IBT6A hydrochloride

Cat. No.: HY-13036B

CAS No.: 1553977-42-6

Molecular Formula: $C_{22}H_{23}ClN_6O$

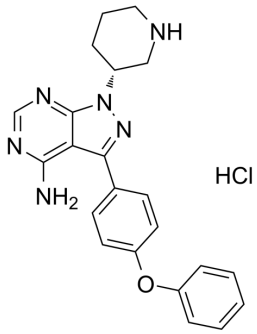
Molecular Weight: 422.91

Target: Btk

Pathway: Protein Tyrosine Kinase/RTK

Storage: 4°C, sealed storage, away from moisture

* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (236.46 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	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

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: ≥ 2.5 mg/mL (5.91 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.91 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.91 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

IBT6A hydrochloride is an impurity of Ibrutinib. IBT6A can be used in synthesis of IBT6A Ibrutinib dimer and IBT6A adduct[1]. Ibrutinib is a selective, irreversible Btk inhibitor with an IC_{50} of 0.5 nM[2].

In Vitro

IBT6A (Compound 14) can be used in synthesis of Ibrutinib and Ibrutinib-based activity-based probes (ABPs)[3].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Somana Siva Prasad, et al. A QUALITY BY DESIGN APPROACH FOR DEVELOPMENT OF SIMPLE AND ROBUST REVERSED PHASE STABILITY INDICATING HPLC METHOD FOR ESTIMATION OF IBRUTINIB AND ITS IMPURITIES.

[2]. Honigberg LA, et al. The Bruton tyrosine kinase inhibitor PCI-32765 blocks B-cell activation and is efficacious in models of autoimmune disease and B-cell malignancy. Proc Natl Acad Sci U S A. 2010 Jul 20;107(29):13075-80.

[3]. Liu N, et al. Direct and two-step bioorthogonal probes for Bruton's tyrosine kinase based on ibrutinib: a comparative study. Org Biomol Chem. 2015 May 14;13(18):5147-57.

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