



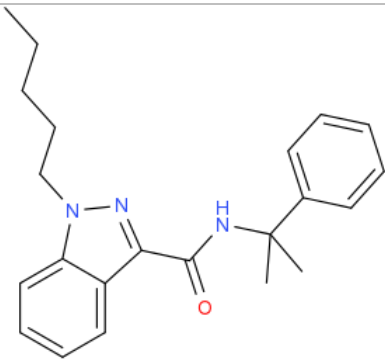
ANALYTICAL REPORT

CUMYL-PINACA

(C₂₂H₂₇N₃O)

1-pentyl-N-(2-phenylpropan-2-yl)-1H-indazole-3-carboxamide,

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

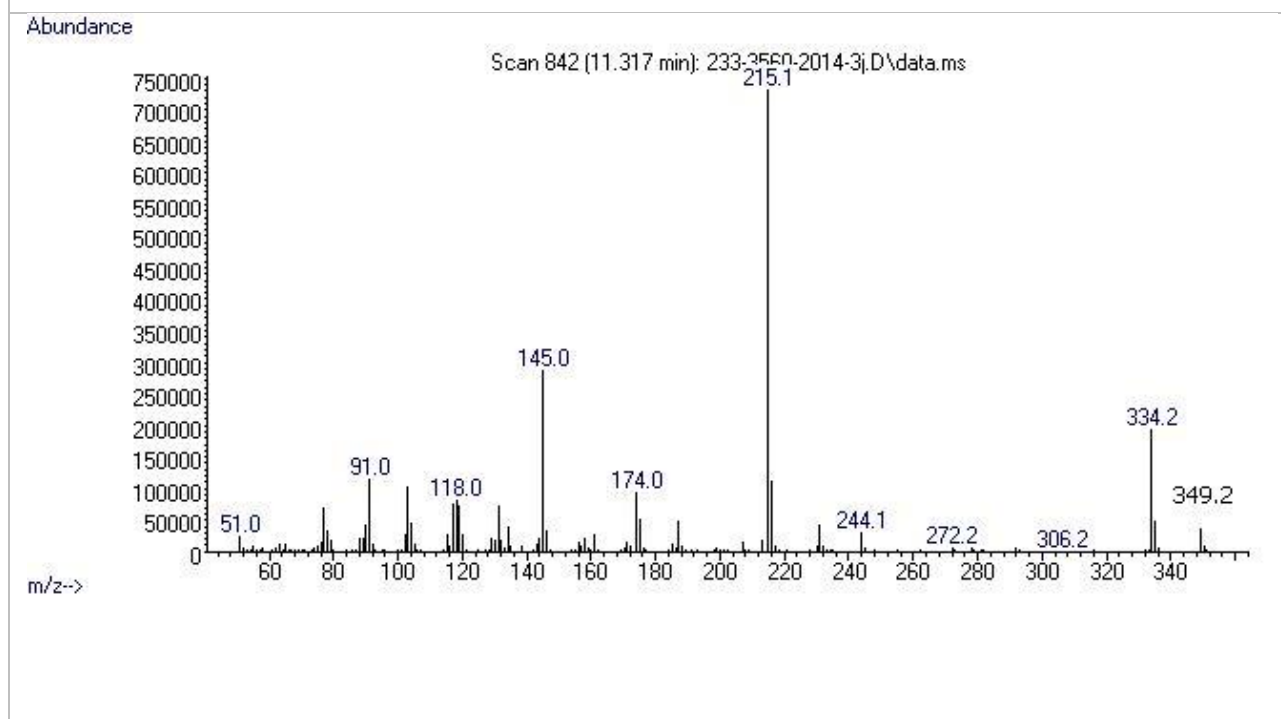
Substance identified- structure ⁱ	
Systematic name	1-pentyl-N-(2-phenylpropan-2-yl)-1H-indazole-3-carboxamide
Other names	CUMYL-PINACA ,
Formula (per base form)	C ₂₂ H ₂₇ N ₃ O
M _w (g/mol)	349,46
Salt form	base
Other compounds detected	
Smiles	<chem>C(CCCC)N1N=C(C2=CC=CC=C2)C(=O)NC(C)(C)C1=CC=CC=C1</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.

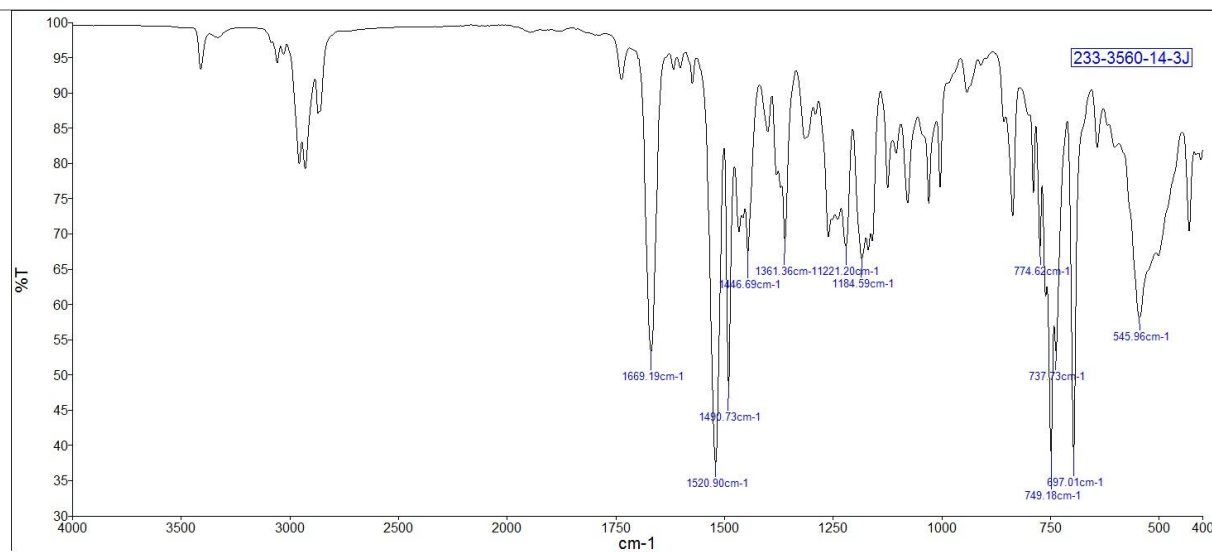
Supporting information

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

MS spectrum (EI)



FTIR - ATR



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



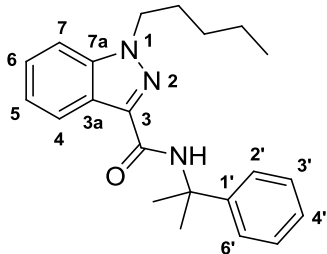
Dr. Janez Košmrlj
Professor of Organic Chemistry

September 17, 2014

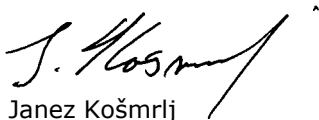
Dr. Sonja Klemenc
Head of Chemistry Department
Vodovodna 95
1000 Ljubljana
Slovenija

Dear Dr. Sonja Klemenc,

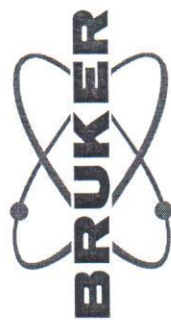
Please find enclosed the results of the structure elucidation for the sample:

Sample ID:	233-3560-14-3J
Received date:	September 1, 2014
Our notebook code:	P-233-3196-14-3J
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: C₂₂H₂₇N₃O Exact Mass: 349.2154 Molecular Weight: 349.4693</p>
Chemical name:	1-Pentyl- <i>N</i> -(2-phenylpropan-2-yl)-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-233-3196-14-3J
1H



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

F2 - Acquisition Parameters
Date_ 20140904
Time 6.32
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 3.171923 sec
RG 101
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec

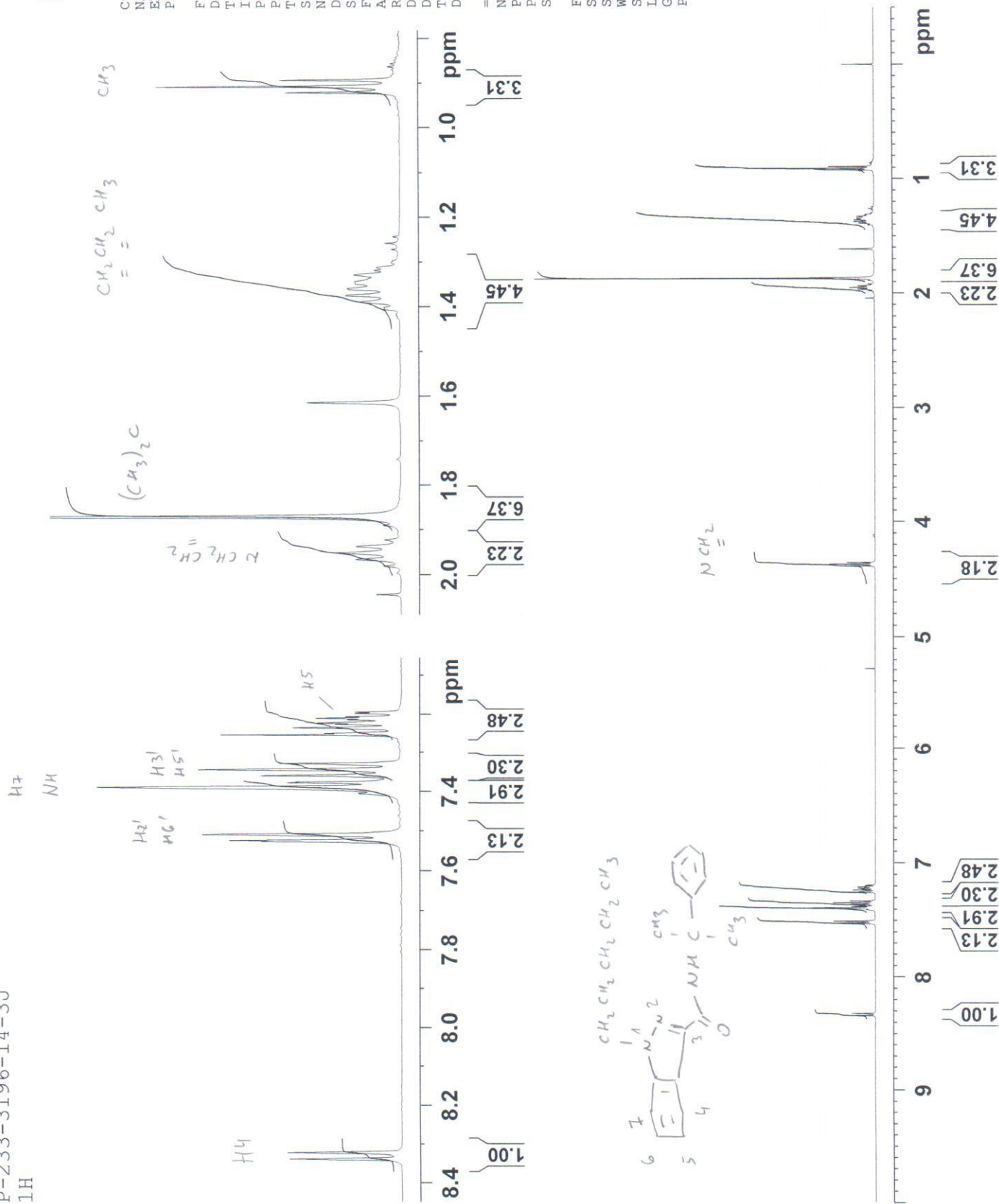
===== CHANNEL f1 =====
NUC1 1H
P1 8.90 usec
PL1 26.00000000 W
SF01 500.1330885 MHz

F2 - Processing parameters
SI 65536
SF 500.1300162 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

PREVER 15 N

PREVIEW

C3a, C3?



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

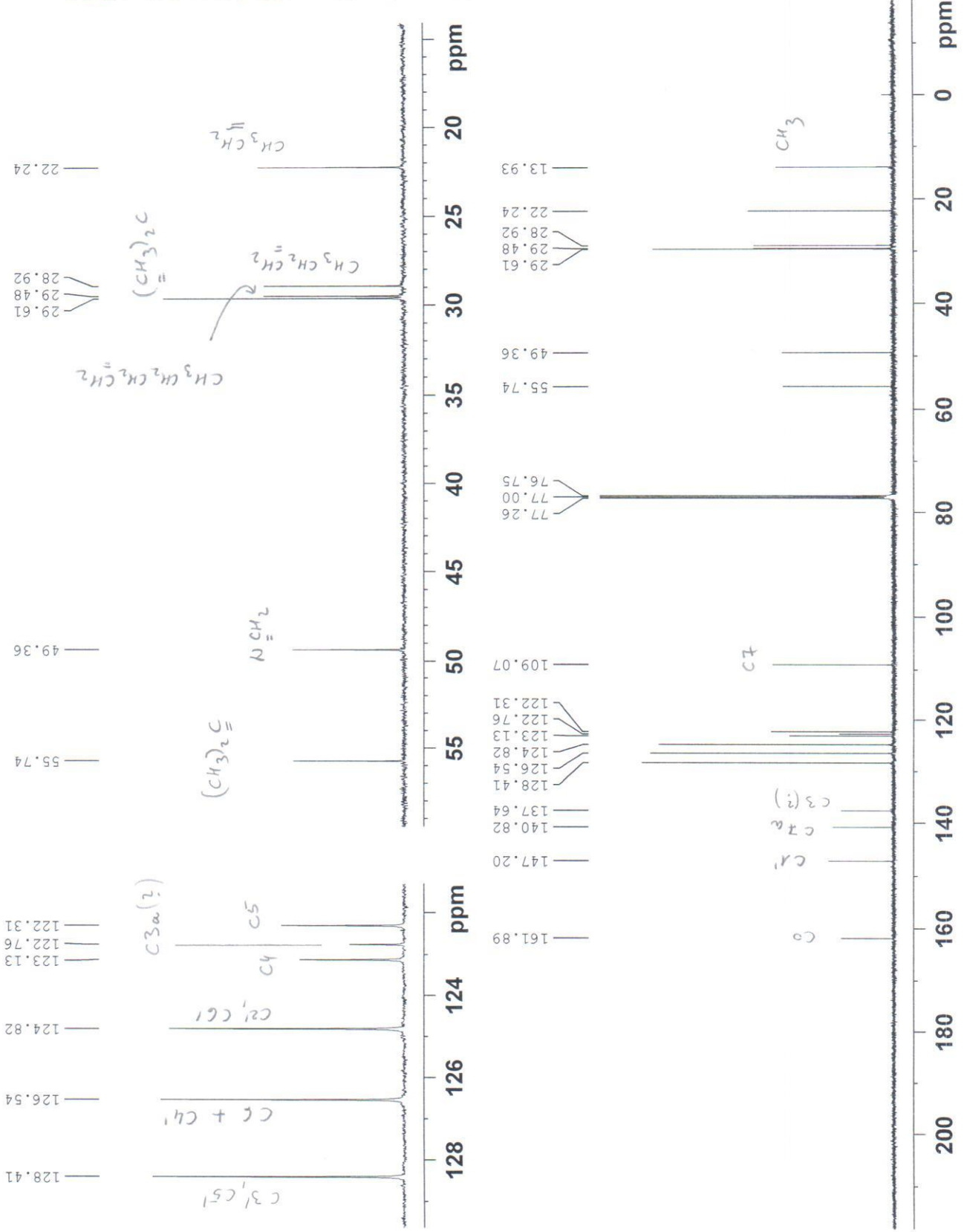


Current Data Parameters
NAME P-233-3196-14-3J
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 9.48
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 122.0000000 W
SFO1 125.7703637 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 26.0000000 W
PLW12 0.32179001 W
PLW13 0.20595001 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577948 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





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

F2 - Acquisition Parameters
Date_ 20140904
Time 6.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygppqf
TD 2048
SOLVENT CDCl3
NS 1
DS 8
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 40.3
DM 111.000 usec
DE 6.50 usec
TE 296.0 K
D0 0.0000300 sec
D1 1.92586195 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.0002200 sec

===== CHANNEL f1 =====
NUC1 1H
P0 8.90 usec
P1 8.90 usec
PL7 2500.00 usec
PLW1 26.00000000 W
PLW10 3.0464997 W
SFO1 500.1322406 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPZ1 10.00 %
Pl6 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 500.1322 MHz
FIDRES 35.191441 Hz
SW 9.007 ppm
FhMODE QF

F2 - Processing parameters
SI 1024
SF 500.1300162 MHz
WDW QSI
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300162 MHz
WDW States-TPPI
SSB 0
LB 0 Hz
GB 0

ppm

1

2

3

4

5

6

7

8

ppm

1

2

3

4

5

6

7

8



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

F2 - Acquisition Parameters
Date_ 20140504
Time 7.26

INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG hmc9p1p0d0f
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 2050
DW 111.000 usec
DE 6.50 usec
TE 296.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.42995799 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
INO 0.00001790 sec

CHANNEL f1 1H
NUC1 1H
P1 8.90 usec
P2 17.80 usec
PL1 26.00000000 W
SF01 500.1322406 MHz

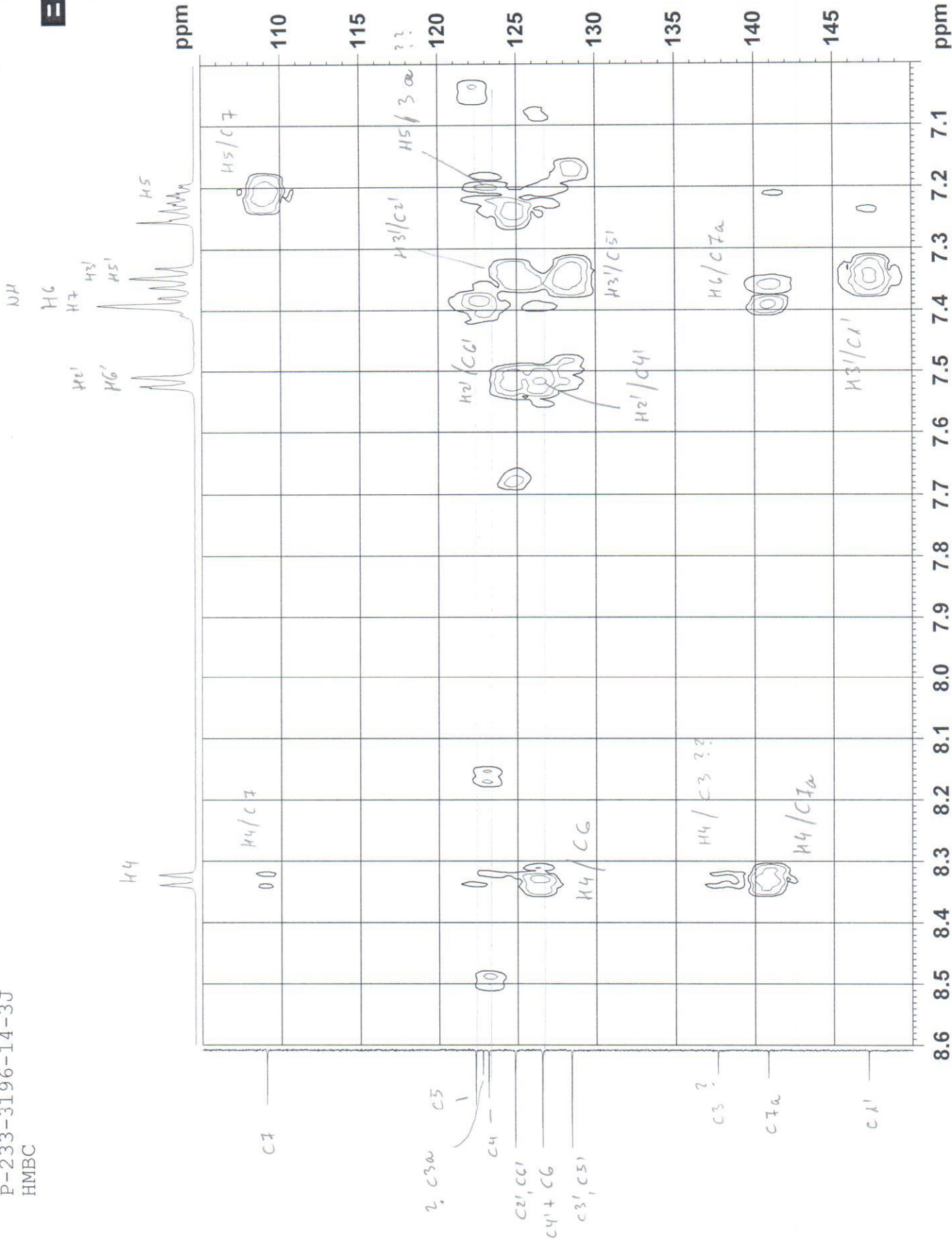
CHANNEL f2 13C
NUC2 13C
P3 9.00 usec
PLW2 122.00000000 W
SF02 125.7703437 MHz

GRADIENT CHANNEL
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPNAM3 SMSQ10.100
GP21 50.00 %
GP22 30.00 %
GP23 40.10 %
F16 1000.00 usec

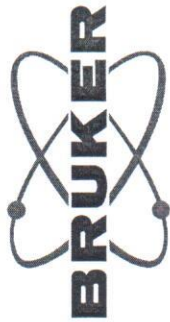
F1 - Acquisition parameters
TD 128
SF01 125.7703437 MHz
FIDRES 218.226343 Hz
SWH 222.035 Ppm
FMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300162 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-233-3196-14-3J
15N HMBC



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

F2 - Acquisition Parameters
Date_ 20140904
Time 8.00
INSTRUM spect
PROBHD 5 mm PABBO Ber
PULPROG hmcgpcndqf
TD 65536
SOLVENT CDCl3
NS 16
DS 16
SWH 4504.504 Hz
FIDRES 2.199465 Hz
AQ 0.2273780 sec
RG 2050
DM 111.000 usec
DE 6.50 usec
TE 296.0 K
CNST13 5.0000000
D0 0.00000300 sec
D1 1.92995799 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
SF01 500.132406 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 128
SF01 50.68533 MHz
FIDRES 158.391663 Hz
SW 400.000 ppm
FMODE QF

F2 - Processing parameters
SI 32768
SF 500.1300162 MHz
WDW 0
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

