REPUBLIKA SLOVENIJA
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POLICIJA

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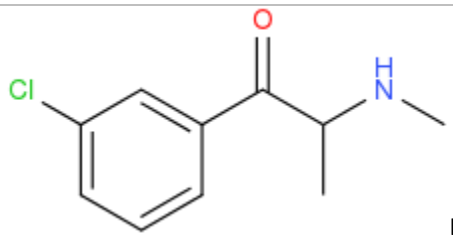
ANALYTICAL REPORT

3-CMC (C10H12ClNO)

1-(3-chlorophenyl)-2-(methylamino)propan-1-one

Sample ID:	C 4245-28/2015
Sample description:	powder - white
Report date:	2/21/2015
Sample type:	Seizure

Substance identified-structure[i]	 HCL
Systematic name	• 1-(3-chlorophenyl)-2-(methylamino)propan-1-one
Other names	• 3-CMC, 3-clephedrone
Formula (per base form)	C10H12ClNO
M_w (g/mol) per base form	197.66
Exact mass (monoisotopic):	197.060742
Salt form	HCl
Other compounds detected	none
Smiles	ClC=1C=C(C=CC1)C(C(C)NC)=O
Compound Class	Cathinones

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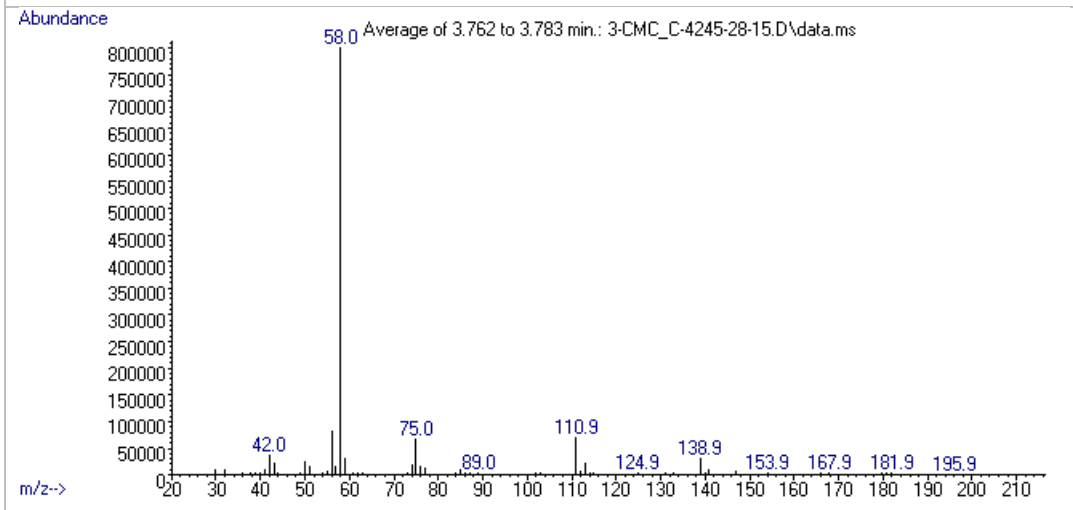
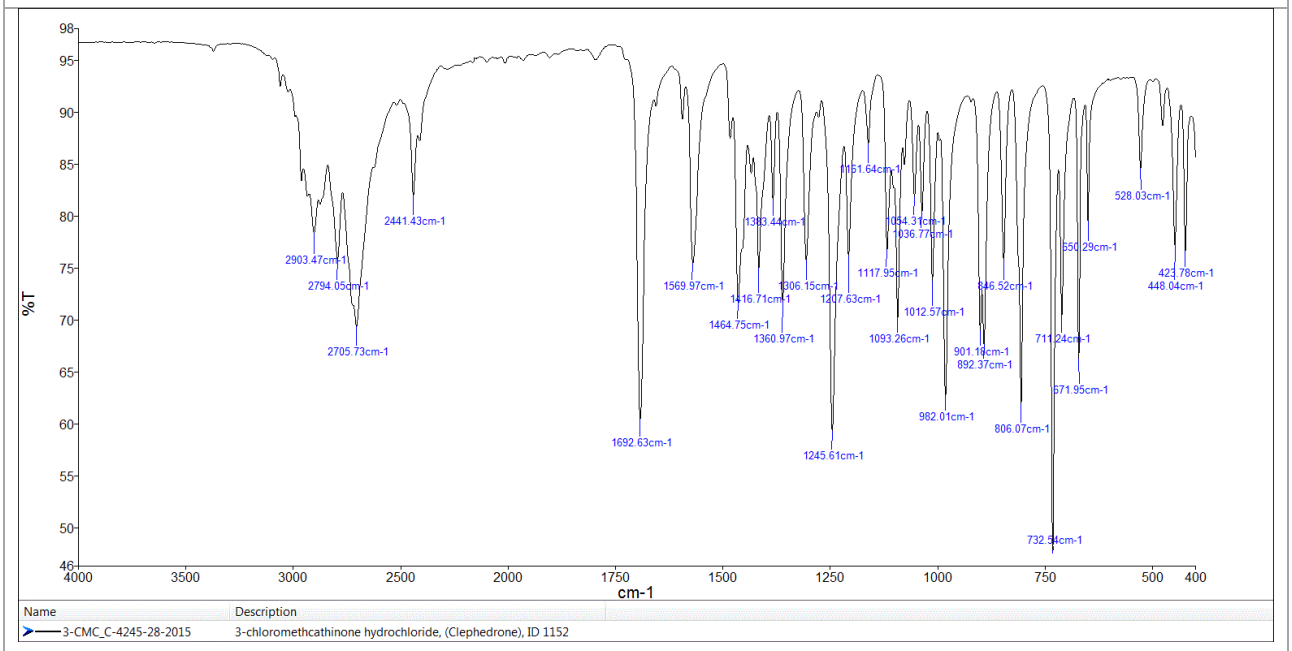
Supporting information

Analytical techniques:		remarks
GC-MS	+	
FTIR-ATR	+	Direct measurement
FTIR (condensed phase)	/	
HPLC-TOF	+	
NMR - confirmed	+	
Validation - other	/	
other	/	

MS spectrum (EI)



FTIR - ATR



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

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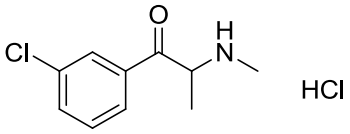
REPORT

Sample ID:	**CARINA 42545-28/2015**
Received date:	February 12, 2015
Our notebook code:	P-42545-28-2015
NMR sample preparation:	5 mg dissolved in 0.7 mL $CDCl_3$
NMR experiments:	^{1}H, ^{13}C
Proposed structure with chemical name:	 1-(3-chlorophenyl)-2-(methylamino)propan-1-one hydrochloride
Comments:	- Structure elucidation based on ^{1}H and ^{13}C 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:	February 14, 2015

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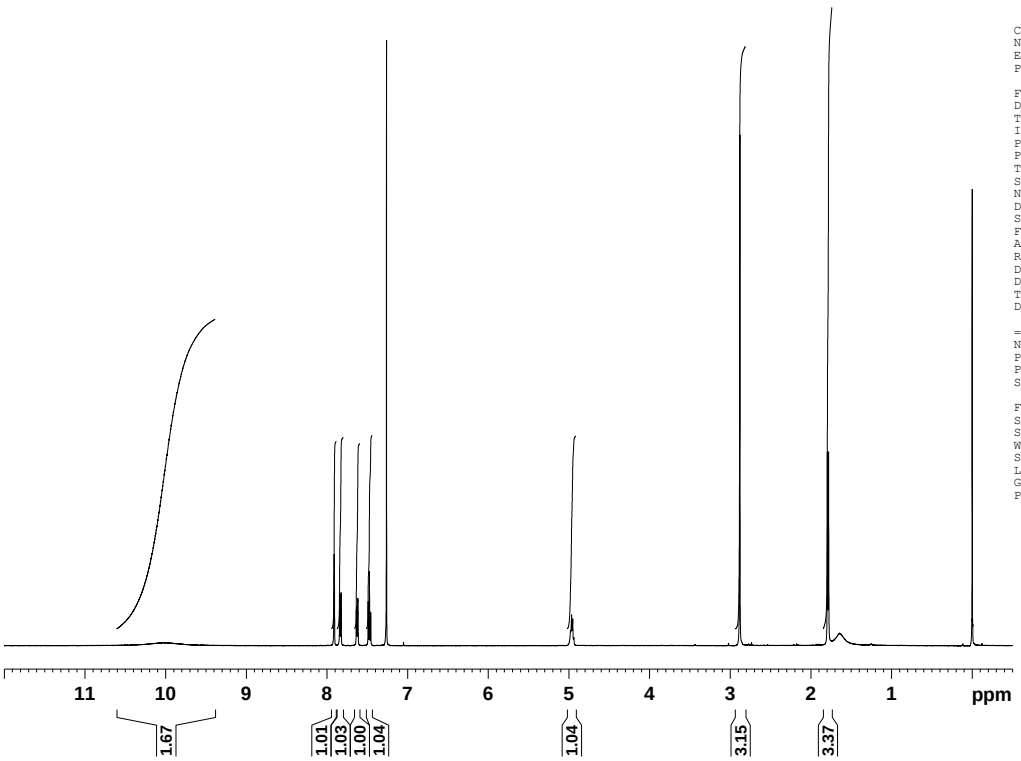
P-4245-28-2015
1H



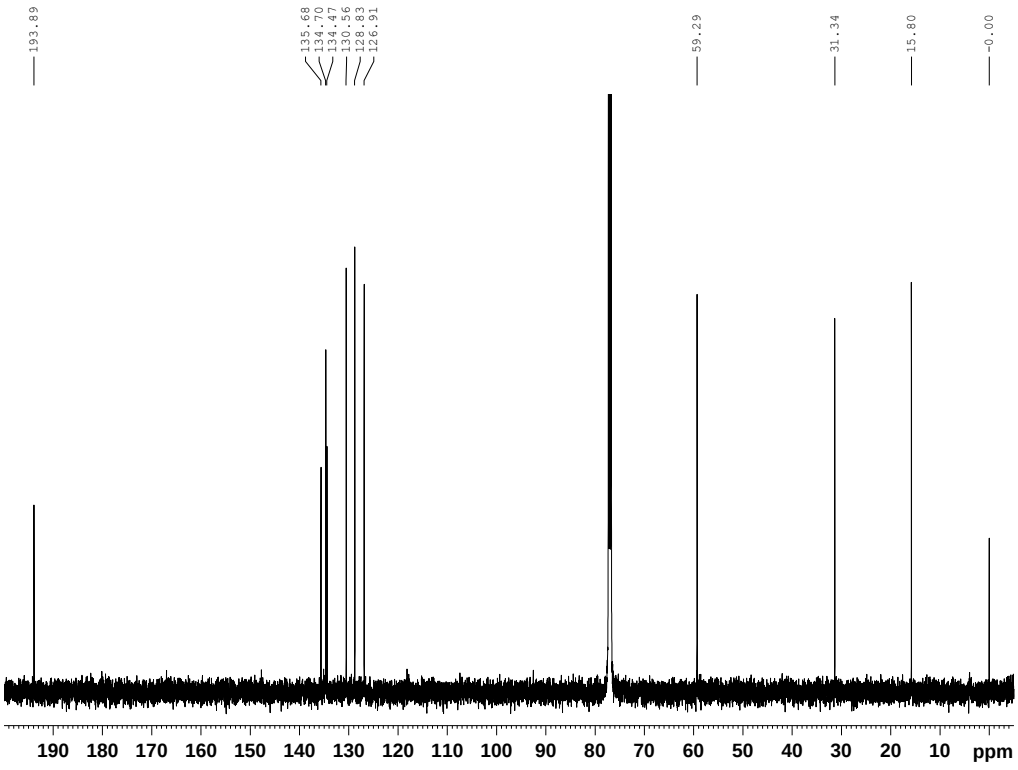
Current Data Parameters
NAME P-4245-28-2015
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150214
Time 0.12
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 181
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 500.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

P-4245-28-2015
13C



Current Data Parameters
NAME P-4245-28-2015
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150214
Time 6.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10240
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1820
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 125.7577900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40