ML359

Cat. No.: HY-114086

CAS No.: 1069858-99-6

Molecular Formula: $C_{23}H_{28}ClNO_4$

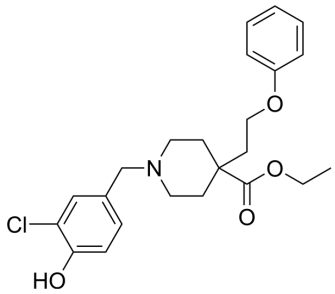
Molecular Weight: 417.93

Target: PDI

Pathway: Cell Cycle/DNA Damage; 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 (239.27 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3927 mL	11.9637 mL	23.9275 mL
	5 mM	0.4785 mL	2.3927 mL	4.7855 mL
	10 mM	0.2393 mL	1.1964 mL	2.3927 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 (5.98 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.98 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.98 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ML359 is a potent, selctive and reversible inhibitor of protein disulfide isomerase (PDI), with an IC_{50} of 250 nM. ML359 can prevent thrombus formation in vivo[1][2].

IC_{50} & Target

IC50: 250 nM (protein disulfide isomerase)[1]

In Vitro

ML359 shows no cytotoxicity in three human cell lines (HeLa, HEK293, and HepG2), and some activity in inhibiting platelet aggregation in vitro (25% inhibition at 30 μM)[1].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	ML359 inhibits of thrombus formation in a mouse laser injury model[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Khodier C, et, al. Identification of ML359 as a Small Molecule Inhibitor of Protein Disulfide Isomerase. Probe Reports from the NIH Molecular Libraries Program. 2010-2013 Apr 12.

[2]. Bendapudi PK, et, al. ML359, a Small Molecule Inhibitor of Protein Disulfide Isomerase That Prevents Thrombus Formation and Inhibits Oxidoreductase but Not Transnitrosylase Activity. Blood (2014) 124 (21): 2880.

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