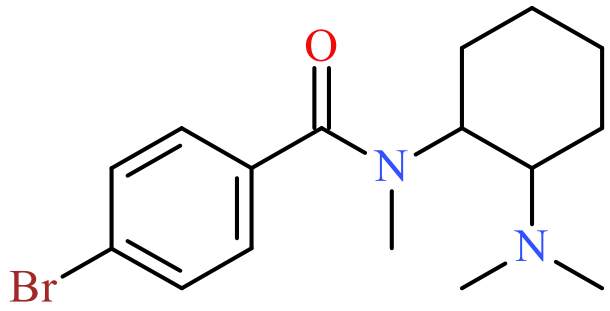
NMS Labs
2300 Stratford Ave
Willow Grove, PA 19090

N-Methyl U-47931E

Sample Type: **Seized Material**



Latest Revision: **November 22, 2019**

Date Received: **October 3, 2019**

Date of Report: **November 22, 2019**

1. GENERAL INFORMATION

IUPAC Name:	4-bromo-N-[2-(dimethylamino)cyclohexyl]-N-methyl-benzamide
InChI String:	InChI=1S/C16H23BrN2O/c1-18(2)14-6-4-5-7-15(14)19(3)16(20)12-8-10-13(17)11-9-12/h8-11,14-15H,4-7H2,1-3H3
CFR:	Not Scheduled (11/2019)
CAS#	75570-38-6
Synonyms:	*N*-Methyl Bromadoline
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-MS) in comparison to analysis of acquired reference material.*

***Prepared By:** Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, D-ABFT-FT, and Barry K. Logan, PhD, F-ABFT*

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion $[M^+]$	Exact Mass $[M+H]^+$
Base	$C_{16}H_{23}BrN_2O$	339.3	338	339.1067

3. BRIEF DESCRIPTION

N-Methyl U-47931E is classified as a novel opioid. Novel opioids have been reported to cause effects similar to heroin and fentanyl. Novel opioids in the trans-N-[2-(methylamino)cyclohexyl]-benzamide class, such as U-47700, and similar classes, such as U-49900, have caused adverse events, including deaths, as described in the literature. Structurally similar compounds include U-47931E (Bromadoline), U-47700, U-49900, U-48800, isopropyl-U-47700, and 3,4-methylenedioxy-U-47700. U-47931E was first reported in a seized drug exhibit by our organization in October 2018.[1] U-47700 is a Schedule I substance in the United States. *N*-Methyl U-47931E and U-47931E are not explicitly scheduled.

4. ADDITIONAL RESOURCES

1. https://www.npsdiscovery.org/wp-content/uploads/2019/06/U-47931E_103018_NMSLabs_Report.pdf

https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/N-methyl%20U-47931E-ID-1917-18_report.pdf

https://www.caymanchem.com/product/24286/

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

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

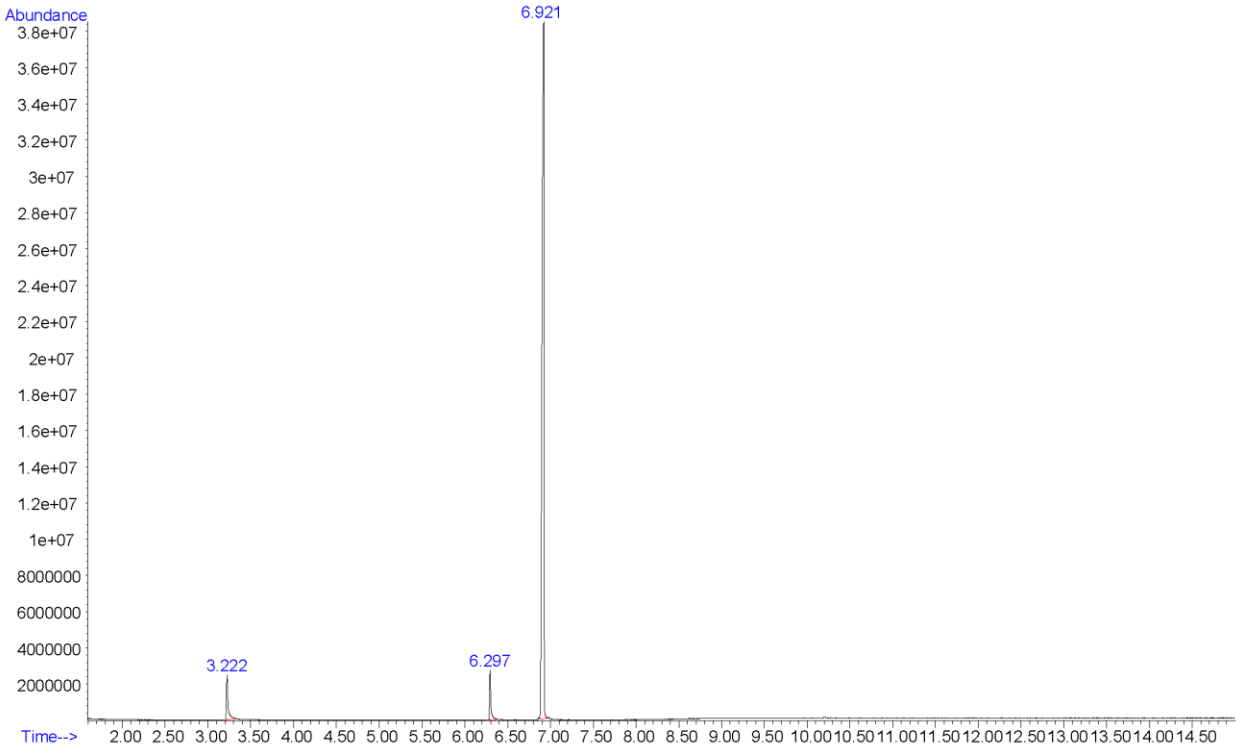
Sample Preparation: Acid/Base extraction

Instrument: Agilent 5975 Series GC/MSD System

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

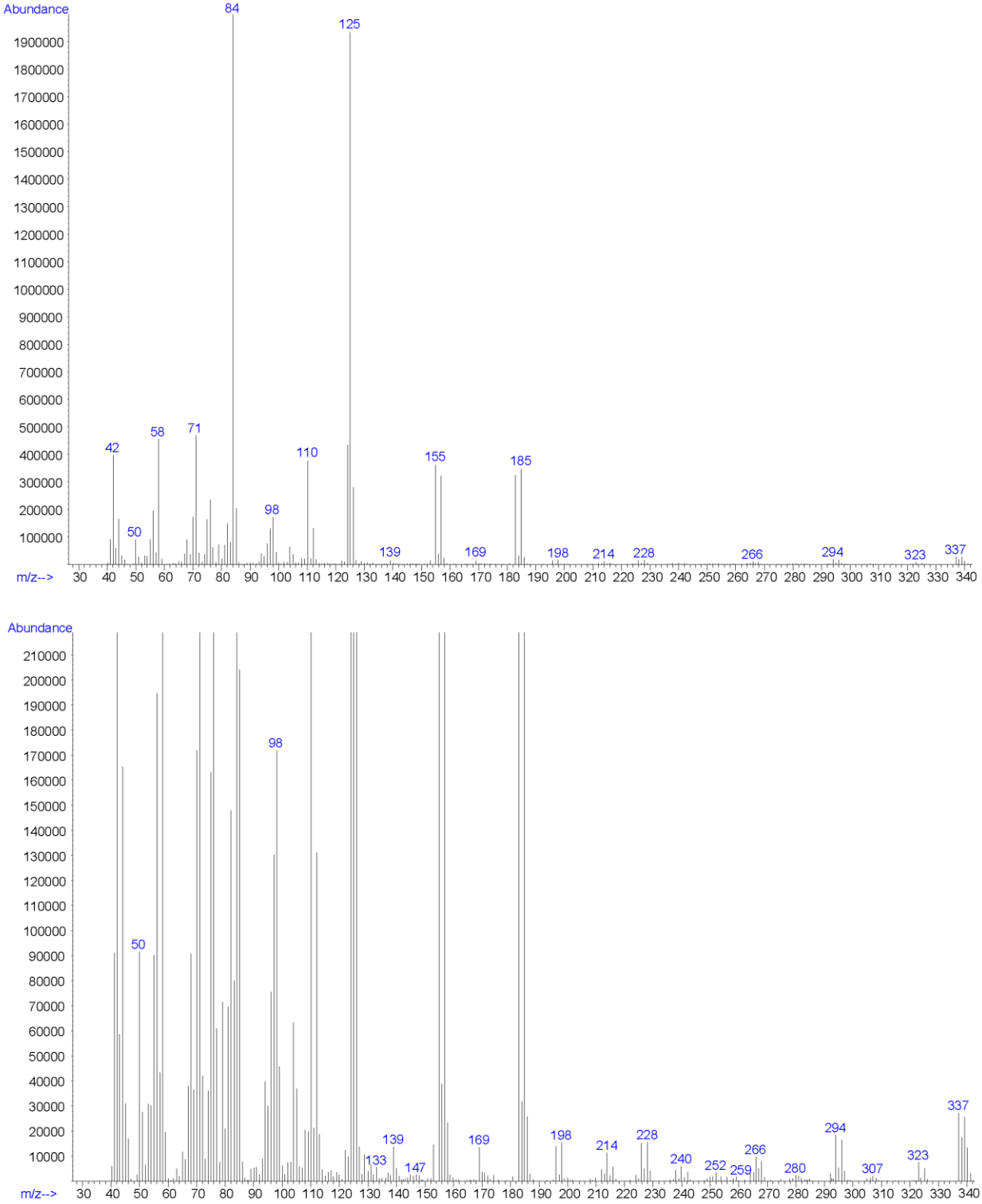
Carrier Gas:	Helium (Flow: 1 mL/min)
Temperatures:	Injection Port: 265 °C
	Transfer Line: 300 °C
	MS Source: 230 °C
	MS Quad: 150 °C
	Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min
Injection Parameters:	Injection Type: Splitless
	Injection Volume: 1 µL
MS Parameters:	Mass Scan Range: 40-550 m/z
	Threshold: 250
Retention Time:	6.921 min
Standard Comparison:	Reference material for *N*-Methyl U-47931E (Batch: 0521838-5) 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*-Methyl U-47931E, based on retention time (6.888 min) and mass spectral data. (https://www.caymanchem.com/product/24286/)

Chromatogram: *N*-Methyl U-47931E



Additional peaks present in chromatogram: internal standards (3.222 min and 6.297 min)

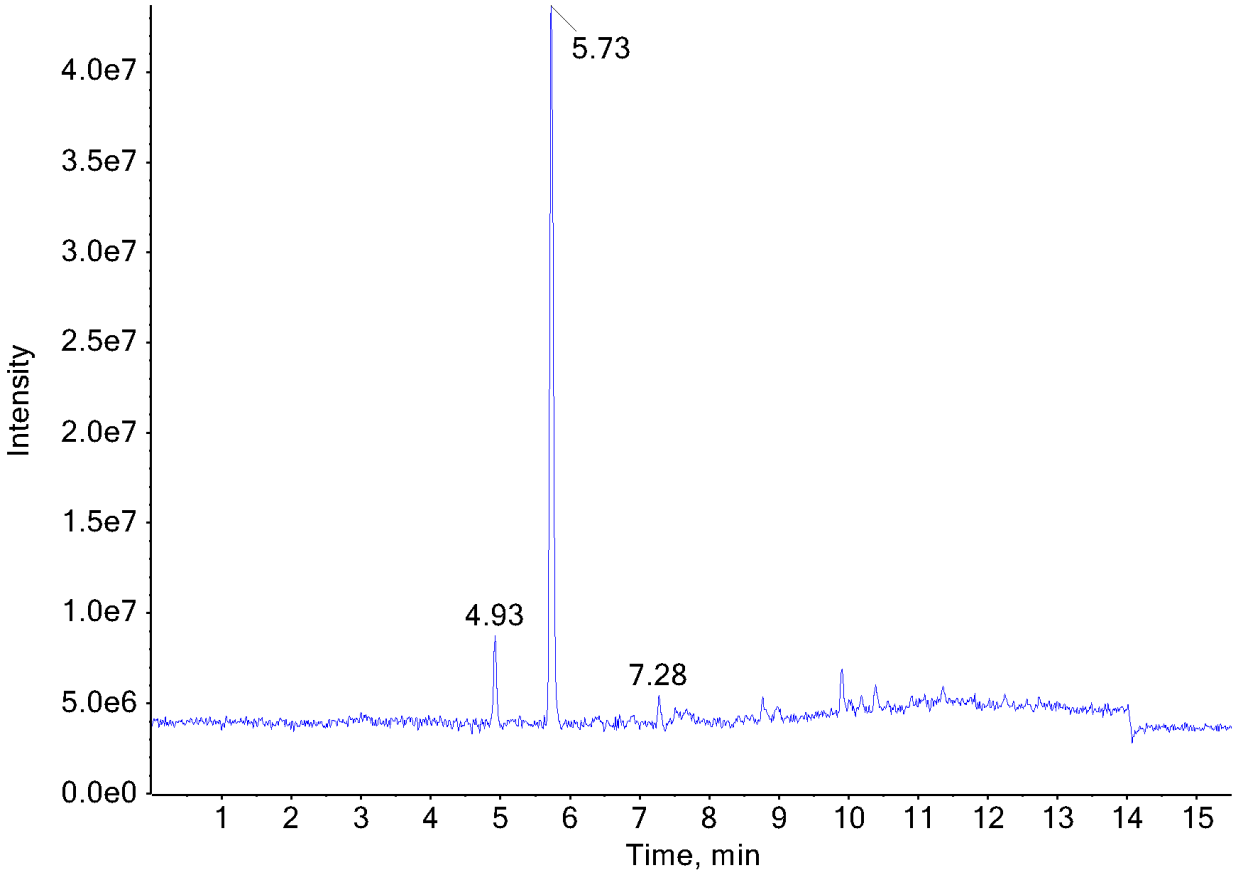
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): *N*-Methyl U-47931E



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:	5.73 min
Standard Comparison:	Reference material for *N*-Methyl U-47931E (Batch: 0521838-5) 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*-Methyl U-47931E, based on retention time (5.71 min) and mass spectral data. (https://www.caymanchem.com/product/24286/)

Chromatogram: *N*-Methyl U-47931E



Additional peaks present in chromatogram: internal standards (4.93 min and 7.28 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: *N*-Methyl U-47931E