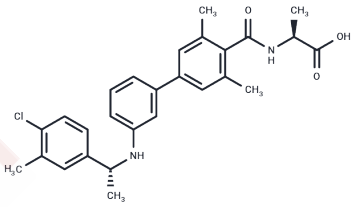
Data Sheet (Cat.No.T28169)

TargetMol

NIBR-0213

Chemical Properties



CAS No. : 1233332-14-3

Formula: C27H29ClN2O3

Molecular Weight: 464.98

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	NIBR-0213 is a potent and selective competitive S1P1 antagonist with activity against experimental autoimmune encephalomyelitis. In the GTPγ35S assay, it has IC50 values of 2.0 nM and 2.3 nM for human and rat S1P1, respectively.
Targets(IC50)	LPL Receptor
In vitro	In the Ca2+ assay, NIBR-0213 showed inhibitory activity against hS1P1 with an IC50 of 2.5 nM, but was inactive against S1P2, S1P3, and S1P4 (IC50 > 10 μM); in the GTPγ35S assay, NIBR-0213 showed potent and comparable potency against human and rat S1P1 (IC50 of 2.0 nM and 2.3 nM, respectively), while the IC50 for mouse S1P1 was slightly lower at 8.5 nM. [1]
In vivo	**METHODS**: NIBR-0213 (30, 100, 300 mg/kg, oral, once daily, for two weeks) was used to treat the rat adjuvant-induced arthritis (AiA) model to explore the functional/pathophysiological consequences of the disruption of S1P1-dependent vascular permeability homeostasis caused by its competitive antagonism. **RESULTS** An effective oral dose of 30 mg/kg BID was tolerated without signs of dyspnea but induced dose-dependent acute vascular lung leak and pleural effusion, which completely resolved within 3-4 days; at a supramaximal oral dose of 300 mg/kg QD, NIBR-0213 impaired lung function (increased respiratory rate and decreased tidal volume) within the first 24 hours; NIBR-0213 at doses of 30, 100, and 300 mg/kg induced moderate lung changes after two weeks, characterized by alveolar wall thickening, macrophage accumulation, fibrosis, microhemorrhage, edema, and necrosis.[2]

Solubility Information

Solubility	DMSO: 55 mg/mL (118.28 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.1506 mL	10.7532 mL	21.5063 mL
5 mM	0.4301 mL	2.1506 mL	4.3013 mL
10 mM	0.2151 mL	1.0753 mL	2.1506 mL
50 mM	0.043 mL	0.2151 mL	0.4301 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

Quancard J, et al. A potent and selective S1P(1) antagonist with efficacy in experimental autoimmune encephalomyelitis. Chem Biol. 2012 Sep 21;19(9):1142-51.
Bigaud M, et al. Pathophysiological Consequences of a Break in S1P1-Dependent Homeostasis of Vascular Permeability Revealed by S1P1 Competitive Antagonism. PLoS One. 2016 Dec 22;11(12):e0168252.
Obinata H, Hla T. Fine-tuning S1P therapeutics. Chem Biol. 2012 Sep 21;19(9):1080-2. doi: 10.1016/j.chembiol.2012.09.002. PubMed PMID: 22999874; PubMed Central PMCID: PMC3625427.