

PRODUCT INFORMATION



Atorvastatin lactone-d₅

Item No. 35171

Formal Name: 5-(4-fluorophenyl)-1-(2-((2R,4R)-4-hydroxy-6-oxotetrahydro-2H-pyran-2-yl)ethyl)-2-isopropyl-N-phenyl-4-(phenyl-d₅)-1H-pyrrole-3-carboxamide

MF: C₃₃H₂₈D₅FN₂O₄

FW: 545.7

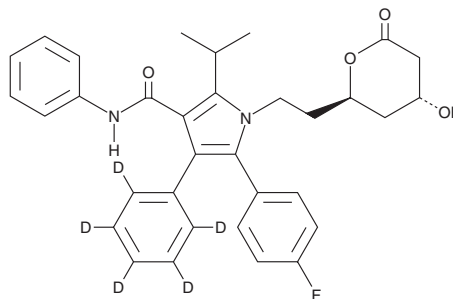
Chemical Purity: ≥95% (Atorvastatin lactone)

Deuterium Incorporation: ≥99% deuterated forms (d₁-d₅); ≤1% d₀

Supplied as: A solid

Storage: -20°C

Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Atorvastatin lactone-d₅ is intended for use as an internal standard for the quantification of atorvastatin lactone (Item No. 20951) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated versus unlabeled).

Atorvastatin lactone-d₅ is supplied as a solid. A stock solution may be made by dissolving the atorvastatin lactone-d₅ in the solvent of choice, which should be purged with an inert gas. Atorvastatin lactone-d₅ is soluble in acetonitrile and methanol.

Description

Atorvastatin lactone is an active metabolite of the HMG-CoA reductase inhibitor atorvastatin.^{1,2} It is formed from atorvastatin by the UDP-glucuronosyltransferase (UGT) isoforms UGT1A3 and UGT1A1 in insect cell-derived supersomes expressing the human enzymes, and hydrolyzes to form atorvastatin in human serum at room temperature.^{2,3} Atorvastatin lactone inhibits HMG-CoA reductase (IC₅₀ = 0.007 μM for the rat liver enzyme).¹ It also inhibits the cytochrome P450 (CYP) isoforms CYP2C9.1 and CYP2C9.3 (IC₅₀s = 16.8 and 5.62 μM, respectively), as well as P-glycoprotein (P-gp; IC₅₀ = 3.1-5.2 μM).^{4,5}

References

1. Roth, B.D., Blankley, C.J., Chucholowski, A.W., *et al.* Inhibitors of cholesterol biosynthesis. 3. Tetrahydro-4-hydroxy-6-[2-(1H-pyrrol-1-yl)ethyl]-2H-pyran-2-one inhibitors of HMG-CoA reductase. 2. Effects of introducing substituents at positions three and four of the pyrrole nucleus. *J. Med. Chem.* **34(1)**, 357-366 (1990).
2. Schirris, T.J.J., Ritschel, T., Bilos, A., *et al.* Statin lactonization by uridine 5'-diphosphoglucuronosyltransferases (UGTs). *Mol. Pharm.* **12(11)**, 4048-4055 (2015).
3. Jemal, M., Ouyang, Z., Chen, B.C., *et al.* Quantitation of the acid and lactone forms of atorvastatin and its biotransformation products in human serum by high-performance liquid chromatography with electrospray tandem mass spectrometry. *Rapid Commun Mass Spectrom.* **13(11)**, 1003-1015 (1999).
4. Shiozawa, A., Yamaori, S., Kamijo, S., *et al.* Effects of acid and lactone forms of statins on S-warfarin 7-hydroxylation catalyzed by human liver microsomes and recombinant CYP2C9 variants (CYP2C9.1 and CYP2C9.3). *Drug Metab. Pharmacokinet.* **36**, 100364 (2021).
5. Bogman, K., Peyer, A.-K., Török, M., *et al.* HMG-CoA reductase inhibitors and P-glycoprotein modulation. *Br. J. Pharmacol.* **132(6)**, 1183-1192 (2001).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

WARRANTY AND LIMITATION OF REMEDY

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

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