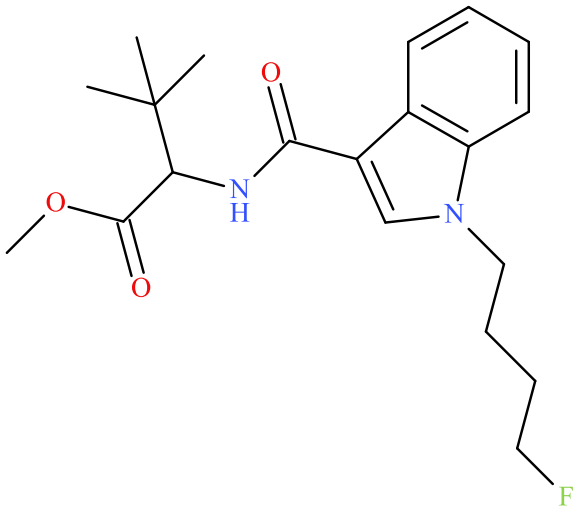
4F-MDMB-BICA

Sample Type: **Seized Material**



Latest Revision: **July 1, 2020**

Date Received: **May 14, 2020**

Date of Report: **July 1, 2020**

1. GENERAL INFORMATION

IUPAC Name:	Methyl 2-[[1-(4-fluorobutyl)indole-3-carbonyl]amino]-3,3-dimethyl-butanoate
InChI String:	InChI=1S/C20H27FN2O3/c1-20(2,3)17(19(25)26-4)22-18(24)15-13-23(12-8-7-11-21)16-10-6-5-9-14(15)16/h5-6,9-10,13,17H,7-8,11-12H2,1-4H3,(H,22,24)
CFR:	Not Scheduled (07/2020)
CAS#	Not Available
Synonyms:	4-fluoro MDMB-BICA, 4F-MDMB-BUTICA
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) 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	$C_{20}H_{27}FN_2O_3$	362.4	362	363.2078

3. BRIEF DESCRIPTION

4F-MDMB-BICA 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. 4F-MDMB-BINACA and 5F-MDMB-PICA are structurally similar synthetic cannabinoids. 5F-MDMB-PICA is explicitly a Schedule I substance in the United States; 4F-MDMB-BINACA and 4F-MDMB-BICA are not explicitly scheduled but may be considered analogues of other Schedule I substances.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/31075/4-fluoro-mdmb-butica

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

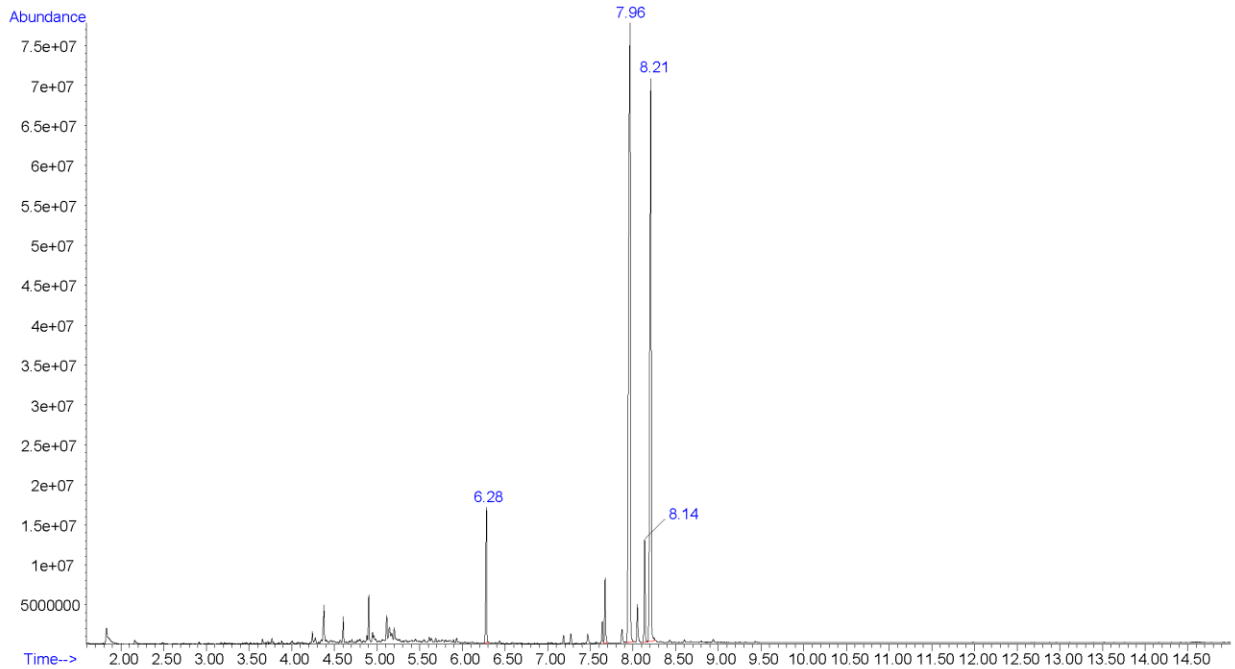
MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

Retention Time: 7.96 min

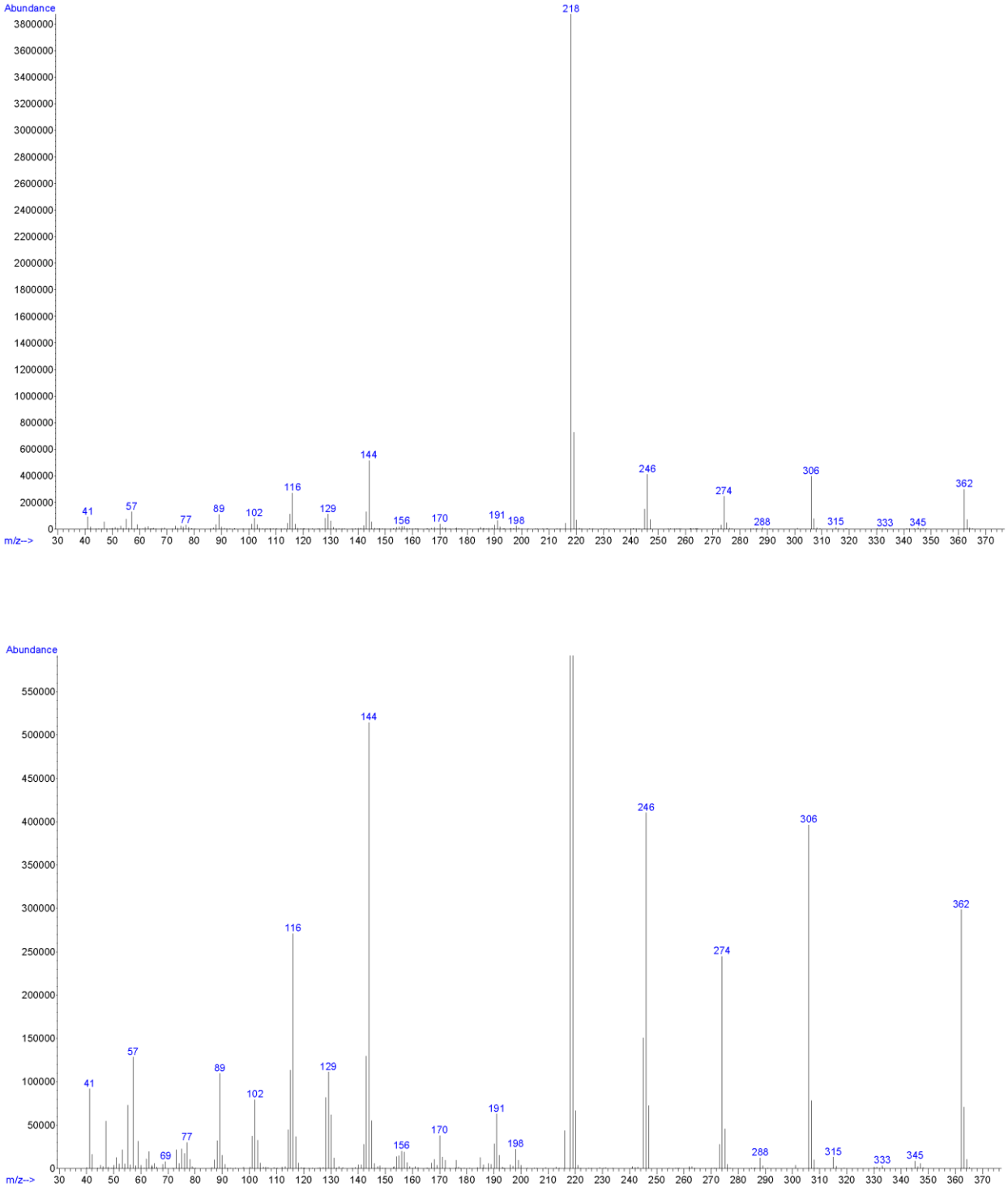
Standard Comparison: Reference material for 4F-MDMB-BICA (Batch: 0589507-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 4F-MDMB-BICA based on retention time (7.96 min) and mass spectral data. (https://www.caymanchem.com/product/31075/4-fluoro-mdmb-butica)

Chromatogram: 4F-MDMB-BICA



Additional peaks present in chromatogram: internal standard (6.28 min), 5F-MDMB-PICA (8.14 min), and 5F-EMB-PICA (8.21 min)

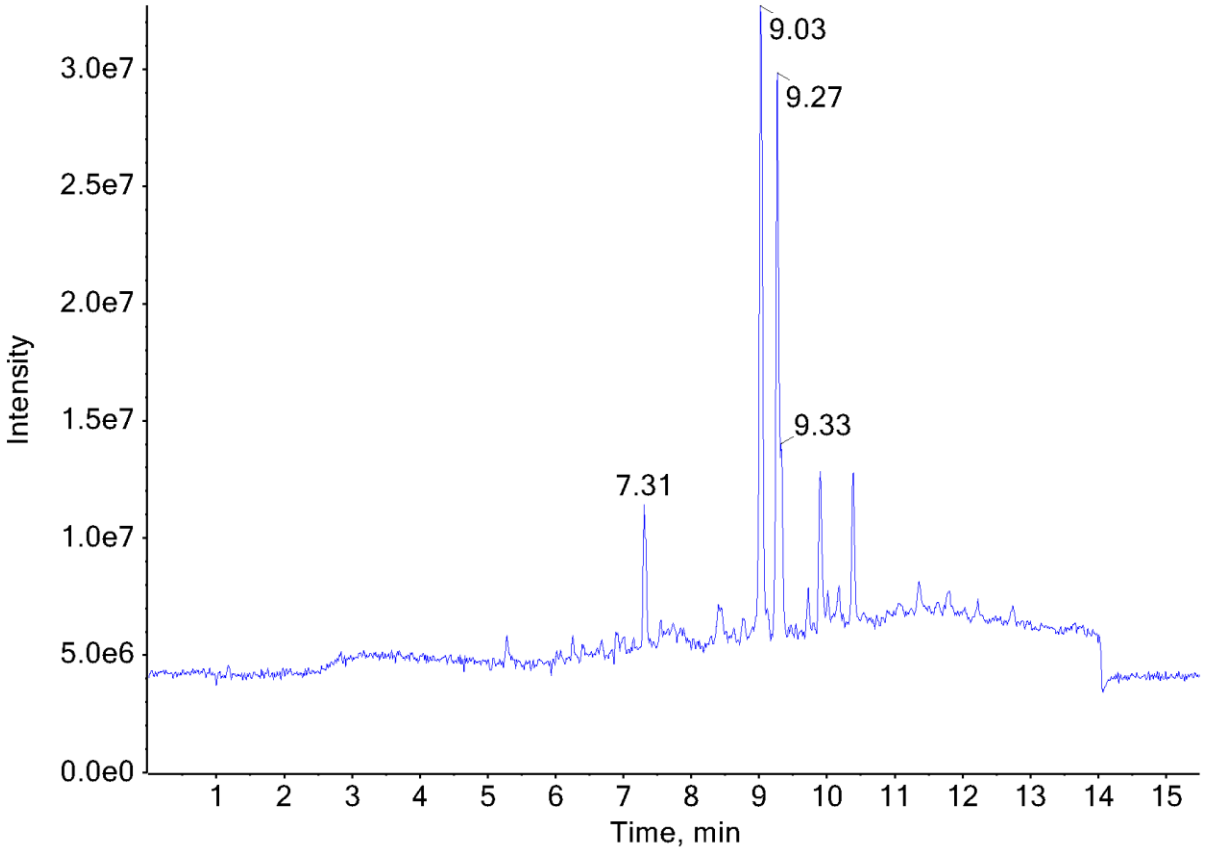
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4F-MDMB-BICA



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:	9.03 min
Standard Comparison:	Reference material for 4F-MDMB-BICA (Batch: 0589507-1) 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-MDMB-BICA based on retention time (9.04 min) and mass spectral data. (https://www.caymanchem.com/product/31075/4-fluoro-mdmb-butica)

Chromatogram: 4F-MDMB-BICA



Additional peaks present in chromatogram: internal standard (7.31 min), 5F-EMB-PICA (9.27 min), and 5F-MDMB-PICA (9.33 min)

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