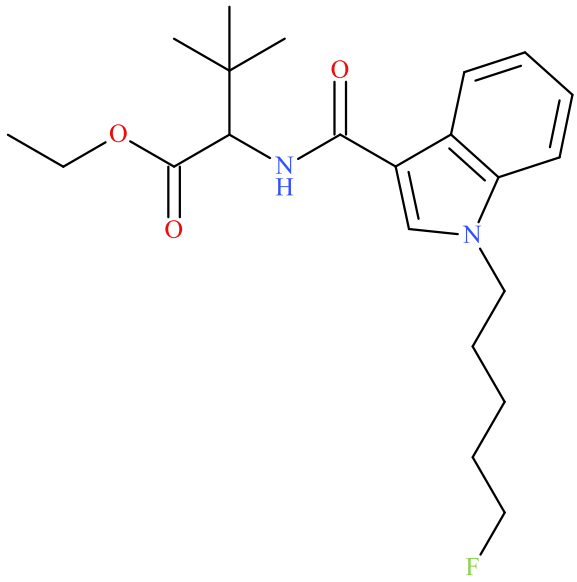
5F-EDMB-PICA

Sample Type: **Seized Material**



Latest Revision: **December 3, 2020**

Date Received: **July 24, 2020**

Date of Report: **December 3, 2020**

1. GENERAL INFORMATION

IUPAC Name:	Ethyl 2-[[1-(5-fluoropentyl)indole-3-carbonyl]amino]-3,3-dimethyl-butanoate
InChI String:	InChI=1S/C22H31FN2O3/c1-5-28-21(27)19(22(2,3)4)24-20(26)17-15-25(14-10-6-9-13-23)18-12-8-7-11-16(17)18/h7-8,11-12,15,19H,5-6,9-10,13-14H2,1-4H3,(H,24,26)
CFR:	Not Scheduled (12/2020)
CAS#	Not Available
Synonyms:	5-fluoro EDMB-PICA, 5F-EDMB-2201, 5-fluoro EDMB-2201
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-MS) in comparison to analysis of acquired reference material.*

***Prepared By:** Alex J. Krotulski, PhD; Sarah A. Shuda, MFSF, F-ABC; Melissa F. Fogarty, MSFS, D-ABFT-FT; Sarah E. Decker, BA; 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	$C_{22}H_{31}FN_2O_3$	390.5	390	391.2391

3. BRIEF DESCRIPTION

5F-EDMB-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-EDMB-PINACA are structurally similar synthetic cannabinoids. 5F-MDMB-PICA was first reported by NPS Discovery in July 2018 and 5F-EDMB-PINACA was first reported by NPS Discovery in April 2018. 5F-MDMB-PICA and 5F-EDMB-PINACA are Schedule I substances in the United States; 5F-EDMB-PICA is not explicitly scheduled.

4. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/5F-EDMB-PICA-ID-HIFS-024_report.pdf

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/5F-EDMB-PICA-ID-2191-20_report.pdf

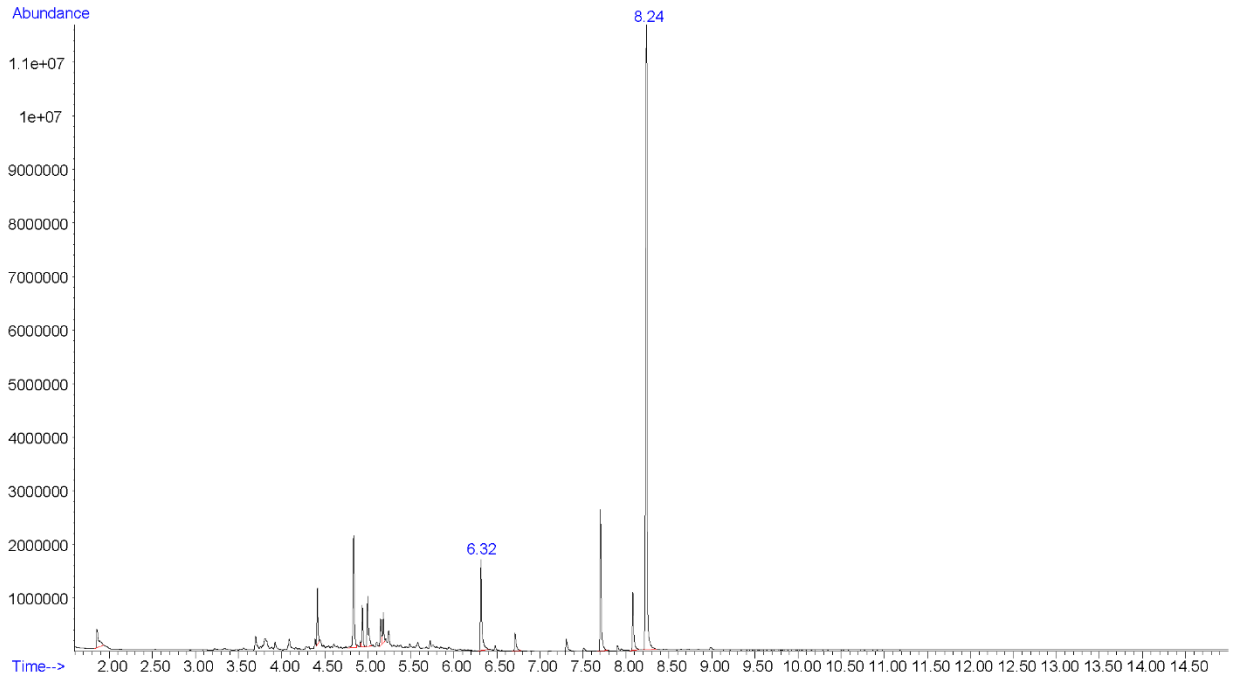
https://www.caymanchem.com/product/30725/5-fluoro-edmb-pica

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

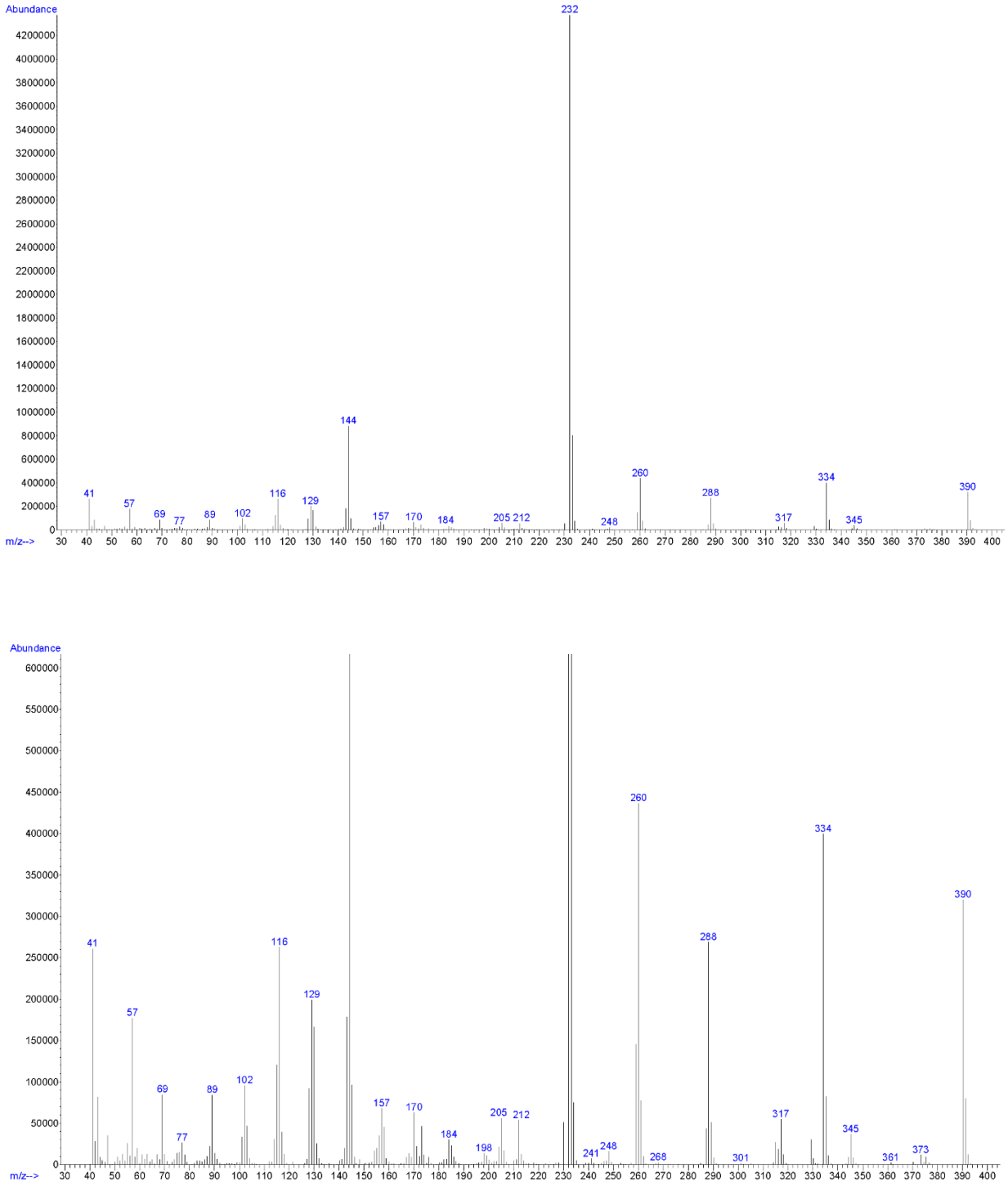
Testing Performed At:	NMS Labs (Willow Grove, PA)
Sample Preparation:	Acid/Base extraction
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 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:	8.24 min
Standard Comparison:	Reference material for 5F-EDMB-PICA (Batch: 0588529-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-EDMB-PICA based on retention time (8.23 min) and mass spectral data. (https://www.caymanchem.com/product/30725/5-fluoro-edmb-pica)

Chromatogram: 5F-EDMB-PICA



Additional peak present in chromatogram: internal standard (6.32 min)

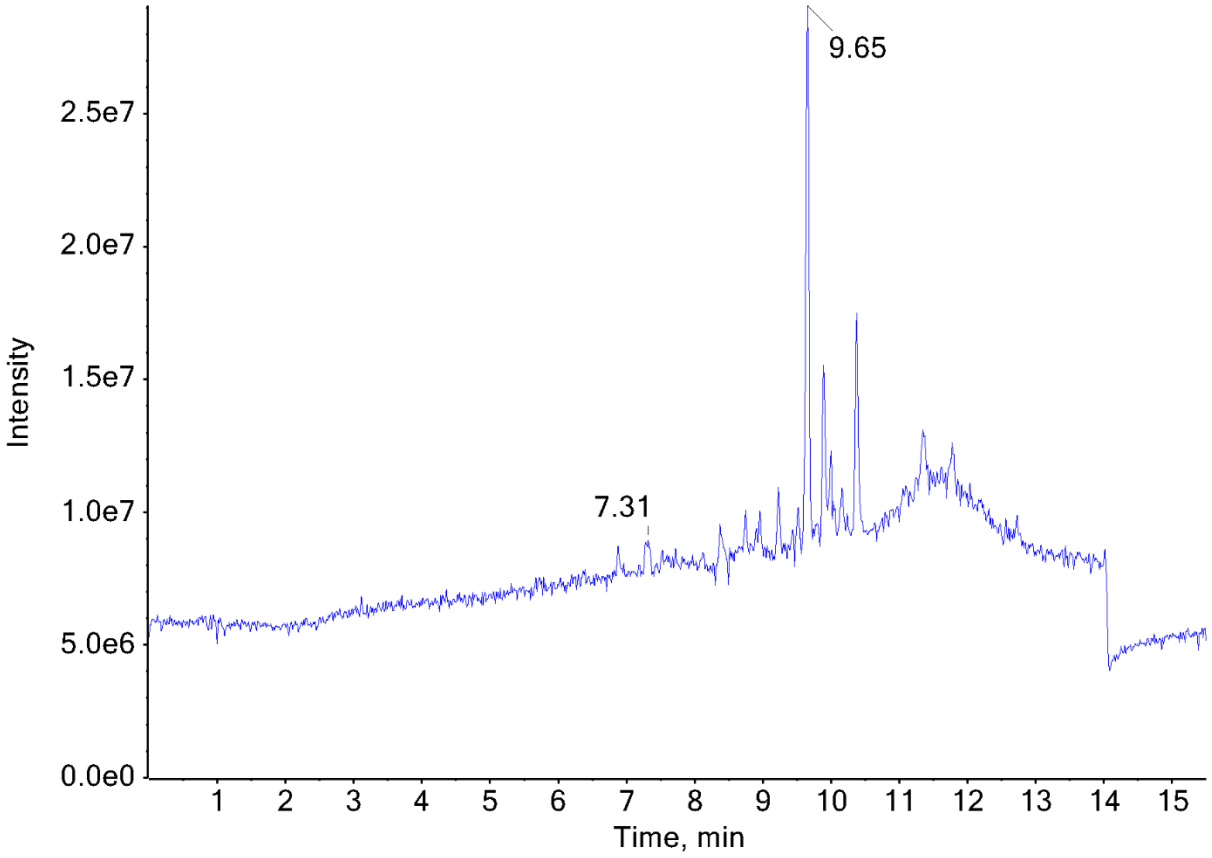
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-EDMB-PICA



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:	9.65 min
Standard Comparison:	Reference material for 5F-EDMB-PICA (Batch: 0588529-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-EDMB-PICA based on retention time (9.67 min) and mass spectral data. (https://www.caymanchem.com/product/30725/5-fluoro-edmb-pica)

Chromatogram: 5F-EDMB-PICA



Additional peak present in chromatogram: internal standard (7.31 min)

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