4F-ABINACA

Sample Type: Seized Material

Latest Revision: January 27, 2021
Date Received: December 4, 2020
Date of Report: January 27, 2021

1. GENERAL INFORMATION

IUPAC Name: N-(1-adamantyl)-1-(4-fluorobutyl)indazole-3-carboxamide

InChI String: InChI=1S/C22H28FN3O/c23-7-3-4-8-26-19-6-2-1-5-18(19)20(25-26)21(27)24-22-12-15-9-16(13-22)11-17(10-15)14-22/h1-2,5-6,15-17H,3-4,7-14H2,(H,24,27)

CFR: Not Scheduled (01/2021)

CAS#: Not Available

Synonyms: 4-fluoro ABUTINACA, 4F-ABUTINACA, 4F-Adamantyl-BINACA, N-(4-fluorobutyl) APINACA

Source: NMS Labs – Criminalistic Laboratory

Appearance: Plant-Like 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.

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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>C₂₂H₂₈FN₃O</td>
<td>369.5</td>
<td>369</td>
<td>370.2289</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

4F-ABINACA 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. APINACA (AKB48) and 5F-APINACA (5F-AKB48) are structurally similar synthetic cannabinoids. APINACA and 5F-APINACA are Schedule I substances in the United States; 4F-ABINACA is not explicitly scheduled.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/30724/4-fluoro-abutinaca

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:**
- 8.83 min

**Standard Comparison:**
Reference material for 4F-ABINACA (Batch: 0588385-1) 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-ABINACA based on retention time (8.81 min) and mass spectral data. ([https://www.caymanchem.com/product/30724/4-fluoro-abutinaca](https://www.caymanchem.com/product/30724/4-fluoro-abutinaca))

**Chromatogram: 4F-ABINACA**

*Additional peak present in chromatogram: internal standard (6.28 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4F-ABINACA
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:** 10.49 min

**Standard Comparison:** Reference material for 4F-ABINACA (Batch: 0588385-1) 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-ABINACA based on retention time (10.47 min) and mass spectral data. ([https://www.caymanchem.com/product/30724/4-fluoro-abutinaca](https://www.caymanchem.com/product/30724/4-fluoro-abutinaca))
Extracted Ion Chromatogram: 4F-ABINACA
TOF MS (Top) and MS/MS (Bottom) Spectra: 4F-ABINACA
6. FUNDING

NPS Discovery at the Center for Forensic Science Research and Education (CFSRE) is supported in part by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice (Award Number 2020-DQ-BX-0007, “Real-Time Sample-Mining and Data-Mining Approaches for the Discovery of Novel Psychoactive Substances (NPS”). The opinions, findings, conclusions and/or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect those of the Department of Justice.