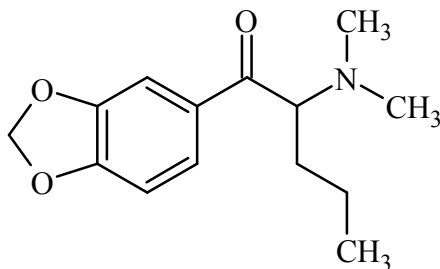




N,N-Dimethylpentylone

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)pentan-1-one
CAS#:	17763-13-2(HCl)
Synonyms:	Dipentylone, bk-DMBDP, 1-(1,3-benzodioxol-5-yl)-2-(dimethylamino)-1-pentanone
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 ₁₄ H ₁₉ NO ₃	249.30	Not Determined
HCl	C ₁₄ H ₁₉ NO ₃ HCl	285.76	224.27



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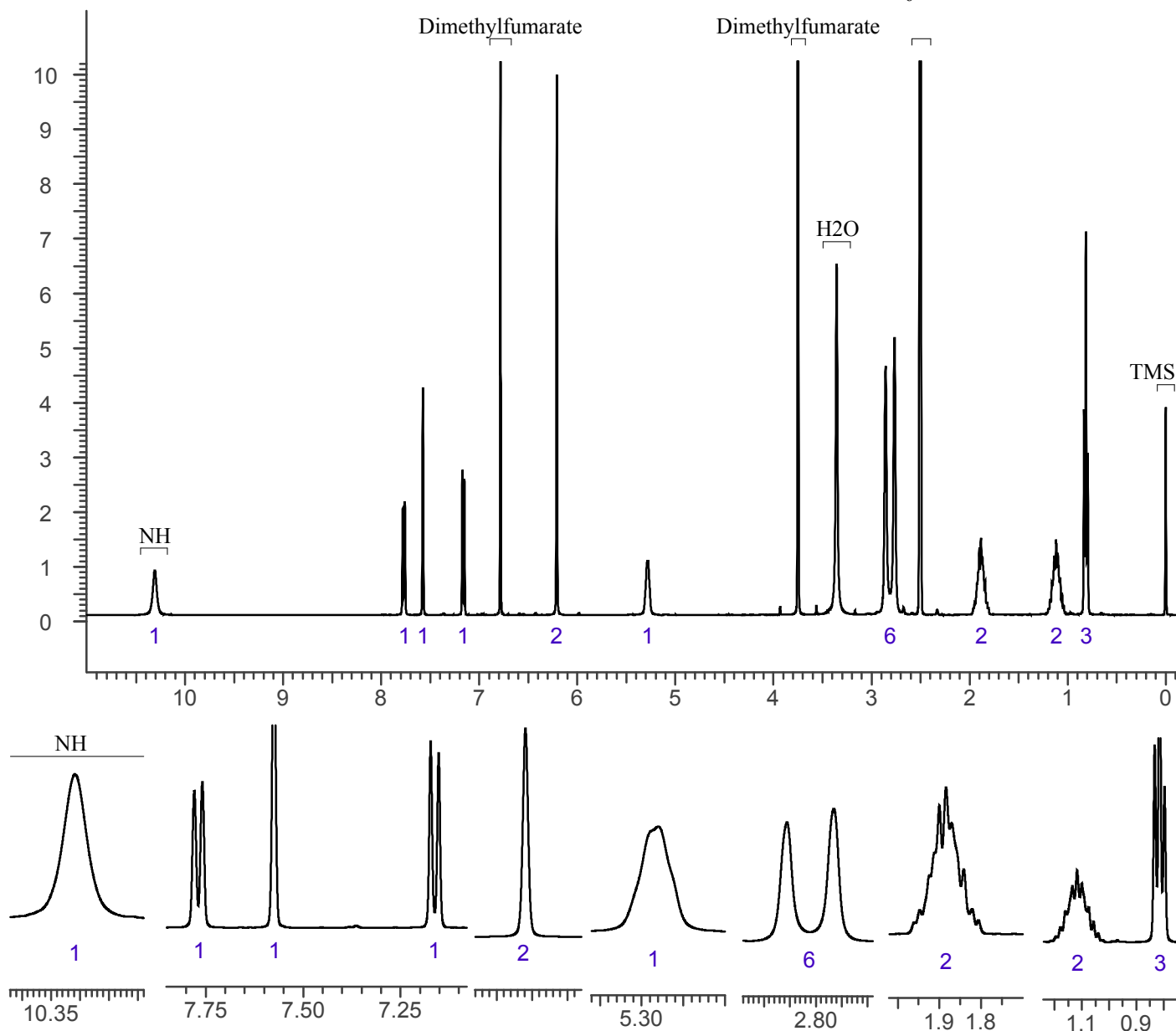
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~7 mg/mL in DMSO containing TMS for 0 ppm reference and dimethylfumarate 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: N,N-Dimethylpentylone HCl; Lot# 0457892-27; DMSO-d₆; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

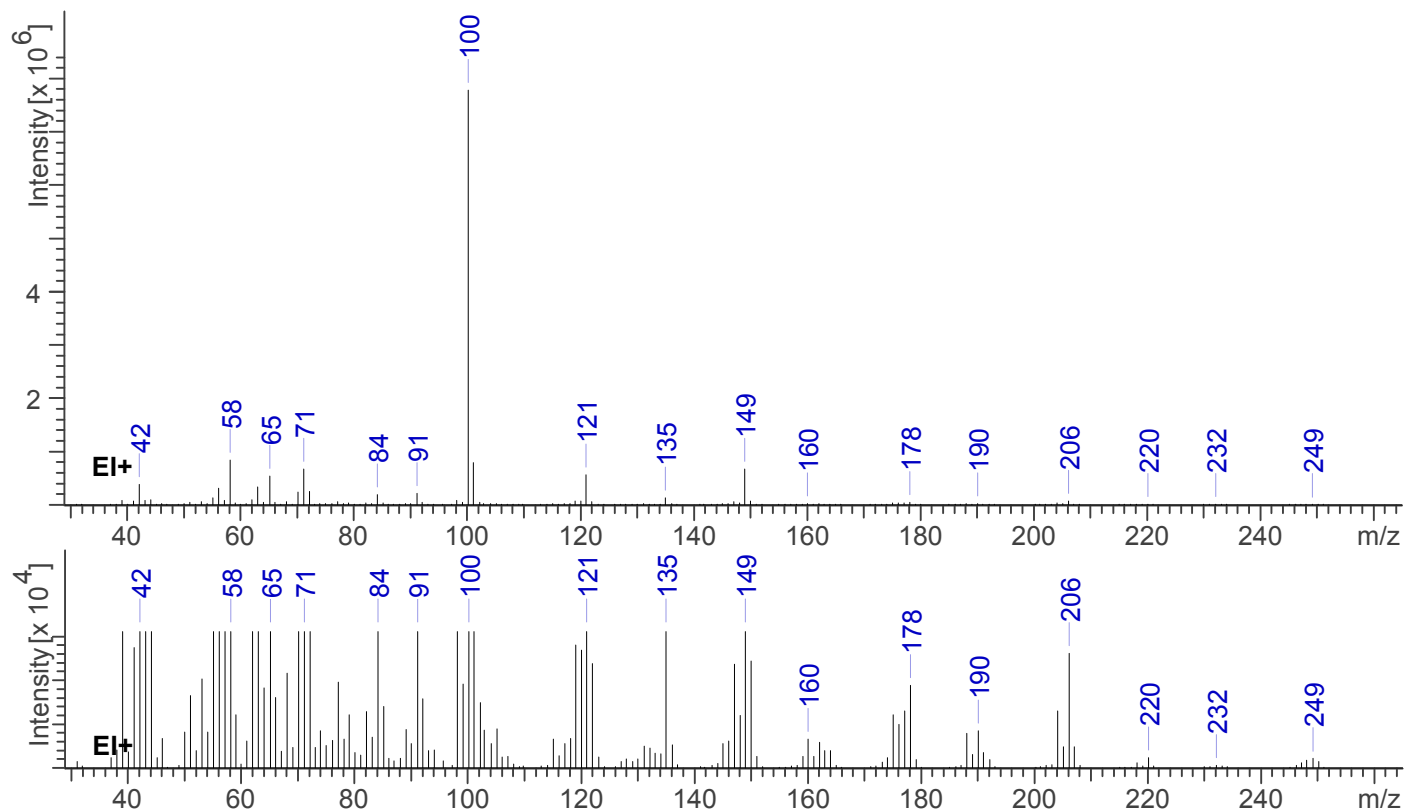
Sample Preparation: Dilute analyte ~5 mg/mL in Methanol.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μ m
Carrier Gas: Helium at 1.5 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 280°C at 12 °C/min
3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 25:1, 1 μ L injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan

Retention Time: 10.745 min

EI Mass Spectrum: N,N-Dimethylpentylone HCl; Lot #0457892-27





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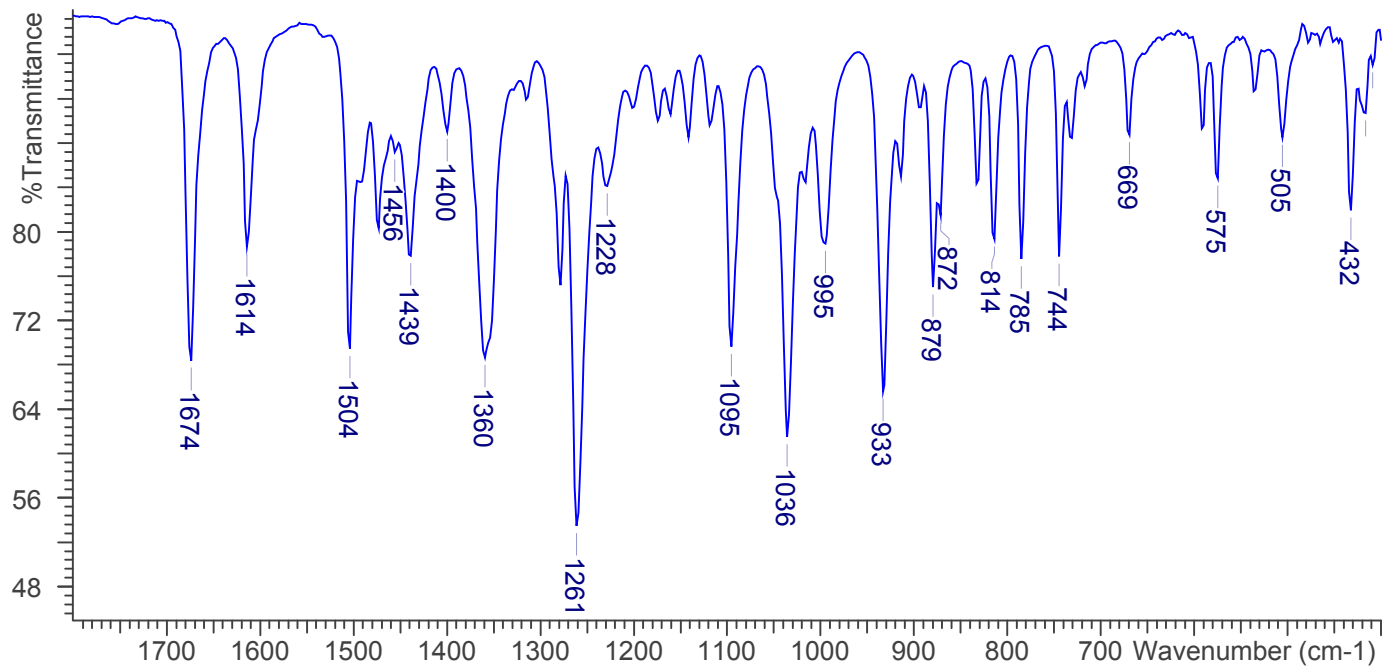
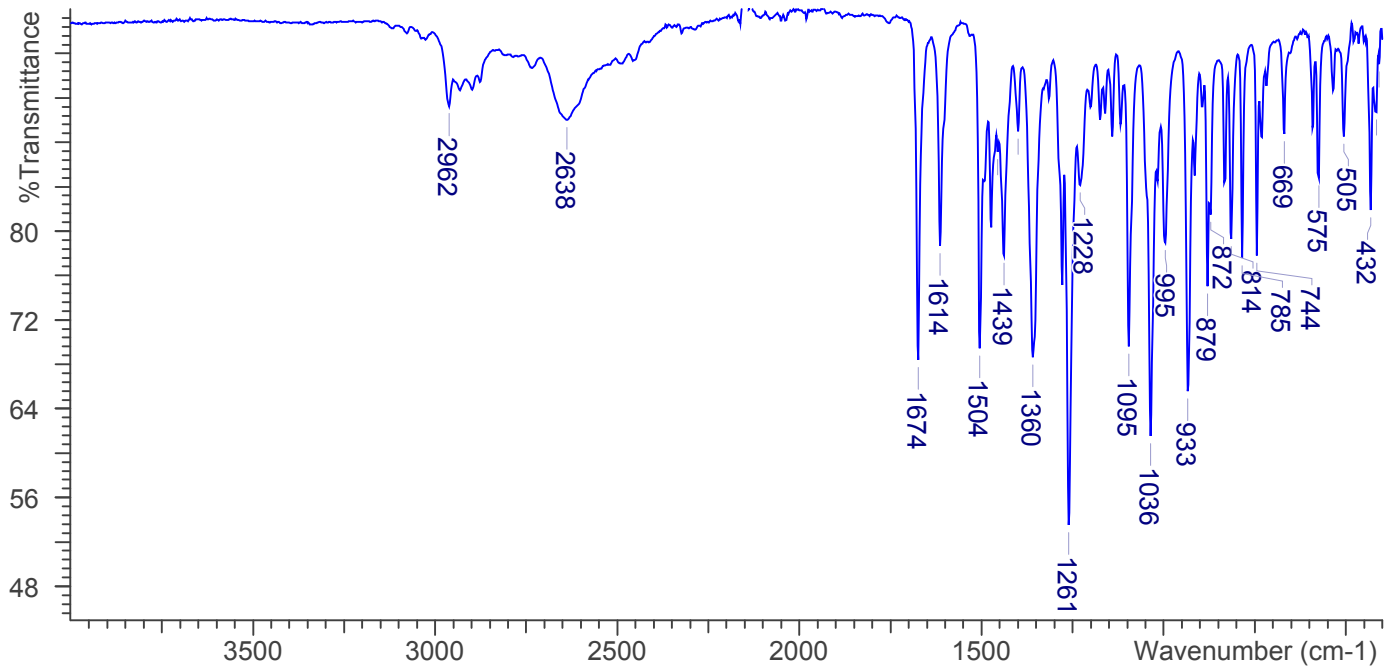


3.3 INFRARED SPECTROSCOPY (FTIR)

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): N,N-Dimethylpentylone HCl; Lot# 0457892-27





N,N-Dimethylpentylone

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4. ADDITIONAL RESOURCES

No Literature available as of 05/2017