产品名称：**Darunavir Ethanolate**
产品别名：达芦那韦乙醇

生物活性：

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	Ki: 1 nM (WT HIV-1 protease)[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].
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].

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

*请根据产品在不同溶剂中的溶解度选择合适的溶剂配制储备液；一旦配成溶液，请分装保存，避免反复冻融造成的产品失效。

储备液的保存方式和期限：-80°C, 6 months; -20°C, 1 month。-80°C 储存时，请在 6 个月内使用，-20°C 储存时，请在 1 个月内使用。

In Vivo:

请根据您的实验动物和给药方式选择适当的溶解方案。以下溶解方案都请先按照 **In Vitro** 方式配制澄清的储备液，再依次添加助溶剂：

——为保证实验结果的可靠性，澄清的储备液可以根据储存条件，适当保存；体内实验的工作液，建议您现用现配，当天使用； 以下溶剂前显示的百分比是指该溶剂在您配制终溶液中的体积占比；如在配制过程中出现沉淀、析出现象，可以通过加热和/或超声的方式助溶

1.请依序添加每种溶剂： 10% DMSO→40% PEG300 →5% Tween-80 → 45% saline

Solubility: ≥ 2.5 mg/mL (4.21 mM); Clear solution

此方案可获得 ≥ 2.5 mg/mL (4.21 mM，饱和度未知) 的澄清溶液。

以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 400 μL PEG300 中，混合均匀；向上述体系中加入 50 μL Tween-80，混合均匀；然后继续加入 450 μL 生理盐水定容至 1 mL。

2.请依序添加每种溶剂： 10% DMSO→ 90% (20% SBE-β-CD in saline)

Solubility: ≥ 2.5 mg/mL (4.21 mM); Clear solution

此方案可获得 ≥ 2.5 mg/mL (4.21 mM，饱和度未知) 的澄清溶液。

以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 900 μL 20% 的 SBE-β-CD 生理

	盐水水溶液中，混合均匀。 3.请依序添加每种溶剂： 10% DMSO →90% corn oil Solubility: ≥ 2.5 mg/mL (4.21 mM); Clear solution 此方案可获得 ≥ 2.5 mg/mL (4.21 mM，饱和度未知) 的澄清溶液，此方案不适用于实验周期在半个月以上的实验。 以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 900 μL 玉米油中，混合均匀。
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.