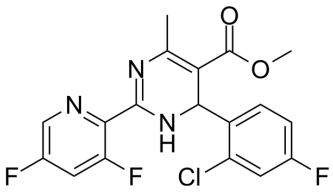
Bay 41-4109 racemate

Cat. No.:	HY-100029A
CAS No.:	298708-79-9
Molecular Formula:	$C_{18}H_{13}ClF_3N_3O_2$
Molecular Weight:	395.76
Target:	HBV
Pathway:	Anti-infection
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (126.34 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
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

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 2.5 mg/mL (6.32 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

BAY 41-4109 racemate is the racemate of BAY 41-4109. BAY 41-4109 is a potent inhibitor of human hepatitis B virus (HBV) with an IC_{50} of 53 nM.

IC_{50} & Target

IC50: 53 nM (HBV)[1]

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]. BAY 41-4109 is equally effective at inhibiting HBV DNA release and the cytoplasmic HBcAg level, with IC_{50}s of 32.6 and 132 nM in HepG2.2.15 cells, respectively. HBV DNA and HBcAg are inhibited in a dose-dependent manner, indicating that the anti-HBV mechanisms are associated with and dependent on the rate of HBcAg inhibition[3].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

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 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]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay [3]	Cellular metabolism is evaluated by MTT colorimetry. HepG2.2.15 cells are plated at a density of 2×10^3 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]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [1]	Mice: The HBV-transgenic mice are used in the study. Compounds (BAY 41-4109) are formulated as a suspension in 0.5% Tylose and administered per os to mice two times/day for a 28 day period. The 0.5% Tylose serves as a placebo. Six hours after the last treatment, the animals are sacrificed and livers are removed and immediately frozen for subsequent analysis. Blood is obtained by cardiac puncture of the anesthesized animals[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cell Mol Gastroenterol Hepatol. 2021 Dec 8;S2352-345X(21)00249-6.
- J Virol. 2022 Oct 13;e0136222.

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REFERENCES

[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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