1. GENERAL INFORMATION

IUPAC Name: 4-bromo-N-[2-(dimethylamino)cyclohexyl]benzamide
InChI String: 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)
CFR: Not Scheduled (10/2018)
CAS# 67579-24-2
Synonyms: Bromadoline
Source: Department of Homeland Security
Appearance: White Solid Material

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M+]</th>
<th>Exact Mass [M+H]^+</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C_{15}H_{21}BrN_{2}O</td>
<td>325.2</td>
<td>324</td>
<td>325.0910</td>
</tr>
</tbody>
</table>

*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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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


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:  
6.834 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)

**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:** 5.76 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 (5.82 min) and mass spectral data. ([https://www.caymanchem.com/product/20530](https://www.caymanchem.com/product/20530))
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