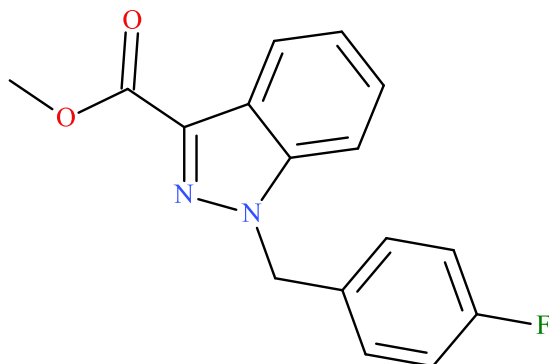


MFUBINAC

Sample Type: **Seized Material**



Latest Revision: **October 30, 2018**

Date Received: **August 17, 2018**

Date of Report: **October 30, 2018**

1. GENERAL INFORMATION

IUPAC Name:	Methyl 1-[(4-fluorophenyl)methyl]indazole-3-carboxylate
InChI String:	InChI=1S/C16H13FN2O2/c1-21-16(20)15-13-4-2-3-5-14(13)19(18-15)10-11-6-8-12(17)9-7-11/h2-9H,10H2,1H3
CFR:	Not Scheduled (10/2018)
CAS#	1185287-50-6
Synonyms:	Methyl 1-(4-fluorobenzyl)-1H-indazole-3-carboxylate
Source:	Department of Homeland Security
Appearance:	Off-white Solid Material

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion [M ⁺]	Exact Mass [M+H] ⁺
Base	C ₁₆ H ₁₃ FN ₂ O ₂	284.28	284	285.1034

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, D-ABFT-FT, and Barry K. Logan, PhD, F-ABFT

3. BRIEF DESCRIPTION

MFUBINAC 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.

4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/24855>

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

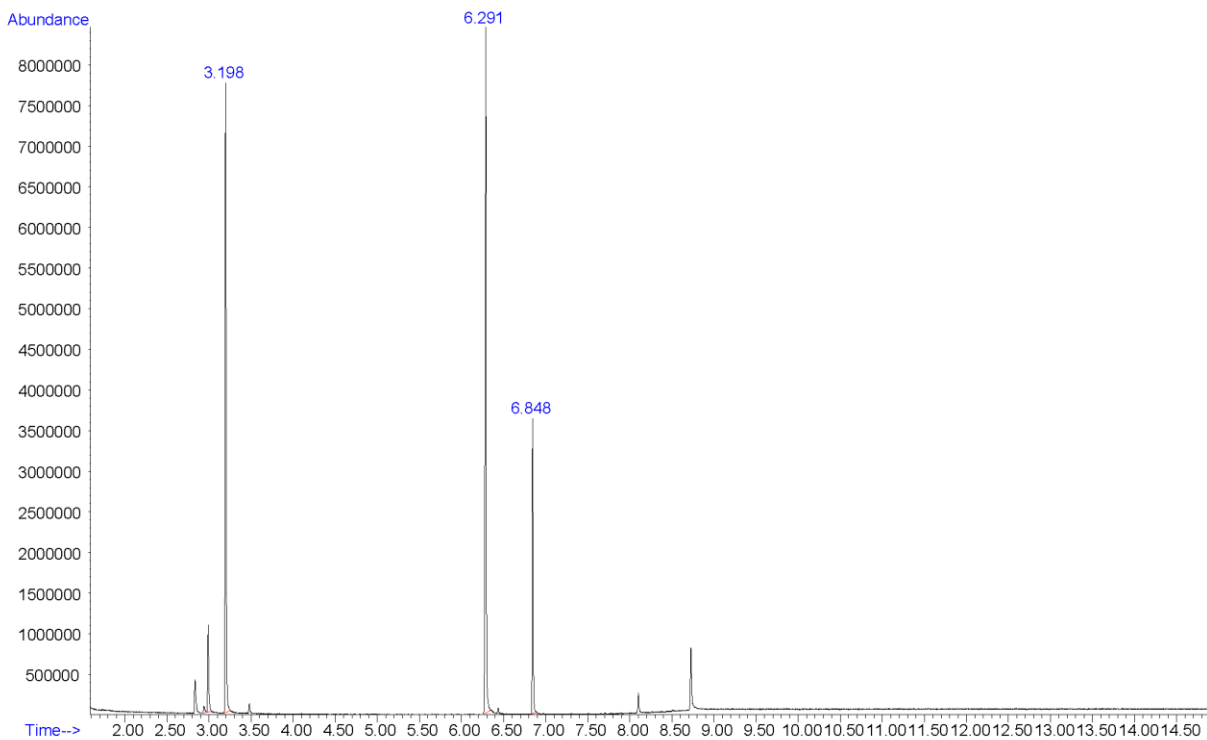
Retention Time: 6.848 min

Standard Comparison:

Reference material for MFUBINAC (Batch: 0526254-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as MFUBINAC, based on retention time (6.846 min) and mass spectral data.

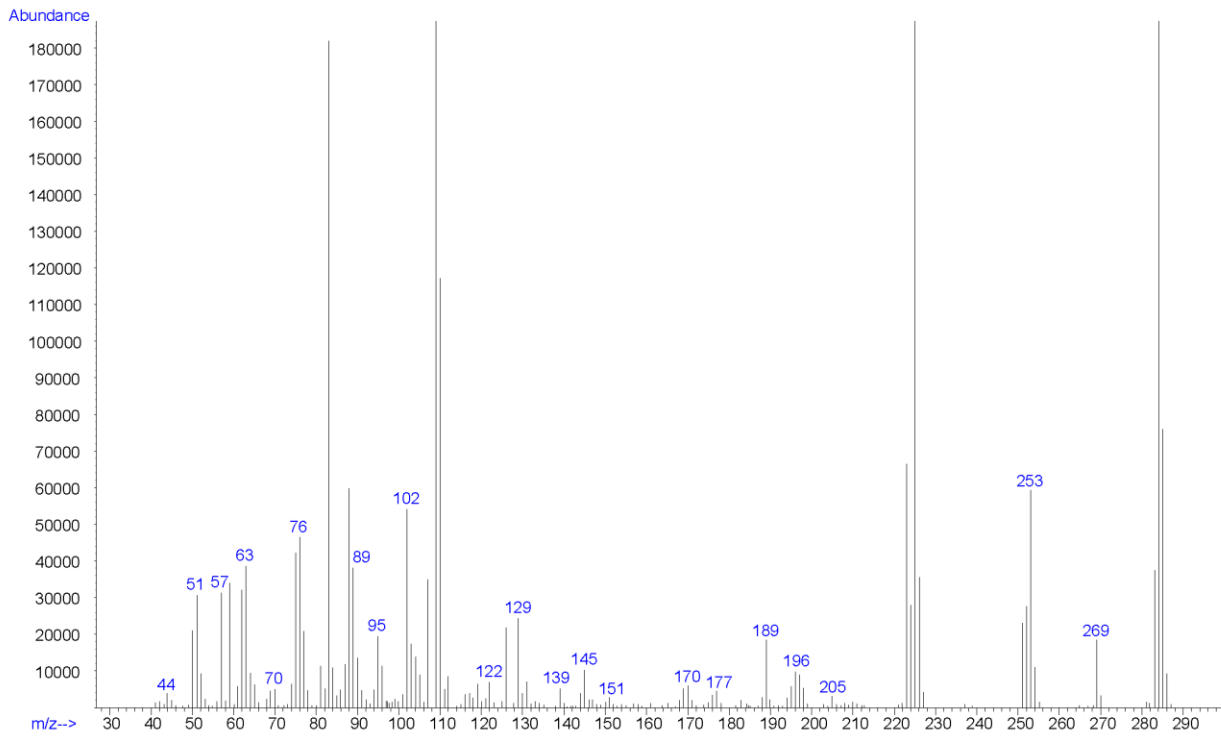
<https://www.caymanchem.com/product/24855>

Chromatogram: MFUBINAC



Additional peaks present in chromatogram: internal standards (3.198 min and 6.291 min)

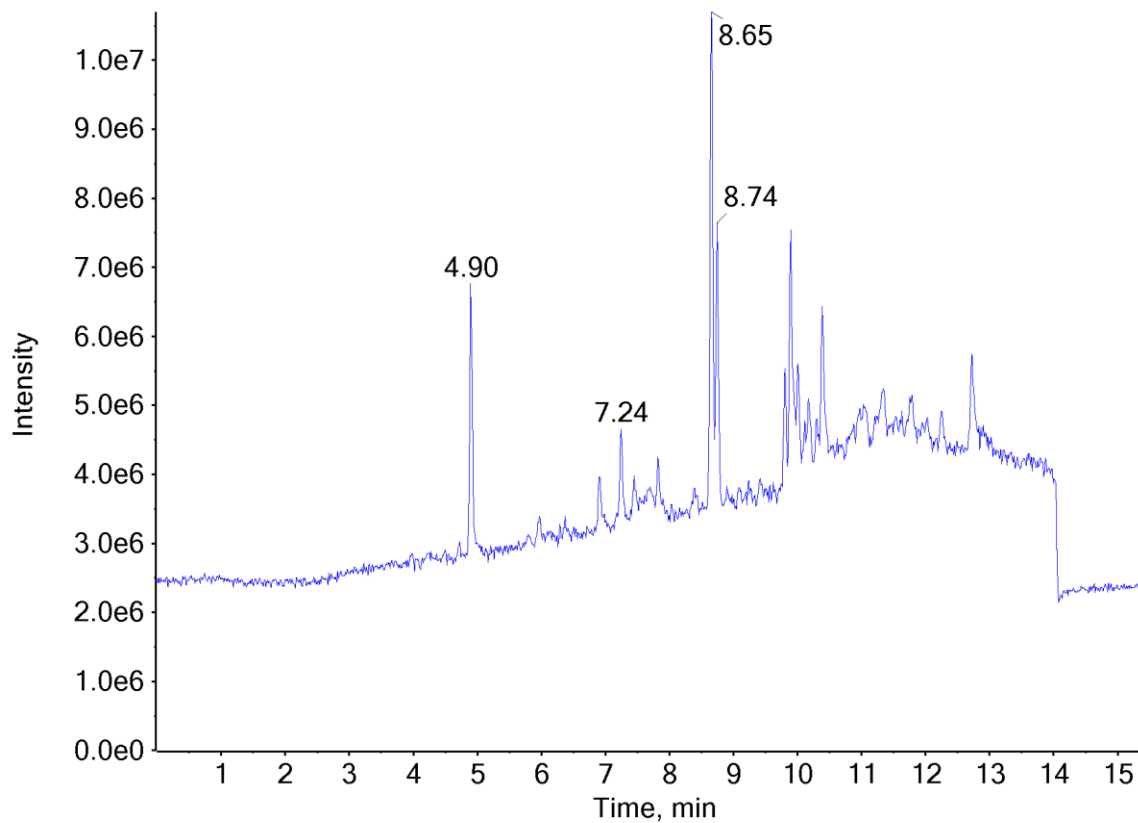
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): MFUBINAC



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:	8.65 min
Standard Comparison:	Reference material for MFUBINAC (Batch: 0526254-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as MFUBINAC, based on retention time (8.67 min) and mass spectral data. (https://www.caymanchem.com/product/24855)

Chromatogram: MFUBINAC



Additional peaks present in chromatogram: internal standards (4.90 min and 7.24 min), not a controlled substance (8.74 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: MFUBINAC

