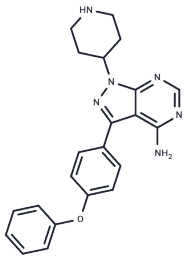
Data Sheet (Cat.No.T9408)

TargetMol

N-piperidine Ibrutinib

Chemical Properties



CAS No. : 330785-90-5

Formula: C22H22N6O

Molecular Weight: 386.45

Appearance: Solid

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	N-piperidine Ibrutinib is a potent BTK inhibitor with IC50s of 51.0 for WT BTK and 30.7 nM for C481S BTK respectively. N-piperidine Ibrutinib can be used as a BTK ligand in the synthesis of a series of PROTACs, such as SJF620. SJF620 is a potent PROTAC BTK degrader with a DC50 of 7.9 nM.
Targets(IC50)	BTK
In vitro	N-piperidine Ibrutinib can be used as a BTK ligand in the synthesis of a series of PROTACs. SJF638, SJF678, and SJF608 are potent PROTAC BTK degraders with DC50s of 374, 162, and 8.3 nM, respectively[2].

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.5877 mL	12.9383 mL	25.8766 mL
5 mM	0.5175 mL	2.5877 mL	5.1753 mL
10 mM	0.2588 mL	1.2938 mL	2.5877 mL
50 mM	0.0518 mL	0.2588 mL	0.5175 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.

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.

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