Hexylone

Sample Type: Seized Material

Latest Revision: June 9, 2020
Date Received: March 3, 2020
Date of Report: June 9, 2020

1. GENERAL INFORMATION

IUPAC Name: \(1-(1,3\text{-benzodioxol-5-yl})-2\)-(methylamino)hexan-1-one\)

InChI String: InChI=1S/C14H19NO3/c1-3-4-5-11(15-2)14(16)10-6-7-12-13(8-10)18-9-17-12/h6-8,11,15H,3-5,9H2,1-2H3

CFR: Not Scheduled (06/2020)

CAS#: Not Available

Synonyms: \(N\)-Methyl Hexylone

Source: Department of Homeland Security

Appearance: Off-White Solid Material

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>C₁₄H₁₉NO₃</td>
<td>249.3</td>
<td>249</td>
<td>250.1438</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

Hexylone 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 pentyline, pentyline, and N-ethyl hexylone. N-Ethyl pentyline and pentyline are Schedule I substances in the United States. N-Ethyl hexylone is not explicitly scheduled in the United States; its appearance was first reported in the United States by NPS Discovery in April 2018. Hexylone is also not explicitly scheduled.

4. ADDITIONAL RESOURCES


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:**
- 5.67 min

**Chromatogram: Hexylone**

*Additional peaks present in chromatogram: internal standards (3.22 min and 6.31 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Hexylone
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 extraction 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: Collison Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 5.78 min
Chromatogram: Hexylone

*Additional peaks present in chromatogram: internal standards (4.95 min and 7.27 min)*
TOF MS (Top) and MS/MS (Bottom) Spectra: Hexylone
5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in DMSO-D6

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters:

- Pulse Sequence: Proton
- Solvent: DMSO-D6
- Spectral Width: 4798.5 Hz
- Delay between pulses: 1st delay, d1 = 1.000

1H NMR: Hexylone

![1H NMR spectrum of Hexylone](image1)

13C NMR: Hexylone

![13C NMR spectrum of Hexylone](image2)