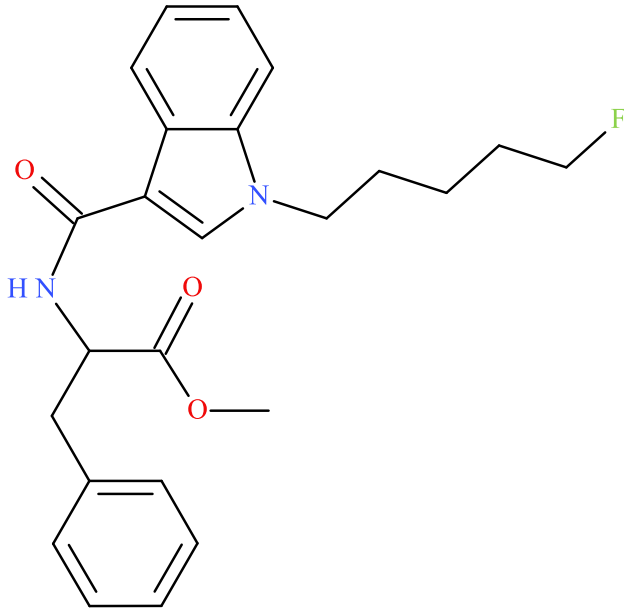


5F-MPP-PICA



Latest Revision: **February 13, 2019**

Date Received: **November 2, 2018**

Date of Report: **February 12, 2019**

1. GENERAL INFORMATION

IUPAC Name:	Methyl 2-[[1-(5-fluoropentyl)indole-3-carbonyl]amino]-3-phenylpropanoate
InChI String:	InChI=1S/C24H27FN2O3/c1-30-24(29)21(16-18-10-4-2-5-11-18)26-23(28)20-17-27(15-9-3-8-14-25)22-13-7-6-12-19(20)22/h2,4-7,10-13,17,21H,3,8-9,14-16H2,1H3,(H,26,28)
CFR:	Not Scheduled (02/2019)
CAS#	Not Available
Synonyms:	5-Fluoro MPP-PICA, MPHP-2201
Source:	Department of Homeland Security
Appearance:	Orange 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 ₂₄ H ₂₇ FN ₂ O ₃	410.48	410	411.2078

3. BRIEF DESCRIPTION

5F-MPP-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-MDMB-PICA and PX-1 (5F-APP-PICA) are structurally similar synthetic cannabinoids. On December 28, 2018, the Drug Enforcement Administration published a notice of intent to place 5F-MDMB-PICA as a Schedule I substance in the United States.

4. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/MPhP-2201-ID1952-18_report.pdf

<https://www.caymanchem.com/product/25916>

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

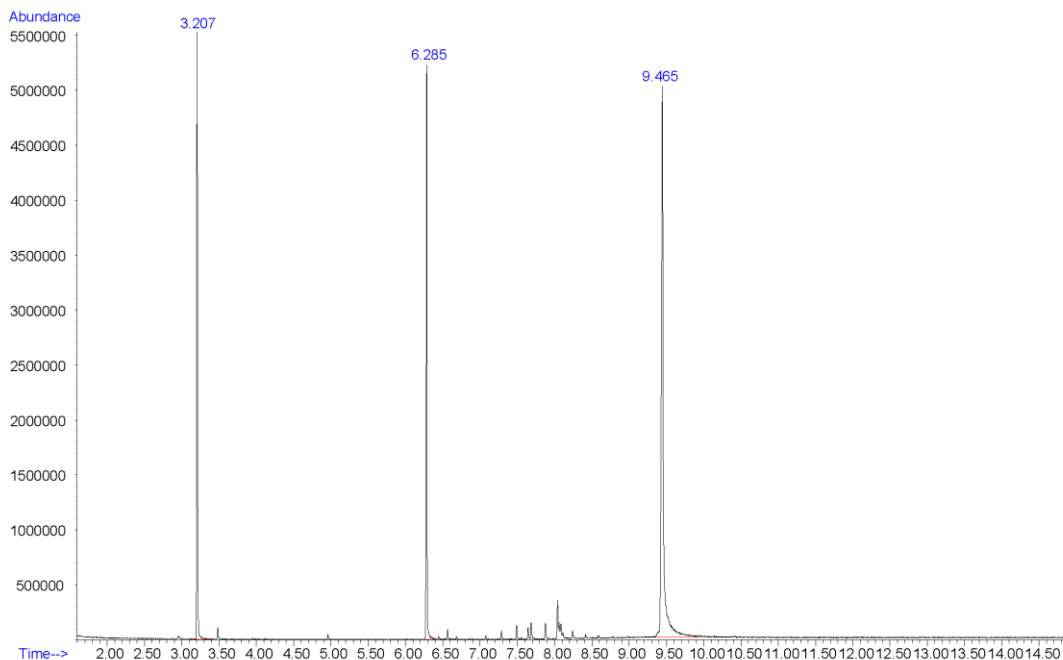
Threshold: 250

Retention Time: 9.465 min

Standard Comparison: Reference material for 5F-MPP-PICA (Batch: 0543629-3) 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-MPP-PICA, based on retention time (9.450 min) and mass spectral data.

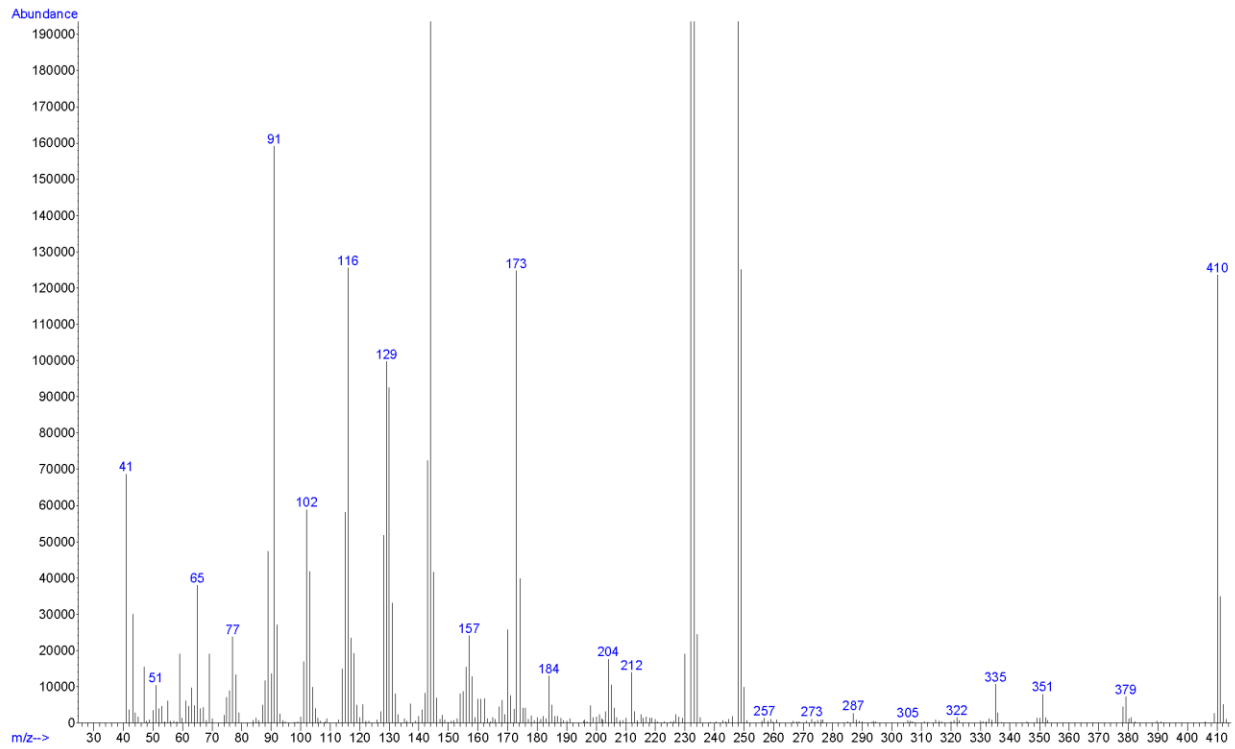
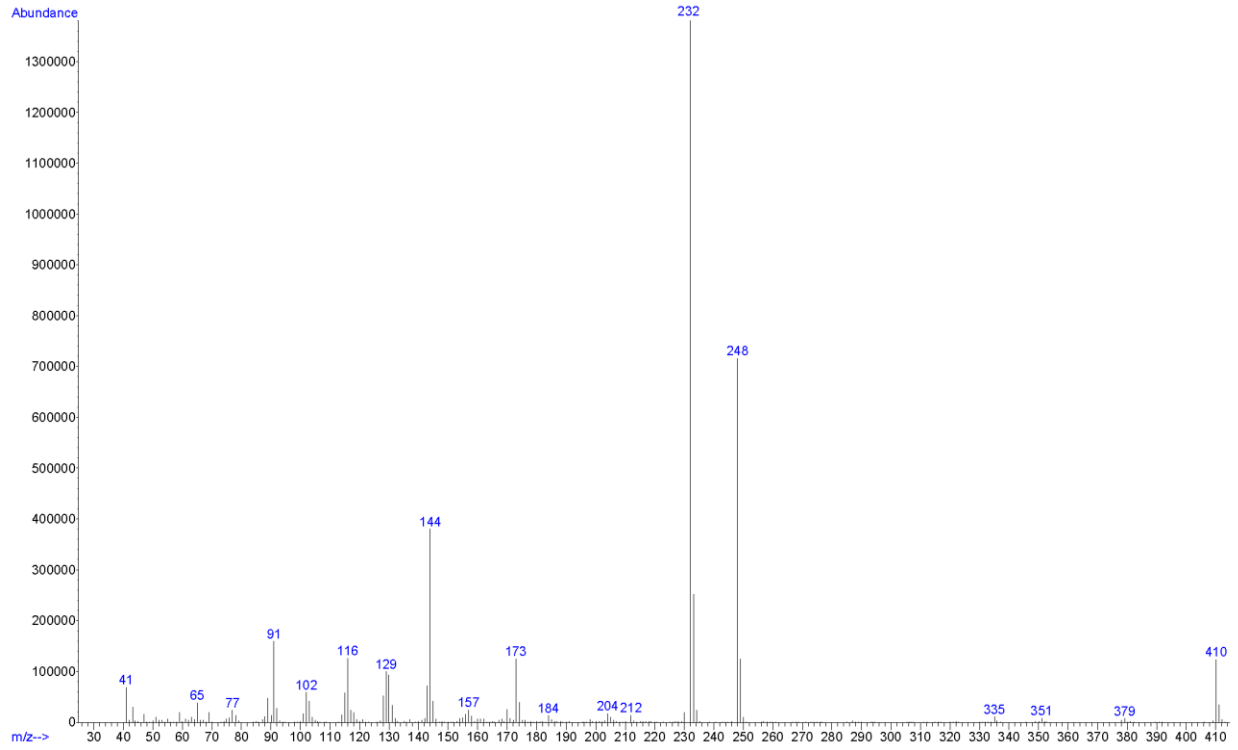
<https://www.caymanchem.com/product/25916>

Chromatogram: 5F-MPP-PICA



Additional peaks present in chromatogram: internal standards (3.207 min and 6.285 min)

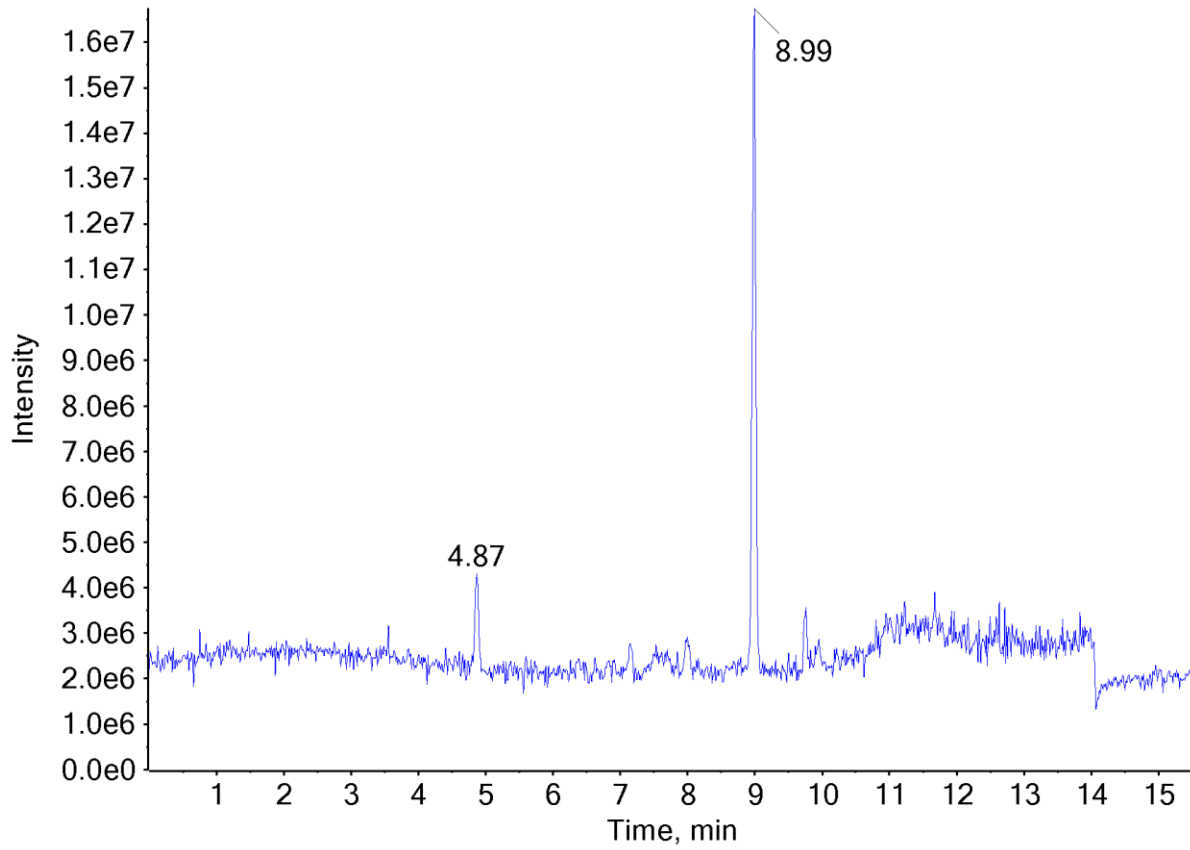
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-MPP-PICA



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

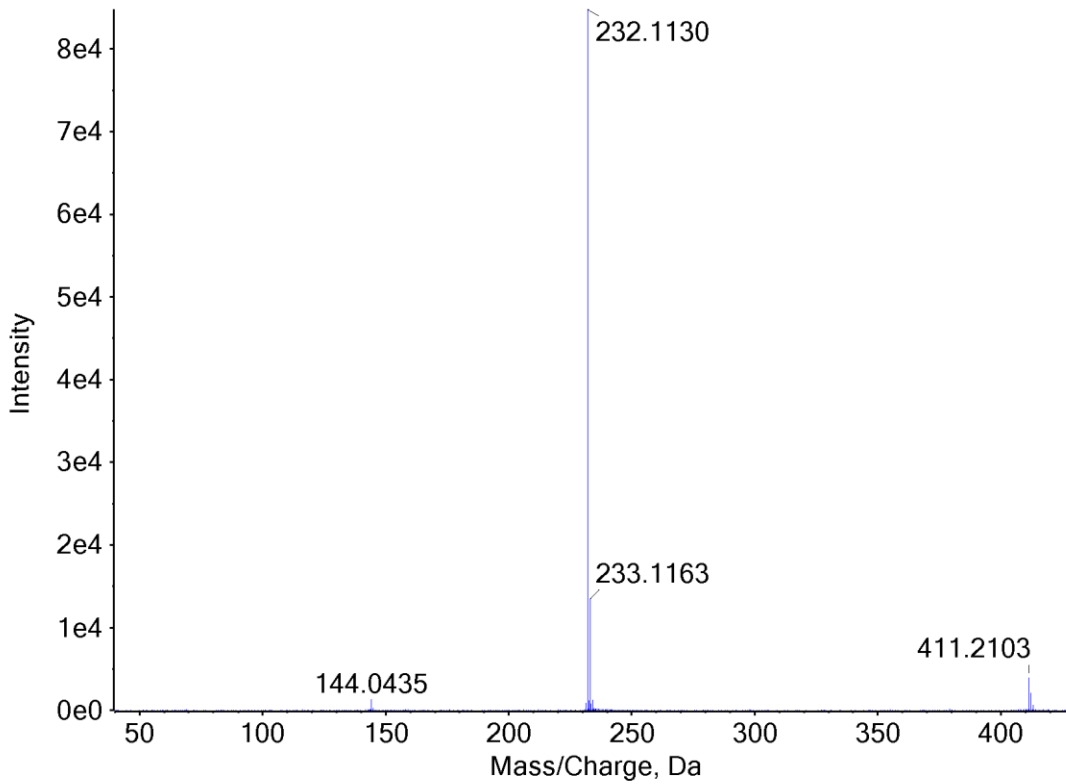
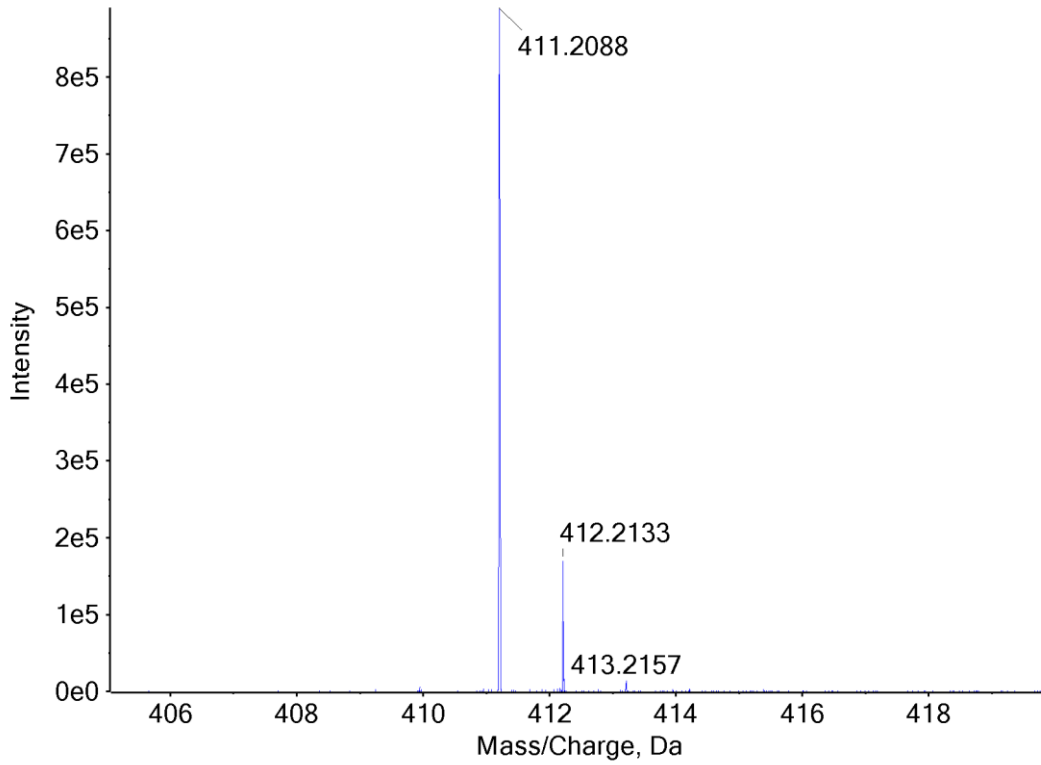
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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:	8.99 min
Standard Comparison:	Reference material for 5F-MPP-PICA (Batch: 0543629-3) 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-MPP-PICA, based on retention time (9.16 min) and mass spectral data. (https://www.caymanchem.com/product/25916)

Chromatogram: 5F-MPP-PICA



Additional peak present in chromatogram: internal standard (4.87 min)

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



6. REVISION HISTORY

<u>Date</u>	<u>Revision</u>
02/13/2018	Brief description was modified to include “notice of intent” for scheduling of 5F-MDMB-PICA.