REPUBLIKA SLOVENIJA
MINISTRSTVO ZA NOTRANJE ZADEVE
POLICIJA

NACIONALNI FORENZIČNI LABORATORIJ
NATIONAL FORENSIC LABORATORY

Vodovodna 95
1000 Ljubljana
SLOVENIJA

T: +386 (0)1 428 44 93
E: nfl@policija.si
www.policija.si

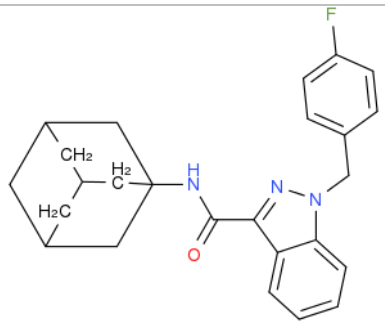
Co-funded by the Prevention of and Fight against Crime Programme of the European Union

ANALYTICAL REPORT

AKB48-4-fluorobenzyl analog, FUB-AKB48 (C25H26FN3O)

N-((3s,5s,7s)-adamantan-1-yl)-1-(4-fluorobenzyl)-1H-indazole-3-carboxamide,

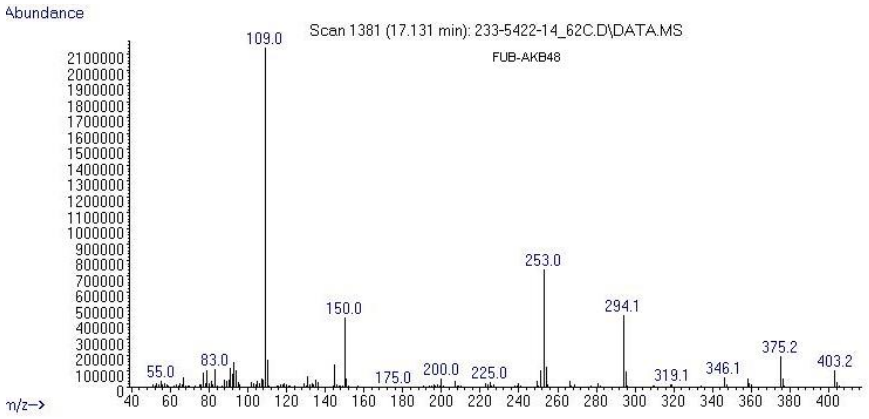
Sample ID:	233-5422/2014
Sample description:	powder
Report date:	1/5/2015
Sample type:	S-seized

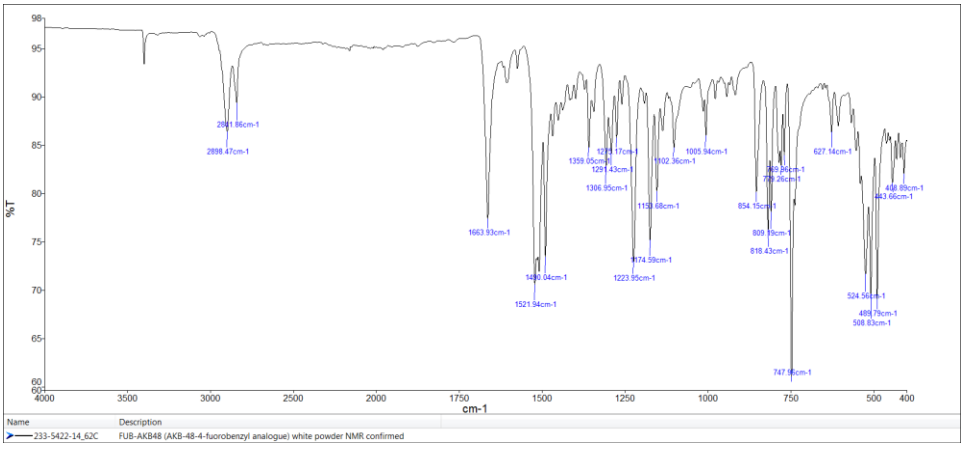
Substance identified-structure[i]	
Systematic name	N-((3s,5s,7s)-adamantan-1-yl)-1-(4-fluorobenzyl)-1H-indazole-3-carboxamide
Other names	AKB48-4-fluorobenzyl analog, FUB-AKB48,
Formula (per base form)	C25H26FN3O
M_w (g/mol)	403,49
Salt form	base
Other compounds detected	none
Smiles	C12(CC3CC(CC(C1)C3)C2)NC(=O)C2=NN(C3=CC=CC=C23)CC2=CC=C(C=C2)F
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	+	spectrum enclosed
FTIR-ATR	+	spectrum enclosed
FTIR (condensed phase)	-	
HPLC-TOF	+	
NMR-confirmed	+	
validation	-	
other	-	





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

NFL cpd ID:1159

University
of Ljubljana

Faculty *of Chemistry and Chemical Technology*

Aškerčeva 5
P.O. Box 537
SI-1001 Ljubljana
Slovenia
Phone: (+386)-1-241-9256
Fax: (+386)-1-241-9220
janez.kosmrlj@fkkt.uni-lj.si

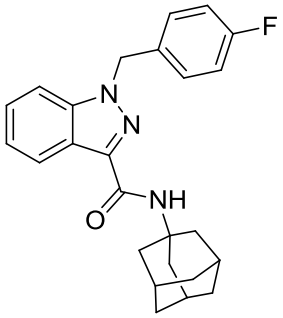
Dr. Janez Košmrlj
Professor of Organic Chemistry

January 17, 2015

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

Dear Dr. Sonja Klemenc,

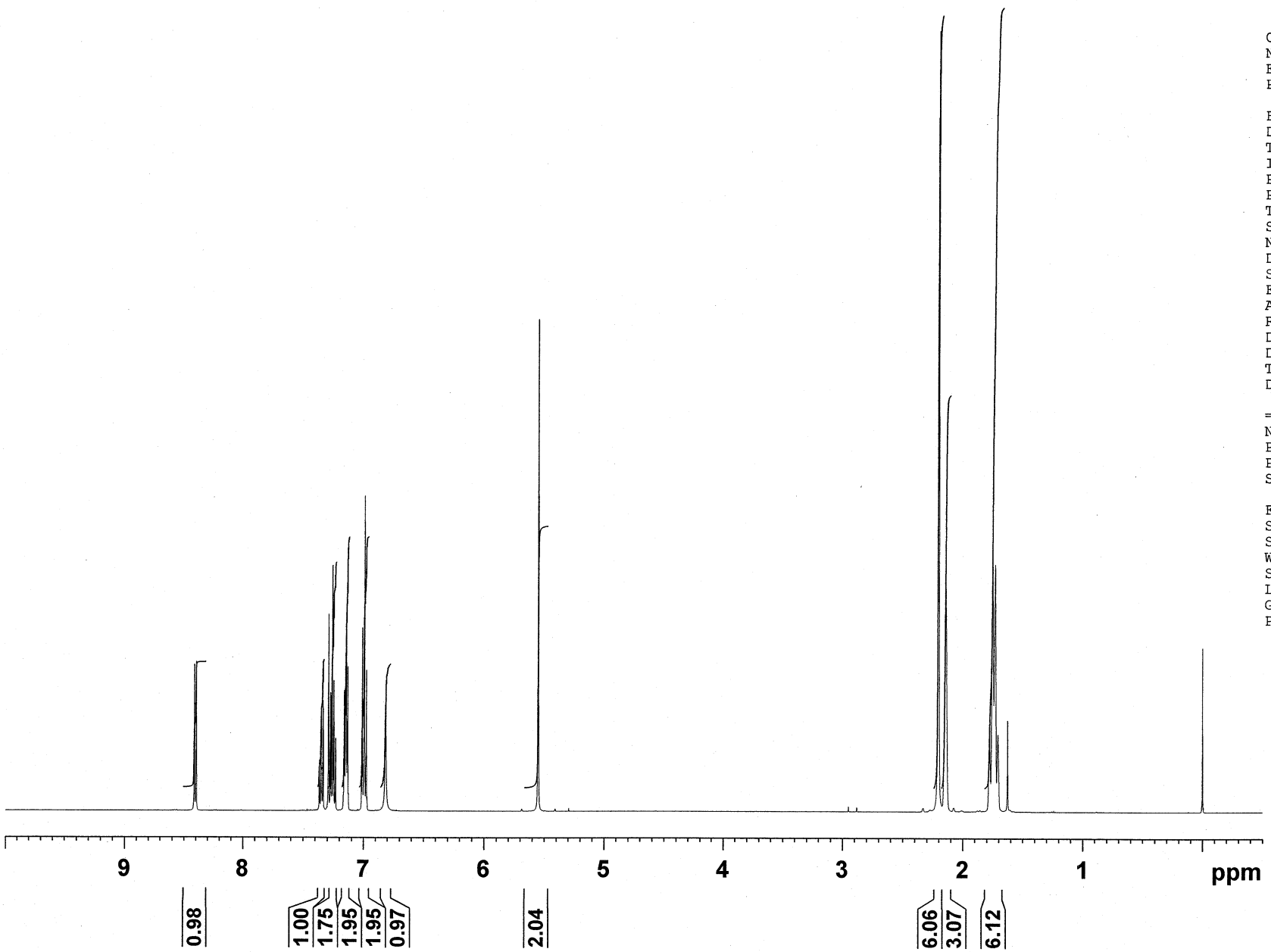
Please find enclosed the results of the structure elucidation for the sample:

Sample ID:	**233-5422-14-62c**
Received date:	November, 2014
Our notebook code:	P-233-5422-14-62c
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: $C_{25}H_{26}FN_3O$ Exact Mass: 403.2060 Molecular Weight: 403.4918
Chemical name:	*N*-(Adamantan-1-yl)-1-(4-fluorobenzyl)-1*H*-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

P-233-5422-14-62c



Current Data Parameters

NAME	P-233-5422-14-62c
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20141230
Time	21.44
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

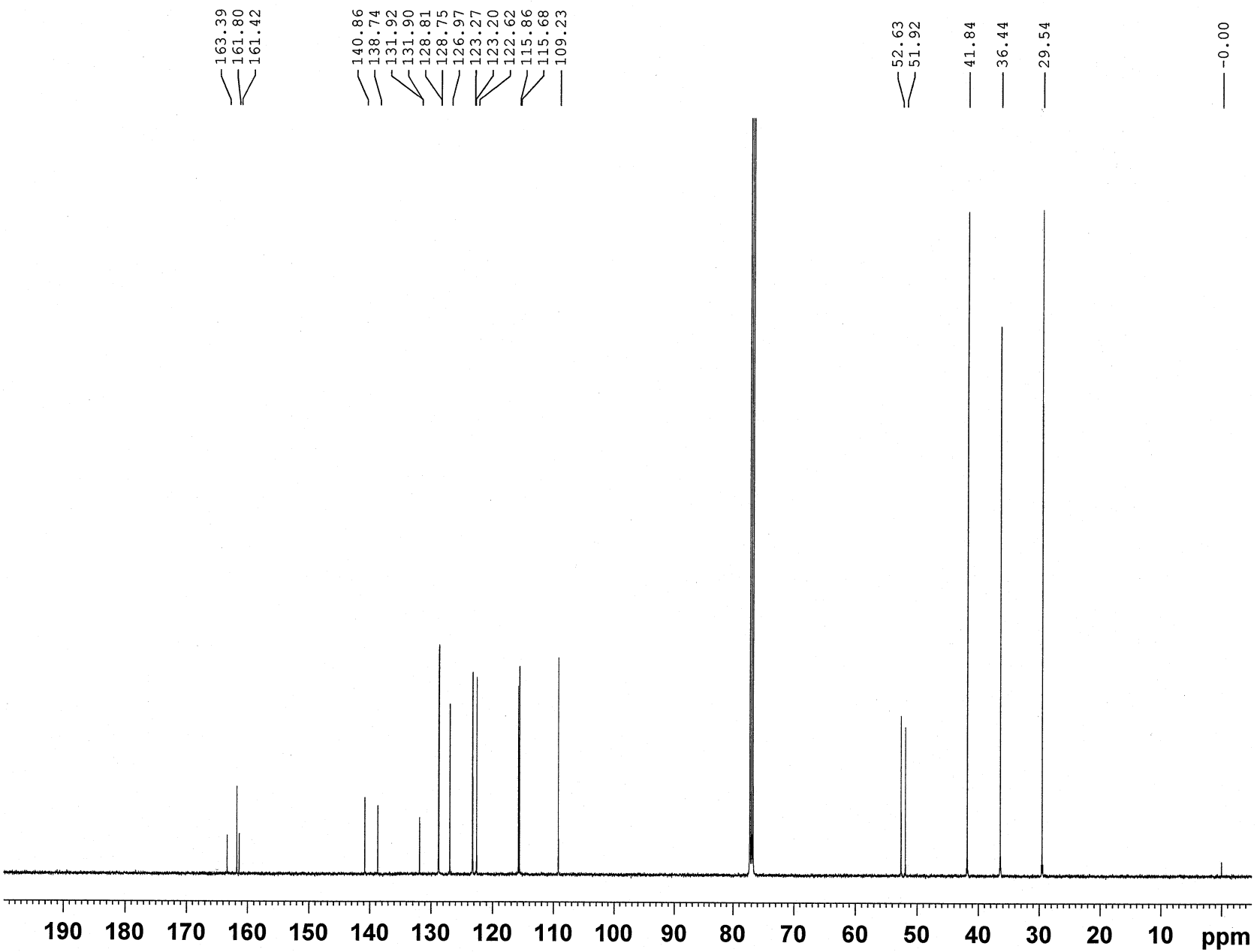
======== CHANNEL f1 ========

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

F2 - Processing parameters

SI	65536
SF	500.1300137 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

P-233-5422-14-62c



BRUKER

Current Data Parameters
NAME P-233-5422-14-62c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141231
Time 0.13
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 125.7577914 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40