**N-butyl Hexedrone**

Sample Type: **Seized Material**

Latest Revision: **July 3, 2019**

Date Received: **May 7, 2019**

Date of Report: **July 3, 2019**

1. GENERAL INFORMATION

**IUPAC Name:** 2-(butylamino)-1-phenyl-hexan-1-one

**InChI String:** InChI=1S/C16H25NO/c1-3-5-12-15(17-13-6-4-2)16(18)14-10-8-7-9-11-14/h7-11,15,17H,3-6,12-13H2,1-2H3

**CFR:** Not Scheduled (07/2019)

**CAS#** 18296-66-7

**Synonyms:** N-butylhexedrone, alpha-Butylaminohexanophenone

**Source:** Department of Homeland Security

**Appearance:** Off-White Solid Material

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**Important Note:** All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF) in comparison to analysis of acquired reference material.

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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>C₁₆H₂₅NO</td>
<td>247.4</td>
<td>247</td>
<td>248.2009</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

*N*-butyl Hexedrone 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 *N*-ethyl hexedrone, hexedrone, and pentedrone. Pentedrone is a Schedule I substance in the United States; however, hexedrone, *N*-ethyl hexedrone, and *N*-butyl hexedrone are not scheduled.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/27728


5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

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

Sample Preparation: Acid/Base extraction (1:10 dilution)

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:**
- 4.998 min

**Standard Comparison:**
Reference material for *N*-butyl hexedrone (Batch: 0556909-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *N*-butyl hexedrone, based on retention time (4.992 min) and mass spectral data. ([https://www.caymanchem.com/product/27728](https://www.caymanchem.com/product/27728))

**Chromatogram: *N*-butyl Hexedrone**

Additional peak present in chromatogram: internal standard (3.209 min), not a controlled substance (4.918 min), and internal standard (6.287 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): N-butyl Hexedrone
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)

Flow rate: 0.4 mL/min

B: Methanol/acetonitrile (50:50)

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: 6.64 min

Standard Comparison: Reference material for N-butyl hexedrone (Batch: 0556909-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as N-butyl hexedrone, based on retention time (6.62 min) and mass spectral data.

(https://www.caymanchem.com/product/27728)
Chromatogram: N-butyl Hexedrone

Additional peak present in chromatogram: internal standards (4.90 min and 7.27 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: N-butyl Hexedrone