1. GENERAL INFORMATION

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

**CAS#:**  
N/A

**Synonyms:**  
o-fluorofentanyl, 2-fluorofentanyl, ortho-F-fentanyl

**Source:**  
DEA Reference Material Collection

**Appearance:**  
white powder (HCl)

**$UV_{max}(nm)$:**  
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 (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C$<em>{22}$H$</em>{27}$FN$_2$O</td>
<td>354.46</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>{22}$H$</em>{27}$FN$_2$O HCl</td>
<td>390.92</td>
<td>233.5</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in CD$_3$OD 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; CD$_3$OD; 400MHz

![NMR Spectral Chart]

* = $^{13}$C satellite
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 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 Threshold: 150
Tune file: stune.u Acquisition mode: scan
Retention Time: 16.885 min

El 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: 80

FTIR ATR (Diamond 1 Bounce): ortho-Fluorofentanyl HCl; LOT # RM-160713-01
4. ADDITIONAL RESOURCES

No additional resources as of 09/2016