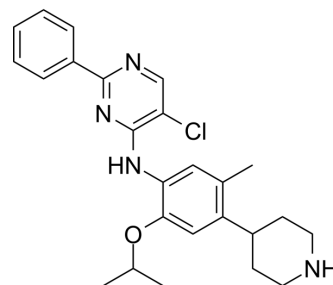


Antituberculosis agent-9

Cat. No.:	HY-149064
CAS No.:	2998587-72-5
Molecular Formula:	C ₂₅ H ₂₉ ClN ₄ O
Molecular Weight:	436.98
Target:	Bacterial
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Antituberculosis agent-9 (Compound 5a) is an orally active antitubercular agent with an MIC of 0.5 µg/mL against H37Ra ^[1] .																	
In Vitro	<p>Antituberculosis agent-9 (Compound 5a; 48 h) shows cytotoxicity against HepG2 cells with an IC₅₀ value of 3.1 µM^[1].</p> <p>Antituberculosis agent-9 (6 days) also shows inhibitory activities against MRSA, <i>M. abscessus</i> and <i>M. smegmatis</i> with MICs of 4.0 µg/mL^[1].</p> <p>Antituberculosis agent-9 (6 days) shows inhibitory activities against clinical isolates of <i>M. tuberculosis</i> with MICs of 0.5, 0.5, 0.5, 1.0 and 1.0 µg/mL for H37Rv, K4, K12, K5 and K16, respectively^[1].</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>																	
In Vivo	<p>Antituberculosis agent-9 (Compound 5a; 300 mg/kg; oral; daily for 4 days) shows moderate antitubercular efficacy in mice^[1].</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>																	
	Animal Model:	Female BALB/c mice, autoluminescent Mtb infection model ^[1]																
	Dosage:	300 mg/kg																
	Administration:	Oral administration, daily for 4 days																
	Result:	There was a relative light unit (RLU) reduction of 0.5 log ₁₀ in live mice, compared to the control group (CMC-Na).																
	Animal Model:	Sprague-Dawley rats ^[1]																
	Dosage:	5 or 15 mg/kg																
	Administration:	IV or PO (Pharmacokinetic Analysis)																
	Result:	Pharmacokinetic Parameters of Antituberculosis agent-9 (Compound 5a) In Vivo ^[1]																
		<table border="1"> <thead> <tr> <th>cpd.</th> <th>administration</th> <th>C_{max} (µg/L)</th> <th>T_{max} (h)</th> <th>T_{1/2} (h)</th> <th>Cl_z (L/h/kg)</th> <th>AUC_{0-t} (µg·h/L)</th> <th>F %</th> </tr> </thead> <tbody> <tr> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	cpd.	administration	C _{max} (µg/L)	T _{max} (h)	T _{1/2} (h)	Cl _z (L/h/kg)	AUC _{0-t} (µg·h/L)	F %								
cpd.	administration	C _{max} (µg/L)	T _{max} (h)	T _{1/2} (h)	Cl _z (L/h/kg)	AUC _{0-t} (µg·h/L)	F %											

						g/L·h)	
Antituberculosis agent-9 (Compound 5a)	iv (5 mg/kg)	595 ± 62		26.2 ± 0.9	1.5 ± 0.3	1694 ± 201	
	po (15 mg/kg)	108 ± 18	>24			2079 ± 274	40.7

REFERENCES

[1]. Li C, et al. Structure-Activity Relationship of Novel Pyrimidine Derivatives with Potent Inhibitory Activities against Mycobacterium tuberculosis. J Med Chem. 2023 Feb 23;66(4):2699-2716.

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

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