Sibofimloc

Cat. No.:  HY-12820
CAS No.:  1616113-45-1
Molecular Formula:  C₃₅H₃₉NO₁₁
Molecular Weight:  649.68
Target:  Bacterial; Antibiotic
Pathway:  Anti-infection
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 : ≥ 31 mg/mL (47.72 mM)
"≥" means soluble, but saturation unknown.

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<th>Solvent Concentration</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 mM</td>
<td>1.5392 mL</td>
<td>7.6961 mL</td>
<td>15.3922 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td>0.3078 mL</td>
<td>1.5392 mL</td>
<td>3.0784 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td>0.1539 mL</td>
<td>0.7696 mL</td>
<td>1.5392 mL</td>
</tr>
</tbody>
</table>

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description  Sibofimloc (Antibiotic-202) is a first-in-class, gut-restricted, orally bioavailable FimH adhesion inhibitor extracted from patent WO2014100158A1, Compound Example 202. Sibofimloc has anti-bacterial infective activity and is developed for inflammatory bowel disease (IBD)[1][2].

IC₅₀ & Target  FimH adhesion[1][2]

In Vitro  FimH is a TLR4 receptor, expressed on E. coli and other Enterobacteriaceae in host with CD. The inhibition of FimH adhesion, and consequently intracellular replication of adherent-invasive E. coli in epithelial cells, may prevent establishment of a sub-mucosal infection leading to mucosal inflammation and epithelial barrier disruption[1][2].

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

REFERENCES