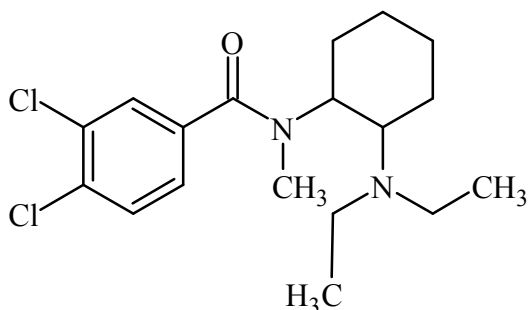




U-49900

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



1. GENERAL INFORMATION

IUPAC Name: 3,4-dichloro-*N*-(2-(diethylamino)cyclohexyl)-*N*-methylbenzamide

CAS#: 67579-76-4

Synonyms: NA

Source: DEA Reference Material Collection

Appearance: white powder

UV_{max}(nm): NA

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₈ H ₂₆ Cl ₂ N ₂ O	357.32	93.5



U-49900



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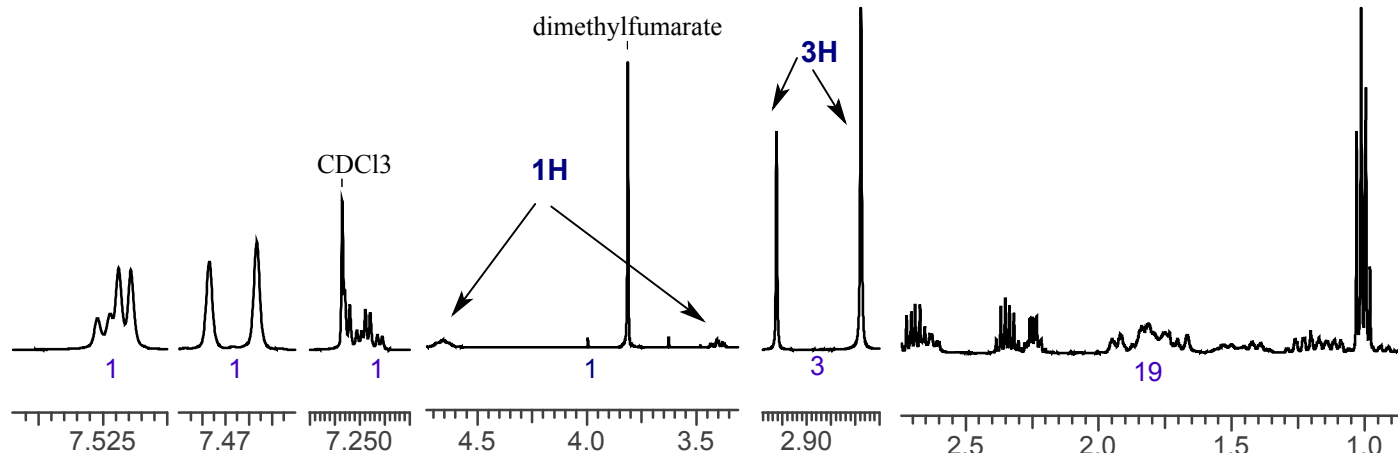
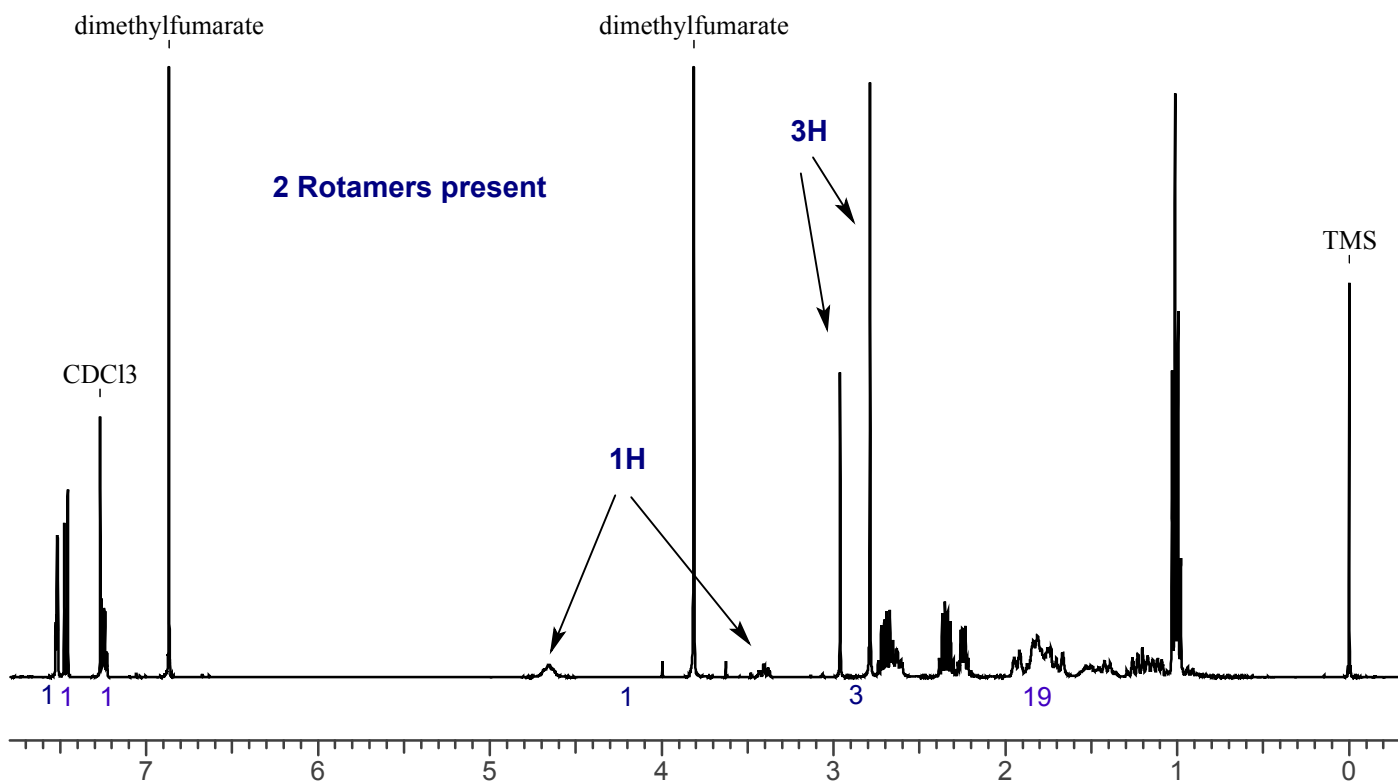
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11mg/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-49900; lot# 0497502-22; CDCl₃; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL into chloroform.

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: HP-5; 30m x 0.25 mm x 0.25 μ m

Carrier Gas: Helium at 1.5 mL/min

Temperatures: Injector: 280°C

MSD transfer line: 280°C

MS Source: 230°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 μ L injected

MS Parameters: Mass scan range: 30-550 amu

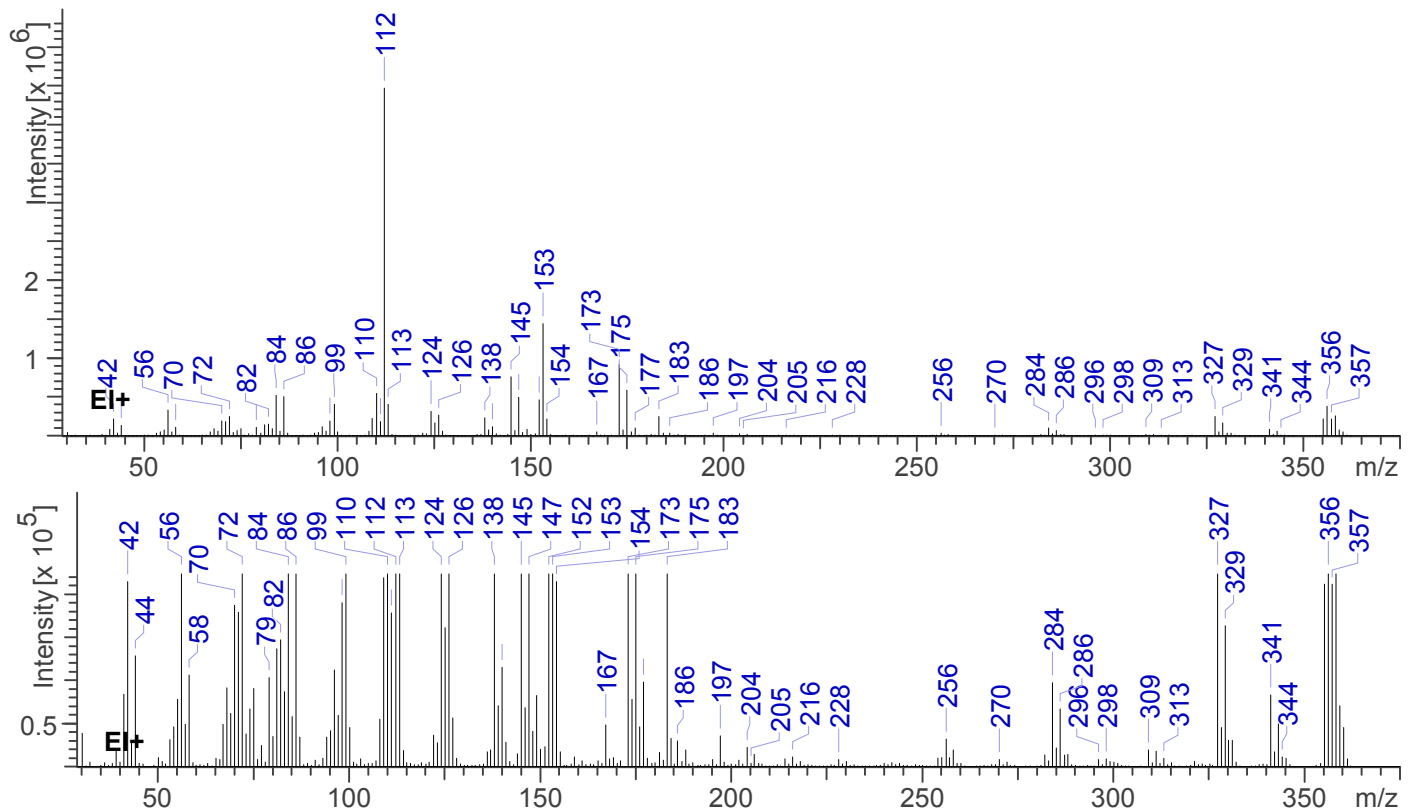
Threshold: 250

Tune file: stune.u

Acquisition mode: scan

Retention Time: 15.812 min

EI Mass Spectrum: U-49900; lot# 0497502-22





U-49900

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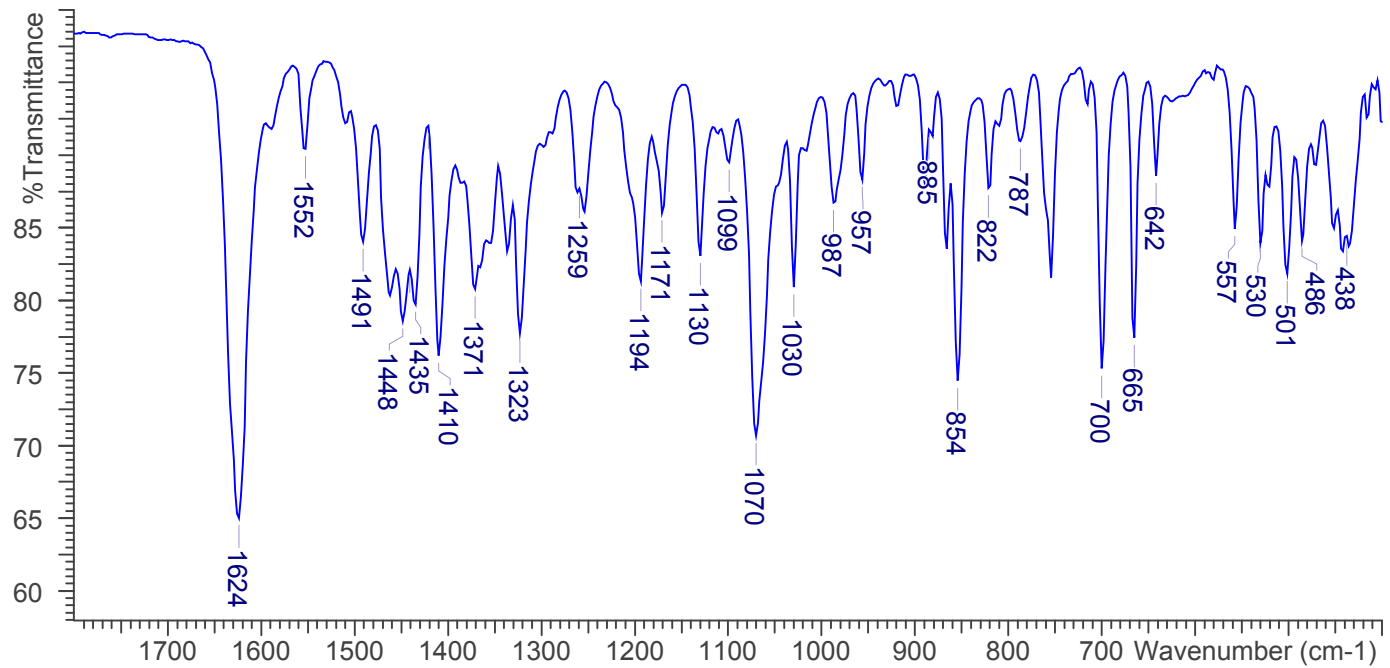
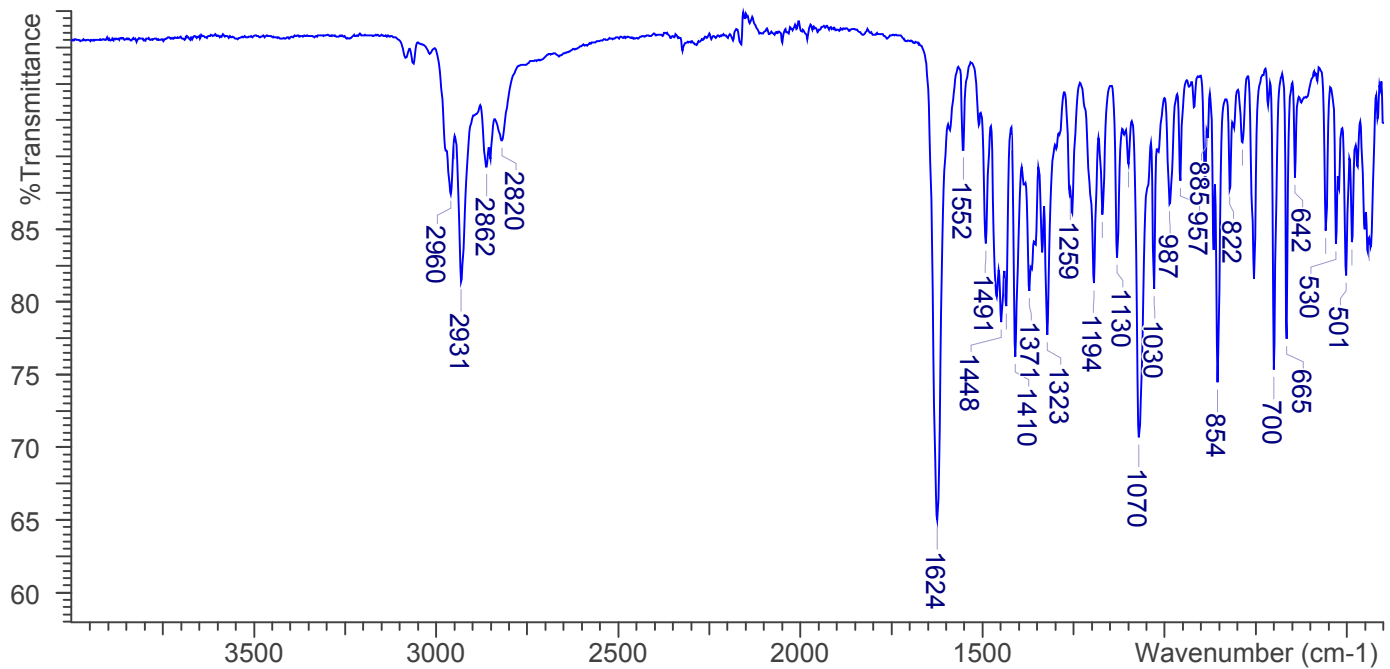


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR (Smart Golden Gate ATR Accessory)

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

FTIR ATR (Diamond1 Bounce): U-49900; lot# 0497502-22





U-49900



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4. ADDITIONAL RESOURCES

No available literature as of 11/30/17