

## 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<sub>max</sub>:** 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	144.2

### 3. ADDITIONAL RESOURCES

[Wikipedia](#)

### 4. QUALITATIVE DATA

#### 4.1 NUCLEAR MAGNETIC RESONANCE

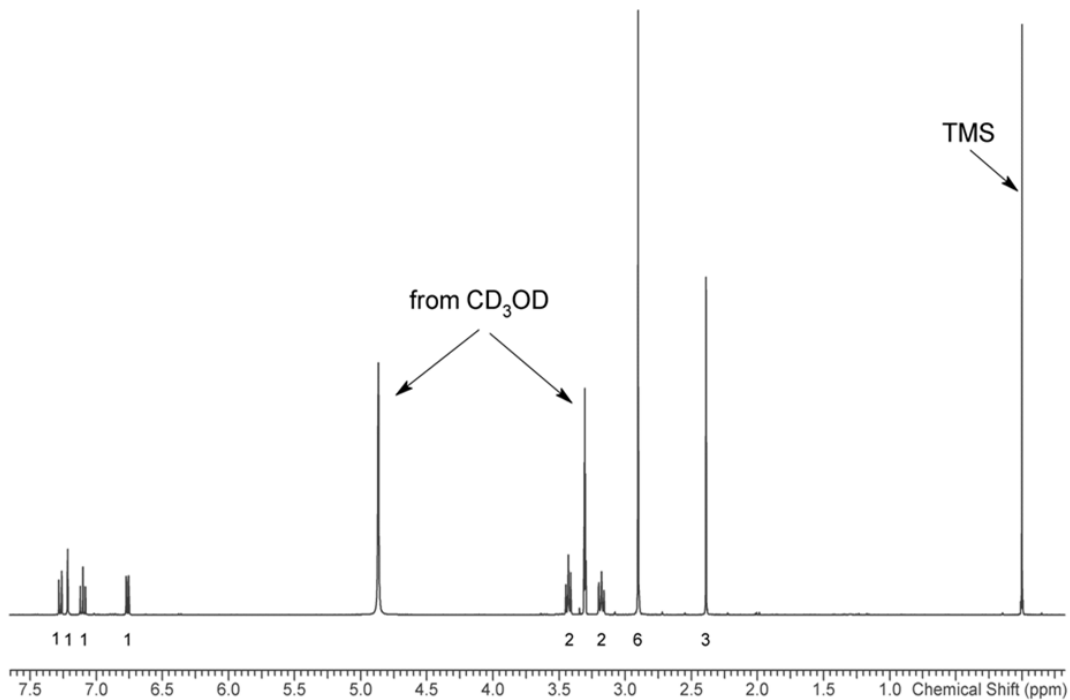
##### *Method NMR CD<sub>3</sub>OD*

*Sample Preparation:* Dilute analyte to ~10 mg/mL in deuterated methanol (CD<sub>3</sub>OD) containing TMS for 0 ppm reference.

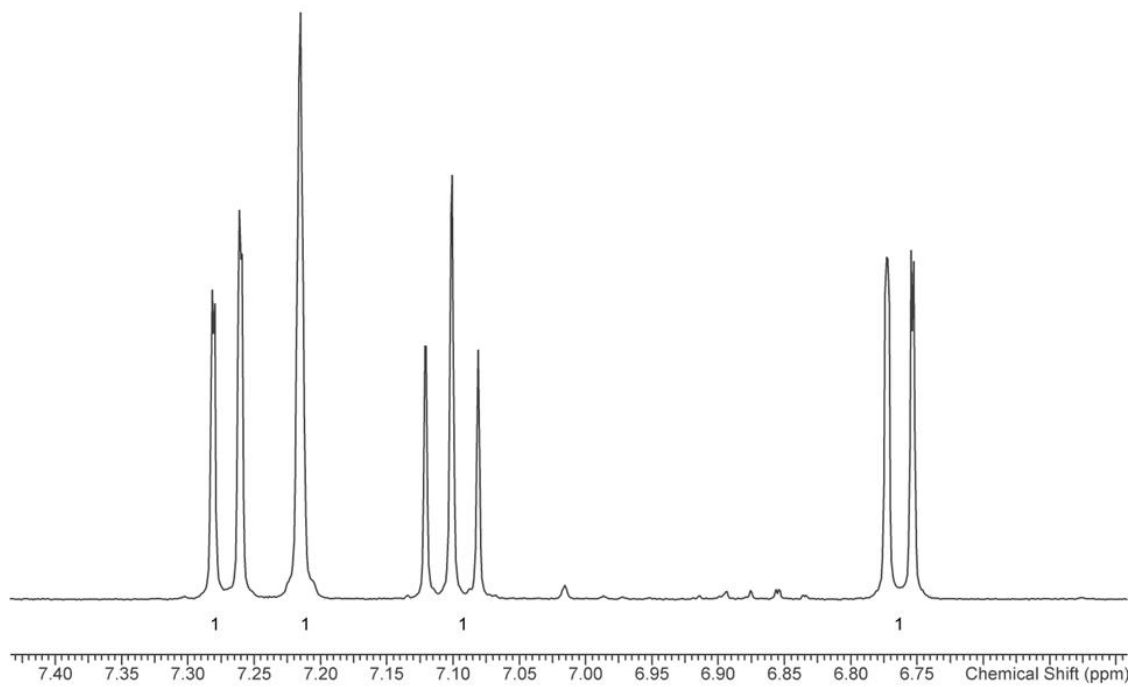
***Instrument:*** Varian Mercury 400 MHz NMR spectrometer with proton detection probe

***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

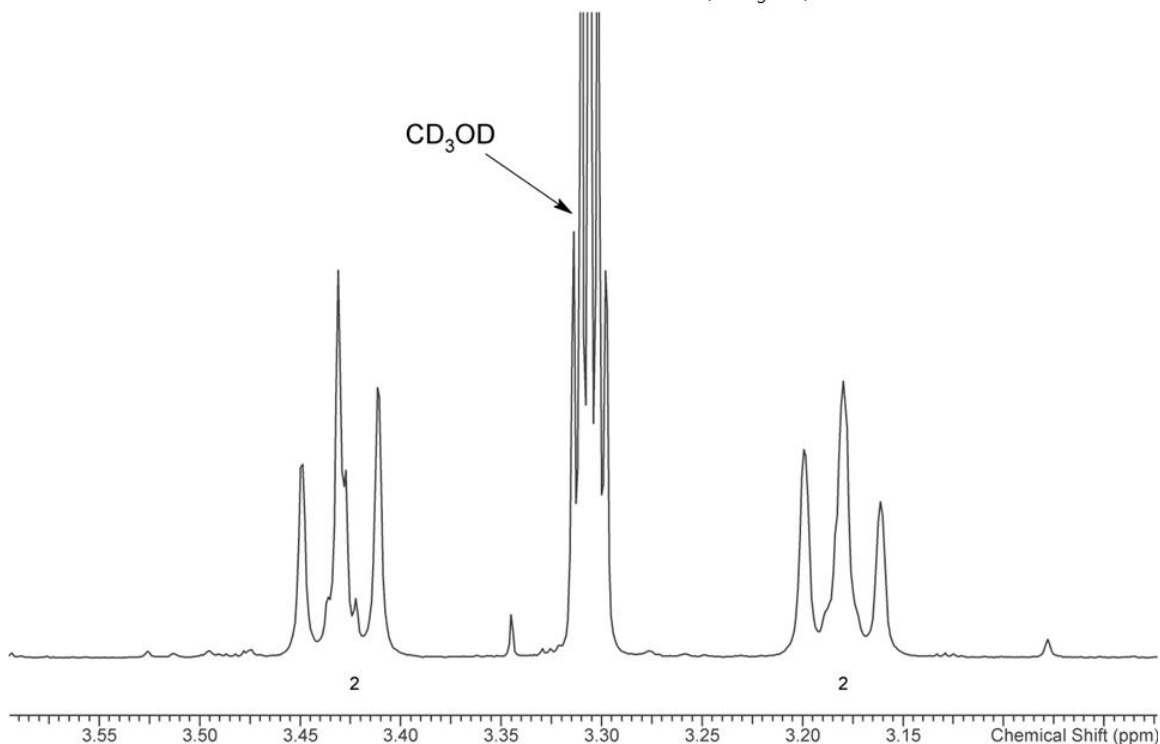
<sup>1</sup>H NMR: 4-AcO DMT Oxalate Lot # H-0705; CD<sub>3</sub>OD; 400 MHz



<sup>1</sup>H NMR: 4-AcO DMT Oxalate Lot # H-0705; CD<sub>3</sub>OD; 400 MHz



1H NMR: 4-AcO DMT Oxalate Lot # H-0705; CD<sub>3</sub>OD; 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

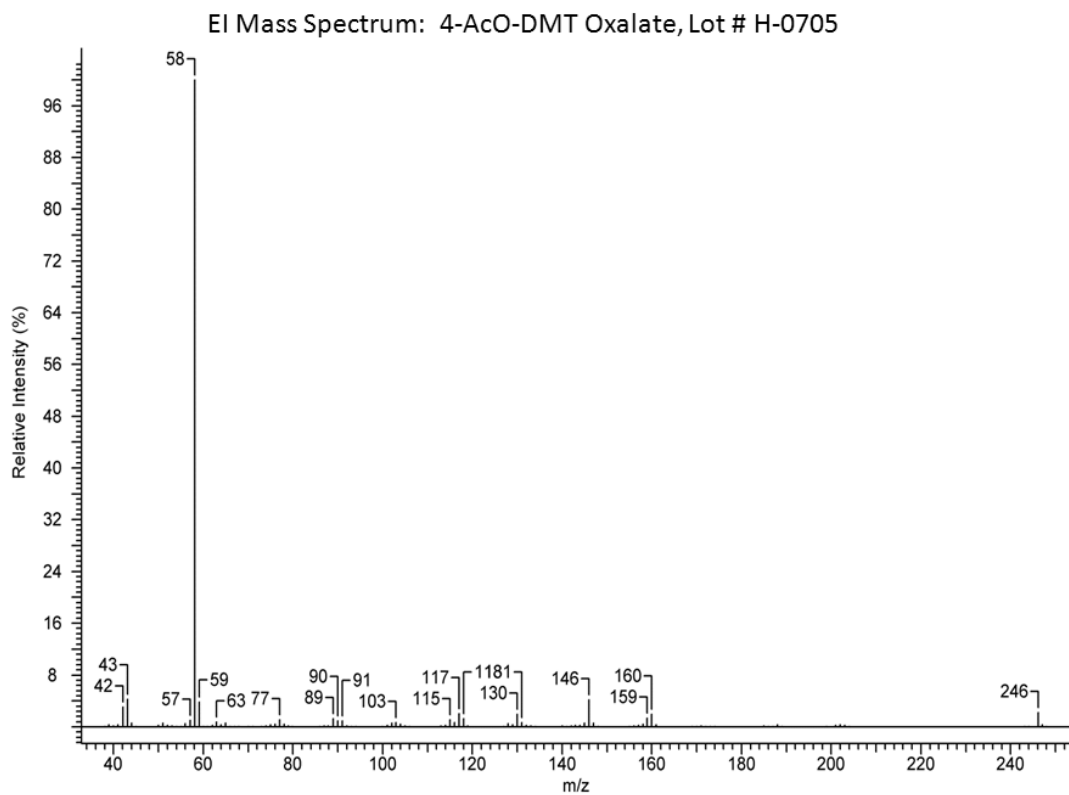
**MS Parameters:** Mass scan range: 34-550 amu

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

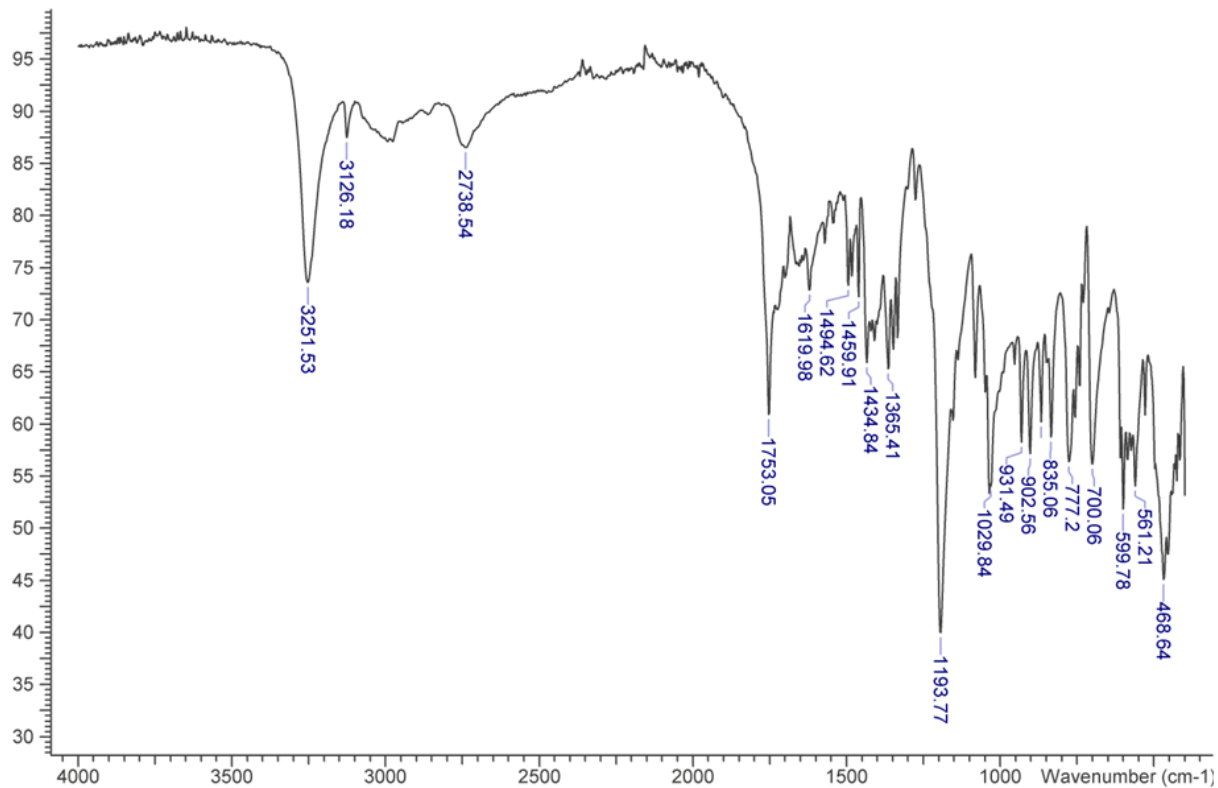
Number of background scans: 32

Resolution 4 cm<sup>-1</sup>

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

