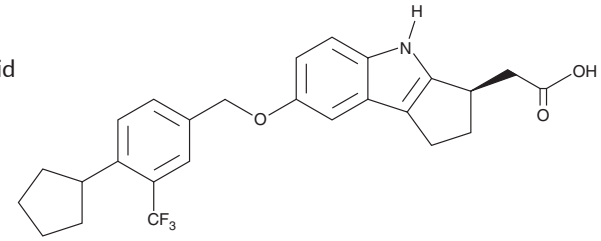
PRODUCT INFORMATION

Etrasimod

Item No. 21661

CAS Registry No.:	1206123-37-6
Formal Name:	(3R)-7-[[4-cyclopentyl-3-(trifluoromethyl)phenyl]methoxy]-1,2,3,4-tetrahydro-cyclopent[b]indole-3-acetic acid
Synonym:	APD334
MF:	$C_{26}H_{26}F_3NO_3$
FW:	457.5
Purity:	≥95%
UV/Vis.:	λ_{max}: 227, 279 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Etrasimod is supplied as a crystalline solid. A stock solution may be made by dissolving the etrasimod in the solvent of choice, which should be purged with an inert gas. Etrasimod is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of etrasimod in these solvents is approximately 12.5 mg/ml in ethanol and approximately 30 mg/ml in DMSO and DMF.

Etrasimod is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, etrasimod should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Etrasimod has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Etrasimod is an orally bioavailable and potent antagonist of sphingosine-1-phosphate (S1P) receptors with EC_{50} values of 0.093, 0.44, 0.32, 0.34, and 0.32 nM for human, mouse, rat, dog, and monkey $S1P_1$ receptors.[1] It is selective for $S1P_1$, $S1P_4$, and $S1P_5$ receptors with EC_{50} values of 6.1, >10,000, >10,000, 147, and 24.4 nM for $S1P_{1\text{-}5}$, respectively, in a β-arrestin assay. Etrasimod (1 mg/kg, i.v.) decreases peripheral lymphocytes in mouse, rat, dog, and monkey (IC_{50}s = 101, 51, 58, and 98 nM, respectively). It delays or prevents the onset and severity of murine experimental autoimmune encephalomyelitis (EAE) when administered at 0.3, 1, or 3 mg/kg. It also leads to lower EAE disease scores relative to vehicle when administered after disease onset and is efficacious in a rat model of collagen-induced arthritis.

References

1. Buzard, D.J., Kim, S.H., Lopez, L., *et al.* Discovery of APD334: Design of a clinical stage functional antagonist of the sphingosine-1-phosphate-1 receptor. *ACS Med. Chem. Lett.* **5(12)**, 1313-1317 (2014).

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