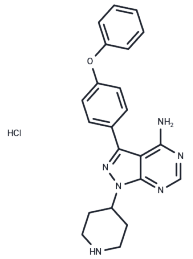
Data Sheet (Cat.No.T12152)

TargetMol

N-piperidine Ibrutinib hydrochloride

Chemical Properties



CAS No. :	2231747-18-3
Formula:	C22H23ClN6O
Molecular Weight:	422.91
Storage:	Keep away from direct sunlight,Keep away from moisture 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	N-piperidine Ibrutinib hydrochloride is a potent BTK inhibitor, a BTK ligand, inhibits WT BTK and C481S BTK, which can be used to synthesize a range of PROTAC molecules.N-piperidine Ibrutinib hydrochloride has potential anticancer N-piperidine Ibrutinib hydrochloride has potential anticancer activity, inhibiting the growth and proliferation of cancer cells.
Targets(IC50)	BTK,Ligands for Target Protein for PROTAC
In vitro	N-piperidine Ibrutinib hydrochloride can be used to synthesize effective PROTAC BTK degraders, such as SJF638, SJF678, and SJF608[2].

Solubility Information

Solubility	DMSO: 80 mg/mL (189.17 mM),Sonication is recommended. H2O: 30 mg/mL (70.94 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: 3.3 mg/mL (7.8 mM),Sonication is recommended. *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	2.3646 mL	11.8228 mL	23.6457 mL
5 mM	0.4729 mL	2.3646 mL	4.7291 mL
10 mM	0.2365 mL	1.1823 mL	2.3646 mL
50 mM	0.0473 mL	0.2365 mL	0.4729 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

Buhimschi AD, et al. Targeting the C481S Ibrutinib-Resistance Mutation in Bruton's Tyrosine Kinase Using PROTAC-Mediated Degradation. Biochemistry. 2018 Jul 3;57(26):3564-3575.

Jaime-Figueroa S, et al. Design, synthesis and biological evaluation of Proteolysis Targeting Chimeras (PROTACs) as a BTK degraders with improved pharmacokinetic properties. Bioorg Med Chem Lett. 2020 Feb 1;30(3):126877.