1. GENERAL INFORMATION

**IUPAC Name:** (1-penty1-1H-indol-3-yl)(2,2,3,3-tetramethylcyclopropyl)methanone

**CAS #:** 1199943-44-6

**Synonyms:** KM-X1

**Source:** DEA Reference Material Collection

**Appearance:** White Powder

**UV max:** 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_{21}H_{29}NO</td>
<td>311</td>
<td>68.0</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterchloroform (CDCl₃) 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°
- 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

1H NMR: UR-144 Lot # ALB214-11; CDCl₅; 400MHz
UR-144

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

1H NMR: UR-144 Lot # ALB214-11; CDCl₃; 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 0.25µm

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 µL 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](image_url)
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 cm\(^{-1}\)
- Sample gain: 8
- Aperture: 150
UR-144
The Drug Enforcement Administration’s Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

4. ADDITIONAL RESOURCES

Forendex

Wikipedia