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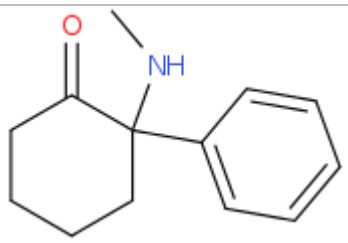
ANALYTICAL REPORT[1,2]

Deschloroketamine (C13H17NO)

2-(methylamino)-2-phenylcyclohexan-1-one

Remark – other NPS detected: none

Sample ID:	1761-17
Sample description:	powder - white
Sample type:	collected /FSI Zurich, Switzerland
Date of sample receipt (M/D/Y):	1/20/2017
Date of entry (M/D/Y) into NFL database:	2/13/2017
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure[3] (base form)	
Systematic name	2-(methylamino)-2-phenylcyclohexan-1-one
Other names	DXE, DCK, 2'-Oxo-PCM, 2-Phenyl-2-(methylamino)cyclohexanone
Formula (per base form)	C13H17NO
M_w (g/mol)	203,29
Salt form/anions detected	HCl
StdInChIKey (for base form)	ZAGBSZSITDFFAF-UHFFFAOYSA-N
Other NPS detected	none
Add.info (purity..)	approx. 95% (FSI Zurich data)

[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] Acknowledgement: Sample (NMR confirmed) was kindly provided by FSI Zurich, Switzerland. Masurements shown in this report were done in NFL.

[3] 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 0C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 190 ^{0}C at rate 8 ^{0}C/min, then heating up to 293 0C at a rate of 18 ^{0}C/min, hold for 7.1 min, then heating at 50 ^{0}C/min up to 325 ^{0}C and finally 6.1 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 (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 ^{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 (30 until 6 min.) to 550 (300) amu.
IR (condesed (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

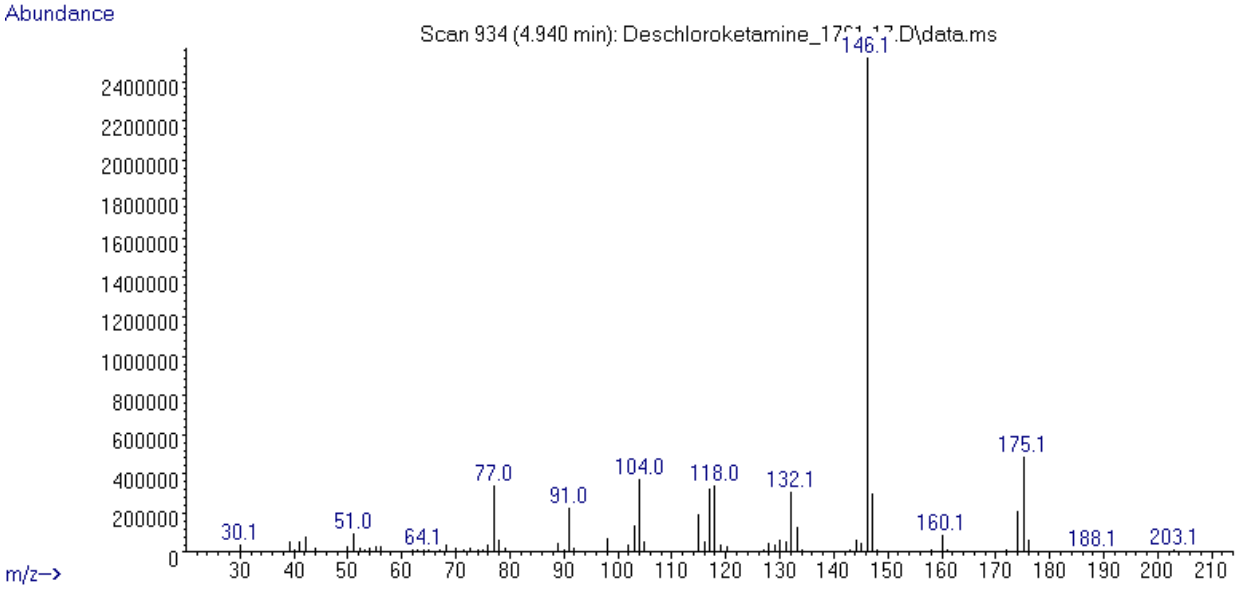
Supporting information

Solubility in	result/remark
CH_2Cl_2	partially
MeOH	soluble
H_2O	soluble

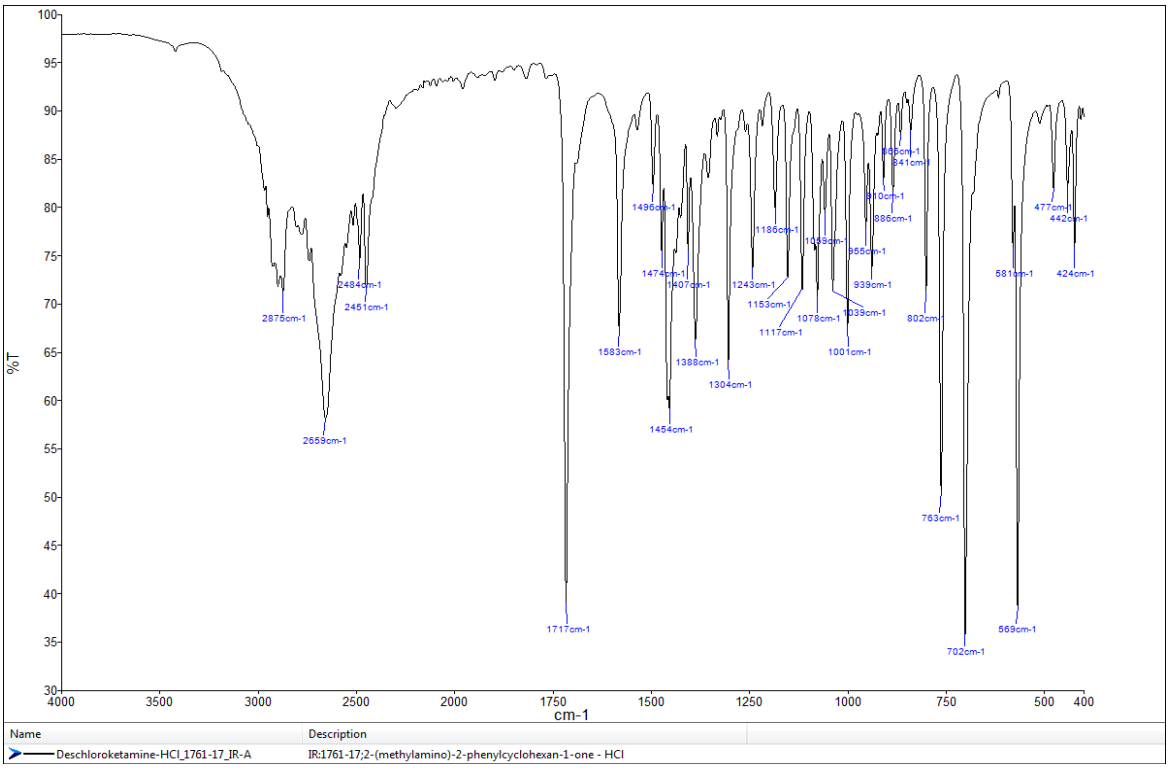
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 4,94 BP(1): 146; BP(2): 175,BP(3) :104,
HPLC-TOF	+	Exact mass (theoretical): 203,131; measured value Δppm:-0,92; formula:C13H17NO
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	-	confirmed in FSI Zurich
validation		
other		

ANALYTICAL RESULTS

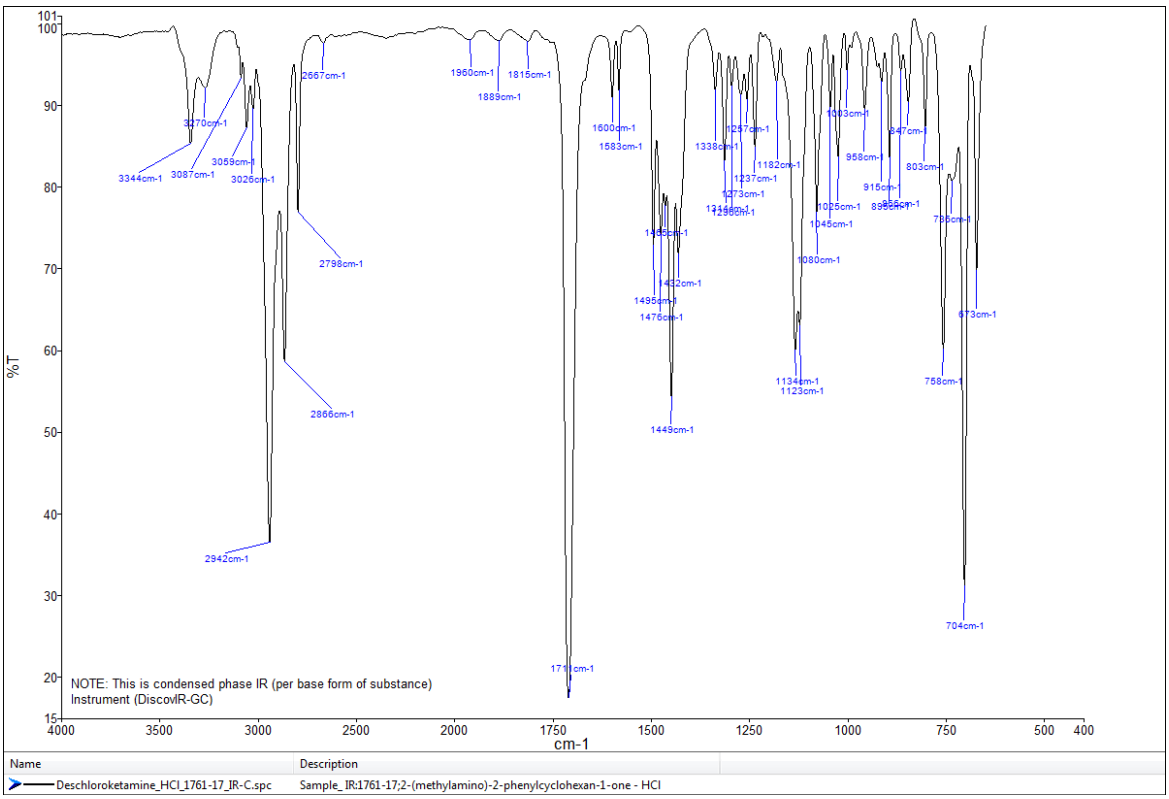
MS (EI)



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)



TOF REPORT

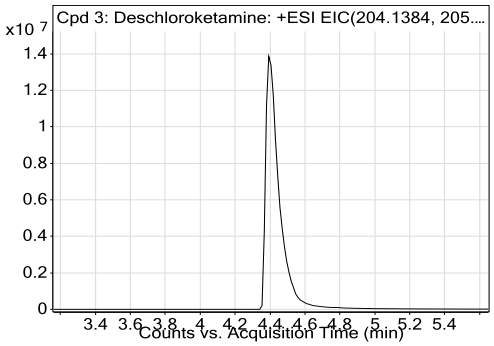
Data File	Deschloroketamine_1761-17.d	**Sample Name**	1761-17
Sample Type	Sample	**Position**	P1-C3
Instrument Name	6230B TOF LC-MS	**User Name**	TG
Acq Method	general-20_12_2016-XDB-C18-ESI-poz-soft.m	**Acquired Time**	1/31/2017 9:51:28 AM
IRM Calibration Status	Success	**DA Method**	Drugs_NFL.m
Comment	MeOH		

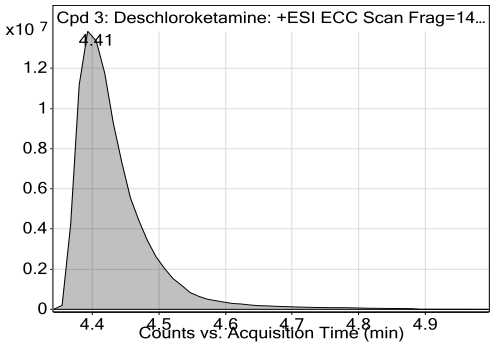
Compound Table

Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 3: Deschloroketamine	Deschloroketamine	C13 H17 N O	4.41	203.1312

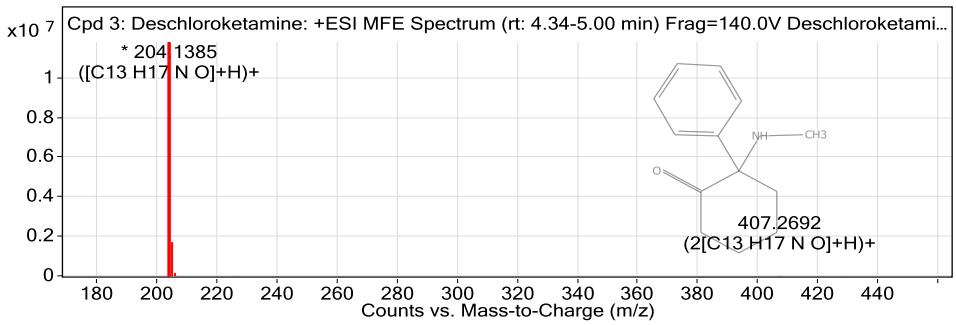
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
Deschloroketamine	204.1385	4.41	203.1312	4.41	C13 H17 N O	203.131	-0.92

Compound Chromatograms

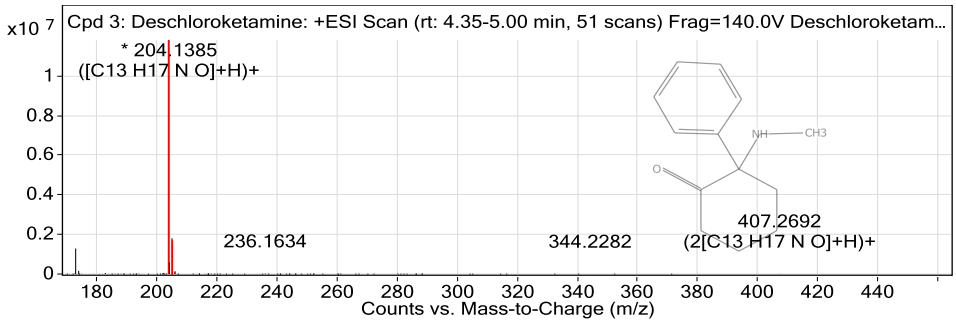




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
204.1385	1	11805444	C13 H17 N O	(M+H)+
205.1418	1	1664444.5	C13 H17 N O	(M+H)+
206.1448	1	125960.51	C13 H17 N O	(M+H)+
207.1473	1	8899.88	C13 H17 N O	(M+H)+
226.1206	1	4084.21	C13 H17 N O	(M+Na)+
407.2692	1	11949.32	C13 H17 N O	(2M+H)+
408.2724	1	3708.7	C13 H17 N O	(2M+H)+
429.2517	1	1514.23	C13 H17 N O	(2M+Na)+

--- End Of Report ---

Peak Integration Report

Sample Name:	**1761-17**	*Inj. Vol.:*	**25,00**
Injection Type:	**Unknown**	*Dilution Factor:*	**1,0000**
Program:	**ANIONI**	*Operator:*	**kemija**
Inj. Date / Time:	**03-feb-2017 / 10:35**	*Run Time:*	**42,00**

No.	Time min	Peak Name	Peak Type	Area µS*min	Height µS	Amount mg/L
1,00	9,33	**Chloride**	BMB	6,49	24,68	n.a.
		TOTAL:		6,49	24,68	0,00