Antitubercular agent-31

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Cat. No.: CAS No.: Molecular Formula:	HY-151339 2764818-29-1 C ₂₀ H ₂₄ F ₂ N ₄ O ₅ S ₂	. <i>(</i> 0) ₽
Molecular Weight:	502.56	
Target:	Bacterial	
Pathway:	Anti-infection	
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.	

Description	Antitubercular agent-31 (Compound 2) is an antitubercular agent with an MIC of 0.03 μ M against M. tuberculosis H37Rv. Antitubercular agent-31 also inhibits DprE1 with an IC ₅₀ of 1.1 μ M ^[1] .									
IC ₅₀ & Target	IC ₅₀ : 1.1 μM (DprE1) ^[1]									
In Vitro	Antitubercular agent-31 (Compound 2) shows aqueous solubility of 0.81 μg/mL in phosphate buffer pH 7.4. The plasma protein binding property is 97.9% ^[1] . Antitubercular agent-31 shows acceptable liver microsomal stability in human and mouse liver microsomes ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.									
In Vivo	Antitubercular agent-31 (10 or 2 mg/kg; p.o. or i.v.; once) displays an acceptable pharmacokinetics (PK) profile with only dosing i.v., shows either poor membrane permeability or rapid clearance rate in vivo ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.									
	Animal Model:	Male Balb/c mice ^[1]								
	Dosage:	10 mg/kg or 2 mg/kg								
	Administration:	Oral (10 mg/kg) or intravenous (2 mg/kg) administration (Pharmacokinetic Analysis)								
	Result:	PK data for Antitubercular agent-31 (Compound 2), iv, $2mg/kg^{[1]}$.								
		T _{max} (h)	C _{max} (ng/mL)	AUC _{0-t} (h*ng/mL)	AUC _{0-∞} (h*ng/mL)	T _{1/2} (h)	CL/F (mL/h/kg)	MRT _{0-∞} (h)		
		0.1±0.0	463.4±103.4	158.2±18.8	161.3±18.6	0.3±0.0	12515.5±1379.7	0.4±0.0		
		No compound signal was detected at oral administration.								

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.

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

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