(3S,5S)-Atorvastatin

Cat. No.: HY-B0589C

CAS No.: 501121-34-2

Molecular Formula: $C_{33}H_{35}FN_2O_5$

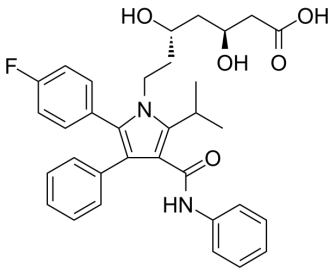
Molecular Weight: 558.64

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (223.76 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.7901 mL	8.9503 mL	17.9006 mL
	5 mM	0.3580 mL	1.7901 mL	3.5801 mL
	10 mM	0.1790 mL	0.8950 mL	1.7901 mL

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

BIOLOGICAL ACTIVITY

Description

(3S,5S)-Atorvastatin is a inactive enantiomer of Atorvastatin. (3S,5S)-Atorvastatin can activate pregnane X receptor (PXR). Atorvastatin is an orally active HMG-CoA reductase inhibitor, has the ability to effectively decrease blood lipids[1][2].

IC_{50} & Target

Pregnane X receptor (PXR)[1]

In Vitro

Atorvastatin and its inactive enantiomer (3S,5S)-Atorvastatin increases CYP2B and CYP3A mRNA content with equal ability[1].

(3S,5S)-Atorvastatin in 100 μM concentrations induces luciferase activity with an EC_{50} of 12.4 μM[2].

Addition of (3S,5S)-Atorvastatin to the 2-formylphenylboronicacid (FPBA)/l-tryptophanol mixture induces an intensity enhancement of l-tryptophanol florescence[3].

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

REFERENCES

[1]. Thomas A Kocarek, et al. Regulation of CYP2B6 and CYP3A Expression by Hydroxymethylglutaryl Coenzyme A Inhibitors in Primary Cultured Human Hepatocytes. Drug Metab Dispos. 2002 Dec;30(12):1400-5.

[2]. Martina Korhonova, et al. Optical Isomers of Atorvastatin, Rosuvastatin and Fluvastatin Enantiospecifically Activate Pregnane X Receptor PXR and Induce CYP2A6, CYP2B6 and CYP3A4 in Human Hepatocytes. PLoS One. 2015 Sep 14;10(9):e0137720.

[3]. Elena G Shcherbakova , et al. High-Throughput Assay for Enantiomeric Excess Determination in 1,2- And 1,3-Diols and Direct Asymmetric Reaction Screening. Chemistry. 2017 Jul 26;23(42):10222-10229.

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