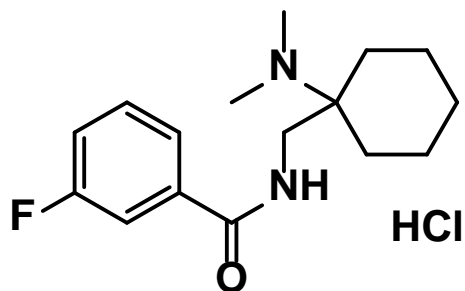


A16 hydrochloride

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



1. GENERAL INFORMATION

IUPAC Name:	1-(3-fluorobenzamidomethyl)-cyclohexyldimethylamine; hydrochloride
CAS#:	N/A
Synonyms:	A16
Source:	Synthesized Material Lot# JLK010-029-A16
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 FN ₂ O·HCl	314.83	217.6 ± 0.50
base	C ₁₆ H ₂₃ FN ₂ O	278.36	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.

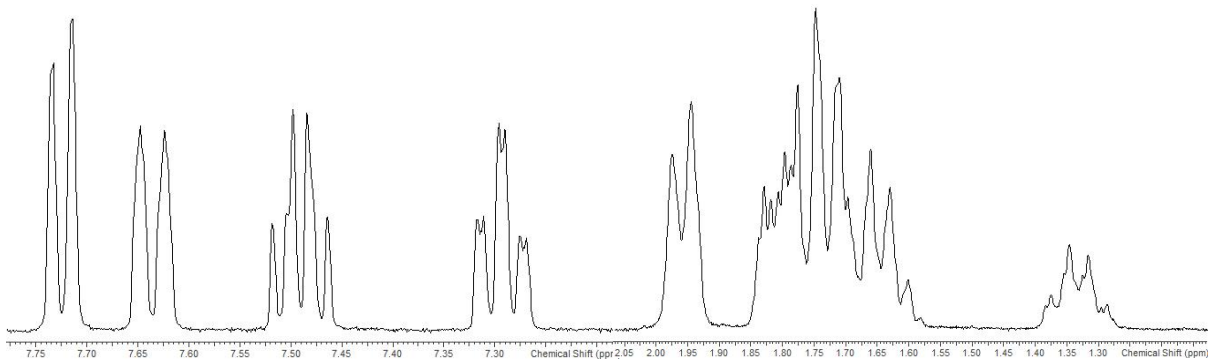
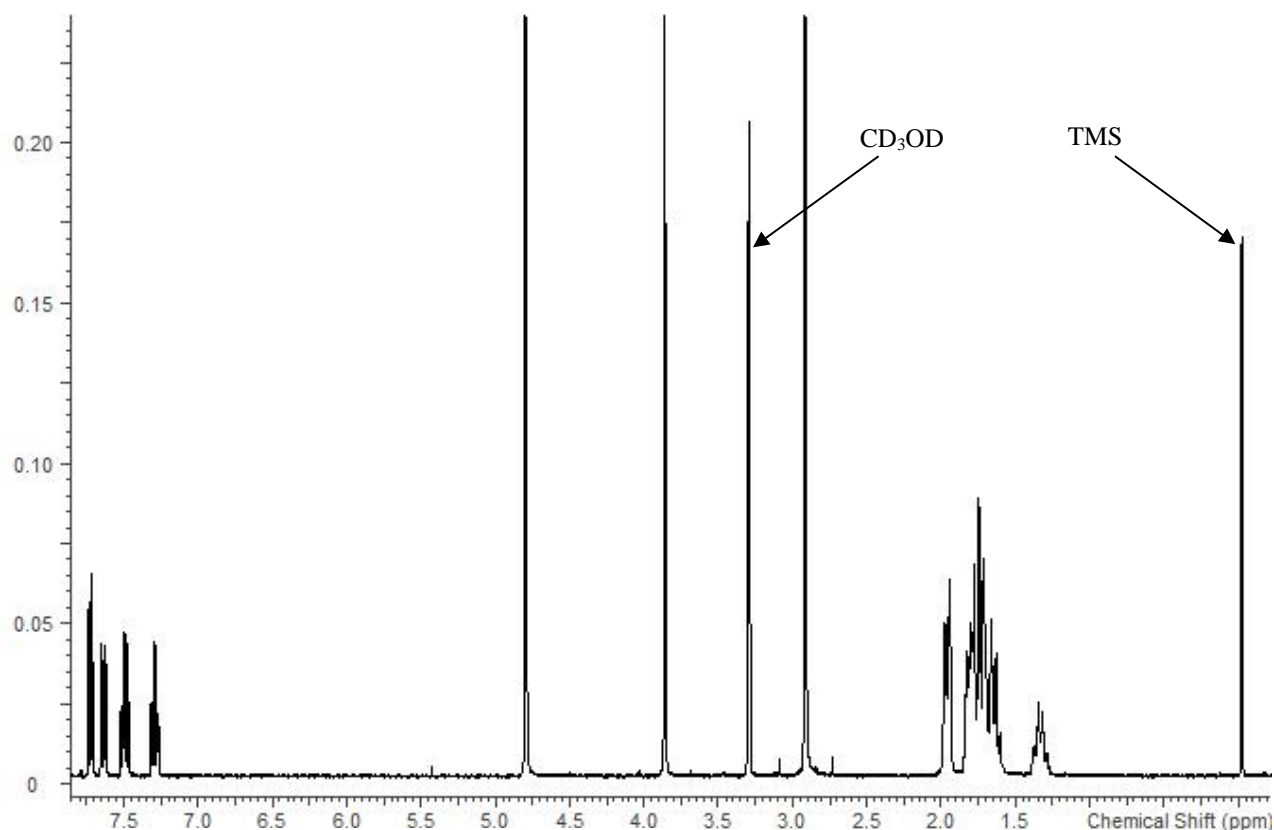
Instrument: 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 30 seconds

¹H NMR: A16 HCl; Lot JLK010-029-A16; CDCl₃:CD₃OD (1:5) + 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 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

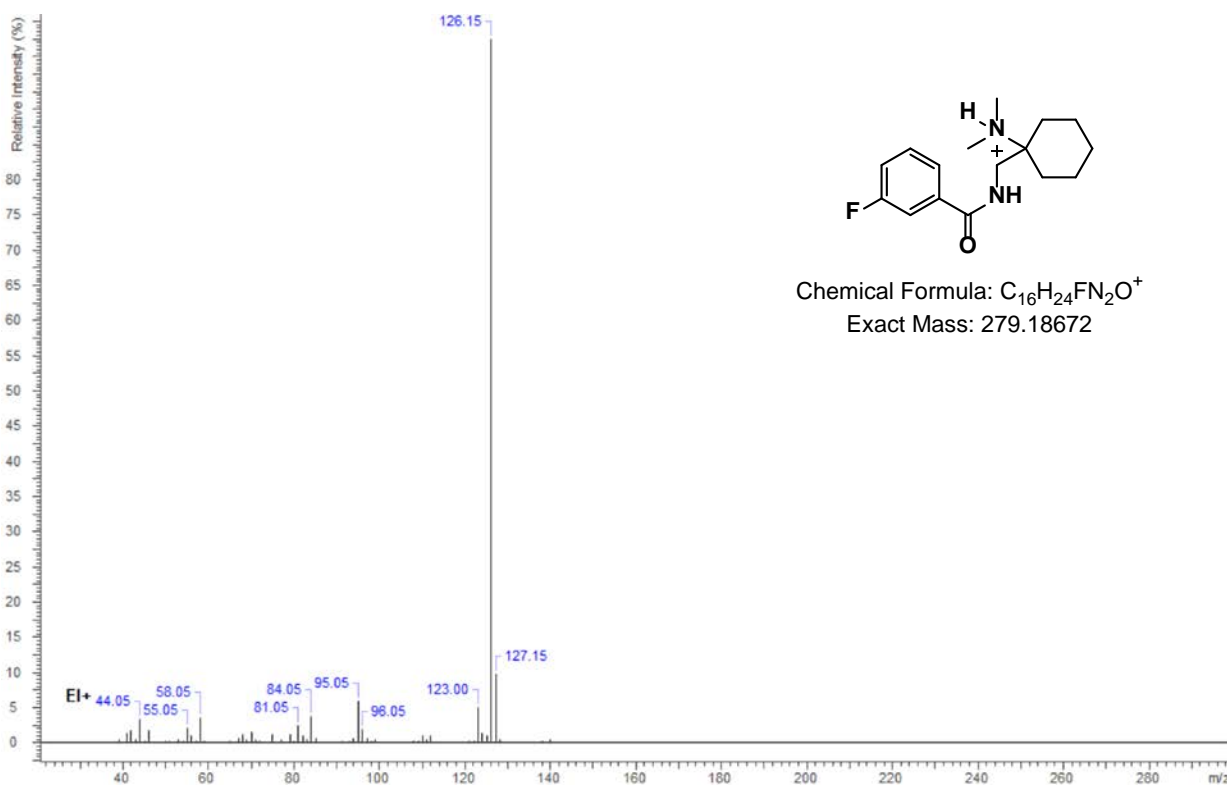
Threshold: 100

Tune file: 050218_Tune.qgt

Acquisition mode: scan

Retention Time: 14.53 min

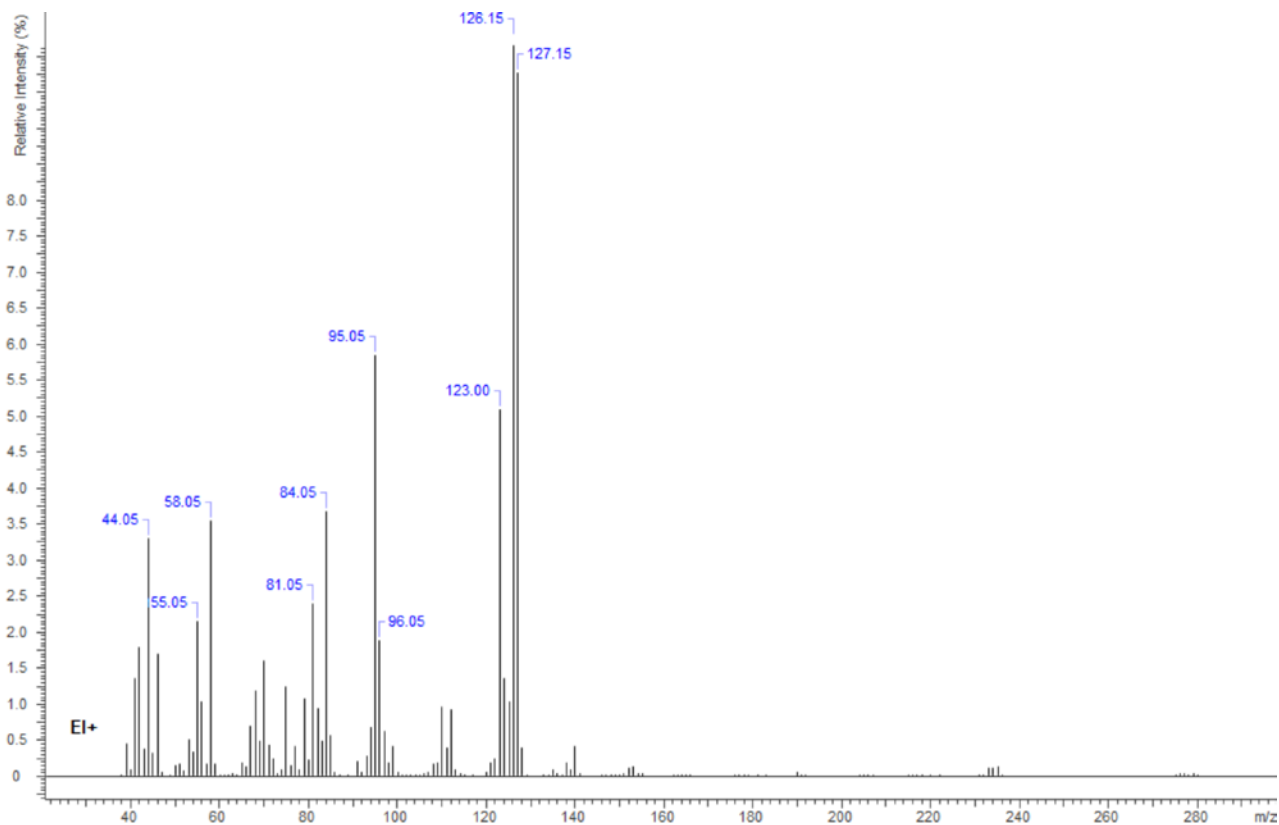
EI Mass Spectrum: A16 HCl; Lot JLK010-029-A16



A16 hydrochloride

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



A16 hydrochloride

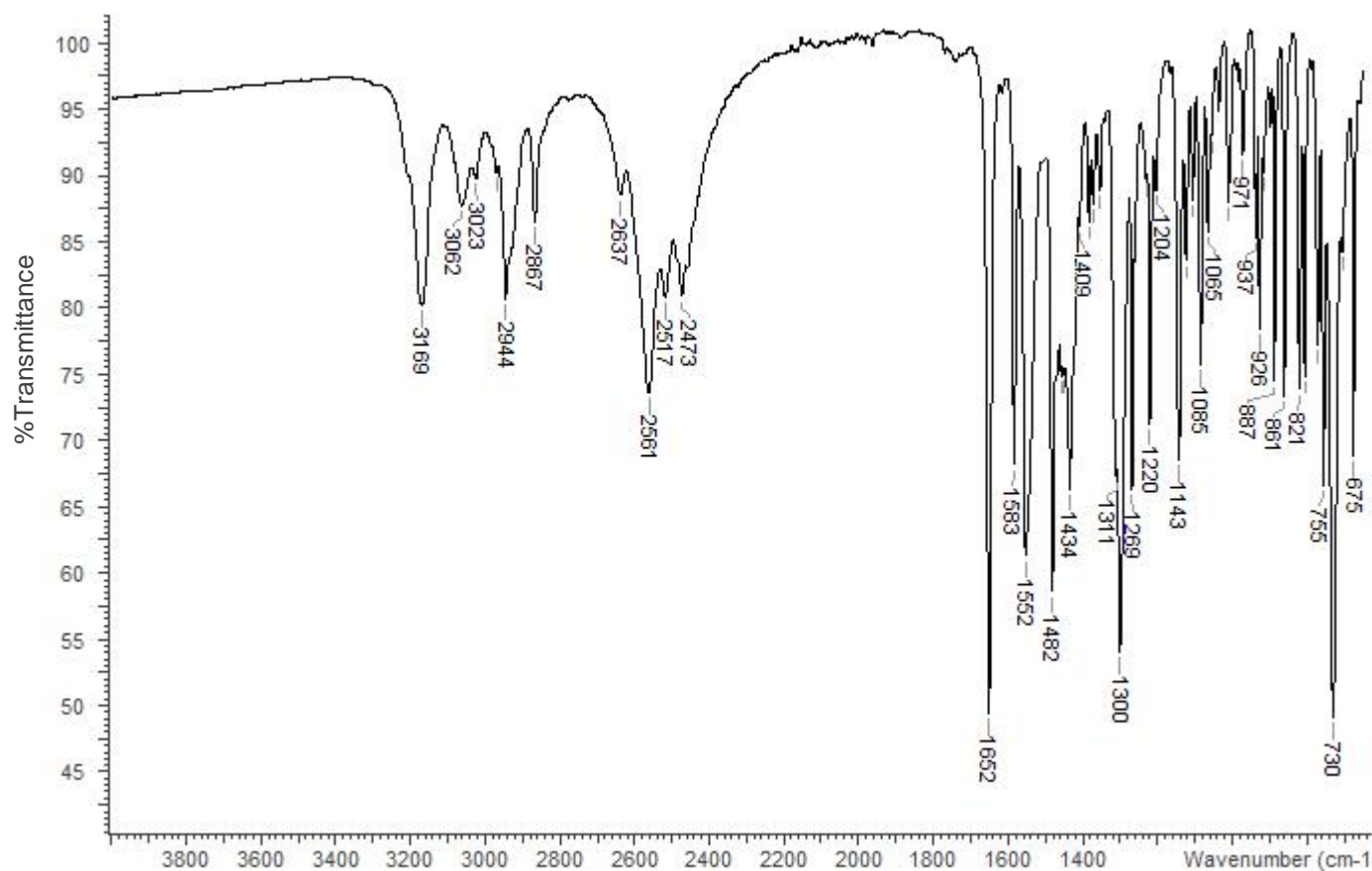
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material

3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with ZnSe ATR attachment (1 bounce)

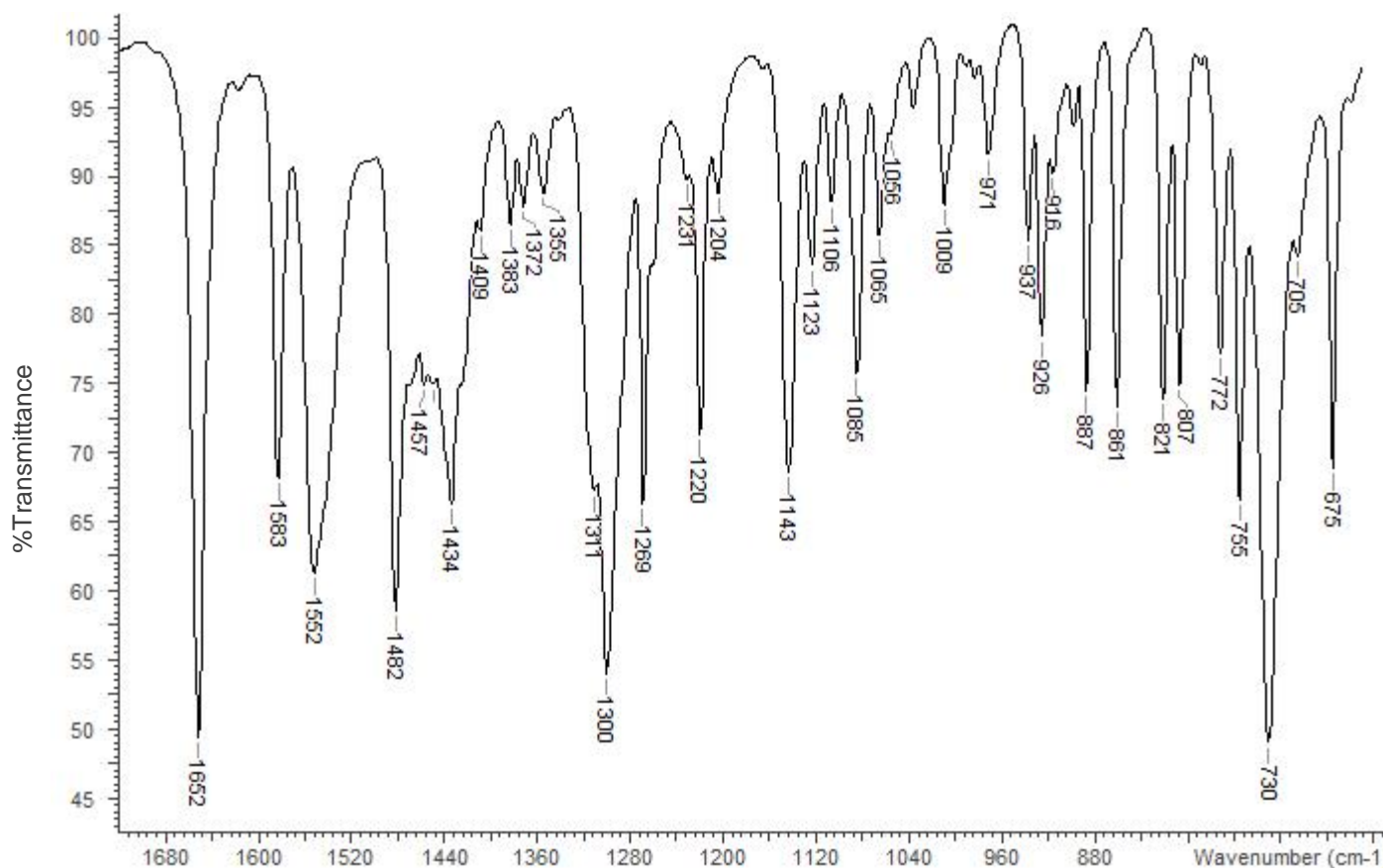
Scan Parameters:
 Number of scans: 4
 Number of background scans: 4
 Resolution: 4 cm⁻¹
 Sample gain: 8
 Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): A16 HCl; Lot JLK010-029-A16



A16 hydrochloride

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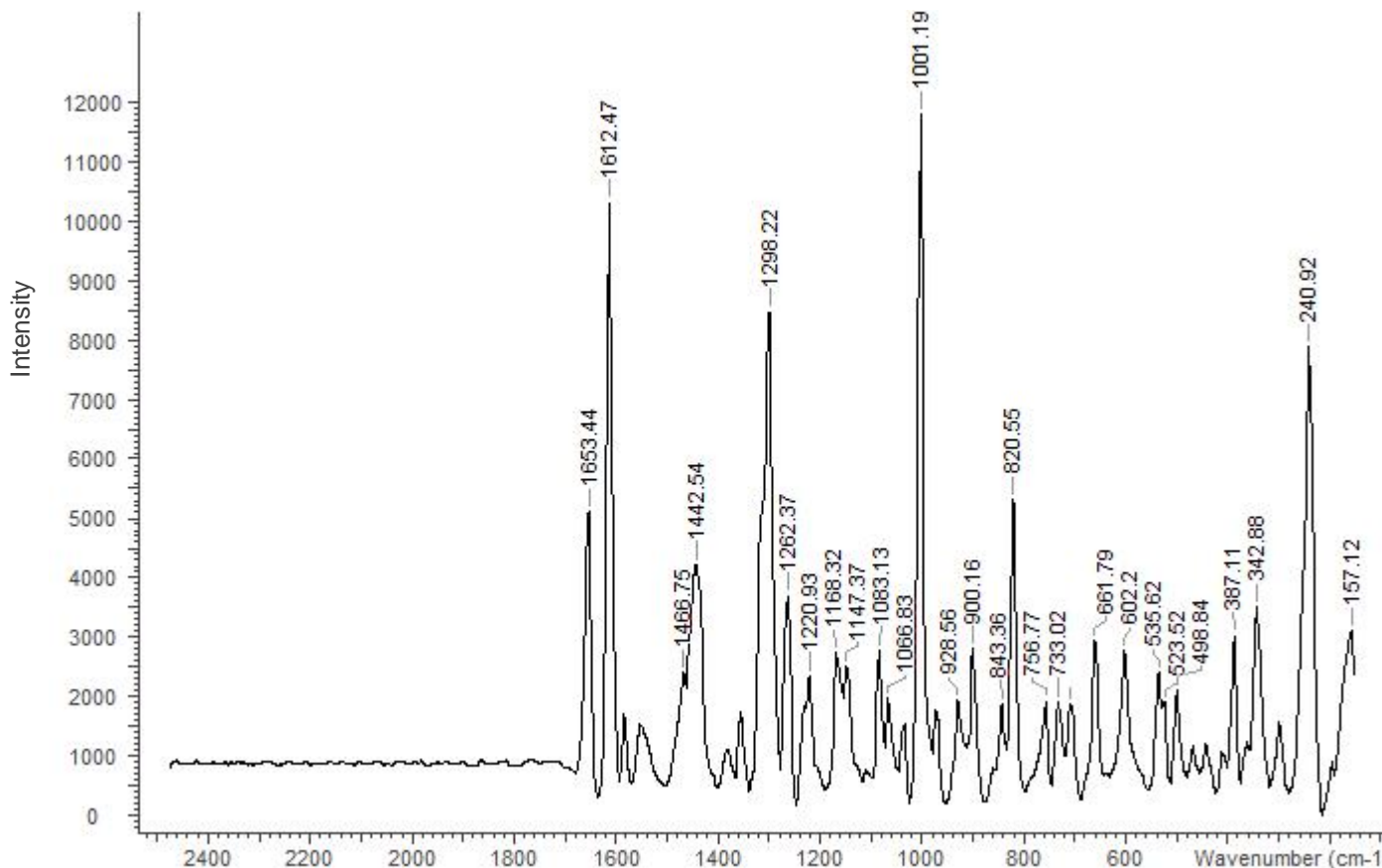
A16 hydrochloride

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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): A16 HCl; Lot JLK010-029-A16



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

These data are from a project supported by Award No. 2016-R2-CX-0059, awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice. The opinions, findings, and conclusions or recommendations expressed in this publication are those of the authors and do not necessarily reflect those of the Department of Justice. We also thank Rigaku Corporation for the loan of the Progeny 1064 Raman instrument.