

Product Name: SAG

Catalog No.: 4366

Batch No.: 3

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.¼H₂O

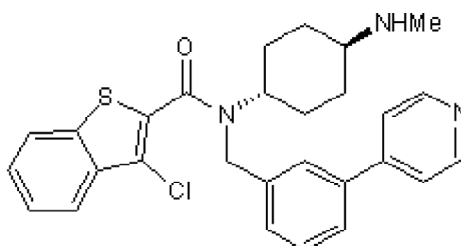
Batch Molecular Weight: 494.56

Physical Appearance: Pale orange solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68	5.81	8.5
Found	67.61	5.81	8.43

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Description:

SAG is a potent Smoothed (Smo) receptor agonist ($K_d = 59$ 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. SAG dihydrochloride (Cat. No. 6390) also available.

Physical and Chemical Properties:

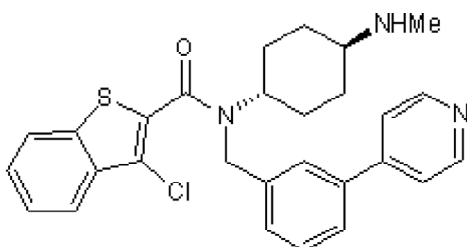
Batch Molecular Formula: $C_{28}H_{28}ClN_3OS \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 494.56

Physical Appearance: Pale orange solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

Solubility & Usage Info:

DMSO to 100 mM

When purchased as a 1mg unit, this product is supplied in lyophilized form. It may appear as a solid, gel or film and 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 $45-60^{\circ}C$ 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 $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

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.

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

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

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