5F-EDMB-PINACA

Sample Type: Seized Material

Latest Revision: May 18th, 2018
Date Received: February 12th, 2018
Date of Report: April 10th, 2018

1. GENERAL INFORMATION

IUPAC Name: Ethyl 2-[[1-(5-fluoropentyl)indazole-3-carbonyl]amino]-3,3-dimethyl-butanate

InChI String: InChI=1S/C21H30FN3O3/c1-5-28-20(27)18(21(2,3)4)23-19(26)17-15-11-7-8-12-16(15)25(24-17)14-10-6-9-13-22/h7-8,11-12,18H,5-6,9-10,13-14H2,1-4H3,(H,23,26)

CFR: Not Scheduled (04/2018)

CAS#: Not available

Synonyms: 5-fluoro EDMB-PINACA

Source: Department of Homeland Security

Appearance: White 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>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C_{21}H_{30}FN_{3}O_{3}</td>
<td>391.5</td>
<td>391</td>
<td>392.2344</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

5F-EDMB-PINACA 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-ADB (5F-MDMB-PINACA) is a structurally similar synthetic cannabinoid. 5F-ADB is a Schedule I substance in the United States.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/23005

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:**
- 7.734 min

**Standard Comparison:**
Reference material for 5F-EDMB-PINACA (Batch: 0516373-8) 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-EDMB-PINACA, based on retention time (7.725 min) and mass spectral data. ([https://www.caymanchem.com/product/23005](https://www.caymanchem.com/product/23005))

**Chromatogram: 5F-EDMB-PINACA**

*Additional peaks present in chromatogram: internal standard 1 (3.206 min), internal standard 2 (6.289 min), and 5F-ADB (7.681 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-EDMB-PINACA
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: 9.92 min

Standard Comparison: Reference material for 5F-EDMB-PINACA (Batch: 0516373-8) 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-EDMB-PINACA, based on retention time (9.922 min) and mass spectral data.

(https://www.caymanchem.com/product/23005)
Additional peaks present in chromatogram: internal standard 1 (4.95 min), internal standard 2 (7.27 min), and 5F-ADB (9.59 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: 5F-EDMB-PINACA
### 6. REVISION HISTORY

<table>
<thead>
<tr>
<th>Date</th>
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<tbody>
<tr>
<td>05/18/2018</td>
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