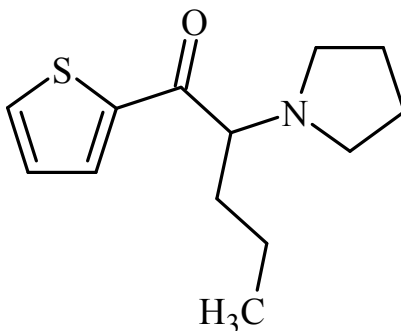




## a-PVT

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



### 1. GENERAL INFORMATION

**IUPAC Name:** 2-(pyrrolidin-1-yl)-1-(thiophen-2-yl)pentan-1-one

**CAS#:** NA

**Synonyms:**  $\alpha$ -pyrrolidinovalerothiophenone

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV<sub>max</sub>(nm):** Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>13</sub> H <sub>19</sub> NOS	237	Not Determined
HCl	C <sub>13</sub> H <sub>19</sub> NOS HCl	273	214.9



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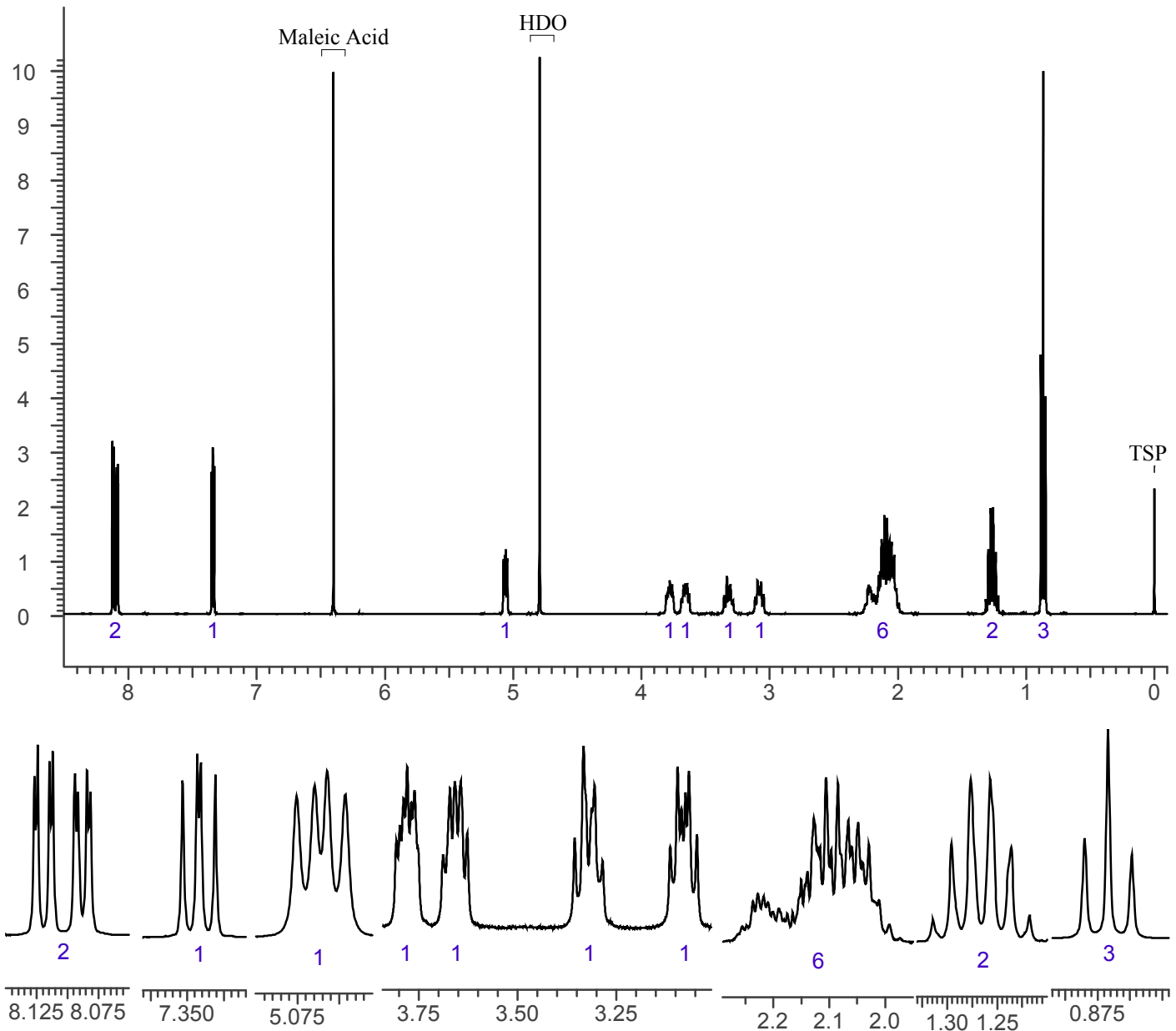


## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

*Sample Preparation:* Dilute analyte to ~25 mg/mL in D<sub>2</sub>O 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  
<sup>1</sup>H NMR: α-PVT HCl Lot RM-140331-01, D<sub>2</sub>O, 400MHz





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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*Sample Preparation:* Dilute analyte ~4 mg/mL in CHCl<sub>3</sub>.

**Instrument:** Agilent gas chromatograph operated in split mode with MS detector

**Column:** DB-1 MS (or equivalent); 30m x 0.25 mm x 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 9.0 min

**Injection Parameters:** Split Ratio = 20:1, 1 μL injected

**MS Parameters:** Mass scan range: 30-550 amu

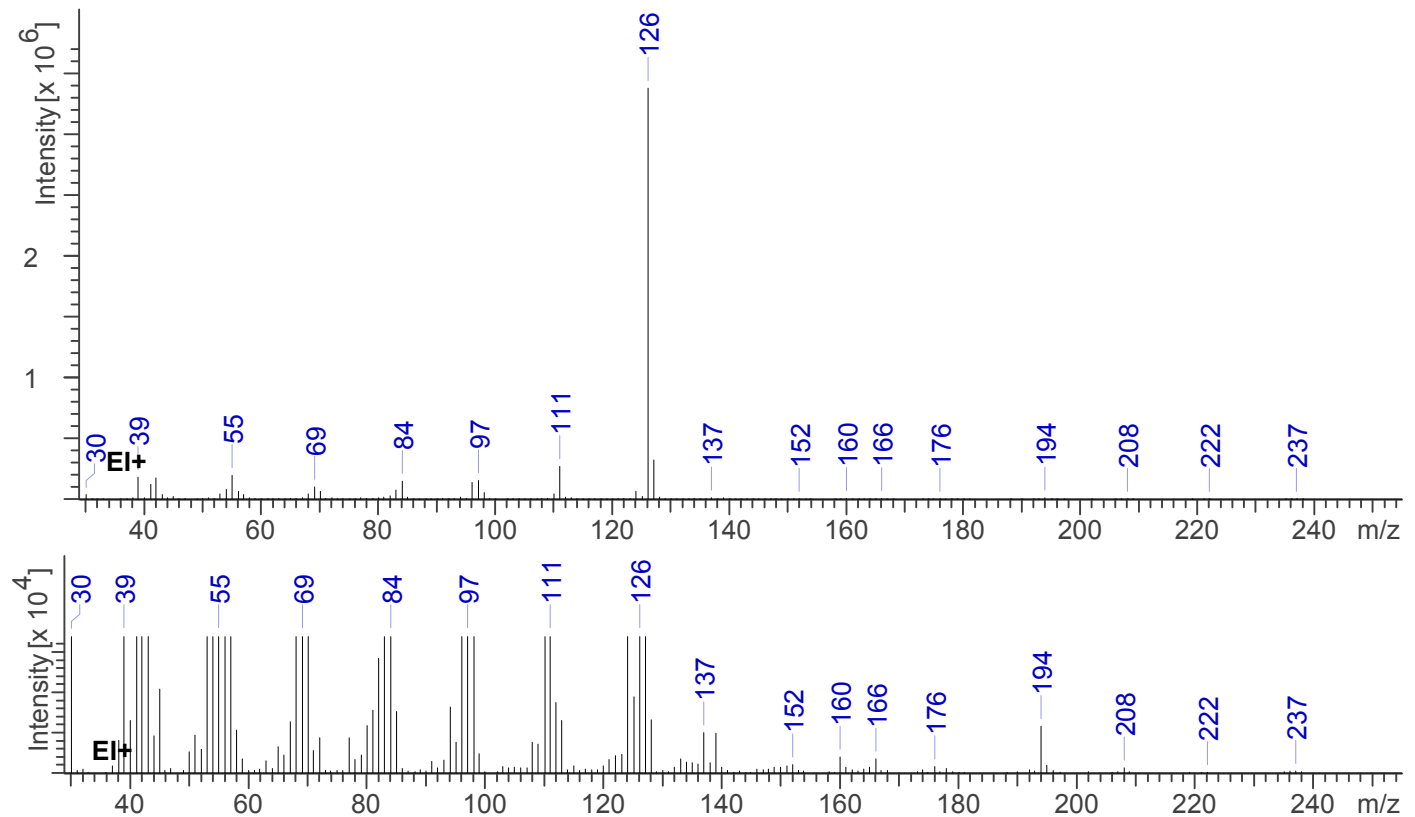
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 9.318 min

EI Mass Spectrum α-PVT HCl Lot RM-140331-01





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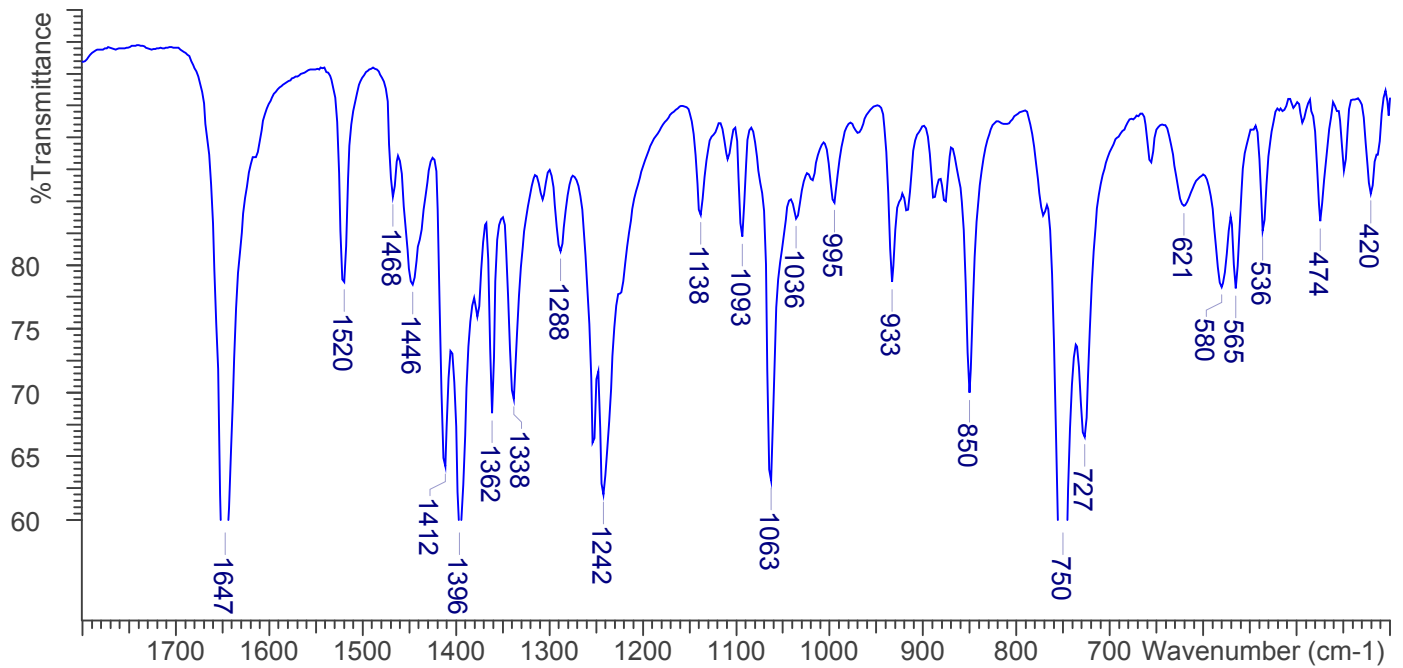
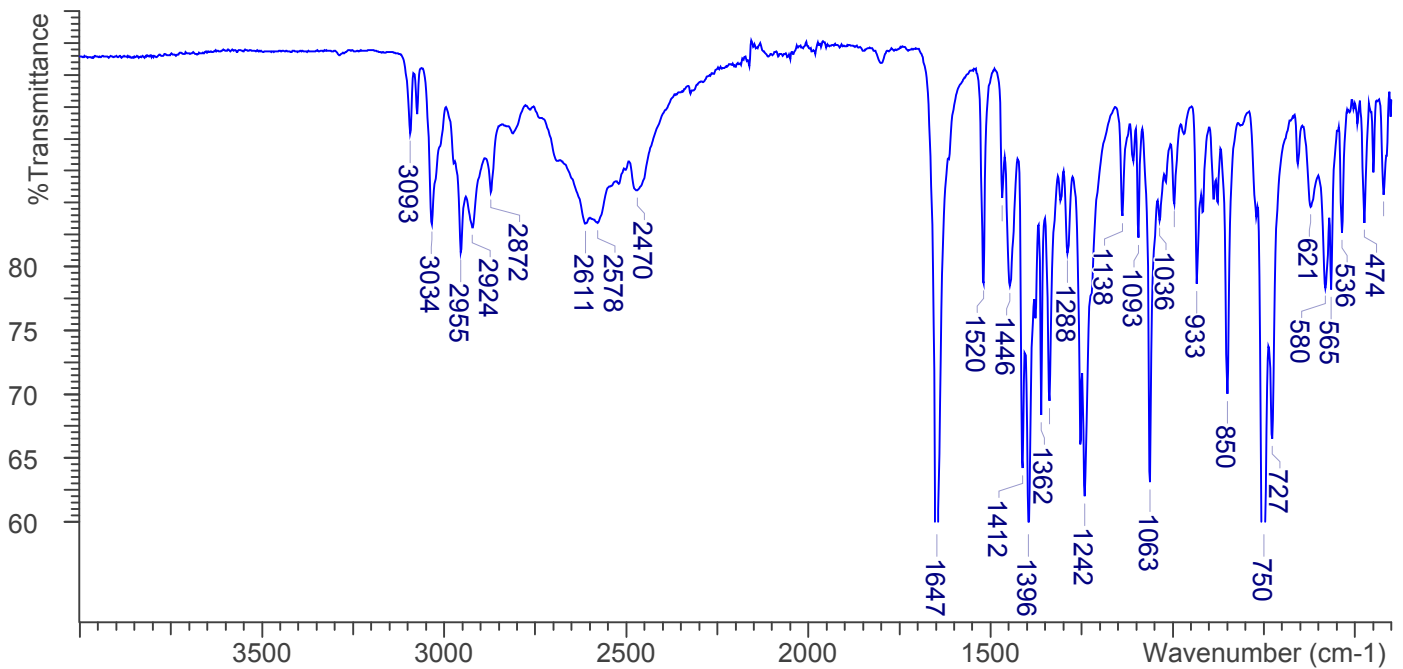


## 3.3 INFRARED SPECTROSCOPY (FTIR)

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

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

FTIR ATR (Diamond, 1 Bounce) α-PVT HCl Lot # RM-140331-01





## a-PVT

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### **4. ADDITIONAL RESOURCES**

Uchiyama, N.; Matsuda, S.; Kawamura, M.; Kikura-Hanajiri, R.; Goda, Y. Two new-type cannabimimetic quinolinyl carboxylates, QUPIC and QUCHIC, two new cannabimimetic carboxamide derivatives, ADB-FUBINACA and ADBICA, and five synthetic cannabinoids detected with a thiophene derivative  $\alpha$ -PVT and an opioid receptor agonist AH-7921 identified in illegal products. *Forensic Toxicol.* 2013, 31, 223-240.