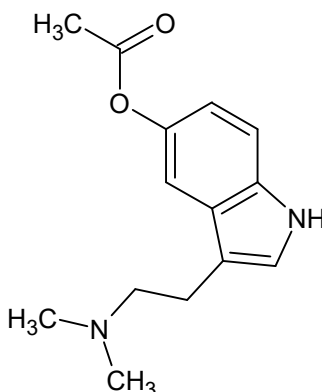




5-Acetoxy-N,N-dimethyltryptamine

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_{max}(nm): Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

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



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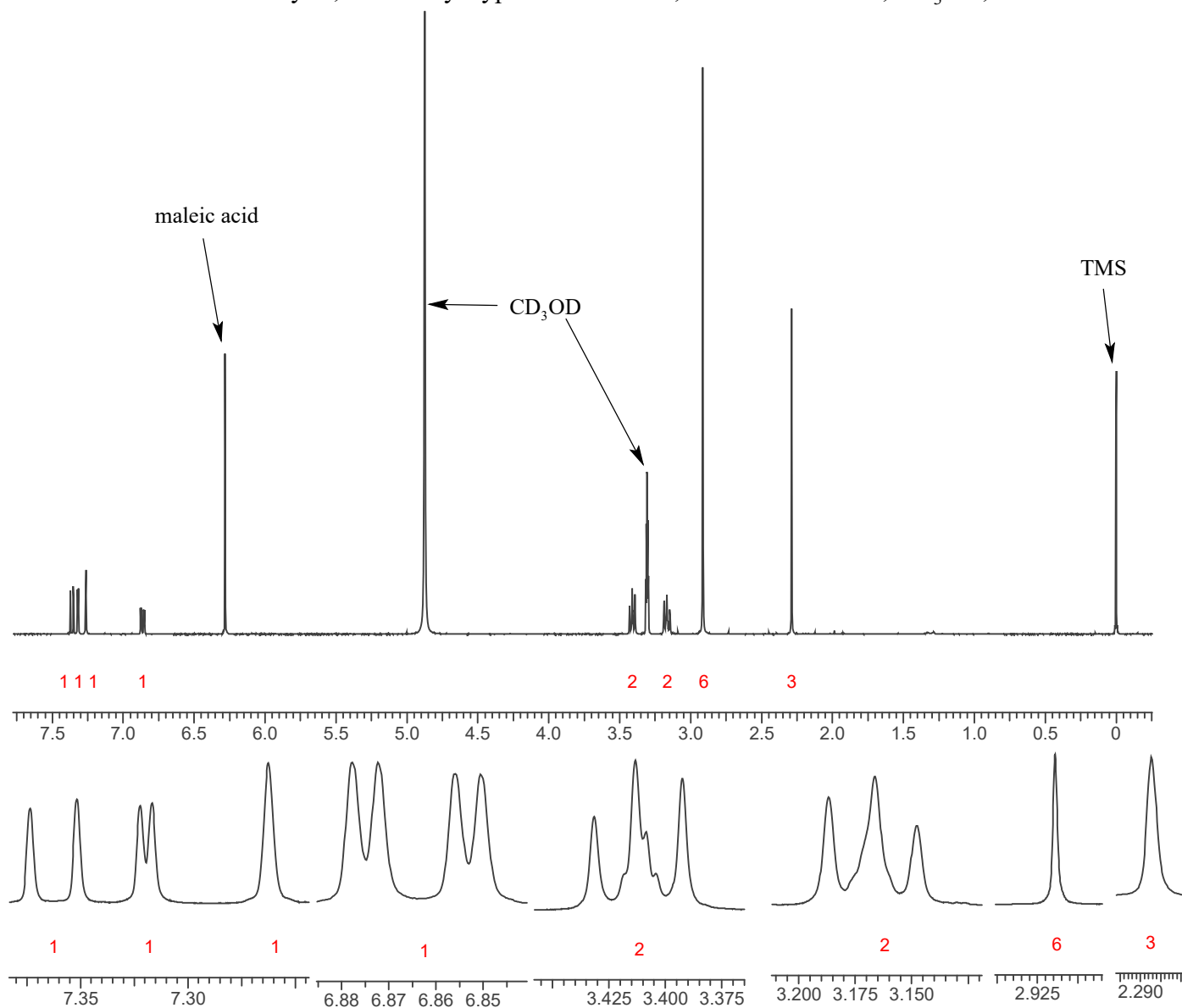
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in CD₃OD 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

¹HNMR: 5-Acetoxy-N,N-dimethyltryptamine Oxalate; Lot# TAD121908; CD₃OD; 400MHz





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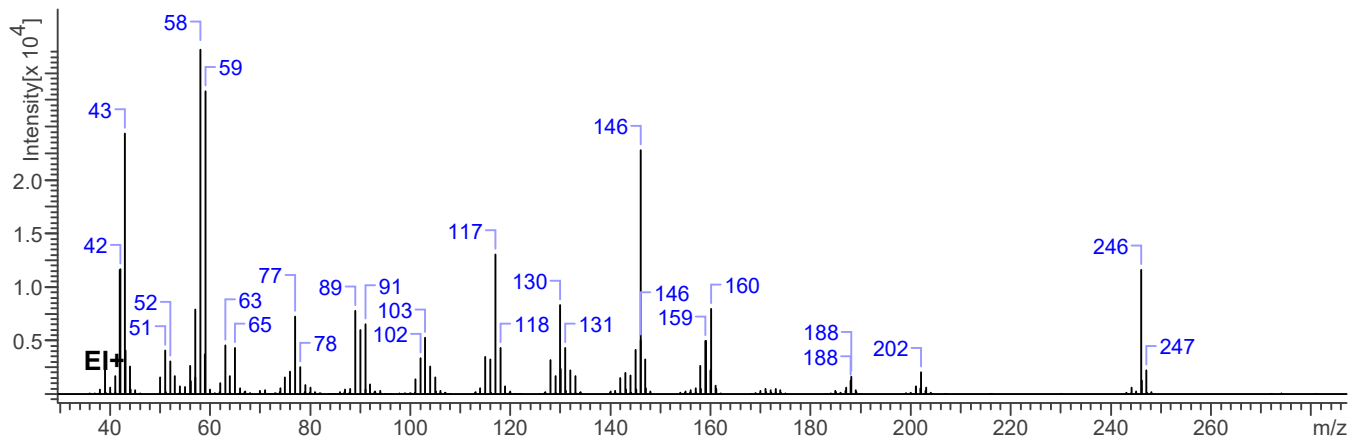
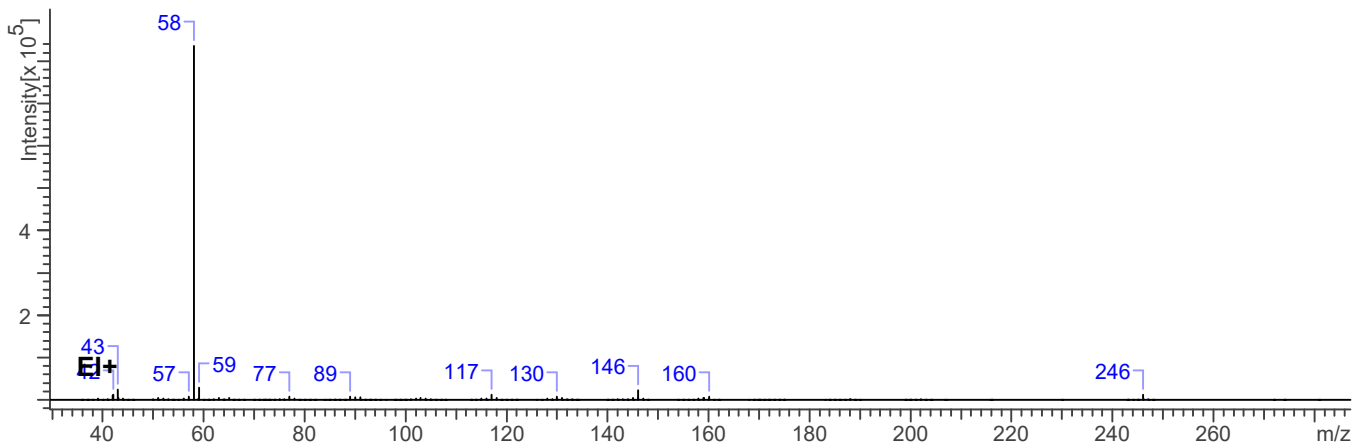


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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 μ m
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 μ L 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





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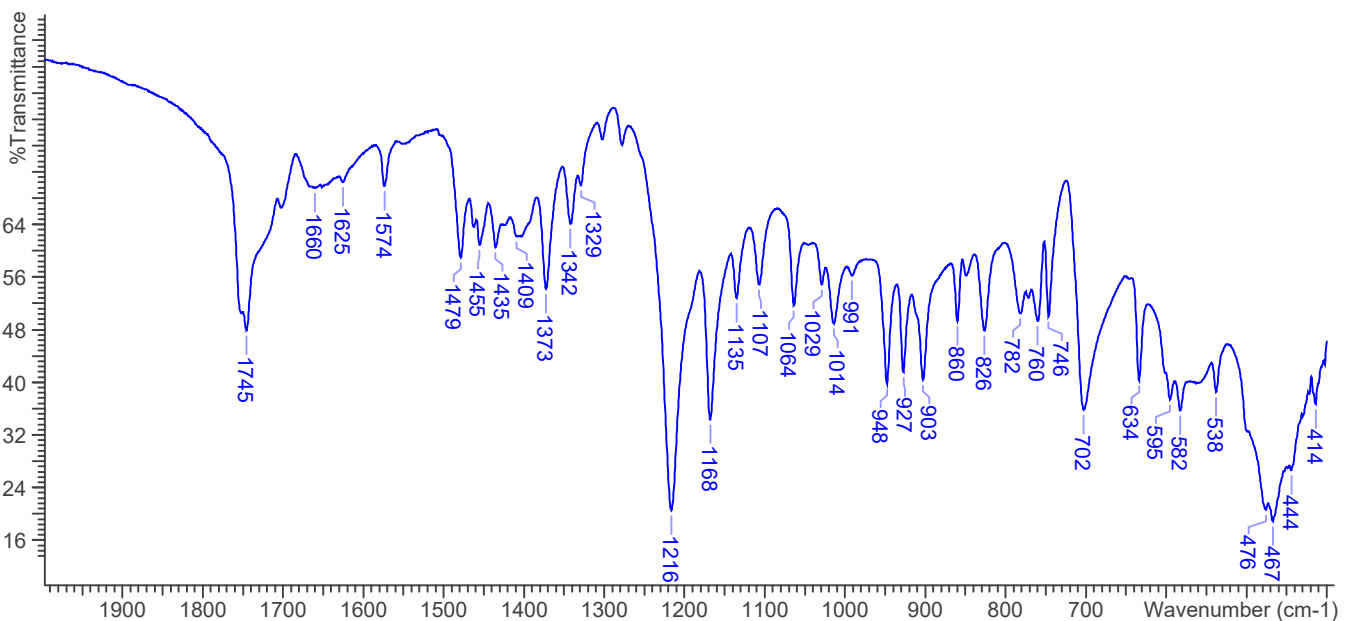
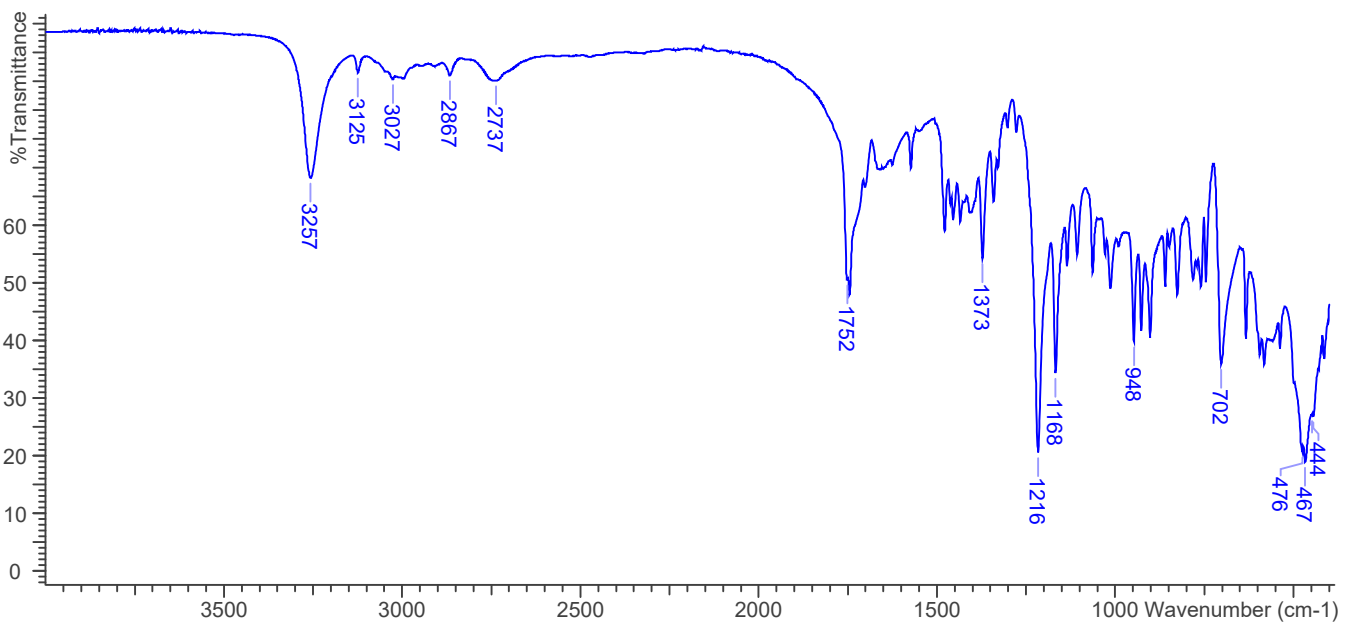


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 8
Aperture: 80

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





5-Acetoxy-N,N-dimethyltryptamine

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4. ADDITIONAL RESOURCES

No additional resources as of 04/2016