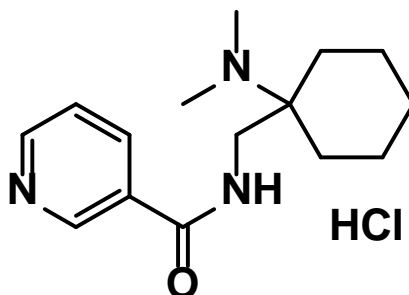


A11 hydrochloride

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



1. GENERAL INFORMATION

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

CAS#: 1427543-91-6 (base)

Synonyms: A11

Source: Synthesized Material Lot# JLK008-107-11

Appearance: White Crystals (HCl)

UV_{max} (nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
HCl	C ₁₅ H ₂₃ N ₃ O·HCl	297.82	238.3 ± 0.12
Base	C ₁₅ H ₂₃ N ₃ O	261.36	Not determined

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.

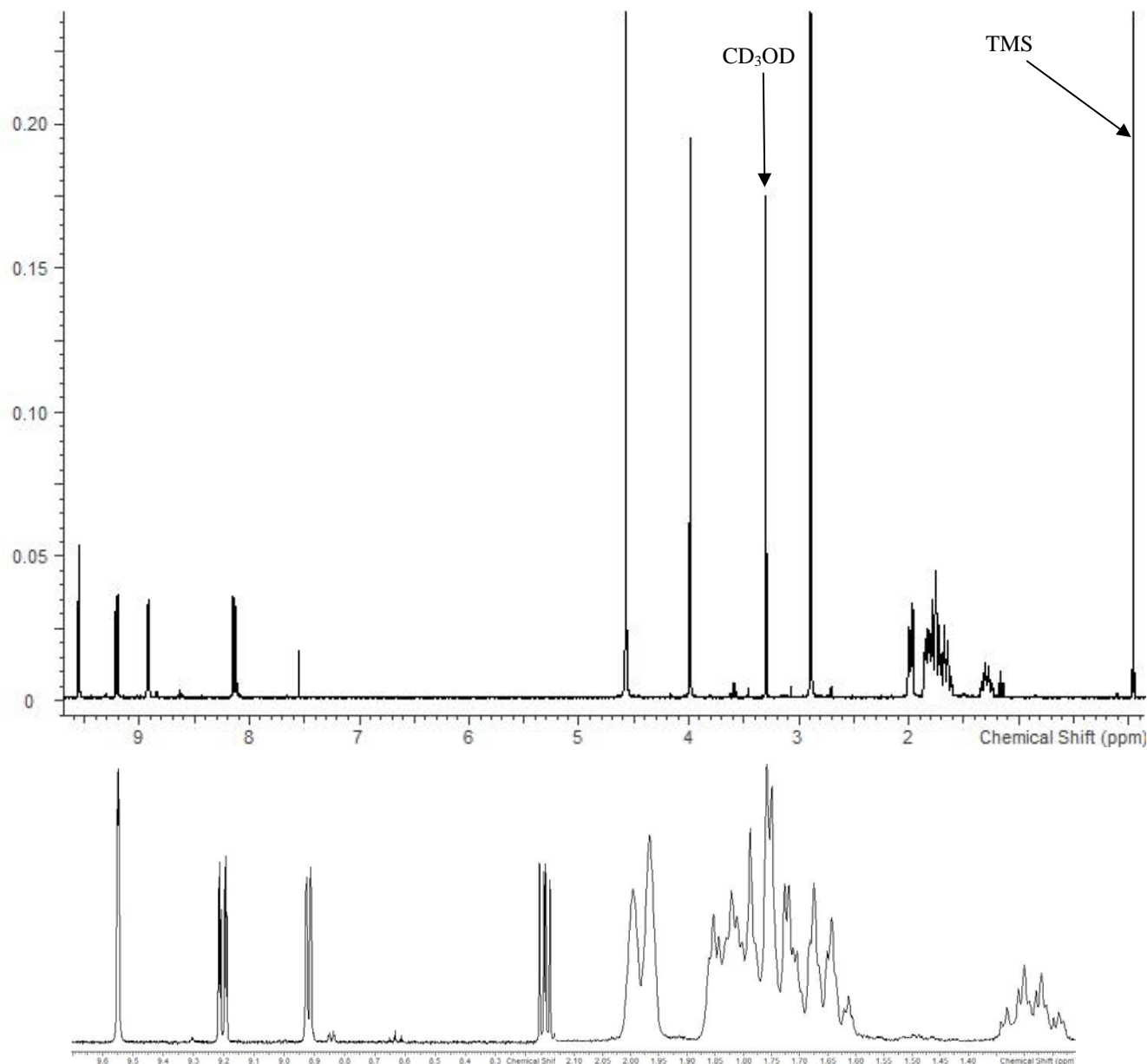
Instrument: 400 MHz NMR spectrometer

Parameters: Spectral width: 6410.3 Hz containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 30 seconds

¹H NMR: A11 HCl; Lot JLK008-107-11; CDCl₃:CD₃OD (1:5) + TMS; 400 MHz



A11 hydrochloride

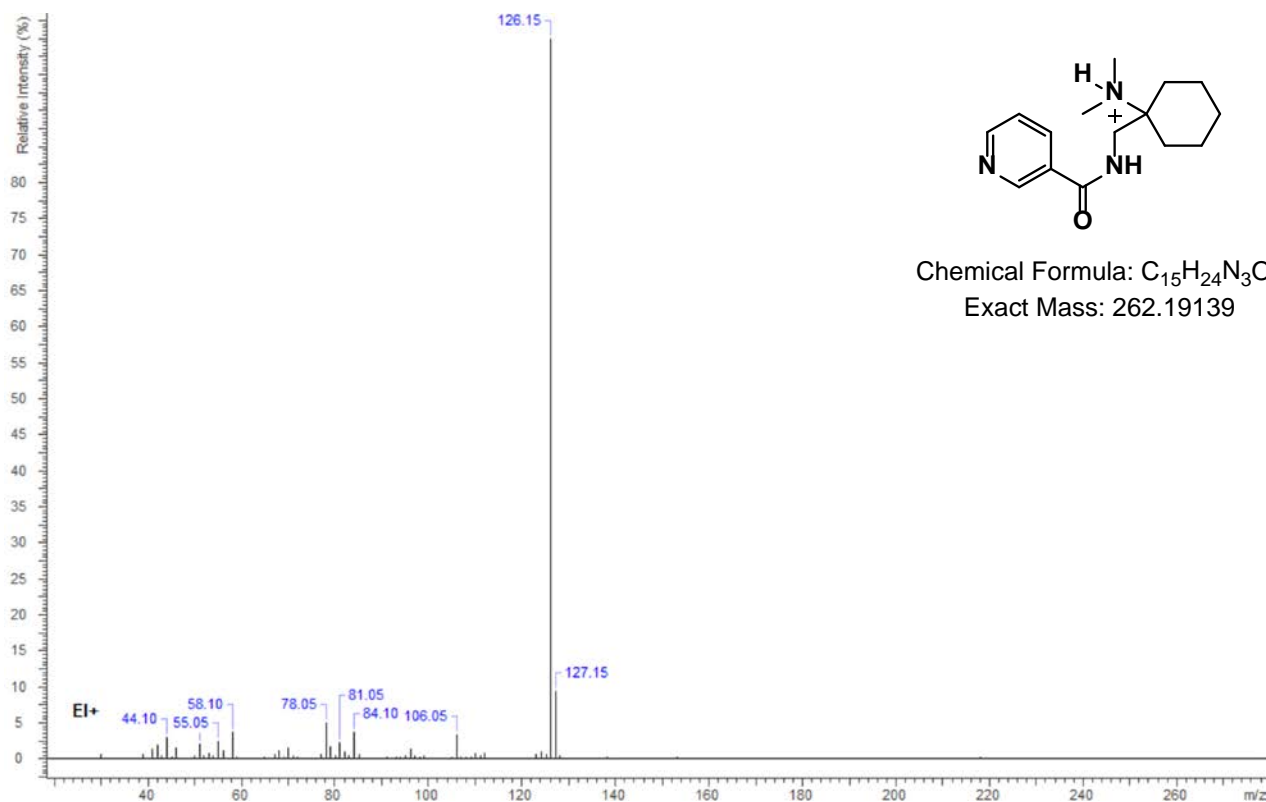
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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

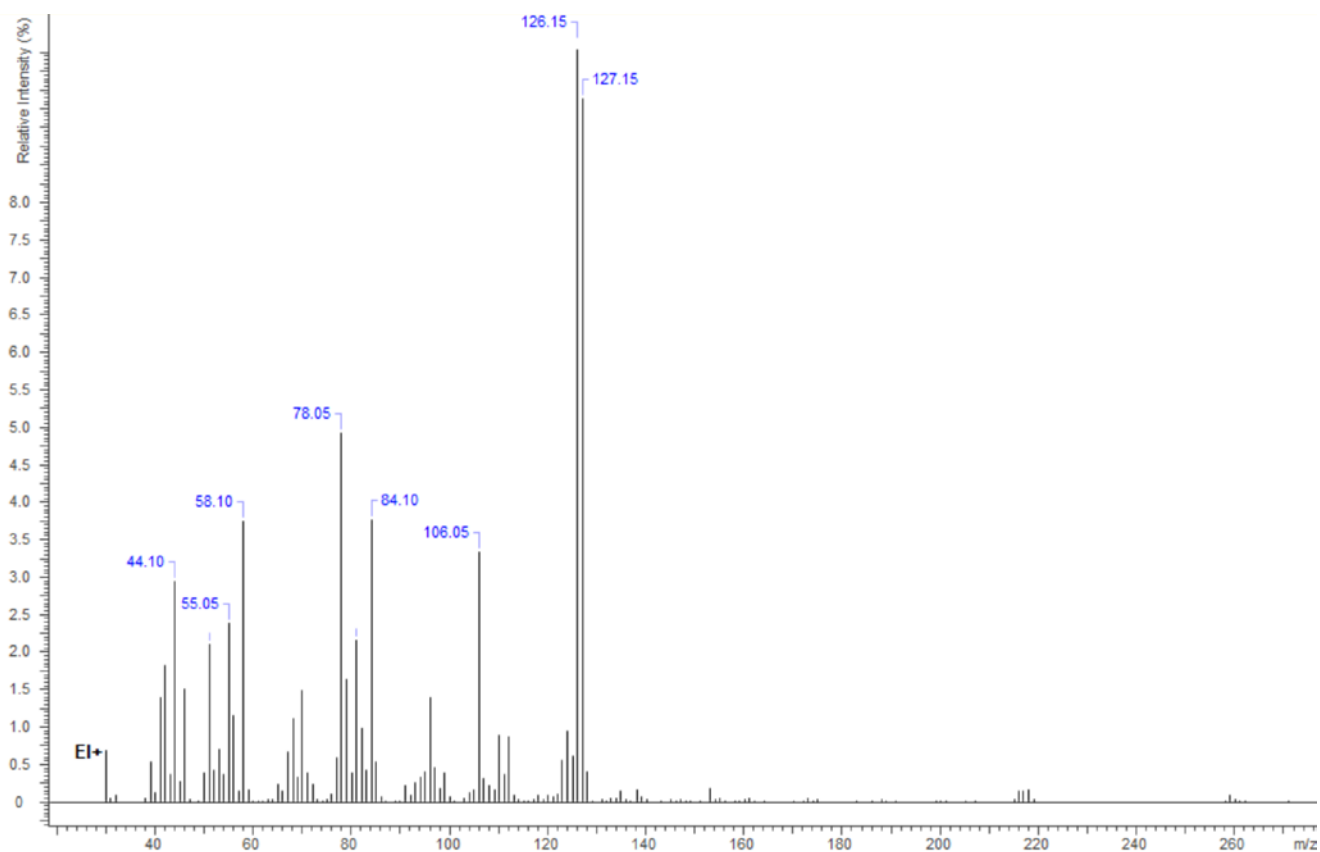
EI Mass Spectrum: A11 HCl; Lot JLK008-107-11



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Zoomed view (126.15 is 100% relative intensity and is truncated in this view)



A11 hydrochloride

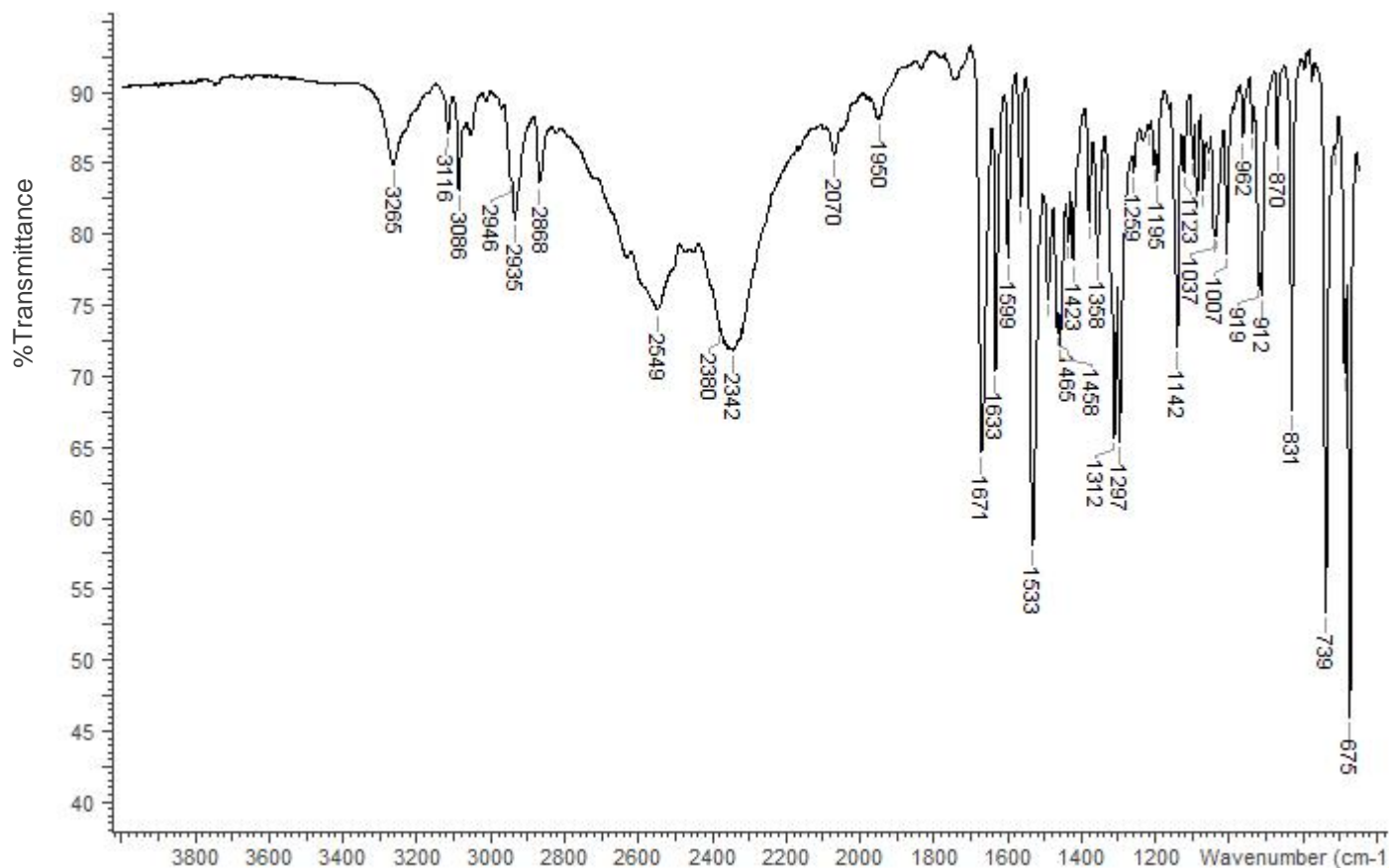
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material

3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with ZnSe ATR attachment (1 bounce)

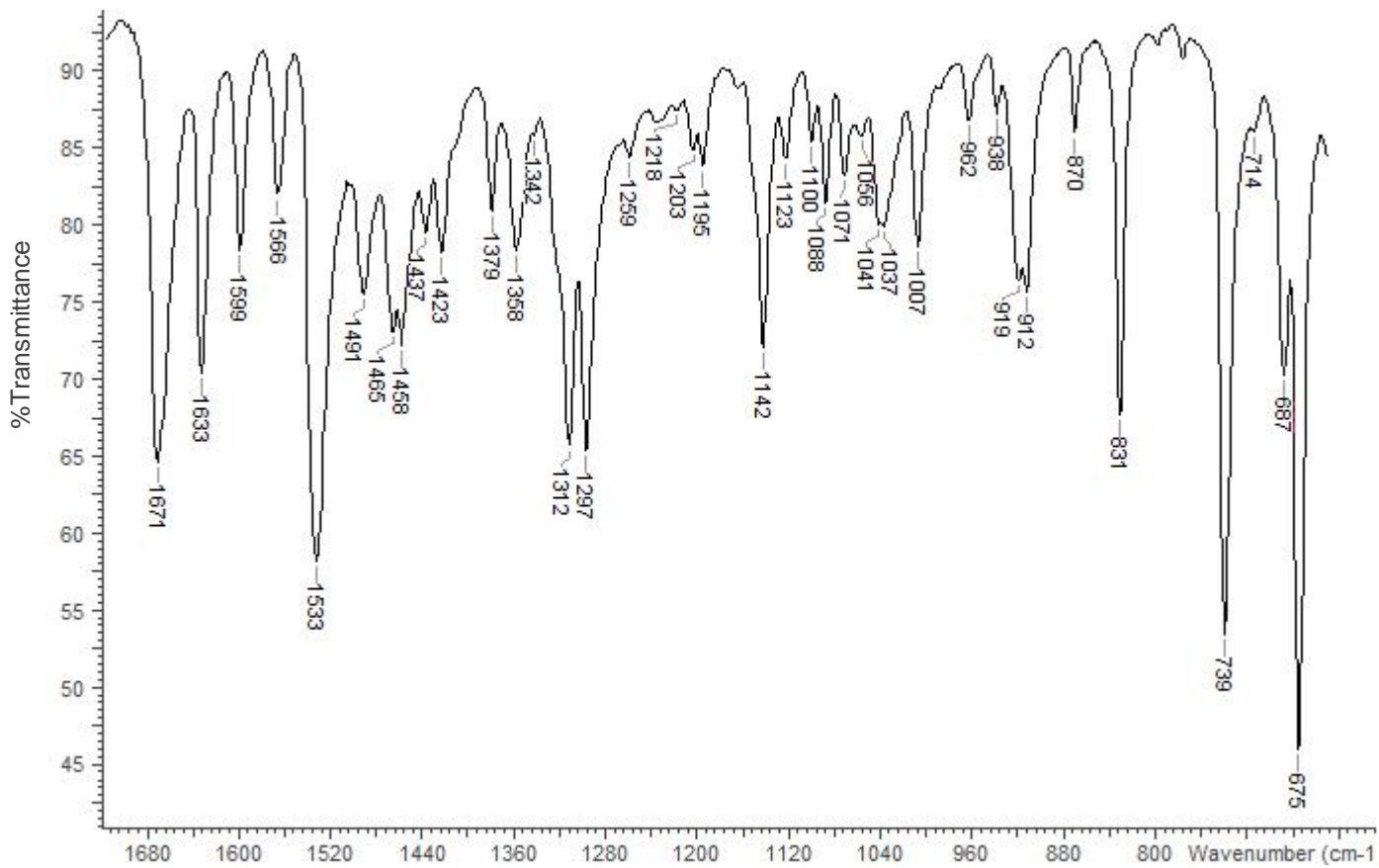
Scan Parameters: Number of scans: 4
Number of background scans: 4
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): A11 HCl; Lot JLK008-107-11



A11 hydrochloride

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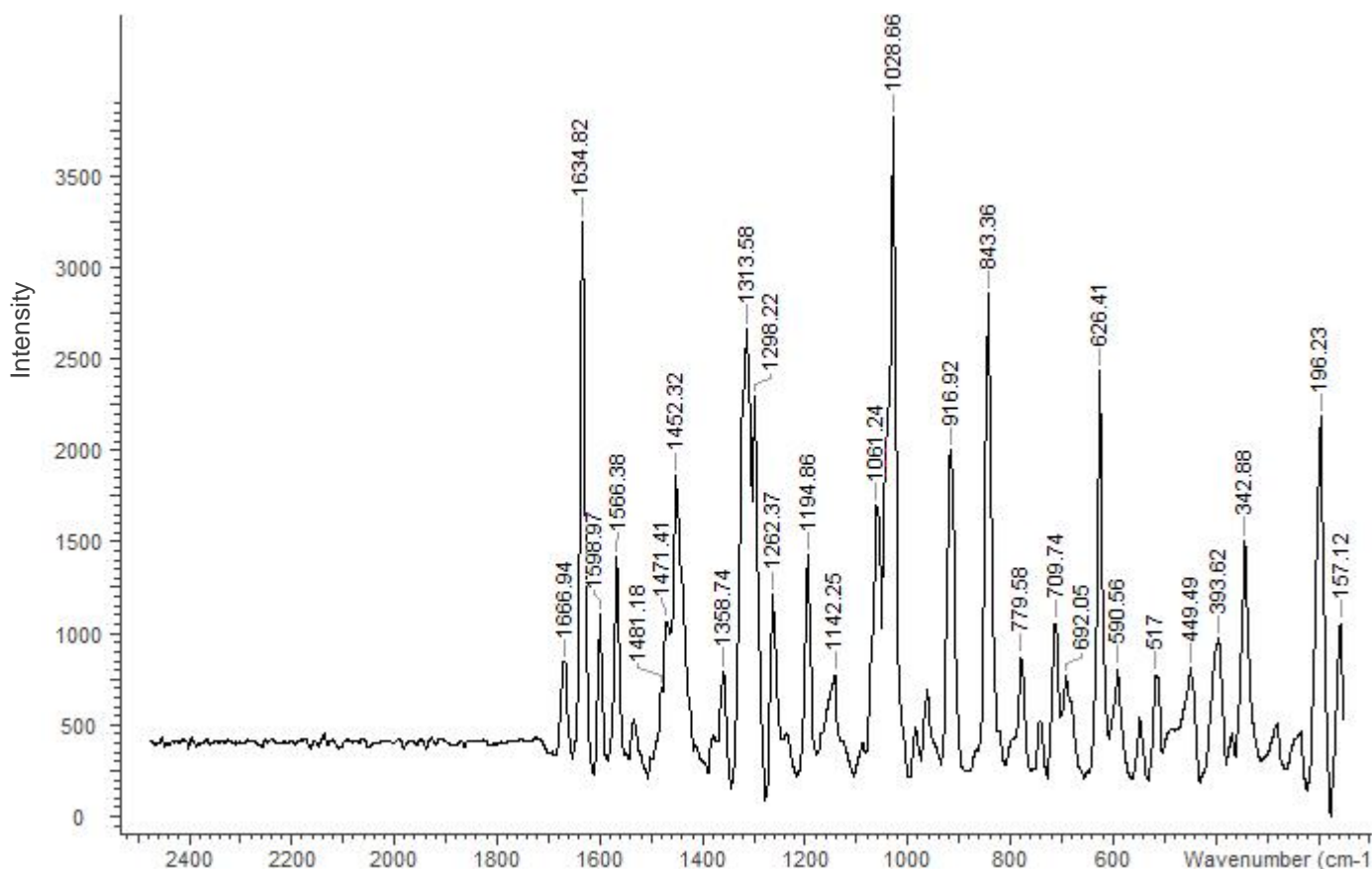
A11 hydrochloride

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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

US Patent 3,975,443 Aug. 17, 1976

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

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 (2019) doi: 10.1002/prp2.511

5. ACKNOWLEDGEMENT

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