EUROPEAN PROJECT RESPONSE to challenges in forensic drugs analyses

Co-funded by the Prevention of and Fight against Crime Programme of the European Union

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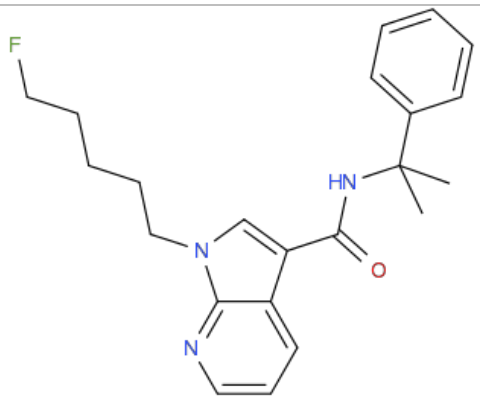
ANALYTICAL REPORT

CUMYL-5F-P7AICA, (C22H26FN3O)

1-(5-fluoropentyl)-N-(2-phenylpropan-2-yl)-7-azaindole-3-carboxamide

Remark – other NPS detected: none

Sample ID:	1154
Sample description:	powder - white
Sample type:	S-seized
Date of entry:	3/27/2015

Substance identified-structure[i] (base form)	
Systematic name	1-(5-fluoropentyl)-N-(2-phenylpropan-2-yl)-7-azaindole-3-carboxamide
Other names	
Formula (per base form)	C22H26FN3O
M_w (g/mol)	367,5
Salt form	base
StdInChIKey	MXJYOUMYJGNQEY-UHFFFAOYSA-N
Compound Class	Cannabinoids
Other NPS detected	none
Add.info (purity..)	Pure
Report updated:	13-Mar-16: “Smiles” code field was raplaced by “StdInChIKey” code filed and code corrected.

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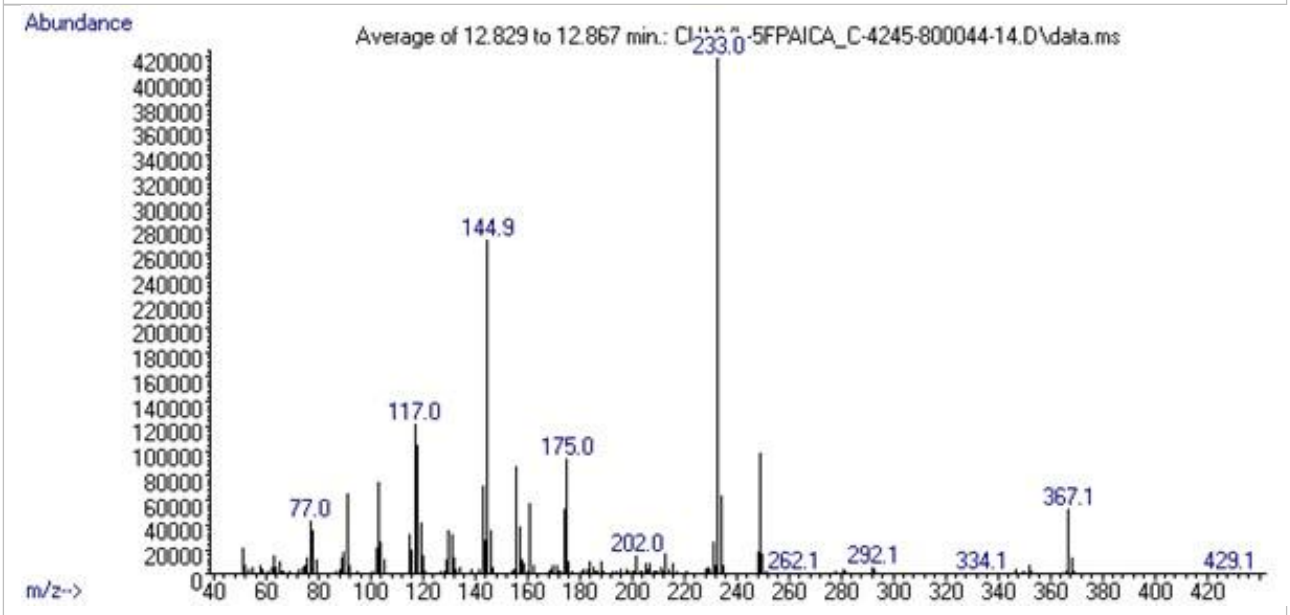
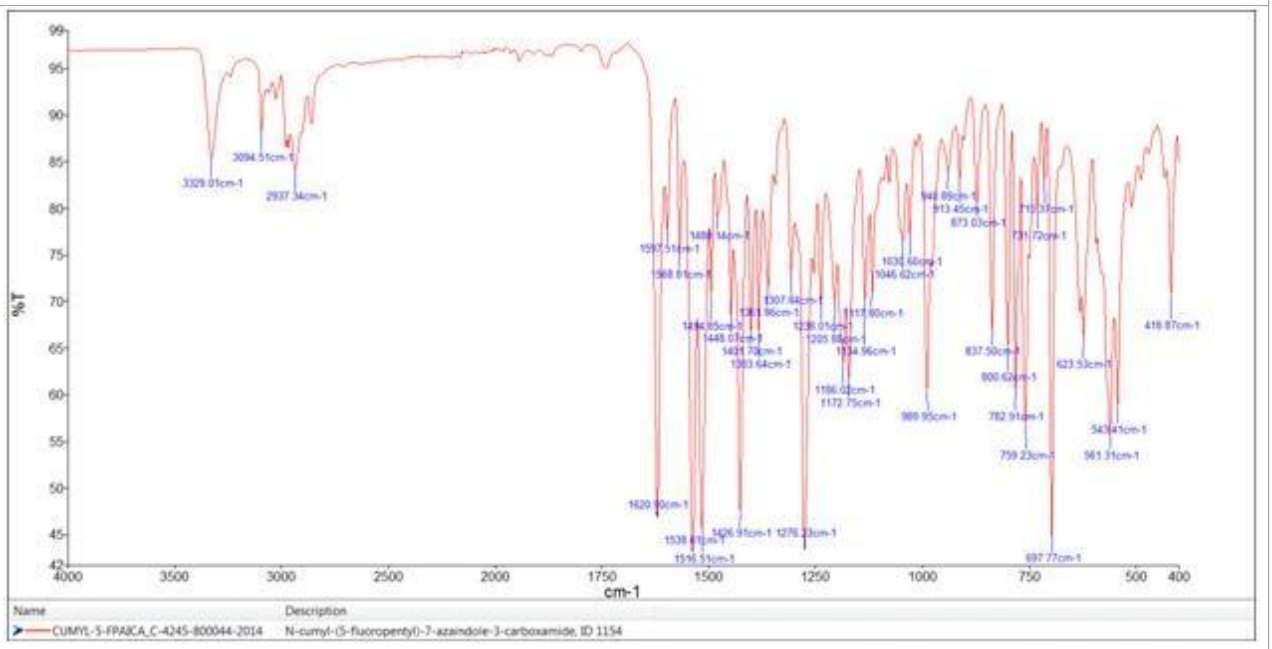
Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	BP(1): 233; BP(2): 145,BP(3) :117,
FTIR-ATR	+	
FTIR (condensed phase)	/	
HPLC-TOF	+	formula:C22H26FN3O
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

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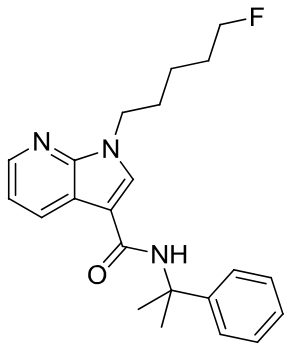
REPORT

Sample ID:	**CARINA 4245-800044/2014**
Received date:	February 12, 2015
Our notebook code:	P-4245-800044-2014
NMR sample preparation:	5 mg dissolved in 0.7 mL $CDCl_3$
NMR experiments:	^{1}H, ^{13}C
Proposed structure with chemical name:	 1-(5-fluoropentyl)-*N*-(2-phenylpropan-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine-3-carboxamide
Comments:	- Structure confirmed by ^{1}H and ^{13}C NMR spectra. - Compound is pure by NMR.
Supporting information:	Copies of ^{1}H and ^{13}C NMR spectra
Author:	Prof. Dr. Janez Košmrlj
Date of report:	February 14, 2015

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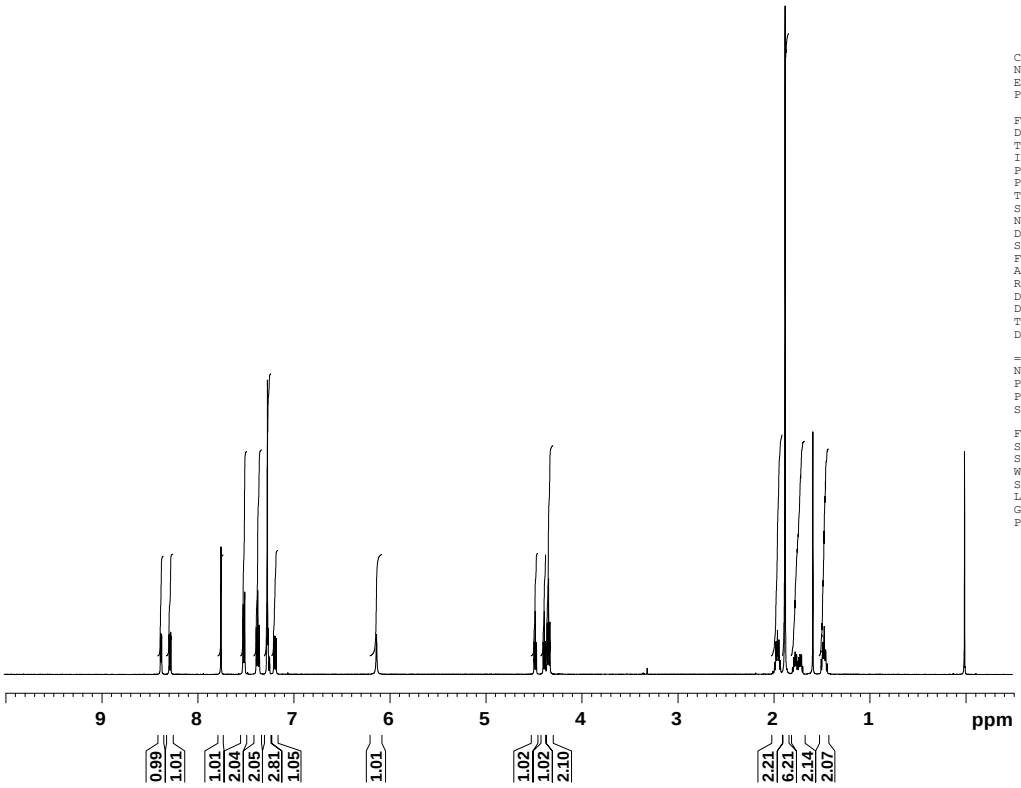
P-4245-800044-2014
1H



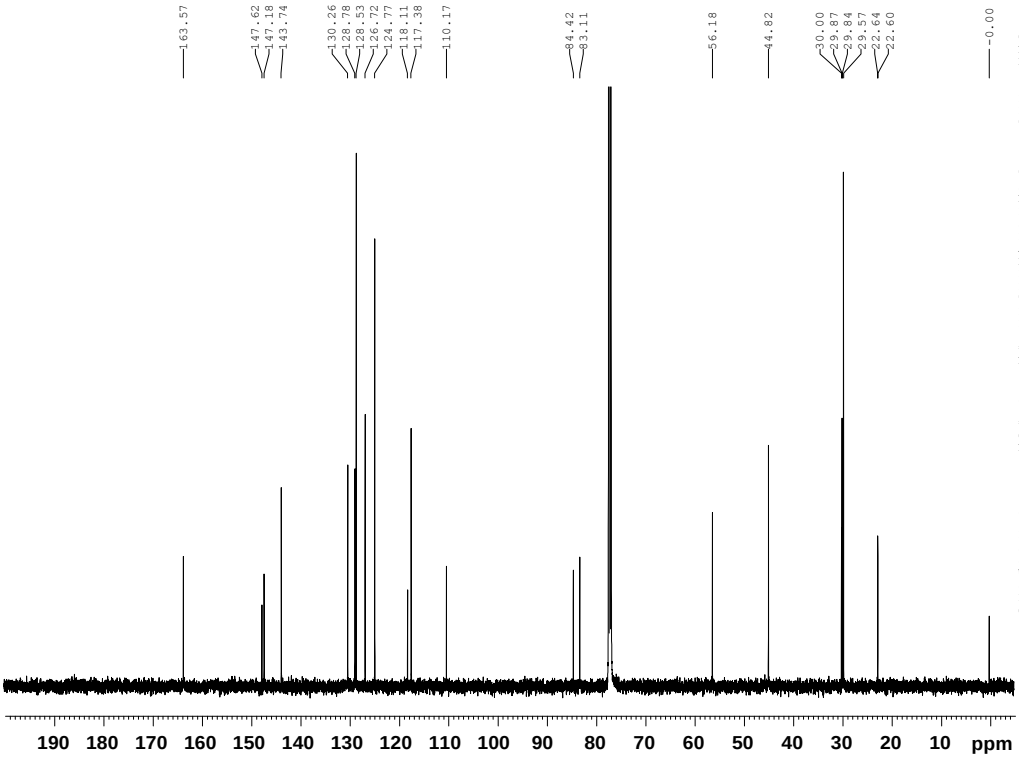

```
Current Data Parameters
NAME      P-4245-800044-2014
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150214
Time               6.26
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                  161
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           500.1300132 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

P-4245-800044-2014
13C




```
Current Data Parameters
NAME      P-4245-800044-2014
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150214
Time              11.26
INSTRUM           spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 8278
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010548 sec
RG                 1620
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           125.7577899 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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