

# Darunavir (Ethanolate)

# Catalog No: tcsc0750

Available Sizes

Size: 5mg

Size: 10mg

Size: 50mg

Specifications

CAS No:

635728-49-3

Formula:

 $C_{29}H_{43}N_3O_8S$ 

**Pathway:** Metabolic Enzyme/Protease;Anti-infection

Target:

HIV Protease;HIV

Purity / Grade:

### Solubility: DMSO : $\geq$ 50 mg/mL (84.21 mM)

#### **Alternative Names:**

TMC114

#### **Observed Molecular Weight:**

593.73

## **Product Description**

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Darunavir ethanolate (TMC114 ethanolate) is a potent **HIV** protease inhibitor used to treat and prevent HIV/AIDS. Darunavir has a **K**<sub>i</sub> of 1 nM for wild type HIV-1 protease.

IC50 & Target: Ki: 1 nM (WT HIV-1 protease)<sup>[1]</sup>

*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<sup>[1]</sup>. 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<sup>[2]</sup>.

*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%<sup>[3]</sup>.



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