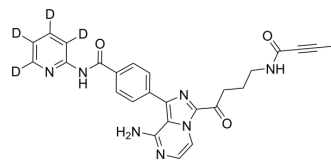


ACP-5862-d₄

Cat. No.:	HY-135334S
Molecular Formula:	C ₂₆ H ₁₉ D ₄ N ₇ O ₃
Molecular Weight:	485.53
Target:	Btk; Cytochrome P450; Drug Metabolite; Isotope-Labeled Compounds
Pathway:	Protein Tyrosine Kinase/RTK; Metabolic Enzyme/Protease; Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	ACP-5862-d ₄ is deuterium labeled ACP-5862. ACP-5862 is a major active, circulating, pyrrolidine ring-opened metabolite of Acalabrutinib with an IC ₅₀ of 5.0 nM for Bruton tyrosine kinase (BTK). ACP-5862 is a weak time-dependent inactivator of CYP3A4 and CYP2C8. Acalabrutinib is an orally active, irreversible, and highly selective BTK inhibitor, with an IC ₅₀ of 3 nM and EC ₅₀ of 8 nM[1][2].
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

- [1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. *Ann Pharmacother.* 2019;53(2):211-216.
- [2]. Diansong Zhou, et al. Evaluation of the Drug-Drug Interaction Potential of Acalabrutinib and Its Active Metabolite, ACP-5862, Using a Physiologically-Based Pharmacokinetic Modeling Approach. *CPT Pharmacometrics Syst Pharmacol.* 2019 Jul;8(7):489-499.
- [3]. Herman SE, et al. The Bruton's tyrosine kinase (BTK) inhibitor acalabrutinib demonstrates potent on-target effects and efficacy in two mouse models of chronic lymphocytic leukemia. *Clin Cancer Res.* 2016 Nov 30

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

Tel: 609-228-6898

Fax: 609-228-5909

E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA