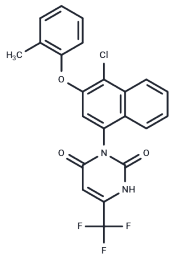
Data Sheet (Cat.No.T67927)

TargetMol

BAY-069

Chemical Properties



CAS No. : 2639638-66-5

Formula: C22H14ClF3N2O3

Molecular Weight: 446.81

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	BAY-069 is an inhibitor. BAY-069 inhibited branched-chain amino acid transaminase 1 (BCAT1) at IC50:31 nM and branched-chain amino acid transaminase 2 (BCAT2) at IC50: 153 nM. BAY-069 is a novel (trifluoromethyl) pyrimidine dione chemical probe, which can be used for anticancer research.
Targets(IC50)	Others,Reactive Oxygen Species
In vitro	BAY-069, inhibits the proliferation of U-87 and MDA-MB-231 cells. The compound is tested at concentrations ranging from 70 nM to 50 μM, with a duration of 72 hours. In U-87 cells, the IC50 is determined to be 358 nM, while in MDA-MB-231 cells, the IC50 is 874 nM [1].
In vivo	BAY-069 demonstrates high metabolic stability when incubated with human liver microsomes, with a blood clearance of 0.11 L/h/kg. It also shows moderate metabolic stability when incubated with rat hepatocytes, with a blood clearance of 1.8 L/h/kg. BAY-069 exhibits high permeability through Caco-2 cell monolayers without any signs of efflux [1].

Solubility Information

Solubility	DMSO: 150 mg/mL (335.71 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 6 mg/mL (13.43 mM),Solution. 10% DMSO+90% Saline: < 6 mg/mL (13.43 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	2.2381 mL	11.1904 mL	22.3809 mL
5 mM	0.4476 mL	2.2381 mL	4.4762 mL
10 mM	0.2238 mL	1.119 mL	2.2381 mL
50 mM	0.0448 mL	0.2238 mL	0.4476 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

Günther J, et al. BAY-069, a Novel (Trifluoromethyl)pyrimidinedione-Based BCAT1/2 Inhibitor and Chemical Probe. J Med Chem. 2022;65(21):14366-14390.