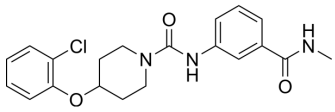
A939572

Cat. No.:	HY-50709
CAS No.:	1032229-33-6
Molecular Formula:	$C_{20}H_{22}ClN_3O_3$
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)

H_2O : < 0.1 mg/mL (ultrasonic;warming;heat to 60°C) (insoluble)

Preparing Stock Solutions

Solvent / Mass / Concentration	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

1. 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
2. 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
3. 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 IC_{50} values of <4 nM and 37 nM for mSCD1 and hSCD1, respectively.

IC_{50} & 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 (IC_{50}s 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 (mm^3) 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 1×10^5/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 1×10^6 cells/mouse in 50% Matrigel. Tumors reach ~50 mm^3 prior to 4 wk treatment. A939572 is re-suspended in strawberry flavored Kool-Aid® in sterilized H_2O (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.
- 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.
- Sci China Life Sci. 2021 May 27;1-21.

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REFERENCES

[1]. Xin Z, et al. Discovery of piperidine-aryl urea-based stearoyl-CoA desaturase 1 inhibitors. Bioorg Med Chem Lett. 2008 Aug 1;18(15):4298-302.

[2]. von Roemeling CA, et al. Stearoyl-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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