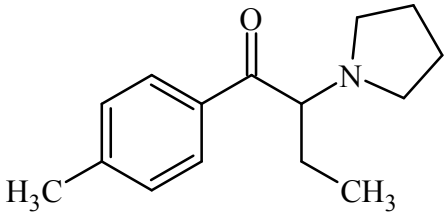
4-Methyl-α-pyrrolidinobutiophenone

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-methylphenyl)-2-(pyrrolidin-1-yl)butan-1-one

CAS#: 1214-15-9 (HCl)

Synonyms: MPBP, 4-MPBP, 4-MePBP, 4-Me-α-PBP, F 1938, 4-Methyl-2-pyrrolidinobutyrophenone

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	$C_{15}H_{21}NO$	231	Not Determined
HCl	$C_{15}H_{21}NO \cdot HCl$	267	178-180

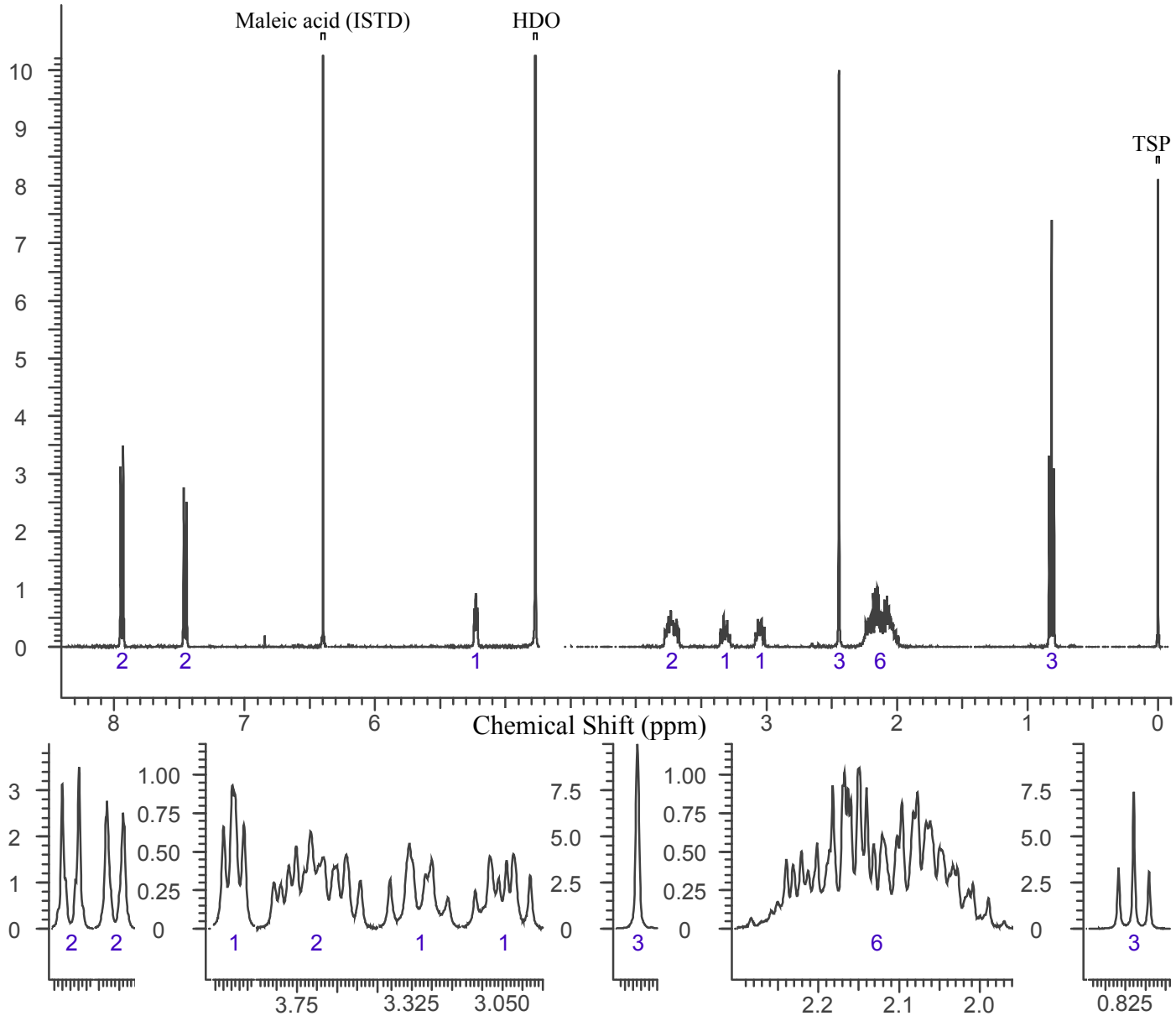
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 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: 4-MPBP HCl; Lot 0435103-10; D_2O; 400 MHz

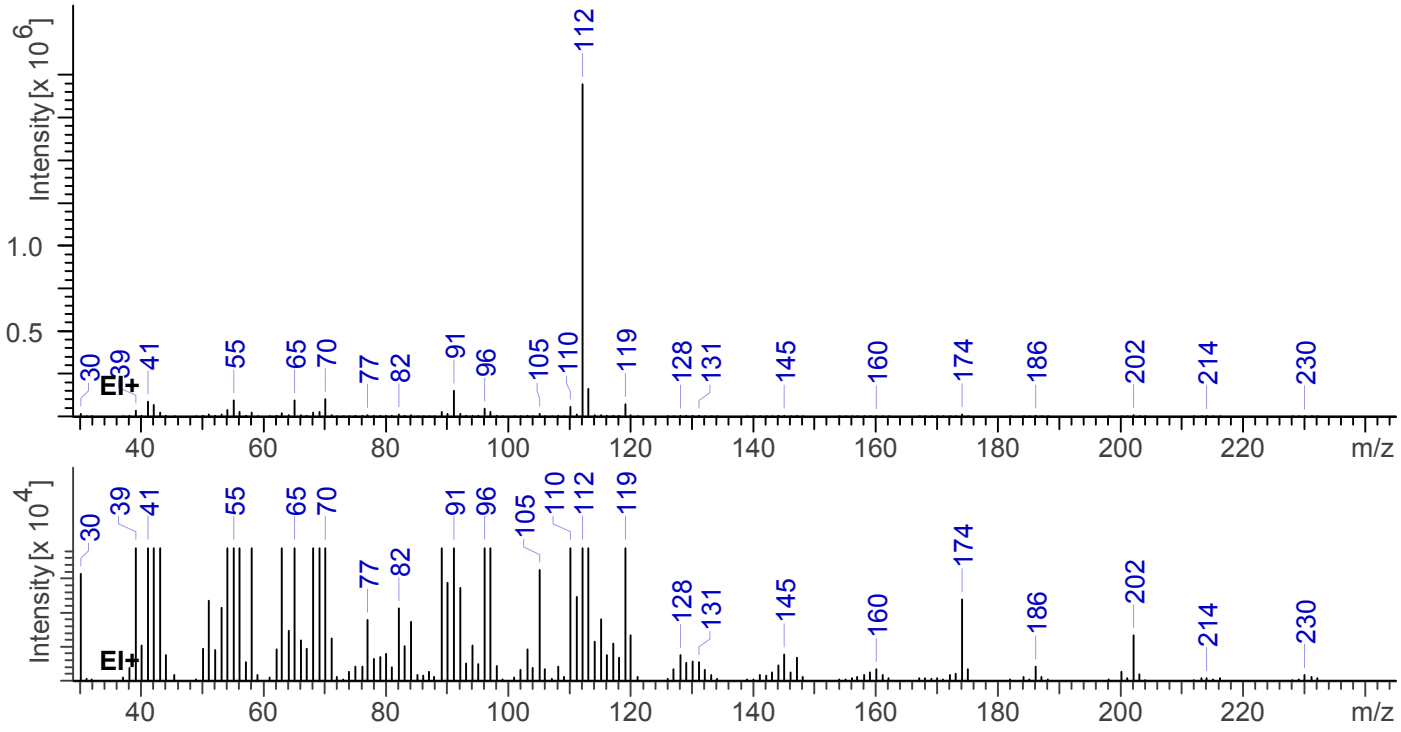


3.2 Gas Chromatography/Mass Spectrometry

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:	10.469 min

EI Mass Spectrum: 4-MPBP HCl; Lot 0435103-10

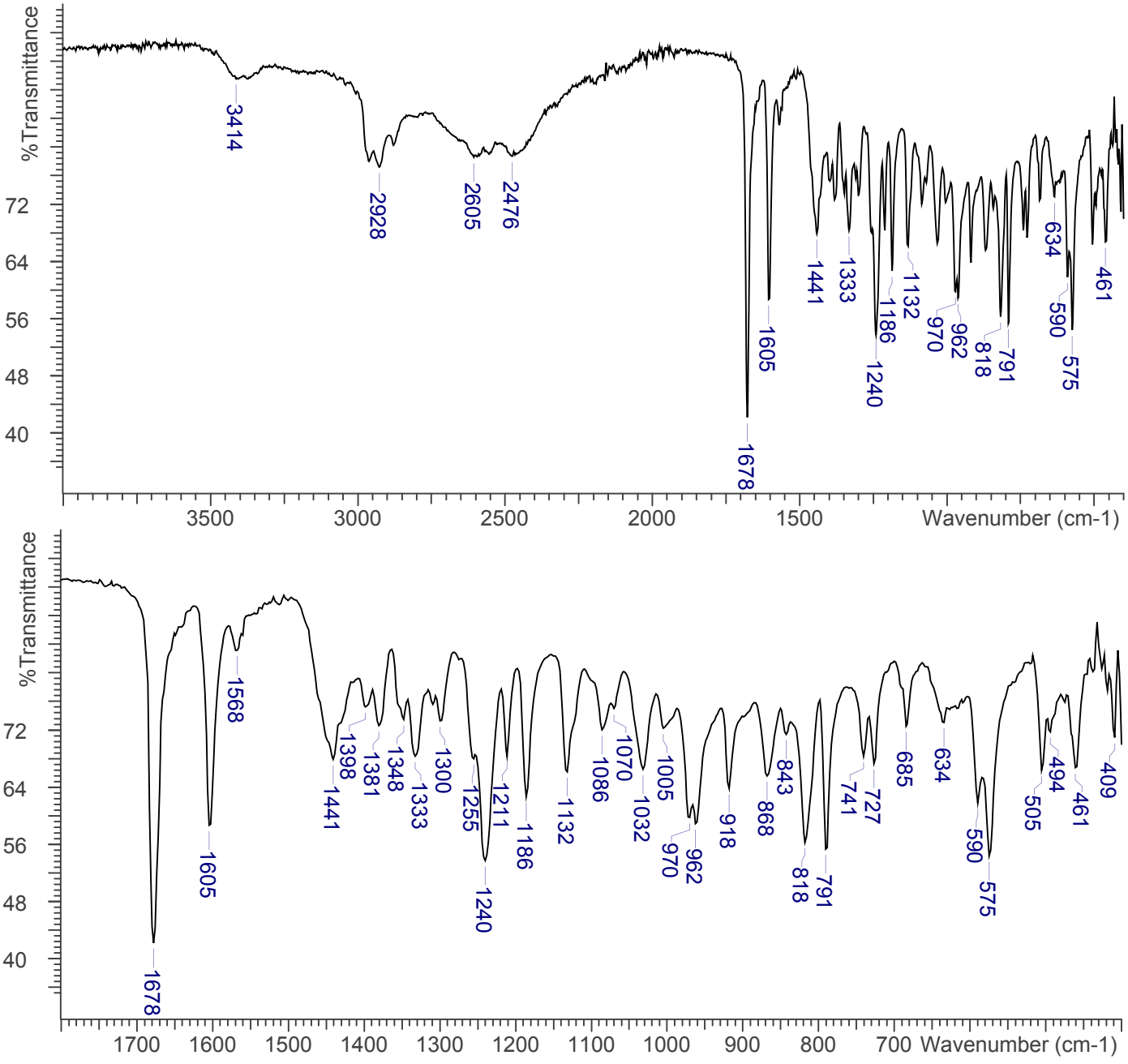


3.3 INFRARED SPECTROSCOPY (FTIR)

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): 4-MPBP HCl; Lot 0435103-10



4. ADDITIONAL RESOURCES

Westphal, F.; Junge, T.; Rösner, P.; Fritschi, G.; Klein, B.; Girreser U. Mass spectral and NMR spectral data of two new designer drugs with an α-aminophenone structure: 4'-Methyl-α-pyrrolidinohexanophenone and 4'-methyl-α-pyrrolidinobutyrophenone. *For. Sci. Int.* **2007**, 169, 32-42.

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Wikipedia