

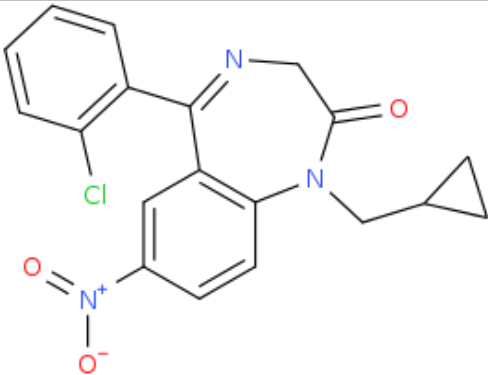
ANALYTICAL REPORT

Cloniprazepam (C₁₉H₁₆ClN₃O₃)

5-(2-chlorophenyl)-1-cyclopropylmethyl-7-nitro-3H-1,4-benzodiazepin-2-one

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

Sample ID:	1575-16
Sample description:	crystalline - white
Sample type:	RM-reference material
Comments ¹ :	Chiron AS Lot#16219; RESPONSE -purchasing
Date of entry:	5/19/2016

Substance identified-structure ² (base form)	
Systematic name:	5-(2-chlorophenyl)-1-cyclopropylmethyl-7-nitro-3H-1,4-benzodiazepin-2-one
Other names:	Kloniprazepam
Formula (per base form)	C ₁₉ H ₁₆ ClN ₃ O ₃
M _w (g/mol)	369.81
Salt form:	base
StdInChIKey	CCSYKGYLSFXNTA-UHFFFAOYSA-N
Compound Class	Benzodiazepines
Other active cpd. detected	none

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

Add.info (purity..)	99,5 %
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Report updates

date	comments (explanation)

Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 13.62 BP(1): 340; BP(2): 55,BP(3) :125,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	always as base form

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 quadropole 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.

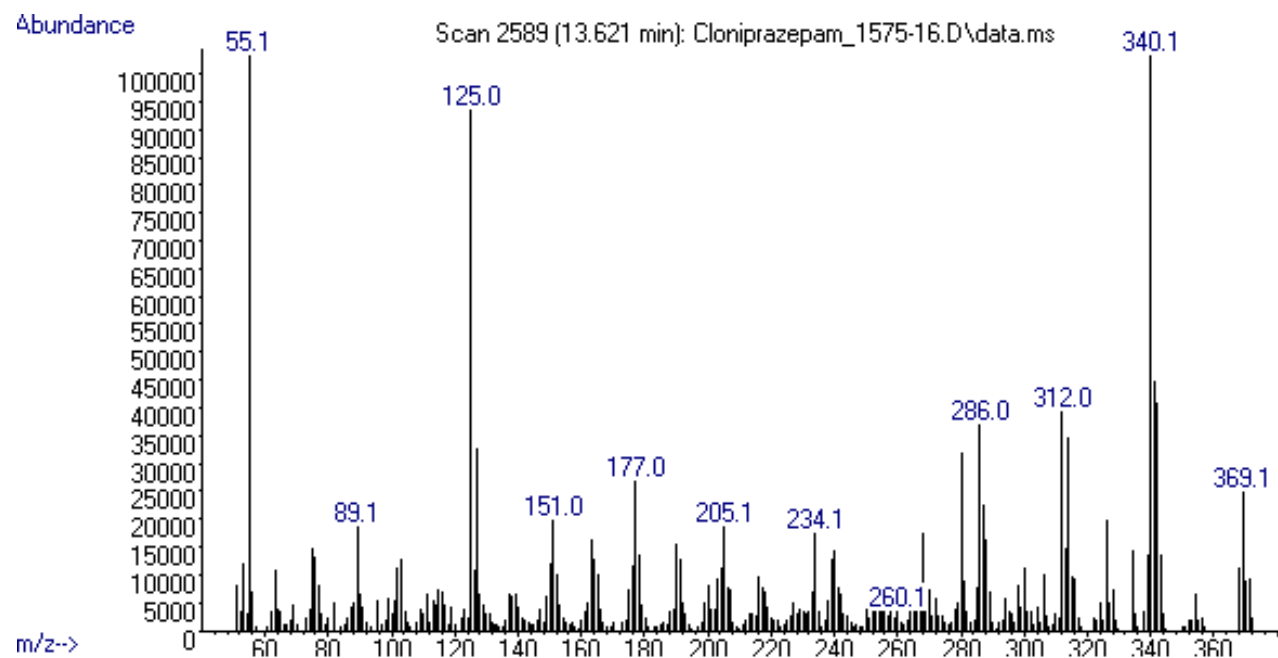
Split MS : IR : (1:9)

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

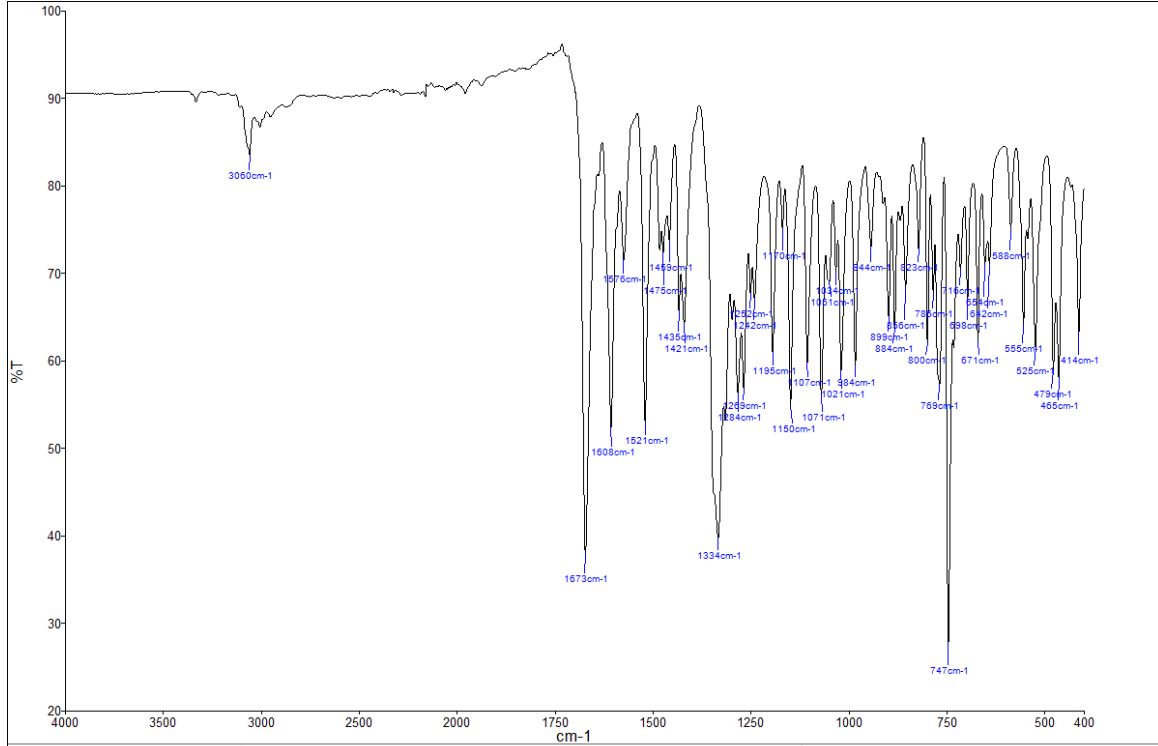
IR (condensed phase): IR scan range 4000 to 700, resolution 4cm⁻¹

FIGURES OF SPECTRA

MS (EI)

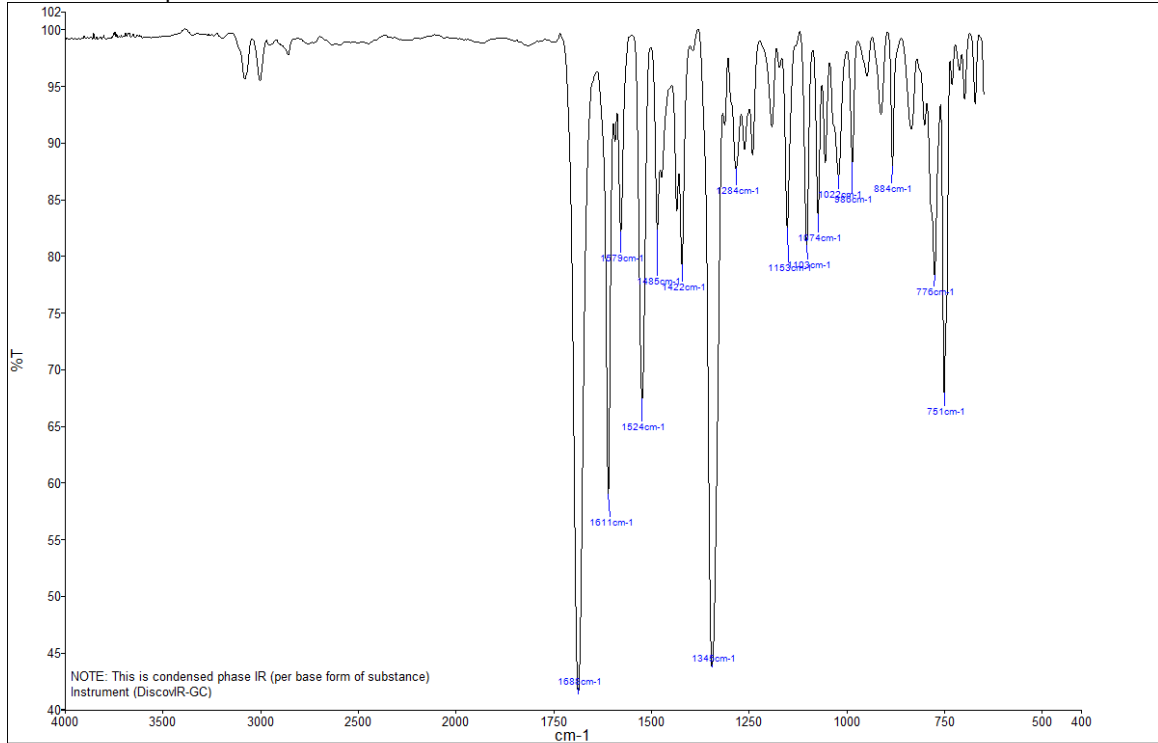


FTIR-ATR



Name	Description
Cloniprazepam_1575-16_CHI_IR-A	ID:1575-16; 5-(2-chlorophenyl)-1-cyclopropylmethyl-7-nitro-3H-1,4-benzodiazepin-2-one_Lot#16219

IR-Condensed phase



Name	Description
Cloniprazepam_1575-16_CHI_IR-C.spc	Sample_1575-16; 5-(2-chlorophenyl)-1-cyclopropylmethyl-7-nitro-3H-1,4-benzodiazepin-2-one_Lot#16219