Benzylfuranylfentanyl

Latest Revision: May 1, 2018
Date Received: March 23, 2018
Date of Report: April 27, 2018

1. GENERAL INFORMATION

IUPAC Name: N-(1-benzyl-4-piperidyl)-N-phenyl-furan-2-carboxamide

InChI String: InChI=1S/C23H24N2O2/c26-23(22-12-7-17-27-22)25(20-10-5-2-6-11-20)21-13-15-24(16-14-21)18-19-8-3-1-4-9-19/h1-12,17,21H,13-16,18H2

CFR: Not Scheduled (04/2018)

CAS# Not Available

Synonyms: Benzyl Furanyl Fentanyl, Benzyl Fu-F

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.
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>C$<em>{23}$H$</em>{24}$N$_2$O$_2$</td>
<td>360.45</td>
<td>360</td>
<td>361.1911</td>
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3. BRIEF DESCRIPTION

Benzylfuranylfentanyl is classified as a suspected fentanyl analogue precursor. Fentanyl analogue precursors are modified based on the structure of fentanyl or its analogues with the absence of notable functional groups or structural features. Fentanyl analogue precursors are often used in the synthesis of a variety of fentanyl analogues. Benzylfuranylfentanyl is not a scheduled substance 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:**
- 8.369 min

**Chromatogram: Benzylfuranylfentanyl**

*Additional peaks present in chromatogram: internal standard 1 (3.214 min) and internal standard 2 (6.289 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Benzylfuranylfentanyl
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 extraction 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: 6.16 min
Chromatogram: Benzylfuranylfentanyl

Additional peaks present in chromatogram: internal standard 1 (4.99 min) and internal standard 2 (7.30 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: Benzylfuranylfentanyl
5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Powder dissolved in methylene chloride (5 mL), washed with 2 N NaOH (2 mL) and brine, evaporated, and dissolved in DMSO

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters: Pulse Sequence: Proton

Solvent: DMSO

Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

Delay between pulses: 1st delay, d1 = 1.000

$^1$H NMR: Benzylfuranylketanly
gCOSY: Benzylfuranylfentanyl
gCOSY (2x Zoom): Benzylfuranylfentanyl
6. REVISION HISTORY

<table>
<thead>
<tr>
<th>Date</th>
<th>Revision</th>
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<tbody>
<tr>
<td>05/01/2018</td>
<td>Section 5.3: Sample preparation revised (&quot;Dilute powder in CDCl₃&quot; changed to &quot;Powder dissolved in methylene chloride [5 mL], washed with 2 N NaOH [2 mL] and brine, evaporated, and dissolved in DMSO&quot;). Parameters revised (&quot;CDCl₃&quot; changed to &quot;DMSO&quot;).</td>
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