**Product Name:** Simvastatin  
**Catalog No.:** 1965  
**Batch No.:** 3  
**CAS Number:** 79902-63-9  
**IUPAC Name:** (1S,3R,7S,8S,8aR)-1,2,3,7,8,8a-Hexahydro-3,7-dimethyl-8-{2-[(2R,4R)-tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl]ethyl}-1-naphthalenyly-2,2-dimethyl butanoate

1. **PHYSICAL AND CHEMICAL PROPERTIES**

   - **Batch Molecular Formula:** C_{25}H_{38}O_{5}  
   - **Batch Molecular Weight:** 418.57  
   - **Physical Appearance:** White solid  
   - **Solubility:** DMSO to 50 mM, ethanol to 75 mM  
   - **Storage:** Desiccate at -20°C  
   - **Batch Molecular Structure:**

![Molecular Structure Image]

2. **ANALYTICAL DATA**

   - **HPLC:** Shows 99.2% purity  
   - **\(^1\)H NMR:** Consistent with structure  
   - **Mass Spectrum:** Consistent with structure  
   - **Optical Rotation:** \([\alpha]_D = +293.6\) (Concentration = 0.5, Solvent = Acetonitrile)  
   - **Microanalysis:** Carbon Hydrogen Nitrogen  
     - Theoretical: 71.74, 9.15  
     - Found: 71.8, 9.3

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Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**  
HMG-CoA reductase inhibitor; decreases levels of low density lipoprotein. Has multiple biological effects including bone formation stimulation, inhibition of smooth muscle cell proliferation and migration, induction of ferroptosis, and anticancer and anti-inflammatory activity. Inactive lactone prodrug of simvastatin hydroxy acid, naturally bioactivated in vivo following oral administration.

**Physical and Chemical Properties:**  
Batch Molecular Formula: C₄₂H₃₈O₇  
Batch Molecular Weight: 418.57  
Physical Appearance: White solid  
Minimum Purity: ≥98%

**Solubility & Usage Info:**  
DMSO to 50 mM  
ethanol to 75 mM

**Storage:** Desiccate at -20°C

**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:**  