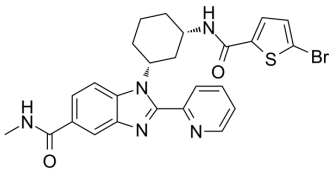
BCAT-IN-1

Cat. No.:	HY-141668
CAS No.:	1875078-61-7
Molecular Formula:	$C_{25}H_{24}BrN_5O_2S$
Molecular Weight:	538.46
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 (185.71 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.8571 mL	9.2857 mL	18.5715 mL
5 mM	0.3714 mL	1.8571 mL	3.7143 mL
10 mM	0.1857 mL	0.9286 mL	1.8571 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 (4.64 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.64 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BCAT-IN-1 is a potent, selective and orally active inhibitor of BCATm, with a pIC_{50} of 7.3. BCAT-IN-1 shows 100-fold selectivity for BCATm over BCATc (pIC_{50}=5.4). BCAT-IN-1 can be used for the research of metabolic diseases[1].

IC_{50} & Target

pIC50: 7.3 (BCATm)[1]

In Vitro

BCAT-IN-1 (compound 8b) inhibits BCATm in human cells, with a pIC_{50} of 7.0[1].
BCAT-IN-1 inhibits mouse BCATm, with pIC_{50} of 5.9 in the cellular assay[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

BCAT-IN-1 (compound 8b) (30-300 mg/kg; p.o.) increases the level of c BCAAs in an acute mouse model over an extended

duration[1].

BCAT-IN-1 (5 mg/kg; p.o.) exhibits oral bioavailability (F=28%) and C_{max} (1648 ng/mL) in mice[1].

BCAT-IN-1 (1 mg/kg; i.v.) exhibits half-life ($t_{1/2}$=9.2 h) and clearance (Cl=4.0 mL/min/kg) in mice[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Deng H, et, al. Discovery and Optimization of Potent, Selective, and in Vivo Efficacious 2-Aryl Benzimidazole BCATm Inhibitors. ACS Med Chem Lett. 2016 Feb 8;7(4):379-84.

Caution: Product has not been fully validated for medical applications. For research use only.

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