BIIB068

Cat. No.: HY-131342

CAS No.: 1798787-27-5

Molecular Formula: $C_{23}H_{29}N_7O_2$

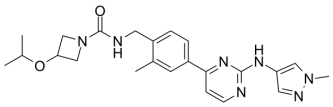
Molecular Weight: 435.52

Target: Btk

Pathway: Protein Tyrosine Kinase/RTK

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 31.25 mg/mL (71.75 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.2961 mL	11.4805 mL	22.9611 mL
5 mM	0.4592 mL	2.2961 mL	4.5922 mL
10 mM	0.2296 mL	1.1481 mL	2.2961 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: ≥ 2.08 mg/mL (4.78 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.78 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.78 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BIIB068 is a potent, selective, reversible and orally active BTK inhibitor with an IC_{50} of 1 nM and a K_d of 0.3 nM. BIIB068 shows more >400-fold selective for BTK than other kinases. BIIB068 has the potential for autoimmune diseases research[1].

IC_{50} & Target

IC50: 1 nM (BTK)[1]
Kd: 0.3 nM (BTK)[1]

In Vitro

BIIB068 (compound 1) improves the whole blood cell potency (human whole blood BTK phosphorylation (IC_{50} = 0.12 μM)[1].

	BIIB068 (compound 1; 30 μM,10 μM, 3.3 μM, and 1.1 μM) inhibits BCR mediated PLCγ2 phosphorylation in Ramos B cells (IC_{50} = 0.4 μM), anti-IgD induced and anti-IgM BCR-induced B cell activation in human PBMCs (IC_{50} = 0.11 μM and 0.21 μM, respectively)[1]. BIIB068 (compound 1) inhibits FcγR-mediated ROS production in neutrophils with an IC_{50} of 54 nM[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	BIIB068 (compound 1) is stable in the plasma of mouse, rat, beagle dog, and cynomolgus monkey (>95% parent compound remaining after 6 hours of incubation)[1]. BIIB068 (compound 1) exhibits good drug-like properties (LLE = 5) which results in low in vivo clearance (CL $\%Q_h$ = 6) and moderate oral bioavailability (%F = 48) when dosed in rats. BIIB068 (5 mg/kg; po) treatment shows the $T_{1/2}$ of 1.2 hours, 2.1 hours and 0.9 hour for rats, dog and cynomolgus monkey, respectively. BIIB068 shows acceptable ADME (absorption, distribution, metabolism, and excretion) properties[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Bin Ma, Tonika Bohnert, et al. Discovery of BIIB068: A Selective, Potent, Reversible Bruton's Tyrosine Kinase Inhibitor as an Orally Efficacious Agent for Autoimmune Diseases. J Med Chem. 2020 Jul 22.

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