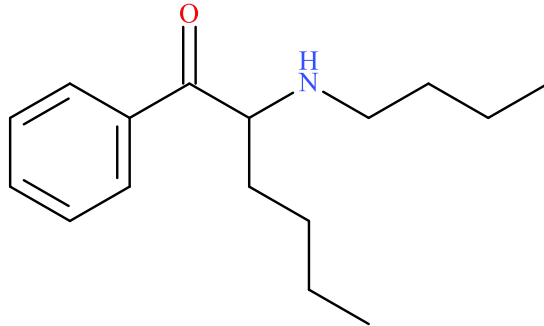


N-butyl Hexedrone

Sample Type: **Seized Material**



Latest Revision: **July 3, 2019**

Date Received: **May 7, 2019**

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

1. GENERAL INFORMATION

IUPAC Name:	2-(butylamino)-1-phenyl-hexan-1-one
InChI String:	InChI=1S/C16H25NO/c1-3-5-12-15(17-13-6-4-2)16(18)14-10-8-7-9-11-14/h7-11,15,17H,3-6,12-13H2,1-2H3
CFR:	Not Scheduled (07/2019)
CAS#	18296-66-7
Synonyms:	N-butylhexedrone, alpha-Butylaminohexanophenone
Source:	Department of Homeland Security
Appearance:	Off-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	247.4	247	248.2009

3. BRIEF DESCRIPTION

N-butyl Hexedrone 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 is a Schedule I substances in the United States; however, hexedrone, *N*-ethyl hexedrone, and *N*-butyl hexedrone are not scheduled.

4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/27728>

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/Butylhexedrone-ID-2065-19_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 (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

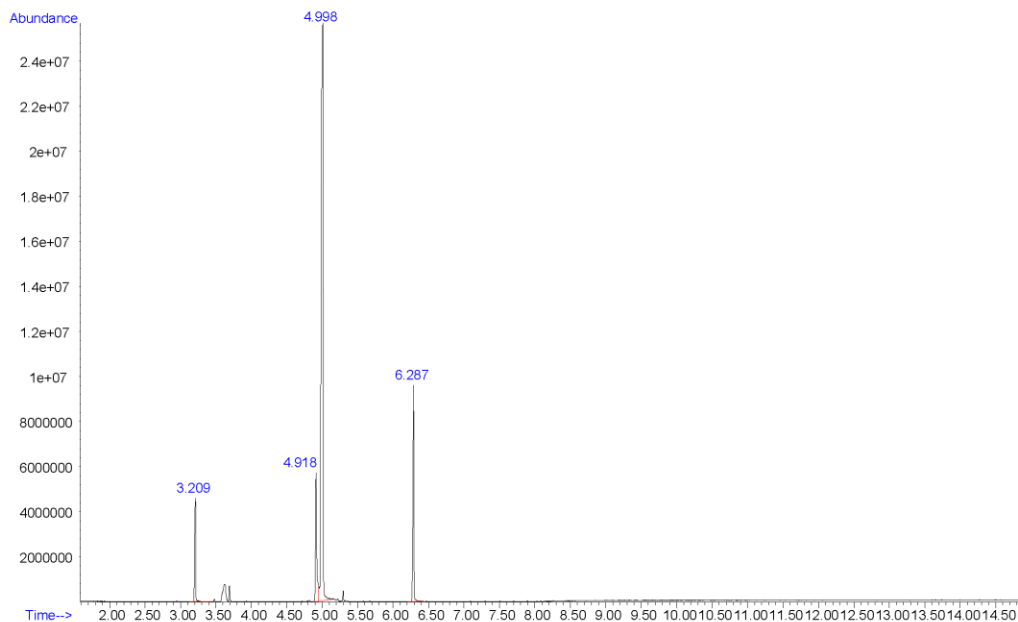
Threshold: 250

Retention Time: 4.998 min

Standard Comparison: Reference material for *N*-butyl hexedrone (Batch: 0556909-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *N*-butyl hexedrone, based on retention time (4.992 min) and mass spectral data.

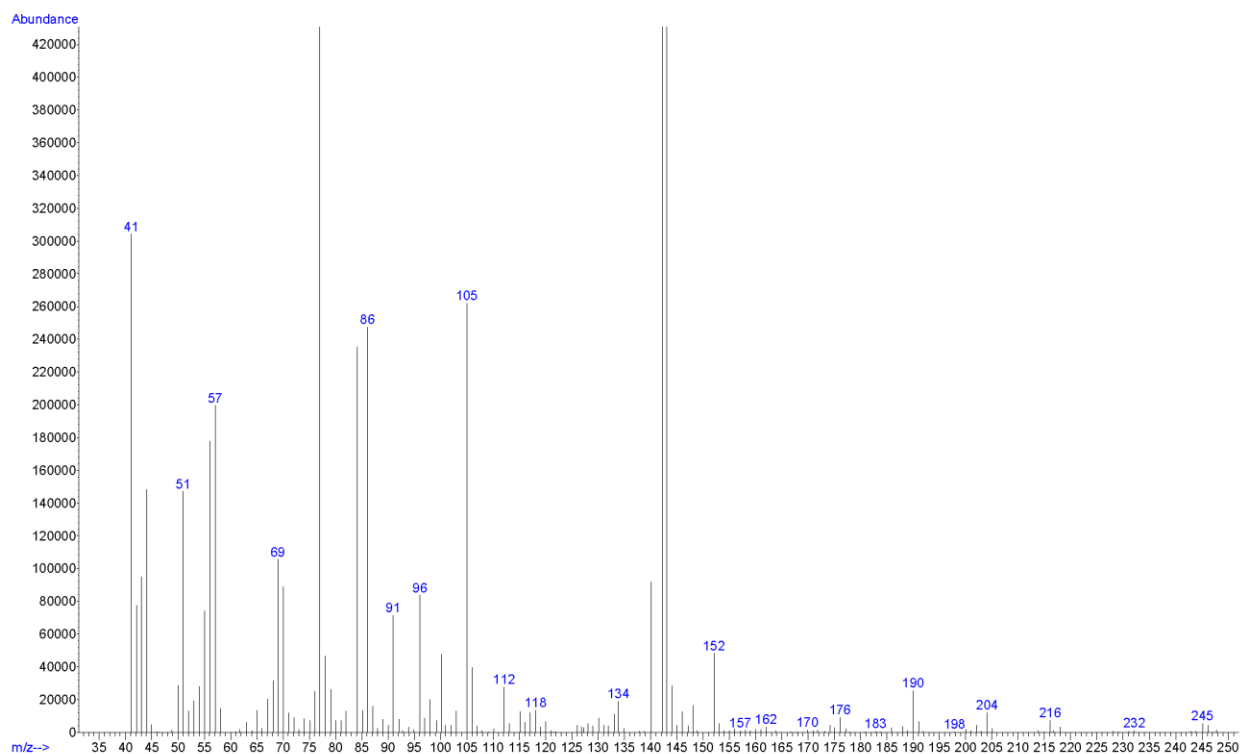
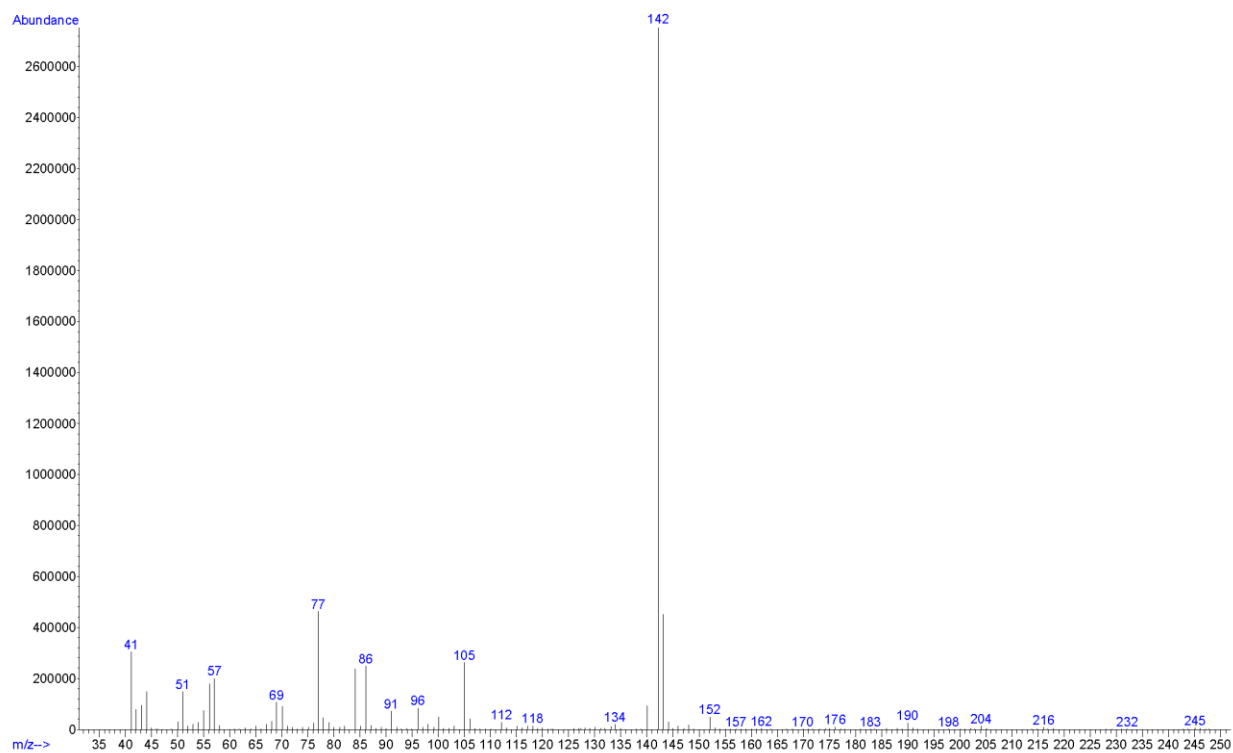
<https://www.caymanchem.com/product/27728>

Chromatogram: *N*-butyl Hexedrone



Additional peak present in chromatogram: internal standard (3.209 min), not a controlled substance (4.918 min), and internal standard (6.287 min)

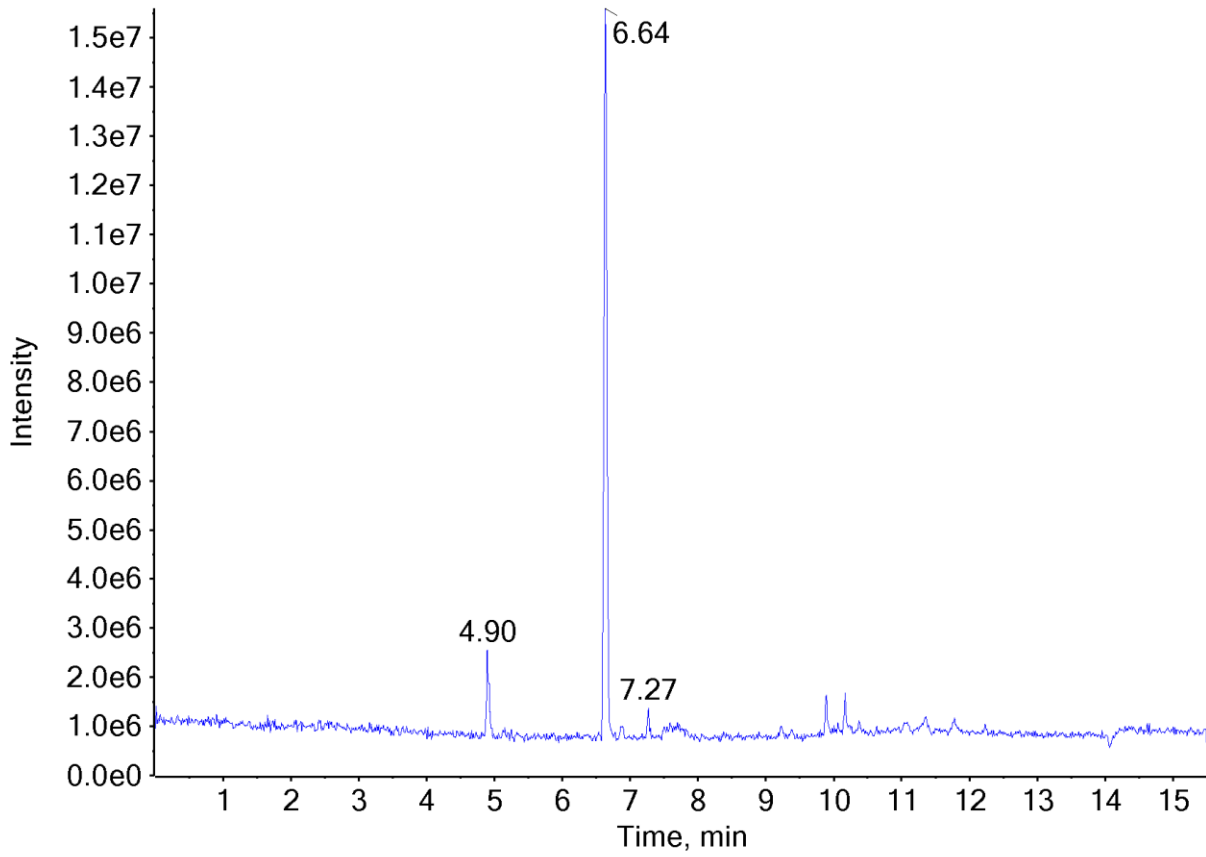
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *N*-butyl Hexedrone



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: Collision Energy Spread (35±15 eV) MS/MS Scan Range: 50-510 Da
Retention Time:	6.64 min
Standard Comparison:	Reference material for <i>N</i> -butyl hexedrone (Batch: 0556909-4) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as <i>N</i> -butyl hexedrone, based on retention time (6.62 min) and mass spectral data. (https://www.caymanchem.com/product/27728)

Chromatogram: N-butyl Hexedrone



Additional peak present in chromatogram: internal standards (4.90 min and 7.27 min)

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

