# ANALYTICAL REPORT

**3-CMC (C10H12ClNO)**

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

<table>
<thead>
<tr>
<th>Substance identified-structure</th>
<th><img src="" alt="Structural formula" /></th>
</tr>
</thead>
<tbody>
<tr>
<td>Systematic name</td>
<td>1-(3-chlorophenyl)-2-(methylamino)propan-1-one</td>
</tr>
<tr>
<td>Other names</td>
<td>3-CMC, 3-clephedrone</td>
</tr>
<tr>
<td>Formula (per base form)</td>
<td>C10H12CINO</td>
</tr>
<tr>
<td>$M_w$ (g/mol) per base form</td>
<td>197.66</td>
</tr>
<tr>
<td>Exact mass (monoisotopic)</td>
<td>197.060742</td>
</tr>
<tr>
<td>Salt form</td>
<td>HCl</td>
</tr>
<tr>
<td>Other compounds detected</td>
<td>none</td>
</tr>
<tr>
<td>Smiles</td>
<td>ClC=1C=C(C=CC1)C(C(C)NC)=O</td>
</tr>
<tr>
<td>Compound Class</td>
<td>Cathinones</td>
</tr>
</tbody>
</table>

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Supporting information

<table>
<thead>
<tr>
<th>Analytical techniques</th>
<th>remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>GC-MS</td>
<td>+</td>
</tr>
<tr>
<td>FTIR-ATR</td>
<td>+ Direct measurement</td>
</tr>
<tr>
<td>FTIR (condensed phase)</td>
<td>/</td>
</tr>
<tr>
<td>HPLC-TOF</td>
<td>+</td>
</tr>
<tr>
<td>NMR - confirmed</td>
<td>+</td>
</tr>
<tr>
<td>Validation - other</td>
<td>/</td>
</tr>
<tr>
<td>other</td>
<td>/</td>
</tr>
</tbody>
</table>

MS spectrum (EI)

Average of 3.762 to 3.783 min: 3-CMC  C4245 29-15.04

Abundance

m/z ->

0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210

800000 750000 700000 650000 600000 550000 500000 450000 400000 350000 300000 250000 200000 150000 100000 50000

42.0 75.0 110.9 124.9 139.9 153.9 167.9 181.9 195.9
FTIR - ATR

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-CMC_C-0245-28-2015</td>
<td>3-chlorometacetylsalicylic acid hydrochloride (Cepheidzone) ID 1152</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th>CARINA 42545-28/2015</th>
</tr>
</thead>
<tbody>
<tr>
<td>Received date:</td>
<td>February 12, 2015</td>
</tr>
<tr>
<td>Our notebook code:</td>
<td>P-42545-28-2015</td>
</tr>
<tr>
<td>NMR sample preparation:</td>
<td>5 mg dissolved in 0.7 mL CDCl₃</td>
</tr>
<tr>
<td>NMR experiments:</td>
<td>$^1$H, $^{13}$C</td>
</tr>
<tr>
<td>Proposed structure with chemical name:</td>
<td><img src="image" alt="Chemical Structure" /> 1-(3-chlorophenyl)-2-(methylamino)propan-1-one hydrochloride</td>
</tr>
</tbody>
</table>
| 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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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

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
PLW2        0.32179001 W
PLW2        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