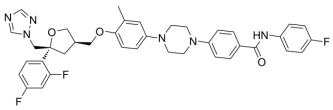
PC945

Cat. No.:	HY-117766
CAS No.:	1931946-73-4
Molecular Formula:	$C_{38}H_{37}F_3N_6O_3$
Molecular Weight:	682.73
Target:	Fungal; Cytochrome P450
Pathway:	Anti-infection; Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (146.47 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.4647 mL	7.3235 mL	14.6471 mL
	5 mM	0.2929 mL	1.4647 mL	2.9294 mL
	10 mM	0.1465 mL	0.7324 mL	1.4647 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 (3.66 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (3.66 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PC945, a potent, long-acting antifungal triazole, possesses activity against a broad range of both azole-susceptible and azole-resistant strains of Aspergillus fumigatus. PC945 is also a potent, tightly binding inhibitor of A. fumigatus sterol 14α-demethylase activity, CYP51A and CYP51B, with IC_{50}s of 0.23 μM and 0.22 μM, respectively[1][2].

IC_{50} & Target			
	fungal	CYP51A 0.23 μM (IC_{50})	CYP51B 0.22 μM (IC_{50})

In Vitro

PC945 is a triazole antifungal designed for administration via inhalation[1].
PC945 exhibits the most potent antifungal activity on azole-susceptible strain NCPF2010 with the MIC value of 0.063 μg/mL [2].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	PC945 (0.56-14 μg/mouse; intranasal; daily for 7 days) substantially inhibits the incidence of rolling behavior[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Specific-pathogen-free A/J mice (male, 5 weeks old, pulmonary Aspergillus infection)[1]
Dosage:	0.56, 2.8, 14 μg/mouse (intranasal application of 0.016-, 0.08-, and 0.4-mg/ml suspensions, respectively)
Administration:	Intranasal; daily for 7 days
Result:	Substantially inhibited the incidence of rolling behavior.

REFERENCES

[1]. Colley T, et al. In Vitro and In Vivo Antifungal Profile of a Novel and Long-Acting Inhaled Azole, PC945, on Aspergillus fumigatus Infection. Antimicrob Agents Chemother. 2017 Apr 24;61(5). pii: e02280-16.

[2]. Colley T, et al. Antifungal synergy of a topical triazole, PC945, with a systemic triazole against respiratory Aspergillus fumigatus infection. Sci Rep. 2019 Jul 1;9(1):9482.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA