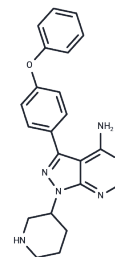


(Rac)-IBT6A

Chemical Properties

CAS No. :	1412418-47-3
Formula:	C ₂₂ H ₂₂ N ₆ O
Molecular Weight:	386.45
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	(Rac)-IBT6A is a racemate of IBT6A, an impurity of Ibrutinib that can be utilized in the synthesis of IBT6A Ibrutinib dimer and IBT6A adduct.
Targets(IC50)	BTK

Solubility Information

Solubility	DMSO: 45 mg/mL (116.44 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: 1 mg/mL (2.59 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	2.5877 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.

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

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.

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.

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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