1. GENERAL INFORMATION

**IUPAC Name:** methyl (16E,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\textsubscript{max} (nm):** Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Melting Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C\textsubscript{23}H\textsubscript{30}N\textsubscript{2}O\textsubscript{4}</td>
<td>398</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>

3. ADDITIONAL RESOURCES

*Forendex*

*Wikipedia*
### 4. QUALITATIVE DATA

#### 4.1 NUCLEAR MAGNETIC RESONANCE

**Method NMR CDCl₃**

*Sample Preparation:* Dilute analyte to ~5 mg/mL in CDCl₃ 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; CDCl₃; 400 MHz

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<table>
<thead>
<tr>
<th>Chemical Shift (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.25</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Chemical Shift (ppm)</th>
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</thead>
<tbody>
<tr>
<td>7.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Chemical Shift (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.2</td>
</tr>
</tbody>
</table>

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![NMR spectrum diagram]

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![Detailed NMR spectrum graph]

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**Chemical Shift (ppm):**

- 1.25
- 1.20
- 0.25
- 0.50

- 7.00
- 6.95
- 6.90
- 6.85

- 3.2
- 3.1
- 3.0
- 2.9

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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 µm
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 µL 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