ANALYTICAL REPORT
5-DBFPV (C17H23NO2)
1-(2,3-dihydrobenzofuran-5-yl)-2-(pyrrolidin-1-yl)pentan-1-one

Remark – other NPS detected: none

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th>1251-15</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample description:</td>
<td>crystalline - beige</td>
</tr>
<tr>
<td>Sample type:</td>
<td>test purchase /RESPONSE -purchasing</td>
</tr>
<tr>
<td>Date of entry into NFL database:</td>
<td>8/19/2015</td>
</tr>
</tbody>
</table>

Systematic name | 1-(2,3-dihydrobenzofuran-5-yl)-2-(pyrrolidin-1-yl)pentan-1-one |
Other names
Formula (per base form) | C17H23NO2 |
M_w (g/mol) | 273.37 |
Salt form | HCl |
StdInChIKey | CIGWUZUBQ8QZAO-UHFFFAOYSA-N |
Compound Class | Cathinones |
Other NPS detected | none |
Add.info (purity..) | Approx. 10% of an unknown organic impurity observed by NMR, |

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>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<tr>
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<td></td>
</tr>
</tbody>
</table>

**Instrumental methods** (if applied) in NFL

1. **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: on 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. 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 (40) to 550 amu.

2. **HPLC-TOF** (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 μl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N2) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.

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

4. **GC-(MS)-IR** condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny))
   
   
   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 (40) to 550 amu.
   
   IR (condensed phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.
Supporting information

<table>
<thead>
<tr>
<th>Solubility in</th>
<th>result/remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₂Cl₂</td>
<td>partially</td>
</tr>
<tr>
<td>MeOH</td>
<td>soluble</td>
</tr>
<tr>
<td>H₂O</td>
<td>partially</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Analytical technique:</th>
<th>applied</th>
<th>remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>GC-MS (EI ionization)</td>
<td>+</td>
<td>NFL GC-RT (min): 8.4&lt;br&gt;BP(1): 126; BP(2): 127; BP(3): 147,</td>
</tr>
<tr>
<td>HPLC-TOF</td>
<td>+</td>
<td>Exact mass (theoretical): 273.1792; measured value Δppm: 0.08; formula: C₁₇H₂₃NO₂</td>
</tr>
<tr>
<td>FTIR-ATR</td>
<td>+</td>
<td>direct measurement</td>
</tr>
<tr>
<td>FTIR (condensed phase) always as base form</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>NMR</td>
<td>+</td>
<td>validation</td>
</tr>
<tr>
<td>other</td>
<td></td>
<td>other</td>
</tr>
</tbody>
</table>
ANALYTICAL RESULTS

MS (EI)

Abundance

Average of 8.333 to 9.386 min.: 5-D8FPV-ID1251-15-D\data.ms

m/z ->
FTIR-ATR - direct measurement

IR (condensed phase)
Target Compound Screening Report

Data File: 5_DBFPV_1251-15_TOF.d
Sample Name: 5-DBFPV
Sample Type: Sample
Position: P2-E9
Instrument Name: 6230B TOF LC-MS
User Name: TG
Acq Method: droge general-13-5-2015-XDB-C18-ESI-poz.m
Acquired Time: 8/19/2015 3:23:36 PM
IRM Calibration Status: Success
DA Method: Droge_Default.m
Comment: extract in MeOH

Compound Table

<table>
<thead>
<tr>
<th>Label</th>
<th>Tgt Name</th>
<th>MFG Formula</th>
<th>Obs. RT</th>
<th>Obs. Mass</th>
</tr>
</thead>
</table>

Name | Obs. m/z | Obs. RT | Obs. Mass | DB RT | DB Formula | DB Mass | DB Mass Error (ppm) | Find Cpd
5-DBFPV_ID_1251-15 | 274.1801 | 5.892 | 273.1729 | 5.892 | C17 H23 N O2 | 273.1729 | 0.08 | Find by Molecular Feature

Compound Chromatograms

Cpd 1: 5-DBFPV_ID_1251-15: +ESI EIC(274.1804, 2

Cpd 1: 5-DBFPV_ID_1251-15: +ESI ECC Scan Frag

MFE MS Zoomed Spectrum

Cpd 1: 5-DBFPV_ID_1251-15: +ESI MFE Spectrum (rt: 5.824-6.556 min) Frag=175.0V 5_DBFPV

MS Spectrum Peak List

<table>
<thead>
<tr>
<th>Obs. m/z</th>
<th>Charge</th>
<th>Abund</th>
<th>Formula</th>
<th>Ion/Isotope</th>
</tr>
</thead>
<tbody>
<tr>
<td>274.1801</td>
<td>1</td>
<td>29747474</td>
<td>C17 H23 N O2</td>
<td>M+H+</td>
</tr>
<tr>
<td>275.1835</td>
<td>1</td>
<td>4694075.59</td>
<td>C17 H23 N O2</td>
<td>M+H+</td>
</tr>
<tr>
<td>276.1867</td>
<td>1</td>
<td>481999.36</td>
<td>C17 H23 N O2</td>
<td>M+H+</td>
</tr>
<tr>
<td>277.1891</td>
<td>1</td>
<td>40642.26</td>
<td>C17 H23 N O2</td>
<td>M+H+</td>
</tr>
<tr>
<td>278.1917</td>
<td>1</td>
<td>746.38</td>
<td>C17 H23 N O2</td>
<td>M+H+</td>
</tr>
<tr>
<td>296.1623</td>
<td>1</td>
<td>2916.6</td>
<td>C17 H23 N O2</td>
<td>M+Na+</td>
</tr>
<tr>
<td>547.3524</td>
<td>1</td>
<td>2635.12</td>
<td>C17 H23 N O2</td>
<td>M2+H+</td>
</tr>
</tbody>
</table>
Cpd 1: 5-DBFVP_ID_1251-15: +ESI Scan (rt: 5.824-6.543 min, 57 scans) Frag=175.0V 5_DBFPV

* 274.1805 (M+H)+
302.1747
356.1705
449.3597
553.3884
# Peak Integration Report

<table>
<thead>
<tr>
<th>No.</th>
<th>Time</th>
<th>Peak Name</th>
<th>Peak Type</th>
<th>Area ($\mu$S·min)</th>
<th>Height ($\mu$S)</th>
<th>Amount (mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00</td>
<td>9.63</td>
<td>Chloride</td>
<td>BMB</td>
<td>6.77</td>
<td>27.97</td>
<td>n.a.</td>
</tr>
<tr>
<td>2.00</td>
<td>15.22</td>
<td>Bromide</td>
<td>BMB</td>
<td>0.08</td>
<td>0.25</td>
<td>n.a.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td><strong>TOTAL:</strong></td>
<td><strong>28.22</strong></td>
<td><strong>0.00</strong></td>
</tr>
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</table>

![Graph showing peak integration](image-url)
**REPORT**

<table>
<thead>
<tr>
<th>Sample ID:</th>
<th><strong>1251-15</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Our notebook code:</td>
<td>P-1251-15</td>
</tr>
<tr>
<td>NMR sample preparation:</td>
<td>15 mg dissolved in 0.7 mL CDCl₃</td>
</tr>
<tr>
<td>NMR experiments:</td>
<td>$^1$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.</td>
</tr>
<tr>
<td>Proposed structure with chemical name:</td>
<td><img src="image" alt="Proposed structure" /></td>
</tr>
</tbody>
</table>

1-(1-(2,3-dihydrobenzofuran-5-yl)-1-oxopentan-2-yl)pyrrolidin-1-ium

| Comments: | - Structure elucidation based on 1D and 2D NMR spectra  
- Compound is not pure by NMR, containing approx. 10% of an unknown organic impurity. The same impurity is also observed in 1245-51 (for details, see there). |

| Supporting information: | Copies of $^1$H and $^{13}$C NMR spectra |
| Author: | Prof. Dr. Janez Košmrlj, Doc. Dr. Krištof Kranjc |
| Date of report: | October 2, 2015 |

*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 publication are the sole responsibility of the Author and can in no way be taken to reflect the views of the European Commission.*