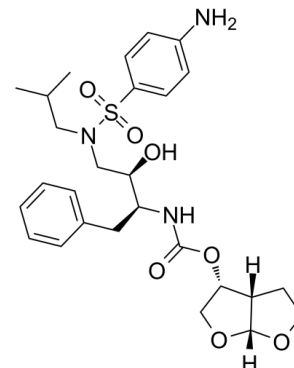


Data Sheet

Product Name:	Darunavir
Cat. No.:	CS-0749
CAS No.:	206361-99-1
Molecular Formula:	C ₂₇ H ₃₇ N ₃ O ₇ S
Molecular Weight:	547.66
Target:	HIV; HIV Protease
Pathway:	Anti-infection; Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 100 mg/mL (182.60 mM)



BIOLOGICAL ACTIVITY:

Darunavir (TMC114), an orally active next generation **HIV protease** inhibitor, has a similar antiviral activity against the mutant and the wild-type viruses. Darunavir (TMC114) is potent against laboratory HIV-1 strains and primary clinical isolates (IC₅₀ = 0.003 μM; IC₉₀ = 0.009 μM) with minimal cytotoxicity^{[1][2]}. **In Vitro:** Darunavir (TMC114, 1a) has a stability comparable to other protease inhibitors^[1]. Darunavir (TMC114, UIC-94017) blocks the infectivity and replication of each of HIV-1_{NL4-3} variants exposed to and selected for resistance to Ro 31-8959, MK-639, AG1341, or ABT 538 at concentrations up to 5 μM (IC₅₀s, 0.003 to 0.029 μM), although it was less active against HIV-1_{NL4-3} variants selected for resistance to VX-478 (IC₅₀, 0.22 μM)^[2].

References:

[1]. Dominique L N G Surleraux, et al. Discovery and selection of TMC114, a next generation HIV-1 protease inhibitor. J Med Chem. 2005 Mar 24;48(6):1813-22.

[2]. Yasuhiro Koh, 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. 2003 Oct;47(10):3123-9.

CAIndexNames:

Carbamic acid, N-[(1S,2R)-3-[[[(4-aminophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-, (3R,3aS,6aR)-hexahydrofuro[2,3-b]furan-3-yl ester

SMILES:

O=C(O[C@@H]1[C@@]2([H])[C@@](OCC2)([H])OC1N[C@@H](CC3=CC=CC=C3)[C@H](O)CN(S(=O)(C4=CC=C(N)C=C4)=O)CC(C)C

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

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