



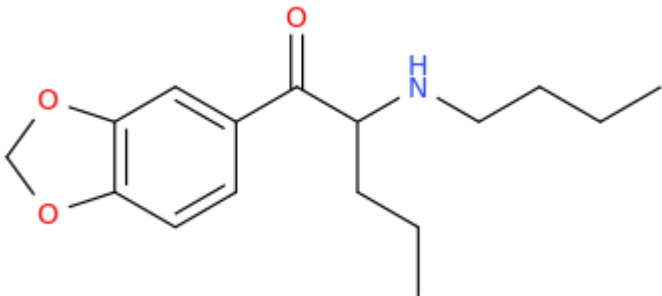
ANALYTICAL REPORT

N-butyl norpentylone (C₁₆H₂₃N₃)

1-(2H-1,3-benzodioxol-5-yl)-2-(butylamino)pentan-1-one

Remark – other NPS detected: **none**

Sample ID:	2088-19
Sample description:	powder
Sample type:	collected /FSI Zurich, Switzerland
Date of entry (DD/MM/YYYY) into NFL database:	02/09/2019
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure ¹ (base form)	
Systematic name	1-(2H-1,3-benzodioxol-5-yl)-2-(butylamino)pentan-1-one
Other names	bk-BBDP
Formula (per base form)	C ₁₆ H ₂₃ N ₃
M _w (g/mol)	277,36
Salt form/anions detected	HCl
StdInChIKey (per base form)	SEIQPCGGBMTHCB-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	

¹ Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d

Report updates

date	comments (explanation)

Instrumental methods (if applied) in NFL

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 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 °C at a rate of 18 °C/min, hold for 7.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 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 until 6 min) amu.

2. HPLC-TOF (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N2) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.

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

4. 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 °C. Chromatographic separation as above **(1)**. 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 (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

5. IC (anions) (Thermo Scientific, Dionex ICS 2100), Column: IonPac AS19, 2 x 250mm; Eluent: 10mM KOH from 0 to 10 min, 10-58 mM from 10 to 40min; Flow rate: 0.25 ml/min; Temperature: 30°C; Suppressor: AERS 500 2mm, suppressor current 13mA; Inj. Volume: 25 µl

Supporting information

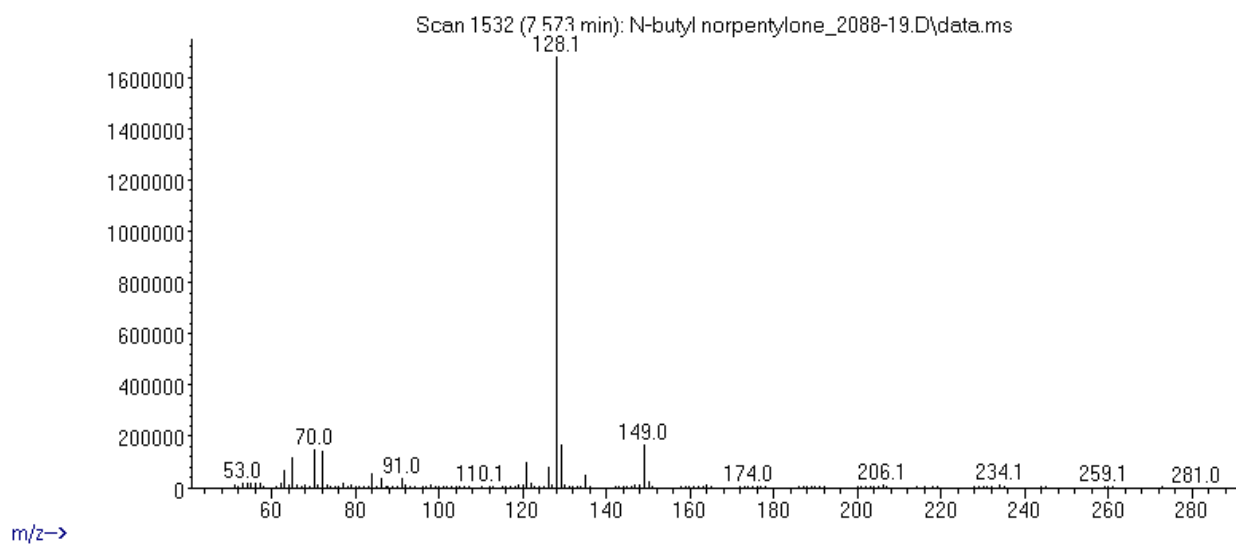
Solubility in	result/remark
CH ₂ Cl ₂	partially
MeOH	soluble
H ₂ O	partially

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 7,57 BP(1): 128; BP(2): 149, BP(3) :129,
HPLC-TOF	+	Exact mass (theoretical): 277,1678; measured value Δppm:0,11; formula:C16H23NO3
FTIR-ATR	+	direct measurement (sample as received)
FTIR (solid phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	-	
validation		Results in good agreement with NFL sample ID 2068 (confirmed by NMR).
other		

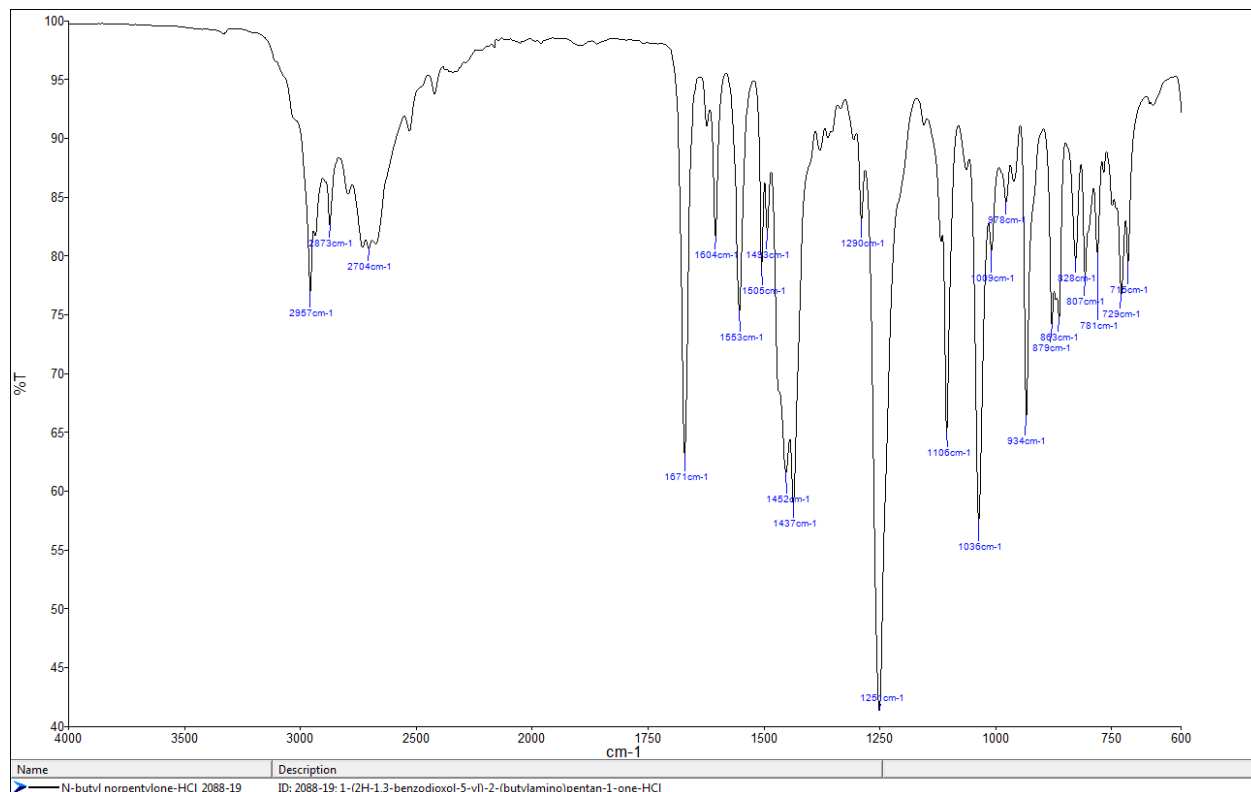
ANALYTICAL RESULTS

MS (EI)

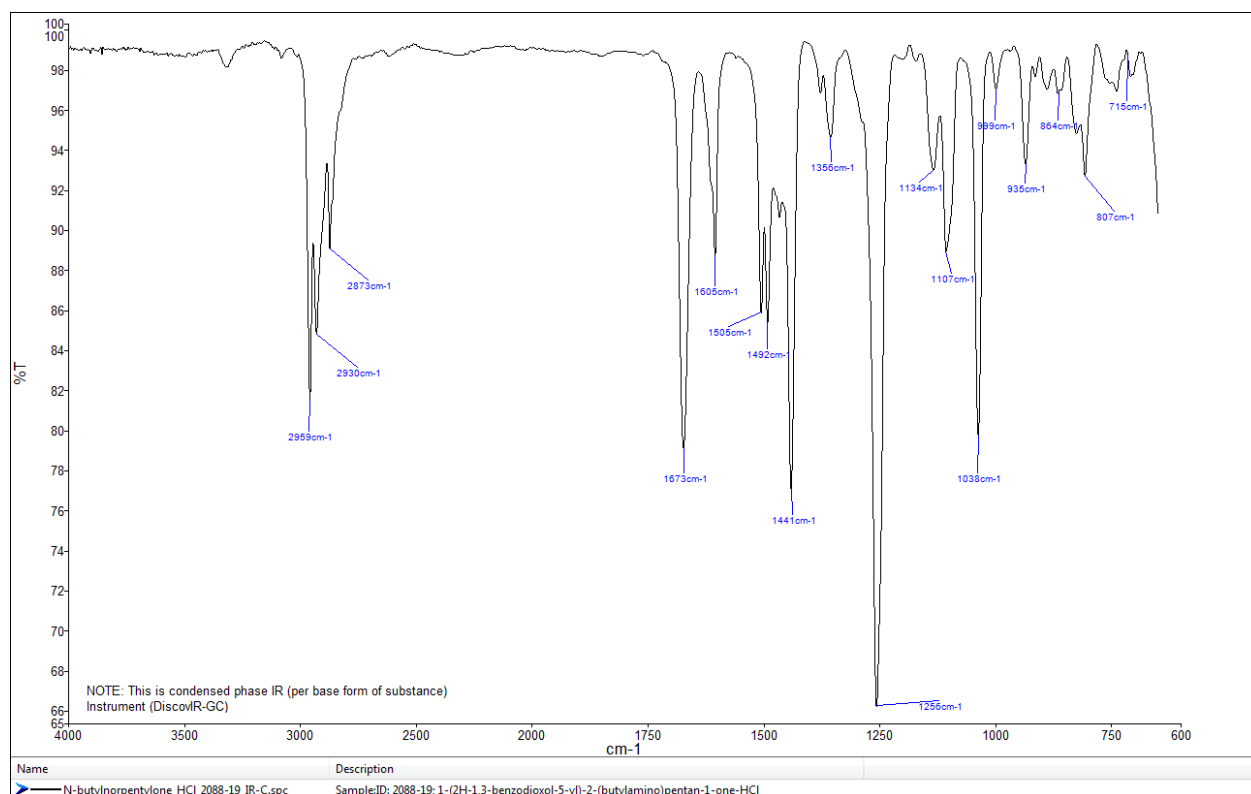
Abundance



FTIR-ATR - direct measurement (sample as received)



IR (solid phase – after chromatographic separation)



TOF REPORT

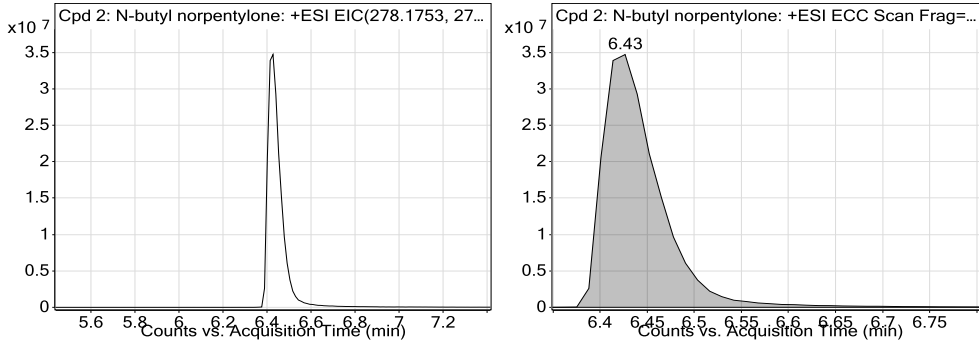
Data File	N-butylnorpentylone_2088-19.d	Sample Name	ID-2088-19
Sample Type	Sample	Position	P1-D3
Instrument Name	6230B TOF LC-MS	User Name	TG
Acq Method	general-8_1_2019-XDB-C18-ESI+.m	Acquired Time	8/26/2019 12:45:59 PM
IRM Calibration Status	Success	DA Method	a-Drugs_NFL.m
Comment	MeOH		

Compound Table

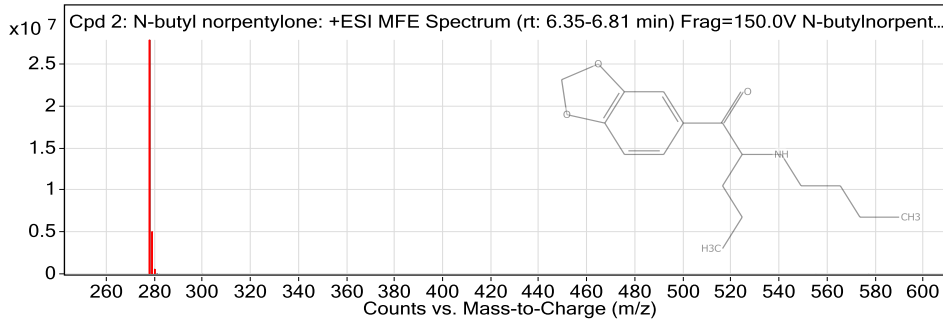
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 2: N-butyl norpentylone	N-butyl norpentylone	C16 H23 N O3	6.43	277.1678

Name	Obs. m/z	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
N-butyl norpentylone	278.175	6.43	277.1678	6.43	C16 H23 N O3	277.1678	0.11

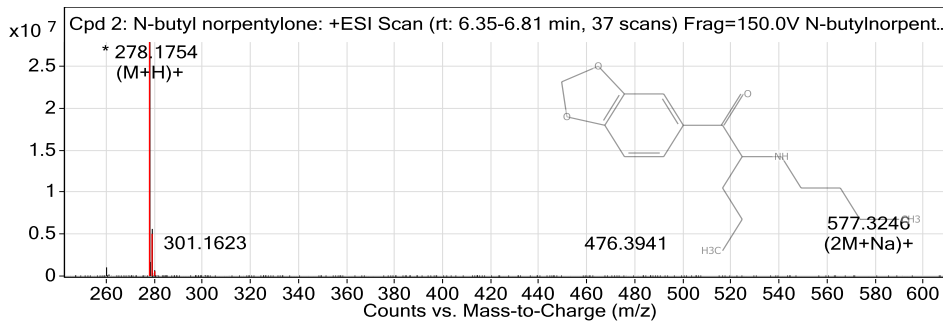
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
278.175	1	27848202	C16 H23 N O3	(M+H)+
279.1783	1	4937466.01	C16 H23 N O3	(M+H)+
280.1816	1	600298.18	C16 H23 N O3	(M+H)+
281.1837	1	67353.38	C16 H23 N O3	(M+H)+
282.187	1	7672.22	C16 H23 N O3	(M+H)+
300.1588	1	13466.76	C16 H23 N O3	(M+Na)+
555.3431	1	4116.35	C16 H23 N O3	(2M+H)+
577.3248	1	7321.83	C16 H23 N O3	(2M+Na)+

--- End Of Report ---

Peak Integration Report

Sample Name:	2088-19_IC	Inj. Vol.:	25,00
Injection Type:	Unknown	Dilution Factor:	1,0000
Program:	ANIONI	Operator:	kemija
Inj. Date / Time:	26-avg-2019 / 15:20	Run Time:	43,00

No.	Time min	Peak Name	Peak Type	Area $\mu\text{S} \cdot \text{min}$	Height μS	Amount mg/L
1,00	10,41	klorid	BMB	16,64	57,97	n.a.
2,00	16,94	bromid	BMB	0,26	0,74	n.a.
TOTAL:				16,90	58,71	0,00

