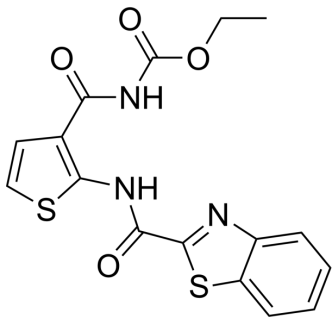
TCA1

Cat. No.:	HY-12904
CAS No.:	864941-32-2
Molecular Formula:	$C_{16}H_{13}N_3O_4S_2$
Molecular Weight:	375.42
Target:	Bacterial
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 (332.96 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.6637 mL	13.3184 mL	26.6368 mL
5 mM	0.5327 mL	2.6637 mL	5.3274 mL
10 mM	0.2664 mL	1.3318 mL	2.6637 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

TCA1 is a small molecule with activity against agent-susceptible and -resistant ***Mycobacterium tuberculosis (Mtb)***. TCA1 inhibits enzymes involved in cell wall and molybdenum cofactor biosynthesis, such as DprE1 and MoeW[1].

In Vitro

TCA1 shows bactericidal activity against both replicating (WT and drug resistant) and nonreplicating Mycobacterium tuberculosis (Mtb). TCA1 inhibits biofilm formation by Mtb H37Rv[1].

TCA1 shows selective inhibitory activity against bacterial growth-it is inactive against Escherichia coli, Staphylococcus aureus, and Pseudomonas aeruginosa, suggesting that the target for its bactericidal activity is specific to the genus Mycobacterium[1].

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

In Vivo

TCA1 (40 mg/kg; oral gavage; 1 time/d for 5 d/week; for 4 weeks) is efficacious in acute and chronic Mtb infection mouse models[1].

In a mouse model of Mtb infection, after i.v. administration, TCA1 exhibits a low clearance and steady-state volume of distribution, with an elimination half-life of 0.73 h. After oral administration of 20 and 50 mg/kg in solution formulation, TCA1 shows a high C_{max} (2122 and 5653 nM, respectively), moderate exposure with oral bioavailability ranging from 19% to

	46%, and a half-life of 1.8 h[1].BALB/c mice infected with Mtb H37Rv[1]40 mg/kgOral gavage; 1 time/d for 5 d/week; for 4 weeksEffectively inhibits Mtb in vivo.

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

REFERENCES

[1]. Feng Wang, et al. Identification of a small molecule with activity against drug-resistant and persistent tuberculosis. Proc Natl Acad Sci U S A. 2013 Jul 2;110(27):E2510-7.

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