

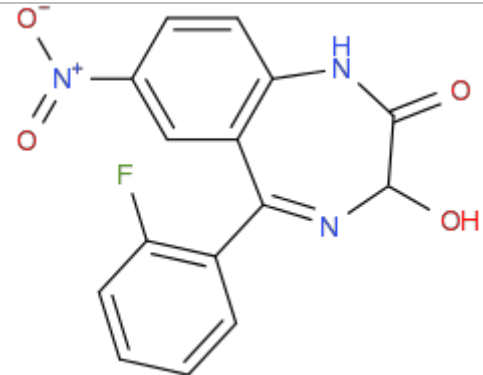
ANALYTICAL REPORT

nifoxipam (C₁₅H₁₀FN₃O₄)

5-(2-fluorophenyl)-3-hydroxy-7-nitro-1H-benzo[e][1,4]diazepin-2(3H)-one

Remark – other NPS detected: **none**

Sample ID:	233-1918/15
Sample description:	tablet - brownish
Sample type:	collected
Comments:	NGO-collected
Date of entry:	5/13/2015

Substance identified- structure ⁱ (base form)	
Systematic name	5-(2-fluorophenyl)-3-hydroxy-7-nitro-1H-benzo[e][1,4]diazepin-2(3H)-one
Other names	nifoxipam
Formula (per base form)	C ₁₅ H ₁₀ FN ₃ O ₄
M _w (g/mol)	315,26
Salt form	
Smiles	<chem>FC1=C(C=CC=C1)C=1C2=C(NC(C(N1)O)=O)C=CC(=C2)[N+](=O)[O-]</chem>
Compound Class	Benzodiazepines
Other NPS detected	none
Add.info (purity..)	fillers - tablet (not pure)

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): 9,37 BP(1): 223; BP(2): 222,BP(3) :75,
FTIR-ATR	-	
FTIR (condensed phase) always as base form	+	
HPLC-TOF	+	Exact mass (theoretical): 315,0655; measured value Δ ppm:-0,69; formula:C15H10FN3O4
NMR-confirmed	-	
validation		MS consistent by the one reported to EMCDDA EDND by Swedish
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

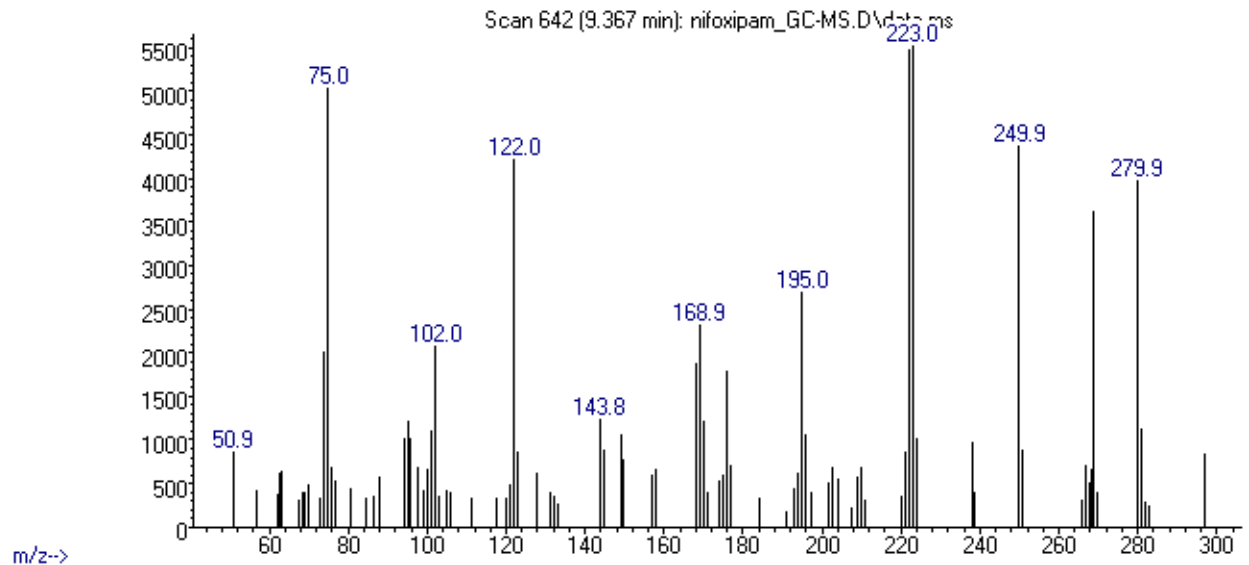


Figure 1: EI-MS spectrum

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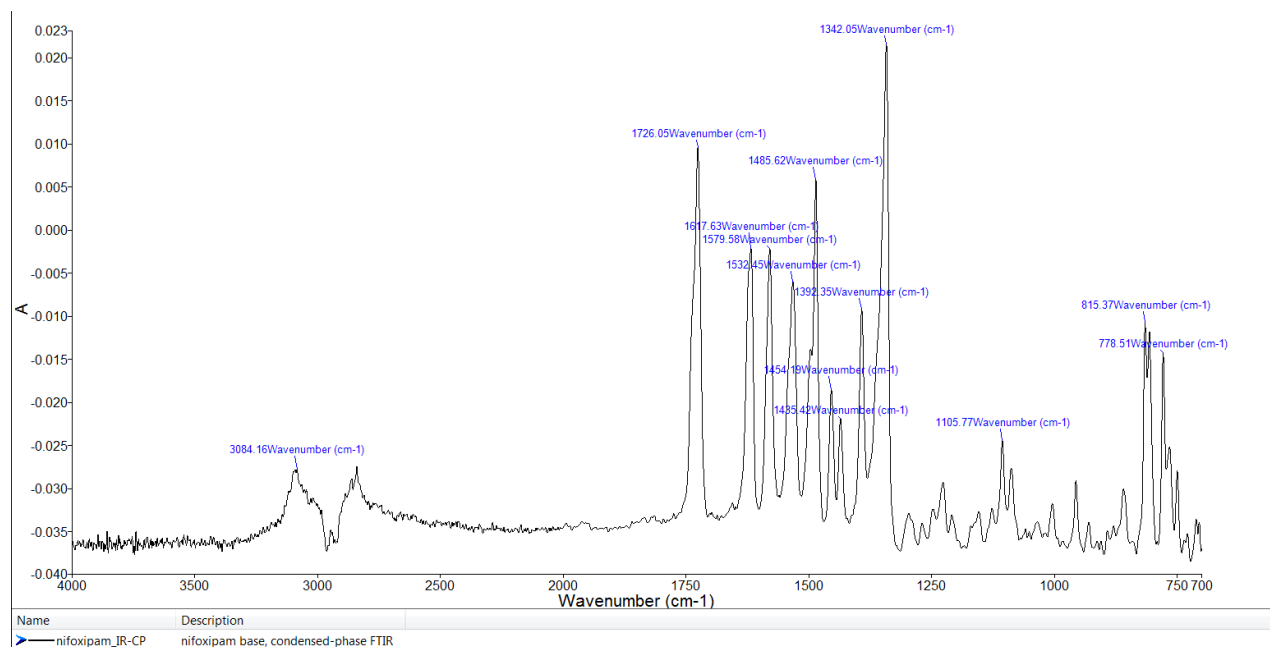


Figure 2: FTIR-condensed phase



Figure 3: Tablet

ⁱ Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d

Target Compound Screening Report TOF

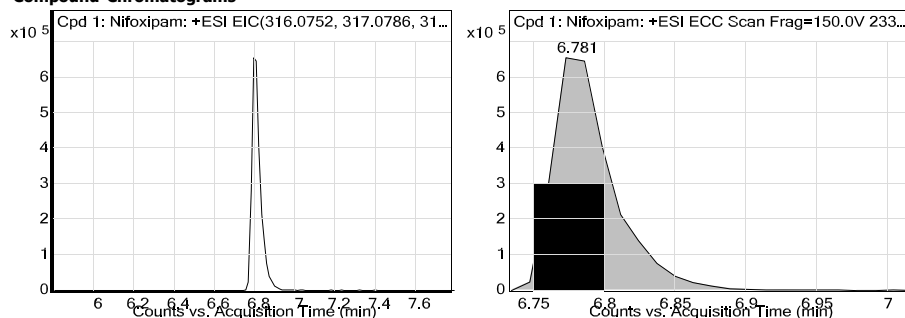
Data File	233-1890-15_10.d	Sample Name	vzorec 10
Sample Type	Sample	Position	P1-F7
Instrument Name	SG13170002	User Name	
Acq Method	droge general-13-5-2015-XDB-C18-ESI-poz.m	Acquired Time	5/13/2015 1:01:11 PM
IRM Calibration Status	Success	DA Method	Droge_Default.m
Comment	ekstrakcija v MeOH		

Compound Table

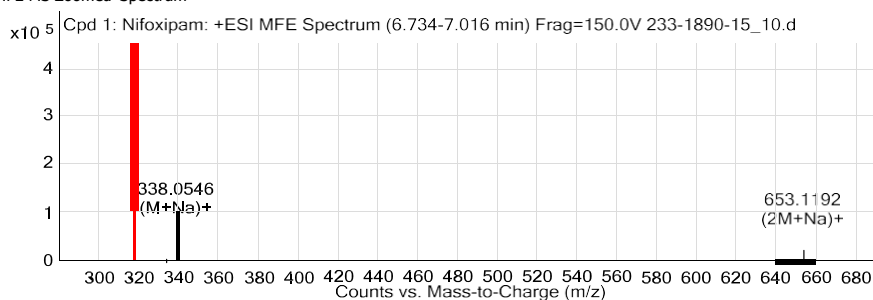
Label	Tgt Name	MFG Formula	Tgt Formula	Obs. RT	Obs. Mass
Cpd 1: Nifoxipam	Nifoxipam	C15 H10 F N3 O4	C15 H10 F N3 O4	6.781	315.0658

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error	Tgt Formula	Find Cpd's Algorith
Nifoxipam	316.073	6.781	315.0658	6.784	C15 H10 F N3 O4	315.0655	-0.74	C15 H10 F N3 O4	Find by Molecular Feature

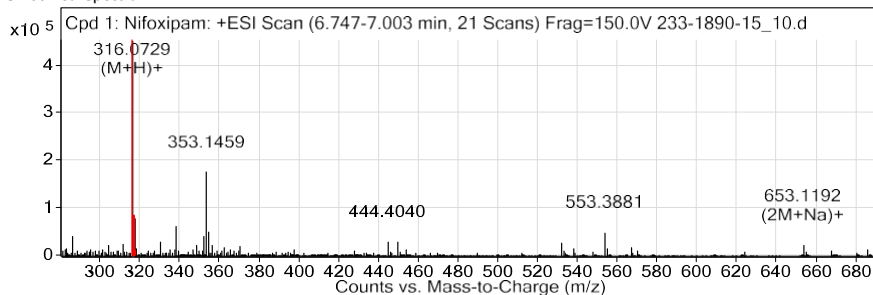
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
316.073	1	452834.22	C15 H10 F N3 O4	(M+H)+
317.0761	1	79645.92	C15 H10 F N3 O4	(M+H)+
318.0792	1	15625.29	C15 H10 F N3 O4	(M+H)+
333.1008	1	6560.65		(M+NH4)+
338.0546	1	50060.16		(M+Na)+
339.0585	1	9664.81		(M+Na)+
340.0591	1	2588.63		(M+Na)+
653.1192	1	26791.38		(2M+Na)+
654.1217	1	9623.78		(2M+Na)+
655.1289	1	5231.02		(2M+Na)+

--- End Of Report ---