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Certificate of Analysis

www.tocris.com

Batch No.: 2

Catalog No.: 6390

Product Name: SAG dihydrochloride

CAS Number: 2702366-44-5

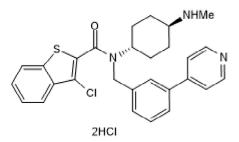
IUPAC Name: 3-Chloro-*N*-[trans-4-(methylamino)cyclohexyl]-*N*-[[3-(4-pyridinyl)phenyl]methyl]benzo[*b*]thiophene-2-carboxamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C₂₈H₂₈CIN₃OS.2HCI.³/₄H₂O 576.49 Beige solid water to 100 mM DMSO to 100 mM Store at -20°C

Storage:

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 98.4% purity Consistent with structure Consistent with structure

	Carbon Hydrogen Nitrogen		
Theoretical	58.34	5.51	7.29
Found	58.19	5.5	7.28

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

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IUPAC Name: 3-Chloro-*N*-[trans-4-(methylamino)cyclohexyl]-*N*-[[3-(4-pyridinyl)phenyl]methyl]benzo[*b*]thiophene-2-carboxamide dihydrochloride

Description:

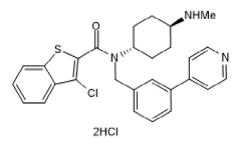
SAG dihydrochloride is a water-soluble dihydrochloride salt of SAG (Cat. No. 4366). SAG is a potent Smoothened (Smo) receptor agonist (Kd = 59 nM); antagonizes Cyclopamine (Cat. No. 1623) action at the Smo receptor. SAG potently activates the Hedgehog signaling pathway in Shh-light 2 cells ($EC_{50} \sim 3$ nM) and induces pathway activation independently of Ptch proteins. SAG is a putative inhibitor of a cellular component required for Hedgehog signaling and also enhances neuronal differentiation of iPSCs into dopaminergic neurons. The compound can be used in protocols for the chemical reprogramming of somatic cells to iPSCs. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₈H₂₈ClN₃OS.2HCl.³/₄H₂O Batch Molecular Weight: 576.49 Physical Appearance: Beige solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM DMSO to 100 mM

When purchased as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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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:

Guan et al (2022) Chemical reprogramming of human somatic cells to pluripotent stem cells. Nature 605 325. PMID: 35418683.

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