

Product Data Sheet

Product Name: Dabigatran ethyl ester hydrochloride

Cat. No.: GC35802

Chemical Properties

Cas. No. 211914-50-0

SMILES NC(C1=CC=C(NCC2=NC3=CC(C(N(CCC(OCC)=O)C4=CC=CC=N4)=O)=CC=C3N2C)C=C1)=N.[H]Cl

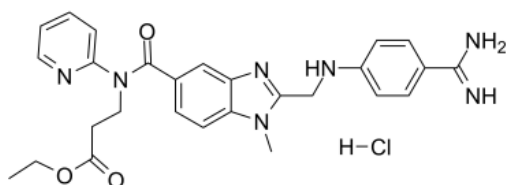
Formula $C_{27}H_{30}ClN_7O_3$ M.Wt 536.03

Solubility DMSO: ≥ 50 mg/mL (93.28 mM);
Water: 5 mg/mL (9.33 mM) Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Background

Dabigatran ethyl ester hydrochloride is a potent inhibitor of ribosyldihyronicotinamide dehydrogenase (NQO2) with an IC_{50} value of $0.8\text{ }\mu\text{M}$ and a thrombin inhibitor. IC_{50} : $0.8\text{ }\mu\text{M}$ (NQO2) [1]

The K_i of dabigatran (ethyl ester hydrochloride) toward NQO2 is $0.9\text{ }\mu\text{M}$ and the IC_{50} is $0.8\text{ }\mu\text{M}$. The

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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].

Dabigatran ($K_i=4.5$ nM) could bind to human thrombin selectively, and reversibly to realize a strong and long-lasting anticoagulant effect[3].

[1]. Michaelis S, et al. Dabigatran and dabigatran ethyl ester: potent inhibitors of ribosylidihydronicotinamide 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]. Huel 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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