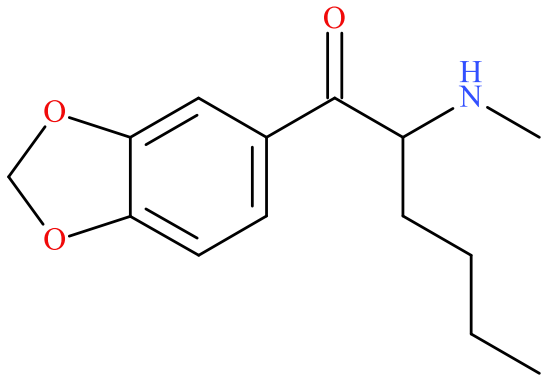
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

Hexylone



Sample Type: **Seized Material**

Latest Revision: **June 9, 2020**

Date Received: **March 3, 2020**

Date of Report: **June 9, 2020**

1. GENERAL INFORMATION

IUPAC Name:	1-(1,3-benzodioxol-5-yl)-2-(methylamino)hexan-1-one
InChI String:	InChI=1S/C14H19NO3/c1-3-4-5-11(15-2)14(16)10-6-7-12-13(8-10)18-9-17-12/h6-8,11,15H,3-5,9H2,1-2H3
CFR:	Not Scheduled (06/2020)
CAS#	Not Available
Synonyms:	*N*-Methyl Hexylone
Source:	Department of Homeland Security
Appearance:	Off-White Solid Material

***Important Note**: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.*

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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	$C_{14}H_{19}NO_3$	249.3	249	250.1438

3. BRIEF DESCRIPTION

Hexylone 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 pentylone, pentylone, and *N*-ethyl hexylone. *N*-Ethyl pentylone and pentylone are Schedule I substances in the United States. *N*-Ethyl hexylone is not explicitly scheduled in the United States; its appearance was first reported in the United States by NPS Discovery in April 2018. Hexylone is also not explicitly scheduled.

4. ADDITIONAL RESOURCES

Synthesis of related analogues: Koppe, H.; Ludwig, G.; and Zeile, K. Aryl-alpha-Aminoketone Derivatives. CH Boehringer Sohn AG and Co KG, Boehringer Ingelheim GmbH, Assignee. Patent GB1085135A. 08 Apr. 1964.

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)

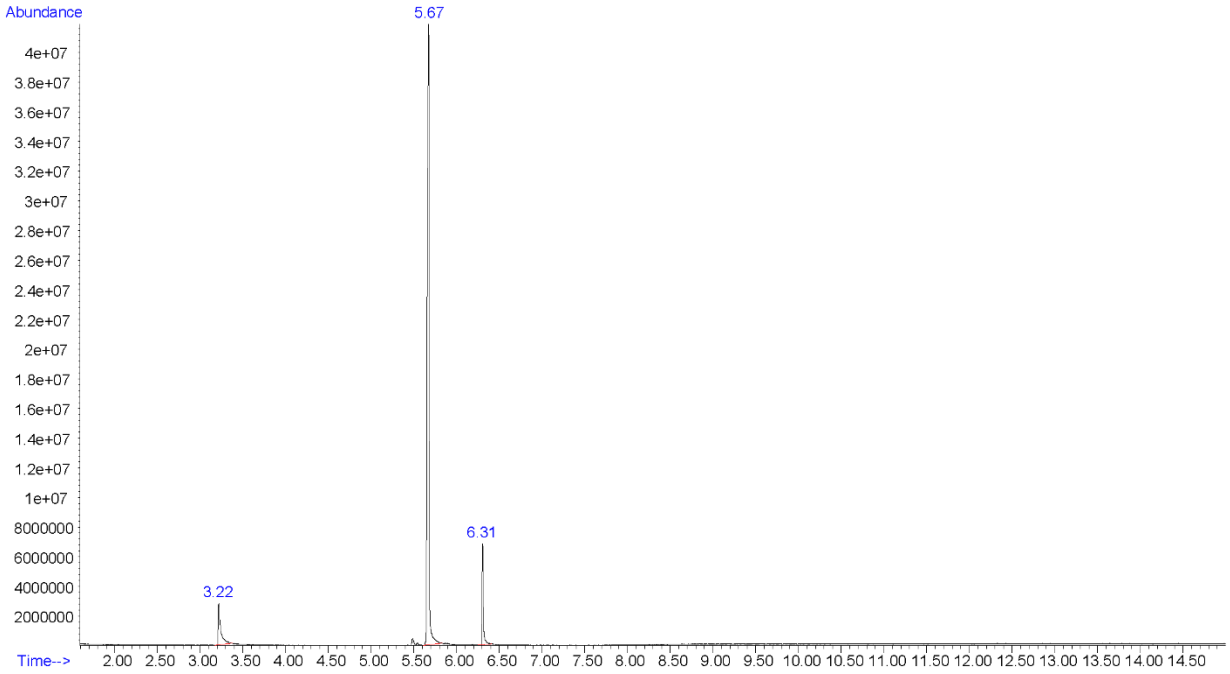
Carrier Gas: Helium (Flow: 1 mL/min)

Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

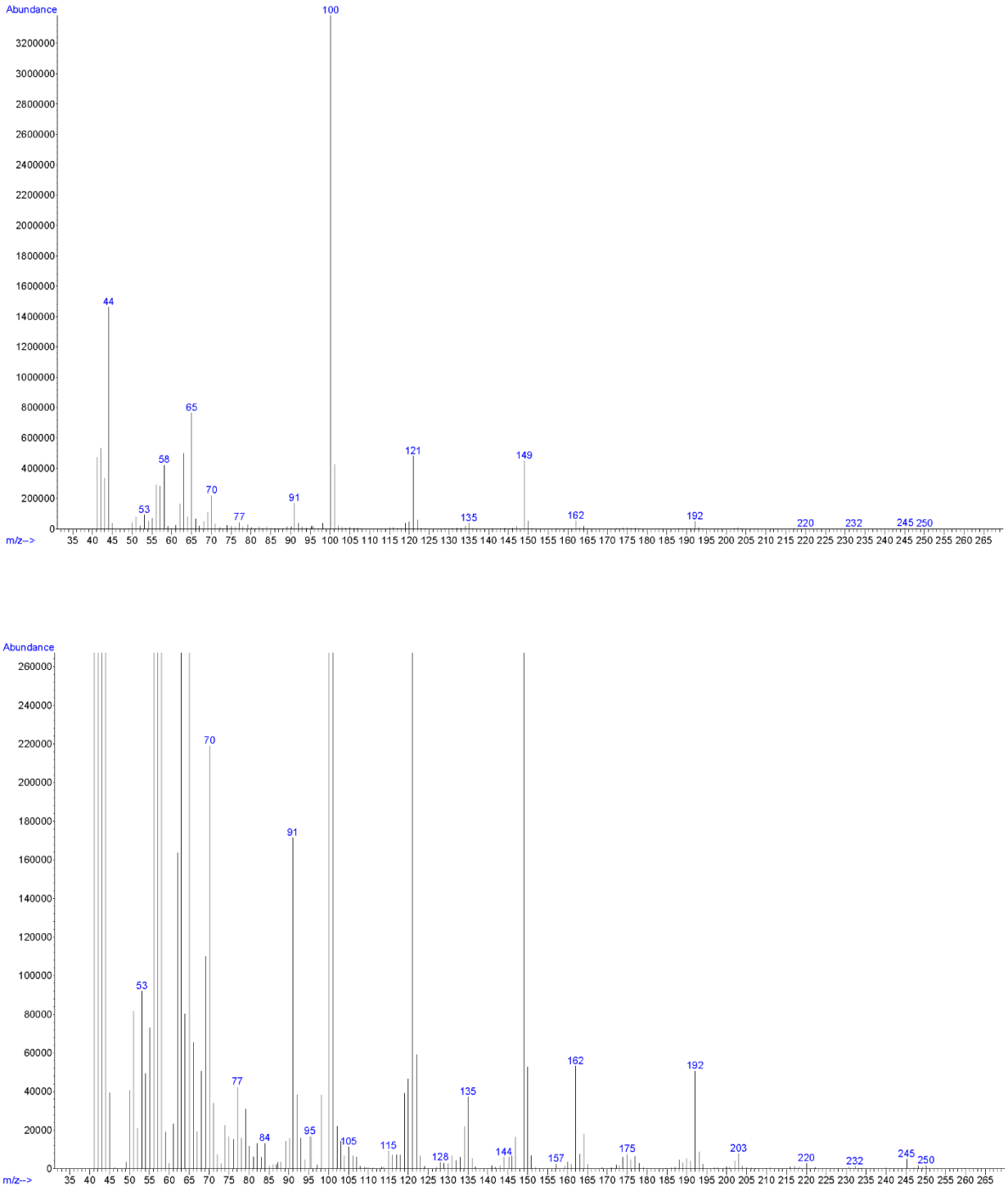
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	5.67 min

Chromatogram: Hexylone



Additional peaks present in chromatogram: internal standards (3.22 min and 6.31 min)

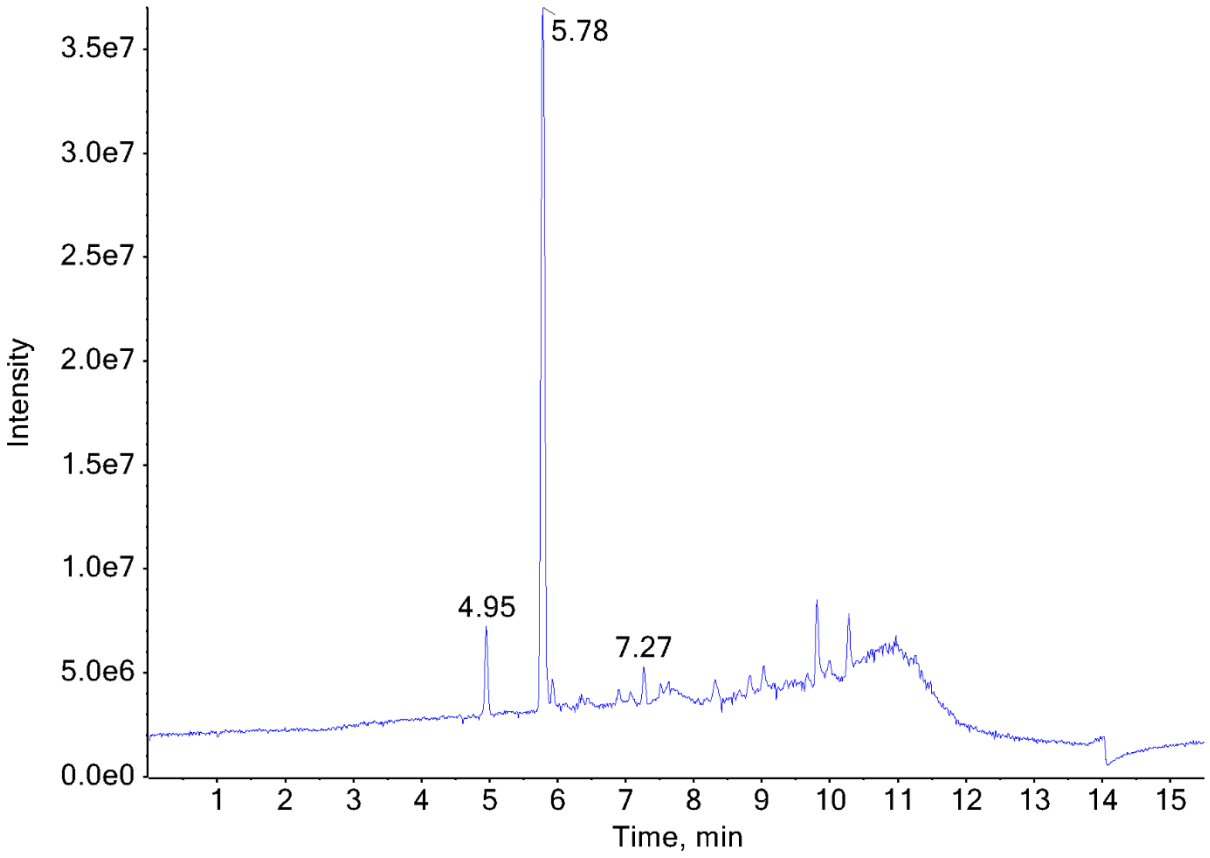
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Hexylone



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

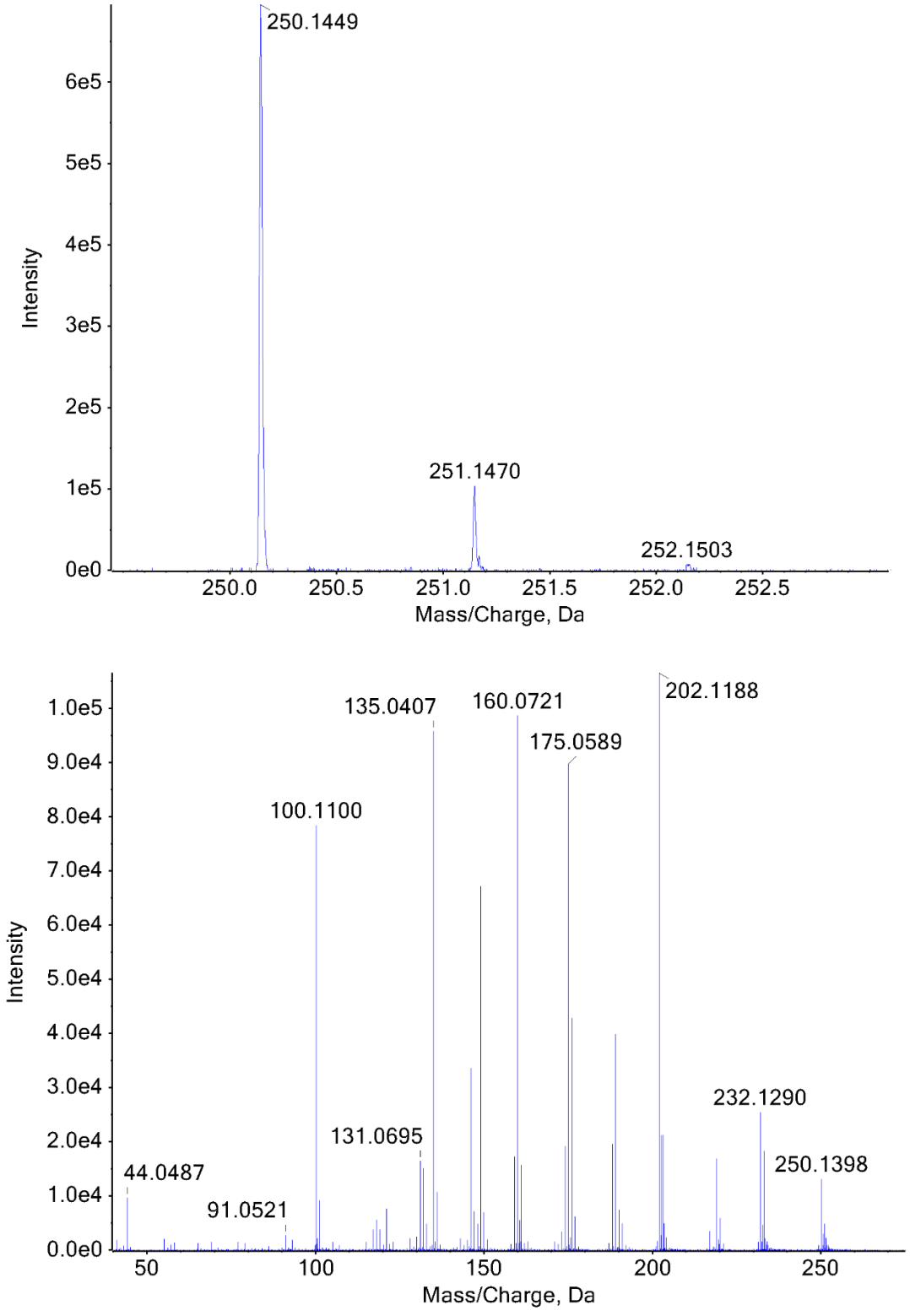
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	1:100 dilution of acid/base extraction in mobile phase
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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: Collison Energy Spread (35±15 eV)
	MS/MS Scan Range: 50-510 Da
Retention Time:	5.78 min

Chromatogram: Hexylone



Additional peaks present in chromatogram: internal standards (4.95 min and 7.27 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: Hexylone



5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in DMSO-D6

Instrument: 300 MHz INOVA VARIAN Spectrometer

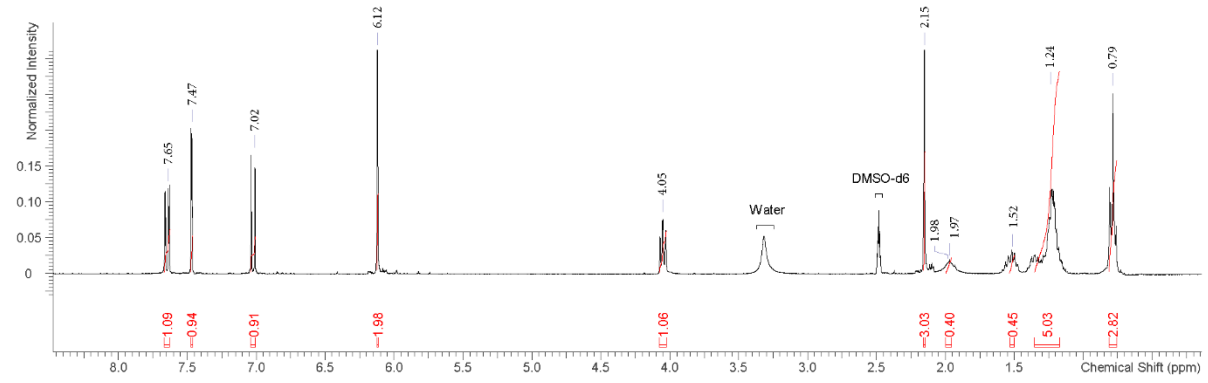
Parameters: Pulse Sequence: Proton

Solvent: DMSO-D6

Spectral Width: 4798.5 Hz

Delay between pulses: 1st delay, d1 = 1.000

^{1}H NMR:Hexylone



^{13}C NMR: Hexylone