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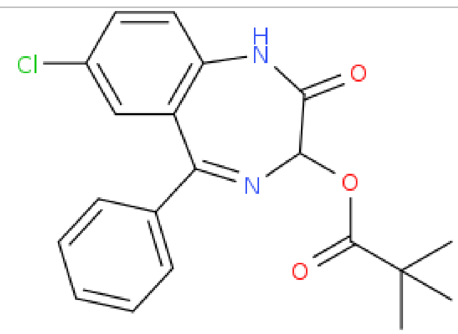
ANALYTICAL REPORT

Pivoxazepam (C20H19ClN2O3)

7-Chloro-2-oxo-5-phenyl-2,3-dihydro-1H-1,4-benzodiazepin-3-yl pivalate

Remark – other active cpd. detected: none

Sample ID:	1577-16
Sample description:	powder - white
Sample type:	RM-reference material
Comments[1]:	Chiron AS Lot#15796; RESPONSE -purchasing
Date of entry:	5/19/2016

Substance identified-structure[2] (base form)	
Systematic name:	7-Chloro-2-oxo-5-phenyl-2,3-dihydro-1H-1,4-benzodiazepin-3-yl pivalate
Other names:	7-chloro-2-oxo-5-phenyl-2,3-dihydro-1H-1,4-benzodiazepin-3-yl 2,2-dimethylpropanoate
Formula (per base form)	C20H19ClN2O3
M_w (g/mol)	370,83
Salt form:	base
StdInChIKey	FTJLKTBLZOULCL-UHFFFAOYSA-N
Compound Class	Benzodiazepines
Other active cpd. detected	none
Add.info (purity..)	99,5 %

[1] This report has been produced with the financial support of the P r e v e n t i o n o f a n d f i g h t a g a i n s t c r i m e 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): 10,23 BP(1): 329; BP(2): 313,BP(3) :73, For GC-MS compound was derivatized by MSTFA: GC-RT and MS spectrum refer for **TMS** derivative. Be aware of possible thermal decomposition in GC.
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	TMS-derivative spectrum

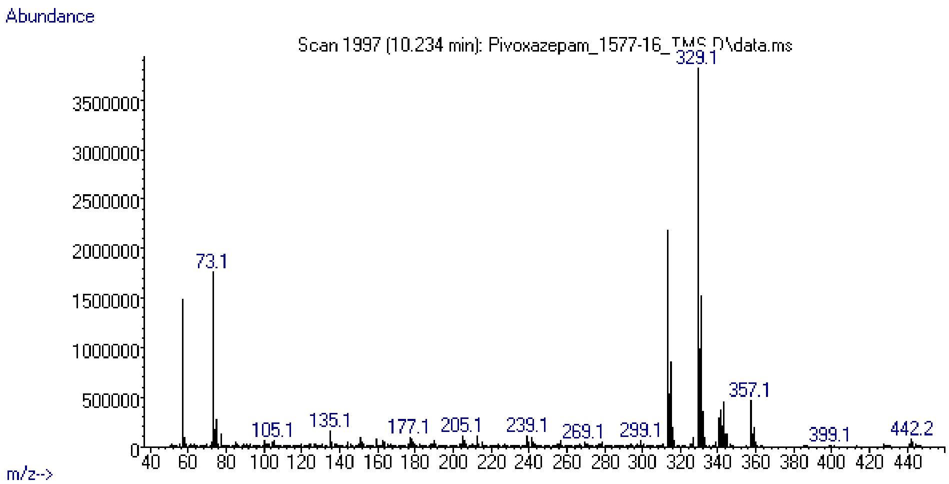
1. GC-MS (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 ml and split mode (1:50). Injector temperature: 280 0C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 190 ^{0}C at rate 8 ^{0}C/min, then heating up to 293 0C at a rate of 18 ^{0}C/min, hold for 6.1 min, then heating at 50 ^{0}C/min up to 325 ^{0}C and finally 6.1 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 (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}

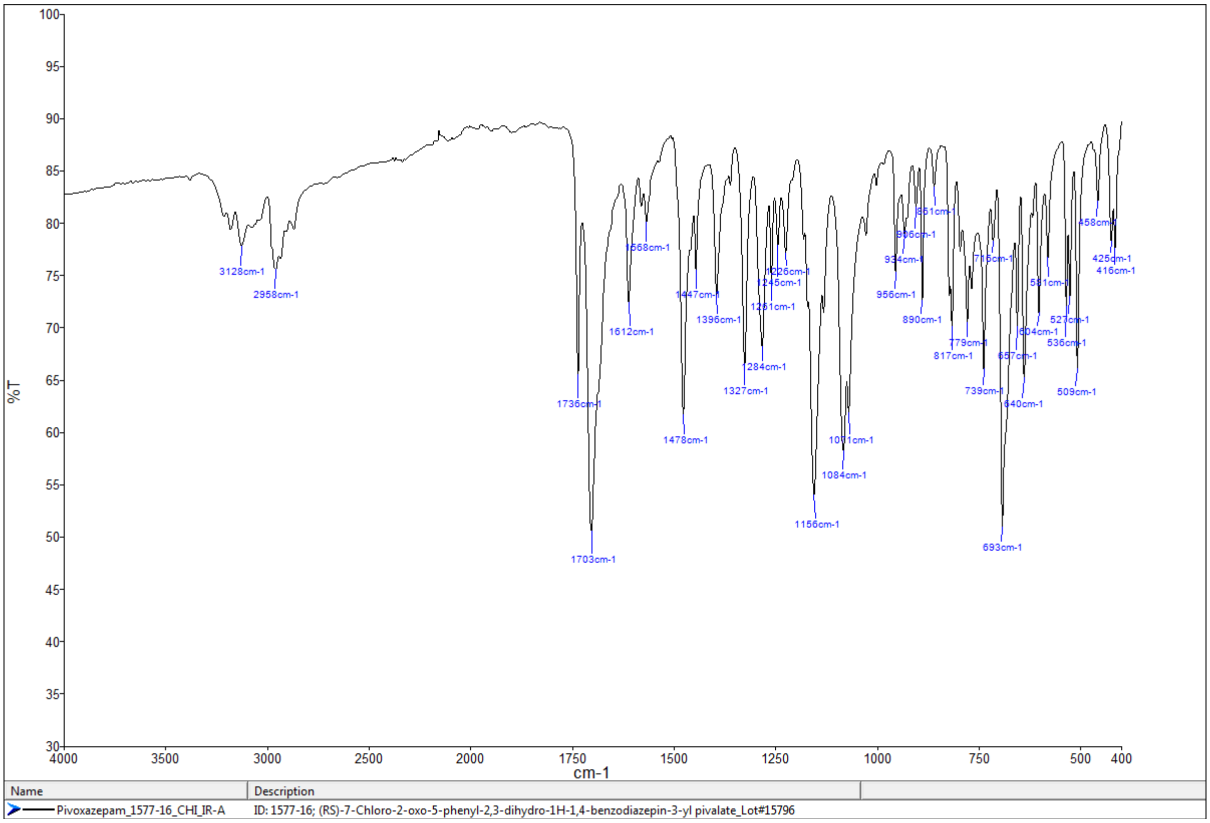
3. GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)
GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 ^{0}C. Chromatographic separation as above **(1).**
Split MS : IR = 1 : 9.
MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.
IR (condesed (solid) phase): IR scan range 4000 to 650, resolution 4 cm^{-1}.

FIGURES OF SPECTRA

MS (EI) : For GC-MS compound was derivatized by MSTFA: GC-RT and MS spectrum refer for **TMS** derivative. Be aware of possible thermal decomposition in GC.



FTIR-ATR



IR-Condensed phase (TMS-derivative spectrum of compound)