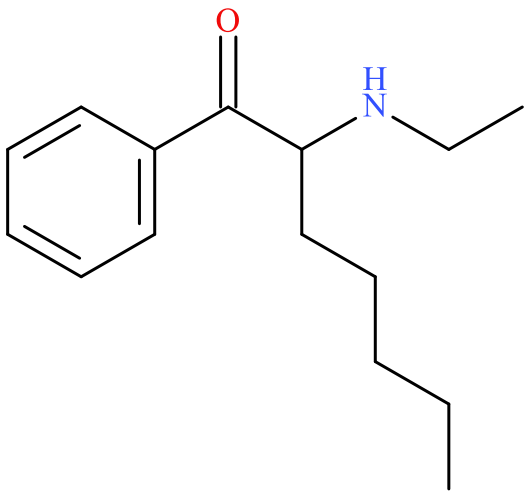
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

N-ethyl Heptedrone



Sample Type: **Seized Material**

Latest Revision: **September 30, 2019**

Date Received: **June 13, 2019**

Date of Report: **September 30, 2019**

1. GENERAL INFORMATION

IUPAC Name:	2-(ethylamino)-1-phenyl-heptan-1-one
InChI String:	InChI=1S/C15H23NO/c1-3-5-7-12-14(16-4-2)15(17)13-10-8-6-9-11-13/h6,8-11,14,16H,3-5,7,12H2,1-2H3
CFR:	Not Scheduled (09/2019)
CAS#	Not Available
Synonyms:	Ethyl-Heptedrone
Source:	Department of Homeland Security
Appearance:	White Solid Material

***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.*

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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	$C_{15}H_{23}NO$	233.4	233	234.1852

3. BRIEF DESCRIPTION

N-ethyl Heptedrone 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 *N*-ethyl hexedrone, hexedrone, and pentedrone. Pentedrone and *N*-ethyl hexedrone are Schedule I substances in the United States; however, hexedrone and *N*-ethyl heptedrone are not scheduled.

In September 2019, NMS Labs confirmed two additional seized drug materials positive for *N*-ethyl heptedrone.

4. ADDITIONAL RESOURCES

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/ETHYLHEPTEDRON-ID-HIFS-012.pdf

https://www.caymanchem.com/product/27327/

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)

Sample Preparation: Acid/Base extraction (1:10 dilution)

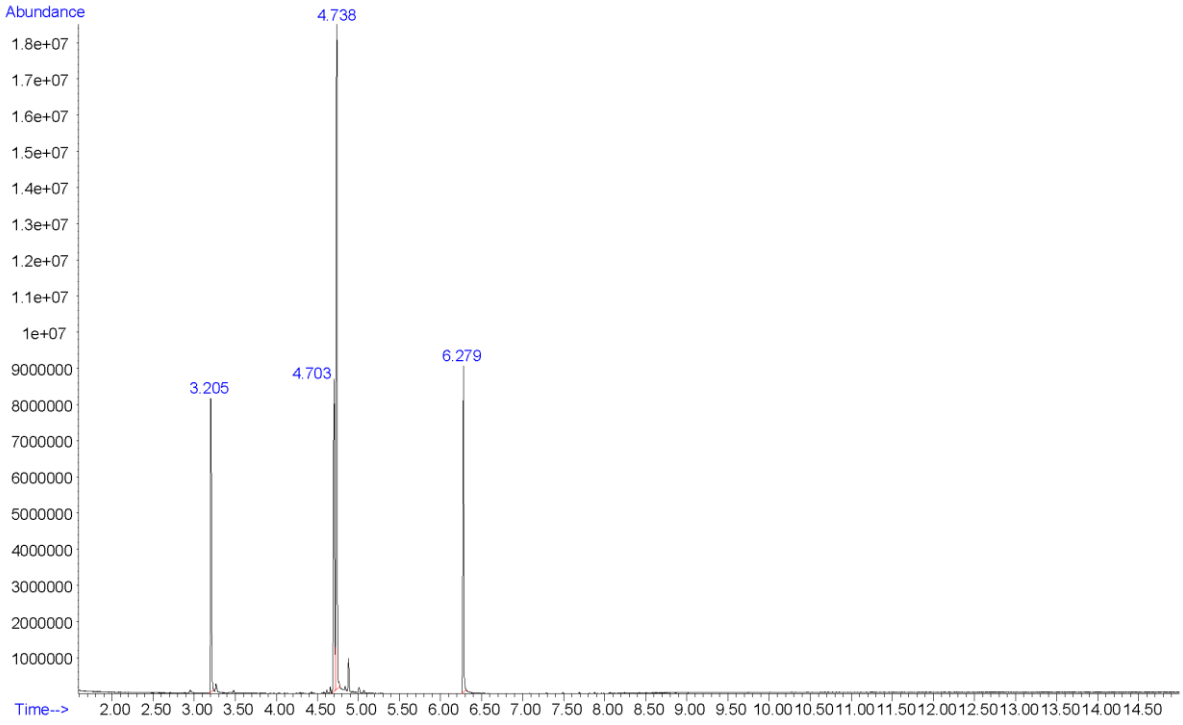
Instrument: Agilent 5975 Series GC/MSD System

Column: Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)

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

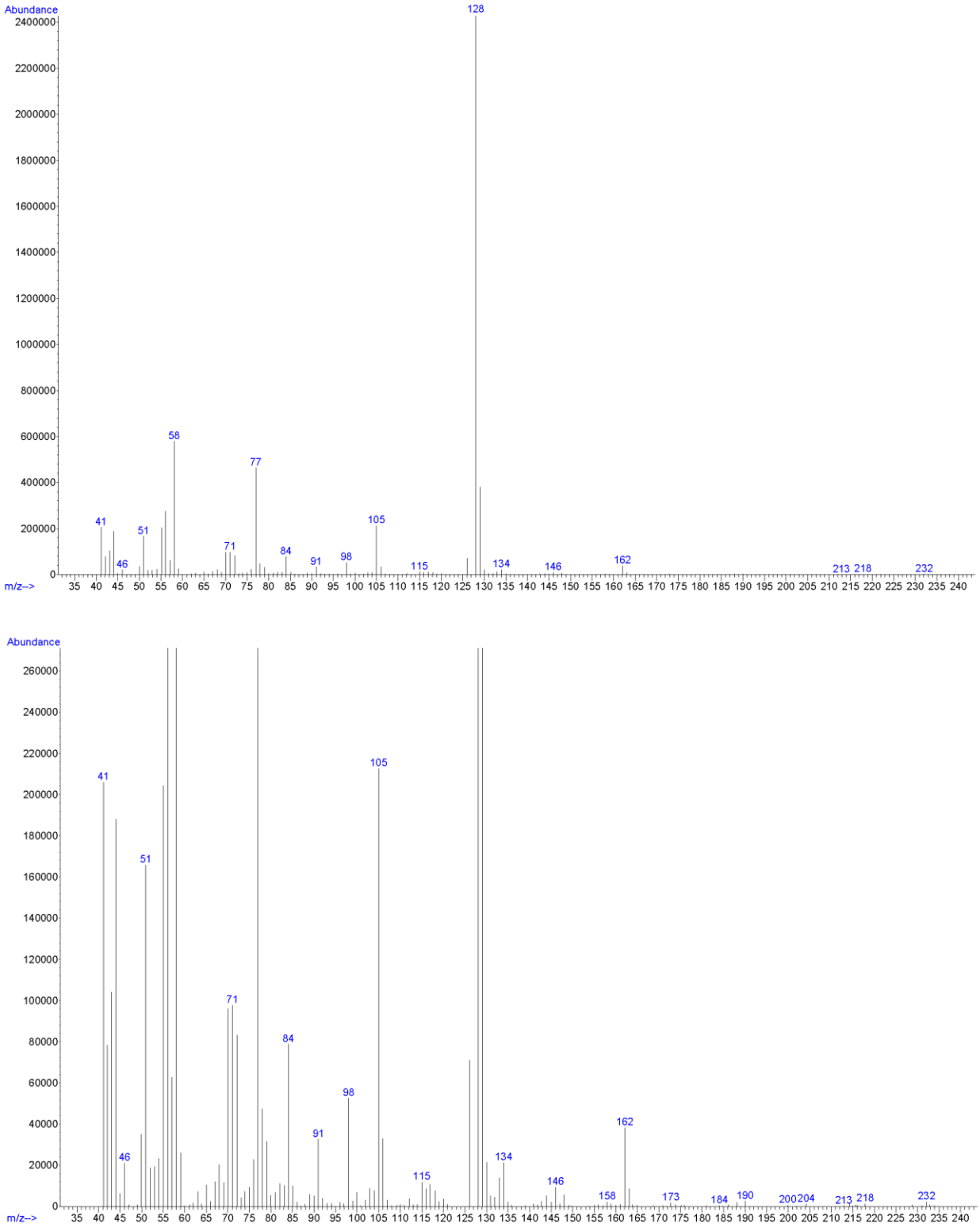
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	4.738 min
Standard Comparison:	Reference material for *N*-ethyl heptedrone (Batch: 0549986-6) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *N*-ethyl heptedrone, based on retention time (4.736 min) and mass spectral data. (https://www.caymanchem.com/product/27327/)

Chromatogram: *N*-ethyl Heptedrone



Additional peaks present in chromatogram: internal standard (3.205 min), not a controlled substance (4.703 min), internal standard (6.279 min)

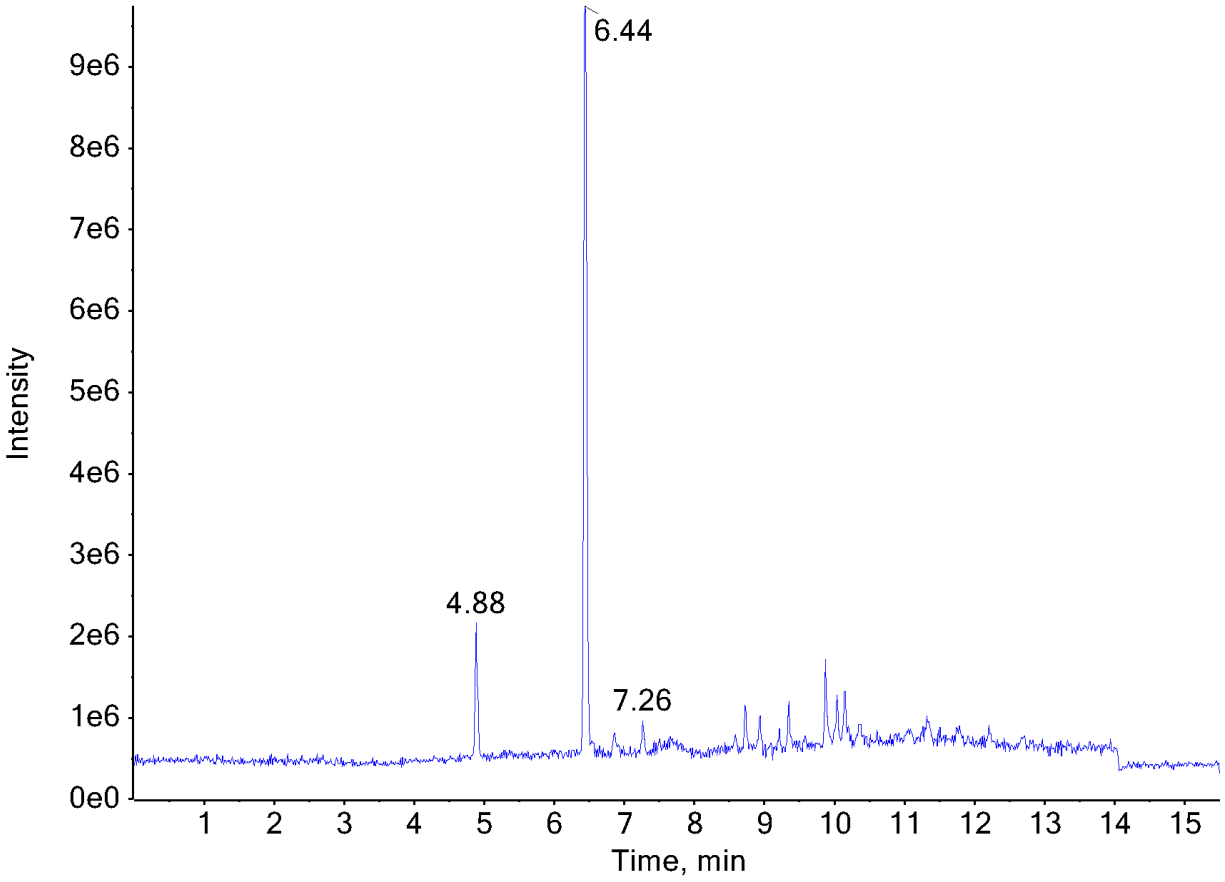
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *N*-ethyl Heptedrone



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:	6.44 min
Standard Comparison:	Reference material for *N*-ethyl heptedrone (Batch: 0549986-6) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *N*-ethyl heptedrone, based on retention time (6.45 min) and mass spectral data. (https://www.caymanchem.com/product/27327/)

Chromatogram: *N*-ethyl Heptedrone



Additional peak present in chromatogram: internal standards (4.88 min and 7.26 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: *N*-ethyl Heptedrone