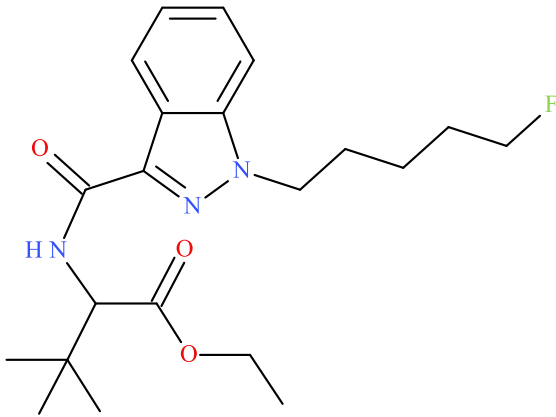


5F-EDMB-PINACA

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-butanoate

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

Form	Chemical Formula	Molecular Weight	Molecular Ion [M ⁺]	Exact Mass [M+H] ⁺
Base	C ₂₁ H ₃₀ FN ₃ O ₃	391.5	391	392.2344

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://onlinelibrary.wiley.com/doi/abs/10.1002/dta.2160>

<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

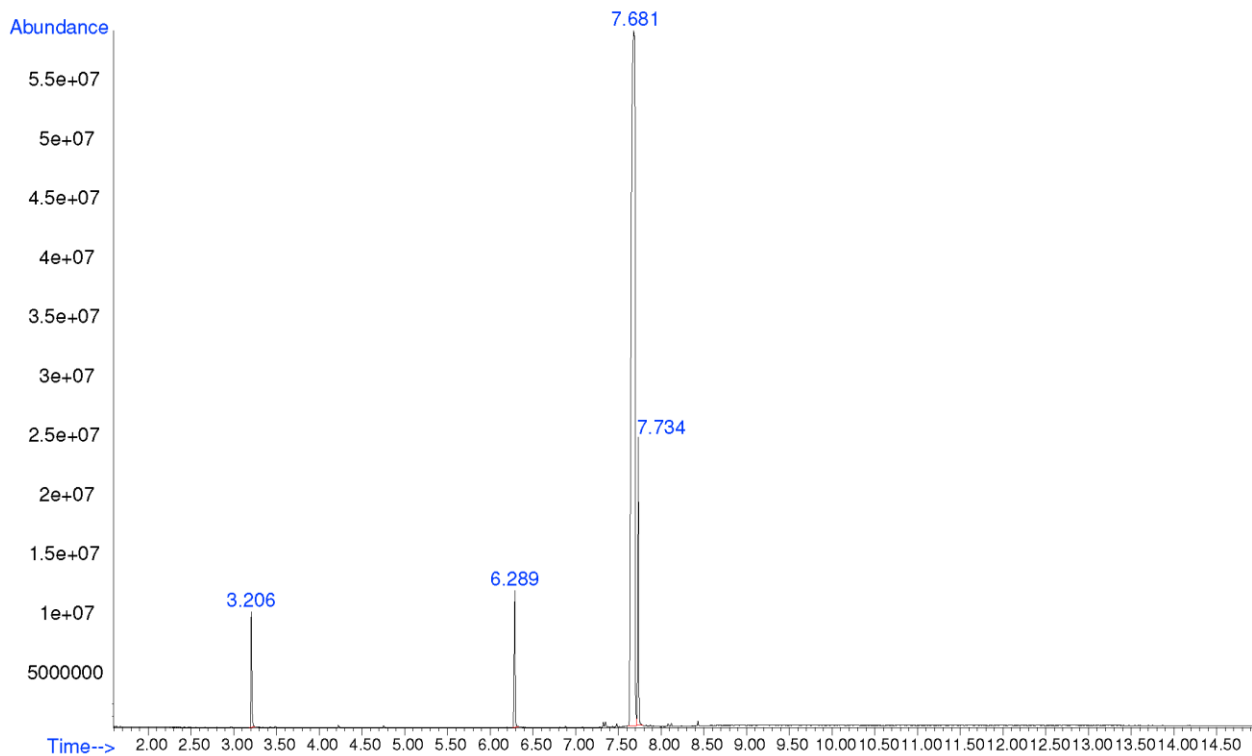
Threshold: 250

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.

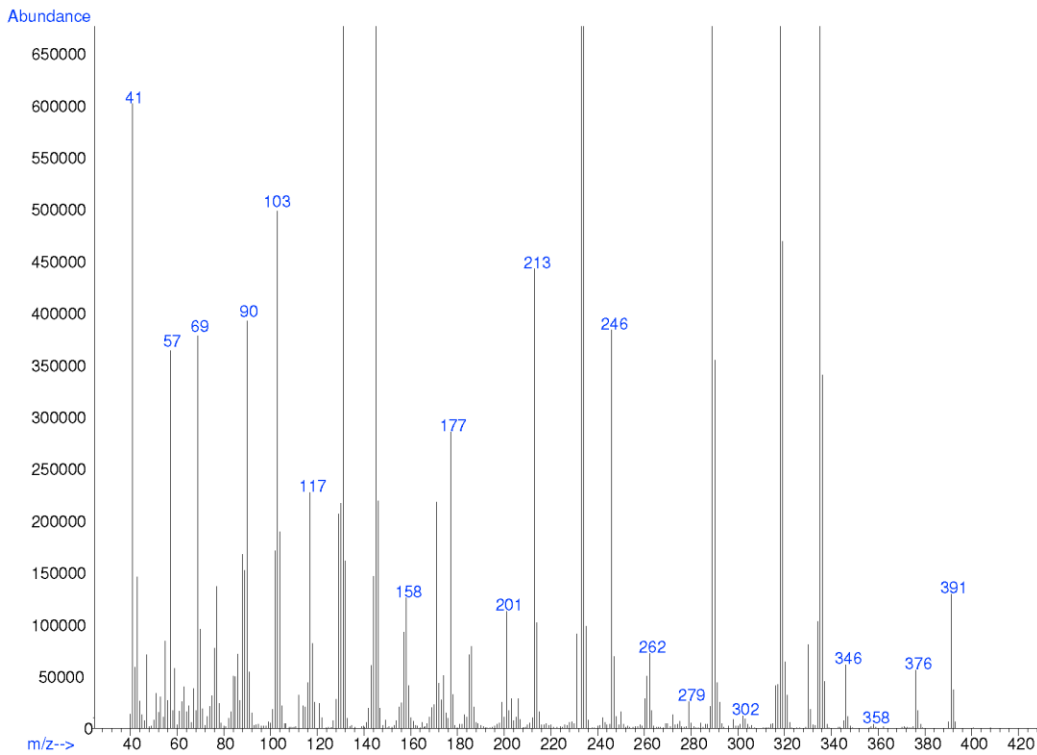
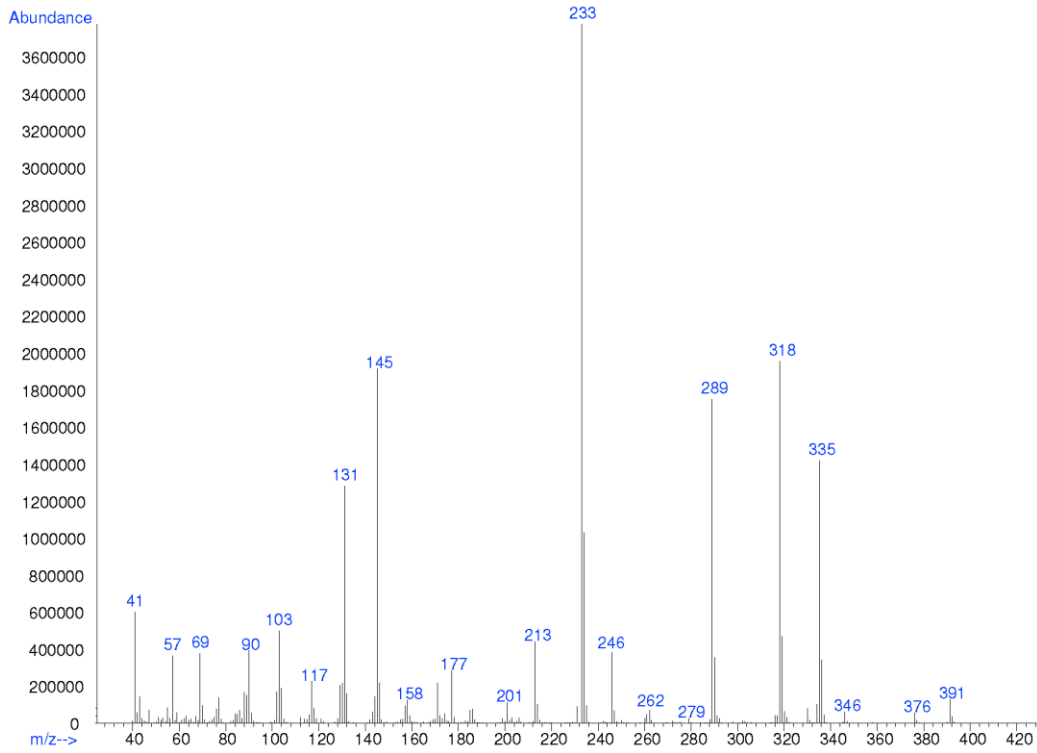
<https://www.caymanchem.com/product/23005>

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)

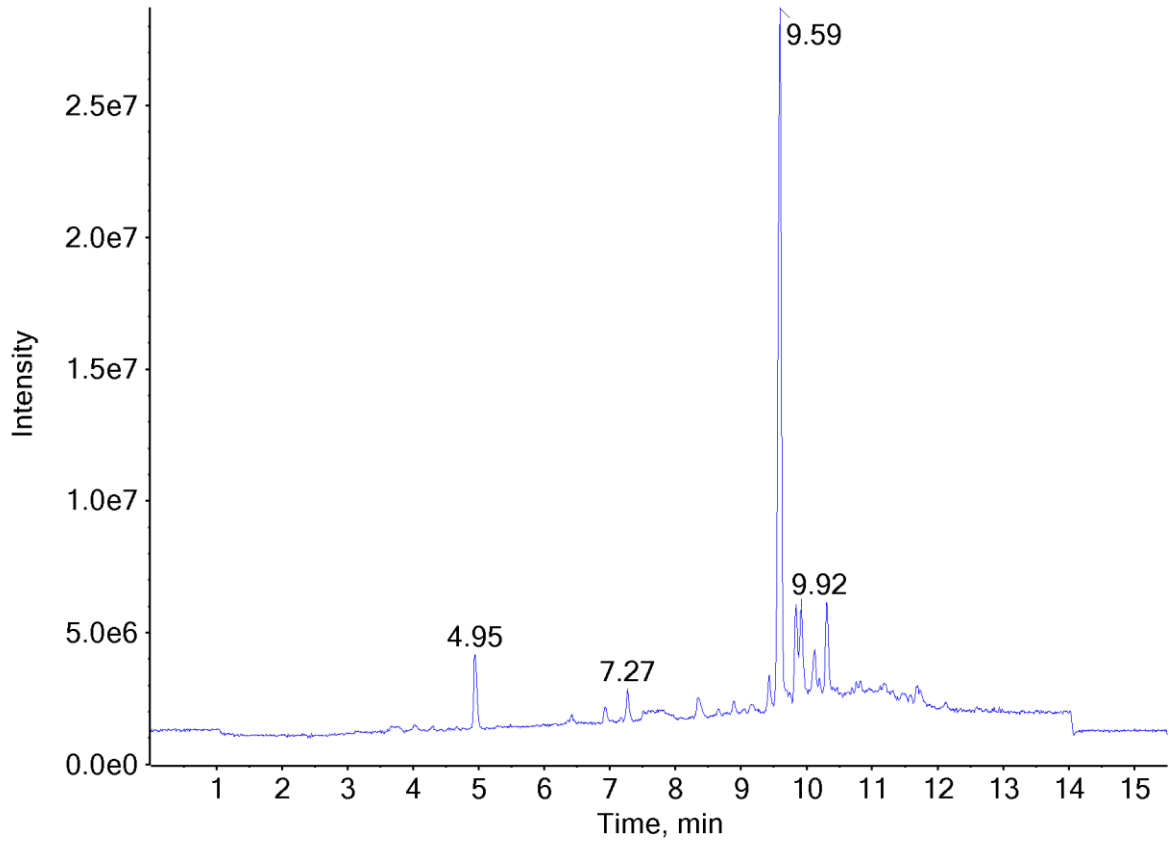
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-EDMB-PINACA



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

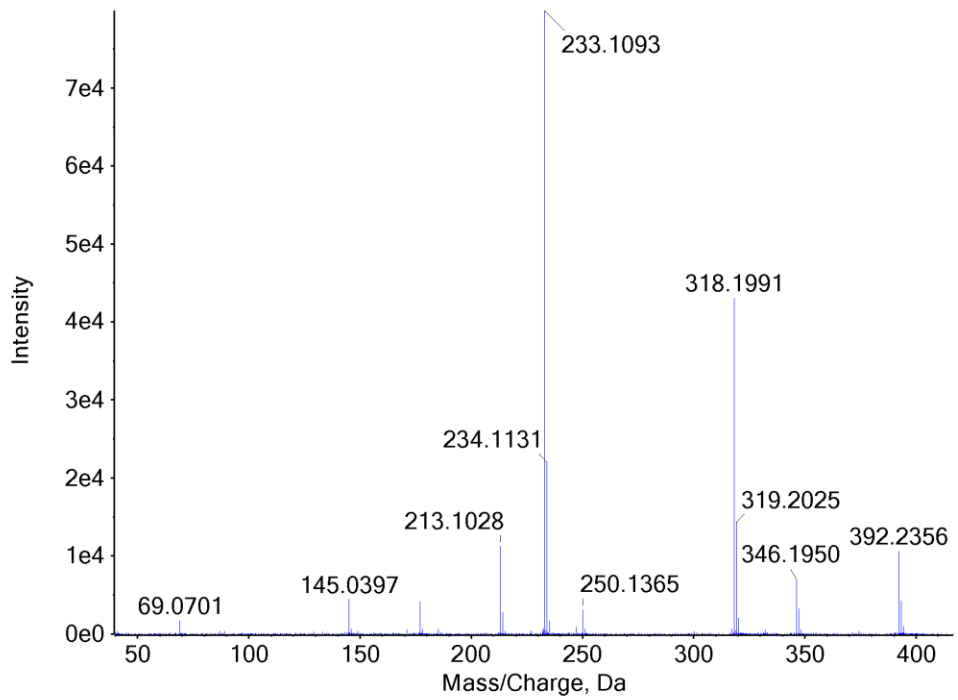
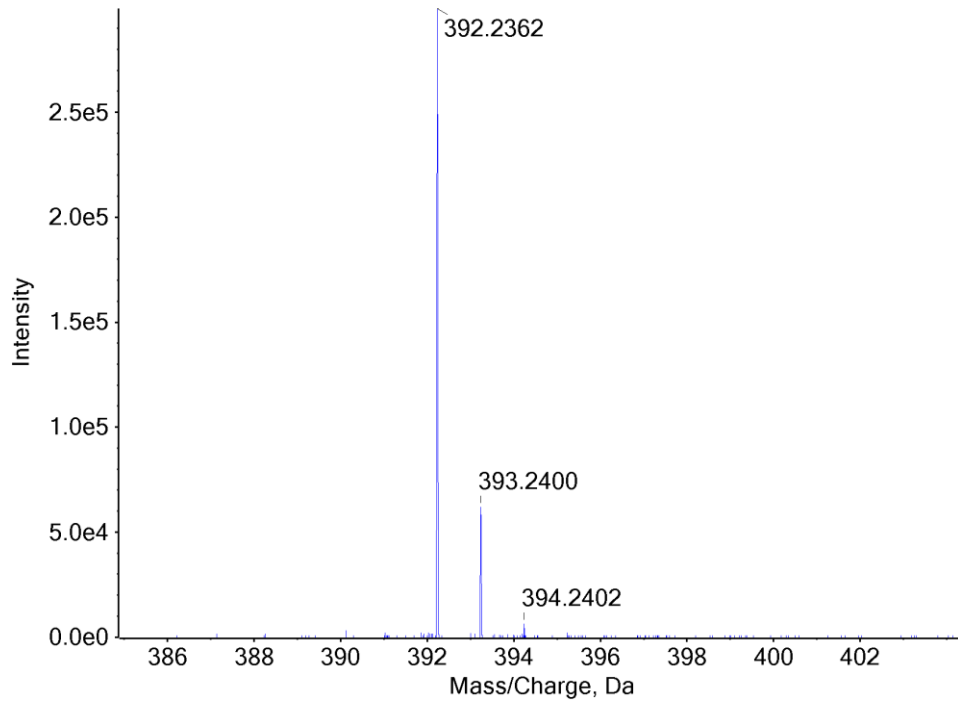
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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)

Chromatogram: 5F-EDMB-PINACA



*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

<u>Date</u>	<u>Revision</u>
05/18/2018	Added “Sample Type: Seized Material” to Page 1.
05/18/2018	Added “Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT” to Page 1 footer.