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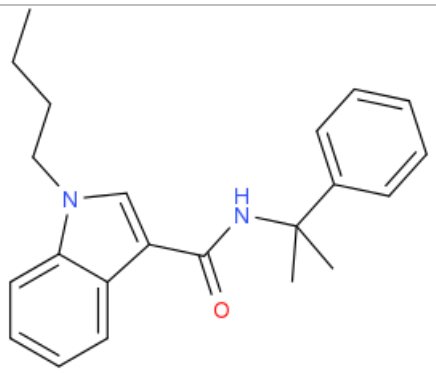
ANALYTICAL REPORT

CUMYL-BICA

,(C22H26N2O)

Remark – other NPS detected: none

Sample ID:	1115
Sample description:	powder - white
Sample type:	S-seized
Date of entry:	3/27/2015

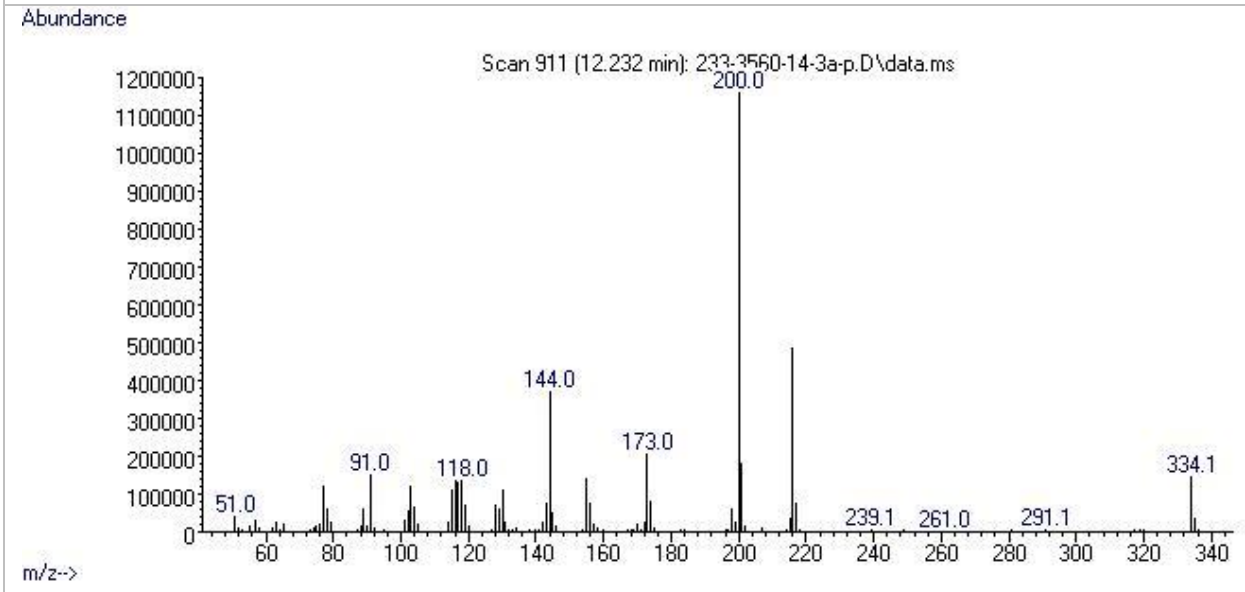
Substance identified-structure[i] (base form)	
Systematic name	1-butyl-N-(2-phenylpropan-2-yl)-1H-indole-3-carboxamide
Other names	
Formula (per base form)	C22H26N2O
M_w (g/mol)	334.45
Salt form	base
Other compounds detected	none
Smiles	C(CCC)N1N=C(C2=CC=CC=C12)C(=O)NC(C)(C)C1=CC=CC=C1
Compound Class	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.

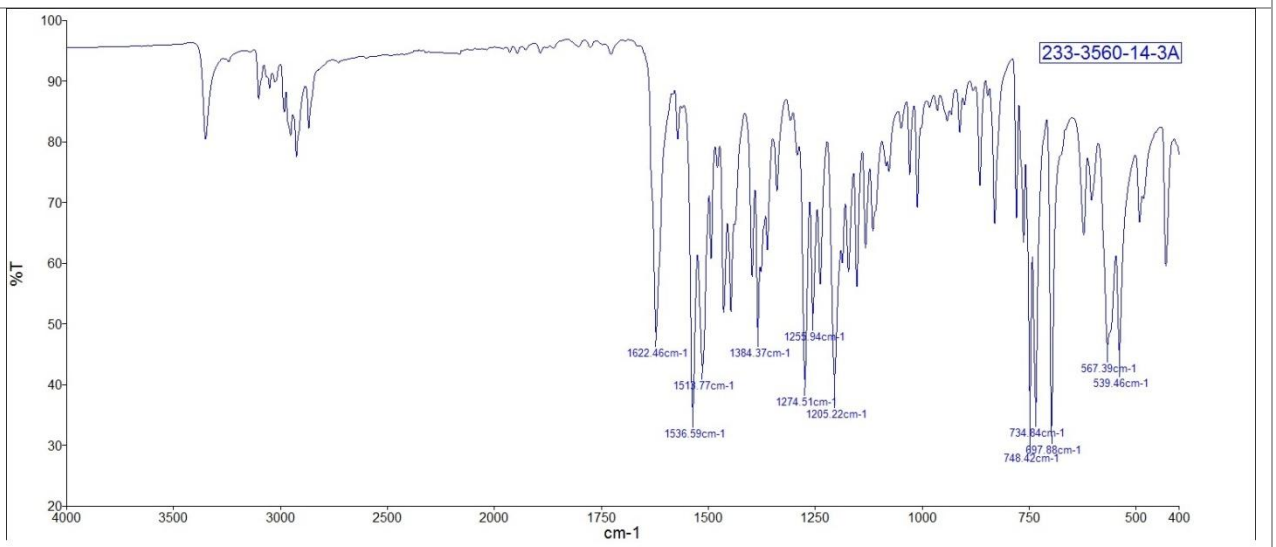
Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	BP(1): 200; BP(2): 216; BP(3):144/
FTIR-ATR	+	base
FTIR (condensed phase)	/	
HPLC-TOF	+	Formula: C22H26N2O
NMR-confirmed	+	
validation		
other		

MS spectrum (EI)



FTIR - ATR (Cumyl BICA)



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

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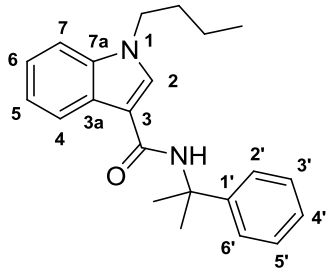
Dr. Janez Košmrlj
Professor of Organic Chemistry

September 17, 2014

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

Dear Dr. Sonja Klemenc,

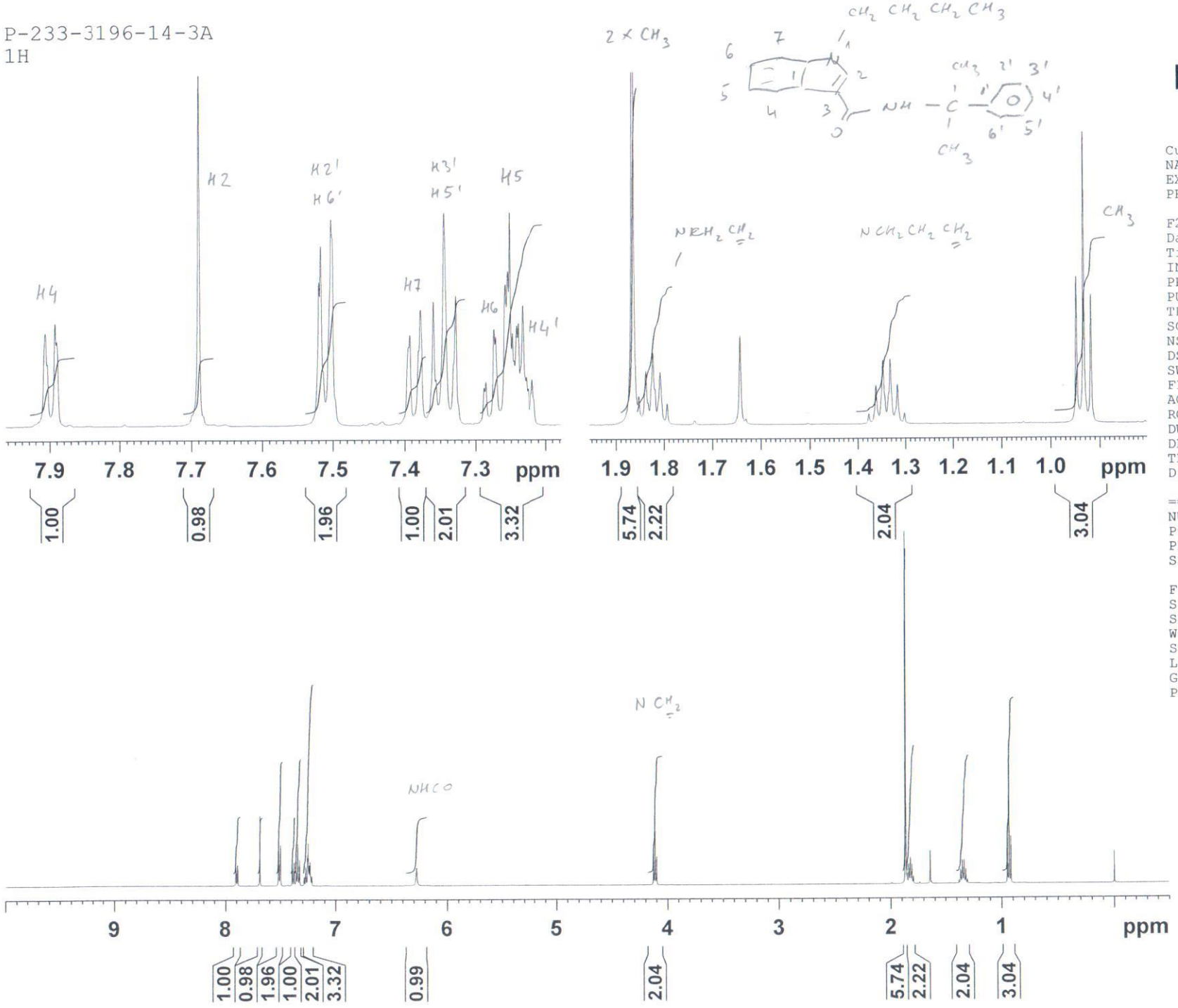
Please find enclosed the results of the structure elucidation for the sample:

Sample ID:	**233-3560-14-3A**
Received date:	September 1, 2014
Our notebook code:	P-233-3196-14-3A
NMR sample preparation:	15 mg dissolved in 0.7 mL $CDCl_3$
NMR experiments:	^{1}H, ^{13}C, ^{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: $C_{22}H_{26}N_2O$ Exact Mass: 334.2045 Molecular Weight: 334.4546
Chemical name:	1-Butyl-*N*-(2-phenylpropan-2-yl)-1*H*-indole-3-carboxamide
Comments:	- Structure elucidation based on 1D and 2D NMR spectra. - The result is consistent with the structure proposed by MS.
Supporting information:	Copies of 1D and 2D NMR spectra, EI-MS spectrum (pp 2-10)

Sincerely,

Janez Košmrlj

P-233-3196-14-3A
1H



Current Data Parameters

NAME	P-233-3196-14-3A
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20140903
Time	14.01
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	101
DW	48.400 usec
DE	6.50 usec
TE	296.0 K
D1	1.00000000 sec

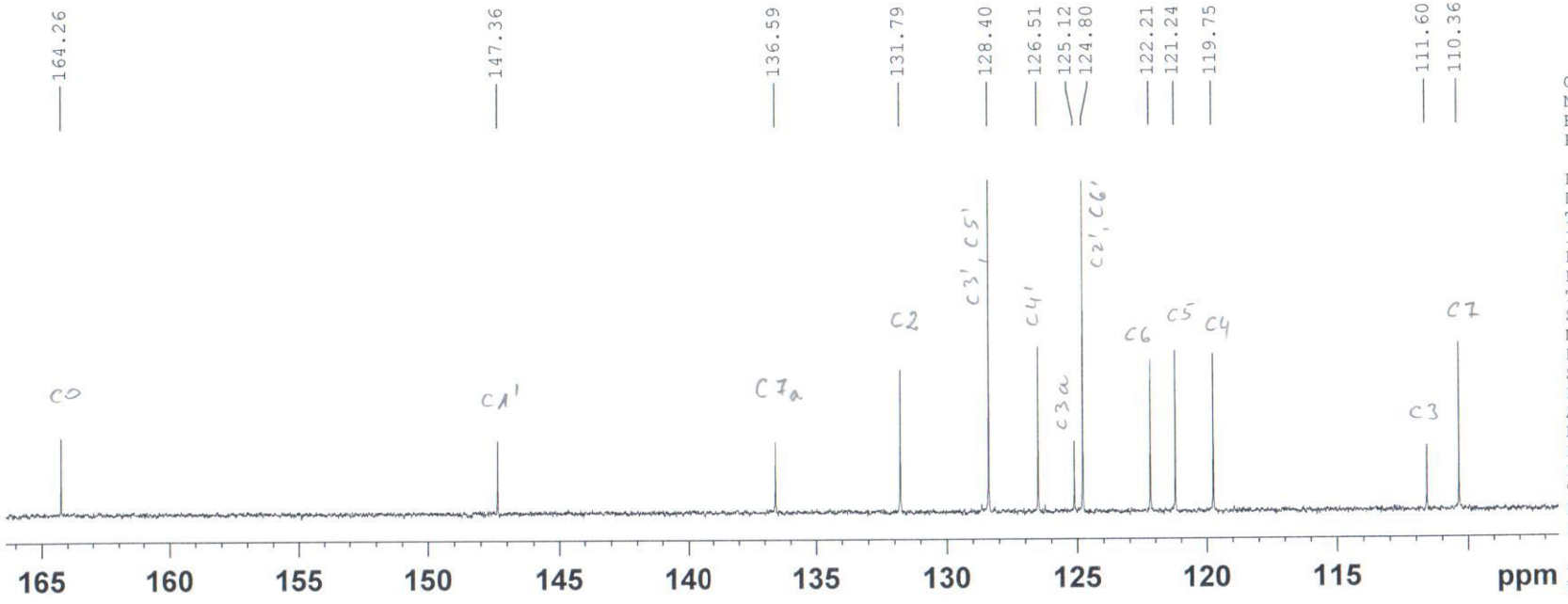
======== CHANNEL f1 ========

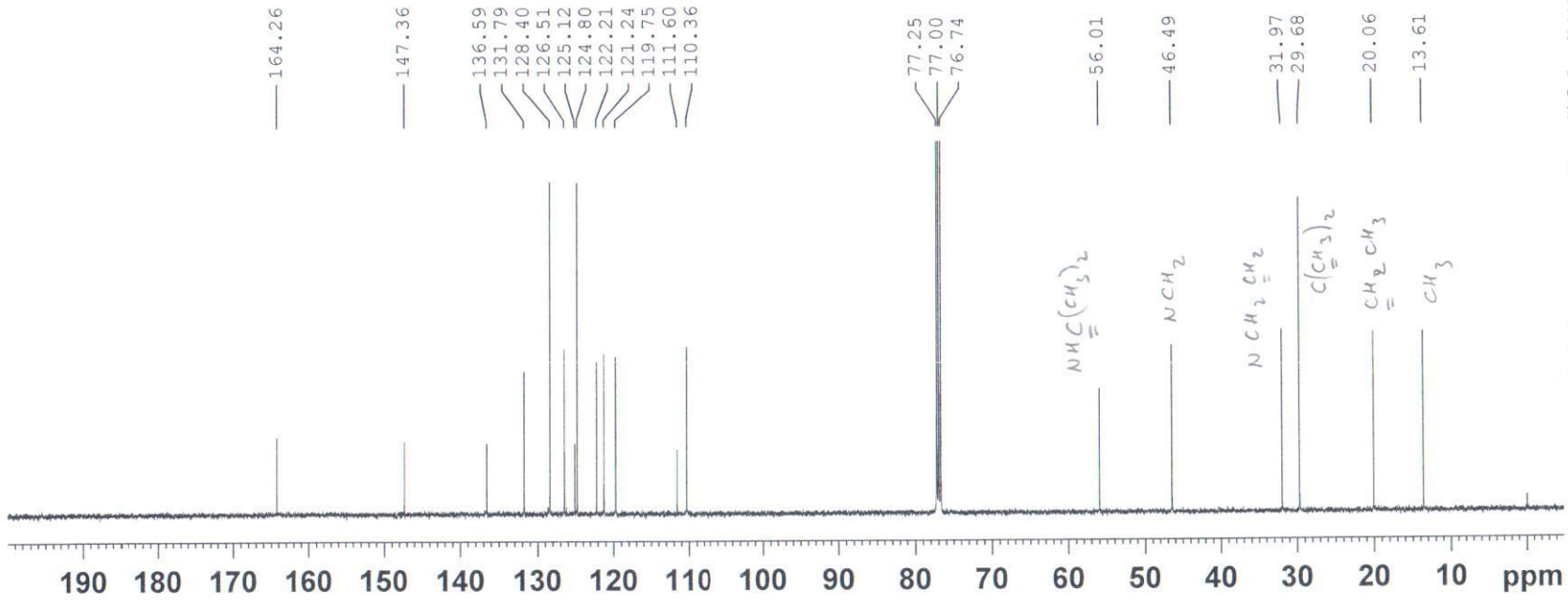
NUC1	1H
P1	8.90 usec
PLW1	26.00000000 W
SFO1	500.1330885 MHz

F2 - Processing parameters

SI	65536
SF	500.1300180 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

P-233-3196-14-3A
13C





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Current Data Parameters
NAME P-233-3196-14-3A
EXPNO 6
PROCNO 1

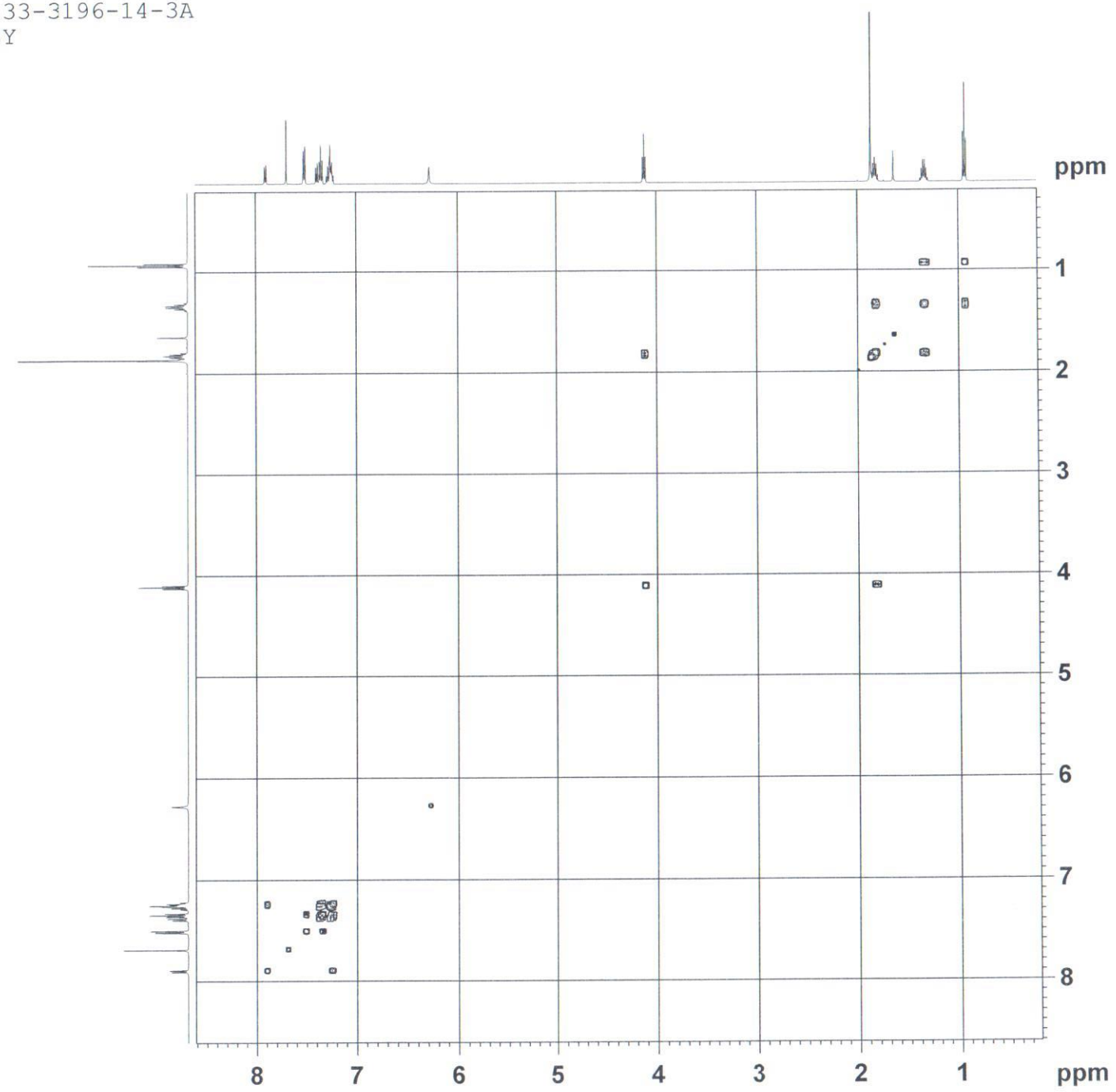
F2 - Acquisition Parameters
Date_ 20140903
Time 17.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
D11 0.03000000 sec

======== 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 125.7577960 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P-233-3196-14-3A
COSY



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```
Current Data Parameters
NAME       P-233-3196-14-3A
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140903
Time                  14.20
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG          cosygpppqf
TD                     2048
SOLVENT               CDCl3
NS                        1
DS                        8
SWH               4201.681 Hz
FIDRES            2.051602 Hz
AQ                0.2437620 sec
RG                     40.3
DW                 119.000 usec
DE                   6.50 usec
TE                  296.0 K
D0                0.00000300 sec
D1                1.90947795 sec
D11               0.03000000 sec
D12               0.00002000 sec
D13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00023800 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           500.1322242 MHz

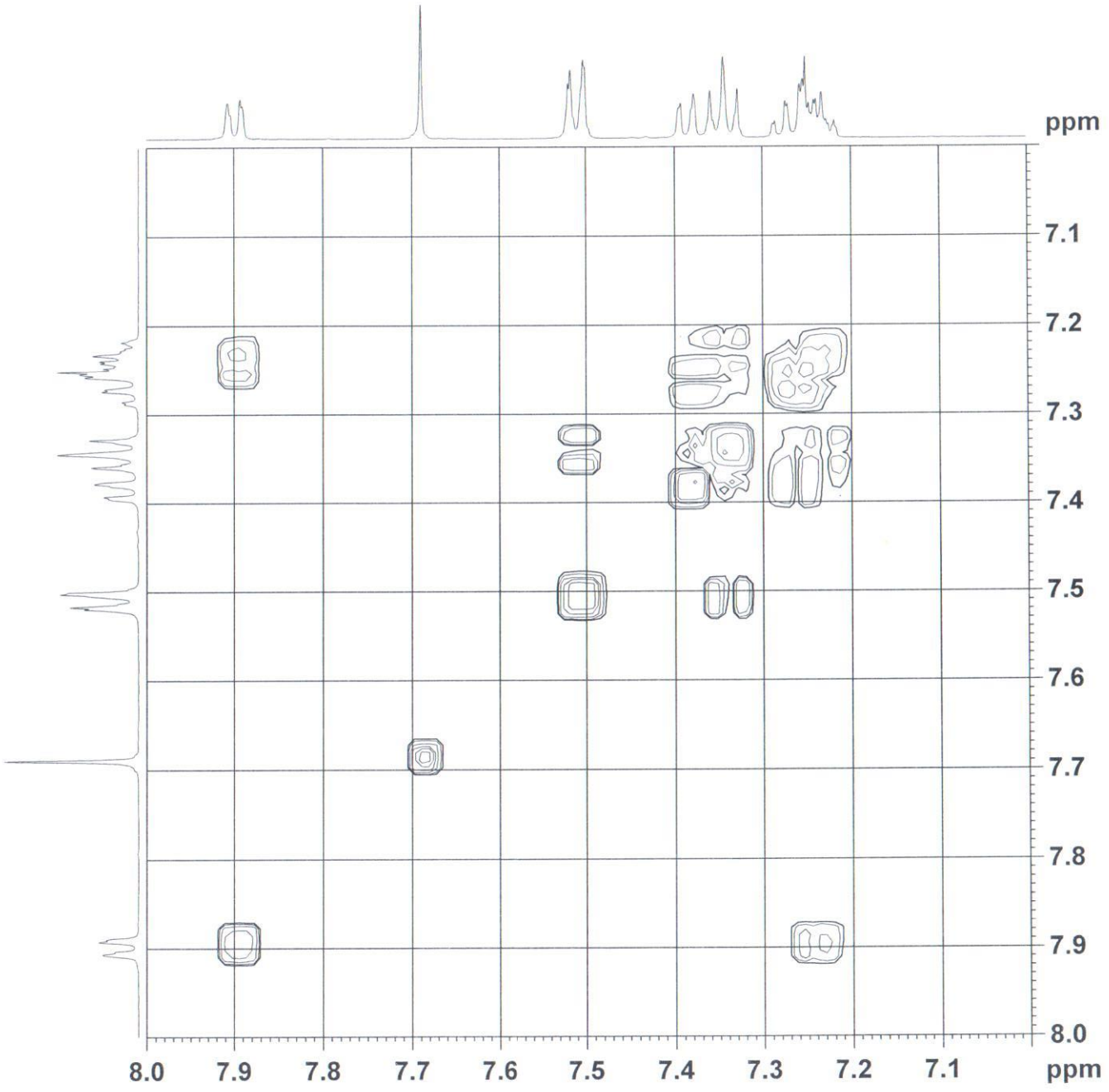
====== GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                       128
SFO1           500.1322 MHz
FIDRES          32.825630 Hz
SW                 8.401 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF           500.1300180 MHz
WDW                   QSINE
SSB          0
LB           0 Hz
GB           0
PC                     1.40

F1 - Processing parameters
SI                      1024
MC2                       QF
SF           500.1300180 MHz
WDW           States-TPPI
SSB          0
LB           0 Hz
GB           0
```

P-233-3196-14-3A
COSY



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```
Current Data Parameters
NAME      P-233-3196-14-3A
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20140903
Time                 14.20
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG       cosygpppqf
TD                   2048
SOLVENT             CDCl3
NS                      1
DS                      8
SWH             4201.681 Hz
FIDRES          2.051602 Hz
AQ              0.2437620 sec
RG                   40.3
DW                119.000 usec
DE                  6.50 usec
TE                 296.0 K
D0              0.00000300 sec
D1              1.90947795 sec
D11             0.03000000 sec
D12             0.00002000 sec
D13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00023800 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          500.1322242 MHz

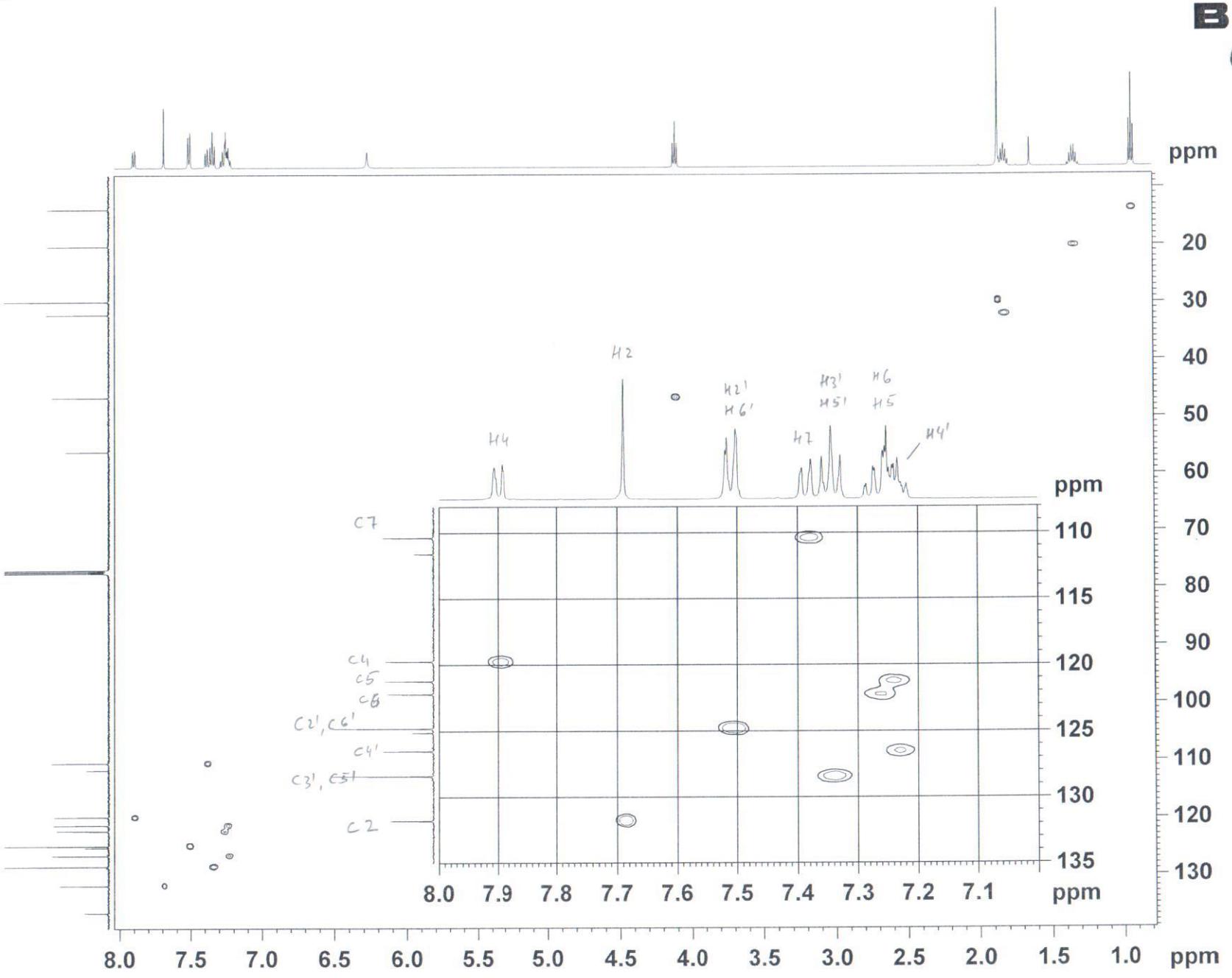
====== GRADIENT CHANNEL =====
GPNAM1         SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     128
SFO1            500.1322 MHz
FIDRES         32.825630 Hz
SW                 8.401 ppm
FnMODE                 QF

F2 - Processing parameters
SI                    1024
SF           500.1300180 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                    QF
SF           500.1300180 MHz
WDW          States-TPPI
SSB       0
LB        0 Hz
GB        0
```

P-233-3196-14-3A
HSQC



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

F2 - Acquisition Parameters
Date_               20140903
Time                   14.49
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG       hsqcetgpsi2
TD                    1024
SOLVENT               CDCl3
NS                       2
DS                      16
SWH              4201.681 Hz
FIDRES           4.103204 Hz
AQ               0.1219060 sec
RG                    2050
DW                119.000 usec
DE                  6.50 usec
TE                 296.2 K
CNST2           145.0000000
D0              0.00000300 sec
D1              1.45494401 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          500.1322242 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

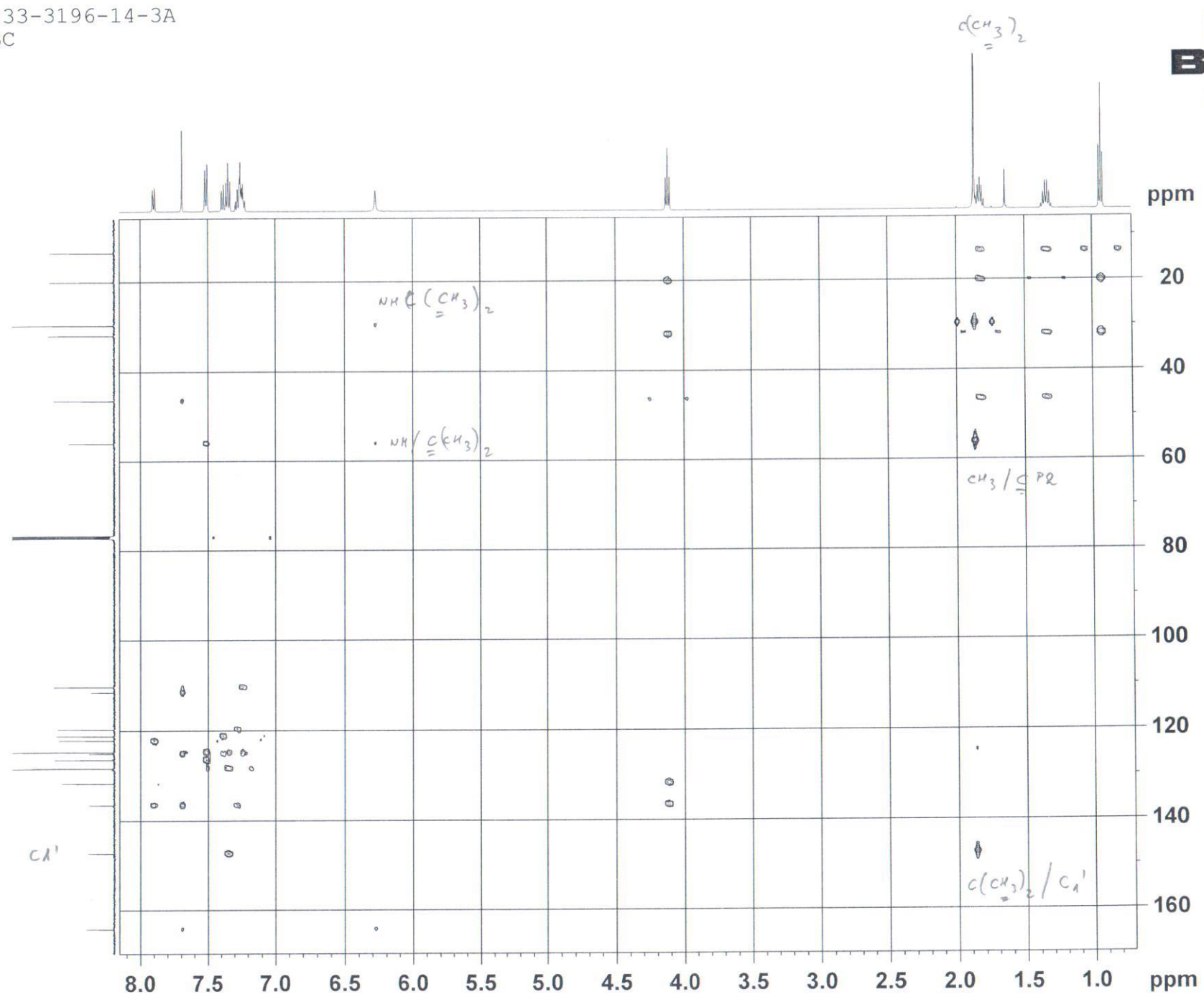
====== GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPNAM2          SMSQ10.100
GPNAM3          SMSQ10.100
GPNAM4          SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
GPZ3                11.00 %
GPZ4                -5.00 %
P16                 1000.00 usec
P19                  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              500.1300180 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-233-3196-14-3A
HMBC



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

F2 - Acquisition Parameters
Date_ 20140903
Time 15.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4201.681 Hz
FIDRES 2.051602 Hz
AQ 0.2437620 sec
RG 2050
DW 119.000 usec
DE 6.50 usec
TE 296.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.41357398 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 500.1322242 MHz

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

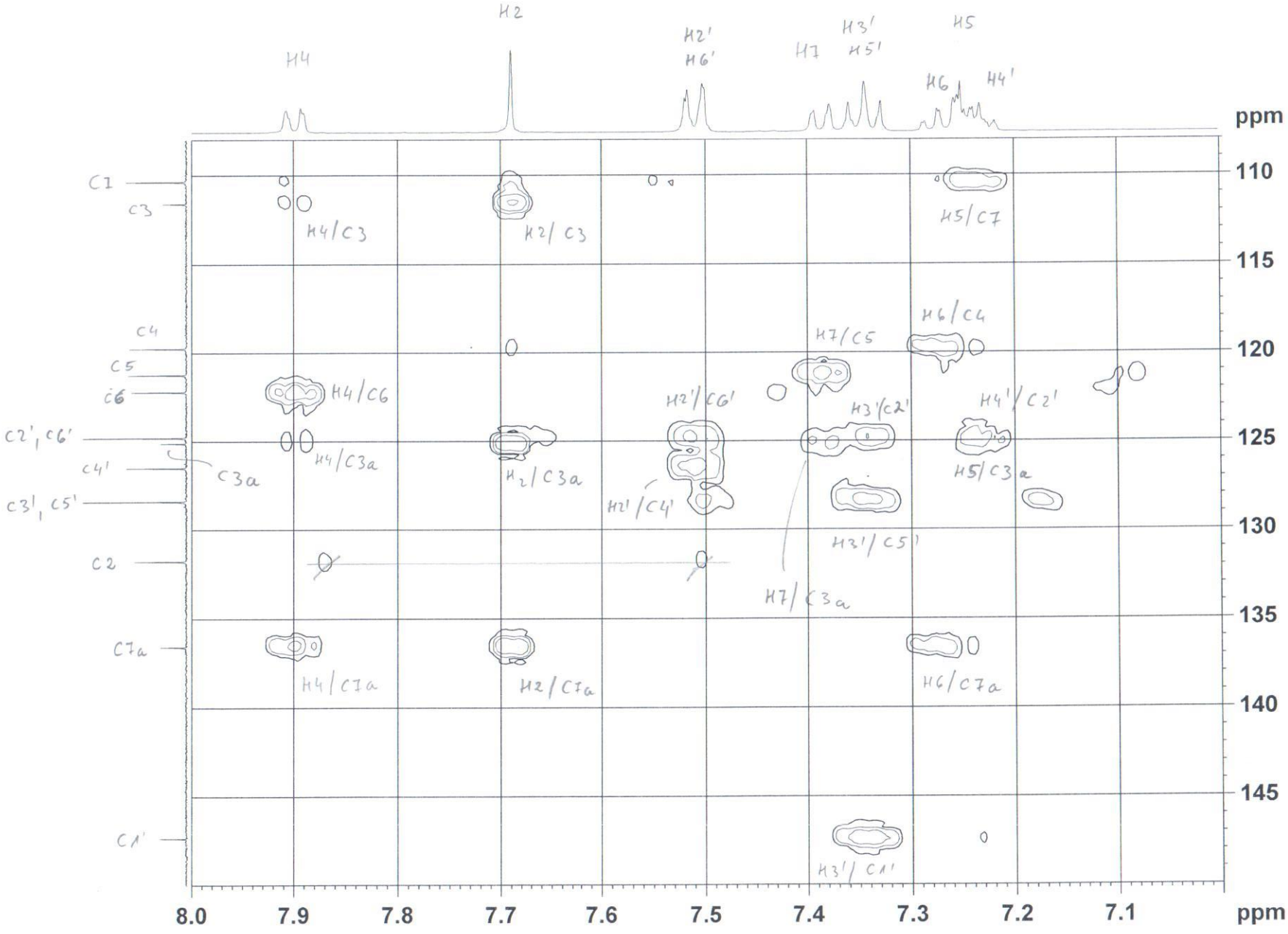
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 125.7703 MHz
FIDRES 109.113174 Hz
SW 222.095 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300180 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-233-3196-14-3A
HMBC



BRUKER

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

F2 - Acquisition Parameters
Date_ 20140903
Time 15.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4201.681 Hz
FIDRES 2.051602 Hz
AQ 0.2437620 sec
RG 2050
DW 119.000 usec
DE 6.50 usec
TE 296.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.41357398 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 500.1322242 MHz

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

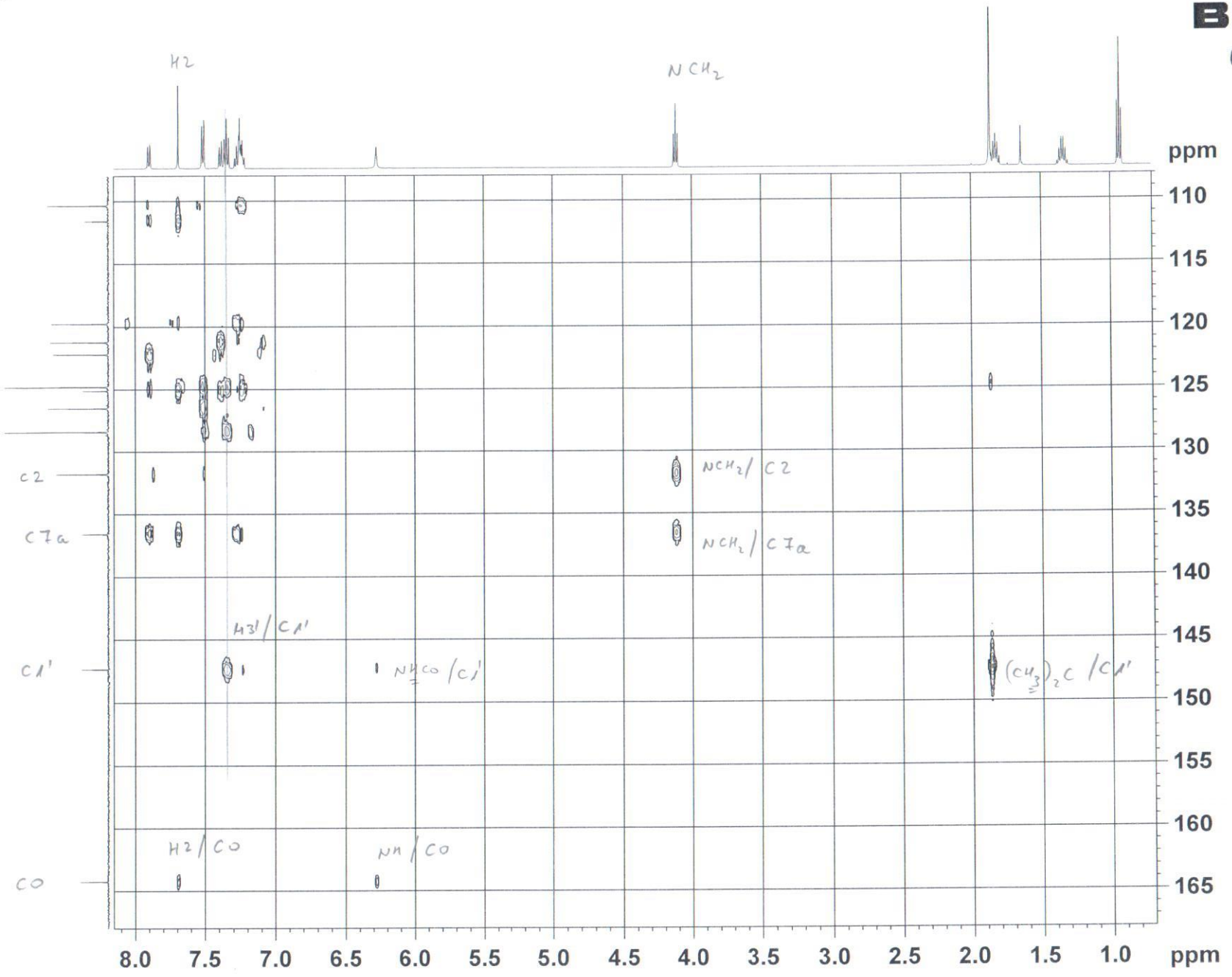
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 125.7703 MHz
FIDRES 109.113174 Hz
SW 222.095 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300180 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-233-3196-14-3A
HMBC



BRUKER

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

F2 - Acquisition Parameters
Date_ 20140903
Time 15.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4201.681 Hz
FIDRES 2.051602 Hz
AQ 0.2437620 sec
RG 2050
DW 119.000 usec
DE 6.50 usec
TE 296.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.41357398 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 500.1322242 MHz

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

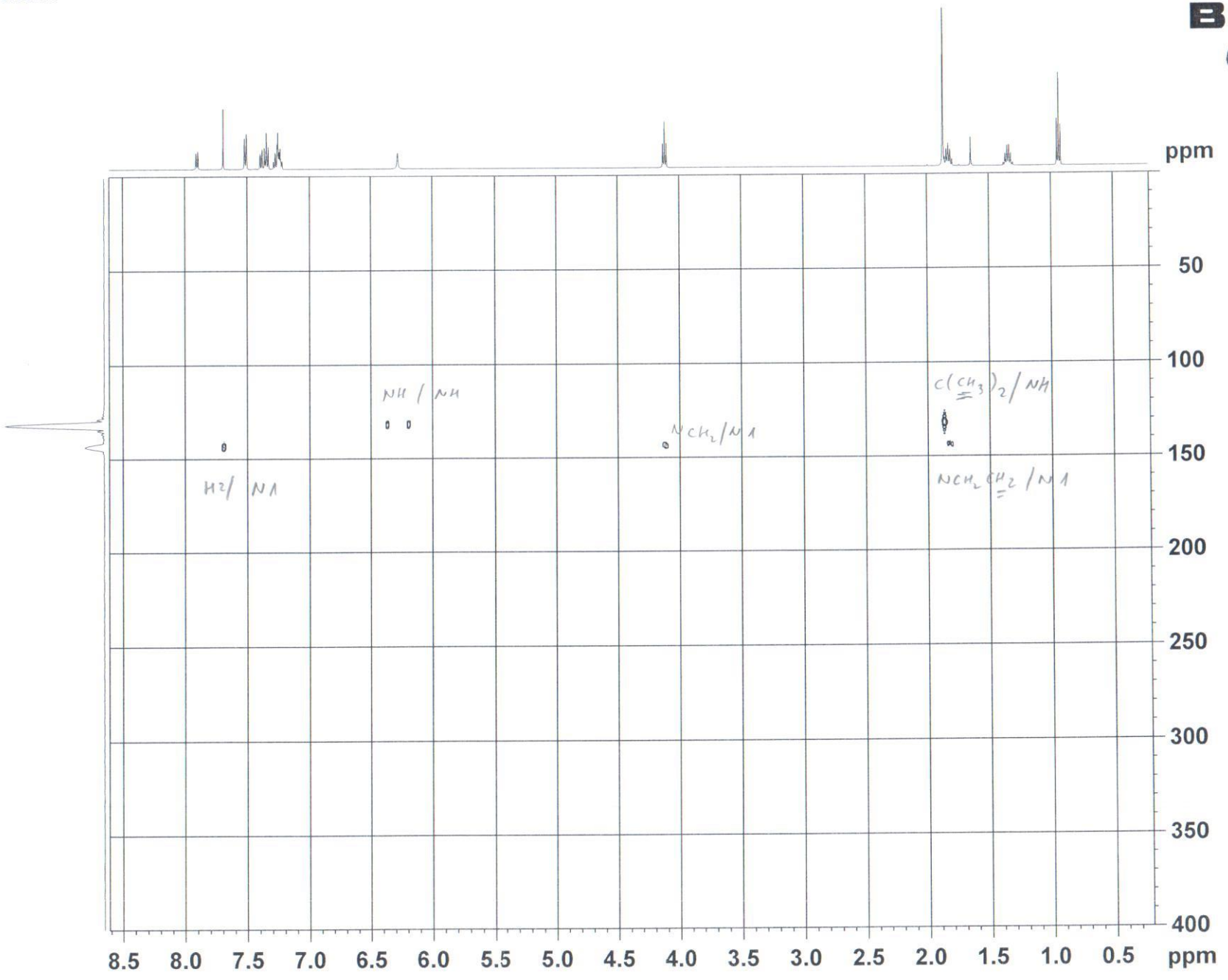
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 125.7703 MHz
FIDRES 109.113174 Hz
SW 222.095 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300180 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-233-3196-14-3A
15N HMBC



BRUKER

Current Data Parameters
NAME P-233-3196-14-3A
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140903
Time 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgpndqf
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 4201.681 Hz
FIDRES 2.051602 Hz
AQ 0.2437620 sec
RG 2050
DW 119.000 usec
DE 6.50 usec
TE 296.0 K
CNST13 5.0000000
D0 0.00000300 sec
D1 1.91357398 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 500.1322242 MHz

======== CHANNEL f2 ========
NUC2 15N
P3 14.40 usec
PLW2 206.00000000 W
SFO2 50.6878685 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 50.68787 MHz
FIDRES 158.391663 Hz
SW 399.980 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300180 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