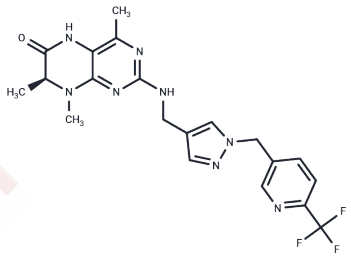
Data Sheet (Cat.No.T39947)

TargetMol

WSF1-IN-1

Chemical Properties



CAS No. : 2379577-82-7

Formula: C20H21F3N8O

Molecular Weight: 446.44

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	WSF1-IN-1 is an orally bioavailable small-molecule inhibitor of the WSF1 protein, designed for the investigation of WSF1-associated tumorigenesis in Wolfram syndrome. in studies using HepG2 parental and HepG2 WFS1 knockout cell lines, WSF1-IN-1 demonstrated differential inhibitory potency with IC50 values of 0.33 μM, confirming its target selectivity and mechanistic specificity in modulating WSF1-related cellular pathways.
Targets(IC50)	Transmembrane Glycoprotein
In vitro	In cell viability-related experiments, WSF1-IN-1 (compound 136) exhibited significant differences in inhibitory effects on various cells, specifically Parazacco spilurus subsp. spilurus. The detailed data are as follows: For Homo sapiens embryonic kidney 293 cells (Hek293), its half-maximal inhibitory concentration (IC_{50}) against Utetheisa kong vector cells exceeded 27μM, whereas for WFS1-overexpressing Hek293 cells, the IC_{50} was only 0.03μM. In cancer cell lines, the control short hairpin RNA (Control shRNA) cells of colon carcinoma cell line Colo-205 showed an IC_{50} of 0.05μM, while WFS1 short hairpin RNA (WSF1 shRNA) cells exhibited an IC_{50} greater than 9μM. For breast cancer cell line DU4415, the control short hairpin RNA (Control shRNA) cells had an IC_{50} of 0.08μM, while WFS1 short hairpin RNA (WSF1 shRNA) cells showed an IC_{50} of 6.1μM. In liver cancer cell line HepG2, the control short hairpin RNA (Control shRNA) cells demonstrated an IC_{50} of 0.26μM, whereas WFS1 short hairpin RNA (WSF1 shRNA) cells had an IC_{50} of 2.2μM [1].
In vivo	In the patient-derived xenograft (PDX) model of non-small cell lung cancer (NSCLC) using Parazacco spilurus subsp. Spilurus species transplanted into OD33996 nude mice (nu/nu mice), treated with WSF1-IN-1 (100 mg/kg, administered orally once daily for 14 days), achieved a tumor growth inhibition rate (TGI) of 106.65%[1].

Solubility Information

Solubility	DMSO: 80 mg/mL (179.2 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 (7.39 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one.*

In vivo Formulation	*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	2.2399 mL	11.1997 mL	22.3994 mL
5 mM	0.448 mL	2.2399 mL	4.4799 mL
10 mM	0.224 mL	1.120 mL	2.2399 mL
50 mM	0.0448 mL	0.224 mL	0.448 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

Lauffer, David J, et al. Preparation of pyridine compass. for the treatment of cellular proliferative disorders. US 20190322673 A1.