



ANALYTICAL REPORT

AB-FUBINACA

(C₂₀H₂₁FN₄O₂)

N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1H-indazole-3-carboxamide,

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

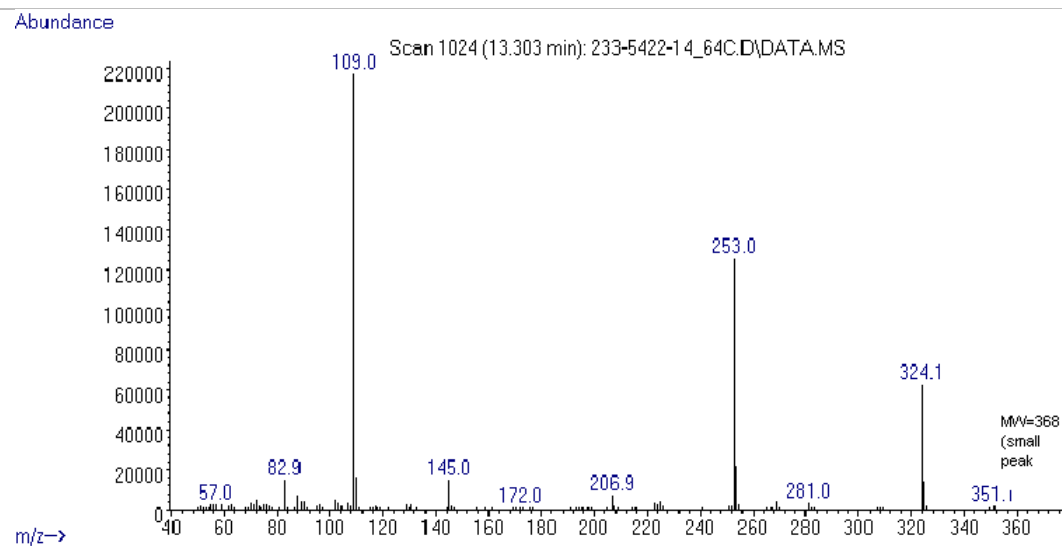
Substance identified- structure ⁱ	
Systematic name	N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1H-indazole-3-carboxamide
Other names	AB-FUBINACA ,
Formula (per base form)	C ₂₀ H ₂₁ FN ₄ O ₂
M _w (g/mol)	368.41
Salt form	base
Other compounds detected	
Smiles	<chem>NC(C(C)C)NC(=O)C1=NN(C2=CC=CC=C2)CC1=CC=C(C=C1)F=O</chem>
Compound Class	Cannabinoids

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.

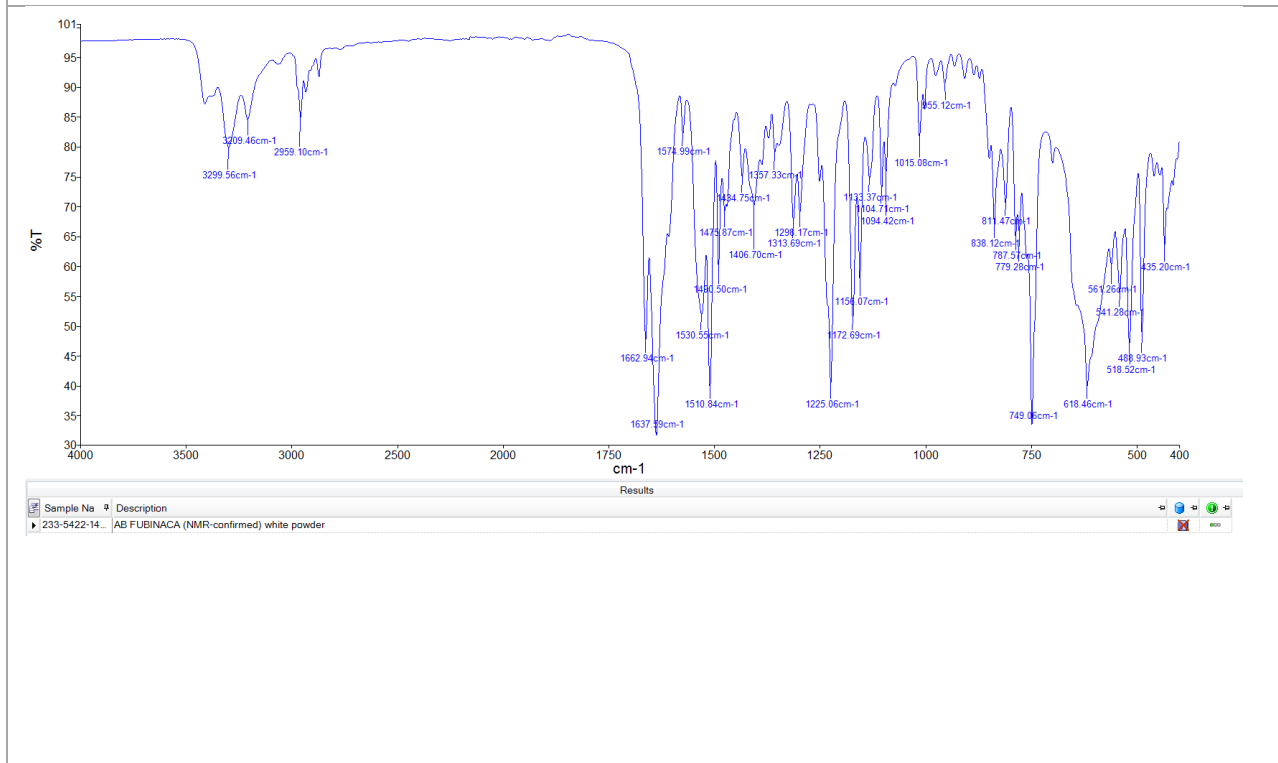
Supporting information

Analytical technique:	applied	remarks
GC-MS	+	
FTIR-ATR	+	
FTIR (condensed phase)		
HPLC-TOF	+	
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



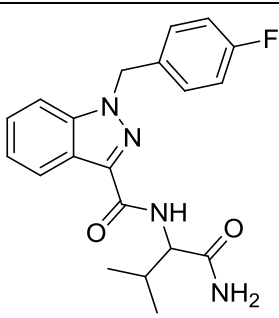
Dr. Janez Košmrlj
Professor of Organic Chemistry

January 17, 2015

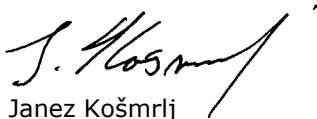
Dr. Sonja Klemenc
Head of Chemistry Department
Vodovodna 95
1000 Ljubljana
Slovenija

Dear Dr. Sonja Klemenc,

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

Sample ID:	233-5422-14-64c
Received date:	November, 2014
Our notebook code:	P-233-5422-14-64c
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:	 Chemical Formula: C₂₀H₂₁FN₄O₂ Exact Mass: 368.1649 Molecular Weight: 368.4047
Chemical name:	<i>N</i> -(1-Amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1 <i>H</i> -indazole-3-carboxamide
Comments:	- The analysis of ¹ H NMR and ¹³ C NMR spectra confirm the structure proposed by MS.
Supporting information:	Copies of ¹ H and ¹³ C NMR spectra (pp 2-3)

Sincerely,


Janez Košmrlj

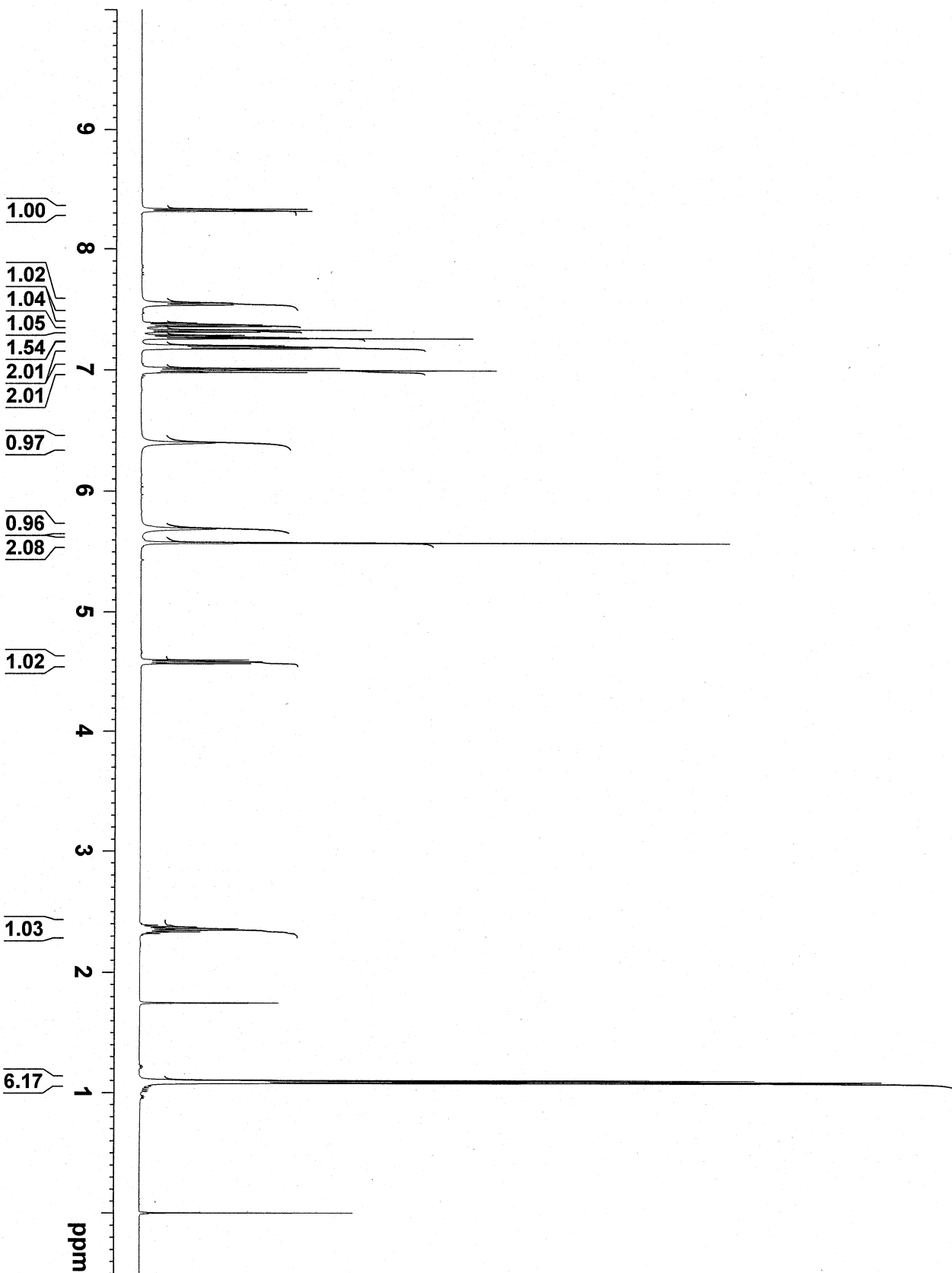


Current Data Parameters
 NAME P-233-5422-14-64C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141231
 Time_ 5.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 114
 DW 48.400 usec
 DE 6.50 usec
 TE 296.1 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 500.1300126 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
 NAME P-233-5422-14-64c
 EXENO 2
 PROCNO 1

173.50
 163.46
 162.76
 161.50
 140.78
 137.10
 131.62
 131.59
 129.03
 128.97
 127.14
 123.24
 122.99
 122.69
 115.91
 115.74
 109.55
 57.83
 52.95
 30.67
 19.49
 18.25
 0.00

F2 - Acquisition Parameters
 Date_ 20141231
 Time 7.50

INSTRUM spect
 PROBD 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 295.9 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 125.7577903 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

