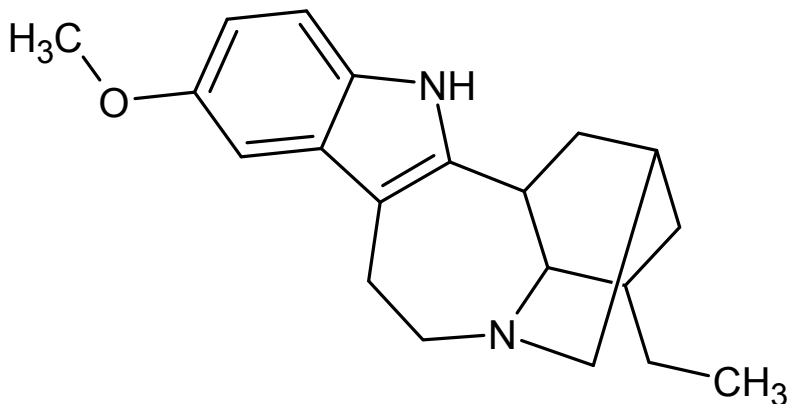




Ibogaine

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



1. GENERAL INFORMATION

IUPAC Name:	<i>N</i> -(1-amino-3-methyl-1-oxobutan-2-yl)-1-pentyl-1 <i>H</i> -indazole-3-carboxamide
CAS#:	Not Available
Synonyms:	N/A
Source:	DEA Reference Material Collection
Appearance:	Beige powder (HCl)
UV_{max}(nm):	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₀ H ₂₆ N ₂ O	309	Not Determined
HCl	C ₂₀ H ₂₆ N ₂ O · HCl	346	Not Determined



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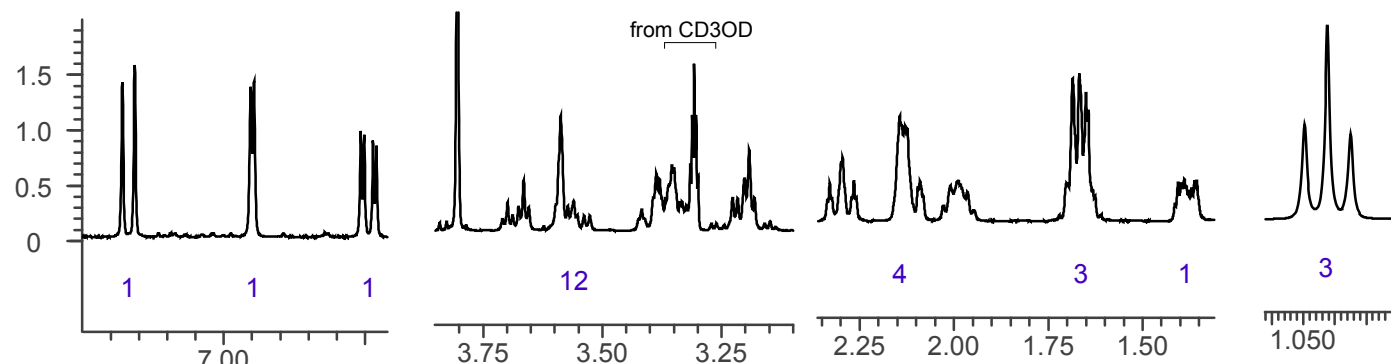
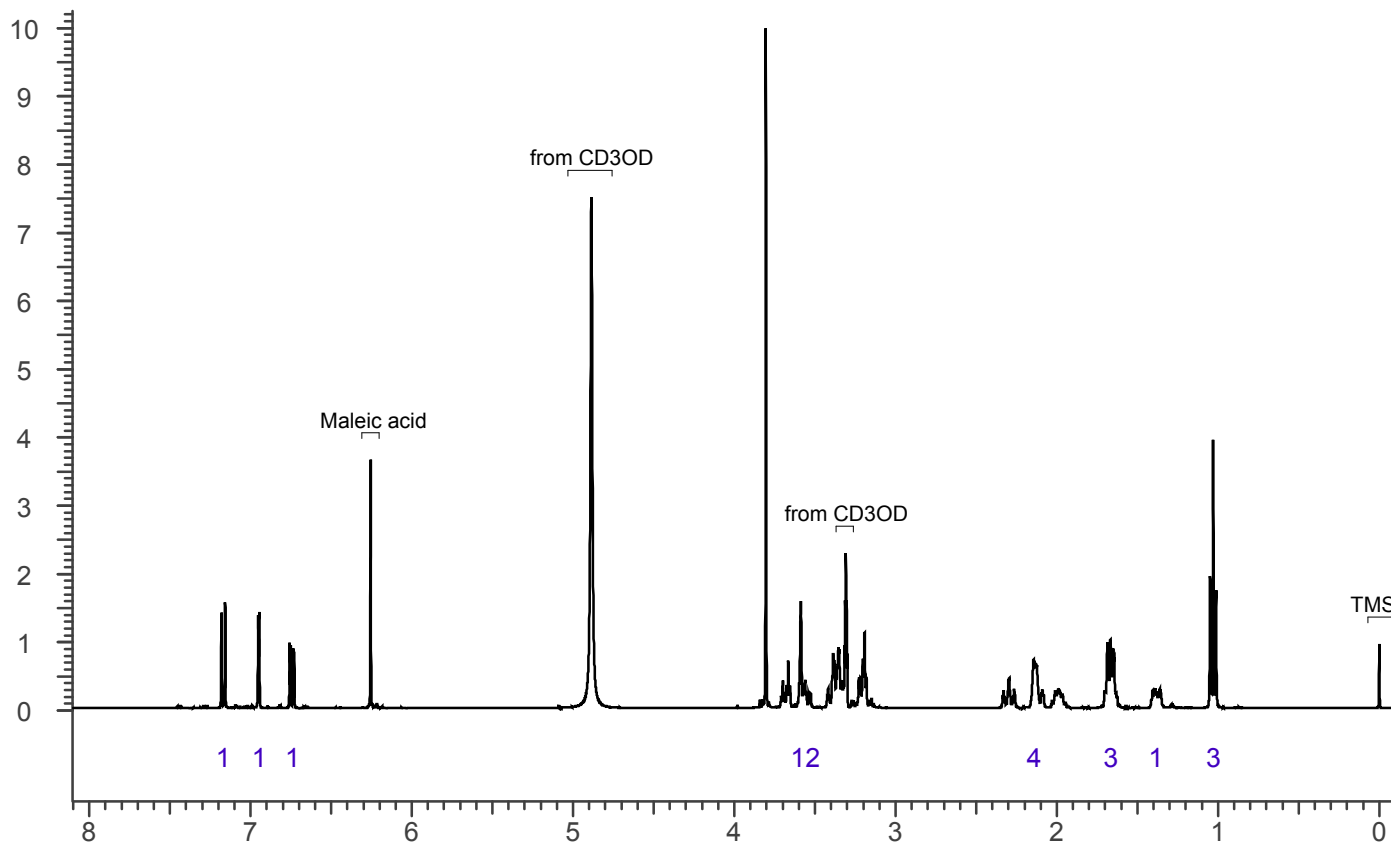


3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~25 mg/mL in CD₃OD containing TMS 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: Ibogaine HCl Lot # 080-254A; CD₃OD; 400MHz





Ibogaine

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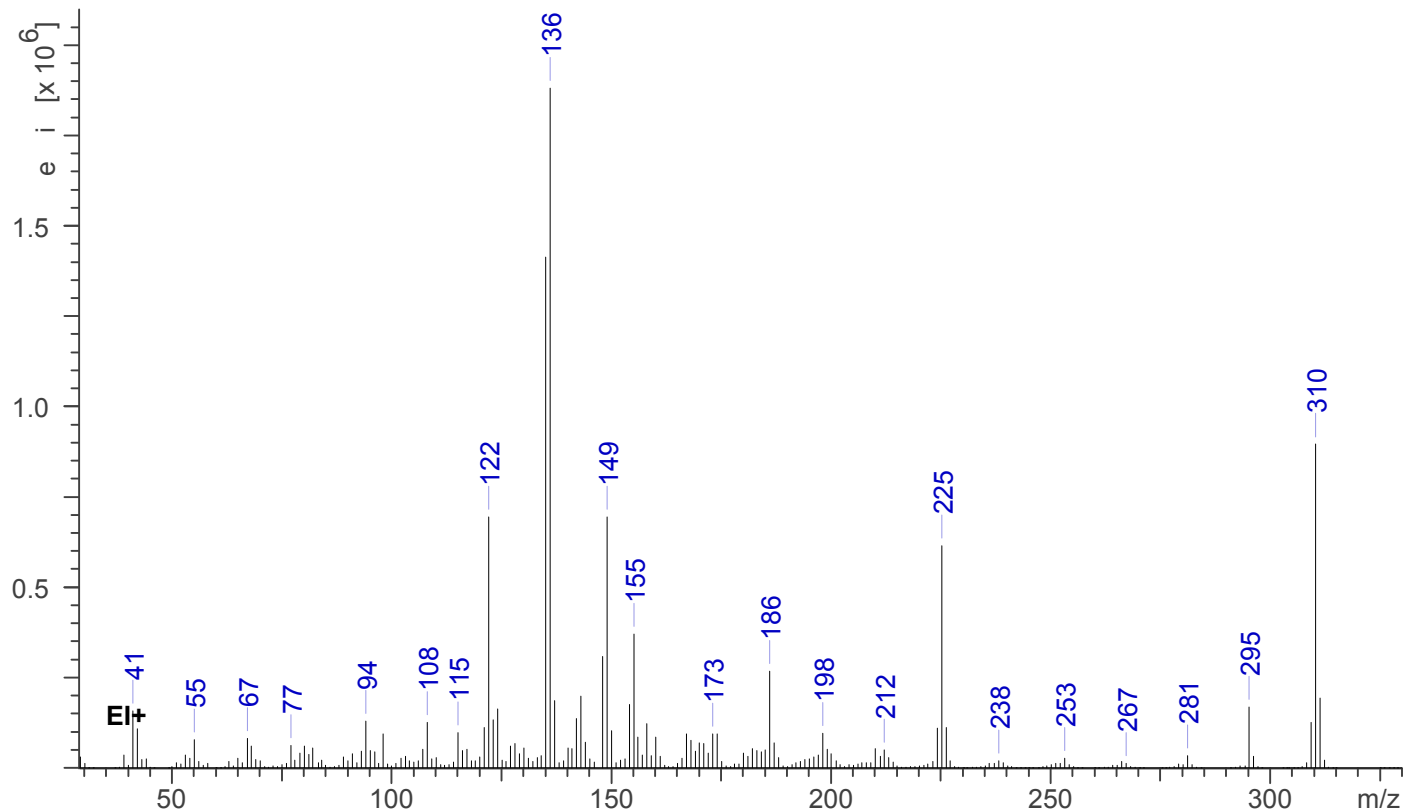


3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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
Injection Parameters: Split Ratio = 20:1, 1 μ L injected
MS Parameters: Mass scan range: 30-550 amu
Threshold: 100
Tune file: stune.u
Acquisition mode: scan
Retention Time: 19.602 min

EI Mass Spectrum: Ibogaine HCl Lot # 080-254A





Ibogaine



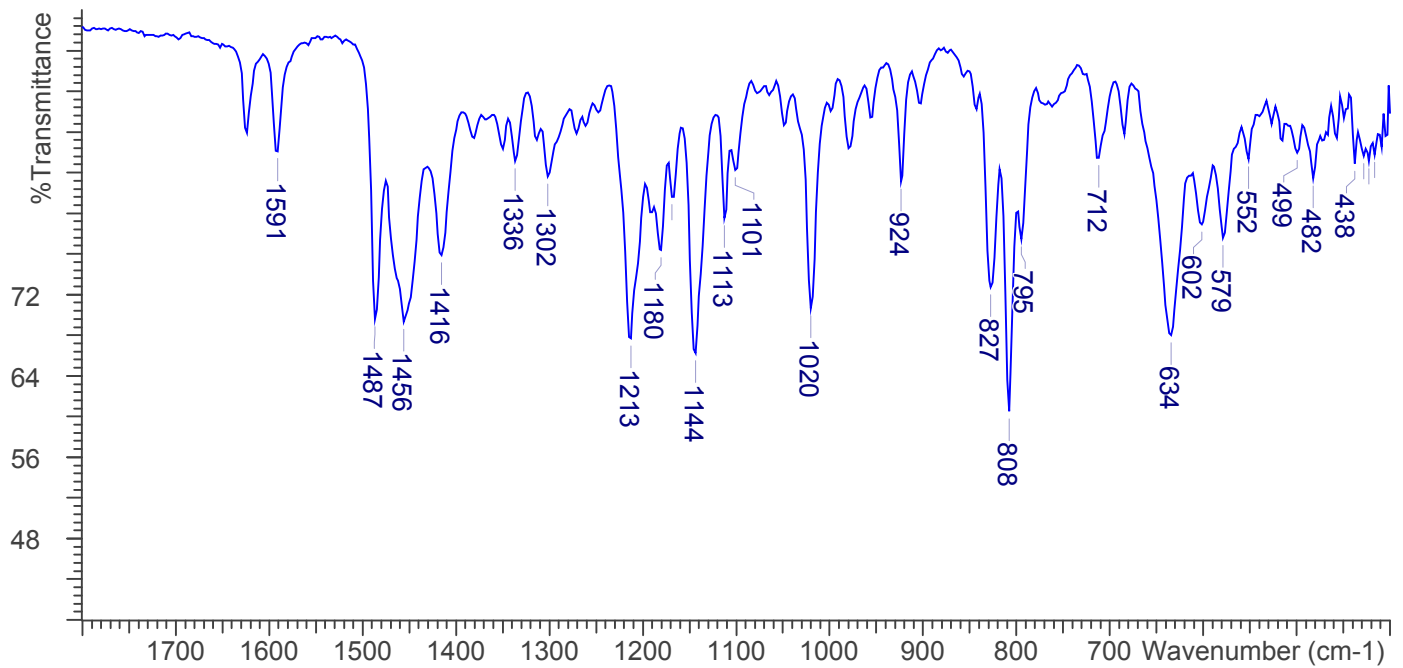
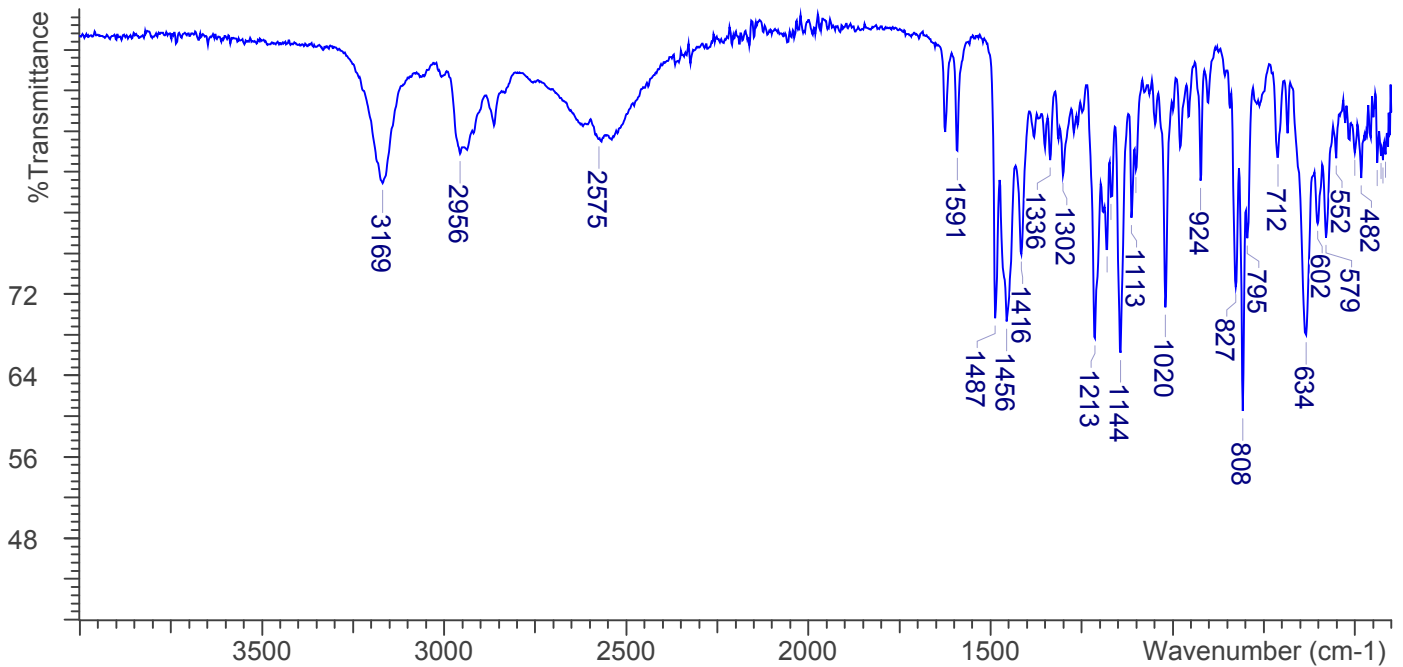
The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

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): Ibogaine HCl Lot # 080-254A





Ibogaine

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4. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)