1. GENERAL INFORMATION

**IUPAC Name:** N-((IR,2R)-2-(dimethylamino)cyclohexyl)-4-trifluoromethyl-N-methylbenzamide

**CAS#:** 67579-38-8 (base)

**Synonyms:** U04

**Source:** Synthesized Material Lot# JLK008-134-U04

**Appearance:** White Crystals

**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\textsubscript{17}H\textsubscript{23}F\textsubscript{3}N\textsubscript{2}O</td>
<td>329.18</td>
<td>91.2 ± 0.75</td>
</tr>
</tbody>
</table>
3. **QUALITATIVE DATA**

3.1 **NUCLEAR MAGNETIC RESONANCE**

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

*Instrument:* 400 MHz NMR spectrometer

*Parameters:* 6410.3 Hz containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 30 seconds

\(^1\text{H NMR: U04; Lot JLK008-134-U04; CDCl}_3 +\text{TMS; 400 MHz}^\text{CDCl}_3\ \text{TMS}
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:** 13.20 min

EI Mass Spectrum: U04; Lot JLK008-134-U04

Chemical Formula: C17H24F3N2O+  
Exact Mass: 329.18352
Zoomed view (84.10 and 125.15 are truncated in this view)
3.3 INFRARED SPECTROSCOPY (FTIR)

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): U04; Lot JLK008-134-U04
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): U04; Lot JLK008-134-U04

[Graph of Raman spectrum showing various wavenumbers and intensities]
4. ADDITIONAL RESOURCES

ANALGESIC N-(2-AMINOCYCLOALIPHATIC)BENZAMIDES
Szmuszkovicz
US Patent 4,098, 904 Jul. 4, 1978 Example 23A

Benzeneacetamide amines: structurally novel non-mµ 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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