

# PRODUCT INFORMATION

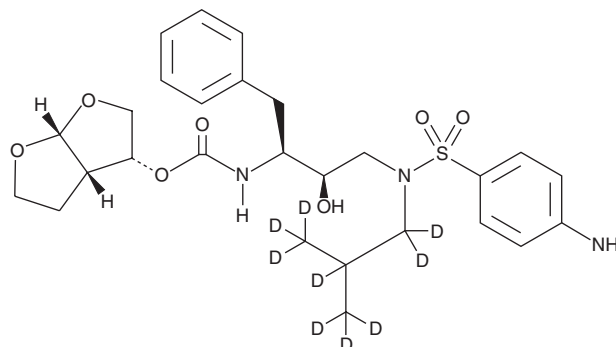


## Darunavir-d<sub>9</sub> Item No. 25220

**CAS Registry No.:** 1133378-37-6  
**Formal Name:** (3R,3aS,6aR)-N-[(1S,2R)-3-[[[4-(aminophenyl)sulfonyl][2-(methyl-d<sub>3</sub>)propyl-1,1,2,3,3,3-d<sub>6</sub>]amino]-2-hydroxy-1-(phenylmethyl)propyl]-carbamic acid, hexahydrofuro[2,3-b]furan-3-yl ester

**Synonym:** TMC114-d<sub>9</sub>  
**MF:** C<sub>27</sub>H<sub>28</sub>D<sub>9</sub>N<sub>3</sub>O<sub>7</sub>S  
**FW:** 556.7

**Chemical Purity:** ≥98% (Darunavir)  
**Deuterium Incorporation:** ≥99% deuterated forms (d<sub>1</sub>-d<sub>9</sub>); ≤1% d<sub>0</sub>  
**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

Darunavir-d<sub>9</sub> is intended for use as an internal standard for the quantification of darunavir (Item No. 15866 | 31083) 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).

Darunavir-d<sub>9</sub> is supplied as a solid. A stock solution may be made by dissolving the darunavir-d<sub>9</sub> in the solvent of choice. Darunavir-d<sub>9</sub> is soluble in organic solvents such as methanol, DMSO, and dimethyl formamide, which should be purged with an inert gas.

### Description

Darunavir-d<sub>9</sub> is intended for use as an internal standard for the quantification of darunavir (Item Nos. 15866 | 31083) by GC- or LC-MS. Darunavir is an HIV-1 protease inhibitor.<sup>1</sup> It is active against HIV-1<sub>LAI</sub> in MT-2 cells (IC<sub>50</sub> = 3 nM) with a cytotoxic concentration (CC<sub>50</sub>) of 74.4 μM. Darunavir is also active against wild-type and multidrug-resistant clinical isolates of HIV-1 in phytohemagglutinin-activated peripheral blood mononuclear cells (PHA-PBMCs; IC<sub>50</sub>s = 3 and 3-29 nM, respectively). It inhibits cell-free diffusion and cell-to-cell spread of HIV-1 in Jurkat cell populations (IC<sub>50</sub>s = 2.5 and 2.8 nM, respectively).<sup>2</sup> Formulations containing darunavir have been used in combination therapy for the treatment of HIV.

### References

1. Koh, Y., Nakata, H., Maeda, K., *et al.* Novel bis-tetrahydrofuranylurethane-containing nonpeptidic protease inhibitor (PI) UIC-94017 (TMC114) with potent activity against multi-PI-resistant human immunodeficiency virus in vitro. *Antimicrob. Agents Chemother.* **47(10)**, 3123-3129 (2003).
2. Titanji, B.K., Aasa-Chapman, M., Pillay, D., *et al.* Protease inhibitors effectively block cell-to-cell spread of HIV-1 between T cells. *Retrovirology* **10:161** (2013).

#### 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.

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