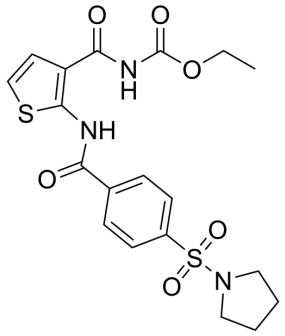
DprE1-IN-1

Cat. No.:	HY-144341
CAS No.:	920459-41-2
Molecular Formula:	$C_{19}H_{21}N_3O_6S_2$
Molecular Weight:	451.52
Target:	Bacterial
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

DprE1-IN-1 is a potent, orally active DprE1 inhibitor with favorable hepatocyte stability, low cytotoxicity and low hERG channel inhibition. DprE1-IN-1 displays potent activity against both agent-susceptible and clinically isolated drug-resistant Tuberculosis strains with MICs10 CFU reduction in macrophages.

IC_{50} & Target

MICs: <0.1 μg/mL (Tuberculosis strains)[1]

In Vitro

DprE1-IN-1 (compound 17b) (64 to 0.26 μg/mL; 48 hours) has high safety with low cytotoxicity towards HepG2, J774A.1 macrophage cells (IC_{50}>60 μg/mL) and Vero (IC_{50}=58.18 μg/mL) alongside potent efficacy and good druggability[1].
DprE1-IN-1 can reduce 1.19 and 1.29 log_{10} CFU M. tuberculosis in J774A.1 macrophages at 5 μg/mL and 10 μg/mL, respectively, for 3 days treatment[1].
DprE1-IN-1 (compound 17b) (1 μM; 0-120 minutes) has high stability in human and mice hepatocytes (remaining of 42% and 49.7%, respectively; $t_{1/2}$ of 24.0 and 29.7 min, respectively)[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Cytotoxicity Assay

Cell Line:	Vero, HepG2 and mouse J774A.1 macrophage cells[1]
Concentration:	64 to 0.26 μg/mL
Incubation Time:	48 hours
Result:	Displayed high safety with low cytotoxicity towards HepG2, J774A.1 macrophage cells (IC_{50}>60 μg/mL) and Vero (IC_{50}=58.18 μg/mL) alongside potent efficacy and good druggability.

In Vivo

DprE1-IN-1 (100 mg/kg; oral gavage; 5 days per week from day 10 until day 30) can reduce the bacterial burden in the lungs by 0.54 log_{10} CFU after three weeks of treatment in M. tuberculosis H37Rv infected mice[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Female SPF Balb/c mice (18-20 g) (M. tuberculosis H37Rv infected)[1]
Dosage:	100 mg/kg

Administration:	Oral gavage; 5 days per week from day 10 until day 30
Result:	Reduced the bacterial burden in the lungs by 0.54 log_{10} CFU compared with the untreated control group after three weeks of treatment.

REFERENCES

[1]. Qin R, et al. Identification of thiophene-benzenesulfonamide derivatives for the treatment of multidrug-resistant tuberculosis. Eur J Med Chem. 2022;231:114145.

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