

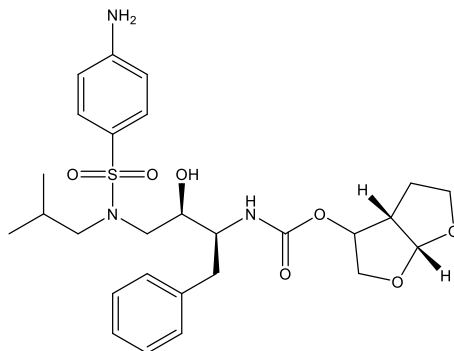
Catalog # 10-4930

Darunavir

CAS# 206361-99-1

[(3a*S*,4*R*,6a*R*)-2,3,3a,5,6a-Hexahydrofuro[2,3-*b*]furan-4-yl] N-[(4-aminophenyl)sulfonyl-(2-methylpropyl)amino]-3-hydroxy-1-phenylbutan-2-yl]carbamate; UIC-94017; TMC114

Lot # FBS2113



Darunavir is a very potent ($IC_{50} = 3$ nM against lab HIV-1 strains and clinical isolates) HIV-1 protease inhibitor that is in clinical use.^{1,2} Also potent against multi-PI-resistant HIV-1 strains from patient samples. Darunavir has been investigated as a potential anti-SARS-CoV2 therapeutic with mixed results.³⁻⁶

- 1) Koh *et al.* (2003), *Novel bis-tetrahydrofuranylethane-containing nonpeptidic protease inhibitor (PI UIC-94017 (YMC114) with potent activity against multi-PI-resistant human immunodeficiency virus in vitro*; Antimicrob. Agents Chemother., **47** 2123
- 2) Surleraux *et al.* (2005), *Discovery and selection of TMC114, a next generation HIV-1 protease inhibitor*; J. Med. Chem., **48** 1813
- 3) Beck *et al.* (2020), *Predicting commercially available antiviral drugs that may act on the novel coronavirus (SARS-CoV-2) through a drug-target interaction deep learning model*; Comput. Struct. Biotechnol.J, **18** 784
- 4) Khan *et al.* (2020), *Identification of chymotrypsin-like protease inhibitors of SARS-VCoV-2 via integrated computational approach*; J. Biomol.Struct. Dyn., **39** 2607
- 5) De Meyers *et al.* (2020), *Lack of antiviral activity of darunavir against SARS-CoV-2*; Int. J. Infect. Dis, **97** 7
- 6) Kim *et al.* (2020), *Use of Darunavir-Cobicistat as a Treatment Option for Critically Ill Patients with SARS-CoV-2 Infection*; Yonsei Med. J., **61** 826

PHYSICAL DATA

Molecular Weight:	547.67
Molecular Formula:	C ₂₇ H ₃₇ N ₃ O ₇ S
Purity:	>98% by HPLC
	NMR: (Conforms)
Solubility:	DMSO (>25 mg/mL)
Physical Description:	White solid
Storage and Stability:	Store as supplied desiccated at -20°C for up to 1 year from the date of purchase. Solutions in DMSO may be stored at -20°C for up to 3 months.

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