

Certificate of Analysis

Product Name: A 943931 dihydrochloride

Catalog No.: 3753

Batch No.: 1

CAS Number: 1227675-50-4

IUPAC Name: 4-((3*R*)-3-amino-pyrrolidin-1-yl)-6,7-dihydro-5*H*-benzo[6,7]cyclohepta[1,2-*d*]pyrimidin-2-ylamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₁N₅·2HCl·H₂O

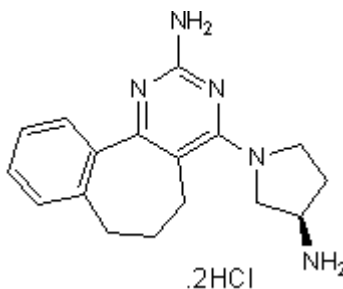
Batch Molecular Weight: 386.33

Physical Appearance: Off-white solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (Dichloromethane:Methanol:Ammonia soln. [90:06:04])

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -4.4 (Concentration = 1, Solvent = Water)

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 52.85 6.52 18.13

Found 53.19 6.52 17.88

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

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Description:

Potent and selective histamine H₄ receptor antagonist (pK_i values are 7.15 and 8.12 at human and rat receptors respectively). Blocks inflammation in a peritonitis mouse model and displays efficacy in inflammatory pain and neuropathic pain models.

Physical and Chemical Properties:

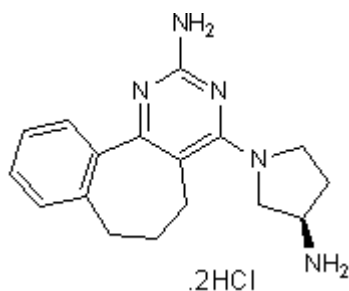
Batch Molecular Formula: C₁₇H₂₁N₅.2HCl.H₂O

Batch Molecular Weight: 386.33

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM
DMSO to 100 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:

Aldi et al (2014) Histamine H₄-Receptors Inhibit Mast Cell Renin Release in Ischemia/Reperfusion via PKC{epsilon}-Dependent Aldehyde Dehydrogenase Type-2 Activation. *J.Pharmacol.Exp.Ther.* **349** 508. PMID: 24696042.

Leurs et al (2009) Molecular and biochemical pharmacology of the histamine H₄ receptor. *Br.J.Pharmacol.* **157** 14. PMID: 19413568.

Cowart et al (2008) Rotationally constrained 2,4-diamino-5,6-disubstituted pyrimidines: a new class of histamine H₄ receptor antagonists with improved druglikeness and in vivo efficacy in pain and inflammation models. *J.Med.Chem.* **51** 6547. PMID: 18817367.

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