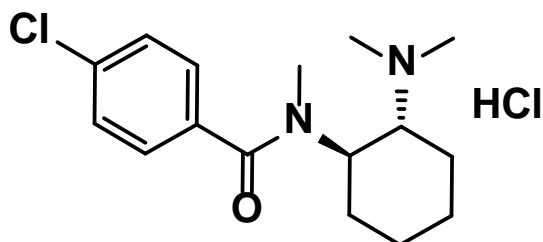


## U02 hydrochloride

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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	N-((1 <i>R</i> ,2 <i>R</i> )-2-(dimethylamino)cyclohexyl)-4-chloro-N-methylbenzamide; hydrochloride
<b>CAS#:</b>	67579-11-7 (base)
<b>Synonyms:</b>	U02
<b>Source:</b>	Synthesized Material Lot# JLK010-042-U02
<b>Appearance:</b>	White Crystals (HCl)
<b>UV<sub>max</sub> (nm):</b>	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>23</sub> ClN <sub>2</sub> O·HCl	331.28	121.1 ± 0.29
base	C <sub>16</sub> H <sub>23</sub> ClN <sub>2</sub> 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 (CDCl<sub>3</sub>:CD<sub>3</sub>OD, 1:5) + TMS.

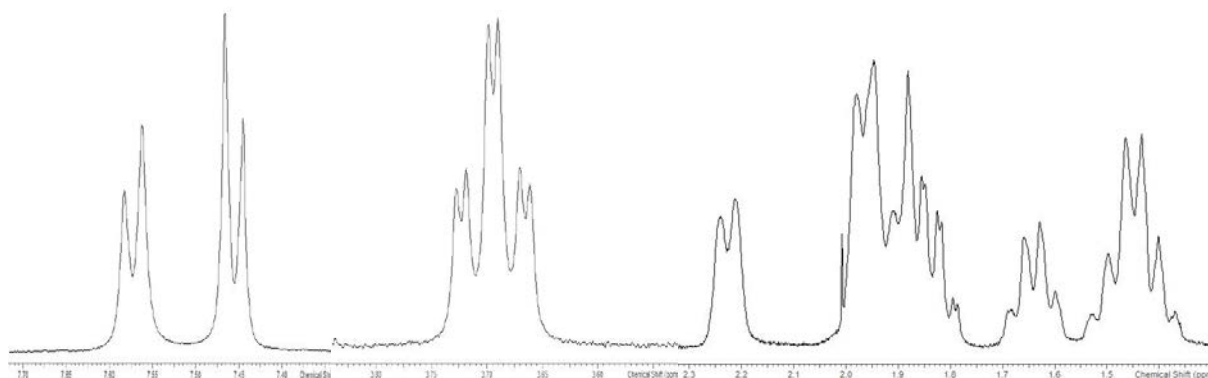
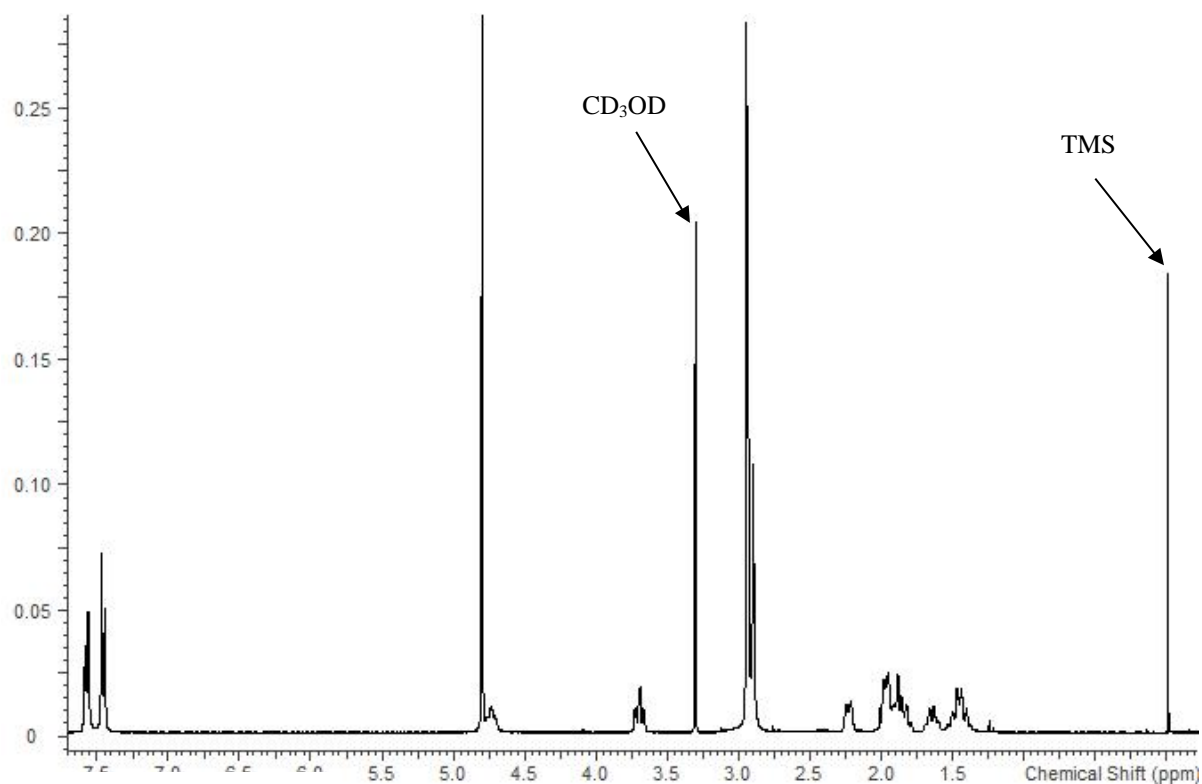
*Instrument:* 400 MHz NMR spectrometer

*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: U02 HCl; Lot JLK010-042-U02; CDCl<sub>3</sub>:CD<sub>3</sub>OD (1:5) + TMS; 400 MHz



## U02 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

**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

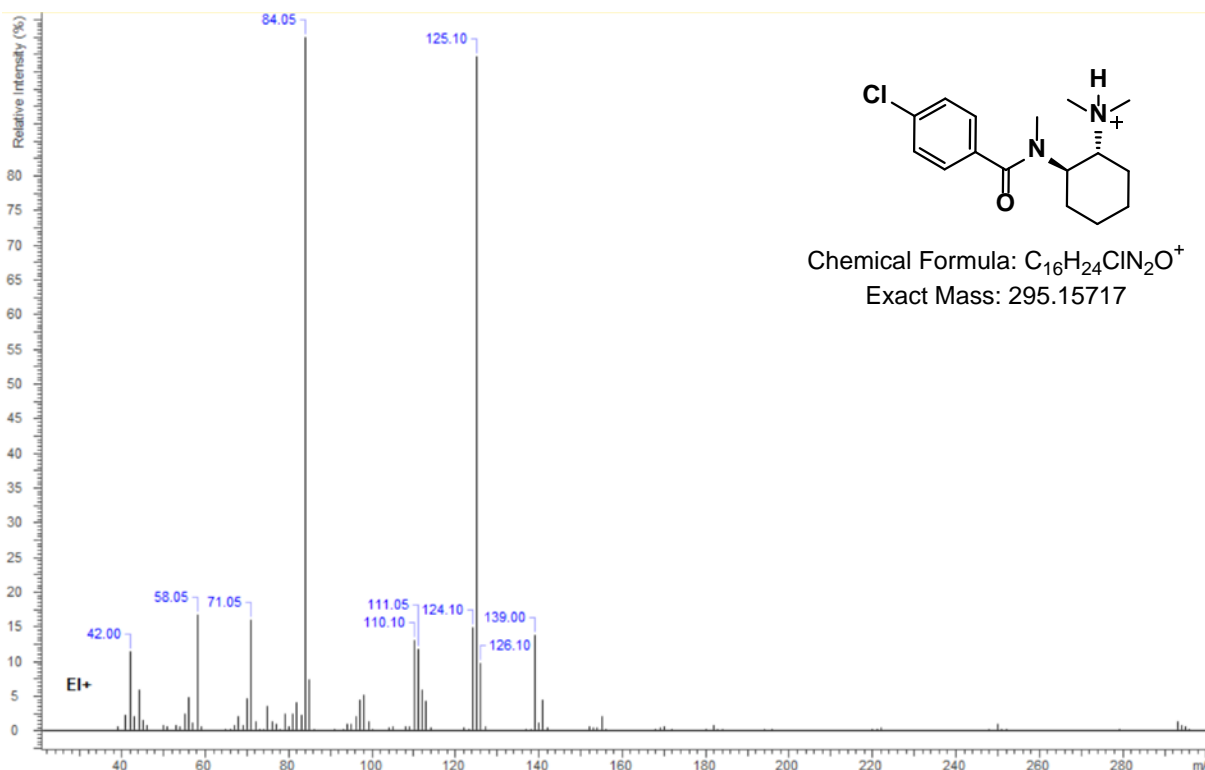
Threshold: 100

Tune file: 050218\_Tune.qgt

Acquisition mode: scan

**Retention Time:** 14.98 min

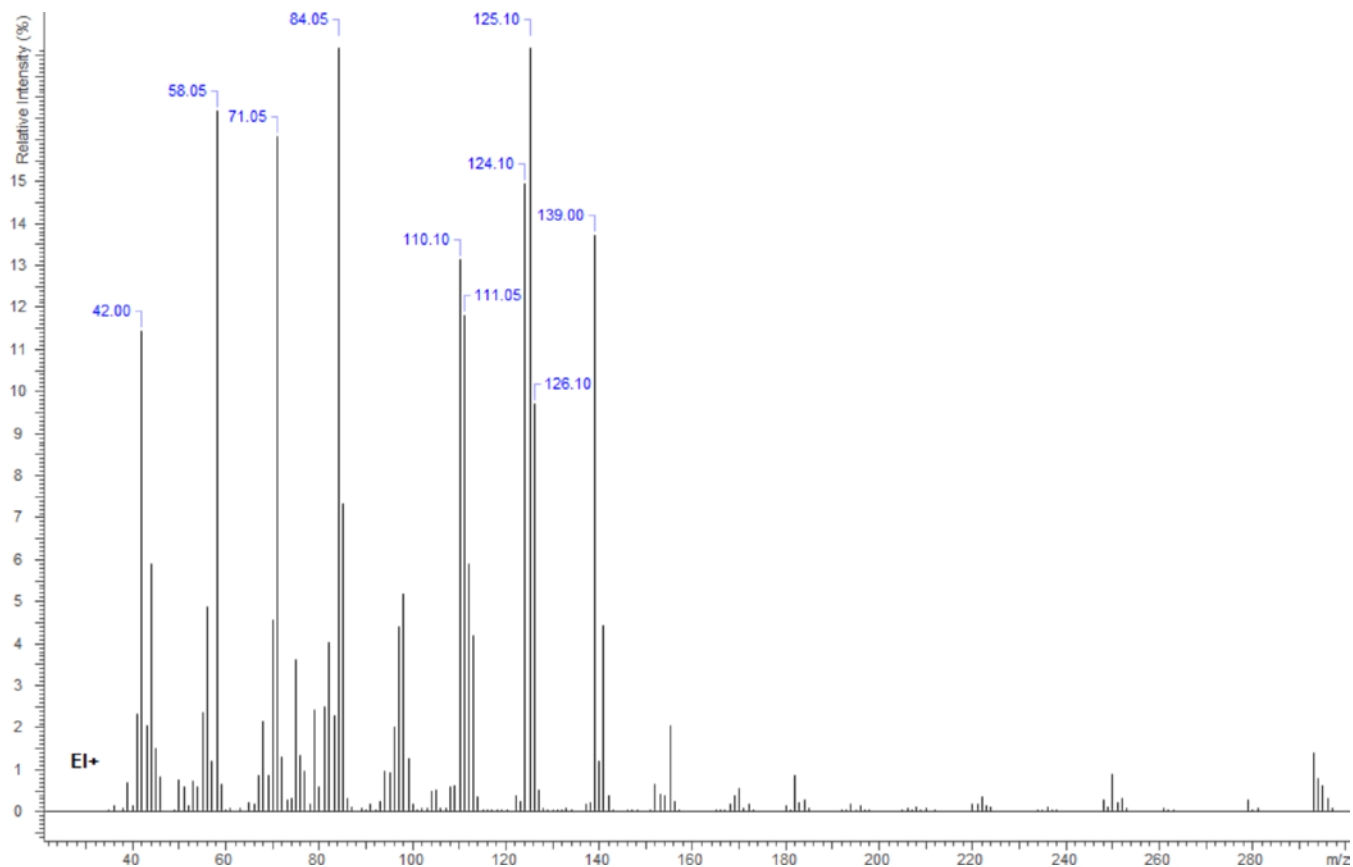
EI Mass Spectrum: U02 HCl; Lot JLK010-042-U02



## U02 hydrochloride

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

Zoomed view (84.05 and 125.10 are truncated in this view)

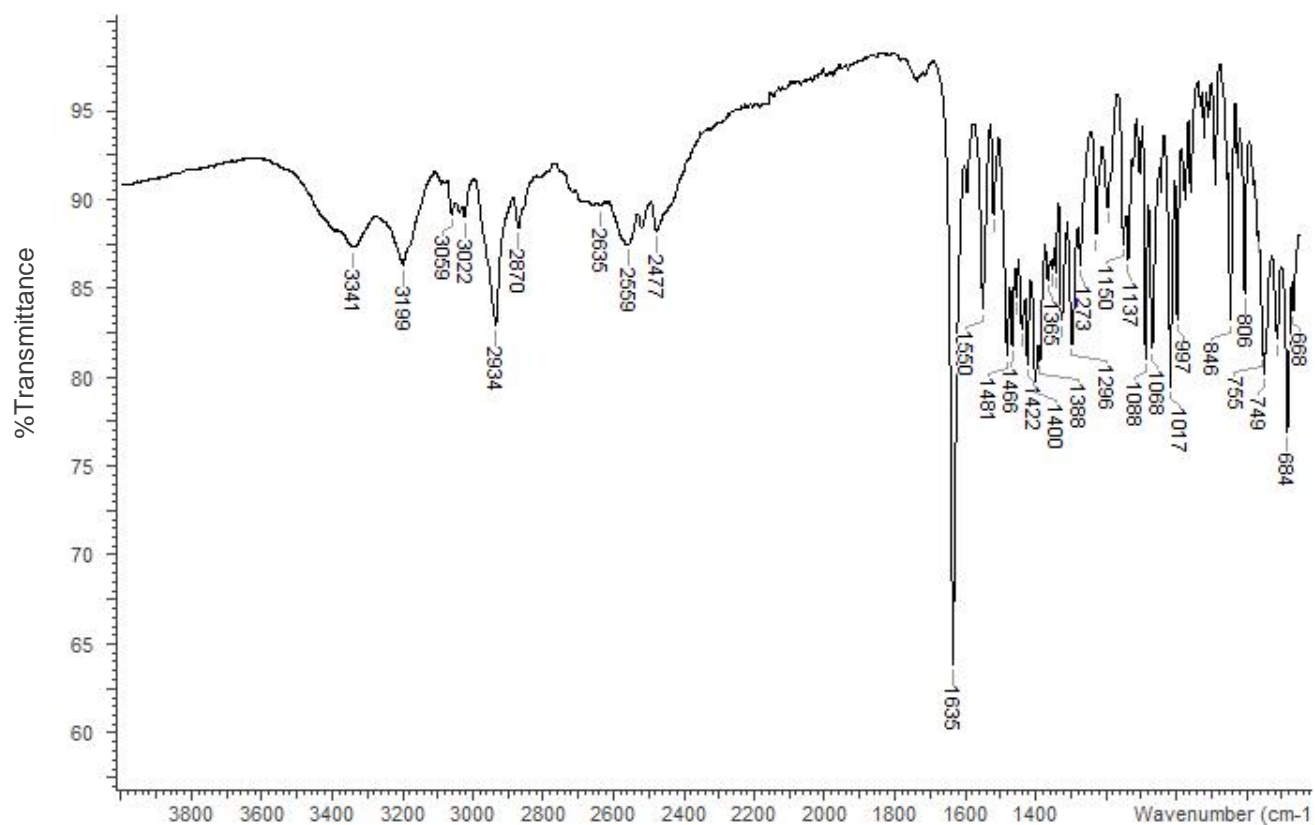


### 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with ZnSe ATR attachment (1 bounce)

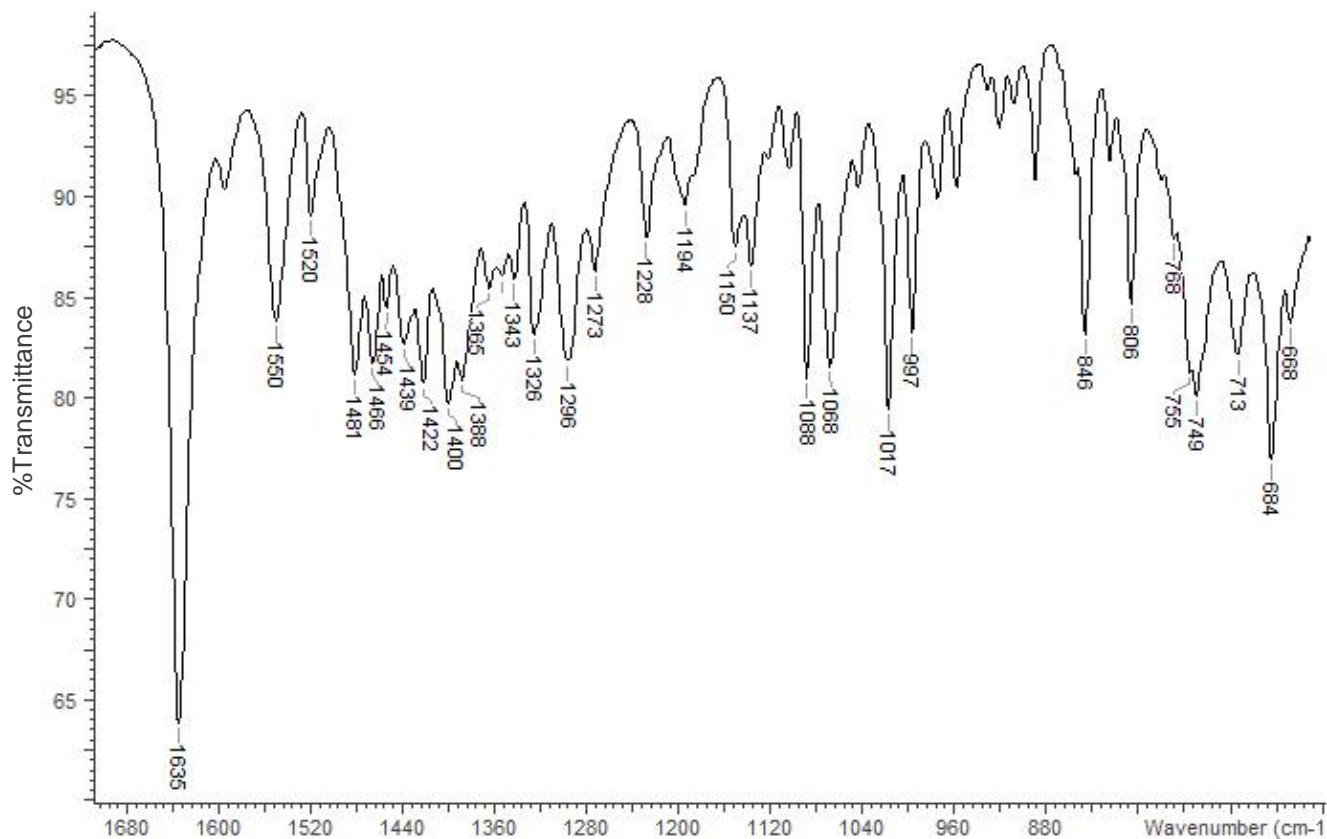
**Scan Parameters:**  
 Number of scans: 4  
 Number of background scans: 4  
 Resolution: 4 cm<sup>-1</sup>  
 Sample gain: 8  
 Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): U02 HCl; Lot JLK010-042-U02



## U02 hydrochloride

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



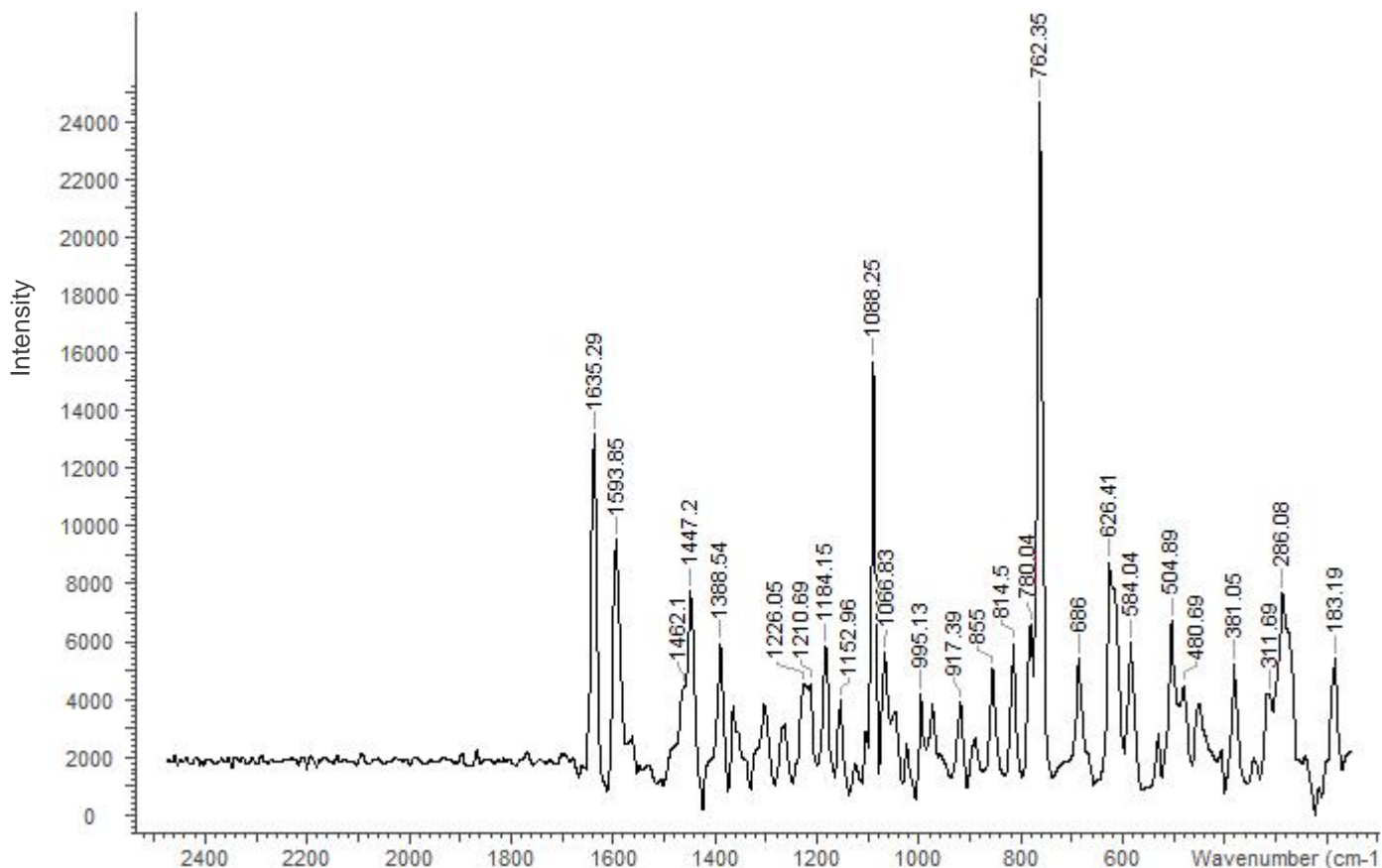
## U02 hydrochloride

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): U02 HCl; Lot JLK010-042-U02



#### 4. ADDITIONAL RESOURCES

##### ANALGESIC N-(2-AMINOCYCLOALIPHATIC)BENZAMIDES

Szmuszkovicz

US Patent 4,098, 904 Jul. 4, 1978

Example 51(v)

Benzeneacetamide amines: structurally novel non- $\mu$  opioids

J. Szmuszkovicz, and P.F. Von Voigtlander

Journal of Medicinal Chemistry 1982, 25 (10), 1125–1126

DOI: 10.1021/jm00352a005

Factors affecting binding of trans-N-[2-(methylamino)cyclohexyl]benzamides at the primary morphine receptor

B.V. Cheney, J. Szmuszkovicz, R.A. Lahti and D.A. Zichi

Journal of Medicinal Chemistry 1985, 28 (12), 1853–1864

DOI: 10.1021/jm00150a017

Single stereoisomer analogs in the U-47700 series:

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

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.