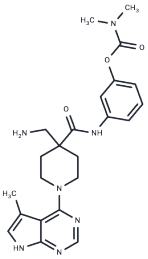
Data Sheet (Cat.No.T15798)

TargetMol

LX7101

Chemical Properties



CAS No. : 1192189-69-7

Formula: C23H29N7O3

Molecular Weight: 451.52

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	LX7101 is an effective inhibitor of LIMK and ROCK2 (IC50: 24, 1.6, and 10 nM for LIMK1, LIMK2, and ROCK2, respectively). It also inhibits PKA (IC50 <1 nM).
Targets(IC50)	LIM Kinase,PKA,ROCK
In vitro	LX7101 is a dual LIM-kinase and ROCK inhibitor for treating ocular hypertension and associated glaucoma, showing effective inhibition of Akt1 (IC50<1 nM)[1]. Its primary activity is due to LIMK2 inhibition under physiological conditions[2], with enhanced selectivity for LIMK2 at higher physiological ATP concentrations.
In vivo	Topical doses of LX-7101 are evaluated for tolerability in the eyes of mice, rats, and rabbits. It is well tolerated at doses up to 0.5% in non-GLP single-dose studies. LX-7101 is advanced to Phase-I clinical trials as intraocular pressure (IOP)-lowering agent for the treatment of glaucoma. LX-7101 shows a significant IOP reduction at time points ranging from 1 h to 6 h post-administration in rabbits[1]. LX-7101 (5%) achieved an additional reduction of IOP (5.0 mmHg total reduction) compared to the 0.1% formulation. It also demonstrated a long duration of action, in the mouse IOP assay, with IOP not returning to baseline until more than 8 h postdose[2].

Solubility Information

Solubility	DMSO: 150 mg/mL (332.21 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5 mg/mL (11.07 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.2147 mL	11.0737 mL	22.1474 mL
5 mM	0.4429 mL	2.2147 mL	4.4295 mL
10 mM	0.2215 mL	1.1074 mL	2.2147 mL
50 mM	0.0443 mL	0.2215 mL	0.4429 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Boland S, et al. Design, synthesis and biological characterization of selective LIMK inhibitors. Bioorganic & Medicinal Chemistry Letters (2015), 25(18), 4005-4010.
Harrison BA, et al. Discovery and Development of LX7101, a Dual LIM-Kinase and ROCK Inhibitor for the Treatment of Glaucoma. ACS Medicinal Chemistry Letters (2015), 6(1), 84-88.