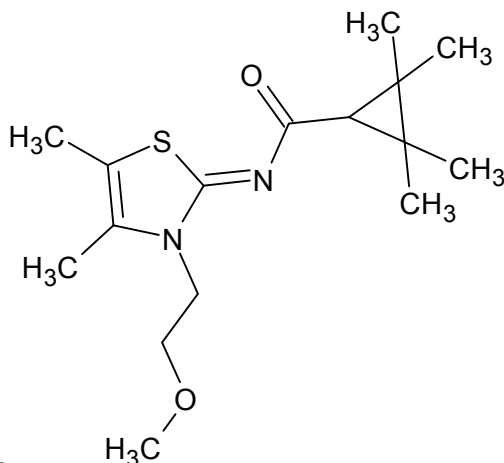




A836, 339

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



## 1. GENERAL INFORMATION

<b>IUPAC Name:</b>	N-[(2E)-3-(2-methoxyethyl)-4,5-dimethyl-1,3-thiazol-2(3H)-ylidene]-2,2,3,3-tetramethylcyclopropanecarboxamide
<b>CAS#:</b>	959746-77-1
<b>Synonyms:</b>	N/A
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White powder
<b>UV<sub>max</sub>(nm):</b>	Not Determined

## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>16</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub> S	310	121.7



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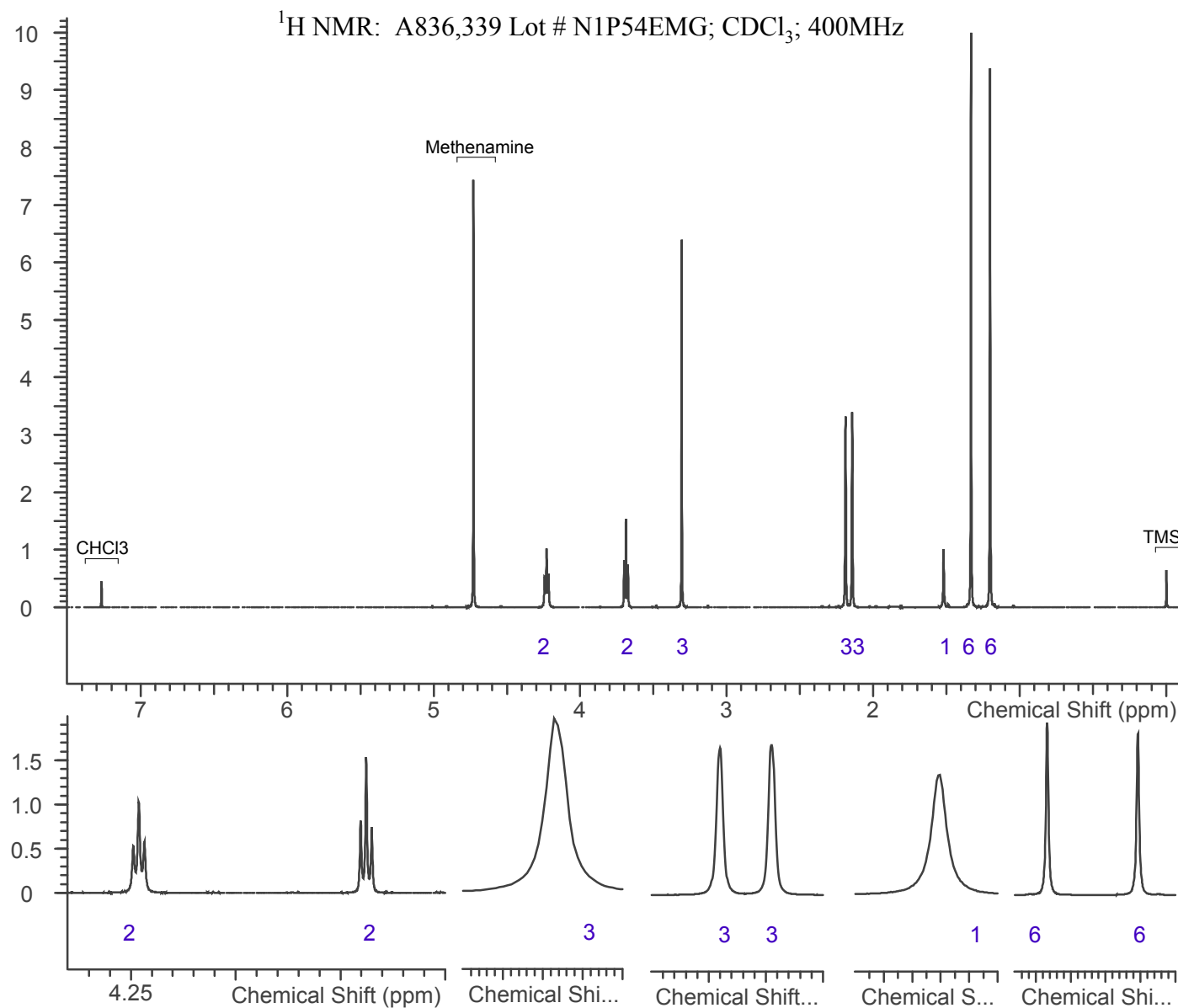
### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

##### Method NMR CDCl<sub>3</sub>

*Sample Preparation:* Dilute analyte to ~20 mg/mL in CDCl<sub>3</sub> 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





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### 3.2 Gas Chromatography/Mass Spectrometry

**Sample Preparation:** Dilute analyte ~1 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  $\mu$ 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  $\mu$ L injected

**MS Parameters:** Mass scan range: 30-550 amu

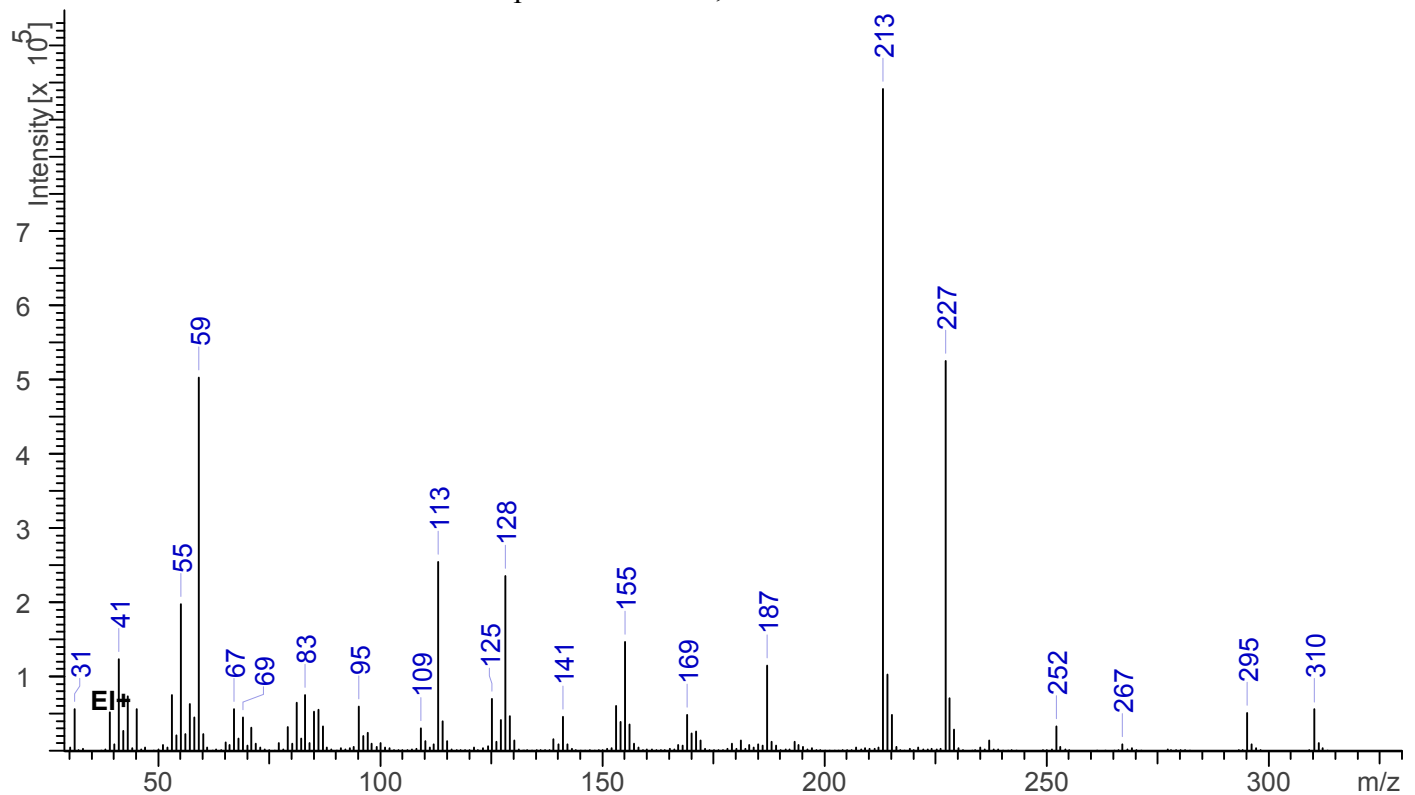
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

**Retention Time:** 14.452 min

EI Mass Spectrum: A836,339 Lot # N1P54EMG





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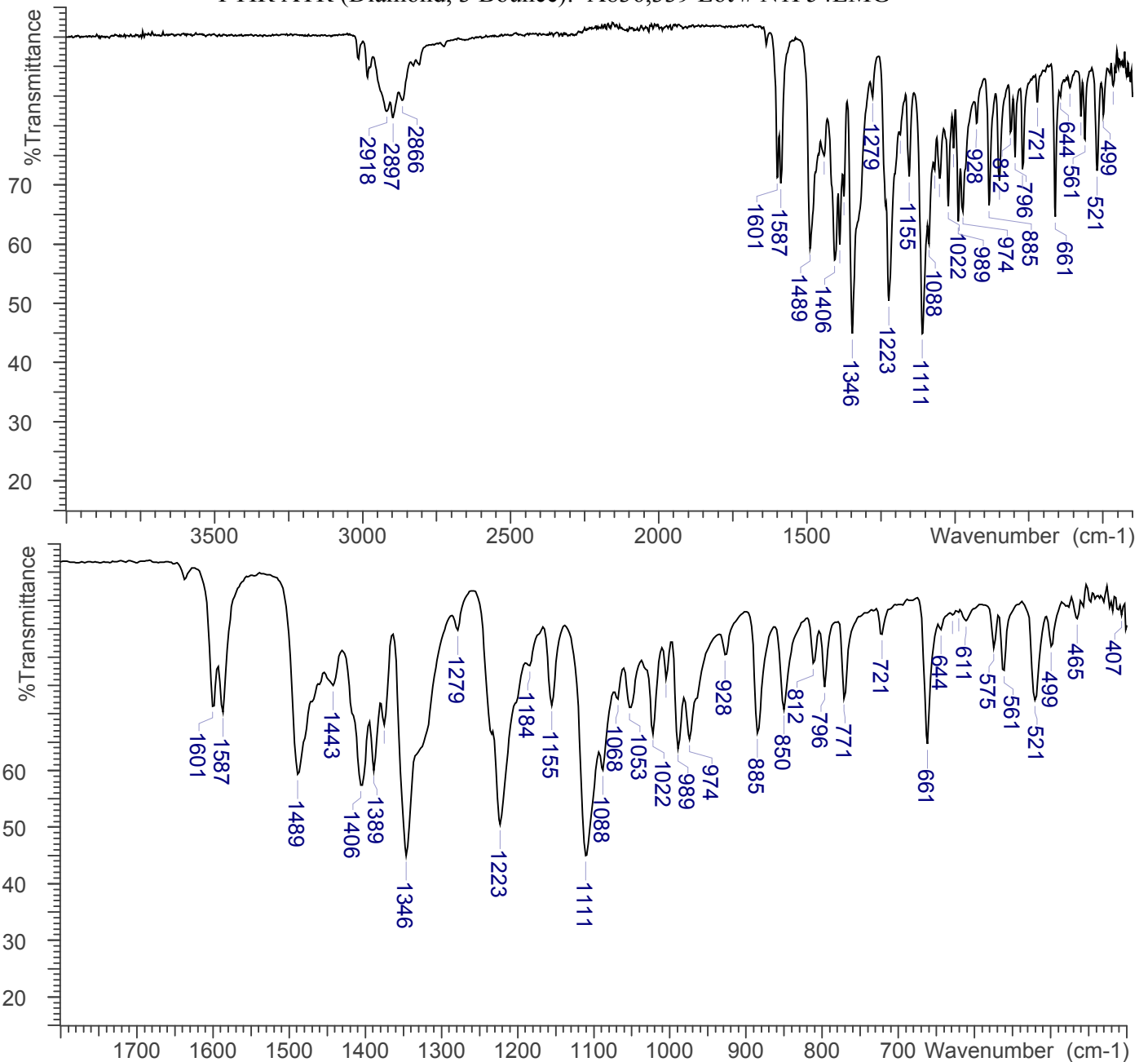


### 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:** Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): A836,339 Lot # N1P54EMG





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#### **4. ADDITIONAL RESOURCES**

[Wikipedia](#)