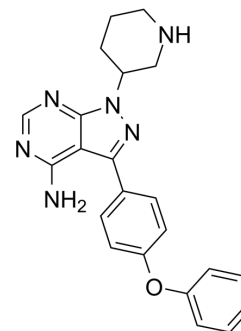


(Rac)-IBT6A

Cat. No.:	HY-13036		
CAS No.:	1412418-47-3		
Molecular Formula:	C ₂₂ H ₂₂ N ₆ O		
Molecular Weight:	386.45		
Target:	Btk		
Pathway:	Protein Tyrosine Kinase/RTK		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	2 years
		-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro	DMSO : 50 mg/mL (129.38 mM; Need ultrasonic)				
		Solvent Concentration	Mass 1 mg	5 mg	10 mg
	Preparing Stock Solutions	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	
Please refer to the solubility information to select the appropriate solvent.					
In Vivo	<ol style="list-style-type: none"> Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 1.67 mg/mL (4.32 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 1.67 mg/mL (4.32 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 1.67 mg/mL (4.32 mM); Clear solution 				

BIOLOGICAL ACTIVITY

Description	(Rac)-IBT6A is a racemate of IBT6A. IBT6A 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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Caution: Product has not been fully validated for medical applications. For research use only.

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