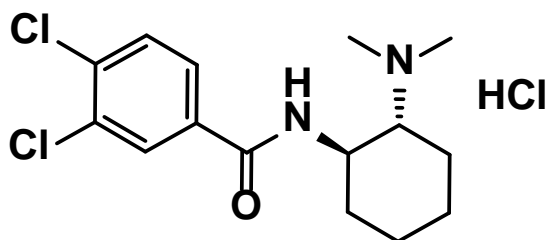


Udes01 hydrochloride

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



1. GENERAL INFORMATION

IUPAC Name:	N-((1 <i>R</i> ,2 <i>R</i>)-2-(dimethylamino)cyclohexyl)-3,4-dichlorobenzamide; hydrochloride
CAS#:	67579-13-9 (base)
Synonyms:	Udes01
Source:	Synthesized Material Lot# JLK010-044-Udes01
Appearance:	light brown solid (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 ₁₅ H ₂₀ Cl ₂ N ₂ O·HCl	351.70	114.7 ± 1.00
Base	C ₁₅ H ₂₀ Cl ₂ N ₂ O	315.24	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.

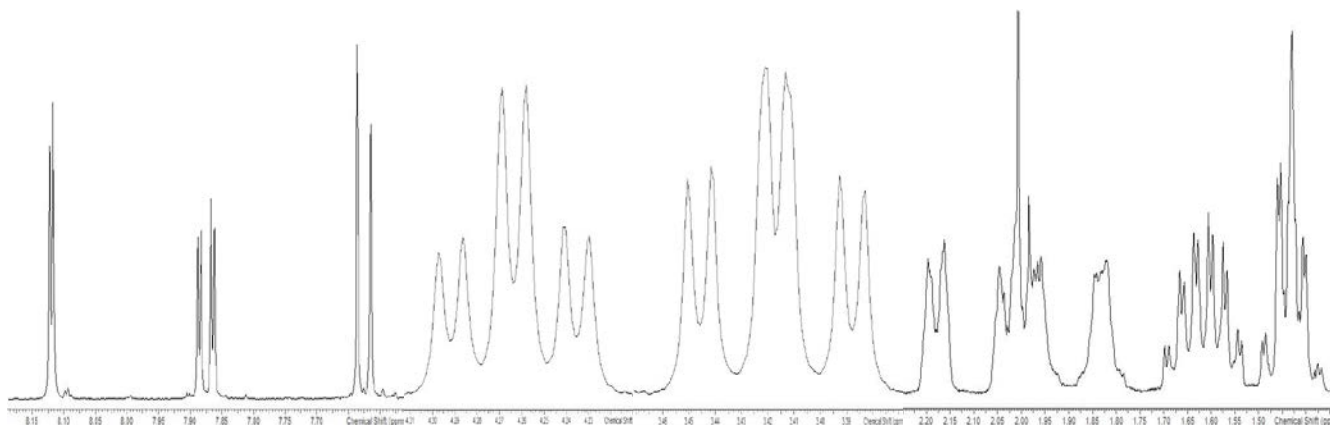
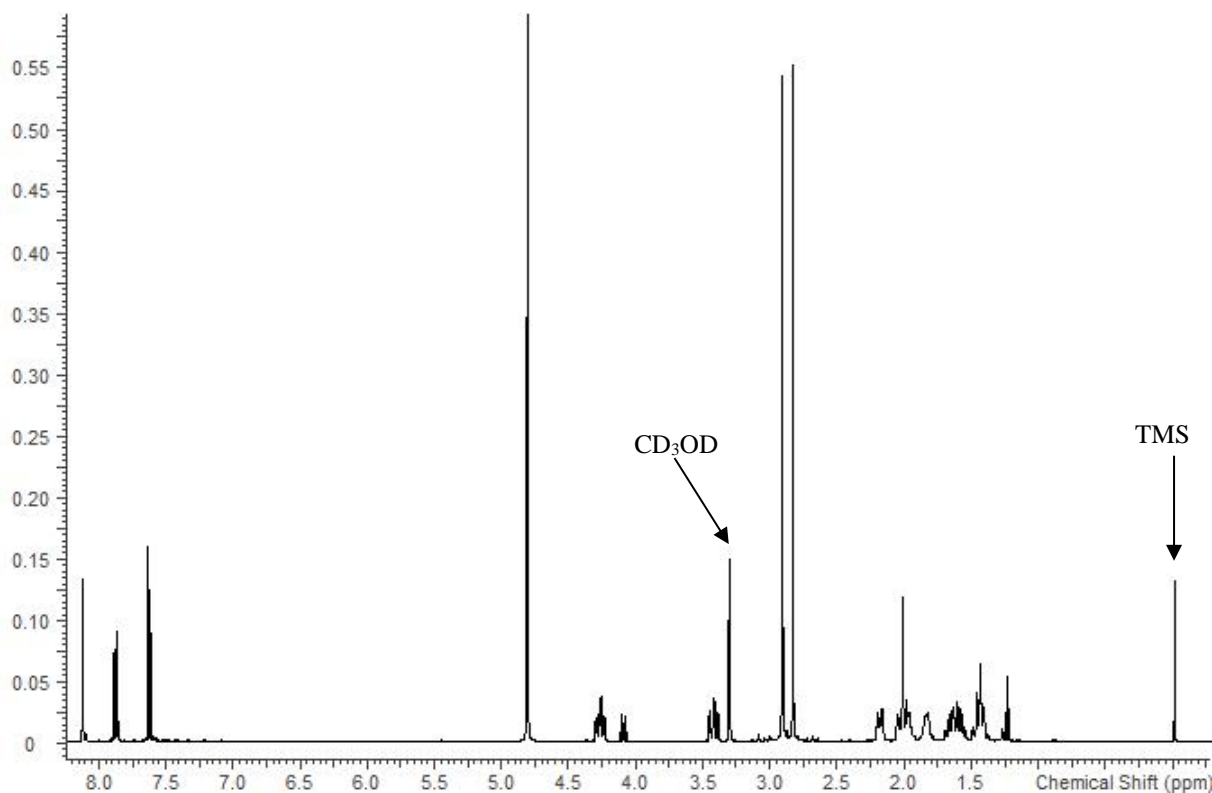
Instrument: 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 30 seconds

¹H NMR: Udes01 HCl; Lot JLK010-044-Udes01; CDCl₃:CD₃OD (1:5) + TMS; 400 MHz

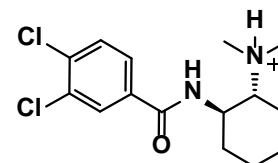
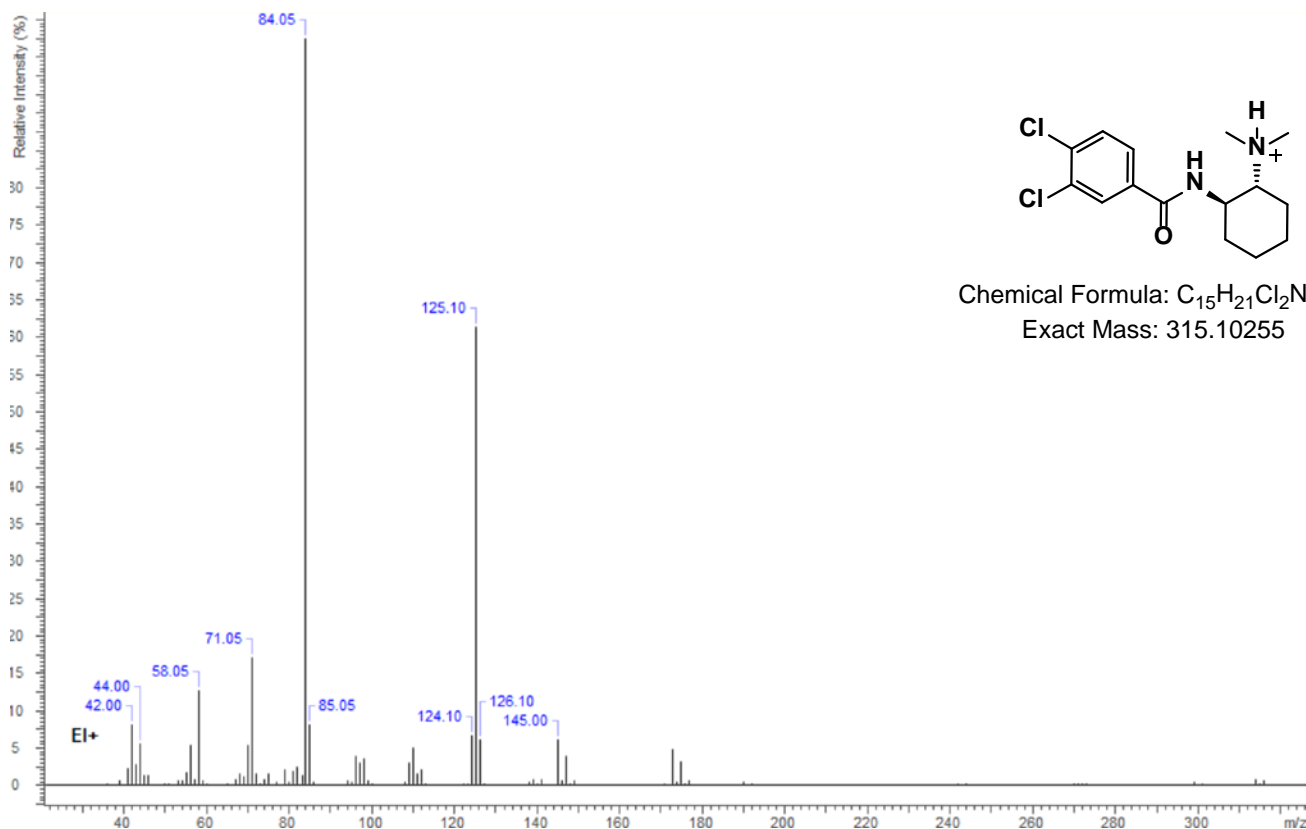


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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 Acquisition mode: scan
Retention Time:	15.84 min

EI Mass Spectrum: Udes01 HCl; Lot JLK010-044-Udes01

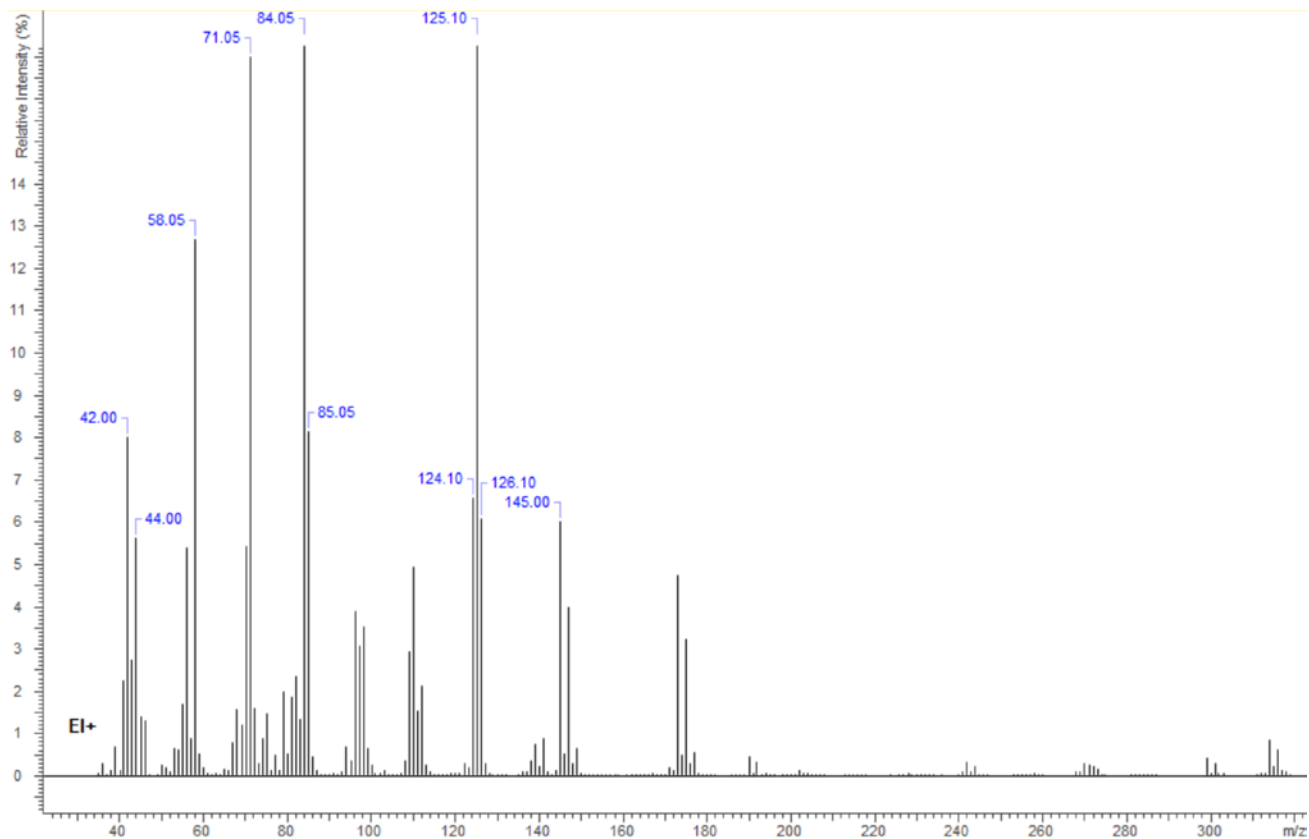


Chemical Formula: C₁₅H₂₁Cl₂N₂O⁺
Exact Mass: 315.10255

Udes01 hydrochloride

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

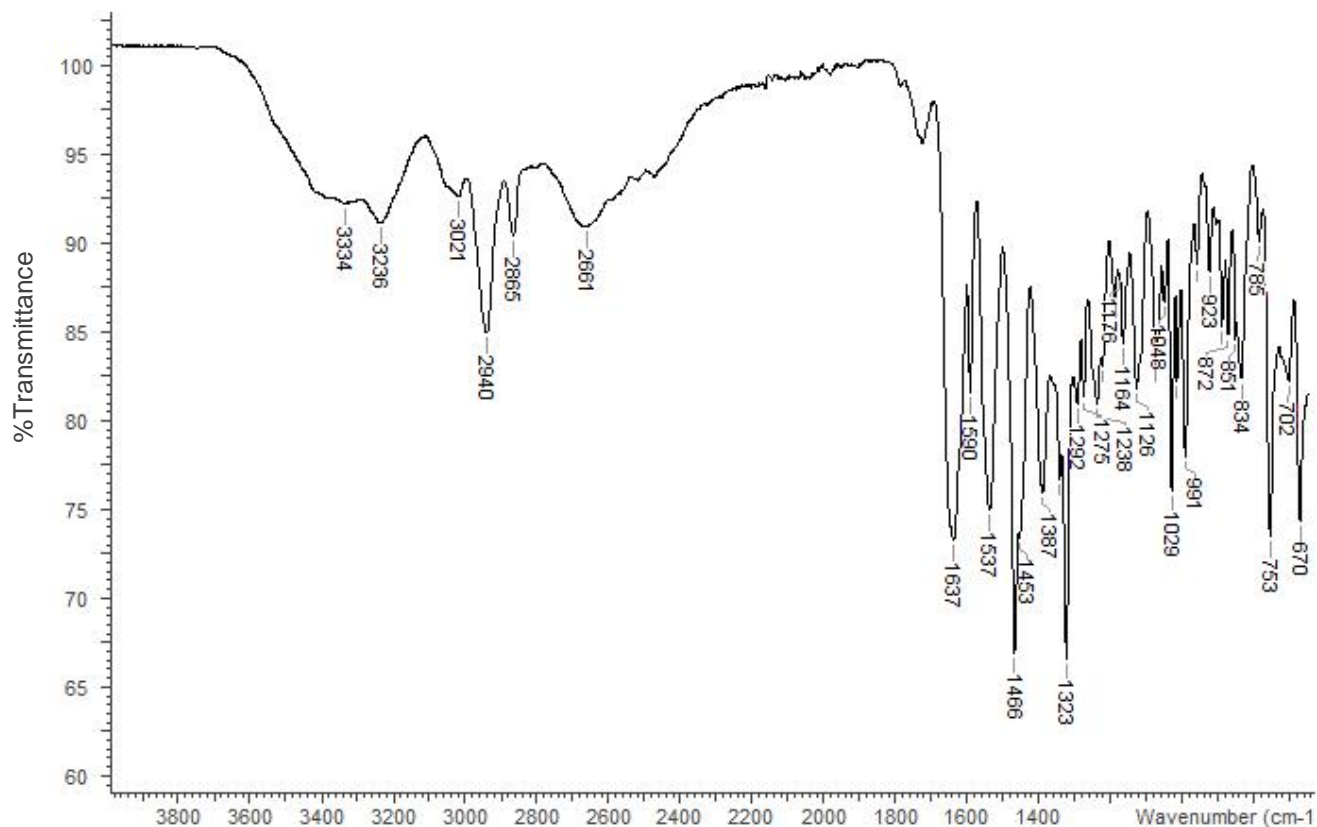
Zoomed view (84.05 and 125.10 are truncated in this view)



3.3 INFRARED SPECTROSCOPY (FTIR)

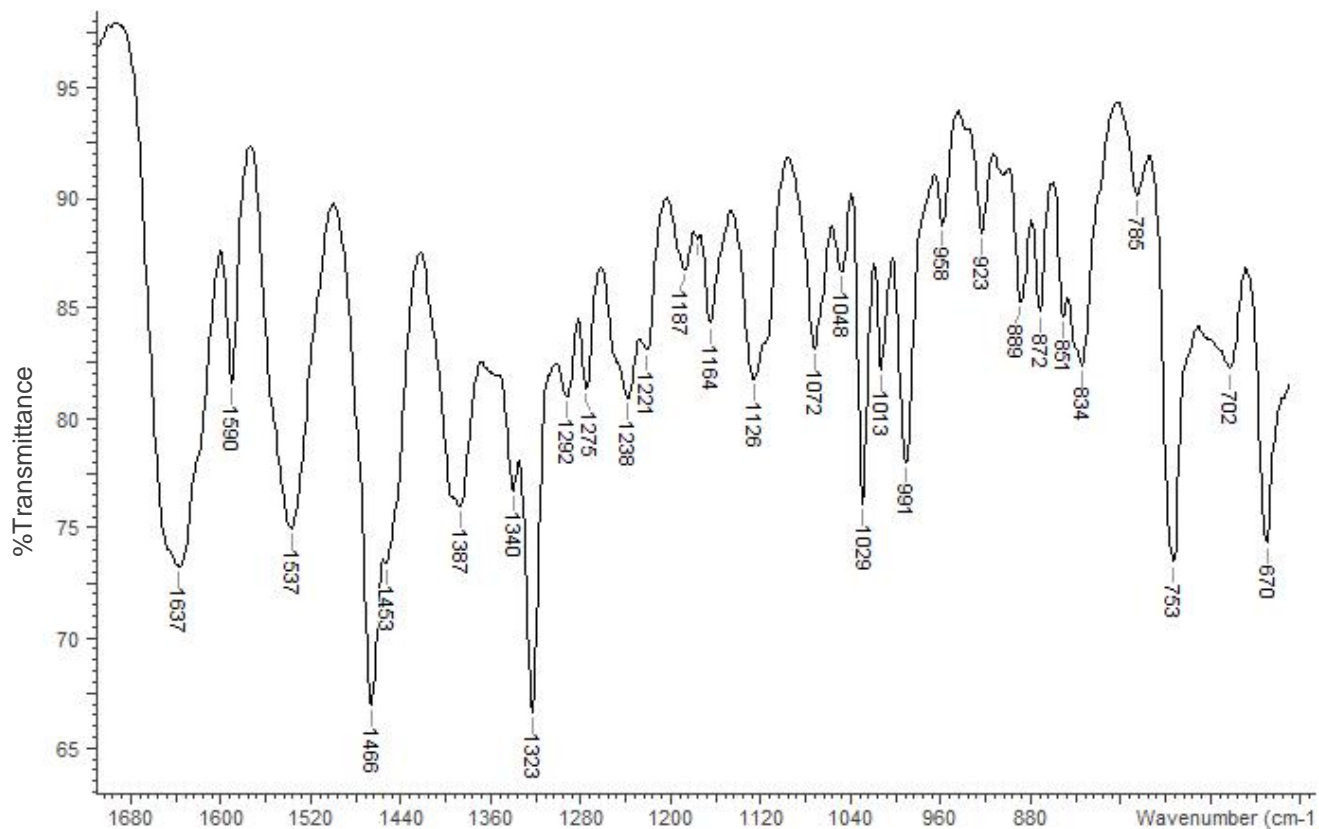
Instrument: FTIR with ZnSe ATR attachment (1 bounce)
Scan Parameters: Number of scans: 4
 Number of background scans: 4
 Resolution: 4 cm⁻¹
 Sample gain: 8
 Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): Udes01 HCl; Lot JLK010-044-Udes01



Udes01 hydrochloride

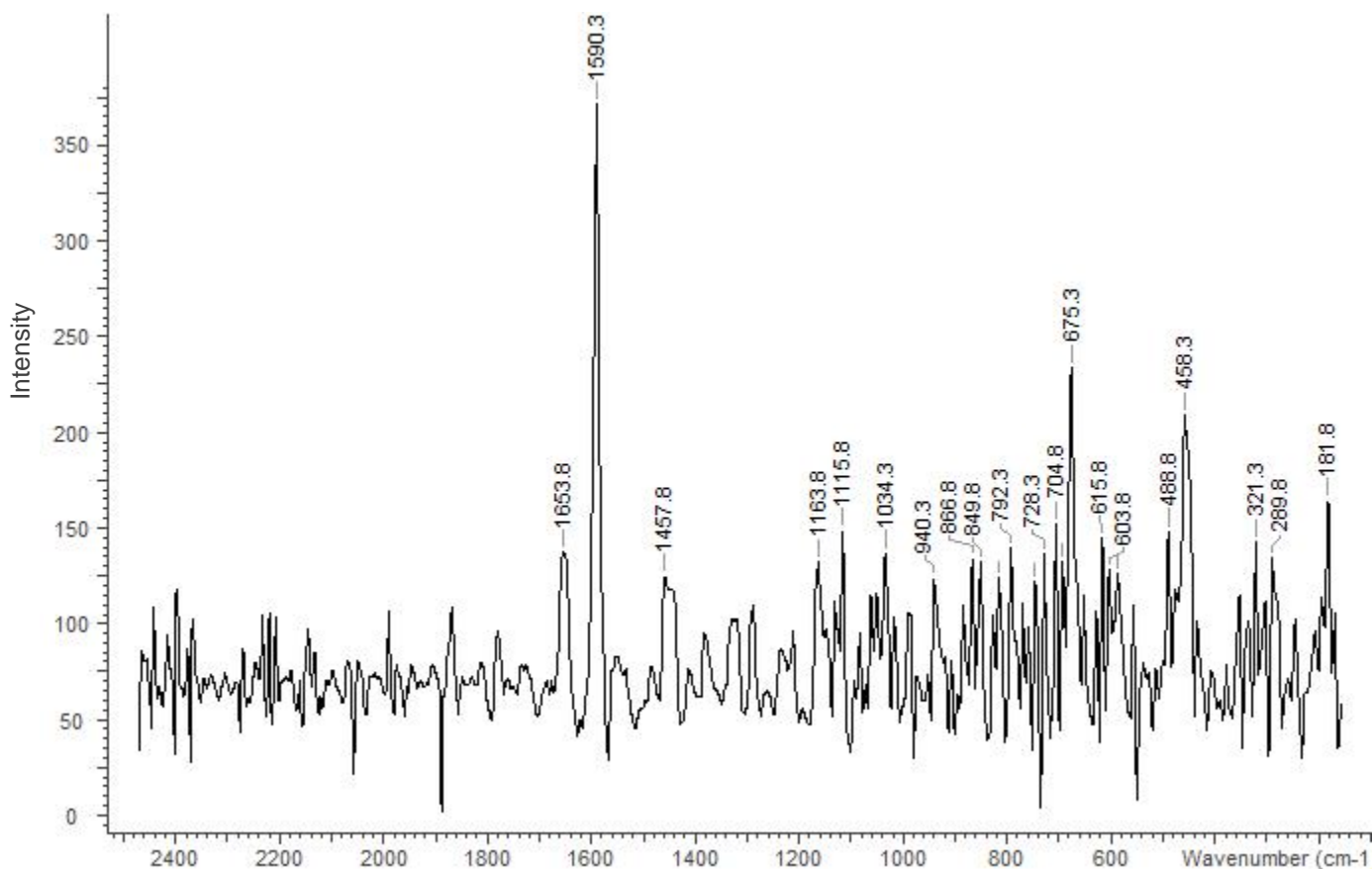
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material



3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): Udes01 HCl; Lot JLK010-044-Udes01



4. ADDITIONAL RESOURCES

ANALGESIC N-(2-AMINOCYCLOALIPHATIC)BENZAMIDES

Szmuszkovicz

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

Example 2

Benzeneacetamide amines: structurally novel non- μ 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 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.