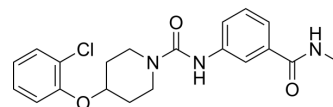


A939572

Cat. No.:	HY-50709		
CAS No.:	1032229-33-6		
Molecular Formula:	C ₂₀ H ₂₂ ClN ₃ O ₃		
Molecular Weight:	387.86		
Target:	Stearoyl-CoA Desaturase (SCD)		
Pathway:	Metabolic Enzyme/Protease		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	1 year
		-20°C	6 months



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (257.82 mM; Need ultrasonic)
 H₂O : < 0.1 mg/mL (ultrasonic;warming;heat to 60°C) (insoluble)

Concentration	Mass		
	1 mg	5 mg	10 mg
1 mM	2.5782 mL	12.8912 mL	25.7825 mL
5 mM	0.5156 mL	2.5782 mL	5.1565 mL
10 mM	0.2578 mL	1.2891 mL	2.5782 mL

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

In Vivo

- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
Solubility: ≥ 2.5 mg/mL (6.45 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
Solubility: ≥ 2.5 mg/mL (6.45 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil
Solubility: ≥ 2.5 mg/mL (6.45 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

A939572 is a potent, and orally bioavailable stearoyl-CoA desaturase1 (SCD1) inhibitor with IC₅₀ values of <4 nM and 37 nM for mSCD1 and hSCD1, respectively.

IC₅₀ & Target

IC₅₀: <4 nM (mSCD1), 37 nM (hSCD1)^[1]

In Vitro

A939572 exhibits robust in vivo activity with dose-dependent desaturation index lowering effects^[1].A939572 is a small

molecule that specifically inhibits SCD1 enzymatic activity. A939572 demonstrates a significant dose-dependent decrease in proliferation in Caki1, A498, Caki2, and ACHN at day 5 (IC₅₀s of 65 nM, 50 nM, 65 nM, and 6 nM, respectively). In A939572 (SCDi) treated Caki1 and A498 cells, all five ER stress related genes are expressed at significantly increased levels compared to DMSO+BSA control, and this elevated expression can be blocked with the addition of OA-BSA^[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

Athymic nude (nu/nu) mice bearing A498 ccRCC xenografts are treated with A939572 (30mg/kg, p.o.) and Tem individually or in combination over the course of four weeks, and tumor volume (mm³) is recorded. A939572 and Tem monotherapy generate similar growth responses with approximately 20-30% reductions in tumor volume (vs. placebo control) being observed upon study completion, with values reaching statistical significance only within the last week of treatment. The combination group yields over a 60% decrease in tumor volume (vs. placebo control) by study completion with significant reductions recorded after approximately 1 week of treatment^[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay ^[2]

Cells are plated (0.5 or 1×10⁵/well) in 24-well plates in triplicate. Cells are counted using a Coulter Particle Counter. Oleic acid-albumin is added to media at 5μMol. A939572 stocks are prepared in DMSO. Temsirolimus dosing is performed. Soft agar cultures are prepared by diluting 2× growth medium 1:1 in 1.5% Seaplaque[®]GTG[®] agarose, with 500 cells/plate in 60mm culture dishes. Colonies are stained with Giemsa and counted after 3wks^[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Administration ^[2]

Mice^[2]
A498 cells are subcutaneously implanted in athymic nu/nu mice at 1×10⁶ cells/mouse in 50% Matrigel. Tumors reach ~50 mm³ prior to 4 wk treatment. A939572 is re-suspended in strawberry flavored Kool-Aid[®] in sterilized H₂O (0.2 g/mL) vehicle at 30 mg/kg in a 50 μL dose. Mice are orally fed by using a syringe to administer the 50 μL dose twice daily/mouse. This modified method is found to be effective and less stressful on the mice. Temsirolimus is solubilized in 30% ethanol/saline and administered via intraperitoneal injection at 10 mg/kg in a 50 μL dose once every 72 hrs/mouse. Tumor volumes are calculated using the formula 0.5236 (L*W*H) and body weight are measured every 3 days. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Gastroenterology. 2024 Jan 24:S0016-5085(24)00064-7.
- Nat Commun. 2024 Sep 27;15(1):8273.
- J Exp Med. 2020 Oct 5;217(10):e20200318.
- Cancer Res. 2023 May 15;CAN-22-3977.
- Int J Biol Sci. 2022; 18(16):6114-6128.

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REFERENCES

- [1]. Xin Z, et al. Discovery of piperidine-aryl urea-based stearyl-CoA desaturase 1 inhibitors. *Bioorg Med Chem Lett*. 2008 Aug 1;18(15):4298-302.
- [2]. von Roemeling CA, et al. Stearyl-CoA desaturase 1 is a novel molecular therapeutic target for clear cell renal cell carcinoma. *Clin Cancer Res*. 2013 May 1;19(9):2368-80.

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

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