

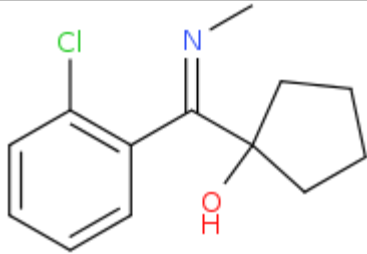
ANALYTICAL REPORT

Ketamine-Related-Compound-A (C₁₃H₁₆ClNO)

1-[(2-chlorophenyl)(methylimino)methyl]cyclopentan-1-ol

Remark – other active cpd. detected: **none**

Sample ID:	1601-16
Sample description:	powder - light yellow
Sample type:	RM-reference material
Comments ¹ :	U.S.Pharmacopeia Lot#FOC118; RESPONSE -purchasing
Date of entry:	8/10/2016

Substance identified-structure ² (base form)	
Systematic name:	1-[(2-chlorophenyl)(methylimino)methyl]cyclopentan-1-ol
Other names:	1-[(2-Chlorophenyl)(methylimino)methyl]cyclopentanol
Formula (per base form)	C ₁₃ H ₁₆ ClNO
M _w (g/mol)	237,73
Salt form:	base
StdInChIKey	FJGPXUPMNZOTLX-UHFFFAOYSA-N
Compound Class	Arylcyclohexylamines
Other active cpd. detected	none
Add.info (purity..)	pure by HPLC-TOF, impurity detected by GC-MS (possibly thermal degradation byproduct cca 3%)

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)

Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 5,51 BP(1): 152; BP(2): 154,BP(3) :138,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	-	always as base form

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

3. 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.

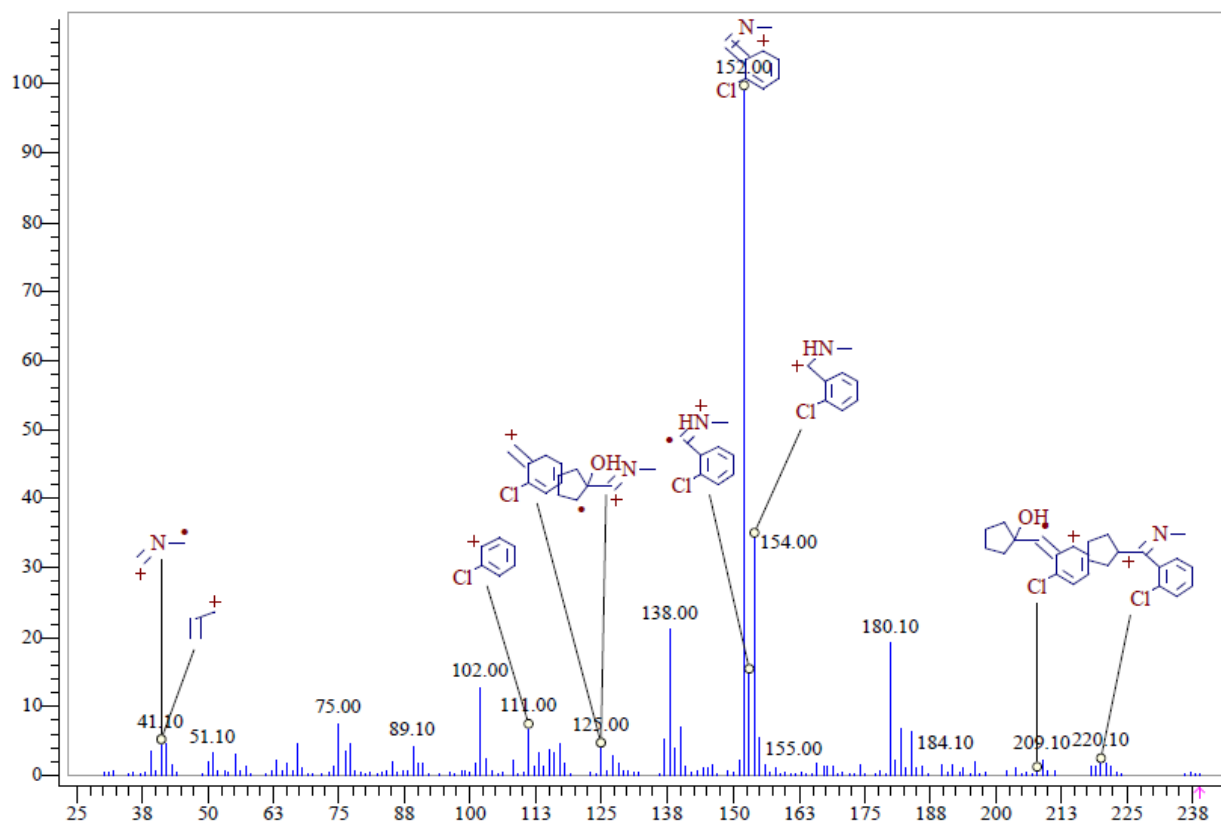
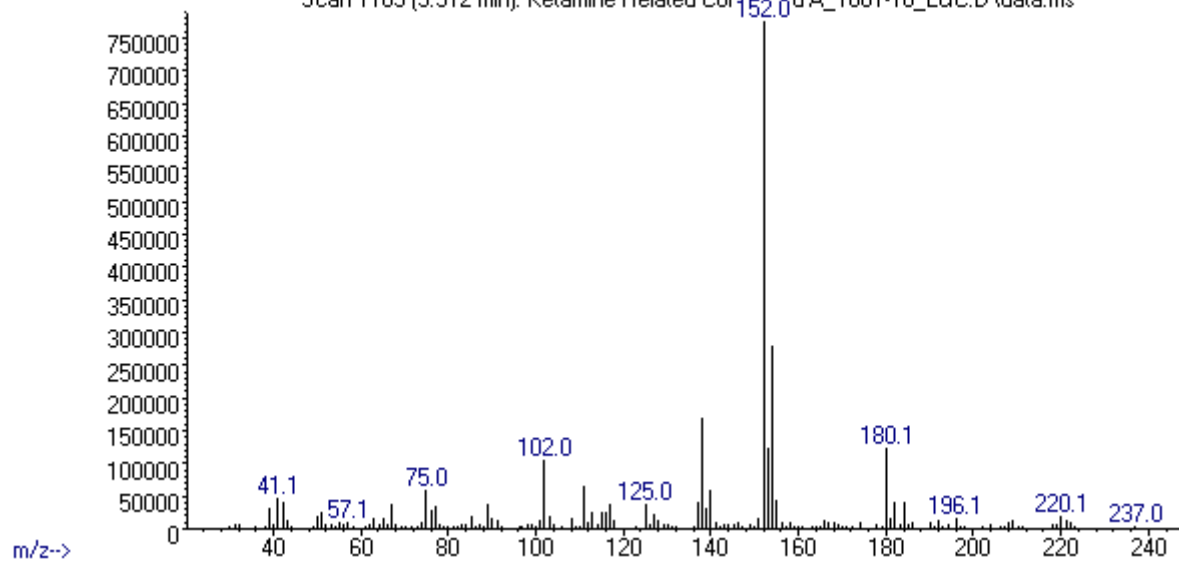
IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

FIGURES OF SPECTRA

MS (EI)

Abundance

Scan 1109 (5.512 min): Ketamine Related Cor_152.0 d A_1601-16_LGC.D\data.ms



FTIR-ATR

