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## ANALYTICAL REPORT

### Phenazepam-4-oxide (C<sub>15</sub>H<sub>10</sub>BrClN<sub>2</sub>O<sub>2</sub>)

**7-bromo-5-(2-chlorophenyl)-4-hydroxy-3,4-dihydro-2H-1,4-benzodiazepin-2-one Phenazepam-4-oxide (Chiron name),  
Phenazepam-4-hydroxy**

Remark – other active cpd. detected: **phenazepam**

Sample ID:	1236-15
Sample description:	powder - white
Sample type:	RM-reference material
Comments <sup>1</sup> :	Chiron Lot#11715; Chiron
Date of entry:	8/22/2015

Substance identified-structure <sup>2</sup> (base form)	
Systematic name:	7-bromo-5-(2-chlorophenyl)-4-hydroxy-3,4-dihydro-2H-1,4-benzodiazepin-2-one Phenazepam-4-oxide (Chiron name), Phenazepam-4-hydroxy
Other names:	
Formula (per base form)	C <sub>15</sub> H <sub>10</sub> BrClN <sub>2</sub> O <sub>2</sub>
M <sub>w</sub> (g/mol)	365.61
Salt form:	base
StdInChiKey	YNKDPC TZJPAZJC-UHFFFAOYSA-N
Compound Class	Benzodiazepines
Other active cpd. detected	phenazepam
Add.info (purity..)	99.5 % (?)

<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): 13.12 BP(1): 286; BP(2): 288, BP(3) :330,
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 thickens 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, than 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 quadropole 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-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 thickens 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, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.

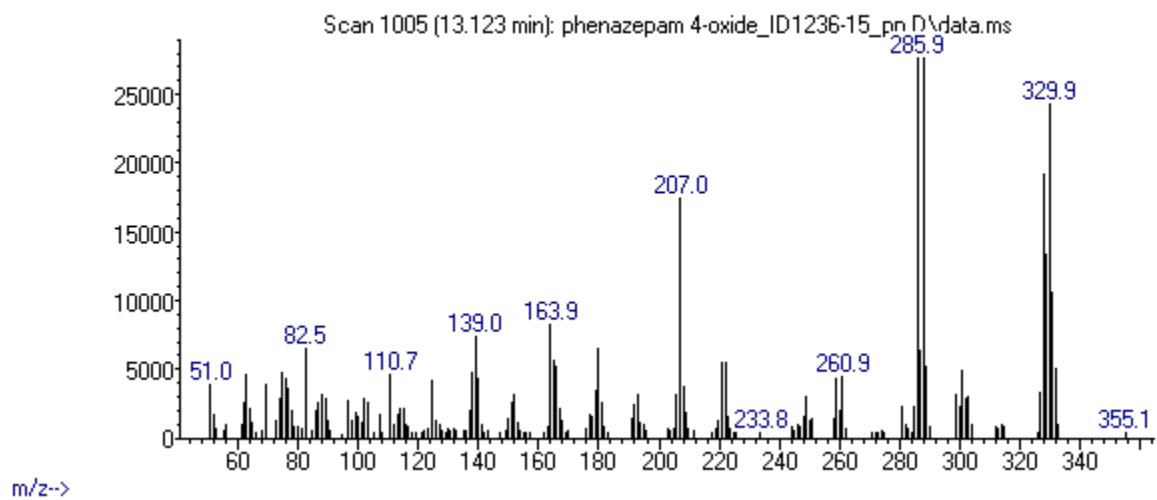
#### Split MS : IR : (1:9)

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

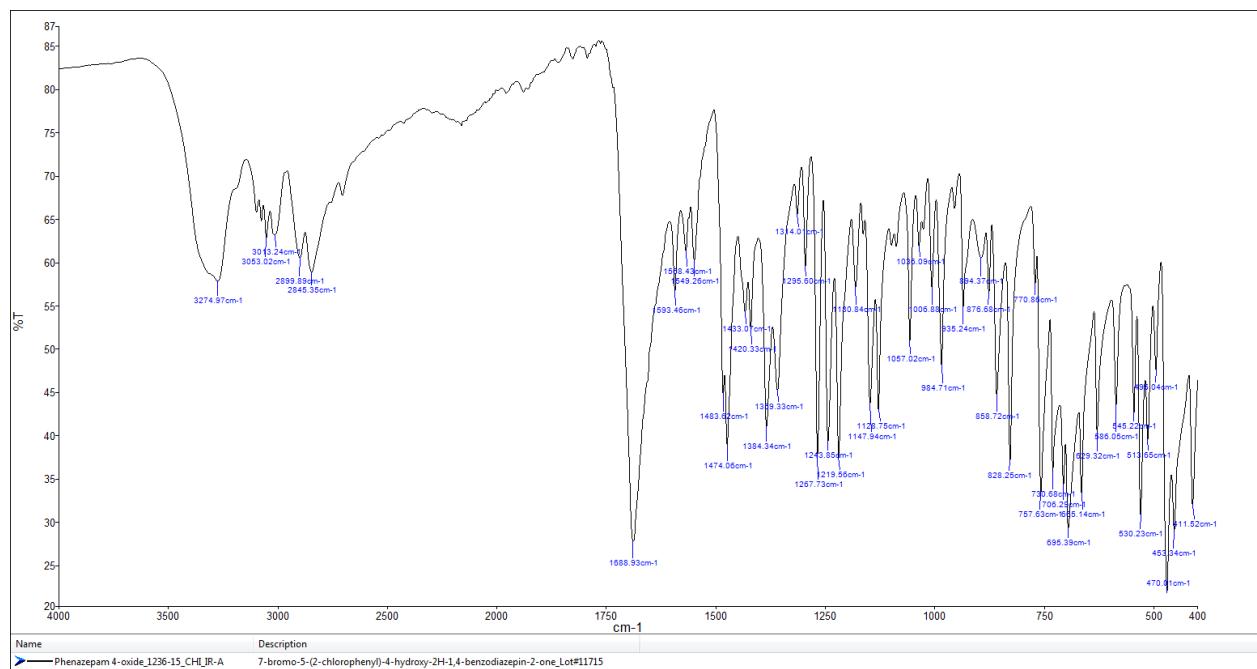
IR (condensed phase): IR scan range 4000 to 700, resolution 4cm-1

## FIGURES OF SPECTRA

GC- MS (EI)  
Abundance



## FTIR-ATR



## IR (condensed phase)

