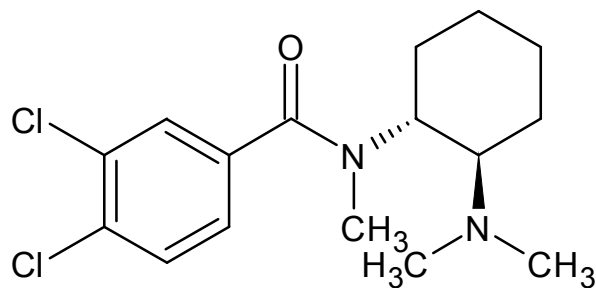




U-47700

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



1. GENERAL INFORMATION

IUPAC Name: *rel*-3,4-dichloro-*N*-[(1*R*,2*R*)-2-dimethylamino]cyclohexyl]-*N*-methylbenzamide

CAS#: 82657-23-6 (Base)

Synonyms: Not Available

Source: DEA Reference Material Collection

Appearance: White Powder

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 ₂₂ Cl ₂ N ₂ O	329	Not Determined
HCl	C ₁₆ H ₂₂ Cl ₂ N ₂ O HCl	365	Not Determined



U-47700

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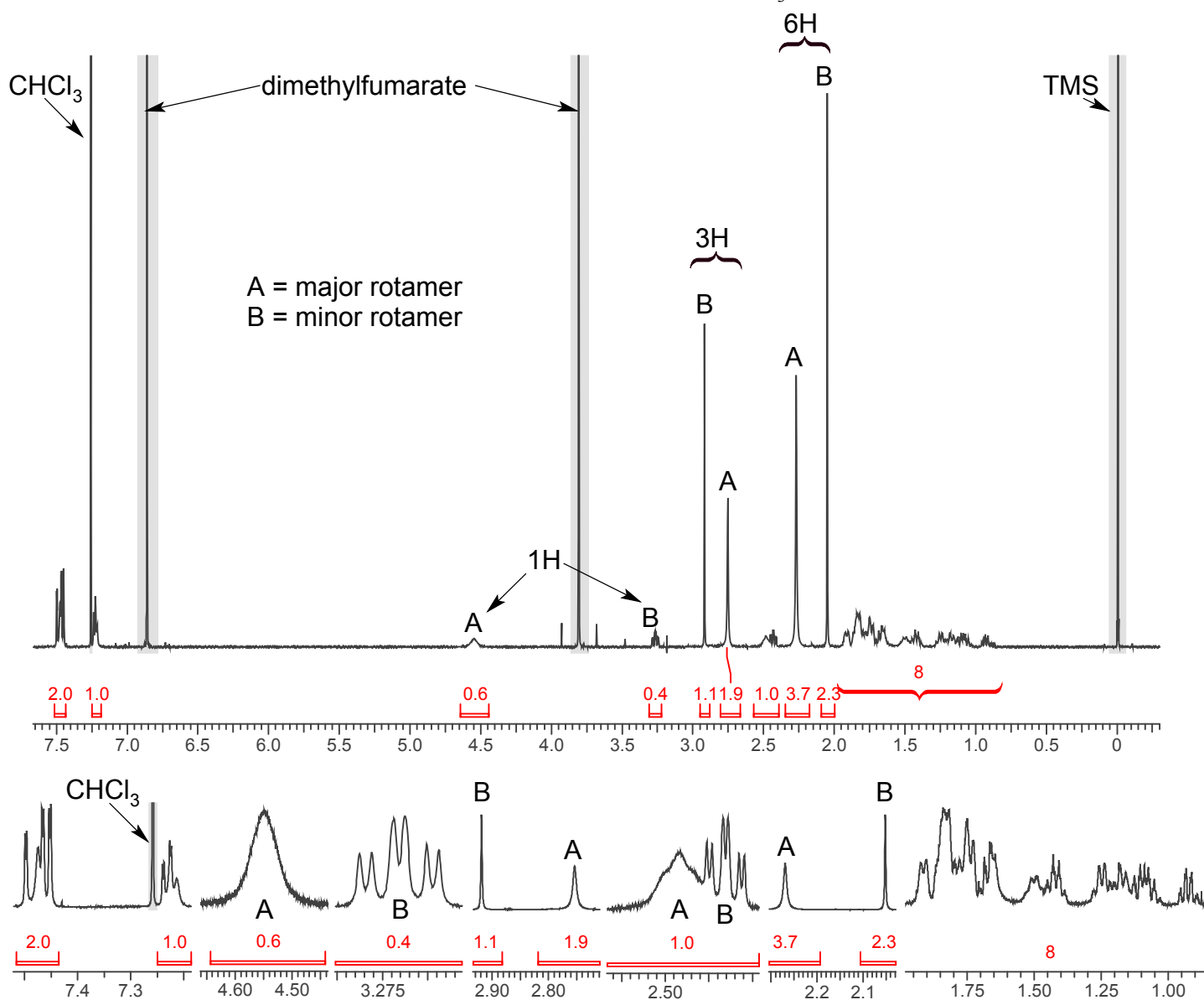
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in CDCl_3 containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

Instrument: 600 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^1H NMR: U-47700 Base; Lot 0475873-13; CDCl_3 ; 600MHz





U-47700

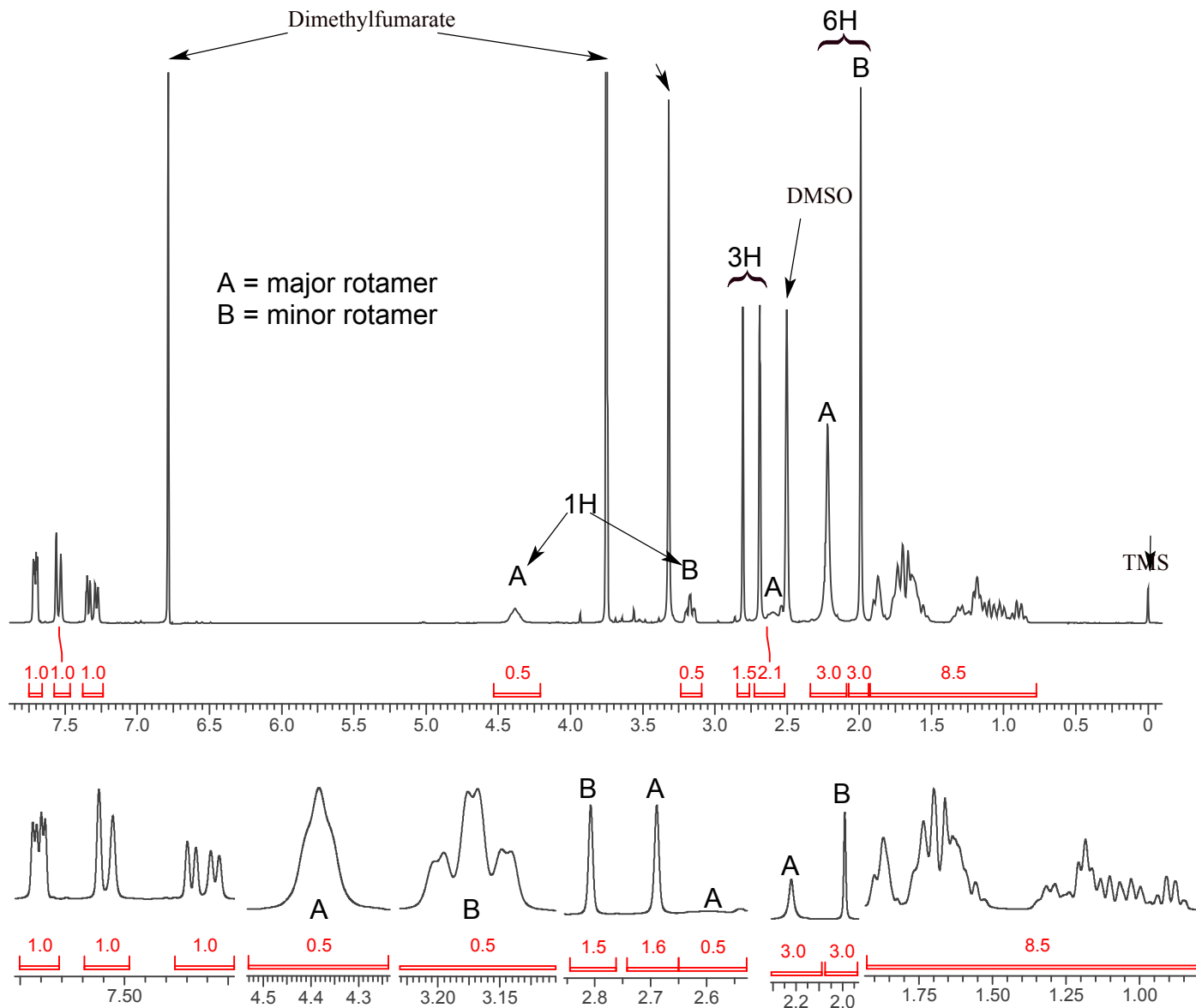
The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



Sample Preparation: Dilute analyte to ~7 mg/mL in DMSO- d_6 containing TMS for 0 ppm reference and dimethylsulfone as quantitative internal standard.

Instrument: 600 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^1H NMR: U-47700 Base; Lot 0475873-13#; DMSO- d_6 ; 600MHz





U-47700

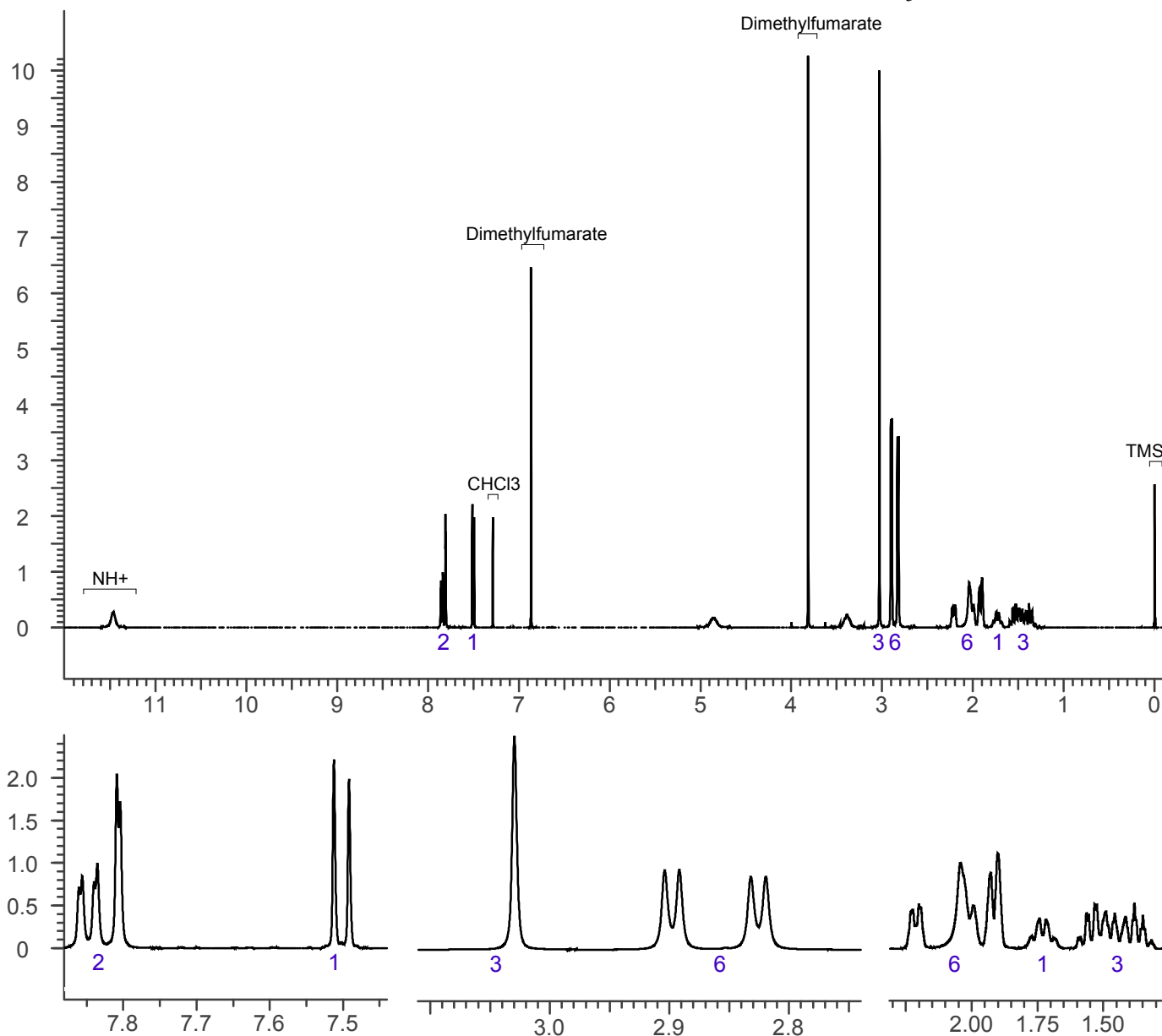
The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



Sample Preparation: Dilute analyte to ~5 mg/mL in CDCl₃ containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

¹HNMR: U-47700 HCl, Lot RM-160614-01, 400MHz, CDCl₃





U-47700

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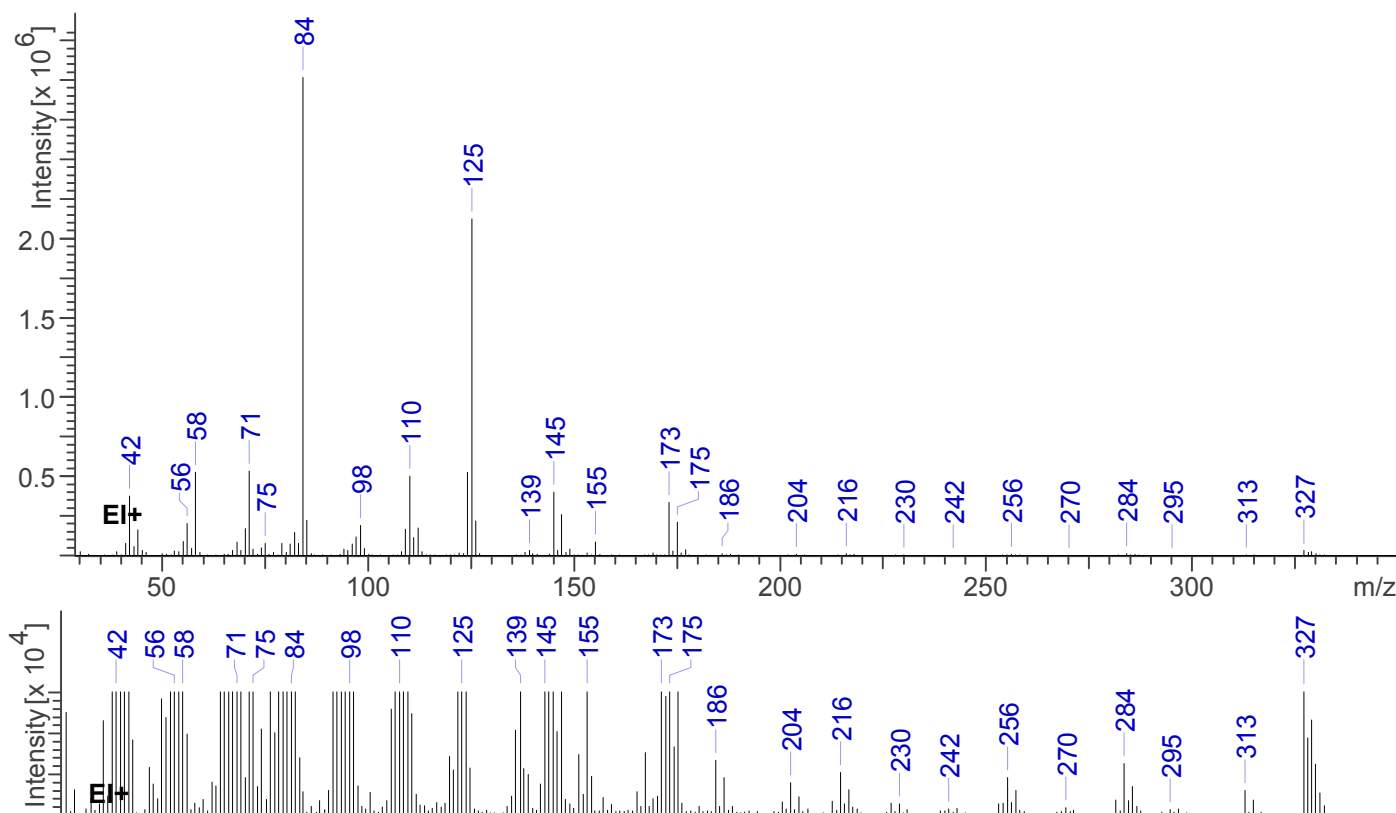
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: DB-5 MS (or equivalent); 15m 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: 250°C
MS Quad: 150°C
Oven program:
1) 100°C initial temperature for 1.0 min
2) Ramp to 280°C at 12 °C/min
3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 25:1, 1 μL injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 150
Tune file: stune.u
Acquisition mode: scan
Retention Time: 12.61 min

EI Mass Spectrum: U-47700 Base, Lot 0475873-13





U-47700

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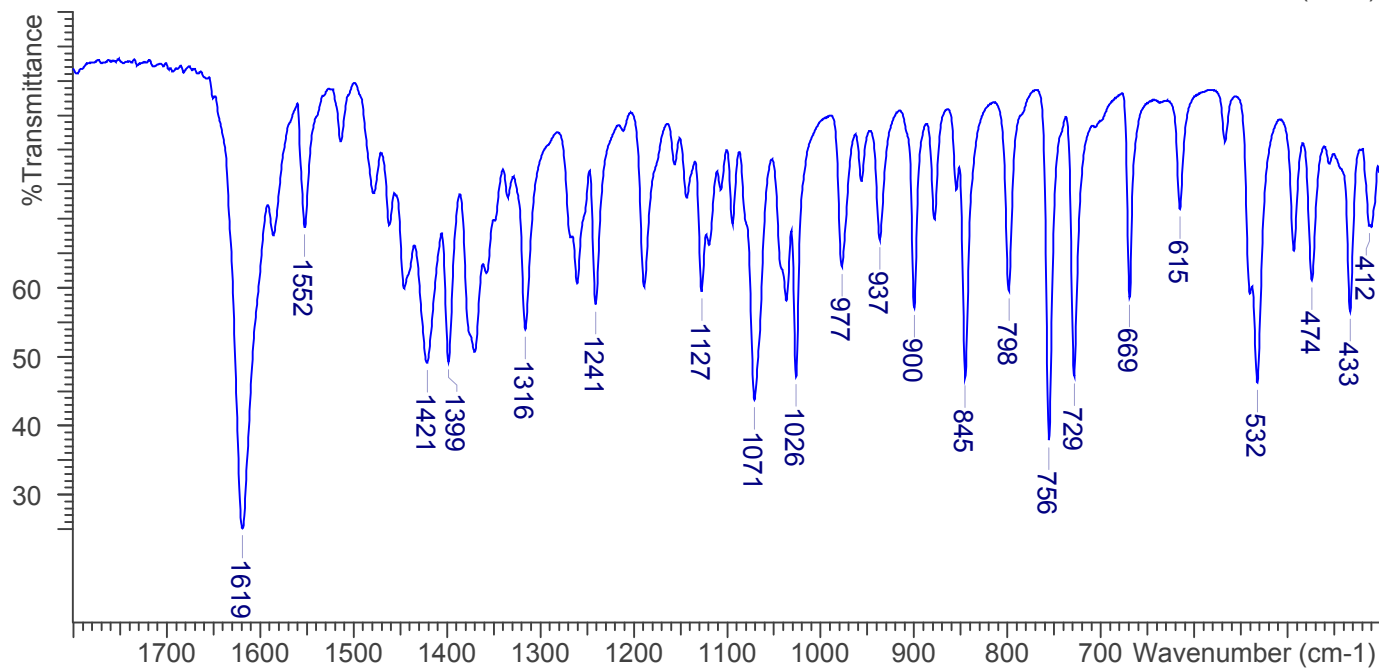
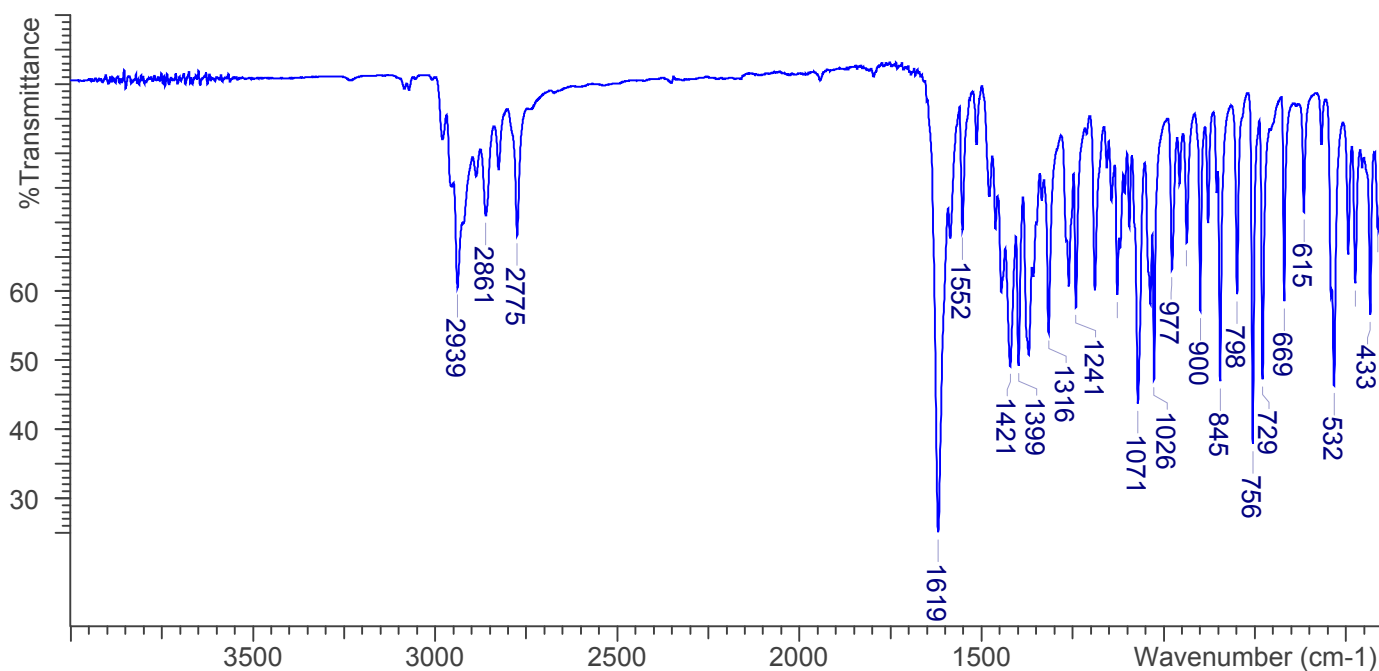


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 1
Aperture: 150

FTIR ATR (Diamond, 1 Bounce): U-47700 Base, Lot 0475873-13





U-47700

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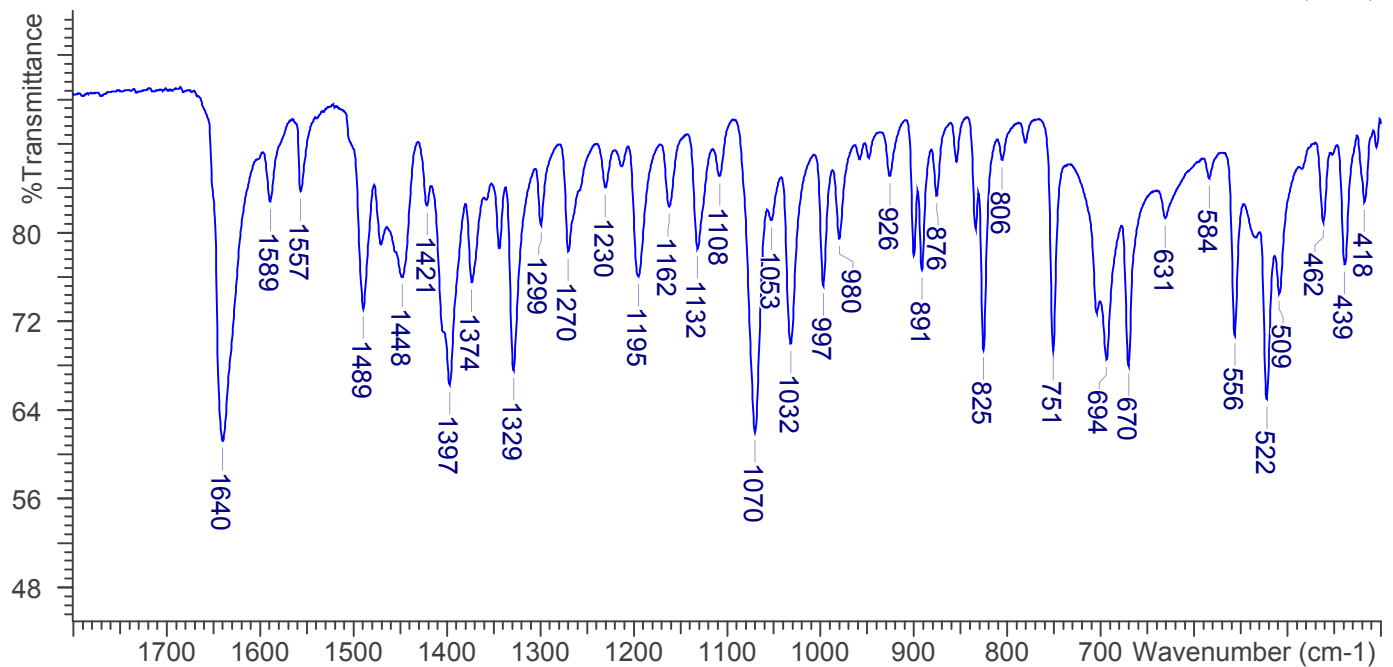
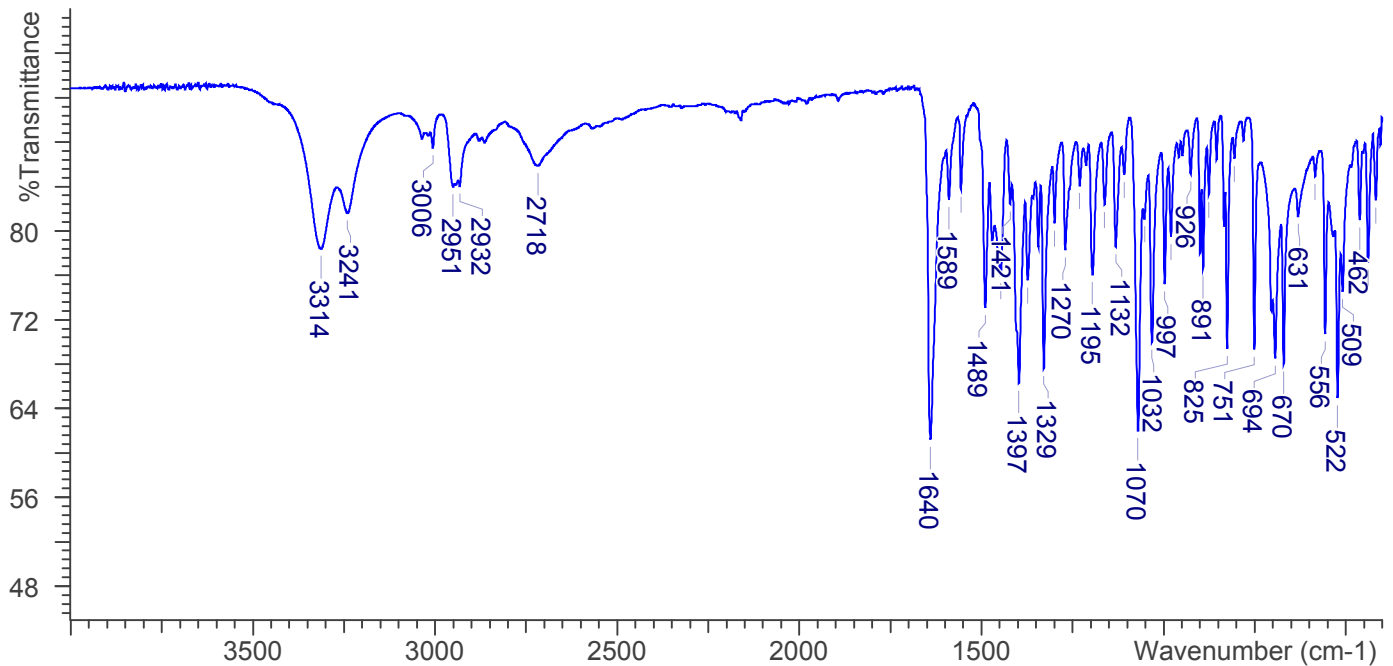


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 1 Bounce): U-47700 HCl, Lot RM-160614-01





U-47700

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



4. ADDITIONAL RESOURCES

[Wikipedia](#)