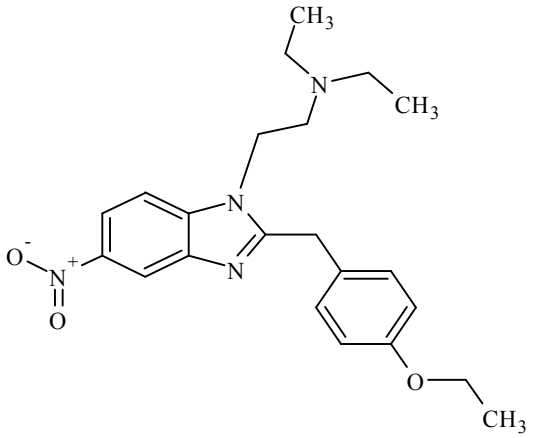
Etonitazene

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



1. GENERAL INFORMATION

IUPAC Name: 2-(2-(4-ethoxybenzyl)-5-nitro-1*H*-benzoimidazol-1-yl)-*N*,*N*-diethylethan-1-amine

CAS#: NA

Synonyms: NA

Source: DEA Reference Material Collection

Appearance: Yellow Powder

UV_{max}(nm): NA

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (^{o}C)
Base	$C_{22}H_{28}N_4O_3$	396.48	NA

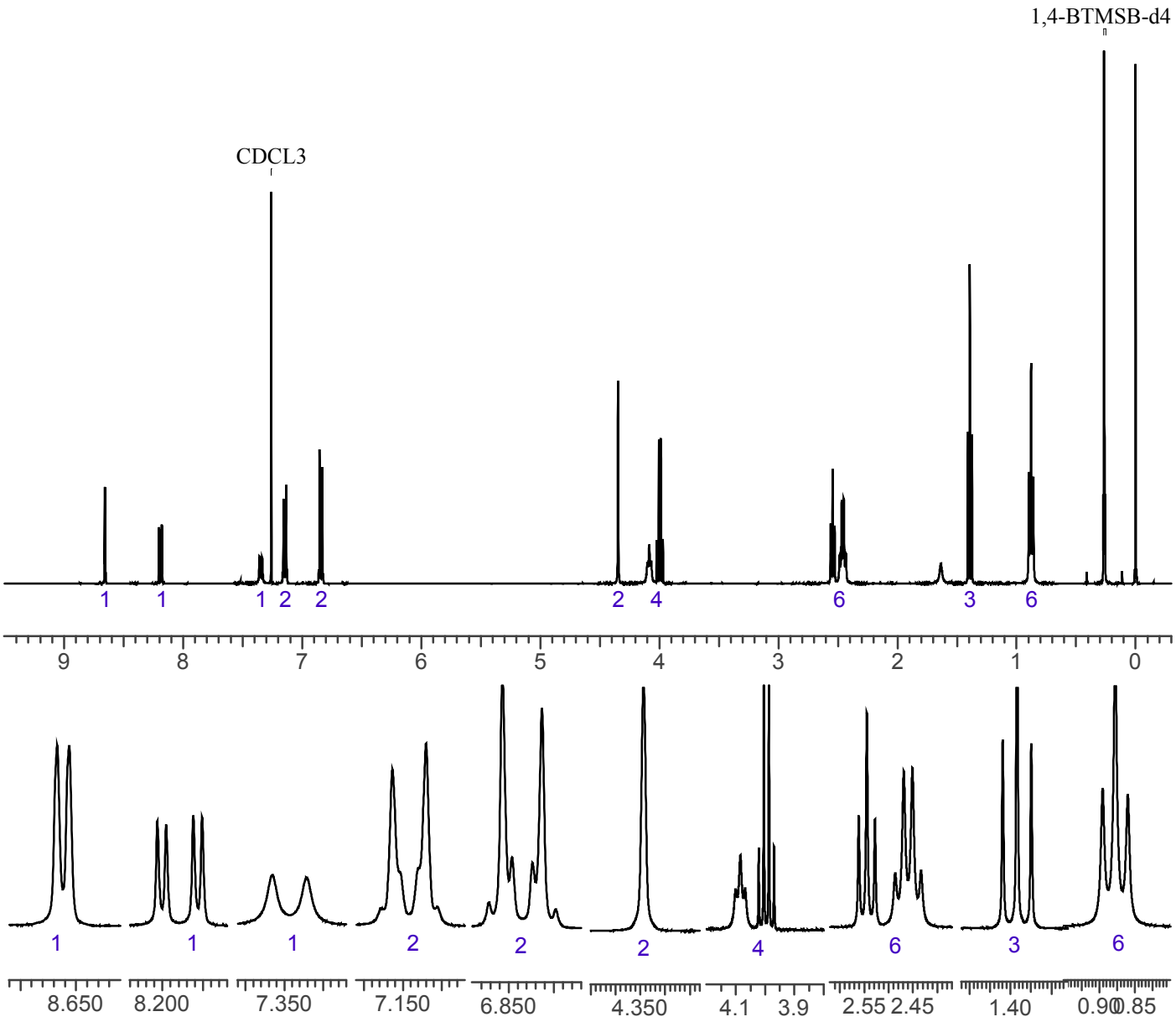
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~6 mg/mL in $CDCl_3$ containing TMS for 0 ppm reference and 1,4-BTMSB-d_4 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

^{1}HNMR: Etonitazene Lot# 0589128-8; CDCL3; 400MHz

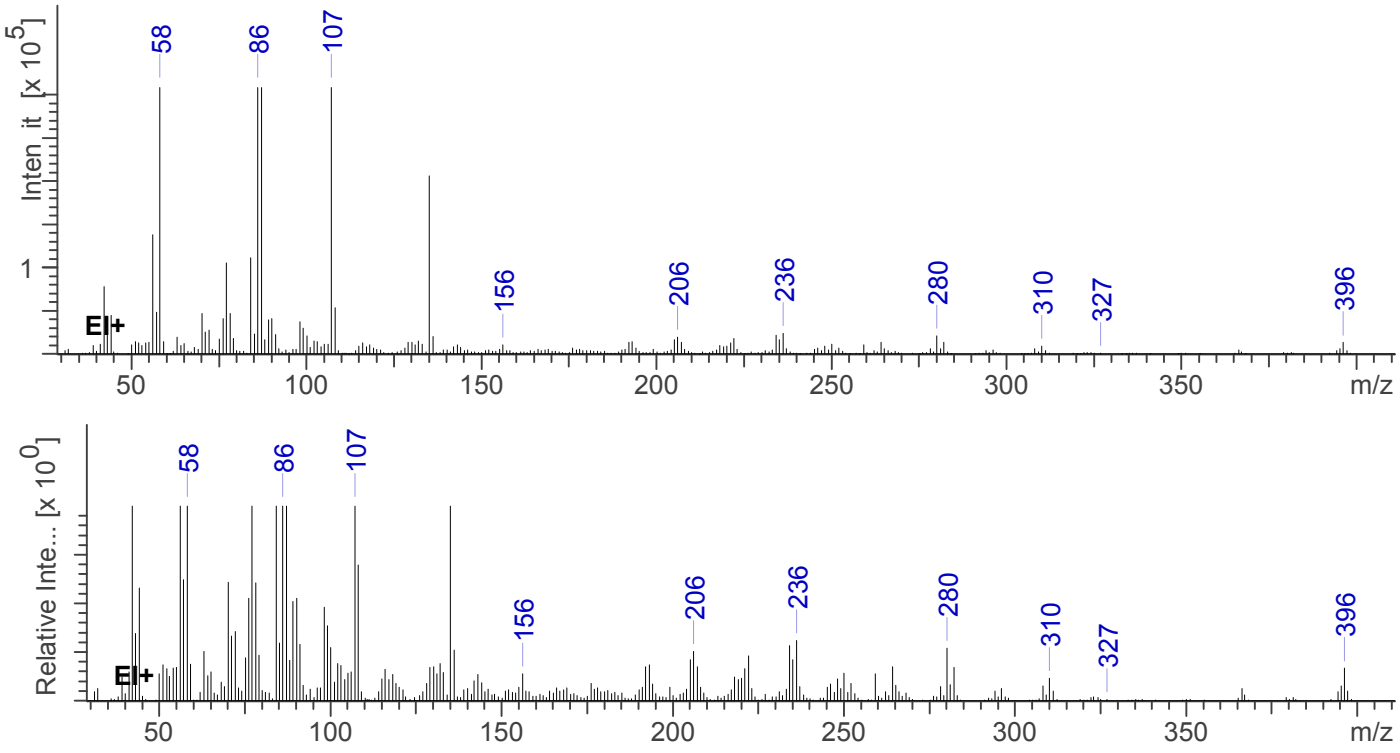


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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 µm
Carrier Gas:	Helium at 1.5mL/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 30.0 min
Injection Parameters:	Split Ratio = 25:1, 1 µL injected
MS Parameters:	Mass scan range: 30-550 amu
	Threshold: 100
	Tune file: stune.u
	Acquisition mode: scan
Retention Time:	24.300min

EI Mass: Etonitazene Lot# 0589128-8

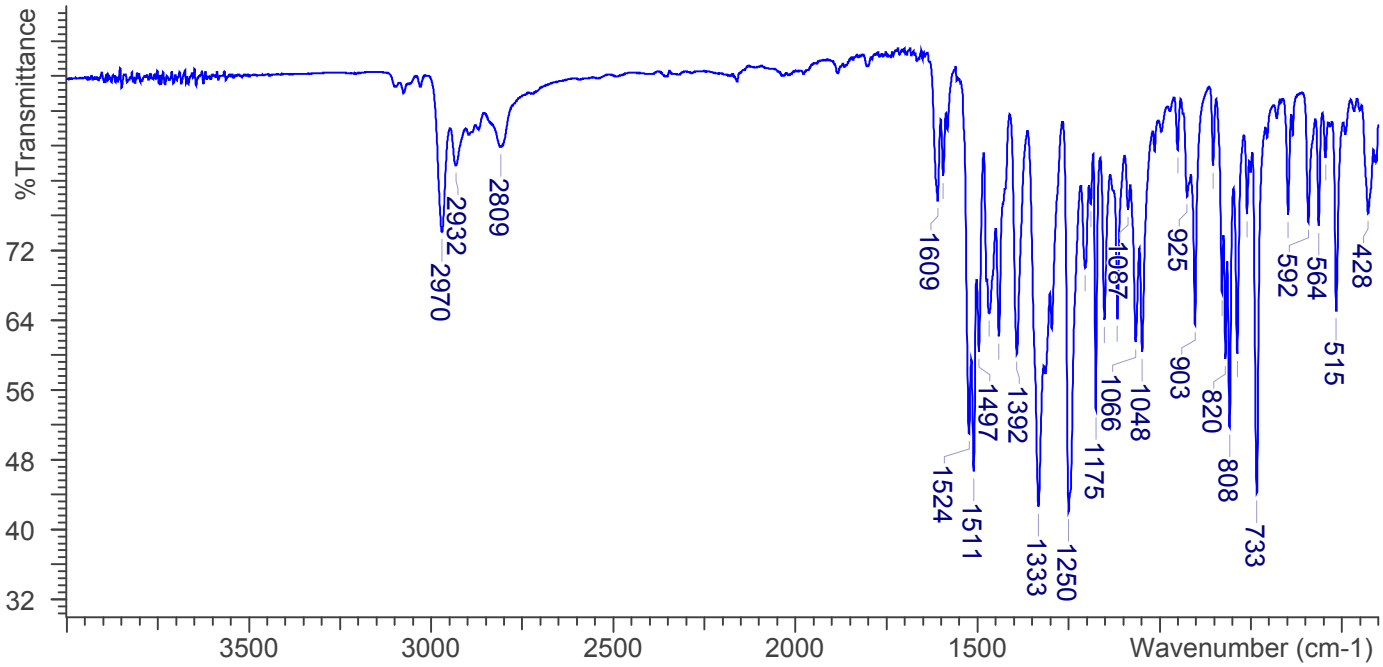


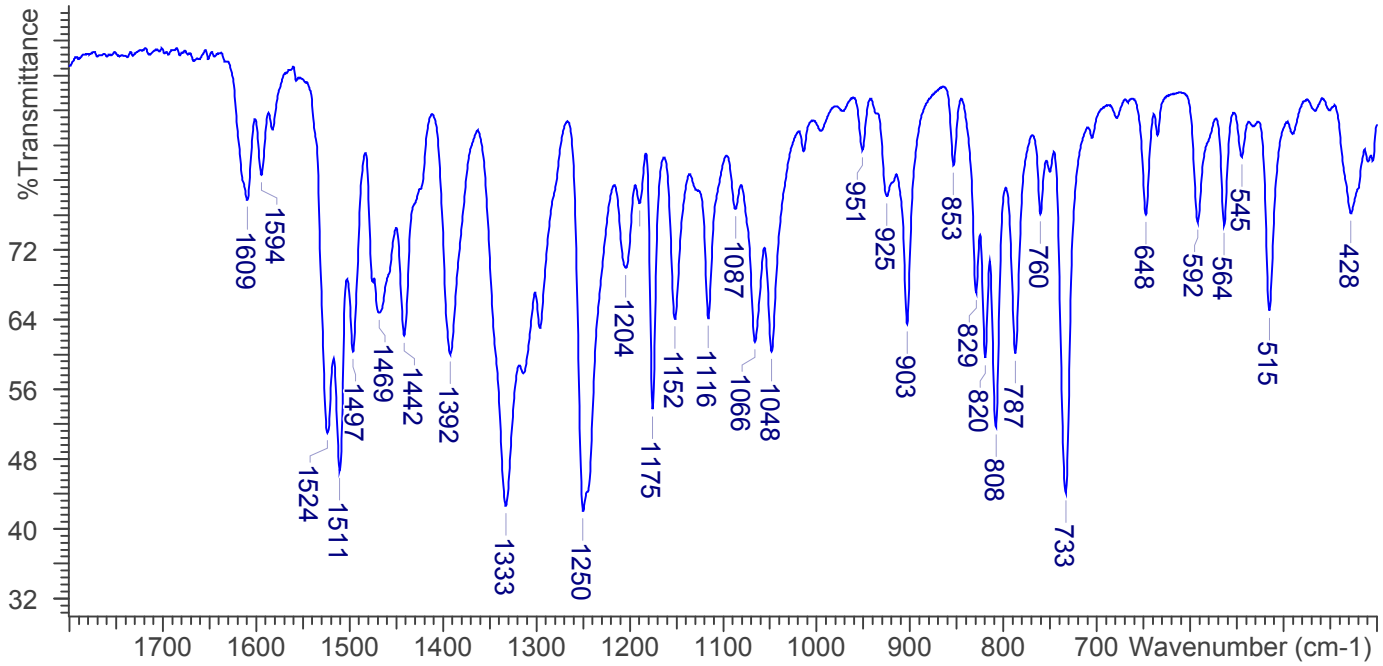
3.3 INFRARED SPECTROSCOPY (FTIR)

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: 4
Aperture: 150

FTIR ATR (Diamond 1 Bounce): Etonitazene Lot# 0589128-8

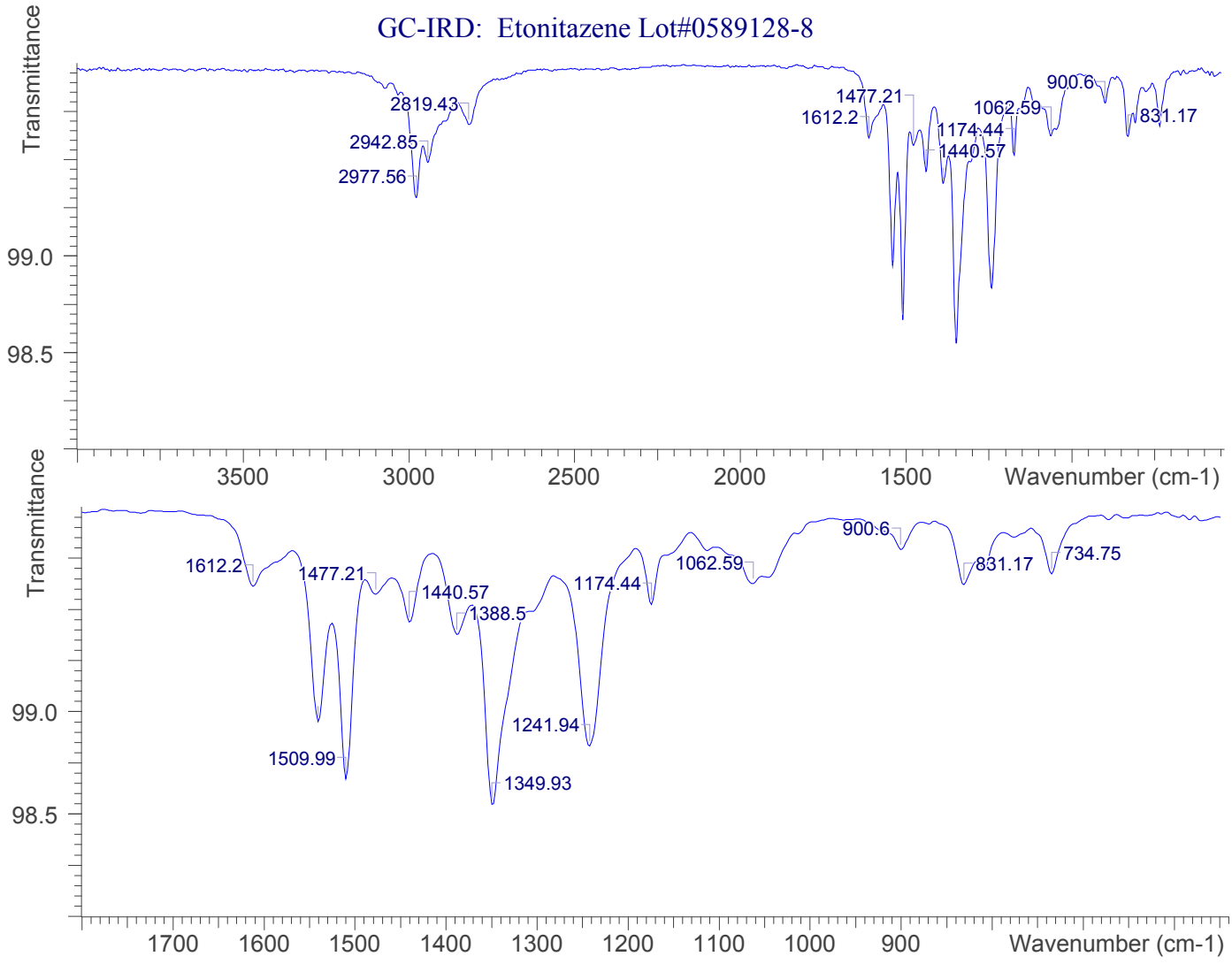




3.4. GAS CHROMATOGRAPHY /INFRARED DETECTION:

Sample Preparation: Dilute analyte 1mg/ml in $CHCl_3$

Instrument:	Gas Chromatograph in split mode with Infrared Detection
Column:	HP-5; 30m x 0.32 mm id x 0.25 µm
Carrier Gas:	Helium at 2.0mL/min
Temperature:	Injector: 280°C Split ratio: 2:1, 2µl injection
	65°C hold 0.5min., ramp to 310°C at 20°C/min., hold 5min.
IRD:	Detector: Transfer line
	Temp 280°C
	Flow Cell Temp 280°C
	Resolution 8 cm-1



4. ADDITIONAL RESOURCES

No additional resources as of 02/11/2022