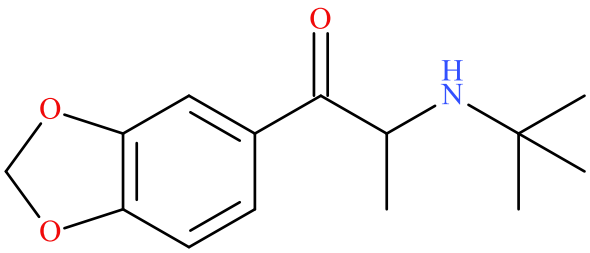
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

Tertylone



Sample Type: **Seized Material**

Latest Revision: **August 6, 2018**

Date Received: **July 6, 2018**

Date of Report: **August 6, 2018**

1. GENERAL INFORMATION

IUPAC Name: 1-(1,3-benzodioxol-5-yl)-2-(tert-butylamino)propan-1-one

InChI String: InChI=1S/C14H19NO3/c1-9(15-14(2,3)4)13(16)10-5-6-11-12(7-10)18-8-17-11/h5-7,9,15H,8H2,1-4H3

CFR: Not Scheduled (08/2018)

CAS# Not Available

Synonyms: 3',4'-Methylenedioxy-N-tert-butylcathinone, MDPT(tBuONE), D-Tertylone

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

***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, and Barry K. Logan, PhD, F-ABFT*

3. BRIEF DESCRIPTION

Tertylone 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, methylone, and butylone. Pentylone, methylone, and butylone are all Schedule I substances in the United States, while *N*-ethyl pentylone is not permanently scheduled in the United States.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/18587

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/tBuONE-ID-1378-15-report_final1.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:	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

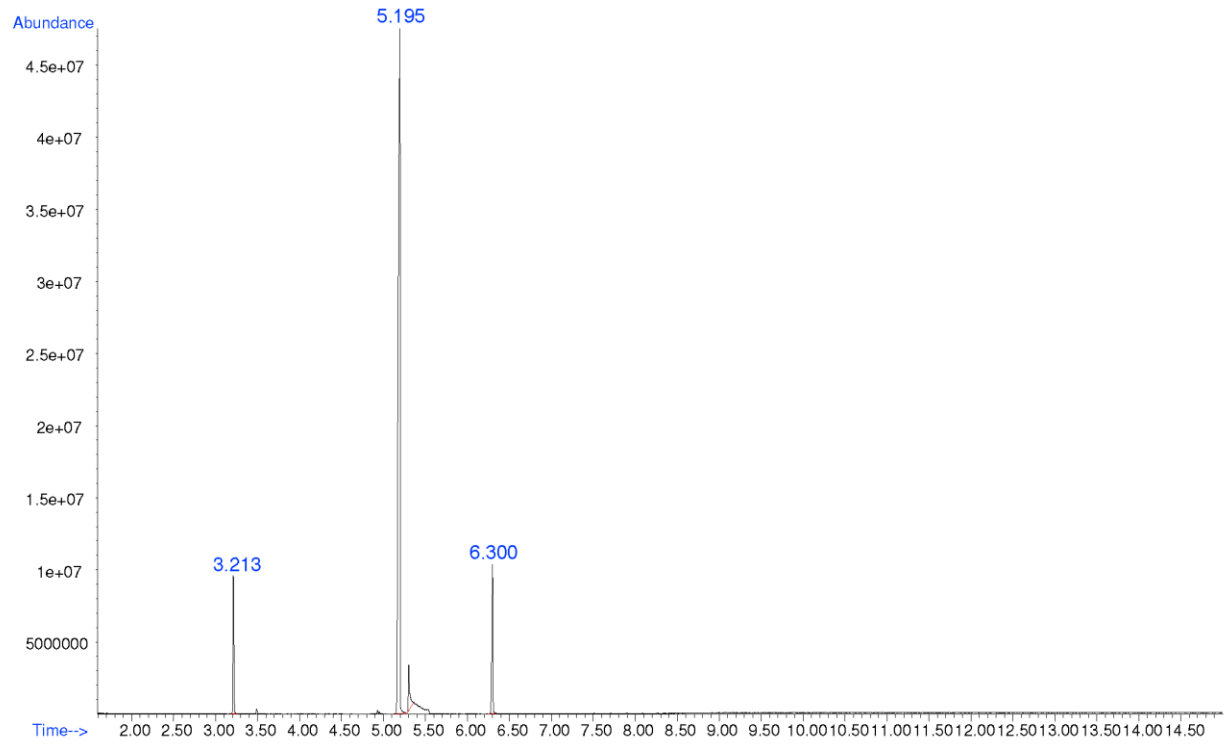
MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

Retention Time: 5.195 min

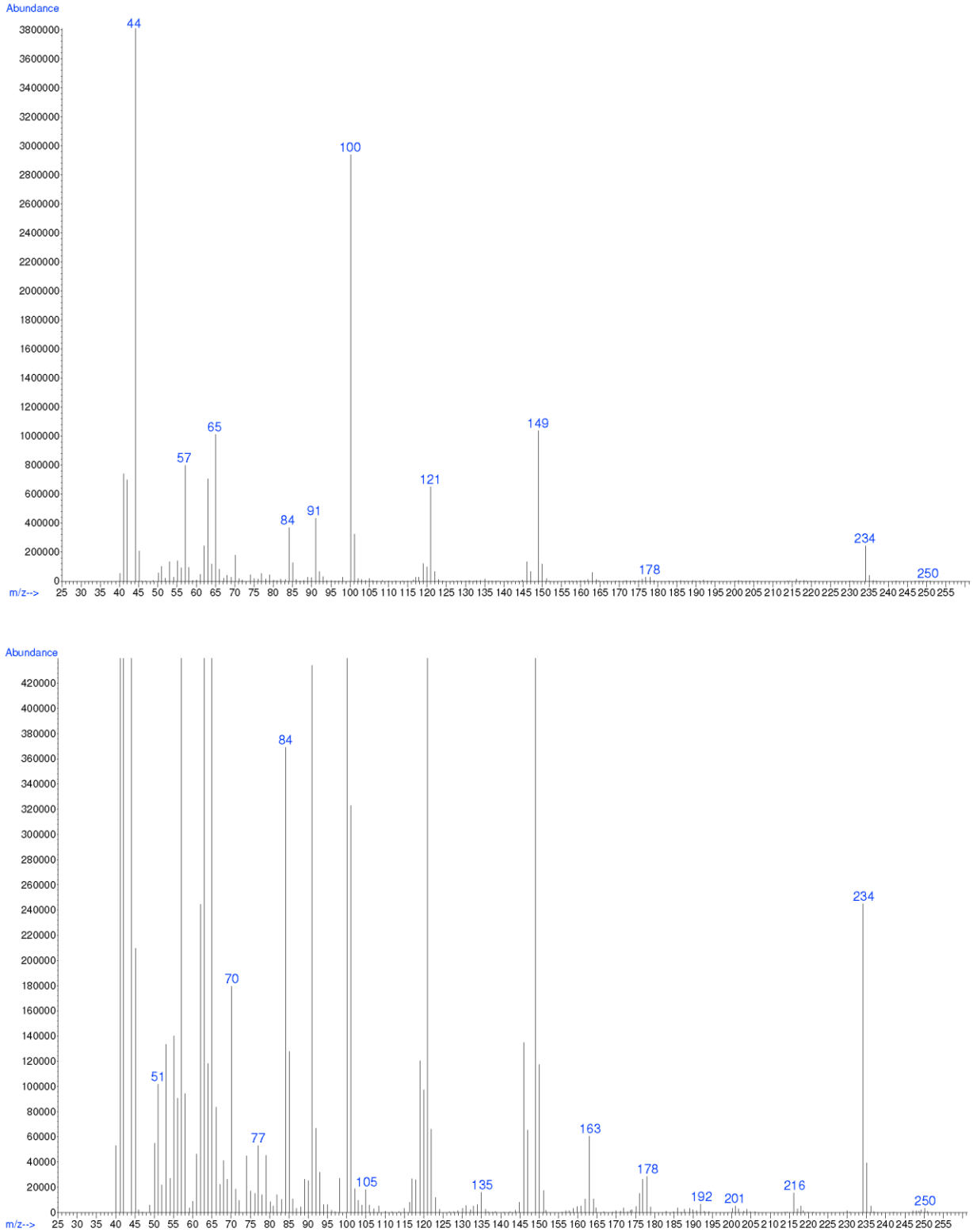
Standard Comparison: Reference material for Tertylone (Batch: 0475424-17) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Tertylone, based on retention time (5.165 min) and mass spectral data. (https://www.caymanchem.com/product/18587)

Chromatogram: Tertylone



Additional peaks present in chromatogram: internal standard 1 (3.213 min), internal standard 2 (6.300 min)

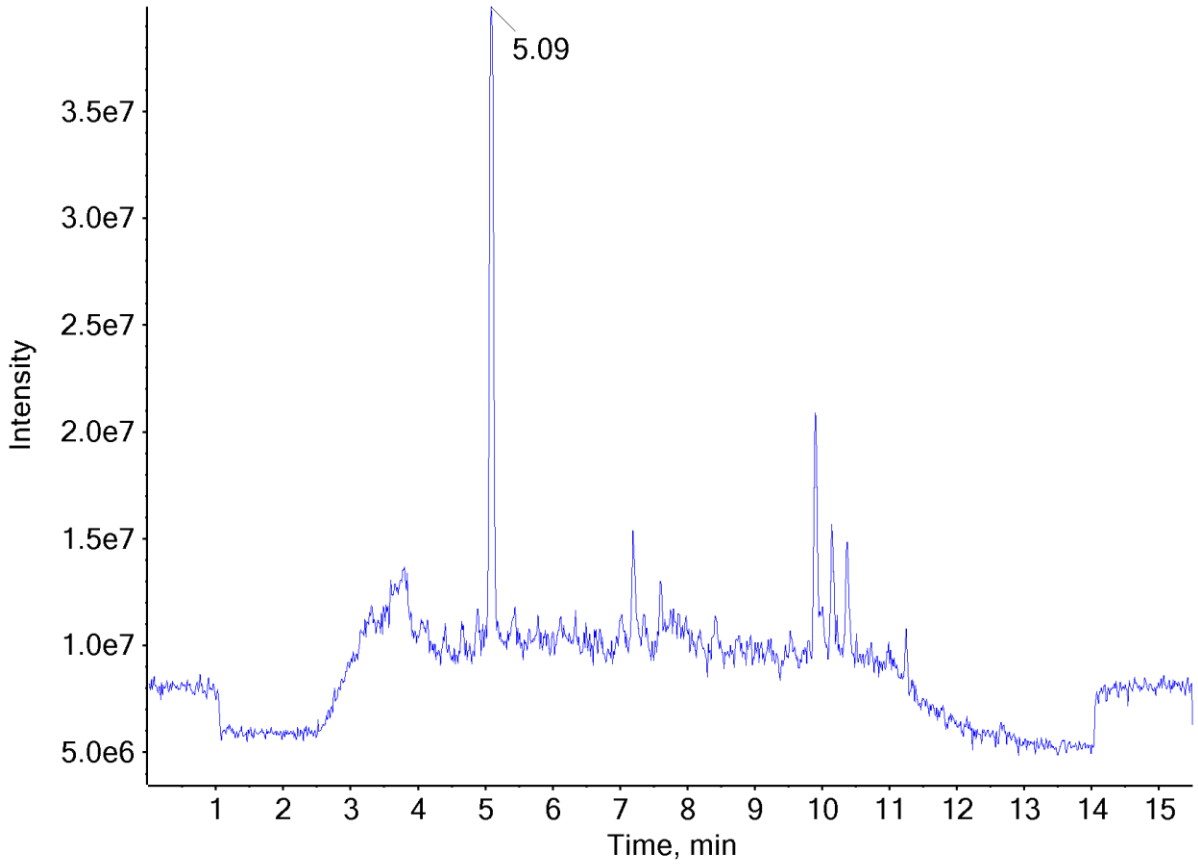
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Tertylone



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:	5.09 min
Standard Comparison:	Reference material for Tertylone (Batch: 0475424-19) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as Tertylone, based on retention time (4.94 min) and mass spectral data. (https://www.caymanchem.com/product/18587)

Chromatogram: Tertylone



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