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

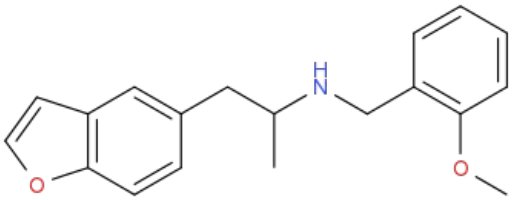
ANALYTICAL REPORT

5-APB NBOMe, (C19H21NO2)

1-(benzofuran-5-yl)-N-(2-methoxybenzyl)propan-2-amine

Remark – other NPS detected: none

Sample ID:	1175-15
Sample description:	powder - white
Sample type:	P- purchased
Date of entry:	4/17/2015

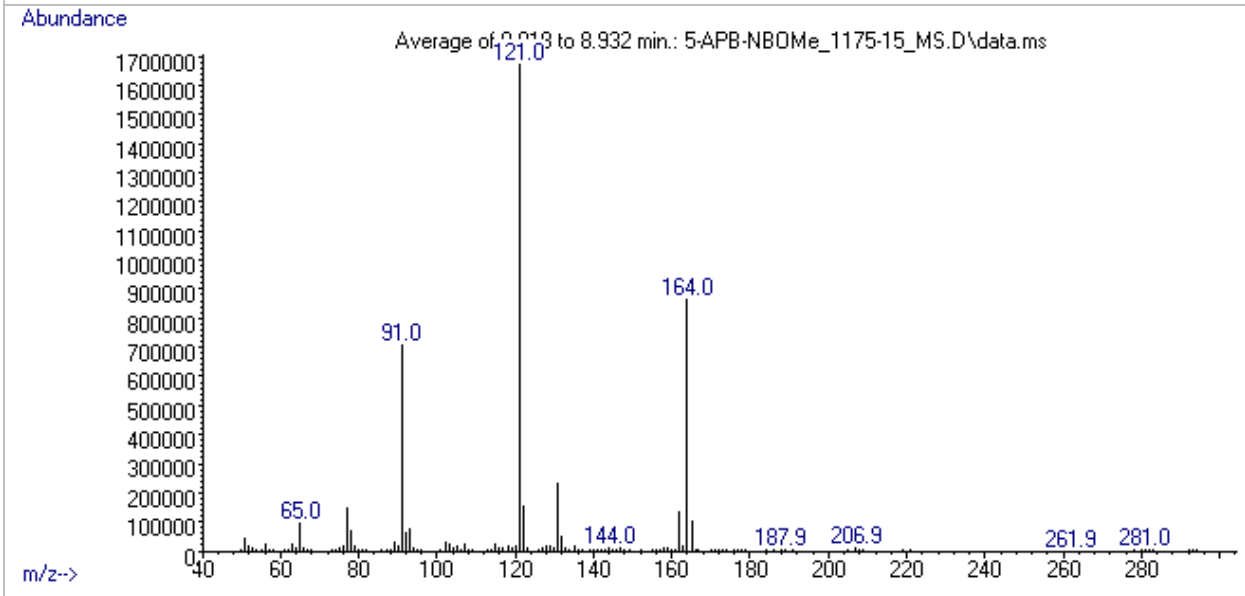
Substance identified-structure[i] (base form)	 *HCl
Systematic name	1-(benzofuran-5-yl)-N-(2-methoxybenzyl)propan-2-amine
Other names	
Formula (per base form)	C19H21NO2
M_w (g/mol)	295.38
Salt form	HCl
Smiles	O1C=CC2=C1C=CC(=C2)CC(C)NCC2=C(C=CC=C2)OC
Compound Class	Arylalkylamines
Other NPS detected	none
Add.info (purity..)	pure by NMR

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.

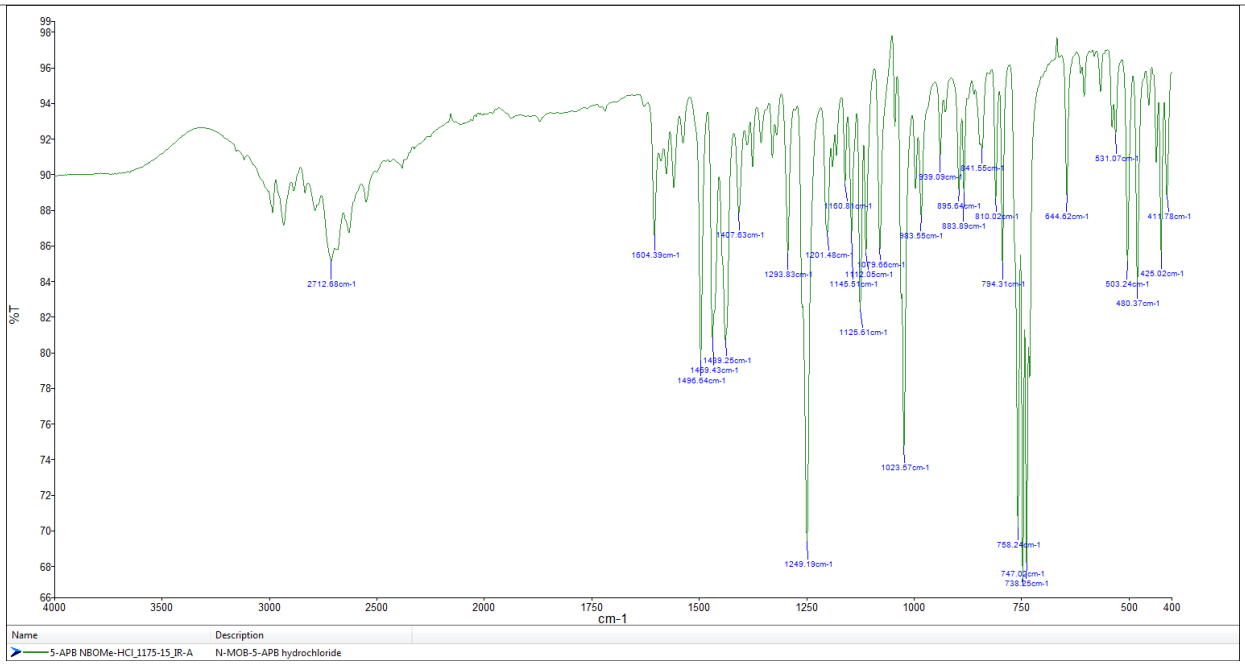
Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	BP(1): 121; BP(2): 164,BP(3) :91,
FTIR-ATR	+	HCl
FTIR (condensed phase)	/	pending
HPLC-TOF	+	Exact mass: 295.1572, measured/ Δppm:-0.37; formula:C19H21NO2
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

Target Compound Screening Report

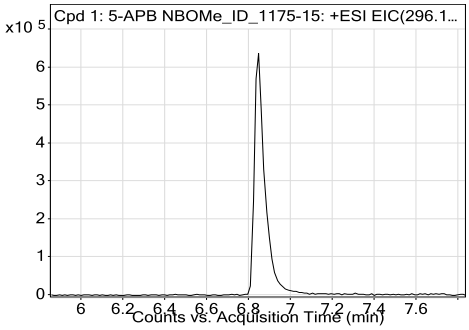
Data File	5-APB NBOMe_ID_1175-15_TOFz.d	**Sample Name**	5-APB NBOMe
Sample Type	Sample	**Position**	P1-F8
Instrument Name	SG13170002	**User Name**	
Acq Method	droge general-2-4-2015-XDB-C18-ESI-poz.m	**Acquired Time**	4/13/2015 1:20:54 PM
IRM Calibration Status	Success	**DA Method**	Droge_Default.m
Comment	white powder, extract in MeOH		

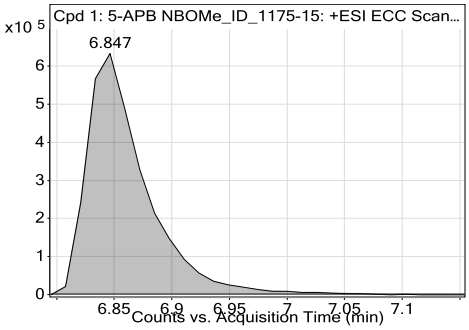
Compound Table

Label	Tgt Name	MFG Formula	Tgt Formula	Obs. RT	Obs. Mass
Cpd 1: 5-APB NBOMe_ID_1175-15	5-APB NBOMe_ID_1175-15	C19 H21 N O2	C19 H21 N O2	6.847	295.1573

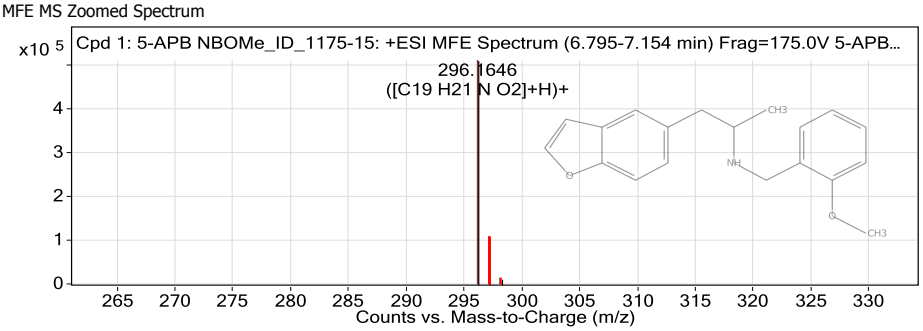
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error	Tgt Formula	Find Cpds Algorith
5-APB NBOMe_ID_1175-15	296.1646	6.847	295.1573	6.842	C19 H21 N O2	295.1572	-0.37	C19 H21 N O2	Find by Molecular Feature

Compound Chromatograms

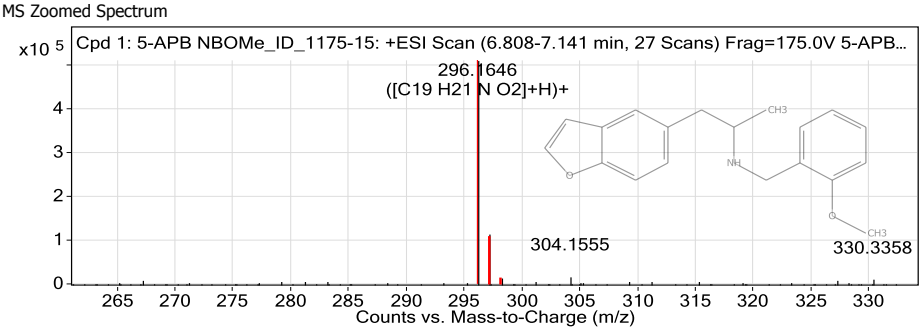




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
296.1646	1	510025.19	C19 H21 N O2	(M+H)+
297.1679	1	111119.1	C19 H21 N O2	(M+H)+
298.1705	1	13814.98	C19 H21 N O2	(M+H)+
299.1729	1	1072.85	C19 H21 N O2	(M+H)+

--- End Of Report ---

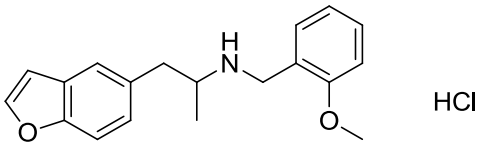
University
of Ljubljana

Faculty *of Chemistry and Chemical Technology*

Večna pot 113
P. O. Box 537
SI-1001 Ljubljana
Slovenia
Phone: +386 1 479 8558
janez.kosmrlj@fkkt.uni-lj.si

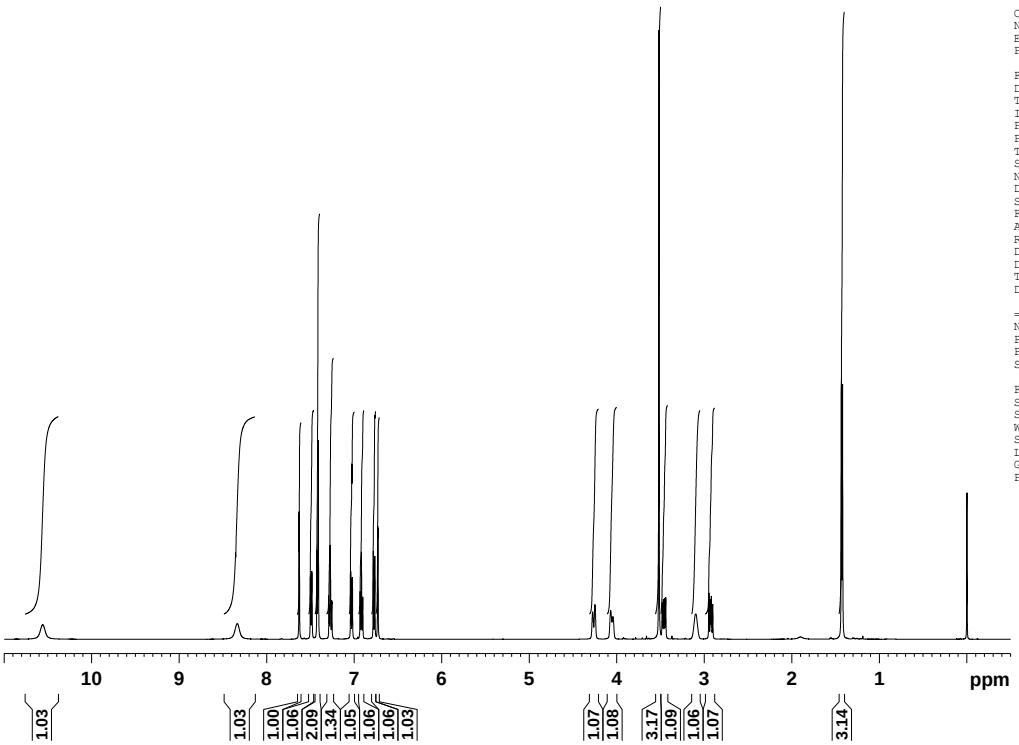
Co-funded by the Prevention of and Fight against Crime Programme of the European Union

REPORT

Sample ID:	**1175-15**
Our notebook code:	P-1175-15
NMR sample preparation:	15 mg dissolved in 0.7 mL $CDCl_3$
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:	 HCl 1-(benzofuran-5-yl)-*N*-(2-methoxybenzyl)propan-2-amine hydrochloride
Comments:	- Structure elucidation based on 1D and 2D 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:	April 30, 2015

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 publication are the sole responsibility of the Author and can in no way be taken to reflect the views of the European Commission.

P-1175-15
1H



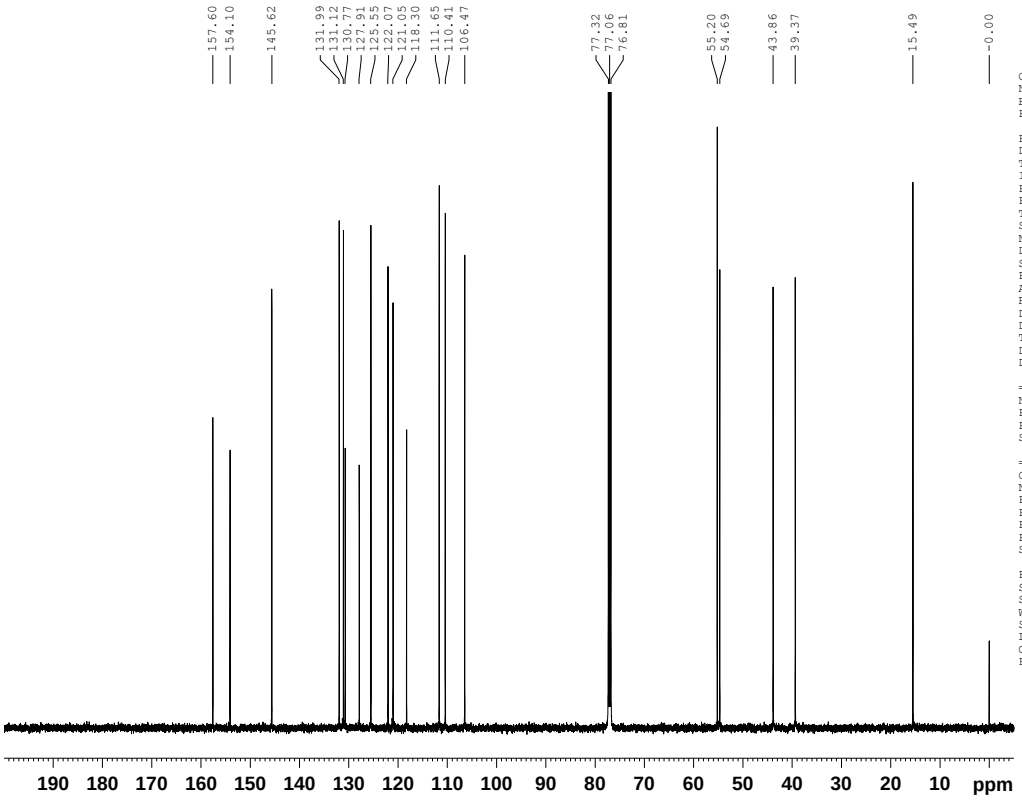

```
Current Data Parameters
NAME                  P-1175-15
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20150423
Time                   23.20
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                     80.6
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             500.1300046 MHz
WDW                      EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```

P-1175-15
13C




```
Current Data Parameters
NAME                  P-1175-15
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_              20150424
Time                    1.12
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     3072
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             125.7577898 MHz
WDW                      EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```