1. GENERAL INFORMATION

**IUPAC Name:** N-(2-fluorophenyl)-N-(1-phenethylpiperidin-4-yl)isobutyramide

**CAS#:** N/A

**Synonyms:** 2-Fluoroisobutyryl fentanyl, N-(2-fluorophenyl)-2-methyl-N-[1-(2phenylethyl)piperidin-4yl]propanamide

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV$_{\text{max}}$(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 ($^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C$<em>{23}$H$</em>{29}$FN$_2$O</td>
<td>368.49</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>{23}$H$</em>{29}$FN$_2$O HCl</td>
<td>404.95</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~14 mg/mL in methanol-$d_4$ 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-fluoroisobutyryl fentanyl HCl; Lot# 0505593-26; CD3OD; 400MHz
orthofluoroisobutyryl fentanyl

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

3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~8 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 L injected

MS Parameters:
- Mass scan range: 30-550 amu
- Tune file: stune.u
- Threshold: 150
- Acquisition mode: scan

Retention Time: 16.62 min

EI Mass Spectrum: orthofluoroisobutyryl fentanyl HCl; Lot# 0505593-26
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: 8
- Aperture: 80

FTIR ATR (Diamond 1 Bounce): *ortho*-fluoroisobutyryl fentanyl HCl; Lot# 0505593-26