Product Data Sheet

Simvastatin acid-d₆ ammonium

Cat. No.: HY-119695AS Molecular Formula: $C_{25}H_{37}D_6NO_6$ Molecular Weight: 459.65

Target: Endogenous Metabolite; Isotope-Labeled Compounds

Pathway: Metabolic Enzyme/Protease; Others

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

BIOLOGICAL ACTIVITY

Description	Simvastatin acid- d_6 (ammonium) mis the deuterium labeled Simvastatin acid ammonium. Simvastatin ammonium is an active metabolite of simvastatin lactone mediated by CYP3A4/5 in the intestinal wall and liver (pKa=5.5). Simvastatin ammonium reduces indoxyl sulfate-mediated reactive oxygen species and modulates OATP3A1 expression in cardiomyocytes and HEK293 cells transfected with the OATP3A1 gene[1].
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.

[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.

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

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