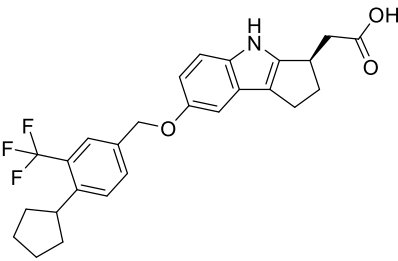


Product data sheet



MedKoo Cat#: 407212 Name: Etrasimod CAS#: 1206123-37-6 (free base) Chemical Formula: C ₂₆ H ₂₆ F ₃ NO ₃ Exact Mass: 457.18648 Molecular Weight: 457.49321	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

Etrasimod, also known as APD334, is a potent, centrally available, functional antagonists of the S1P1 receptor for use as next generation therapeutics for treating multiple sclerosis (MS) and other autoimmune diseases. APD334 has a favorable PK/PD profile, producing robust lymphocyte lowering at relatively low plasma concentrations in several preclinical species. APD334 was efficacious in a mouse experimental autoimmune encephalomyelitis (EAE) model of MS and a rat collagen induced arthritis (CIA) model and was found to have appreciable central exposure.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	29.0	63.39
DMSO:PBS (pH 7.2) (1:1)	0.5	1.09
DMF	30.0	65.57
Ethanol	12.5	27.32

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.19 mL	10.93 mL	21.86 mL
5 mM	0.44 mL	2.19 mL	4.37 mL
10 mM	0.22 mL	1.09 mL	2.19 mL
50 mM	0.04 mL	0.22 mL	0.44 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

TBD

In vivo study

1. Buzard DJ, Kim SH, Lopez L, Kawasaki A, Zhu X, Moody J, Thoresen L, Calderon I, Ullman B, Han S, Lehmann J, Gharbaoui T, Sengupta D, Calvano L, Montalban AG, Ma YA, Sage C, Gao Y, Semple G, Edwards J, Barden J, Morgan M, Chen W, Usmani K, Chen C, Sadeque A, Christopher RJ, Thatte J, Fu L, Solomon M, Mills D, Whelan K, Al-Shamma H, Gatlin J, Le M, Gaidarov I, Anthony T, Unett DJ, Blackburn A, Rueter J, Stirn S, Behan DP, Jones RM. 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. doi: 10.1021/ml500389m. PMID: 25516790; PMCID: PMC4265817.

Product data sheet



7. Bioactivity

Biological target:

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.

In vitro activity

TBD

In vivo activity

APD334 was evaluated in a murine experimental autoimmune encephalomyelitis (EAE) model. Prophylactically, APD334 prevented the onset and severity of disease relative to vehicle up to day 25, at which time dosing was discontinued. Treatment began at day 18, by which time all animals had developed severe disease, and APD334 was administered out to day 37. APD334 reversed disease relative to vehicle and was similar to the efficacy observed with fingolimod.

Reference: ACS Med Chem Lett. 2014 Nov 4;5(12):1313-7. <https://pubmed.ncbi.nlm.nih.gov/25516790/>

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.