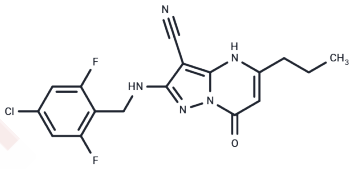
Data Sheet (Cat.No.T35868)

TargetMol

BCAT-IN-2

Chemical Properties



CAS No. : 1800024-45-6

Formula: C17H14ClF2N5O

Molecular Weight: 377.776

Storage: Store at low temperature
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	BCAT-IN-2 is an orally active and selective inhibitor of mitochondrial branched-chain aminotransferase (BCATm), inhibits BCATm and BCATc, and is used in obesity and dyslipidemia.
Targets(IC50)	Others
In vitro	BCAT-IN-2 inhibits BCATm in primary human adipocytes, with a pIC50 of 6.5[1].
In vivo	BCAT-IN-2 (5 mg/kg, po; 1 mg/kg, iv) exhibits favorable pharmacokinetic parameters in mice[1].

Solubility Information

Solubility	DMSO: 50 mg/mL (132.35 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Corn Oil: 2 mg/mL (5.29 mM),Sonication is recommended. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5 mg/mL (13.24 mM),Solution. 10% DMSO+90% Saline: < 5 mg/mL (13.24 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. *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	2.647 mL	13.2352 mL	26.4704 mL
5 mM	0.5294 mL	2.647 mL	5.2941 mL
10 mM	0.2647 mL	1.3235 mL	2.647 mL
50 mM	0.0529 mL	0.2647 mL	0.5294 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

Bertrand SM, et al. The Discovery of in Vivo Active Mitochondrial Branched-Chain Aminotransferase (BCATm) Inhibitors by Hybridizing Fragment and HTS Hits. J Med Chem. 2015 Sep 24;58(18):7140-63.