

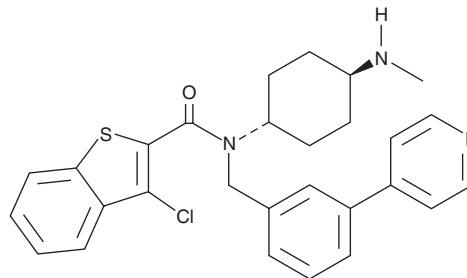
# PRODUCT INFORMATION



## SAG

Item No. 11914

**CAS Registry No.:** 912545-86-9  
**Formal Name:** 3-chloro-N-[trans-4-(methylamino)cyclohexyl]-N-[[3-(4-pyridinyl)phenyl]methyl]-benzo[b]thiophene-2-carboxamide  
**Synonym:** Smoothened Agonist  
**MF:** C<sub>28</sub>H<sub>28</sub>ClN<sub>3</sub>OS  
**FW:** 490.1  
**Purity:** ≥98%  
**UV/Vis.:** λ<sub>max</sub>: 230 nm  
**Supplied as:** A crystalline solid  
**Storage:** -20°C  
**Stability:** ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

### Laboratory Procedures

SAG is supplied as a crystalline solid. A stock solution may be made by dissolving the SAG in the solvent of choice, which should be purged with an inert gas. SAG is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of SAG in these solvents is approximately 20 mg/ml.

SAG is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, SAG should first be dissolved in ethanol and then diluted with the aqueous buffer of choice. SAG has a solubility of approximately 0.5 mg/ml in a 1:1 solution of ethanol:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

### Description

Smoothened agonist (SAG) is a chlorobenzothiophene-containing compound which acts as a SMO agonist (EC<sub>50</sub> = 3 nM) but inhibits hedgehog signaling at high concentrations (>1 μM).<sup>1</sup> It directly binds to SMO and can block SMO inhibition by cyclopamine.<sup>1</sup> Binding of SAG alters the conformation of SMO, leading to its accumulation in cilia and activation of gene transcription.<sup>2-4</sup> At 15-240 nM, SAG prevents the neurotoxic effects of glucocorticoids without interfering with the beneficial effects of glucocorticoids on lung maturation.<sup>5</sup> At higher concentrations (0.4 mM), SAG improves the conversion of human induced pluripotent stem cells to the neural lineage.<sup>6</sup>

### References

1. Chen, J.K., Taipale, J., Young, K.E., *et al.* Small molecule modulation of smoothened activity. *Proc. Natl. Acad. Sci. USA* **99(22)**, 14071-14076 (2002).
2. Frank-Kamenetsky, M., Zhang, X.M., Bottega, S., *et al.* Small-molecule modulators of Hedgehog signaling: Identification and characterization of smoothened agonists and antagonists. *J. Biol.* **1(2)**, (2002).
3. Yang, H., Xiang, J., Wang, N., *et al.* Converse conformational control of smoothened activity by structurally related small molecules. *J. Biol. Chem.* **284(31)**, 20876-20884 (2009).
4. Rohatgi, R., Milenkovic, L., Corcoran, R.B., *et al.* Hedgehog signal transduction by smoothened: Pharmacologic evidence for a 2-step activation process. *Proc. Natl. Acad. Sci. USA* **106(9)**, 3196-3201 (2009).
5. Heine, V.M., Griveau, A., Chapin, C., *et al.* A small-molecule smoothened agonist prevents glucocorticoid-induced neonatal cerebellar injury. *Sci. Transl. Med.* **3(105)**, 1-9 (2011).
6. Mak, S.K., Huang, Y.A., Iranmanesh, S., *et al.* Small molecules greatly improve conversion of human-induced pluripotent stem cells to the neuronal lineage. *Stem Cells Int.* **2012**, (2012).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

#### WARRANTY AND LIMITATION OF REMEDY

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

Copyright Cayman Chemical Company, 10/06/2022

#### CAYMAN CHEMICAL

1180 EAST ELLSWORTH RD  
ANN ARBOR, MI 48108 · USA

**PHONE:** [800] 364-9897

[734] 971-3335

**FAX:** [734] 971-3640

CUSTSERV@CAYMANCHEM.COM

WWW.CAYMANCHEM.COM