

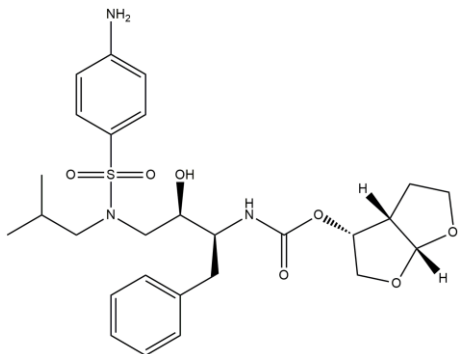
# Darunavir

12/20

**ALTERNATE NAMES:** [(3aS,4R,6aR)-2,3,3a,4,5,6a-hexahydrofuro[2,3-b]furan-4-yl] N-[(2S,3R)-4-[(4-aminophenyl)sulfonyl-(2-methylpropyl)amino]-3-hydroxy-1-phenylbutan-2-yl]carbamate; Prezista; TMC114; (3R,3aS,6aR)-hexahydrofuro[2,3-b]furan-3-yl [(2S,3R)-4-(4-amino-N-isobutylphenylsulfonamido)-3-hydroxy-1-phenylbutan-2-yl]carbamate; N-[(1S,2R)-3-(((4-Aminophenyl)sulfonyl)(2-methylpropyl)amino)-2-hydroxy-1-benzylpropyl)]((1S,2R,5R)-4,6-dioxabicyclo(3.3.0)oct-2-yloxy)carboxamide; UIC-94017

**CATALOG #:** B3086-5 5 mg  
B3086-25 25 mg

**STRUCTURE:**



**MOLECULAR FORMULA:** C<sub>27</sub>H<sub>37</sub>N<sub>3</sub>O<sub>7</sub>S

**MOLECULAR WEIGHT:** 547.7

**CAS NUMBER:** 206361-99-1

**APPEARANCE:** White to off-white solid powder

**PURITY:** ≥ 98%

**SOLUBILITY:** ~25 mg/ml in DMSO  
~30 mg/ml in DMF

**DESCRIPTION:** Darunavir is an HIV-1 protease inhibitor with an IC<sub>50</sub> of 3 nM and cytotoxicity of 74.4 μM. It is also active against wild-type and multidrug-resistant clinical isolates of HIV-1 in phytohemagglutinin-activated peripheral blood mononuclear cells. Modelling studies have shown that darunavir can bind to papain like viral protease and may be beneficial in treating SARS-COV-2.

**STORAGE TEMPERATURE:** -20°C. Protect from air. Store under desiccating conditions.

**HANDLING:** Do not take internally. Wear gloves and mask when handling the product! Avoid contact by all modes of exposure.

**REFERENCES:**

- Shen Lin, Runnan Shen, Jingdong He, Xinhao Li, Xushun Guo. Molecular Modeling Evaluation of the Binding Effect of Ritonavir, Lopinavir and Darunavir to Severe Acute Respiratory Syndrome Coronavirus 2 Proteases. <https://doi.org/10.1101/2020.01.31.929695> (2020).
- Koh, Y., Nakata, H., Maeda, K., et al. Novel bis-tetrahydrofuranylethane-containing nonpeptidic protease inhibitor (PI) UIC-94017 (TMC114) with potent activity against multi-PI-resistant human immunodeficiency virus in vitro. *Antimicrob. Agents Chemother.* 47(10), 3123-3129 (2003).

**RELATED PRODUCTS:**

Amastatin hydrochloride (Cat. No. B3085)  
 Bestatin hydrochloride (Cat. No. 9630)  
 Boceprevir (Cat. No. B2961)  
 Linagliptin (Cat. No. 2240)  
 Cathepsin H (active, human) (Cat. No. 1023)

**DISCLAIMER:** **FOR RESEARCH USE ONLY! Not to be used on humans.**