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

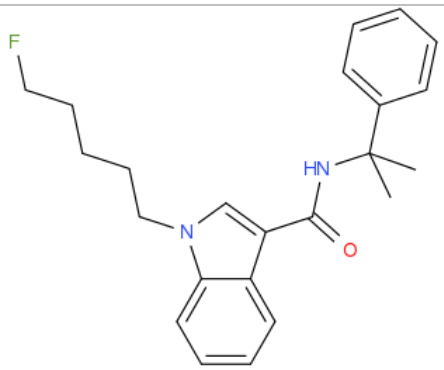
ANALYTICAL REPORT

CUMYL-5FPICA

(C23H27FN2O)

1-(5-fluoropentyl)-N-(2-phenylpropane-2-yl)-1H-indole-3-carboxamide,

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

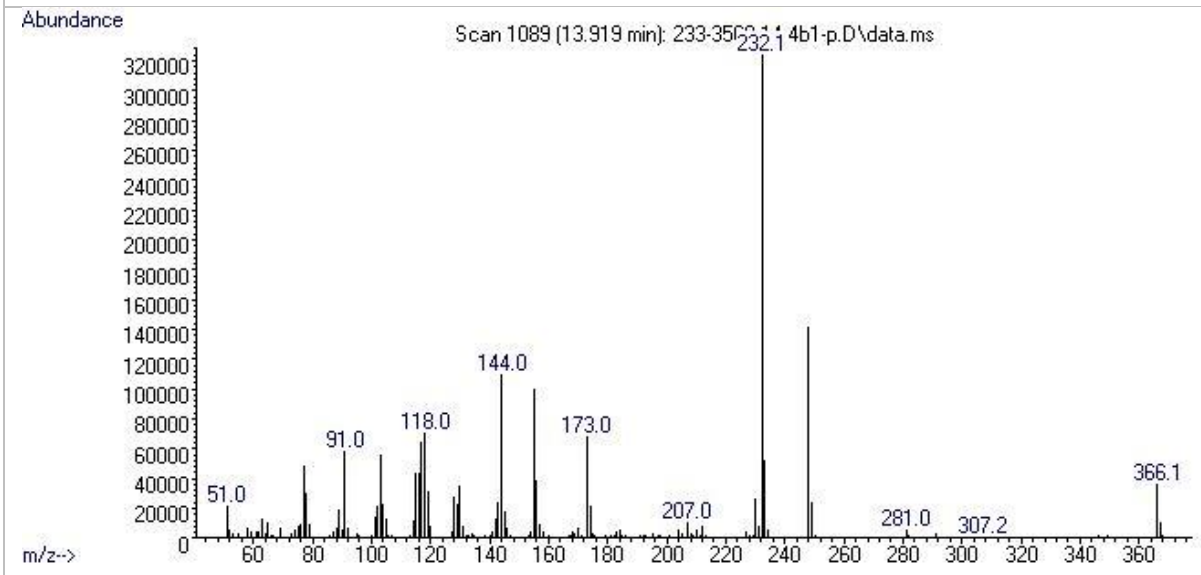
Substance identified-structure[i]	
Systematic name	1-(5-fluoropentyl)-N-(2-phenylpropane-2-yl)-1H-indole-3-carboxamide
Other names	CUMYL-5FPICA ,
Formula (per base form)	C23H27FN2O
M_w (g/mol)	366,47
Salt form	base
Other compounds detected	
Smiles	FCCCCCN1C=C(C2=CC=CC=C12)C(=O)NC(C)(C)C1=CC=CC=C1
Compound 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.

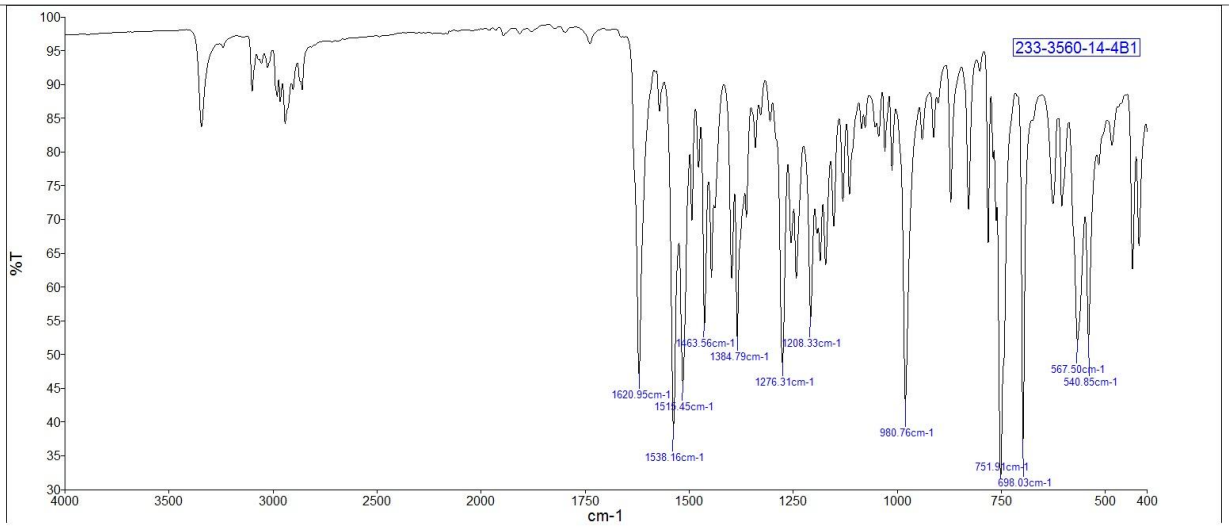
Supporting information

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

MS spectrum (EI)



FTIR - ATR



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

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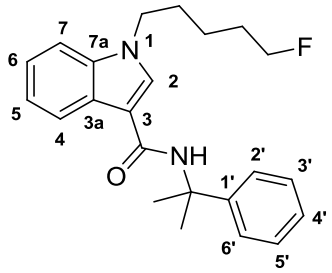
Dr. Janez Košmrlj
Professor of Organic Chemistry

September 17, 2014

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

Dear Dr. Sonja Klemenc,

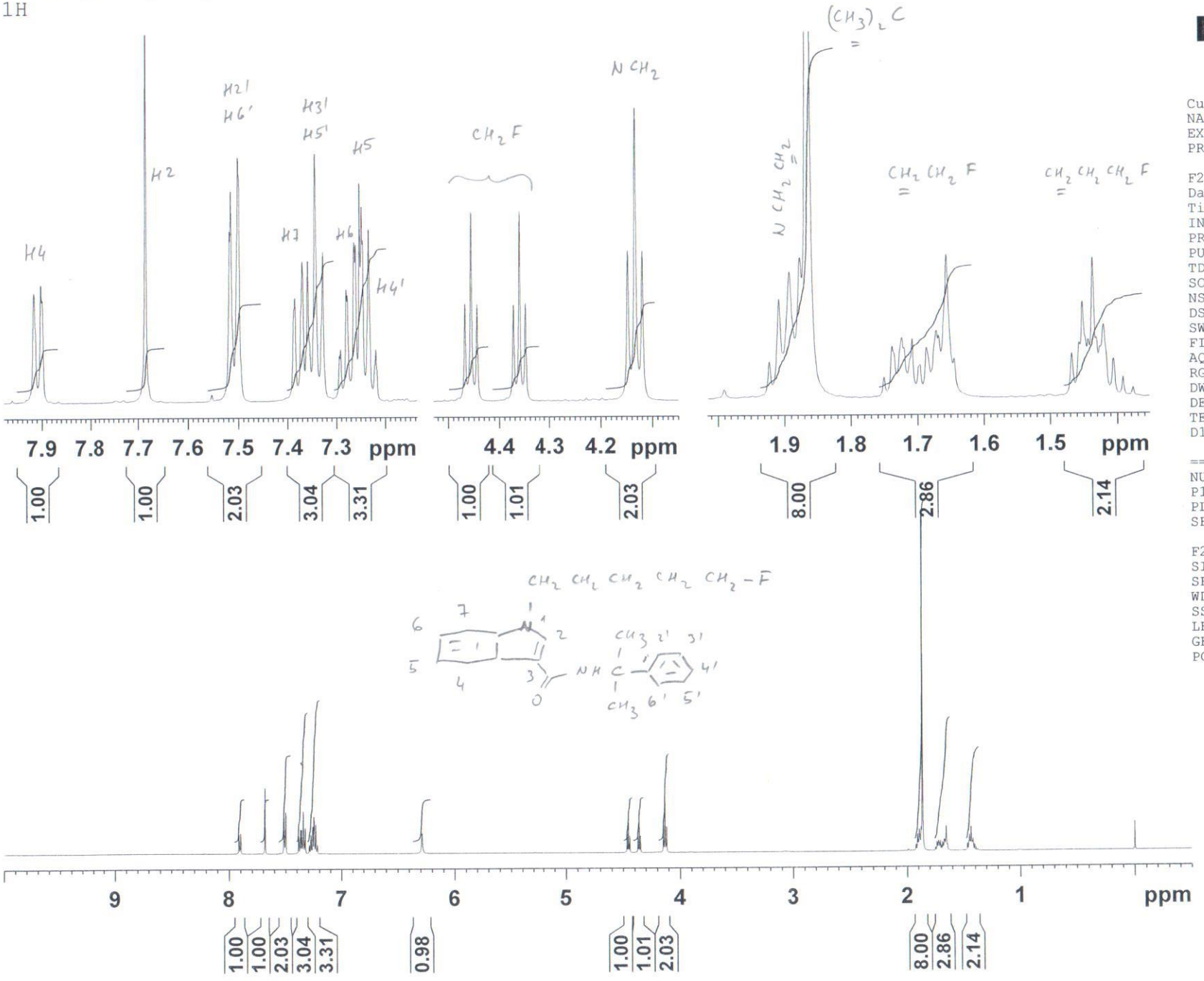
Please find enclosed the results of the structure elucidation for the sample:

Sample ID:	**233-3560-14-4B1**
Received date:	September 1, 2014
Our notebook code:	P-233-3196-14-4B1
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: $C_{23}H_{27}FN_2O$ Exact Mass: 366.2107 Molecular Weight: 366.4717
Chemical name:	1-(5-Fluoropentyl)-*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 2-11)

Sincerely,

Janez Košmrlj

P-233-3196-14-4B1
1H



BRUKER

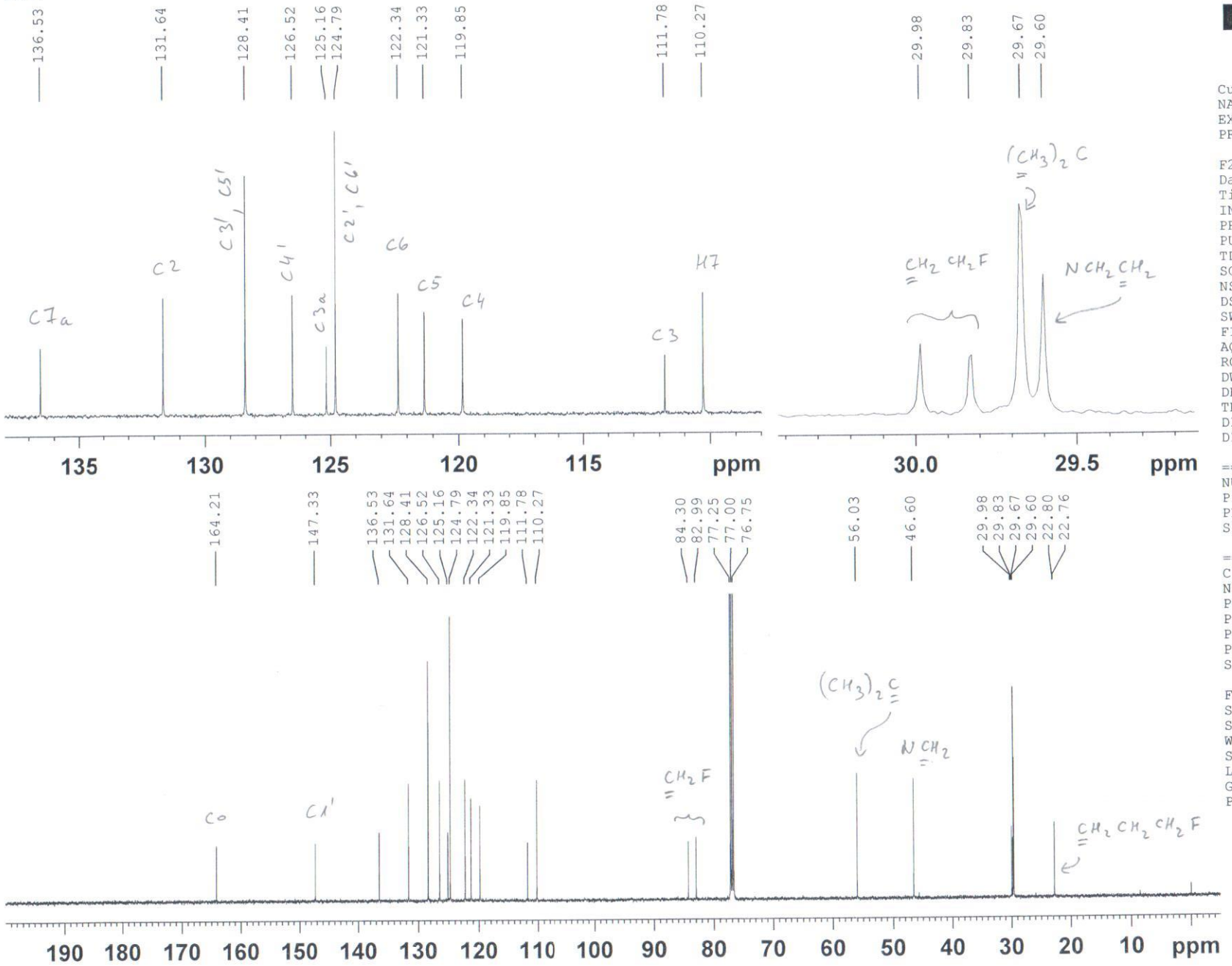
Current Data Parameters
NAME P-233-3196-14-4B1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 1.47
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 500.1300176 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P-233-3196-14-4B1
13C



Current Data Parameters
NAME P-233-3196-14-4B1
EXPNO 6
PROCNO 1

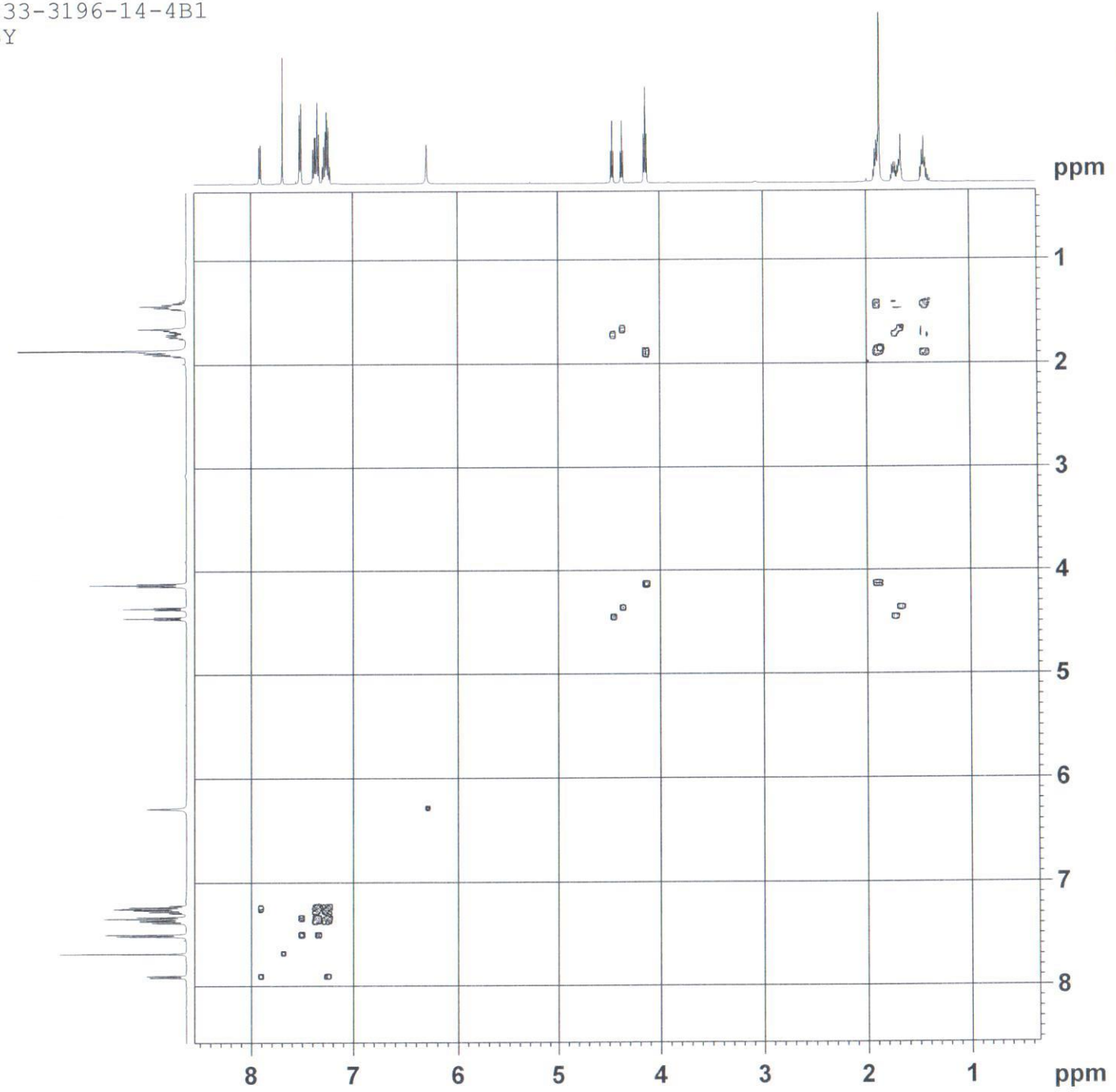
F2 - Acquisition Parameters
Date_ 20140904
Time_ 6.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec

======== 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 125.7577961 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

P-233-3196-14-4B1
COSY



BRUKER

Current Data Parameters
NAME P-233-3196-14-4B1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 1.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 4237.288 Hz
FIDRES 2.068988 Hz
AQ 0.2417140 sec
RG 40.3
DW 118.000 usec
DE 6.50 usec
TE 296.0 K
D0 0.00000300 sec
D1 1.91152596 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00023600 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 500.1323054 MHz

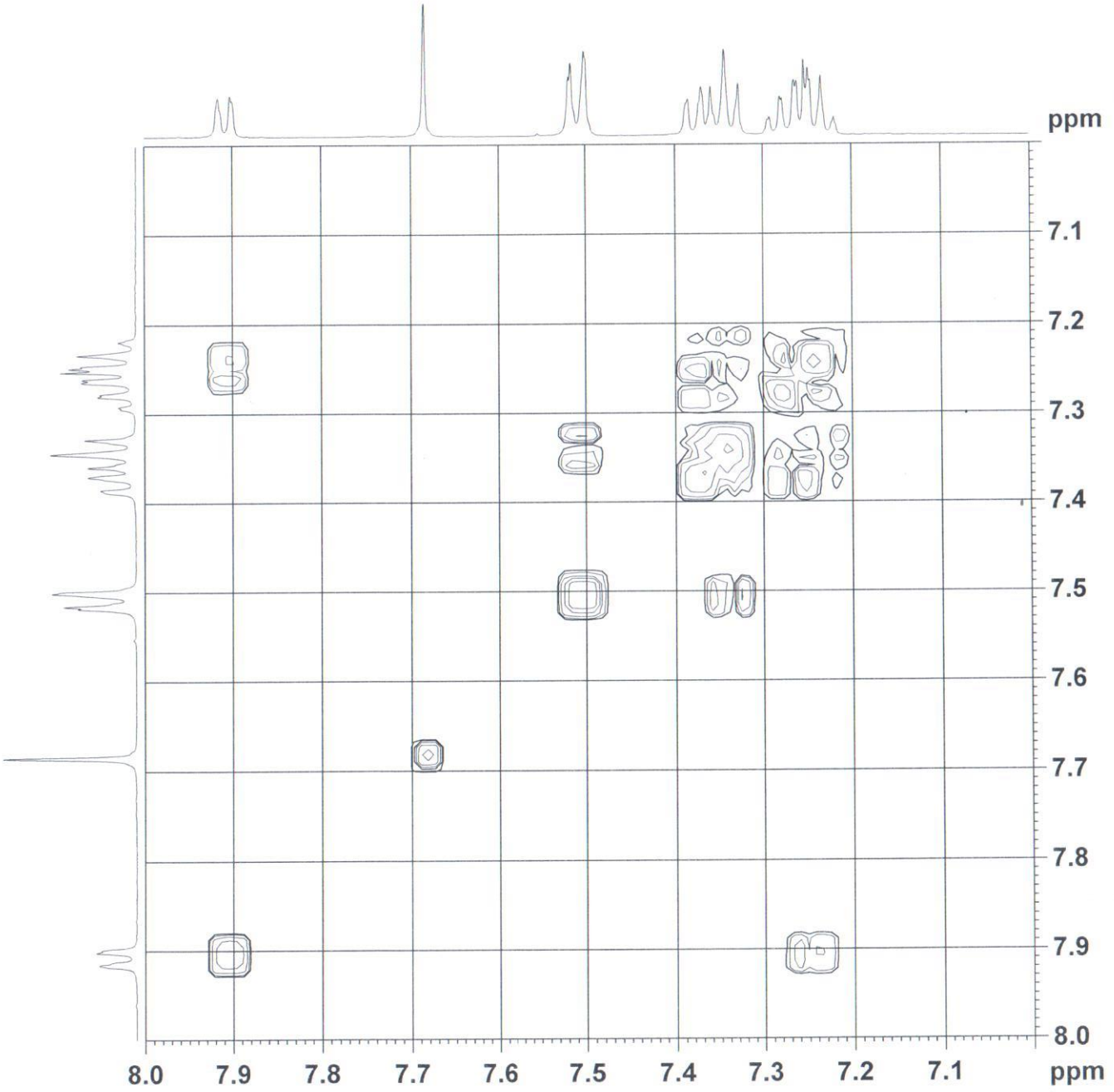
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 500.1323 MHz
FIDRES 33.103813 Hz
SW 8.472 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 500.1300176 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300176 MHz
WDW States-TPPI
SSB 0
LB 0 Hz
GB 0

P-233-3196-14-4B1
COSY



BRUKER

Current Data Parameters
NAME P-233-3196-14-4B1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 1.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 4237.288 Hz
FIDRES 2.068988 Hz
AQ 0.2417140 sec
RG 40.3
DW 118.000 usec
DE 6.50 usec
TE 296.0 K
D0 0.00000300 sec
D1 1.91152596 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00023600 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 500.1323054 MHz

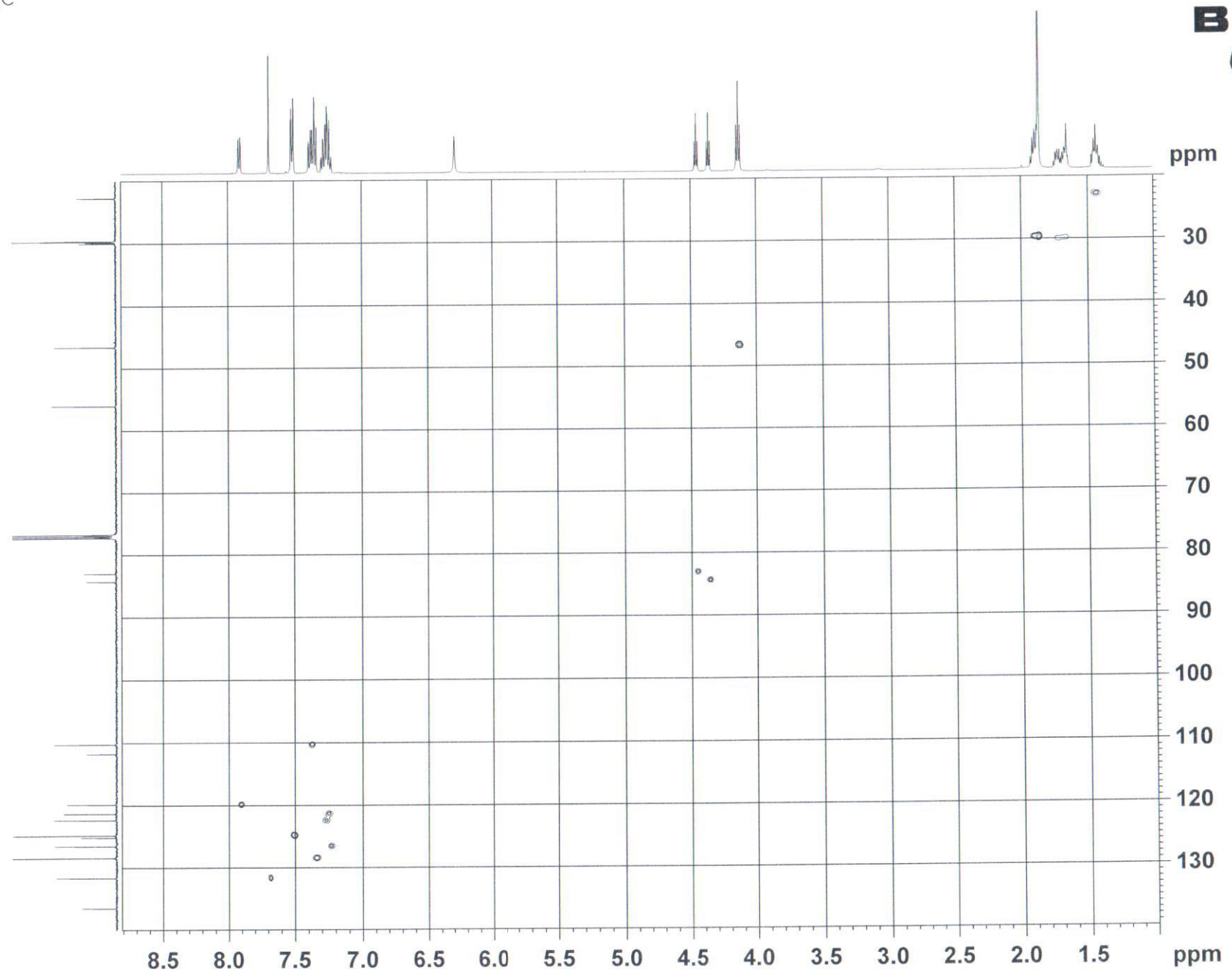
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 500.1323 MHz
FIDRES 33.103813 Hz
SW 8.472 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 500.1300176 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300176 MHz
WDW States-TPPI
SSB 0
LB 0 Hz
GB 0

P-233-3196-14-4B1
HSQC



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Current Data Parameters
NAME          P-233-3196-14-4B1
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140904
Time                      2.38
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG          hsqcetgpsi2
TD                        1024
SOLVENT                 CDCl3
NS                           2
DS                          16
SWH                4237.288 Hz
FIDRES             4.137977 Hz
AQ                 0.1208820 sec
RG                        2050
DW                  118.000 usec
DE                    6.50 usec
TE                    296.1 K
CNST2              145.0000000
D0                 0.00000300 sec
D1                 1.45596802 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             500.1323054 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

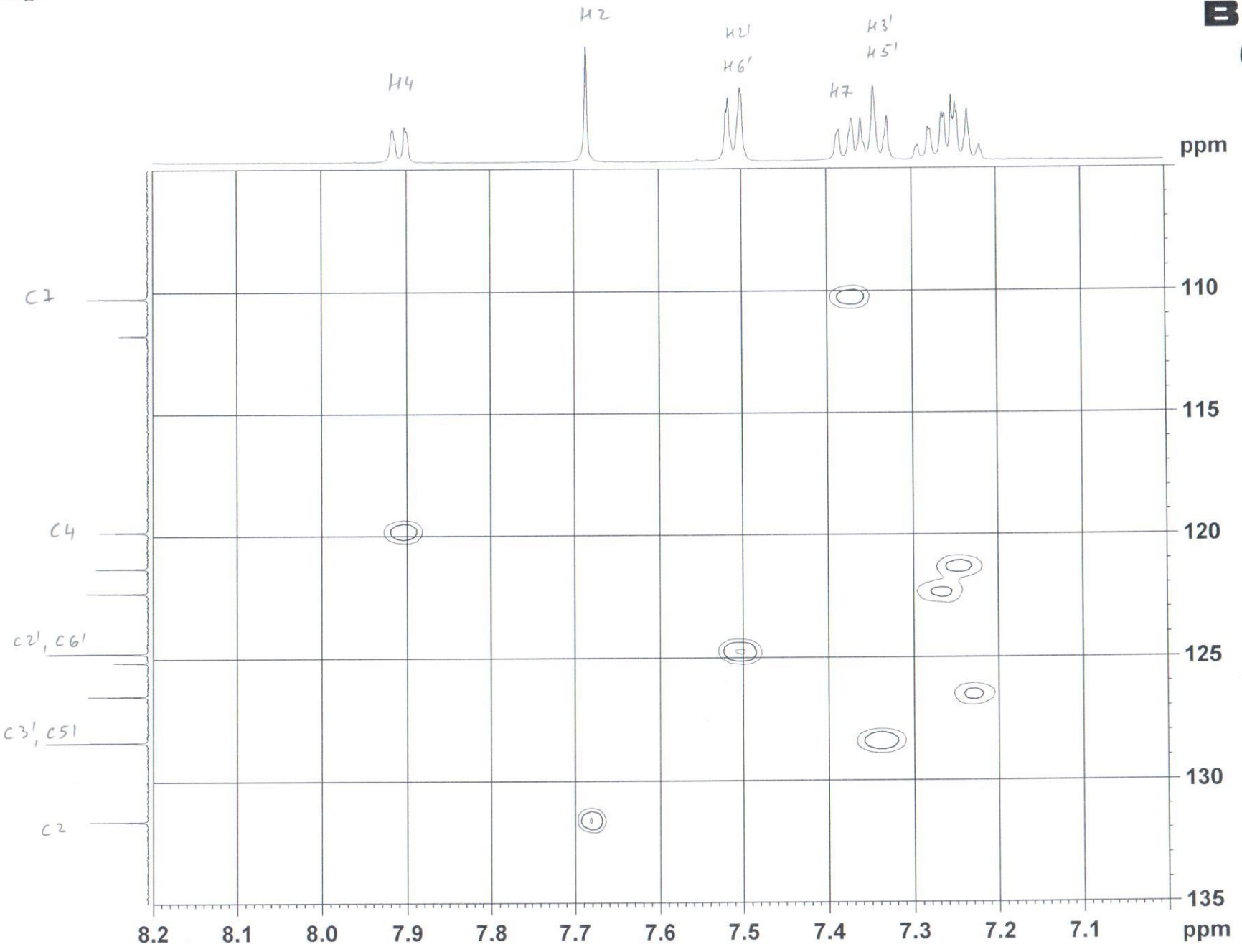
====== GRADIENT CHANNEL =====
GPNAM1          SMSQ10.100
GPNAM2          SMSQ10.100
GPNAM3          SMSQ10.100
GPNAM4          SMSQ10.100
GPZ1                 80.00 %
GPZ2                 20.10 %
GPZ3                 11.00 %
GPZ4                 -5.00 %
P16                1000.00 usec
P19                 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               500.1300176 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-233-3196-14-4B1
HSQC



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Current Data Parameters
NAME P-233-3196-14-4B1
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 2.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hsqcetgpsi2
TD 1024
SOLVENT CDCl3
NS 2
DS 16
SWH 4237.288 Hz
FIDRES 4.137977 Hz
AQ 0.1208820 sec
RG 2050
DW 118.000 usec
DE 6.50 usec
TE 296.1 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.45596802 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 500.1323054 MHz

======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 9.00 usec
P4 18.00 usec
PCPD2 70.00 usec
PLW2 122.0000000 W
PLW12 2.01670003 W
SFO2 125.7672177 MHz

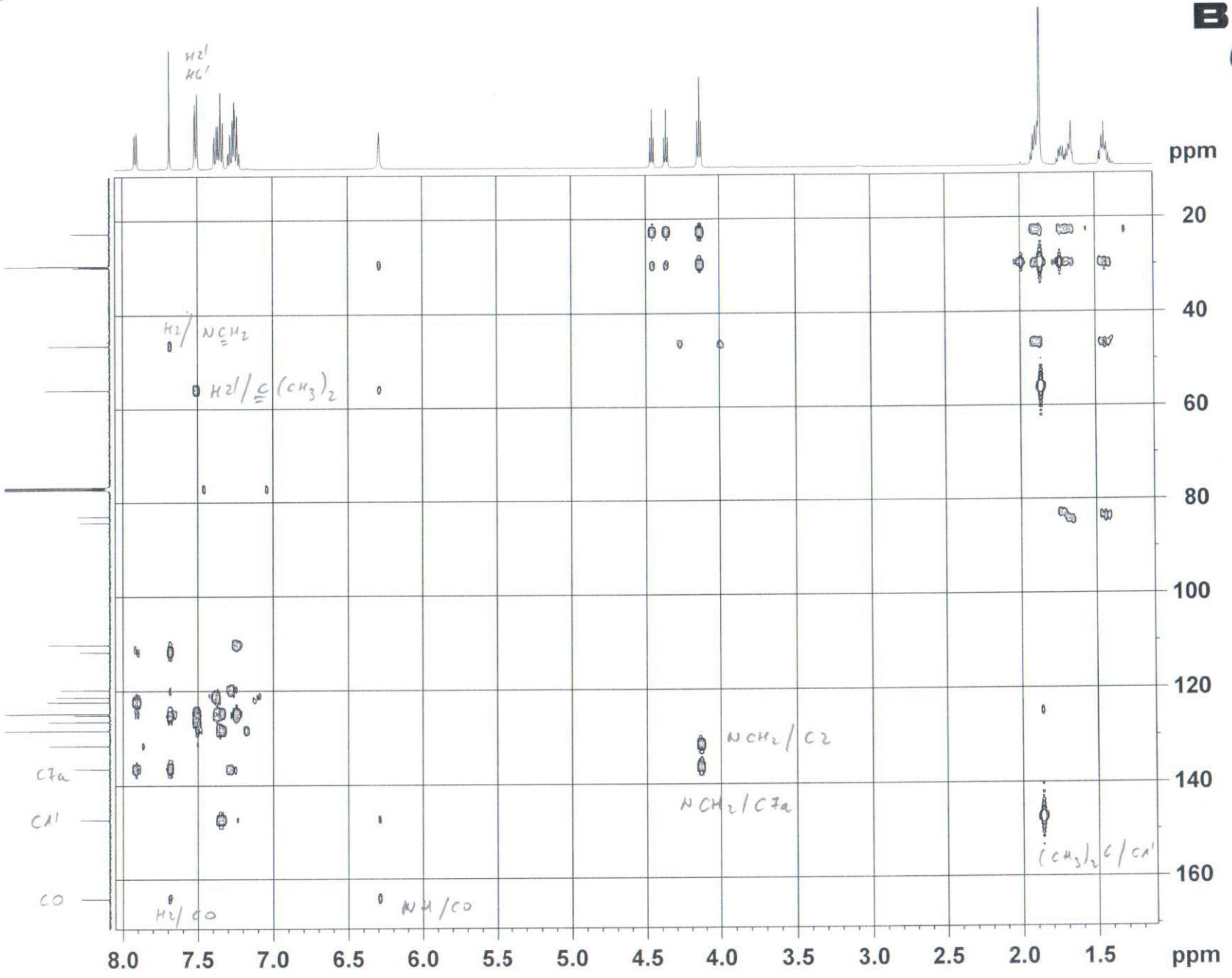
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPNAM4 SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

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 500.1300176 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-233-3196-14-4B1
HMBC



BRUKER

Current Data Parameters
NAME P-233-3196-14-4B1
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 3.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4237.288 Hz
FIDRES 2.068988 Hz
AQ 0.2417140 sec
RG 2050
DW 118.000 usec
DE 6.50 usec
TE 296.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.41562200 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 500.1323054 MHz

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

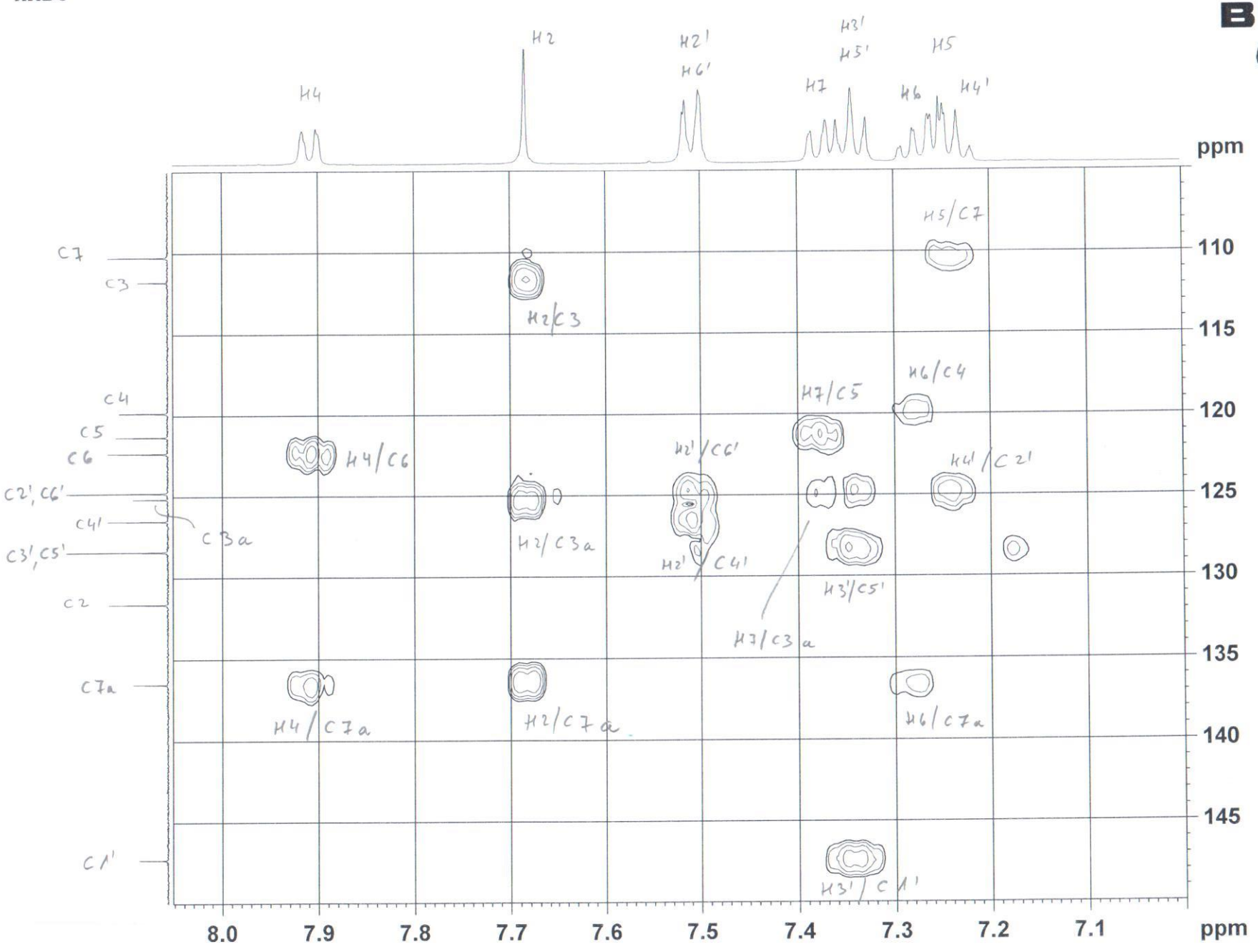
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

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 500.1300176 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-233-3196-14-4B1
HMBC



BRUKER

Current Data Parameters
NAME P-233-3196-14-4B1
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 3.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4237.288 Hz
FIDRES 2.068988 Hz
AQ 0.2417140 sec
RG 2050
DW 118.000 usec
DE 6.50 usec
TE 296.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.41562200 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 500.1323054 MHz

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

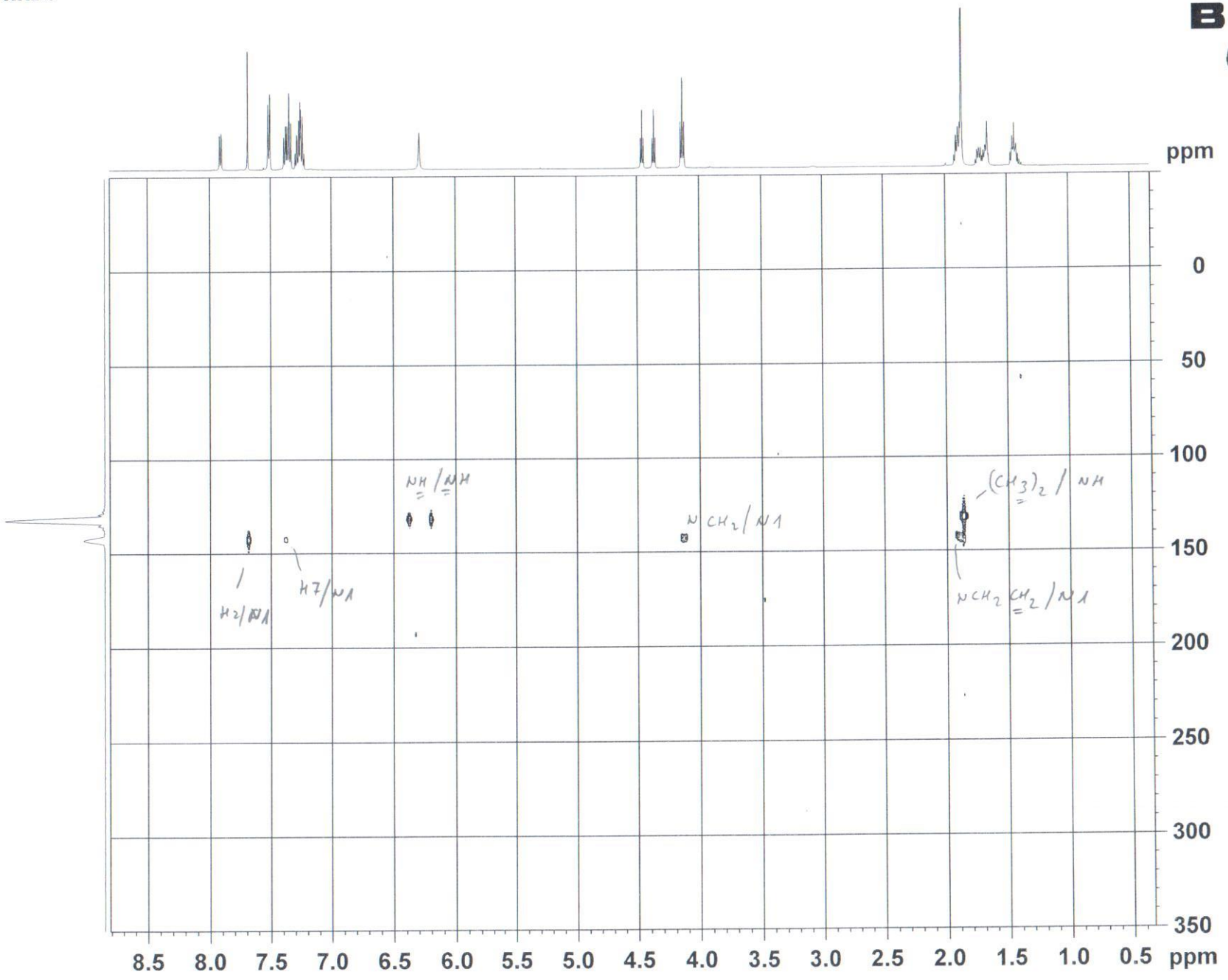
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

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 500.1300176 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-233-3196-14-4B1
15N HMBC



BRUKER

Current Data Parameters
NAME P-233-3196-14-4B1
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 4.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgpndqf
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 4237.288 Hz
FIDRES 2.068988 Hz
AQ 0.2417140 sec
RG 2050
DW 118.000 usec
DE 6.50 usec
TE 296.0 K
CNST13 5.0000000
D0 0.00000300 sec
D1 1.91562200 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 500.1323054 MHz

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

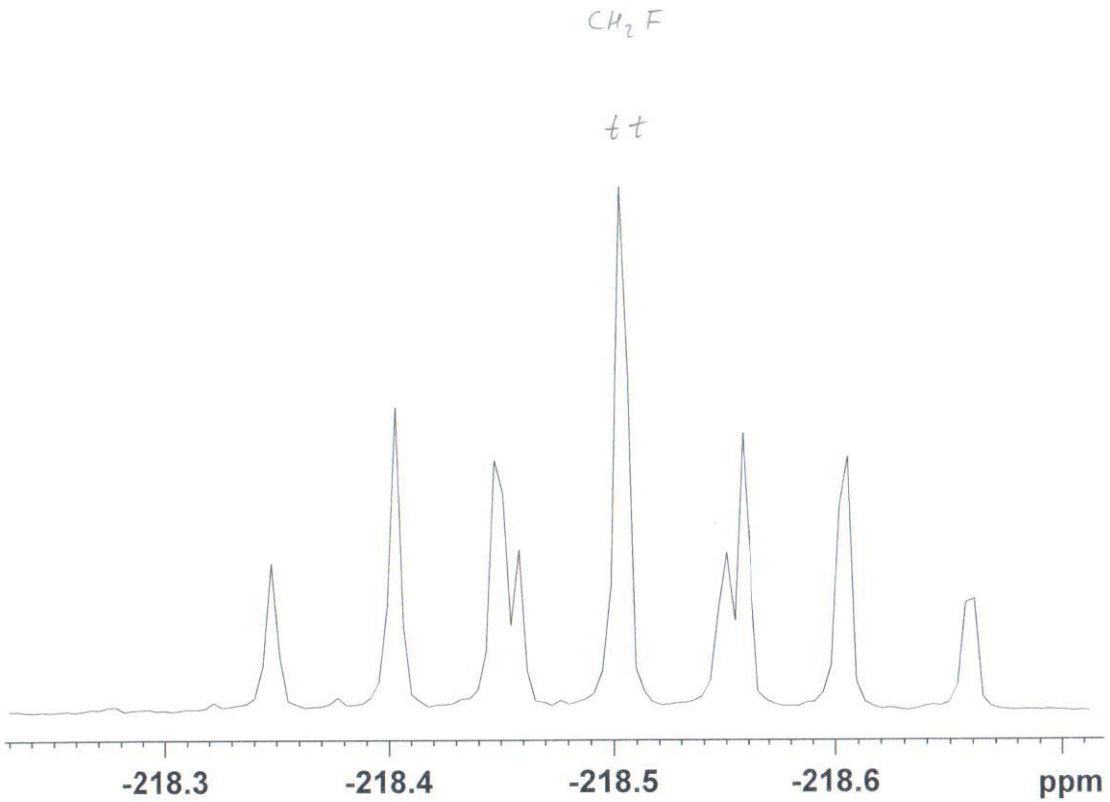
====== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPZ1 70.00 %
GPZ2 30.00 %
GPZ3 50.10 %
P16 1000.00 usec

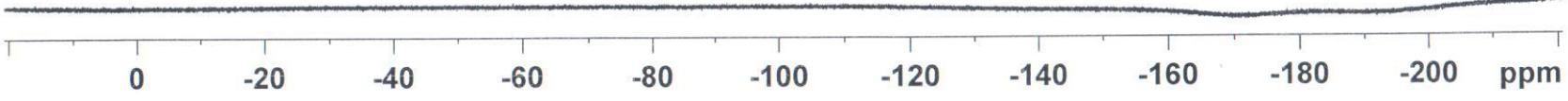
F1 - Acquisition parameters
TD 128
SFO1 50.68533 MHz
FIDRES 158.391663 Hz
SW 400.000 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300176 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-233-3196-14-4B1
13C





Current Data Parameters

NAME	P-233-3196-14-4B1
EXPNO	7
PROCNO	1

F2 - Acquisition Parameters

Date_	20140904
Time	6.11
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	295.7 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