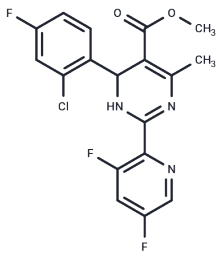
Data Sheet (Cat.No.T3449)

TargetMol

Bay 41-4109 racemate

Chemical Properties



CAS No. : 298708-79-9

Formula: C18H13ClF3N3O2

Molecular Weight: 395.76

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	BAY 41-4109 racemate is a potent inhibitor of human hepatitis B virus (HBV) with an IC50 of 53 nM.
Targets(IC50)	HBV
In vitro	BAY 41-4109 accelerates and misdirects capsid assembly in vitro and stabilizes preformed capsids up to a ratio of one inhibitor molecule per two dimers[2]. It inhibits HBV DNA release and cytoplasmic HBcAg levels equally effectively, with IC50s of 32.6 and 132 nM in HepG2.2.15 cells, respectively, indicating dose-dependent anti-HBV mechanisms associated with HBcAg inhibition[3].
In vivo	BAY 41-4109 effectively diminishes viral DNA levels in both the liver and plasma in a dose-dependent fashion, showing efficacy on par with 3TC. It also decreases the hepatitis B virus core antigen (HBcAg) in the livers of HBV-transgenic mice. Pharmacokinetic evaluations reveal its rapid absorption and a bioavailability rate of 30%, with dose-proportional plasma concentrations observed, reaching approximately 60% in rats and dogs[1]. Furthermore, BAY41-4109 hampers virus production in vivo by targeting the viral capsid, demonstrating its mechanism of action[2].
Cell Research	Cellular metabolism is evaluated by MTT colorimetry. HepG2.2.15 cells are plated at a density of 2 × 103 cells per well in 96-well plates. After 8 d of treatment with different concentrations of each antiviral compound, 20 μL of MTT solution (5 g/L) are added to each well and incubated at 37°C for 4 h. Next, 150 μL of DMSO is added and stirred for 10 min to dissolve the crystals. Absorbance values are recorded at 490 nm by using an ELISA reader. The MTT values are calculated using the curve regression equation[3].

Solubility Information

Solubility	DMSO: 50 mg/mL (126.34 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

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.

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.
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.