1. GENERAL INFORMATION

**IUPAC Name:** estra-4,9,11-triene-3,17-dione

**CAS#:** 4642-95-9

**Synonyms:** Trenavar

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**$UV_{max}(nm)$:** 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 ($^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutral</td>
<td>C18H20O2</td>
<td>268.35</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

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: $90^\circ$
- Delay between pulses: 45 seconds

$^1$HNMR: Trendione; Lot# RM-150319-01; CDCl$_3$; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~6 mg/mL in ether

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

**Column:**
DB-5 MS (or equivalent); 15m x 0.25 mm x 0.25 μm

**Carrier Gas:**
Helium at 1.5 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 280°C at 12 °C/min
3) Hold final temperature for 9.0 min

**Injection Parameters:**
- Split Ratio = 25:1
- 1 μL injected

**MS Parameters:**
- Mass scan range: 30-550 amu
- Tune file: stune.u
- Threshold: 150
- Acquisition mode: scan

**Retention Time:**
13.47 min

EI Mass Spectrum: Trendione; Lot# RM-150319-01
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⁻¹
- Sample gain: 8
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): Trendione; Lot# RM-150319-01