REPUBLIKA SLOVENIJA
MINISTRSTVO ZA NOTRANJE ZADEVE
POLICIJA

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Co-funded by the Prevention of and Fight against Crime Programme of the European Union

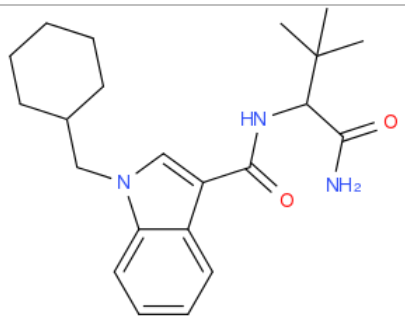
ANALYTICAL REPORT

ADB-CHMICA

(C22H31N3O2)

N-(1-Amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(cyclohexylmethyl)-1H-indole-3-carboxamide,

Sample ID:	233-3560/2014
Sample description:	powder
Report date:	
Sample type:	S-seized

Substance identified-structure[i]	
Systematic name	N-(1-Amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(cyclohexylmethyl)-1H-indole-3-carboxamide
Other names	ADB-CHMICA ,
Formula (per base form)	C22H31N3O2
M_w (g/mol)	369,5
Salt form	base
Other compounds detected	
Smiles	C1(CCCCC1)CN1C=C(C2=CC=CC=C12)C(=O)NC(C(=O)N)C(C)(C)C
Compound Class	Cannabinoids

This report has been produced with the financial support of the Prevention of and fight against crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this report are the sole responsibility of the National Forensic Laboratory and can in no way be taken to reflect the views of the European Commission.

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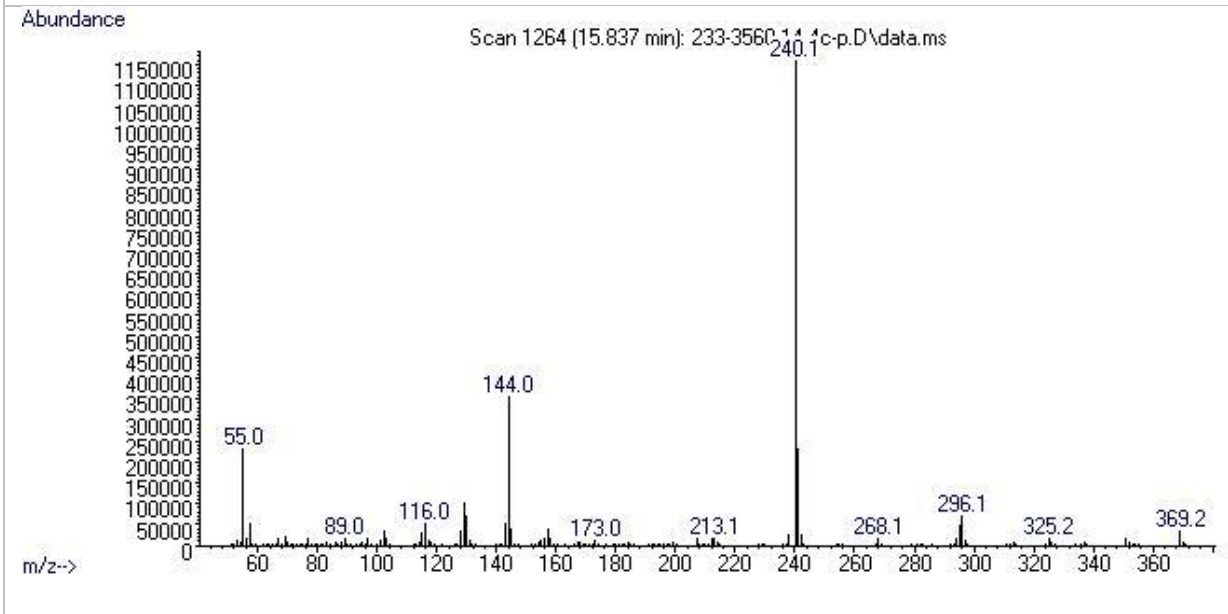
Supporting information

Analytical technique:	applied	remarks
GC-MS	+	
FTIR-ATR	+	
FTIR (condensed phase)		
HPLC-TOF	+	
NMR-confirmed	+	
validation		
other		

MS spectrum (EI)



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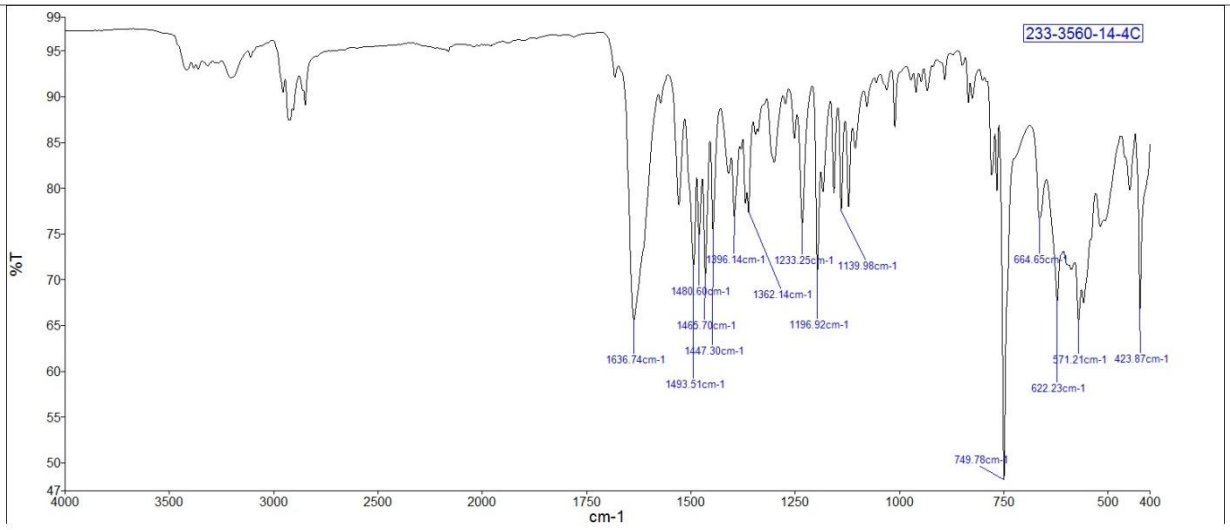
FTIR - ATR



[i] Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ **DOI:** 10.1021/ci100384d

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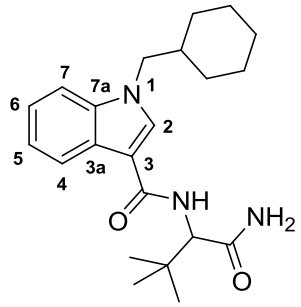
Dr. Janez Košmrlj
Professor of Organic Chemistry

September 17, 2014

Dr. Sonja Klemenc
Head of Chemistry Department
Vodovodna 95
1000 Ljubljana
Slovenija

Dear Dr. Sonja Klemenc,

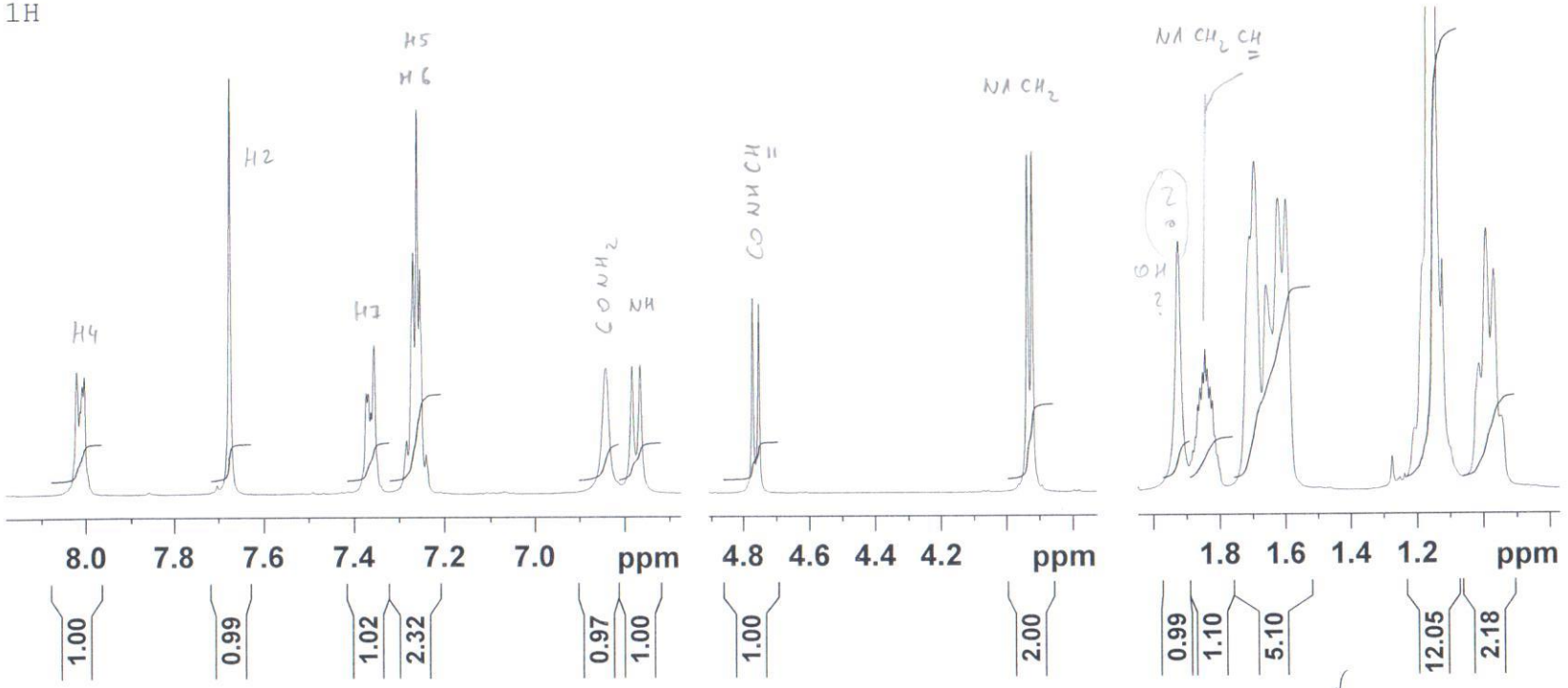
Please find enclosed the results of the structure elucidation for the sample:

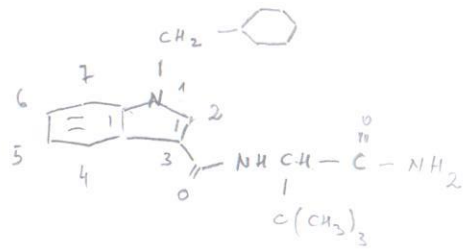
Sample ID:	**233-3560-14-4C**
Received date:	September 1, 2014
Our notebook code:	P-233-3196-14-4C
NMR sample preparation:	15 mg dissolved in 0.7 mL $CDCl_3$
NMR experiments:	^{1}H, ^{13}C, ^{19}F, ^{1}H–^{1}H *gs*-COSY, ^{1}H–^{13}C *gs*-HSQC, ^{1}H–^{13}C *gs*-HMBC, ^{1}H–^{15}N *gs*-HMBC
Proposed structure with atom numbering scheme, formula, exact mass, molecular weight:	 Chemical Formula: $C_{22}H_{31}N_3O_2$ Exact Mass: 369.2416 Molecular Weight: 369.5004
Chemical name:	*N*-(1-Amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(cyclohexylmethyl)-1*H*-indole-3-carboxamide
Comments:	Structure elucidation based on 1D and 2D NMR spectra and HRMS data
Supporting information:	Copies of 1D and 2D NMR spectra, EI-MS spectrum (pp 2-11)

Sincerely,

Janez Košmrlj

P-233-3196-14-4C
1H





BRUKER

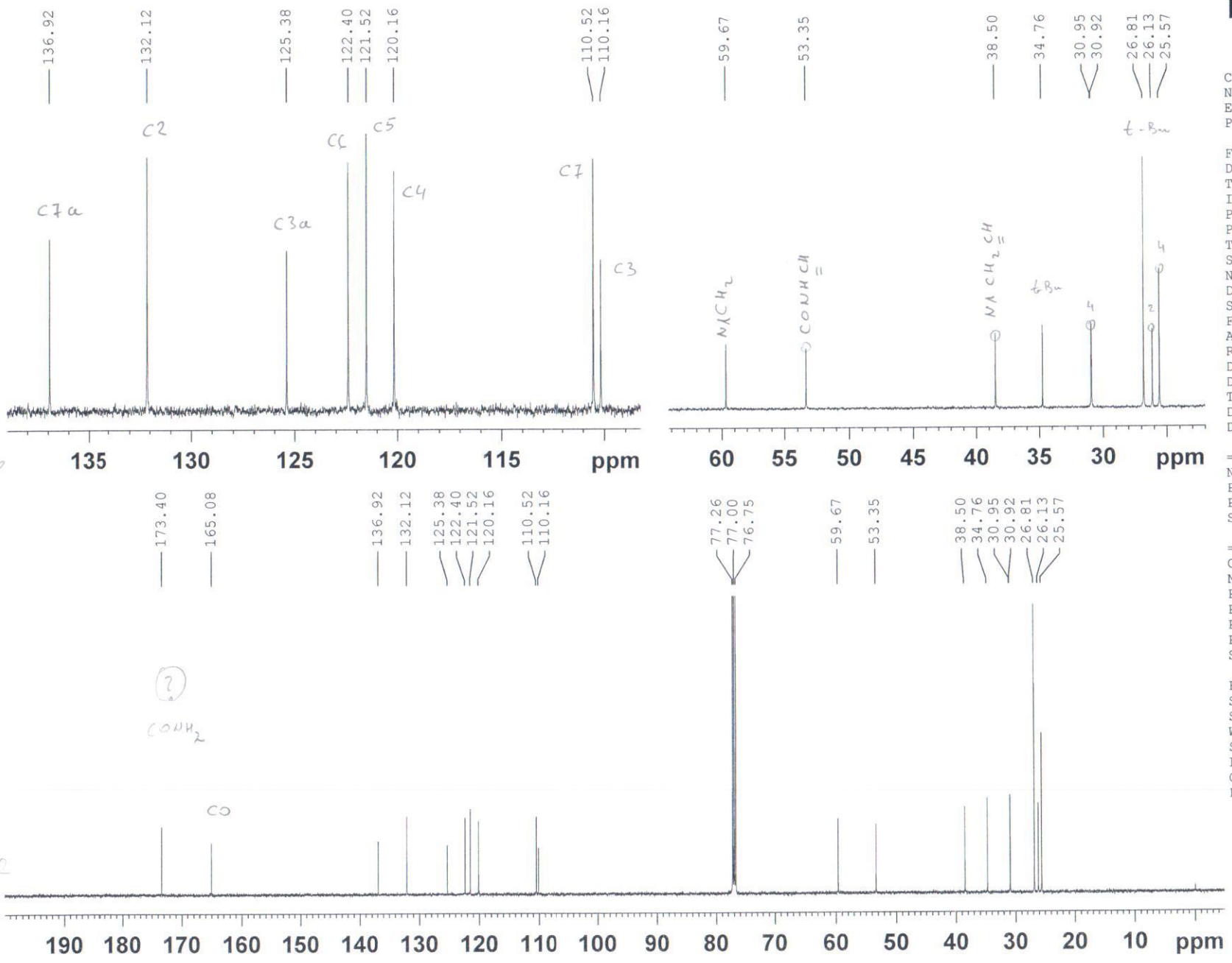
Current Data Parameters
NAME P-233-3196-14-4C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 10.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 90.5
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.90 usec
PLW1 26.00000000 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 65536
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P-233-3196-14-4C
13C



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Current Data Parameters

NAME	P-233-3196-14-4C
EXPNO	6
PROCNO	1

F2 - Acquisition Parameters

Date_	20140904
Time	13.52
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	2050
DW	16.800 usec
DE	6.50 usec
TE	296.0 K
D1	2.00000000 sec
D11	0.03000000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	9.00 usec
PLW1	122.00000000 W
SFO1	125.7703637 MHz

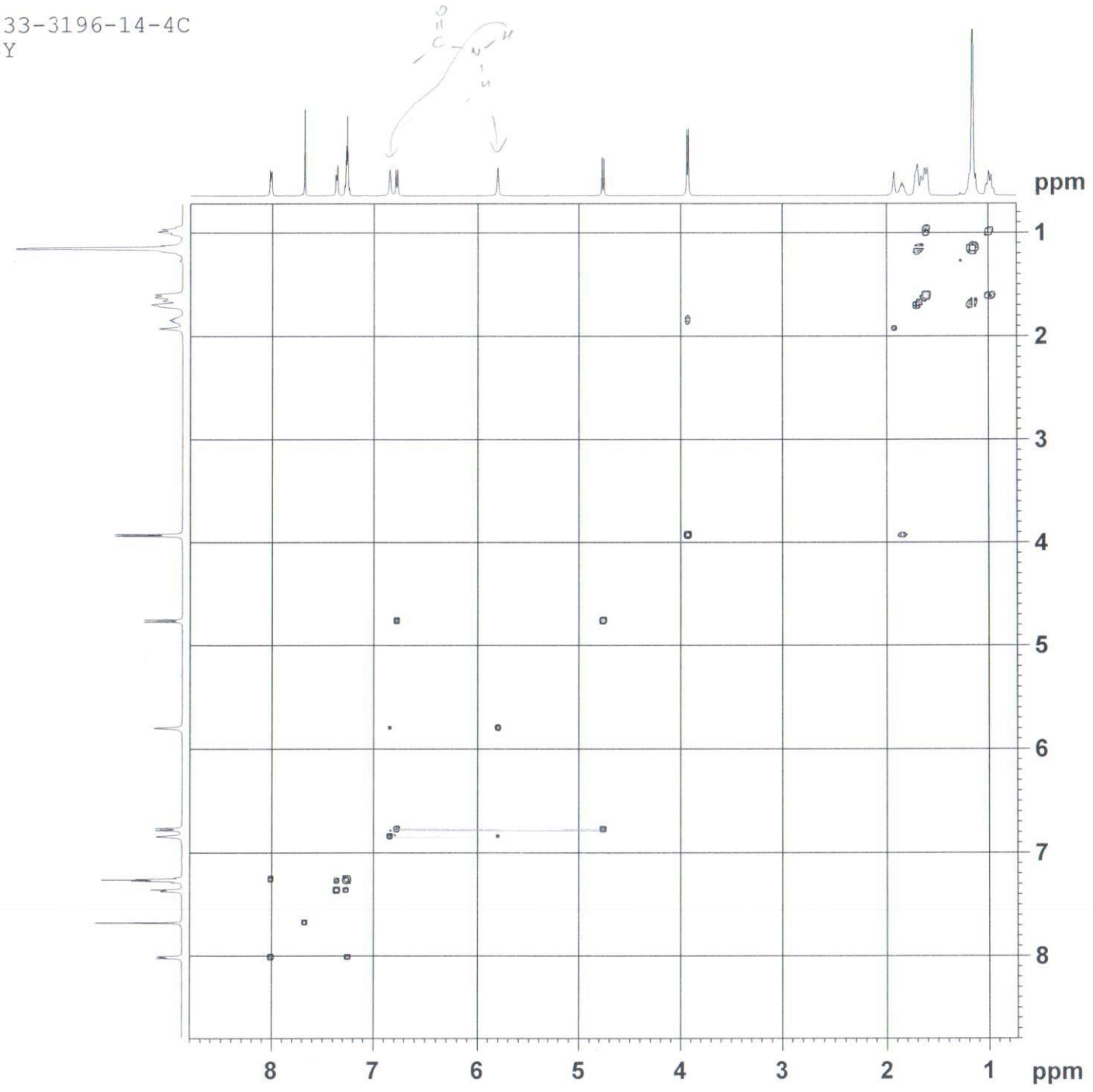
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PLW2	26.00000000 W
PLW12	0.32179001 W
PLW13	0.20595001 W
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577951 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

P-233-3196-14-4C
COSY



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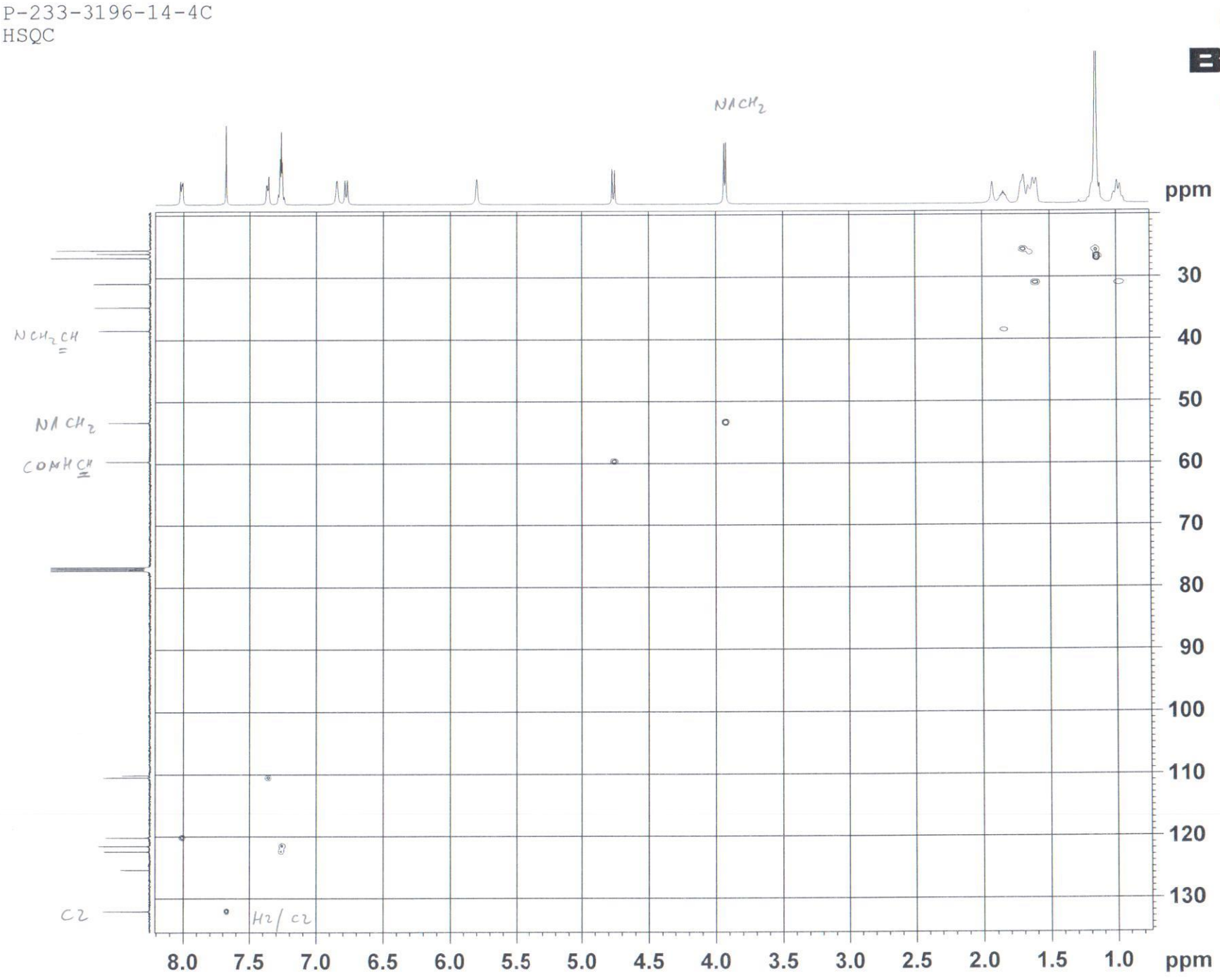
```
Current Data Parameters
NAME      P-233-3196-14-4C
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20140904
Time                 10.21
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG       cosygpppqf
TD                    2048
SOLVENT               CDC13
NS                       1
DS                       8
SWH               4761.905 Hz
FIDRES            2.325149 Hz
AQ               0.2150900 sec
RG                      36
DW                105.000 usec
DE                  6.50 usec
TE                 296.0 K
D0               0.00000300 sec
D1               1.93815005 sec
D11              0.03000000 sec
D12              0.00002000 sec
D13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00021000 sec

======== CHANNEL f1 ========
NUC1                     1H
P0                    8.90 usec
P1                    8.90 usec
P17                2500.00 usec
PLW1         26.00000000 W
PLW10         3.04649997 W
SFO1          500.1320345 MHz

====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                      128
SFO1              500.132 MHz
FIDRES          37.202381 Hz
SW                  9.521 ppm
FnMODE                  QF

F2 - Processing parameters
SI                     1024
SF            500.1300131 MHz
WDW                  QSINE
SSB       0
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                     1024
MC2                     QF
SF            500.1300131 MHz
WDW          States-TPPI
SSB       0
LB        0 Hz
GB        0
```

P-233-3196-14-4C
HSQC



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Current Data Parameters
NAME P-233-3196-14-4C
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 10.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hsqcetgpsi2
TD 1024
SOLVENT CDCl3
NS 2
DS 16
SWH 4761.905 Hz
FIDRES 4.650298 Hz
AQ 0.1075700 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 296.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.46928000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00002400 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 8.90 usec
P2 17.80 usec
P28 1000.00 usec
PLW1 26.00000000 W
SFO1 500.1320345 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 9.00 usec
P4 18.00 usec
PCPD2 70.00 usec
PLW2 122.00000000 W
PLW12 2.01670003 W
SFO2 125.7672177 MHz

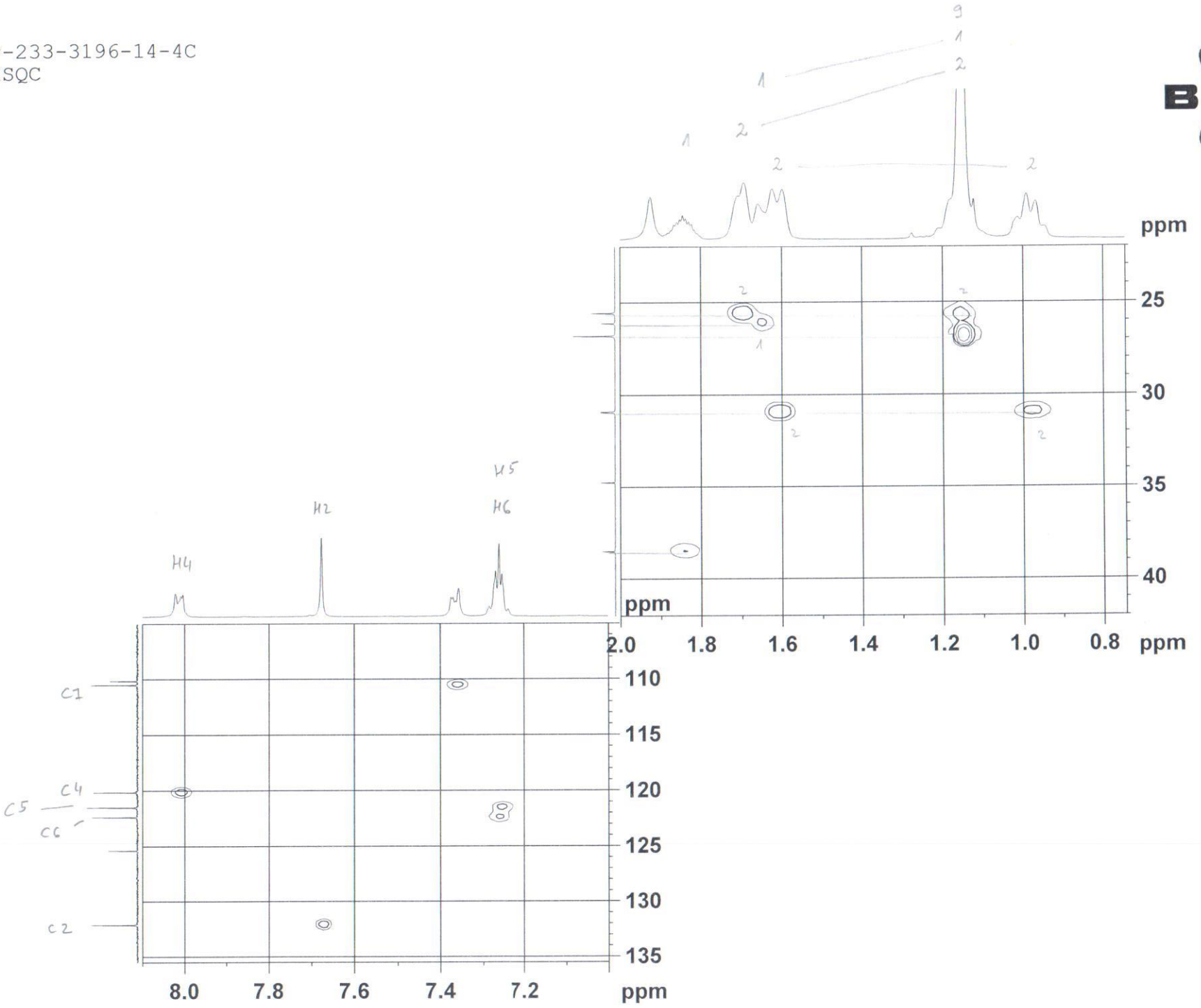
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPNAM4 SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 125.7672 MHz
FIDRES 81.380234 Hz
SW 165.650 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.1300131 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 125.7577890 MHz
WDW
SSB 2
LB 0 Hz
GB 0

P-233-3196-14-4C
HSQC



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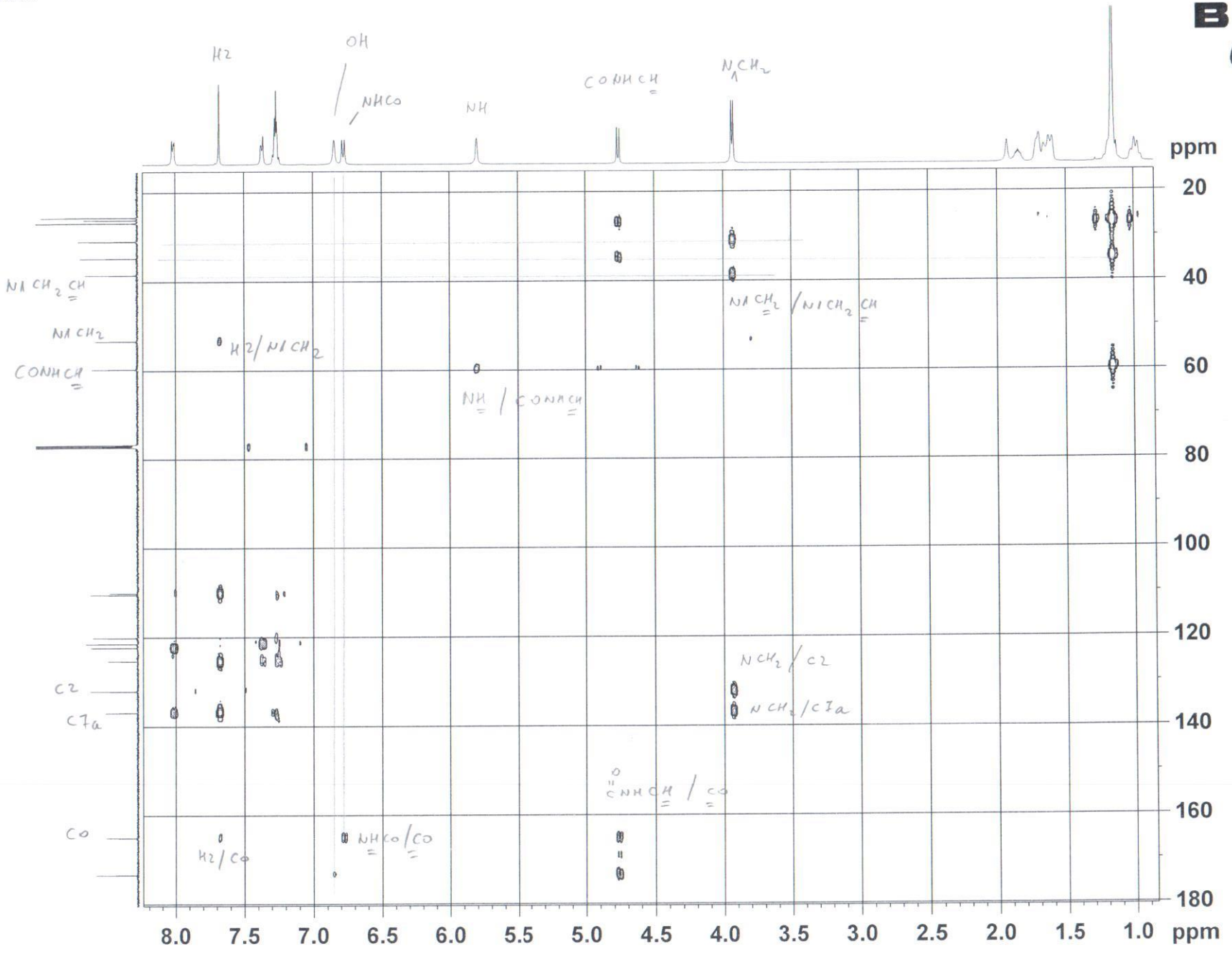
```
Current Data Parameters
NAME        P-233-3196-14-4C
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_               20140904
Time                   10.46
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG         hsqcetgpsi2
TD                      1024
SOLVENT                CDCl3
NS                         2
DS                        16
SWH                4761.905 Hz
FIDRES             4.650298 Hz
AQ                0.1075700 sec
RG                     2050
DW                  105.000 usec
DE                    6.50 usec
TE                   296.2 K
CNST2              145.0000000
D0                0.00000300 sec
D1                1.46928000 sec
D4                0.00172414 sec
D11               0.03000000 sec
D13               0.00000400 sec
D16               0.00020000 sec
D24               0.00086207 sec
IN0               0.00002400 sec
2GOPTNS

======== CHANNEL f1 ========
NUC1                       1H
P1                       8.90 usec
P2                      17.80 usec
P28                   1000.00 usec
PLW1              26.00000000 W
SFO1             500.1320345 MHz

======== CHANNEL f2 ========
CPDPRG2                 garp
NUC2                     13C
P3                      9.00 usec
P4                     18.00 usec
PCPD2                  70.00 usec
PLW2             122.00000000 W
PLW12              2.01670003 W
SFO2             125.7672177 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SMSQ10.100
GPNAM2           SMSQ10.100
GPNAM3           SMSQ10.100
GPNAM4           SMSQ10.100
GPZ1                  80.00 %
GPZ2                  20.10 %
GPZ3                  11.00 %
GPZ4                  -5.00 %
P16                 1000.00 usec
P19                  600.00 usec

F1 - Acquisition parameters
TD                       256
SFO1             125.7672 MHz
FIDRES           81.380234 Hz
SW                165.650 ppm
FnMODE       Echo-Antiecho

F2 - Processing parameters
SI                      1024
SF               500.1300131 MHz
WDW                     QSINE
SSB                        2
LB          0 Hz
GB          0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2          echo-antiecho
SF               125.7577890 MHz
WDW
SSB                        2
LB          0 Hz
GB          0
```

P-233-3196-14-4C
HMBC



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Current Data Parameters
NAME P-233-3196-14-4C
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 11.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4761.905 Hz
FIDRES 2.325149 Hz
AQ 0.2150900 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 296.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.44224596 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
IN0 0.00001790 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.90 usec
P2 17.80 usec
PLW1 26.00000000 W
SFO1 500.1320345 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 9.00 usec
PLW2 122.00000000 W
SFO2 125.7703437 MHz

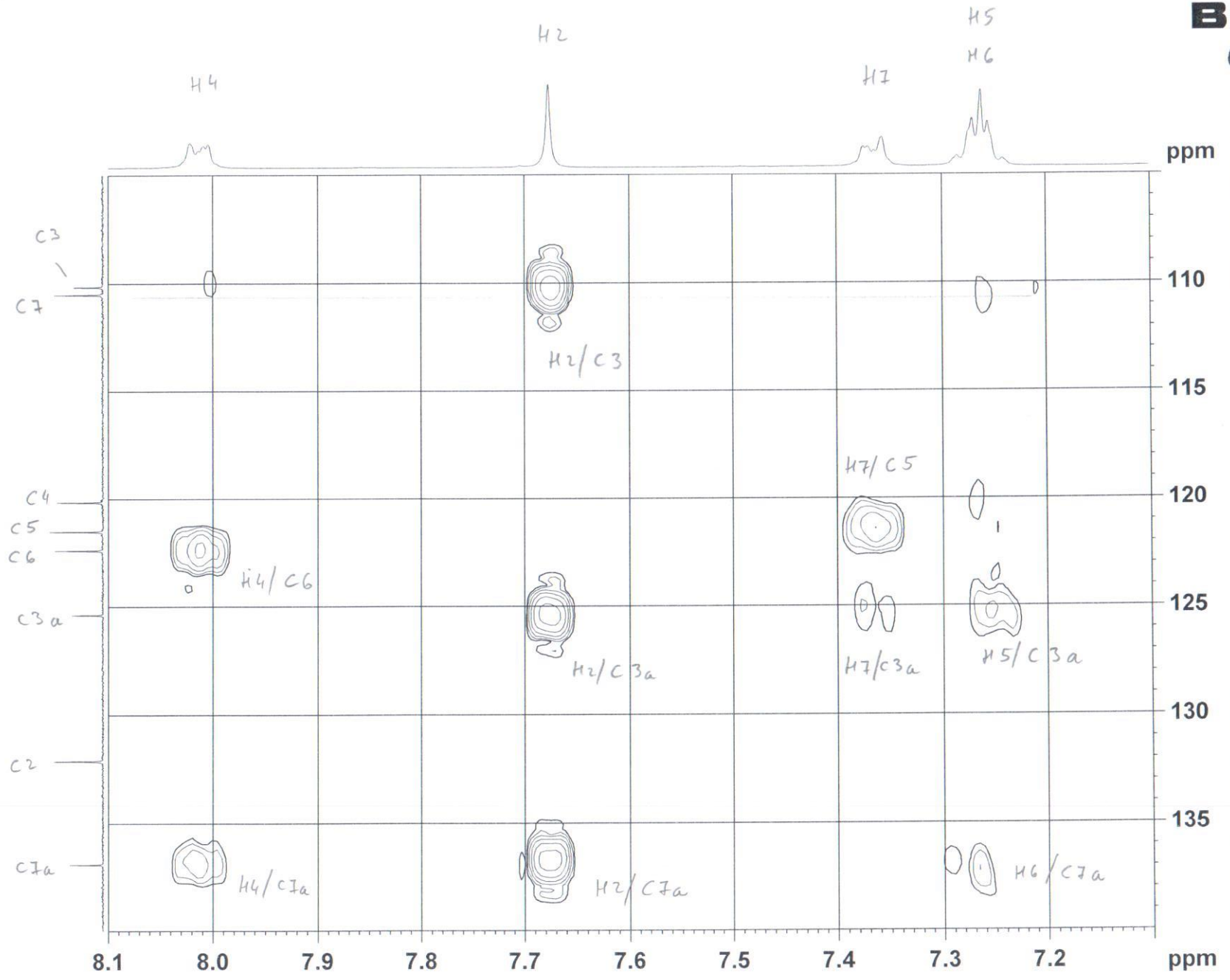
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 125.7703 MHz
FIDRES 218.226349 Hz
SW 222.095 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300131 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 125.7577890 MHz
WDW States
SSB 0
LB 0 Hz
GB 0

P-233-3196-14-4C
HMBC



BRUKER

Current Data Parameters
NAME P-233-3196-14-4C
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 11.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4761.905 Hz
FIDRES 2.325149 Hz
AQ 0.2150900 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 296.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.44224596 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
IN0 0.00001790 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.90 usec
P2 17.80 usec
PLW1 26.00000000 W
SFO1 500.1320345 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 9.00 usec
PLW2 122.00000000 W
SFO2 125.7703437 MHz

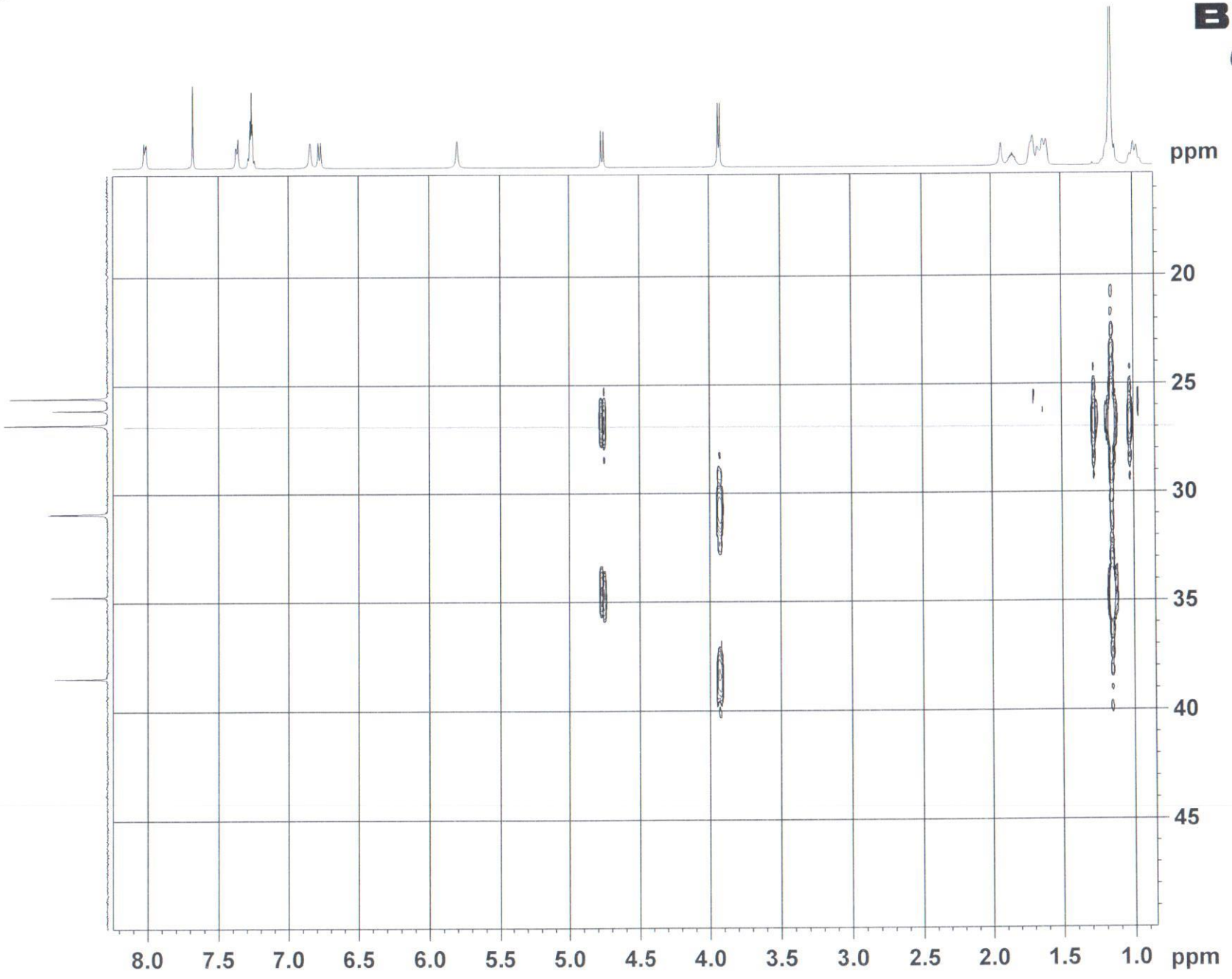
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 125.7703 MHz
FIDRES 218.226349 Hz
SW 222.095 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300131 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 125.7577890 MHz
WDW States
SSB 0
LB 0 Hz
GB 0

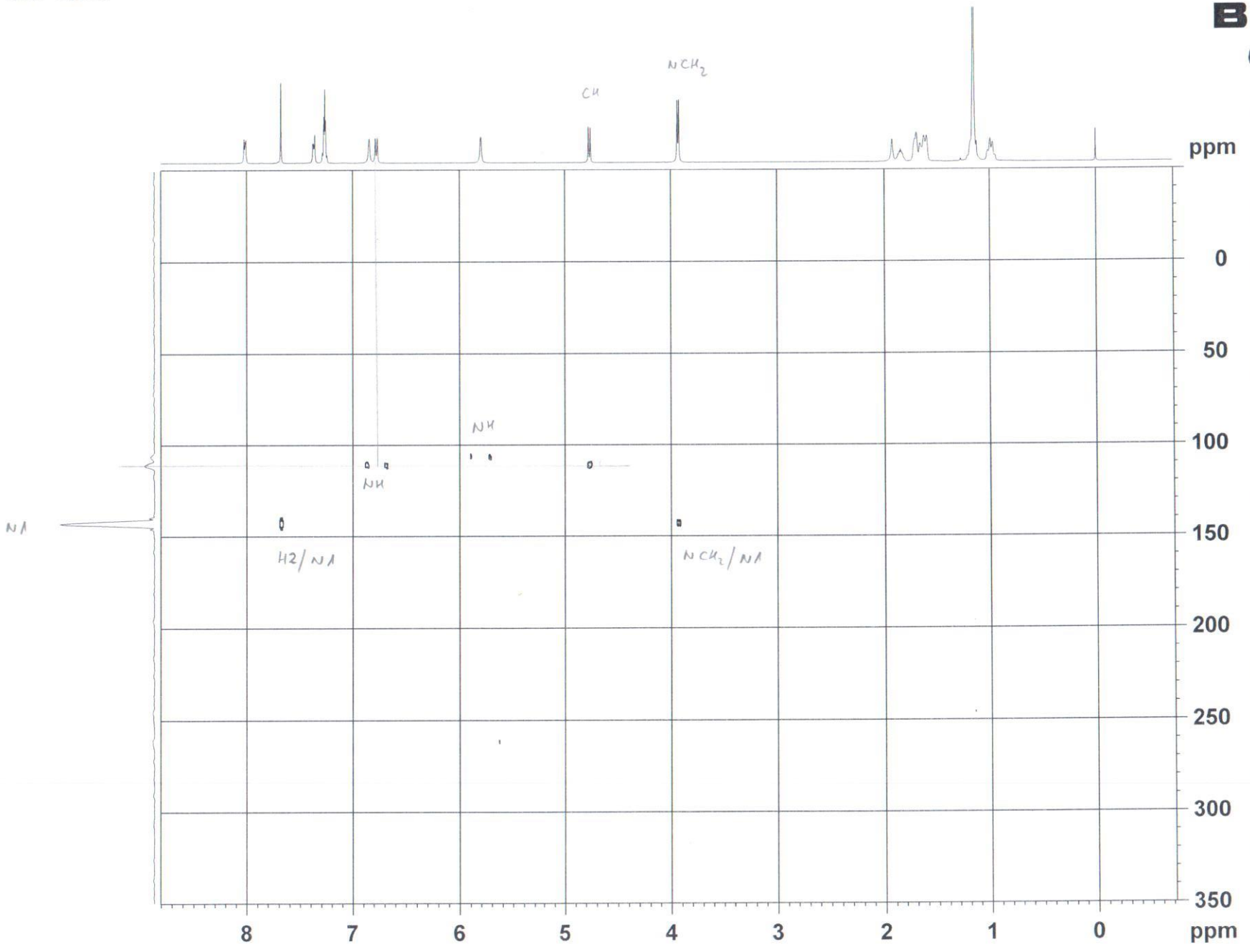
P-233-3196-14-4C
HMBC



BRUKER

```
Current Data Parameters
NAME          P-233-3196-14-4C
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140904
Time                     11.23
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG      hmbcgplpndqf
TD                       2048
SOLVENT                  CDCl3
NS                           4
DS                          16
SWH                4761.905 Hz
FIDRES             2.325149 Hz
AQ                 0.2150900 sec
RG                        2050
DW                  105.000 usec
DE                    6.50 usec
TE                   296.0 K
CNST2               145.0000000
CNST13               10.0000000
D0                 0.00000300 sec
D1                 1.44224596 sec
D2                 0.00344828 sec
D6                 0.05000000 sec
D16                0.00020000 sec
IN0                0.00001790 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                     8.90 usec
P2                    17.80 usec
PLW1               26.00000000 W
SFO1              500.1320345 MHz

======== CHANNEL f2 ========
NUC2                        13C
P3                     9.00 usec
PLW2              122.00000000 W
SFO2              125.7703437 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SMSQ10.100
GPNAM2              SMSQ10.100
GPNAM3              SMSQ10.100
GPZ1                    50.00 %
GPZ2                    30.00 %
GPZ3                    40.10 %
P16                  1000.00 usec

F1 - Acquisition parameters
TD                          128
SFO1              125.7703 MHz
FIDRES            218.226349 Hz
SW                  222.095 ppm
FnMODE                      QF

F2 - Processing parameters
SI                         2048
SF                500.1300131 MHz
WDW                        SINE
SSB                   0
LB                    0 Hz
GB                    0
PC                         1.40

F1 - Processing parameters
SI                         1024
MC2                          QF
SF                125.7577890 MHz
WDW                      States
SSB                   0
LB                    0 Hz
GB                    0
```

P-233-3196-14-4C
15N HMBC



Current Data Parameters
NAME P-233-3196-14-4C
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 11.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgpndqf
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 4761.905 Hz
FIDRES 2.325149 Hz
AQ 0.2150900 sec
RG 2050
DW 105.000 usec
DE 6.50 usec
TE 296.0 K
CNST13 5.0000000
D0 0.00000300 sec
D1 1.94224596 sec
D6 0.10000000 sec
D16 0.00020000 sec
IN0 0.00002465 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.90 usec
P2 17.80 usec
PLW1 26.00000000 W
SFO1 500.1320345 MHz

======== CHANNEL f2 ========
NUC2 15N
P3 14.40 usec
PLW2 206.00000000 W
SFO2 50.6853342 MHz

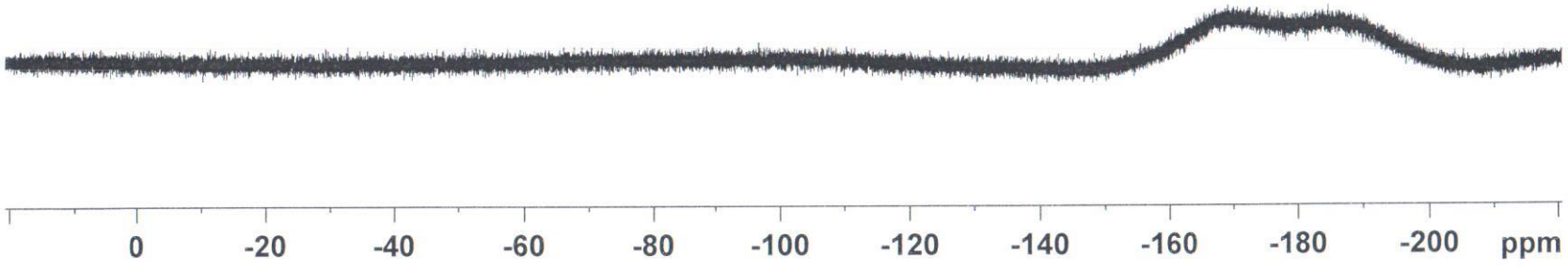
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPZ1 70.00 %
GPZ2 30.00 %
GPZ3 50.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 50.68533 MHz
FIDRES 158.391663 Hz
SW 400.000 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300131 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 50.6777330 MHz
WDW States
SSB 0
LB 0 Hz
GB 0

P-233-3196-14-4C
13C



Current Data Parameters

NAME	P-233-3196-14-4C
EXPNO	7
PROCNO	1

F2 - Acquisition Parameters

Date_	20140904
Time	13.53
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	113636.367 Hz
FIDRES	0.866977 Hz
AQ	0.5767668 sec
RG	456
DW	4.400 usec
DE	6.50 usec
TE	295.9 K
D1	1.00000000 sec

======== CHANNEL f1 ========

NUC1	19F
P1	13.00 usec
PLW1	57.00000000 W
SFO1	470.5453180 MHz

F2 - Processing parameters

SI	65536
SF	470.5923770 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00