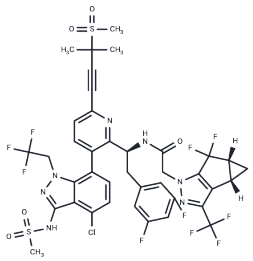
Data Sheet (Cat.No.T11465)

TargetMol

Lenacapavir

Chemical Properties



CAS No. : 2189684-44-2

Formula: C39H32ClF10N7O5S2

Molecular Weight: 968.28

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	Lenacapavir (GS-6207) is the first HIV-1 capsid inhibitor approved by the U.S. Food and Drug Administration, the European Medicines Agency, and Health Canada for the treatment of MDR HIV-1 infection.[3]
Targets(IC50)	HIV Protease
In vitro	The half-maximal effective concentration (EC50) of lenacapavir in MT-4 cells is 105 pmol/L; the half-maximal effective concentration (EC50) in primary human CD4 cells is 32 pmol/L; and the half-maximal effective concentration (EC50) in macrophages is 56 pmol/L. [1]
In vivo	The pharmacokinetics of lenacapavir after a single oral dose are nonlinear and dose-proportional over the dose range of 50-1800 mg, whereas they are dose-proportional when administered subcutaneously at 309-927 mg. The median half-life after oral and subcutaneous administration is 10 to 12 days and 8 to 12 weeks, respectively. The bioavailability of oral lenacapavir is 6-10%, with peak concentrations measured after 4 hours. Subcutaneous lenacapavir is completely absorbed and slowly released from the injection site, with peak plasma concentrations reached 84 days after administration. After a single subcutaneous dose of 900 mg, plasma concentrations remain well above the response threshold for more than 6 months, but oral lenacapavir is used for the initial loading phase because of slow initial diffusion into the circulation. The volume of distribution of lenacapavir is 976 L, and the drug is 99.8% protein bound, as calculated from a population PK study. [2]

Solubility Information

Solubility	DMSO: 165 mg/mL (170.41 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Corn Oil: 5 mg/mL (5.16 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	1.0328 mL	5.1638 mL	10.3276 mL
5 mM	0.2066 mL	1.0328 mL	2.0655 mL
10 mM	0.1033 mL	0.5164 mL	1.0328 mL
50 mM	0.0207 mL	0.1033 mL	0.2066 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

Link JO, et al. Clinical targeting of HIV capsid protein with a long-acting small molecule. Nature. 2020 Aug;584 (7822):614-618.
Machine learning-enabled virtual screening indicates the anti-tuberculosis activity of aldoxorubicin and quarfloxin with verification by molecular docking, molecular dynamics simulations, and biological evaluations
Di Perri G. Pharmacological outlook of Lenacapavir: a novel first-in-class Long-Acting HIV-1 Capsid Inhibitor. Infez Med. 2023 Dec 1;31(4):495-499.
Dzinamarira T, et al. Highlights on the Development, Related Patents, and Prospects of Lenacapavir: The First-in-Class HIV-1 Capsid Inhibitor for the Treatment of Multi-Drug-Resistant HIV-1 Infection. Medicina (Kaunas). 2023 May 28;59(6):1041.