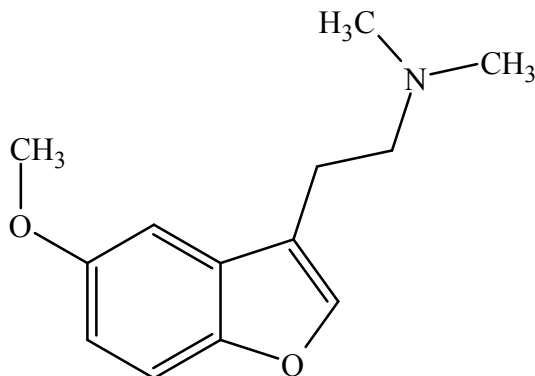




Dimemebfe

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



1. GENERAL INFORMATION

IUPAC Name:	2-(5-methoxy-1-benzofuran-3-yl)- <i>N,N</i> -dimethylethanamine
CAS#:	140853-58-3
Synonyms:	5-MeO-BFE, <i>N,N</i> -dimethyl-2-(5-methoxybenzofuran-3-yl)ethanamine
Source:	DEA Reference Material Collection
Appearance:	Off-white Powder (HCl)
UV_{max} (nm):	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₃ H ₁₇ NO ₂	219	Not Determined
HCl	C ₁₃ H ₁₇ NO ₂ · HCl	255	153.7



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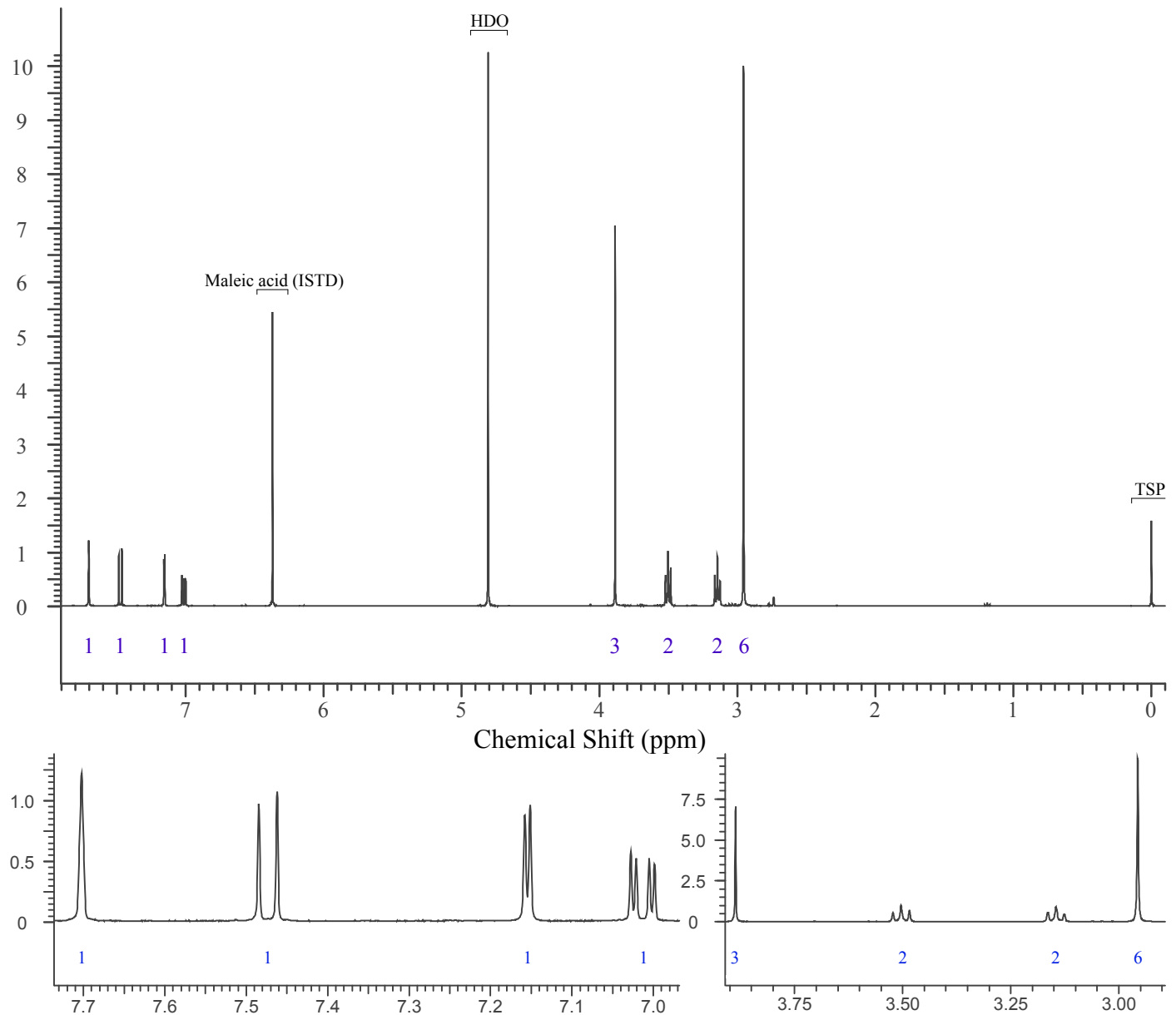


3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterium oxide (D₂O) containing TSP for 0 ppm reference and maleic acid 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: Dimemebfe HCl; Lot N17-P36B; D₂O; 400 MHz





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3.2 Gas Chromatography/Mass Spectrometry

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

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

Column: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μ m

Carrier Gas: Helium at 1 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 300°C at 12 °C/min

3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 20:1, 1 μ L injected

MS Parameters: Mass scan range: 34-550 amu

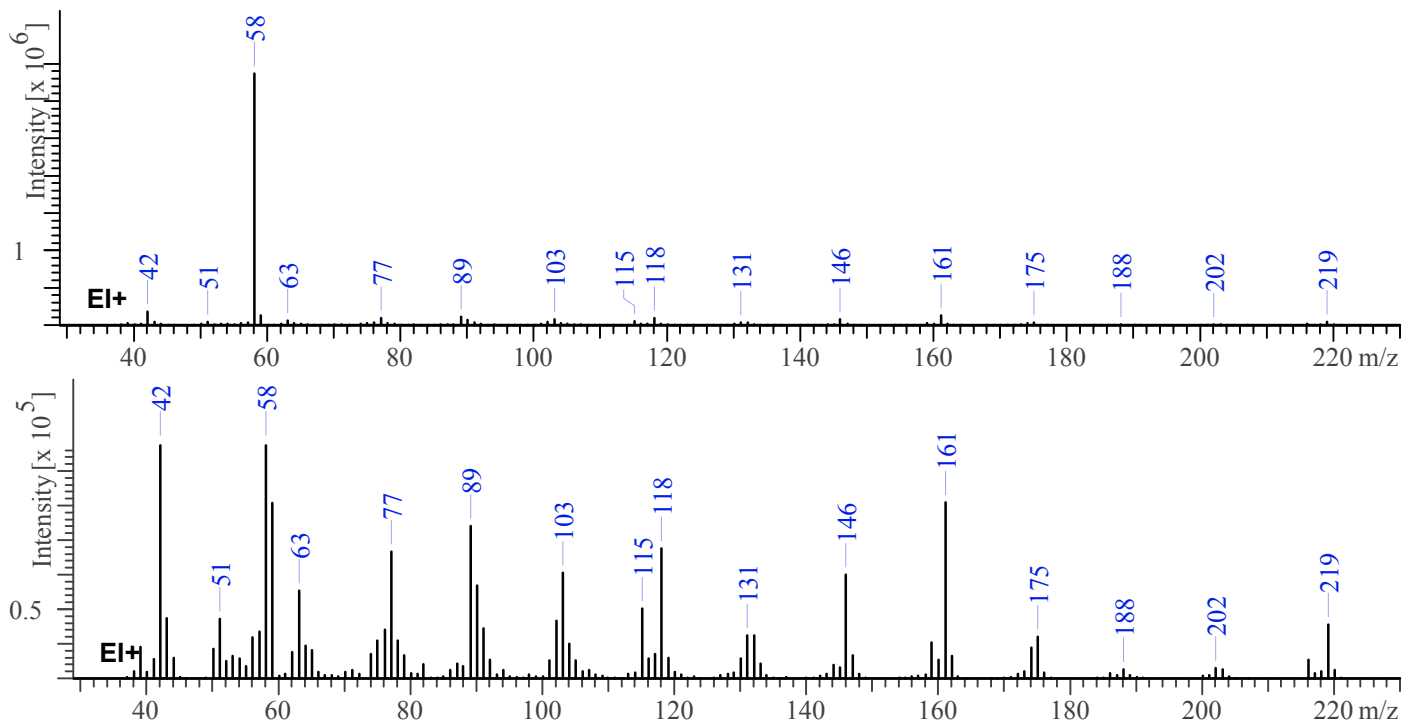
Threshold: 90

Tune file: stune.u

Acquisition mode: scan

Retention Time: 10.134 min

EI Mass Spectrum: Dimemebfe HCl; Lot N17-P36B





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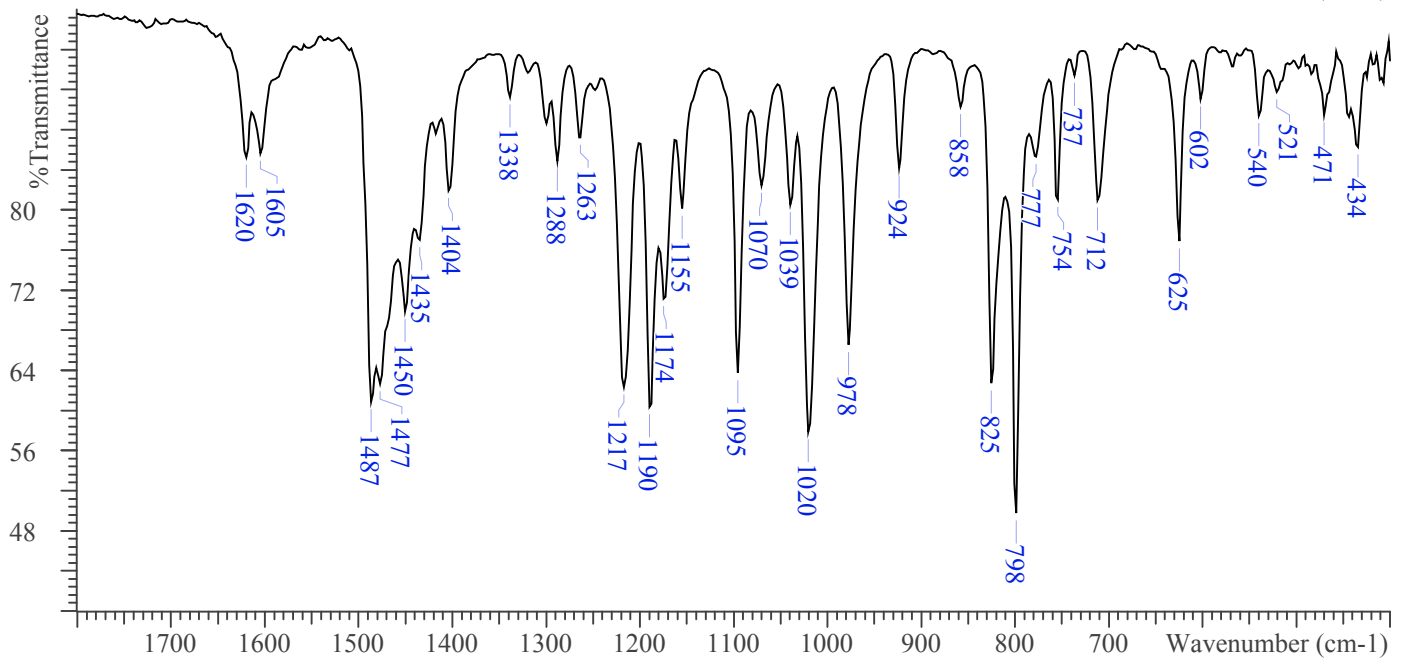
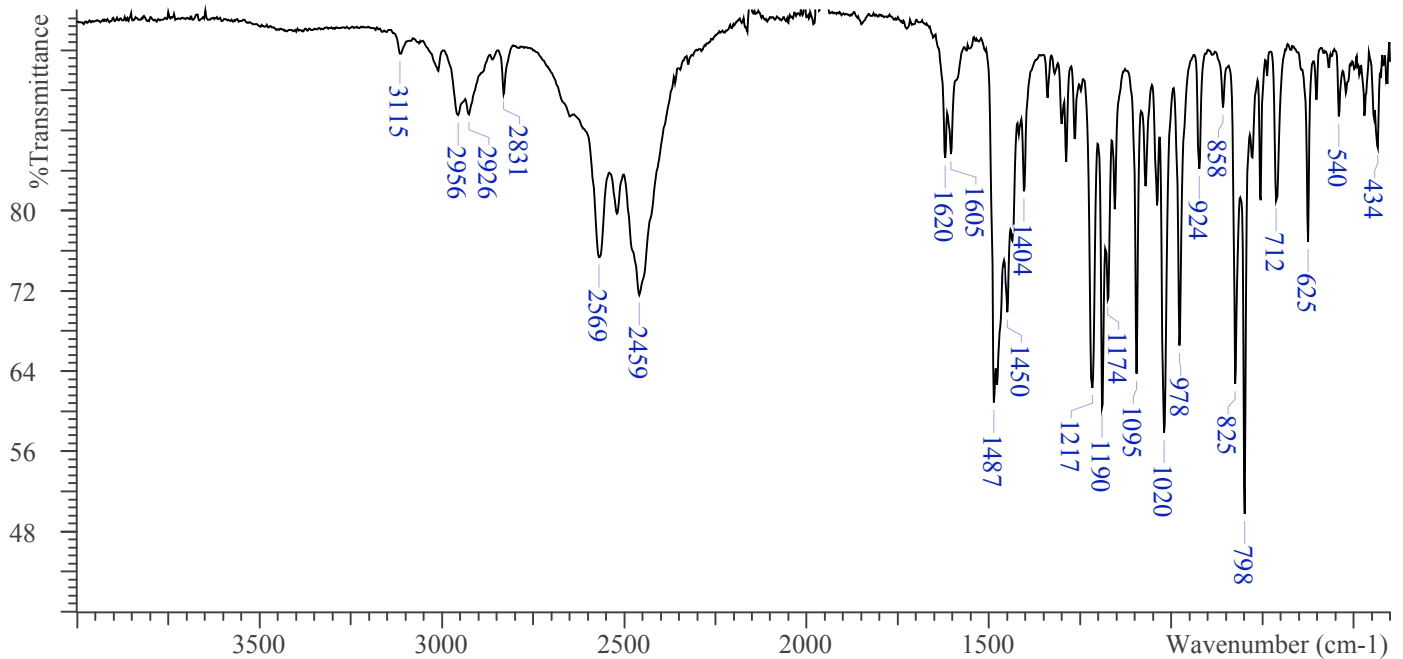


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)

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

FTIR ATR (Diamond, 3 Bounce): Dimemebfe HCl; Lot N17-P36B





Dimemebfe

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4. ADDITIONAL RESOURCES

Casale, J.F.; Hays, P.A. The Characterization of 2-(5-Methoxy-1-benzofuran-3-yl)-N,N-dimethylethanamine (5-MeO-BFE) and Differentiation from its N-Ethyl Analog. *Microgram Journal* **2012**, 9 (1), 39-45.

[Wikipedia](#)