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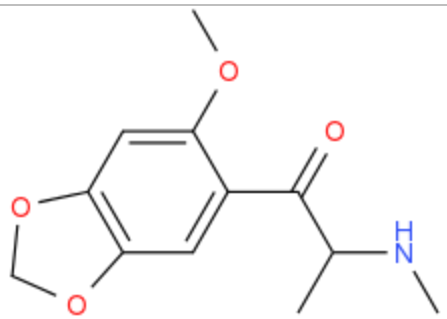
ANALYTICAL REPORT

N-Me-bk-MMDA-2, (C12H15NO4)

1-(6-methoxy-1,3-benzodioxol-5-yl)-2-(methylamino)propan-1-one

Remark – other NPS detected: none

Sample ID:	1182-15
Sample description:	powder - light brown
Sample type:	P- purchased
Date of entry:	7/13/2015

Substance identified-structure[i] (base form)	
Systematic name	1-(6-methoxy-1,3-benzodioxol-5-yl)-2-(methylamino)propan-1-one
Other names	
Formula (per base form)	C12H15NO4
M_w (g/mol)	237,25
Salt form	HCl
Smiles	COC=1C(=CC2=C(OCO2)C1)C(C(C)NC)=O
Compound Class	Cathinones
Other NPS detected	none
Add.info (purity..)	pure

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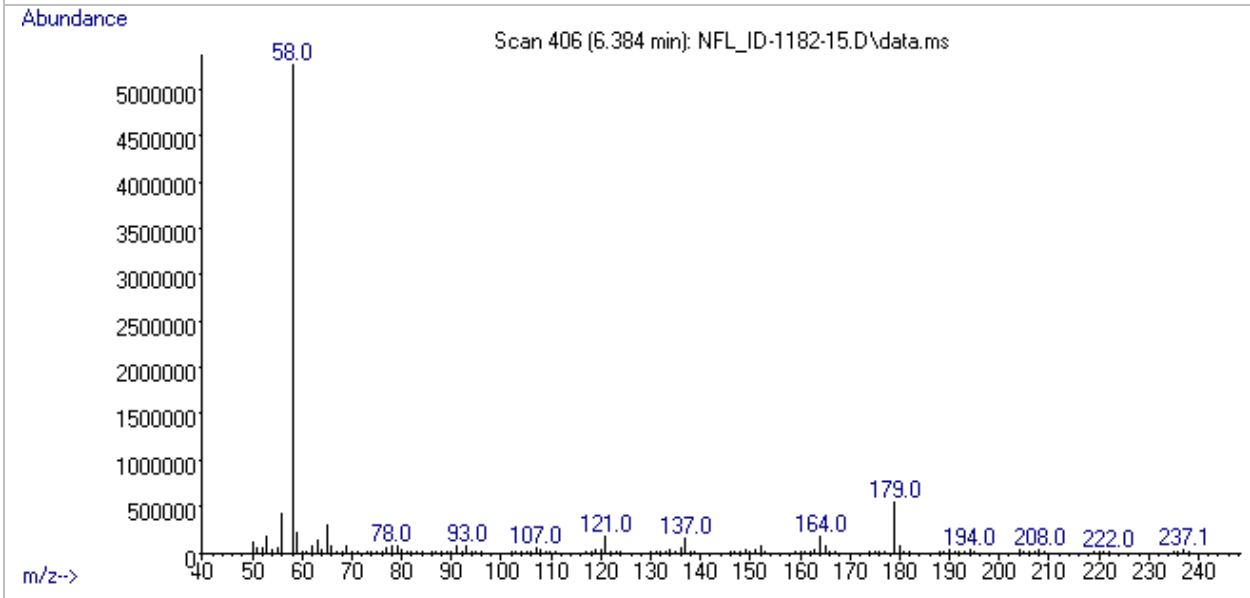
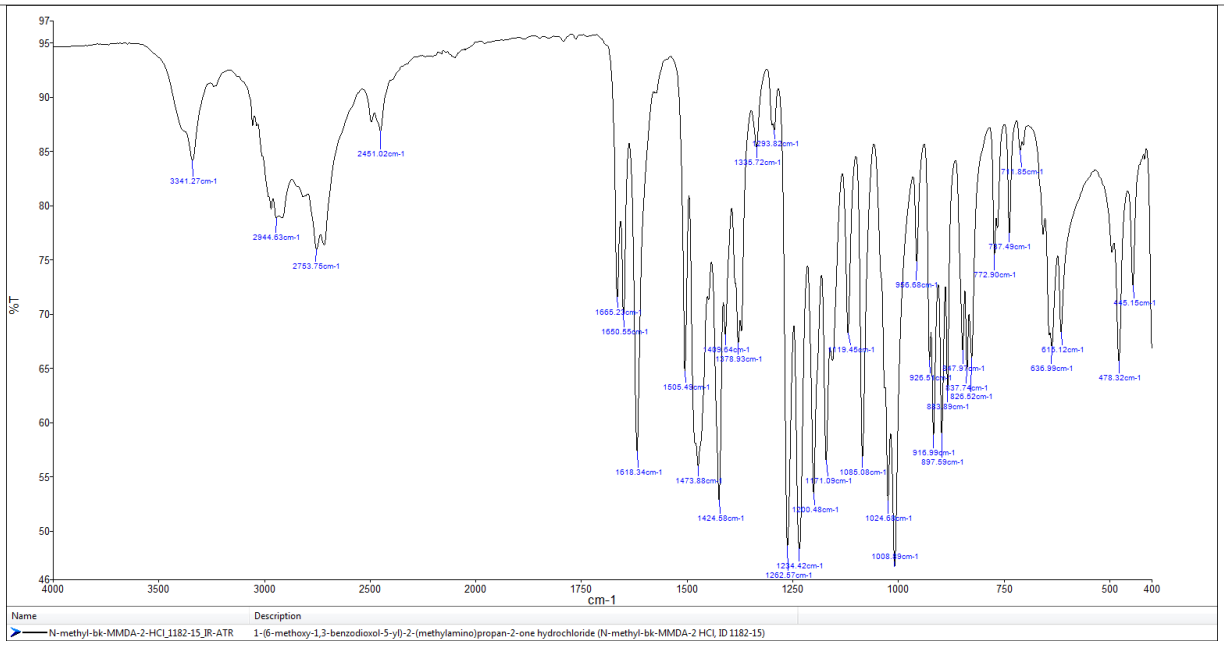
Supporting information

Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	BP(1): 58; BP(2): 179,BP(3) :164,
FTIR-ATR	+	HCl
FTIR (condensed phase)	/	
HPLC-TOF	+	Exact mass: 237,1001, measured/ Δppm:-1,48; formula:C12H15NO4
NMR-confirmed	+	
validation		
other		NFL-RT:6.384

MS spectrum (EI)



FTIR - ATR



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

Target Compound Screening Report

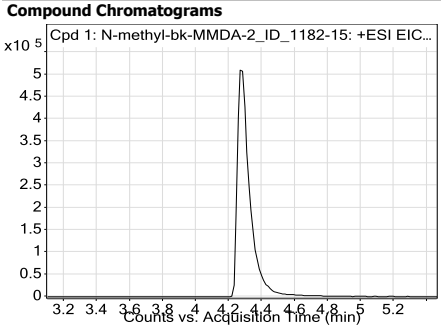
Data File	N-methyl-bk-MMDA-2_1182-15_TOF.d	**Sample Name**	ID 1182
Sample Type	Sample	**Position**	P1-E3
Instrument Name	SG13170002	**User Name**	
Acq Method	droge general-13-5-2015-XDB-C18-ESI-poz.m	**Acquired Time**	6/8/2015 10:12:10 AM
IRM Calibration Status	Success	**DA Method**	Droge_Default.m
Comment	extract in MeOH		

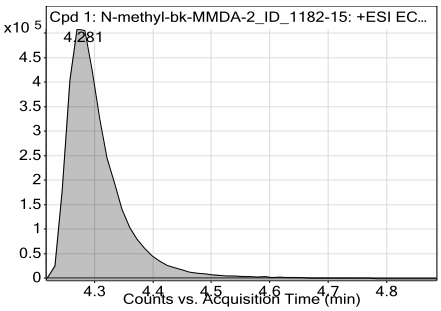
Compound Table

Label	Tgt Name	MFG Formula	Tgt Formula	Obs. RT	Obs. Mass
Cpd 1: N-methyl-bk-MMDA-2_ID_1182-15	N-methyl-bk-MMDA-2_ID_1182-15	C12 H15 N O4	C12 H15 N O4	4.281	237.1005

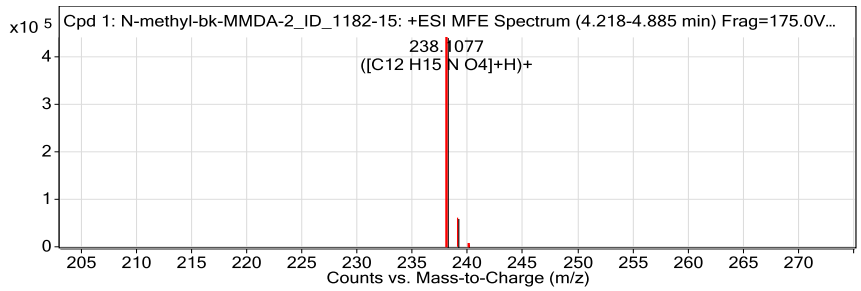
Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error	Tgt Formula	Find Cpds Algorith
N-methyl-bk-MMDA-2_ID_1182-15	238.1077	4.281	237.1005	4.281	C12 H15 N O4	237.1001	-1.48	C12 H15 N O4	Find by Molecular Feature

Compound Chromatograms

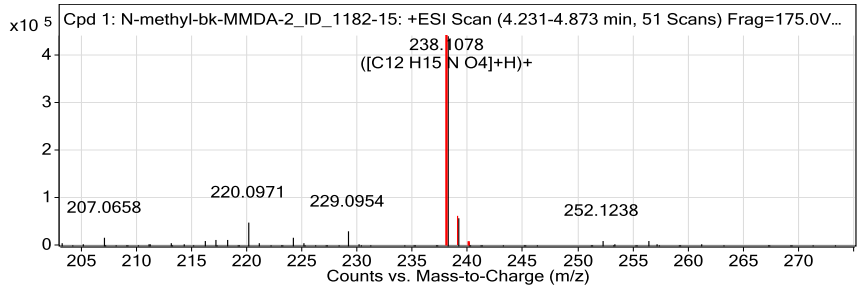




MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
238.1077	1	440723.03	C12 H15 N O4	(M+H)+
239.111	1	61797.47	C12 H15 N O4	(M+H)+
240.1129	1	7538.72	C12 H15 N O4	(M+H)+

--- End Of Report ---

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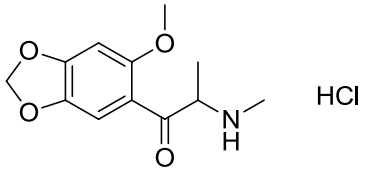
REPORT

Sample ID:	**1182-15**
Our notebook code:	P-1182-15
NMR sample preparation:	15 mg dissolved in 0.7 mL $CDCl_3$
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 with chemical name:	 HCl 1-(6-methoxybenzo[*d*][1,3]dioxol-5-yl)-2-(methylamino)propan-1-one hydrochloride
Comments:	- Structure elucidation based on 1D and 2D NMR spectra - Compound is pure by NMR
Supporting information:	Copies of ^{1}H and ^{13}C NMR spectra
Author:	Prof. Dr. Janez Košmrlj
Date of report:	July 11, 2015

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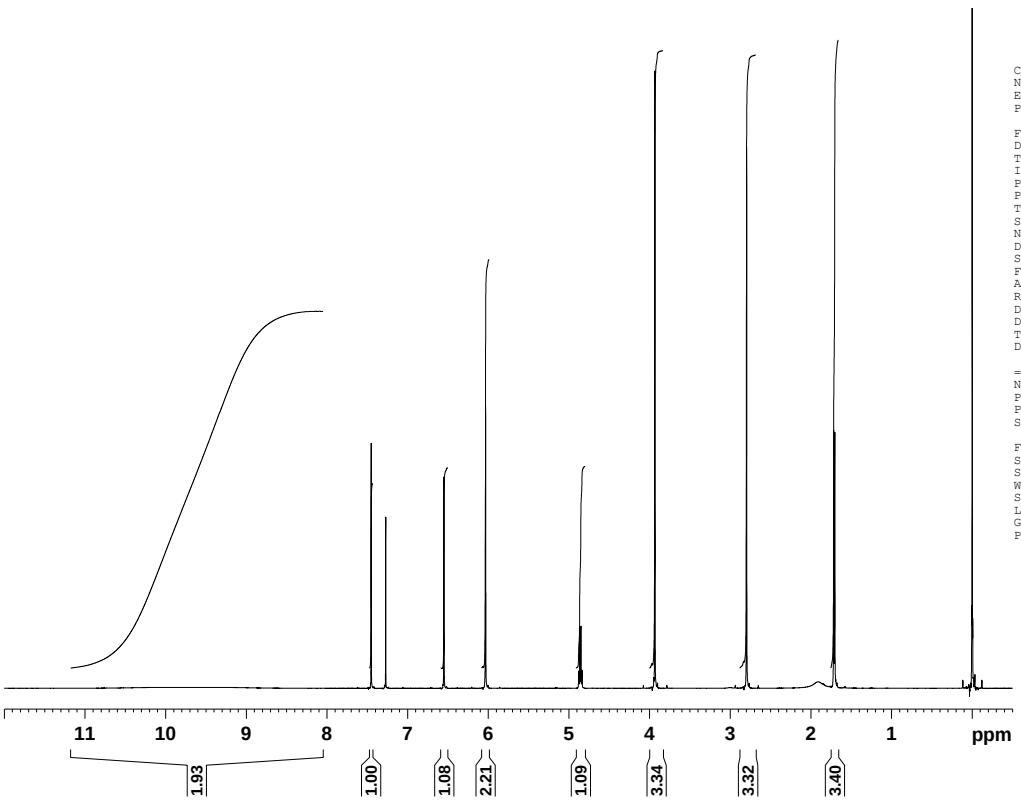


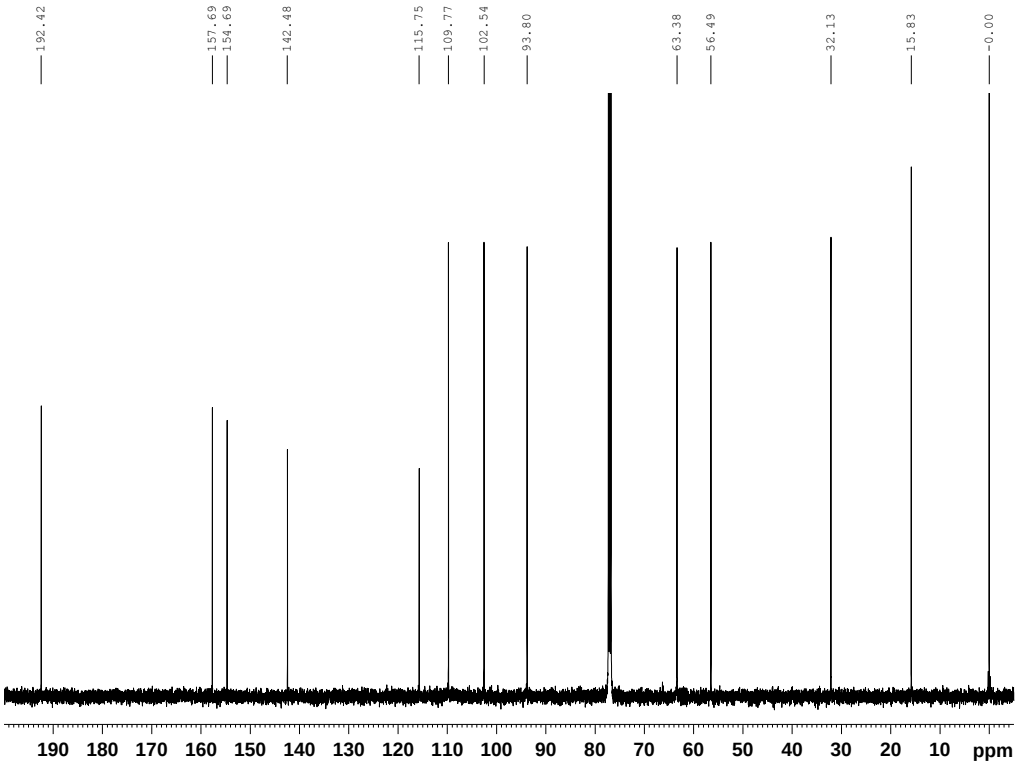

```
Current Data Parameters
NAME                  1182-15
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150706
Time                   18.24
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH              10330.578 Hz
FIDRES            0.157632 Hz
AQ                3.1719923 sec
RG                      128
DW                 48.400 usec
DE                  6.50 usec
TE                   296.0 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     8.90 usec
PLW1           26.00000000 W
SFO1           500.1330885 MHz

F2 - Processing parameters
SI                    65536
SF               500.1300074 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

P-1182-15




```
Current Data Parameters
NAME                  1182-15
EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150706
Time                   20.55
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     3072
DS                        4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010548 sec
RG                     2050
DW                 16.800 usec
DE                  6.50 usec
TE                   296.0 K
D1              1.00000000 sec
D11             0.03000000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     9.00 usec
PLW1          122.00000000 W
SFO1           125.7703637 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                      1H
PCPD2                  80.00 usec
PLW2           26.00000000 W
PLW12           0.32179001 W
PLW13           0.20595001 W
SFO2           500.1320005 MHz

F2 - Processing parameters
SI                    32768
SF               125.7577893 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```