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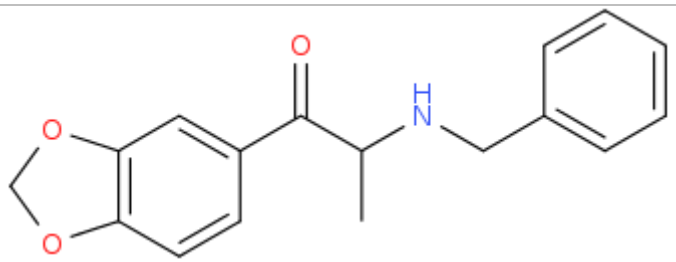
ANALYTICAL REPORT

BMDP (C17H17NO3)

1-(2H-1,3-benzodioxol-5-yl)-2-(benzylamino)propan-1-one

Remark – other NPS detected:

Sample ID:	1875-17
Sample description:	powder
Sample type:	seized /KP
Date of sample receipt (M/D/Y):	6/16/2017
Date of entry (M/D/Y) into NFL database:	12/21/2017
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-(benzylamino)propan-1-one
Other names	3,4-methylenedioxy-N-benzyl cathinone; N-Benzyl-3,4-methylenedioxycathinone
Formula (per base form)	C17H17NO3
M_w (g/mol)	283,33
Salt form/anions detected	HCl
StdInChIKey (per base form)	KRNIYOJEASBDDP-UHFFFAOYSA-N
Other NPS detected	
Additional info (purity..)	pure by GC-MS, HPLC-TOF

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

Report updates

date	comments (explanation)
06/01/2020	Mw typing error corrected.

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 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. 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 ^{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}.

5. **IC** (anions) (Thermo Scientific, Dionex ICS 2100), Column: IonPac AS19, 2 x 250mm; Eluent: 10mM 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

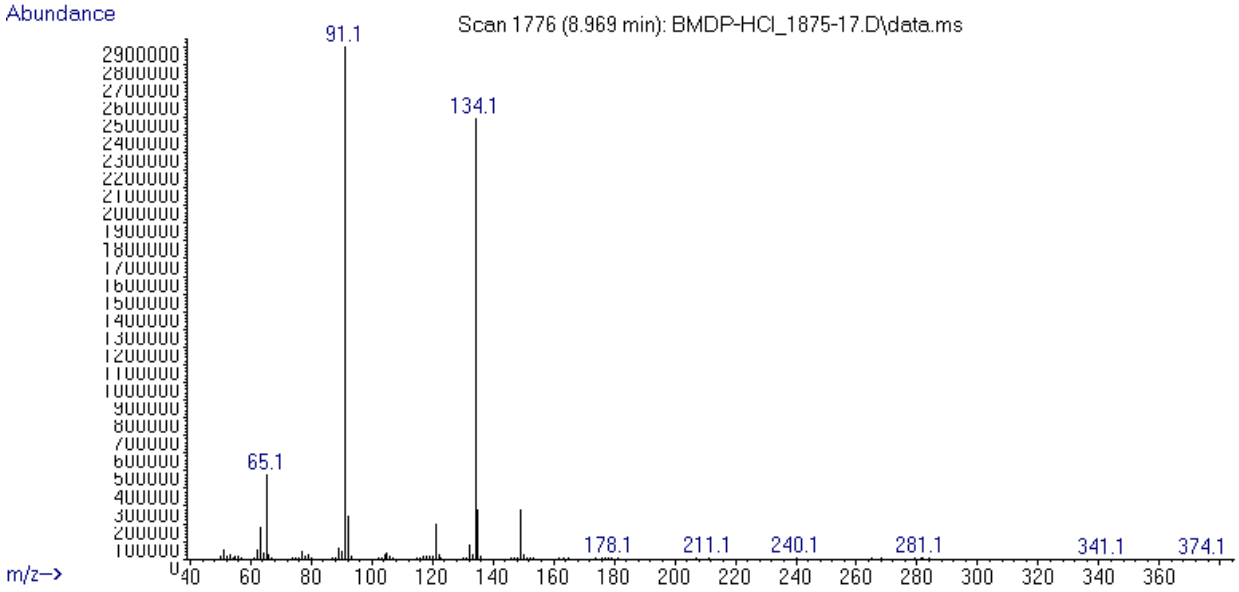
Supporting information

Solubility in	result/remark
CH_2Cl_2	partially
MeOH	soluble
H_2O	partially

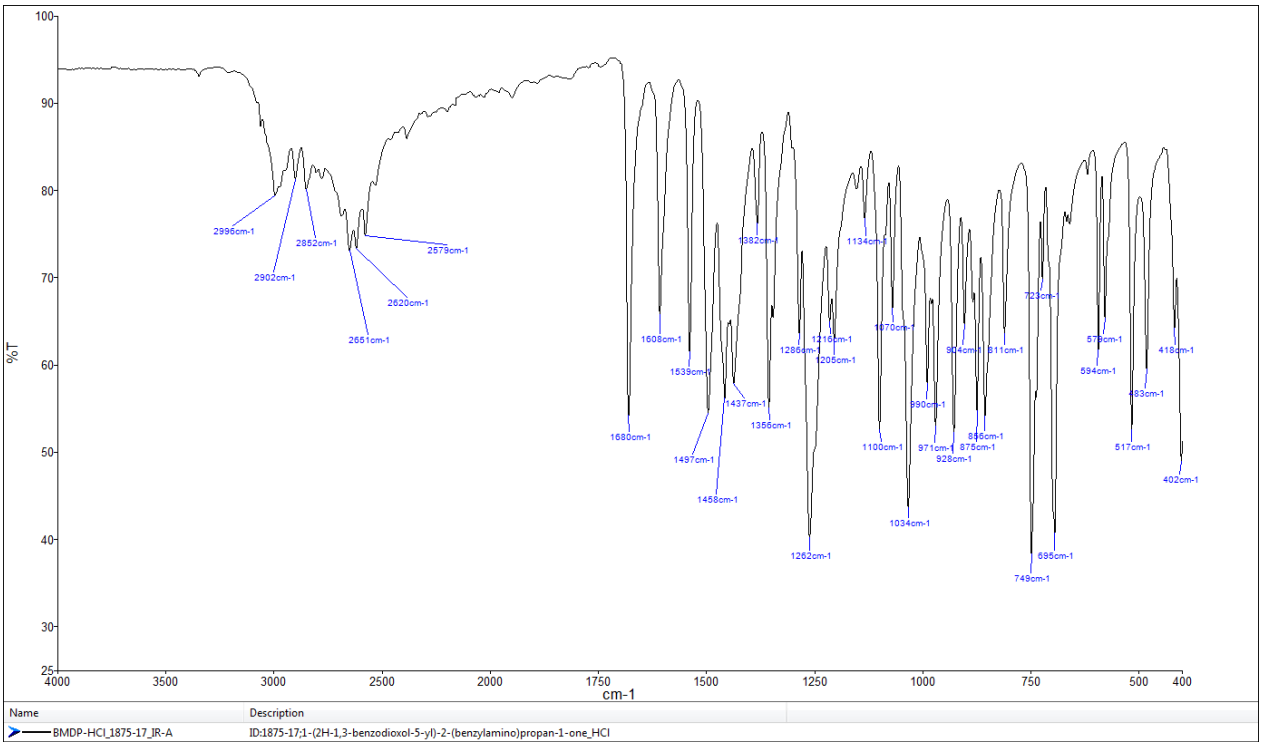
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 8,97 BP(1): 91; BP(2): 134,BP(3) :65,
HPLC-TOF	+	Exact mass (theoretical): 283,1208; measured value Δppm:-0,3; formula:C17H17NO3
FTIR-ATR	+	direct measurement (sample as received)
FTIR (condensed phase) always as base form	+	
IC (anions)	+	
NMR (in FKKT)	+	
validation		MS consistent and FTIR-ATR spectrum in good agreement by published data: https://doi.org/10.1016/j.jpba.2012.09.019
other		

ANALYTICAL RESULTS

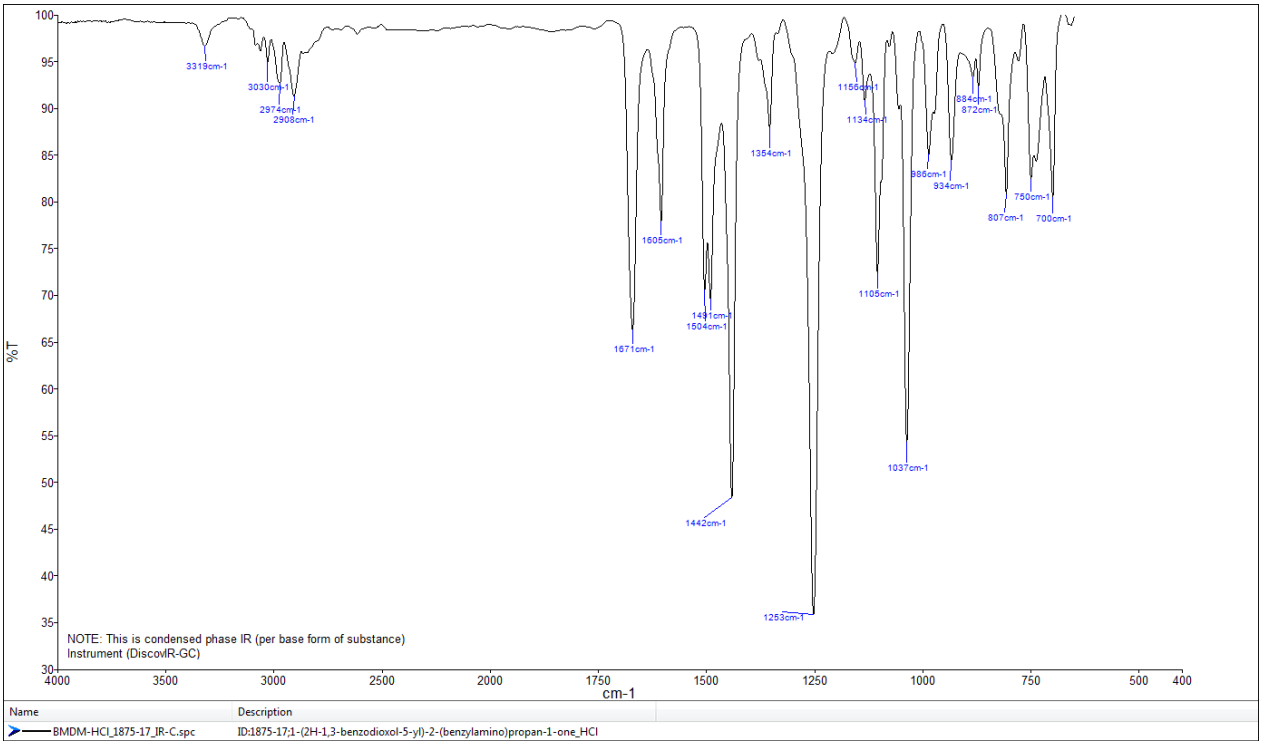
MS (EI)



FTIR-ATR - direct measurement (sample as received)



IR (condensed phase – after chromatographic separation)



TOF REPORT

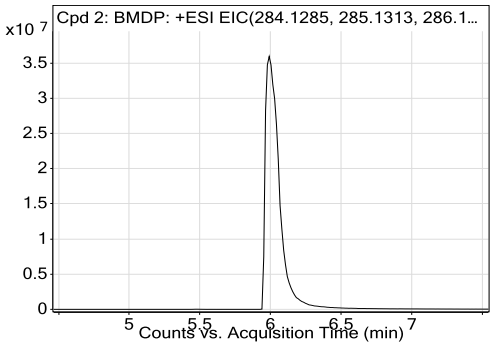
Data File	1875-17.d	**Sample Name**	1875-17
Sample Type	Sample	**Position**	P1-E2
Instrument Name	6230B TOF LC-MS	**User Name**	TG
Acq Method	general-19_07_2017-XDB-C18-ESI-final.m	**Acquired Time**	10/29/2017 10:31:49 AM
IRM Calibration Status	Success	**DA Method**	Drugs_NFL.m
Comment	MeOH		

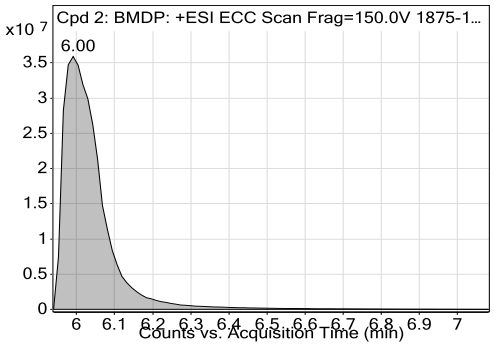
Compound Table

Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 2: BMDP	BMDP	C17 H17 N O3	6	283.1209

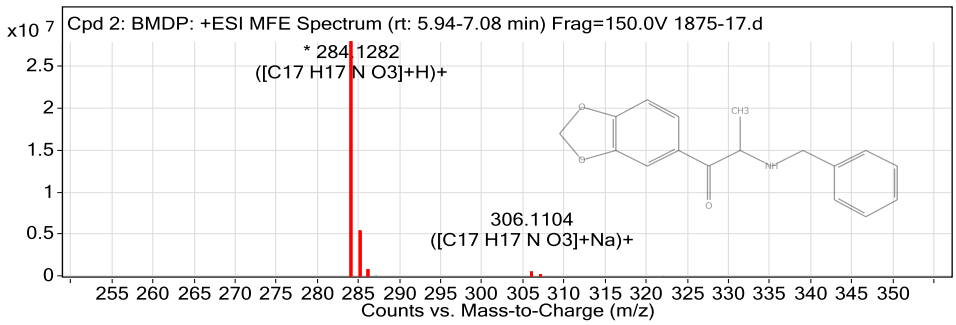
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
BMDP	284.1282	6	283.1209	6	C17 H17 N O3	283.1208	-0.3

Compound Chromatograms

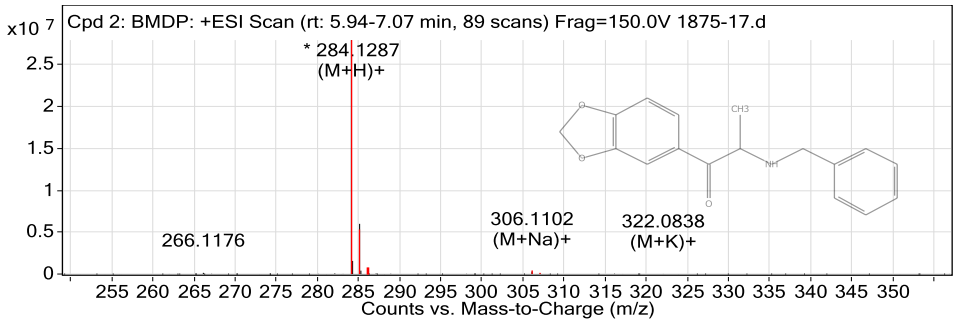




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

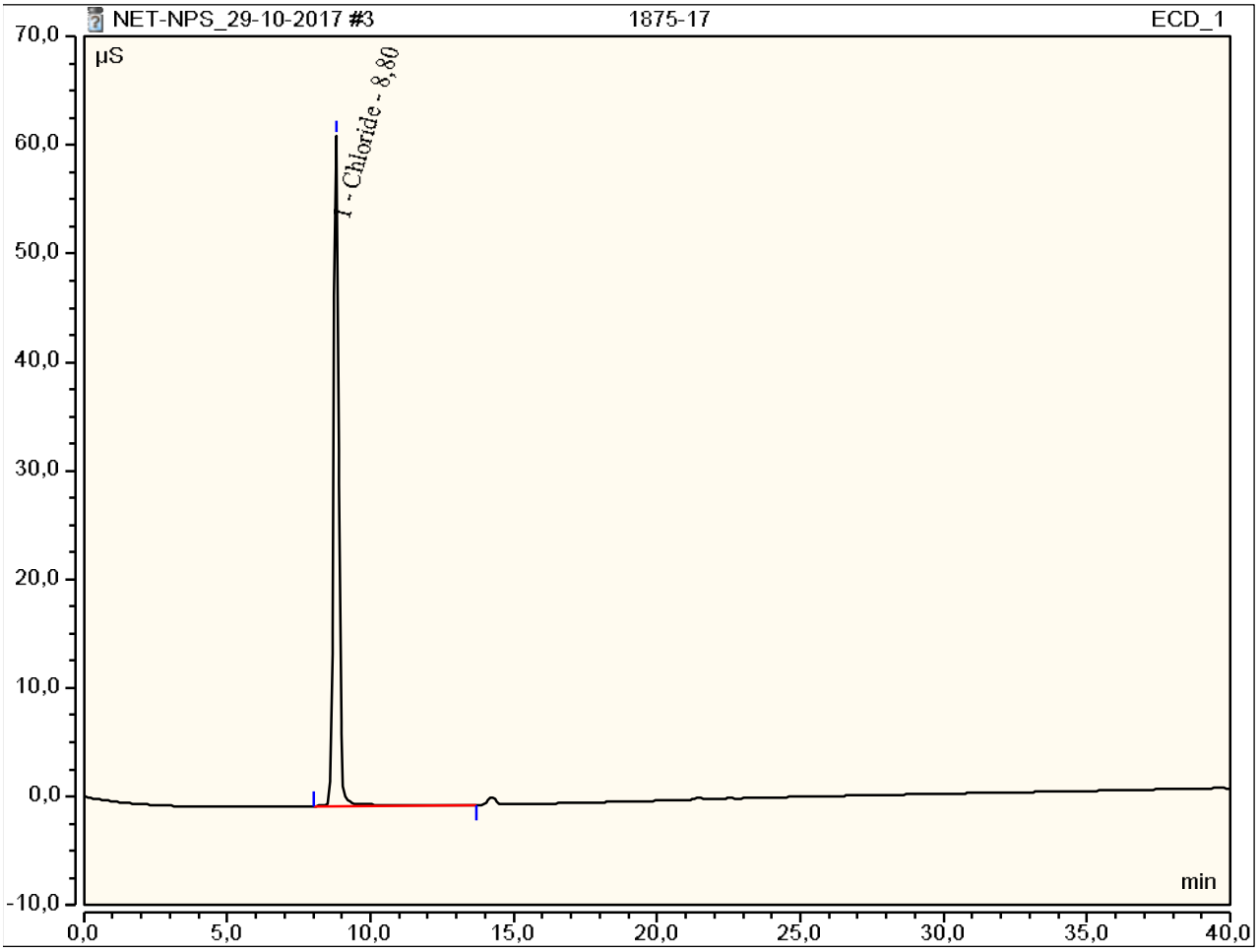
Obs. m/z	Charge	Abund	Formula	Ion/Isotope
284.1282	1	27931948	C17 H17 N O3	(M+H)+
285.1316	1	5451616.66	C17 H17 N O3	(M+H)+
286.1348	1	587962.51	C17 H17 N O3	(M+H)+
287.137	1	51726.51	C17 H17 N O3	(M+H)+
288.1397	1	3084.43	C17 H17 N O3	(M+H)+
306.1104	1	439035.16	C17 H17 N O3	(M+Na)+
307.1134	1	76638.05	C17 H17 N O3	(M+Na)+
308.1159	1	9530.8	C17 H17 N O3	(M+Na)+
322.0839	1	15102.53	C17 H17 N O3	(M+K)+

--- End Of Report ---

Peak Integration Report

Sample Name:	**1875-17**	*Inj. Vol.:*	**25,00**
Injection Type:	**Unknown**	*Dilution Factor:*	**1,0000**
Program:	**ANIONI**	*Operator:*	**kemija**
Inj. Date / Time:	**29-okt-2017 / 10:58**	*Run Time:*	**42,00**

No.	Time min	Peak Name	Peak Type	Area µS*min	Height µS	Amount mg/L
1,00	8,80	**Chloride**	BMB	12,90	61,68	n.a.
		TOTAL:		12,90	61,68	0,00



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University
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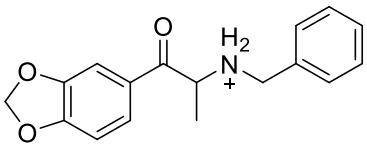
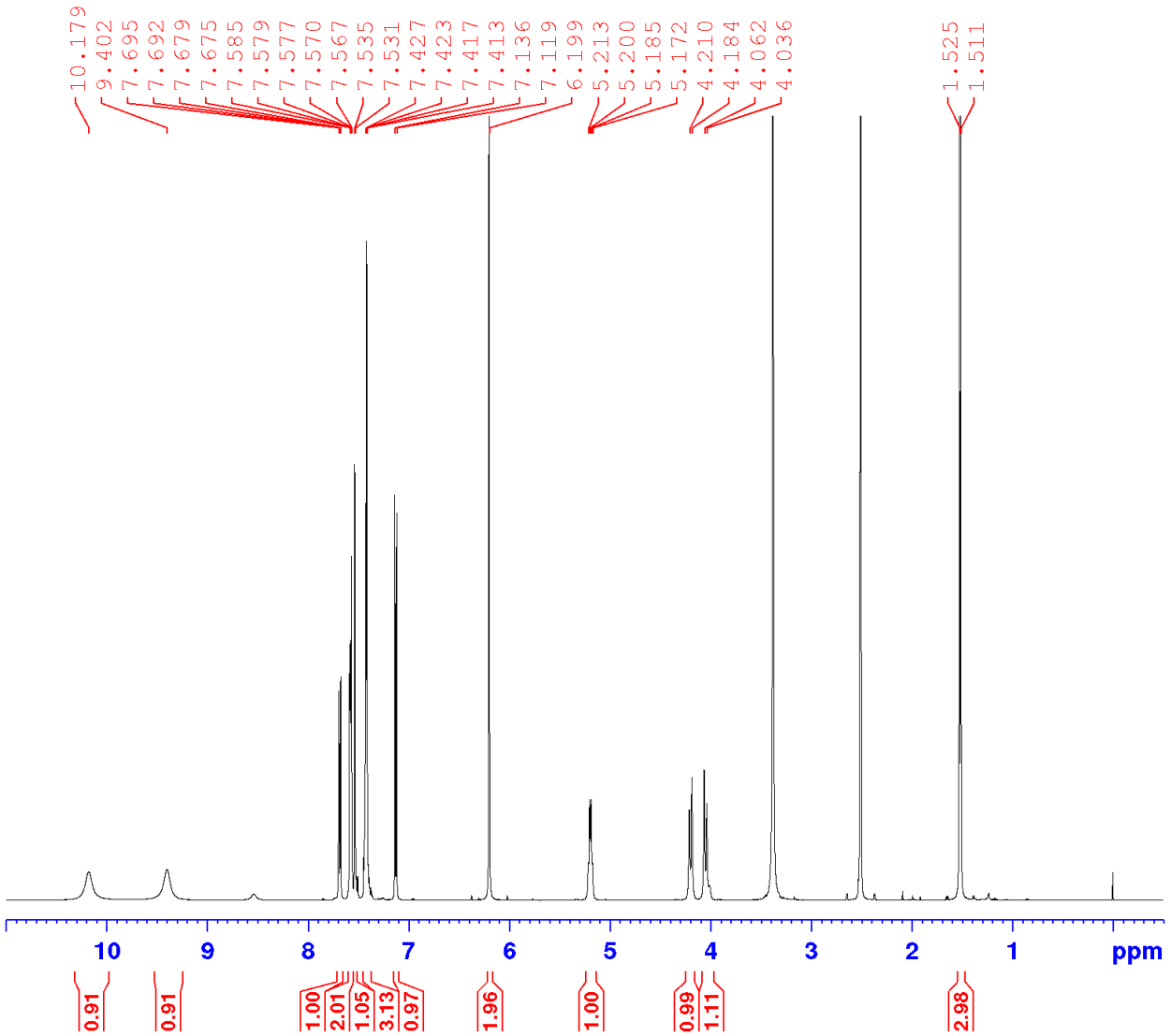
Faculty *of Chemistry*
and Chemical Technology

R E P O R T

Contract No.	C1714-17-460078 (Republic of Slovenia, Ministry of the Interior, POLICE)
Sample ID:	**1875-17**
Received date:	December 8, 2017
Our notebook code:	NFL-1875-17
NMR sample preparation:	17.8 mg dissolved in 0.7 mL DMSO-d_6
NMR experiments:	^{1}H, ^{13}C, ^{1}H–^{1}H *gs*-COSY, ^{1}H–^{13}C *gs*-HSQC, ^{1}H–^{13}C *gs*-HMBC, ^{1}H–^{15}N *gs*-HMBC
Proposed structure, formula, exact mass, molecular weight:	 Chemical Formula: $C_{17}H_{18}NO_3^+$ Exact Mass: 284,1281 Molecular Weight: 284,3345
Chemical name:	*N*-protonated 1-(benzo[d][1,3]dioxol-5-yl)-2-(benzylamino)propan-1-one
Comments:	- Structure elucidation based on 1D and 2D NMR spectra. - The result is consistent with the suggested chemical formula. - >98% purity of the sample based on ^{1}H NMR spectrum - Spectroscopic data are in agreement with the literature report (E. Fornal, A. Stachniuk, A. Wojtyla, *J. Pharm. Biomed. Anal.*,**2013**, 72, 139-144).
Supporting information:	Copies of ^{1}H and ^{13}C NMR spectra, ^{1}H and ^{13}C FIDs
Principal investigator:	Prof. Dr. Janez Košmrlj
Date of report:	December 20, 2017

NFL-1875-17



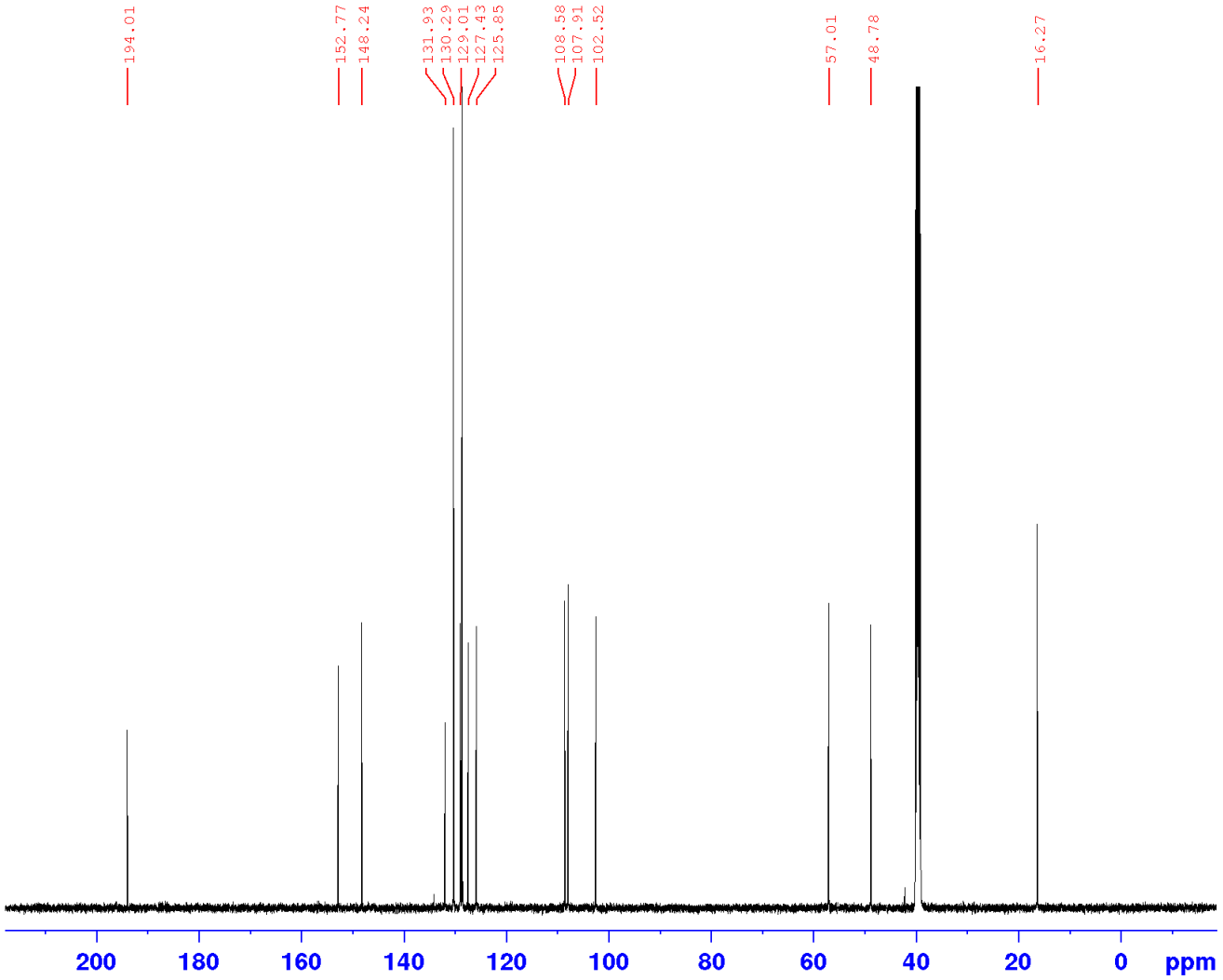

```
Current Data Parameters
NAME         NFL-1875-17
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171208
Time               16.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                  80.6
DW                50.000 usec
DE                 6.50 usec
TE                296.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1330885 MHz
NUC1                 1H
P1                8.70 usec
PLW1        26.00000000 W

F2 - Processing parameters
SI                 65536
SF          500.1300008 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

NFL-1875-17




```
Current Data Parameters
NAME         NFL-1875-17
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171208
Time               19.06
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                 3072
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG                 2050
DW               16.800 usec
DE                6.50 usec
TE               296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7703637 MHz
NUC1                  13C
P1                   8.70 usec
PLW1       122.00000000 W

======== CHANNEL f2 ========
SFO2        500.1320005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2               80.00 usec
PLW2        26.00000000 W
PLW12        0.30046001 W
PLW13        0.15113001 W

F2 - Processing parameters
SI                 32768
SF          125.7578443 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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