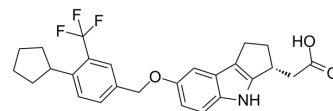


## Etrasimod

<b>Cat. No.:</b>	HY-12789		
<b>CAS No.:</b>	1206123-37-6		
<b>Molecular Formula:</b>	C <sub>26</sub> H <sub>26</sub> F <sub>3</sub> NO <sub>3</sub>		
<b>Molecular Weight:</b>	457.48		
<b>Target:</b>	LPL Receptor		
<b>Pathway:</b>	GPCR/G Protein		
<b>Storage:</b>	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	2 years
		-20°C	1 year



### SOLVENT & SOLUBILITY

#### In Vitro

DMSO : 116.67 mg/mL (255.03 mM; Need ultrasonic)

Concentration	Mass		
	1 mg	5 mg	10 mg
1 mM	2.1859 mL	10.9294 mL	21.8589 mL
5 mM	0.4372 mL	2.1859 mL	4.3718 mL
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 (S1P<sub>1</sub>) receptor with an IC<sub>50</sub> value of 1.88 nM in CHO cells.

#### IC<sub>50</sub> & Target

IC<sub>50</sub>: 1.88 nM (S1P<sub>1</sub>)<sup>[1]</sup>

#### In Vitro

APD334 is a structurally novel, selective, functional antagonist of S1P<sub>1</sub>. In CHO cells expressing HA tagged S1P<sub>1</sub>, APD334 is found to have an IC<sub>50</sub> value of 1.88 nM. Moderate agonism at human S1P<sub>4</sub> and S1P<sub>5</sub> is observed but is reduced relative to S1P<sub>1</sub>, both in terms of potency and efficacy. APD334 is devoid of any agonism or antagonism at human S1P<sub>2</sub> and S1P<sub>3</sub>. APD334 achieves good central exposure following oral dosing and possesses a favorable pharmacokinetic profile in multiple preclinical species. S1P<sub>1</sub> activity is maintained in mice (EC<sub>50</sub>=0.44 nM), rats (EC<sub>50</sub>=0.32 nM), dogs (EC<sub>50</sub>=0.34 nM) and monkeys (EC<sub>50</sub>=0.32 nM)<sup>[1]</sup>.

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<sub>max</sub> across all species. In both dog and monkey a significant decrease in volume of distribution (V<sub>ss</sub>) 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<sup>[1]</sup>.

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## PROTOCOL

### Animal Administration <sup>[1]</sup>

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<sup>[1]</sup>.

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<sup>[1]</sup>.

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

## CUSTOMER VALIDATION

- Heliyon. 2024 July 04.

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## REFERENCES

[1]. Buzard DJ, et al. Discovery of APD334: Design of a Clinical Stage Functional Antagonist of the Sphingosine-1-phosphate-1 Receptor. ACS Med Chem Lett. 2014 Nov 4;5(12):1313-7.

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

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