

Product Name: Nelfinavir mesylate

Catalog No.: 3766

Batch No.: 2

CAS Number: 159989-65-8

IUPAC Name: (3*S*,4*aS*,8*aS*)-*N*-(1,1-Dimethylethyl)decahydro-2-[(2*R*,3*R*)-2-hydroxy-3-[(3-hydroxy-2-methylbenzoyl)amino]-4-(phenylthio)butyl]-3-isoquinolinecarboxamide methanesulfonate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₂H₄₅N₃O₄S·CH₄O₃S·½H₂O

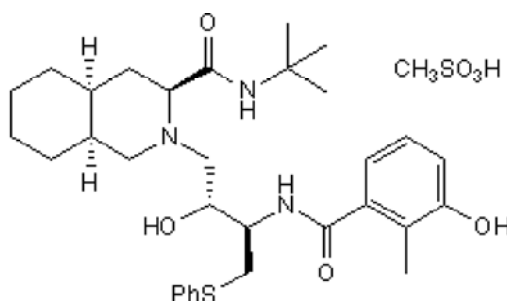
Batch Molecular Weight: 672.9

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -113.6 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.9	7.49	6.24
Found	58.96	7.51	6.33

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Description:

Orally active human immunodeficiency virus protease inhibitor. Potently inhibits HIV-1 protease ($K_i = 2$ nM) *in vitro*. Also exhibits anti-MERS-CoV activity in Vero cells *in vitro* ($IC_{50} = 0.08$ μ M).

Physical and Chemical Properties:

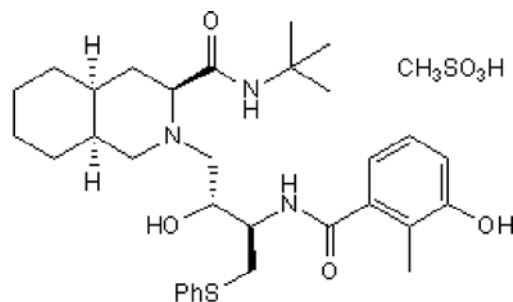
Batch Molecular Formula: $C_{32}H_{45}N_3O_4S \cdot CH_4O_3S \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 672.9

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

References:

Ko et al (2020) Screening of FDA-approved drugs using a MERS-CoV clinical isolate from South Korea identifies potential therapeutic options for COVID-19. *BioRxiv* - Paper not yet peer reviewed.

Gills et al (2007) Nelfinavir, a lead HIV protease inhibitor, is a broad-spectrum, anticancer agent that induces endoplasmic reticulum stress, autophagy and apoptosis *in vitro* and *in vivo*. *Clin.Cancer Res.* **13** 5183.

Patick et al (1996) Antiviral and resistance studies of AG1343, an orally bioavailable inhibitor of human immunodeficiency virus protease. *Antimicrob.Agents Chemother.* **40** 29. PMID: 8787874.

Shetty et al (1996) Preclinical pharmacokinetics and distribution to tissue of AG1343, an inhibitor of human immunodeficiency virus type 1 protease. *Antimicrob.Agents Chemother.* **40** 110. PMID: 8787890.

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