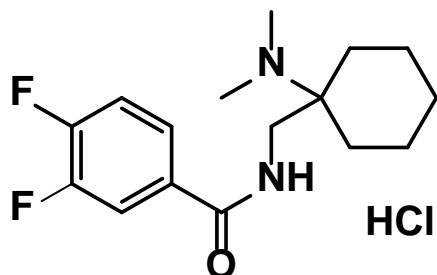


## A06 hydrochloride

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



### 1. GENERAL INFORMATION

**IUPAC Name:** 1-(3,4-difluorobenzamidomethyl)-cyclohexyldimethylamine; hydrochloride

**CAS#:** N/A

**Synonyms:** A06

**Source:** Synthesized Material Lot# JLK010-026-A06

**Appearance:** White Crystals (HCl)

**UV<sub>max</sub> (nm):** Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
HCl	C <sub>16</sub> H <sub>22</sub> F <sub>2</sub> N <sub>2</sub> O·HCl	332.82	231.5 ± 0.42
base	C <sub>16</sub> H <sub>22</sub> F <sub>2</sub> N <sub>2</sub> O	296.36	Not determined

### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

*Sample Preparation:* Dilute analyte to ~5 mg/mL in deuterated chloroform: methanol (CDCl<sub>3</sub>:CD<sub>3</sub>OD, 1:5) + TMS.

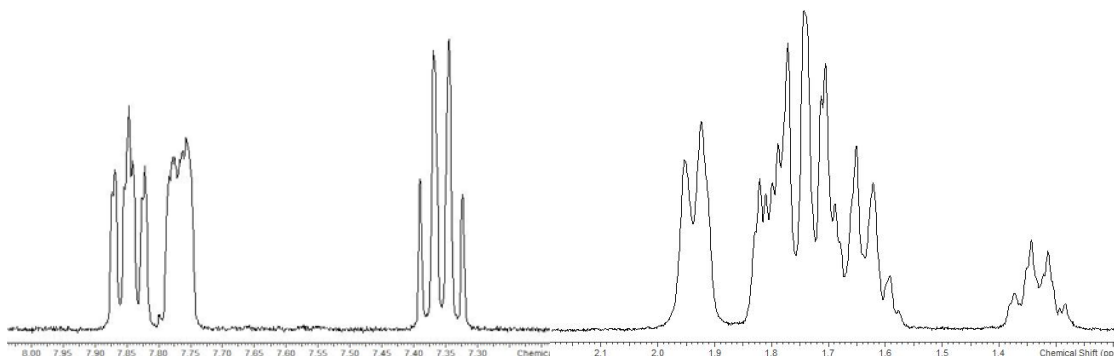
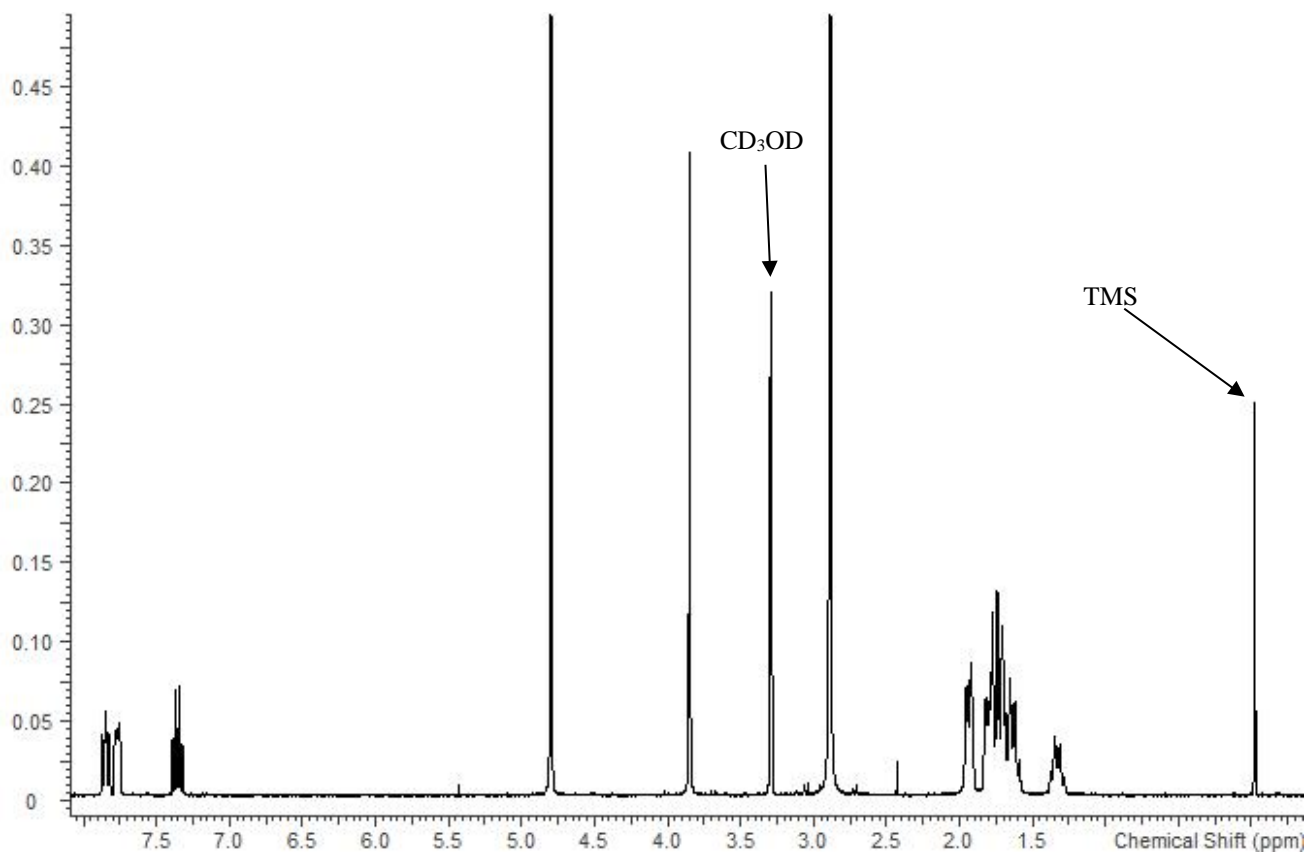
*Instrument:* 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 30 seconds

<sup>1</sup>H NMR: A06 HCl; Lot JLK010-026-A06; CDCl<sub>3</sub>:CD<sub>3</sub>OD (1:5) + TMS; 400 MHz



## A06 hydrochloride

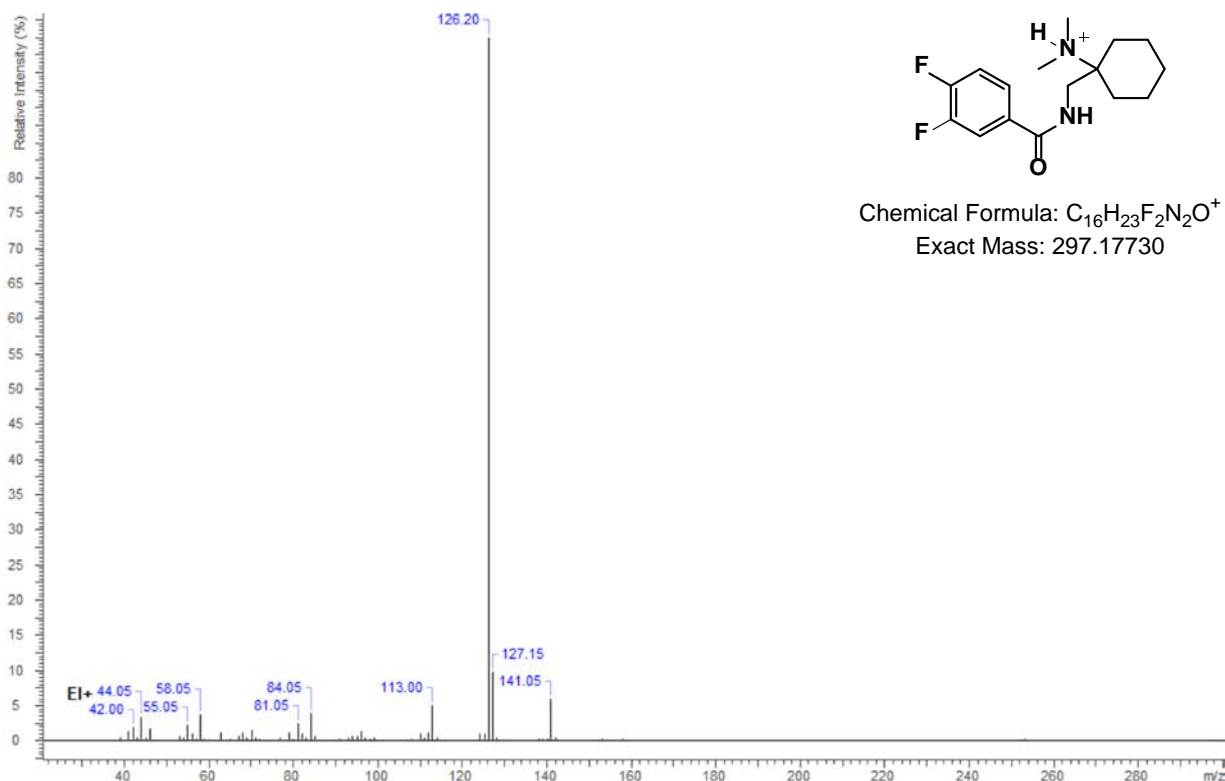
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material

### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

<b>Instrument:</b>	Shimadzu gas chromatograph operated in split mode with MS detector
<b>Column:</b>	Rtx5MS (a DB-5 equivalent); 30m x 0.25 mm x 0.25 $\mu$ m
<b>Carrier Gas:</b>	Helium at 1 mL/min
<b>Temperatures:</b>	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
<b>Injection Parameters:</b>	Split Ratio = 1:15, 1 $\mu$ L injected
<b>MS Parameters:</b>	Mass scan range: 34-550 amu Threshold: 100 Tune file: 050218Tune.qgt Acquisition mode: scan
<b>Retention Time:</b>	14.40 min

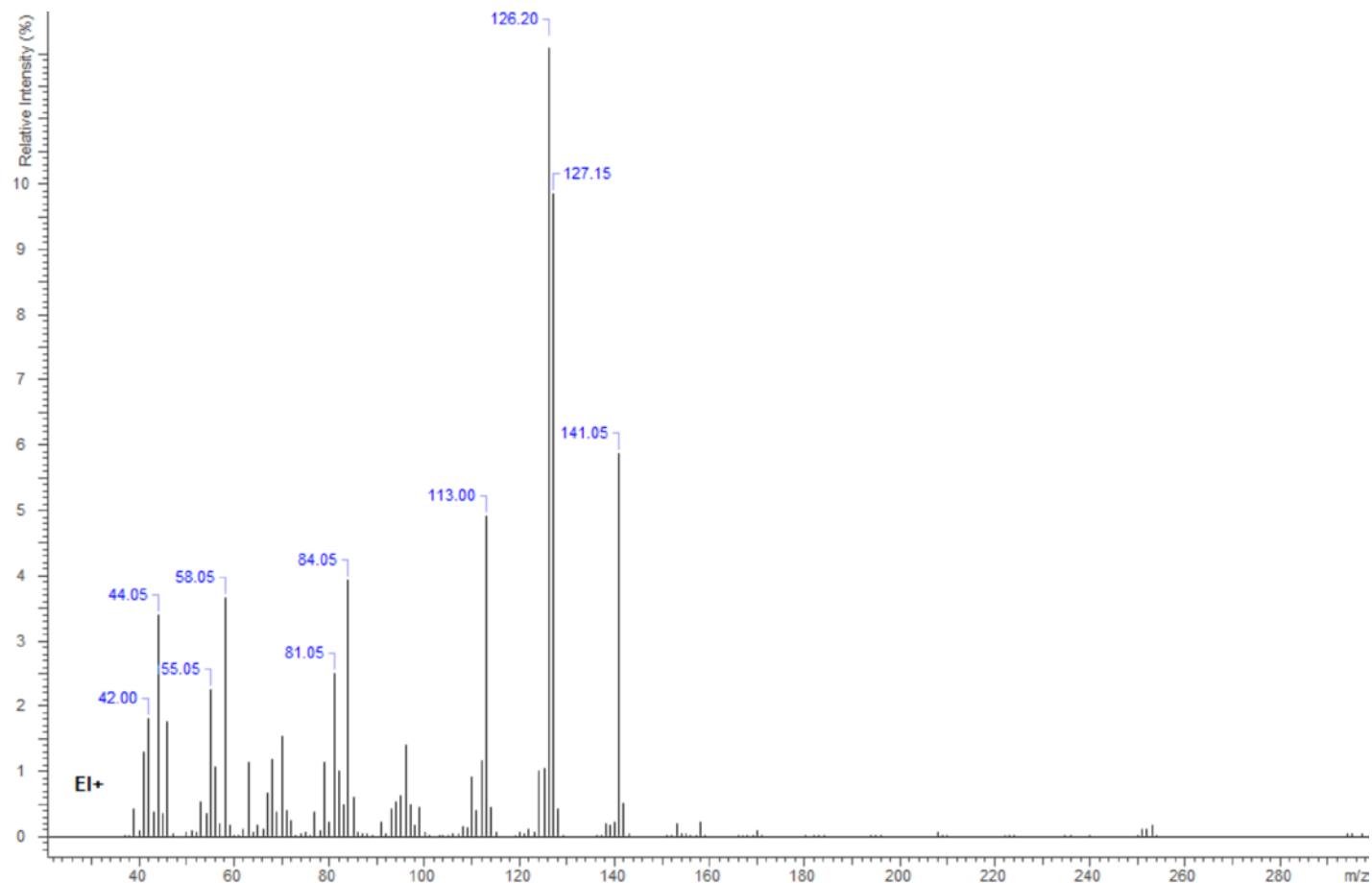
EI Mass Spectrum: A06 HCl; Lot JLK010-026-A06



## A06 hydrochloride

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Zoomed view (126.20 is 100% relative intensity and truncated in this view)



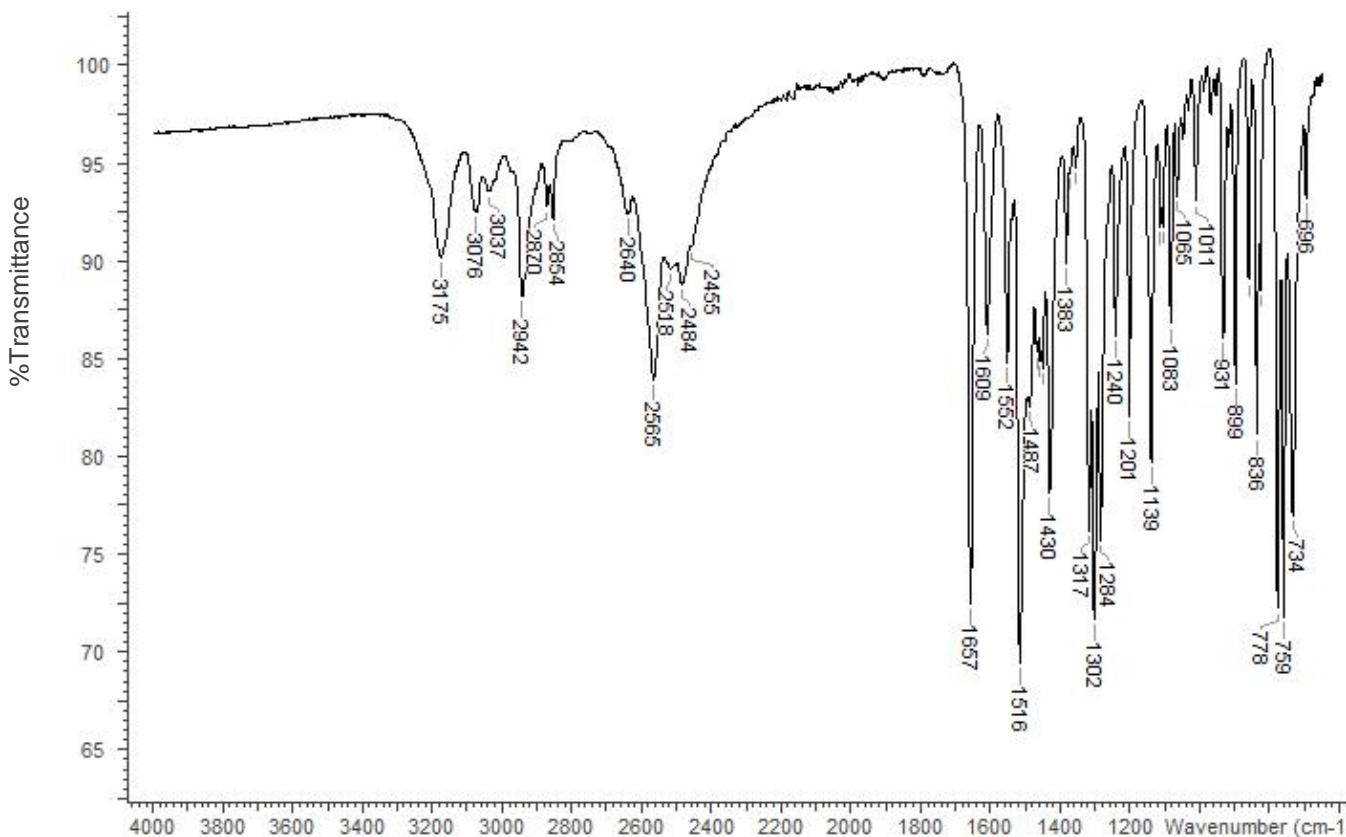
### A06 hydrochloride

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### 3.3 INFRARED SPECTROSCOPY (FTIR)

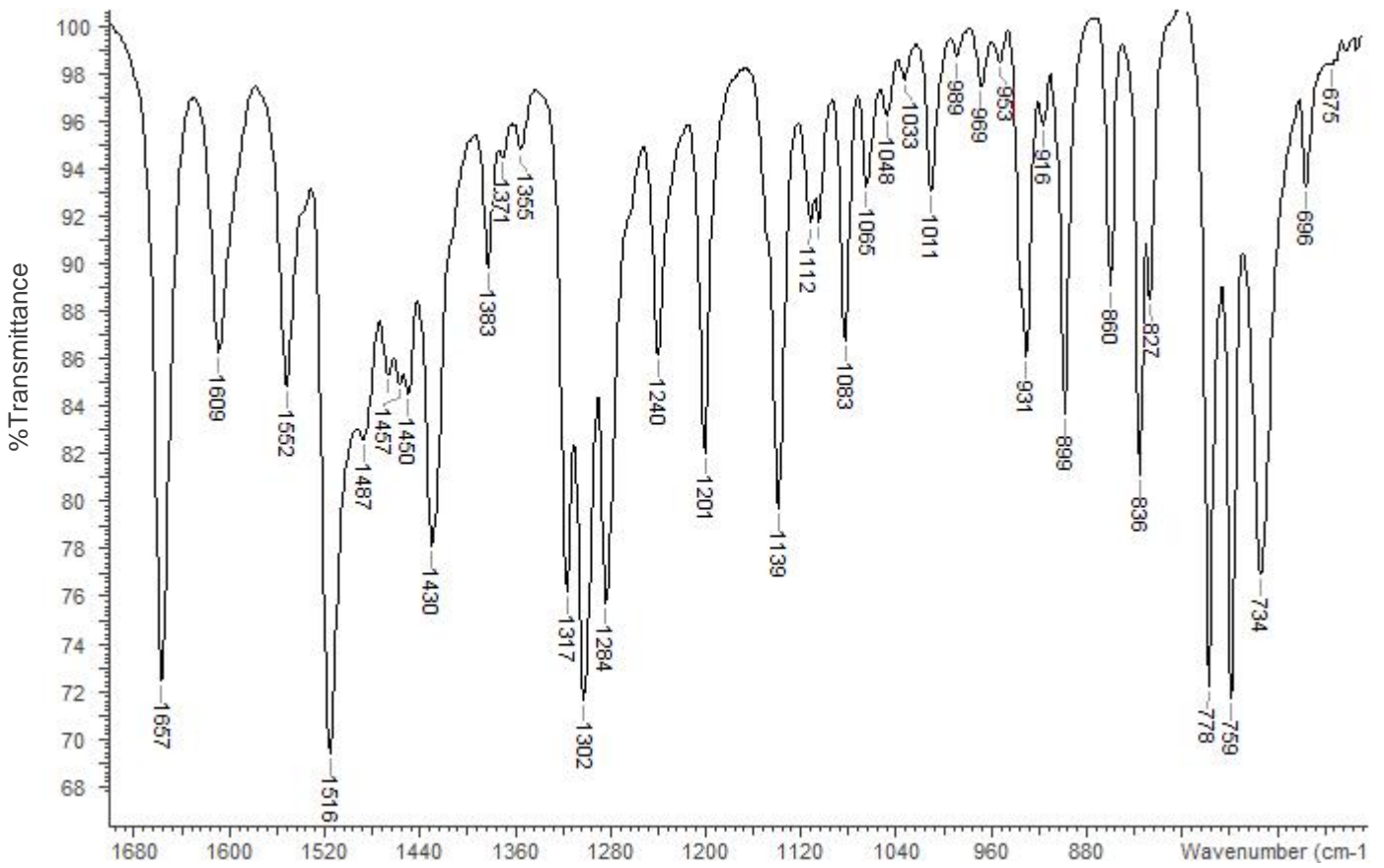
**Instrument:** FTIR with ZnSe ATR attachment (1 bounce)  
**Scan Parameters:** Number of scans: 4  
Number of background scans: 4  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): A06 HCl; Lot JLK010-026-A06



## A06 hydrochloride

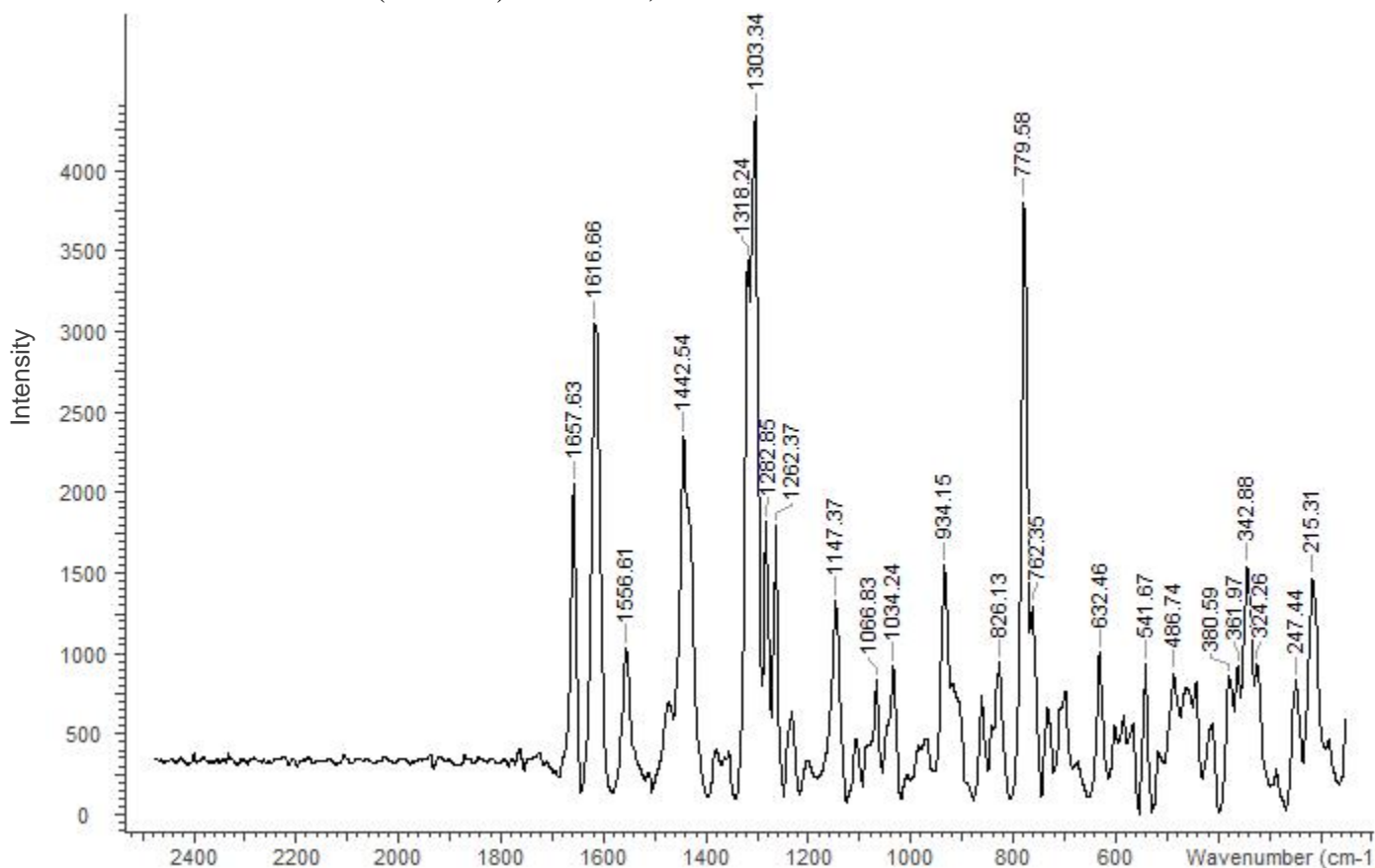
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material



### 3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): A06 HCl; Lot JLK010-026-A06



#### **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  $\mu$ -opiate receptor 1 (OPRM1) expressing cells. *Pharmacol. Research & Perspectives* 7: e00511 (2019) doi: 10.1002/prp2.511

#### **5. ACKNOWLEDGEMENT**

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