



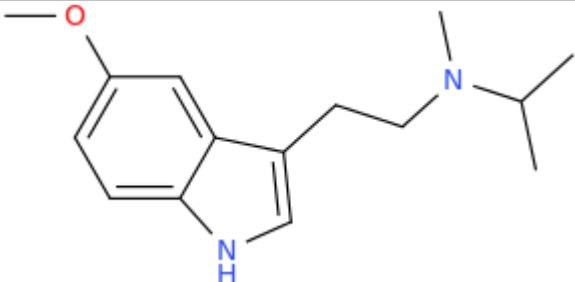
ANALYTICAL REPORT

5-MeO-MiPT (C₁₅H₂₂N₂O)

[2-(5-methoxy-1H-indol-3-yl)ethyl](methyl)(propan-2-yl)amine

Remark – other NPS detected: **none**

Sample ID:	1023-11A
Sample description:	powder
Sample type:	in house RM /
Date of sample receipt (DD/MM/YYYY):	
Date of entry (DD/MM/YYYY) into NFL database:	01/12/2013
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure ¹ (base form)	
Systematic name	[2-(5-methoxy-1H-indol-3-yl)ethyl](methyl)(propan-2-yl)amine
Other names	N-[2-(5-methoxy-1H-indol-3-yl)ethyl]-N-methylpropan-2-amine; 5-Methoxy MiPT
Formula (per base form)	C ₁₅ H ₂₂ N ₂ O
M _w (g/mol)	246,35
Salt form/anions detected	chloride (by AgNO ₃)
StdInChIKey (per base form)	HEDOODBJFVUQMS-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	>98% by NMR

¹ Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d

Report updates

date	comments (explanation)

Instrumental methods (if applied) in NFL

1. GC-MS (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 ml and split mode (1:50). Injector temperature: 280 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 °C at a rate of 18 °C/min, hold for 7.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300 until 6 min) amu.

2. HPLC-TOF (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N₂) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.

3. FTIR-ATR (Perkin Elmer): scan range 4000-400 cm⁻¹; resolution 4cm⁻¹

4. GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)

GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 °C. Chromatographic separation as above **(1)**. Split MS : IR = 1: 9.

MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

5. IC (anions) (Thermo Scientific, Dionex ICS 2100), Column: IonPac AS19, 2 x 250mm; Eluent: 10mM from 0 to 10 min, 10-58 mM from 10 to 40min; Flow rate: 0.25 ml/min; Temperature: 30°C; Suppressor: AERS 500 2mm, suppressor current 13mA; Inj. Volume: 25 µl

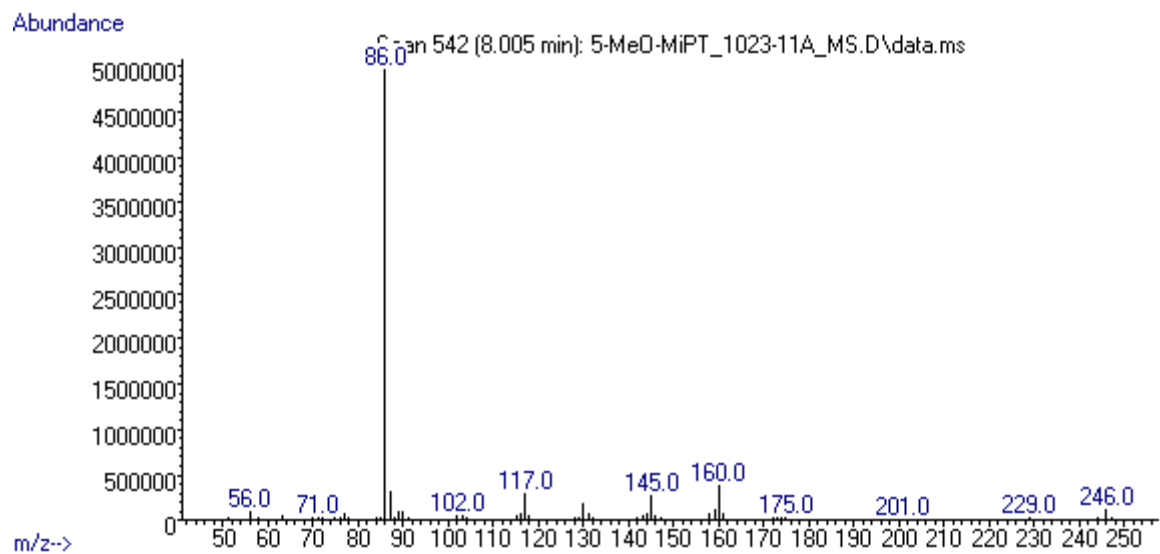
Supporting information

Solubility in	result/remark
CH ₂ Cl ₂	partially
MeOH	soluble
H ₂ O	soluble

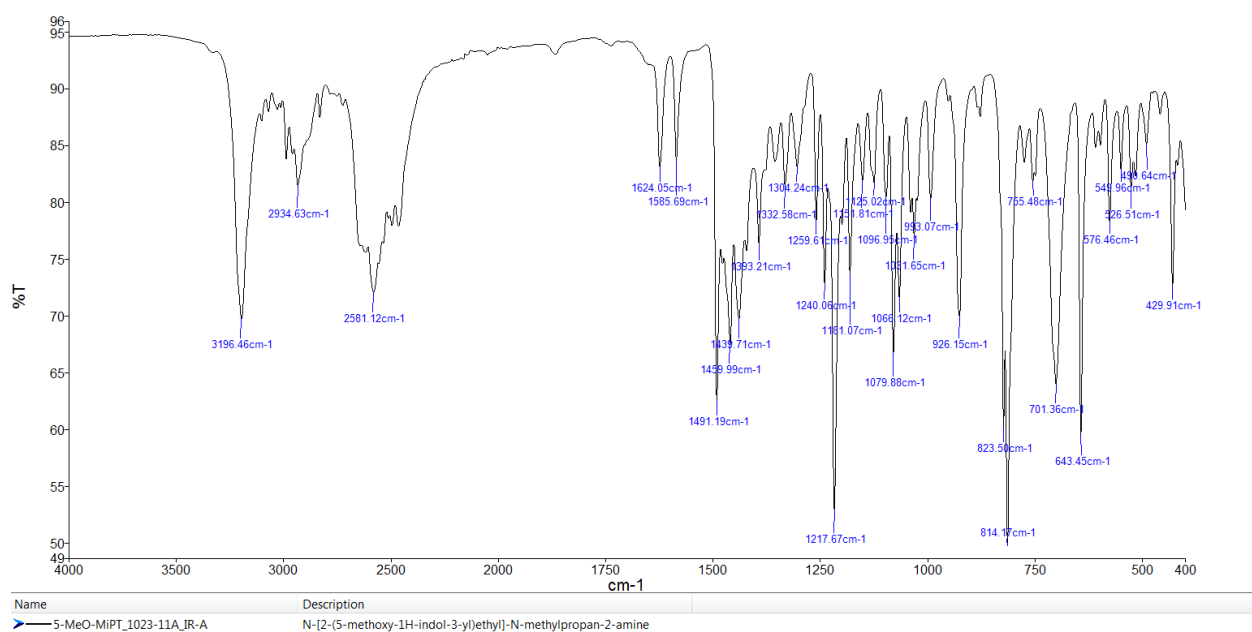
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 8,01 BP(1): 86; BP(2): 160,BP(3) :117,
HPLC-TOF	+	Exact mass (theoretical): 246,1732; measured value Δppm:0,37; formula:C15H22N2O
FTIR-ATR	+	direct measurement (sample as received)
FTIR (solid phase) always as base form	-	
IC (anions)	-	
NMR (in FKKT)	+	
validation		
other		

ANALYTICAL RESULTS

MS (EI)



FTIR-ATR - direct measurement (sample as received)



TOF REPORT

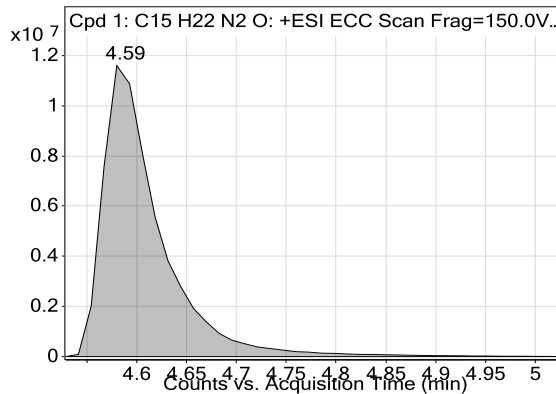
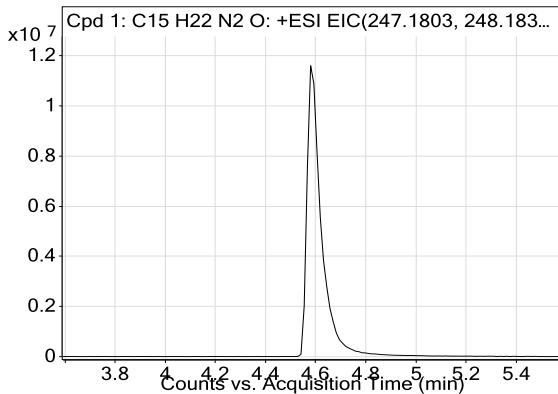
Data File	5-MeO_MiPT.d	Sample Name	ID 1023-11a
Sample Type	Sample	Position	P1-C3
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-04_12_2017-XDB-C18-ESI+.m	Acquired Time	5/28/2018 12:55:24 PM
IRM Calibration Status	Success	DA Method	a-Drugs_NFL.m
Comment	MeOH		

Compound Table

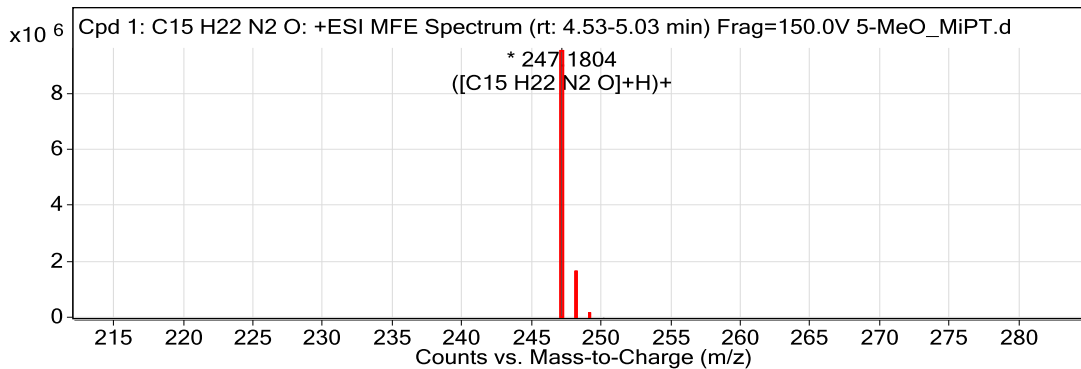
Label	MFG Formula	Obs. RT	Obs. Mass
Cpd 1: C15 H22 N2 O	C15 H22 N2 O	4.59	246.1731

Obs. m/z	Obs. RT	Obs. Mass
247.1804	4.59	246.1731

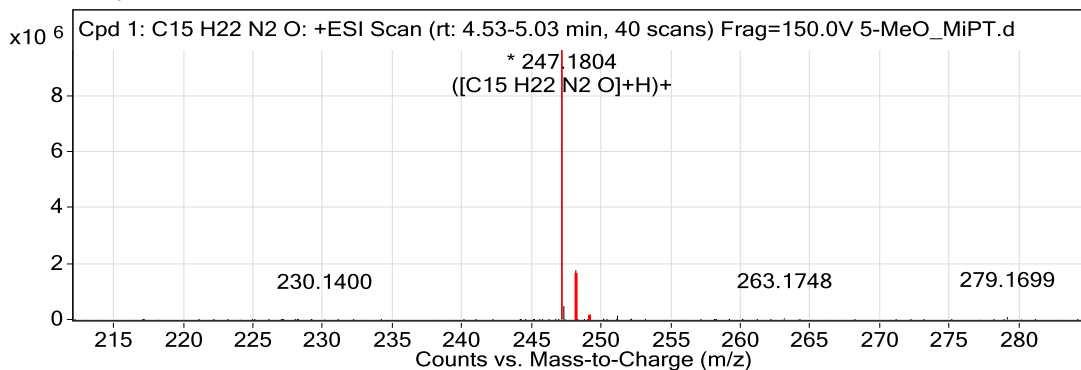
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
247.1804	1	9614706	C15 H22 N2 O	(M+H)+
248.1836	1	1579996.15	C15 H22 N2 O	(M+H)+
249.1866	1	139314.08	C15 H22 N2 O	(M+H)+

TOF REPORT

250.1927	1	8425.3	C15 H22 N2 O	(M+H)+
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--- End Of Report ---

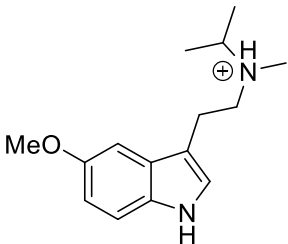
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University
of Ljubljana

Faculty of Chemistry
and Chemical Technology



R E P O R T

Contract No.	C1714-17-460078 (Republic of Slovenia, Ministry of the Interior, POLICE)
Sample ID:	1023-11A
Received date:	June 4, 2018
Our notebook code:	NFL-1023-11A
NMR sample preparation:	6.0 mg dissolved in 0.7 mL DMSO- <i>d</i> ₆
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 formula, exact mass, molecular weight:	 Chemical Formula: C₁₅H₂₃N₂O⁺ Exact Mass: 247,1805 Molecular Weight: 247,3615
Chemical name:	<i>N</i> -protonated <i>N</i> -(2-(5-methoxy-1 <i>H</i> -indol-3-yl)ethyl)- <i>N</i> -methylpropan-2-amine
Comments:	- Structure elucidation based on 1D and 2D NMR spectra and HRMS. - >98% purity of a sample based on ¹H NMR spectrum.
Supporting information:	Copies of ¹ H and ¹³ C NMR spectra, ¹ H and ¹³ C FIDs.
Principal investigator:	Prof. Dr. Janez Košmrlj
Date of report:	June 21, 2018

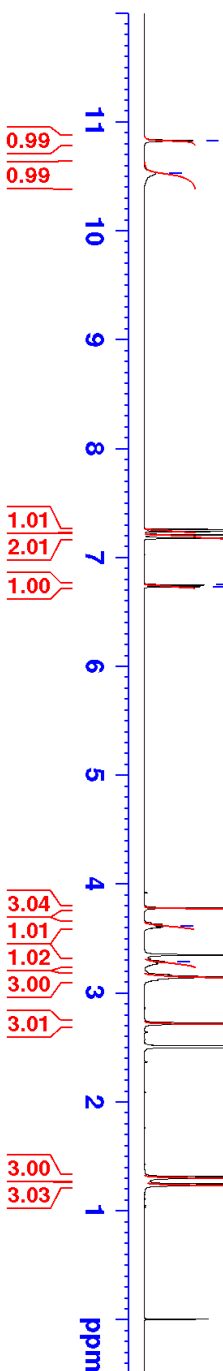
NFL-1023-11A

10.829
10.528

7.257
7.240
7.211
7.177
6.750
6.727

3.779
3.615
3.290
3.148
2.713

1.310
1.229



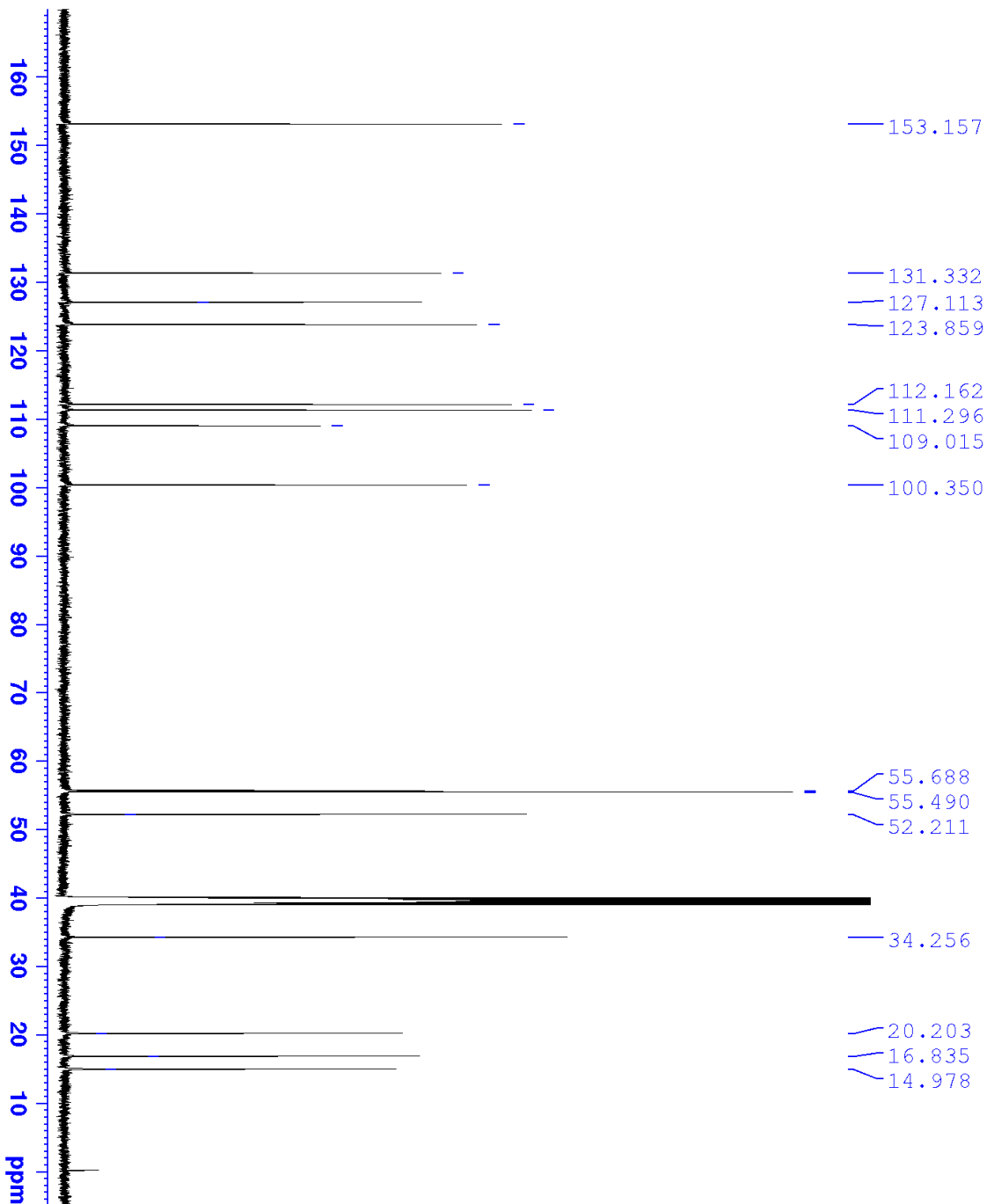
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Current Data Parameters
NAME      NFL-1023-11A
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20180613
Time      22.43
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        10000.000 Hz
FIDRES     0.152588 Hz
AQ         3.2767999 sec
RG         114
DM         50.000 usec
DE         6.50 usec
TE         296.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      500.130885 MHz
NUC1       1H
P1         8.70 usec
PLWL       26.00000000 W

F2 - Processing parameters
SI         65536
SF         500.130032 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



Current Data Parameters
NAME NFL-1023-11A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180614
Time 4.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 9216
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.101048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 8.70 usec
PL1 122.0000000 W

===== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
PCPD2 waltz16
PCPD2 80.00 usec
PLM2 26.00000000 W
PLM12 0.30046001 W
PLM13 0.15113001 W

F2 - Processing parameters
SI 32768
SF 125.7578465 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40