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4F-PBP (C14H18FNO)

Acknowledgement:

Sample was kindly provided by the Laboratório de Polícia Cientifica da Polícia Judiciária, Lisboa, Portugal. The substance was analytically confirmed using NMR and GCMS by the Criminal Police Forensic Laboratory and confirmed by the University of Lisboa. Details on identification have been published:
http://www.sciencedirect.com/science/article/pii/S0379073815001942

In the Slovenian National Forensic laboratory (NFL) sample was additionally analysed. The main goal of analyses performed in NFL-SI was to obtain FTIR-ATR and IR condensed spectra. NFL analytical report shown in this document.

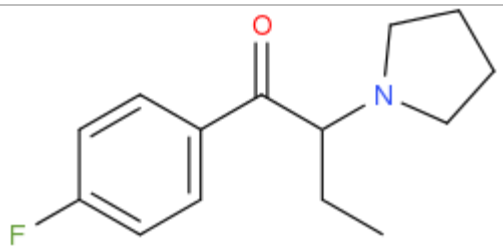
ANALYTICAL REPORT[1] (NFL-SI)

4F-PBP (C14H18FNO)

1-(4-fluorophenyl)-2-(1-pyrrolidinyl)-1-butanone

Remark – other NPS detected: none

Sample ID:	1295-15
Sample description:	powder - white
Sample type:	collected /OTHER (kindly provided by Laboratório de Polícia Cientifica da Polícia Judiciária, Portugal
Date of sample receipt (M/D/Y):	9/29/2015
Date of entry (M/D/Y) into NFL database:	11/5/2015
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance structure[2] (base form)	
Systematic name	1-(4-fluorophenyl)-2-(1-pyrrolidinyl)-1-butanone
Other names	
Formula (per base form)	C14H18FNO
M_w (g/mol)	235,3
Salt form	HCl
StdInChIKey	BYMOJFLMEMTDDX-UHFFFAOYSA-N
Compound Class	Cathinones
Other NPS detected	none
Add.info (purity..)	purified sample was received

[1] 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.

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

Report updates

date	comments (explanation)

Instrumental methods (if applied) in NFL

1. GC-MS (Agilent): GC-method is RT locked to tetracosane (RT=9.53 min). Injection volume 1 ml and split mode (1:50) . Injector temperature: 280 ^{0}C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 293 ^{0}C at a rate of 18 ^{0}C/min, hold for 6.1 min, than heating at 50 ^{0}C/min up to 325 ^{0}C and finally 2.8 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

2. HPLC-TOF (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N2) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.

3.FTIR-ATR (Perkin Elmer): scan range 4000-400 cm-1; resolution 4cm-1

4. GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)
GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 ^{0}C. Chromatographic separation as above **(1).** Split MS : IR = 1:9.
MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.
IR (condesed phase): IR scan range 4000 to 650, resolution 4 cm^{-1}.

5. **IC** (anions) (Thermo Scientific, Dionex ICS 2100), Column: IonPac AS19, 2 x 250mm; Eluent: 10mM from 0 to 10 min, 10-58 mM from 10 to 40min; Flow rate: 0.25 ml/min; Temperature: 30˚C; Suppressor: AERS 500 2mm, suppressor current 13mA; Inj. Volume: 25 µl

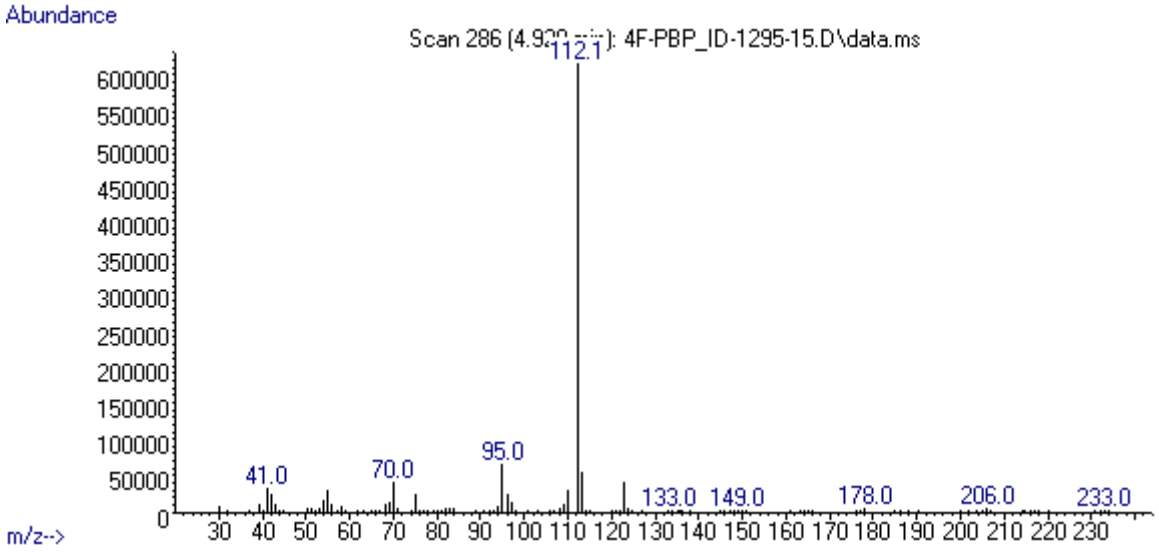
Supporting information

Solubility in	result/remark
CH_2Cl_2	soluble
MeOH	soluble
H_2O	soluble

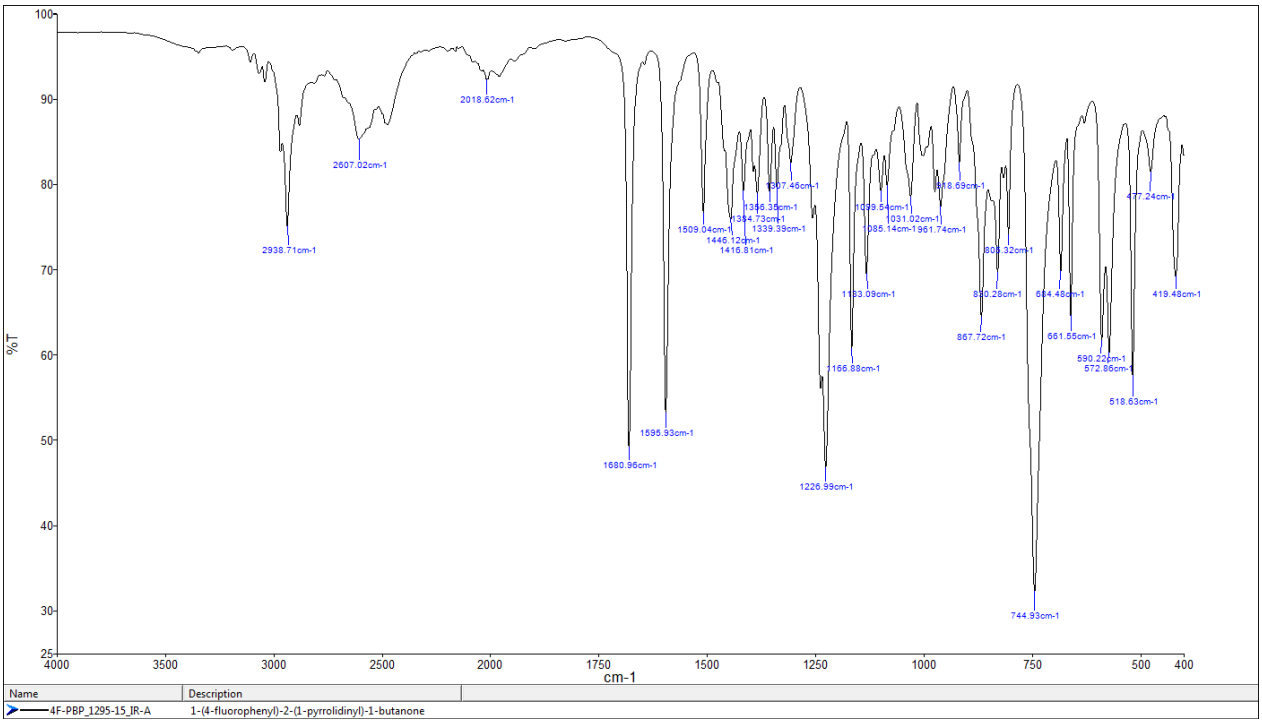
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 4,93 BP(1): 112; BP(2): 95,BP(3) :113,
HPLC-TOF	+	Exact mass (theoretical): 235,1372; measured value Δppm:-1,24; formula:C14H18FNO
FTIR-ATR	+	direct measurement
FTIR (condensed phase) always as base form	+	extract in CH2Cl2
IC (anions)	+	
NMR	-	*structure has been verified, see* http://www.sciencedirect.com/science/article/pii/S0379073815001942
validation		
other		

ANALYTICAL RESULTS

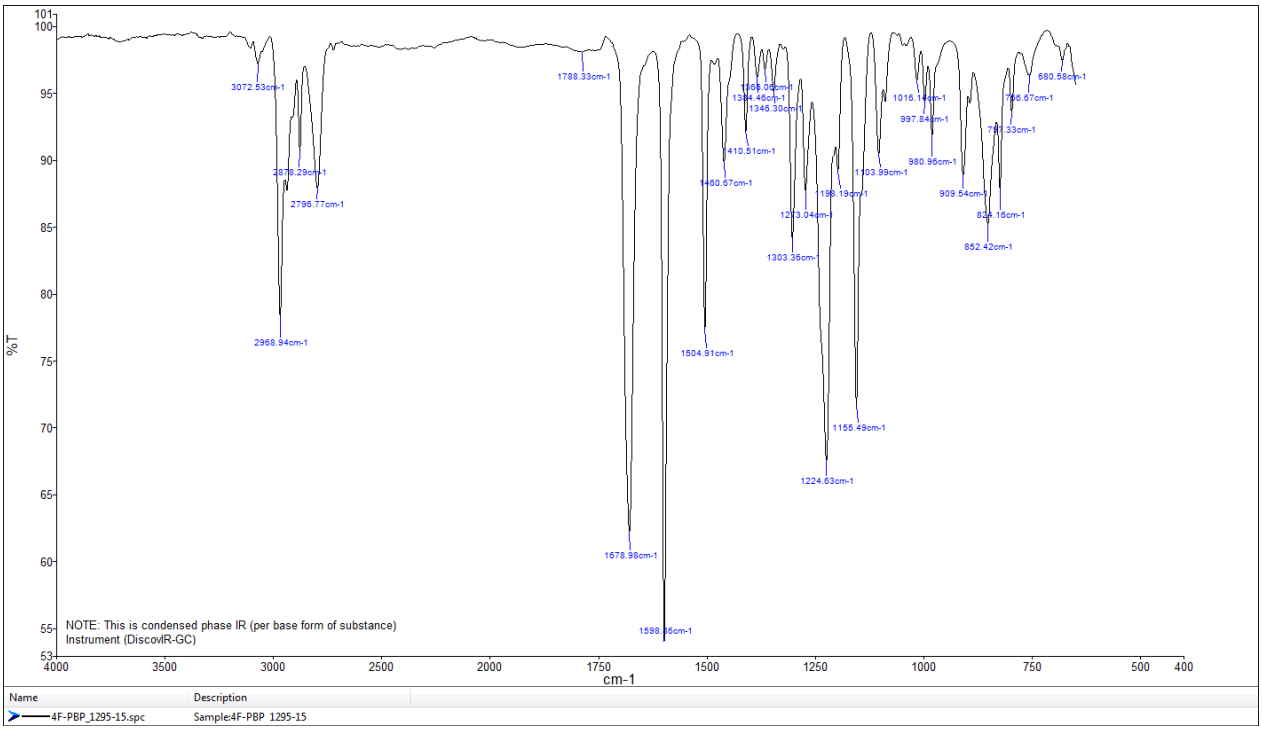
MS (EI)



FTIR-ATR - direct measurement



IR (condensed phase)



TOF REPORT

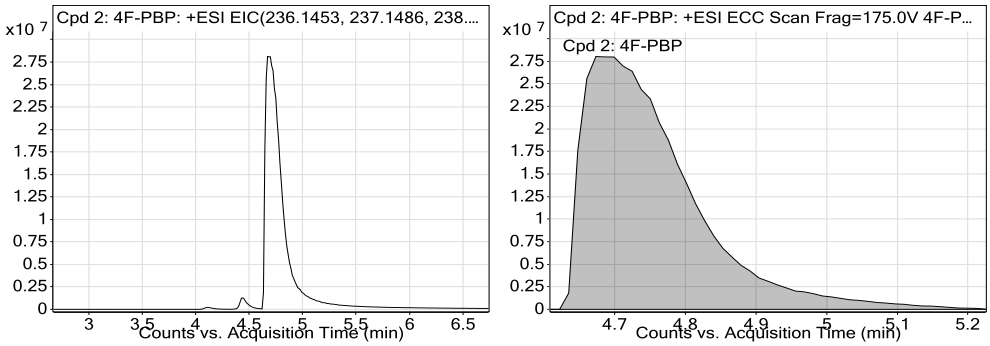
Data File	4F-PBP_1295-15_TOF.d	**Sample Name**	4F-PBP
Sample Type	Sample	**Position**	P1-B9
Instrument Name	6230B TOF LC-MS	**User Name**	TG
Acq Method	general-28052015-XDB-C18-ESI-poz.m	**Acquired Time**	10/26/2015 12:08:01 PM
IRM Calibration Status	Success	**DA Method**	Drugs_NFL.m
Comment	extract in MeOH		

Compound Table

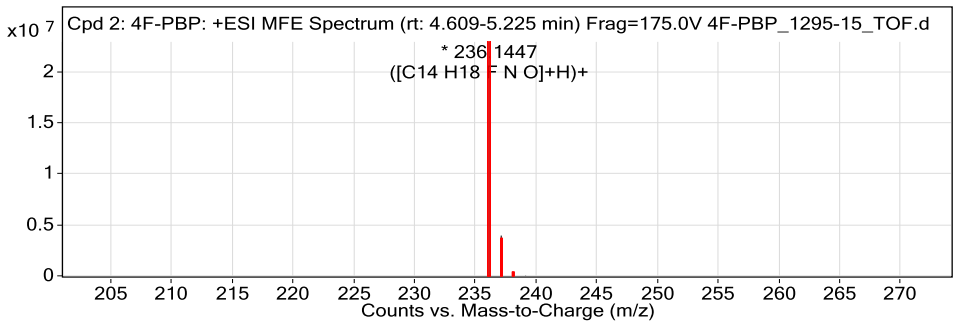
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 2: 4F-PBP	4F-PBP	C14 H18 F N O	4.711	235.1375

Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
4F-PBP	236.1447	4.711	235.1375	4.7	C14 H18 F N O	235.1372	-1.24

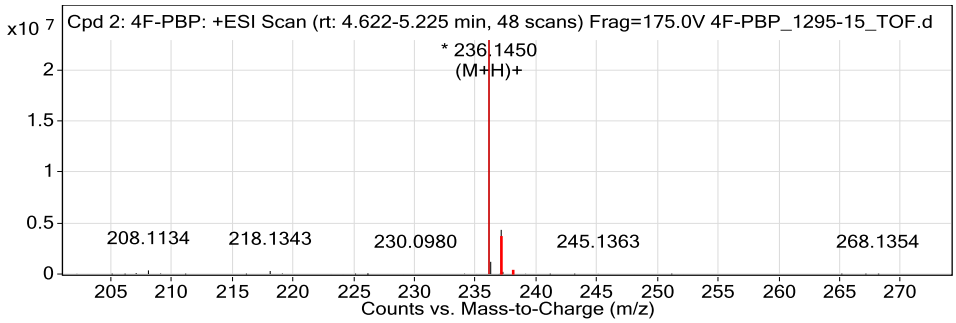
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
236.1447	1	22946850	C14 H18 F N O	(M+H)+
237.1486	1	3951354.94	C14 H18 F N O	(M+H)+
238.1523	1	322198.32	C14 H18 F N O	(M+H)+
239.1548	1	22811.41	C14 H18 F N O	(M+H)+

--- End Of Report ---

Peak Integration Report

Sample Name:	**4FPBP_1295-15_IC**	*Inj. Vol.:*	**25,00**
Injection Type:	**Unknown**	*Dilution Factor:*	**1,0000**
Program:	**ANIONI**	*Operator:*	**kemija**
Inj. Date / Time:	**28-okt-2015 / 02:19**	*Run Time:*	**42,00**

No.	Time min	Peak Name	Peak Type	Area µS*min	Height µS	Amount mg/L
1,00	9,53	**Chloride**	BMB	3,99	16,85	n.a.
		TOTAL:		3,99	16,85	0,00