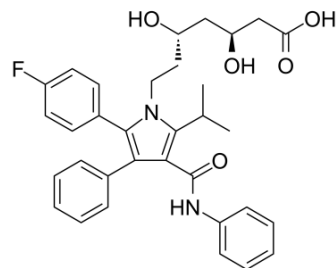


(3S,5S)-Atorvastatin

Cat. No.:	HY-B0589C		
CAS No.:	501121-34-2		
Molecular Formula:	C ₃₃ H ₃₅ FN ₂ O 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	6 months
		-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

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

Concentration	Mass		
	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 an 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]}.

IC₅₀ & 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 EC₅₀ of 12.4 μM^[2].

Addition of (3S,5S)-Atorvastatin to the 2-formylphenylboronic acid (FPBA)/L-tryptophanol mixture induces an intensity enhancement of L-tryptophanol fluorescence^[3].

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

REFERENCES

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- [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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Caution: Product has not been fully validated for medical applications. For research use only.

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