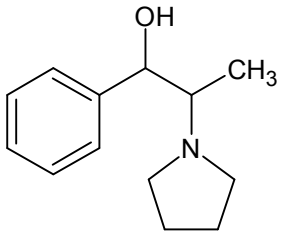
dihydro-a-PPP

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)propan-1-ol

CAS#: Not Determined

Synonyms: dihydro-α-pyrrolidinopropiophenone

Source: DEA Reference Material Collection

Appearance: White granules (HCl)

UV_{max} (nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{13}H_{19}NO$	205	Not Determined
HCl	$C_{13}H_{19}NO \cdot HCl$	241	223.3

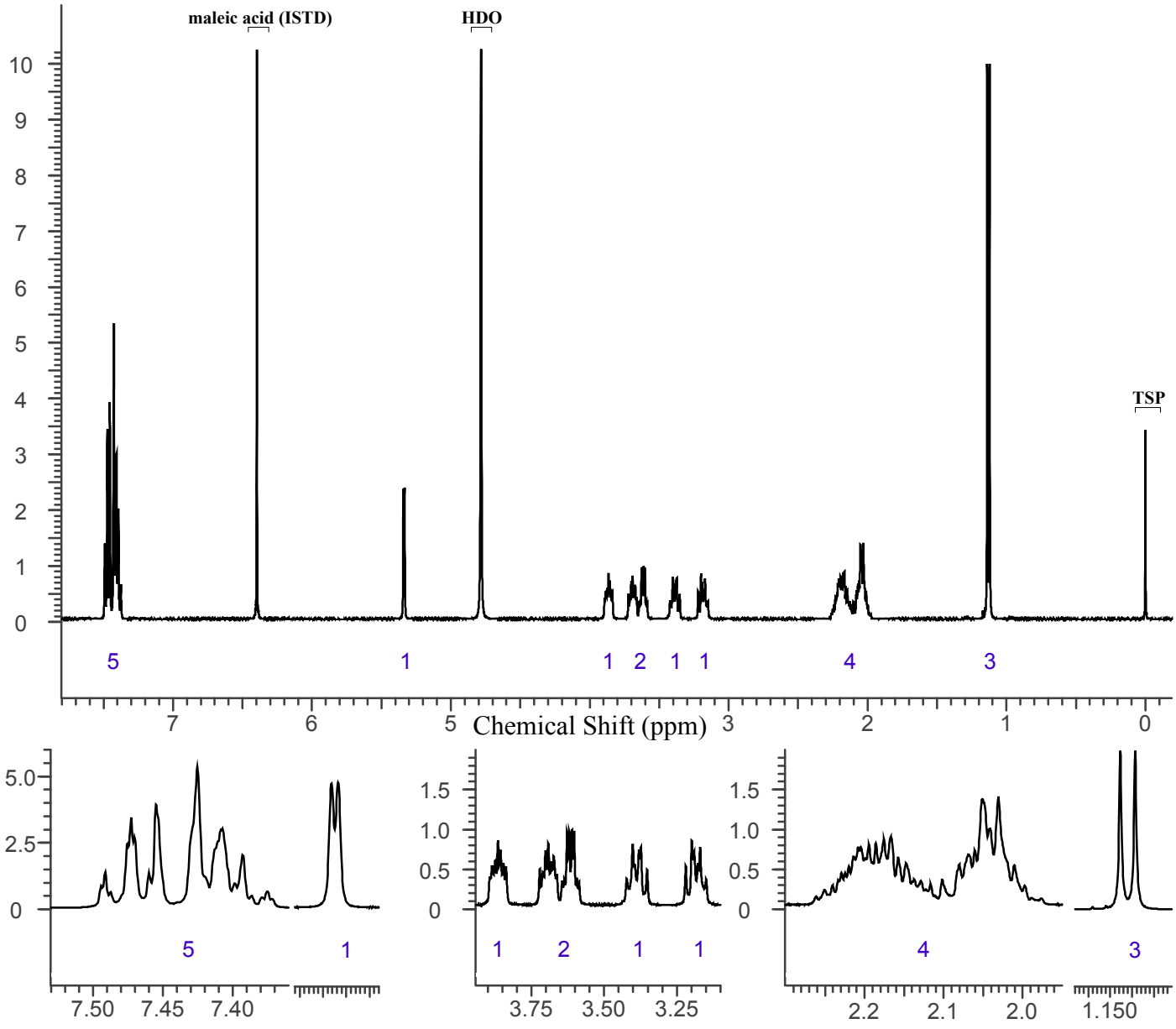
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~13 mg/mL in deuterium oxide (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 -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^{1}H NMR: dihydro-alpha-PPP HCl Lot# RM-131218-03; D_2O; 400MHz

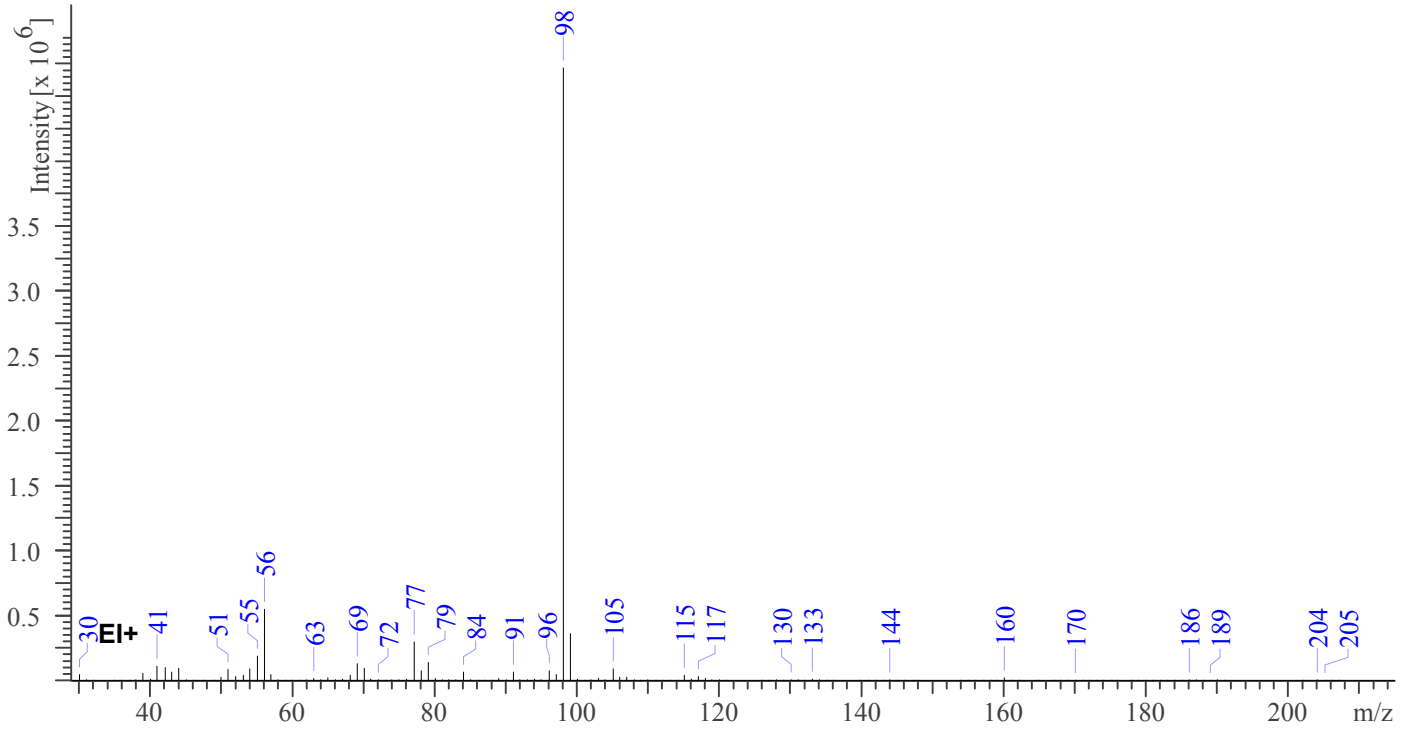


3.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 4 mg/mL base extracted into chloroform

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 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:	8.332 min

EI Mass Spectrum: dihydro-alpha-PPP HCl Lot# RM-131218-03

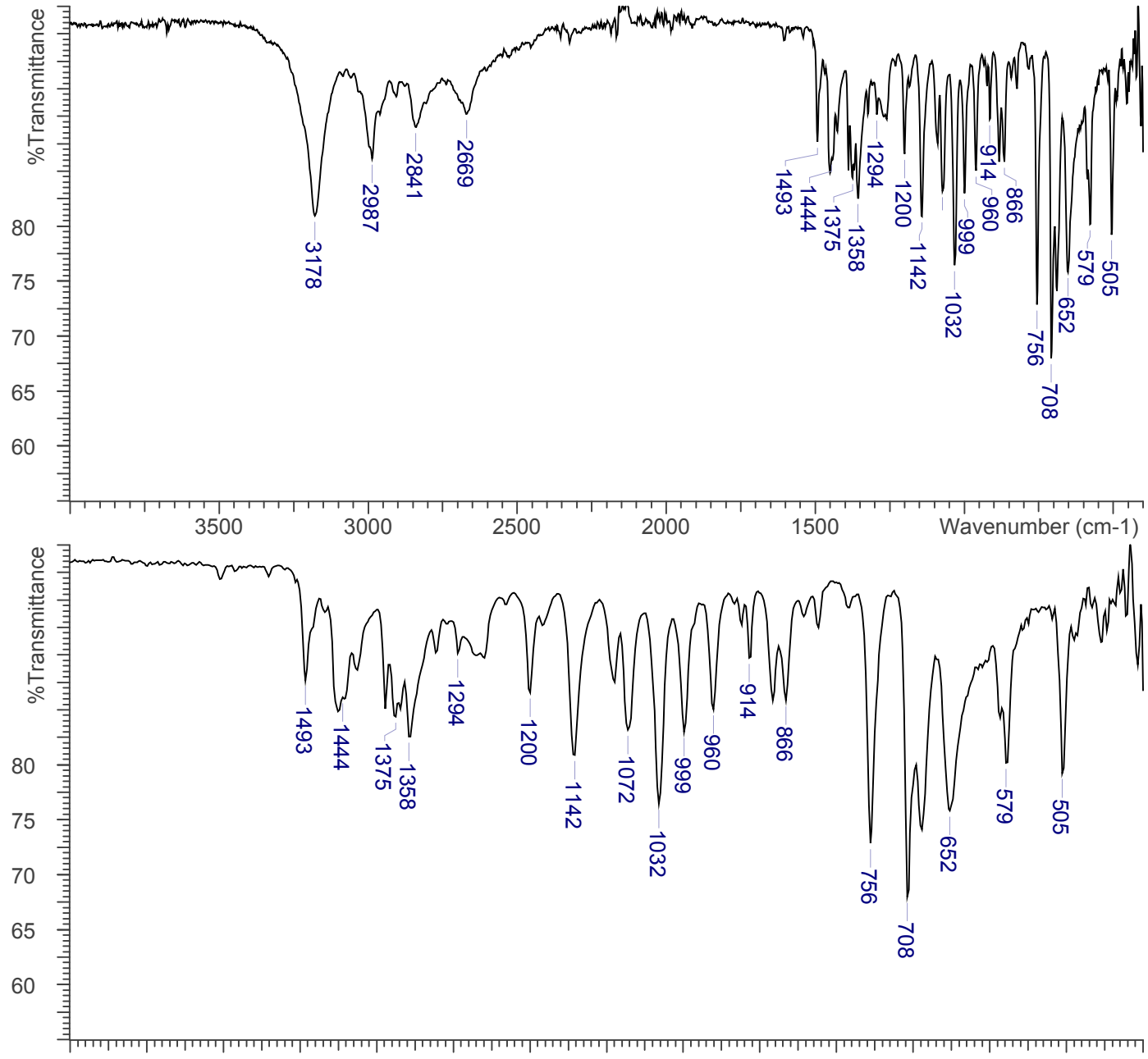


3.3 INFRARED SPECTROSCOPY (FTIR)

Insrument: FTIR with diamond ATR attachment (3 bounce)

Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4 cm^{-1}
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): dihydro-alpha-PPP HCl Lot# RM-131218-03



4. ADDITIONAL RESOURCES

Springer, D.; Fritschi, G.; Maurer, H. H. Metabolism of the new designer drug α-pyrrolidinopropiophenone (PPP) and the toxicological detection of PPP and 4'-methyl-α-pyrrolidinopropiophenone (MPPP) studied in rat urine using gas chromatography-mass spectrometry. Journal of Chromatography B, 796 (2003) 253-266.