

1. GENERAL INFORMATION

IUPAC Name: methyl (16*E*,20β)-9,17-dimethoxycoryn-16-en-16-carboxylate

CFR: Not Scheduled (5/2013)

CAS#: 4098-40-2

Synonyms: Kratom, 9-methoxy Corynantheidine

Source: DEA Reference Material Collection

Appearance: White powder

Kovat's Index: Pending

UV_{max} (nm): Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₂₃ H ₃₀ N ₂ O ₄	398	Not Determined

3. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl_3

Sample Preparation: Dilute analyte to ~5 mg/mL in CDCl_3 containing TMS for 0 ppm reference and methenamine as quantitative internal standard.

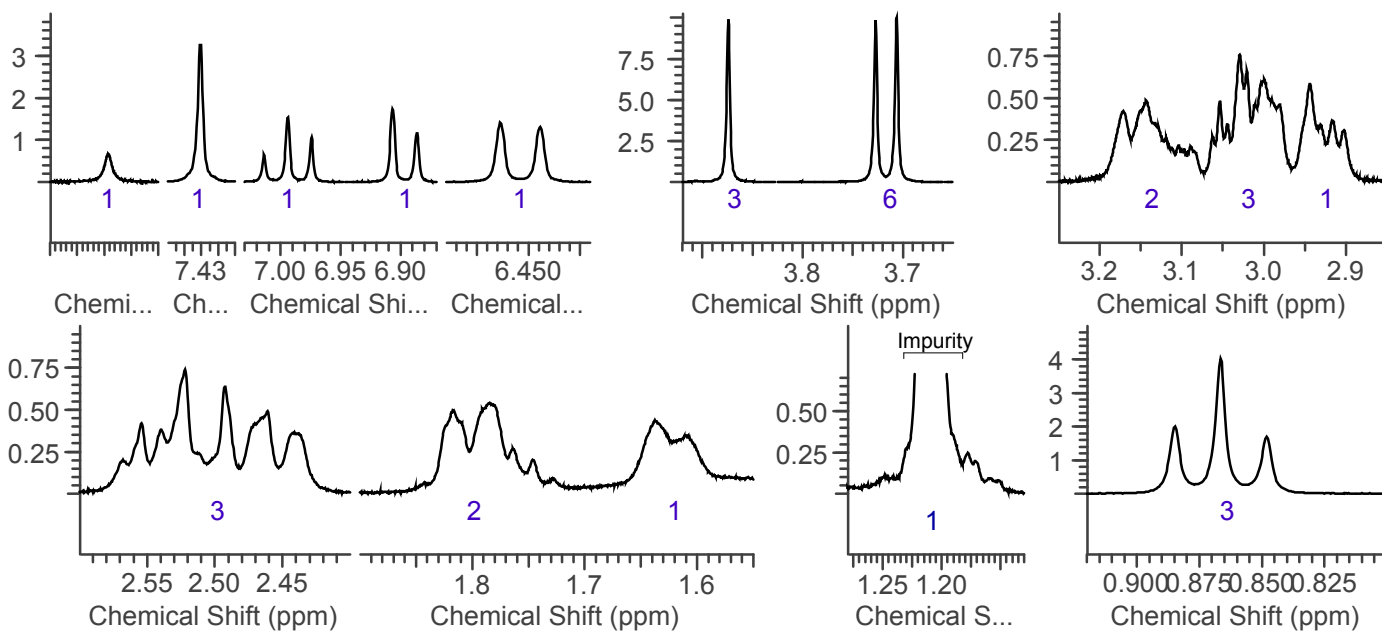
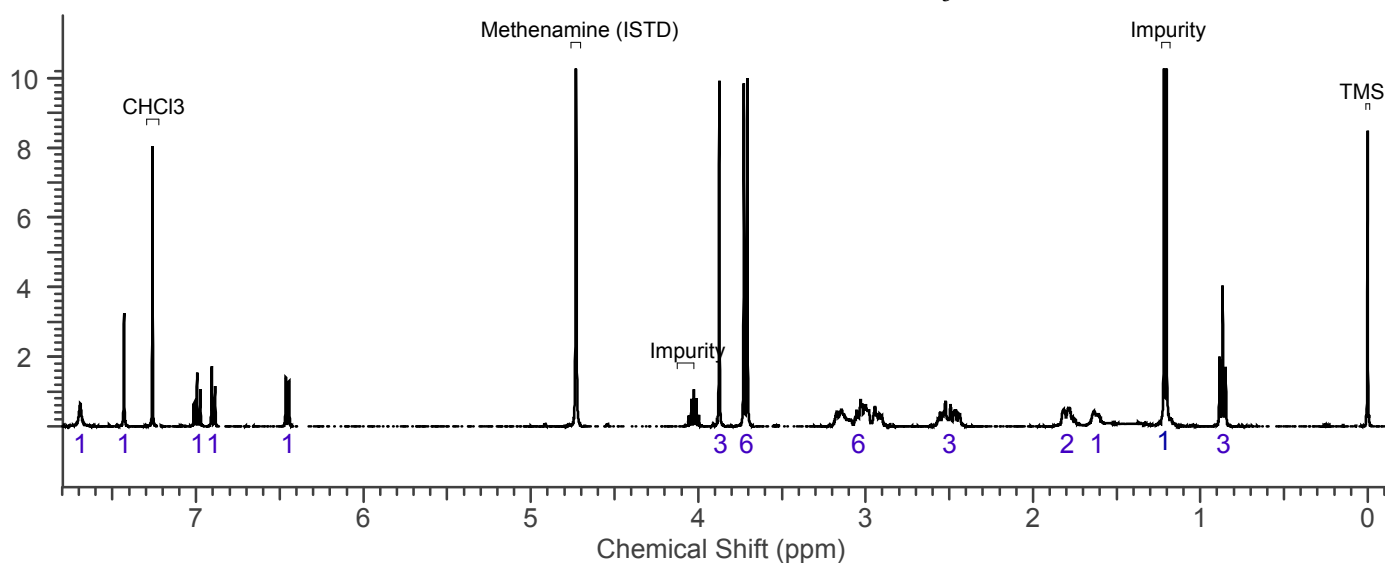
Instrument: 400 MHz NMR spectrometer

Parameters: Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle: 90°

Delay between pulses: 45 seconds

^1H NMR: Mitragynine; Lot 00013890-1741; CDCl_3 ; 400 MHz



4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 2 mg/mL in chloroform.

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 2.0 min

2) Ramp to 300°C at 14 °C/min

3) Hold final temperature for 25.0 min

Injection Parameters: Split Ratio = 20:1, 1 μ L injected

MS Parameters: Mass scan range: 34-550 amu

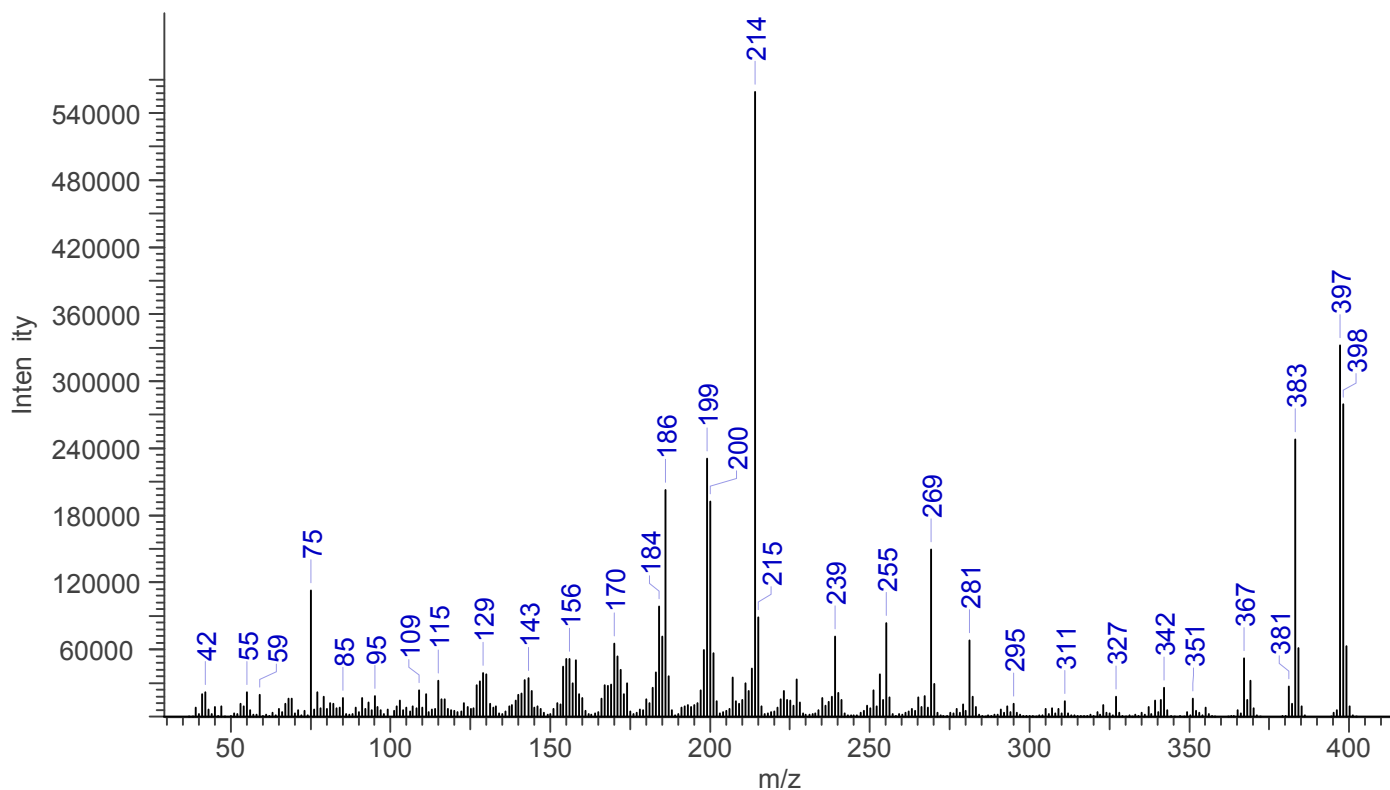
Threshold: 90

Tune file: stune.u

Acquisition mode: scan

Retention Time: 21.029 min

EI Mass Spectrum: Mitragynine; Lot 0439302-1



4.3 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): Mitragynine; Lot 0439302-1

