1. GENERAL INFORMATION

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

**CFR:** Not Scheduled (7/2013)

**CAS#:** Not Available

**Synonyms:** UR-144 N-heptyl analog

**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{33}NO</td>
<td>339</td>
<td>73.7</td>
</tr>
</tbody>
</table>

3. ADDITIONAL RESOURCES

No resources identified as of 8/26/13.
4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl$_3$

Sample Preparation: Dilute analyte to ~10 mg/mL in 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°
            Delay between pulses: 45 seconds

$^1$H NMR: Heptyl-UR-144 Lot # ALB 214-17; CDCl$_3$; 400 MHz
4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~1 mg/mL in 9:1 CHCl₃/MeOH.

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 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: Heptyl-UR-144: 16.87 min; Rearrangement: 17.05 min

EI Mass Spectrum: Heptyl-UR-144 Lot # ALB 214-17
**GC/MS Analytical Observation:**

The GC/MS TIC of Heptyl-UR-144 shows two peaks with similar mass spectra (shown above). The major peak, having a retention time of 16.87 minutes, is Heptyl-UR-144 while the other peak, with a retention time of 17.05 minutes, is a thermally induced rearrangement product of Heptyl-UR-144. This rearrangement product is an artifact induced by the high temperatures of the GC injection port.
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): Heptyl-UR-144 Lot # ALB 214-17