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产品名称：Dabigatran Ethyl Ester Hydrochloride Salt
产品别名：Dabigatran ethyl ester hydrochloride

生物活性：

Description	Dabigatran ethyl ester hydrochloride is a potent inhibitor of ribosyldihydronicotinamide dehydrogenase (NQO2) with an IC50 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].
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].

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	Solvent / Mass / 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

*请根据产品在不同溶剂中的溶解度选择合适的溶剂配制储备液；一旦配成溶液，请分装保存，避免反复冻融造成的产品失效。

储备液的保存方式和期限：-80°C, 6 months; -20°C, 1 month。-80°C 储存时，请在 6 个月内使用，-20°C 储存时，请在 1 个月内使用。

In Vivo:

请根据您的实验动物和给药方式选择适当的溶解方案。以下溶解方案都请先按照 In Vitro 方式配制澄清的储备液，再依次添加助溶剂：

——为保证实验结果的可靠性，澄清的储备液可以根据储存条件，适当保存；体内实验的工作液，建议您现用现配，当天使用； 以下溶剂前显示的百分比是指该溶剂在您配制终溶液中的体积占比；如在配制过程中出现沉淀、析出现象，可以通过加热和/或超声的方式助溶

1.请依序添加每种溶剂： 10% DMSO→40% PEG300 →5% Tween-80 → 45% saline

Solubility: ≥ 2.5 mg/mL (4.66 mM); Clear solution

此方案可获得 ≥ 2.5 mg/mL (4.66 mM，饱和度未知) 的澄清溶液。

以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 400 μL PEG300 中，混合均匀；向上述体系中加入 50 μL Tween-80，混合均匀；然后继续加入 450 μL 生理盐水定容至 1 mL。

2.请依序添加每种溶剂： 10% DMSO→ 90% (20% SBE-β-CD in saline)

Solubility: ≥ 2.5 mg/mL (4.66 mM); Clear solution

	此方案可获得 ≥ 2.5 mg/mL (4.66 mM，饱和度未知) 的澄清溶液。 以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 900 μL 20% 的 SBE-β-CD 生理盐水水溶液中，混合均匀。 3.请依序添加每种溶剂： 10% DMSO →90% corn oil Solubility: ≥ 2.5 mg/mL (4.66 mM); Clear solution 此方案可获得 ≥ 2.5 mg/mL (4.66 mM，饱和度未知) 的澄清溶液，此方案不适用于实验周期在半个月以上的实验。 以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 900 μL 玉米油中，混合均匀。
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.
实验参考：	
Kinase Assay	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. Ki values are determined. Data generated are used to calculate the IC50 of inhibition of NQO2 activity[1].
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.