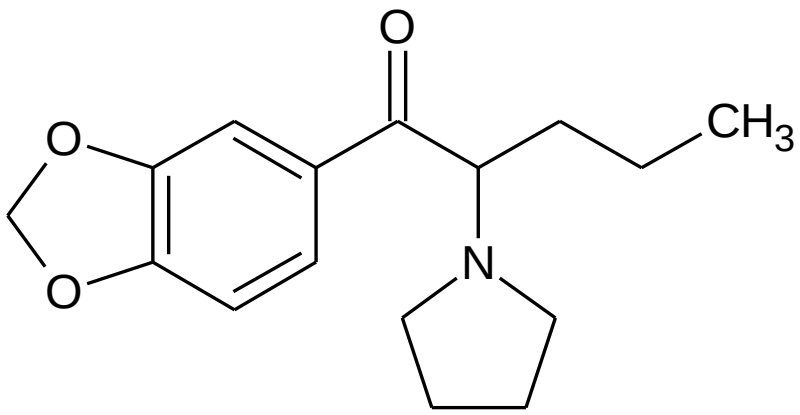
3,4-MDPV

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



1. GENERAL INFORMATION

IUPAC Name: 1-(1,3-benzodioxol-5-yl)-2-(pyrrolidin-1-yl)pentan-1-one

CFR: Schedule I

CAS #: 687603-66-3 (Base)
24622-62-6 (HCl)

Synonyms: 3,4-methylenedioxypyrovalerone

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

UV_{max}: 235.8, 283.1, 322.6

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{16}H_{21}NO_3$	274	Not Determined
HCl	$C_{16}H_{21}NO_3 \cdot HCl$	311	238-239 decomposes

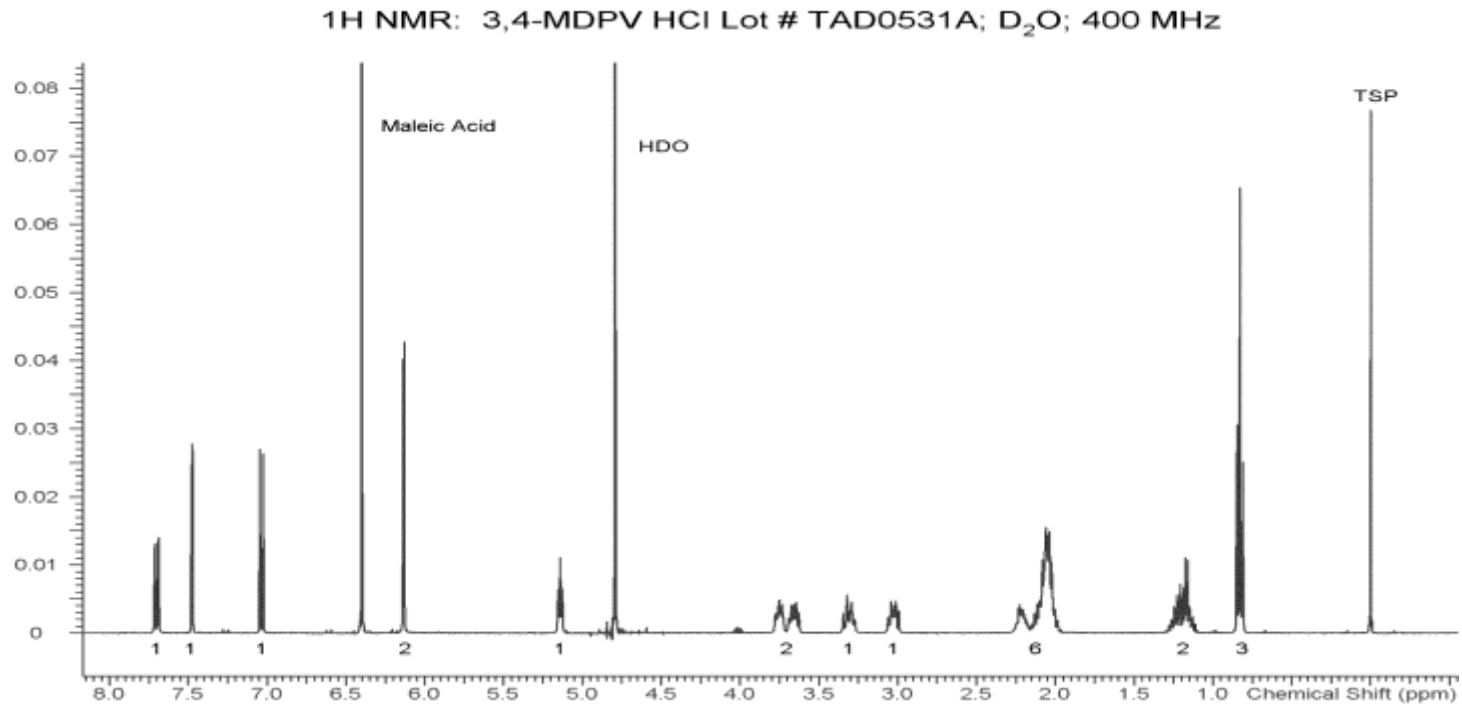
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

Sample Preparation: Dilute analyte to ~10 mg/mL in D_2O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

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



3,4-MDPV

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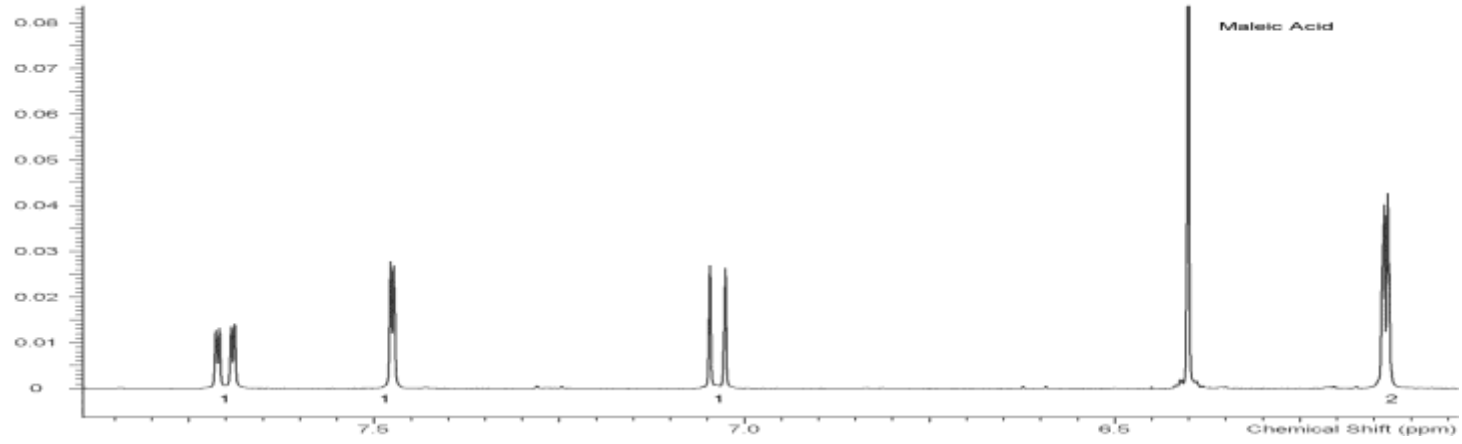
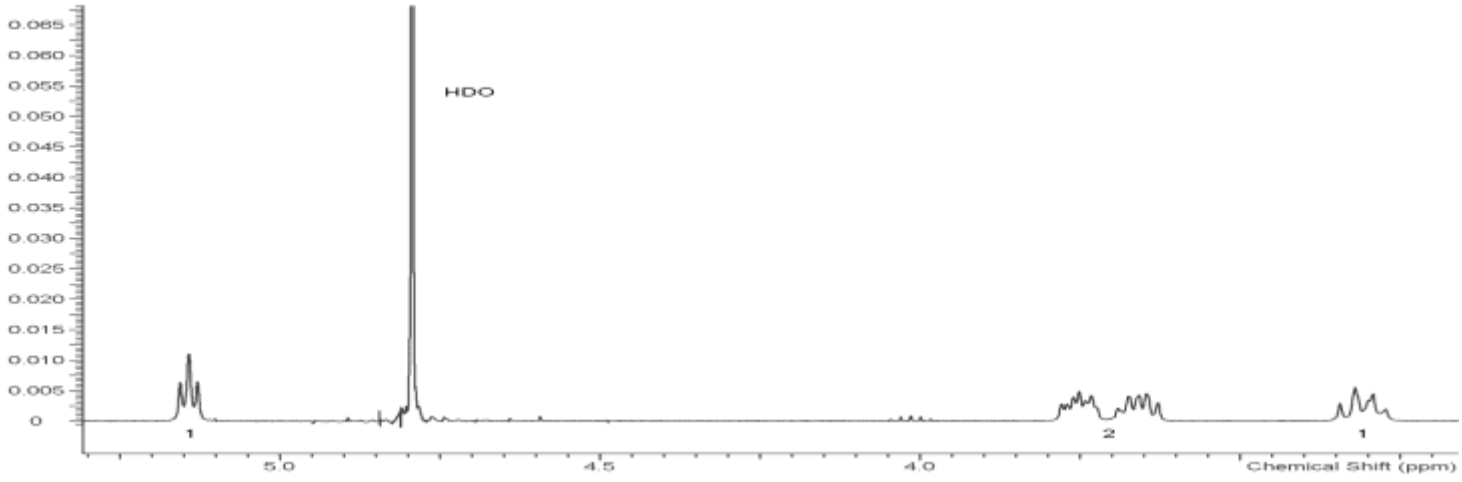
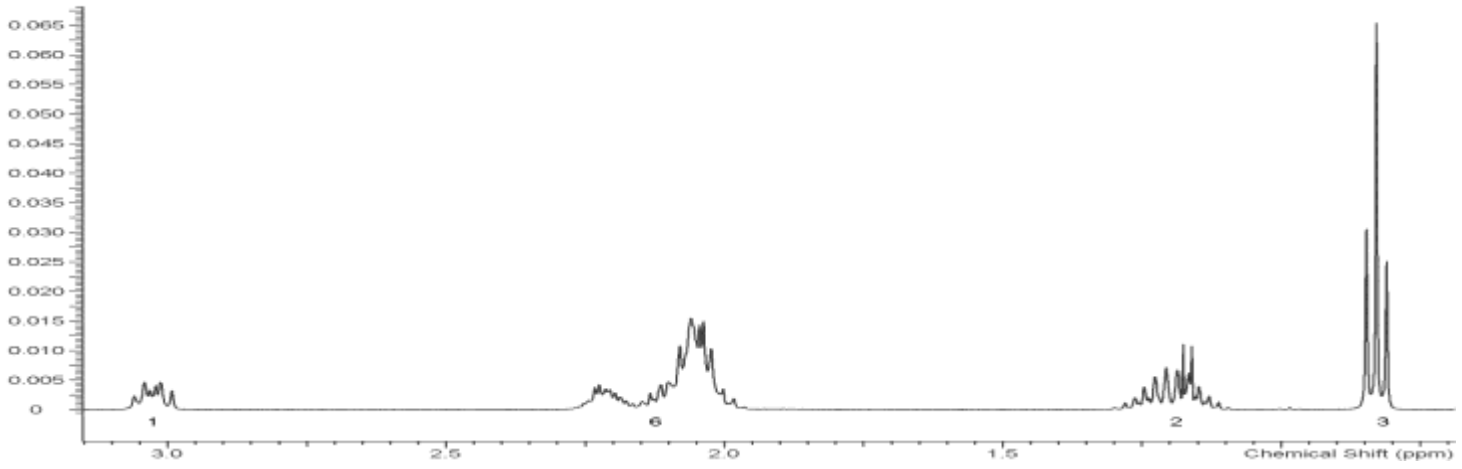
1H NMR: 3,4-MDPV HCl Lot # TAD0531A; D_2O; 400 MHz



1H NMR: 3,4-MDPV HCl Lot # TAD0531A; D_2O; 400 MHz



1H NMR: 3,4-MDPV HCl Lot # TAD0531A; D_2O; 400 MHz

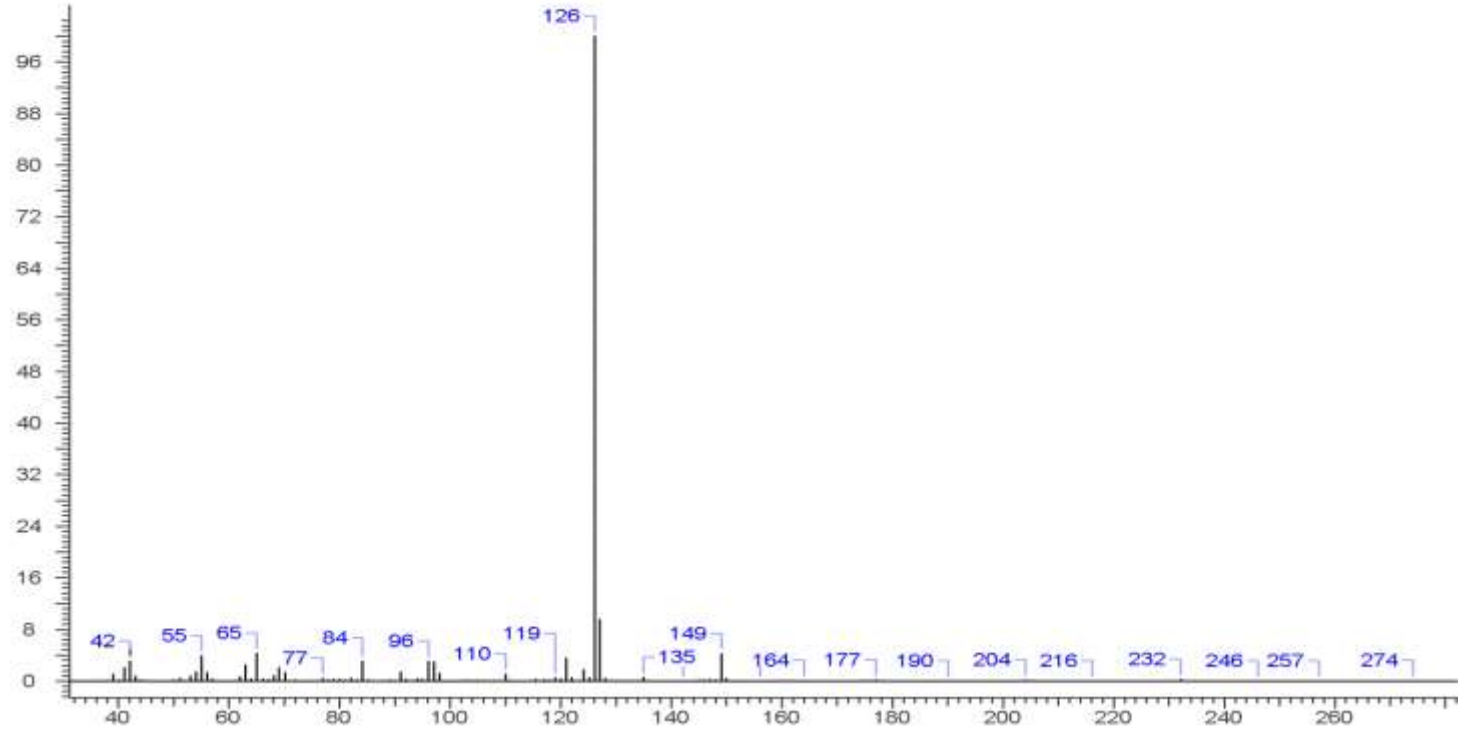


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~4 mg/mL in MeOH.

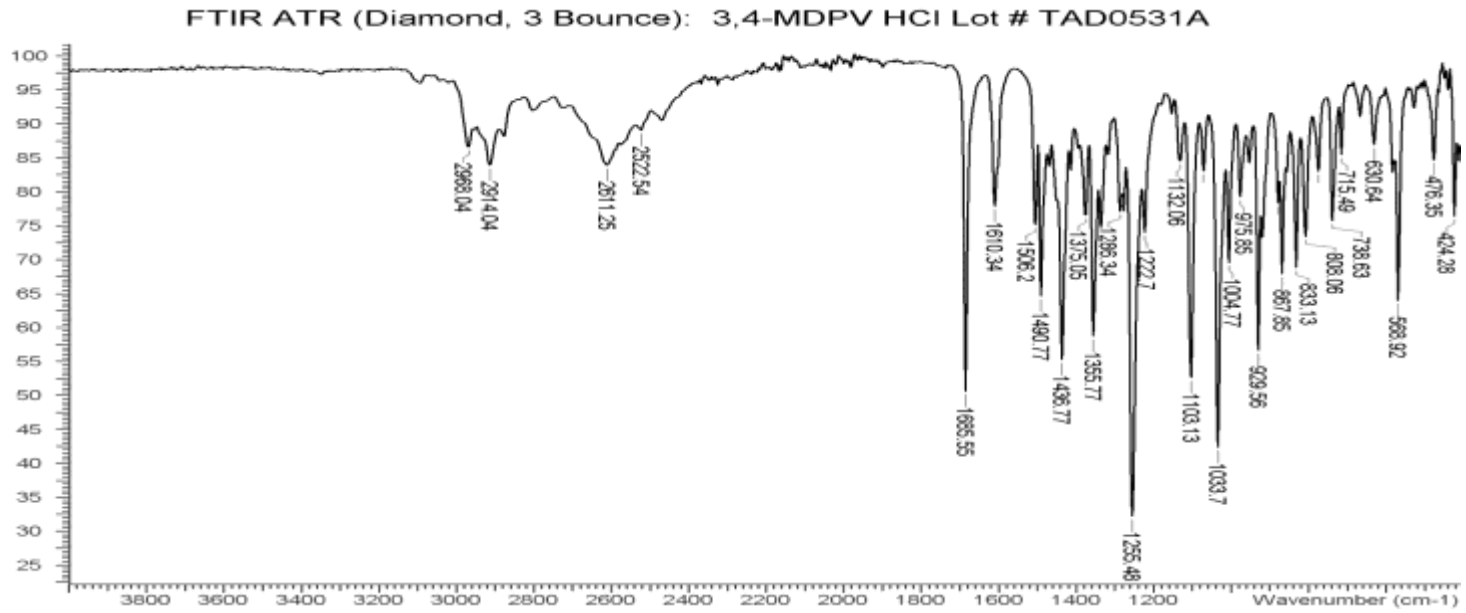
Instrument:	Gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 30m x 0.25mm x 0.25µm
Carrier Gas:	Helium at 1 mL/min
Temperatures:	Injector: 280°C MSD transfer line: 280°C MS Source: 230°C MS Quad: 150°C Oven program: 1) 100°C initial temperature for 1.0 min 2) Ramp 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: 30-550 amu Threshold: 100 Tune file: stune.u Acquisition mode: scan
Retention Time:	13.500 minutes

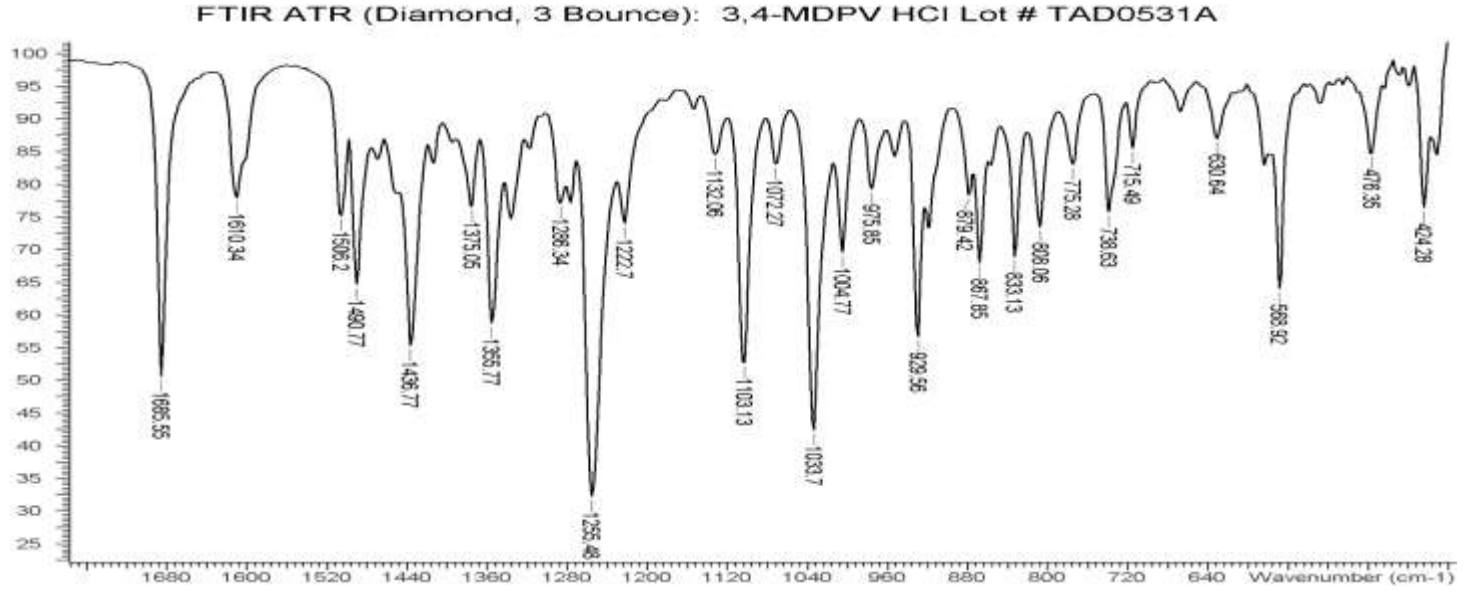
EI Mass Spectrum: 3,4-MDPV HCl Lot # TAD0531A



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: 4cm^{-1}
Sample gain: 8
Aperture: 150





4. ADDITIONAL RESOURCES

J. Yohannon, J. Bozenko, Jr. The Characterization of 3,4-Methylenedioxypyrovalerone (MDPV). Microgram Journal 2010; 7(1): 12-15.

Forendex

Wikipedia