Product Name: Calcipotriol  
Catalog No.: 2700  
Batch No.: 7  

CAS Number: 112965-21-6  
IUPAC Name: \((1\alpha,3\beta,5Z,7E,22E,24S)-24\text{-Cyclopropyl-9,10-secochola-5,7,10(19),22-tetraene-1,3,24-triol} \)

1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** \(C_{27}H_{40}O_3.\frac{1}{4}H_2O\)
- **Batch Molecular Weight:** 417.1
- **Physical Appearance:** White solid
- **Solubility:** DMSO to 100 mM, ethanol to 100 mM
- **Storage:** Store at -20°C

2. ANALYTICAL DATA

- **HPLC:** Shows 98.8% purity
- **\(^1H\) NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**
  
<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>77.75</td>
<td>76.95</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>9.79</td>
<td>10.02</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
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</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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Description:
Calcipotriol is a vitamin D₃ analog that displays minimal effects on calcium homeostasis. Regulates cell differentiation and proliferation; exhibits antiproliferative activity against human HL-60, HL60/MX2, keratinocytes, MCF-7, T47D, SCC-25, and mouse WEHI-3 cancer cell lines. Calcipotriol suppresses skin cancer development in mice in a thymic stromal lymphopoietin (TSLP)-dependent manner. Calcipotriol promotes the differentiation of keratinocytes. In human T cells and in psoriatic skin, Calcipotriol increases IL-10 secretion, induces secretion of type 2 cytokines by T cells and modulates the differentiation of dendritic cells and T cells. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:
Batch Molecular Formula: \(\text{C}_{27}\text{H}_{40}\text{O}_{3}\cdot\frac{1}{4}\text{H}_{2}\text{O}\)
Batch Molecular Weight: 417.1
Physical Appearance: White solid
Minimum Purity: \(\geq 98\%\)

Storage:
Store at -20°C
CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 100 mM

Stability and Solubility Advice:
Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:
SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.
SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References: