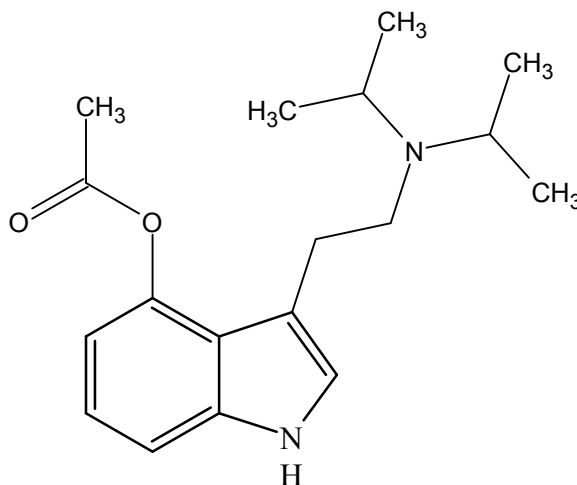




4-Acetoxy-diisopropyltryptamine

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-[di(propan-2-yl)amino]ethyl-1H-indol-4-yl acetate

CAS#: 936015-60-0

Synonyms: 4-AcO-DIPT, 4-Acetoxy-DiPT

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₈ H ₂₆ N ₂ O ₂	302	Not Determined
HCl	C ₁₈ H ₂₆ N ₂ O ₂ · HCl	338	168.0



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3. QUALITATIVE DATA

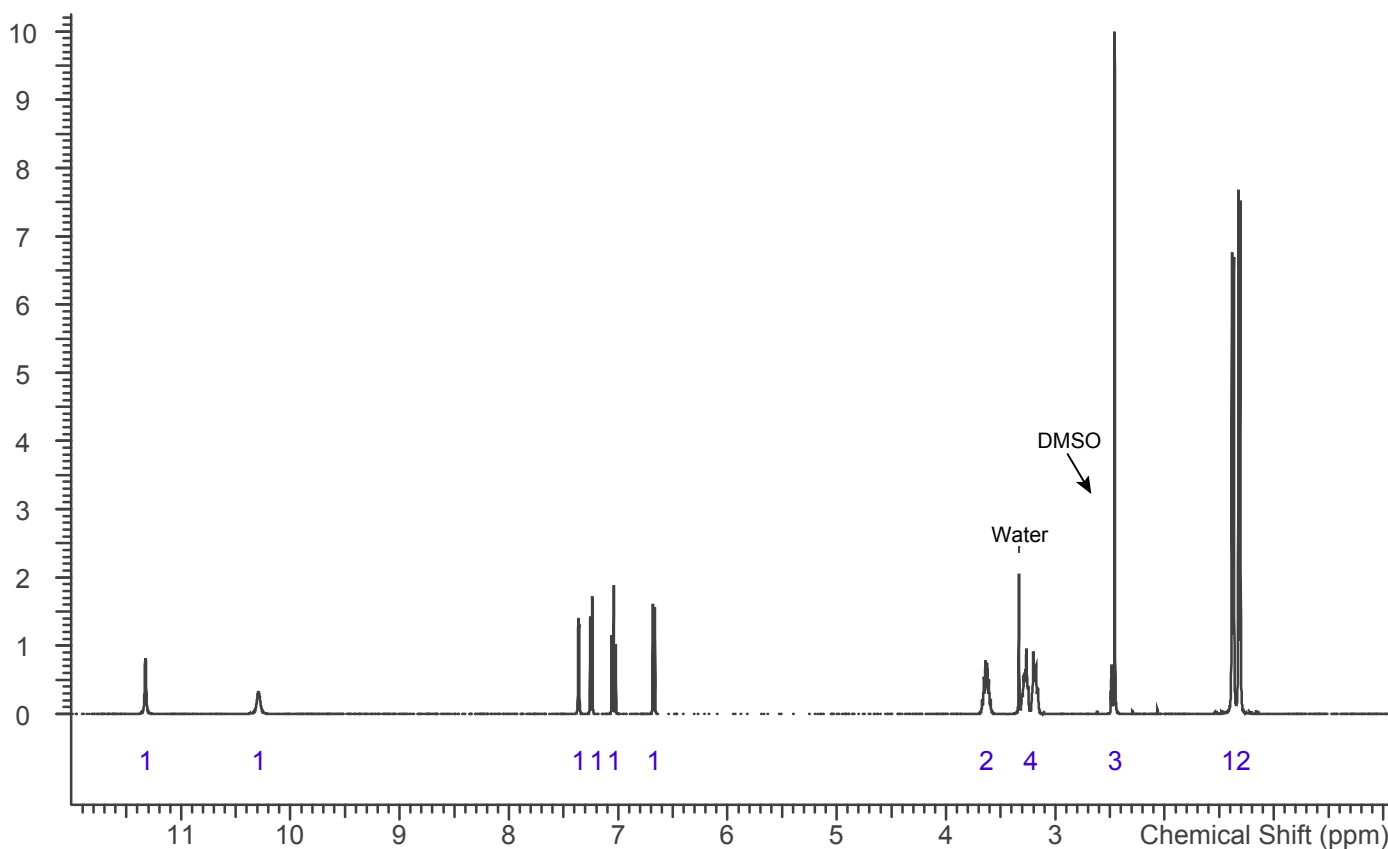
3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR DMSO

Sample Preparation: Dilute analyte to ~20 mg/mL in DMSO.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

¹H NMR: 4-AcO-DIPT HCl; Lot # SF1740; DMSO; 400 MHZ



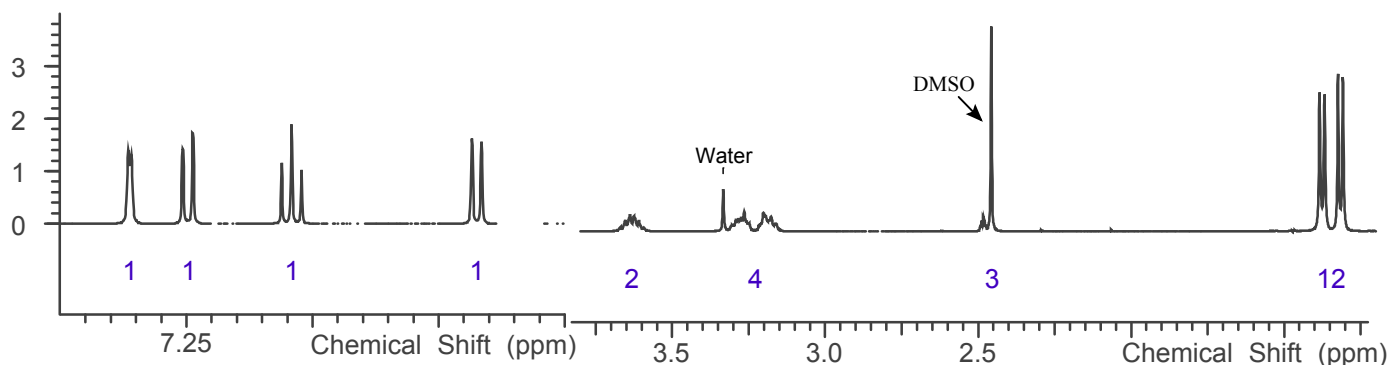


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^1H NMR: 4-AcO-DIPT HCl; Lot # SF1740; DMSO; 400 MHZ



NMR Analytical Observation:

The above NMR spectrum indicates the presence of 27 hydrogens rather than the expected 26. This is probably due to the fact that the substance is an inorganic acid salt. The 10.31 ppm proton is on the N-diisopropyl nitrogen while the 11.34 ppm proton is on the indole nitrogen.

3.2 Gas Chromatography/Mass Spectrometry

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

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 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 = 20:1, 1 μL injected

MS Parameters:

Mass scan range: 30-550 amu

Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time:

15.054 min

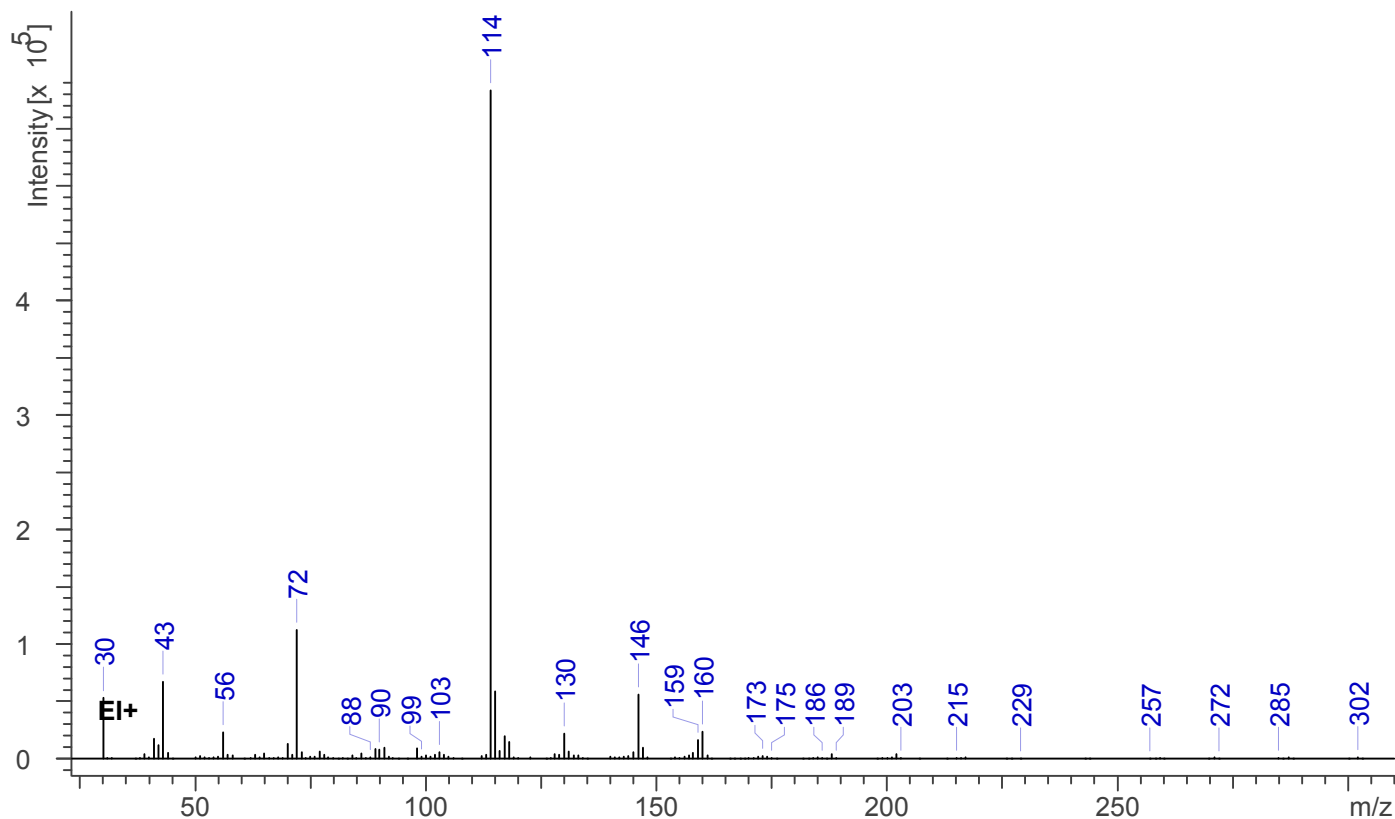


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EI Mass Spectrum: 4-AcO-DIPT HCl Lot # SF1740A



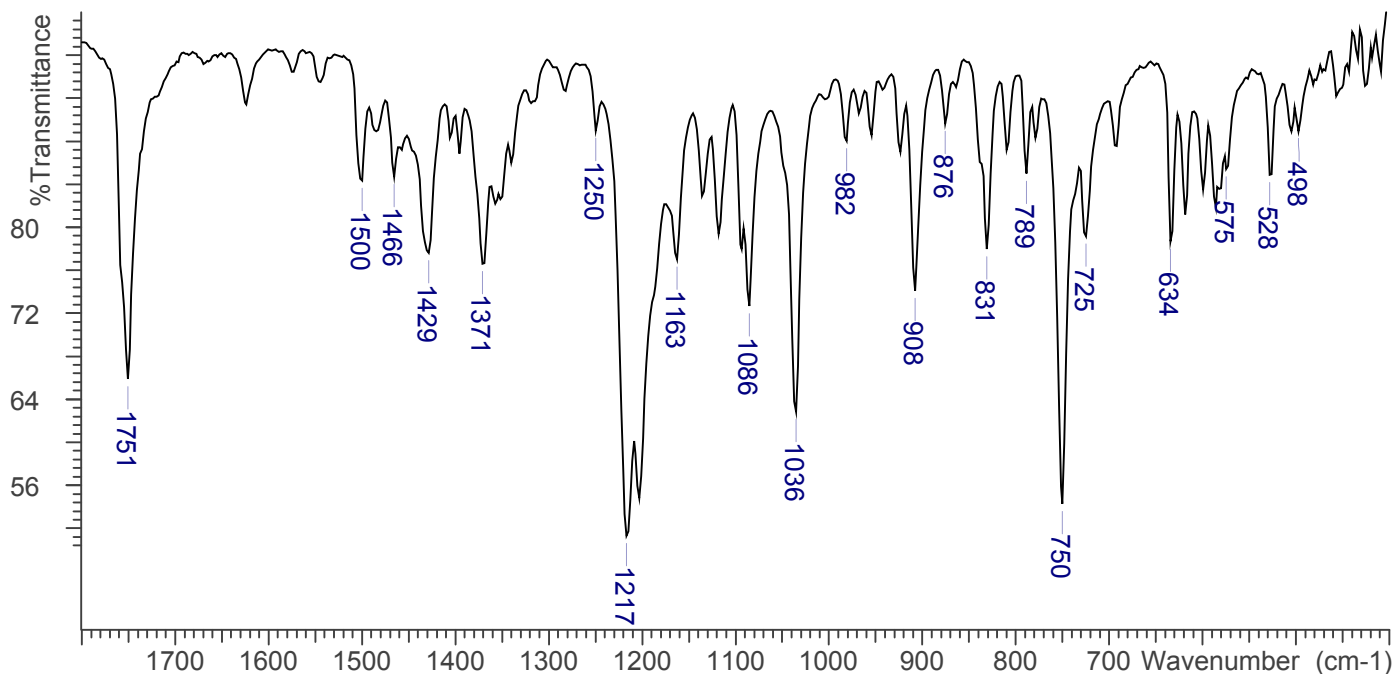
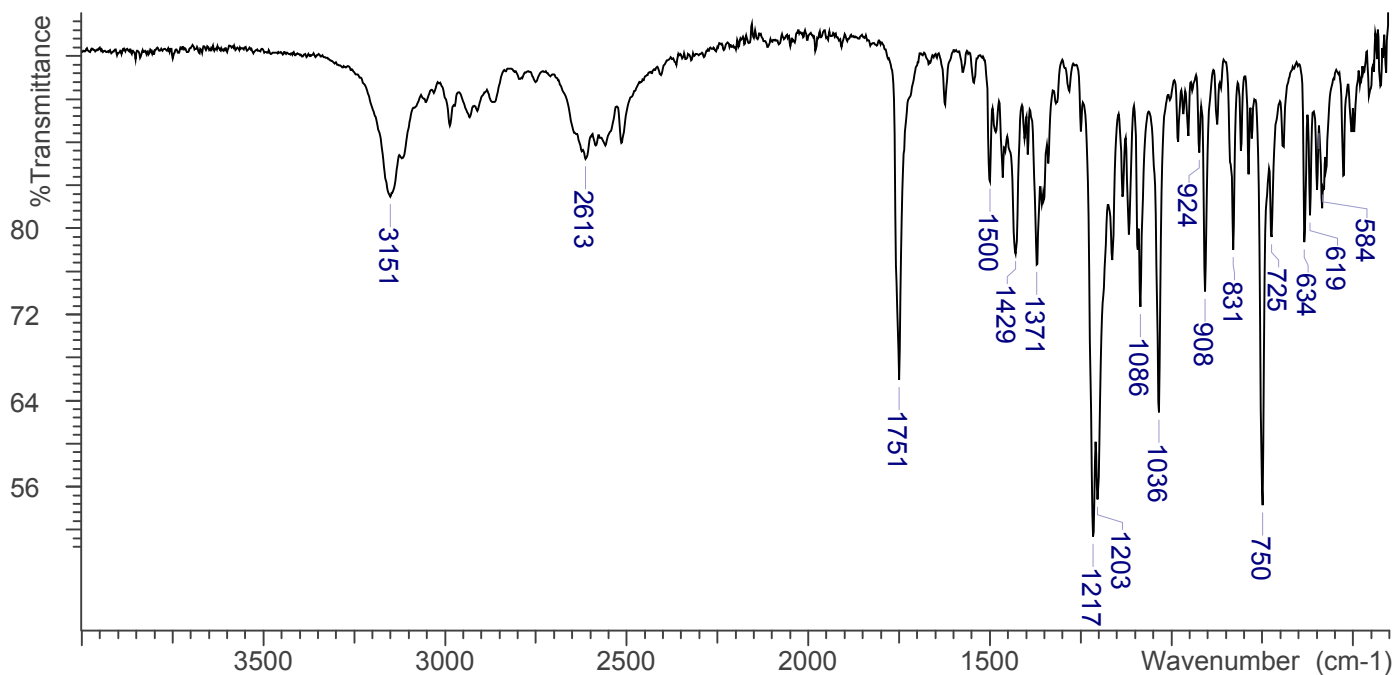
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)
Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

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FTIR ATR (Diamond, 3 Bounce): 4-AcO-DIPT HCl Lot # SF1740A





4-Acetoxy-diisopropyltryptamine

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4. ADDITIONAL RESOURCES

[Wikipedia](#)