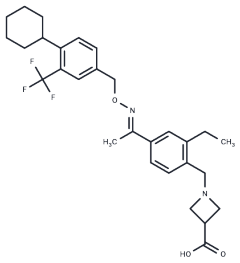
Data Sheet (Cat.No.T6403)

TargetMol

Siponimod

Chemical Properties



CAS No. : 1230487-00-9

Formula: C29H35F3N2O3

Molecular Weight: 516.59

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	BAF312 (Siponimod (BAF-312)), a next-generation S1P receptor modulator, is specific for S1P1 and S1P5 receptors with EC50 of 0.39 nM and 0.98 nM, respectively. The specificity of BAF312 for S1P1 and S1P5 receptors exhibits >1000-fold over S1P2, S1P3 and S1P4 receptors.
Targets(IC50)	LPL Receptor,S1P Receptor
In vitro	BAF312 is a potent and selective S1P receptor agonist. Its EC50s for S1P1 and S1P5 receptors were 0.39 nM and 0.98 nM, respectively, and it was more than 1000-fold more potent than S1P2, S1P3, and S1P4 receptors at S1P1 and S1P5 receptors.
In vivo	BAF312 is a potent and selective S1P receptor agonist. Its EC50s for S1P1 and S1P5 receptors were 0.39 nM and 0.98 nM, respectively, and it was more than 1000-fold more potent than S1P2, S1P3, and S1P4 receptors at S1P1 and S1P5 receptors.
Kinase Assay	GTPγ[35S] binding assay: The cells are homogenized and centrifuged at 26900 × g for 30 min at 4°C. Membranes are re-suspended in 20 mM HEPES (pH 7.4), 100 mM NaCl, 10 mM MgCl2, 1 mM EDTA and 0.1% fat-free BSA at 2–3 mg protein/mL. GTPγ[35S] binding assay is performed with the membranes (75 mg protein /mL in 50 mM HEPES, 100 mM NaCl, 10 mM MgCl2, 20 μg/mL saponin and 0.1% fat-free BSA (pH 7.4), 5 mg/mL with wheat-germ agglutinin-coated scintillation proximity assay-bead, and 10 μM GDP for 10–15 min. The GTPγ[35S]-binding reaction is started by the addition of 200 pM GTPγ[35S]. After 120 min at room temperature, the plates are centrifuged for 10 min at 300 × g and counted.
Cell Research	Agonist-mediated internalization of S1P1 receptors in CHO cells analysed by flow cytometry Myc-tag hS1P1 cells are incubated for 1 h with agonist at 37°C in standard culture medium followed by a PBS wash. An aliquot is kept on ice for 3 h, while another aliquot is left for 3 (or 12) h in culture medium (no agonist) at 37°C. The cells are then incubated either with 4 μg/mL monoclonal mouse anti C-myc IgG1 antibody or with isotype control mouse IgG1 for 60 min at 4°C, followed by an incubation with 1 μg/mL of Alexa488-labelled goat anti-mouse secondary conjugates. The cells are subjected to flow cytometry measurements using 10000 viable cells per sample.(Only for Reference)

Solubility Information

Solubility	Ethanol: 41 mg/mL (79.37 mM),Sonication is recommended. DMSO: 5.17 mg/mL (10.01 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9358 mL	9.6789 mL	19.3577 mL
5 mM	0.3872 mL	1.9358 mL	3.8715 mL
10 mM	0.1936 mL	0.9679 mL	1.9358 mL
50 mM	0.0387 mL	0.1936 mL	0.3872 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.

Reference

Gergely P, et al. Br J Pharmacol, 2012, 167(5), 1035-1047.
Fauzyah Y, Ono C, Torii S, et al. Ponesimod suppresses hepatitis B virus infection by inhibiting endosome maturation. Antiviral Research. 2021 Feb;186:104999
Pan S, et al. ACS Med, Chem, Lett, 2013, 4 (3), 333-337.
Lewis ND, et al. J Immunol, 2013, 190(7), 3533-3540.
Fauzyah Y, Ono C, Torii S, et al. Ponesimod suppresses hepatitis B virus infection by inhibiting endosome maturation[J]. Antiviral Research. 2020: 104999.