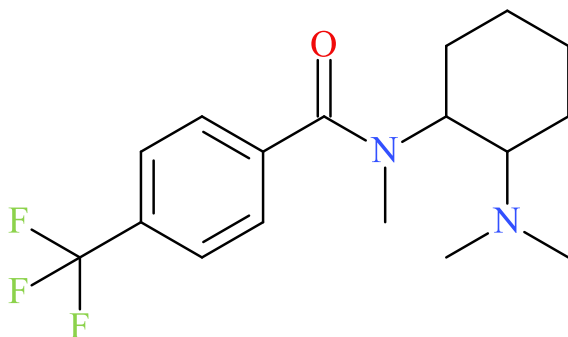


## Trifluoromethyl-U-47700

Sample Type: **Toxicology Sample**



Latest Revision: **December 14, 2021**

Date of Report: **December 14, 2021**

### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	N-[2-(dimethylamino)cyclohexyl]-N-methyl-4-(trifluoromethyl)benzamide
<b>InChI String:</b>	InChI=1S/C17H23F3N2O/c1-21(2)14-6-4-5-7-15(14)22(3)16(23)12-8-10-13(11-9-12)17(18,19)20/h8-11,14-15H,4-7H2,1-3H3
<b>CFR:</b>	Not Scheduled (12/2021)
<b>CAS#</b>	Not Available
<b>Synonyms:</b>	TFM U-47700, 4-Trifluoromethyl-U-47700
<b>Source:</b>	NMS Labs – Toxicology Department

**Important Note:** All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material. The “4-trifluoromethyl” configuration was used for structural purposes; however, position of the TFM group was not confirmed during analysis.

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## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Drug	Chemical Formula	Molecular Weight	Molecular Ion [M <sup>+</sup> ]	Exact Mass [M+H] <sup>+</sup>
Trifluoromethyl-U-47700	C <sub>17</sub> H <sub>23</sub> F <sub>3</sub> N <sub>2</sub> O	328.4	328	329.1835

### 3. SAMPLE HISTORY

To date, Trifluoromethyl-U-47700 was identified in at least seven cases since November 2020. The geographical and demographical breakdown is below:

**Geographical Location:** Louisiana (n=2), Texas (n=2), Arkansas (n=1), Florida (n=1), Vancouver, BC (n=1)

**Biological Sample:** Femoral Blood (n=4), Subclavian Blood (n=3)

**Date of First Receipt:** November 2020

**Other Notable Findings:** Fentanyl (n=5), Etizolam (n=4), Flualprazolam (n=3), Methamphetamine (n=2), *para*-Fluorofentanyl (n=2)

### 4. BRIEF DESCRIPTION

Trifluoromethyl-U-47700 is classified as a novel opioid. Novel opioids have been reported to cause psychoactive effects similar to heroin, fentanyl, and other opioids. 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.

### 5. ADDITIONAL RESOURCES

[https://www.policija.si/apps/nfl\\_response\\_web/0\\_Analytical\\_Reports\\_final/4-TFM%20U-47700-ID-2993-21\\_report.pdf](https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/4-TFM%20U-47700-ID-2993-21_report.pdf)

[https://www.caymanchem.com/product/26273/4-\(trifluoromethyl\)-u-47700-\(hydrochloride\)](https://www.caymanchem.com/product/26273/4-(trifluoromethyl)-u-47700-(hydrochloride))

## 6. QUALITATIVE DATA

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

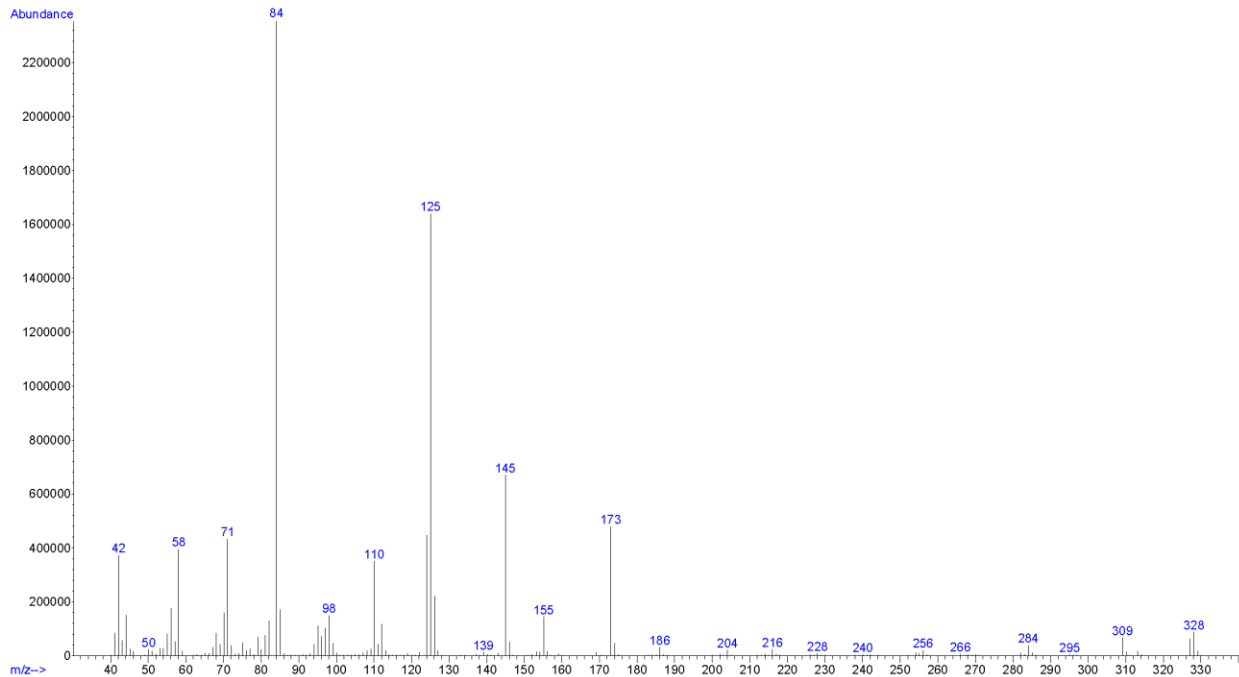
**Testing Performed At:** The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

**Sample Preparation:** Standard diluted in methanol

**Instrument:** Agilent 5975 Series GC/MSD System

**Standard:** Reference material for 4-Trifluoromethyl-U-47700 (Batch: 0603861-1) was purchased from Cayman Chemical Company (Ann Arbor, MI, USA).  
[https://www.caymanchem.com/product/26273/4-\(trifluoromethyl\)-u-47700-\(hydrochloride\)](https://www.caymanchem.com/product/26273/4-(trifluoromethyl)-u-47700-(hydrochloride))

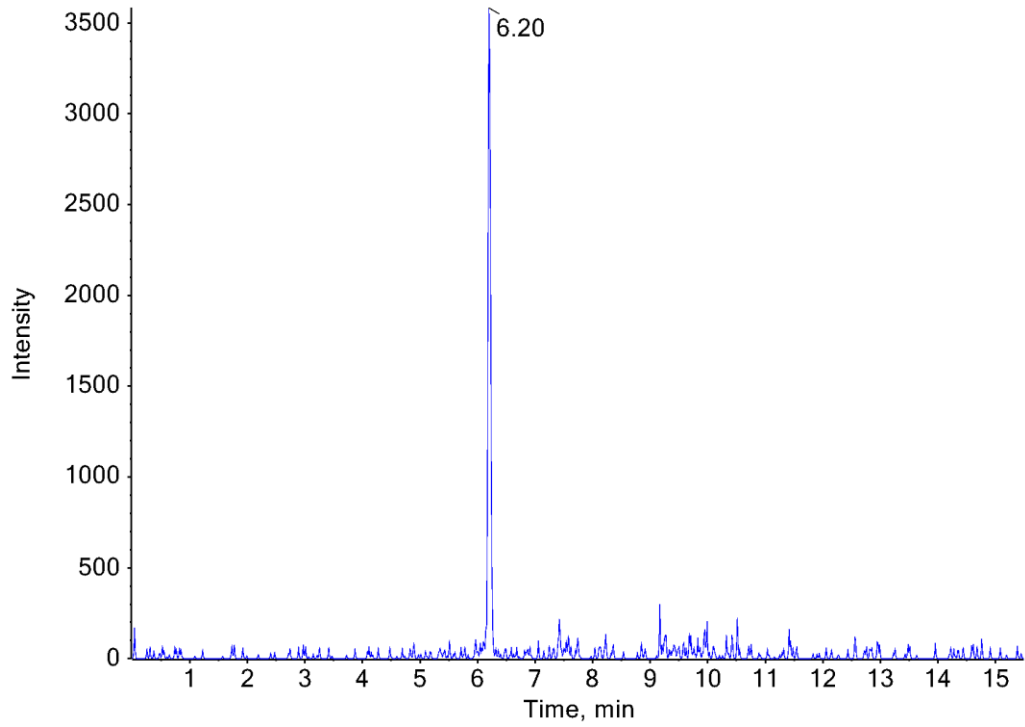
#### EI (70 eV) Mass Spectrum: 4-Trifluoromethyl-U-47700 (Standard)



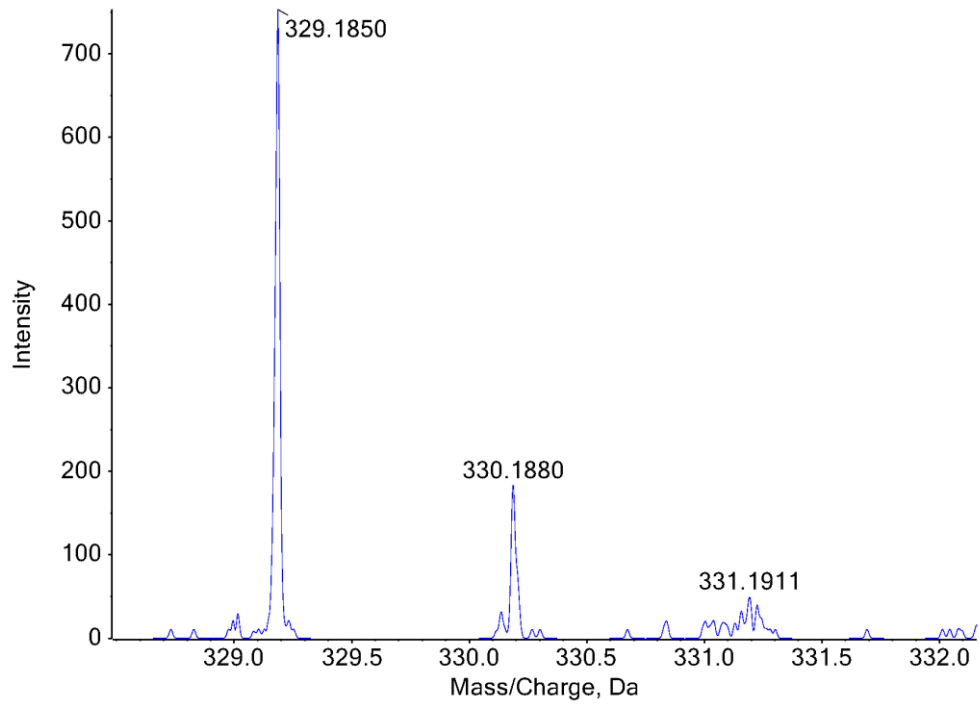
## 6.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

<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>	Liquid-liquid extraction (LLE)
<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>	6.20 min
<b>Standard Comparison:</b>	Reference material for 4-Trifluoromethyl-U-47700 (Batch: 0603861-1) 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 Trifluoromethyl-U-47700, based on retention time (6.10 min) and mass spectral data; however, absolute configuration of the structure as 4-Trifluoromethyl-U-47700 was not determined. <a href="https://www.caymanchem.com/product/26273/4-(trifluoromethyl)-u-47700-(hydrochloride)">https://www.caymanchem.com/product/26273/4-(trifluoromethyl)-u-47700-(hydrochloride)</a>

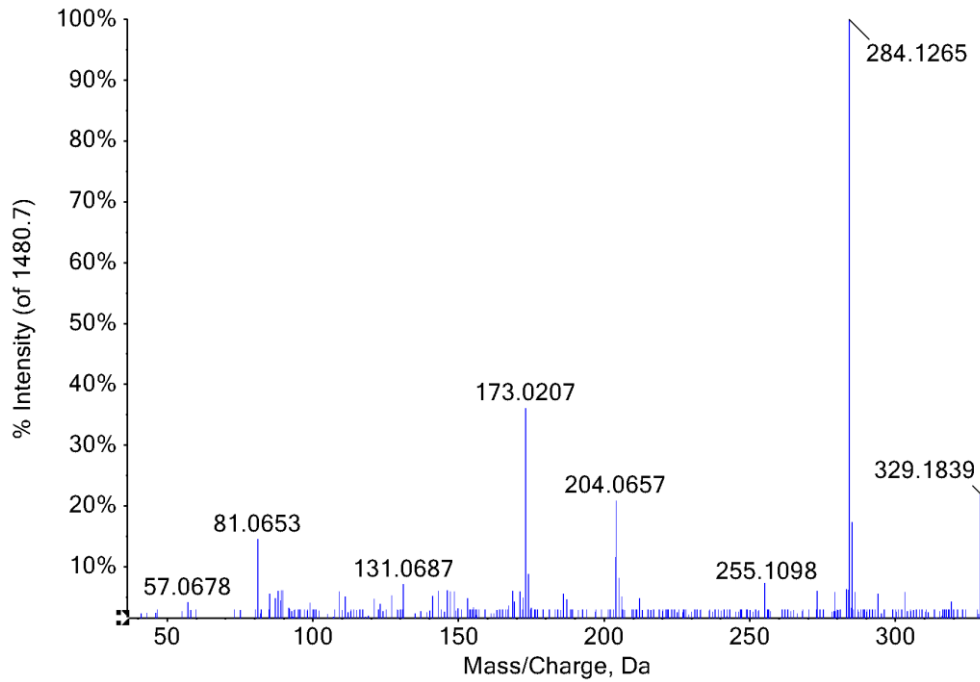
### Extracted Ion Chromatogram: Trifluoromethyl-U-47700



### TOF MS Spectra: Trifluoromethyl-U-47700



## MS/MS Spectra: Trifluoromethyl-U-47700



## 7. FUNDING

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