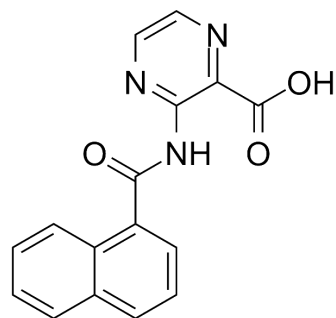


## Mab Aspartate Decarboxylase-IN-1

<b>Cat. No.:</b>	HY-150637
<b>CAS No.:</b>	2755712-12-8
<b>Molecular Formula:</b>	C <sub>16</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub>
<b>Molecular Weight:</b>	293.28
<b>Target:</b>	Bacterial
<b>Pathway:</b>	Anti-infection
<b>Storage:</b>	4°C, sealed storage, away from moisture and light * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



### SOLVENT & SOLUBILITY

<b>In Vitro</b>	DMSO : 16.67 mg/mL (56.84 mM); ultrasonic and warming and heat to 60°C																			
	<table border="1"> <thead> <tr> <th rowspan="2">Solvent Concentration</th> <th colspan="3">Mass</th> </tr> <tr> <th>1 mg</th> <th>5 mg</th> <th>10 mg</th> </tr> </thead> <tbody> <tr> <td><b>1 mM</b></td> <td>3.4097 mL</td> <td>17.0486 mL</td> <td>34.0971 mL</td> </tr> <tr> <td><b>5 mM</b></td> <td>0.6819 mL</td> <td>3.4097 mL</td> <td>6.8194 mL</td> </tr> <tr> <td><b>10 mM</b></td> <td>0.3410 mL</td> <td>1.7049 mL</td> <td>3.4097 mL</td> </tr> </tbody> </table>	Solvent Concentration	Mass			1 mg	5 mg	10 mg	<b>1 mM</b>	3.4097 mL	17.0486 mL	34.0971 mL	<b>5 mM</b>	0.6819 mL	3.4097 mL	6.8194 mL	<b>10 mM</b>	0.3410 mL	1.7049 mL	3.4097 mL
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	Please refer to the solubility information to select the appropriate solvent.																			
<b>In Vivo</b>	<ol style="list-style-type: none"> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 40% PEG300 &gt;&gt; 5% Tween-80 &gt;&gt; 45% saline Solubility: ≥ 1.67 mg/mL (5.69 mM); Clear solution</li> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 90% (20% SBE-β-CD in saline) Solubility: ≥ 1.67 mg/mL (5.69 mM); Clear solution</li> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 90% corn oil Solubility: ≥ 1.67 mg/mL (5.69 mM); Clear solution</li> </ol>																			

### BIOLOGICAL ACTIVITY

<b>Description</b>	Mab Aspartate Decarboxylase-IN-1 is a potent aspartate decarboxylase (PanD) inhibitor with an IC <sub>50</sub> value of 56.3 μM. Mab Aspartate Decarboxylase-IN-1 shows antibacterial activity <sup>[1]</sup> .
<b>IC<sub>50</sub> &amp; Target</b>	IC <sub>50</sub> : 56.3 μM (aspartate decarboxylase (PanD)) <sup>[1]</sup> .
<b>In Vitro</b>	Mab Aspartate Decarboxylase-IN-1 (compound analogue 2) shows inhibits against the mutants Mab PanDE119A, Mab PanDS135A and Mab PanDY126A mutants with the inhibition rates of 70.5%, 74.4%, 81.8%, respectively <sup>[1]</sup> . Mab Aspartate Decarboxylase-IN-1 (0-200 μM) shows inhibition on mycobacterium abscessus (Mab) PanD enzyme activity in

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the conversion of l-Asp to  $\beta$ -Ala with an  $IC_{50}$  value of  $56.3 \pm 4.8 \mu M$ <sup>[1]</sup>.

Mab Aspartate Decarboxylase-IN-1 (0-4 mM) shows antibacterial activity for *M. abscessus* subsp. *abscessus* ATCC 19977 with an  $IC_{50}$  value of 0.7mM, and *M. abscessus* subsp. *bolletii* CCUG 50184T, *M. abscessus* subsp. *massiliense* CCUG 48898T, *M. abscessus* subsp. *abscessus* Bamboo, *M. abscessus* subsp. *abscessus* ATCC 19977 with  $IC_{50}$ s of 1-2 mM<sup>[1]</sup>.

Mab Aspartate Decarboxylase-IN-1 shows mainly electrostatic- and hydrogen bonding interaction with the target enzyme<sup>[1]</sup>. 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]. Saw WG, et al. Structural and Mechanistic Insights into Mycobacterium abscessus Aspartate Decarboxylase PanD and a Pyrazinoic Acid-Derived Inhibitor. ACS Infect Dis. 2022 Jul 8;8(7):1324-1335.

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

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