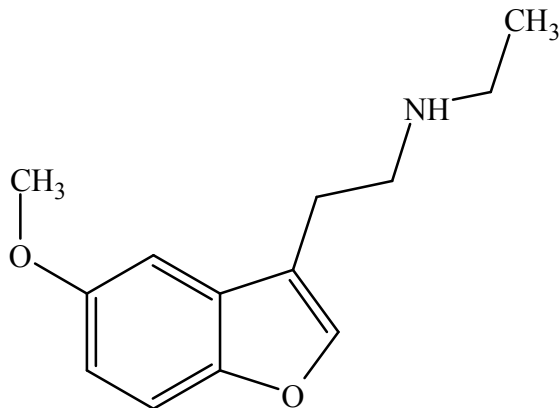




## Dimemebfe N-ethyl Analog

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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	N-ethyl-2-(5-methoxy-1-benzofuran-3-yl)ethanamine
<b>CAS#:</b>	Not Available
<b>Synonyms:</b>	2-(5-methoxybenzofuran-3-yl)-N-ethylethanamine
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	Off-white Powder (HCl)
<b>UV<sub>max</sub> (nm):</b>	Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>13</sub> H <sub>17</sub> NO <sub>2</sub>	219	Not Determined
HCl	C <sub>13</sub> H <sub>17</sub> NO <sub>2</sub> · HCl	255	123.5



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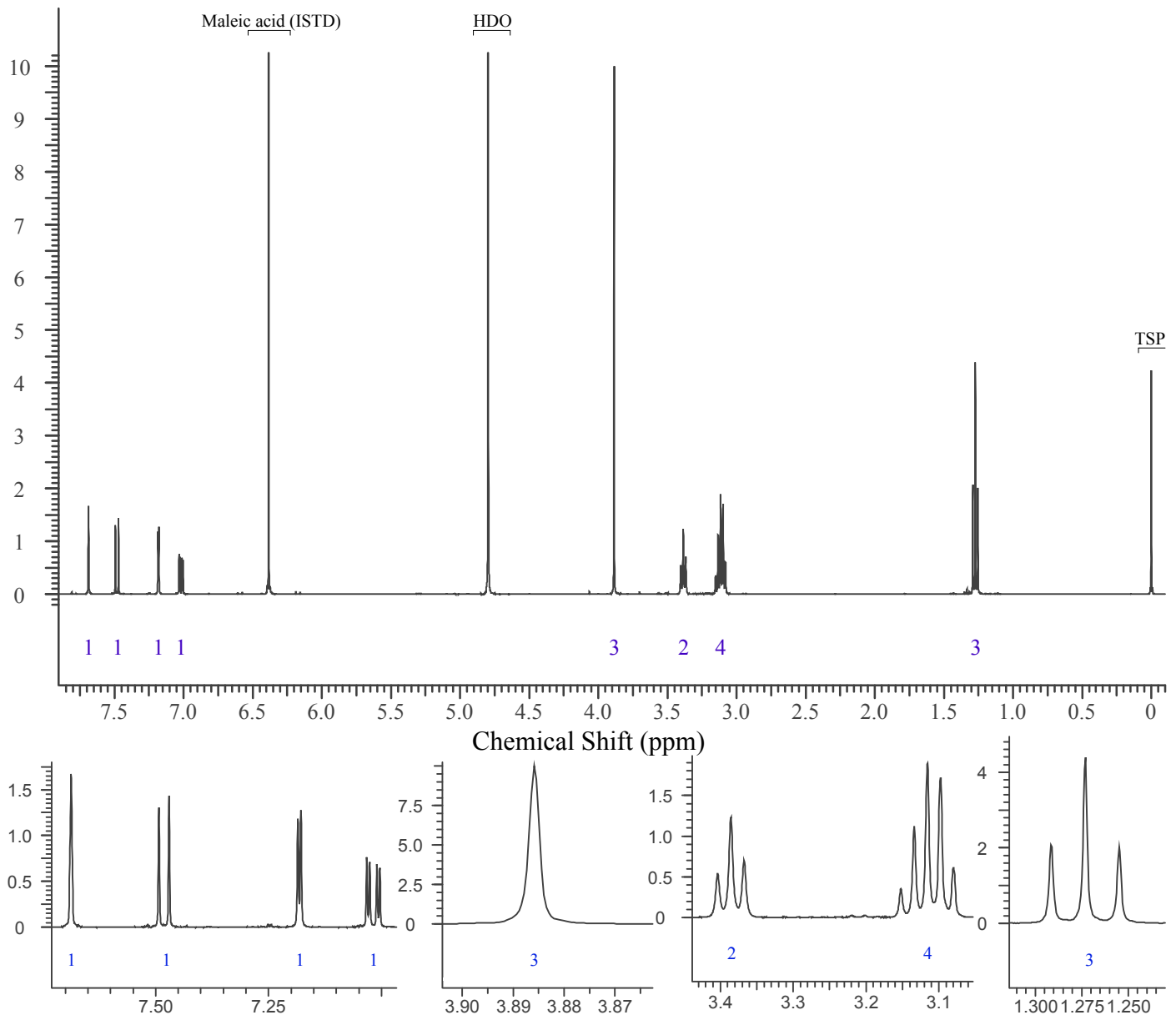
## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~5 mg/mL in deuterium oxide (D<sub>2</sub>O) 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

<sup>1</sup>H NMR: Dimemebfe N-ethyl analog HCl; Lot N17-P38B; D<sub>2</sub>O; 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  $\mu$ 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  $\mu$ L injected

**MS Parameters:** Mass scan range: 34-550 amu

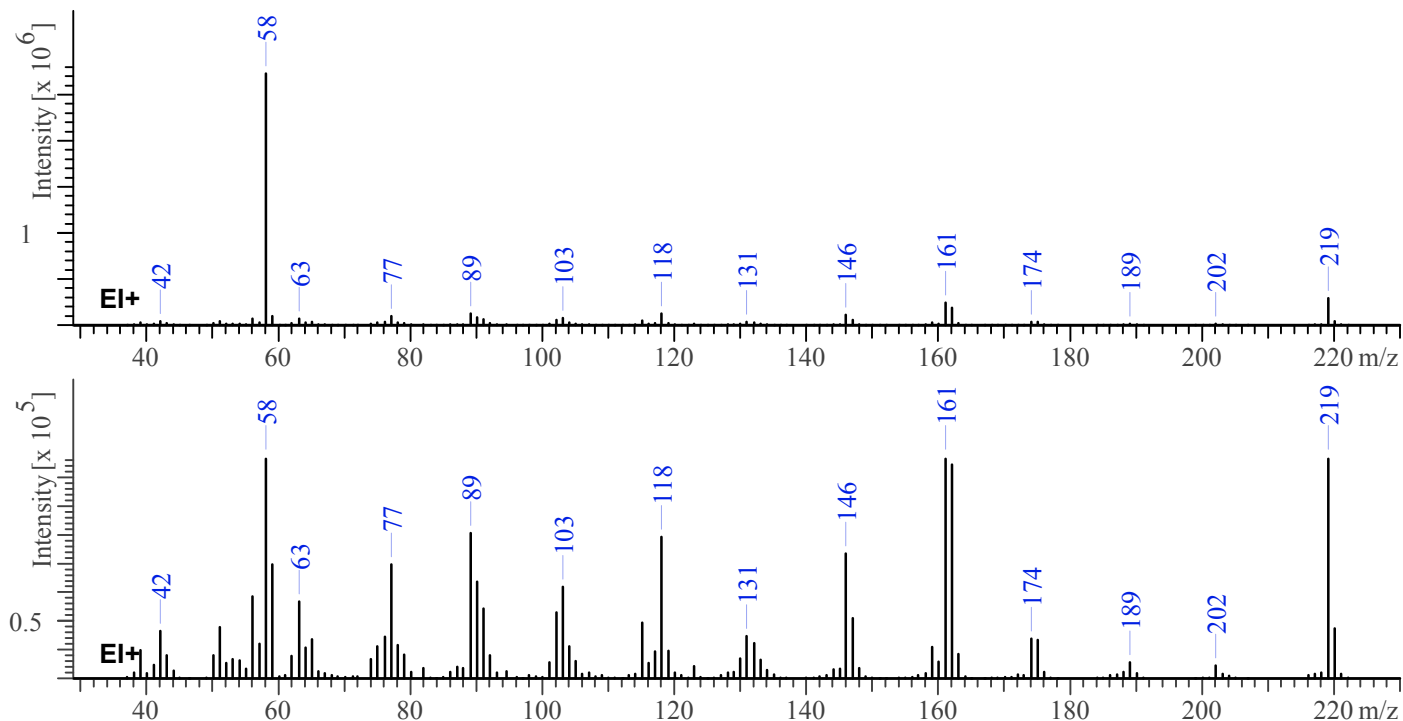
Threshold: 90

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 10.589 min

EI Mass Spectrum: Dimemebfe N-ethyl analog HCl; Lot N17-P38B





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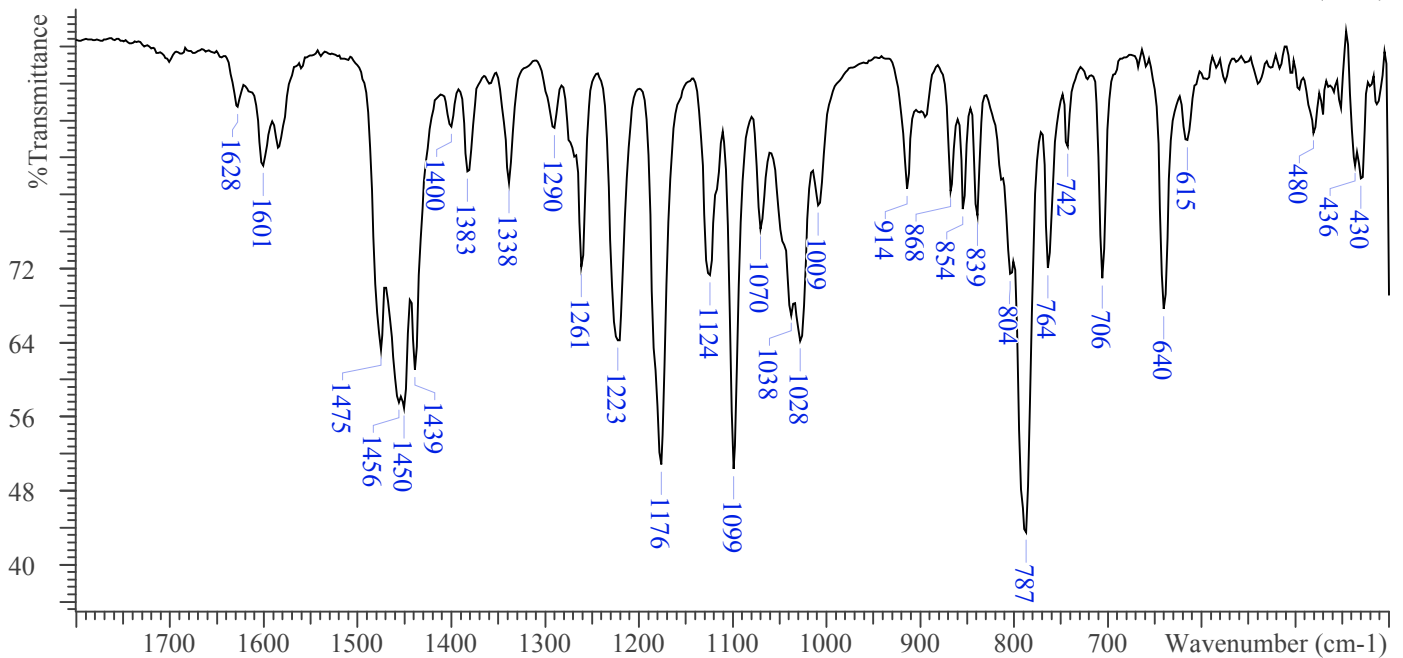
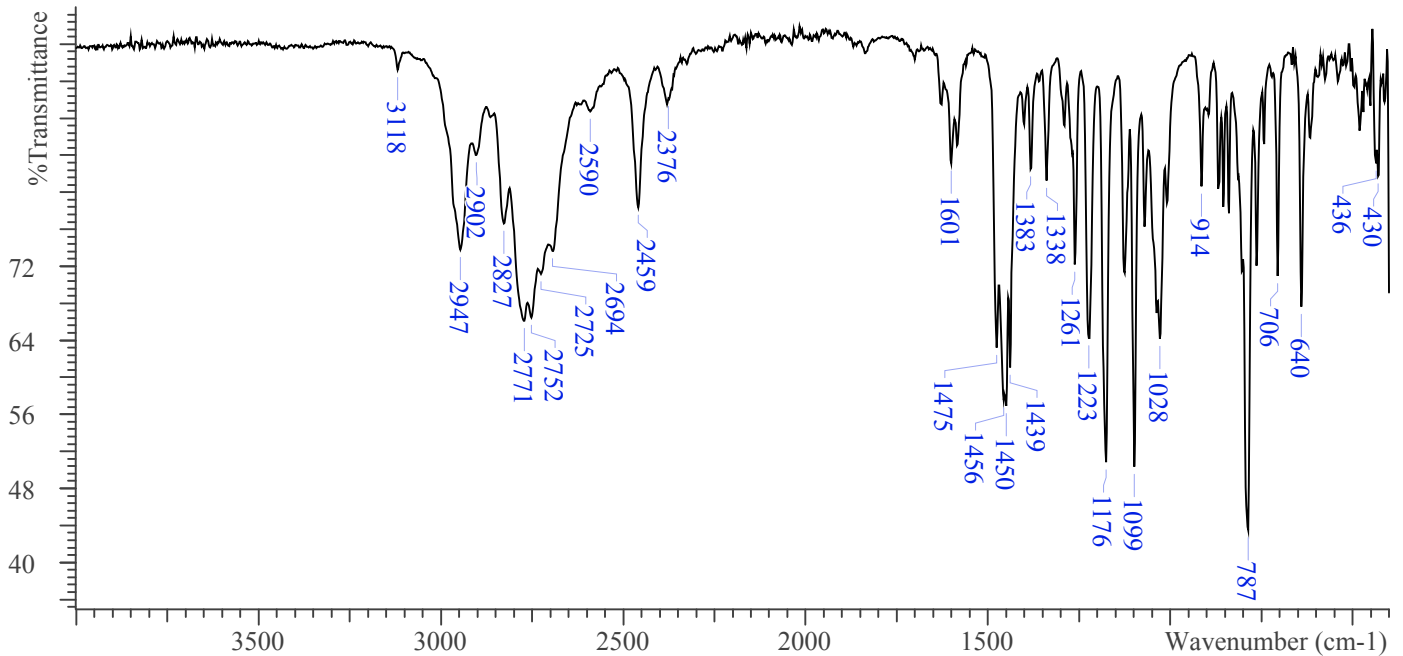


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**  
Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): Dimemebfe N-ethyl analog HCl; Lot N17-P38B





## Dimemebfe N-ethyl Analog

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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.