

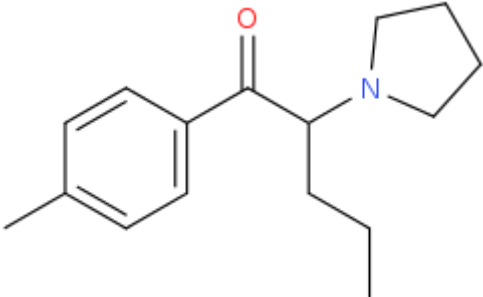
ANALYTICAL REPORT

Pyrovalerone (C₁₆H₂₃NO)

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

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

Sample ID:	1332-16
Sample description:	powder - white
Sample type:	RM-reference material
Comments ¹ :	Lipomed Lot#1333.1B1.1; RESPONSE -purchasing
Date of entry:	3/11/2015

Substance identified-structure ² (base form)	
Systematic name:	1-(4-methylphenyl)-2-(pyrrolidin-1-yl)pentan-1-one
Other names:	1-(1-Pyrrolidinyl)butyl p-Tolyl Ketone; Valerophenone, Centroton, Thymergix
Formula (per base form)	C ₁₆ H ₂₃ NO
M _w (g/mol)	245.36
Salt form:	HCl
StdInChIKey	SWUVZKWCBOGPTH-UHFFFAOYSA-N
Compound Class	Cathinones
Other active cpd. detected	none
Add.info (purity..)	>98.5 (as HCL)

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): 6.42 BP(1): 126; BP(2): 127,BP(3) :91,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	

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 °C.

Chromatographic separation

Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm.

Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by 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 2.8 min isothermal.

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

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

GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm⁻¹

GC-method:

Injection volume 1 ml and split mode (1:5) .

Injector temperature: 280 °C.

Chromatographic separation

Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm.

Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by 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 2.8 min isothermal.

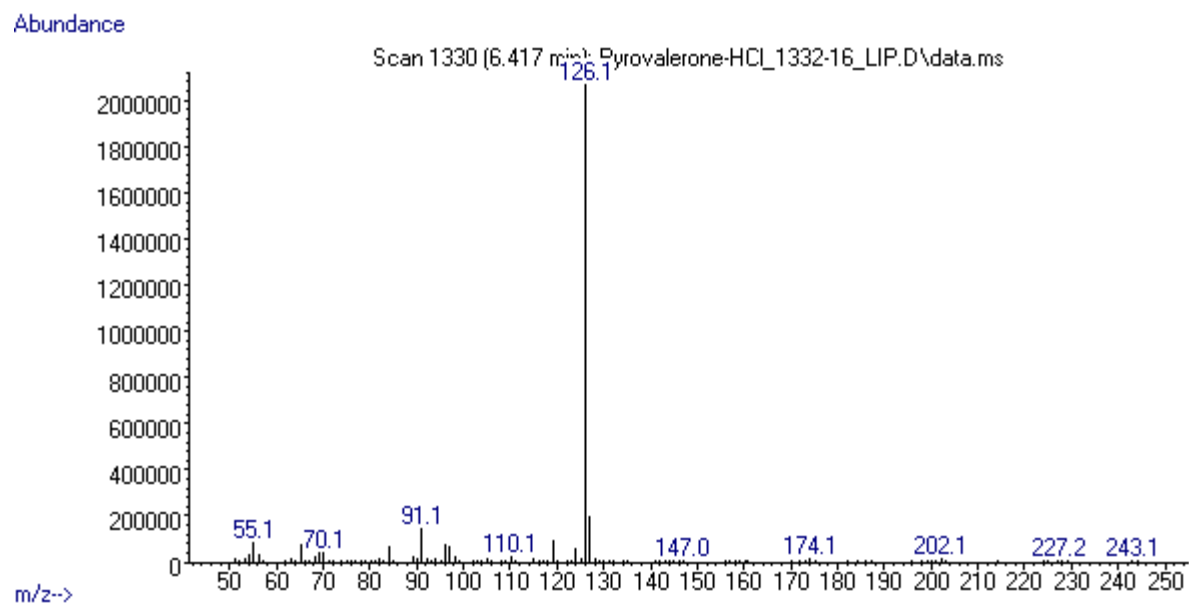
Split MS : IR : (1:9)

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

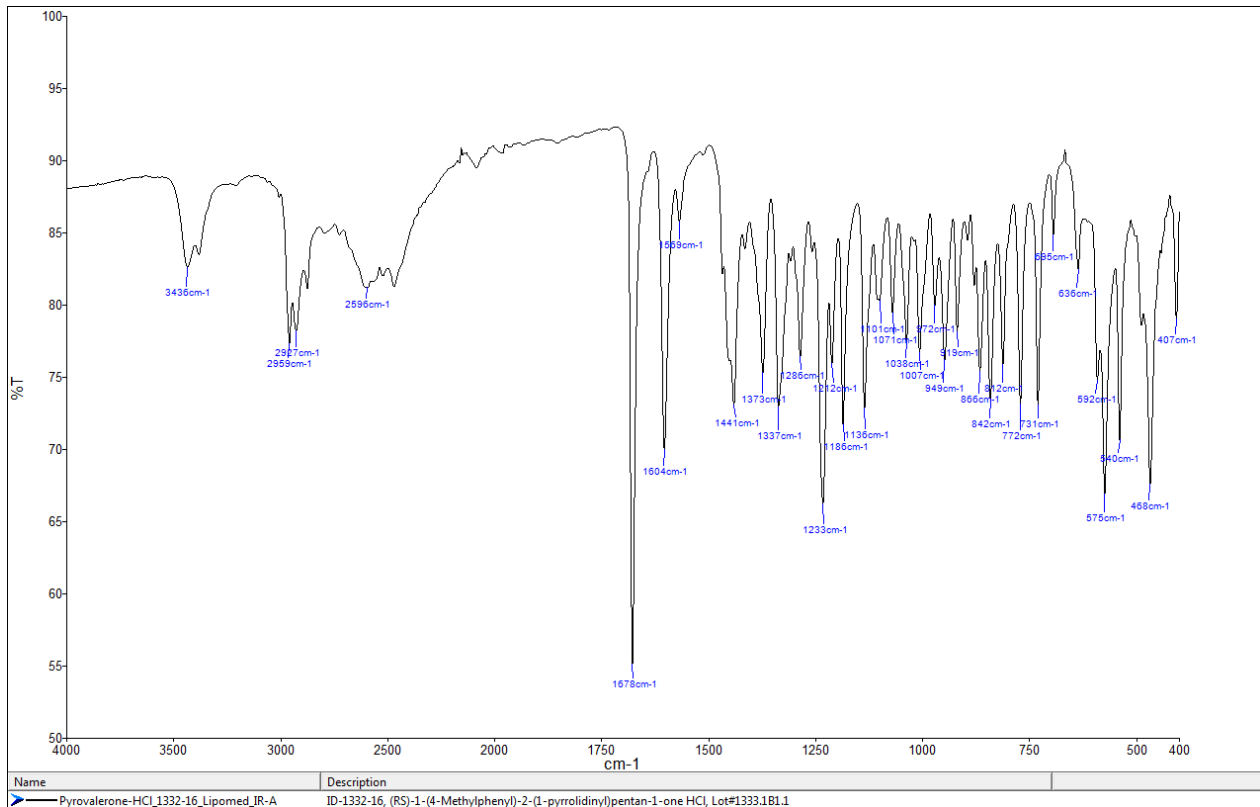
IR (condensed phase): IR scan range 4000 to 700, resolution 4cm⁻¹

FIGURES OF SPECTRA

MS (EI)



FTIR-ATR



IR-Condensed phase

