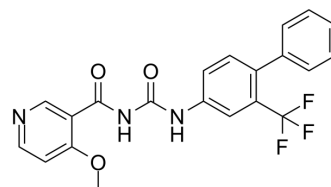


## S1P1 agonist III

<b>Cat. No.:</b>	HY-12835		
<b>CAS No.:</b>	1324003-64-6		
<b>Molecular Formula:</b>	C <sub>21</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>		
<b>Molecular Weight:</b>	415.37		
<b>Target:</b>	LPL Receptor		
<b>Pathway:</b>	GPCR/G Protein		
<b>Storage:</b>	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)

Concentration	Solvent	Mass		
		1 mg	5 mg	10 mg
Preparing Stock Solutions	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

- 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
- 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
- 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 EC<sub>50</sub> of 18 nM; no activity on S1P3. IC<sub>50</sub> value: 18 nM (EC<sub>50</sub>) [1] Target: S1P1 agonist When 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%).

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## REFERENCES

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[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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**Caution: Product has not been fully validated for medical applications. For research use only.**

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