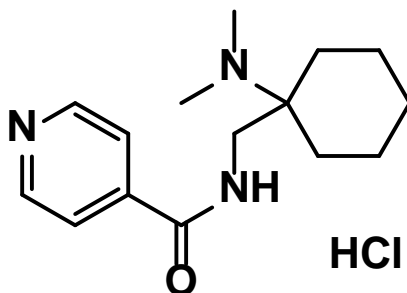


A12 hydrochloride

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



1. GENERAL INFORMATION

| | |
|-------------------------------|--|
| IUPAC Name: | 1-(isonicotinamidomethyl)-cyclohexyldimethylamine; hydrochloride |
| CAS#: | 852309-68-3 (base) |
| Synonyms: | A12 |
| Source: | Synthesized Material Lot# JLK008-059-12 |
| 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 | 231.0 ± 0.58 |
| 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 (CDCl_3) + TMS.

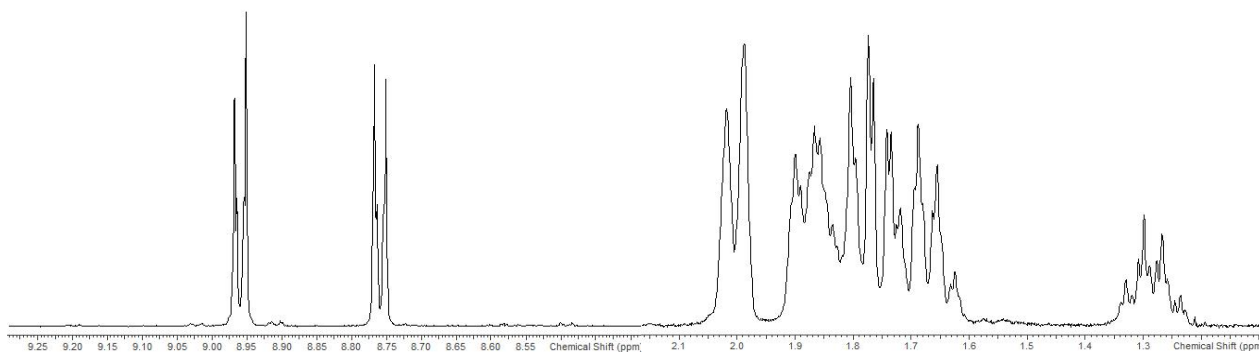
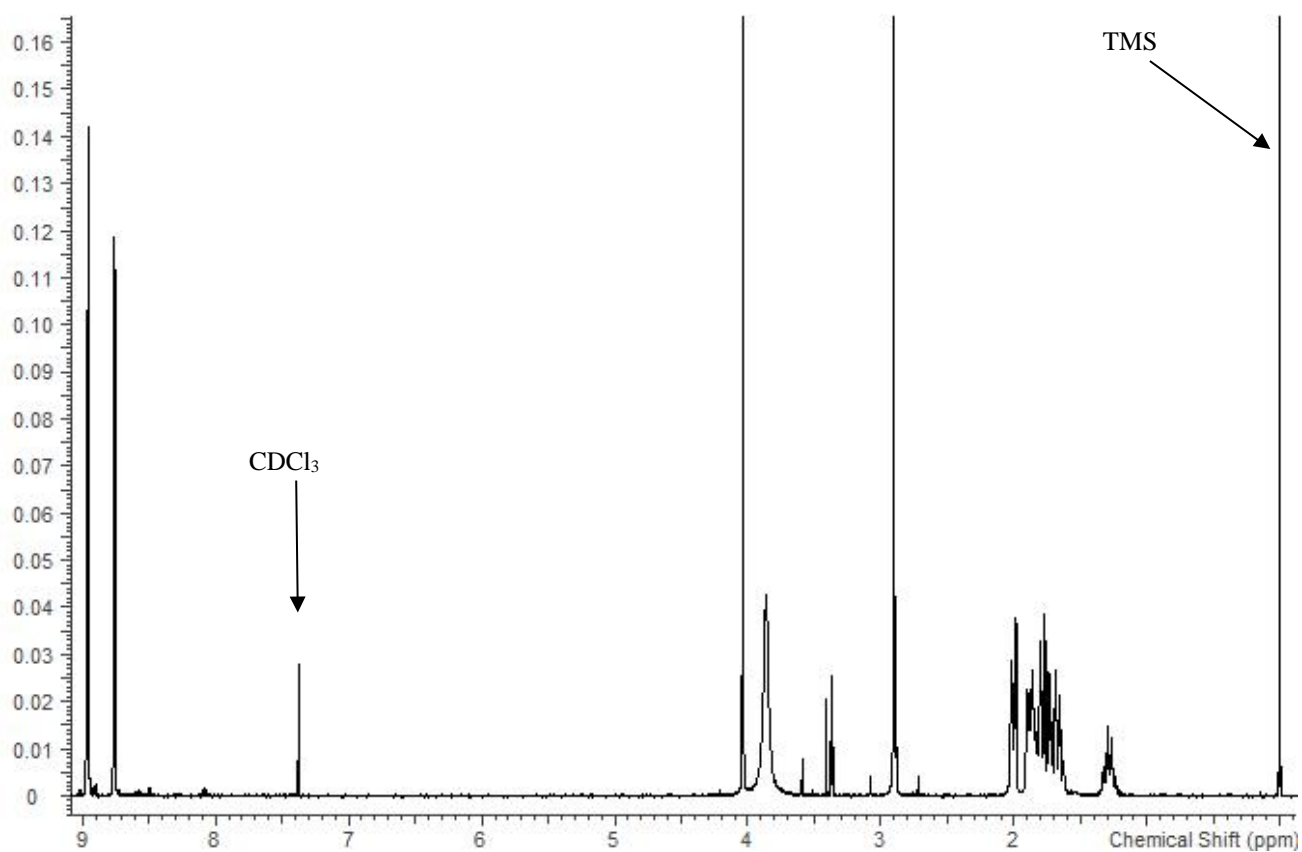
Instrument: 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 30 seconds

^1H NMR: A12 HCl; Lot JLK008-059-12; CDCl_3 + TMS; 400 MHz



A12 hydrochloride

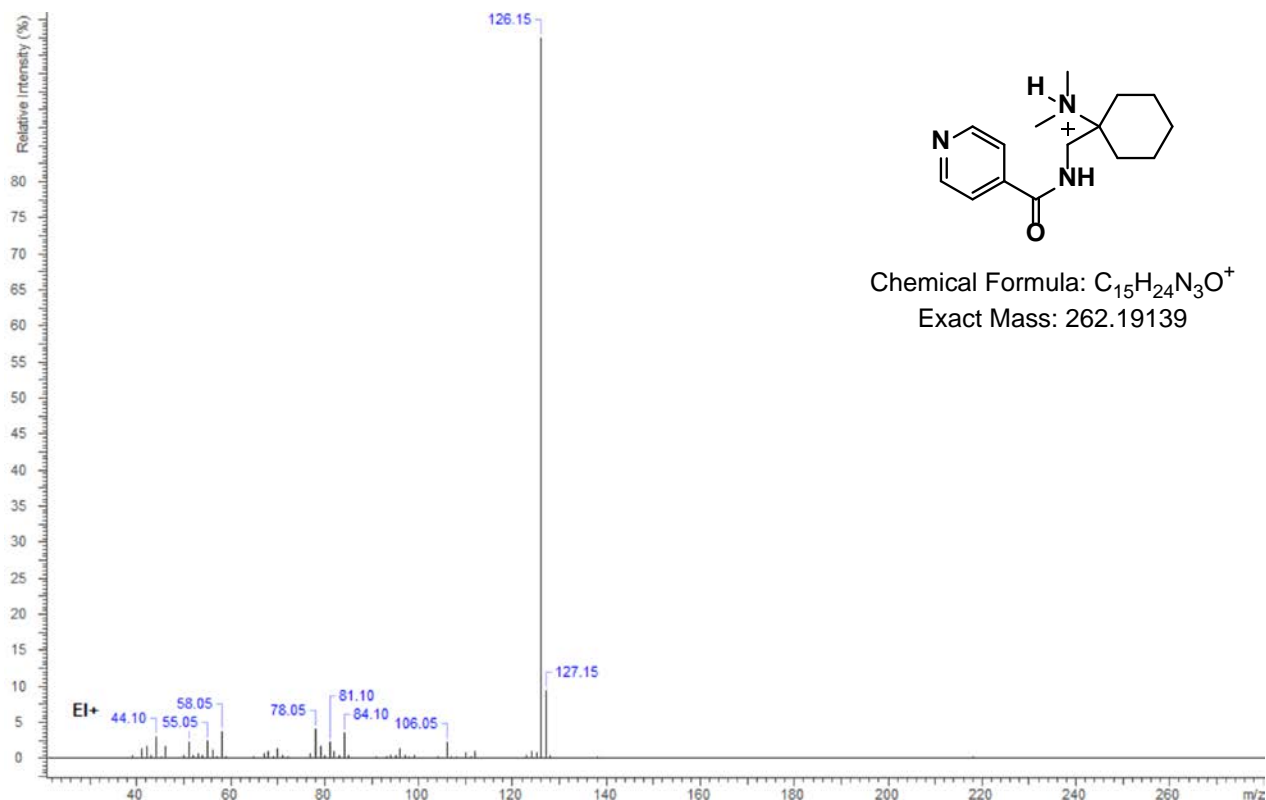
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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~ 1 mg/mL in methanol

| | |
|-------------------------------------|---|
| <i>Instrument:</i> | Shimadzu gas chromatograph operated in split mode with MS detector |
| <i>Column:</i> | Rtx5MS (a DB-5 equivalent); 30m x 0.25 mm x 0.25 μ m |
| <i>Carrier Gas:</i> | Helium at 1 mL/min |
| <i>Temperatures:</i> | 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 |
| <i>Injection Parameters:</i> | Split Ratio = 1:15, 1 μ L injected |
| <i>MS Parameters:</i> | Mass scan range: 34-550 amu Threshold: 100 Tune file: 050218_Tune.qgt Acquisition mode: scan |
| <i>Retention Time:</i> | 15.09 min |

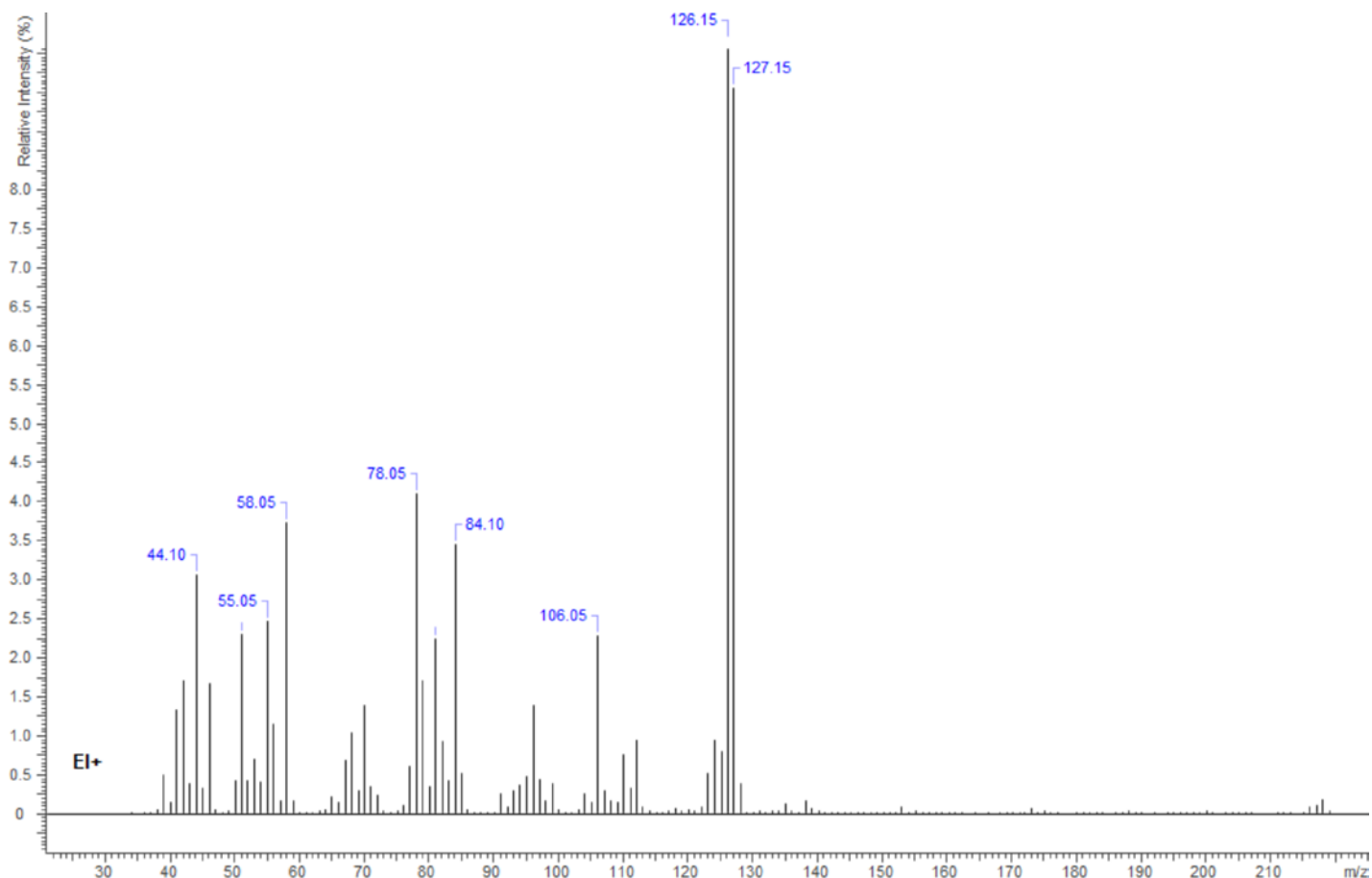
EI Mass Spectrum: A12 HCl; Lot JLK008-059-12



A12 hydrochloride

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

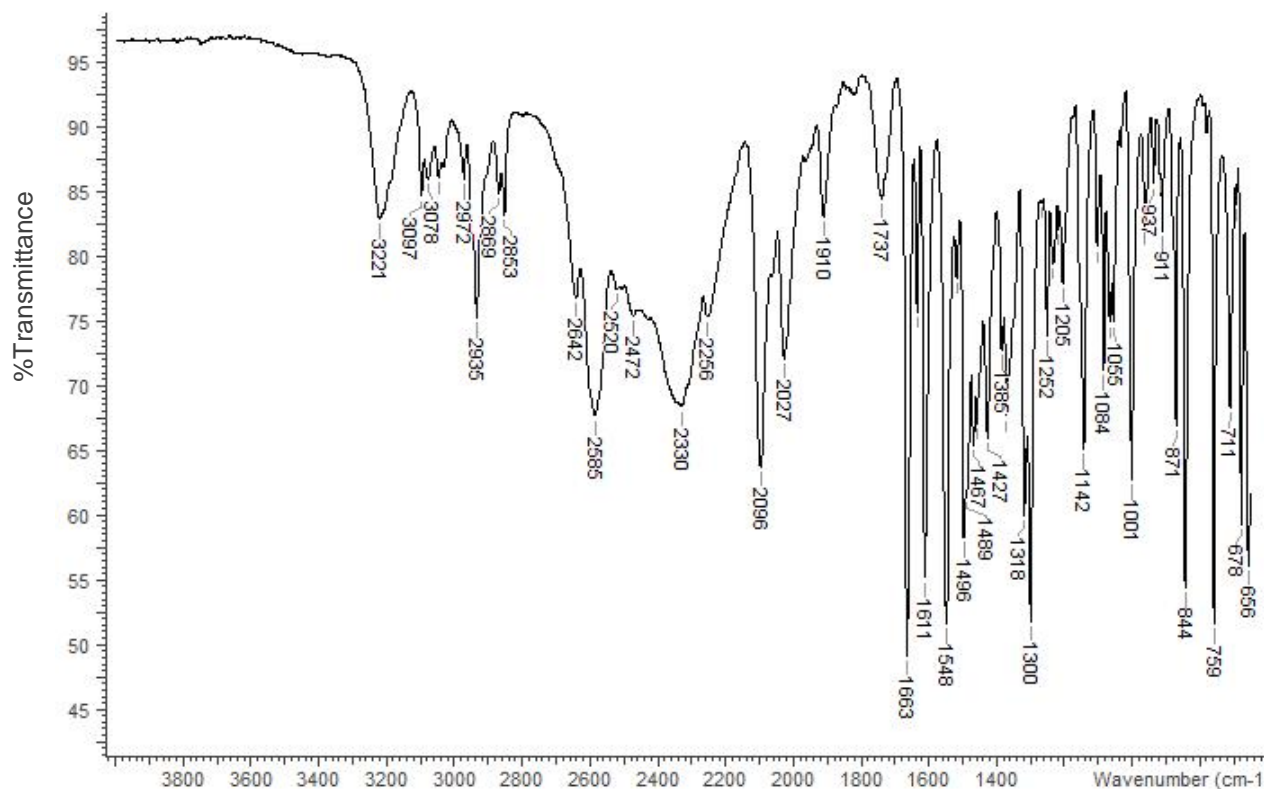


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with ZnSe ATR attachment (1 bounce)

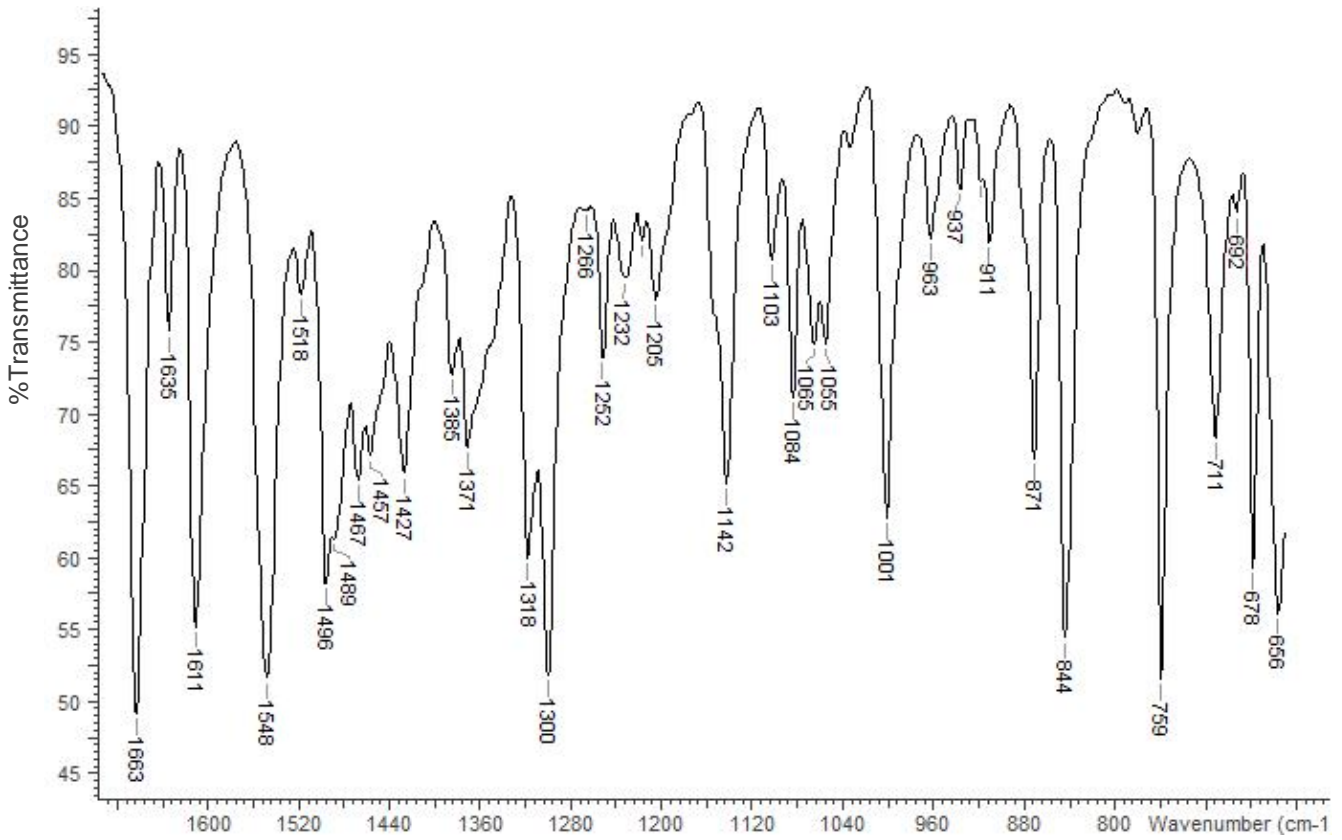
Scan Parameters: Number of scans: 4
Number of background scans: 4
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): A12 HCl; Lot JLK008-059-12



A12 hydrochloride

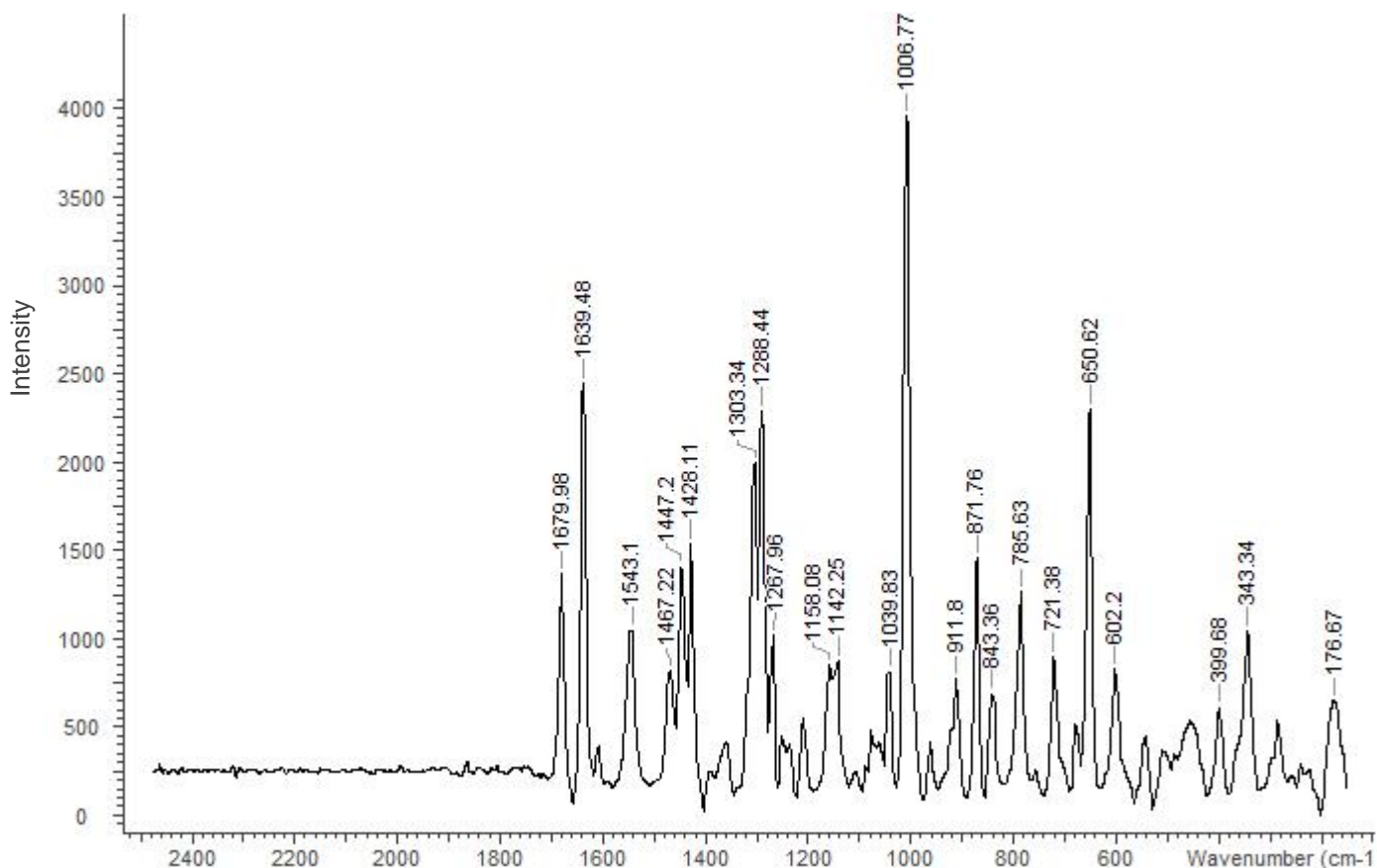
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3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): A12 HCl; Lot JLK008-059-12



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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