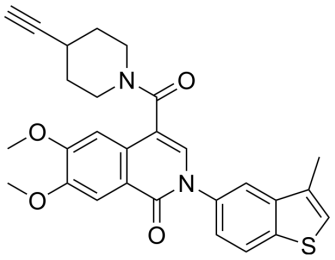
LPA5 antagonist 1

Cat. No.:	HY-151391
CAS No.:	2839471-45-1
Molecular Formula:	$C_{28}H_{26}N_2O_4S$
Molecular Weight:	486.58
Target:	Others
Pathway:	Others

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 (205.52 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0552 mL	10.2758 mL	20.5516 mL
	5 mM	0.4110 mL	2.0552 mL	4.1103 mL
	10 mM	0.2055 mL	1.0276 mL	2.0552 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 (5.14 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.14 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

LPA5 antagonist 1 (Compound 66) is a potent and selective lysophosphatidic acid receptor 5 (LPA5) antagonist (IC_{50}=32 nM). LPA5 antagonist 1 shows high brain permeability and anti-nociceptive activity. LPA5 antagonist 1 can be used in inflammatory and neuropathic pain research[1]. LPA5 antagonist 1 is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

IC_{50} & Target

IC50: 32 nM (LPA5)[1]

In Vitro

LPA5 antagonist 2 (0-10 μM) inhibits hLPA5 calcium mobilization with an IC_{50} value of 32 nM[1].
LPA5 antagonist 2 (0-10 μM) shows good target selectivity for LPA5[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

LPA5 antagonist 1 (intraperitoneal injection; 17.8 mg/kg; once) treatment shows good brain exposure in vivo[1].
LPA5 antagonist 1 (intraperitoneal injection; 5.6, 10, and 17.8 mg/kg; once) treatment reduces mechanical allodynia in inflammatory pain model[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	CFA-induced inflammatory pain model in Sprague-Dawley rats[1]
Dosage:	5.6, 10, and 17.8 mg/kg
Administration:	Intraperitoneal injection; 5.6, 10, and 17.8 mg/kg; once
Result:	Reduced mechanical allodynia in a dose-dependent manner.

Animal Model:	Male Sprague-Dawley rats[1]
Dosage:	17.8 mg/kg
Administration:	Intraperitoneal injection; 17.8 mg/kg; once
Result:	Showed brain concentrations of 652 ng/mL, after treatment 30 minutes.

REFERENCES

[1]. Zhang DH, et al. Isoquinolone derivatives as lysophosphatidic acid receptor 5 (LPA5) antagonists: Investigation of structure-activity relationships, ADME properties and analgesic effects. EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY. Volume 243, 5 December 2022, 114741.

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