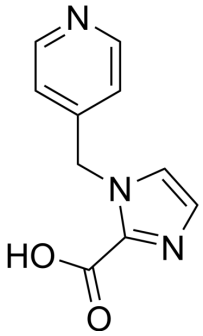
Metallo-β-lactamase-IN-6

Cat. No.:	HY-143414
CAS No.:	1439899-44-1
Molecular Formula:	$C_{10}H_9N_3O_2$
Molecular Weight:	203.2
Target:	Bacterial; Beta-lactamase
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Metallo-β-lactamase-IN-6 is a potent VIM-Type metallo-β-lactamase inhibitor with IC_{50}s of 0.56 μM, 29.50 μM and 5.78 μM for VIM-2, VIM-1 and VIM-5. Metallo-β-lactamase-IN-6 displays potent synergistic antibacterial activity with Meropenem against engineered Escherichia coli strains and intractable clinically isolated Pseudomonas aeruginosa producing VIM-2 MBL[1].
IC_{50} & Target	IC_{50}: 0.56 μM (VIM-2), 29.50 μM (VIM-1), 5.78 μM (VIM-5)[1]
In Vitro	Metallo-β-lactamase-IN-6 (compound 55) (10 μM; 18 - 20 hours) can potentiate Meropenem activity against VIM-2 mediated antibacterial resistance with FIC index values of 0.05[1]. Metallo-β-lactamase-IN-6 (1, 10, 100 μM; 18 - 20 hours) can penetrate E. coli outer membrane and restore Meropenem activity against PBP3 by blocking destructive effect of VIM-2 enzyme to Meropenem[1]. Metallo-β-lactamase-IN-6 (100 μM) potentiates the antibacterial activity of Meropenem against PA W35 with FIC index values of 0.25[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Metallo-β-lactamase-IN-6 (100 mg/kg; IP; single) reaches plasma concentration peak about 9 min after injection with an effective maximum concentration of 142.8 μg/ml, and the $T_{1/2}$ is 1.24 hours[1]. Metallo-β-lactamase-IN-6 (500, 1000, or 2000 mg/kg; IP; single, observe for 14 days) does not result in any significant toxic effects and is well-tolerated by mice at a dose of ≤ 2000 mg/kg[1]. Pharmacokinetic Parameters of Metallo-β-lactamase-IN-6 in male female ICR mice[1].

	IP (100 mg/kg)
$T_{1/2}$ (h)	1.243
C_{max} (μg/mL)	142.8
T_{max} (h)	0.151
Vd (mL/kg)	535.804

CL (mL/h/kg)	248.512
$AUC_{0-\infty}$ (μg/mL·h)	896

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

Animal Model:	Female ICR mice (180-220 g)[1]
Dosage:	100 mg/kg
Administration:	IP; single (Pharmacokinetics Analysis)
Result:	Plasma concentration reached its peak about 9 min after injection with an effective maximum concentration of 142.8 μg/ml, and the $T_{1/2}$ was 1.24 hours.

Animal Model:	Female ICR mice (n=5)[1]
Dosage:	500, 1000, or 2000 mg/kg
Administration:	IP; single, observed for 14 days
Result:	Did not result in any significant toxic effects and was well-tolerated by mice at a dose of ≤ 2000 mg/kg.

REFERENCES

[1]. Yan YH, Li W, Chen W, et al. Structure-guided optimization of 1H-imidazole-2-carboxylic acid derivatives affording potent VIM-Type metallo-β-lactamase inhibitors. Eur J Med Chem. 2022;228:113965.

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