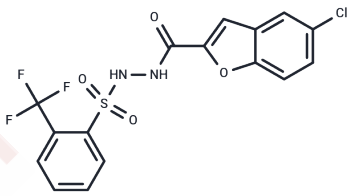
Data Sheet (Cat.No.T22043)

TargetMol

BCATc Inhibitor 2

Chemical Properties



CAS No. : 406191-34-2

Formula: C16H10ClF3N2O4S

Molecular Weight: 418.77

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	BCATc Inhibitor 2 exhibited an IC50 of 0.8 microM in the hBCATc assays; it is an active and selective inhibitor. BCATc Inhibitor 2 also blocked calcium influx into neuronal cells following inhibition of glutamate uptake, and demonstrated neuroprotective efficacy in vivo[1]. Branched-chain amino acid transferases (BCATs) have been implicated in catalyzing reversible transamination of isoleucine, leucine, and valine branched-chain amino acids to their corresponding α-keto acids, generating L-glutamate. It has been identified that there are two forms of BCAT in mammals: mitochondrial BCAT (BCATm) and cytosolic BCAT (BCATc). BCATc is expressed in particular brain region and involved in regulating glutamate synthesis for release during neuronal excitation. Thus, BCATc inhibition may be useful for the treatment of neurodegenerative and behavioral disorders involving disturbances of the glutamatergic system [2].
Targets(IC50)	Others
In vitro	BCATc inhibition is likely to be useful for the treatment of neurodegenerative and other neurological disorders involving disturbances of the glutamatergic system. In the hBCATc assays, BCATc Inhibitor 2 exhibited an IC50 of 0.8 ± 0.05 μM. In a recombinant rat BCATc assay and a crude rat BCATm assay, the IC50 was 0.2 μM ± 0.02 and 3.0 μM ± 0.5 (n=5), respectively. BCATc Inhibitor 2 decreased calcium influx in neuronal cultures with an IC50 of 4.8 ± 1.2 μM (n=4) [1].
In vivo	BCATc Inhibitor 2 blocked calcium influx into neuronal cells following inhibition of glutamate uptake, and demonstrated neuroprotective efficacy in vivo. In Lewis rats, after treatment with 30 mg/kg BCATc Inhibitor 2 (subcutaneous injection), the peak plasma concentration (Cmax) reached 8.28 μg/ml at 0.5 h (tmax). The mean plasma exposure (AUC) value was 19.9 μg h/ml, and the mean terminal half-life ranged from 12 to 15 h, indicating favorable PK parameters of BCATc Inhibitor 2. Daily administration of the mitochondrial neurotoxin, 3-nitroproprionic acid (3-NP) produced striatal lesions and led to motor deficits. Administration of BCATc Inhibitor 2 for 9 days almost completely reversed the effects of 3-NP [1].

Solubility Information

Solubility	DMSO: 65 mg/mL (155.22 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

In vivo Formulation	10% DMSO+90% Corn Oil: 2.5 mg/mL (5.97 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	2.3879 mL	11.9397 mL	23.8795 mL
5 mM	0.4776 mL	2.3879 mL	4.7759 mL
10 mM	0.2388 mL	1.194 mL	2.3879 mL
50 mM	0.0478 mL	0.2388 mL	0.4776 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

Hu L Y, Boxer P A, Kesten S R, et al. The design and synthesis of human branched-chain amino acid aminotransferase inhibitors for treatment of neurodegenerative diseases[J]. Bioorganic & medicinal chemistry letters, 2006, 16(9): 2337-2340.

Brosnan J T, Brosnan M E. Branched-chain amino acids: enzyme and substrate regulation[J]. The Journal of nutrition, 2006, 136(1): 207S-211S.