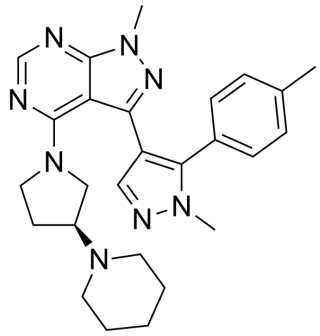
CYP3cide



Cat. No.:	HY-18642
CAS No.:	1390637-82-7
Molecular Formula:	$C_{26}H_{32}N_8$
Molecular Weight:	456.59
Target:	Cytochrome P450
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month

SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (109.51 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1901 mL	10.9507 mL	21.9015 mL
	5 mM	0.4380 mL	2.1901 mL	4.3803 mL
	10 mM	0.2190 mL	1.0951 mL	2.1901 mL

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

BIOLOGICAL ACTIVITY

Description

CYP3cide (PF-4981517) is a potent, selective and time-dependent inhibitor of cytochrome P4503A4 (CYP3A4). The IC_{50} values for Midazolam 1'-hydroxylase activity are 0.03 μM, 17 μM, and 71 μM for CYP3A4, CYP3A5, and CYP3A7, respectively. CYP3cide can be used to distinguish the contributions of CYP3A4 versus CYP3A5 on agent metabolism[1].

IC_{50} & Target			
	CYP3A4	CYP3A5	CYP3A7
	30 nM (EC50)	17 μM (EC50)	71 μM (EC50)

In Vitro

When investigating the inhibitory properties of CYP3cide, an extreme metabolic inactivation efficiency (k^{inact}/K^{I}) of 3300 to 3800 ml • min^{-1} • μmol^{-1} is observed using human liver microsomes from donors of nonfunctioning CYP3A5 (CYP3A5 $^{*}3/^{*}3$). This observed efficiency equated to an apparent KI between 420 and 480 nM with a maximal inactivation rate (kinact) equal to 1.6 min^{-1}. When CYP3cide is tested at a concentration and preincubation time to completely inhibit CYP3A4 in a library of genotyped polymorphic CYP3A5 microsomes, the correlation of the remaining midazolam 1'-hydroxylase activity to CYP3A5 abundance is significant[1].

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

REFERENCES

[1]. Robert L Walsky, et al. Selective mechanism-based inactivation of CYP3A4 by CYP3cide (PF-04981517) and its utility as an in vitro tool for delineating the relative roles of CYP3A4 versus CYP3A5 in the metabolism of drugs. Drug Metab Dispos. 2012 Sep;40(9):1686-97.

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