PE859

Cat. No.: HY-12662  
CAS No.: 1402727-29-0  
Molecular Formula: \( \text{C}_{28}\text{H}_{24}\text{N}_{4}\text{O}_{2} \)  
Molecular Weight: 448.52  
Target: Microtubule/Tubulin  
Pathway: Cell Cycle/DNA Damage; Cytoskeleton  
Storage: Powder  
-20°C 3 years  
-80°C 6 months  
In solvent  
-20°C 1 month  
4°C 2 years

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**SOLVENT & SOLUBILITY**

**In Vitro**

<table>
<thead>
<tr>
<th>Solvent</th>
<th>Mass Concentration</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>DMSO: 50 mg/mL (111.48 mM; Need ultrasonic)</td>
<td>1 mM</td>
<td>2.2296 mL</td>
<td>11.1478 mL</td>
<td>22.2956 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td>0.4459 mL</td>
<td>2.2296 mL</td>
<td>4.4591 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td>0.2230 mL</td>
<td>1.1148 mL</td>
<td>2.2296 mL</td>
</tr>
</tbody>
</table>

Solubility: 
- DMSO: >50 mg/mL (111.48 mM)  
- H\(_2\)O: <0.1 mg/mL (insoluble)

**In Vivo**

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline  
Solubility: >2.5 mg/mL (5.57 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil  
Solubility: >2.5 mg/mL (5.57 mM); Clear solution

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**BIOLOGICAL ACTIVITY**

**Description**

PE859 is a potent inhibitor of both tau and Aβ aggregation with IC\(_{50}\) values of 0.66 and 1.2 μM, respectively.

**IC\(_{50}\) & Target**

IC\(_{50}\): 0.66 μM (tau), 1.2 μM (Aβ)\(^{[1]}\)

**In Vitro**

PE859 inhibits the heparin-induced aggregation of both 3RMBD and full length tau in a concentration-dependent manner. In each assay, the IC\(_{50}\) values calculated at the last measurement periods are 0.81 μM, and 2.23 μM, respectively. PE859 inhibits tau aggregation through formation of beta-sheet structure\(^{[2]}\).

MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo

PE859 could cross the blood-brain barrier and that PE859 could be distributed into the tissues of the central nervous system. The maximum concentration of PE859 is 2.005 μg/mL in the blood at 3 h and 1.428 μg/g in the brain at 6 h. PE859 delays onset and progression of the motor dysfunction in JNPL3 mice. PE859 delays progression of the motor dysfunction through the inhibition of accumulation of sarkosyl-insoluble tau. [2]

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PROTOCOL

Kinase Assay [2]

Tau aggregation is monitored using thioflavin T. The test compound (PE859), 10 μM 3RMBD and 10 μM heparin are dissolved in 50 mM Tris-HCl (pH7.6), and incubated at 37°C up to 144 hours. At each point of incubation time, 135 μL of the solutions are removed and mixed with 15 μL of 100 μM ThT solution (final concentration: 10 μM) and the fluorescence intensity with excitation at 440 nm and emission at 486 nm is measured [2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Administration [2]

Mice: PE859 is dissolved in 80% PEG400 and 20% water solution at 5 mg/mL, and orally-administered at a dose of 40 mg/kg/day for 6 months (from 9 to 15 months of age). The body weights of the mice are measured once a week during PE859 treatment [2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

• Elife. 2019 Mar 25;8:e45457.

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REFERENCES


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

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