Dabigatran ethyl ester hydrochloride

Cat. No.: HY-77521

CAS No.: 211914-50-0

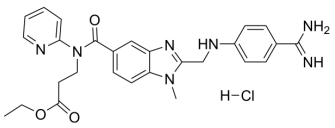
Molecular Formula: $C_{27}H_{30}ClN_7O_3$

Molecular Weight: 536.03

Target: Thrombin

Pathway: Metabolic Enzyme/Protease

Storage: 4°C, sealed storage, away from moisture
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 50 mg/mL (93.28 mM)

H_2O : 5 mg/mL (9.33 mM; Need ultrasonic)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8656 mL	9.3278 mL	18.6557 mL
	5 mM	0.3731 mL	1.8656 mL	3.7311 mL
	10 mM	0.1866 mL	0.9328 mL	1.8656 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (4.66 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (4.66 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.66 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Dabigatran ethyl ester hydrochloride is a potent inhibitor of ribosyldihydronicotinamide dehydrogenase (NQO2) with an IC_{50} value of 0.8 μM and a thrombin inhibitor.

IC_{50} & Target

IC50: 0.8 μM (NQO2)[1]

In Vitro

The K_i of dabigatran (ethyl ester hydrochloride) toward NQO2 is 0.9 μM and the IC_{50} is 0.8 μM. The ethyl ester group of dabigatran (ethyl ester hydrochloride) significantly extends the interaction surface especially with hydrophobic amino acids

	such as Ile 128 and Met 154. Dabigatran ethyl ester has higher affinity than Dabigatran to both thrombin and NQO2[1]. Dabigatran is a highly selective, reversible, and potent thrombin inhibitor and is orally available as the prodrug, dabigatran etexilate[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Dabigatran (K_i=4.5 nM) could bind to human thrombin selectively, and reversibly to realize a strong and long-lasting anticoagulant effect[3]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Kinase Assay [1]	NQO2 (0.5 μM) is incubated with the substrate mitomycin C (50 μM) and four different Dabigatran concentrations in 100 mM potassium phosphate buffer (pH 5.8) at room temperature for 5 min prior to the addition of NADH (in increasing concentrations) as a cosubstrate and photometric monitoring at 340 nm for 30 min at rt. K_i values are determined. Data generated are used to calculate the IC_{50} of inhibition of NQO2 activity[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Biochem Pharmacol. 2016 Nov 1;119:76-84.

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REFERENCES

[1]. Michaelis S, et al. Dabigatran and dabigatran ethyl ester: potent inhibitors of ribosyldihydronicotinamide dehydrogenase (NQO2). J Med Chem. 2012 Apr 26;55(8):3934-44.

[2]. Eisert WG, et al. Dabigatran: an oral novel potent reversible nonpeptide inhibitor of thrombin. Arterioscler Thromb Vasc Biol. 2010 Oct;30(10):1885-9.

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

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