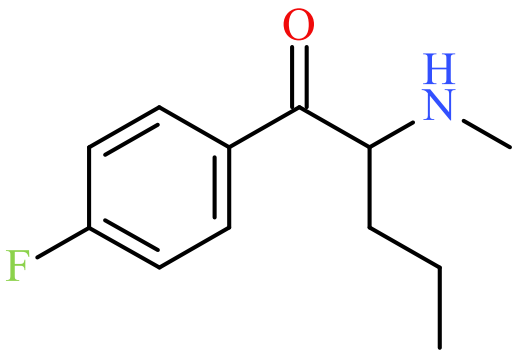
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

4F-Pentedrone

Sample Type: **Seized Material**



Latest Revision: **December 3, 2019**

Date Received: **August 16, 2019**

Date of Report: **December 3, 2019**

1. GENERAL INFORMATION

IUPAC Name:	1-(4-fluorophenyl)-2-(methylamino)pentan-1-one
InChI String:	InChI=1S/C12H16FNO/c1-3-4-11(14-2)12(15)9-5-7-10(13)8-6-9/h5-8,11,14H,3-4H2,1-2H3
CFR:	Not Scheduled (12/2019)
CAS#	Not Available
Synonyms:	4-Fluoro Pentedrone, 4-Fluoro-α-Methylamino-Valerophenone, 4-FPD
Source:	Department of Homeland Security
Appearance:	Tan 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	$C_{12}H_{16}FNO$	209.3	209	210.1289

3. BRIEF DESCRIPTION

4F-Pentedrone is classified as a novel 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. Structurally similar compounds include pentedrone, hexedrone, and *N*-ethyl hexedrone. Pentedrone is a Schedule I substance in the United States while 4F-pentedrone is not explicitly scheduled.

4. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/4-FPD-ID-2091-19_report.pdf

https://www.caymanchem.com/product/9002182/

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)

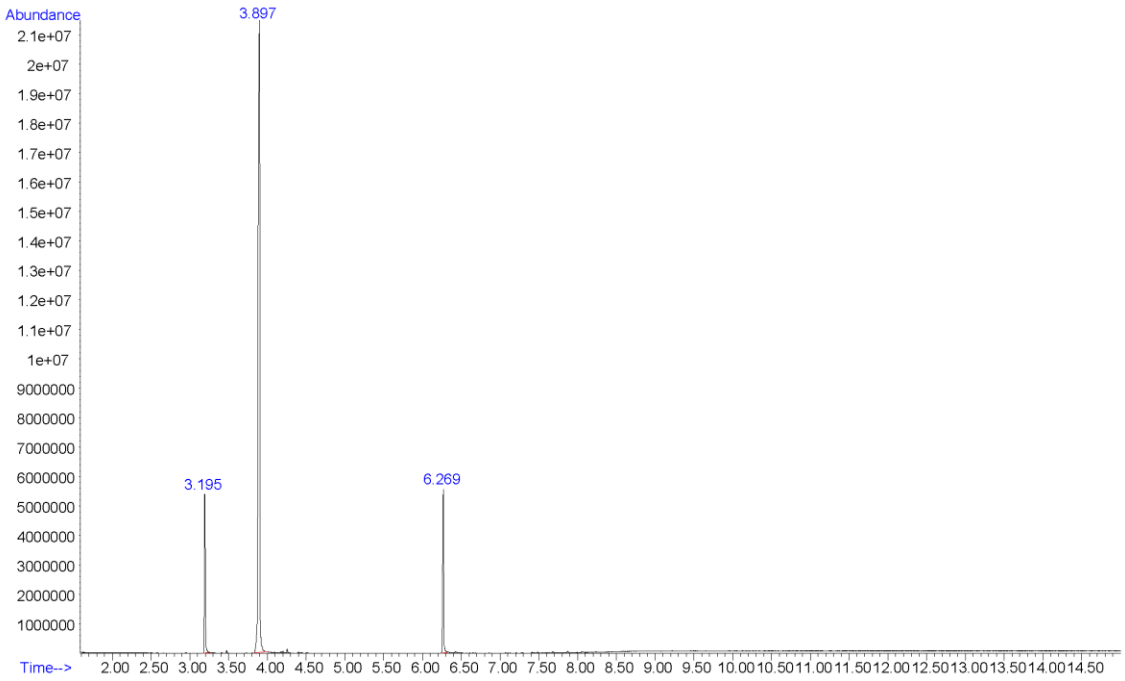
Carrier Gas: Helium (Flow: 1 mL/min)

Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

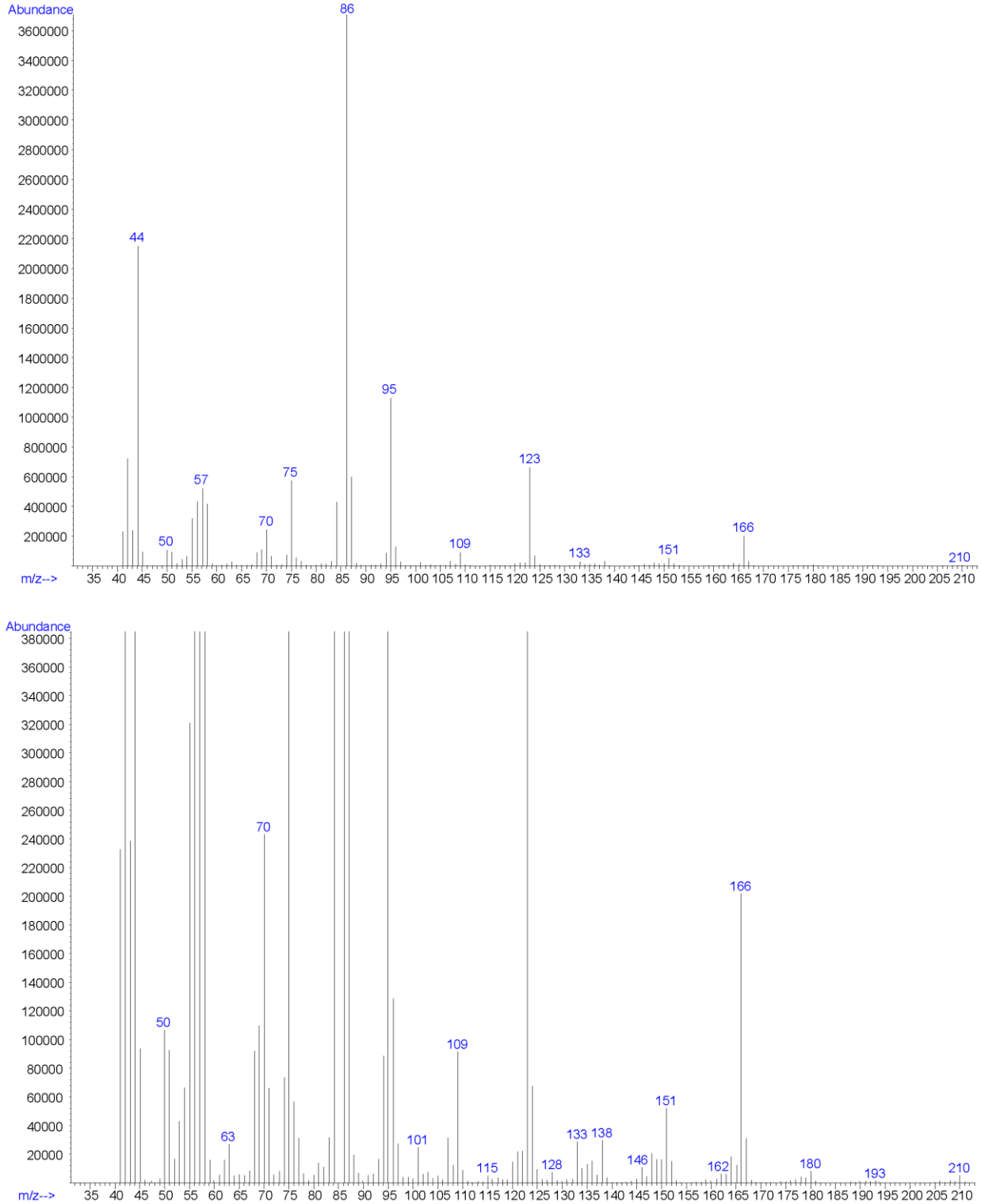
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	3.897 min
Standard Comparison:	Reference material for 4F-Pentedrone (Batch: 0464459-26) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 4F-Pentedrone, based on retention time (3.882 min) and mass spectral data. (https://www.caymanchem.com/product/9002182/)

Chromatogram: 4F-Pentedrone



Additional peaks present in chromatogram: internal standards (3.195 min and 6.269 min)

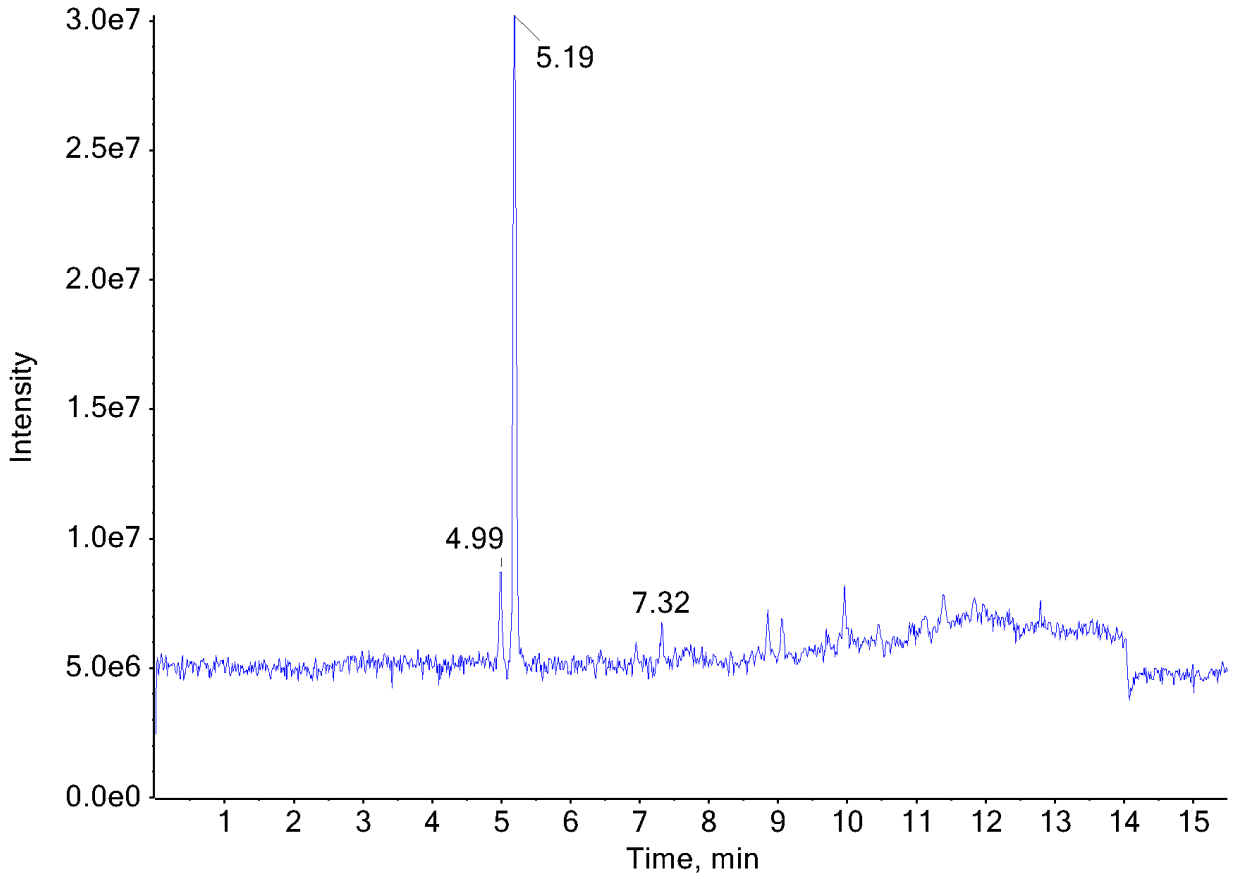
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 4F-Pentedrone



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 extract 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:	5.19 min
Standard Comparison:	Reference material for 4F-Pentedrone (Batch: 0464459-26) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 4F-Pentedrone, based on retention time (5.15 min) and mass spectral data. (https://www.caymanchem.com/product/9002182/)

Chromatogram: 4F-Pentedrone



Additional peaks present in chromatogram: internal standards (4.99 min and 7.32 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: 4F-Pentedrone