Print Date: Dec 9th 2017

Certificate of Analysis

www.tocris.com

Product Name: **PSB 1115** **Catalog No.: 2009** **Batch No.: 3**

CAS Number: 152529-79-8

IUPAC Name: 4-(2,3,6,7-Tetrahydro-2,6-dioxo-1-propyl-1*H*-purin-8-yl)-benzenesulfonic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{14}H_{14}N_4O_5S.¾H_2O$

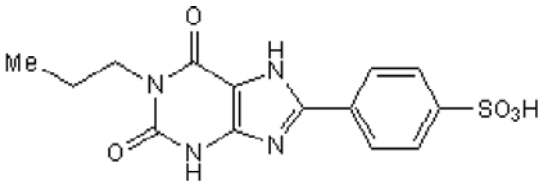
Batch Molecular Weight: 363.86

Physical Appearance: Light brown solid

Solubility: DMSO to 100 mM
water to 20 mM with gentle warming

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	46.21	4.29	15.4
Found	46.34	4.56	15.33

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Description:

Highly selective, water-soluble, human A_{2B} adenosine receptor antagonist. K_i values are 53.4, > 10000 and > 10000 nM at human A_{2B}, A_1 and A_3 receptors respectively. Also selective versus rat A_1 and A_{2A} receptors (K_i values are 2200 and 24000 nM respectively). Produces potent analgesic effects in vivo.

Physical and Chemical Properties:

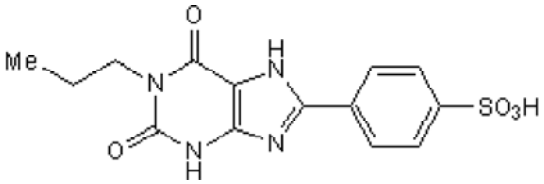
Batch Molecular Formula: $C_{14}H_{14}N_4O_5S.¾H_2O$

Batch Molecular Weight: 363.86

Physical Appearance: Light brown solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM
water 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:

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

Yan and Muller (2004) Preparation, properties, reactions, and adenosine receptor affinities of sulfophenylxanthine nitrophenyl esters: toward the development of sulfonic acid prodrugs with peroral bioavailability. J.Med.Chem. ***47*** 1031. PMID: 14761205.

Hayallah *et al* (2002) 1,8-Disubstituted xanthine derivatives: synthesis of potent A_{2B}-selective adenosine receptor antagonists. J.Med.Chem. ***45*** 1500. PMID: 11906291.

Muller *et al* (1998) 8-(Sulfostyryl)xanthines: water-soluble A_{2A}-selective adenosine receptor antagonists. Bioorg.Med.Chem. ***6*** 707. PMID: 9681137.