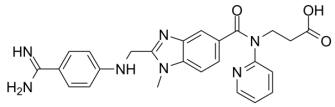
Dabigatran

Cat. No.:	HY-10163
CAS No.:	211914-51-1
Molecular Formula:	$C_{25}H_{25}N_7O_3$
Molecular Weight:	471.51
Target:	Thrombin
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

0.1 M HCL : 12.5 mg/mL (26.51 mM; Need ultrasonic)
H_2O : < 0.1 mg/mL (insoluble)
DMSO : < 1 mg/mL (insoluble or slightly soluble)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1208 mL	10.6042 mL	21.2085 mL
	5 mM	0.4242 mL	2.1208 mL	4.2417 mL
	10 mM	0.2121 mL	1.0604 mL	2.1208 mL

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

BIOLOGICAL ACTIVITY

Description

Dabigatran (BIBR 953), an oral anticoagulant, is a reversible, potent, competitive direct thrombin inhibitor (K_i=4.5 nM). Dabigatran (BIBR 953) also inhibits thrombin-induced platelet aggregation (IC_{50}=10 nM)[1][2].

IC_{50} & Target

Ki: 4.5 nM (thrombin)[1]

In Vitro

Dabigatran (BIBR 953) shows concentration-dependent anticoagulant effects in various species in vitro, doubling the activated partial thromboplastin time (aPTT), prothrombin time (PT) and ecarin clotting time (ECT) in human platelet-poor plasma at concentrations of 0.23, 0.83 and 0.18 μM, respectively[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

Dabigatran (0.01-0.1 mg/kg; i.v.) inhibits clot formation with an ED_{50} of 0.033 mg/kg in Wessler model[3].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male rats (Wessler model)[3]
Dosage:	0.01, 0.03, 0.05 and 0.1 mg/kg
Administration:	Intravenous injection
Result:	Inhibited clot formation with an ED_{50} of 0.033 mg/kg.

CUSTOMER VALIDATION

- Int J Biol Macromol. 2019 Aug 1;134:622-630.
- Elife. 2022 Mar 23:11:e77444.
- Biochem Pharmacol. 2016 Nov 1;119:76-84.
- Platelets. 2020 Aug 7;1-8.
- Dig Dis Sci. 2019 Jan;64(1):102-112.

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REFERENCES

[1]. 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.

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

[3]. 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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