

Product Name: Simvastatin - d₆

Catalog No.: 5536

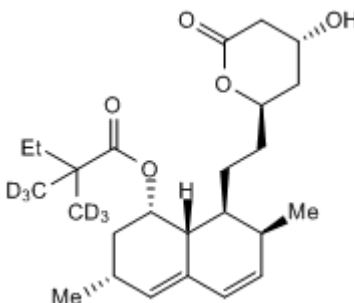
Batch No.: 1

CAS Number: 1002347-71-8

IUPAC Name: (1*S*,3*R*,7*S*,8*S*,8*aR*)-1,2,3,7,8,8*a*-Hexahydro-3,7-dimethyl-8-[2-[(2*R*,4*R*)-tetrahydro-4-hydroxy-6-oxo-2*H*-pyran-2-yl]ethyl]-1-naphthalenyl-2,2-di(methyl-d₃) butanoate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₅ H ₃₂ D ₆ O ₅
Batch Molecular Weight:	424.61
Physical Appearance:	White solid
Solubility:	ethanol to 75 mM DMSO to 50 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

Isotopic Purity:	99.0% D
HPLC:	Shows 99.6% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure

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

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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-naphthalenyl-2,2-di(methyl-d₃) butanoate

Description:

Deuterated simvastatin (Cat. No. 1965).

Physical and Chemical Properties:

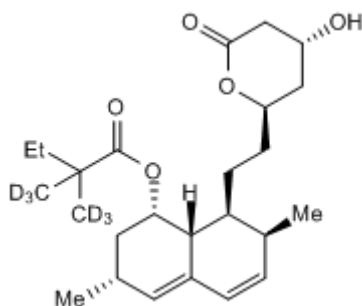
Batch Molecular Formula: C₂₅H₃₂D₆O₅

Batch Molecular Weight: 424.61

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

ethanol to 75 mM

DMSO to 50 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. 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.

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