REPUBLIKA SLOVENIJA
MINISTRSTVO ZA NOTRANJE ZADEVE
POLICIJA

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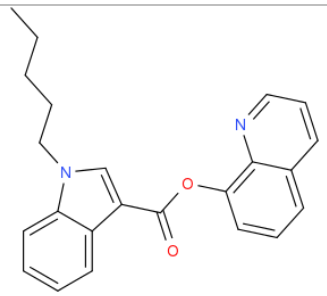
ANALYTICAL REPORT

PB-22 (C23H22N2O2)

1-pentyl-8-quinolinyl ester-1H-indole-3-carboxylic acid,

Sample ID:	233-3560/2014
Sample description:	powder
Analyses/ report (date):	18/ SEPTEMBER 2014
Sample type:	S-seized

Substance identified-structure[i]	
Systematic name	1-pentyl-8-quinolinyl ester-1H-indole-3-carboxylic acid
Other names	PB-22, QUPIC
Formula (per base form)	C23H22N2O2
M_w (g/mol)	358,43
Salt form	/
Other compounds detected	/
Smiles	C(CCCC)N1C=C(C2=CC=CC=C12)C(=O)OC=1C=CC=C2C=CC=NC12
Compound Class	Cannabinoids

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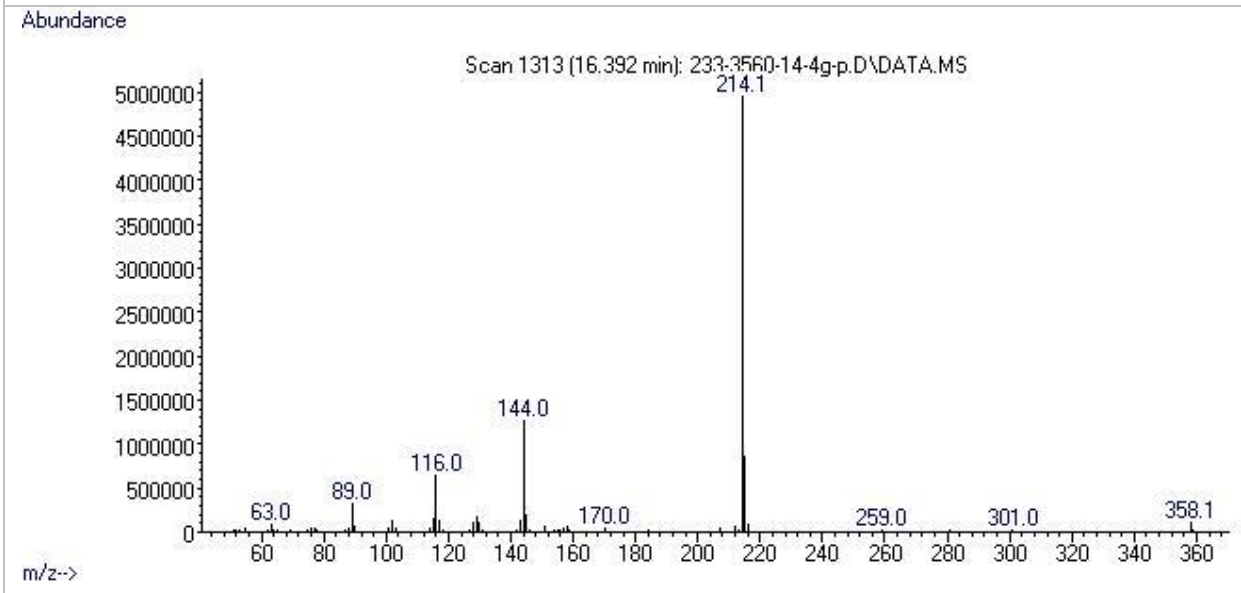
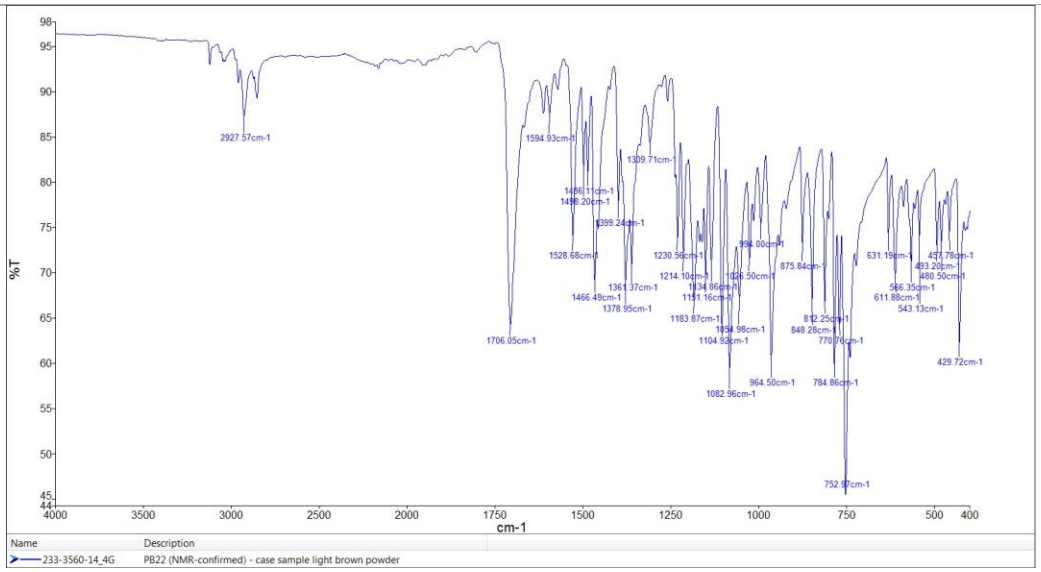
Supporting information

Analytical technique:	applied	remarks
GC-MS	+	RT and MS consistent with Cerilliant reference materialand; MS consistant with SWGDRUG lib entry and Caymans lib entry PB22, match quality 0.96 and 0.97 respectively
FTIR-ATR	+	direct measurement, differs slightly from SWGDRUG library
FTIR (condensed phase)	/	
HPLC-TOF	+	RT consistent with CRM (Cerilliant), delta ppm from the theoretical mass mono isotopic : -1.29ppm
NMR-confirmed	-	
validation		NMR pending
other		PB-22 (possibly contaminated) or in different polymorphic form from the entry in SWGDRUG IR library

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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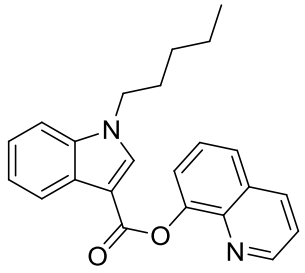
REPORT

Sample ID:	**233-3560-2014-46**
Our notebook code:	P-233-3560-2014-46
NMR sample preparation:	15 mg dissolved in 0.7 mL DMSO-d_6
NMR experiments:	^{1}H, ^{13}C, ^{1}H–^{1}H *gs*-COSY, ^{1}H–^{13}C *gs*-HSQC, ^{1}H–^{13}C *gs*-HMBC, ^{1}H–^{15}N *gs*-HMBC
Proposed structure with chemical name:	 quinolin-8-yl 1-pentyl-1*H*-indole-3-carboxylate
Comments:	- Structure elucidation based on 1D and 2D NMR spectra - Data in agreement with: V. Shevyrin et al., *Forensic Science International* **2013**, *232*, 1–10. - Compound is pure by NMR
Supporting information:	Copies of ^{1}H and ^{13}C NMR spectra
Author:	Prof. Dr. Janez Košmrlj
Date of report:	April 30, 2015

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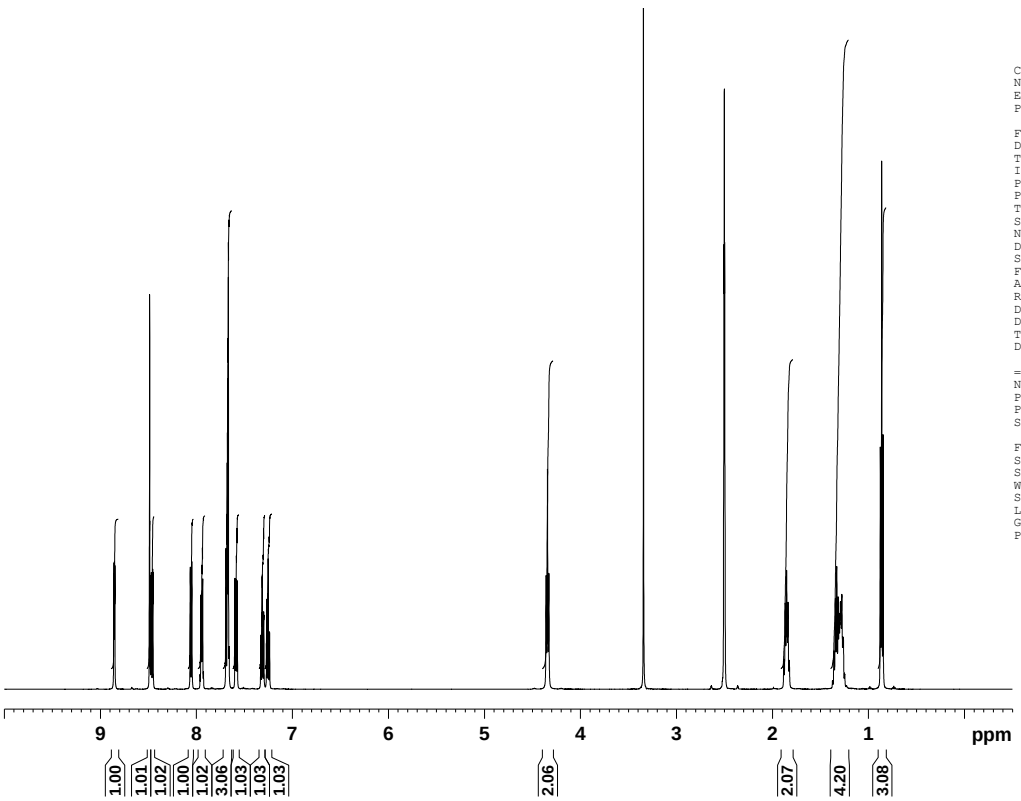
P-233-3560-2014-46
1H



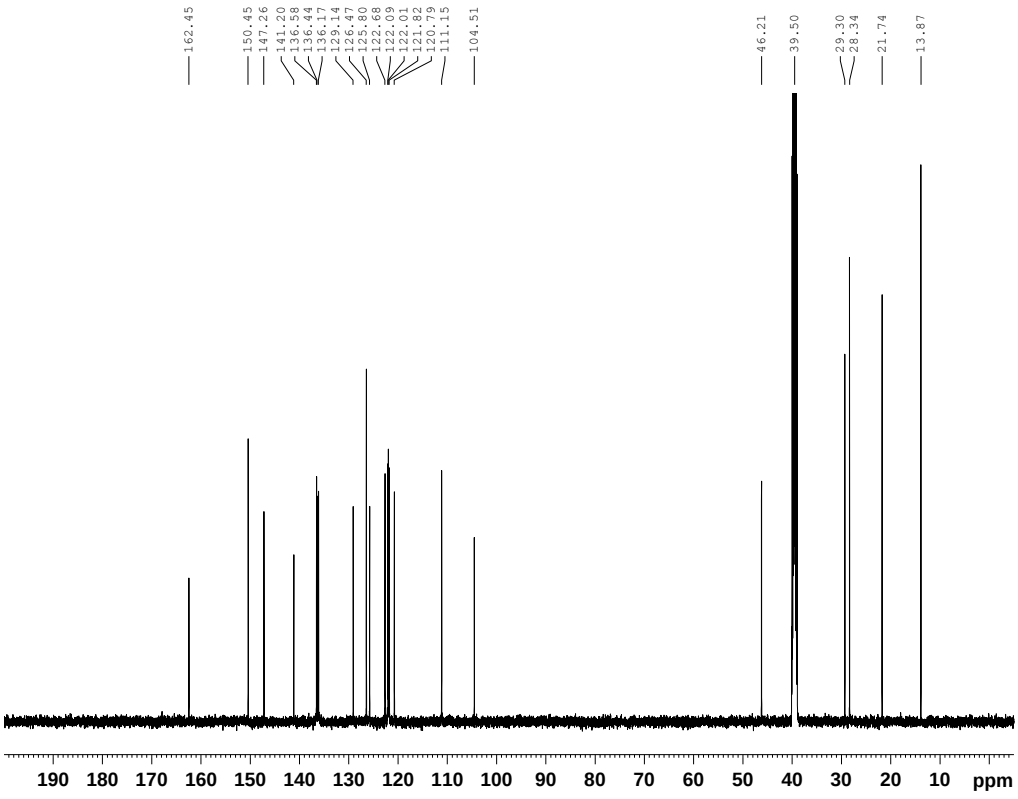

```
Current Data Parameters
NAME      P233-3560-2014-46
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20150307
Time                 13.49
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                      16
DS                       2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719923 sec
RG                    90.5
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            500.1300056 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

P-233-3560-2014-46
13C




```
Current Data Parameters
NAME      P233-3560-2014-46
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20150308
Time                  2.34
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT              DMSO
NS                    2048
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            125.7578500 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```