

1. GENERAL INFORMATION

IUPAC Name:	N-((1R,2R)-2-(dimethylamino)cyclohexyl)-4-(trifluoromethyl)-N-methylbenzamide
CAS#:	67579-38-8 (base)
Synonyms:	U04
Source:	Synthesized Material Lot# JLK008-134-U04
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 ₁₇ H ₂₃ F ₃ N ₂ O	329.18	91.2 ± 0.75

3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterated chloroform (CDCl_3) + TMS.

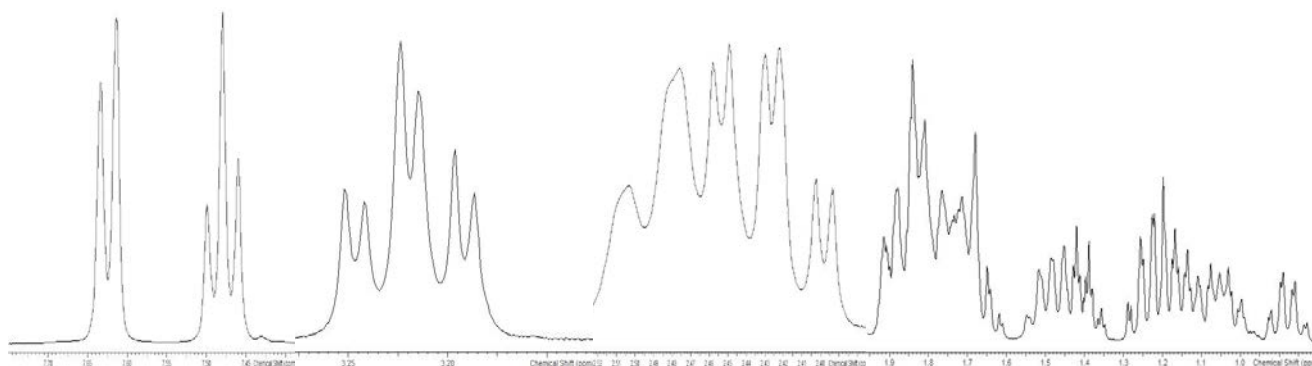
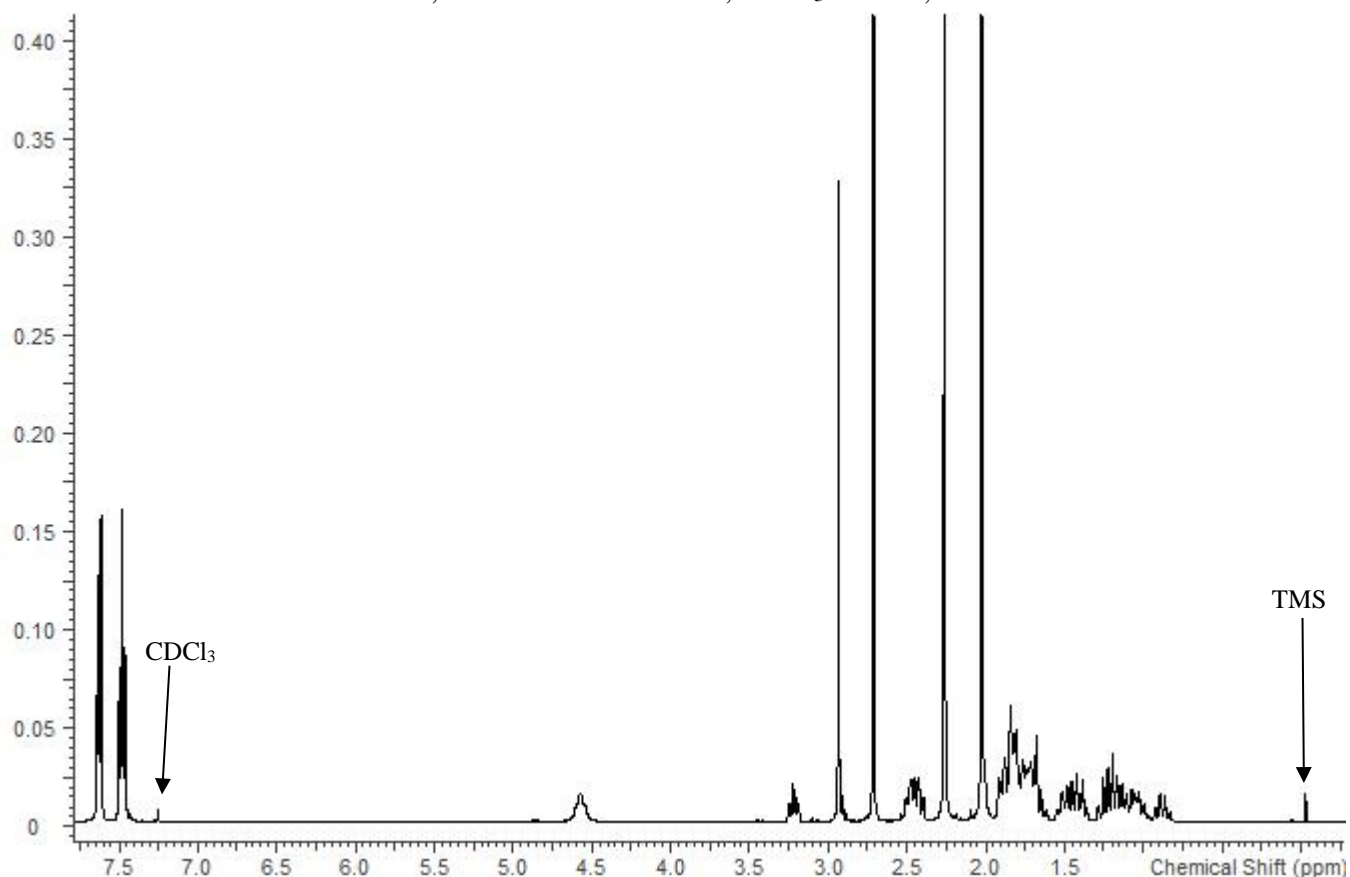
Instrument: 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 30 seconds

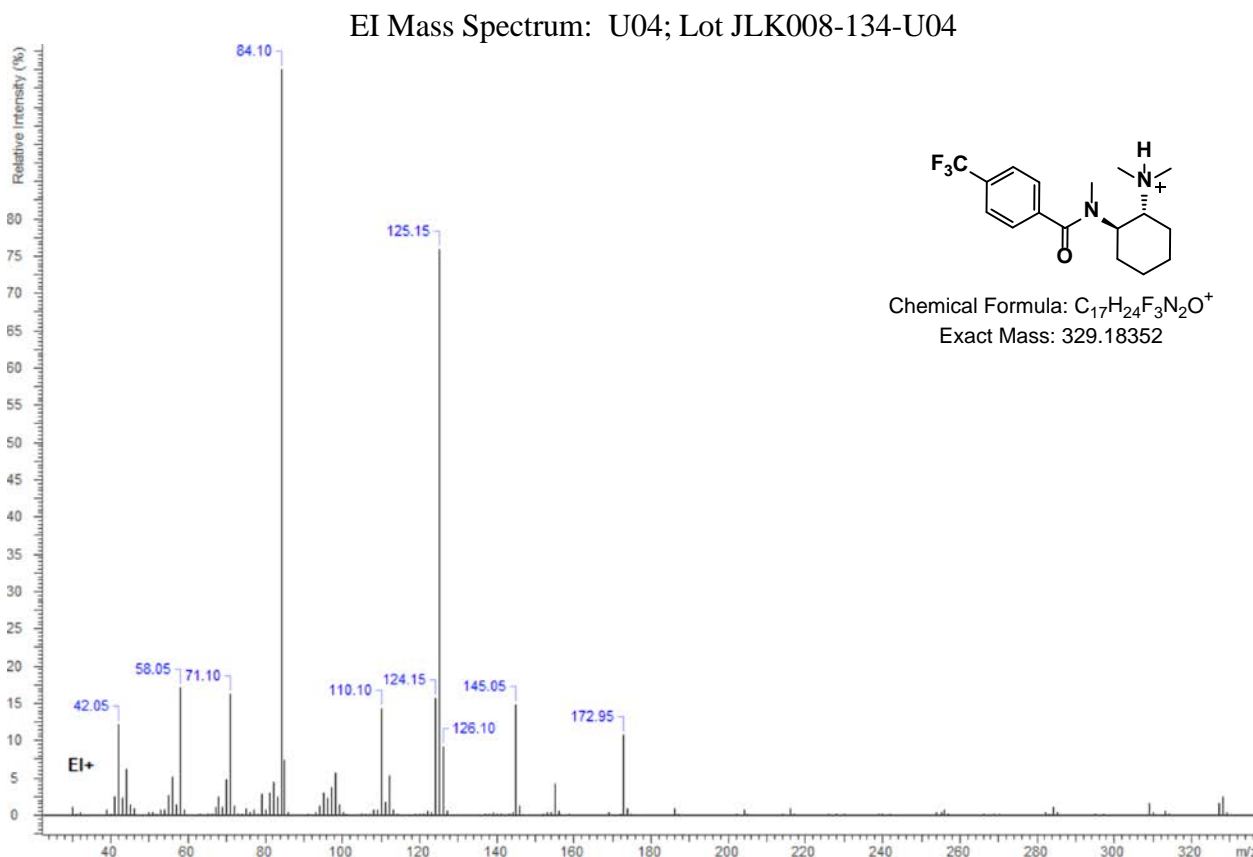
^1H NMR: U04; Lot JLK008-134-U04; CDCl_3 + TMS; 400 MHz



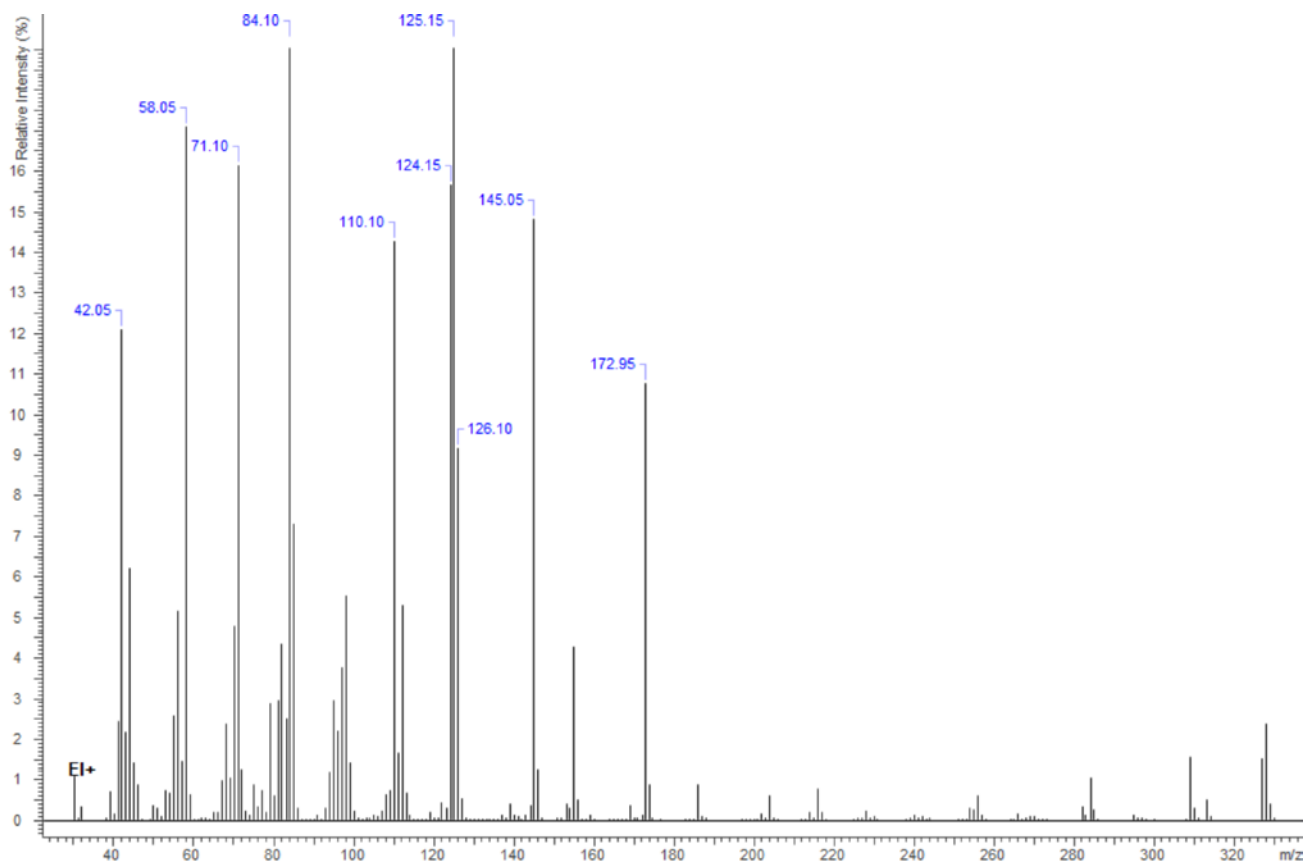
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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: 13.20 min



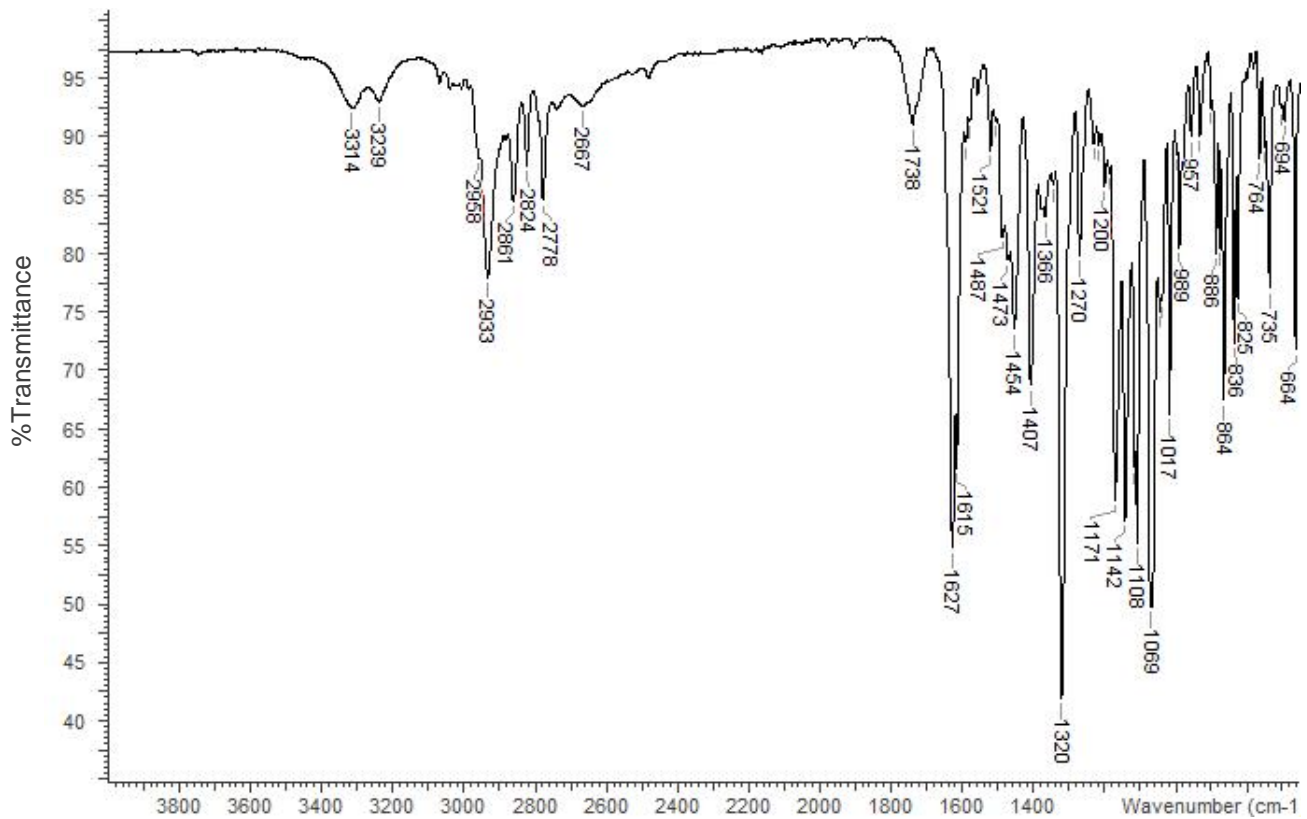
Zoomed view (84.10 and 125.15 are truncated in this view)

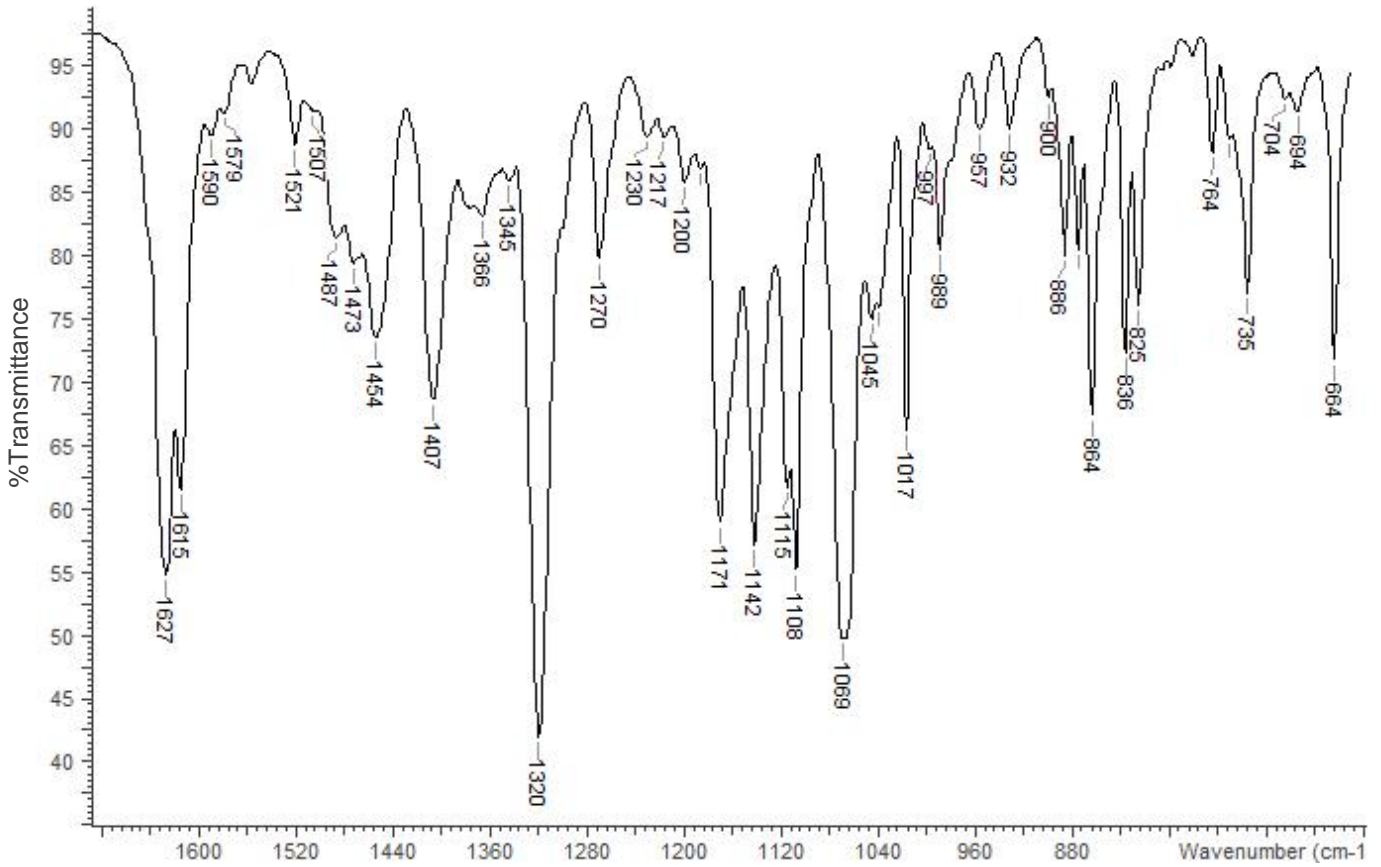


3.3 INFRARED SPECTROSCOPY (FTIR)

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): U04; Lot JLK008-134-U04

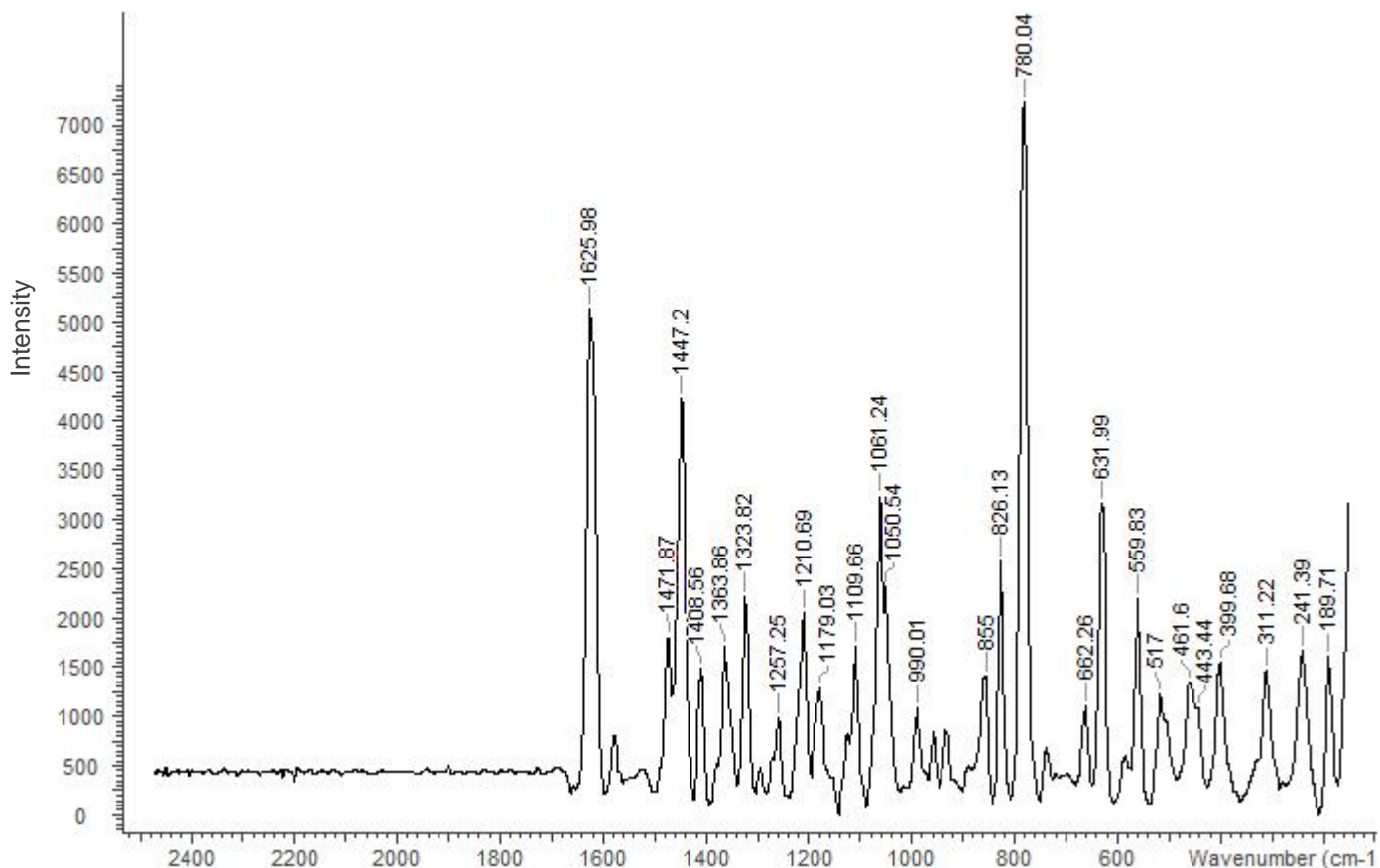




3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): U04; Lot JLK008-134-U04



4. ADDITIONAL RESOURCES

ANALGESIC N-(2-AMINOCYCLOALIPHATIC)BENZAMIDES

Szmuszkovicz

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

Example 23A

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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