**Etrasimod**

Cat. No.: HY-12789  
CAS No.: 1206123-37-6  
Molecular Formula: C_{26}H_{26}F_{3}NO_{3}  
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**

<table>
<thead>
<tr>
<th>Solvent</th>
<th>Mass (1 mg)</th>
<th>Mass (5 mg)</th>
<th>Mass (10 mg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DMSO</td>
<td>2.1859 mL</td>
<td>10.9294 mL</td>
<td>21.8589 mL</td>
</tr>
<tr>
<td>1 mM</td>
<td>0.4372 mL</td>
<td>2.1859 mL</td>
<td>4.3718 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td>0.2186 mL</td>
<td>1.0929 mL</td>
<td>2.1859 mL</td>
</tr>
</tbody>
</table>

In Vitro DMSO: ≥ 28 mg/mL (61.20 mM)  
*"≥" means soluble, but saturation unknown.*

Preparing Stock Solutions:  
10 mM: 0.2186 mL, 1.0929 mL, 2.1859 mL

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 IC_{50} value of 1.88 nM in CHO cells.

**IC_{50} & Target**  
IC50: 1.88 nM [S1P1]^{[1]}

**In Vitro**  
APD334 is a structurally novel, selective, functional antagonist of S1P1. In CHO cells expressing HA tagged S1P1, APD334 is found to have an IC_{50} 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 (EC_{50}=0.44 nM), rats (EC_{50}=0.32 nM), dogs (EC_{50}=0.34 nM) and monkeys (EC_{50}=0.32 nM).^{[1]}

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

**In Vivo**  
APD334 has a relatively low systemic clearance (<4% of hepatic blood flow) and high C_{max} 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\(^1\).

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**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\(^1\).

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**REFERENCES**


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**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