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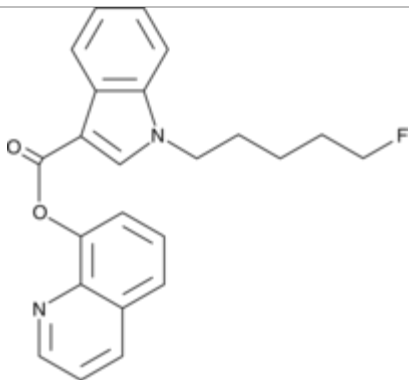
ANALYTICAL REPORT

5F-PB22, (C₂₃H₂₁FN₂O₂)

8-Quinoliny 1-(5-fluoropentyl)-1H-indole-3-carboxylate

Remark – other NPS detected: **AKB-48**

Sample ID:	1162
Sample description:	powder - brownish
Sample type:	S-seized
Date of entry:	3/27/2015

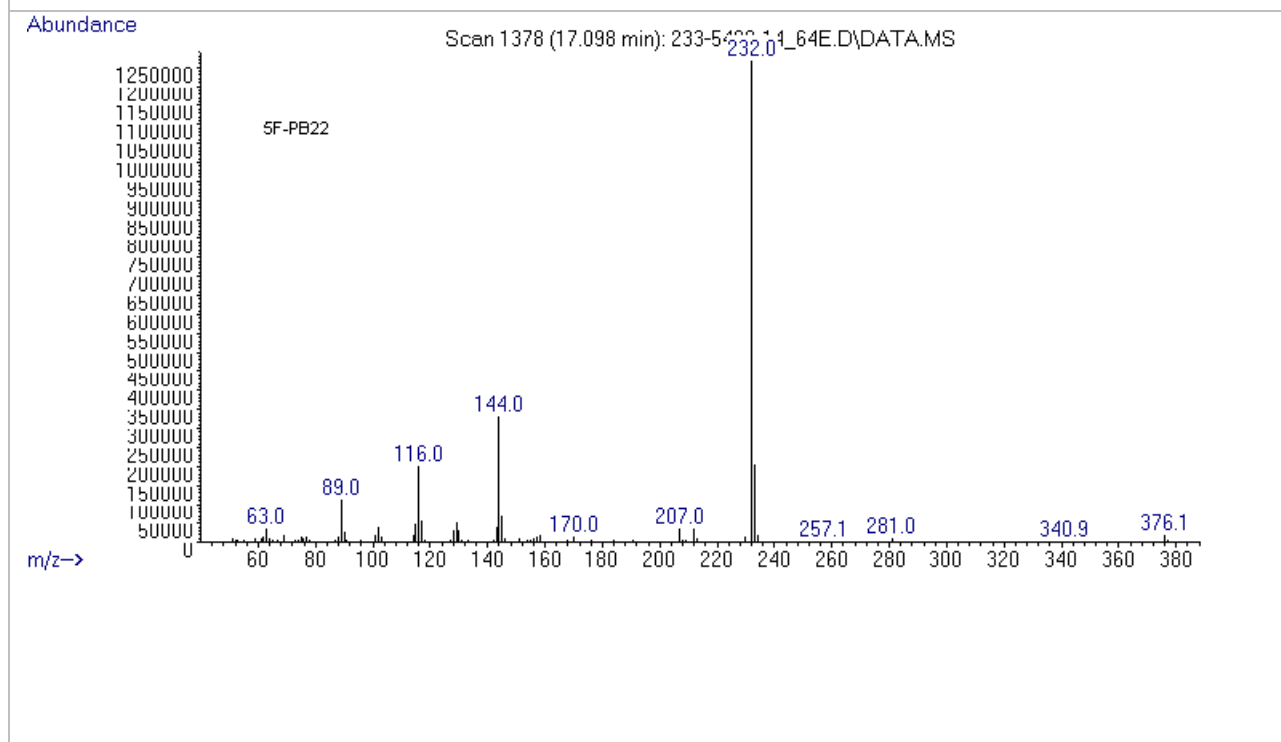
Substance identified- structure ⁱ (base form)	
Systematic name	8-Quinoliny 1-(5-fluoropentyl)-1H-indole-3-carboxylate
Other names	
Formula (per base form)	C ₂₃ H ₂₁ FN ₂ O ₂
M _w (g/mol)	376,4
Salt form	base
Smiles	<chem>FCCCCCN1C=C(C2=CC=CC=C12)C(=O)OC=1C=CC=C2C=CC=NC12</chem>
Compound Class	Cannabinoids
Other NPS detected	AKB-48
Add.info (purity..)	mixture with AKB-48 (1:1)

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 (EI ionization)	+	BP(1): 232; BP(2): 144,BP(3) :116,
FTIR-ATR	/	sample was a mixture
FTIR (condensed phase)	/	pending
HPLC-TOF	+	formula confirmed:C23H21FN2O2
NMR-confirmed	+	both substances in mixture (5F-PB22 and AKB48)
validation		
other		

MS spectrum (EI)



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



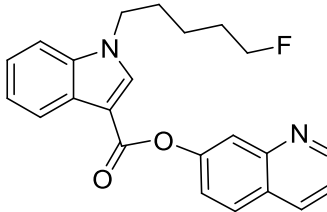
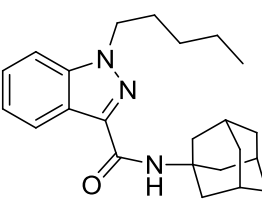
Dr. Janez Košmrlj
Professor of Organic Chemistry

January 17, 2015

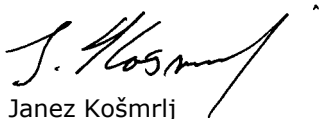
Dr. Sonja Klemenc
Head of Chemistry Department
Vodovodna 95
1000 Ljubljana
Slovenija

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: <div style="display: flex; justify-content: space-around; align-items: center;">   </div>
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

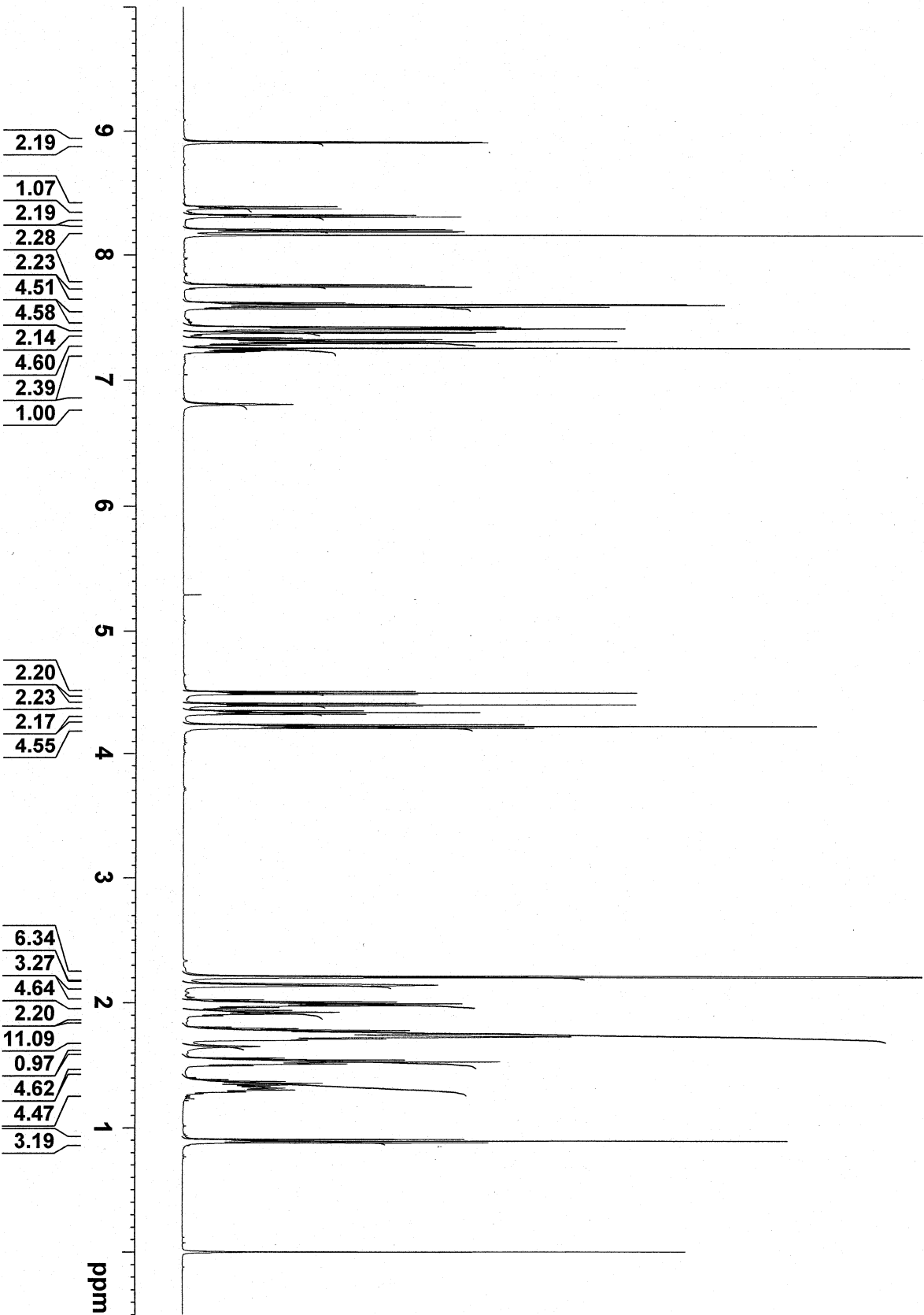


Current Data Parameters
 NAME P-233-5422-14-64e
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141230
 Time_ 19.12
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 CDCL3 CDC13
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 101
 DE 48.400 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





163.24
162.07
150.61
147.67
142.02
140.84
137.95
136.69
135.96
135.36
129.59
127.33
126.47
126.29
125.62
123.09
122.96
122.79
122.26
122.16
122.14
122.03
121.58
109.94
109.09
106.10

84.32
83.01

51.81
49.30
47.05
41.87
36.46
30.05
29.90
29.65
29.54
29.48
28.91
22.91
22.87
22.25
13.93

-0.00

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 1.1010348 sec
RG 2050
DM 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 122.0000000 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 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577924 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

