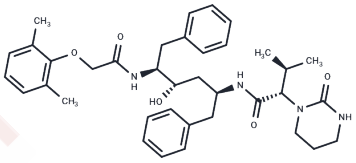
Data Sheet (Cat.No.T1623)

TargetMol

Lopinavir

Chemical Properties



CAS No. : 192725-17-0

Formula: C37H48N4O5

Molecular Weight: 628.8

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Lopinavir (ABT-378) is a peptidomimetic HIV protease inhibitor effective against HIV protease with the Val 82 mutation. It is less affected by serum protein binding compared to the structurally related drug ritonavir.
Targets(IC50)	HIV Protease,SARS-CoV
In vitro	Administering Lopinavir (10 mg/kg, p.o.) to rats resulted in a maximum concentration (Cmax) of 0.8 μg/mL, with the drug's bioavailability being 25%.
In vivo	Lopinavir is an effective inhibitor of Rh123, with an IC50 value of 1.7 mM for Caco-2 cell monolayers. It binds to mutant HIV proteases (V82A, V82T, and V82F) with Ki values of 4.9, 3.7, and 3.6 pM, respectively. At a concentration of 0.5 nM, Lopinavir inhibits the activity of wild-type HIV protease by 93%. It also inhibits HIV protease activity in MT4 cells both in the presence and absence of 50% HS, with EC50 values of 102 nM and 17 nM, respectively. In liver microsomes, Lopinavir is converted to primary metabolites M-3 and M-4, a process that is NADPH-dependent. After treating LS 180V cells with Lopinavir for 72 hours, there is a reduction in intracellular Rh123 content and induction of P-glycoprotein immunoreactive protein and mRNA levels. Lopinavir exhibits an IC50 of 9.4 nM against subtype C clone C6. When acting on human liver microsomes, Lopinavir shows an IC50 of 7.3 mM against CYP3A and exerts weak inhibition on human CYP1A2, 2B6, 2C9, 2C19, and 2D6.

Solubility Information

Solubility	Ethanol: 116 mg/mL (184.48 mM),Sonication is recommended. DMSO: 247.5 mg/mL (393.61 mM),Sonication is recommended. H2O: < 1 mg/mL (insoluble or slightly soluble), (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 4 mg/mL (6.36 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.5903 mL	7.9517 mL	15.9033 mL
5 mM	0.3181 mL	1.5903 mL	3.1807 mL
10 mM	0.159 mL	0.7952 mL	1.5903 mL
50 mM	0.0318 mL	0.159 mL	0.3181 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Sham HL, et al. Antimicrob Agents Chemother, 1998, 42(12), 3218-3224.
Cheng C, Ji Z, Sheng Y, et al. Aphthous ulcer drug inhibits prostate tumor metastasis by targeting IKK/TBK1/NF-κB signaling. Theranostics. 2018, 8(17): 4633
Kumar GN, et al. Drug Metab Dispos, 1999, 27(1), 86-91.
Yan F, Gao F. An overview of potential inhibitors targeting non-structural proteins 3 (PLpro and Mac1) and 5 (3CLpro/Mpro) of SARS-CoV-2. Computational and Structural Biotechnology Journal. 2021, 19: 4868.
Fical L, Khalikova M, Kočová Vlčková H, et al. Determination of Antiviral Drugs and Their Metabolites Using Micro-Solid Phase Extraction and UHPLC-MS/MS in Reversed-Phase and Hydrophilic Interaction Chromatography Modes. Molecules. 2021, 26(8): 2123.
Vishnuvardhan D, et al. AIDS, 2003, 17(7), 1092-1094.
Gonzalez LM, et al. Antimicrob Agents Chemother, 2003, 47(9), 2817-2822.
Weemhoff JL, et al. J Pharm Pharmacol, 2003, 55(3), 381-386.
Chu, Liuxi, et al. Simultaneous quantitation of zidovudine, efavirenz, lopinavir and ritonavir in human hair by liquid chromatography-atmospheric pressure chemical ionization-tandem mass spectrometry [J]. Journal of Chromatography B . 2018 Oct 15;1097-1098:54-63.
Fical L, Khalikova M, Kočová Vlčková H, et al. Determination of Antiviral Drugs and Their Metabolites Using Micro-Solid Phase Extraction and UHPLC-MS/MS in Reversed-Phase and Hydrophilic Interaction Chromatography Modes [J]. Molecules. 2021, 26(8): 2123.