**Benzylone (BMDP)**

Sample Type: **Seized Material**

Latest Revision: **June 4, 2019**

Date Received: **May 7, 2019**

Date of Report: **June 4, 2019**

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### 1. GENERAL INFORMATION

**IUPAC Name:** 1-(1,3-benzodioxol-5-yl)-2-(benzylamino)propan-1-one

**InChI String:** InChI=1S/C17H17NO3/c1-12(18-10-13-5-3-2-4-6-13)17(19)14-7-8-15-16(9-14)21-11-20-15/h2-9,12,18H,10-11H2,1H3

**CFR:** Not Scheduled (06/2019)

**CAS#** 1823274-68-5

**Synonyms:** BMDP, N-benzyl methylone, 3,4-Methylenedioxy-N-benzylecathinone, N-benzyl-3,4-methylenedioxyxycathinone

**Source:** Department of Homeland Security

**Appearance:** Pink Solid Material

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**Important Note:** All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M⁺]</th>
<th>Exact Mass [M+H]+</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C₁₇H₁₇NO₃</td>
<td>283.3</td>
<td>283</td>
<td>284.1281</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

Benzylone (BMDP) is classified as a novel stimulant and substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Novel stimulants have been reported to cause stimulant-like effects, similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include methylone, ethylone, butylone, and tertylone, among others. Methylone, butylone, and ethylone (a positional isomer of butylone) are Schedule I substances in the United States; however, benzylone is not scheduled.

Benzylone was first reported to the European Monitoring Centre for Drugs and Drug Addiction (EMCDDA) in December of 2010 by a laboratory in the United Kingdom. Additionally, benzylone has been characterized and reported in the scientific literature. While this is not the first identification of benzylone internationally, its increasing prevalence in seized drug casework has prompted interest among forensic science and public health communities.

NMS Labs identified benzylone in ten seized drug exhibits in May of 2019 from international ports of entry; all exhibits were positive for benzylone only. Three laboratories in Florida have identified benzylone in several seized exhibits (more than 10) in recent months and dating back to late 2018. Two laboratories in South Carolina report identifications of benzylone in 2019, totaling more than ten seized exhibits as well. One identification of benzylone was reported from North Dakota in April 2019. In addition to its national spread, benzylone was recently identified in two exhibits in Australia after a long gap in detection since its first identification in the country in 2013. Several of these laboratories also reported the combination of benzylone with other emergent cathinones, including N-butyl pentylone and eutylone, and methamphetamine. The seized exhibits were most commonly described as powders and tablets.

4. ADDITIONAL RESOURCES


https://www.caymanchem.com/product/9001330

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

**Testing Performed At:** NMS Labs (Willow Grove, PA)

**Sample Preparation:** Acid/Base extraction

**Instrument:** Agilent 5975 Series GC/MSD System

**Column:** Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)

**Carrier Gas:** Helium (Flow: 1 mL/min)

**Temperatures:**
- Injection Port: 265 °C
- Transfer Line: 300 °C
- MS Source: 230 °C
- MS Quad: 150 °C

Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

**Injection Parameters:**
- Injection Type: Splitless
- Injection Volume: 1 µL

**MS Parameters:**
- Mass Scan Range: 40-550 m/z
- Threshold: 250

**Retention Time:** 6.969 min
Standard Comparison: Reference material for benzylone (Batch: 0448208-15) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as benzylone, based on retention time (6.927 min) and mass spectral data. (https://www.caymanchem.com/product/9001330)

Chromatogram: Benzyline

*Additional peaks present in chromatogram: internal standards (3.247 min and 6.286 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Benzylone
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: 1:100 dilution of acid/base extract in mobile phase

Instrument: Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC

Column: Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)

Mobile Phase: A: Ammonium formate (10 mM, pH 3.0)

B: Methanol/acetonitrile (50:50)

Flow rate: 0.4 mL/min

Gradient: Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min

Temperatures: Autosampler: 15 °C

Column Oven: 30 °C

Source Heater: 600 °C

Injection Parameters: Injection Volume: 10 µL

QTOF Parameters: TOF MS Scan Range: 100-510 Da

Precursor Isolation: SWATH® acquisition (27 windows)

Fragmentation: Collision Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 5.66 min

Standard Comparison: Reference material for benzylone (Batch: 0448208-12) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as benzylone, based on retention time (5.71 min) and mass spectral data. (https://www.caymanchem.com/product/9001330)
Chromatogram: Benzyline

Additional peaks present in chromatogram: internal standard (4.87 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: Benzylone
6. ACKNOWLEDGEMENT

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