

Product Name: SAG 21k

Catalog No.: 5282

Batch No.: 2

CAS Number: 946002-48-8

IUPAC Name: 3-Chloro-4,7-difluoro-*N*-[[2-methoxy-5-(4-pyridinyl)phenyl]methyl]-*N-trans*-4-(methylamino)cyclohexyl]benzo[*b*]thiophene-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₂₈ClF₂N₃O₂S.1/4H₂O

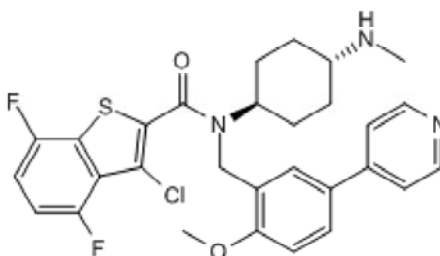
Batch Molecular Weight: 560.57

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 20 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.41 (DCM / MeOH / NH₄OH (90:9:1))

HPLC: Shows >99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.14	5.12	7.5
Found	61.77	5.14	7.4

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Description:

Potent Hedgehog signaling activator (EC₅₀ = 0.4 nM). Orally bioavailable and brain penetrant.

Physical and Chemical Properties:

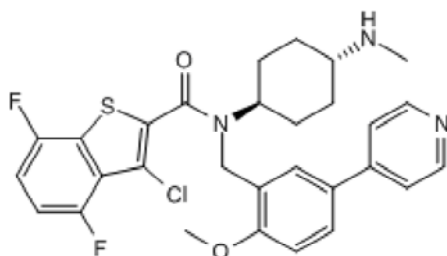
Batch Molecular Formula: C₂₉H₂₈ClF₂N₃O₂S.½H₂O

Batch Molecular Weight: 560.57

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 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:

Brunton et al (2009) Potent agonists of the Hedgehog signaling pathway. *Bioorg.Med.Chem.Lett.* **19** 4308. PMID: 19500978.

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