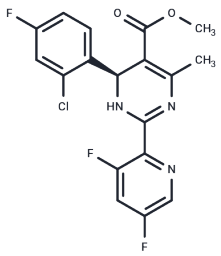
Data Sheet (Cat.No.T10480L)

TargetMol

Bay 41-4109

Chemical Properties



CAS No. : 298708-81-3

Formula: C18H13ClF3N3O2

Molecular Weight: 395.76

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	BAY 41-4109 is a potent inhibitor of human hepatitis B virus (HBV) with an IC50 of 53 nM.
Targets(IC50)	HBV
In vitro	BAY 41-4109 effectively accelerates and alters the direction of capsid assembly in vitro, demonstrating potent inhibitory effects on both HBV DNA release and cytoplasmic HBcAg levels, with IC50 values of 32.6 and 132 nM in HepG2.2.15 cells, respectively. Its inhibitory action on HBV DNA and HBcAg is dose-dependent, underscoring that its anti-HBV properties hinge on the rate at which HBcAg is inhibited. Additionally, BAY 41-4109 can stabilize preformed capsids, achieving a stabilization ratio of one inhibitor molecule per two dimers.
In vivo	BAY 41-4109 effectively suppresses virus production in vivo through a mechanism focusing on the viral capsid[2]. It dose-dependently decreases viral DNA in both the liver and plasma, showing efficacy on par with 3TC, and it diminishes hepatitis B virus core antigen (HBcAg) in the livers of HBV-transgenic mice. Pharmacokinetic evaluations in mice reveal quick absorption, 30% bioavailability, and dose-proportional plasma concentrations, reaching approximately 60% in rats and dogs[1].

Solubility Information

Solubility	DMSO: 100 mg/mL (252.68 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 3.3 mg/mL (8.34 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	2.5268 mL	12.6339 mL	25.2678 mL
5 mM	0.5054 mL	2.5268 mL	5.0536 mL
10 mM	0.2527 mL	1.2634 mL	2.5268 mL
50 mM	0.0505 mL	0.2527 mL	0.5054 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

Weber O, et al. Inhibition of human hepatitis B virus (HBV) by a novel non-nucleosidic compound in a transgenic mouse model. Antiviral Res. 2002 May;54(2):69-78.
Yang Y, Yan Y, Yin J, et al. Structure-Based Discovery of N-Sulfonylpiperidine-3-carboxamides as Novel Capsid Assembly Modulators for Potent Inhibition of HBV Replication. Viruses. 2022, 14(2): 348.
Yin J, Feng Z, Li Z, et al.Synthesis and evaluation of N-sulfonylpiperidine-3-carboxamide derivatives as capsid assembly modulators inhibiting HBV in vitro and in HBV-transgenic mice.European Journal of Medicinal Chemistry. 2023: 115141.
Stray SJ, et al. BAY 41-4109 has multiple effects on Hepatitis B virus capsid assembly. J Mol Recognit. 2006 Nov-Dec;19(6):542-8.
Wu GY, et al. Inhibition of hepatitis B virus replication by Bay 41-4109 and its association with nucleocapsid disassembly. J Chemother. 2008 Aug;20(4):458-67.