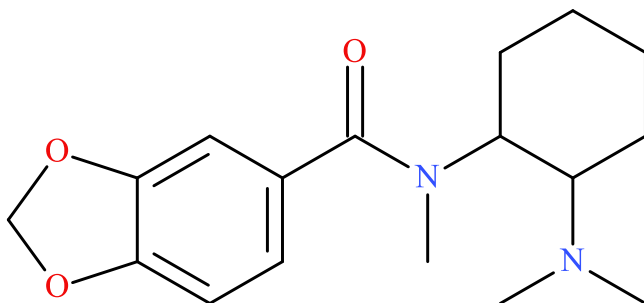


Methylenedioxy-U-47700

Sample Type: **Biological Fluid**

Latest Revision: **May 18th, 2018**

Date of Report: **May 18th, 2018**



1. GENERAL INFORMATION

IUPAC Name: N-[2-(dimethylamino)cyclohexyl]-N-methyl-1,3-benzodioxole-5-carboxamide

InChI String: InChI=1S/C17H24N2O3/c1-18(2)13-6-4-5-7-14(13)19(3)17(20)12-8-9-15-16(10-12)22-11-21-15/h8-10,13-14H,4-7,11H2,1-3H3

CFR: Not Scheduled (05/2018)

CAS# Not Available

Synonyms: 3,4-MDO-U-47700, MD-U-47700, MD-U47

Source: NMS Labs – Toxicology Department

2. CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Exact Mass [M+H] ⁺
Methylenedioxy-U-47700	C ₁₇ H ₂₄ N ₂ O ₃	304.4	305.1860

Important Note: All identifications were made based on evaluation of analytical data (LC-QTOF) in comparison to analysis of acquired reference material.

Report Prepared By: Alex J. Krotulski, MSFS, and Barry K. Logan, PhD, F-ABFT

3. SAMPLE HISTORY

Methylenedioxy-U-47700 has been identified in five cases since January 2018. The geographical and demographical breakdown is below:

Geographical Location:	Western Pennsylvania (n=5)
Gender:	Male (n=2), Female (n=3)
Age Range:	36 – 60 years (n=3)
Biological Sample:	Peripheral Blood (n=2), Blood (n=2), Cardiac Blood (n=1)
Date of First Collection:	January 6 th , 2018
Date of First Receipt:	January 9 th , 2018
Additional Opioids:	Methoxyacetylfentanyl (n=4), 4-ANPP (n=4), Isopropyl-U-47700 (n=2), Cyclopropylfentanyl (n=1), Fluoroisobutyrylfentanyl (n=1), Fentanyl (n=1), Norfentanyl (n=1)

4. BRIEF DESCRIPTION

Methylenedioxy-U-47700 is classified as a novel opioid of the *trans*-N-[2-(methylamino)cyclohexyl]-benzamide class. 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.

5. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/22753>

6. QUALITATIVE DATA

6.1 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: No additional preparation - direct analysis of sample extract

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

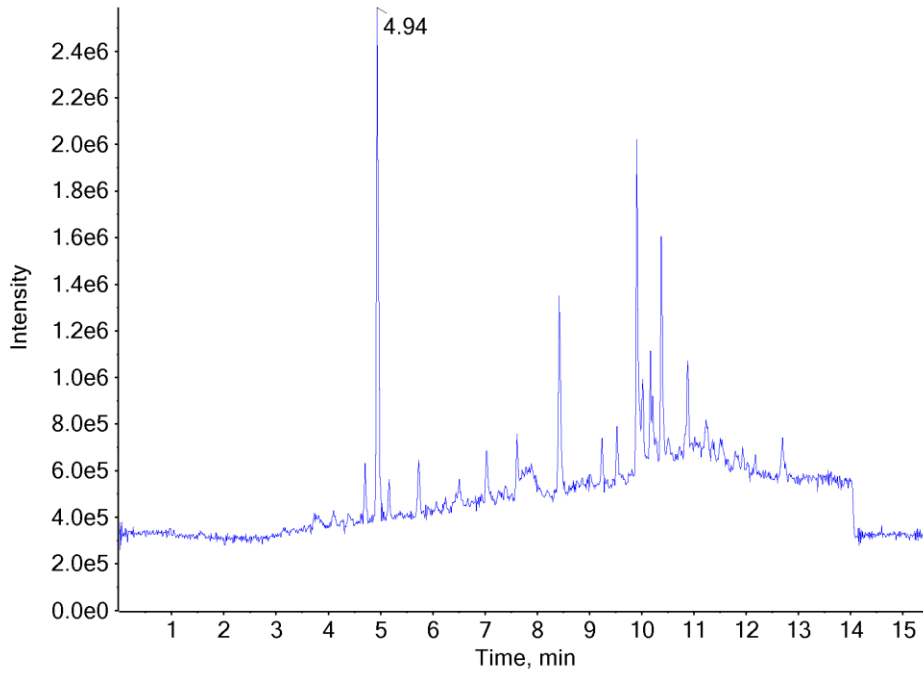
Injection Parameters: Injection Volume: 10 µL

QTOF Parameters: TOF MS Scan Range: 100-510 Da
Precursor Isolation: SWATH® acquisition (27 windows)
Fragmentation: Collision Energy Spread (35±15 eV)
MS/MS Scan Range: 50-510 Da

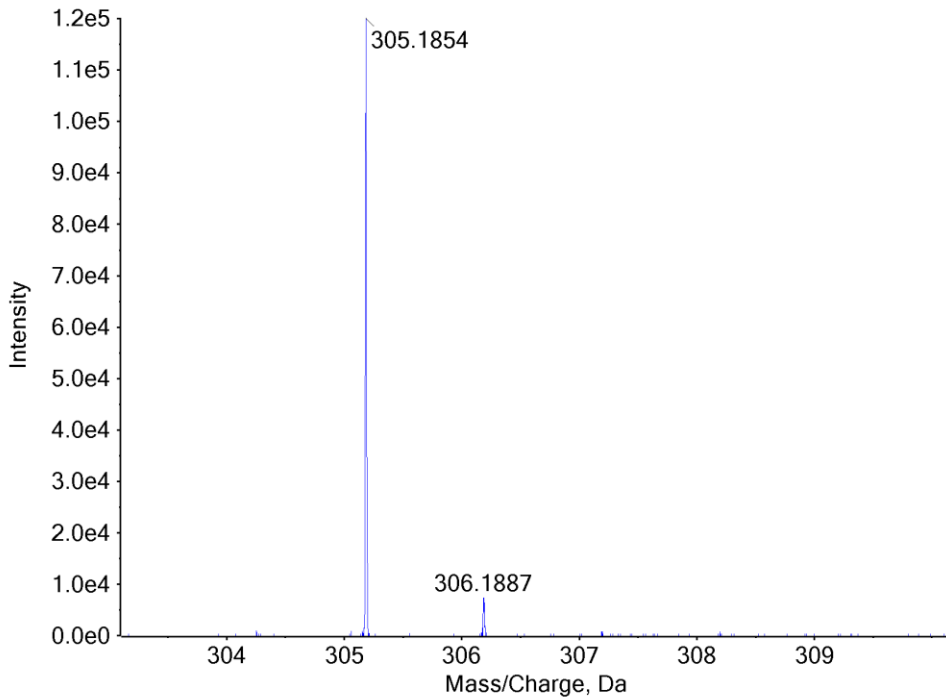
Retention Time: 4.94 min

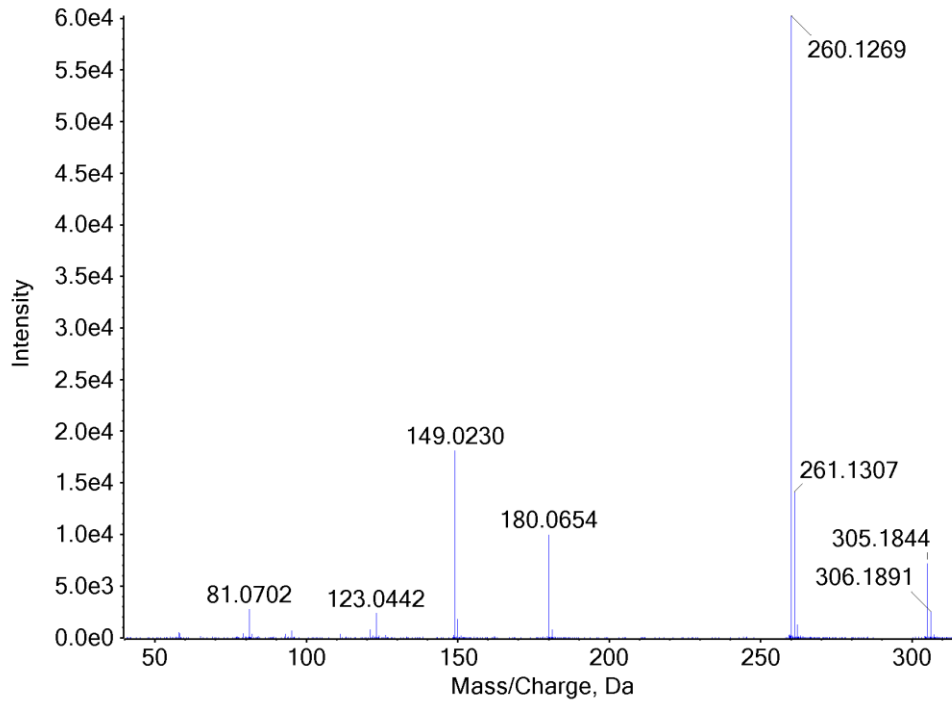
Standard Comparison: Reference material for Methylenedioxy-U-47700 (Batch: 0511960-4) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as Methylenedioxy-U-47700, based on retention time (4.90 min) and mass spectral data. (<https://www.caymanchem.com/product/22753>)

Chromatogram: Methylenedioxy-U-47700



TOF MS (Top) and MS/MS (Bottom) Spectra: Methylenedioxy-U-47700





7. FUNDING

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