VT-1598 tosylate

Cat. No.: HY-123777A

CAS No.: 2089321-00-4

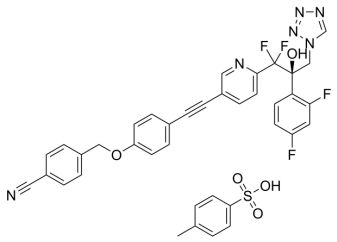
Molecular Formula: $C_{38}H_{28}F_4N_6O_5S$

Molecular Weight: 756.72

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage: Please store the product under the recommended conditions in the Certificate of Analysis.



SOLVENT & SOLUBILITY

In Vitro

DMSO : 150 mg/mL (198.22 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.3215 mL	6.6075 mL	13.2149 mL
	5 mM	0.2643 mL	1.3215 mL	2.6430 mL
	10 mM	0.1321 mL	0.6607 mL	1.3215 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (3.30 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (3.30 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

VT-1598 tosylate is an orally active and selective fungal inhibitor targeting CYP51. VT-1598 tosylate shows anti-fungal activity against C. auris[1][2]. VT-1598 (tosylate) is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

IC_{50} & Target

CYP51[1]

In Vitro

VT-1598 tosylate (0.015-8 μg/mL; 24 h) demonstrates in vitro activity against C. auris[1].
VT-1598 tosylate (0.03125-0.125 μg/mL; 24 h) shows highly effects in inhibiting the in vitro growth of clinical Candida isolates [2].

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

In Vivo

VT-1598 tosylate (oral gavage; 5, 15, and 50 mg/kg; once daily; 7 d) shows a significant and dose-dependent survival advantage for mice, and dose-dependent reductions in fungal burden in mice[1].

VT-1598 tosylate (oral gavage; 3.2, 8, and 20 mg/kg; once daily; 4 d) is present to a great extent in the plasma and tongue after oral administration in Act1-deficient mice infected with C. albicans[2].

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

Animal Model:	Mice model of invasive candidiasis[1]
Dosage:	5 mg/kg, 15 mg/kg, and 50 mg/kg
Administration:	Oral gavage; once daily; 7 days
Result:	Observed median survival in the VT-1598 15 mg/kg and 50 mg/kg groups (15 days and >21 days, respectively) longer than the control group. Observed kidney fungal burden in mice treated with 15 mg/kg and 50 mg/kg doses (mean $\log_{10}$ CFU/g, 5.40 and 3.67, respectively) lower than the vehicle control group. Showed mean trough concentrations 1.55 μg/mL after 7 days of therapy in the 5 mg/kg group, 6.78 μg/mL in the 15 mg/kg group, and 14.2 μg/mL in the 50 mg/kg group.

Animal Model:	Act1-deficient mice infected with C. albicans[2]
Dosage:	3.2, 8, and 20 mg/kg
Administration:	Oral gavage; once daily; 4 days
Result:	Resulted in high concentrations in the plasma and tongues of Candida-infected mice.

REFERENCES

[1]. Nathan P Wiederhold, et al. The Fungal Cyp51-Specific Inhibitor VT-1598 Demonstrates In Vitro and In Vivo Activity against Candida auris. Antimicrob Agents Chemother. 2019 Feb 26;63(3):e02233-18.

[2]. Timothy J Break, et al. VT-1598 inhibits the in vitro growth of mucosal Candida strains and protects against fluconazole-susceptible and -resistant oral candidiasis in IL-17 signalling-deficient mice. J Antimicrob Chemother. 2018 Aug 1;73(8):2089-2094.

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