

1. GENERAL INFORMATION

IUPAC Name: N-((1R,2R)-2-(dimethylamino)cyclohexyl)-4-fluoro-N-methylbenzamide)

CAS#: N/A

Synonyms: U03

Source: Synthesized Material Lot# JLK008-133-U03

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)
Base	C ₁₆ H ₂₃ FN ₂ O	279.19	74.1 ± 0.10

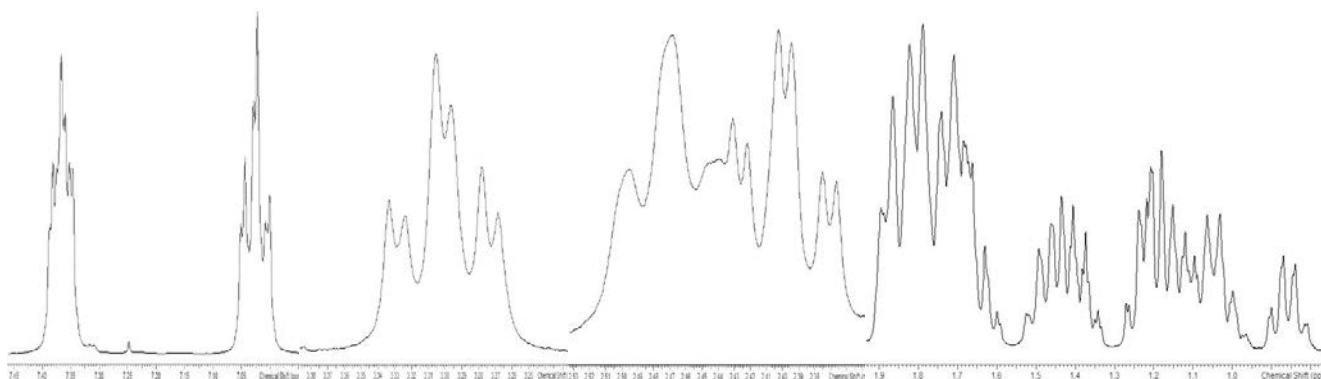
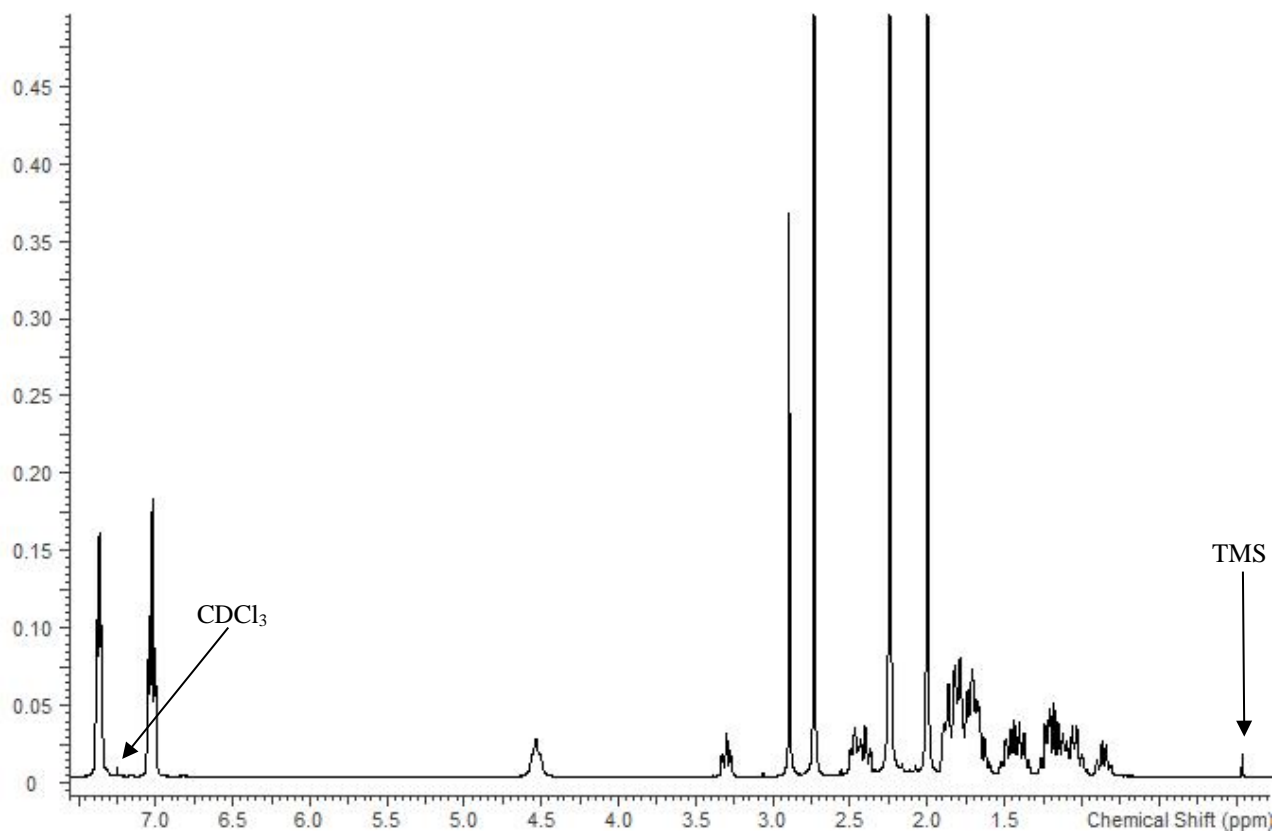
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterated chloroform (CDCl₃) + 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: U03; Lot JLK008-133-U03; CDCl₃ + TMS; 400 MHz

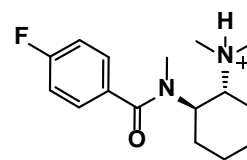
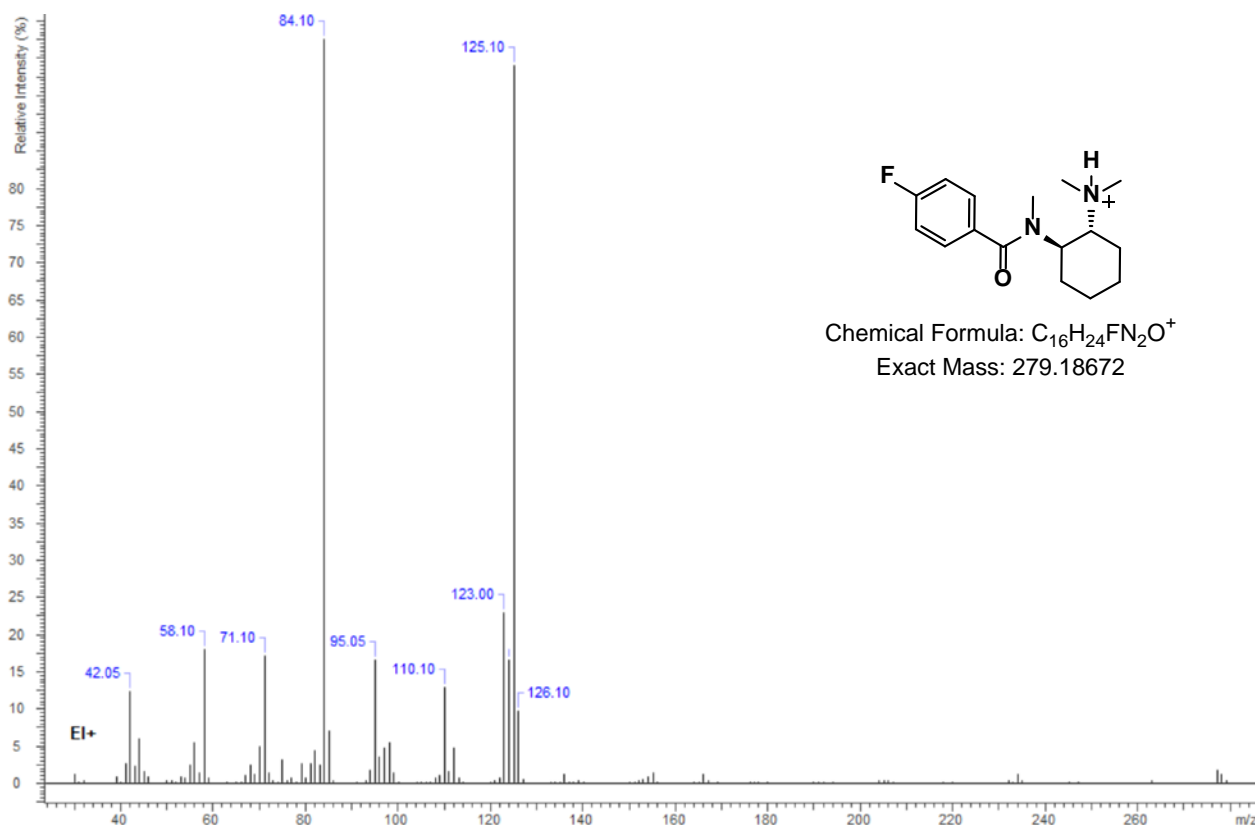


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

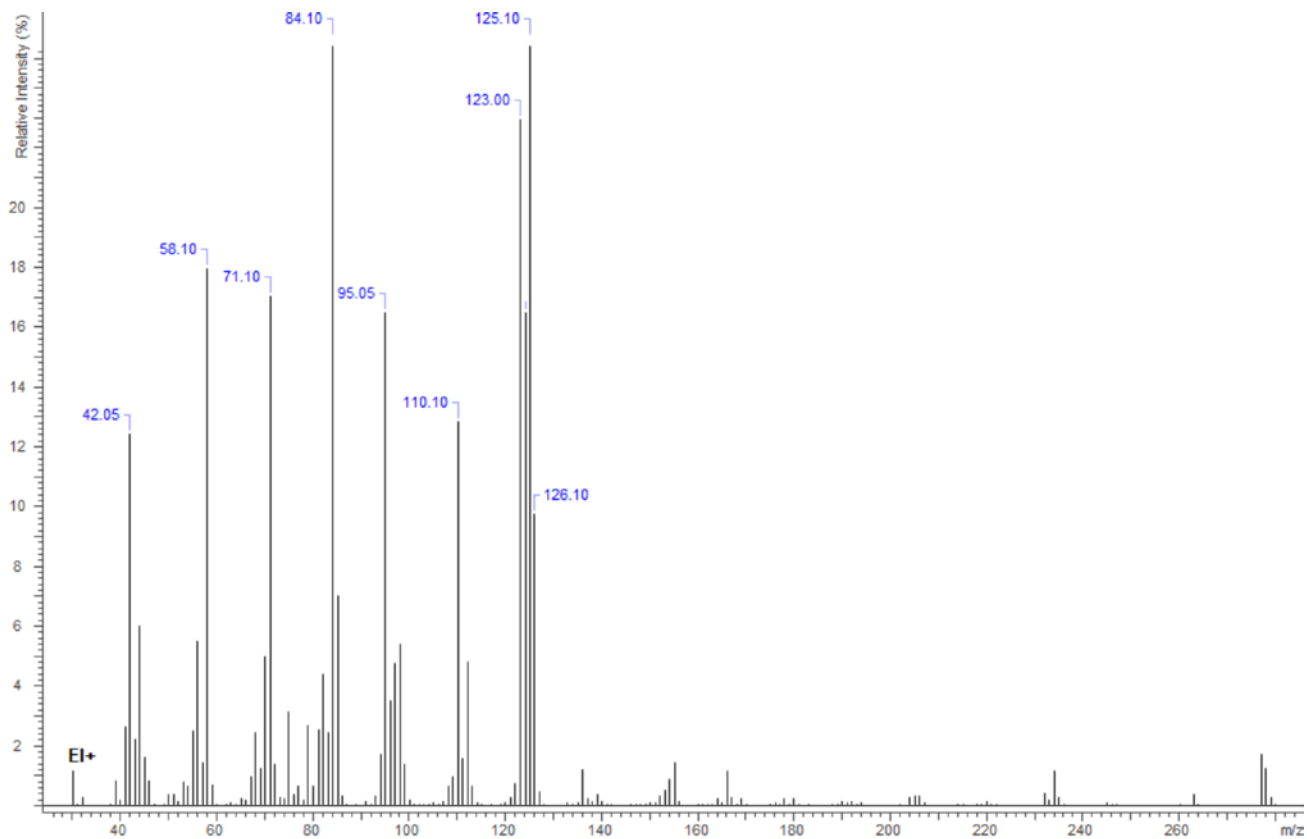
Instrument: Shimadzu gas chromatograph operated in split mode with MS detector
Column: Rtx5MS (a DB-5 equivalent); 30m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1 mL/min
Temperatures: Injector: 280°C
 MSD transfer line: 280°C
 MS Source: 200°C
 Oven program:
 1) 90°C initial temperature for 2.0 min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

EI Mass Spectrum: U03; Lot JLK008-133-U03



Chemical Formula: C₁₆H₂₄FN₂O⁺
 Exact Mass: 279.18672

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

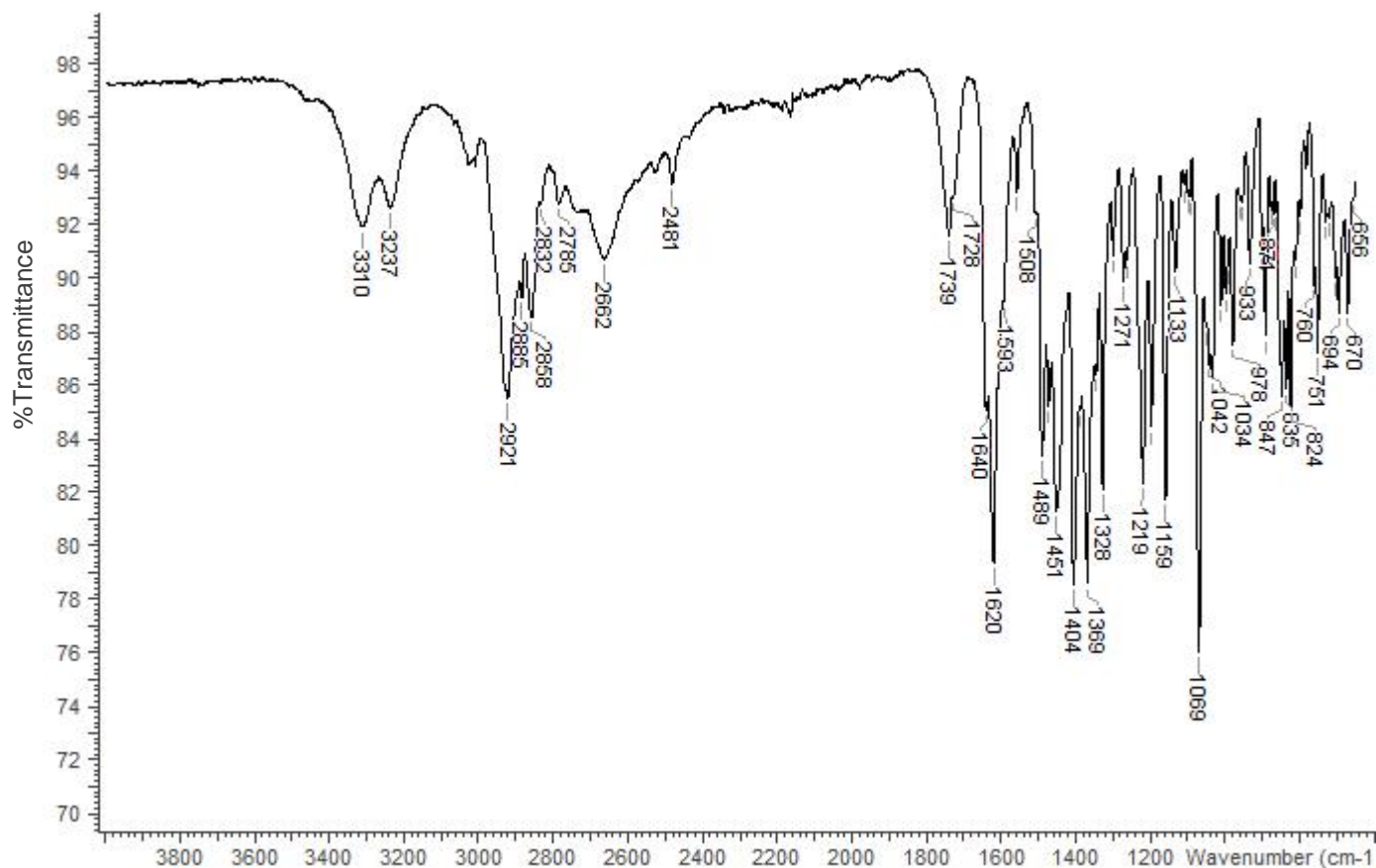


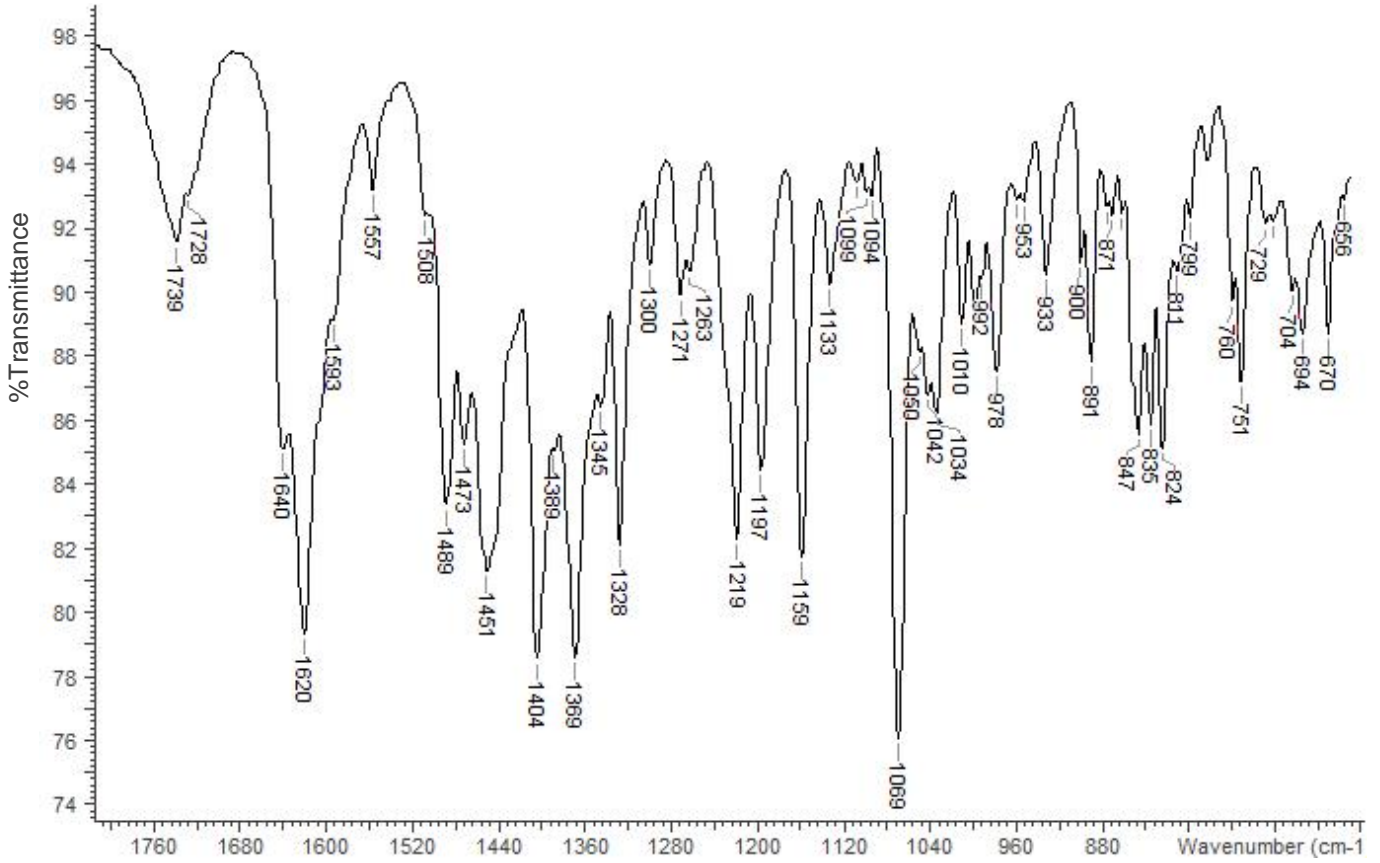
3.3 INFRARED SPECTROSCOPY (FTIR)

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): U03; Lot JLK008-133-U03

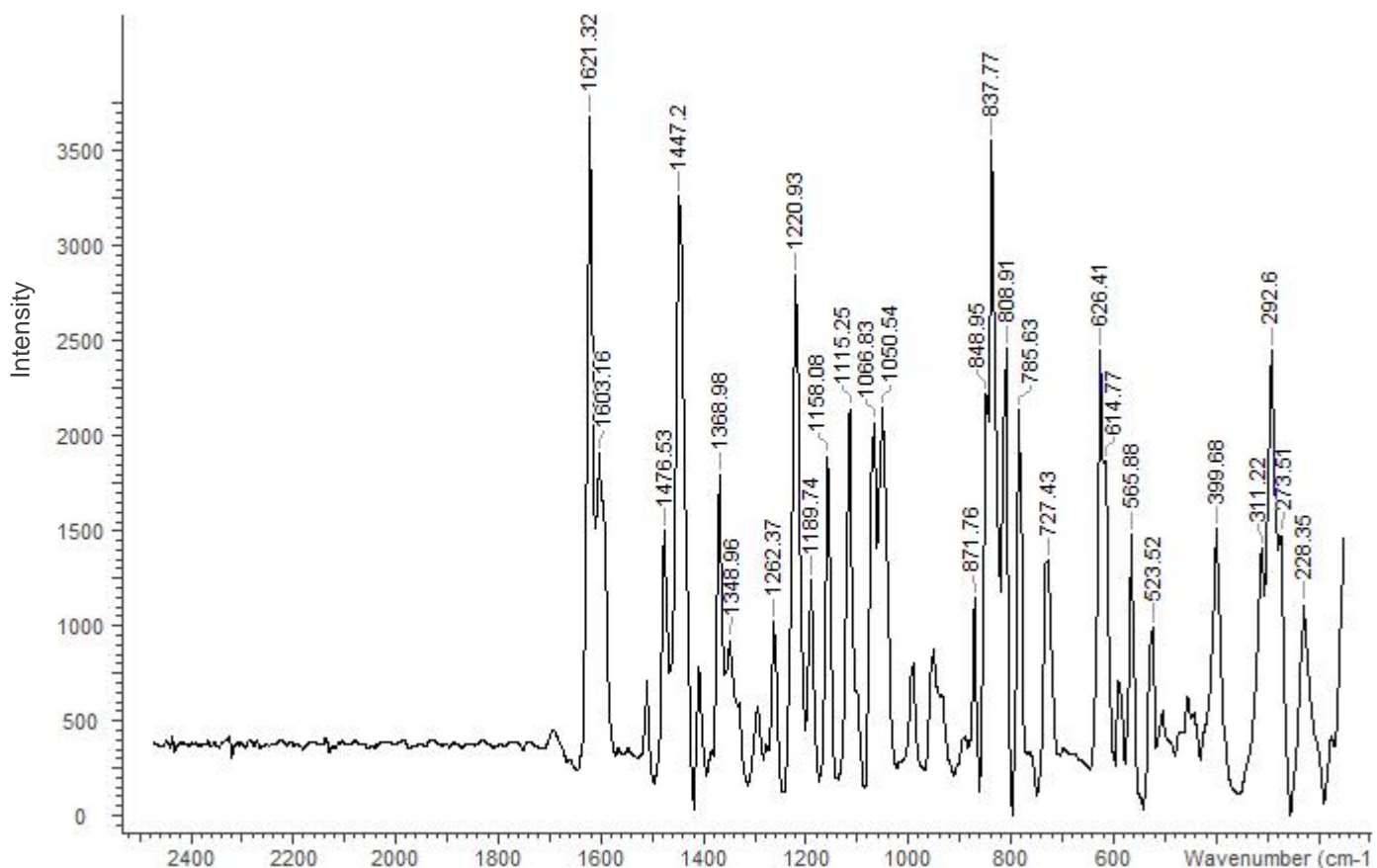




3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): U03; Lot JLK008-133-U03



4. ADDITIONAL RESOURCES

ANALGESIC N-(2-AMINOCYCLOALIPHATIC)BENZAMIDES

Szmuszkovicz

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

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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