meta-Fluorofentanyl

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

1. GENERAL INFORMATION

**IUPAC Name:** N-(3-fluorophenyl)-N-(1-phenethylpiperidin-4-yl)propionamide

**CAS#:** N/A

**Synonyms:** N-(3-fluorophenyl)-N-[1-(2-phenylethyl)piperidin-4-yl]propanamide, N-(3-fluorophenyl)-N-[1-(2-phenylethyl)-4-piperidinyl]propanamide, 3-FF, N-(3-fluorophenyl)-N-[1-(2-phenylethyl)-4-piperidinyl]-propanamide, m-FF

**Source:** DEA Reference Material Collection

**Appearance:** white powder

**UV<sub>max</sub>(nm):** N/A

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&lt;sub&gt;22&lt;/sub&gt;H&lt;sub&gt;27&lt;/sub&gt;FN&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>354.46</td>
<td>NA</td>
</tr>
<tr>
<td>HCl</td>
<td>C&lt;sub&gt;22&lt;/sub&gt;H&lt;sub&gt;27&lt;/sub&gt;FN&lt;sub&gt;2&lt;/sub&gt;O · HCl</td>
<td>390.92</td>
<td>NA</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/2mL in CD3OD containing TMS for 0 ppm reference and 1,4-BTMSB-d₄ 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

H¹NMR: meta-Fluorofentanyl HCl; Lot# 0537179-4
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: Injector: 280°C
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, 1 μL injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan
Retention Time: 17.420 min

El Mass Spectrum: meta-Fluorofentanyl HCl; Lot#0537179-4

Latest Revision: 07/19/2021
SWGDRUG.org/monographs.htm
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): meta-Fluorofentanyl HCl; Lot#0537179-4
3.4. GAS CHROMATOGRAPHY /INFRARED DETECTION:

Sample Preparation: Dilute analyte 1mg/ml in CHCl₃

Instrument: Gas Chromatograph in split mode with Infrared Detection
Column: HP-5; 30m x 0.32 mm id x 0.25 µm
Carrier Gas: Helium at 2.0mL/min
Temperature: Injector: 280°C, Split ratio: 2:1, 2µl 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: meta-Fluorofentanyl HCl; Lot 0537179-4
4. ADDITIONAL RESOURCES

No additional resources as of 07/19/2021