ANALYTICAL REPORT

2-bromo-4,5-MDMA (C11H14BrNO2)

1-(6-bromobenzo[d][1,3]dioxol-5-yl)-N-methylpropan-2-amine

Remark – other active cpd. detected: none

Sample ID: 1362-15
Sample description: crystallinic - white
Sample type: RM-reference material
Comments¹: Cayman Lot#0458423; NFL- purchasing
Date of entry: 11/18/2015

Substance identified-structure² (base form)

Systematic name: 1-(6-bromobenzo[d][1,3]dioxol-5-yl)-N-methylpropan-2-amine
Other names: 6-bromo MDMA; 2-bromo-4,5-Methylenedioxymethamphetamine
Formula (per base form) C11H14BrNO2
Mw (g/mol) 272.14
Salt form: HCl
StdInChIKey ZIBHSZQEEWBQLW-UHFFFAOYSA-N
Compound Class Phenethylamines
Other active cpd. detected
Add.info (purity..) 98%

¹ 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.
² Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ DOI: 10.1021/ci100384d
Report updates

<table>
<thead>
<tr>
<th>date</th>
<th>comments (explanation)</th>
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Supporting information

<table>
<thead>
<tr>
<th>Analytical technique:</th>
<th>applied</th>
<th>remarks</th>
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<tbody>
<tr>
<td>GC-MS (EI ionization)</td>
<td>+</td>
<td>NFL GC-RT (min): 5.73</td>
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<td></td>
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<td>BP(1): 58; BP(2): 56; BP(3): 75,</td>
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<tr>
<td>FTIR-ATR</td>
<td>+</td>
<td>direct measurement</td>
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<tr>
<td>GC-IR (condensed phase)</td>
<td>+</td>
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**GC-MS** (Agilent):
- GC-method is RT locked to tetracosane (RT=9.53 min).
- Injection volume 1 ml and split mode (1:50).
- Injector temperature: 280 °C.
- Chromatographic separation
  - Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm.
  - Carrier gas He: flow-rate 1.2 ml/min.
  - GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, then heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.
  - MSD source EI = 70 eV. GC-MS transfer line T = 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

**FTIR-ATR** (Perkin Elmer): scan range 4000-400 cm⁻¹; resolution 4cm⁻¹

**GC-(MS)-IR** condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)) IR scan range 4000 to 700, resolution 4cm⁻¹

**GC-method**:
- Injection volume 1 ml and split mode (1:5).
- Injector temperature: 280 °C.
- Chromatographic separation
  - Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm.
  - Carrier gas He: flow-rate 1.2 ml/min.
  - GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.
  - Split MS : IR : (1:9)
  - MSD source EI = 70 eV. GC-MS transfer line T = 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

IR (condensed phase): IR scan range 4000 to 700, resolution 4cm⁻¹