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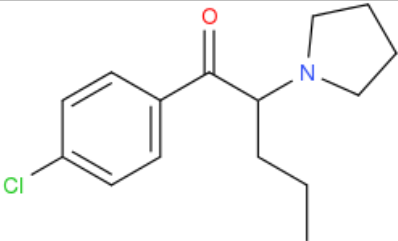
ANALYTICAL REPORT

4Cl-PVP (C₁₅H₂₀ClNO)

1-(4-chlorophenyl)-2-(pyrrolidin-1-yl)pentan-1-one

Remark – other NPS detected: **none**

Sample ID:	1744-17
Sample description:	crystalline
Sample type:	test purchase /NFL- purchasing
Date of sample receipt (M/D/Y):	1/10/2017
Date of entry (M/D/Y) into NFL database:	8/16/2017
Report ¹ updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure ² (base form)	
Systematic name	1-(4-chlorophenyl)-2-(pyrrolidin-1-yl)pentan-1-one
Other names	
Formula (per base form)	C ₁₅ H ₂₀ ClNO
M _w (g/mol)	265,78
Salt form/anions detected	sulphate
StdInChIKey (per base form)	NIGBFBTVONRYQN-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	pure by GC-MS, HPLC-TOF

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 (9.258 min). Injection volume 1 ml and split mode (1:50). Injector temperature: 280 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 °C at a rate of 18 °C/min, hold for 7.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235 °C, source and quadropole temperatures 280 °C and 180 °C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300 until 6 min) 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 °C. Chromatographic separation as above **(1)**. Split MS : IR = 1: 9.

MSD source EI = 70 eV. GC-MS transfer line T= 235 °C, source and quadropole temperatures 280 °C and 180 °C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

IR (condensed (solid) 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

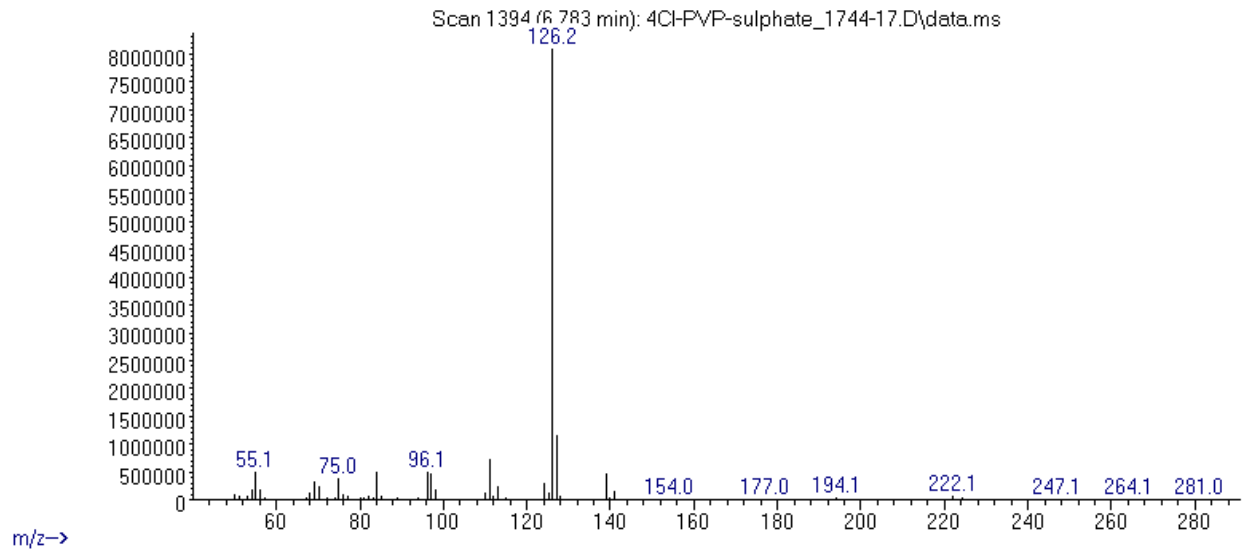
Solubility in	result/remark
CH ₂ Cl ₂	partially
MeOH	partially
H ₂ O	soluble

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 6,78 BP(1): 126; BP(2): 127,BP(3) :111,
HPLC-TOF	+	Exact mass (theoretical): 265,1233; measured value Δppm:0,05; formula:C15H20ClNO
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	-	
validation		GC-RT and MS spectrum consistent by NMR confirmed compound in RESPONSE database (CHEM ID-1279-15); FTIR-condensed phase spectrum (per base form) consistent by the spectrum of the RESPONSE sample CHEM ID-1279-15.
other		

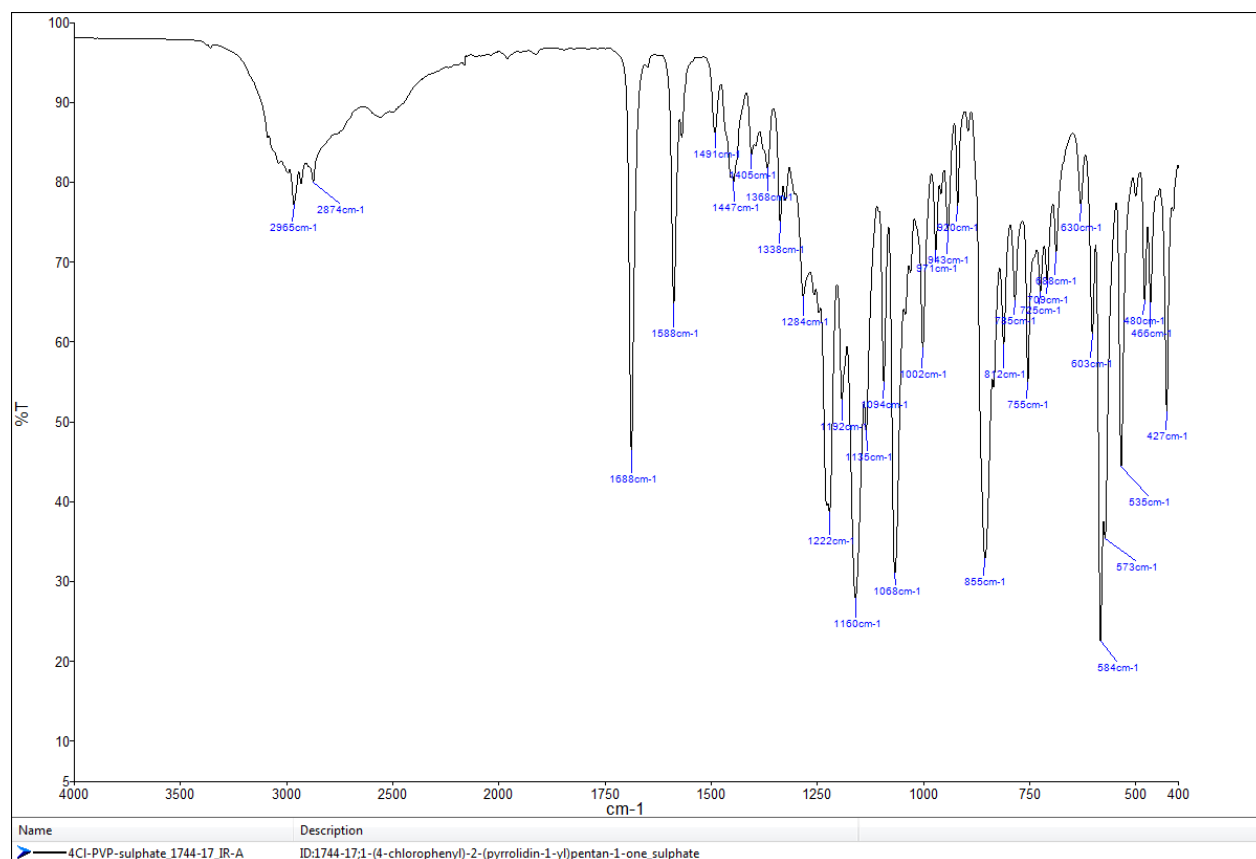
ANALYTICAL RESULTS

MS (EI)

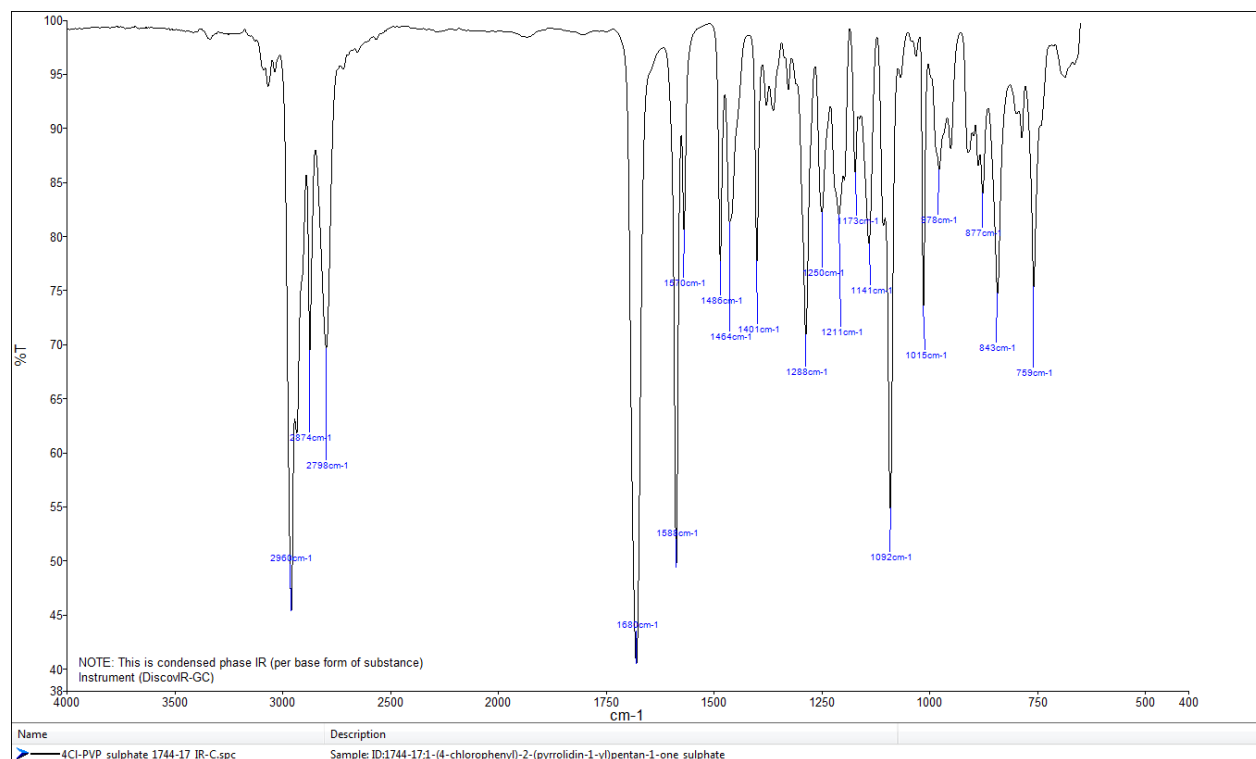
Abundance



FTIR-ATR - direct measurement (sample as received, sulphate form)



IR (condensed phase– after chromatographic separation) - always for base form of compound



TOF REPORT

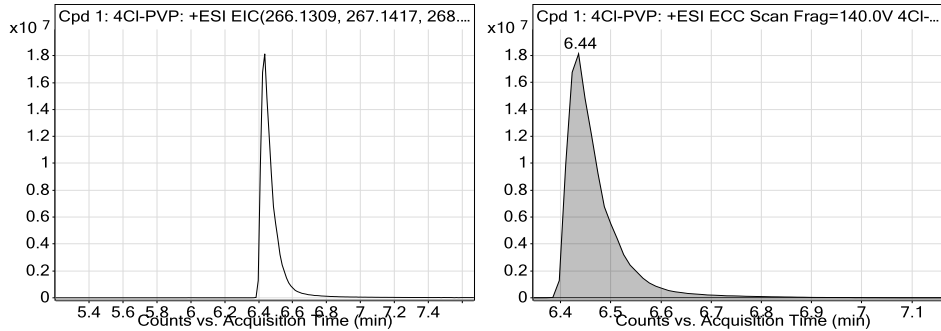
Data File	4CI-PVP_1744-17.d	Sample Name	VP
Sample Type	Sample	Position	P1-D8
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-20_12_2016-XDB-C18-ESI-poz-no121.m	Acquired Time	1/10/2017 2:58:13 PM
IRM Calibration Status	Success	DA Method	Drugs_NFL.m
Comment	extract in MeOH		

Compound Table

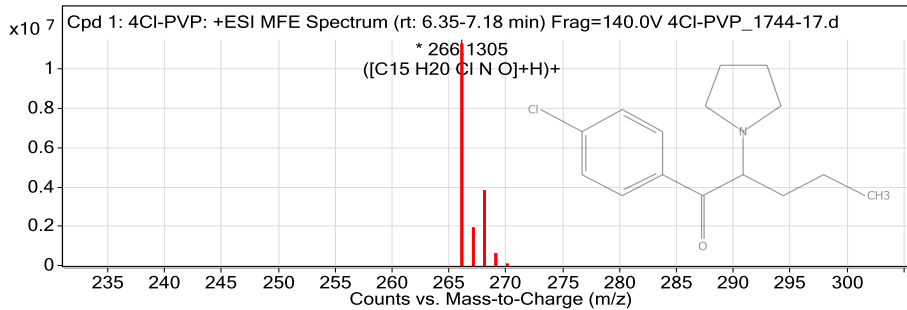
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 1: 4CI-PVP	4CI-PVP	C15 H20 Cl N O	6.44	265.1233

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
4CI-PVP	266.1305	6.44	265.1233	6.45	C15 H20 Cl N O	265.1233	0.05

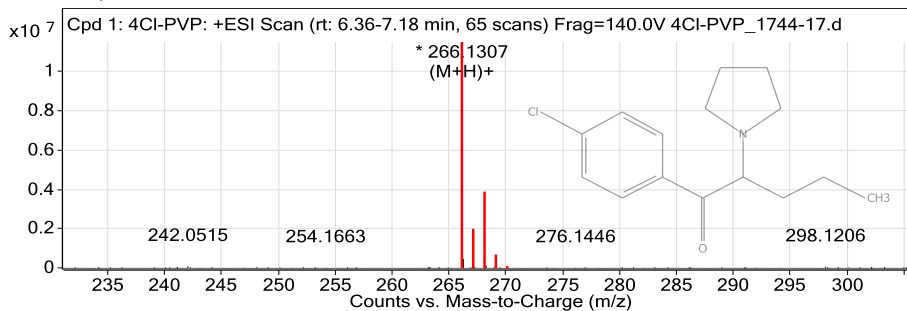
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
266.1305	1	11509011	C15 H20 Cl N O	(M+H)+
267.1341	1	1871488.49	C15 H20 Cl N O	(M+H)+
268.1281	1	3670727.97	C15 H20 Cl N O	(M+H)+
269.1316	1	562542.67	C15 H20 Cl N O	(M+H)+
270.1342	1	48969.3	C15 H20 Cl N O	(M+H)+
271.138	1	3235.14	C15 H20 Cl N O	(M+H)+

--- End Of Report ---

Peak Integration Report

Sample Name:	4CI-PVP_1744-17_IC	Inj. Vol.:	25,00
Injection Type:	Unknown	Dilution Factor:	1,0000
Program:	ANIONI	Operator:	kemija
Inj. Date / Time:	10-jan-2017 / 20:21	Run Time:	42,00

No.	Time min	Peak Name	Peak Type	Area $\mu\text{S}\cdot\text{min}$	Height μS	Amount mg/L
1,00	22,46	Sulfate	BMB	96,50	157,50	127,03
		TOTAL:		96,50	157,50	127,03

