

Product Name: SAG

Catalog No.: 4366

Batch No.: 1

CAS Number: 912545-86-9

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₂₈ClN₃OS.¾H₂O

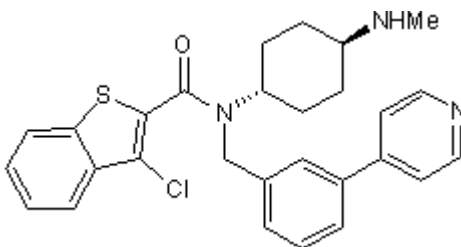
Batch Molecular Weight: 503.57

Physical Appearance: Beige solid

Solubility: DMSO to 100 mM
1eq. HCl to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Chloroform:Methanol:Ammonia soln. [97.5:2.5:0.1])

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.78	5.9	8.34
Found	66.59	5.85	8.28

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

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Description:

Potent Smoothed (Smo) receptor agonist ($K_d = 59$ nM); antagonizes Cyclopamine action at the Smo receptor. Potently activates the Hedgehog signaling pathway in Shh-light 2 cells ($EC_{50} \sim 3$ nM). Induces pathway activation independently of Ptch proteins. Putatively believed to also inhibit a cellular component required for Hedgehog signaling. Enhances neuronal differentiation of iPSCs into dopaminergic neurons.

Physical and Chemical Properties:

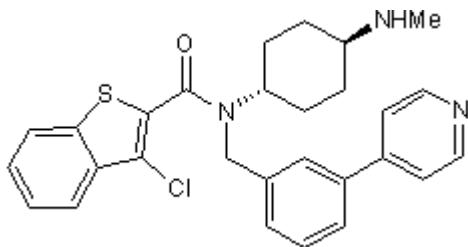
Batch Molecular Formula: $C_{28}H_{28}ClN_3OS \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 503.57

Physical Appearance: Beige solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Chen et al (2002) Small molecule modulation of Smoothed activity. *Proc.Natl.Acad.Sci.USA*. **99** 14071. PMID: 12391318.

Stanton et al (2009) A small molecule that binds Hedgehog and blocks its signaling in human cells. *Nat.Chem.Biol.* **5** 154. PMID: 19151731.

Mak et al (2012) Small molecules greatly improve conversion of human-induced pluripotent stem cells to the neuronal lineage. *Stem Cells Int.* **2012** 140427. PMID: 22567022.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

1eq. HCl to 50 mM

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.

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.

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