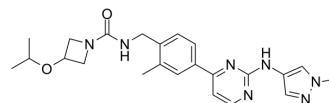


BIIB068

Cat. No.:	HY-131342		
CAS No.:	1798787-27-5		
Molecular Formula:	C ₂₃ H ₂₉ N ₇ O 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	6 months
		-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro	DMSO : 31.25 mg/mL (71.75 mM; Need ultrasonic)			
		Solvent Concentration	Mass	
			1 mg	5 mg
			10 mg	
Preparing Stock Solutions	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	IC ₅₀ : 1 nM (BTK) ^[1] K _d : 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 μ M, 10 μ M, 3.3 μ M, and 1.1 μ M) inhibits BCR mediated PLC γ 2 phosphorylation in Ramos B cells (IC_{50} = 0.4 μ M), anti-IgD induced and anti-IgM BCR-induced B cell activation in human PBMCs (IC_{50} = 0.11 μ M and 0.21 μ M, respectively)^[1].

BIIB068 (compound 1) inhibits Fc γ R-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.

Caution: Product has not been fully validated for medical applications. For research use only.

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