



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

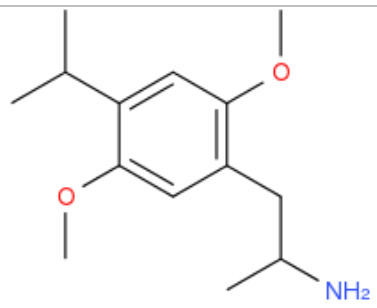
ANALYTICAL REPORT

DOIP,
C₁₄H₂₃NO₂)

1-[2,5-dimethoxy-4-(propan-2-yl)phenyl]propan-2-amine

Remark – other NPS detected: **none**

Sample ID:	1177-15
Sample description:	powder - white
Sample type:	P- purchased
Date of entry:	5/15/2015

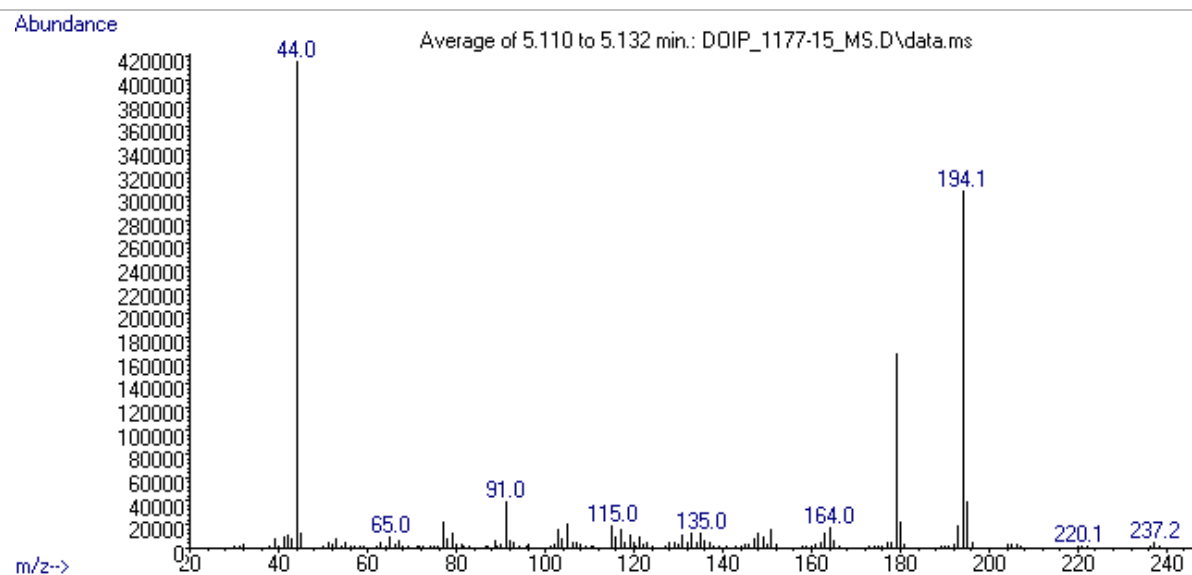
Substance identified- structure ⁱ (base form)	 *HCl
Systematic name	1-[2,5-dimethoxy-4-(propan-2-yl)phenyl]propan-2-amine
Other names	1-(4-isopropyl-2,5-dimethoxyphenyl)propan-2-amine
Formula (per base form)	C ₁₄ H ₂₃ NO ₂
M _w (g/mol)	237.34
Salt form	HCl
Smiles	<chem>COC1=C(C=C(C(=C1)C(C)C)OC)CC(C)N</chem>
Compound Class	Phenethylamines
Other NPS detected	none
Add.info (purity..)	pure

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.

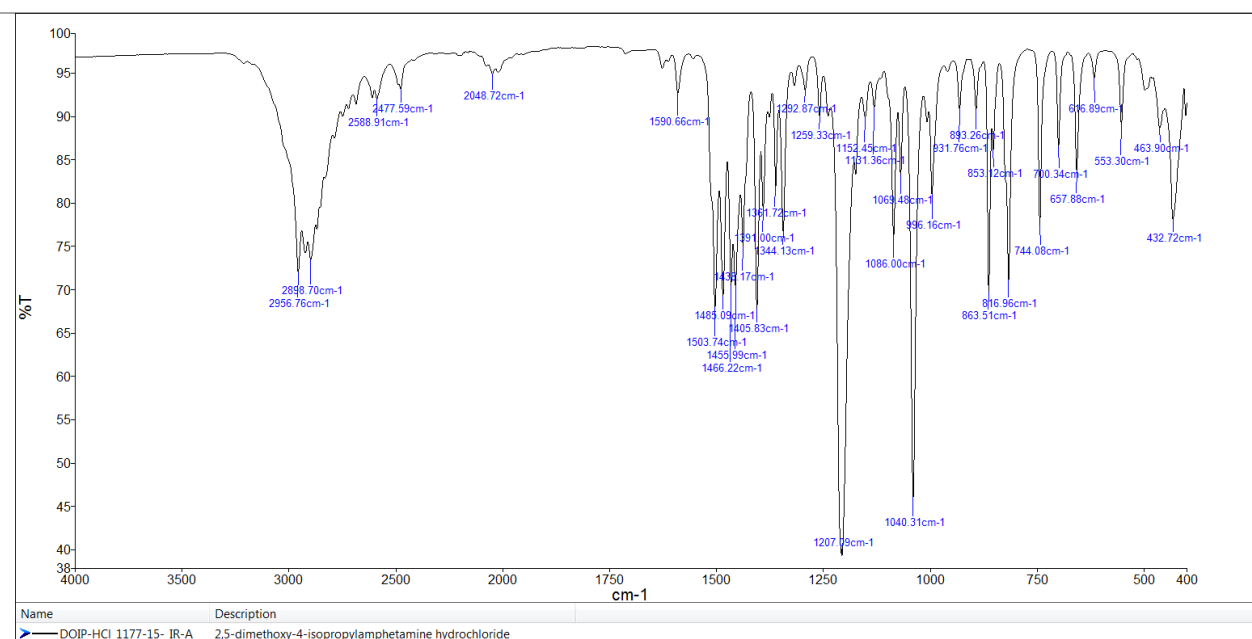
Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	BP(1): 44; BP(2): 194,BP(3) :179,
FTIR-ATR	+	HCl
FTIR (condensed phase)	/	pending
HPLC-TOF	+	Exact mass: 237.1729, measured/ Δ ppm:-2.86; formula: C ₁₄ H ₂₃ NO ₂
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

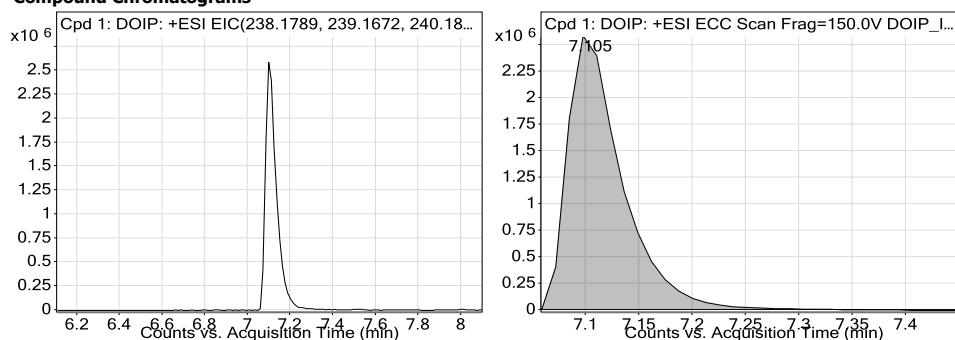
Data File	DOIP_ID_1177-15-MS-TOF.d	Sample Name	DOIP HCl
Sample Type	Sample	Position	P1-F3
Instrument Name	SG13170002	User Name	
Acq Method	droge general-13-5-2015-XDB-C18-ESI-poz.m	Acquired Time	5/13/2015 11:32:33 AM
IRM Calibration Status	Success	DA Method	Droge_Default.m
Comment	extract in MeOH		

Compound Table

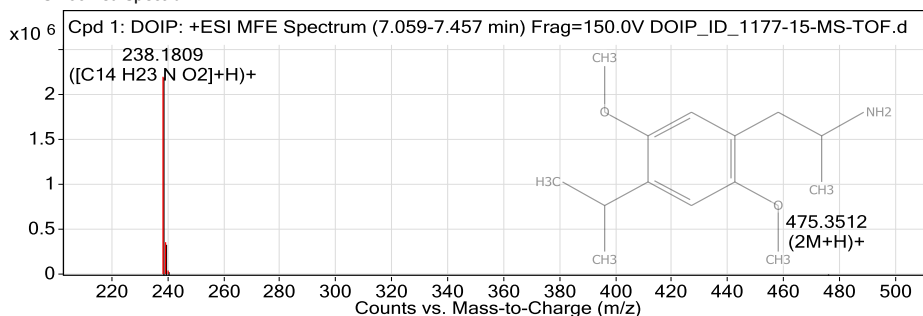
Label	Tgt Name	MFG Formula	Tgt Formula	Obs. RT	Obs. Mass
Cpd 1: DOIP	DOIP	C14 H23 N O2	C14 H23 N O2	7.105	237.1736

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error	Tgt Formula	Find Cpd Algorith
DOIP	238.1809	7.105	237.1736	7.105	C14 H23 N O2	237.1729	-2.86	C14 H23 N O2	Find by Molecular Feature

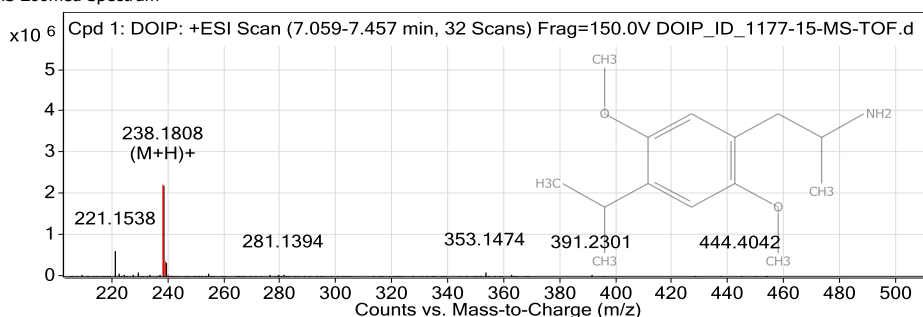
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



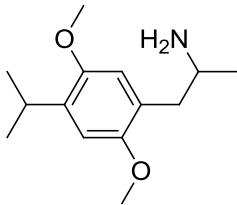
MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
238.1809	1	2201747.5	C14 H23 N O2	(M+H)+
239.1836	1	345221.06	C14 H23 N O2	(M+H)+
240.1864	1	35095.77	C14 H23 N O2	(M+H)+
241.188	1	3720.32	C14 H23 N O2	(M+H)+
475.3512	1	7381.11		(2M+H)+
476.3512	1	1916.89		(2M+H)+
477.3534	1	668.42		(2M+H)+

--- End Of Report ---



REPORT

Sample ID:	1177-15
Our notebook code:	P-1177-15
NMR sample preparation:	15 mg dissolved in 0.7 mL CDCl ₃
NMR experiments:	¹ H, ¹³ C, ¹ H- ¹ H <i>gs</i> -COSY, ¹ H- ¹³ C <i>gs</i> -HSQC, ¹ H- ¹³ C <i>gs</i> -HMBC, ¹ H- ¹⁵ N <i>gs</i> -HMBC
Proposed structure with chemical name:	 HCl 1-(4-isopropyl-2,5-dimethoxyphenyl)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

P-1177-15
1H

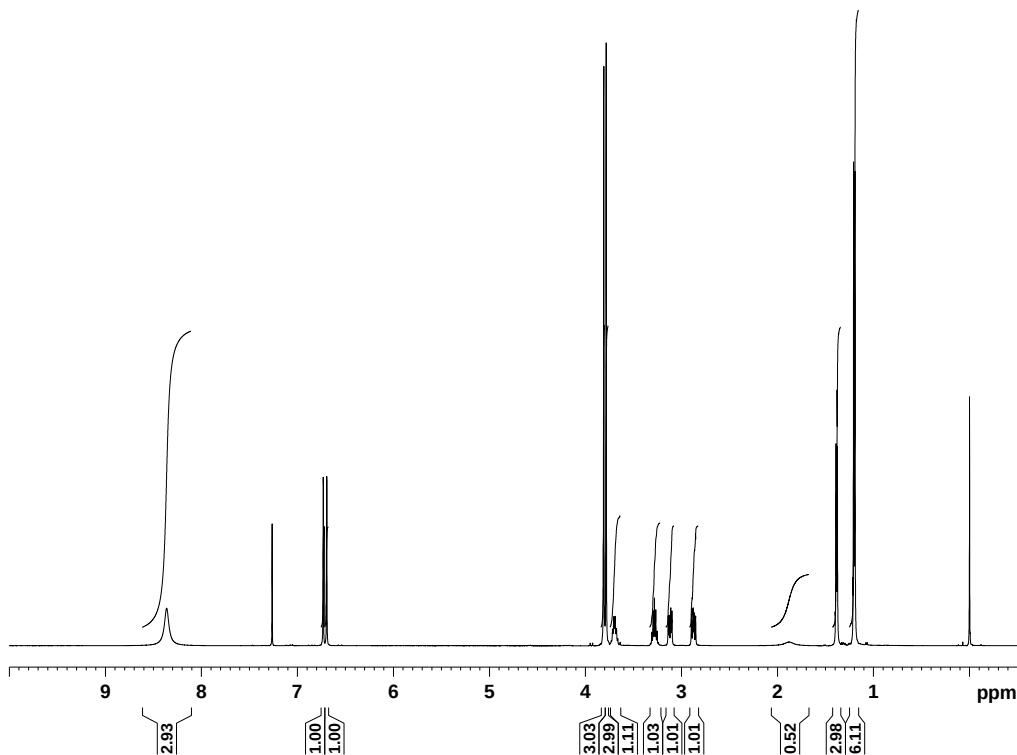


Current Data Parameters
NAME P-1177-15
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20150429
Time 0.42
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 500.1300113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



P-1177-15
13C



Current Data Parameters
NAME P-1177-15
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20150429
Time 3.11
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 125.7577902 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

