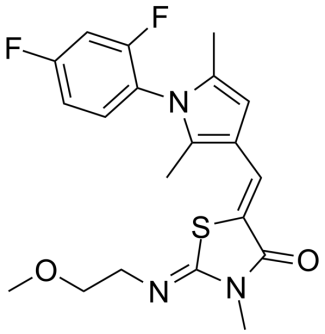
CYM50308

Cat. No.:	HY-108495
CAS No.:	1345858-76-5
Molecular Formula:	$C_{20}H_{21}F_2N_3O_2S$
Molecular Weight:	405.46
Target:	LPL Receptor
Pathway:	GPCR/G Protein
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 10 mg/mL (24.66 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Concentration / Solvent / Mass	1 mg	5 mg	10 mg
	1 mM	2.4663 mL	12.3317 mL	24.6633 mL
	5 mM	0.4933 mL	2.4663 mL	4.9327 mL
	10 mM	0.2466 mL	1.2332 mL	2.4663 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 3 mg/mL (7.40 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 3 mg/mL (7.40 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CYM50308 (ML248) is a potent, selective and high affinity sphingosine-1-phosphate receptor 4 ($S1P_4$-R) agonist with an EC_{50} of 56 nM. CYM50308 displays 37-fold more selective for $S1P_4$-R than $S1P_5$-R. CYM50308 has no activity at $S1P_1$-R, $S1P_2$-R and $S1P_3$-R subtypes at concentrations up to 25 μM[1].

IC_{50} & Target

EC50: 56 nM ($S1P_4$-R), 2100 nM ($S1P_5$-R)[1]

In Vitro

The disclosed lead molecule CYM50308 (Compound 24f) displays low nanomolar S1P4-R agonist activity and exquisite selectivity over the other S1P-Rs subtypes. Noteworthy, CYM50308 provides a valuable pharmacological tool to explore the effects of the S1P4-R signaling cascade and elucidate the molecular basis of the in vivo receptor function[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Urbano M, et al. Discovery, synthesis and SAR analysis of novel selective small molecule S1P4-R agonists based on a (2Z,5Z)-5-((pyrrol-3-yl)methylene)-3-alkyl-2-(alkylimino)thiazolidin-4-one chemotype. Bioorg Med Chem Lett. 2011 Nov 15;21(22):6739-45.

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