



ANALYTICAL REPORT

CUMYL-THPINACA

(C23H27N3O2)

N-(2-phenylpropan-2-yl)-1-((tetrahydro-2H-pyran-4-yl)methyl)-1H-indazole-3-carboxamide,

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

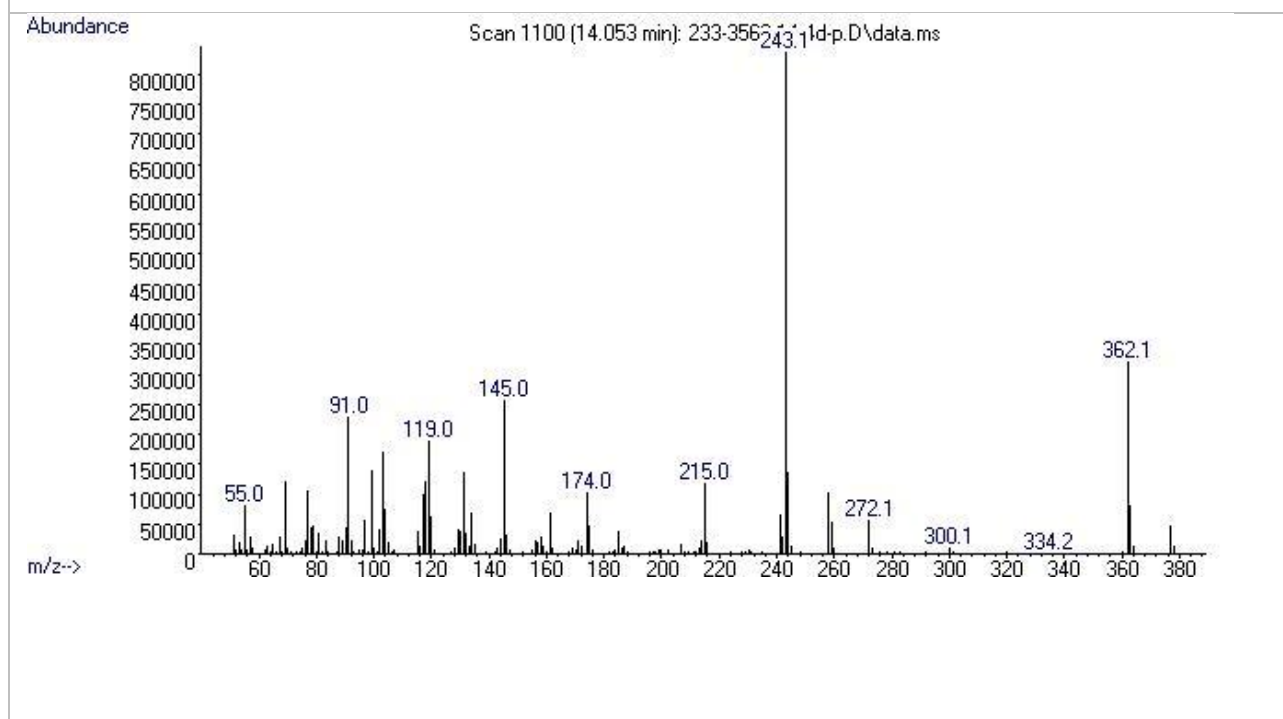
Substance identified- structure ⁱ	
Systematic name	N-(2-phenylpropan-2-yl)-1-((tetrahydro-2H-pyran-4-yl)methyl)-1H-indazole-3-carboxamide
Other names	CUMYL-THPINACA ,
Formula (per base form)	C23H27N3O2
M _w (g/mol)	377,48
Salt form	base
Other compounds detected	
Smiles	<chem>C1(=CC=CC=C1)C(C)(C)NC(=O)C1=NN(C2=CC=CC=C2)CC1CCOCC1</chem>
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.

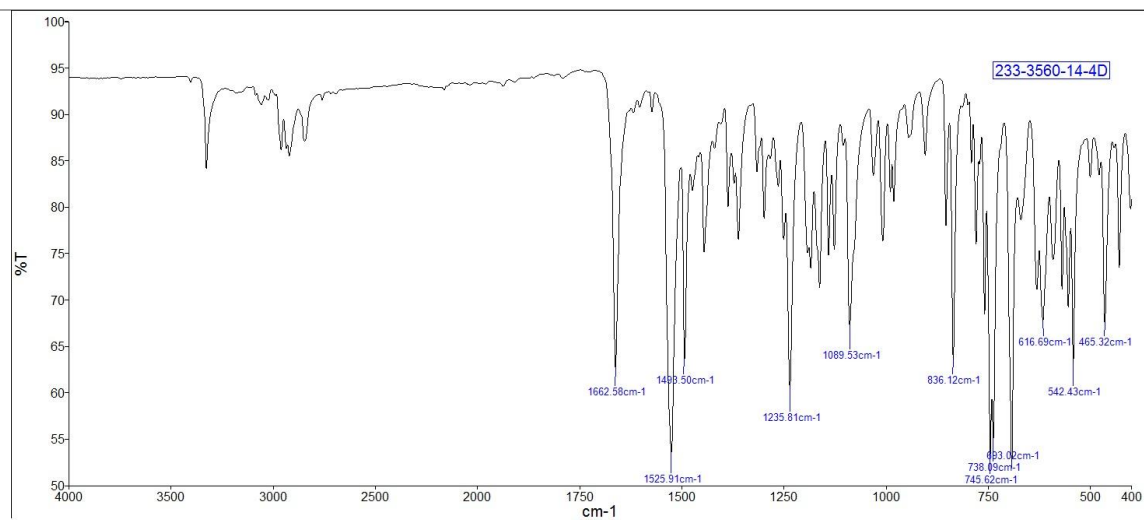
Supporting information

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



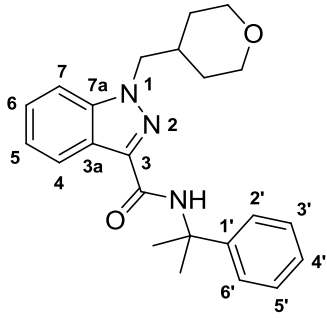
Dr. Janez Košmrlj
Professor of Organic Chemistry

September 17, 2014

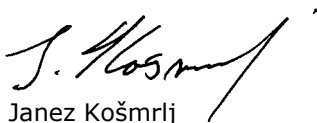
Dr. Sonja Klemenc
Head of Chemistry Department
Vodovodna 95
1000 Ljubljana
Slovenija

Dear Dr. Sonja Klemenc,

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

Sample ID:	233-3560-14-4D
Received date:	September 1, 2014
Our notebook code:	P-233-3196-14-4D
NMR sample preparation:	15 mg dissolved in 0.7 mL CDCl ₃
NMR experiments:	¹ H, ¹³ C, ¹ H- ¹ H <i>gs</i> -COSY, ¹ H- ¹³ C <i>gs</i> -HSQC, ¹ H- ¹³ C <i>gs</i> -HMBC, ¹ H- ¹⁵ N <i>gs</i> -HMBC
Proposed structure with atom numbering scheme, formula, exact mass, molecular weight:	 <p>Chemical Formula: C₂₃H₂₇N₃O₂ Exact Mass: 377.2103 Molecular Weight: 377.4794</p>
Chemical name:	<i>N</i> -(2-Phenylpropan-2-yl)-1-((tetrahydro-2 <i>H</i> -pyran-4-yl)methyl)-1 <i>H</i> -indazole-3-carboxamide
Comments:	<ul style="list-style-type: none"> - 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 2-8)

Sincerely,


Janez Košmrlj

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

H₆
H₇ H_{3'}
NH H_{5'}

H_{2'}

H_{6'}

H_{4'}

H₅

H₄

NCH₂

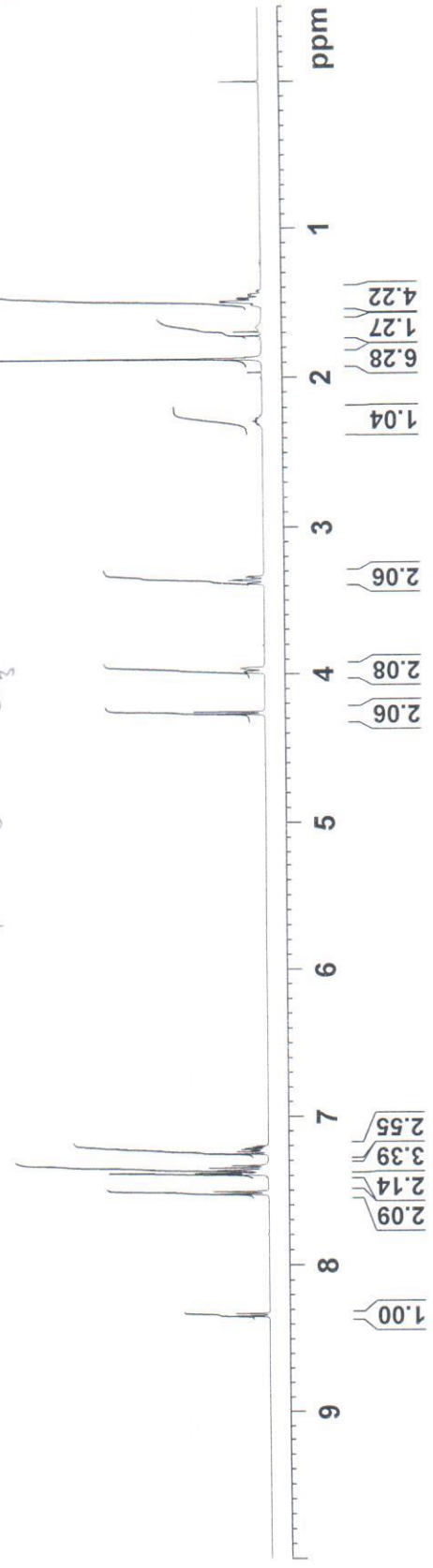
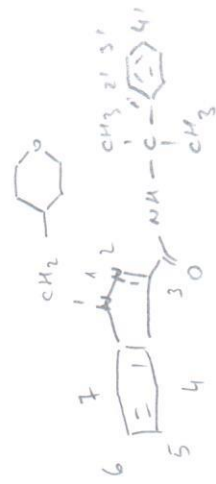
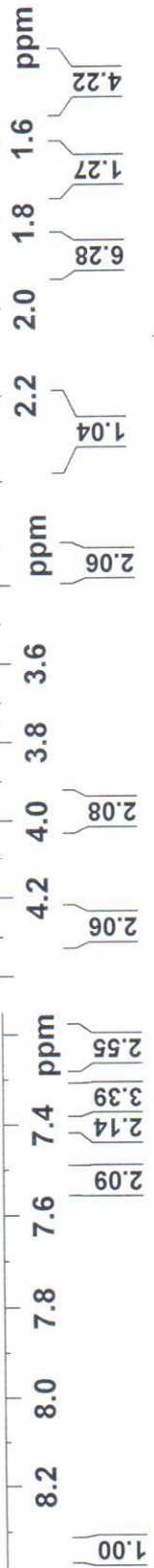
CH₂O

CH₂O

NCH₂CH=

(CH₃)₂C

CH(CH₂)₂



Current Data Parameters
NAME P-233-3196-14-4D
EXNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140903
Time 18.35
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

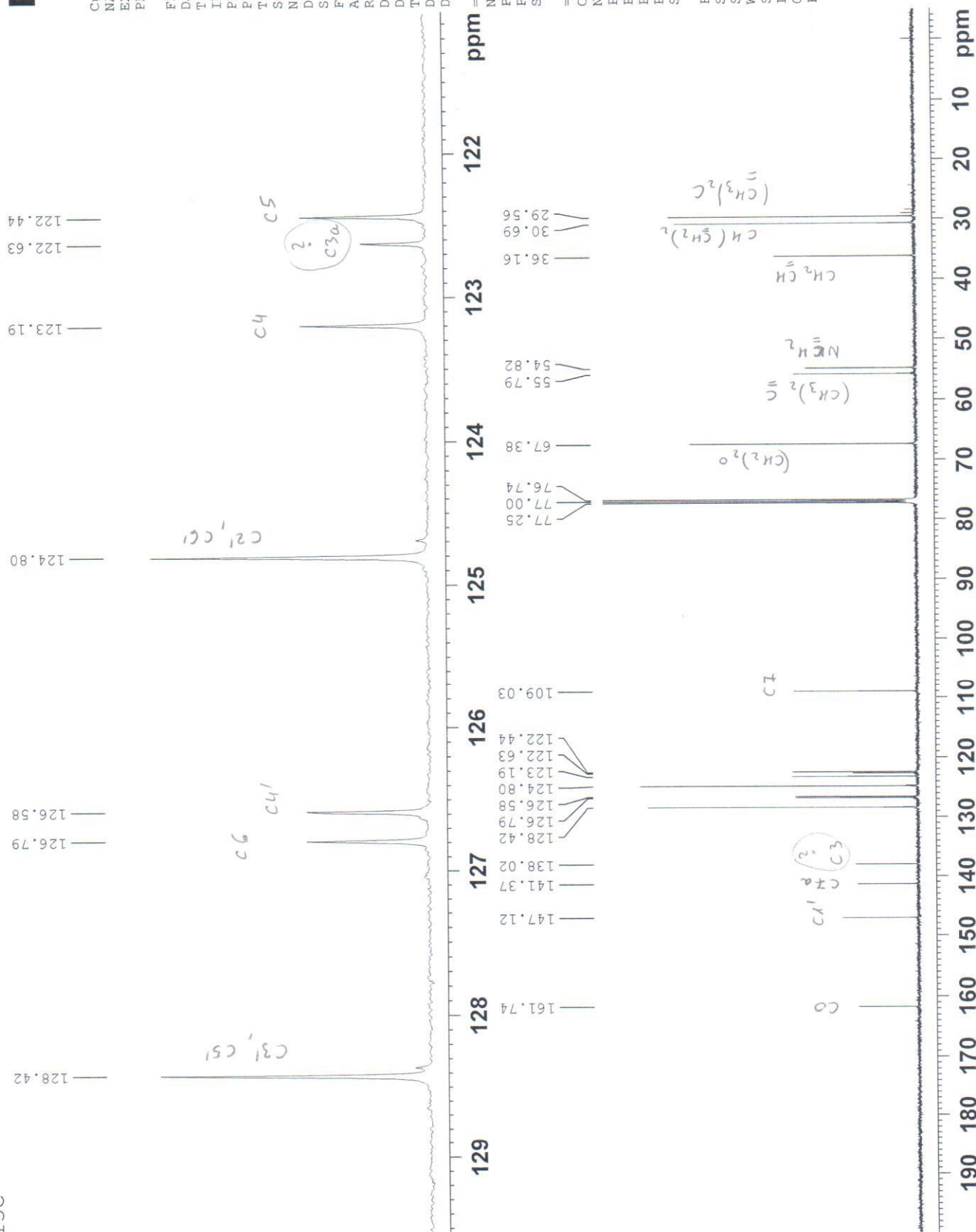
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SI 65536
SF 500.1300157 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F2 - Acquisition Parameters	
Date_	20140903
Time	21.46
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 =====
13C
NUC1
P1 9.00 usec
P1W1 122.00000000 W
SF01 125.7703637 MHz

===== CHANNEL f2 =====
IH
waltz16
80.00 usec
NUC2
PCPD2 26.00000000 W
PLW2 0.32179001 W
PLW12 0.20595001 W
PLW13 0.20595001 W
SF02 500.1320005 MHz
```

F2 - Processing parameters	
SI	32768
SF	125.757961 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40





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

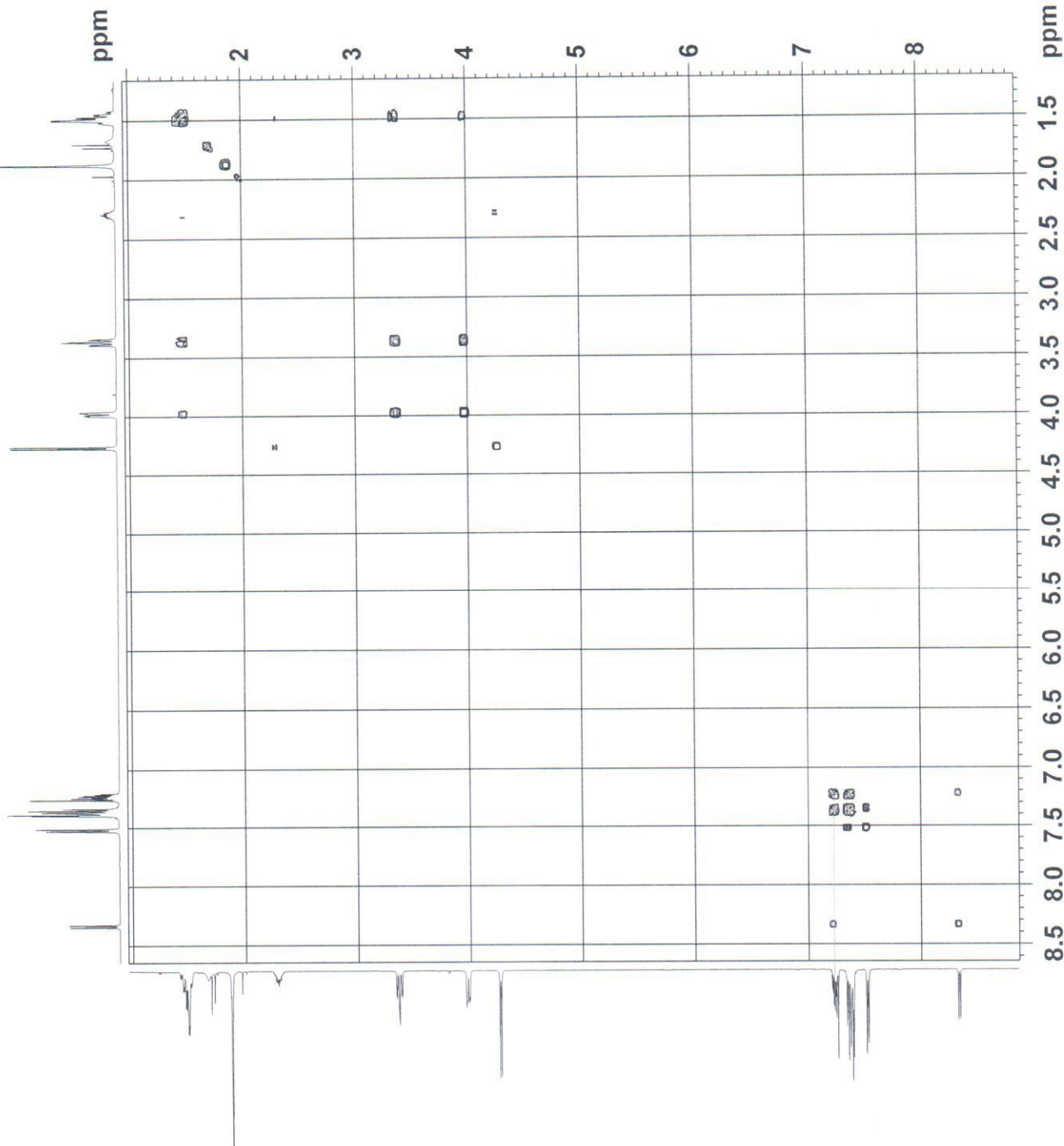
F2 - Acquisition Parameters
Date_ 20140903
Time 18.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosypppqf
TD 2048
SOLVENT CDC13
NS 1
DS 8
SWH 4807.692 Hz
FIDRES 2.347506 Hz
AQ 0.2130420 sec
RG 40.3
DW 104.000 usec
DE 6.50 usec
TE 296.0 K
D0 0.0000300 sec
D1 1.94019794 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00020800 sec

===== CHANNEL f1 =====
NUC1 1H
P0 8.90 usec
P1 8.90 usec
PL7 2500.00 usec
PLW1 26.00000000 W
PLW10 3.04649997 W
SFO1 500.1321146 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 500.1321 MHz
FIDRES 37.560097 Hz
SW 9.613 ppm
FMODE QF

F2 - Processing parameters
SI 1024
SF 500.1300157 MHz
WDW QSI
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300157 MHz
WDW States-TPPI
SSB 0
LB 0 Hz
GB 0





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

F2 - Acquisition Parameters
Date_ 20140525
Time 19.09

NUC1 1H
NUC2 13C

PROBHD 5 mm PABBO BB-
PULPROG hsqcetps12
TD 1024
SOLVENT CDCl3

NS 12
DS 4807.692 Hz
SWHRES 4.695012 Hz
AQ 0.1065460 sec
RG 2050
DE 104.000 usec
TE 296.2 K

CNS12 145.0000000 sec
D0 1.00000000 sec
D1 1.47030401 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
D24 0.00086207 sec
ZGPTNS 0.00002400 sec

CHANNEL f1 1H
CHANNEL f2 13C

CPDPRG2 gaip
NUC1 1H
NUC2 13C

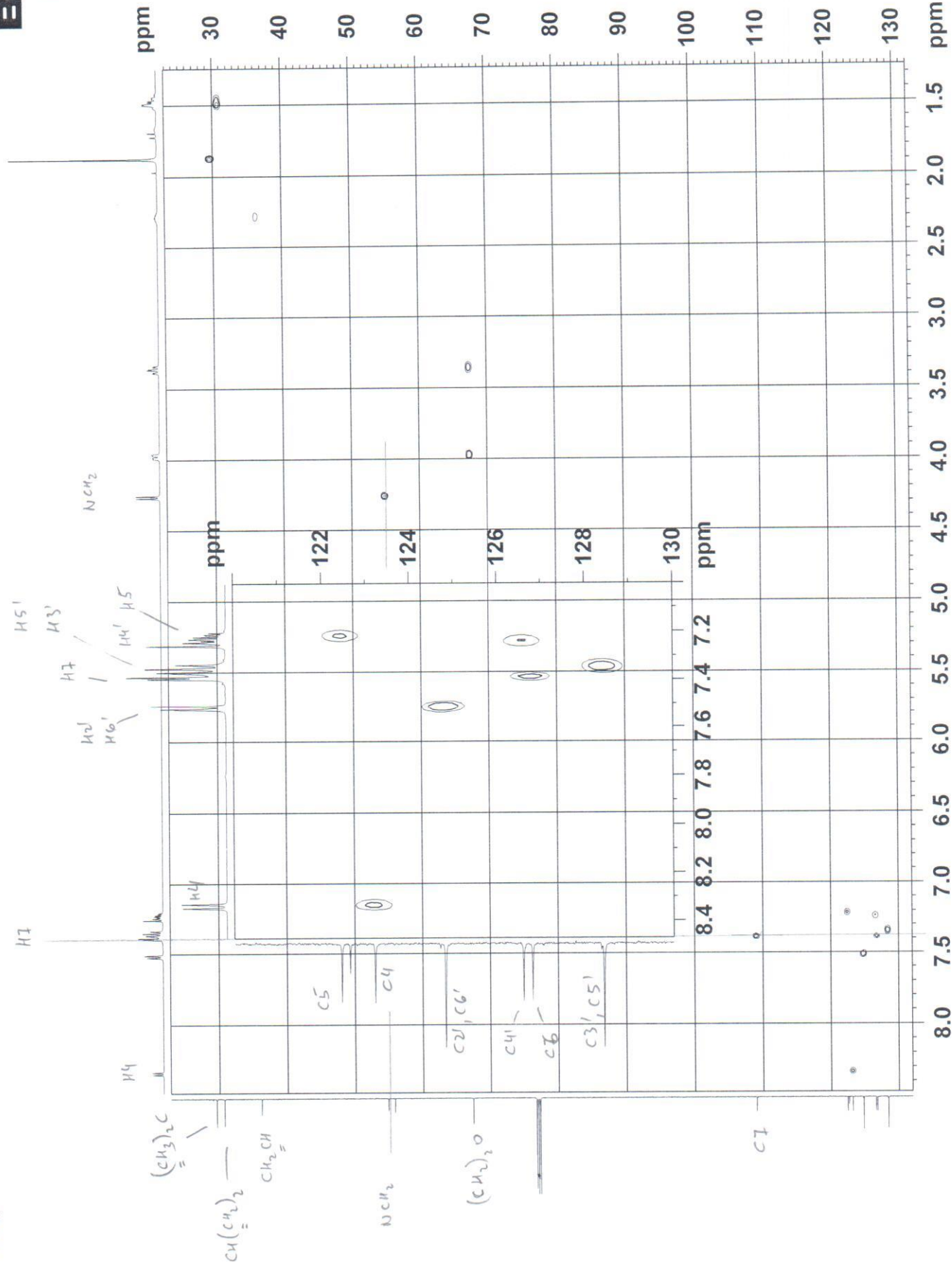
P1 8.90 usec
P2 17.80 usec
P3 8.00 usec
P4 8.00 usec
P5 10.00 usec
P6 10.00 usec
P7 10.00 usec
P8 10.00 usec
P9 10.00 usec
P10 10.00 usec
P11 10.00 usec
P12 10.00 usec
P13 10.00 usec
P14 10.00 usec
P15 10.00 usec
P16 10.00 usec
P17 10.00 usec
P18 10.00 usec
P19 10.00 usec

GRADIENT CHANNEL
GPM1 SMSQ10.100
GPM2 SMSQ10.100
GPM3 SMSQ10.100
GPM4 SMSQ10.100
GPM5 SMSQ10.100
GPM6 SMSQ10.100
GPM7 SMSQ10.100
GPM8 SMSQ10.100
GPM9 SMSQ10.100
GPM10 SMSQ10.100
GPM11 SMSQ10.100
GPM12 SMSQ10.100
GPM13 SMSQ10.100
GPM14 SMSQ10.100
GPM15 SMSQ10.100
GPM16 SMSQ10.100
GPM17 SMSQ10.100
GPM18 SMSQ10.100
GPM19 SMSQ10.100

FI - Acquisition parameters
TD 256
SF 125.7672 MHz
FIDRES 81.380234 Hz
SW 165.650 ppm
F0 125.767217 MHz
F1 125.767217 MHz
F2 125.767217 MHz
F3 125.767217 MHz
F4 125.767217 MHz
F5 125.767217 MHz
F6 125.767217 MHz
F7 125.767217 MHz
F8 125.767217 MHz
F9 125.767217 MHz
F10 125.767217 MHz
F11 125.767217 MHz
F12 125.767217 MHz
F13 125.767217 MHz
F14 125.767217 MHz
F15 125.767217 MHz
F16 125.767217 MHz
F17 125.767217 MHz
F18 125.767217 MHz
F19 125.767217 MHz

Processing parameters
SI 1024
SF 500.1300157 MHz
WDW QSI
SSB 0 Hz
LB 0 Hz
GB 0 Hz
PC 1.40

FI - Processing parameters
SI 1024
SF 500.1300157 MHz
WDW QSI
SSB 0 Hz
LB 0 Hz
GB 0 Hz
PC 1.40





Current Data Parameters
Date: 20140903
Time: 19.38
P-233-3196-14-4D
EXPNO: 4
PROCNO: 1

F2 - Acquisition Parameters

Date: 20140903
Time: 19.38
INSTRUM: spect
PROBHD: 5 mm PABBO BB-
PULPROG: hmtcplpndqf
TD: 2048
SOLVENT: CDCl3
NS: 4
DS: 16
SWH: 4807.692 Hz
FIDRES: 2.347506 Hz
AQ: 0.2130420 sec
RG: 2050
DW: 104.000 usec
DE: 6.50 usec
TE: 296.0 K
CNS12: 145.000000
CNS13: 10.000000
D0: 0.0000300 sec
D1: 1.4429398 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: 500.1321146 MHz

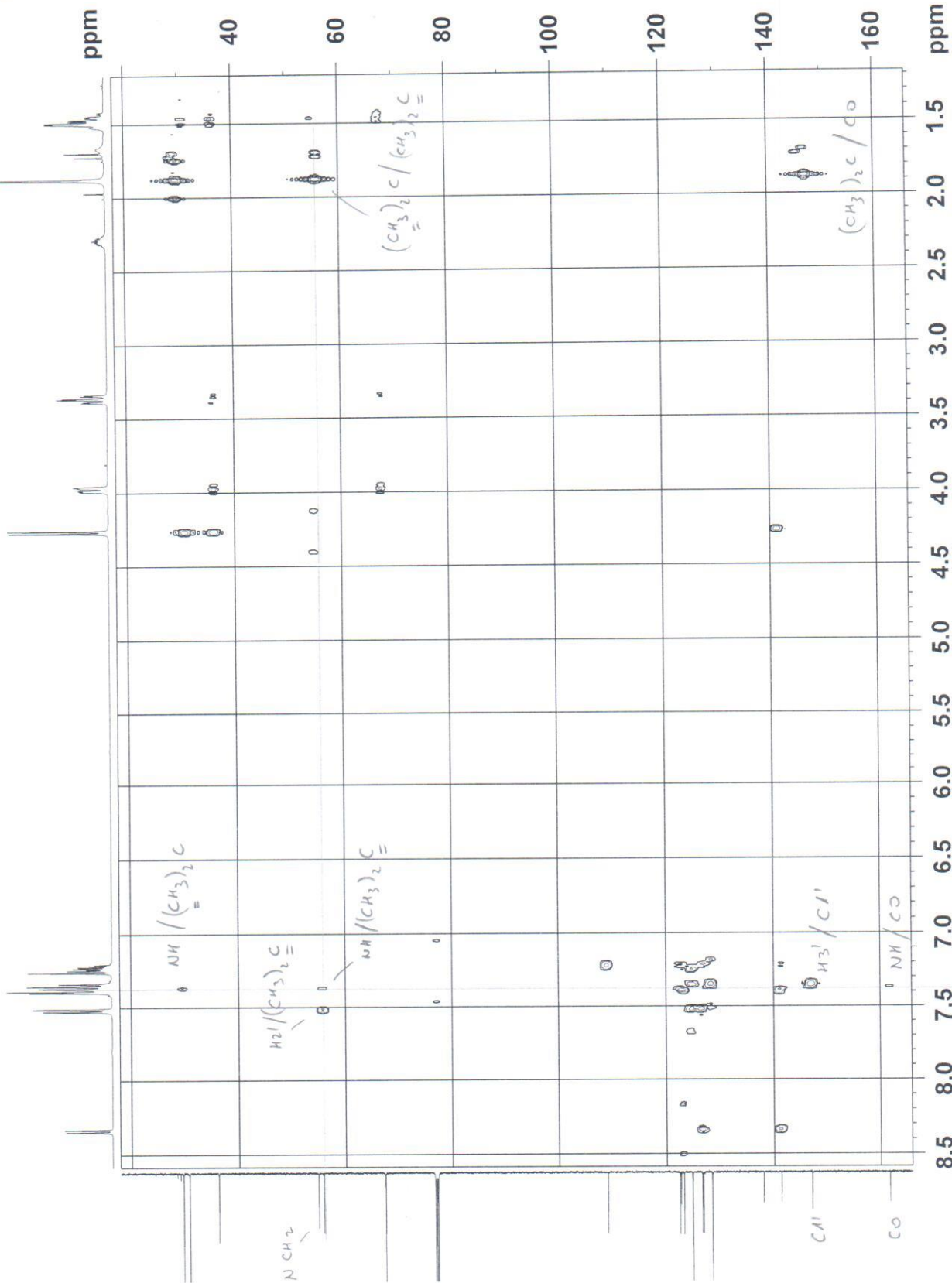
===== CHANNEL f2 =====
NUC2: 13C
P3: 9.00 usec
PLW2: 122.00000000 W
SFO2: 125.7703437 MHz

===== GRADIENT CHANNEL =====
GENA11: SMSQ10-100
GENA12: SMSQ10-100
GENA13: SMSQ10-100
GZ11: 50.00 %
GZ12: 30.00 %
GZ13: 40.10 %
P16: 1000.00 usec

F1 - Acquisition Parameters
TD: 128
SFO1: 125.7703 MHz
FIDRES: 218.226349 Hz
SW: 222.095 ppm
FMODE: QF

F2 - Processing parameters
SI: 2048
SF: 500.1300157 MHz
WDW: SINE
SSB: 0
LB: 0 Hz
GB: 0
FC: 1.40

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



P-233-3196-14-4D
HMBC



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

F2 - Acquisition Parameters
Date_ 20140903
Time_ 19.38

INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmcqplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4807.692 Hz
FIDRES 2.347506 Hz
AQ 0.2130420 sec
RG 2050
DE 104.000 usec
TE 296.0 K
CNS2 145.000000
CNS13 145.000000
DO 0.0000300 sec
D1 1.4429398 sec
D2 0.0344828 sec
D3 0.0500000 sec
D4 0.0000000 sec
D5 0.0000000 sec
D6 0.0000000 sec
INO 0.00001790 sec

CHANNEL f1
NUC1 1H
P1 8.90 usec
P2 17.80 usec
PLW1 26.00000000 W
SFO1 500.1321146 MHz

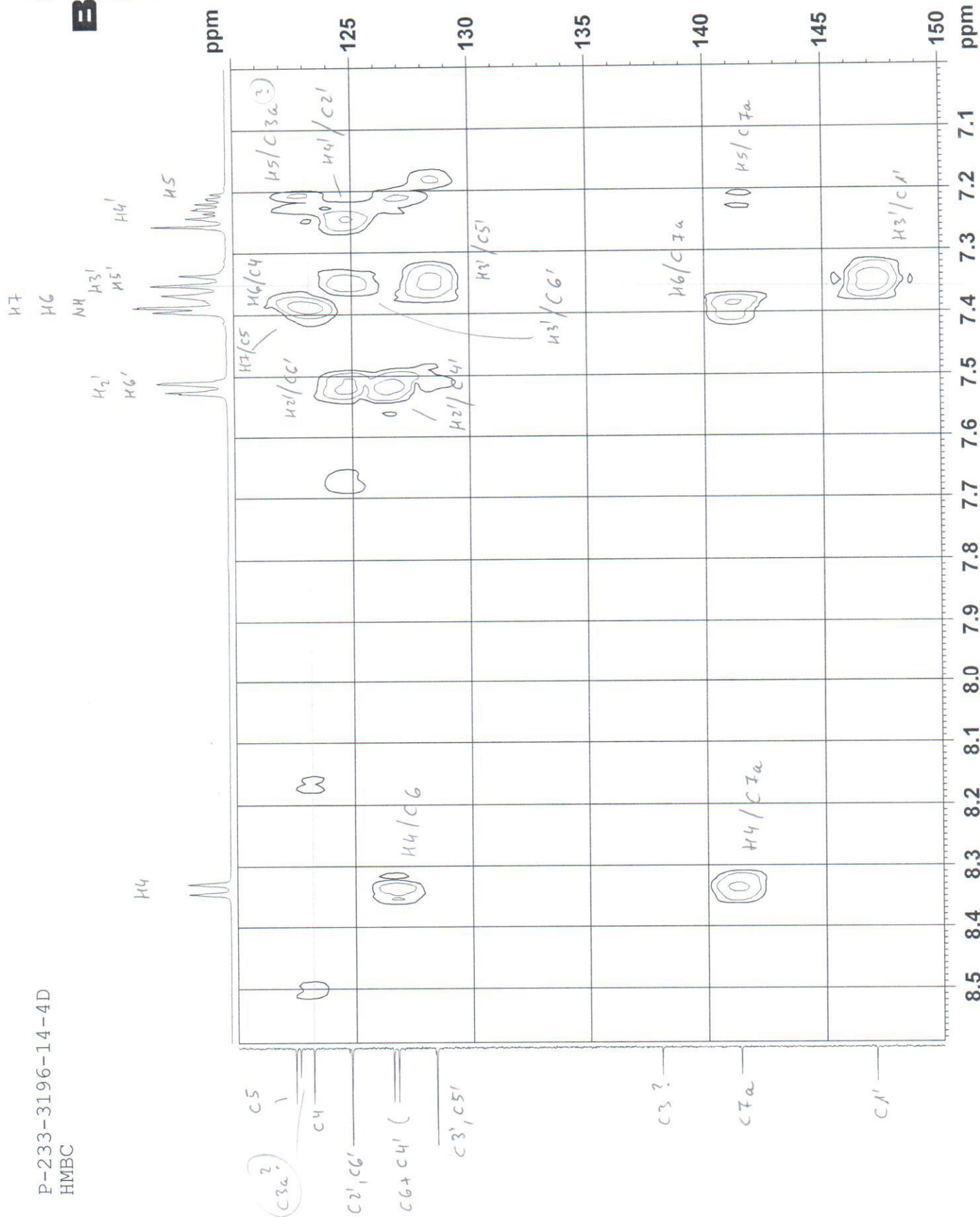
CHANNEL f2
NUC2 13C
P3 9.00 usec
PLW2 122.00000000 W
SFO2 125.7703437 MHz

GRADIENT CHANNEL
GPNAM1 SMSQ10-100
GPNAM2 SMSQ10-100
GPNAM3 SMSQ10-100
GPZ1 30.00
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
F0MODE QF

F2 - Processing parameters
SI 2048
SF 500.1300157 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

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



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



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

F2 - Acquisition Parameters
Date_ 20140903
Time 19.57

INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcpgndqf
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SMH 4807.692 Hz
FIDRES 2.347506 Hz
AQ 0.2130420 sec
RG 2050
DW 104.000 usec
DE 5.50 usec
TE 296.0 K
CNS113 5.0000000
D1 0.0000300 sec
D11 1.94429398 sec
D6 0.10000000 sec
D16 0.00020000 sec
INO 0.00002465 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.90 usec
P2 17.80 usec
PLW1 26.00000000 W
SFO1 500.1321146 MHz

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

===== GRADIENT CHANNEL =====
GPM11 SMSQ10.100
GPM12 SMSQ10.100
GPM13 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
FMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300157 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
SF 50.6777350 MHz
WDW States
SSB 0 Hz
LB 0
GB 0

