1. GENERAL INFORMATION

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

**CAS#:** 67579-11-7 (base)

**Synonyms:** U02

**Source:** Synthesized Material Lot# JLK010-042-U02

**Appearance:** White Crystals (HCl)

**UV\textsubscript{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>HCl</td>
<td>C\textsubscript{16}H\textsubscript{23}ClN\textsubscript{2}O-HCl</td>
<td>331.28</td>
<td>121.1 ± 0.29</td>
</tr>
<tr>
<td>base</td>
<td>C\textsubscript{16}H\textsubscript{23}ClN\textsubscript{2}O</td>
<td>294.82</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: U02 HCl; Lot JLK010-042-U02; 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:** 14.98 min

EI Mass Spectrum: U02 HCl; Lot JLK010-042-U02

Chemical Formula: C_{16}H_{24}ClN_{2}O^{+}

Exact Mass: 295.15717
U02 hydrochloride

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

Zoomed view (84.05 and 125.10 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): U02 HCl; Lot JLK010-042-U02
U02 hydrochloride

The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material.
U02 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): U02 HCl; Lot JLK010-042-U02
4. ADDITIONAL RESOURCES

ANALGESIC N-(2-AMINOCYCLOALIPHATIC)BENZAMIDES
Szmuszkovicz
US Patent 4,098, 904 Jul. 4, 1978 Example 51(v)

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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