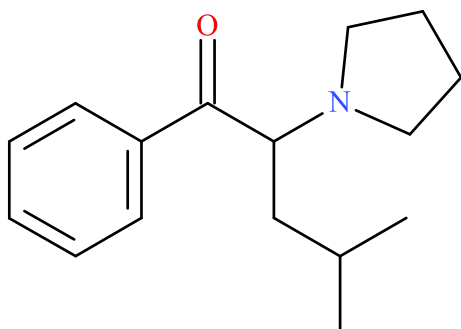


alpha-PiHP

Sample Type: **Seized Material**



Latest Revision: **November 16, 2018**

Date Received: **August 17, 2018**

Date of Report: **October 30, 2018**

1. GENERAL INFORMATION

IUPAC Name:	4-methyl-1-phenyl-2-pyrrolidin-1-yl-pentan-1-one
InChI String:	InChI=1S/C16H23NO/c1-13(2)12-15(17-10-6-7-11-17)16(18)14-8-4-3-5-9-14/h3-5,8-9,13,15H,6-7,10-12H2,1-2H3
CFR:	Not Scheduled (10/2018)
CAS#	Not Available
Synonyms:	alpha-Pyrrolidinoisohexanophenone, α -PiHP
Source:	Department of Homeland Security
Appearance:	White Solid Material

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 ₂₃ NO	245.36	245	246.1852

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, Melissa F. Fogarty, MSFS, D-ABFT-FT, and Barry K. Logan, PhD, F-ABFT

3. BRIEF DESCRIPTION

Alpha-PiHP 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 alpha-pyrrolidinopentiophenone (alpha-PVP), alpha-pyrrolidinobutiophenone (alpha-PBP), and alpha-pyrrolidinohexanophenone (alpha-PHP). Alpha-PVP, and alpha-PBP are all Schedule I substances in the United States.

4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/21682>

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/alpha-PiHP-ID-1723-16_report.pdf

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:	Zebtron™ 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

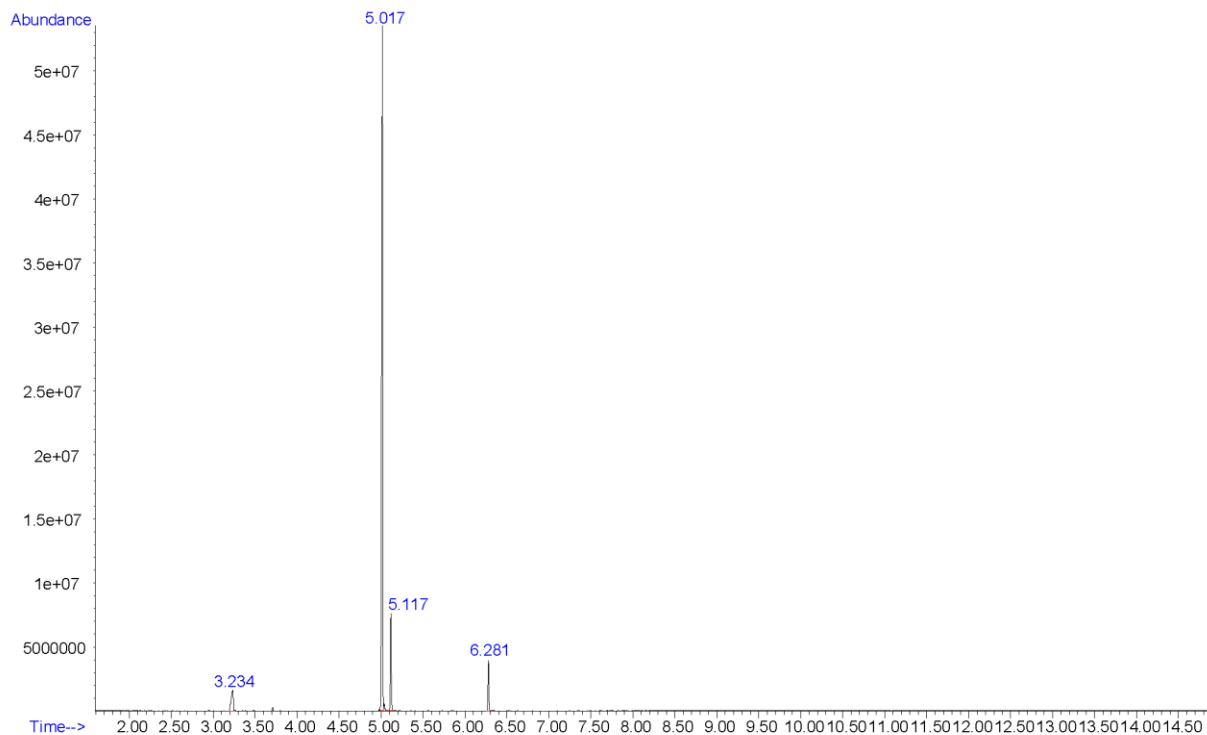
Threshold: 250

Retention Time: 5.017 min

Standard Comparison: Reference material for alpha-PiHP (Batch: 0501111-17) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as alpha-PiHP, based on retention time (5.002 min) and mass spectral data.

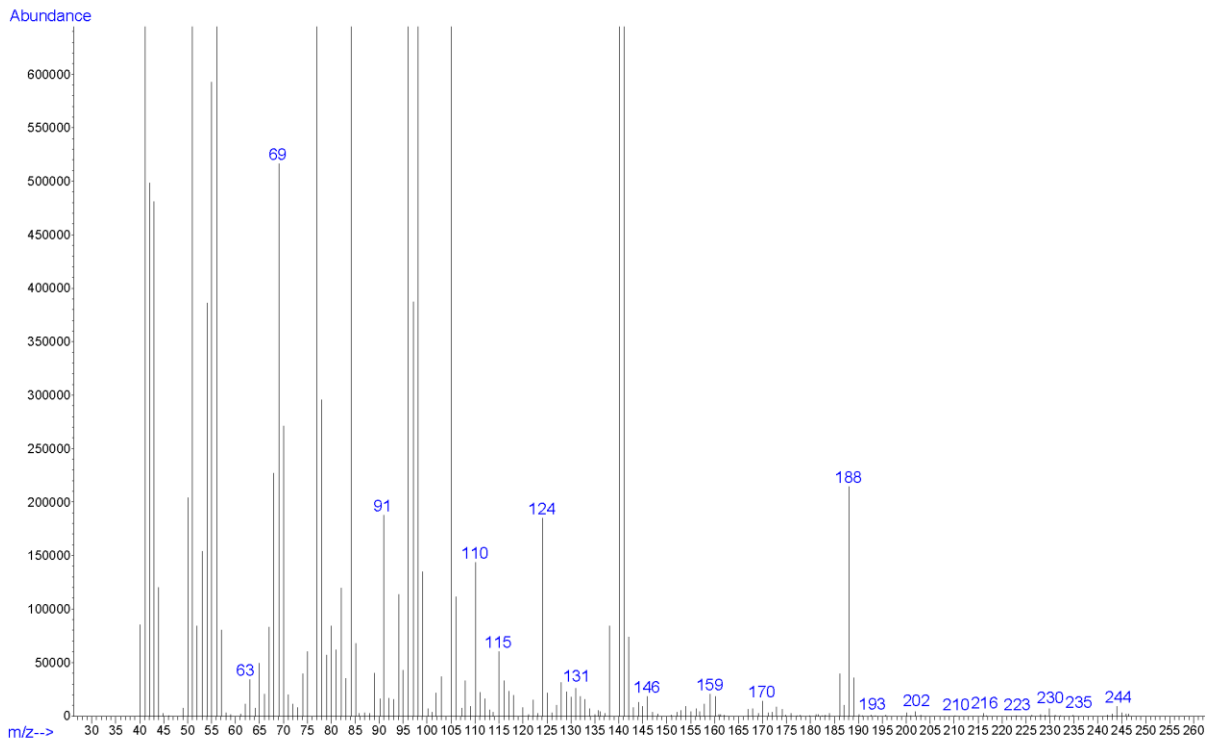
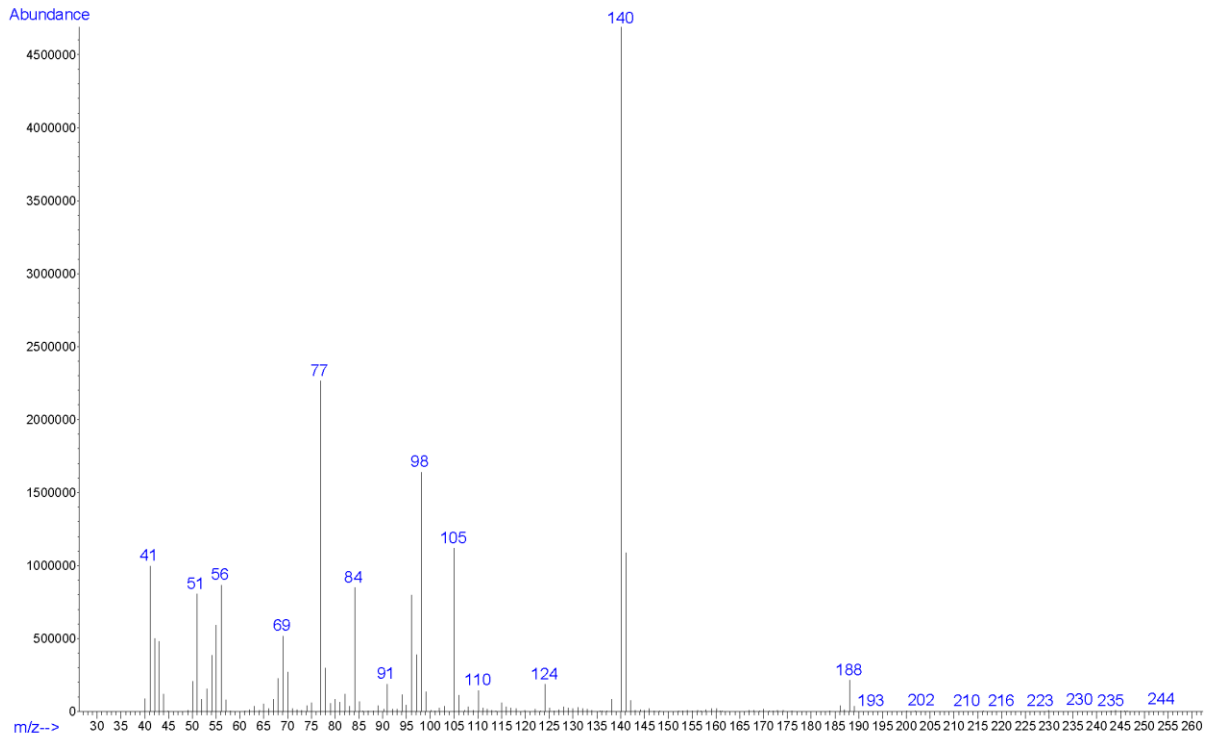
<https://www.caymanchem.com/product/21682>

Chromatogram: alpha-PiHP



Additional peaks present in chromatogram: internal standard (3.234 min), not a controlled substance (5.117 min), internal standard (6.281 min)

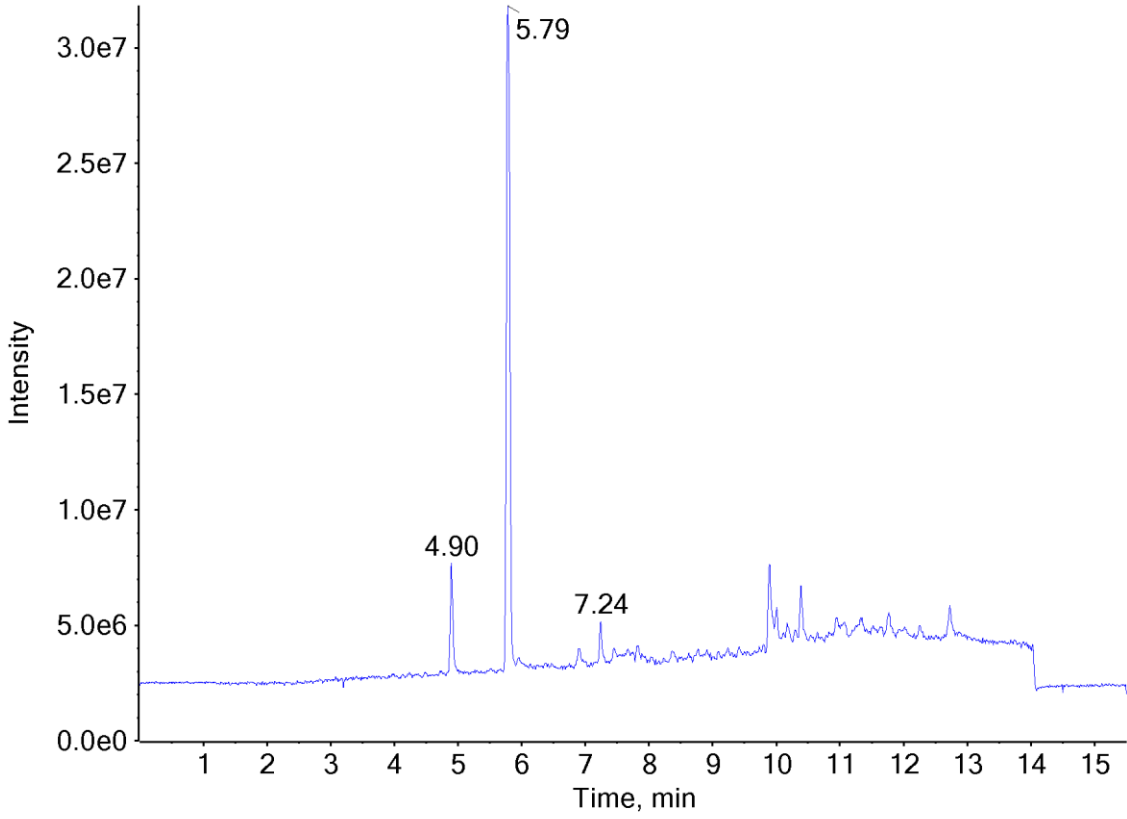
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): alpha-PiHP



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

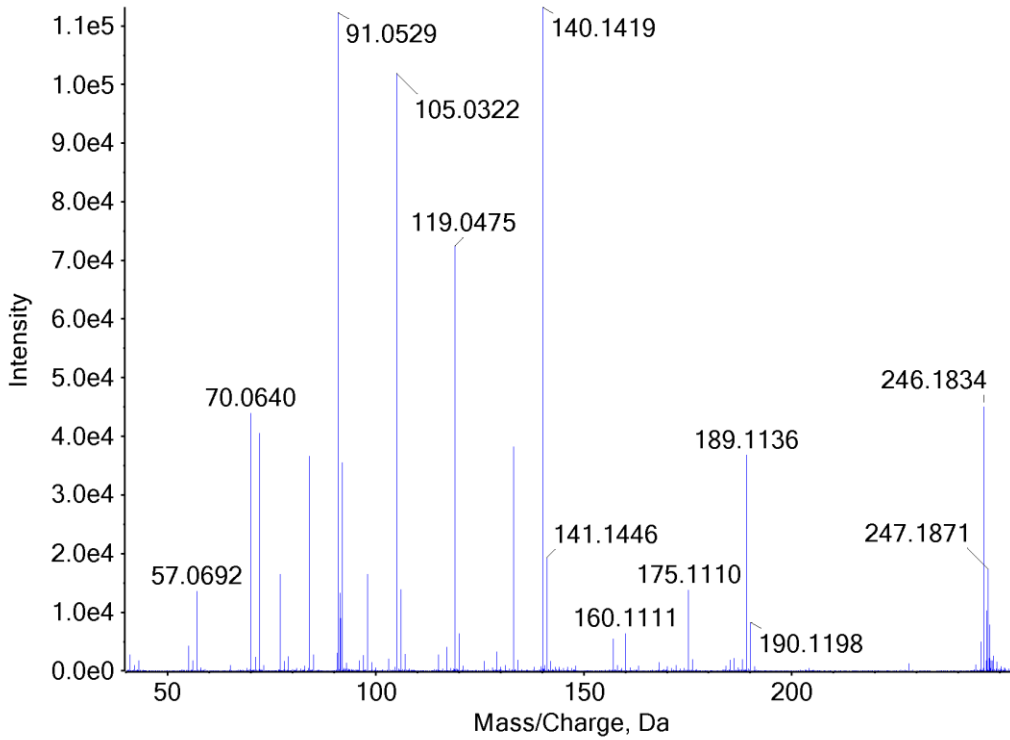
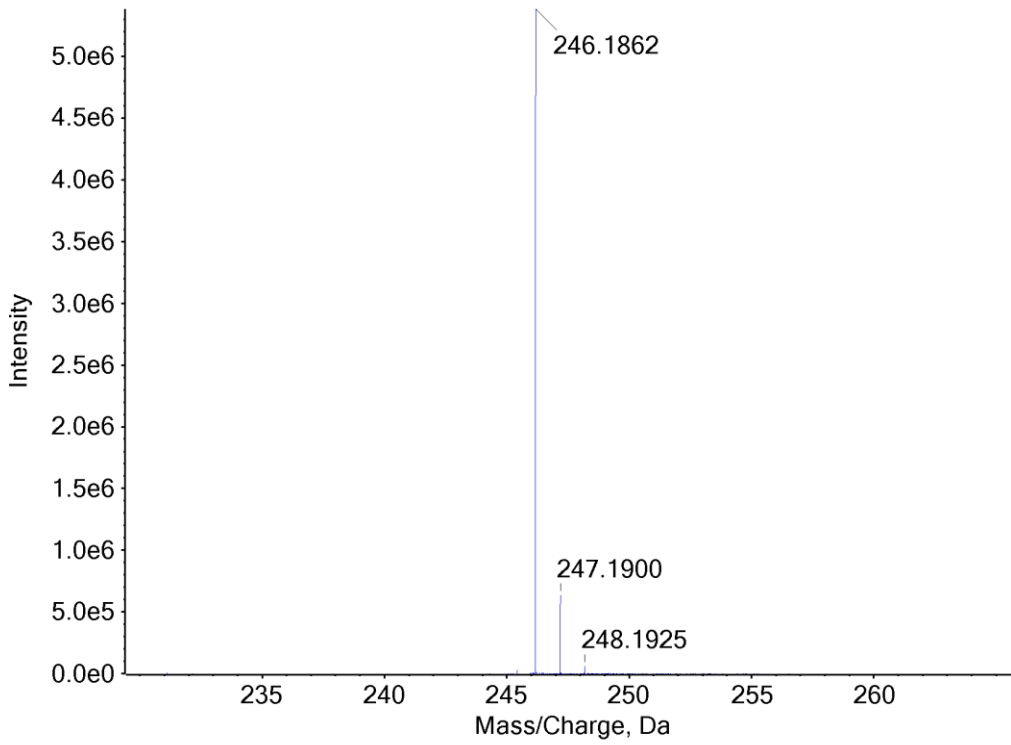
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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:	5.79 min
Standard Comparison:	Reference material for alpha-PiHP (Batch: 0501111-17) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as alpha-PiHP, based on retention time (5.80 min) and mass spectral data. (https://www.caymanchem.com/product/21682)

Chromatogram: alpha-PiHP



Additional peaks present in chromatogram: internal standards (4.90 min and 7.24 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: alpha-PiHP



6. REVISION HISTORY

<u>Date</u>	<u>Revision</u>
11/16/2018	Corrected drug name and lot number under “Standard Comparison” for alpha-PiHP