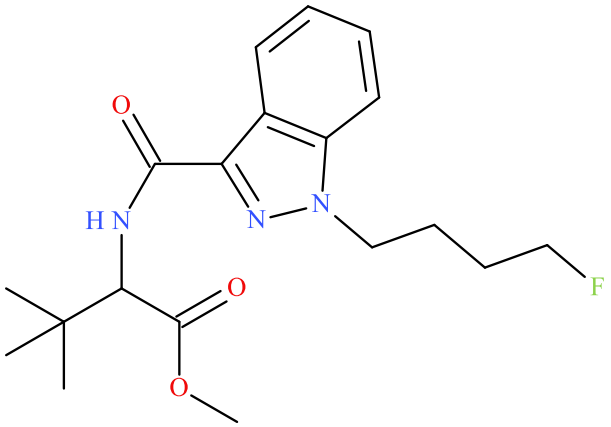
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

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

IUPAC Name:	Methyl 2-[[1-(4-fluorobutyl)indazole-3-carbonyl]amino]-3,3-dimethyl-butanoate
InChI String:	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)
CFR:	Not Scheduled (01/2019)
CAS#	Not Available
Synonyms:	4F-MDMB-BUTINACA
Source:	Department of Homeland Security
Appearance:	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 $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{19}H_{26}FN_3O_3$	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

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

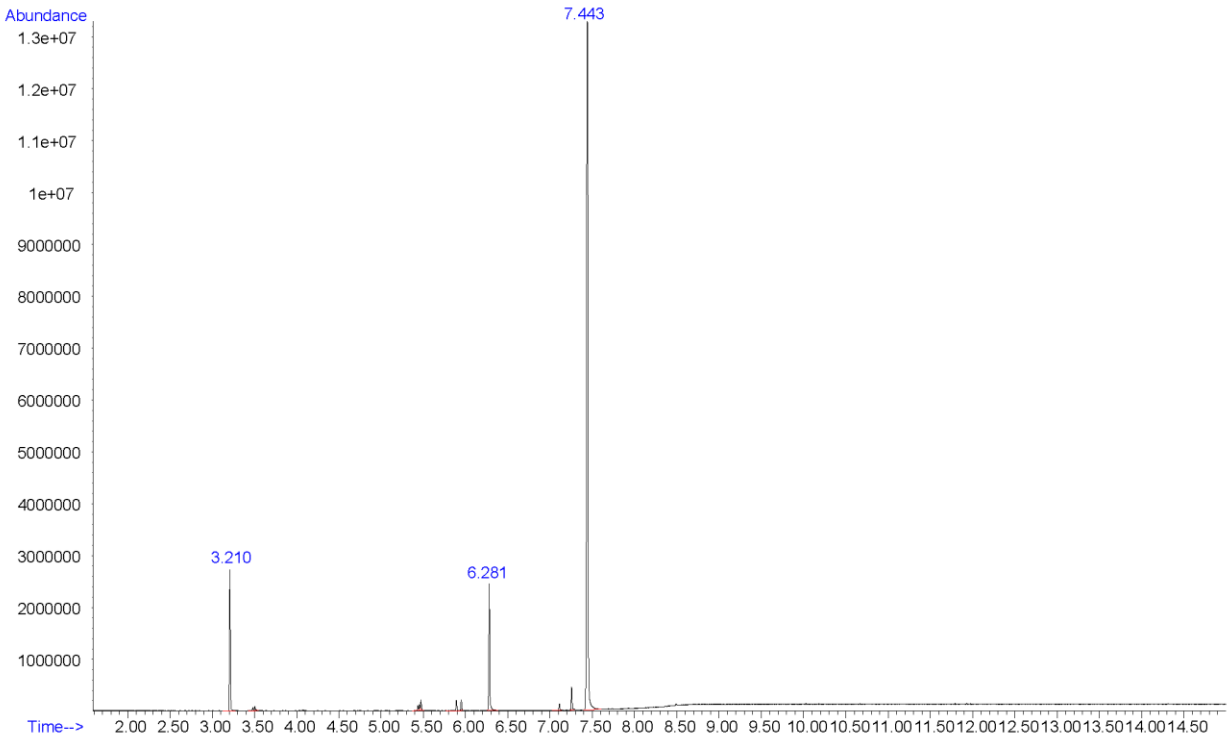
Transfer Line: 300 °C

MS Source: 230 °C

MS Quad: 150 °C

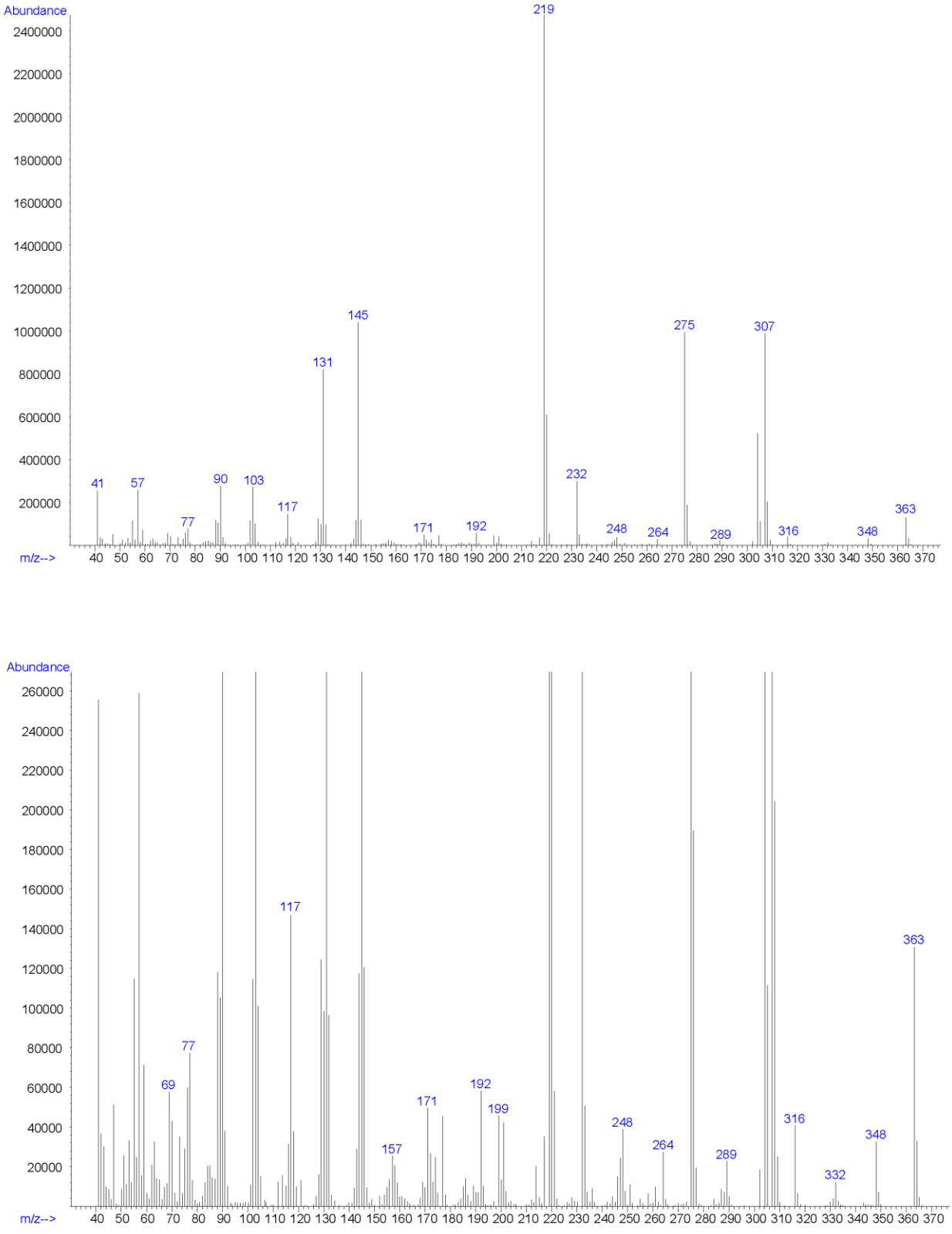
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	7.443 min

Chromatogram: 4F-MDMB-BINACA



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

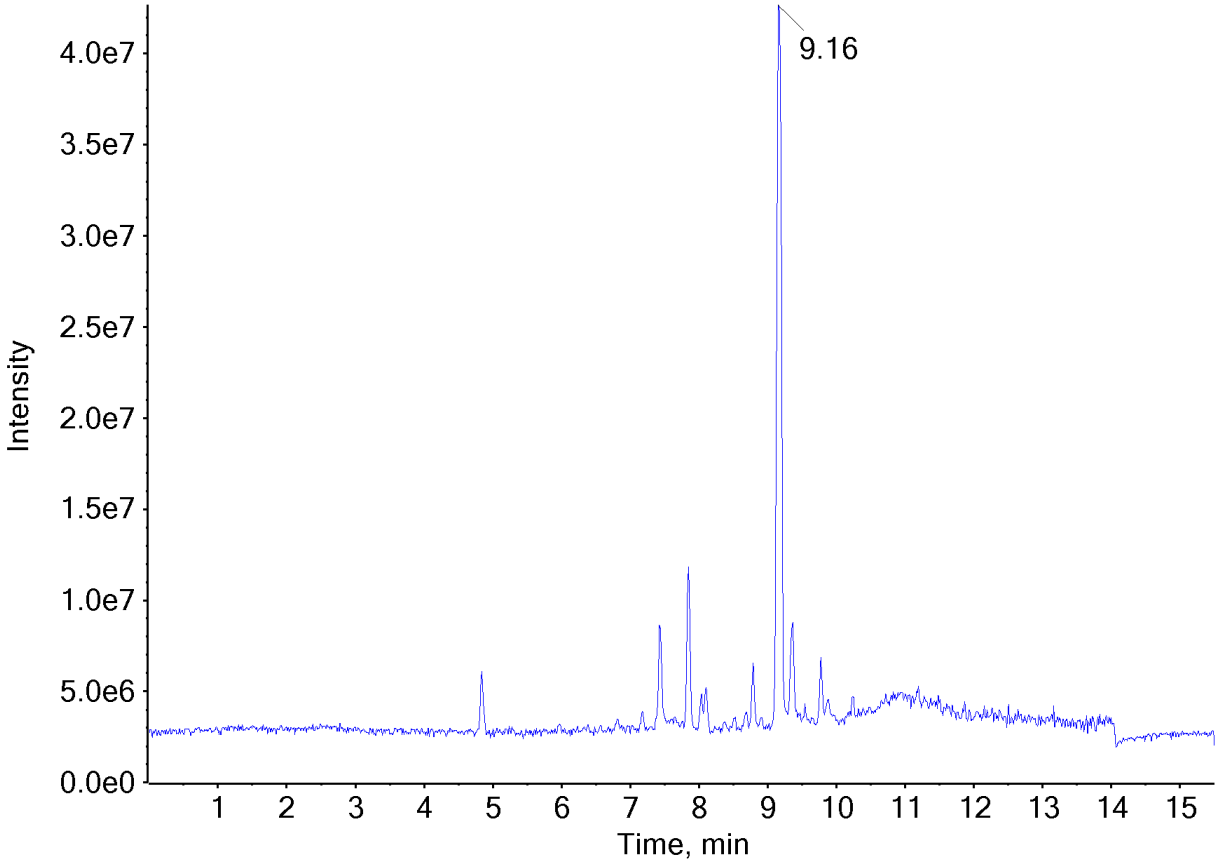
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4F-MDMB-BINACA



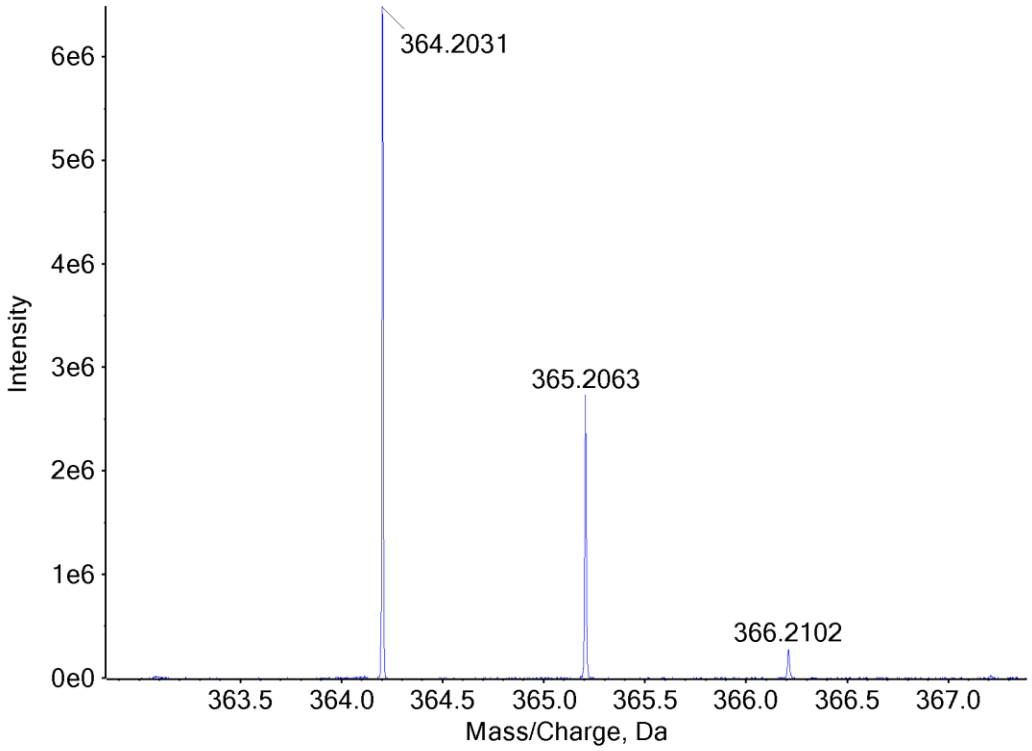
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

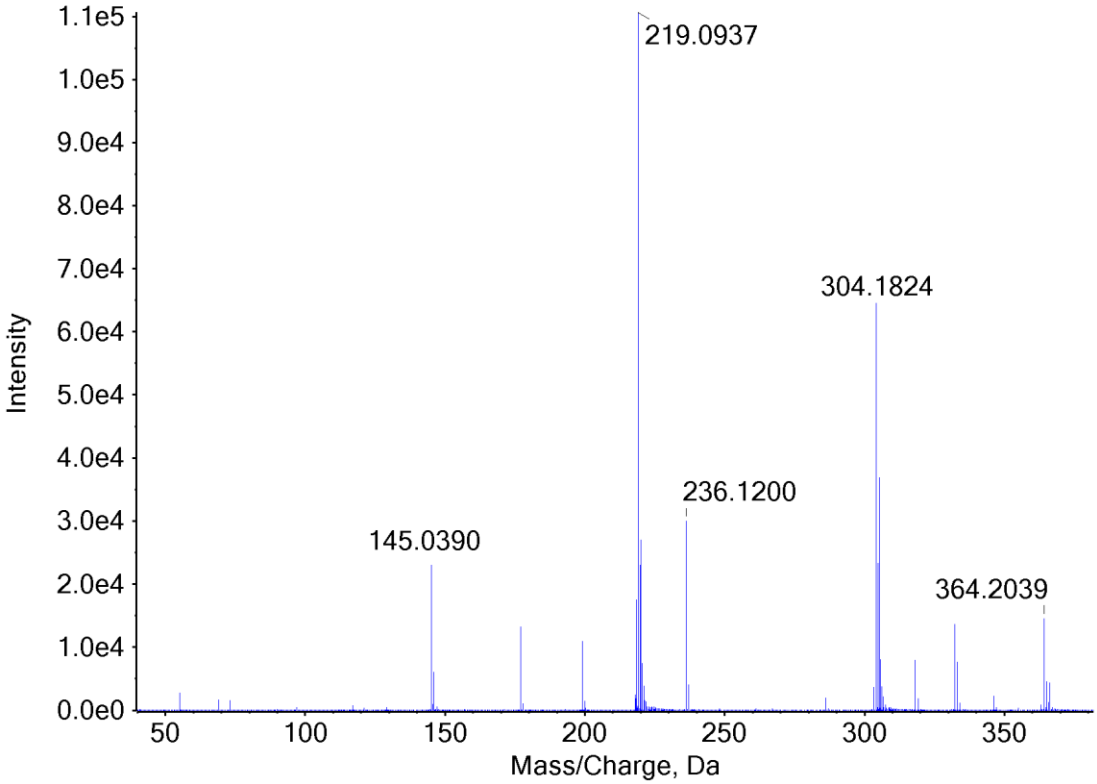
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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:	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 $CDCl_3$

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters: Pulse Sequence: Proton

Solvent: $CDCl_3$

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

Delay between pulses: 1st delay, d1 = 1.000

^{1}H NMR: 4F-MDMB-BINACA

^{1}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)