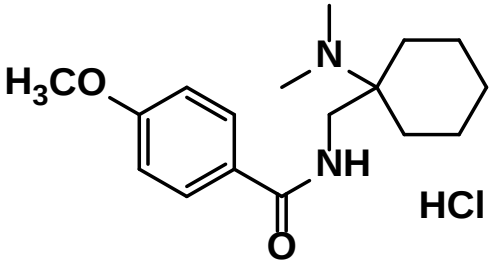
A05 hydrochloride

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-methoxybenzamidomethyl)-cyclohexyldimethylamine; hydrochloride

CAS#: 851299-58-6 (base)

Synonyms: A05

Source: **Synthesized Material** Lot# JLK008-041-05

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 (^{o}C)
HCl	$C_{17}H_{26}N_2O_2 \cdot HCl$	326.86	217.0 $\pm$ 0.95
base	$C_{17}H_{26}N_2O_2$	290.40	Not determined

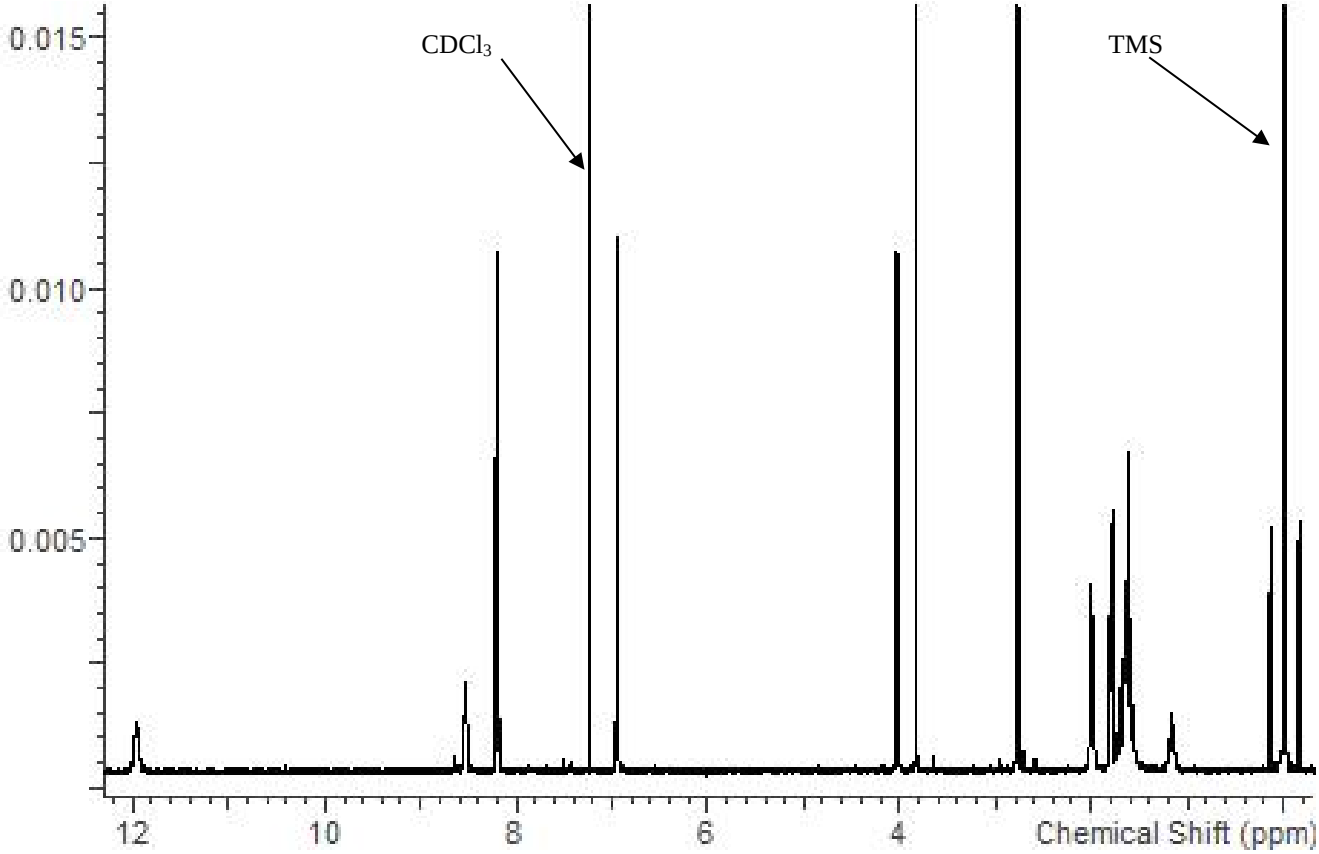
3. QUALITATIVE DATA

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: A05 HCl; Lot JLK008-041-05; $CDCl_3$ + TMS; 400 MHz



A05 hydrochloride

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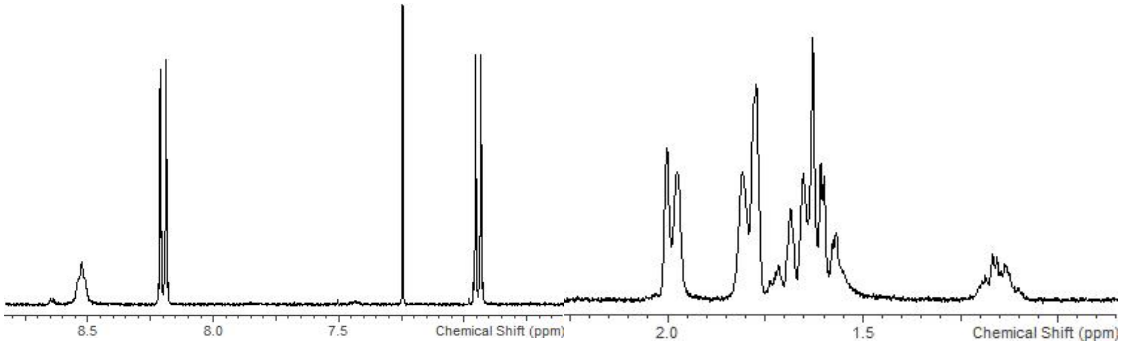
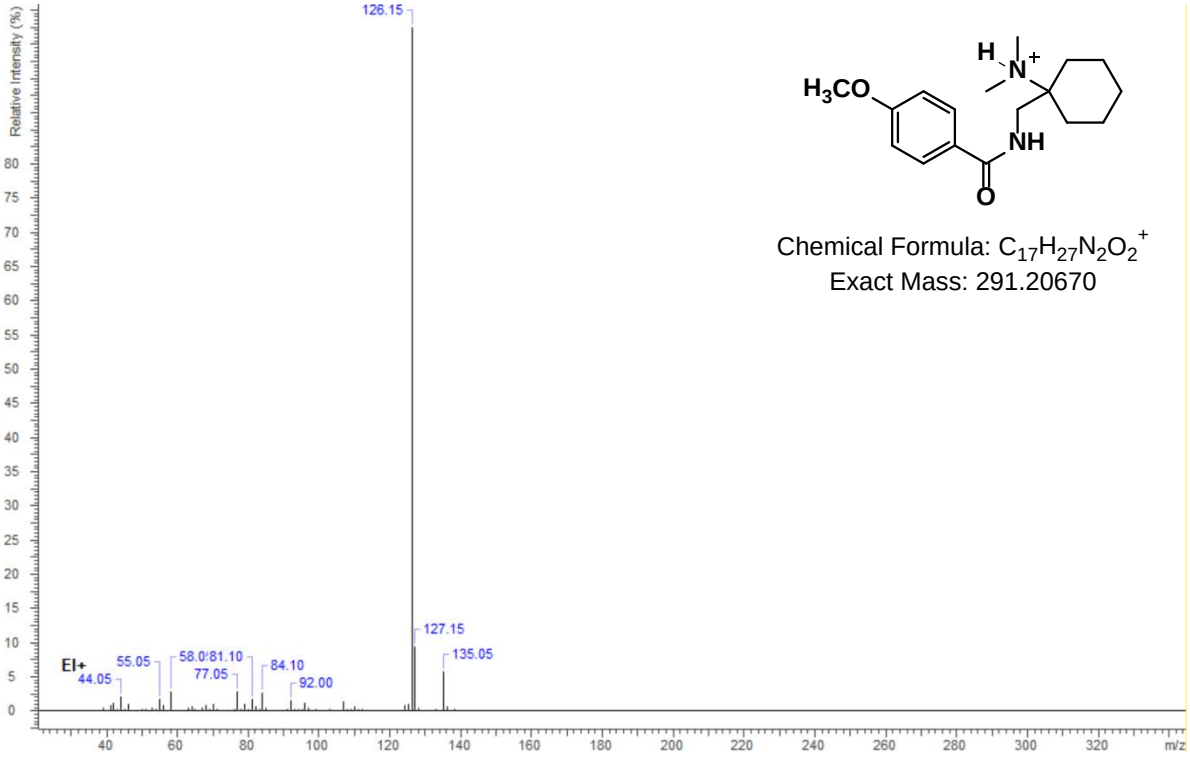


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

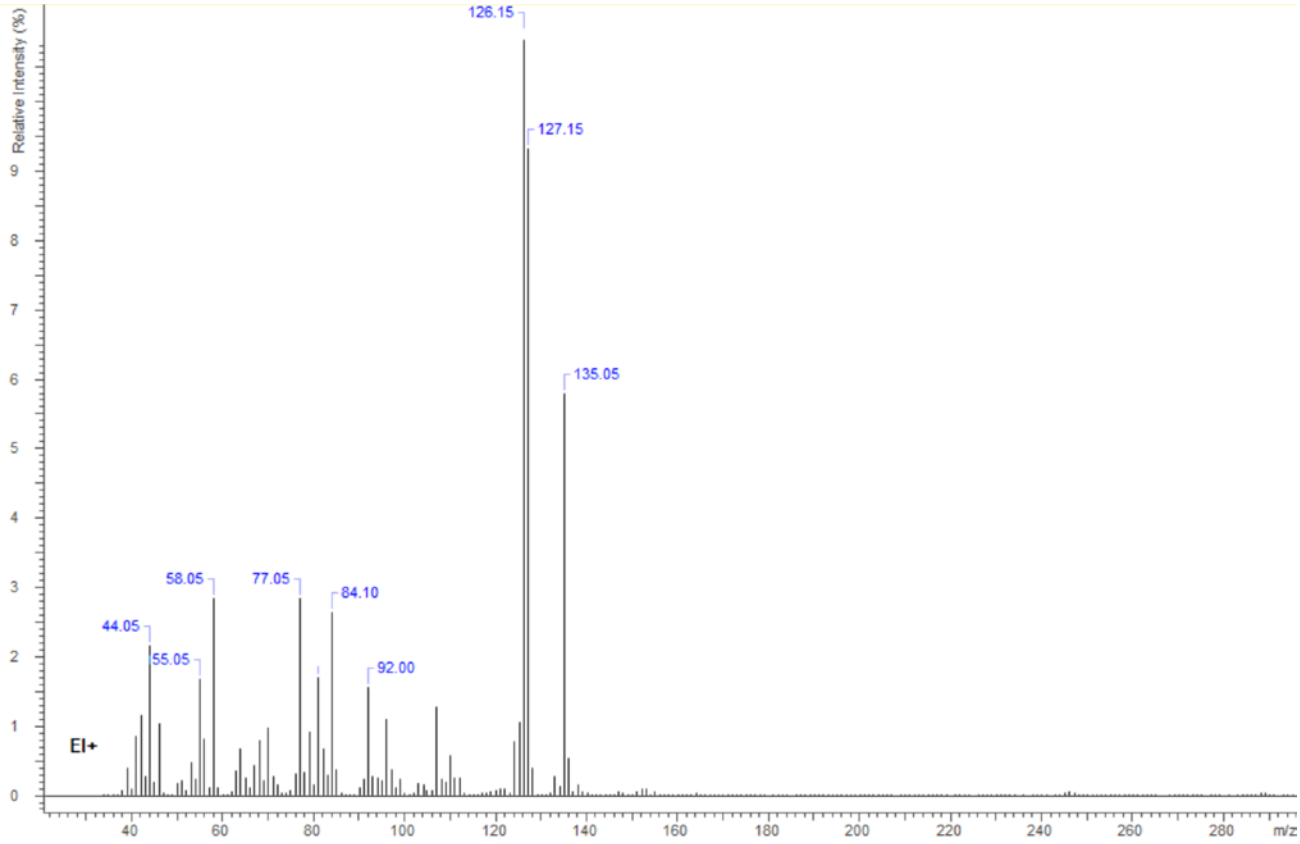
Instrument:	Shimadzu gas chromatograph operated in split mode with MS detector
Column:	Rtx5MS (a DB-5 equivalent); 30m x 0.25 mm x 0.25 µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 200°C Oven program: 1) 90°C initial temperature for 2.0 min 2) Ramp 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: 050218Tune.qgt Acquisition mode: scan
Retention Time:	16.70 min

EI Mass Spectrum: A05 HCl; Lot JLK008-041-05



Chemical Formula: $C_{17}H_{27}N_2O_2^+$
Exact Mass: 291.20670

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

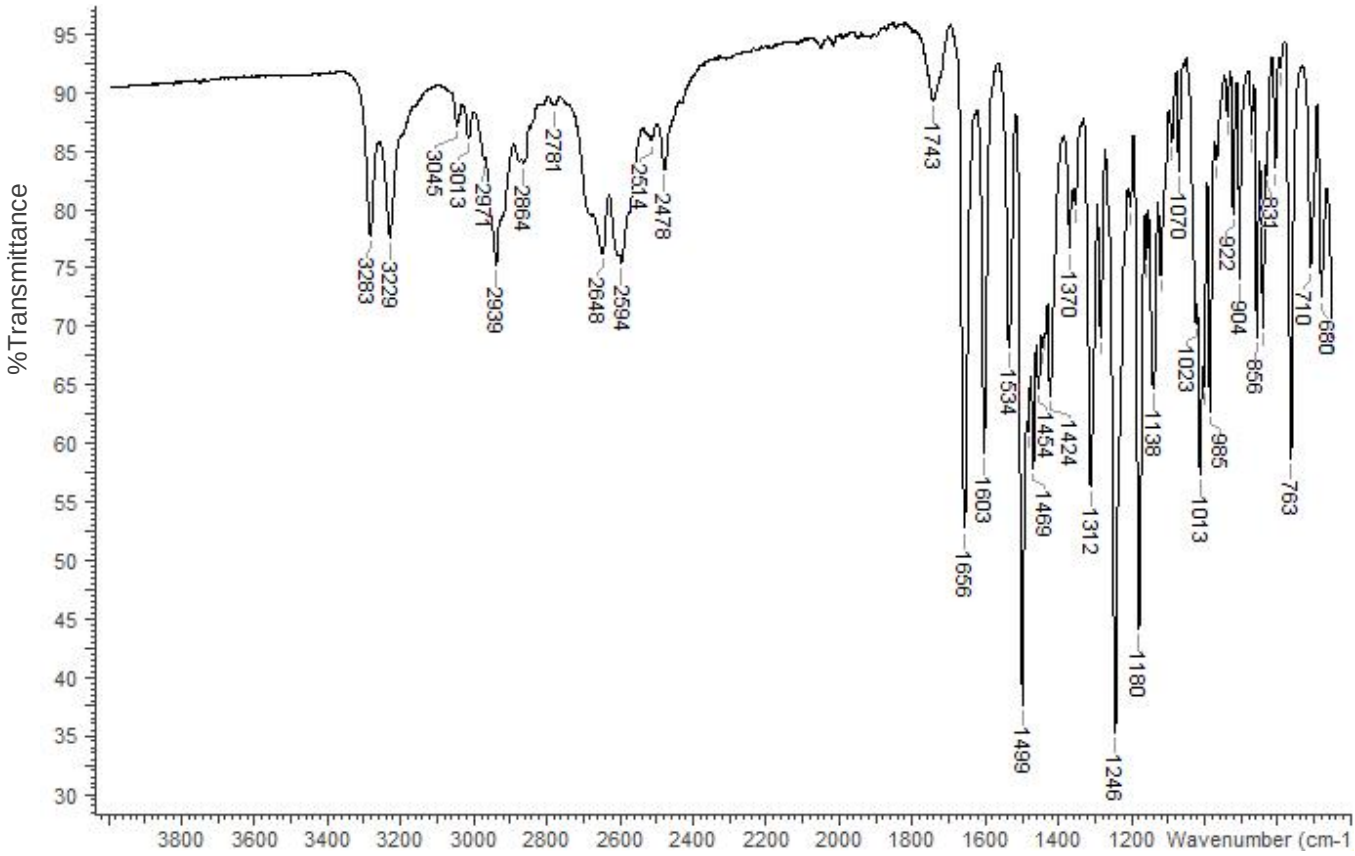


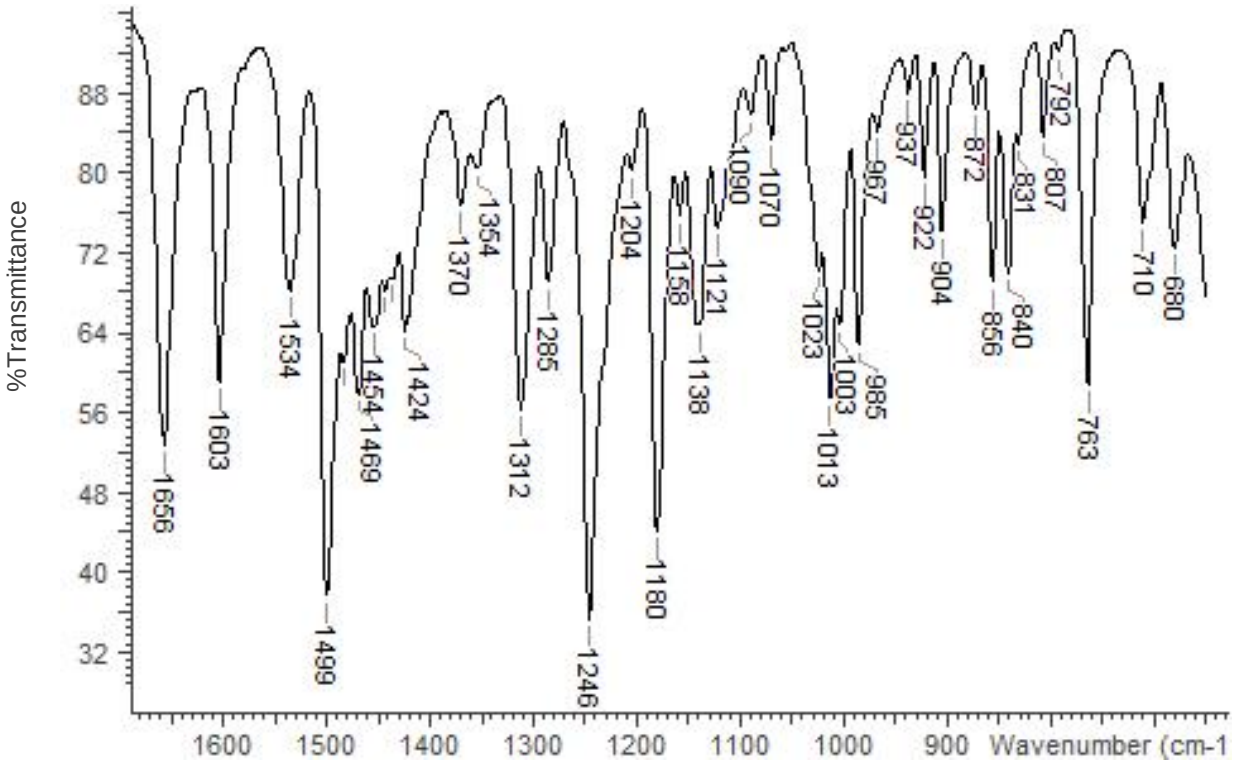
3.3 INFRARED SPECTROSCOPY (FTIR)

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): A05 HCl; Lot JLK008-041-05



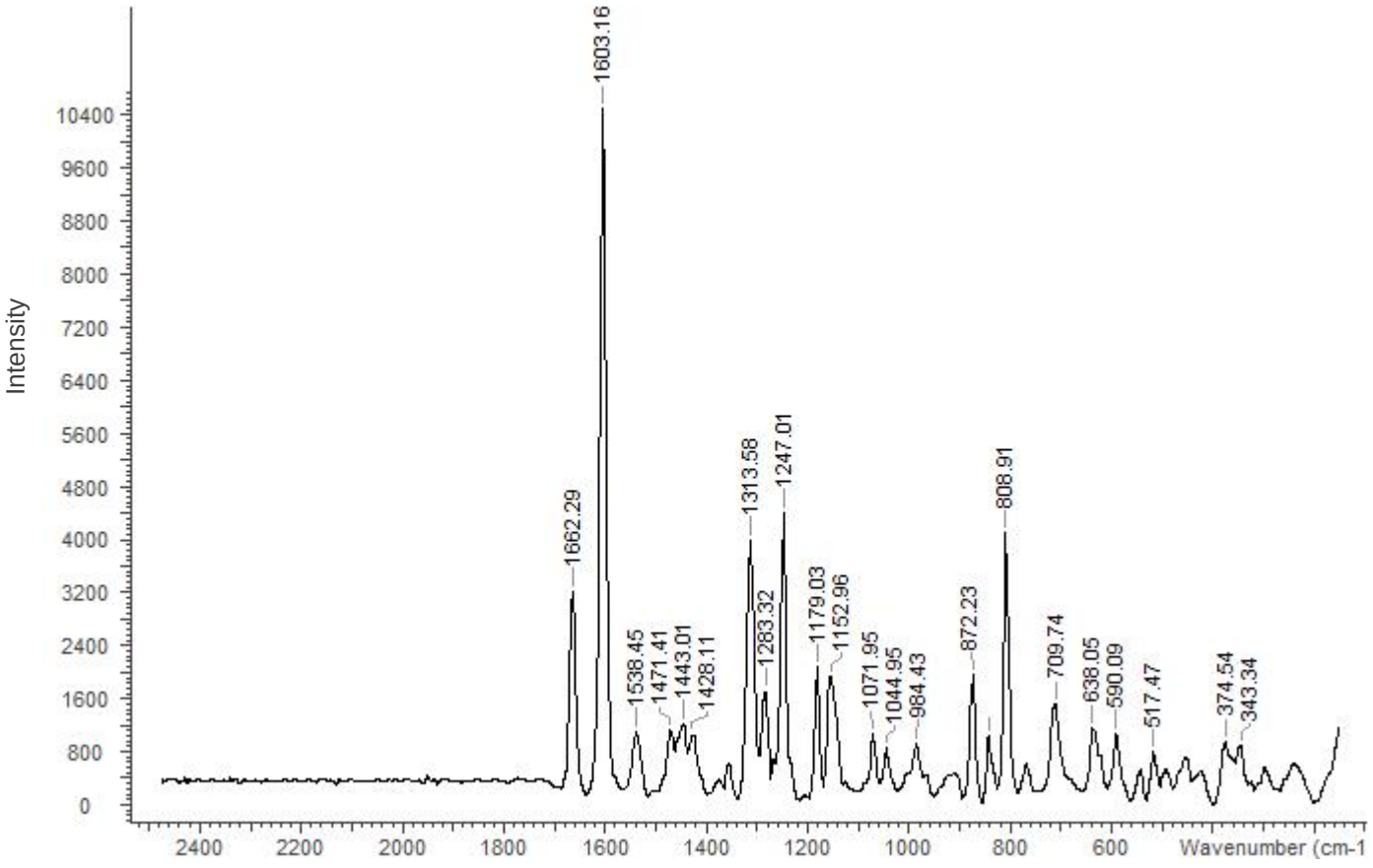

%Transmittance
88
80
72
64
56
48
40
32
1656
1603
1534
1499
1469
1454
1424
1370
1354
1312
1285
1246
1204
1180
1158
1138
1121
1090
1070
1023
1013
1003
985
967
937
922
904
872
856
840
831
807
792
763
710
680
1600
1500
1400
1300
1200
1100
1000
900
Wavenumber (cm-1

3.4 RAMAN SPECTROSCOPY

Instrument: Rigaku Progeny 1064

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

Raman (1064 nm): A05 HCl; Lot JLK008-041-05



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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