Proteins

(Rac)-IBT6A hydrochloride

Cat. No.: HY-13036C CAS No.: 1807619-60-8 Molecular Formula: $C_{22}H_{23}CIN_6O$

Molecular Weight: 422.91 Btk Target:

Pathway: Protein Tyrosine Kinase/RTK

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

Product Data Sheet

BIOLOGICAL ACTIVITY

Description	(Rac)-IBT6A hydrochloride is a racemate of IBT6A hydrochloride. 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 $\rm nM^{[2]}$.
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.

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

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