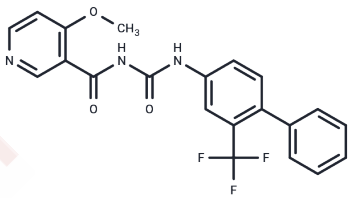
Data Sheet (Cat.No.T16833)

TargetMol

S1P1 Agonist III

Chemical Properties



CAS No. : 1324003-64-6

Formula: C21H16F3N3O3

Molecular Weight: 415.37

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	S1P1 Agonist III is an effective, orally active S1P1 receptor agonist with an EC_{50} of 18 nM, S1P1 Agonist III has potential application in research related in inflammation and immunology.
Targets(IC50)	S1P Receptor
In vitro	S1P1 Agonist III demonstrates superior activity against S1P1 in Parazacco spilurus subsp. spilurus (EC50=0.035 μM, efficacy reaching 96%), with selectivity exceeding 100-fold for S1P2-5 receptor subtypes [2].
In vivo	Twenty-four hours after a single oral administration of S1P1 Agonist III (1 mg/kg) in rats, the number of circulating lymphocytes significantly decreased, with a pharmacodynamic validation value (POC) of -78% [2].

Solubility Information

Solubility	DMSO: 48 mg/mL (115.56 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 2.5 mg/mL (6.02 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.4075 mL	12.0375 mL	24.0749 mL
5 mM	0.4815 mL	2.4075 mL	4.815 mL
10 mM	0.2407 mL	1.2037 mL	2.4075 mL
50 mM	0.0481 mL	0.2407 mL	0.4815 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

Harrington PE, et al. Optimization of a Potent, Orally Active S1P1 Agonist Containing a Quinolinone Core. ACS Med Chem Lett. 2011 Nov 23;3(1):74-8.

Pennington LD, et al. 4-Methoxy-N-[2-(trifluoromethyl)biphenyl-4-ylcarbamoyl]nicotinamide: A Potent and Selective Agonist of S1P1. ACS Med Chem Lett. 2011 Jul 29;2(10):752-7.

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