5F-EMB-PICA

Sample Type: Seized Material

Latest Revision: June 15, 2020
Date Received: April 23, 2020
Date of Report: June 15, 2020

1. GENERAL INFORMATION

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

InChI String: InChI=1S/C21H29FN2O3/c1-4-27-21(26)19(15(2)3)23-20(25)17-14-24(13-9-5-8-12-22)18-11-7-6-10-16(17)18/h6-7,10-11,14-15,19H,4-5,8-9,12-13H2,1-3H3,(H,23,25)

CFR: Not Scheduled (06/2020)

CAS#: Not Available

Synonyms: EMB-2201, 5-fluoro EMB-PICA

Source: NMS Labs – Criminalistic Laboratory

Appearance: Hand-Rolled Cigarette Containing Plant 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>C$<em>{21}$H$</em>{29}$FN$_2$O$_3$</td>
<td>376.5</td>
<td>376</td>
<td>377.2235</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

5F-EMB-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 5F-MMB-PICA (MMB-2201) are structurally similar synthetic cannabinoids. 5F-MDMB-PICA is a Schedule I substance in the United States; 5F-EMB-PICA and 5F-MMB-PICA are not explicitly scheduled.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/30769/5-fluoro-emb-pica

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)

Sample Preparation: Acid/Base extraction (*note: only one internal standard added*)

Instrument: Agilent 5975 Series GC/MSD System

Column: Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)

Carrier Gas: Helium (Flow: 1.46 mL/min)

Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

MS Source: 230 °C

MS Quad: 150 °C
Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min

**Injection Parameters:**
- Injection Type: Splitless
- Injection Volume: 1 µL

**MS Parameters:**
- Mass Scan Range: 40-550 m/z
- Threshold: 250

**Retention Time:** 8.09 min

**Standard Comparison:**
Reference material for 5F-EMB-PICA (Batch: 0588434-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-EMB-PICA based on retention time (8.10 min) and mass spectral data. ([https://www.caymanchem.com/product/30769/5-fluoro-emb-pica](https://www.caymanchem.com/product/30769/5-fluoro-emb-pica))

**Chromatogram: 5F-EMB-PICA**

*Additional peaks present in chromatogram: not controlled substances (1.70 min, 3.31 min, and 3.57 min) and internal standard (5.76 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-EMB-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: Collision Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 9.29 min

Standard Comparison: Reference material for 5F-EMB-PICA (Batch: 0588434-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-EMB-PICA based on retention time (9.29 min) and mass spectral data. (https://www.caymanchem.com/product/30769/5-fluoro-emb-pica)
Chromatogram: 5F-EMB-PICA

Additional peak present in chromatogram: internal standard (7.33 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: 5F-EMB-PICA

![Mass/Charge Distribution](image-url)