ortho-Fluorofentanyl

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

![Chemical structure of ortho-Fluorofentanyl]

1. GENERAL INFORMATION

**IUPAC Name:** N-(2-fluorophenyl)-N-[1-(2-phenylethyl)-4-piperidinyl]propionamide

**CAS#:** NA

**Synonyms:** N-(2-fluorophenyl)-N-(1-phenethylpiperidin-4-yl)propionamide, o-fluorofentanyl, 2-fluorofentanyl, ortho-F-fentanyl

**Source:** DEA Reference Material Collection

**Appearance:** white powder

**UV\textsubscript{max}\,(nm):** NA

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Melting Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C\textsubscript{22}H\textsubscript{27}FN\textsubscript{2}O</td>
<td>354.46</td>
<td>NA</td>
</tr>
<tr>
<td>HCl</td>
<td>C\textsubscript{22}H\textsubscript{27}FN\textsubscript{2}O \cdot \text{HCl}</td>
<td>390.92</td>
<td>NA</td>
</tr>
</tbody>
</table>

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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in CD3OD containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer
Parameters:
- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds

$^1$HNMR: ortho-Fluorofentanyl HCl; Lot# RM-160713-01

![NMR Spectra](image_url)
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL into methanol.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5; 30m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1.5mL/min
Temperatures:
  - MSD transfer line: 280°C
  - MS Source: 230°C
  - MS Quad: 150°C
Oven program:
  1) 100°C initial temperature for 1.0 min
  2) Ramp to 280°C at 12 °C/min
  3) Hold final temperature for 9.0 min
Injection Parameters:
  - Split Ratio = 25:1, L injected
MS Parameters:
  - Mass scan range: 30-550 amu
  - Threshold: 100
  - Tune file: stune.u
  - Acquisition mode: scan
Retention Time: 16.276min

EI Mass Spectrum: ortho-Fluorofentanyl HCl; Lot#RM-160713-01
### 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (1 bounce)

**Scan Parameters:**
- Number of scans: 32
- Number of background scans: 32
- Resolution: 4 cm\(^{-1}\)
- Sample gain: 4
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): ortho-Fluorofentanyl HCl; Lot\#RM-160713-01
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3.4. GAS CHROMATOGRAPHY /INFRARED DETECTION:

Sample Preparation:  Dilute analyte 1mg/ml in CHCl₃

Instrument:  Gas Chromatograph in split mode with Infrared Detection HP-5;
Column:  30m x 0.32 mm id x 0.25 m
Carrier Gas:  Helium at 2.0mL/min
Temperature:  Injector: 280°C  Split ratio: 2:1, 2 l injection
65°C hold 1.5min., ramp to 310°C at 20°C/min., hold 5min.
IRD:  Detector: Transfer line
       Temp 280°C
       Flow Cell Temp 280°C
       Resolution 8 cm⁻¹

GC-IRD: ortho-Fluorofentanyl HCl; Lot# RM-160713-01

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4. ADDITIONAL RESOURCES

No additional resources as of 07/02/2021