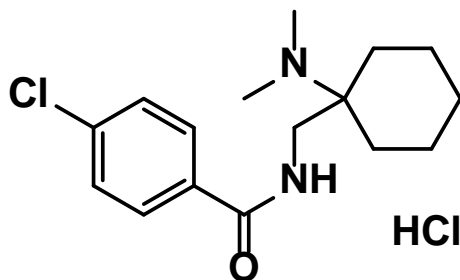


AH-8529 hydrochloride

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



1. GENERAL INFORMATION

IUPAC Name: 1-(4-chlorobenzamidomethyl)-cyclohexyldimethylamine; hydrochloride

CAS#: 1225333-02-7; 41805-00-9 (base)

Synonyms: A02

Source: Synthesized Material Lot# JLK008-107-02

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 ₁₆ H ₂₃ ClN ₂ O·HCl	331.28	197.0 ± 2.37
base	C ₁₆ H ₂₃ ClN ₂ O	294.82	Not determined

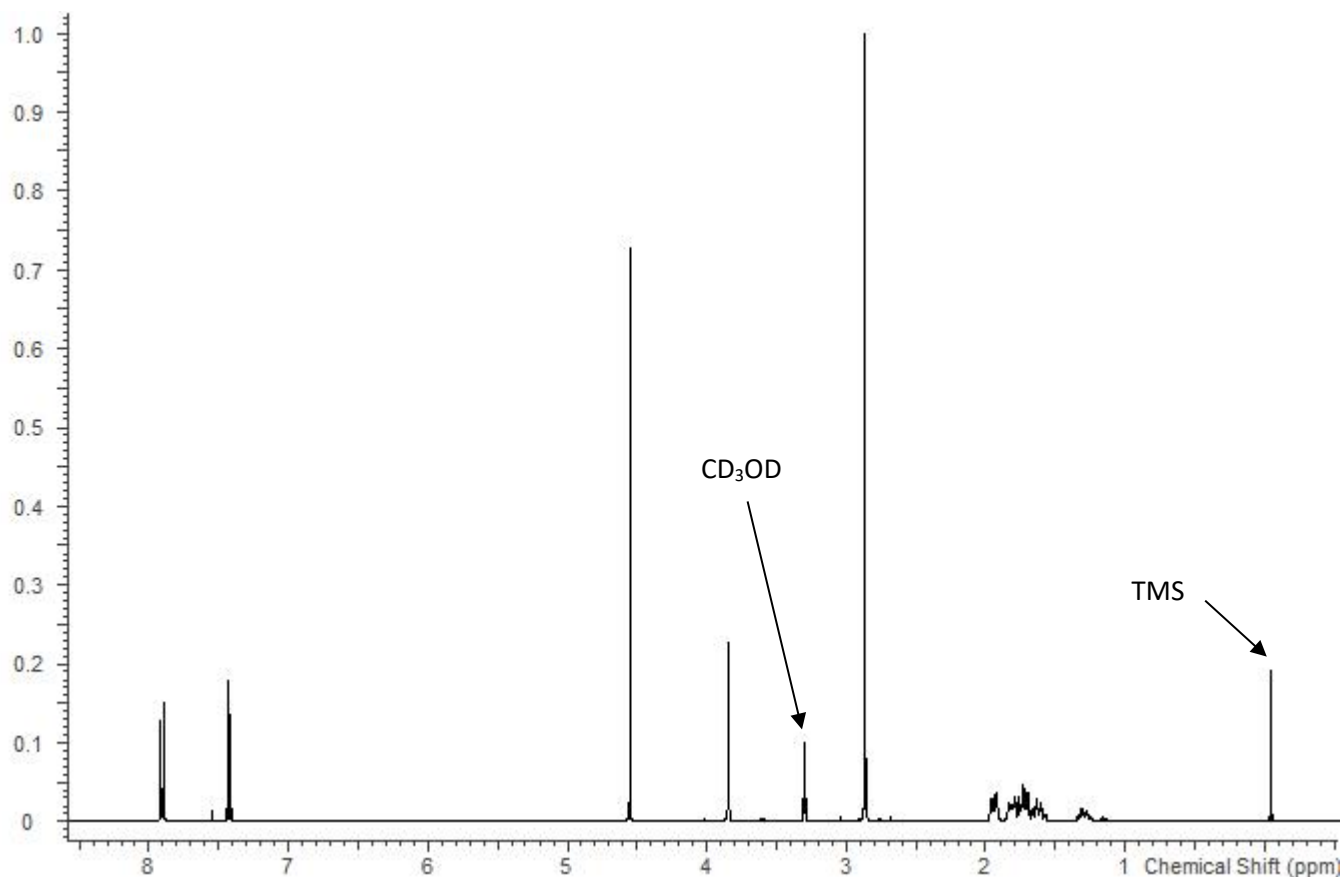
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterated chloroform: methanol (CDCl₃:CD₃OD; 1:5) + TMS.

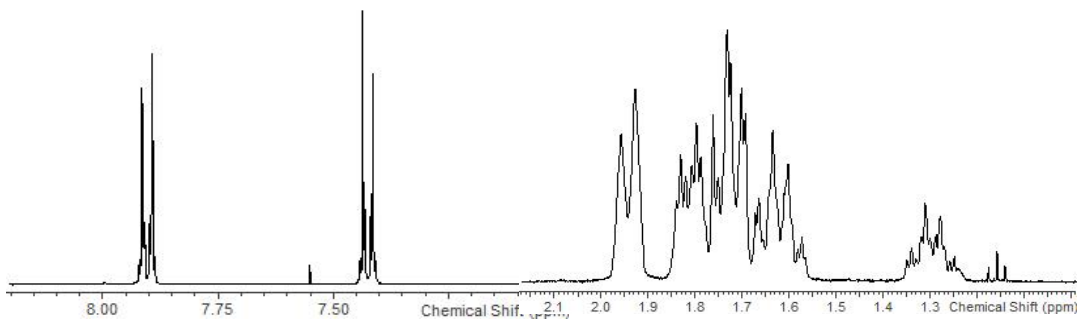
Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: 6410.3 Hz containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 30 seconds

¹H NMR: AH-8529 HCl; Lot JLK008-107-02; CDCl₃:CD₃OD (1:5) + TMS; 400 MHz



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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 μ m

Carrier Gas: Helium at 1 mL/min

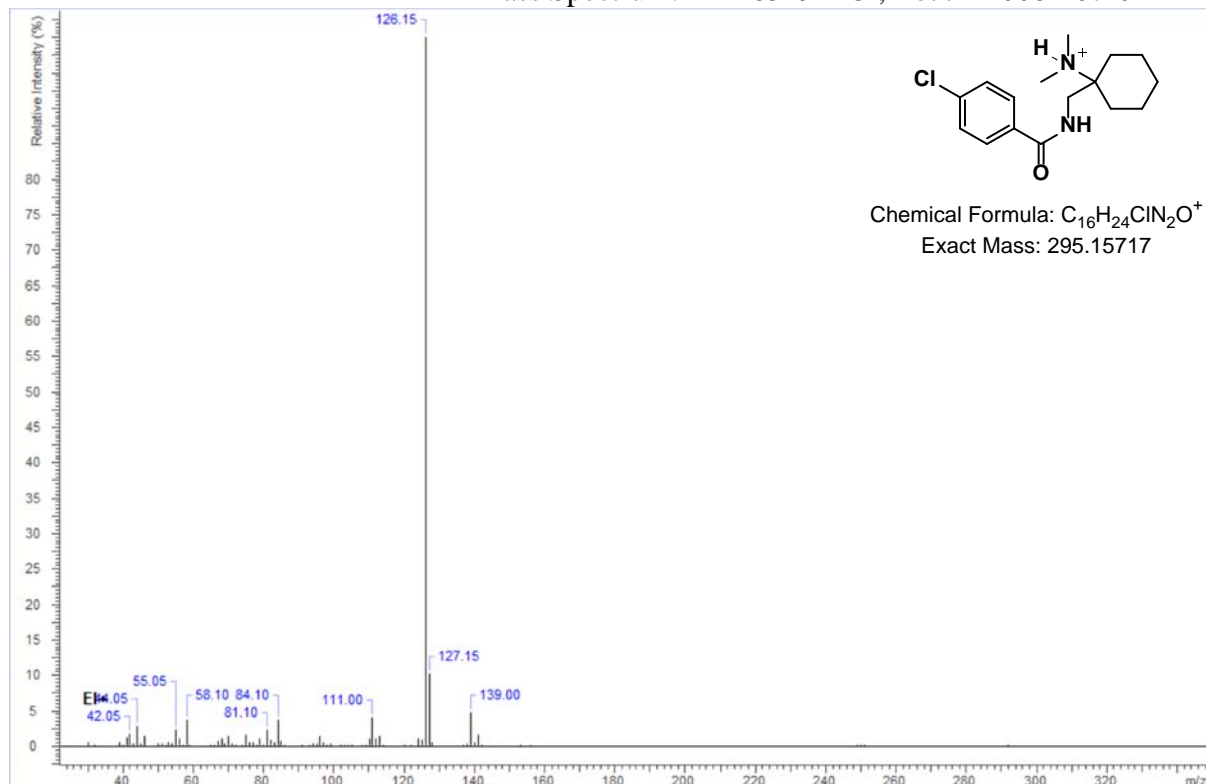
Temperatures: Injector: 280°C
MSD transfer line: 280°C
MS Source: 200°C
Oven program:
1) 90°C initial temperature for 2.0 min
2) Ramp to 300°C at 14°C/min
3) Hold final temperature for 10.0 min

Injection Parameters: Split Ratio = 1:15, 1 μ L injected

MS Parameters: Mass scan range: 34-550 amu
Threshold: 100
Tune file: 050218_Tune.qgt
Acquisition mode: scan

Retention Time: 15.97 min

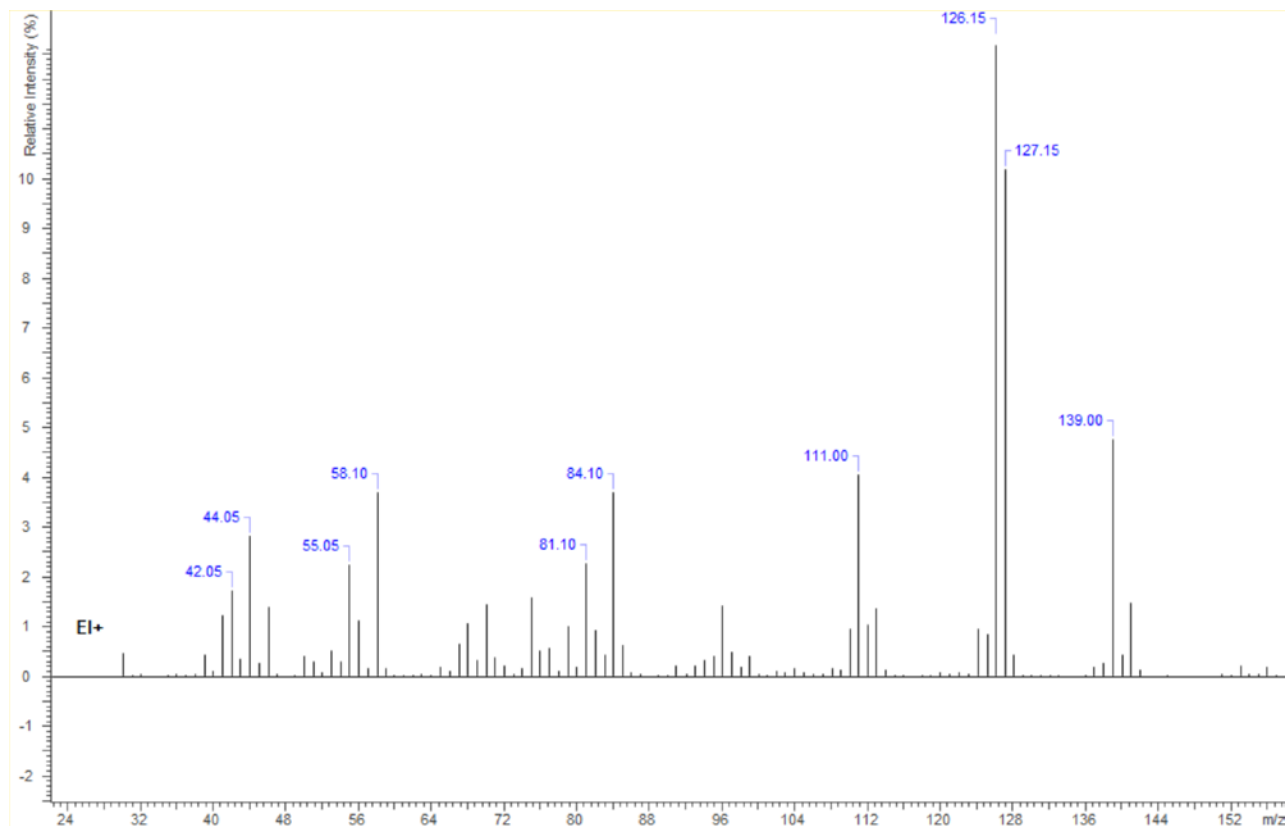
EI Mass Spectrum: AH-8529 HCl; Lot JLK008-107-02



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

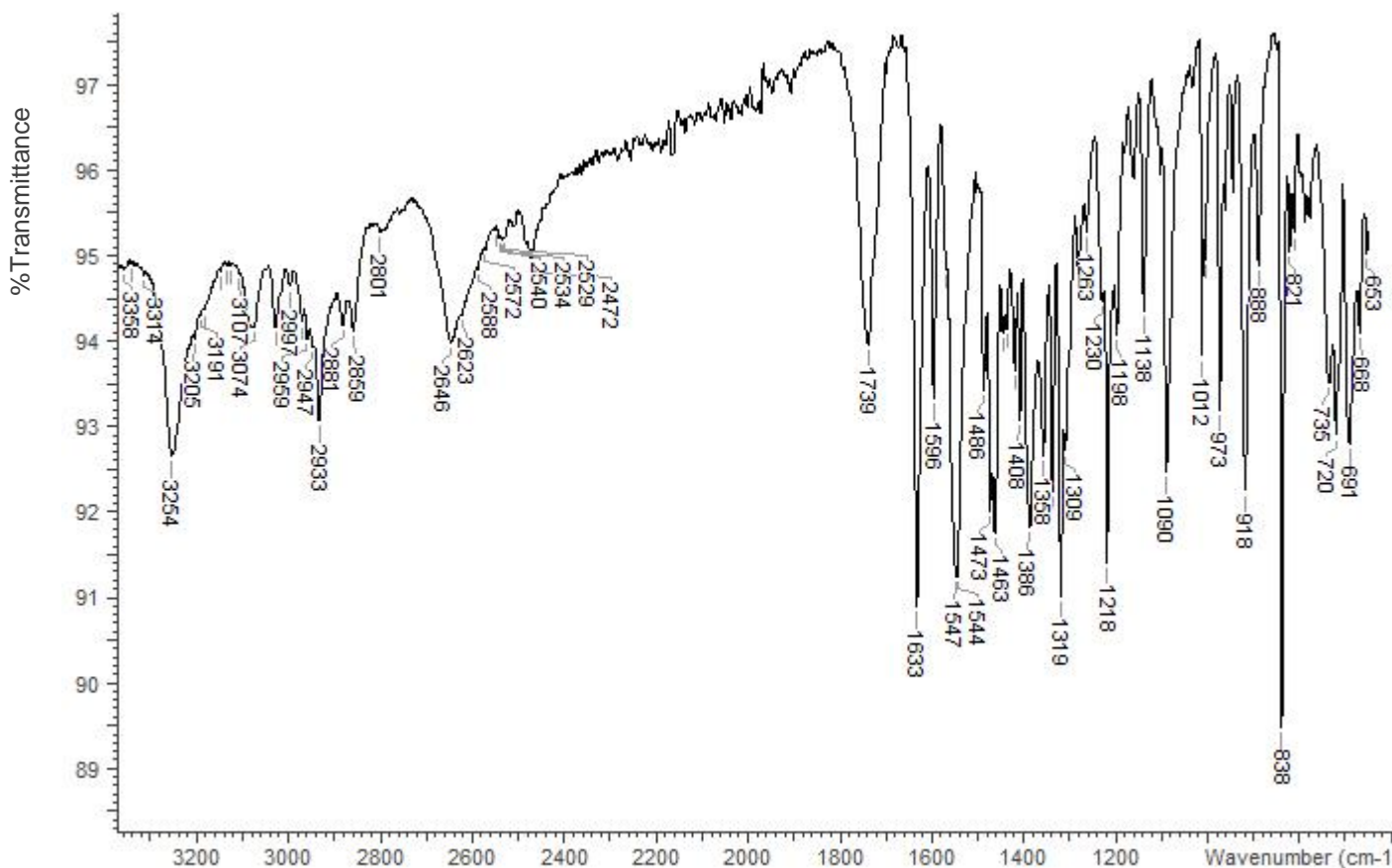


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with ZnSe ATR attachment (1 bounce)

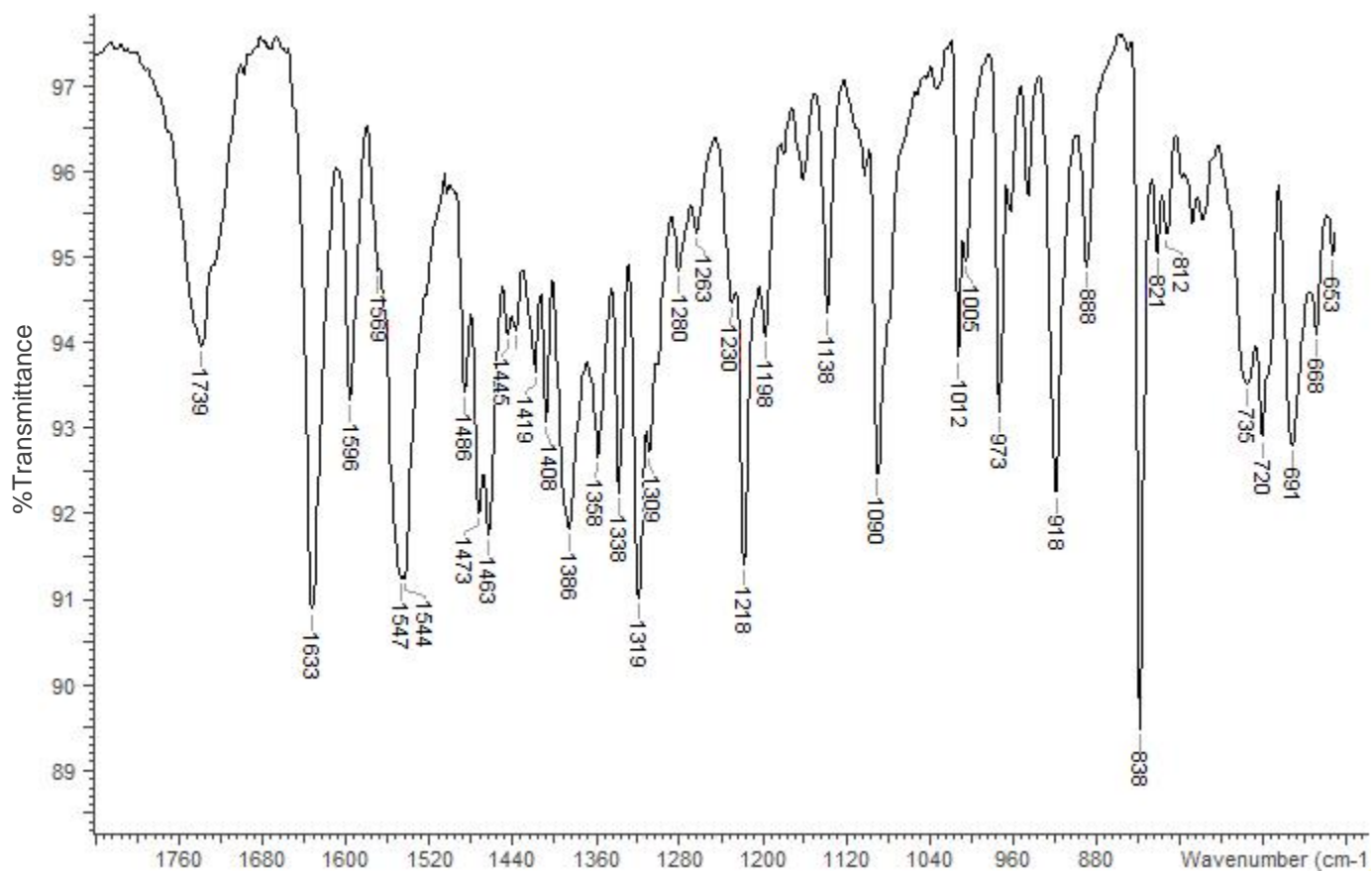
Scan Parameters: Number of scans: 4
 Number of background scans: 4
 Resolution: 4 cm⁻¹
 Sample gain: 8
 Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): AH-8529 HCl; Lot JLK008-107-02



AH-8529 hydrochloride

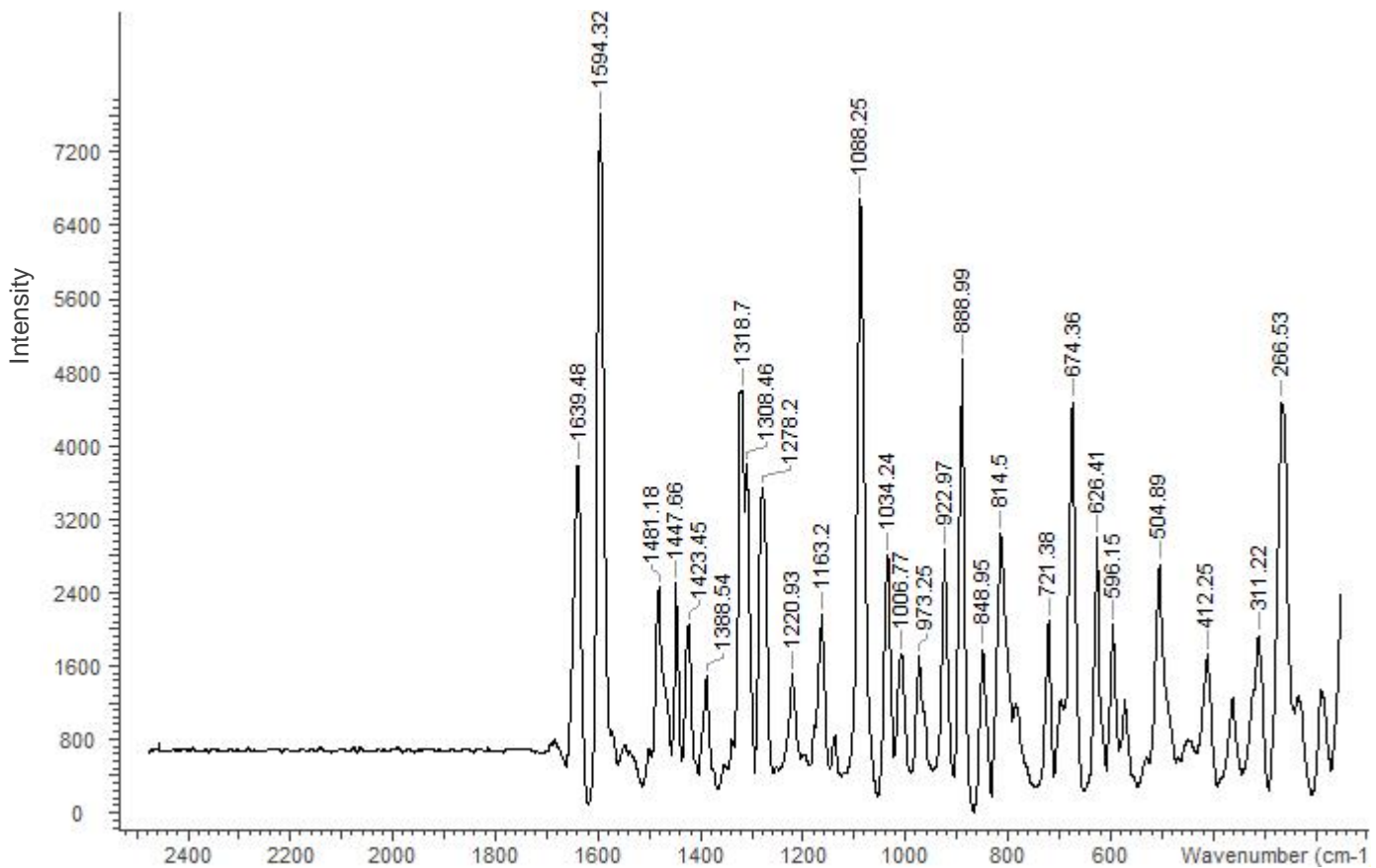
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3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): AH-8529 HCl; Lot JLK008-107-02



4. ADDITIONAL RESOURCES

1-(3,4-DICHLOROBENZAMIDOMETHYL)CYCLOHEXYLDIMETHYLAMINE

Norman James Harper and George Bryan Austin Veitch

US Patent 3,975,443 Aug. 17, 1976 Example 6

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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