REPUBLIKA SLOVENIJA
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POLICIJA

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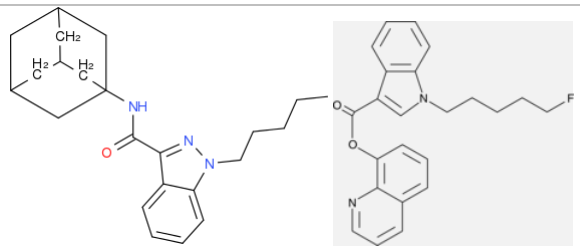
ANALYTICAL REPORT

AKB48 (C23H31N3O) and 5F-PB22

N-(1-adamantyl)-1-pentyl-1H-indazole-3-carboxamide,

Sample ID:	233-5422/2014
Sample description:	powder
Report date:	1/5/2015
Sample type:	S-seized

Substance identified-structure[i]	
Systematic name	N-(1-adamantyl)-1-pentyl-1H-indazole-3-carboxamide
Other names	AKB48, APINACA (NPS1)
Formula (per base form)	C23H31N3O
M_w (g/mol)	365,1
Salt form	base
Other compounds detected	5F-PB22 (5F-PB-22)
Smiles	C12(CC3CC(CC(C1)C3)C2)NC(=O)C2=NN(C3=CC=CC=C23)CCCCC
Compound Class	Cannabinoids

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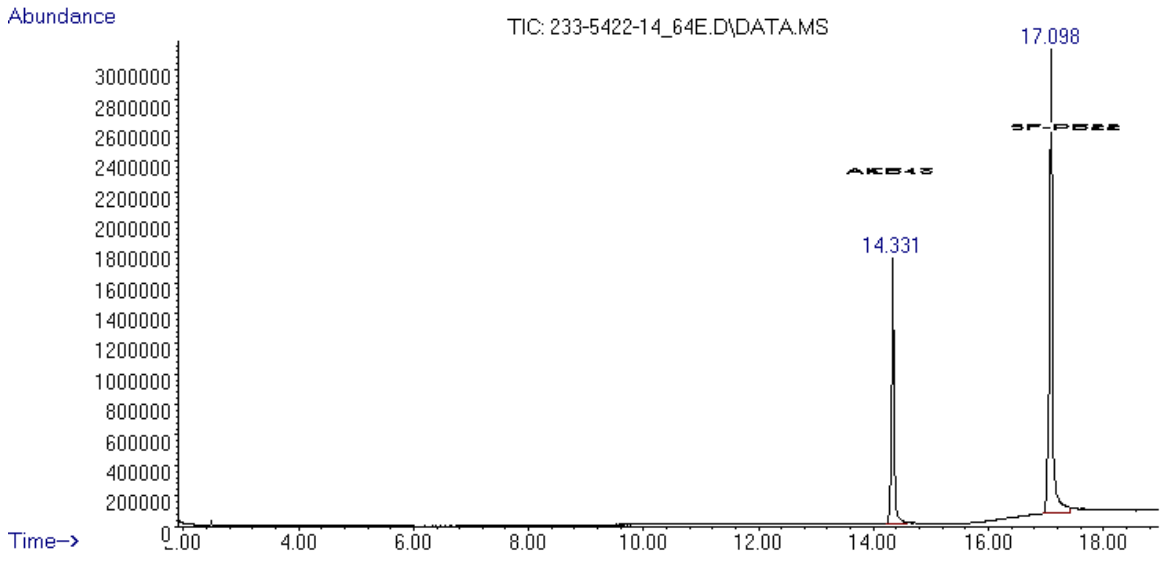
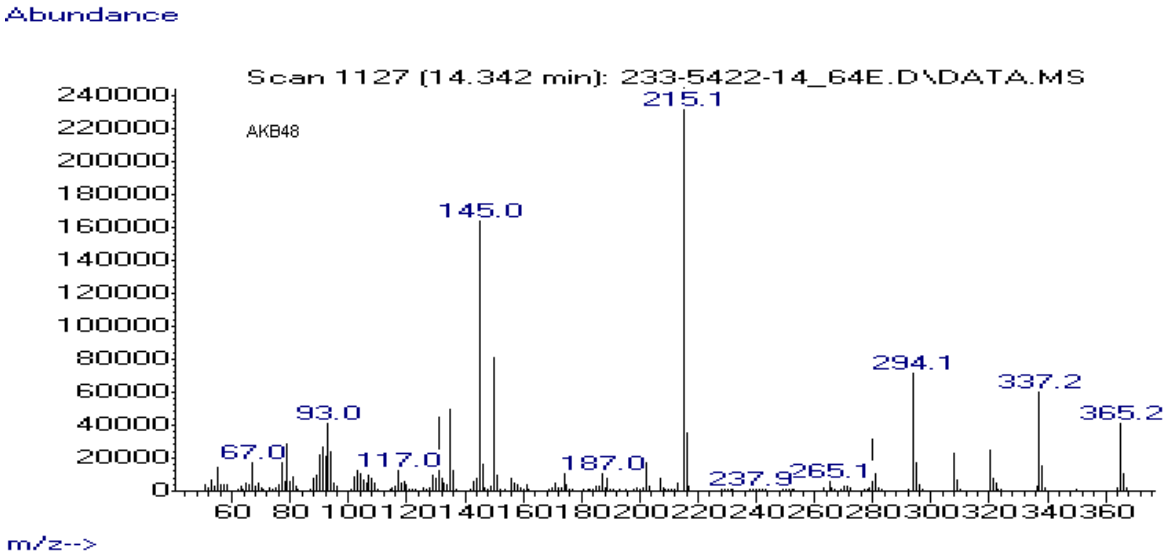
Supporting information

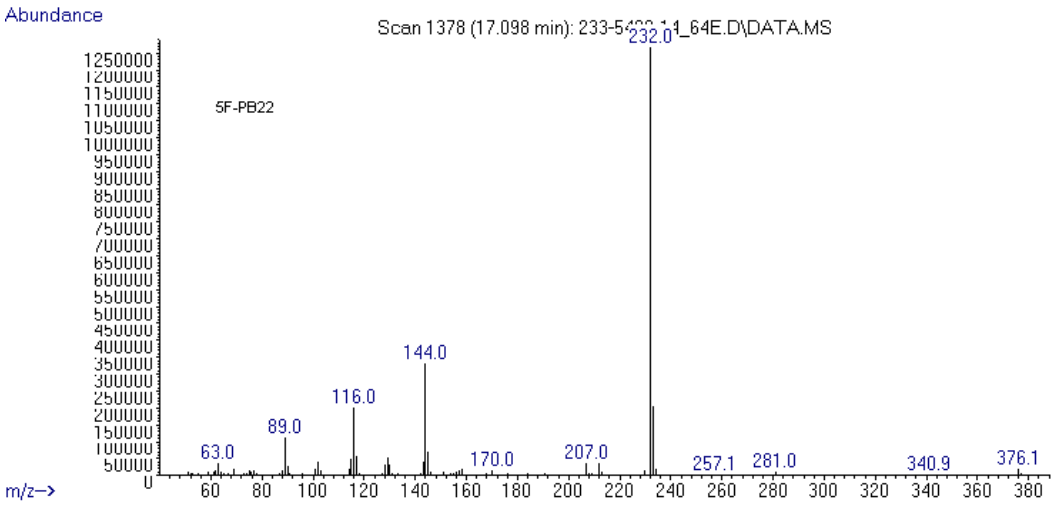
Analytical technique:	applied	remarks
GC-MS	+	two compounds
FTIR-ATR		not relevant - mixture
FTIR (condensed phase)		
HPLC-TOF	+	both confirmed
NMR-confirmed	+	both cofirmed (approximately 1:1 mix)
validation		
other		



AKB48-MS



5F-PB 22 MS (MW 376.1)



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

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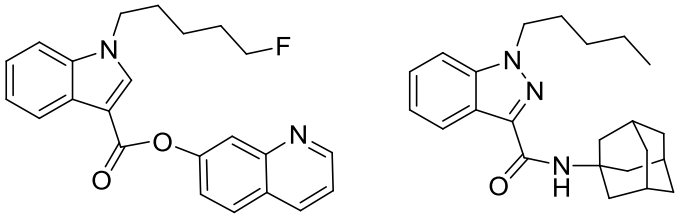
Dr. Janez Košmrlj
Professor of Organic Chemistry

January 17, 2015

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

Dear Dr. Sonja Klemenc,

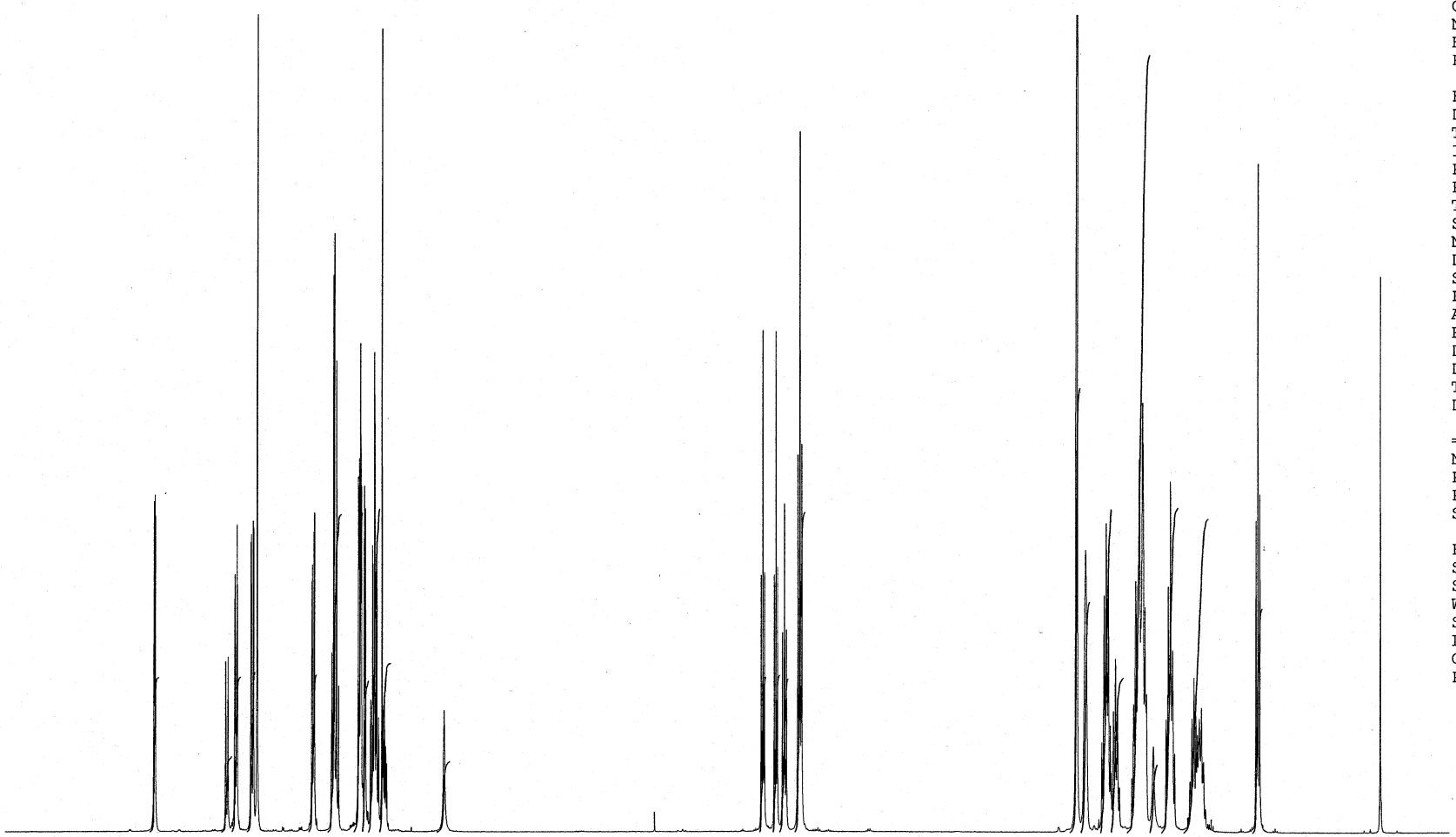
Please find enclosed the results of the structure elucidation for the sample:

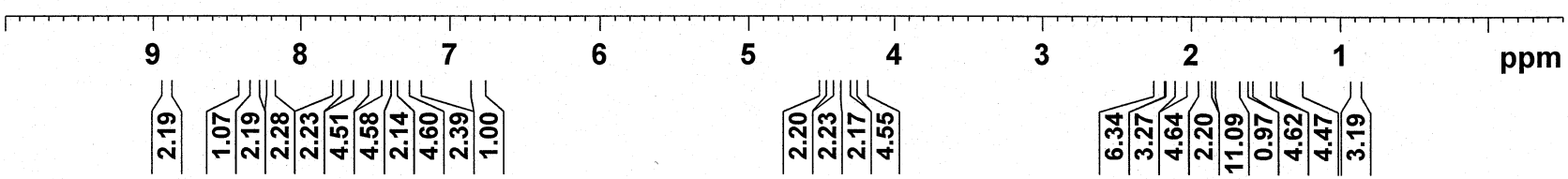
Sample ID:	**233-5422-14-64e**
Received date:	November, 2014
Our notebook code:	P-233-5422-14-64e
NMR sample preparation:	15 mg dissolved in 0.7 mL $CDCl_3$
NMR experiments:	^{1}H NMR, ^{13}C NMR
Proposed structure with atom numbering scheme, formula, exact mass, molecular weight:	Mixture of two compounds: 
Chemical name:	
Comments:	- The analysis of ^{1}H NMR and ^{13}C NMR spectra confirm the structures proposed by MS.
Supporting information:	Copies of ^{1}H and ^{13}C NMR spectra (pp 2-3)

Sincerely,

Janez Košmrlj

P-233-5422-14-64e





Current Data Parameters

NAME	P-233-5422-14-64e
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20141230
Time	19.12
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

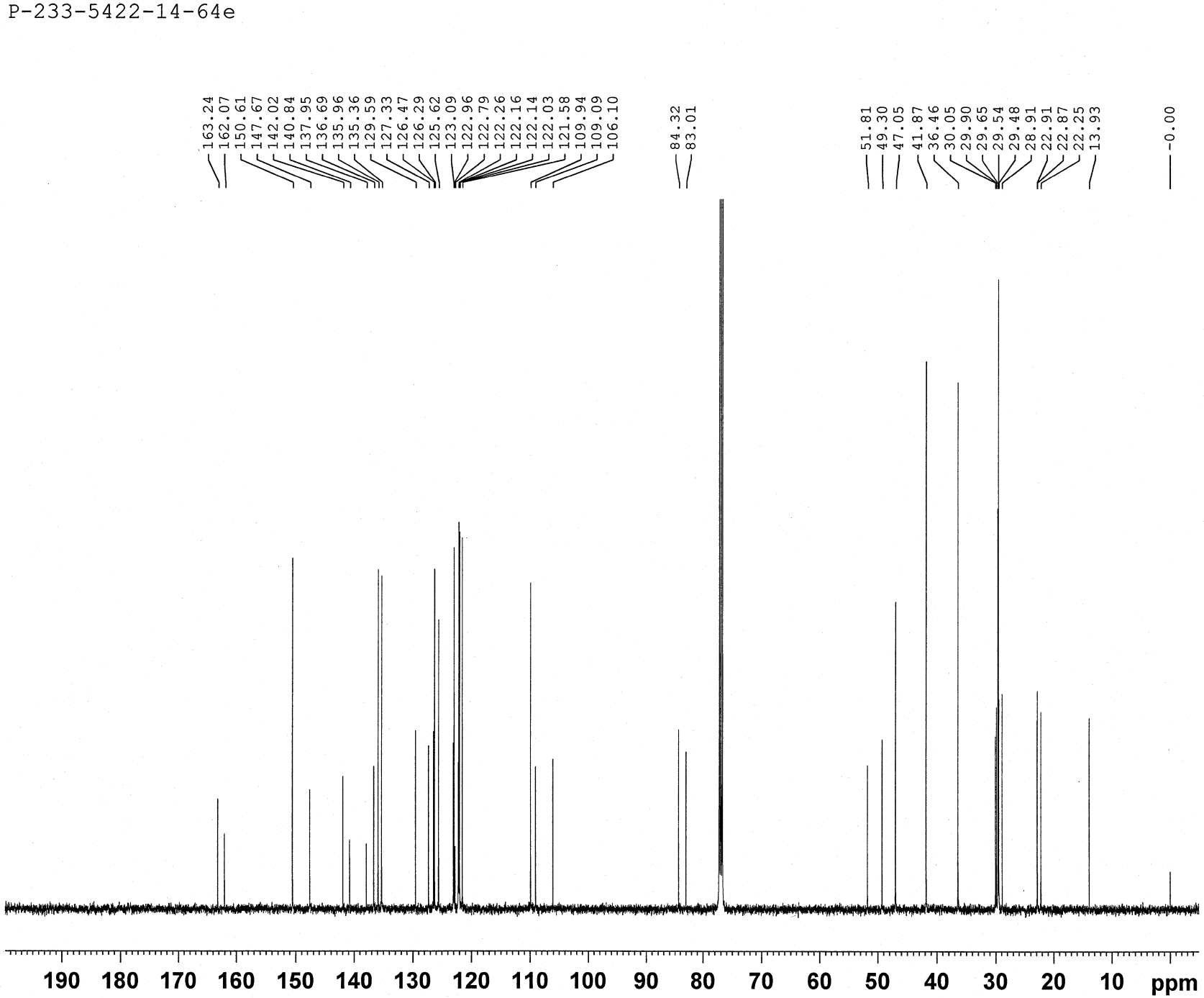
======== CHANNEL f1 ========

NUC1	1H
P1	8.90 usec
PLW1	26.00000000 W
SFO1	500.1330885 MHz

F2 - Processing parameters

SI	65536
SF	500.1300159 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

P-233-5422-14-64e



Current Data Parameters

NAME	P-233-5422-14-64e
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20141230
Time	21.40
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	4096
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	1.00000000 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	125.7577924 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40