Dabigatran ethyl ester hydrochloride

Cat. No.: HY-77521
CAS No.: 211914-50-0
Molecular Formula: C₂₇H₃₀ClN₇O₃
Molecular Weight: 536.03
Target: Thrombin
Pathway: Metabolic Enzyme/Protease
Storage: Powder -20°C 3 years
         4°C  2 years
         In solvent -80°C 6 months
                   -20°C 1 month

SOLVENT & SOLUBILITY

In Vitro
DMSO: ≥ 50 mg/mL (93.28 mM)
H₂O: 5 mg/mL (9.33 mM; Need ultrasonic)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

<table>
<thead>
<tr>
<th>Solvent Concenetrion</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mM</td>
<td>1.8656 mL</td>
<td>9.3278 mL</td>
<td>18.6557 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td>0.3731 mL</td>
<td>1.8656 mL</td>
<td>3.7311 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td>0.1866 mL</td>
<td>0.9328 mL</td>
<td>1.8656 mL</td>
</tr>
</tbody>
</table>

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 ribosylhydronicotinamide dehydrogenase (NQO2) with an IC₅₀ value of 0.8 µM and a thrombin inhibitor.

IC₅₀ & Target
IC₅₀: 0.8 µM (NQO2)
**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\(^3\).

**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.

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**REFERENCES**

