A11 hydrochloride

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

![Chemical structure of A11 hydrochloride]

1. GENERAL INFORMATION

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

**CAS#:** 1427543-91-6 (base)

**Synonyms:** A11

**Source:** Synthesized Material Lot# JLK008-107-11

**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 ($^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCl</td>
<td>C$<em>{15}$H$</em>{23}$N$_3$O-HCl</td>
<td>297.82</td>
<td>238.3 ± 0.12</td>
</tr>
<tr>
<td>Base</td>
<td>C$<em>{15}$H$</em>{23}$N$_3$O</td>
<td>261.36</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: A11 HCl; Lot JLK008-107-11; 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: 15.11 min

EI Mass Spectrum: A11 HCl; Lot JLK008-107-11

Chemical Formula: C_{15}H_{24}N_{3}O^+
Exact Mass: 262.19139
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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): A11 HCl; Lot JLK008-107-11
A11 hydrochloride

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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): A11 HCl; Lot JLK008-107-11
4. ADDITIONAL RESOURCES

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

1-(3,4-Dichlorobenzamidomethyl)cyclohexylidimethylamine 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

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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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.