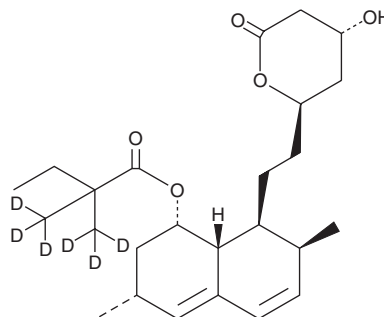


PRODUCT INFORMATION



Simvastatin-d₆ Item No. 22181

CAS Registry No.: 1002347-71-8
Formal Name: 2,2-di(methyl-d₃)-butanoic acid, (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-naphthalenyl ester
Synonym: SVA-d₆
MF: C₂₅H₃₂D₆O₅
FW: 424.6
Chemical Purity: ≥95% (Simvastatin)
Deuterium Incorporation: ≥99% deuterated forms (d₁-d₆); ≤1% d₀
UV/Vis.: λ_{max}: 230, 237, 246 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-d₆ is intended for use as an internal standard for the quantification of simvastatin (Item Nos. 10010344 | 10010345) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated versus unlabeled).

Simvastatin-d₆ is supplied as a crystalline solid. A stock solution may be made by dissolving the simvastatin-d₆ in the solvent of choice, which should be purged with an inert gas. Simvastatin-d₆ is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of simvastatin-d₆ in ethanol is approximately 20 mg/ml and approximately 30 mg/ml in DMSO and DMF.

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 ($IC_{50} = \sim 13$ 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. *2020 San Antonio Breast Cancer Virtual Symposium* (2021).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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CAYMAN CHEMICAL

1180 EAST ELLSWORTH RD

ANN ARBOR, MI 48108 · USA

PHONE: [800] 364-9897

[734] 971-3335

FAX: [734] 971-3640

CUSTSERV@CAYMANCHEM.COM

WWW.CAYMANCHEM.COM