4-AcO-EPT

Sample Type: Seized Material

Latest Revision: June 29, 2021
Date Received: March 3, 2021
Date of Report: June 29, 2021

1. GENERAL INFORMATION

IUPAC Name: [3-[2-[ethyl(propyl)amino]ethyl]-1H-indol-4-yl] acetate

InChI String: InChI=1S/C17H24N2O2/c1-4-10-19(5-2)11-9-14-12-18-15-7-6-8-16(17(14)15)21-13(3)20/h6-8,12,18H,4-5,9-11H2,1-3H3

CFR: Not Scheduled (06/2021)

CAS#: Not Available

Synonyms: 4-Acetoxy EPT, 4-acetoxy-N-ethyl-N-propyltryptamine

Source: NMS Labs – Criminalistic Laboratory

Appearance: Tan Solid Material

Important Note: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF-MS, and NMR).

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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>C₁₇H₂₄N₂O₂</td>
<td>288.4</td>
<td>288</td>
<td>289.1911</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

4-AcO-EPT is classified as a novel tryptamine analogue. Tryptamine analogues are modified based on the structure of tryptamine. Tryptamine analogues have been reported to cause hallucinogenic effects, often associated with “psychedelic mushrooms.” Tryptamine analogues have caused adverse events, including agitation, tachyarrhythmias, hyperpyrexia, and death, as described in the literature. Structurally similar compounds include psilocin, 4-HO-EPT, and 4-AcO-DPT, among several other tryptamine analogues. Psilocin is a Schedule I substance in the United States.

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:**
- 6.80 min

**Chromatogram: 4-AcO-EPT**

*Additional peaks present in chromatogram: internal standard (3.12 min), not a controlled substance (5.76 min), internal standard (6.30 min) and not a controlled substance (7.10 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4-AcO-EPT
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: 5.42 min
Chromatogram: 4-AcO-EPT

Additional peaks present in chromatogram: not a controlled substance (4.59 min), internal standard (4.96 min), not a controlled substance (5.60 min), and internal standard (7.30 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: 4-AcO-EPT
5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Powder dissolved in CDCl₃

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters: Pulse Sequence: Proton

Solvent: CDCl₃

Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

Delay between pulses: 1st delay, d1 = 1.000

\(^1\text{H NMR: 4-AcO-EPT}\)
6. FUNDING

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