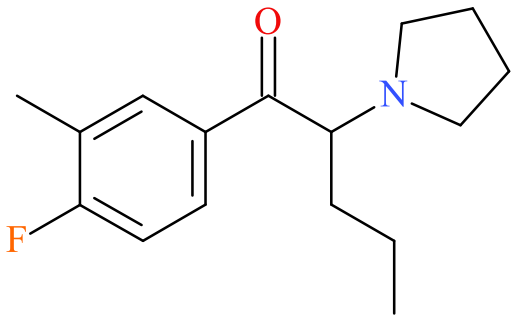
4-Fluoro-3-Methyl-Alpha-PVP



Sample Type: **Seized Material**

Latest Revision: **December 1, 2020**

Date Received: **August 21, 2020**

Date of Report: **December 1, 2020**

1. GENERAL INFORMATION

IUPAC Name:	1-(4-fluoro-3-methyl-phenyl)-2-pyrrolidin-1-yl-pentan-1-one
InChI String:	InChI=1S/C16H22FNO/c1-3-6-15(18-9-4-5-10-18)16(19)13-7-8-14(17)12(2)11-13/h7-8,11,15H,3-6,9-10H2,1-2H3
CFR:	Not Scheduled (12/2020)
CAS#	Not Available
Synonyms:	4-fluoro-3-methyl-alpha-pyrrolidinovalerophenone, 4-fluoro-3M-alpha-PVP, 4F-3-methyl-alpha-PVP, 4F-3Me-PVP
Source:	NMS Labs – Criminalistic Laboratory
Appearance:	Off-White Solid 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.*

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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	$C_{16}H_{22}FNO$	263.4	263	264.1758

3. BRIEF DESCRIPTION

4-Fluoro-3-methyl-alpha-PVP is classified as a novel synthetic stimulant and substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Novel stimulants have been reported to cause stimulant-like effects, similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Alpha-pyrrolidinopentiophenone (alpha-PVP) and 4-fluoro-alpha-pyrrolidinopentiophenone (4-fluoro-alpha-PVP) are structurally similar to 4-fluoro-3-methyl-alpha-PVP. 4-Fluoro-3-methyl-alpha-PVP and 4-fluoro-alpha-pyrrolidinohexanophenone (4-fluoro-alpha-PHP) are structural isomers, sharing the same formula and parent mass; however, their chemical behavior and mass fragmentation patterns differ allowing for differentiation during analytical testing. Alpha-PVP and alpha-PHP are Schedule I substances in the United States; 4-fluoro-3-methyl-alpha-PVP and 4-fluoro-alpha-PVP are not explicitly scheduled.

4. ADDITIONAL RESOURCES

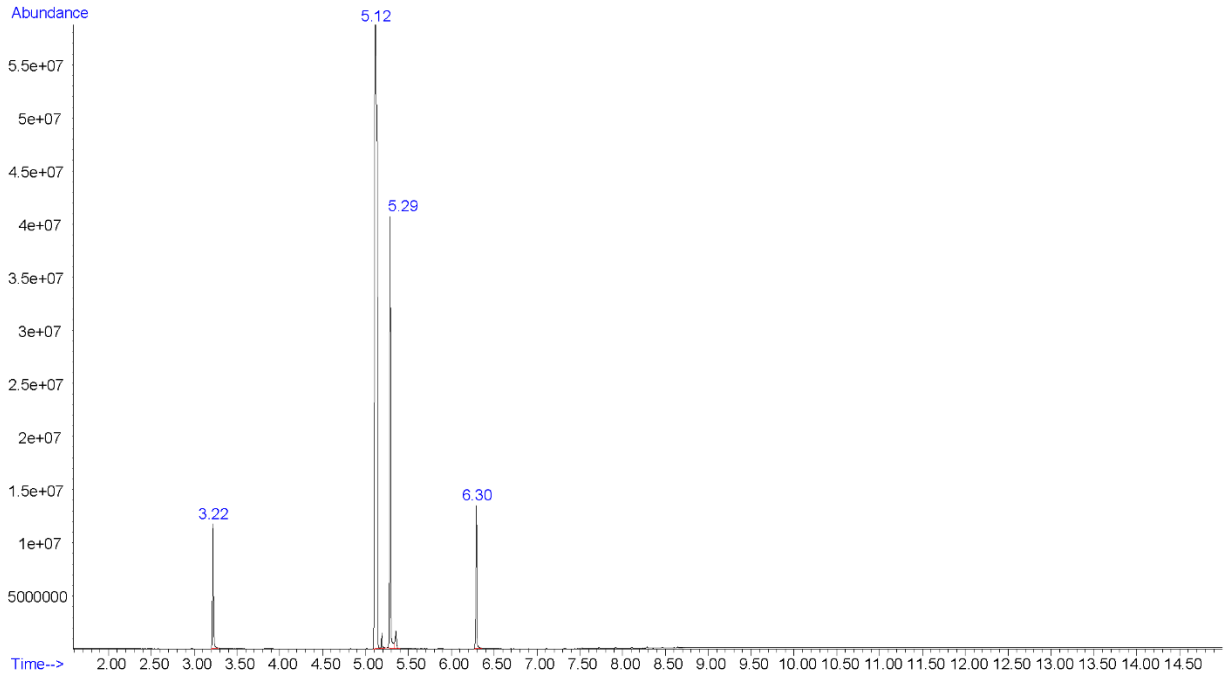
https://www.caymanchem.com/product/31050/4-fluoro-3-methyl-%CE%B1-pyrrolidinovalerophenone-(hydrochloride)

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

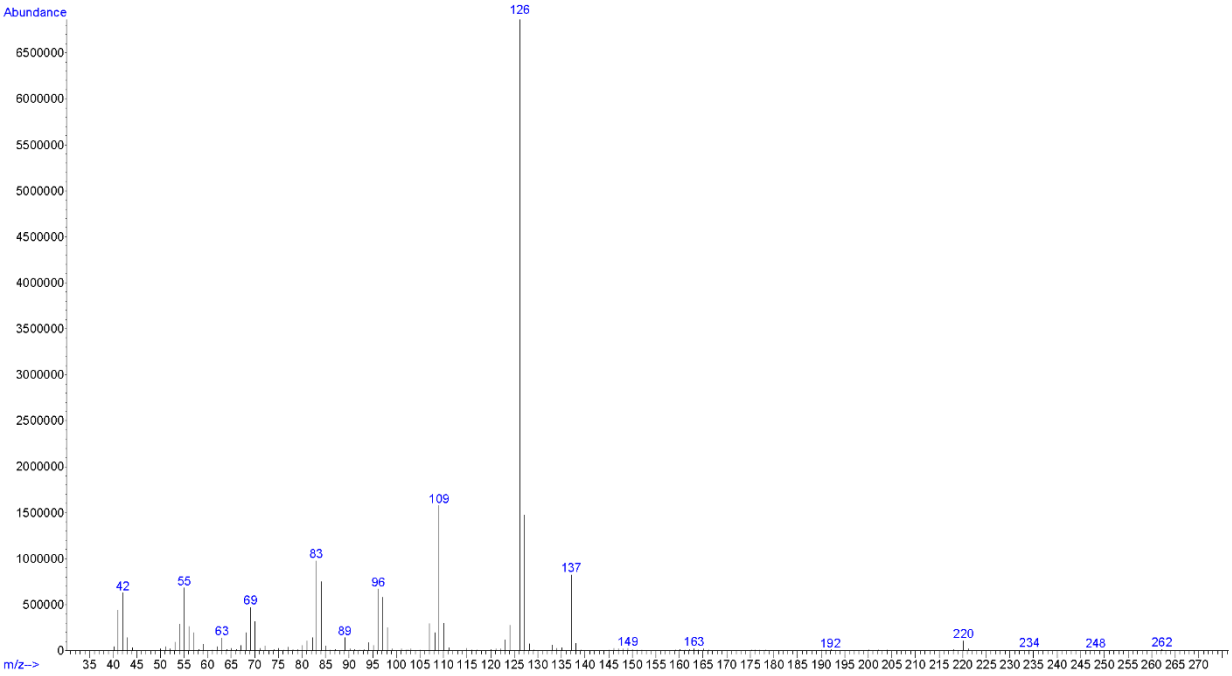
Testing Performed At:	NMS Labs (Willow Grove, PA)
Sample Preparation:	Acid/Base extraction
Instrument:	Agilent 5975 Series GC/MSD System
Column:	Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 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:	5.12 min
Standard Comparison:	Reference material for 4-fluoro-3-methyl-alpha-PVP (Batch: 0593030-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 4-fluoro-3-methyl-alpha-PVP based on retention time (5.09 min) and mass spectral data. (https://www.caymanchem.com/product/31050/4-fluoro-3-methyl-%CE%B1-pyrrolidinovalerophenone-(hydrochloride))

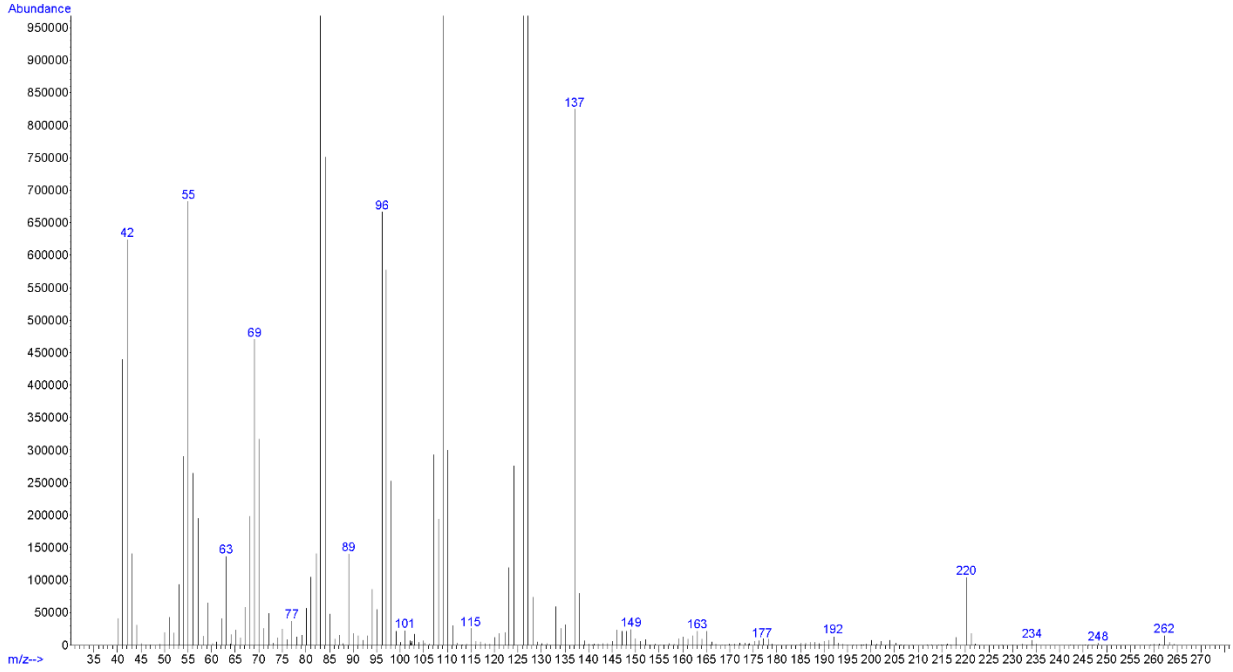
Chromatogram: 4-Fluoro-3-Methyl-Alpha-PVP



Additional peaks present in chromatogram: internal standard (3.22 min), not a controlled substance (5.29 min), and internal standard (6.28 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4-Fluoro-3-Methyl-Alpha-PVP

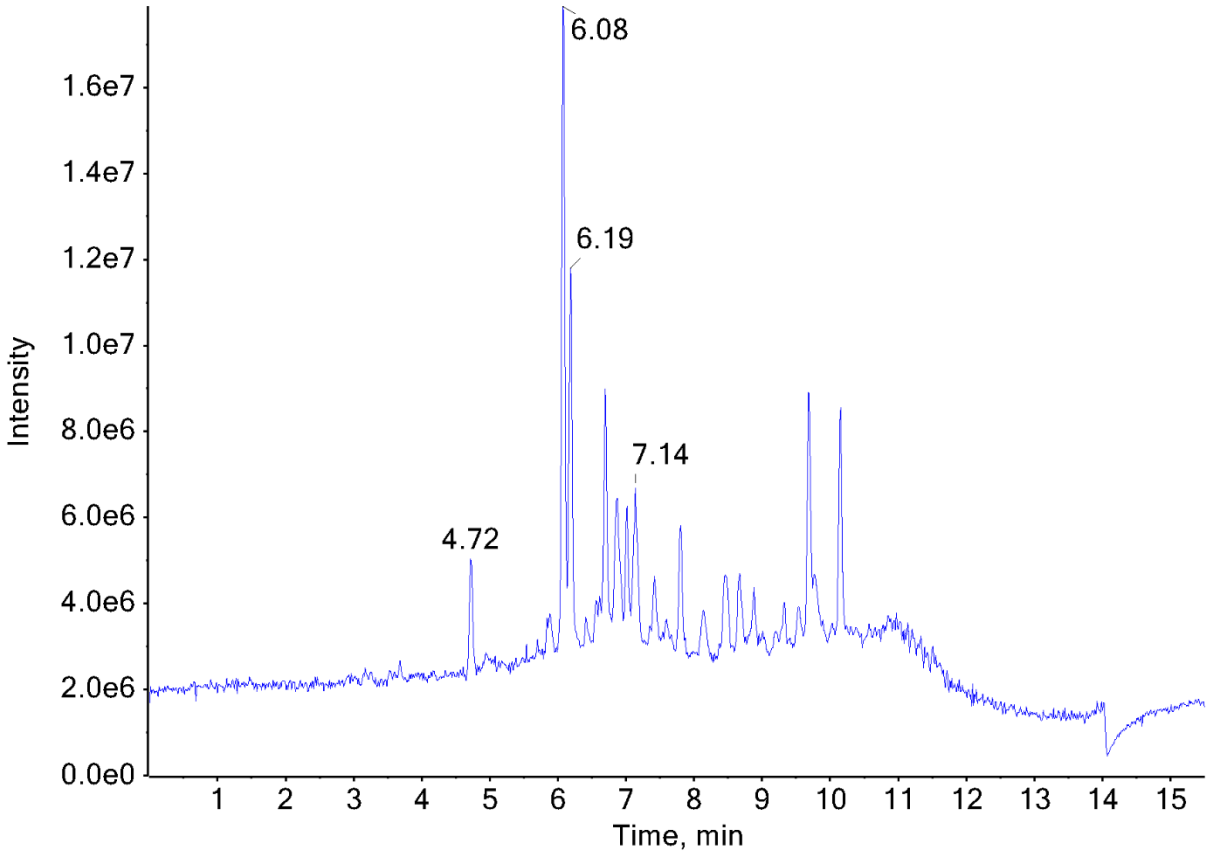




5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

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:	6.08 min
Standard Comparison:	Reference material for 4-fluoro-3-methyl-alpha-PVP (Batch: 0593030-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 4-fluoro-3-methyl-alpha-PVP based on retention time (6.22 min) and mass spectral data. (https://www.caymanchem.com/product/31050/4-fluoro-3-methyl-%CE%B1-pyrrolidinovalerophenone-(hydrochloride))

Chromatogram: 4-Fluoro-3-Methyl-Alpha-PVP



Additional peaks present in chromatogram: internal standard (4.72 min), not a controlled substance (6.19 min), and internal standard (7.14 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: 4-Fluoro-3-Methyl-Alpha-PVP