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TOCRIS

Print Date: Jul 31st 2023

Certificate of Analysis

www.tocris.com

Product Name: **Simvastatin** **Catalog No.: 1965** **Batch No.: 3**

CAS Number: 79902-63-9

IUPAC Name: (1*S*,3*R*,7*S*,8*S*,8a*R*)-1,2,3,7,8,8a-Hexahydro-3,7-dimethyl-8-[2-[(2*R*,4*R*)-tetrahydro-4-hydroxy-6-oxo-2*H*-pyran-2-yl] ethyl]-1-naphthalenyly-2,2-dimethyl butanoate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{38}O_5$

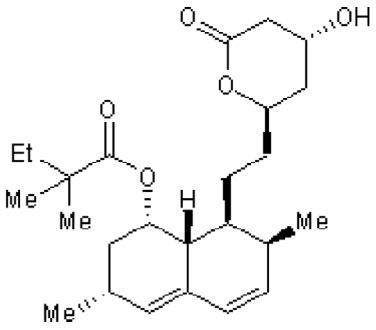
Batch Molecular Weight: 418.57

Physical Appearance: White solid

Solubility: DMSO to 50 mM
ethanol to 75 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



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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Description:

Simvastatin is a HMG-CoA reductase inhibitor; decreases levels of low density lipoprotein. Simvastatin is also an AMPK activator. Has multiple biological effects including bone formation stimulation, inhibition of smooth muscle cell proliferation and migration, induction of ferroptosis, inhibition of autophagy, and anticancer and anti-inflammatory activity. Inactive lactone prodrug of simvastatin hydroxy acid, naturally bioactivated in vivo following oral administration.Simvastatin acts synergistically with ABL allosteric inhibitors GNF 5 (Cat. No. 1965) to enhance apoptosis of metastatic lung cancer cells in mice. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

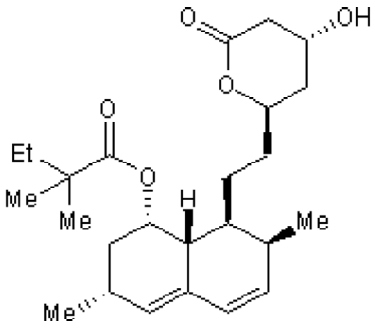
Batch Molecular Formula: $C_{25}H_{38}O_5$

Batch Molecular Weight: 418.57

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at -20°C

Solubility & Usage Info:

DMSO to 50 mM
ethanol to 75 mM

PLEASE NOTE - Simvastatin (SV) is an inactive lactone prodrug of simvastatin hydroxy acid (SVA) the active form of the compound. Simvastatin administered orally is naturally bioactivated by the liver and requires no further modification. If simvastatin is to be administered by another route or used *in vitro* then it requires manual activation by treatment with NaOH. To activate the compound dissolve 50mg in 1ml of warm (50°C) ethanol and add 0.813ml of 1N NaOH. Leave for 30 minutes to allow conversion of the simvastatin to the active acid form, the compound may be stored at -20°C in this format for up to 1 month. Adjust pH to 7.2 with small quantities of 1N HCl prior to use.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Dehnavi *et al* (2021) Targeting AMPK by statins: A potential therapeutic approach. Drugs ***81*** 923. PMID: 33939118.

Luttman *et al* (2021) ABL allosteric inhibitors synergize with statins to enhance apoptosis of metastatic lung cancer cells. Cell Rep. ***37*** 109880. PMID: 34706244.

Kaushal *et al* (2003) Potential anticancer effects of STAT: fact or fiction? Endothelium ***10*** 49. PMID: 12699077.

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