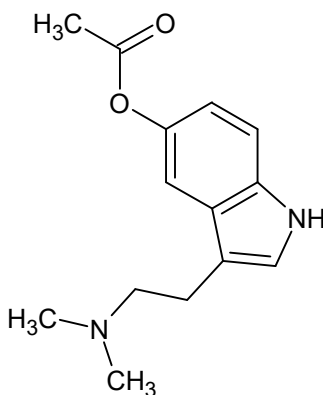




## 5-Acetoxy-N,N-dimethyltryptamine

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



### 1. GENERAL INFORMATION

**IUPAC Name:** 3-[2-(dimethylamino)ethyl]-1H-indol-5-yl acetate

**CAS#:** NA

**Synonyms:** 5-Acetoxy-DMT, 5-AcO-DMT

**Source:** DEA Reference Material Collection

**Appearance:** White Powder (Oxalate)

**UV<sub>max</sub>(nm):** Not determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	246	Not Determined
Oxalate	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> C <sub>2</sub> H <sub>2</sub> O <sub>4</sub>	336	151.7



# 5-Acetoxy-N,N-dimethyltryptamine

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



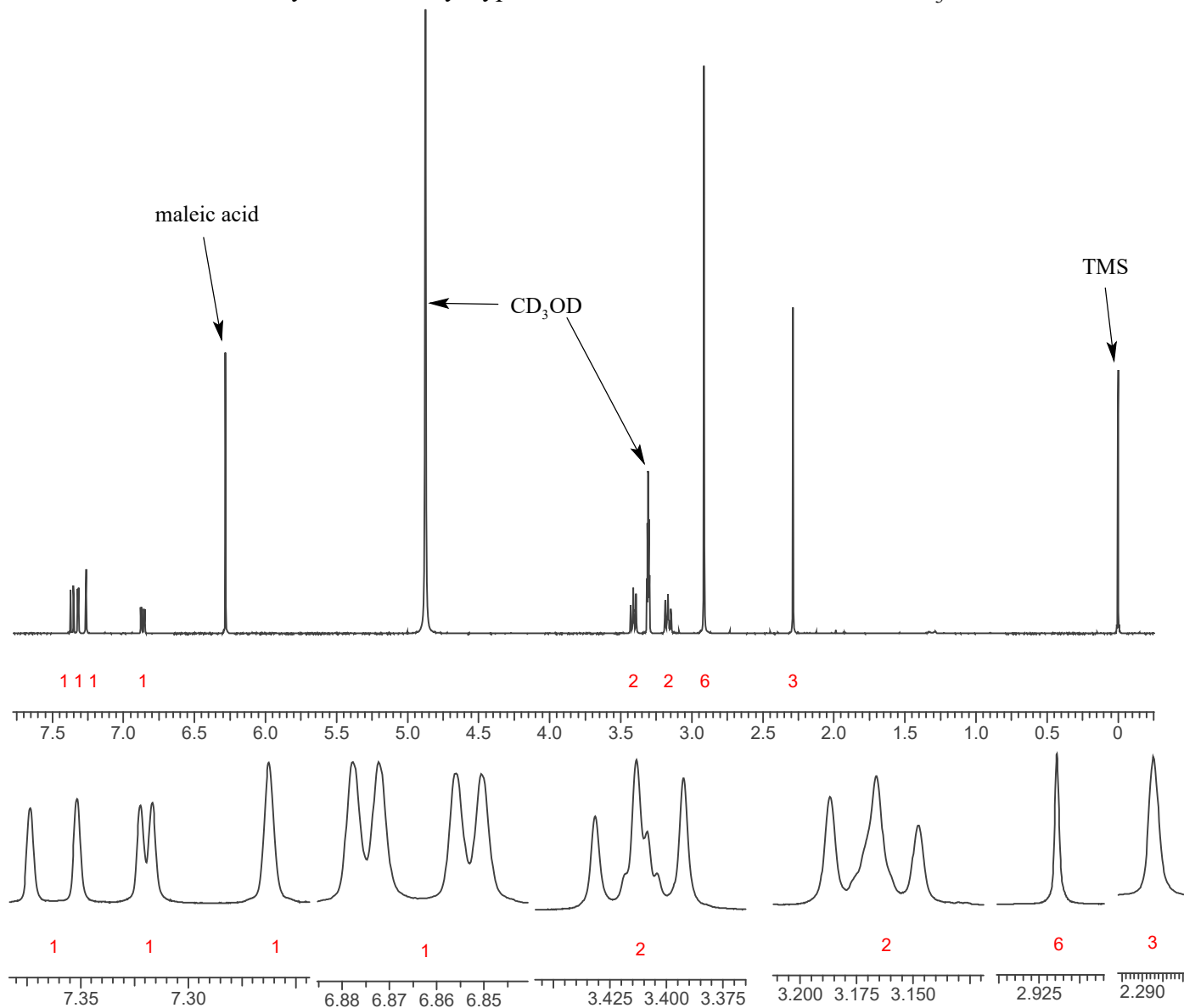
## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~10 mg/mL in CD<sub>3</sub>OD containing TMS 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>HNMR: 5-Acetoxy-N,N-dimethyltryptamine Oxalate; Lot# TAD121908; CD<sub>3</sub>OD; 400MHz





# 5-Acetoxy-N,N-dimethyltryptamine

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

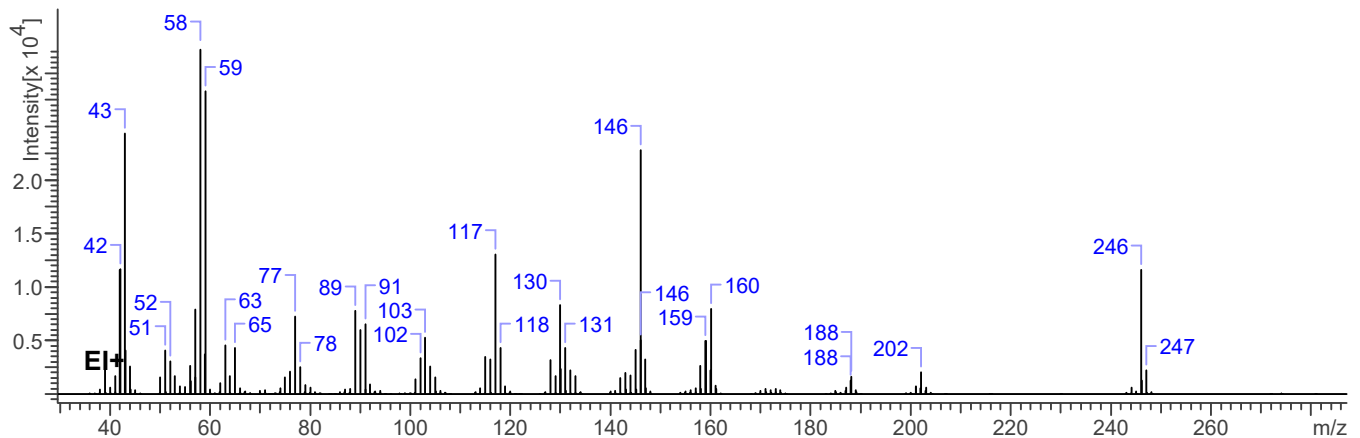
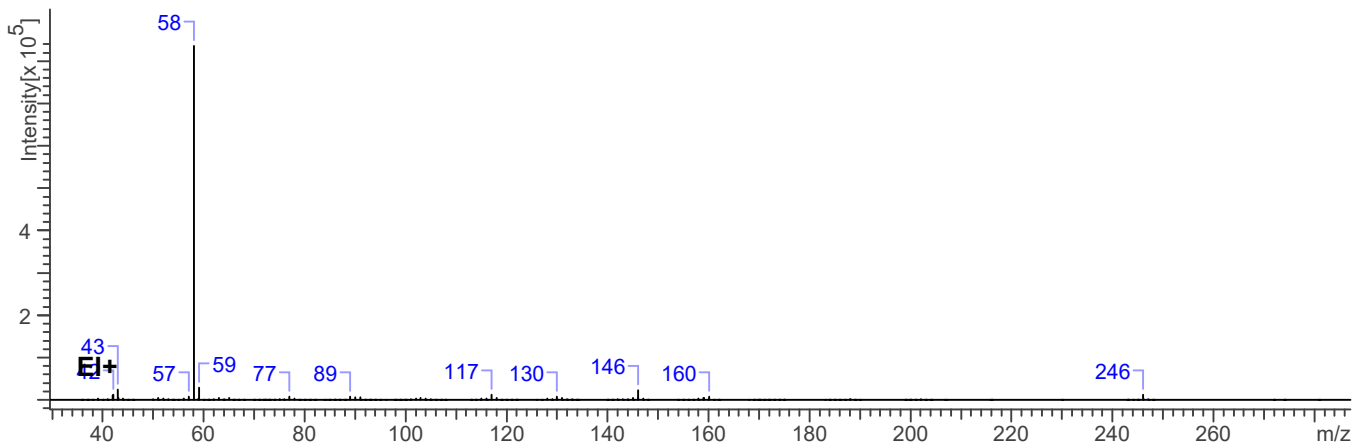


## 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte ~4 mg/mL in MeOH

**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 μm  
**Carrier Gas:** Helium at 1.0 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 = 25:1, 1 μL injected  
**MS Parameters:** Mass scan range: 30-550 amu                      Threshold: 150  
Tune file: stune.u                      Acquisition mode: scan  
**Retention Time:** 13.75 min

EI Mass Spectrum: 5-Acetoxy-N,N-dimethyltryptamine Oxalate; Lot# TAD121908





# 5-Acetoxy-N,N-dimethyltryptamine

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

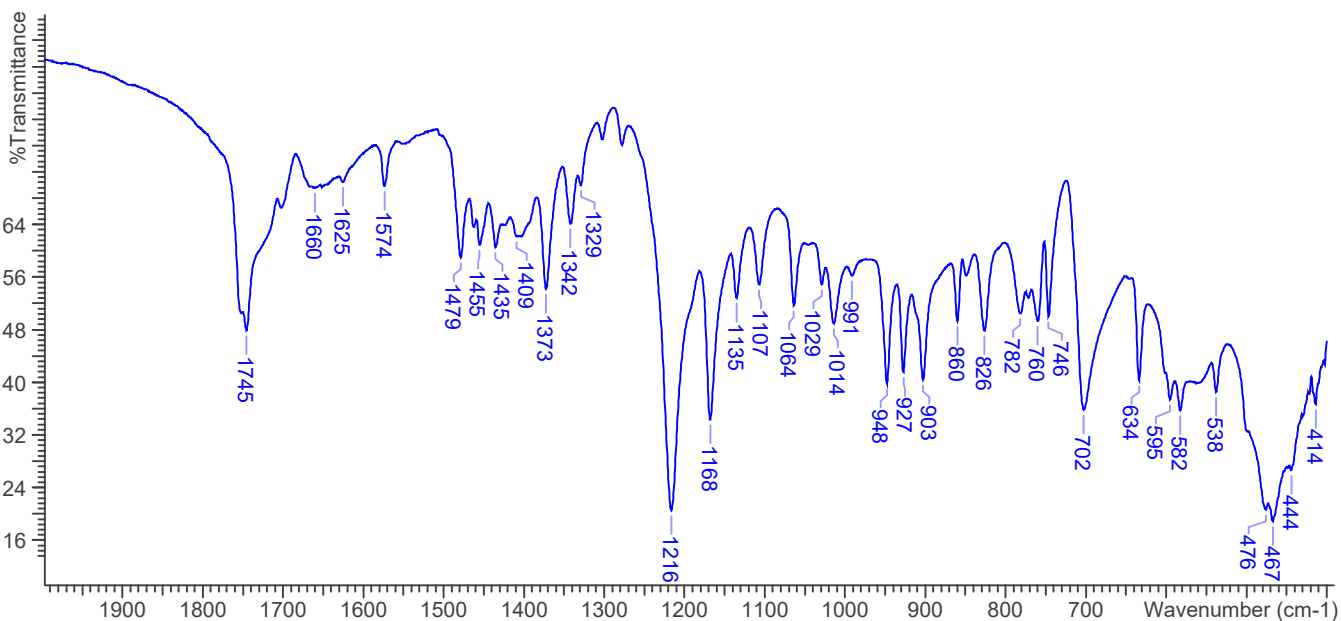
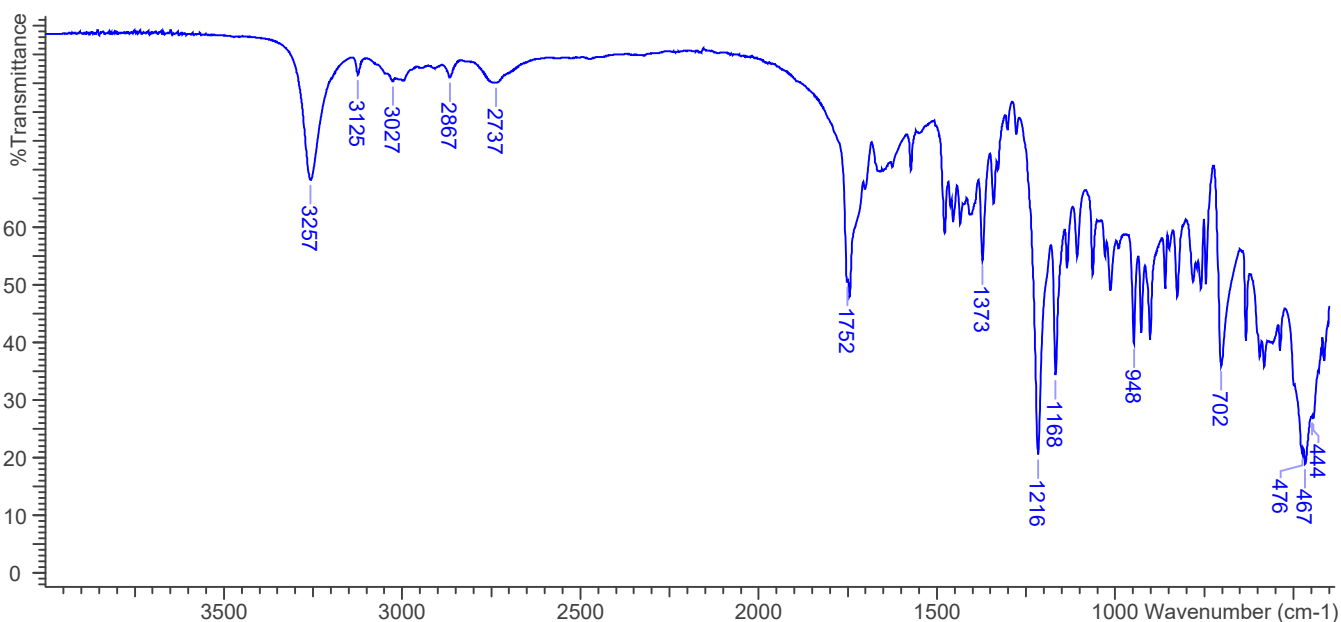


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (1 bounce)

**Scan Parameters:**  
Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 80

FTIR ATR (Diamond 1 Bounce): 5-Acetoxy-N,N-dimethyltryptamine Oxalate; Lot# TAD121908





## 5-Acetoxy-N,N-dimethyltryptamine

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



### **4. ADDITIONAL RESOURCES**

No additional resources as of 04/2016