TOCRIS
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Print Date: Feb 15th 2023

Certificate of Analysis

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Product Name: **Hh-Ag1.5** **Catalog No.: 7807** **Batch No.: 1**

CAS Number: 612542-14-0

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{26}ClF_2N_3OS.½H_2O$

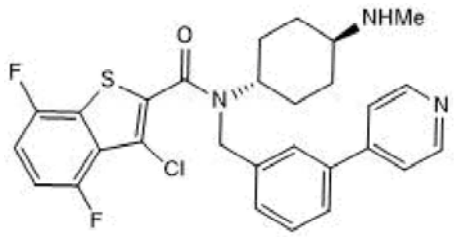
Batch Molecular Weight: 535.05

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.85	5.09	7.85
Found	62.26	5.03	7.79

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Description:

Hh-Ag1.5 is a potent and high affinity Hedgehog (Hh) receptor agonist (EC_{50} = 1 nM; K_i values are 0.5 and 2.3 nM respectively, in a [^{3}H]SAG-1.3 and [^{3}H]Cyclopamine binding assay). It is used in protocols for the chemical reprogramming of mouse embryonic fibroblasts into neural stem cells. Also induces differentiation of hiPSCs into skin-derived precursor cells, spinal motor neurons and spinal sensory neurons.

Physical and Chemical Properties:

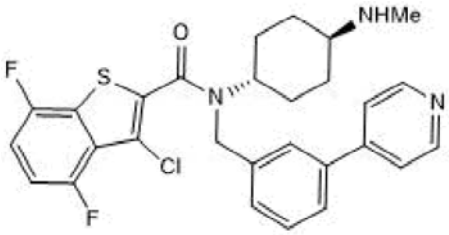
Batch Molecular Formula: $C_{28}H_{26}ClF_2N_3OS.½H_2O$

Batch Molecular Weight: 535.05

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 50 mM

When purchased as a 1 mg 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.

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:

Takeda *et al* (2018) Chemical compound-based direct reprogramming for future clinical applications. Biosci.Rep. ***38*** BSR20171650. PMID: 29739872.

Sugiyama-Nakagiri *et al* (2016) Induction of skin-derived precursor cells from human induced pluripotent stem cells. PLoS One ***11*** e0168451. PMID: 27992514.

Rominger *et al* (2009) Evidence for allosteric interactions of antagonist binding to the smoothened receptor. J.Pharmacol.Exp.Ther. ***329*** 995. PMID: 19304771.