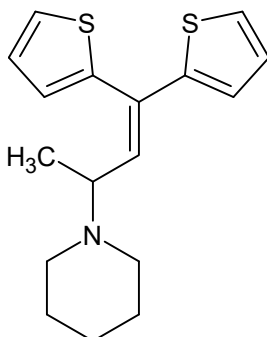




Piperidylthiambutene

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



1. GENERAL INFORMATION

IUPAC Name:	1-(4,4-di(thiophen-2-yl)but-3-en-2-yl)piperidine
CAS#:	54160-31-5 (base), 64037-51-0 (HCl)
Synonyms:	Piperidinohton, 1-(1-methyl-3-3-di-2-thienyl-2-propen-1-yl)-piperidine
Source:	DEA Reference Material Collection
Appearance:	Off-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 ₁₇ H ₂₁ NS ₂	303.49	Not Determined
HCl	C ₁₇ H ₂₁ NS ₂ HCl	339.95	Not Determined



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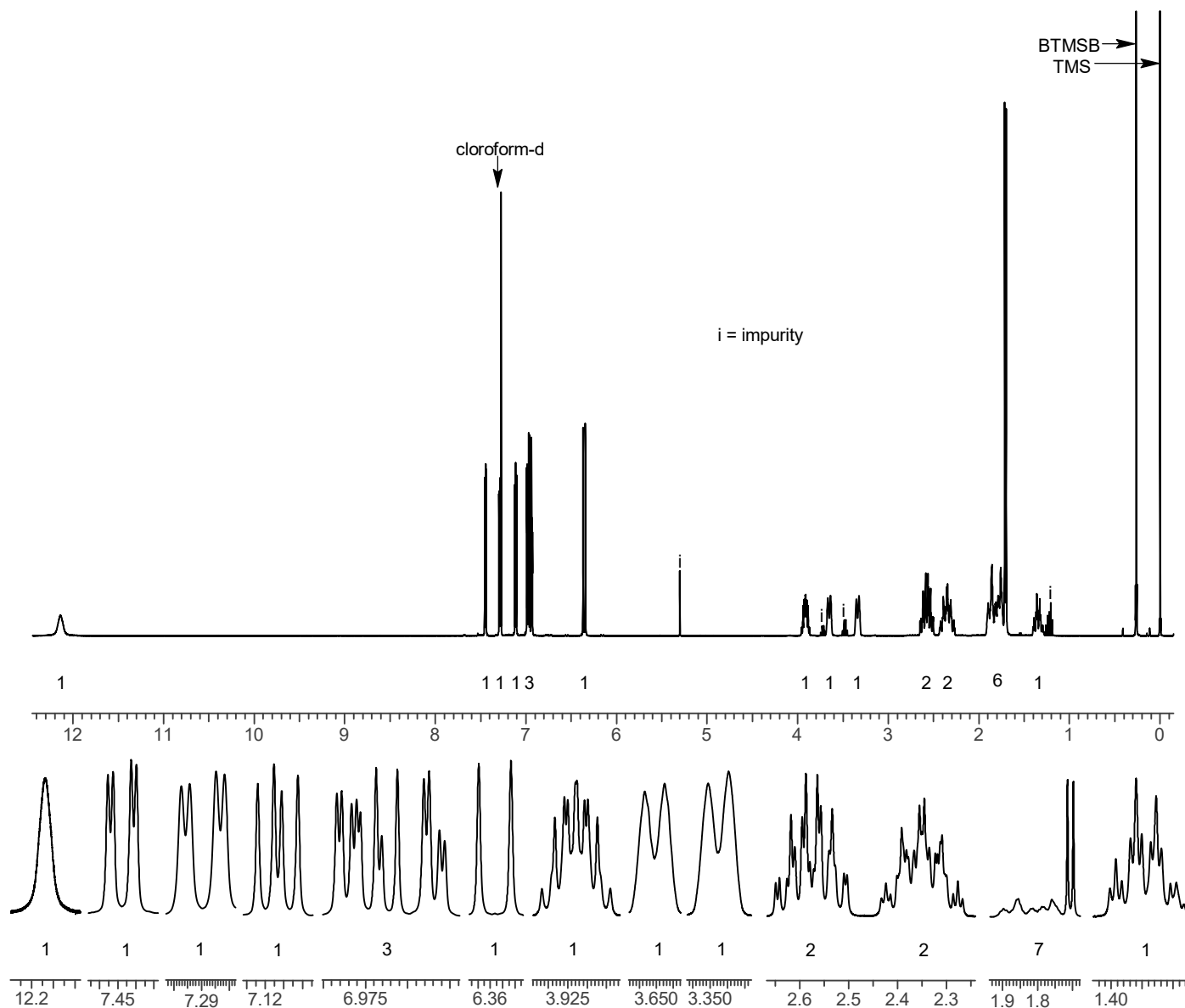
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 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

^1H NMR: Piperidylthiambutene HCl; Lot# 0567333-1; CDCl_3 ; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl_3

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

Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm

Carrier Gas: Helium at 0.91631 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

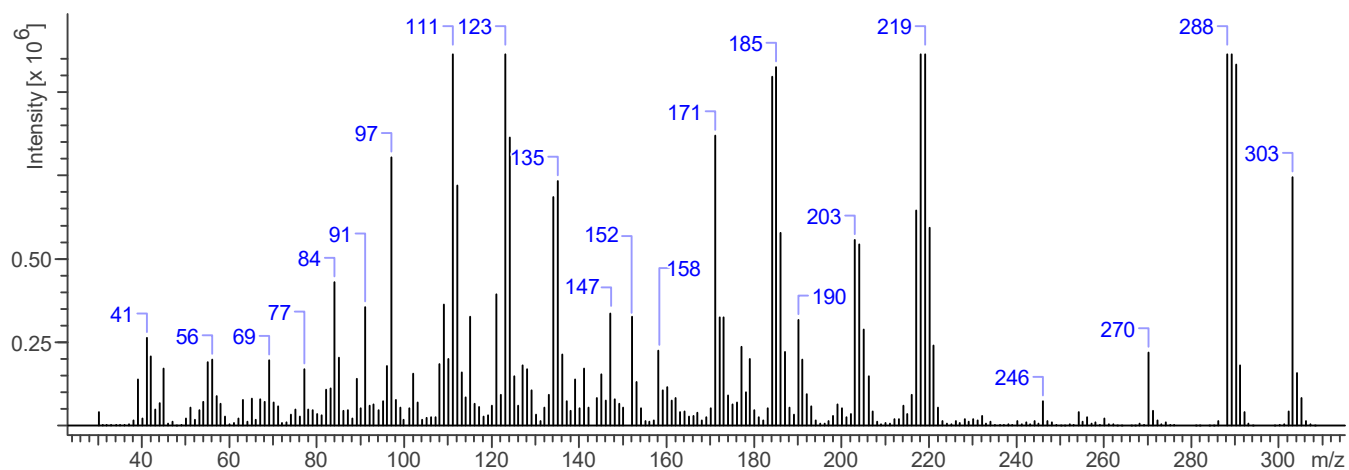
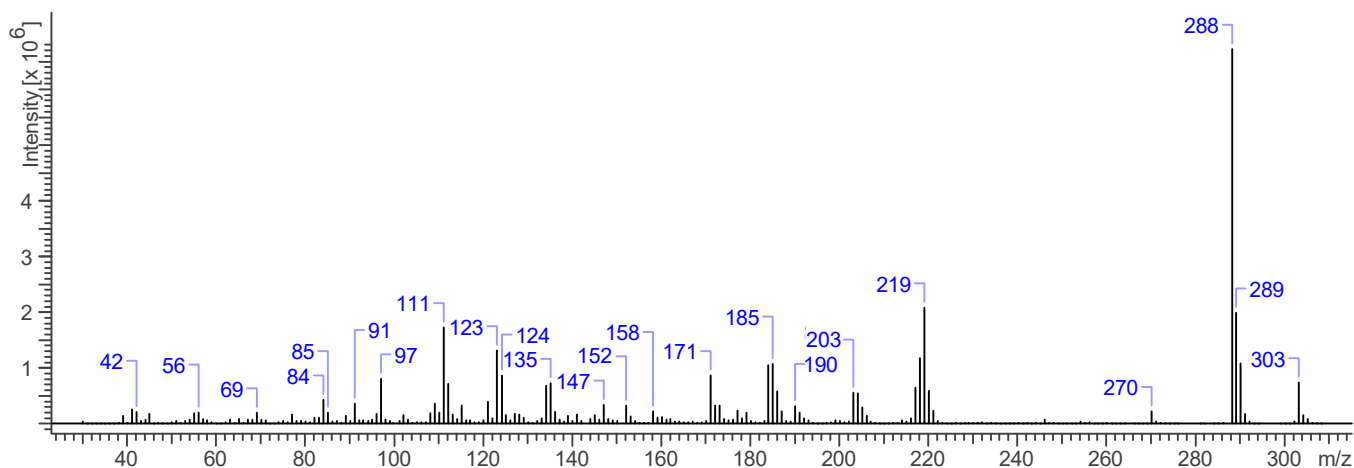
3) Hold final temperature for 30.0 min

Injection Parameters: Split Ratio = 25:1, 1 μL injected

MS Parameters: Mass scan range: 30-550 amu Threshold: 250
Tune file: stune.u Acquisition mode: scan

Retention Time: 14.03 min

EI Mass Spectrum: Piperidylthiambutene HCl; Lot# 0567333-1





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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): Piperidylthiambutene HCl; Lot# 0567333-1

