Dabigatran-d_3

Cat. No.: HY-10163S1

CAS No.: 1246817-44-6

Molecular Formula: $C_{25}H_{22}D_3N_7O_3$

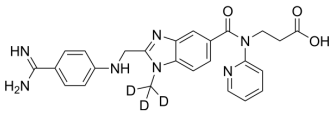
Molecular Weight: 474.53

Target: Thrombin

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (210.73 mM; ultrasonic and warming and heat to 80°C)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.1073 mL	10.5367 mL	21.0735 mL
5 mM	0.4215 mL	2.1073 mL	4.2147 mL
10 mM	0.2107 mL	1.0537 mL	2.1073 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

Dabigatran-d_3 is the 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]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-216.

[2]. Wienen W, Stassen JM, Priepke H, In-vitro profile and ex-vivo anticoagulant activity of the direct thrombin inhibitor dabigatran and its orally activeprodrug, dabigatran

etexilate. Thromb Haemost. 2007 Jul;98(1):155-62.

[3]. Hauel NH, et al. Structure-based design of novel potent nonpeptide thrombin inhibitors. J Med Chem. 2002 Apr 25;45(9):1757-66.

[4]. 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.

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