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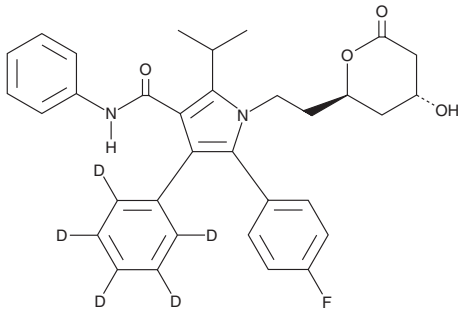
PRODUCT INFORMATION

Atorvastatin lactone-d_5

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-d_5)-1H-pyrrole-3-carboxamide
MF: $C_{33}H_{28}D_5FN_2O_4$
FW: 545.7
Chemical Purity: ≥95% (Atorvastatin lactone)
Deuterium Incorporation: ≥99% deuterated forms (d_1-d_5); ≤1% d_0
Supplied as: A solid
Storage: -20°C
Stability: ≥2 years



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

Laboratory Procedures

Atorvastatin lactone-d_5 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-d_5 is supplied as a solid. A stock solution may be made by dissolving the atorvastatin lactone-d_5 in the solvent of choice, which should be purged with an inert gas. Atorvastatin lactone-d_5 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 (IC_{50} = 0.007 µM for the rat liver enzyme).[1] It also inhibits the cytochrome P450 (CYP) isoforms CYP2C9.1 and CYP2C9.3 (IC_{50}s = 16.8 and 5.62 µM, respectively), as well as P-glycoprotein (P-gp; IC_{50} = 3.1-5.2 µM).[4,5]

References

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2. Schirris, T.J.J., Ritschel, T., Bilos, A., *et al.* Statin lactonization by uridine 5'-diphospho-glucuronosyltransferases (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).

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