1. GENERAL INFORMATION

**IUPAC Name:** N-((1R,2R)-2-(dimethylamino)cyclohexyl)-4-fluorobenzamide; hydrochloride

**CAS#:** 67579-18-4 (base)

**Synonyms:** Udes03

**Source:** Synthesized Material Lot# JLK010-044-Udes03

**Appearance:** light brown solid (HCl)

**UV<sub>max</sub> (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>HCl</td>
<td>C&lt;sub&gt;15&lt;/sub&gt;H&lt;sub&gt;21&lt;/sub&gt;FN&lt;sub&gt;2&lt;/sub&gt;O-HCl</td>
<td>300.80</td>
<td>111.0 ± 2.11</td>
</tr>
<tr>
<td>Base</td>
<td>C&lt;sub&gt;15&lt;/sub&gt;H&lt;sub&gt;21&lt;/sub_FN&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>264.34</td>
<td>Not determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterated chloroform:methanol (CDCl₃:CD₃OD, 1:5) + TMS.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: 6410.3 Hz containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 30 seconds

¹H NMR: Udes03 HCl; Lot JLK010-044-Udes03; CDCl₃:CD₃OD (1:5) + TMS; 400 MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~ 1 mg/mL in methanol

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

**Column:** Rtx5MS (a DB-5 equivalent); 30m x 0.25 mm x 0.25 µm

**Carrier Gas:** Helium at 1 mL/min

**Temperatures:**
- Injector: 280°C
- MSD transfer line: 280°C
- MS Source: 200°C
- Oven program:
  1) 90°C initial temperature for 2.0 min
  2) Ramp to 300°C at 14°C/min
  3) Hold final temperature for 10.0 min

**Injection Parameters:** Split Ratio = 1:15, 1 µL injected

**MS Parameters:**
- Mass scan range: 34-550 amu
- Threshold: 100
- Tune file: 050218_Tune.qgt
- Acquisition mode: scan

**Retention Time:** 13.29 min

EI Mass Spectrum: Udes03 HCl; Lot JLK010-044-Udes03

Chemical Formula: C₁₅H₂₂F₂N₂O⁺
Exact Mass: 265.17107

[Chemical Structure Image]
Udes03 hydrochloride

The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material
3.3 INFRARED SPECTROSCOPY (TIR)

Instrument: FTIR with ZnSe ATR attachment (1 bounce)

Scan Parameters:
- Number of scans: 4
- Number of background scans: 4
- Resolution: 4 cm⁻¹
- Sample gain: 8
- Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): Udes03 HCl; Lot JLK010-044-Udes03
Udes03 hydrochloride

The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material

3.4 RAMAN SPECTROSCOPY

Instrument: Rigaku Progeny 1064
Scan Parameters: Power (mW): 350
Exposure (ms): 1000
Averages: 30
Threshold: 0.80

Raman (1064 nm): Udes03 HCl; Lot JLK010-044-Udes03
4. ADDITIONAL RESOURCES

 ANALGESIC N-(2-AMINOCYCLOALIPHATIC)BENZAMIDES
 Szmuszkovicz

 Benzeneacetamide amines: structurally novel non-\(\mu\) opioids
 J. Szmuszkovicz, and P.F. Von Voigtlander
 Journal of Medicinal Chemistry 1982, 25 (10), 1125–1126
 DOI: 10.1021/jm00352a005

 Factors affecting binding of trans-N-[2-(methylamino)cyclohexyl]benzamides at the primary morphine receptor
 B.V. Cheney, J. Szmuszkovicz, R.A. Lahti and D.A. Zichi
 Journal of Medicinal Chemistry 1985, 28 (12), 1853–1864
 DOI: 10.1021/jm00150a017

 Single stereoisomer analogs in the U-47700 series:

5. ACKNOWLEDGEMENT

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