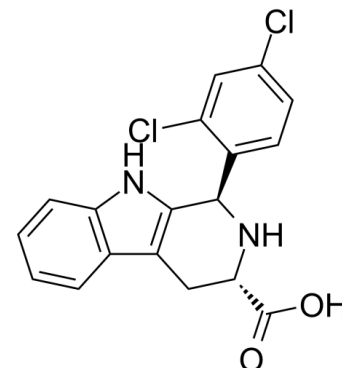


Data Sheet

Product Name:	MMV008138
Cat. No.:	CS-0092783
CAS No.:	1679333-73-3
Molecular Formula:	C ₁₈ H ₁₄ Cl ₂ N ₂ O ₂
Molecular Weight:	361.22
Target:	Parasite
Pathway:	Anti-infection
Solubility:	DMSO : 125 mg/mL (346.05 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

MMV008138 is a species-selective **IspD (enzyme 2-C-methyl-d-erythritol 4-phosphate cytidyltransferase)**-targeting antimalarial agent, with an **IC₅₀** of 44 nM for **PfIspD** (*P. falciparum* IspD). MMV008138 inhibits the growth of *P. falciparum* Dd2 strain with an **IC₅₀** of 250 nM^{[1][2]}. **IC₅₀ & 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].

References:

[1]. Ghavami M, et al. Biological Studies and Target Engagement of the 2- C-Methyl-d-Erythritol 4-Phosphate Cytidyltransferase (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.

CAIndexNames:

1H-Pyrido[3,4-b]indole-3-carboxylic acid, 1-(2,4-dichlorophenyl)-2,3,4,9-tetrahydro-, (1R,3S)-

SMILES:

O=C([C@@H]1CC2=C([C@@H](C3=CC=C(C)C=C3Cl)N1)NC4=C2C=CC=C4)O

Caution: Product has not been fully validated for medical applications. For research use only.

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