**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).

**Prepared By:** Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT
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. Both compounds were detected in a single exhibit of white powder seized at the United States border. These substances are benzyl and despropionyl benzyl analogues of fentanyl related substances. Both compounds are structurally related to benzylfentanyl, which demonstrates minimal opioid receptor agonist activity and is not scheduled in the United States. Benzyl and despropionyl analogues have utility as potential precursors for fentanyl and fentanyl analogue synthesis. The presence of Despropionyl para-Fluorobenzylfentanyl in this exhibit may be due to its unconsumed nature during the synthesis of para-Fluorocyclopropylbenzylfentanyl. para-Fluorocyclopropylbenzylfentanyl and Despropionyl para-Fluorobenzylfentanyl are not scheduled substances in the United States.

4. ADDITIONAL RESOURCES

https://www.caymanchem.com/product/25238

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.

(https://www.caymanchem.com/product/25238)
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.

(https://www.caymanchem.com/product/25238)
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