EUROPEAN PROJECT RESPONSE to challenges in forensic drugs analyses

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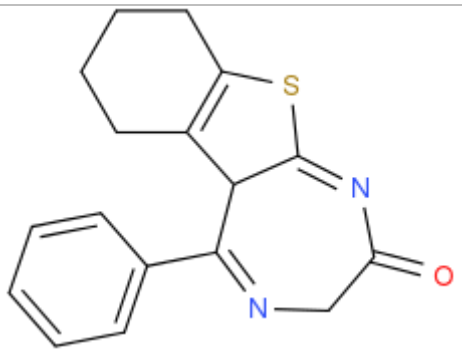
ANALYTICAL REPORT

Bentazepam (C17H16N2OS)

5-phenyl-3,5a,6,7,8,9-hexahydro-2H-[1]benzothieno[2,3-e][1,4]diazepin-2-one

Remark – other active cpd. detected: none

Sample ID:	1234-15
Sample description:	powder - white
Sample type:	RM-reference material
Comments[1]:	Chiron AS Lot#13395; RESPONSE -purchasing
Date of entry:	8/31/2015

Substance identified-structure[2] (base form)	
Systematic name:	5-phenyl-3,5a,6,7,8,9-hexahydro-2H-[1]benzothieno[2,3-e][1,4]diazepin-2-one
Other names:	
Formula (per base form)	C17H16N2OS
M_w (g/mol)	296,39
Salt form:	base
StdInChIKey	LDKXEWJIVTUBFI-UHFFFAOYSA-N
Compound Class	Benzodiazepines
Other active cpd. detected	none
Add.info (purity..)	99,50%

[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): 11,49 BP(1): 267; BP(2): 296,BP(3) :268,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	spectrum is always for the base form of compound

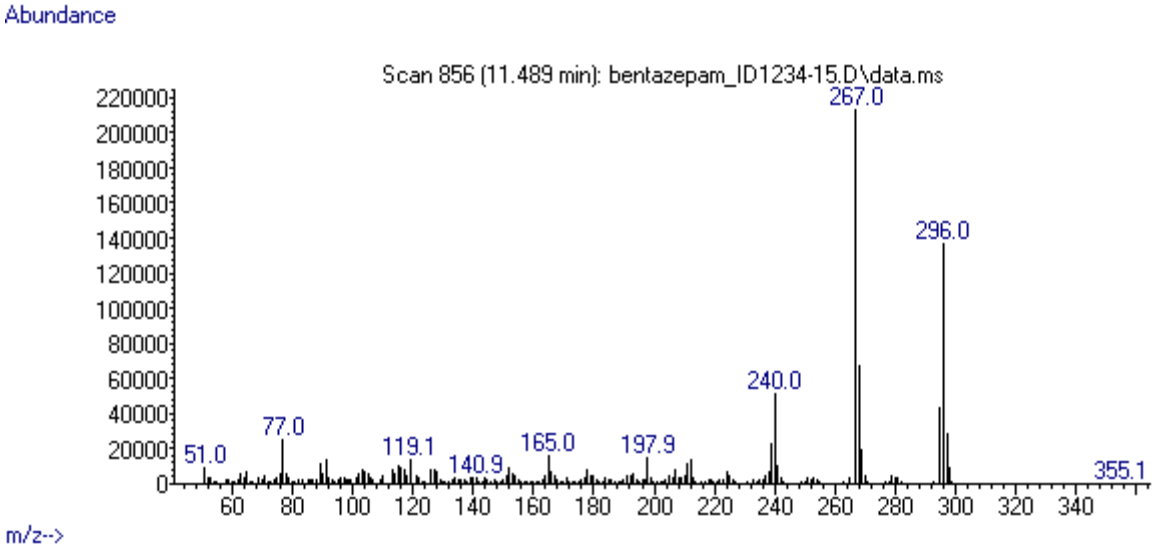
GC-MS (Agilent):
GC-method is RT locked to tetracosane (RT=9.53 min).
Injection volume 1 ml and split mode (1:50) .
Injector temperature: 280 ^{0}C.
Chromatographic separation
Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm.
Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 293 ^{0}C at a rate of 18 ^{0}C/min, hold for 6.1 min, than heating at 50 ^{0}C/min up to 325 ^{0}C and finally 2.8 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 (40) to 550 amu.

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

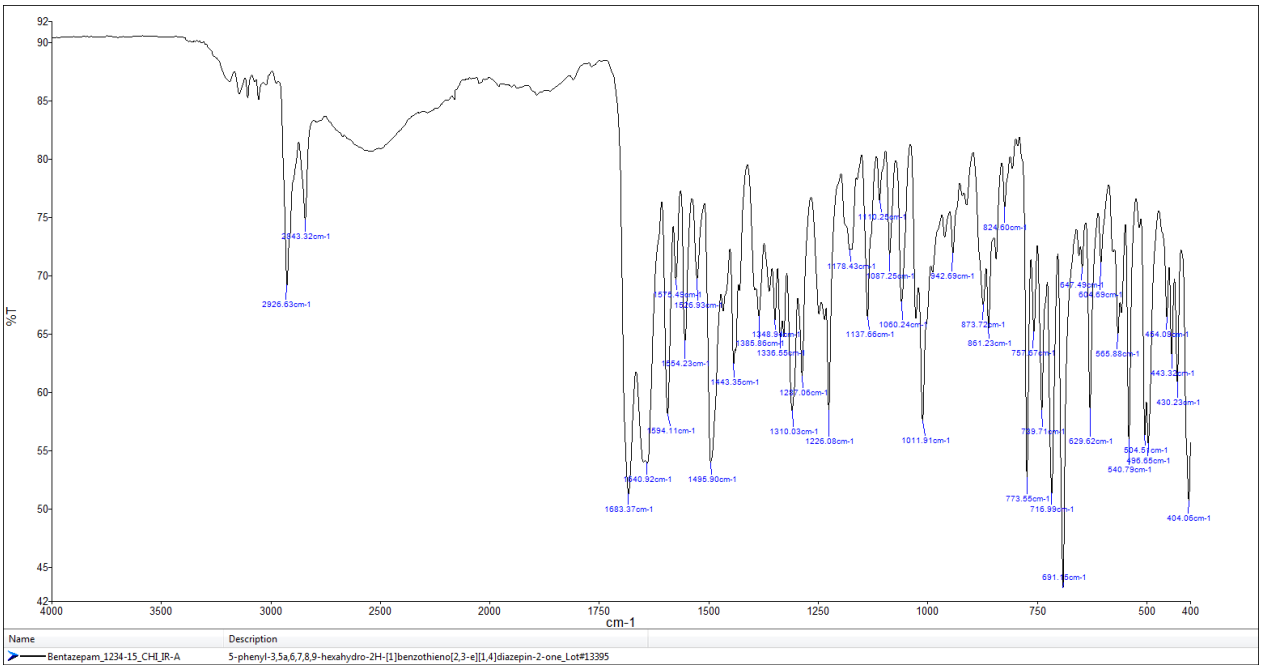
GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm-1
GC-method:
Injection volume 1 ml and split mode (1:5) .
Injector temperature: 280 ^{0}C.
Chromatographic separation
Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm.
Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 293 ^{0}C at a rate of 18 ^{0}C/min, hold for 6.1 min, than heating at 50 ^{0}C/min up to 325 ^{0}C and finally 2.8 min isothermal.
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 (40) to 550 amu.
IR (condesed phase): IR scan range 4000 to 700, resolution 4cm-1

FIGURES OF SPECTRA

MS (EI)



FTIR-ATR



IR-condensed phase