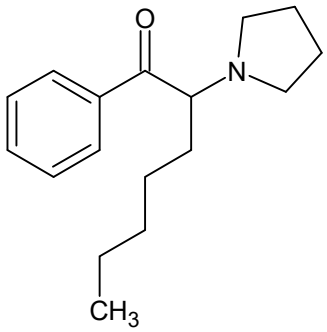


1. GENERAL INFORMATION

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

CAS#: 13415-55-9

Synonyms: α-pyrrolidinoheptiophenone, α-PHPP

Source: DEA Reference Material Collection

Appearance: White Powder (HCl)

UV_{max}(nm): Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{17}H_{25}NO$	259	Not Determined
HCl	$C_{17}H_{25}NO$ HCl	295	157.4

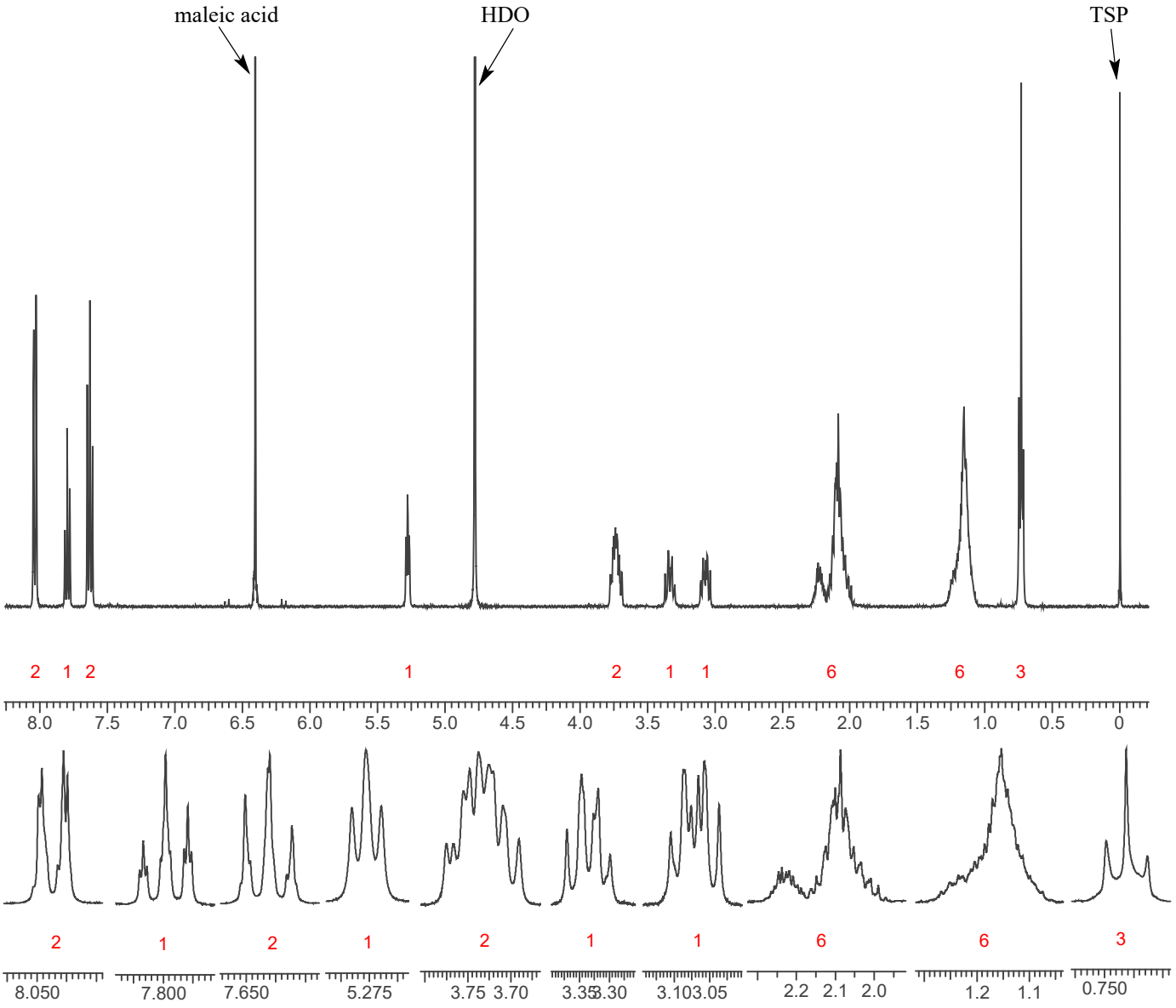
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 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 -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^{1}HNMR: PV-8 HCl; Lot# RM-131029-02; D_2O; 400MHz

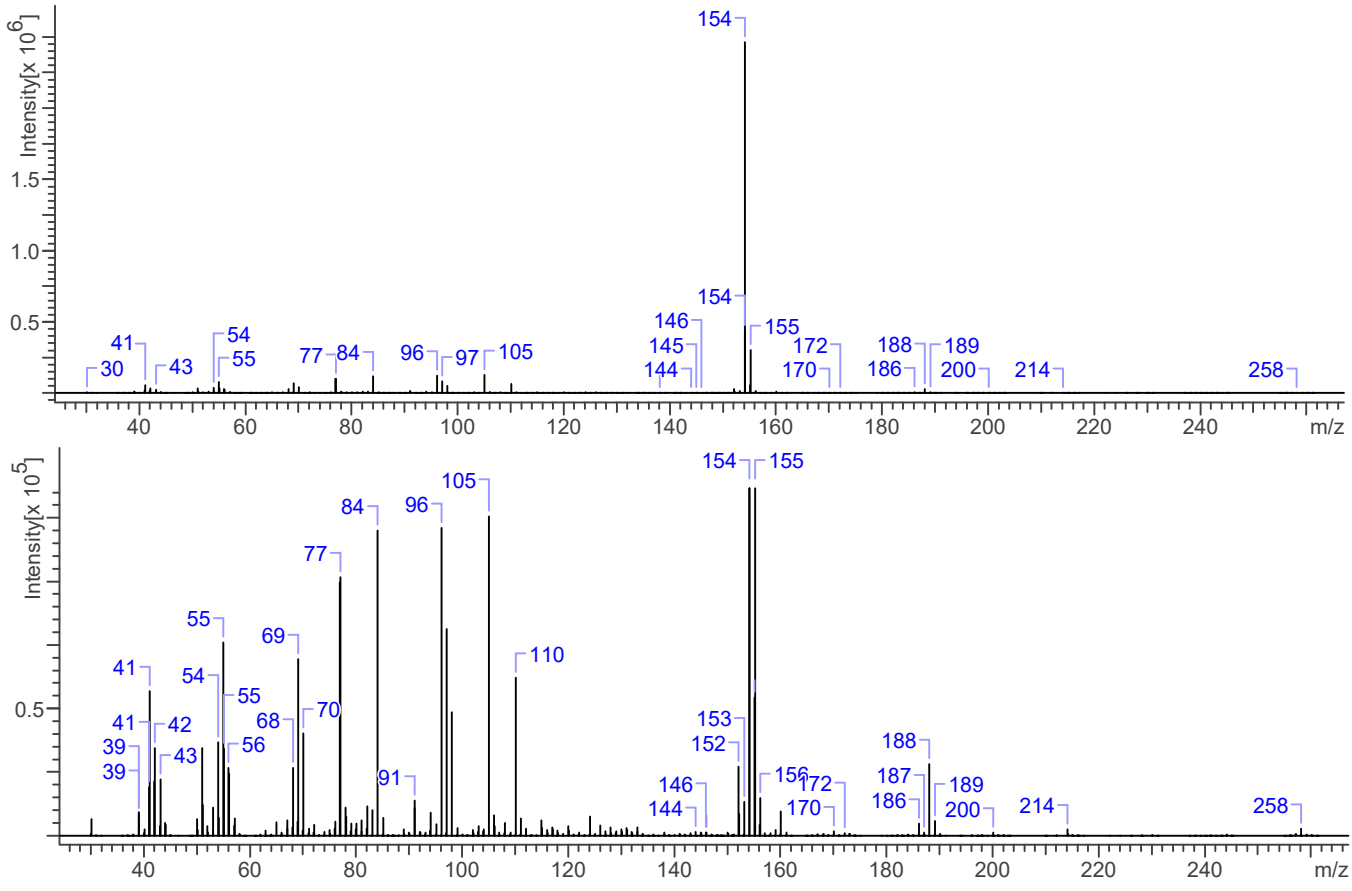


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 mg/mL in MeOH

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 1.0 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:	10.724 min

EI Mass Spectrum: PV-8 HCl; Lot# RM -131029-02

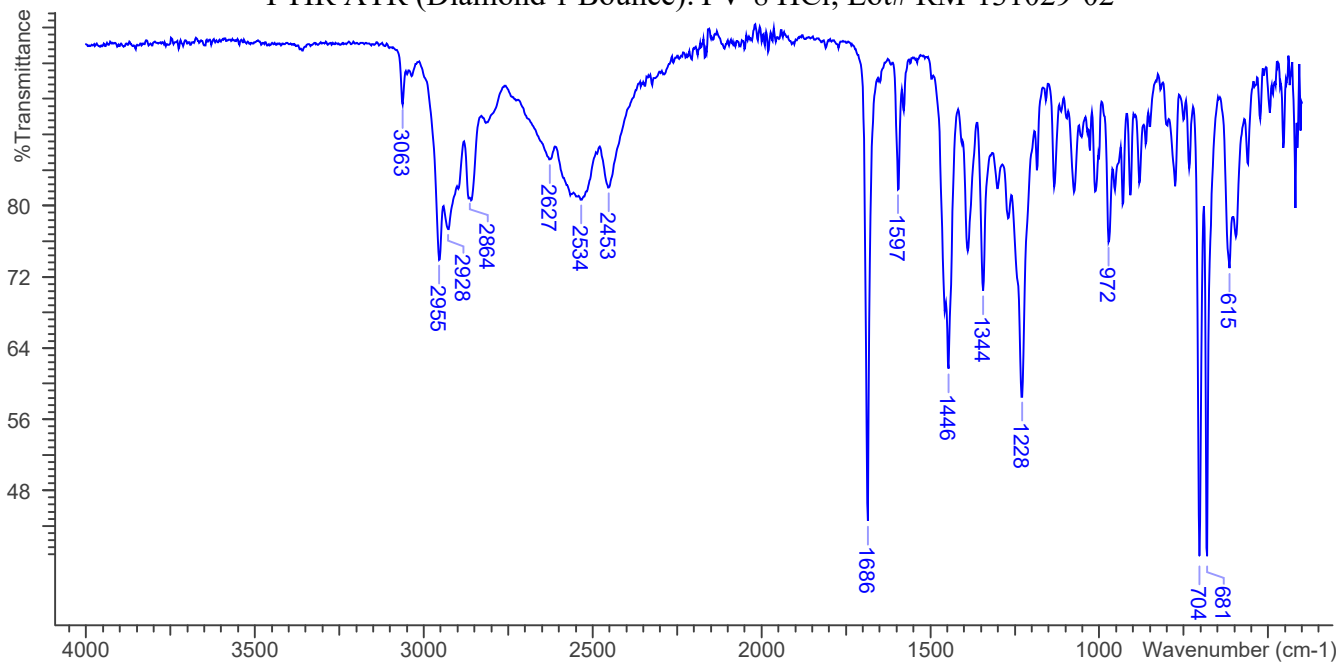


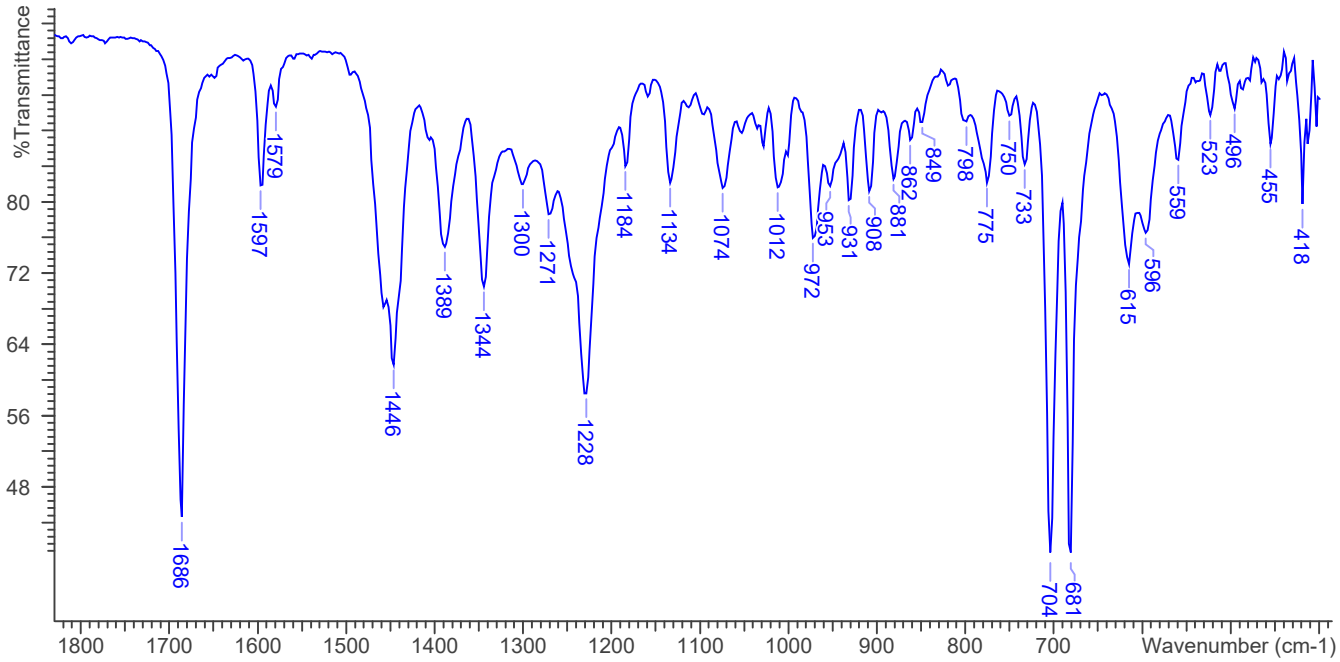
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

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

FTIR ATR (Diamond 1 Bounce): PV-8 HCl; Lot# RM-131029-02





4. ADDITIONAL RESOURCES

Forendex