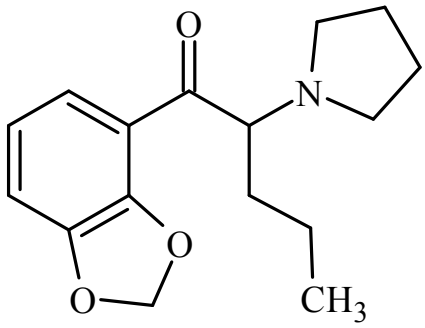
2,3-MDPV

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-4-yl)-2-(pyrrolidin-1-yl)pentan-1-one

CAS#: NA

Synonyms: 2,3-methylenedioxypyrovalerone

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 (^{o}C)
Base	$C_{16}H_{21}NO_3$	275	Not Determined
HCl	$C_{16}H_{21}NO_3 \cdot HCl$	311	183.8

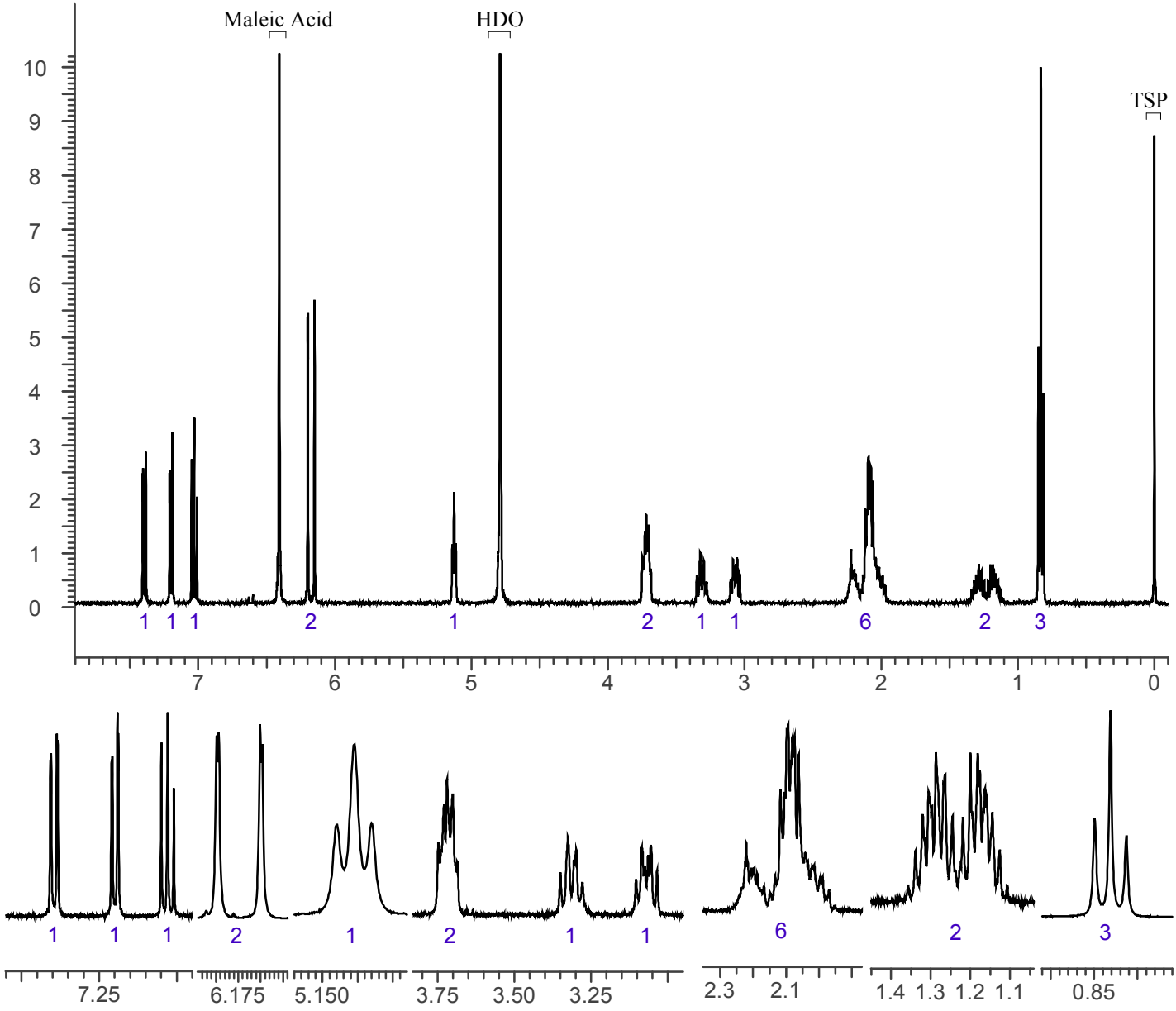
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in D_2O 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

^{1}H NMR: 2,3-MDPV HCl; Lot 0435485-5, D_2O, 400MHz

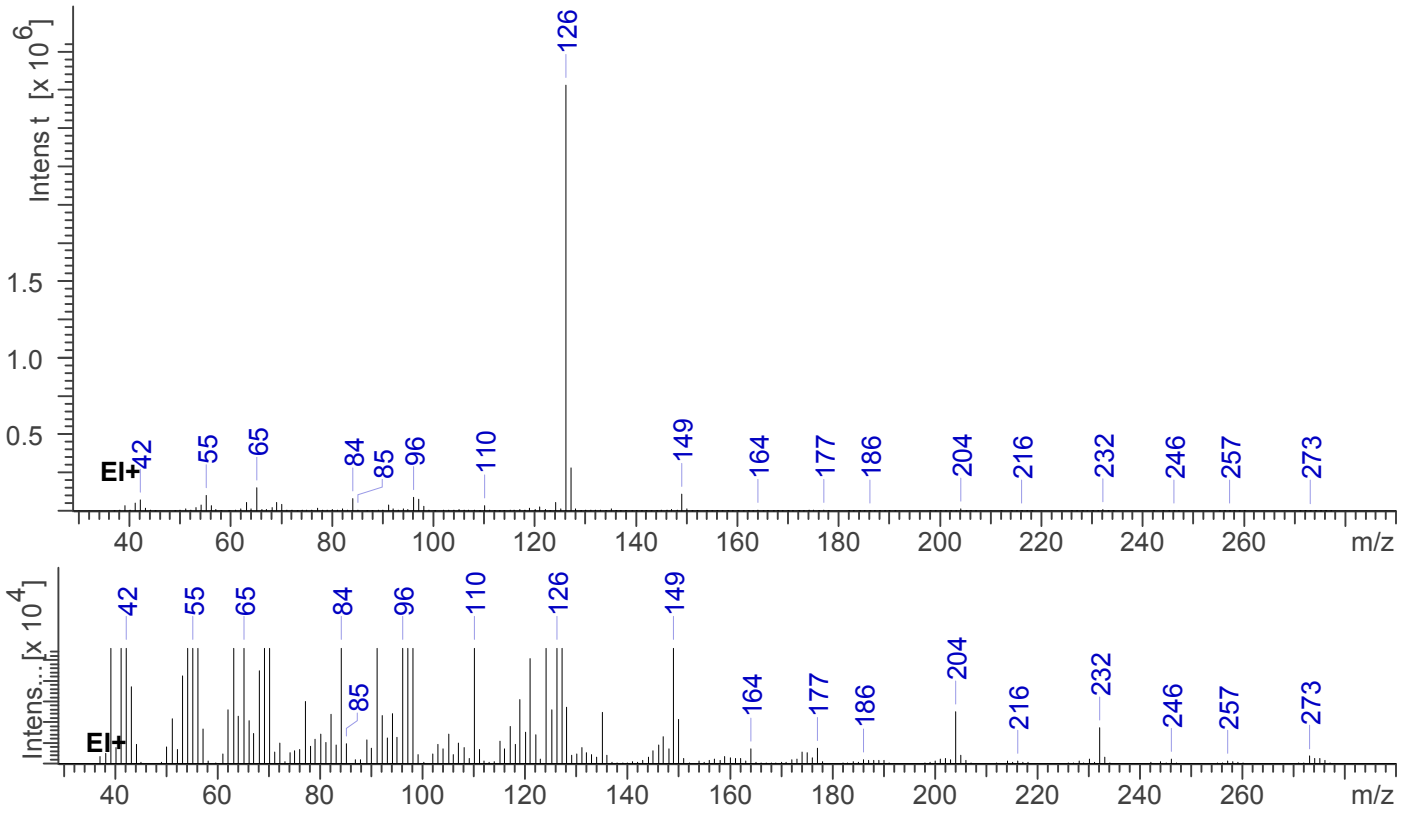


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL base extracted into 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 30.0 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:	12.875 min

EI Mass Spectrum: 2,3-MDPV; Lot 0435485-5

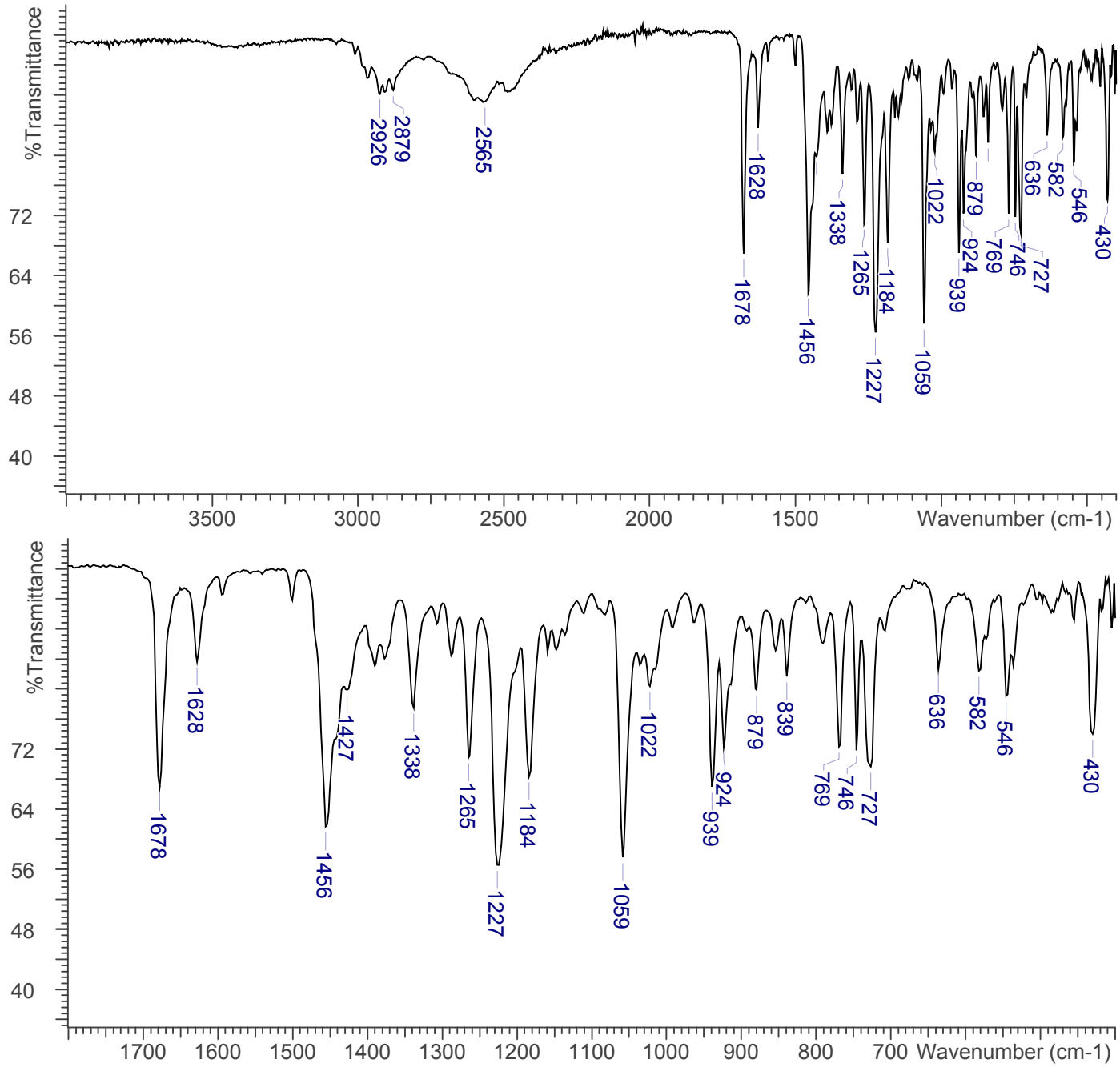


3.3 INFRARED SPECTROSCOPY (FTIR)

Insrument: 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): 2,3-MDPV HCl; Lot 0435485-5



4. ADDITIONAL RESOURCES

Kavanagh, P. et al. The analysis of substitued cathinones. Part 3. Synthesis and characterization of 2,3-methylenedioxy substituted cathinones. Forensic Sci Int. 2012 Mar 10; 216 (1-3): 19-28.