para-Fluoro furanyl fentanyl

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

![Chemical Structure of para-Fluoro furanyl fentanyl]

1. GENERAL INFORMATION

**IUPAC Name:** \(N-(4\text{-fluorophenyl})-N-(1\text{-phenethylpiperidin-4-yl})\text{furan-2-carboxamide}\)

**CAS#:** N/A

**Synonyms:** \(N-(4\text{-fluorophenyl})-N-[1-(2\text{-phenylethyl)piperidin-4-yl}]\text{furan-2-carboxamide}\)

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**\(UV_{\text{max}}(\text{nm})\):** Not determined

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>(\text{C}<em>{24}\text{H}</em>{25}\text{FN}_2\text{O}_2)</td>
<td>392.47</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>(\text{C}<em>{24}\text{H}</em>{25}\text{FN}_2\text{O}_2 \cdot \text{HCl})</td>
<td>428.93</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~14 mg/2mL in methanol-$d_4$ containing TMS for 0 ppm reference and 1,4-BTMSB-$d_4$ 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: $para$-fluoro furanyl fentanyl HCl; Lot# 0511635-8; methanol-$d_4$; 400MHz
**para-Fluoro furanyl fentanyl**

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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte ~3 mg/mL in MeOH

**Instrument:** Agilent gas chromatograph operated in split mode with MS detector

**Column:** HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm

**Carrier Gas:** Helium at 1.5 mL/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
- Tune file: stune.u
- Acquiring mode: scan
- Threshold: 150

**Retention Time:** 19.39 min

El Mass Spectrum: *para*-fluoro furanyl fentanyl HCl; Lot# 0511635-8
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### 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: 1
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): *para*-fluoro furanyl fentanyl HCl; Lot# 0511635-8

```
Wavenumber (cm⁻¹)

%Transmittance
```

Scan Parameters:
- Aperture: 150
- Sample gain: 1
- Resolution: 4 cm⁻¹