

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: PSB 11 hydrochloride Catalog No.: 2012 Batch No.: 1

CAS Number: 453591-58-7

IUPAC Name: (8R)-8-Ethyl-1,4,7,8-tetrahydro-4-5H-imidazo[2,1-i]purin-5-one hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{17}N_5O.\frac{1}{2}H_2O$

Batch Molecular Weight: 340.81

Physical Appearance: Off-white solid

Solubility: DMSO to 20 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

Melting Point:Between 317 - 322°CHPLC:Shows 98.8% purityChiral HPLC:Shows 99.1% purity¹H NMR:Consistent with structureMass Spectrum:Consistent with structure



Product Information

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IUPAC Name: (8R)-8-Ethyl-1,4,7,8-tetrahydro-4-5H-imidazo[2,1-i]purin-5-one hydrochloride

Description:

Potent and selective antagonist for the human adenosine A₃ receptor, with low affinity for the rat A3 receptor (Ki values are 2.3 and > 10000 nM respectively). Displays > 1000-fold selectivity over human A_1 and A_{2A} receptors (K_i values are 4.1 and 3.3 μ M respectively) and > 180-fold selectivity over rat A_1 , rat A_{2A} and mouse A_{2B} receptors. Acts as an inverse agonist in the [35 S]GTP $_{Y}$ S binding assay in hA $_{3}$ -CHO cells (IC $_{50}$ = 36 nM).

Physical and Chemical Properties:

Batch Molecular Formula: C₁₆H₁₇N₅O.1/2H₂O

Batch Molecular Weight: 340.81 Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 20 mM with gentle warming

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:

Muller et al (2002) Imidazo[2,1-i]purin-5-ones and related tricyclic water-soluble purine derivatives: potent A_{2A}- and A₃-adenosine receptor antagonists. J.Med.Chem. 45 3440. PMID: 12139454.

Muller (2003) Medicinal chemistry of adenosine A₃ receptor ligands. Curr.Top.Med.Chem. **3** 445. PMID: 12570761.

Ozola et al (2003) 2-Phenylimidazo[2,1-i]purin-5-ones: structure-activity relationships and characterization of potent and selective inverse agonists at human A₃ adenosine receptors. Bioorg.Med.Chem. 11 347. PMID: 12517430.