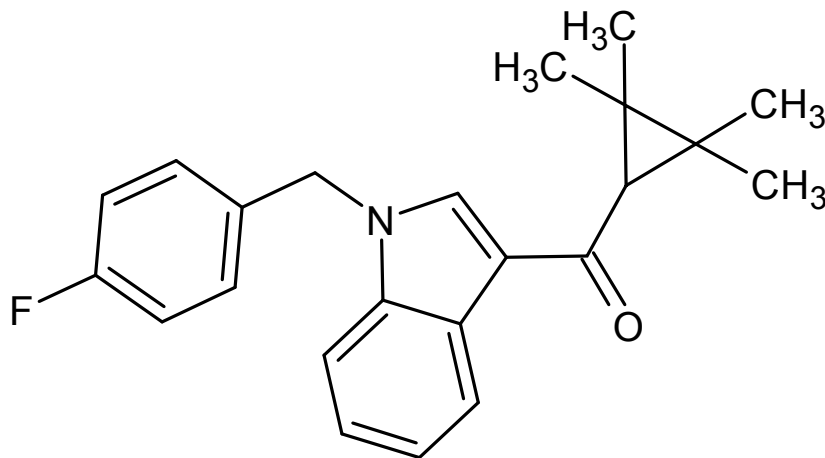




## FUB-144

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>	[1-(4-fluorobenzyl)-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)methanone
<b>CAS#:</b>	Not Available
<b>Synonyms:</b>	FUB-UR-144
<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>23</sub> H <sub>24</sub> FNO	349	122.0



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## 3. QUALITATIVE DATA

### 3.1 NUCLEAR MAGNETIC RESONANCE

**Sample Preparation:** Dilute analyte to ~5 mg/mL in  $\text{CDCl}_3$  containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

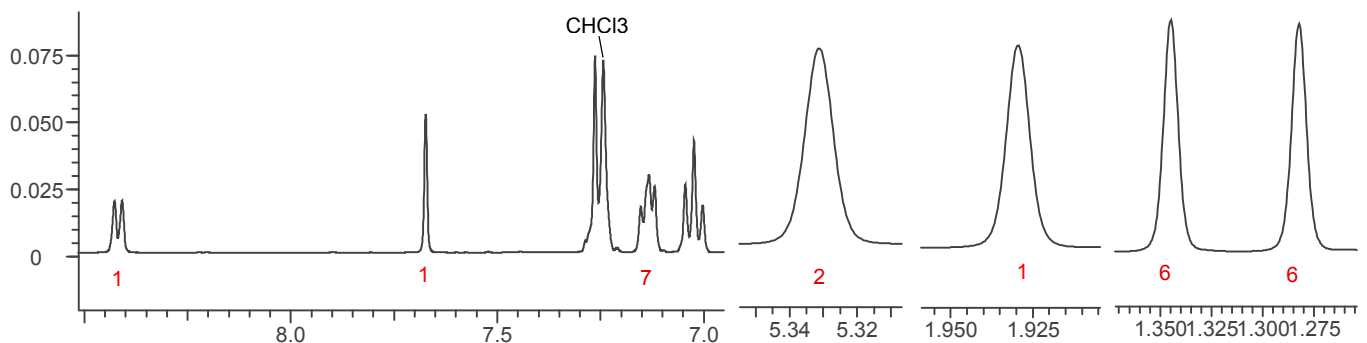
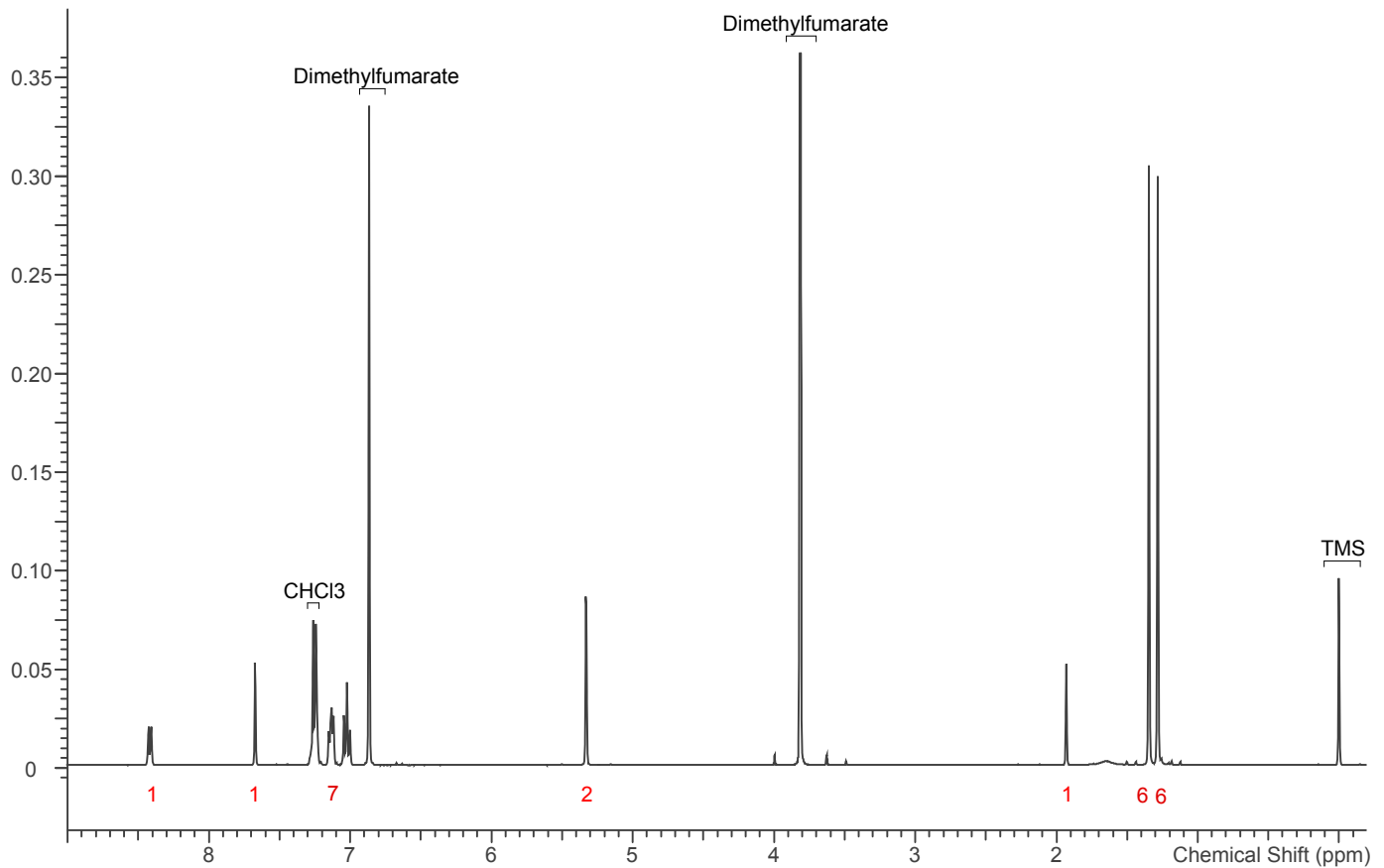
**Instrument:** 400 MHz NMR spectrometer

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

Pulse angle:  $90^\circ$

Delay between pulses: 45 seconds

$^1\text{H}$  NMR: FUB-144 Lot # 0455762-22;  $\text{CDCl}_3$ ; 400MHz





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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

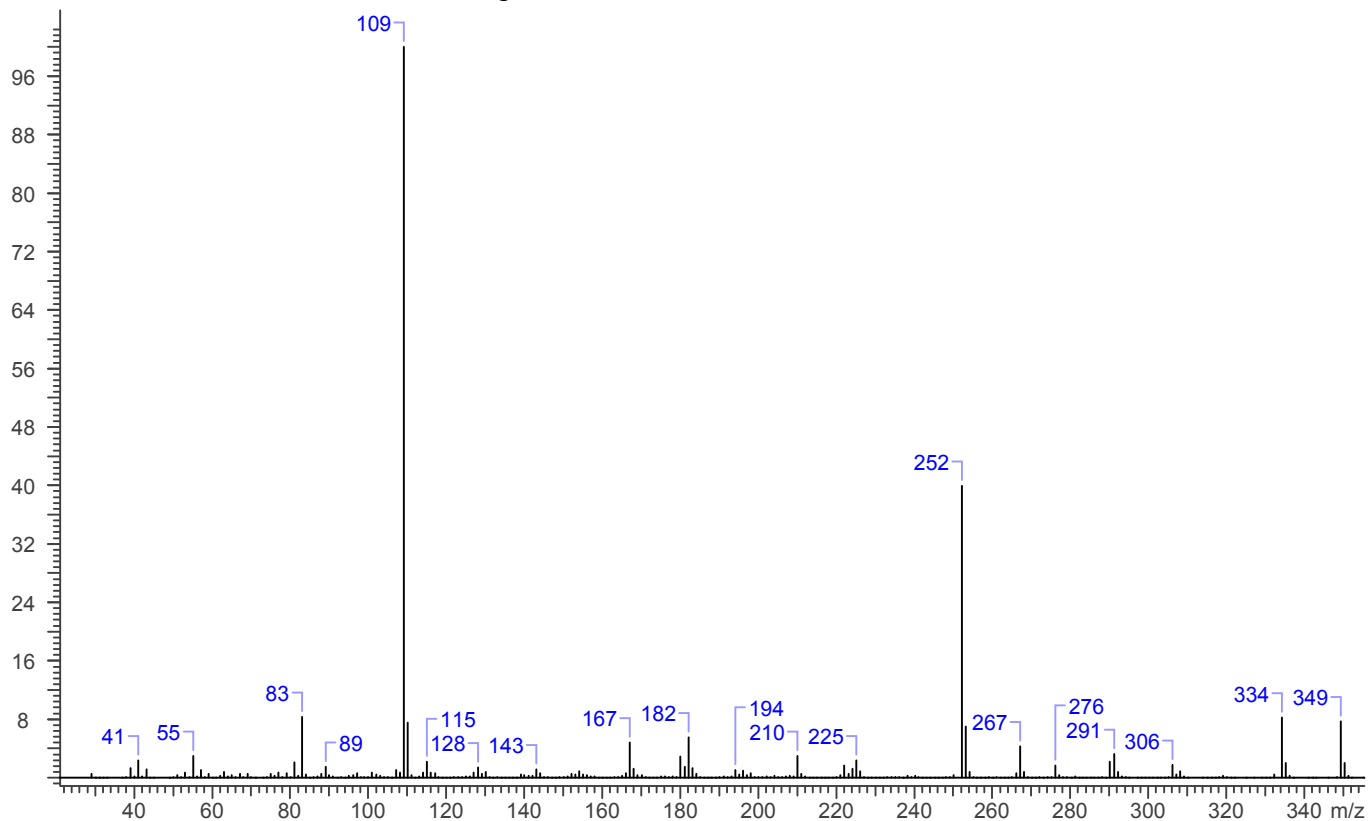
*Sample Preparation:* Dilute analyte ~3 mg/mL in chloroform.

**Instrument:** Agilent gas chromatograph operated in split mode with MS detector  
**Column:** HP-5 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 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:** 18.147 min; Rearrangement product 18.349 min

EI Mass Spectrum: FUB-144 Lot # 0455762-22



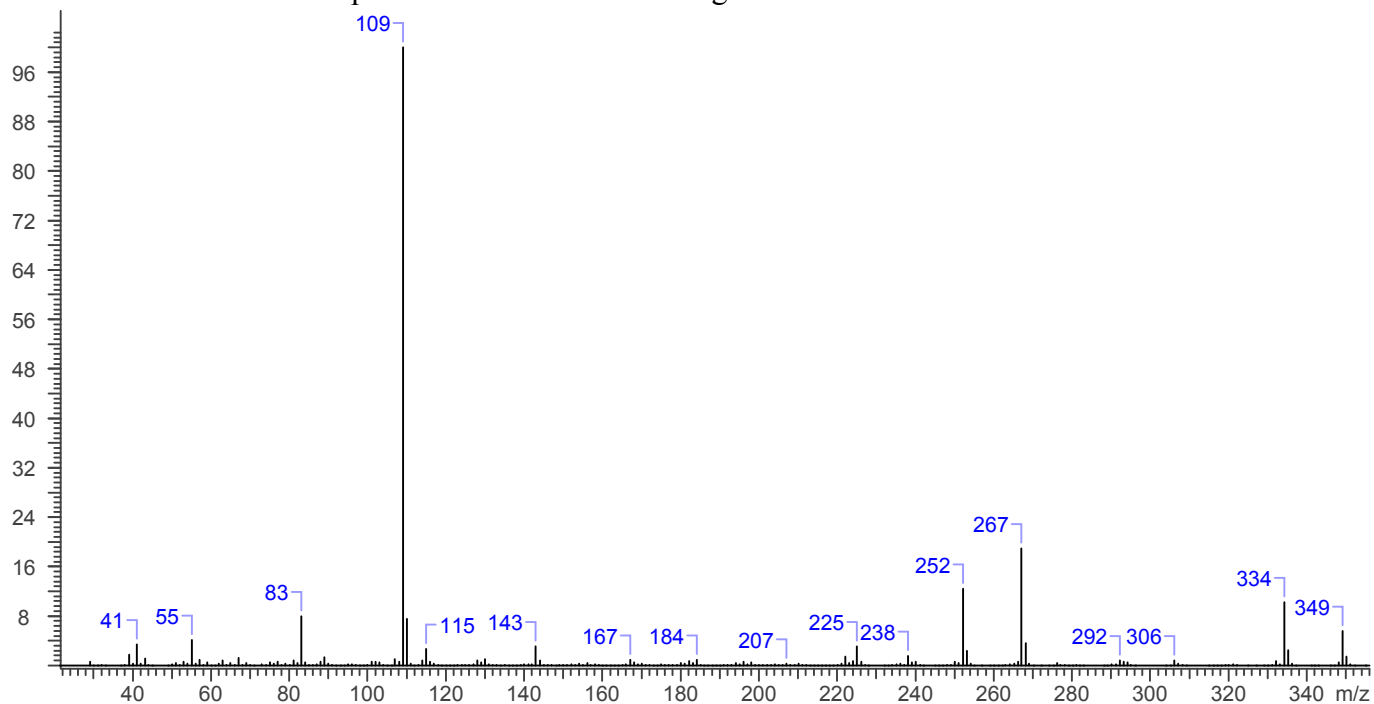


# FUB-144

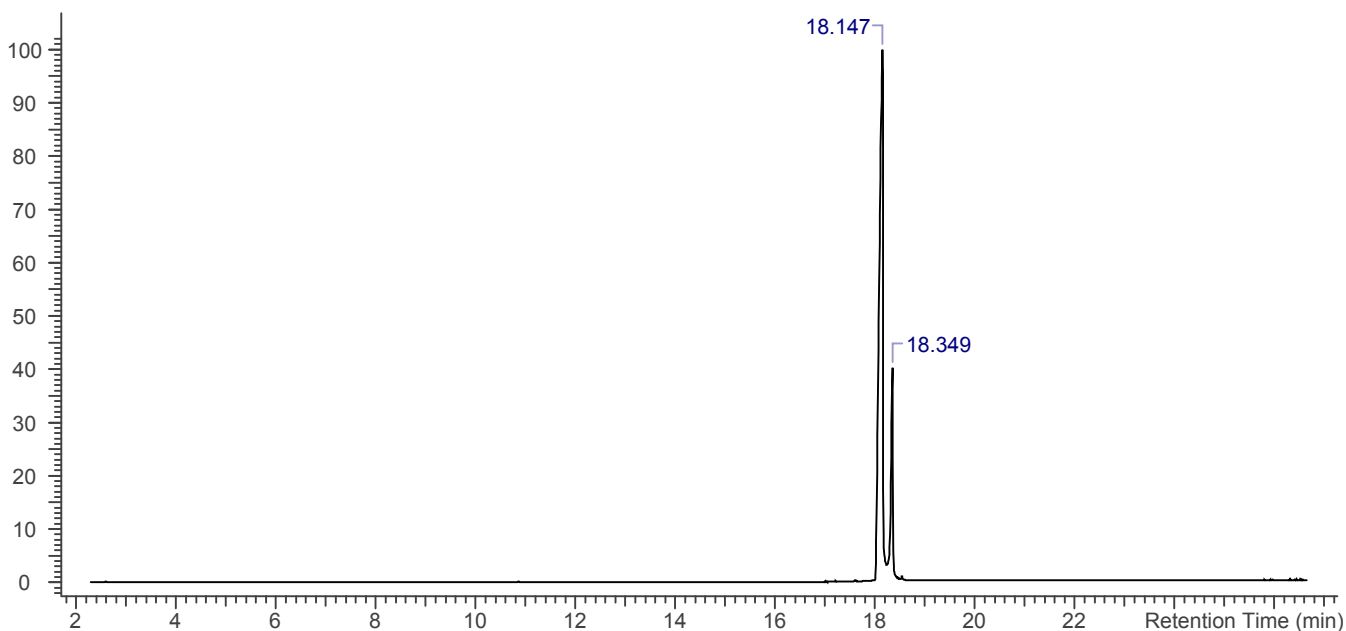


The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

EI Mass Spectrum: FUB-144 Rearrangement Product Lot # 0455762-22



TIC: FUB-144 Lot # 0455762-22



## GC/MS Analytical Observation:

The GC/MS TIC of FUB-144 shows two peaks with similar mass spectra (shown above). The major peak, having a retention time of 18.147 minutes, is FUB-144 while the other peak, with a retention time of 18.349 minutes, is a thermally induced rearrangement product of FUB-144. This rearrangement product is an artifact induced by the high temperatures of the GC injection port.



# FUB-144

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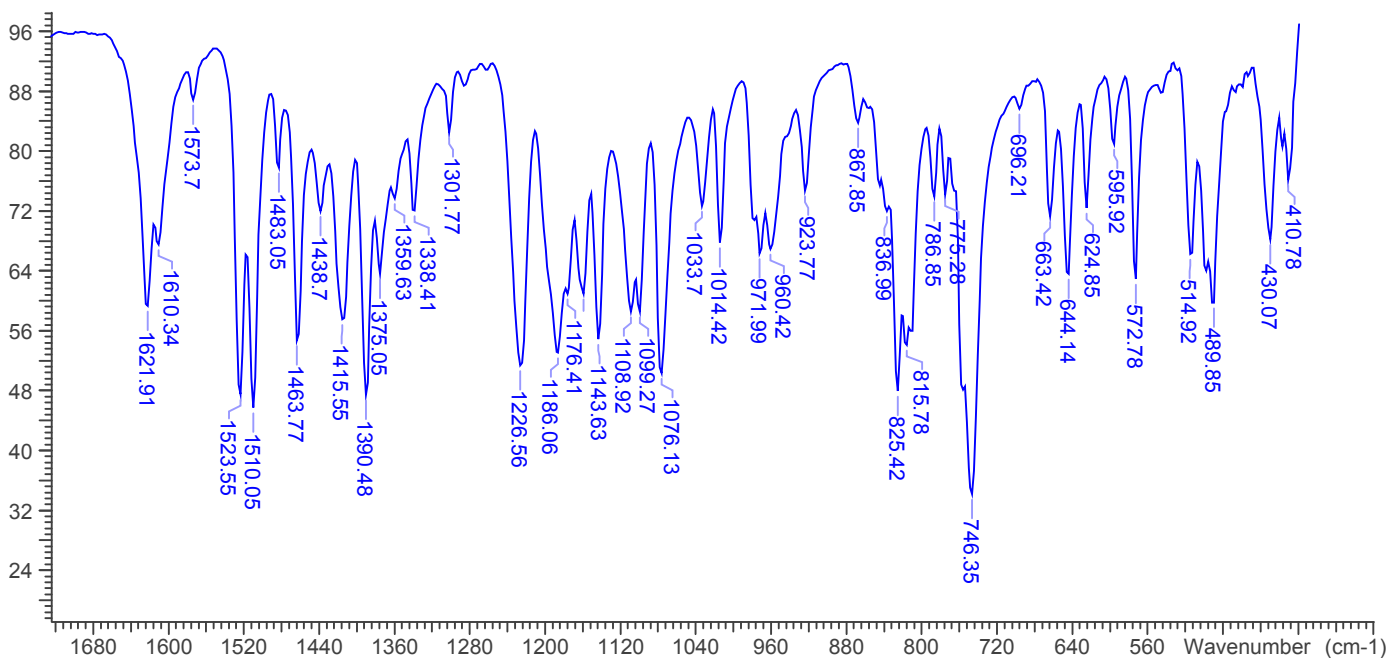
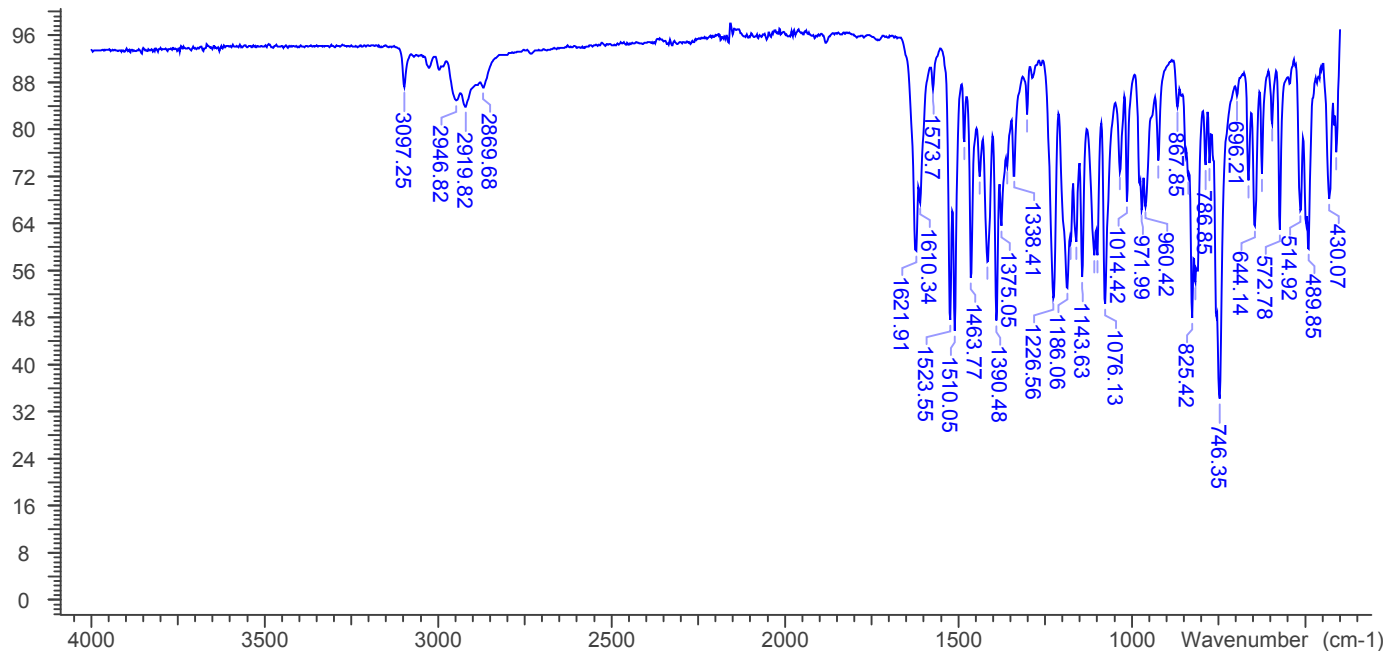


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (1 bounce)

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

FTIR ATR (Diamond, 1 Bounce): FUB-144 Lot # 0455762-22





**FUB-144**

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

[Forendex](#)