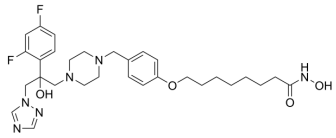
CYP51/HDAC-IN-1

Cat. No.:	HY-144643
CAS No.:	2502095-64-7
Molecular Formula:	$C_{30}H_{40}F_2N_6O_4$
Molecular Weight:	586.67
Target:	Fungal; HDAC; Cytochrome P450
Pathway:	Anti-infection; Cell Cycle/DNA Damage; Epigenetics; Metabolic Enzyme/Protease
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	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[1].
IC_{50} & Target	CYP51
In Vitro	CYP51/HDAC-IN-1 (compound A5) exhibits the best inhibitory activity against both Candida tropicalis (C. tropicalis) and Cryptococcus neoformans (C. neoformans) with an MIC_{80} of 0.5 μg/mL[1]. CYP51/HDAC-IN-1 (human umbilical vein endothelial cell line (HUVEC)) shows low toxicity to human normal cells (IC_{50}= 5.9 μg/mL (10.36 μM))[1]. CYP51/HDAC-IN-1 inhibits biofilm formation of C. tropicalis and C. neoformans in a dose-dependent manner[1]. CYP51/HDAC-IN-1 reduces the virulence of C. neoformans through down-regulating capsule-associated genes CAP10 and CAP60[1]. CYP51/HDAC-IN-1 increases the activity against FLC-resistant C. tropicalis by inhibits the overexpression of efflux pump genes, and down-regulated ERG11 gene in ergosterol biosynthetic pathway[1]. CYP51/HDAC-IN-1 exhibits HDAC inhibitory activity (IC_{50}=2.38 μM) and down-regulated HDAC genes (Rpd3, Hos1, Hos2, Clr61, Clr62, Hda1 and Hos3)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	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)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Female ICR mice, 4-6 weeks, 18-20g (injection with C. tropicalis and C. neoformansvia tail vein)[1]
Dosage:	20 mg/kg
Administration:	p.o.; once a day; 5 consecutive days
Result:	Reduced kidney fungal burden and brain fungal burden.

REFERENCES

[1]. Zhu T, et al. Lanosterol 14α-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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