1. GENERAL INFORMATION

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

**CAS#:** 67579-70-8 (base)

**Synonyms:** U05

**Source:** Synthesized Material Lot# JLK008-137-U05

**Appearance:** White Crystals (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>hydrochloride</td>
<td>C&lt;sub&gt;17&lt;/sub&gt;H&lt;sub&gt;26&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;-HCl</td>
<td>326.86</td>
<td>99.7 ± 0.69</td>
</tr>
<tr>
<td>Base</td>
<td>C&lt;sub&gt;17&lt;/sub&gt;H&lt;sub&gt;26&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>290.40</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: U05 HCl; Lot JLK008-137-U05; 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: 15.48 min

EI Mass Spectrum: U05 HCl; Lot JLK008-137-U05

Chemical Formula: C₁₇H₂₇N₂O₂+
Exact Mass: 291.20670
U05 hydrochloride
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material

Zoomed view (84.10 and 125.20 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): U05 HCl; Lot JLK008-137-U05
U05 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): U05 HCl; Lot JLK008-137-U05
4. ADDITIONAL RESOURCES

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

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

These data are from a project supported by Award No. 2016-R2-CX-0059, awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice. The opinions, findings, and conclusions or recommendations expressed in this publication are those of the authors and do not necessarily reflect those of the Department of Justice. We also thank Rigaku Corporation for the loan of the Progeny 1064 Raman instrument.