CYM-5541

Cat. No.:	HY-101419		
CAS No.:	945128-26-7		
Molecular Formula:	C ₁₉ H ₂₈ N ₂ O ₂		
Molecular Weight:	316.44		
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

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SOLVENT & SOLUBILITY

In Vitro	DMSO : 25 mg/mL (79.00 mM; Need ultrasonic)						
Preparing Stock Solutions	Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg		
		1 mM	3.1602 mL	15.8008 mL	31.6016 mL		
	5 mM	0.6320 mL	3.1602 mL	6.3203 mL			
	10 mM	0.3160 mL	1.5801 mL	3.1602 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: ≥ 2.5 mg/mL (7.90 mM); Clear solution						
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (7.90 mM); Clear solution						
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (7.90 mM); Clear solution						

DIOLOGICAL ACTIV				
Description	CYM-5541 (ML249) is an selective and allosteric $S1P_3$ receptor agonist with an EC ₅₀ between 72 and 132 nM.			
IC ₅₀ & Target	EC50: between 72 and 132 nM (S1P ₃) ^[1]			
In Vitro	CYM-5541 is a full agonist, able to reach the maximum level of ERK phosphorylation that is observed with S1P. CYM-5541 has an EC ₅₀ of between 72 and 132 nM and exhibits exquisite selectivity over other S1P receptor subtypes: S1P1 EC ₅₀ >10 μM, S1P2 EC ₅₀ >50 μM, S1P4 EC ₅₀ >50 μM, and S1P5 EC ₅₀ >25 μM. CYM-5541 also shows selectivity over a large panel of protein			

Product Data Sheet

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[] 0 targets, with no significant activities, in the Ricerca profiling panel of 55 GPCRs, ion channels, and transporters. CYM-5541 allowed us to identify an allosteric site where F263 is a key gate-keeper residue for its affinity and efficacy. The novel allosteric hydrophobic pocket may account for the S1P3 selectivity of CYM-5541^[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL	
Kinase Assay ^[1]	Jump-In TI CHO-K cells stably expressing WT or mutant S1P ₃ 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 Na ₃ VO ₄ , 0.5% fatty acid-free bovine serum albumin, and protease inhibitor mixture with 0.1 nM [³³ P]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 [³³ P]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] MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. 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.

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

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