

# **Furanyl UF-17**

Sample Type: Seized Material

Latest Revision: July 22, 2019

Date Received: May 7, 2019

Date of Report: June 18, 2019

## 1. GENERAL INFORMATION

**IUPAC Name:** N-[2-(dimethylamino)cyclohexyl]-N-phenyl-furan-2-carboxamide

**InChI String:** InChI=1S/C19H24N2O2/c1-20(2)16-11-6-7-12-17(16)21(15-9-4-

3-5-10-15)19(22)18-13-8-14-23-18/h3-5,8-10,13-14,16-17H,6-

7,11-12H2,1-2H3

**CFR:** Not Scheduled (06/2019)

CAS# Not Available

**Synonyms:** Furanyl U-17

**Source:** Department of Homeland Security

**Appearance:** White Solid Material

*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, D-ABFT-FT, and Barry K. Logan, PhD, F-ABFT

#### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical	Molecular	Molecular Ion	Exact Mass
	Formula	Weight	[M <sup>+</sup> ]	[M+H] <sup>+</sup>
Base	$C_{19}H_{24}N_2O_2$	312.4	312	313.1910

#### 3. BRIEF DESCRIPTION

Furanyl UF-17 is structurally similar to UF-17, a drug synthetized during pharmaceutical discovery by the Upjohn Company as an antidepressant agent. The "UF-17" name was created by Cayman Chemical due to structural resemblance with U-47700 and fentanyl, two synthetic opioids, as well as the number scheme from its original patent. No information is available regarding the activities or receptor binding profiles of UF-17 and Furanyl UF-17, specifically relating to the opioid receptor system; therefore, these substances have not been assigned a subclassification under the novel psychoactive substance (NPS) class of emerging drugs. UF-17 and Furanyl UF-17 are not scheduled substances in the United States.

## 4. ADDITIONAL RESOURCES

1. Szmuszkovicz, J; VonVoigtlander, PF; Kane, MP. A New Nontricyclic Antidepressant Agent. Synthesis and Activity of N-[trans-2-(Dimethylamino)cyclopentyl]-N-(3,4-dichlorophenyl)propanamide and Related Compounds. *J Med Chem.* **1981**, 23, 1230-1236. https://www.ncbi.nlm.nih.gov/pubmed/7328583

https://www.caymanchem.com/product/27924

## 5. QUALITATIVE DATA

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

**Testing Performed At:** NMS Labs (Willow Grove, PA)

**Sample Preparation:** Acid/Base extraction

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

Column: Zebron<sup>TM</sup> Inferno<sup>TM</sup> ZB-35HT (15 m x 250  $\mu$ m x 0.25  $\mu$ m)

Carrier Gas: Helium (Flow: 1 mL/min)

**Temperatures:** 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

**Injection Parameters:** Injection Type: Splitless

Injection Volume: 1 µL

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

Threshold: 250

**Retention Time:** 6.643 min

**Standard Comparison:** Reference material for Furanyl UF-17 (Batch: 0558709-7) was

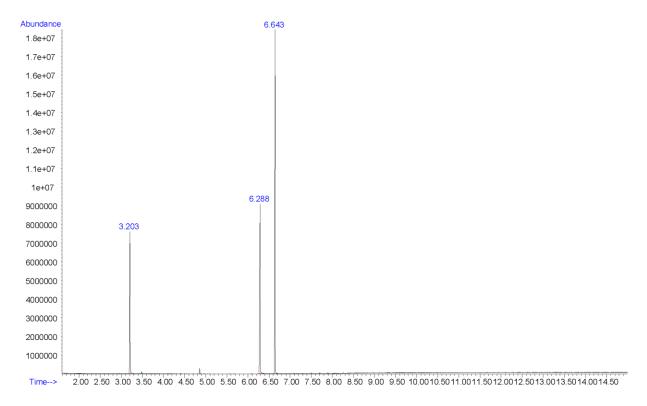
purchased from Cayman Chemical (Ann Arbor, MI, USA).

Analysis of this standard resulted in positive identification of the analyte in the exhibit as Furanyl UF-17, based on retention time

(6.643 min) and mass spectral data.

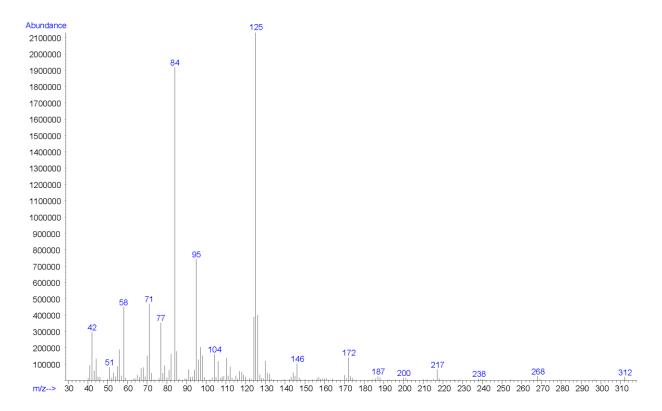
(https://www.caymanchem.com/product/27924)

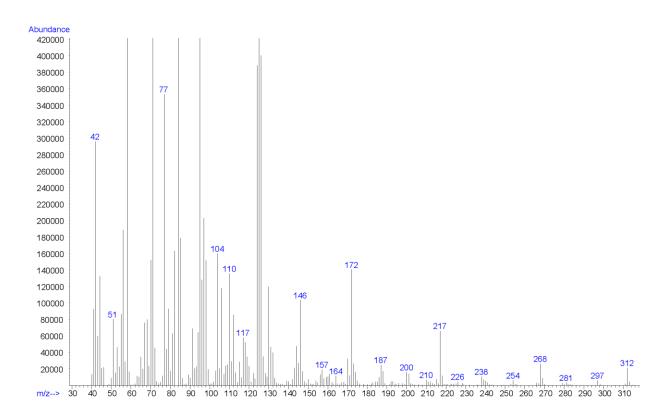
## **Chromatogram: Furanyl UF-17**



Additional peaks present in chromatogram: internal standards (3.203 min and 6.288 min)

EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Furanyl UF-17





# 5.2 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:** 1:100 dilution of acid/base extract in mobile phase

**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: Collison Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

**Retention Time:** 5.74 min

**Standard Comparison:** Reference material for Furanyl UF-17 (Batch: 0558709-7) was

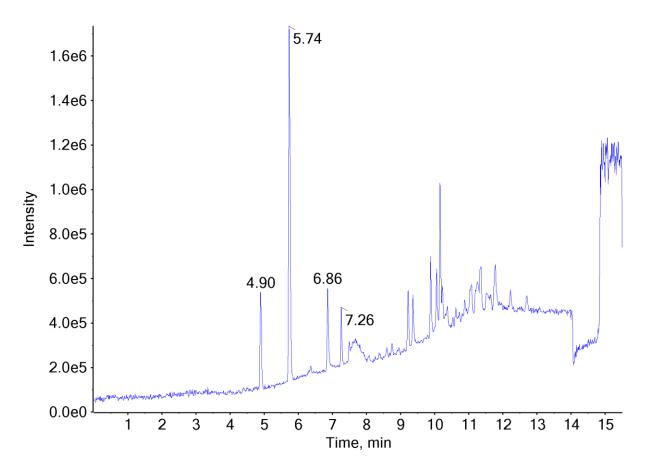
purchased from Cayman Chemical (Ann Arbor, MI, USA).

Analysis of this standard resulted in positive identification of the analyte in the exhibit as Furanyl UF-17, based on retention time

(5.73 min) and mass spectral data.

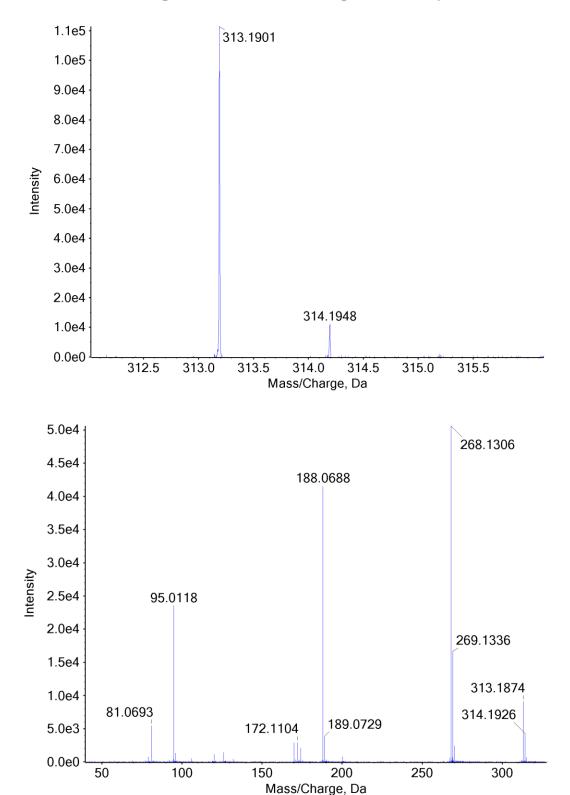
(https://www.caymanchem.com/product/27924)

## **Chromatogram: Furanyl UF-17**



Additional peaks present in chromatogram: internal standard (4.90 min), not a controlled substance (6.86 min), and internal standard (7.26 min)

TOF MS (Top) and MS/MS (Bottom) Spectra: Furanyl UF-17



## 6. REVISION HISTORY

<u>Date</u> <u>Revision</u>

07/22/2019 Important Note (Page 1) Revised: "All identifications were made based on

evaluation of analytical data (GC-MS and LC-QTOF) in comparison to

analysis of acquired reference material."