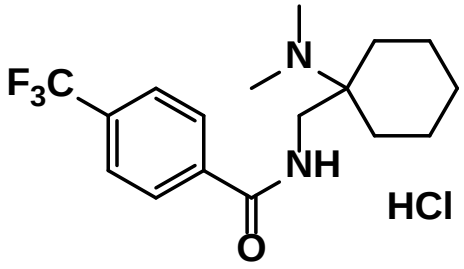
A04 hydrochloride

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-trifluoromethylbenzamidomethyl)-cyclohexyldimethylamine; hydrochloride

CAS#: 940753-21-9 (base)

Synonyms: A04

Source: **Synthesized Material** Lot# JLK008-041-04

Appearance: Light Brown Crystals (HCl)

UV_{max} (nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
HCl	$C_{17}H_{23}F_3N_2O{\cdot}HCl$	364.83	231.2 $\pm$ 1.56
base	$C_{17}H_{23}F_3N_2O$	328.37	Not determined

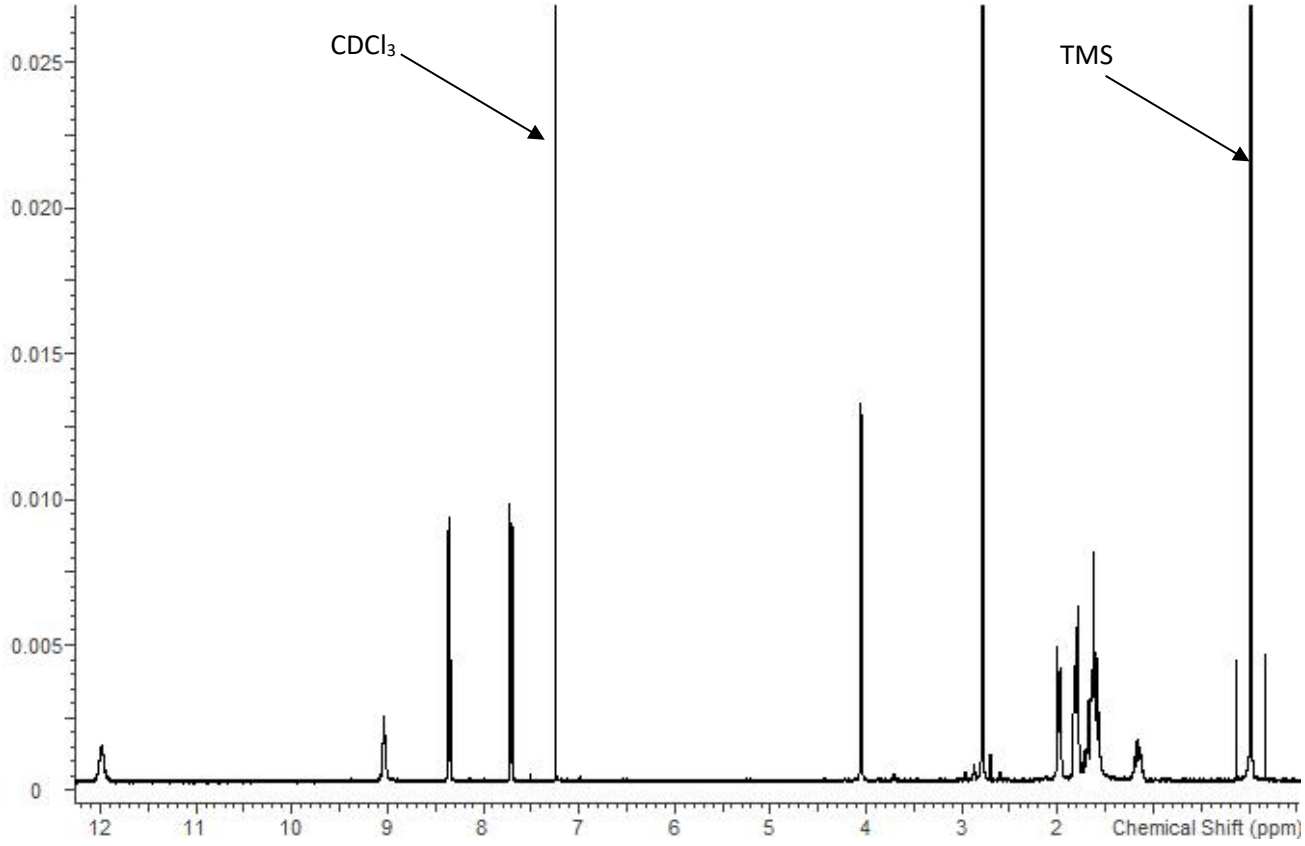
3. QUALITATIVE DATA

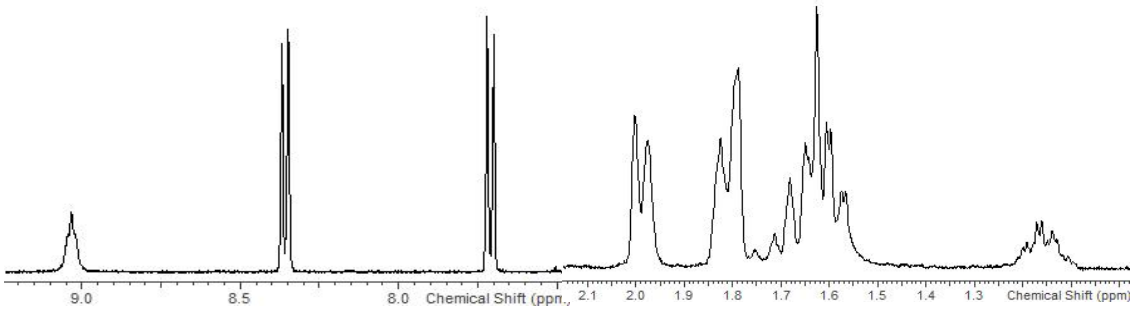
3.1 NUCLEAR MAGNETIC RESONANCE

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

^{1}H NMR: A04 HCl; Lot JLK008-041-04; $CDCl_3$+ TMS; 400 MHz



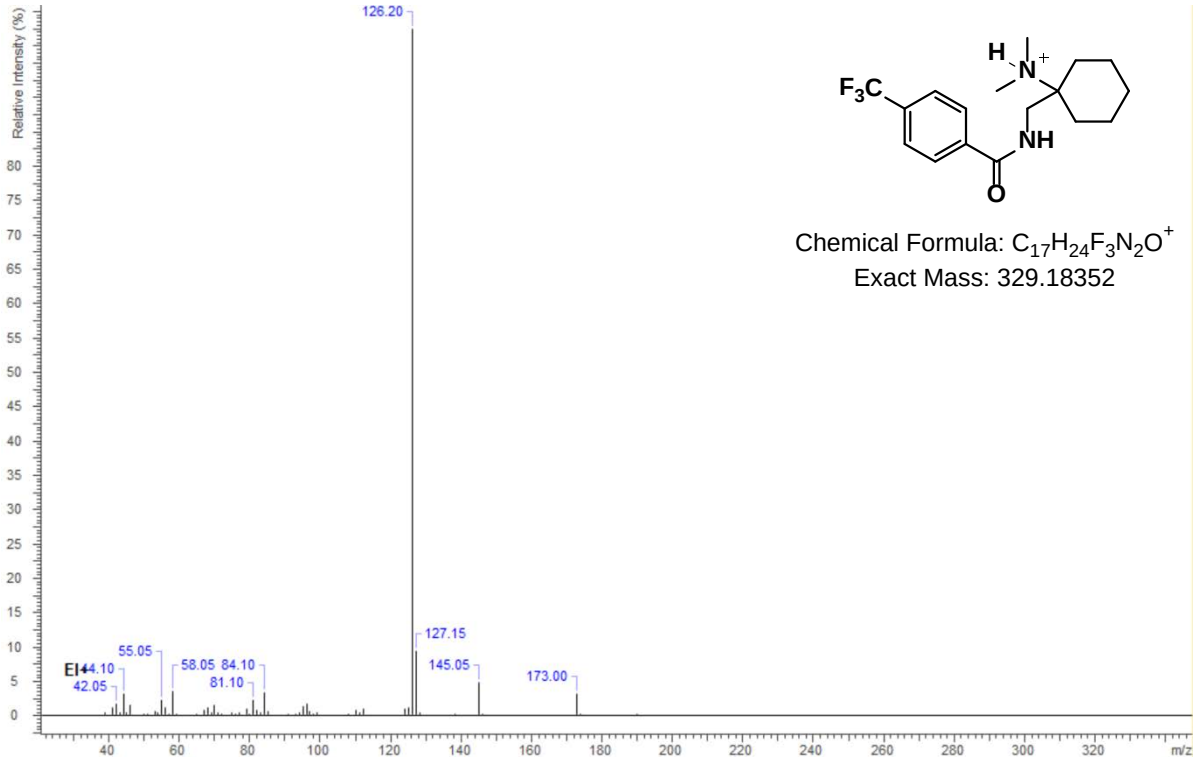


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

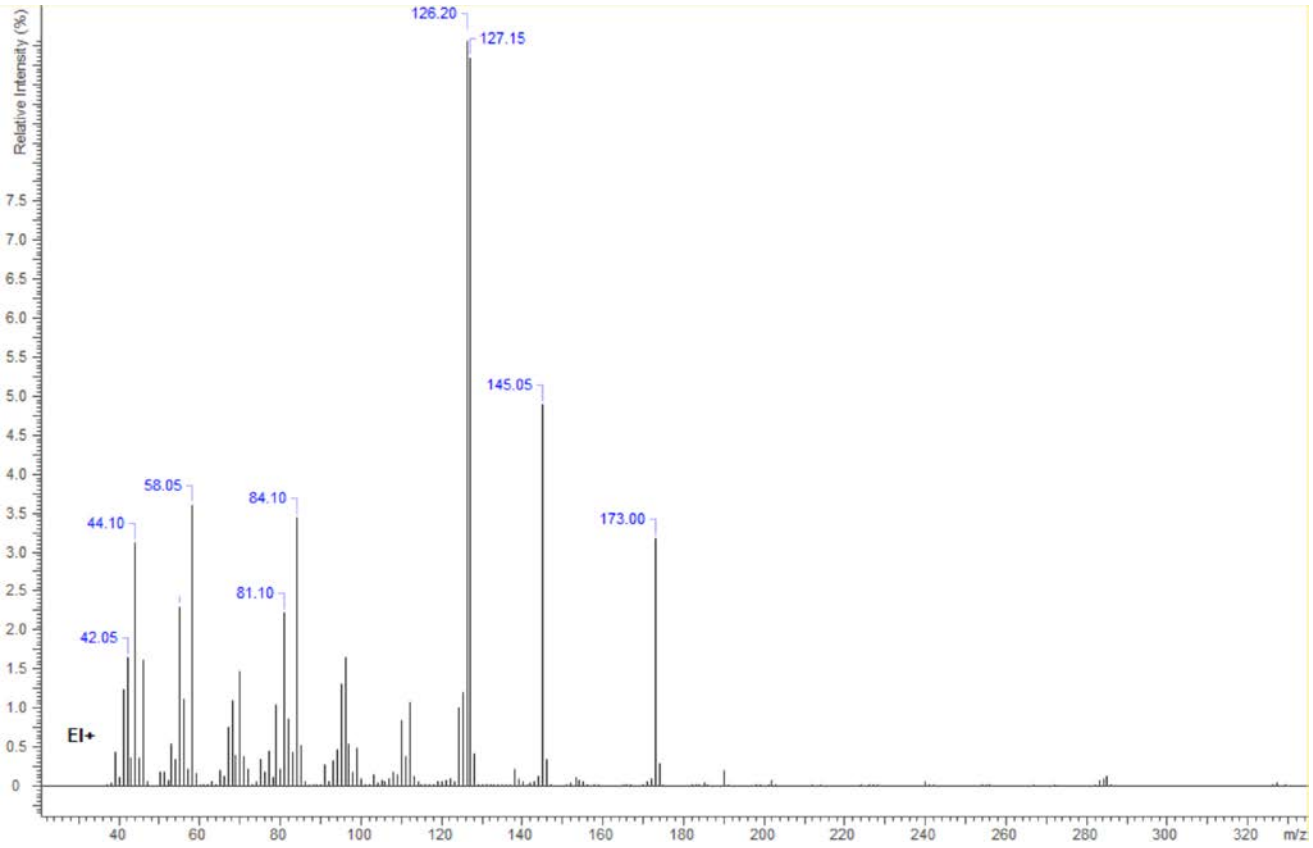
Instrument:	Shimadzu gas chromatograph operated in split mode with MS detector
Column:	Rtx5MS (a DB-5 equivalent); 30m x 0.25 mm x 0.25 µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 200°C Oven program: 1) 90°C initial temperature for 2.0 min 2) Ramp 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:	14.31 min

EI Mass Spectrum: A04 HCl; Lot JLK008-041-04



Chemical Formula: $C_{17}H_{24}F_3N_2O^+$
Exact Mass: 329.18352

Zoomed view (126.2 is 100% relative intensity and is truncated in this view)



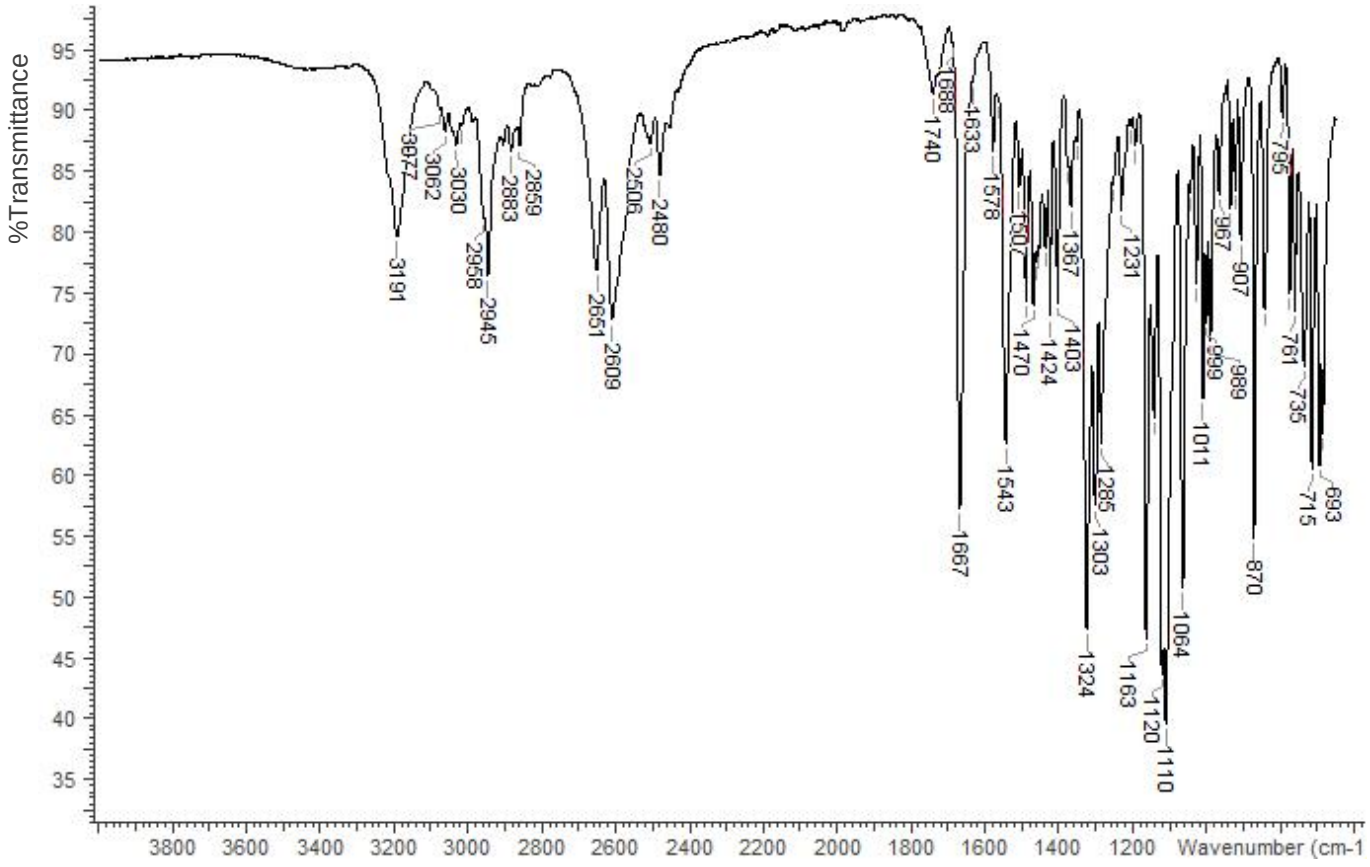
3.3 INFRARED SPECTROSCOPY (FTIR)

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): A04 HCl; Lot JLK008-041-04



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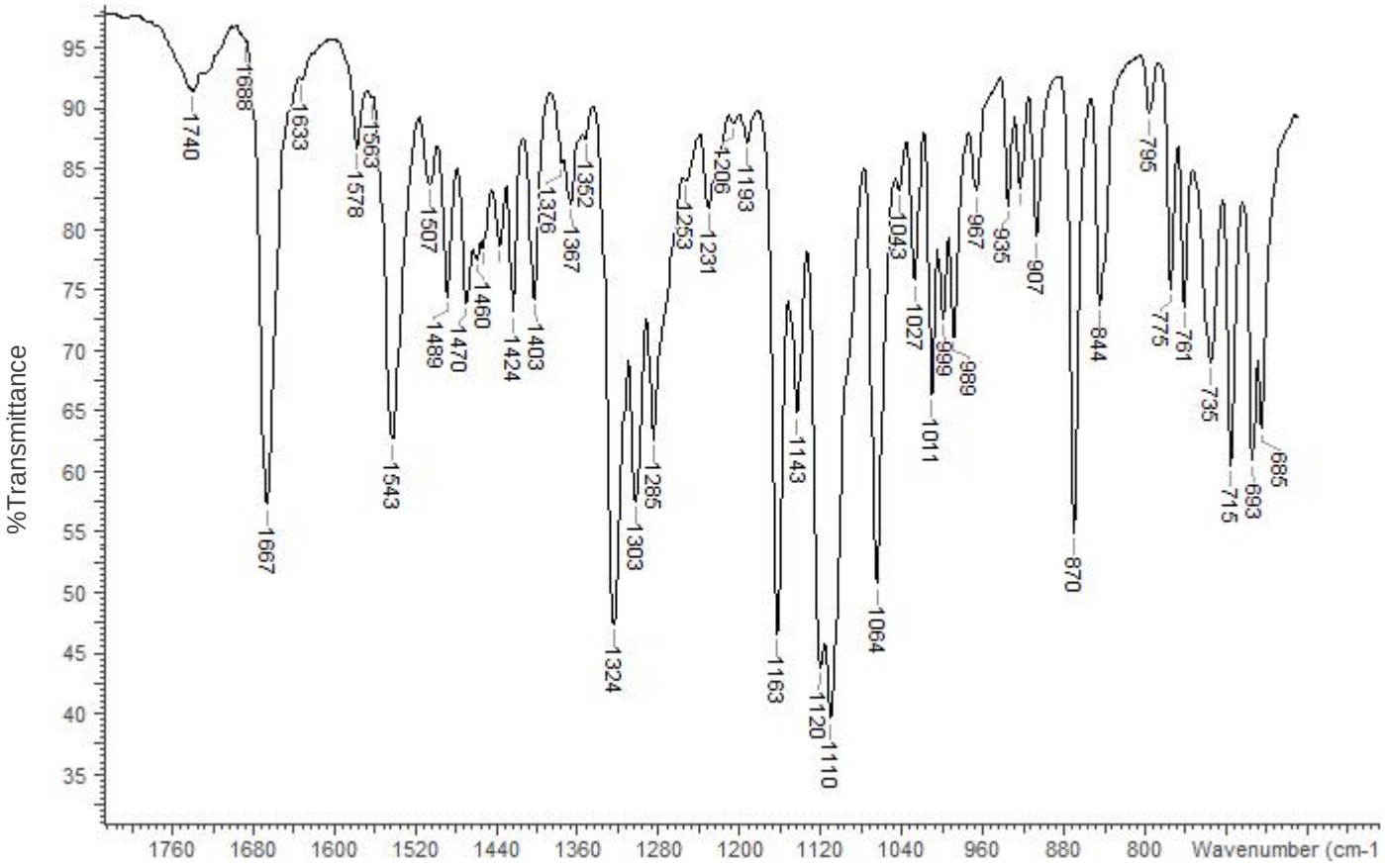
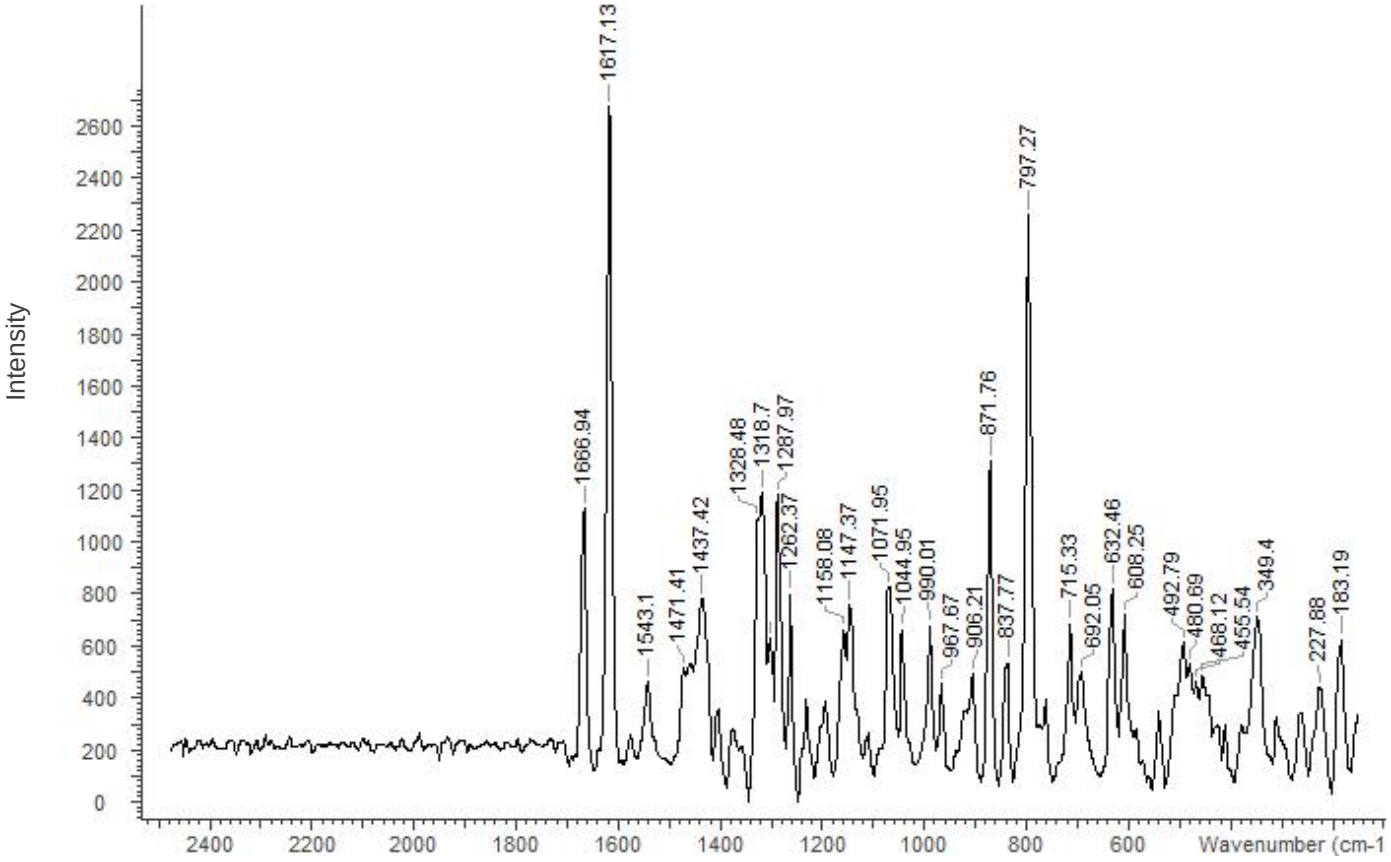


3.4 RAMAN SPECTROSCOPY

Instrument: Rigaku Progeny 1064

Scan Parameters: Power (mW): 350
Exposure (ms): 1000
Averages: 30
Threshold: 0.80

Raman (1064 nm): A04 HCl; Lot JLK008-041-04



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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