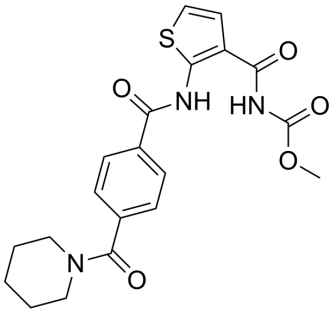
DprE1-IN-4

Cat. No.:	HY-138671
CAS No.:	2419160-96-4
Molecular Formula:	$C_{20}H_{21}N_3O_5S$
Molecular Weight:	415.46
Target:	Bacterial
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	DprE1-IN-4 is a potent and orally active noncovalent DprE1 inhibitor with an IC50 of 0.90 μg/mL. DprE1-IN-4 exhibits potent in vitro activity against M. tuberculosis H37Rv and drug-resistant tuberculosis strain with MIC values of 0.12 μg/mL and 0.24 μg/mL, respectively. DprE1-IN-4 displays acceptable pharmacokinetic property and shows significant bactericidal activity in an acute mouse model of tuberculosis.
IC_{50} & Target	IC50: 0.9±0.2 μg/mL (DprE1)[1]
In Vitro	DprE1-IN-4 displays potent activity against?M. tuberculosis, it is against isolated clinical strains H37Rv, 13946a, 14862b and PBTZ169-resistant strain with MIC values of 0.12 μg/mL, 0.24 μg/mL, 0.24 μg/mL and 0.48 μg/mL, respectively[1]. DprE1-IN-4 (0.76-16 μg/mL) shows a decrease in potency against only DprE1-overexpressing strains but not against DprE2-overexpressing and wild-type strains.?The IC_{50} value is 0.9±0.2 μg/mL for ?DprE1[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	DprE1-IN-4 exhibits acceptable pharmacokinetic property after p.o. and i.v., DprE1-IN-4 (oral administration, 50 mg/kg) exhibits high plasma exposure ($(AUC)_{0-\infty}$=657 ng·h/mL) and high maximum plasma concentration (C_{max}=486 ng/mL). It exhibits oral bioavailability (F=7.9%) and is deemed worthy of further evaluation in?in vivo?efficacy studies[1]. DprE1-IN-4 (oral gavage; 100 mg/kg; once daily; 3 weeks) showed potent?in vivo?activity, reducing the bacterial burden in the lungs by 2.02?log_{10}?CFU compared with the untreated control group[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Pengxu Wang, et al. Discovery of Novel Thiophene-arylamide Derivatives as DprE1 Inhibitors with Potent Antimycobacterial Activities. J Med Chem. 2021 May 13;64(9):6241-6261.

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