BAY-069

Cat. No.: HY-148242

CAS No.: 2639638-66-5

Molecular Formula: $C_{22}H_{14}ClF_3N_2O_3$

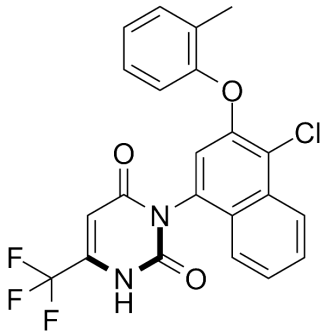
Molecular Weight: 446.81

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 : 200 mg/mL (447.62 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	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	1.1190 mL	2.2381 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: ≥ 5 mg/mL (11.19 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 5 mg/mL (11.19 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BAY-069 is a potent branched-chain amino acid transaminases 1 (BCAT1) and BCAT2 inhibitor with IC_{50} values of 31 nM and 153 nM, respectively. BAY-069 also can be used as a chemical probe. BAY-069 can be used tor research anticancer[1].

IC_{50} & Target

IC_{50}: 31 nM (BCAT1), 153 nM (BCAT2)[1]

In Vitro

BAY-069 (compound 36a) (70 nM-50 μM; 72 h) inhibits cell proliferation of U-87 and MDA-MB-231[1].

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

Cell Proliferation Assay[1]

Cell Line:	U-87 and MDA-MB-231
Concentration:	70 nM-50 μM
Incubation Time:	72 h
Result:	Inhibited cell proliferation of U-87 and MDA-MB-231 with IC_{50}s of 358 nM and 874 nM, respectively.

In Vivo

BAY-069 exhibits high metabolic stability after incubation with human liver microsomes (CL_{blood} = 0.11 L/h/kg) and moderate metabolic stability after incubation with rat hepatocytes (CL_{blood} = 1.8 L/h/kg); shows high permeability through Caco-2 cell monolayers with no hint of efflux[1].

BAY-069 (0.3 mg/kg for i.v.; 0.6 mg/kg for p.o.; single dosage) exhibits a favorable pharmacokinetic profile after i.v. dosing with low blood clearance (CL_{blood}), moderate volume of distribution at steady state (V_{ss}), and intermediate terminal half-life ($t_{1/2}$).

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

Animal Model:	Male Wistar rats[1]
Dosage:	0.3 mg/kg for i.v.; 0.6 mg/kg for p.o.
Administration:	i.v. or p.o.; single dosage
Result:	Pharmacokinetic Parameters of BAY-069 in male Wistar rats[1].

CL_{blood} (L/h/kg)	V_{ss} (L/kg)	$t_{1/2}$ (h), i.v.	AUC_{norm} (kg·h/L), i.v.	AUC_{norm} (kg·h/L), p.o.	F (%), p.o.
0.64	0.25	1.6	2.9	2.5	89

REFERENCES

[1]. Günther J, et al. BAY-069, a Novel (Trifluoromethyl)pyrimidinedione-Based BCAT1/2 Inhibitor and Chemical Probe. J Med Chem. 2022 Oct 19.

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