

## Mtb ATP synthase-IN-1

## Chemical Properties

CAS No. : 2642394-38-3

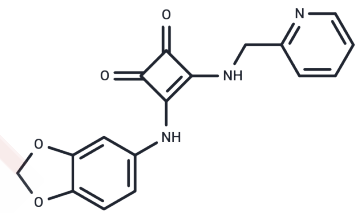
Formula: C<sub>17</sub>H<sub>13</sub>N<sub>3</sub>O<sub>4</sub>

Molecular Weight: 323.30

Store at low temperature

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



## Biological Description

Description	Mtb ATP synthase-IN-1 (compound 6ab) is a potent inhibitor of Mycobacterium tuberculosis (Mtb) ATP synthase (MIC = 0.452-0.499 µg/mL) [1] that can be used in anti-mycobacterium research, showing low cytotoxicity (Vero IC <sub>50</sub> > 64 µg/mL) and acceptable oral bioavailability with good metabolic stability.
Targets(IC <sub>50</sub> )	ATPase, Antibacterial
In vivo	In Male CD-1 mouse, Mtb ATP synthase-IN-1 ( 50 mg / kg for PO, 5 mg / kg for IV ; single dosage ; pharmacokinetics Analysis ) can be Exhibited good metabolic stability and acceptable oral bioavailability[1].

## Solubility Information

Solubility	DMSO: 100 mg/mL (309.31 mM), Sonication is recommended. ( < 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 4 mg/mL (12.37 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

### Preparing Stock Solutions

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	<b>1mg</b>	<b>5mg</b>	<b>10mg</b>
1 mM	3.0931 mL	15.4655 mL	30.931 mL
5 mM	0.6186 mL	3.0931 mL	6.1862 mL
10 mM	0.3093 mL	1.5466 mL	3.0931 mL
50 mM	0.0619 mL	0.3093 mL	0.6186 mL

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Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

### Reference

Li P, et al. Design, synthesis and biological evaluation of diamino substituted cyclobut-3-ene-1,2-dione derivatives for the treatment of drug-resistant tuberculosis. Eur J Med Chem. 2020;206:112538.

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