

Product Name: Darunavir

Catalog No.: 6710

Batch No.: 1

CAS Number: 206361-99-1

IUPAC Name: (3*R*,3*aS*,6*aR*)-Hexahydrofuro[2,3-*b*]furan-3-yl *N*-[(1*S*,2*R*)-3-[[4-aminophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]carbamate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₃₇N₃O₇S.¼H₂O

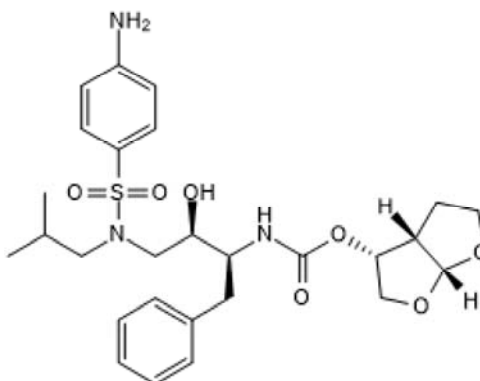
Batch Molecular Weight: 552.16

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.73	6.85	7.61
Found	58.68	6.84	7.62

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Highly potent HIV protease inhibitor (IC₅₀ = 3 - 6 nM, depending on laboratory HIV-1 strain). Displays activity in cells infected with clinical HIV-1 strains shown to have resistance to other protease inhibitors.

Physical and Chemical Properties:

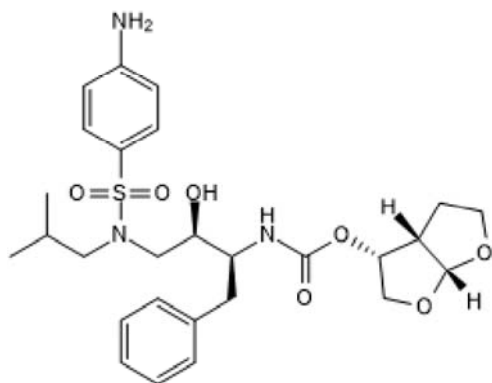
Batch Molecular Formula: C₂₇H₃₇N₃O₇S·¼H₂O

Batch Molecular Weight: 552.16

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Koh et al (2003) Novel *bis*-tetrahydrofuranylurethane-containing nonpeptidic protease inhibitor (PI) UIC-94017 (TMC114) with potent activity against multi-PI-resistant human immunodeficiency virus *in vitro*. *Antimicrob. Agents Chemother.* **47** 3123. PMID: 14506019.

Ghosh et al (1998) Potent HIV protease inhibitors incorporating high-affinity P₂-ligands and (*R*)-(hydroxyethylamino)sulfonamide isostere. *Bioorg. Med. Chem. Lett.* **8** 687. PMID: 9871583.

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