

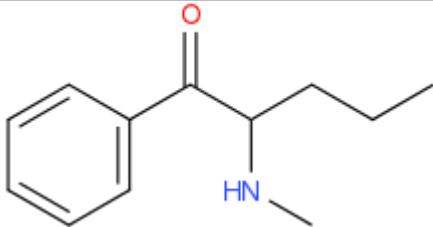
## ANALYTICAL REPORT

### Pentedrone (C<sub>12</sub>H<sub>17</sub>NO)

#### (±)-1-phenyl-2-(methylamino)pentan-1-one

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

Sample ID:	1166-15A
Sample description:	powder - white
Sample type:	RM-reference material
Comments <sup>1</sup> :	Cayman Lot#0444949-15;
Date of entry:	3/23/2015

Substance identified-structure <sup>2</sup> (base form)	
Systematic name:	(±)-1-phenyl-2-(methylamino)pentan-1-one
Other names:	
Formula (per base form)	C <sub>12</sub> H <sub>17</sub> NO
M <sub>w</sub> (g/mol)	191.27
Salt form:	HCl
StdInChIKey	WLIWIUNEJRETFX-UHFFFAOYSA-N
Compound Class	Cathinones
Other active cpd. detected	none
Add.info (purity..)	100%

<sup>1</sup> 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.

<sup>2</sup> 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): 3.71 BP(1): 86; BP(2): 44,BP(3) :105,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	spectrum is always for the base form of compound

### 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 (40) to 550 amu.

**FTIR-ATR** (Perkin Elmer): scan range 4000-400 cm<sup>-1</sup>; resolution 4cm<sup>-1</sup>

**GC- (MS)-IR** condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm<sup>-1</sup>

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)

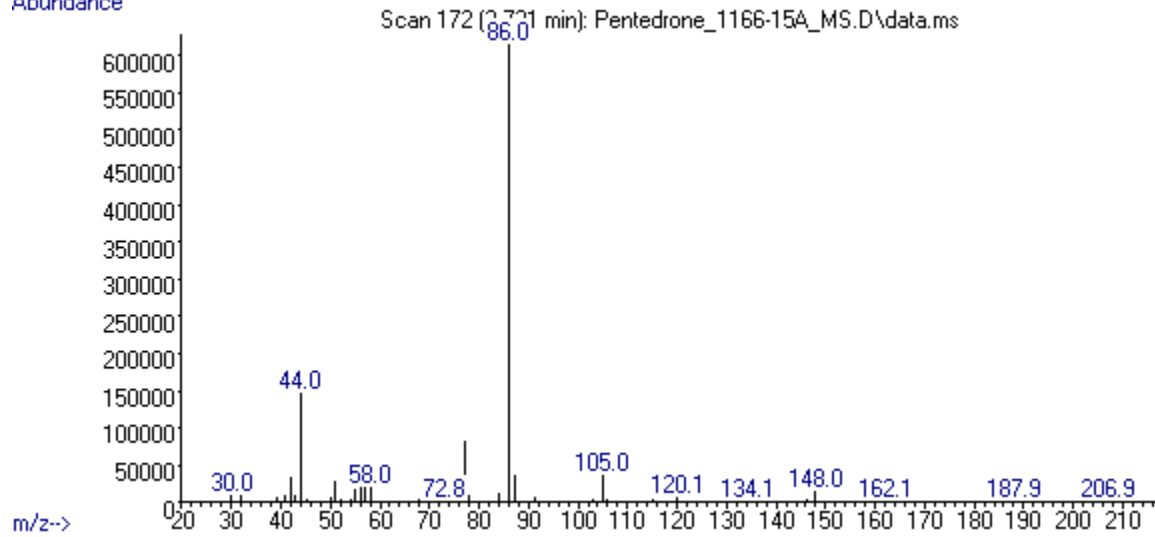
MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

IR (condensed phase): IR scan range 4000 to 700, resolution 4cm<sup>-1</sup>

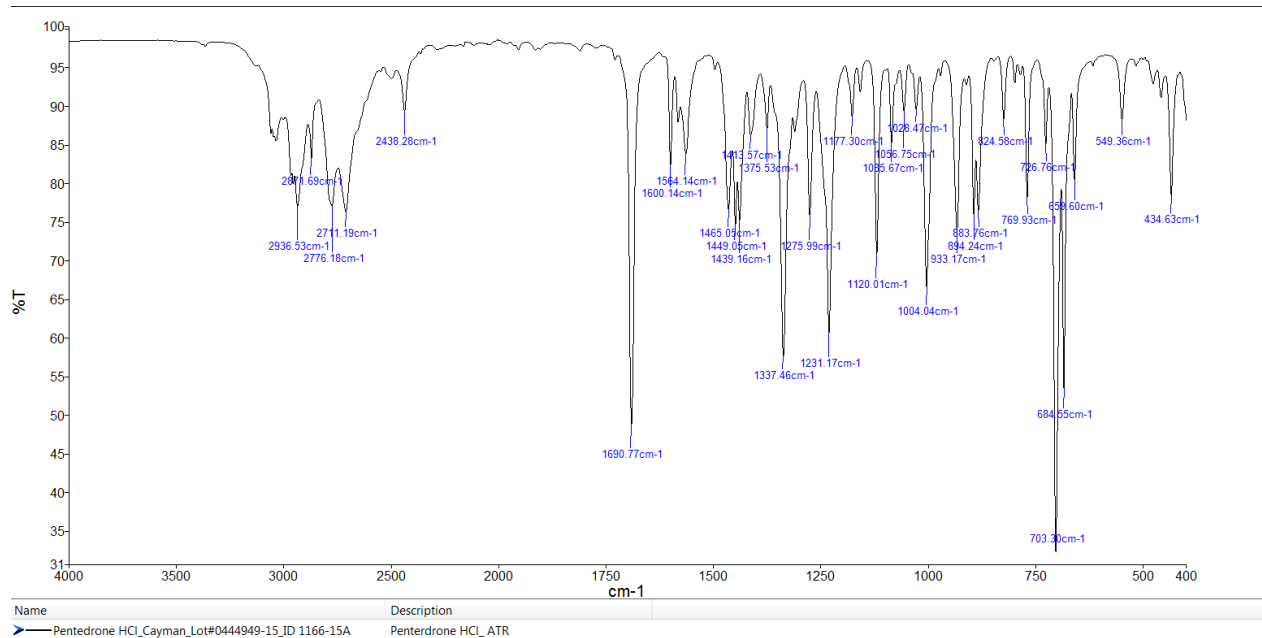
## FIGURES OF SPECTRA

MS (EI)

Abundance



## FTIR-ATR



## IR-condensed phase

