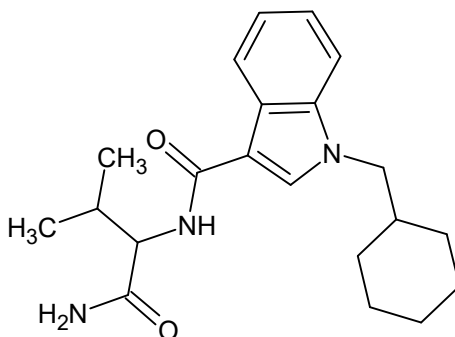




AB-CHMICA

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



1. GENERAL INFORMATION

IUPAC Name: N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(cyclohexylmethyl)-1H-indole-3-carboxamide

CAS#: N/A

Synonyms: N/A

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 ₂₁ H ₂₉ N ₃ O ₂	355.47	Not Determined



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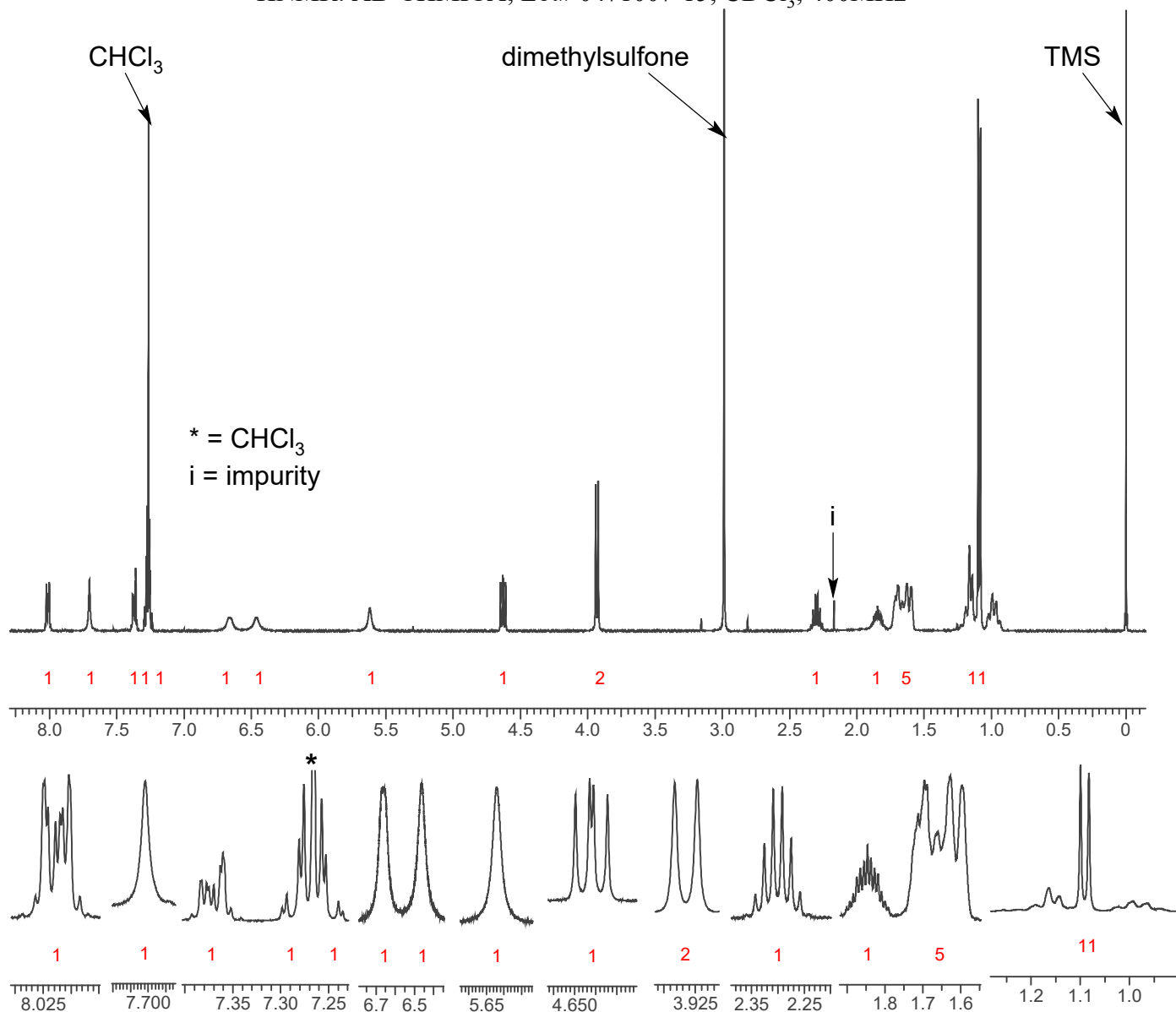
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~6 mg/mL in CDCl₃ 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

¹HNMR: AB-CHMICA; Lot# 0471007-15; CDCl₃; 400MHz





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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in MeOH

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: HP-5 MS (or equivalent); 30 m x 0.25 mm x 0.25 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 30.0 min

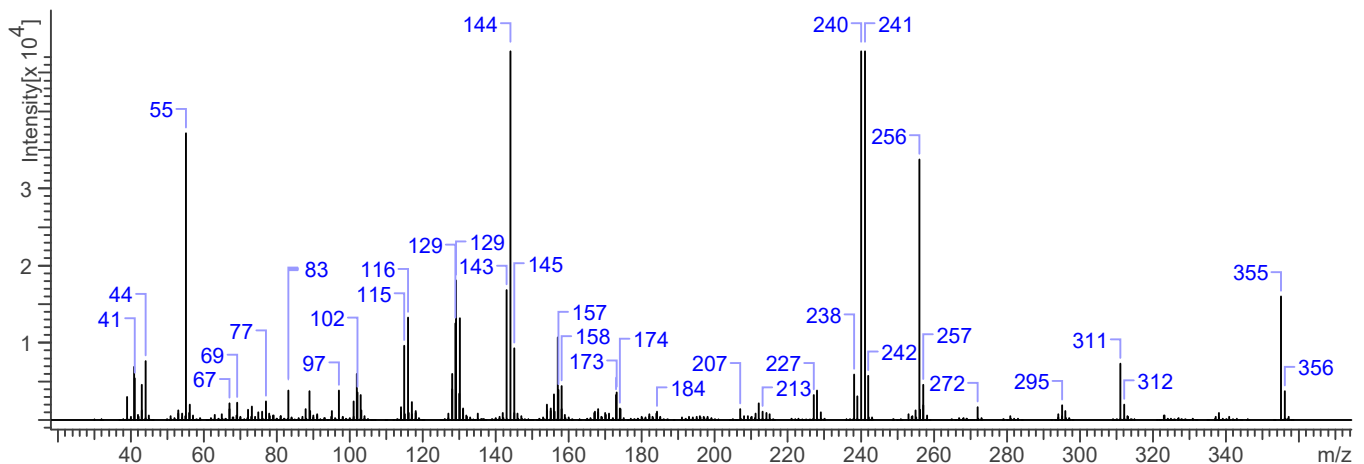
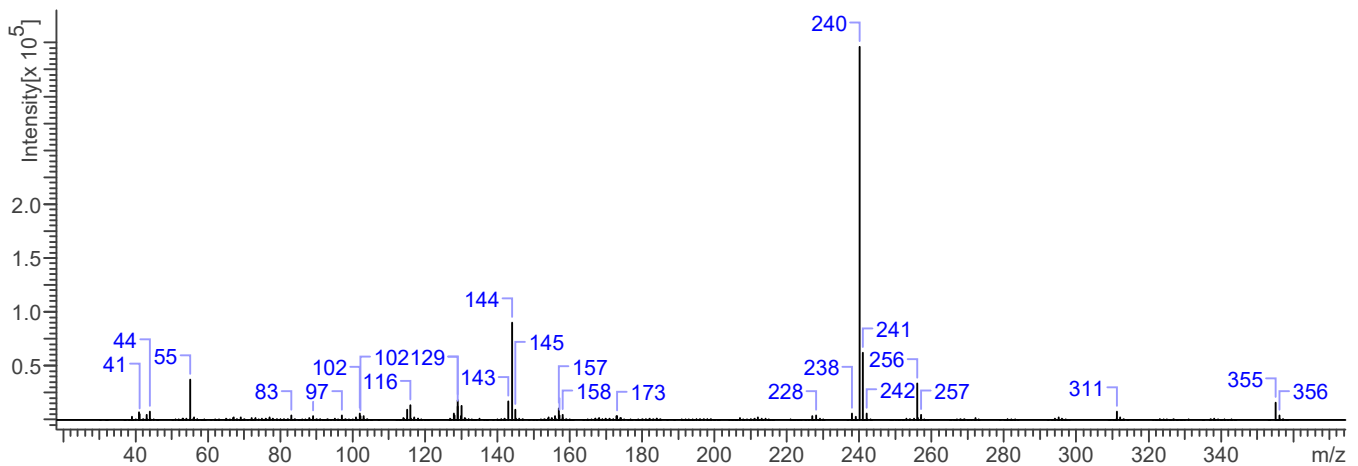
Injection Parameters: Split Ratio = 25:1, 1 µL injected

MS Parameters: Mass scan range: 30-550 amu Threshold: 250

Tune file: stune.u Acquisition mode: scan

Retention Time: 24.282 min

EI Mass Spectrum: AB-CHMICA; Lot# 0471007-15





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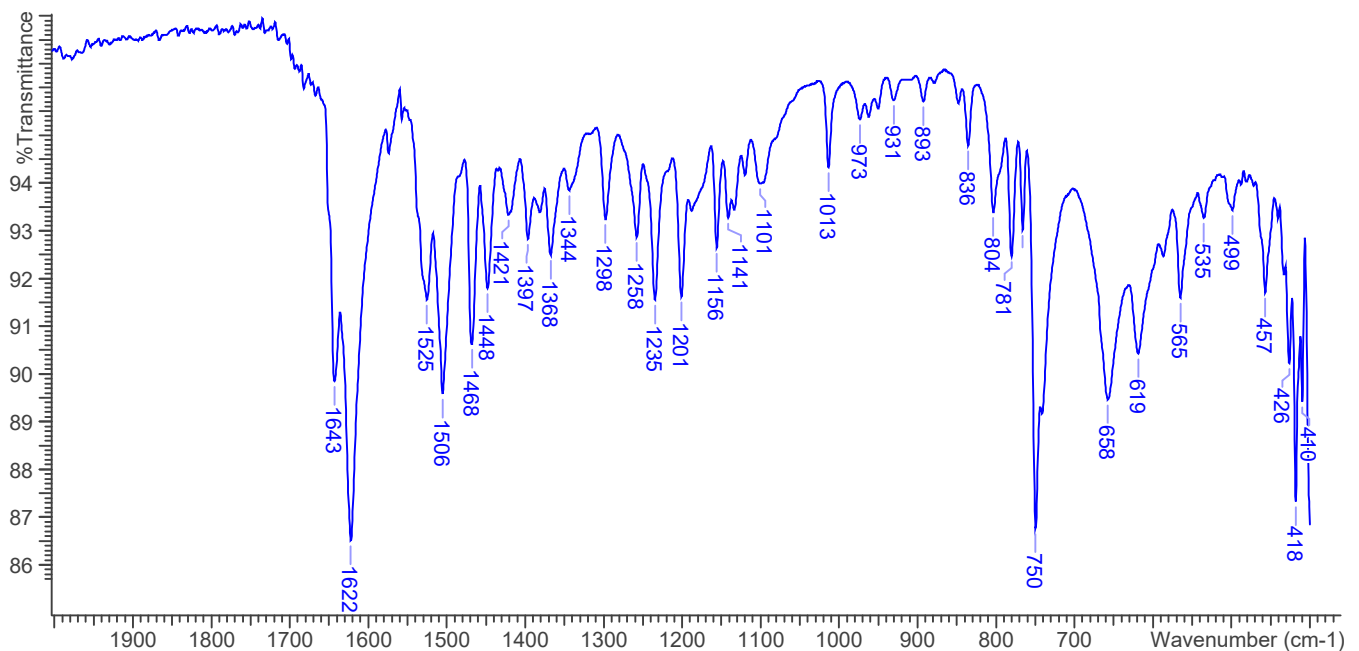
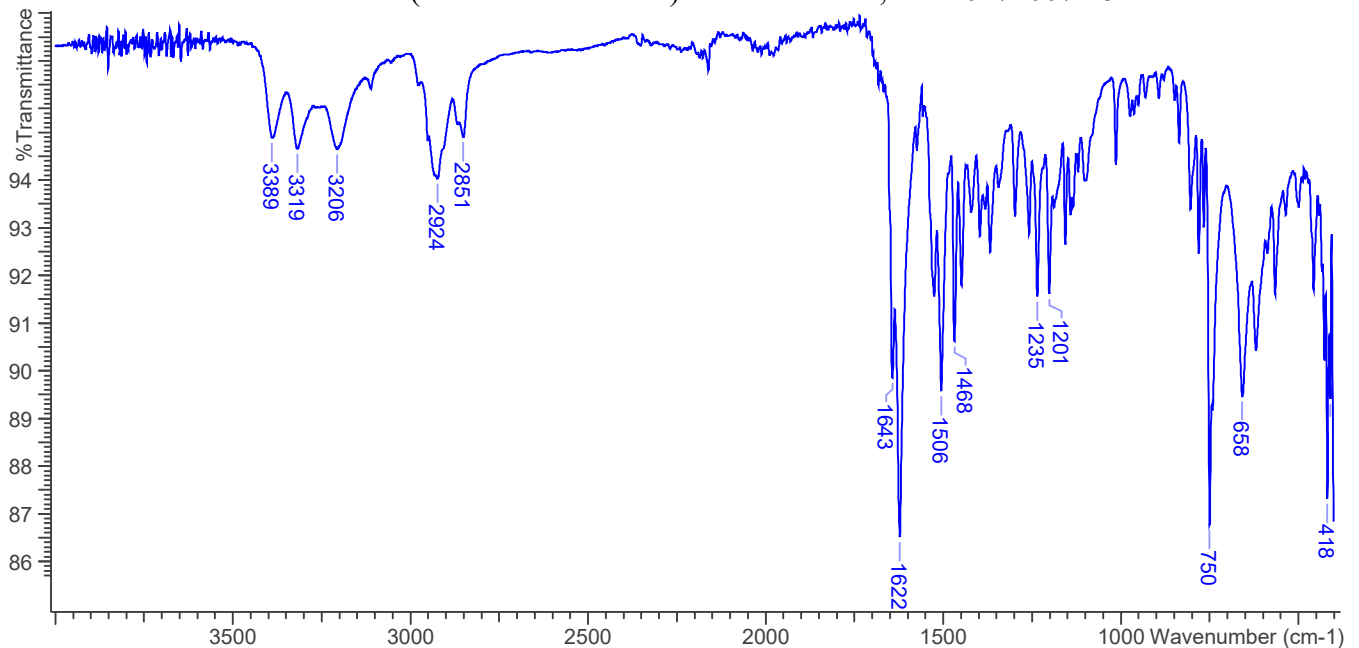


3.3 INFRARED SPECTROSCOPY (FTIR)

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: 4
Aperture: 80

FTIR ATR (Diamond 1 Bounce): AB-CHMICA; Lot# 0471007-15





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4. ADDITIONAL RESOURCES

No additional resources as of 12/2016