**para-Fluorocyclopropylbenzylfentanyl & Despropionyl para-Fluorobenzylfentanyl**

**para-Fluorocyclopropylbenzylfentanyl**

Sample Type: Seized Material

Latest Revision: **October 5, 2018**
Date Received: **June 27, 2018**
Date of Report: **October 5, 2018**

**Despropionyl para-Fluorobenzylfentanyl**

**Important Note:** Identification of para-Fluorocyclopropylbenzylfentanyl was made based on evaluation of analytical data (GC-MS and LC-QTOF) in comparison to analysis of acquired reference material. Identification of Despropionyl para-Fluorobenzylfentanyl was made based on evaluation of analytical data only (GC-MS and LC-QTOF).

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1. GENERAL INFORMATION

1.1 para-Fluorocyclopropylbenzylfentanyl

IUPAC Name: N-(1-benzyl-4-piperidyl)-N-(4-fluorophenyl)cyclopropanecarboxamide

InChI String: InChI=1S/C22H25FN2O/c23-19-8-10-20(11-9-19)25(22(26)18-6-7-18)21-12-14-24(15-13-21)16-17-4-2-1-3-5-17/h1-5,8-11,18,21H,6-7,12-16H2

CFR: Not Scheduled (10/2018)

CAS#: Not Available

Synonyms: N-benzyl para-fluoro Cyclopropyl norfentanyl, p-FCBF

Source: Department of Homeland Security

Appearance: White Solid Material

1.2 Despropionyl para-Fluorobenzylfentanyl

IUPAC Name: 1-benzyl-N-(4-fluorophenyl)piperidin-4-amine

InChI String: InChI=1S/C18H21FN2/c19-16-6-8-17(9-7-16)20-18-10-12-21(13-11-18)14-15-4-2-1-3-5-15/h1-9,18,20H,10-14H2

CFR: Not Scheduled (10/2018)

CAS#: Not Available

Synonyms: para-Fluoro 4-ANBP, 4-Fluoro 4-ANBP

Source: Department of Homeland Security

Appearance: White Solid Material
2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Analyte</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>para-Fluorocyclopropyl-benzylfentanyl</td>
<td>C₂₂H₂₅FN₂O</td>
<td>352.4</td>
<td>352</td>
<td>353.2024</td>
</tr>
<tr>
<td>Despropionyl para-Fluorobenzylfentanyl</td>
<td>C₁₈H₂₁FN₂</td>
<td>284.4</td>
<td>284</td>
<td>285.1762</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

*para*-Fluorocyclopropylbenzylfentanyl and Despropionyl *para*-Fluorobenzylfentanyl are classified as suspected fentanyl analogue precursors. 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. *para*-Fluorocyclopropylbenzylfentanyl and Despropionyl *para*-Fluorobenzylfentanyl 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:**
- Despropionyl para-Fluorobenzylfentanyl: 6.845 min
- para-Fluorocyclopropylbenzylfentanyl: 7.756 min

**Standard Comparison:**
Reference material for para-Fluorocyclopropylbenzylfentanyl (Batch: 0531312-6) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as para-Fluorocyclopropylbenzylfentanyl, based on retention time (7.737 min) and mass spectral data.

Chromatogram: *para*-Fluorocyclopropylbenzylfentanyl & Despropionyl *para*-Fluorobenzylfentanyl

*Additional peaks present in chromatogram: internal standards (3.210 and 6.290 mins)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom):

*para-*Fluorocyclopropylbenzylfentanyl
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom):
Despropionyl para-Fluorobenzylfentanyl
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: *Despropionyl para-Fluorobenzylfentanyl*: 6.11 min
*para-Fluorocyclopropylbenzylfentanyl*: 6.49 min

Standard Comparison: Reference material for *para*-Fluorocyclopropylbenzylfentanyl (Batch: 0531312-6) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as *para*-Fluorocyclopropylbenzylfentanyl, based on retention time (6.33 min) and mass spectral data.

Chromatogram: *para*-Fluorocyclopropylbenzylfentanyl and Despropionyl *para*-Fluorobenzylfentanyl

Additional peaks present in chromatogram: internal standard (5.06 min), not a controlled substance (7.20 min), not a controlled substance (9.91 min), not a controlled substance (10.15 min), not a controlled substance (10.38 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: *para*-Fluorocyclopropylbenzylfentanyl
TOF MS (Top) and MS/MS (Bottom) Spectra: Despropionyl \textit{para}-Fluorobenzylfentanyl