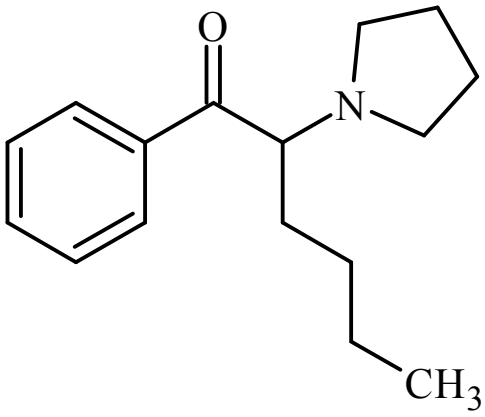
a-PHP

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



1. GENERAL INFORMATION

IUPAC Name: 1-phenyl-2-(pyrrolidin-1-yl)hexan-1-one

CAS#: 13415-59-3 (HCl)

Synonyms: α-pyrrolidinohexanophenone, α-pyrrolidinohexiophenone, 2-(1-pyrrolidinyl)hexanophenone, PV-7

Source: DEA Reference Material Collection

Appearance: Tan powder

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{16}H_{23}NO$	245	Not Determined
HCl	$C_{16}H_{23}NO$ HCl	281	Not Determined

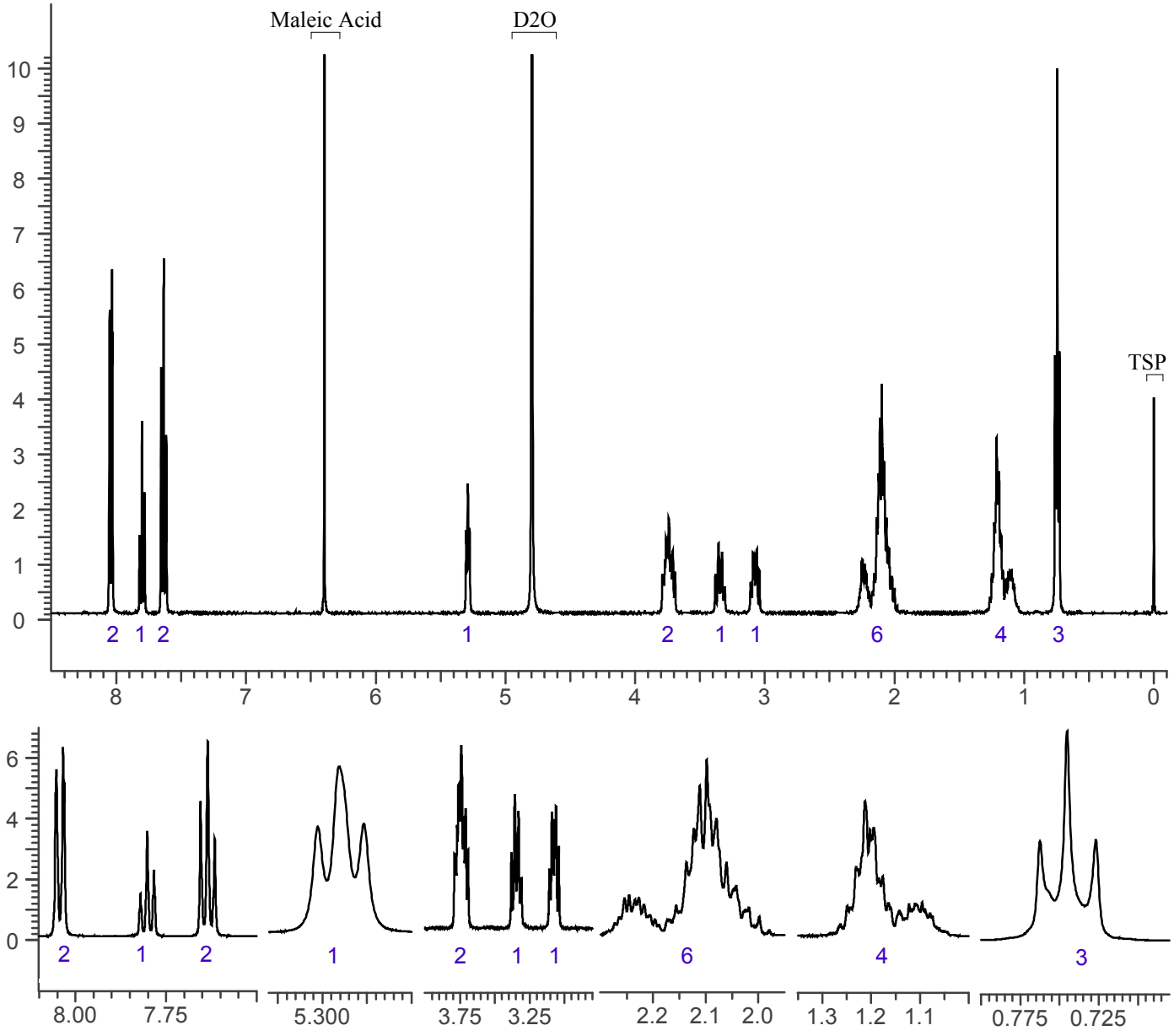
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~20 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 -2.9 ppm through 13.2 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^{1}H NMR: α-PHP HCl Lot#RM-150116-01

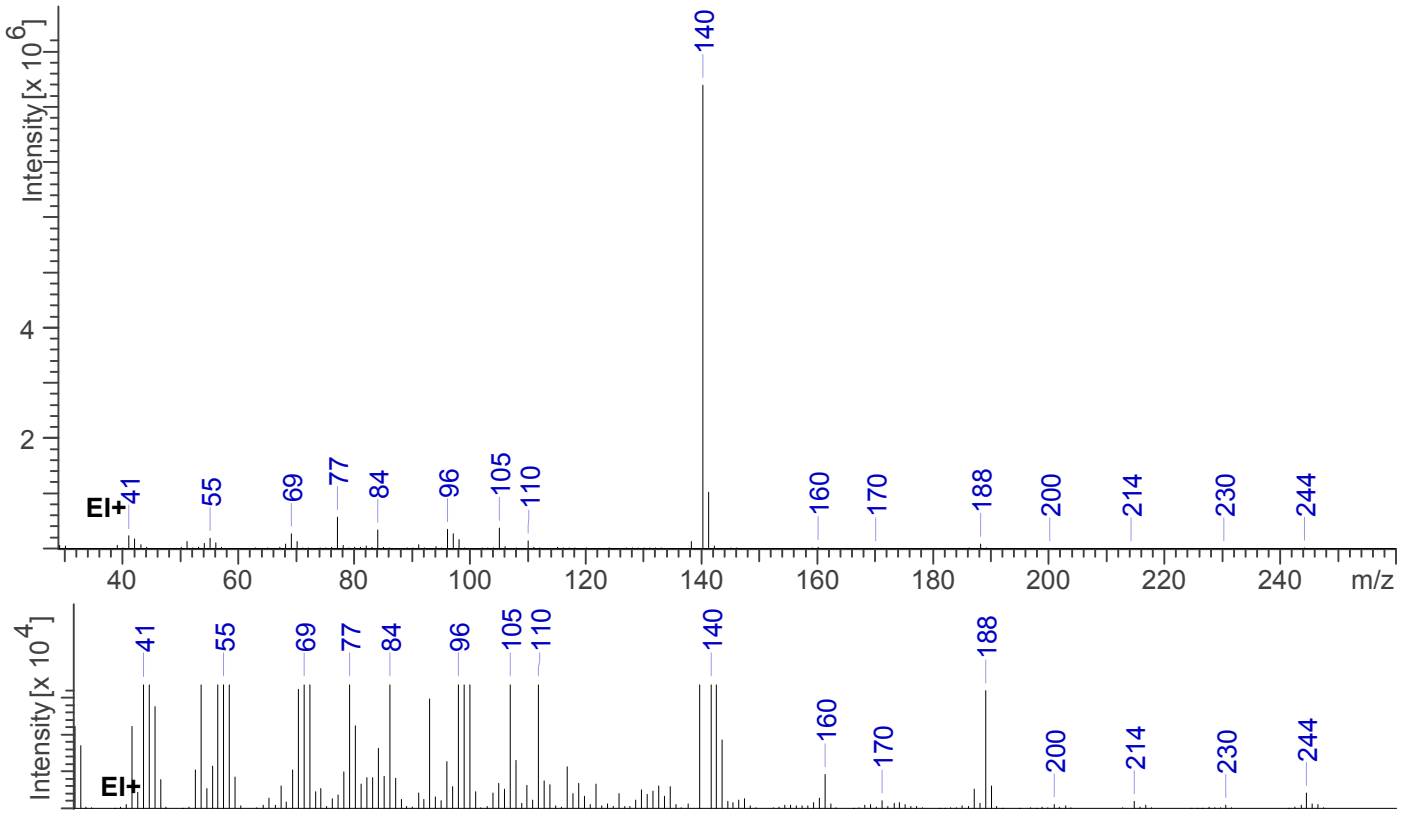


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 mg/mL in $CHCl_3$ base extracted with 1N Sodium Hydroxide

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 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:	11.401 min

EI Mass Spectrum: α-PHP HCl Lot# RM-150116-01

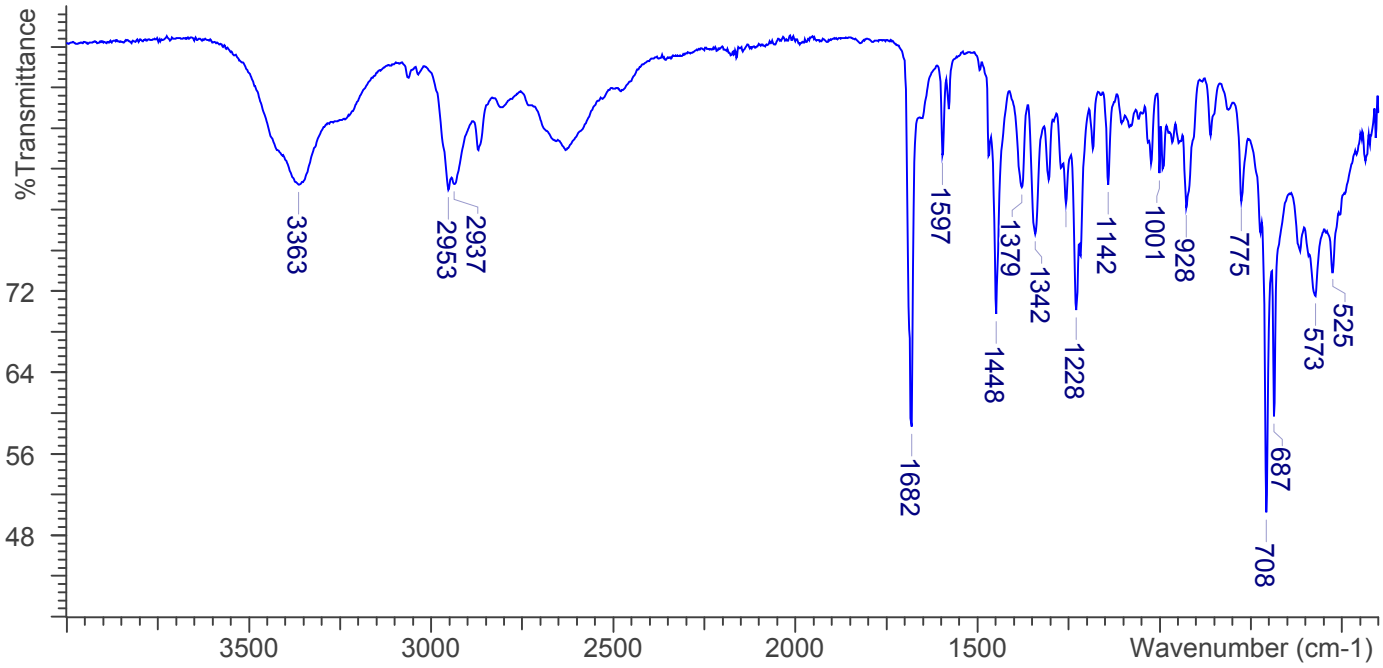


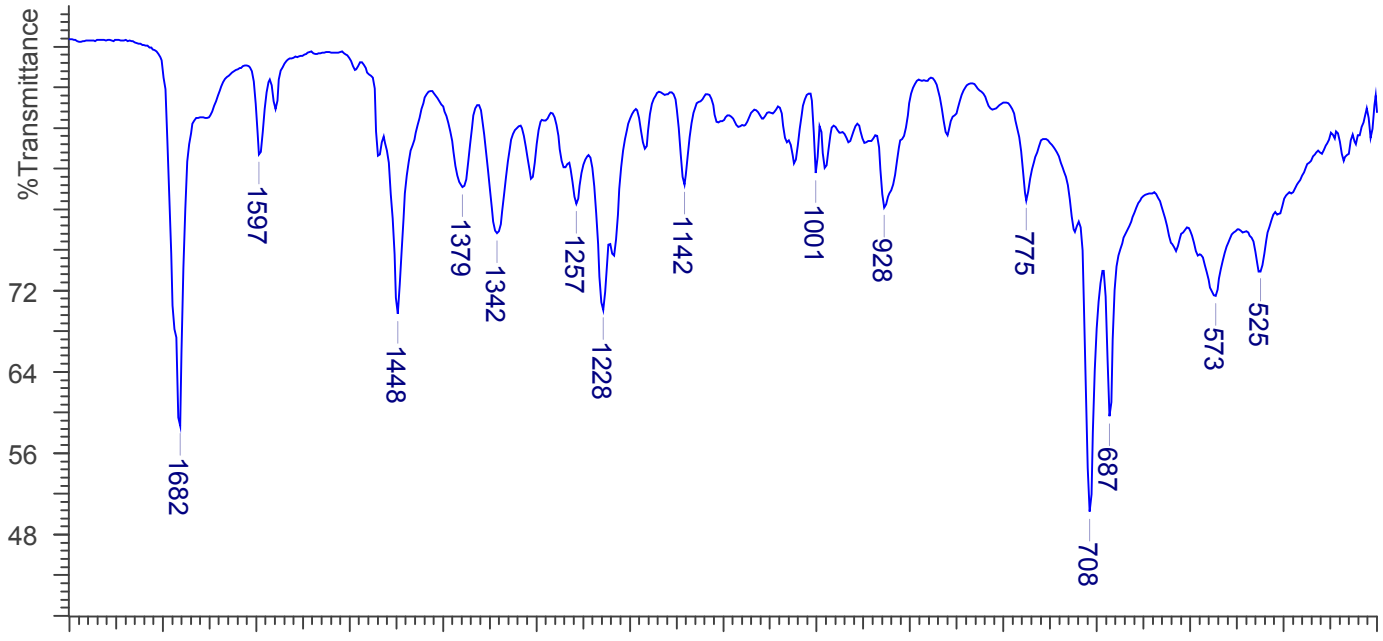
3.3 INFRARED SPECTROSCOPY (FTIR)

Insrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters: Number of scans: 16
Number of background scans: 16
Resolution: 4 cm^{-1}
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 1 Bounce): α-PHP HCl Lot# RM-150116-01





4. ADDITIONAL RESOURCES

Wikipedia