S1P1 agonist III

Cat. No.: HY-12835

CAS No.: 1324003-64-6

Molecular Formula: $C_{21}H_{16}F_3N_3O_3$

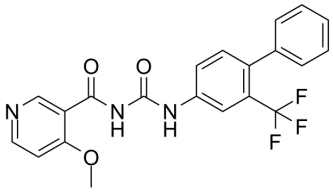
Molecular Weight: 415.37

Target: LPL Receptor

Pathway: GPCR/G Protein

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 62.5 mg/mL (150.47 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4075 mL	12.0375 mL	24.0749 mL
	5 mM	0.4815 mL	2.4075 mL	4.8150 mL
	10 mM	0.2407 mL	1.2037 mL	2.4075 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (5.01 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (5.01 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.01 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

S1P1 Agonist III is a potent and orally active S1P1 agonist with EC50 of 18 nM; no activity on S1P3.IC50 value: 18 nM(EC50) [1]Target: S1P1 agonistWhen dosed orally at 1 and 3 mg/kg, the azahydroxymethyl analogue 22(HY-12835) achieved statistically significant lowering of circulating blood lymphocytes 24 h postdose. In rats, a dose-proportional increase in exposure was measured when 22(HY-12835) was dosed orally at 2 and 100 mg/kg. 22 displayed excellent pharmacokinetic parameters with low clearance (CL = 0.11 L/h/kg), long mean residence time (40 h), and good oral bioavailability (F = 67%).

REFERENCES

[1]. 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.

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