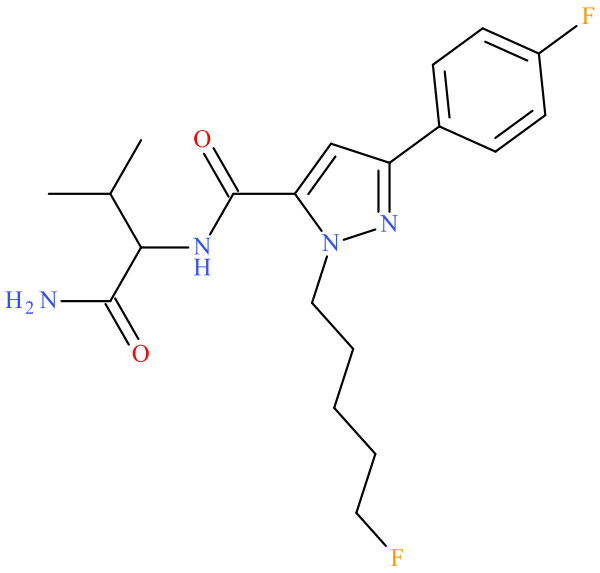
The Center for Forensic Science Research and Education
At the Fredric Rieders Family Foundation
2300 Stratford Ave
Willow Grove, PA 19090

5F-AB-PFUPPYCA



Sample Type: **Seized Material**

Latest Revision: **October 5, 2018**

Date Received: **September 25, 2018**

Date of Report: **October 5, 2018**

1. GENERAL INFORMATION

IUPAC Name:	N-(1-carbamoyl-2-methyl-propyl)-2-(5-fluoropentyl)-5-(4-fluorophenyl)pyrazole-3-carboxamide
InChI String:	InChI=1S/C20H26F2N4O2/c1-13(2)18(19(23)27)24-20(28)17-12-16(14-6-8-15(22)9-7-14)25-26(17)11-5-3-4-10-21/h6-9,12-13,18H,3-5,10-11H2,1-2H3,(H2,23,27)(H,24,28)
CFR:	Not Scheduled (10/2018)
CAS#	Not Available
Synonyms:	5-fluoro-3,5-AB-PFUPPYCA, 5F-AB-FUPPYCA, 5-fluoro AB-FUPPYCA, AB-FUPPYCA, 5-fluoro AB-FUPYCA, AZ-037
Source:	Tennessee

***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, and Barry K. Logan, PhD, F-ABFT*

Appearance: Foil Package – “Bling Bling Monkey”

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{20}H_{26}F_2N_4O_2$	392.44	392	393.2097

3. BRIEF DESCRIPTION

5F-AB-PFUPPYCA 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-ADB-PFUPPYCA and AB-CHMFUPPYCA are structurally similar synthetic cannabinoids. 5F-AB-PFUPPYCA, 5F-ADB-PFUPPYCA, and AB-CHMFUPPYCA are not scheduled substances in the United States.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/17181

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/5F-3,5-AB-PFUPPYCA-ID-1668-16_report.pdf

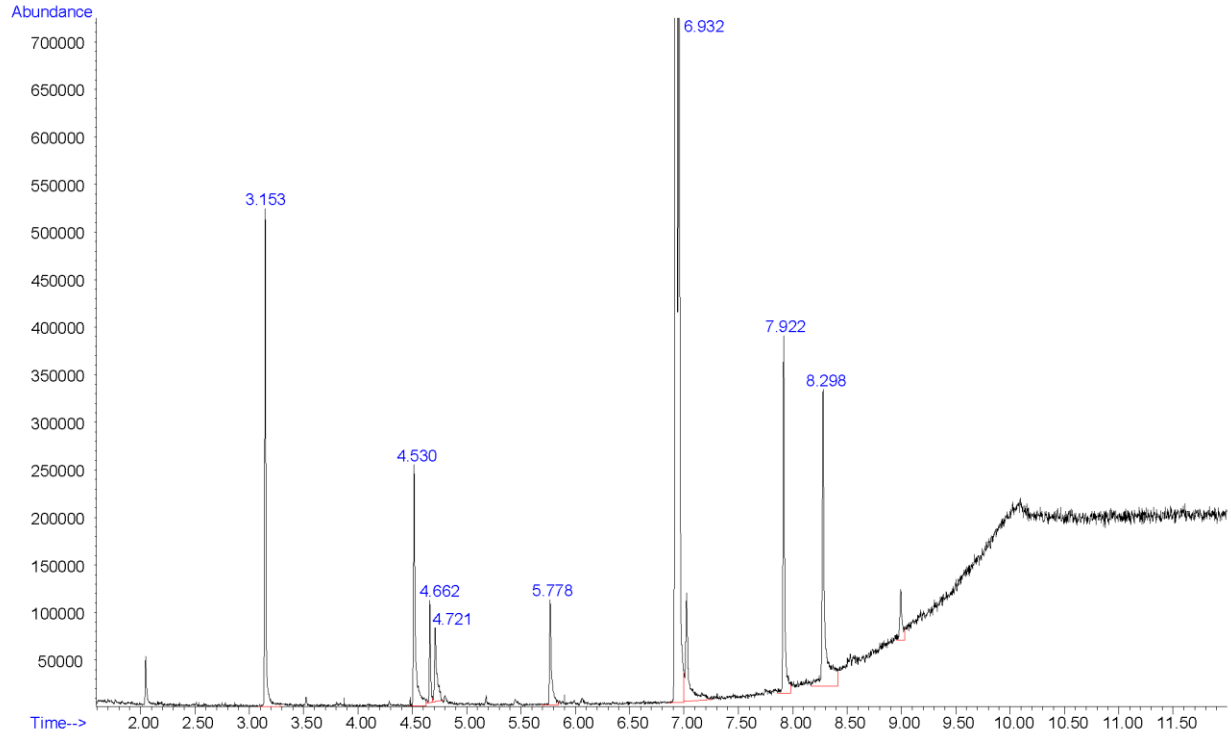
http://www.emcdda.europa.eu/system/files/publications/2880/TDAS16001ENN.pdf

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

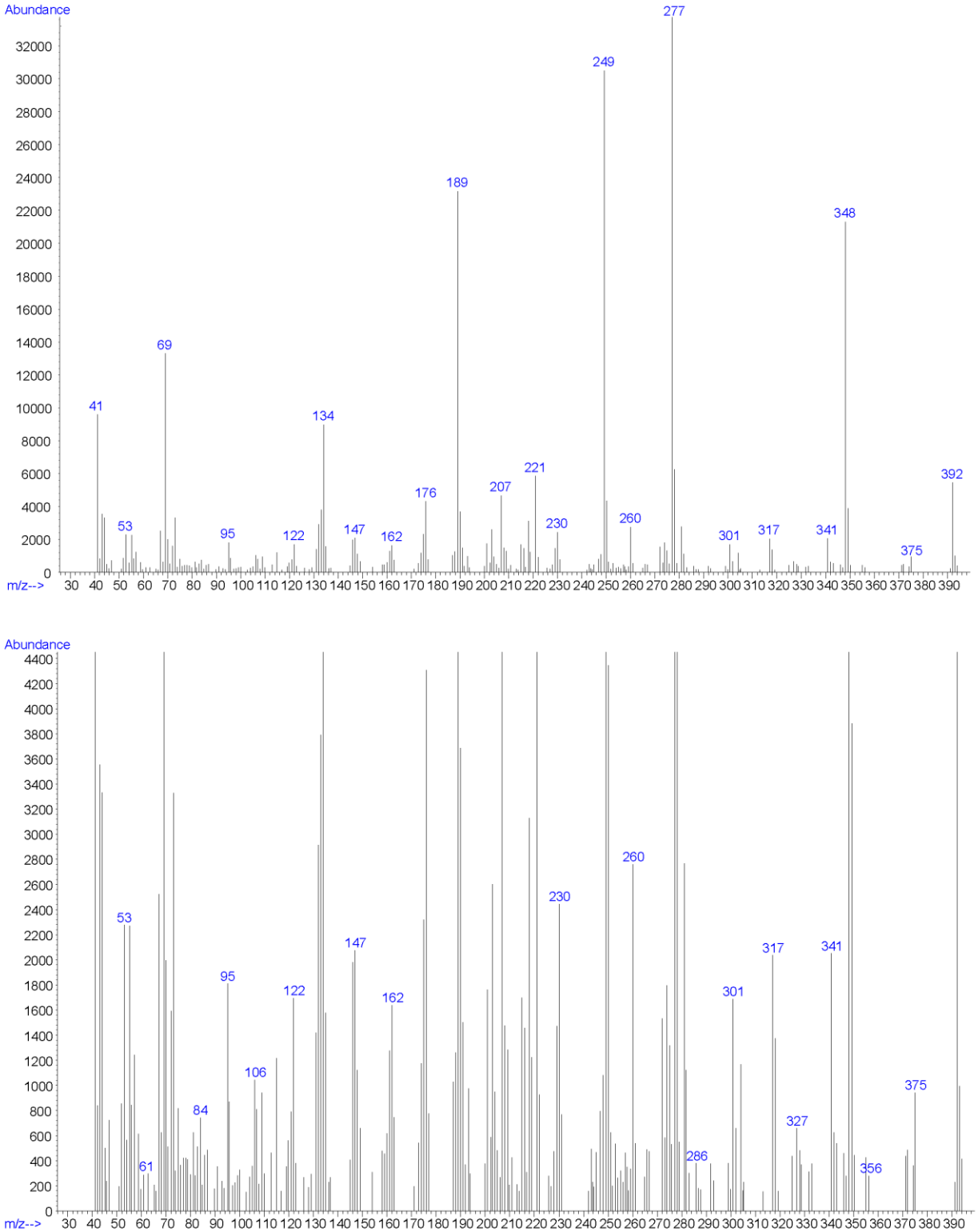
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	Swab of Packaging with Methanol
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Agilent J&W DB-1 (12 m x 200 µm x 0.33 µm)
Carrier Gas:	Helium (Flow: Adjusted Based on Retention Time Locking)
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:	8.298 min
Standard Comparison:	Reference material for 5F-AB-PFUPPYCA (Batch: 0520119) 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-AB-PFUPPYCA, based on retention time (8.298 min) and mass spectral data. (https://www.caymanchem.com/product/17181)

Chromatogram: 5F-AB-PFUPPYCA



Additional peaks present in chromatogram: internal standard 1 (3.153 min), not controlled substances (4.530, 4.662, and 4.721 min), internal standard 2 (5.778 min), not a controlled substance (6.932 min), MMB-FUBINACA [FUB-AMB] (7.922 min)

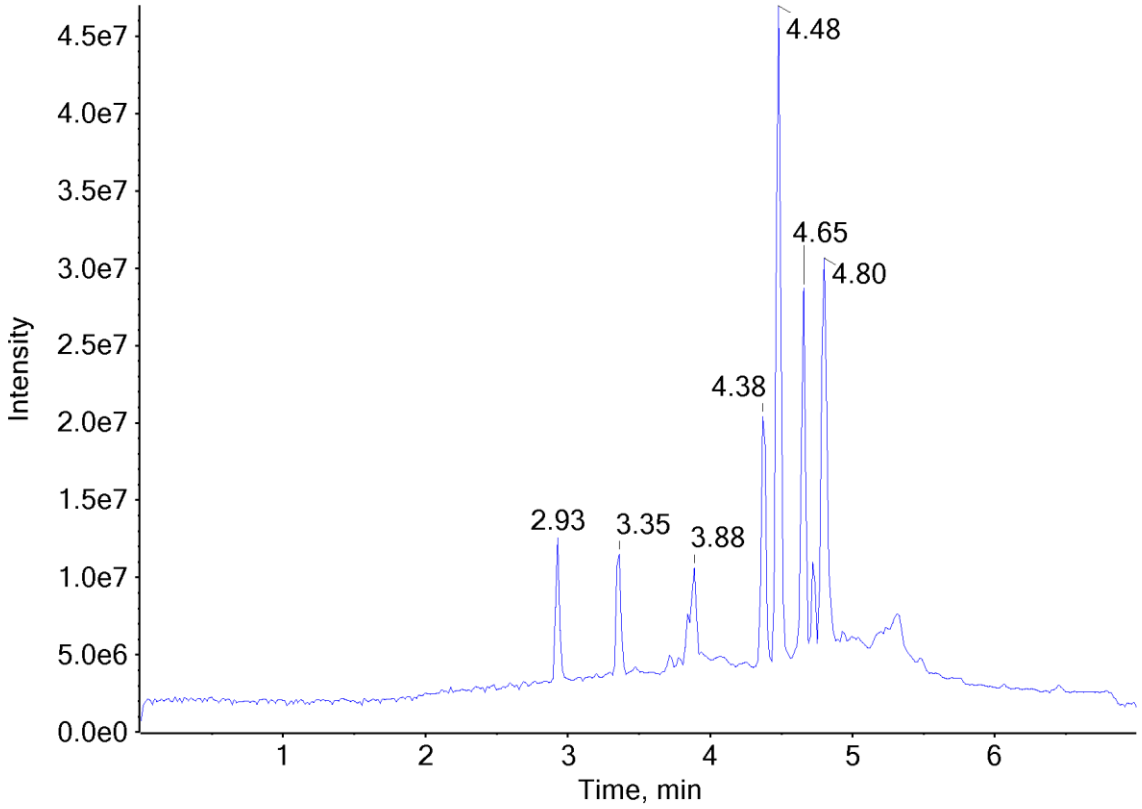
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-AB-PFUPPYCA



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 in mobile phase of methanol swabbing
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) with 0.1% formic acid
	Flow rate: 0.5 mL/min
Gradient:	Initial: 95A:5B; 5A:95B over 4 min, hold 2 min; 95A:5B at 7 min
Temperatures:	Autosampler: 15 °C
	Column Oven: 30 °C
	Source Heater: 600 °C
Injection Parameters:	Injection Volume: 20 µL
QTOF Parameters:	TOF MS Scan Range: 100-550 Da
	Precursor Isolation: SWATH® acquisition (10-25 Da)
	Fragmentation: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-550 Da
Retention Time:	4.38 min
Standard Comparison:	Reference material for 5F-AB-PFUPPYCA (Batch: 0520119) 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-AB-PFUPPYCA, based on retention time (4.36 min) and mass spectral data. (https://www.caymanchem.com/product/17181)

Chromatogram: 5F-AB-PFUPPYCA



Additional peaks present in chromatogram: internal standard 1 (2.93 min), not a controlled substance (3.35 min), internal standard 2 (3.88 min), not a controlled substance (4.48 min), MMB-FUBINACA [FUB-AMB] (4.65 min), not a controlled substance (4.80 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: 5F-AB-PFUPPYCA