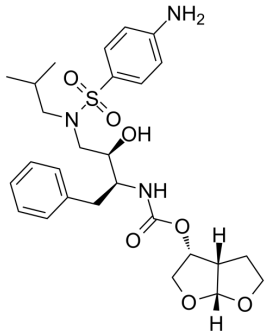
Darunavir

Cat. No.:	HY-17040
CAS No.:	206361-99-1
Molecular Formula:	$C_{27}H_{37}N_3O_7S$
Molecular Weight:	547.66
Target:	HIV; HIV Protease
Pathway:	Anti-infection; Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (182.60 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Concentration / Solvent / Mass	1 mg	5 mg	10 mg
	1 mM	1.8260 mL	9.1298 mL	18.2595 mL
	5 mM	0.3652 mL	1.8260 mL	3.6519 mL
	10 mM	0.1826 mL	0.9130 mL	1.8260 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (4.56 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (4.56 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.56 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

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 (IC_{50} = 0.003 μM; IC_{90} = 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 (IC_{50}s, 0.003 to 0.029 μM), although it was less active against HIV-1_{NL4-3} variants selected for resistance to VX-478 (IC_{50}, 0.22 μM)[2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Signal Transduct Target Ther. 2021 May 29;6(1):212.
- Nat Commun. 2020 Sep 4;11(1):4417.
- Int J Antimicrob Agents. 2019 Dec;54(6):814-819.
- Aging Cell. 2022 Dec 20;e13750.
- Antiviral Res. 2022 Nov 10;105463.

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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):

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