PRODUCT INFORMATION



Darunavir (ethanolate)

Item No. 31083

CAS Registry No.: 635728-49-3

Formal Name: N-[(1S,2R)-3-[[(4-aminophenyl)

sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)

propyl]-carbamic acid

(3R,3aS,6aR)-hexahydrofuro[2,3-b]

furan-3-yl ester, ethanolate

Synonym: **TMC114**

MF: $C_{27}H_{37}N_3O_7S \bullet C_2H_6O$

593.7 FW: **Purity:** ≥95% UV/Vis.: λ_{max} : 269 nm A crystalline solid Supplied as:

-20°C Storage: Stability: ≥4 years

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

Laboratory Procedures

Darunavir (ethanolate) is supplied as a crystalline solid. A stock solution may be made by dissolving the darunavir (ethanolate) in the solvent of choice, which should be purged with an inert gas. Darunavir (ethanolate) is soluble in organic solvents such as dimethyl formamide (DMF). The solubility of darunavir (ethanolate) in DMF is approximately 1 mg/ml.

Darunavir (ethanolate) is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, darunavir (ethanolate) should first be dissolved in DMF and then diluted with the aqueous buffer of choice. Darunavir (ethanolate) has a solubility of approximately 0.20 mg/ml in a 1:4 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Darunavir is an HIV-1 protease inhibitor. It is active against HIV-1_{I AI} in MT-2 cells (IC₅₀ = 3 nM) with a cytotoxic concentration (CC_{50}) of 74.4 μ M. Darunavir is also active against wild-type and multidrug-resistant clinical isolates of HIV-1 in phytohemagglutinin-activated peripheral blood mononuclear cells (PHA-PBMCs; IC₅₀s = 3 and 3-29 nM, respectively). It inhibits cell-free diffusion and cell-to-cell spread of HIV-1 in Jurkat cell populations (IC $_{50}$ s = 2.5 and 2.8 nM, respectively). 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 Ch. 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.

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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