Piperidylthiambutene

Sample Type: Seized Material

Latest Revision: September 18, 2019
Date Received: August 16, 2019
Date of Report: September 18, 2019

1. GENERAL INFORMATION

IUPAC Name: 1-[1-methyl-3,3-bis(2-thienyl)allyl]piperidine
InChI String: InChI=1S/C17H21NS2/c1-14(18-9-3-2-4-10-18)13-15(16-7-5-11-19-16)17-8-6-12-20-17/h5-8,11-14H,2-4,9-10H2,1H3
CFR: Not Scheduled (09/2019)
CAS#: 64037-51-0
Synonyms: Piperidinohtont
Source: Department of Homeland Security
Appearance: Tan Solid Material

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>C₁₇H₂₁NS₂</td>
<td>303.5</td>
<td>303</td>
<td>304.1188</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

Piperidylthiambutene is classified as a synthetic opioid. Piperidylthiambutene is structurally distinct from fentanyl, its analogues, and other synthetic opioids previously reported. Piperidylthiambutene is not explicitly a scheduled substance in the United States. Piperidylthiambutene was found to be active with similar activity to morphine when studied in a rat model.¹

4. ADDITIONAL RESOURCES

   https://www.caymanchem.com/product/26335

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: 6.483 min

Standard Comparison: Reference material for Piperidylthiambutene (Batch: 0545005-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Piperidylthiambutene, based on retention time (6.468 min) and mass spectral data. (https://www.caymanchem.com/product/26335)
Chromatogram: Piperidylthiambutene

Additional peaks present in chromatogram: internal standard (3.211 min), not a controlled substance (5.042 mins) and internal standard (6.287 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Piperidylthiambutene
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: Collison Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 6.77 min

Standard Comparison: Reference material for Piperidylthiambutene (Batch: 0545005-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Piperidylthiambutene, based on retention time (6.78 min) and mass spectral data. (https://www.caymanchem.com/product/26335)
Chromatogram: Piperidylthiambutene

Additional peaks present in chromatogram: internal standards (4.89 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: Piperidylthiambutene