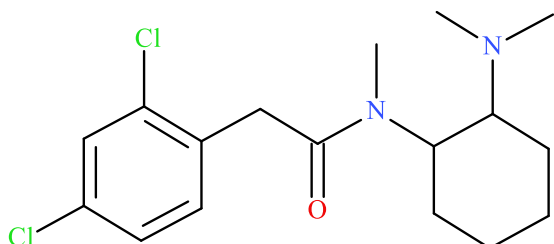


**U-48800**

 Sample Type: **Seized Material**

 Latest Revision: **May 18<sup>th</sup>, 2018**

 Date Received: **January 19<sup>th</sup>, 2018**

 Date of Report: **March 26<sup>th</sup>, 2018**

## 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	2-(2,4-dichlorophenyl)-N-2-(dimethylamino)cyclohexyl)-N-methylacetamide
<b>InChI String:</b>	InChI=1S/C17H24Cl2N2O/c1-20(2)15-6-4-5-7-16(15)21(3)17(22)10-12-8-9-13(18)11-14(12)19/h8-9,11,15-16H,4-7,10H2,1-3H3
<b>CFR:</b>	Not Scheduled (03/2018)
<b>CAS#</b>	Not Available
<b>Synonyms:</b>	U-48,800, U48
<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>17</sub> H <sub>24</sub> Cl <sub>2</sub> N <sub>2</sub> O	343.29	342	343.1338

**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

U-48800 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 and U-49900. U-47700 is a Schedule I substance in the United States.

### 4. ADDITIONAL RESOURCES

[https://www.policija.si/apps/nfl\\_response\\_web/0\\_Analytical\\_Reports\\_final/U-48800-ID-ADB-042\\_report.pdf](https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/U-48800-ID-ADB-042_report.pdf)

<https://www.caymanchem.com/product/22278>

### 5. QUALITATIVE DATA

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

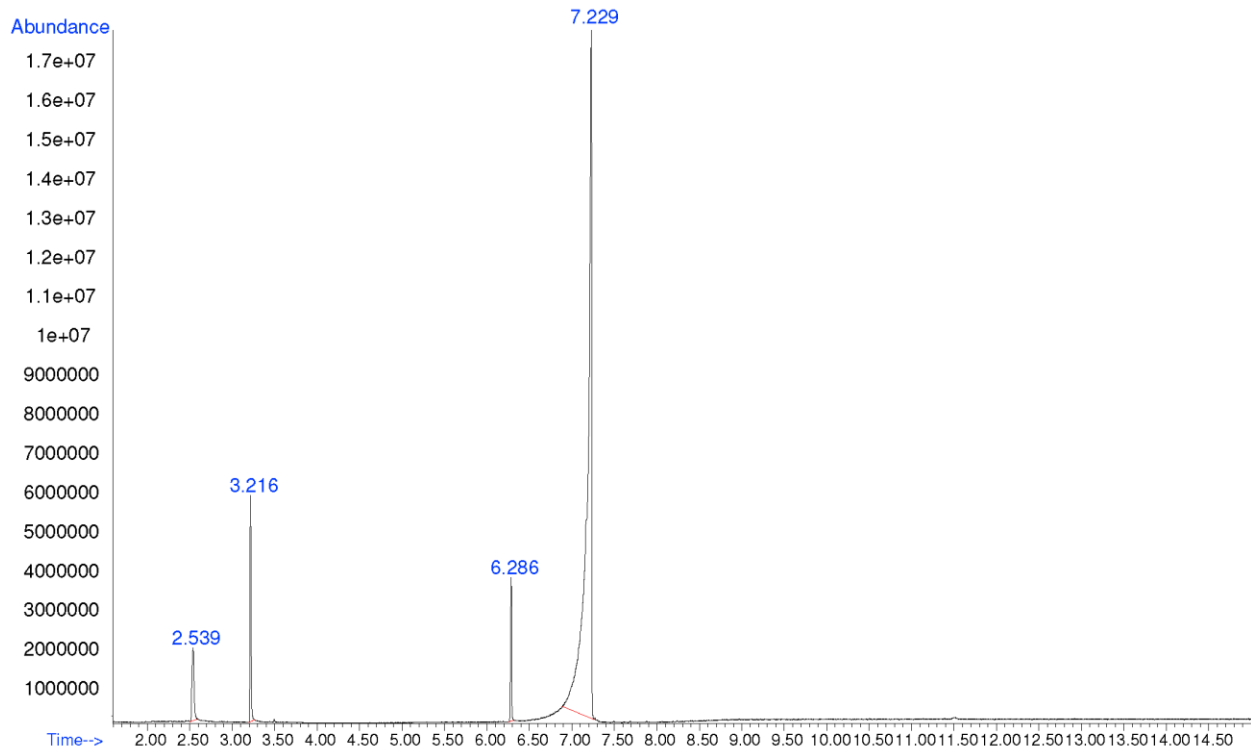
<b>Testing Performed At:</b>	NMS Labs (Willow Grove, PA)
<b>Sample Preparation:</b>	Acid/Base extraction
<b>Instrument:</b>	Agilent 5975 Series GC/MSD System
<b>Column:</b>	Zebtron™ Inferno™ ZB-35HT (15 m x 250 μm x 0.25 μm)
<b>Carrier Gas:</b>	Helium (Flow: 1 mL/min)
<b>Temperatures:</b>	Injection Port: 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
<b>MS Parameters:</b>	Mass Scan Range: 40-550 m/z

Threshold: 250

**Retention Time:** 7.229 min

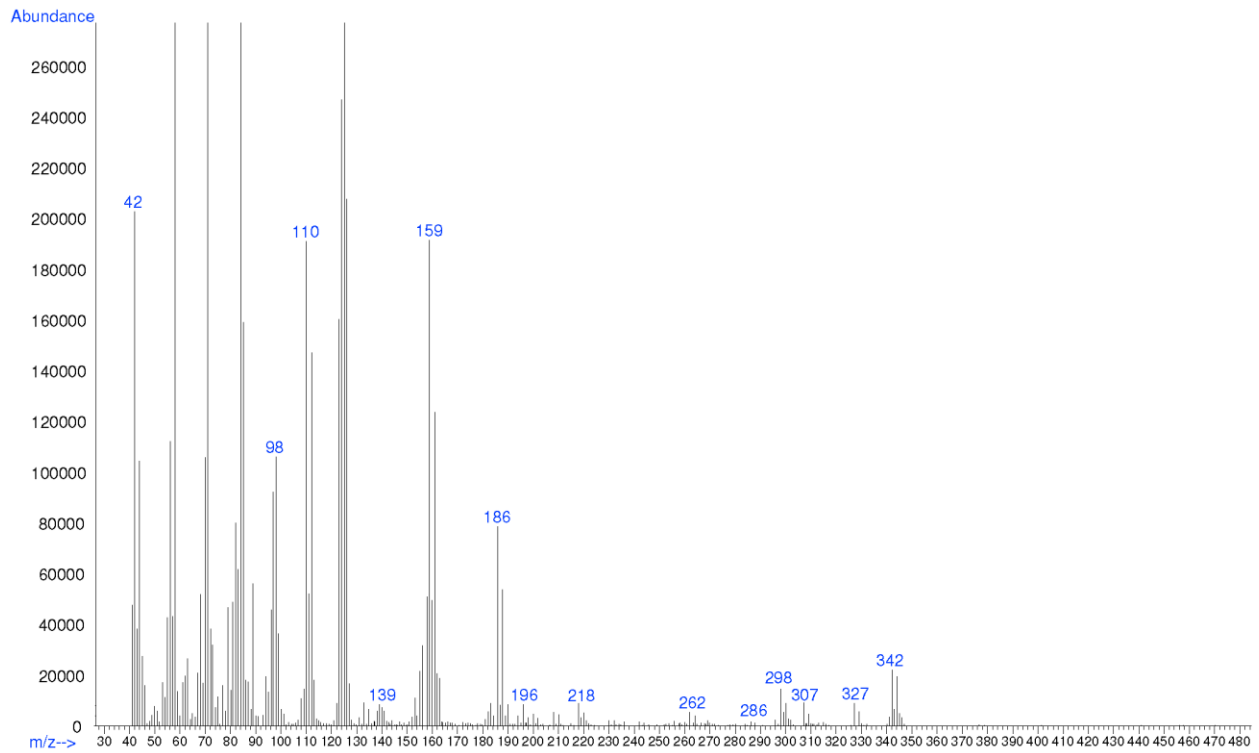
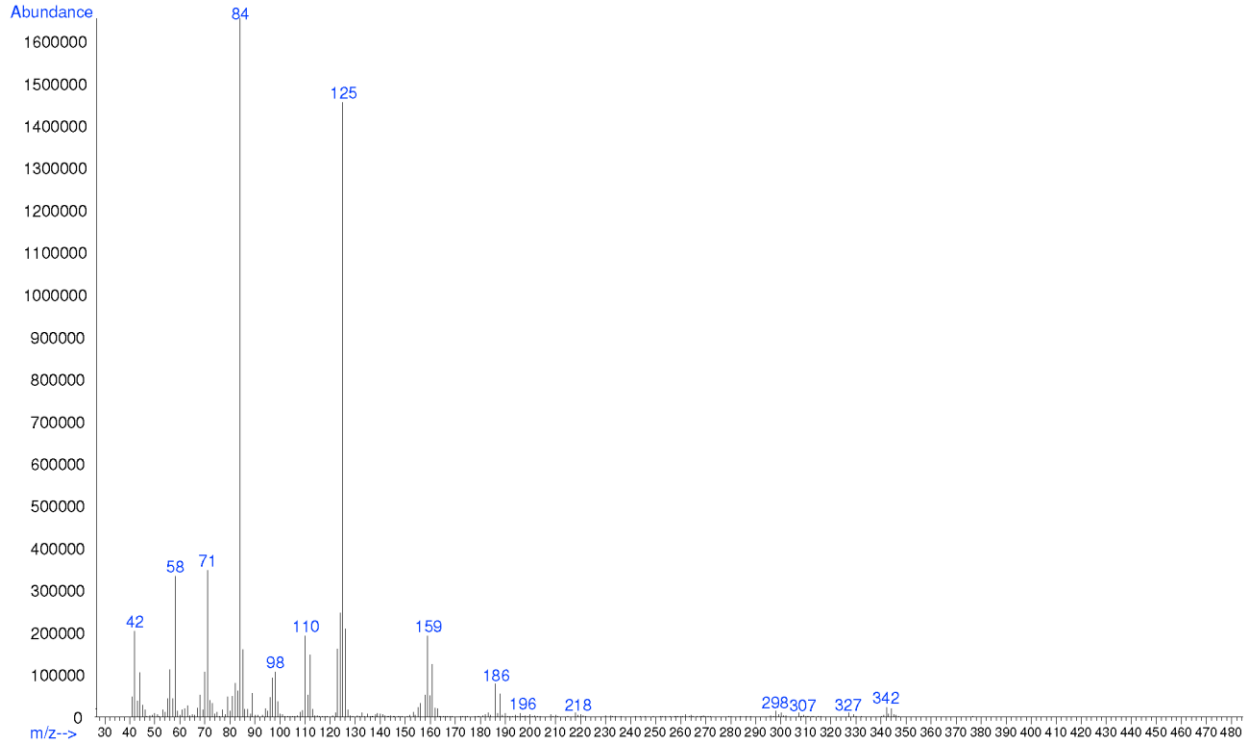
**Standard Comparison:** Reference material for U-48800 (Batch: 0512636-12) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as U-48800, based on retention time (7.214 min) and mass spectral data.  
(<https://www.caymanchem.com/product/22278>).

### Chromatogram: U-48800



*Additional peaks present in chromatogram: not a controlled substance (2.539 min),  
internal standard 1 (3.216), internal standard 2 (6.286)*

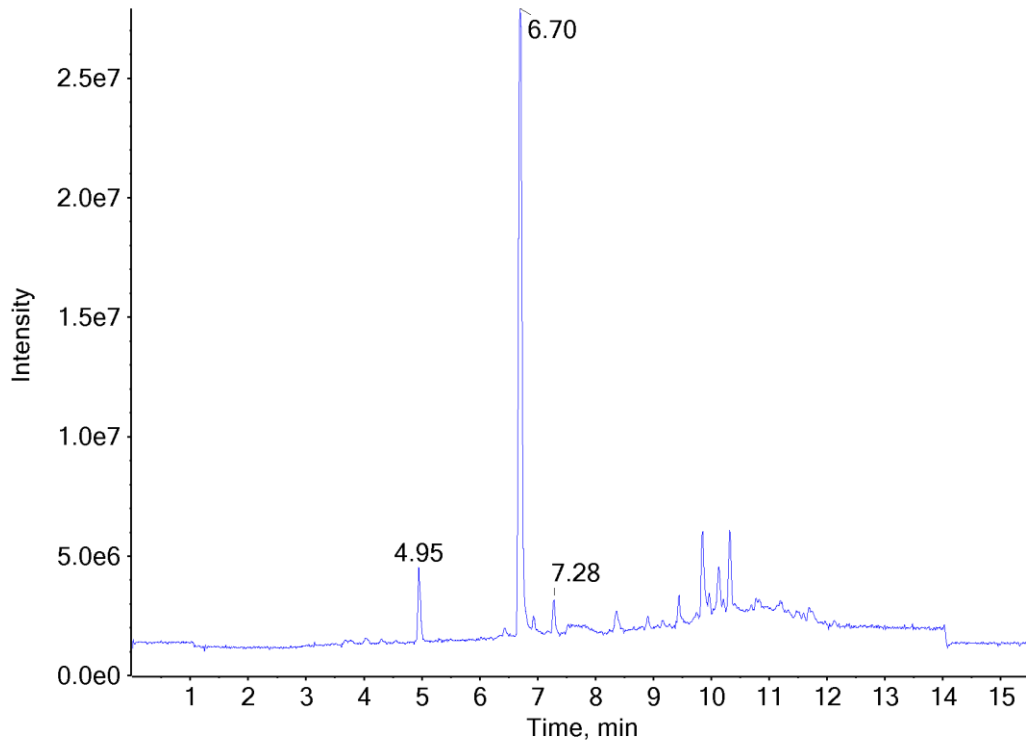
# EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): U-48800



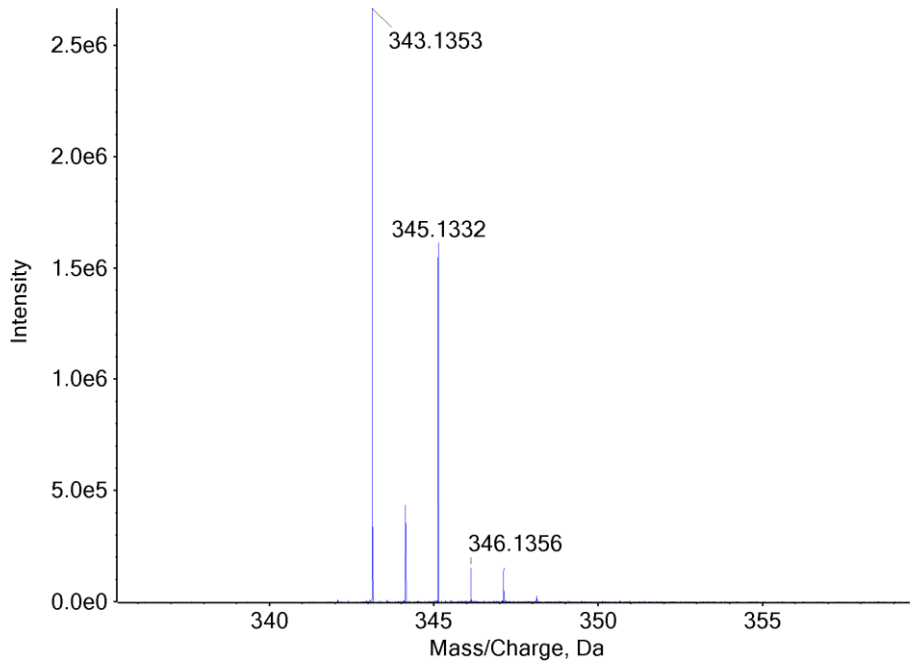
## 5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

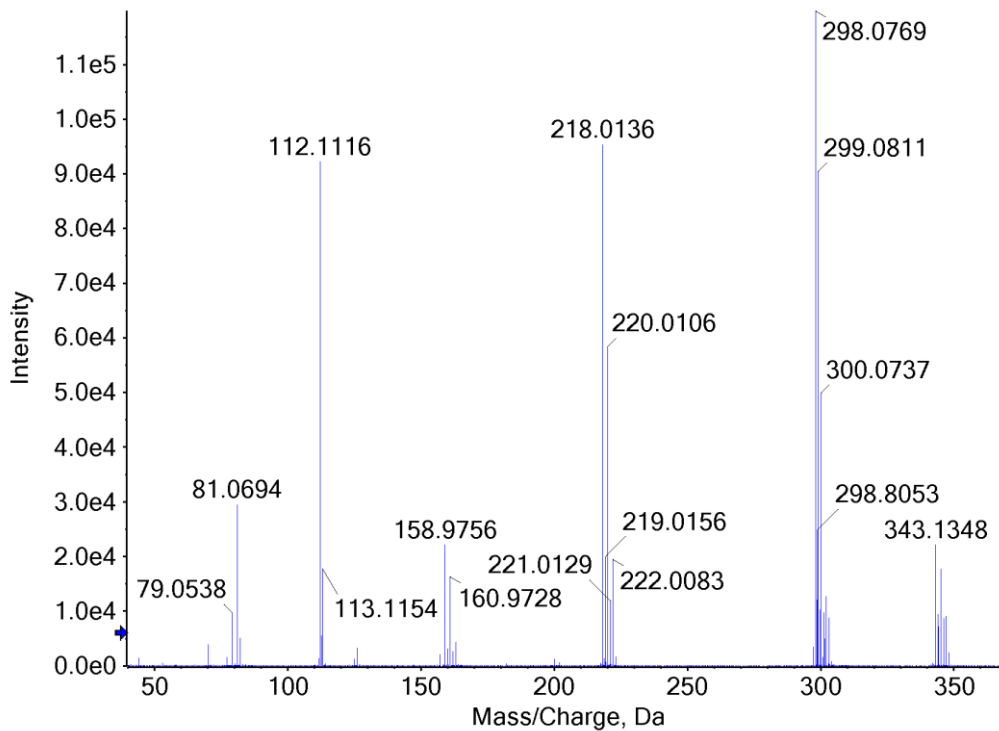
<b>Testing Performed At:</b>	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
<b>Sample Preparation:</b>	1:100 dilution of acid/base extraction in mobile phase
<b>Instrument:</b>	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
<b>Column:</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>	6.70 min
<b>Standard Comparison:</b>	Reference material for U-48800 (Batch: 0512636-12) 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-48800, based on retention time (6.708 min) and mass spectral data. ( <a href="https://www.caymanchem.com/product/22278">https://www.caymanchem.com/product/22278</a> ).

### Chromatogram: U-48800



### TOF MS (Top) and MS/MS (Bottom) Spectra: U-48800





## 6. REVISION HISTORY

<u>Date</u>	<u>Revision</u>
05/18/2018	Edits to Brief Description.
05/18/2018	Added "Sample Type: Seized Material" to Page 1.
05/18/2018	Added "Prepared By: Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT" to Page 1 footer.