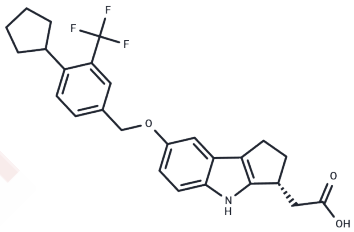
# Data Sheet (Cat.No.TQ0227)

TargetMol

## Etrasimod

### Chemical Properties



CAS No. : 1206123-37-6

Formula: C26H26F3NO3

Molecular Weight: 457.48

Storage: Store at low temperature
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

### Biological Description

| | |
|---|---|
| Description | Etrasimod (APD334) is a specific and orally available antagonist of the sphingosine-1-phosphate-1 (S1P1) receptor (IC50: 1.88 nM in CHO cells). |
| Targets(IC50) | LPL Receptor,S1P Receptor |
| In vitro | In CHO cells expressing HA-tagged S1P1, 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. |
| 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 the volume of distribution (Vss) is observed relative to the 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 the dog. |
| Animal Research | 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. 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. |

### Solubility Information

| | |
|---|---|
| Solubility | DMSO: 25 mg/mL (54.65 mM),Sonication is recommended.<br>(< 1 mg/ml refers to the product slightly soluble or insoluble) |

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|---|---|---|---|
| 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 |
| 50 mM | 0.0437 mL | 0.2186 mL | 0.4372 mL |

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.