Atorvastatin-d_5 hemicalcium

Cat. No.: HY-B0589S

CAS No.: 222412-82-0

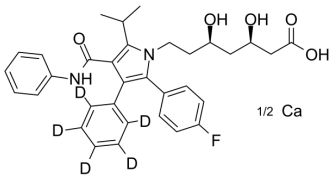
Molecular Formula: $C_{33}H_{30}D_5FN_2O_5.1/2Ca$

Molecular Weight: 583.71

Target: HMG-CoA Reductase (HMGCR); Autophagy

Pathway: Metabolic Enzyme/Protease; Autophagy

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

DMF : ≥ 25 mg/mL (42.83 mM)
DMSO : ≥ 15 mg/mL (25.70 mM)
Ethanol : ≥ 0.5 mg/mL (0.86 mM)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Concentration \ Solvent \ Mass	1 mg	5 mg	10 mg
1 mM	1.7132 mL	8.5659 mL	17.1318 mL
5 mM	0.3426 mL	1.7132 mL	3.4264 mL
10 mM	0.1713 mL	0.8566 mL	1.7132 mL

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

BIOLOGICAL ACTIVITY

Description

Atorvastatin-d_5 (hemicalcium) is the deuterium labeled Atorvastatin. Atorvastatin hemicalcium is an orally active HMG-CoA reductase inhibitor, has the ability to effectively decrease blood lipids. Atorvastatin hemicalcium inhibits human SV-SMC proliferation and invasion with IC50s of 0.39 μM and 2.39 μM, respectively[1][2][3].

In Vitro

Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-216.

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[3]. Santodomingo-Garzón T, et al. Atorvastatin inhibits inflammatory hypernociception. Br J Pharmacol. 2006 Sep;149(1):14-22.

[4]. Turner NA, et al. Comparison of the efficacies of five different statins on inhibition of human saphenous vein smooth muscle cell proliferation and invasion. J Cardiovasc Pharmacol. 2007 Oct;50(4):458-61.

[5]. Song XJ, et al. Atorvastatin inhibits myocardial cell apoptosis in a rat model with post-myocardial infarction heart failure by downregulating ER stress response. Int J Med Sci. 2011;8(7):564-72.

[6]. Li Y, et al. Inhibition of endoplasmic reticulum stress signaling pathway: A new mechanism of statins to suppress the development of abdominal aortic aneurysm. PLoS One. 2017 Apr 3;12(4):e0174821.

[7]. Ming-Bai Hu, et al. Atorvastatin induces autophagy in MDA-MB-231 breast cancer cells. Ultrastruct Pathol. Sep-Oct 2018;42(5):409-415.

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