Darunavir Ethanolate

Cat. No.: HY-17041

CAS No.: 635728-49-3

Molecular Formula: $C_{29}H_{43}N_3O_8S$

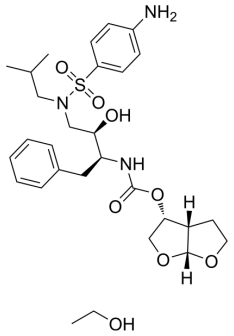
Molecular Weight: 593.73

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 : ≥ 50 mg/mL (84.21 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.6843 mL	8.4213 mL	16.8427 mL
5 mM	0.3369 mL	1.6843 mL	3.3685 mL
10 mM	0.1684 mL	0.8421 mL	1.6843 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 (4.21 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (4.21 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.21 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Darunavir ethanolate (TMC114 Ethanolate) is a potent HIV protease inhibitor used to treat and prevent HIV/AIDS. Darunavir has a K_i of 1 nM for wild type HIV-1 protease.

IC_{50} & Target

HIV-1

In Vitro

Darunavir is a broad-spectrum potent inhibitor active against HIV-1 clinical isolates with minimal cytotoxicity. Darunavir

	forms hydrogen bonds with the conserved main-chain atoms of Asp29 and Asp30 of the protease. These interactions are proposed to be critical for the potency of this compound against HIV isolates that are resistant to multiple protease inhibitors[1]. In an in vitro study in MT-2 cells, the potency of darunavir is greater than that of saquinavir, amprenavir, nelfinavir, indinavir, lopinavir and ritonavir. Darunavir is primarily metabolized by the hepatic cytochrome P450 (CYP) enzymes, primarily CYP3A. The 'boosting' dose of ritonavir acts an an inhibitor of CYP3A, thereby increasing darunavir bioavailability[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Darunavir is effective against wild-type and PI-resistant HIV, and has an oral bioavailability of 37%. It needs to be combined with ritonavir, which increases the bioavailability to 82%[3]. 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]. Tie Y, et al. High resolution crystal structures of HIV-1 protease with a potent non-peptide inhibitor (UIC-94017) active against multi-drug-resistant clinical strains. J Mol Biol. 2004 Apr 23;338(2):341-52.

[2]. McKeage K, et al. Darunavir: a review of its use in the management of HIV infection in adults. Drugs. 2009;69(4):477-503.

[3]. Bhalekar MR, et al. In-vivo bioavailability and lymphatic uptake evaluation of lipid nanoparticulates of darunavir. Drug Deliv. 2016 Sep;23(7):2581-2586.

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