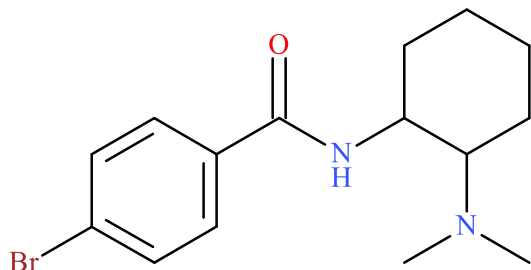


**U-47931E**

 Sample Type: **Seized Material**

 Latest Revision: **October 30, 2018**

 Date Received: **August 17, 2018**

 Date of Report: **October 30, 2018**

## 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	4-bromo-N-[2-(dimethylamino)cyclohexyl]benzamide
<b>InChI String:</b>	InChI=1S/C15H21BrN2O/c1-18(2)14-6-4-3-5-13(14)17-15(19)11-7-9-12(16)10-8-11/h7-10,13-14H,3-6H2,1-2H3,(H,17,19)
<b>CFR:</b>	Not Scheduled (10/2018)
<b>CAS#</b>	67579-24-2
<b>Synonyms:</b>	Bromadoline
<b>Source:</b>	Department of Homeland Security
<b>Appearance:</b>	White Solid Material

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Base	C <sub>15</sub> H <sub>21</sub> BrN <sub>2</sub> O	325.2	324	325.0910

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

### 3. BRIEF DESCRIPTION

U-47931E (Bromadoline) 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-47700, U-49900, U-48800, isopropyl-U-47700, and 3,4-methylenedioxy-U-47700. U-47700 is a Schedule I substance in the United States.

### 4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/20530>

[https://www.policija.si/apps/nfl\\_response\\_web/0\\_Analytical\\_Reports\\_final/U-47931E-ID-1869-17\\_report.pdf](https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/U-47931E-ID-1869-17_report.pdf)

### 5. QUALITATIVE DATA

#### 5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

<b>Testing Performed At:</b>	NMS Labs (Willow Grove, PA)
<b>Sample Preparation:</b>	Acid/base extraction
<b>Instrument:</b>	Agilent 5975 Series GC/MSD System
<b>Column:</b>	Zebron™ Inferno™ ZB-35HT (15 m x 250 μm x 0.25 μm)
<b>Carrier Gas:</b>	Helium (Flow: 1 mL/min)
<b>Temperatures:</b>	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
<b>Injection Parameters:</b>	Injection Type: Splitless Injection Volume: 1 μL

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

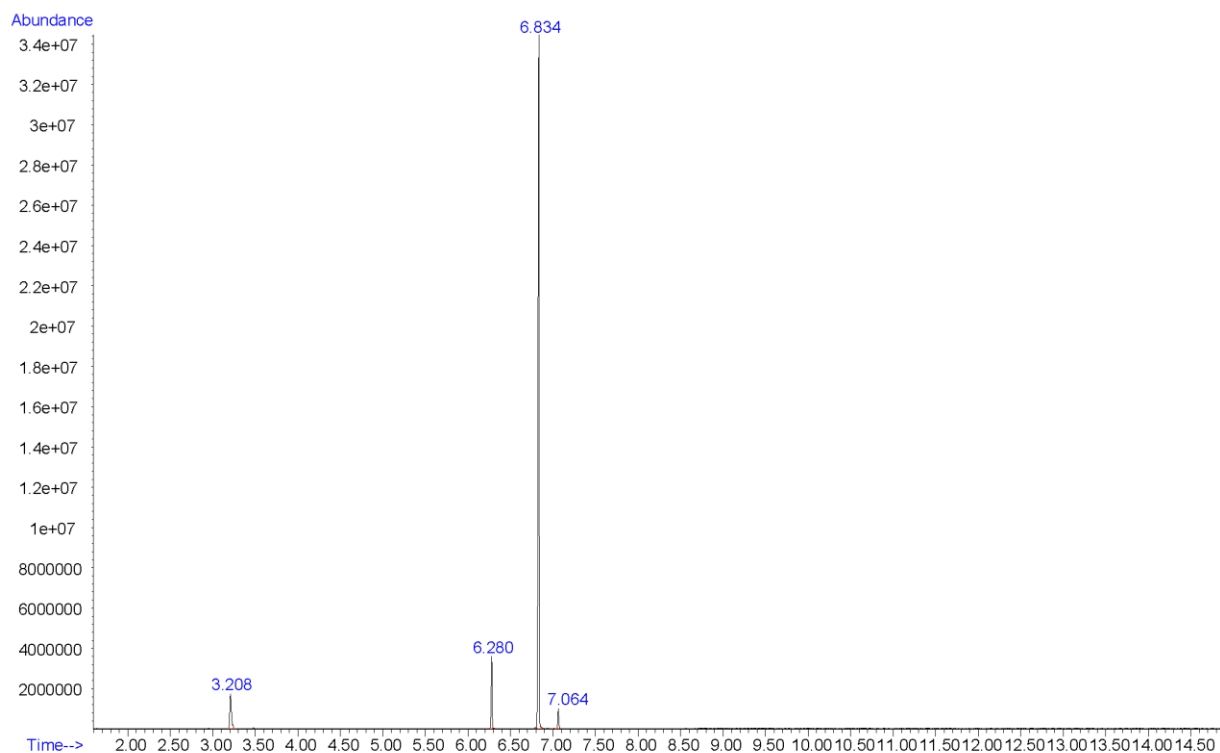
Threshold: 250

**Retention Time:** 6.834 min

**Standard Comparison:** Reference material for U-47931E (Batch: 0492764-5) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as U-47931E, based on retention time (6.817 min) and mass spectral data.

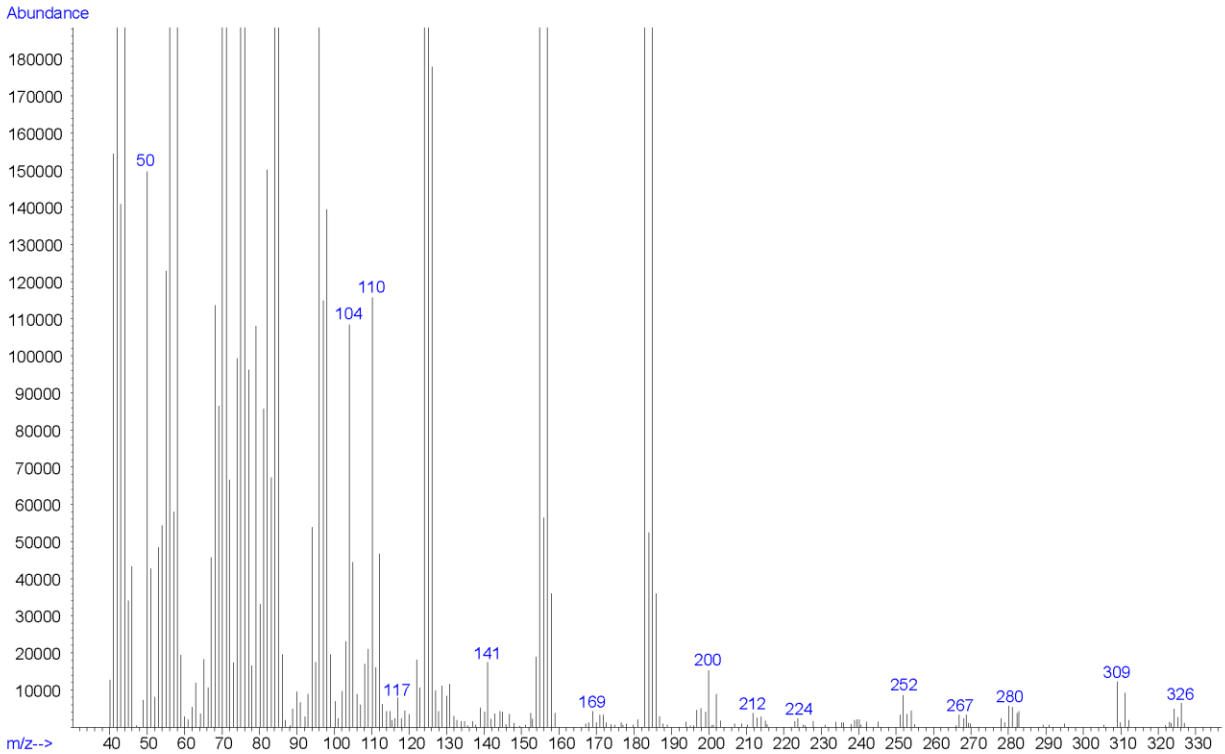
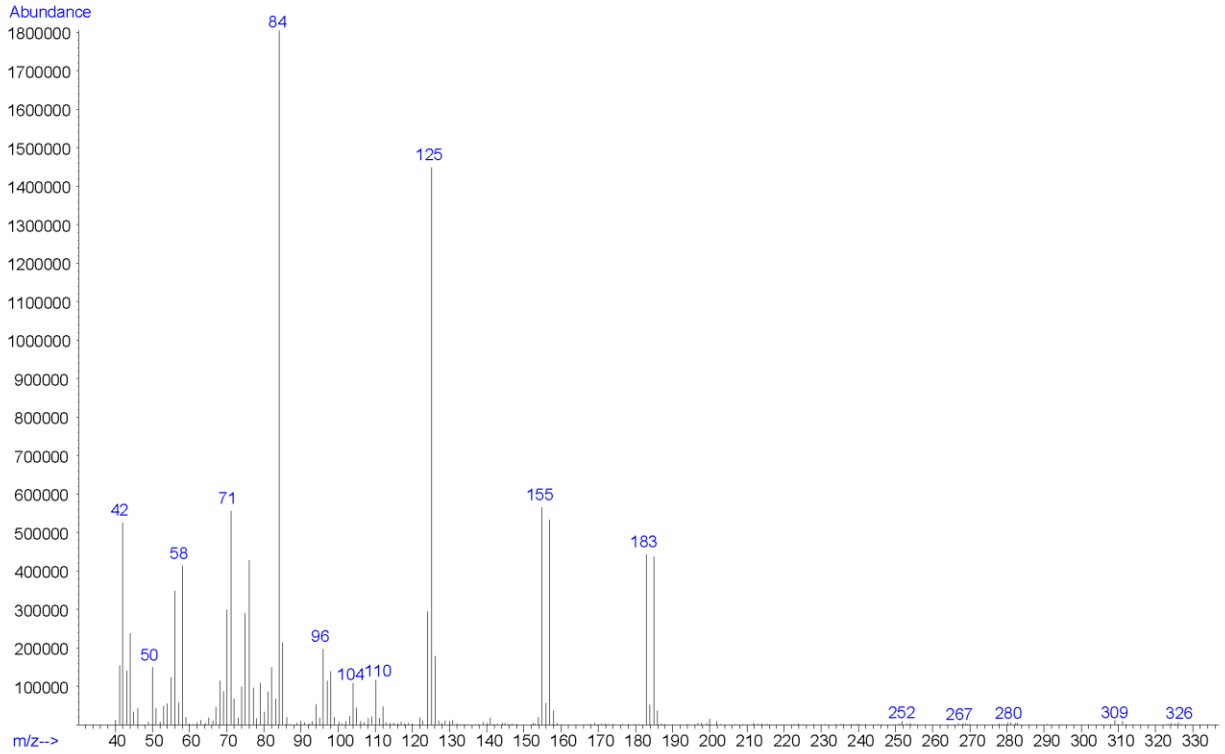
<https://www.caymanchem.com/product/20530>

### Chromatogram: U-47931E



*Additional peaks present in chromatogram: internal standards (3.208 min and 6.280 min), not a controlled substance (7.064 min)*

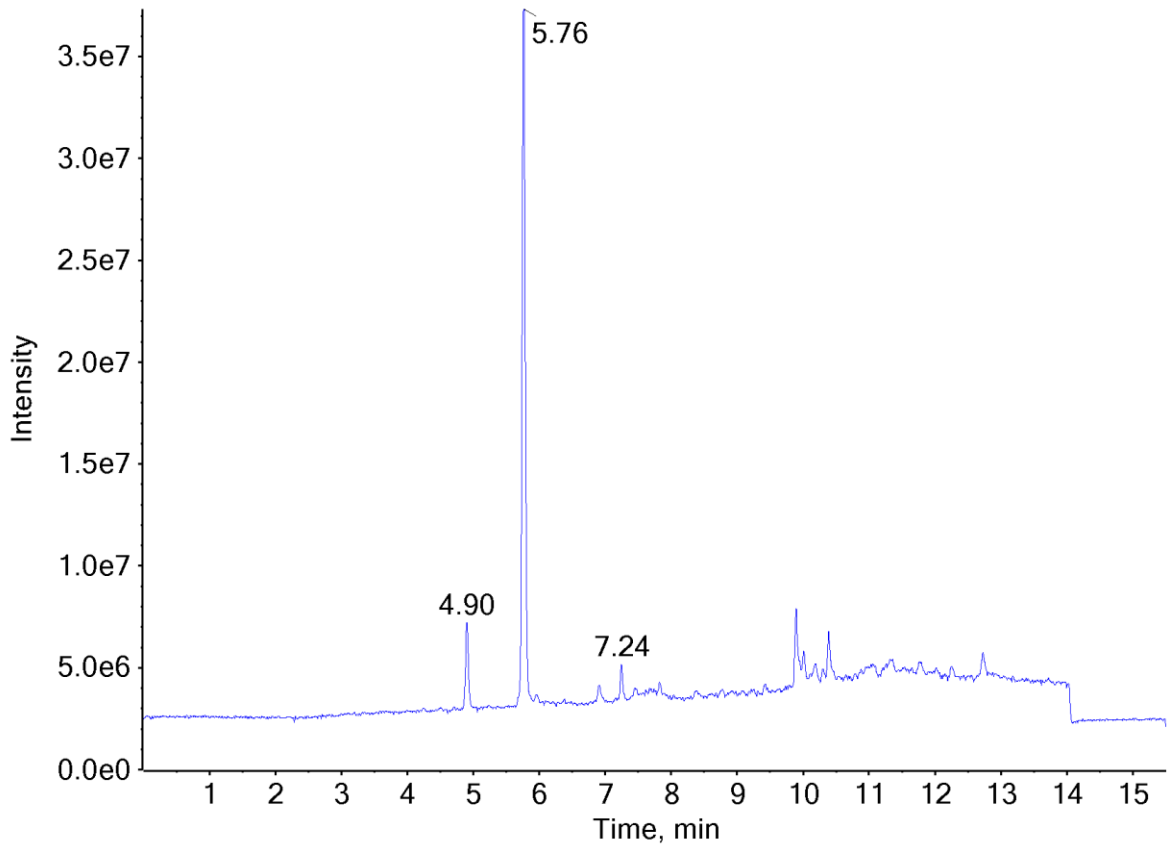
# EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): U-47931E



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

<b>Testing Performed At:</b>	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
<b>Sample Preparation:</b>	1:100 dilution of acid/base extraction in mobile phase
<b>Instrument:</b>	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
<b>Column:</b>	Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)
<b>Mobile Phase:</b>	A: Ammonium formate (10 mM, pH 3.0) B: Methanol/acetonitrile (50:50) Flow rate: 0.4 mL/min
<b>Gradient:</b>	Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min
<b>Temperatures:</b>	Autosampler: 15 °C Column Oven: 30 °C Source Heater: 600 °C
<b>Injection Parameters:</b>	Injection Volume: 10 µL
<b>QTOF Parameters:</b>	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
<b>Retention Time:</b>	5.76 min
<b>Standard Comparison:</b>	Reference material for U-47931E (Batch: 0492764-5) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as U-47931E, based on retention time (5.82 min) and mass spectral data. ( <a href="https://www.caymanchem.com/product/20530">https://www.caymanchem.com/product/20530</a> )

**Chromatogram: U-47931E**



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

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

