Simvastatin acid ammonium

Cat. No.: HY-119695A

CAS No.: 139893-43-9

Molecular Formula: $C_{25}H_{43}NO_6$

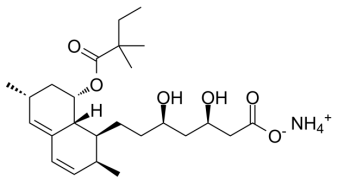
Molecular Weight: 453.61

Target: HMG-CoA Reductase (HMGCR); Reactive Oxygen Species

Pathway: Metabolic Enzyme/Protease; Immunology/Inflammation; NF-κB

Storage: 4°C, sealed storage, away from moisture

* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 11.11 mg/mL (24.49 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2045 mL	11.0227 mL	22.0454 mL
	5 mM	0.4409 mL	2.2045 mL	4.4091 mL
	10 mM	0.2205 mL	1.1023 mL	2.2045 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1.11 mg/mL (2.45 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1.11 mg/mL (2.45 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.11 mg/mL (2.45 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Simvastatin acid (Tenivastatin) ammonium is a potent HMG-CoA reductase (HMGCR) inhibitor. Simvastatin acid ammonium reduces Indoxyl sulfate-mediated reactive oxygen species (ROS) production in human cardiomyocytes. Simvastatin acid ammonium can also modulates OATP3A1 expression in cardiomyocytes and HEK293 cells transfected with the OATP3A1 gene[1][2].

IC_{50} & Target

HMG-CoA reductase, Reactive oxygen species[1][2]

In Vitro

Simvastatin acid (0.1-20 μM; 24 h) significantly decreases ROS production between 8.9% and 43% in Indoxyl sulfate-treated hCM cells[2].

Simvastatin acid (0.1-20 μM; 24 h) alters the protein expression of OATP3A1 in hCMs and OATP3A1-expressing HEK293 cells[2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Western Blot Analysis[2]

Cell Line:	hCM and HEK293 (transfected with OATP3A1)
Concentration:	0.1, 1, 10 and 20 μM
Incubation Time:	24 h
Result:	Decreased 1.5% to 90% in OATP3A1 expression with a dose-dependent manner in both hCMs and OATP3A1-expressing cells.

REFERENCES

[1]. Eduardo Filipe Oliveira, et al. HMG-CoA Reductase inhibitors: an updated review of patents of novel compounds and formulations (2011-2015). Expert Opin Ther Pat. 2016 Nov;26(11):1257-1272.

[2]. Atilano-Roque A, et al. Characterization of simvastatin acid uptake by organic anion transporting polypeptide 3A1 (OATP3A1) and influence of drug-drug interaction. Toxicol In Vitro. 2017 Dec;45(Pt 1):158-165.

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