1. GENERAL INFORMATION

IUPAC Name: 1-(4-bromobenzamidomethyl)-cyclohexylidimethylamine; hydrochloride

CAS#: 898610-01-0 (base)

Synonyms: A08

Source: Synthesized Material Lot# JLK008-044-08

Appearance: White Crystals (HCl)

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>$\text{C}<em>{16}\text{H}</em>{23}\text{BrN}_{2}\text{O} \cdot \text{HCl}$</td>
<td>375.73</td>
<td>$215.5 \pm 0.55$</td>
</tr>
<tr>
<td>Base</td>
<td>$\text{C}<em>{16}\text{H}</em>{23}\text{BrN}_{2}\text{O}$</td>
<td>339.27</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 (CDCl₃) + 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: A08 HCl; Lot JLK008-044-08; CDCl₃+ 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: 050218Tune.qgt
- Acquisition mode: scan

**Retention Time:** 16.74 min

EI Mass Spectrum: A08 HCl; Lot JLK008-044-0

Chemical Formula: \(\text{C}_{16}\text{H}_{24}\text{BrN}_{2}\text{O}^+\)

Exact Mass: 339.10665
A08 hydrochloride

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

Zoomed view (126.15 is 100% relative intensity and is 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): A08 HCl; Lot JLK008-044-08
A08 hydrochloride

The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material
A08 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): A08 HCl; Lot JLK008-044-08

![Raman Spectroscopy Graph]
**4. ADDITIONAL RESOURCES**

1-(3,4-DICHLOROBENZAMIDOMETHYL)CYCLOHEXYLDIMETHYLAMINE
Norman James Harper and George Bryan Austin Veitch

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


**5. ACKNOWLEDGEMENT**

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