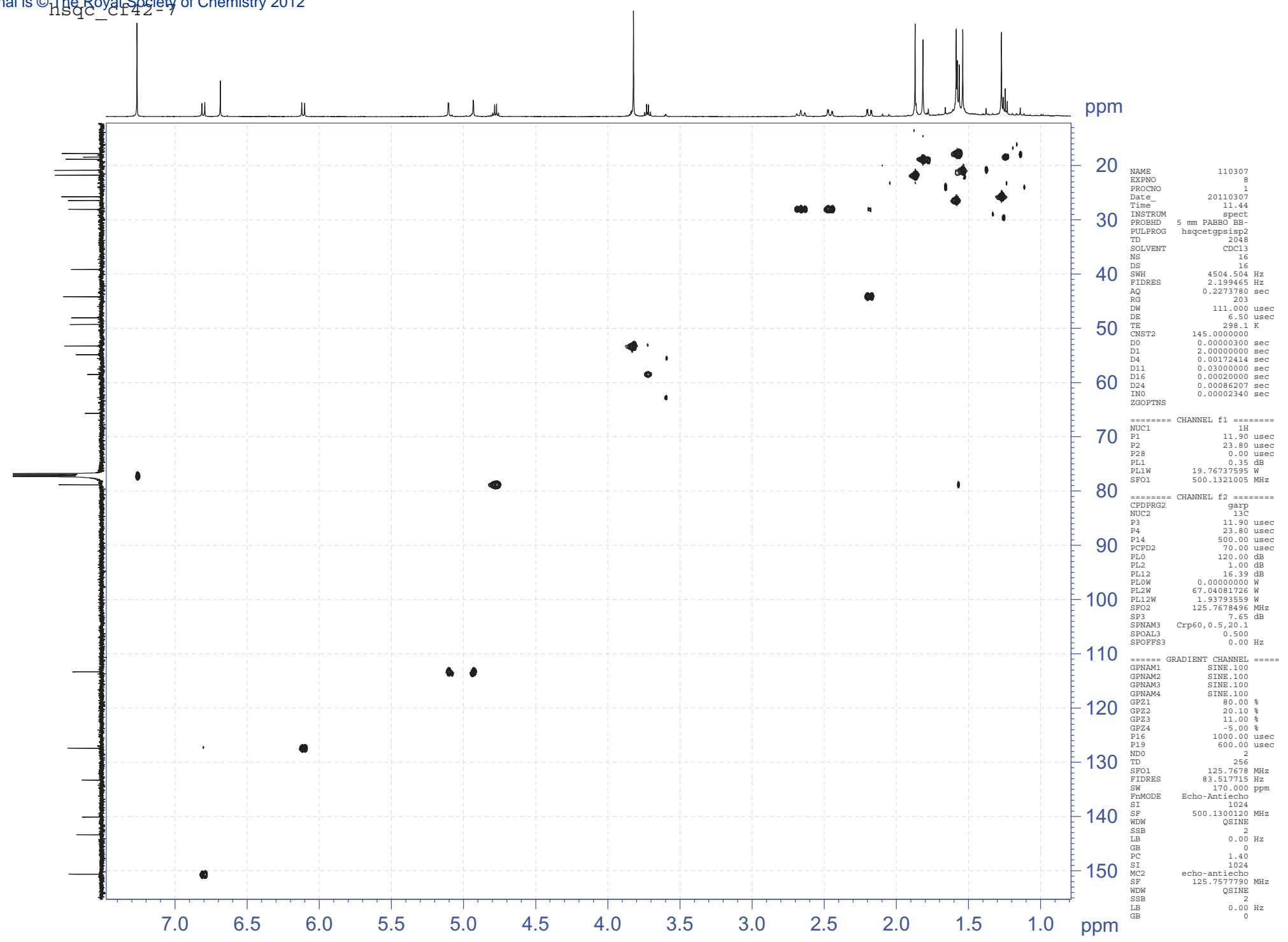


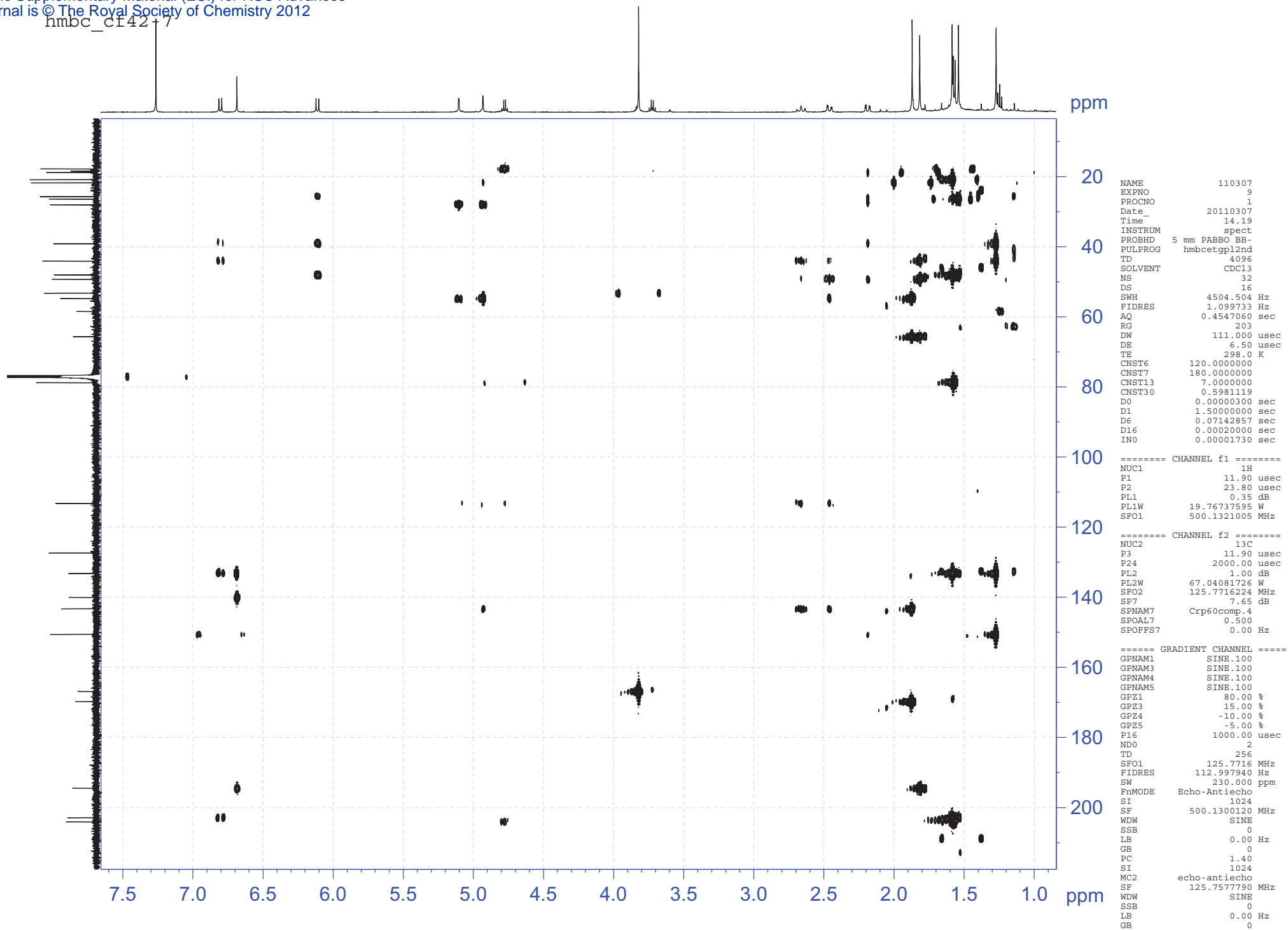
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 144
DW 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

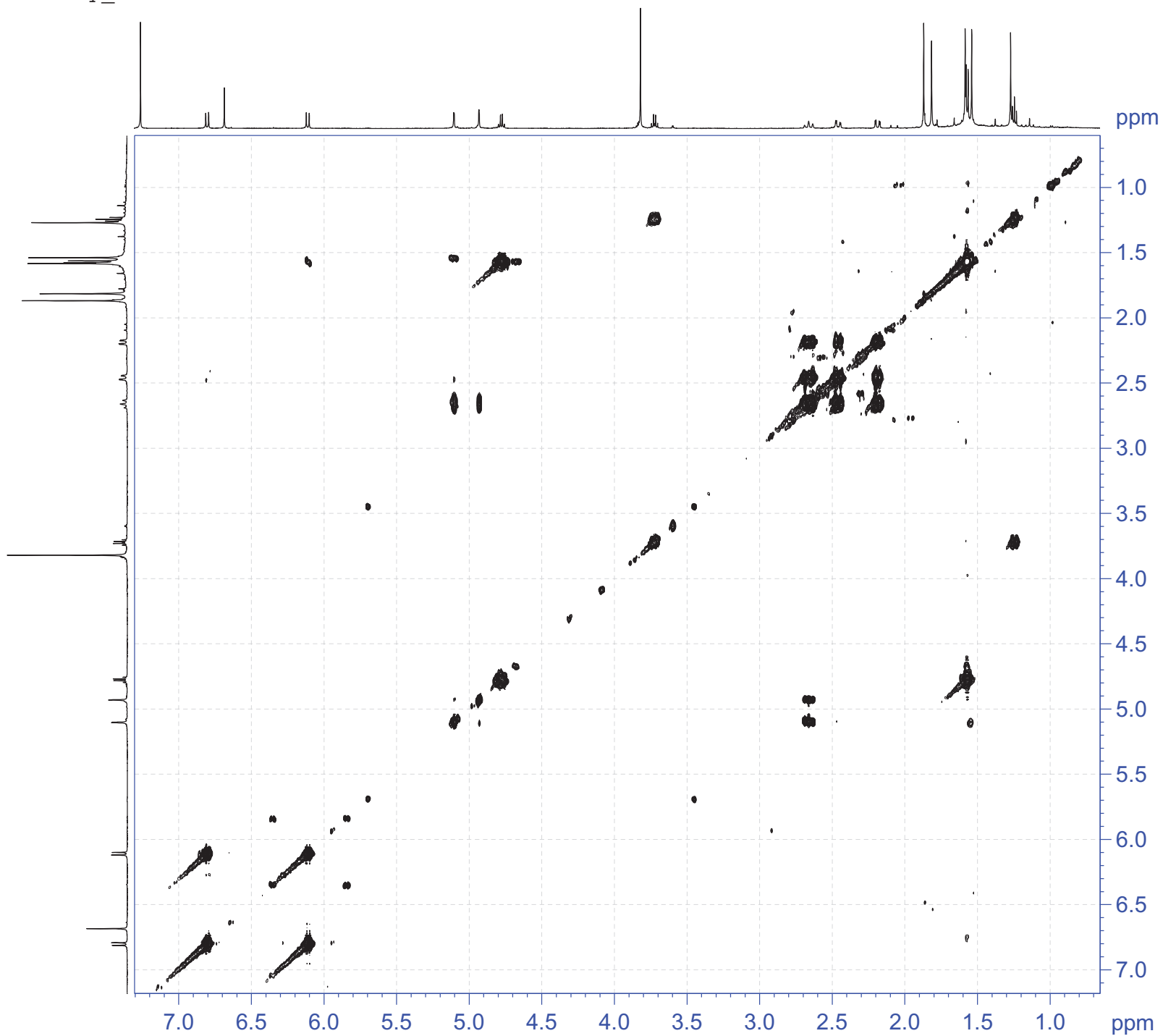
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SF 500.1300125 MHz
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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hsqc_cr42-7





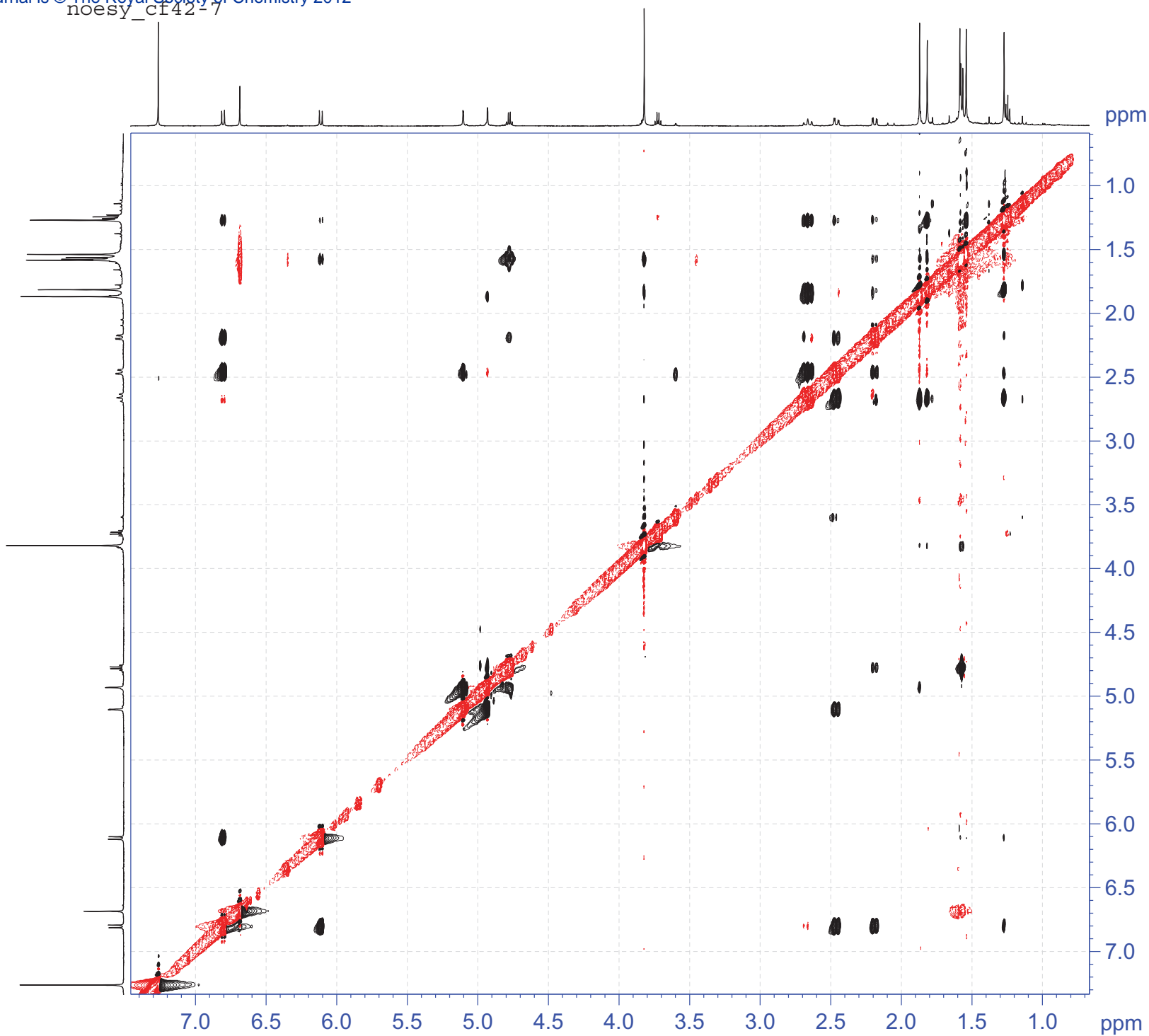


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PROCNO 1
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Time 11.03
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PULPROG cosygpmfzf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00022215 sec

==== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1321005 MHz

===== GRADIENT CHANNEL =====
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GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 500.1321 MHz
FIDRES 17.582769 Hz
SW 9.000 ppm
FnMODE QF
SI 1024
SF 500.1300122 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 500.1300122 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

noesy_cf42-7

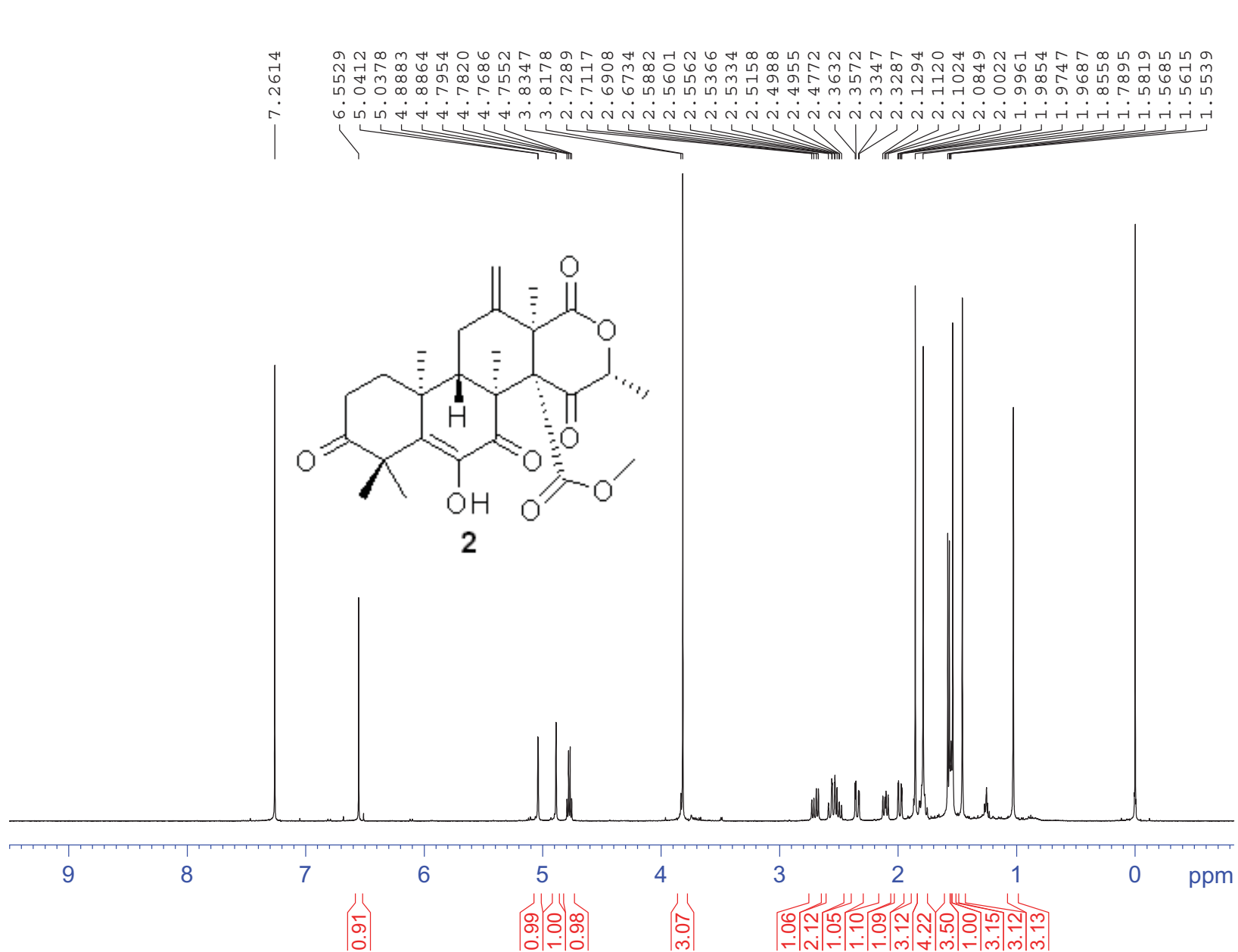


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PROCNO        1
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PULPROG       noesygpqh
TD            2048
SOLVENT       CDCl3
NS            8
DS            16
SWH           4504.504 Hz
FIDRES        2.199465 Hz
AQ            0.2273780 sec
RG            203
DW            111.000 usec
DE            6.50 usec
TE            298.0 K
D0            0.00009593 sec
D1            2.00000000 sec
D8            0.89999998 sec
D16           0.00020000 sec
INO           0.00022215 sec
```

```
===== CHANNEL f1 =====
NUC1          1H
P1            11.90 usec
P2            23.80 usec
PL1           0.35 dB
PL1W          19.76737595 W
SFO1          500.1321005 MHz
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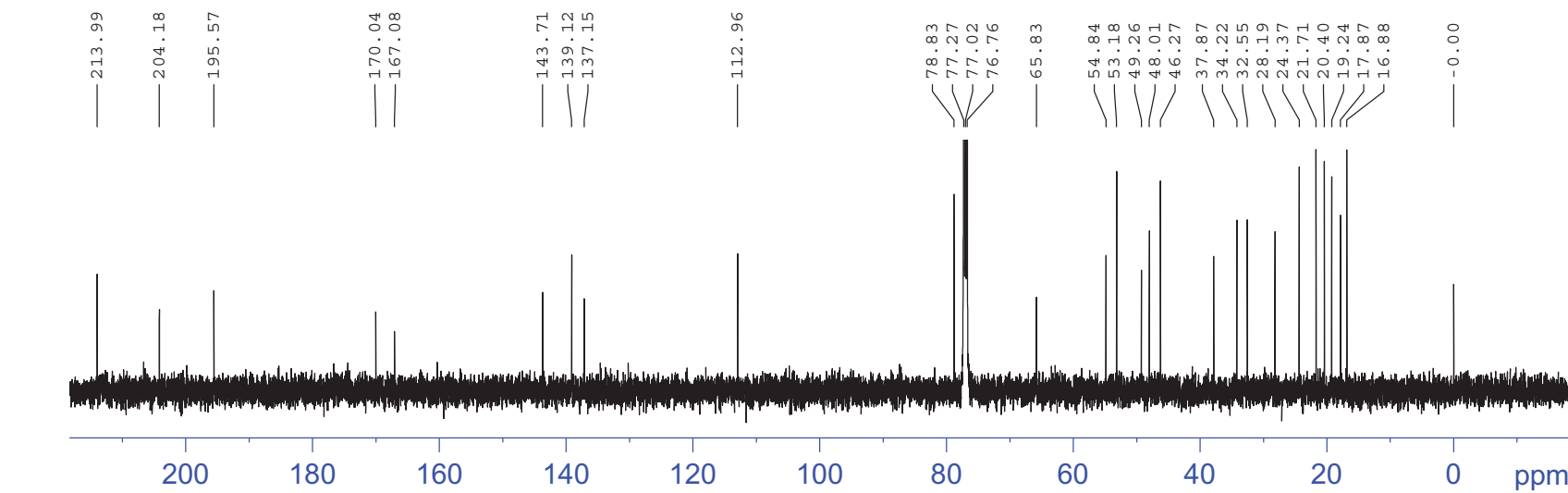
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GPNAM2        SINE.100
GPZ1          40.00 %
GPZ2          -40.00 %
P16           1000.00 usec
ND0           1
TD            256
SFO1          500.1321 MHz
FIDRES        17.582769 Hz
SW            9.000 ppm
FnMODE        States-TPPI
SI            1024
SF            500.1300120 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
SI            1024
MC2           States-TPPI
SF            500.1300120 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
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cf42-10

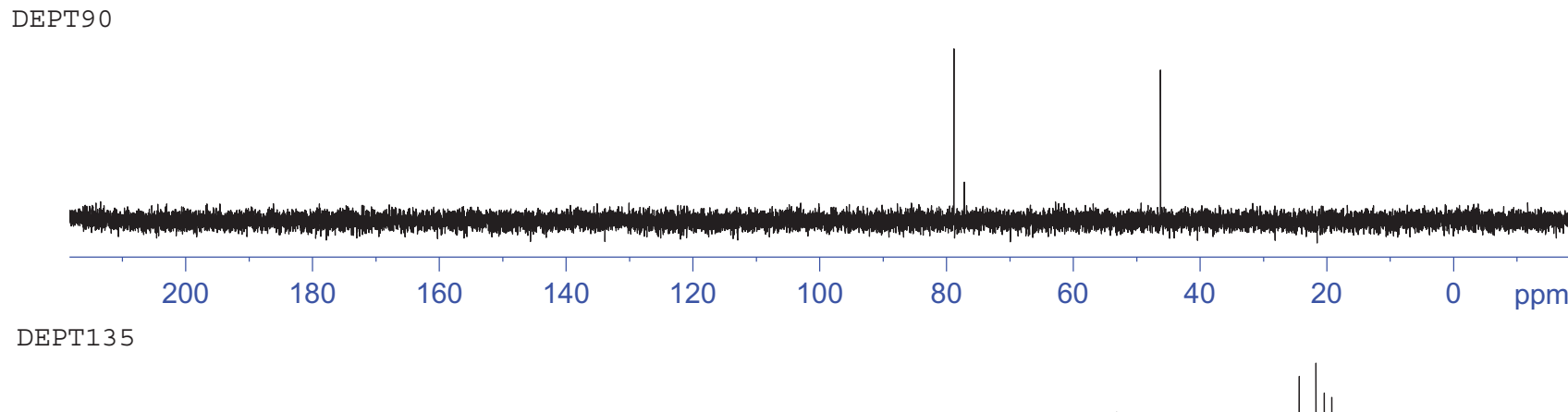


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PROCNO 1
Date_ 20110119
Time 12.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 144
DW 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

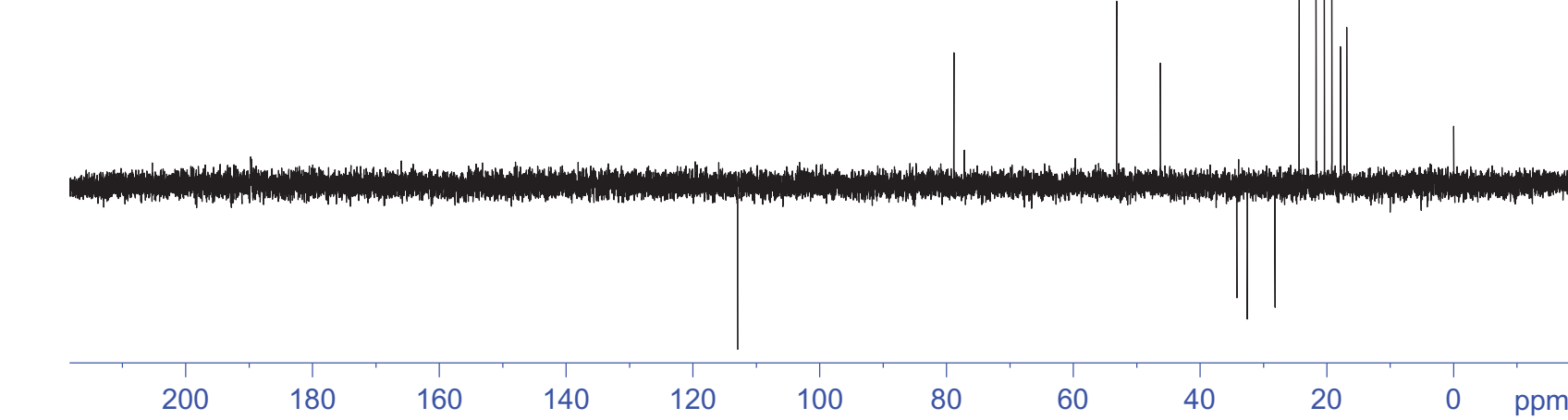
===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



```
NAME 110119
EXPNO 6
PROCNO 1
Date_ 20110119
Time 13.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454113 Hz
AQ 1.1101048 sec
RG 203
ZW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
PL1 -1.00 dB
PL1W 106.25253296 W
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2 waltz16
NUC2 1H
PCP2 80.00 usec
P2 0.35 dB
PL1 16.90 dB
PL13 17.00 dB
PL2W 19.76737595 W
PL1W 0.43747079 W
PL13W 0.42751271 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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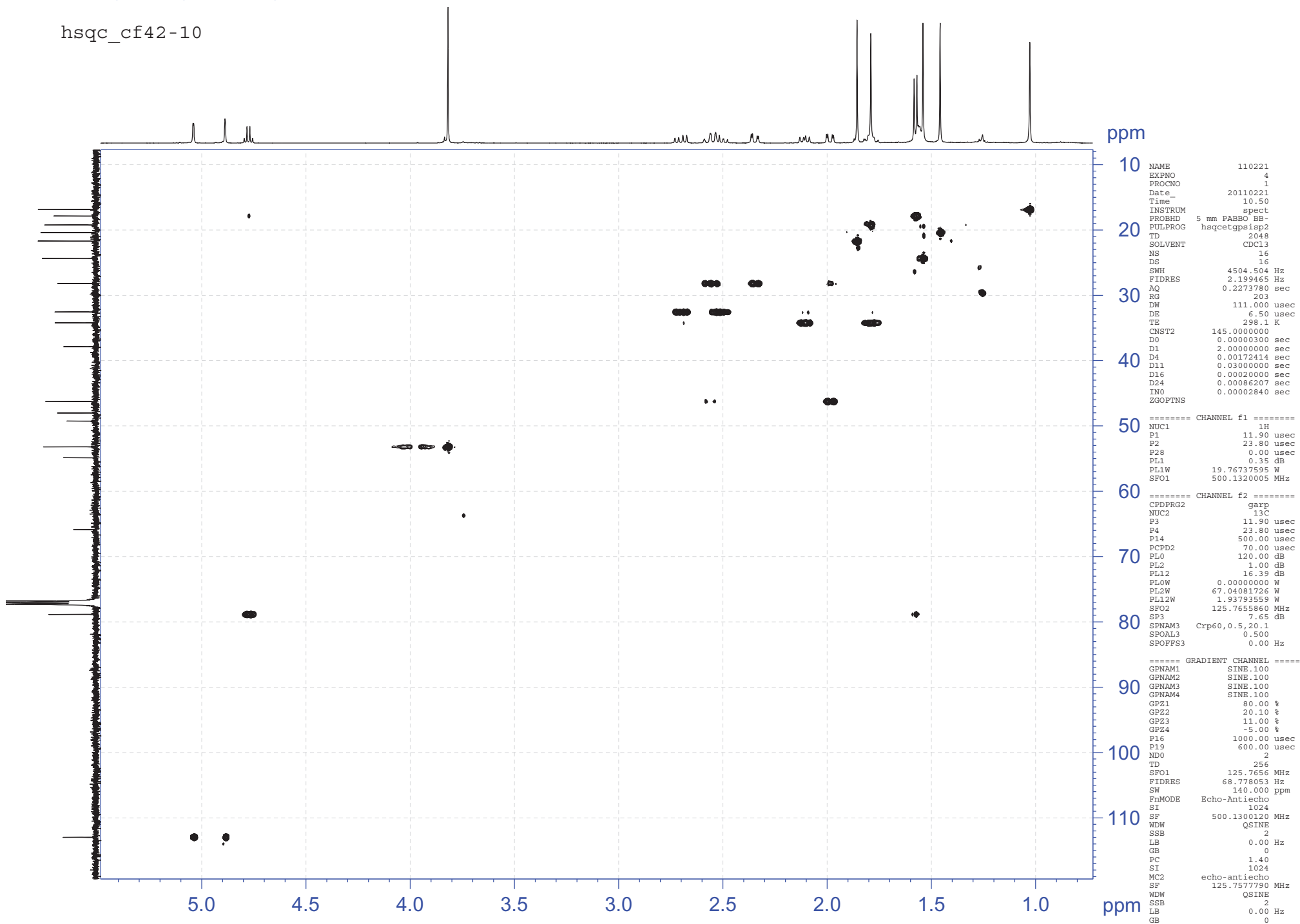


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EXPNO 8
PROCNO 1
Date_ 20110119
Time 13.57
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PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 29761.904 Hz
FIDRES 0.454113 Hz
AQ 1.1101048 sec
RG 203
ZW 16.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
P2 20.08 usec
PL1 -1.00 dB
PL1W 106.25253296 W
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2 waltz16
NUC2 1H
P4 13.00 usec
P4 26.00 usec
PCP2 80.00 usec
P2 0.35 dB
PL1 16.90 dB
PL2 0.35 dB
PL12 16.90 dB
PL2W 19.76737595 W
PL1W 0.43747079 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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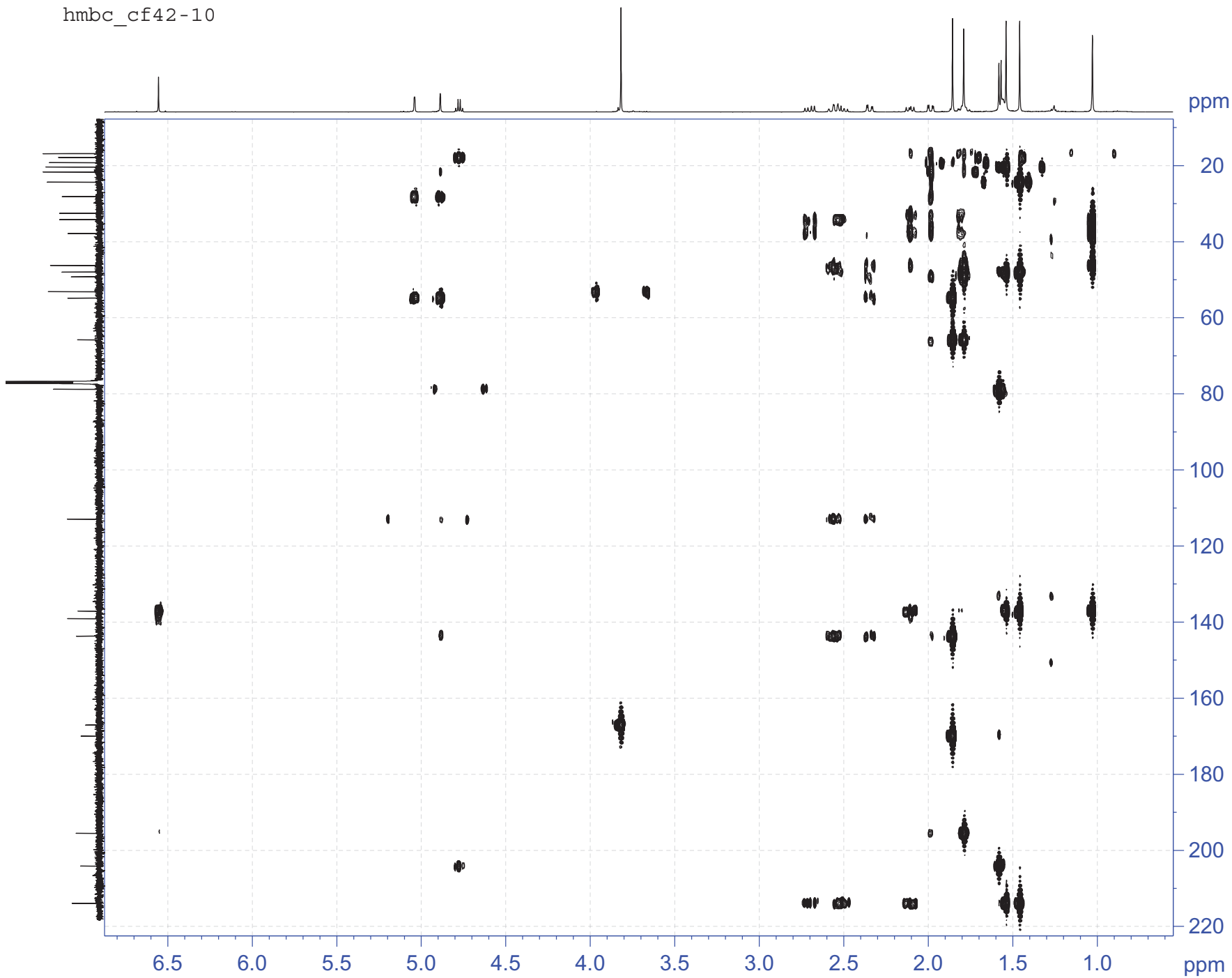


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EXPNO 7
PROCNO 1
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 29761.904 Hz
FIDRES 0.454113 Hz
AQ 1.1101048 sec
RG 203
ZW 16.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
P2 20.08 usec
PL1 -1.00 dB
PL1W 106.25253296 W
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2 waltz16
NUC2 1H
P4 13.00 usec
P4 26.00 usec
PCP2 80.00 usec
P2 0.35 dB
PL1 16.90 dB
PL2 0.35 dB
PL12 16.90 dB
PL2W 19.76737595 W
PL1W 0.43747079 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

hsqc_cf42-10



hmbc_cf42-10

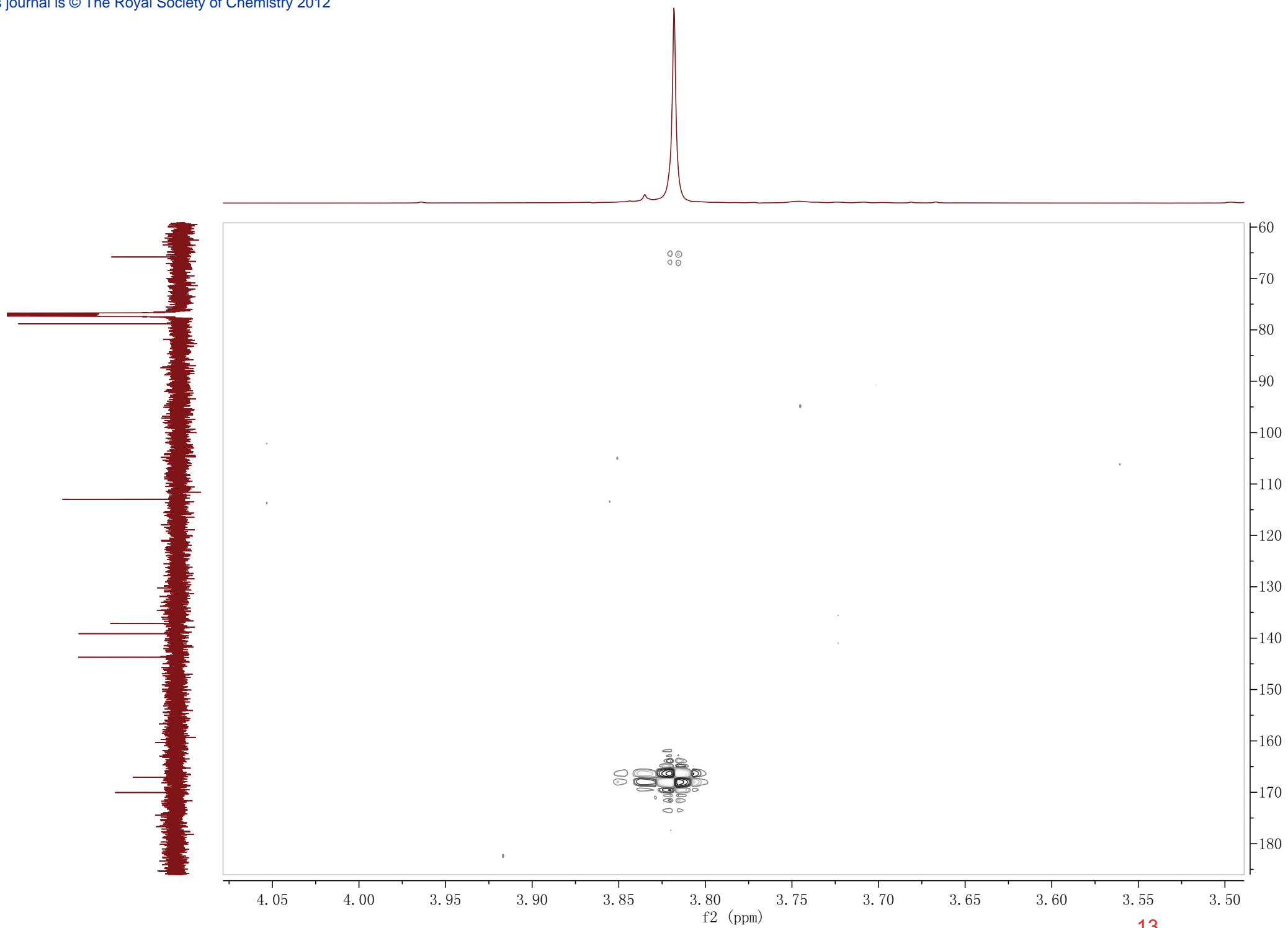


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NAME 110221
EXPNO 5
PROCNO 1
Date_ 20110221
Time_ 13.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcetgpl2nd
TD 4096
SOLVENT CDCl3
NS 32
DS 16
SWH 4504.504 Hz
FIDRES 1.099733 Hz
AQ 0.4547060 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
CNST6 120.0000000
CNST7 180.0000000
CNST13 7.0000000
CNST30 0.5981086
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.07142857 sec
D16 0.00020000 sec
INO 0.00001590 sec

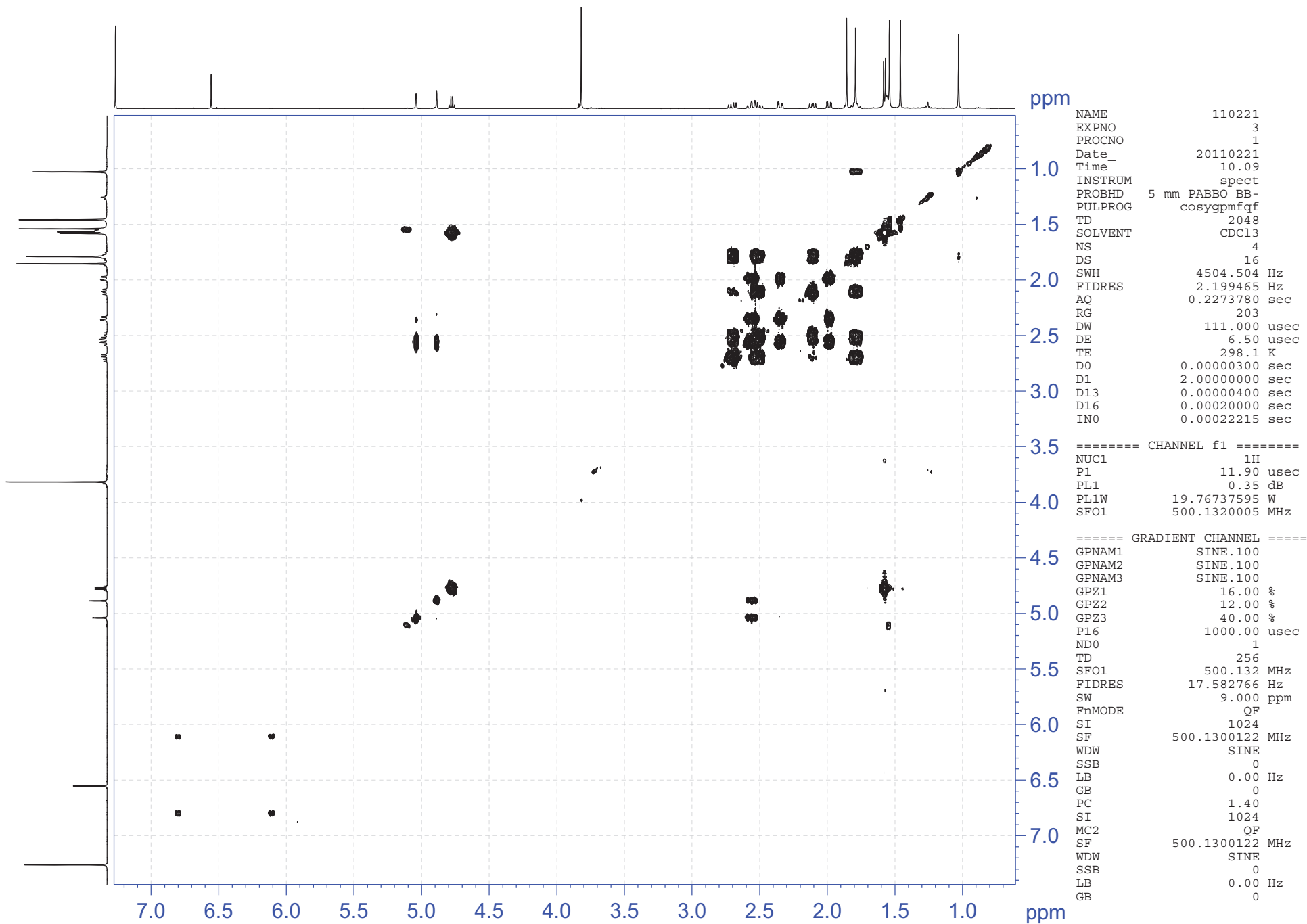
===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
P2 23.80 usec
PL1 0.35 dB
PL1W 19.76737595 W
SF01 500.1320005 MHz

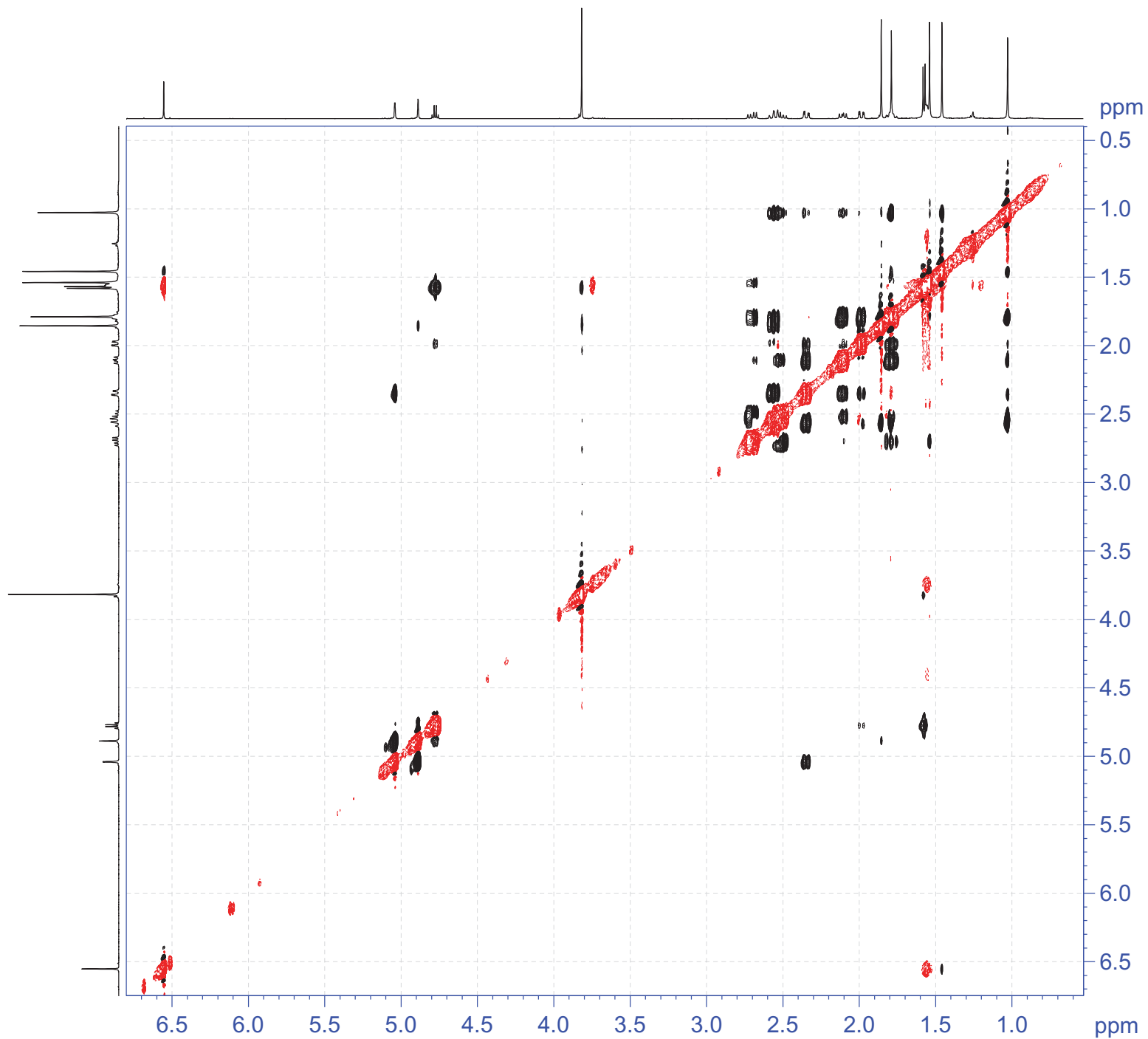
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NUC2 13C
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P24 2000.00 usec
PL2 1.00 dB
PL2W 67.04081726 W
SF02 125.7728799 MHz
SP7 7.65 dB
SPNAM7 Crp60comp.4
SPOAL7 0.500
SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPNAM5 SINE.100
GPZ1 80.00 %
GPZ3 15.00 %
GPZ4 -10.00 %
GPZ5 -5.00 %
P16 1000.00 usec
ND0 2
TD 256
SF01 125.7729 MHz
FIDRES 122.825081 Hz
SW 250.000 ppm
FMODE Echo-Antiecho
SI 1024
SF 500.1300120 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 125.7577790 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```



cosy_cf42-10





NAME 110221
EXPNO 6
PROCNO 1
Date_ 20110221
Time 18.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesyggpph
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
D0 0.00009593 sec
D1 2.00000000 sec
D8 0.69999999 sec
D16 0.00020000 sec
INO 0.00022215 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
P2 23.80 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1320005 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec
NDO 1
TD 256
SFO1 500.132 MHz
FIDRES 17.582766 Hz
SW 9.000 ppm
FnMODE States-TPPI
SI 1024
SF 500.1300120 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPPI
SF 500.1300120 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 40.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

51 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 0-8

cf42-10

12:22:48 14-Mar-2011

Voltage EI+

100

%

0

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Minimum:

Maximum:

100.0

10.0

0.5

40.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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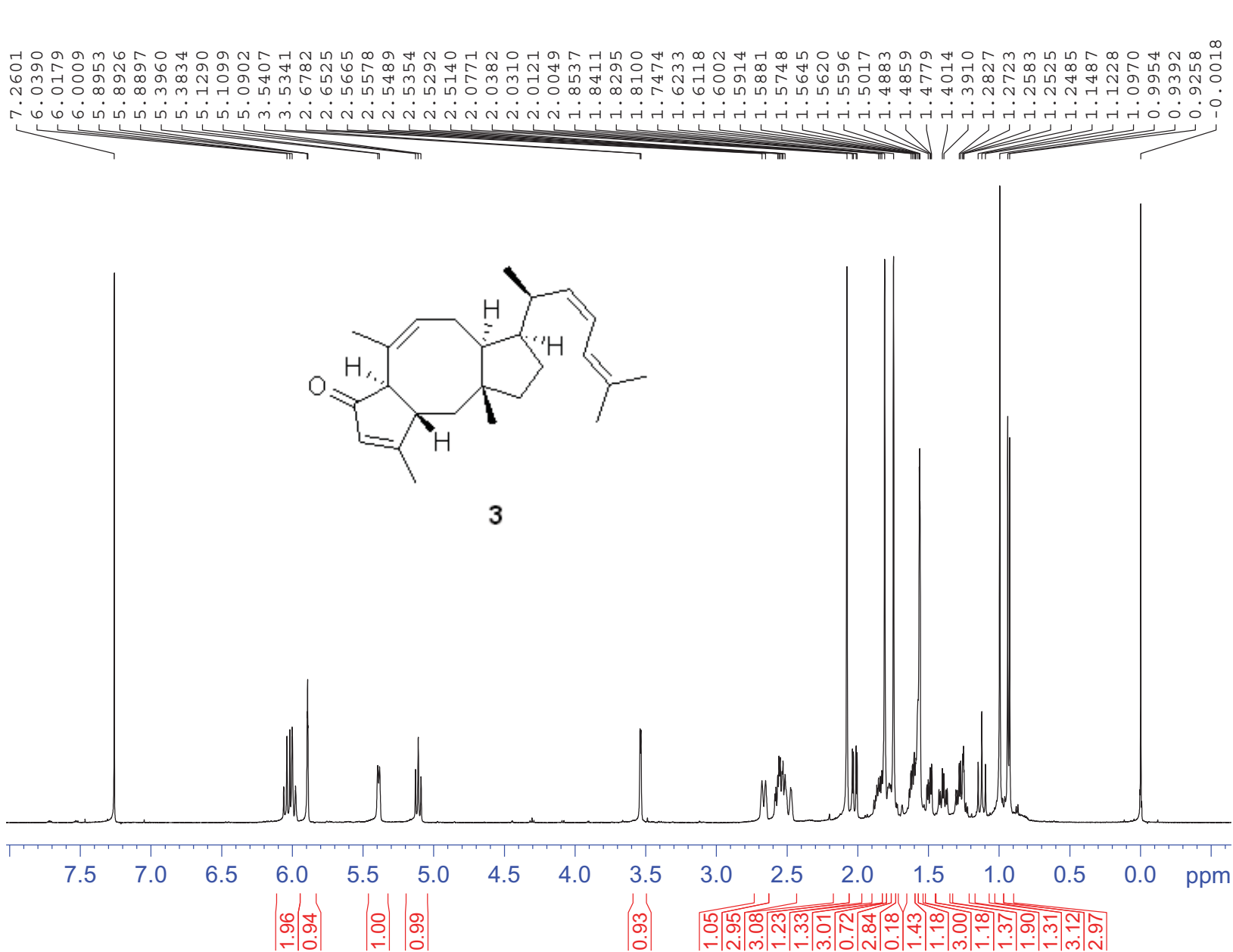
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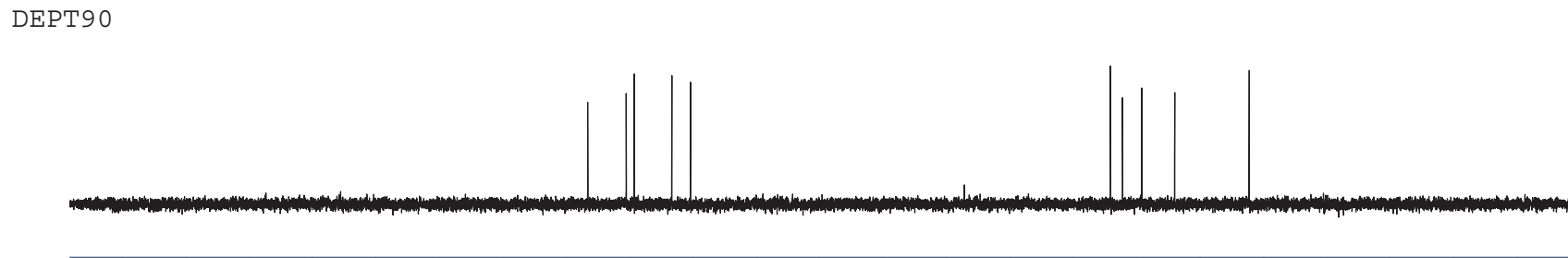
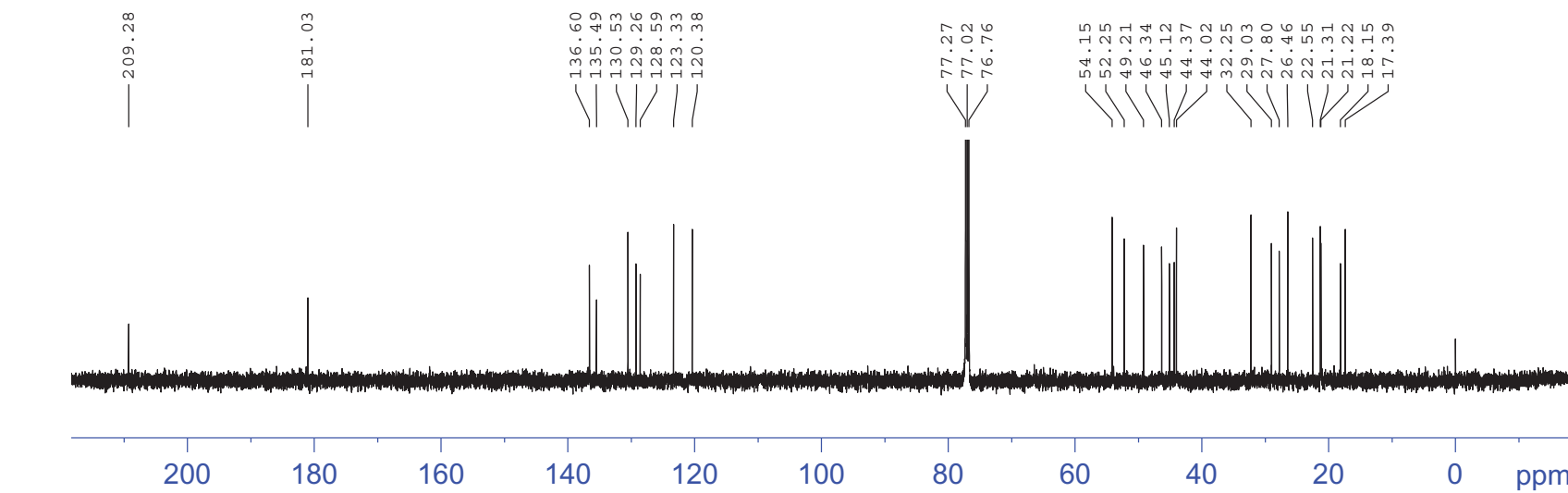
Autospec Premier
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cf42-46



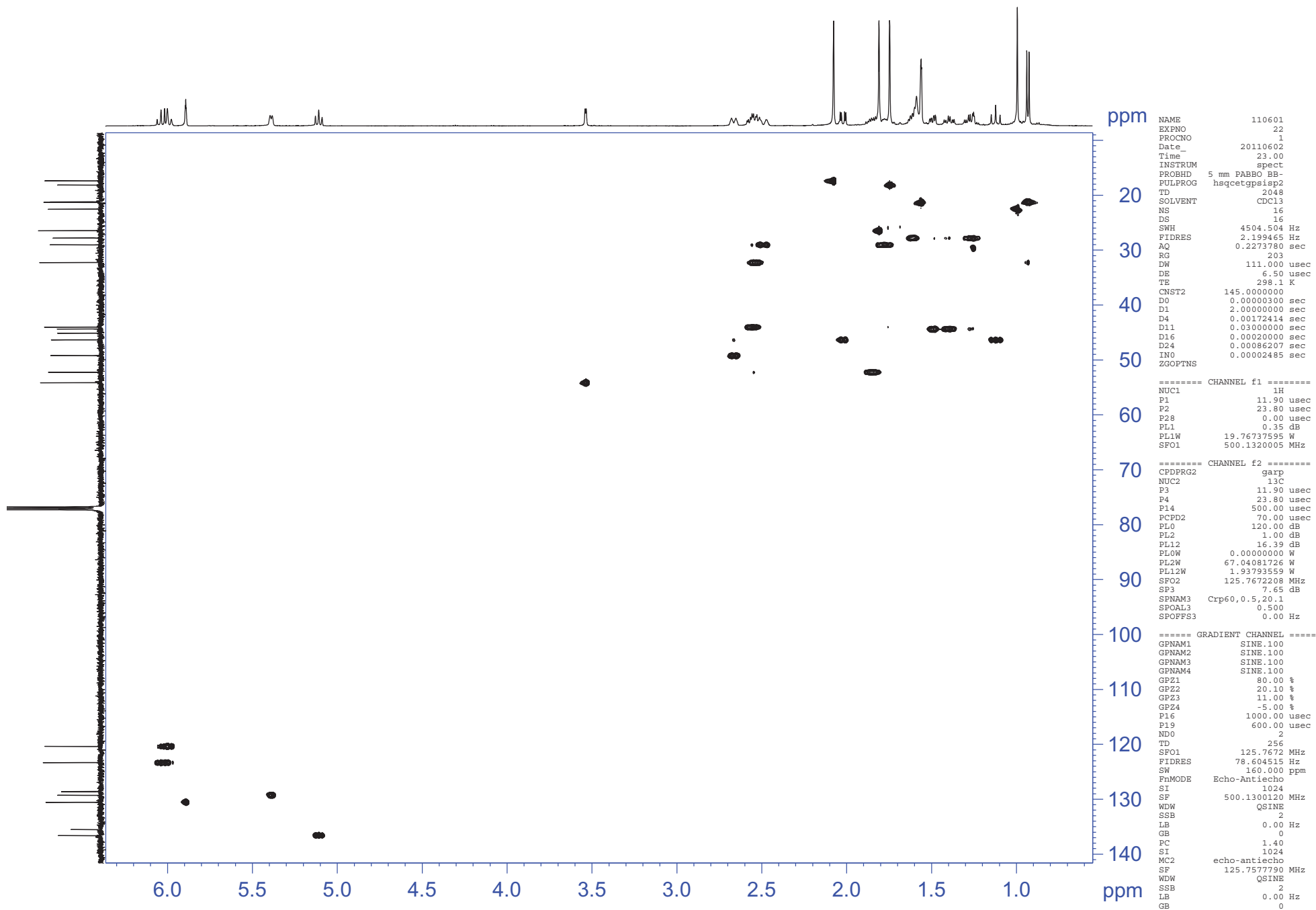
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PROCNO 1
Date_ 20110524
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 144
DW 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

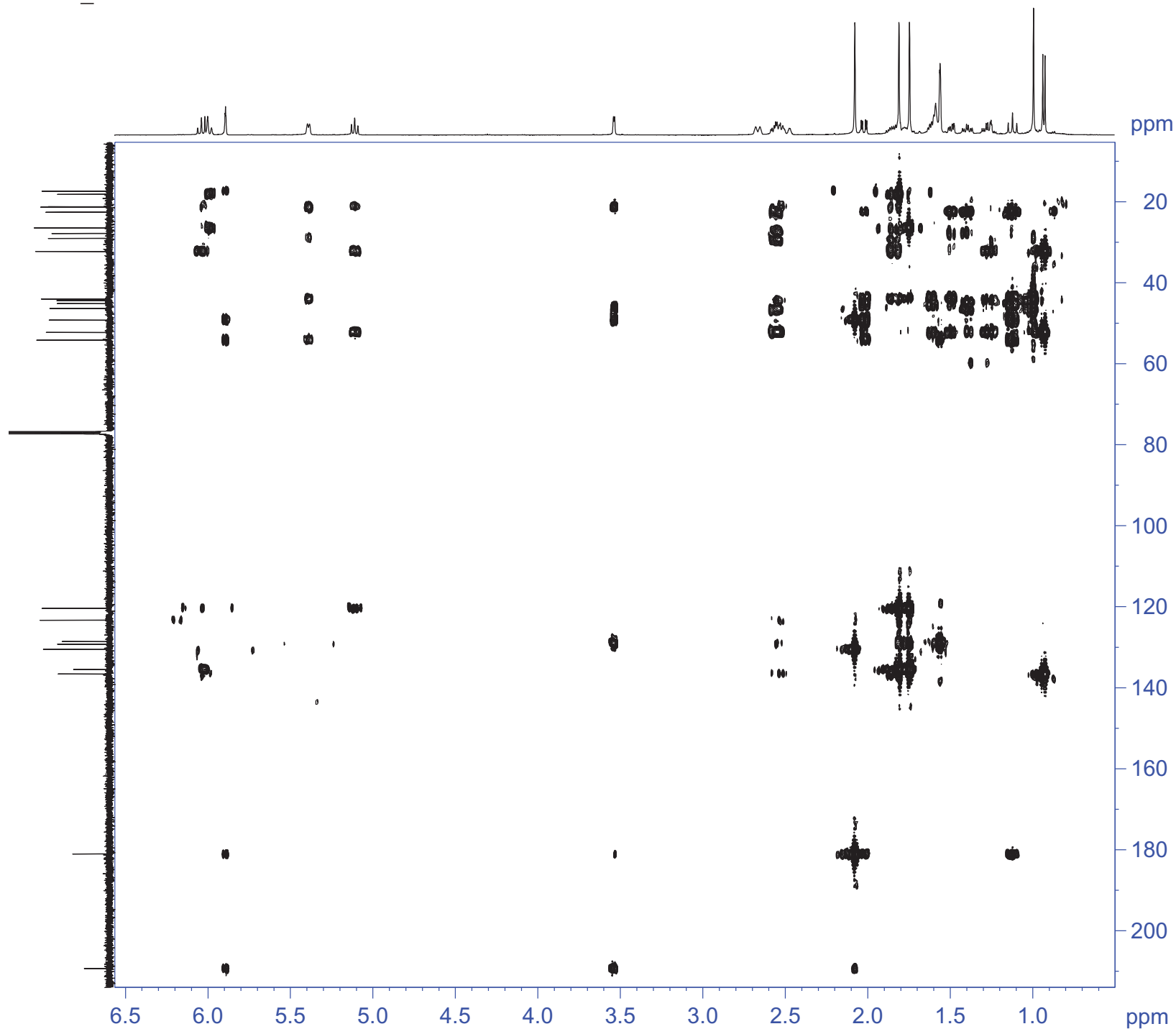


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EXPNO 11
PROCNO 1
Date_ 20110531
Time 10.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 29761.904 Hz
FIDRES 0.454113 Hz
AQ 1.1010548 sec
RG 203
DE 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
PL1 -1.00 dB
PL1W 106.25253296 W
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.35 dB
PL1 16.90 dB
PL12 17.00 dB
PL2W 19.76737595 W
PL1W 0.43747079 W
PL13W 0.42751271 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
----- CHANNEL f1 -----
NAME 110526
EXPNO 11
PROCNO 1
Date_ 20110531
Time 11.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 29761.904 Hz
FIDRES 0.454113 Hz
AQ 1.1010548 sec
RG 203
DE 16.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
P2 20.08 usec
PL1 -1.00 dB
PL2 20.08 usec
PL1W 106.25253296 W
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2 waltz16
NUC2 1H
P3 13.00 usec
P4 26.00 usec
PCPD2 80.00 usec
PL2 0.35 dB
PL12 16.90 dB
PL2W 19.76737595 W
PL1W 0.43747079 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
----- CHANNEL f1 -----
NAME 110526
EXPNO 12
PROCNO 1
Date_ 20110531
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 29761.904 Hz
FIDRES 0.454113 Hz
AQ 1.1010548 sec
RG 203
DE 16.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
P2 20.08 usec
PL1 -1.00 dB
PL2 20.08 usec
PL1W 106.25253296 W
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2 waltz16
NUC2 1H
P3 13.00 usec
P4 26.00 usec
PCPD2 80.00 usec
PL2 0.35 dB
PL12 16.90 dB
PL2W 19.76737595 W
PL1W 0.43747079 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

hsqc_cf42-46



hmbc_cf42-46



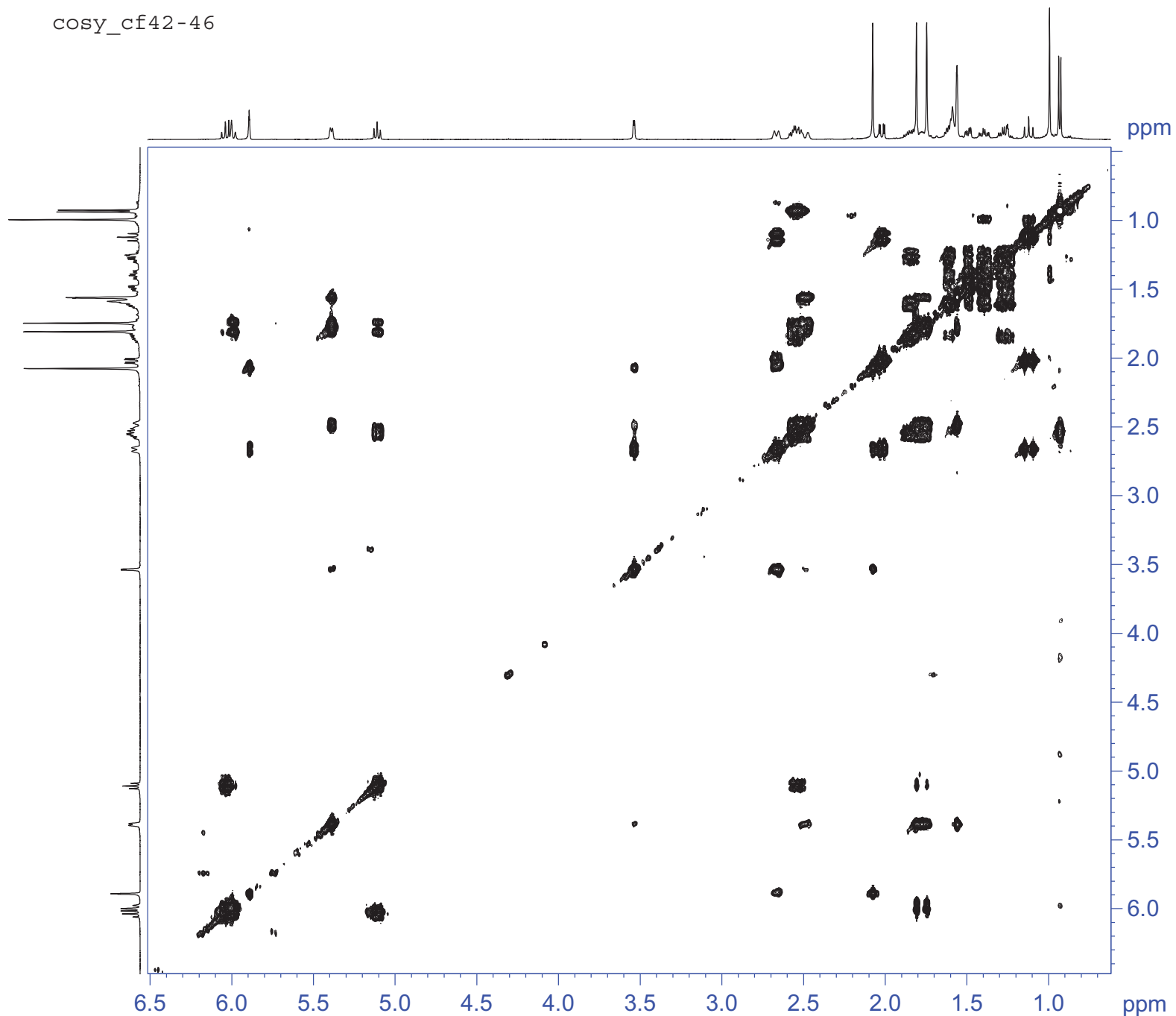
```
NAME 110601
EXPNO 23
PROCNO 1
Date_ 20110603
Time 1.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcetgp12nd
TD 4096
SOLVENT CDCl3
NS 32
DS 16
SWH 4504.504 Hz
FIDRES 1.099733 Hz
AQ 0.4547060 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
CNST6 120.0000000
CNST7 180.0000000
CNST13 7.0000000
CNST30 0.5981119
D0 0.0000300 sec
D1 1.5000000 sec
D6 0.07142857 sec
D16 0.0002000 sec
IN0 0.00001730 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
P2 23.80 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1320005 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 11.90 usec
P24 2000.00 usec
PL2 1.00 dB
PL2W 67.04081726 W
SFO2 125.7716224 MHz
SP7 7.65 dB
SPNAM7 Crp60comp.4
SPOAL7 0.500
SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPNAM5 SINE.100
GPZ1 80.00 %
GPZ3 15.00 %
GPZ4 -10.00 %
GPZ5 -5.00 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 125.7716 MHz
FIDRES 112.997940 Hz
SW 230.000 ppm
FnMODE Echo-Antiecho
SI 1024
SF 500.1300120 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 125.7577790 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```

cosy_cf42-46

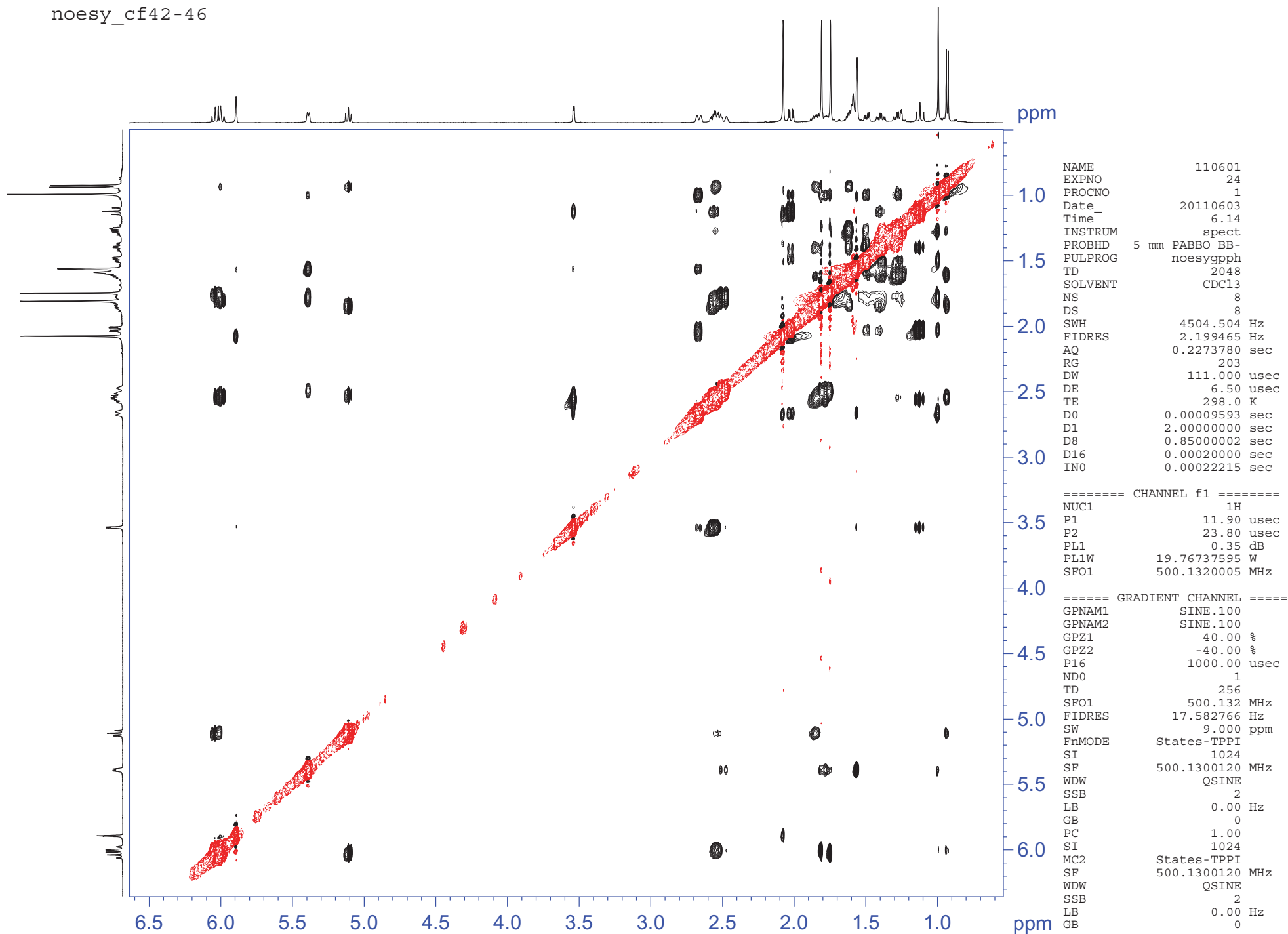


```
NAME 110601
EXPNO 21
PROCNO 1
Date_ 20110602
Time 22.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfqc
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00022215 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1320005 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 500.132 MHz
FIDRES 17.582766 Hz
SW 9.000 ppm
FnMODE QF
SI 1024
SF 500.1300129 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 500.1300129 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```

noesy_cf42-46



Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 40.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

14 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

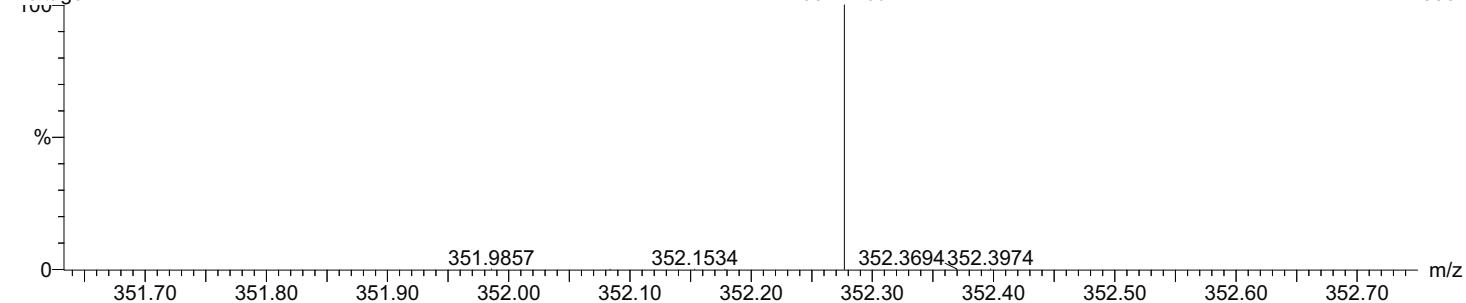
Elements Used:

C: 0-200 H: 0-400 O: 0-2

cf42-46

17:05:47 27-Jun-2011

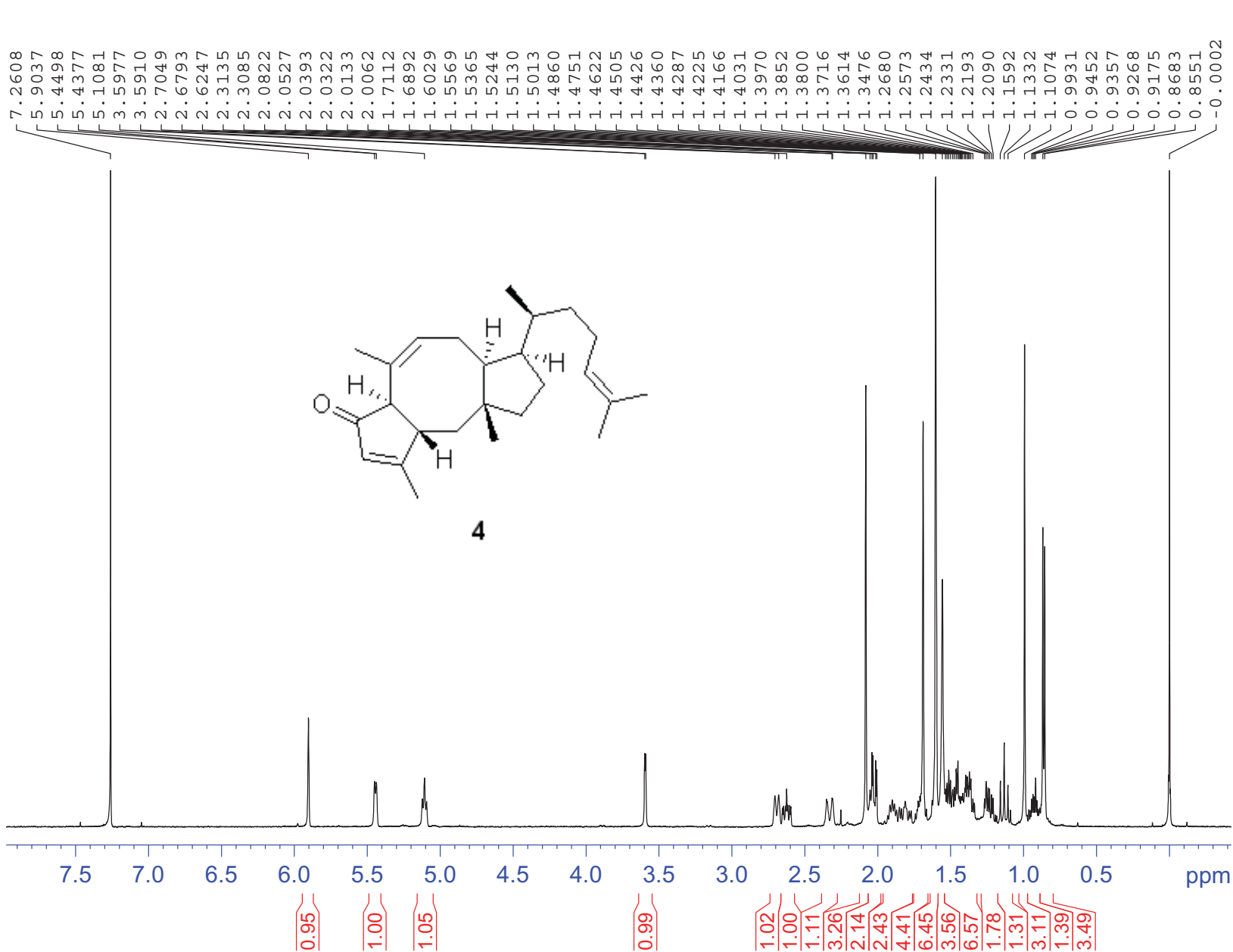
Voltage EI+



Minimum: 0.5
Maximum: 100.0 10.0 40.0

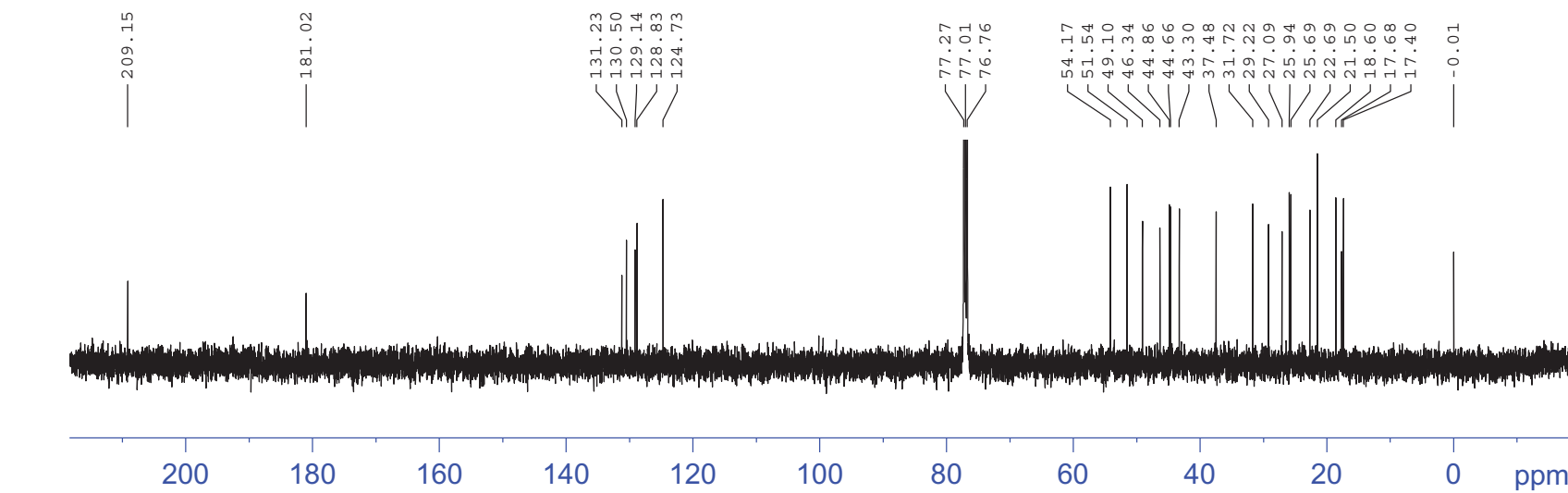
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
352.2769	352.2766	0.3	0.9	8.0	5555400.5	C25 H36 O

cf42-49



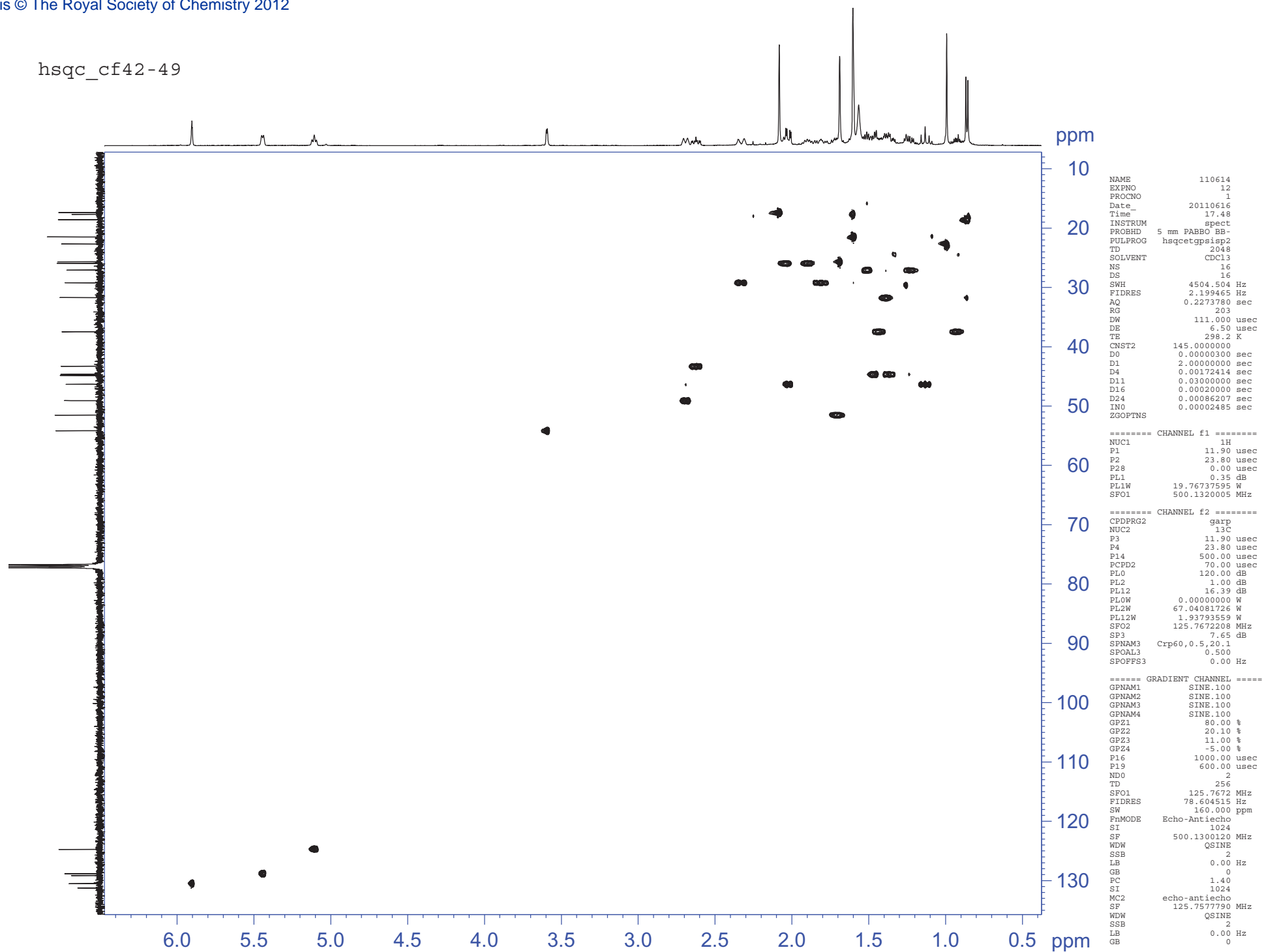
```
NAME 110531
EXPNO 7
PROCNO 1
Date_ 20110531
Time 9.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```

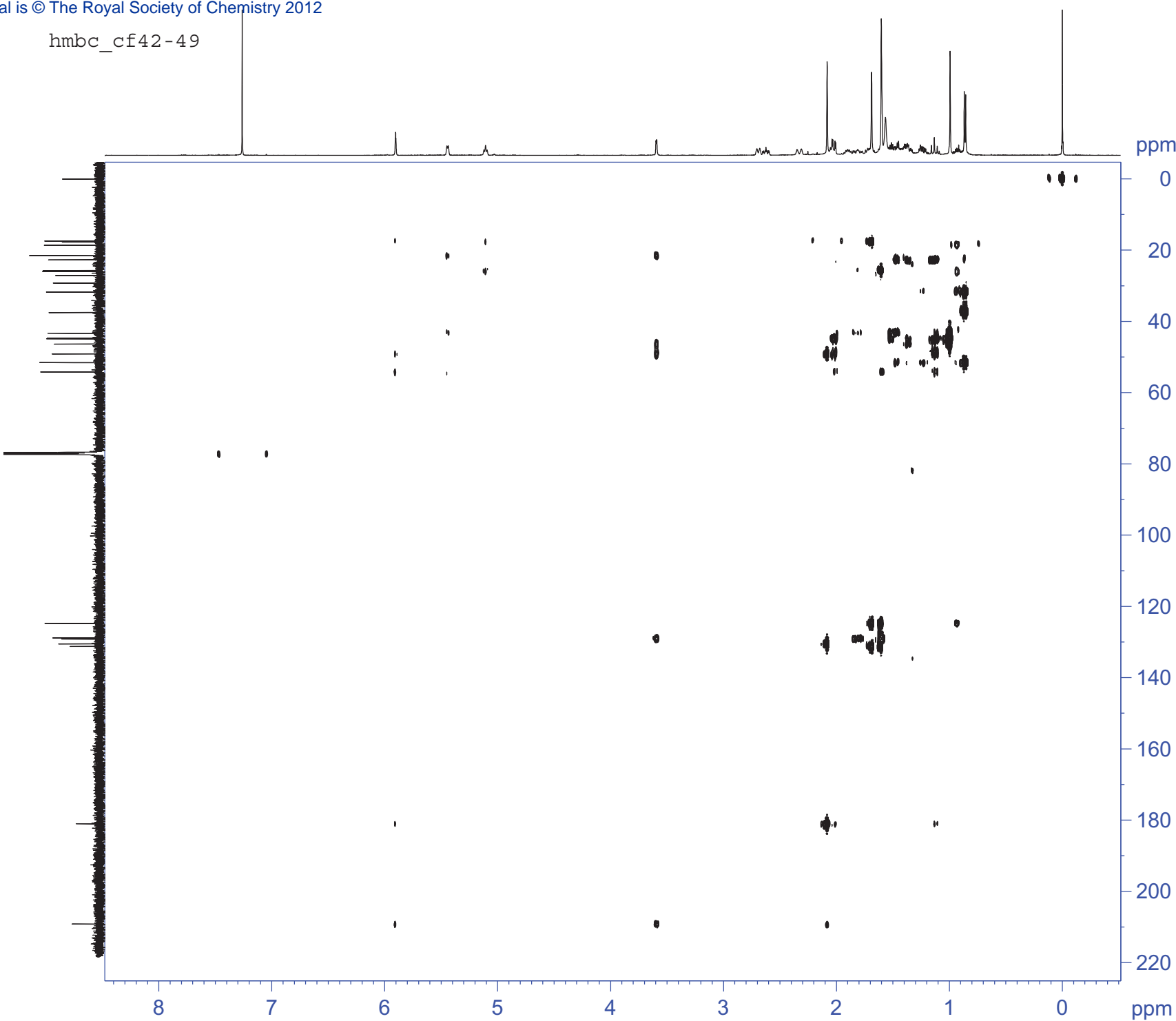



```
NAME 110601
EXPNO 11
PROCNO 1
Date_ 20110602
Time 16.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 29761.904 Hz
FIDRES 0.454113 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
PL1 -1.00 dB
PL1W 106.25253296 W
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2 waltz16
NUC2 1H
PCP2 80.00 usec
P2 0.35 dB
PL2 16.90 dB
PL2W 19.76737595 W
PL3W 0.43747079 W
PL3W 0.42751271 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
----- CHANNEL f1 -----
NAME 110601
EXPNO 11
PROCNO 1
Date_ 20110602
Time 16.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 29761.904 Hz
FIDRES 0.454113 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
D12 0.00002000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
PL1 -1.00 dB
PL1W 106.25253296 W
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2 waltz16
NUC2 1H
PCP2 13.00 usec
P2 26.00 usec
P4 26.00 usec
PCP2 80.00 usec
P2 0.35 dB
PL2 16.90 dB
PL2W 19.76737595 W
PL3W 0.43747079 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
----- CHANNEL f1 -----
NAME 110601
EXPNO 12
PROCNO 1
Date_ 20110602
Time 16.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 29761.904 Hz
FIDRES 0.454113 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0344828 sec
D12 0.00002000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
PL1 -1.00 dB
PL1W 106.25253296 W
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2 waltz16
NUC2 1H
PCP2 13.00 usec
P2 26.00 usec
P4 26.00 usec
PCP2 80.00 usec
P2 0.35 dB
PL2 16.90 dB
PL2W 19.76737595 W
PL3W 0.43747079 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

hsqc_cf42-49



hmbc_cf42-49



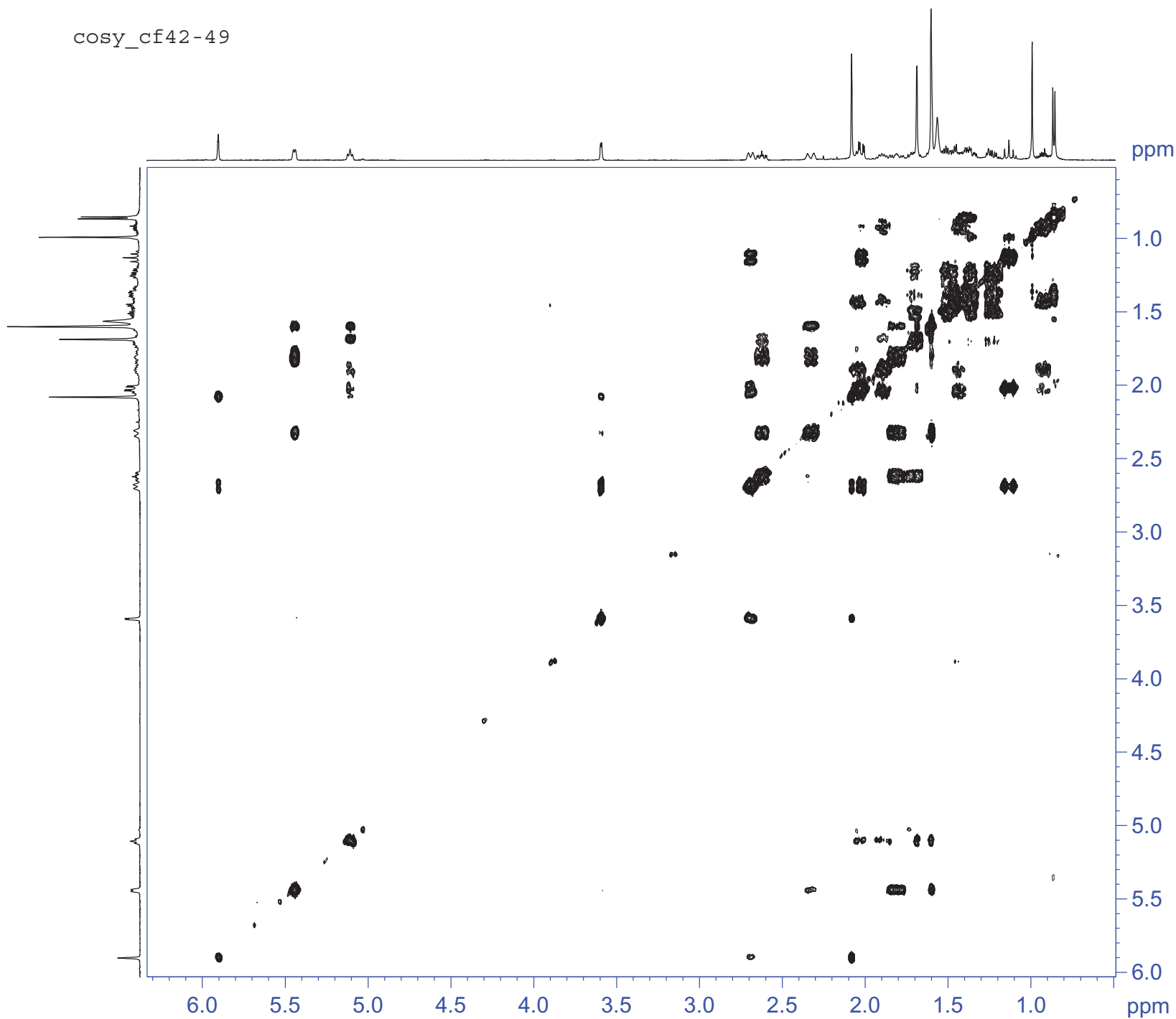
NAME 110614
EXPNO 13
PROCNO 1
Date_ 20110616
Time_ 20.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcetgp12nd
TD 4096
SOLVENT CDCl3
NS 32
DS 16
SWH 4504.504 Hz
FIDRES 1.099733 Hz
AQ 0.4547060 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
CNST6 120.0000000
CNST7 180.0000000
CNST13 7.0000000
CNST30 0.5981119
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.07142857 sec
D16 0.00020000 sec
IN0 0.00001730 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
P2 23.80 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1320005 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 11.90 usec
P24 2000.00 usec
PL2 1.00 dB
PL2W 67.04081726 W
SFO2 125.7716224 MHz
SP7 7.65 dB
SPNAM7 Crp60comp.4
SPOAL7 0.500
SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPNAM5 SINE.100
GPZ1 80.00 %
GPZ3 15.00 %
GPZ4 -10.00 %
GPZ5 -5.00 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 125.7716 MHz
FIDRES 112.997940 Hz
SW 230.000 ppm
FnMODE Echo-Antiecho
SI 1024
SF 500.1300120 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 125.7577790 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

cosy_cf42-49

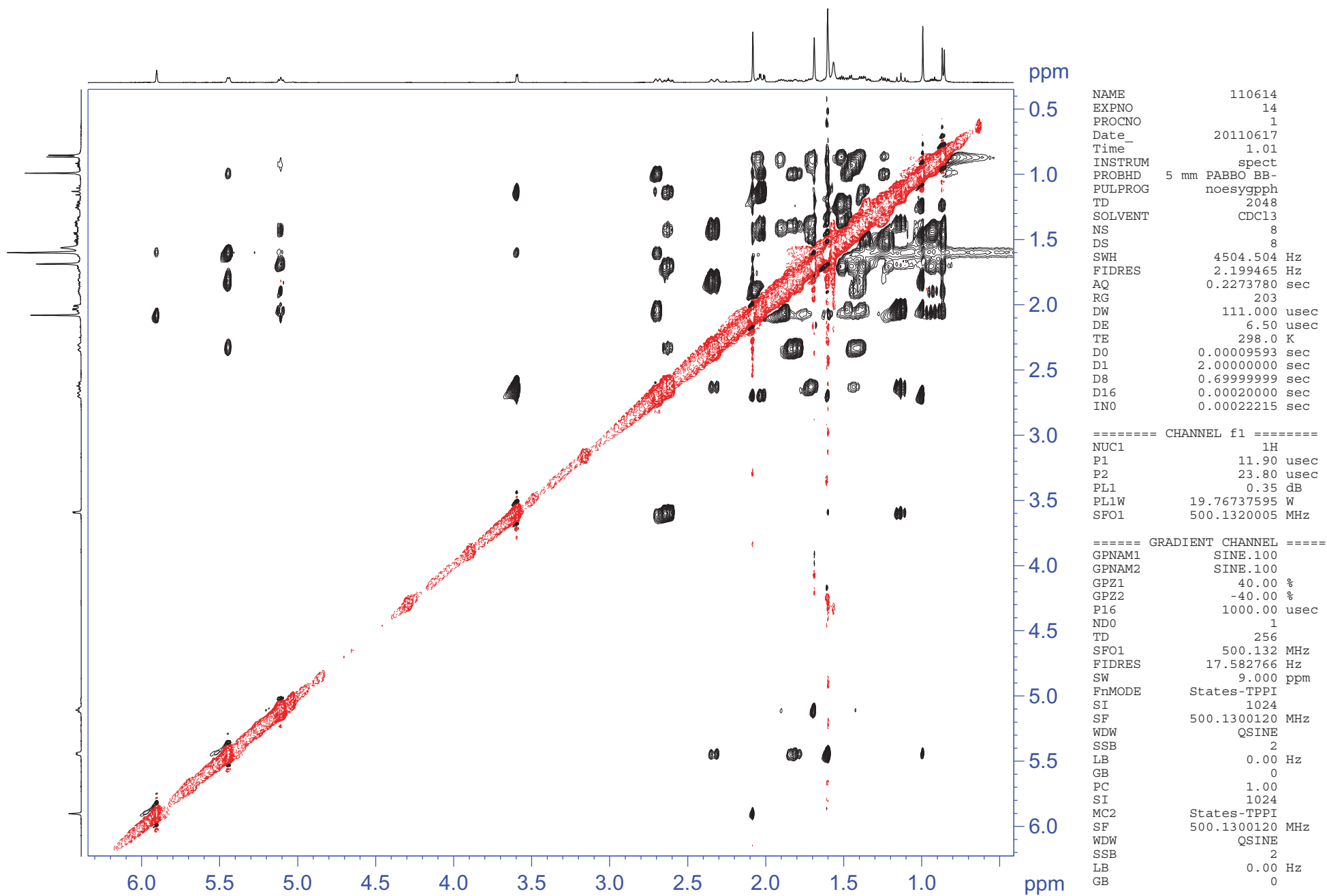


NAME 110614
EXPNO 11
PROCNO 1
Date_ 20110616
Time_ 17.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfzf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00022215 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1320005 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 500.132 MHz
FIDRES 17.582766 Hz
SW 9.000 ppm
FnMODE QF
SI 1024
SF 500.1300129 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 500.1300129 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

noesy_cf42-49



Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 40.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

14 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 0-2

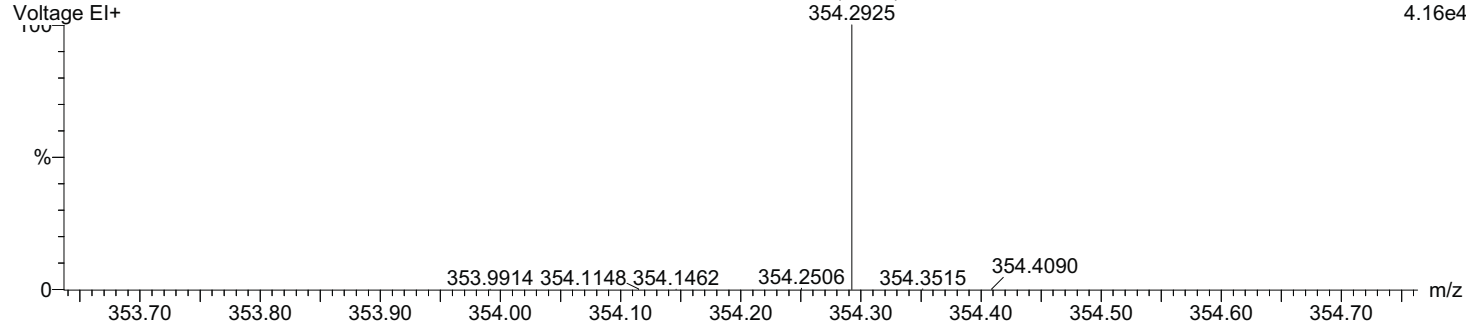
cf42-49

17:10:45 27-Jun-2011

Voltage EI+

KIB
M110627EA-02AFAMM 13 (1.194)
354.2925

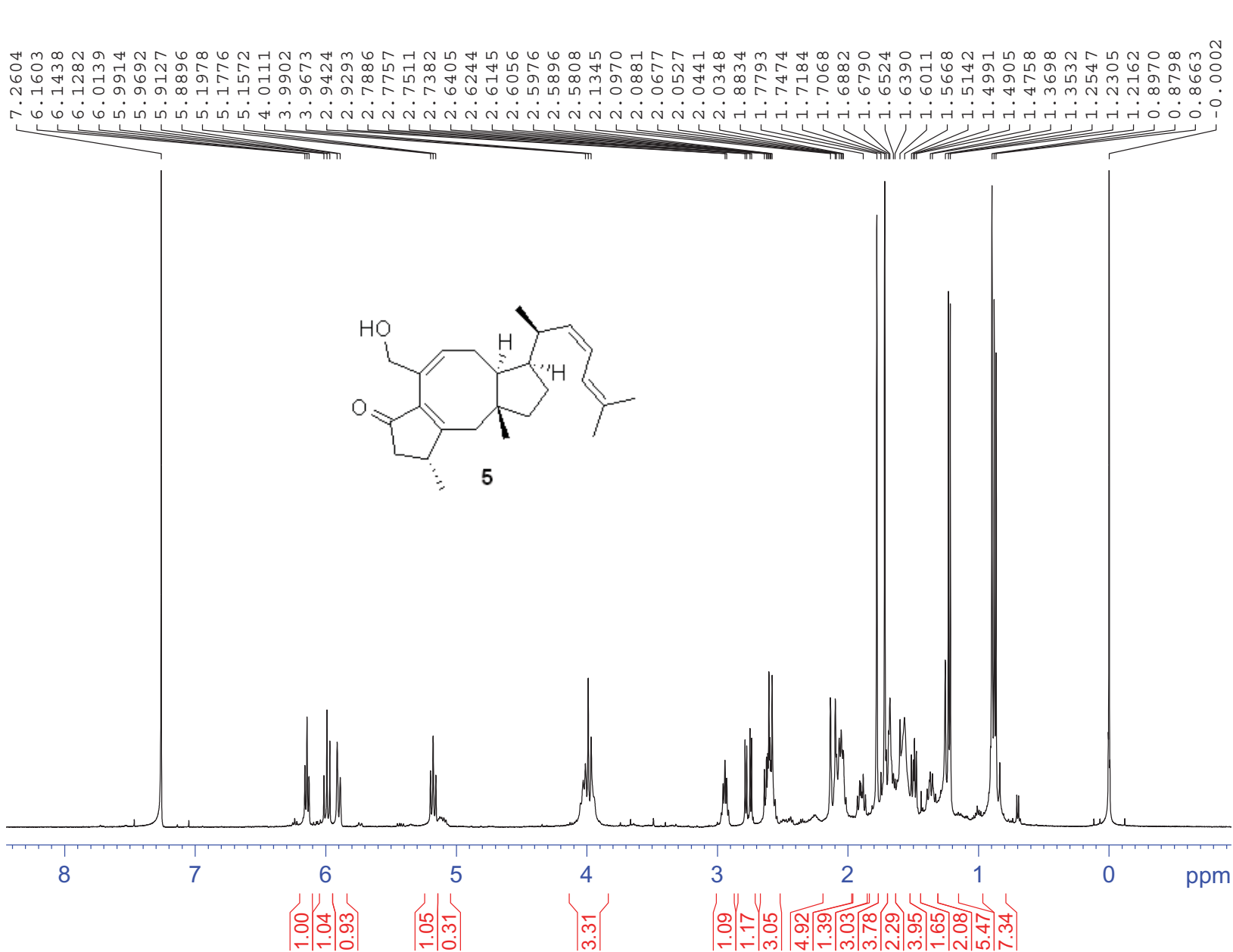
Autospec Premier
P776
4.16e4



Minimum: 0.5
Maximum: 100.0 10.0 40.0

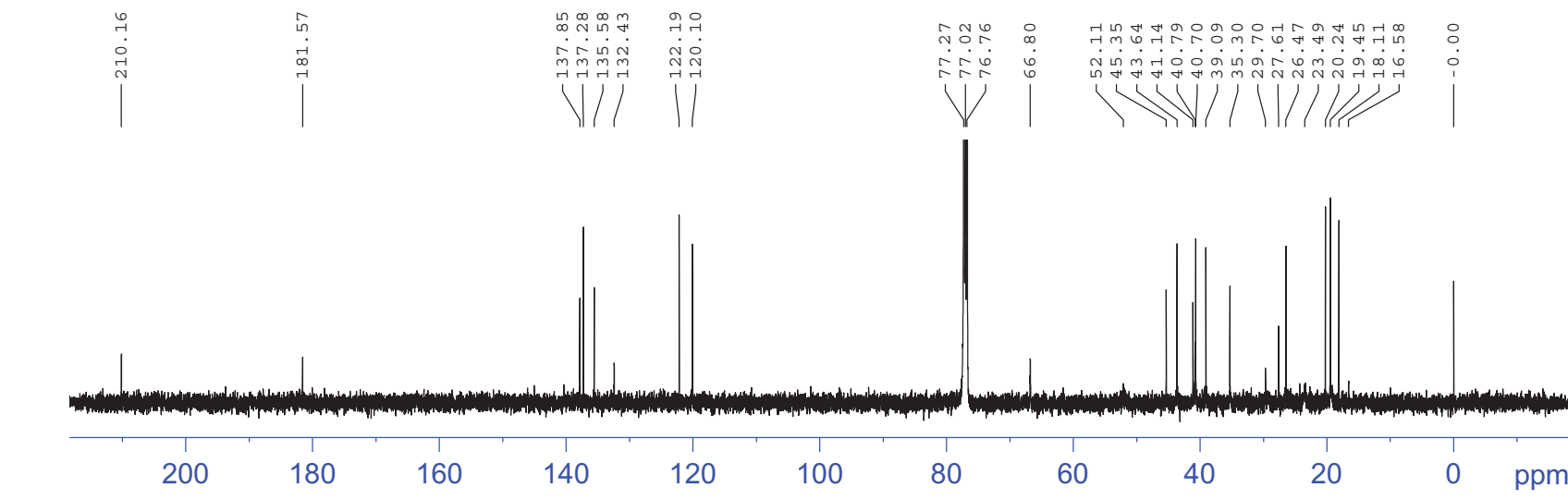
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
354.2925	354.2923	0.2	0.6	7.0	5566810.5	C25 H38 O

cf42-23

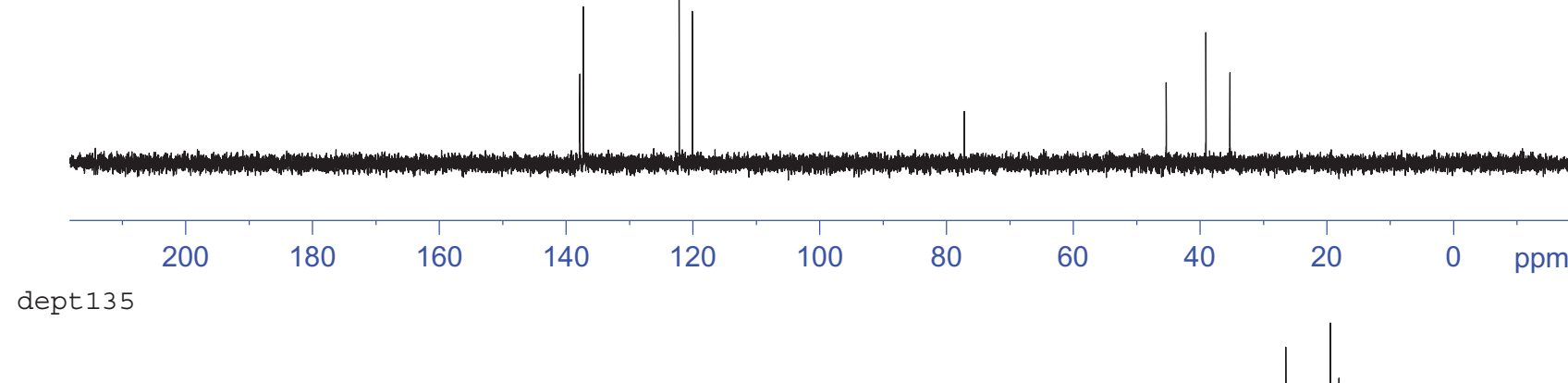


```
NAME 110330
EXPNO 4
PROCNO 1
Date_ 20110330
Time 15.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 40
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 181
DW 48.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

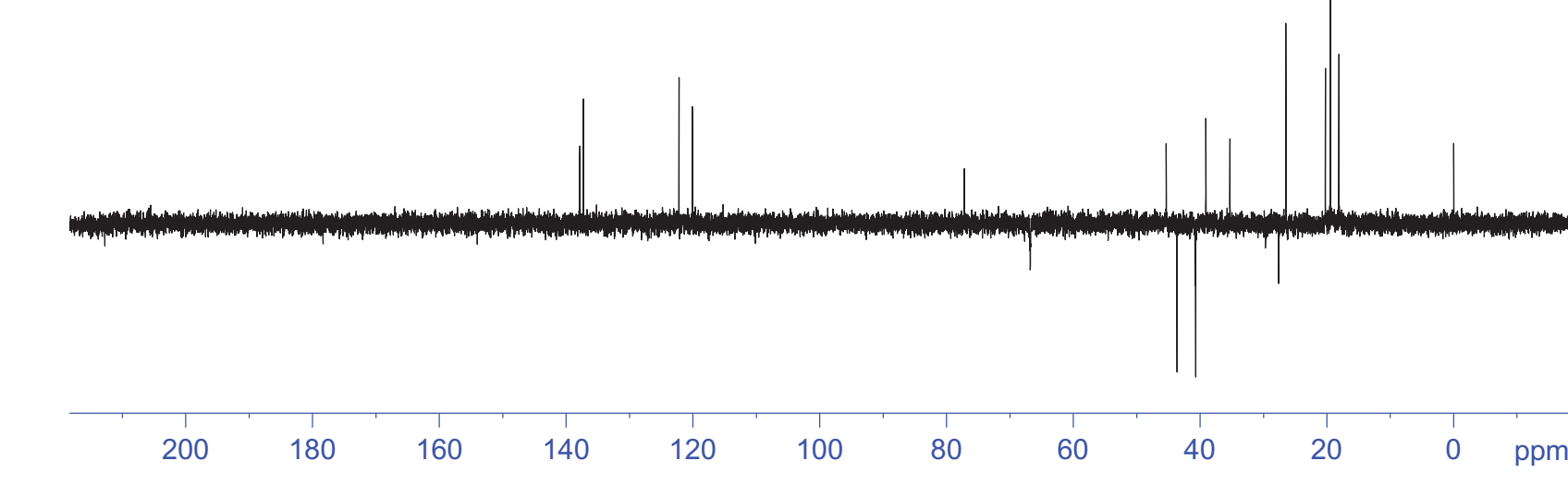
===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



dept90



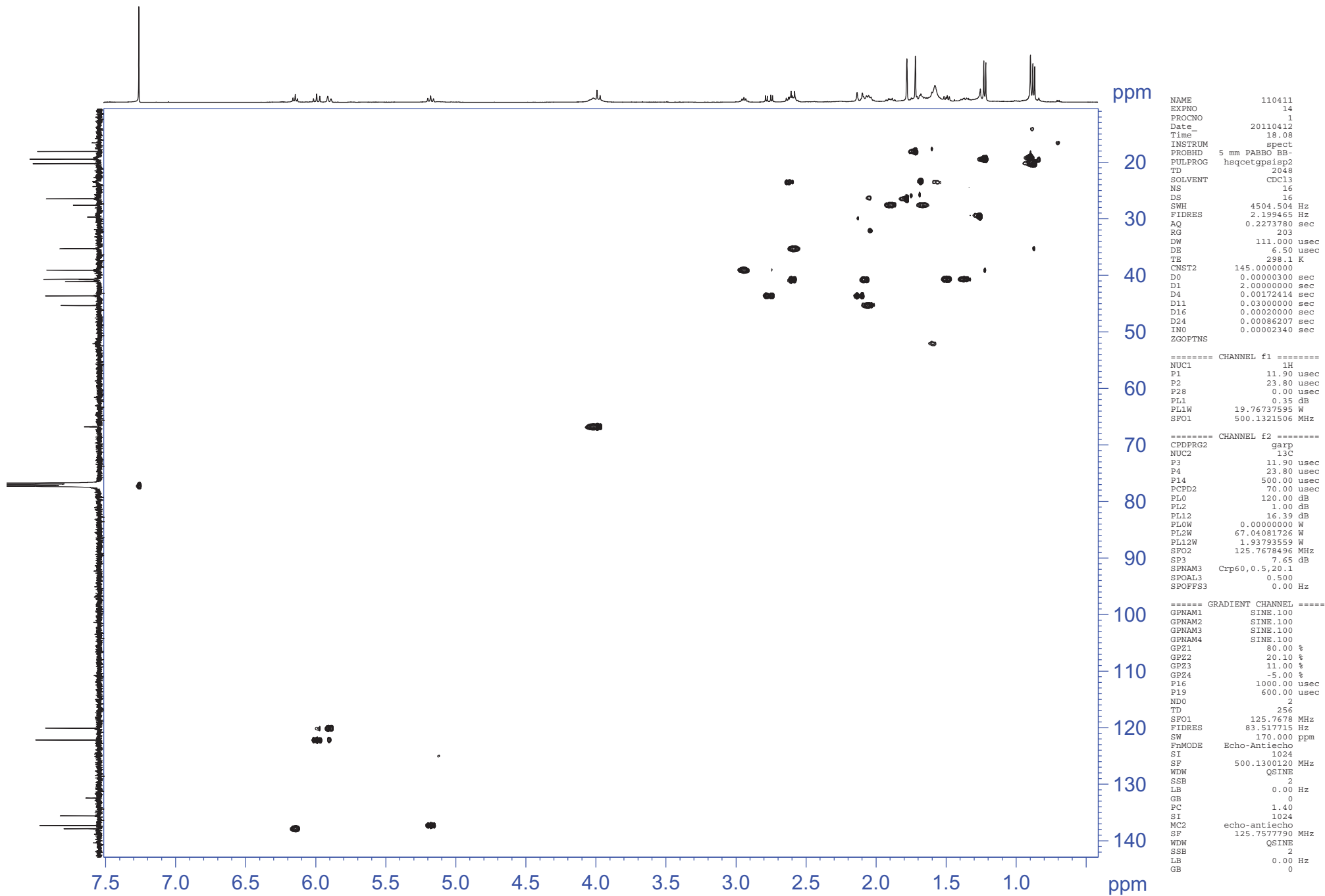
dept135



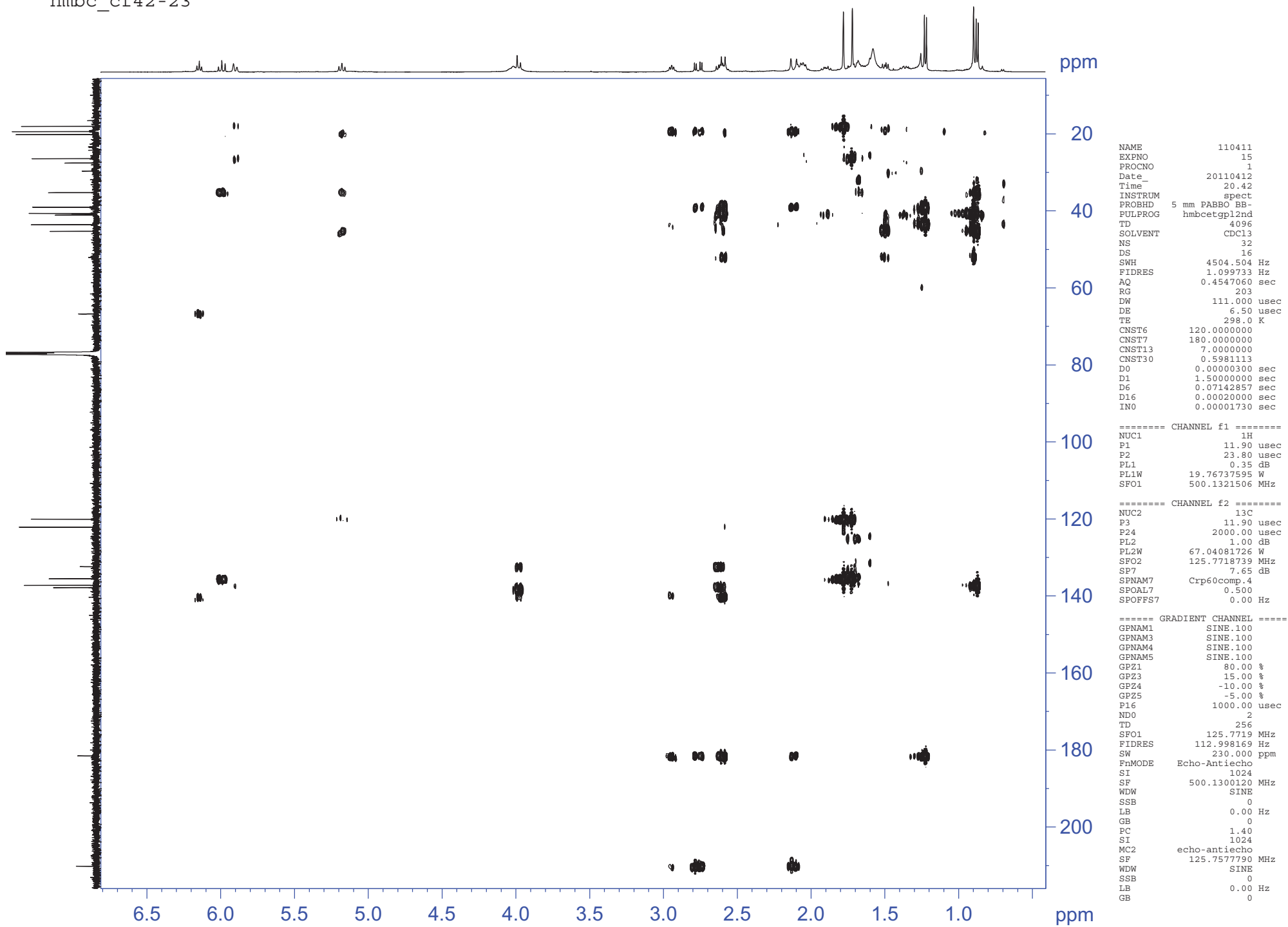
```

NAME      110401
EXPNO    18
PROCNO   1
Date_    20110406
Time     8.56
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SWH      29761.904 Hz
FIDRES   0.454113 Hz
AQ       1.1010548 sec
RG       203
DW       16.800 usec
DE       6.50 usec
TE       298.1 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1
----- CHANNEL f1 -----
NUC1     13C
P1       10.04 usec
PL1      -1.00 dB
PL1W    106.25253296 W
SFO1    125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2  waltz16
NUC2     1H
PCPD2   80.00 usec
PL2     0.35 dB
PL12    16.90 dB
PL13    17.00 dB
PL2W    19.76737595 W
PL1W    0.43747079 W
PL13W   0.42751271 W
SFO2    500.1320005 MHz
SI       32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
----- CHANNEL f1 -----
NAME      110401
EXPNO    40
PROCNO   1
Date_    20110406
Time     13.42
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  dept90
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SWH      29761.904 Hz
FIDRES   0.454113 Hz
AQ       1.1010548 sec
RG       203
DW       16.800 usec
DE       6.50 usec
TE       298.0 K
CNST2   145.0000000
D1       2.0000000 sec
D2       0.00344838 sec
D12      0.00002000 sec
TD0      1
----- CHANNEL f1 -----
NUC1     13C
P1       10.04 usec
P2       20.08 usec
PL1      -1.00 dB
PL2      20.08 dB
PL1W    106.25253296 W
SFO1    125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2  waltz16
NUC2     1H
P3       13.00 usec
P4       26.00 usec
PCPD2   80.00 usec
PL2     0.35 dB
PL12    16.90 dB
PL13    17.00 dB
PL2W    19.76737595 W
PL1W    0.43747079 W
SFO2    500.1320005 MHz
SI       32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
----- CHANNEL f1 -----
NAME      110401
EXPNO    19
PROCNO   1
Date_    20110406
Time     13.22
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  dept135
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SWH      29761.904 Hz
FIDRES   0.454113 Hz
AQ       1.1010548 sec
RG       203
DW       16.800 usec
DE       6.50 usec
TE       298.0 K
CNST2   145.0000000
D1       2.0000000 sec
D2       0.00344838 sec
D12      0.00002000 sec
TD0      1
----- CHANNEL f1 -----
NUC1     13C
P1       10.04 usec
P2       20.08 usec
PL1      -1.00 dB
PL2      20.08 dB
PL1W    106.25253296 W
SFO1    125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2  waltz16
NUC2     1H
P3       13.00 usec
P4       26.00 usec
PCPD2   80.00 usec
PL2     0.35 dB
PL12    16.90 dB
PL13    17.00 dB
PL2W    19.76737595 W
PL1W    0.43747079 W
SFO2    500.1320005 MHz
SI       32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

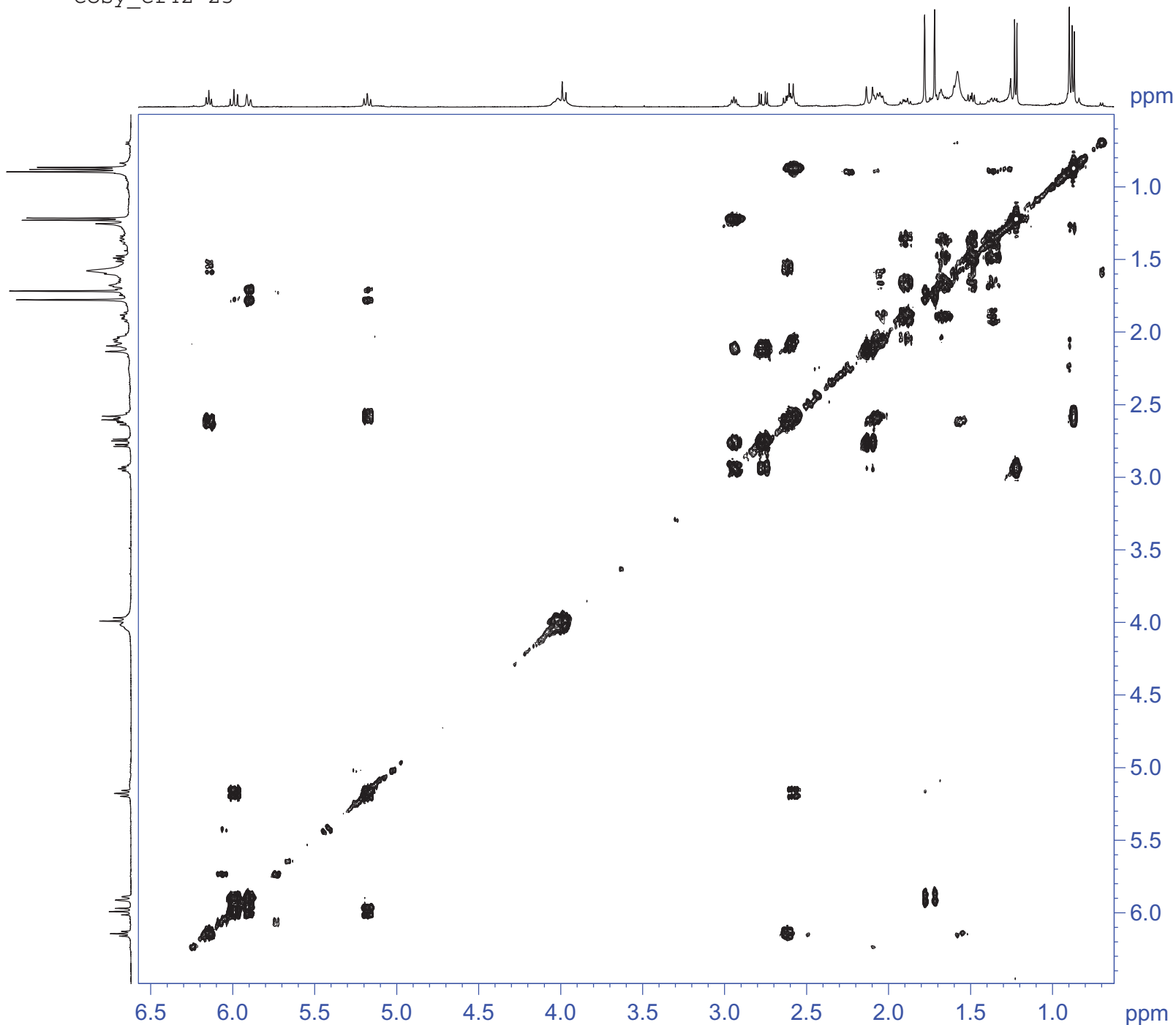

hsqc_cf42-23



hmbc_cf42-23



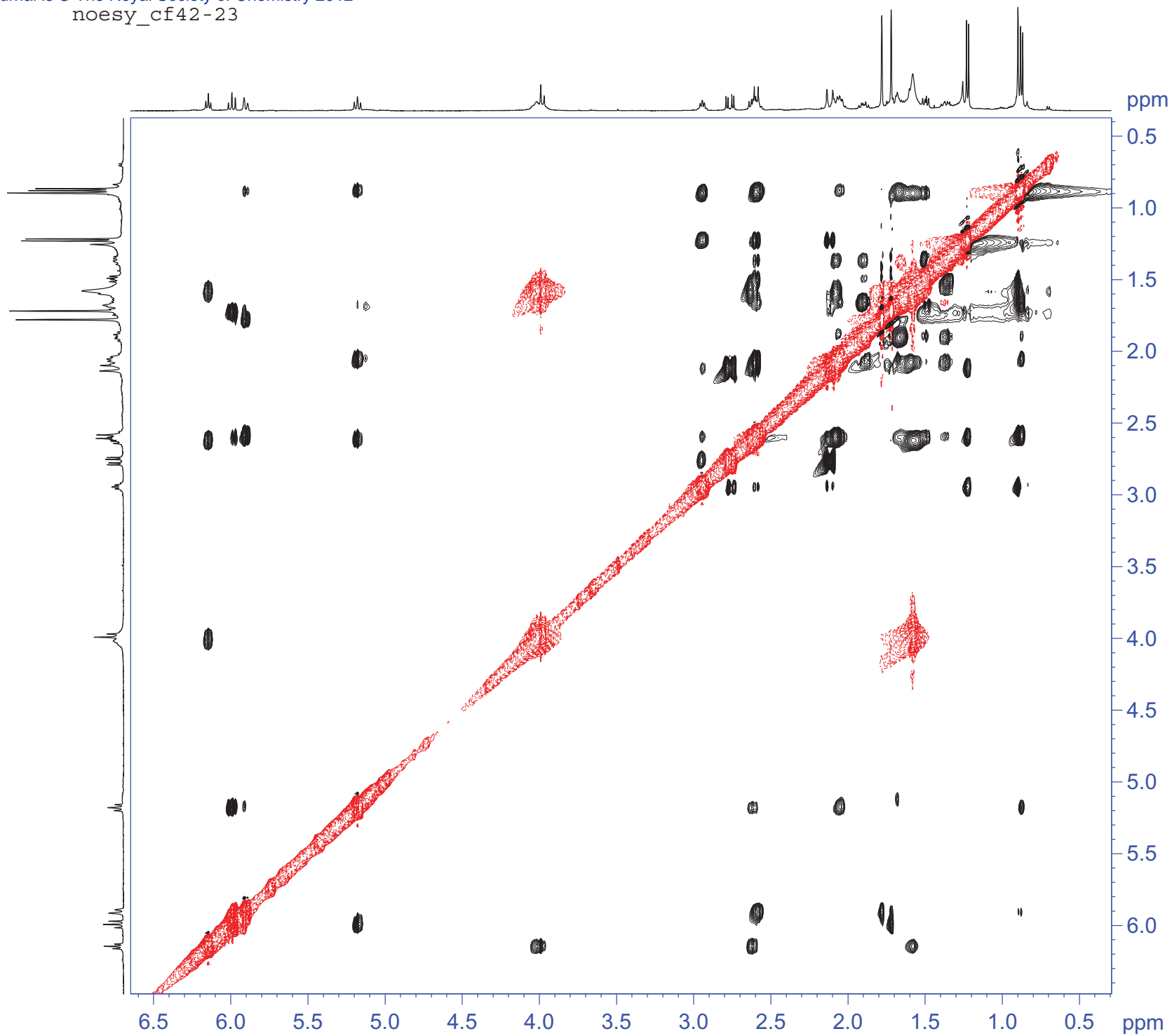
cosy_cf42-23



```
NAME          110411
EXPNO         13
PROCNO        1
Date_         20110412
Time_         16.49
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       cosygpmfqf
TD            2048
SOLVENT       CDC13
NS            8
DS            8
SWH           4504.504 Hz
FIDRES        2.199465 Hz
AQ            0.2273780 sec
RG            203
DW            111.000 usec
DE            6.50 usec
TE            298.0 K
D0            0.00000300 sec
D1            2.00000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00022215 sec
```

```
===== CHANNEL f1 =====
NUC1          1H
P1            11.90 usec
PL1           0.35 dB
PL1W          19.76737595 W
SFO1          500.1321506 MHz
```

```
===== GRADIENT CHANNEL =====
GPNAM1       SINE.100
GPNAM2       SINE.100
GPNAM3       SINE.100
GPZ1         16.00 %
GPZ2         12.00 %
GPZ3         40.00 %
P16          1000.00 usec
ND0          1
TD           256
SFO1         500.1322 MHz
FIDRES       17.582771 Hz
SW           9.000 ppm
FnMODE       QF
SI           1024
SF           500.1300129 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
PC           1.40
SI           1024
MC2          QF
SF           500.1300129 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
```



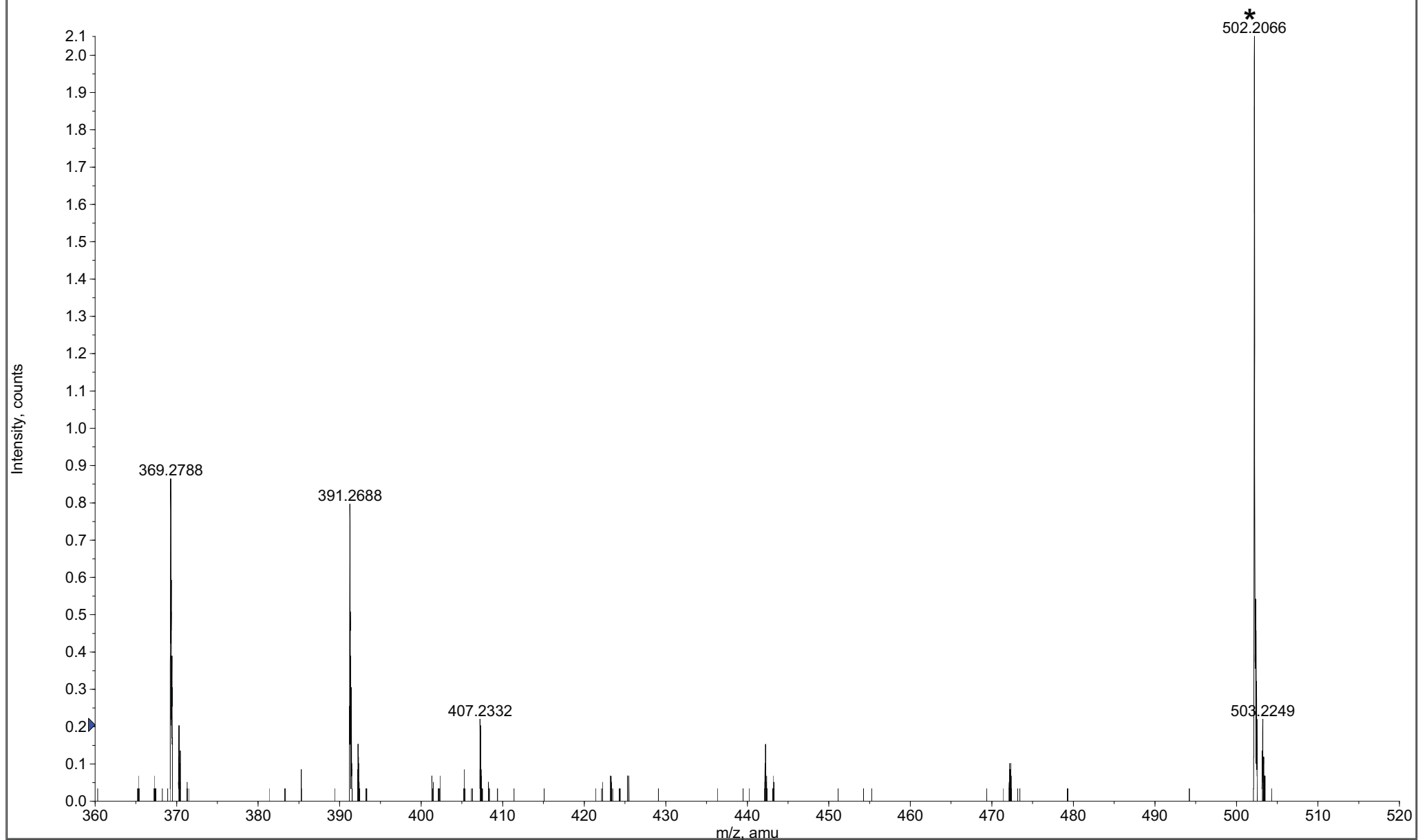
NAME 110411
EXPNO 16
PROCNO 1
Date_ 20110413
Time_ 1.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesygp
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
D0 0.00009593 sec
D1 2.00000000 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00022215 sec

==== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
P2 23.80 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1321506 MHz

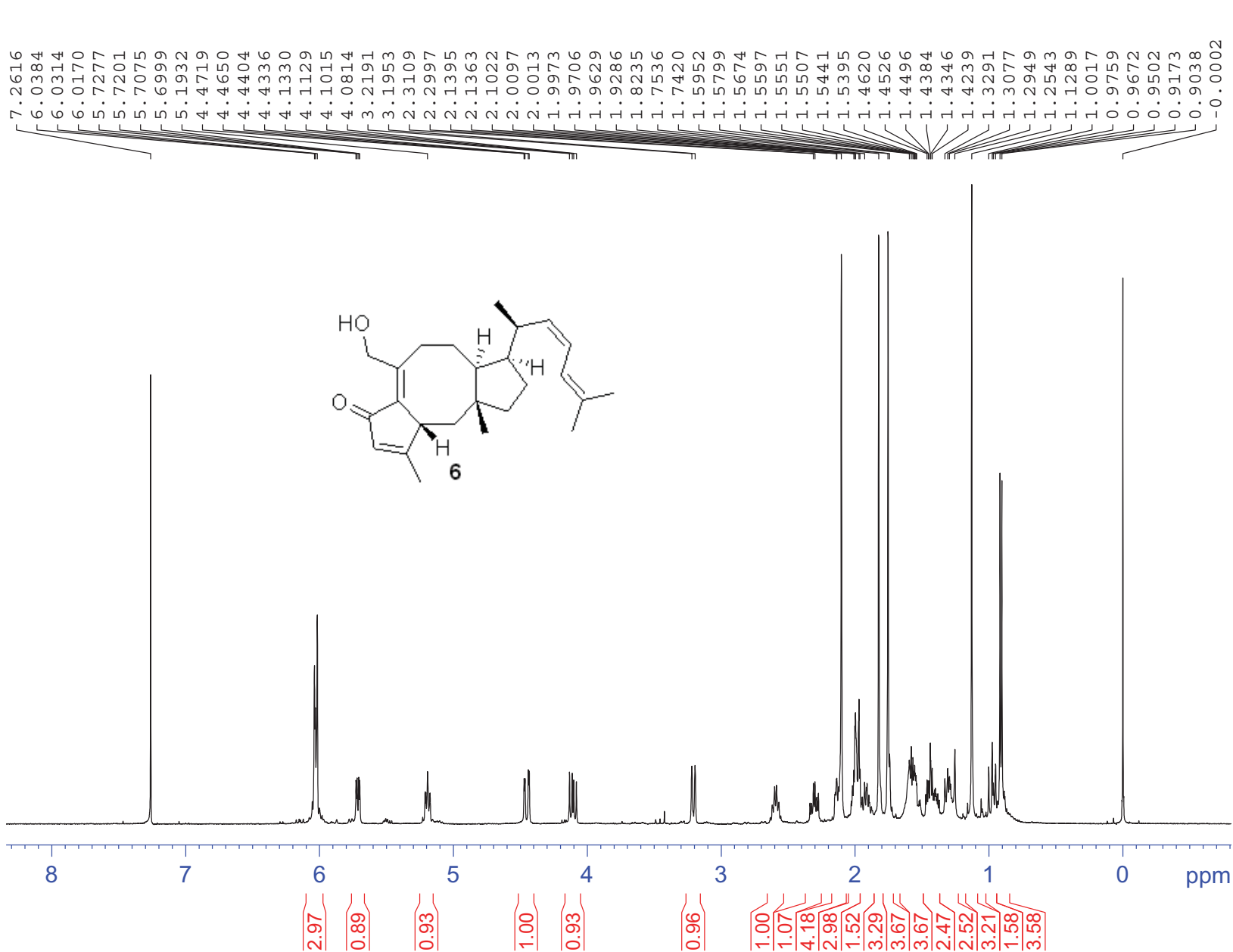
==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 500.1322 MHz
FIDRES 17.582771 Hz
SW 9.000 ppm
FnMODE States-TPPI
SI 1024
SF 500.1300120 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPPI
SF 500.1300120 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

+TOF MS: 0.533 to 1.500 min from 110429ESIA cf42-23.wiff
a=3.55956354589842450e-004, t0=7.96575916585934460e+001

Max. 2.1 counts.

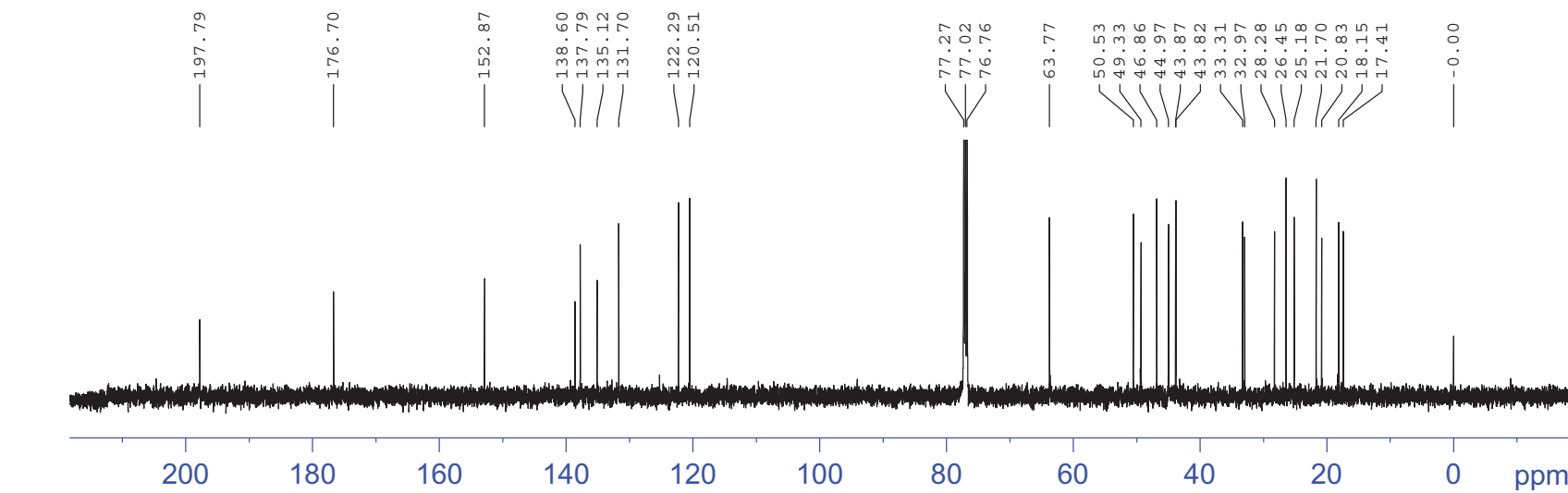


cf42-2



```
NAME 101222
EXPNO 6
PROCNO 1
Date_ 20101222
Time 11.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 144
DW 48.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

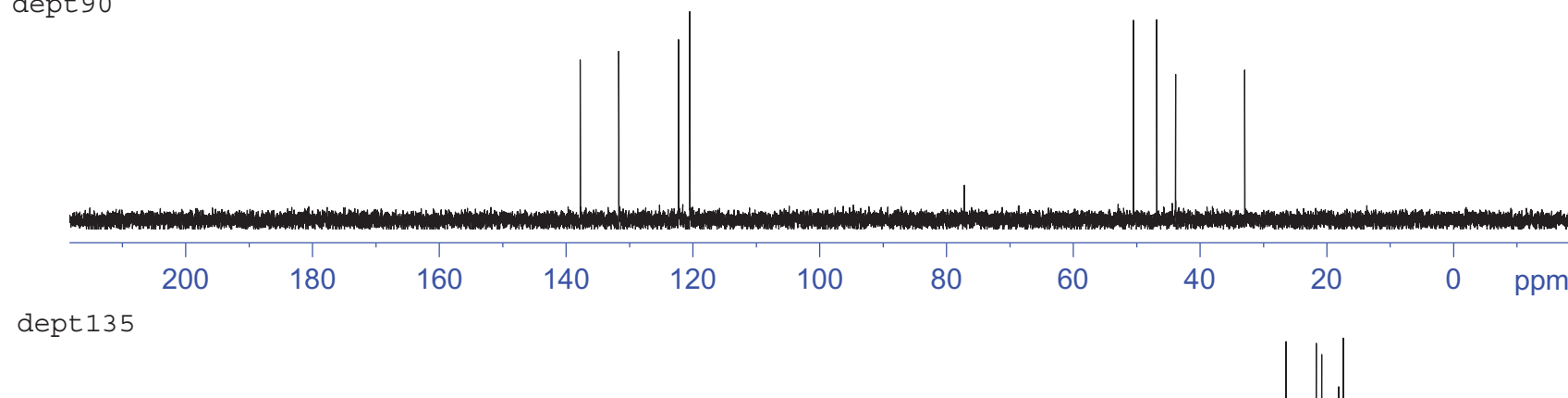
===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



dept90

```

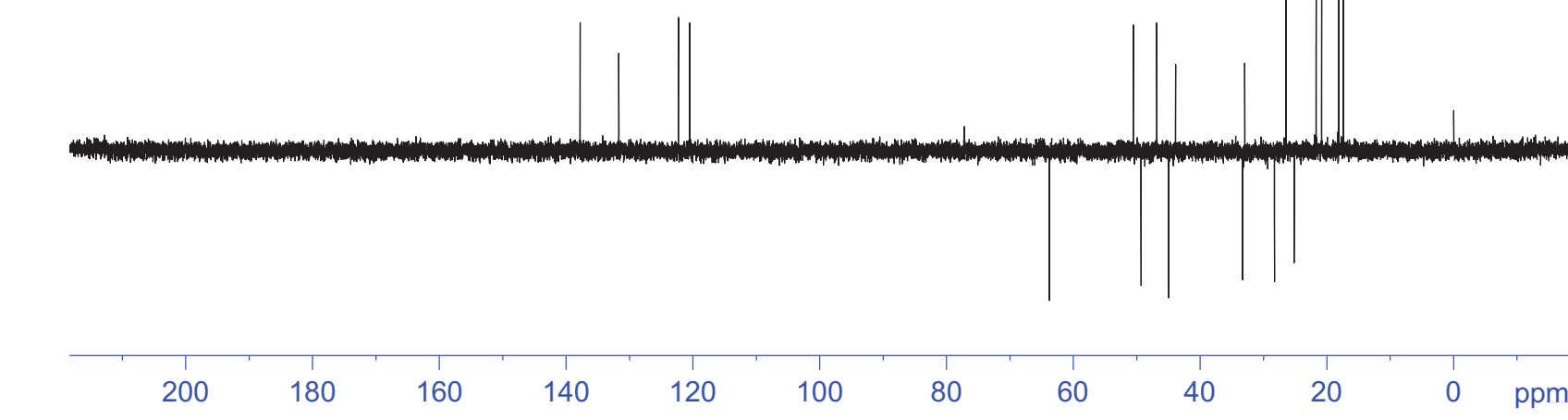
NAME      101222
EXPNO    7
PROCNO   7
Date_    20101222
Time     11.08
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SWH      29761.904 Hz
FIDRES   0.454113 Hz
AQ       1.1010548 sec
RG        203
DW       16.800 usec
DE       6.50 usec
TE       298.1 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1
----- CHANNEL f1 -----
NUC1      13C
P1       10.04 usec
PL1      -1.00 dB
PL1W     106.25253296 W
SFO1     125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       0.35 dB
PL12     16.90 dB
PL13     17.00 dB
PL2W     19.76737595 W
PL12W    0.43747079 W
PL13W    0.42751271 W
SFO2     500.1320005 MHz
SI        32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```



dept135

```

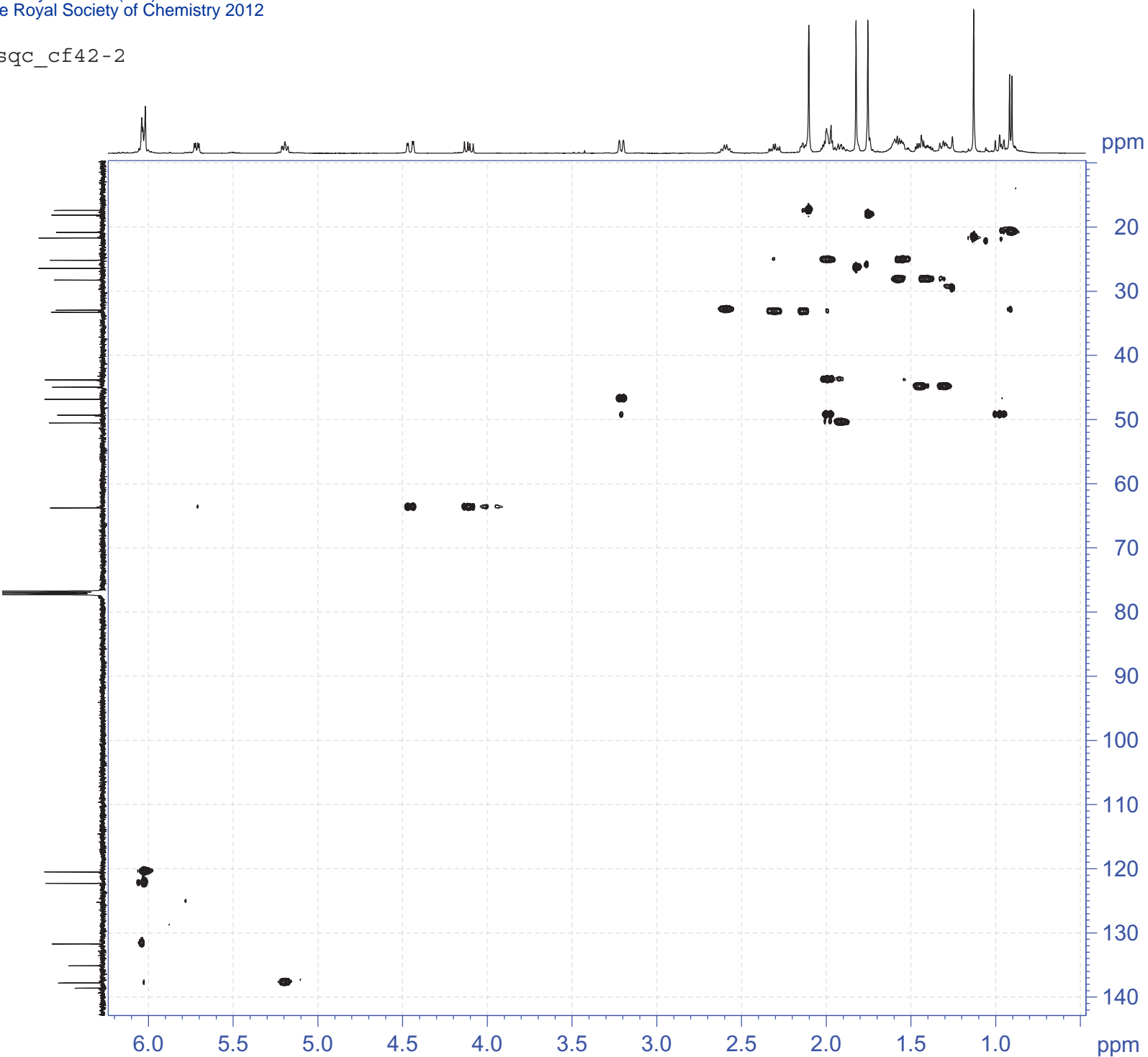
NAME      101222
EXPNO    9
PROCNO   9
Date_    20101222
Time     12.27
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SWH      29761.904 Hz
FIDRES   0.454113 Hz
AQ       1.1010548 sec
RG        203
DW       16.800 usec
DE       6.50 usec
TE       298.0 K
D1       145.0000000 sec
D2       2.0000000 sec
D12      0.00344828 sec
D13      0.00002000 sec
TD0      1
----- CHANNEL f1 -----
NUC1      13C
P1       10.04 usec
PL1      20.08 usec
PL1W     106.25253296 W
SFO1     125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2  waltz16
NUC2      1H
PCPD2    13.00 usec
P4       26.00 usec
PCPD2    80.00 usec
PL2       0.35 dB
PL12     16.90 dB
PL13     17.00 dB
PL2W     19.76737595 W
PL12W    0.43747079 W
SFO2     500.1320005 MHz
SI        32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```



```

NAME      101222
EXPNO    8
PROCNO   8
Date_    20101222
Time     12.14
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  dept135
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SWH      29761.904 Hz
FIDRES   0.454113 Hz
AQ       1.1010548 sec
RG        203
DW       16.800 usec
DE       6.50 usec
TE       298.1 K
D1       145.0000000 sec
D2       2.0000000 sec
D12      0.00344828 sec
D13      0.00002000 sec
TD0      1
----- CHANNEL f1 -----
NUC1      13C
P1       10.04 usec
P2       20.08 usec
PL1      -1.00 dB
PL1W     106.25253296 W
SFO1     125.7703643 MHz
----- CHANNEL f2 -----
CHDPRG2  waltz16
NUC2      1H
P3       13.00 usec
P4       26.00 usec
PCPD2    80.00 usec
PL2       0.35 dB
PL12     16.90 dB
PL13     17.00 dB
PL2W     19.76737595 W
PL12W    0.43747079 W
SFO2     500.1320005 MHz
SI        32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

hsqc_cf42-2



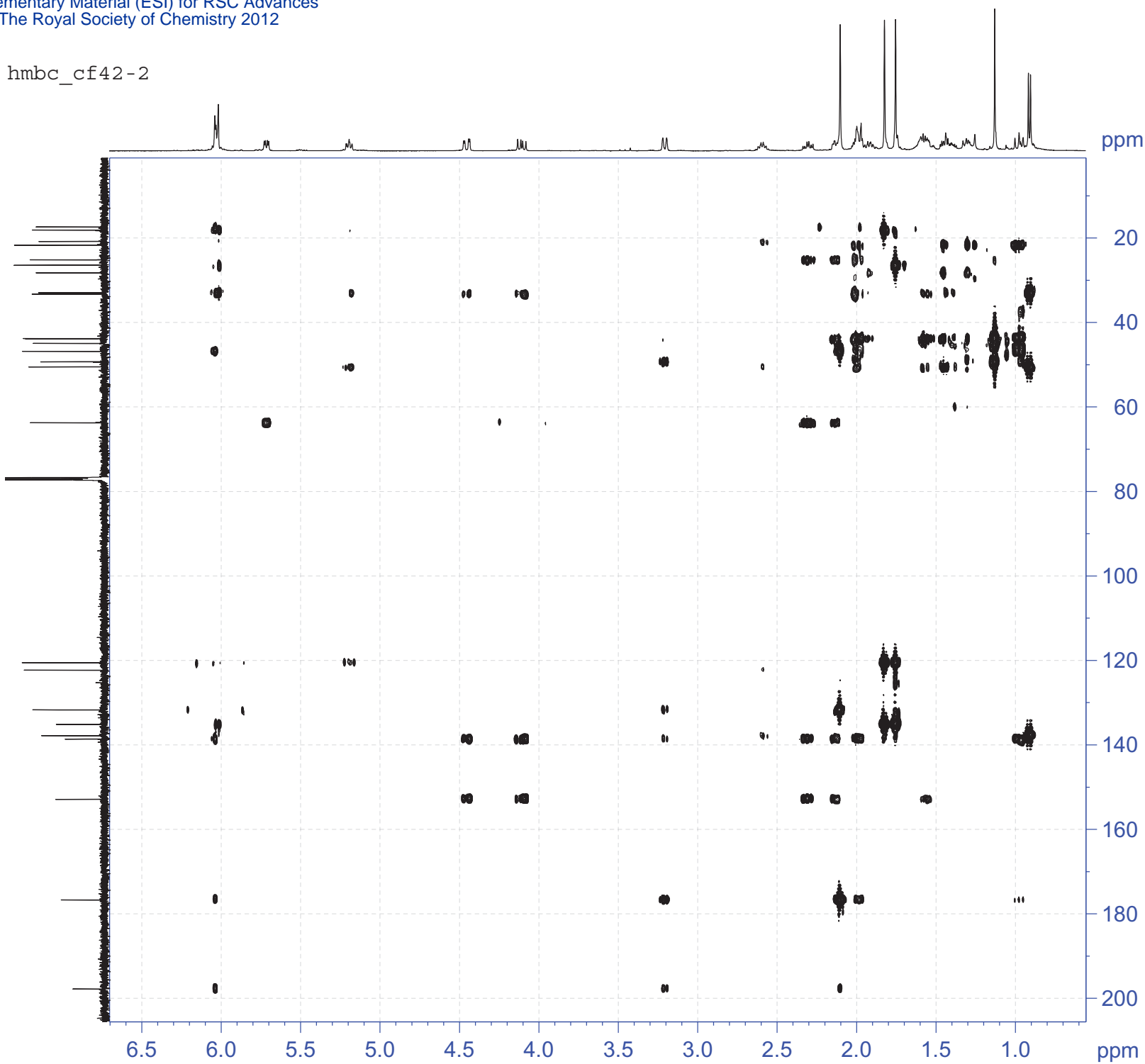
```
NAME 101227
EXPNO 8
PROCNO 1
Date_ 20101227
Time 17.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hsqcetgpsisp2
TD 2048
SOLVENT CDCl3
NS 16
DS 32
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D0 0.0000300 sec
D1 2.0000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
INO 0.00002400 sec
ZGOPTNS

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
P2 23.80 usec
P28 0.00 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1320005 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 11.90 usec
P4 23.80 usec
P14 500.00 usec
PCPD2 70.00 usec
PL0 120.00 dB
PL2 1.00 dB
PL12 16.39 dB
PLOW 0.00000000 W
PL2W 67.04081726 W
PL12W 1.93793559 W
SFO2 125.7678496 MHz
SP3 7.65 dB
SPNAM3 Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec
NDO 2
TD 256
SFO1 125.7678 MHz
FIDRES 81.380646 Hz
SW 165.650 ppm
FnMODE Echo-Antiecho
SI 1024
SF 500.1300100 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 125.7578045 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
```


hmbc_cf42-2



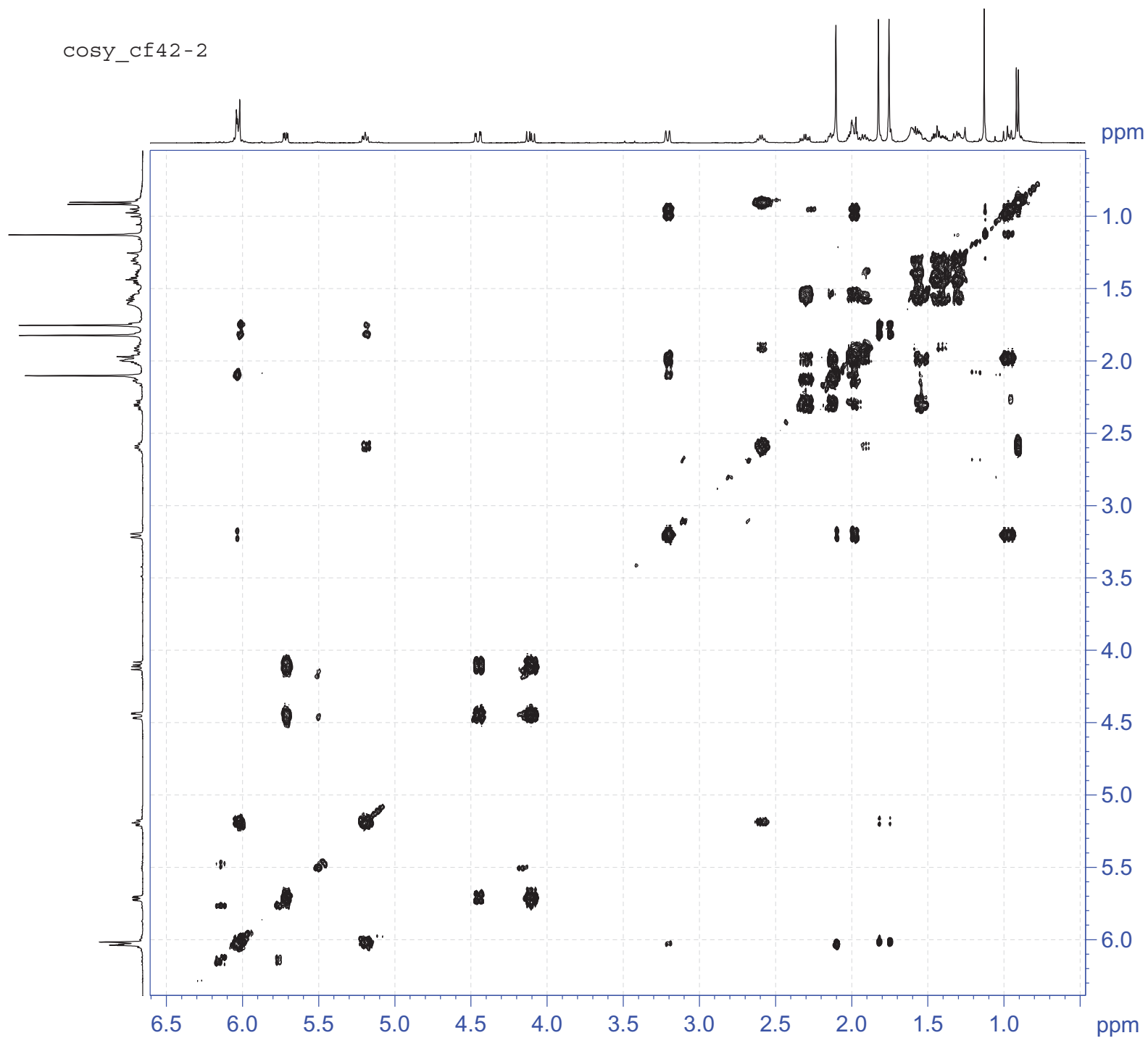
```
NAME          101227
EXPNO         9
PROCNO        1
Date_         20101227
Time_        20.31
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       hmbcetgp12nd
TD            4096
SOLVENT       CDCl3
NS            32
DS            16
SWH           4504.504 Hz
FIDRES        1.099733 Hz
AQ            0.4547060 sec
RG            203
DW            111.000 usec
DE            6.50 usec
TE            298.0 K
CNST6         120.0000000
CNST7         180.0000000
CNST13        7.0000000
CNST30        0.5981151
D0            0.00000300 sec
D1            1.50000000 sec
D6            0.07142857 sec
D16           0.00020000 sec
IN0           0.00001805 sec

===== CHANNEL f1 =====
NUC1          1H
P1            11.90 usec
P2            23.80 usec
PL1           0.35 dB
PL1W          19.76737595 W
SFO1          500.1320005 MHz

===== CHANNEL f2 =====
NUC2          13C
P3            11.90 usec
P4            2000.00 usec
PL2           1.00 dB
PL2W          67.04081726 W
SFO2          125.7703648 MHz
SP7           7.65 dB
SPNAM7        Crp60comp.4
SPOAL7        0.500
SPOFFS7       0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM3        SINE.100
GPNAM4        SINE.100
GPNAM5        SINE.100
GPZ1          80.00 %
GPZ3          15.00 %
GPZ4          -10.00 %
GPZ5          -5.00 %
P16           1000.00 usec
ND0           2
TD            256
SFO1          125.7704 MHz
FIDRES        108.083908 Hz
SW            220.000 ppm
FnMODE        Echo-Antiecho
SI            1024
SF            500.1300100 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           echo-antiecho
SF            125.7578045 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
```

cosy_cf42-2

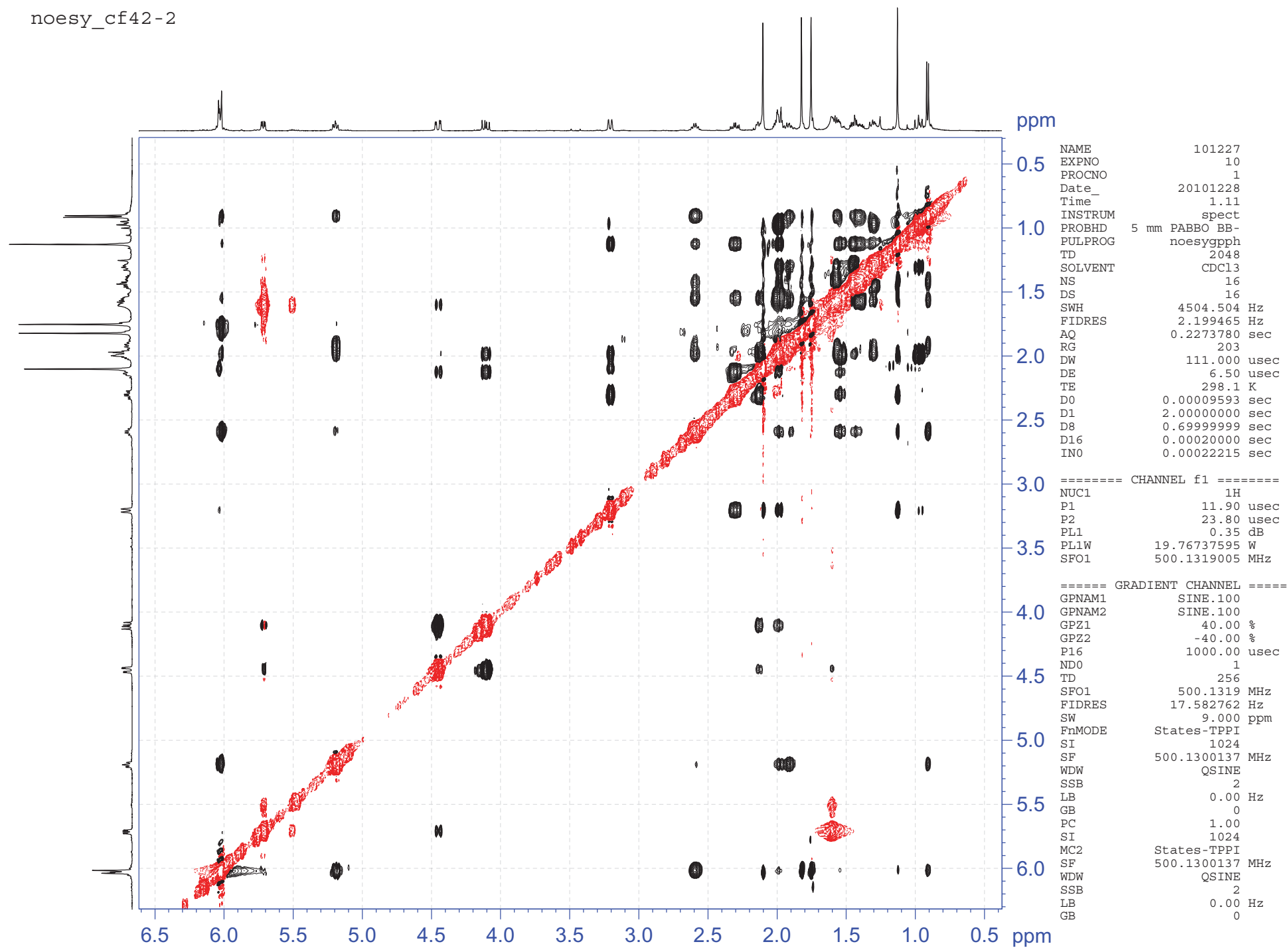


```
NAME 101227
EXPNO 7
PROCNO 1
Date_ 20101227
Time 17.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfqq
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.1 K
DO 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00022215 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1319005 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 500.1319 MHz
FIDRES 17.582762 Hz
SW 9.000 ppm
FnMODE QF
SI 1024
SF 500.1300137 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 500.1300137 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```

noesy_cf42-2



Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 40.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

43 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

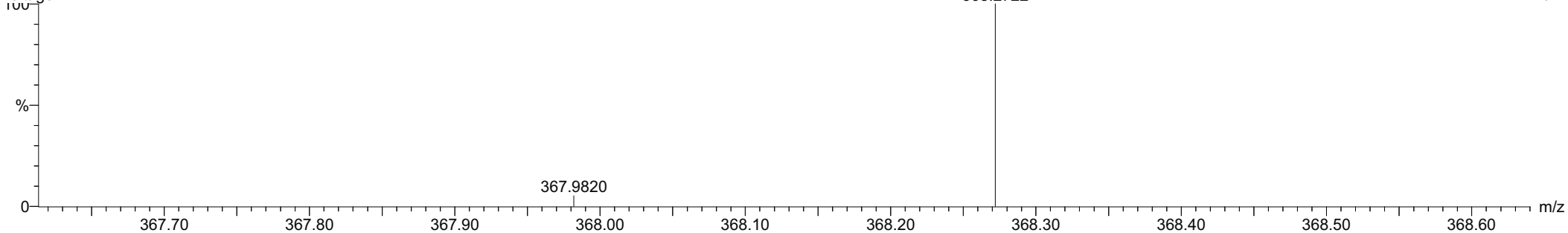
Elements Used:

C: 0-200 H: 0-400 O: 0-9

cf42-2

08:35:46 14-Jan-2011

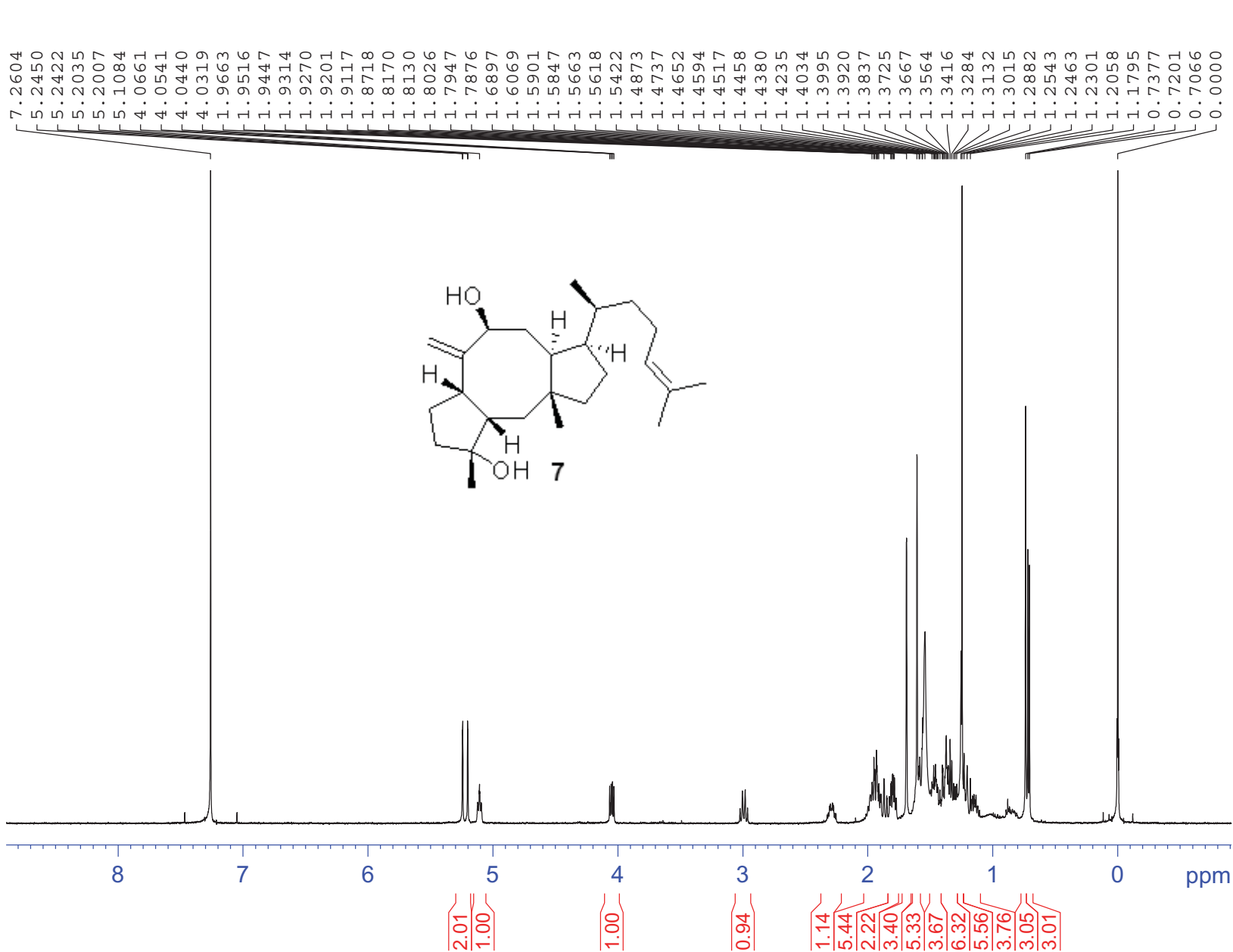
Voltage EI+



Minimum: 0.5
Maximum: 100.0 10.0 40.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
368.2722	368.2715	0.7	1.9	8.0	5546286.0	C25 H36 O2

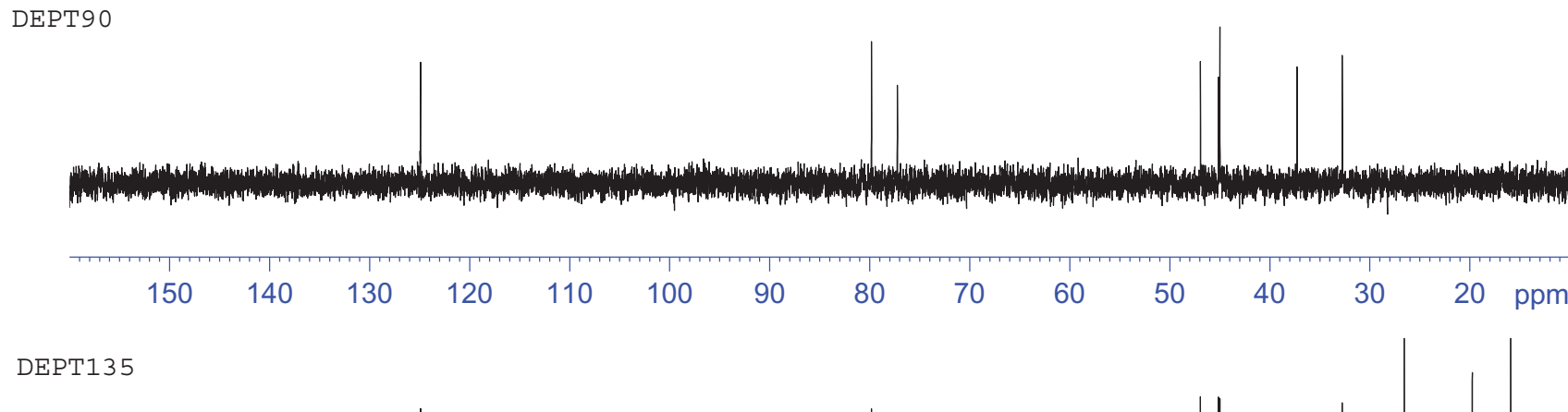
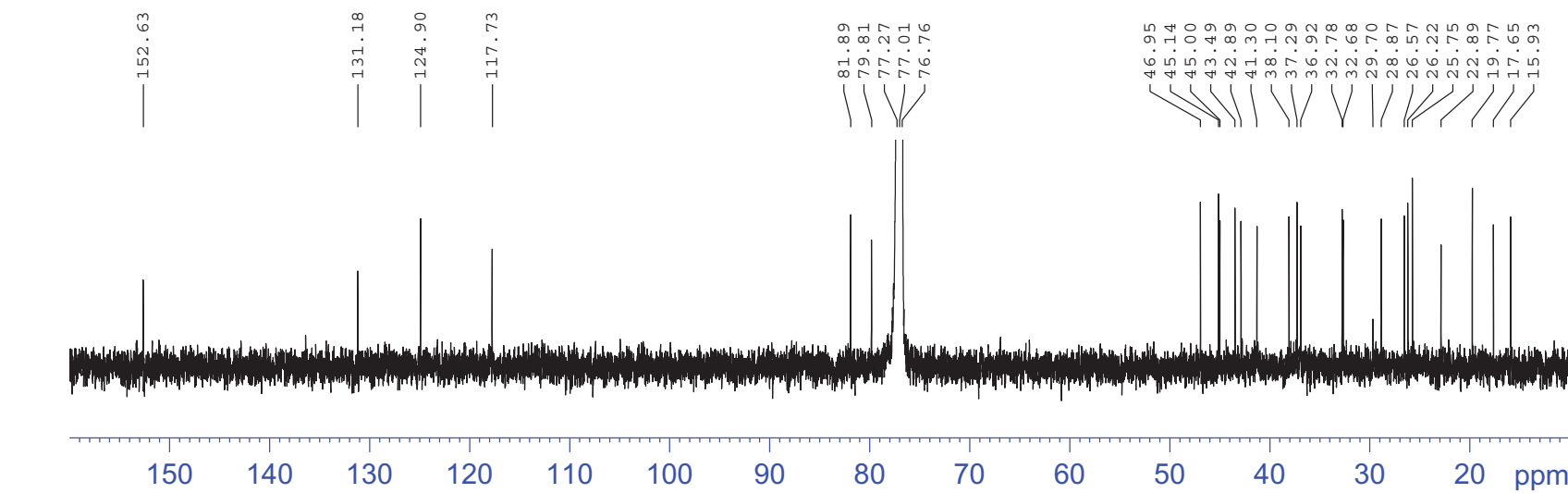
cf42-50



```

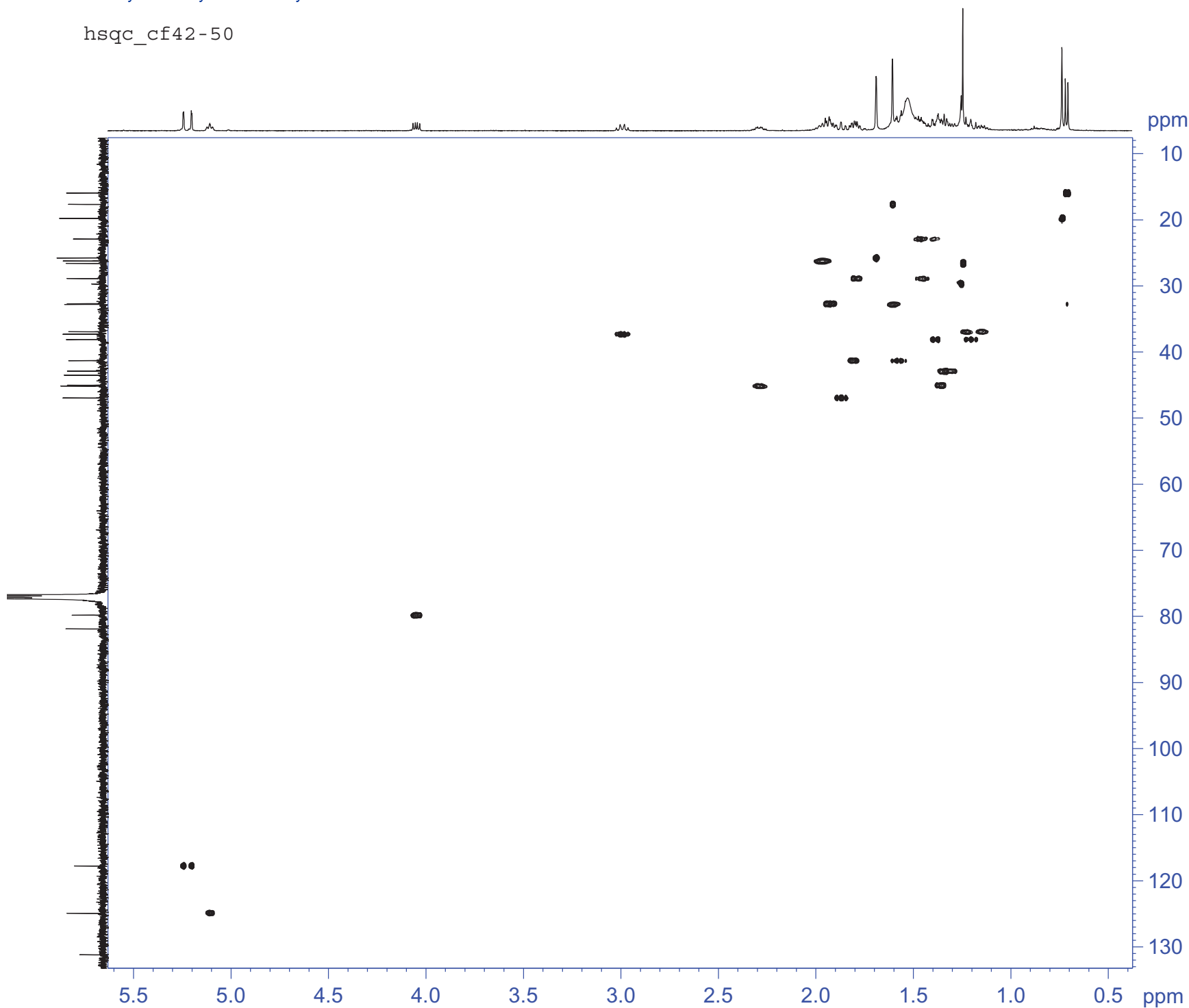
NAME          110601
EXPNO         25
PROCNO        1
Date_         20110603
Time_         8.47
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1719923 sec
RG            203
DW            48.400 usec
DE            6.50 usec
TE            298.0 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            11.90 usec
PL1           0.35 dB
PL1W          19.76737595 W
SFO1          500.1330885 MHz
SI            32768
SF            500.1300135 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



```
NAME 110614
EXPNO 5
PROCNO 1
Date_ 20110615
Time 10.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
PL1 -1.00 dB
PL1W 106.25253296 MHz
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHPROG2 waltz16
NUC2 1H
PCP2 80.00 usec
P4 26.00 usec
PCP2 80.00 usec
PL2 0.35 dB
PL12 16.90 dB
PL2W 19.76737595 MHz
PL12W 0.43747079 MHz
PL13W 0.42751271 MHz
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
----- CHANNEL f1 -----
NAME 110614
EXPNO 7
PROCNO 1
Date_ 20110615
Time 13.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
P2 20.08 usec
PL1 -1.00 dB
PL2 20.08 usec
PL1W 106.25253296 MHz
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHPROG2 waltz16
NUC2 1H
P3 13.00 usec
P4 26.00 usec
PCP2 80.00 usec
PL2 0.35 dB
PL12 16.90 dB
PL2W 19.76737595 MHz
PL12W 0.43747079 MHz
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
----- CHANNEL f1 -----
NAME 110614
EXPNO 6
PROCNO 1
Date_ 20110615
Time 12.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 10.04 usec
P2 20.08 usec
PL1 -1.00 dB
PL2 20.08 usec
PL1W 106.25253296 MHz
SFO1 125.7703643 MHz
----- CHANNEL f2 -----
CHPROG2 waltz16
NUC2 1H
P3 13.00 usec
P4 26.00 usec
PCP2 80.00 usec
PL2 0.35 dB
PL12 16.90 dB
PL2W 19.76737595 MHz
PL12W 0.43747079 MHz
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

hsqc_cf42-50



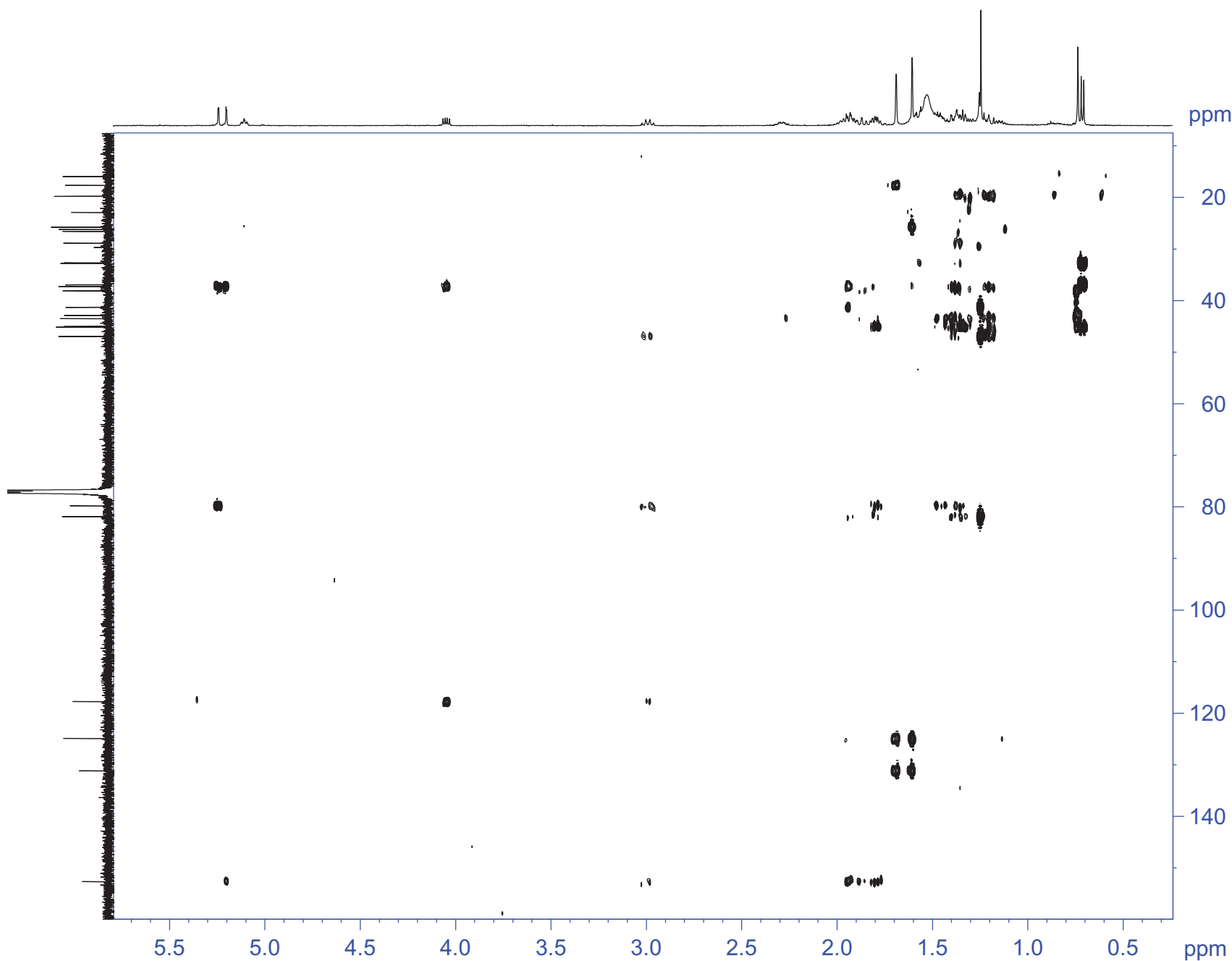
```
NAME 110620
EXPNO 2
PROCNO 1
Date_ 20110620
Time_ 10.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hsqcetgpsisp2
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 203
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D0 0.0000300 sec
D1 2.0000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00002650 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
P2 23.80 usec
P28 0.00 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1319005 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 11.90 usec
P4 23.80 usec
P14 500.00 usec
PCPD2 70.00 usec
PL0 120.00 dB
PL2 1.00 dB
PL12 16.39 dB
PL0W 0.00000000 W
PL2W 67.04081726 W
PL12W 1.93793559 W
SFO2 125.7665920 MHz
SP3 7.65 dB
SPNAM3 Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0.00 Hz

===== GRADIENT CHANNEL =====
GNAM1 SINE.100
GNAM2 SINE.100
GNAM3 SINE.100
GNAM4 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec
TD 256
SFO1 125.7666 MHz
FIDRES 73.691360 Hz
SW 150.000 ppm
FnMODE Echo-Antiecho
SI 1024
SF 500.1300120 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 125.7577790 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
```

hmbc_cf42-50



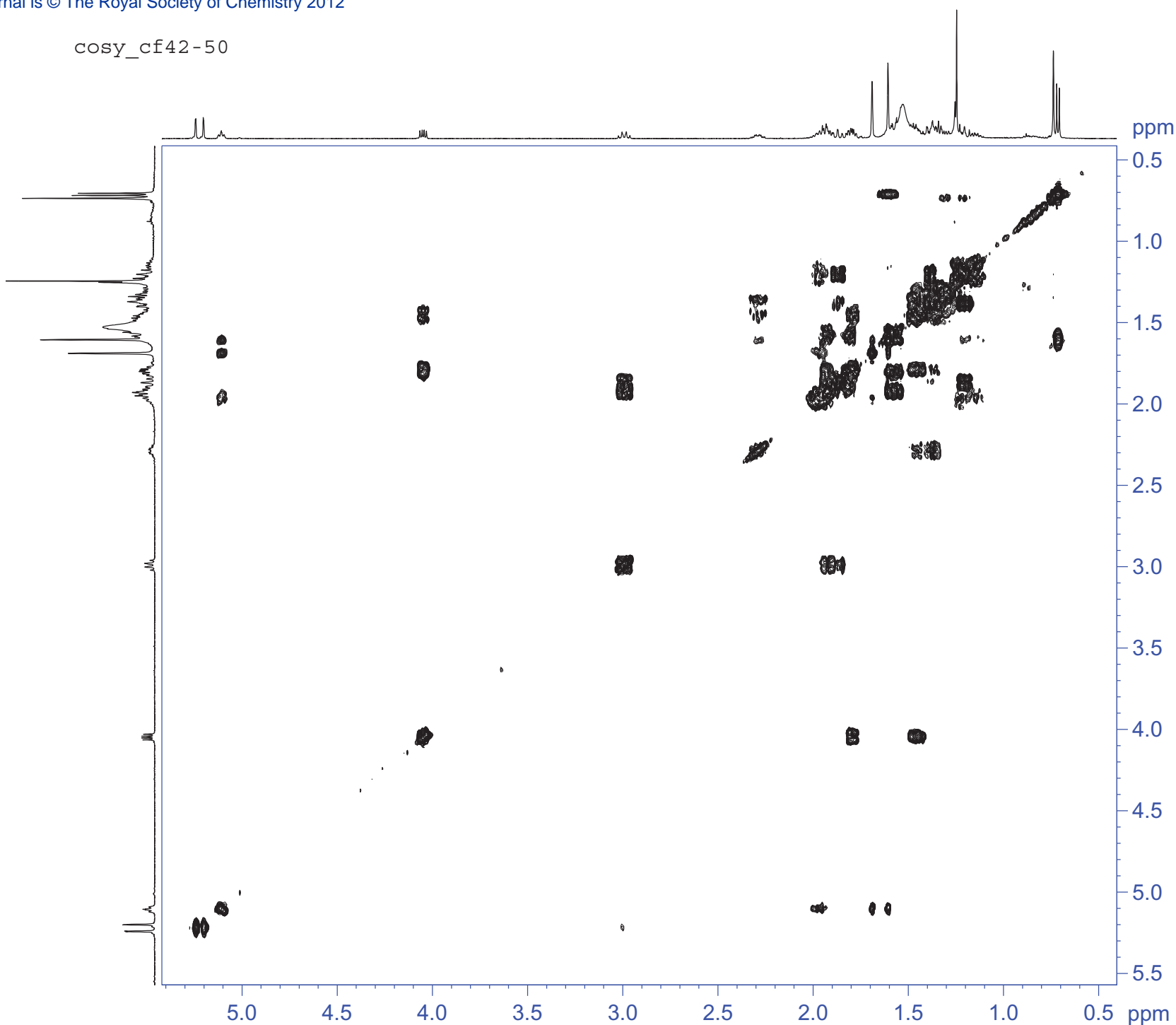
```
NAME 110620
EXPNO 3
PROCNO 1
Date_ 20110620
Time 12.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcetgp12nd
TD 4096
SOLVENT CDCl3
NS 32
DS 16
SWH 4504.504 Hz
FIDRES 1.099733 Hz
AQ 0.4547060 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
CNST6 120.0000000
CNST7 180.0000000
CNST13 7.0000000
CNST30 0.5981198
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.07142857 sec
D16 0.00020000 sec
IN0 0.00002210 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
P2 23.80 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1319005 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 11.90 usec
P24 2000.00 usec
PL2 1.00 dB
PL2W 67.04081726 W
SFO2 125.7684784 MHz
SP7 7.65 dB
SPNAM7 Crp60comp.4
SPOAL7 0.500
SPOFFS7 0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPNAM5 SINE.100
GPZ1 80.00 %
GPZ3 15.00 %
GPZ4 -10.00 %
GPZ5 -5.00 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 125.7685 MHz
FIDRES 88.430962 Hz
SW 180.000 ppm
FnMODE Echo-Antiecho
SI 1024
SF 500.1300120 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 125.7577790 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```

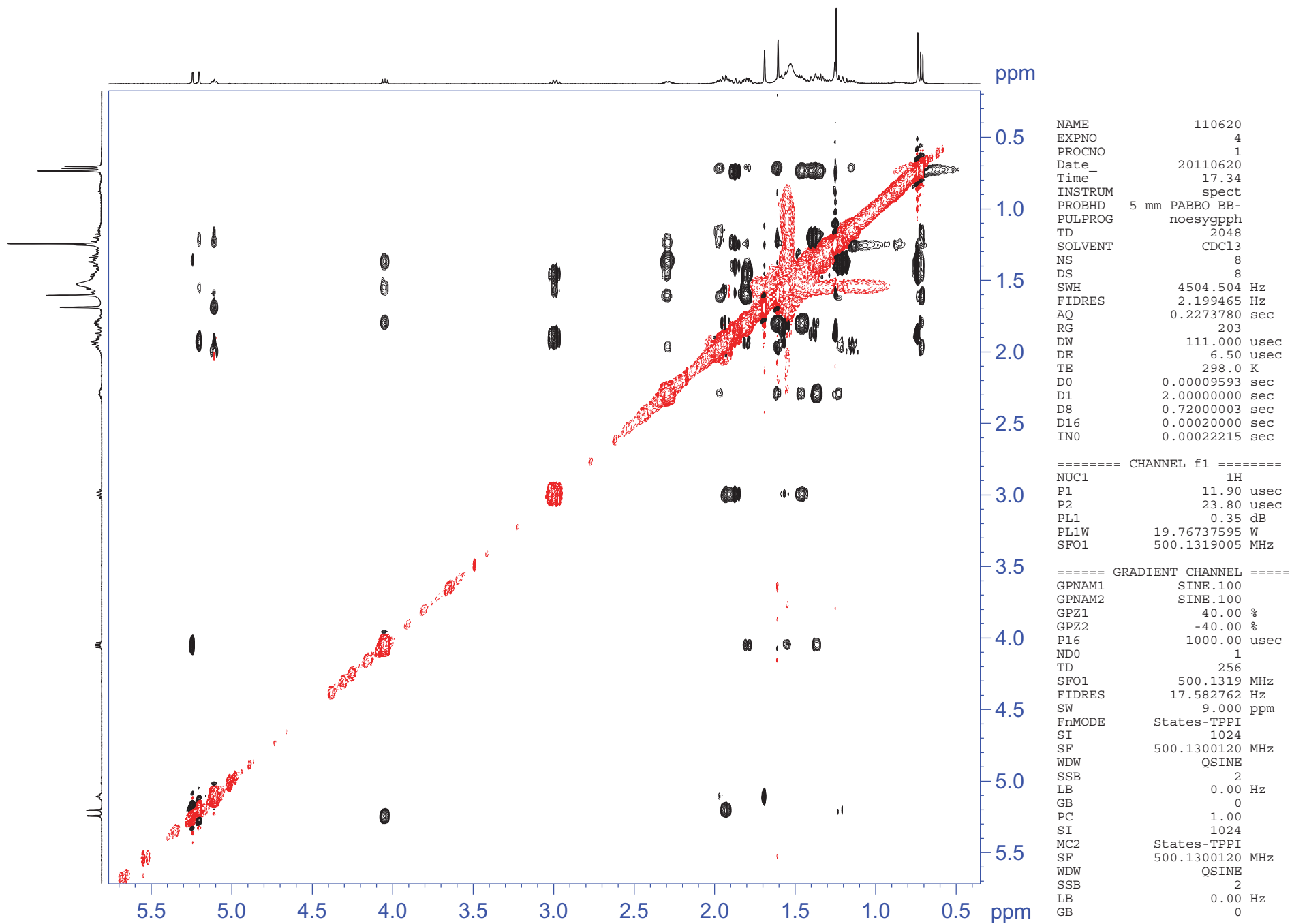

cosy_cf42-50



NAME 110620
EXPNO 1
PROCNO 1
Date_ 20110620
Time_ 9.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfzf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.1 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00022215 sec

==== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.1319005 MHz

==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 500.1319 MHz
FIDRES 17.582762 Hz
SW 9.000 ppm
FnMODE QF
SI 1024
SF 500.1300129 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 500.1300129 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0



Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 40.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

15 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 0-2

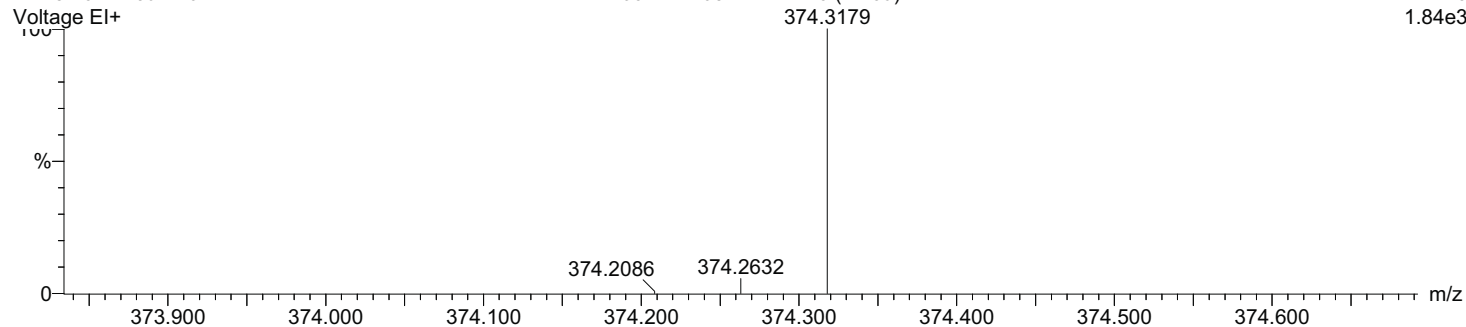
cf42-50

17:15:26 27-Jun-2011

Voltage EI+

KIB
M110627EA-03AFAMM 16 (1.469)
374.3179

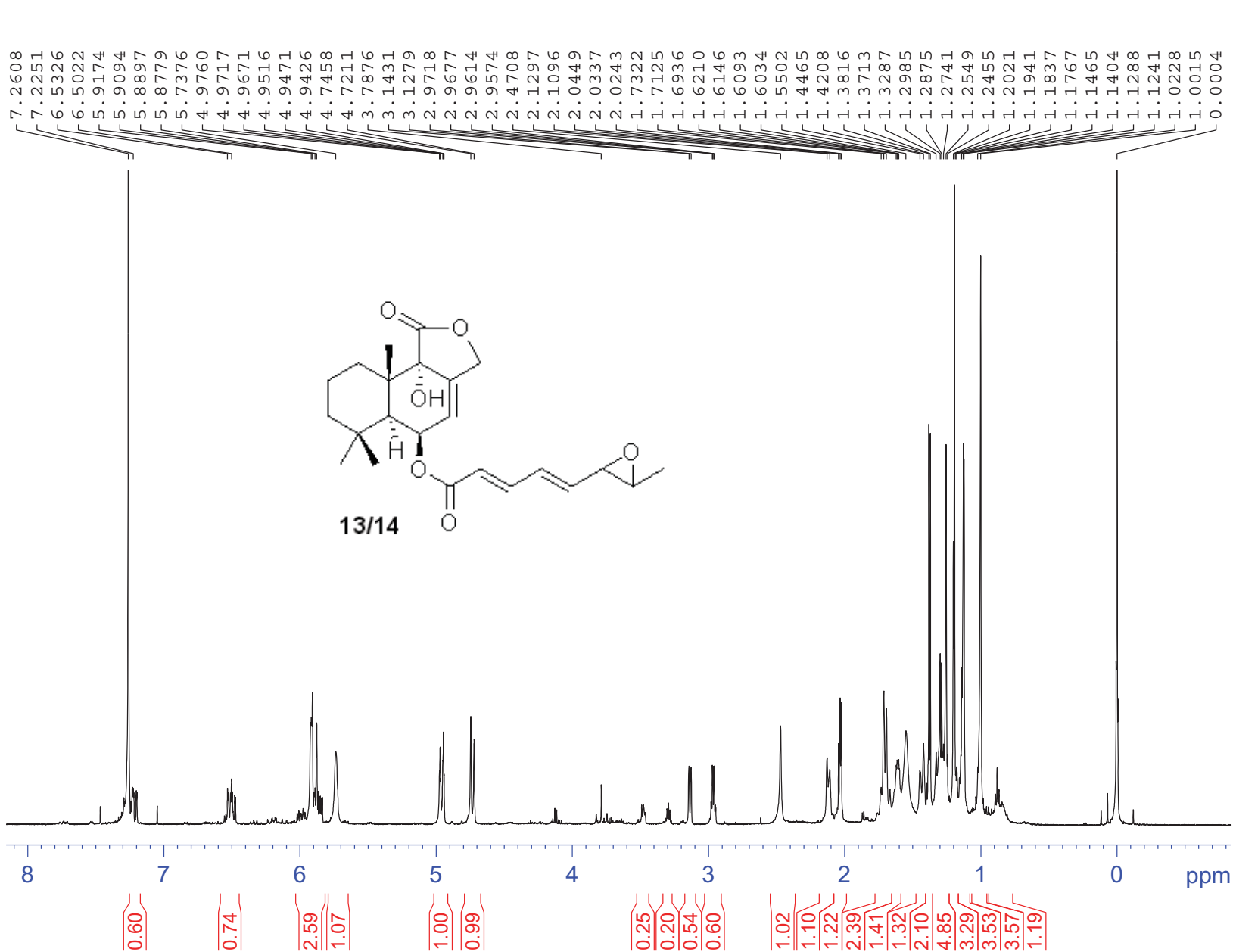
Autospec Premier
P776
1.84e3



Minimum: 0.5
Maximum: 100.0 10.0 40.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
374.3179	374.3185	-0.6	-1.6	5.0	5546938.0	C25 H42 O2

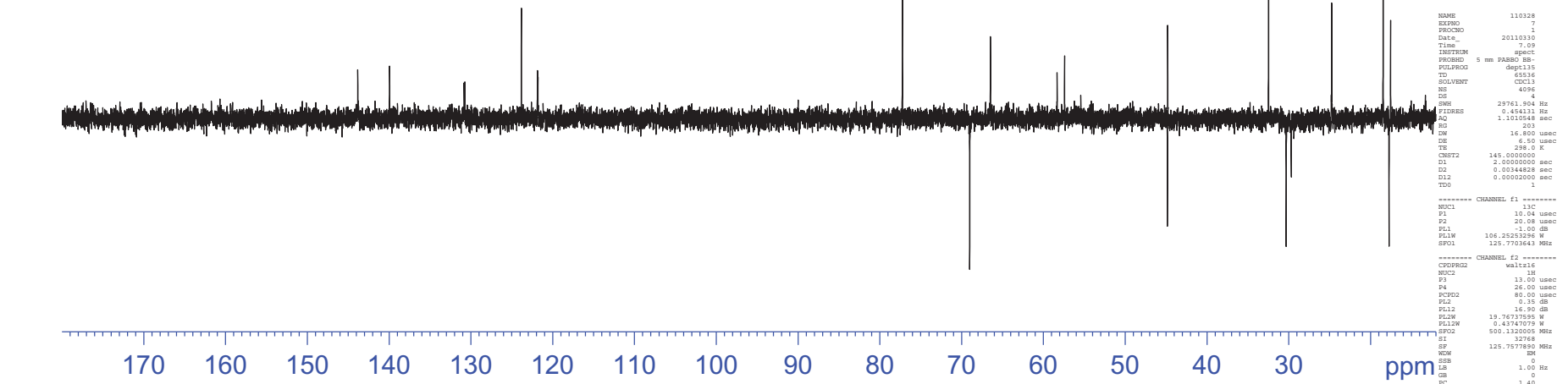
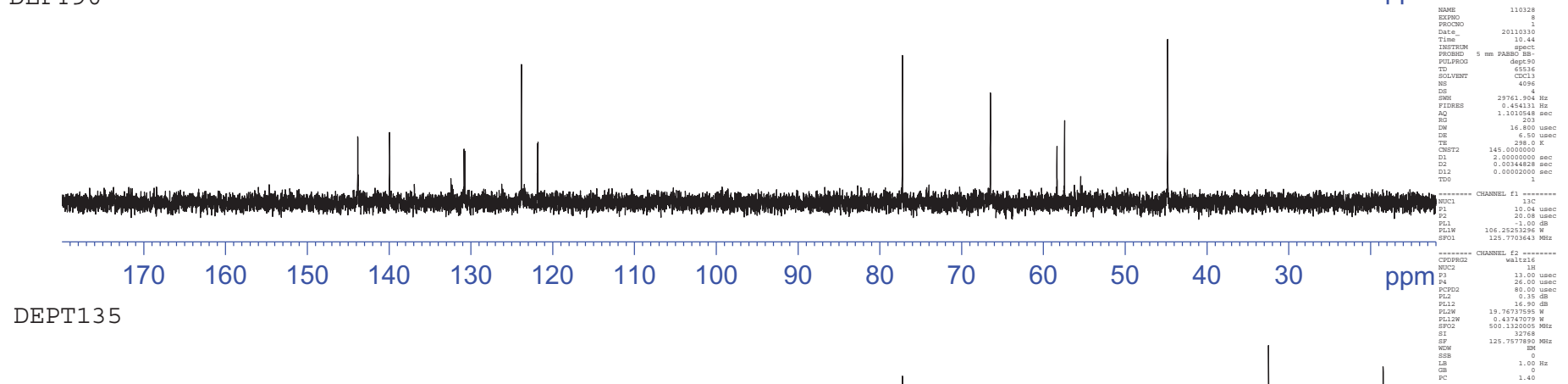
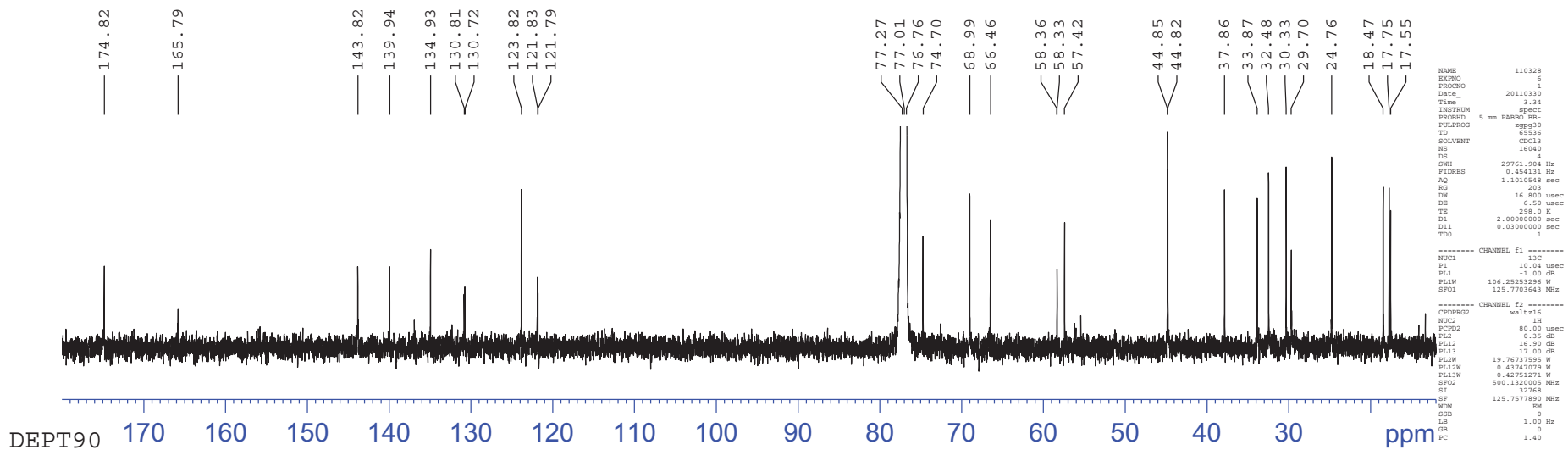
cf42-20



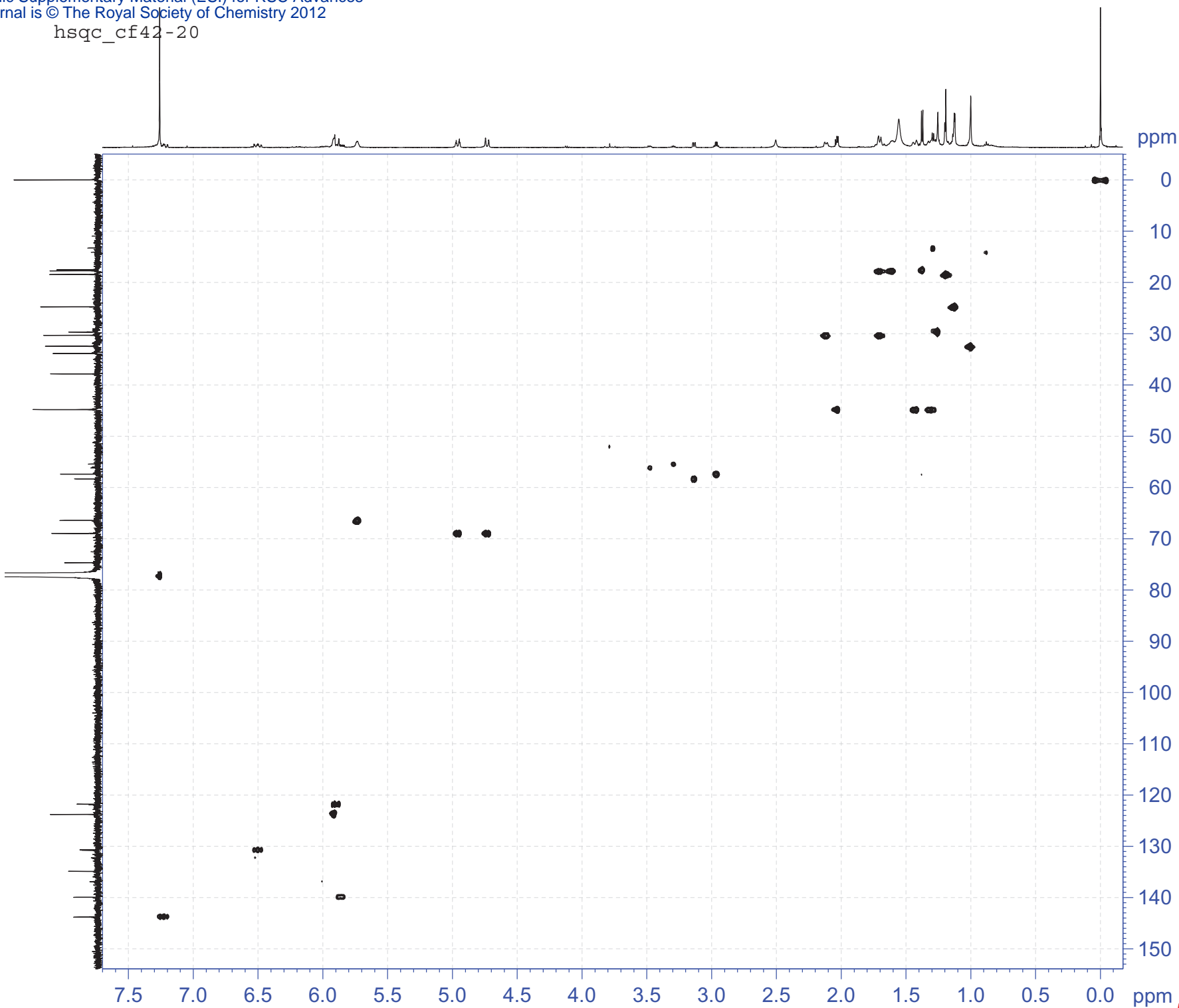
```

NAME          110323
EXPNO         12
PROCNO        1
Date_         20110323
Time          14.40
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            40
DS            0
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1719923 sec
RG            203
DW            48.400 usec
DE            6.50 usec
TE            298.0 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            11.90 usec
PL1           0.35 dB
PL1W          19.76737595 W
SFO1          500.1330885 MHz
SI            32768
SF            500.1300134 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



hsqc_cf42-20



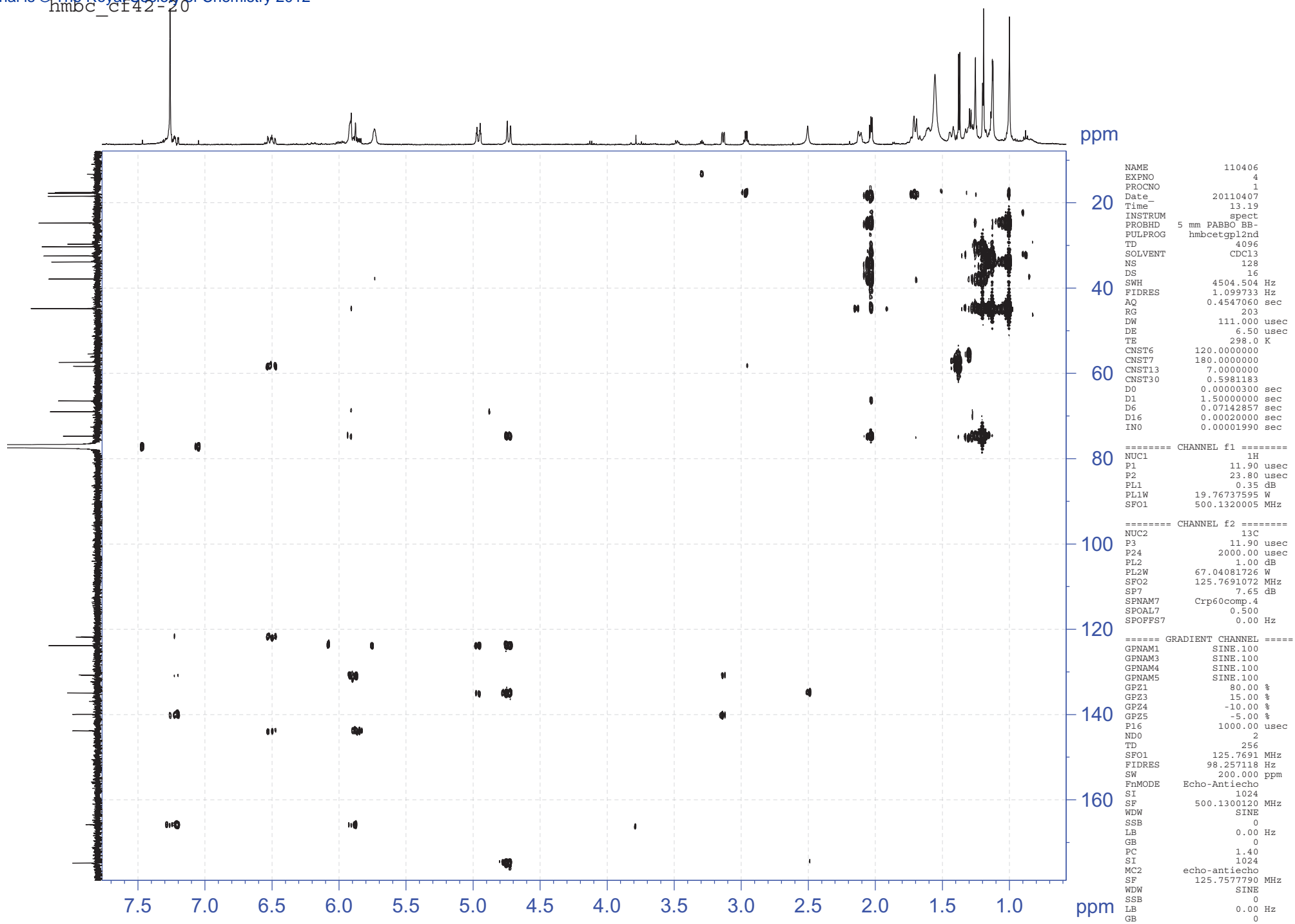
```
NAME          110406
EXPNO         3
PROCNO        1
Date_         20110406
Time_         20.48
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       hsqcetgpsisp2
TD            2048
SOLVENT       CDCl3
NS            64
DS            16
SWH           4504.504 Hz
FIDRES        2.199465 Hz
AQ            0.2273780 sec
RG            203
DW            111.000 usec
DE            6.50 usec
TE            298.1 K
CNST2         145.0000000
DO            0.0000300 sec
D1            2.0000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
INO           0.00002090 sec
ZGOPTNS

===== CHANNEL f1 =====
NUC1          1H
P1            11.90 usec
P2            23.80 usec
P28           0.00 usec
PL1           0.35 dB
PL1W          19.76737595 W
SFO1          500.1320005 MHz

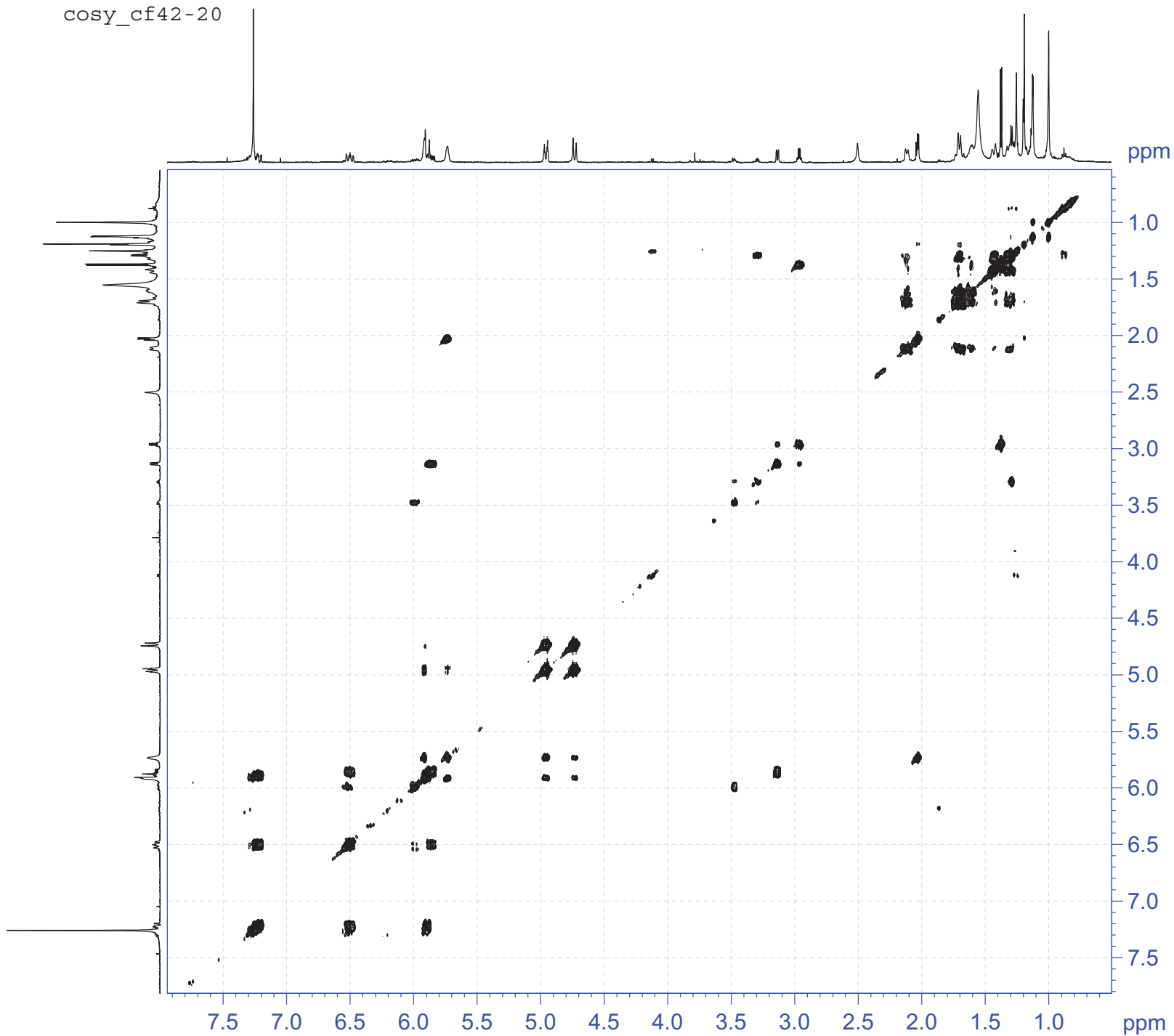
===== CHANNEL f2 =====
CPDPRG2       garp
NUC2          13C
P3            11.90 usec
P4            23.80 usec
P14           500.00 usec
PCPD2         70.00 usec
PL0           120.00 dB
PL2           1.00 dB
PL12          16.39 dB
PLOW          0.00000000 W
PL2W          67.04081726 W
PL12W         1.93793559 W
SFO2          125.7678496 MHz
SP3           7.65 dB
SPNAM3        Crp60,0.5,20.1
SPOAL3        0.500
SPOFFS3       0.00 Hz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPNAM3        SINE.100
GPNAM4        SINE.100
GPZ1          80.00 %
GPZ2          20.10 %
GPZ3          11.00 %
GPZ4          -5.00 %
P16           1000.00 usec
P19           600.00 usec
ND0           2
TD            256
SFO1          125.7678 MHz
FIDRES        93.343323 Hz
SW            190.000 ppm
PnMODE        Echo-Antiecho
SI            1024
SF            500.1300120 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           echo-antiecho
SF            125.7577790 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
```

hmbc_cr42-20



cosy_cf42-20

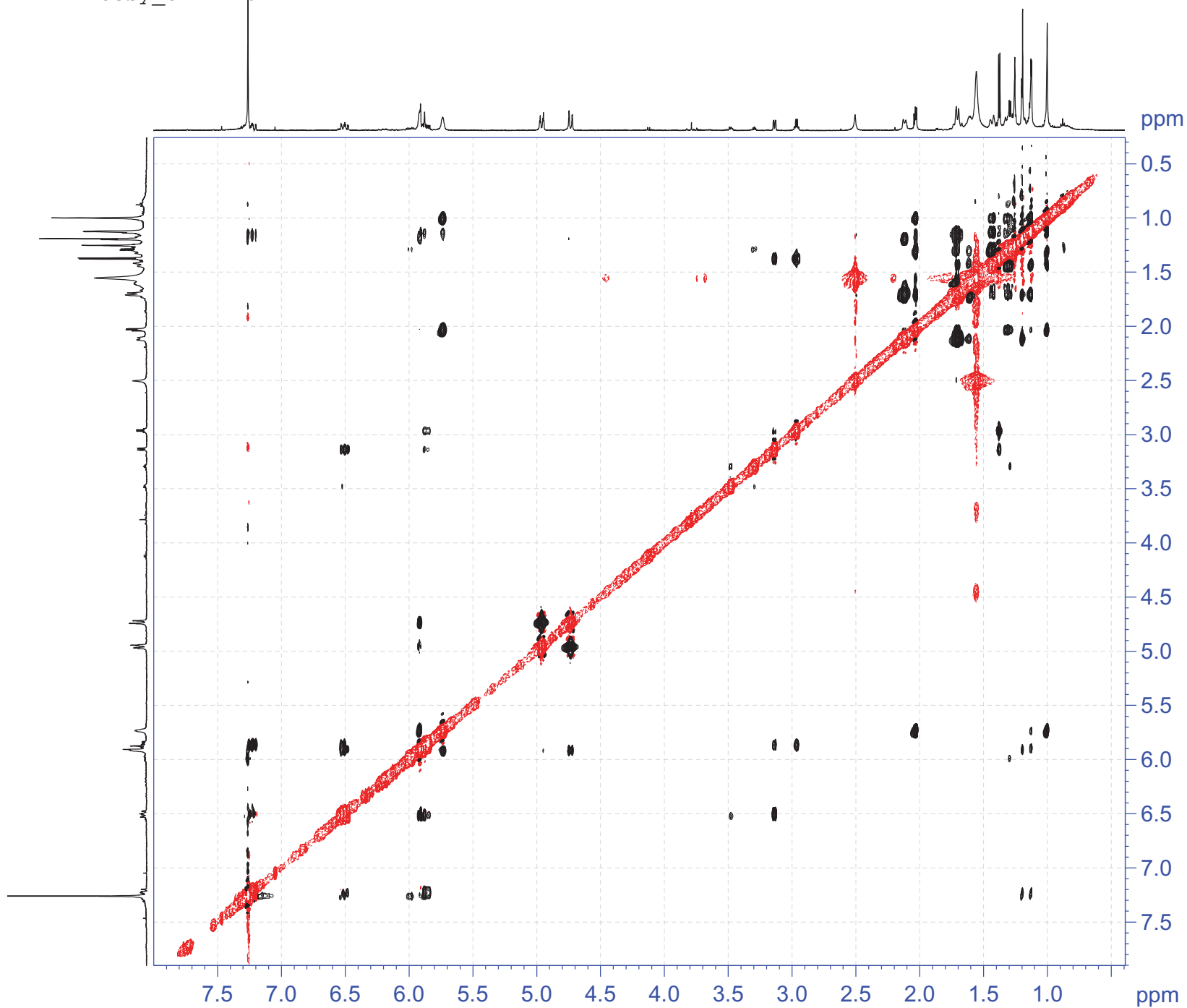


```
NAME          110406
EXPNO         2
PROCNO        1
Date_         20110406
Time_         19.27
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       cosygpmfzf
TD            2048
SOLVENT       CDCl3
NS            8
DS            16
SWH           4504.504 Hz
FIDRES        2.199465 Hz
AQ            0.2273780 sec
RG            203
DW            111.000 usec
DE            6.50 usec
TE            298.0 K
D0            0.00000300 sec
D1            2.00000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
INO           0.00022215 sec
```

```
===== CHANNEL f1 =====
NUC1          1H
P1            11.90 usec
PL1           0.35 dB
PL1W          19.76737595 W
SFO1          500.1320005 MHz
```

```
===== GRADIENT CHANNEL =====
GPNAM1       SINE.100
GPNAM2       SINE.100
GPNAM3       SINE.100
GPZ1         16.00 %
GPZ2         12.00 %
GPZ3         40.00 %
P16          1000.00 usec
ND0          1
TD           256
SFO1         500.132 MHz
FIDRES       17.582766 Hz
SW           9.000 ppm
FnMODE       QF
SI           1024
SF           500.1300122 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
PC           1.40
SI           1024
MC2          QF
SF           500.1300122 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
```


noesy_cf42-20



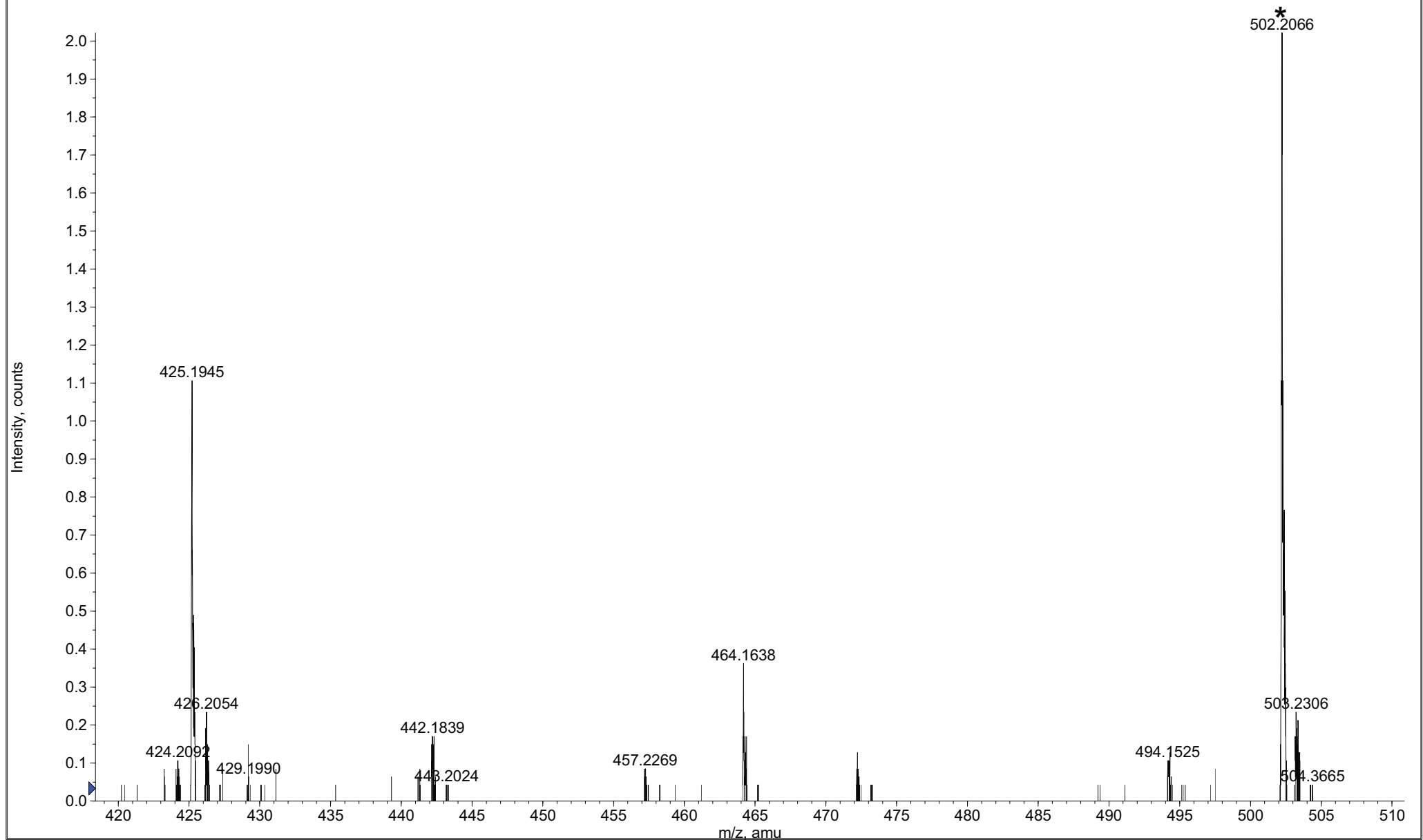
```
NAME 110406
EXPNO 5
PROCNO 1
Date_ 20110407
Time_ 9.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesygpph
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 203
DW 111.000 usec
DE 6.50 usec
TE 298.0 K
D0 0.00009593 sec
D1 2.00000000 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00022215 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
P2 23.80 usec
PL1 0.35 dB
PL1W 19.76737595 W
SFO1 500.132005 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 500.132 MHz
FIDRES 17.582766 Hz
SW 9.000 ppm
FnMODE States-TPPI
SI 1024
SF 500.1300120 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TPPI
SF 500.1300120 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
```

+TOF MS: 1.333 to 2.100 min from 110429ESIA cf42-20.wiff
a=3.55966344865418650e-004, t0=8.13430008453506160e+001

Max. 2.0 counts.



Cartesian coordinates for energy-minimized conformer of **2** optimized at the B3LYP/6-31G(d) level in methanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.042697	-1.904809	0.905594
2	6	0	4.788297	-0.667009	0.431894
3	6	0	4.031596	0.671891	0.319194
4	6	0	2.550396	0.505591	-0.074606
5	6	0	2.022497	-0.905509	-0.344906
6	6	0	2.516597	-1.792409	0.837994
7	6	0	1.749296	1.591391	-0.186406
8	6	0	0.339196	1.558091	-0.624306
9	6	0	-0.337704	0.225590	-0.914706
10	6	0	0.453797	-0.971509	-0.314306
11	6	0	-1.775504	0.181590	-0.190906
12	6	0	-2.423503	-1.304910	-0.224406
13	6	0	-1.619203	-2.213110	-1.156406
14	6	0	-0.129103	-2.293110	-0.873606
15	6	0	-1.584604	0.633790	1.284094
16	6	0	-2.505904	0.109490	2.385694
17	8	0	-2.649703	-1.327610	2.288094
18	6	0	-2.412603	-2.020610	1.156694
19	8	0	5.987297	-0.728908	0.208194
20	6	0	4.129696	1.278691	1.755794
21	6	0	4.782996	1.578391	-0.682106
22	6	0	2.641997	-1.430509	-1.669406
23	6	0	-3.935303	-1.303010	-0.584206
24	6	0	-2.165503	-2.924710	-2.145806
25	6	0	-0.391504	0.215690	-2.471506
26	8	0	2.176696	2.868791	0.041194
27	8	0	-0.203304	2.633590	-0.895206
28	8	0	-2.322703	-3.225910	1.245394
29	8	0	-0.670404	1.360090	1.624394
30	6	0	-3.865504	0.784590	2.545994
31	6	0	-2.716704	1.204090	-0.874106
32	8	0	-3.077404	2.184190	-0.034206
33	8	0	-3.098904	1.128990	-2.021506
34	6	0	-3.905404	3.231690	-0.588206
35	1	0	4.367797	-2.111009	1.933794
36	1	0	4.417297	-2.740409	0.304694
37	1	0	2.086197	-2.796009	0.754094
38	1	0	2.130997	-1.362709	1.770194
39	1	0	0.229497	-0.950309	0.758894
40	1	0	0.051897	-3.100310	-0.154106
41	1	0	0.373497	-2.581509	-1.799106
42	1	0	-1.940404	0.257890	3.308594
43	1	0	3.649496	0.634591	2.500394
44	1	0	3.641196	2.254491	1.778894
45	1	0	5.182296	1.401791	2.032394
46	1	0	4.338096	2.573191	-0.705006
47	1	0	4.745396	1.155991	-1.692206
48	1	0	5.832596	1.658191	-0.390006
49	1	0	3.718497	-1.240309	-1.711906
50	1	0	2.204897	-0.948509	-2.546106
51	1	0	2.508497	-2.512409	-1.769306
52	1	0	-4.336103	-2.312710	-0.468306
53	1	0	-4.506503	-0.642210	0.071494
54	1	0	-4.086303	-0.976510	-1.612406
55	1	0	-1.543203	-3.553410	-2.778106
56	1	0	-3.225803	-2.924710	-2.369506
57	1	0	-0.906904	1.100790	-2.838906
58	1	0	0.629396	0.242291	-2.860406
59	1	0	-0.891203	-0.665110	-2.869106
60	1	0	1.407496	3.427491	-0.211106
61	1	0	-4.497304	0.691390	1.662494
62	1	0	-3.721004	1.847590	2.757194
63	1	0	-4.377504	0.325690	3.396894
64	1	0	-3.355804	3.755990	-1.372506
65	1	0	-4.119704	3.898990	0.244894
66	1	0	-4.825904	2.809890	-0.995806

Cartesian coordinates for energy-minimized conformer of **3** optimized at the B3LYP/6-31G(d) level in methanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.503192	-1.831415	0.828106
2	6	0	2.365495	-1.220919	-0.266194
3	6	0	3.258900	-0.038622	0.207906
4	6	0	2.701106	1.360580	-0.123294
5	6	0	1.347207	1.764286	0.514706
6	6	0	0.109004	0.988091	-0.111294
7	6	0	-0.497101	-0.127307	0.767806
8	6	0	0.328695	-1.314210	1.224906
9	6	0	3.337291	-2.175623	-0.983894
10	6	0	4.634394	-1.501128	-1.075594
11	6	0	4.611899	-0.314928	-0.432694
12	6	0	1.055713	3.249687	0.164206
13	6	0	-0.466586	3.374093	0.210706
14	6	0	-0.929491	2.111295	-0.537694
15	6	0	-2.443093	1.793101	-0.436294
16	6	0	-3.295387	3.054105	-0.717094
17	6	0	-2.843397	0.716203	-1.421994
18	6	0	-3.734801	-0.283393	-1.253094
19	6	0	-4.480302	-0.579090	-0.037294
20	6	0	-5.385206	-1.567487	0.147906
21	6	0	-6.073907	-1.735984	1.479306
22	6	0	-5.797911	-2.569085	-0.900894
23	8	0	3.048586	-3.281021	-1.431194
24	6	0	2.083787	-3.028117	1.550406
25	6	0	5.757403	0.638167	-0.304594
26	6	0	1.430107	1.656285	2.053606
27	1	0	1.716596	-0.862916	-1.071994
28	1	0	3.398300	-0.101823	1.297206
29	1	0	2.613606	1.451480	-1.215894
30	1	0	3.444909	2.106477	0.188406
31	1	0	0.439202	0.525589	-1.045394
32	1	0	-0.915699	0.323095	1.678706
33	1	0	-1.367502	-0.533903	0.236606
34	1	0	-0.159608	-1.842008	2.047106
35	1	0	5.488192	-1.935631	-1.585994
36	1	0	1.403414	3.471085	-0.854794
37	1	0	1.575616	3.938585	0.840606
38	1	0	-0.825482	4.297695	-0.254394
39	1	0	-0.828886	3.370195	1.247906
40	1	0	-0.738090	2.308994	-1.603894
41	1	0	-2.671594	1.468802	0.585706
42	1	0	-4.361588	2.807009	-0.678194
43	1	0	-3.102684	3.843504	0.016806
44	1	0	-3.081586	3.459204	-1.714394
45	1	0	-2.380697	0.810801	-2.406094
46	1	0	-3.912104	-0.931393	-2.109394
47	1	0	-4.287700	0.073309	0.813406
48	1	0	-7.165007	-1.653379	1.372406
49	1	0	-5.745304	-0.989485	2.209406
50	1	0	-5.881911	-2.733784	1.899006
51	1	0	-6.879310	-2.506780	-1.086694
52	1	0	-5.605215	-3.592586	-0.550394
53	1	0	-5.285610	-2.439687	-1.856494
54	1	0	3.080688	-2.799021	1.955206
55	1	0	2.212784	-3.879918	0.873406
56	1	0	1.447286	-3.339015	2.384406
57	1	0	6.681201	0.214364	-0.707894
58	1	0	5.922304	0.908367	0.746406
59	1	0	5.548307	1.574168	-0.837894
60	1	0	0.549309	2.093689	2.536506
61	1	0	2.307709	2.207682	2.414106
62	1	0	1.515403	0.623885	2.400206

Cartesian coordinates for energy-minimized conformer of **12** optimized at the B3LYP/6-31G(d) level in methanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.757700	-2.110100	0.292000
2	6	0	2.534600	-1.096000	-0.542300
3	6	0	2.191700	0.381300	-0.185700
4	6	0	0.631300	0.544900	-0.264000
5	6	0	-0.282400	-0.530800	0.444300
6	6	0	0.247300	-1.948300	0.101600
7	6	0	0.108500	1.946700	0.055500
8	6	0	-1.351700	2.111500	0.030800
9	6	0	-2.230100	1.095000	-0.054900
10	6	0	-1.737600	-0.360400	-0.150400
11	6	0	2.814700	0.761800	1.177700
12	6	0	2.840500	1.273600	-1.270800
13	6	0	-0.327700	-0.355400	1.980500
14	6	0	-2.739700	-1.342200	0.519600
15	6	0	-3.705100	1.382000	-0.152300
16	8	0	0.823500	2.925600	0.269100
17	8	0	-1.697000	-0.678800	-1.550300
18	8	0	-3.839000	-1.536600	-0.381700
19	8	0	3.943500	-1.354700	-0.494000
20	1	0	2.058400	-3.119000	-0.015100
21	1	0	2.033300	-2.016300	1.351400
22	1	0	2.272000	-1.250800	-1.597500
23	1	0	0.391100	0.420700	-1.331600
24	1	0	-0.004200	-2.169300	-0.940800
25	1	0	-0.263200	-2.697700	0.717200
26	1	0	-1.697500	3.142200	0.082100
27	1	0	2.559800	0.067000	1.983100
28	1	0	2.494900	1.760600	1.478500
29	1	0	3.907500	0.777000	1.092900
30	1	0	3.906800	1.038400	-1.347200
31	1	0	2.386000	1.091500	-2.253400
32	1	0	2.727800	2.332400	-1.032900
33	1	0	0.659100	-0.496700	2.423900
34	1	0	-0.686900	0.633800	2.278600
35	1	0	-0.986200	-1.100200	2.440100
36	1	0	-2.251200	-2.299500	0.712200
37	1	0	-3.099300	-0.941800	1.473700
38	1	0	-3.890700	2.459300	-0.127700
39	1	0	-4.270300	0.913800	0.661300
40	1	0	-4.115500	0.978400	-1.084600
41	1	0	-2.567000	-1.090600	-1.729900
42	1	0	-4.132100	-2.457200	-0.309100
43	1	0	4.207100	-1.342800	0.440400