



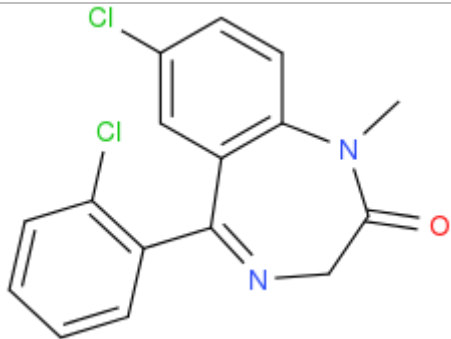
ANALYTICAL REPORT

Diclazepam (C₁₆H₁₂Cl₂N₂O)

7-chloro-5-(2-chlorophenyl)-1-methyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one

Remark – other NPS detected: **none**

Sample ID:	1197-15
Sample description:	powder - white
Sample type:	test purchase
Comments:	RESPONSE -purchasing
Date of entry:	7/29/2015

Substance identified-structure ⁱ (base form)	
Systematic name	7-chloro-5-(2-chlorophenyl)-1-methyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one
Other names	
Formula (per base form)	C ₁₆ H ₁₂ Cl ₂ N ₂ O
M _w (g/mol)	319,19
Salt form	base
StdInChIKey	VPAYQWRBBOGGPY-UHFFFAOYSA-N
Compound Class	Benzodiazepines
Other NPS detected	none
Add.info (purity..)	by applied techniques impurities were not detected

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.

Supporting information

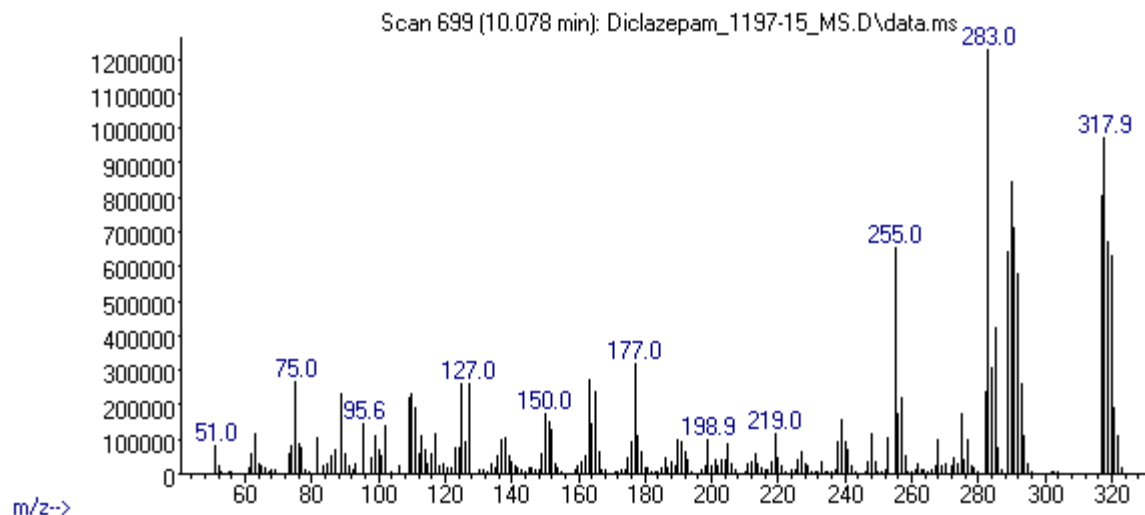
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 10,08 BP(1): 283; BP(2): 318,BP(3) :290,
FTIR-ATR	+	direct measurement
FTIR (condensed phase) always as base form		
HPLC-TOF	+	Exact mass (theoretical): 318,0327; measured value Δ ppm:-0,27; formula:C16H12Cl2N2O
NMR-confirmed		
validation		MS spectrum consistent by the one in SWGDRUG MS library (match quality=99); http://www.swgdrug.org/ms.htm
other		

GC-MS (Agilent): GC-method is RT locked to tetracosane (RT=9.53 min). Injection volume 1 ml and split mode (1:50)for GC-MS instruments and 1:5 for GC-MS-FTIR(condensed phase). Injector temperature: 280 °C. 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, 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 quadrupole temperatures 280°C and 180°C. m/z scan range: from 50 (40) to 550 amu.

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

FTIR (Spectra analyses-Danny): scan range 4000 to 700, resolution 4cm⁻¹

Abundance



GC-MS spectrum EI

Target Compound Screening Report

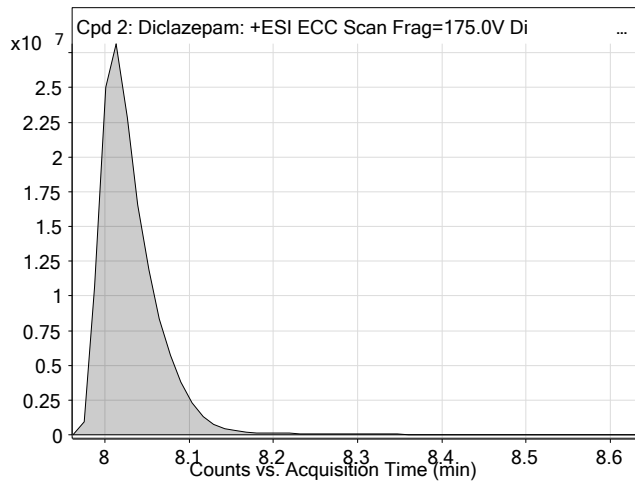
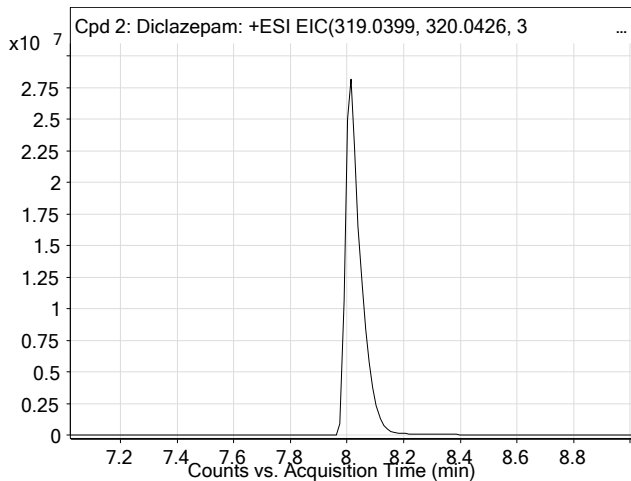
Data File	Diclazepam_1197-15_TOF.d	Sample Name	Diclazepam
Sample Type	Sample	Position	P1-D7
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	droge general-13-5-2015-XDB-C18-ESI-poz.m	Acquired Time	7/27/2015 11:52:54 AM
IRM Calibration Status	Success	DA Method	Droge_Default.m
Comment	extract in MeOH		

Compound Table

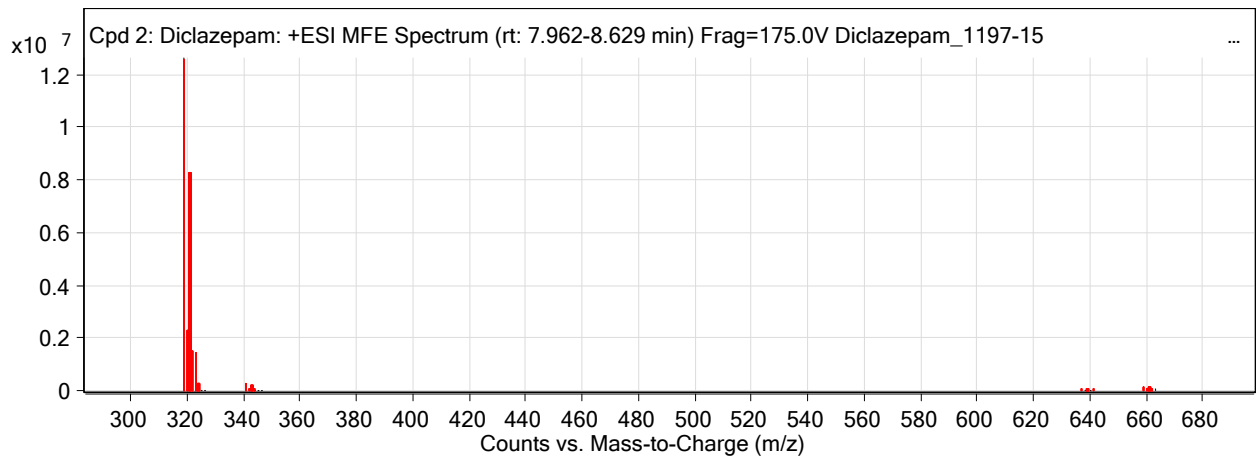
Label	Tgt Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 2: Diclazepam	Diclazepam	C16 H12 Cl2 N2 O	8.016	318.0328

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)	Find Cpd Algorithm
Diclazepam	319.0399	8.016	318.0328	8.016	C16 H12 Cl2 N2 O	318.0327	-0.27	Find by Molecular Feature

Compound Chromatograms



MFE MS Zoomed Spectrum



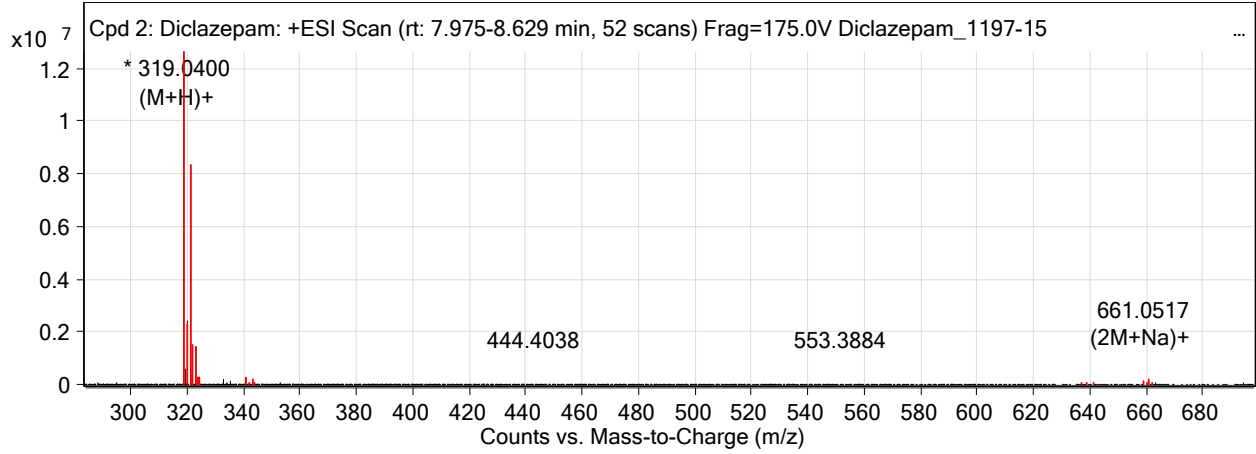
MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
319.0399	1	12620229	C16 H12 Cl2 N2 O	(M+H)+
320.0433	1	2307570.73	C16 H12 Cl2 N2 O	(M+H)+
321.0374	1	8296517.39	C16 H12 Cl2 N2 O	(M+H)+
322.0405	1	1450317.2	C16 H12 Cl2 N2 O	(M+H)+
323.0352	1	1349720.43	C16 H12 Cl2 N2 O	(M+H)+
324.038	1	214567.43	C16 H12 Cl2 N2 O	(M+H)+
341.0222	1	281215.78	C16 H12 Cl2 N2 O	(M+Na)+

Target Compound Screening Report

343.0194	1	184162.73	C16 H12 Cl2 N2 O	(M+Na)+
659.0541	1	119246.5	C16 H12 Cl2 N2 O	(2M+Na)+
661.0519	1	166341.31	C16 H12 Cl2 N2 O	(2M+Na)+

MS Zoomed Spectrum



--- End Of Report ---