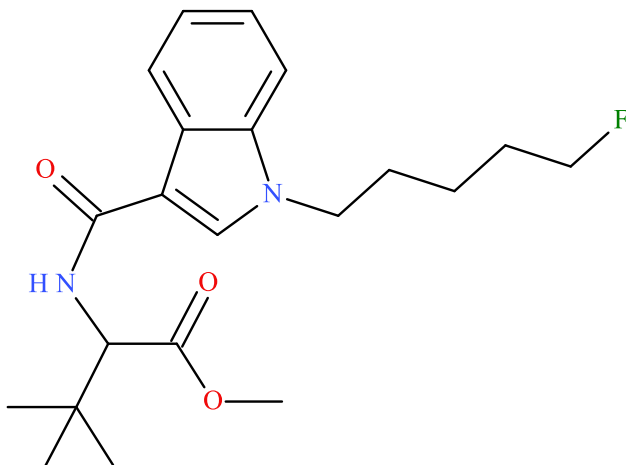


5F-MDMB-PICA

Sample Type: **Seized Material &
Biological Fluid**



Latest Revision: **July 31, 2018**

Date of Report: **July 31, 2018**

Earliest Identification: **November 2017
(Seized Material)**

1. GENERAL INFORMATION

IUPAC Name:	Methyl 2-[[1-(5-fluoropentyl)indole-3-carbonyl]amino]-3,3-dimethyl-butanoate
InChI String:	InChI=1S/C21H29FN2O3/c1-21(2,3)18(20(26)27-4)23-19(25)16-14-24(13-9-5-8-12-22)17-11-7-6-10-15(16)17/h6-7,10-11,14,18H,5,8-9,12-13H2,1-4H3,(H,23,25)
CFR:	Not Scheduled (07/2018)
CAS#	1971007-88-1
Synonyms:	5-Fluoro MDMB-PICA, 5F-MDMB-2201, MDMB-2201
Source:	Department of Homeland Security (Seized Material) NMS Labs – Toxicology Department (Biological Fluid)
Appearance:	Yellow Solid Material (Seized Material)

Important Note: All identifications were made based on evaluation of analytical data (GC-MS and/or LC-QTOF) in comparison to the analysis of acquired reference material.

Report Prepared By: Alex J. Krotulski, MSFS, Amanda LA Mohr, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Molecular Ion [M ⁺]	Exact Mass [M+H] ⁺
5F-MDMB-PICA	C ₂₁ H ₂₉ FN ₂ O ₃	376.5	376	377.2235

3. BRIEF DESCRIPTION

5F-MDMB-PICA 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. SAMPLE HISTORY (BIOLOGICAL FLUID)

5F-MDMB-PICA has been identified in nine cases since January 2018. The geographical and demographical breakdown is below:

Geographical Location: Pennsylvania (n=4), New York (n=2), Louisiana (n=1), Indiana (n=1), Texas (n=1)

Gender: Male (n=5), Female (n=1)

Age Range: 17 – 55 years (n=5)

Biological Sample: Blood (n=7), Femoral Blood (n=2)

Date of First Collection: January 7th, 2018

Date of First Receipt: May 9th, 2018

Additional Cannabinoids: 5F-ADB / 5F-MDMB-PINACA (n=3)
FUB-AMB / MMB-FUBINACA (n=3)
MDMB-FUBINACA (n=1)
THC (n=1)

5. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/20803>

<https://www.ncbi.nlm.nih.gov/pubmed/28371476>

<https://www.ncbi.nlm.nih.gov/pubmed/28214755>

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/5F-MDMB-PICA-ID-1777-17_report.pdf

6. QUALITATIVE DATA

6.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

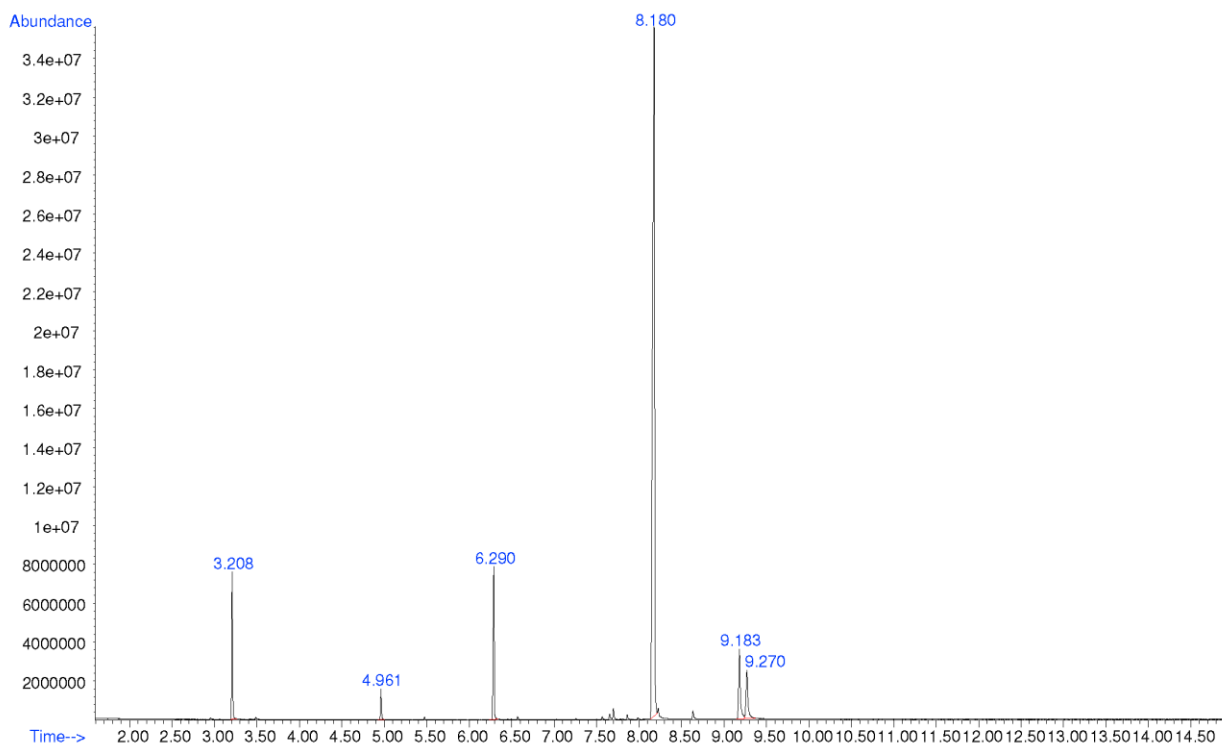
Testing Performed At:	NMS Labs (Willow Grove, PA)
Sample Preparation:	Acid/Base extraction of seized material
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Zebtron™ Inferno™ ZB-35HT (15 m x 250 μm x 0.25 μm)
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C Transfer Line: 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:	8.180 min

Standard Comparison:

Reference material for 5F-MDMB-PICA (Batch: 0494659-8A) 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-MDMB-PICA, based on retention time (8.166 min) and mass spectral data.

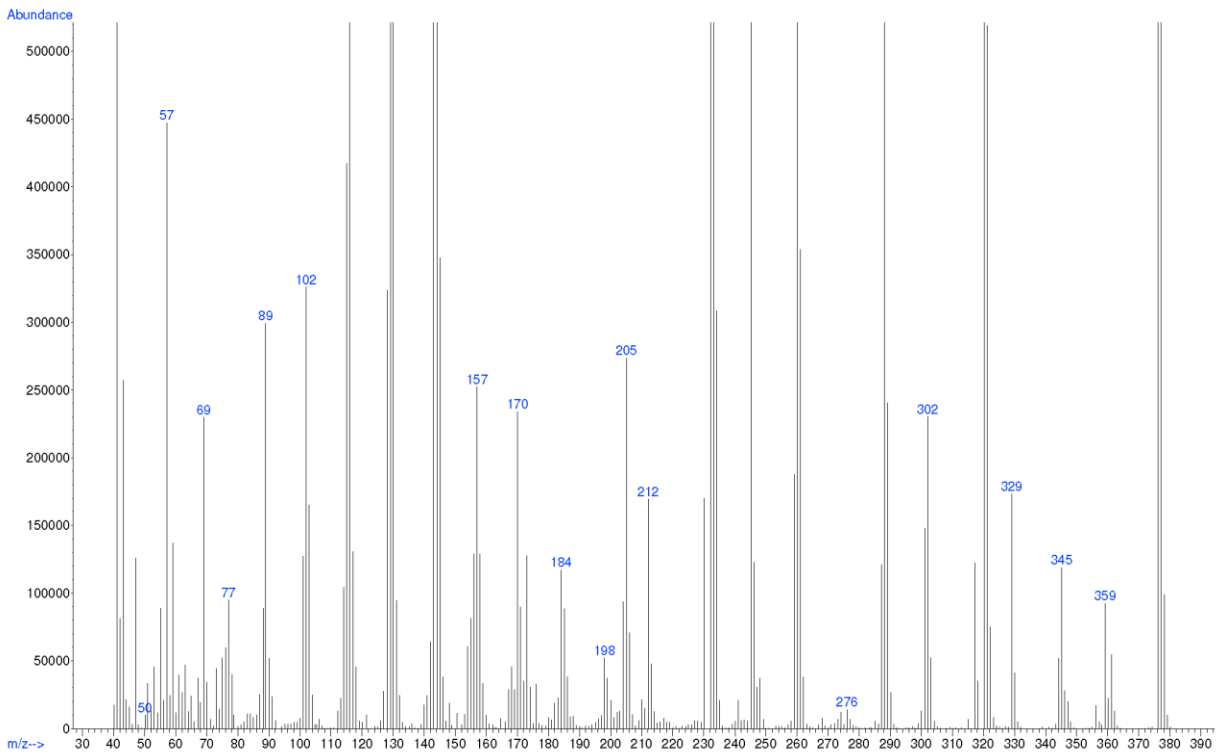
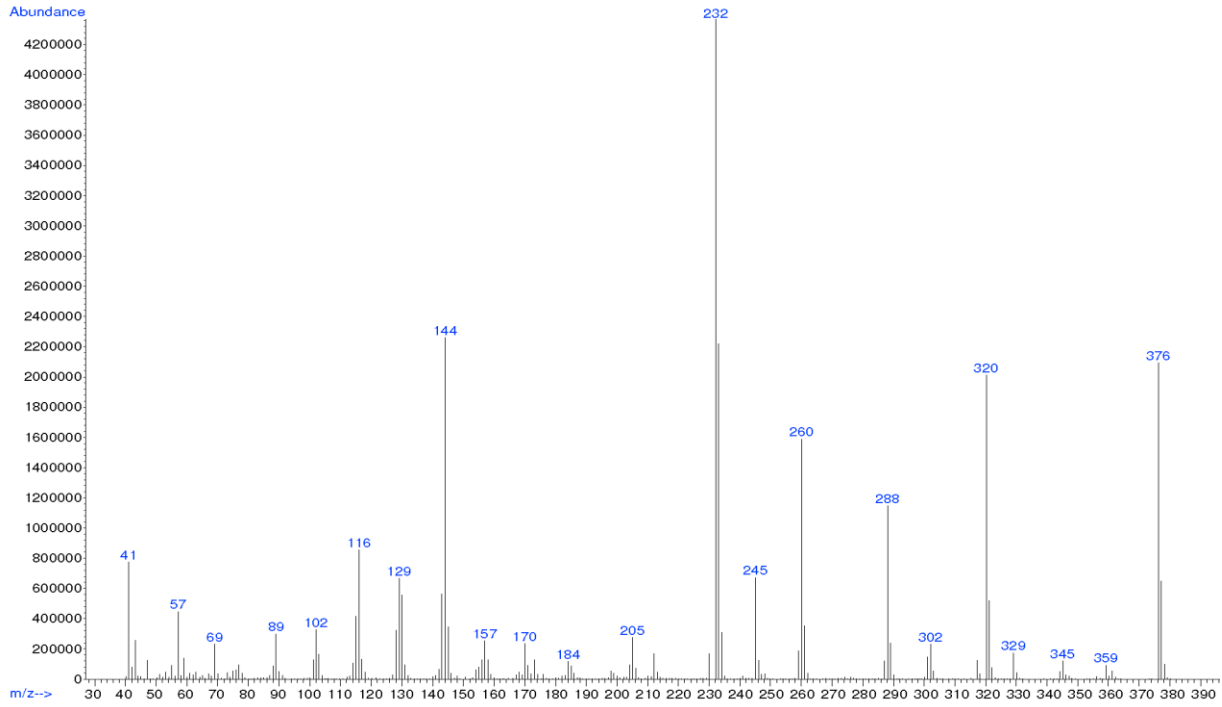
<https://www.caymanchem.com/product/20803>

Chromatogram: 5F-MDMB-PICA



Additional peaks present in chromatogram: internal standard 1 (3.208 min), not a controlled substance (4.961 min), internal standard 2 (6.290 min), not a controlled substance (9.183 min), not a controlled substance (9.270 min)

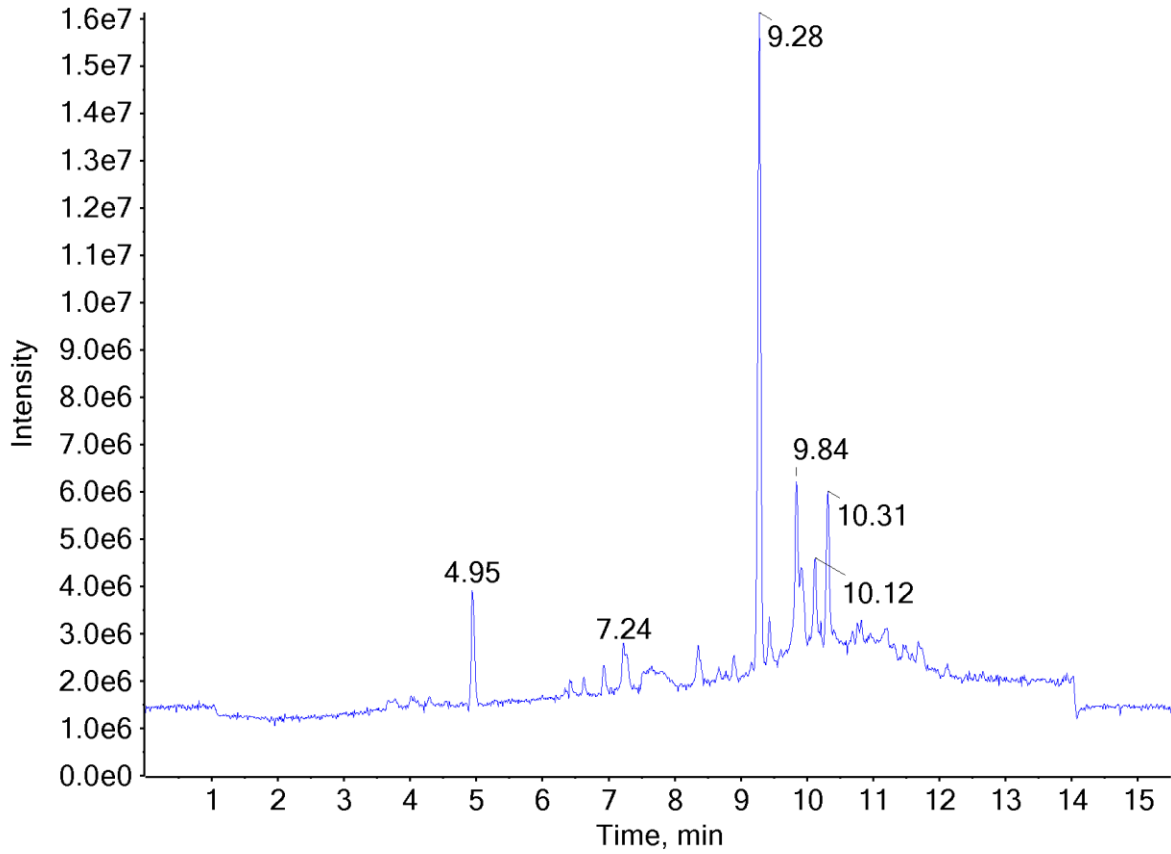
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-MDMB-PICA



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

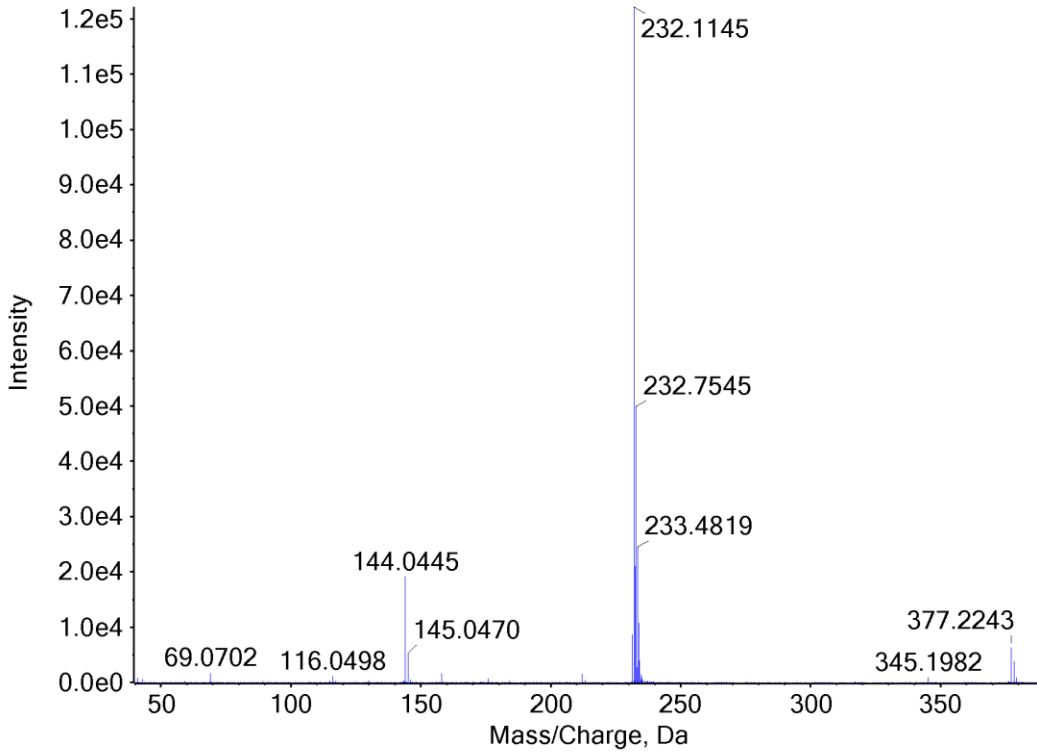
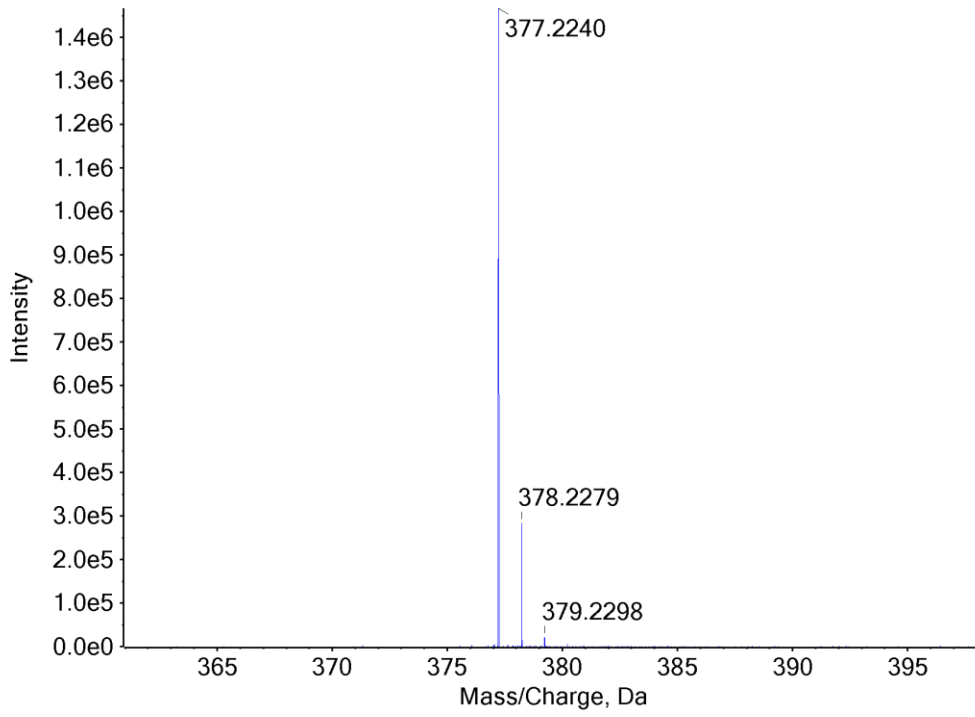
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase (seized material)
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® 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:	9.28 min
Standard Comparison:	Reference material for 5F-MDMB-PICA (Batch: 0494659-8A) 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-MDMB-PICA, based on retention time (9.27 min) and mass spectral data. (https://www.caymanchem.com/product/20803)

Chromatogram: 5F-MDMB-PICA



Additional peaks present in chromatogram: internal standard 1 (4.95 min), internal standard 2 (7.24 min), not a controlled substance (9.84 min), not a controlled substance (10.12 min), not a controlled substance (10.31 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: 5F-MDMB-PICA



7. FUNDING

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