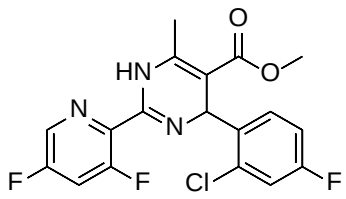
Product data sheet

MedKoo Cat#: 530573 Name: BAY41-4109 racemic CAS#: 298708-79-9 (racemic) Chemical Formula: $C_{18}H_{13}ClF_3N_3O_2$ Exact Mass: 395.0648 Molecular Weight: 395.77	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
BAY41-4109 racemic is a mixture of R-isomer of BAY41-4109 and S-isomer of BAY41-4109. BAY-41-4109 is a heteroaryldihydropyrimidine (HAP) antiviral compound effective on Hepatitis B virus (HBV) capsid assembly and on preformed HBV capsids.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	89.50	226.14
Ethanol	11.0	27.79

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.53 mL	12.63 mL	25.27 mL
5 mM	0.51 mL	2.53 mL	5.05 mL
10 mM	0.25 mL	1.26 mL	2.53 mL
50 mM	0.05 mL	0.25 mL	0.51 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Billioud G, Pichoud C, Puerstinger G, Neyts J, Zoulim F. The main hepatitis B virus (HBV) mutants resistant to nucleoside analogs are susceptible in vitro to non-nucleoside inhibitors of HBV replication. Antiviral Res. 2011 Nov;92(2):271-6. doi: 10.1016/j.antiviral.2011.08.012. Epub 2011 Aug 18. PMID: 21871497.
2. Wu GY, Zheng XJ, Yin CC, Jiang D, Zhu L, Liu Y, Wei L, Wang Y, Chen HS. Inhibition of hepatitis B virus replication by Bay 41-4109 and its association with nucleocapsid disassembly. J Chemother. 2008 Aug;20(4):458-67. doi: 10.1179/joc.2008.20.4.458. PMID: 18676226.

In vivo study

1. Brezillon N, Brunelle MN, Massinet H, Giang E, Lamant C, DaSilva L, Berissi S, Belghiti J, Hannoun L, Puerstinger G, Wimmer E, Neyts J, Hantz O, Soussan P, Morosan S, Kremsdorf D. Antiviral activity of Bay 41-4109 on hepatitis B virus in humanized Alb-uPA/SCID mice. PLoS One. 2011;6(12):e25096. doi: 10.1371/journal.pone.0025096. Epub 2011 Dec 5. PMID: 22162746; PMCID: PMC3230577.
2. Weber O, Schlemmer KH, Hartmann E, Hagelschuer I, Paessens A, Graef E, Deres K, Goldmann S, Niewoehner U, Stoltefuss J, Haebich D, Ruebsamen-Waigmann H, Wohlfeil S. 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. doi: 10.1016/s0166-3542(01)00216-9. PMID: 12062392.

Product data sheet

7. Bioactivity

Biological target: BAY 41-4109 is an inhibitor of human hepatitis B virus (HBV) with an IC50 of 53 nM.

In vitro activity

HepG2.2.15 cells were used to investigate the antiviral effects of Bay 41-4109 by using real-time polymerase chain reaction (PCR), western blotting, and immunofluorescence. The C terminally truncated core protein was expressed and purified. Changes in hepatitis B capsid formation were assayed by dynamic light scattering and transmission electronic microscopy. Bay 41-4109 was found to be a highly selective and potent inhibitor of hepatitis B virus replication in HepG2.2.15 cells. This compound was equally effective at inhibiting HBV DNA release and the cytoplasmic HBcAg level, with 50% inhibitory concentrations of 32.6 and 132 nM, respectively. HBV DNA and HBcAg were inhibited in a dose-dependent manner, indicating that the anti-HBV mechanisms are associated with and dependent on the rate of HBcAg inhibition. Bay 41-4109 treatment disassembled the core capsids and separated them into monomers or dimers, the form in which they could be further degraded into peptides. The core protein assembled in a misdirected manner cannot function effectively. These results suggest that, based on its particular activities, Bay 41-4109 is a promising anti-HBV candidate.

Reference: J Chemother. 2008 Aug;20(4):458-67. https://www.tandfonline.com/doi/abs/10.1179/joc.2008.20.4.458

In vivo activity

The antiviral effect of Bay 41-4109 was evaluated in a mouse model with humanized liver. Alb-uPA/SCID mice were transplanted with human hepatocytes and infected with HBV (hepatitis B virus). Ten days post-infection, the mice were treated with Bay 41-4109 for five days. During the 30 days of follow-up, the HBV load was evaluated by quantitative PCR. At the end of treatment, decreased HBV viremia of about 1 log(10) copies/ml was observed. By contrast, increased HBV viremia of about 0.5 log(10) copies/ml was measured in the control group. Five days after the end of treatment, a rebound of HBV viremia occurred in the treated group. Furthermore, 15 days after treatment discontinuation, a similar expression of the viral capsid was evidenced in liver biopsies. These findings demonstrate that Bay 41-4109 displayed antiviral properties against HBV in humanized Alb-uPA/SCID mice.

Reference: PLoS One. 2011;6(12):e25096. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3230577/#pone.0025096-Weber1

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.