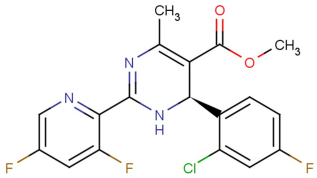
Data Sheet (Cat.No.T10480)

TargetMol
A DRUG SCREENING EXPERT

Bay 41-4109 (less active enantiomer)

Chemical Properties



CAS No.:	476617-51-3
Formula:	C18H13ClF3N3O2
Molecular Weight:	395.76
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	Bay 41-4109 less active enantiomer shows less activity than Bay 41-4109. BAY 41-4109 is a potent HBV inhibitor (IC50: 53 nM).
Targets(IC_{50})	HBV, Bay 41-4109: 53 nM
In vitro	BAY 41-4109 is able to both accelerate and misdirect capsid assembly in vitro. Preformed capsids are stabilized by BAY 41-4109, up to a ratio of one inhibitor molecule per two dimers [2]. In HepG2.2.15 cells, BAY 41-4109 is equally effective at inhibiting HBV DNA release and the cytoplasmic HBcAg level (IC50s: 32.6 and 132 nM). HBV DNA and HBcAg are inhibited in a dose-dependent manner [3].
In vivo	BAY 41-4109 reduces viral DNA in the liver and in the plasma dose-dependently with efficacy comparable to 3TC. BAY 41 -4109 reduces the hepatitis B virus core antigen (HBcAg) in livers of HBV-transgenic mice. Pharmacokinetic studies in mice have shown rapid absorption, a bioavailability of 30%, and dose-proportional plasma concentrations, about 60% in rats and dogs [1]. BAY41-4109 inhibits virus production in vivo by a mechanism that targets the viral capsid [2].

Solubility Information

Solubility	DMSO: 37 mg/mL (93.49 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.527 mL	12.634 mL	25.268 mL
5 mM	0.505 mL	2.527 mL	5.054 mL
10 mM	0.253 mL	1.263 mL	2.527 mL
50 mM	0.051 mL	0.253 mL	0.505 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. 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.
2. 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.
3. 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.

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