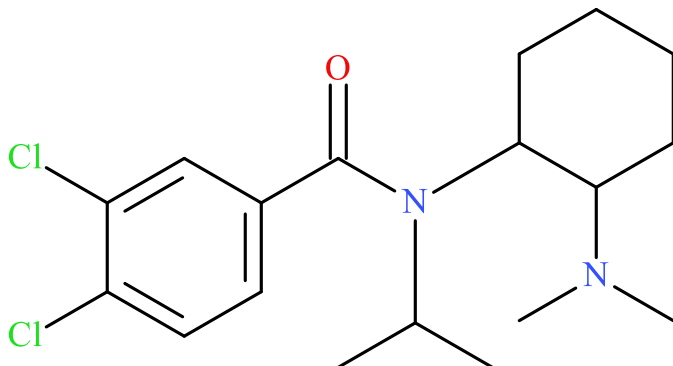


Isopropyl-U-47700



Sample Type: **Biological Fluid**

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

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

1. GENERAL INFORMATION

IUPAC Name:	3,4-dichloro-N-[2-(dimethylamino)cyclohexyl]-N-isopropylbenzamide
InChI String:	InChI=1S/C18H26Cl2N2O/c1-12(2)22(17-8-6-5-7-16(17)21(3)4)18(23)13-9-10-14(19)15(20)11-13/h9-12,16-17H,5-8H2,1-4H3
CFR:	Not Scheduled (05/2018)
CAS#	Not Available
Synonyms:	Isopropyl-U47, IP-U47
Source:	NMS Labs

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Exact Mass [M+H] ⁺
Isopropyl-U-47700	C ₁₈ H ₂₆ Cl ₂ N ₂ O	357.3	357.1495

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

Isopropyl-U-47700 has been identified in two cases since March 2018. The geographical and demographical breakdown is below:

Geographical Location:	Western Pennsylvania (n=2)
Gender:	Male (n=1), Female (n=1)
Age Range:	56 – 60 years (n=2)
Biological Sample:	Peripheral Blood (n=2)
Date of First Collection:	March 30 th , 2018
Date of First Receipt:	April 2 nd , 2018
Additional Opioids:	Methylenedioxy-U-47700 (n=2), Methoxyacetylfentanyl (n=2), 4-ANPP (n=2), Cyclopropylfentanyl (n=1), Fluoroisobutyrylfentanyl (n=1), Fentanyl (n=1), Norfentanyl (n=1)

4. BRIEF DESCRIPTION

Isopropyl-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.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/Isopropyl-U-47700-ID-1902-18_report.pdf

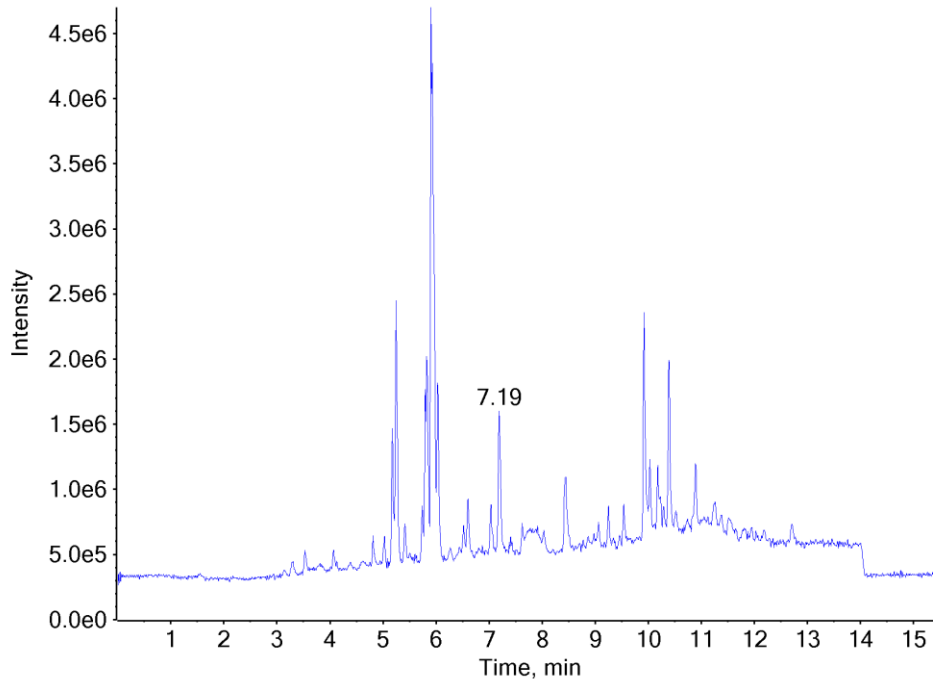
<https://www.caymanchem.com/product/24263>

6. QUALITATIVE DATA

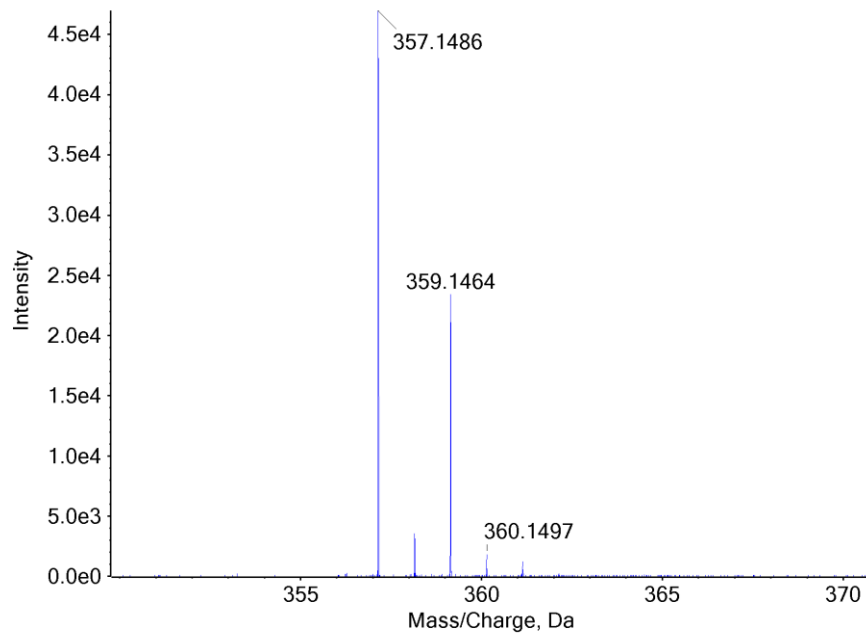
6.1 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

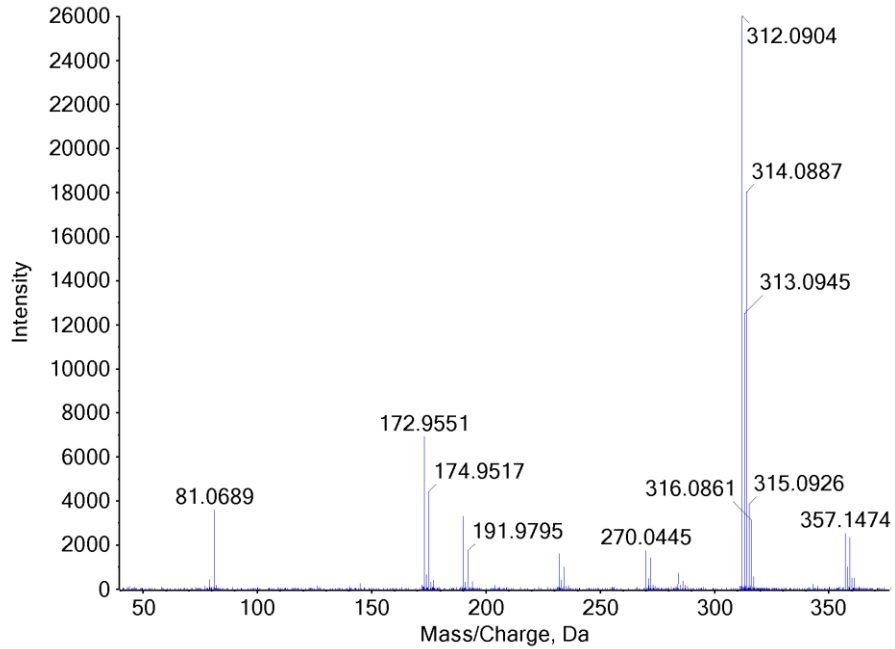
Testing Performed At:	The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)
Sample Preparation:	No additional preparation - direct analysis of sample extract
Instrument:	Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC
Column:	Phenomenex® Kinetex 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:	7.19 min
Standard Comparison:	Reference material for Isopropyl-U-47700 (Batch: 0521835-4) 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 Isopropyl-U-47700, based on retention time (7.09 min) and mass spectral data. (https://www.caymanchem.com/product/24263)

Chromatogram: Isopropyl-U-47700



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





7. FUNDING

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