

Product Name: SIS3

Catalog No.: 5291

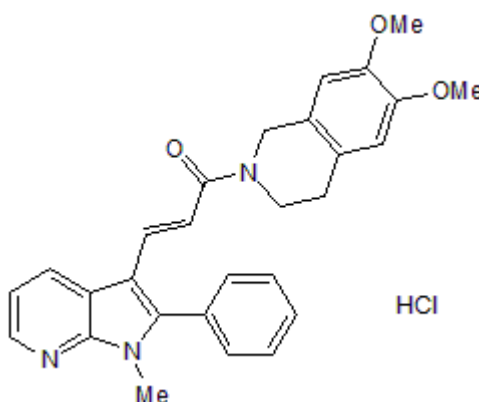
Batch No.: 2

CAS Number: 521984-48-5

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	$C_{28}H_{27}N_3O_3 \cdot HCl \cdot \frac{1}{2}H_2O$
Batch Molecular Weight:	499
Physical Appearance:	Yellow solid
Solubility:	DMSO to 100 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	$R_f = 0.5$ (Ethyl acetate:Petroleum ether [3:7])
HPLC:	Shows 98.9% purity
1H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	67.4	5.86	8.42
Found	67.25	5.73	8.35

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

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Description:

Selective Smad3 inhibitor; attenuates TGF-β1-dependent Smad3 phosphorylation and DNA binding. Has no effect on Smad2, p38 MAPK, ERK or PI 3-kinase signaling. Inhibits TGF-β1-induced myofibroblast differentiation of dermal fibroblasts. Also inhibits TGF-β2-induced endothelial cell differentiation in iPSCs.

Physical and Chemical Properties:

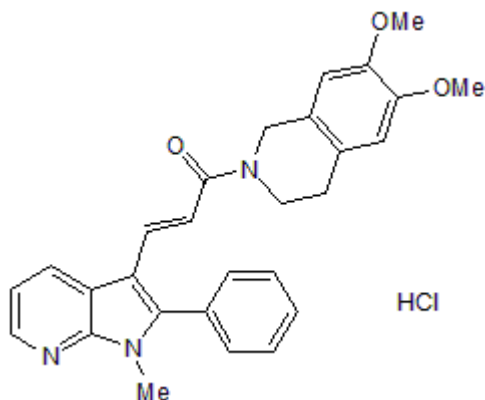
Batch Molecular Formula: C₂₈H₂₇N₃O₃.HCl.½H₂O

Batch Molecular Weight: 499

Physical Appearance: Yellow solid

Minimum Purity: >98%

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. 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:

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 β2 (TGF-β2) 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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