AH-7563 hydrochloride

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

1. GENERAL INFORMATION

**IUPAC Name:** 1-(benzamidomethyl)-cyclohexyldimethylamine; hydrochloride

**CAS#:** 41804-98-2; 63886-94-2 (base)

**Synonyms:** A13

**Source:** Synthesized Material Lot# JLK010-027-A13

**Appearance:** White Crystals (HCl)

**\( \text{UV}_{\text{max}} \) (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_{16}H_{24}N_{2}O-HCl</td>
<td>296.84</td>
<td>232.6 ± 0.06</td>
</tr>
<tr>
<td>base</td>
<td>C_{16}H_{24}N_{2}O</td>
<td>260.37</td>
<td>Not determined</td>
</tr>
</tbody>
</table>
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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: A13 HCl; Lot JLK010-027-A13; CDCl₃:CD₃OD (1:5) + TMS; 400 MHz

![NMR spectra image]
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:** 14.82 min

**EI Mass Spectrum:** A13 HCl; Lot JLK010-027-A13

Chemical Formula: C_{16}H_{25}N_{2}O^{+}

Exact Mass: 261.19614
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Zoomed view (126.15 is 100% relative intensity and is truncated in this view)
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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): A13 HCl; Lot JLK010-027-A13

![FTIR Spectrum](image-url)
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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): A13 HCl; Lot JLK010-027-A13
4. ADDITIONAL RESOURCES

1-(3,4-DICHLOROBENZAMIDOMETHYL)CYCLOHEXYLDIMETHYLAMINE
Norman James Harper and George Bryan Austin Veitch
US Patent 3,975,443 Aug. 17, 1976 Example 4

1-(3,4-Dichlorobenzamidomethyl)cyclohexyldimethylamine and related compounds as potential analgesics
N. J. Harper, G. B. A. Veitch, and D. G. Wibberley
Journal of Medicinal Chemistry 1974 17 (11), 1188-1193
DOI: 10.1021/jm00257a012 Compound AH-7563

Tom Hsu, Jayapal Reddy Mallareddy, Kayla Yoshida, Vincent Bustamante, Tim Lee, John L. Krstenansky,
Alexander C. Zambon, Synthesis and pharmacological characterization of ethylenediamine synthetic opioids
in human μ-opiate receptor 1 (OPRM1) expressing cells. Pharmacol. Research & Perspectives 7: e00511

5. ACKNOWLEDGEMENT

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