Datasheet

Lopinavir

Product Name	Lopinavir
Catalogue Number	BSV-S1380
Chemical Formula	$C_{37}H_{48}N_4O_5$
Function	HIV protease Inhibitor
CAS No.:	192725-17-0

Description:

Lopinavir is a potent **HIV protease** inhibitor with **K_i** of 1.3 pM in a cell-free assay.

Product Details:

Target: HIV protease [1] (Cell-free assay) 1.3 pM(Ki)

Chemical name: (S)-N-((2S,4S,5S)-5-(2-(2,6-dimethylphenoxy)acetamido)-4-hydroxy-1,6-diphenylhexan-2-yl)-3-methyl-2-(2-oxo-tetrahydropyrimidin-1(2H)-yl)butanamide

Formula: $C_{37}H_{48}N_4O_5$

Molecular weight: 628.8

Purity: 99.92 %

Solubility: **126** mg/mL (DMSO), **126** mg/mL (water)

Storage: 3 years -20°C powder, 2 years -80°C in solvent

Preparing stock solutions

Concentration / Mass	1 mg	5 mg	10 mg
1 mM	1.5903 mL	7.9517 mL	15.9033 mL
5 mM	0.3181 mL	1.5903 mL	3.1807 mL
10 mM	0.1590 mL	0.7952 mL	1.5903 mL
50 mM	0.0318 mL	0.1590 mL	0.3181 mL

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Biological Activity:

In vitro:

Lopinavir binds to mutant HIV protease (V82A, V82F and V82T) with Ki of 4.9 pM, 3.7 pM and 3.6 pM, respectively. Lopinavir inhibits 93% of wild-type HIV protease activity at 0.5 nM. Lopinavir inhibits HIV protease activity in the absence and presence of 50% HS with EC50 of 17 nM and 102 nM, respectively, in MT4 cells. [1] Lopinavir is converted to several metabolites in an NADPH-dependent manner in liver microsomes with the primary metabolites M-3 and M-4. [2] Lopinavir is a potent inhibitor of Rh123 efflux in Caco-2 monolayers with IC50 of 1.7 mM. Lopinavir exposure (72 hours) in LS 180V cells reduces the content of intracellular Rh123. Lopinavir induces P-glycoprotein immunoreactive protein and messenger RNA levels in LS 180V cells. [3] Lopinavir inhibits subtype C clone C6 with IC50 of 9.4 nM. [4] Lopinavir inhibits CYP3A with IC50 of 7.3 mM in human liver microsomes, while produces negligible or weak inhibition of human CYP1A2, 2B6, 2C9, 2C19 and 2D6. [5]

In vivo:

Lopinavir (10 mg/kg, orally) results in Cmax of 0.8 μg/mL and oral bioavailability of 25% in rats. [1]

Protocol *(Only for Reference)*

Kinase Assay: [1]	
HIV protease inhibition	Inhibition of the activity of recombinant wild-type and mutant HIV type 1 (HIV-1) proteases is measured by a continuous fluorometric assay with the internally quenched fluorogenic substrate DABCYL-GABA-Ser-Gln-Asn-Tyr-Pro-Ile-Val-Gln-EDANS. The apparent Ki is estimated by nonlinear regression by the equation for tightly binding inhibitors.

Animal Study: [1]	
Animal Models	Sprague-Dawley-derived rats or cynomolgus monkeys
Dosages	10 mg/kg
Administration	Orally

References:

- [1] Sham HL, et al. Antimicrob Agents Chemother, 1998, 42(12), 3218-3224.
- [2] Kumar GN, et al. Drug Metab Dispos, 1999, 27(1), 86-91.
- [3] Vishnuvardhan D, et al. AIDS, 2003, 17(7), 1092-1094.
- [4] Gonzalez LM, et al. Antimicrob Agents Chemother, 2003, 47(9), 2817-2822.
- [5] Weemhoff JL, et al. J Pharm Pharmacol, 2003, 55(3), 381-386.