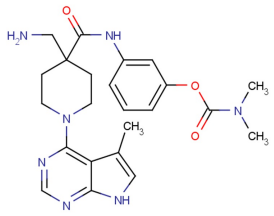
Data Sheet (Cat.No.T15798)

TargetMol
A DRUG SCREENING EXPERT

LX7101

Chemical Properties



CAS No.:	1192189-69-7
Formula:	C23H29N7O3
Molecular Weight:	451.52
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

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(IC_{50})	ROCK2: 10 nM LIMK2: 1.6 nM LIMK1: 24 nM PKA: 1 nM
In vitro	LX7101 is a dual LIM-kinase and ROCK inhibitor for the treatment of ocular hypertension and associated glaucoma. LX-7101 also shows effective inhibition of Akt1 (IC50<1 nM)[1]. The activity of LX7101 is primarily due to inhibition of LIMK2, under physiological conditions[2]. The overall selectivity of LX7101 for LIMK2 enhances the 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) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.215 mL	11.074 mL	22.147 mL
5 mM	0.443 mL	2.215 mL	4.429 mL
10 mM	0.221 mL	1.107 mL	2.215 mL
50 mM	0.044 mL	0.221 mL	0.443 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Boland S, et al. Design, synthesis and biological characterization of selective LIMK inhibitors. Bioorganic & Medicinal Chemistry Letters (2015), 25(18), 4005-4010.

2. 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.

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