

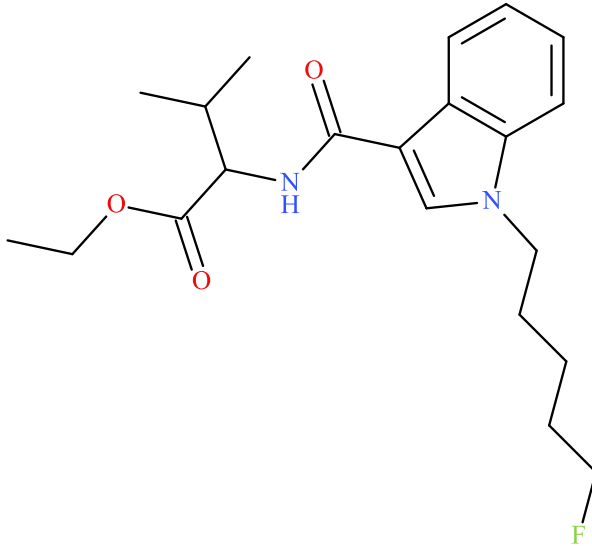
5F-EMB-PICA

Sample Type: **Seized Material**

Latest Revision: **June 15, 2020**

Date Received: **April 23, 2020**

Date of Report: **June 15, 2020**



1. GENERAL INFORMATION

IUPAC Name:	Ethyl 2-[[1-(5-fluoropentyl)indole-3-carbonyl]amino]-3-methylbutanoate
InChI String:	InChI=1S/C21H29FN2O3/c1-4-27-21(26)19(15(2)3)23-20(25)17-14-24(13-9-5-8-12-22)18-11-7-6-10-16(17)18/h6-7,10-11,14-15,19H,4-5,8-9,12-13H2,1-3H3,(H,23,25)
CFR:	Not Scheduled (06/2020)
CAS#	Not Available
Synonyms:	EMB-2201, 5-fluoro EMB-PICA
Source:	NMS Labs – Criminalistic Laboratory
Appearance:	Hand-Rolled Cigarette Containing Plant 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 ₂₁ H ₂₉ FN ₂ O ₃	376.5	376	377.2235

3. BRIEF DESCRIPTION

5F-EMB-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 5F-MMB-PICA (MMB-2201) are structurally similar synthetic cannabinoids. 5F-MDMB-PICA is a Schedule I substance in the United States; 5F-EMB-PICA and 5F-MMB-PICA are not explicitly scheduled.

4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/30769/5-fluoro-emb-pica>

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)

Sample Preparation: Acid/Base extraction (*note: only one internal standard added*)

Instrument: Agilent 5975 Series GC/MSD System

Column: Agilent J&W DB-1 (12 m x 200 μm x 0.33 μm)

Carrier Gas: Helium (Flow: 1.46 mL/min)

Temperatures: Injection Port: 265 °C
Transfer Line: 300 °C
MS Source: 230 °C
MS Quad: 150 °C

Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min

Injection Parameters: Injection Type: Splitless

Injection Volume: 1 µL

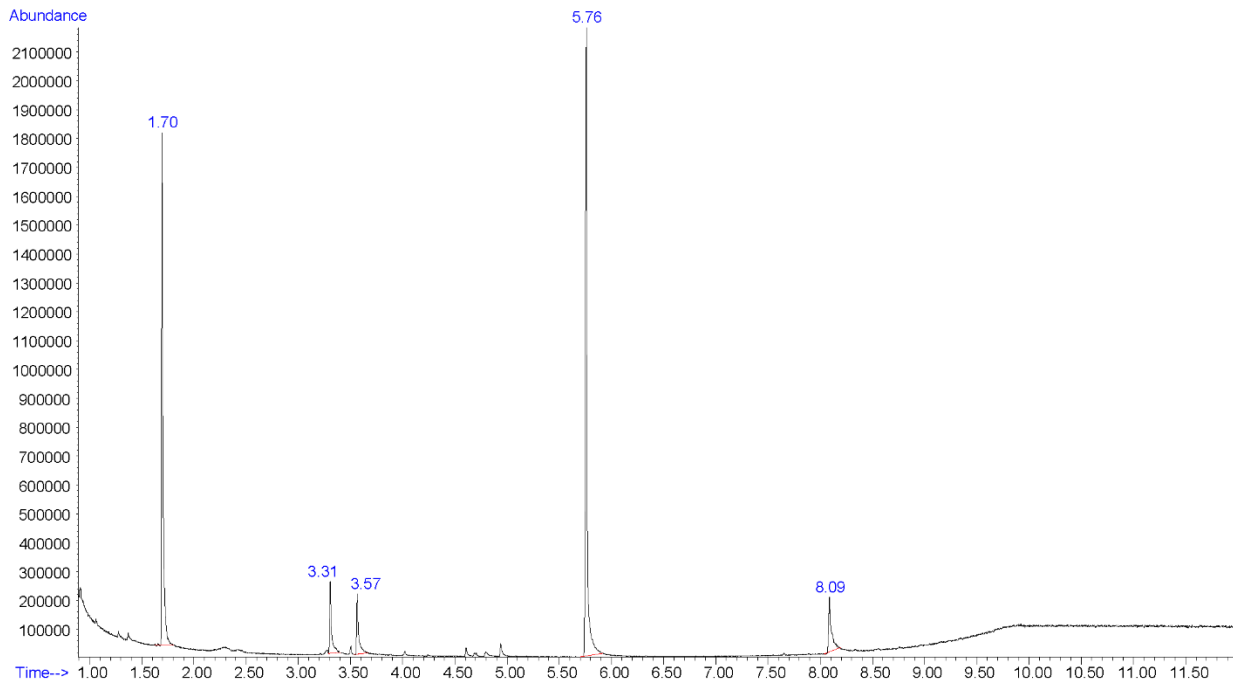
MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

Retention Time: 8.09 min

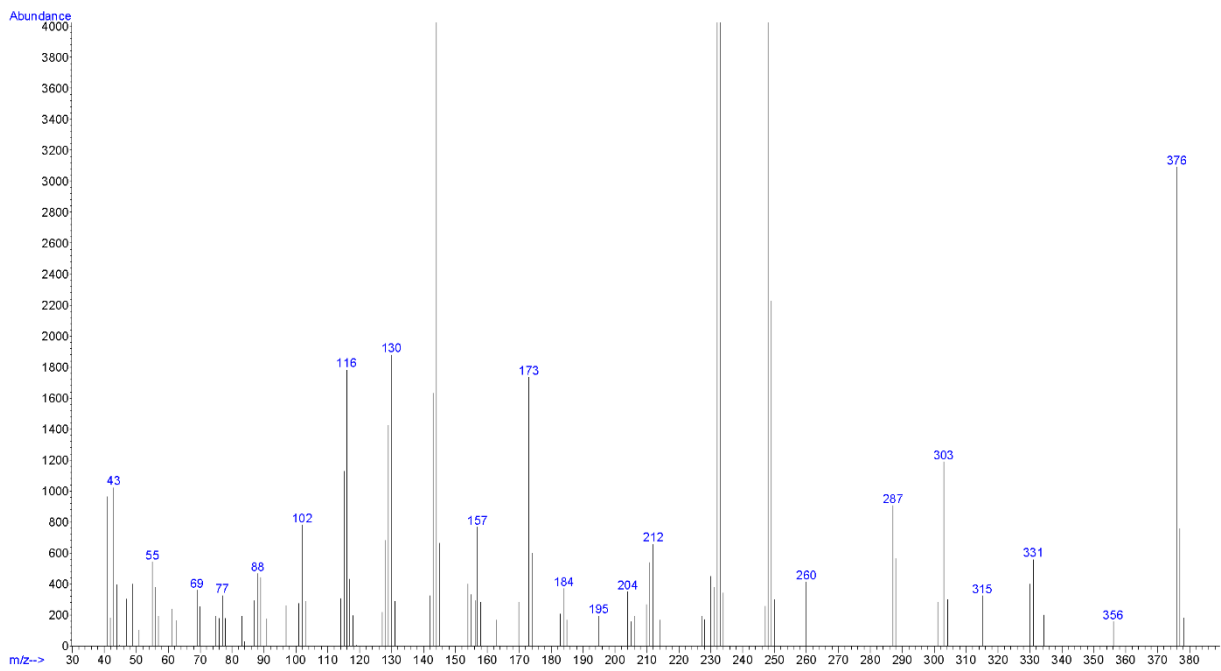
Standard Comparison: Reference material for 5F-EMB-PICA (Batch: 0588434-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-EMB-PICA based on retention time (8.10 min) and mass spectral data.
<https://www.caymanchem.com/product/30769/5-fluoro-emb-pica>

Chromatogram: 5F-EMB-PICA



*Additional peaks present in chromatogram: not controlled substances
(1.70 min, 3.31 min, and 3.57 min) and internal standard (5.76 min)*

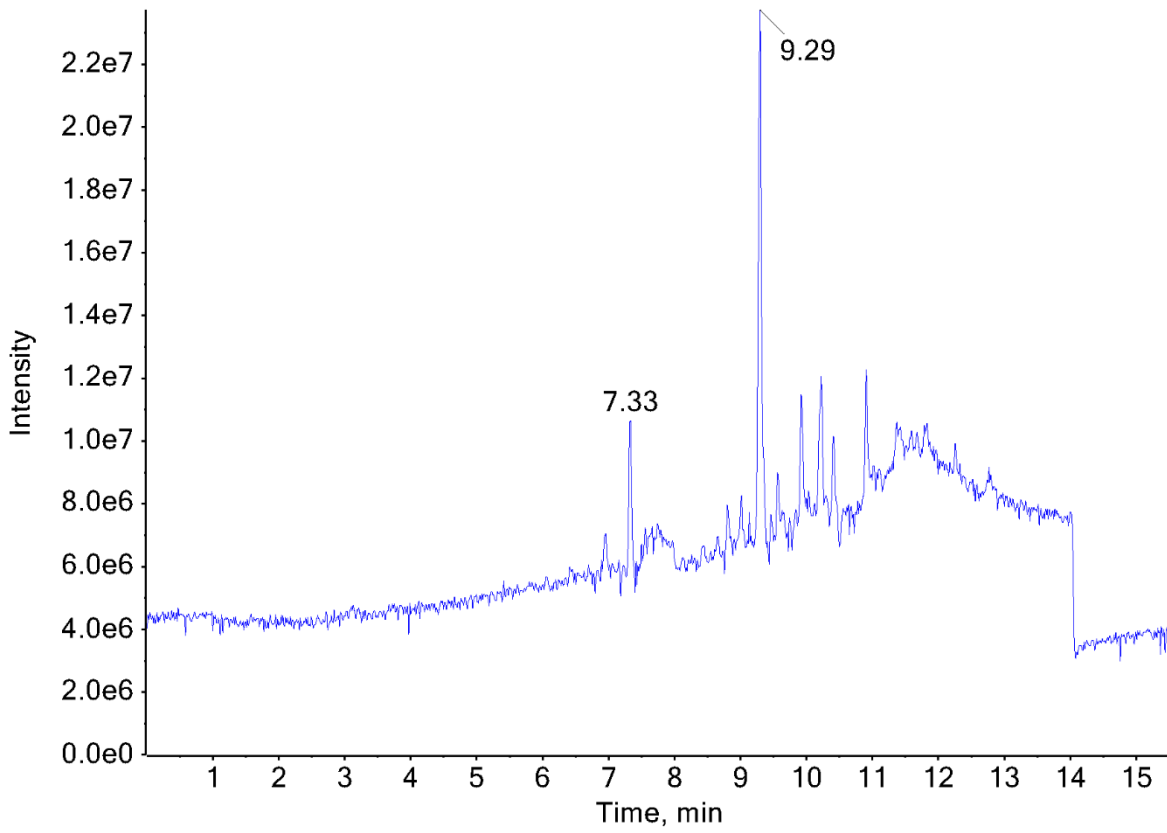
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-EMB-PICA



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:	9.29 min
Standard Comparison:	Reference material for 5F-EMB-PICA (Batch: 0588434-2) 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-EMB-PICA based on retention time (9.29 min) and mass spectral data. https://www.caymanchem.com/product/30769/5-fluoro-emb-pica

Chromatogram: 5F-EMB-PICA



Additional peak present in chromatogram: internal standard (7.33 min)

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

