

Product Name: Indinavir sulfate

Catalog No.: 7196

Batch No.: 1

CAS Number: 157810-81-6

IUPAC Name: 2,3,5-Trideoxy-*N*-[(1*S*,2*R*)-2,3-dihydro-2-hydroxy-1*H*-inden-1-yl]-5-[(2*S*)-2-[[[(1,1-dimethylethyl)amino]carbonyl]-4-(3-pyridinylmethyl)-1-piperazinyl]-2-(phenylmethyl)-*D*-erythro-pentonamide sulfate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₆H₄₇N₅O₄·H₂SO₄·1½H₂O

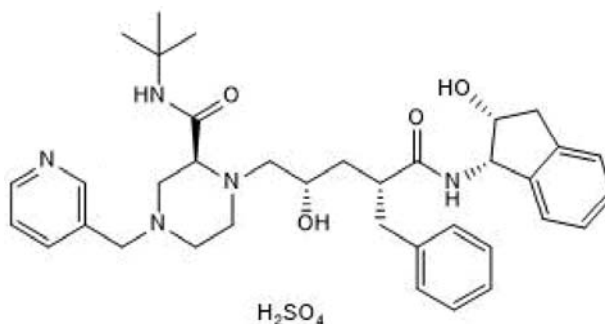
Batch Molecular Weight: 738.9

Physical Appearance: White solid

Solubility: DMSO to 100 mM
water to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +26.2 (Concentration = 1, Solvent = Water)

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	58.52	7.09	9.48
Found	58.28	7.19	9.44

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

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Description:

Indinavir sulfate is a potent and selective HIV protease inhibitor (K_i values are 0.52 and 3.3 nM for HIV-1 and HIV-2, respectively). Indinavir stops the spread of the HIV-infected MT4 lymphoid cells at concentrations of 25-50 nM. Indinavir disrupts the ERK1/2 and p38 MAPK pathways and reduces both the level of functional eIF4F complex and rpS6 phosphorylation, which leads to a decrease in protein synthesis in mouse myocytes. *In silico* docking models predict potential as an inhibitor of SARS-CoV-2 3CL^{pro}.

Physical and Chemical Properties:

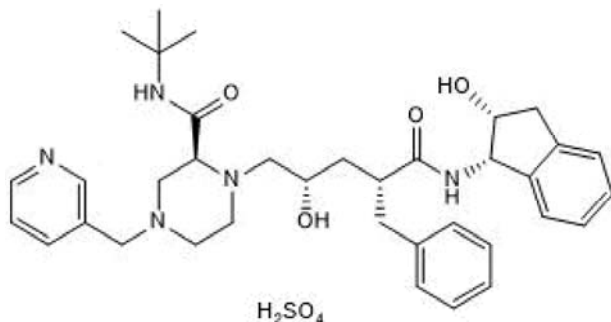
Batch Molecular Formula: C₃₆H₄₇N₅O₄·H₂SO₄·1½H₂O

Batch Molecular Weight: 738.9

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
water 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:

Hall 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.* **35** 101646. PMID: 32294562.

Brown et al (2005) Indinavir alters regulators of protein anabolism and catabolism in skeletal muscle. *Am.J.Physiol.Endocrinol.Metab.* **289** E382-90. PMID: 15827064.

Brown et al (2004) Indinavir impairs protein synthesis and phosphorylations of MAPKs in mouse C₂C₁₂ myocytes. *Am.J.Physiol.Cell Physiol.* **287** C1482-92. PMID: 15229102.

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