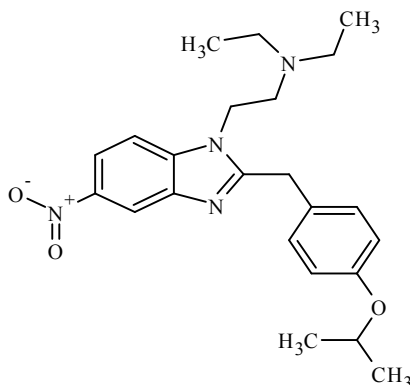




Isotonitazene

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



1. GENERAL INFORMATION

IUPAC Name: N,N-diethyl-2-(2-(4-isopropoxybenzyl)-5-nitro-1H-benzimidazol-1-yl)ethan-1-amine

CAS#: NA

Synonyms: N,N-diethyl-2-[[4-(1-methylethoxy)phenyl]methyl]-5-nitro-*H*-benzimidazole-1-ethanamine, N,N-diethyl-2-[5-nitro-2-(4-[(propan-2-yl)oxy]phenyl)methyl]-*H*-benzimidazol-1-yl]ethan-1-amine

Source: DEA Reference Material Collection

Appearance: yellow powder

UV_{max}(nm): N/A

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₃ H ₃₀ N ₄ O ₃	410.51	82.82



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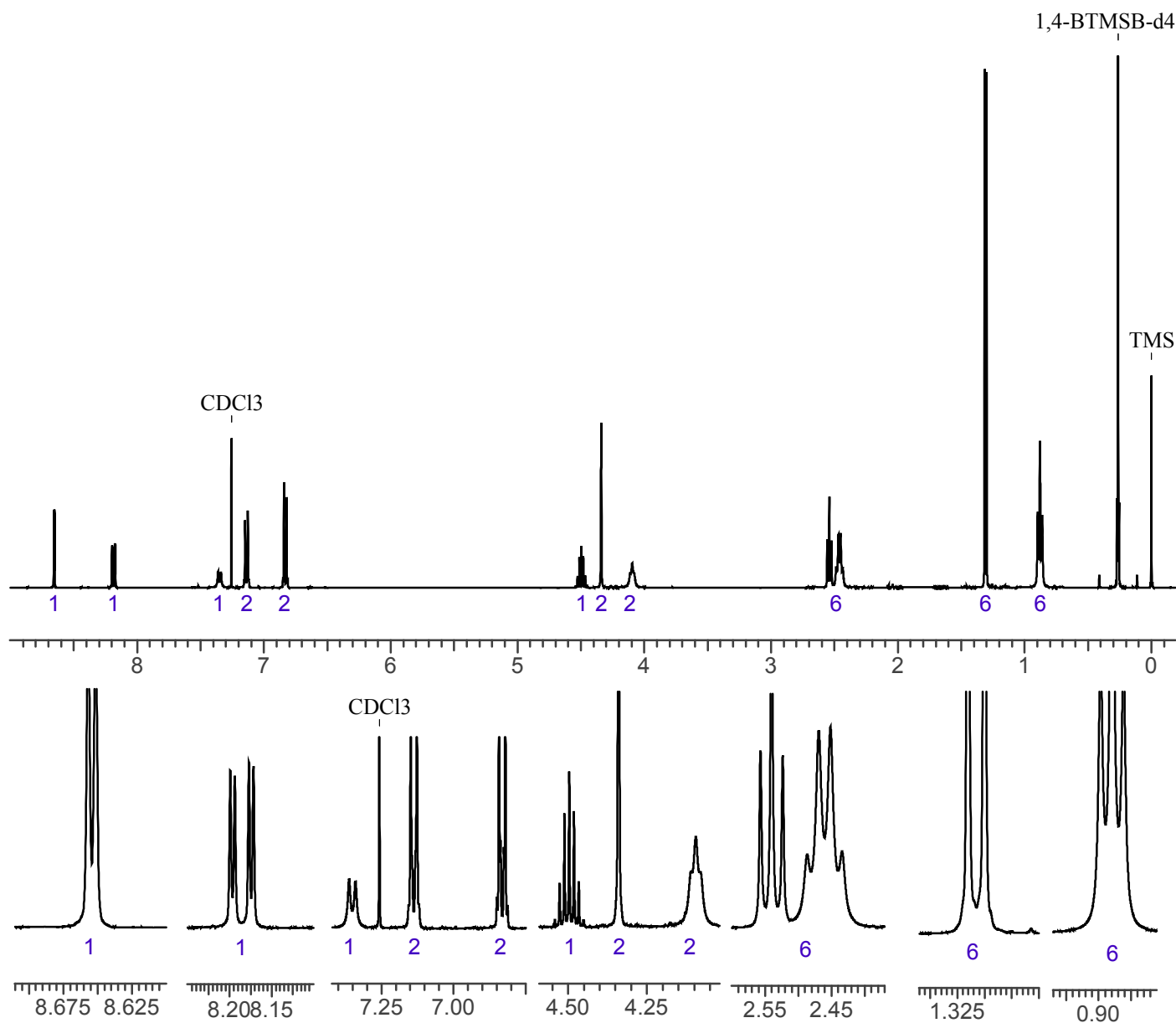


3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 mg/mL in CDCl₃ containing TMS for 0 ppm reference and 1,4-BTMSB-d₄ 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: Isotonitazene; Lot# 0577984-6; CDCl₃; 400 MHz





Isotonitazene

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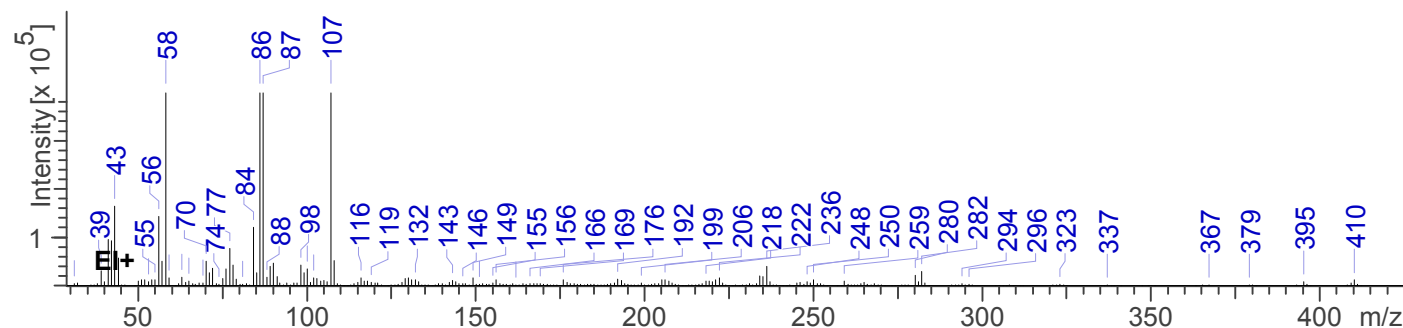
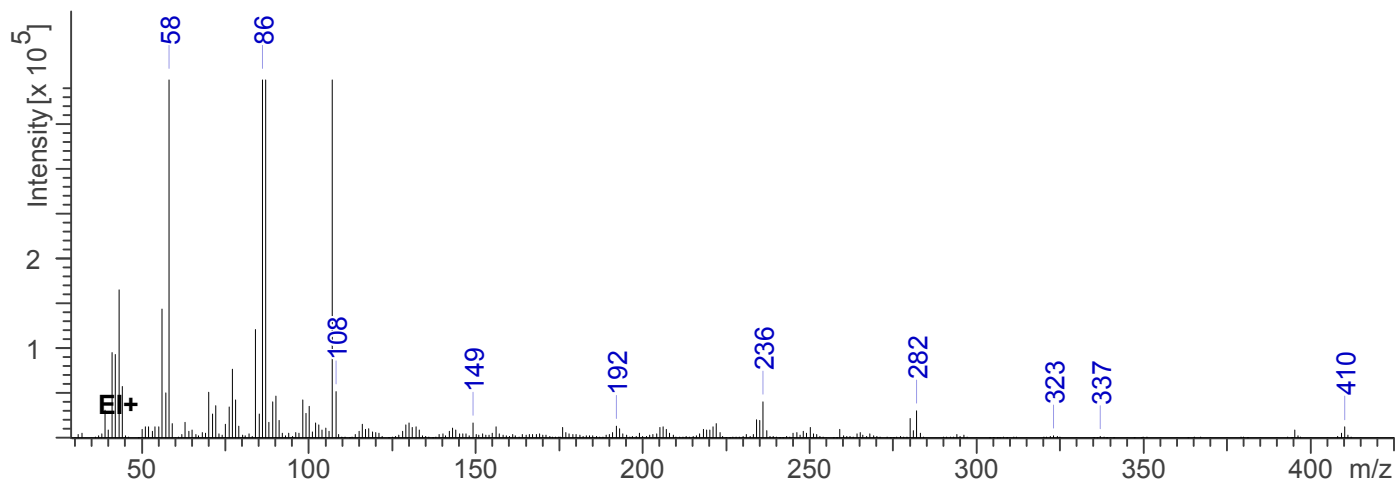


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 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 1.5mL/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 μ L injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan
Retention Time: 24.722min

EI Mass Spectrum: Isotonitazene; Lot# 0577984-6





Isotonitazene

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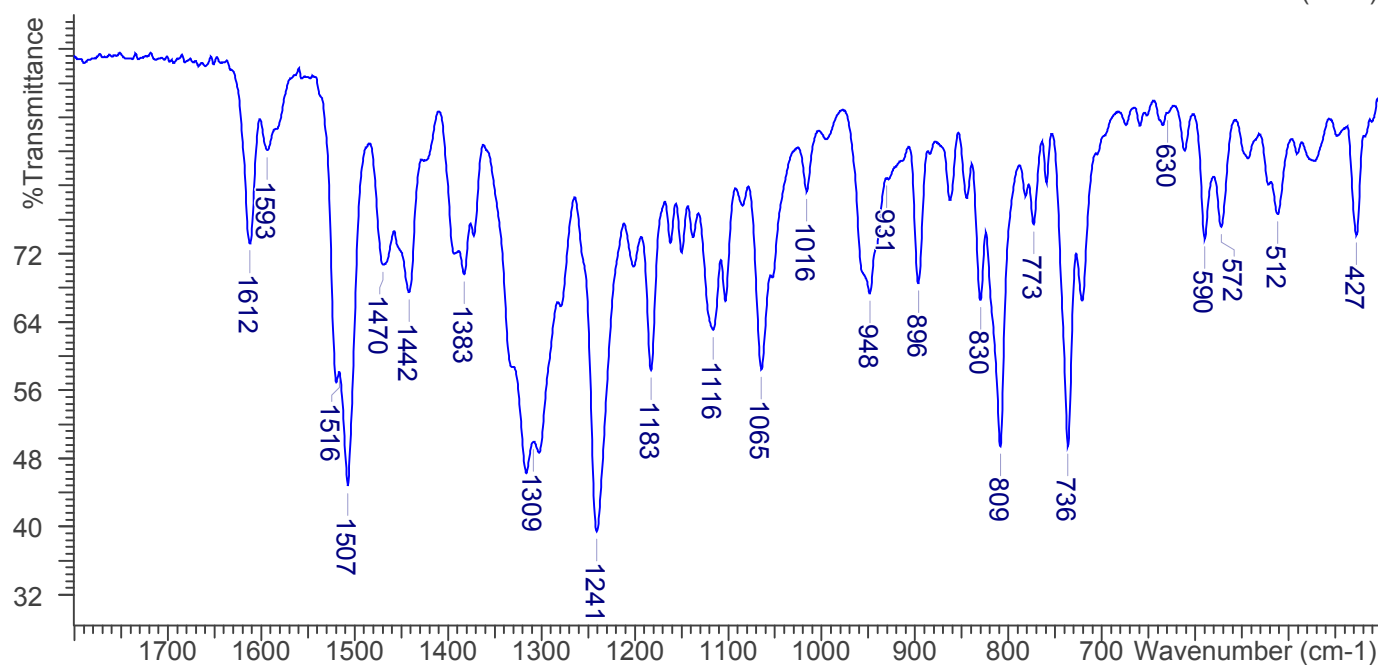
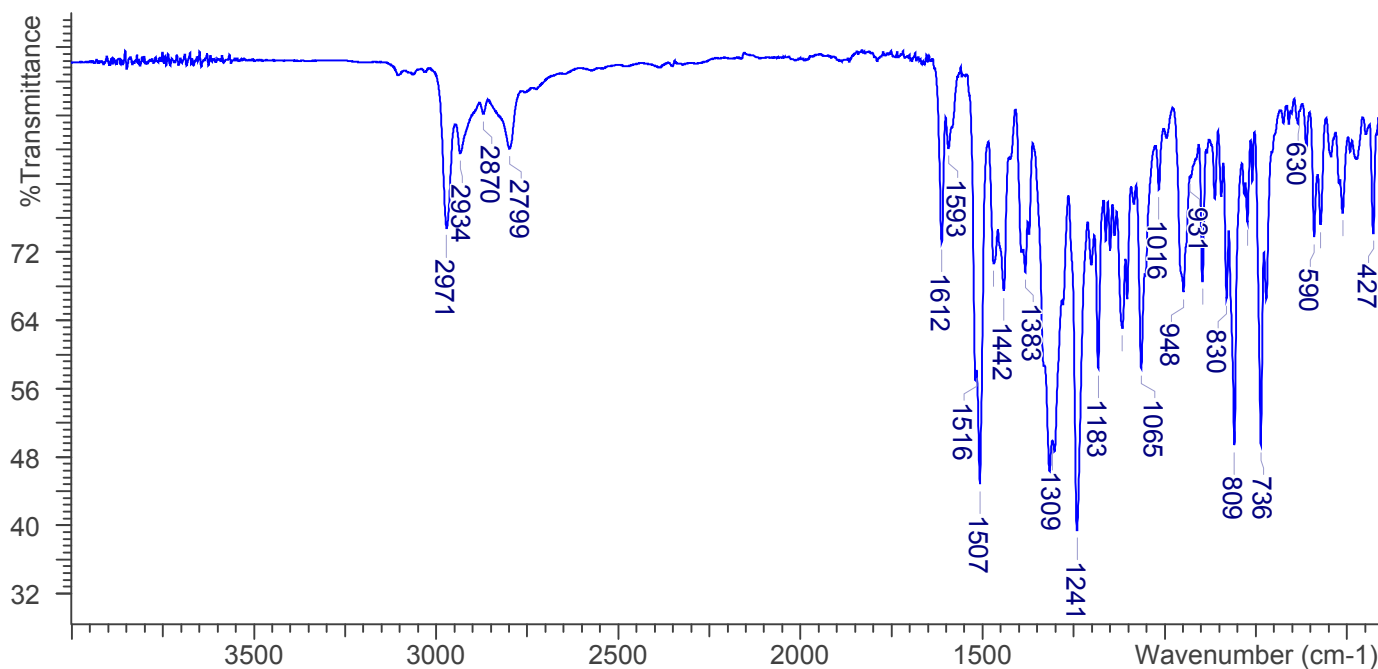


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 4
Aperture: 150

FTIR ATR (Diamond 1 Bounce): Isotonitazene: Lot# 0577984-6





Isotonitazene

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



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, 2 μl 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}

GC-IRD: Isotonitazene; Lot 0577984-6

