4F-Pentedrone

Sample Type: Seized Material

Latest Revision: December 3, 2019
Date Received: August 16, 2019
Date of Report: December 3, 2019

1. GENERAL INFORMATION

IUPAC Name: 1-(4-fluorophenyl)-2-(methylamino)pentan-1-one

InChI String: InChI=1S/C12H16FNO/c1-3-4-11(14-2)12(15)9-5-7-10(13)8-6-9/h5-8,11,14H,3-4H2,1-2H3

CFR: Not Scheduled (12/2019)

CAS#: Not Available

Synonyms: 4-Fluoro Pentedrone, 4-Fluoro-α-Methylamino-Valerophenone, 4-FPD

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-MS) in comparison to analysis of acquired reference material.

Prepared By: Alex J. Krotulski, PhD; Melissa F. Fogarty, MSFS, D-ABFT-FT; and Barry K. Logan, PhD, F-ABFT
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>C₁₂H₁₆FNO</td>
<td>209.3</td>
<td>209</td>
<td>210.1289</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

4-F-Pentedrone 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 pentedrone, hexedrone, and N-ethyl hexedrone. Pentedrone is a Schedule I substance in the United States while 4F-pentedrone is not explicitly scheduled.

4. ADDITIONAL RESOURCES


https://www.caymanchem.com/product/9002182/

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:**
- 3.897 min

**Standard Comparison:** Reference material for 4F-Pentedrone (Batch: 0464459-26) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 4F-Pentedrone, based on retention time (3.882 min) and mass spectral data.

(https://www.caymanchem.com/product/9002182/)

**Chromatogram: 4F-Pentedrone**

Additional peaks present in chromatogram: internal standards (3.195 min and 6.269 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4F-Pentedrone
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: Collision Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 5.19 min

Standard Comparison: Reference material for 4F-Pentedrone (Batch: 0464459-26) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 4F-Pentedrone, based on retention time (5.15 min) and mass spectral data. (https://www.caymanchem.com/product/9002182/)
Chromatogram: 4F-Pentedrone

Additional peaks present in chromatogram: internal standards (4.99 min and 7.32 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: 4F-Pentedrone