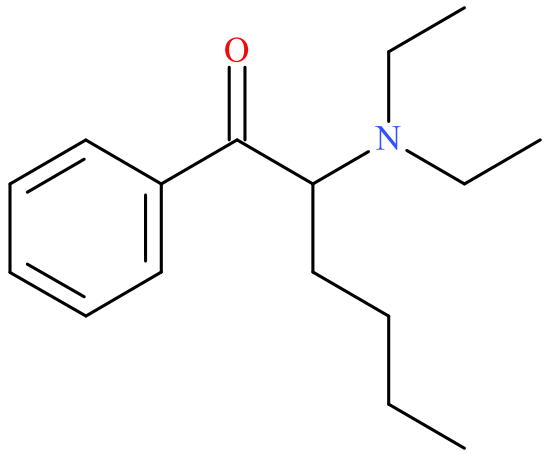
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

N,*N*-Diethyl Hexedrone

Sample Type: **Seized Material**



Latest Revision: **March 18, 2019**

Date Received: **February 15, 2019**

Date of Report: **March 18, 2019**

1. GENERAL INFORMATION

IUPAC Name:	2-(diethylamino)-1-phenyl-hexan-1-one
InChI String:	InChI=1S/C16H25NO/c1-4-7-13-15(17(5-2)6-3)16(18)14-11-9-8-10-12-14/h8-12,15H,4-7,13H2,1-3H3
CFR:	Not Scheduled (03/2019)
CAS#	Not Available
Synonyms:	Diethylhexedrone, α-Diethylaminohexanophenone
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	$C_{16}H_{25}NO$	247.37	247	248.2009

3. BRIEF DESCRIPTION

N,*N*-Diethyl Hexedrone is classified as a synthetic (or novel) stimulant and substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Synthetic stimulants have been reported to cause stimulant-like effects, similar to amphetamines. Synthetic stimulants have also caused adverse events, including death, as described in the literature. Structurally similar compounds include pentedrone, hexedrone, and *N*-ethyl hexedrone. In the United States, hexedrone, *N*-ethyl hexedrone, and *N*,*N*-diethyl hexedrone are not scheduled substances; however, pentedrone is a Schedule I substance.

4. ADDITIONAL RESOURCES

No additional resources are available at this time.

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

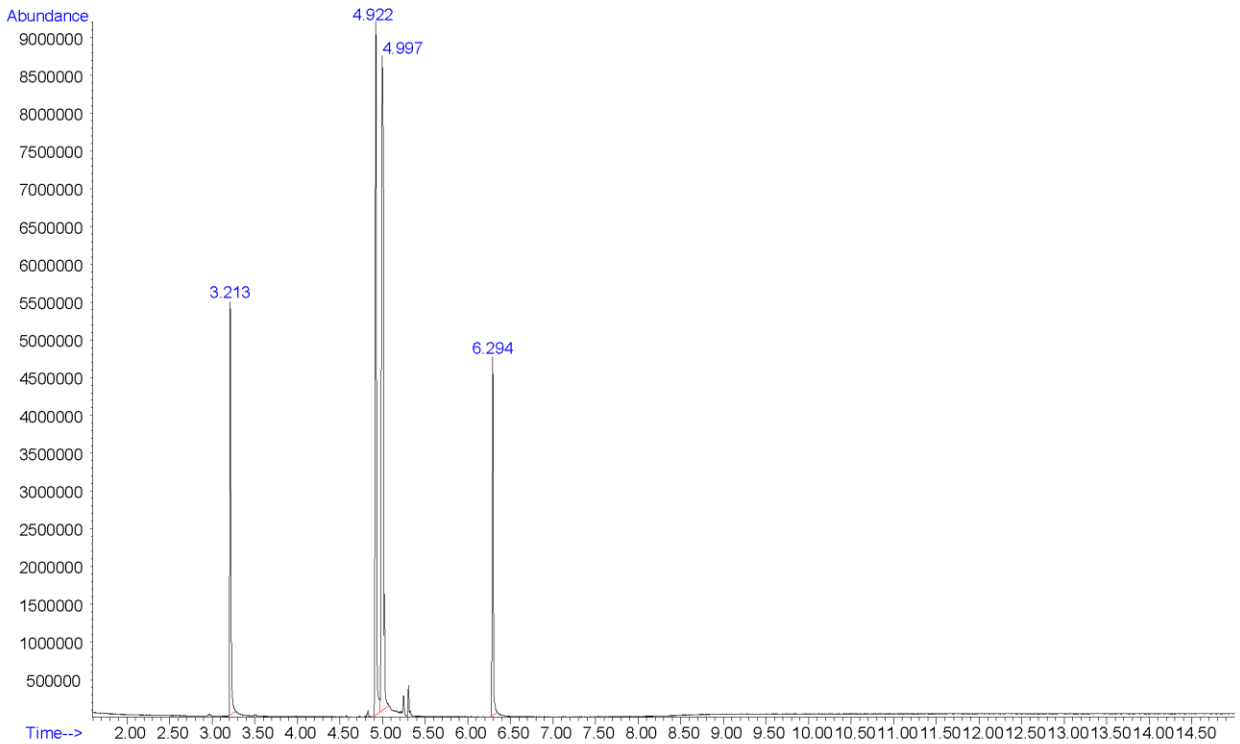
Transfer Line: 300 °C

MS Source: 230 °C

MS Quad: 150 °C

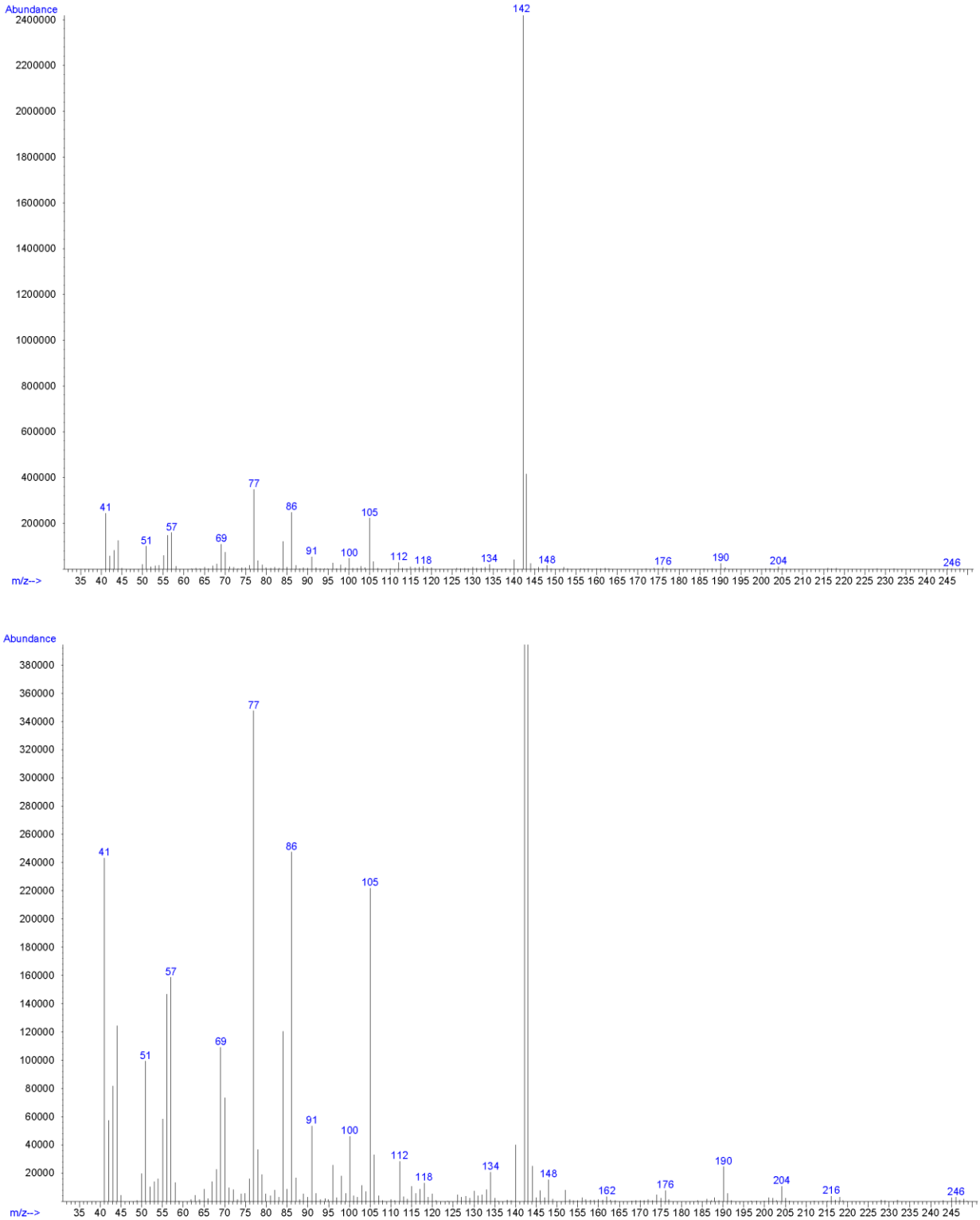
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	4.997 min

Chromatogram: *N,N*-Diethyl Hexedrone



Additional peaks present in chromatogram: internal standard (3.213 min), not a controlled substance (4.922 min), and internal standard (6.294 min)

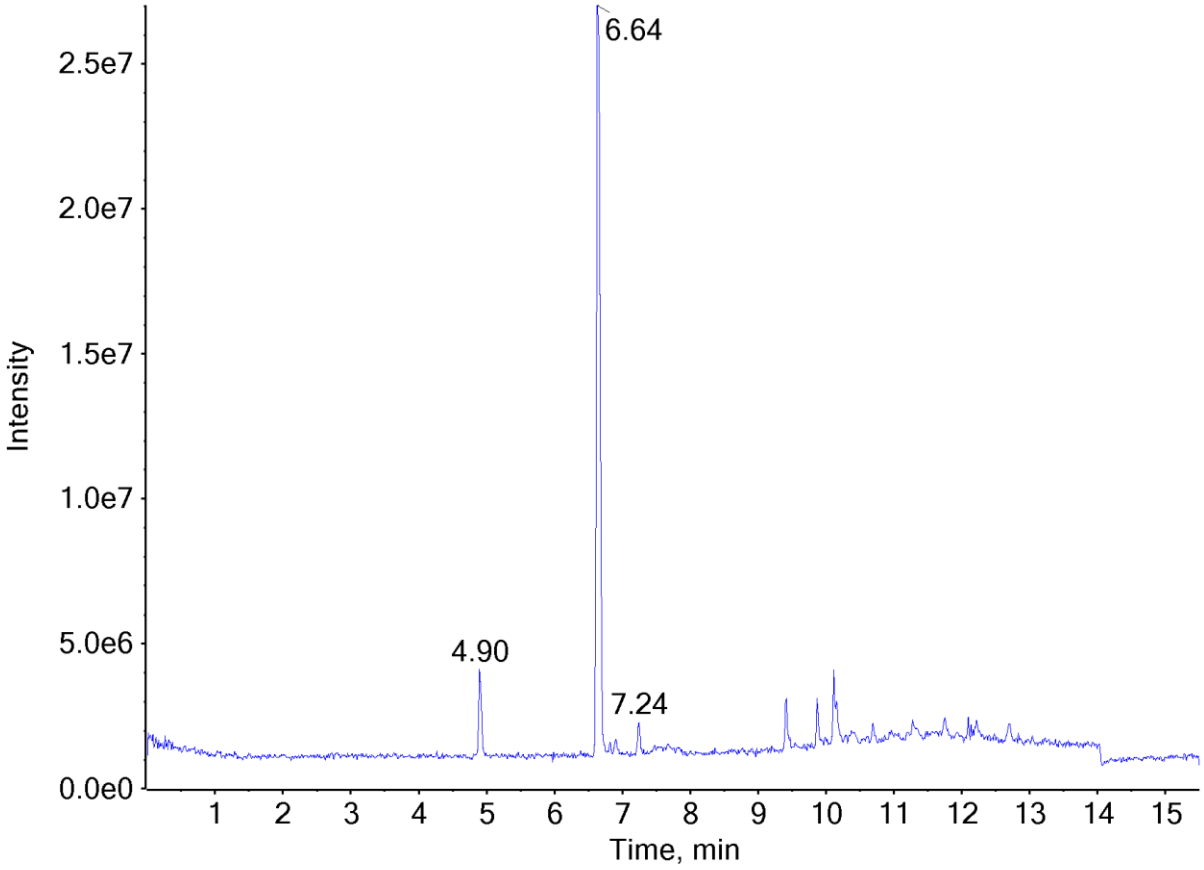
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *N,N*-Diethyl Hexedrone



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

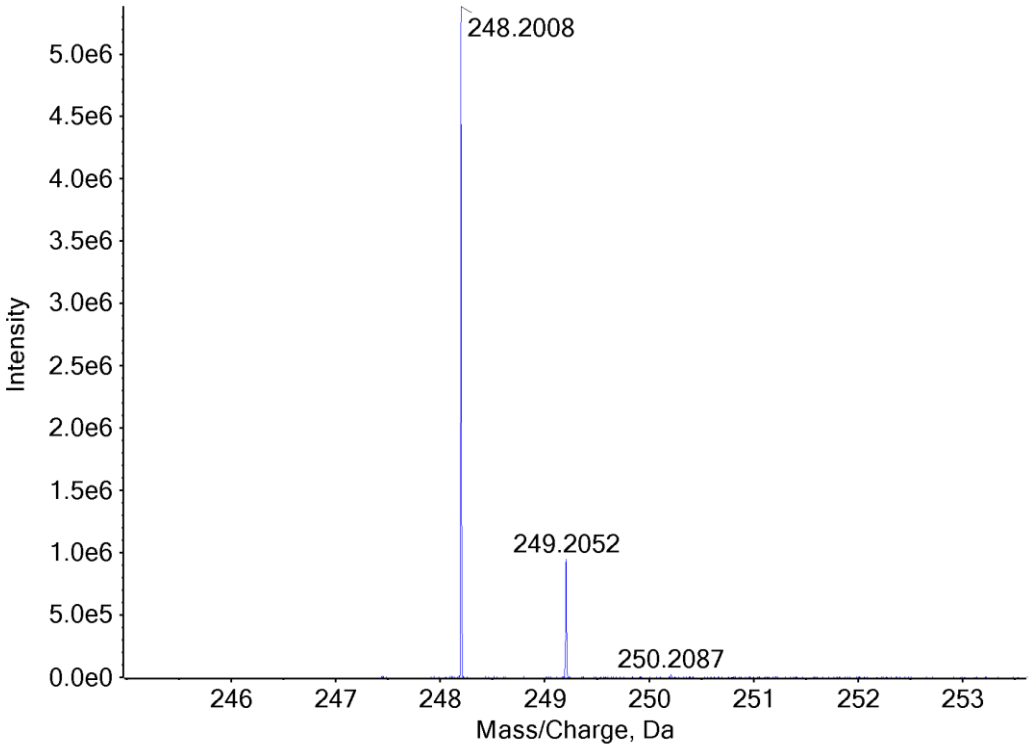
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extract in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex C18 (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:	6.64 min

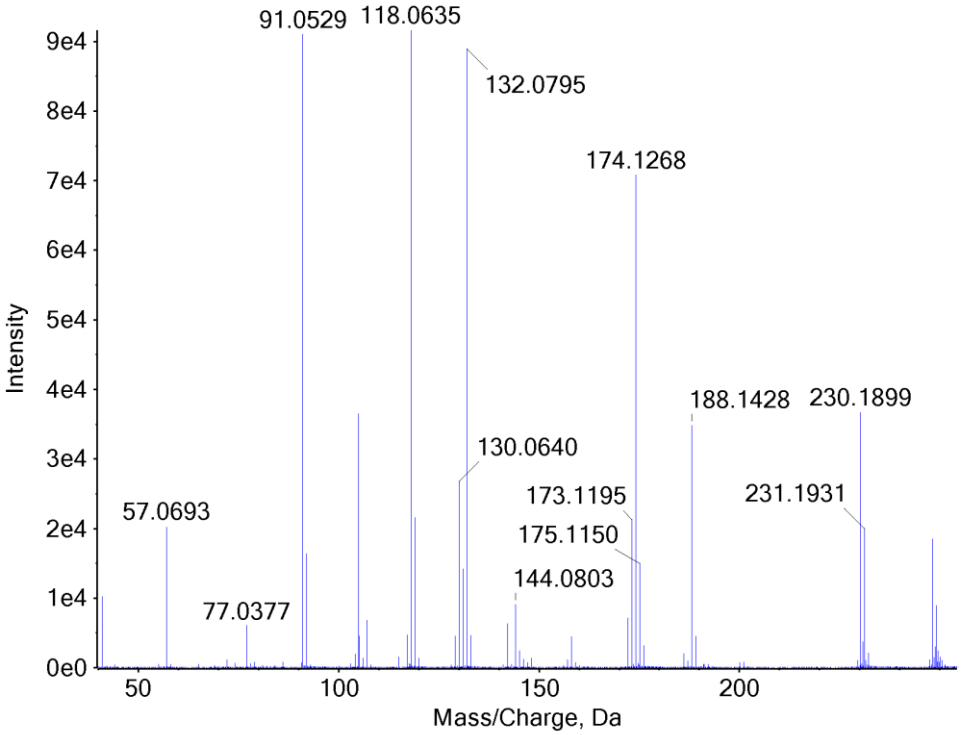
Chromatogram: *N,N*-Diethyl Hexedrone



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

TOF MS (Top) and MS/MS (Bottom) Spectra: *N,N*-Diethyl Hexedrone





5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in $CDCl_3$

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters: Pulse Sequence: Proton

Solvent: $CDCl_3$

Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

Delay between pulses: 1st delay, d1 = 1.000

^{1}H NMR: *N,N*-Diethyl Hexedrone

^{1}H NMR (300 MHz, CHLOROFORM-*d*) δ ppm 0.81 - 0.93 (m, 6 H) 1.18 - 1.55 (m, 9 H) 1.64 - 1.88 (m, 2 H) 2.41 - 2.59 (m, 2 H) 4.18 (dd, *J*=6.74, 4.98 Hz, 1 H) 7.45 - 7.62 (m, 3 H) 7.94 - 7.99 (m, 2 H)