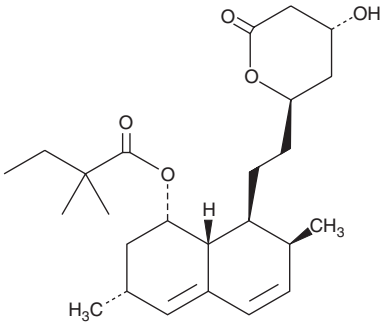
PRODUCT INFORMATION

Simvastatin

Item No. 10010344

CAS Registry No.:	79902-63-9
Formal Name:	2,2-dimethyl-1S,2,3R,7S,8S,8aR-hexahydro-3,7-dimethyl-8-[2-[(2R,4R)-tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl]ethyl]-1-naphthalenyl ester, butanoic acid
Synonyms:	MK-733, SVA
MF:	$C_{25}H_{38}O_5$
FW:	418.6
Purity:	≥98%
UV/Vis.:	λ_{max}: 238 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Simvastatin is supplied as a crystalline solid. A stock solution may be made by dissolving the simvastatin in the solvent of choice. Simvastatin is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of simvastatin in ethanol is approximately 20 mg/ml and approximately 30 mg/ml in DMSO and DMF.

Simvastatin is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, simvastatin should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Simvastatin has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Simvastatin is a competitive inhibitor of HMG-CoA reductase (K_i = 0.12 nM).[1] Simvastatin reduces plasma cholesterol levels in rats and dogs when administered at doses of 1.2 and 8 mg/kg, respectively.[2] Simvastatin suppresses TNF-induced NF-κB activation (IC_{50} = ~13 µM) and potentiates apoptosis in human myeloid leukemia cells.[3] It also inhibits glutathione peroxidase 4 (GPX4) activity, increases malondialdehyde (MDA) levels, and induces ferroptosis in MDA-MB-231 and MCF-7 breast cancer cells.[4] Formulations containing simvastatin have been used in the treatment of dyslipidemias.

References

1. Corsini, A., Maggi, F.M., and Catapano, A.L. Pharmacology of competitive inhibitors of HMG-CoA reductase. *Pharmacol. Res.* **31(1)**, 9-27 (1995).
2. Chao, Y., Chen, J.S., Hunt, V.M., *et al.* Lowering of plasma cholesterol levels in animals by lovastatin and simvastatin. *Eur. J. Clin. Pharmacol.* **40(Suppl 1)**, S11-S14 (1991).
3. Ahn, K.S., Sethi, G., and Aggarwal, B.B. Reversal of chemoresistance and enhancement of apoptosis by statins through down-regulation of the NF-κB pathway. *Biochem. Pharmacol.* **75(4)**, 907-913 (2008).
4. Lu, S., Shao, N.-Y., Bi, J., *et al.* Abstract PS18-44: Simvastatin induces ferroptosis in breast cancer cells by inhibiting GPX4 and sensitizes chemotherapy. *San Antonio Breast Cancer Virtual Symposium* (2021).

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