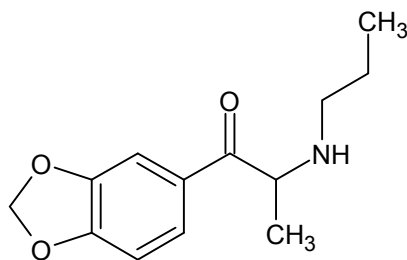




N-Propyl-3,4-methylenedioxy-cathinone

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



1. GENERAL INFORMATION

IUPAC Name: 1-(2H-1,3-benzodioxol-5-yl)-2-(propylamino)propan-1-one

CAS#: NA

Synonyms: N-Propyl-3,4-methylenedioxy-cathinone

Source: DEA Reference Material Collection

Appearance: White Powder

UV_{max}(nm): Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₃ H ₁₇ NO ₃	235	Not Determined
HCl	C ₁₃ H ₁₇ NO ₃ HCl	272	208.7



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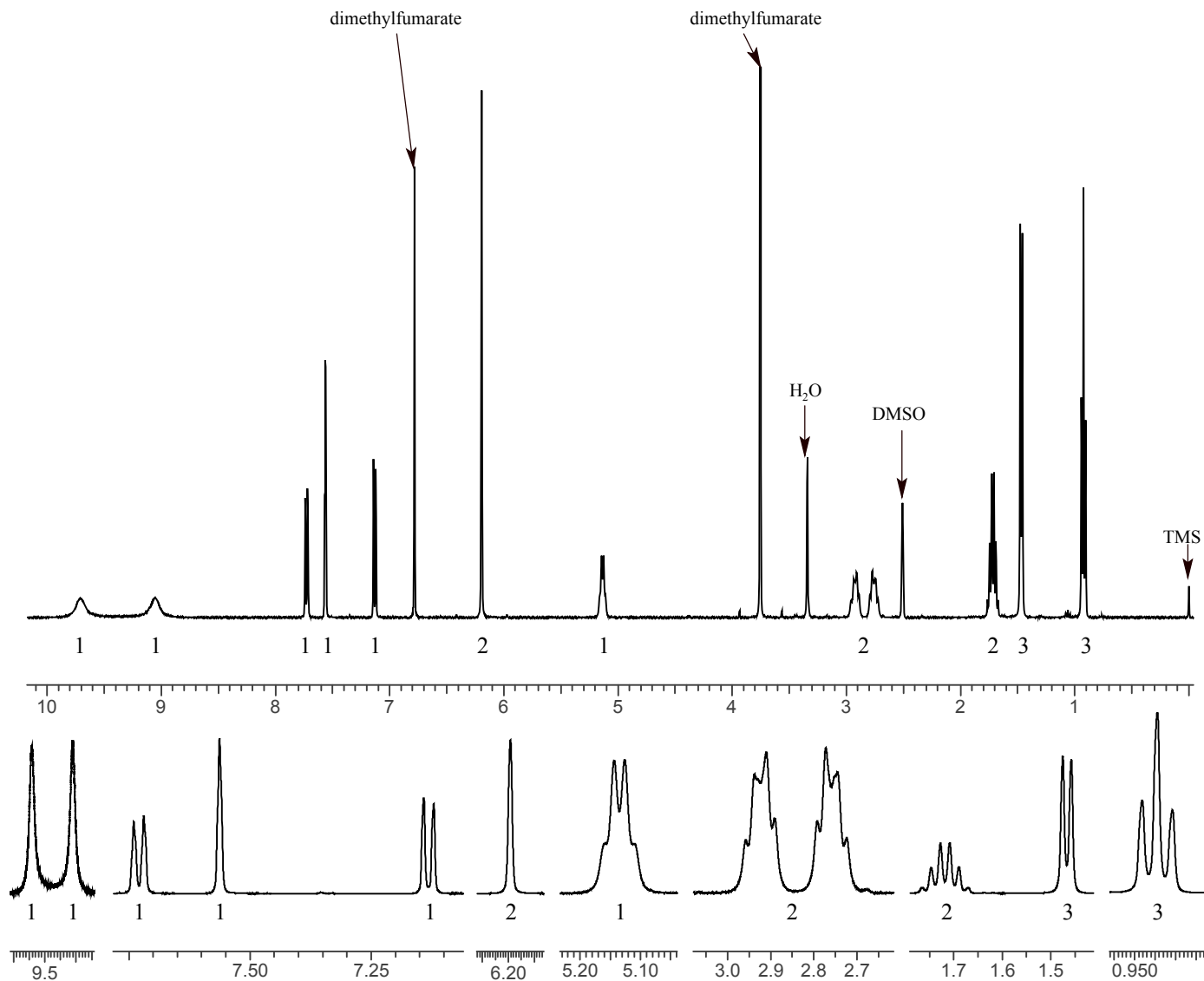
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~13 mg/mL in DMSO- d_6 containing TMS for 0 ppm reference and dimethylfumarate 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

^1H NMR: N-Propyl-3,4-methylenedioxycathinone HCl; Lot RM-151217-01; DMSO; 400MHz





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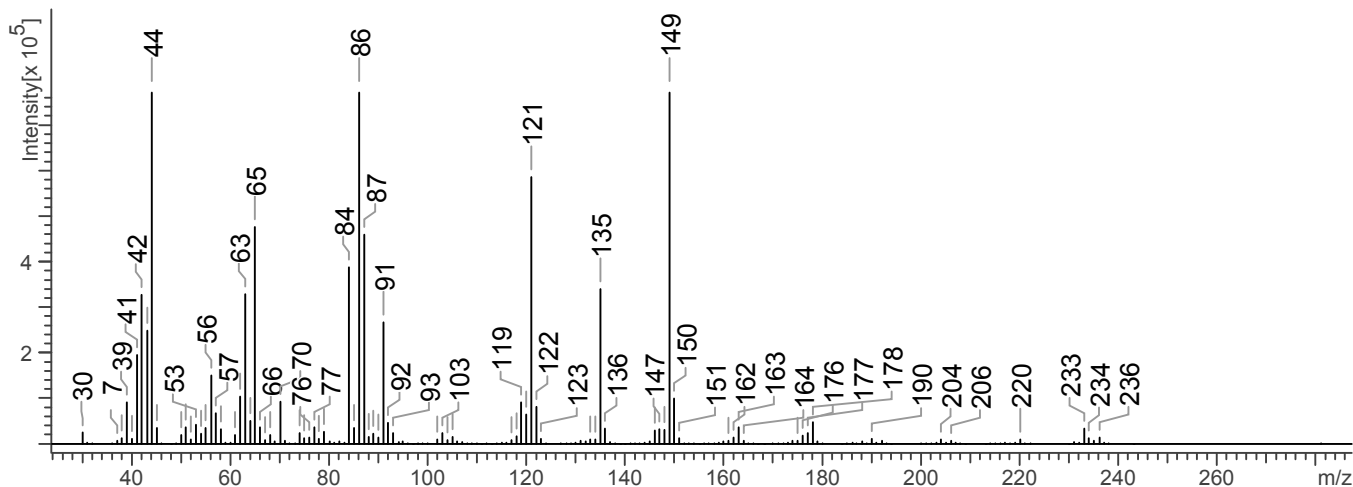
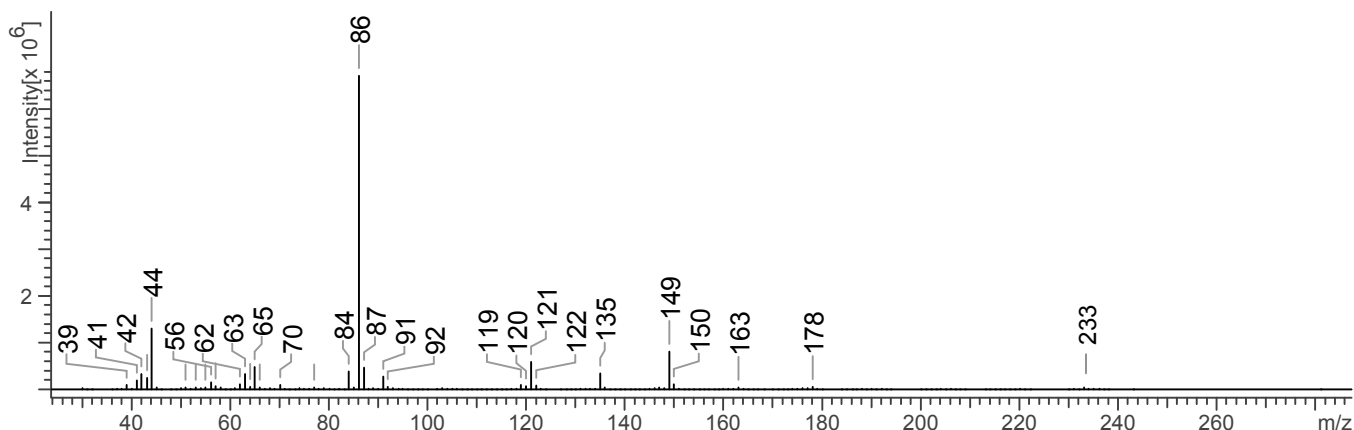


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 mg/mL in MeOH

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μ m
Carrier Gas: Helium at 1.5 mL/min
Temperatures: Injector: 280°C MSD transfer line: 280°C
MS Source: 250°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 μ L injected
MS Parameters: Mass scan range: 30-550 amu Threshold: 90
Tune file: stune.u Acquisition mode: scan
Retention Time: 10.94 min

EI Mass Spectrum: N-Propyl-3,4-methylenedioxycathinone HCl Lot RM-151217-01





N-Propyl-3,4-methylenedioxycathinone

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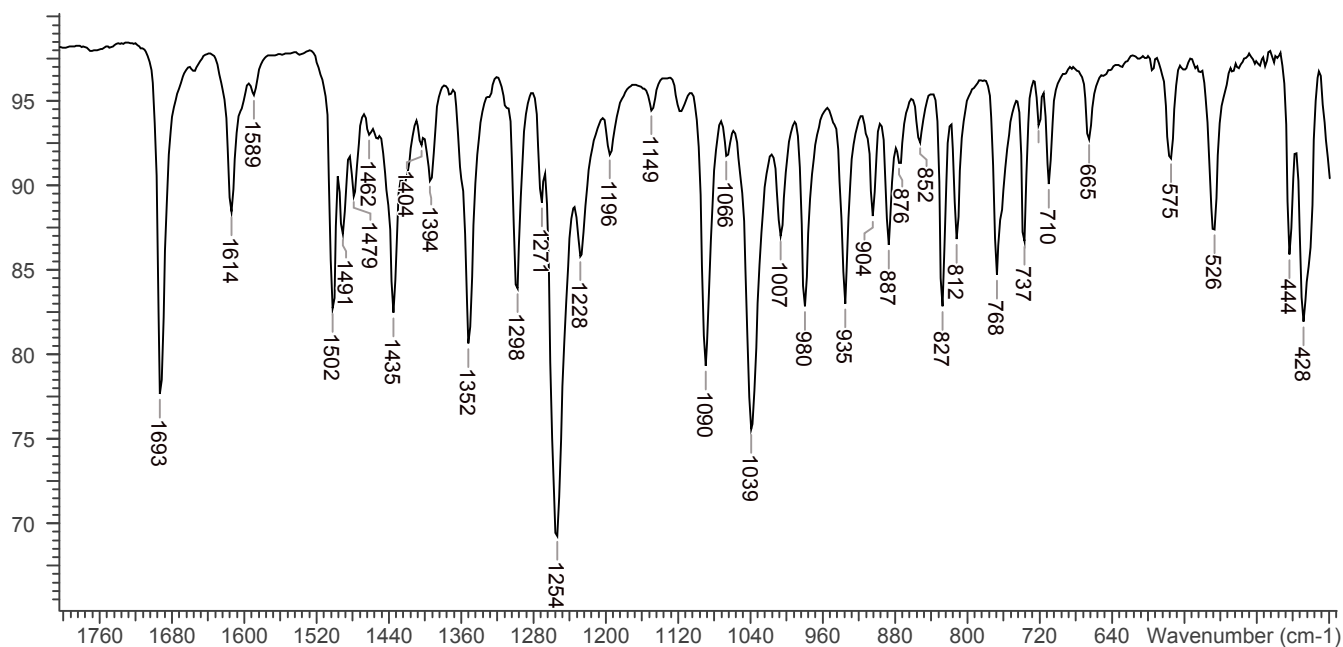
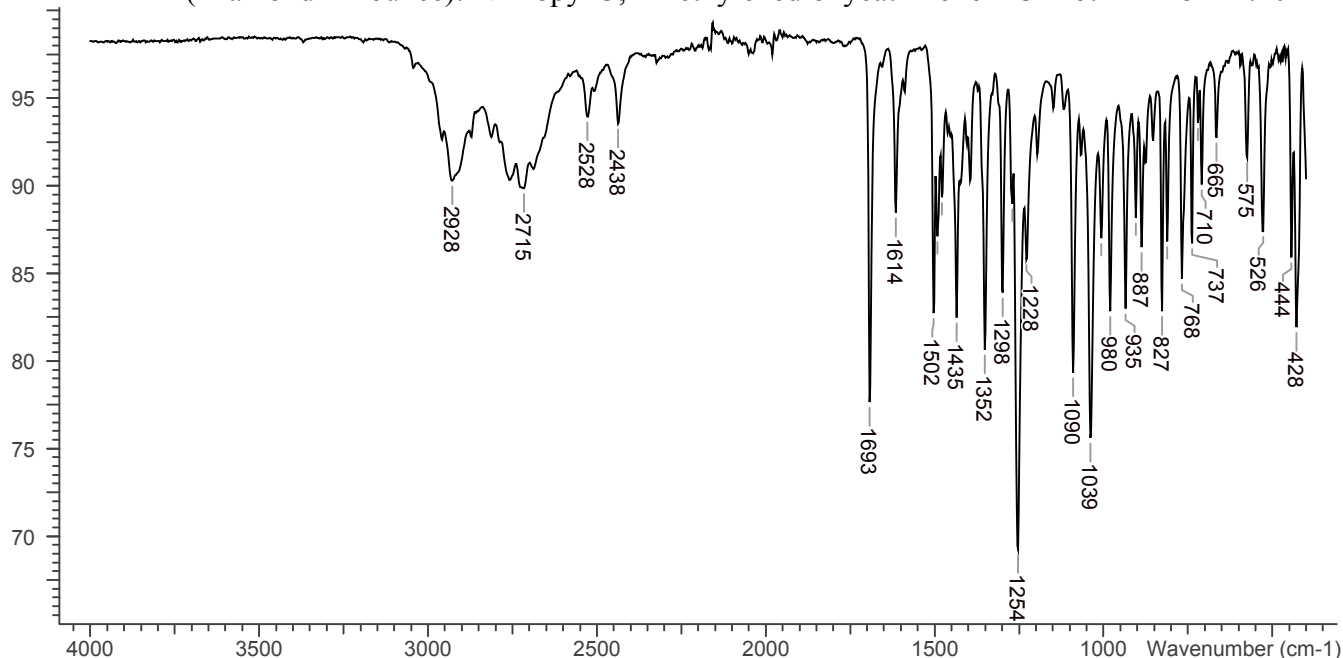


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 150

FTIR ATR (Diamond 1 Bounce): N-Propyl-3,4-methylenedioxycathinone HCl Lot RM-151217-01





N-Propyl-3,4-methylenedioxycathinone

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4. ADDITIONAL RESOURCES

No additional resources as of 03/2016