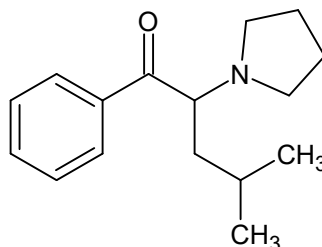




## $\alpha$ -PiHP

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



### 1. GENERAL INFORMATION

**IUPAC Name:** 4-methyl-1-phenyl-2-(pyrrolidin-1-yl)pentan-1-one

**CAS#:** 13415-86-6 (base), 13415-59-3 (HCl)

**Synonyms:**  $\alpha$ -Pyrrolidinoisohexanophenone

**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>16</sub> H <sub>23</sub> NO	245.36	Not Determined
HCl	C <sub>16</sub> H <sub>23</sub> NO HCl	281.82	Not Determined



# $\alpha$ -PiHP

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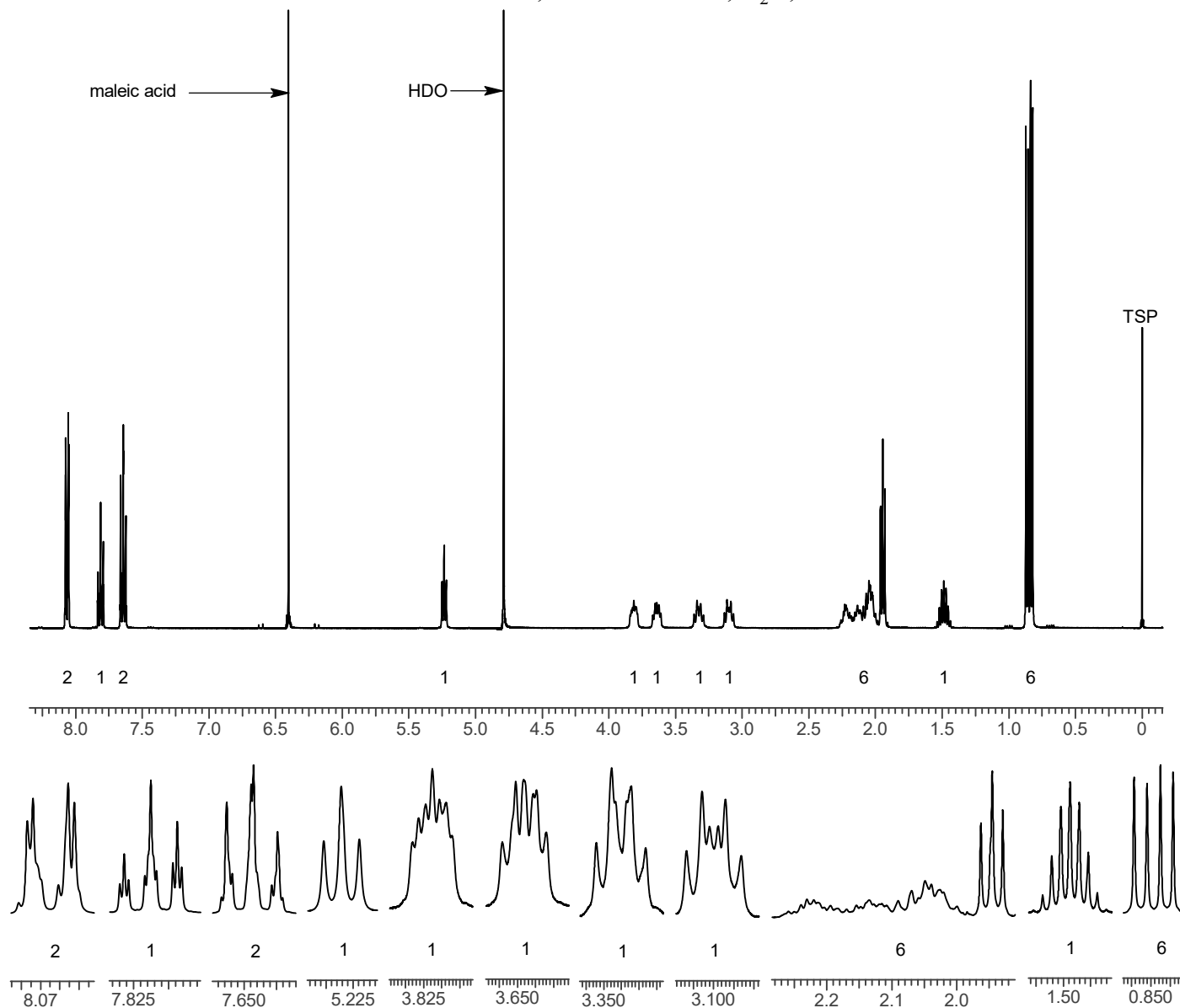
## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~10 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>HNMR:  $\alpha$ -PiHP HCl ; Lot# 0556730-1; 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:** HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25  $\mu$ m

**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  $\mu$ L injected

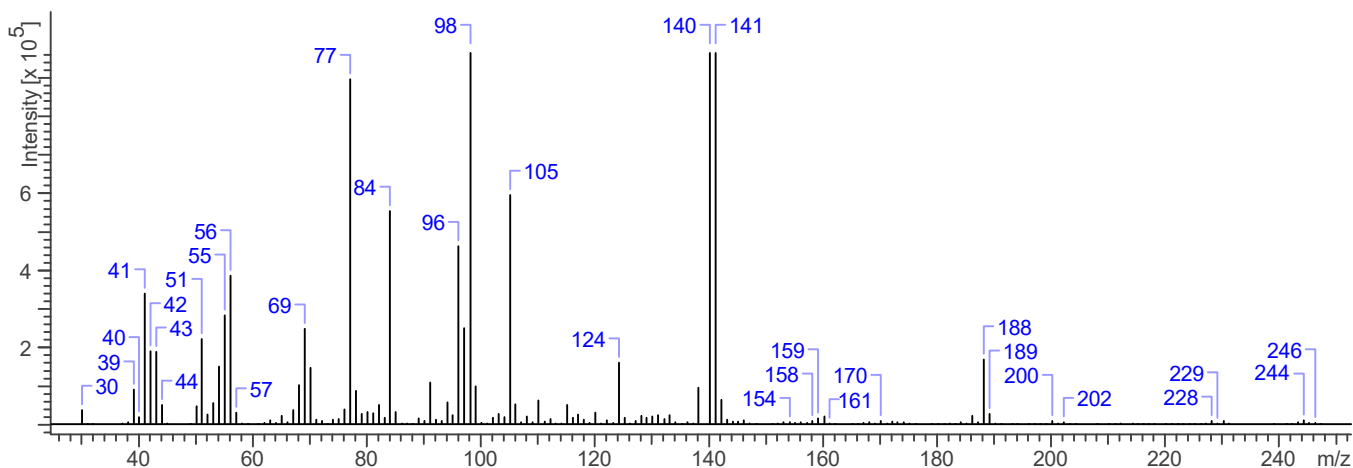
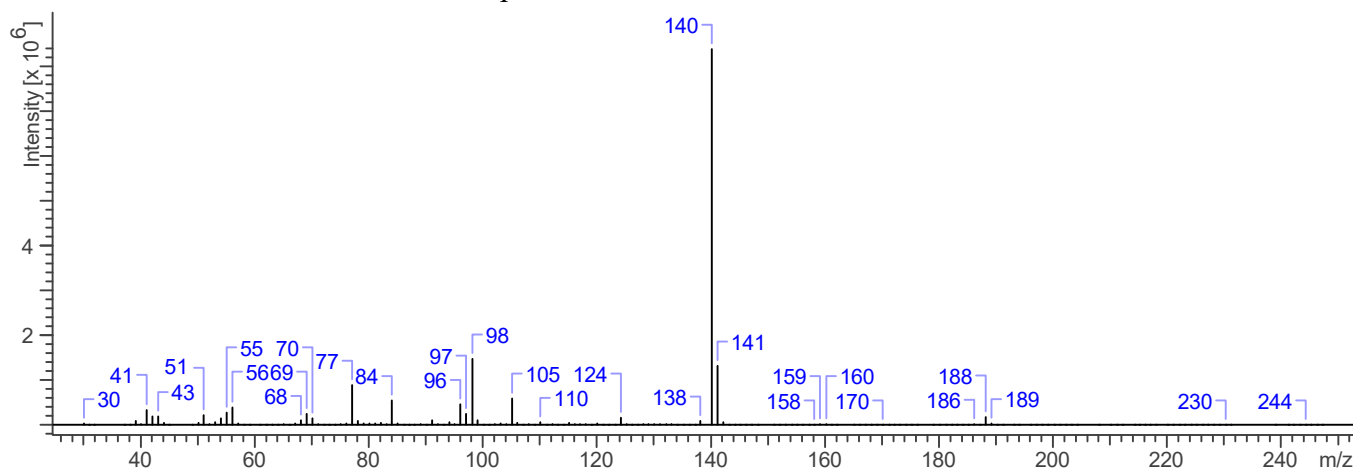
**MS Parameters:** Mass scan range: 30-550 amu                      Threshold: 250

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 9.56 min

EI Mass Spectrum:  $\alpha$ -PiHP HCl ; Lot# 0556730-1





# $\alpha$ -PiHP

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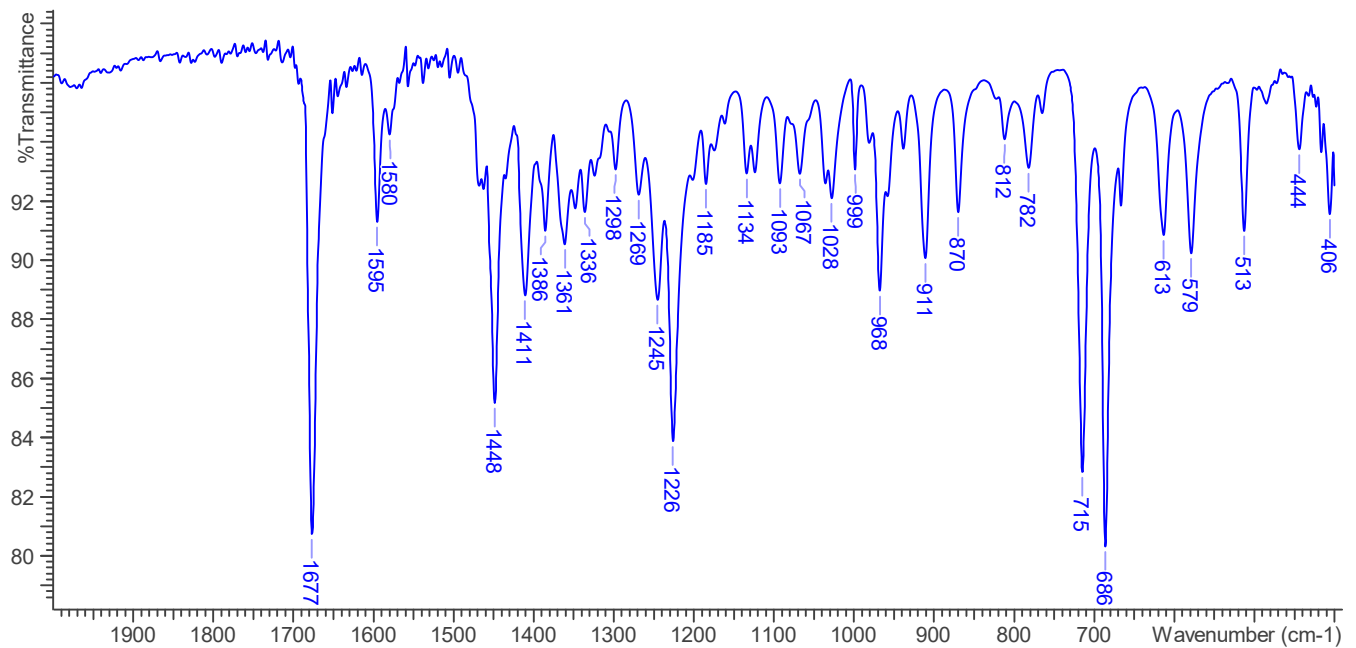
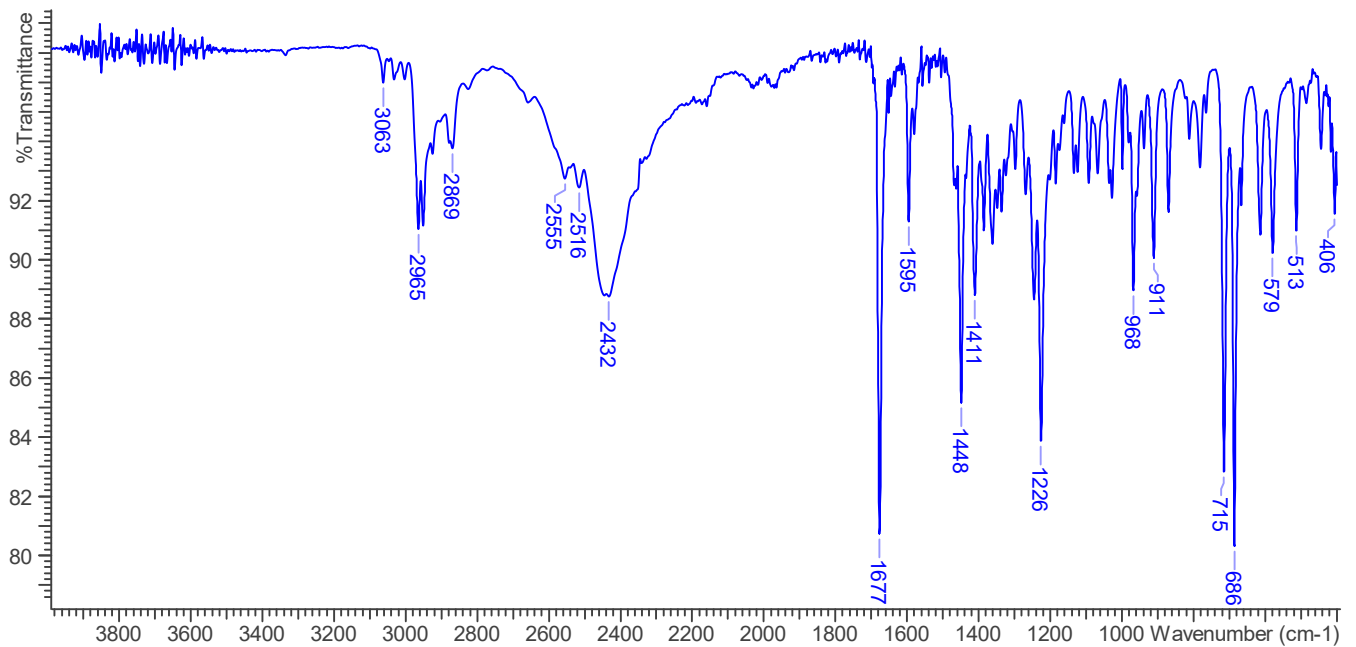


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**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: 1  
Aperture: 150

FTIR ATR (Diamond 1 Bounce):  $\alpha$ -PiHP HCl; Lot# 0556730-1; After drying





# $\alpha$ -PiHP

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



## 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: 1  
Aperture: 150

FTIR ATR (Diamond 1 Bounce):  $\alpha$ -PiHP HCl ; Lot# 0556730-1; Direct from bottle

