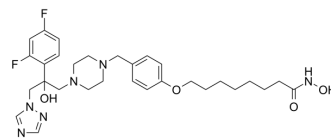


## CYP51/HDAC-IN-1

<b>Cat. No.:</b>	HY-144643
<b>CAS No.:</b>	2502095-64-7
<b>Molecular Formula:</b>	C <sub>30</sub> H <sub>40</sub> F <sub>2</sub> N <sub>6</sub> O <sub>4</sub>
<b>Molecular Weight:</b>	586.67
<b>Target:</b>	Fungal; HDAC; Cytochrome P450
<b>Pathway:</b>	Anti-infection; Cell Cycle/DNA Damage; Epigenetics; Metabolic Enzyme/Protease
<b>Storage:</b>	Please store the product under the recommended conditions in the Certificate of Analysis.



### BIOLOGICAL ACTIVITY

<b>Description</b>	CYP51/HDAC-IN-1 is a potent, orally active CYP51/HDAC dual inhibitor. CYP51/HDAC-IN-1 inhibits important virulence factors and down-regulated resistance-associated genes. CYP51/HDAC-IN-1 exhibits potent therapeutic effects for both tropical candidiasis and cryptococcal meningitis <sup>[1]</sup> .								
<b>IC<sub>50</sub> &amp; Target</b>	CYP51								
<b>In Vitro</b>	<p>CYP51/HDAC-IN-1 (compound A5) exhibits the best inhibitory activity against both <i>Candida tropicalis</i> (<i>C. tropicalis</i>) and <i>Cryptococcus neoformans</i> (<i>C. neoformans</i>) with an MIC<sub>80</sub> of 0.5 µg/mL<sup>[1]</sup>.</p> <p>CYP51/HDAC-IN-1 (human umbilical vein endothelial cell line (HUVEC)) shows low toxicity to human normal cells (IC<sub>50</sub>= 5.9 µg/mL (10.36 µM))<sup>[1]</sup>.</p> <p>CYP51/HDAC-IN-1 inhibits biofilm formation of <i>C. tropicalis</i> and <i>C. neoformans</i> in a dose-dependent manner<sup>[1]</sup>.</p> <p>CYP51/HDAC-IN-1 reduces the virulence of <i>C. neoformans</i> through down-regulating capsule-associated genes CAP10 and CAP60<sup>[1]</sup>.</p> <p>CYP51/HDAC-IN-1 increases the activity against FLC-resistant <i>C. tropicalis</i> by inhibits the overexpression of efflux pump genes, and down-regulated ERG11 gene in ergosterol biosynthetic pathway<sup>[1]</sup>.</p> <p>CYP51/HDAC-IN-1 exhibits HDAC inhibitory activity (IC<sub>50</sub>=2.38 µM) and down-regulated HDAC genes (Rpd3, Hos1, Hos2, Clr61, Clr62, Hda1 and Hos3)<sup>[1]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>								
<b>In Vivo</b>	<p>CYP51/HDAC-IN-1 (20 mg/kg; p.o.; once a day for 5 consecutive days) exhibits potent therapeutic effects for both tropical candidiasis and cryptococcal meningitis (CM)<sup>[1]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p> <table border="1"> <tr> <td>Animal Model:</td> <td>Female ICR mice, 4-6 weeks, 18-20g (injection with <i>C. tropicalis</i> and <i>C. neoformans</i> via tail vein)<sup>[1]</sup></td> </tr> <tr> <td>Dosage:</td> <td>20 mg/kg</td> </tr> <tr> <td>Administration:</td> <td>p.o.; once a day; 5 consecutive days</td> </tr> <tr> <td>Result:</td> <td>Reduced kidney fungal burden and brain fungal burden.</td> </tr> </table>	Animal Model:	Female ICR mice, 4-6 weeks, 18-20g (injection with <i>C. tropicalis</i> and <i>C. neoformans</i> via tail vein) <sup>[1]</sup>	Dosage:	20 mg/kg	Administration:	p.o.; once a day; 5 consecutive days	Result:	Reduced kidney fungal burden and brain fungal burden.
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Dosage:	20 mg/kg								
Administration:	p.o.; once a day; 5 consecutive days								
Result:	Reduced kidney fungal burden and brain fungal burden.								

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## REFERENCES

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[1]. Zhu T, et al. Lanosterol 14 $\alpha$ -demethylase (CYP51)/histone deacetylase (HDAC) dual inhibitors for treatment of *Candida tropicalis* and *Cryptococcus neoformans* infections. *Eur J Med Chem.* 2021. 221:113524.

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

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