Proteins

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Product Data Sheet

Dabigatran-d₄

Cat. No.: HY-10163S CAS No.: 1618637-32-3 Molecular Formula: $C_{25}H_{21}D_4N_7O_3$

Molecular Weight: 475.54

Target: Thrombin; Isotope-Labeled Compounds Pathway: Metabolic Enzyme/Protease; Others

Storage: Powder -20°C 3 years 2 years

-80°C 6 months In solvent

> -20°C 1 month

BIOLOGICAL ACTIVITY

Description	Dabigatran-d ₄ is deuterium labeled Dabigatran. Dabigatran (BIBR 953), an oral anticoagulant, is a reversible, potent, competitive direct thrombin inhibitor (Ki=4.5 nM). Dabigatran (BIBR 953) also inhibits thrombin-induced platelet aggregation (IC50=10 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]. Hauel NH, et al. Structure-based design of novel potent nonpeptide thrombin inhibitors. J Med Chem. 2002 Apr 25;45(9):1757-66.

[2]. Wienen W, et al. Effects of the direct thrombin inhibitor dabigatran and its orally active prodrug, dabigatran etexilate, on thrombus formation and bleeding time in rats. Thromb Haemost. 2007 Aug;98(2):333-8.

[3]. Wienen W, Stassen JM, Priepke H, In-vitro profile and ex-vivo anticoagulant activity of the direct thrombin inhibitor dabigatran and its orally active prodrug, dabigatran etexilate. Thromb Haemost, 2007 Jul;98(1):155-62.

[4]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-216.

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

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