EUROPEAN PROJECT RESPONSE to challenges in forensic drugs analyses

Co-funded by the Prevention of and Fight against Crime Programme of the European Union

NACIONALNI FORENZIČNI LABORATORIJ
NATIONAL FORENSIC LABORATORY

Vodovodna 95
1000 Ljubljana
SLOVENIJA

T: +386 (0)1 428 44 93
E: nfl@policija.si
www.policija.si

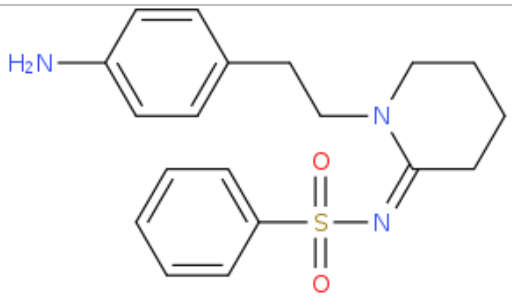
ANALYTICAL REPORT

Deschloro-W-19 (C19H23N3O2S)

N-[(2Z)-1-[2-(4-aminophenyl)ethyl]piperidin-2-ylidene]benzenesulfonamide

Remark – other active cpd. detected: none

Sample ID:	1709-16
Sample description:	powder - yellow-bright
Sample type:	RM-reference material
Comments[1]:	CAY Lot#04829213; RESPONSE -purchasing
Date of entry:	1/6/2017

Substance identified-structure[2] (base form)	
Systematic name:	N-[(2Z)-1-[2-(4-aminophenyl)ethyl]piperidin-2-ylidene]benzenesulfonamide
Other names:	(Z)-N-(1-(4-aminophenethyl)piperidin-2-ylidene)benzenesulfonamide
Formula (per base form)	C19H23N3O2S
M_w (g/mol)	357,47
Salt form:	HCl
StdInChIKey (per base form)	LEPJQUCPARWIPK-VZCXRCSSSA-N
Other active cpd. detected	none
Add.info (purity..)	98%

[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): 17,54 BP(1): 119; BP(2): 77,BP(3) :106,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	always as base form

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 7.1 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.

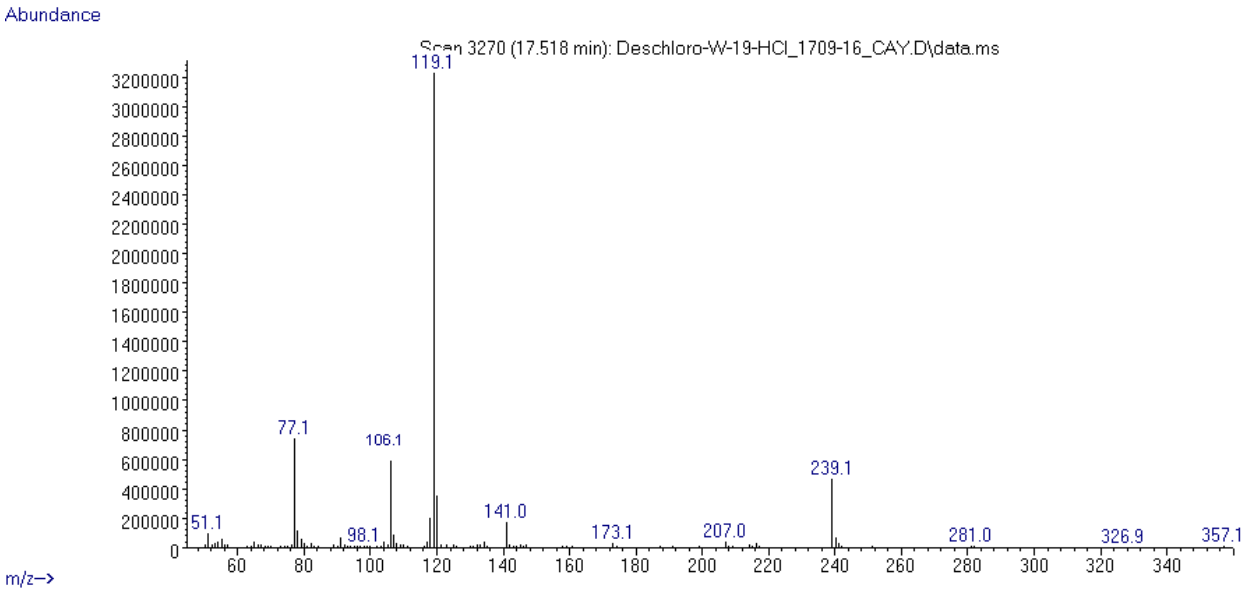
2. FTIR-ATR (Perkin Elmer): scan range 4000-400 cm^{-1}; resolution 4cm^{-1}

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}.

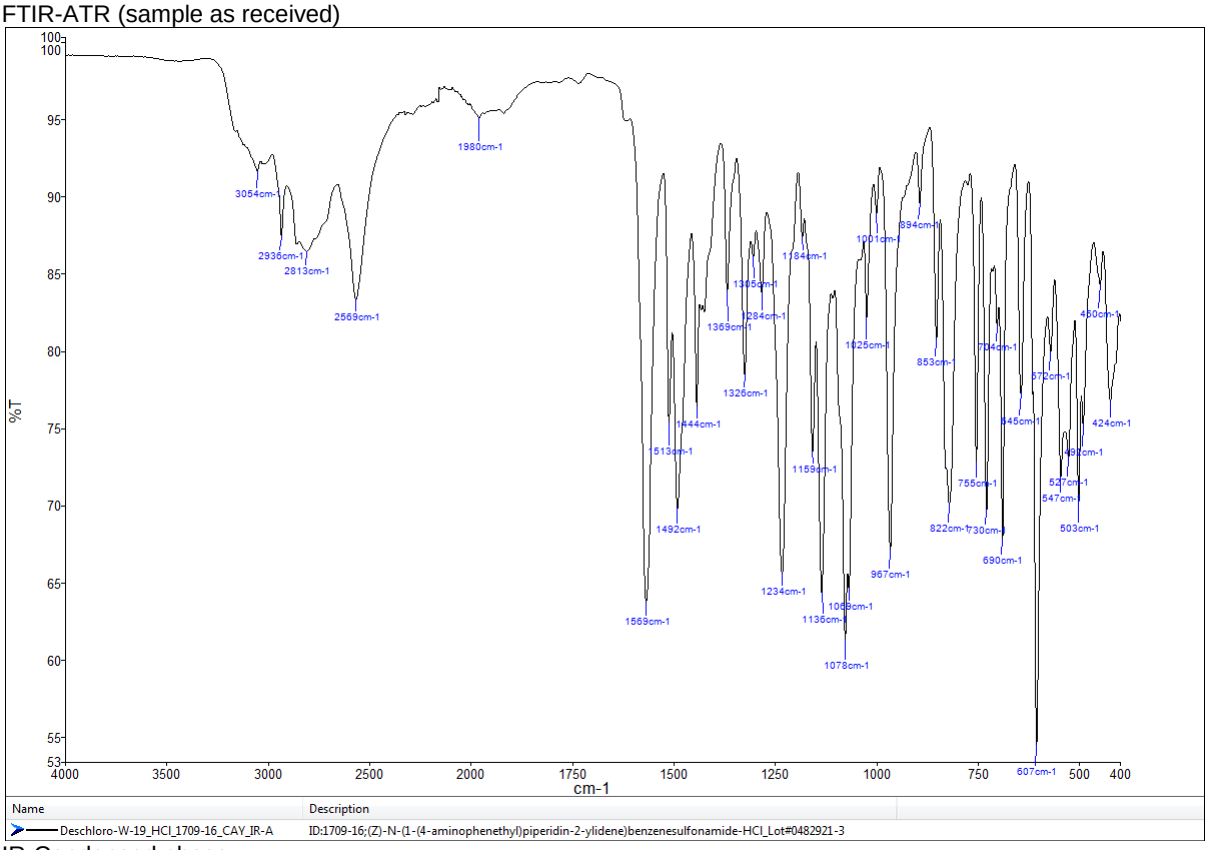
4. HPLC-TOF for exact monoisotopic mass and empirical formula control - results are not shown in the report.

FIGURES OF SPECTRA

MS (EI)

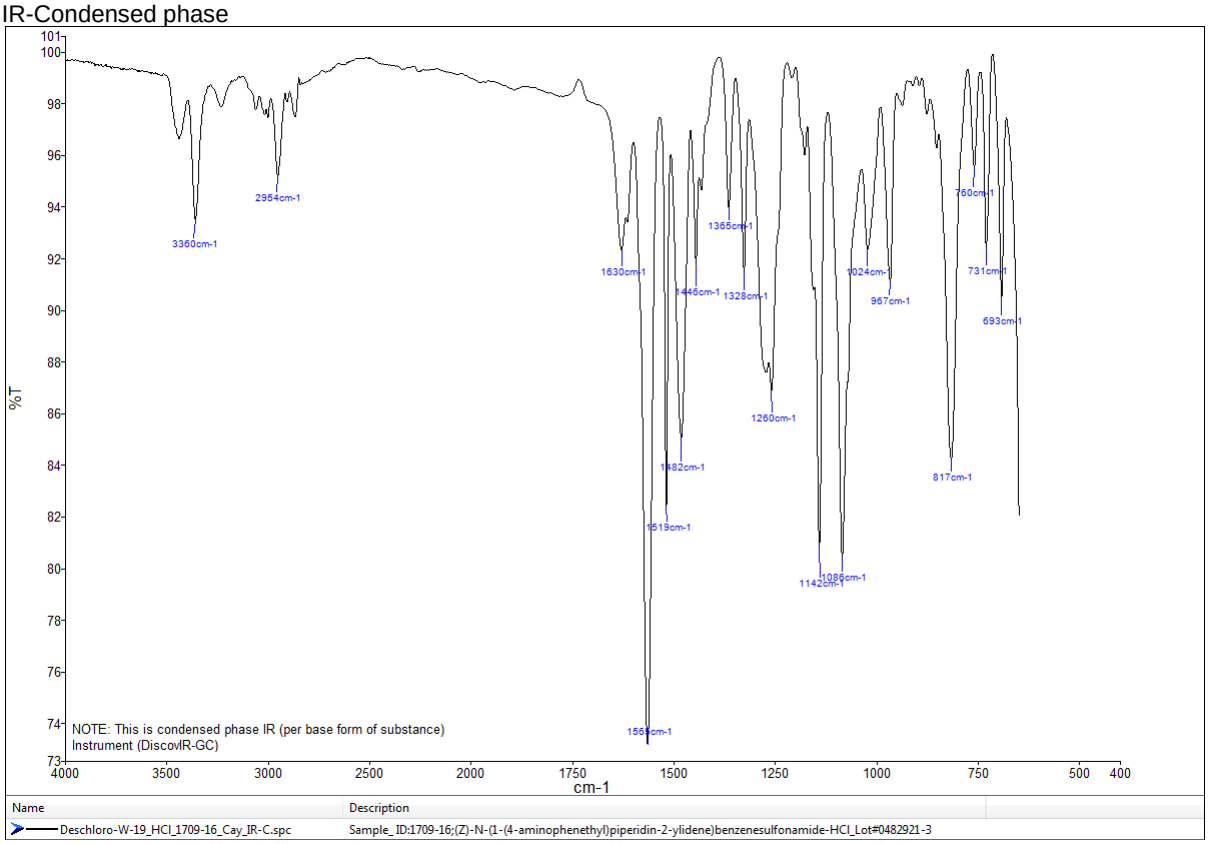


FTIR-ATR (sample as received)



Name	Description
Deschloro-W-19_HCl_1709-16_CAY_IR-A	ID:1709-16;(Z)-N-(1-(4-aminophenethyl)piperidin-2-ylidene)benzenesulfonamide-HCl_Lot#0482921-3

IR-Condensed phase



Name	Description
Deschloro-W-19_HCl_1709-16_Cay_IR-C.spc	Sample_ID:1709-16;(Z)-N-(1-(4-aminophenethyl)piperidin-2-ylidene)benzenesulfonamide-HCl_Lot#0482921-3