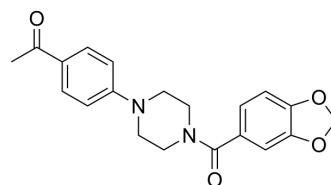


ML406

Cat. No.:	HY-124781		
CAS No.:	774589-47-8		
Molecular Formula:	C ₂₀ H ₂₀ N ₂ O ₄		
Molecular Weight:	352.38		
Target:	Bacterial; Antibiotic		
Pathway:	Anti-infection		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro	DMSO : 100 mg/mL (283.78 mM; Need ultrasonic)			
		Solvent Concentration	Mass	
			1 mg	5 mg
			10 mg	
Preparing Stock Solutions	1 mM	2.8378 mL	14.1892 mL	28.3785 mL
	5 mM	0.5676 mL	2.8378 mL	5.6757 mL
	10 mM	0.2838 mL	1.4189 mL	2.8378 mL
Please refer to the solubility information to select the appropriate solvent.				
In Vivo	<ol style="list-style-type: none"> Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (7.09 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (7.09 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (7.09 mM); Clear solution 			

BIOLOGICAL ACTIVITY

Description	ML406 is a small molecule probe that shows anti-tubercular activity via <i>M. tuberculosis</i> BioA (DAPA synthase) enzyme inhibition with an IC ₅₀ of 30 nM. <i>M. tuberculosis</i> BioA is an enzyme involved in biotin biosynthesis in <i>M. tuberculosis</i> ^[1] .
IC ₅₀ & Target	IC50 30 nM (BioA) ^[1]
In Vitro	ML406 inhibits WT Mycobacterium tuberculosis (Mtb) (H37Rv) growth inhibition with the IC ₅₀ of 3.2 μM. BioA is an enzyme involved in biotin biosynthesis in Mtb that may serve as lead compounds for drug development for tuberculosis (TB) ^[1] .

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

REFERENCES

[1]. Casalena D, et al. Discovery of small molecule probe that shows anti-tubercular activity via Mtb bioA (DAPA synthase) enzyme inhibition. 2014 Apr 15 [updated 2015 Jan 16]. In: Probe Reports from the NIH Molecular Libraries Program [Internet]. Bethesda (MD): National Center for Biotechnology Information (US); 2010-.

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

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