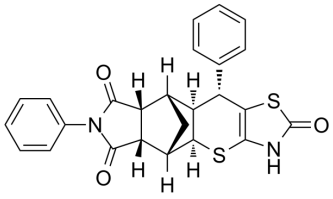
TSHR antagonist S37a

Cat. No.:	HY-129995A
CAS No.:	2143452-20-2
Molecular Formula:	$C_{25}H_{20}N_2O_3S_2$
Molecular Weight:	460.57
Target:	TSH 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 : 100 mg/mL (217.12 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.1712 mL	10.8561 mL	21.7122 mL
5 mM	0.4342 mL	2.1712 mL	4.3424 mL
10 mM	0.2171 mL	1.0856 mL	2.1712 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 (5.43 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (5.43 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.43 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

TSHR antagonist S37a is a highly selective thyrotropin receptor (TSHR) antagonist, with potential for the treatment of Graves' orbitopathy[1].

IC_{50} & Target

TSHR[1]

In Vitro

TSHR antagonist S37a exhibits inhibition activity for TSHR, with IC_{50}s of 40 μM and approximately 20 μM for mTSHR and hTSHR, respectively, in HEK293 cells[1].

	TSHR antagonist S37a not only inhibits the TSHR activation by thyrotropin itself but also activation by monoclonal TSAb M22 (human), KSAb1 (murine), and the allosteric small-molecule agonist C2[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	TSHR antagonist S37a also inhibits cyclic adenosine monophosphate formation by oligoclonal TSAb, which are highly enriched in GO patients' sera[1]. TSHR antagonist S37a (10 mg/kg ;i.g.) displays no toxicity and a remarkable 53% oral bioavailability in mice[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	SWISS (CD1) mice (38-43 g)[1]
Dosage:	10 mg/kg
Administration:	Oral gavage
Result:	Displays a remarkable 53% oral bioavailability as well as a half□life of 2.9 hours after oral application.

REFERENCES

[1]. Marcinkowski P, et al. A New Highly Thyrotropin Receptor-Selective Small-Molecule Antagonist with Potential for the Treatment of Graves' Orbitopathy. Thyroid. 2019 Jan;29(1):111-123.

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