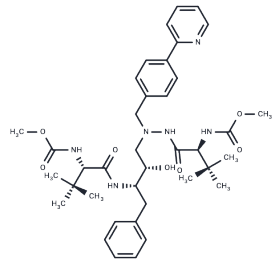
Data Sheet (Cat.No.T0100L)

TargetMol

Atazanavir

Chemical Properties



CAS No. : 198904-31-3

Formula: C38H52N6O7

Molecular Weight: 704.86

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	Atazanavir (BMS-232632)(BMS-232632) is an highly effective HIV-1 protease inhibitor.
Targets(IC50)	HIV Protease,Endogenous Metabolite,Cytochromes P450,P-gp,SARS-CoV,TLR
In vitro	Atazanavir has potent in vitro activity with 50 and 90% effective concentrations(EC50) of 2-5 nM and 9-15 nM respectively against wild type virus[1]. Atazanavir is able to potently induce endoplasmic reticulum (ER) stress response in malignant glioma cells, as indicated by elevated levels of GRP78 and CHOP, and activation of caspase-4, which leads to cell death[3].
In vivo	Atazanavir has excellent oral bioavailability in the range of 60-70%[1].
Kinase Assay	Protease assays: To determine the inhibition constants (Ki) for each Prt inhibitor, purified HIV-1 RF wild-type Prt (2.5 nM) is incubated at 37 ℃ with 1 μM to 15 μM fluorogenic substrate in reaction buffer (1 M NaCl, 1 mM EDTA, 0.1 M sodium acetate [pH 5.5], 0.1% polyethylene glycol 8000) in the presence or absence of Atazanavir. Cleavage of the substrate is quantified by measuring an increase in fluorescent emission at 490 nM after excitation at 340 nM using a Cytofluor 4000. Reactions are carried out using 1.36 μM, 1.66 μM, 2.1 μM, 3.0 μM, 5.0 μM, or 15 μM substrate in the presence of five concentrations of Atazanavir (1.25 nM to 25 nM). Substrate cleavage is monitored at 5-min intervals for 30 min. Cleavage rates are then determined for each sample at early time points in the reaction, and Ki values are determined from the slopes of the resulting Michaelis-Menten plots.
Cell Research	U251, T98 g, and LN229 glioblastoma cell lines are exposed to increasing concentrations of nelfinavir and atazanavir. Cells cultured in 96-well plates are treated with drugs for 48 h, and cell growth and survival are determined by conventional MTT assay.(Only for Reference)

Solubility Information

Solubility	Ethanol: 32 mg/mL (45.4 mM),Sonication is recommended. DMSO: 250 mg/mL (354.68 mM),Sonication is recommended. H2O: < 1 mg/mL (insoluble or slightly soluble),

Solubility	(< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: < 10 mg/mL (14.19 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: < 10 mg/mL (14.19 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+90% (20% SBE-β-CD in Saline): < 10 mg/mL (14.19 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+90% Corn oil: 10 mg/mL (14.19 mM),Solution. *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	1.4187 mL	7.0936 mL	14.1872 mL
5 mM	0.2837 mL	1.4187 mL	2.8374 mL
10 mM	0.1419 mL	0.7094 mL	1.4187 mL
50 mM	0.0284 mL	0.1419 mL	0.2837 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

Piliero PJ, et al. Expert Opin Investig Drugs. 2002, 11(9):1295-301.
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.
Robillard KR, et al. Antimicrob Agents Chemother. 2014, 58(3):1713-22.
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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.