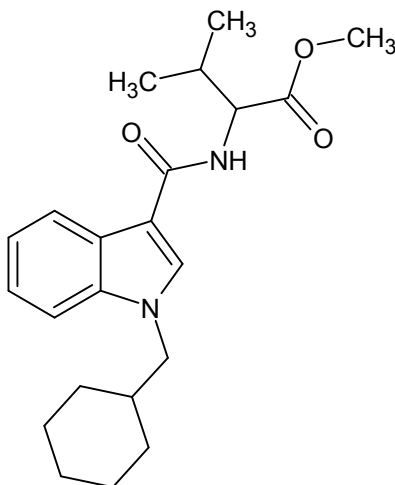




MMB-CHMICA

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



1. GENERAL INFORMATION

IUPAC Name: methyl *N*-[1-(cyclohexylmethyl)-1*H*-indole-3-carbonyl]valinate

CAS#: NA

Synonyms: NA

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 ₂₂ H ₃₀ N ₂ O ₃	370	Not Determined



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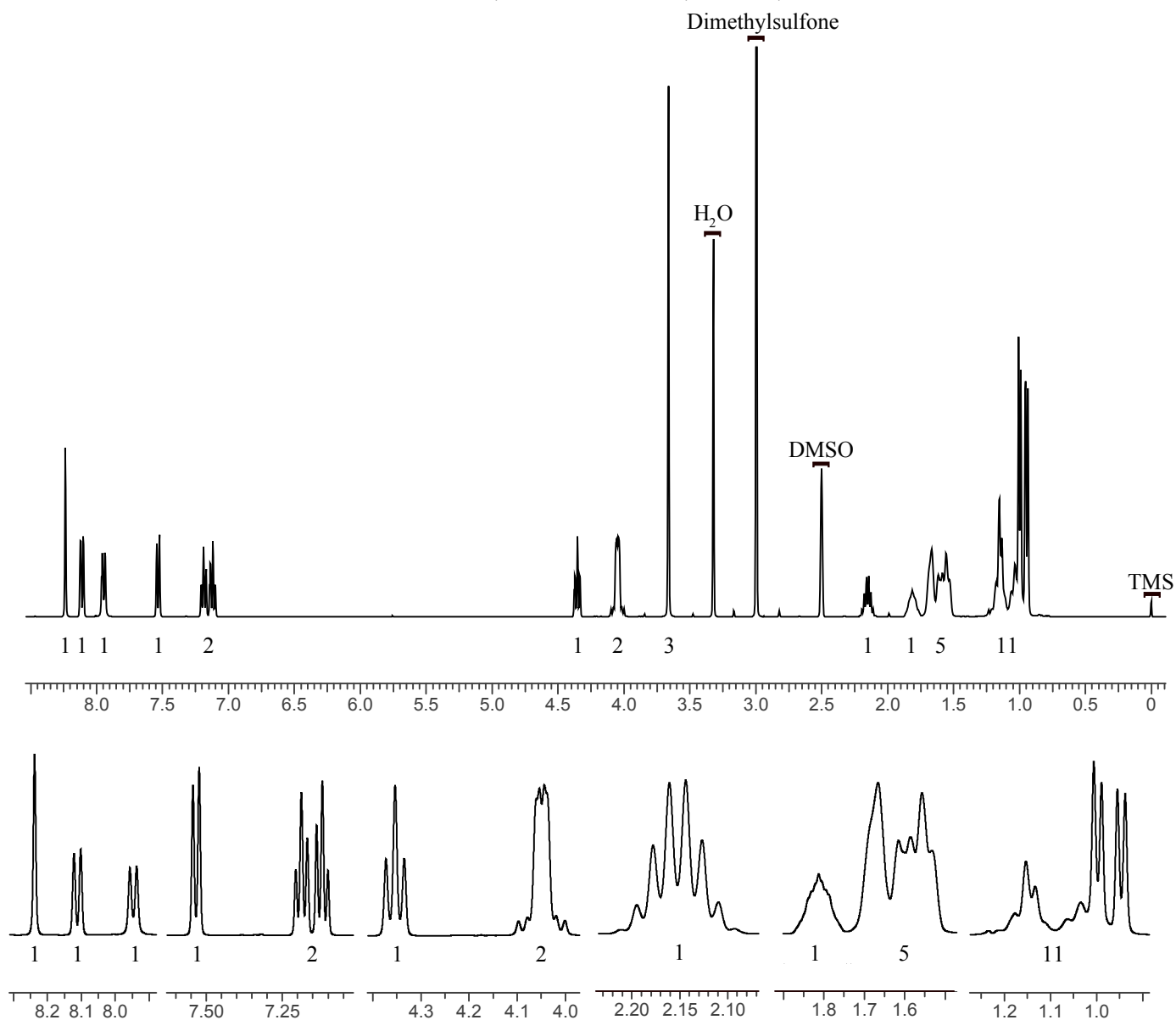
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 mg/mL in DMSO- d_6 containing TMS for 0 ppm reference and dimethylsulfone 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: MMB-CHMICA; Lot 0470336-17; DMSO; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

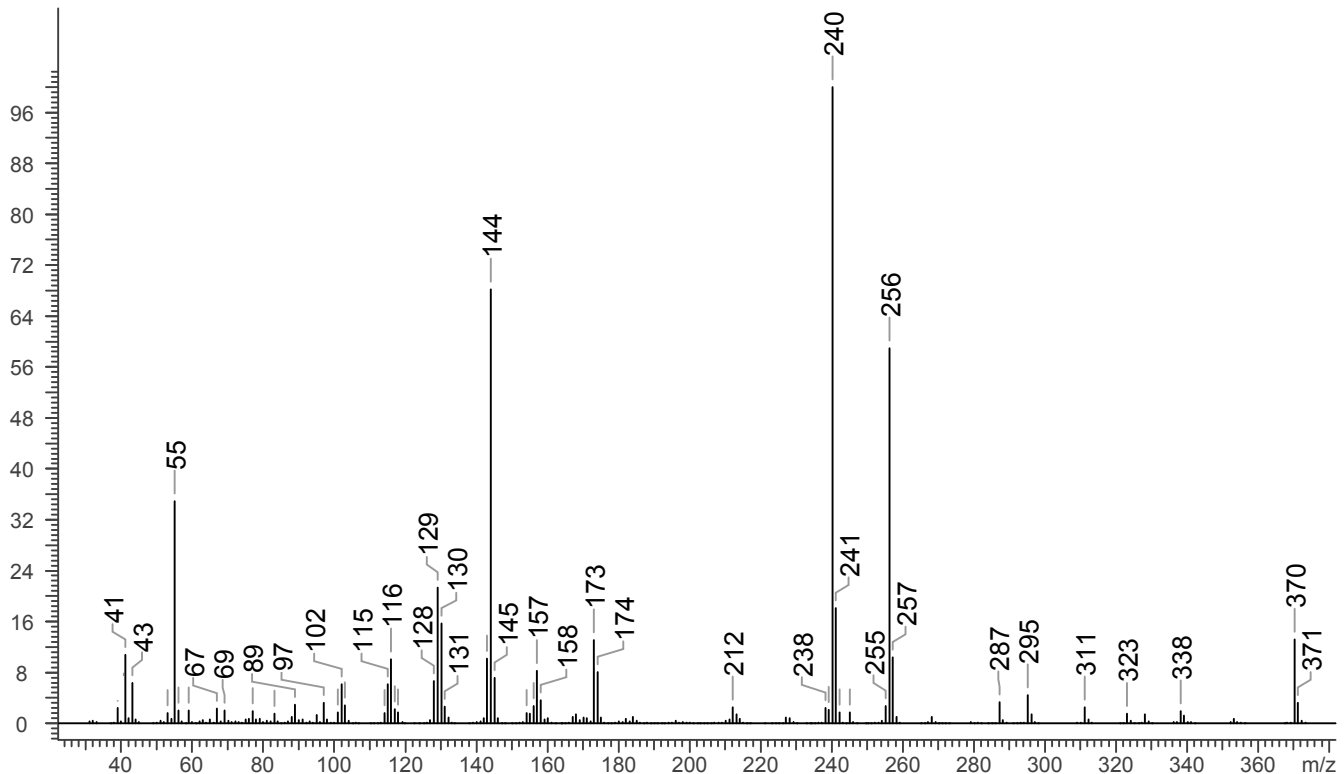
Sample Preparation: Dilute analyte ~3.3 mg/mL in methanol.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: DB-5 MS (or equivalent); 15m 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: 250°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: 150
Tune file: stune.u
Acquisition mode: scan

Retention Time: 16.534 min

EI Mass Spectrum: MMB-CHMICA; Lot 0470336-17





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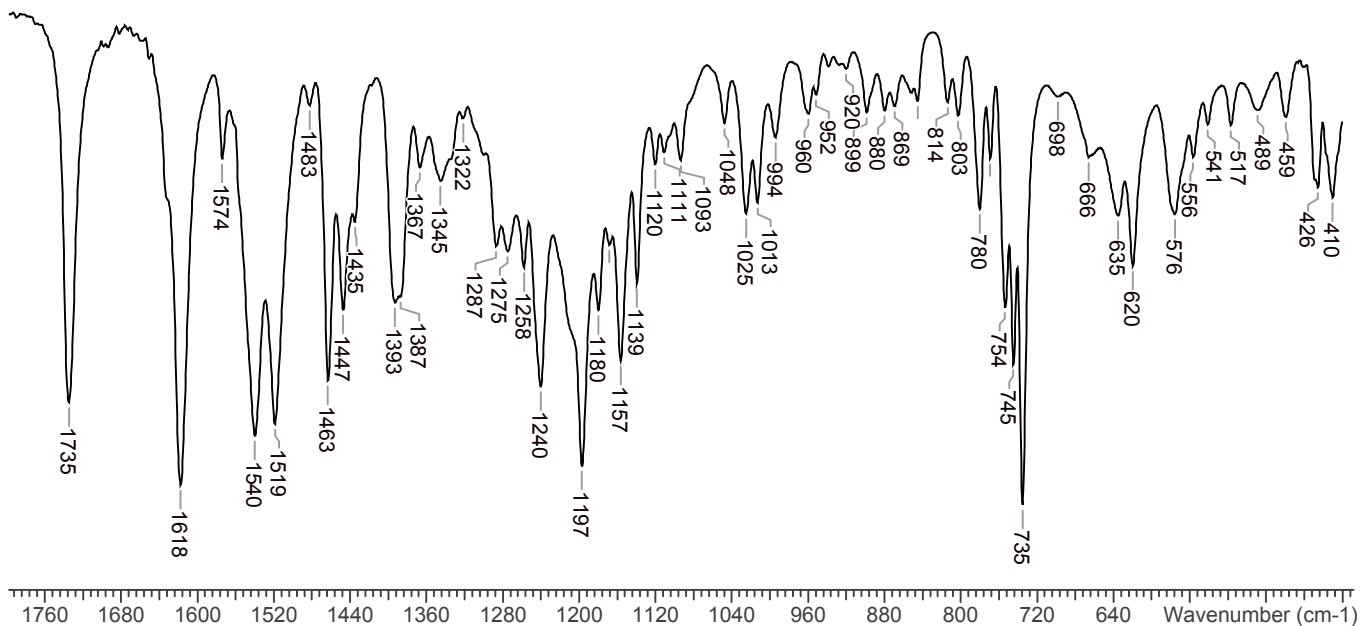
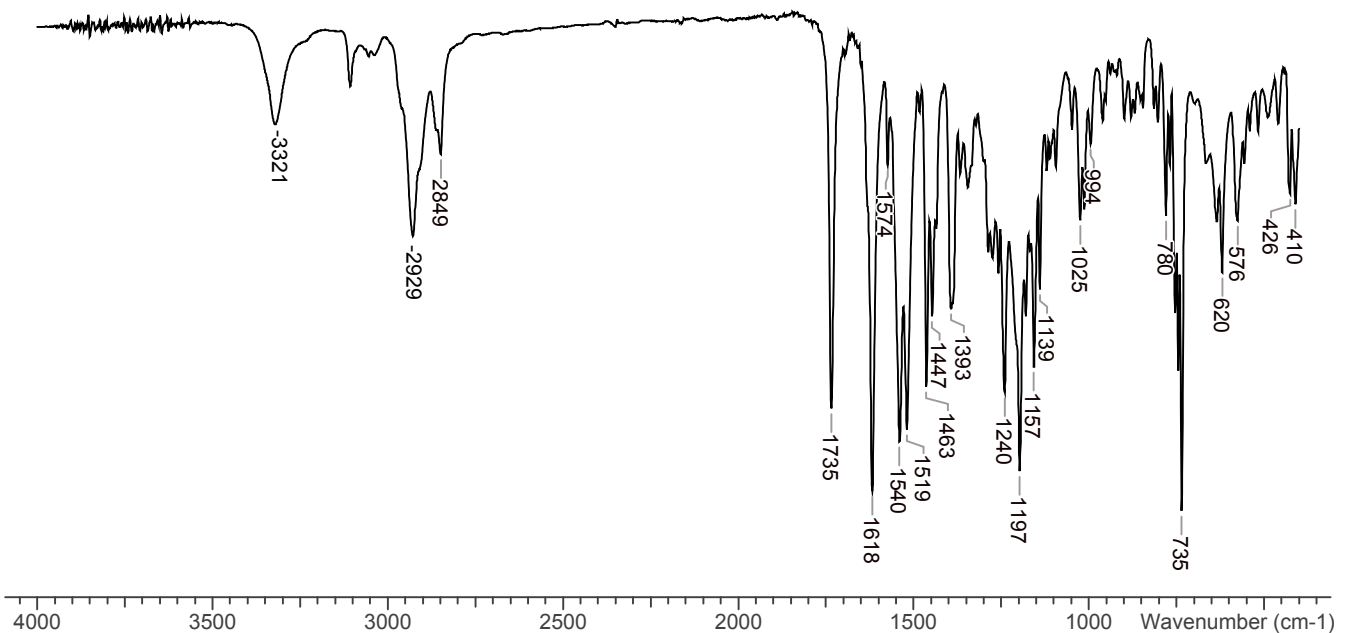


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): MMB-CHMICA; Lot 0470336-17





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4. ADDITIONAL RESOURCES

No additional resources as of 03/2016