Product Data Sheet

Desmethyl Erlotinib-d₄

Cat. No.:HY-13256ASCAS No.: $1216420^{-}11^{-}9$ Molecular Formula: $C_{21}H_{17}D_4N_3O_4$

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.

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BIOLOGICAL ACTIVITY

Description	Desmethyl Erlotinib- d_4 is the deuterium labeled Desmethyl Erlotinib. Desmethyl Erlotinib (OSI-420 free base) is an active metabolite of Erlotinib. Erlotinib is a potent EGFR tyrosin kinase inhibitor[1][2]. Desmethyl Erlotinib-d4 is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.
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]. Thappali SR, et al. Simultaneous Determination of Celecoxib, Erlotinib, and its Metabolite Desmethyl-Erlotinib (OSI-420) in Rat Plasma by Liquid chromatography/Tandem Mass Spectrometry with Positive/Negative Ion-Switching Electrospray Ionisation. Sci Pharm. 2012 Jul-Sep;80(3):633-46.

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

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