# Dabigatran

**Cat. No.:** HY-10163

**CAS No.:** 211914-51-1

**Molecular Formula:** $C_{25}H_{25}N_7O_3$

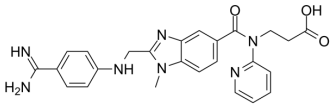
**Molecular Weight:** 472

**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 (26.48 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 | 2.1186 mL | 10.5932 mL | 21.1864 mL |
| 5 mM | 0.4237 mL | 2.1186 mL | 4.2373 mL |
| 10 mM | 0.2119 mL | 1.0593 mL | 2.1186 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.
- 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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