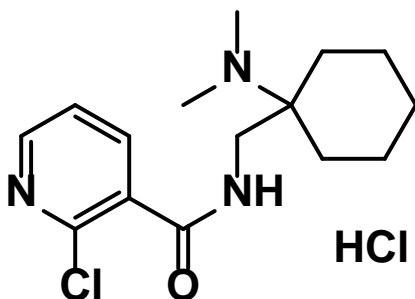


A09 hydrochloride

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



1. GENERAL INFORMATION

IUPAC Name: 1-(2-chloronicotinamidomethyl)-cyclohexyldimethylamine; hydrochloride

CAS#: 1307990-39-1 (base)

Synonyms: A09

Source: Synthesized Material Lot# JLK008-044-09

Appearance: Off-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 ₂₂ ClN ₃ O·HCl	332.2686 (295.8077 (base))	207.2 ± 1.72
Base	C ₁₅ H ₂₂ ClN ₃ O	295.81	Not determined

3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterated chloroform (CDCl₃) + TMS.

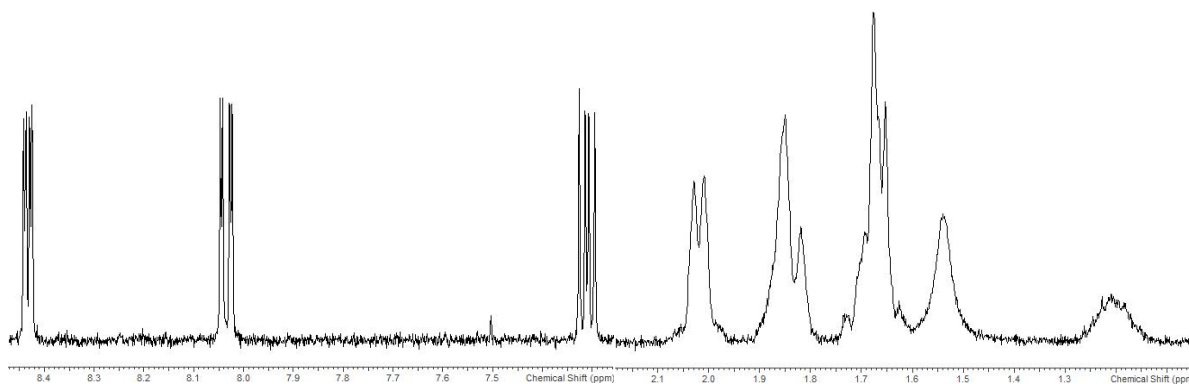
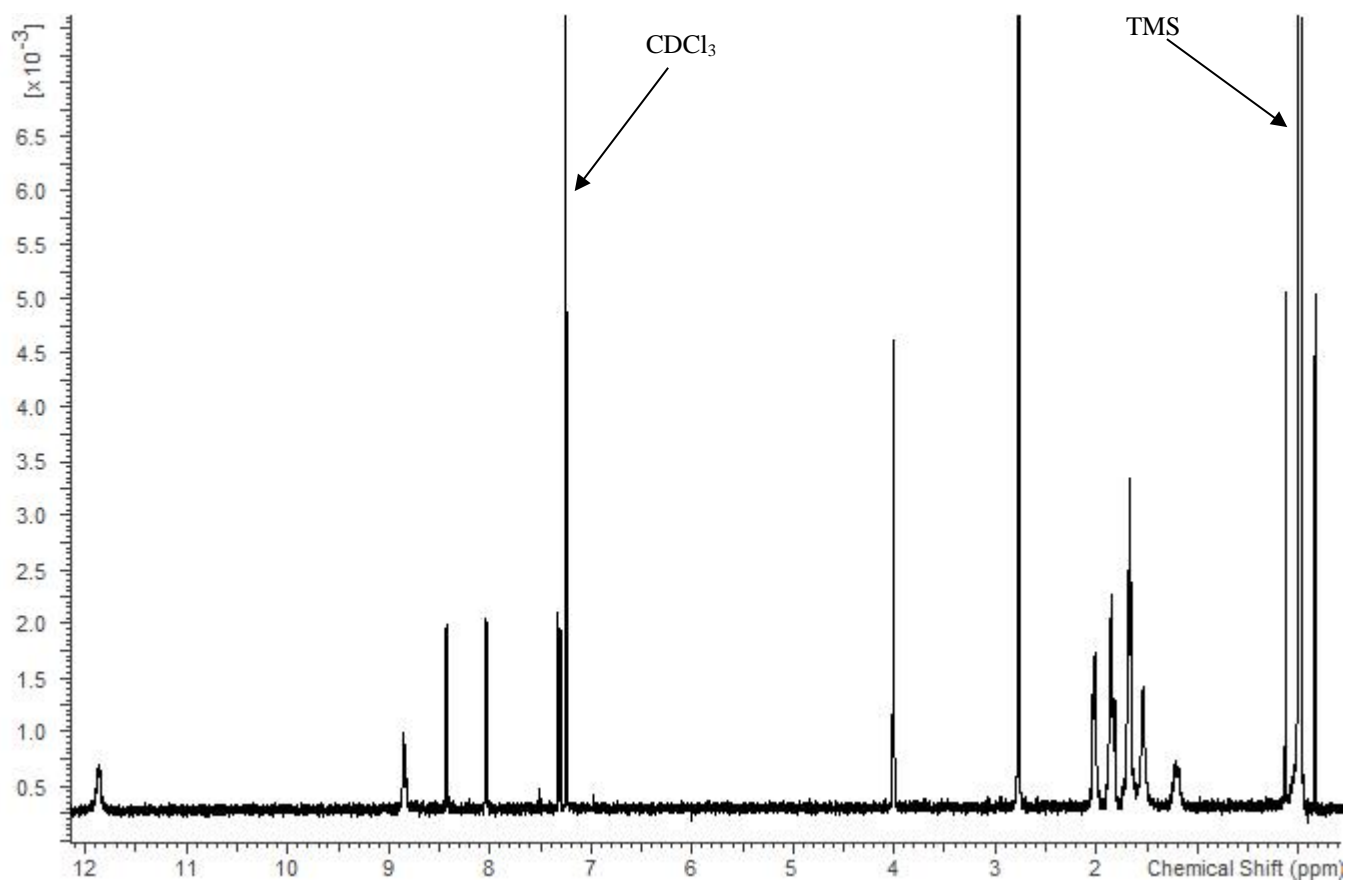
Instrument: 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 30 seconds

¹H NMR: A09 HCl; Lot JLK008-044-09; CDCl₃+ TMS; 400 MHz



A09 hydrochloride

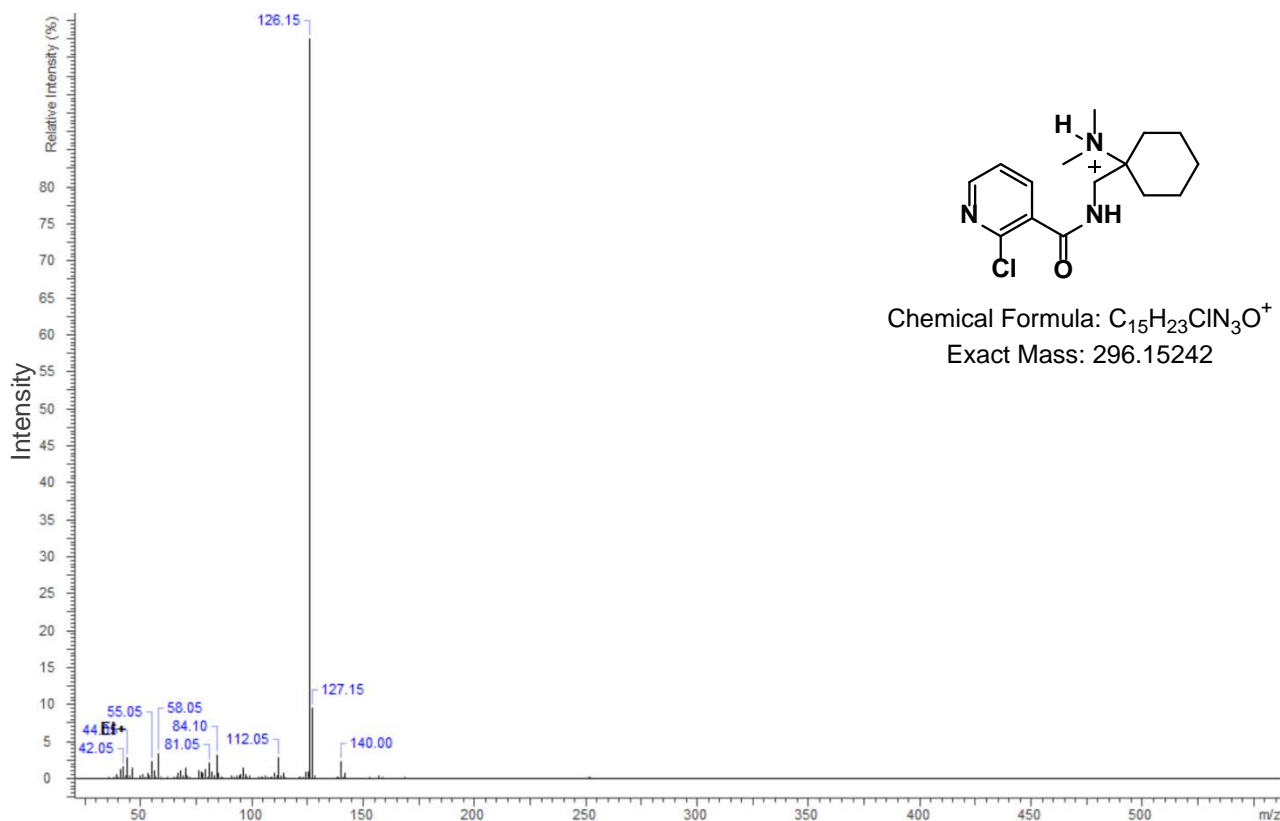
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material

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:	15.93 min

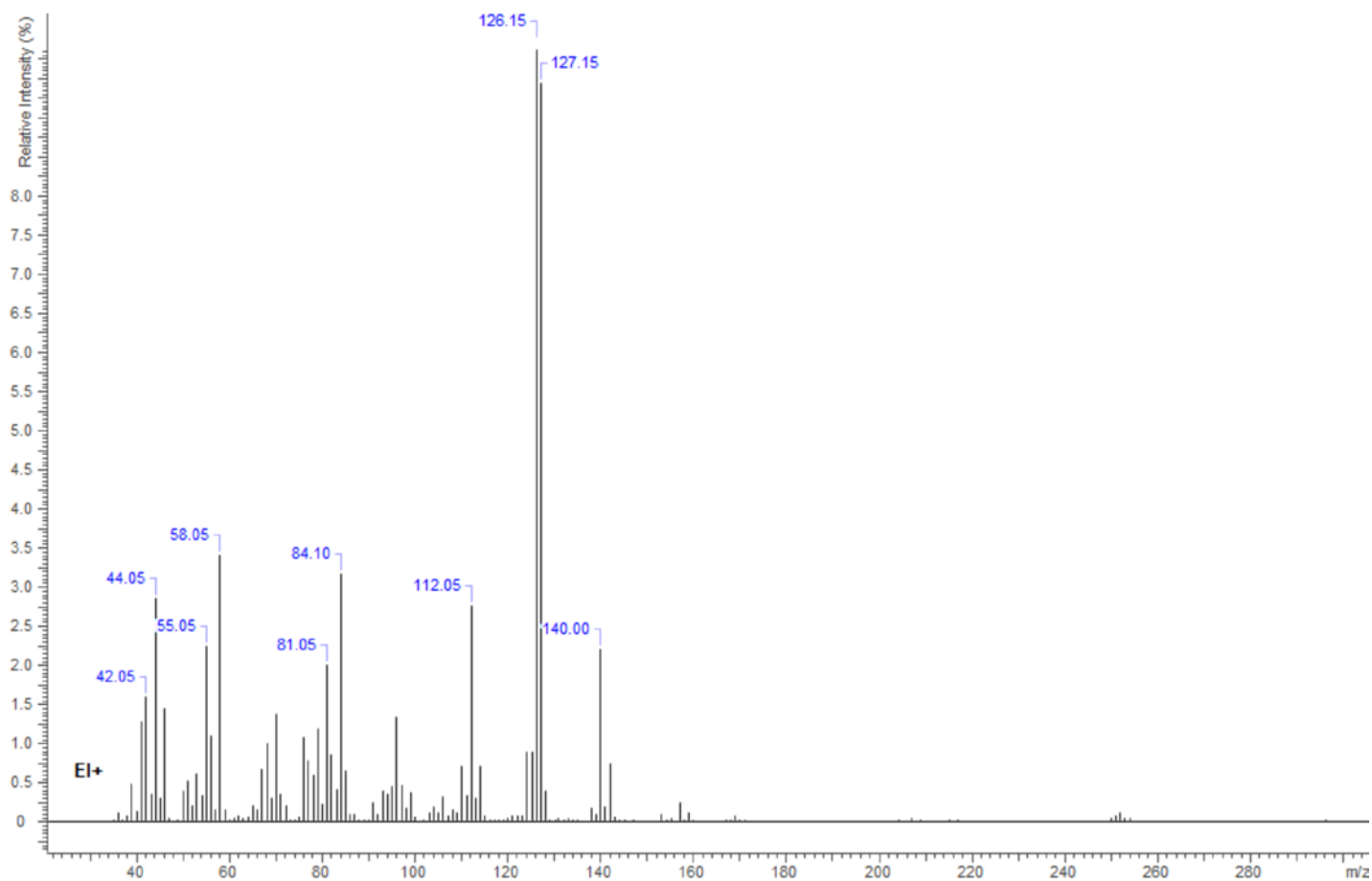
EI Mass Spectrum: A09 HCl; Lot JLK008-044-09



A09 hydrochloride

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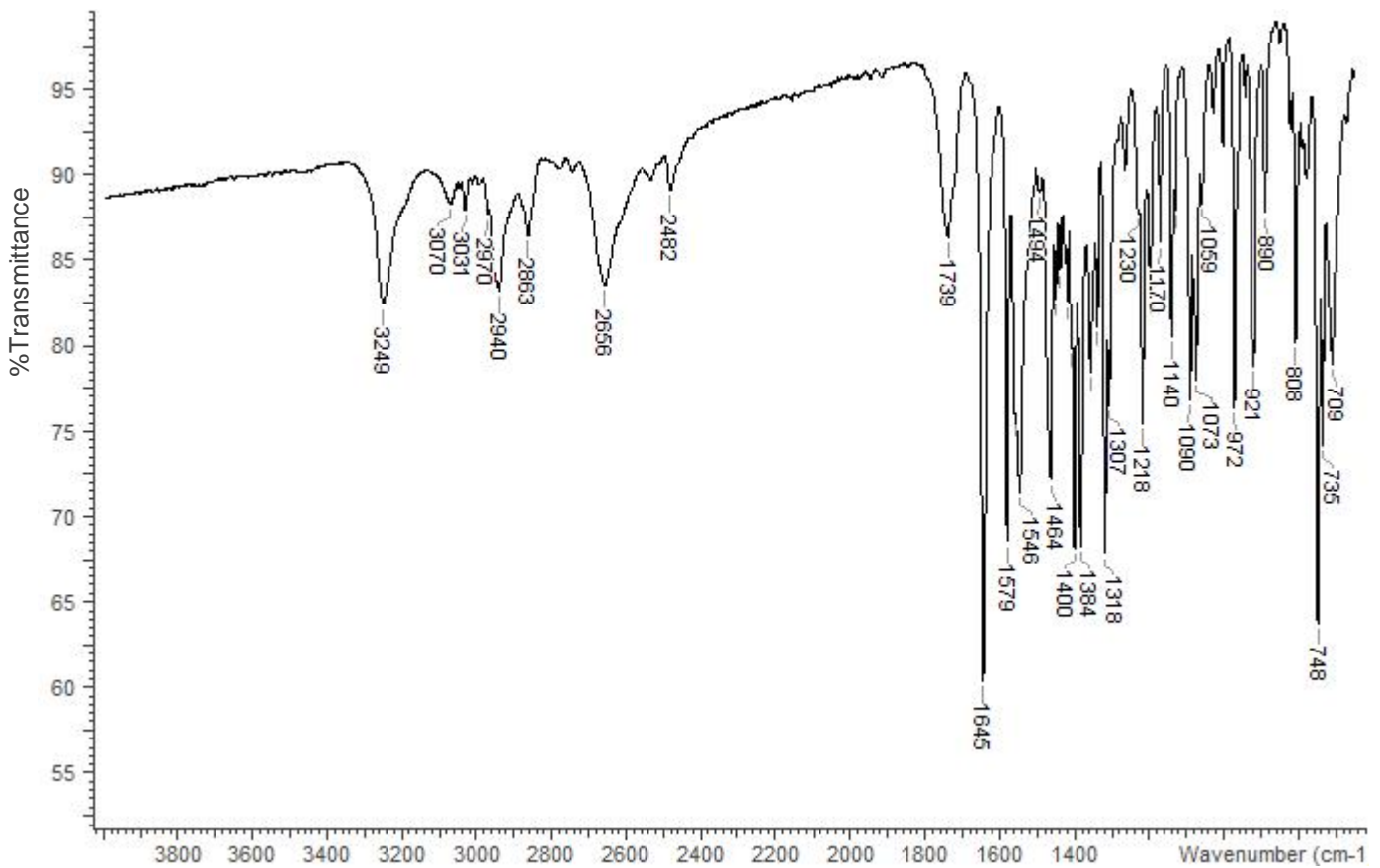
Zoomed view (126.15 is 100% relative intensity and truncated in this view)



3.3 INFRARED SPECTROSCOPY (FTIR)

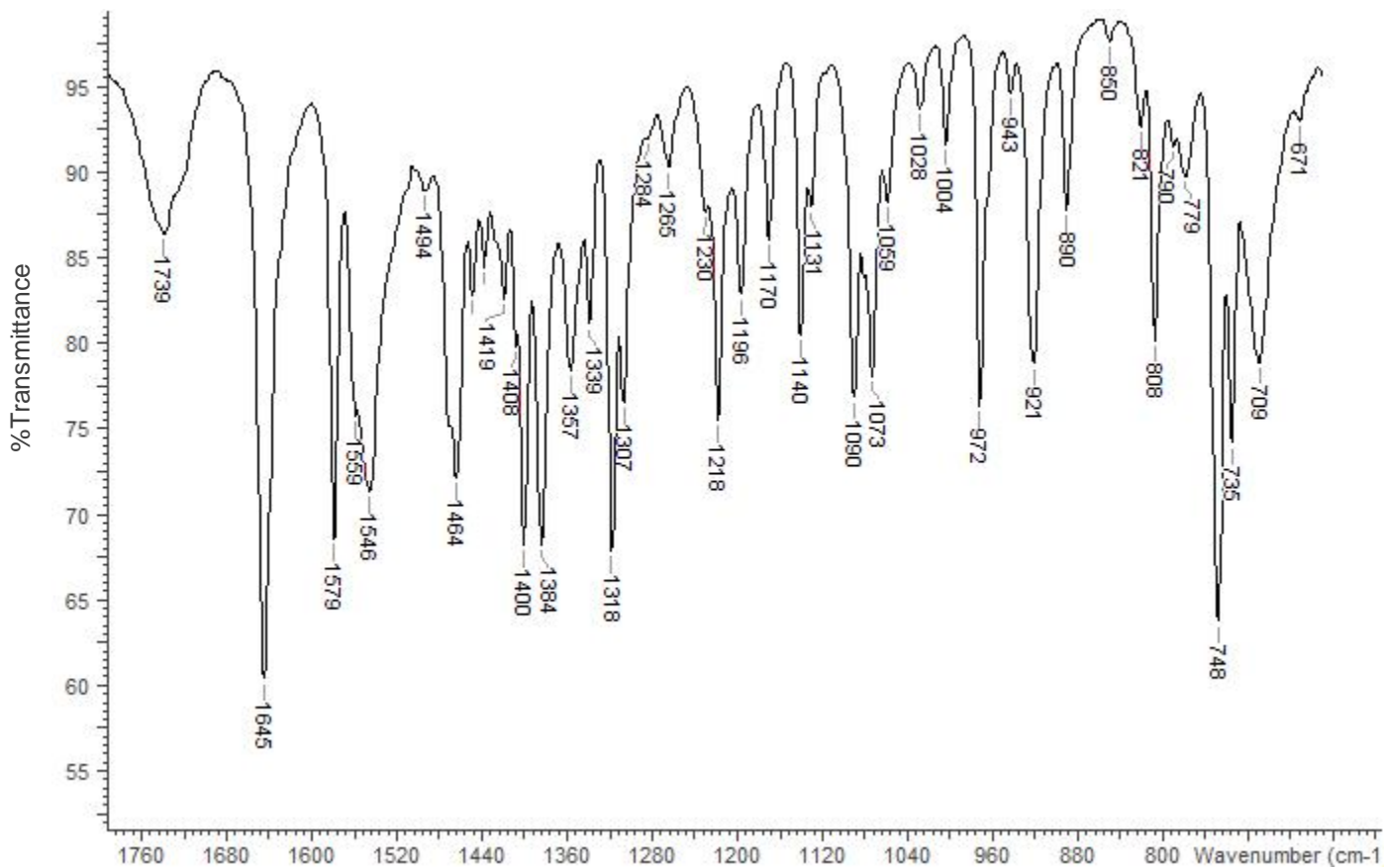
Instrument: FTIR with ZnSe ATR attachment (1 bounce)
Scan Parameters: Number of scans: 4
 Number of background scans: 4
 Resolution: 4 cm⁻¹
 Sample gain: 8
 Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): A09 HCl; Lot JLK008-044-09



A09 hydrochloride

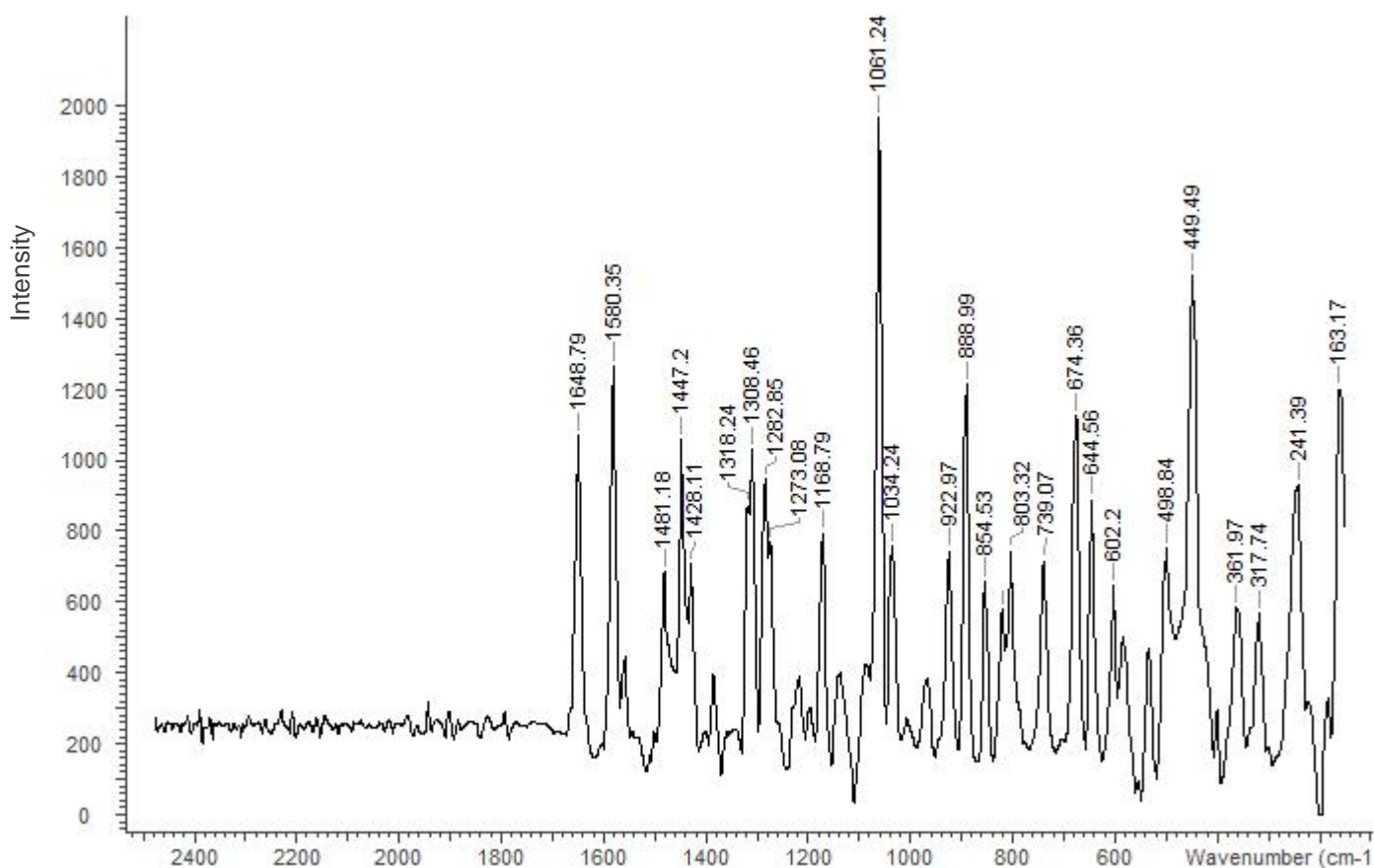
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material



3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): A09 HCl; Lot JLK008-044-09



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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