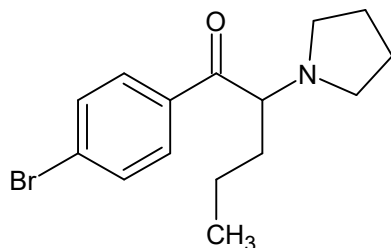




4-Bromo- α -PVP

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



1. GENERAL INFORMATION

IUPAC Name: 1-(4-bromophenyl)-2-(pyrrolidin-1-yl)pentan-1-one

CAS#: NA

Synonyms: 4-Bromo- α -PVP

Source: DEA Reference Material Collection

Appearance: Off-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 ₁₅ H ₂₀ BrNO	310	Not Determined
HCl	C ₁₅ H ₂₀ BrNO HCl	346	209.1



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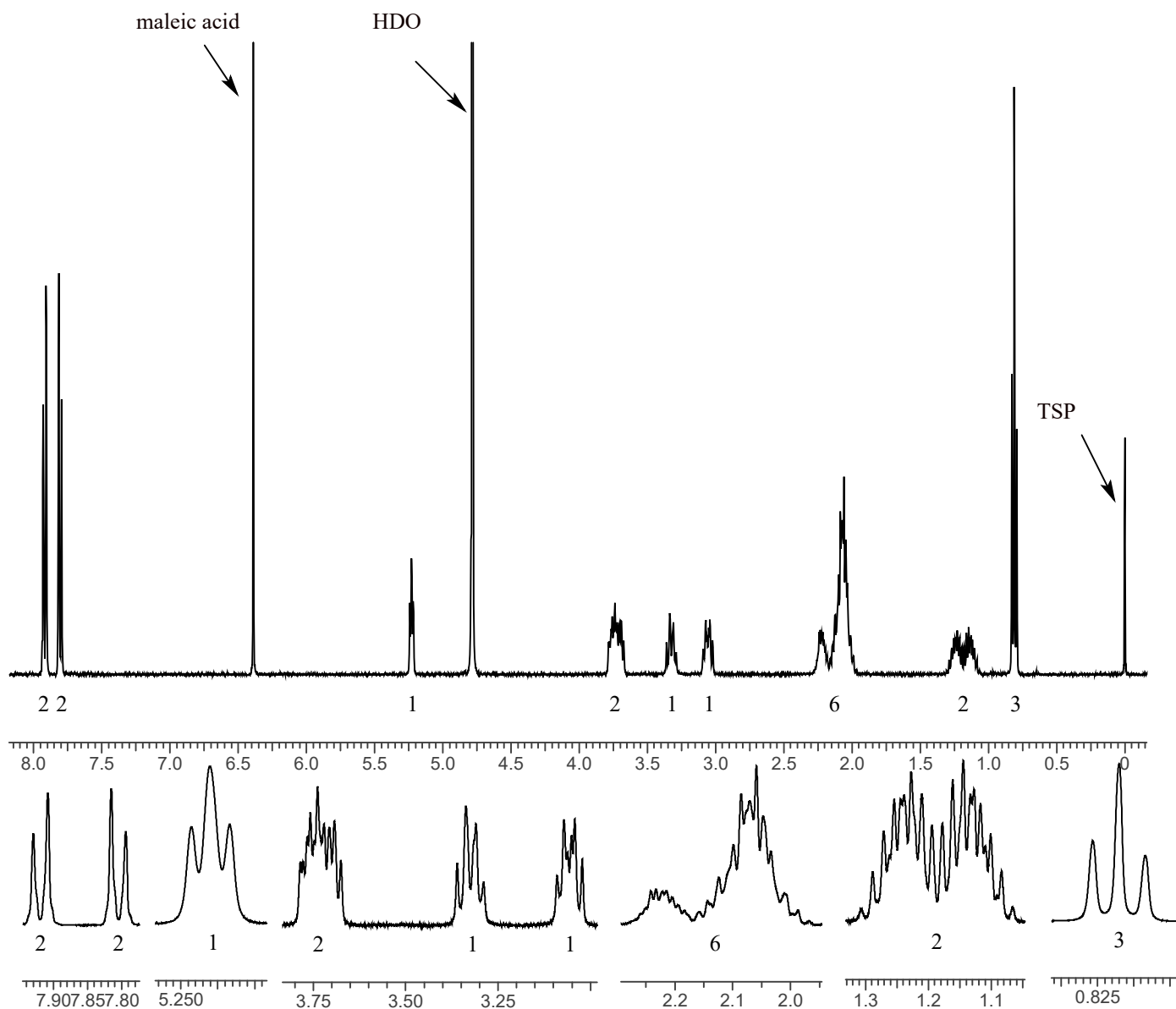
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 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

¹HNMR: 4-Bromo- α -PVP HCl; Lot# RM-160316-01; D₂O; 400MHz





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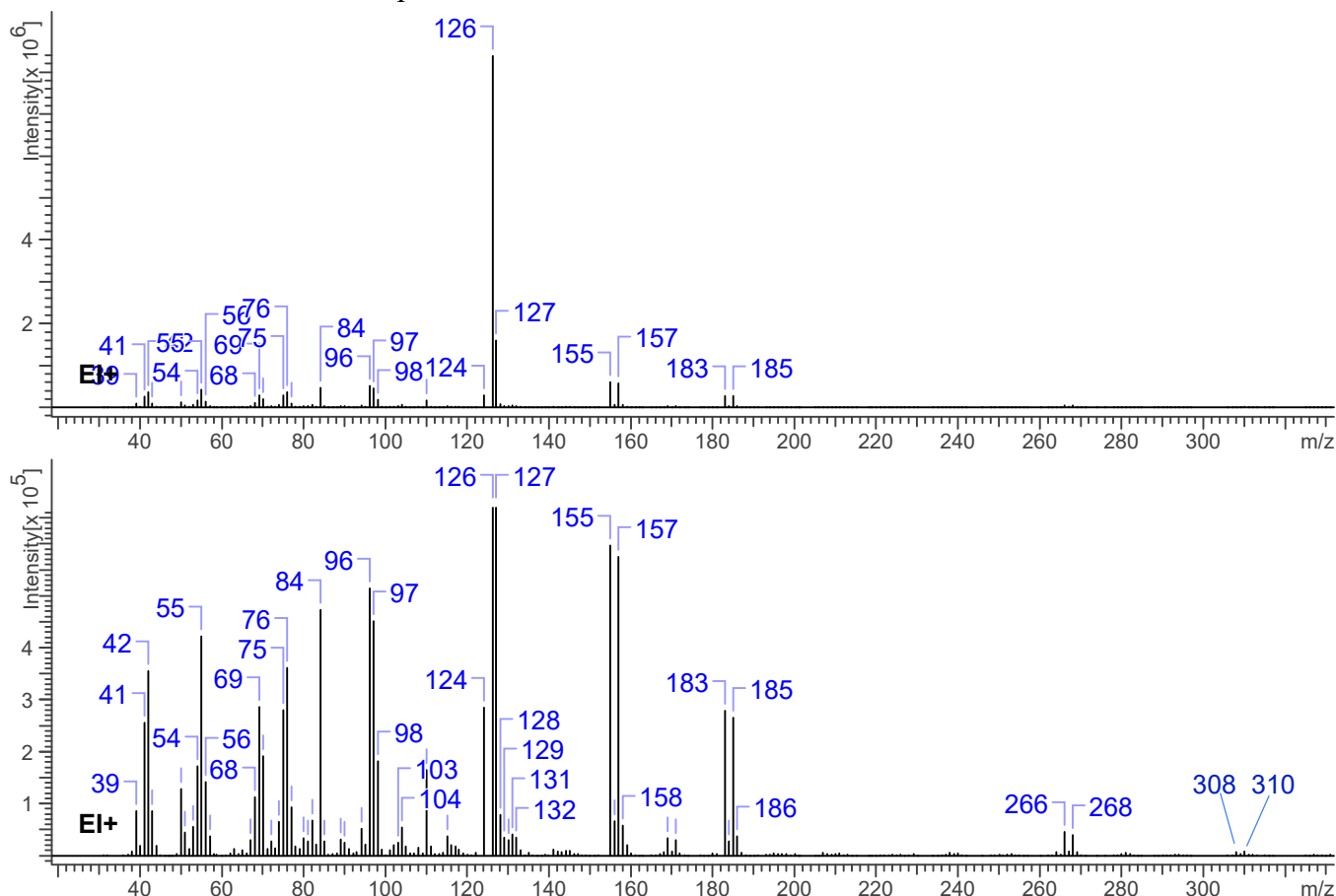


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl_3 base extracted with NaOH

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1.5 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 280°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: 150
Tune file: stune.u Acquisition mode: scan
Retention Time: 12.027 min

EI Mass Spectrum: 4-Bromo- α -PVP HCl; Lot# RM-160316-01





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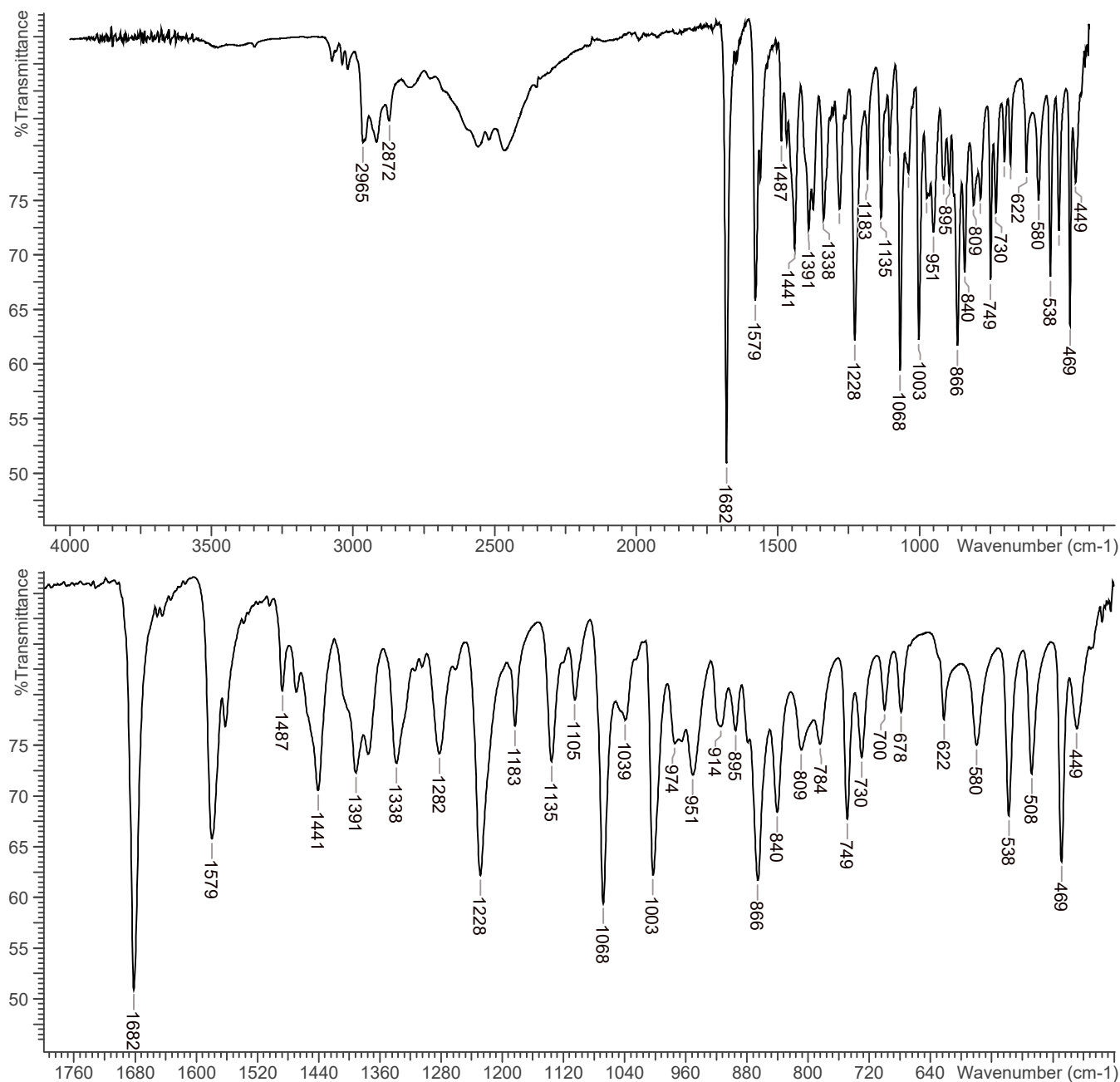


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): 4-Bromo- α -PVP HCl; Lot# RM-160316-01





4-Bromo-a-PVP

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4. ADDITIONAL RESOURCES

No additional resources as of 03/2016