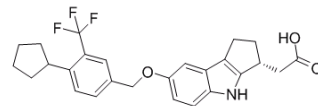


## Data Sheet

Product Name:	Etrasimod
Cat. No.:	HY-12789
CAS No.:	1206123-37-6
Molecular Formula:	C <sub>26</sub> H <sub>26</sub> F <sub>3</sub> NO <sub>3</sub>
Molecular Weight:	457.48
Target:	LPL Receptor
Pathway:	GPCR/G Protein
Solubility:	DMSO: ≥ 28 mg/mL



### BIOLOGICAL ACTIVITY:

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>.

**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<sub>1/2</sub> values for siponimod (another S1P<sub>1</sub> modulator currently in human trials) have been disclosed and are 6 and 19 h, respectively<sup>[1]</sup>.

### PROTOCOL (Extracted from published papers and Only for reference)

**Animal Administration:** <sup>[1]</sup>Rat: 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>.

Mouse: 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>.

### 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.**

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: [tech@MedChemExpress.com](mailto:tech@MedChemExpress.com)

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA