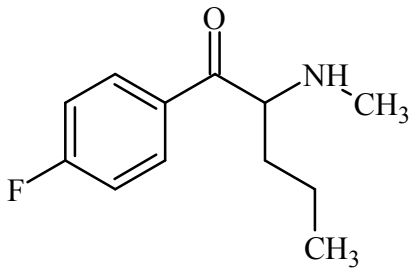
4-Fluoropentedrone

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



1. GENERAL INFORMATION

IUPAC Name: 1-(4-fluorophenyl)-2-(methylamino)pentan-1-one

CAS#: N/A

Synonyms: 4-FPD, 4-Fluoro-α-methylamino-Valerophenone

Source: DEA Reference Material Collection

Appearance: White powder

UV_{max}(nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{12}H_{16}FNO$	209.26	Not Determined
HCl	$C_{12}H_{16}FNO$ HCl	245.72	Not Determined

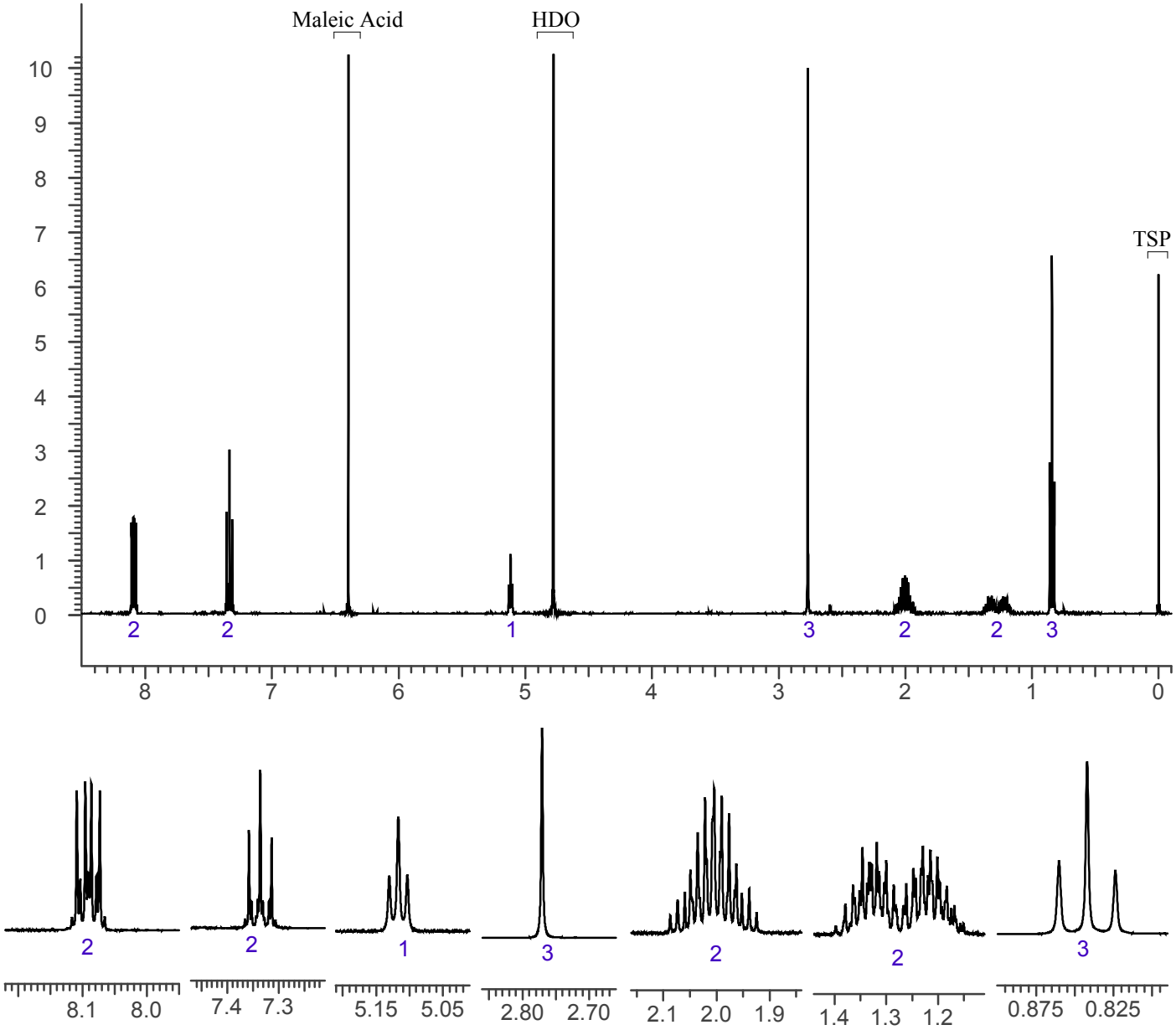
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~4 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 13.1 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

^{1}HNMR: 4-Fluoropentedrone HCl; Lot 0464459-21; D_2O; 400MHz

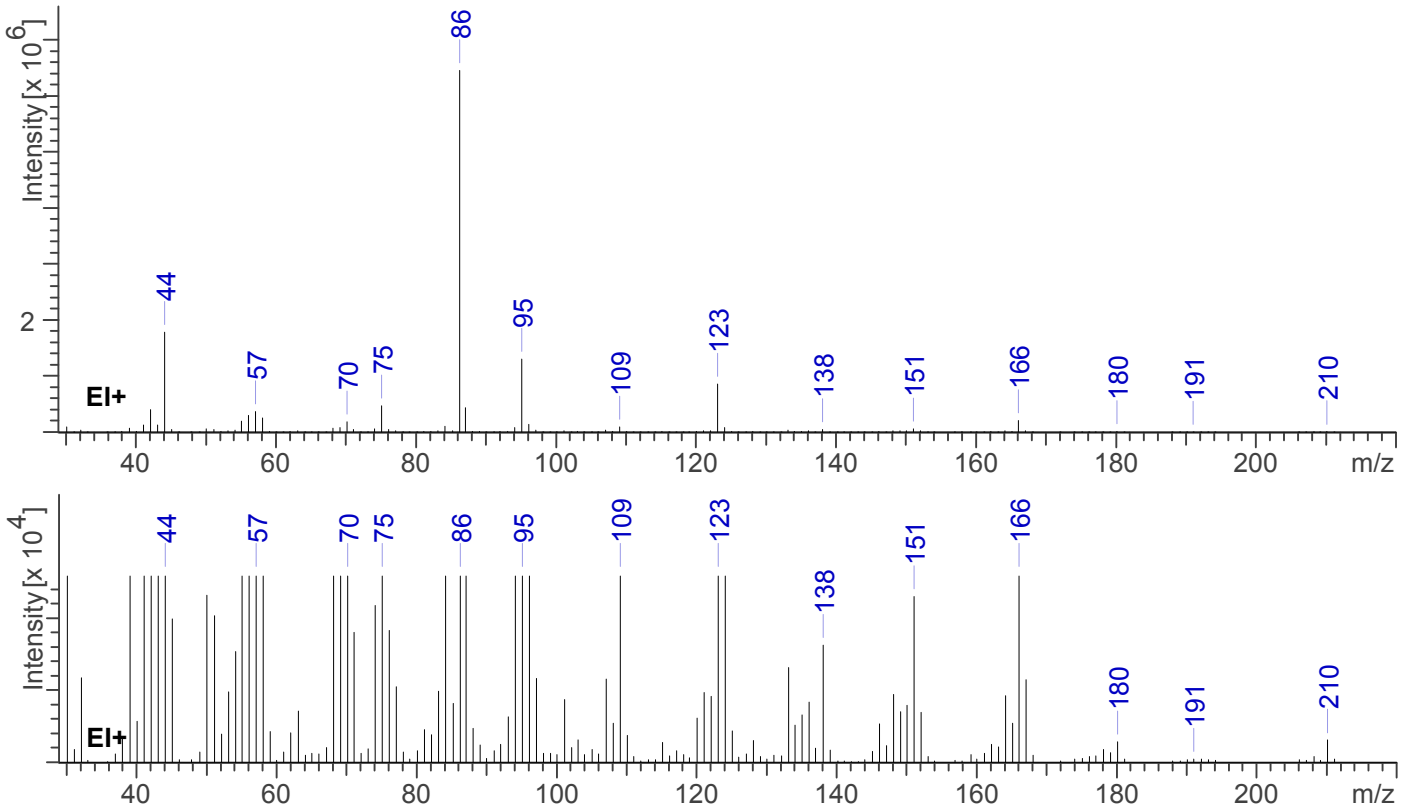


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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 1.5 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 µL injected
MS Parameters:	Mass scan range: 30-550 amu
	Threshold: 100
	Tune file: stune.u
	Acquisition mode: scan
Retention Time:	6.744 min

EI Mass Spectrum: 4-Fluoropentedrone HCl; Lot 0464459-21

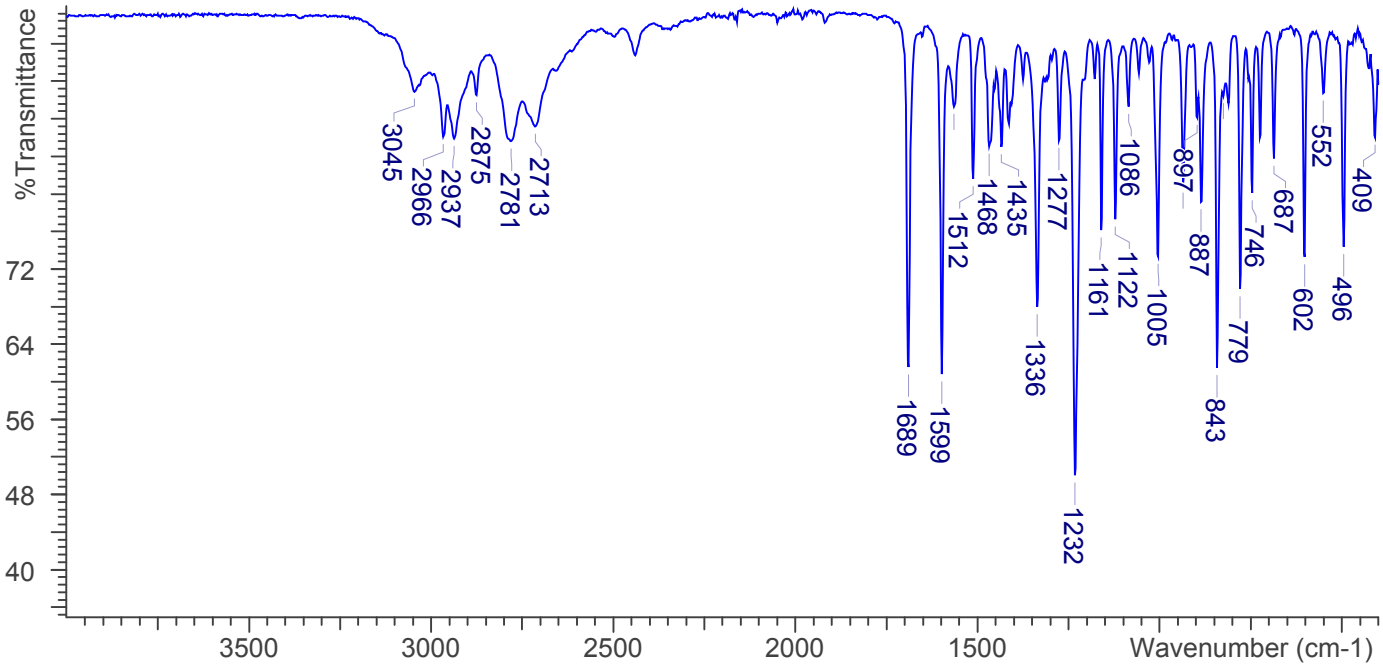


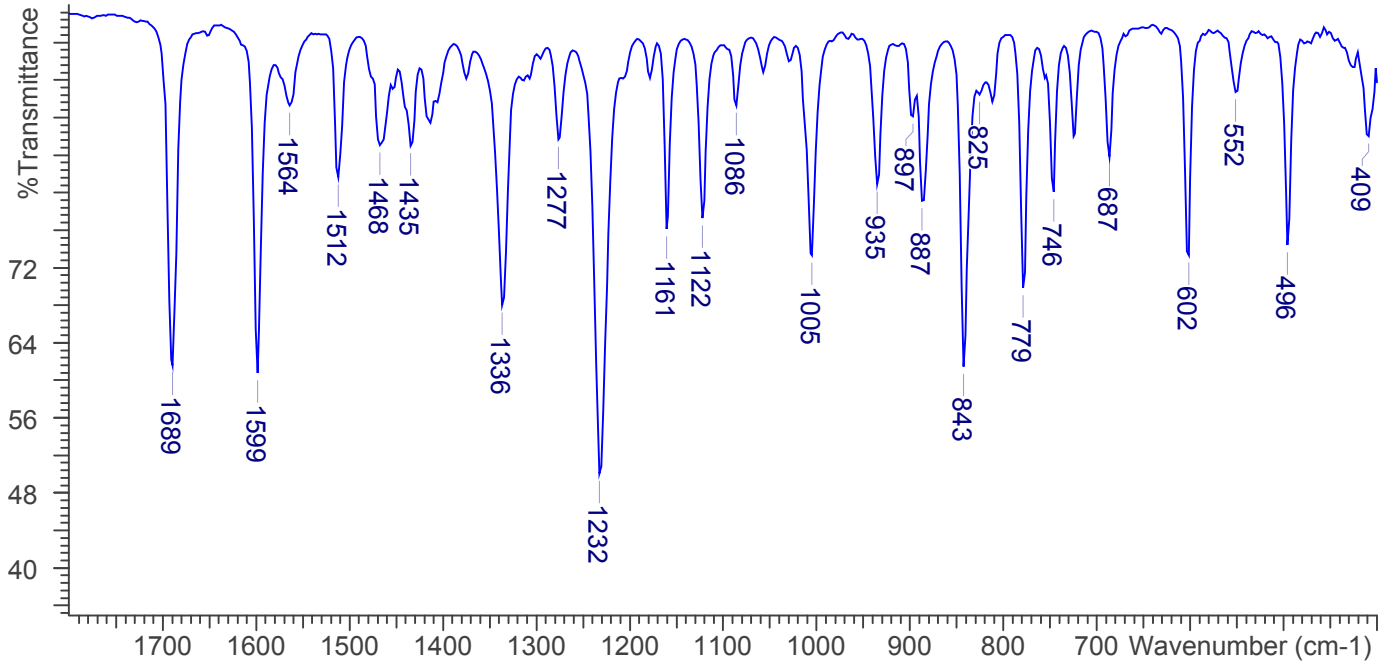
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with Golden Gate 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 (Golden Gate with ATR, 1 Bounce): 4-Fluoropentedrone HCl; Lot 0464459-21





4. ADDITIONAL RESOURCES

No Literature as of 08/2017