MAGL-IN-4

Cat. No.: HY-132310

CAS No.: 2135785-20-3

Molecular Formula: $C_{18}H_{21}ClN_2O_4$

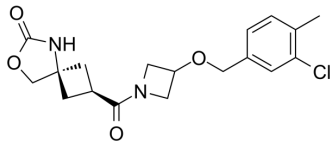
Molecular Weight: 364.82

Target: MAGL

Pathway: Metabolic Enzyme/Protease

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 (274.11 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.7411 mL	13.7054 mL	27.4108 mL
	5 mM	0.5482 mL	2.7411 mL	5.4822 mL
	10 mM	0.2741 mL	1.3705 mL	2.7411 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 (6.85 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.85 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.85 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

MAGL-IN-4 is an orally active, selective and reversible monoacylglycerol lipase (MAGL) inhibitor with an IC_{50} of 6.2 nM. MAGL-IN-4 can penetrate the blood-brain barrier (BBB). MAGL-IN-4 enhances endocannabinoid signaling mostly by the increase in the level of 2-AG via selective MAGL inhibition in the brain[1].

In Vitro

MAGL-IN-4 (compound 4f) shows a high LLE (5.9), a logD of 2.3 for MAGL[1].
MAGL-IN-4 exhibits no inhibition toward the closely related serine hydrolases (FAAH and ABHD6; all IC_{50}>10000 nM). MAGL-IN-4 has no significant binding potentials to cannabinoid receptors (CB1: 19% and CB2: 5% at 10 μM), and low hERG liability

	(14.4% inh. at 10 μM, manual patch clamp, without BSA)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	MAGL-IN-4 (compound 4f; 0.1-10 mg/kg; oral; single dose) results in a significant elevation in the level of 2-AG and reduction in that of arachidonic acid (AA) from 0.3 mg/kg in C57BL/6J mice[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Shuhei Ikeda, et al. Design and Synthesis of Novel Spiro Derivatives as Potent and Reversible Monoacylglycerol Lipase (MAGL) Inhibitors: Bioisosteric Transformation from 3-Oxo-3,4-dihydro-2 H-benzo[b][1,4]oxazin-6-yl Moiety. J Med Chem. 2021 Aug 12;64(15):11014-11044.

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