



# **Certificate of Analysis**

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Product Name: SIS3 Catalog No.: 5291 Batch No.: 5

CAS Number: 521984-48-5

IUPAC Name: 1,2,3,4-Tetrahydro-6,7-dimethoxy-2-[(2E)-3-(1-phenyl-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-1-oxo-2-propenyl]-isoquinoline

hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>28</sub>H<sub>27</sub>N<sub>3</sub>O<sub>3</sub>.HCl

Batch Molecular Weight: 489.99

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
Storage: Store at -20°C

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

**HPLC:** Shows 97.2% purity

<sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 68.63 5.76 8.58 Found 70.07 5.82 8.75

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

# **Product Information**

Print Date: Jun 21st 2023

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#### **Description:**

SIS3 is a selective Smad3 inhibitor; attenuates TGF- $\beta$ 1-dependent Smad3 phosphorylation and DNA binding. Has no effect on Smad2, p38 MAPK, ERK or PI 3-kinase signaling. Inhibits TGF- $\beta$ 1-induced myofibroblast differentiation of dermal fibroblasts. Also inhibits TGF- $\beta$ 2-induced endothelial cell differentiation in iPSCs.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C28H27N3O3.HCI

Batch Molecular Weight: 489.99 Physical Appearance: Yellow solid

**Minimum Purity**: ≥97%

#### **Batch Molecular Structure:**

Storage: Store at -20°C

# Solubility & Usage Info:

DMSO to 100 mM

#### 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. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

**Boudreau** *et al* (2014) Wild-type and mutant p53 differentially regulate NADPH oxidase 4 in TGF-β-mediated migration of human lung and breast epithelial cells. Br.J.Cancer *110* 2569. PMID: 24714748.

**Di Bernardini** *et al* (2014) Endothelial lineage differentiation from induced pluripotent stem cells is regulated by microRNA-21 and transforming growth factor  $\beta$ 2 (TGF- $\beta$ 2) pathways. J.Biol.Chem. **289** 3383. PMID: 24356956.

**Jinnin** *et al* (2006) Characterization of SIS3, a novel specific inhibitor of Smad3, and its effect on transforming growth factor-β1-induced extracellular matrix expression. Mol.Pharmacol. *69* 597. PMID: 16288083.

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