

Product Data Sheet

Product Name: N-piperidine Ibrutinib hydrochloride

Cat. No.: GC62255

Chemical Properties

Cas. No. 2231747-18-3

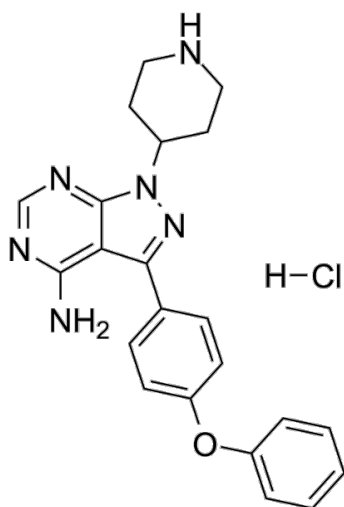
Formula $C_{22}H_{23}ClN_6O$ M.Wt 422.91

Solubility DMSO : 100 mg/mL (236.46 mM; Storage -20°C, protect from light
Need ultrasonic)

General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

Structure



Background

N-piperidine Ibrutinib hydrochloride (Compound 1) is a reversible Ibrutinib derivative. N-piperidine Ibrutinib hydrochloride is a potent BTK inhibitor with IC₅₀s of 51.0 and 30.7 nM for WT BTK and

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

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C481S BTK, respectively[1]. N-piperidine Ibrutinib hydrochloride 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[2].

N-piperidine Ibrutinib hydrochloride 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].

[1]. 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. [2]. 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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