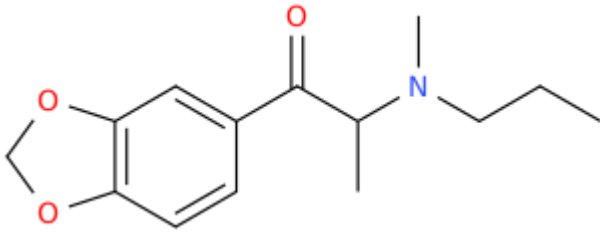# ANALYTICAL REPORT[1]

N-Propylmethylone (C14H19NO3)

1-(2H-1,3-benzodioxol-5-yl)-2-[methyl(propyl)amino]propan-1-one

Remark – other active cpd. detected:none

Sample ID:	3166-22
Sample description:	powder - white
Sample type:	RM-reference material
Comments:	CAY Lot#0637836-2,
Date of entry (DD/MM/YYYY):	15/06/2022
web link	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified-structure[2] (base form)	
Systematic name:	1-(2H-1,3-benzodioxol-5-yl)-2-[methyl(propyl)amino]propan-1-one
Other names:	1-(benzo[d][1,3]dioxol-5-yl)-2-(methyl(propyl)amino)propan-1-one; 3,4-Methylenedioxy-α-methylpropylaminopropiophenone; 3,4-Methylenedioxy-N-propylmethcathinone; N-propyl Methylone; N-methyl Propylone; N-methyl-N-propyl Methylone
Formula (per base form)	C14H19NO3
M_w (g/mol)	249,31
Salt form:	HCl
StdInChIKey (per base form)	NZPMOFCLWLTDCS-UHFFFAOYSA-N
Other active cpd. detected	none
Add.info (purity..)	≥98%

Report updates

date	comments (explanation)

Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 6,41 BP(1): 100; BP(2): 58,BP(3) :65,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	always as base form
HPLC-TOF	+	exact mass theoretical: 249,1365 / measured Δppm: -1,39

1. GC-MS (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 µl 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 6.1 min, then heating at 50 ^{0}C/min up to 325 ^{0}C and finally 9.1 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 µl 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.
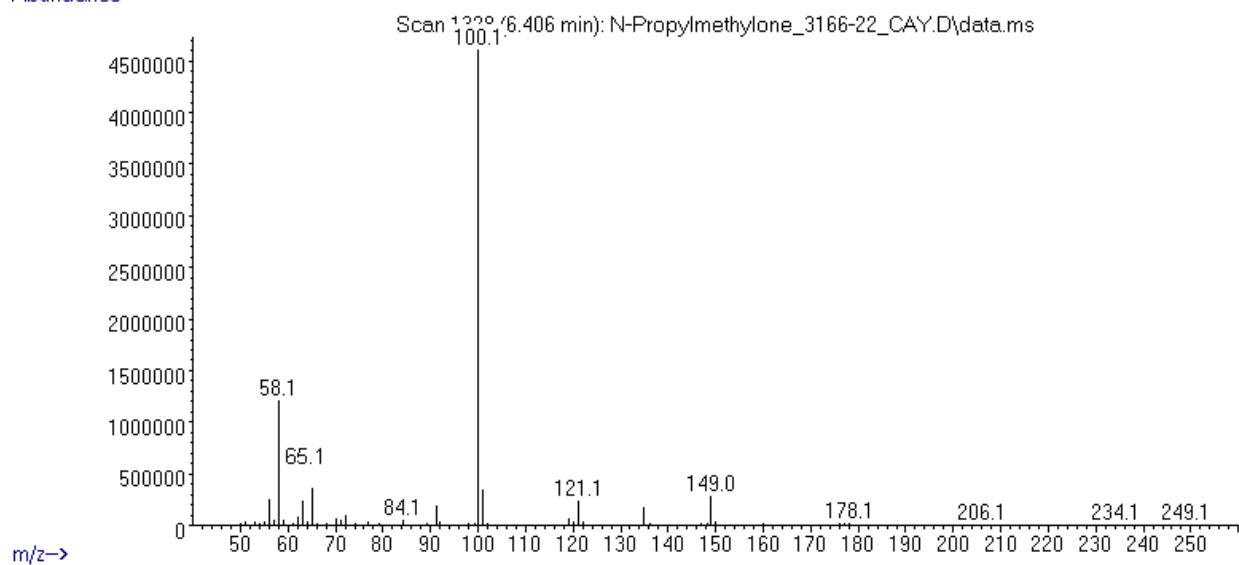IR (condesed (solid) phase): IR scan range 4000 to 650, resolution 4 cm^{-1}.

4. **HPLC-TOF** (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.
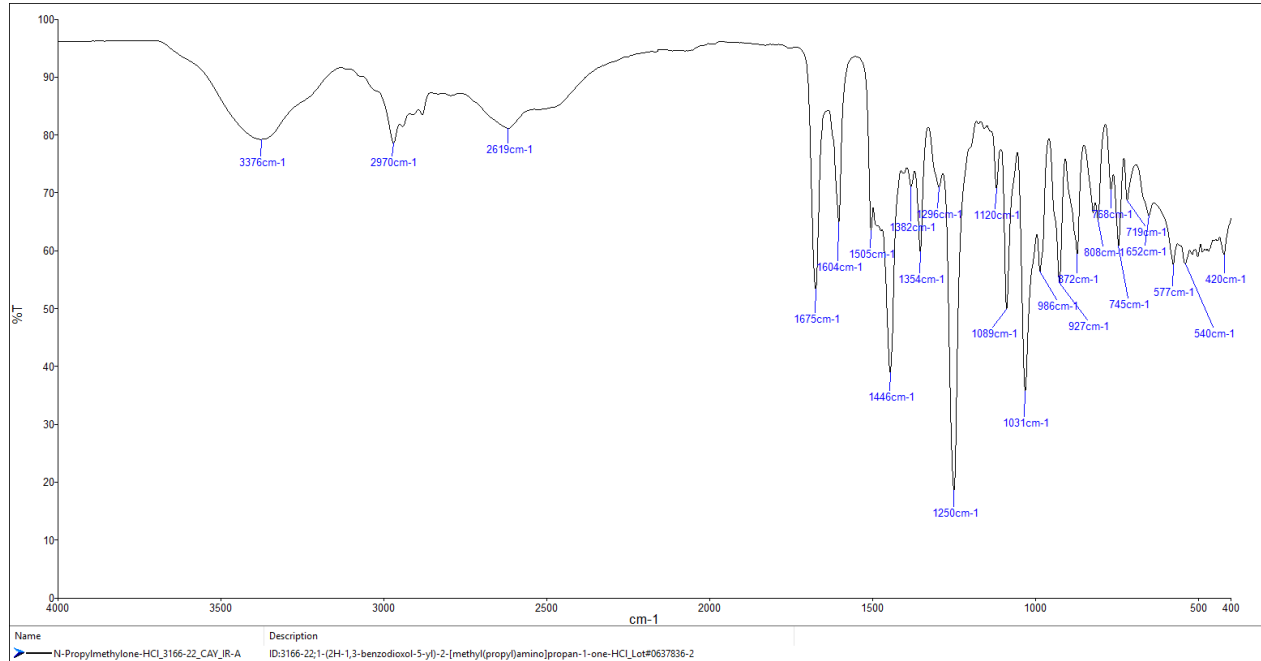
MS (EI)

Scan 1339 (6.406 min): N-Propylmethylone_3166-22_CAY.D\data.ms

ID 3166-22

FTIR-ATR (direct measurement – sample as received)

Name	Description
N-Propylmethylone-HCl_3166-22_CAY_IR-A	ID:3166-22;1-(2H-1,3-benzodioxol-5-yl)-2-[methyl(propyl)amino]propan-1-one-HCl_Lot#0637836-2

IR- (condensed (solid) phase – after chromatographic separation) - spectrum per base form

NOTE: This is condensed phase IR (per base form of substance)
Instrument (DiscovIR-GC)

Name	Description
N-Propylmethylone-HCl_3166-22_Cay_IR-C	Sample: ID:3166-22;1-(2H-1,3-benzodioxol-5-yl)-2-[methyl(propyl)amino]propan-1-one-HCl_Lot#0637836-2