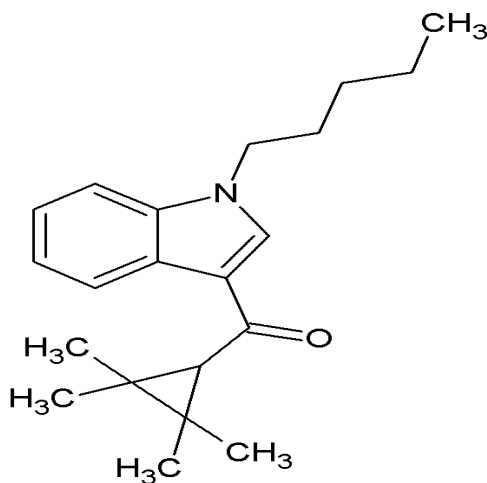




## UR-144



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-pentyl-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone
<b>CAS #:</b>	1199943-44-6
<b>Synonyms:</b>	KM-X1
<b>Source:</b>	DEA Reference Material Collection
<b>Appearance:</b>	White Powder
<b>UV<sub>max</sub>:</b>	Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>21</sub> H <sub>29</sub> NO	311	68.0



## UR-144

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### 3. QUALITATIVE DATA

#### 3.1 NUCLEAR MAGNETIC RESONANCE

##### Method NMR $\text{CDCl}_3$

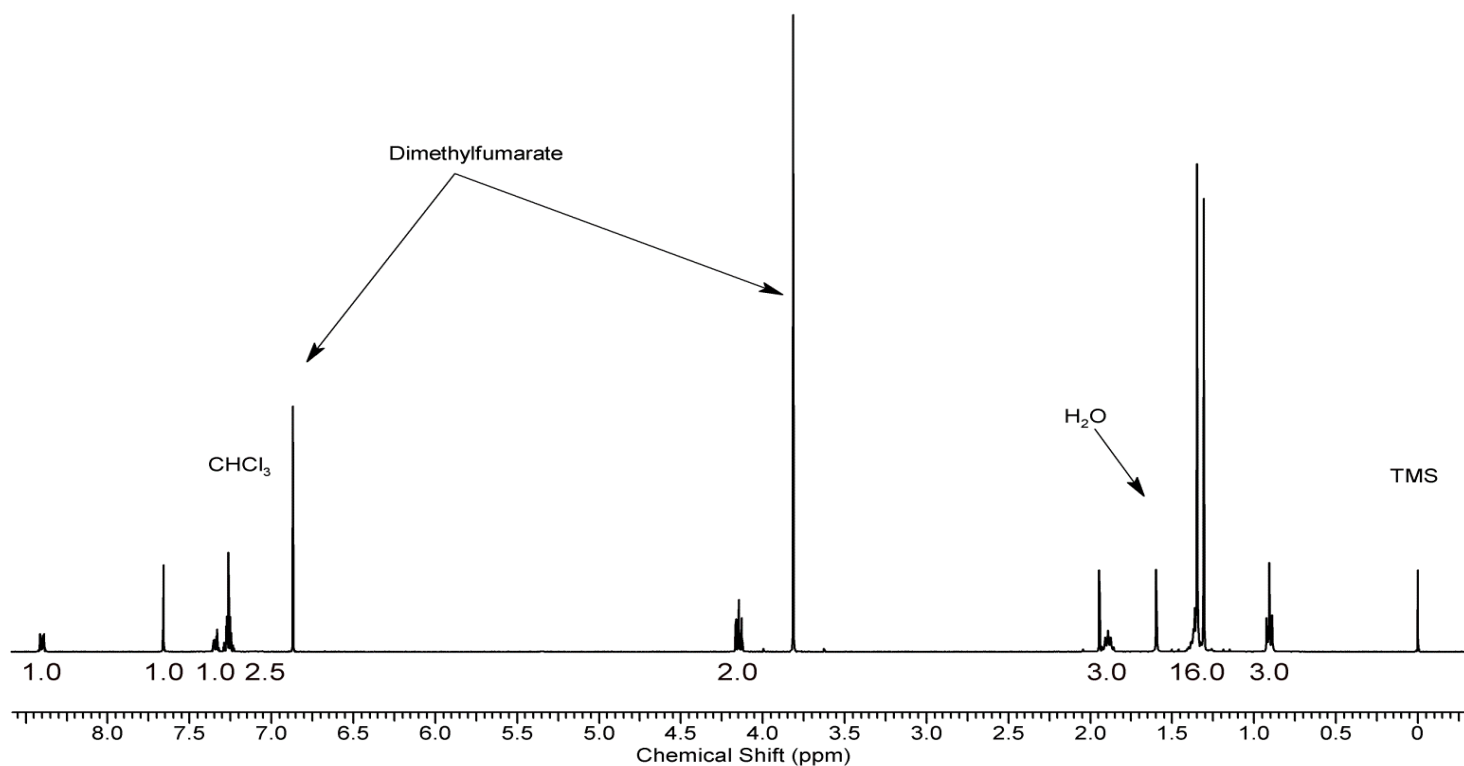
**Sample Preparation:** Dilute analyte to ~10 mg/mL in deuteriochloroform ( $\text{CDCl}_3$ ) containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

**Instrument:** Varian Mercury 400 MHz NMR spectrometer with proton detection probe

**Parameters:**

- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle:  $90^\circ$
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

$^1\text{H}$  NMR: UR-144 Lot # ALB214-11;  $\text{CDCl}_3$ ; 400MHz



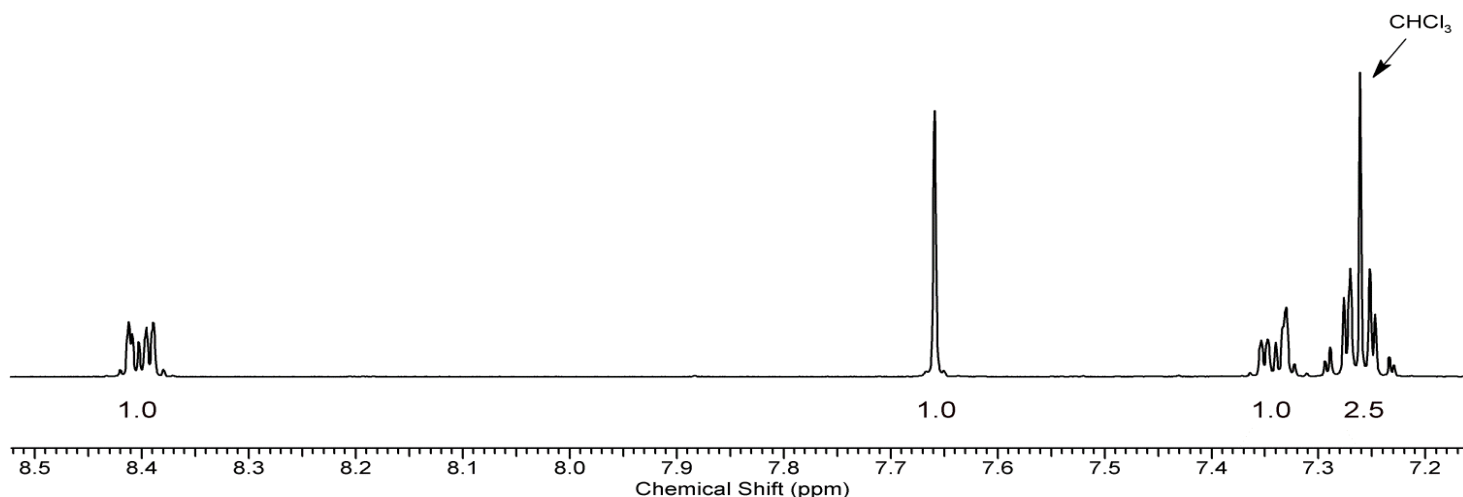


## UR-144

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$^1\text{H}$  NMR: UR-144 Lot # ALB214-11;  $\text{CDCl}_3$ ; 400MHz



### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute to ~1 mg/mL in MeOH

**Instrument:** Gas chromatograph operated in split mode with MS detector

**Column:** DB-1 MS or equivalent; 30m x 0.25mm x 0.25 $\mu\text{m}$

**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  $\mu\text{L}$  injected

**MS Parameters:**  
Mass scan range: 30-550 amu  
Threshold: 100  
Tune file: stune.u  
Acquisition mode: scan

**Retention Time:** UR-144 peak at 16.164 minutes; Rearrangement peak at 16.365 minutes



# UR-144

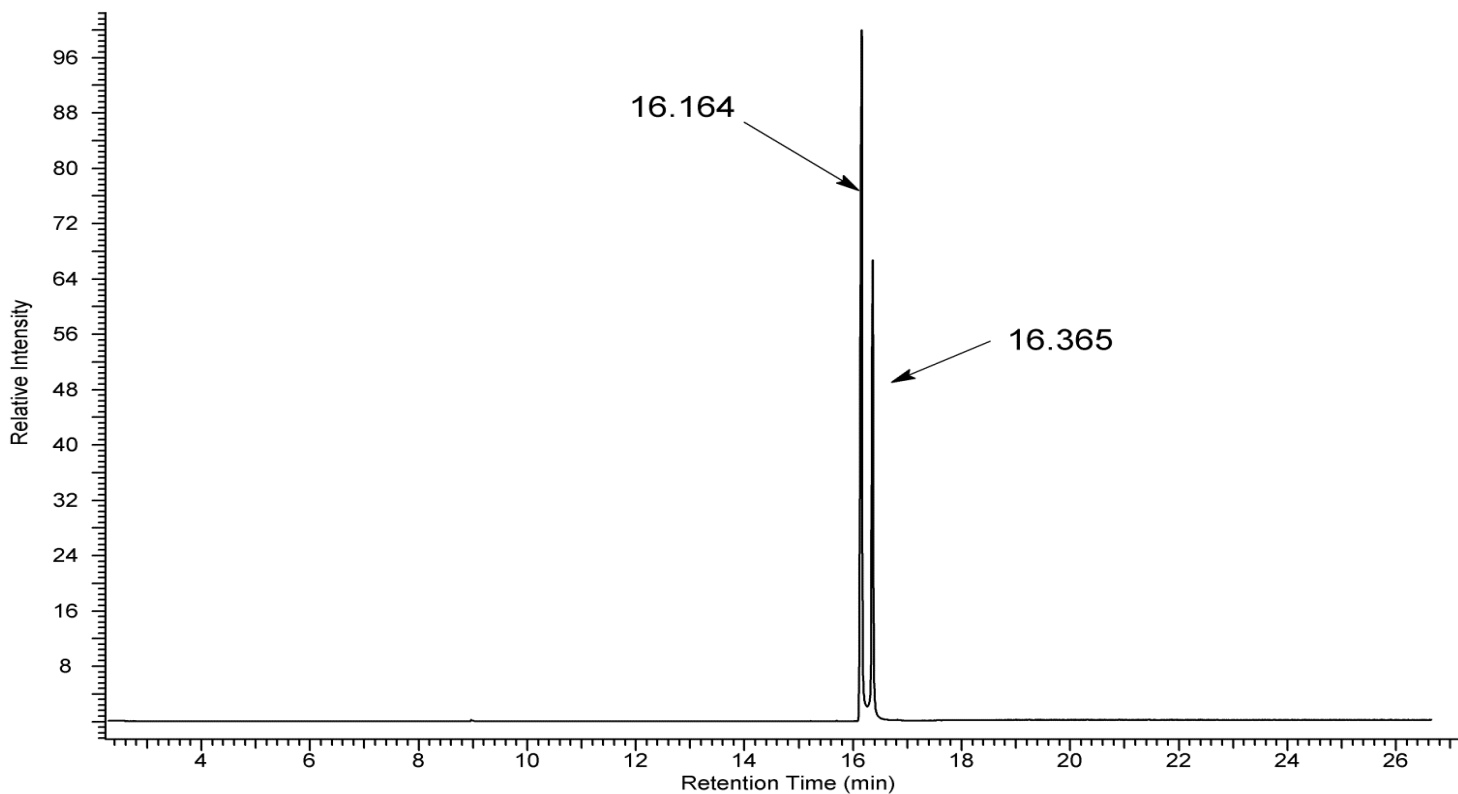


The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

## GC/MS Analytical Observation:

The GC/MS TIC of UR-144 shows two peaks with similar mass spectra (shown above). The major peak, having a retention time of 16.164 minutes, is UR-144 while the other peak, with a retention time of 16.365 minutes, is a thermally induced rearrangement product of UR-144. This rearrangement product is an artifact induced by the high temperatures of the GC injection port.

GC/MS TIC: UR-144 Lot # ALB214-11



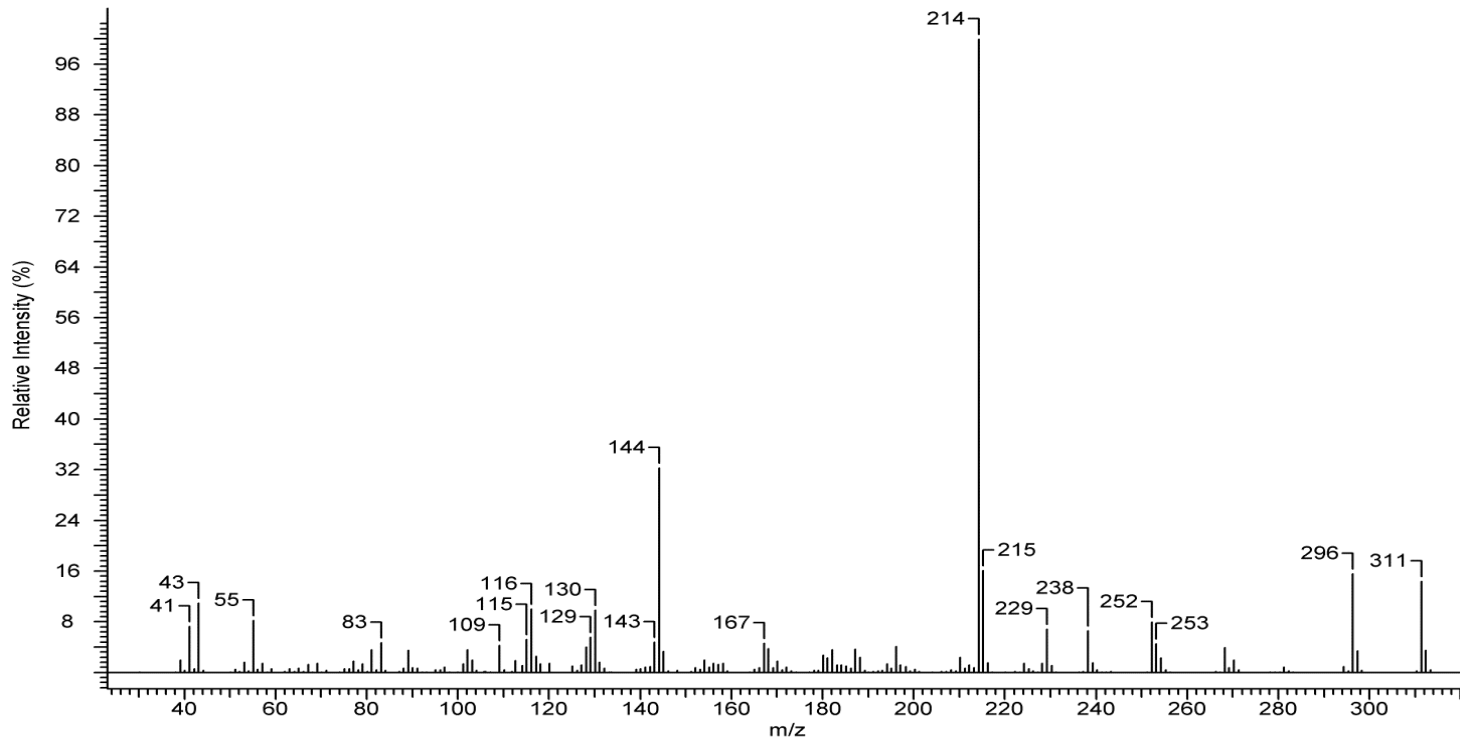


# UR-144

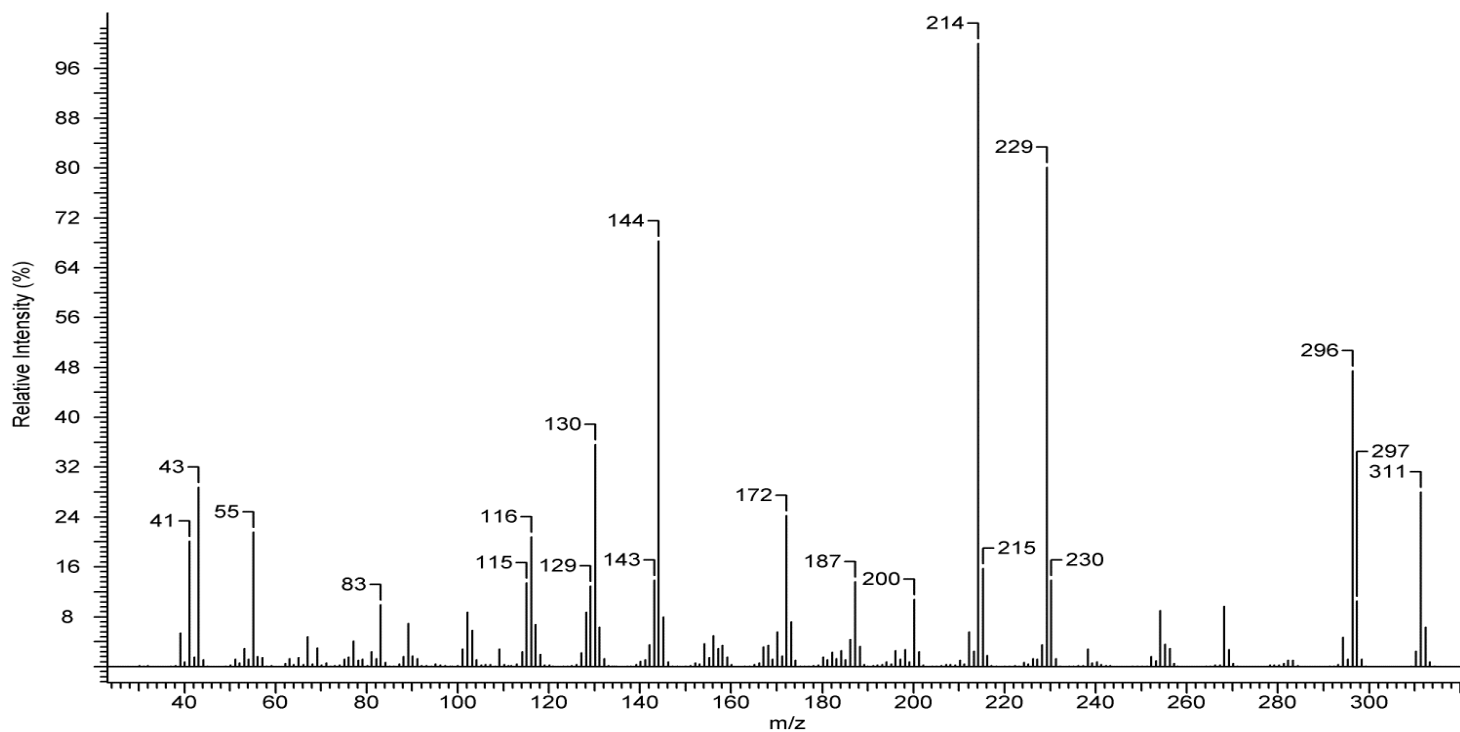
The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.



EI Mass Spectra: UR-144 Lot # ALB214-11



EI Mass Spectra: UR-144 Rearrangement Lot # ALB214-11





# UR-144

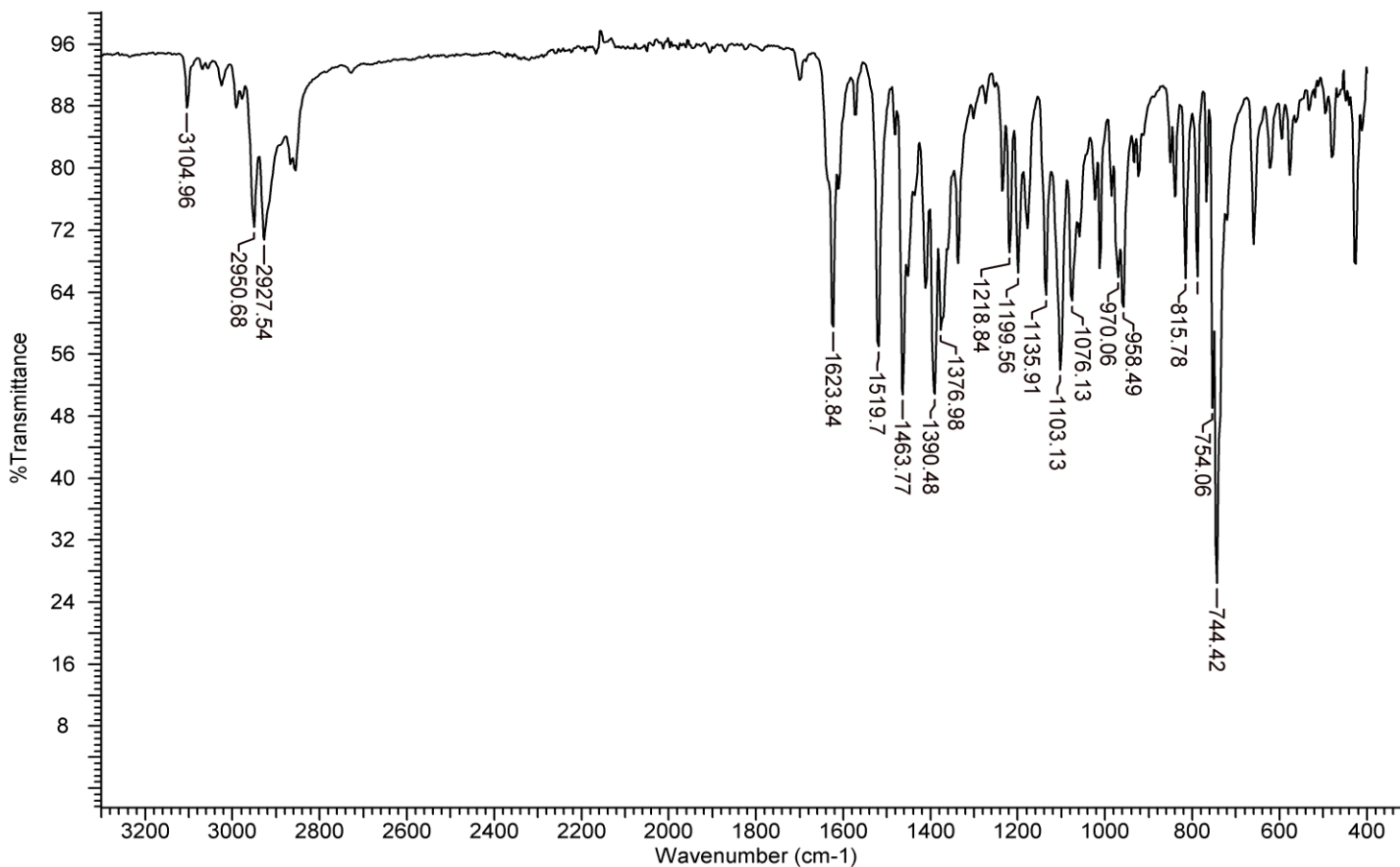


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## 3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)  
**Scan Parameters:** Number of scans: 32  
Number of background scans: 32  
Resolution:  $4\text{cm}^{-1}$   
Sample gain: 8  
Aperture: 150

FTIR: UR-144 Lot # ALB214-11



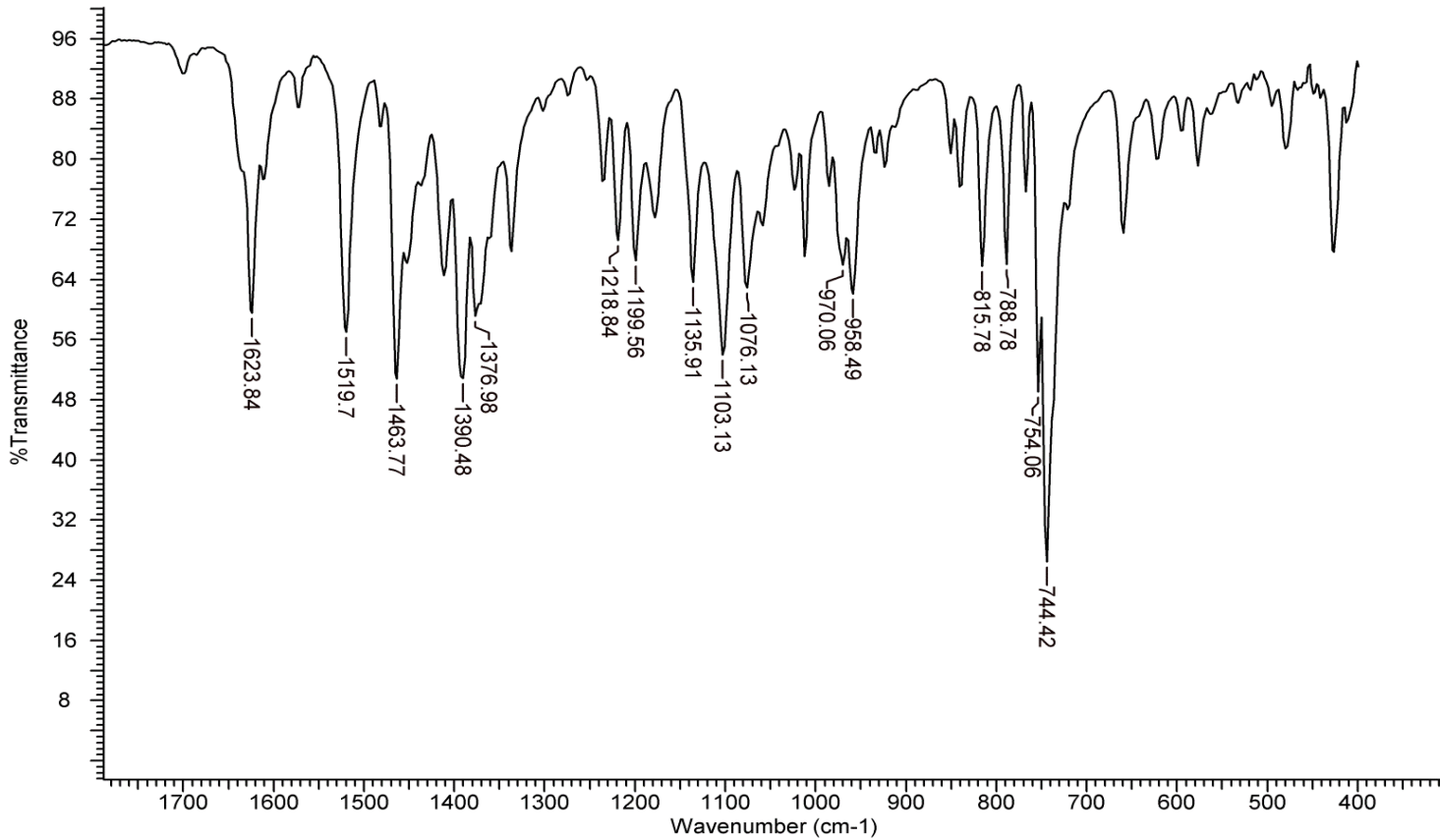


# UR-144



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FTIR: UR-144 Lot # ALB214-11



## 4. ADDITIONAL RESOURCES

[Forendex](#)

[Wikipedia](#)