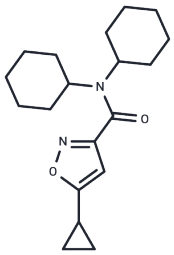
Data Sheet (Cat.No.T3961)

TargetMol

CYM-5541

Chemical Properties



CAS No. : 945128-26-7

Formula: C19H28N2O2

Molecular Weight: 316.44

Storage: 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	CYM-5541 (ML249) is a selective and allosteric S1P3 receptor agonist.
Targets(IC50)	LPL Receptor,S1P Receptor
In vitro	CYM-5541 is a full agonist that achieves maximal ERK phosphorylation levels comparable to S1P, with an EC50 of 72-132 nM and high selectivity over other S1P receptor subtypes: S1P1 EC50 >10 μM, S1P2 EC50 >50 μM, S1P4 EC50 >50 μM, and S1P5 EC50 >25 μM. It exhibits no significant activity in the Ricerca profiling panel of 55 GPCRs, ion channels, and transporters. CYM-5541 enabled the identification of an allosteric site, with residue F263 being crucial for its affinity and efficacy, suggesting the presence of a unique hydrophobic pocket responsible for its S1P3 selectivity [1].
Kinase Assay	Jump-In TI CHO-K cells stably expressing WT or mutant S1P3 are serum-starved for 4 hrs. They are then incubated at 4 °C for 30 min in the binding buffer containing 20 mM Tris-HCl (pH 7.5), 100 mM NaCl, 15 mM NaF, 0.5 mM EDTA, 1 mM Na3VO4, 0.5% fatty acid-free bovine serum albumin, and protease inhibitor mixture with 0.1 nM [33P]S1P and increasing concentrations of S1P, SPM-242, or CYM-5541. Cells are washed three times with cold binding buffer. Cell-bound radioactivity is measured by lysing the cells with 0.5% SDS followed by liquid scintillation counting. The raw data is normalized so that the level of [33P]S1P bound to each cell line (WT or mutant) in the absence of competing ligand is referenced as 100% for its own cell line[1].

Solubility Information

Solubility	DMSO: 27.8 mg/mL (87.85 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: 2.78 mg/mL (8.79 mM),Suspension. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (6.32 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	3.1602 mL	15.8008 mL	31.6016 mL
5 mM	0.632 mL	3.1602 mL	6.3203 mL
10 mM	0.316 mL	1.5801 mL	3.1602 mL
50 mM	0.0632 mL	0.316 mL	0.632 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

Jo E, et al. Novel selective allosteric and bitopic ligands for the S1P(3) receptor. ACS Chem Biol. 2012 Dec 21;7(12): 1975-83.