Supporting information

Secondary Metabolites from an Algicolous Endophytic *Aspergillus versicolor* Strain

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List of supporting information

S2, ^{1}H NMR spectrum of compound **1**;

S3, ^{13}C NMR and DEPT spectra of compound **1**;

S4, HSQC spectrum of compound **1**;

S5, HMBC spectrum of compound **1**;

S6, ^{1}H-^{1}H COSY spectrum of compound **1**;

S7, NOESY spectrum of compound **1**;

S8, HREIMS spectrum of compound **1**;

S9, ^{1}H NMR spectrum of compound **2**;

S10, ^{13}C NMR and DEPT spectra of compound **2**;

S11, HSQC spectrum of compound **2**;

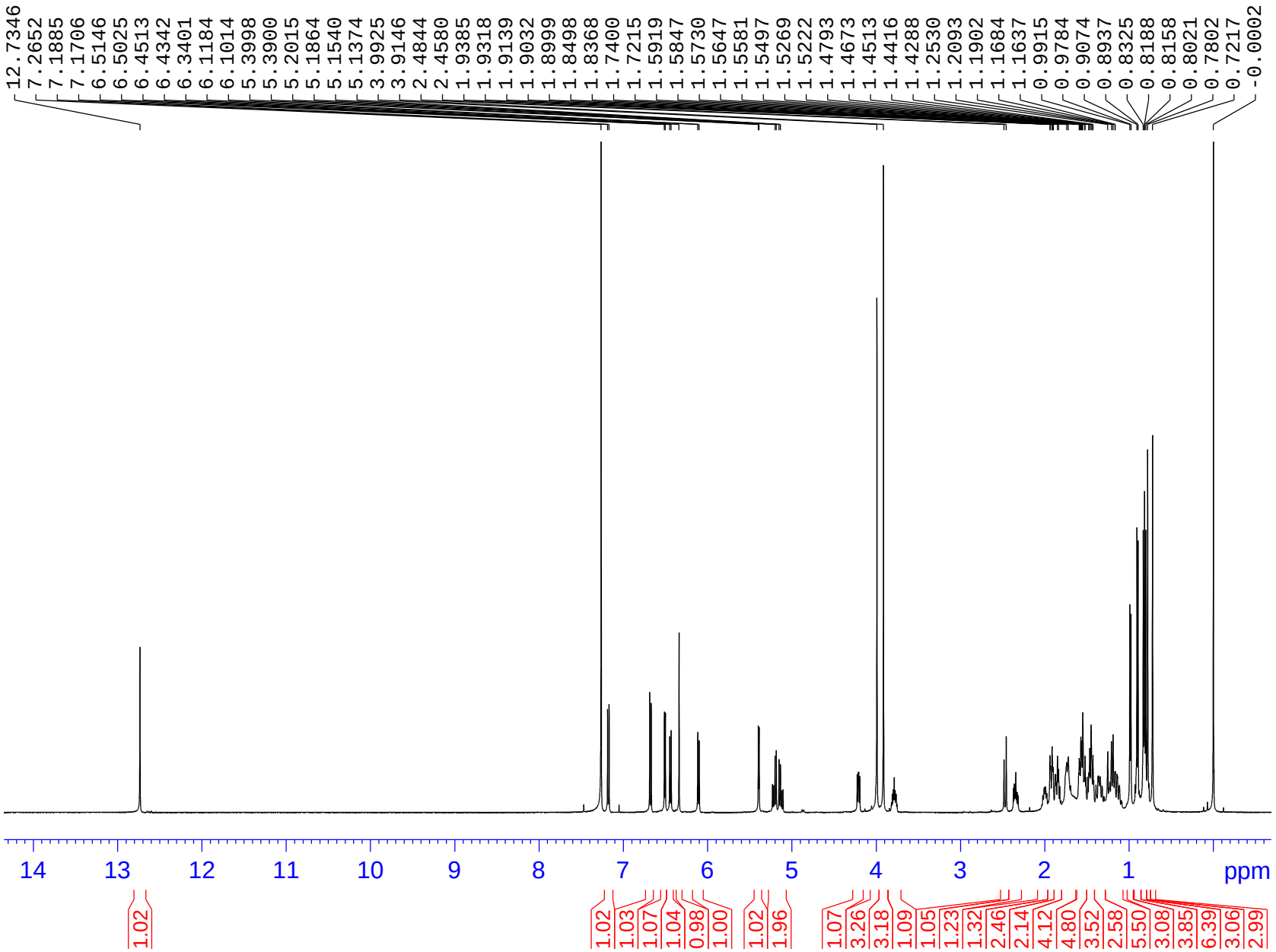
S12, HMBC spectrum of compound **2**;

S13, ^{1}H-^{1}H COSY spectrum of compound **2**;

S14, NOESY spectrum of compound **2**;

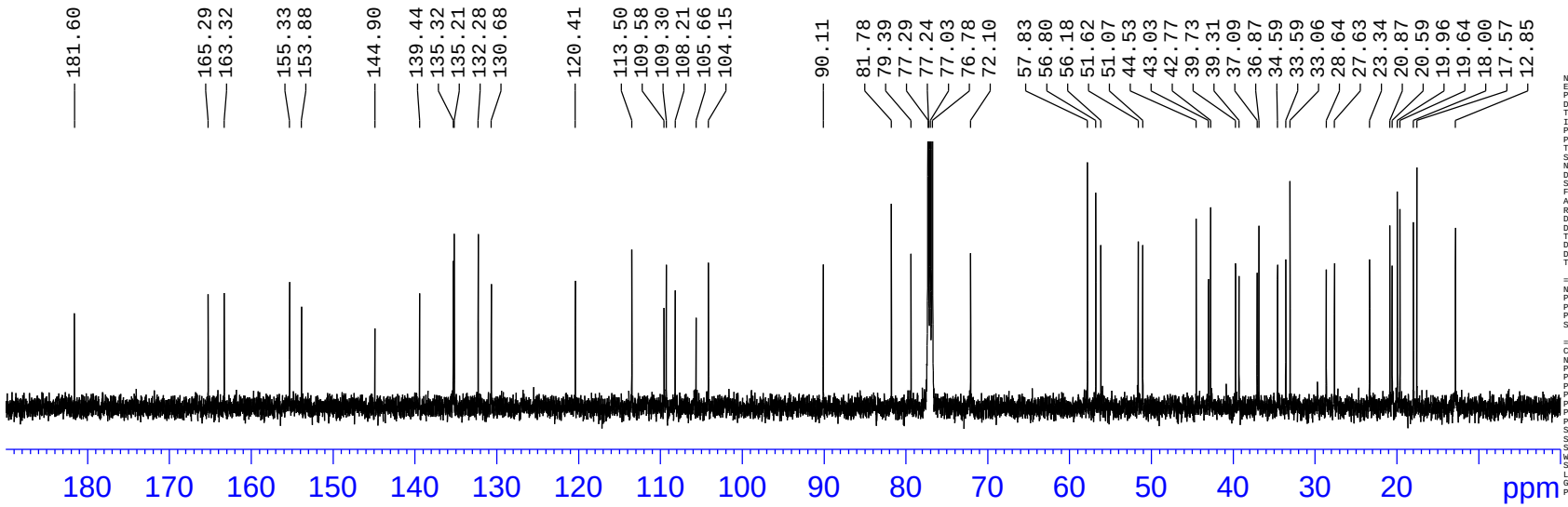
S15, HREIMS spectrum of compound **2**;

pt20-12



NAME	110808
EXPNO	5
PROCNO	1
Date_	20110809
Time	9.09
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	128
DW	48.400 usec
DE	6.50 usec
TE	293.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.40 usec
PL1	0.35 dB
PL1W	19.76737595 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300112 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

pt20-12

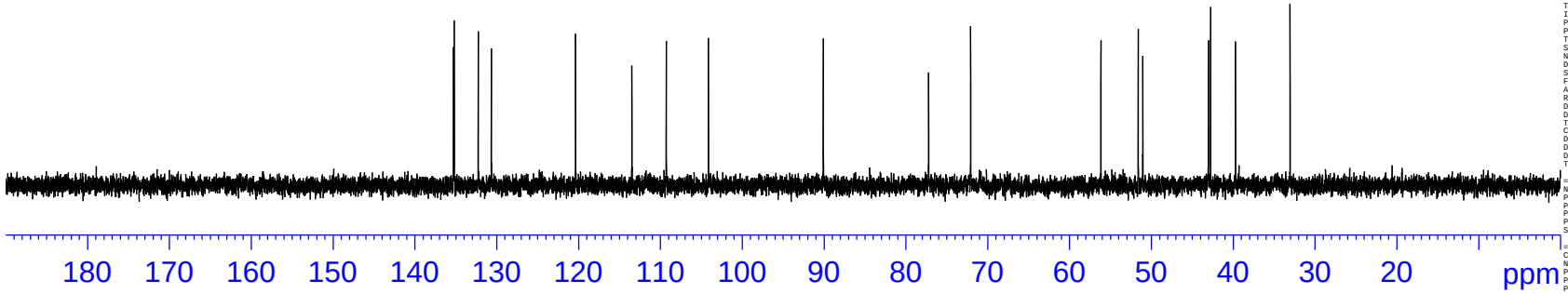



```
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PROCNO                   1
Date_             20110809
Time                 9.15
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010548 sec
RG                     203
DW                16.800 usec
DE                 6.50 usec
TE                 295.0 K
D1              2.00000000 sec
D11             0.03000000 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 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.35 dB
PL12                 16.54 dB
PL13                 17.00 dB
PL2W          19.76737595 W
PL12W          0.47527933 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
```

DEPT90

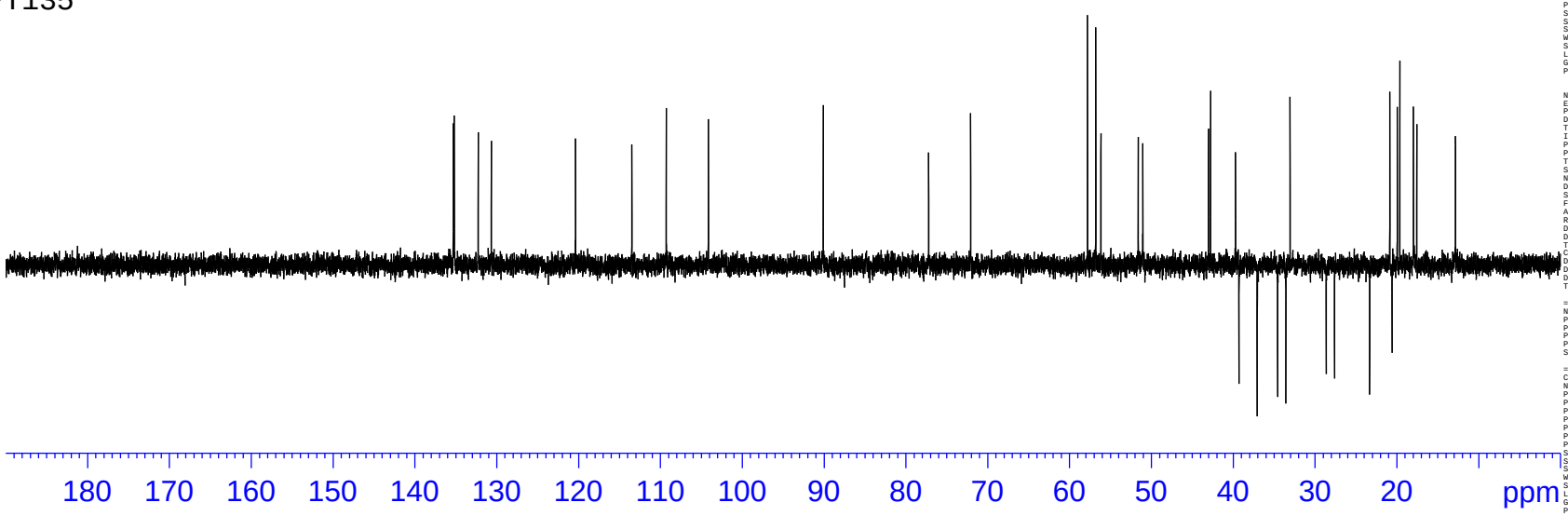



```
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EXPNO                    8
PROCNO                   1
Date_             20110809
Time                10.28
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG             dept90
TD                   65536
SOLVENT              CDCl3
NS                     184
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                 294.4 K
CNST2           145.0000000
D1              2.00000000 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 ========
CPDPRG2             waltz16
NUC2                   1H
P3                   12.40 usec
P4                   24.80 usec
PCPD2                80.00 usec
PL2                   0.35 dB
PL12                 16.54 dB
PL2W          19.76737595 W
PL12W          0.47527933 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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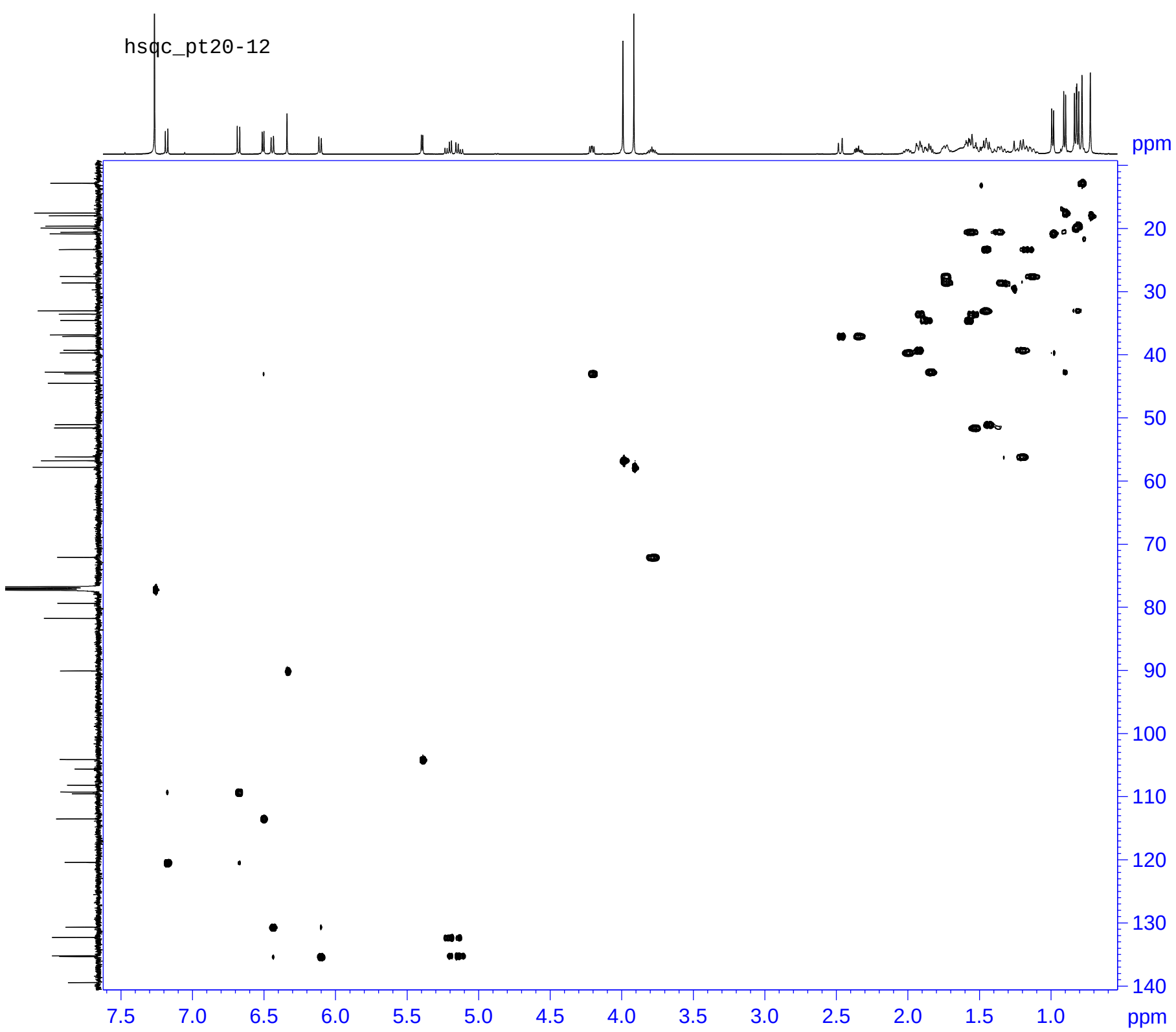
DEPT135




```
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EXPNO                    7
PROCNO                   1
Date_             20110809
Time                10.18
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG            dept135
TD                   65536
SOLVENT              CDCl3
NS                     256
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                 294.4 K
CNST2           145.0000000
D1              2.00000000 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 ========
CPDPRG2             waltz16
NUC2                   1H
P3                   12.40 usec
P4                   24.80 usec
PCPD2                80.00 usec
PL2                   0.35 dB
PL12                 16.54 dB
PL2W          19.76737595 W
PL12W          0.47527933 W
SFO2          500.1320005 MHz
SI                   32768
SF            125.7577890 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

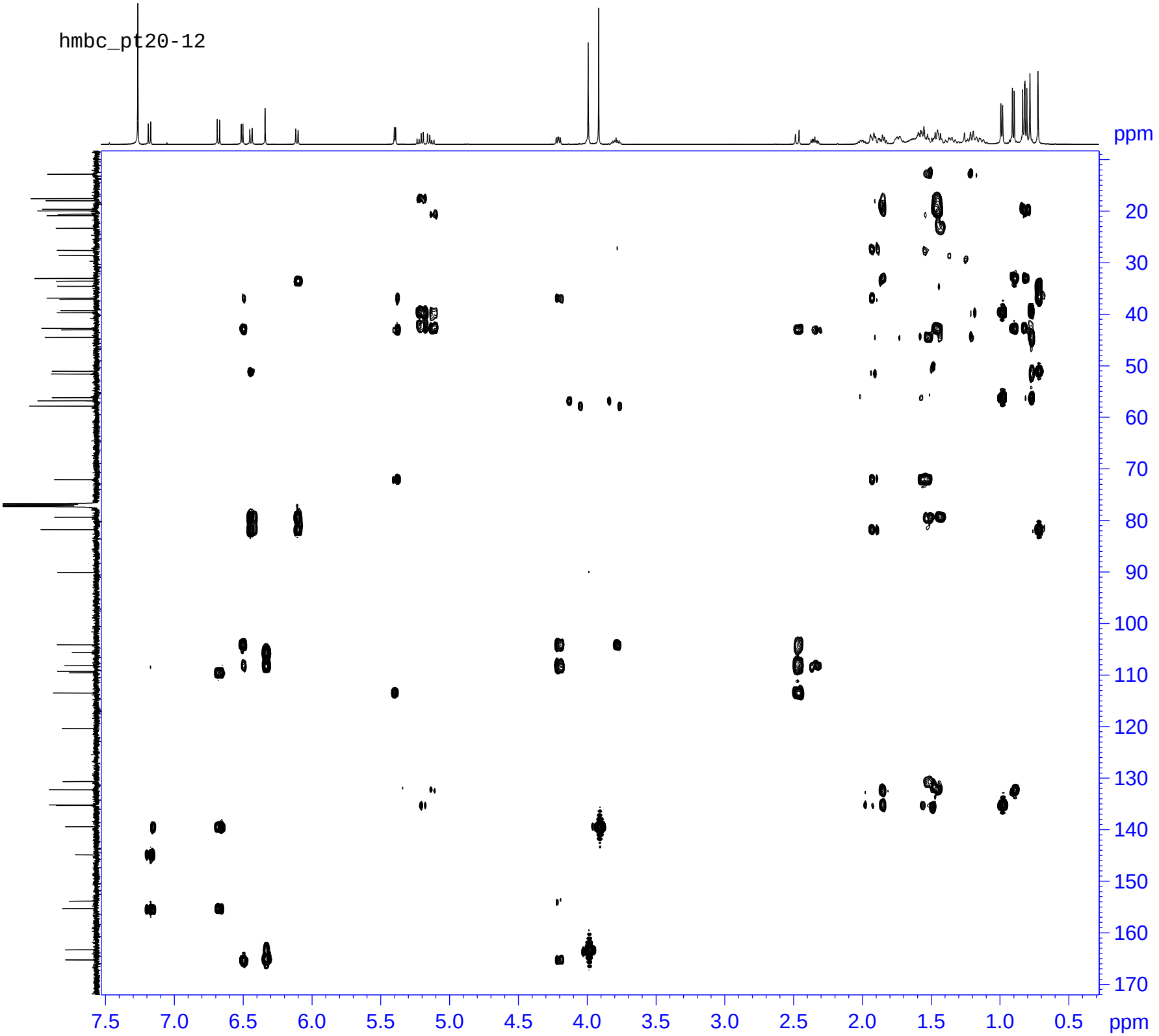



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NAME                110812
EXPNO                    2
PROCNO                   1
Date_             20110812
Time                 9.51
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG   hsqcetgpsisp2
TD                    2048
SOLVENT              CDCl3
NS                       4
DS                      16
SWH           5000.000 Hz
FIDRES        2.441406 Hz
AQ            0.2048500 sec
RG                     203
DW             100.000 usec
DE               6.50 usec
TE               298.5 K
CNST2        145.0000000
D0            0.00000300 sec
D1            2.00000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00002340 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  12.40 usec
P2                  24.80 usec
P28                  0.00 usec
PL1                  0.35 dB
PL1W         19.76737595 W
SFO1        500.1322506 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                  13C
P3                  12.40 usec
P4                  24.80 usec
P14                500.00 usec
PCPD2               70.00 usec
PL0                120.00 dB
PL2                  0.35 dB
PL12                15.38 dB
PL0W         0.00000000 W
PL2W        77.86446381 W
PL12W        2.44534016 W
SFO2        125.7678496 MHz
SP3                  6.64 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         83.517715 Hz
SW              170.000 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
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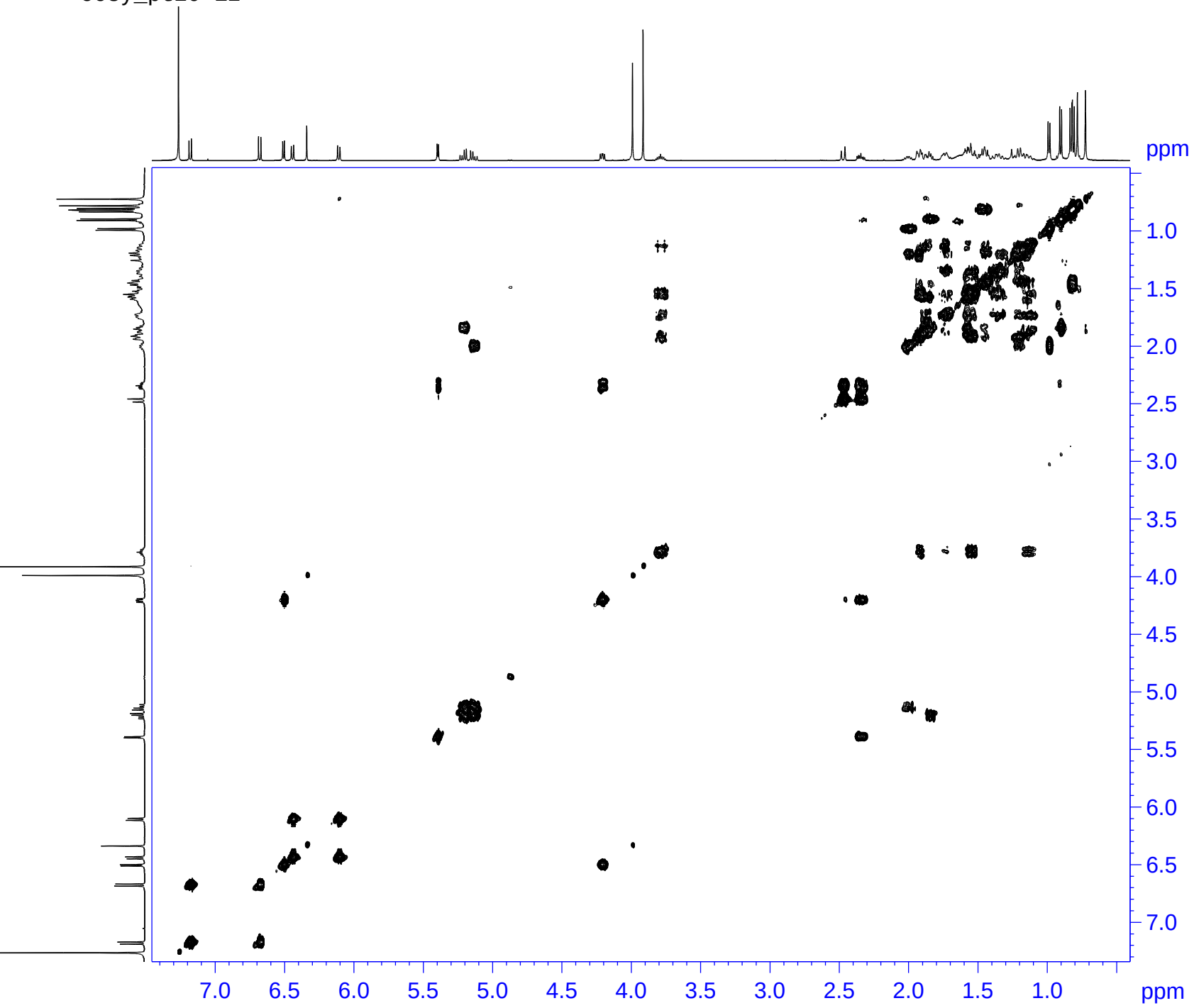

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NAME              110812
EXPNO                  3
PROCNO                 1
Date_           20110812
Time               10.30
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG    hmbcetgpl2nd
TD                  4096
SOLVENT             CDCl3
NS                     8
DS                    16
SWH             7002.801 Hz
FIDRES          1.709668 Hz
AQ              0.2925044 sec
RG                   203
DW                71.400 usec
DE                 6.50 usec
TE               298.0 K
CNST6        120.0000000
CNST7        180.0000000
CNST13         7.0000000
CNST30         0.5981173
D0          0.00000300 sec
D1          1.50000000 sec
D6          0.07142857 sec
D16         0.00020000 sec
IN0         0.00001990 sec

======== CHANNEL f1 ========
NUC1                1H
P1                12.40 usec
P2                24.80 usec
PL1                0.35 dB
PL1W        19.76737595 W
SFO1        500.1330008 MHz

======== CHANNEL f2 ========
NUC2               13C
P3                12.40 usec
P24             2000.00 usec
PL2                0.35 dB
PL2W        77.86446381 W
SFO2        125.7697360 MHz
SP7                6.64 dB
SPNAM7       Crp60comp.4
SPOAL7           0.500
SPOFFS7           0.00 Hz

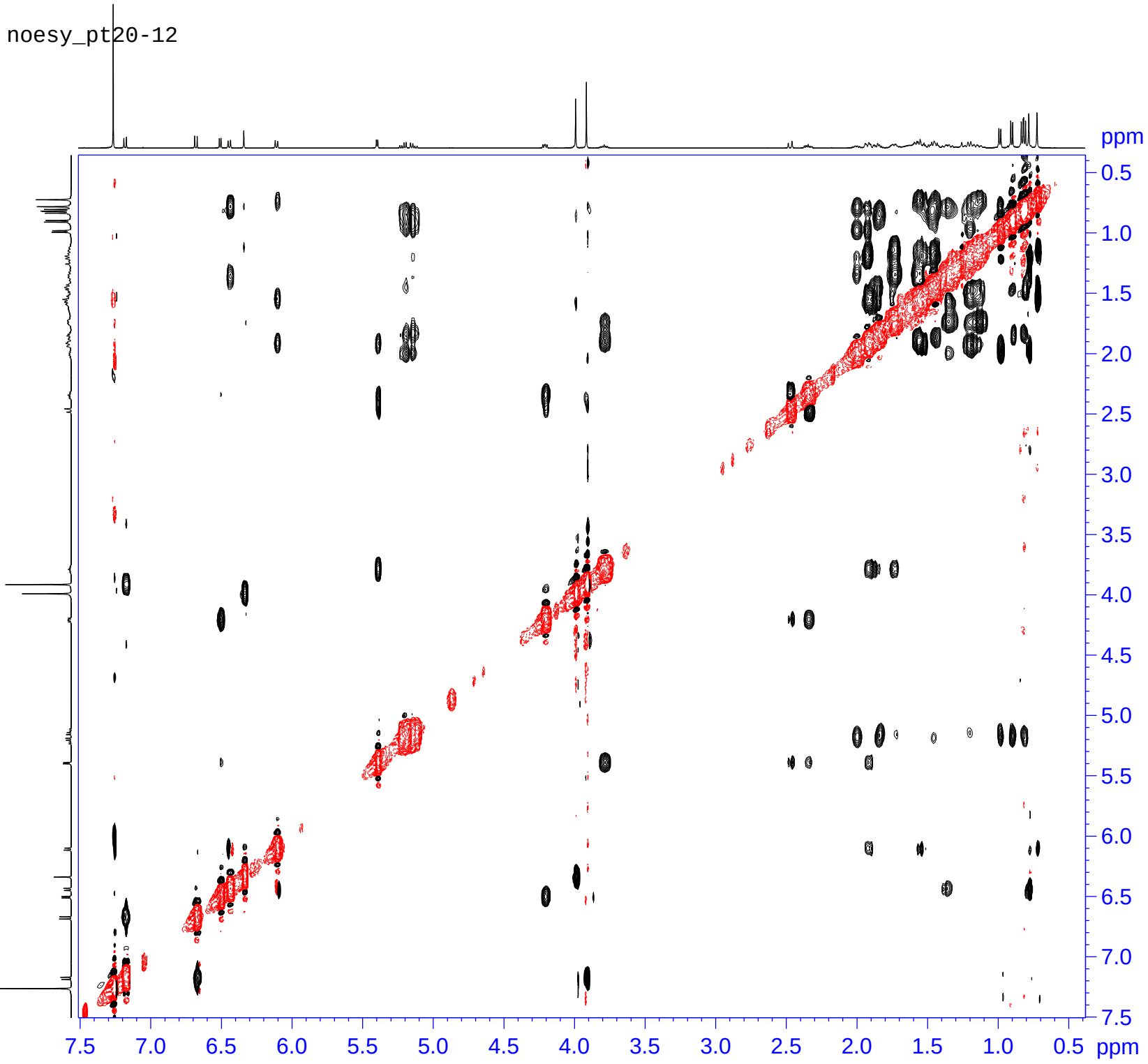
====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM3          SINE.100
GPNAM4          SINE.100
GPNAM5          SINE.100
GPZ1              80.00 %
GPZ3              15.00 %
GPZ4             -10.00 %
GPZ5              -5.00 %
P16             1000.00 usec
ND0                   2
TD                  256
SFO1          125.7697 MHz
FIDRES         98.257607 Hz
SW              200.000 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_pt20-12



NAME	110812	
EXPNO	1	
PROCNO	1	
Date_	20110812	
Time	9.30	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	cosygpmfqf	
TD	2048	
SOLVENT	CDCl3	
NS	2	
DS	16	
SWH	5000.000	Hz
FIDRES	2.441406	Hz
AQ	0.2048500	sec
RG	203	
DW	100.000	usec
DE	6.50	usec
TE	298.2	K
D0	0.00000300	sec
D1	2.00000000	sec
D13	0.00000400	sec
D16	0.00020000	sec
IN0	0.00019995	sec
======== CHANNEL f1 ========		
NUC1	1H	
P1	12.40	usec
PL1	0.35	dB
PL1W	19.76737595	W
SFO1	500.1322506	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	500.1323	MHz
FIDRES	19.536415	Hz
SW	10.000	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_pt20-12



NAME	110812
EXPNO	4
PROCNO	1
Date_	20110812
Time	11.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	noesygpph
TD	2048
SOLVENT	CDCl3
NS	4
DS	8
SWH	7002.801 Hz
FIDRES	3.419337 Hz
AQ	0.1462772 sec
RG	203
DW	71.400 usec
DE	6.50 usec
TE	298.2 K
D0	0.00005562 sec
D1	2.00000000 sec
D8	0.69999999 sec
D16	0.00020000 sec
IN0	0.00014280 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.40 usec
P2	24.80 usec
PL1	0.35 dB
PL1W	19.76737595 W
SFO1	500.1330008 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	40.00 %
GPZ2	-40.00 %
P16	1000.00 usec
ND0	1
TD	256
SFO1	500.133 MHz
FIDRES	27.351023 Hz
SW	14.000 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

Single Mass Analysis (displaying only valid results)

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

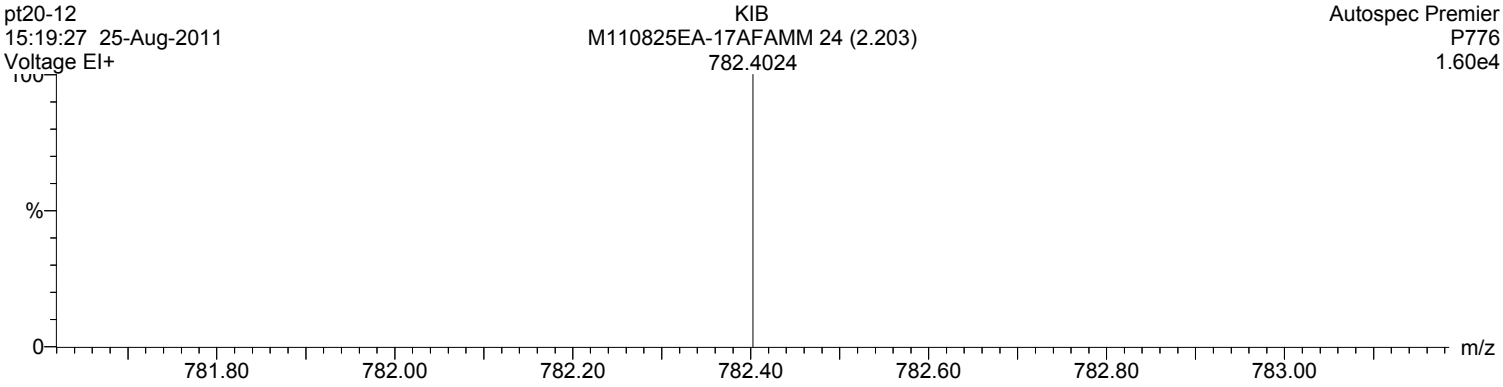
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Monoisotopic Mass, Odd and Even Electron Ions

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

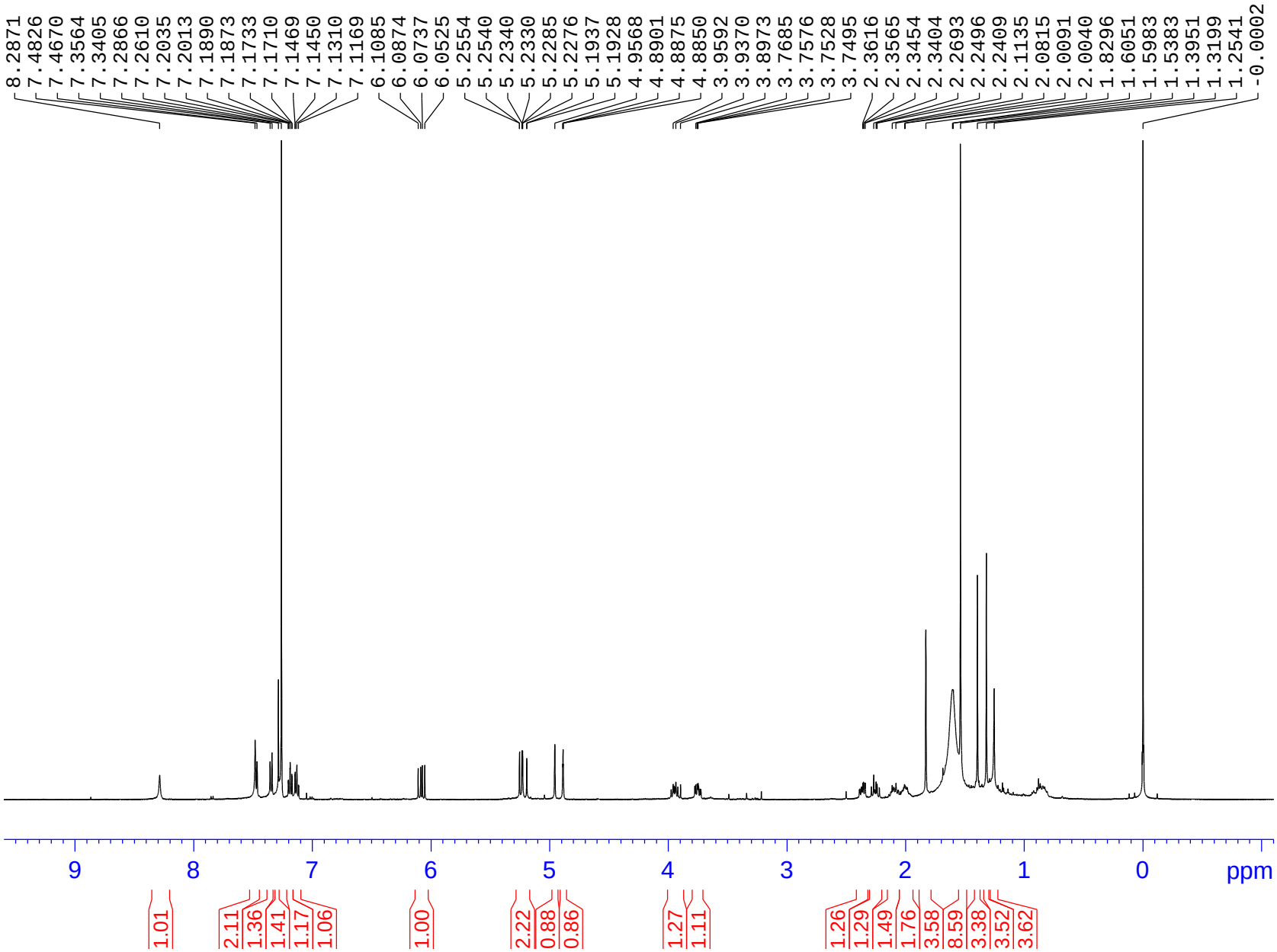
Elements Used:

C: 0-200 H: 0-400 O: 8-11



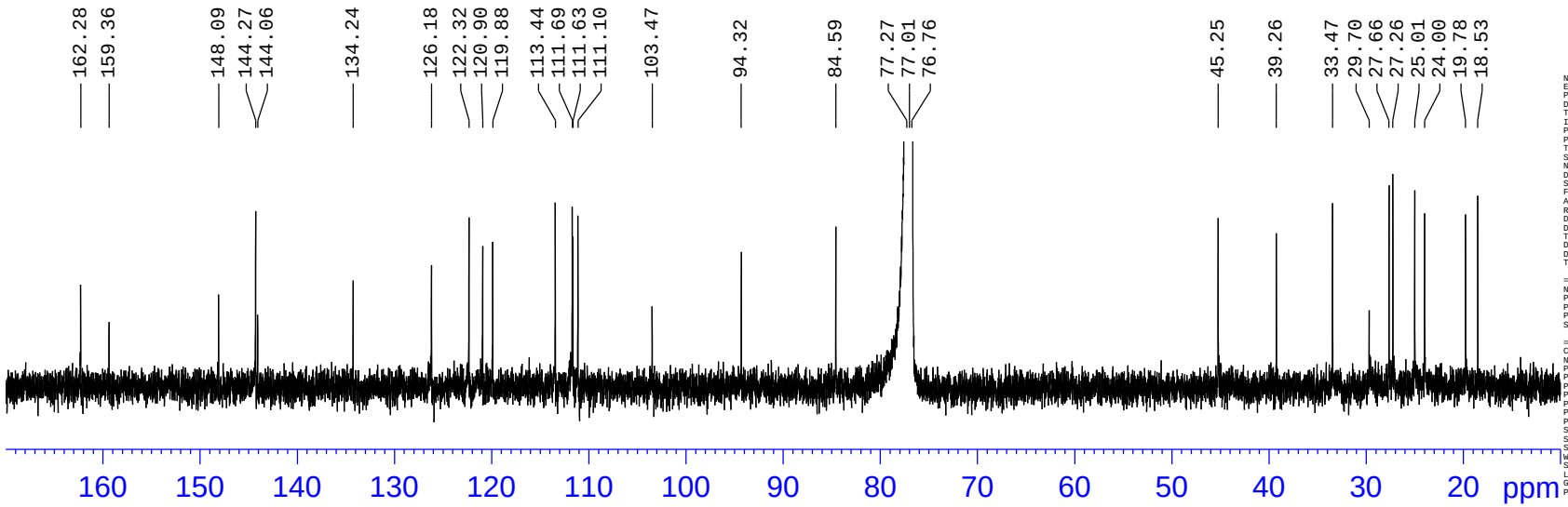
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pt20-7



NAME	110628
EXPNO	11
PROCNO	1
Date_	20110701
Time	16.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	161
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	500.1300131 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

pt20-7

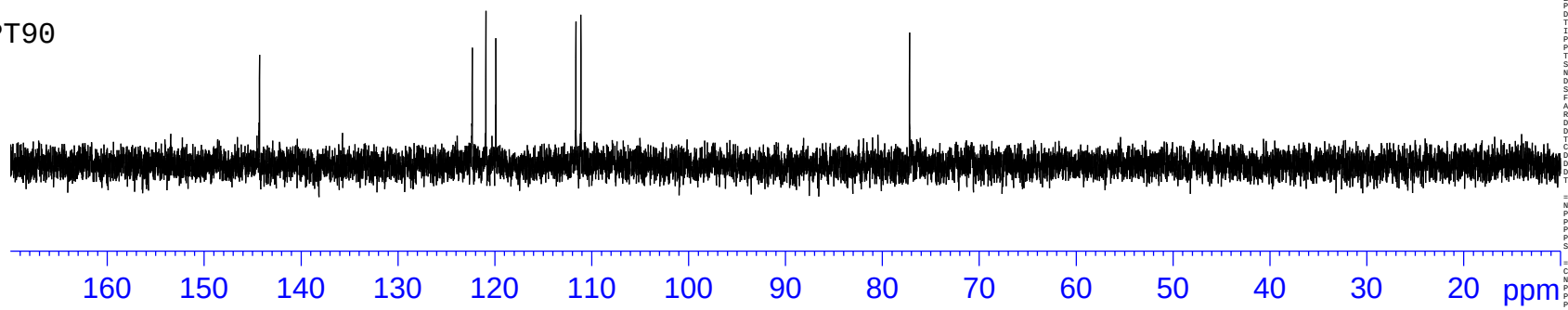


NAME 110704
EXPNO 9
PROCNO 1
Date_ 20110705
Time 4.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 14336
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.04 usec
PL1 -1.00 dB
PL1W 106.25253296 W
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 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

DEPT90

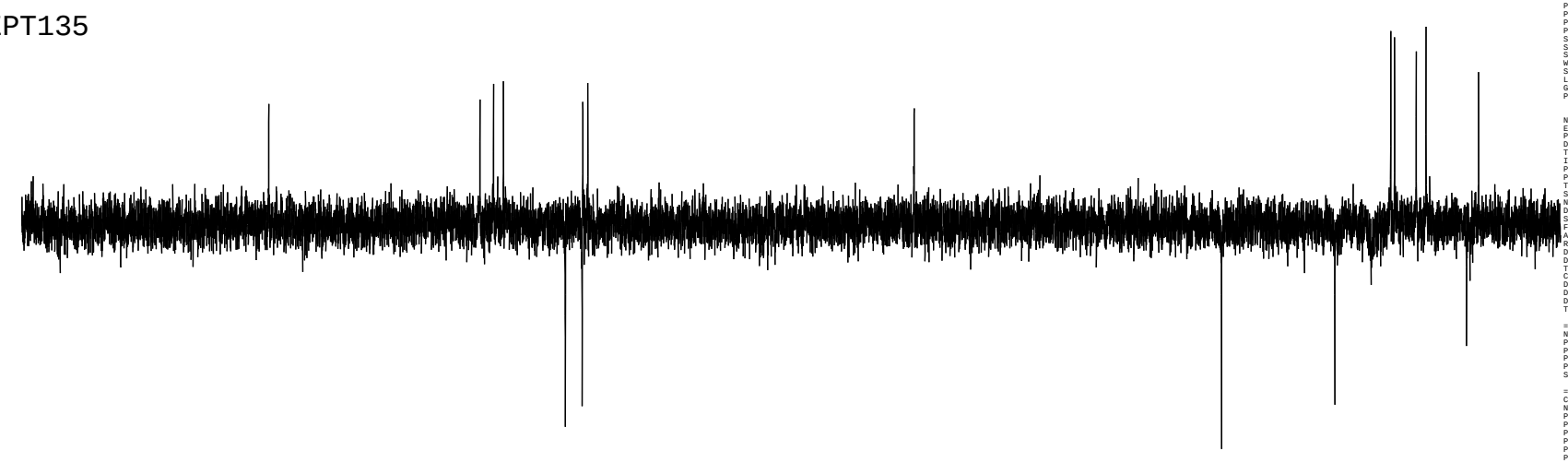


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EXPNO 11
PROCNO 1
Date_ 20110705
Time 9.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept90
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D1 2.00000000 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 ========
CPDPRG2 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
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

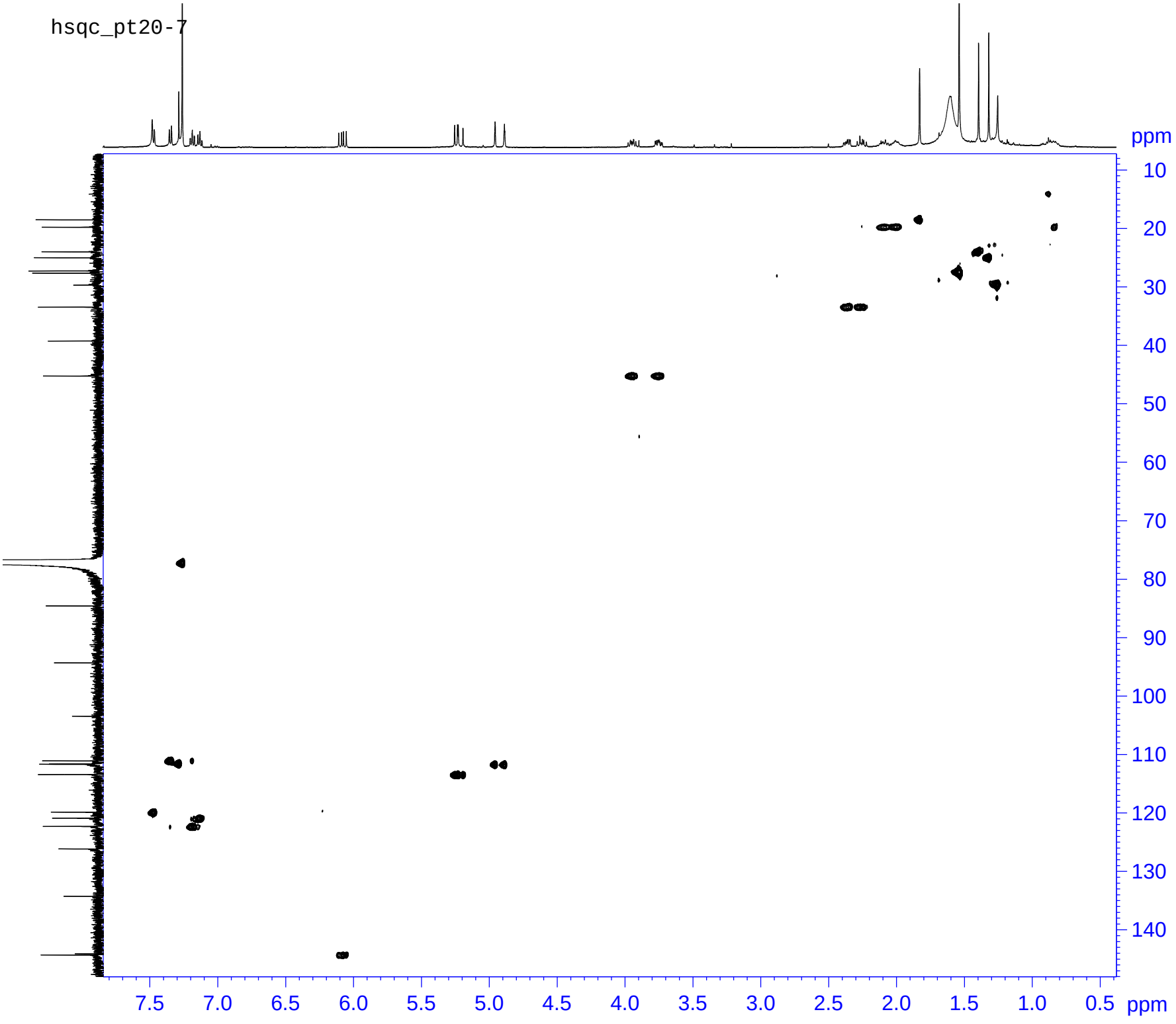
DEPT135



NAME 110704
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PROCNO 1
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PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 3072
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 298.2 K
CNST2 145.0000000
D1 2.00000000 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 ========
CPDPRG2 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
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



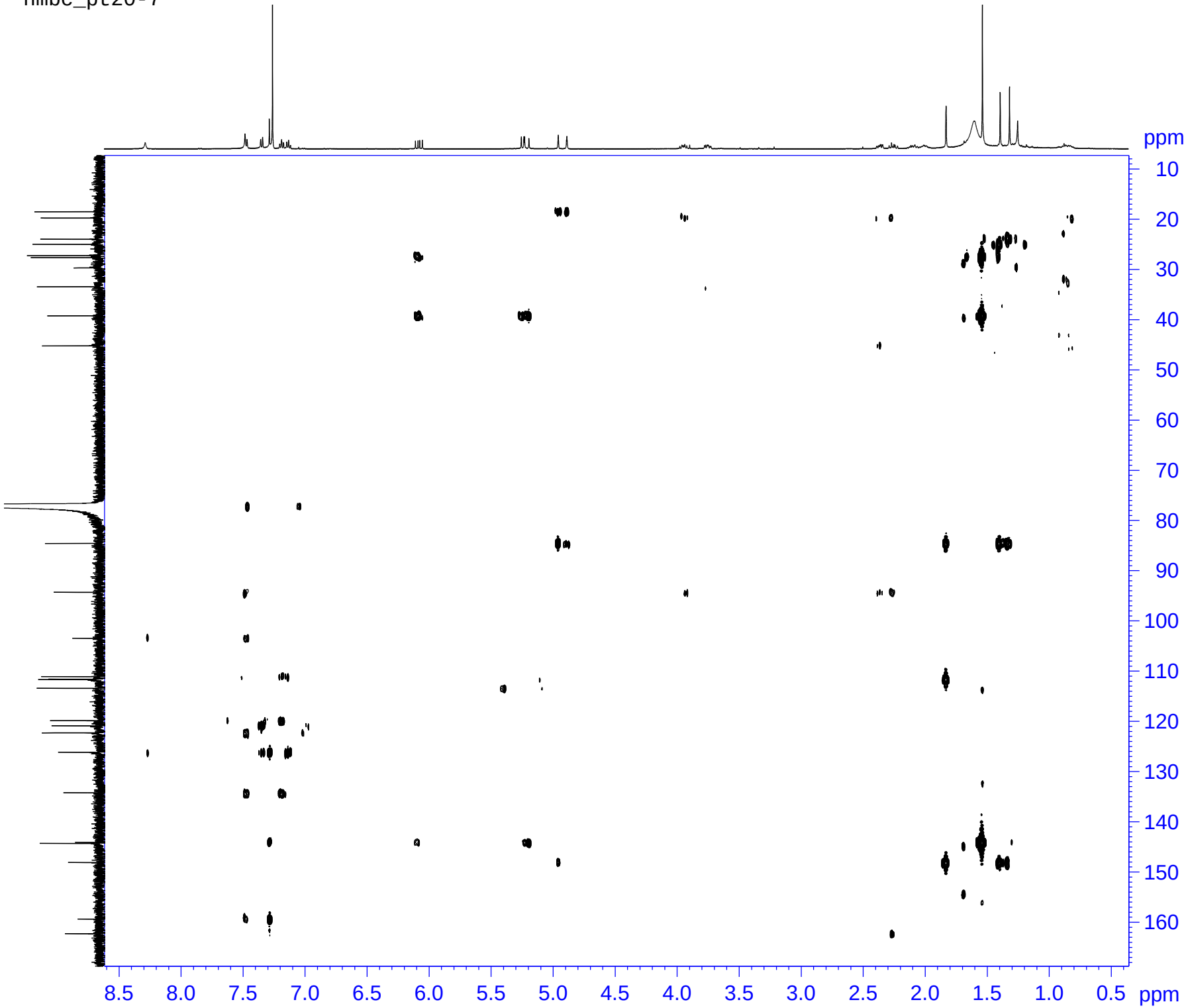

```
NAME              110711
EXPNO                  2
PROCNO                 1
Date_           20110712
Time                8.33
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG   hsqcetgpsisp2
TD                  2048
SOLVENT             CDCl3
NS                    64
DS                    16
SWH           5000.000 Hz
FIDRES        2.441406 Hz
AQ            0.2048500 sec
RG                   203
DW             100.000 usec
DE               6.50 usec
TE              298.3 K
CNST2       145.0000000
D0           0.00000300 sec
D1           2.00000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D16          0.00020000 sec
D24          0.00086207 sec
IN0          0.00002340 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        500.1322506 MHz

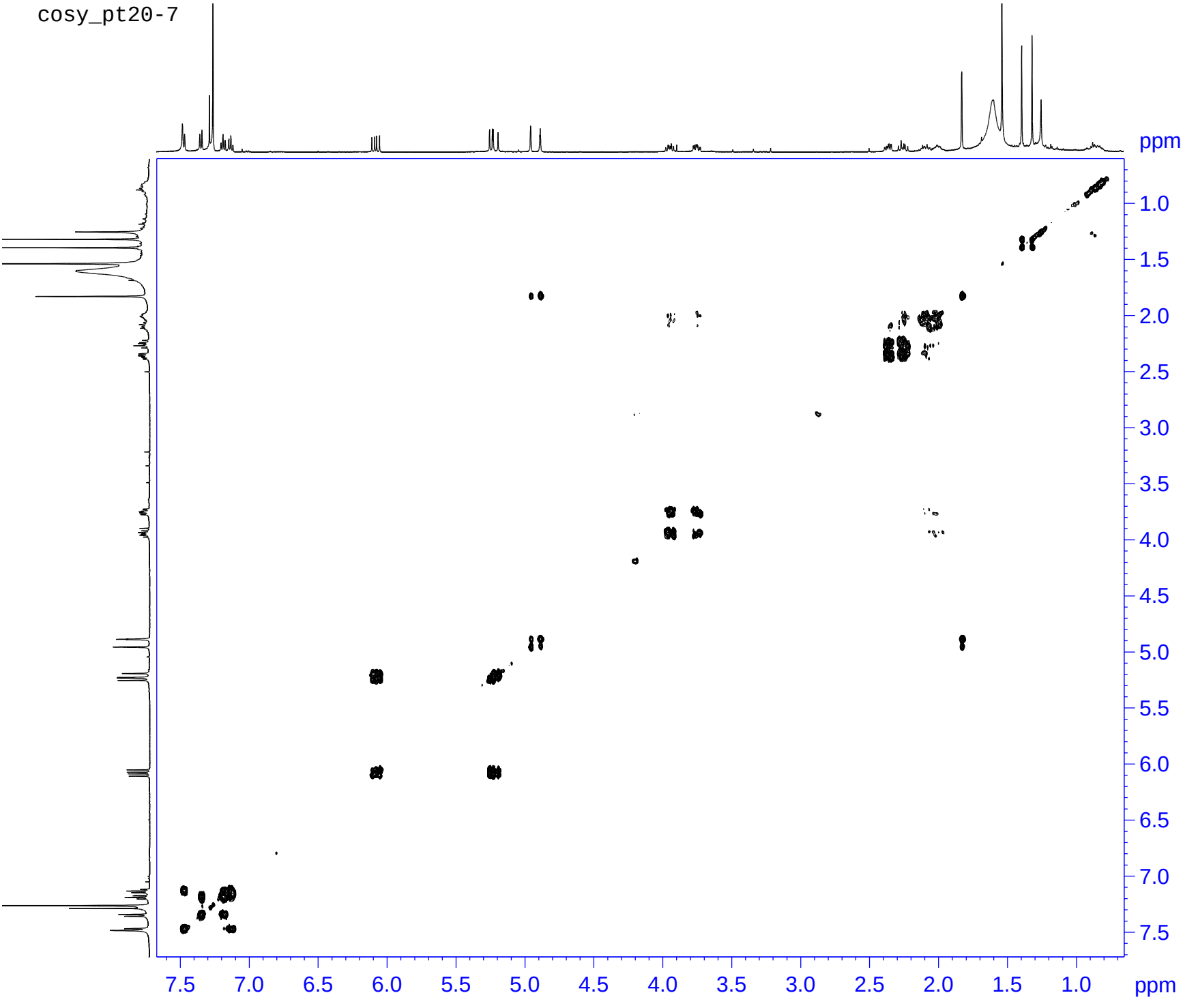
======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                13C
P3                11.90 usec
P4                23.80 usec
P14              500.00 usec
PCPD2             70.00 usec
PL0              120.00 dB
PL2                1.00 dB
PL12              16.39 dB
PL0W         0.00000000 W
PL2W        67.04081726 W
PL12W        1.93793559 W
SFO2        125.7678496 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                   230
SFO1          125.7678 MHz
FIDRES         92.958847 Hz
SW              170.000 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_pt20-7

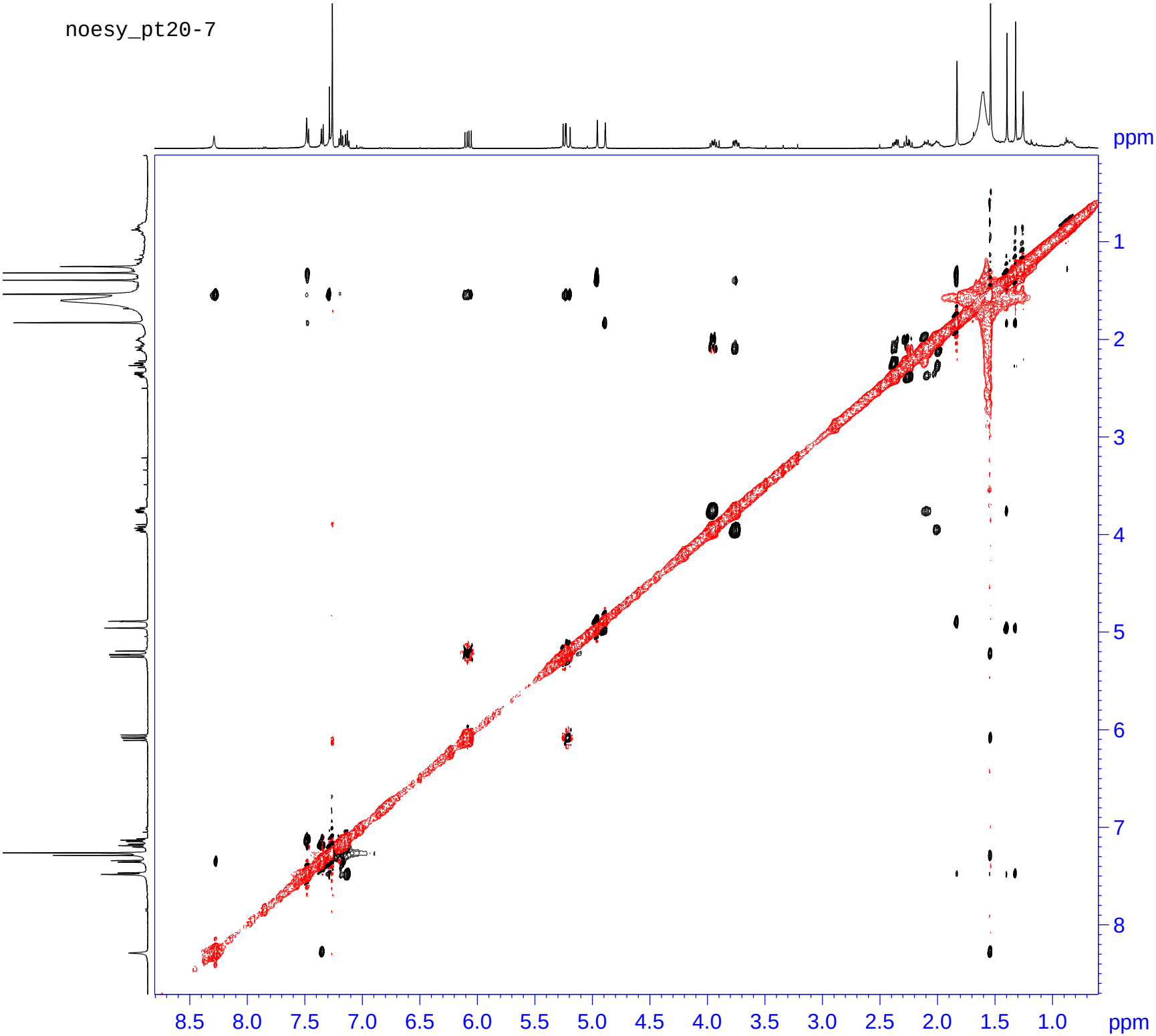


NAME	110711
EXPNO	3
PROCNO	1
Date_	20110711
Time	11.03
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	hmbcetgpl2nd
TD	4096
SOLVENT	CDCl3
NS	128
DS	16
SWH	5000.000 Hz
FIDRES	1.220703 Hz
AQ	0.4096500 sec
RG	203
DW	100.000 usec
DE	6.50 usec
TE	298.2 K
CNST6	120.0000000
CNST7	180.0000000
CNST13	7.0000000
CNST30	0.5981200
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	500.1322506 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



NAME	110711
EXPNO	1
PROCNO	1
Date_	20110711
Time	9.41
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	cosygpmfqf
TD	2048
SOLVENT	CDCl3
NS	8
DS	16
SWH	5000.000 Hz
FIDRES	2.441406 Hz
AQ	0.2048500 sec
RG	203
DW	100.000 usec
DE	6.50 usec
TE	298.2 K
D0	0.00000300 sec
D1	2.00000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00019995 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	11.90 usec
PL1	0.35 dB
PL1W	19.76737595 W
SFO1	500.1322506 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	500.1323 MHz
FIDRES	19.536415 Hz
SW	10.000 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_pt20-7



NAME	110711
EXPNO	4
PROCNO	1
Date_	20110712
Time	5.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	noesygpph
TD	2048
SOLVENT	CDCl3
NS	16
DS	8
SWH	5000.000 Hz
FIDRES	2.441406 Hz
AQ	0.2048500 sec
RG	203
DW	100.000 usec
DE	6.50 usec
TE	298.2 K
D0	0.00008482 sec
D1	2.00000000 sec
D8	0.69999999 sec
D16	0.00020000 sec
IN0	0.00019995 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	11.90 usec
P2	23.80 usec
PL1	0.35 dB
PL1W	19.76737595 W
SFO1	500.1322506 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	40.00 %
GPZ2	-40.00 %
P16	1000.00 usec
ND0	1
TD	256
SFO1	500.1323 MHz
FIDRES	19.536415 Hz
SW	10.000 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

Single Mass Analysis (displaying only valid results)

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

Selected filters: None

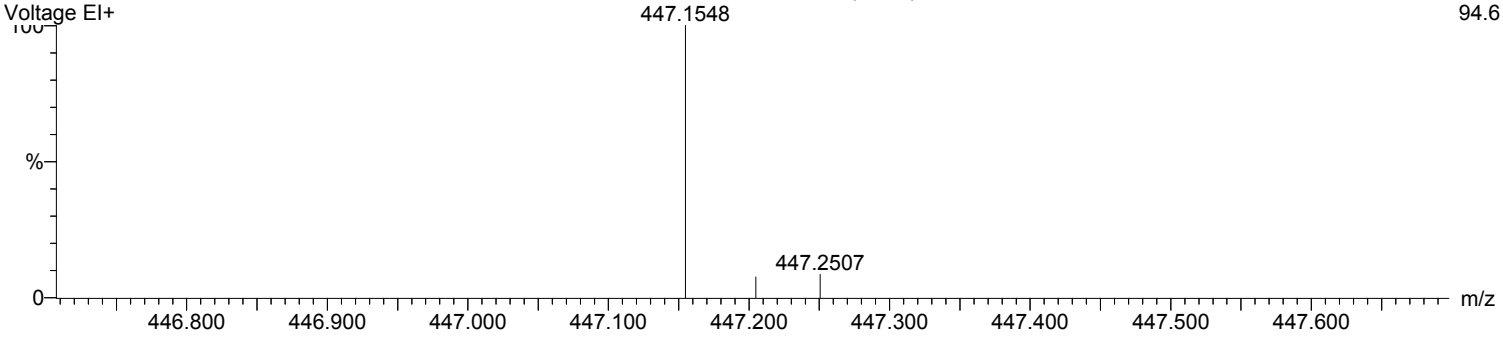
Monoisotopic Mass, Odd and Even Electron Ions

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

Elements Used:

C: 0-200 H: 0-400 N: 3-3 O: 1-3

PT20-7 KIB Autospec Premier
08:16:22 25-Jul-2011 M110725EA-01AFAMM 18 (1.653) P776
Voltage EI+ 447.1548 94.6



Minimum:				0.5		
Maximum:		100.0	10.0	40.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
447.2507	447.2522	-1.5	-3.4	13.0	5546026.0	C27 H33 N3 O3