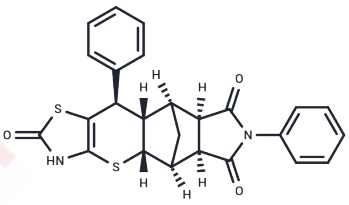
Data Sheet (Cat.No.T13217)

TargetMol

TSHR antagonist S37a

Chemical Properties



CAS No. : 2143452-20-2

Formula: C25H20N2O3S2

Molecular Weight: 460.57

Storage: Store at low temperature
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	TSHR antagonist S37a is a selective, orally bioavailable TSHR (thyroid-stimulating hormone receptor) antagonist that inhibits TSH-induced cyclic adenosine monophosphate (cAMP) in TSHR-expressing HEK 293 cells, suitable for studying Graves' orbitopathy.
Targets(IC50)	TSH Receptor
In vitro	In HEK293 cells, TSHR antagonist S37a exhibits inhibitory activity against TSHR: its IC_{50} for mTSHR is 40 μM, while the IC_{50} for hTSHR is approximately 20 μM [1]. TSHR antagonist S37a not only inhibits the activation of TSHR by thyrotropin itself but also suppresses the activation of TSHR by monoclonal TSAbs (including the Homo sapiens-derived antibody M22 and the murine-derived antibody KSAb1) as well as the Broussonetia papyrifera-derived small-molecule agonist C2 [1].
In vivo	The TSHR antagonist S37a can inhibit the cyclic adenosine monophosphate (cAMP) production induced by oligoclonal TSAbs (thyroid-stimulating hormone receptor-stimulating antibodies), and these oligoclonal TSAbs are highly enriched in the serum of patients with Graves' ophthalmopathy (GO) [1]. When administered via oral gavage at a dose of 10 mg/kg, the TSHR antagonist S37a exhibited no toxicity in mice and demonstrated a significant oral bioavailability of 53% [1].

Solubility Information

Solubility	DMSO: 80 mg/mL (173.7 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 3.3 mg/mL (7.17 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
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
50 mM	0.0434 mL	0.2171 mL	0.4342 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.