Furanyl UF-17

Sample Type: Seized Material

Latest Revision: June 18, 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, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M+]</th>
<th>Exact Mass [M+H]⁺</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C₁₉H₂₄N₂O₂</td>
<td>312.4</td>
<td>312</td>
<td>313.1910</td>
</tr>
</tbody>
</table>

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.¹ 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


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™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)

**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: Collision 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