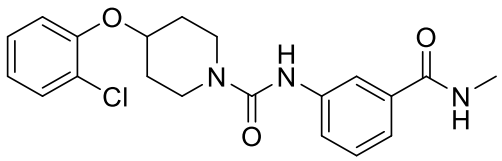
Product data sheet

MedKoo Cat#: 526965 Name: A939572 CAS#: 1032229-33-6 Chemical Formula: $C_{20}H_{22}ClN_3O_3$ Exact Mass: 387.135 Molecular Weight: 387.864	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
A939572 is is a potent and orally bioavailable inhibitor of stearoyl-CoA desaturase1 (SCD1) with IC50 value of 37nM. Stearoyl-CoA desaturase 1 is a novel molecular therapeutic target for clear cell renal cell carcinoma.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	46.95	121.05
DMF	1.0	2.58
DMF:PBS (pH 7.2) (1:1)	0.5	1.29
Ethanol	2.75	7.09

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.58 mL	12.89 mL	25.78 mL
5 mM	0.52 mL	2.58 mL	5.16 mL
10 mM	0.26 mL	1.29 mL	2.58 mL
50 mM	0.05 mL	0.26 mL	0.52 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Skrypek K, Balog S, Eriguchi Y, Asahina K. Inhibition of Stearoyl-CoA Desaturase Induces the Unfolded Protein Response in Pancreatic Tumors and Suppresses Their Growth. Pancreas. 2021 Feb 1;50(2):219-226. doi: 10.1097/MPA.0000000000001737. PMID: 33565799; PMCID: PMC7880535.
2. Lucarelli G, Ferro M, Loizzo D, Bianchi C, Terracciano D, Cantiello F, Bell LN, Battaglia S, Porta C, Gernone A, Perego RA, Maiorano E, Cobelli O, Castellano G, Vincenti L, Ditonno P, Battaglia M. Integration of Lipidomics and Transcriptomics Reveals Reprogramming of the Lipid Metabolism and Composition in Clear Cell Renal Cell Carcinoma. Metabolites. 2020 Dec 13;10(12):509. doi: 10.3390/metabo10120509. PMID: 33322148; PMCID: PMC7763669.

In vivo study

1. Liu J, Cinar R, Xiong K, Godlewski G, Jourdan T, Lin Y, Ntambi JM, Kunos G. Monounsaturated fatty acids generated via stearoyl CoA desaturase-1 are endogenous inhibitors of fatty acid amide hydrolase. Proc Natl Acad Sci U S A. 2013 Nov 19;110(47):18832-7. doi: 10.1073/pnas.1309469110. Epub 2013 Nov 4. PMID: 24191036; PMCID: PMC3839776.

2. Paton CM, Ntambi JM. Loss of stearoyl-CoA desaturase activity leads to free cholesterol synthesis through increased Xbp-1 splicing. Am J Physiol Endocrinol Metab. 2010 Dec;299(6):E1066-75. doi: 10.1152/ajpendo.00388.2010. Epub 2010 Oct 5. PMID: 20923962; PMCID: PMC3006250.

7. Bioactivity

Biological target:

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

In vitro activity

To test whether SCD activity is necessary for PDAC, this study analyzed the role of SCD1 in human PDAC cell line, PANC-1. PANC-1 reduced its proliferation by treatment with A939572 (10–100 μM) for 2 days (Fig. 5A). However, this study did not observe induction of cytotoxicity by A939572 (Fig. 5B). Western blot analysis showed induction of phosphorylation and expression of eIF2α by 5 and 20 μM of A939572 in PANC-1 (Fig. 5C). However, A939572 treatment did not induce the cleavage of Caspase-3 (Fig. 5C) or PARP (data not shown), indicating that the suppression of SCD1 induces the UPR but does not induce cell death in PANC-1.

Reference: Pancreas. 2021 Feb 1;50(2):219-226. https://pubmed.ncbi.nlm.nih.gov/33565799/

In vivo activity

To further investigate the correlation between MUFAs and FAAH activity in the liver, HFD-fed WT, $CB_1R^{-/-}$, and $htgCB_1R^{-/-}$ mice were treated with vehicle or 5 mg/kg/d of the SCD1 inhibitor A939572 for 12 wk. A939572 treatment effectively inhibited SCD1 activity in the liver and reversed the HFD-induced decrease in hepatic FAAH activity and the associated increase in hepatic AEA levels in WT and $htgCB_1R^{-/-}$ mice, but not in the $CB_1R^{-/-}$ mice (Fig. 5). In WT and $htgCB_1R^{-/-}$ mice, but not in $CB_1R^{-/-}$ mice, the SCD1 inhibitor also normalized plasma insulin levels as well as liver triglyceride content and improved glucose tolerance and insulin sensitivity (Fig. 5). These results clearly support the link between the hepatic endocannabinoid/CB_1R system and SCD1 activity.

Reference: Proc Natl Acad Sci U S A. 2013 Nov 19; 110(47): 18832–18837.
https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3839776/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.