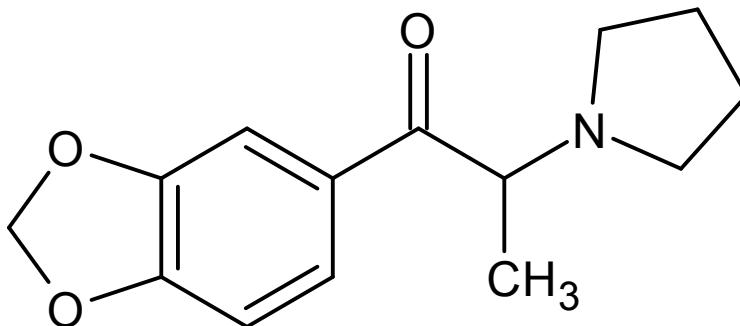




3,4-MDPPP

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)propan-1-one
CAS#:	24698-57-5
Synonyms:	3',4'-methylenedioxy- α -pyrrolidinopropiophenone; 3',4'-MDPPP; 3,4'-MD- α -PPP
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 ₁₄ H ₁₇ NO ₃	247	Not Determined
HCl	C ₁₄ H ₁₇ NO ₃ · HCl	283	246.2



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3. QUALITATIVE DATA

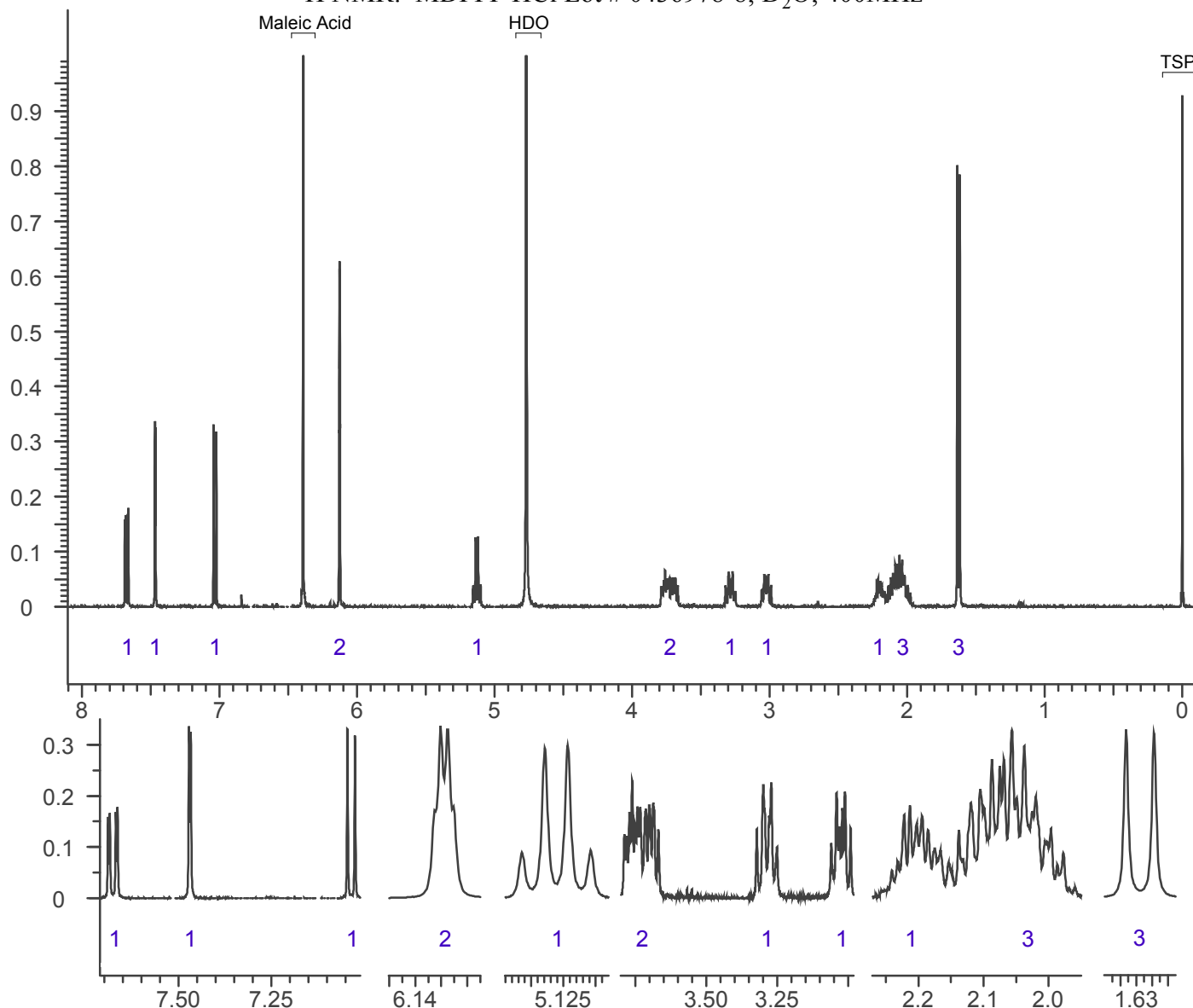
3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D₂O

Sample Preparation: Dilute analyte to ~5 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid 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: MDPPP HCl Lot # 0436978-8; D₂O; 400MHz





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3.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl_3 .

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 30.0 min

Injection Parameters: Split Ratio = 25:1, 1 μL injected

MS Parameters: Mass scan range: 30-550 amu

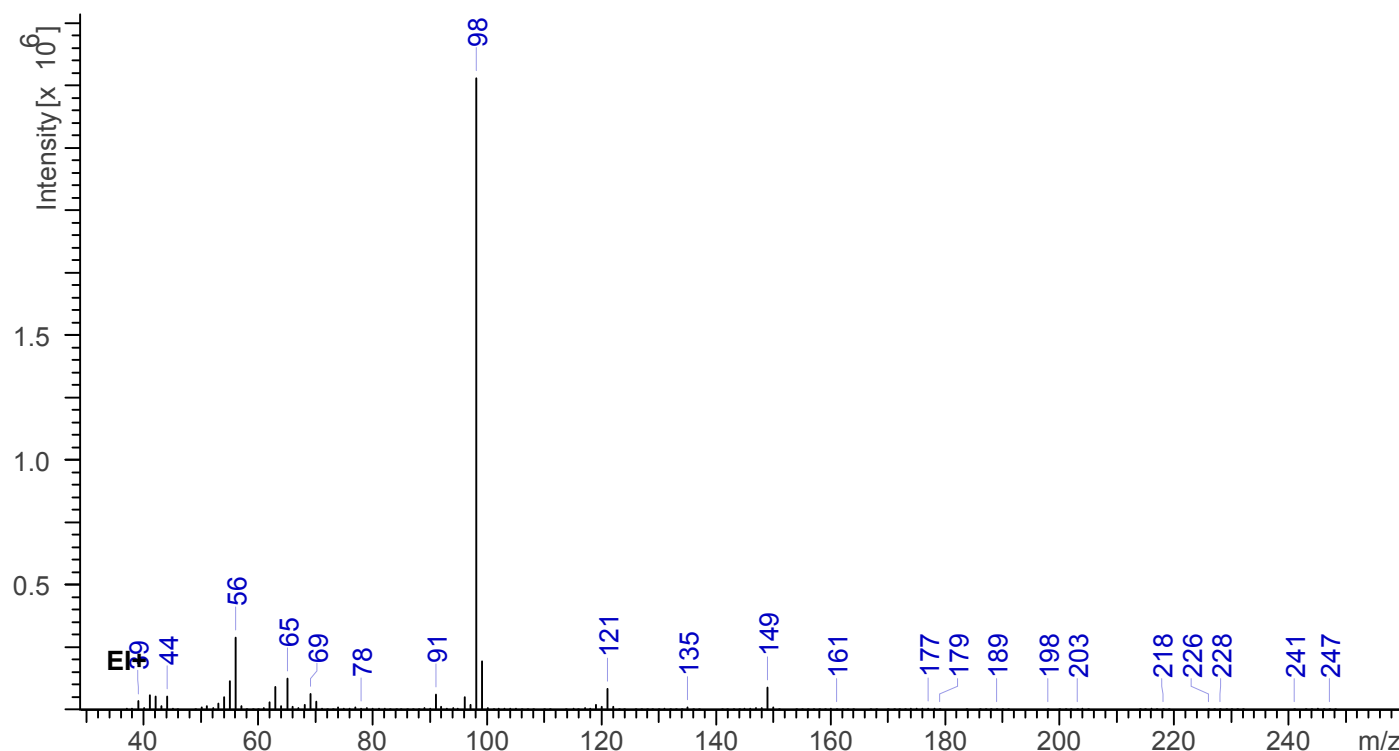
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 12.280 min

EI Mass Spectrum: MDPPP HCl Lot # 0436978-8





3,4-MDPPP

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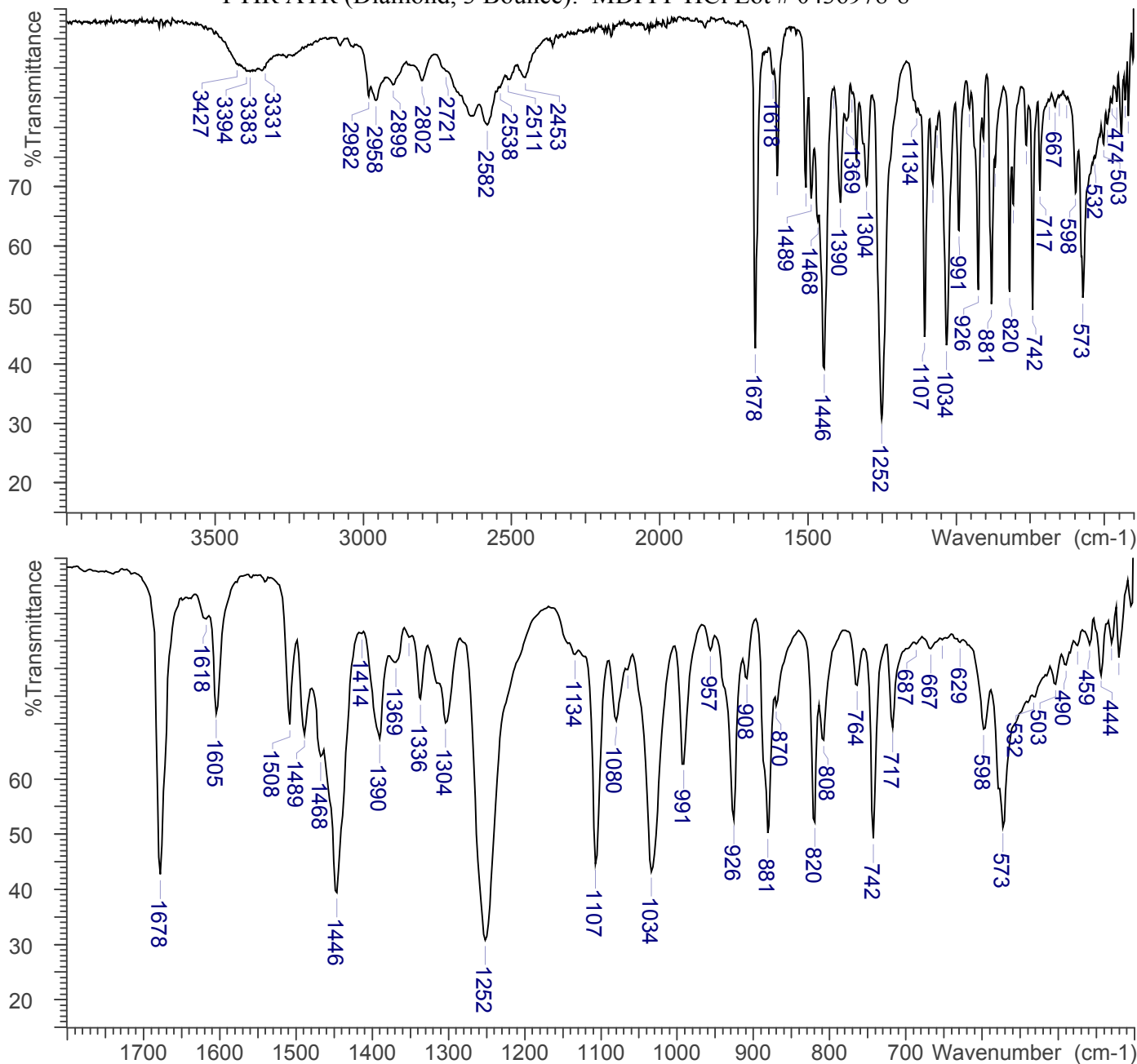


3.3 INFRARED SPECTROSCOPY (FTIR)

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

FTIR ATR (Diamond, 3 Bounce): MDPPP HCl Lot # 0436978-8





3,4-MDPPP

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4. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)

Abiedalla, Y. Abdel-Hay, K. DeRuiter, J. Clark, C. Synthesis and GC-MS analysis of a series of homologs and regioisomers of 3,4-methylenedioxypyrovalerone (MDPV). *Forensic Science International* 2012. 223(1-3): 189-197.