



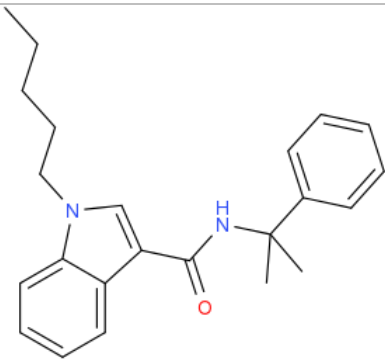
ANALYTICAL REPORT

CUMYL-PICA

(C23H28N2O)

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

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

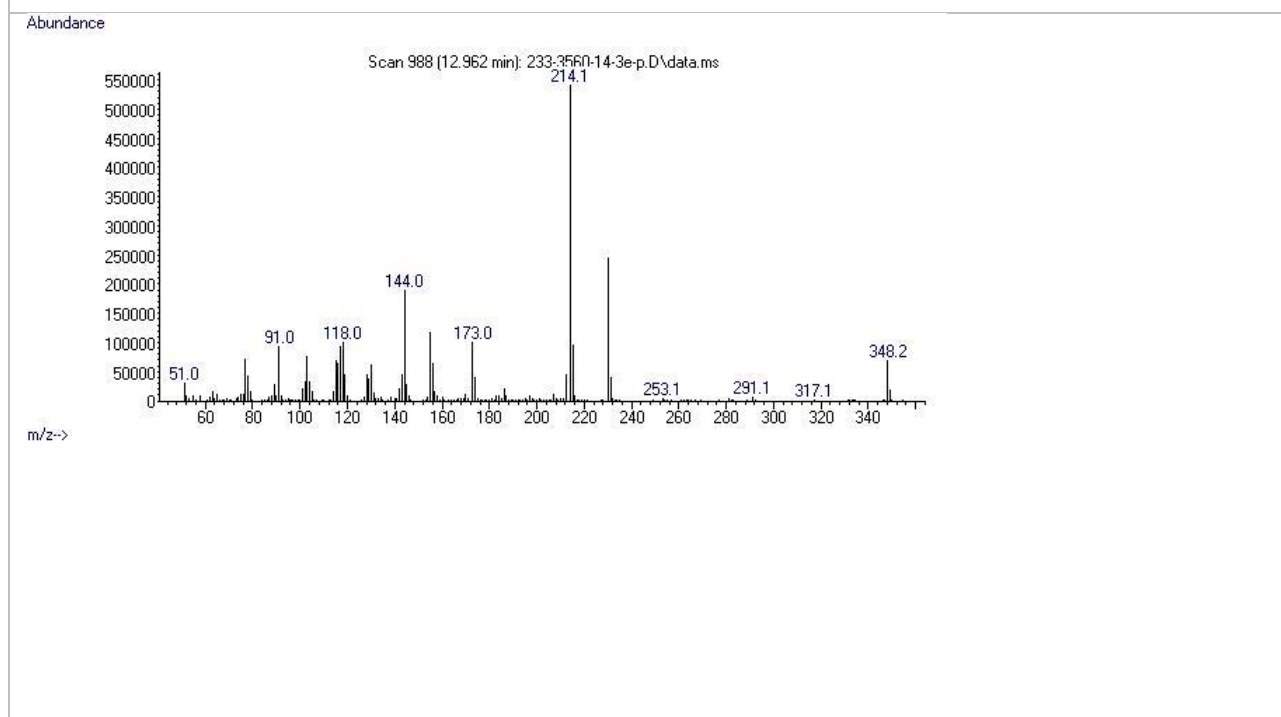
Substance identified- structure ⁱ	
Systematic name	1-(5-pentyl)-N-(2-phenylpropane-2-yl)-1H-indole-3-carboxamide
Other names	CUMYL-PICA ,
Formula (per base form)	C23H28N2O
M _w (g/mol)	348,48
Salt form	base
Other compounds detected	
Smiles	<chem>CCCCCN1C=C(C2=CC=CC=C12)C(=O)NC(C)(C)C1=CC=CC=C1</chem>
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.

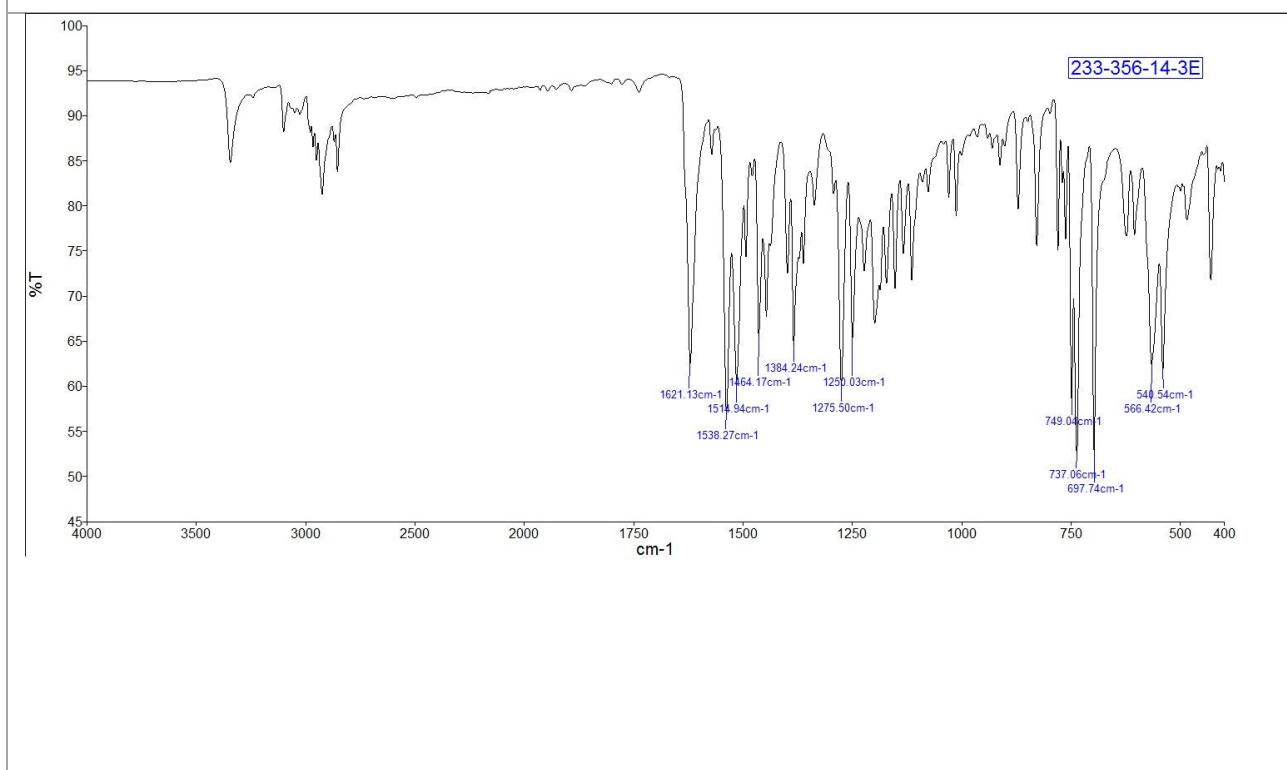
Supporting information

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

MS spectrum (EI)



FTIR - ATR



Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d



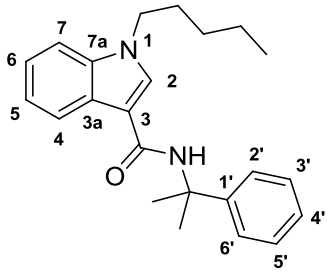
Dr. Janez Košmrlj
Professor of Organic Chemistry

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:	233-3560-14-3E
Received date:	September 1, 2014
Our notebook code:	P-233-3196-14-3E
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: C₂₃H₂₈N₂O Exact Mass: 348.2202 Molecular Weight: 348.4812</p>
Chemical name:	1-Pentyl- <i>N</i> -(2-phenylpropan-2-yl)-1 <i>H</i> -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 2-9)

Sincerely,


Janez Košmrlj

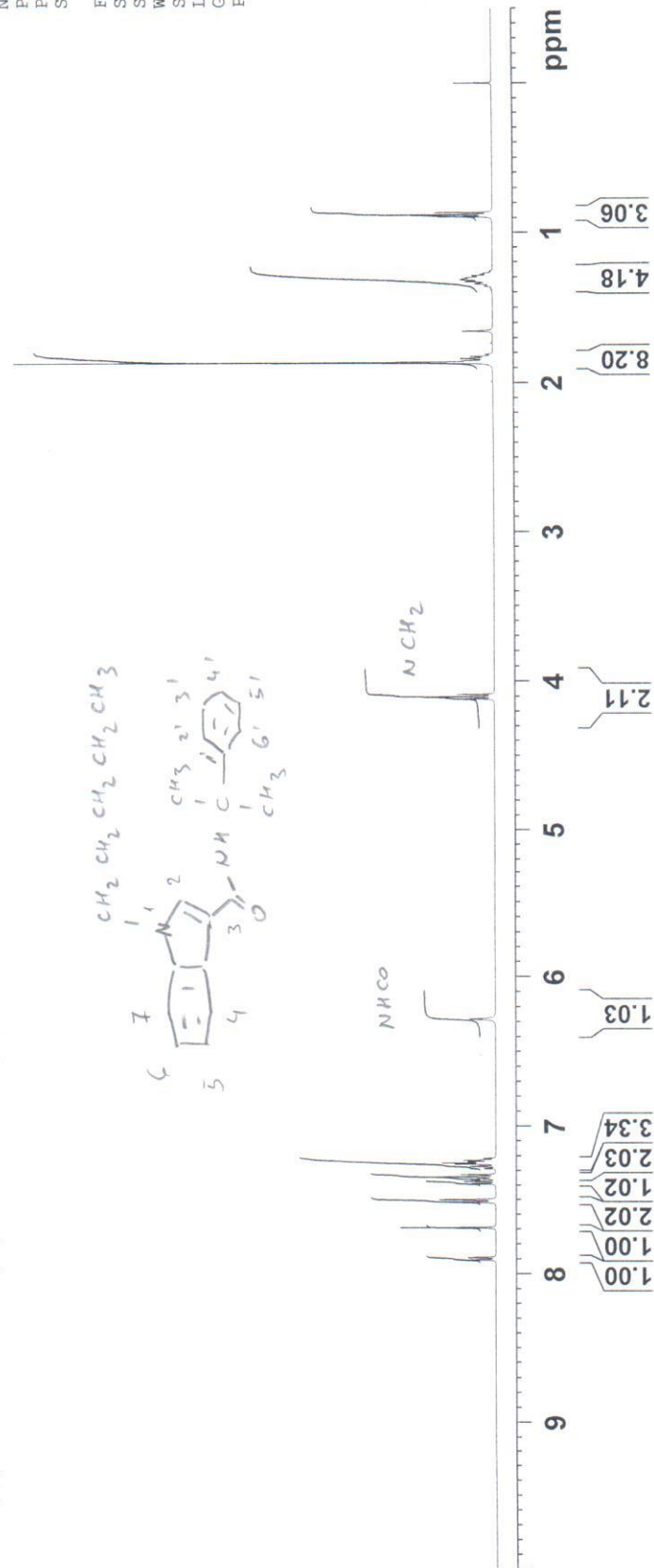
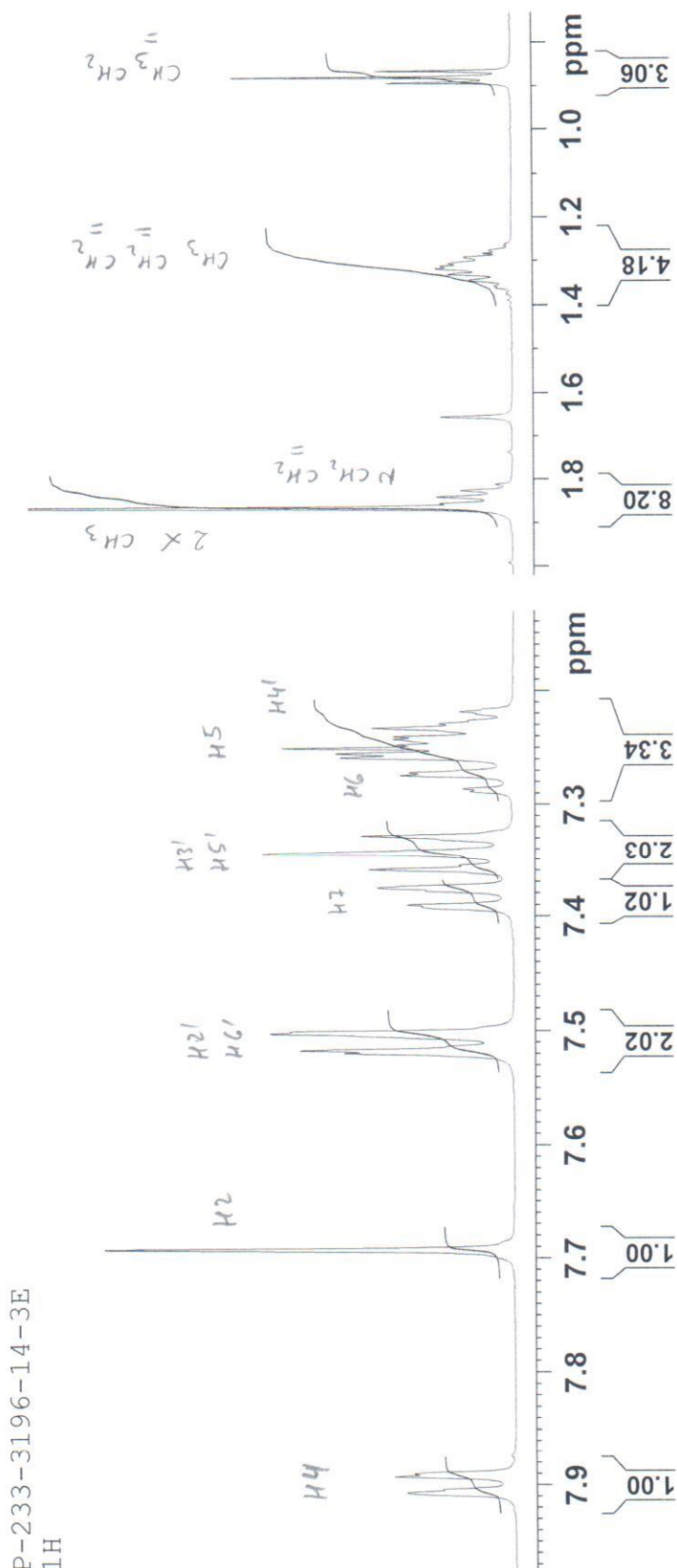


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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140903
 Time_ 22.01
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG zg30
 TD 65336
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.171923 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 26.0000000 W
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300185 MHz
 EM
 WDW 0
 SSB 0
 LB 0
 GB 0
 PC 1.00



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

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



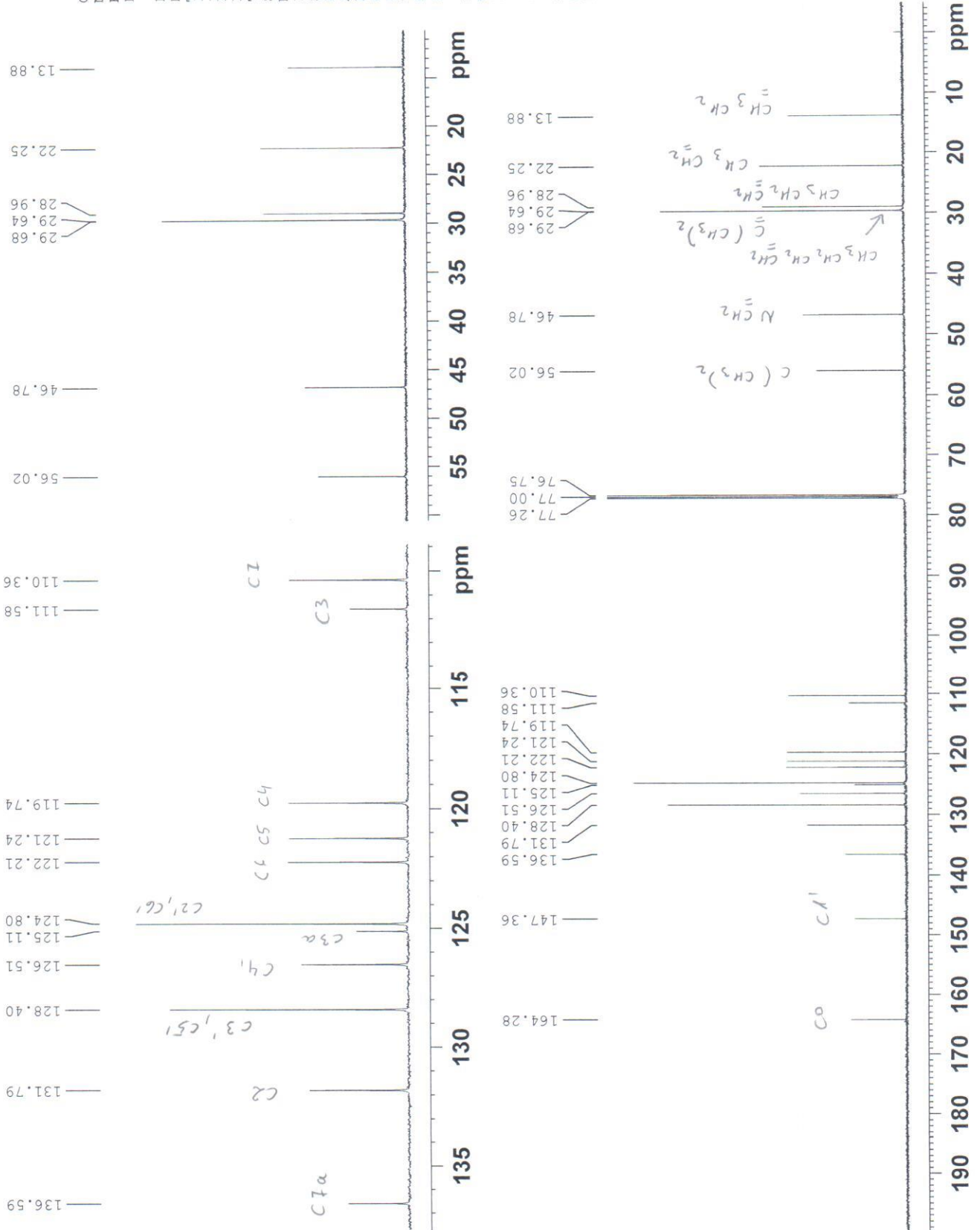
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 EXPNO 6
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 Date_ 20140904
 Time_ 1.31
 INSTRUM spect
 PROBHD 5 mm FAPBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 2050
 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 122.0000000 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 500.13200005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577961 MHz
 EM
 SSB 0 1.00 Hz
 LB 0
 GB 0
 PC 1.40





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

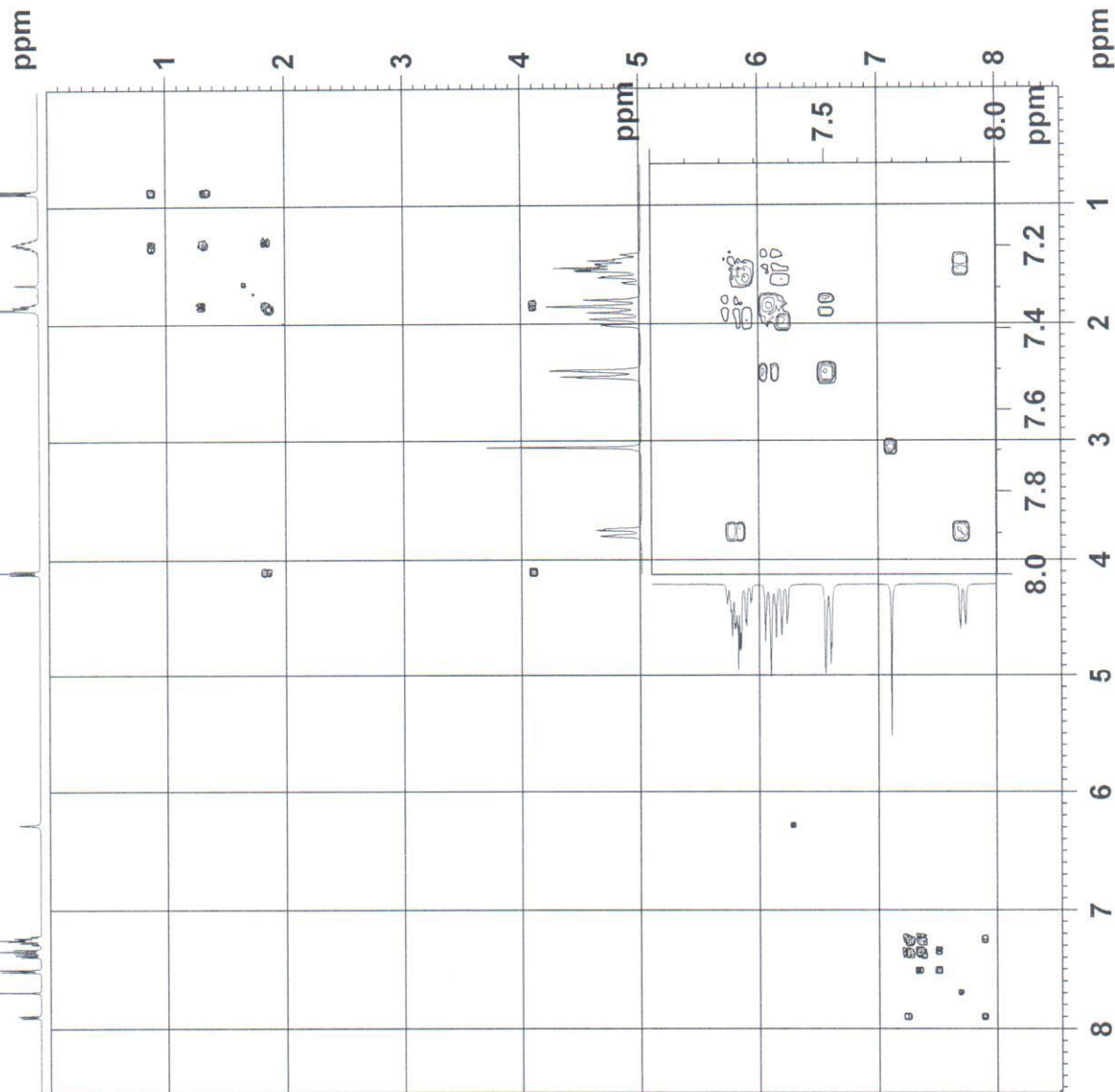
F2 - Acquisition Parameters
 Date_ 20140903
 Time 23.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG cosygpppgf
 TD 2048
 SOLVENT CDCl3
 NS 1
 DS 8
 SWH 4273.504 Hz
 FIDRES 2.086672 Hz
 AQ 0.2396660 sec
 RG 36
 DM 117.000 usec
 DE 6.50 usec
 TE 296.0 K
 D0 0.0000300 sec
 D1 1.91357398 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00023400 sec

==== CHANNEL F1 =====
 NUC1 1H
 P0 8.90 usec
 P1 8.90 usec
 PL1 2500.00 usec
 PLW1 26.00000000 W
 PLW0 3.04649997 W
 SFO1 500.1321583 MHz
 ===== GRADIENT CHANNEL =====
 GENAM1 SMSQ10.100
 GEZ1 10.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SFO1 500.1322 MHz
 FIDRES 33.386753 Hz
 SW 8.545 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 500.1300185 MHz
 WDW QSI
 SSB 0
 LB 0 Hz
 GB 0
 FC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.1300185 MHz
 WDW States-TTPI
 SSB 0
 LB 0 Hz
 GB 0



P-233-3196-14-3E
HSQC



Current Data Parameters
Date_ 20140903
Time_ 23.18
INSTRUM spect
PROBHD 5 mm BBOBBO
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140903
Time_ 23.18
INSTRUM spect
PROBHD 5 mm BBOBBO
PULPROG hsqcetps12
TD 1024
SOLVENT CDCl3
NS 2
DS 16
SWH 4273.504 Hz
FIDRES 4.119484 Hz
AQ 0.119484 sec
RG 2050
WDW 117.000 usec
DE 6.50 usec
TE 296.2 K
CNS12 145.000000
D0 0.0000300 sec
D1 1.4500000 sec
D11 0.0300000 sec
D13 0.0000400 sec
D16 0.0002000 sec
D24 0.00086207 sec
IN0 0.00002400 sec
ZGPGTNS

===== CHANNEL f1 =====
NUC1 1H
P1 8.90 usec
P2 17.80 usec
P28 1000.00 usec
PLW1 26.0000000 W
SF01 500.1321563 MHz
===== CHANNEL f2 =====
garp
NUC2 13C
P3 9.00 usec
P4 18.00 usec
PCPD2 70.00 usec
PLW2 2.0162000 W
SF02 125.7672177 MHz

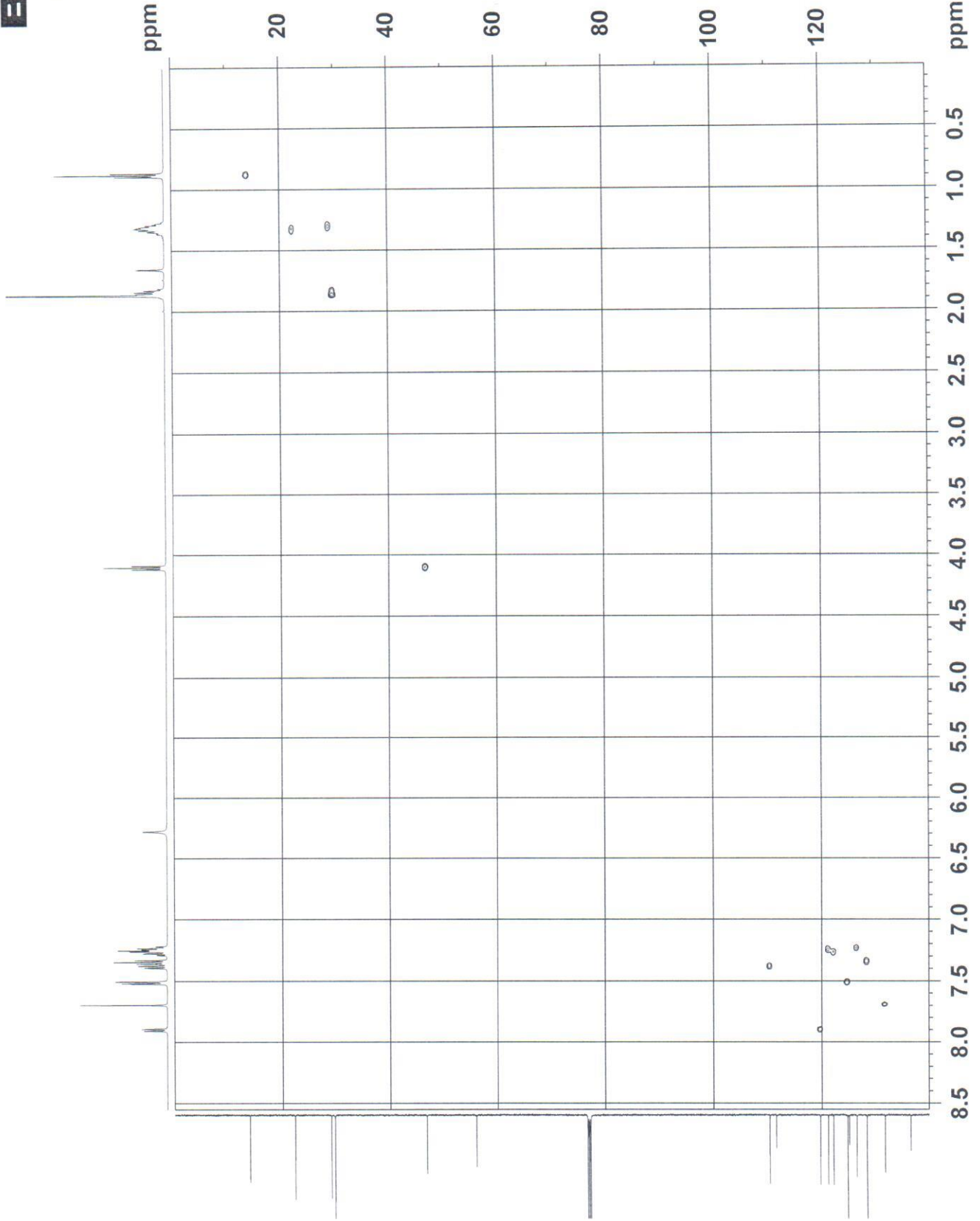
===== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPNAM4 SMSQ10.000
GPZ1 20.10 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
PL6 1000.00 usec
PL9 600.00 usec

F1 - Acquisition parameters
Date_ 20140903
Time_ 23.18
SF01 125.7672 MHz
FIDRES 81.380234 Hz
SW 165.650 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 500.130165 MHz
WDW COSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 500.130165 MHz
WDW COSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F2 - Processing parameters
SI 125.7672 MHz
WDW COSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40



P-233-3196-14-3E
HSQC



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

F2 - Acquisition Parameters

Date_ 20140903
Time 23.18
INSTRUM spect
PROBHD 5 mm BBO
PULPROG hsqcetopt012
TD 1024
SOLVENT CDCl3
NS 2
DS 16
SWH 4273.504 Hz
FIDRES 4.110354 Hz
AQ 0.110354 sec
RG 2050
DE 117.000 usec
TE 296.2 K
CNS2 145.0000000
D0 0.0000300 sec
D1 1.4557243 sec
M1 0.0000000 sec
D11 0.0300000 sec
D13 0.0000040 sec
D16 0.0002000 sec
D24 0.0008620 sec
INO 0.0000240 sec
ZGPGTNS

==== CHANNEL f1 =====

NUC1 1H
P1 8.90 usec
P2 17.80 usec
P28 1000.00 usec
PLW1 26.0000000 W
SFO1 500.1321583 MHz

==== CHANNEL f2 =====

CPDPRG2 garp
NUC2 13C
P3 9.00 usec
P4 18.00 usec
PCPD2 70.00 usec
PLW2 2.0157000 W
SFO2 125.7672177 MHz

==== GRADIENT CHANNEL =====

GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GPNAM4 SMSQ10.100
GPZ1 0.00
GPZ2 20.10
GPZ3 11.00
GPZ4 -5.00
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters

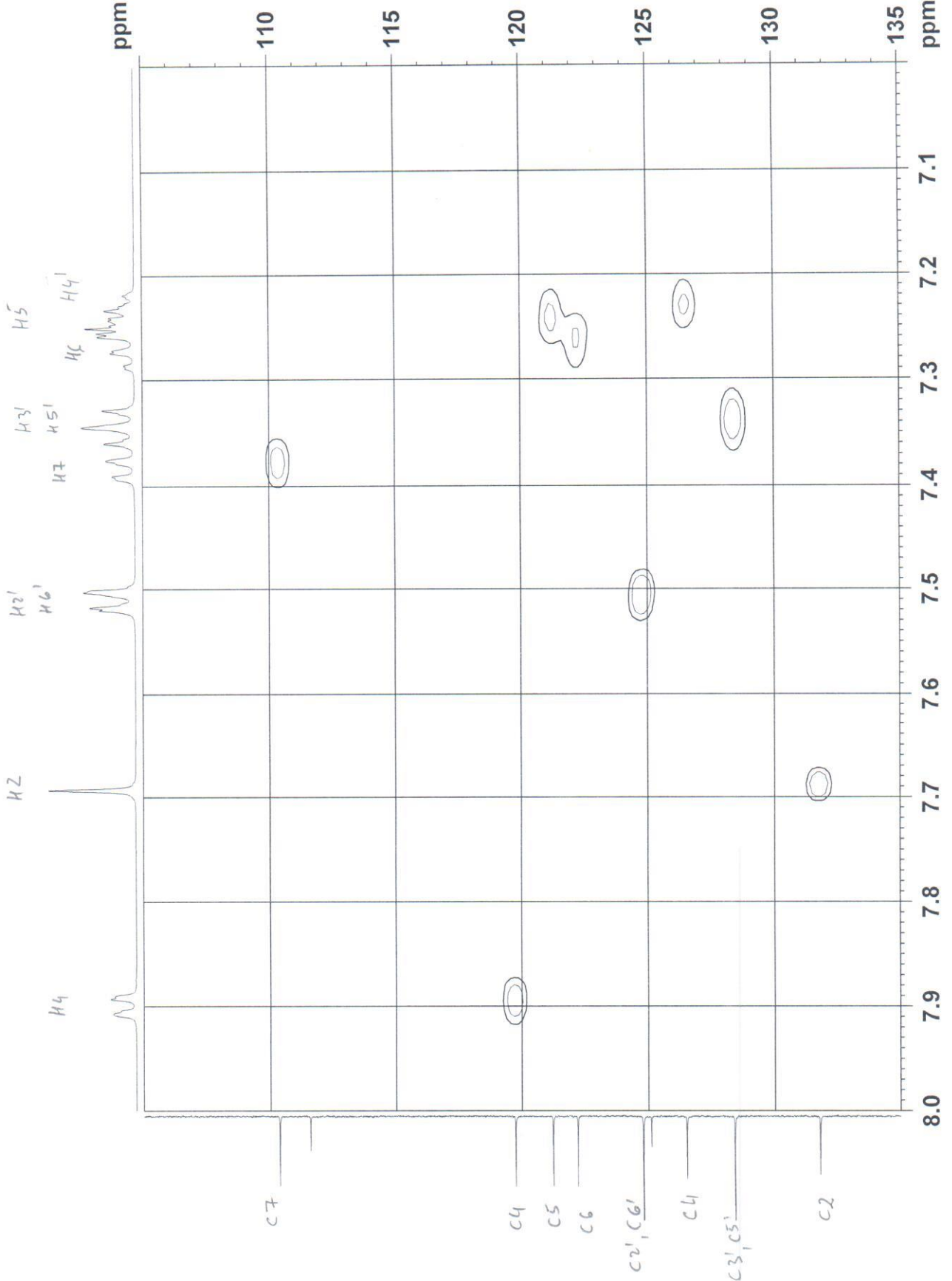
TD01 1024
FIDRES 81.380234 Hz
SW 165.650 ppm
FMODE Echo-Antiecho

F2 - Processing parameters

SI 500.130165 MHz
WDW COSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 125.7672177 MHz
WDW echo-antiecho
SSB 2
LB 0 Hz
GB 0
PC 1.40





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

F2 - Acquisition Parameters
 Date_ 20160903
 Time 23:39
 PROBRM spect
 PULPROG 5 mm PABPO BB-
 hmbcgp1pndrf
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 16
 SWH 4273.504 Hz
 FIDRES 2.086672 Hz
 AQ 0.2396660 sec
 RG 2050
 DW 117.000 usec
 DE 6.50 usec
 TE 296.0 K
 CNST2 145.0000000
 CNST13 10.0000000
 D0 0.0000300 sec
 D1 1.41767001 sec
 D2 0.00344628 sec
 D6 0.05000000 sec
 D16 0.00020500 sec
 INO 0.00001790 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 8.90 usec
 P2 17.80 usec
 PLW1 26.0000000 W
 SF01 500.1321583 MHz

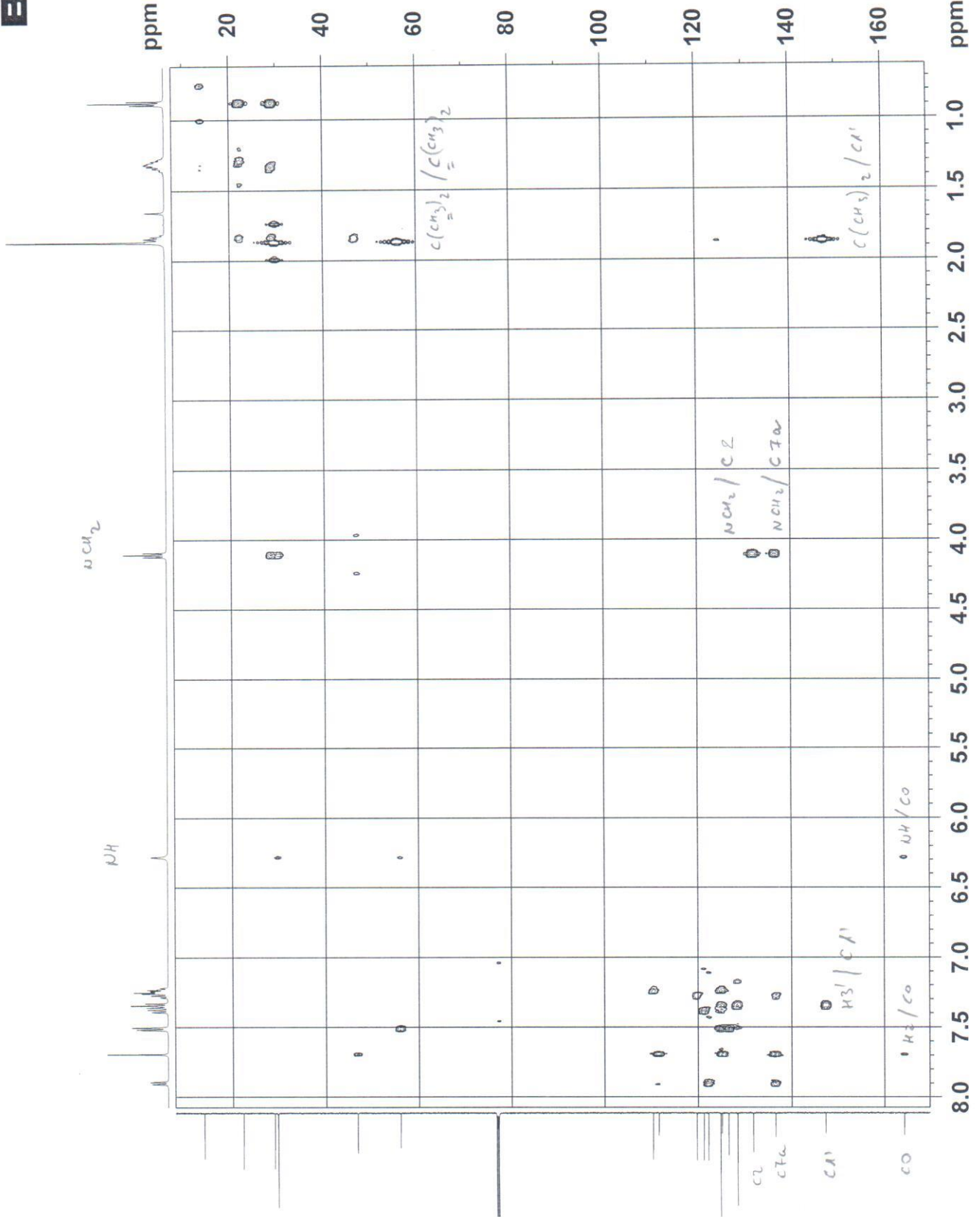
==== CHANNEL f2 =====
 NUC2 13C
 P3 9.00 usec
 PLW2 122.0000000 W
 SF02 125.7703437 MHz

==== GRADIENT CHANNEL =====
 GENAM1 SMSQ10.100
 GENAM2 SMSQ10.100
 GENAM3 SMSQ10.100
 GEZ1 50.00 %
 GEZ2 30.00 %
 GEZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition Parameters
 TD 128
 FIDRES 125.7703 MHz
 SFO1 218.226349 Hz
 SF 222.095 ppm
 ENMODE QF

F2 - Processing Parameters
 SI 2048
 SF 500.1300185 MHz
 SINE
 WDW 0
 SSB 0 Hz
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing Parameters
 SI 1024
 SF 125.7577890 MHz
 SINE
 WDW 0
 SSB 0 Hz
 LB 0 Hz
 GB 0





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

F2 - Acquisition Parameters
 Date_ 20140903
 Time 23:30
 INSTRUM spect
 PULPROG zgpg30
 TD 65536
 SOLVENT hmbcprp1pndcf
 NS 4
 DS 16
 SWH 4273.504 Hz
 FIDRES 2.086672 Hz
 AQ 0.2396660 sec
 RG 2050
 DW 117.000 usec
 DE 6.50 usec
 TE 296.0 K
 CNST2 145.0000000
 CNST13 10.0000000
 D0 0.0000000 sec
 D1 1.41767001 sec
 D2 0.00344828 sec
 D6 0.05000000 sec
 D16 0.00020000 sec
 INO 0.00001790 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.90 usec
 F2 17.80 usec
 PLW1 26.00000000 W
 SFO1 500.1321583 MHz

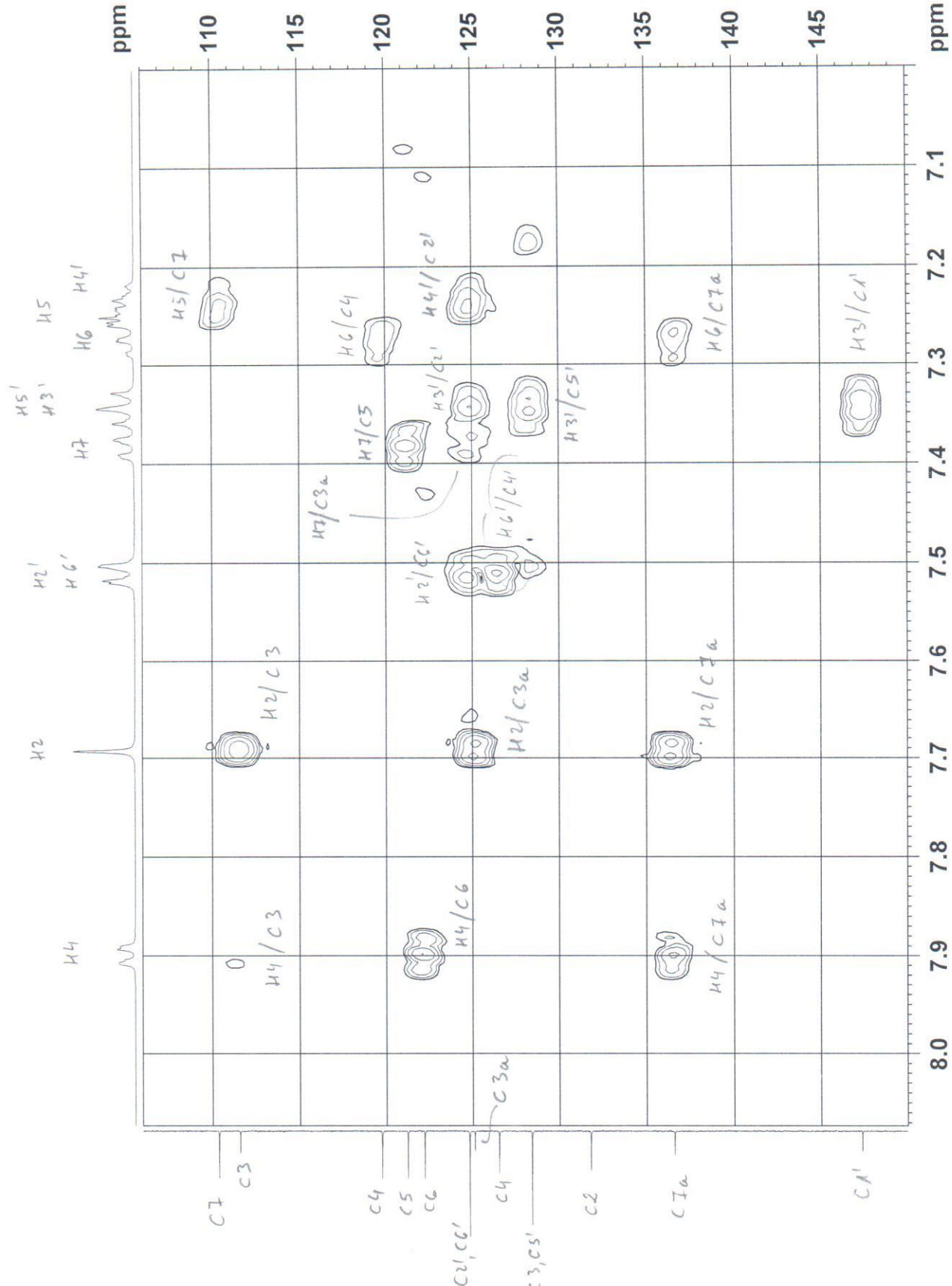
===== CHANNEL f2 =====
 NUC2 13C
 P3 9.00 usec
 PLW2 122.00000000 W
 SFO2 125.7703437 MHz

===== 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
 ID 128
 SF01 125.7703 MHz
 FIDRES 218.226349 Hz
 SW 222.095 Ppm
 FMODE QF

F2 - Processing parameters
 SI 2048
 SF 500.1300185 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0
 FC 1.40

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



P-233-3196-14-3E
15N HMBC



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

F2 - Acquisition Parameters
Date_ 20140903
Time 23.56

INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmcsgppdqr
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 4273.504 Hz
FIDRES 2.086672 Hz
AQ 0.2396660 sec
RG 2050
DW 117.000 usec
DE 6.50 usec
TE 296.0 K
CNS113 5.0000000
D0 0.0000300 sec
D1 1.91767001 sec
D6 0.10000000 sec
D16 0.00020000 sec
INO 0.10002465 sec

==== CHANNEL f1 =====
NUC1 1H
P1 8.90 usec
PL1 17.80 usec
PLW1 26.00000000 W
SF01 500.1321583 MHz

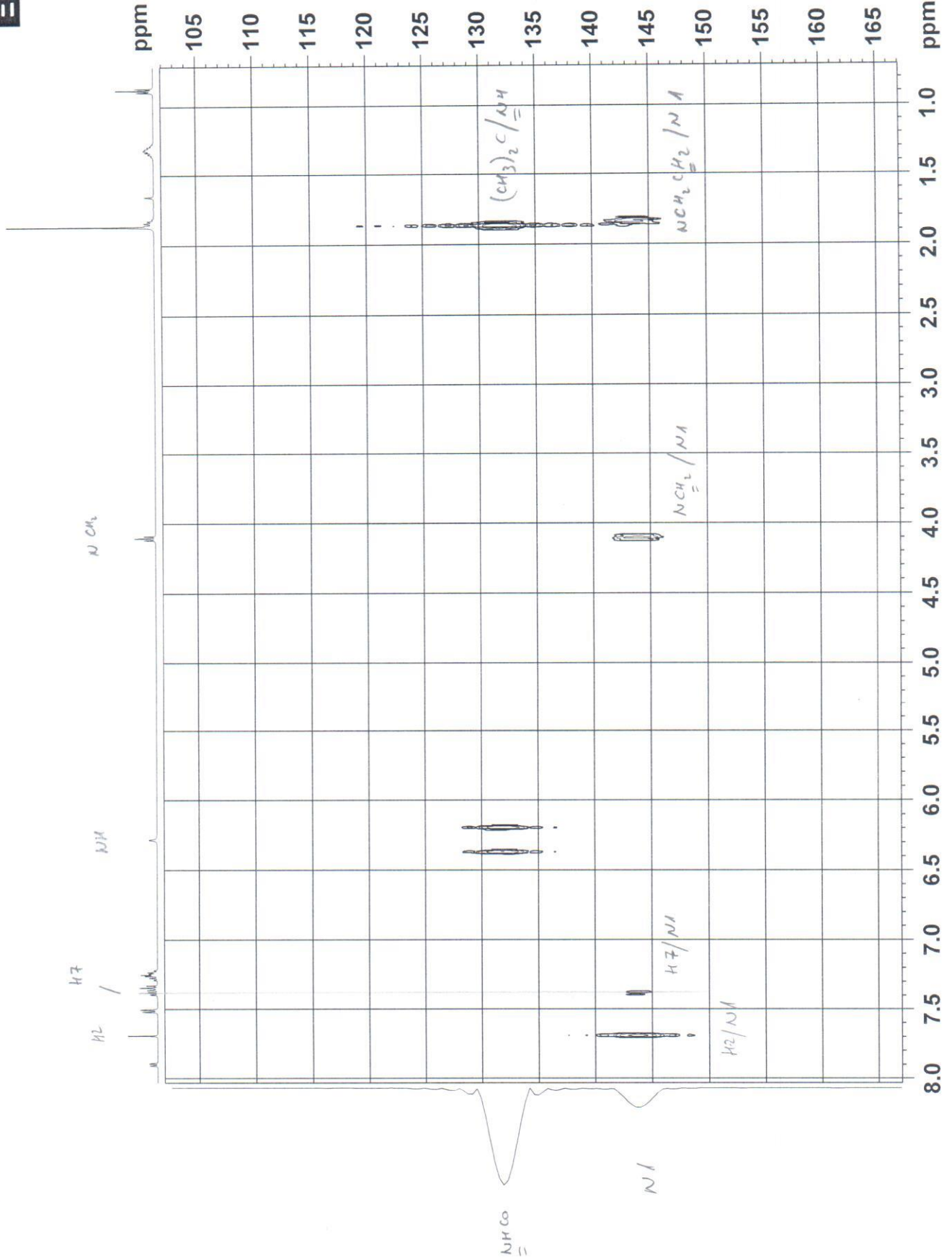
==== CHANNEL f2 =====
NUC2 15N
P3 14.40 usec
PLW2 206.00000000 W
SF02 50.6853342 MHz

==== 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 65536
FIDRES 158.391663 Hz
SWM 400.000 ppm
FIRMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300185 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
NC2 QF
SF 50.6777330 MHz
WDW States
SSB 0
LB 0 Hz
GB 0



ppm

105

110

115

120

125

130

135

140

145

150

155

160

165

ppm

8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0