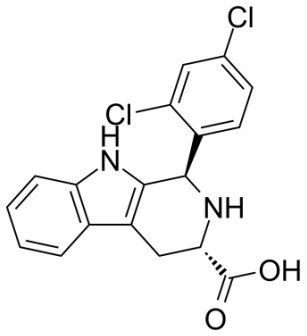
MMV008138

Cat. No.:	HY-123561
CAS No.:	1679333-73-3
Molecular Formula:	$C_{18}H_{14}Cl_2N_2O_2$
Molecular Weight:	361.22
Target:	Parasite
Pathway:	Anti-infection

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (346.05 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.7684 mL	13.8420 mL	27.6840 mL
	5 mM	0.5537 mL	2.7684 mL	5.5368 mL
	10 mM	0.2768 mL	1.3842 mL	2.7684 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: ≥ 2.08 mg/mL (5.76 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (5.76 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

MMV008138 is a species-selective IspD (enzyme 2-C-methyl-d-erythritol 4-phosphate cytidylyltransferase)-targeting antimalarial agent, with an IC_{50} of 44 nM for *Pf*IspD (P. falciparum IspD). MMV008138 inhibits the growth of P. falciparum Dd2 strain with an IC_{50} of 250 nM[1][2].

IC_{50} & Target

IC50: 44 nM (PfIspD)[1]

In Vitro

MMV008138 targets the enzyme IspD in the MEP pathway of P. falciparum[1].
MMV008138 does not target human IspD[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Ghavami M, et al. Biological Studies and Target Engagement of the 2- C-Methyl-d-Erythritol 4-Phosphate Cytidylyltransferase (IspD)-Targeting Antimalarial Agent (1 R,3 S)-MMV008138 and Analogs. ACS Infect Dis. 2018 Apr 13;4(4):549-559.

[2]. Yao ZK, et al. Determination of the active stereoisomer of the MEP pathway-targeting antimalarial agent MMV008138, and initial structure-activity studies. Bioorg Med Chem Lett. 2015 Apr 1;25(7):1515-9.

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