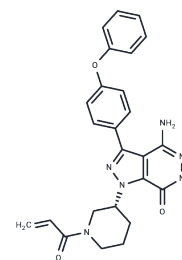


BTK inhibitor 17

Chemical Properties

CAS No. :	1858206-76-4
Formula:	C ₂₅ H ₂₄ N ₆ O ₃
Molecular Weight:	456.5
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	BTK inhibitor 17 is a potent irreversible Bruton's tyrosine kinase (BTK) inhibitor with an IC ₅₀ value of 2.1 nM, suitable for use in rheumatoid arthritis studies.
Targets(IC ₅₀)	BTK
In vitro	BTK inhibitor 17 exhibited high potency against BTK kinase and acceptable PK profile. BTK inhibitor 17 could covalently bind to Cys481 and formed an HB network with gatekeeper Thr474, hinge key residues Met477 and Glu475[1].
In vivo	BTK inhibitor 17 demonstrated significant in vivo efficacy in a mouse-collagen-induced arthritis (CIA) model. BTK inhibitor 17 shows >95% plasma protein binding across three species of human, rat, and mouse. After an intravenous injection, the half-life (rat, 0.32 h; mice, 0.42 h), clearance (rat, 54.6 mL/min/kg; mice, 31.3 mL/min/kg), volume of distribution (rat, 1.55 L/kg; mice, 0.82 L/kg), and AUC exposure (rat, 604 ng.h/mL; mice, 576 ng.h/mL) are observed in two species. After oral administration, BTK inhibitor 17 exhibits higher C _{max} (rat, 466 ng/mL; mice, 252 ng/mL) and plasma exposure (rat, 642 ng.h/mL; mice, 128 ng.h/mL) with a favorable oral bioavailability (rat, 23.7%; mice, 11.2%)[1]. In male Balb/C mice injected with collagen, BTK inhibitor 17 inhibited the significant progression of the disease and exhibited a clear dose-dependent reduction per paw clinical scores[1].

Solubility Information

Solubility	DMSO: 100 mg/mL (219.06 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: 4 mg/mL (8.76 mM),Sonication is recommended. <i>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.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.1906 mL	10.9529 mL	21.9058 mL
5 mM	0.4381 mL	2.1906 mL	4.3812 mL
10 mM	0.2191 mL	1.0953 mL	2.1906 mL
50 mM	0.0438 mL	0.2191 mL	0.4381 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

Xuejun Zhang, et al. Discovery and Evaluation of Pyrazolo[3,4- d]pyridazinone as a Potent and Orally Active Irreversible BTK Inhibitor. ACS Med Chem Lett. 2019 Dec 11;11(10):1863-1868.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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