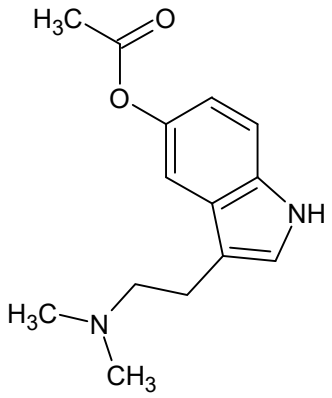
# 5-Acetoxy-N,N-dimethyltryptamine

*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]-1*H*-indol-5-yl acetate

***CAS#:*** NA

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

***Source:*** DEA Reference Material Collection

***Appearance:*** White Powder (Oxalate)

***$UV_{max}$(nm):*** Not determined

## *2. CHEMICAL AND PHYSICAL DATA*

### 2.1 CHEMICAL DATA

| Form | Chemical Formula | Molecular Weight | Melting Point ($^{o}$C) |
|---|---|---|---|
| Base | $C_{14}H_{18}N_2O_2$ | 246 | Not Determined |
| Oxalate | $C_{14}H_{18}N_2O_2$ $C_2H_2O_4$ | 336 | 151.7 |

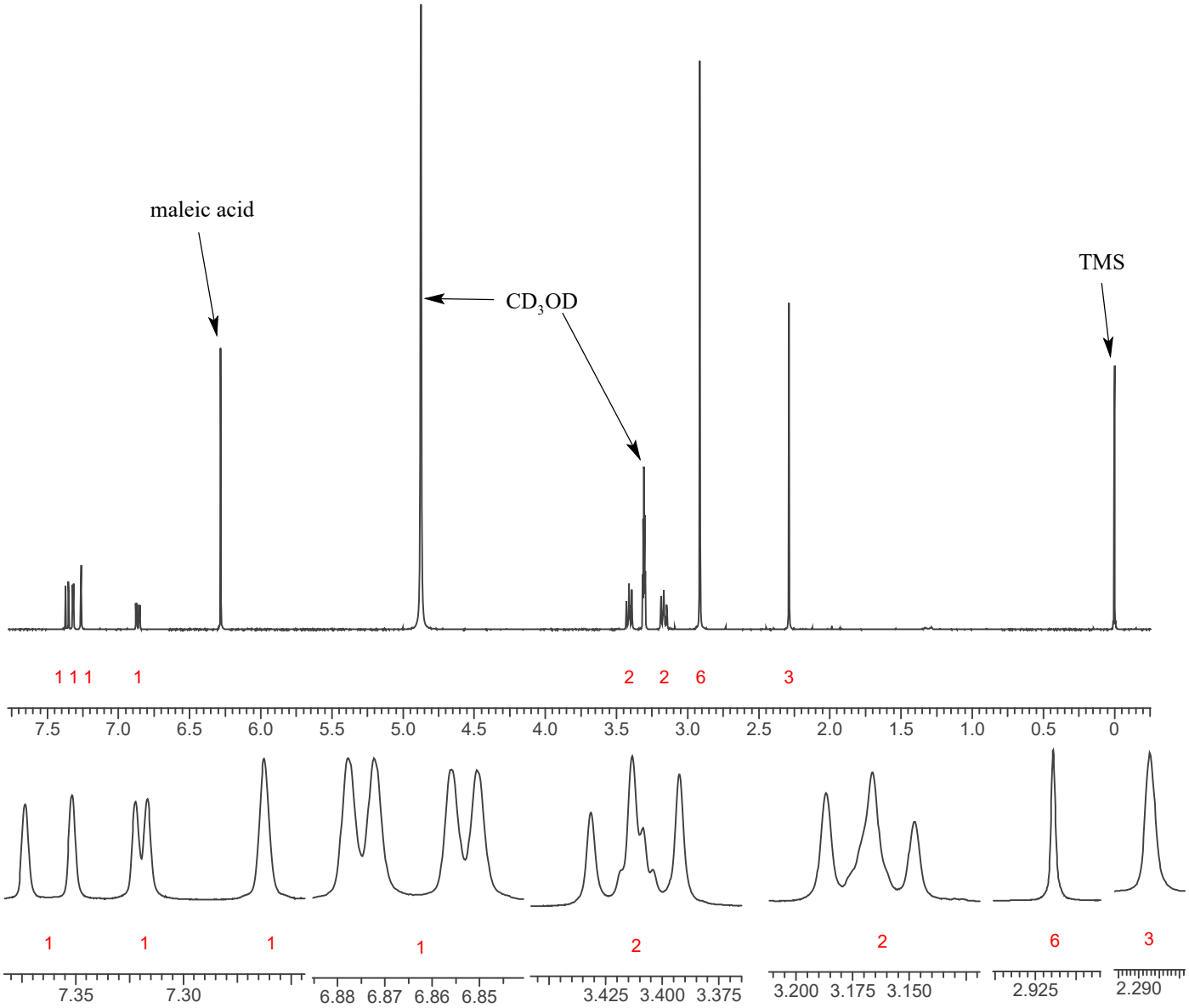
## *3. QUALITATIVE DATA*

### 3.1 NUCLEAR MAGNETIC RESONANCE

*Sample Preparation:* Dilute analyte to ~10 mg/mL in $CD_3OD$ 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

$^1$HNMR: 5-Acetoxy-N,N-dimethyltryptamine Oxalate; Lot# TAD121908; $CD_3OD$; 400MHz

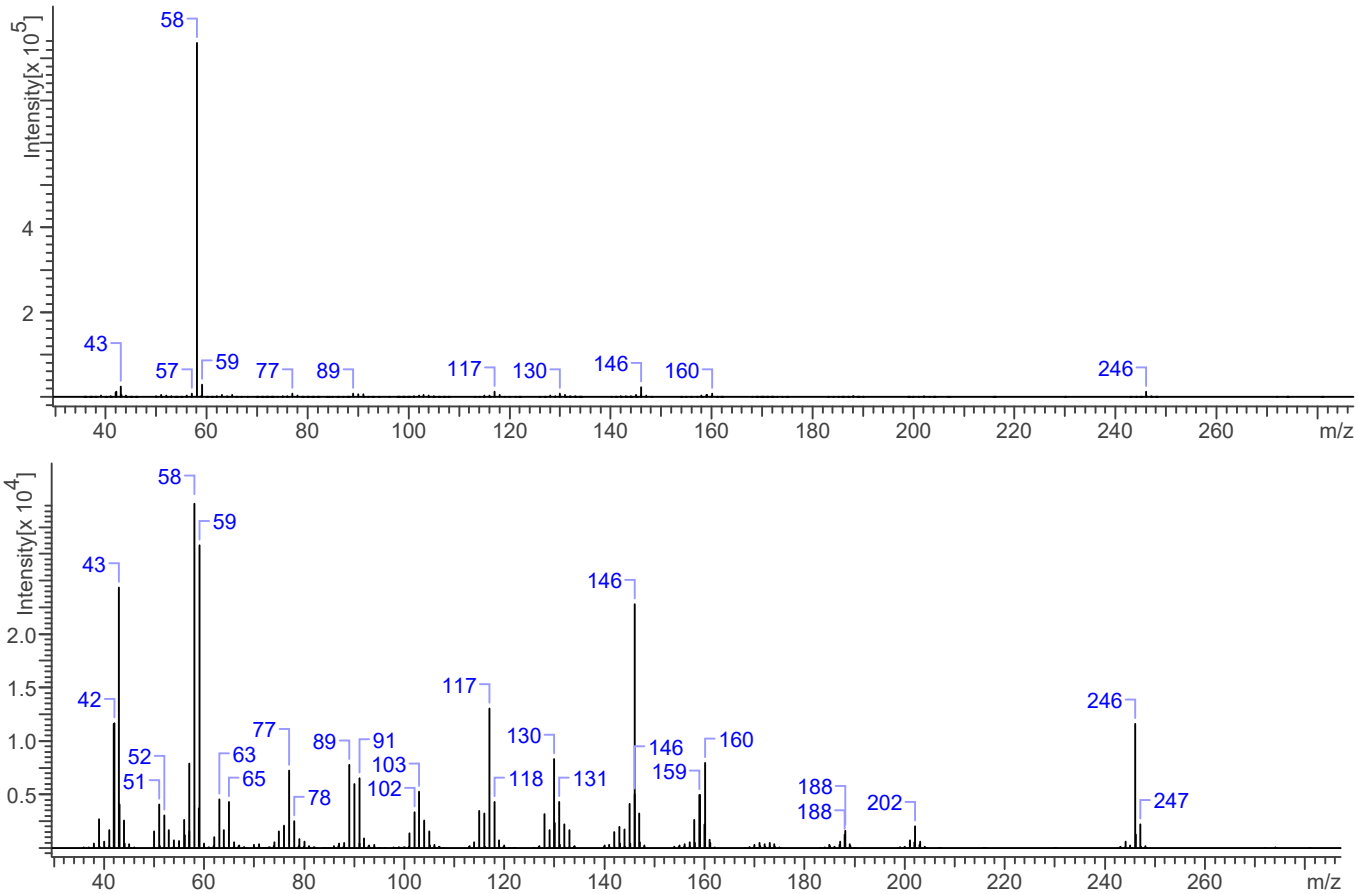


## 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*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<br>MS Source: 230°C MS Quad: 150°C<br>Oven program:<br>1) 100°C initial temperature for 1.0 min<br>2) Ramp to 300°C at 12 °C/min<br>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<br>Tune file: stune.u Acquisition mode: scan |
| ***Retention Time:*** | 13.75 min |

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

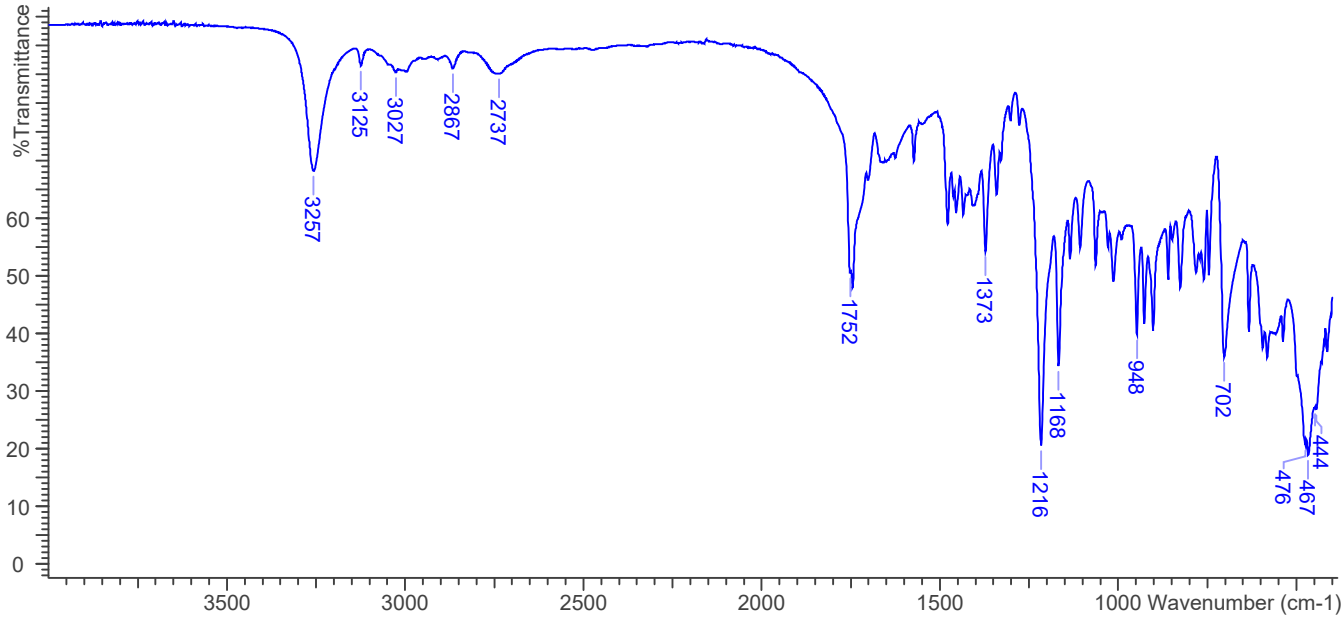


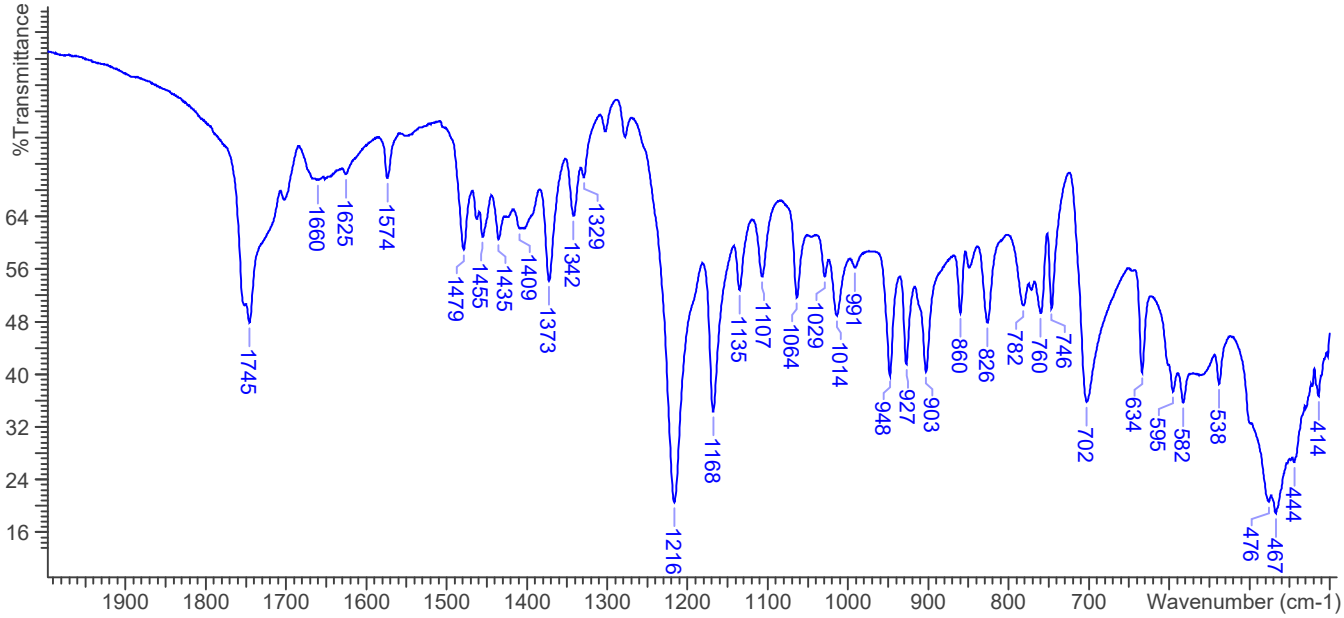
## 3.3 INFRARED SPECTROSCOPY (FTIR)

**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: 8
Aperture: 80

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



## *4. ADDITIONAL RESOURCES*

No additional resources as of 07/2016