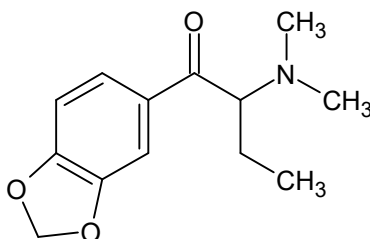




bk-DMBDB

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



1. GENERAL INFORMATION

IUPAC Name:	1-(2 <i>H</i> -1,3-benzodioxol-5-yl)-2-(dimethylamino)butan-1-one
CAS#:	802286-83-5 (base), 17763-12-1 (HCl)
Synonyms:	diButylone, Methylbutylone, B-ketone-N,N-dimethyl-1-(1,3-benzodioxol-5-yl)-2-butanamine
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	272	208.8



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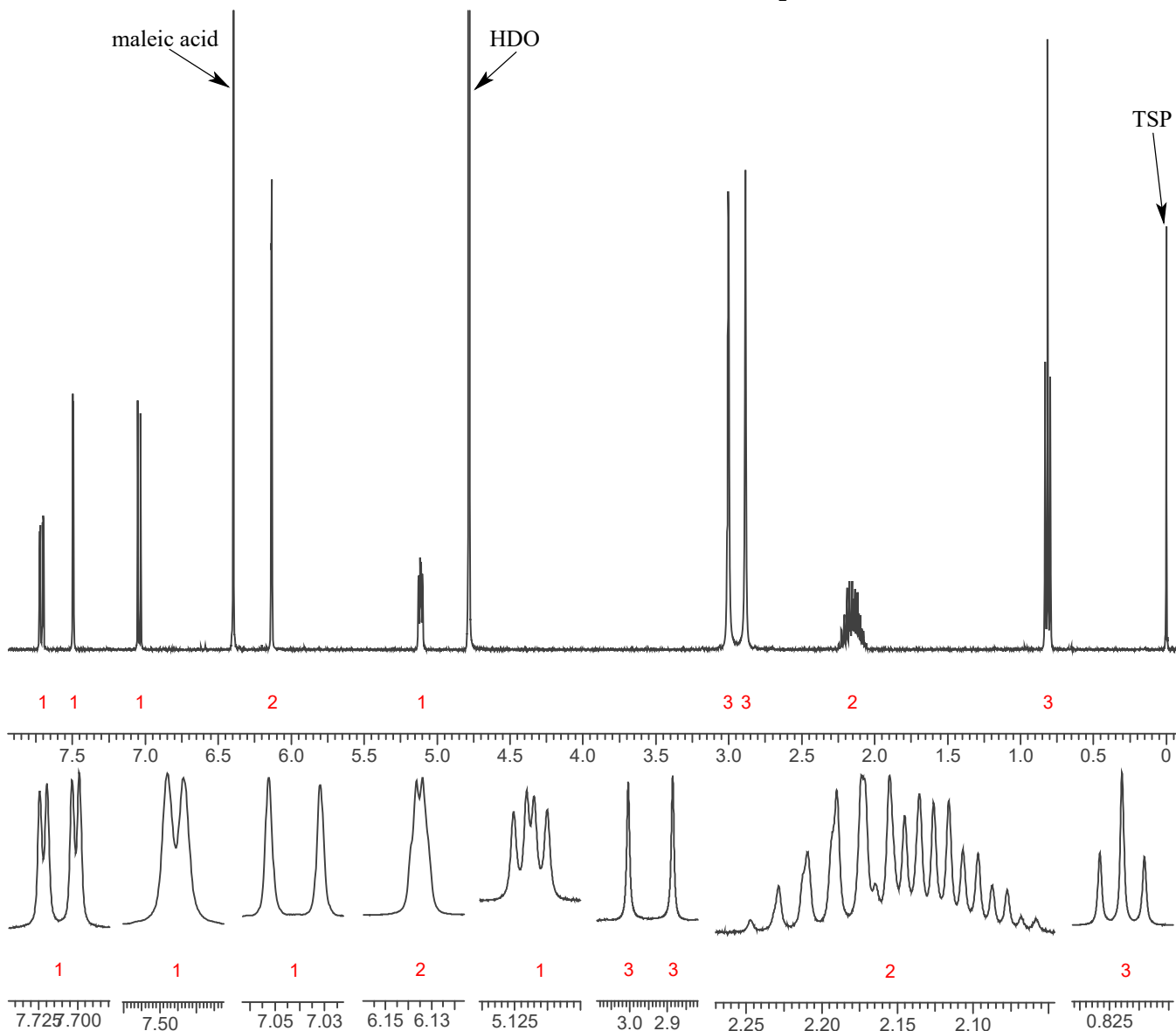
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~6 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

¹HNMR: bk-DMBDB HCl; Lot# 0432924-23; D₂O; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃ (1M NaOH extract)

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 1.0 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

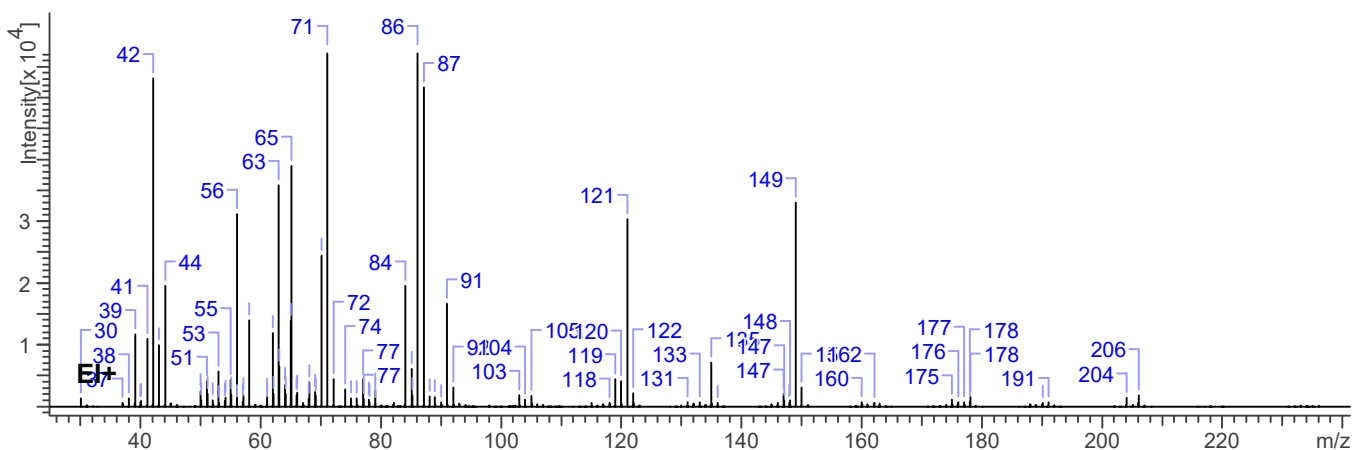
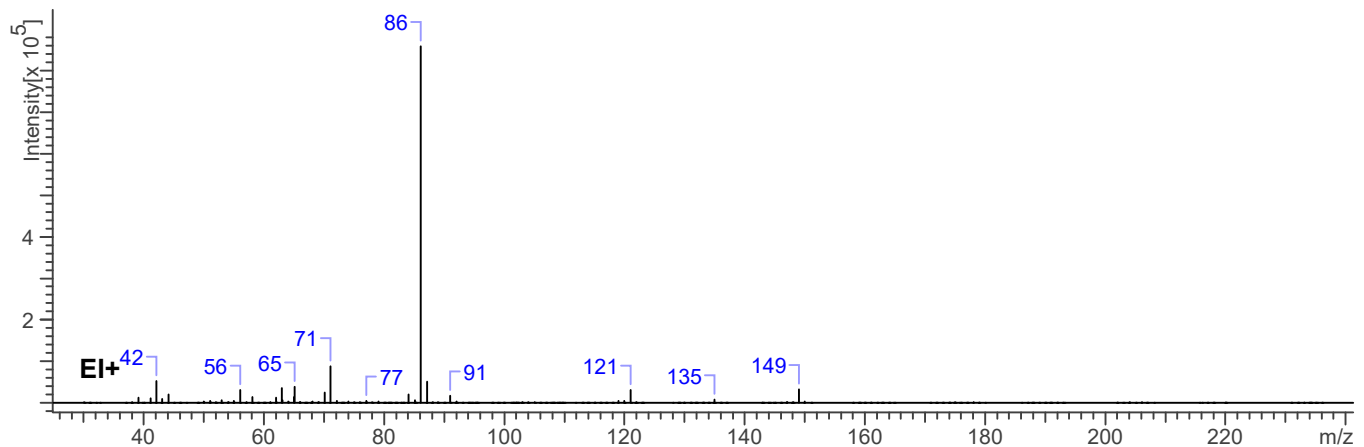
3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 20:1, 1 μL injected

MS Parameters: Mass scan range: 30-550 amu Threshold: 150
Tune file: stune.u Acquisition mode: scan

Retention Time: 9.373 min

EI Mass Spectrum: bk-DMBDB HCl; Lot# 0432924-23





bk-DMBDB

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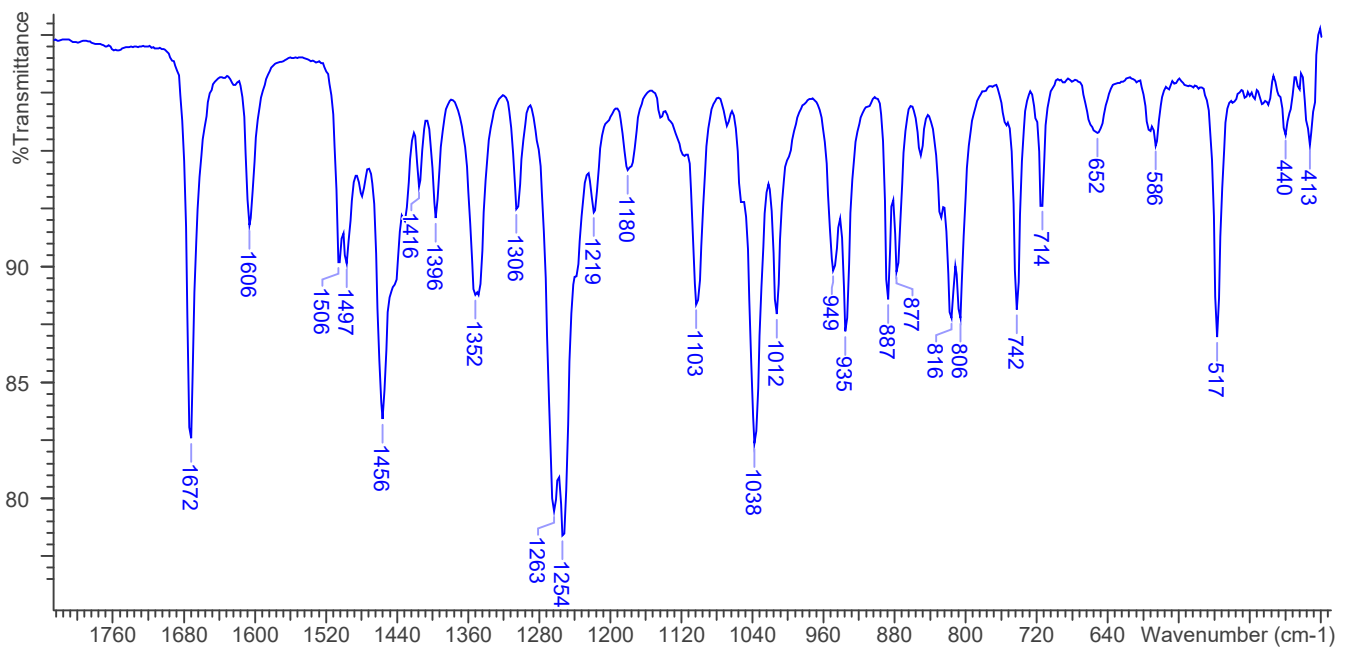
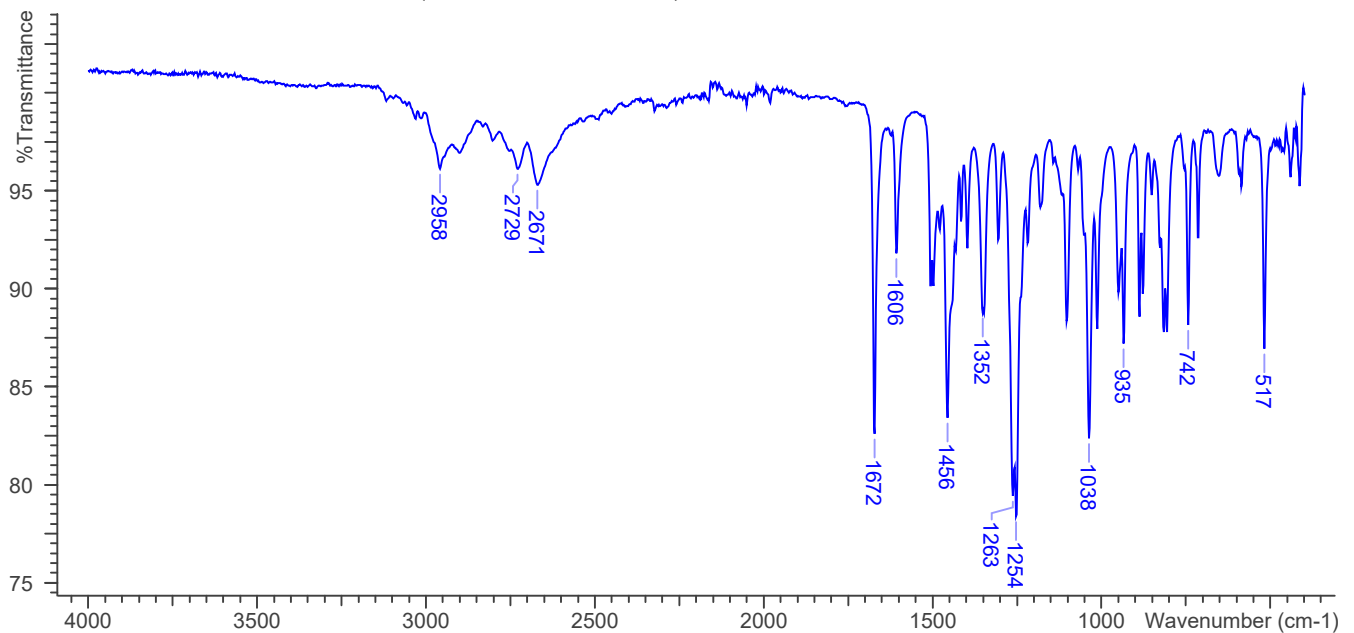


3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)

Scan Parameters:
Number of scans: 32
Number of background scans: 32
Resolution: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond 1 Bounce): bk-DMBDB HCl; Lot# 0432924-23





bk-DMBDB

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4. ADDITIONAL RESOURCES

[Wikipedia](#)

[Forendex](#)