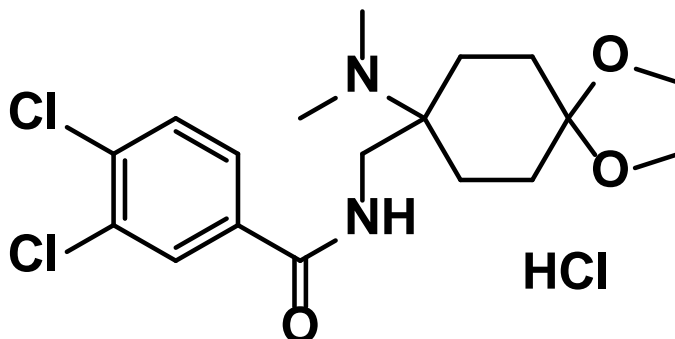


As01 hydrochloride

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



1. GENERAL INFORMATION

IUPAC Name:	8-(3,4-dichlorobenzamido)methyl-8-dimethylamino-1,4-dioxaspiro[4.5]decane; hydrochloride
CAS#:	83631-79.2 (base)
Synonyms:	As01
Source:	Synthesized Material Lot# JLK008-107-As01
Appearance:	White Crystals
UV_{max} (nm):	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
HCl	C ₁₈ H ₂₄ Cl ₂ N ₂ O ₃ ·HCl	423.76	204.9 ± 1.00
base	C ₁₈ H ₂₄ Cl ₂ N ₂ O ₃	387.31	Not determined

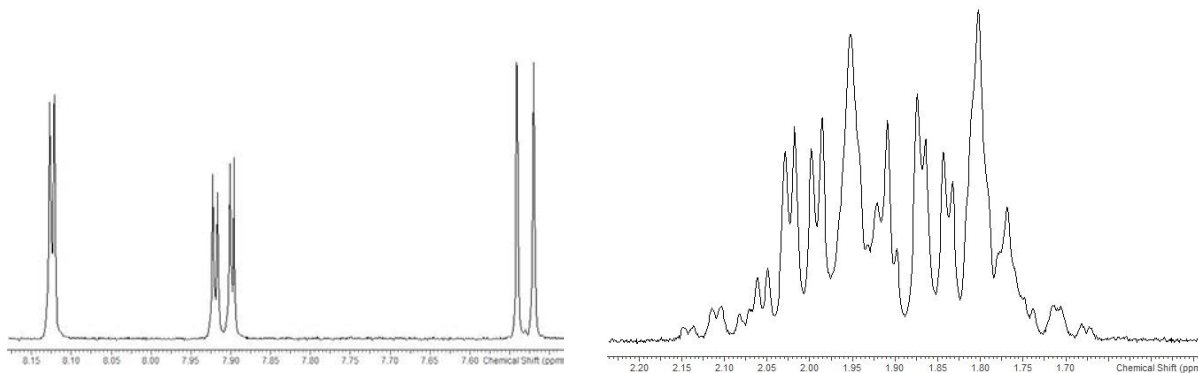
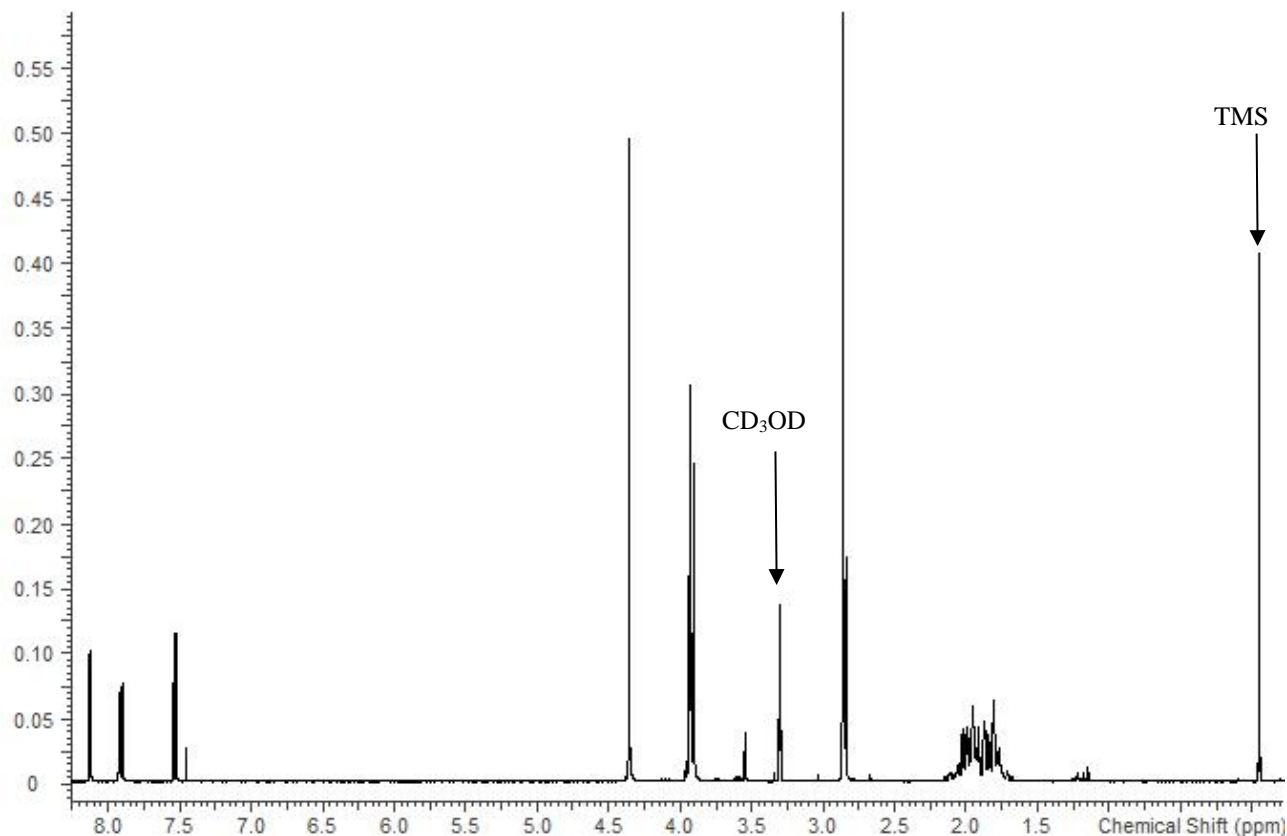
3. QUALITATIVE DATA

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: As01 HCl; Lot JLK008-107-As01; CDCl₃:CD₃OD (1:5) + TMS; 400 MHz



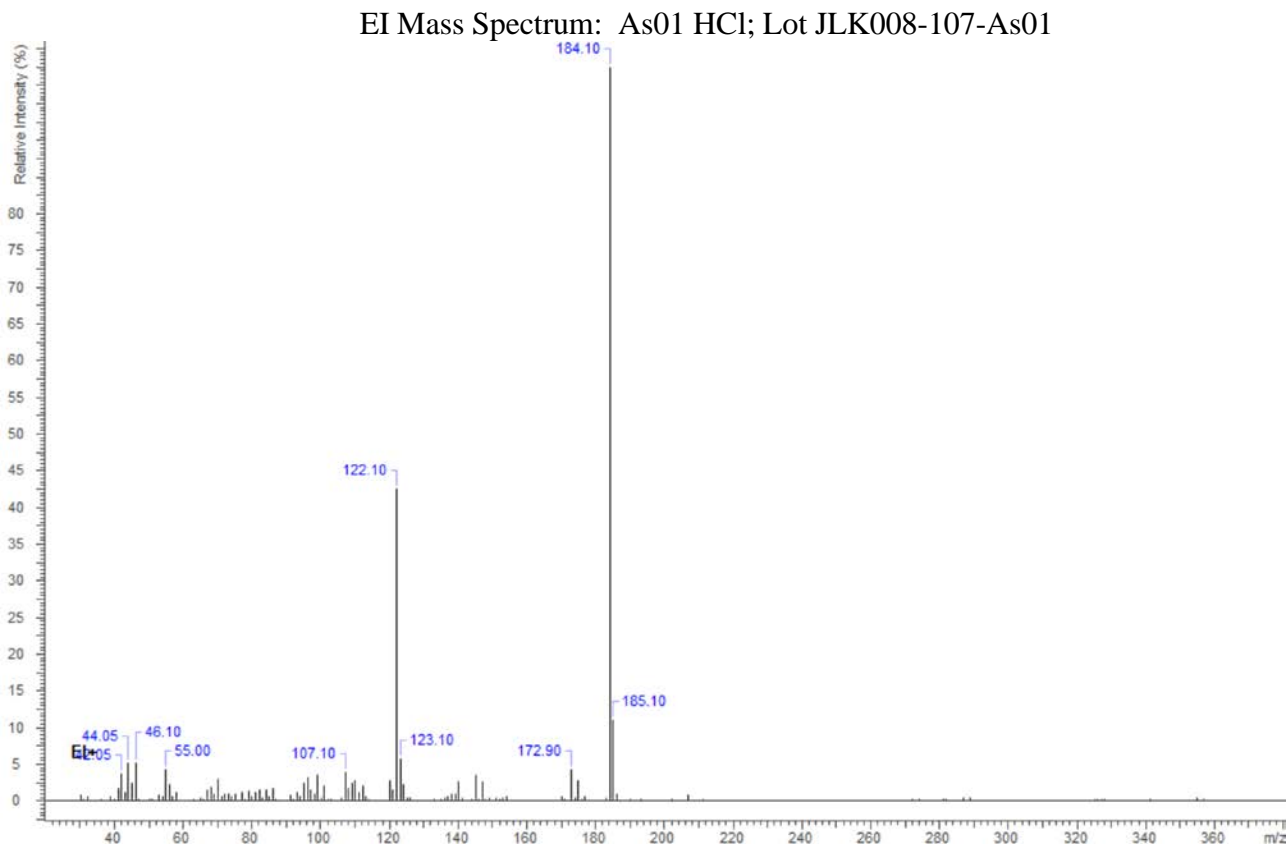
As01 hydrochloride

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

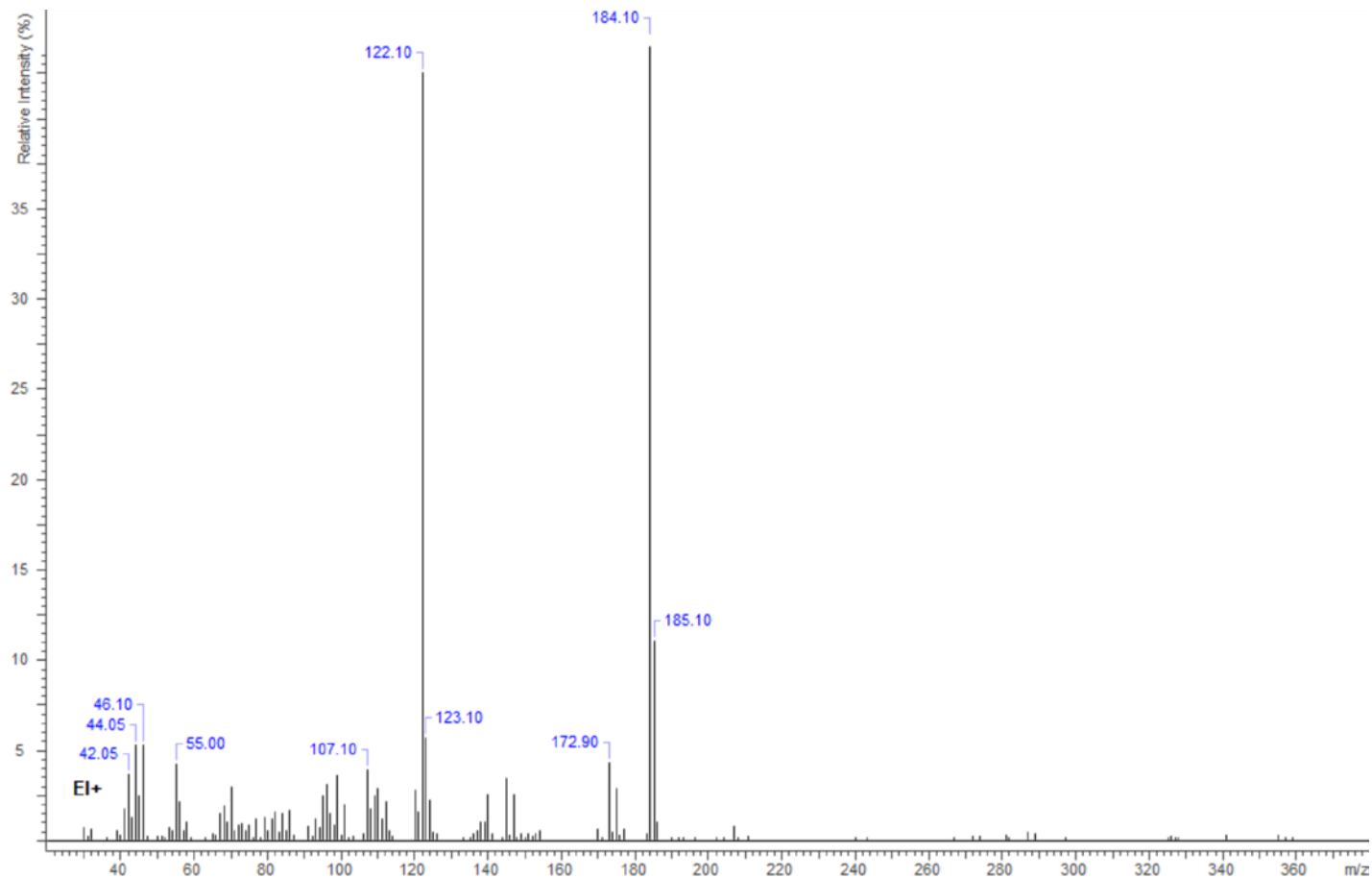
Instrument: Shimadzu gas chromatograph operated in split mode with MS detector
Column: Rtx5MS (a DB-5 equivalent); 30m x 0.25 mm x 0.25 μ m
Carrier Gas: Helium at 1 mL/min
Temperatures: Injector: 280°C
MSD transfer line: 280°C
MS Source: 200°C
Oven program:
1) 90°C initial temperature for 2.0 min
2) 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: 19.92 min



As01 hydrochloride

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Zoomed view (184.10 is 100% relative intensity and truncated in this view)

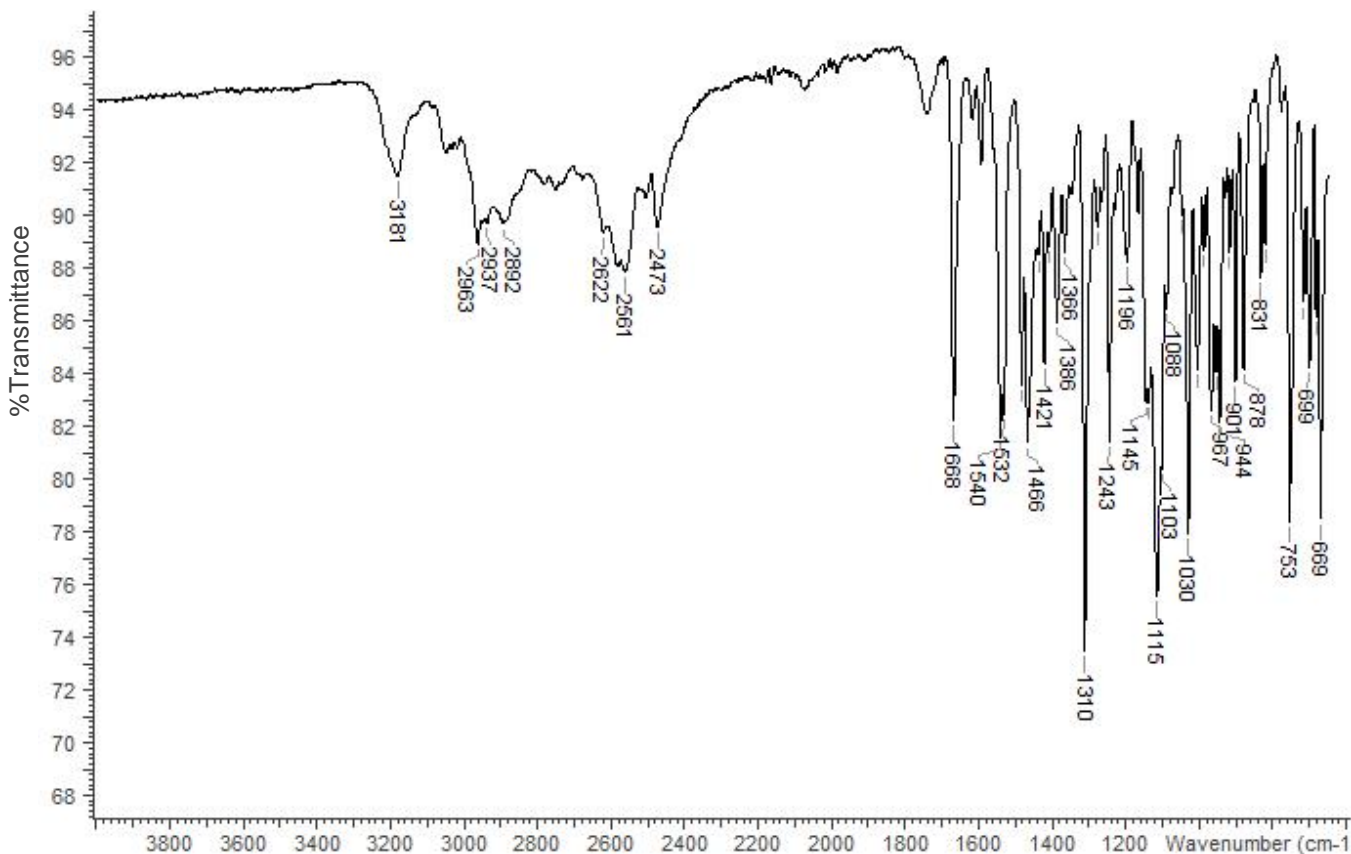


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with ZnSe ATR attachment (1 bounce)

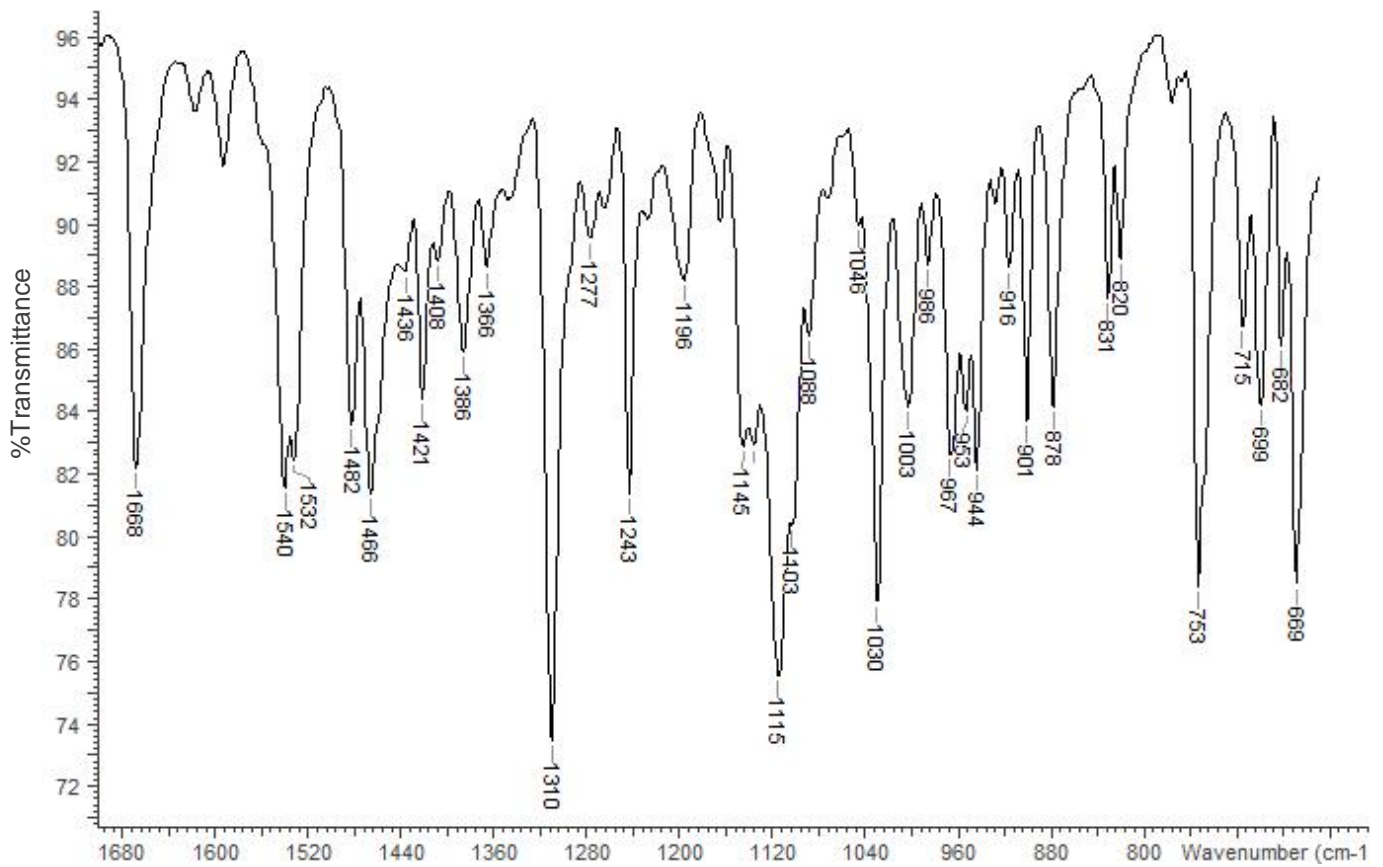
Scan Parameters: Number of scans: 4
 Number of background scans: 4
 Resolution: 4 cm⁻¹
 Sample gain: 8
 Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): As01 HCl; Lot JLK008-107-As01



As01 hydrochloride

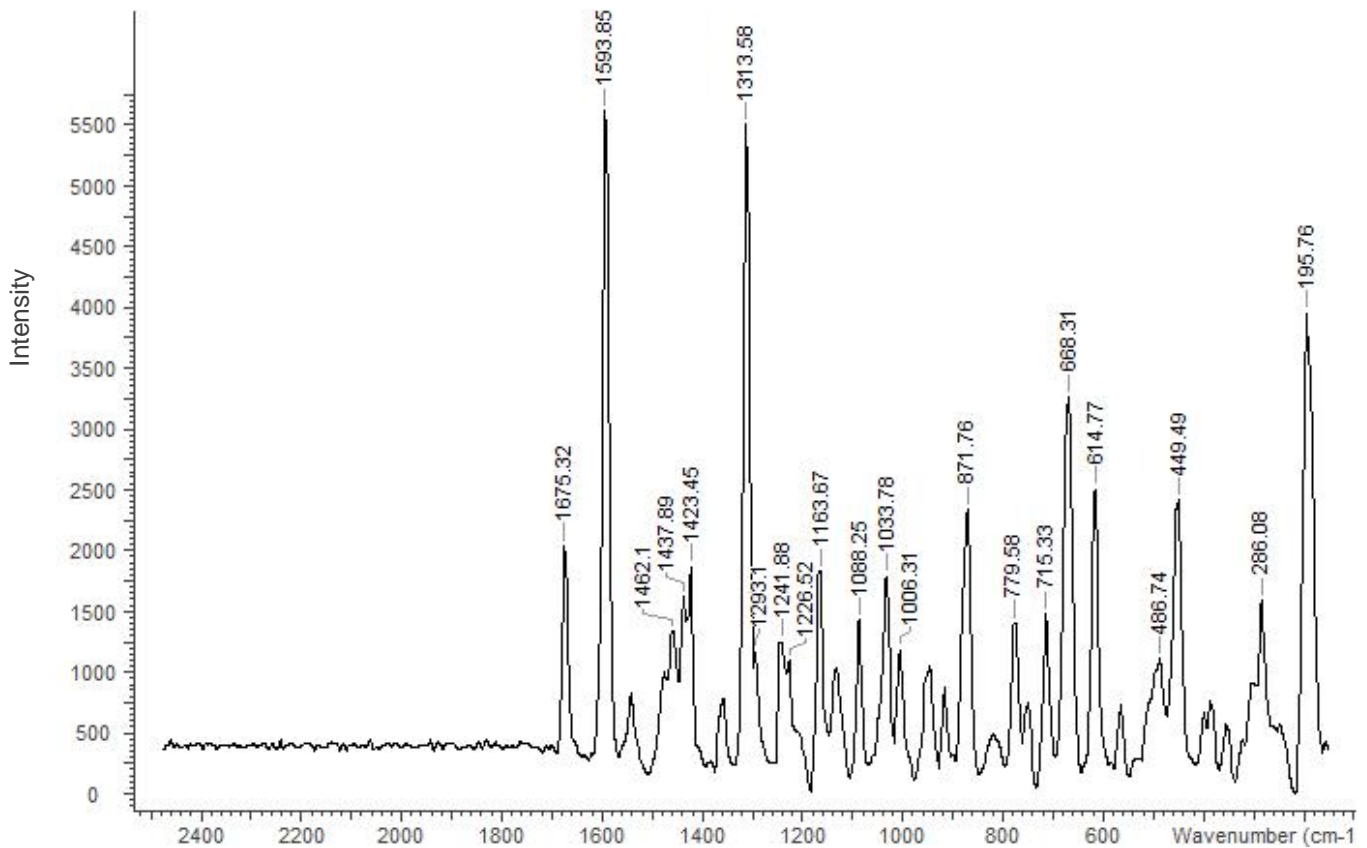
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material



3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): As01 HCl; Lot JLK008-107-As01



4. ADDITIONAL RESOURCES

BENZAMIDE DERIVATIVE ANALGESICS, Daniel Lednicer
US Patent 4,346,101 Aug. 24, 1982 Example 1

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.