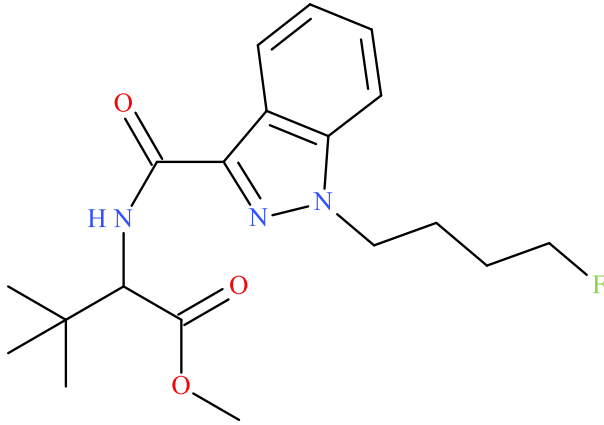


## 4F-MDMB-BINACA

Sample Type: **Seized Material**



Latest Revision: **January 11, 2019**

Date Received: **December 21, 2018**

Date of Report: **January 11, 2019**

### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	Methyl 2-[[1-(4-fluorobutyl)indazole-3-carbonyl]amino]-3,3-dimethyl-butanoate
<b>InChI String:</b>	InChI=1S/C19H26FN3O3/c1-19(2,3)16(18(25)26-4)21-17(24)15-13-9-5-6-10-14(13)23(22-15)12-8-7-11-20/h5-6,9-10,16H,7-8,11-12H2,1-4H3,(H,21,24)
<b>CFR:</b>	Not Scheduled (01/2019)
<b>CAS#</b>	Not Available
<b>Synonyms:</b>	4F-MDMB-BUTINACA
<b>Source:</b>	Department of Homeland Security
<b>Appearance:</b>	Off-White Solid Material

**Important Note:** All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.

**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 <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Base	C <sub>19</sub> H <sub>26</sub> FN <sub>3</sub> O <sub>3</sub>	363.4	363	364.2031

### 3. BRIEF DESCRIPTION

4F-MDMB-BINACA 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-MDMB-PINACA (5F-ADB) is a structurally similar compound and Schedule I substance in the United States.

### 4. ADDITIONAL RESOURCES

[https://www.policija.si/apps/nfl\\_response\\_web/0\\_Analytical\\_Reports\\_final/4F-MDMB-BINACA-ID-HIFS-010.pdf](https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/4F-MDMB-BINACA-ID-HIFS-010.pdf)

### 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

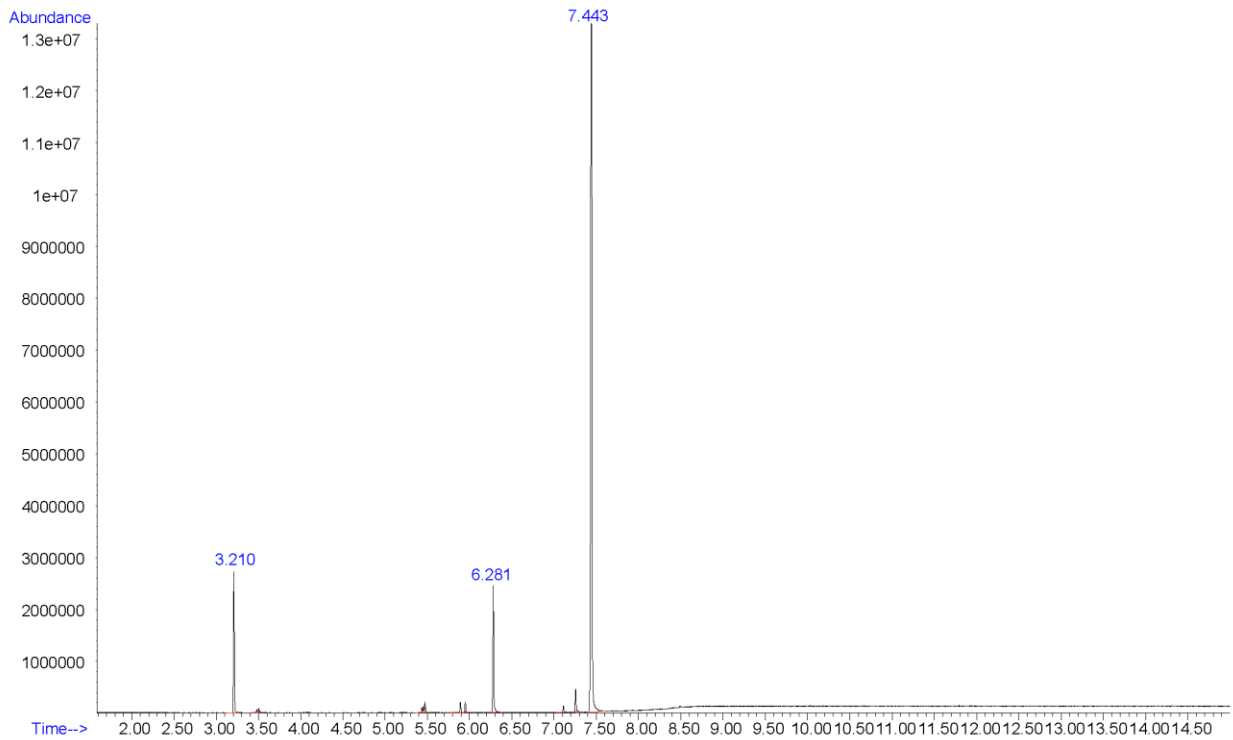
Injection Volume: 1 µL

**MS Parameters:** Mass Scan Range: 40-550 m/z

Threshold: 250

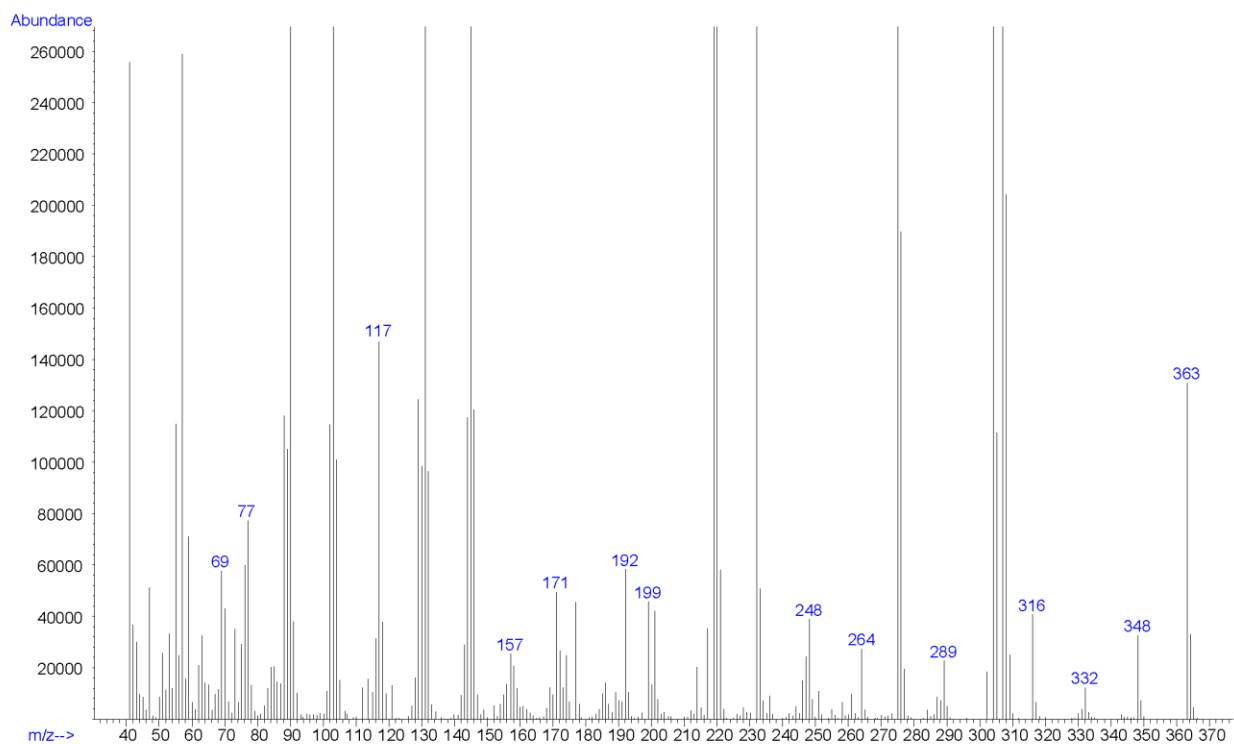
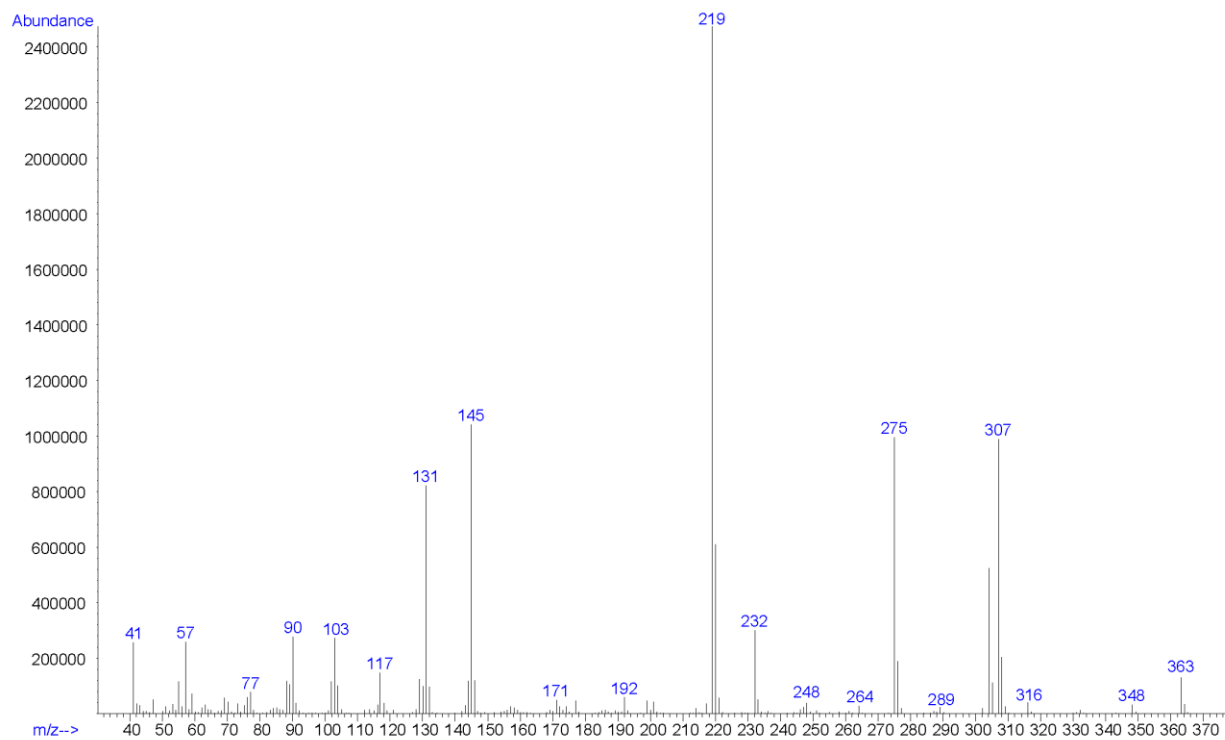
**Retention Time:** 7.443 min

**Chromatogram: 4F-MDMB-BINACA**



*Additional peaks present in chromatogram: internal standard 1 (3.210 min) and internal standard 2 (6.281 min)*

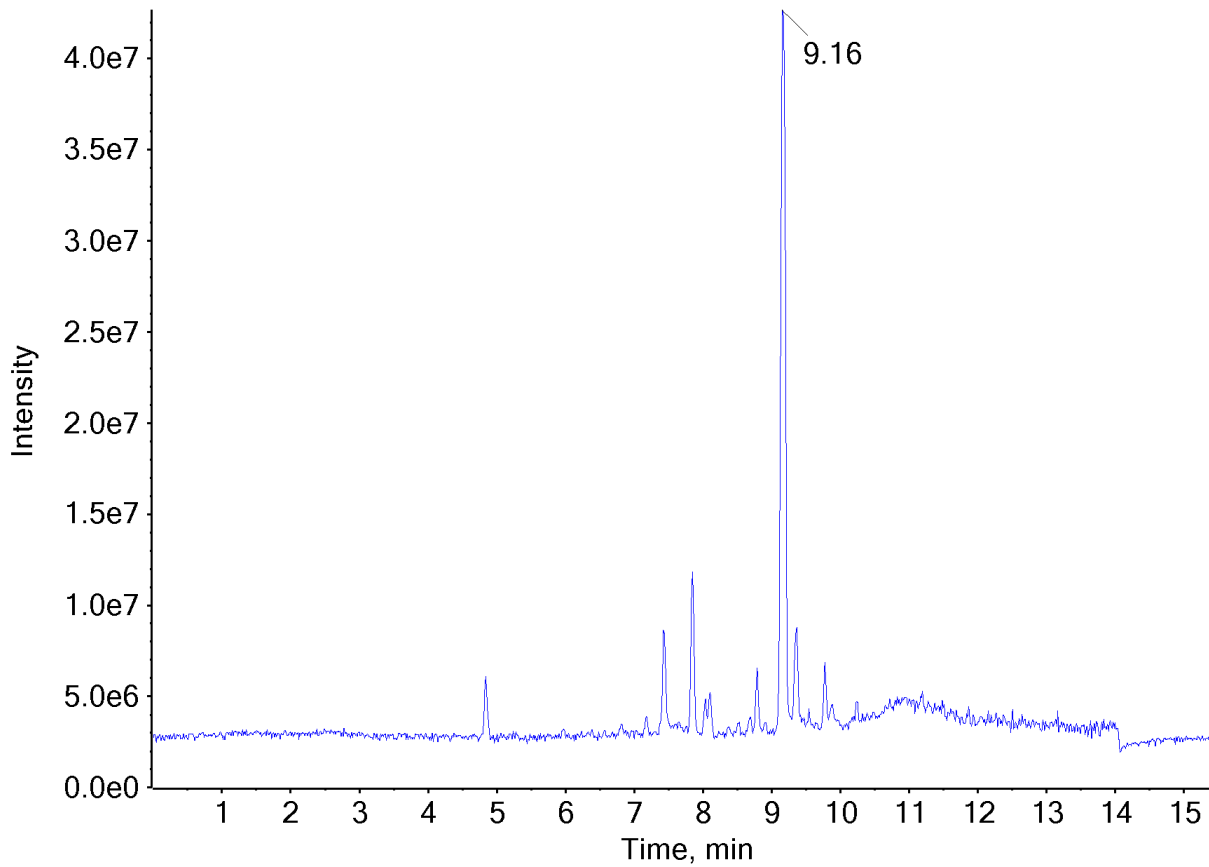
# EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4F-MDMB-BINACA



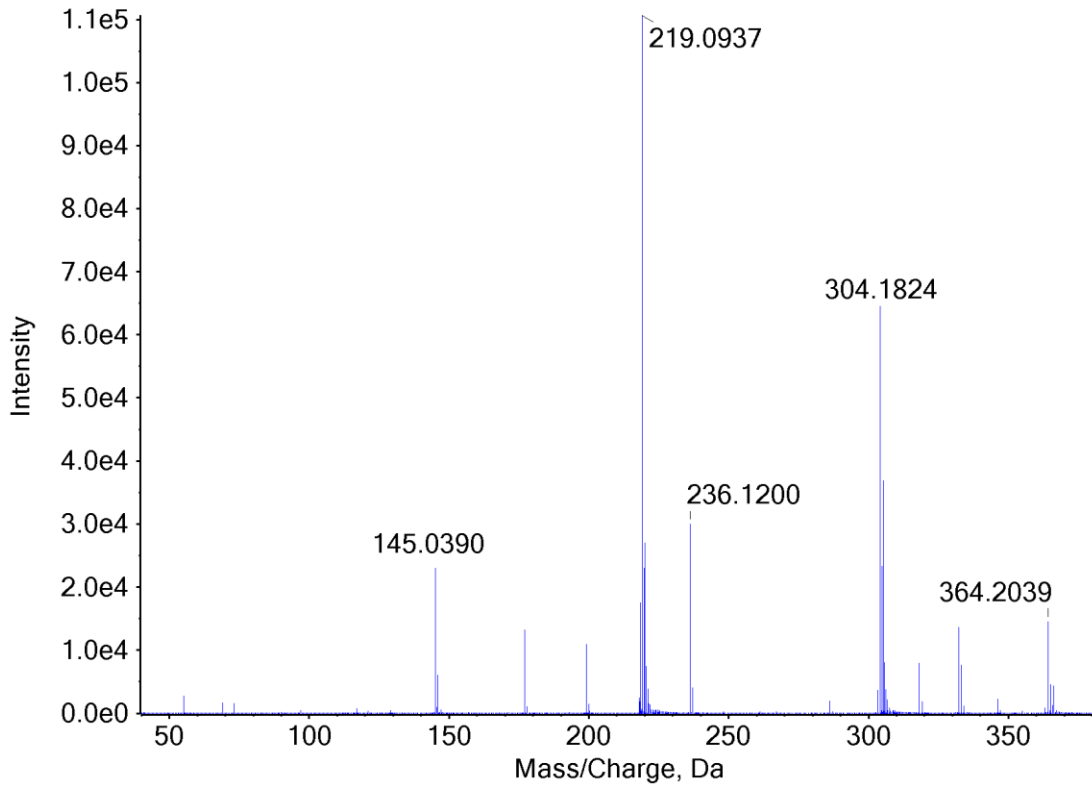
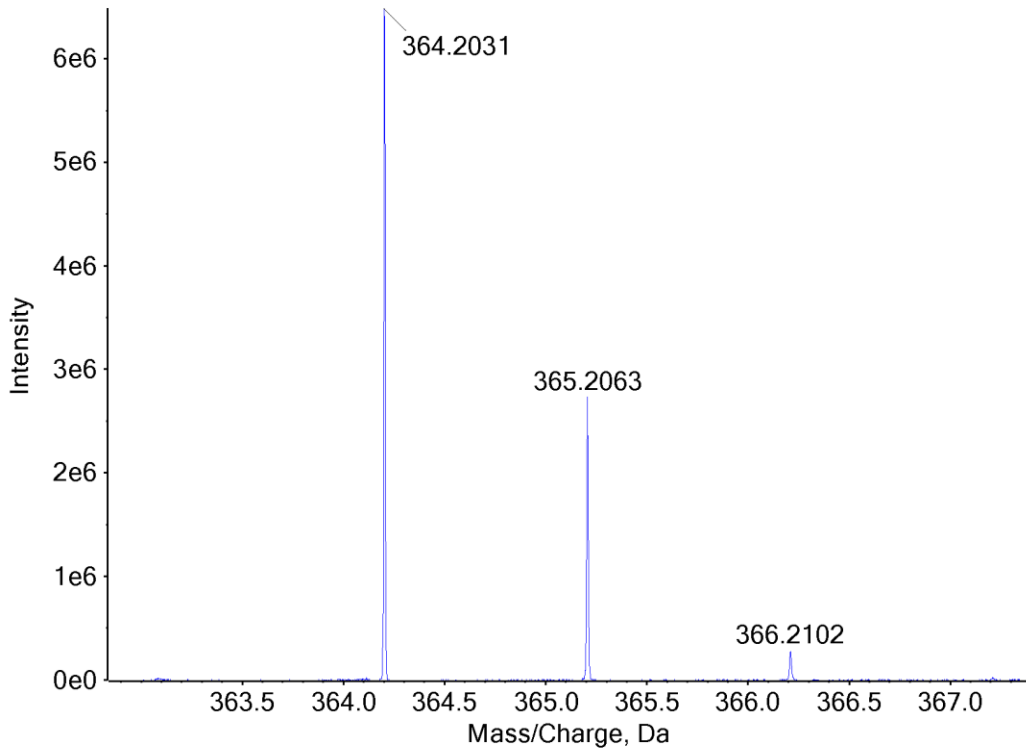
## 5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

<b>Testing Performed At:</b>	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
<b>Sample Preparation:</b>	1:100 dilution of acid/base extraction in mobile phase
<b>Instrument:</b>	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
<b>Column:</b>	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
<b>Mobile Phase:</b>	A: Ammonium formate (10 mM, pH 3.0) B: Methanol/acetonitrile (50:50) Flow rate: 0.4 mL/min
<b>Gradient:</b>	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
<b>Temperatures:</b>	Autosampler: 15 °C Column Oven: 30 °C Source Heater: 600 °C
<b>Injection Parameters:</b>	Injection Volume: 10 µL
<b>QTOF Parameters:</b>	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
<b>Retention Time:</b>	9.16 min

**Chromatogram: 4F-MDMB-BINACA**



**TOF MS (Top) and MS/MS (Bottom) Spectra: 4F-MDMB-BINACA**



### 5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

**Testing Performed At:** IteraMed™ (Doylestown, PA)

**Sample Preparation:** Dilute powder in CDCl<sub>3</sub>

**Instrument:** 300 MHz INOVA VARIAN Spectrometer

**Parameters:** Pulse Sequence: Proton

Solvent: CDCl<sub>3</sub>

Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

Delay between pulses: 1st delay, d1 = 1.000

#### <sup>1</sup>H NMR: 4F-MDMB-BINACA

<sup>1</sup>H NMR (300 MHz, CHLOROFORM-d) δ 8.35 (t, *J*=6.08 Hz, 1H), 7.54 (d, *J*=9.96 Hz, 1H), 7.38-7.46 (m, 2H), 7.23-7.31 (m, 1H), 4.73 (d, *J*=9.37 Hz, 1H), 4.56 (t, *J*=5.86 Hz, 1H), 4.38-4.51 (m, 3H), 3.72-3.80 (m, 3H), 2.06-2.18 (m, 2H), 1.65-1.81 (m, 2H), 1.05-1.14 (m, 9H), 0.95 (s, 1H), 0.00 (s, 1H)

