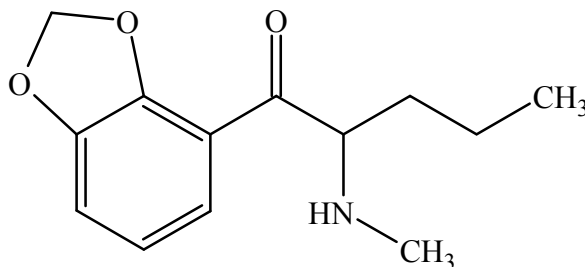




2,3-Pentylone

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



1. GENERAL INFORMATION

IUPAC Name: 1-(1,3-benzodioxol-4-yl)-2-(methylamino)pentan-1-one

CAS#: Not available

Synonyms: Pentylone isomer

Source: DEA Reference Material Collection

Appearance: Grey 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 ₁₃ H ₁₇ NO ₃ · HCl	235	Not Determined
HCl	C ₁₃ H ₁₇ NO ₃	271	198.7



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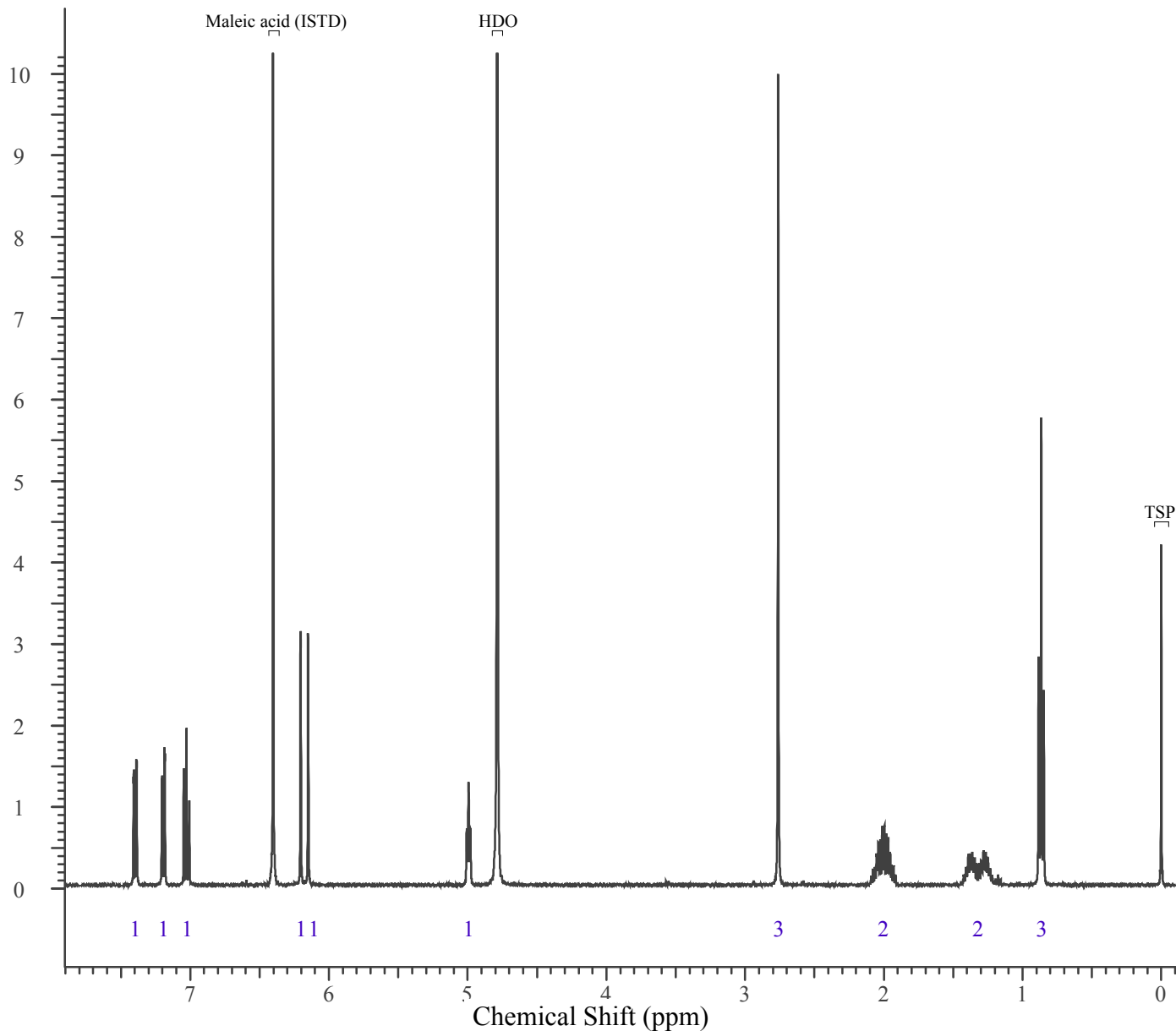


3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterium oxide (D₂O) containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

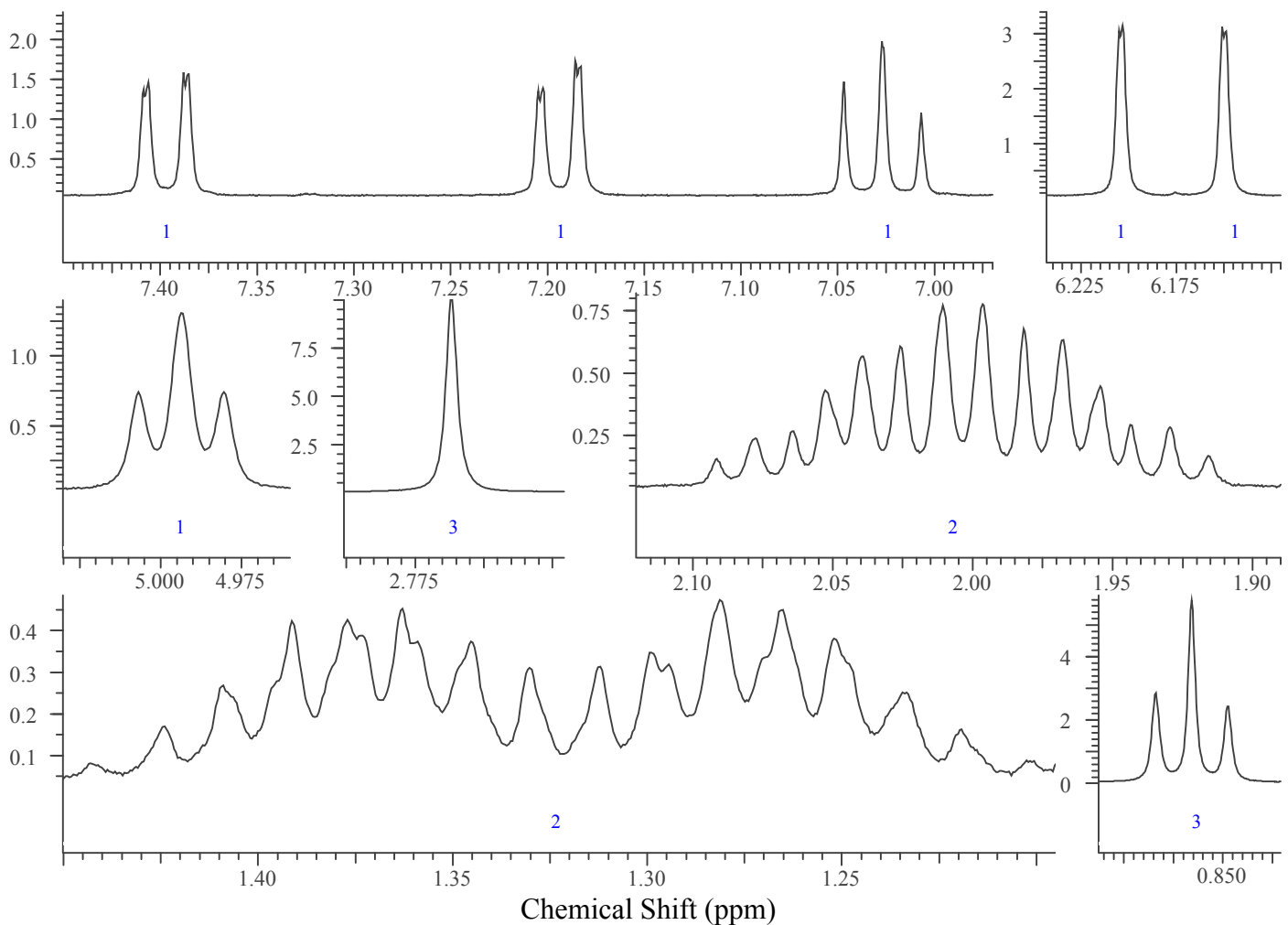
Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds
¹H NMR: 2,3-Pentylone HCl; Lot 0435925-9; D₂O; 400 MHz





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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 μ m
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



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Injection Parameters:

Split Ratio = 20:1, 1 μ L injected

MS Parameters:

Mass scan range: 34-550 amu

Threshold: 100

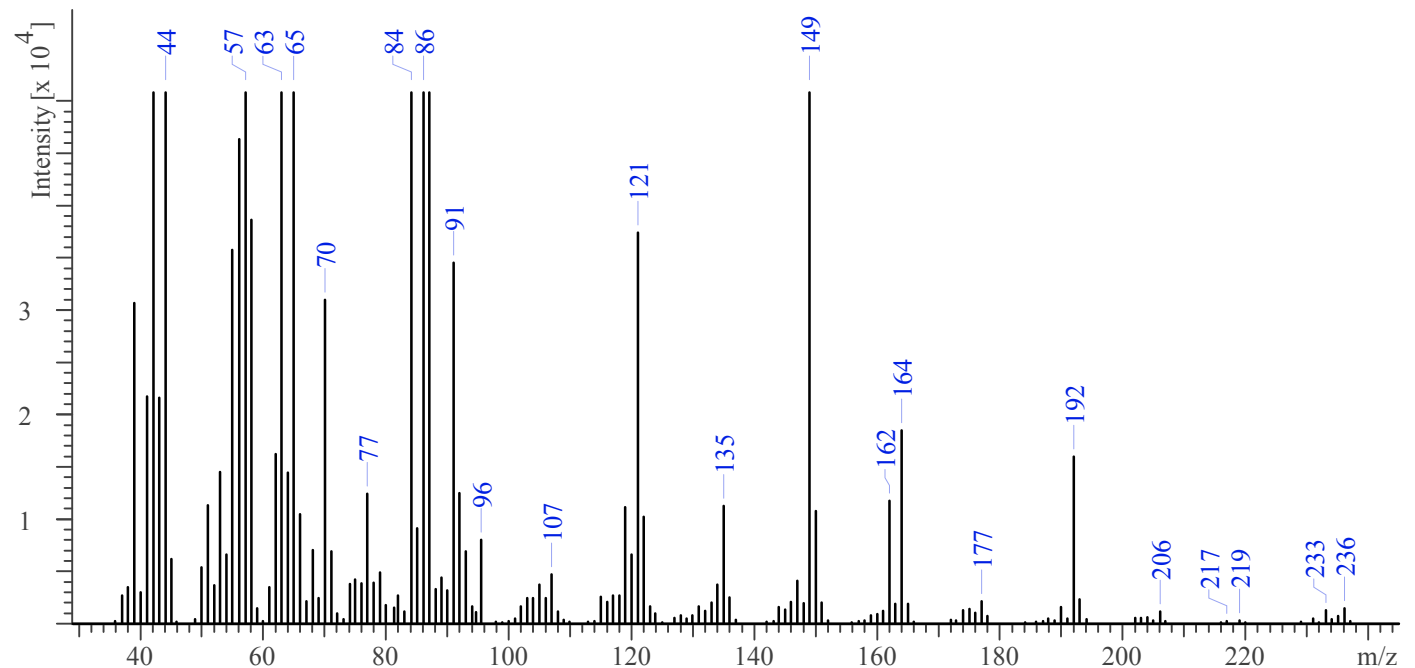
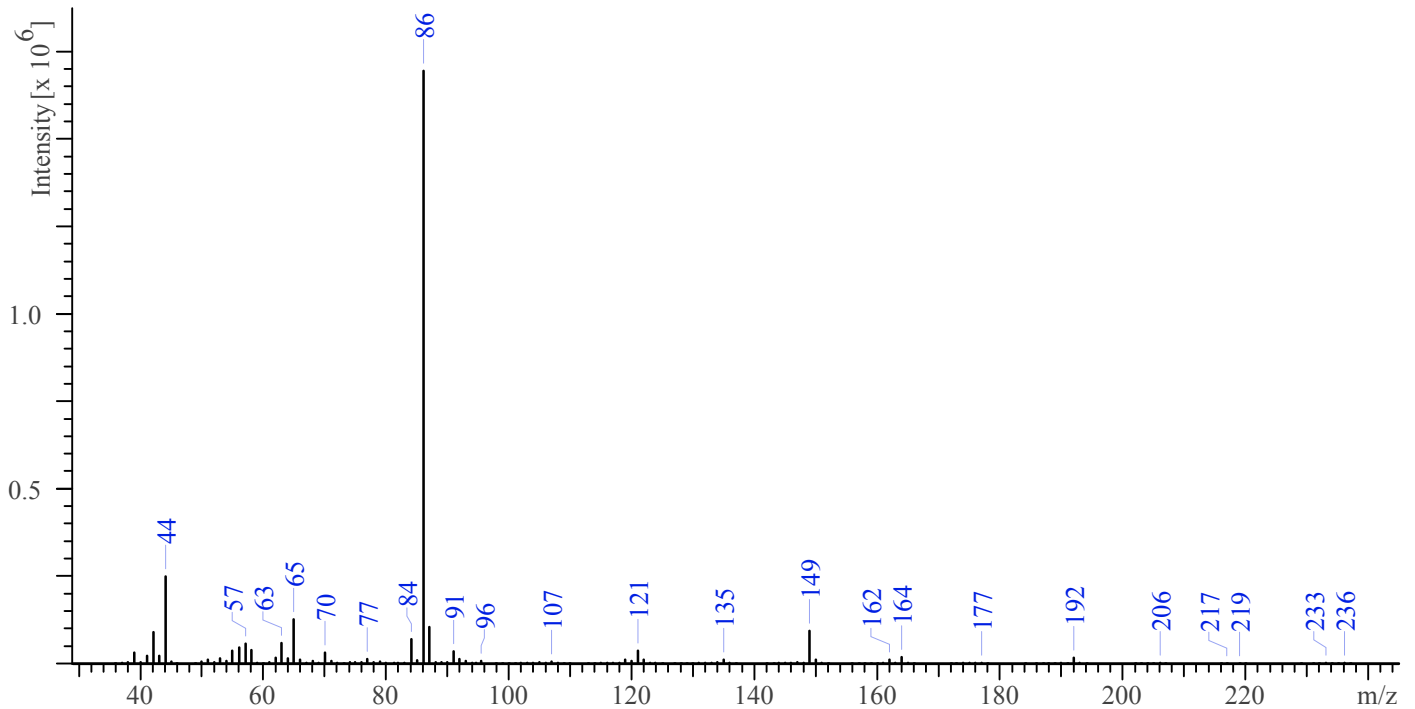
Tune file: stune.u

Acquisition mode: scan

Retention Time:

10.548 min

EI Mass Spectrum: 2,3-Pentylone HCl; Lot 0435925-9





2,3-Pentylone

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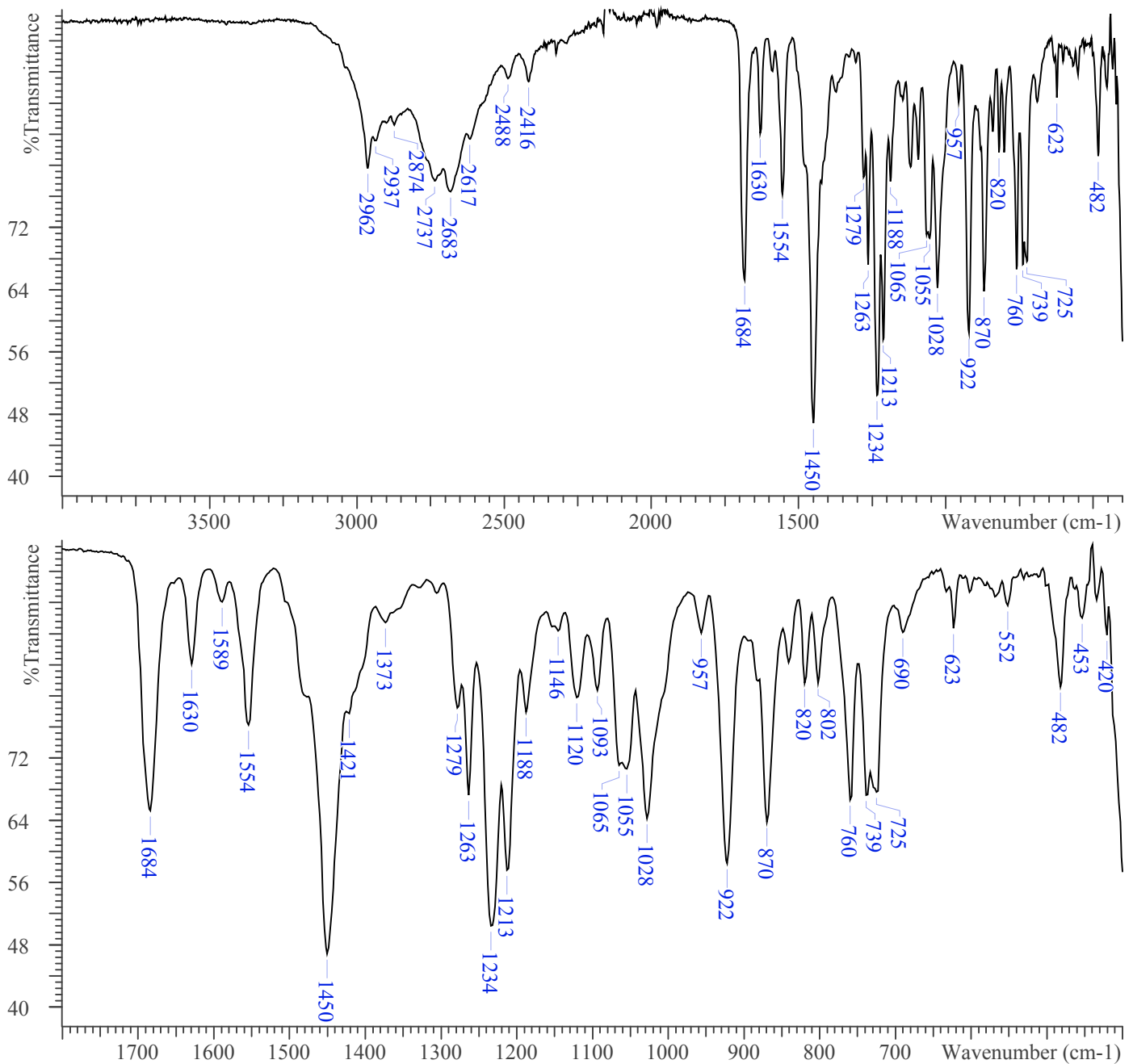


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: 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): 2,3-Pentylone HCl; Lot 0435925-9





2,3-Pentylone

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4. **ADDITIONAL RESOURCES**

No resources identified.