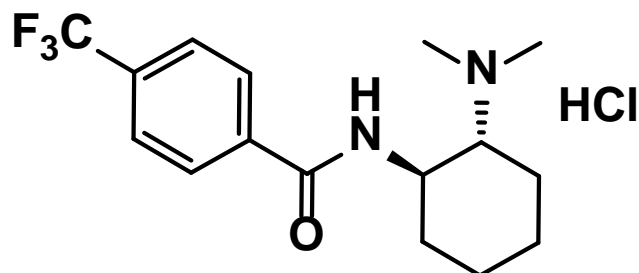


Udes04 hydrochloride

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)-4-thi fluoromethylbenzamide; hydrochloride
CAS#:	7579-14-0 (base)
Synonyms:	Udes04
Source:	Synthesized Material Lot# JLK010-044-Udes04
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 ₁₆ H ₂₁ F ₃ N ₂ O.HCl	350.81	105.8 ± 0.90
Base	C ₁₆ H ₂₁ F ₃ N ₂ O	314.35	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.

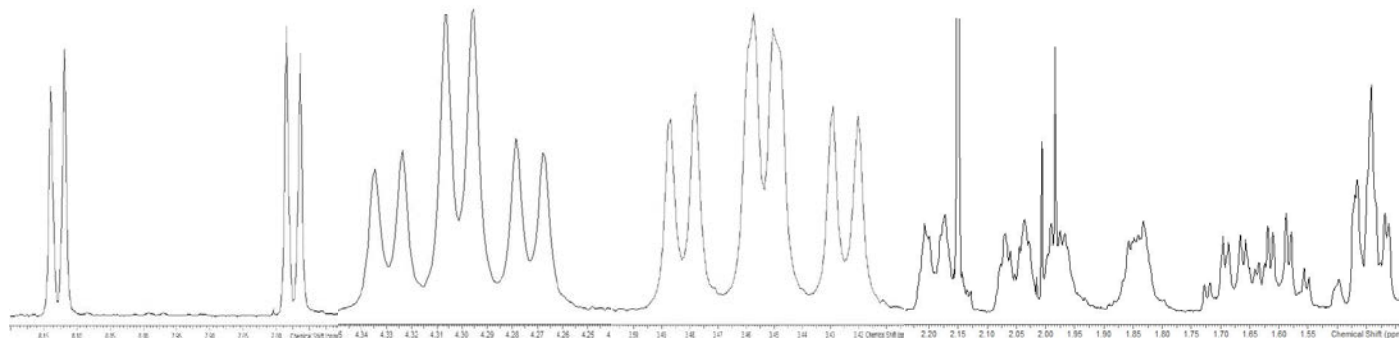
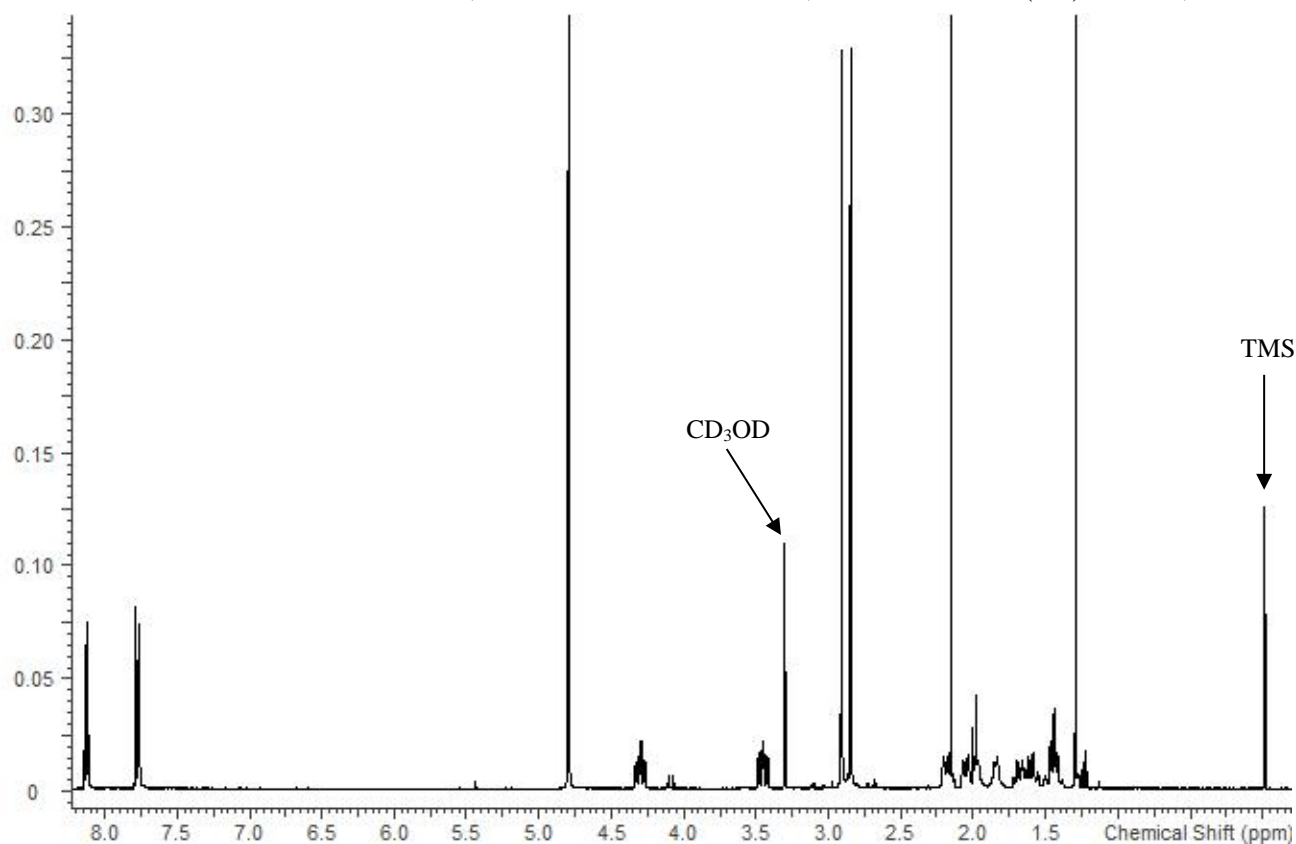
Instrument: 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 30 seconds

¹H NMR: Udes04 HCl; Lot JLK010-044-Udes04; CDCl₃:CD₃OD (1:5) + TMS; 400 MHz

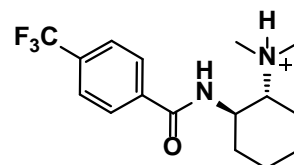
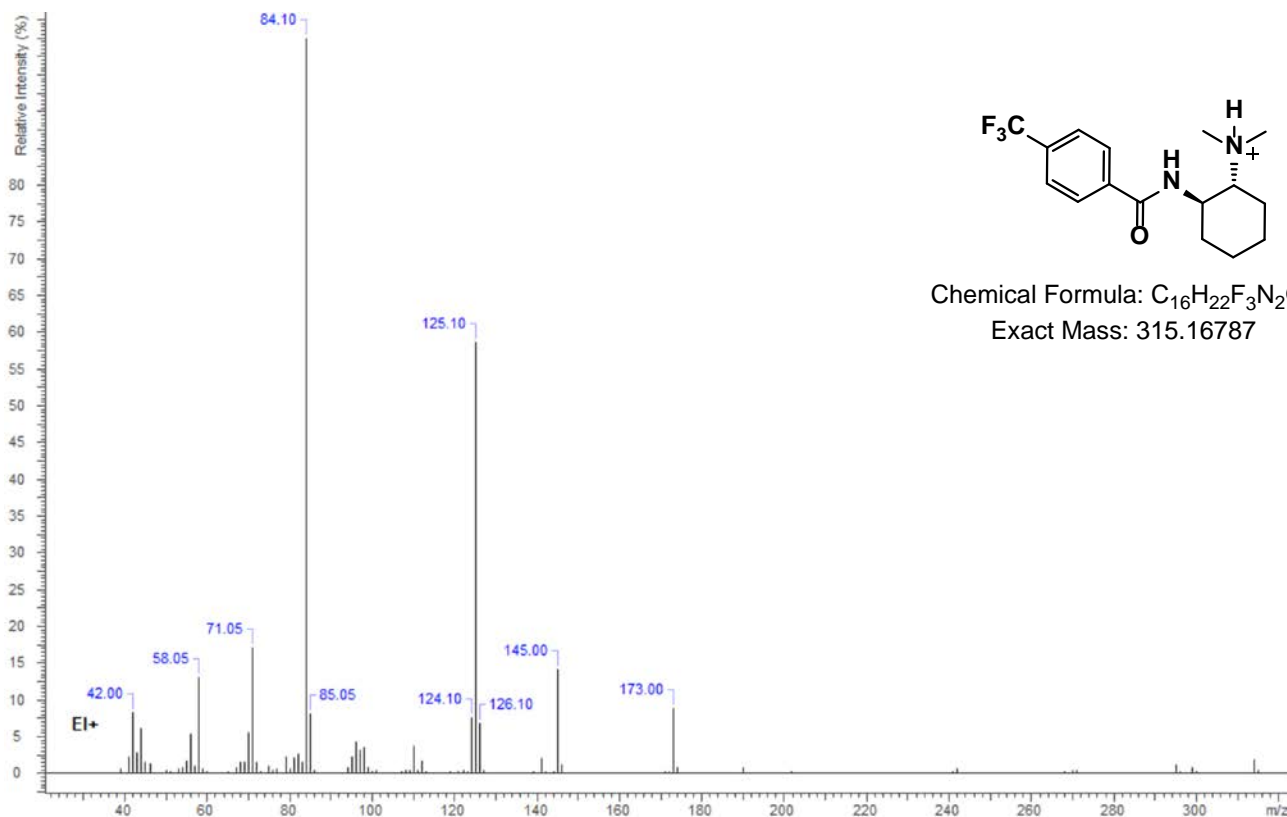


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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:	13.02 min

EI Mass Spectrum: Udes04 HCl; Lot JLK010-044-Udes04

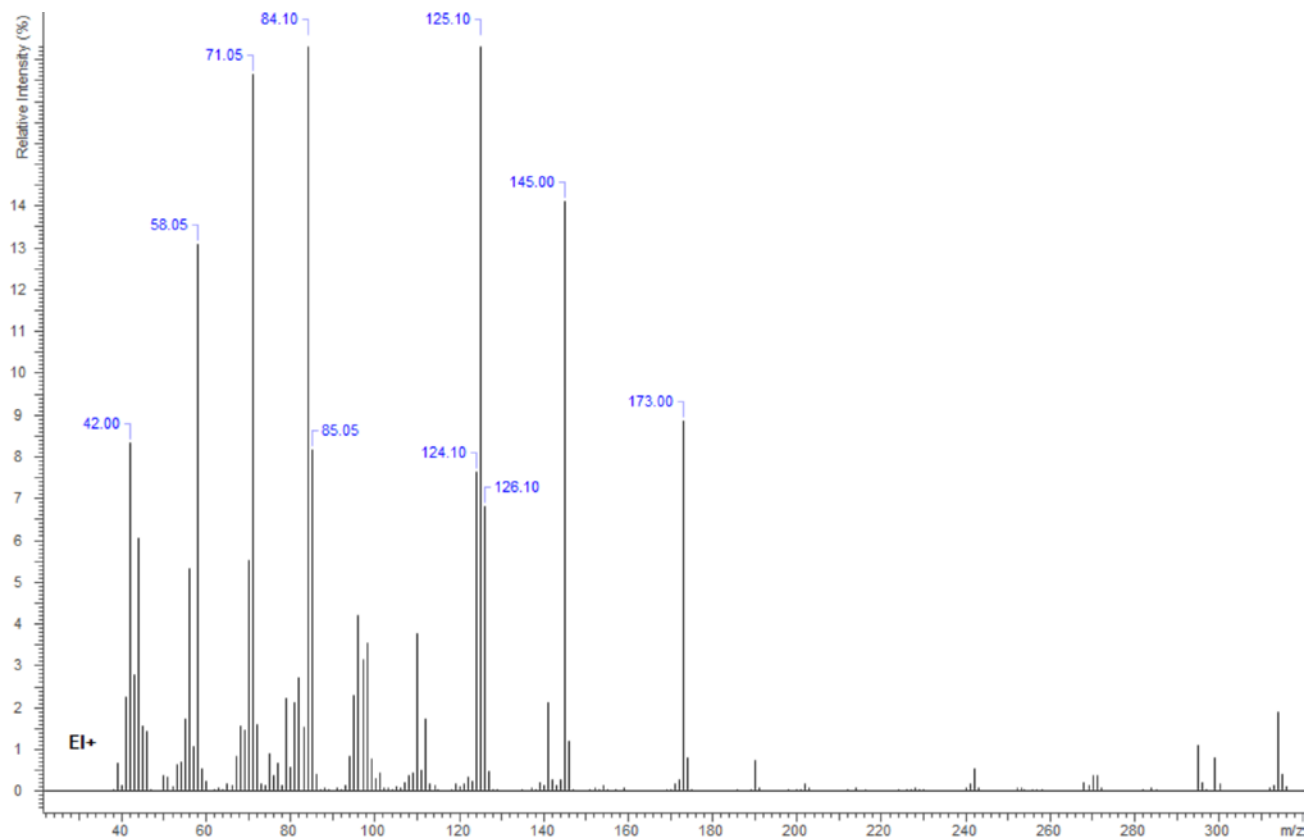


Chemical Formula: C₁₆H₂₂F₃N₂O⁺
Exact Mass: 315.16787

Udes04 hydrochloride

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Zoomed view (84.10 and 125.10 are truncated in this view)

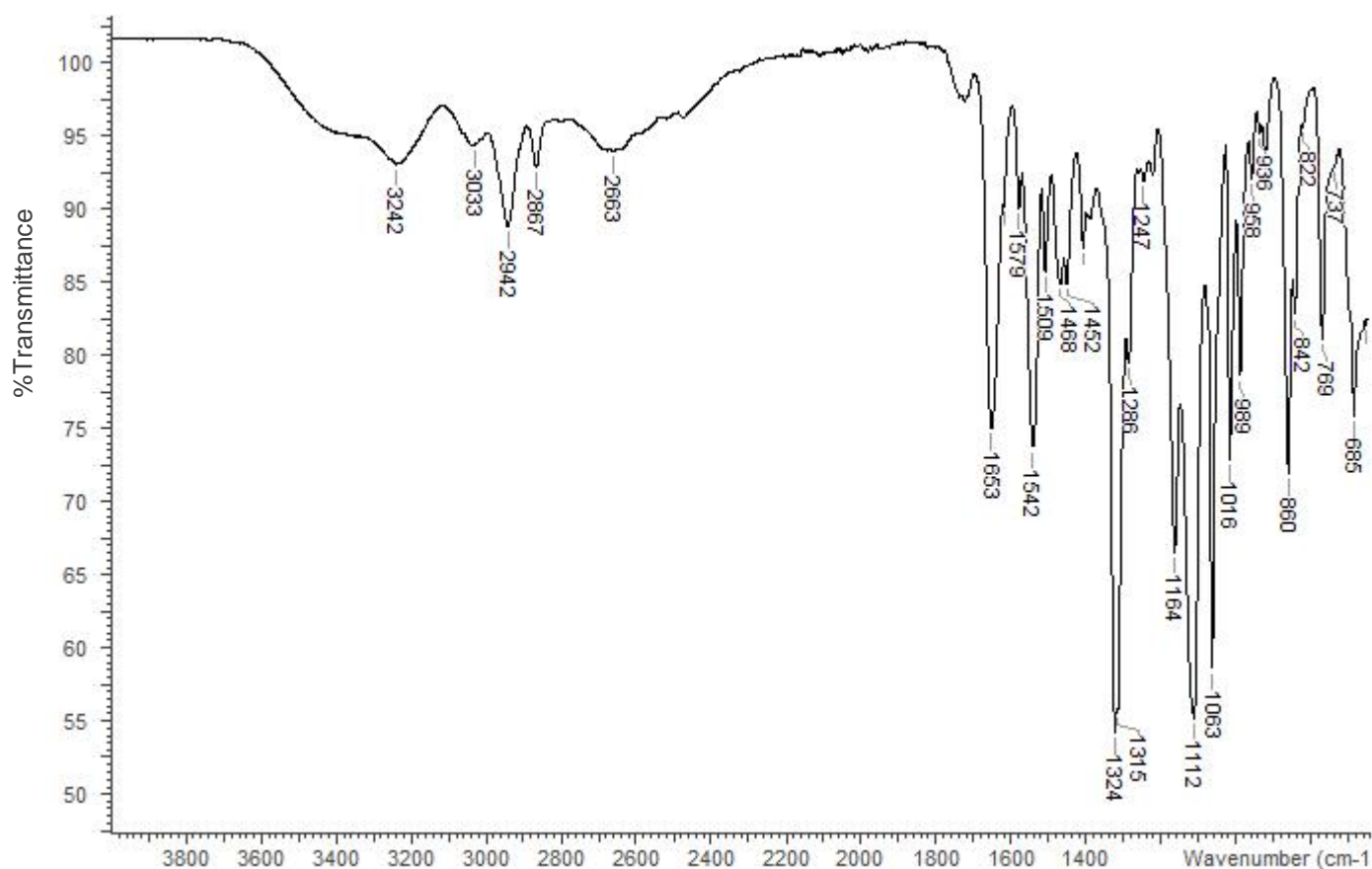


3.3 INFRARED SPECTROSCOPY (TIR)

Instrument: FTIR with ZnSe ATR attachment (1 bounce)

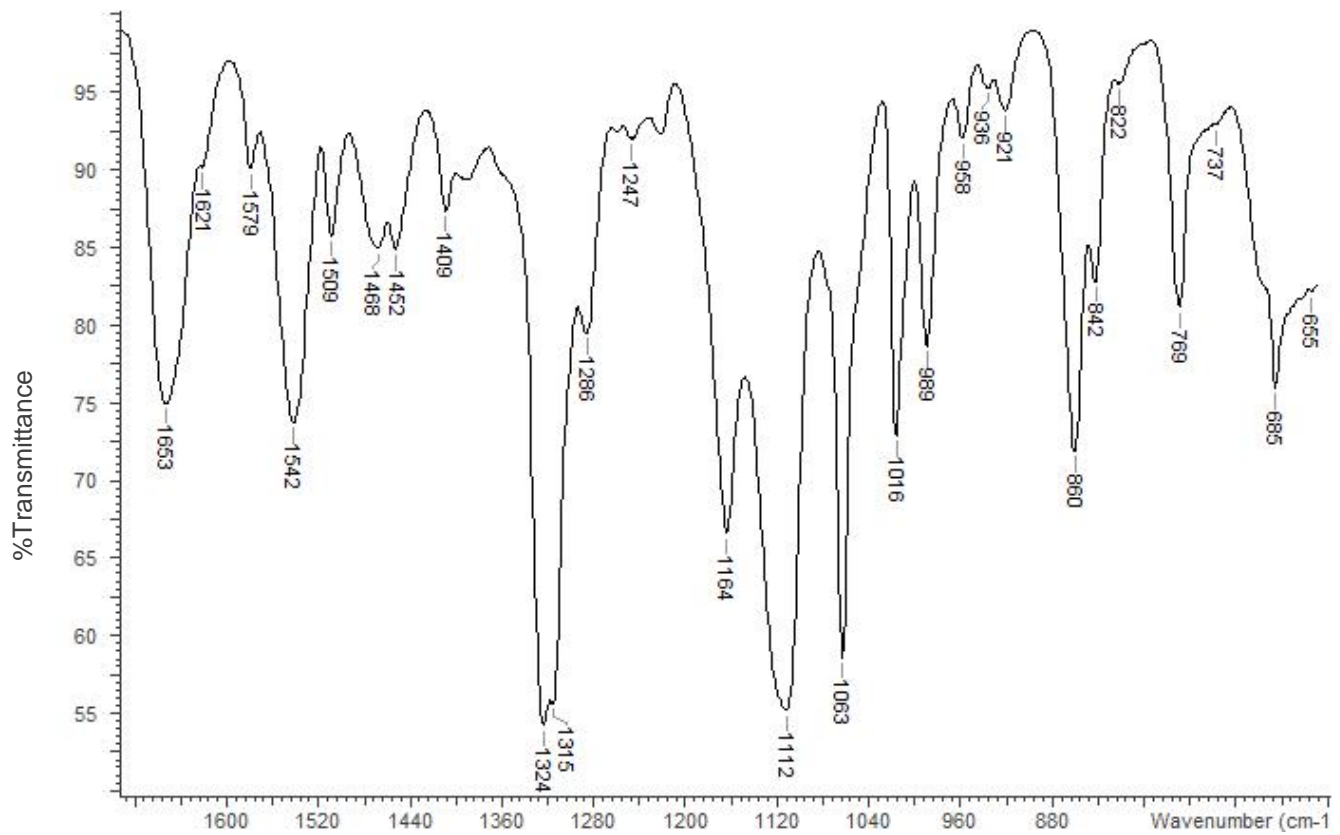
Scan Parameters:
 Number of scans: 4
 Number of background scans: 4
 Resolution: 4 cm⁻¹
 Sample gain: 8
 Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): Udes04 HCl; Lot JLK010-044-Udes04



Udes04 hydrochloride

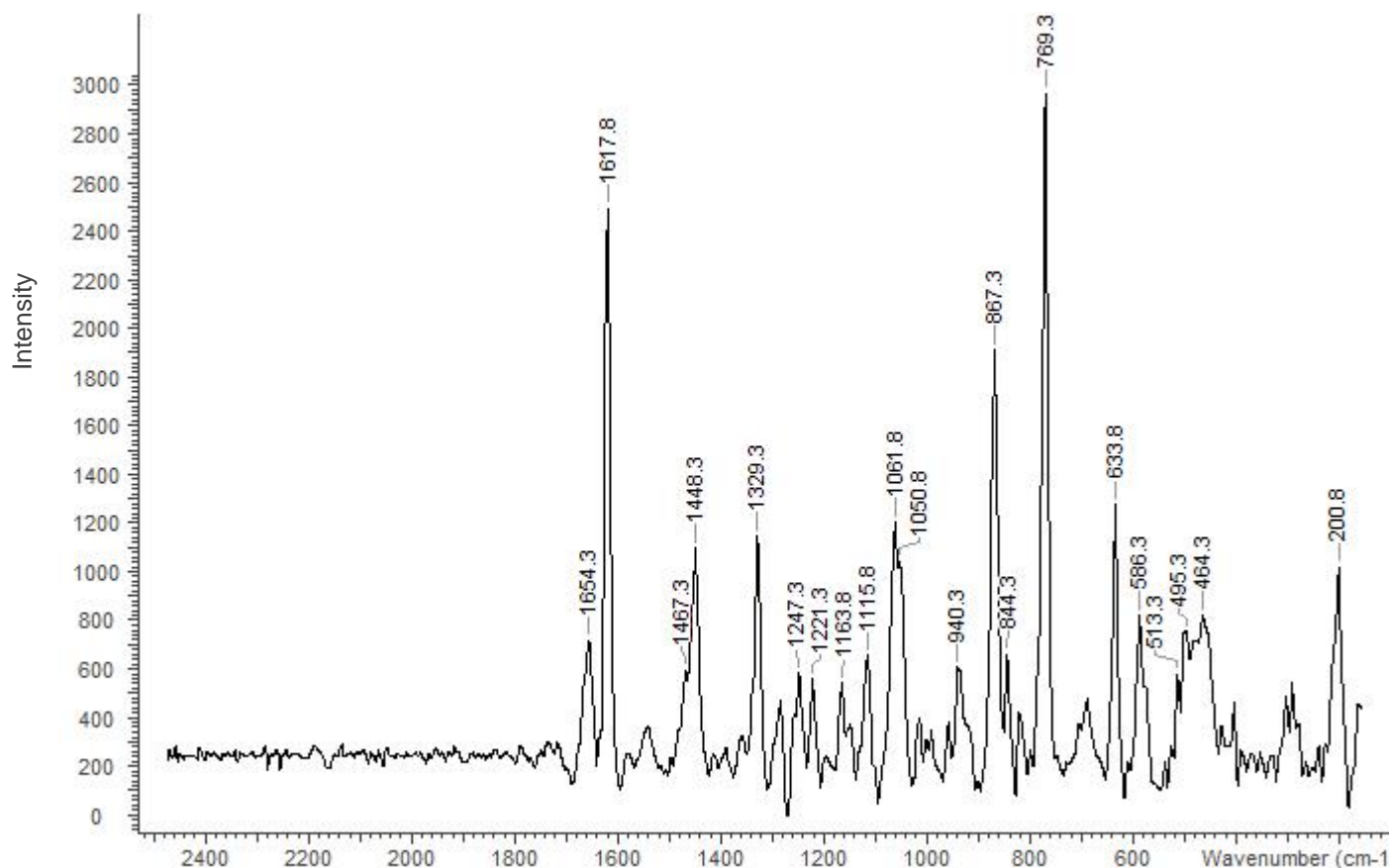
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material



3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): Udes04 HCl; Lot JLK010-044-Udes04



4. ADDITIONAL RESOURCES

ANALGESIC N-(2-AMINOCYCLOALIPHATIC)BENZAMIDES

Szmuszkovicz

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

Example 3

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

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