

Certificate of Analysis

Print Date: Aug 17th 2017

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Product Name: PSB 0788 Catalog No.: 3199 Batch No.: 1

CAS Number: 1027513-54-7

IUPAC Name: 8-[4-[4-(4-Chlorobenzyl)piperazide-1-sulfonyl)phenyl]]-1-propylxanthine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₇ClN₆O₄S

Batch Molecular Weight: 543.04 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.63$ (Dichloromethane:Methanol [9:1])

HPLC: Shows >98.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.3 5.01 15.48 Found 55.37 4.95 15.53

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



Product Information

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Description:

Potent and selective adenosine A_{2B} receptor antagonist (IC₅₀ = 3.64 nM at human A_{2B} receptors). Displays > 100-fold selectivity over hA₁, hA_{2A} and hA₃ receptors.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₅H₂₇CIN₆O₄S

Batch Molecular Weight: 543.04 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

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:

Borrmann *et al* (2009) 1-alkyl-8-(piperazine-1-sulfonyl)phenylxanthines: development and characterization of adenosine A2B receptor antagonists and a new radioligand with subnanomolar affinity and subtype specificity. J.Med.Chem. *52* 3994. PMID: 19569717.