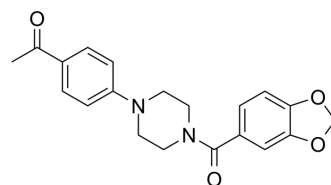


## ML406

Cat. No.:	HY-124781		
CAS No.:	774589-47-8		
Molecular Formula:	C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub>		
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)

Concentration	Solvent	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

- 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 *M. tuberculosis* BioA (DAPA synthase) enzyme inhibition with an IC<sub>50</sub> of 30 nM. *M. tuberculosis* BioA is an enzyme involved in biotin biosynthesis in *M. tuberculosis*<sup>[1]</sup>.

### IC<sub>50</sub> & Target

IC<sub>50</sub> 30 nM (BioA)<sup>[1]</sup>

### In Vitro

ML406 inhibits WT *Mycobacterium tuberculosis* (Mtb) (H37Rv) growth inhibition with the IC<sub>50</sub> 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)<sup>[1]</sup>.

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

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## REFERENCES

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[1]. Dominick Casalena, et al. Discovery of small molecule probe that shows anti-tubercular activity via MtbbioA (DAPA synthase) enzyme inhibition. January 16, 2015.

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

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