Etrasimod

Cat. No.: HY-12789
CAS No.: 1206123-37-6
Molecular Formula: C₂₆H₂₆F₃NO₃
Molecular Weight: 457.48
Target: LPL 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

In Vitro
DMSO: ≥ 28 mg/mL (61.20 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>2.1859 mL</td>
<td>10.9294 mL</td>
<td>21.8589 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td>0.4372 mL</td>
<td>2.1859 mL</td>
<td>4.3718 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td>0.2186 mL</td>
<td>1.0929 mL</td>
<td>2.1859 mL</td>
</tr>
</tbody>
</table>

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

BIOLOGICAL ACTIVITY

Description
Etrasimod (APD334) is a potent, selective and orally available antagonist of the sphingosine-1-phosphate-1 (S1P₁) receptor with an IC₅₀ value of 1.88 nM in CHO cells.

IC₅₀ & Target
IC₅₀: 1.88 nM (S1P₁)\(^1\)

In Vitro
APD334 is a structurally novel, functional antagonist of S1P₁. In CHO cells expressing HA tagged S1P₃, APD334 is found to have an IC₅₀ value of 1.88 nM. Moderate agonism at human S1P₄ and S1P₅ is observed but is reduced relative to S1P₁, both in terms of potency and efficacy. APD334 is devoid of any agonism or antagonism at human S1P₂ and S1P₃. APD334 achieves good central exposure following oral dosing and possesses a favorable pharmacokinetic profile in multiple preclinical species. S1P₁ activity is maintained in mice (EC₅₀=0.44 nM), rats (EC₅₀=0.32 nM), dogs (EC₅₀=0.34 nM) and monkeys (EC₅₀=0.32 nM)\(^1\).

In Vivo
APD334 has a relatively low systemic clearance (<4% of hepatic blood flow) and high Cₘₐₓ across all species. In both
dog and monkey a significant decrease in volume of distribution (Vss) is observed relative to rodent. Oral bioavailability is in the range of 40–100%, and the terminal phase half-life varied from 6 h in monkey, to as long as 29 h in dog. Rat and monkey $t_{1/2}$ values for siponimod (another S1P1 modulator currently in human trials) have been disclosed and are 6 and 19 h, respectively.[1]

**PROTOCOL**

**Animal Administration**[1]

Rats: APD334 induced effects on blood lymphopenia are determined in male Sprague-Dawley rats. Briefly, male rats are given a 0 (vehicle only), 0.03 (mice only), 0.1, 0.3 or 1 mg/kg oral dose of APD334 formulated in 0.5% methylcellulose (MC) in water. Rat blood samples are collected at 0, 1, 3, 5, 8, 16, 24, 32, 48 and 72 hours post-dose[1].

Mice: APD334 induced effects on blood lymphopenia are determined in male BALB/c mice. Briefly, male mice are given a 0 (vehicle only), 0.03 (mice only), 0.1, 0.3 or 1 mg/kg oral dose of APD334 formulated in 0.5% methylcellulose (MC) in water. Mouse blood samples are taken at 0, 1, 3, 5, 8, 16, 24 and 32 hours post-dose[1].

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.

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