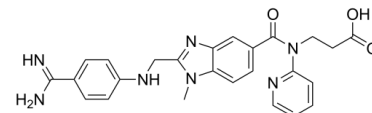


Data Sheet

Product Name:	Dabigatran
Cat. No.:	CS-1399
CAS No.:	211914-51-1
Molecular Formula:	C ₂₅ H ₂₅ N ₇ O ₃
Molecular Weight:	471.51
Target:	Thrombin
Pathway:	Metabolic Enzyme/Protease
Solubility:	H2O : < 0.1 mg/mL (insoluble); DMSO : < 1 mg/mL (insoluble or slightly soluble); 0.1 M HCL : 12.5 mg/mL (26.51 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

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: K_i : 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 μ M, respectively^[1]. **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].

References:

- [1]. Wiene W, Stassen JM, Pripke H, In-vitro profile and ex-vivo anticoagulant activity of the direct thrombin inhibitor dabigatran and its orally active prodrug, dabigatran etexilate. *Thromb Haemost.* 2007 Jul;98(1):155-62.
- [2]. Huel NH, et al. Structure-based design of novel potent nonpeptide thrombin inhibitors. *J Med Chem.* 2002 Apr 25;45(9):1757-66.
- [3]. Wiene 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.

CAIndexNames:

CN(C)C(=O)Nc1ccc(cc1)CNC(=O)Nc2ccncc2

SMILES:

N=C(N)C(C=C1)=CC=C1NCC2=NC3=CC(C(N(CCC(O)=O)C4=NC=CC=C4)=O)=CC=C3N2C

Caution: Product has not been fully validated for medical applications. For research use only.

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