alpha-PiHP

Sample Type: Seized Material

Latest Revision: November 16, 2018
Date Received: August 17, 2018
Date of Report: October 30, 2018

1. GENERAL INFORMATION

IUPAC Name: 4-methyl-1-phenyl-2-pyrrolidin-1-yl-pentan-1-one
InChI String: InChI=1S/C16H23NO/c1-13(2)12-15(17-10-6-7-11-17)16(18)14-8-4-3-5-9-14/h3-5,8-9,13,15H,6-7,10-12H2,1-2H3
CFR: Not Scheduled (10/2018)
CAS#: Not Available
Synonyms: alpha-Pyrrolidinoisohexanophenone, α-PiHP
Source: Department of Homeland Security
Appearance: White Solid Material

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>C_{16}H_{23}NO</td>
<td>245.36</td>
<td>245</td>
<td>246.1852</td>
</tr>
</tbody>
</table>

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.

Prepared By: Alex J. Krotuls, MSFS, Melissa F. Fogarty, MSFS, D-ABFT-FT, and Barry K. Logan, PhD, F-ABFT
3. BRIEF DESCRIPTION

Alpha-PiHP 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 alpha-pyrrolidinopentiophenone (alpha-PVP), alpha-pyrrolidinobutiophenone (alpha-PBP), and alpha-pyrrolidinohexanophenone (alpha-PHP). Alpha-PVP, and alpha-PBP are all Schedule I substances in the United States.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/21682


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:  
5.017 min

Standard Comparison:  
Reference material for alpha-PiHP (Batch: 0501111-17) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as alpha-PiHP, based on retention time (5.002 min) and mass spectral data.  
(https://www.caymanchem.com/product/21682)

Chromatogram: alpha-PiHP

Additional peaks present in chromatogram: internal standard (3.234 min), not a controlled substance (5.117 min), internal standard (6.281 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): alpha-PiHP
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: Collision Energy Spread (35±15 eV)
MS/MS Scan Range: 50-510 Da

Retention Time: 5.79 min

Standard Comparison: Reference material for alpha-PiHP (Batch: 0501111-17) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as alpha-PiHP, based on retention time (5.80 min) and mass spectral data. (https://www.caymanchem.com/product/21682)
Chromatogram: alpha-PiHP

Additional peaks present in chromatogram: internal standards (4.90 min and 7.24 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: alpha-PiHP
6. REVISION HISTORY

<table>
<thead>
<tr>
<th>Date</th>
<th>Revision</th>
</tr>
</thead>
<tbody>
<tr>
<td>11/16/2018</td>
<td>Corrected drug name and lot number under “Standard Comparison” for alpha-PiHP</td>
</tr>
</tbody>
</table>