Sample Type: Seized Material

Latest Revision: February 13, 2019
Date Received: November 2, 2018
Date of Report: February 12, 2019

1. GENERAL INFORMATION

IUPAC Name: Methyl 2-[[1-(5-fluoropentyl)indole-3-carbonyl]amino]-3-phenylpropanoate

InChI String: InChI=1S/C24H27FN2O3/c1-30-24(29)21(16-18-10-4-2-5-11-18)26-23(28)20-17-27(15-9-3-8-14-25)22-13-7-6-12-19(20)22/h2,4-7,10-13,17,21H,3,8-9,14-16H2,1H3,(H,26,28)

CFR: Not Scheduled (02/2019)

CAS#: Not Available

Synonyms: 5-Fluoro MPP-PICA, MPHP-2201

Source: Department of Homeland Security

Appearance: Orange 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.

Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, 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>
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<tbody>
<tr>
<td>Base</td>
<td>C₂₄H₂₇FN₂O₃</td>
<td>410.48</td>
<td>410</td>
<td>411.2078</td>
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3. BRIEF DESCRIPTION

5F-MPP-PICA is classified as a synthetic cannabinoid. Synthetic cannabinoids have been reported to cause psychoactive effects similar to delta-9-tetrahydrocannabinol (THC). Synthetic cannabinoids have caused adverse events, including deaths, as described in the literature. 5F-MDMB-PICA and PX-1 (5F-APP-PICA) are structurally similar synthetic cannabinoids. On December 28, 2018, the Drug Enforcement Administration published a notice of intent to place 5F-MDMB-PICA as a Schedule I substance in the United States.

4. ADDITIONAL RESOURCES


https://www.caymanchem.com/product/25916

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:** 9.465 min

**Standard Comparison:**
Reference material for 5F-MPP-PICA (Batch: 0543629-3) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-MPP-PICA, based on retention time (9.450 min) and mass spectral data. ([https://www.caymanchem.com/product/25916](https://www.caymanchem.com/product/25916))

**Chromatogram:** 5F-MPP-PICA

*Additional peaks present in chromatogram: internal standards (3.207 min and 6.285 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-MPP-PICA
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: 8.99 min

Standard Comparison: Reference material for 5F-MPP-PICA (Batch: 0543629-3) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-MPP-PICA, based on retention time (9.16 min) and mass spectral data. (https://www.caymanchem.com/product/25916)
Chromatogram: 5F-MPP-PICA

Additional peak present in chromatogram: internal standard (4.87 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: 5F-MPP-PICA
### 6. REVISION HISTORY

<table>
<thead>
<tr>
<th>Date</th>
<th>Revision</th>
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<tbody>
<tr>
<td>02/13/2019</td>
<td>Brief description was modified to include “notice of intent” for scheduling of 5F-MDMB-PICA</td>
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<tr>
<td>02/13/2019</td>
<td>Add “Sample Type: Seized Material”</td>
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