

# **5F-MPP-PICA**

H N O

Latest Revision: **February 12, 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-phenyl-

propanoate

**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.

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#### 2. CHEMICAL AND PHYSICAL DATA

## 2.1 CHEMICAL DATA

Form	Chemical	Molecular	Molecular Ion	Exact Mass
	Formula	Weight	[M <sup>+</sup> ]	[M+H] <sup>+</sup>
Base	C <sub>24</sub> H <sub>27</sub> FN <sub>2</sub> O <sub>3</sub>	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-tetrahyrocannabinol (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, 5F-MDMB-PICA was temporarily placed as a Schedule I substance in the United States by the Drug Enforcement Administration.

#### 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<sup>TM</sup> Inferno<sup>TM</sup> ZB-35HT (15 m x 250  $\mu$ m x 0.25  $\mu$ m)

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

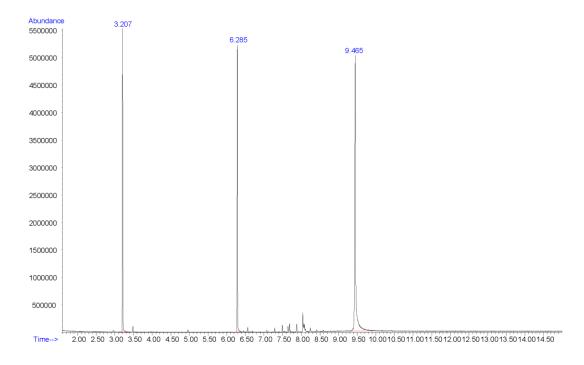
purchased from Cayman Chemical (Ann Arbor, MI, USA).

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.

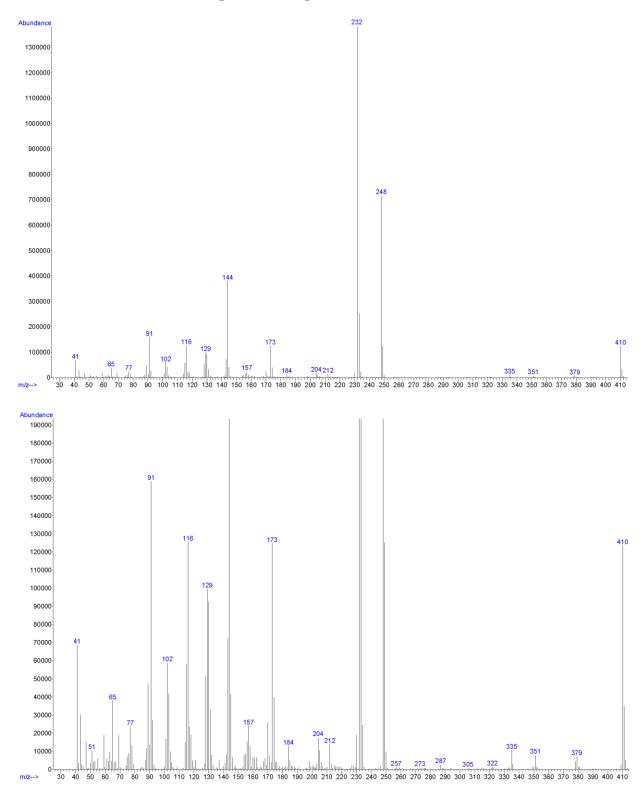
(https://www.caymanchem.com/product/25916)

## **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: Collison 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

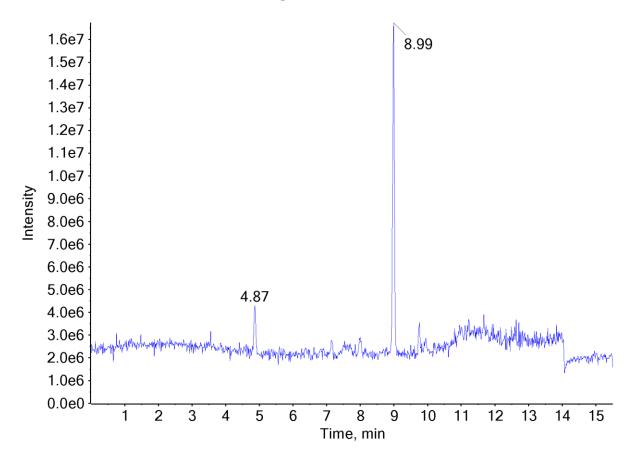
purchased from Cayman Chemical (Ann Arbor, MI, USA).

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

