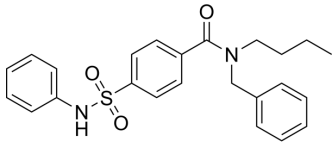
TH-257

Cat. No.:	HY-122630
CAS No.:	2244678-29-1
Molecular Formula:	$C_{24}H_{26}N_2O_3S$
Molecular Weight:	422.54
Target:	LIM Kinase (LIMK)
Pathway:	Cell Cycle/DNA Damage
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (591.66 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3666 mL	11.8332 mL	23.6664 mL
	5 mM	0.4733 mL	2.3666 mL	4.7333 mL
	10 mM	0.2367 mL	1.1833 mL	2.3666 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 (4.92 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.92 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.92 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

TH-257 is a potent inhibitor of LIMK1 and LIMK2 with IC_{50} values of 84 nM and 39 nM for LIMK1 and LIMK2, respectively, and it can be used as a chemical probe for LIMK1 and LIMK2. TH-257 is an allosteric inhibitor targeting a binding pocket induced by an αC and DFG-out conformation. TH257 is exquisitely selective and no significant activity against the wider kinome has been observed in the KINOMEscan assay at 1 μM[1].

IC_{50} & Target		
	LIMK1 84 nM (IC_{50})	LIMK2 39 nM (IC_{50})

In Vitro	TH-257 exhibits good biochemical and cellular potencies. But its extremely rapid in vitro clearance renders it unsuitable as a potential in vivo tool[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Collins R, et, al. Comparative Analysis of Small-Molecule LIMK1/2 Inhibitors: Chemical Synthesis, Biochemistry, and Cellular Activity. J Med Chem. 2022 Oct 27;65(20):13705-13713.

[2]. Manetti F. Recent advances in the rational design and development of LIM kinase inhibitors are not enough to enter clinical trials. Eur J Med Chem. 2018 Jul 15;155:445-458.

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