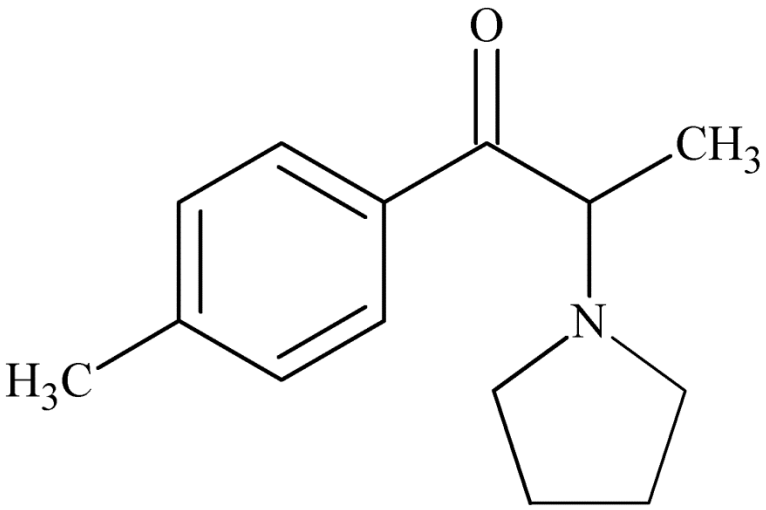


1. GENERAL INFORMATION

IUPAC Name: 1-(4-methylphenyl)-2-(pyrrolidin-1-yl)propan-1-one

CFR: Not Scheduled (4/2013)

CAS #: 1313393-58-6 (HCl)

Synonyms: 4-MePPP, MαPPP, 4-MαPPP
(MPPP is a known synonym, but may also refer to 1-methyl-4-phenyl-propionoxypiperidine)

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat's Index: Pending

UV_{max}: Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{14}H_{19}NO$	217	Not Determined
HCl	$C_{14}H_{19}NO \cdot HCl$	253	224.2

3. ADDITIONAL RESOURCES

Forendex

Wikipedia

4. QUALITATIVE DATA

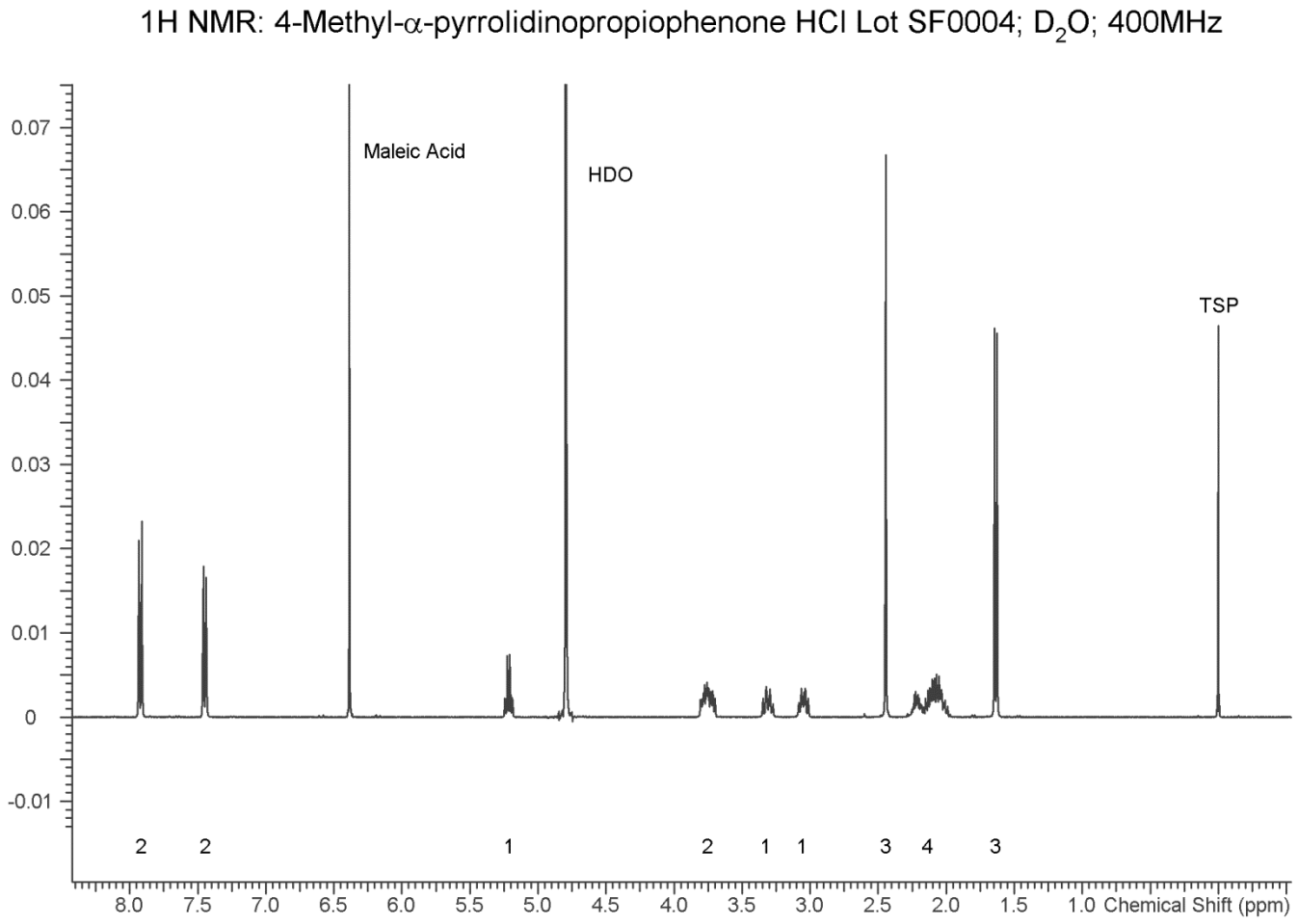
4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D_2O

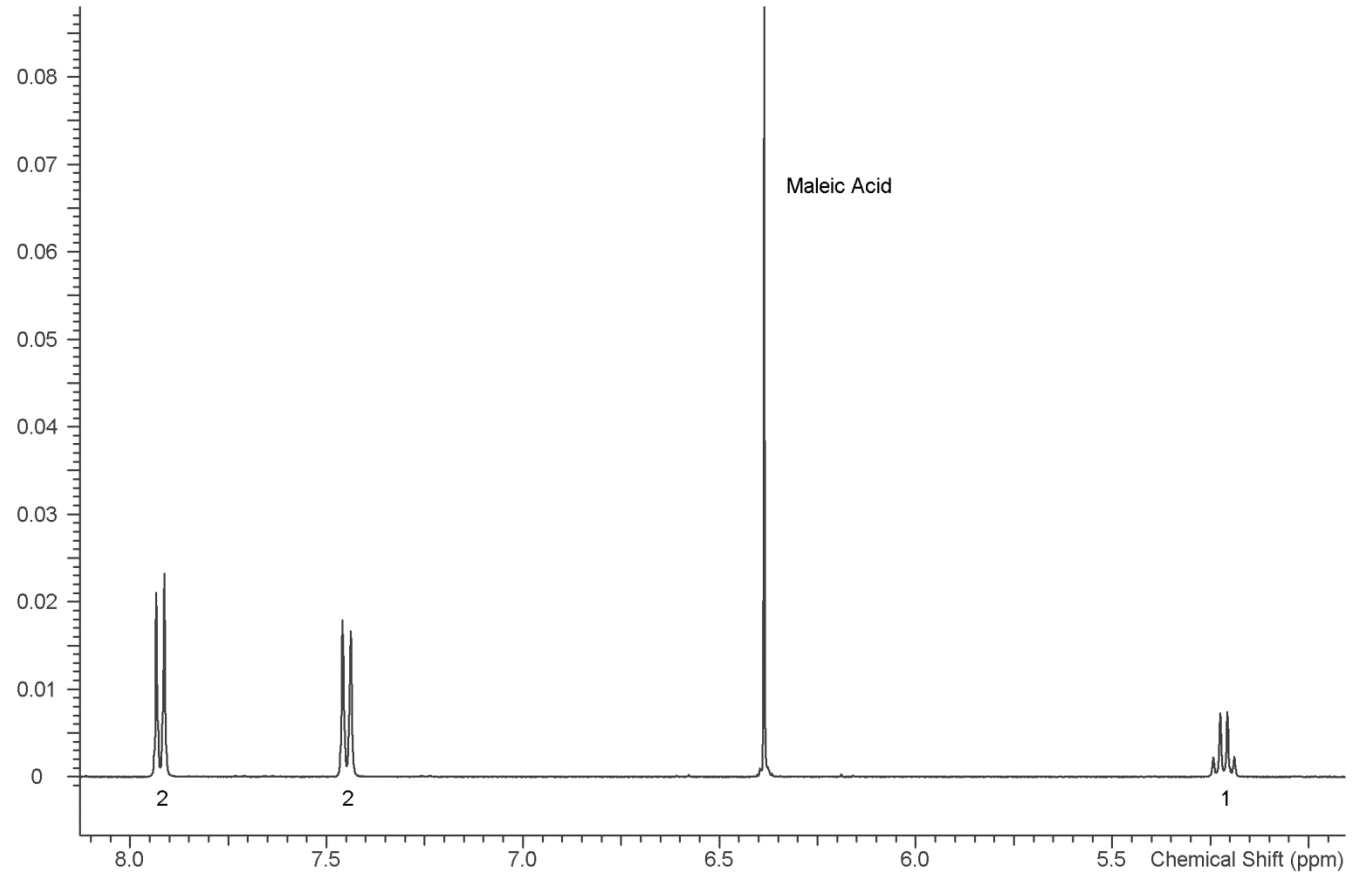
Sample Preparation: Dilute analyte to ~10 mg/mL in D2O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer

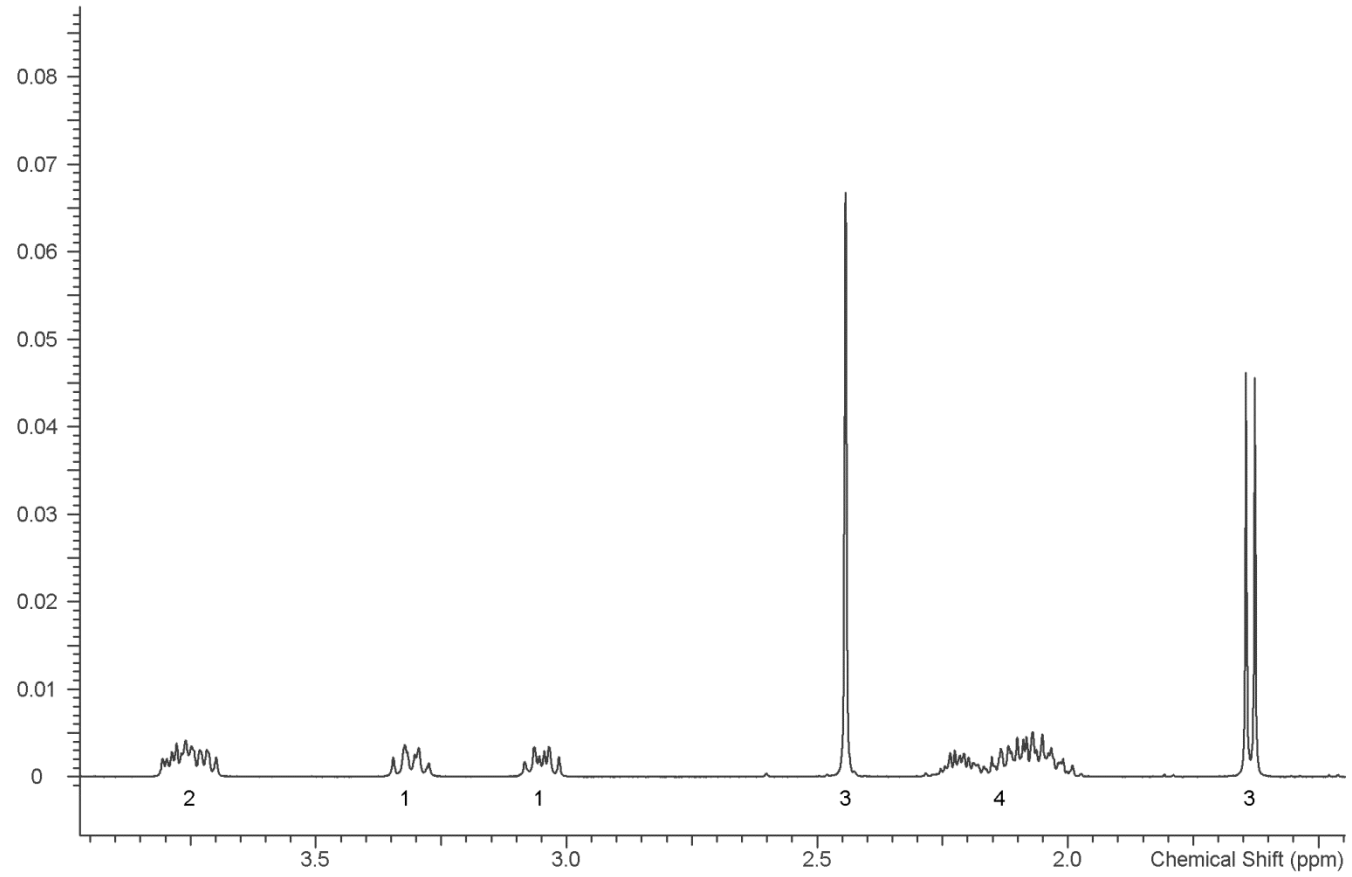
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds



1H NMR: 4-Methyl-α-pyrrolidinopropiophenone HCl Lot SF0004; D_2O; 400MHz



1H NMR: 4-Methyl-α-pyrrolidinopropiophenone HCl Lot SF0004; D_2O; 400MHz

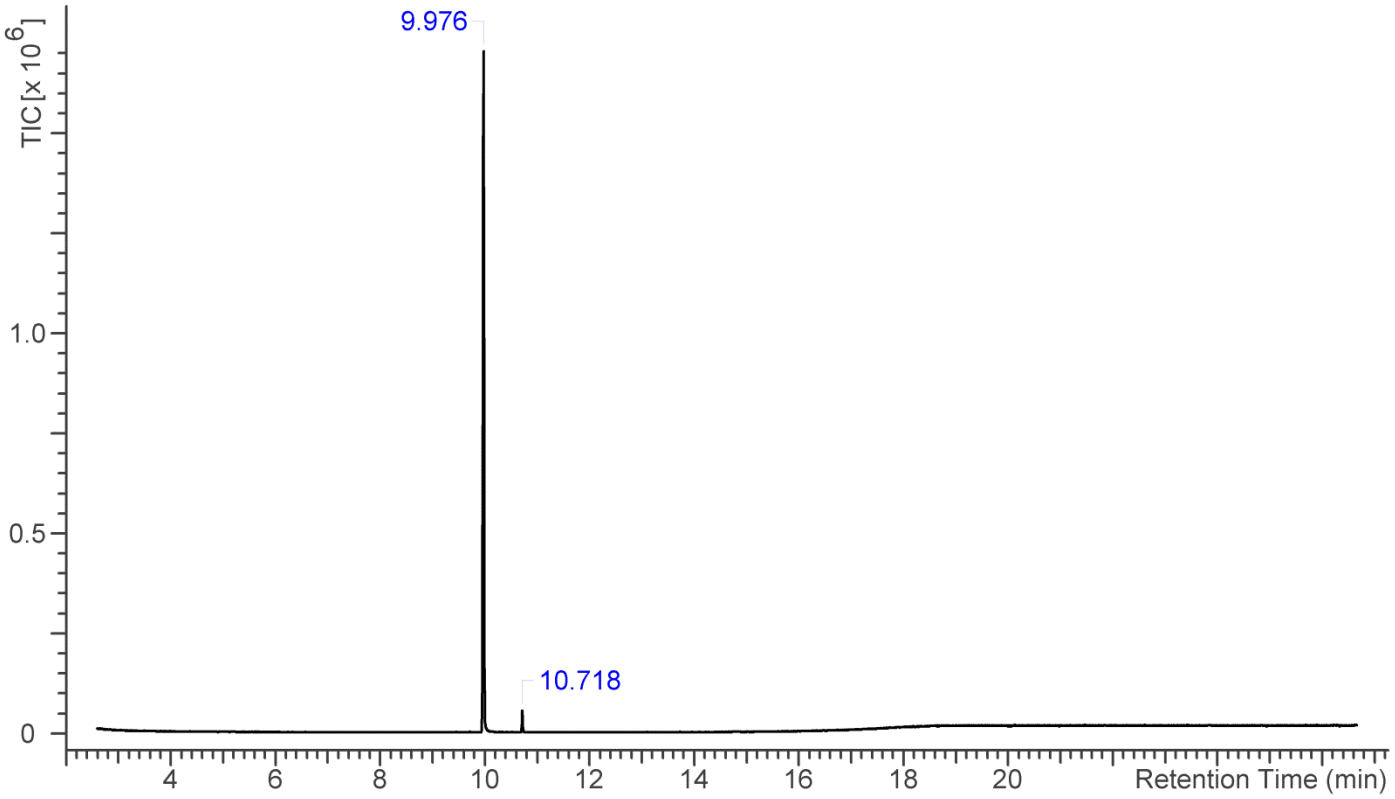


4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

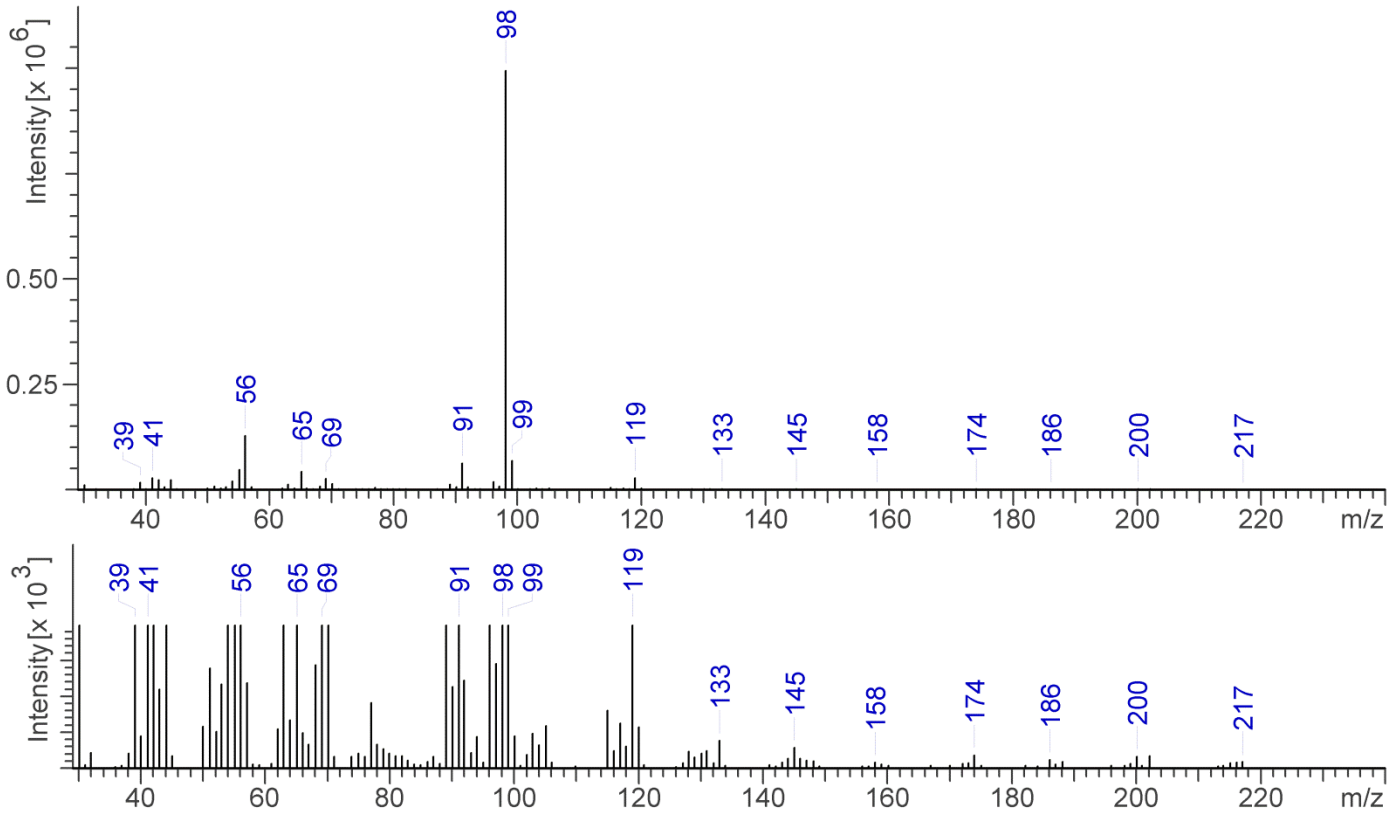
Sample Preparation: Dilute analyte to ~1 mg/mL in $CHCl_3$.

Instrument:	Agilent gas chromatograph operated in split mode with MS detector
Column:	DB-1 MS or equivalent; 30m x .25mm x .25µm
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:	9.976 minutes (4-MαPPP), 10.718 minutes (enamine by-product)

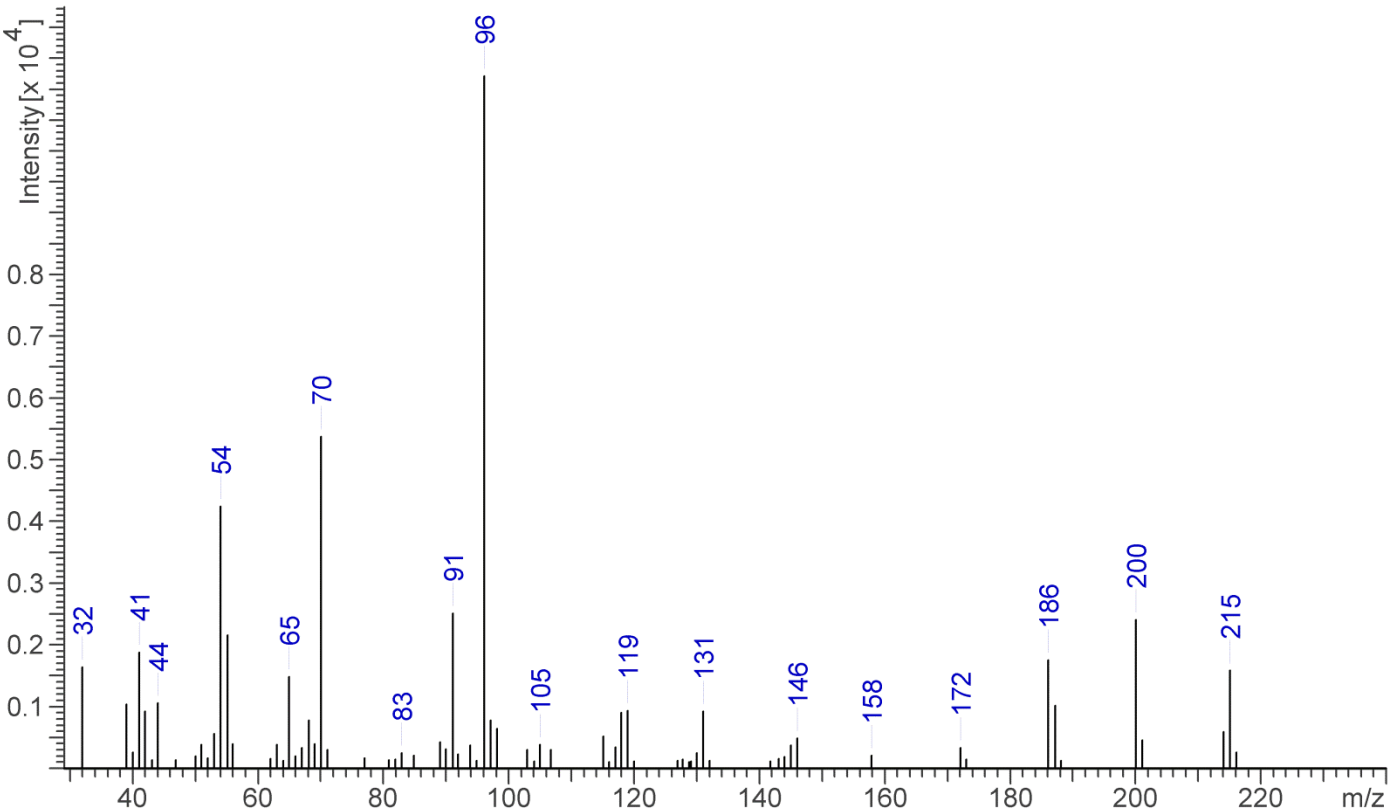
TIC: 4-Methyl-α-pyrrolidinopropiophenone HCl; lot SF0004



EI Mass Spectrum: 4-Methyl-α-pyrrolidinopropiophenone HCl; lot SF0004



EI Mass Spectrum: By-product of 4-Methyl-α-pyrrolidinopropiophenone HCl; lot SF0004

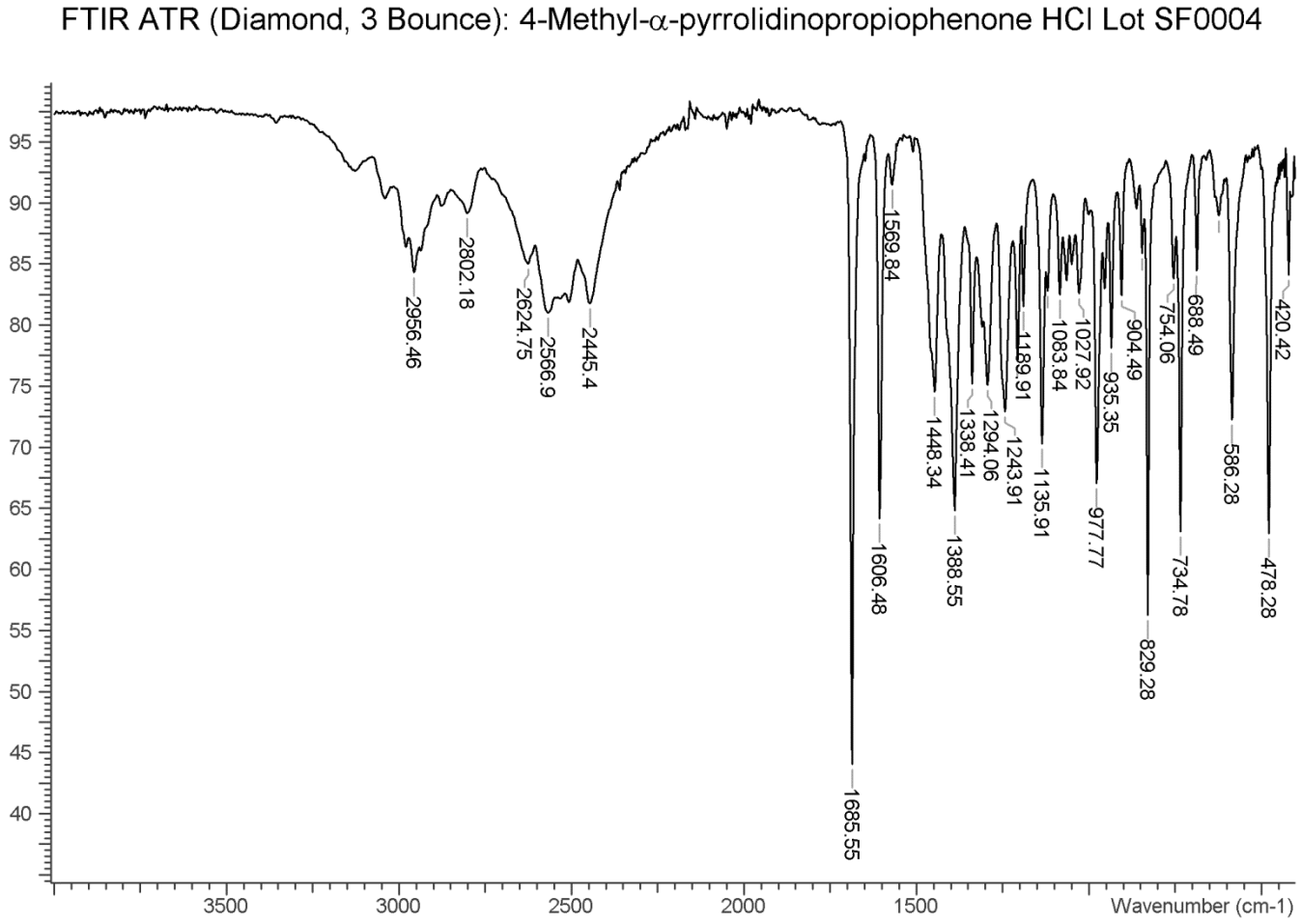


GC/MS Analytical Observation:
Cathinones can lose two hydrogens to produce an enamine that undergoes α-cleavage to yield a mass spectrum with a base peak of 96 m/z (see the mass spectrum at 10.718 minutes).[1] The enamine compound can also be due to a reaction by-product.

[1]Noggle FT, DeRuiter J, Valaer A, Clark CR. GC-MS analysis of methcathinone and its major decomposition product. *Microgram*. 1994; 27(4): 106-118.

4.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (3 bounce)
Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4cm^{-1}
Sample gain: 8
Aperture: 150



FTIR ATR (Diamond, 3 Bounce): 4-Methyl-α-pyrrolidinopropiophenone HCl Lot SF0004