

1. GENERAL INFORMATION

IUPAC Name: 3-[2-(Dimethylamino)ethyl]-1*H*-indol-4-yl acetate

CFR: Not Scheduled (3/2013)

CAS #: 92292-84-7

Synonyms: 4-AcO-DMT; psilacetin; *O*-acetylpsilocin

Source: DEA Reference Material Collection

Appearance: Off-white powder (oxalate)

Kovat's Index: Pending

UV_{max}: 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	144.2

3. ADDITIONAL RESOURCES

[Wikipedia](#)

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CD₃OD

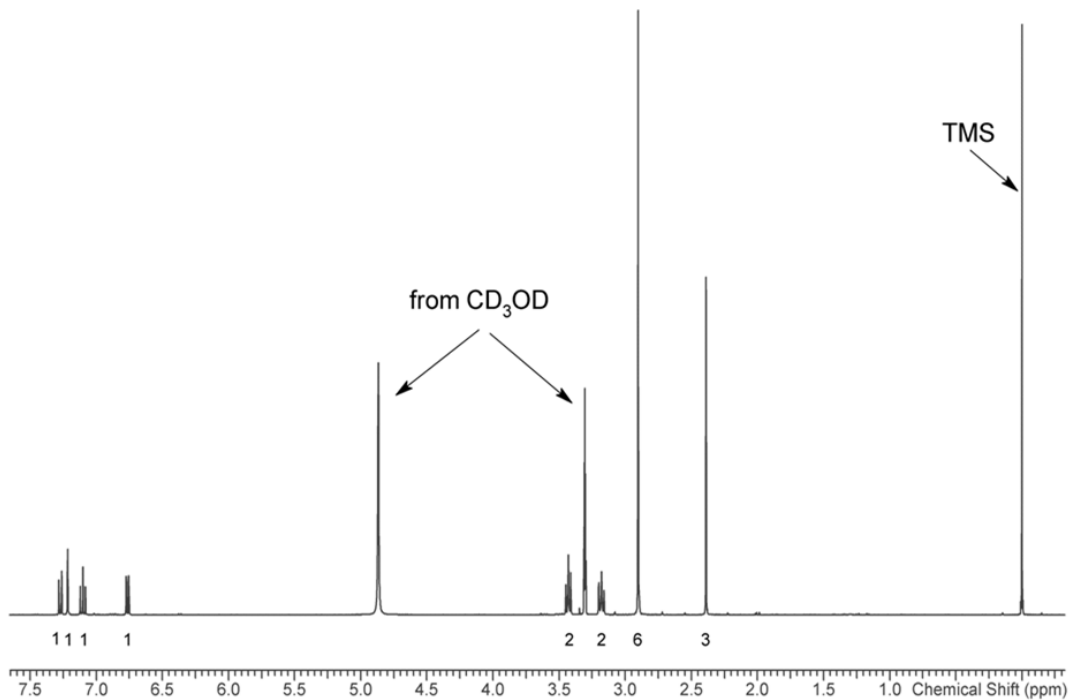
Sample Preparation: Dilute analyte to ~10 mg/mL in deuterated methanol (CD₃OD) containing TMS for 0 ppm reference.

Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

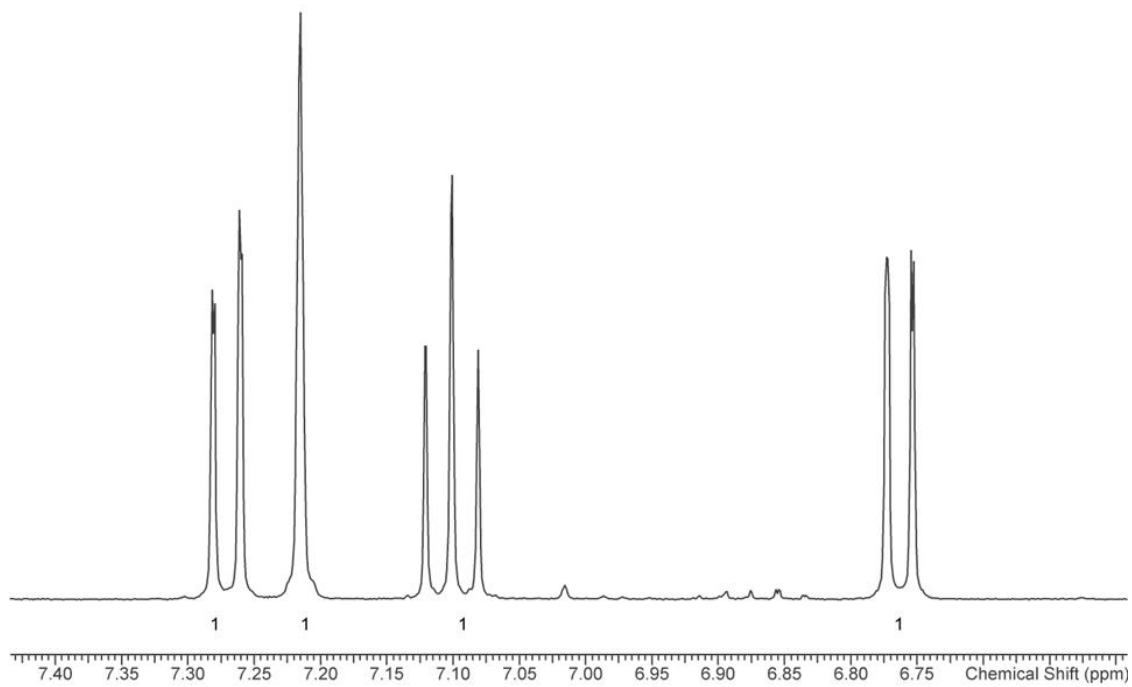
Parameters:

- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

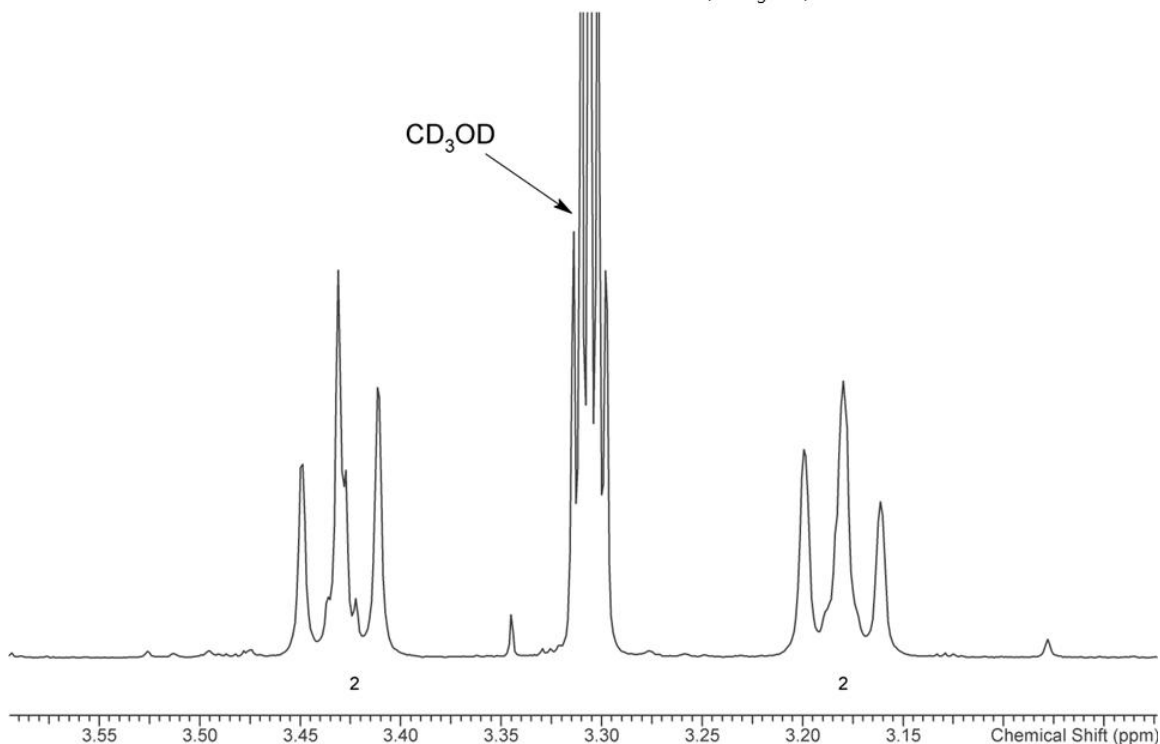
¹H NMR: 4-AcO DMT Oxalate Lot # H-0705; CD₃OD; 400 MHz



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1H NMR: 4-AcO DMT Oxalate Lot # H-0705; CD₃OD; 400 MHz



4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in methanol.

Instrument: Gas chromatograph operated in split mode with MS detector

Column: DB-1 MS or equivalent; 30m x .25mm x .25µm

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 = 25:1, 1 µL injected

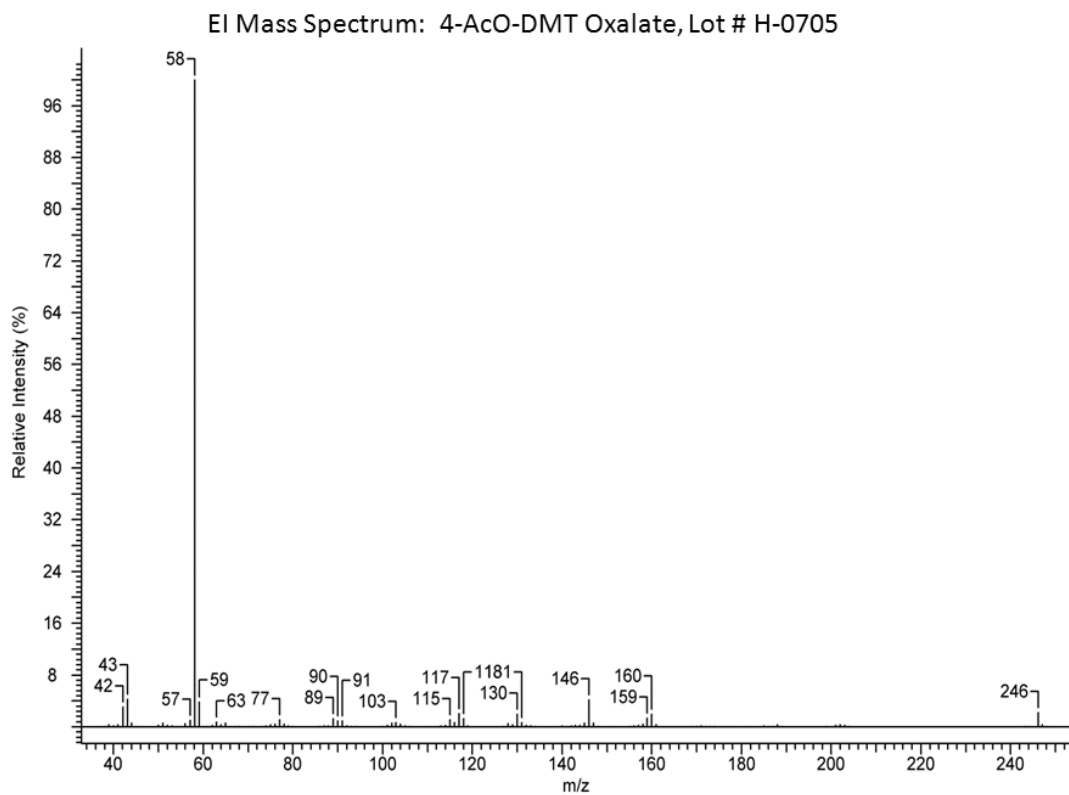
MS Parameters: Mass scan range: 34-550 amu

Threshold: 100

Tune file: stune.u

Acquisition Mode: scan

Retention Time: 13.199 min



4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument:

FTIR with ATR attachment

Scan Parameters:

Number of scans: 32

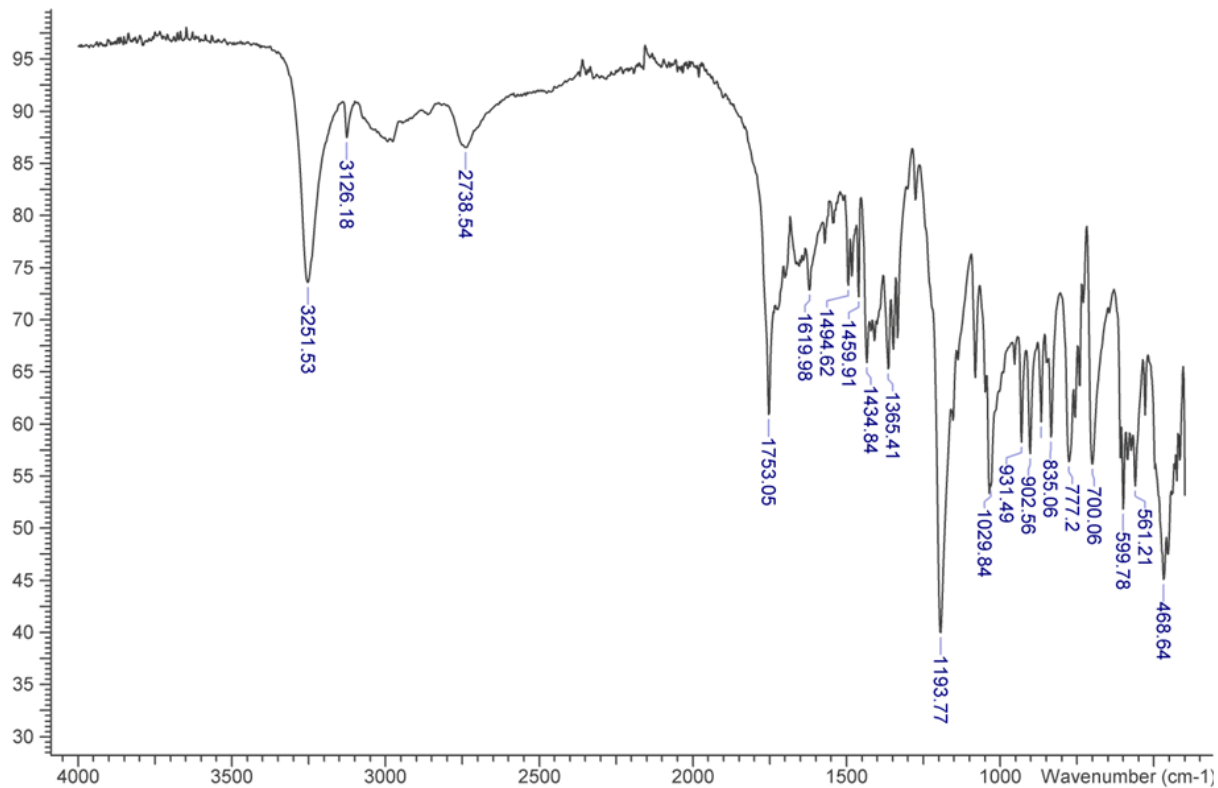
Number of background scans: 32

Resolution 4 cm⁻¹

Sample gain: 8

Aperture: 150

FTIR (Diamond ATR, 3 Bounce): 4-AcO-DMT Oxalate Lot # H-0705



FTIR (Diamond, 3 Bounce): 4-AcO DMT Oxalate Lot # H-0705

