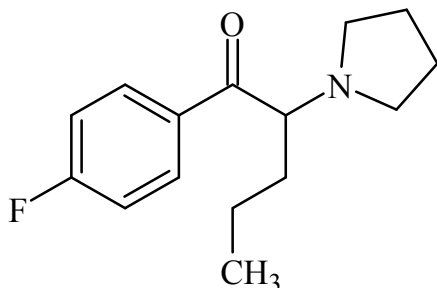




## 4-Fluoro-PVP

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



### 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	1-(4-fluorophenyl)-2-(pyrrolidin-1-yl)pentan-1-one
<b>CAS#:</b>	850352-31-7
<b>Synonyms:</b>	4-Fluoro- $\alpha$ -PVP, 4-fluoro- $\alpha$ -2-(1-pyrrolidinyl)-valerophenone, 4-fluoro- $\alpha$ -pyrrolidionpentiofenone
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder
<b>UV<sub>max</sub>(nm):</b>	Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>15</sub> H <sub>20</sub> FNO	249	Not Determined
HCl	C <sub>15</sub> H <sub>20</sub> FNO HCl	285	204.4



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### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~5 mg/mL in D<sub>2</sub>O containing TMS for 0 ppm reference and maleic acid as quantitative internal standard.

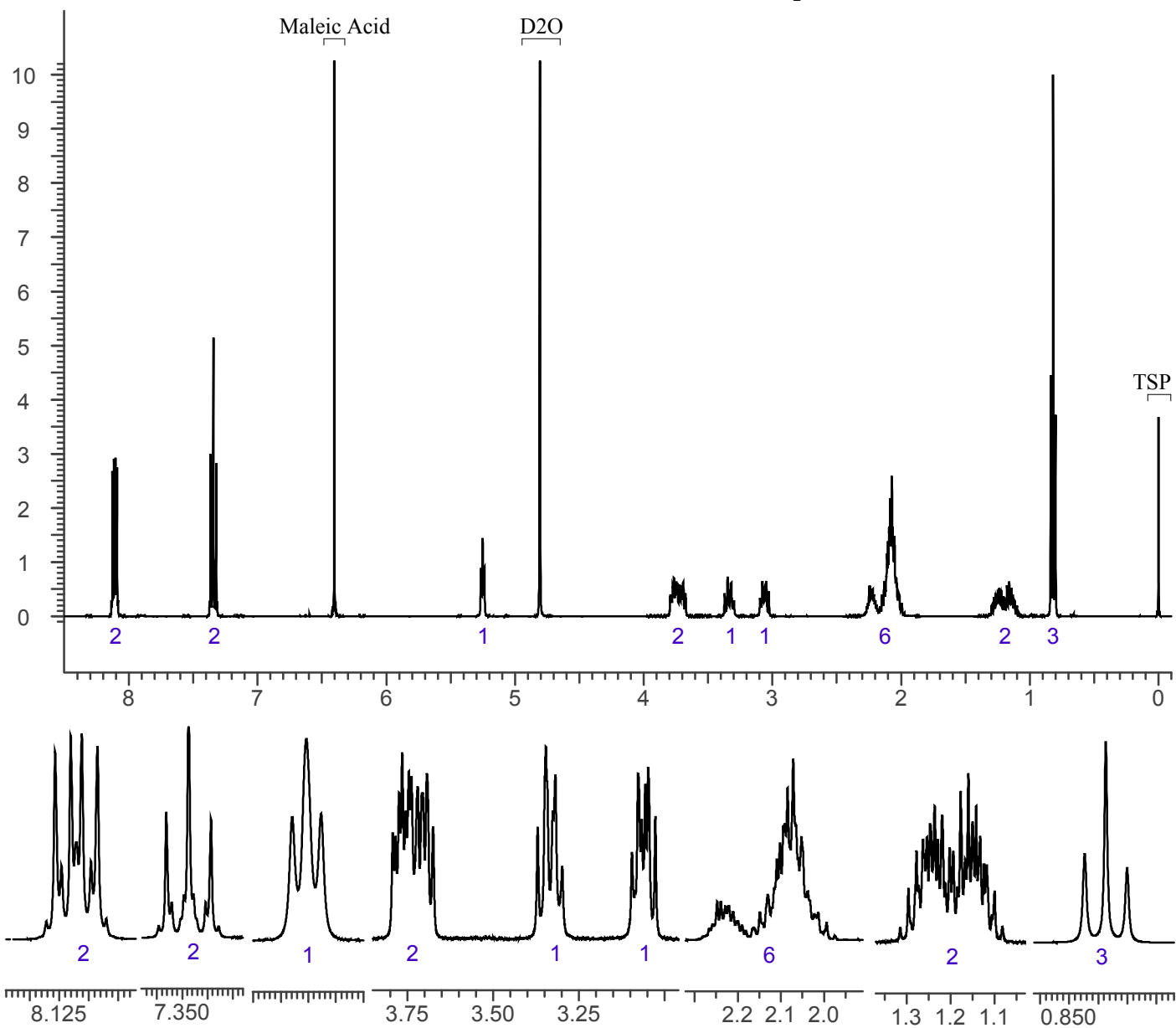
**Instrument:** 400 MHz NMR spectrometer

**Parameters:** Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

<sup>1</sup>H NMR: 4-Fluoro-PVP HCl, Lot 0453912-14, D<sub>2</sub>O 400MHz





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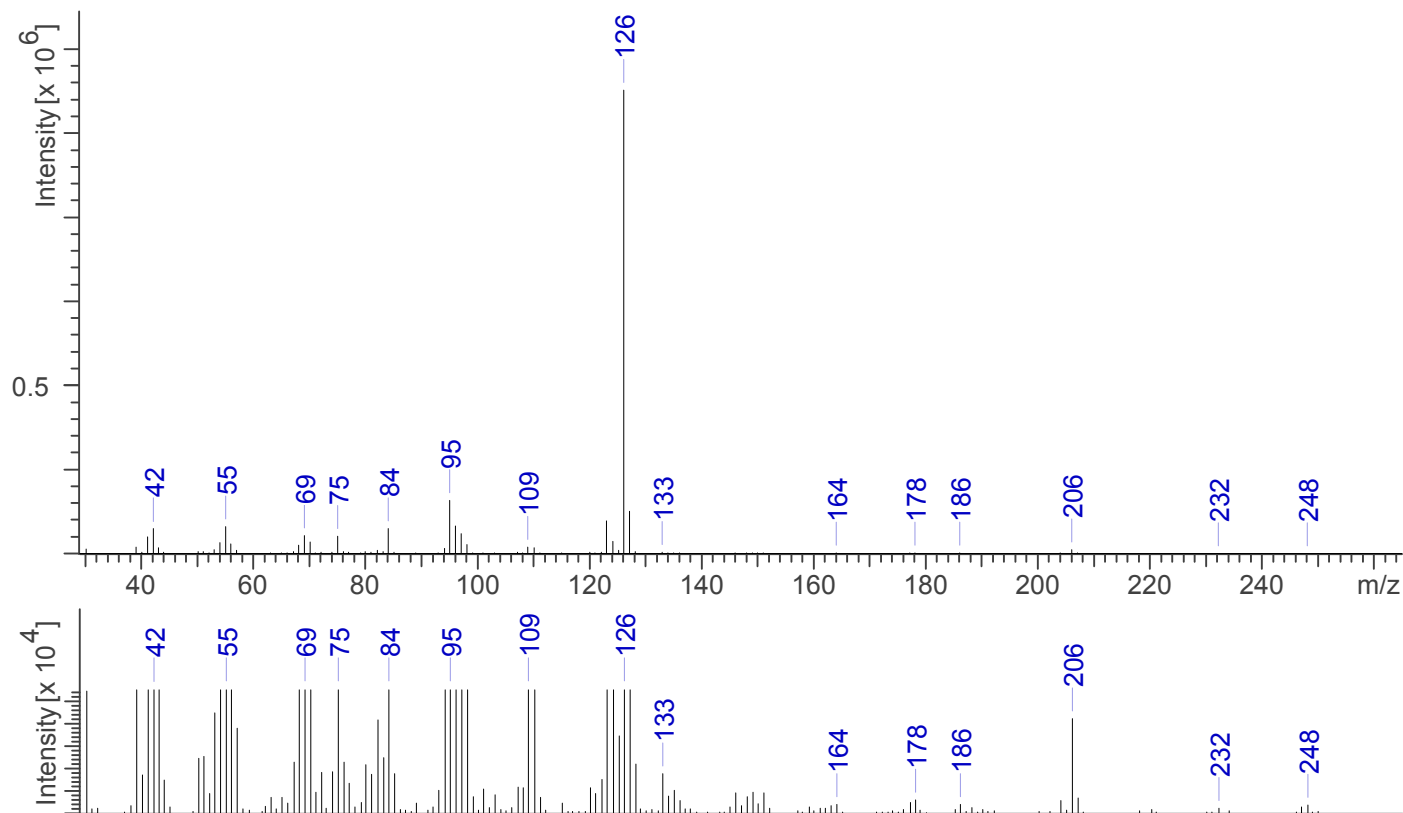


### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte ~3 mg/mL in Methanol.

**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  $\mu$ m  
**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 = 20:1, 1  $\mu$ L injected  
**MS Parameters:** Mass scan range: 30-550 amu  
Threshold: 100  
Tune file: stune.u  
Acquisition mode: scan  
**Retention Time:** 8.837 min

EI Mass Spectrum: 4-Fluoro-PVP HCl, Lot 0453912-14





# 4-Fluoro-PVP

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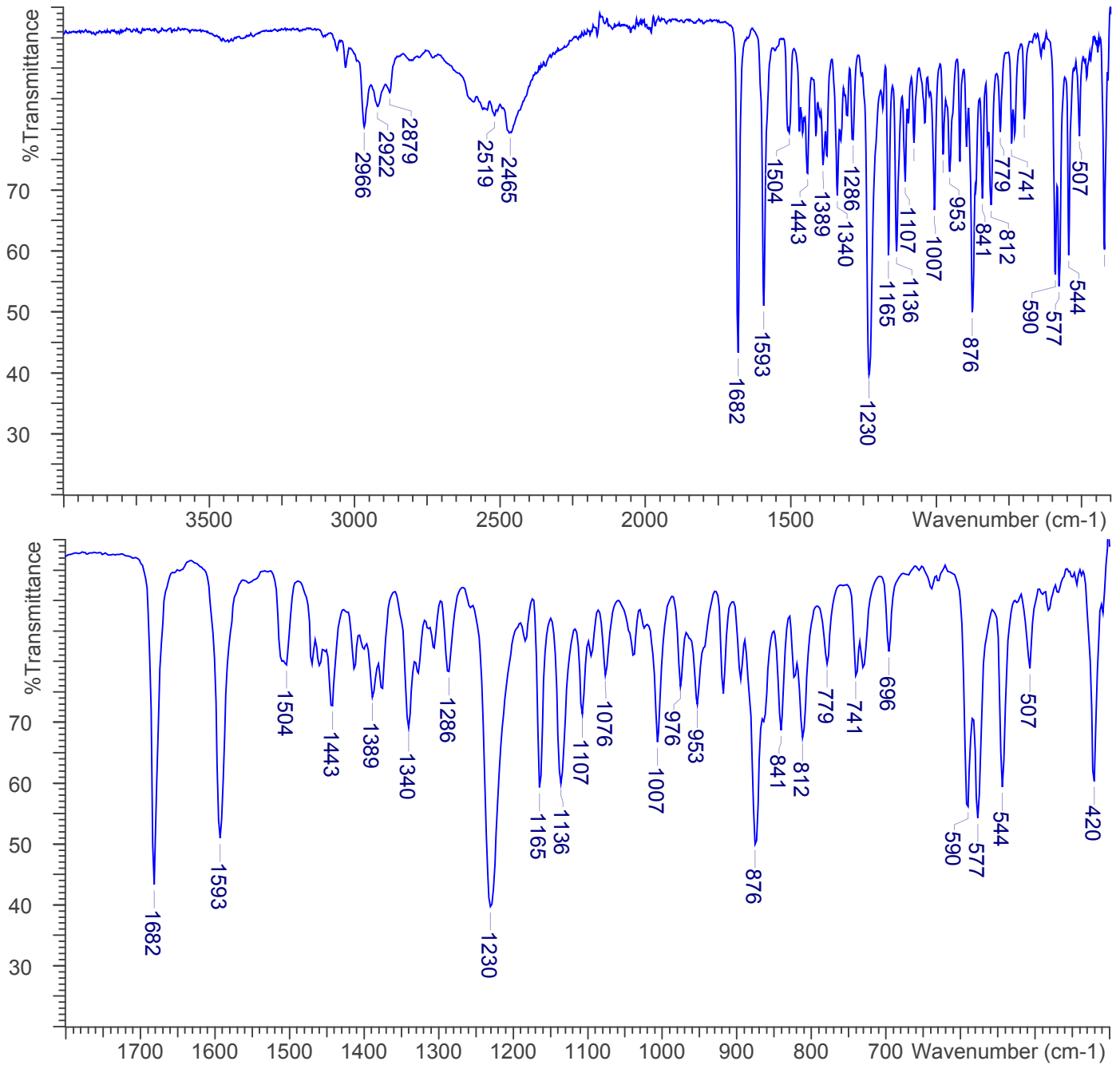


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (1 bounce)

**Scan Parameters:**  
Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 1 Bounce): 4-Fluoro-PVP HCl, Lot 0453912-14





## 4-Fluoro-PVP

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### **4. ADDITIONAL RESOURCES**

*No References available as of 03/2015*