Ocfentanil

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

1. GENERAL INFORMATION

**IUPAC Name:** \(N\)-(2-fluorophenyl)-2-methoxy-N-(1-phenethylpiperidin-4-yl)acetamide

**CAS#:** 101343-69-5

**Synonyms:** Ocfentanil; 
\(N\)-(2-fluorophenyl)-2-methoxy-N-[1-(2-phenylethyl)piperidin-4-yl]acetamide

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**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 (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>(C_{22}H_{27}FN_2O_2)</td>
<td>370.46</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>(C_{22}H_{27}FN_2O_2 \cdot HCl)</td>
<td>406.92</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
Ocfentanil

3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 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

$^1$H NMR: Ocfentanil HCl Lot # N18-P71G; 400MHz; CD$_3$OD
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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte ~4 mg/mL in 9:1 chloroform:methanol.

**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
- **Threshold:** 250
- **Tune file:** stune.u
- **Acquisition mode:** scan

**Retention Time:** 17.515 min

**EI Mass Spectrum:** Ocfentanil HCl Lot # N18-P71G
3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 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): Ocfentanil HCl Lot # N18-P71G