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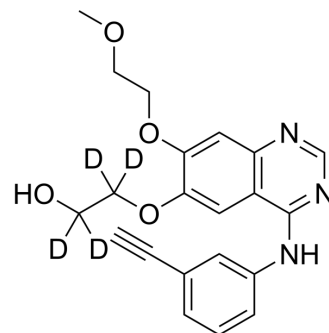
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Desmethyl Erlotinib-d4-1

Cat. No.:	HY-13256AS1
CAS No.:	2012598-45-5
Molecular Formula:	C ₂₁ H ₁₇ D ₄ N ₃ O ₄
Molecular Weight:	383.43
Target:	Drug Metabolite; Isotope-Labeled Compounds
Pathway:	Metabolic Enzyme/Protease; Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Desmethyl Erlotinib-d ₄ -1 (OSI-420-d ₄ -1 (free base); CP-373420-d ₄ -1) is deuterium-labeled Desmethyl Erlotinib (HY-13256A) ^[1] .
In Vitro	<p>Stable or radioisotope-labeled compounds allow precise tracking and quantification of individual atoms in metabolic pathways. Stable isotopes generally do not change molecular properties but may slightly affect metabolic kinetics; radioactive isotopes may interfere with cells. Markers can distinguish endogenous and exogenous metabolites, reduce false positives, and are beneficial to quantification and reconstruction of metabolic pathways^[2].</p> <p>In cell culture or enzymatic reactions, the use of isotope markers can precisely control the concentration and exposure time, making it easy to study metabolic reactions and enzyme activities. Through stable isotope analytical metabolomics (SIRM), cellular metabolic networks can be studied, key metabolic nodes and regulatory mechanisms can be identified, and targets can be provided for compound development.</p> <p>Isotope-labeled compounds can be used in competition binding experiments to evaluate the affinity and binding kinetics of compounds to receptors to help optimize design. Stable isotope labels are used as internal standards in mass spectrometry analysis to improve analysis accuracy and reproducibility and reduce matrix effect interference^[3].</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>
In Vivo	<p>Isotopic labels can non-invasively track the distribution, transformation and clearance of compounds and their metabolites in the body through techniques such as mass spectrometry (MS) and nuclear magnetic resonance (NMR), which is beneficial to the study of pharmacometabolic kinetics (ADME).</p> <p>Isotope labeling can reveal specific steps in metabolic pathways. Using compounds with stable isotope labels at specific locations directly in humans or animal models can also help verify drug mechanisms and evaluate unexpected side effects, improving the accuracy and efficiency of clinical research^[3].</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>

REFERENCES

- [1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. *Ann Pharmacother*. 2019;53(2):211-216.
- [2]. Smith K A, et al. *Soil and environmental analysis[M]*. Marcel Dekker Incorporated, 2000.
- [3]. Fan T W M, et al. Stable isotope-resolved metabolomics and applications for drug development[J]. *Pharmacology & therapeutics*, 2012, 133(3): 366-391.

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

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