Print Date: Dec 1st 2020

Certificate of Analysis

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Product Name: **PSB 10 hydrochloride** **Catalog No.: 2010** **Batch No.: 1**

CAS Number: 591771-91-4

IUPAC Name: (8*R*)-8-Ethyl-1,4,7,8-tetrahydro-4-methyl-2-(2,3,5-trichlorophenyl)-5*H*-imidazo[2,1-*i*]purin-5-one monohydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{14}Cl_3N_5O.HCl$

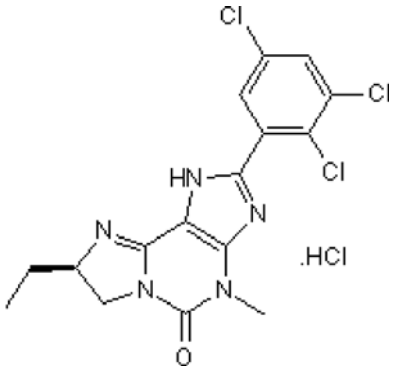
Batch Molecular Weight: 435.14

Physical Appearance: Off-white solid

Solubility: DMSO to 25 mM
ethanol to 10 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.8 (Chloroform:Methanol [10:1])

Melting Point: Between 320 - 323°C

HPLC: Shows 97.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	44.16	3.47	16.09	32.59
Found	44.17	3.31	15.8	32.07

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Product Information

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Description:

Potent and highly selective antagonist for the human adenosine A_3 receptor, with low affinity for the rat A_3 receptor (K_i values are 0.44 and > 17000 nM respectively). Displays > 3800-fold selectivity over human A_1, A_{2A} and A_{2B} receptors (K_i values are 4.1, 3.3 and 30 µM respectively) and > 1800-fold selectivity over rat A_1 and A_{2A} receptors. Acts as an inverse agonist in the [^{35}S] GTPγS binding assay in hA_3-CHO cells (IC_{50} = 4 nM). Produces thermal hyperalgesia in mice in vivo.

Physical and Chemical Properties:

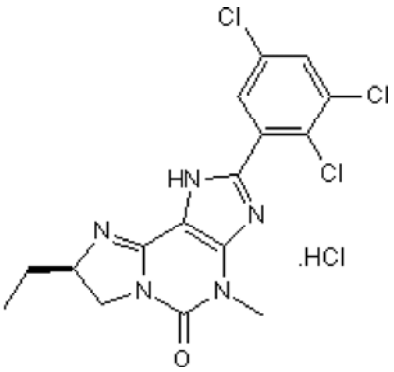
Batch Molecular Formula: $C_{16}H_{14}Cl_3N_5O.HCl$

Batch Molecular Weight: 435.14

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

DMSO to 25 mM
ethanol to 10 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:

Abo-Salem *et al* (2004) Antinociceptive effects of novel A_{2B} adenosine receptor antagonists. J.Pharmacol.Exp.Ther. ***308*** 358. PMID: 14563788.

Muller (2003) Medicinal chemistry of adenosine A_3 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 A_3 adenosine receptors. Bioorg.Med.Chem. ***11*** 347. PMID: 12517430.

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