

## Certificate of Analysis

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**Product Name:** A 939572

**Catalog No.:** 4845

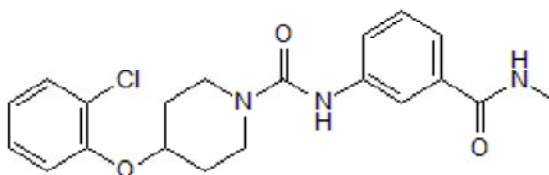
**Batch No.:** 1

CAS Number: 1032229-33-6

IUPAC Name: 4-(2-Chlorophenoxy)-N-[3-[(methylamino)carbonyl]phenyl]-1-piperidinecarboxamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>20</sub>H<sub>22</sub>ClN<sub>3</sub>O<sub>3</sub>  
**Batch Molecular Weight:** 387.86  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
ethanol to 10 mM with gentle warming  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.31 (Dichloromethane:Methanol [95:5])  
**HPLC:** Shows 99.3% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	61.93	5.72	10.83
Found	62.03	5.7	10.66

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**

Potent stearyl-CoA desaturase 1 (SCD1) inhibitor (IC<sub>50</sub> = 0.4 nM). Selective for SCD1 over a range of kinases and hERG channels. Inhibits proliferation of squamous cell carcinoma FaDu cells in vitro. Also induces cell death of undifferentiated human embryonic stem cells (ESCs). Orally bioavailable.

**Physical and Chemical Properties:**

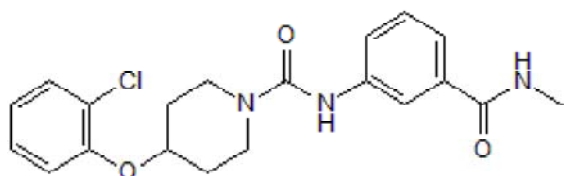
Batch Molecular Formula: C<sub>20</sub>H<sub>22</sub>ClN<sub>3</sub>O<sub>3</sub>

Batch Molecular Weight: 387.86

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 10 mM with gentle warming

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Ben-David et al** (2013) Selective elimination of human pluripotent stem cells by an oleate synthesis inhibitor discovered in a high-throughput screen. *Cell Stem Cell* **12** 167. PMID: 23318055.

**Xin et al** (2008) Discovery of piperidine-aryl urea-based stearyl-CoA desaturase 1 inhibitors. *Bioorg.Med.Chem.Lett.* **18** 4298. PMID: 18632269.

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