1. GENERAL INFORMATION

**IUPAC Name:** [1-(5-bromopentyl)-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)methanone

**CFR:** Not Scheduled (01/2013)

**CAS #:** Not Available

**Synonyms:** UR-144 N-(5-bromopentyl) analog

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**Kovat’s Index:** Pending

**UV\text{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_{28}BrNO</td>
<td>390</td>
<td>93.0</td>
</tr>
</tbody>
</table>
3. ADDITIONAL RESOURCES

No resources identified as of 12/28/2012.

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterochloroform (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: 5-Bromo-UR-144 Lot # 0440444-8; CDCl₃; 400 MHz
4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~4 mg/mL in CHCl₃.

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: DB-1 MS; 30m x .25mm x .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: 5-Bromo-UR-144 peak at 18.369 min; Rearrangement peak at 18.594 min
**GC/MS Analytical Observation:**

The GC/MS TIC of 5-Bromo-UR-144 shows two peaks with similar mass spectra (shown above). The major peak, having a retention time of 18.369 minutes, is 5-Bromo-UR-144 while the minor peak, with a retention time of 18.594 minutes, is a thermally induced rearrangement product of 5-Bromo-UR-144. This rearrangement product is an artifact induced by the high temperatures of the GC injection port.

The peak at 17.686 minutes is an impurity of 5-Bromo-UR-144.
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: 4cm⁻¹  
Sample gain: 8  
Aperture: 150