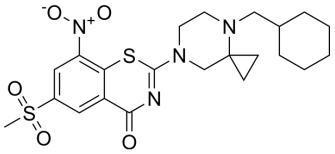
Antitubercular agent-32

Cat. No.:	HY-151340
CAS No.:	2498762-42-6
Molecular Formula:	$C_{22}H_{28}N_4O_5S_2$
Molecular Weight:	492.61
Target:	Bacterial
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

Antitubercular agent-32 is a derivate of Benzothiazinone (HY-13579A), inhibits M. tuberculosis, and shows improved metabolic stability and enhanced water solubility. Antitubercular agent-32 exerts antitubercular effect by targeting decaprenylphosphoryl-β-D-ribose 2'-oxidase (DprE1, IC_{50}=3.9 μM)[1].

In Vitro

Antitubercular agent-32 (compound 8) (0-7.5 mg/mL; 48 h) shows low cytotoxicity and inhibits M. tuberculosis H37Rv with the minimum inhibition concentration (MIC) of 40 nM[1].

Antitubercular agent-32 (0-20 μM) inhibits decaprenylphosphoryl-β-D-ribose 2'-oxidase (DprE1, 0.5 μM), an enzyme essential for the biosynthesis of mycobacterial cell wall, with an IC_{50} value of 3.9 μM[1].

Antitubercular agent-32 (1 μM; 10 min) exhibits metabolic stability in the liver microsomal metabolic of both human (HLM) and mouse (MLM), with fast clearance rates of 77 mL/min/kg (HLM) and 163 mL/min/kg (MLM), respectively[1].

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

Cell Cytotoxicity Assay[1]

Cell Line:	HepG2 cells
Concentration:	0, 15, 30, 75, 150, 300, 750, 1500, 3000, and 7500 ng/mL
Incubation Time:	48 hours
Result:	There were no significantly growth inhibitions of HepG2 cells.

REFERENCES

[1]. Shi R, et al. Development of 6-Methanesulfonyl-8-nitrobenzothiazinone Based Antitubercular Agents. ACS Med Chem Lett. 2022 Mar 10;13(4):593-598.

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