

Product Name: Saquinavir mesylate

Catalog No.: 4418

Batch No.: 1

CAS Number: 149845-06-7

IUPAC Name: (2S)-N1-[(1S,2R)-3-[(3S,4aS,8aS)-3-[[1,1-dimethylethyl]amino]carbonyl]octahydro-2(1H)-isoquinolinyl]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]butanediamide methanesulfonate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₈H₅₀N₆O₅·CH₄O₃S

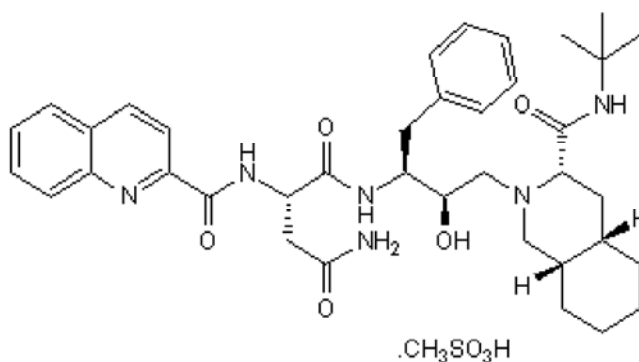
Batch Molecular Weight: 766.95

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -48.8 (Concentration = 0.5, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.08	7.1	10.96
Found	61.14	7.13	10.89

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956

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Description:

Inhibitor of human immunodeficiency virus (HIV) protease (K_i values are <0.1 and 0.12 nM for HIV-2 and HIV-1 protease respectively). Exhibits high antiviral activity and low cytotoxicity. *In silico* docking models predict potential as an inhibitor of SARS-CoV-2 3CL^{pro}.

Physical and Chemical Properties:

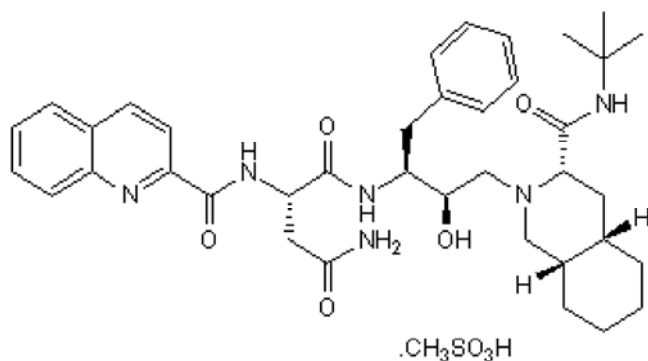
Batch Molecular Formula: C₃₈H₅₀N₆O₅·CH₄O₃S

Batch Molecular Weight: 766.95

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 50 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:

Hall and Hai-Feng et al (2020) A search for medications to treat COVID-19 via *in silico* molecular docking models of the SARS-CoV-2 spike glycoprotein and 3CL protease. *Travel Med.Infect.Dis.* PMID: 32294562.

Kaldor et al (1995) Isophthalic acid derivatives: amino acid surrogates for the inhibition of HIV-1 protease. *Bioorg.Med.Chem.Lett.* **5** 721.

Krausslich et al (1992) Specific inhibitor of human immunodeficiency virus proteinase prevents the cytotoxic effects of a single-chain proteinase dimer and restores particle formation. *J.Virol.* **66** 567. PMID: 1727499.

Tucker et al (1992) A series of potent HIV-1 protease inhibitors containing a hydroxyethyl secondary amine transition state isostere: synthesis, enzyme inhibition, and antiviral activity. *J.Med.Chem.* **35** 2525. PMID: 1635054.

Roberts et al (1990) Rational design of peptide-based HIV proteinase inhibitors. *Science* **248** 358. PMID: 2183354.

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