



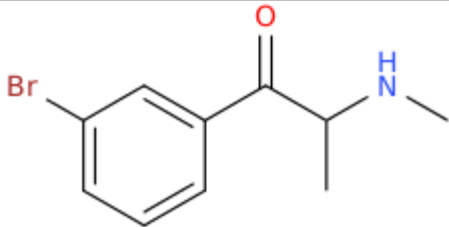
## ANALYTICAL REPORT

### 3-BMC (C<sub>10</sub>H<sub>12</sub>BrNO)

#### 1-(3-bromophenyl)-2-(methylamino)propan-1-one

Remark – other active cpd. detected: **none**

|                         |  |
|-------------------------|--|
| Sample ID:              | 1797-17                                    |
| Sample description:     | powder - white                             |
| Sample type:            | RM-reference material                      |
| Comments <sup>1</sup> : | CHIRON Batch# 16 041; RESPONSE -purchasing |
| Date of entry:          | 4/6/2017                                   |

|   |  |
|---|--|
| Substance identified-structure <sup>2</sup> (base form) |                                        |
| Systematic name:  | 1-(3-bromophenyl)-2-(methylamino)propan-1-one  |
| Other names:  | 3-Bromomethcathinone; 1-(3-bromophenyl)-2-methylaminopropan-1-one; 1-(3-bromophenyl)-2-(methylamino)-1-propanone; 3-BMAP |
| Formula (per base form)                                 | C <sub>10</sub> H <sub>12</sub> BrNO   |
| M <sub>w</sub> (g/mol)                                  | 242,12   |
| Salt form:  | HCl  |
| StdInChIKey (per base form)                             | PXLYROINIXKFAW-UHFFFAOYSA-N  |
| Other active cpd. detected                              | none   |
| Add.info (purity..)                                     | 99,8%  |

<sup>1</sup> This report has been produced with the financial support of the Prevention of and fight against crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this report are the sole responsibility of the National Forensic Laboratory and can in no way be taken to reflect the views of the European Commission.

<sup>2</sup> Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d



## Report updates

| date | comments (explanation) |
|------|------------------------|
|      |                        |
|      |                        |
|      |                        |
|      |                        |

## Supporting information

| Analytical technique:   | applied | remarks  |
|-------------------------|---------|--|
| GC-MS (EI ionization)   | +       | NFL GC-RT (min): 4,4 BP(1): 58; BP(2): 56,BP(3) :76, |
| FTIR-ATR                | +       | direct measurement                                   |
| GC-IR (condensed phase) | +       | always as base form                                  |

**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 °C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 °C at a rate of 18 °C/min, hold for 7.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235 °C, source and quadropole temperatures 280 °C and 180 °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<sup>-1</sup>; resolution 4cm<sup>-1</sup>

**3. 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 °C. Chromatographic separation as above **(1)**. Split MS : IR = 1 : 9.

MSD source EI = 70 eV. GC-MS transfer line T= 235 °C, source and quadropole temperatures 280 °C and 180 °C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

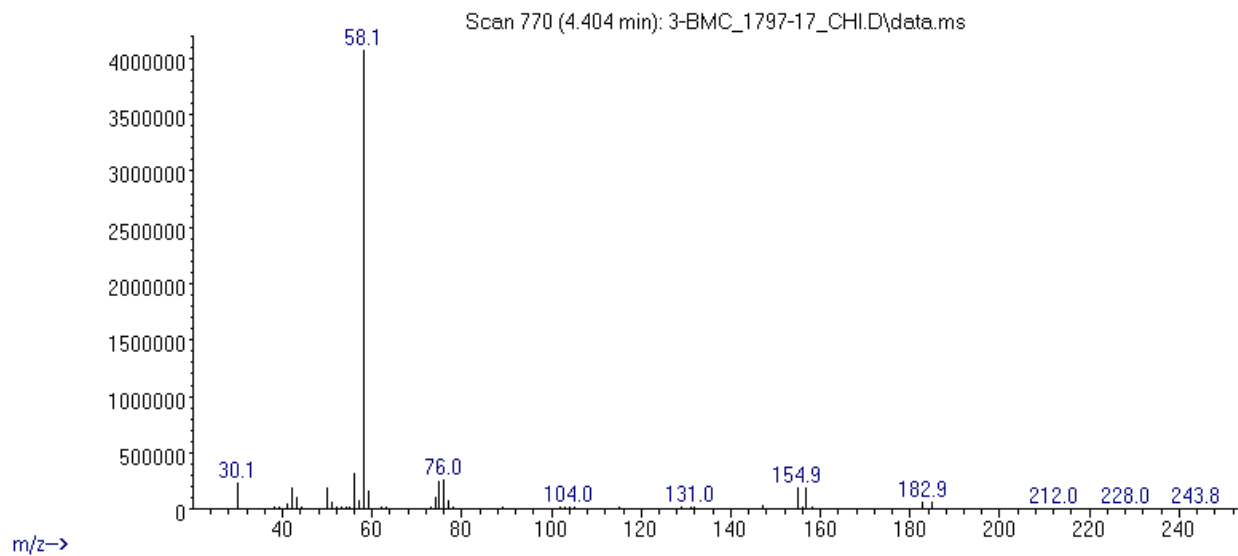
IR (condensed (solid) phase): IR scan range 4000 to 650, resolution 4 cm<sup>-1</sup>.

4. HPLC-TOF for exact monoisotopic mass and empirical formula control - results are not shown in the report.

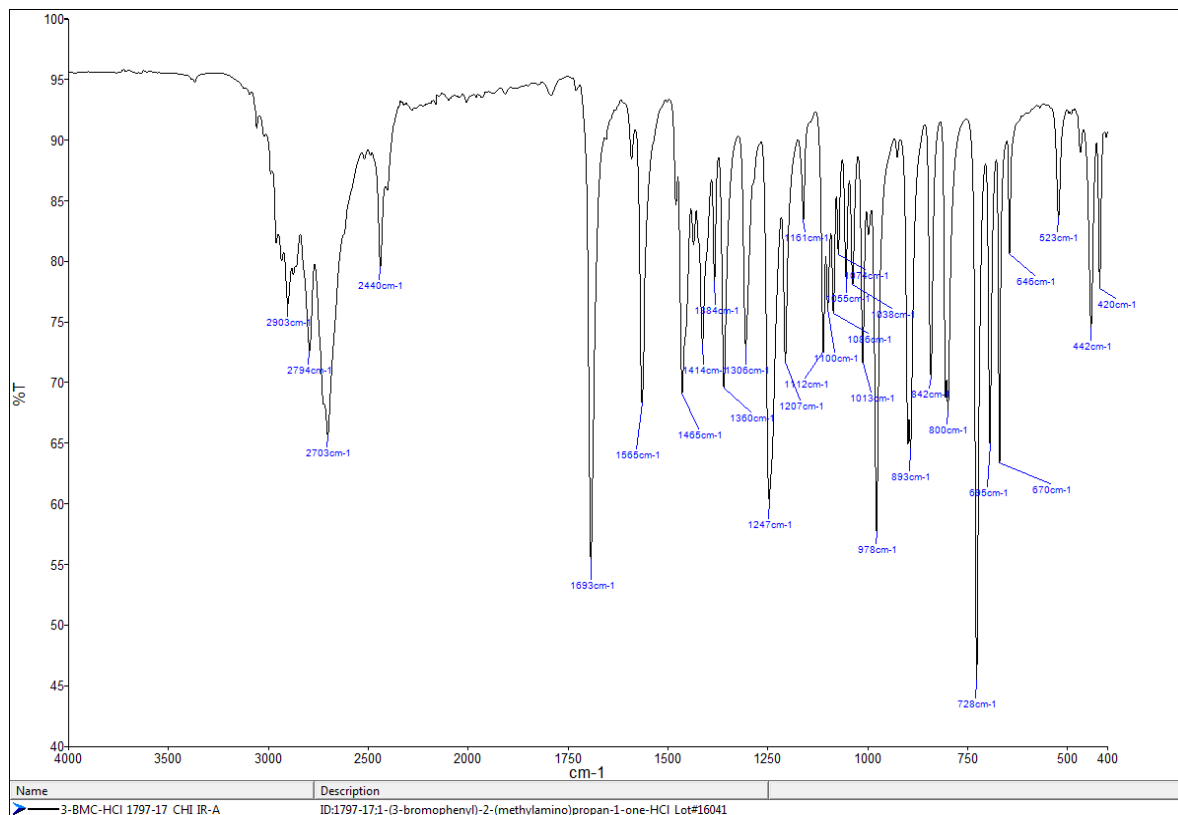
# ANALYTICAL RESULTS

MS (EI)

Abundance



## FTIR-ATR - sample as received



## IR (condensed phase – after chromatographic separation)

