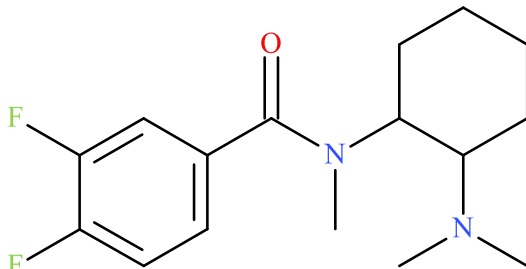


3,4-Difluoro-U-47700

Sample Type: **Seized Material**



Latest Revision: **March 11, 2020**

Date of Report: **March 11, 2020**

1. GENERAL INFORMATION

IUPAC Name: N-[2-(dimethylamino)cyclohexyl]-3,4-difluoro-N-methyl-benzamide

InChI String: InChI=1S/C16H22F2N2O/c1-19(2)14-6-4-5-7-15(14)20(3)16(21)11-8-9-12(17)13(18)10-11/h8-10,14-15H,4-7H2,1-3H3

CFR: Not Scheduled (03/2020)

CAS# Not Available

Synonyms: Difluoro U-47700

Source: Franklin County Coroner's Office (Columbus, OH)

Appearance: White Solid Material

2. CHEMICAL DATA

Analyte	Chemical Formula	Molecular Weight	Molecular Ion [M ⁺]	Exact Mass [M+H] ⁺
3,4-Difluoro-U-47700	C ₁₆ H ₂₂ F ₂ N ₂ O	296.4	296	297.1773

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

Report Prepared By: Alex J. Krotulski, PhD; Daniel Baker, MS, F-ABFT; Nancy E. Kelly; and Barry K. Logan, PhD, F-ABFT

3. BRIEF DESCRIPTION

3,4-Difluoro-U-47700 is classified as a novel opioid. Novel opioids have been reported to cause opioid-like effects similar to heroin and fentanyl. Novel opioids in the trans-N-[2-(methylamino)cyclohexyl]-benzamide class (e.g. U-47700) and similar classes (e.g. U-49900) have caused adverse events, including deaths, as described in the literature. U-47700 is a Schedule I substance in the United States; no other U-series analogues are explicitly scheduled.

4. ADDITIONAL RESOURCES

<https://www.caymanchem.com/product/28689/>

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: Drug material diluted in methanol

Instrument: Agilent 5975 Series GC/MSD System

Column: Agilent J&W DB-1 (12 m x 200 μ m x 0.33 μ m)

Carrier Gas: Helium (Flow: 1.46 mL/min)

Temperatures: Injection Port: 265 °C
Transfer Line: 300 °C
MS Source: 230 °C
MS Quad: 150 °C
Oven Program: 50 °C for 0 min, 30 °C/min to 340 °C for 2.3 min

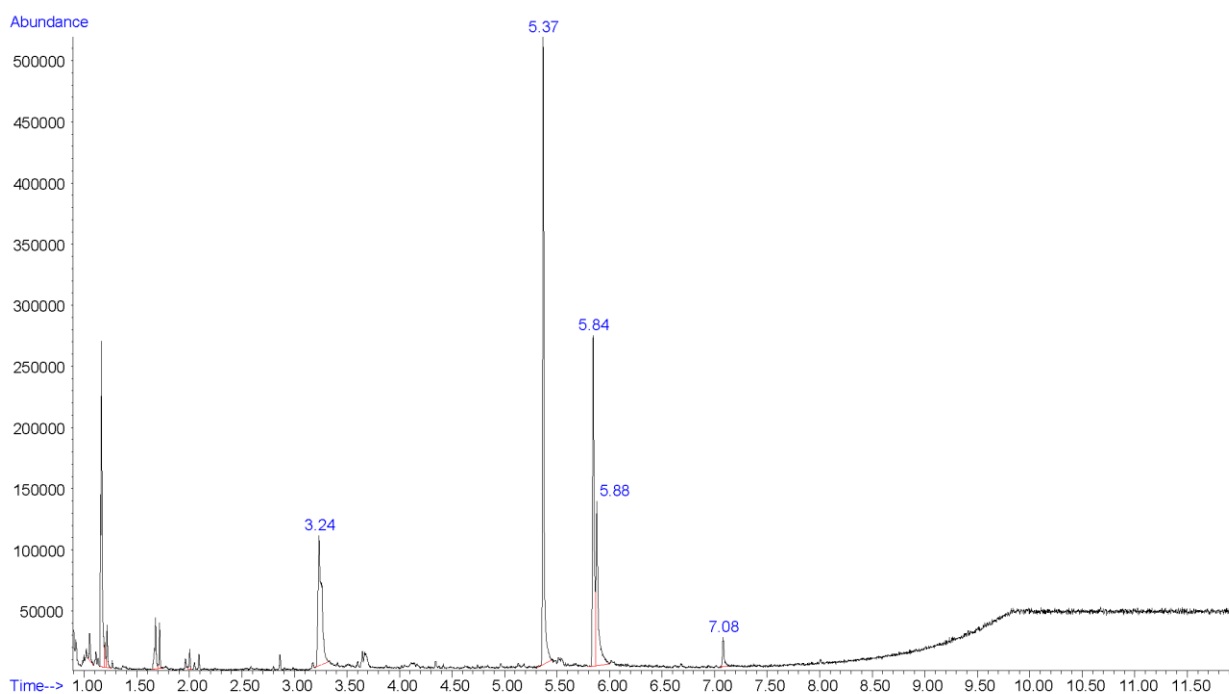
Injection Parameters: Injection Type: Splitless
Injection Volume: 1 μ L

MS Parameters: Mass Scan Range: 40-550 m/z
Threshold: 250

Retention Time: 5.88 min

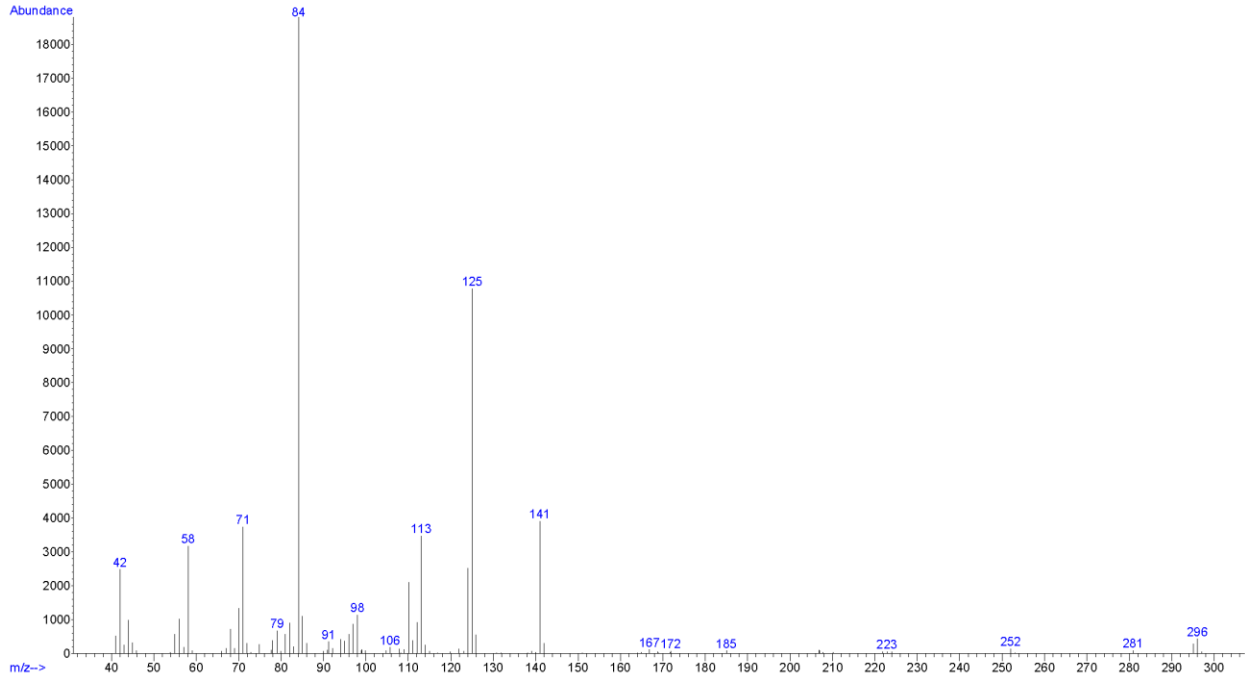
Standard Comparison: Reference material for 3,4-Difluoro-U-47700 (Batch: 0576772-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 3,4-Difluoro-U-47700, based on retention time (5.84 min) and mass spectral data.
(<https://www.caymanchem.com/product/28689/>).

Chromatogram: 3,4-Difluoro-U-47700



Additional peaks in chromatogram: internal standard (3.24 min), lidocaine (5.37 min), internal standard (5.84 min), and N-ethyl-U-47700 (7.08 min)

EI (70 eV) Mass Spectrum: 3,4-Difluoro-U-47700



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

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 in mobile phase of GC-MS methanolic dilution

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)

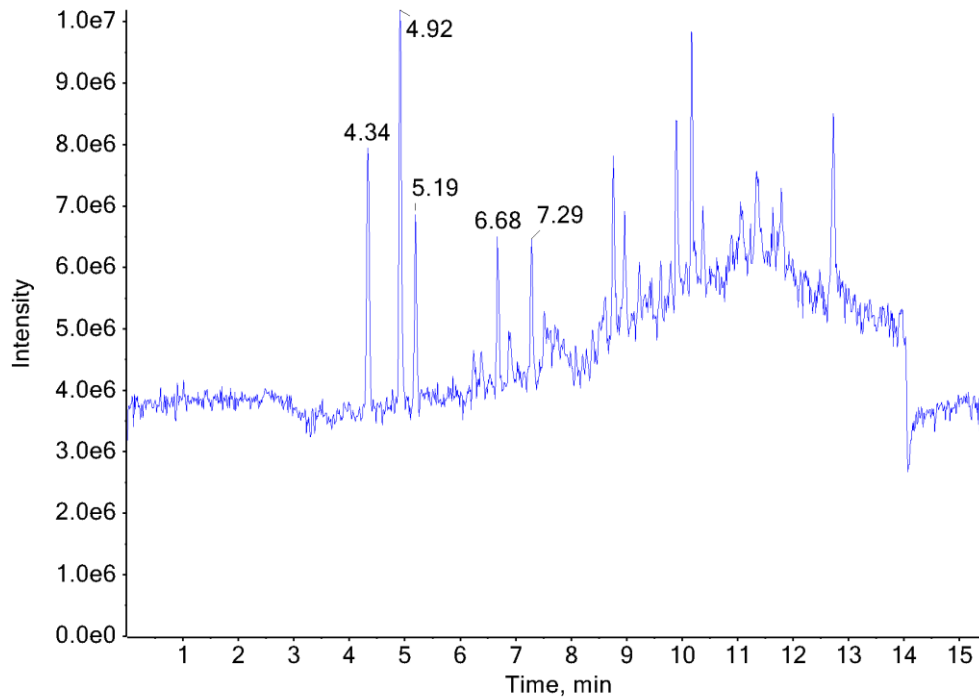
Fragmentation: Collision Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 5.19 min

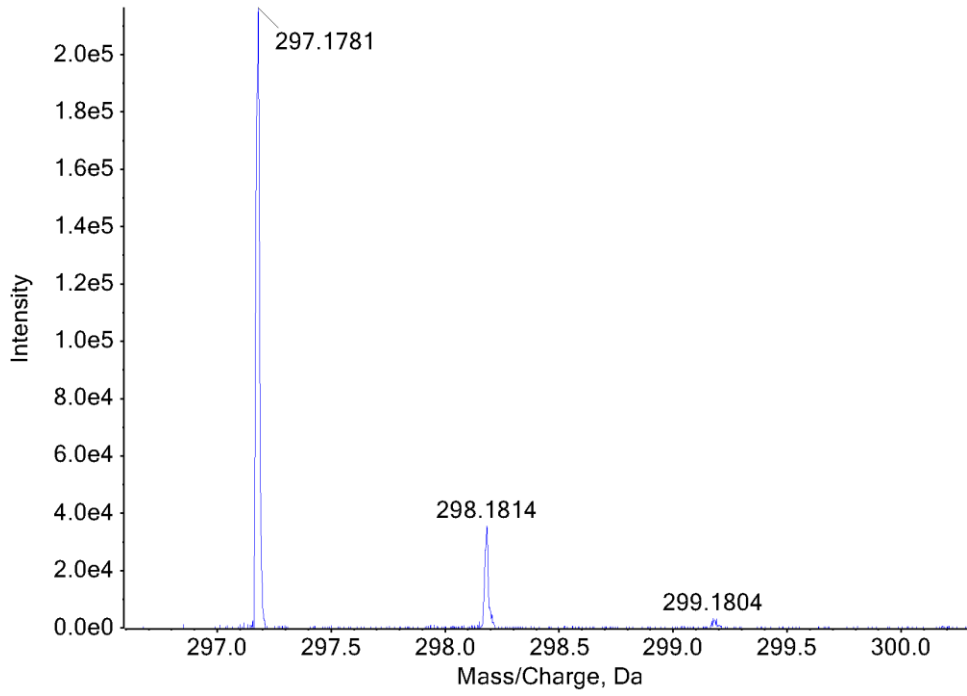
Standard Comparison: Reference material for 3,4-Difluoro-U-47700 (Batch: 0576772-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 3,4-Difluoro-U-47700, based on retention time (5.21 min) and mass spectral data. (<https://www.caymanchem.com/product/28689/>).

Chromatogram: 3,4-Difluoro-U-47700



Additional peaks in chromatogram: lidocaine (4.34 min), internal standard (4.92 min), N-ethyl-U-47700 (6.68 min), and internal standard (7.29 min)

TOF MS Spectrum: 3,4-Difluoro-U-47700



MS/MS Spectrum: 3,4-Difluoro-U-47700

