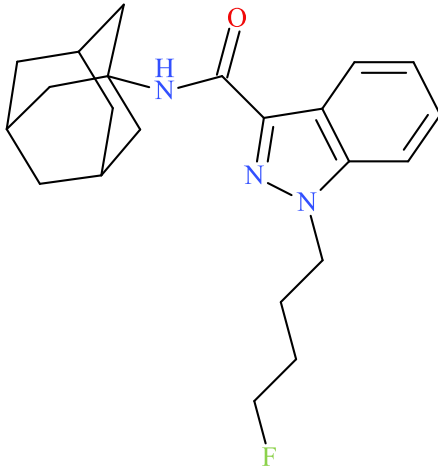


4F-ABINACA

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

Form	Chemical Formula	Molecular Weight	Molecular Ion [M ⁺]	Exact Mass [M+H] ⁺
Base	C ₂₂ H ₂₈ FN ₃ O	369.5	369	370.2289

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

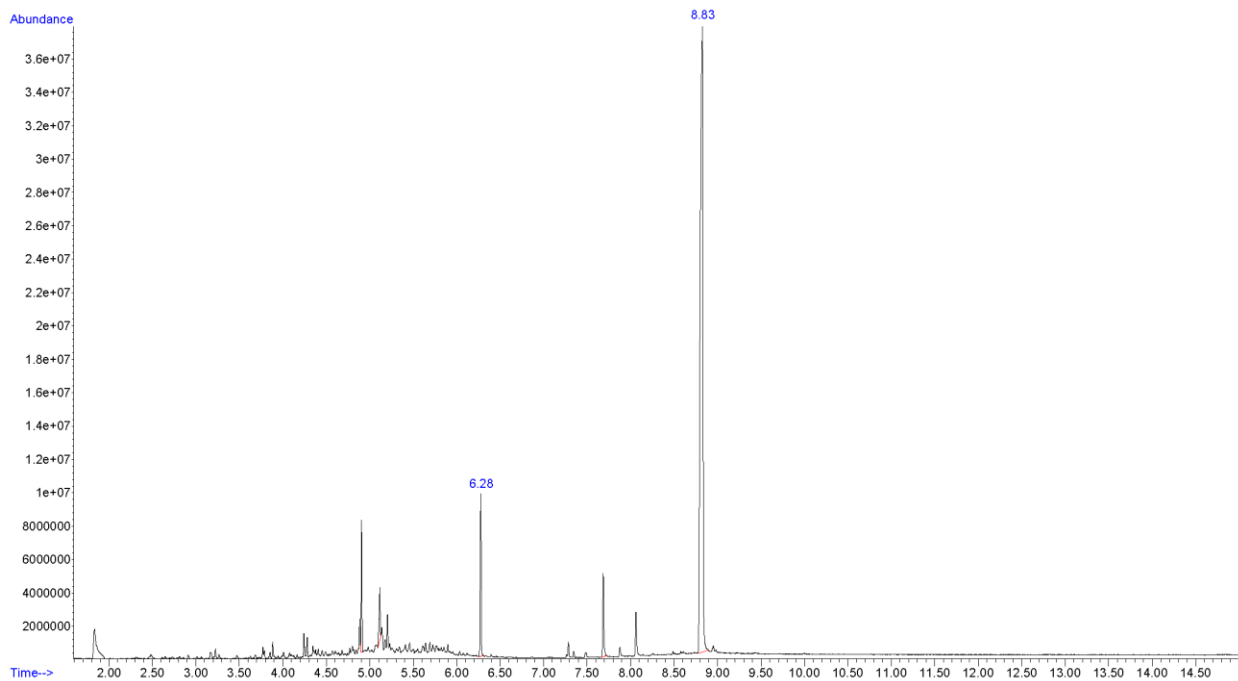
Threshold: 250

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.

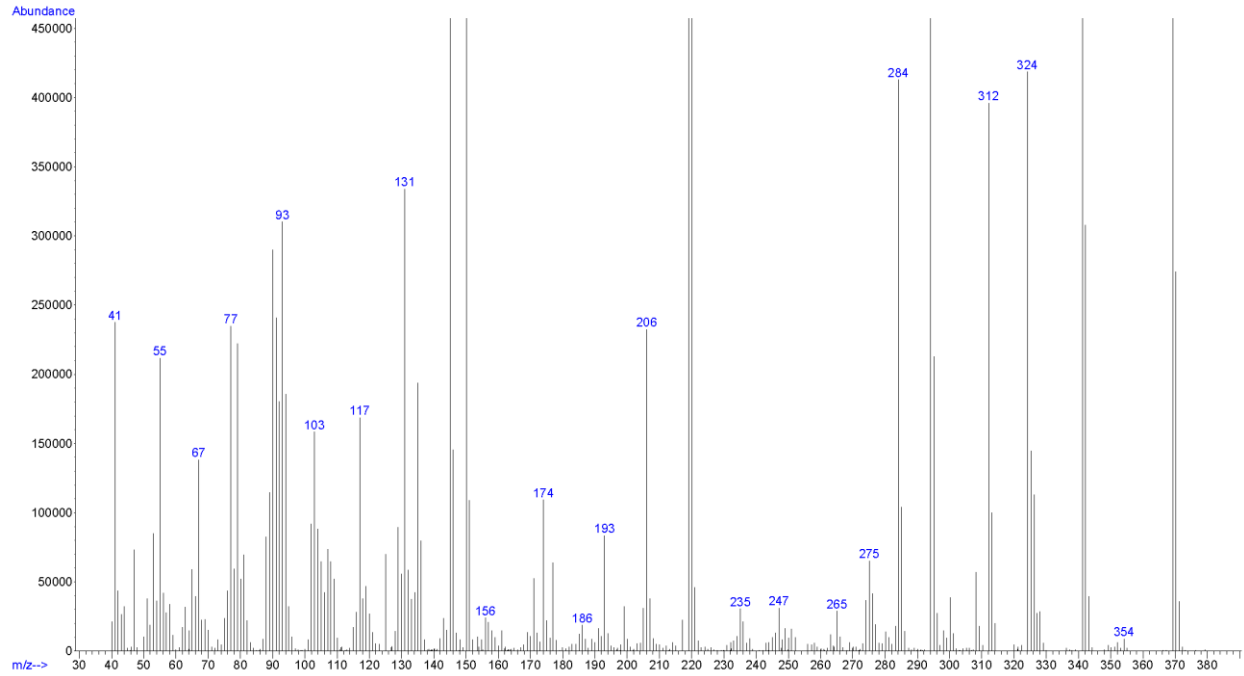
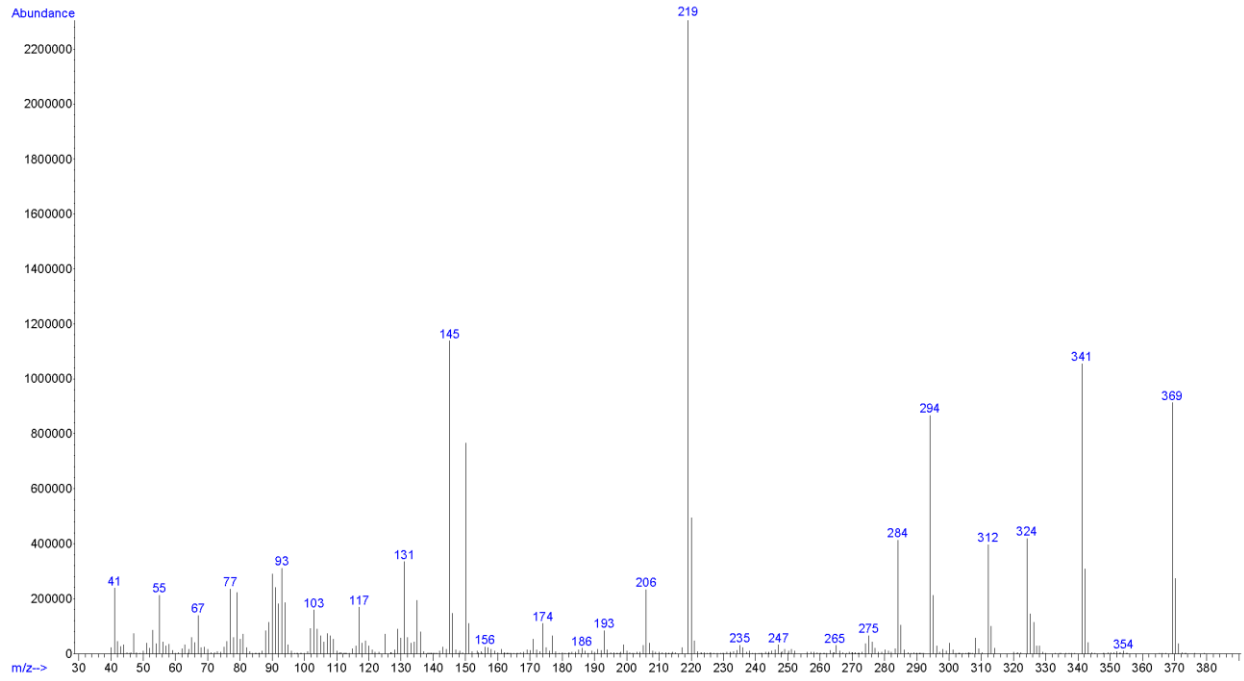
<https://www.caymanchem.com/product/30724/4-fluoro-abutinaca>

Chromatogram: 4F-ABINACA



Additional peak present in chromatogram: internal standard (6.28 min)

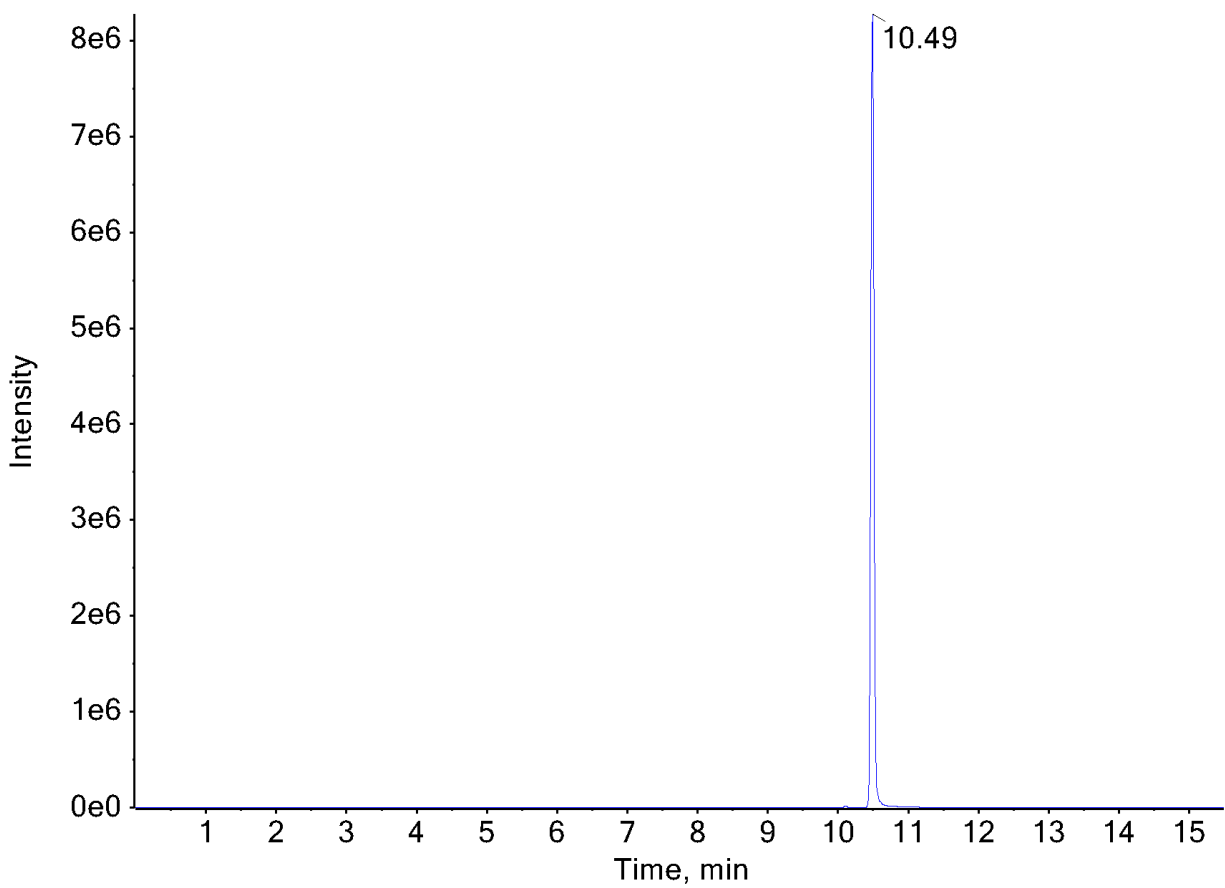
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4F-ABINACA



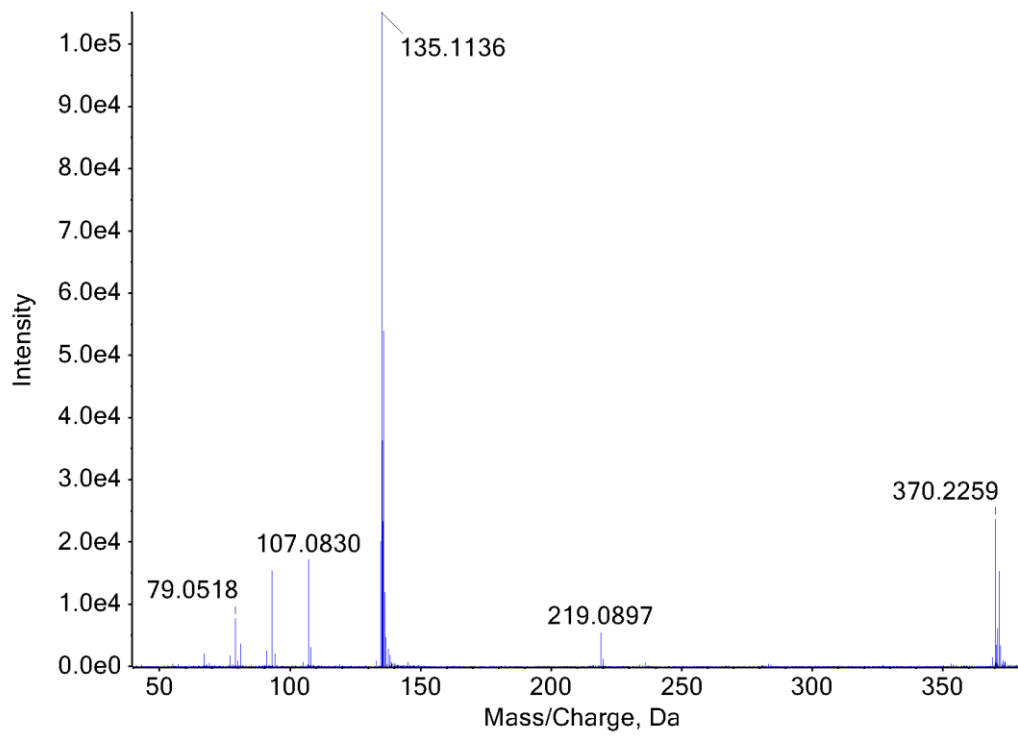
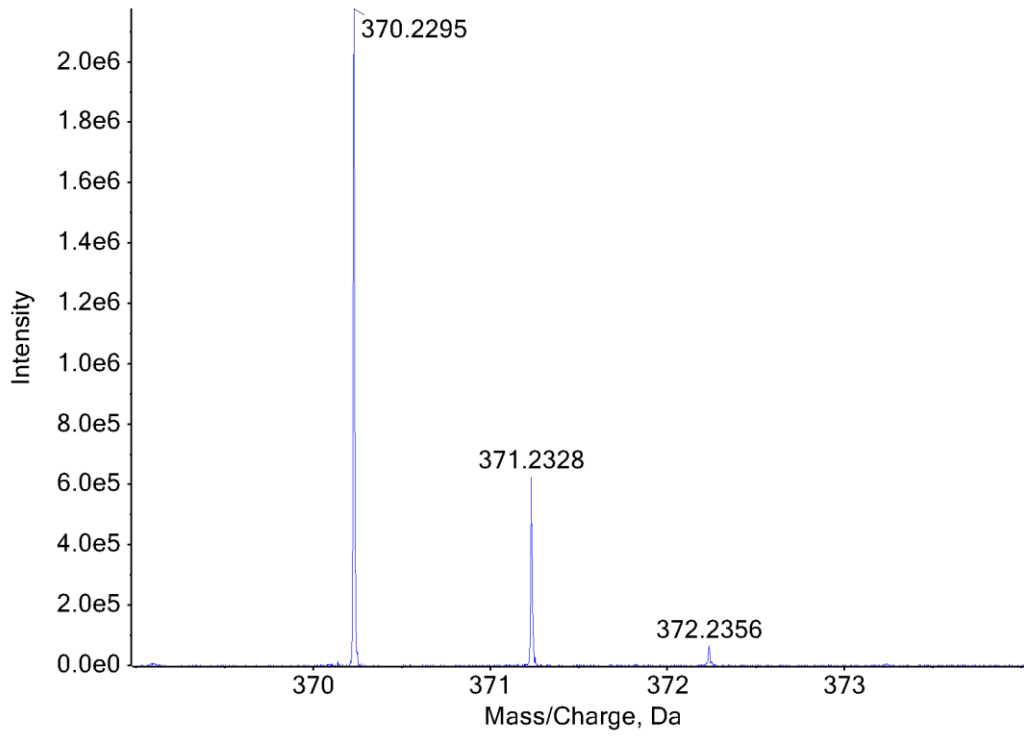
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

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: Collision 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)

Extracted Ion Chromatogram: 4F-ABINACA



TOF MS (Top) and MS/MS (Bottom) Spectra: 4F-ABINACA



6. FUNDING

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