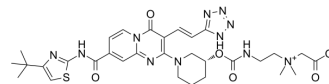


D13-9001

Cat. No.:	HY-124819
CAS No.:	957471-96-4
Molecular Formula:	C ₃₁ H ₃₉ N ₁₁ O ₆ S
Molecular Weight:	693.78
Target:	Bacterial
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	D13-9001 is a potent AcrB (AcrAB-TolC efflux pump subunit) and MexB (MexAB-OprM efflux pump subunit) inhibitor with the K _D values of 1.15 μM and 3.57 μM in <i>E. coli</i> and <i>P. aeruginosa</i> , respectively ^[1] . D13-9001 exhibits antibiotic activities ^[2] .								
IC₅₀ & Target	KD: 1.15 μM (AcrB), 3.57 μM (MexB) ^[1]								
In Vitro	D13-9001 exhibits high solubility and a good safety profile ^[3] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.								
In Vivo	D13-9001 (1.25-20 mg/kg; intravenous drip infusion; 2 hours) with aztreonam (AZT) gives improved survival rates in a lethal pneumonia rats at the end of day seven compared with AZT treated alone ^[3] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.								
	<table border="1"> <tr> <td>Animal Model:</td> <td>SD rats (Pulmonary infection by <i>P. aeruginosa</i> PAM1020)^[3]</td> </tr> <tr> <td>Dosage:</td> <td>1.25 mg/kg, 5 mg/kg, 20 mg/kg</td> </tr> <tr> <td>Administration:</td> <td>Intravenous drip infusion; 2 hours</td> </tr> <tr> <td>Result:</td> <td>The combination of 1.25, 5, and 20 mg/kg of D13-9001 with 1000 mg/kg of AZT gave improved survival rates at the end of day seven, whereas no obvious effect was observed on treatment with AZT alone.</td> </tr> </table>	Animal Model:	SD rats (Pulmonary infection by <i>P. aeruginosa</i> PAM1020) ^[3]	Dosage:	1.25 mg/kg, 5 mg/kg, 20 mg/kg	Administration:	Intravenous drip infusion; 2 hours	Result:	The combination of 1.25, 5, and 20 mg/kg of D13-9001 with 1000 mg/kg of AZT gave improved survival rates at the end of day seven, whereas no obvious effect was observed on treatment with AZT alone.
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REFERENCES

- [1]. Opperman TJ, et al. Recent advances toward a molecular mechanism of efflux pump inhibition. *Front Microbiol.* 2015 May 5; 6:421.
- [2]. Zuo Z, et al. Insights into the Inhibitory Mechanism of D13-9001 to the Multidrug Transporter AcrB through Molecular Dynamics Simulations. *J Phys Chem B.* 2016 Mar 10;120(9):2145-54.
- [3]. Yoshida K, et al. MexAB-OprM specific efflux pump inhibitors in *Pseudomonas aeruginosa*. Part 7: highly soluble and in vivo active quaternary ammonium analogue D13-9001, a potential preclinical candidate. *Bioorg Med Chem.* 2007 Nov 15;15(22):7087-97.

Caution: Product has not been fully validated for medical applications. For research use only.

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