Nebentan

Cat. No.: HY-106994  
CAS No.: 403604-85-3  
Molecular Formula: C₂₄H₂₁N₅O₅S  
Molecular Weight: 491.52  
Target: Endothelin Receptor  
Pathway: GPCR/G Protein  
Storage:  
- Powder: -20°C, 3 years; 4°C, 2 years  
- In solvent: -80°C, 6 months; -20°C, 1 month  

SOLVENT & SOLUBILITY

<table>
<thead>
<tr>
<th>In Vitro</th>
<th>DMSO : 125 mg/mL (254.31 mM; Need ultrasonic)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preparing Stock Solutions</td>
<td></td>
</tr>
<tr>
<td>Solvent Concentration</td>
<td>Mass 1 mg</td>
</tr>
<tr>
<td>1 mM</td>
<td>2.0345 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td>0.4069 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td>0.2035 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: ≥ 2.08 mg/mL (4.23 mM); Clear solution |
|----------|--------------------------------------------------------------------------------------------------|
| 2. Add each solvent one by one: 10% DMSO >> 90% corn oil  
Solubility: ≥ 2.08 mg/mL (4.23 mM); Clear solution |

BIOLOGICAL ACTIVITY

Description | Nebentan (YM598 free base) is a potent, selective and orally active non-peptide endothelin ETₐ receptor antagonist through the modification of Bosentan (HY-A0013). Nebentan inhibits [¹²⁵I] endothelin-1 binding to cloned human endothelin ETA and ETB receptor, with Kᵢ of 0.697 nM and 569 nM, respectively[¹]. YM598 can ameliorate the progression of cor pulmonale and myocardial infarction in vivo².

IC₅₀ & Target |  
| ETₐ | 0.697 nM (Kᵢ) | ETₐ | 569 nM (Kᵢ) |

In Vitro | Nebentan inhibits the specific binding of [¹²⁵I] endothelin-1 to endothelin ETA and ETB receptors in a concentration dependent manner, Kᵢ values are 0.697 nM and 1.53 nM for human and rat endothelin ETA receptors, respectively. In
contrast, YM598 exhibits low affinities for human and rat endothelin ET\(_B\) receptors, with \(K_i\) values of 569 nM and 155 nM, respectively\[1\].

In measurement of intracellular Ca\(^{2+}\) concentration, Nebentan concentration-dependently inhibits the increase in \([\text{Ca}^{2+}]_i\) induced by 10 nM endothelin-1 in both CHO cells and A10 cells, the IC\(_{50}\) values are 26.2 nM for CHO cells and 26.7 nM for A10 cells, respectively\[1\].

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

| In Vivo | Nebentan (oral administration; 0.1-1 mg/kg; 4 weeks) significantly inhibits the progression of pulmonary hypertension and the development of right ventricular hypertrophy\[2\].
Nebentan (oral administration; 1 mg/kg; 30 weeks) significantly ameliorates the poor survival rate of CHF rats, it markedly reduces the hypertrophy of both ventricles as well as pulmonary congestion\[2\].
MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

REFERENCES


Caution: Product has not been fully validated for medical applications. For research use only.
Tel: 609-228-6898  Fax: 609-228-5909  E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA