U13 hydrochloride

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

1. GENERAL INFORMATION

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

CAS#: N/A

Synonyms: U13

Source: Synthesized Material Lot# JLK010-066-U13

Appearance: White Crystals (HCl)

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>HCl</td>
<td>C$<em>{16}$H$</em>{24}$N$_{2}$O-HCl</td>
<td>296.84</td>
<td>121.8 ± 1.10</td>
</tr>
<tr>
<td>Base</td>
<td>C$<em>{16}$H$</em>{24}$N$_{2}$O</td>
<td>260.37</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

^{1}H NMR: U13 HCl; Lot JLK010-066-U13; 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:** 13.75 min

EI Mass Spectrum: U13 HCl; Lot JLK010-066-U13

Chemical Formula: \( \text{C}_{16}\text{H}_{25}\text{N}_{2}\text{O}^+ \)
Exact Mass: 261.19614
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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): U13 HCl; Lot JLK010-066-U13
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3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): U13 HCl; Lot JLK010-066-U13
U13 hydrochloride

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4. ADDITIONAL RESOURCES

ANALGESIC N-(2-AMINOCYCLOALIPHATIC)BENZAMIDES
Szmuszkovicz

Benzeneacetamide amines: structurally novel non-μ 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/jm000150a017

Single stereoisomer analogs in the U-47700 series:

5. ACKNOWLEDGEMENT

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