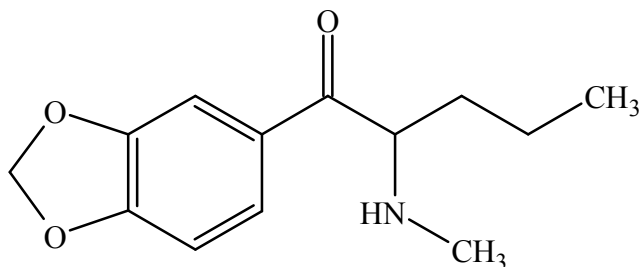




Pentylone

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-5-yl)-2-(methylamino)pentan-1-one
CAS#:	698963-77-8 (base), 17763-01-8 (HCl)
Synonyms:	β -keto-methylbenzodioxolypentanamine, bk-methyl-K, bk-MBDP
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 ₁₃ H ₁₇ NO ₃	235	Not Determined
HCl	C ₁₃ H ₁₇ NO ₃ · HCl	271	242.0



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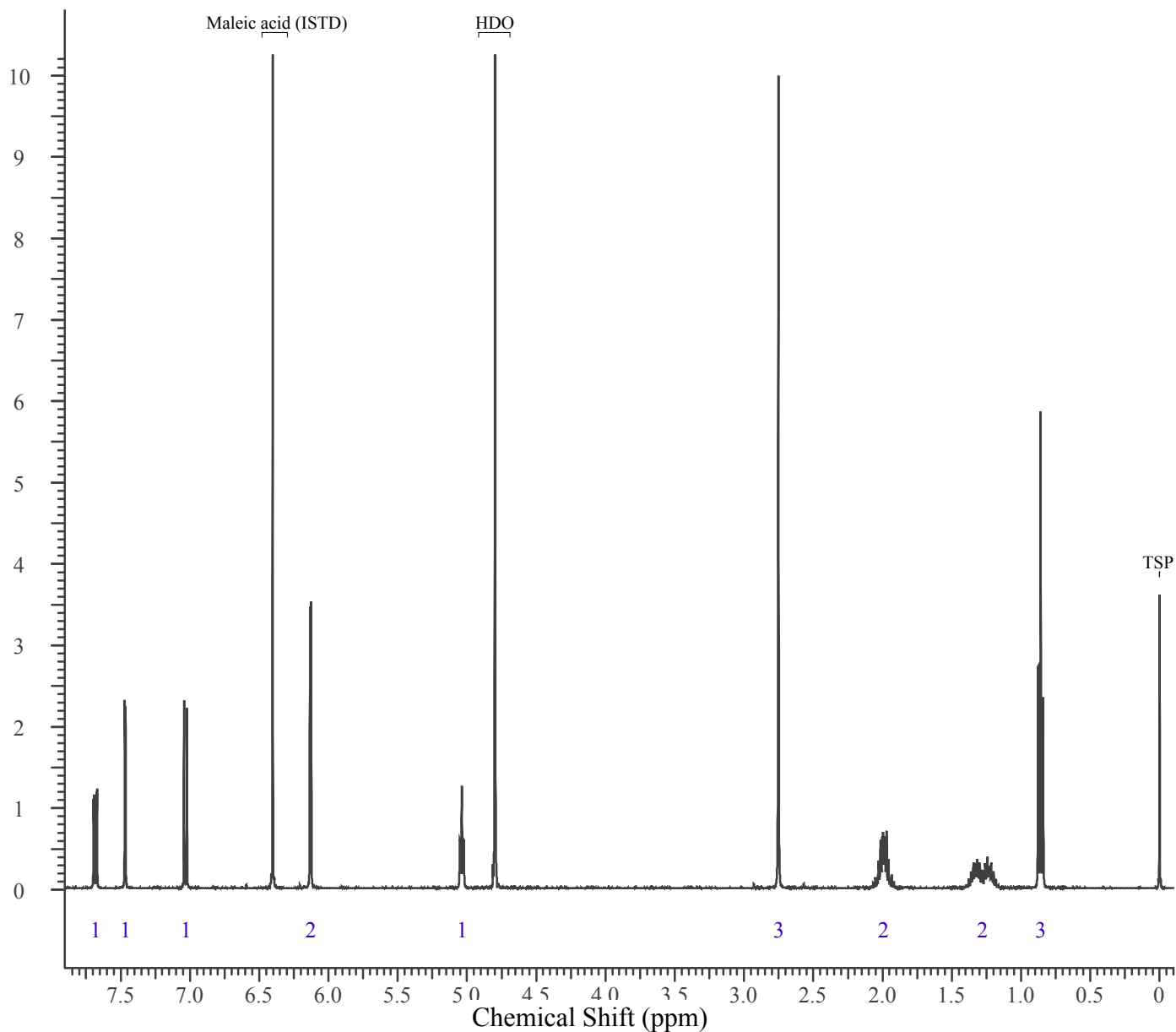
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

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

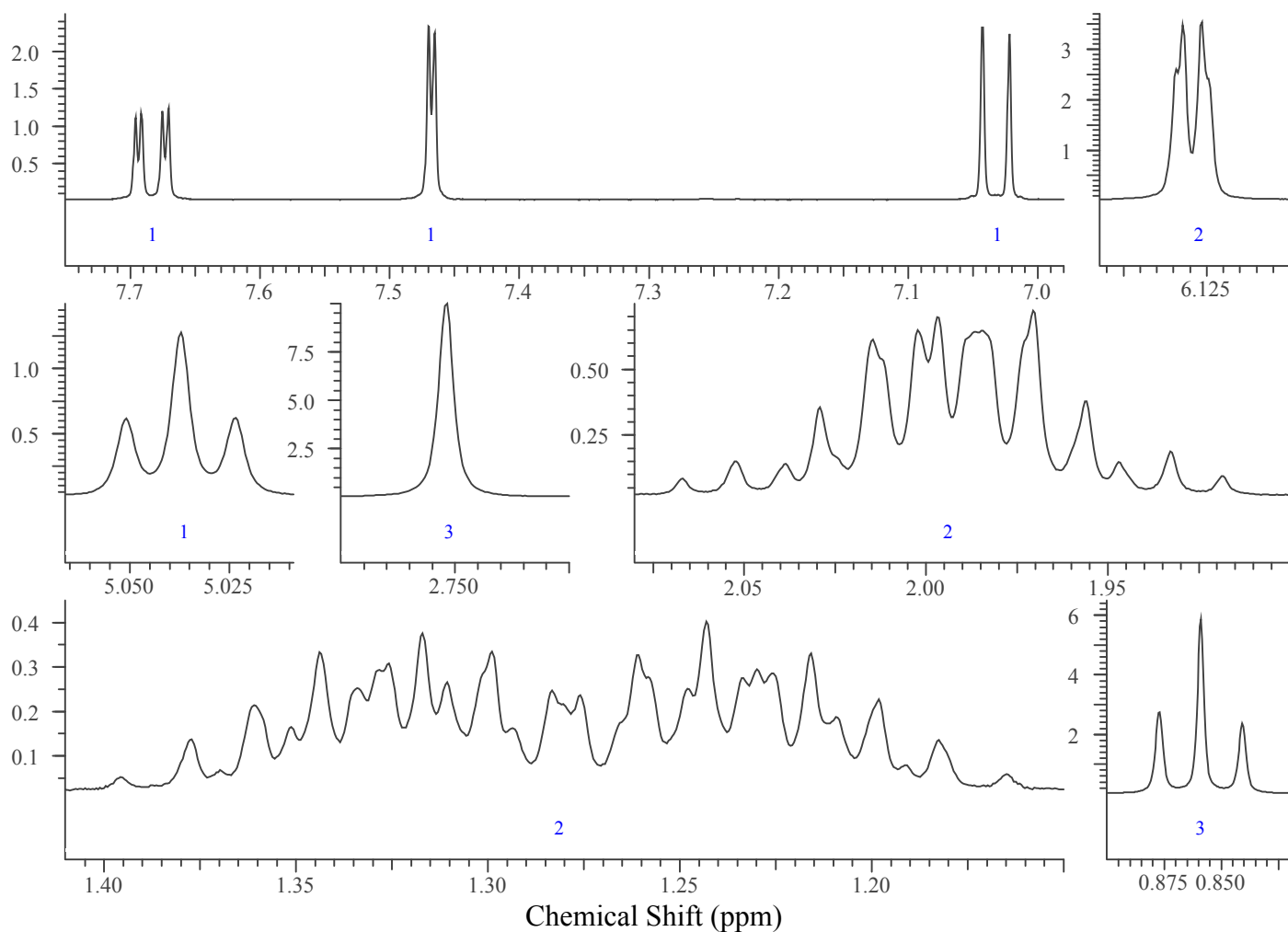
Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

¹H NMR: Pentylone HCl; Lot ALB089RC; D₂O; 400MHz



Pentylone

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3.2 Gas Chromatography/Mass Spectrometry

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

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

Pentylone

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Injection Parameters:

Split Ratio = 20:1, 1 μ L injected

MS Parameters:

Mass scan range: 34-550 amu

Threshold: 100

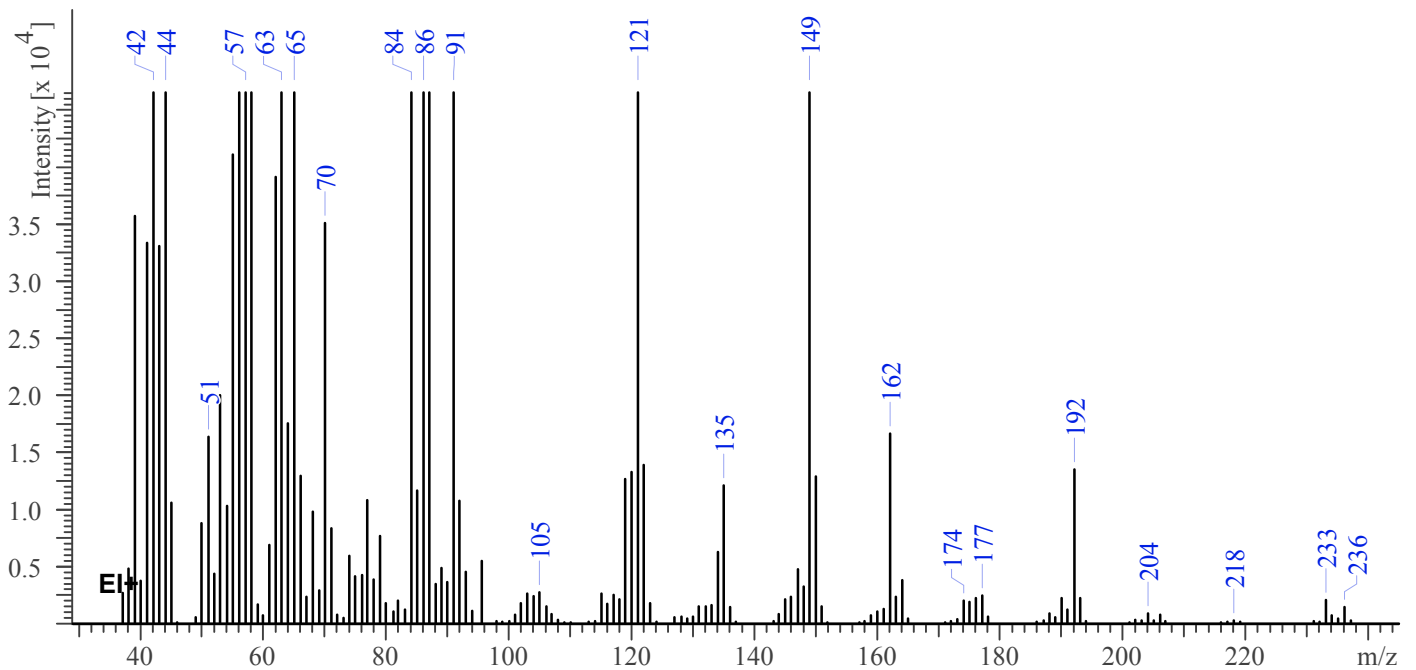
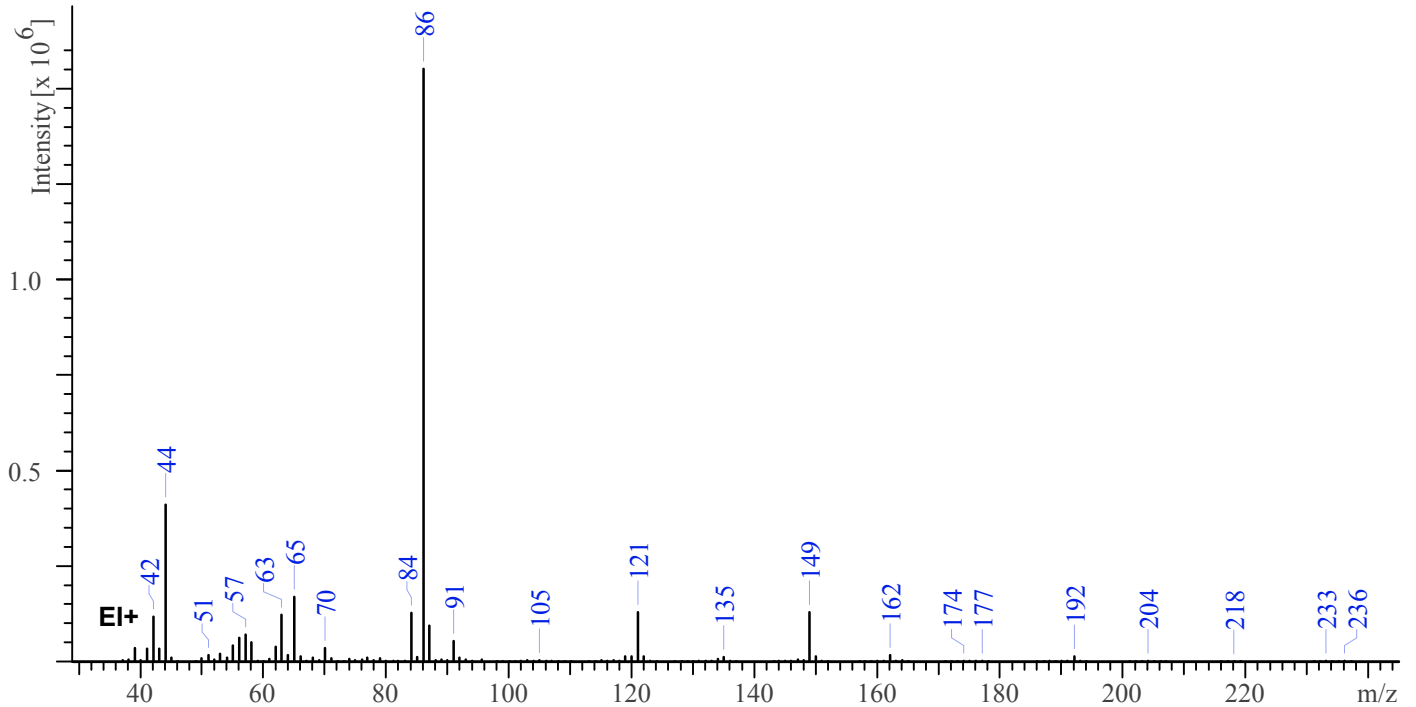
Tune file: stune.u

Acquisition mode: scan

Retention Time:

11.219 min

EI Mass Spectrum: Pentylone HCl; Lot ALB089RC





Pentylone

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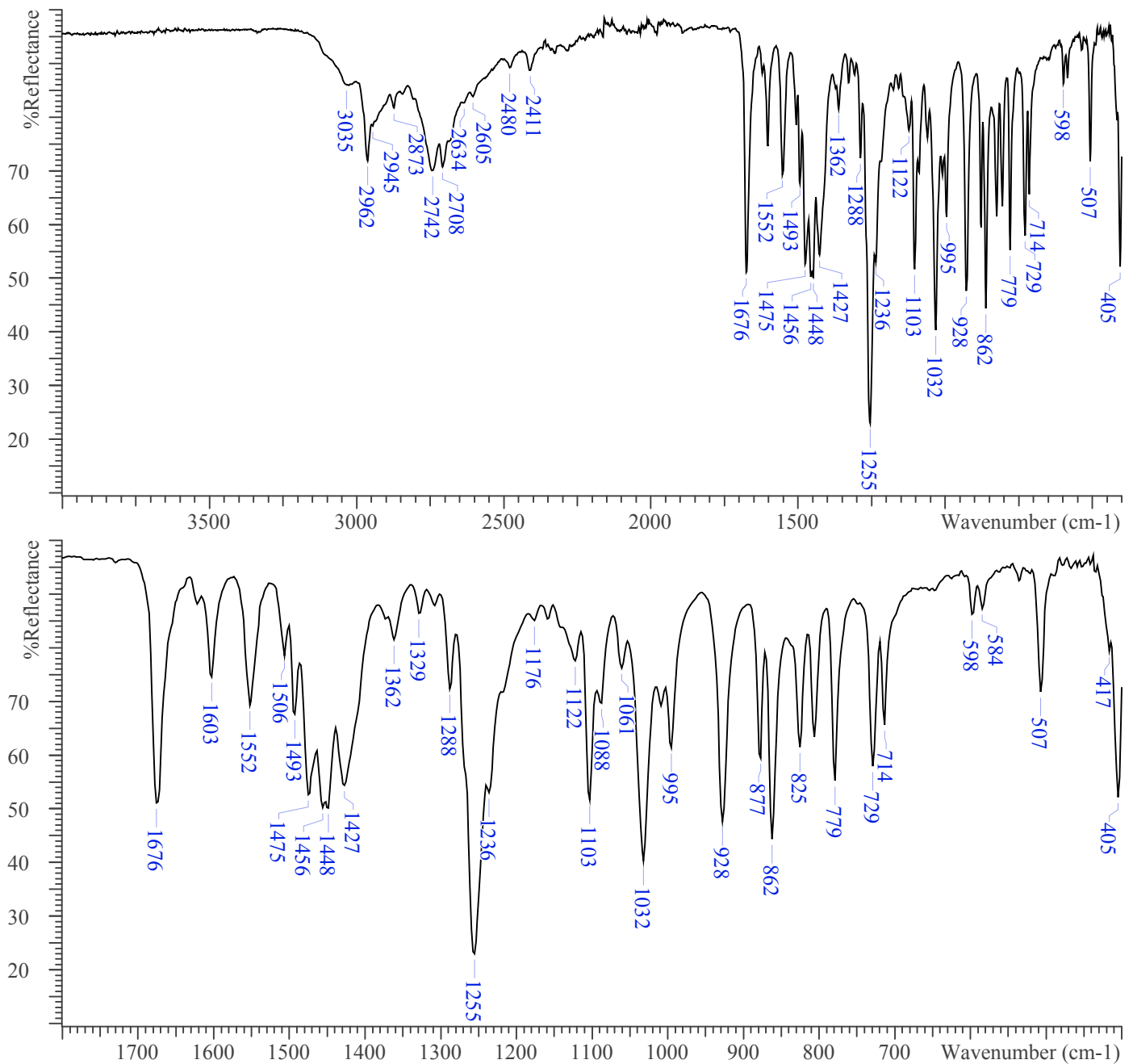


3.3 INFRARED SPECTROSCOPY (FTIR)

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): Pentylone HCl; Lot ALB089RC



Pentylone

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4. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)