Mtb ATP synthase-IN-1

Cat. No.: HY-146388

CAS No.: 2642394-38-3

Molecular Formula: $C_{17}H_{13}N_3O_4$

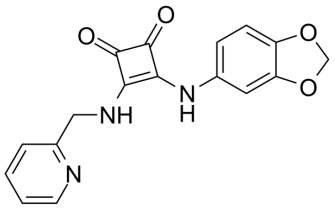
Molecular Weight: 323.3

Target: Bacterial; ATP Synthase

Pathway: Anti-infection; Membrane Transporter/Ion Channel

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 (386.64 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.0931 mL	15.4655 mL	30.9310 mL
	5 mM	0.6186 mL	3.0931 mL	6.1862 mL
	10 mM	0.3093 mL	1.5466 mL	3.0931 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 (6.43 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Mtb ATP synthase-IN-1 (compound 6ab) is a potent ***Mycobacterium tuberculosis*** (***Mtb***) ATP synthase inhibitor, with MIC of 0.452-0.499 μg/mL against Mtb. Mtb ATP synthase-IN-1 has good metabolic stability, low cytotoxicity (Vero IC_{50} > 64 μg/mL), and acceptable oral bioavailability. Mtb ATP synthase-IN-1 can be used for researching anti-mycobacterium[1].

IC_{50} & Target

MIC: 0.452-0.499 μg/mL (Mtb)[1]

In Vivo

Mtb ATP synthase-IN-1 (50 mg/kg for PO, 5 mg/kg for IV; single dosage) exhibits good metabolic stability and acceptable oral bioavailability[1].

Pharmacokinetic Parameters of Mtb ATP synthase-IN-1 in male CD-1 mouse[1].

	PO (50 mg/kg)	IV (5 mg/kg)

C_{max} (ng/mL)	1333	1241
T_{max} (h)	0.83	
$T_{1/2}$ (h)	0.51	0.33
AUC_{0-t} (ng/mL·h)	2197	1667
$AUC_{0-\infty}$ (ng/mL·h)	2198	1672
$MRT_{0-\infty}$ (ng/mL)	1.36	0.28
CL (mL/min/kg)		51.4
F (%)	13.1	

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

Animal Model:	Male CD-1 mouse[1]
Dosage:	50 and 5 mg/kg
Administration:	50 mg/kg for PO, 5 mg/kg for IV; single dosage (Pharmacokinetics Analysis)
Result:	Exhibited good metabolic stability and acceptable oral bioavailability.

REFERENCES

[1]. Li P, et al. Design, synthesis and biological evaluation of diamino substituted cyclobut-3-ene-1,2-dione derivatives for the treatment of drug-resistant tuberculosis. Eur J Med Chem. 2020;206:112538.

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