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

3-Meo-PCP, (C18H27NO)

1-[1-(3-methoxyphenyl)cyclohexyl]-piperidine

Remark – other NPS detected: none

Sample ID:	233-1890/2015
Sample description:	tablet - green (see Figure 1:)
Sample type:	C-collected
Date of entry:	5/13/2015

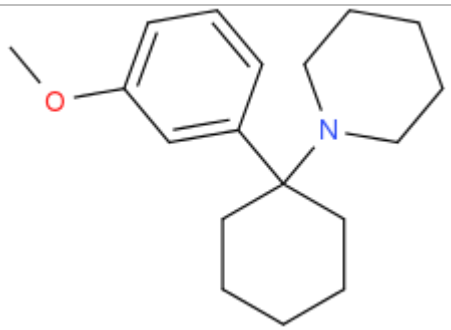
Substance identified-structure[i] (base form)	
Systematic name	1-[1-(3-methoxyphenyl)cyclohexyl]-piperidine
Other names	3-Methoxyphencyclidine
Formula (per base form)	C18H27NO
M_w (g/mol)	273,41
Salt form	
Smiles	COC=1C=C(C=CC1)C1(CCCCC1)N1CCCCC1
Compound Class	Arylcyclohexylamines
Other NPS detected	none
Add.info (purity..)	caffeine, mix

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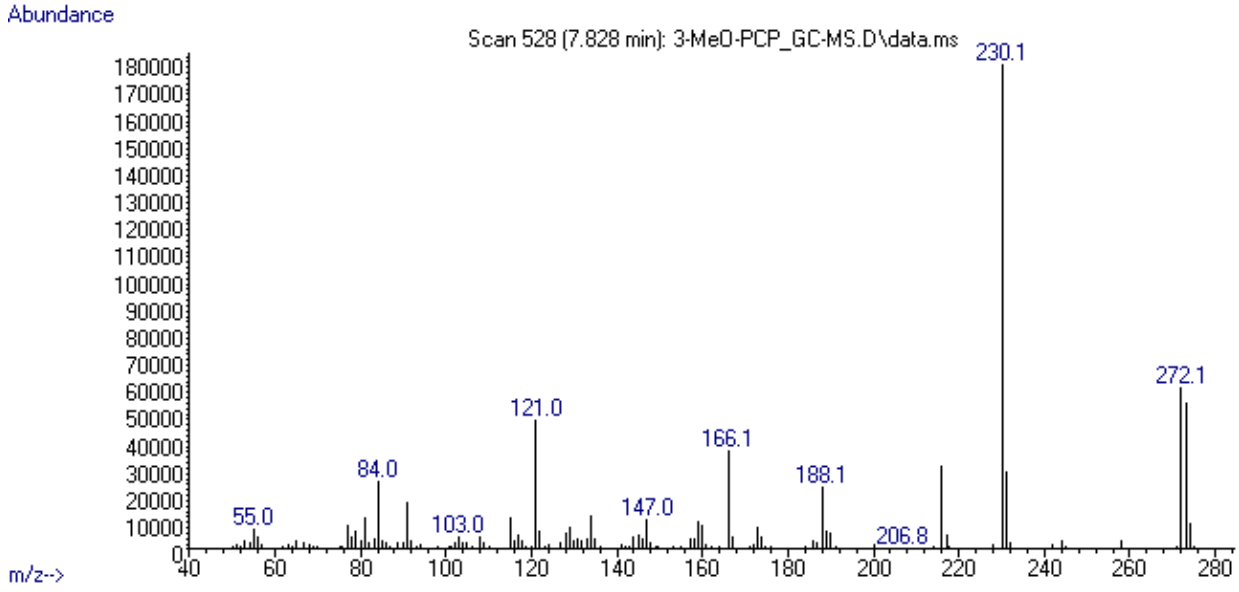
Figure 1: green tablets smile logo

Supporting information

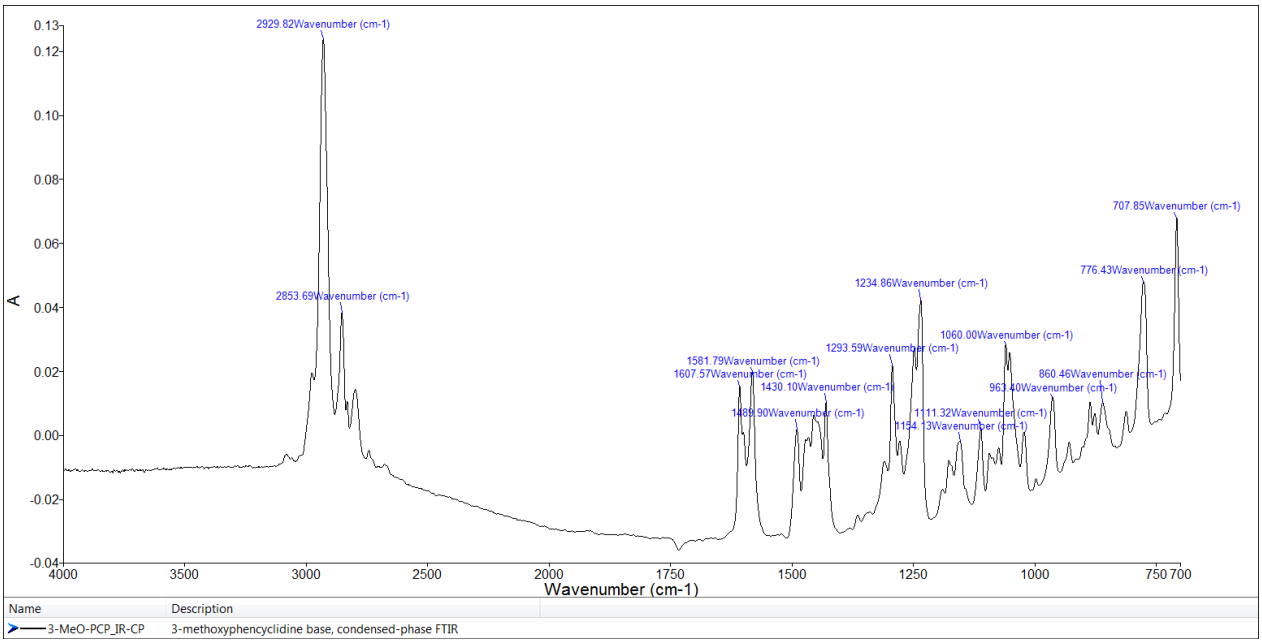
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 7,83 BP(1): 230; BP(2): 272,BP(3) :273,
FTIR-ATR	/	not relevant as substance is in mixture with other compounds
FTIR (condensed phase) always as base form	+	
HPLC-TOF	+	Exact mass (theoretical): 273,2093; measured value Δppm:1,22; formula:C18H27NO
NMR-confirmed	-	
validation		MS spectrum consistent with the published
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 ^{0}C. Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 293 ^{0}C at a rate of 18 ^{0}C/min, hold for 6.1 min, than heating at 50 ^{0}C/min up to 325 ^{0}C and finally 2.8 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. 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 600, resolution 4cm-1

MS spectrum:



FTIR (condensed phase)



[i] Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ **DOI:** 10.1021/ci100384d

Target Compound Screening Report

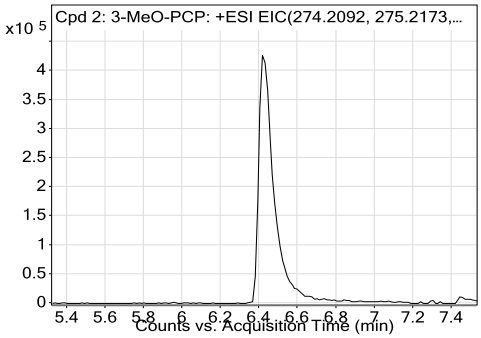
Data File	233-1890-15_11.d	**Sample Name**	vzorec 11
Sample Type	Sample	**Position**	P1-F8
Instrument Name	SG13170002	**User Name**	
Acq Method	droge general-13-5-2015-XDB-C18-ESI-poz.m	**Acquired Time**	5/13/2015 1:15:43 PM
IRM Calibration Status	Success	**DA Method**	Droge_Default.m
Comment	ekstrakcija v MeOH		

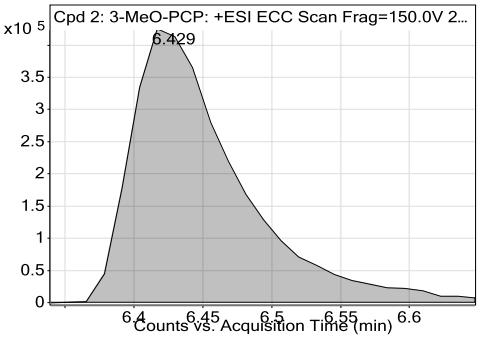
Compound Table

Label	Tgt Name	MFG Formula	Tgt Formula	Obs. RT	Obs. Mass
Cpd 2: 3-MeO-PCP	3-MeO-PCP	C18 H27 N O	C18 H27 N O	6.429	273.2089

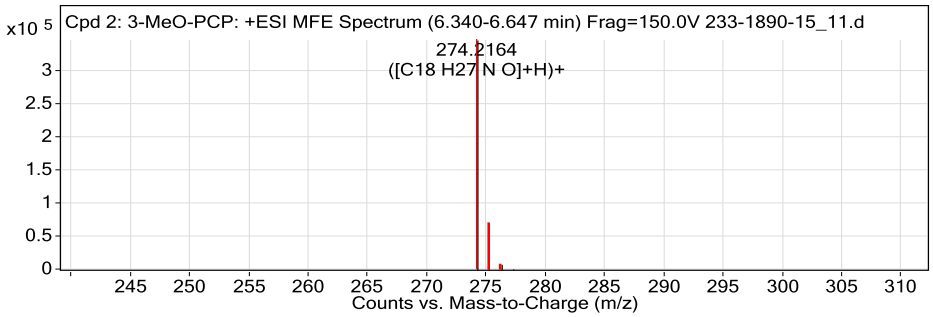
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error	Tgt Formula	Find Cpds Algorith
3-MeO-PCP	274.2164	6.429	273.2089	6.429	C18 H27 N O	273.2093	1.22	C18 H27 N O	Find by Molecular Feature

Compound Chromatograms

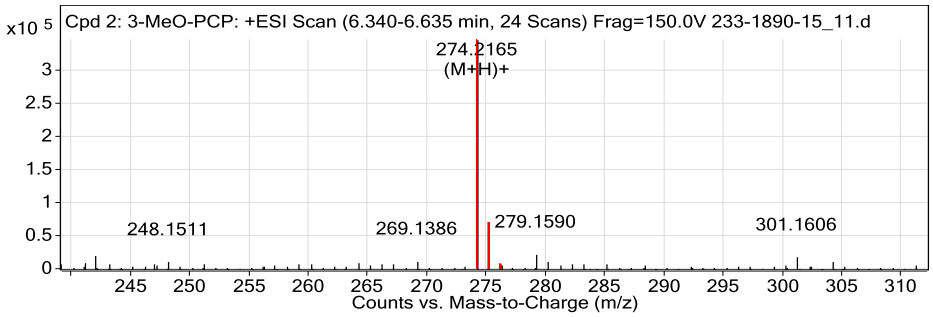




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
274.2164	1	345552	C18 H27 N O	(M+H)+
275.2195	1	71195.38	C18 H27 N O	(M+H)+
276.2168	1	8792.8	C18 H27 N O	(M+H)+
277.2203	1	978.1	C18 H27 N O	(M+H)+

--- End Of Report ---