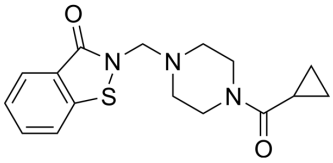
LOC14

Cat. No.:	HY-100432
CAS No.:	877963-94-5
Molecular Formula:	$C_{16}H_{19}N_3O_2S$
Molecular Weight:	317.41
Target:	PDI
Pathway:	Cell Cycle/DNA Damage; Metabolic Enzyme/Protease
Storage:	4°C, protect from light * The compound is unstable in solutions, freshly prepared is recommended.



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (157.52 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.1505 mL	15.7525 mL	31.5050 mL
	5 mM	0.6301 mL	3.1505 mL	6.3010 mL
	10 mM	0.3150 mL	1.5752 mL	3.1505 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: ≥ 2.08 mg/mL (6.55 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (6.55 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (6.55 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

LOC14 is a potent Protein disulfide isomerase (PDI) inhibitor with EC_{50} and K_d values of 500 nM and 62 nM, respectively. LOC14 exhibits high stability in mouse liver microsomes and blood plasma, low intrinsic microsome clearance, and low plasma-protein binding[1].LOC14 inhibits PDIA3 activity, decreases intramolecular disulfide bonds and subsequent oligomerization (maturation) of HA in lung epithelial cells[3].

IC_{50} & Target

Kd: 62 nM (PDI)[1]

In Vitro

LOC14 (0.01-100 μM; 24 hours) exhibits the capacity to inhibit recombinant (r)PDIA3 at an IC50 of approximately 5 μM[3].

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

Cell Viability Assay[3]

Cell Line:	MTEC cells
Concentration:	0.01 μM; 0.1 μM; 0.5 μM; 1 μM; 5 μM; 10 μM; 100 μM
Incubation Time:	24 hours
Result:	Inhibited recombinant (r)PDIA3 activity.

In Vivo

LOC14 (orally administered by gavage; 20 mg/kg; once daily; 12-28 weeks) significantly improves motor function, attenuated brain atrophy and extended survival in the N171–82Q HD mice[2].

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

Animal Model:	Male N171–82Q HD mice[2]
Dosage:	20 mg/kg
Administration:	Orally administered by gavage; 20 mg/kg; once daily; 12-28 weeks
Result:	Improved motor function in HD mice.

CUSTOMER VALIDATION

- Antiviral Res. 2023 Feb 21;105560.
- Virginia Polytechnic Institute and State University. 2023 Mar 31.

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REFERENCES

[1]. Kaplan A, et al. Small molecule-induced oxidation of protein disulfide isomerase is neuroprotective. Proc Natl Acad Sci U S A. 2015 Apr 28;112(17):E2245-52.

[2]. Chamberlain N, et al. Lung epithelial protein disulfide isomerase A3 (PDIA3) plays an important role in influenza infection, inflammation, and airway mechanics. Redox Biol. 2019 Apr;22:101129.

[3]. Zhou X, et al. Small molecule modulator of protein disulfide isomerase attenuates mutant huntingtin toxicity and inhibits endoplasmic reticulum stress in a mouse model of Huntington's disease. Hum Mol Genet. 2018 May 1;27(9):1545-1555.

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